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Computational Analysis of Drug Targets and Prediction of Protein-Compound Interactions

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ABSTRACT

Computational prediction of compound-protein interactions generated a substantial amount of interest in the recent years owing to the importance of the knowledge of these interaction for drug discovery and drug repurposing efforts. Research suggests that the currently known drug targets constitute only a fraction of a complete set of drug targets, limiting our ability to identify suitable targets to develop new drugs or to repurpose current drugs for new diseases. These efforts are further thwarted by our limited knowledge of protein-drug (and more generally protein-compound) interactions, where only a subset of drug targets is typically known for the currently used drugs. This thesis focuses on the most populous category of drug targets, which are proteins, and addresses three main goals. The first goal is to computationally characterize the current drug targets among human proteins in order to identify a collection of markers that can be used to find novel/potential drug targets. We discover several useful markers that can be used to accelerate the process of identifying previously unknown drug targets. The second goal investigates potential weaknesses in the context of computational prediction of interaction between proteins and compounds. We find that current predictors of compound-protein interactions often rely on similarity between drugs and compounds to make predictions, i.e., they predict interactions with compounds that are similar to the compounds that are known to interact with a given protein and vice versa. We note that proteins are often composed of discernable units, called domains, and some of them play central role in binding compounds. However, when relying on the fact that a given domain interacts with a given compound it should be acknowledged that some other proteins with the same domain (which makes them similar) may not interact with this compound. We study this problem and find thousands of these cases. We empirically investigate whether current computational predictors of compound-protein interactions can be effectively used to differentiate these binding and non-binding cases. We show that while the existing methods achieve very high predictive performance for typically used (easy) test datasets, only some of them are able to achieve modest levels of predictive performance for this specific (difficult) scenario. Consequently, the third goal designs, develops, tests and deploys a new solution that aims to improve predictive performance for this difficult scenario. We develop a consensus model that

combines predictions from several current and well-performing predictors by using machine learning and applying additional inputs that quantify properties and similarity of compounds and proteins. Our ablation analysis shows that these additional inputs are crucial for the success of our new model, which is shown to statistically outperform the current solutions. We deploy the resulting predictor (MetaBoostCPI) as a convenient webserver for public use.

Chapter 1. **Introduction**

Drugs are chemical substances that we use to treat, prevent, or cure diseases. Drugs work via molecular-level interactions with biological molecules including proteins, nucleic acids and lipids, which are collectively referred to as drug targets. Significant majority of drugs targets, in the order of over 95%, are proteins [1]. This motivates our focus on the computational analysis and prediction of protein-drug interactions. We use the term "drug target" as a synonym for protein drug target in the remainder of this document. The drug-protein interactions either inhibit or stimulate the cellular functions of the target proteins and these changes lead to the (desired) therapeutic effects and also potentially to (undesired) side effects [2]. Perhaps surprisingly, the precise mechanism of action including the targets protein and details of the underlying interactions are unknown for some of the drugs. Pharmaceutical research and development and drug discovery revolve around targeting the right/therapeutic biomolecules that are linked to the disease of interest with minimal effects on other "off-targets", i.e., side-effects could be caused by interactions of a given drug with unintended target proteins. Therefore, knowledge of a comprehensive collection of targets for a given drug and the complete list of all potential drug targets are essential to a variety of drug discovery and design applications. These applications include screening drug candidates that targets specific disease-associated proteins [3-6], drug repurposing/repositioning (i.e., finding targets associated with diseases that are not yet known to benefit from an existing drug) [7-13], identification of side-effects resulting from interactions with the non-therapeutic off-targets [14-18], and elucidation of the a complete set of drug targets [1, 19-24].

Out of over 20,000 human proteins, so far only around 600 (3%) are targeted by the current drugs [25], while it is estimated that the number of proteins that can interact with drug-like molecules (druggable proteins) is as high as 22% [23]. Therefore, we have a long way to go to identify a complete collection of potential drug targets. One way to accomplish that is to find key properties/markers that differentiate current drug targets from the other proteins, which then can be used to identify potential/novel drug targets.

The currently limited knowledge of drug-protein interactions can be extended with the help of computational methods that predict whether a given drug-protein pair interacts [26-32]. These predictions can be used to facilitate discovery of new interactions by focusing the expensive and time-consuming experiments that are employed to discover and validate potential interactions on a subset of more promising targets [33-35]. The results that they generate can be also utilized to develop databases of pre-computed putative drug-protein interactions [36-38] and to decipher the underlying therapeutic mechanisms and side-effects of drugs [18, 39-41]. One of the key principles used by these predictors is similarity between proteins and similarity between compounds [42], i.e., similar drugs may interact with the same targets, and similar targets may interact with the same drug. Many of these methods have reached high levels of predictive performance [30-32, 43-48]. However, proteins do not have a monolithic structure and sequence. In fact, many proteins include discernable segments, called domains, that recur in other proteins and may even fold independently (have independent structure from the rest of the protein) [49-52]. Also, proteins often have more than one domain [53].

Since protein and compound similarity is one of the key factors that drive prediction of interactions [30], a potential problem for these predictors is when similar proteins (e.g., those that share a domain) may bind or not bind the same compound. More specifically, one protein that has a compound-binding domain may bind a given compound while another protein that has the same domain may not bind the same compound. This is because the ability to bind may depend on the remainder of the protein architecture, i.e., other domains that it includes. This poses several interesting questions:

- how common is the scenario that proteins that share a compound-interacting domain "switch" their ability to interact with this compound?

- can current predictors of protein-compound interactions provide accurate predictions for these interactions?
- can a new method that improves upon current methods for these interactions be developed?

Therefore, we define three goals for this dissertation:

Goal 1 Analysis of current human drug targets and other human proteins to develop markers that can be used to identify novel drug targets. This work is presented in Chapter 3 and was recently published [54].

Goal 2 Analysis of the abundance of compound-protein interaction where proteins share domains and assessment of predictive performance of current predictors of protein-compound interactions for this scenario. This goal is subdivided into two objectives: Sub-goal 2.1 that finds out how common is the scenario in which a single domain protein binds a certain compound while other proteins that have this domain do not interact with that compound; and Sub-goal 2.2 that evaluates current predictors on a large dataset of these interactions. More specifically, we evaluate current predictors on a challenging dataset of interaction with proteins that share domains and compare these results with the results that they secure using mode typical test data. This work is described in Chapter 4.

Goal 3 Conceptualization, development, comparative testing and deployment of a new method that provides accurate prediction of compound-protein interactions for proteins that share domains. This study is summarized in Chapter 5.

Chapter 2. **Background**

In this chapter, we describe general concepts and definitions that are used in this thesis. This section serves as an introduction for a reader who is not familiar with this area of research and also as a reference to clarify meaning of the terms used in the following chapters.

2.1. **Drugs**

Drugs are chemical substances which we use to prevent, treat, or cure diseases. They generate therapeutic/desired effects and side-effects (undesired effects) through interactions with biological targets that include proteins, DNA, RNA, and membrane components such as lipid and carbohydrates [55]. Drugs are essential tools in today's medicine. They range from everyday use Ibuprofen that we take for headache and anti-allergy Claritin to drugs like Paclitaxel and Revlimid for life-threatening diseases like cancer. Their history goes back to ancient times when humans observed that consuming certain plants has positive health effects. In modern times the area called pharmacology is dedicated to studying and engineering drugs. Nowadays, drugs undergo rigorous tests before they reach the market. They have to be proven to be safe and efficacious in clinical trials, which means they must provide benefits (therapeutic effects) that outweighs their risk (side-effects).

2.1.1. **Drug discovery**

Discovering new drugs is very long and expensive process [56]. This is mostly because many of the drug candidates do not pass the efficacy or safety tests in clinical or preclinical tests [57]. While in the past drugs were found by accidental exposure to natural compounds, modern drug discovery is mainly driven by knowledge of interactions between drug and targets (target-based approach).

The target-based approach usually starts with selection of molecular targets that are believed to be linked the onset or progression of a disease. The next step is to find candidate compounds that can reach the target and interact with it resulting in perturbations in its activity. This sometimes involves knowledge of the 3D structure of the target and design of a compound that can fit in its cavities. Nevertheless, the compounds that actually interact with the target ("hits") are usually found after trying many (thousands or even millions) different compounds. Therefore, the knowledge of interactions between compounds and proteins is very important for the target-based drug discovery.

2.1.2. **Small molecules**

Small molecules have certain properties that make them particularly appropriate when searching for compounds that "hit" the target biomolecule. They have the ability to reach tissues and biomolecules of interest when taken orally, while other bigger compounds may not be able to pass through the cellular membranes and other natural barriers in the body. This property is referred to as bioavailability. Even though there are other types of therapeutics, like biologics, that do not fit into this category, a large majority of approved therapeutics are small molecules. Furthermore, a concept of drug-like small molecule is formulated in the so called "rule of 5" introduced by Lipinski [58]. This rule specifies physicochemical properties that are common among most successful drugs and make them more likely to be bioavailable and able to bind to proteins (bioactive). Small molecules are usually studied in chemistry and information about them is stored in databases like PubChem [59] and CHEMBL [60]. These databases identify these molecules by their unique IDs and their atomic structure represented in standard formats, such as SMILES[61]. Furthermore, physical and chemical properties as well as interactions with biomolecules (bioactivity) are often recorded in these databases. Figure 2-1 shows an example compound entry in PubChem and the main information attached to it.

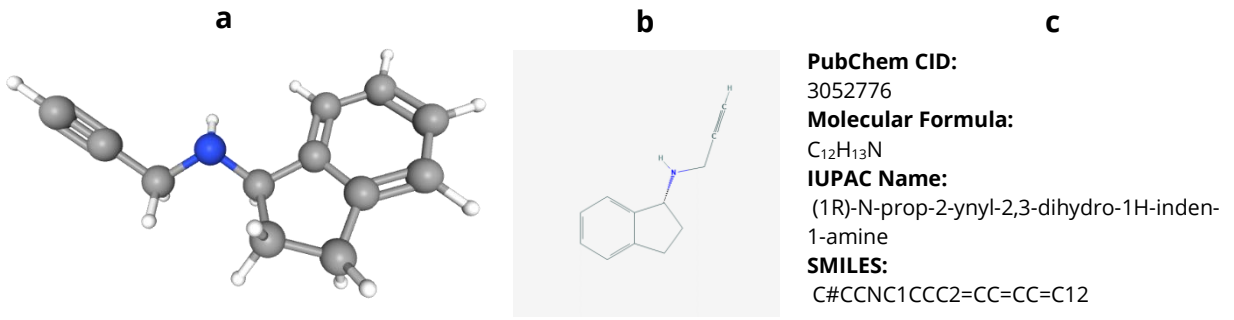


Figure 2-1. Example of a small molecule and information from PubChem. The figure shows 3D structure (Panel a), 2D structure (Panel b) and a selection of information (Panel c) about Rasagiline all taken from PubChem.

2.2. **Proteins**

Proteins are biological molecule that are at the center of virtually all cellular functions and not surprisingly they are the primary drug targets. In fact, 89% of 1578 FDA-approved drugs work by targeting proteins [25] and 96% of drug targets are proteins [20]. This motivates our focus on protein targets, i.e., we use the drug target as the synonym for protein drug target.

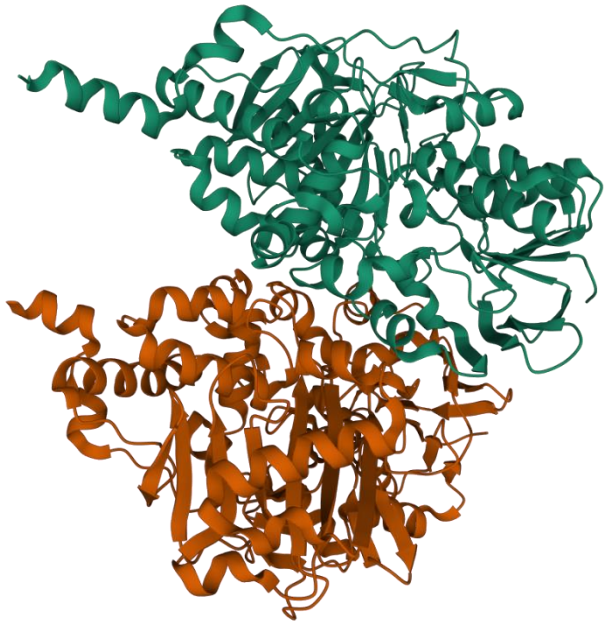
2.2.1. **Protein sequence, structure and intrinsic disorder**

Despite their great variation in size, shape and function, proteins are built by chaining amino acids together, with only 20 different amino acid types. The sequence of these amino acid determines the structure that the protein will adopt in the 3D space (a process known as protein folding), which in turn determines its interactions and function. The "sequence to structure to function" paradigm holds true for the globular/structured proteins. However, some sequences or sequence regions, which are called intrinsically disordered, are functional when being unstructured [62, 63], in which case the paradigm is shortened to "sequence to function". The wide-spread presence of the intrinsic disorder, particularly in eukaryotes [64-66], is one of the factors that motivates the development of the methods that predict drug-protein interactions using protein sequences, rather than protein structures, as the input.

2.2.2. **Protein representation and databases**

Information about proteins including their sequence, 3D structure, disorder and function is stored in public databases, such as UniProt (sequences) [67], Protein Data Bank (PDB) (structures) [68]

and DisProt (disorder) [69]. The sequence (a.k.a. primary structure) of a protein is typically shown as a string consisting of 20-character alphabet, each character denoting one of the 20 amino acid types. Figure 2-2 shows human Mono Amine Oxidase-B (MAO-B) protein, which is an enzyme formed as a complex of two chains with the same sequence. The figure shows the sequence and the corresponding 3D structure of this protein.



```
        10         20         30         40         50
MSNKCDVVVV GGGISGMAAA KLLHDSGLNV VVLEARDRVG GRTYTLRNQK
        60         70         80         90        100
VKYVDLGGSY VGPTQNRILR LAKELGLETY KVNEVERLIH HVKGKSYPFR
       110        120        130        140        150
GPFPPVWNPI TYLDHNNFWR TMDDMGREIP SDAPWKAPLA EEWDNMTMKE
       160        170        180        190        200
LLDKLCWTES AKQLATLFVN LCVTAETHEV SALWFLWYVK QCGGTTRIIS
       210        220        230        240        250
TTNGGQERKF VGGSGQVSER IMDLLGDRVK LERPVIYIDQ TRENVLVETL
       260        270        280        290        300
NHEMYEAKYV ISAIPPTLGM KIHFNPPLPM MRNQMITRVP LGSVIKCIVY
       310        320        330        340        350
YKEPFWRKKD YCGTMIIDGE EAPVAYTLDD TKPEGNYAAI MGFILAHKAR
       360        370        380        390        400
KLARLTKEER LKKLCELYAK VLGSLEALEP VHYEEKNWCE EQYSGGCYTT
       410        420        430        440        450
YFPPGILTQY GRVLRQPVDR IYFAGTETAT HWSGYMEGAV EAGERAAREI
       460        470        480        490        500
LHAMGKIPED EIWQSEPESV DVPAQPITTT FLERHLPSVP GLLRLIGLTT
       510        520
IFSATALGFL AHKRGLLVRV
```

Figure 2-2. Sequence and 3D structure of human MAO-B protein. The structure (on the left) is taken from PDB (PDB ID: 2BK3) and the sequence (on the right) is taken from UniProt (UniProt ID: P27338).

UniProt is the central database for protein sequences mainly coming from genomic data, with its Swiss-Prot subset that relies on the human curation [70]. PDB, the main database for protein 3D structure, is populated by structured derived primarily using the X-Ray crystallography as well as some other structure determination technologies, such as Nuclear Magnetic Resonance (NMR) and cryo-Electron Macroscopy (cryo-EM). While the rapid development of genomic technologies have provided abundance of protein sequences (including complete set of human proteins), 3D structures are available for only a small fraction of proteins since the experimental determination of structure is slow and expensive [71]. This is yet another reason why the sequence-based methods are preferred for the prediction of the drug-protein interactions.

2.2.3. **Protein domains**

Proteins are not monolithic in their "design". Parts of protein sequence and structure may recur in many proteins, while these proteins may include other regions that make them different. The recurring regions are called protein domains and are usually similar in sequence and function, being the result of common ancestry. Therefore, homology (similarity) in the protein world is usually studied at the level of domains. For instance, one of the common ways to classify proteins into families is based on inclusion and similarity of their domains.

Protein domains are usually detected and characterized based on sequence. The main database of sequence-based domains is Pfam [52], which includes manually curated domain annotations (Pfam-A) found by alignment of protein sequences. However, some repositories of domains, like CATH [50, 72] and SCOP [51, 73], use structure-based detection and classification of domains to detect more distant homologies that are not discoverable by sequence alone. Figure 2-3 shows an example of a structure of a protein (Pyruvate Kinase) and its 3 domains.

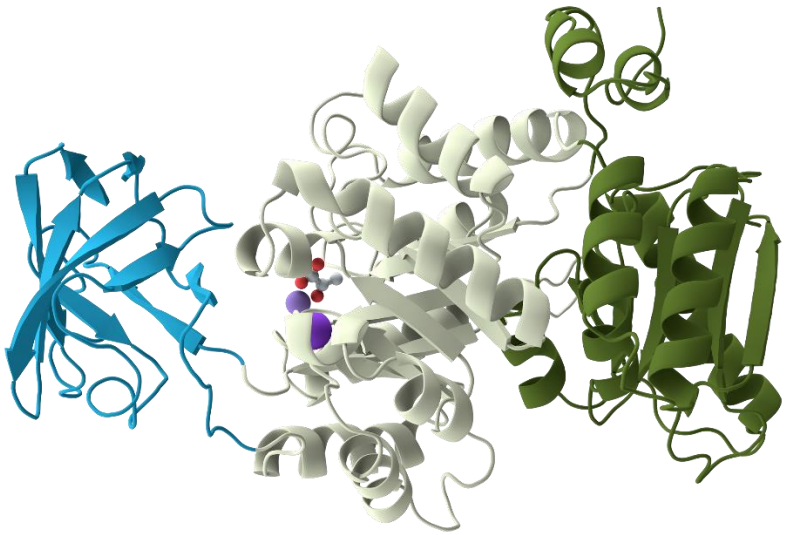


Figure 2-3. Human Pyruvate Kinase with its 3 domains shown by different colors [From Wikipedia]

2.3. **Compound-protein interactions**

Most drugs work by binding to their target protein(s) and interfering with their cellular function. Side effects of drugs could be the result of interactions with other molecules than the

intended/therapeutic target (i.e., off-target). The knowledge of these interactions is very important in guiding different steps of drug discovery and to minimize potential side effects. These interactions can be determined using experiments where a given protein and a compound are exposed in a solution and we measure how much of the protein will stay unbound and how much of it has interacted with the compound. This tendency to interact is usually called affinity and is quantified by different measures like Ki, Kd, IC50 and EC50.

High-throughput screening has allowed these experiments to be done between a given protein and large pool (library) of compounds in a few days. This is usually used for searching for compounds that can bind to an already selected target. A biproduct of this process is the record of the interactions that have not happened. Therefore, databases like PubChem Bioassay [74] or CHEML [60, 75] and BindingDB [76], store result of thousands of these experiments. Interestingly, the inverse experiments where a given drug/compound is screened against thousands of proteins are rarely, if ever, done. In a typical scenario, drugs are screened against a relatively small panel of targets [77, 78]. For instance, SafetyScreen44 panel screens against 44 targets [79], Novartis screens against 24 targets [80], Pfizer against between 30 targets [81], and Roche uses a panel of 48 targets [82]. To compare, human proteome includes over 20,000 canonical proteins and over 70,000 isoforms.

On a molecular level, the drug-protein interaction happens because of the compatibility of the physical properties and shapes of the drug and the protein. It is believed that certain subset of proteins, called druggable proteins, are more susceptible to bind to small molecules, due to their accessibility to drugs and their structural features, like having pockets that small molecules can fit in (binding pocket). Therefore, they are more likely to be drug targets.

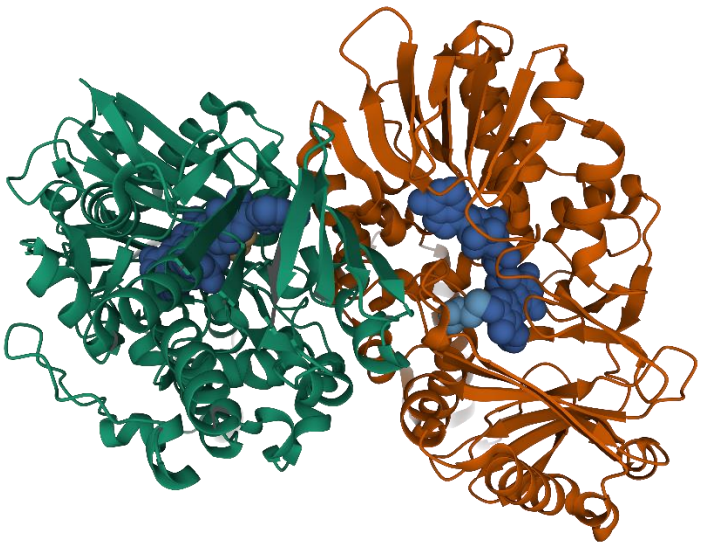


Figure 2-4. The structure of human MAO-B protein bound to Rasagiline. The structure of the drug-protein complex is taken from PDB (PDB ID: 2BK3). The dark blue molecule shown in space-fill representation is the small molecule.

2.4. **Prediction of compound-protein interactions**

Despite the existence of high-throughput screening, the large number of compounds (in millions) and proteins (in dozens of thousands) does not allow to experimentally determine all possible interactions. This is especially true considering the relatively small size of the inverse experiments where drugs are screened against panels of protein targets. Therefore, the interaction data for majority of compound-protein pairs is yet to be determined. This has motivated the development of the many computational methods that predict these interactions [26-32]. These tools (a.k.a. virtual screening) aim to narrow down the search space for the experimental methods by suggesting the most probable candidate interactions.

Depending on whether the protein structure is used or not, these predictors can be categorized into two groups: protein structure-based methods and chemogenomic methods that do not rely on protein structures. The structure-based tools are inherently limited to proteins with 3D structure, which are only a fraction of all proteins. Representative examples of structure-based methods include PatchSurfer [83, 84] that uses a reduced representation of the structural information (e.g., numeric vector that summarizes geometry and physicochemical properties of binding pockets) to speed up predictions, approaches that that performs computationally expensive docking of [85,

86], and methods like eFindSite [87, 88] and SMAP [89, 90] that utilize threading/similarity-based approach. The chemogenomic methods rely on information that is widely available for proteins and compounds, which includes protein sequence and compound structure. They work by extracting information from the protein sequence (its similarity to known drug targets), drug structure (its similarity to known drugs), and a variety of interaction data (protein-protein, protein-disease, etc.) and the principle that similar proteins have similar interacting compounds.

The ability to make predictions for virtually all proteins makes the chemogenomic methods particularly appealing. These methods utilize the abundant post-genomic data (i.e., protein sequences, protein-protein interaction data, etc.) that are growing at a faster rate than protein 3D structures or bioassay data. Therefore, they can provide a first-line screening and searching tools for drug discovery. The main principle used in these methods is the fact that similarity in both the compound and protein side results in similar interactions [30]. Therefore, these methods use the similarity in protein sequence (usually coming from sequence alignment) and in compound structure (usually from comparison of SMILES structures) and try to extrapolate the currently known compound-protein interactions. While this is the main idea behind these tools, they have been extended to add other sources of information and data mining techniques in their prediction process. Some of the ideas that have been introduced in recent years include the use of heterogenous information like association networks (e.g. between drugs, proteins and disease) [91, 92], drug side effects data [93] and even Electronic Health Records (EHR) data [94], in addition to applying advanced machine learning techniques [43, 47, 95-97]. This complexity of methods and heterogeneity of data has resulted in high levels of accuracy and, at the same time, has made a reliable evaluation and comparison of these methods more challenging. In recent years, several reviews of the methods in the field have been published with different categorization schemes that has made the complexity of the field more manageable [30, 32, 98].

2.5. **Evaluation of CPI prediction**

The drug-protein prediction is usually modeled as a binary classification problem, where given the information about the protein and the compound the predictive model predicts whether or not they interact. We call interacting pairs “positive pairs” (or positive interaction) and non-interacting pairs “negative”. The binary prediction is often accompanied by a propensity score that estimates the

likelihood of interaction. Some methods predict numeric affinity, providing a more detailed insight about the interaction. The predictions generated by the binary predictors are typically assessed with classification metrics like Area Under the ROC Curve (AUC) and Area Under the Precision-Recall curve (AUPR). The results produced by the predictors of affinity are typically evaluated with measures such as correlation, Mean Absolute Error (MAE), Mean Squared Error (MSE), and concordance index. We focus on the binary classification problem since more methods fall into this category. When dealing with tools that predict affinity, we either convert their results to binary or use the predicted affinity as a propensity score.

In nature, only a small fraction of all possible compound-protein pairs interacts. Therefore, binary classification formulation of compound interaction has the inevitable problem of extreme class imbalance. Moreover, there is an opposite imbalance in the available data. While the number of experimentally validated interacting pairs is reasonably large, the amount of validated non-interacting pairs is relatively small and under-represents the actual set. For example, Figure 2-5 shows the distribution of Ki, Kd, IC50 and EC50 values in the BindingDB and the range of values that are considered a positive (green) and negative (red) interaction. A positive interaction commonly assumed to correspond to value of less than 1μM and a negative interaction with a value of more than 30μM for these quantities [99, 100]. In Figure 2-5 values are shown with their -log (negative of natural logarithm), which is a common way to present their values and makes presentation of their distributions easier.

We observe that majority of the experiments correspond to positive interactions. The bias towards positive interactions likely stems from the fact that a typical scenario focuses on interactions that are presumed to be likely and a non-interaction is considered undesired. In addition, many predictors of CPI are trained and tested in a setting where only positive interaction data is based on experimental results, e.g., they use training/test data extracted from databases. such as DrugBank[101], which store only positive interactions. For these methods, the negative interactions are usually generated by randomly sampling the pairs without a known positive interaction (pairs with unknown label). This is a fundamental flaw since the status of interactions for these presumed negatives is actually unknown. We collect both interacting and non-interacting drug-protein pairs using experimental data, ensuring that they are properly validated. This is possible because of a recent increase in the amount of the negative experimental data, which is

now sufficient to create imbalanced datasets that do not have to rely on randomly sampled negatives We plan to accommodate for the under-representation of the negative interaction data by using metrics that are robust against class imbalance, such as AUPR [102].

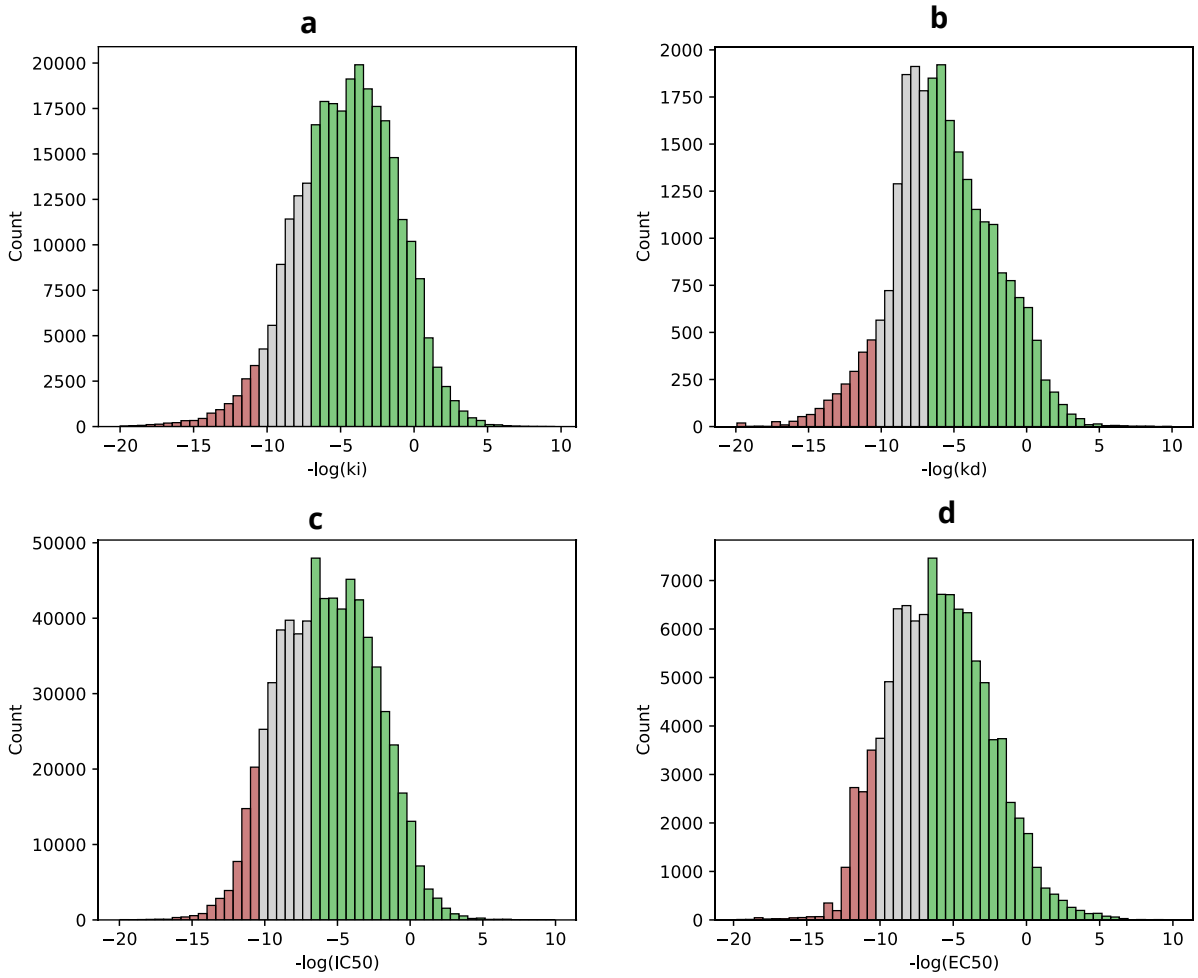


Figure 2-5. Distribution of affinity measures in BindingDB. Affinity values are shown negated (natural) logarithm of their values for easier representation.

Chapter 3. **Analysis of current human drug targets and other human proteins to develop markers that can be used to identify novel drug targets**

3.1. **Introduction**

Knowledge of the drug-target interactions is essential for numerous applications including screening of drug candidates [3-6], drug repurposing [7-13], characterization and mitigation of side-effects of drugs [14-18], and prediction of novel protein-drug interactions [31, 38, 103-107]. We focus on the drug-protein interactions and we use the term "drug target" as a synonym for the protein drug target. While early works reported about 400 human drug targets [108, 109], subsequent studies annotate as many as over 600 drug targets in human [25]. However druggable proteins, usually defined as the set of proteins that could bind to drug-like (orally bioavailable) molecules, is expected to be much larger [1, 19-22]. Early estimates place the number of human druggable proteins around 3 thousand [108, 109]. A more recent analysis approximates this number at 4.5 thousand [23], which corresponds to about 22% of the human genome. These observations point to the fact that many of the drug targets remain to be discovered and characterized. The search for potential targets has relied on the concept of druggability, which was defined based on the presence of structure that favors interactions with drug-like compounds [108-110]. However, the potential drug target proteins not only must be able to bind to drug-like molecules, but the protein should be linked to a disease, so that the corresponding interaction could potentially provide desired therapeutic effects [108]. Therefore, we consider both conditions in our search for potential drug targets.

One of key elements in the quest to find potential targets is to identify functional and structural characteristics that differentiate drug targets from the non-drug targets [111-119]. In one of the earliest works, Chen *et al.* concentrated on the analysis of structural fold types, target family representation and similarity, pathway associations, tissue distribution, and chromosome location for the drug targets [111]. A similar analysis that considered cellular functions, pathway associations, tissue distribution, and subcellular and chromosome location of the drug targets was published soon after by Lauss and colleagues [112]. More recent studies have shifted the focus towards characteristic features of the target protein sequence and structure. Bakheet and Doig used a relatively small set of 148 targets to analyze several sequence properties (chain length, hydrophobicity, charge, and isoelectric point), putative secondary structure and transmembrane regions, inclusion of signal peptides, selected set of post-translational modifications (PTMs), as well as the previously studied subcellular location and functions [117]. Subsequently, Bull and Doig investigated a similar set of characteristics using a much larger set of 1324 drug targets [118]. They considered sequence properties, native secondary structure and signal peptides, selected PTMs, and a few new properties: the number of germline variants, expression levels, and the number of protein-protein interactions (PPIs) [118]. The most recent study by Park, Lee and colleagues expanded the above list of characteristics by inclusion of gene essentiality and tissue specificity [119]. Moreover, several articles narrowly focused on characteristics that quantify topological features of the underlying PPI networks [113-116]. While these studies have considered a broad range of functional and structural features of drug targets, they compared the current drug targets against the current non targets (other human proteins that are not the target of any current drug). However, many of these currently non-target proteins could become drug targets in the future. They could be druggable [23] and many of them are linked to a disease. Using the current non-target proteins to investigate differences between drug targets and non-targets in order to define drug targets ultimately creates a bias toward describing the currently known drug targets. Consequently, this reduces our ability to use these characteristics to identify a complete set of target proteins.

Our study is novel in four ways. **First,** we contrast the current drug targets (**D dataset**) not only against all currently non-target proteins (**N dataset**), which was also done in prior studies, but also against two subsets of the current non-targets:

- **Nd dataset**: proteins that are likely to be a target in the future, because they are known to be associated with multiple diseases (we call them likely targets for short)

- **Nn dataset**: proteins that are unlikely to be a target in the future, because they don't have any known disease associations (we call them unlikely-to-be-target or unlikely for short)

Second, we further compare the D, N, Nd and Nn proteins against highly promiscuous drug targets that interact with many drugs (**Dh dataset**) and drug targets that interact with smaller number of drugs (**Dl dataset**). This full-spectrum analysis allows us to pinpoint characteristics that differentiate between current drug target and those that are likely or unlikely to be a drug target in the future, as well as features that are specific to promiscuous vs. non-promiscuous drug targets. We provide the complete D dataset in the Appendix A. **Third,** we focus on the characteristics that can be quantified directly from the protein sequence or are available proteome-wide. This facilitates their use as potential markers across the entire human proteome. This is in contrast to several related studies that are limited to a relatively small subset of human proteins with solved structures [22, 38, 104, 118, 120]. **Fourth,** we include several important sequence-derived characteristics that were missed in the past studies including putative intrinsic disorder, residue-level conservation, presence and number of alternative splicing isoforms, inclusion of domains, and solvent accessibility (surface area). Moreover, we still cover some of the key characteristics from the prior works, such as the topological features of PPIs, cellular functions and subcellular locations.

3.2. **Materials and Methods**

3.2.1. **Data collection**

Datasets of current drug targets (D dataset), highly promiscuous drug targets (Dh dataset) and low-interaction drug targets (Dl dataset).

We collect a comprehensive set of drug targets by combining interaction information extracted from several large bioactive compounds-protein interaction databases. We filter these bioactive compounds to include only approved and experimental drugs. Furthermore, we focus on human proteins by excluding protein fragments and proteins from other organisms. We maximize the

coverage by first collecting an inclusive set of interactions (including all bioactive compounds and protein chains) and then applying the two filters to obtain a large high-quality set of drugs and proteins.

The data collection protocol follows the work in [103, 121]. We extract the source data from three large repositories: Drug2gene[122], TTD [123] and GtP[124]**.** Drug2gene is one of the most inclusive repositories that aggregates 19 source databases including TTD and GtP and several other major databases like ChEMBL[125] and DrugBank [126]. However, Drug2gene includes older and substantially smaller version of the TTD and GtP resources. Therefore, we integrated the latest versions of these two databases into our dataset. These databases provide a list of drug-protein pairs that use different identifiers and which include other information that could be useful to identify these molecules (like drug structure). The arguably most popular way to identify drugs and proteins are the PubChem CIDs and UniProt accession numbers, respectively. We use these identifiers to map data between the resources. First, we remove the data collected from TTD and GTP that lacks PubChem CID or UniProt identifiers. Next, we map the proteins in Drug2gene that are represented by Entrez Gene ID into the corresponding UniProt accession numbers. After mapping and combining these datasets and removing duplicates, we obtain 2,490,057 interactions for 591,684 bioactive compounds and 4,128 proteins. Next, we filter this list of compounds using the list of drugs obtained from the DrugBank and ChEMBL. We remove the compounds that do not have the same CID or SMILES structure when compared to the list of DrugBank and ChEMBL drugs. Finally, we remove non-human proteins using a reference human proteome from UniProt. This resulted in 33,104 interactions between 4,405 drugs (PubChem CID) and 1,638 proteins (UniProt identifiers). We provide the complete D dataset in the Appendix A. Moreover, we generate an expanded set of drug targets (**D+ dataset**) that includes proteins in the D dataset plus human proteins that share high sequence similarity to drug targets in other organisms. More specifically, following recent works [38, 104, 127], human proteins that share at least 90% sequence identity quantified using BLAST with default parameters [128] to any of the drug targets (human or otherwise) were added into the D+ dataset. Consequently, the D+ dataset has 1,762 proteins all proteins in D and 124 extra proteins that were included based on the high similarity; we list these proteins in the Appendix A. We include D+ set in our analyses to make sure that our conclusions would not be affected if by this extension, even though the fact that D+ dataset has

very little overall difference with D dataset, makes any statistically significant difference between these sets unlikely.

The number of drug targets in our dataset is slightly higher than the sizes of the datasets used in related studies (in the inverse chronological order): 1604 in [113], 1578 in [119], 1324 in [118], and 1030 in [1]. Compared to popular databases, such as KEGG DRUG and DrugBank, our dataset features a more complete set of interactions (33,104 vs. 14,222 and 23,380, respectively [121]) while focusing on a smaller and relevant set of drugs that specifically target human proteins (4,405 vs. 5,045 and 10,562, respectively [121]).

Number of drug interactions for our drug targets ranges between 1 to 443. We investigate whether structural and functional characteristics of highly promiscuous drug targets are different from the drug targets that interact with a few proteins. To do that we extracted two subsets of the drug targets, the highly promiscuous targets (Dh dataset) that correspond to the top quartile of the targets with the highest interaction counts, and the low-interaction drug targets (Dl dataset) that include the bottom quartile of the drug targets with the lowest numbers of interactions.

Dataset of current non-targets (N dataset)

We contrast the structural and functional characteristics of the proteins in the D, D+, Dh and Dl datasets against the proteins that are currently not drug targets (as of May 2018 when we performed this study). We collect these current non-targets (N dataset) by selecting proteins from the UniProt's human proteome that are not in the D dataset. The selection process follows two rules. First, we match the size of the N dataset to the size of the D dataset to ensure robust statistical comparisons between different datasets. Second, when down-sampling the human proteins, we ensure that the selected proteins have similar size as the proteins in the D dataset. More specifically, for each protein in the D dataset we pick a human non-drug target at random (without replacement) that has a matching sequence length (with 10% tolerance). We introduce the latter rule since the amount of intrinsic disorder in proteins is dependent on proteins length [129]. The same selection process was used in several related studies [130-132] to eliminate protein size bias when studying intrinsic disorder. We provide the list of the 1,638 size-matched proteins that constitute the N dataset in Appendix A. Moreover, the first sub-section in the "Results and discussion" section describes how we develop the Nd dataset (likely targets; currently non-drug

targets that are associated with multiple diseases) and Nn dataset (unlikely targets; the currently non-drug targets that have no known disease associations).

3.2.2. **Characterization of protein properties**

We characterize a broad collection of characteristics of human proteins that include their disease associations, structural properties derived from the sequence (putative intrinsic disorder and surface), sequence properties (domain annotations, alternative splicing and residue-level conservation), topological properties of the corresponding PPI network (centrality measures and hubs), and functional properties (GO annotations and predicted protein-binding regions). We extract these characteristics directly from the protein sequence or other protein annotations that are available proteome-wide. This means that they could be used as potential markers for drug targets that cover the entire human proteome.

Disease associations

We collect the protein-disease association data from DisGeNET [13]. DisGeNET integrates several curated databases and offers arguably one of the most complete levels of coverage for human diseases. This database provides association between disease MeSH IDs and Entrez Gene IDs and also provides a mapping between Entrez Gene IDs and UniProt identifiers. We map these annotations to our dataset using the UniProt identifiers.

Sequence-derived Structural properties

We annotate two relevant structural properties that are accurately derivable from the protein sequences: intrinsic disorder and solvent accessibility. We are unable to directly collect structural data since majority of the proteins in the D, D+ and N datasets do not have solved structures.

Intrinsically disordered proteins and protein regions lack a stable tertiary structure in isolation [62, 133, 134]. Proteins with disordered regions are crucial for many key cellular functions including molecular recognition and assembly, cell cycle and cell death regulation, signal transduction, transcription, translation, and viral cycle [131, 132, 135-153]. They are also the main contributors to the dark proteome [154, 155]. Intrinsic disorder is abundant in the human proteins. Computational studies estimate that about 19% amino acids in eukaryotic proteins are intrinsically disordered [66] and over 40% human proteins have at least one long disordered region with 30 or

more consecutive residues [156]. These proteins are particularly relevant to this study since they are associated with several human diseases [151, 157-159] and since they attract recent interest as potent drug targets [160-164]. Intrinsic disorder can be predicted accurately from protein sequence using computational methods [165-169]. We use one of the leading disorder predictors, IUPred [170, 171]. This selection is motivated by the fact that IUPred is computationally efficient (i.e., it can be used to process large datasets of proteins, such as the D and N datasets) and since it provides accurate predictions [168, 169]. We use the IUPred's results to compute the disorder content (fraction of disordered residues in a given protein) and the length of the putative disordered regions.

Solvent accessibility provides a crucial context for the analysis of the residue-level conservation since it allows us to separate conserved residues that are localized on the surface (which include residues that are instrumental for the drug-protein interaction) from those located in the protein core (which are likely responsible for structural stability of the protein). We predict the relative accessible surface area using the ASAquick method [172]. This method predicts solvent accessibility from a single sequence (without alignment), and thus it much faster than the other predictors that require calculation of multiple sequence alignment. It also provides accurate prediction, which is why it was recently used in related studies [173-175]. We convert the numeric relative solvent accessibility of residues into a binary annotation (solvent exposed vs. buried) using a threshold of 0.15. This value adequately splits the bimodal distribution of solvent accessibility values for the residues in the combined D and N datasets (Figure 3-1). We use these results to quantify the fraction of the putative surface residues in a given protein.

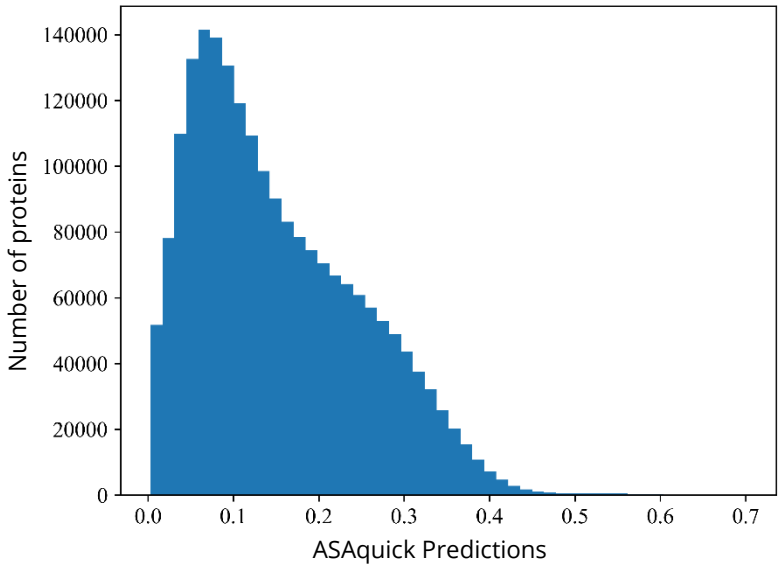


Figure 3-1. Distribution of the putative solvent accessibility values generated with ASAquick method for the residues in the D and N datasets. A threshold of 0.15 was selected to binarize the putative solvent accessibility scores, i.e., solvent exposed residues > 0.15, buried ≤ 0.15.

We assess quality of these predictions by comparing values of the fraction of the native surface residues that are computed using a limited set of proteins that have structures against the fraction of the predicted surface residues for the same set of proteins. We utilize mapping generated with the SIFTS resource [176] that is available in UniProt to identify structures of the human proteins from the D and N datasets in the PDB database [177]. We consider structures that cover at least 90% of the corresponding full protein sequences collected from UniProt to ensure that they correspond to a similar set of residues that are covered by the predictions which rely on the full protein chains. We compute the native solvent accessibility from these structures in three steps. First, we remove other molecules (including other protein chains) from the PDB structures. Second, we use DSSP [178, 179] to compute solvent accessibility values. Third, we convert the solvent accessibility into the relative solvent accessibility values using the normalization procedure that is described in the ASAquick article [172]. We were able to collect the native solvent accessibility values for 373 drug targets (including 343 proteins from the D dataset, 55 from the Dh dataset and 103 from the Dl dataset) and 73 proteins non-drug targets (including 39 from the Nd dataset and 12 from the Nn dataset). This corresponds to (373+73)/(1762+1,638) = 13% structural coverage of the human proteins in our datasets. Figure 3-2 compares the distributions of

the fractions of the surface residues computed from the protein structures against the fractions that are based on the predicted solvent accessibility for the seven considered datasets. The distributions that rely on the native vs. putative solvent accessibility for each of the seven datasets are very similar. The differences are not statistically significant (*p*-values range between 0.17 for the N dataset and 0.88 for the Nd dataset). These results suggest that the solvent accessibility predicted with ASAquick provides an accurate approximation of the native fraction of the surface residues.

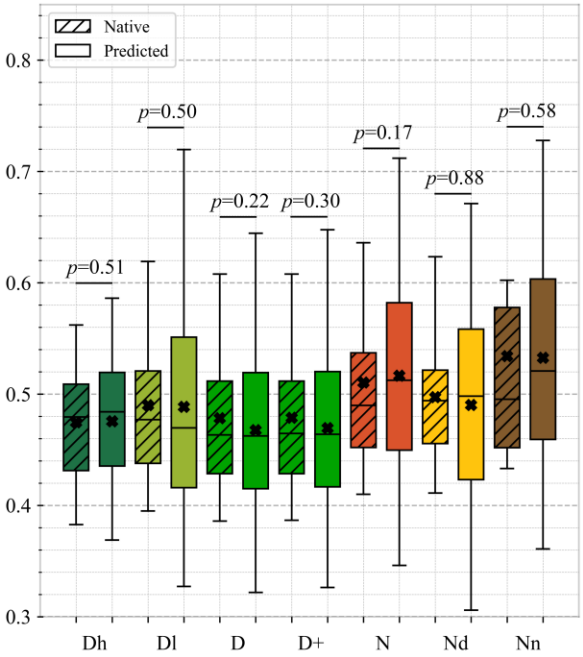


Figure 3-2. Comparison of content (fraction) of surface residues in seven protein sets for both native and putative values. The whiskers show the 5 and 95 percentiles, the middle bar is the median, and the cross marker is the average. The p-values shown above the whiskers quantify the significance of differences between putative and native values. We explain calculation of statistical tests in section "Statistical and similarity analyses"

Protein sequence properties

We use protein sequences to annotate the domains, alternative splicing isoforms and sequence conservation. We collect the domain annotations from Pfam [180] using UniProt identifiers, and we use these annotations to compute the domain boundaries (fraction of the domain-assigned residues) and the number of domains per protein. We obtain the number of alternative splicing isoforms from the UniProt database [181]. We calculate residue-level conservation scores using the relative entropy measure [182] from the PSSMs generated with PSI-BLAST [183]. We use a threshold to convert the numeric conservation scores to binary, i.e., a given residue is either conserved (if its conservation score > threshold) or non-conserved (otherwise). We select the

threshold that corresponds to the 80th percentile of the distribution of the conservation scores for the residues in the combined D and N datasets (Figure 3-3). The corresponding threshold value of 0.63 corresponds to an inflection point in the distribution tail where the conserved residues should be located. Using these annotations, we quantify the rate of the conserved residues in the protein sequence and among the residues located on the putative protein surface, given that this is where the drug-protein interaction occurs.

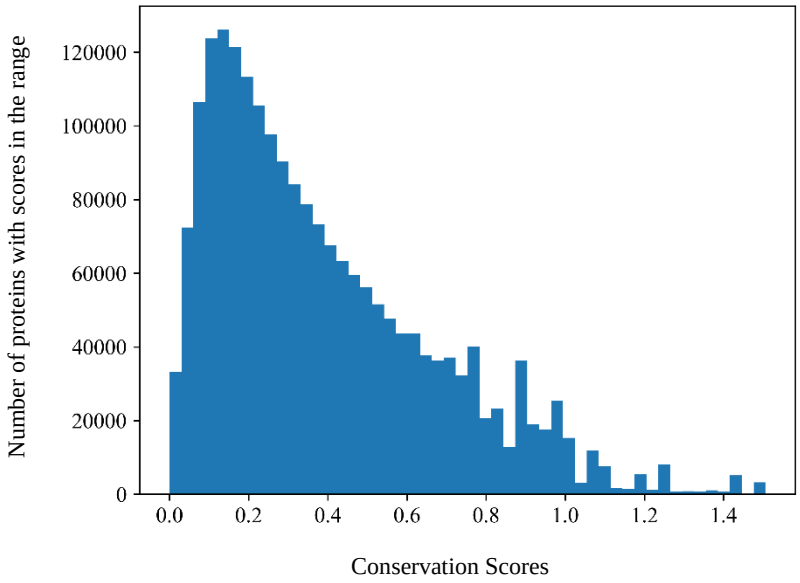


Figure 3-3. Histogram of the conservation scores for the residues in the D and N datasets. A threshold of 0.63, which corresponds to the 80th percentile of the distribution, was selected to binarize the score.

Topological properties of the protein-protein interaction network

Motivated by work in [113-116], we quantify the topological characteristics of drug targets and non-drug targets in the human PPI network. We collect the interaction network from the MENTHA resource [180] and directly map it to our datasets using UniProt identifiers. MENTHA integrates data coming from several popular databases of PPIs, such as IntAct [184], MINT [185], DIP [186], BioGRID [187] and MatrixDB [188], providing arguably one of the most comprehensive coverage levels. Several different centrality measures can be used to define topological characteristics of proteins in PPI networks [189]. We consider a comprehensive set of measures including betweenness centrality [190], eigenvector centrality [191], closeness centrality [192], information

centrality [193], degree centrality [194], subgraph centrality[195], network centrality[196] and local average connectivity[197]). We reduce this set by removing measures that are redundant (highly correlated). The corresponding subset of four measures (eigenvector, closeness, betweenness and information centrality) has relatively low mutual correlations (<0.6) while being highly correlated (>0.8) with at least one of the removed measures. We give the corresponding correlations between these measures on our datasets in Figure 3-4. The eigenvector centrality is an extension of the node degree in which connections to more important nodes have more impact on the score. The nodes that are connected to many highly connected nodes end up having higher score than nodes which are connected to the same number of less-connected nodes [191]. The closeness centrality measures the average length of the shortest path from the node to other nodes. The nodes with higher closeness centrality on average have smaller distance to the other nodes [192]. The betweenness centrality quantifies the frequency with which a given node appears in the shortest paths between nodes in the network. Thus, removal of nodes with high betweenness centrality has big impact on the shortest paths between nodes [190]. Finally, information centrality is based on information along the paths from a given node to the other nodes [193].

	DC	IC	EC	SC	BC	CC	NC	LAC
DC	1.00							
IC	0.41	1.00						
EC	0.91	0.42	1.00					
SC	0.82	0.15	0.83	1.00				
BC	0.77	0.12	0.54	0.62	1.00			
CC	0.17	0.23	0.18	0.08	0.06	1.00		
NC	0.93	0.27	0.87	0.93	0.75	0.12	1.00	
LAC	0.67	0.53	0.80	0.51	0.26	0.20	0.65	1.00

Figure 3-4. Matrix of correlations between centrality measures. Pearson correlations between the measures of Betweenness Centrality (BC), Eigenvector Centrality (EC), Closeness Centrality (CC), Information Centrality (IC), Degree Centrality (DC), Subgraph Centrality (SC), Network Centrality (NC) and Local Average Connectivity (LAC) computed over the combined set of proteins from the D and N datasets. There gray shaded numbers are high correlations (>0.8) between the two measures and the green shading highlights the selected measures.

Besides quantifying several different topological features, we also annotate hub proteins, defined as proteins that interact with many proteins [198]. While early works on hub proteins defined them using a fixed minimal number of [198], more recent studies use a floating threshold defined as a certain percentage of the most connected nodes in a given interactome [199-201]. This results in different cut-offs that define hubs for different interactomes (different organisms) and emphasizes

the fact that hubs are a property of the whole interactome system rather than a property of individual proteins. We use the latter definition using the cut-off that corresponds to the 90th percentile of the interaction counts in the complete human PPI network, which is consistent with several recent studies [199-201]. Therefore, we annotate hub proteins as those that have the number of PPIs in the complete interactome collected from MENTHA that is higher than this threshold (i.e., $\geq$ 77 interactions).

Hub proteins have increased levels of intrinsic disorder [131, 202] and the disordered regions are often employed to carry out protein-protein interactions [135, 203, 204]. The disordered protein-binding regions are also linked to certain human diseases [205]. Thus, we also annotate putative disordered protein binding regions. We use ANCHOR [206] to predict the disordered protein-binding residues and we aggregate this information to compute the content of disordered protein binding residues for the proteins in our datasets. The selection of this method is motivated by the fact that it is accurate and popular, and provides fast predictions (i.e., is capable of processing our large datasets) [165, 207, 208].

Functional properties

We annotate cellular functions and subcellular locations of the drug targets and the non-drug targets using the Gene Ontology (GO) terms [209], which we collect using the PANTHER system [210]. We annotate and separately analyze the molecular functions, biological processes, and cellular components, where the latter define the subcellular locations.

3.2.3. **Statistical and semantic-similarity analyses**

We compare the structural and functional characteristics between the current targets, currently non-targets and likely targets using statistical tests of significance of differences. We quantify the significance of the differences using the *t*-test if the underlying measure of the structural/functional property has normal distribution, and Wilcoxon rank-sum test otherwise. We use the Anderson-Darling test with the *p*-value cutoff of 0.05 to test normality. We use the Fisher's exact test when comparing binary characteristics, including disease associations and presence of hubs.

We annotate the cellular functions and subcellular locations associated with each set of proteins using enrichment analysis offered by the PANTHER system [210]. This system generates a list of

annotations that are statistically over-represented when compared with the annotations present in the whole human proteome. PANTHER quantifies the ratios of enrichment and the corresponding *p*-values for each GO term when compared with the reference human proteome. We focus on the GO terms that occur at least 10 times in our datasets (to ensure robustness of statistical analysis), and we annotate a given term as associated with a particular set of proteins if its ratio > 2 (at least two-fold increase) and the associated *p*-value (quantified using the False Discovery Rate correction) is < 0.05.

We use these semantic similarity measures as a proxy to estimate the level of overlap in functional characteristics between our proteins sets. We calculate this semantic similarity using the GOSemSim package [211] with default parameters (Wang *et al.* measure [212]) and the set of human proteins as the reference set.

3.3. **Results and discussion**

3.3.1. **Likely and unlikely drug target proteins**

The set of the current non-targets probably includes a relatively large number of proteins that can potentially be drug targets in the future. The necessary conditions to be a drug target include being able to bind a drug-like molecules (druggability) and to alter the state of a disease as the result of that interaction [108-110]. Thus, one way to separate likely and unlikely future target proteins is to analyze protein-disease associations, i.e., proteins that are not associated with diseases cannot satisfy the second condition. Figure 3-5 shows the fractions of the disease-associated proteins among the current targets and non-targets side by side, across different classes of diseases. As expected, the number of the disease-associated proteins is significantly higher for the current targets compared to the current non-targets. This difference is statistically significant for each of the 23 diseases classes (*p*-values < 0.0001). Theoretically, each drug target should have some disease association (known or unknown) that explains its therapeutic use. Therefore, expectedly, about 94% of the proteins in our drug target set have at least one disease annotation. This attests to the relatively high coverage (rate of completeness) of these disease association annotations. To compare, only about 64% of the non-drug targets are disease-associated. It would be reasonable to say that future drug targets are most likely among this disease associated subset and the remaining 36% have a low chance being a drug target.

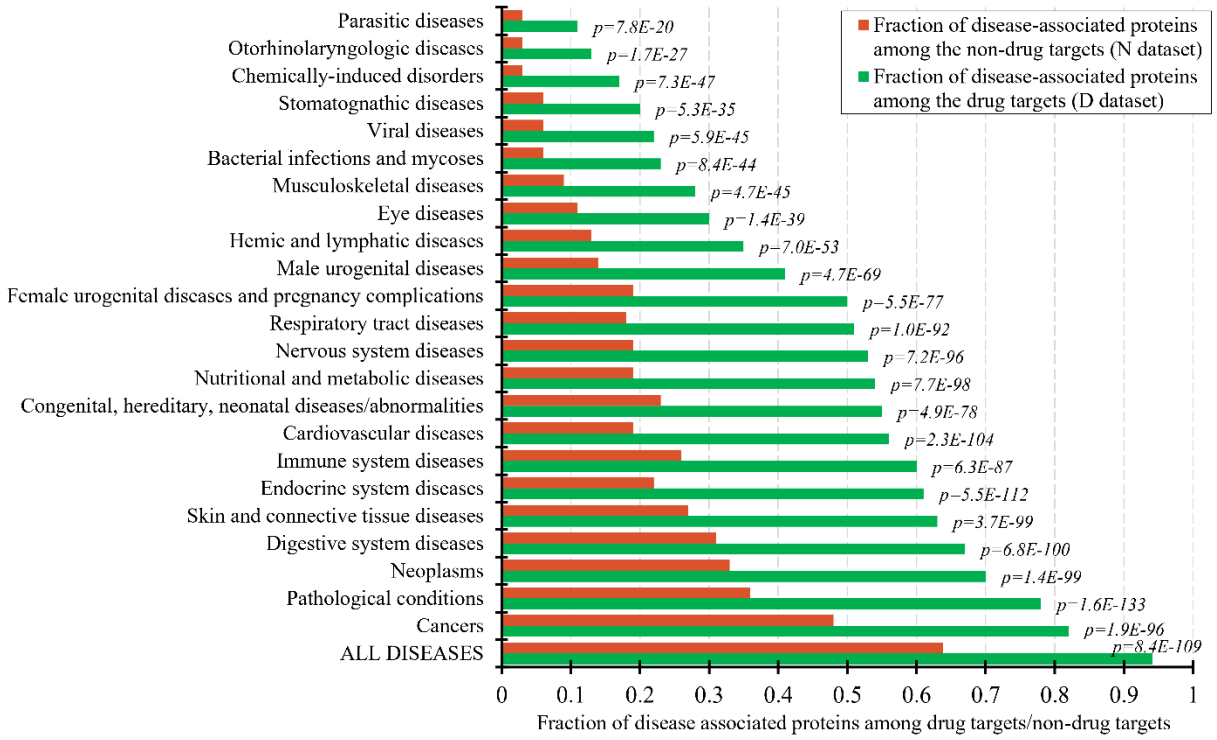


Figure 3-5. Disease-associated fraction of proteins for different categories of diseases and shown for both current targets (green) and current non-targets (red). The p-values quantify the significance of the differences between the two fractions using the Fisher's exact test. The disease classes are sorted by the value of the fraction of the drug targets.

Figure 3-6 further analyzes relation between current targets, current non-targets and disease associations, this time with a focus on the number of diseases associations of each protein. Figure 3-6A reveals that disease-associated proteins are more likely to be found in the set of drug targets than in the set of non-targets. About 60% of proteins that are associated with at least one disease are drug targets. This fraction grows higher for the proteins that are associated with more disease. Also, Figure 3-6A shows that this increase is sharper initially and then plateaus for higher number (10 or more) disease associations. Therefore, we hypothesize that the current non-target proteins with a relatively large number of disease associations can be used as a proxy for likely future targets. Using Figure 3-6A we choose a threshold of 13 as a high number of disease associations. Figure 3-6B shows the same diagram plotted between K=0 and K=40 to focus on the proximity of the threshold and where the change in the rate of variation happens. Using this threshold, we define the set of **likely target** proteins (**Nd set**) as the subset of current non-targets (N) with ≥13 disease associations. Figure 3-6C is a Venn diagram that visualizes overlap between these sets. The set of

proteins with ≥1 and ≥13 disease associations are shown with black borders, the current targets (dataset D) with green border, and the non-drug targets (dataset N) with red border. Figure 3-6C shows that virtually all drug targets are associated with at least one disease (black border rectangle with number of diseases K ≥ 1), while a large portion of the non-drug targets lacks any disease associations (brown area in Figure 3-6C). The latter set of proteins constitutes the set of the unlikely targets (**Nn set**).

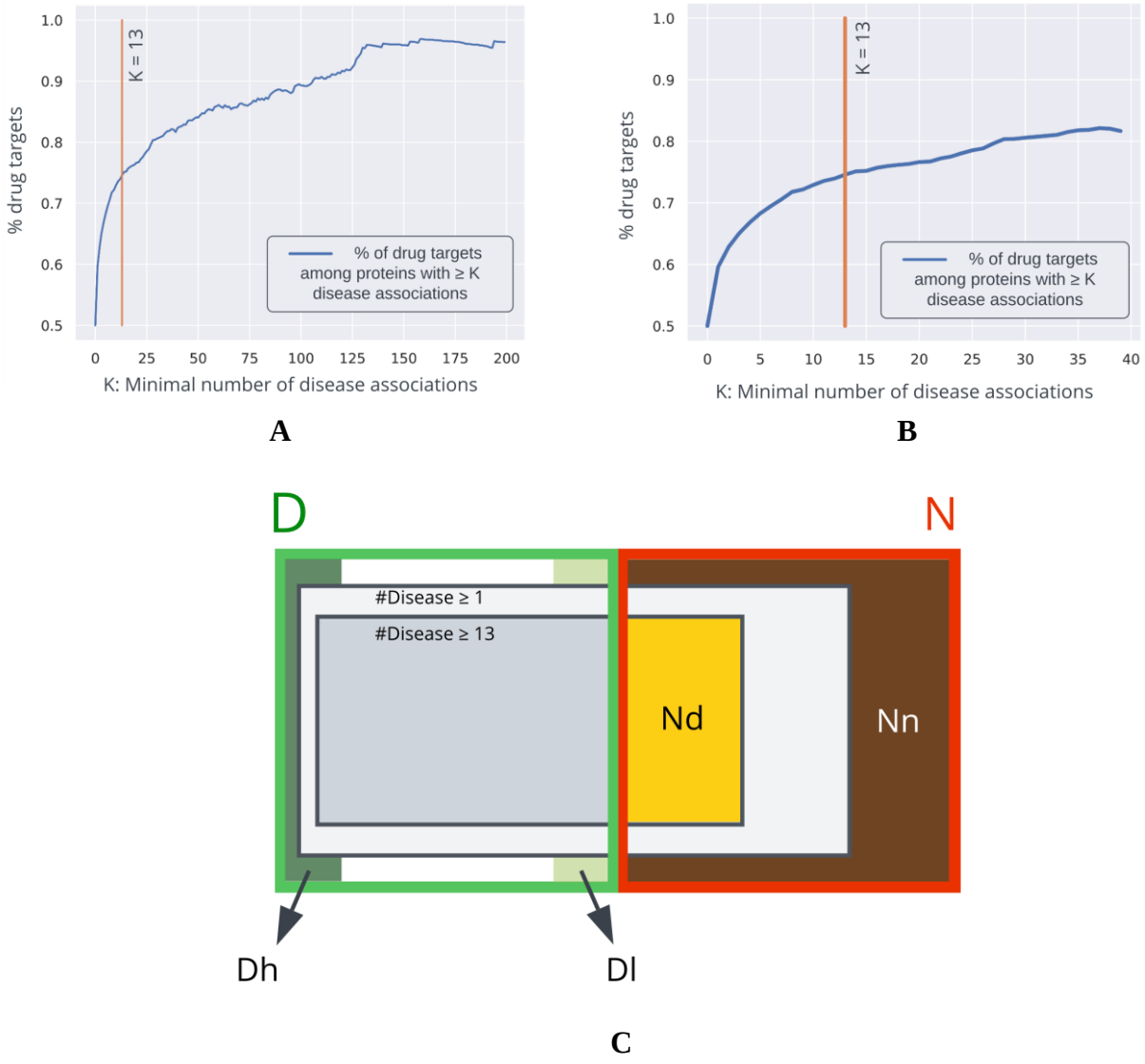


Figure 3-6. Relation between current targets, current non-targets and diseases associations. Panel A shows the fraction of the drug targets among proteins associated with a given minimal number of diseases K. Panel B shows the same plot focused on the K values below 40 to better represent selection of the threshold. Panel C is a Venn diagram that visualizes overlap between the disease associated proteins (with K = 1 and K = 13), current targets (dataset D; green border), and the current non-targets (dataset N; red border). Among the current non-targets, we define the Nn dataset of unlikely targets (brown area) that have no disease associations, and the Nd dataset of likely targets (orange area),

i.e., the current non-targets that are associated with 13 or more diseases. We also annotate Dh and Dl that represent the current targets that have high and low number of drug interactions, respectively

We validate the definition of likely and unlikely targets using the 124 current non-target proteins that have high sequence similarity to drug targets in other organisms (D+ dataset). We find that D+ set has much more in common with Nd set than with Nn set. 67% (83 out 124) proteins in D+ were in Nd, while only 4% (5 of the 124) were in Nn, considering that Nn and Nd are similar in size (4,869 versus 4,287). The high degree of overlap suggests that the Nd dataset should include a substantial number of druggable proteins. which in addition to their high disease association makes them more likely as a drug target. We note that the 4% overlap with Nn likely stems from some (albeit likely low) level of incompleteness of the disease association data.

Observations in Figure 3-7 further strengthen the hypothesis that the Nd and Nn datasets are relatively good representations of the likely and unlikely targets, respectively. It quantifies the level of similarity (as measured by semantic similarity in annotations) between each pair of these proteins sets (N, D, Nd, and Nn) in the context of cellular functions and subcellular. We perform this analysis separately for each of the three GO terms categories: molecular functions, biological processes, and cellular components; the latter is a proxy for the subcellular location. First, we generate a set of GO terms that are enriched in each of these datasets, i.e., GO terms over-represented in a given dataset when compared to the human proteome. Next, we calculate semantic similarity between the enriched GO terms of the four protein sets N, D, Nd, and Nn. The details of these calculations are presented in section 2.3. The gray lines in Figure 3-7 shows the semantic similarity values for each GO term category while the blue lines show the average across the three categories. The left-most set of results reveals that the cellular functions and subcellular location of the current drug targets (D dataset) are similar to the likely targets (Nd dataset). The second set of results, which compares the current drug targets against the unlikely targets (Nn dataset), shows lack of semantic similarity in the and subcellular locations and modestly reduced levels of semantic similarity in the annotations of molecular functions. The corresponding average semantic similarity with D is lower (0.145) for Nn by a factor of two when compared with the semantic similarity for Nd set (0.303). The other two sets of results, which compare the likely targets against the unlikely targets (Nd-Nn) and the current targets against current non-targets (D-N), reveal the lack of semantic similarity in the biological processes and subcellular locations annotations, while

showing semantic similarity in the molecular functions annotations. The average semantic similarities for these two dataset pairs are low and equal 0.177 and 0.115, respectively, suggesting that the corresponding two pairs of datasets include proteins involved in distinct cellular processes and subcellular locations. To sum up, the above analysis demonstrates that the likely target proteins (Nd) share much higher levels of overlap in functional and subcellular location annotations than other sets (N and Nn) to the set of current targets (D). This finding, which uses an independent source of information from the definition of likely targets (based on disease association), further validates the selection of the likely and unlikely sets of proteins.

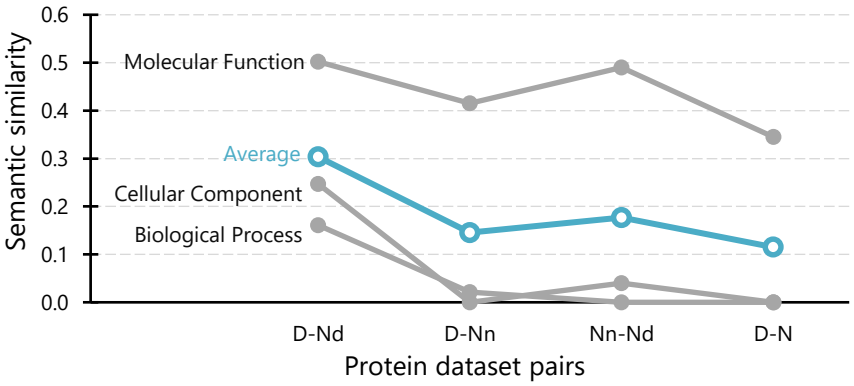


Figure 3-7. Semantic similarities in annotations of functions and subcellular locations between the current targets (D dataset), likely targets (Nd dataset), unlikely targets (Nn dataset), and current non-targets (N dataset). These semantic similarities are separately calculated and shown with grey markers for the three categories of GO terms and for the average of the three is shown with blue markers. We describe details of these calculations in section 3.2.3.

3.3.2. **Comparative analysis of sequence-derived structural and functional characteristics of the current targets, likely targets and unlikely targets**

Identifying functional and structural characteristics that differentiate drug targets from the rest of proteins can provide invaluable insights for finding novel drug targets. We focus specifically on the characteristics that can be extracted from the protein and information that are available proteome-wide (GO annotations and protein-protein interaction networks). We compare a broad range of these characteristics between the four set of proteins described in the previous section (D, N, Nd and Nn), the D+ set, which is an expansion of current drug targets by adding the human proteins that are not currently drug target but are highly similar to drug targets in other organisms, and the Dh and Dl which are current targets that have respectively high and low number of drug interactions (Figure 3-6C).

Characteristics derived from the protein sequence

Figure 3-8 focuses on the characteristics derived directly from the protein sequence, including the residue-level conservation (content of conserved residues in protein chains), number of domains and the content of domain-annotated residues, and the number of the alternative splicing isoforms. Figure 3-8A shows that the current drug targets (both D and D+ datasets) have significantly fewer conserved residues than the current non-targets, likely targets, unlikely targets proteins (p-value < 0.05). The likely targets (orange) have significantly lower numbers of conserved residues compared to the unlikely targets (brown) (*p*-value < 0.05). Moreover, the highly-promiscuous drug targets (Dh) have significantly lower numbers of the conserved amino acids than the current non-targets and the non-target proteins (*p*-value < 0.05), while maintaining similar levels compared to the likely targets. Altogether, relatively low numbers of the conserved residues are characteristics for the current drug targets and these numbers are also relatively low among the likely targets. Interestingly, the residue-level conservation of the residues on the protein surface, where the protein-drug interaction occurs, follows the same pattern (Figure 5E). This finding complements prior results that show that drug targets have lower evolutionary rates and higher similarity to orthologous genes [213].

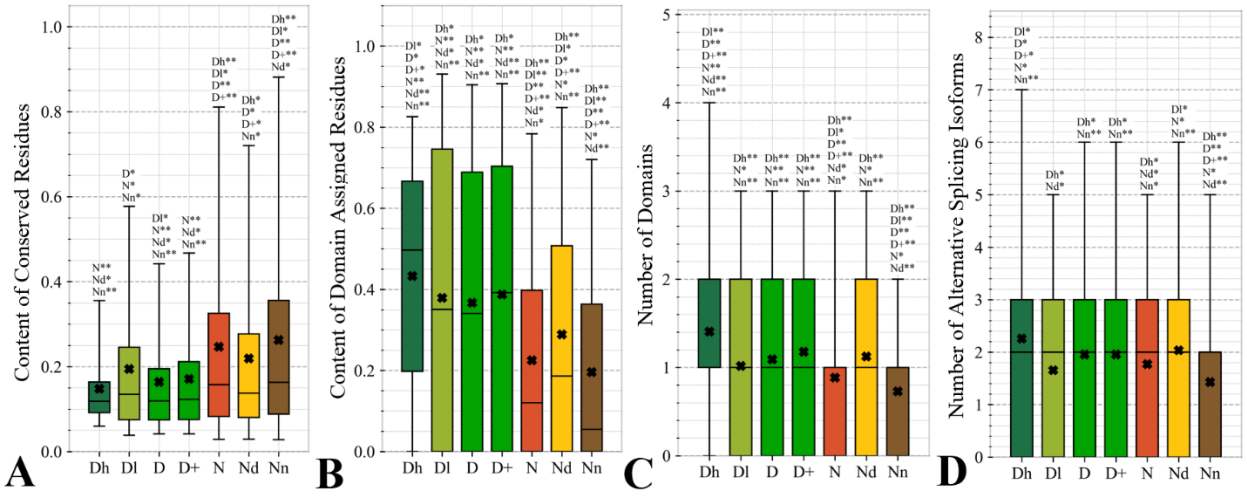


Figure 3-8. Distributions of the values of the sequence-derived characteristics for the seven sets of proteins (Panels A) shows the fraction of conserved residues. Panels B and C focus on the protein domains while Panel D quantifies the number of splicing isoforms. The whiskers show the 5 and 95 percentiles, the middle bar is the median, and the cross marker is the average. The annotations above the whiskers show the significance of differences with the other protein sets; only significant differences are listed where N* means p-value<0.05 and N** means p-value<0.0001 when compared with the N dataset. We explain calculation of statistical tests in section 3.2.3

Figure 3-8B and C reveal that current drug targets (both D and D+ datasets) have substantially more domains and have larger amounts of domain-annotated residues when compared to the unlikely targets (p-value < 0.001). At the same time, they have comparable number of domains and more similar levels of the content when contrasted with the likely targets. Furthermore, the likely targets have significantly higher levels of domain annotations when contrasted against the unlikely targets (*p*-value < 0.0001). The underlying reasons for this enrichment could be two-fold. First, there could be proportionally more multi-domain proteins among the current targets and the likely targets. Consequently, inclusion of a larger number of domains could increase the likelihood that these proteins host at least one druggable domain. However, our result could also mean that these proteins are more studied and understood, and thus their domain annotations are more complete. Moreover, the fact that at least close to half of proteins in all considered datasets have domain annotations, which suggests that they are functionally annotated, confirms robustness of our semantic similarity analysis in Figure 3-7.

The current drug targets (both D and D+ datasets) and likely targets have significantly more splicing isoforms compared to the unlikely targets (*p*-value < 0.05) and this increase is even higher for the promiscuous drug targets (*p*-value < 0.001). This suggests that enrichment in the number of alternative splicing variants could serve as a marker for likely target proteins. The alternative splicing was found to contribute to drug resistance [214, 215], which supports veracity of our result. Interestingly, recent studies suggest that targeting alternative splicing events could lead to therapeutic opportunities [215, 216]. Our analysis also reveals that majority of the current drug targets and the likely targets have multiple isoforms. Thus, gene level analysis of drug targets may not be adequate, considering that these genes would encode multiple proteins.

Overall, we identified three potential sequence-derived markers of likely targets. The current targets and likely target proteins share lower numbers of conserved residues and are more likely to have multiple domains and isoforms when compared to the unlikely targets. We also note that the results for the original set of current human drug targets (D dataset) are consistent with the results for the expanded set of targets (D+ dataset).

Sequence-derived structural properties

This study is the first to analyze two relevant sequence-derived structural characteristics that can be accurately predicted from the protein sequence: intrinsic disorder and solvent accessibility. Proteins with disordered regions are associated with a wide range of human diseases [151, 157-159] while solvent accessibility determines protein surface where the drug-protein interaction happens. We note that while authors in [119] computed putative solvent accessibility, they used it only to analyze results concerning enrichment in the PTMs.

Figure 3-9A, 3.5B and 3.5C quantify two key aspects of the disorder: the overall content of disordered residues and the length of disordered regions. Proteins with higher disorder content are functionally distinct from structured proteins while long disordered regions correspond to disordered protein domains [65, 217, 218]. We observe that current drug targets (both D and D+ datasets) are significantly less disordered (by a factor of two) and include much shorter disordered regions when compared with the current non-targets, including likely t and unlikely targets (p-value < 0.001). This is in agreement with a recent study that demonstrates that the current drug targets are biased to exclude disordered proteins [22]. There are several reasons for this bias. The protein structures are used during the rational drug design process [219-222] and to gain mechanistic insights into the protein-drug interactions [223-225]. The structures are also indispensable for modeling associated with drug repurposing and repositioning [226, 227]. This is while proteins with disordered regions are much less likely to have structures [154], partly because since they are explicitly avoided in the structural genomics pipeline [228-230]. Interestingly, the highly promiscuous drug targets are enriched in disorder when contrasted with the overall set of drug targets and the low promiscuity drug targets (p-value < 0.0001), while their disorder levels are comparable to the likely targets. This coincides with the observation that disordered regions are capable of interactions with multiple partners [231, 232]. Our results suggest that although low disorder amounts are a strong marker for the current drug targets, the set of likely targets includes large amounts of disorder. In fact, the disordered proteins may become the key to unlocking a substantial portion of yet to be discovered drug targets [22, 161], especially given their association with numerous human diseases [151, 157-159].

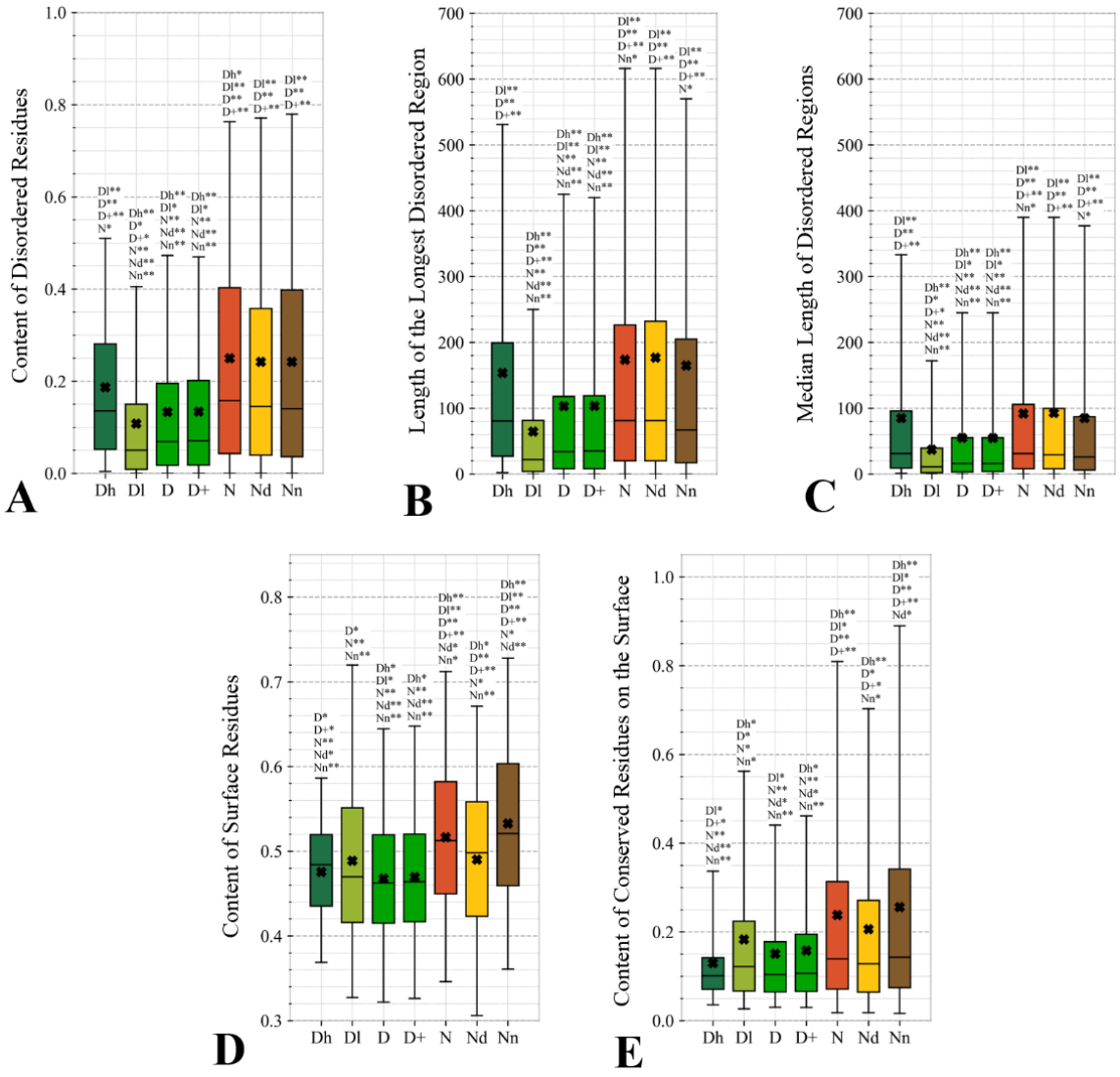


Figure 3-9. Distributions of the values of the sequence-derived structural characteristics. Panels A, B, and C quantify the abundance of intrinsic disorder while Panels D and E quantify the fraction of surface and the fraction of conserved residues on the surface, respectively. The whiskers show the 5 and 95 percentiles, the middle bar is the median, and the cross marker is the average. The annotations above the whiskers show the significance of differences with the other protein sets; only significant differences are listed where N* means p-value 0.05 and N** means p-value 0.0001 when compared with the N dataset. We explain calculation of statistical tests in section 3.2.3

The amount of the putative surface residues for the current drug targets (both D and D+ datasets) is significantly smaller that for the current non-targets, including the likely and unlikely targets (*p*-value < 0.0001), see Figure 3-9D. This could be driven by the fact that current drug targets are often membrane proteins [233, 234], which means that they have relatively low surface area compared to other proteins. They are also mostly structured proteins [22] that are more likely to have globular shape with more buried residues compared to more irregularly shaped/elongated

disordered proteins [139, 235]. Moreover, presence of disordered regions on the protein surface also leads to an increase of the surface area compared to structured conformations [236]. Interestingly, the likely targets have comparable content of the putative surface residues with the low promiscuity drug targets, which is also significantly smaller when contrasted with the unlikely targets (p-value < 0.0001). This again, like in the case of the results in Figure 3-8, shows that the likely targets are more similar to drug targets than to the unlikely targets. Finally, we observe that the number of conserved residues on the putative surface (Figure 3-9E) maintains the same relation between the different protein sets as the overall number of conserved residues shown in Figure 3-8A, i.e., significantly lower for current targets (both D and D+ datasets), and lower for the likely compared to the unlikely targets (*p*-value < 0.05).

Topological features of the PPI networks

Topological features of the PPI networks are among the most studied characteristics of the drug targets [113-116, 118, 119]. A unique aspect of our analysis is that we focus on a set of orthogonal measures, i.e., measures that have low mutual correlations. This results in a more focused and balanced analysis given the high degree of correlation between many of these measures. Figure 3-10 reveals that the entire set of four measures of centrality has significantly higher values for current targets (both D and D+ datasets) compared to the unlikely targets (*p*-value < 0.0001). This confirms the results from prior studies that similarly show that drug targets have more connected and denser local network neighborhoods [114-116, 213]. The novel element in our study is that we find that all considered network centrality measures for the likely targets are even higher than for the current targets (orange vs. green in Figure 3-10; p-value < 0.05). Consequently, they are also significantly higher than for the unlikely targets (orange vs. brown in Figure 3-10; p-value < 0.0001). Thus, our study suggests that these measures can be used as strong markers of drug targets.

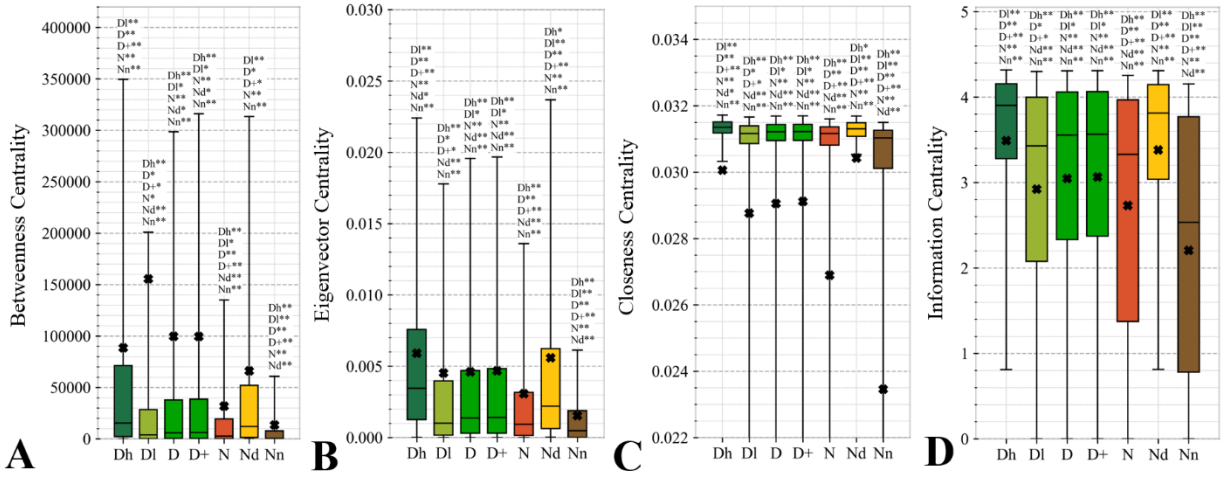


Figure 3-10. Distributions of the values of the selected orthogonal PPI network properties. Panels A, B, C, and D concern the betweenness centrality, eigenvector centrality, closeness centrality, and information centrality measures, respectively. The whiskers show the 5 and 95 percentiles, the middle bar is the median, and the cross marker is the average. The annotations above the whiskers show the significance of differences with the other protein sets; only significant differences are listed where N* means p-value 0.05 and N** means p-value 0.0001 when compared with the N dataset. We explain calculation of statistical tests in section 3.2.3.

Figure 3-11 analyzes the abundance of the PPI network hubs among the current drug targets, likely targets and unlikely targets. Approximately 17% of current targets (for both D and D+ datasets) are hubs and this rate is significantly higher than the 12% rate for the current non-targets (green vs red; p-value < 0.0001). Similarly large difference was observed in [114]. Our study reveals additional important details. We observe that the rate of hubs is very high among the highly promiscuous targets (25%) and likely targets (24%), and these rates are significantly higher than the 12% rate for the current non-targets (*p*-value < 0.0001) and the 5% rate for the unlikely targets (*p*-value < 0.0001). This suggests that high connectivity in the PPI network is a strong marker for drug targets.

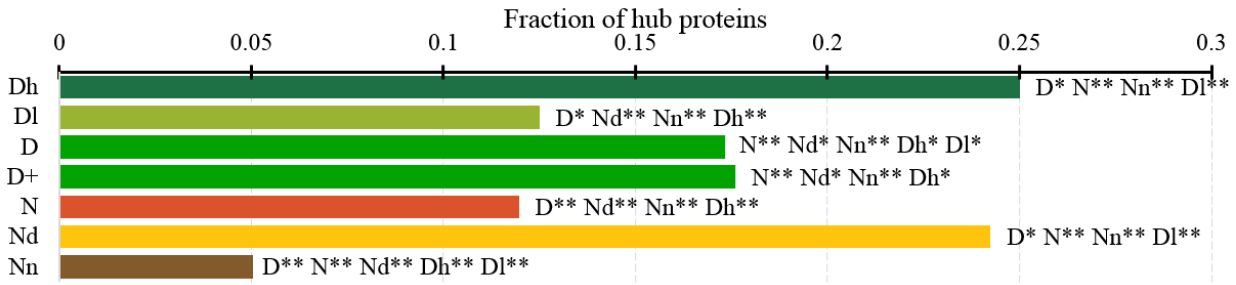


Figure 3-11. Fraction of hub proteins for the seven protein sets. The annotation next to the bars show the significance of differences with the other protein sets; only significant differences are listed where N* means p-value 0.05 and N** means p-value 0.0001 when compared with the N dataset. We explain calculation of statistical tests in section 3.2.3.

3.3.3. **Functions and subcellular locations of current targets and likely target proteins**

Several studies analyzed cellular functions and subcellular locations of the drug targets [112, 117, 237]. The green bars in Figure 8 provide a list of significantly enriched functions and locations for our set current drug targets. Our results indicate that most of the current targets are enzymes, including kinases and oxidoreductases, followed by substatial numbers of channels, and in particular ion channels. They are often involved in binding, signalling, regulation and transport. These finding are in close agreement with the results in [117]. Figure 3-12 also shows that current targets are primarily found in membranes, with a large number also found in the cytoplasm and the intracellular space. This is consistent with results in [117, 237], and these subcellular locations also agree with the observation that membrane proteins are the prime targets for the development of therapeutics [233, 234].

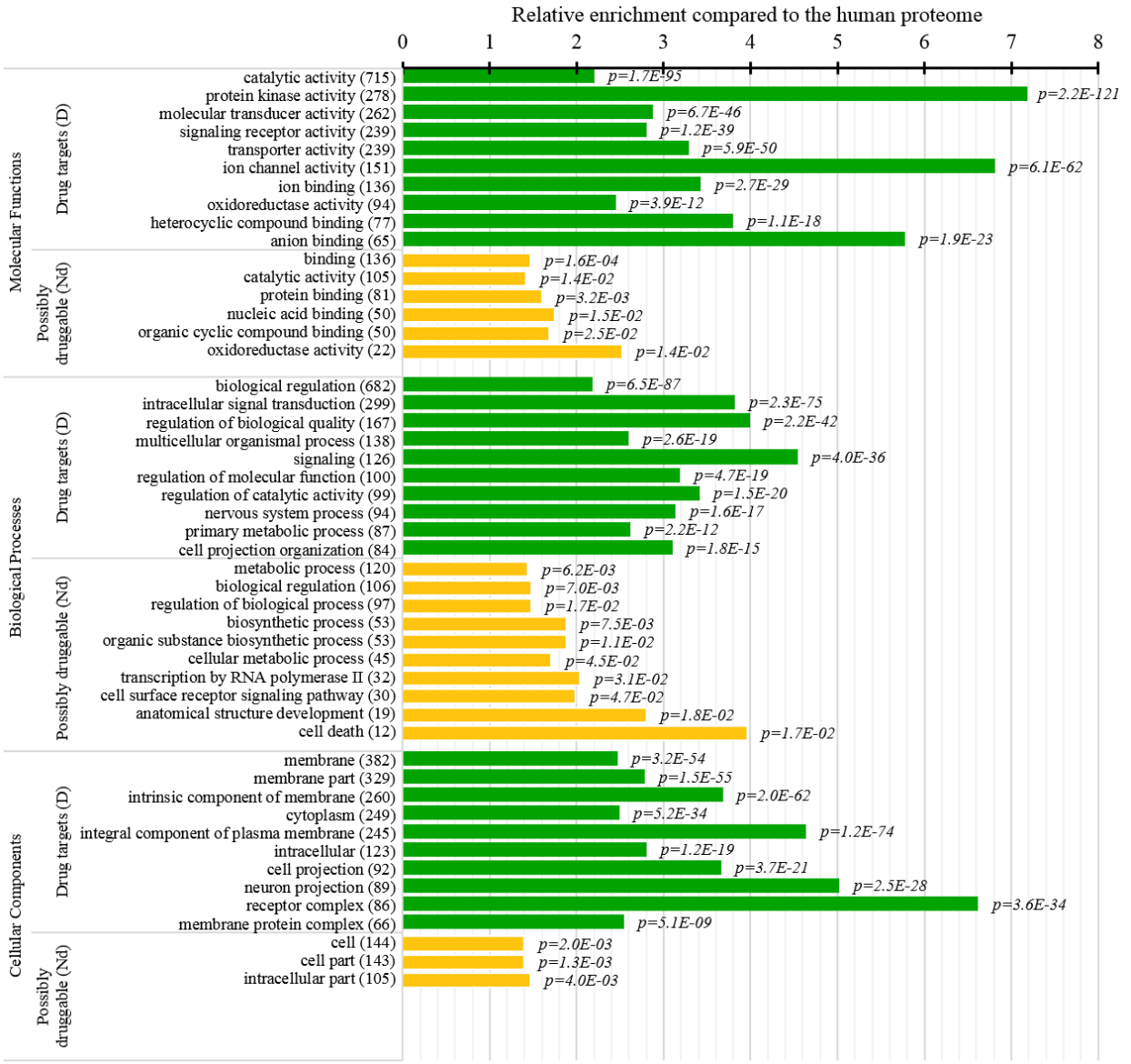


Figure 3-12. Molecular functions, processes, and subcellular locations that are enriched among the drug targets (D dataset) and the likely target proteins (Nd dataset). We show the top 10 (with the highest counts) over-represented (significantly enriched) GO terms for the current targets (green bars) and the likely targets (orange bars). The bars quantify the ratios of enrichment relative to the human proteome and the corresponding p-values are shown on the right. GO terms are identified on the left, including their names and the number of the corresponding proteins in the given dataset. We explain calculation of statistical tests in section 3.2.3.

This study is the first to perform this type of analysis for the likely targets (orange bars in Figure 3-12). Our analysis suggests that the likely target proteins share commonalities with the current targets. They are similarly involved in the catalysis, signaling, and binding. However, the likely targets tend to bind proteins and nucleic acids, instead of anions and ions which are the main

partners for current targets. Moreover, the likely target proteins are often involved in the metabolic and biosynthesis processes, and in the cell death cycle. The preference for the protein-protein and protein-nucleic acids binding and the cell death cycle involvement are supported by their significant enrichment in the intrinsic disorder (compared to the drug targets, see Figure 3-9A and 5B), and the fact that disordered regions are known to facilitate these types of functions [66, 141-144, 232, 238-240]. We further investigate this in Figure 3-13 that analyzes differences in the content of the putative disordered protein-protein binding regions. These results confirm the enrichment in the corresponding functional annotations for the likely target proteins. The likely targets include a substantial amount of the disordered protein-binding regions, on average about 14% of residues. Moreover, current targets (both D and D+ datasets) are significantly depleted in these protein-binding regions (on average only 7% of residues) when compared with the likely target proteins (*p*-value < 0.0001). Interestingly, Figure 3-12 also reveals that the likely target proteins are localized across the cell and they do not have a specifically associated subcellular location, unlike the current targets that are found mostly in the membranes and cytoplasm. Overall, our empirical analysis provides new insights into the cellular functions and subcellular locations of the current and likely targets.

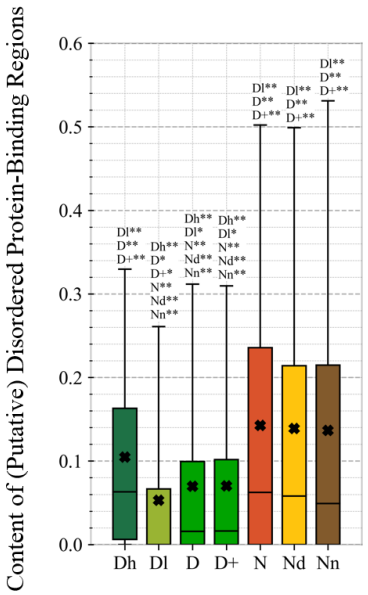


Figure 3-13. Content (fraction) of putative protein binding regions in the seven protein sets. The annotation next to the bars show the significance of differences with the other protein sets; only significant differences are listed where N* means p-value 0.05 and N** means p-value 0.0001 when compared with the N dataset. We explain calculation of statistical tests in section "Statistical and similarity analyses"

3.4. **Summary and conclusions**

Recent research approximates that 4500 proteins in human proteome could potentially be drug targets [23], while there are about 1600 proteins that have been targeted by drugs (1750 drug targets if we include proteins that share high sequence similarity to drug targets that were annotated in other organisms). Finding properties that could be used as markers of drug targets would strengthen our ability to identify novel targets. We contrast the current targets against the likely and unlikely targets to identify markers that could be used in search for targets in drug discovery, repurposing and repositioning. This is a different approach from prior studies that only compare current drug targets against current non-targets [111-119], thus being more prone to describing current drug targets rather than identifying not yet discovered targets. We specify a set of likely and unlikely targets based on presence and number of disease associations, and confirm validity of this selection via semantic similarity analysis in functional annotations.

We cover a wide range of sequence-derived characteristics to define the markers. These characteristics can be computed across the entire human proteome, allowing for a proteome-wide study. We investigate several important characteristics that were missed in the past studies including putative intrinsic disorder, residue-level conservation, presence and number of alternative splicing isoforms, inclusion of domains, and putative solvent accessibility (surface area), as well as the key features from the prior works, such as the topological features of PPIs, cellular functions and subcellular locations. Figure 3-14 summarizes the results. It shows the difference in the values of the key markers when comparing the likely targets (in orange), the non-unlikely targets (in brown), and all current non-targets (in red) and the expanded set (D+) of current human targets human proteins similar to targets in other organisms (in light green) against the current human drug targets (D; in dark green). We observe that the likely target proteins are significantly more similar to the current drug targets than the unlikely targets for majority of the markers. These markers include high abundance of alternative splicing isoforms, relatively large number of domains, higher degree of centrality in the corresponding PPI network (and correspondingly much higher rate of hubs), lower number of conserved residues and lower number of residues on the putative (sequence-derived) surface. Thus, these factors could serve as high-quality markers for potentials for being drug target. Moreover, Figure 3-14 shows that current drug targets (both D and D+ datasets) have significantly depleted levels of intrinsic disorder and

intrinsically disordered protein-binding regions when compared with the much higher levels in likely and unlikely targets. This suggests that the high levels of disorder combined with the presence of the abovementioned markers should be used together to effectively enlarge the current collection of drug targets. This is in accord with several recent studies that postulate inclusion of the disorder-enriched proteins into the set of druggable proteins [22, 161, 241-246].

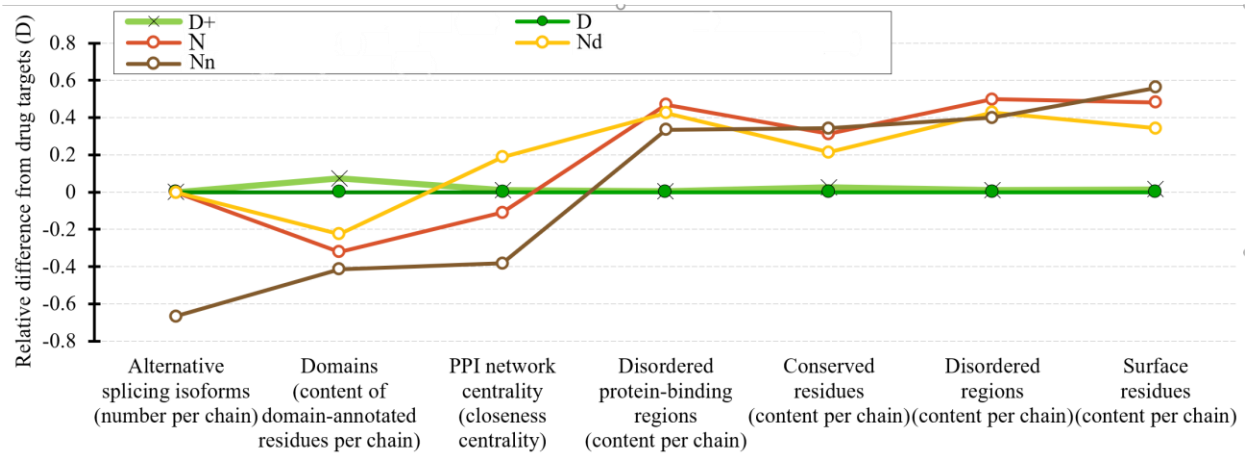


Figure 3-14. Overview of the sequence-derived markers. The y-axis quantifies the relative difference of the values of a given protein set X compared to the values of current targets (D) set defined as: (median(X)-median(D))/IQR(D), where IQR means the interquartile range. The markers are sorted in the ascending order by the difference for the unlikely targets (in brown).

Our analysis also shows that the likely target proteins are functionally similar to the current drug targets, being involved in the catalysis, signaling, and binding. The main difference is that the likely target proteins tend to have interactions with proteins and nucleic acids, unlike the current drug targets that favor interactions with anions and ions. Figure 3-14 points to the high amount of the disordered protein-binding regions for the likely target proteins compared to the current drug targets, which is in concert with the disordered nature of the likely target proteins. This is in agreement with the literature that shows that disordered regions often facilitate protein-protein interactions [135, 142, 203, 204, 232]. Finally, we show that the likely targets are involved in the metabolic and biosynthesis processes and that they are localized across the cell, without a preference for specific subcellular locations. This is unlike the current drug targets that are located primarily in the membranes.

To sum up, our empirical analysis leads us to formulate several markers that are suitable for the identification of new drug targets, and produces interesting insights into the cellular functions and subcellular locations of the current and likely candidates for future targets.

Chapter 4. **Analysis of compound-protein interaction focusing on the proteins containing compound-binding domains**

4.1. **Introduction**

In this chapter we focus on the task of predicting interactions for proteins-compound pairs. We extend beyond the protein-drug interactions by including molecules/compounds that may not be currently an approved or experimental drug. Therefore, we deliberately use the term "compound", which is the commonly used for this purpose. Since drugs work mainly by binding specific proteins and modulating their function, knowledge of these interactions is very important for drug discovery and repurposing. The ultimate goal is to find currently unknown interactions between small molecule compounds (described in Chapter 2) and human proteins.

As we discuss in Chapters 1 and 2, experimental data is available for a relatively limited collection of protein-compound pairs. Therefore, in-silico predictive approaches have been developed to fill this gap [26-32]. We focus on methods that do not rely on protein structures since they can be applied to a much broader group of proteins when compared to the protein-structure based predictors. These predictors were recently shown to achieve very high levels of accuracy in predicting interactions between compounds and proteins [31, 32].

Many proteins have modular architectures, being composed of multiple domains. Binding sites of small molecule compounds usually cover one domain [247], suggesting that individual domains mediate interactions with small molecules. Furthermore, poly-pharmacology (multi-target nature) of drugs is thought to be the result of domain-based architecture of proteins [248, 249]. In other words, the observations that drugs interact with individual domains and that the same interacting

domain can appear in several different proteins can explain how drugs can interact with multiple proteins [248]. Therefore, multiple studies investigated associations of compounds and domains in order to provide insights into compound-protein interactions[247, 250].

Associations between domains and compounds have been analyzed in recent studies [247, 250]. Kruger *et al.* have created a manually curated catalogue of domains and their interactions and a heuristic process to transfer them to new proteins [247]. They also built a database that facilitates manual curation of these interactions [251]. These resources rely on finding a set of domain-compound associations using single-domain proteins and then propagating these associations to proteins that contain that domain. However, they did not empirically study whether and how many of these inferred associations lead to actual interaction for the proteins for which associations have been propagated to. We examine this problem using experimental data on the compound-protein interactions that we collected from BindingDB [76] and domain annotations from Pfam [252].

To illustrate the situation better, Figure 4-1 shows an example of a domain-level interaction with the compound with PubChem CID: 44335601 that has high affinity (120nM). Since this protein consist of a single domain (Pfam ID: PF00089) that spans virtually the entire sequence, it is reasonable to assume that this interaction occurs between this domain and the compound. We find that the same compound interacts with another protein that has this domain (Thrombin and coagulation factor; UniProt ID: P00734), suggesting that this is likely because of the presence of this domain. However, this same domain appears in three other proteins that are experimentally shown not to interact with that compound (UniProt IDs: P00742, P00750, P00747). Table 4.1 shows the corresponding records in BindingDB that we use to extract the affinity data.

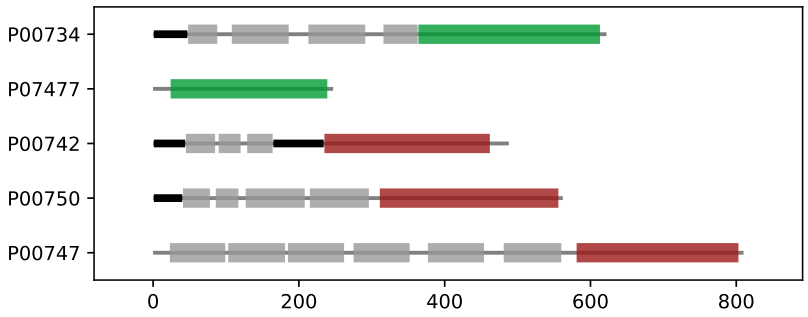


Figure 4-1. Example of five proteins that share the same domain and were experimentally evaluated for interaction with the same compound (PubChem CID: 44335601). UniProt identifiers of these proteins are shown on the y-axis, and the length (number of residues) is shown in x-axis. Individual rows show proteins that share same domain (Pfam ID: PF00089) identified using green box if a given protein interacts with the compound vs. red box if the protein does not interact with the compound. The grey boxes identify other domains. The thick black lines identify long sequence regions (> 30 residues long) that are sufficiently long to potentially contain other domains, while the thin light grey lines show the regions shorter than 30 residues.

Table 4.1. BindingDB records (selected columns) for proteins in Figure 4-1

BindingDB ID (for pair)	Target UniProt ID	Target Name	Ki (nM)	Kd (nM)	IC50 (nM)	EC50 (nM)	Institution
50096699	P00734	Thrombin and coagulation factor X	0.056	-	-	-	Merck Lab.
50799221	P00734	Thrombin and coagulation factor X	0.056	-	-	-	Univ. of Queensland
50096691	P07477	Trypsin-1	120	-	-	-	Merck Lab.
50096700	P00742	Coagulation factor X	95000	-	-	-	Merck Lab.
50096692	P00750	Tissue-type plasminogen activator	137000	-	-	-	Merck Lab.
50096690	P00747	Plasminogen	165000	-	-	-	Merck Lab.

This example shows a case where an interaction of a given protein with a compound is determined by factors that extend beyond a domain-compound interaction. It is possible that the reason why the three proteins do not interact with this compound is because the other domains in these proteins somehow impact their ability for this interaction. This means that interactions should not be assumed solely based on the presence of the same compound-interacting domain. The first objective of this chapter, which is our Sub-goal 2.1, is to investigate how common are these scenarios.

We anticipate that the scenario shown in Figure 4.1 may also cause difficulties for methods that predict compounds-protein interactions using protein sequence. Many of the current predictors rely on protein and compound molecular similarities to make predictions [107], i.e., similar targets share interactions with the same drugs and similar drugs interact with the same proteins. Here, similar proteins (which share the same domain) may or may not interact with the same compound.

This is different from the scenarios/datasets on which the current methods are commonly tested, where the interacting proteins that are typically different from the non-interacting proteins (i.e., they usually do not share domains), thus being relatively easy to differentiate. While the current methods have been shown to offer high predictive performance on these "easy" datasets [31, 32], to the best of our knowledge, the published evaluations never explicitly tested for this challenging scenario. Thus, our Sub-goal 2.2 investigates accuracy of the current predictors of compounds-protein interactions for these difficult cases.

Therefore, this chapter defines two sub-goals:

Sub-goal 2.1. We quantify how common are the cases where proteins that share the same binding domain may interact or not interact with a given compound. In other words, we collect and count cases in which a given domain that interacts with a given compound results in non-interaction with the same compound when this domain is included in another protein.

Sub-goal 2.2. Test a comprehensive collection of existing compound-protein interaction predictors on a dataset of cases extracted in the Sub-goal 2.2. More specifically, we empirically test a representative collection of current tools on a range of datasets, from the most challenging that are composed solely of the difficult cases explained above to the typical datasets that are commonly applied for benchmarking, with the underlying objective to study a relation between predictive performance and dataset difficulty.

4.2. **Sub-goal 2.1. Analysis of the abundance of compound-protein interaction where proteins share domains**

We collect a set of high-confidence cases where a domain (single-domain protein) binds a certain compound while there are examples of both binding and non-binding proteins that include the same domain. We use experimentally measured binding affinity values that are available in BindingDB to assign binary labels (positive for binding and negative for non-binding) to compound-protein pairs.

4.2.1. **Data sources**

Collection of compound-protein binding affinity data from BindingDB

We extracted binding data between human proteins and compounds from BindingDB [76]. BindingDB is arguably the most complete database of interactions between proteins and small molecules, where the underlying data is extracted from literature and other source databases including CHEMBL[60] and PubChem[74]. This database is usually updated monthly. We used version m72021 from July 2021. BindingDB provides measurement of binding affinity between compounds and proteins. The affinities as measured with Ki, Kd, IC50 and EC50 and usually at least one of them is present for each interaction record, depending on the type of experiments which produced the measurement. The database also provides several identifiers for drugs and proteins and secondary information, such as links to external databases. UniProt accession IDs for proteins and PubChem CIDs for compounds are commonly used in literature. UniProt accession IDs and PubChem CIDs are available for most of the records in BindingDB and thus we use them to uniquely identify compounds and proteins. We observe that including records lacking either of these two identifiers would increase the size of our data by only about 1%. Mapping protein sequences and SMILES structures of compounds to the corresponding identifiers is prone to errors and so we decided to exclude these records.

Collection of protein domain annotations from Pfam

Next, we annotate the resulting proteins that we collect from BindingDB with domains. We collect domain annotations from Pfam [252] using its RESTful API. The API takes the Uniprot ID of a protein and returns the domain annotations in the xml format. We use Pfam-A annotations which are manually curated and cover well-characterized protein domain families with high quality alignments [253]. We do not use Pfam-B since it has lower quality and is generated automatically using alignment [253]. The annotation includes a list of domains identified by their Pfam ID and their location in the sequence identified by the beginning and ending residues.

4.2.2. **Internal data model**

We represent the interactions as a set of compound-protein pairs (represented by their PubChem CID and UniProt IDs) and a binary interaction (positive for binding and negative for non-binding)

assigned to each pair. Moreover, for each protein ID, we can find all compounds that it interacts with (positive label), and for each compound ID we can find all proteins that interact with that compound (positive label). We also have domain annotations from Pfam-A (identified by Pfam ID) assigned to each protein identifier, together with the beginning and end residues for each domain region. Furthermore, using the Pfam ID we can find all proteins that contain that domain.

Conversion of BindingDB affinities to binary annotations of interactions

The binding affinities, which are quantified with Ki, Kd, IC50 and EC50 in BindingDB, measure strength of interactions between compounds and proteins. Lower values mean higher intensity and higher values mean lower intensity of interaction. For practical purposes (such as drug discovery), there are maximum values above which the compound can be assumed to not interact and affinity values below certain levels are considered a strong interaction. We found multiple different threshold in the literature that were used to identify positive and negative interactions [99, 100]. To ensure that our binary interactions have high confidence, we chose the most conservative thresholds and enforced that all measures that are provided for a given interactions must agree. Consequently, we converted affinities into binary interactions using the following rules:

- If all of affinity values (Ki, Kd, IC50 and EC50) that are provided for a given record (compound-protein pair) were smaller than 1μM, then we consider the pair as a positive interaction.
- Conversely, if all provided values are greater than 30μM, then we consider the pair as a negative interaction.
- Otherwise, we do not include the pair.

4.2.3. **Identification of compound-binding domains which appear on both binding and non-binding proteins**

We apply the following 3-step procedure to identify the “difficult” cases that follow the scenario shown in Figure 4.1:

1- Find single-domain protein(s) that interact with a given compound.

2- Find other proteins that contain the same domain.

3- Ensure that these proteins, after removing any possible duplicates, contain both binding and non-binding examples

These three steps are repeated for all single-domain proteins that have interactions with compounds (positive label)

Finding single-domain proteins

We define the single-domain proteins as those that satisfy these two conditions:

1- Have one domain annotation;

2- Have no more than 30 non-domain residues on each side of that domain segment. This step is meant to ensure that the remainder of the protein sequence (outside of the annotated domain) is unlikely to harbor other domains, or play a significant role in compound interactions.

Removing redundancy

Finally, we ensure that the proteins for which we have interaction data for the same compound and which share the domain are different from each other. We use a domain scanning protocol to check whether their domain composition is different, which if true guarantees that they are different. We cannot rely on UniProt IDs since sometimes the same protein may have different IDs when it comes from different organisms or from different individuals in the same organism. Each protein is represented as an ordered sequence of segments defined as domain identifiers and long sequence regions (>30 residues long), and we assume that two proteins are different when their ordered sequences of segments differ.

We show a pseudo-code for the procedure to identify the “difficult” cases in Algorithm 1.

Algorithm 1. Extracting set of difficult cases

Inputs
D: Compound-protein interaction dataset
M: Domain annotations
Outputs
H: Difficult compound-protein pairs
CD: Corresponding compound-domain pairs
Begin
H={}
CD={}
P_D = *proteins_in(D)* Extract the set of proteins in *D*
P_{sd} = *M.find_single_domain_proteins*(P_D) Find the set of single-domain proteins in *D*
foreach *p* **in** P_{sd} **do**
C_p = {*c*|(*c*,*p*, *True*) ∈ *D*} Find the set C_p all compounds that interact with *p*
if $C_p \neq \emptyset$ **do**
m = *M.single_domain_of (p)* Let *m* be the single domain of *p*
Q = *M.proteins_with(m)* Find set *Q* of all proteins that contain the domain *m*
Q_{pos} = {}
Q_{neg} = {}
for *q* **in** *Q* **do** # for all proteins in *Q*
If (*c*,*q*, *True*) ∈ *D* **do** Those that interact with *c* will go to Q_{pos}
Q_{pos}.*add(q)*
If (*c*,*q*, *False*) ∈ *D* **do** And those that don't interact with *c* go to Q_{neg}
Q_{neg}.*add(q)*
If $Q_{pos} \neq \emptyset$ *and* $Q_{neg} \neq \emptyset$ **do** If we have both binding and non-binding examples
Q_{pos} = *M.reduce*(Q_{pos}) Remove possible redundancies in Q_{pos}
Q_{neg} = *M.reduce*(Q_{neg}) Remove possible redundancies in Q_{neg}
CD.add(c,m) Include (c, m) in the output compound-domain pairs
for *q* **in** $Q_{pos} \cup Q_{neg}$ **do** Include the pos. and neg. proteins as difficult
H.add(c,q)
End

4.2.4. **Results for Sub-goal 2.1**

In Goal 2.1, we investigate the abundance of the scenario where different proteins sharing a compound-binding domain may or may not bind the same compound (the scenario illustrated in Figure 4.1). To this end, we applied the process (defined in section 4.2.3) for finding the examples of this scenario on our interaction data (explained in section 4.2.2). The number of resulting cases at different steps of process is listed in Table 4.2.

Table 4.2. Summary of the examples found in Sub-goal 2.1. Number of domain-compound pairs, number of domains involved and number of compounds involved at each step of the process are shown

Step in the process	Domain-compound pairs	Domains	Compounds
All domain-compound interactions found	44,656	205	44,391
Interactions with pos. and neg. protein examples	1,425	43	1,424
After removing redundancy	479	23	479

The last row is the final set of high-quality and non-redundant examples that show that even with the most stringent definitions there is a significant number of these challenging cases. We obtained 479 compound-domain pairs for which we identified both negative and positive interaction at the protein level. These pairs cover 23 different domains and 479 different compounds. This collection of examples is provided in Appendix B. We expect that the actual number of these cases is much higher since the amount of the negative (non-interacting) data is severely under-represented in current databases. Still, the sheer number of the cases that we identified and the diversity of domains that they represent clearly demonstrate that this is a relatively common scenario. These cases constitute Testset1, which we dub the *difficult* test set. This dataset includes 1337 compound-protein pairs (655 negatives and 682 positives) between 204 proteins and 479 compounds.

4.3. **Sub-goal 2.2. Assessment of predictive performance of current predictors of protein-compound interactions**

As discussed in the introduction of this chapter, the examples found in Sub-goal 2.1 may cause problems for methods that rely on sequence similarity between proteins to make predictions of compound-protein interactions, i.e., in this case the similar/domain-sharing proteins are not guaranteed to provide consistent annotations of binding with the same compound. We use Testset1 to evaluate predictive performance for a representative and large collection of current predictors of compound-protein interactions. We also compare these results against results produced on traditional/typical datasets that include a broader variety of compound-protein pairs.

4.3.1. **Datasets for training and testing**

A common problem concerning empirical evaluation of current methods for prediction of the compound-protein interactions is that they are trained and tested on (very) different datasets with different metrics and using different test protocols. This makes it virtually impossible to reliably compare these methods. We attempt to provide a more consistent evaluation protocol where all methods are trained and tested using the same datasets and predictive performance is measured using the same metrics. We develop a training set which does not overlap with data in any of our test datasets, and train all selected and representative methods, including baseline/reference

predictors, on this *common training set*. Below we explain how we collect the training and test datasets.

In Sub-goal 2.1, we describe the process for extracting a set of high-confidence binary compound-protein interactions. We use this procedure to annotate interactions from BindingDB, which we utilize to develop three test datasets (including Testset1) and the common training set. Each of these datasets is composed of a set of compound-protein pairs where the compounds are represented by their PubChem CIDs and SMILES string and proteins are represented by their UniProt IDs and amino acid sequences.

Since the number of available (labeled) positive pairs is generally larger than the number of (labeled) negative pairs, the latter number is usually the main constraint in building datasets. Therefore, we ensure that each dataset includes a sufficiently large number of negative examples, and then we sample positive examples to the same ratio across datasets. This ensures that results of specific methods can be reliably compared across datasets. We use random sampling to obtain positive-to-negative ratio that is close to a balanced 1:1 ratio, since this ratio is commonly used in other works [43, 254-257]. We illustrate the overall procedure that we use to collect the training and test datasets in Figure 4-2, and we discuss details below.

Testset1 (difficult)

We use Testset1 to evaluate compound-protein binding predictors on the "difficult" scenario i.e., to predict binding vs non-binding for proteins that share binding domains. The positives and negatives in this dataset already have a close to a 1-1 ratio. Therefore, we did not sample this dataset and use the exact ratio from this dataset as the reference to sample data for the other datasets.

Testset3 (typical)

Testset3 reflects a typical test dataset used in literature where the underlying data is selected at random (possibly with some resampling to adjust the positive to negative ratio) from a source database [43, 254-257]. Therefore, to build Testset3, we randomly select 10% of all negative pairs collected from BindingDB, and randomly sample positive pairs to establish the desired positive-to-negative ratio (the same ratio as in Testset1).

Testset2 (intermediate)

Testset2 is an intermediate dataset we collect using a procedure in-between the typical Testset3 and the difficult Testset1. The underlying principle is to extend Testset1 with complete interactomes for its proteins and compounds. Therefore, to build Testset2, we collect binary-labeled compound-protein pairs from BindingDB that have a compound or a protein in common with the compounds and proteins found in Testset1, respectively. We keep all resulting negative pairs and randomly subsample positives to obtain the desired positive-to-negative ratio (the same ratio as in Testset1).

Common training set

The common training set is used to train all the methods which we test. Therefore, it is designed to reflect a typical training set used in training of these methods (close to a random selection of pairs, with a balanced positive-to-negative ratio). Therefore, we build the common training set to have the same positive-to-negative as our three test sets and not have any intersection (shared compound-protein pairs) with any of them. To do this, we take the set of all binary interactions and remove any pairs that is in Testset1, Testset2, or Testset3. In the remaining pairs we keep all the negatives and resample the positive pairs to establish the desired positive-to negative-ratio.

Figure 4-2 shows the schematic illustration of the process of obtaining the three test sets and the common training set. Table 4.3 shows the number of pairs, proteins and compounds for these datasets. These four datasets are available at http://biomine.cs.vcu.edu/servers/MetaBoostCPI.

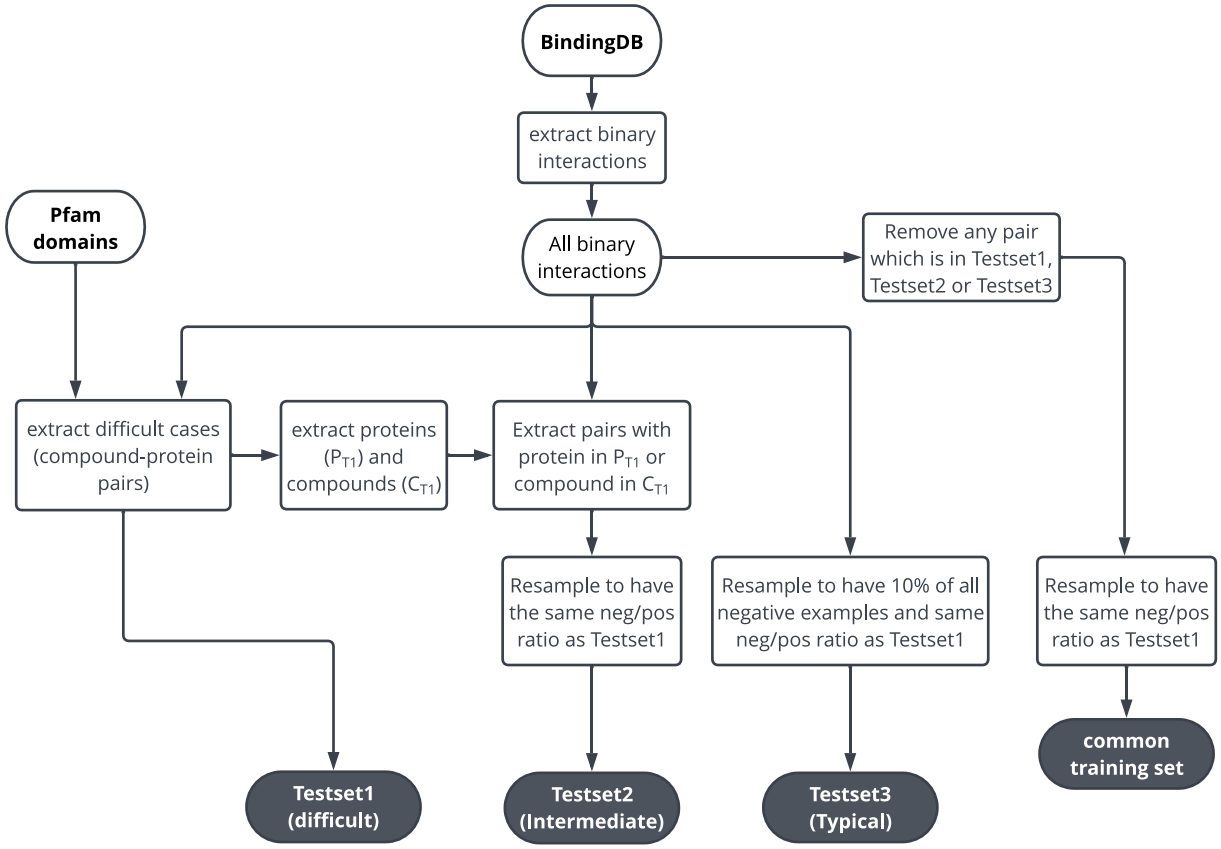


Figure 4-2. The schematic illustration for a process that we use to collect the three test sets (Testset1, Testset2, and Testset3), and the common training set.

Table 4.3. Summary of the three test datasets and the common training set that we use for the Sub-goal 2.2. We include the number of compound-protein pairs in the set (Pairs), number of positive pairs (Positives), number of negative pairs (Negatives), number of proteins (Proteins) and number of compounds (Compounds) in each dataset.

Dataset name	Pairs	Positives	Negatives	Proteins	Compounds
Testset1 (difficult)	1,337	682	655	204	479
Testset2 (intermediate)	30,199	15,404	14,795	278	26,275
Testset3 (typical)	36,145	18,437	17,708	2,995	34,787
Common training set	268,232	136,824	131,408	4,624	222,638

4.3.2. **Survey and selection of chemogenomic predictors of drug-protein interactions**

We briefly overview methods that predict compound-protein interactions to select a representative group that we use in our comparative analysis.

We focus on the methods that predict compound-protein interactions without requiring protein tertiary (3D) structure. The protein structure-based methods are mostly based on molecular docking, which is computationally expensive and not suitable to genome-scale studies and predictions. This is because protein structure is available for a subset of proteins and it cannot be obtained for a large collection of the intrinsically disordered proteins. There are dozens of the protein sequence-based predictors and thus we consider a subset of methods (higher impact, more recent and available to the end users) based on the following criteria:

1. **Journal impact**: We include methods that are published in higher impact journals, defined as those which are in the top quartile of at least one area in which they are listed according to the Web of Science ranking.

2. **Publication year:** We include methods which have been published in 2017 or later. This is motivated by an observation that newer tools typically improve over the older solutions.

3. **Availability:** We include methods that have link to an implementation (source code or web server) in their article. We need the implementations to be able to train and test these methods on our datasets. This also ensured that these methods are available to the end users.

Table 4.4 lists 36 methods that we select using the above criteria. This table also summarizes key characteristics related to their inputs and predictive approaches. We introduce and discuss these characteristics below.

Predictive models

The methods can be divided based on their predictive approach into similarity-based, molecular-representation-based, and network-based approaches.

Similarity-based approach (SIM): this class of methods hinge on the quantification of similarity (or conversely distance) between compounds and between proteins. Their prediction of interaction for a given protein-compound pair relies on identifying similar compounds and proteins that have known interaction information (using a chosen similarity measure), and utilizing this information to make predictions.

The similarity between compounds and between proteins can be defined in many ways. Arguably most common similarity metric for proteins is based on results the sequence alignment [258] and for compounds is based on the Tanimoto (Jaccard) similarity between compound fingerprints[30]. Other approaches include measuring Tanimoto similarity between side effect profiles of compounds based on drug side effect or disease association for compounds and biological function or interaction annotations for proteins. Different ways of measuring similarity and even combination of them have been studied extensively in the literature [29, 30, 259].

Network-based approach (NET): These methods build a network (graph) where compounds and proteins are nodes and their interactions are edges. The underlying problem is cast as link prediction in the resulting graphs. Graphs usually includes additional node types like diseases, side effects, other molecules, as well as other edge types like Protein-Protein Interactions (PPIs), drug-disease associations, and protein-disease associations. Such heterogenous graph with different types of edges and nodes are used in other related areas, such as recommender systems and social networks, and are typically called knowledge graphs. One of the drawbacks of these methods is that it is difficult to ensure that information is not leaking between the training and test datasets, making it difficult to robustly compare different methods.

Molecular representation learning approach (MolRL): These methods typically rely on deep neural networks and the idea of learning a numeric representation (encoding) from molecular representations of proteins and compounds in an end-to-end and data-driven fashion. The main advantage of these methods is that they typically use universally/proteome-wide available representations about compounds and proteins, namely compound structure (usually represented as SMILES string) and protein amino acid sequence, as the input. This makes them more widely applicable and also easier to compare with each other. Their predictive models are binary classifiers that are generated using a training dataset. These methods become popular recently motivated by the successes of Deep Representation Learning in other fields, such as Natural Language Processing and protein structure prediction. They rely on a variety of deep learning architectures like Recurrent Neural Networks (such as biLSTM), Convolutional Neural Network (CNN), and Graph Neural Networks [260-263]. More recently, some of these methods utilize transformers [43, 254].

These categories are not completely disjoint and some methods may overlap a couple of these architectures. For example, compound-compound or protein-protein similarities are sometimes used as edges in the network-based approaches[257, 264]. Also, deep learning is sometimes used by the network-based method, though usually not for molecular representations of compounds and proteins but rather for descriptors that are defined based on connectivity in the underlying networks[45, 265, 266].

Additional/secondary input features

In addition to the typical inputs, which are the protein sequence and drug structure, some methods (especially network-based methods) use other information for training and prediction. We identify three commonly used types of input features.

Protein domains and compound substructures (SUB): The information about the protein domains and substructures that a given drug is made of are. This type of input is relevant to our study because we focus on the role of domains in the predictions of compound-protein interactions. Therefore, we included this information when describing individual predictors.

Protein-protein interactions (PPI): Interaction profile of a protein with other proteins is a potentially valuable source of information for prediction of their interaction with small molecules. This is because PPIs identify related proteins and proteins that are more likely to be drug targets (as we discuss in Chapter 3). Many methods, including some recent tools, use this information.

Phenotypic or indirect information (PHE): This includes information about drugs and compounds that is not a direct attribute of the molecule itself but rather associated phenotypic-level information, such as side-effect, indications/diagnoses associated with compounds, functional annotations, and/or disease association of proteins. This distinction between molecular and phenotypic information was proposed by Hinnerichs *et al*[255].

Table 4.4. Selected sequence-based predictors of compound-protein interactions. The first column is the year a given method was published. The second column is the name of the method together with citation. The third column shows the predictive approach according to categories described in the text. Columns 4, 5, 6 indicate whether a given method uses specific types of input information for training or prediction (we describe these inputs in the text). The last column shows whether the implementation allows for retraining the model on custom datasets, which is required for our comparative analysis.

Year	Name	Approach	Additional/secondary Inputs			Implementation
			SUB	PPI	PHE	Retrainable
2022	FusionDTA [267]	MolRL				
2022	NerLTR-DTA [268]	MolRL				
2022	**BACPI [269]**	**MolRL**				✓
2021	DeepDTAF [270]	MolRL				
2021	**HyperAttentionDTI [271]**	**MolRL**				✓
2021	**KGE_NFM [257]**	**NET**		✓	✓	✓
2021	**MolTrans [254]**	**MolRL**	✓			✓
2021	AEFS [256]	MolRL		✓	✓	
2021	DTI-Voodoo [255]	NET		✓	✓	
2021	MultiDTI [265]	NET		✓	✓	
2021	**GraphDTA [261]**	**MolRL**				✓
2021	PretrainDPI [272]	MolRL				
2021	DTI-CDF [273]	MolFea			✓	
2021	GCN-DNN [274]	MolRL				
2020	**DeepPurpose [275]**	**MolRL**				✓
2020	TargetPredict [276]	NET		✓	✓	
2020	**MDeePred [277]**	**MolRL**				✓
2020	**TransformerCPI [43]**	**MolRL**				✓
2020	AOPEDF [278]	NET		✓	✓	
2020	TriModel [279]	MolRL		✓	✓	
2020	drugVQA [280]	MolRL				
2020	DeepCDA [281]	MolRL				
2020	GCN-DTI [274]	MolRL				
2020	CMMC/TMMC [282]	MolFea			✓	
2020	deepDTnet [283]	MolFea		✓	✓	
2019	**DeepConv-DTI [284]**	**MolRL**				✓
2019	**DeepAffinity [262]**	**MolRL**	✓			✓
2019	NeoDTI [285]	MolRL		✓	✓	
2019	**GNN-CPI [260]**	**MolRL**				✓
2019	Zong2019 [286]	MolRL		✓	✓	
2019	LRF-DTIs [287]	MolFea				
2018	**DeepDTA [263]**	**MolRL**				✓
2018	**CONNECTOR [288]**	**SIM**			✓	✓
2018	DDR [259]	SIM	✓		✓	
2017	DTINet [264]	NET			✓	✓
2017	Zong2017 [266]	NET		✓	✓	

Implementations

We find that the source code provided by authors of many of these methods is aimed towards replicating training and testing experiments rather than being a ready-to-use interface or tool for prediction. While such implementation is less useful in practical applications, for our purpose, it enables us to retrain and retest them on our training and test datasets, facilitating our assessment. Therefore, we define 3 inclusion criteria that are necessary to select a given tool for our comparative study: 1) a given tool can be retrained on a custom training dataset; 2) it produces predictions in a reasonable amount of time (no more than 5 minutes), given the large size of Testset3; and 3) its code must work with little to no adjustments/modifications (it is not buggy or incomplete). We identify methods that satisfy these criteria in the last column of Table 4.4. Importantly, this collection of methods is relatively large (14 tools), covers all types of approaches (SIM, NET and MolRL), and these methods use different types of additional inputs, such as SUB, PPI and PHE. It also includes a mixture of newer (2021 and 2002) and older (2018 and 2019) methods. This suggests that this selection relatively well represents the larger population of all tools.

4.3.3. **Evaluation framework**

Each data point in our datasets (compound-protein pair) has a binary label representing interaction vs. non-interaction status. The corresponding predictors take the protein and compound information (sequence and/or identifier) as the input and they typically predict a numeric propensity score for interaction. The proteins are usually represented by one-letter encoded amino acid sequence (Section 2.2.2), and drugs by their SMILES-formatted structure (Section 2.1.2). The three test datasets (Testset1, Testset2 and Testset3) maintain the same ratio of positive vs. negative pairs (Table 4.3), which is consistent with how current predictors are trained and tested [47, 289]. We summarize the training and prediction process in Figure 4-3.

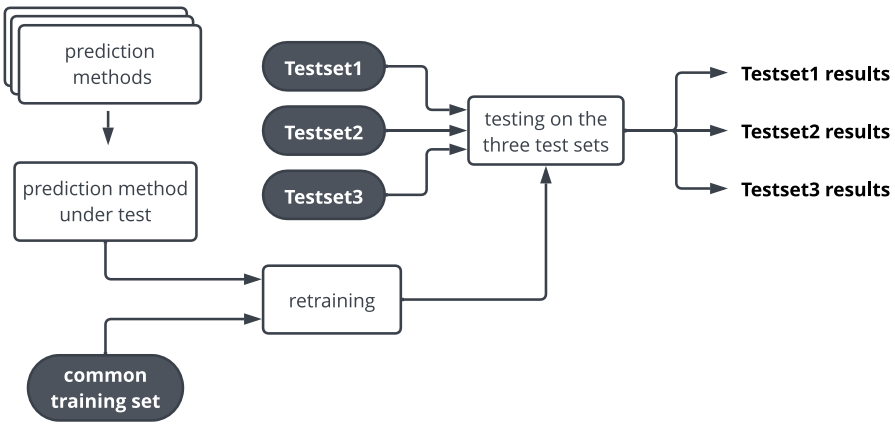


Figure 4-3. Schematic of the process to train and test the considered predictors.

4.3.4. **Evaluation metrics and statistical significance**

Motivated by how the current methods are evaluated in the literature, we apply the commonly used metrics to perform assessment. We include AUC and AUPR (explained in Section 2.5) that we compute by comparing predicted values and the corresponding binary labels. These metrics are capable of measuring the classification performance across different binarization thresholds, if the binary predictions are accompanied by scores that represent the level of confidence/or probability for predicting a positive label. All predictors that we include in the assessment provide such scores. Therefore, we can use AUC and AUPR that quantify performance that is not dependent on a choice of a threshold. We also provide MCC and F1 which assess binary predictions, which we obtain by applying a threshold to the putative scores. We use a different threshold for each method, such that the corresponding binary predictions generate a correct rate-of-prediction; meaning a threshold that produces binary predictions with the correct ratio between predicted-positives to predicted-negatives for a given test dataset. This way we can directly compare values of the binary metrics across different methods.

We also evaluate statistical significance of differences in predictive performance between selected pairs of methods. This allows us to analyze whether a given tool provides statistically better (i.e., consistently better) results when compared to another method on a range of different datasets. We apply the following process to measure statistical significance (separately for any given test set and metric):

1. We sample (with replacement) half of the pairs in a given test set 100 times to generate 100 different datasets

2. We calculate metrics for the two methods on these 100 datasets to obtain 100 values for each of the methods.

3. We test normality of distribution of these measured values using the Anderson-Darling test with *p*-value cutoff of 0.05. If they are normal then we use a paired *t*-test to assess the significance; otherwise, we perform a paired Wilcoxon test.

4. If the resulting *p*-value < 0.05 then we consider one method as statistically better than the other method.

4.3.5. **Protein-based and compound-based predictors as baselines**

Different test datasets may have different levels of difficulty, which ultimately impacts the predictive performance that is achievable for these datasets. Some test datasets could be more similar to the training dataset and one way this could happen is when training and test dataset share similar bias. The compound-side and protein-side bias has been mentioned in recent works [43, 255] but was never studied adequately. This bias refers to a situation where compound-protein interaction predictors achieve a high classification performance by simply recalling information from training data for similar compounds or proteins, possibly by copying results from the most similar compound or protein. For example, if a compound from a given test compound-protein pair (or a training compound that is similar to the test compound) is present in the training dataset and always annotated as binding in the training set, then this fact could be simply recalled to make the prediction. If most of the similar compounds in the training and test datasets are highly biased (they are either mostly binding or mostly non-binding) and this bias is consistent between training and test dataset, then a naïve prediction that copies bias from the training dataset into the test dataset could produce highly accurate results, without actually producing useful results. We study this issue for each of the three test datasets by applying compound-side and protein-side bias generated using the training dataset. We formulate these two baselines (baseline-C and Baseline-P) below and illustrate their biases in section 4.3.7.

Compound-based baseline (Baseline-C)

Baseline-C represents prediction based on the bias on the compound side. Baseline-C makes prediction for a test pair *(c, p)* by finding all pairs with compound *c* in the training set (or *c'*, the most similar compound in the training set, if *c* cannot be found in the training set), draws a random pair *(c, p'')* (or a random *(c', p'')* pair) from this set, and outputs label of this training pair as the prediction. The similarity between compounds is measured with the Tanimoto coefficient between their PubChem compound fingerprints, where the most similar compound *c'* is the compound with the highest Tanimoto coefficient with compound *c*.

Protein-based baseline (Baseline-P)

Baseline-P works in the same way as the Baseline-C, except it relies on the bias on the protein side. It predicts label for a given test pair *(c, p)* by finding all the pairs of the protein *p* in the training set (or *p'*, the most similar protein in the training set if *p* cannot be found in the training set), draws a random pair *(c'', p)* (or a random *(c'', p')* pair) from this set, and outputs the label of this training pair as the prediction. The similarity between proteins is measured by sequence identity quantified in percent and calculated with the MMseqs2 method [290, 291]. The most similar protein *p'* is the protein in the training dataset that has the maximal sequence identity with *p*.

The predictive performance of these two baselines is directly attributed to the bias shared between the training and test datasets. They provide reference results to evaluate predictors on a specific test dataset. More specifically, only the methods that improve over the better of the two baselines should be considered accurate.

4.3.6. **Results - Prediction performance on the three test sets.**

Table 4-5 shows the predictive performance for the 14 selected methods (section 4.3.2) and the two baselines (section 4.3.5) on the three test sets (section 4.3.1). We primarily focus on AUC to discuss the results, however, in most cases the other metric provides consistent observations. We mention when there is considerable difference between observations that are coming from the other metrics.

Table 4.5. Performance of the 14 selected methods and the two baselines on Testset1, Testset2 and Testset3. The methods are sorted by their AUC on Testset1. For baselines, the standard deviation of the metric is shown in parentheses under the (average) value of the metric; this is based on 100 runs for each baseline on each dataset. Annotations on the superscript show the significance of difference compared to Baseline-C. '+' means significantly higher, '−' means significantly lower and '=' means no significant difference. Calculation of statistical significance test is described in section 4.3.4. All measurements are normal and thus the statistics exclusively rely on the t-test.

		Testset1 (difficult)				**Testset2 (intermediate)**				**Testset3 (typical)**			
		AUC	**AUPR**	**MCC**	**F1**	**AUC**	**AUPR**	**MCC**	**F1**	**AUC**	**AUPR**	**MCC**	**F1**
Baselines	Baseline-P	0.496 $^{-}$ (±0.021)	0.490 $^{-}$ (±0.017)	0.037 $^{=}$ (±0.033)	0.513 $^{=}$ (±0.017)	0.634 $^{-}$ (±0.006)	0.727 $^{-}$ (±0.005)	0.224 $^{-}$ (±0.010)	0.720 $^{-}$ (±0.004)	0.772 $^{-}$ (±0.003)	0.847 $^{-}$ (±0.003	0.483 $^{-}$ (±0.006	0.836 $^{-}$ (±0.002
	Baseline-C	0.517 (±0.009)	0.520 (±0.011)	0.015 (±0.014)	0.501 (±0.007)	0.813 (±0.003)	0.867 (±0.003	0.540 (±0.007)	0.834 (±0.002)	0.851 (±0.003)	0.917 (±0.002)	0.532 (±0.005)	0.850 (±0.002)
Current predictors	GNN-CPI	0.502 $^{=}$	0.512 $^{=}$	0.087 $^{+}$	0.521 $^{=}$	0.732 $^{-}$	0.724 $^{-}$	0.332 $^{-}$	0.652 $^{-}$	0.807 $^{-}$	0.766 $^{-}$	0.493 $^{-}$	0.757 $^{-}$
	CONNECTOR	0.511 $^{=}$	0.522 $^{=}$	0.033 $^{=}$	0.542 $^{+}$	0.772 $^{-}$	0.789 $^{-}$	0.446 $^{-}$	0.661 $^{-}$	0.845 $^{=}$	0.819 $^{-}$	0.568 $^{+}$	0.793 $^{-}$
	BACPI	0.520 $^{=}$	0.542 $^{+}$	0.098 $^{+}$	0.512 $^{=}$	0.832 $^{+}$	0.804 $^{-}$	0.501 $^{-}$	0.705 $^{-}$	0.902 $^{+}$	0.911 $^{=}$	0.680 $^{+}$	0.783 $^{-}$
	MDeePred	0.526 $^{=}$	0.530 $^{=}$	0.052 $^{=}$	0.564 $^{+}$	0.812 $^{=}$	0.824 $^{-}$	0.492 $^{-}$	0.694 $^{-}$	0.894 $^{+}$	0.898 $^{-}$	0.652 $^{+}$	0.764 $^{-}$
	HyperAttentionDTI	0.556 $^{+}$	0.601 $^{+}$	0.101 $^{+}$	0.616 $^{+}$	0.823 $^{+}$	0.813 $^{-}$	0.510 $^{-}$	0.712 $^{-}$	0.883 $^{+}$	0.864 $^{-}$	0.652 $^{+}$	0.729 $^{-}$
	DeepAffinity-dom	0.577 $^{+}$	0.636 $^{+}$	0.109 $^{+}$	0.551 $^{+}$	0.878 $^{+}$	0.936 $^{+}$	0.569 $^{+}$	0.845 $^{+}$	0.951 $^{+}$	0.974 $^{+}$	0.742 $^{+}$	0.907 $^{+}$
	KGE_NFM	0.589 $^{+}$	0.593 $^{+}$	0.172 $^{+}$	0.642 $^{+}$	0.862 $^{+}$	0.866 $^{=}$	0.598 $^{+}$	0.751 $^{-}$	0.887 $^{+}$	0.871 $^{-}$	0.651 $^{+}$	0.833 $^{-}$
	DeepAffinity	0.616 $^{+}$	0.678 $^{+}$	0.179 $^{+}$	0.586 $^{+}$	0.914 $^{+}$	0.955 $^{+}$	0.648 $^{+}$	0.873 $^{+}$	0.951 $^{+}$	0.974 $^{+}$	0.744 $^{+}$	0.908 $^{+}$
	DeepPurpose	**0.632** $^{+}$	**0.645** $^{+}$	**0.220** $^{+}$	**0.551** $^{+}$	**0.902** $^{+}$	**0.908** $^{+}$	**0.712** $^{+}$	**0.831** $^{=}$	**0.923** $^{+}$	**0.929** $^{+}$	**0.804** $^{+}$	**0.892** $^{+}$
	TransformerCPI	**0.652** $^{+}$	**0.632** $^{+}$	**0.252** $^{+}$	**0.630** $^{+}$	**0.889** $^{+}$	**0.874** $^{+}$	**0.658** $^{+}$	**0.790** $^{-}$	**0.899** $^{+}$	**0.902** $^{-}$	**0.756** $^{+}$	**0.732** $^{-}$
	GraphDTA	**0.666** $^{+}$	**0.712** $^{+}$	**0.269** $^{+}$	**0.631** $^{+}$	**0.904** $^{+}$	**0.950** $^{+}$	**0.619** $^{+}$	**0.863** $^{+}$	**0.930** $^{+}$	**0.963** $^{+}$	**0.690** $^{+}$	**0.888** $^{+}$
	MolTrans	**0.669** $^{+}$	**0.672** $^{+}$	**0.237** $^{+}$	**0.626** $^{+}$	**0.942** $^{+}$	**0.943** $^{+}$	**0.757** $^{+}$	**0.881** $^{+}$	**0.968** $^{+}$	**0.964** $^{+}$	**0.835** $^{+}$	**0.919** $^{+}$
	DeepDTA	**0.671** $^{+}$	**0.641** $^{+}$	**0.282** $^{+}$	**0.648** $^{+}$	**0.780** $^{-}$	**0.755** $^{-}$	**0.423** $^{-}$	**0.718** $^{-}$	**0.793** $^{-}$	**0.776** $^{-}$	**0.443** $^{-}$	**0.727** $^{-}$
	DeepConvDTI	**0.676** $^{+}$	**0.651** $^{+}$	**0.309** $^{+}$	**0.651** $^{+}$	**0.901** $^{+}$	**0.903** $^{+}$	**0.716** $^{+}$	**0.752** $^{-}$	**0.929** $^{+}$	**0.913** $^{=}$	**0.790** $^{+}$	**0.891** $^{+}$

Starting with the baselines, we observe that both baselines achieve high levels of performance on Testset2 and Testset3 while they perform poorly on Testset1. Both Baseline-C and Baseline-P are close to a random prediction on Testset1 (AUC at around 0.5), which shows that neither compound nor protein bias (their tendency to be binding or non-binding) are helpful to make predictions on this dataset. On the other hand, baselines on Testset3 are very accurate, showing that such typical test datasets can produce high levels of predictive performance due to their similarity to training data and high degree of shared bias (between the training and test datasets). Furthermore, on both Testset1 and Testset2, Baseline-C is statistically significantly more accurate than Baseline-P (p-value < 0.05), which means that the compound bias is much stronger predictor of interactions then the protein bias. These observations are consistent across all 4 metrics used (AUC, AUPR, MCC, and F1). We present a more detailed analysis of the baseline results in section 4.3.7.

The 14 selected methods are sorted based on their AUC on Testset1, which ranges between 0.502 and 0.676 (Table 4.5). We observe a consistent (across both baselines and all methods) and large

drop in performance on Testset1 compared to the other two test sets. For Testsst1, there is a measurable difference in performance between methods; while some methods secure modest and significantly better than baseline (random-level) values of AUC (between 0.60 and 0.68), others perform similar to a random level (AUC < 0.55). The fact that better Baseline-C fails to produce meaningfully accurate predictions and the large drop in performance on Testset1 compared to Testset2 and Testset3 means that Testset1 is much more challenging, which is expected and consistent with our hypothesis.

Testset2 is an intermediate dataset which is built using interactomes of the compounds and proteins from Testset1. The baselines produce relatively accurate predictions and some methods make very accurate predictions (AUC > 0.9). While there is a consistent drop in performance from Testset3 to Testset2 across different methods and baselines, the results on Testset2 are consistently closer to results on Testset3 than to Testset1. AUCs of the 14 methods range from 0.732 to 0.942. However, still some of the methods perform statistically no better than the Baseline-C, including GNN-CPI, CONNECTOR, DeepDTA and MDeePred. This suggest that the difficulty for prediction on Testset1 is less likely to be a result of specific properties of compounds or proteins.

The results on Testset3, which represents a typical test scenario used in literature, show that while the performance metrics seem to be very high on this dataset (AUCs are as high as 0.968 for MolTrans), the baseline-C also achieves very high level of performance (AUC of 0.851). Considering the fact that Baseline-C is a naïve approach and only uses compound for prediction and is blind to the protein, it seems that the bias in Testset1 makes it an “easy” prediction task. It is also interesting that some of the methods are significantly worse than baseline-level performance, including GNN-CPI and DeepDTI (p-value < 0.05).

We can discern several groups of methods. We find that several methods, such as DeepAffinity, MolTrans, GraphDTA, and DeepConvDTI, are statistically better than the best baseline across all metrics and datasets (p-value < 0.05). Some methods are statistically similar or worse than Baseline-C on at least one of the datasets based on AUC, including GNN-CPI, CONNECTOR, BACPI, MDeePred, and DeepDTA. Interestingly, DeepDTA produces relatively accurate results on Testset1 but performs poorly on Testset2 and Testset3, suggesting that this method is not optimized to take advantage of the compound and protein biases.

For Testset1, we observe that the existing methods achieve only modest predictive performance, and there is a lot of room for improvement. However, there are still multiple methods which perform significantly better than the best baseline, suggesting that their results are useful and could be perhaps used to design a consensus method. Another important conclusion is that while most of the existing methods achieve very high scores on Testset3 (AUC > 0.85), the high AUC of baseline-C for this dataset reveals that this is an inherently "easy" prediction task, where the bias especially on the compound side is a strong predictor of interactions. This strongly suggests that proper analysis of predictive performance must be done in relation to a suitable baseline.

The fact that Testset3 represents an easy prediction task suggest that more sophisticated prediction methods on this dataset would have limited value. The range of predictor performance is "squished" between the baseline performance (AUC=0.851) and a practical limit of the predictive performance measured with AUC, which is smaller than 1 and dictated by inevitable errors and imperfections in the data. The fact that the existing methods approach a likely near perfect AUC of ~0.97 suggests that there is little room for improvement.

Following, we analyze the baseline results and explain how the training dataset bias can be used to explain difference in performance for Baseline-C and Baseline-P across the three test datasets.

4.3.7. **Analysis of baseline predictions**

Baseline-P and Baseline-C are used to quantify whether the biases in the training and test datasets, if present, can be used to make accurate predictions. They rely on the level to which the tendency of a given compound to interact (with any protein) is a strong predictor of interaction in our test sets; the same is true for the tendency of protein to interact (with any compound). To make this clearer, we use the term **compound bias for binding** to refer to the fraction of times a given compound has appeared in a positive (binding) pair as opposed to negative (non-binding) pairs in the training set. Similarly, we use the term **protein bias for binding** to refer to the fraction of times the protein has appeared in a positive pair as opposed to negative pairs in the training set. We quantify how these biases for proteins and compounds correlate with their likelihood of being in a positive pair in each of the test sets, and use this correlation to explain why specific baselines work well or poorly for specific datasets.

Figure 4-4 shows the histograms of the protein bias (in panel a, b, and c) and the compound bias (in panels d, e, and f) for the compound-protein pairs in the three test sets. The histograms for positive pairs are shown in green and above the *x*-axis and the negative pairs are shown in red and below the *x*-axis. This facilitates side-by-side comparison of histograms. Being close to 1 on the *x*-axis means the most similar protein/compound is almost always binding in the training set, and beings close to zero means that it is almost always non-binding in the training set. If positive (binding) pairs are more on the right side and negative pairs on the left side, and there is little data in the middle, then this means these highly biased proteins tend to have the same bias as the test dataset. Such strong and consistent between training and test dataset bias can be exploited to achieve high predictive performance. We can study this separately for the bias on the protein side (in panel a, b, and c) and the compound side (in panels d, e, and f).

Comparing panels a, b, and c in Figure 4-4 reveals that on Testset1, both positive and negative pairs are randomly distributed with respect to their protein-bias (i.e., the corresponding Baseline-P would perform poorly), while in Testset2 and Testset3 there are more positive pairs than negative pairs on the right-end of the histogram (where the proteins are highly biased to be binding). Furthermore, on Testset3 this effect is stronger, negatives are shifted to the left, and there is less data in the middle. Altogether, these factors increase accuracy of the labels that are transferred/predicted from the most similar training protein sequence. Consequently, Baseline-P should perform relatively well on Testset2 and even better for Testset3. This agrees with the results in Table 4-5.

Panels d, e, and f in Figure 4-4 show a more extreme scenario on the compound side. Compounds in all three test sets seem to be either almost always binding or almost always non-binding. This is why the histograms are concentrated on both sides of the plot, with virtually no values in the middle. On Testset1, however, this bias does not correlate with the label in the test dataset (i.e., on both sides of the plot, the green and red bars have similar size). This means that labels transferred from the most similar training compound do not have the same labels as the native label on the Testset1. This is why Baseline-C perform poorly on Testset1. On the other hand, the label from Testset2 and Testset3 are in strong agreement with the labels from the training set. This is because the histograms are pushed to the extremes/end, the right-most bars are heavily biased to be positive while the left-most bars are strongly biased to be negative/non-binding. This means that

binding/non-binding labels from the most similar training compound are in good agreement with the test labels, which translates into very high predictive performance for this Baseline-C approach. This concurs with the results in Table 4-5.

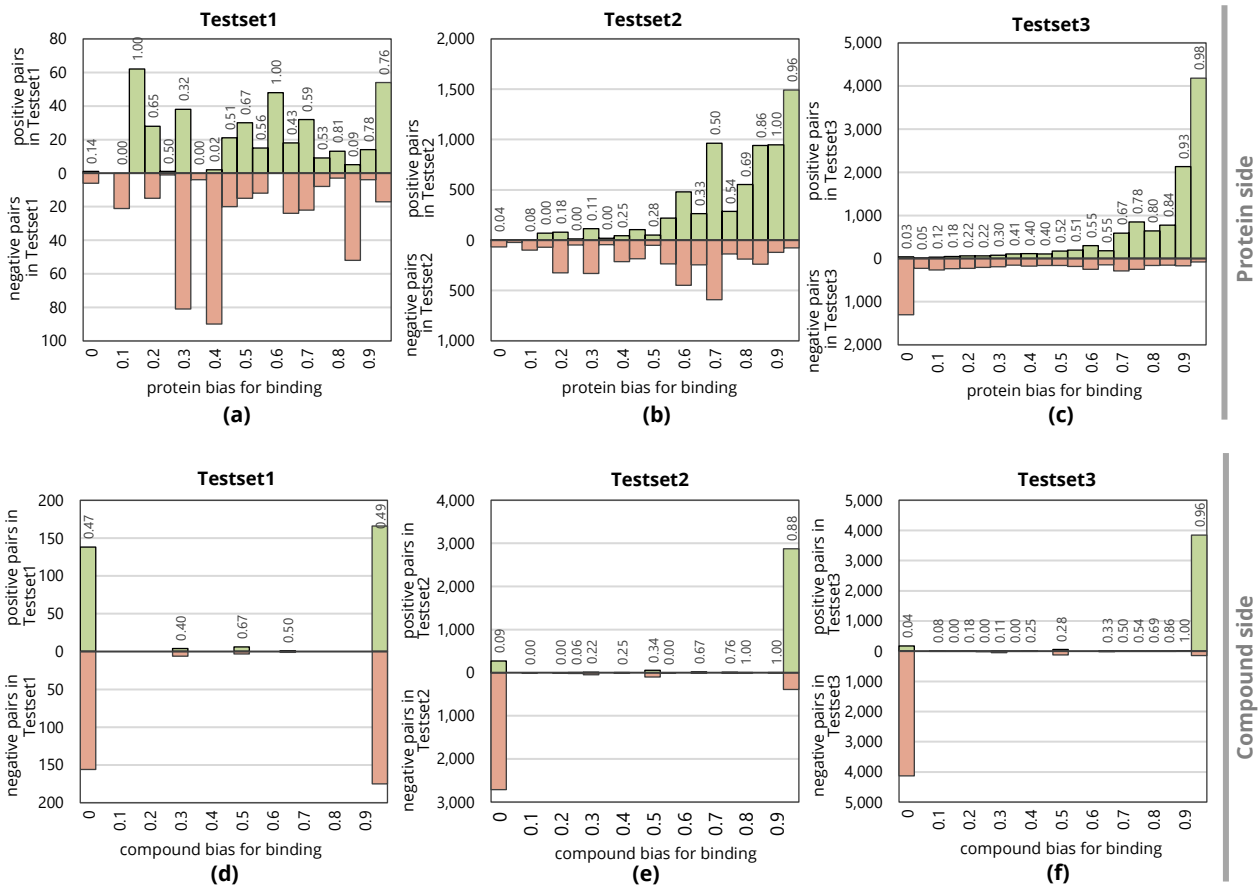


Figure 4-4. Distribution (histogram) of protein bias (panel a, b, c), and compound bias (panel d, e, f) for positive/interacting (green bars) and negative/non-interacting (red bars) pairs in each of the three test sets. Protein bias represents the fraction of times proteins are annotated as binding (as opposed to non-binding) in the training set. Compound bias is an equivalent fraction for compounds. The green histograms show the distribution for positive (binding) pairs in the given test set, and the red histogram shows the distribution for negative (non-binding) pairs. For example, in panel e, the green bar at the right-most side of the upper histogram contains most of the distribution of the positive pairs in Testset2 and shows that most of the positive/interacting pairs in the Testset2 have a very high (> 0.95) bias. The number 0.88 annotated on top of this bar means 88% of the Testset2 pairs that have a compound with a bias in the corresponding range (bias > 0.95) are labeled positive/interacting.

Comparing the compound side and protein side, apart from the Testset1, the reason why Baseline-C is better than baseline-P is that almost all compounds tend to be extremely biased (there is little to no data in the middle) and on Testset2 and Testset3 the bias directly correlates with their label on the test set. This bias on the protein side is weaker (there are still relatively a lot of proteins that

are in the middle), and thus less useful for the prediction. Moreover, neither of the baselines works well on Testset1 because proteins in this set are not biased (Figure 4-4a) and the bias for compounds is inconsistent between training and test dataset (Figure 4-4d). This is why simple, similarity-based methods would not work for this type of the "difficult" prediction problem, and why more sophisticated methods are needed.

4.4. **Conclusions and discussion**

In the Sub-goal 2.1, we identify domain-compound associations that may or may not transfer to their host proteins. In other words, presence of a domain that is shown to interact with a given compound does not guarantee that all proteins that have this domain will also bind this compound. We find that even with the currently limited availability of the compound-protein interaction data (particularly for the non-binding) and a conservative definition of binding and non-binding, thousands of these examples could be found. After removing redundancy, we are left with 459 such compound-domain pairs. This finding is particularly problematic for recent works that rely on assignment of compound-interaction to domains and propagating these compound interactions to all proteins that have those domains[250, 292]. While presence of a compound-interacting domain is helpful to hypothesize that another protein that includes this domain may bind this compound, our study shows that additional steps are needed before that annotation of interaction can be transferred.

More importantly, the above pattern could also affect ability of the current predictors of compound-protein interactions to make accurate predictions. This is because these tools often rely on similarity between proteins and between compound, and here high similarity between proteins (that share domains) may result in incorrect predictions. We study this issue empirically in Sub-Sub-goal 2.2 using three datasets: Testset1, which corresponds to data collected in Sub-goal 2.1, Testset3 that represents a typical benchmark dataset, and Testset2, which is in-between these other two datasets. We find that while the current predictors score very high performance on typical Testset3 test dataset, which agrees with the results in literature, they perform either poorly or modestly accurately on Testset1. This demonstrates the need to develop a new solution that would provide more accurate results for data like in Testset1. We find that several methods perform

modestly well and significantly better than best baselines for Testset1, which suggests that a new solution could perhaps take a form of a meta-predictor.

Moreover, our analysis of baselines shows that while the current methods secure very high AUCs for the typical test dataset, Testset3 (AUC=0.96), a simple similarity-based baseline also achieves high AUC of 0.85. This suggests that the current test datasets are "easy", in the sense that the predictors can take advantage of the existing biases in these test datasets and similarity of these biases to the biases in the training datasets. Therefore, we postulate that the performance of predictors on such datasets must be evaluated in relative terms to the corresponding baseline. Only the methods that significantly outperform the baselines should be considered as accurate. Moreover, as some of the current methods likely approach a theoretical ceiling of the predictive performance, further and meaningful improvements are rather unlikely and potentially not very impactful. This suggest that focus should shift to more challenging scenarios where the baselines no longer perform well, meaning that bias and similarity do not produce accurate results.

One option is to consider the so called cold-start scheme, where the compounds and proteins in the training and test dataset are dissimilar. This limits the ability of the baseline to find suitably similar proteins or compounds in the training dataset. Current implementations of the cold-start scheme remove "similarity" between training and test data based on a simple exclusion of identical proteins and compounds with identical IDs [257, 267]. This is insufficient and correspond to a barely "warm"-start scheme. Our results suggest that this should be based on measuring similarity and ensuring that is it low between compound-proteins pairs in the training and test datasets. However, this is difficult to realize since similarity must be measured for both compounds and proteins and somehow combined for the corresponding compound-protein pairs.

Another option is to consider the scenario represented by Testset1. This scenario directly challenges the ability to transfer annotations of the domain-compound interactions across proteins that share domains. Our empirical results demonstrate that this scenario also substantially diminishes the ability of current predictors of compound-proteins interactions to generate accurate results. Moreover, we find that this scenario cannot be solved with a simple, similarity- and bias-based approach, which is why the baselines fail. We focus our attention this problem. The Goal 3, which we address in the next Chapter, finds a new and accurate solution for this problem.

Chapter 5. **Conceptualization, development, comparative testing and deployment of a new method that provides accurate prediction of compound-protein interactions for proteins that share domains**

5.1. **Introduction**

Chapter 4 shows that while the existing predictors of compound-protein interactions perform very well on a typical test dataset, they perform either poorly or only modestly well on Testset1. Moreover, the similarity- and bias-based baseline predictions also generate inaccurate results for this dataset. Altogether, this means that the underlying problem is unsolved and there is a lot of room for improvement. The availability of several modestly performing methods that use different predictive approaches and inputs motivated us to investigate whether an ensemble of these methods could provide improvement and produce higher levels of accuracy. Our hypothesis is to evaluate if modest quality predictions could be combined together to secure high-quality predictions. Therefore, we select and combine a subset of the methods that significantly better than the baselines and that provide at least modest levels of predictive quality. Furthermore, to develop this new meta-predictor, we collect a new training and validation set that we use for empirical design and parametrization. These datasets share similar characteristics to the Testset1 (difficult), while being disjoint with all datasets described in Chapter 4.

We first examine a simple weighted combination of the outputs of the selected predictors, which we obtain by training a logistic regression model. We progressively upgrade this meta-model by adding useful inputs and demonstrate how these upgrades impact predictive performance. Finally, we compare the best meta-model against the existing methods and the baselines to evaluate

whether it is capable of producing accurate and better results on Testset1. We also compare the results on the other test sets (Testset2 and Testset3) that are closer to a typical test scenario that is currently used in literature.

5.2. **Materials and methods**

We provide details of the datasets and tools that we use for develop the meta-predictor. The evaluation framework (i.e., use of training and test sets, the assessment metrics and statistical tests) is the same as the one used in Chapter 4 (Sections 4.3.3 and 4.3.4). Moreover, to ensure that evaluation on Testset1 is reliable, we hold out the Testset1 for the final evaluation only and develop the consensus method using a separate training dataset and validation dataset, which are disjoint from Testset1 and other datasets (Testset2, Testset3, and the common training set).

5.2.1. **Datasets**

Since we use Testset1 to perform comparative tests, we collect new data that shares similar characteristics with Testset1 (i.e., inclusion of binding and non-binding proteins that share binding domain), to develop training and validation datasets. We apply the same procedure that we use to collect Testset1 (see Section 4.2.3) but we utilize domain annotations from InterPro [293, 294], instead of Pfam-A. The Pfam-A annotations that we use to derive Testset1 are manually curated and available for a subset of proteins. In contrast, InterPro combines domain annotations from several source databases including Pfam and is arguably the most comprehensive databases of these annotations. Using these more inclusive but less accurate domain annotations allows us to collect a much bigger set of relevant compound-protein pairs. Next, we remove overlap between the new dataset of compound-protein pairs and the other datasets by removing any pair which is in Testset1, Testset2, Testset3, or in the main/common training set from the new dataset.

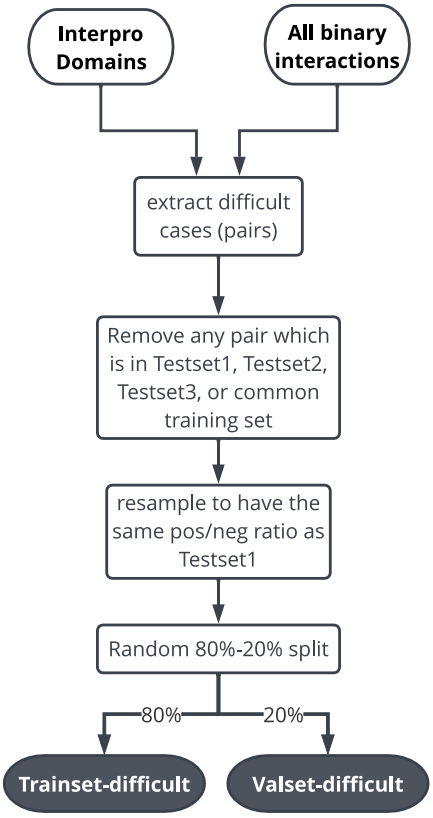


Figure 5-1. Schematic of the steps for building training and validation setfor development of consensus method

We randomly divide the resulting compound-protein interaction dataset into training dataset (Trainset-difficult) and validation set (Valset-difficult) with the ratio 80% to 20%. We summarize these datasets in Table 5.1 and visualize the entire process to collect these datasets in Figure 5-1. Trainset-difficult is used for training consensus models and Valset-difficult for model selection, hyperparameter tuning, and selecting input features.

Both of these datasets are available at http://biomine.cs.vcu.edu/servers/MetaBoostCPI

Table 5.1. Summary of the Trainset-difficult and Valset-difficult datasets that we use to develop the meta-predictor. We provide the number of compound-protein pairs (Pairs), number of positive pairs (Positives), number of negative pairs (Negatives), number of proteins (Proteins) and number of compounds (Compounds).

Dataset name	Pairs	Positives	Negatives	Proteins	Compounds
Trainset-difficult	18,436	9,852	8,584	832	3,540
Valset-difficult	4,373	2,532	1,841	352	1,408

5.2.2. **Developing consensus method**

As the first step in developing the new meta-method, we select a subset of current predictors of compound-protein interactions that we use as the inputs. We select methods that are statistically better than the baselines (p-value < 0.05) and that provide at least modest levels of predictive quality (AUC > 0.62) on Testset1. Using results in Table 4.5, these criteria result in selection of six methods: DeepPurpose, TransformerCPI, GraphDTA, MolTrans, DeepDTA and DeepConvDTI.

We start with a very simple method that only combines the results from these six methods using a simple weighted sum (Consensus-1), to evaluate whether this approach would improve over the results of individual predictions on the validation set (Valset-difficult). Then, we develop and evaluate three additional ideas to seek further improvements, resulting in the Consensus2, Consensus3, and Consensus4 solutions. In this development phase, we maximize the AUC on the Valset-difficult dataset to guide the design decisions (selection of features, models, and hyper parameters). Following, we describe details of these designs.

Consensus-1: Logistic regression with input predictors only.

We use a weighted average of the prediction from the six methods that we compute using logistic regression and the Trainset-difficult dataset. This is a step-up from a simpler unweighted average, since we optimize the weights to the Valset-difficult dataset. Therefore, outputs from the six predictors make up the first group of features that we use to develop the meta-predictor. We normalize the output from each predictor to have a mean of 0 and standard deviation of 1, so these outputs can be reliably combined together.

Consensus-2. Gradient boosted tree with input predictors only.

We study whether using a more advanced model to combine the six predictions would result in improved predictive performance. Thus, Consensus-2 model uses the same inputs as the Consensus-1 and applies Gradient Boosted Tree (GBT) instead of regression. We selected this classifier by comparing it with a few other algorithms, specifically Random Forest, Decision Tree, and ElasticNet, on the Valset-difficult dataset. GBT secured slightly better AUC and thus we

selected it for Consensus-2. The selection of the GBT algorithm is also supported by its recent use for many related prediction problems [295-299].

Consensus-3. Gradient boosted tree with input predictors and molecular features.

We extend the Consensus-2 by inclusion of additional inputs. We observe that the six predictions lack the context of the information about the input compound and protein. Such information could provide useful context for the predictions, since we expect that individual input predictors may perform differently for different types of proteins and compounds. We derive a small set of molecular features that describe the input protein sequence and the structure of the input compound. We explicitly limit the size of the feature set given the relatively small size of our training and validation datasets (Table 5.1).

We describe the input protein sequence using composition of the 20 amino acid types. This 20-dimensional feature vector is computed as the number of amino acids of a given type divided by the total number of residues in the protein sequence.

We use nine features to quantify key characteristics of the compound structure expressed using the SMILES string format. These descriptors are commonly used to describe small compounds and are included in PubChem. The commonly used cheminformatics package, RDKit (https://www.rdkit.org), was used for implementations of these features

1. *Molecular Weight:* Total mass of atoms in the compound reported in daltons and calculated as a sum of the mass of each constituent atom multiplied by the number of atoms of that element in the molecular formula.
2. *XLogP3:* Predicted octanol-water partition coefficient, computed using the Cheng *et al* algorithm [300]
3. *Hydrogen Bond Donor Count:* The number of hydrogen bond donors in this compound.
4. *Hydrogen Bond Acceptor Count:* The number of hydrogen bond acceptors in this compound.
5. *Rotatable Bond Count:* Number of rotatable binds in the compound
6. *Topological Polar Surface Area:* An estimate of the polar surface area (in $Å^2$) of a molecule, computed as the surface sum over polar atoms in the molecule. The implementation is based on Ertl *et al* [301].

7. *Heavy Atom Count:* Number of heavy atoms (non-hydrogen atoms) in the compound.
8. *Formal Charge:* Difference between the number of valence electrons of each atom and the number of electrons the atom is associated with.
9. *Complexity:* An estimate of how complicated the compound structure is, computed using the Bertz/Hendrickson/Ihlenfeldt formula [302, 303].

In total, Consensus-3 uses 6 + 20 + 9 = 35 input features.

Consensus-4. Gradient boosted tree with input predictors, molecular features, and similarity-based features.

Given the wide-spread use of compound and protein similarity for the prediction of compound-protein interactions [30], we develop additional features that focus on this aspect. This will again provide a useful context for the six predictions, given that some of these methods are more reliant on having a similar protein and/or compound in the training set while others may not use this information.

We design the similarity-based features to represent the level to which the input compounds and the input proteins are similar to the proteins and compounds in the training dataset of these predictors, which is the "common training set" described in Section 4.3.1. We note that the Trainset-difficult, Valset-difficult and Testset1 are disjoins with the common training dataset. Moreover, we do not use the interactions data extracted from the information in the training dataset for the similar proteins and/or compounds, but rather quantify whether and how many similar proteins and compounds can be found. This means that such model could be potentially used to address the cold-start scenario.

For a given input compound, we compute its similarity with the compounds in the common training dataset using Tanimoto coefficient based on the fingerprints extracted from the SMILES structures. We calculate three features that quantify similarity to the most similar training compound, average of the highest five similarities, and average of the top 100 highest similarities with the training compounds. Similarly, for the a given protein sequence, we quantify its similarity with sequences in the training dataset using percent sequence identity from the pairwise sequence alignment computed using MMseqs2 [258, 290]. Using these results, we derive three features that

quantify similarity to the most similar training protein, average of the highest five similarities, and average of the top 100 highest similarities with the training proteins.

We summarize these three groups of features, including the six predictions, the molecular features and the similarity-based features in Table 5.2. In total, Consensus-4 utilizes 6 + 29 + 6 = 41 features.

Table 5.2. Summary of different types of inputs used by the meta-predictors.

Feature Groups	Features	Description
Input predictions 6 Features	pred_MolTrans	Normalized prediciton scores from the six selected predictors
	pred_DeepDTA	
	pred_DeepConvDTI	
	pred_GraphDTA	
	pred_DeepPurpose	
	pred_TransformerCPI	
Molecular features 29 Features	Molecular Weight	Molecular properties of the compound
	XLogP3	
	Hydrogen Bond Donor Count	
	Hydrogen Bond Acceptor Count	
	Rotatable Bond Count	
	Topological Polar Surface Area	
	Heavy Atom Count	
	Formal Charge	
	Complexity	
	AAC_A, …, AAC_Y	20 amino acid compositions for the protein
Similarity-based features 6 Features	TOP_1_SIM_C	Similarity to training compounds
	TOP_5_SIM_C	
	TOP_100_SIM_C	
	TOP_1_SIM_P	Similarity to training proteins
	TOP_5_SIM_P	
	TOP_100_SIM_P	

5.3. **Results**

5.3.1. **Comparison of meta-predictors**

Table 5.3 summarizes results generated by the four designs of the meta-predictors on the Valset-difficult and Testset1 datasets. The results are sorted by AUC on Testset1 and show and the significance of differences against the simplest Consensus-1 and the most complex Consensus-4 (calculated using the process explained in Section 4.3.4).

Consensus-1 is a relatively simple method and we use it to evaluate whether such simple solution would still improve over the current predictors. While overall Consensus-1 seems to improve over the best results from the current tools, these improvements are not always statistically significant and, in some cases, the best current methods perform better. For instance, AUC of Consensus-1 for Testset1 is significantly and statistically higher that AUCs of the six predictors (p-value < 0.05). However, for Valset-difficult dataset, while Consensus-1 secures higher AUC than the six predictors, the differences to one of the predictors (GraphDTA) is not statistically significant. At the same time, AUPR of GraphDTA is higher than AUPR of Consensus-1 on Testset1 while being lower on Valset-difficult. Altogether, we find that this simple meta-predictor produces modest and relatively consistent improvements over the input predictors, suggesting that meta-prediction is a viable option to improve predictive performance for this challenging predictive problem.

Table 5.3. Results on the validation dataset (right) and Testset1 (left)generated by the four meta-predictors (Consensus-1, Consensus-2, Consensus-3, and Consensus-4) and the six input predictors. The methods are sorted by their AUC on Testset1. Annotations in the superscript report significance of differences when compared to Consensus-1 while annotations in subscript show the significance of differences against Consensus-4. '+' means significantly higher, '−' means significantly lower and '=' means no significant difference according to the statistical significance test described in section 4.3.4. For example, "0.632 $^{-}_{-}$" in the top left corner means the AUC = 0.632 obtained by DeepPurpose on Testset1 is significantly lower than the AUCs of Consensus-4 and Consensus-1 on this dataset. Statistical significance test is described in Section 4.3.4. All measurements are normal and thus the statistics exclusively rely on the t-test.

		Testset1				**Valset-difficult**			
		AUC	**AUPR**	**MCC**	**F1**	**AUC**	**AUPR**	**MCC**	**F1**
Predictors used as input to the meta-predictor	DeepPurpose	0.632 $^{-}_{-}$	0.645 $^{-}_{-}$	0.220 $^{-}_{-}$	0.551 $^{-}_{-}$	0.682 $^{-}_{-}$	0.704 $^{-}_{-}$	0.262 $^{-}_{-}$	0.699 $^{-}_{-}$
	TransformerCPI	0.652 $^{-}_{-}$	0.632 $^{-}_{-}$	0.252 $^{-}_{-}$	0.630 $^{-}_{-}$	0.715 $^{-}_{-}$	0.739 $^{-}_{-}$	0.289 $^{-}_{-}$	0.715 $^{-}_{-}$
	GraphDTA	0.666 $^{-}_{-}$	0.712 $^{+}_{-}$	0.269 $^{=}_{-}$	0.631 $^{-}_{-}$	0.763 $^{=}_{-}$	0.724 $^{-}_{-}$	0.291 $^{-}_{-}$	0.789 $^{=}_{-}$
	MolTrans	0.669 $^{-}_{-}$	0.672 $^{-}_{-}$	0.237 $^{-}_{-}$	0.626 $^{-}_{-}$	0.754 $^{-}_{-}$	0.729 $^{-}_{-}$	0.326 $^{=}_{-}$	0.761 $^{-}_{-}$
	DeepDTA	0.671 $^{-}_{-}$	0.641 $^{-}_{-}$	0.282 $^{=}_{-}$	0.648 $^{-}_{-}$	0.718 $^{-}_{-}$	0.707 $^{-}_{-}$	0.315 $^{-}_{-}$	0.734 $^{-}_{-}$
	DeepConvDTI	0.676 $^{-}_{-}$	0.651 $^{-}_{-}$	0.309 $^{=}_{-}$	0.651 $^{-}_{-}$	0.735 $^{-}_{-}$	0.746 $^{-}_{-}$	0.352 $^{=}_{-}$	0.752 $^{-}_{-}$
Consensus	Consensus-1	0.715 $^{}_{-}$	0.692 $^{}_{-}$	0.293 $^{}_{-}$	0.753 $^{}_{-}$	0.772 $^{}_{-}$	0.759 $^{}_{-}$	0.346 $^{}_{-}$	0.792 $^{}_{-}$
	Consensus-2	0.721 $^{=}_{-}$	0.719 $^{+}_{-}$	0.315 $^{=}_{-}$	0.777 $^{+}_{-}$	0.773 $^{=}_{-}$	0.768 $^{=}_{-}$	0.366 $^{=}_{-}$	0.823 $^{+}_{-}$
	Consensus-3	0.752 $^{+}_{-}$	0.749 $^{+}_{-}$	0.339 $^{+}_{=}$	0.792 $^{+}_{-}$	0.812 $^{+}_{-}$	0.803 $^{+}_{-}$	0.383 $^{+}_{-}$	0.804 $^{+}_{-}$
	Consensus-4	**0.793** $^{+}$	**0.785** $^{+}$	**0.366** $^{+}$	**0.835** $^{+}$	**0.841** $^{+}$	**0.830** $^{+}$	**0.405** $^{+}$	**0.835** $^{+}$
Oracle		0.983 $^{+}_{+}$	0.979 $^{+}_{+}$	0.923 $^{+}_{+}$	0.986 $^{+}_{+}$	0.973 $^{+}_{+}$	0.961 $^{+}_{+}$	0.882 $^{+}_{+}$	0.920 $^{+}_{+}$

Interestingly, the improvements of Consensus-2 over Consensus-1 are rather modest. While Consensus-2, which applies a more sophisticated model generated by GBT, generates higher predictive performance across all metrics and both datasets, these differences are not statistically significant for AUC and MCC. This suggests that introduction of a more complex model does not lead to substantial improvements.

On the other hand, we observe that introduction of the additional molecular and similarity-based features produces large and statistically significant improvements. Consensus-3 improves over Consensus-2 across all metrics and for both datasets. Similarly, Consensus-4 further improves over Consensus-3 across the four metrics and for both datasets. This demonstrates that the context that these features provides for the input predictions is useful to formulate a more accurate meta-prediction. Moreover, the two sets of features provide improvements in different ways, suggesting that they complement each other, resulting in an accurate Consensus-4.

We observe that Consensus-4 provides the best predictive performance across all four metrics on the Valset-difficult validation dataset and Testset1. It generates predictions with AUC = 0.79 on Testset1 and AUC = 0.84 on Valset-difficult, which suggests that this model delivers accurate

results. To compare, the currently best DeepConvDTI obtains AUC = 0.68 on Testset1 and 0.73 on Valset-difficult. The improvements when comparing Consensuus-4 to all other approaches, including the six best current predictors and the three meta-predictors (Consensus-1, Consensus-2 and Consensus-3) are statistically significant (p-value < 0.05), except for comparison using MCC on Testset1 with Consensus-3 where the results are still better by the difference is not significant. Given these favorable results, we use Consensus-4 as our best meta-predictor and name it MetaBoostCPI.

We observe that the progression of the improvements by the consecutive meta-predictor designs (Consensus-1, Consensus-2, Consensus-3 and Consensus-4) is consistent and occurs on both validation dataset and Testset1. We also note that the results on the validation dataset are consistently better than the results on Testset1. This can be attributed to the fact that the validation Valset-difficult dataset is more similar to the Trainset-difficult, since they apply the same type of domain annotations.

Finally, we produce an additional baseline that approximates an upper limit of the predictive performance for a meta-model. This “oracle” predictor is formulated by always selecting the most accurate prediction generated by the six input methods (highest prediction value when the label is binding and lowest when the label is non-binding). Results in Table 5.2 show that oracle secures AUC = 0.98 on Testset1 and 0.97 on Valset-difficult. We find that MetaBoostCPI performs very well by improving AUC on Testset1 from 0.68 (the best current method on this dataset, DeepConvDTI) to 0.79, and on Valset-difficult from 0.76 (the best current method on this dataset, GraphDTA) to 0.84. However, the oracle-based result reveals that further improvements are still possible.

In the next section, we compare MetaBoostCPI with the collection of the 14 representative current methods on multiple test datasets.

5.3.2. **Performance of MetaBoostCPI on the test datasets**

We find that MetaBoostCPI (Consensus-4 model) makes significant improvements on Tesetset1 when compared to the six best current tools on this dataset. Table 5.4 compares this meta-model

with a wider set of 14 representative methods we select in Chapter 4 on the three test datasets: Tesetset1 (difficult), Tesetset2 (intermediate), and Tesetset3 (typical).

Table 5.4. Comparison of the results produced by the best meta-predictor (MetaBoostCPI) with the 14 representative predictorsof compound-protein interactions and the two baselines on Testset1, Testset2 and Testset3. The methods are sorted by their AUCs on Testset1. For baselines, the standard deviation of the metric is shown in parentheses under the (average) value of the metric; this is based on 100 runs for each baseline on each dataset. Annotations in the superscript report significance of differences when compared to MetaBoostCPI. '+' means significantly higher, '−' means significantly lower and '=' means no significant difference, according to the statistical significance test described in Section 4.3.4. All measurements are normal and thus the statistics exclusively rely on the t-test.

		Testset1(difficult)				**Testset2 (intermediate)**				**Testset3 (typical)**			
		AUC	**AUPR**	**MCC**	**F1**	**AUC**	**AUPR**	**MCC**	**F1**	**AUC**	**AUPR**	**MCC**	**F1**
Baselines	Baseline-P	0.496 $^{-}$ ±0.021	0.490 $^{-}$ ±0.017	0.037 $^{-}$ ±0.033	0.513 $^{-}$ ±0.017	0.634 $^{-}$ ±0.006	0.727 $^{-}$ ±0.005	0.224 $^{-}$ ±0.010	0.720 $^{-}$ ±0.004	0.772 $^{-}$ ±0.003	0.847 $^{-}$ ±0.003	0.483 $^{-}$ ±0.006	0.836 $^{-}$ ±0.002
	Baseline-C	0.517 $^{-}$ ±0.009	0.520 $^{-}$ ±0.011	0.015 $^{-}$ ±0.014	0.501 $^{-}$ ±0.007	0.813 $^{-}$ ±0.003	0.867 $^{-}$ ±0.003	0.540 $^{-}$ ±0.007	0.834 $^{-}$ ±0.002	0.851 $^{=}$ ±0.003	0.917 $^{=}$ ±0.002	0.532 $^{=}$ ±0.005	0.850 $^{=}$ ±0.002
Current predictors	GNN-CPI	0.502 $^{-}$	0.512 $^{-}$	0.087 $^{-}$	0.521 $^{-}$	0.732 $^{-}$	0.724 $^{-}$	0.332 $^{-}$	0.652 $^{-}$	0.807 $^{-}$	0.766 $^{-}$	0.493 $^{-}$	0.757 $^{-}$
	CONNECTOR	0.511 $^{-}$	0.522 $^{-}$	0.033 $^{-}$	0.542 $^{-}$	0.772 $^{-}$	0.789 $^{-}$	0.446 $^{-}$	0.661 $^{-}$	0.845 $^{-}$	0.819 $^{-}$	0.568 $^{-}$	0.793 $^{-}$
	BACPI	0.520 $^{-}$	0.542 $^{-}$	0.098 $^{-}$	0.512 $^{-}$	0.832 $^{-}$	0.804 $^{-}$	0.501 $^{-}$	0.705 $^{-}$	0.902 $^{-}$	0.911 $^{-}$	0.680 $^{-}$	0.783 $^{-}$
	MDeePred	0.526 $^{-}$	0.530 $^{-}$	0.052 $^{-}$	0.564 $^{-}$	0.812 $^{-}$	0.824 $^{-}$	0.492 $^{-}$	0.694 $^{-}$	0.894 $^{-}$	0.898 $^{-}$	0.652 $^{-}$	0.764 $^{-}$
	HyperAttentionDTI	0.556 $^{-}$	0.601 $^{-}$	0.101 $^{-}$	0.616 $^{-}$	0.823 $^{-}$	0.813 $^{-}$	0.510 $^{-}$	0.712 $^{-}$	0.883 $^{-}$	0.864 $^{-}$	0.652 $^{-}$	0.729 $^{-}$
	DeepAffinity-dom	0.577 $^{-}$	0.636 $^{-}$	0.109 $^{-}$	0.551 $^{-}$	0.878 $^{-}$	0.936 $^{+}$	0.569 $^{-}$	0.845 $^{=}$	0.951 $^{+}$	0.974 $^{+}$	0.742 $^{+}$	0.907 $^{+}$
	KGE_NFM	0.589 $^{-}$	0.593 $^{-}$	0.172 $^{-}$	0.642 $^{-}$	0.862 $^{-}$	0.866 $^{-}$	0.598 $^{-}$	0.751 $^{-}$	0.887 $^{-}$	0.871 $^{-}$	0.651 $^{-}$	0.833 $^{-}$
	DeepAffinity	0.616 $^{-}$	0.678 $^{-}$	0.179 $^{-}$	0.586 $^{-}$	0.914 $^{=}$	0.955 $^{+}$	0.648 $^{=}$	0.873 $^{+}$	0.951 $^{+}$	0.974 $^{+}$	0.744 $^{=}$	0.908 $^{+}$
	DeepPurpose	0.632 $^{-}$	0.645 $^{-}$	0.220 $^{-}$	0.551 $^{-}$	0.902 $^{-}$	0.908 $^{-}$	0.712 $^{-}$	0.831 $^{-}$	0.923 $^{=}$	0.929 $^{-}$	0.804 $^{+}$	0.892 $^{+}$
	TransformerCPI	0.652 $^{-}$	0.632 $^{-}$	0.252 $^{-}$	0.630 $^{-}$	0.889 $^{-}$	0.874 $^{-}$	0.658 $^{-}$	0.790 $^{-}$	0.899 $^{-}$	0.902 $^{-}$	0.756 $^{+}$	0.732 $^{-}$
	GraphDTA	0.666 $^{-}$	0.712 $^{-}$	0.269 $^{-}$	0.631 $^{-}$	0.904 $^{-}$	0.950 $^{+}$	0.619 $^{-}$	0.863 $^{+}$	0.930 $^{=}$	0.963 $^{+}$	0.690 $^{-}$	0.888 $^{+}$
	MolTrans	0.669 $^{-}$	0.672 $^{-}$	0.237 $^{-}$	0.626 $^{-}$	0.942 $^{+}$	0.943 $^{+}$	0.757 $^{+}$	0.881 $^{+}$	0.968 $^{+}$	0.964 $^{+}$	0.835 $^{+}$	0.919 $^{+}$
	DeepDTA	0.671 $^{-}$	0.641 $^{-}$	0.282 $^{-}$	0.648 $^{-}$	0.780 $^{-}$	0.755 $^{-}$	0.423 $^{-}$	0.718 $^{-}$	0.793 $^{-}$	0.776 $^{-}$	0.443 $^{-}$	0.727 $^{-}$
	DeepConvDTI	0.676 $^{-}$	0.651 $^{-}$	0.309 $^{-}$	0.651 $^{-}$	0.901 $^{-}$	0.903 $^{-}$	0.716 $^{=}$	0.752 $^{-}$	0.929 $^{=}$	0.913 $^{-}$	0.790 $^{+}$	0.891 $^{+}$
	MetaBoostCPI	0.793	0.785	0.366	0.835	0.912	0.918	0.709	0.849	0.925	0.936	0.742	0.878

As expected, our empirical results reveal show that MetaBoostCPI significantly improves over all 14 methods and both baselines for Testset1 (p-value < 0.05). The fact that MetaBoostCPI achieves such high levels of predictive performance suggests that it could be considered as a viable solution to the problem posed in Chapter 4.

Table 5.4 shows that MetaBoostCPI achieves competitive levels of predictive performance on Testset2 and Testset3. While not being the best on these two datasets, MetaBoostCPI is substantially better than the best baseline, AUC = 0.912 vs. 0.813 on Testset2 and AUC = 0.925 vs. 0.851 on Testset3. This means that our new meta-predictor produces accurate results across all three test datasets. We note that MolTrans is significantly better than MetaBoostCPI on Testset2

and Testset3, but this tool performs poorly for Testset1. Moreover, as we argue in the previous chapter, there are many methods that provide highly accurate results for typical test scenarios represented by Testset3 and thus further improving results for these scenarios has arguably lesser impact than solving the problem that corresponds to Testset1.

5.4. **Analysis of the contribution of individual features in the MetaBoostCPI model**

Motivated by the favorable performance of MetaBoostCPI, we study importance/impact of its input features on the predictive quality. We use the feature importance scores produced by the implementation of Gradient Boosted Tree in the XGBoost package to quantify contributions of individual features. These scores are calculated using the number of times a given feature is used to split the data across all trees [304]. Therefore, it represents how often MetaBoostCPI rely on that feature to make predictions.

Figure 5-2 shows the feature importance scores sorted by their values from the most important to the least important where features with a zero score are removed. As expected, the predictions of MetaBoostCPI are mainly driven by the outputs from the top-performing predictors. However, not all predictors contribute equally, with the results produced by MolTrans, DeepConvDTI, DeepPurpose, and TransformerCPI being the most useful. The other useful inputs are the TOP_1_SIM_P and TOP_1_SIM_C features that quantify similarity to the most similar protein and the most similar compound in the training set, respectively, essentially revealing whether similar proteins and compounds are present. These features likely provide useful context for the predictions from the current methods. For example, some of the input predictors might work well for compounds or proteins that are similar to the data in the training dataset, while others may provide better predictions where this similarity is low. The use of these features would allow identifying such relations. Our analysis also shows that while several of the molecular features from the compound side, such as Molecular Weight and Topological Polar Surface Area and XLogP3, modestly contribute to the prediction, contribution from the protein amino acid compositions is minimal. This could be because we represented the protein sequence using a rather simple amino acid vector. Use of a more sophisticated representation of the protein chain could strengthen our model, which we discuss in our future work section.

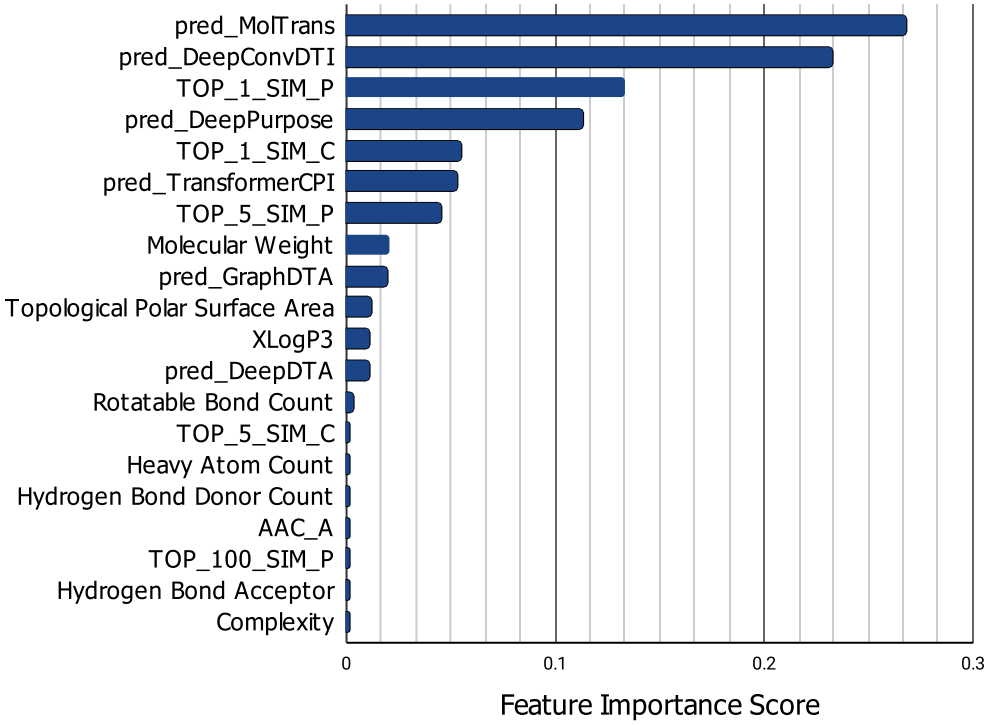


Figure 5-2. The plot of feature importance scores for MetaBoostCPI. Features are sorted by the value of their scores from the most important (top) to the least important (bottom). Only features with the non-zero scores are shown.

Overall, the observations from the importance of features are consistent with the what we observed by comparing different consensus models. However, such more fine-grained characterization of features provide better insights into the working of the model and intrinsic value of the input features, informing our future work.

5.5. **Webserver**

Motivated by the results produced by MetaBoostCPI, we make it publicly available by deploying it as a webserver at http://biomine.cs.vcu.edu/servers/MetaBoostCPI. The end users need only a web-browser and Internet connection to access the web-sever webpage and use our model. They input a protein sequence and a SMILES-based representation of a compound using simple web form, click start and wait for the predictions to complete. The computations including running the six predictors, computing compound and protein features (MolFea and SIM features) and running the consensus model are done on the server side (i.e., the Biomine Lab server at the Virginia

Commonwealth University). Users do not need to take any extra steps, use their hardware, install software, or have any knowledge of programming, to complete the prediction process. This makes this tool accessible to a wide range of users, from usually more computer-savvy computer scientists and bioinformaticians to potentially less computing-experienced biophysicists, biochemists, structural biologists, and other scientists and developers. This stands in contrast to the existing predictors that are primarily available as source code, which is suitable to reproduce experiments but not easy to use to make predictions. The predictions from MetaBoostCPI are returned in the web-browser window and by email, if provided on the entry page. The server generates the outputs of the six input methods on top of the predictions from the MetaBoostCPI model.

5.6. **Conclusions and discussion**

This chapter pursues Goal 3 motivated by modest levels of predictive performance of the existing methods for differentiating binding and non-binding protein with compound-interacting domains. We develop an innovative meta-predictor using predictions from six top-performing existing predictors, a modern machine learning algorithm, and molecular and similarity-based features.

We show that a simple weighted average of the predictions from these six methods, which we generate with logistic regression, provides modest improvements when tested on the difficult Testset1. We examine several ideas to improve this simple consensus design. We find that using a more sophisticated machine learning model, the Gradient Boosted Tree (GBT) is insufficient to make statistically significant improvements over the more basic logistic regression. However, incorporating additional molecular and similarity features leads to statistically significantly and substantial gains in predictive quality. We believe that these features provide a useful context for the GBT model to figure out which input predictors should be used for which input proteins and compounds. This “selection” depends on the intrinsic characteristics of proteins and compounds as well as their (extrinsic) similarity to the training proteins and compounds. Our empirical tests reveal that intrinsic and extrinsic characteristics are complementary and they both produce improvements.

The resulting MetaBoostCPI meta-model significantly improves over the current solutions on Testset1, and can be used as a viable solution to accurately differentiate between binding and non-

binding proteins that share compound-interacting domains. Furthermore, the results on Testset3 show that MetaBoostCPI also achieves competitive performance on generic/typical prediction scenarios. We deploy MetaBoostCPI as a convenient webserver to make it available for public use.

Chapter 6. **Summary**

We pursue three goals related to the analysis of drugs/compounds, their target proteins and prediction of compound-protein interactions.

In the first goal (Chapter 3), we characterize sequence-based properties of the current drug targets and extract a set of markers that describe these proteins. Even though we do not address interactions with specific drugs or compounds, these results help us to better understand drug-protein interactions in the context of properties of proteins. A unique contribution of this work is to consider several new-to-this-field protein properties and bring disease association into this picture. The latter allows us to more accurately identify the non-targets, leading to arguably more useful results when compared to prior studies that only compare current drug targets against current non-targets [111-119]. We formulate several interesting markers that can be used to identify new and likely drug-target proteins. They include high number of alternative splicing isoforms, large number of domains, higher degree of centrality in the corresponding protein-protein interaction networks, relatively lower number of conserved residues and residues on the putative (sequence-derived) surface. Importantly, these characteristics can be computed across the entire human proteome, facilitating a comprehensive search for putative drug targets. We also find that current drug targets have low levels of intrinsic disorder and intrinsically disordered protein-binding regions when compared with much higher levels among the likely drug-targets and unlikely drug-targets. This suggests that novel drug targets should be searched among the disordered proteins, agreeing with recent studies that point to inclusion of these proteins into the set of druggable proteins [22, 161, 241-246]. Finally, we also generate interesting insights concerning cellular functions and subcellular locations of the likely drug-target proteins. We

demonstrate that they are possibly involved in the metabolic and biosynthesis processes and localized across the cell, without a preference for specific subcellular locations. These results were published in a journal article [54].

While Goal 1 analyzes drug targets, Goal 2 (Chapter 4) focuses on the topic of compound-protein interactions. In Sub-goal 2.1, we identify binding and non-binding proteins that share compound-interacting domains and evaluate their abundance. Using a strict/conservative process, we find hundreds of such "problematic" compound-domain pairs. This is particularly problematic for works that propagate compound-domain interactions to all proteins that have those domains[250, 292]. More importantly, this pattern/scenario likely affects ability of current predictors of compound-protein interactions to make accurate predictions. These tools often rely on similarity between proteins and between compound, and in this scenario the high similarity between proteins (that share domains) may lead to incorrect predictions. We study this issue empirically in Sub-goal 2.2 using three datasets: Testset1, which includes data collected in Sub-goal 2.1, Testset3 that represents a typical benchmark dataset, and Testset2, which is in-between Testset1 and Testset3. In line with literature, we find that current predictors perform very well on the typical Testset3. Moreover, while they perform relatively well on the intermediate Testset2, we discover that they perform either poorly or only modestly well on Testset1. This reveals the need to develop new solutions that would provide more accurate predictions for Testset1.

Moreover, under Sub-goal 2.2, we formulate and analyze two baseline predictions that rely in intrinsic bias and similarity between training and test datasets. We find that these baselines secure accurate results for Testset3, suggesting that the current test datasets are "easy". This means that current predictors can and likely take advantage of the biases and similarity between training and test datasets to generate accurate results. Our results strongly suggest that the performance of predictors on such "easy" datasets must be evaluated in a context of these baselines. We also conclude that several current methods, such as DeepAffinity, GraphDTA, and MolTrans, produce significantly better results on Testset3 when compared to the baseline.

The third goal (Chapter 5) is motivated by the finding that current tools do not provide accurate results for Testset1 and that this problem cannot be solved with a simple, similarity- and bias-based approach, which is why the baselines produce poor results. We develop an innovative meta-

predictor that relies on predictions from six existing predictors, GBT model, and molecular and similarity-based features. We empirically demonstrate that use of the molecular and similarity features leads to substantial gains in predictive quality. Our MetaBoostCPI meta-model significantly improves over the current solutions on Testset1, including the baselines. We argue that it can be used as a viable solution to accurately differentiate between binding and non-binding proteins that share compound-interacting domains. We also show that MetaBoostCPI provides competitive predictive performance on generic/typical prediction scenarios, which correspond to Testset3. We implement and deploy MetaBoostCPI as a convenient and publicly available webserver at http://biomine.cs.vcu.edu/servers/MetaBoostCPI.

Lastly, this work has allowed us to provide answers to the three questions that we pose in the Introduction. We find that the scenario that proteins that share a compound-interacting domain "switch" their ability to interact with the same compound is relatively common. The current predictors of protein-compound interactions provide at best modestly accurate predictions for this scenario. Finally, a new method that improves upon the current methods and provides accurate predictions for these interactions can be developed.

6.1. **Major Contributions**

My contributions to Goal 1 include:

- collection and integration of the drug-protein interactions from several databases
- collection of predictions and annotations for the proteins in the database
- defining and collection of the datasets
- comparative statistical analysis
- examination of the results
- development of markers that are useful to identify likely target proteins
- formulation of insights concerning cellular functions and subcellular locations of the likely target proteins

For Goal 2:

- collection of the binding data and preprocessing and collecting domain annotations
- collection and annotation of the datasets including Testset1, Testset2, Testset3 and common training set
- analysis of abundance of binding and non-binding proteins that share compound-interacting domains
- review of current predictors of compound-protein interactions
- selection, installation and running of the selected 14 predictors of compound-protein interactions
- development and empirical analysis of baselines
- production and analysis of comparative results of the 14 predictors and baselines on Testset1, Testset2, and Testset3

For Goal 3:

- development of Trainset-difficult and Valset-difficult datasets
- design and development of meta-models
- empirical comparative assessment of meta-models
- empirical comparison of MetaBoostCPI on Testset1, Testset2, and Testset3
- implementation and deployment as the MetaBoostCPI webserver

6.2. **Future work**

Theoretical upper limits of the predictive performance defined by the oracle consensus model (Section 5.3.1) suggest that there is room for further improvements for Testset1. One option for future work is to include additional inputs with focus on protein domains, compound substructures, inclusion of information derived from protein-protein interaction networks, drug side-effects and indications, and protein-disease associations, to name a few. Especially, the sequence-derived markers that we identify in Goal 1, and which are effective in differentiating drug target proteins from the non-targets, are strong candidates to develop better features to describe the protein

sequence. This would be especially valuable in the light of the relatively low value of the currently used amino acid composition.

A common practice in the field of machine learning is to perform an exploratory data analysis to characterize training and test datasets with respect to their properties, such as feature distributions, similarity between examples, outliers, and different biases. While this is less practiced in bioinformatics fields, in Section 4.3.7 we characterize a certain type of bias where compounds and proteins are heavily biased either towards binding or towards non-binding and illustrate how this bias leads to inflated AUC levels on typical test datasets. We plan to analyze other properties and assess their differences between training and test sets to investigate whether they also impact predictive quality of our meta-model. More specifically, looking at possible sources of shared biases between Trainset-difficult and Valset-difficult can provide insights for the reasons for the drop of performance from Valset-difficult to Testset1, which is consistent across all methods including the consensus. Also, studying the similarity (i.e., sequence similarity for proteins and fingerprint similarity for compounds) or a combination of both of them within each dataset and across different datasets can provide a more complete picture about commonalities and differences between these datasets.

Most of the predictors in Goal 2.2 were based on deep neural networks. While the amount of available data in generic compound-protein interaction datasets allows for training deep neural networks, the available data for our specific prediction tasks are more than an order of magnitude smaller (as can be observed by comparing the size of common training set with 268,232 pairs with the size of Trainset-difficult with 18,436 pairs), which prevents effective training of deep neural network with large number of parameters from the ground up. We may consider transfer learning, where a predictive model could be pre-trained using a more generic set of compound-protein interactions (such as the common training dataset) and then fine-tune it using smaller and problem-specific datasets (such as Trainset-difficult and Valset-difficult). Another approach that has been recently used for predictive problems with low numbers of labeled data in the context of prediction of compound protein affinity/binding prediction is meta-learning [305]. In a recent work, the challenge has been arising from the dearth of interaction data for (a subset of) individual compounds [306]. Similarly, for our problem, meta-learning could be utilized to tackle the

challenges around effectively training complex models with the relatively small size of datasets for the difficult cases (Trainset-difficult and Valsets-difficult).

Another angle to explore in the future is to focus on the regression task that predict numeric values of affinity measured by Ki, Kd, IC50, and EC50. The numeric values provide more information than the binary interaction label. One solution would be to consider a meta-predictor with custom-developed features and a regressor model. The particularly challenging aspect is to accommodate for the various measures of affinity (Ki, Kd, IC50, and EC50).

LIST OF PUBLICATIONS

Journal Publications

- Zhang, J., **Ghadermarzi, S.**, Katuwawala, A., & Kurgan, L. (2021). DNAgenie: accurate prediction of DNA-type-specific binding residues in protein sequences. *Briefings in Bioinformatics*, 22(6), bbab336. (https://doi.org/10.1093/bib/bbab336)

- **Ghadermarzi, S.**, Krawczyk, B., Song, J., & Kurgan, L. (2021). XRRpred: accurate predictor of crystal structure quality from protein sequence. *Bioinformatics*, 37(23), 4366-4374. (https://doi.org/10.1093/bioinformatics/btab509)

- Hu, G., Katuwawala, A., Wang, K., Wu, Z., **Ghadermarzi, S.**, Gao, J., & Kurgan, L. (2021). flDPnn: Accurate intrinsic disorder prediction with putative propensities of disorder functions. *Nature communications*, 12(1), 1-8. (https://doi.org/10.1038/s41467-021-24773-7)

- Katuwawala, A., **Ghadermarzi, S.**, Hu, G., Wu, Z., & Kurgan, L. (2021). QUARTERplus: Accurate disorder predictions integrated with interpretable residue-level quality assessment scores. *Computational and structural biotechnology journal*, 19, 2597-2606. (https://doi.org/10.1016/j.csbj.2021.04.066)

- Zhang, J., **Ghadermarzi, S.**, & Kurgan, L. (2020). Prediction of protein-binding residues: dichotomy of sequence-based methods developed using structured complexes versus disordered proteins. *Bioinformatics*, 36(18), 4729-4738. (https://doi.org/10.1093/bioinformatics/btaa573)

- **Ghadermarzi, S.**, Li, X., Li, M., & Kurgan, L. (2019). Sequence-derived markers of drug targets and potentially druggable human proteins. *Frontiers in genetics*, 1075. (https://doi.org/10.3389/fgene.2019.01075)

Conference Publications

- **Ghadermarzi, S.**, Katuwawala, A., Oldfield, C. J., Barik, A., & Kurgan, L. (2019). Disordered Function Conjunction: On the in-silico function annotation of intrinsically disordered regions. In *PACIFIC SYMPOSIUM ON BIOCOMPUTING 2020* (pp. 171-182). (https://doi.org/10.1142/9789811215636_0016)

Book Chapters

- Katuwawala, A., **Ghadermarzi, S.**, & Kurgan, L. (2019). Computational prediction of functions of intrinsically disordered regions. *Progress in Molecular Biology and Translational Science*, 166, 341-369. (https://doi.org/10.1016/bs.pmbts.2019.04.006)

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APPENDIX A

D dataset

The list of proteins in the dataset of current drug targets (D dataset) is provided below in the following format (sorted by the number of drug interactions)

IDX|***UNIPROT_ID*** (***NUM_DISEASE***) [***DRUGLIST***]

IDX: Sequential index
NUM_DISEASE: number of disease annotation
DRUG_LIST: comma separated list of PubChem CIDs of the interacting drugs

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527|P54855(17) [2913, 1057]
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532|P35557(71) [46908929, 39562]
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534|Q13126(66) [10041129, 188350]
535|P05186(61) [5478883, 26879]
536|P14091(14) [24800541, 16126898]
537|Q12908(24) [53492727, 10133]
538|Q13093(58) [9939609, 9918381]
539|Q9Y2Q3(182) [5326960, 6]
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543|Q401N2(21) [32051, 6000]
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545|Q9Y4D2(0) [3034010, 3572]
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548|P15085(9) [16741275, 24768537]
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551|Q9UL51(13) [65637, 9869877]
552|P41250(19) [1088, 12717]
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554|O14939(26) [10198924, 445639]
555|P61160(18) [447966, 588963]
556|P00505(36) [447742, 1051]
557|O95665(2) [54385, 119192]
558|P23434(10) [12717, 1088]
559|Q07817(142) [24978538, 12597]
560|Q13133(35) [2758, 16734800]
561|Q13332(7) [2088, 3305]
562|O00182(50) [101798, 119138]
563|P63165(43) [3151041, 54676538]
564|Q08493(3) [3671, 5092]
565|Q9NY46(5) [216327, 11967800]
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567|O14924(9) [3351, 10219]
568|Q9HAW9(17) [10894, 21138]
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570|P25098(54) [1973720, 1870615]
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579|Q12884(65) [44513473, 11516136]
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590|P18505(7) [31304, 104781]
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593|Q9Y210(54) [444899, 441298]
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644|Q9H598(4) [5665, 1088, 12717]
645|Q9NTQ9(9) [957, 636403, 3371]
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647|Q96S37(13) [255968, 5342, 2333]
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676|P43004(38) [52941485, 11412540, 107883]
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678|Q9NR96(215) [2090, 3652, 12449]
679|Q9UP38(22) [16779, 31475, 14868]
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695|P49116(31) [11751922, 445354, 444795]
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707|Q14790(179) [42601552, 12000240, 24800541]
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771|Q7Z2H8(5) [439280, 3744, 6305]
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773|P14679(88) [1057, 7638, 9015]
774|Q92952(2) [2993, 10237, 6000, 44623946]
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777|P22607(188) [9809715, 53235510, 11154925, 51039095]
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781|Q86XQ3(0) [5994, 5280723, 60663, 5280360]
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796|P48048(37) [1989, 2368, 3478, 199]
797|P80404(12) [5950, 1060, 1051, 5665]

798|Q13304(6) [18068, 5957, 6031, 8629]
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803|P68371(14) [2082, 4030, 4622, 11351021]
804|P09382(122) [101798, 119138, 11953346, 1567]
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859|Q15858(63) [56959, 129228, 216327, 219078, 11967800]
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879|P51843(107) [72462, 107782, 4122, 42725, 35803]
880|P04278(110) [102146, 10633, 44450327, 19582, 27812]
881|P00918(65) [5284549, 3284, 2720, 2343, 2910]
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883|P56696(15) [121892, 3932, 2351, 5413, 214350]
884|Q9GZV3(5) [19646, 36811, 249, 10198924, 187]
885|Q5XXA6(33) [4488, 3386, 16129778, 60663, 3371]
886|Q9P0L9(17) [16231, 3371, 313, 525, 311]
887|P01584(709) [54675783, 61635, 123600, 10341154, 3671]
888|Q9H0H5(14) [54676538, 11293, 2016, 12449, 54675783]
889|P07101(85) [6140, 6057, 3125, 441350, 44257]
890|P33316(8) [11536503, 145729, 11680992, 11637769, 554527]
891|P50052(90) [11238823, 172198, 2540, 9825285, 10257882]
892|P39086(8) [447196, 10036135, 5282253, 5284627, 127894]
893|P10826(81) [444795, 5289501, 5381, 60164, 449171]
894|P35869(166) [3117, 2750, 2361, 41684, 21307]
895|P32239(41) [16129675, 9870520, 4506, 108187, 3960]
896|P62508(11) [5280961, 11742, 448537, 5284643, 9549223]
897|P08709(118) [183797, 204102, 1792, 42601552, 24800541]
898|O43497(13) [16362, 5576, 1547484, 11967800, 60663]
899|Q00975(12) [5282138, 199, 2950, 16135415, 5745207]
900|Q9Y2T6(12) [16078, 2391, 4671, 644019, 104850]
901|P09668(26) [42601552, 24800541, 44398651, 44398659, 13186895, 24901101]
902|Q8TCC7(13) [123979, 10258, 148200, 11948288, 1175, 44814423]
903|P49019(23) [56950369, 9060, 16098, 938, 51576, 71567]
904|Q05940(27) [5770, 3822, 22297, 6018, 101616, 1615]
905|Q13936(32) [4485, 2520, 39186, 4499, 60663, 60753]
906|P40763(375) [400769, 131411, 5284513, 16659841, 2750, 129869]
907|P42261(21) [2910, 2196, 4843, 4118151, 127894, 126569]
908|P41594(29) [9926832, 15585158, 162834, 44557636, 5042, 129228]
909|Q9Y243(51) [43860, 25227436, 176167, 148177, 24788740, 6918736]
910|Q16850(7) [5335, 441383, 43233, 2812, 1349907, 5510]
911|P10276(88) [444795, 449171, 108143, 5289501, 5381, 60164]
912|Q9HC97(6) [54676038, 2391, 3440, 2471, 5722, 3845]
913|P49286(23) [10220503, 10305301, 896, 115348, 82148, 208902]
914|P20648(40) [3883, 4594, 9578005, 4679, 9568614, 5029]
915|Q12791(84) [2733, 216327, 5757, 214350, 5413, 37393]
916|Q92736(57) [888, 2519, 6914273, 4914, 5361, 5957]
917|O15496(47) [53323583, 53319614, 51346870, 25166397, 10067704, 155815]
918|P14902(73) [3505109, 69590, 405012, 6305, 11979, 11122]
919|P42336(403) [16654980, 3973, 49784945, 10427712, 51001932, 50905713]
920|Q99816(31) [903966, 2016, 13791, 10168, 4343310, 3108]
921|P00326(77) [1048, 77022, 13017, 3406, 11815987, 17429]
922|P15559(164) [68238, 89105, 2361, 394347, 54676038, 5813717]
923|P50281(151) [42601552, 44383797, 448002, 24768528, 119031, 9933197]
924|P00519(120) [24826799, 5291, 10302451, 5328940, 644241, 3062316]
925|P10827(44) [9863447, 5819, 5803, 8730, 5920, 9862248]
926|P21817(70) [6914273, 5361, 2519, 5957, 4914, 888]
927|Q15842(17) [4201, 3488, 32778, 3033825, 5505, 443423]
928|Q8TDV5(12) [5283468, 4671, 27902, 5311093, 11691484, 56971]
929|P36544(24) [46196517, 9930121, 25147644, 60854, 4032, 9794392]
930|P03951(23) [11304895, 183797, 6852140, 204102, 6852141, 6857702]
931|Q9UNI1(7) [446501, 10324367, 24820112, 4634717, 444650, 46228924]
932|O15552(9) [1032, 24857286, 264, 176, 6590, 7991]
933|Q9NRA0(28) [219100, 44158028, 448008, 15604015, 107970, 44158029]
934|Q9Y5Y9(30) [5411, 56959, 3610, 5467, 7176, 10770]
935|O14843(0) [7991, 24857286, 1032, 176, 6590, 264]
936|Q9NS75(19) [4887, 177941, 5717, 60842, 6913104, 11508736]
937|Q9HCF6(9) [5591, 77999, 4044, 4485, 4829, 5280335]
938|Q9UBX1(10) [46937105, 24901101, 5289258, 13186895, 10324367, 46228924]
939|Q15661(14) [11840929, 3447, 37126, 657077, 4413, 159772]
940|Q14832(19) [446355, 9834591, 213056, 33032, 5042, 188803]
941|P11217(24) [446801, 124823, 1051, 657140, 445723, 445722]
942|O95259(40) [3559, 71329, 3696, 2247, 2798, 441074, 5405]
943|Q8TF76(0) [2856, 2396, 3973, 5005498, 9549303, 6419766, 447966]
944|Q86V90(0) [11967800, 66553195, 52195, 2893, 7699, 5497, 10770]
945|P56817(26) [24748050, 3699841, 24748051, 449218, 44251605, 25134249, 49837968]
946|Q9Y233(17) [11610553, 3108, 5722, 204105, 44141871, 11581936, 10239]
947|P48167(6) [1088, 656665, 4485, 12717, 32051, 31304, 10303232]
948|P51582(3) [161647, 6830, 5957, 145729, 6133, 148197, 9875516]
949|Q15788(30) [656952, 11395145, 10274777,

10286462 , 6102690 , 6102691 , 656953]
950|Q06432(0) [65866 , 2162 , 39186 , 4507 , 4485 , 3784 , 2950]
951|P00742(86) [11634458 , 10182969 , 4581 , 10280735 , 5496659 , 9875401 , 11641515]
952|P50579(25) [1069140 , 2082 , 4030 , 19910 , 3334 , 6855 , 23647763]
953|P21554(97) [104850 , 2543 , 9826744 , 6398473 , 10278470 , 16078 , 11226090]
954|Q9UBY5(26) [11568387 , 11625765 , 44394293 , 44407394 , 10051843 , 10322404 , 44407386]
955|P29371(30) [219077 , 5311424 , 44623946 , 10328936 , 104974 , 23649245 , 133090]
956|P13569(192) [1548943 , 3488 , 4497 , 5280961 , 16220172 , 3333 , 5280443]
957|Q06278(10) [43157 , 2435 , 3108 , 2179 , 3324 , 11967800 , 4055]
958|P23458(87) [44205240 , 16722836 , 25126798 , 46216796 , 25062766 , 16659841 , 46866319]
959|Q04206(155) [114829 , 16109598 , 9820526 , 127864 , 16109538 , 16109600 , 10181390]
960|Q13698(26) [39186 , 4485 , 3333 , 2520 , 153994 , 208898 , 1547484]
961|P00797(228) [24800541 , 6324659 , 44317193 , 44251605 , 44345978 , 16126898 , 5493444]
962|Q07820(124) [3503 , 24978538 , 54675783 , 722193 , 12597 , 1780 , 141870]
963|P11926(90) [445062 , 123865 , 1051 , 1055 , 3009 , 446425 , 1045]
964|Q92633(43) [10322404 , 44394293 , 44407386 , 44407394 , 11625765 , 10051843 , 11568387]
965|Q86VL8(0) [3108 , 119570 , 16362 , 3151 , 2756 , 216210 , 10531]
966|P23415(18) [31304 , 16078 , 4485 , 32051 , 656665 , 6167 , 441071]
967|Q9NYK1(95) [159603 , 12620 , 46241268 , 10309114 , 57469 , 60737 , 3652]
968|Q9HBW0(67) [62532 , 44407394 , 11625765 , 10322404 , 44394293 , 44407386 , 11568387]
969|P49841(96) [6419766 , 5005498 , 11285002 , 11313622 , 176167 , 2856 , 5326739]
970|P30874(63) [56237 , 448601 , 5311430 , 16129681 , 71349 , 2247 , 9941444]
971|P53582(2) [4030 , 2740174 , 3334 , 19910 , 1069140 , 2082 , 6855]
972|P78527(67) [16203712 , 3973 , 16204163 , 51001932 , 16204164 , 16203710 , 16204165]
973|O60755(1) [1878823 , 1993 , 187 , 108144 , 1599306 , 31729 , 1568843]
974|P35498(65) [208898 , 216327 , 4506 , 4753 , 11967800 , 5734 , 5284583]
975|P51681(256) [3002977 , 11614352 , 49871007 , 3001322 , 9574343 , 11285792 , 3009355]
976|Q9UHC3(13) [69590 , 32051 , 199 , 338 , 16231 , 4413 , 3033 , 2244]
977|Q9BYP7(2) [447966 , 5005498 , 9549303 , 3973 , 2856 , 6419766 , 11712649 , 2396]
978|O95180(11) [60663 , 1547484 , 3333 , 941361 , 2200 , 11967800 , 934 , 516892]
979|Q9H244(38) [5957 , 11273179 , 9854012 , 60606 , 6918456 , 9871419 , 5472 , 16066663]
980|Q9Y3S1(12) [6419766 , 5005498 , 3973 , 447966 , 2396 , 2856 , 9549303 , 11712649]
981|P78536(109) [11452716 , 11402671 , 24768528 , 24800541 , 42601552 , 119031 , 448002 , 23627203]
982|P48050(5) [1103 , 1045 , 888 , 444899 , 54683953 , 1102 , 5413 , 32051]
983|Q9UNQ0(171) [2950 , 119373 , 151115 , 176870 , 6063342 , 148201 , 2361 , 11790]
984|Q9UN88(9) [4506 , 2789 , 2441 , 3261 , 31304 , 104781 , 2170 , 31640]
985|P41231(38) [6133 , 145729 , 5361 , 44623946 , 161647 , 148197 , 9875516 , 5957]
986|P01375(1069) [216326 , 40632 , 6918412 , 5639 , 4413 , 3083542 , 5426 , 4740]
987|Q13822(38) [44407394 , 44394293 , 4031 , 13211563 , 11568387 , 10322404 , 11625765 , 44407386]
988|P34947(28) [5005498 , 6419766 , 11712649 , 3973 , 9549303 , 2396 , 447966 , 2856]
989|P48169(6) [3448 , 10237 , 32051 , 4266 , 3373 , 31304 , 107926 , 104781]
990|Q86TI2(12) [10376704 , 11516136 , 44513473 , 11573427 , 11493219 , 11949652 , 10932707 , 11500899]
991|P23416(2) [6167 , 31304 , 32051 , 656665 , 1088 , 441071 , 16078 , 12717]
992|O14842(11) [11005 , 445639 , 121871 , 77999 , 445580 , 5280934 , 985 , 24857286]
993|P55017(60) [6307 , 2315 , 2910 , 2343 , 3639 , 4170 , 2720 , 4870]
994|Q5T6X5(12) [750 , 5950 , 9750 , 5962 , 6322 , 5951 , 6262 , 5961]
995|O94759(21) [444899 , 784 , 5892 , 32051 , 3371 , 2812 , 4189 , 3198]
996|Q9HBX9(10) [65599 , 3324 , 1473386 , 4118928 , 35802 , 210320 , 824727 , 2844395]
997|Q6V1X1(9) [11516136 , 11500899 , 11573427 , 11949652 , 11493219 , 44513473 , 10932707 , 10376704]
998|P08473(121) [5362417 , 24800541 , 656629 , 3038505 , 443380 , 4369380 , 1234 , 42601552]
999|Q96FL8(5) [2756 , 10531 , 216210 , 4993 , 3151 , 2749 , 3108 , 16362 , 2247]
1000|O43781(2) [160355 , 3540 , 6918454 , 153999 , 5005498 , 3973 , 10172943 , 3078519 , 3542]
1001|P48039(22) [10305301 , 82148 , 44623946 , 10220503 , 208902 , 115348 , 23581869 , 10531 , 896]
1002|Q12879(37) [2130 , 68736 , 22880 , 3821 , 180081 , 888 , 750 , 6468 , 71077]
1003|P42262(21) [4843 , 127894 , 3003157 , 2196 , 10518 , 2910 , 126569 , 10036135 , 167842]
1004|P80365(66) [5060832 , 36054272 , 5289613 , 4432326 , 36054265 , 10114 , 4570352 , 11670435 , 5151632]
1005|P34995(24) [49843471 , 448457 , 5311044 , 5280363 , 5280723 , 5282411 , 5280360 , 45266502 , 5312153]
1006|P39900(115) [448002 , 24800541 , 10565532 , 119031 , 24751752 , 46937107 , 25271580 , 46937106 , 46937108]
1007|Q15118(39) [10267580 , 6918454 , 11712649 , 447966 , 10296883 , 3973 , 24748573 , 448008 , 2396]
1008|P62805(20) [24800541 , 3025986 , 5005498 , 42601552 , 4592 , 11338033 , 448008 , 160355 , 17754027]
1009|Q96RG2(2) [447966 , 3973 , 2396 , 448008 , 2856 , 6419766 , 11712649 , 9549303 , 5005498]
1010|Q13258(17) [11462174 , 448457 , 5280363 , 45270144 , 42641863 , 49843471 , 11508736 , 5280723 , 5280360]
1011|P22310(15) [17100 , 102210 , 121892 , 2913 , 4761 , 5405 , 28718 , 2725 , 11230]
1012|P18054(52) [3610 , 3503 , 4493 , 1780 , 10168 , 3698 , 107715 , 3117 , 19910]
1013|P13631(27) [3312 , 5289501 , 60164 , 9887303 , 449171 , 444795 , 108143 , 5381 , 2605]
1014|P09619(154) [5329102 , 9809715 , 25031915 , 10366136 , 151194 , 5329099 , 11485656 , 9933475 , 10074640]
1015|P09237(155) [128564 , 44302022 , 119031 , 42601552 , 10565532 , 9933197 , 466151 , 5362422 , 24800541]
1016|Q13370(24) [3698 , 3758 , 17754438 , 110635 , 5663 , 24316 , 4197 , 2753 , 2754]
1017|P21397(67) [4235 , 3675 , 68802 , 3759 , 26757 , 4380 , 10192617 , 5530 , 60824]
1018|Q9UHL4(0) [23646087 , 11516136 , 44513473 , 11573427 , 44387758 , 11500899 , 10096344 , 23646100 , 11493219]
1019|P43250(9) [5005498 , 447966 , 2856 , 9549303 , 6419766 , 3973 , 2396 , 11712649 , 448008]
1020|P00374(103) [46883536 , 21109 , 126941 , 446753 , 448810 , 104758 , 446752 , 148121 , 5583]
1021|Q12809(74) [71329 , 3114 , 2157 , 60753 , 4932 , 2247 , 3081185 , 2769 , 5405]
1022|P32297(25) [10235 , 10517 , 10176764 , 3389 , 4032 , 115237 , 1615 , 3559 , 3604]
1023|O15399(3) [71077 , 888 , 22880 , 2130 , 6468 , 3821 , 750 , 68736 , 180081]
1024|Q5TEH5(0) [24800541 , 204102 , 447733 , 152951 , 10324367 , 447732 , 42601552 , 46228924 , 11641515 , 183797]
1025|P05023(16) [8612 , 5359268 , 441207 , 3647 , 2749 , 33887 , 6437380 , 6604423 , 28620 , 2724385]
1026|P55210(47) [24800541 , 448573 , 42601552 , 2179 , 24144 , 12000240 , 10219 , 3108 , 10168 , 3503]
1027|Q4U2R8(10) [11948288 , 4911 , 3639 , 10258 , 2333 , 44814423 , 181976 , 148200 , 123979 , 1175]
1028|P43088(19) [5282226 , 5311100 , 9868491 , 5312153 , 5311221 , 5280360 , 5311027 , 11508736 , 448457 , 5280363]
1029|P09960(31) [24768560 , 44129621 , 1082702 , 7023019 , 22690393 , 2776332 , 44129624 , 44129620 , 15547703 , 22692237]
1030|P42574(291) [24800541 , 12000240 , 42601552 , 44395211 , 54675783 , 207112 , 447400 , 46937133 , 44395477 , 46937089]
1031|P43116(55) [5282381 , 5280363 , 25114442 , 11508736 , 18376177 , 5280723 , 5280360 , 9890801 , 49843471 , 448457]
1032|P43119(16) [11508736 , 45270144 , 5282415 , 5311044 , 5311243 , 6918140 , 5282381 , 11462174 , 5280723 , 10501053]
1033|Q96RJ0(2) [1614 , 36303 , 2366 , 1615 , 4581 , 5610 , 5826 , 1001 , 32893 , 2200]
1034|P43681(50) [5310966 , 9824145 , 5310967 , 10131048 , 170361 , 5850 , 3604 , 4032 , 25147644 , 23576]
1035|P30559(24) [5311010 , 9895468 , 644077 , 11634973 , 53330936 , 11340891 , 172997 , 439302 , 60943 , 14257660]
1036|Q9H228(4) [44394248 , 44394116 , 44394169 , 44394220 , 44344193 , 44394117 , 44394149 , 107970 , 44394161 , 44394247]
1037|P78508(37) [3478 , 1989 , 4201 , 5503 , 4543 , 32778 , 91610 , 121891 , 9565 , 2727]
1038|Q9HC16(23) [1552036 , 3244425 , 1811924 , 3781338 , 2082 , 4343310 , 68684 , 12449 , 151506 , 21109]
1039|P47989(60) [1349907 , 5288320 , 1046 , 446425 , 134018 , 65457 , 2094 , 675 , 43157 , 11979]
1040|P31639(18) [11988953 , 10453870 , 9871420 , 44814423 , 9824918 , 5278 , 9887712 , 25195624 , 11949646 , 24812758]
1041|Q9HBH1(1) [5583 , 213043 , 5578 , 159596 , 24466 , 6178111 , 4064 , 148121 , 4993 , 9571037]
1042|P21453(30) [44394248 , 44394116 , 327045 , 44394117 , 44394161 , 44344193 , 107970 , 44394169 , 44394220 , 44394247 , 44394149]
1043|P30518(37) [216237 , 9895468 , 5311010 , 439302 , 644076 , 644077 , 3038506 , 60943 , 119369 , 172997 , 151171]
1044|P21731(34) [123879 , 6918030 , 54343 , 5362391 , 9938840 , 5311100 , 5312138 , 6449876 , 2449 , 5280363 , 5280360]
1045|P07437(24) [5978 , 9854073 , 2082 , 13342 , 36314 , 4030 , 148124 , 6445540 , 40839 , 6167 , 11354606]
1046|O60341(43) [46868080 , 46868074 , 46868078 , 46867800 , 46867937 , 5530 , 46867935 , 46867802 , 46867943 , 46868082 , 46867941]
1047|P00750(161) [204102 , 152951 , 183797 , 6540268 , 42601552 , 11641515 , 564 , 24800541 , 1507 , 445843 , 4474224]
1048|Q9P0X4(2) [8280 , 3291 , 9883933 , 5576 , 11967800 , 2520 , 1547484 , 60663 , 5486971 , 16362 , 6476]
1049|Q494W8(3) [16005981 , 46196517 , 10176607 , 10518 , 3003157 , 101616 , 5475 , 24795080 , 187 , 10888091 , 11151363]
1050|P61925(0) [16122633 , 16122635 , 11175137 , 11314340 , 11608401 , 3540 , 10172943 , 3542 , 12412578 , 11840906 , 16122634]
1051|Q13490(51) [44567560 , 44567555 , 24939290 , 24737642 , 44567563 , 44567572 , 46940575 , 49836020 , 44567564 , 44567571 , 44567568]

1052|Q13621(60) [4121 , 4849 , 3440 , 41781 , 2732 , 2315 , 3278 , 4873 , 5560 , 2471 , 3647]
1053|P37288(9) [72081 , 9895468 , 216237 , 439302 , 3038506 , 60943 , 5311010 , 644077 , 151171 , 119369 , 644076]
1054|P27169(224) [12279383 , 102914 , 11559 , 18303 , 44578434 , 86736 , 559675 , 44578433 , 86852 , 14936438 , 257369 , 13204]
1055|P35236(4) [3647 , 10212 , 16654690 , 16654689 , 16654688 , 13001 , 16217011 , 3246767 , 1973720 , 10168 , 1780 , 16654691]
1056|Q96PF2(3) [76098 , 16122633 , 11608401 , 6419766 , 448008 , 2856 , 11712649 , 2396 , 9549303 , 447966 , 3973 , 5005498]
1057|O15244(33) [199 , 21138 , 3151 , 4342 , 123600 , 216210 , 44814423 , 10531 , 3108 , 16231 , 155774 , 16362]
1058|P11388(82) [2179 , 5362259 , 36462 , 2950 , 3885 , 9865515 , 115150 , 4212 , 72116 , 10180 , 108143 , 31703]
1059|P14555(104) [1372 , 51346870 , 53323583 , 10954847 , 11063341 , 10067704 , 53319614 , 3711 , 25166397 , 3710 , 155815 , 446400]
1060|Q99500(11) [107970 , 44394247 , 44394116 , 44394169 , 44394117 , 44361291 , 44394220 , 44394149 , 44394161 , 44344193 , 2727678 , 44394248]
1061|P33527(140) [148201 , 2396 , 444455 , 2333 , 11967809 , 1715 , 5342 , 13806 , 3037617 , 8820 , 11790 , 31200]
1062|Q9Y5Y4(23) [11508736 , 448457 , 45270144 , 5280363 , 42641863 , 11292191 , 3715 , 49843471 , 11462174 , 123879 , 5280360 , 44158492]
1063|Q9HBY8(1) [6419766 , 447966 , 2396 , 11608401 , 9549303 , 11712649 , 16122633 , 448008 , 76098 , 5005498 , 3973 , 2856]
1064|P13866(18) [44560296 , 25195624 , 44560297 , 24812758 , 44814423 , 9887712 , 11949646 , 44560294 , 9824918 , 11988953 , 44560302 , 44560286]
1065|P30536(74) [33746 , 6433109 , 31640 , 3033621 , 3261 , 11967800 , 204105 , 2717 , 2811 , 37632 , 3380 , 3117]
1066|P09874(197) [63306 , 657038 , 1511 , 23725625 , 25070031 , 936 , 9796068 , 148140 , 44819241 , 9925908 , 44403396 , 9931954]
1067|P04626(334) [208908 , 10437018 , 11511120 , 9915743 , 10184653 , 9874913 , 6444692 , 11349170 , 10458325 , 11488320 , 11620908 , 6918508 , 153241]
1068|P04054(103) [5311052 , 3599 , 71415 , 6714002 , 131505 , 2090 , 5311067 , 237 , 10133 , 84088 , 155815 , 129148 , 7329]
1069|P00915(18) [5284627 , 216468 , 5355 , 2732 , 5734 , 5284549 , 1986 , 3295 , 4107 , 68844 , 4100 , 370 , 3038]
1070|Q92831(41) [25066642 , 53258426 , 56663055 , 56683417 , 53258425 , 53258302 , 3581192 , 56666522 , 44448303 , 65064 , 56669931 , 56676753 , 56663053]
1071|P03372(392) [3606 , 154257 , 448537 , 5991 , 104741 , 5035 , 2733526 , 5756 , 5870 , 5757 , 216416 , 2800 , 5284643]
1072|Q13224(33) [3821 , 71077 , 52919 , 180081 , 219101 , 3559 , 68736 , 888 , 6468 , 156328 , 22880 , 750 , 2130]
1073|O95977(4) [44394169 , 44394247 , 44344210 , 107970 , 44394149 , 44394248 , 44394117 , 44394161 , 327045 , 44394220 , 44344193 , 44344194 , 44344404]
1074|O43570(23) [5734 , 216468 , 68844 , 5355 , 2732 , 1986 , 5284549 , 3295 , 5284627 , 4100 , 119607 , 3038 , 2662]
1075|P08185(29) [3033993 , 5755 , 5875 , 443980 , 4506 , 6918155 , 31307 , 6215 , 5311412 , 9642 , 15209 , 5311000 , 5311167]
1076|P47901(7) [60943 , 644077 , 5311010 , 9895468 , 10298385 , 14257660 , 119369 , 644076 , 53330936 , 10034060 , 11340891 , 439302 , 11634973]
1077|P10632(57) [11967800 , 17754438 , 148201 , 16362 , 2247 , 21109 , 3151 , 3698 , 59823 , 170364 , 16363 , 208908 , 4506]
1078|P22460(27) [216327 , 4932 , 1727 , 104826 , 3356 , 39186 , 2474 , 9571004 , 5413 , 4485 , 441074 , 2798 , 208898]
1079|Q08499(60) [154575 , 166553 , 3025803 , 11561674 , 9896267 , 5092 , 151170 , 5722 , 5723 , 17754438 , 449193 , 3758 , 3182 , 3671]
1080|P22894(90) [94413 , 128564 , 151506 , 69521 , 54671203 , 12473 , 1066 , 42601552 , 53317936 , 9933197 , 24800541 , 73761 , 119031 , 1269845]
1081|P43115(43) [11508736 , 5312153 , 49843471 , 5282381 , 5280363 , 5280360 , 5311100 , 3559 , 1615 , 5311044 , 6918140 , 115237 , 2159 , 3389]
1082|P18507(27) [37632 , 4506 , 4999 , 3033621 , 2441 , 2811 , 4890 , 3261 , 31640 , 31304 , 2170 , 2789 , 104781 , 3369]
1083|P20248(71) [4564 , 6852201 , 4565 , 160355 , 4566 , 447656 , 447655 , 1540 , 10224714 , 447961 , 9601217 , 449087 , 5289411 , 447649]
1084|Q02083(13) [74288 , 575358 , 1355 , 44398718 , 46229793 , 46229839 , 46229841 , 46230476 , 20514378 , 46229840 , 46229792 , 46229791 , 46229794 , 46229746]
1085|P30556(235) [60919 , 172198 , 5281037 , 130881 , 132706 , 3749 , 2541 , 3082475 , 60846 , 3961 , 65999 , 9825285 , 158781 , 60921]
1086|A8MPY1(1) [4890 , 4506 , 104781 , 37632 , 31304 , 4999 , 2811 , 4266 , 31640 , 3369 , 2441 , 3261 , 3448 , 3033621]
1087|O95749(7) [4395717 , 53319062 , 44452371 , 447277 , 5276507 , 25023860 , 53321690 , 25023863 , 5276503 , 447278 , 16122553 , 24832031 , 5276520 , 130956]
1088|P47870(7) [2811 , 5281077 , 2441 , 31640 , 3369 , 4506 , 2170 , 31304 , 4890 , 2789 , 37632 , 3261 , 3033621 , 104781]
1089|Q02127(24) [15433 , 4064 , 54684141 , 3899 , 15942657 , 1543 , 159866 , 54723327 , 10239 , 54727975 , 54727972 , 4112111 , 51347395 , 54727985]
1090|O00748(29) [79690 , 138508 , 13005 , 62539 , 10902085 , 3321360 , 176445 , 10879668 , 146089 , 26257 , 237515 , 44455840 , 11747 , 76915]
1091|Q9UKV0(98) [419176 , 6445533 , 6918638 , 9804992 , 4261 , 11538455 , 5352062 , 6918837 , 24756910 , 10313 , 5311 , 10309899 , 88129 , 53340666]
1092|P11940(18) [659036 , 2866904 , 327044 , 327045 , 3082 , 3132640 , 288875 , 752652 , 5392 , 11061 , 24892221 , 547914 , 1595804 , 2327]
1093|O00591(7) [3369 , 3033621 , 2811 , 37632 , 2789 , 104781 , 31304 , 4999 , 4890 , 4506 , 3261 , 2441 , 31640 , 2170]
1094|Q99928(4) [3033621 , 4506 , 104781 , 31640 , 4999 , 2441 , 2811 , 2170 , 31304 , 2789 , 4890 , 37632 , 3369 , 3261]
1095|Q8WUI4(14) [10313 , 88129 , 6918837 , 53340666 , 11538455 , 5352062 , 9804992 , 6918638 , 4261 , 10309899 , 419176 , 2746 , 6445533 , 9865515 , 24756910]
1096|P78334(6) [37632 , 2811 , 104781 , 3369 , 4890 , 2441 , 3033621 , 3261 , 2170 , 2789 , 4999 , 4506 , 33746 , 31304 , 31640]
1097|Q8N1C3(1) [2789 , 3261 , 4506 , 2170 , 104781 , 3033621 , 4999 , 2811 , 4890 , 31304 , 37632 , 33746 , 3369 , 31640 , 2441]
1098|O95136(25) [44394117 , 44394247 , 44344194 , 44394220 , 1720828 , 44344404 , 44394169 , 44344210 , 44394161 , 44394248 , 44344193 , 44394149 , 107970 , 44394116 , 1568843]
1099|P28476(5) [3033621 , 4890 , 31640 , 3261 , 4999 , 4266 , 3369 , 130021 , 2441 , 104781 , 4506 , 2811 , 37632 , 31304 , 3448]
1100|P24046(1) [3448 , 37632 , 130021 , 31304 , 31640 , 104781 , 2811 , 4506 , 4999 , 3033621 , 3369 , 4266 , 4890 , 3261 , 2441]
1101|P08754(7) [11532642 , 11696933 , 11553599 , 11595656 , 11561507 , 11675664 , 11661302 , 11641511 , 11660784 , 11690308 , 11625733 , 11641883 , 11674801 , 11689506 , 11532035]
1102|Q9UQL6(19) [88129 , 2746 , 4996 , 24756910 , 9865515 , 419176 , 11538455 , 9804992 , 5311 , 6918638 , 10313 , 53340666 , 6445533 , 5352062 , 10309899]
1103|O00418(12) [3078519 , 3542 , 3973 , 5005498 , 6918454 , 10172943 , 11712649 , 447966 , 9549303 , 160355 , 2856 , 3540 , 6419766 , 2396 , 153999]
1104|P34972(66) [115237 , 10624 , 568235 , 16078 , 11695365 , 119828 , 11515193 , 44274794 , 10253143 , 20514378 , 44406743 , 42617987 , 4218308 , 104850 , 1548942]
1105|P05771(50) [16122633 , 76098 , 11608401 , 153999 , 176167 , 448008 , 6918670 , 2856 , 6419766 , 2396 , 447966 , 3973 , 11712649 , 9549303 , 5005498 , 11442891]
1106|P15121(87) [16058629 , 16058630 , 53359 , 1613 , 153948 , 5724 , 10114 , 25210476 , 11292191 , 4369325 , 337359 , 1944 , 157839 , 160024 , 1549120 , 448658]
1107|P37231(357) [170364 , 644213 , 400010 , 5591 , 5280961 , 400769 , 3033 , 447458 , 154000 , 2750 , 4829 , 5329099 , 4075 , 77999 , 204109 , 3715]
1108|Q13315(279) [806859 , 13791 , 76915 , 3435 , 660051 , 2392140 , 1580955 , 2122 , 3973 , 53708 , 141870 , 307963 , 1599306 , 4342 , 20544 , 3108]
1109|O14764(21) [31304 , 3369 , 3261 , 4890 , 3033621 , 2441 , 33746 , 4999 , 37632 , 3448 , 2170 , 104781 , 2789 , 2811 , 31640 , 4506]
1110|Q14432(14) [19987169 , 2754 , 3033825 , 3973 , 53708 , 3671 , 24316 , 16960 , 2182 , 5663 , 204105 , 4197 , 449193 , 17754438 , 2753 , 3698]
1111|P08235(89) [31378 , 5839 , 5311505 , 11876263 , 5754 , 3034004 , 5994 , 5833 , 3333 , 68873 , 5743 , 443872 , 4497 , 16734800 , 5755 , 10133]
1112|P30968(45) [16130938 , 16137348 , 49800011 , 36523 , 3038517 , 11250647 , 25077993 , 10348973 , 657181 , 50225 , 25077405 , 16136245 , 16131215 , 25074887 , 25074470 , 5311128]
1113|P25774(35) [11695261 , 46228924 , 10152654 , 9547943 , 13186895 , 5288616 , 10201696 , 24901101 , 10324367 , 5288259 , 11514361 , 14060550 , 46937176 , 11651881 , 24800541 , 11464526]
1114|Q13547(78) [9804992 , 6918837 , 5222465 , 9865515 , 11538455 , 5311 , 53340666 , 5352062 , 4775 , 3121 , 2746 , 6445533 , 6918638 , 4261 , 264 , 4996 , 11609955]
1115|P05129(28) [5005498 , 176167 , 2856 , 6419766 , 11712649 , 16122633 , 2396 , 6918670 , 448008 , 76098 , 9549303 , 447966 , 11314340 , 25227436 , 11608401 , 153999 , 3973]
1116|P14324(13) [4674 , 23730246 , 57637 , 23730244 , 5245 , 1195 , 23730364 , 23730248 , 68740 , 60852 , 448400 , 1023 , 130956 , 2088 , 44452371 , 23730136 , 15230201]
1117|Q14191(83) [612424 , 24816706 , 7475369 , 10168 , 2016 , 13752 , 16467159 , 1973720 , 22430877 , 4680274 , 1568843 , 7329 , 2090 , 2743305 , 16347 , 12449 , 3746037]
1118|Q15822(3) [10235 , 3604 , 115237 , 1615 , 1057 , 441290 , 2968 , 3389 , 24244 , 39765 , 2366 , 4032 , 21233 , 50192 , 3559 , 5831 , 5281042]
1119|P27815(33) [154575 , 204105 , 1676 , 3108 , 19987169 , 9827968 , 110635 , 5722 , 1712095 , 4197 , 5092 , 3671 , 151170 , 3182 , 16960 , 9896267 , 449193 , 2754]
1120|P20813(194) [16362 , 148201 , 11332763 , 2361 , 11229234 , 12229396 , 59823 , 2355 , 448632 , 154104 , 182137 , 51049968 , 16363 , 2247 , 11790 , 4506 , 3151 , 1349907]
1121|O75469(183) [1684 , 176870 , 2812 , 104741 , 4763 , 3401 , 16734800 , 5757 , 3333 , 55245 , 4485 , 10133 , 441298 ,

446313 , 36314 , 56950369 , 10229498 , 53232]
1122|P35408(65) [3389 , 9890801 , 5311044 , 3559 , 5280360 , 2159 , 1615 , 11677589 , 49843471 , 5280723 , 9803828 , 6918140 , 115237 , 5282381 , 5282411 , 5280363 , 448457 , 11508736]
1123|Q9Y5N1(13) [44418490 , 3077 , 16119086 , 2366 , 2913 , 24771368 , 11697697 , 9948102 , 44418482 , 6450823 , 25070031 , 16049886 , 9976892 , 24745335 , 774 , 16119082 , 3389 , 41376 , 17747460]
1124|Q16644(3) [3542 , 6419766 , 3078519 , 5005498 , 2856 , 448008 , 76098 , 11608401 , 11712649 , 9549303 , 10172943 , 153999 , 6918454 , 3540 , 160355 , 447966 , 2396 , 16122633 , 3973]
1125|Q9Y2D0(0) [72139 , 36811 , 462919 , 6307 , 216468 , 5287541 , 76509 , 11117301 , 2732 , 12066940 , 3295 , 14611919 , 19772348 , 389641 , 5356 , 169682 , 11967800 , 16122590 , 12066941]
1126|P30542(32) [11270783 , 21874557 , 5311037 , 158795 , 10117987 , 11561692 , 9860294 , 3758 , 3035850 , 9576912 , 2519 , 216466 , 219024 , 6439091 , 64627 , 9953065 , 123683 , 60961 , 2153]
1127|Q14524(140) [3180 , 4935 , 3025 , 3356 , 3114 , 56339 , 4060 , 7699 , 3292 , 38945 , 441074 , 52195 , 4178 , 34633 , 4913 , 4906 , 48041 , 3676 , 10770]
1128|P10275(333) [6010 , 13765 , 3397 , 9880 , 9904 , 4493 , 224004 , 251636 , 2375 , 5995 , 261000 , 6013 , 10635 , 55245 , 15951529 , 6446 , 9824562 , 5878 , 6011]
1129|Q13639(24) [3052762 , 53354764 , 9805719 , 6918314 , 216236 , 71451950 , 3052778 , 2769 , 11430856 , 3388 , 11961293 , 9860294 , 5362436 , 177336 , 656665 , 154104 , 68867 , 108182 , 119584]
1130|P06401(132) [104741 , 6279 , 16734800 , 130904 , 9270 , 6917715 , 55245 , 5994 , 5311505 , 9577221 , 13109 , 36709 , 4369524 , 6230 , 11683 , 40973 , 6540478 , 9051 , 13559281]
1131|P38398(209) [4404908 , 1432578 , 1720828 , 2090 , 17113 , 24817194 , 3108 , 3240818 , 3746037 , 19646 , 1878823 , 680935 , 265580 , 1568843 , 2291046 , 2914644 , 5005498 , 5198 , 65758 , 24792593]
1132|O75762(42) [16590 , 3026 , 6989 , 16315 , 49381 , 11715 , 12228 , 6005 , 24823 , 5469318 , 3117 , 65036 , 16666 , 21782 , 11617 , 177 , 7847 , 880 , 89594 , 16078]
1133|P08912(1) [174174 , 444031 , 6646 , 4848 , 2381 , 24199 , 9577995 , 9571002 , 3494 , 71183 , 5910 , 441071 , 4926 , 2160 , 4167 , 60809 , 187 , 107867 , 2551 , 442021]
1134|Q05513(35) [3540 , 2856 , 2396 , 9549303 , 176167 , 11712649 , 10172943 , 11608401 , 16122633 , 6918454 , 76098 , 6419766 , 447966 , 160355 , 3973 , 153999 , 3542 , 5005498 , 444899 , 3078519]
1135|P35218(14) [36811 , 216468 , 19772348 , 5287541 , 11117301 , 72139 , 6852128 , 389641 , 12066941 , 3295 , 12066940 , 16122590 , 76509 , 462919 , 169682 , 2732 , 6307 , 5356 , 10112 , 11967800 , 14611919]
1136|Q92887(109) [47318 , 5074 , 3478 , 158781 , 4122 , 176870 , 21138 , 16231 , 11286230 , 2247 , 2333 , 2812 , 119373 , 3108 , 3639 , 5405 , 3559 , 119259 , 3333 , 31729 , 10133]
1137|P29274(49) [11270783 , 123683 , 60961 , 11561692 , 65710 , 9576912 , 64627 , 3035850 , 10680 , 158795 , 5311037 , 6439091 , 208820 , 2153 , 219024 , 10117987 , 216466 , 2519 , 855908 , 9860294 , 21874557]
1138|O15245(59) [2179 , 155774 , 175540 , 1349907 , 3478 , 3559 , 2265 , 3108 , 3639 , 5405 , 4342 , 3333 , 16231 , 119259 , 183797 , 199 , 1549093 , 21138 , 2812 , 2576 , 123600]
1139|Q92769(69) [3994 , 2466 , 49855250 , 88129 , 53340666 , 24756910 , 10313 , 9804992 , 6918837 , 4261 , 5352062 , 11538455 , 264 , 6445533 , 9865515 , 6918638 , 10309899 , 419176 , 2746 , 5311 , 4996]
1140|P23141(32) [185195 , 2893 , 79690 , 76915 , 62539 , 176445 , 10013998 , 26257 , 237515 , 11493344 , 138508 , 10902085 , 4912 , 13005 , 39042 , 3321360 , 146089 , 11747 , 182197 , 44455840 , 10879668]
1141|P00533(966) [10184653 , 6445562 , 176870 , 22024915 , 124437 , 6918508 , 71496458 , 6918403 , 5329099 , 153241 , 11511120 , 10437018 , 4510 , 3081361 , 123631 , 11349170 , 6444692 , 11488320 , 9915743 , 208908 , 10458325]
1142|P34913(50) [47379736 , 11053022 , 44235174 , 3001386 , 49782570 , 6420120 , 4359 , 104741 , 53323158 , 25073288 , 49782569 , 44234911 , 6420121 , 25070135 , 53320344 , 11167602 , 44235634 , 4357 , 44234913 , 43608139 , 4358 , 11160856]
1143|O00141(74) [3540 , 5326739 , 448008 , 3078519 , 5005498 , 447966 , 3542 , 10172943 , 1694 , 2856 , 10267580 , 3973 , 9549303 , 2396 , 6419766 , 160355 , 16122633 , 11608401 , 6918454 , 153999 , 76098 , 11712649]
1144|Q8IUX4(6) [3108 , 327045 , 2832737 , 3003803 , 3377088 , 3244341 , 42725 , 6472026 , 72139 , 67686 , 3442589 , 4343310 , 16269005 , 32681 , 100472 , 6301 , 166553 , 16347 , 1937568 , 18573524 , 19910 , 2220273]
1145|Q8NER1(103) [104826 , 2998 , 1548943 , 1548942 , 65036 , 2913 , 42617987 , 16007367 , 11256560 , 24752296 , 3245451 , 3559 , 20514378 , 21138 , 588415 , 4628 , 638024 , 5311093 , 9910486 , 2170 , 2435 , 1719873]
1146|P18031(66) [449162 , 17759780 , 1757 , 445784 , 114829 , 47318 , 17758920 , 444764 , 9547959 , 10305301 , 447994 , 1854 , 447695 , 2194 , 1628 , 447450 , 25111933 , 9547919 , 6914659 , 10114 , 1829 , 9547958 , 5327154]
1147|P23280(6) [1057 , 6852128 , 12066941 , 216468 , 14611919 , 19772348 , 5356 , 3295 , 16129778 , 3161908 , 2732 , 169682 , 72139 , 16122590 , 11967800 , 389641 , 36811 , 10112 , 5287541 , 11117301 , 76509 , 6307 , 12066940]
1148|O00167(11) [3156995 , 44602029 , 3238160 , 2775706 , 307963 , 2090 , 1985 , 1745499 , 701332 , 6469502 , 4031 , 263177 , 1392 , 13791 , 2490338 , 3236502 , 1614257 , 3108 , 10212 , 1552036 , 3237439 , 327045 , 824727]
1149|P56524(49) [11844893 , 9865515 , 23634895 , 11538455 , 6445533 , 11844892 , 10309899 , 10313 , 419176 , 4261 , 24756910 , 2746 , 11844891 , 6918638 , 23634892 , 23634893 , 9804992 , 23634894 , 53340666 , 5352062 , 88129 , 6918837 , 23634770]
1150|P23219(140) [3825 , 54677470 , 5280581 , 4781 , 4614 , 1983 , 5161 , 5359 , 4075 , 6335412 , 156391 , 60726 , 3033 , 3342 , 4495 , 54676228 , 4044 , 3394 , 338 , 2244 , 3672 , 3826 , 4037]
1151|O15379(56) [2466 , 10313 , 49855250 , 264 , 3994 , 5352062 , 6918638 , 5311 , 2746 , 24756910 , 6445533 , 9804992 , 208908 , 4261 , 419176 , 11609955 , 53340666 , 4996 , 10309899 , 11538455 , 88129 , 9865515 , 6918837]
1152|Q99685(15) [20449950 , 2359 , 5043631 , 70261 , 45484105 , 139950 , 13072144 , 12704 , 4362 , 7347 , 65389 , 44550866 , 4526314 , 12351263 , 44274794 , 13258570 , 25057 , 3117 , 44560662 , 3572 , 512831 , 606562 , 44560663]
1153|Q9H3N8(20) [3559 , 115237 , 25070031 , 2159 , 11697697 , 3389 , 119828 , 1547484 , 10624 , 17747460 , 2170 , 41376 , 24745335 , 3077 , 16106 , 2725 , 2247 , 2818 , 2913 , 774 , 4761 , 119570 , 9976892]
1154|Q5JVE8(0) [10182969 , 216210 , 183797 , 10250490 , 9549258 , 446345 , 204102 , 11634458 , 11641515 , 447362 , 6540267 , 447359 , 10343728 , 6540268 , 42628060 , 104625 , 446346 , 24800541 , 152951 , 10095865 , 42601552 , 9549257 , 24794406]
1155|Q16445(9) [10518 , 2170 , 2441 , 31304 , 104781 , 3261 , 10133 , 10531 , 3448 , 4064 , 107926 , 31640 , 3003157 , 10237 , 2789 , 65914 , 4506 , 4266 , 3380 , 3373 , 2893 , 2576 , 32051]
1156|P12821(491) [91270 , 107807 , 5464343 , 5484727 , 5463984 , 5362124 , 5462501 , 5311447 , 42601552 , 5388962 , 56330 , 107994 , 44093 , 5464344 , 5362119 , 92400 , 72022 , 5464097 , 3033702 , 5464096 , 32681 , 5362129 , 55891 , 6604423]
1157|P09917(156) [3052 , 3600 , 4992 , 71398 , 60490 , 124087 , 54675783 , 1066 , 60923 , 71751 , 12473 , 6439232 , 69521 , 10368812 , 133021 , 3610 , 94413 , 151506 , 3086671 , 73761 , 1269845 , 53317936 , 56237 , 11508736]
1158|P10145(524) [81530 , 2265 , 15250 , 3118 , 11604 , 7798 , 11167 , 25644 , 16231 , 2950 , 28803 , 8196 , 1057 , 15286 , 123600 , 11293 , 61247 , 10168 , 19996 , 14242 , 11852 , 3672772 , 6540 , 10868]
1159|Q02880(22) [2179 , 5379 , 42890 , 124093 , 4421 , 9952884 , 4212 , 3948 , 62959 , 152946 , 41867 , 10180 , 149096 , 2764 , 60464 , 3229 , 4583 , 4539 , 9571107 , 31703 , 287180 , 2762 , 3357 , 51081]
1160|P08253(384) [5362422 , 94413 , 1269845 , 119031 , 53317936 , 69521 , 151506 , 466151 , 16108938 , 128564 , 6918336 , 24768528 , 24800541 , 10039403 , 60937 , 73761 , 42601552 , 3342298 , 10610500 , 448002 , 10492779 , 12473 , 1066 , 9933197]
1161|O94956(9) [6324616 , 119373 , 3404 , 130881 , 3333 , 5311236 , 2333 , 176870 , 46181428 , 5405 , 2812 , 3433 , 3463 , 1017 , 3117 , 2247 , 3478 , 21138 , 3488 , 5335 , 3108 , 175540 , 11967809 , 11286230 , 119259]
1162|P08913(32) [5702063 , 4893 , 5707 , 5268 , 439260 , 2726 , 443951 , 3519 , 5504 , 5816 , 2803 , 2216 , 8969 , 47811 , 213046 , 2435 , 28864 , 5775 , 4636 , 5311068 , 4850 , 54746 , 31101 , 4205 , 6005]
1163|P30939(2) [21138 , 4440 , 5078 , 8969 , 1150 , 5002 , 197706 , 5073 , 8226 , 10531 , 3389 , 4106 , 77993 , 8223 , 28693 , 182137 , 2818 , 60149 , 23897 , 11610526 , 60857 , 4585 , 60809 , 5358 , 3559]
1164|P47898(4) [1615 , 8223 , 44623946 , 8969 , 3389 , 9966051 , 115237 , 119570 , 2818 , 11954293 , 9860294 , 10624 , 3822 , 11430856 , 5074 , 4106 , 28693 , 11961293 , 5358 , 197706 , 10100 , 2159 , 3559 , 71768094 , 1355]
1165|P18825(19) [838 , 213046 , 219050 , 31101 , 4636 , 5707 , 443951 , 4205 , 6005 , 439260 , 2216 , 5268 , 2435 , 28864 , 54746 , 5775 , 3519 , 2803 , 4850 , 5702063 , 5504 , 4893 , 47811 , 8969 , 2726 , 5311068]
1166|P18089(68) [4636 , 5311068 , 4893 , 28864 , 2726 , 4205 , 3519 , 8969 , 4740 , 31101 , 838 , 5702063 , 5775 , 4768 , 5504 , 219050 , 439260 , 54746 , 2803 , 2435 , 5707 , 5736 , 47811 , 5268 , 443951 , 6005]
1167|P06276(73) [10879668 , 1933 , 15083623 , 1547484 , 77991 , 10902085 , 54766 , 10198924 , 26257 , 2131 , 62539 , 5983 , 1935 , 5936 , 5420 , 11747 , 79690 , 138508 , 13005 , 3108 , 446980 , 237515 , 3321360 , 20689 , 15192 , 76915]
1168|P29275(30) [6439091 , 9953065 , 219024 , 2893 , 10117987 , 11561692 , 21874557 , 3035850 , 158795 , 5311037 , 16071896 , 10531 , 123683 , 1676 , 216466 , 2519 , 9860294 , 16960 , 19987169 , 9576912 , 11270783 , 1188 , 7 , 1892 , 2153 , 60961]
1169|P27487(117) [5494422 , 6918537 , 24800541 , 23646100 , 4369359 , 11426348 , 42608447 , 10932707 , 205131 , 10198228 , 11243969 , 2734054 , 10376704 , 23646087 , 9887755 , 46209133 , 11516136 , 11450633 , 11659120 , 11949652 , 25022354 , 44513473 , 5459374 , 11572962 , 44387758 , 15991577 , 10096344]
1170|Q9NPD5(42) [3117 , 3404 , 158781 , 176870 , 5212 , 3463 , 3478 , 175540 , 2333 , 2812 , 119259 , 5284373 , 24988881 , 5335 , 3108 , 46181428 , 14982 , 2247 , 5405 , 11967809 , 3333 , 130881 , 3433 , 119373 , 21138 , 11286230 , 6324616]

1171|P22748(20) [2343,3295,6852128,5356,36811,72139,389641,5284627,169682,12066941,11117301,12066940,5287541,2315,4100,6307,10112,1003,11967800,3038,16122590,19772348,76509,2732,3647,1986,14611919,3639]
1172|Q8TDS4(23) [53320057,24954204,53325309,53325627,16098,24955289,938,53324022,51576,53326893,15605500,53321367,637542,53326575,56950369,24955288,53317449,10931,53318740,53326616,53324024,53325308,5310993,53318768,53321351,24955642,53318741,25025505]
1173|Q9Y6L6(62) [3333,3433,11286230,24988881,2812,3463,54687,46181428,11967809,3478,5212,5405,158781,3117,175540,119259,2333,6324616,21138,130881,5335,3108,5284373,14982,2247,176870,3404,119373]
1174|P29475(164) [10198539,347590,11149707,10261068,123895,15689,24894151,19049152,9797857,1649,447029,19049087,15552206,22617750,19049121,3311,12778906,107984,447030,1893,18721726,132862,10221335,44396192,1433,18721725,18721724,18721729]
1175|P43235(77) [5288867,6918602,44391415,24901101,44398651,5289428,44398660,46228924,10062713,10152654,44398689,44398780,5288988,10062714,44398665,11514361,5288259,11464526,44398659,14060550,13186895,44391459,5288616,11651881,44398650,10201696,10324367,11695261,44398688]
1176|P35228(332) [18721729,11149707,15552206,24894151,2146,123895,18721726,10104379,107984,19049121,1649,22617750,1433,44322997,19049152,15689,107782,44396192,10198539,18721724,5754,12778906,18721725,9797857,657073,132862,10261068,19049087,10221335]
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1178|O95747(1) [10427712,176870,10127622,11427553,10113978,11314340,11712649,3025986,208908,16722836,176167,153999,11667893,11656518,6918454,11485656,17755052,11213558,24889392,151194,11338033,156414,10074640,11234052,11409972,3038522,11364421,24779724,447077,15983966]
1179|P46063(19) [327045,2750,5282060,15945601,3746037,31236,3243567,2540,1781,669633,2768975,5289501,107738,3238778,1973720,948382,11852,1057,2396,1780,2179,51040,2333,2758,10168,3698,54675783,3503,3885,1694]
1180|Q92772(5) [11656518,11213558,11667893,208908,11712649,3038522,176167,447077,11338033,3025986,6918454,176870,11409972,17755052,11314340,10127622,11234052,11427553,10113978,156414,11485656,151194,24779724,10427712,16722836,153999,11364421,10074640,24889392,15983966]
1181|Q13523(9) [15983966,176167,11364421,11213558,11338033,156414,176870,16722836,151194,11234052,3038522,153999,11656518,447077,208908,10427712,6918454,11667893,11409972,17755052,11314340,11712649,24889392,11427553,11485656,10074640,10127622,10113978,3025986,24779724]
1182|Q9BQI3(15) [11234052,24779724,10113978,3025986,176870,15983966,156414,447077,10127622,11314340,10427712,11485656,6918454,11656518,11213558,11409972,17755052,151194,11667893,11338033,208908,16722836,11364421,24889392,11427553,3038522,153999,10074640,176167,11712649]
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1184|Q8TDR2(0) [11213558,447077,11656518,10113978,11427553,11409972,153999,11364421,17755052,11314340,11712649,16722836,3025986,151194,24889392,156414,10127622,11338033,176167,24779724,11667893,176870,10074640,11485656,10427712,15983966,208908,6918454,11234052,3038522]
1185|Q15208(10) [3025986,11409972,447077,11485656,10074640,11338033,15983966,153999,11364421,151194,208908,11427553,11656518,11667893,10427712,10127622,17755052,11712649,176870,3038522,11314340,16722836,10113978,24779724,11213558,6918454,156414,176167,24889392,11234052]
1186|O75385(15) [3038522,11485656,15983966,6918454,10074640,16722836,3025986,11234052,153999,151194,10127622,24779724,447077,17755052,11667893,11656518,176167,11338033,11427553,208908,11364421,10113978,11314340,11409972,11712649,176870,11213558,24889392,10427712,156414]
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1189|P32298(13) [208908,10127622,3025986,11314340,11485656,11213558,11409972,15983966,176870,10113978,447077,11427553,151194,11364421,24889392,3038522,11338033,153999,11667893,10074640,11234052,176167,11712649,16722836,24779724,10427712,6918454,17755052,11656518,156414]
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1196|O60331(4) [24779724,10113978,10427712,11667893,3038522,11656518,11234052,11314340,153999,3025986,151194,10074640,11213558,17755052,11485656,15983966,16722836,24889392,6918454,208908,11409972,11712649,11427553,11338033,176167,156414,447077,176167,10074640,24779724,24889392,3025986,6918454,151194,17755052,208908]
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1216|O75460(39) [10113978, 10074640, 3038522, 11213558, 15983966, 11314340, 16722836, 176870, 10127622, 6918454, 153999, 11712649, 151194, 208908, 24779724, 11427553, 11409972, 447077, 3025986, 156414, 11338033, 11485656, 10427712, 11667893, 176167, 24889392, 17755052, 11656518, 11234052, 11364421]
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1236|P11308(75) [16231,70464,5918,6307,3969,31729,2327,119259,10621,4578,10168,114811,2831167,3474,658365,50248,2179,5335,2794,2016,2082,5593,2482,2307977,327044,5510,19646,2815581,13752,2132993,166553]
1237|Q9UQ88(6) [11667893,11364421,151194,16722836,17755052,10127622,11427553,11213558,11485656,11338033,208908,11409972,10074640,153999,24779724,156414,11656518,11314340,10427712,6918454,11712649,10113978,3025986,160355,11234052,176870,176167,447077,3038522,15983966,24889392]
1238|Q8IY84(3) [11712649,156414,11485656,11667893,15983966,10127622,11409972,11364421,11213558,24889392,10074640,176167,176870,151194,10113978,208908,11427553,17755052,11656518,447077,11314340,6918454,10427712,11338033,24779724,3025986,153999,16722836,11442891,11234052,3038522]
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1255|P31152(2) [11338033,10113978,208908,160355,151194,10074640,10127622,11234052,11427553,17755052,11485656,24889392,3038522,11712649,11213558,176870,156414,16722836,15983966,176167,11409972,11656518,24779724,11364421,10427712,11667893,11314340,6918454,153999,447077,3025986]
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1269|Q9H093(4) [24889392, 156414, 447077, 10074640, 11234052, 11364421, 3025986, 11656518, 11712649, 16722836, 151194, 11314340, 17755052, 10127622, 11667893, 208908, 153999, 176870, 15983966, 160355, 3038522, 11213558, 6918454, 11427553, 10113978, 11338033, 24779724, 11409972, 11485656, 10427712, 176167]
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1295|O75716(2) [447077,153999,11667893,11427553,11712649,160355,24889392,10113978,3025986,11409972,17755052,151194,10427712,11314340,10127622,208908,11485656,11364421,10074640,11234052,176870,11338033,11213558,24779724,16722836,3038522,156414,15983966,176167,447966,6918454,11656518]
1296|Q04771(41) [208908,11213558,3025986,10427712,11364421,176870,10127622,24779724,15983966,11427553,24889392,10074640,11234052,156414,11338033,17755052,151194,3038522,11409972,160355,447966,11485656,153999,10113978,11656518,11712649,11667893,176167,6918454,16722836,11314340,447077]
1297|Q9UBN7(59) [9804992,6918638,50908800,88129,52949685,10309899,5311,24756910,419176,2466,5352062,11844892,11844893,4261,52947269,11609955,52947250,53340666,52948832,52950031,6445533,11538455,11844891,10313,208908,6918837,4996,9865515,3994,2746,49855250,23640756]
1298|Q9NY57(4) [24779724,176870,11314340,24889392,11338033,3025986,11213558,15983966,208908,10427712,6918454,11656518,10127622,17755052,156414,11234052,16722836,11712649,153999,11667893,151194,176167,3038522,10113978,447077,10074640,11409972,447966,11427553,11485656,11364421,160355]
1299|Q9UF33(5) [447966,176167,11712649,10427712,10074640,151194,447077,11213558,11338033,11409972,15983966,6918454,11667893,3038522,10127622,17755052,3025986,11485656,10113978,11364421,11427553,176870,11314340,208908,156414,24889392]
1300|P36894(50) [6918454,10113978,24779724,10427712,11712649,10074640,208908,153999,11234052,24889392,160355,11427553,11364421,11667893,3025986,11338033,10127622,176167,11213558,156414,17755052,11409972,16722836,11656518,447077,11485656,3038522,11314340,447966,176870,15983966,151194]
1301|Q9P2K8(17) [11338033,447077,153999,447966,10127622,10074640,176167,11409972,15983966,151194,11234052,11656518,160355,11364421,3025986,24779724,156414,17755052,11667893,3038522,176870,16722836,10113978,11712649,11213558,10427712,208908,11427553,11485656,11314340,24889392,6918454]
1302|Q9UKE5(10) [11712649,11213558,447966,11234052,176167,10113978,11667893,11656518,15983966,3025986,10427712,16722836,11338033,11314340,10074640,24779724,11427553,208908,447077,17755052,11364421,10127622,160355,6918454,24889392,11409972,151194,3038522,11485656,153999,176870,156414]
1303|Q13237(6) [10074640,10127622,11667893,17755052,3038522,15983966,176167,153999,16722836,11427553,24779724,11314340,208908,151194,11656518,11364421,11409972,11712649,176870,10113978,448008,156414,160355,3025986,11485656,24889392,11338033,11234052,447077,10427712,11213558,6918454]
1304|O15118(82) [10219,1720828,2197,107985,5074,14369,1608140,17113,1552036,4380,5405,5289501,42725,65758,2161,1599306,4122,1580955,166553,1878823,3503,24817194,10206,162834,41684,3240818,3455,1568843,19910,19646,1238,680935]
1305|Q13233(47) [11213558,16666708,10074640,10127622,17755052,11667893,176167,16722836,3038522,153999,11427553,24779724,10172827,11314340,11656518,151194,11364421,11234052,176870,11409972,11712649,156414,10113978,447077,24889392,11338033,15983966,3025986,11485656,208908,10427712,6918454]
1306|Q99640(6) [153999,15983966,447077,11234052,10127622,6918454,156414,10074640,24779724,447966,16722836,3038522,176167,11712649,10427712,10113978,151194,17755052,11409972,11656518,160355,3025986,11338033,176870,11427553,208908,11364421,11213558,11667893,11485656,24889392,11314340]
1307|P53671(13) [15983966,17755052,447077,176167,11314340,447966,11667893,11712649,11338033,6918454,10074640,11234052,208908,156414,24779724,10127622,11213558,10427712,16722836,3038522,24889392,176870,11364421,153999,11485656,11409972,3025986,10113978,151194,11656518,160355,11427553]
1308|Q13131(72) [11656518,16722836,6918454,176167,11338033,11667893,447966,11409972,151194,176870,17755052,11213558,11314340,11234052,447077,11364421,10427712,15983966,10113978,24779724,208908,160355,11712649,10074640,11485656,153999,10127622,11427553,3038522,448008,24889392,156414,3025986]
1309|P21918(10) [47811,3389,68950,3372,1615,59227,107930,681,1547484,11154555,5265,16,31101,42601552,2818,1355,6005,115237,3822,3559,37459,119828,10624,18104,5281881,2726,2159,9860294,28864,5452,54746,12454,119570]
1310|P50613(22) [24889392,24779724,11364421,153999,208908,11712649,176870,156414,11338033,160355,16722836,11409972,3025986,11213558,15983966,11656518,6918454,11667893,10113978,11427553,11314340,11285002,17755052,11485656,3038522,6918852,11234052,176167,447077,10427712,10127622,151194,10074640]
1311|P29376(5) [447077,11314340,176870,11712649,15983966,153999,11427553,151194,16722836,11656518,6918454,156414,11485656,3038522,208908,11409972,3025986,176167,10074640,11667893,10427712,24889392,17755052,447966,11234052,11364421,24779724,10127622,10113978,448008,11213558,160355,11338033]
1312|Q96L34(6) [447077,11234052,447966,153999,24889392,6918454,11409972,10074640,208908,151194,16722836,3025986,176167,17755052,11656518,160355,24779724,10113978,11712649,11364421,11314340,156414,11485656,3038522,176870,10427712,448008,11427553,11213558,11338033,11667893,15983966,10127622]
1313|O00444(29) [3038522,11213558,24889392,176167,11667893,10127622,11610113,10427712,156414,153999,11485656,16722836,11656518,11234052,24779724,160355,11364421,10113978,176870,10074640,11409972,11314340,3025986,151194,11338033,15983966,447077,447966,11427553,11712649,208908,17755052,6918454]
1314|P49759(2) [24779724,208908,11364421,11667893,176167,11234052,11409972,16722836,11338033,3025986,6918454,17755052,4564,10427712,447966,11656518,10127622,447077,11485656,153999,11213558,160355,156414,11712649,3038522,10113978,11314340,11427553,24889392,151194,10074640,176870,15983966]
1315|Q8TD19(1) [156414,447077,160355,176167,11234052,17755052,11667893,10113978,11409972,176870,153999,3038522,24889392,16722836,11712649,11427553,11338033,15983966,11656518,6918454,11485656,24779724,447966,11213558,208908,151194,11314340,10074640,10127622,3025986,448008,11364421,10427712]
1316|Q9H0K1(10) [448008,24889392,11314340,3038522,11427553,17755052,156414,151194,11656518,24779724,6918454,11234052,10127622,176167,11213558,11712649,447077,10113978,16722836,10074640,160355,15983966,176870,10427712,208908,11409972,11364421,447966,3025986,11485656,11338033,11667893,153999]
1317|Q9ULX7(8) [3295,69809,6852128,5287541,20184392,389641,216468,76509,4100,44424363,11117301,14611919,169682,44424366,11967800,44424364,15729847,5356,19772348,25258361,2732,68844,72139,96876,25258363,5284549,12066941,6307,12066940,25258360,16122590,36811,1986]
1318|Q9P289(6) [24889392,11234052,11485656,3025986,156414,160355,153999,151194,15983966,10074640,11667893,11409972,208908,11656518,10427712,11364421,16722836,10127622,3038522,176167,17755052,176870,448008,24779724,10113978,11712649,11314340,6918454,11338033,11213558,447966,447077,11427553]
1319|Q13470(2) [11338033,11485656,11427553,3025986,11667893,447966,16722836,11314340,11656518,11364421,11234052,10113978,151194,208908,160355,3038522,176167,11213558,447077,11712649,24779724,10127622,6918454,10074640,11409972,24889392,17755052,10427712,448008,153999,156414,176870,15983966]
1320|P33981(32) [208908,11213558,11485656,11364421,11667893,15983966,11234052,176167,160355,10127622,11409972,447966,10074640,156414,153999,6918454,11712649,11314340,3025986,10113978,17755052,151194,11338033,11656518,10427712,448008,176870,16722836,24889392,3038522,24779724,11427553,447077]
1321|Q00526(6) [153999,176167,447077,176870,151194,11712649,11364421,24779724,11427553,24889392,10113978,11667893,10127622,16722836,3025986,11285002,11314340,6918454,160355,11234052,11656518,11213558,15983966,156414,10427712,208908,17755052,11485656,3038522,11338033,11409972,10074640,448008]
1322|Q16816(0) [10127622,11213558,448008,11427553,16722836,176870,153999,3025986,11485656,6918454,151194,11656518,11712649,208908,10113978,17755052,176167,3038522,11409972,447966,11338033,24889392,24779724,11234052,10427712,447077,160355,15983966,156414,11364421,10074640,11314340,11667893]
1323|Q16584(23) [11667893,11409972,447077,16722836,156414,10074640,176870,11314340,42642645,11485656,11656518,176167,6918454,11338033,11213558,151194,11427553,

153999 , 3038522 , 447966 , 17755052 , 10127622 , 24889392 , 208908 , 15983966 , 11712649 , 24779724 , 10113978 , 11234052 , 10427712 , 160355 , 11364421 , 3025986]
1324|P28566(4) [10531 , 119828 , 28693 , 8226 , 197706 , 4440 , 8969 , 115237 , 4585 , 2818 , 3559 , 4106 , 5358 , 60854 , 1355 , 77993 , 5073 , 2159 , 3396 , 5736 , 182137 , 3389 , 5078 , 5002 , 10624 , 1150 , 443884 , 8223 , 60809 , 119570 , 60149 , 1615 , 60857]
1325|P54646(68) [208908 , 10113978 , 448008 , 15983966 , 11485656 , 3025986 , 11213558 , 10074640 , 16722836 , 24779724 , 151194 , 156414 , 11314340 , 11667893 , 11656518 , 17755052 , 11364421 , 153999 , 10427712 , 447077 , 3038522 , 176870 , 160355 , 11338033 , 24889392 , 176167 , 11712649 , 11427553 , 447966 , 11234052 , 11409972 , 10127622 , 6918454]
1326|Q14164(21) [447077 , 11234052 , 10127622 , 11485656 , 11667893 , 11442891 , 208908 , 24779724 , 153999 , 10074640 , 11712649 , 11314340 , 448008 , 3038522 , 11409972 , 11552706 , 176870 , 6918454 , 11656518 , 16722836 , 176167 , 11338033 , 24889392 , 151194 , 3025986 , 17755052 , 10427712 , 10113978 , 11427553 , 15983966 , 156414 , 160355 , 11213558 , 11364421]
1327|O60733(129) [45482339 , 45482338 , 45482342 , 44562726 , 45482340 , 45482337 , 45482343 , 44241583 , 44346482 , 11360688 , 45482332 , 44562673 , 44563072 , 16118459 , 9906670 , 44563042 , 44329617 , 44330207 , 16118461 , 16118318 , 16118320 , 44563074 , 4670 , 44563043 , 16118319 , 25166397 , 44562672 , 45482333 , 45482334 , 44562729 , 44563075 , 45482335 , 45482341 , 44563073]
1328|P50750(39) [11427553 , 17755052 , 3025986 , 6918454 , 10113978 , 10427712 , 11656518 , 151194 , 11285002 , 3038522 , 153999 , 24779724 , 11485656 , 11712649 , 15983966 , 11314340 , 11234052 , 11667893 , 11409972 , 16722836 , 24889392 , 11364421 , 46926350 , 208908 , 447077 , 176167 , 5330286 , 156414 , 10074640 , 160355 , 176870 , 11338033 , 10127622 , 11213558]
1329|P31644(6) [3003157 , 10518 , 107926 , 4506 , 4064 , 4266 , 4912 , 65914 , 2441 , 4999 , 10531 , 10133 , 31304 , 3380 , 37632 , 32051 , 2789 , 3373 , 3033621 , 2893 , 4890 , 2811 , 5556 , 216456 , 10237 , 2118 , 2170 , 3448 , 9908684 , 104781 , 31640 , 3261 , 2576 , 3369]
1330|P29597(62) [11409972 , 11314340 , 176167 , 11712649 , 6918454 , 46866319 , 15983966 , 11213558 , 11427553 , 11656518 , 176870 , 448008 , 3038522 , 151194 , 153999 , 16722836 , 10127622 , 3025986 , 10427712 , 17755052 , 10074640 , 447077 , 160355 , 208908 , 11667893 , 11485656 , 447966 , 11234052 , 156414 , 24889392 , 11364421 , 11338033 , 24779724 , 10113978]
1331|Q13153(80) [16722836 , 11314340 , 11485656 , 3025986 , 11712649 , 153999 , 24779724 , 11234052 , 25227462 , 15983966 , 6918454 , 208908 , 448008 , 176167 , 160355 , 176870 , 151194 , 447966 , 11656518 , 11338033 , 10427712 , 11667893 , 11427553 , 10113978 , 10127622 , 447077 , 10074640 , 3038522 , 11364421 , 11213558 , 156414 , 24889392 , 17755052 , 11409972]
1332|Q9Y468(12) [3156743 , 3242481 , 1973720 , 4396341 , 282398 , 2384580 , 1815815 , 32681 , 719632 , 1066 , 2348 , 2812 , 246835 , 3261980 , 16129778 , 54676538 , 645503 , 3842656 , 3245728 , 1580955 , 893703 , 3236936 , 68089 , 44201975 , 246831 , 4814 , 680935 , 2732927 , 1870615 , 659036 , 18573526 , 820311 , 661085 , 290012]
1333|P68400(29) [15983966 , 16722836 , 17755052 , 156414 , 11364421 , 24889392 , 10113978 , 176167 , 24779724 , 160355 , 10074640 , 447077 , 3025986 , 11409972 , 448008 , 10127622 , 11213558 , 11338033 , 11427553 , 447966 , 11234052 , 10427712 , 208908 , 11656518 , 6918454 , 11712649 , 11485656 , 153999 , 3038522 , 11314340 , 1694 , 151194 , 176870 , 11667893 , 24748573]
1334|P08254(270) [1269845 , 16108938 , 44302165 , 151506 , 44302430 , 10492779 , 4369141 , 44305706 , 128564 , 1066 , 24800541 , 44302432 , 132519 , 10039403 , 10474389 , 119031 , 44270901 , 3342298 , 12473 , 53317936 , 44302167 , 17754156 , 448002 , 9933197 , 44329644 , 24178109 , 15485452 , 94413 , 73761 , 69521 , 44333947 , 10610500 , 1948 , 42601552 , 10073353]
1335|Q07869(168) [2315 , 154000 , 16103190 , 3463 , 11236126 , 204109 , 11395145 , 2750 , 16103189 , 16103197 , 10467 , 9890879 , 16103192 , 170364 , 16734800 , 10274777 , 5694 , 39042 , 2763 , 11149906 , 3339 , 3503 , 206044 , 11711595 , 114924 , 447458 , 5289501 , 15797 , 10229498 , 9909438 , 4829 , 11483970 , 3034285 , 2796 , 6603901]
1336|O94806(3) [10427712 , 11409972 , 11667893 , 11234052 , 160355 , 153999 , 76098 , 10113978 , 24779724 , 11364421 , 15983966 , 10127622 , 156414 , 16722836 , 208908 , 24889392 , 16122633 , 11213558 , 17755052 , 11314340 , 11608401 , 11485656 , 11338033 , 151194 , 11427553 , 447077 , 3025986 , 11712649 , 11656518 , 176167 , 6918454 , 176870 , 10074640 , 448008 , 3038522]
1337|P08172(17) [3696 , 2381 , 2229 , 441071 , 2160 , 71183 , 4848 , 11519070 , 187 , 11434515 , 10938 , 442021 , 15376 , 71203 , 2230 , 30843 , 107867 , 4629 , 3450 , 444031 , 3494 , 6172 , 2784 , 174174 , 4634 , 60809 , 154059 , 4934 , 443879 , 2370 , 44259 , 3042 , 24199 , 5910 , 2551]
1338|P35462(32) [57267 , 54746 , 4917 , 6918314 , 219050 , 5095 , 37459 , 5355 , 4926 , 5073 , 688272 , 6005 , 54562 , 31101 , 47811 , 4850 , 2726 , 60149 , 28864 , 11697676 , 3559 , 16362 , 443951 , 119570 , 5736 , 3964 , 3033769 , 5281881 , 5265 , 681 , 59227 , 2818 , 115368 , 3151 , 57242 , 4452]
1339|P27338(30) [21910 , 3052776 , 71164 , 71627 , 4380 , 68555 , 5576 , 4688 , 26757 , 5530 , 3435 , 11967800 , 2134 , 71307 , 15433 , 5494443 , 4235 , 5289613 , 3759 , 4064 , 3748 , 21558 , 3675 , 68804 , 46937129 , 29142 , 2750 , 4362 , 11616886 , 12717 , 23659732 , 131682 , 233979 , 16750123 , 16739244 , 10192617]
1340|P28222(30) [5736 , 5073 , 2818 , 219050 , 443951 , 4106 , 9966051 , 4440 , 5358 , 77993 , 60149 , 5074 , 77992 , 54746 , 8969 , 3388 , 28693 , 71351 , 197706 , 123606 , 60795 , 4830 , 9805719 , 10531 , 60854 , 60809 , 66004 , 1150 , 47811 , 5078 , 28864 , 4636 , 60857 , 3822 , 4585 , 31101]
1341|P29474(359) [10221335 , 24894151 , 1433 , 10103242 , 1649 , 39836 , 19049087 , 15552206 , 22617750 , 44516953 , 1894 , 12778906 , 181426 , 18721726 , 9793827 , 132862 , 44396192 , 47938 , 44313550 , 449633 , 19049152 , 9797857 , 18721724 , 18721725 , 10198539 , 19049121 , 347590 , 11149707 , 10261068 , 44313313 , 107984 , 123895 , 15689 , 18721729 , 44322997 , 10104379]
1342|Q9NYY3(28) [15983966 , 9549303 , 6918454 , 153999 , 11427553 , 10113978 , 11409972 , 11485656 , 3025986 , 447077 , 10427712 , 2856 , 11712649 , 11213558 , 3973 , 3038522 , 151194 , 10127622 , 11656518 , 2396 , 6419766 , 24779724 , 11667893 , 156414 , 176870 , 24889392 , 447966 , 11364421 , 11234052 , 11314340 , 208908 , 11338033 , 5005498 , 16722836 , 176167 , 17755052 , 10074640]
1343|P43166(3) [20184392 , 5284549 , 19772348 , 16122590 , 10112 , 3295 , 44424363 , 12066941 , 11117301 , 25258361 , 6852128 , 216468 , 11967800 , 96876 , 5734 , 12066940 , 36811 , 5356 , 15729847 , 68844 , 76509 , 2732 , 25258363 , 5355 , 6307 , 1986 , 5287541 , 5284627 , 69809 , 169682 , 389641 , 4100 , 25258360 , 72139 , 44424364 , 14611919 , 44424366]
1344|O14733(130) [3973 , 11338033 , 3038522 , 447966 , 11656518 , 11234052 , 11364421 , 17755052 , 10127622 , 151194 , 16722836 , 11213558 , 156414 , 6419766 , 9549303 , 10113978 , 176870 , 447077 , 153999 , 11314340 , 15983966 , 24889392 , 11485656 , 3025986 , 11667893 , 5005498 , 2396 , 208908 , 6918454 , 11712649 , 176167 , 10074640 , 24779724 , 2856 , 11427553 , 10427712 , 11409972]
1345|P11229(12) [5749 , 187 , 3494 , 44259 , 4634 , 2784 , 3290 , 2370 , 11434515 , 2230 , 71183 , 442021 , 154059 , 5910 , 2911 , 9577995 , 15376 , 10938 , 60809 , 4848 , 11519070 , 3042 , 2818 , 107867 , 2551 , 4629 , 9862248 , 2229 , 5572 , 444031 , 174174 , 2160 , 2381 , 9571002 , 71203 , 441071 , 4934]
1346|Q86Y07(4) [11213558 , 11485656 , 10427712 , 208908 , 153999 , 24779724 , 11409972 , 24889392 , 3025986 , 11234052 , 10113978 , 11314340 , 11338033 , 11667893 , 11656518 , 176870 , 11427553 , 11364421 , 6419766 , 17755052 , 15983966 , 16722836 , 447966 , 2396 , 3038522 , 5005498 , 176167 , 156414 , 151194 , 10074640 , 3973 , 11712649 , 2856 , 9549303 , 10127622 , 6918454 , 447077]
1347|Q9Y253(26) [3676681 , 1973720 , 2435 , 11852 , 265341 , 4593 , 54676538 , 10621 , 722121 , 2768975 , 5289501 , 10168 , 1967 , 2016 , 265580 , 5282176 , 54675783 , 3746037 , 3698 , 1870753 , 21138 , 316274 , 2090 , 5198 , 2179 , 701332 , 1369 , 3151041 , 70464 , 8209243 , 3885 , 1870615 , 327044 , 265436 , 5405 , 299996 , 31475]
1348|P51617(57) [447077 , 3038522 , 11338033 , 3025986 , 10074640 , 11314340 , 24779724 , 11364421 , 11409972 , 2856 , 151194 , 2396 , 10113978 , 5005498 , 16722836 , 24889392 , 11667893 , 11213558 , 176167 , 11234052 , 10127622 , 156414 , 15983966 , 9549303 , 17755052 , 208908 , 153999 , 11656518 , 10427712 , 6918454 , 6419766 , 11427553 , 3973 , 11485656 , 447966 , 176870 , 11712649]
1349|Q7L7X3(3) [11656518 , 3038522 , 153999 , 24889392 , 11364421 , 447077 , 151194 , 10074640 , 24779724 , 11485656 , 11409972 , 10113978 , 17755052 , 176167 , 6419766 , 208908 , 9549303 , 3973 , 6918454 , 11712649 , 11213558 , 447966 , 11427553 , 176870 , 11234052 , 3025986 , 16722836 , 10427712 , 2856 , 11314340 , 11667893 , 10127622 , 15983966 , 156414 , 2396 , 5005498 , 11338033]
1350|Q6PHR2(5) [176167 , 15983966 , 11427553 , 6918454 , 10427712 , 11213558 , 156414 , 24779724 , 16722836 , 11656518 , 24889392 , 11667893 , 10127622 , 2396 , 153999 , 5005498 , 447077 , 151194 , 11314340 , 11338033 , 11712649 , 10113978 , 11364421 , 447966 , 11485656 , 17755052 , 2856 , 11234052 , 10074640 , 11409972 , 3025986 , 176870 , 208908 , 6419766 , 3973 , 3038522 , 9549303]
1351|Q8IYT8(2) [11409972 , 11712649 , 153999 , 2856 , 6419766 , 11314340 , 11427553 , 447077 , 10427712 , 11364421 , 208908 , 11667893 , 176167 , 176870 , 11234052 , 151194 , 17755052 , 11485656 , 9549303 , 11213558 , 10127622 , 3973 , 24889392 , 2396 , 156414 , 15983966 , 16722836 , 6918454 , 11338033 , 3025986 , 447966 , 5005498 , 11656518 , 24779724 , 3038522 , 10113978 , 10074640]
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1354|Q8TD08(7) [156414, 15983966, 24779724, 10172943, 176870, 11427553, 11712649, 3038522, 153999, 3078519, 24889392, 3542, 11409972, 176167, 151194, 447077, 11667893, 6918454, 10113978, 17755052, 11213558, 10074640, 11656518, 16722836, 11234052, 3973, 11314340, 11485656, 3025986, 208908, 5005498, 11338033, 10427712, 10127622, 160355, 3540, 11364421]
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1439|Q13554(7) [10074640 , 11427553 , 10427712 , 156414 , 10113978 , 153999 , 11656518 , 11409972 , 76098 , 11213558 , 176870 , 176167 , 5005498 , 2856 , 11712649 , 208908 , 24889392 , 11314340 , 11338033 , 11234052 , 24779724 , 447077 , 447966 , 16122633 , 10127622 , 11364421 , 6419766 , 6918454 , 23624249 , 11667893 , 9549303 , 3025986 , 17755052 , 15983966 , 151194 , 2396 , 16722836 , 160355 , 11608401 , 3973 , 11485656 , 3038522]
1440|Q96RI1(93) [10168 , 28803 , 10245972 , 39042 , 16362 , 11852 , 3401 , 10868 , 10229498 , 1989 , 104741 , 10026128 , 2750 , 2812 , 16181 , 7346 , 41684 , 6540 , 7329 , 37175 , 16734800 , 115157 , 21138 , 520196 , 8178 , 2391 , 62485 , 5326713 , 8041 , 447715 , 2998 , 3034285 , 3503 , 31253 , 16316 , 19996 , 5289501 , 6 , 8907 , 10133 , 3082 , 3333]
1441|Q7KZI7(112) [11338033 , 17755052 , 11712649 , 3038522 , 9549303 , 16722836 , 176167 , 2856 , 11608401 , 11667893 , 10427712 , 3025986 , 11213558 , 5005498 , 11234052 , 447966 , 208908 , 448008 , 10074640 , 10127622 , 160355 , 447077 , 11364421 , 156414 , 3973 , 15983966 , 176870 , 11485656 , 76098 , 16122633 , 6419766 , 24779724 , 153999 , 11314340 , 6918454 , 10113978 , 11427553 , 24889392 , 2396 , 11656518 , 11409972 , 151194]
1442|Q8N568(0) [6918454 , 208908 , 10127622 , 447966 , 16122633 , 16722836 , 176870 , 176167 , 76098 , 9549303 , 11712649 , 160355 , 153999 , 11314340 , 3025986 , 11409972 , 11234052 , 11485656 , 10074640 , 10427712 , 11608401 , 6419766 , 11338033 , 11427553 , 11656518 , 2396 , 11364421 , 24889392 , 448008 , 3038522 , 5005498 , 17755052 , 156414 , 447077 , 2856 , 11667893 , 10113978 , 24779724 , 3973 , 151194 , 15983966 , 11213558]
1443|Q04759(25) [3973 , 2856 , 11608401 , 17755052 , 447077 , 15983966 , 3038522 , 10074640 , 176870 , 156414 , 3025986 , 208908 , 11485656 , 11314340 , 76098 , 447966 , 11712649 , 11234052 , 11338033 , 11364421 , 11656518 , 160355 , 11427553 , 24779724 , 24889392 , 448008 , 176167 , 11213558 , 10427712 , 16722836 , 5005498 , 6419766 , 11667893 , 153999 , 2396 , 9549303 , 151194 , 16122633 , 10127622 , 11409972 , 10113978 , 6918454]
1444|Q14012(7) [2856 , 15983966 , 24779724 , 6419766 , 10172943 , 176870 , 153999 , 11234052 , 11409972 , 10074640 , 11712649 , 10427712 , 3038522 , 3078519 , 160355 , 3973 , 3542 , 11485656 , 11656518 , 5005498 , 6918454 , 176167 , 151194 , 11213558 , 11427553 , 11314340 , 9549303 , 156414 , 16722836 , 2396 , 11667893 , 208908 , 11338033 , 3025986 , 447966 , 10113978 , 17755052 , 447077 , 3540 , 24889392 , 10127622 , 11364421]
1445|P11802(160) [57379345 , 11656518 , 5330286 , 11667893 , 176167 , 6918852 , 3038522 , 16722836 , 156414 , 5289419 , 11409972 , 151194 , 46220502 , 5287969 , 6918834 , 11314340 , 448008 , 448991 , 11610113 , 176870 , 10427712 , 11485656 , 15983966 , 447077 , 3025986 , 153999 , 24779724 , 208908 , 11234052 , 11364421 , 11213558 , 11338033 , 5327686 , 24889392 , 11712649 , 10074640 , 11285002 , 10113978 , 11427553 , 6918454 , 10127622 , 17755052]
1446|Q9H2X6(32) [2396 , 153999 , 11712649 , 9549303 , 24779724 , 15983966 , 10172943 , 176870 , 6419766 , 11364421 , 156414 , 447077 , 3540 , 11338033 , 5005498 , 208908 , 3025986 , 160355 , 11485656 , 10127622 , 3973 , 447966 , 16722836 , 10427712 , 11667893 , 17755052 , 6918454 , 10074640 , 176167 , 151194 , 11314340 , 11213558 , 11656518 , 3542 , 11234052 , 2856 , 10113978 , 11409972 , 3038522 , 24889392 , 11427553 , 3078519]
1447|Q13557(8) [447966 , 176870 , 2396 , 447077 , 10427712 , 208908 , 448008 , 11712649 , 3038522 , 11314340 , 11427553 , 10074640 , 10113978 , 153999 , 11364421 , 11213558 , 3973 , 24889392 , 176167 , 11667893 , 5005498 , 15983966 , 16722836 , 151194 , 2856 , 11608401 , 160355 , 11338033 , 11234052 , 24779724 , 6419766 , 16122633 , 10127622 , 6918454 , 11409972 , 11485656 , 76098 , 9549303 , 3025986 , 11656518 , 156414 , 17755052]
1448|Q13976(65) [176167 , 11409972 , 2396 , 447966 , 17755052 , 153999 , 9549303 , 24889392 , 10127622 , 2856 , 11213558 , 208908 , 447077 , 11364421 , 11656518 , 3025986 , 10074640 , 3973 , 24779724 , 11712649 , 11427553 , 5005498 , 11338033 , 176870 , 160355 , 11667893 , 16122633 , 448008 , 11608401 , 10113978 , 15983966 , 151194 , 11234052 , 11314340 , 76098 , 156414 , 16722836 , 6918454 , 11485656 , 10427712 , 6419766 , 3038522]
1449|Q13464(52) [24889392 , 447077 , 6419766 , 6918454 , 3025986 , 10074640 , 2396 , 16722836 , 24779724 , 5005498 , 176167 , 11667893 , 153999 , 448008 , 3973 , 11409972 , 2856 , 11314340 , 3038522 , 208908 , 151194 , 10113978 , 11364421 , 11234052 , 10127622 , 11427553 , 11338033 , 11552706 , 11656518 , 448042 , 9549303 , 25227436 , 17755052 , 15983966 , 10296883 , 447966 , 11213558 , 11485656 , 11712649 , 156414 , 176870 , 10427712]
1450|Q16513(4) [10427712 , 24779724 , 447966 , 11213558 , 11314340 , 15983966 , 151194 , 11656518 , 11427553 , 6918454 , 10127622 , 208908 , 11409972 , 3078519 , 11712649 , 9549303 , 11364421 , 11667893 , 3025986 , 11485656 , 10074640 , 2856 , 153999 , 24889392 , 11338033 , 5005498 , 3542 , 447077 , 176167 , 3973 , 2396 , 16722836 , 160355 , 3038522 , 176870 , 11234052 , 10172943 , 17755052 , 3540 , 10113978 , 6419766 , 156414]
1451|Q9NWZ3(35) [16722836 , 11314340 , 3025986 , 2396 , 17755052 , 176870 , 5005498 , 208908 , 447077 , 10074640 , 15983966 , 11667893 , 11409972 , 3038522 , 6419766 , 10113978 , 11427553 , 76098 , 151194 , 24779724 , 11485656 , 10427712 , 24889392 , 11364421 , 11338033 , 11213558 , 11608401 , 448008 , 16122633 , 176167 , 447966 , 156414 , 153999 , 11234052 , 11987888 , 3973 , 11656518 , 6918454 , 10127622 , 9549303 , 11712649 , 2856]
1452|P24723(21) [16722836 , 76098 , 447966 , 10074640 , 11234052 , 5005498 , 6419766 , 2856 , 160355 , 11656518 , 15983966 , 11364421 , 447077 , 3025986 , 156414 , 11608401 , 10427712 , 11314340 , 9549303 , 24889392 , 11712649 , 11213558 , 3973 , 24779724 , 10113978 , 11338033 , 17755052 , 11667893 , 153999 , 10127622 , 176167 , 6918454 , 11427553 , 2396 , 16122633 , 11409972 , 10114 , 448008 , 208908 , 176870 , 3038522 , 11485656 , 151194]
1453|O75676(1) [16122633 , 448008 , 10074640 , 153999 , 24779724 , 10127622 , 2396 , 447077 , 10427712 , 11485656 , 9549303 , 6419766 , 15983966 , 208908 , 10113978 , 24889392 , 11427553 , 76098 , 11234052 , 3025986 , 11656518 , 25227436 , 156414 , 11712649 , 6918454 , 5005498 , 11338033 , 3973 , 3038522 , 447966 , 11667893 , 176167 , 151194 , 11213558 , 16722836 , 17755052 , 176870 , 11608401 , 2856 , 11314340 , 11409972 , 160355 , 11364421]
1454|Q14680(18) [151194 , 2396 , 24779724 , 176167 , 176870 , 3025986 , 16722836 , 11409972 , 10074640 , 447077 , 11213558 , 3542 , 11338033 , 24889392 , 11427553 , 447966 , 156414 , 10113978 , 11364421 , 6419766 , 10172943 , 5005498 , 11234052 , 11485656 , 160355 , 3078519 , 3973 , 3540 , 153999 , 11712649 , 448008 , 10127622 , 10427712 , 2856 , 11667893 , 6918454 , 15983966 , 9549303 , 11656518 , 3038522 , 208908 , 17755052 , 11314340]
1455|Q8TDX7(4) [11667893 , 11485656 , 448008 , 17755052 , 11314340 , 10427712 , 176167 ,

3038522, 156414, 11427553, 6419766, 16722836, 6918454, 160355, 2396, 153999, 11409972, 11712649, 2856, 3542, 151194, 15983966, 11656518, 24779724, 10127622, 10074640, 5005498, 3540, 208908, 3973, 11338033, 3025986, 11234052, 10172943, 9549303, 447966, 447077, 11364421, 24889392, 3078519, 11213558, 176870, 10113978]

1456|Q96SB4(22) [3025986, 17755052, 10127622, 11234052, 447966, 11667893, 208908, 24779724, 176870, 10074640, 448008, 151194, 11712649, 11314340, 16722836, 3078519, 11485656, 3038522, 3973, 11409972, 6918454, 153999, 11656518, 3542, 176167, 2396, 9549303, 10113978, 5005498, 2856, 6419766, 10172943, 156414, 11213558, 10427712, 447077, 11427553, 11338033, 24889392, 11364421, 3540, 15983966, 160355]

1457|O75604(10) [655601, 3151, 3760, 3926, 4156, 228244, 2799, 2333, 2247, 10219, 4030, 54677971, 5289501, 6307, 24144, 2170, 4343310, 10206, 2540, 5722, 2812, 12454, 2478, 3132640, 2090, 2178, 1780, 4842, 6708773, 16129778, 3108, 655083, 2453, 32681, 3474, 2318, 54677972, 13791, 19675, 5405, 16362, 54676538, 3503]

1458|Q9NQU5(10) [10113978, 11338033, 5005498, 151194, 208908, 6419766, 156414, 11213558, 176870, 2396, 11234052, 16722836, 2856, 447966, 10074640, 3078519, 6918454, 11656518, 11667893, 176167, 15983966, 3542, 10127622, 160355, 3038522, 448008, 11712649, 3973, 153999, 11485656, 3025986, 11314340, 17755052, 24889392, 9549303, 11427553, 447077, 24779724, 10427712, 3540, 11409972, 11364421, 10172943]

1459|Q92630(10) [11409972, 176870, 16722836, 17755052, 10074640, 3540, 10427712, 9549303, 5005498, 176167, 6419766, 3542, 160355, 10113978, 151194, 11314340, 11712649, 6918454, 11213558, 153999, 2856, 11667893, 24889392, 3038522, 2396, 447077, 3973, 15983966, 3078519, 448008, 10172943, 10127622, 24779724, 11234052, 156414, 11364421, 11656518, 11485656, 3025986, 11338033, 11427553, 447966, 208908]

1460|P08631(8) [9549303, 17755052, 176167, 24889392, 11608401, 11656518, 6918454, 11409972, 3973, 3038522, 2396, 151194, 16122633, 176870, 24779724, 208908, 448008, 11314340, 76098, 11712649, 10074640, 11485656, 153999, 11234052, 10113978, 447077, 11667893, 447966, 11364421, 10127622, 6419766, 15983966, 11427553, 10296883, 160355, 11213558, 3025986, 156414, 16722836, 2856, 5005498, 11338033, 10427712]

1461|P43403(55) [11667893, 17755052, 11234052, 6419766, 6918454, 2856, 2396, 11485656, 5005498, 10113978, 11656518, 10296883, 4566, 9549303, 10074640, 153999, 160355, 11314340, 11427553, 3025986, 156414, 15983966, 176870, 11338033, 11712649, 10127622, 3973, 447966, 16722836, 176167, 24889392, 151194, 208908, 11213558, 11364421, 10427712, 24779724, 448008, 11409972, 447077, 57379345, 3038522, 11442891]

1462|Q9P286(14) [208908, 11213558, 447966, 11656518, 10172943, 16722836, 10127622, 176870, 176167, 9549303, 3540, 160355, 11234052, 11712649, 153999, 11314340, 3025986, 11409972, 10427712, 11485656, 10074640, 6419766, 11338033, 2396, 11427553, 3973, 11364421, 448008, 17755052, 156414, 3038522, 447077, 3542, 5005498, 3078519, 24889392, 2856, 11667893, 10113978, 151194, 15983966, 24779724, 6918454]

1463|Q02156(45) [76098, 11427553, 16122633, 4064, 208908, 160355, 6918454, 24889392, 11314340, 11667893, 447077, 24779724, 447966, 2396, 10074640, 5005498, 9549303, 3025986, 11338033, 3973, 16722836, 2856, 153999, 11213558, 11234052, 11712649, 11364421, 6918670, 156414, 11485656, 11409972, 11656518, 15983966, 17755052, 10113978, 10427712, 11608401, 176167, 10127622, 176870, 151194, 3038522, 6419766]

1464|Q9HC98(8) [3078519, 176870, 2396, 447077, 11712649, 448008, 153999, 3973, 11314340, 3038522, 2856, 160355, 11427553, 11667893, 10113978, 24889392, 10127622, 10074640, 15983966, 10427712, 3540, 11364421, 151194, 10172943, 11213558, 447966, 176167, 3542, 11338033, 5005498, 11234052, 16722836, 6419766, 24779724, 11485656, 3025986, 6918454, 17755052, 11409972, 208908, 9549303, 11656518, 156414]

1465|P51813(17) [11712649, 3973, 2856, 11656518, 16722836, 208908, 151194, 11234052, 24889392, 5005498, 11409972, 160355, 6918454, 176870, 4708, 448008, 11338033, 11314340, 447966, 11667893, 2396, 10074640, 11608401, 3038522, 447077, 176167, 16122633, 24779724, 76098, 9549303, 11364421, 153999, 11485656, 10127622, 156414, 6419766, 3025986, 11427553, 15983966, 10113978, 10427712, 11213558, 17755052]

1466|Q9BXA7(6) [153999, 10127622, 11234052, 11656518, 11364421, 11338033, 6419766, 11485656, 3025986, 447966, 151194, 156414, 11427553, 2856, 57379345, 3973, 10074640, 10427712, 9549303, 24889392, 11608401, 10113978, 11314340, 160355, 11712649, 11213558, 176167, 6918454, 76098, 208908, 11409972, 24779724, 17755052, 176870, 11667893, 3038522, 2396, 15983966, 448008, 447077, 5005498, 16122633, 16722836]

1467|Q9H422(3) [11364421, 156414, 15983966, 3038522, 208908, 176167, 11667893, 447966, 3542, 6419766, 9549303, 11712649, 10074640, 11213558, 3540, 2856, 11427553, 24748573, 11485656, 2396, 6918454, 447077, 5005498, 11338033, 176870, 3973, 11409972, 10172943, 16722836, 3078519, 153999, 24889392, 10113978, 24779724, 10127622, 10427712, 151194, 11234052, 160355, 11314340, 17755052, 3025986, 11656518]

1468|Q86V86(19) [447077, 10172943, 11409972, 176870, 2856, 11364421, 448008, 3025986, 17755052, 10113978, 24795070, 11712649, 11338033, 2396, 9549303, 24779724, 11485656, 11213558, 6918454, 447966, 11667893, 3973, 24889392, 6419766, 11427553, 5005498, 15983966, 11314340, 156414, 10127622, 208908, 10074640, 3540, 11234052, 153999, 151194, 3038522, 10427712, 3542, 176167, 16722836, 11656518, 160355, 3078519]

1469|Q9HBH9(5) [2856, 153999, 11213558, 11667893, 208908, 447966, 17755052, 3025986, 16722836, 160355, 3542, 10113978, 11364421, 24889392, 3540, 11427553, 3038522, 448008, 3973, 10074640, 57379345, 11712649, 6419766, 176870, 10172943, 3078519, 5005498, 156414, 24779724, 11234052, 176167, 447077, 10127622, 15983966, 2396, 10427712, 11656518, 6918454, 11409972, 9549303, 11338033, 151194, 11314340, 11485656]

1470|Q9UM73(138) [176870, 24779724, 11234052, 16722836, 11338033, 151194, 11712649, 11656518, 10296883, 11364421, 10074640, 10113978, 10427712, 57379345, 208908, 156414, 6419766, 9549303, 448008, 2396, 11213558, 160355, 11409972, 11667893, 153999, 24889392, 11626560, 49806720, 11427553, 3025986, 11485656, 11751922, 6918454, 447077, 11314340, 15983966, 10127622, 2856, 17755052, 5005498, 3038522, 176167, 3973, 447966]

1471|Q05655(90) [10427712, 17755052, 447077, 11608401, 24889392, 16122633, 151194, 24779724, 10114, 2856, 11314340, 3038522, 6918670, 6419766, 208908, 11364421, 11213558, 156414, 15983966, 176167, 9549303, 11656518, 10113978, 11667893, 6918454, 76098, 447966, 11409972, 16722836, 11234052, 10074640, 10127622, 11427553, 2396, 176870, 10569483, 3025986, 160355, 11485656, 3973, 11712649, 11338033, 5005498, 153999]

1472|Q13177(22) [176167, 9549303, 76098, 160355, 153999, 3025986, 16122633, 24779724, 11213558, 15983966, 10427712, 6918454, 208908, 6419766, 447966, 11427553, 11656518, 176870, 3973, 448008, 3038522, 11712649, 11314340, 17755052, 11485656, 10074640, 11409972, 447077, 11608401, 2856, 57379345, 11338033, 11667893, 10113978, 2396, 11234052, 151194, 11364421, 10127622, 24889392, 10296883, 16722836, 5005498, 156414]

1473|P45984(47) [11656518, 176167, 11667893, 3038522, 5005498, 17755052, 11409972, 3542, 15983966, 3973, 151194, 176870, 447966, 11213558, 2856, 10296883, 3078519, 448008, 11314340, 2396, 447077, 10113978, 24779724, 11364421, 208908, 160355, 11485656, 11234052, 10172943, 6419766, 10427712, 11712649, 10074640, 11427553, 11285002, 24889392, 9549303, 10127622, 153999, 16722836, 6918454, 3540, 3025986, 156414, 11338033]

1474|Q5JY90(0) [3025986, 11485656, 16722836, 448008, 15983966, 11314340, 160355, 176167, 11409972, 3038522, 6419766, 57379345, 11427553, 10296883, 156414, 11656518, 17755052, 24779724, 6918454, 10113978, 11667893, 2396, 11712649, 10074640, 11608401, 153999, 2856, 176870, 10127622, 151194, 9549303, 16122633, 5005498, 447966, 3973, 76098, 11234052, 447077, 10427712, 24889392, 11364421, 11751922, 208908, 11213558, 11338033]

1475|P07333(93) [3025986, 11485656, 160355, 11338033, 10113978, 6419766, 11751922, 10427712, 3973, 2396, 11409972, 176167, 11314340, 24779724, 11427553, 6918454, 24767976, 151194, 17755052, 153999, 9884318, 11656518, 11712649, 176870, 16722836, 3038522, 24889392, 156414, 15983966, 5330286, 447077, 448008, 10366136, 208908, 11667893, 447966, 5005498, 11213558, 10127622, 11364421, 2856, 9933475, 11234052, 10074640, 9549303]

1476|Q9P1W9(20) [10074640, 11427553, 10113978, 160355, 10127622, 3540, 153999, 24748573, 3038522, 10427712, 6918454, 9549303, 24779724, 447966, 3078519, 10172943, 5005498, 176870, 11213558, 11656518, 16722836, 3025986, 2856, 11364421, 11338033, 11234052, 208908, 11314340, 24795070, 11712649, 151194, 3973, 447077, 448008, 11485656, 24889392, 2396, 156414, 15983966, 11667893, 11409972, 17755052, 3542, 176167, 6419766]

1477|O15530(24) [24889392, 24779724, 3025986, 11314340, 10127622, 10427712, 11213558, 11364421, 6419766, 176870, 3078519, 10074640, 448008, 447077, 11485656, 2396, 447966, 17755052, 2856, 11442891, 15983966, 11409972, 10027278, 11712649, 3540, 11656518, 11338033, 6918454, 11667893, 11234052, 9549303, 160355, 151194, 208908, 3973, 11427553, 10113978, 153999, 10172943, 156414, 5005498, 16722836, 3038522, 176167, 3542]

1478|O96013(23) [24779724, 17755052, 10172943, 25227462, 10113978, 11485656, 3078519,

10074640 , 160355 , 156414 , 6918454 , 11213558 , 11427553 , 3540 , 9549303 , 16058637 , 11712649 , 10427712 , 176167 , 11314340 , 6419766 , 3542 , 11234052 , 3973 , 208908 , 2396 , 447966 , 3025986 , 24889392 , 15983966 , 11338033 , 151194 , 447077 , 176870 , 3038522 , 2856 , 11364421 , 16722836 , 11442891 , 153999 , 11656518 , 11409972 , 5005498 , 11667893 , 10127622]
1479|Q99549(1) [4593 , 3973 , 4278 , 2179 , 1547484 , 3117 , 10382715 , 2327 , 5233 , 2170 , 3333 , 1694 , 361655 , 5405 , 101616 , 2812 , 4362 , 53708 , 2913 , 1967 , 36811 , 21138 , 3503 , 4843 , 4493 , 5227 , 5074 , 3455 , 2265 , 16362 , 114924 , 2754 , 133621 , 5289501 , 3151 , 23897 , 1045 , 2717 , 3542 , 3885 , 6603842 , 1649 , 2277 , 3311 , 20544]
1480|P07947(19) [9549303 , 11338033 , 151194 , 25066467 , 15983966 , 10302451 , 3025986 , 24889392 , 176870 , 11364421 , 11712649 , 153999 , 59174488 , 10297043 , 3973 , 10127622 , 24779724 , 5005498 , 10074640 , 11314340 , 2856 , 156414 , 11667893 , 16722836 , 6918454 , 2396 , 6419766 , 447077 , 24795070 , 24826799 , 11427553 , 160355 , 17755052 , 10113978 , 208908 , 3038522 , 11234052 , 448008 , 11485656 , 176167 , 11409972 , 10427712 , 11213558 , 447966 , 11656518 , 11442891]
1481|P51955(36) [11667893 , 176167 , 10427712 , 11485656 , 11409972 , 3540 , 2396 , 151194 , 447966 , 10172943 , 11656518 , 11338033 , 153999 , 6918454 , 160355 , 2856 , 11608401 , 11427553 , 24779724 , 24889392 , 10113978 , 11213558 , 448008 , 15983966 , 5005498 , 3542 , 3038522 , 10074640 , 11314340 , 16122633 , 6419766 , 11364421 , 17755052 , 11712649 , 3025986 , 9549303 , 76098 , 10127622 , 11234052 , 3973 , 447077 , 176870 , 16722836 , 208908 , 3078519 , 156414]
1482|P48730(20) [11364421 , 11427553 , 10113978 , 160355 , 10074640 , 11667893 , 153999 , 17755052 , 24779724 , 129236 , 6419766 , 447077 , 11314340 , 11712649 , 9549303 , 2856 , 3038522 , 3542 , 3078519 , 16722836 , 151194 , 156414 , 2396 , 11656518 , 6918454 , 5005498 , 15983966 , 10127622 , 24889392 , 447966 , 176870 , 10172943 , 11608401 , 76098 , 16122633 , 11234052 , 11338033 , 11213558 , 3025986 , 3540 , 10427712 , 11485656 , 3973 , 176167 , 208908 , 11409972]
1483|P23443(65) [3973 , 2750 , 11213558 , 6918454 , 11409972 , 9549303 , 6419766 , 11427553 , 151194 , 11314340 , 17755052 , 24779724 , 3078519 , 176870 , 10267580 , 11667893 , 3025986 , 10074640 , 11485656 , 153999 , 11364421 , 176167 , 2396 , 11712649 , 2856 , 448008 , 15983966 , 3038522 , 160355 , 208908 , 156414 , 10172943 , 10427712 , 24889392 , 11656518 , 3540 , 447966 , 10127622 , 10113978 , 11234052 , 11338033 , 1694 , 447077 , 16722836 , 5005498 , 3542]
1484|Q8IWQ3(2) [11656518 , 24889392 , 3078519 , 3540 , 10172943 , 2856 , 9549303 , 11213558 , 11667893 , 11409972 , 151194 , 11234052 , 10074640 , 3038522 , 3973 , 24779724 , 15983966 , 10427712 , 3025986 , 11485656 , 447077 , 2396 , 16122633 , 11427553 , 6419766 , 11314340 , 3542 , 10127622 , 448008 , 11712649 , 76098 , 153999 , 11608401 , 17755052 , 176870 , 160355 , 176167 , 10113978 , 208908 , 447966 , 11364421 , 156414 , 11338033 , 5005498 , 6918454 , 16722836]
1485|Q15139(47) [3540 , 176870 , 11364421 , 10172943 , 6419766 , 11234052 , 447077 , 153999 , 3025986 , 160355 , 24779724 , 76098 , 11712649 , 10074640 , 11338033 , 5005498 , 24889392 , 10113978 , 2396 , 17755052 , 208908 , 11427553 , 10127622 , 16122633 , 176167 , 6918454 , 16722836 , 3973 , 447966 , 11656518 , 11667893 , 3542 , 3038522 , 9549303 , 11314340 , 11409972 , 156414 , 11213558 , 151194 , 11485656 , 448008 , 3078519 , 2856 , 10427712 , 15983966 , 11608401]
1486|P41240(37) [1694 , 11314340 , 6419766 , 5005498 , 447077 , 9549303 , 3973 , 176870 , 10074640 , 15983966 , 156414 , 16722836 , 24889392 , 10302451 , 3078519 , 153999 , 151194 , 10427712 , 2396 , 6918454 , 3542 , 11364421 , 11656518 , 17755052 , 3025986 , 10113978 , 11409972 , 11712649 , 176167 , 3038522 , 3540 , 448008 , 160355 , 10172943 , 11234052 , 208908 , 24779724 , 447966 , 11427553 , 2856 , 10127622 , 11973736 , 11485656 , 11667893 , 11213558 , 11338033]
1487|P42684(19) [176167 , 11314340 , 644241 , 2856 , 11427553 , 10113978 , 10427712 , 11409972 , 153999 , 448008 , 11712649 , 447966 , 447077 , 3038522 , 6419766 , 5328940 , 156414 , 24779724 , 2396 , 10074640 , 15983966 , 16122633 , 160355 , 16722836 , 6918454 , 11608401 , 11364421 , 3062316 , 5005498 , 11656518 , 3025986 , 11213558 , 10127622 , 11338033 , 17755052 , 176870 , 76098 , 9549303 , 208908 , 11667893 , 24889392 , 11234052 , 5291 , 151194 , 10302451 , 11485656 , 3973]
1488|P22455(112) [3025986 , 160355 , 6918454 , 9809715 , 11656518 , 11314340 , 156414 , 17755052 , 10074640 , 10113978 , 2856 , 176870 , 53235510 , 2396 , 153999 , 447077 , 10427712 , 3973 , 51039095 , 208908 , 448008 , 3038522 , 24889392 , 11427553 , 15983966 , 11364421 , 16722836 , 151194 , 11213558 , 11667893 , 11338033 , 5005498 , 11234052 , 6419766 , 11409972 , 11485656 , 11608401 , 24826799 , 24779724 , 76098 , 9549303 , 57379345 , 16122633 , 176167 , 10127622 , 11712649 , 447966]
1489|Q13188(15) [176167 , 11213558 , 10427712 , 151194 , 11667893 , 11234052 , 2856 , 10074640 , 11485656 , 17755052 , 10113978 , 3038522 , 2396 , 11427553 , 16122633 , 5005498 , 176870 , 11364421 , 11314340 , 10172943 , 3078519 , 156414 , 11409972 , 9549303 , 3540 , 24779724 , 10127622 , 24889392 , 3973 , 76098 , 153999 , 11712649 , 448008 , 208908 , 11608401 , 15983966 , 160355 , 11338033 , 11751922 , 3025986 , 3542 , 11656518 , 6419766 , 447077 , 447966 , 6918454 , 16722836]
1490|P04049(156) [151194 , 156414 , 9549303 , 11234052 , 11364421 , 11338033 , 176167 , 11409972 , 11667893 , 10127622 , 25161177 , 24779724 , 447077 , 15983966 , 5005498 , 11608401 , 160355 , 2856 , 2396 , 11213558 , 448008 , 208908 , 3038522 , 10427712 , 153999 , 76098 , 11167602 , 11314340 , 176870 , 16122633 , 11712649 , 6419766 , 10113978 , 11656518 , 3973 , 17755052 , 11427553 , 6918454 , 447721 , 42611257 , 10074640 , 16722836 , 44462760 , 3025986 , 11485656 , 24889392 , 447966]
1491|P51812(74) [11409972 , 6419766 , 11427553 , 11314340 , 11712649 , 11667893 , 10113978 , 10427712 , 3542 , 3025986 , 11213558 , 17755052 , 11608401 , 447077 , 3973 , 3540 , 25227436 , 11234052 , 76098 , 5005498 , 160355 , 6918454 , 24889392 , 11656518 , 10127622 , 156414 , 11338033 , 15983966 , 447966 , 448008 , 2396 , 176167 , 10074640 , 3078519 , 2856 , 16722836 , 208908 , 151194 , 16122633 , 24779724 , 3038522 , 9549303 , 11364421 , 153999 , 11485656 , 10172943 , 176870]
1492|P49137(22) [11656518 , 2396 , 11314340 , 11234052 , 76098 , 153999 , 11427553 , 11338033 , 10127622 , 11712649 , 24889392 , 16122633 , 447077 , 3038522 , 10172943 , 6419766 , 16058637 , 3973 , 17755052 , 448008 , 156414 , 176870 , 10113978 , 11364421 , 3540 , 11485656 , 3542 , 11409972 , 160355 , 447966 , 208908 , 9549303 , 16722836 , 11667893 , 11213558 , 2856 , 11608401 , 3025986 , 151194 , 15983966 , 176167 , 24779724 , 10427712 , 5005498 , 10074640 , 3078519 , 6918454]
1493|P46098(19) [108000 , 11151363 , 11961293 , 2159 , 216236 , 3052778 , 5074 , 5284583 , 44623946 , 119828 , 71768094 , 115237 , 656665 , 446220 , 3510 , 119570 , 6337614 , 3033818 , 5011 , 6918107 , 888 , 9966051 , 46196517 , 1615 , 39186 , 9794392 , 21138 , 42601552 , 4168 , 187 , 65997 , 71785 , 1355 , 25070031 , 154104 , 2264 , 2170 , 6000 , 16005981 , 3559 , 4914 , 10624 , 24795080 , 4595 , 2099 , 5284566 , 3389]
1494|Q8IW41(2) [447966 , 208908 , 11314340 , 16722836 , 3542 , 1694 , 24889392 , 3973 , 11608401 , 5005498 , 24779724 , 6419766 , 76098 , 11409972 , 2396 , 151194 , 11485656 , 16122633 , 3025986 , 11667893 , 11712649 , 160355 , 10172943 , 3038522 , 176167 , 2856 , 176870 , 447077 , 17755052 , 10427712 , 448008 , 15983966 , 10113978 , 11427553 , 6918454 , 10127622 , 10074640 , 11656518 , 3540 , 11364421 , 156414 , 11338033 , 153999 , 11234052 , 3078519 , 11213558 , 9549303]
1495|Q15418(21) [24779724 , 11364421 , 10172943 , 2856 , 11485656 , 11667893 , 11409972 , 3540 , 5005498 , 176167 , 11234052 , 6419766 , 16722836 , 3542 , 11338033 , 76098 , 3025986 , 9549303 , 11213558 , 3078519 , 6918454 , 17755052 , 11608401 , 447966 , 10127622 , 11656518 , 153999 , 16122633 , 447077 , 208908 , 11712649 , 160355 , 3038522 , 10113978 , 11314340 , 2396 , 3973 , 11427553 , 10074640 , 156414 , 448008 , 1694 , 24889392 , 151194 , 176870 , 10427712 , 15983966]
1496|S4R381(0) [208908 , 447966 , 11485656 , 153999 , 11338033 , 151194 , 57379345 , 5005498 , 2856 , 176167 , 6918454 , 1633 , 6419766 , 16122633 , 10113978 , 24889392 , 447077 , 24826799 , 10074640 , 448008 , 10427712 , 16722836 , 11409972 , 447622 , 15983966 , 11364421 , 24779724 , 11712649 , 11667893 , 3025986 , 11427553 , 11656518 , 11167602 , 11234052 , 11213558 , 76098 , 11314340 , 11608401 , 3973 , 160355 , 10127622 , 2396 , 9549303 , 176870 , 156414 , 3038522 , 17755052]
1497|Q02750(136) [11712649 , 3025986 , 3973 , 10427712 , 11234052 , 447077 , 10172943 , 6419766 , 11364421 , 24889392 , 10113978 , 2856 , 447966 , 3542 , 176167 , 448008 , 3038522 , 9549303 , 176870 , 11485656 , 11409972 , 11338033 , 10074640 , 1694 , 24779724 , 151194 , 11427553 , 16722836 , 3540 , 10127622 , 11314340 , 11656518 , 208908 , 6918454 , 15983966 , 11707110 , 11213558 , 5005498 , 153999 , 2396 , 156414 , 11667893 , 160355 , 17755052 , 10172827 , 3078519 , 25227436 , 16222096]
1498|O14920(65) [11409972 , 11485656 , 3025986 , 9549303 , 153999 , 11667893 , 17755052 , 11213558 , 11656518 , 11608401 , 76098 , 6918454 , 10113978 , 5005498 , 447077 , 2856 , 11314340 , 10127622 , 6419766 , 11234052 , 24779724 , 176870 , 11338033 , 156414 , 11552706 , 10427712 , 2396 , 160355 , 448008 , 3540 , 24889392 , 208908 , 11364421 , 447966 , 3038522 , 16122633 , 151194 , 15983966 , 10172943 , 3542 , 10074640 , 11712649 , 176167 , 11442891 , 16722836 , 3078519 , 11427553 , 3973]
1499|P45983(168) [11712649 , 10172943 , 10127622 , 3078519 , 16722836 , 10427712 , 24889392 , 11656518 , 2396 , 24779724 , 11364421 , 11667893 , 10113978 , 10275001 , 11409972 , 11485656 , 160355 , 151194 , 176870 , 2856 , 16058637 , 153999 , 156414 , 6918454 , 11234052 , 11314340 , 6419766 , 10296883 , 10267580 , 11427553 , 1694 , 9549303 , 3025986 , 3540 , 11338033 , 447077 , 15983966 , 447966 , 3038522 , 5005498 , 10430360 , 176167 , 208908 , 3973 , 17755052 , 11213558 , 10074640 , 3542]
1500|P08069(215) [208908 , 153999 , 447966 , 6918454 , 72435 , 51039095 , 11656518 , 5005498 , 11485656 , 10074640 , 11213558 , 10296883 , 447077 , 57379345 , 11427553 , 10113978 , 10127622 , 11409972 , 10427712 , 448008 , 16122633 ,

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1501|Q499Y8(0) [6918454,151194,10113978,11656518,3078519,160355,11314340,447077,24779724,3038522,9549303,11338033,15983966,6419766,153999,11712649,11667893,3540,2856,5005498,176870,44224261,10172943,2396,447966,11213558,3025986,10427712,176167,11552706,16750106,208908,3973,24889392,16722836,156414,11409972,11427553,5171,10127622,3542,10074640,17755052,11234052,11485656,16129582,10296883,11364421]
1502|P31751(81) [9549303,25227436,2396,11667893,6419766,10113978,11485656,448008,11427553,11364421,11409972,176167,16122634,11213558,16122633,11234052,3973,10427712,3540,11608401,3025986,10127622,11175137,11338033,208908,10172943,447966,151194,11314340,447077,24889392,5005498,176870,156414,16722836,6918454,11656518,24779724,17755052,2856,153999,10074640,160355,11712649,3078519,15983966,3542,3038522]
1503|O15264(8) [11338033,3038522,3973,176167,10267580,151194,10172943,5005498,17755052,10113978,24779724,10427712,15983966,3540,16722836,11364421,156414,2856,11656518,11409972,16122633,11608401,3078519,160355,24889392,11234052,3025986,447966,208908,11712649,153999,10074640,448008,3542,11667893,447077,11485656,2396,76098,10127622,176870,6918454,11314340,9549303,6419766,1694,11427553,11213558]
1504|O75582(11) [25227436,24889392,151194,9549303,10127622,208908,3078519,3540,11485656,76098,17755052,11608401,11234052,176870,176167,3973,11213558,447077,11667893,11427553,11364421,11409972,3542,10427712,1694,448008,10113978,3038522,10172943,10267580,6419766,153999,24779724,11314340,2856,6918454,2396,11656518,447966,11712649,15983966,160355,11338033,10074640,5005498,3025986,16122633,16722836,156414]
1505|Q03164(107) [4343310,5381,3108,2234553,3842920,8026,50942,3246767,13986,5475,6470206,30717,2315667,2739563,24792601,12938,10718,3236558,361939,2090,19529,1561922,3295,13791,4380,3603333,722121,2179,2075,2200,4097,7475369,3377088,655916,327045,2799,11296583,22430877,547914,24817194,7191,42725,94280,24792593,14369,2832895,3117,235434,3138364]
1506|Q03181(82) [213013,3034285,10168,11236126,5289501,11483970,10467,11293,7329,10868,2950,10229498,2265,114924,6603901,21805,1046,25644,11604,8041,444795,4197,18056,115157,12589,5921,3672772,204109,9803963,3503,1123,21307,28803,16362,8095,3969,8467,2750,62485,41684,11742,11852,206044,11395145,11711595,19996,16734800,16316,39042]
1507|Q14DU5(0) [3078519,447966,447077,208908,11427553,10127622,3025986,6419766,11667893,156414,176870,10113978,11314340,1694,2396,151194,448008,3540,3542,11712649,25227436,3973,16122633,11656518,11608401,11409972,176167,11213558,9549303,24889392,15983966,11364421,10074640,57379345,2856,160355,10172943,17755052,11234052,76098,11338033,3038522,153999,24779724,11485656,6918454,10427712,5005498,16722836,10296883]
1508|P06213(138) [11314340,11712649,3025986,10113978,15983966,151194,16722836,11364421,11442891,11338033,24871491,24779724,10275001,447966,448008,156414,76098,11667893,10127622,3033769,3973,447077,10296883,6419766,57379345,11608401,176167,2396,11656518,11213558,11427553,6918454,11485656,11234052,10427712,9549303,2856,10074640,17755052,11409972,24889392,3038522,160355,5005498,176870,16137271,208908,153999,16122633,11640390]
1509|O96017(110) [24779724,11751922,3038522,208908,2396,3078519,160355,156414,6918454,11427553,11485656,24889392,9549303,11213558,10427712,76098,176167,6419766,11712649,3542,11152667,11314340,11234052,10275001,11610113,11338033,447966,3540,15983966,153999,448008,3973,151194,3025986,447077,176870,10113978,16722836,11409972,2856,16122633,11364421,11656518,10074640,5005498,10172943,17755052,11608401,11667893,10127622]
1510|Q15759(8) [22049997,9871074,447966,3025986,9549303,153999,11712649,11409972,10341154,176870,11667893,11234052,2396,15983966,10427712,24779724,6918454,3542,10113978,448008,10074640,3540,17755052,10172943,6419766,3038522,11338033,11656518,208908,10267580,11213558,11427553,447077,3973,160355,2856,16722836,1694,11314340,24889392,11167602,11364421,5005498,11485656,10127622,156414,176167,151194,3078519,10409068]
1511|Q9UQB9(13) [10113978,24779724,10172943,17755052,160355,10074640,156414,176167,11364421,2396,15983966,11442891,11667893,11338033,16722836,208908,151194,6419766,9549303,153999,176870,24856041,11608401,3038522,11485656,447077,11234052,11314340,11656518,11712649,6918454,11213558,2856,5005498,447966,46885626,11427553,24995524,3025986,24889392,11409972,3078519,10127622,3540,448008,16122633,3542,10427712,76098,3973]
1512|P52333(77) [160355,6918454,16722836,11712649,15991573,5330286,151194,9926791,57379345,17755052,11213558,11409972,176167,10296883,16659841,10127622,3038522,153999,11485656,2396,448008,2856,11667893,11234052,176870,10427712,15983966,46866319,10113978,11656518,45375955,11314340,25062766,6419766,11364421,156414,447077,208908,10074640,447966,46216796,11977753,11338033,5005498,11427553,24779724,3973,24889392,3025986,9549303]
1513|P51151(5) [3455,1552036,17113,3114023,10219,2576,162834,3095276,2291046,16187479,1568843,3542,1878823,16490,3240818,3746037,3127493,2197,2768954,160355,5289501,1608140,327045,22430825,1599306,65758,2812,5405,42725,3503,41684,1580955,265580,19646,19910,24817194,1720828,1238,187,2161,1811924,680935,5074,70846,4380,3885,107985,1432578,16362,1694,4493]
1514|P48736(286) [15983966,25033539,24889392,9849735,6852165,25254071,176870,16654980,3025986,50905713,11485656,11234052,3973,11338033,16736978,11213558,11977753,447077,44516953,3038522,208908,11409972,176167,151171,10113978,10074640,153999,11647372,24779724,11667893,11427553,17755052,10427712,44137675,10296883,11314340,11625818,11712649,49784945,11364421,56649450,51001932,54575456,24989044,156414,151194,16722836,6918454,11656518,25167777,10127622]
1515|P11309(66) [151194,11364421,153999,11667893,24748573,448008,10172943,11338033,3038522,10427712,11234052,11712649,9549303,176167,3540,16722836,156414,76098,17755052,11656518,2396,10127622,208908,11608401,5005498,11314340,447966,6918454,24889392,57899889,160355,11213558,6419766,3025986,176870,11485656,24795070,2856,611002,16122633,3973,24779724,15983966,10074640,3542,10296883,11409972,447077,11427553,10113978,3078519]
1516|P35368(14) [3822,2170,115237,2435,5073,3157,10624,1615,33625,2159,4747,5265,60602,119828,5816,6082,2818,17747460,10836,1355,439260,164089,3677,208898,4184,5074,2092,60820,30487,3559,72106,119570,6041,129211,148842,4636,60809,5826,5268,5775,11597698,5401,5312125,13542,2368,4893,38521,3389,6077,216249,2913]
1517|P53350(99) [11338033,24889392,3973,3038522,2856,3542,176167,448008,17755052,11442891,176870,16722836,53357478,11213558,11409972,151194,11314340,2396,3078519,447966,10427712,208908,10127622,16058637,11552706,10461508,447077,160355,3540,10074640,156414,153999,11712649,11364421,15983966,24779724,10172943,10113978,11427553,6918736,11485656,9549303,3025986,11234052,131682,11667893,11656518,6419766,35595,6918454,5005498]
1518|P34969(18) [71360,2159,11430856,10531,3559,11954293,2913,2726,5074,4847,1615,4184,4585,197033,11961293,11292933,9966051,2818,213046,1150,119828,60809,3822,68848,9805719,2170,44623946,119570,23897,16362,4748,49381,1355,19241,27400,10212,3372,62865,60854,5265,28693,71768094,3389,8969,5073,5452,10624,115237,5736,4106,42601552,5358]
1519|P07949(222) [447077,11656518,15983966,11667893,3081361,57379345,25102847,24826799,11314340,11427553,3038522,10113978,6419766,17755052,10296883,11485656,208908,25031915,216239,11234052,160355,156414,176167,5329102,448008,11442891,3025986,11213558,11338033,10427712,11167602,447966,11364421,9549303,3973,2396,176870,24779724,11712649,11751922,153999,151194,5005498,11282283,24889392,10127622,11409972,24767976,10074640,16722836,2856,6918454]
1520|P17612(37) [3542,11667893,11712649,11656518,11409972,176167,6918454,24889392,11427553,16122634,160355,17755052,12412578,208908,448008,151194,3973,11234052,11314340,10113978,5005498,2396,10050566,3025986,11338033,10427712,9549303,11364421,10074640,10172943,3078519,24779724,11840906,16122635,11608401,10127622,16122633,3540,15983966,11213558,447966,447077,11175137,16722836,6419766,153999,156414,449241,3038522,176870,2856,11485656]
1521|P16234(175) [57379345,11167602,3973,448008,11608401,11409972,24826799,10074640,2396,447077,9809715,153999,76098,6918454,160355,151194,16722836,25031915,

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1522|P35916(99) [176167,
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1523|P04062(105) [3237705,
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1554|P54132(71) [2265 , 20544 , 5917 , 4814 , 3433 , 16362 , 1694 , 5289501 , 2435 , 3885 , 10219 , 11967800 , 175540 , 3973 , 2998 , 9363 , 21138 , 4362 , 119259 , 3311 , 3478 , 5405 , 5723 , 89105 , 11296583 , 1780 , 4342 , 3746037 , 3333 , 249 , 1967 , 2754 , 3277 , 2017 , 11967809 , 23897 , 4197 , 1973720 , 5722 , 2812 , 6603842 , 1392 , 1066 , 5282060 , 2277 , 1676 , 4593 , 104762 , 1123 , 1649 , 5074 , 4578 , 2123 , 3698 , 2179 , 10036135 , 3074827 , 2090 , 3503 , 4122 , 4843 , 114924 , 2750 , 2753 , 1893 , 2762 , 16231 , 3455 , 1355 , 6603901 , 5593 , 53708 , 6764 , 361655 , 2369 , 1993 , 31475 , 10168 , 3671 , 2216 , 3108 , 1989]
1555|P15428(64) [2197 , 2540 , 3708374 , 1984 , 1811924 , 5459671 , 1561922 , 3108 , 16231 , 3324 , 2082 , 660989 , 5723 , 32681 , 4842 , 4284 , 11289 , 10219 , 5722 , 2179 , 612424 , 2426546 , 24144 , 1694 , 3698 , 10651 , 107992 , 3244425 , 1893 , 3238649 , 11852 , 11790 , 683816 , 1780 , 227681 , 2333 , 4506 , 3503 , 3034012 , 2092 , 3277 , 4380 , 2932343 , 10036135 , 1057 , 5153171 , 76915 , 2828376 , 3828 , 2998 , 16590 , 4577033 , 3333 , 72139 , 3240818 , 8569 , 11293 , 2219849 , 53708 , 12028 , 16315 , 6918508 , 2950 , 1676 , 4593 , 10168 , 2435 , 3238154 , 1050 , 2122 , 2750 , 3474 , 7329 , 1719874 , 3237465 , 3117 , 10245972 , 115015 , 1322 , 3245624 , 4197 , 1967 , 2753]
1556|P35968(217) [6450551 , 9549303 , 176870 , 24812719 , 24779724 , 25116064 , 447077 , 156414 , 4030 , 9797919 , 6918454 , 5329099 , 11610113 , 10302451 , 208908 , 10275001 , 11234052 , 10113978 , 10427712 , 11314340 , 9911830 , 16122633 , 5289418 , 11349170 , 11973736 , 9811611 , 24889392 , 11608401 , 11667893 , 11409972 , 9808844 , 24826799 , 3081361 , 448008 , 17755052 , 11338033 , 46207586 , 3025986 , 160355 , 16722836 , 42642645 , 447966 , 151194 , 15991573 , 10074640 , 9549295 , 16662431 , 6420138 , 11712649 , 11656518 , 11427553 , 11364421 , 57379345 , 24767976 , 10296883 , 25102847 , 11552706 , 10458325 , 6419766 , 10127622 , 2396 , 9933475 , 15983966 , 2856 , 5005498 , 10138259 , 9823820 , 9868037 , 24901704 , 3973 , 3038522 , 51039095 , 16040289 , 176167 , 5329102 , 11213558 , 9809715 , 11485656 , 153999 , 11751922 , 76098 , 11167118 , 53235510 , 25031915 , 11442891 , 11167602]
1557|P24941(127) [5327686 , 10224714 , 176870 , 11285002 , 11427553 , 5287969 , 447656 , 10127622 , 11338033 , 16718576 , 5326739 , 151194 , 3078519 , 680935 , 6918834 , 17754027 , 5327096 , 9601217 , 5005498 , 16122633 , 176167 , 160355 , 16113377 , 6852201 , 10113978 , 118458 , 16739650 , 153999 , 11712649 , 17755052 , 5289419 , 11234052 , 6918852 , 3038522 , 87031 , 449087 , 4592 , 2608 , 156414 , 57379345 , 24901723 , 1369 , 10074640 , 447966 , 11213558 , 447961 , 208908 , 448991 , 11314340 , 449088 , 447960 ,

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1558|Q99714(31) [51040 , 15286 , 3117 , 593113 , 11293 , 3245131 , 21307 , 2333 , 10660 , 2123 , 2327 , 16231 , 3333 , 107992 , 4842 , 3324 , 7916 , 547914 , 648831 , 2057112 , 10245972 , 21138 , 5593 , 3239879 , 2753 , 5227 , 4064 , 2913 , 2179 , 3244425 , 5335 , 10313 , 2540 , 3474 , 1548942 , 11289 , 4593 , 2277 , 665652 , 3503 , 1676 , 1815815 , 612424 , 3237465 , 2092 , 28688 , 3698 , 1694 , 155774 , 1561922 , 2216 , 10219 , 10168 , 3243850 , 2165979 , 2355 , 2304617 , 11852 , 6307 , 24144 , 1984 , 6604423 , 5074 , 4278 , 2435 , 4380 , 3238649 , 3240818 , 11790 , 1057 , 3108 , 660989 , 3542 , 193949 , 53708 , 19996 , 25670 , 115015 , 2750 , 3277 , 3973 , 4670 , 5289501 , 2315 , 361655 , 3118 , 11241 , 41684 , 1893 , 2950 , 2866904 , 6605027 , 10651 , 7329 , 12492 , 114924 , 36811 , 15474019]
1559|P49798(18) [4278 , 2396 , 4761 , 107992 , 10245190 , 1568843 , 1676 , 2750 , 1045 , 4593 , 44602029 , 10245972 , 53708 , 3542 , 2768954 , 50287 , 23897 , 3762 , 683816 , 12449 , 2743305 , 3983561 , 10212 , 3151 , 739358 , 5917 , 3298363 , 3092847 , 44112 , 3286 , 123600 , 115015 , 6603842 , 4197 , 3117 , 20544 , 1392 , 1273944 , 175540 , 3973 , 219081 , 361655 , 70464 , 3138330 , 3245131 , 2123 , 1694 , 208820 , 2812 , 5005498 , 1066 , 3455 , 2831167 , 127599 , 16351 , 1892 , 104762 , 2435 , 10531 , 1993 , 31729 , 1234 , 124663 , 2216 , 10168 , 4362 , 1811924 , 2090 , 107883 , 2234617 , 3108 , 547914 , 2913 , 2327 , 4380 , 3698 , 2562 , 4680274 , 107715 , 4342 , 16231 , 1967 , 13752 , 10133 , 2914644 , 3885 , 14899645 , 2229 , 68186 , 3244425 , 10569483 , 5074 , 348986 , 114924 , 3433 , 3503 , 3746037 , 3559]
1560|Q9NUW8(14) [11293 , 123600 , 130881 , 19910 , 2265 , 15158 , 3686 , 2576 , 5593 , 121871 , 1030 , 213013 , 115150 , 10168 , 106729 , 16189712 , 54675783 , 122081 , 107715 , 2396 , 11245 , 11241 , 1549789 , 65909 , 3503 , 2178 , 21138 , 3760 , 5510 , 3156917 , 5335 , 51040 , 121752 , 5074 , 16837 , 6708773 , 31957 , 10206 , 1989 , 2453 , 3969 , 3151041 , 6034 , 10133 , 7916 , 1967 , 2950 , 7191 , 22430815 , 2132 , 16362 , 2170 , 32681 , 2327 , 2750 , 10230 , 16231 , 9273 , 10621 , 1895388 , 3108 , 3455 , 2562 , 4487 , 2812 , 3610 , 47472 , 170344 , 4337923 , 68089 , 10245972 , 246831 , 35970 , 8041 , 4284 , 2264 , 192197 , 115015 , 61247 , 3229428 , 4592 , 1780 , 5233 , 18635 , 10531 , 14052 , 4456136 , 4174 , 4842 , 5326713 , 1355 , 6764 , 26323 , 3295 , 3885 , 175540 , 1781 , 1057]
1561|O75164(18) [21109 , 2016 , 3132640 , 54677971 , 3138330 , 1066 , 3455 , 660989 , 3746037 , 10172943 , 2855211 , 10621 , 7329 , 3003803 , 2478 , 3758 , 2366 , 24792593 , 2165605 , 3138375 , 1870615 , 2762 , 3926 , 3118 , 1349907 , 2090 , 2182 , 2179 , 67686 , 3138373 , 14052 , 2794 , 1967 , 10212 , 11293 , 3760 , 3151041 , 131411 , 3298512 , 6 , 547914 , 2812 , 54675783 , 14369 , 32681 , 2876323 , 68089 , 2866904 , 3286 , 1369 , 3139316 , 441383 , 5074 , 4119575 , 2743305 , 683816 , 5392 , 11852 , 2327 , 3125446 , 3406 , 1720828 , 12454 , 801418 , 24892221 , 16347 , 3240461 , 16190692 , 54676538 , 612424 , 31475 , 3126341 , 3515 , 19910 , 10168 , 219081 , 3138364 , 51040 , 28446 , 2998359 , 10036135 , 3120949 , 115163 , 4680274 , 1973720 , 5510 , 598513 , 4619 , 3117 , 13752 , 3229428 , 10206 , 2453 , 752652 , 16362 , 12449 , 685814 , 3244425 , 76915]
1562|Q9UIF8(0) [76915 , 3610 , 1017 , 2876323 , 24761713 , 10168 , 12454 , 5510 , 4961961 , 647499 , 3298512 , 1989 , 3132640 , 659036 , 18573525 , 2984762 , 3760 , 3236936 , 3242481 , 68089 , 5074 , 19910 , 2343 , 10219 , 1561922 , 2812 , 3229428 , 3377088 , 9550559 , 131411 , 3503 , 10235 , 72900 , 3108 , 1829960 , 21501 , 2122 , 10258 , 2247 , 2315667 , 31475 , 1967 , 2333 , 3151041 , 290012 , 3542 , 612424 , 648831 , 2327 , 2950 , 5359646 , 3731631 , 3932 , 54676538 , 2743305 , 3237465 , 15723 , 645503 , 3435 , 660989 , 911675 , 2229 , 3126341 , 1547484 , 332697 , 32681 , 5804 , 1973720 , 14369 , 3686 , 194595 , 661085 , 752652 , 4110197 , 3245728 , 41684 , 1780 , 16362 , 2754 , 567825 , 16129778 , 2366 , 8210 , 265580 , 3474 , 4760 , 1870615 , 10621 , 11852 , 70846 , 54675783 , 54677971 , 1066 , 2197 , 124087 , 36303 , 3746037 , 3118 , 3244425 , 2179 , 4119575 , 21109]
1563|Q08209(55) [71851 , 3334 , 5921 , 5585 , 3748 , 5541 , 21109 , 2883 , 1548942 , 4122 , 2754 , 4107 , 11643449 , 3639 , 441383 , 1981 , 4912 , 4197 , 5335 , 1349907 , 4843 , 35802 , 3333 , 14385 , 2264 , 2082 , 3686 , 1057 , 2197 , 14868 , 2361 , 2749 , 2732 , 10219 , 2812 , 3516 , 2123 , 4156 , 10531 , 14052 , 5405 , 54676038 , 4174 , 2435 , 44112 , 3055 , 13765 , 16231 , 2482 , 2725 , 2753 , 119259 , 2750 , 54677971 , 3435 , 2366 , 2577 , 1030 , 3561 , 17134 , 4855 , 2484 , 16129778 , 21138 , 50942 , 2758 , 10660 , 3117 , 3559 , 3406 , 5576 , 11683 , 39042 , 3168 , 36811 , 1046 , 3478 , 3698 , 1547484 , 12124 , 2333 , 2467 , 3151 , 4760 , 2893 , 6761 , 3182 , 107782 , 2170 , 4030 , 2265 , 5593 , 11286230 , 2913 , 3973 , 182137 , 3108 , 57469 , 2247 , 124087 , 2132 , 4506 , 5510 , 31072 , 11790 , 4753 , 123600 , 5198 , 2478 , 16574 , 131204 , 2391 , 3324 , 2176 , 175540 , 5722]
1564|P51679(50) [14385 , 2082 , 2170 , 1030 , 3561 , 17134 , 3055 , 16129778 , 2482 , 2725 , 4912 , 36811 , 3478 , 2577 , 2467 , 3151 , 21138 , 31072 , 3168 , 14052 , 2758 , 3117 , 54676038 , 5593 , 6761 , 44112 , 107782 , 4855 , 5576 , 2265 , 2176 , 123600 , 2264 , 175540 , 3686 , 2913 , 119259 , 2893 , 54677971 , 3435 , 3182 , 124087 , 50942 , 11790 , 4753 , 10660 , 3559 , 2750 , 4030 , 182137 , 3108 , 13765 , 2247 , 3324 , 5722 , 3334 , 12124 , 2333 , 4506 , 5510 , 4760 , 2883 , 5335 , 3333 , 1548942 , 11286230 , 2197 , 441383 , 2749 , 5921 , 5585 , 2732 , 3973 , 10219 , 4197 , 57469 , 4122 , 65015 , 4843 , 2478 , 4174 , 2435 , 131204 , 1057 , 3698 , 1981 , 2391 , 3406 , 2132 , 16231 , 71851 , 2361 , 3748 , 1349907 , 5541 , 21109 , 2812 , 35802 , 3516 , 2123 , 2366 , 10531 , 2754 , 4107 , 11643449 , 2484 , 3639 , 14868 , 1547484 , 5405 , 5198 , 16574 , 11683 , 39042 , 1046 , 4156 , 2753]
1565|P32241(49) [10219 , 3055 , 14052 , 39042 , 16129778 , 182137 , 5593 , 3406 , 36811 , 4855 , 71851 , 2725 , 2913 , 4030 , 31072 , 57469 , 2754 , 50942 , 2893 , 4506 , 3559 , 2478 , 2435 , 2170 , 2265 , 4843 , 131204 , 5585 , 35802 , 10531 , 124087 , 14868 , 3686 , 11643449 , 1030 , 17134 , 16231 , 4107 , 1057 , 2366 , 4912 , 2484 , 1548942 , 4156 , 6761 , 1046 , 5722 , 5405 , 3168 , 54677971 , 3435 , 3639 , 2132 , 2123 , 5510 , 3182 , 11286230 , 2176 , 3108 , 4760 , 10660 , 107782 , 3973 , 2361 , 2482 , 11790 , 2577 , 4753 , 123600 , 2391 , 2467 , 5198 , 4174 , 11683 , 5576 , 13765 , 3516 , 2750 , 2753 , 3333 , 44112 , 1981 , 1547484 , 119259 , 1349907 , 2082 , 3561 , 2883 , 44623946 , 2758 , 3324 , 2264 , 3334 , 54676038 , 16574 , 21138 , 2732 , 2749 , 2197 , 2247 , 5335 , 441383 , 2812 , 12124 , 3748 , 3117 , 4197 , 2333 , 5921 , 4122 , 3698 , 5541 , 21109 , 175540 , 3151 , 14385 , 3478]
1566|P49146(14) [4107 , 5585 , 11286230 , 4156 , 2482 , 2197 , 12124 , 2435 , 1030 , 3973 , 3333 , 1548942 , 5921 , 5541 , 21138 , 4753 , 2577 , 2265 , 44112 , 17134 , 4843 , 1981 , 2391 , 182137 , 11643449 , 2247 , 5576 , 10660 , 1057 , 119259 , 2753 , 2883 , 4506 , 3055 , 2484 , 5722 , 187 , 14052 , 10219 , 39042 , 2732 , 2170 , 1547484 , 123600 , 3334 , 14868 , 3748 , 3559 , 3698 , 2725 , 21109 , 2176 , 5510 , 71851 , 3516 , 3435 , 3324 , 131204 , 3478 , 3108 , 4760 , 31072 , 2264 , 11790 , 2478 , 3182 , 2132 , 50942 , 13765 , 4197 , 3151 , 3406 , 441383 , 2893 , 2333 , 4174 , 2361 , 16129778 , 175540 , 36811 , 2749 , 2366 , 10531 , 2750 , 2754 , 3561 , 2758 , 3639 , 4912 , 35802 , 2467 , 2913 , 16231 , 1046 , 2812 , 3168 , 14385 , 3686 , 124087 , 5198 , 6761 , 16574 , 2123 , 3117 , 54676038 , 4122 , 5335 , 4855 , 4030 , 5593 , 107782 , 2082 , 5405 , 54677971 , 11683 , 1349907 , 57469]
1567|P08575(136) [11683 , 3973 , 2361 , 2435 , 2265 , 2732 , 2170 , 131204 , 21109 , 3334 , 2176 , 4912 , 50942 , 2577 , 10660 , 11790 , 4753 , 3561 , 2913 , 3639 , 5510 , 1030 , 5576 , 124087 , 5593 , 12124 , 54676038 , 1548942 , 13765 , 3055 , 2812 , 57469 , 4760 , 54677971 , 3108 , 10219 , 2123 , 4855 , 2750 , 16574 , 9547959 , 31072 , 16231 , 182137 , 5541 , 1981 , 175540 , 2758 , 2391 , 4843 , 11286230 , 3516 , 17134 , 3748 , 4156 , 123600 , 39042 , 3151 , 11643449 , 5405 , 1547484 , 35802 , 2883 , 4122 , 2754 , 2893 , 4030 , 3324 , 3182 , 2333 , 14385 , 3478 , 3435 , 3117 , 1349907 , 5585 , 2082 , 3698 , 2753 , 2482 , 2197 , 3168 , 441383 , 5722 , 5335 , 36811 , 10531 , 2725 , 3686 , 21138 , 2264 , 4506 , 1046 , 6761 , 16129778 , 4197 , 14052 , 2366 , 5921 , 1057 , 2132 , 3559 , 2478 , 2484 , 107782 , 5198 , 4107 , 2467 , 2749 , 3406 , 4174 , 44112 , 3333 , 14868 , 71851 , 119259 , 2247]
1568|P30988(44) [2170 , 6761 , 5335 , 2750 , 3168 , 4122 , 2758 , 2264 , 16231 , 5541 , 11643449 , 16574 , 1548942 , 70691388 , 2391 , 3748 , 123600 , 2732 , 3516 , 12124 , 10531 , 5405 , 2333 , 13765 , 21109 , 3333 , 1547484 , 11683 , 2176 , 4197 , 71851 , 14052 , 21138 , 4912 , 2725 , 11286230 , 3055 , 2754 , 2812 , 4030 , 1046 , 54677971 , 3435 , 2749 , 5921 , 36811 , 2753 , 441383 , 2913 , 4174 , 57469 , 3639 , 3973 , 2478 , 3151 , 3324 , 3478 , 2893 , 3334 , 131204 , 44112 , 4843 , 175540 , 5593 , 14868 , 5585 , 2883 , 14385 , 124087 , 2482 , 2197 , 2577 , 3698 , 4156 , 10219 , 4506 , 16129778 , 2132 , 2484 , 2247 , 50942 , 3108 , 2366 , 1349907 , 2082 , 54676038 , 4760 , 5722 , 10660 , 182137 , 3559 , 5510 , 2123 , 3182 , 2265 , 3686 , 107782 , 1981 , 35802 , 3561 , 1057 , 2361 , 3406 , 4855 , 2435 , 5576 , 11790 , 4753 , 39042 , 4107 , 1030 , 5198 , 17134 , 31072 , 119259 , 3117 , 2467]
1569|P25929(16) [4122 , 4855 , 3117 , 3182 , 5921 , 3108 , 10660 , 14052 , 1057 , 119259 , 182137 , 11683 , 124087 , 1547484 , 2197 , 57469 , 3686 , 2132 , 1548942 , 21109 , 13765 , 2812 , 31072 , 10531 , 17134 , 11643449 , 4843 , 3561 , 3324 , 2754 , 2366 , 2577 , 1349907 , 5335 , 3698 , 12124 , 50942 , 5198 , 3748 , 175540 , 2247 , 54676038 , 44112 , 16129778 , 11286230 , 5722 , 3435 , 11790 , 39042 , 4753 , 2082 , 1046 , 10219 , 2883 , 107782 , 4506 , 2264 , 2176 , 6761 , 2913 , 14868 , 187 , 3333 , 2361 , 4760 , 7504 , 5541 , 2753 , 2391 , 3334 , 5510 , 2750 , 2482 , 2333 , 2467 , 4156 , 4030 , 2732 , 2725 , 2435 , 4107 , 123600 , 3639 , 14385 , 131204 , 4174 , 71851 , 2749 , 35802 , 1981 , 2265 , 2123 , 3055 , 3478 , 3516 , 5405 , 2758 , 3559 , 2170 , 16574 , 3151 , 1030 , 4197 , 3406 , 4912 , 2484 , 21138 , 441383 , 16231 , 2478 , 5593 , 3168 , 5585 , 54677971 , 2893 , 5576 , 3973 , 36811]
1570|P25024(78) [2264 , 2082 , 2366 , 10219 , 3478 , 2197 , 2812 , 1349907 , 3324 , 5510 , 4174 , 2484 , 2265 , 2893 , 1981 , 10531 , 3973 , 123600 , 3516 , 131204 , 3748 , 3698 , 9865554 , 1057 , 35802 , 2176 , 4753 , 3182 , 2435 , 16231 , 2478 , 182137 , 2361 , 57469 , 2750 , 2758 , 54676038 , 4197 , 3406 , 1547484 , 54677971 , 5722 , 11643449 , 3055 , 2123 , 4030 , 2732 , 4855 , 124087 , 10660 , 12124 , 3561 , 9838712 , 4156 , 4912 , 4506 , 16574 , 11683 , 2467 , 2577 , 5198 , 11286230 , 2170 , 175540 , 2247 , 5593 , 3334 , 11790 , 1548942 , 3559 , 1046 , 2132 , 5335 , 5541 , 5585 , 2391 , 16007088 , 3151 , 44112 , 13765 , 2754 , 3108 ,

2753, 441383, 5576, 6761, 1030, 4107, 3168, 36811, 2913, 4760, 3686, 119259, 3639, 4122, 3117, 14052, 4843, 2749, 39042, 3435, 31072, 3333, 17134, 21109, 107782, 71851, 14868, 21138, 2333, 5405, 2725, 14385, 2883, 5921, 16129778, 2482, 50942]
1571|P33032(4) [44112, 2754, 3055, 10219, 16129664, 3108, 107782, 4506, 1057, 2753, 5593, 2132, 6761, 11683, 2812, 182137, 1046, 3334, 3324, 5541, 2883, 2750, 16197727, 21109, 4030, 54677971, 12124, 5335, 2366, 50942, 3516, 21138, 175540, 4912, 2265, 3698, 5585, 3748, 5576, 54676038, 123600, 2170, 16129778, 16574, 2247, 2913, 57469, 2176, 10660, 39042, 4753, 119259, 2082, 2264, 4197, 36811, 17134, 14868, 5198, 4760, 11643449, 3333, 13765, 4843, 10531, 2482, 5510, 2577, 4122, 3561, 2732, 11328898, 2435, 2333, 1349907, 2467, 3639, 31072, 71851, 3686, 3182, 3117, 2123, 124087, 2197, 1981, 14385, 11286230, 14052, 5405, 131204, 3478, 1548942, 4174, 3151, 1547484, 1030, 2749, 35802, 11790, 4107, 2484, 2758, 3559, 3406, 441383, 5722, 2478, 2361, 3973, 2391, 3168, 2893, 16231, 5921, 2725, 3435, 4855, 4156]
1572|Q16236(220) [1568843, 3377088, 13791, 8178, 19996, 16316, 660989, 3082, 2478, 2836838, 3503, 18573528, 213013, 84098, 67686, 3034285, 1614257, 6540, 2750, 8124, 2170, 16188984, 4404908, 197033, 5233, 651913, 1893, 151506, 15439, 16960, 160355, 3114023, 133621, 6307, 657497, 2913, 31475, 7347, 1392, 3242535, 312183, 3244566, 9820526, 5392, 54676538, 54675783, 1720828, 1123, 104741, 4342, 8872, 11742, 6603901, 35758, 4961961, 2179, 101744, 11006, 2166261, 31200, 1548942, 10850, 3114024, 27648, 114924, 62485, 12589, 39040, 3559, 12968, 4156, 13113, 6301, 16231, 658365, 2247, 115157, 10958, 1694, 11604, 14369, 9298, 5289501, 348986, 3138330, 3156709, 3885, 16653, 3781338, 1895388, 104926, 68363, 1057, 225371, 8467, 2137779, 2365, 5459650, 344675, 4572075, 2355, 3326, 16637, 9551522, 76915, 10245972, 10660, 7475414, 8907, 2082, 7395618, 3672772, 22571, 657677, 650127, 44142959, 273053, 65768, 2450, 7475368]
1573|P41968(13) [5405, 57469, 5335, 21138, 3698, 2913, 441383, 119259, 2732, 10219, 2361, 16129778, 2265, 44112, 1981, 5198, 5585, 2333, 71851, 4197, 17134, 2754, 11643449, 3055, 2170, 2749, 50942, 2197, 54677971, 175540, 3559, 4843, 5510, 1057, 16231, 4156, 182137, 2482, 3117, 3108, 6761, 36811, 3478, 3334, 10660, 5722, 16129664, 5921, 3151, 3973, 2132, 4030, 3516, 4912, 1030, 4174, 2435, 4753, 11790, 5576, 3406, 11683, 2758, 5541, 14385, 5593, 14052, 35802, 4506, 3639, 1046, 131204, 31072, 16574, 10531, 21109, 3168, 2247, 14868, 2725, 3748, 107782, 1547484, 2753, 2264, 4107, 2467, 6323491, 54676038, 11286230, 2484, 2750, 12124, 2812, 39042, 3561, 2082, 3686, 2478, 124087, 1349907, 2577, 4122, 2366, 11328898, 2883, 3182, 2391, 16197727, 2893, 2176, 3324, 1548942, 4855, 2123, 4760, 3333, 3435, 123600, 13765]
1574|P08311(36) [50942, 3686, 124087, 57469, 131204, 35802, 2732, 2812, 13765, 21138, 2132, 2754, 107782, 1046, 3748, 2467, 1057, 3108, 4855, 441383, 1030, 2577, 1349907, 182137, 2333, 10219, 14052, 3516, 24800541, 2176, 2366, 3151, 4122, 5405, 5921, 5541, 10660, 3117, 123600, 4030, 11790, 2893, 2484, 2482, 2197, 5335, 4760, 2391, 3559, 31072, 1548942, 2082, 2264, 3561, 2749, 16574, 2247, 36811, 4174, 11286230, 6761, 2265, 17134, 4506, 2753, 10531, 2435, 4912, 3333, 5593, 16129778, 1981, 2361, 3334, 39042, 5576, 107706, 3406, 4197, 3639, 2750, 14385, 119259, 4753, 2913, 3698, 5510, 42601552, 2170, 4156, 16231, 2725, 54676038, 71851, 3182, 14868, 3324, 446833, 21109, 5722, 44112, 3973, 11643449, 2478, 175540, 12124, 2758, 3435, 11683, 3055, 5198, 4107, 2123, 3478, 5585, 54677971, 1547484, 3168, 4843, 2883]
1575|P30411(40) [2732, 119259, 175540, 2577, 5198, 10660, 16231, 11790, 2913, 1046, 21138, 17134, 5541, 2758, 11643449, 4753, 4843, 10531, 4912, 2366, 2893, 4107, 16129778, 1349907, 107782, 4030, 3561, 11286230, 2197, 2176, 4156, 57469, 54677971, 14052, 441383, 3151, 3117, 3055, 5405, 2123, 1548942, 3748, 5576, 2484, 2264, 131204, 31072, 50942, 5510, 2132, 16574, 2478, 5585, 1057, 3559, 3108, 14868, 2247, 4760, 2265, 3686, 21109, 3698, 3324, 9831652, 439201, 11498853, 124087, 71851, 2435, 1981, 2750, 39042, 3333, 36811, 5593, 4122, 3973, 2361, 44112, 4197, 3182, 13765, 3168, 2391, 2482, 182137, 5722, 71364, 4855, 6761, 44623946, 5335, 14385, 3478, 5921, 3435, 1030, 11683, 3516, 123600, 2725, 2082, 2467, 35802, 1547484, 2812, 12124, 54676038, 3406, 2883, 2170, 3334, 4506, 2749, 2754, 3639, 2753, 4174, 2333, 10219]
1576|Q99720(24) [36811, 2123, 2264, 2913, 5585, 11286230, 3478, 6761, 4030, 3324, 5405, 3151, 3108, 39042, 2361, 3406, 2391, 2333, 2132, 13765, 4855, 4107, 57469, 16574, 3748, 5198, 2754, 50942, 175540, 4156, 10531, 44112, 4506, 14385, 16231, 71851, 54677971, 53389, 2893, 3435, 31072, 16129778, 2197, 3686, 2883, 14868, 14052, 5593, 2170, 2482, 2812, 35802, 1547484, 4197, 2366, 11790, 1030, 4753, 10660, 2082, 1057, 3168, 54676038, 4912, 123600, 11683, 2577, 119259, 17134, 3516, 53359, 4760, 2478, 2467, 3639, 4843, 2732, 2435, 3055, 3117, 182137, 4122, 5541, 4174, 2753, 1548942, 5510, 12124, 5722, 2176, 21138, 2750, 3698, 10219, 11430856, 2758, 3333, 3008, 3559, 2725, 21109, 131204, 2749, 3182, 1046, 124087, 107782, 5576, 441278, 3973, 1981, 2484, 2247, 441383, 1349907, 3561, 5335, 5360696, 5921, 3334, 2265, 11643449]
1577|P32245(43) [6323491, 5593, 124087, 3406, 14385, 71851, 2725, 3055, 39042, 182137, 31072, 36811, 16129664, 57469, 2754, 50942, 4030, 1349907, 2478, 2758, 2170, 3639, 2265, 4843, 2082, 3559, 2435, 2893, 3686, 131204, 2482, 1030, 17134, 5585, 4912, 2484, 35802, 10531, 14868, 4156, 1046, 5405, 54677971, 16231, 3435, 4107, 2366, 2132, 1548942, 2123, 6761, 71768094, 11286230, 2176, 16129778, 3168, 10660, 3973, 4855, 5510, 4760, 2391, 107782, 2361, 5198, 11790, 44112, 2577, 4753, 123600, 175540, 5722, 3516, 3108, 2753, 1981, 2467, 119259, 11683, 5576, 16197727, 11328898, 44623946, 13765, 2750, 2913, 3324, 3333, 1547484, 3334, 11643449, 16574, 3561, 2883, 2197, 4506, 2264, 54676038, 21138, 2732, 2749, 5335, 441383, 2812, 4174, 12124, 1057, 3748, 2247, 3182, 5921, 3117, 3151, 4197, 2333, 4122,
3478, 3698, 5541, 10219, 21109, 14052]
1578|P21452(15) [4122, 11790, 3324, 17134, 2123, 50942, 21109, 10660, 3168, 3748, 6761, 182137, 44112, 5541, 4107, 11643449, 104974, 5198, 5510, 3151, 3639, 16574, 2732, 10219, 4156, 2361, 2913, 3698, 1046, 3406, 36811, 2247, 14385, 2435, 3686, 3055, 1547484, 44623946, 2333, 4506, 4753, 123600, 2478, 131204, 107782, 4855, 2812, 2265, 2391, 2366, 5722, 71851, 2758, 5405, 11527495, 5921, 219077, 1349907, 2484, 3973, 14052, 11683, 3333, 39042, 10328936, 3117, 5576, 119259, 14868, 54677971, 441383, 2753, 1030, 3561, 2750, 2482, 16129778, 3435, 1981, 3182, 3334, 3559, 4174, 5311424, 3108, 57469, 2883, 5335, 35802, 4030, 2082, 1548942, 2132, 12124, 13765, 31072, 2754, 16231, 3478, 2893, 2197, 2725, 2749, 4912, 2467, 4843, 4760, 5593, 3516, 11286230, 4197, 2577, 10531, 5585, 21138, 2176, 175540, 54676038, 2264, 2170, 1057, 124087]
1579|P11509(69) [2725, 4174, 36811, 2754, 3334, 2082, 2264, 2478, 2170, 39042, 5335, 12124, 3748, 31072, 441383, 2361, 1548942, 1547484, 3698, 2123, 16574, 2750, 2391, 5405, 2812, 2197, 44112, 2482, 2913, 2753, 1057, 11643449, 3686, 2366, 14385, 4506, 16231, 1349907, 54677971, 131204, 2355, 3324, 2577, 175540, 2758, 4912, 182137, 35802, 123600, 3516, 5722, 3639, 10531, 3117, 3333, 1981, 4760, 124087, 3168, 2176, 4122, 4843, 11790, 21109, 4753, 3108, 2893, 2883, 1046, 2467, 5585, 2732, 2132, 3435, 2484, 2265, 3561, 10660, 11229234, 16129778, 11683, 3182, 1030, 4107, 5510, 148201, 11332763, 14052, 4030, 4156, 21138, 4197, 2435, 51049968, 54676038, 5198, 4855, 5541, 5576, 50942, 14868, 107782, 3559, 3478, 2247, 5593, 2333, 1048, 2749, 119259, 11286230, 3055, 57469, 10219, 3406, 5921, 17134, 6761, 3151, 71851, 3973, 13765]
1580|P32238(17) [54676038, 16231, 1981, 1046, 2484, 107782, 5198, 3406, 12124, 2725, 3478, 2478, 2435, 1547484, 4030, 2391, 6761, 14052, 17134, 1057, 3333, 5921, 39042, 3561, 119259, 4912, 5405, 11286230, 4156, 5541, 2812, 3973, 60182, 3324, 3334, 10660, 4753, 2247, 5722, 65937, 13765, 1548942, 124087, 10531, 3698, 50942, 16129675, 3639, 2482, 31072, 2754, 2749, 2577, 14868, 21109, 54677971, 2758, 2197, 2893, 71851, 5576, 3182, 5510, 2467, 2082, 4174, 10343641, 21138, 4506, 122077, 5593, 123600, 2264, 2123, 4122, 16129778, 1030, 4197, 175540, 2265, 11643449, 3516, 16574, 4760, 2176, 2361, 2366, 3748, 11790, 2732, 3108, 51353551, 3168, 5335, 57469, 3559, 2132, 2883, 3151, 3686, 11683, 2913, 182137, 4855, 36811, 5585, 35802, 3117, 2753, 1349907, 44112, 2333, 131204, 3435, 4107, 14385, 2750, 3055, 4843, 10219, 441383, 44623946, 2170]
1581|P25105(36) [2753, 2247, 3698, 54676038, 3478, 4753, 2264, 3973, 3406, 5541, 3686, 2478, 3748, 2913, 2451, 119259, 4506, 14052, 4107, 4156, 2577, 2482, 36811, 2082, 3055, 5585, 1057, 2170, 3435, 108156, 10531, 175540, 44112, 13765, 21109, 3168, 17134, 182137, 4122, 12124, 4030, 2123, 5198, 16129778, 2265, 3117, 3333, 2435, 2883, 35802, 1981, 5593, 2499, 3151, 119175, 16231, 441383, 3559, 1030, 11683, 2725, 2366, 21138, 65923, 3516, 3108, 123600, 2484, 1046, 4912, 2732, 5335, 65889, 2467, 2750, 16574, 119368, 71851, 54677971, 4197, 5921, 11790, 2812, 1349907, 133017, 10219, 2361, 1547484, 2197, 4843, 11643449, 5405, 3639, 50942, 10660, 5722, 57469, 4174, 2758, 4760, 2749, 107782, 2754, 3182, 2176, 31072, 5576, 2132, 124087, 39042, 11286230, 131204, 14868, 3334, 2893, 3324, 5510, 1548942, 3561, 6761, 44370579, 4855, 14385, 2391, 2333]
1582|P05181(174) [2725, 4753, 2333, 5576, 11790, 3182, 2754, 12124, 4197, 3168, 16129778, 2577, 1349907, 5198, 2753, 4506, 11643449, 3334, 4855, 1981, 3478, 2247, 14052, 3117, 2750, 2482, 119259, 4843, 3151, 16574, 182137, 3435, 54677971, 10660, 4122, 5510, 3406, 4156, 51049968, 31072, 16960, 2197, 5585, 5593, 2467, 441383, 36811, 11683, 71851, 124087, 39042, 54676038, 1030, 2812, 4912, 21109, 2176, 3324, 2758, 175540, 3559, 2361, 1548942, 4107, 6761, 10219, 10783, 2749, 2366, 2391, 57469, 2732, 5722, 17134, 3516, 14868, 5541, 2883, 2170, 3333, 4174, 4760, 4030, 2435, 21138, 148201, 11332763, 14385, 35802, 3973, 3561, 5405, 2082, 2264, 3108, 11286230, 1547484, 3748,

1046 , 2265 , 2132 , 16590 , 44112 , 2950 , 19987169 , 1057 , 131204 , 5921 , 2913 , 5335 , 3698 , 2484 , 3686 , 11229234 , 3639 , 2123 , 50942 , 107782 , 16231 , 2893 , 3055 , 2478 , 10531 , 13765 , 123600]
1583|Q92830(13) [4843 , 3032361 , 115244 , 2170 , 3117 , 4855 , 2540 , 911675 , 4097 , 3163418 , 3814414 , 3607 , 1861634 , 6237 , 3828 , 3561 , 3748 , 54676538 , 294256 , 3245563 , 10767 , 3474 , 2963649 , 122077 , 3109 , 1052 , 2950 , 1829960 , 24761713 , 4119575 , 4506 , 11046239 , 3236575 , 2426546 , 1050 , 3245493 , 11296583 , 39299 , 32681 , 3108 , 2913 , 160355 , 539709 , 2450 , 2724 , 3758 , 6466196 , 2113270 , 3406 , 3730 , 3245728 , 54676537 , 107715 , 22571 , 11852 , 2799 , 2176 , 5392 , 114924 , 1967 , 3503 , 16315 , 6307 , 124663 , 20906 , 2017 , 446816 , 12454 , 67686 , 5153171 , 10798271 , 5576 , 7347 , 7699 , 18573528 , 41684 , 229296 , 2743305 , 121871 , 14868 , 2132993 , 194699 , 1017 , 35455 , 6603901 , 2123 , 16129778 , 2750 , 5074 , 76915 , 11061 , 5917 , 4842 , 683816 , 6603842 , 439201 , 4342 , 115015 , 10404 , 10036135 , 31475 , 10219 , 104762 , 51040 , 104741 , 2466 , 53708 , 1649 , 11967809 , 4487 , 3243567 , 2333 , 1780 , 8210 , 115237 , 16685 , 54675783 , 4456136 , 2264 , 104850 , 1694 , 12620 , 108143 , 25066642 , 3239105 , 3239295]
1584|Q9Y271(37) [2750 , 5405 , 5541 , 4855 , 14385 , 16231 , 2123 , 2247 , 2333 , 16574 , 2478 , 182137 , 6436135 , 123600 , 3055 , 107782 , 5722 , 3406 , 2170 , 4887 , 13765 , 175540 , 11643449 , 2758 , 50942 , 3333 , 17134 , 5198 , 441383 , 119259 , 4912 , 11286230 , 21109 , 39042 , 3117 , 5921 , 2893 , 124087 , 71851 , 2176 , 2913 , 3334 , 3168 , 2732 , 5585 , 11683 , 54677971 , 2132 , 5281040 , 2484 , 1030 , 44112 , 3108 , 21138 , 4107 , 12124 , 14868 , 4156 , 2197 , 10660 , 54676038 , 2812 , 60842 , 2264 , 6913104 , 3686 , 2577 , 1349907 , 2435 , 2391 , 2366 , 5576 , 2753 , 4506 , 6761 , 1057 , 10531 , 5593 , 3559 , 2749 , 35802 , 3516 , 4760 , 10219 , 5510 , 4174 , 4197 , 3151 , 36811 , 11790 , 3478 , 6436123 , 4753 , 2082 , 1981 , 2725 , 2883 , 57469 , 2161 , 3182 , 11508736 , 2467 , 4122 , 3639 , 3324 , 3973 , 1547484 , 2361 , 2754 , 3561 , 16129778 , 1046 , 14052 , 2482 , 6509849 , 3698 , 31072 , 2265 , 4843 , 3748 , 1548942 , 5335 , 131204 , 3435 , 5717 , 4030]
1585|P08246(111) [54686804 , 54677971 , 21109 , 5921 , 2749 , 36811 , 2812 , 1547484 , 2482 , 54678950 , 14052 , 71851 , 3698 , 2132 , 1046 , 3973 , 3151 , 3108 , 2478 , 5198 , 5585 , 2577 , 5593 , 3478 , 3334 , 4843 , 131204 , 2753 , 4156 , 441383 , 2883 , 5510 , 39042 , 54676038 , 3182 , 2484 , 5335 , 2913 , 16129778 , 11286230 , 2893 , 14868 , 175540 , 3324 , 46228924 , 1981 , 35802 , 14385 , 31072 , 124087 , 6761 , 2082 , 4760 , 4197 , 17134 , 3117 , 2758 , 11643449 , 2265 , 2750 , 107706 , 2435 , 5576 , 3686 , 107782 , 44112 , 50942 , 4855 , 5541 , 47499 , 3559 , 24800541 , 1057 , 3406 , 4107 , 11790 , 4753 , 3168 , 13765 , 4122 , 5722 , 10660 , 2732 , 3748 , 16574 , 119259 , 3516 , 4174 , 10324367 , 54735926 , 123600 , 2361 , 2725 , 10531 , 42601552 , 3561 , 21138 , 4912 , 2366 , 4506 , 11683 , 4030 , 3055 , 1030 , 3333 , 2247 , 2391 , 2467 , 2264 , 12124 , 182137 , 1349907 , 5405 , 70683024 , 2754 , 16231 , 2333 , 57469 , 2123 , 65837 , 3435 , 2170 , 2176 , 2197 , 1548942 , 10219 , 3639]
1586|B2RXH2(0) [1694 , 36811 , 665652 , 54675783 , 5722 , 63306 , 2391 , 16188943 , 4380 , 824727 , 2426546 , 3240818 , 11622909 , 2478 , 10168 , 2753 , 4059 , 3092847 , 5153171 , 2310 , 1050 , 1548942 , 3236874 , 3126341 , 11790 , 3237465 , 4027541 , 1322 , 660989 , 3055 , 2855211 , 1878823 , 8395 , 612424 , 3168 , 119259 , 2768954 , 1713166 , 666418 , 4107 , 24144 , 911675 , 3138364 , 245369 , 104838 , 2743305 , 549445 , 327045 , 3333 , 4110197 , 10783 , 2453 , 2122 , 2768974 , 4842 , 3474 , 3746037 , 3865676 , 3781338 , 16190692 , 12555 , 2762 , 3114023 , 1967 , 3503 , 157922 , 10531 , 1649 , 2092 , 3138370 , 2562 , 11289 , 19910 , 68872 , 2540 , 3114022 , 3295 , 3698 , 14052 , 228526 , 193949 , 4197 , 10219 , 4021578 , 2466 , 3648616 , 5585 , 3973 , 3324 , 107992 , 2170 , 8144119 , 104762 , 2739563 , 12492 , 68089 , 2315 , 10235 , 2179 , 3885 , 3277 , 2161 , 175540 , 2307977 , 1066 , 3616 , 16362 , 10651 , 3108 , 32681 , 3647 , 3114024 , 2327 , 2178 , 2876323 , 10206 , 1780 , 2435 , 2355 , 4592 , 126569 , 16231 , 6466196 , 2343 , 54677971 , 36303 , 115015 , 5289501]
1587|P25101(138) [9912992 , 14385 , 4912 , 5510 , 3973 , 2333 , 3406 , 2247 , 3698 , 6918493 , 119259 , 4753 , 2264 , 178103 , 4156 , 4843 , 2482 , 5541 , 3748 , 2913 , 1057 , 2170 , 14052 , 4107 , 216235 , 2577 , 36811 , 44623946 , 17134 , 12124 , 2123 , 44112 , 107782 , 13765 , 4855 , 5585 , 3168 , 16231 , 2361 , 54676038 , 182137 , 4122 , 3559 , 1981 , 104865 , 16129778 , 5593 , 2478 , 3117 , 2366 , 159594 , 3151 , 2883 , 35802 , 10531 , 2176 , 1030 , 2725 , 5198 , 3516 , 2484 , 3108 , 1046 , 3055 , 11683 , 5335 , 16574 , 21138 , 2132 , 123600 , 71851 , 54677971 , 5921 , 2812 , 2732 , 10219 , 2467 , 2750 , 11643449 , 4197 , 5405 , 11790 , 1349907 , 16004692 , 3639 , 50942 , 4506 , 10257882 , 2265 , 1547484 , 443289 , 21109 , 5576 , 10660 , 57469 , 441383 , 2754 , 175540 , 31072 , 5722 , 2758 , 4760 , 124087 , 11286230 , 2749 , 3182 , 9910224 , 3334 , 3324 , 2082 , 2435 , 39042 , 4030 , 3435 , 3333 , 131204 , 14868 , 2893 , 2391 , 1548942 , 2753 , 3561 , 4174 , 6761 , 3686 , 3478 , 177236 , 2197]
1588|O76074(50) [175540 , 17134 , 3151 , 4156 , 2467 , 11465695 , 11286230 , 14868 , 119259 , 5198 , 6761 , 4680 , 50942 , 5318980 , 2197 , 4506 , 4760 , 2132 , 3559 , 3406 , 3639 , 4855 , 1046 , 16574 , 3108 , 10219 , 5335 , 1548942 , 3334 , 5921 , 2754 , 1057 , 1030 , 2753 , 3055 , 2170 , 5593 , 2812 , 3182 , 2478 , 3561 , 3973 , 3686 , 44112 , 2123 , 11683 , 2893 , 2435 , 9892860 , 4174 , 3478 , 2758 , 2577 , 21109 , 54676038 , 447108 , 5585 , 1547484 , 3516 , 3758 , 4107 , 107782 , 3748 , 10660 , 110635 , 2749 , 131204 , 5541 , 2264 , 16960 , 3333 , 19987169 , 123600 , 16129778 , 4912 , 1981 , 11643449 , 3435 , 4843 , 31072 , 182137 , 5212 , 14052 , 36811 , 2391 , 3698 , 4753 , 4030 , 5576 , 2333 , 2725 , 35802 , 10531 , 2883 , 151170 , 124087 , 6918523 , 441383 , 54677971 , 2732 , 11790 , 12124 , 57469 , 21138 , 2176 , 2482 , 13765 , 2366 , 2484 , 2361 , 14385 , 2750 , 3324 , 3671 , 110634 , 4122 , 2265 , 3168 , 2247 , 4197 , 2082 , 5405 , 1349907 , 3117 , 5510 , 16231 , 5722 , 39042 , 2913 , 71851]
1589|P29466(148) [31072 , 16231 , 44112 , 2391 , 2435 , 3108 , 24800541 , 5335 , 2753 , 2197 , 4156 , 5921 , 2333 , 5198 , 124087 , 175540 , 182137 , 3334 , 4843 , 3324 , 3698 , 71851 , 2577 , 1349907 , 5585 , 3333 , 3168 , 2799 , 3516 , 57469 , 3406 , 5510 , 2482 , 2176 , 39042 , 50942 , 12000240 , 2732 , 2758 , 3435 , 11683 , 2247 , 2366 , 4855 , 3055 , 2170 , 3182 , 54677971 , 2361 , 2812 , 4197 , 3561 , 10168 , 2178 , 4912 , 1057 , 16574 , 1547484 , 2893 , 12124 , 10219 , 21109 , 441383 , 2883 , 4506 , 5722 , 42601552 , 54675783 , 2265 , 5593 , 5541 , 2484 , 2132 , 1030 , 2749 , 6761 , 2866904 , 2725 , 4030 , 648831 , 11643449 , 3503 , 4122 , 4760 , 11286230 , 14868 , 1548942 , 119259 , 14052 , 153270 , 4174 , 17134 , 10660 , 36811 , 2750 , 2264 , 13765 , 123600 , 3748 , 3559 , 1046 , 4107 , 16129778 , 2467 , 3117 , 3478 , 2913 , 2123 , 35802 , 24144 , 5576 , 3151 , 3973 , 107782 , 21138 , 131204 , 5405 , 3639 , 5288581 , 1981 , 54676038 , 3686 , 2754 , 2179 , 4753 , 10531 , 11790 , 14385 , 2478 , 2082]
1590|P04035(49) [2725 , 2732 , 3973 , 5312662 , 5510 , 3748 , 50942 , 2170 , 36811 , 3117 , 64715 , 2913 , 107782 , 21138 , 54677971 , 2265 , 14309406 , 2754 , 131204 , 3324 , 446156 , 9867642 , 3639 , 35802 , 1057 , 54687 , 1981 , 12124 , 71851 , 4506 , 1547484 , 446157 , 123600 , 3435 , 1046 , 21109 , 5335 , 2812 , 16574 , 54454 , 53232 , 44112 , 5722 , 2478 , 2577 , 2753 , 4030 , 2082 , 2484 , 2749 , 16231 , 441383 , 5198 , 119259 , 5921 , 2244 , 3698 , 4843 , 124087 , 5585 , 68167 , 4174 , 14868 , 1349907 , 2264 , 3406 , 2758 , 3516 , 10660 , 16129778 , 2750 , 11683 , 5593 , 39042 , 2893 , 14052 , 2482 , 60823 , 13765 , 4122 , 2123 , 2435 , 5405 , 3478 , 2361 , 54684141 , 3151 , 2467 , 3055 , 5576 , 3182 , 4855 , 4197 , 5541 , 3561 , 3108 , 31072 , 2132 , 14385 , 1030 , 2197 , 1662 , 54676038 , 4912 , 3686 , 6761 , 4156 , 10219 , 3334 , 2333 , 4753 , 10531 , 11790 , 11643449 , 175540 , 2883 , 182137 , 2391 , 11286230 , 1548942 , 3168 , 57469 , 4760 , 3333 , 5282452 , 3559 , 4107 , 2176 , 17134 , 2366 , 2247]
1591|P0DMS8(24) [2132 , 3686 , 2197 , 3516 , 5510 , 9953065 , 31072 , 11683 , 2478 , 4156 , 2893 , 10133 , 5722 , 2732 , 182137 , 4855 , 5921 , 2366 , 2753 , 16574 , 2361 , 2391 , 3334 , 124087 , 5198 , 1349907 , 2577 , 35802 , 175540 , 7 , 36811 , 21874557 , 2754 , 5576 , 2333 , 5585 , 3639 , 3324 , 4843 , 2123 , 1057 , 14385 , 1981 , 3478 , 5405 , 5335 , 16231 , 3151 , 14868 , 4753 , 3455 , 3559 , 3748 , 3698 , 3117 , 54676038 , 3973 , 44112 , 131204 , 16129778 , 4107 , 4030 , 2435 , 107782 , 2264 , 2082 , 219024 , 11790 , 123600 , 13765 , 1676 , 2913 , 4760 , 10036135 , 4174 , 10660 , 2170 , 2749 , 5541 , 5593 , 10117987 , 119259 , 2750 , 2883 , 2484 , 14052 , 3108 , 2758 , 3435 , 1548942 , 17134 , 1046 , 4912 , 2812 , 1547484 , 11643449 , 2467 , 4506 , 71851 , 10219 , 10531 , 2265 , 2247 , 21109 , 2176 , 11270783 , 12124 , 16071896 , 1030 , 3561 , 9860294 , 39042 , 21138 , 9896267 , 50942 , 44623946 , 3168 , 3055 , 158795 , 3406 , 441383 , 4122 , 54677971 , 11286230 , 3333 , 57469 , 6761 , 3182 , 2482 , 2725 , 4197]
1592|P13945(94) [4753 , 3779 , 3324 , 39147 , 5405 , 16231 , 107782 , 2913 , 1548942 , 3559 , 5585 , 39468 , 39042 , 124087 , 4156 , 2391 , 3748 , 36811 , 2812 , 2264 , 4843 , 3561 , 2482 , 9865528 , 11286230 , 3698 , 44112 , 31072 , 131204 , 119259 , 3973 , 14385 , 4174 , 1547484 , 2247 , 3435 , 4760 , 2577 , 3117 , 439260 , 4122 , 14052 , 3151 , 175540 , 36920 , 4030 , 3677 , 57469 , 71739 , 3516 , 2749 , 11790 , 5576 , 448991 , 123600 , 5722 , 10531 , 2732 , 2883 , 5541 , 2754 , 2333 , 6761 , 4912 , 2361 , 16129778 , 2123 , 14868 , 3182 , 2176 , 4197 , 50942 , 10219 , 3639 , 838 , 2366 , 2893 , 2478 , 21109 , 2484 , 6439232 , 2467 , 5335 , 54676038 , 71851 , 5510 , 2758 , 1057 , 441383 , 54677971 , 2197 , 3686 , 5593 , 1046 , 10660 , 5921 , 21138 , 2475 , 4946 , 155774 , 1981 , 35802 , 3406 , 4855 , 11683 , 2132 , 3478 , 2082 , 12124 , 4506 , 2435 , 2265 , 3168 , 3108 , 182137 , 16574 , 2585 , 1349907 , 2750 , 11643449 , 1030 , 3035442 , 17134 , 13765 , 2170 , 5198 , 3334 , 2159 , 2753 , 3333 , 2725 , 4107 , 3055]
1593|P25103(56) [1030 , 6451149 , 2170 , 104974 , 2725 , 5198 , 3108 , 1548942 , 3055 , 3516 , 9852175 , 5335 , 21138 , 1046 , 11683 , 10531 , 2132 , 123600 , 71851 , 16574 , 2366 , 2812 , 10219 , 5921 , 2467 , 54677971 , 188927 , 2732 , 2750 , 5585 , 11790 , 3639 , 50942 , 4506 , 108167 , 4197 , 1547484 , 5405 , 1349907 , 21109 , 10660 , 2361 , 57469 , 9917021 , 175540 , 5722 , 4174 , 2754 , 124087 , 219090 , 2749 , 2758 , 4760 , 3334 , 11286230 , 3324 , 2082 , 3182 , 39042 , 3333 , 5576 , 131204 , 2484 , 4030 , 2391 , 3561 , 2893 , 3478 , 2753 , 6761 , 4912 , 219077 , 6918365 , 2333 , 3406 , 2247 , 3698 , 14385 , 3086681 , 3151 , 5510 , 2478 , 3973 , 26757 , 119259 , 4753 , 54676038 , 3686 , 4156 , 4843 , 2482 , 2264 , 2913 , 1057 , 3748 , 5541 , 3435 , 14052 , 4107 , 2577 , 36811 , 107782 , 10328936 , 14868 , 17134 , 2265 , 115237 , 12124 , 31072 , 2123 , 44112 , 6450815 , 16231 , 4855 , 182137 , 6918331 , 177287 , 3168 , 1981 , 4122 , 13765 , 3559 , 16129778 , 10311306 , 5593 , 2197 , 35802 , 11643449 , 2435 , 2176 , 3117 , 2883 , 441383 , 9832383]

1594|Q99700(73) [1234, 3240461, 265436, 3238124, 361655, 647884, 310612, 265580, 2725, 107715, 6469502, 10172943, 6603842, 6, 3333, 2247, 21749, 3932, 16362, 11293, 1967, 12454, 246835, 44201498, 1286501, 4070375, 1608140, 3117, 19646, 65758, 10651, 10206, 2799, 3237705, 2113270, 3119467, 2090, 3455, 28688, 5005498, 23009, 3926, 4116926, 3151, 2732927, 160355, 327044, 2927638, 5187962, 4777942, 3168, 101616, 6063342, 1238, 2562, 1369, 2016, 2179, 3094465, 19910, 2265, 68363, 1719874, 3245163, 76915, 1694, 4342, 4487, 3559, 12449, 1811924, 22430825, 225371, 2166261, 26695, 108144, 2740698, 5074, 21138, 10104227, 4454112, 5405, 16190984, 1568843, 4593, 13791, 3503, 255945, 24792601, 3435, 2938038, 2794, 36811, 24792593, 2747, 4122, 3244425, 11289, 3108, 1392, 115368, 16960, 2229, 2812, 3542, 4031, 648075, 2717, 394347, 54675783, 4795607, 2307977, 3246767, 2170, 10219, 441383, 2913, 1878823, 4961961, 3885, 31593, 3746037, 4396341, 3090880, 2333, 16269005, 28803, 1720828, 2466, 19675, 44142959, 45480035, 3760, 2165605, 3404, 3762, 4014178]
1595|P14780(502) [2435, 2132, 1030, 131204, 2482, 441383, 2913, 4912, 10219, 44112, 3108, 2753, 6761, 13765, 2333, 2082, 54677971, 2754, 3435, 5722, 10660, 3342298, 2247, 44302165, 119031, 3561, 10531, 4174, 3559, 15485452, 2577, 3639, 5405, 3333, 2123, 448002, 5576, 175540, 3334, 2749, 36811, 1046, 2467, 21138, 4122, 11790, 2732, 24751752, 4753, 1057, 2478, 16231, 123600, 1547484, 5335, 94413, 4030, 39042, 3324, 2176, 4107, 4506, 5921, 14052, 54676038, 42601552, 124087, 73761, 3168, 5541, 11643449, 107782, 2361, 3182, 114829, 5593, 3698, 57469, 50942, 2197, 54675783, 3748, 128564, 53317936, 1981, 35802, 151506, 21109, 3406, 16129778, 2893, 71851, 1269845, 1349907, 69521, 5585, 14385, 12473, 12124, 11683, 44270901, 3151, 4760, 14868, 2366, 4855, 3478, 2484, 2391, 2883, 31072, 2725, 182137, 3117, 3055, 3686, 10039403, 16574, 2812, 2758, 2264, 3516, 17134, 4197, 119259, 2265, 5510, 4843, 11286230, 1066, 1548942, 2170, 5198, 2750, 16108938, 9933197, 3973, 4156]
1596|P57059(16) [1548942, 16129778, 1981, 2391, 3117, 3698, 182137, 2247, 2123, 2216, 54676038, 115237, 4122, 2159, 3389, 5510, 3435, 1057, 3748, 1615, 2482, 107782, 208898, 3677, 2478, 2753, 39042, 3561, 5585, 14385, 3334, 3182, 3686, 2170, 13765, 5541, 3973, 44112, 6761, 4174, 4912, 175540, 2913, 2893, 2749, 3478, 14868, 4753, 4843, 208822, 36811, 11643449, 2577, 2750, 2132, 37632, 3324, 131204, 4030, 10660, 5405, 4156, 4506, 50942, 31072, 2197, 2264, 3055, 11286230, 10219, 3333, 119570, 2333, 21138, 10531, 4760, 2366, 16574, 5335, 3639, 35802, 2725, 2754, 11954293, 23897, 2758, 40589, 2082, 5576, 2812, 54677971, 11683, 1349907, 11790, 57469, 2883, 124087, 3168, 1547484, 5722, 16362, 4197, 8966, 2732, 12124, 5593, 2435, 1030, 12454, 123600, 2265, 441383, 21109, 2176, 3559, 2361, 71851, 119828, 17134, 4855, 133621, 3516, 197033, 3108, 2467, 2368, 5921, 119259, 16231, 4107, 216249, 1355, 1046, 3406, 2484, 3151, 14052, 38521, 5198, 10624]
1597|P25021(16) [42601552, 4843, 2247, 16231, 11697697, 54677971, 182137, 2913, 2361, 4760, 11643449, 2750, 2123, 2484, 24745335, 3435, 2725, 2265, 115237, 4855, 14052, 17134, 3001055, 44112, 1547484, 124087, 5722, 71851, 10660, 3033637, 5335, 39042, 2732, 10624, 5921, 107782, 4156, 4912, 2333, 2264, 50942, 2883, 2159, 2753, 2197, 2170, 50287, 175540, 4174, 11683, 2366, 9976892, 1981, 3151, 4122, 3389, 1548942, 3516, 3559, 5510, 10531, 1030, 2749, 1057, 2176, 119570, 131204, 17747460, 2478, 5541, 6761, 2754, 4107, 35802, 4753, 36811, 3406, 54676038, 3117, 31072, 41376, 4197, 7741, 11954293, 3333, 21109, 71768094, 3055, 3108, 3334, 5593, 5702160, 14868, 21138, 2482, 14385, 119828, 10219, 5405, 3478, 4097, 3561, 5198, 11286230, 3324, 12124, 2082, 16129778, 16574, 4506, 3973, 1046, 2467, 1615, 1349907, 2577, 2391, 2132, 4030, 2756, 2893, 11790, 123600, 44623946, 3168, 2812, 1548992, 441383, 5576, 5585, 3748, 25070031, 3698, 13765, 2758, 65895, 3686, 119259, 57469, 3639, 3182, 2435]
1598|Q92731(186) [4197, 179337, 5284643, 11683, 11286230, 10660, 5722, 3182, 5510, 2247, 2082, 9912639, 5991, 656952, 656936, 1349907, 12124, 4506, 104741, 3561, 5576, 2484, 14868, 10219, 1547484, 2754, 3686, 21109, 11643449, 13765, 2482, 4122, 4760, 192197, 1548942, 175540, 2366, 2577, 16734800, 14052, 5756, 119259, 2478, 6102690, 2732, 1030, 50942, 5870, 2913, 656953, 2361, 441383, 5035, 5280961, 3435, 3055, 124087, 4912, 2733526, 2327, 131204, 2725, 14385, 11368987, 2264, 2758, 3151, 3478, 10286462, 3168, 123600, 107782, 6761, 39042, 2123, 44112, 31072, 4107, 2333, 3639, 1046, 3406, 1057, 1981, 4855, 2753, 3698, 5921, 35802, 2812, 4030, 4843, 2197, 2265, 5198, 21138, 182137, 3559, 154257, 5757, 2893, 567825, 71851, 683816, 2176, 54676038, 3108, 4174, 3973, 5335, 3333, 5405, 2749, 57469, 2132, 16574, 36811, 16750040, 16129778, 4156, 54677971, 2750, 2467, 3117, 448537, 5585, 10531, 3748, 216416, 4753, 17134, 11790, 3334, 5541, 3516, 2883, 11149479, 5593, 16231, 3324, 2170, 2435, 2391, 6102691]
1599|P41145(25) [2159, 3435, 57469, 50942, 3559, 2197, 5488548, 4156, 128563, 13765, 4197, 5585, 1547484, 2913, 2725, 14868, 1057, 3108, 5510, 2361, 441383, 16574, 4855, 2082, 175540, 5284570, 11286230, 2132, 3698, 11790, 2482, 4058, 21138, 44129648, 3151, 179340, 3406, 3686, 6761, 2123, 5593, 5462508, 131204, 3748, 3561, 1349907, 54676038, 2758, 44112, 119259, 21109, 2478, 5576, 5335, 11683, 66553195, 2749, 4107, 2247, 441278, 3333, 3334, 17134, 5405, 5284594, 2750, 1046, 60768, 5360515, 2333, 5311304, 2754, 3182, 115237, 1548942, 10100, 16129778, 5198, 4174, 3478, 3055, 4030, 182137, 119828, 115208, 4843, 2435, 2264, 1030, 10101, 36811, 10219, 5361918, 10660, 2176, 6445230, 2893, 107782, 2577, 4912, 2467, 16231, 4122, 5288826, 123600, 2391, 3345, 2265, 31072, 3973, 3516, 3168, 44623946, 5722, 4753, 2366, 2484, 35802, 1981, 14385, 3117, 5284569, 14052, 124087, 5361092, 39042, 5284596, 2812, 13493, 5284595, 2753, 22267, 644073, 5541, 54677971, 71851, 3324, 3639, 11643449, 2883, 2732, 5359421, 4506, 12124, 5921, 2170, 10531, 4760]
1600|P41143(16) [4843, 3345, 2577, 10101, 4174, 10668, 2435, 2264, 3055, 182137, 36811, 5405, 2176, 31072, 5361918, 3973, 4912, 2893, 5288826, 4030, 11790, 2265, 16362, 10531, 24762741, 5510, 2484, 16231, 3168, 123600, 5284569, 1981, 2391, 2366, 124087, 2750, 5361092, 3455, 4122, 5722, 11683, 3516, 4753, 3955, 14052, 35802, 3117, 54677971, 44112, 13493, 39042, 5359421, 10219, 5284596, 22267, 71851, 3324, 3639, 11643449, 5284595, 2753, 5541, 2883, 13505, 5462508, 2732, 2159, 5921, 3435, 57469, 5576, 6761, 2467, 4506, 50942, 2197, 5488548, 4156, 10624, 4760, 5198, 14868, 3559, 441383, 16574, 14385, 4855, 1057, 13765, 4197, 11286230, 12124, 2361, 5585, 2913, 2132, 2812, 2482, 2725, 4058, 175540, 44129648, 2082, 5284603, 2123, 2170, 3406, 5284570, 1547484, 3698, 5593, 21138, 3108, 3151, 5284371, 119259, 3748, 1349907, 54676038, 2478, 2758, 5335, 131204, 441278, 3561, 17134, 5284594, 1046, 5311304, 3334, 2754, 4107, 107782, 10660, 10100, 66553195, 2749, 119570, 21109, 2247, 5360515, 3333, 3686, 3182, 3478, 1548942, 1030, 16129778, 2333]
1601|P25100(13) [2123, 148842, 4855, 16231, 182137, 3559, 5593, 216249, 11286230, 3117, 1547484, 3334, 164089, 4184, 3151, 5576, 39042, 3677, 4030, 2176, 38521, 131204, 2818, 2391, 2753, 1030, 3561, 2159, 2725, 3168, 5722, 5510, 3033538, 2265, 164739, 2333, 2484, 2247, 3108, 11683, 5335, 3686, 2478, 16574, 439260, 60602, 21138, 119259, 4753, 2132, 123600, 54677971, 2368, 72106, 4843, 2732, 5541, 10219, 2750, 2913, 11643449, 4636, 3435, 14052, 5405, 1349907, 1057, 2577, 5585, 21109, 10660, 2812, 17134, 12124, 5312125, 44112, 107782, 4760, 2754, 5265, 175540, 13765, 31072, 4174, 2758, 124087, 33625, 4122, 2749, 1981, 16129778, 3182, 3324, 2082, 4893, 3822, 3333, 2361, 2883, 35802, 14868, 2893, 1548942, 6761, 441383, 4197, 5074, 3478, 3157, 6082, 14385, 4912, 5073, 3406, 3973, 5198, 3698, 3516, 5816, 3869, 208898, 1046, 3055, 10531, 2435, 2264, 5775, 2366, 4156, 2092, 2482, 13542, 71851, 5401, 3748, 54676038, 119570, 5921, 2170, 5268, 4107, 2467, 2197, 129211, 36811, 11790, 3639, 57469, 50942, 4506]
1602|P10636(83) [11286230, 6624620, 1829960, 24239, 101744, 6063342, 11790, 2758, 15474019, 107715, 648831, 2732, 4912, 3151004, 1780, 2913, 68186, 1967, 4592, 16362, 1810986, 21501, 50287, 2435, 2179, 5282060, 2247, 3116068, 54675783, 2950, 5593, 115015, 10168, 19910, 11061, 2855211, 547914, 3245131, 1322, 114924, 6472251, 2392140, 36303, 24867796, 3034012, 78933, 1896320, 3244194, 2265, 219269, 115150, 4362, 10235, 89105, 3237465, 2169358, 911675, 10114, 3686, 1548942, 2147557, 3885, 3610, 2812, 3108, 6301, 3117, 100016, 1811924, 16490, 4122, 3478, 3082, 10230, 3277, 2315667, 265580, 3455, 3435, 11289, 2197, 5917, 3244425, 5185709, 107782, 44112, 10206, 6603842, 26937, 14878, 1993, 2333, 5722, 2743305, 100095, 4760, 104826, 361939, 3316, 2894446, 1066, 3138364, 5480, 12492, 3503, 296597, 5153171, 141870, 50248, 1649, 2768975, 2750, 10382715, 14868, 1694, 3698, 72139, 2799, 4380, 10219, 76915, 4278, 1568843, 949760, 8269, 4343310, 5074, 1878823, 123409, 13791, 5405, 3168, 36811, 122623, 5510, 8609, 2396, 446816, 3138370, 3138330, 612424, 2327, 3242381, 3138375, 361655, 5475, 41684, 10245972, 6603901, 10531]
1603|Q01959(74) [54677971, 57469, 4156, 5722, 119828, 182137, 2482, 2391, 2247, 3182, 2801, 101616, 17134, 2159, 2913, 4107, 4528, 10531, 11790, 4197, 10624, 2577, 11643449, 65650, 4912, 11597698, 2758, 2361, 2750, 444, 2435, 2753, 3639, 3561, 2366, 2264, 124087, 3748, 1981, 9860294, 119570, 14868, 54676038, 2812, 25070031, 4174, 14052, 54841, 2467, 11430856, 2754, 2749, 16574, 2265, 115237, 2170, 1057, 2484, 3516, 5585, 5584, 3435, 1547484, 3151, 5921, 4506, 11622909, 3406, 2176, 5541, 1030, 6917779, 4753, 3168, 1349907, 2893, 16129778, 3686, 5335, 2197, 11286230, 3455, 13765, 3675, 107782, 6761, 4760, 4855, 4158, 3389, 3404, 40589, 4020, 21138, 5210, 4843, 16231, 125017, 1614, 10660, 1046, 175540, 2732, 5198, 10219, 3973, 71851, 119259, 154101, 5593, 39042, 36811, 3117, 5826, 1615, 2333, 11683, 2137, 2478, 5510, 50942, 3334, 131204, 5576,

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1604|P22303(94) [2131,
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1616|P23975(57) [5722,25070031,5002,11430856,2754,4158,4174,65856,2478,5576,2749,16574,2893,1614,3151,3404,449193,3698,65650,2732,11643449,1547484,5736,2750,2435,36811,2176,2995,2771,11683,1349907,119259,3168,6917779,119828,2812,4543,14868,1355,2467,2577,5541,101616,4976,6761,2265,2913,1057,5510,4528,50942,3334,11790,125017,21138,5585,3435,4197,2883,10531,16231,3055,35802,21109,3333,2368,2361,1046,3639,10660,34869,3696,444,2484,12124,54677971,5584,2753,23573,1981,5593,4912,9860294,39042,182137,3455,5335,54841,3947,54676038,31072,2082,16129778,175540,2391,3108,123600,441383,4855,3516,17134,2159,4843,5656,3973,2160,4500,5210,38521,2801,3478,5921,2366,5198,14385,4506,2123,10219,57469,4753,3686,4156,44623946,4760,2482,3561,2333,11286230,13765,4020,3675,9838022,119570,2197,107782,2132,131204,2170,3182,3748,3324,2725,71768094,3117,4107,3389,2247,44112,3559,40589,2758,4011,10624,5405,1030,4122,42601552,13542,4449,4030,2264,71851,124087,11622909,60835,1548942,3406,14052,5826,1615,115237]
1617|P21917(31) [1349907,2812,2577,4122,54676038,2467,2478,16363,2366,16574,688272,71851,2818,3686,124087,2391,10775317,4452,16231,21109,10039198,36811,2197,31101,14385,14868,2750,10705550,3341,2484,2758,219050,54746,3639,123600,5593,10531,2753,5330286,1238,443951,3117,115237,2435,4850,47811,3334,60149,37459,681,49381,44112,4174,3333,12124,10667966,13765,1030,5265,2749,6761,2482,4107,21138,107782,2159,2893,50942,3964,10219,2726,6005,5566,4420454,3406,59227,441383,2448,184841,182137,2732,4506,119828,3561,2754,9860294,2333,5440,11286230,10824155,10420539,54677971,16,2725,5541,11954293,3168,2247,4912,1981,2176,10660,4030,28864,4855,39042,3478,119259,5198,2913,3151,1547484,3516,10116877,17134,3055,131204,11643449,4917,5722,16362,3748,2265,5585,5576,16106,1046,133079,119570,2170,5510,31072,11683,6918248,2361,3973,16129778,57469,5921,5736,2264,3324,3389,4753,11790,68950,4156,3435,2123,3698,10624,4197,2883,2082,1615,5405,14052,5335,1548942,3108,4760,57267,5074,3182,4843,115368,35802,2132,54562,1057,175540,3559,23897]
1618|P11473(346) [1811924,3245163,11061,161562,5288670,288875,612424,3559,124087,6918508,16315,17931,31957,10212,2540,3117,3080557,2333,3698,37175,122077,16269005,3420746,27812,115368,3762,13789,25644,5281107,101616,3746037,20055510,14899645,1057,2170,3237439,25102723,5283734,1967,2950,11350,65790,115150,3503,2812,549445,1322,32681,28803,3082,2090,240112,24776445,7352,2396,2161,10382715,6603901,2450,2194,18573632,3237465,3286,6194,13986,12713,121871,2743305,71905,11967809,3109,7916,115015,6764,2453,16347,5074,3120949,10868,5392,5480,2330,20906,24144,6063342,1046,12449,31200,18104,4278,104850,3885,24361,16362,3760,6,3138375,649156,16837,10672195,219081,108143,2179,6915835,911675,11088,19996,3032279,14868,115157,5288783,7347,20055424,6237,41684,15474019,2017,31475,11683,17434,18573525,3610,1694,14190,6982,10168,1052,10404,1781,542364,3002119,114924,8189,3686,16590,2327,11852,194699,122623,2799,10114,19910,72139,5282060,3244425,15286,13521,5281104,10172943,53708,13113,1238,2794,76915,2435,132862,4680274,446313,3415217,36303,3969,3277,11006,10245972,35455,39299,5289549,10041070,16490,47472,1369,3561,2893,5280453]
1619|Q504U8(0) [2754,4506,1046,11488320,3973,3025986,17134,71851,11620908,5585,35802,3038522,11442891,11667893,11511120,2333,14385,31072,11338033,2396,2758,151194,16722836,5198,119259,14052,10297043,9549303,5335,447966,6419766,176870,2467,3505109,5921,10127622,4912,156414,10296883,1981,176167,3478,2366,3698,3516,10401956,441383,3108,1547484,44112,5329106,2856,17755052,15983966,21138,11712649,2132,3686,12124,2264,3559,5722,3324,6761,123600,39042,11213558,36811,5510,2753,10302451,24794418,2883,2123,54677971,54676038,2577,2478,11640390,10660,3055,107782,10427712,2484,50942,2749,16574,6918454,131204,14868,3639,2750,2170,2247,57469,4174,2435,11643449,11552706,10531,5005498,21109,447077,153999,448008,5593,16129778,2361,2913,24779724,2265,3151,2732,4107,5405,5541,5576,1548942,1030,4030,3406,3435,11790,4753,208908,11409972,4122,24889392,11485656,11683,4760,13765,175540,3117,3333,10219,2391,11608401,76098,2197,3334,2176,22024915,11286230,2482,2893,2725,3182,10113978,2812,46937083,1349907,4843,182137,11656518,4708,1057,3748,124087,2082,160355,11314340,11427553,11364421,16122633,4855,3168,4156,16231,11234052,3561,10074640,57379345,4197]
1620|P41595(22) [5011,3406,5198,131204,16231,62065,5074,11954293,5405,31072,2893,21109,5576,5335,1548942,2176,124087,2725,4199,71851,1030,3055,4912,1046,2264,2333,2247,54677971,71202,8226,1614,107992,11683,28693,4843,14385,68848,11292933,11961293,50942,31101,16574,4753,3478,60809,12124,3559,5510,57469,1355,54676038,2750,5362436,5533,896,107782,1547484,2913,68186,17134,10531,3333,3561,177336,14868,1057,2753,115237,119828,219050,2754,4107,3639,2197,5722,2366,2123,10660,4855,2435,2132,54746,3168,21138,27400,11430856,82148,8969,2265,4184,3108,3117,3973,2484,5585,4122,4760,2818,4850,1615,2082,47811,54562,3822,2467,6761,44623946,2732,2883,3334,441383,35802,114709,2482,11790,5265,36811,5593,4174,3698,28864,11658860,5921,6005,5541,10219,11604525,4828,11286230,9805719,443951,119259,119570,16129778,4506,8223,2361,39042,448400,3324,1349907,10624,2577,

182137,4197,175540,2758,11643449,4106,2478,2749,4030,3435,4156,2159,14052,5160,5568,71781,2170,3151,2391,1150,13765,3516,5311271,3748,123600,5268,2812,3386,44112,3182,1981,3686]
1621|P07550(200) [146294,2577,11790,3410,2749,3442589,1547484,119259,4753,4030,1057,2482,14385,9860294,10531,124087,2265,13765,155774,39147,16129778,71739,9892481,17134,6761,107782,4156,2753,5253,36811,9865528,39042,31072,39468,4946,5510,35330,6918554,2197,2725,4107,31729,11954293,1234,2893,115237,4843,3117,12124,2170,2783,2361,44112,3055,11683,3108,5405,2159,3561,5585,3435,2083,19910,3168,5722,2369,35802,2176,2132,50942,5403,4828,3516,1355,16231,1030,16574,5198,1981,16739244,119570,4506,54676038,1046,2249,3973,3748,32051,2475,2264,4171,3389,175540,3151,3559,2758,1349907,9294,5335,14052,5541,2366,2883,4845,4932,2750,2391,4760,33624,2467,5593,3639,2333,2435,11643449,2754,3677,4916,10184665,3406,44623946,3343,11505444,5152,10660,3779,57469,11504295,2913,131204,4086,6917655,1615,54677971,4122,10219,11286230,4197,123600,14868,441383,2585,31477,3698,54766,63952,3333,5921,2082,37990,2247,182137,21138,4174,1548942,3478,5816,3762,2478,5576,21109,2123,4912,3334,3869,3182,71851,4855,2119,3083544,2484,3324,2812,71768094,3686,2732]
1622|P20309(71) [10938,5576,2883,11519070,2448,4848,119570,4197,11683,2732,50942,4634,4107,443879,36811,3561,174174,441383,2342,14868,9577995,2484,2753,1030,2750,10090005,2749,2551,2265,44419370,3748,3334,2725,5510,107867,16231,16362,2247,3333,2435,21109,12124,5440,4174,2176,5593,3494,44112,5541,187,115237,442021,3435,6126,154059,4753,31072,182137,5198,16129778,54676038,9571002,2467,2754,11434515,5314,2082,2913,2577,2160,444031,5585,16960,441071,5910,50906192,2361,55752,4629,2132,119259,14052,2478,10660,39042,5921,71203,2812,2229,6761,3108,21867154,3686,3324,11643449,1547484,3389,1349907,1057,2159,2366,3478,11790,5722,49381,107782,3168,5335,2170,3973,35802,5405,37632,3182,3042,17134,15376,2230,71851,124087,131204,5487427,54677971,11286230,3559,2758,3117,10219,1046,4760,1981,4122,10531,16065403,23897,21138,16574,2893,14385,175540,1548942,2391,57469,3055,24199,2370,4855,4506,2197,50906191,3406,13765,40589,3698,9860294,4843,60809,50905989,1993,4156,4912,71183,3639,4934,4030,2123,3151,44623946,3516,2784,2381,123600,1615,2482,2264,2333]
1623|P43220(51) [2795,3241177,16363,16157882,45480035,19675,3236724,327045,17113,38531,2081,131411,16188984,187,50248,2799,12454,11289,11310,2220273,2466,3442589,2132,16574,3245025,166553,10172943,801418,1580955,11104,22530,2294842,68943,3828,3758,16231,3127904,3125446,65800,3760,13505,192197,11954283,5918,16187479,2762,588415,16347,3286,1719873,68634,2315,13450,3002820,31729,441383,5359646,3671,288875,204105,37175,446816,67686,3334,119570,108144,310612,3245385,2812,26695,5335,265580,2229,249,123606,115368,44278361,193949,3734228,6301,76915,1552036,6470206,3003803,2361,547914,11643449,2179,614669,2998359,4197,24792593,2016,5510,660989,1878823,98514,3333,24792601,24466,1599306,16191546,1937568,55483,16362,2137779,68684,16639,13789,5074,660708,3245402,1608140,268472,4655877,3351,1432578,175540,1811924,661085,12124,68363,21138,1234,10206,680935,5585,2082,2983151,10651,45480040,808378,3094465,1720828,19646,72462,101744,7329,6063342,9551522,5389584,3168,2453,327044,1568843,1993,10212,2359114,151506,42725,2247,2132993,4619,10517,18573524,19910,394347,5723,581148,6,53708,12555,3940466,16190941,776717,7475368,178144,3542,3746037,68089,2315667,5005498,12449,3559,2090,19003,8395]
1624|O94782(15) [14868,3433,3610,68089,31072,3316,23897,6603842,3326,2092,14878,2333,2396,19646,3117,11289,7572,21102,5381,1392,3936,35375,3005573,193949,6603901,6708773,2750,156419,114811,10206,10651,115244,1967,1892,27448,159977,16362,11046239,5531,61574,175540,2883,5392,14759,68363,5063962,3926,13791,2318,2893,68186,248271,15443,1046,107751,4890,17931,2446,19910,20906,11967809,10718,3759,243274,50259,5282060,361655,10235,4380,108143,71645,104850,10219,3969,2366,192197,47472,22571,7329,2724,1548942,3828,3435,2377,5074,3312,2794,11286230,3607,31475,11412540,3515,31060,2090,27812,3474,2170,104741,4670,2017,107867,11683,26533,2161,3333,2200,67686,3503,4487,4122,1549789,21138,4031,2540,122081,3277,11104,41109,71874,3885,2179,43231,2194,3108,3736,24107,4006,14899645,8798,3741,50248,122077,8138,9363,32170,10831,51040,10212,196122,3698,2812,13986,54676038,11296583,16837,10046567,16351,114924,6764,6237,68909,2576,21414,1238,5405,2330,2799,115015,194699,10531,2484,7191,1547484,2315,2247,5289501,666418,107715,18104,65909,1694,13505,94280,16490,3760,5510,13916,8609,656641,56463,13765,10114,3455]
1625|P04150(213) [4506,3503,17134,5289501,3333,2082,2366,5921,21109,2812,16923,153909,2391,11006,14052,3324,44112,10219,1057,182137,12589,2735009,3182,3559,3435,2132,247839,444036,5281004,3698,1981,31072,10133,6741,16129778,4107,16490,2247,2123,6,8196,28803,3973,2577,3108,9865442,2333,9576789,5198,2749,4843,2725,54677971,13765,2893,4912,31307,4156,3516,41684,11660,5865,14868,2197,123600,2478,28594,443936,4753,7903,15433,107782,4760,5311505,57469,4174,1548942,11683,5335,10168,2264,1547484,3117,9642,16574,5754,32798,1046,3478,2758,6545,3406,2176,16734800,4122,2435,5755,124087,12532,2170,6761,61186,3686,131204,25644,2482,5405,11286230,5576,7347,3748,7329,11852,6505,5743,6215,16231,71851,3034285,6436,3639,6918155,9782,2750,2484,5510,55245,3082,111332,4030,11643449,3168,36811,441383,21138,5585,71414,50942,21805,2883,10531,2754,1030,31253,31236,3334,119259,10660,5311067,115157,2467,2732,3151,11293,8907,441335,84098,9878,3055,35802,175540,2753,39042,12302,1349907,54676038,82153,2265,121752,443958,14385,5593,2913,2361,5541,3118,3561,4855,4197,114924,19996,12329,444025,12124,11790,5722]
1626|P21728(41) [17676,4506,14385,5311360,1981,11286230,4843,16,2265,2264,4197,31101,4107,5335,4912,123600,3404,3973,54746,2725,1057,2818,3686,10783,2749,3406,31729,175540,107715,52919,3435,50942,5593,1649,441383,6603842,2170,1030,53708,4760,5198,5452,11954293,1614,1238,1548942,4174,2758,9860294,11643449,4814,3639,28864,5921,3341,2732,71851,2750,361655,5281881,3561,6077,11683,182137,10624,5722,119828,14052,35802,3389,3117,16129778,4917,3748,60820,8226,2484,5265,2478,3333,44623946,10219,6005,59227,14899645,131204,2435,2159,107930,1349907,2883,681,5585,124087,4855,5510,3334,115237,2726,107782,2123,5541,16231,42601552,2176,5405,1547484,39042,16574,13765,3559,3108,1355,3932,57469,3372,2081,3516,2482,2812,2893,36811,31072,4753,3055,10660,2132,11790,2333,133621,12124,4156,10531,14868,2467,3885,2753,3698,3478,5074,21138,28688,4592,3151,4030,208820,1615,2082,18104,16739244,3822,49381,4122,23897,2247,16362,54676038,5440,2366,119570,2754,54677971,21109,6761,3324,16960,11154555,119259,1046,17134,37459,2197,2577,5576,68950,44112,12454,2913,3182,6603901,47811,3503,2391,4593,3168,2361]
1627|P16473(93) [15394,3239339,8124,4814,28803,666418,2478,2137,208820,26695,3671,2725,3655,3455,3236383,3559,123600,41684,25644,2159,1066,954161,2812,3245385,2133505,175540,81530,10423,101616,3973,6605037,3245025,2355,2754,160355,2753,2576,2053712,5921,4843,7915,1649,10651,3333,28688,2717,26596,3760,655287,2562,53708,4031,228244,3245163,3672772,16316,4197,3245451,3830,36811,3758,11790,19266,47472,665087,1989,4380,5335,10382715,2216,104762,144457,11293,6598,3034012,22530,1993,21138,2170,1238,647884,2365,2090,6605027,16362,170344,8041,2391,660883,133621,2762,3117,6605039,3244425,2930983,249,3326,31253,2333,2836838,2419371,5593,4278,1861634,361655,1815815,3244430,3610,12968,3245931,3969,2950,3238134,2758,4493,10114,6077,68872,2315,2750,8872,7819,54676038,25914,26533,2179,107715,7352,61247,2482,2277,61410,3243710,5723,2200,3478,2166261,25134246,2913,652355,6605024,2396,647201,55918,4122,1046,31475,4578,665652,19996,10168,648831,2132,1701,547914,3237649,11,3542,11245,3002119,2377,10036135,4156,28594,16231,3108,37175,20686,5074,10237,441383,16637,1234,18510,14242,1967,2343,3242198,8095,3239387,115244,4761,11289,101744,645503,6540,3125057,25670]
1628|P28335(38) [3964,5736,60809,2467,1355,2732,8226,2082,2482,124087,1349907,2264,115237,3334,3168,3389,3324,4585,107992,5566,8223,448400,3973,2132,28864,1615,5335,2577,16574,2197,54562,60795,3406,441383,10219,3516,11292933,82148,2726,119570,23897,4636,1238,5533,2812,5160,5073,5011,4184,31072,3108,2435,39042,5265,28693,14052,71768094,4855,71851,9860294,4122,44112,107782,55752,2750,5576,5722,2247,16362,2754,11954293,3435,5452,4030,1548942,17134,10660,71781,219050,4760,60854,3822,10624,4912,68848,21138,14868,12124,33630,4156,11604525,2758,5198,2883,5593,11683,4106,2366,2893,2484,1046,1150,54746,2333,4506,2159,68186,2391,57469,4174,10531,5074,2170,2749,131204,60835,54677971,3478,123600,4843,71202,5311271,119259,6761,1030,4107,3748,16129778,443951,54676038,62065,2361,1057,2913,35802,

2753,4753,13765,11790,11643449,11430856,4449,4748,4197,175540,36811,5541,60149,16231,3686,4205,2123,1547484,21109,9805719,5585,2478,3182,197033,47811,182137,5405,3117,5761,3639,3698,14385,5921,2818,9966051,2176,11286230,11961293,3561,3333,3151,50942,6005,5440,62865,3559,3055,11658860,27400,2725,2265,5510,11683556,31101,1981]
1629|Q96QE3(10) [3781338,1720828,16187479,24978701,1238,4380,2286863,3108,3117,2888937,3973,2914644,660708,2724,2768975,4097,16362,24791741,1701,954161,1599306,3420746,2265,539709,647038,4163388,44602029,4961961,3455,680935,542364,162834,2831167,107715,8041,76915,54677971,4843,3334,65758,3708374,44144252,208820,3503,2179,4487,1046,886096,16574,3542,228526,10219,55918,4777950,1967,31729,11683,70846,4578,2913,647201,2090,3156709,10258,3813687,24817214,3326,2812,4564,53708,911675,10832,4493,10767,2291046,3151,44142242,10531,2827330,14369,1614257,2435,3237465,3168,348986,28803,3240818,1432578,4983363,6,1937568,2197,1392,133621,68363,14604,5585,4122,100472,265580,1863658,18573632,268472,4278,288875,6603842,1811924,4593,1694,19646,17113,3236874,1568843,1608140,820311,756673,5405,100095,5074,2291103,21109,3926,2082,7699,1878823,5917,4103738,3842920,18573526,4343310,160355,549445,5459650,5804,24817194,16269005,2914308,44201975,2234553,327045,24792593,3377088,3433,3698,4366092,3238134,2359114,5510,3139316,1985,7475448,3559,16129778,3236724,4404908,3246760,1552036,194595,1580955,3237655,2277,16306185,3748,2999850,750895,3351,3230434,42725,703905,2753,16190945,3940466,660989,3138330,4261,3095276,361655,1745499,3746037,3238726,4622,12454,3094465,104741,2855211,16059888,3474,3333,5289501,655083,3295,2482,2997734,3730,824727,19910,3885]
1630|Q16539(188) [3324,2391,17755052,5405,11314340,3151,46937120,16722836,2082,2176,2435,9871074,5171,2333,4912,10297982,2366,4174,11364421,160355,16129778,5326869,4506,11427553,17134,54676038,3698,57469,16574,11338033,5287728,3406,2478,10531,2484,5326871,3435,2893,2132,21138,2749,208908,25174101,3561,11790,12124,24963046,176167,6419766,10275001,3108,5541,3973,2725,11667893,11608401,10341154,441383,4369443,2812,35802,15991573,131204,16220188,31072,446816,50942,76098,16231,2170,5005498,2577,2264,5326868,3334,1349907,4122,1057,1030,5327066,2396,4760,5510,42647299,447721,447077,1694,3078519,10113978,2361,2467,9865587,2123,448008,1547484,3168,119259,3542,1046,10074640,3478,10409068,156414,107782,3540,3686,11234052,2265,6761,3516,11643449,11485656,10296883,10172943,22049997,24779724,4156,176870,14385,12106168,5921,5172,36811,5164,182137,3038522,11683,6918454,4030,10427712,3025986,5576,15983966,11656518,39042,24889392,2352168,44112,5198,5289514,5593,2754,1981,153999,3639,54677971,4843,11712649,175540,11406590,4855,3333,2883,10127622,3008319,3055,11442891,21109,3748,1548942,24941253,9549303,3182,447966,124087,71851,5722,46883775,2753,5326866,11373432,151194,2482,2247,11409972,4107,4753,10219,3117,10660,2856,14052,16122633,2197,5282440,129236,11213558,5326870,4197,5335,2750,2913,5585,11286230,13765,11552706,2758,2732,3559,123600,11714580,14868]
1631|P35367(24) [39042,2482,2444,131204,2726,2267,14868,1057,23897,2732,4506,3241,10531,2818,3686,3055,1349907,9860294,3964,2812,33036,3103,164522,65895,14677,10219,37632,16739244,55482,50287,2391,3396,101616,3957,2176,175540,4030,10660,5510,11683,11954293,3478,3698,71768094,71851,3973,2082,2350,5585,24745335,5440,5593,2170,2564,31072,4761,5576,40589,3516,2484,3324,2750,4753,3333,2361,3182,4107,5736,44112,441281,14052,10624,1238,119828,2197,2435,11790,65820,107782,21855,14385,941651,4174,4156,10237,54385,3658,2749,119570,2132,3117,4760,3406,2123,5541,4992,13765,2366,5284514,5566,5587,2342,26035,441383,2478,65906,4843,6834,4066,124087,1547484,3561,36811,2333,9976892,2467,16574,11643449,2577,2795,2247,26987,44623946,2758,5921,5574,3168,19371515,3639,21138,17747460,5198,12454,1355,3151,2754,4615,60854,4912,57697,1981,2265,3827,16129778,6729,119259,3219,11286230,54677971,2725,11697697,2200,11291,3372,1046,4855,16362,123600,3748,5282230,1549000,2753,115237,15723,2160,5281071,6726,1615,6918314,17134,2913,6761,4197,3334,3389,2883,774,42601552,5452,1548942,60795,4830,19861,5282443,3108,2264,197033,170336,4940,5073,5002,5405,182137,133017,16960,3559,5722,57469,12124,50942,60149,4927,3348,25070031,1030,41376,2159,4122,3100,35802,54676038,3162,16231,5335,21109,4748,4585,2678,3435,2893]
1632|P28223(101) [4830,5533,13765,23897,60809,11683,2812,3151,60835,62065,3168,16106,47811,8226,3686,941651,82148,54562,54746,5452,2082,4174,2123,12124,1547484,1548942,11961293,9805719,6005,8223,16739244,2725,27400,4760,71768094,35802,1981,5335,25293,3559,4585,3389,36811,3561,4843,71202,10071196,4449,5510,28693,10257,2750,5576,2478,54676038,1046,448400,1001,11292933,107782,40589,1349907,10219,5160,11286230,2482,119259,3334,3748,1030,4122,16129778,5311271,14385,5198,11697676,119570,14868,11683556,50942,10531,55752,16574,2749,443951,21138,3478,3396,3372,3516,44112,5593,10624,123600,5761,4753,9821951,60149,2754,4506,3108,37632,60785,3333,131204,2435,16007088,71851,16231,16362,5440,11954293,3055,2132,1150,4107,5074,10660,5722,54677971,4156,3964,2265,6761,37459,3182,2170,60854,28864,5585,60262,68867,11430856,130918,3973,2333,2247,5002,3698,3822,4912,2758,31101,4078,4184,5921,3404,71351,49381,125564,5541,62865,3406,4030,2893,31072,2484,4748,21109,11643449,2732,11604525,39042,11658860,2467,1355,5405,2726,5736,4106,5073,2883,68186,2818,6918248,3435,2366,71360,11790,197706,60795,175540,219050,4197,2176,124087,1614,107992,2264,12454,5265,5011,2361,2913,119828,441383,14052,2159,17134,9966051,182137,4205,71781,68848,2577,1615,115237,4828,197033,3117,6077,2197,3324,3639,4855,1057,5566,57469,2753,2391,9860294]
1633|Q5JWF2(180) [228244,327044,2179,2754,4163388,2894446,651353,3091626,28803,650908,3261980,2938038,6063342,50248,4295316,770040,2291413,4118928,3241521,593113,12449,351111,657534,2865112,3442589,2735646,2165979,1369,246835,5389584,808378,11289,24793507,3127493,25134246,2898508,22430860,31475,13752,657977,294256,736069,3156690,5541,3236575,4337923,647038,3237705,3245285,651913,2304617,3238739,3708374,2819985,5240507,1870615,4103738,14604,24793326,3244583,16410213,3126762,19646,234387,16060802,3239387,1870753,801418,2827330,24792050,23009,1473386,3239879,2174167,3799111,4843,893703,3236588,3237465,2984762,3136028,3235671,316274,10133,824155,3145395,267368,332697,3236383,894690,3245402,3095236,44144252,2802499,35758,2834684,16190984,602681,2836838,24761713,3243710,41109,2737716,1286501,2846481,1815811,6472026,2016,246441,843822,3245025,16191563,3156762,8395,4396341,658099,22430904,24466,10104227,1973720,581148,3969,265436,2806901,607728,7329,3639,238499,4343310,3237649,3842920,5187962,645503,683816,3235986,3236583,223613,24816706,1811924,2426546,2763709,68634,722193,6470206,4624023,2162118,16190941,976292,3239200,3244430,660051,31236,2361,1815812,3836519,265341,806859,6624620,3236874,3240006,2180707,22530,3239339,3764070,3240442,3648616,2133505,3240403,5074,3108051,2090,13789,903966,2812,3243609,3090880,3865676,265580,19003,4343274,24856310,361939,3236724,2166261,1530100,3136361,4030278,10219,16306185,26695,100095,4659978,3603333,1810986,3236681,44201975,549445,3731631,535796,3245411,2844395,3551080,657677,660883,1082702,3242288,3243850,660688,788502,240112,1745499,24856270,3244292,3236558,2355,2795,2904782,71209,652720,3246767,573613,3244425,296597,3420746,3242481,2763377,2768974,21749]
1634|P14416(110) [2448,3108,3334,57469,21138,115237,124087,125564,6918314,2482,4926,10824155,9826744,2883,3748,57242,5405,4850,1355,14868,681,4855,5541,4843,3516,123600,3055,3973,2123,131204,2818,16739244,107782,2754,14052,2893,6005,10219,1046,3372,42601552,4753,2197,2812,16106,2247,2333,10420539,10660,3151,1615,3388,5736,6761,5074,115368,3559,31765,36811,12124,208951,4168,4030,37459,4585,5576,2753,5335,3478,197033,4122,5921,11790,3182,2366,62867,10705550,10116877,16363,3324,2342,2577,47811,219050,11430856,1981,17134,5355,68950,4107,119570,21109,4748,2725,55645,54677971,9818479,18104,11154555,119259,6918525,71351,175540,16,44112,688272,54477,60820,667467,23897,54746,3964,114840,5440,4912,52919,4506,4078,60795,5510,2170,5198,27400,5826,2361,2478,2391,11978813,3033769,1238,37632,2265,12454,10836,14385,2467,60149,5002,2749,2913,5073,4174,2264,2580,1614,11286230,3389,10531,2732,40589,2082,2484,54676038,2159,10667966,5593,11683,182137,441383,3698,1057,5095,1030,68634,2132,3686,11292933,10624,4528,1547484,3406,4197,2758,4917,444254,28864,3396,50942,4760,3333,3168,71360,5281881,5330286,35802,3117,60854,11697676,10039198,11954293,1349907,9860294,2176,119828,10775317,4420454,60809,11643449,54562,3639,16231,17676,2726,3561,6077,15443,71851,5722,31101,5566,2435,44623946,443951,16129778,31072,1548942,59227,39042,4156,57267,5585,2750,3435,13765,5311507,16362,13542,187,16574]

1635|Q5TCI8(0) [2754, 1349907, 3516, 2123, 2577, 1548942, 7347, 5459650, 157922, 4030, 6855, 11683, 6604423, 2132, 192197, 41684, 3639, 31343, 4030278, 1057, 35375, 2435, 10831, 5480, 10783, 598513, 1967, 3108, 3236874, 11088, 123606, 3002820, 2883, 17113, 3969, 115368, 2576, 3433, 3724, 3503, 1488408, 2762, 3005573, 14052, 10770, 3333, 104850, 26533, 4760, 4487, 2913, 3885, 16363, 3182, 16015629, 3686, 2794, 14868, 4578, 3760, 124087, 2562, 55918, 3677, 10036135, 3926, 3973, 3117, 2365, 4770, 152951, 196122, 3074827, 8569, 5722, 10850, 2176, 2377, 3781338, 3542, 51040, 4506, 660989, 1234, 6237, 1985, 16231, 2758, 2998359, 1694, 16190945, 3245285, 2178, 6127, 37175, 33925, 15459, 21138, 10382715, 70464, 10237, 7191, 361655, 107985, 31264, 19910, 26937, 119182, 1989, 1123, 170336, 10114, 2159, 101616, 175540, 54675783, 4097, 6077, 21414, 441383, 2265, 3236724, 155774, 10235, 2997693, 3936, 16362, 4622, 2017, 4572075, 3109, 8138, 54677972, 1892, 3515, 4362, 3540, 652629, 3759, 6982, 2333, 176870, 2090, 3241177, 19003, 119259, 666418, 2315, 1547484, 67686, 3404, 208820, 1815815, 3736, 2717, 16188984, 15723, 31072, 6307, 36811, 27648, 182137, 5531, 3245131, 3236065, 3316, 8609, 660708, 3865676, 4621782, 1811924, 5593, 2707, 3334, 2893, 2467, 11289, 2200, 12492, 23897, 57469, 1552036, 24239, 31729, 107715, 12454, 10660, 4165, 2092, 2310, 115163, 16960, 5510, 4064, 5723, 2315667, 35455, 1052, 5541, 2482, 4122, 2950, 2277, 3055, 1561922, 1050, 6603842, 3311, 4855, 6603901, 4107, 26596, 5233, 3326, 3783853, 2247, 4031, 2391, 1392, 3351, 2450, 3156710, 27400, 72157, 16187418, 4842, 32681, 3168, 2081, 10133, 36303, 10221470, 3599497, 3698, 10168, 2327, 9873, 8907, 114811, 4197, 54677971, 15443, 5074, 2478, 104838, 17100, 1549789, 3406, 10219, 3119467, 11310, 13791, 22571, 16190984, 3455, 2366, 10476437, 2812, 54676038, 5335, 1568843, 2082, 2484, 3435, 2170, 3647, 47472, 16351, 5576, 2229, 3080557, 4753, 2113270, 160355, 4174, 3151, 4602, 16574, 5405, 1870615, 2179, 4493, 2369, 2468, 3478, 5289501, 660883]

1636|Q9UNA4(14) [2063649, 225371, 3244776, 949760, 21501, 1993, 15945601, 6466196, 14604, 3092847, 4142675, 10219, 2896475, 5074, 2732927, 163659, 16191546, 166553, 263177, 4680274, 4655877, 1756352, 19266, 24792601, 133621, 2735646, 652629, 2490338, 255948, 3751717, 612424, 1369, 22430877, 394347, 421697, 4456136, 824155, 3698, 11852, 54675783, 3126762, 680935, 6469502, 21453, 3261980, 30717, 31236, 3114023, 2997734, 2724, 1599306, 3238124, 602681, 843822, 1967, 5459650, 12028, 2815581, 16362, 3156995, 273053, 2435, 15987950, 3127284, 3241177, 5405, 3237949, 1719874, 2057115, 3034186, 1090900, 101744, 1870615, 10621, 2762, 16187418, 660989, 598513, 2775706, 3114022, 2576, 3151, 3126341, 10168, 40146, 8569, 1676, 5359646, 19910, 50942, 4021578, 2384580, 3705369, 4777950, 246831, 3218215, 3478, 21109, 3435, 219081, 5934127, 24761713, 646716, 33925, 54676538, 911675, 655601, 13752, 4343526, 4396341, 824727, 1713166, 2990745, 11296583, 327044, 16467159, 2178, 2932343, 3847167, 261282, 3243347, 1937568, 739358, 1878823, 15953533, 4404908, 16347, 3238739, 16187479, 4619, 16739648, 3117, 3156743, 54677972, 2090, 1973720, 2291046, 3094465, 7329, 2997693, 170344, 2277, 1896320, 4150224, 4770, 240112, 2735009, 3090866, 3158622, 24361, 2022387, 2294842, 244136, 2213986, 6472251, 3731631, 361655, 2998, 3799111, 3746037, 136654, 2426546, 2234617, 588415, 2717, 24792050, 2220273, 23009, 2113270, 123435, 3218771, 44201498, 3239925, 3238154, 2053712, 3243567, 3503, 6301, 25102564, 3239339, 3326, 4027541, 2016, 647116, 750895, 2998359, 327045, 2448, 24816636, 235434, 1548942, 16745942, 3885, 31475, 2768975, 1811924, 22571, 54680702, 3794836, 1694, 175540, 659036, 16269005, 3406, 6473420, 119570, 3244425, 3246760, 3842920, 2348004, 22430777, 4278, 1892, 3151041, 2375956, 3150575, 3245025, 1985, 16270080, 2315667, 3242888, 4077789, 2482, 72462, 24793507, 2931883, 16187348, 614669, 3132640, 4777942, 1088, 647884, 1701, 265436, 2327, 1066, 98514, 114811, 54690031, 2739563,

3156710, 5135482, 2369, 5480, 3003803, 2179, 1432578, 2305017, 4343310, 5289501, 255945, 16188943, 719651, 4154053, 2844395, 10767, 605693, 25102556, 3237705, 19646, 6471716, 3138364, 251792, 1810986, 246835, 19675, 22530, 101616, 1561922, 1608140, 348986, 2942924, 1949, 16189712, 669633, 65630, 26695, 2265, 28213, 3163418, 2421810, 3239584, 6, 4572075, 4506, 2384672, 104762, 22430904, 5335, 2234553, 18573525, 288875, 798678, 6603901, 25102723, 19529, 249321, 2132993, 4014178, 16268999, 69594, 25102671, 3114024, 2743305]
1637|Q96KQ7(13) [1608140, 1967, 1547484, 10245972, 65768, 5153171, 3108, 219081, 199, 3125446, 249, 2170, 3478, 3885, 123435, 13113, 6918508, 1052, 1973720, 1050, 2194, 22571, 6469502, 2421810, 10206, 2717, 3813687, 18104, 5405, 2831207, 14878, 194699, 3515, 5289501, 35758, 4493, 2179, 5722, 13765, 65790, 4593, 4365905, 327045, 24761772, 361655, 208820, 2831167, 1066, 3542, 2081, 24978701, 2229, 3074827, 4760, 5074, 11350, 68942, 4680274, 3116068, 10104227, 104741, 3647, 24107, 1234, 288875, 70846, 10237, 55918, 2990797, 1780, 332697, 5459668, 660688, 2384672, 2216, 3760, 10258, 3333, 22530, 3455, 234310, 2466, 68089, 104826, 2743305, 6194, 16362, 54690031, 11683, 1861634, 2369, 16269005, 3298512, 2998, 2366, 2435, 1552036, 3253930, 15250, 28446, 4578, 3138373, 1045, 3969, 19910, 67686, 265580, 2327, 3236588, 3132640, 16351, 1082702, 547914, 10036135, 36303, 4843, 3109, 14369, 10168, 752652, 10782, 1355, 5381, 5392, 4278, 2950, 1349907, 3762, 3406, 3245728, 16960, 65909, 12454, 5480, 68363, 1600802, 3639, 3973, 2913, 5335, 646716, 2762, 4110197, 2484, 10718, 660989, 3117, 3759, 2396, 2178, 3686, 178144, 2017, 10252, 158781, 3298363, 5918, 3239584, 1694, 133621, 2161, 3275, 44112, 76915, 3503, 31475, 3139316, 2265, 1870615, 3005573, 4122, 24792593, 3559, 175540, 3136361, 23897, 54677971, 2450, 2219849, 104762, 60871, 107715, 756673, 2213986, 156419, 2082, 53708, 2739563, 2754, 2794, 685814, 3126341, 3932, 4362, 1549789, 2562, 1993,

2079895, 683816, 1720828, 10230, 107782, 7347, 6603842, 11088, 3138330, 122623, 1752606, 10404, 1989, 3805738, 6603901, 162834, 6473420, 4238274, 9363, 3676681, 1051, 16231, 4119575, 1568843, 2123, 2132993, 3138370, 2333, 16129778, 72139, 2247, 3151041, 13986, 3698, 3245131, 3120949, 124087, 5510, 648831, 3055, 2182, 3433, 10275, 3138364, 10651, 28688, 3156995, 2159, 65758, 21138, 3334, 10212, 5917, 194595, 122081, 3095271, 5593, 612424, 108189, 123600, 13505, 32681, 3277, 2090, 649959, 10783, 22297, 2063649, 657677, 160355, 24792590, 5185709, 2846481, 4619, 54675783, 3151, 5233, 104838, 3713404, 3936, 1046, 104850, 4343310, 65620, 2092, 141870, 4655877, 16837, 71905, 652720, 89105, 10219, 441383, 13916, 10767, 2753, 115150, 50248, 14677, 2197, 20544, 36811, 1561922, 176870, 131411, 5420, 1599306, 14899645, 2318, 3865676, 2812, 1392, 132862, 750895, 3237465, 3540, 54677972, 41684, 10382715, 7191, 3002119, 1238, 35455, 110635, 3242068, 3731631, 6604423, 2467, 54676538, 2576, 3092847, 94280, 2277, 4380, 10612, 2162118, 1811924, 3311, 101616, 14052, 2315667, 24817194, 21307, 115237, 1649, 11967809, 1057, 4342, 3244341]
1638|O75496(20) [3603333, 2057112, 16269005, 2369, 6237, 2758, 16060802, 2167047, 31729, 19910, 3118, 3236575, 57469, 19675, 68089, 6473420, 1234, 3139316, 4197, 1893, 15945601, 3561, 4342, 2113270, 3515, 2562, 19529, 2831167, 6855, 33309, 194699, 1676, 25102671, 1985, 2913, 2831207, 5005498, 2799, 14604, 10036135, 18573631, 101616, 11289, 5282060, 20544, 3783853, 3503, 2391, 65681, 108189, 13916, 2482, 27448, 2997, 13986, 68805, 18573632, 3746037, 6918508, 28061, 2081, 3082, 16270080, 55918, 5510, 54677971, 2866904, 1967, 2827330, 10832, 17134, 4622, 2732927, 67686, 3244583, 6603842, 3953130, 5541, 3117, 72136, 5459650, 3182, 2063649, 1719874, 4030, 68872, 18104, 2450, 11954283, 16190984, 65620, 3478, 182137, 26596, 1719873, 12124, 10206, 5381, 5722, 1778877, 8210, 24761772, 16187479, 5420, 10782, 3138330, 10237, 4122

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54676038 , 10382715 , 3760 ,	547914 , 76915 , 11293 , 2247 ,	3241429 , 50248 , 2467 , 94280	122077 , 13752 , 2750 , 8026]

D+ dataset

The D+ dataset contains all proteins in the D dataset plus the below human proteins that are currently non-target but share high sequence similarity (≥ 90%) to known drug targets from other organisms.

The list of is in the following format.

***IDX*|*UNIPROT_ID* (*NUM_DISEASE*)**

IDX: Sequential index
NUM_DISEASE: number of disease annotation

1|O00506(4)
2|O00555(192)
3|O00764(7)
4|O14594(15)
5|O15144(4)
6|O60391(5)
7|O60939(6)
8|O75874(129)
9|O94768(12)
10|O95461(57)
11|O95819(19)
12|P00156(75)
13|P00352(84)
14|P00403(311)
15|P00491(63)
16|P00748(74)
17|P01215(67)
18|P04083(119)
19|P04406(140)
20|P04792(142)
21|P07339(103)
22|P07998(26)
23|P08319(24)
24|P08758(129)
25|P09211(364)
26|P09919(213)
27|P0DMN0(3)
28|P0DMS9 (0)
29|P11021(126)
30|P11310(27)
31|P13196(9)
32|P13674(8)
33|P14618(58)
34|P16109(393)
35|P16389(21)
36|P17707(23)
37|P19224(34)
38|P19367(114)
39|P19525(81)
40|P22001(133)
41|P22102(16)
42|P22301(759)
43|P22309(143)
44|P22459(5)
45|P22736(73)
46|P23528(39)
47|P24385(353)
48|P24557(32)
49|P24666(118)
50|P26358(177)
51|P28062(71)
52|P28482(326)
53|P29320(70)
54|P31941(26)
55|P32246(78)
56|P33176(18)
57|P34897(12)
58|P37058(23)
59|P39748(41)
60|P40189(89)
61|P40261(41)
62|P41279(75)
63|P42229(121)
64|P43003(38)
65|P43351(29)
66|P46734(22)
67|P48051(38)
68|P48547(6)
69|P48549(16)
70|P48637(30)
71|P49441(6)
72|P49674(21)
73|P51570(10)
74|P51793(16)
75|P51956(3)
76|P53355(80)
77|P54289(15)
78|P54756(9)
79|P61088(28)
80|P63252(32)
81|P83916(12)
82|Q00536(21)
83|Q01453(206)
84|Q02108(13)
85|Q02153(2)
86|Q03721(9)
87|Q04760(57)
88|Q05329(70)
89|Q05397(74)
90|Q06710(64)
91|Q07002(2)
92|Q09470(27)
93|Q13123(6)
94|Q13255(53)
95|Q13393(60)
96|Q13509(49)
97|Q14721(13)
98|Q14749(26)
99|Q15067(28)
100|Q15274(6)
101|Q15878(8)
102|Q16280(1)
103|Q16288(65)
104|Q16678(131)
105|Q2Y0W8 (0)
106|Q68DU8(1)
107|Q6U841(10)
108|Q6ZWB6 (0)
109|Q96BR1(9)
110|Q96CX2(6)
111|Q96D96(7)
112|Q96GD3 (0)
113|Q96L42(30)
114|Q96PR1(2)
115|Q9BY07(4)
116|Q9GZT9(39)
117|Q9HBA0(51)
118|Q9NVS9(14)
119|Q9NZV8(8)
120|Q9P0L2(14)
121|Q9UBN4(11)
122|Q9UNX9(1)
123|Q9Y6M7(11)
124|Q9Y6R1(19)

N dataset

The list of proteins in the dataset of current non-targets (N dataset) is provided below in the following format:

IDX|***UNIPROT_ID*** (***NUM_DISEASE***)

IDX: Sequential index
NUM_DISEASE: number of disease annotation

1|Q7Z398(0)
2|Q9H0E7(9)
3|O00628(44)
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5|Q9NQT6(1)
6|Q49A88(0)
7|Q86SJ2(2)
8|Q9HC77(10)
9|Q8N5F7(2)
10|Q6ZNW5(0)
11|Q9C0H9(7)
12|Q69YN2(10)
13|Q9BZQ8(7)
14|Q96J65(4)
15|Q9UBM7(82)
16|Q8IYK4(0)
17|Q9BW85(1)
18|Q13835(23)
19|Q9UPI3(10)
20|P02545(514)
21|P02549(12)
22|Q7Z3T8(0)
23|Q01804(26)
24|A6H8Z2(0)
25|Q96KX0(0)
26|Q8TDF5(0)
27|P49788(18)
28|Q9HB75(4)
29|P78347(57)
30|Q9UQ07(88)
31|Q5T7W7(0)
32|P52272(4)
33|A0AVT1(0)
34|O76027(1)
35|P01709(0)
36|Q8N8Z8(0)
37|P35244(4)
38|Q6ZTB9(0)
39|P35249(7)
40|Q96RV3(0)
41|Q86UQ5(0)
42|A8MZG2(0)
43|Q9P215(2)
44|Q8NBI5(2)
45|Q9UKL2(0)
46|P00540(27)
47|Q9BXW7(0)
48|Q9H3M7(66)
49|O15320(10)
50|Q15573(0)
51|O75387(5)
52|Q8TEZ7(0)
53|P78562(40)
54|Q8TE96(1)
55|B3EWG5(0)
56|Q6NX45(0)
57|Q8WYB5(50)
58|Q86VW0(0)
59|Q6YHK3(12)
60|Q14587(4)
61|Q9UHF7(39)
62|O94907(119)
63|Q14588(0)
64|Q8N999(0)
65|Q92526(1)
66|Q92521(0)
67|O43790(7)
68|Q92529(17)
69|Q8N3C0(6)
70|Q9ULB4(1)
71|Q5T9C2(2)
72|F5H2V8(0)
73|Q96Q89(10)
74|Q96HA4(0)
75|P86397(0)
76|Q9H210(0)
77|Q99460(1)
78|O60383(9)
79|Q99466(49)
80|Q8TCT6(9)
81|Q9H3Q3(1)
82|Q6P2I3(0)
83|Q8TCT8(3)
84|Q5R3K3(1)
85|Q6UW02(4)
86|Q99990(4)
87|Q8WUF8(2)
88|Q8N1E2(0)
89|O15417(0)
90|Q13349(0)
91|Q8NDA8(0)
92|Q9BU40(0)
93|Q96MG8(1)
94|Q9BSW7(0)
95|P62495(5)
96|Q8IZM9(5)
97|Q86UF1(9)
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99|Q8NH41(0)
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101|Q96A83(1)
102|Q9NWS9(0)
103|P16333(8)
104|Q8TAP6(0)
105|Q9BQ50(3)
106|P49771(41)
107|Q8N1W2(0)
108|O15528(76)
109|O95251(7)
110|Q96M20(0)
111|Q86SU0(5)
112|Q9BZ29(3)
113|Q16670(0)
114|A0MZ66(0)
115|Q9BS34(0)
116|Q9H0B3(0)
117|Q6YN16(5)
118|O15069(0)
119|Q9H6R4(0)
120|O15062(3)
121|Q9H6R6(0)
122|Q9H6R0(0)
123|P60891(35)
124|O95741(0)
125|P29083(2)
126|Q9NW64(0)
127|Q6UXX5(0)
128|Q96D71(2)
129|P05062(30)
130|Q8NAB2(0)
131|Q7Z4H3(1)
132|Q2TBF2(1)
133|Q6UXN2(3)
134|Q9BR01(18)
135|Q8NCJ5(0)
136|F8WAN1(0)
137|A6NHT5(0)
138|P49959(55)
139|Q9HB19(1)
140|P13747(50)
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142|Q5FYB0(0)
143|E9PFP8(0)
144|B0I1T2(1)
145|P56545(12)
146|Q9NWW9(0)
147|Q15935(1)
148|Q00341(9)
149|P78352(19)
150|P10265(0)
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152|Q8IYB7(1)
153|Q969T3(0)
154|O15084(1)
155|O15083(0)
156|P07476(17)
157|Q9Y613(1)
158|P35251(51)
159|Q08170(4)
160|Q8IY18(3)
161|P32926(27)
162|Q00765(24)
163|A4D2P6(0)
164|O00507(9)
165|O00505(2)
166|Q8TCI5(1)
167|Q4V328(0)
168|Q9Y6D5(15)
169|Q53GA4(12)
170|Q9Y6D6(6)
171|A0A286YF58(0)
172|Q8N9M5(0)
173|O75398(9)
174|Q8IYD9(3)
175|O75558(9)
176|Q8TE68(0)
177|Q96P67(0)
178|Q96P63(0)
179|P04280(15)
180|Q9BSJ8(1)
181|Q96R69(0)
182|Q9BSJ2(8)
183|Q9H992(5)
184|P27694(26)
185|Q9BTC8(11)
186|Q7Z5J1(3)
187|Q08378(0)
188|Q8WVD3(1)
189|P98077(4)
190|Q8WXH5(4)
191|P68543(2)
192|Q32M78(0)
193|Q06787(105)
194|P58872(0)
195|Q96RD0(0)
196|P54886(40)
197|Q9H9K5(0)
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213|Q7Z6Z6(0)
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216|Q8N145(0)
217|Q8TCU3(4)
218|Q9UF12(1)
219|A6NI47(0)
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221|Q8N5V2(0)
222|Q8WUA8(0)
223|Q5VY43(5)
224|Q9NY74(1)
225|Q8WUA2(0)
226|Q8WUA7(0)
227|P31943(6)
228|P49407(28)
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230|O15400(0)
231|Q9Y5P8(2)
232|Q9UG22(0)
233|Q9NYT6(0)
234|Q14916(7)
235|Q96DS6(0)
236|Q9UJU2(59)
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244|Q00978(32)
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246|Q8NHW5(0)
247|Q8NA66(1)
248|Q9BX59(0)
249|Q8WZA2(1)
250|Q9HC56(2)
251|Q9HD20(0)
252|Q9NQZ5(2)
253|Q9H6S1(7)
254|Q9UN73(0)
255|Q9NQZ2(0)
256|Q01954(7)
257|Q13585(2)
258|Q9NZJ9(0)
259|Q3MIW9(3)
260|Q9NZJ4(23)
261|Q6UXY8(2)
262|Q6XYQ8(2)
263|P30566(19)
264|A6NFQ2(1)
265|Q96ID5(1)
266|Q8NCE0(4)
267|P38159(11)
268|Q10589(29)
269|Q10588(7)
270|A6NNW6(0)
271|Q99729(3)
272|O00267(4)
273|Q86X51(4)
274|Q8WWQ2(28)
275|Q9Y2E6(2)
276|Q9Y2E4(5)
277|Q6ZTY9(0)
278|P55289(3)
279|Q7Z449(4)
280|O76042(0)
281|P62955(0)
282|P78363(95)
283|P23025(97)
284|Q8TAU3(0)
285|Q9BVJ6(0)
286|Q9BVJ7(3)
287|Q96SZ6(1)
288|O00232(10)
289|A8MWY0(0)
290|Q5T2S8(9)
291|E9PJK4(0)
292|Q15345(0)
293|Q53G59(1)
294|Q9P0M6(4)
295|P28336(8)

296|Q8NGC3(0)
297|A8MWK0(0)
298|Q8N9X3(0)
299|P20916(26)
300|Q9C0D3(0)
301|O95985(1)
302|Q8NGA1(0)
303|Q9UKJ1(5)
304|Q8TCJ0(2)
305|Q8NGA4(0)
306|Q9BZE9(9)
307|P02747(6)
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309|Q8TAB3(11)
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311|Q9UKX3(1)
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313|Q9BXC9(37)
314|Q92618(2)
315|Q53GL7(0)
316|Q53GL0(1)
317|Q96P71(2)
318|Q96P70(1)
319|Q8TE73(13)
320|Q9Y6E2(0)
321|Q9H7Y0(1)
322|Q8N335(13)
323|Q8TAP4(14)
324|P42785(23)
325|P0DPB3(0)
326|Q9NPH3(23)
327|Q92508(16)
328|Q9NRD8(41)
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331|Q13107(12)
332|P61966(16)
333|A0A0A0MTC6(0)
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335|Q8N539(0)
336|P04746(5)
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343|O75185(5)
344|Q0JRZ9(0)
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347|Q3L8U1(0)
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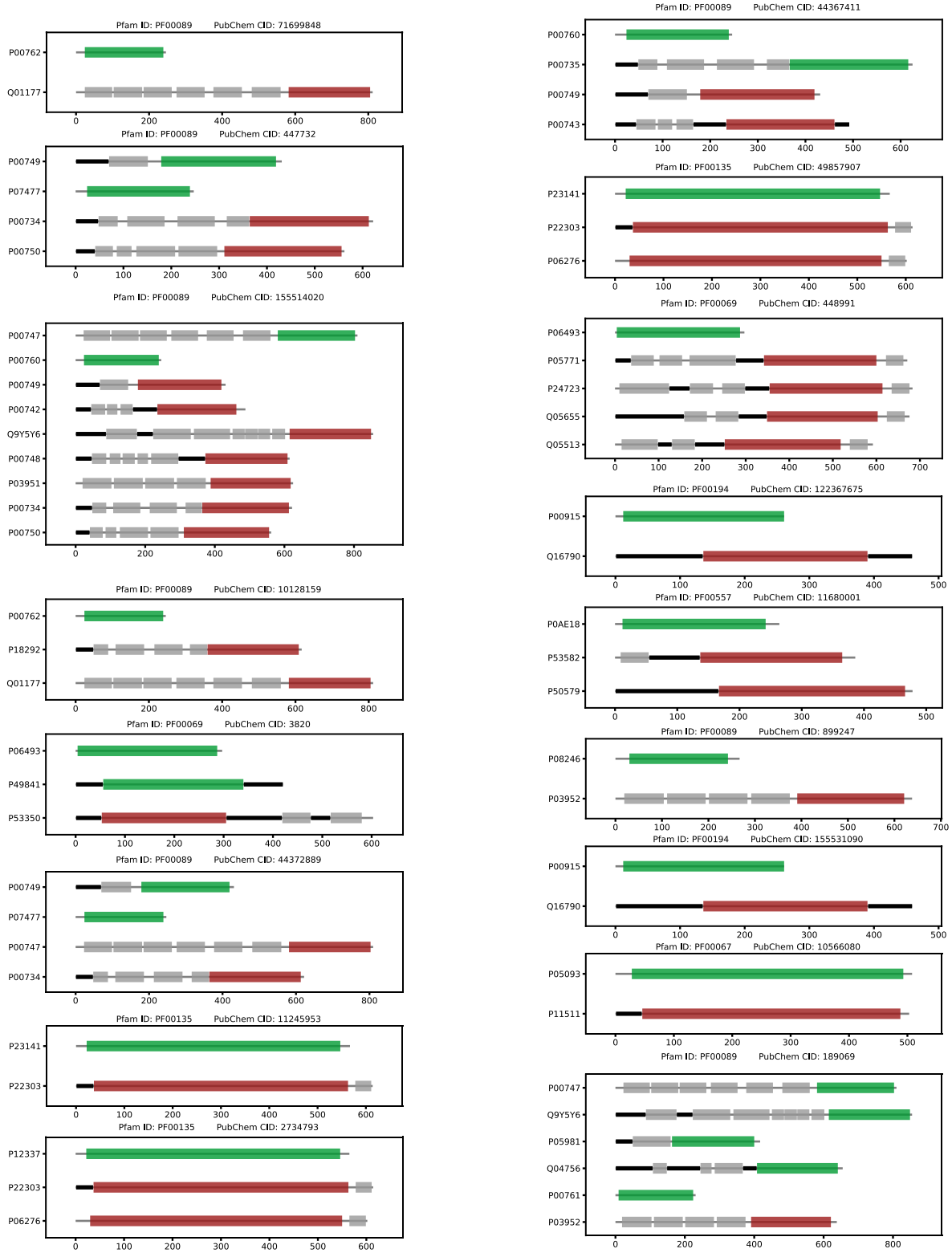
APPENDIX B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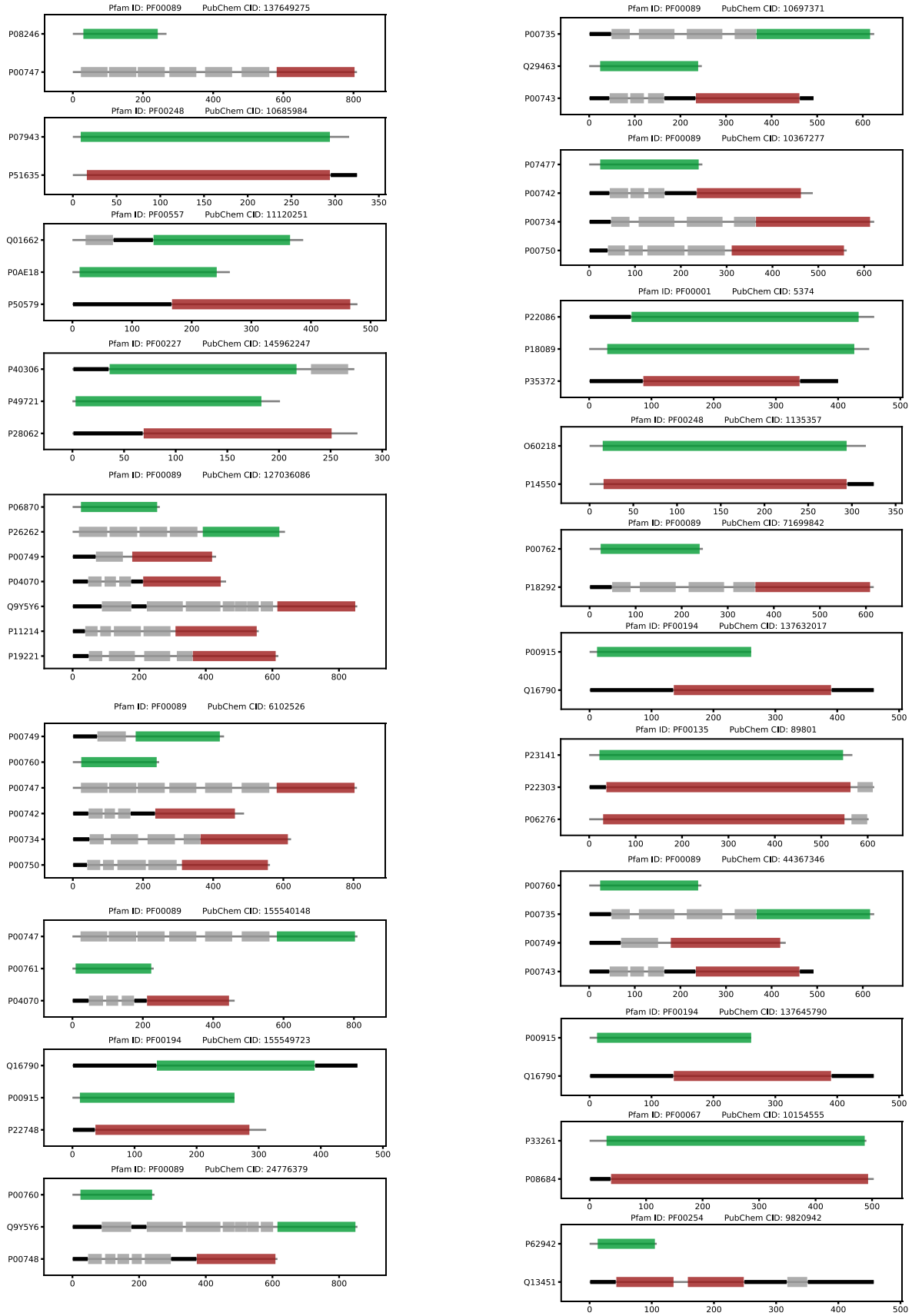
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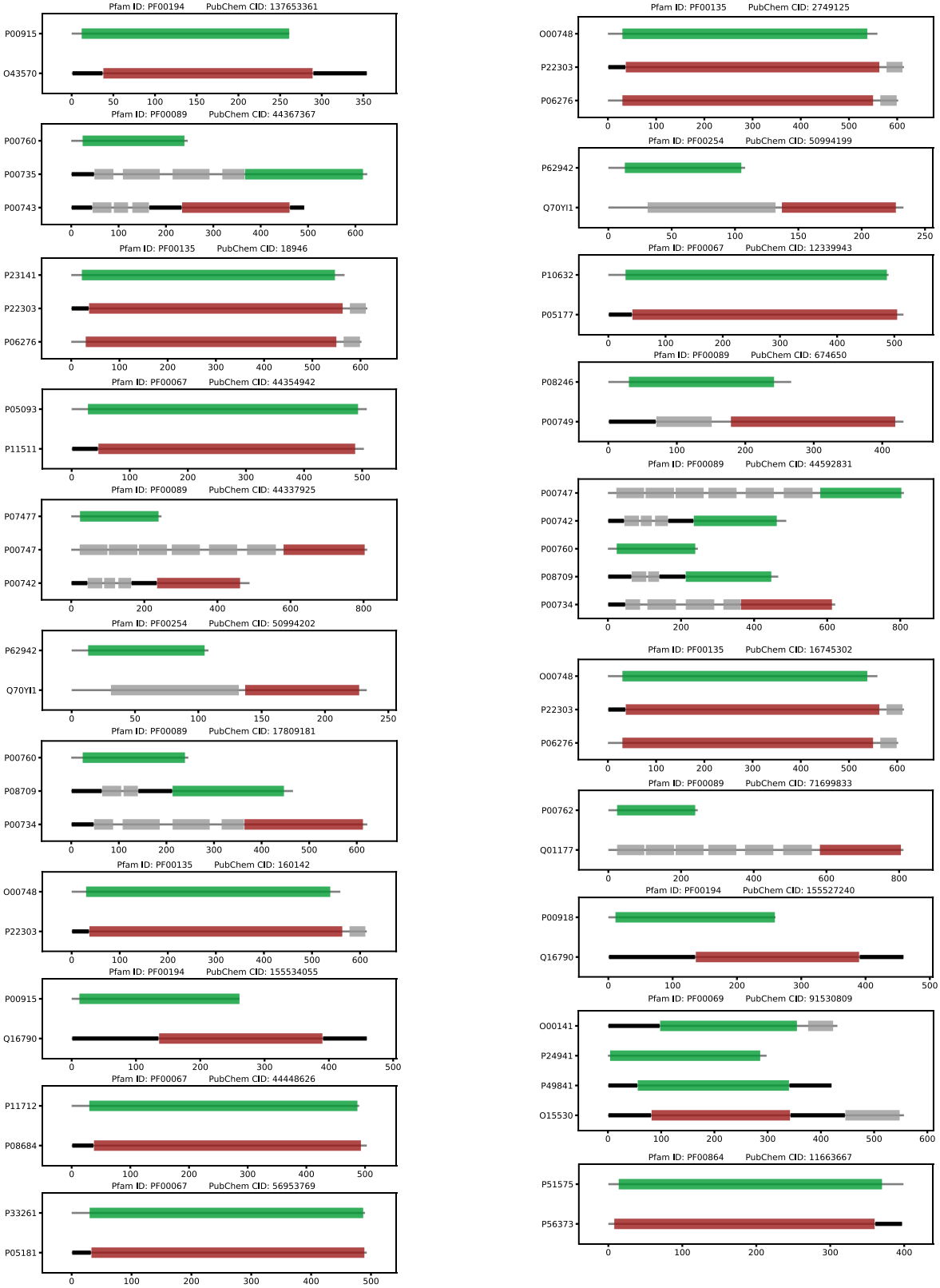
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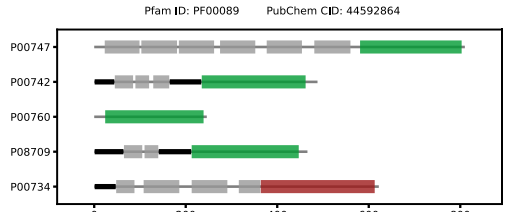
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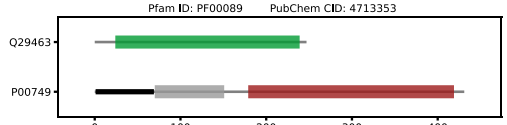
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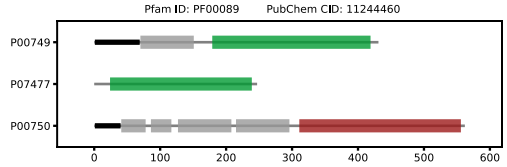
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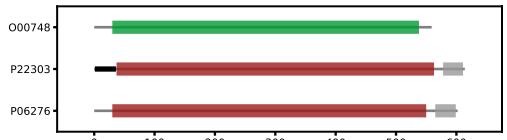
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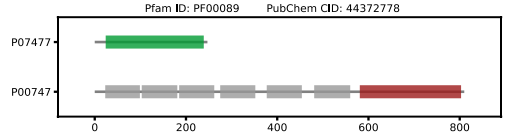
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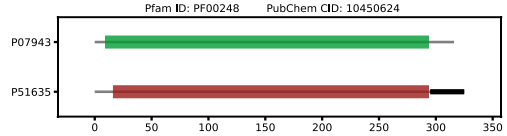
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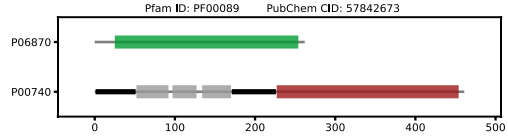
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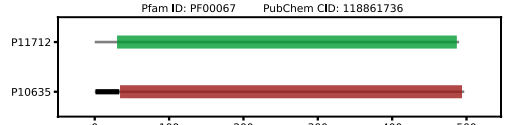
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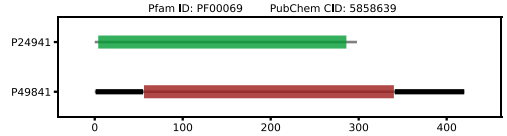
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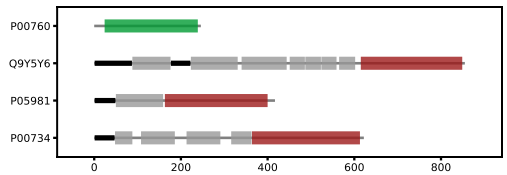
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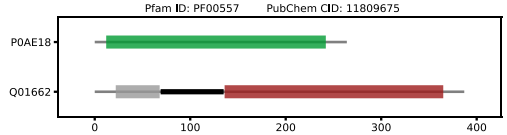
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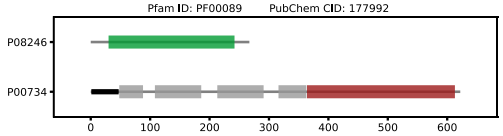
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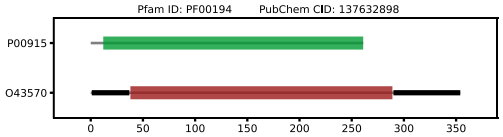
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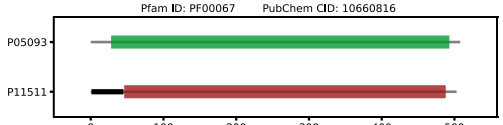
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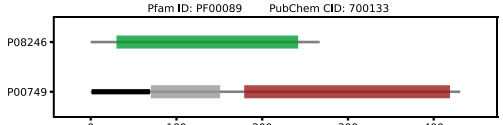
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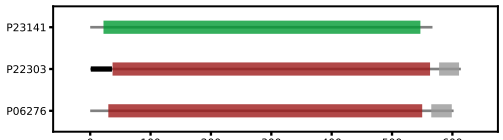
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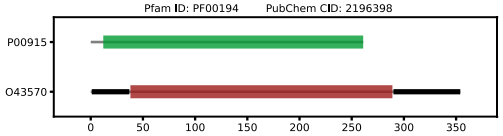
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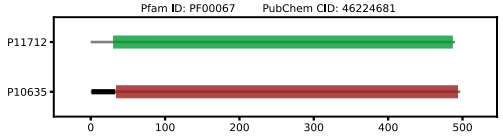
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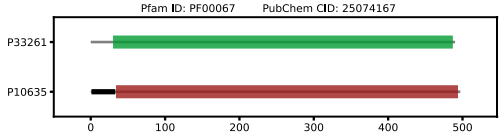
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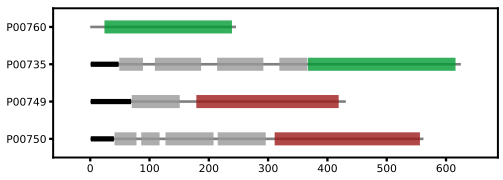
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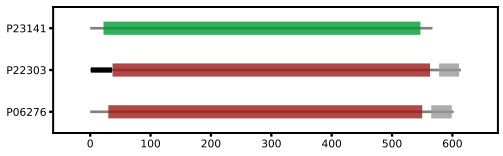
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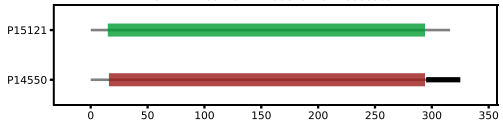
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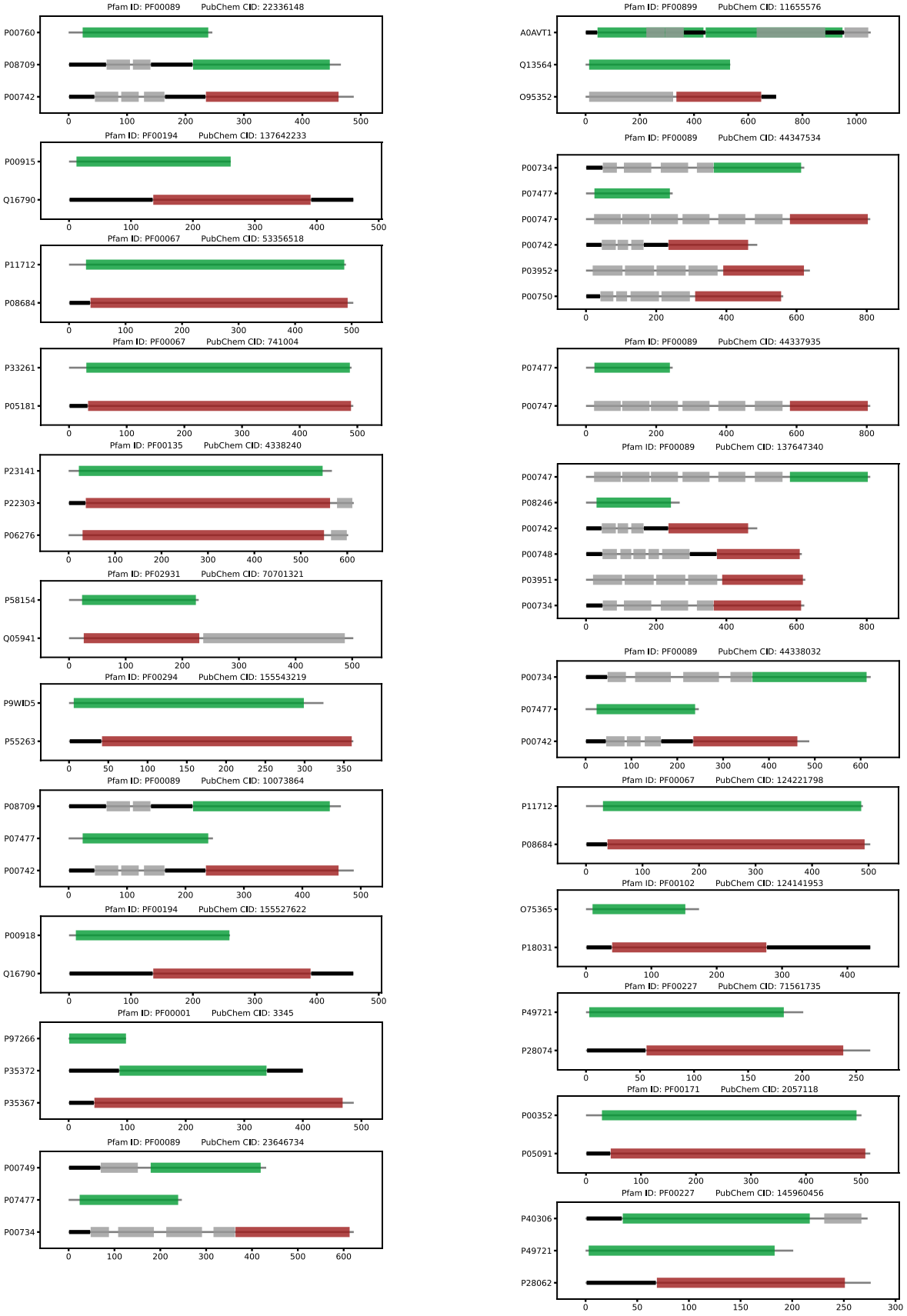
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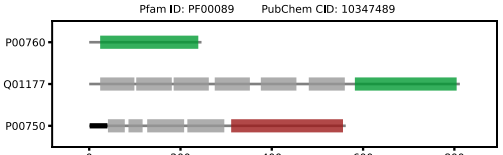
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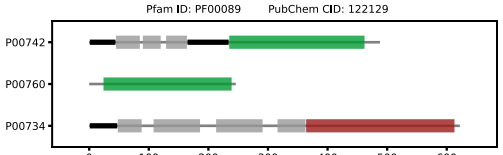
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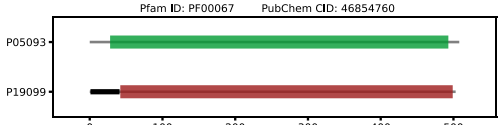
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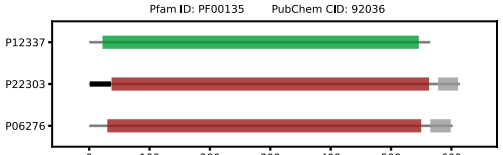
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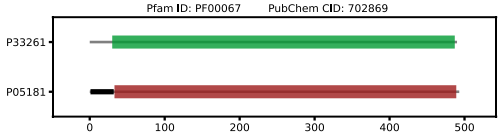
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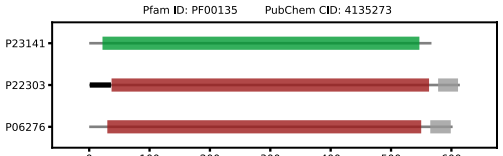
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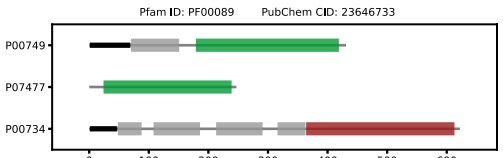
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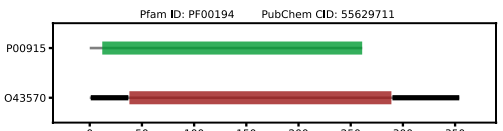
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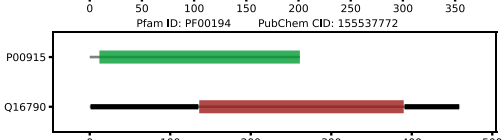
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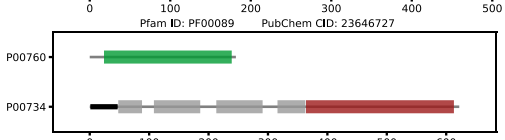
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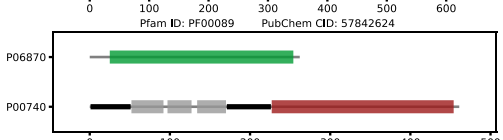
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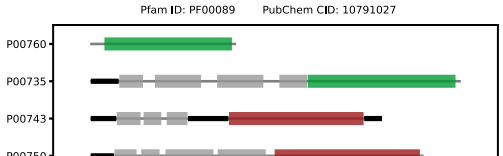
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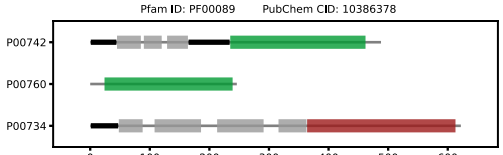
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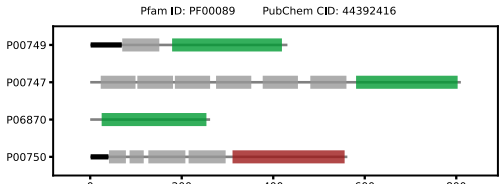
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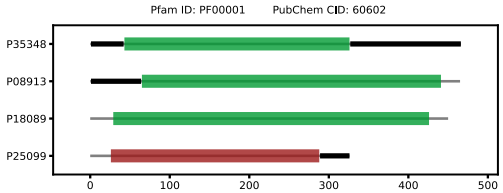
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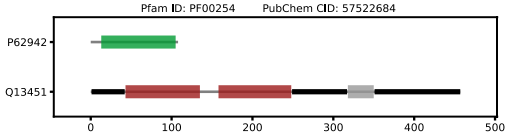
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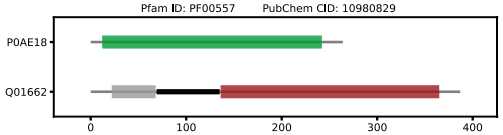
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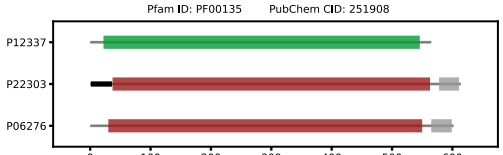
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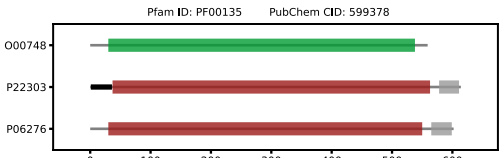
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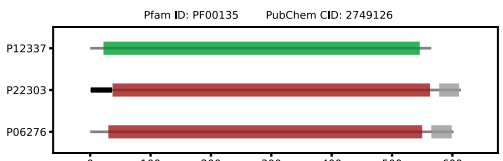
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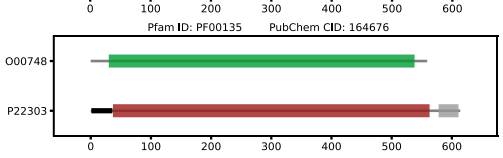
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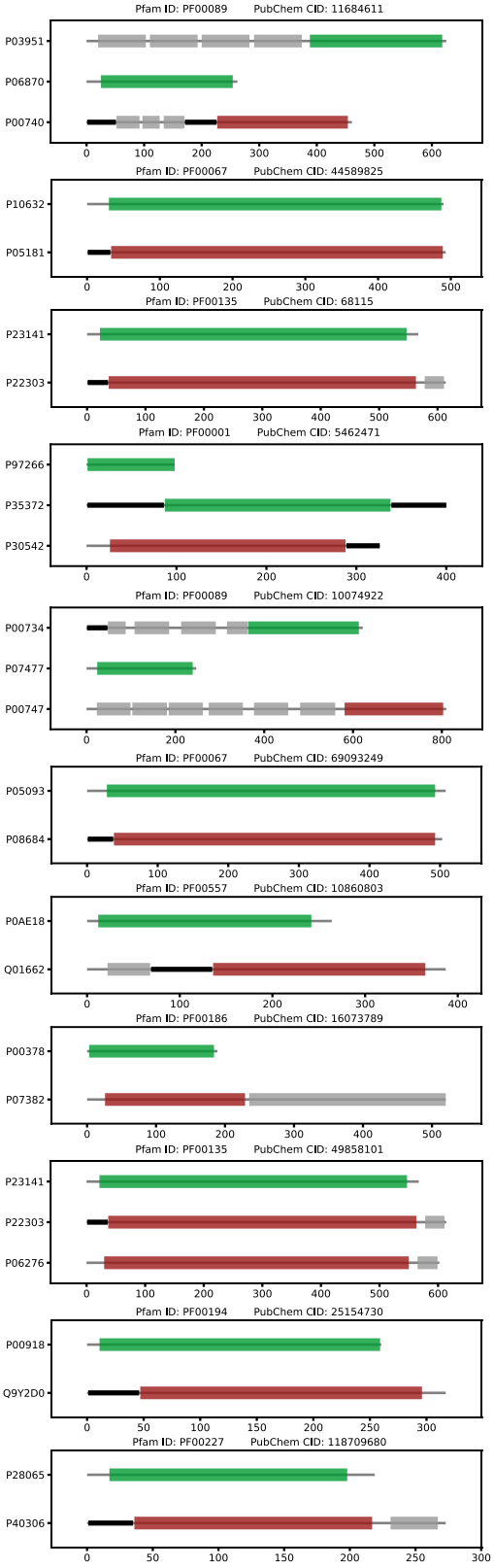
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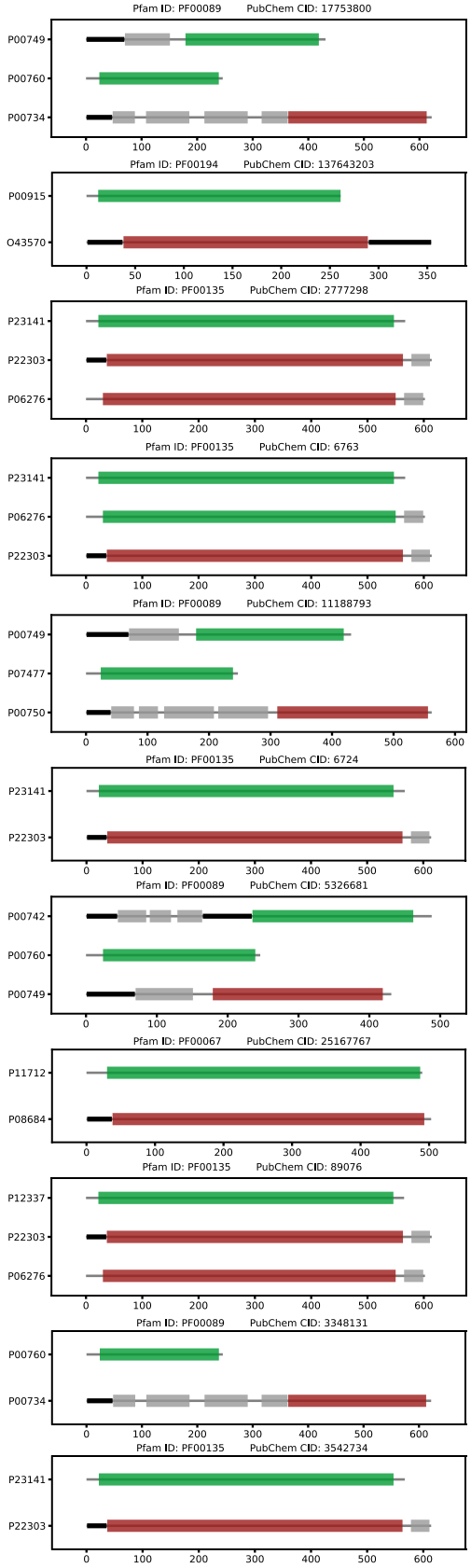
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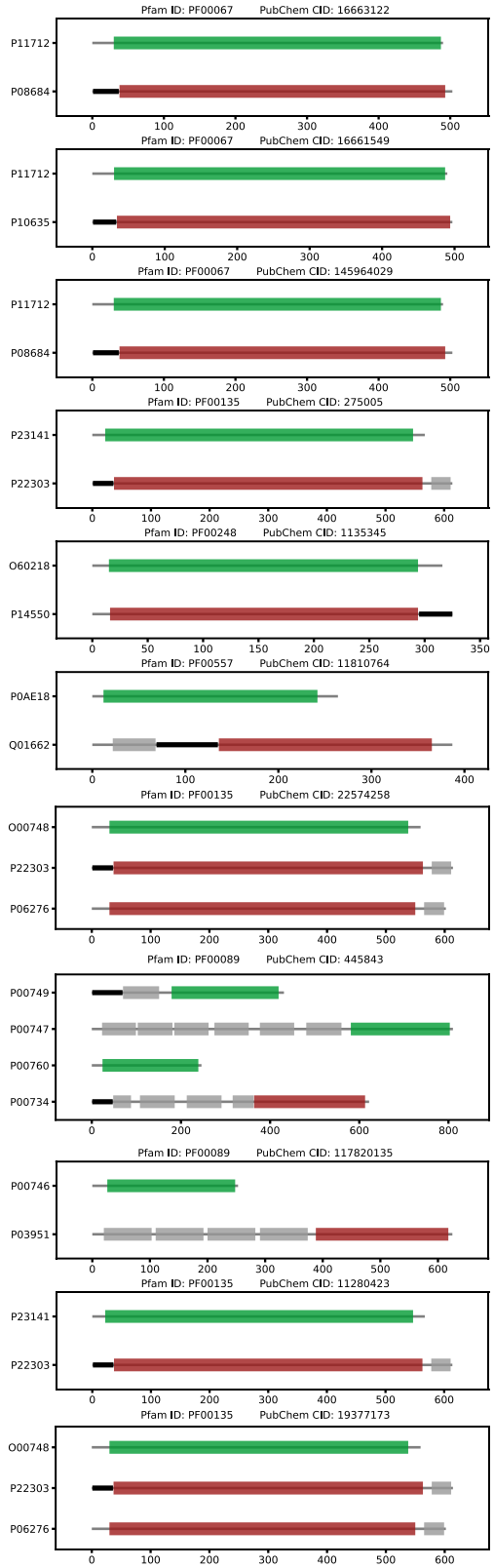
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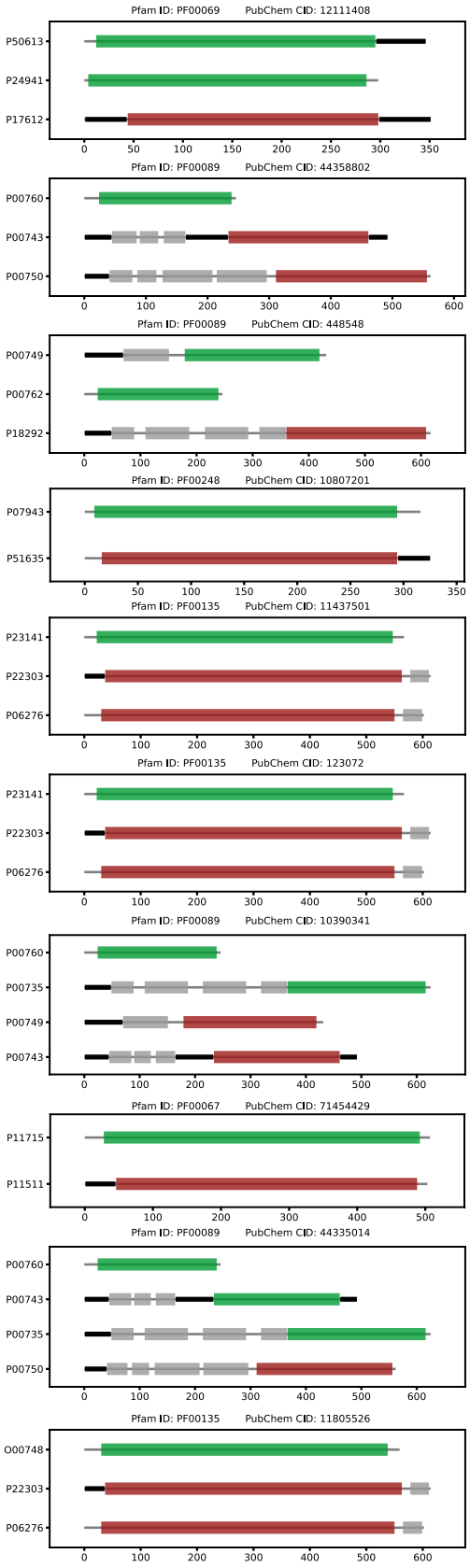
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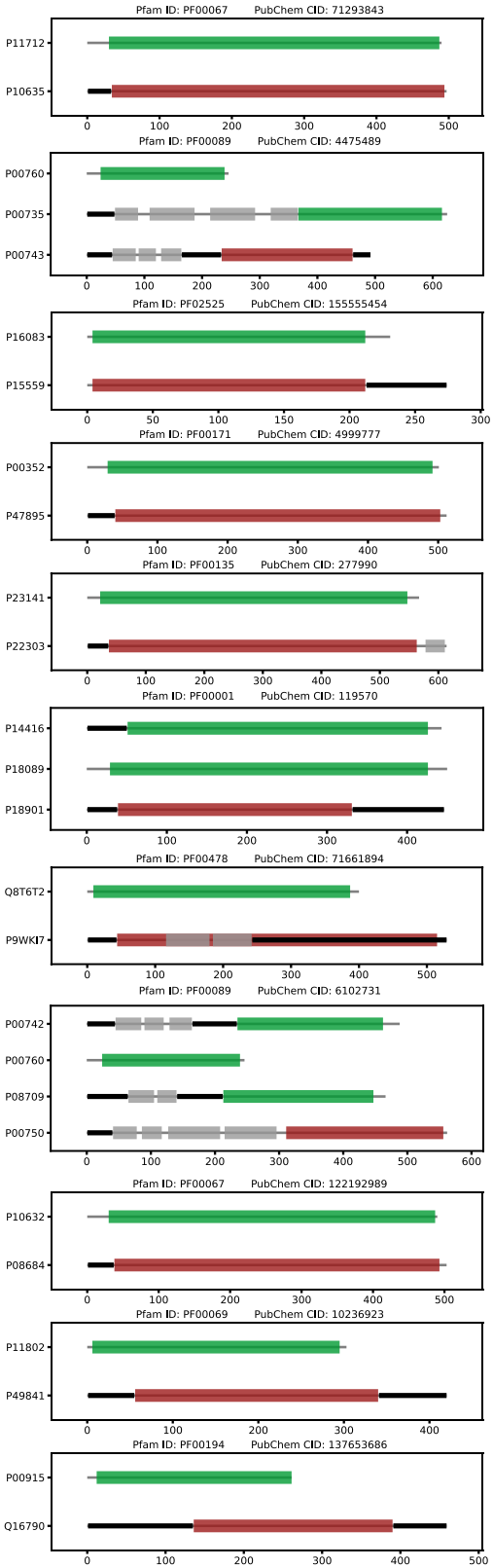
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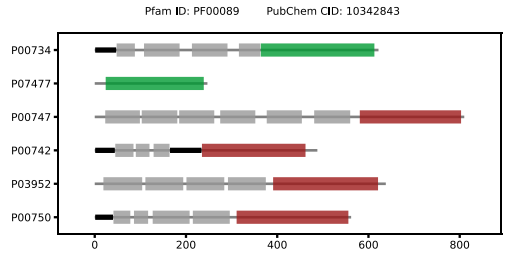
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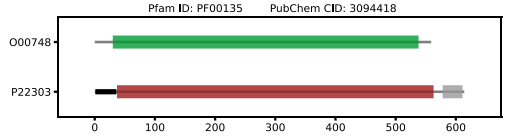
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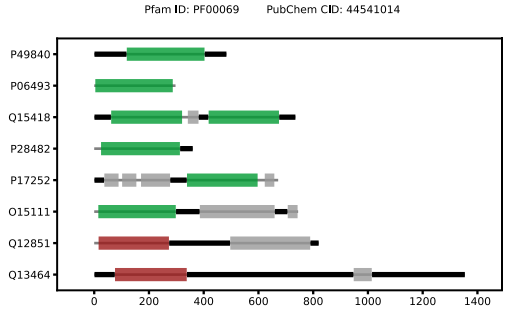
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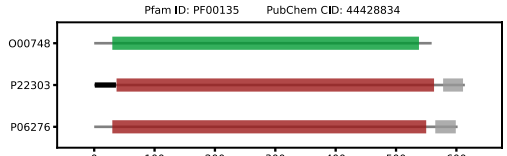
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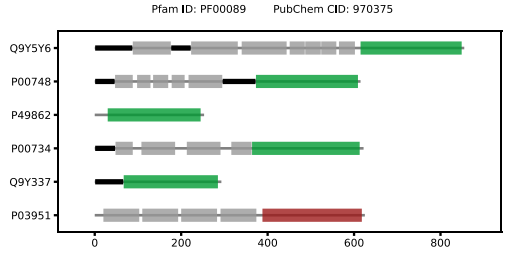
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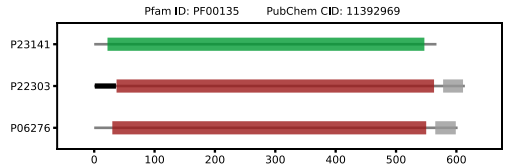
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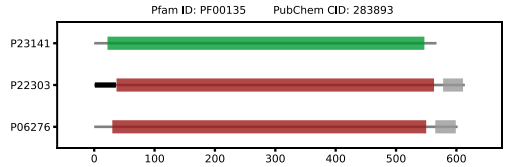
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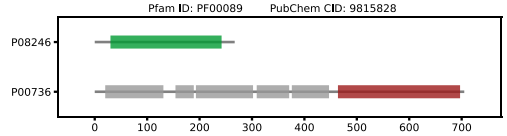
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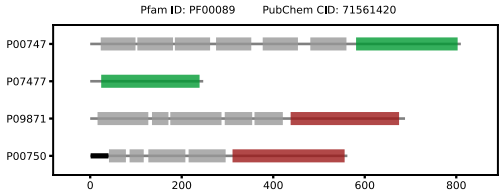
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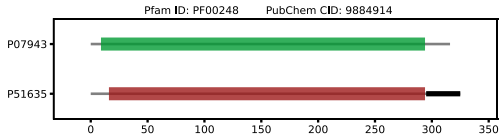
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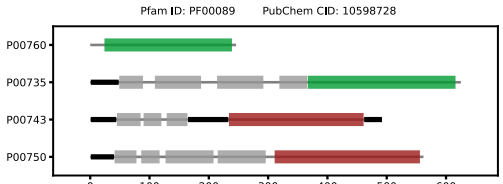
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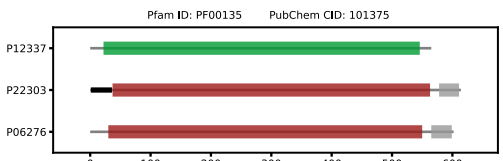
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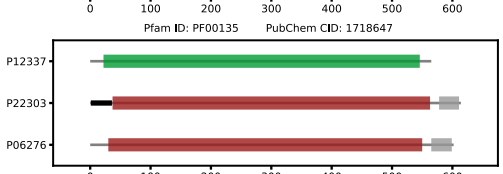
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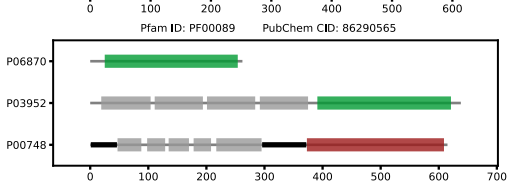
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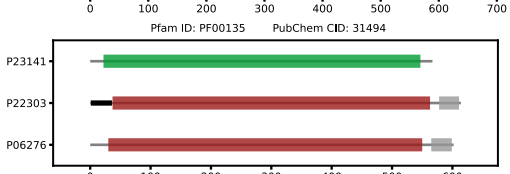
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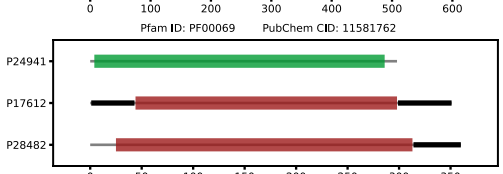
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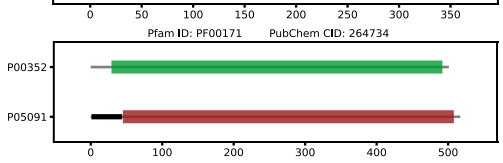
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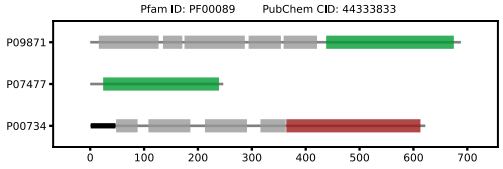
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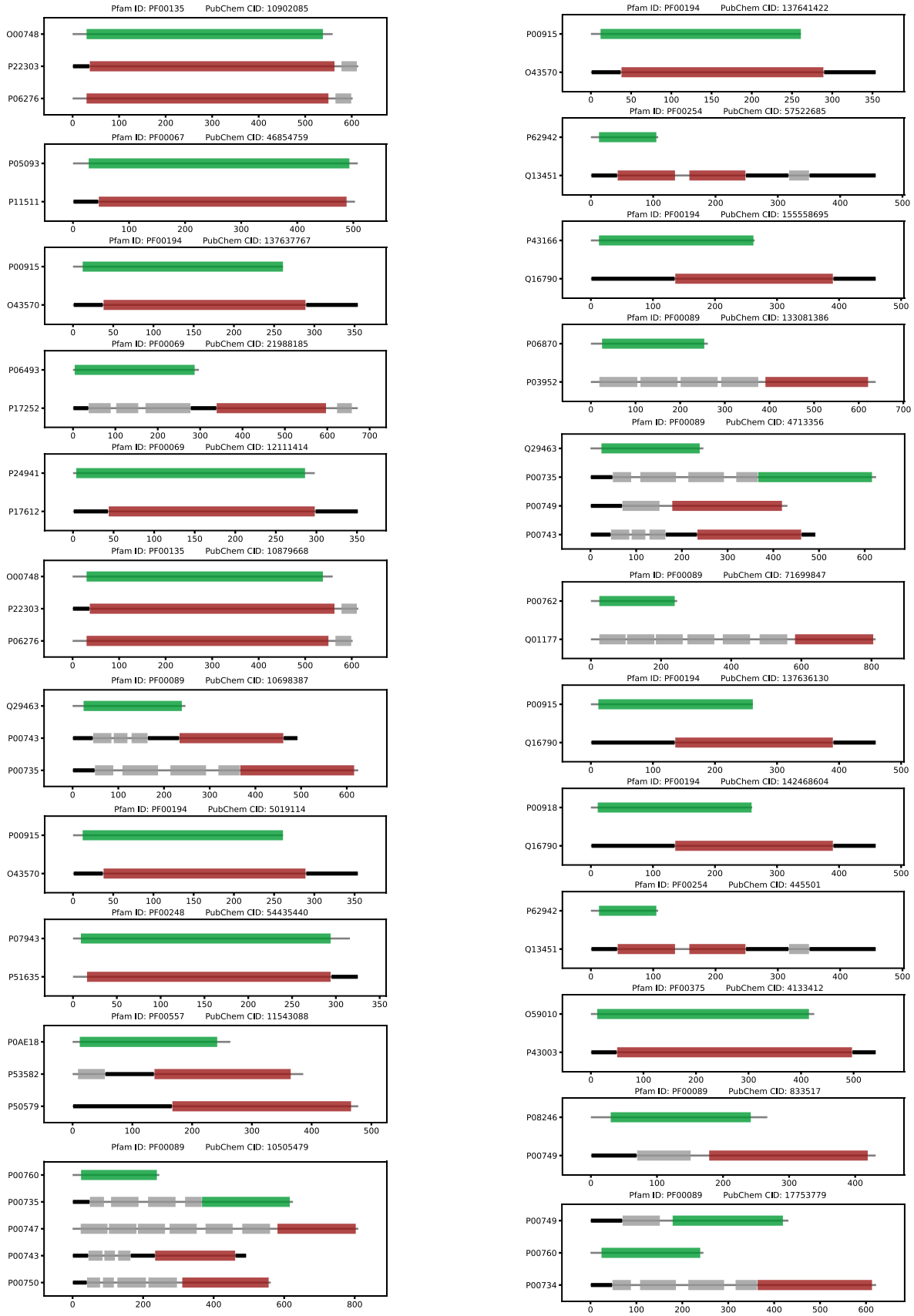
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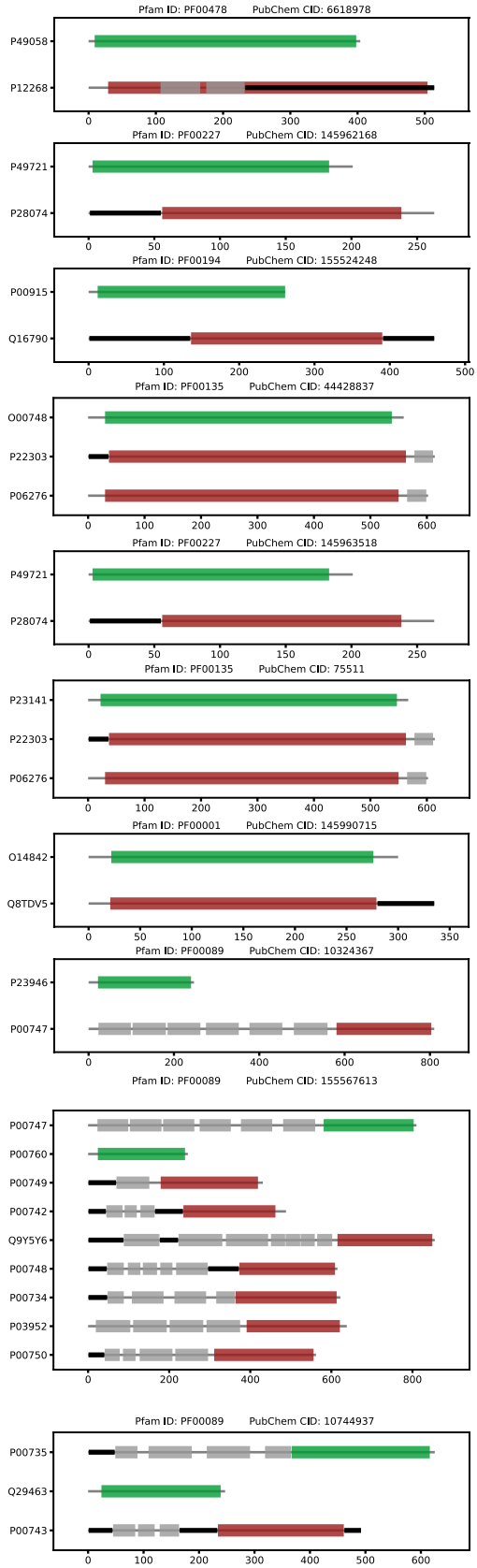
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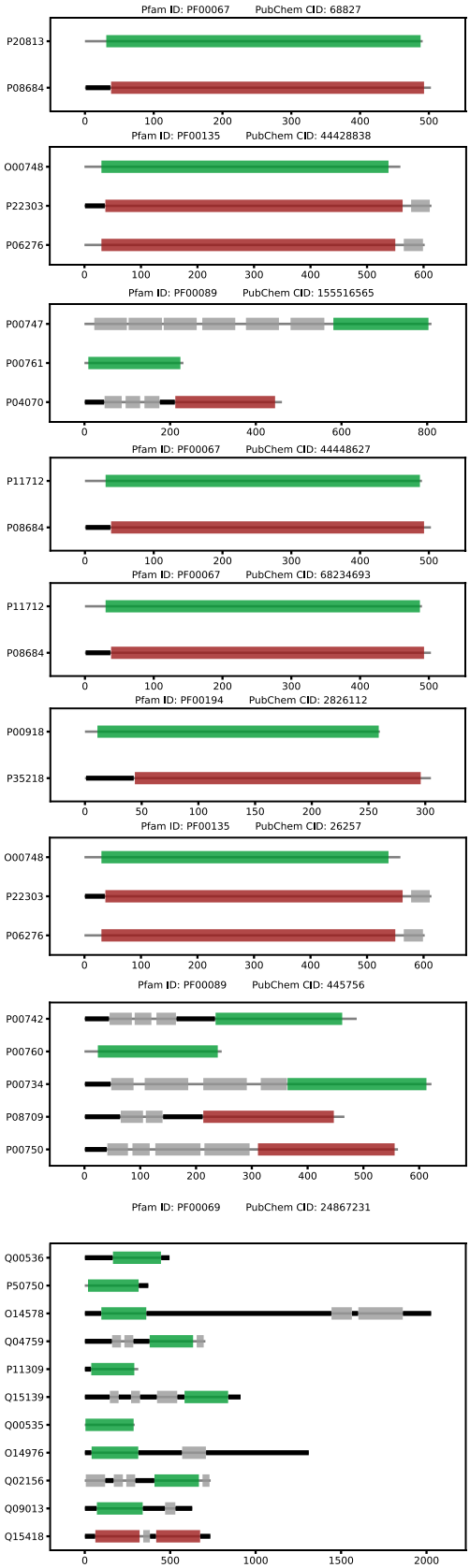
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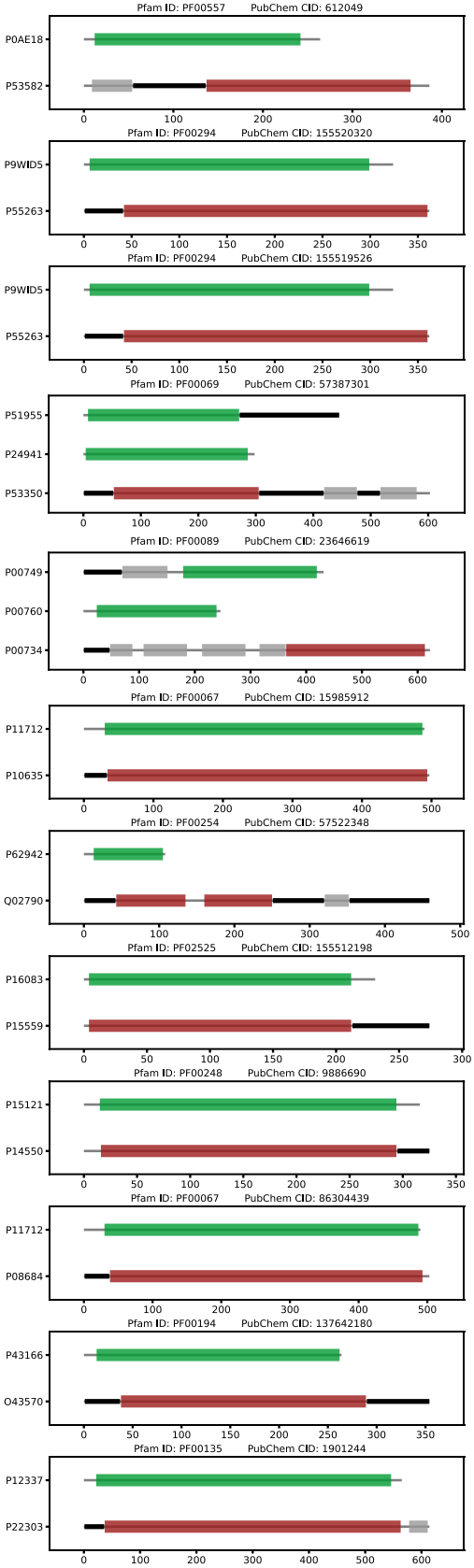
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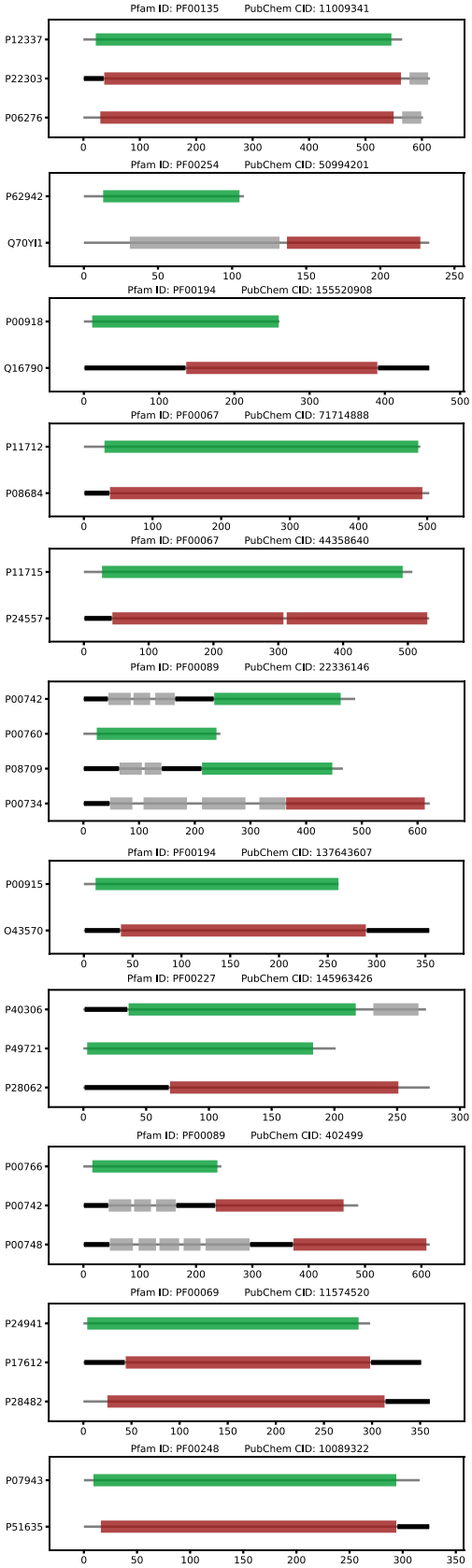
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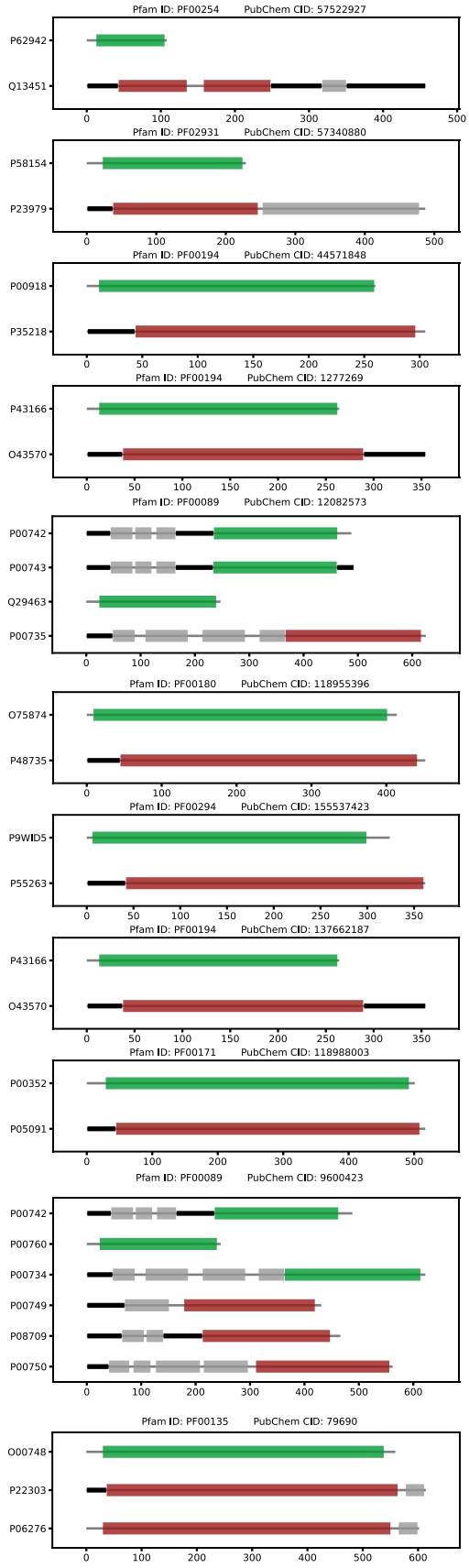
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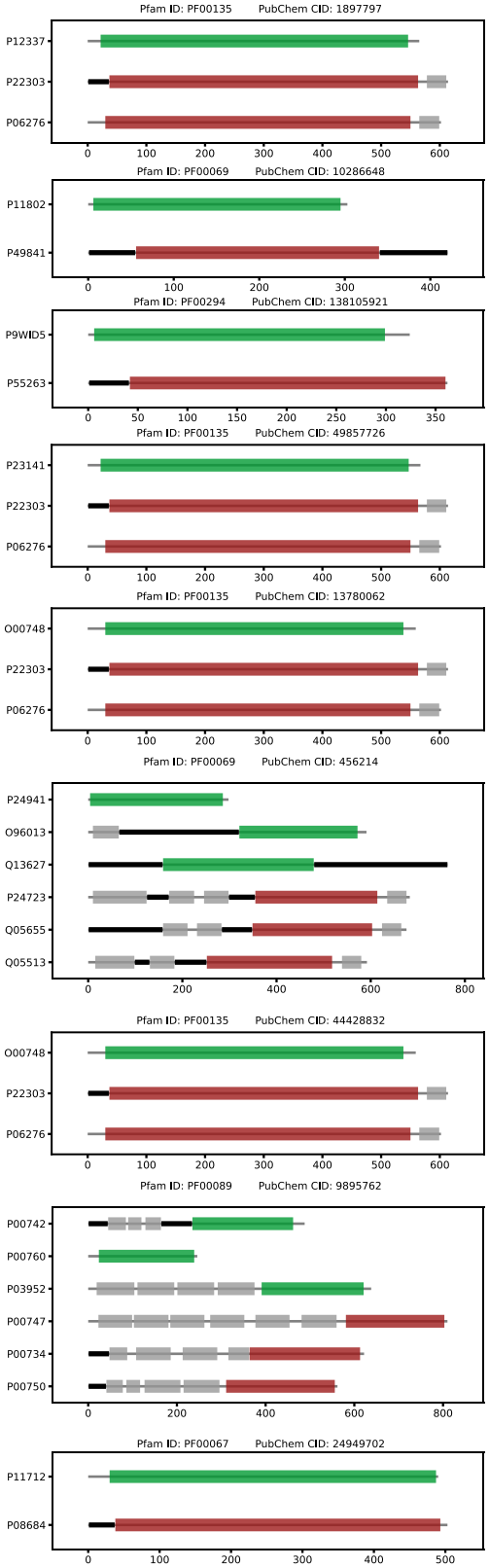
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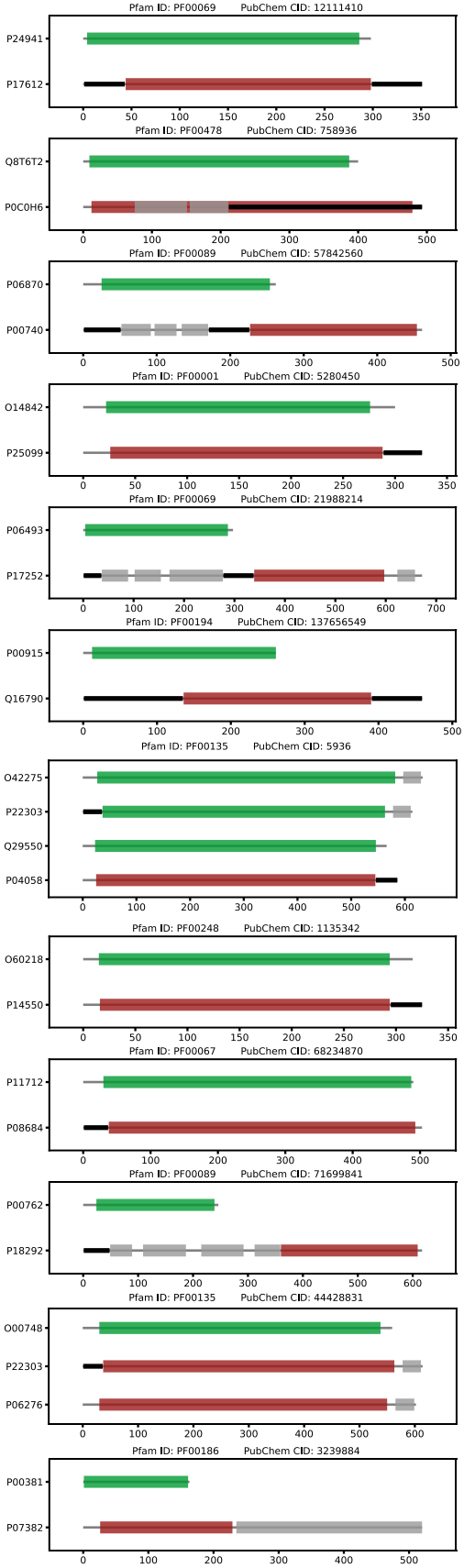
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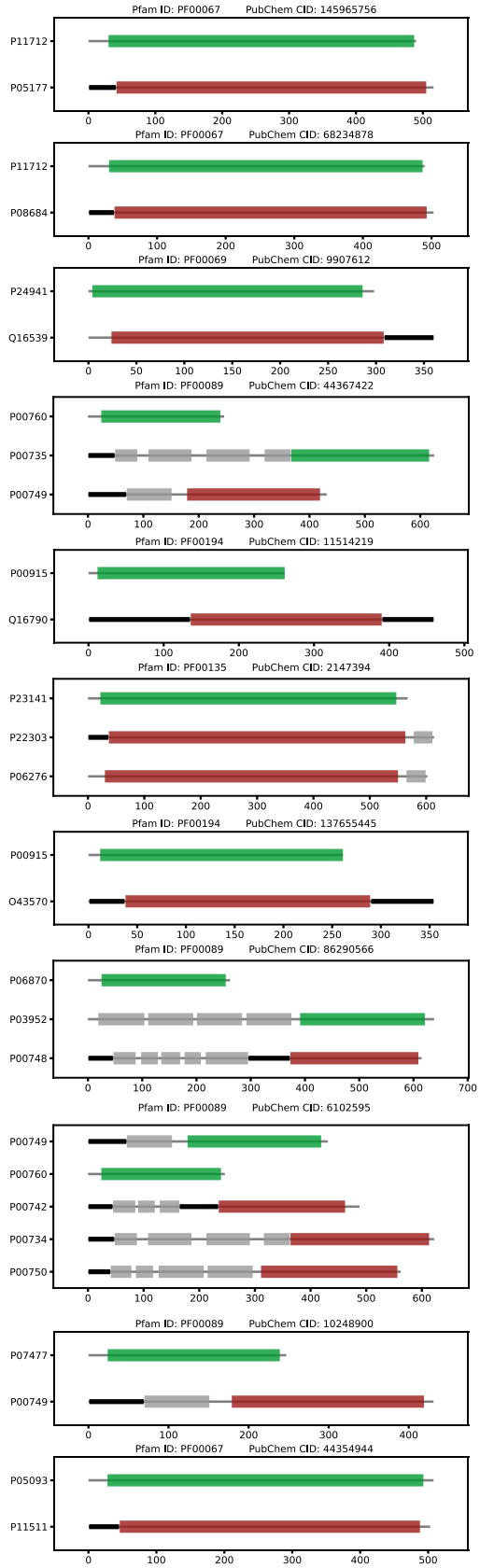
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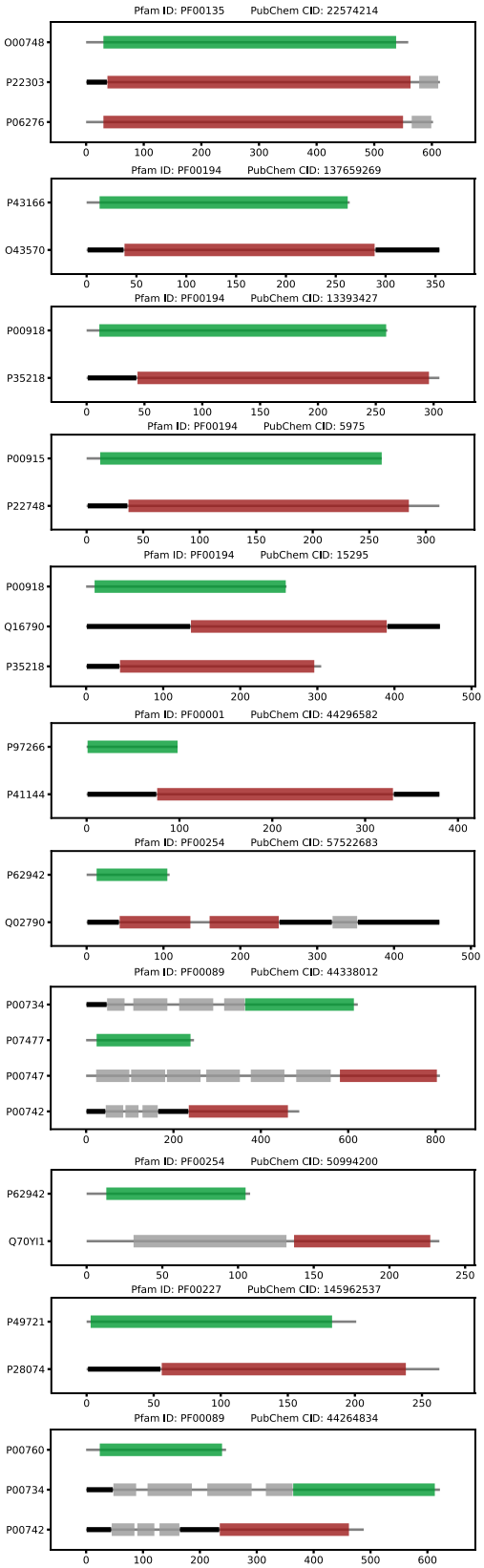
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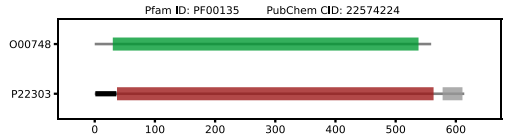
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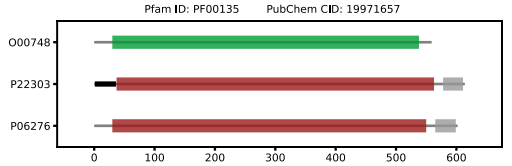
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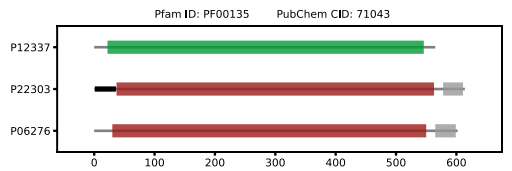
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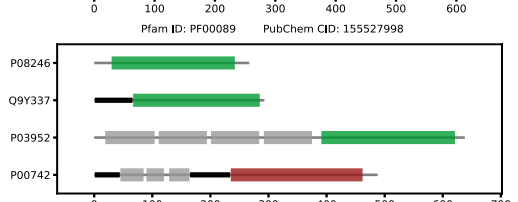
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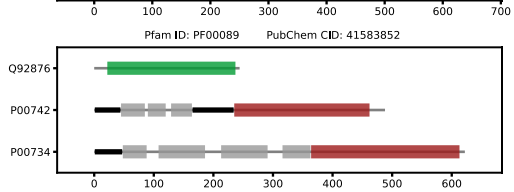
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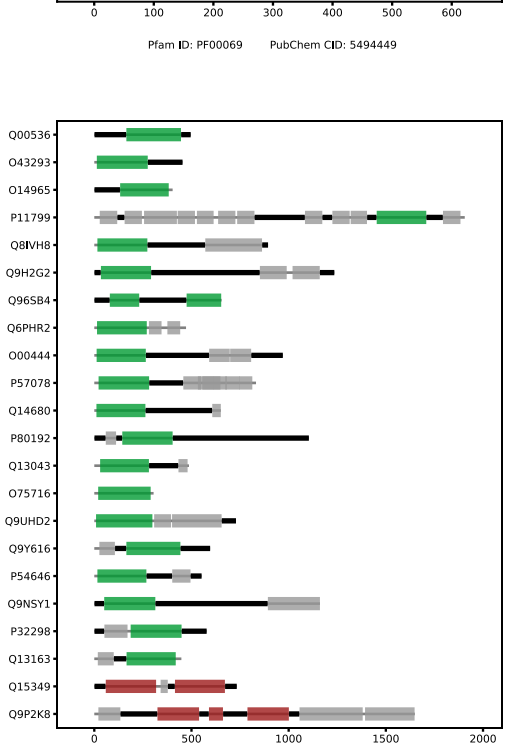
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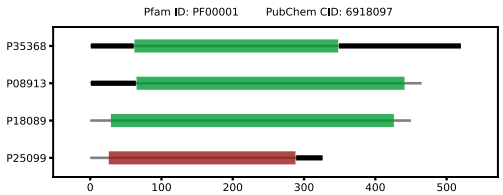
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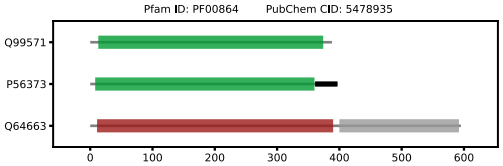
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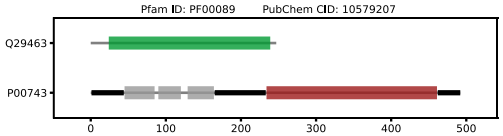
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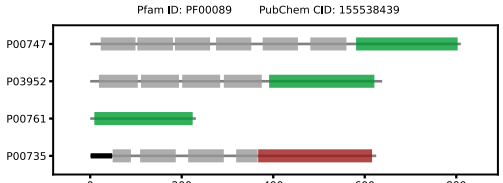
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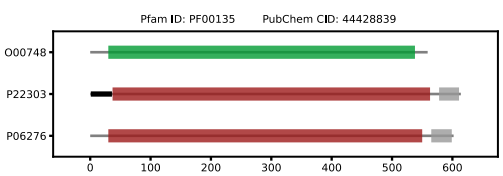
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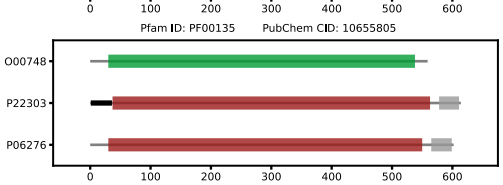
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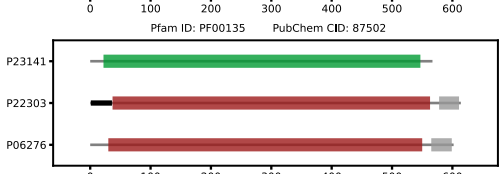
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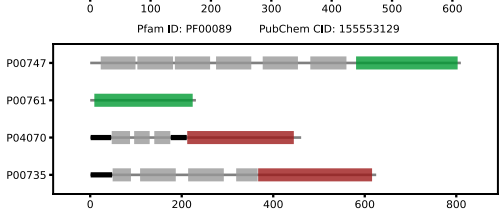
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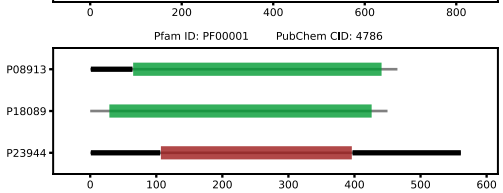
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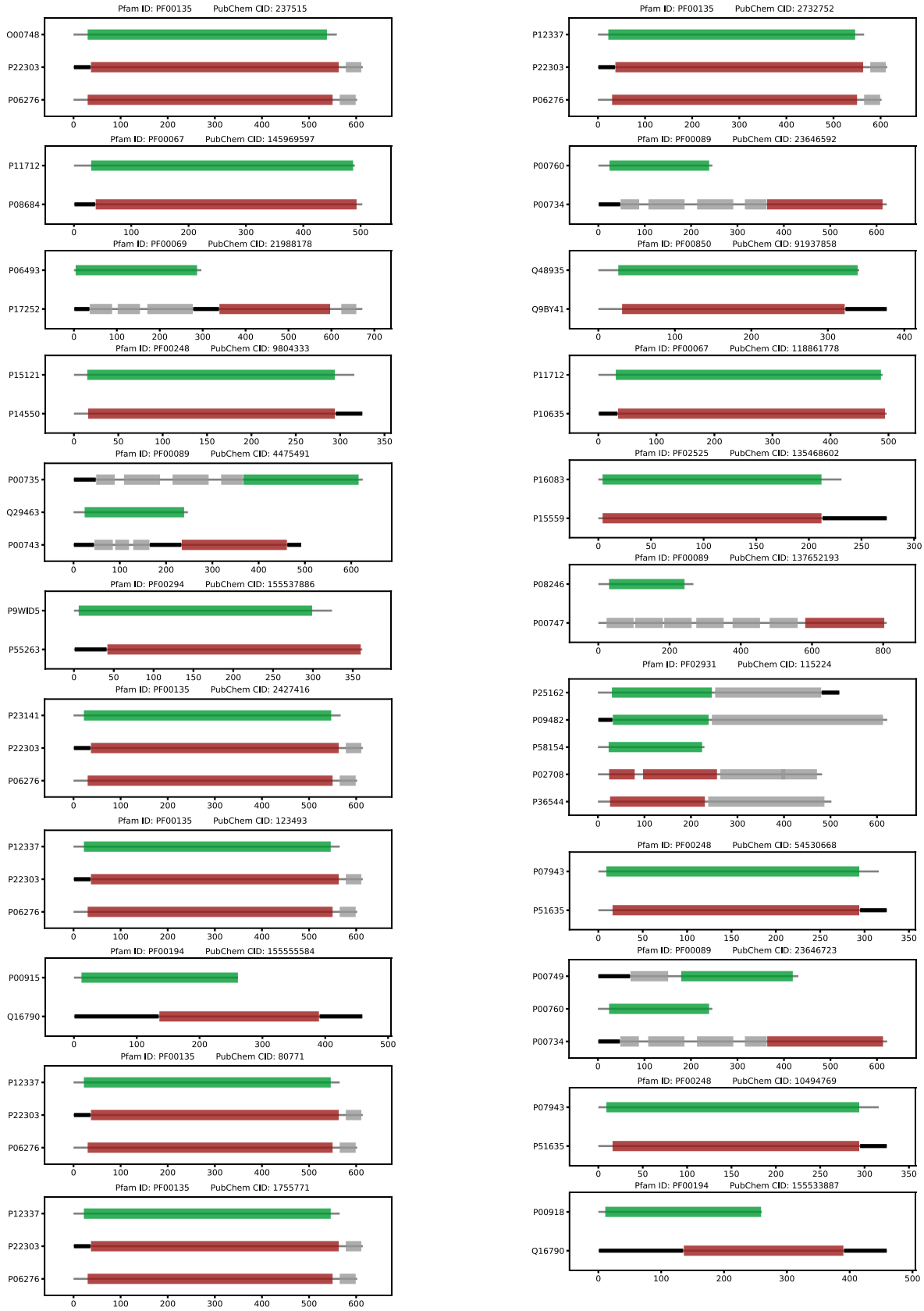
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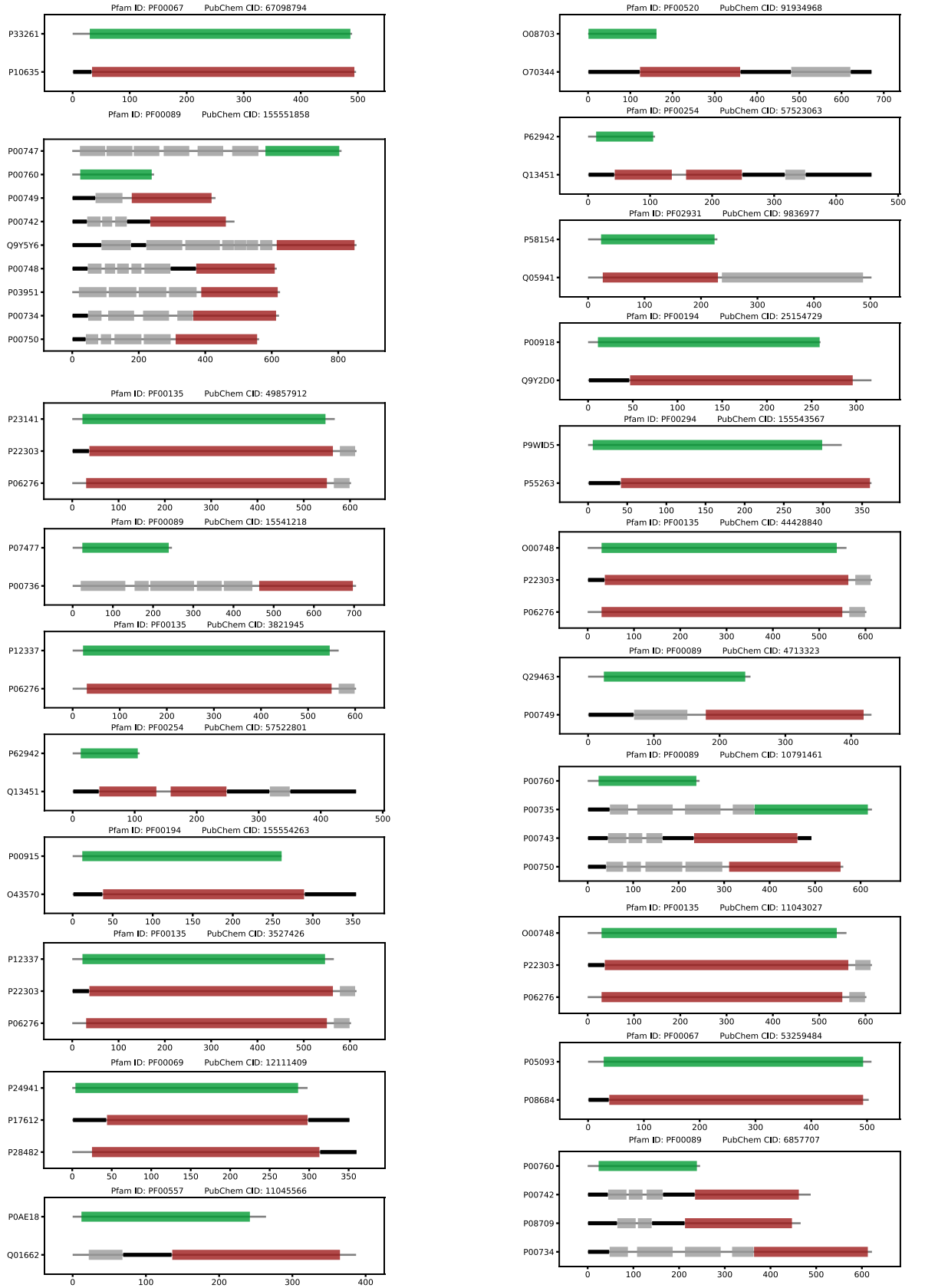
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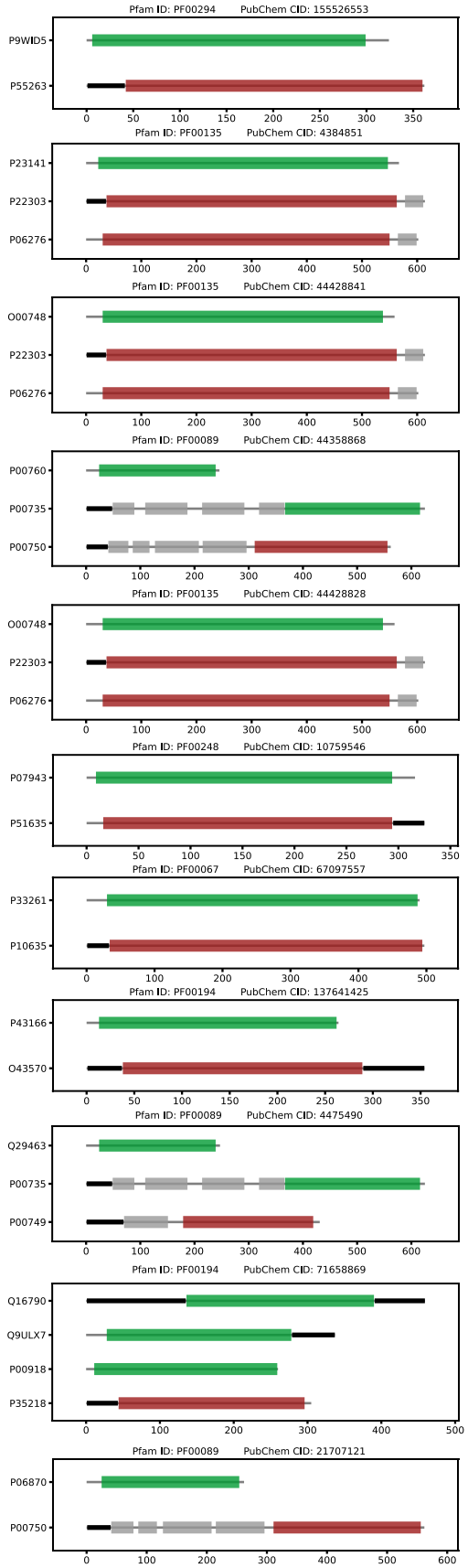
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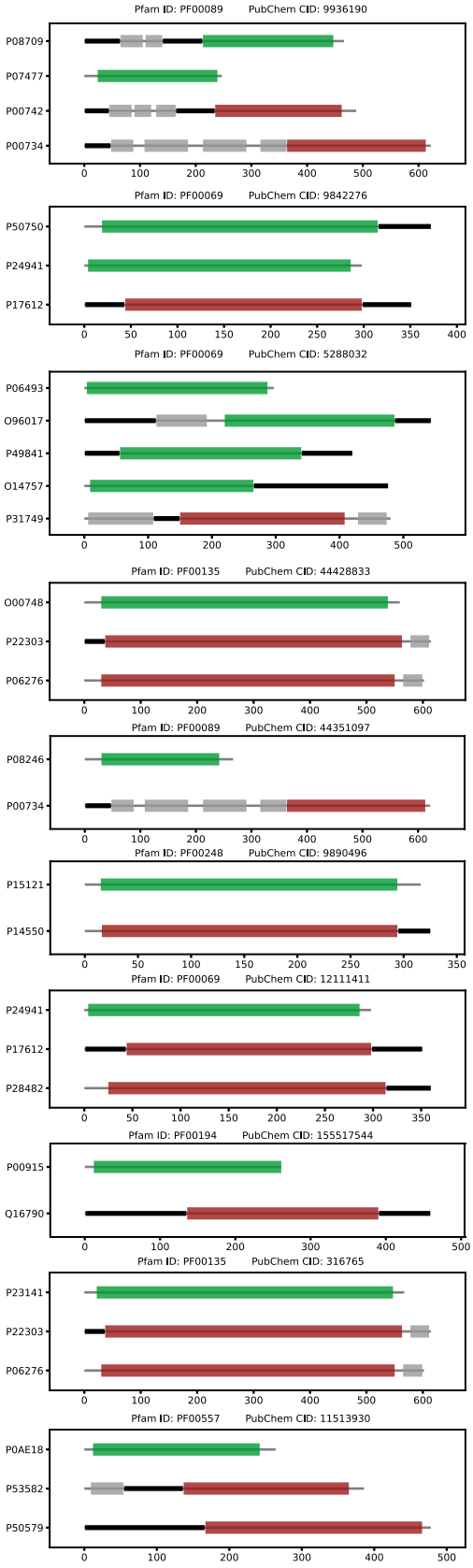
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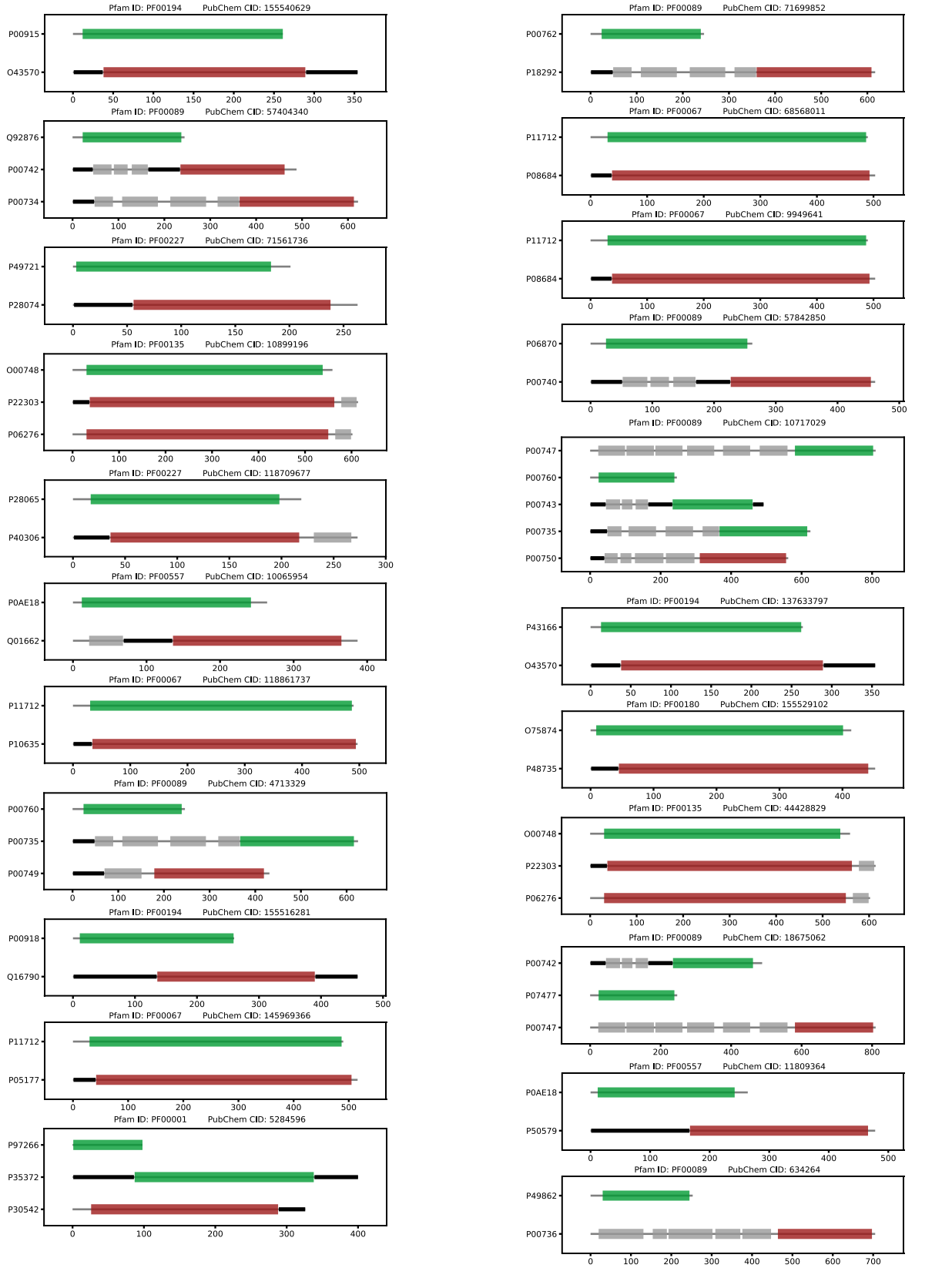
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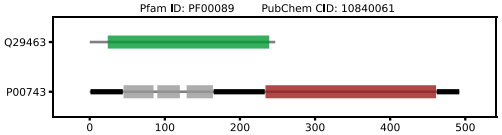
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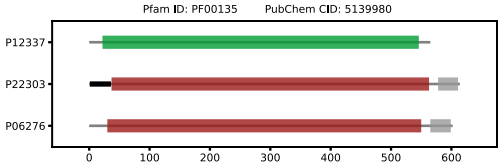
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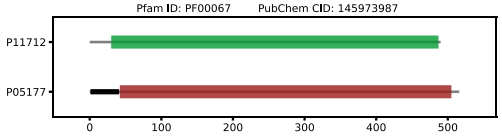
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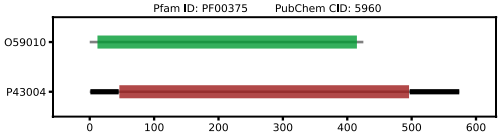
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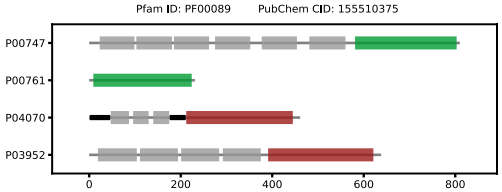
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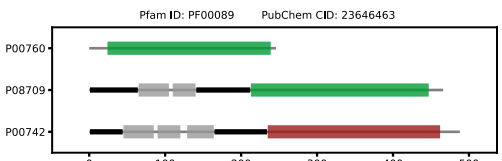
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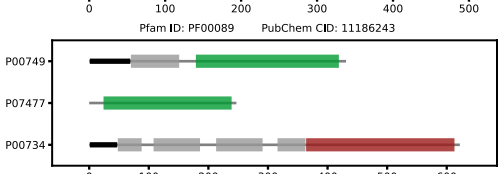
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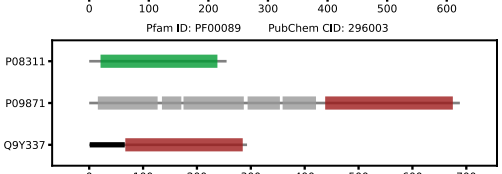
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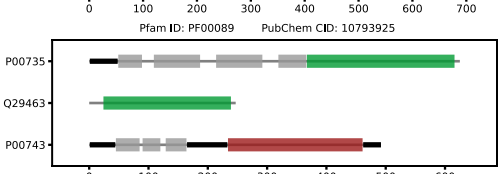
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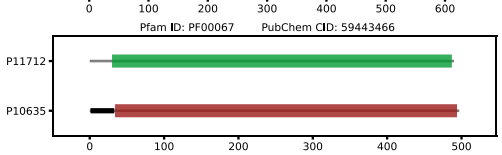
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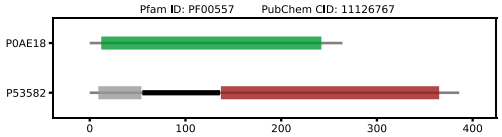
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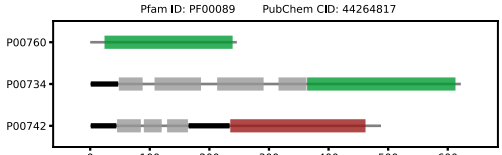
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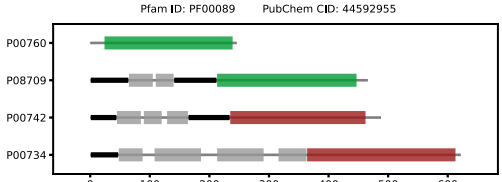
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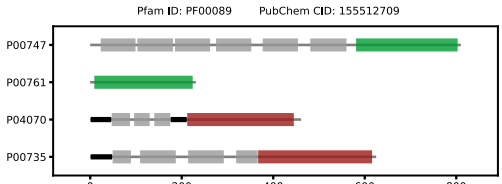
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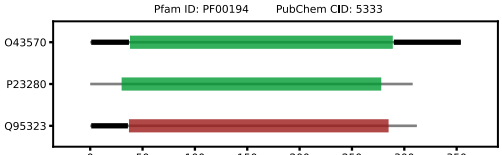
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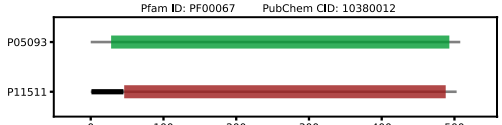
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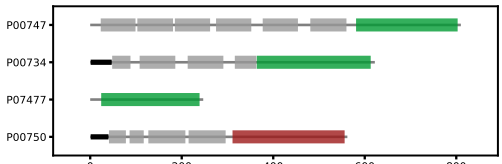
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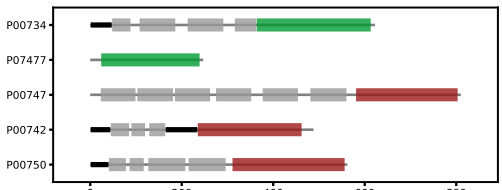
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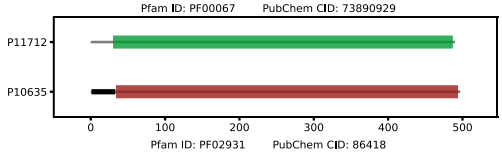
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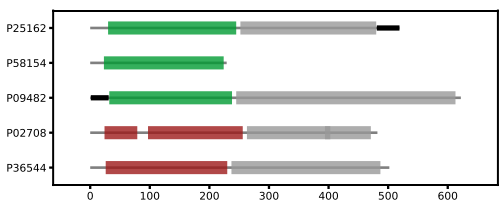
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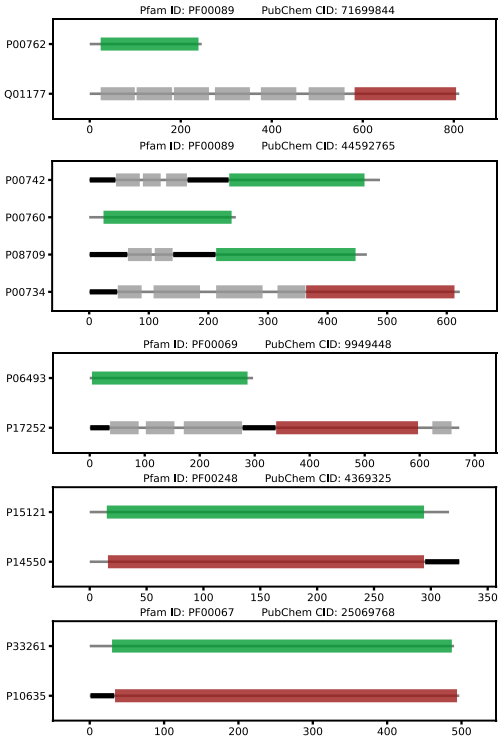
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