IDENTIFICATION OF POTENTIAL INHIBITORS AGAINST N-PROTEIN OF COVID-19 AND ITS CURATION IN THE FORM OF DATABASE

A report submitted in partial fulfilment of the requirements for the degree of

BACHELOR OF TECHNOLOGY

Under the supervision of

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SOLAN, H.P.

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STUDENT'S DECLARATION

I hereby declare that the work presented in the Project report entitled **"DRUG DESIGNING FOR POTENTIAL TARGETS OF COVID-19"** submitted for partial fulfillment of the requirements for the degree of Bachelor of Technology in Bioinformatics Engineering at **Jaypee University of Information Technology, Waknaghat** is an authentic record of my work carried out under the supervision of **Dr. Tiratha Raj Singh, Associate Professor** of Department of Biotechnology and Bioinformatics, Jaypee University of Information Technology, Waknaghat**.** This work has not been submitted elsewhere for the reward of any other degree/diploma. I am fully responsible for the contents of my project report.

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2021

(Dr. Tiratha Raj Singh)

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IDENTIFICATION OF POTENTIAL INHIBITORS AGAINST N-PROTEIN OF COVID-19 AND ITS CURATION IN THE FORM OF DATABASE

We hope our efforts will please our mentors.

ABSTRACT

The project is based on the COVID-19 as it is a recent pandemic and of great importance. The structure of COVID-19 was studied and after gaining awareness of the structure, it was found that attractive drug targets among Corona viruses are the N-proteins/ Nucleocapsid proteins and the S-proteins/ Spike proteins. The N protein is the most abundant in Corona viruses and is responsible for the binding of the RNA. Therefore, N protein constitutes one of the major proteins for the drug designing of COVID-19 disease. In this project we worked on the N-protein. We downloaded the N-protein structure (PDB ID- 6WKP) of SARS-CoV-2 from the RCSB, PDB site. This protein was then analyzed and prepared using Chimera. DrugBank was then explored and we downloaded all FDA-approved drugs, which could potentially be used as inhibitors for the drug designing process of COVID-19 disease. After this, docking studies were performed between the downloaded N-protein and 1000 FDA-approved drugs using Autodock Vina and their binding affinities were recorded. After performing the docking studies, a Database named COVID-19 POTENTIAL DRUG BINDING ENERGY DATABASE was developed using SQL queries in XAMPP version 3.2.4 software. The GUI is provided to retrieve the drug binding affinity against the N-protein. COVID-19 POTENTIAL DRUG BINDING ENERGY DATABASE is a unique and first of its kind database. We will update it as per the availability of new data in near future. COVID-19 POTENTIAL DRUG BINDING ENERGY DATABASE is freely available for the academic and research purpose to provide important information to the scientific community at: http://www.bioinfoindia.org/cdbd.

CHAPTER-1

INTRODUCTION

COVID-19 is a newly developed disease, first found in Wuhan, China in 2019. This disease is caused by a virus called SARS-CoV-2 [1]. It is a communicable disease. As of 6th May, 2021, the number of global COVID-19 cases has risen to 155,926,028 out of which 133,394,505 people have recovered and 3,258,393 deaths recorded. In India the COVID-19 cases has risen to 23,340,938. Out of these 19,382,642 people have recovered and 254,225 deaths recorded. In India, the recovery rate is about 82.75% [2].

As we look evolutionarily, SARS-CoV-2 is quite similar to SARS-CoV, which caused the disease Severe acute respiratory syndrome, i.e., SARS in 2002 in China. It is believed that this virus is having a zoonotic origin. Sequence analysis of genes has shown that coronavirus comes under the genus *Betacoronavirus*, and the subgenus *Sarbecovirus*. This virus is said to be 96% identical to the other bat coronavirus samples [3].

SYMPTOMS OF COVID-19

Conventional symptoms include temperature, cough, tiredness, trouble breathing, and loss of taste and smell. It is seen that predominantly symptoms are mild. Few people have major complex symptoms that advances to acute respiratory distress syndrome (ARDS), multi-organ failure, blood clots, and septic shock. The incubation period is discovered to be of five days but may span from two to fourteen days [4].

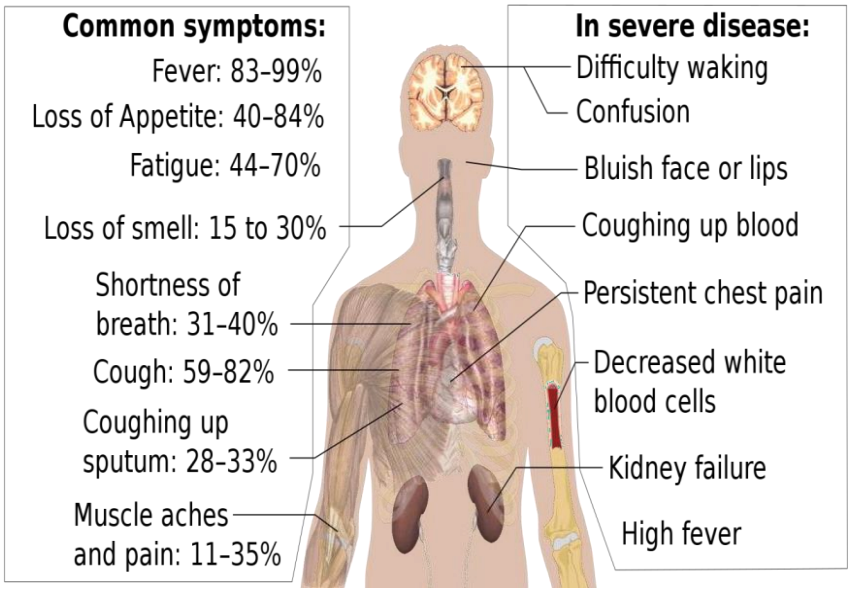

Figure 1. Symptoms of COVID-19 [1]

TRANSMISSION OF DISEASE

As this is a communicable disease, this virus is primarily spread through small droplets developed by sneezing, talking, and coughing. The droplets less often travel long distances through air and usually fall to the ground and other surfaces. People may develop the disease by touching a contaminated surface and then touching their faces. It is extremely contagious during the first three days after the first onset of symptoms [5]. It is still possible to spread the disease before the symptom appears or even when a person is asymptomatic i.e. contains no symptoms at all. The usual method of diagnosis is by real-time reverse transcription-polymerase chain reaction (rRT-PCR) from a nasopharyngeal swab. Based on risk factors and symptoms Chest CT or X-ray imaging could also be used for diagnosis, in individuals having complex symptoms of the disease [6].

STRUCTURE OF SARS-CoV-2 VIRION

The structure of the SARS-CoV-2 virus comprises an outer envelope, a core, the nucleoprotein and a nucleocapsid.

SARS-CoV2 has a diameter of 120nm consisting of a lipid bilayer and a core RNA genome. The lipid bilayer envelope consists of an envelope, membrane and anchored spike proteins. The RNA genome is found to bind the nucleocapsid protein.

S protein: The S protein, also called the spike protein has a homotrimeric structure. It consists of S1 and S2 subunits. The function of the S1 subunit lies as a receptor-binding domain although the S2 subunit helps in forming the spike stalk or helps in fusion. Collectively, each subunit works in virion-host cell receptor binding. The size of S protein is said to be ~150KDa and chemically it is a type of glycoprotein. This protein is said to be immensely glycosylated as it contains N- glycosylation sites numbering to be approximately 21 to 35. The crown-like or corona appearance of the SARS-CoV-2 virus comes from the S or the spike protein [7]. There are in total 2 domains present in the S protein, which are the S1 domain, which is the N- terminal domain and the S2 domain that is the C- terminal domain. The S2 domain contains the putative fusion peptide, HR1 (Heptad repeat 1) and HR2 (Heptad repeat 2). There is another domain called the transmembrane domain [8].

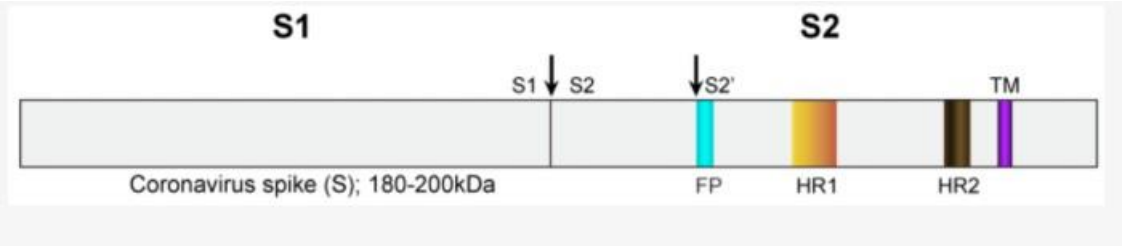

Figure 2. Detailed structure of S protein of Corona virus [2]

M protein: The M protein, also called as the membrane protein, the name suggests functions in giving shape to the virus. It has a dimeric structure. The size of the M protein is thought to be between ~25 to 30KDa.

E protein: The E protein, also called the Envelope protein has a size between ~8-12KDa, it is considered to be a smaller protein. The function of the E protein lies in the assembly and release of the virus.

It has been seen that the SARS-CoV-2 virus, if lacks the E protein, is less lethal. Although, it is seen that the lethality depends upon the type of the strain.

N protein: The N protein, also called the nucleocapsid protein functions in organizing the RNA genome as bead in string. There are in total two domains in the SARS-CoV-2 virus, that is the NTD (N-terminal domain), CTD (C- terminal domain). They both are separated

by a disordered linker. Also, they are said to be flanked in both the termini by disordered tails [9]. The NTD is said to be responsible for RNA binding. It is also noted that the middle terminal and CTD are also capable of RNA binding. The affinity for RNA of both NTD and CTD is said to be enhanced by the three disordered regions [10]. We can also see many other domains, which are having low complexity and are called the low complexity domains, such as the S-rich domain (having a bias for Arginine) and present within the middle linker and a K- rich domain which is seen to be present in the C-terminal disordered tail. In addition to these, we can see some oligomerization domains as well [11]. Combinedly, all the above domains are said to support a role for SARS-CoV-2 protein in the regulation as well as the recruitment of biomolecular condensates.

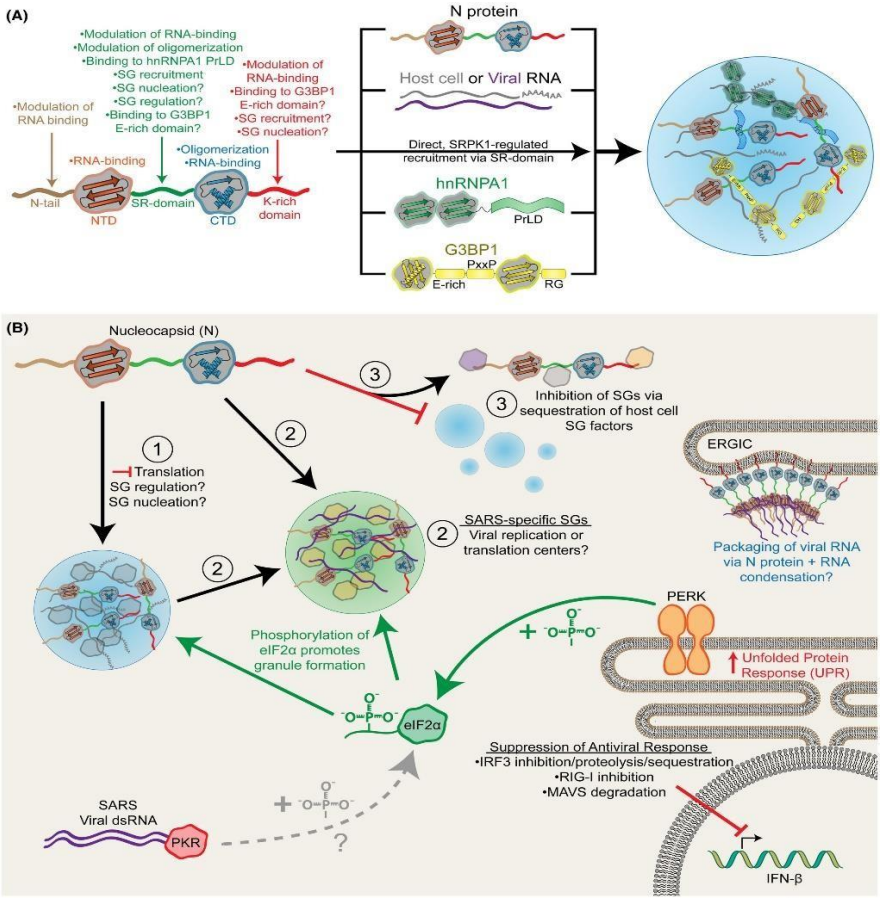

Figure 3. Proposed models for the influence of SARS-CoV-2 N-protein in the regulation and formation of biomolecular condensates [3]

He-hemagglutinin esterase: There is another type of protein called He- **hemagglutinin esterase.** It is present in some strains of coronaviruses such as the *betacoronavirus*. Its function lies in inducing the cell entry of S protein-mediated virions [12].

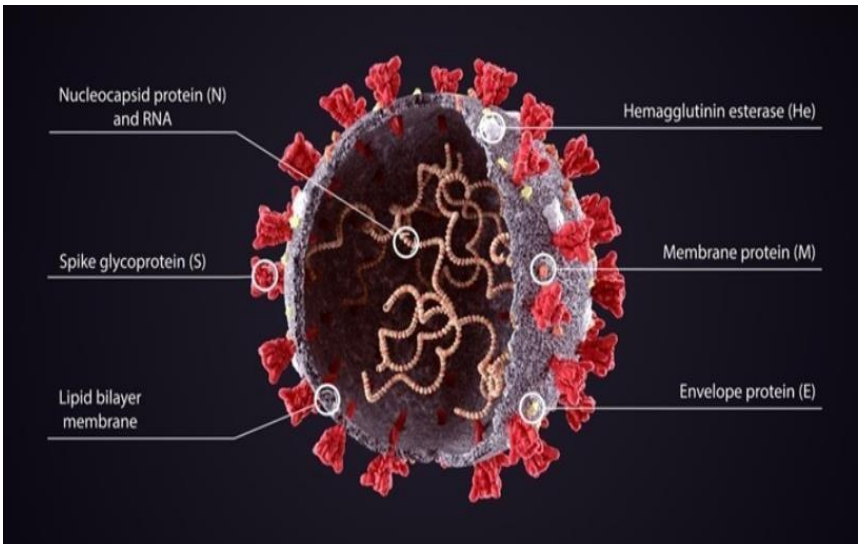

Figure 4. Structure of SARS-CoV-2 virus [4]

CHAPTER 2.

MATERIALS AND METHODS

1) Firstly, the PDB ID 6WKP for N- protein was downloaded from the RCSB's Protein Data Bank (PDB), which was selected as the protein for the docking experiment. The protein was downloaded from the option Download files option as shown below. The resolution of the structure was 2.67 Å.

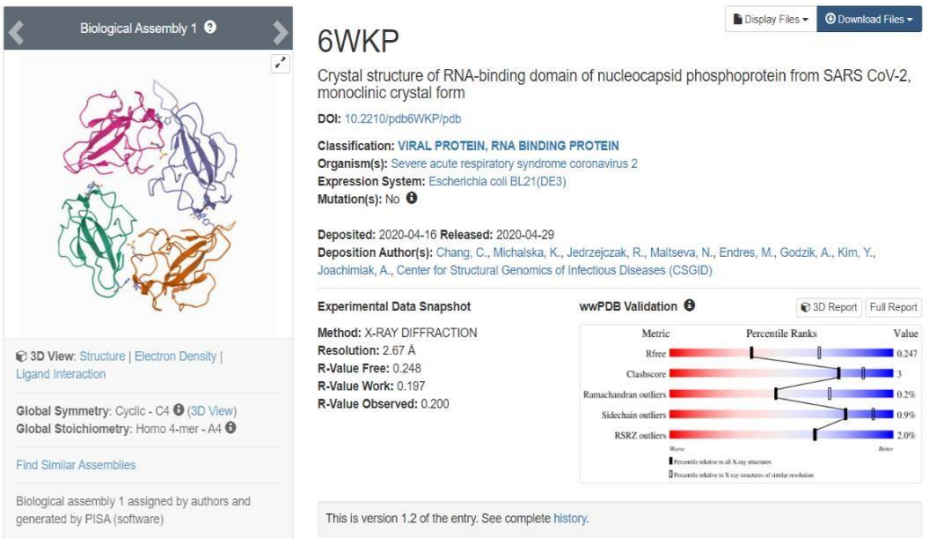

Figure 5. RCSB page showing-6WKP entry at PDB [5]

2) Preparation of the protein was done (6WKP) as we want only a chain so other

chains therefore were deleted from the structure. All non-stranded residues were also deleted using Chimera molecular visualization application software, so that, again, it could be used in Autodock software for docking.

Steps for performing the above are as follows:

- Open chimera. Go to file, open and select the protein(6WKP).
- Go to select, chain, A.
- Go to actions, Atoms and bonds, delete.
- Chain A will be deleted.
- Perform the same steps for chain deletions for other chains and keep only chain B.
- Now, go to Select, residues, all non-stranded.
- Go to actions, Atoms and bonds, delete.
- All non- stranded residues will be deleted.
- Save the above structure as protein.pdb

3) Explore DrugBank:We looked for all the FDA-approved drugs in DrugBank and downloaded them, so that they can be selected as inhibitors for the above protein. Go to downloads, structure and there is a list of drugs in sdf format, download all FDA-approved drugs in sdf format.

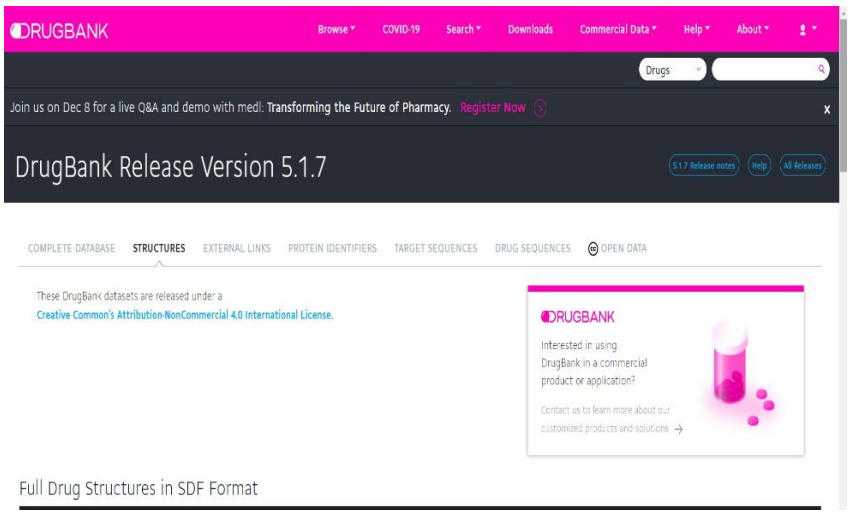

Figure 6. DrugBank page [6]

4) Next, we downloaded each inhibitor one by one PyRx software in the sdf format and then further converted into ligand.mol2 by using UCSF Chimera software, having the following steps:

- Open PyRx.
- Click on Open Babel and then click on the combined structures.sdf file.
- Click on the individual .sdf file that you want to download and save it as ligand.sdf
- Now, prepare this ligand.sdf file using UCSF Chimera molecular visualization application software by clicking on open file, ligand.sdf and save as ligand.mol2.
- Repeat the following steps for all 1000 ligands.

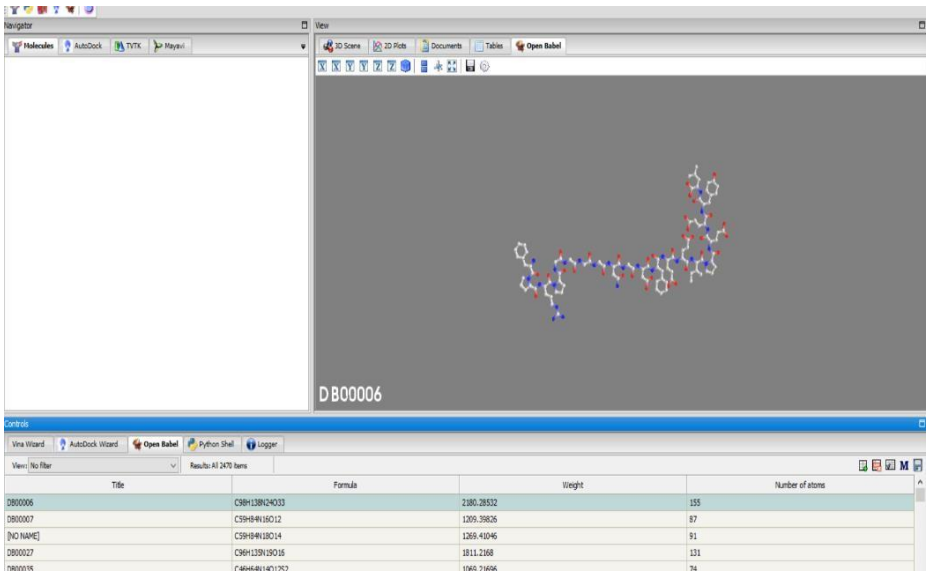

Figure 7. Image showing PyRx software page

5) A folder was created called Docking. Inside the docking folder, various ligand folders with different names were created. Inside the ligand, as the folder keeps protein.pdb and ligand.mol2 files of that particular ligand, along with the config.txt file. Inside the config.txt file, we write about the information necessary for docking, such as the receptor name, the ligand name, center_x, center_y, center_z, size_x, size_y, size_z , energy range and exhaustiveness.

6) After preparing the folders, we prepare for the docking process using mgltools AutoDock software. The steps of the process are as follows:

- Open MGLTools AutoDock software.
- Click on File, preferences, set, start-up directory, write the path of the directory you are currently going to work on, set and dismiss.
- File, read molecule, protein.pdb. Go to edit, add, Hydrogen, Polar only.
- Go to Add, charges, add Kollman charges; Add, atoms, Assign AD4 type; Add, Hydrogen, merge, non-polar, continue; Add, charges, check totals on residue; spread charge deficit, dismiss. Now, save the file as protein.pdbqt.
- Save the protein.pdbqt file in every ligand folder.
- Now, again open mgltools AutoDock software. Click on File, preferences, set, start up directory, write the path of the directory you are currently going to work on, set and dismiss.
- Go to File, read molecule and open ligand.mol2 of a particular ligand folder that you have set in the preferences section.
- Click on Ligand, input, choose, Choose Ligand, select molecule for AutoDock 4 , OK.
- Click on ligand, output and save as ligand.pdbqt.
- Go to file, read molecule and open protein.pdbqt.
- Click on Grid, macromolecule, choose, protein, OK, No, OK.
- Click on grid, grid box, change grid parameters according to the prescribed binding site.
- Then click on File, Output grid dimension file, go to the docking folder you want to save the file in and save as grid.txt.
- Repeat the following steps for all 1000 FDA-approved inhibitors to prepare the molecules for the Docking process.
- At the end of the process a ligand.pdbqt, protein.pdbqt, config.txt, grid.txt files are created for all the 1000 inhibitors and each folder contains these files

7) Now, the actual docking process is done using the software AutoDock Vina version 1.1.2.
    - Now, go to the search bar of your computer and type cmd, command prompt will open.

- Type cd and path of the ligand folder you want to dock.
- Now, go to your C drive, Program files x 86 , Scripps Research Institute, Vina and copy this path i.e "C:\Program Files (x86)\The Scripps Research Institute\Vina"
- Write cd "C:\Program Files (x86)\The Scripps Research Institute\Vina\vina.exe" --receptor protein.pdbqt --ligand ligand.pdbqt --config config.txt --log log.txt --out output.pdbqt and enter.
- This will perform the docking and give us the binding affinities of the docked molecules. The output is generated in log.txt files.
- Repeat these steps for all 1000 inhibitors.

8) After this, the output values i.e. binding affinities were recorded in an excel sheet for all 1000 ligands.
9) Finally, these molecules were sorted using a in house Python code, in ascending order of binding energy to get the top 3 hits.
10) This code was run on Spyder.
11) The code is as follows:

```
Import pandas as pd
data= pd.read_csv("C:\\Users\\Desktop\\docking.csv")
data.sort_values(["Binding affinity"], axis=0, ascending= True, inplace= True)
data
```

12) Next, we have created a Database of the docking results obtained via AutoDock Vina, of these 1000 ligands. The database is created using XAMPP version 3.2.4 software. The steps of creating a database in XAMPP version 3.2.4 are as follows:
    - Go to the search bar of your computer and type cmd, command prompt will open.
    - For going to the root directory enter cd\.
    - Go to the Drive where XAMPP is installed. For this type Drive: in cmd, in this case D:.
    - In cmd enter the path of the bin folder i.e. cd xampp\mysql\bin and then press enter.
    - Now wite the command MySQL -u root -p -h 127.0.0.1 on cmd for

linking it to the local host.

- Now it will be asking for a password. Press Enter and write nothing because no password exists. Now, we are ready to use SQL commands on XAMPP.
- The SQL commands for creating Database are as follows:

```
CREATE TABLE IF NOT EXISTS docking (
  `Index` INT,`DrugBankID` VARCHAR(7) CHARACTER SET utf8,`Ligand`
VARCHAR(47) CHARACTER SET utf8, `Binding_affinity` NUMERIC(3, 1)
                );
INSERT INTO docking VALUES (1,'DB00615','Rifabutin',-
13.6),(2,'DB01395','Drospirenone',-13.6), (3,'DB00320','Dihydroergotamine',-13.2),
(4,'DB00309','Vindesine',-13.2),(5,'DB00390','Digoxin',-13.1),
(6,'DB00207','Azithromycin',-13),(7,'DB01406','Danazol',-12.6),
(8,'DB01200','Bromocriptine',-12.5),(9,'DB08973','Fluclorolone acetonide',-
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11.7),(33,'DB01708','Prasterone',-11.6) (34,'DB04839','Cyproterone acetate',-11.6)
(35,'DB02789','Pregnenolone',-11.6),(36,'DB06595','Midostaurin',-11.5),
(37,'DB06212','Tolvaptan',-11.5),(38,'DB00337','Pimecrolimus',-11.5)
(39,'DB08906','Fluticasone furoate',-11.5),(40,'DB00367','Levonorgestrel',-
11.5),(41,'DB00444','Teniposide',-11.5),(42,'DB00378','Dydrogesterone',-11.4),
(43,'DB01211','Clarithromycin',-11.4),(44,'DB00396','Progesterone',-
```

11.4),(45,'DB00324','Fluorometholone',-11.4),(46,'DB01590','Everolimus',-11.4),(47,'DB06713','Norelgestromin',-11.3),(48,'DB00504','Levallorphan',-11.3),(49,'DB06412','Oxymetholone',-11.3),(50,'DB00253','Medrysone',-11.3),(51,'DB06287','Temsirolimus',-11.3),(52,'DB00223','Diflorasone',-11.2),(53,'DB06230','Nalmefene',-11.2),(54,'DB05990','Obeticholic acid',-11.2),(55,'DB08971','Fluocortolone',-11.2),(56,'DB01216','Finasteride',-11.2),(57,'DB06290','Simeprevir',-11.2),(58,'DB08905','Formestane',-11.2),(59,'DB00294','Etonogestrel',-11.2), (60,'DB06777','Chenodeoxycholic acid',-11.2),(61,'DB08827','Lomitapide',-11.2),(62,'DB08867','Ulipristal',-11.1),(63,'DB00361','Vinorelbine',-11.1),(64,'DB04845','Ixabepilone',-11.1),(65,'DB04573','Estriol',-11.1),(66,'DB00512','Vancomycin',-11.1),(67,'DB06800','Methylnaltrexone',-11),(68,'DB06780','Desoxycorticosterone acetate',-11),(69,'DB00655','Estrone',-11),(70,'DB01177','Idarubicin',-11),(71,'DB00351','Megestrol acetate',-11), (72,'DB00254','Doxycycline',-10.9),(73,'DB08930','Dolutegravir',-10.9),(74,'DB00618','Demeclocycline',-10.9),(75,'DB02659','Cholic Acid',-10.9), (76,'DB03619','Deoxycholic acid',-10.9),(77,'DB00588','Fluticasone propionate',-10.8), (78,'DB01238','Budesonide',-10.8),(79,'DB01586','Ursodeoxycholic acid',-10.8), (80,'DB00547','Desoximetasone',-10.8),(81,'DB04038','Ergosterol',-10.7),(82,'DB00307','Bexarotene',-10.7),(83,'DB00327','Hydromorphone',-10.7),(84,'DB00295','Morphine',-10.7),(85,'DB04574','Estrone sulfate',-10.7),(86,'DB04540','Cholesterol',-10.7),(87,'DB04575','Quinestrol',-10.7),(88,'DB06809','Plerixafor',-10.7),(89,'DB00288','Amcinonide',-10.6),(90,'DB00377','Palonosetron',-10.6),(91,'DB01419','Antrafenine',-10.6),(92,'DB00199','Erythromycin',-10.6),(93,'DB01410','Ciclesonide',-10.6), (94,'DB05013','Ingenol mebutate',-10.5),(95,'DB04348','Taurocholic acid',-10.5),(96,'DB00497','Oxycodone',-10.4),(97,'DB00620','Triamcinolone',-10.4),(98,'DB08901','Ponatinib',-10.4),(99,'DB01420','Testosterone propionate',-10.3), (100,'DB02703','Fusidic acid',-10.3),(101,'DB04868','Nilotinib',-10.3),(102,'DB00434','Cyproheptadine',-10.3),(103,'DB06335','Saxagliptin',-10.2),(104,'DB00318','Codeine',-10.2),(105,'DB08815','Lurasidone',-10.2),(106,'DB06148','Mianserin',-10.2),(107,'DB01380','Cortisone acetate',-10.2),(108,'DB01251','Gliquidone',-10.2),(109,'DB01248','Docetaxel',-10.1),(110,'DB00514','Dextromethorphan',-10.1),(111,'DB06210','Eltrombopag',-10.1),(112,'DB00635','Prednisone',-10.1),

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(580,'DB00432','Trifluridine',-7.2),(581,'DB05271','Rotigotine',-7.2),
(582,'DB06736','Aceclofenac',-7.2),(583,'DB01581','Sulfamerazine',-7.2),

(584,'DB01176','Cyclizine',-7.2),(585,'DB06807','Phenyl aminosalicylate',-7.2), (586,'DB01282','Carbetocin',-7.2), (587,'DB01322','Kava',-7.2), (588,'DB02959','Oxitriptan',-7.2), (589,'DB08943','Isoconazole',-7.2), (590,'DB00193','Tramadol',-7.2), (591,'DB00274','Cefmetazole',-7.2),(592,'DB00263','Sulfisoxazole',-7.2), (593,'DB00185','Cevimeline',-7.2), (594,'DB06217','Vernakalant',-7.2), (595,'DB06695','Dabigatran etexilate',-7.2),(596,'DB00178','Ramipril',-7.2), (597,'DB00495','Zidovudine',-7.2),(598,'DB00459','Acitretin',-7.2), (599,'DB08872','Gabapentin enacarbil',-7.2),(600,'DB00255','Diethylstilbestrol',-7.2), (601,'DB04465','Lactose',-7.2),(602,'DB00322','Floxuridine',-7.2), (603,'DB00532','Mephenytoin',-7.2),(604,'DB00175','Pravastatin',-7.1), (605,'DB00499','Flutamide',-7.1),(606,'DB00285','Venlafaxine',-7.1), (607,'DB00493','Cefotaxime',-7.1), (608,'DB00517','Anisotropine methylbromide',-7.1), (609,'DB01243','Chloroxine',-7.1),(610,'DB00473','Hexylcaine',-7.1), (611,'DB00573','Fenoprofen',-7.1),(612,'DB00150','Tryptophan',-7.1), (613,'DB04846','Celiprolol',-7.1),(614,'DB08880','Teriflunomide',-7.1), (615,'DB01331','Cefoxitin',-7.1),(616,'DB00461','Nabumetone',-7.1),(617,'DB00196','Fluconazole',-7.1),(618,'DB00581','Lactulose',-7.1), (619,'DB06700','Desvenlafaxine',-7.1),(620,'DB04817','Metamizole',-7.1), (621,'DB04951','Pirfenidone',-7.1),(622,'DB00633','Dexmedetomidine',-7.1),(623,'DB01416','Cefpodoxime',-7.1),(624,'DB01627','Lincomycin',-7), (625,'DB00283','Clemastine',-7),(626,'DB04880','Enoximone',-7),(627,'DB00557','Hydroxyzine',-7),(628,'DB00393','Nimodipine',-7),(629,'DB04840','Debrisoquine',-7),(630,'DB01987','Cocarboxylase',-7),(631,'DB00410','Mupirocin',-7),(632,'DB04826','Thenalidine',-7),(633,'DB00440','Trimethoprim',-7),(634,'DB00556','Perflutren',-7), (635,'DB00521','Carteolol',-7),(636,'DB06701','Dexmethylphenidate',-7), (637,'DB01240','Epoprostenol',-7),(638,'DB08889','Carfilzomib',-7), (639,'DB00239','Oxiconazole',-7),(640,'DB00454','Meperidine',-7), (641,'DB06614','Peramivir',-7),(642,'DB00631','Clofarabine',-7), (643,'DB01582','Sulfamethazine',-7),(644,'DB00137','Lutein',-7), (645,'DB06288','Amisulpride',-7),(646,'DB00204','Dofetilide',-7), (647,'DB00250','Dapsone',-7),(648,'DB00640','Adenosine',-7),(649,'DB06762','Pinacidil',-7),(650,'DB00483','Gallamine triethiodide',-7), (651,'DB00080','Daptomycin',-7), (652,'DB00333','Methadone',-6.9),(653,'DB01190','Clindamycin',-6.9), (654,'DB00639','Butoconazole',-6.9),

(655,'DB00345','Aminohippuric acid',-6.9), (656,'DB03312','Brivudine',-6.9),(657,'DB00571','Propranolol',-6.9), (658,'DB01579','Phendimetrazine',-6.9),(659,'DB00494','Entacapone',-6.9),(660,'DB02546','Vorinostat',-6.9),(661,'DB00418','Secobarbital',-6.9), (662,'DB00194','Vidarabine',-6.9),(663,'DB08933','Luliconazole',-6.9), (664,'DB00380','Dexrazoxane',-6.9),(665,'DB08918','Levomilnacipran',-6.9), (666,'DB00287','Travoprost',-6.9),(667,'DB01606','Tazobactam',-6.9), (668,'DB08941','Isoxsuprine',-6.9),(669,'DB00654','Latanoprost',-6.9), (670,'DB01262','Decitabine',-6.9),(671,'DB00476','Duloxetine',-6.9), (672,'DB00187','Esmolol',-6.8),(673,'DB01353','Butobarbital',-6.8), (674,'DB00649','Stavudine',-6.8),(675,'DB00360','Sapropterin',-6.8), (676,'DB00600','Monobenzone',-6.8),(677,'DB00391','Sulpiride',-6.8), (678,'DB04815','Clioquinol',-6.8),(679,'DB00647','Dextropropoxyphene',-6.8), (680,'DB00608','Chloroquine',-6.8),(681,'DB08819','Tafluprost',-6.8) (682,'DB00268','Ropinirole',-6.8),(683,'DB00574','Fenfluramine',-6.8), (684,'DB01616','Alverine',-6.8),(685,'DB01611','Hydroxychloroquine',-6.8), (686,'DB01610','Valganciclovir',-6.8),(687,'DB08868','Fingolimod',-6.8), (688,'DB00308','Ibutilide',-6.8),(689,'DB00234','Reboxetine',-6.8), (690,'DB01600','Tiaprofenicacid',-6.8),(691,'DB06821','Sulfameter',-6.8),(692,'DB01427','Amrinone',-6.8),(693,'DB01191','Dexfenfluramine',-6.8), (694,'DB00312','Pentobarbital',-6.7),(695,'DB04822','Oxeladin',-6.7), (696,'DB00355','Aztreonam',-6.7),(697,'DB00249','Idoxuridine',-6.7),(698,'DB08964','Gemeprost',-6.7),(699,'DB04657','Carboxin',-6.7), (700,'DB00007','Leuprolide',-6.7),(701,'DB00381','Amlodipine',-6.7), (702,'DB00271','Diatrizoate',-6.7),(703,'DB08944','Isoaminile',-6.7), (704,'DB00359','Sulfadiazine',-6.7), (705,'DB01249','Iodixanol',-6.7), (706,'DB01632','5-O-phosphono-alpha-D-ribofuranosyl diphosphate',-6.7), (707,'DB01275','Hydralazine',-6.7), (708,'DB01625','Isopropamide',-6.7),(709,'DB01424','Aminophenazone',-6.6),(710,'DB01241','Gemfibrozil',-6.6),(711,'DB00449','Dipivefrin',-6.6),(712,'DB01597','Cilastatin',-6.6),(713,'DB01319','Fosamprenavir',-6.6), (714,'DB00405','Dexbrompheniramine',-6.6),(715,'DB00484','Brimonidine',-6.6), (716,'DB00428','Streptozocin',-6.6),(717,'DB00422','Methylphenidate',-6.6), (718,'DB01620','Pheniramine',-6.6),(719,'DB08814','Triflusal',-6.6),(720,'DB00183','Pentagastrin',-6.6),(721,'DB08799','Antazoline',-6.6), (722,'DB00409','Remoxipride',-

6.6),(723,'DB00289','Atomoxetine',-6.6), (724,'DB07565','Chloramphenicol succinate',-6.6), (725,'DB00325','Nitroprusside',-6.6), (726,'DB06150','Sulfadimethoxine',-6.5),(727,'DB00336','Nitrofural',-6.5), (728,'DB00014','Goserelin',-6.5),(729,'DB01438','Phenazopyridine',-6.5), (730,'DB00241','Butalbital',-6.5),(731,'DB00577','Valaciclovir',-6.5), (732,'DB04855','Dronedarone',-6.5),(733,'DB00429','Carboprost tromethamine',-6.5),(734,'DB00306','Talbutal',-6.5),(735,'DB06204','Tapentadol',-6.5), (736,'DB00280','Disopyramide',-6.5),(737,'DB00645','Dyclonine',-6.5), (738,'DB06702','Fesoterodine',-6.5),(739,'DB01435','Antipyrine',-6.5), (740,'DB00366','Doxylamine',-6.5),(741,'DB00518','Albendazole',-6.5), (742,'DB00350','Minoxidil',-6.5),(743,'DB06774','Capsaicin',-6.5), (744,'DB06769','Bendamustine',-6.5),(745,'DB00612','Bisoprolol',-6.5), (746,'DB00599','Thiopental',-6.5),(747,'DB08947','Iopamidol',-6.5), (748,'DB04832','Zimelidine',-6.5),(749,'DB06755','Beta carotene',-6.5), (750,'DB01407','Clenbuterol',-6.4);

INSERT INTO docking VALUES(751,'DB00264','Metoprolol',-6.4), (752,'DB00121','Biotin',-6.4),(753,'DB00190','Carbidopa',-6.4), (754,'DB08966','Fursultiamine',-6.4),(755,'DB01194','Brinzolamide',-6.4), (756,'DB00431','Lindane',-6.4),(757,'DB00446','Chloramphenicol',-6.4), (758,'DB00558','Zanamivir',-6.4),(759,'DB00237','Butabarbital',-6.4), (760,'DB00651','Dyphylline',-6.4),(761,'DB00219','Oxyphenonium',-6.4), (762,'DB01362','Iohexol',-6.4),(763,'DB06119','Cenobamate',-6.4), (764,'DB00221','Isoetharine',-6.4),(765,'DB01598','Imipenem',-6.3), (766,'DB02513','Thymol',-6.3),(767,'DB00195','Betaxolol',-6.3), (768,'DB00527','Cinchocaine',-6.3),(769,'DB04948','Lofexidine',-6.3), (770,'DB00176','Fluvoxamine',-6.3),(771,'DB06262','Droxidopa',-6.3), (772,'DB06716','Fospropofol',-6.3),(773,'DB00335','Atenolol',-6.3), (774,'DB00226','Guanadrel',-6.3),(775,'DB00265','Crotamiton',-6.3), (776,'DB02300','Calcipotriol',-6.3),(777,'DB00594','Amiloride',-6.3), (778,'DB00356','Chlorzoxazone',-6.3),(779,'DB06819','Phenylbutyric acid',-6.2), (780,'DB00277','Theophylline',-6.2),(781,'DB00143','Glutathione',-6.2), (782,'DB00152','Thiamine',-6.2),(783,'DB00426','Famciclovir',-6.2), (784,'DB00489','Sotalol',-6.2),(785,'DB00114','Pyridoxal phosphate',-6.2), (786,'DB00281','Lidocaine',-6.2),(787,'DB06826','Unoprostone',-

6.2),(788,'DB03310','Glutathione disulfide',-6.2), (789,'DB00292','Etomidate',-6.2), (790,'DB08949','Inositol nicotinate',-6.2),(791,'DB00217','Bethanidine',-6.1), (792,'DB00636','Clofibrate',-6.1),(793,'DB01187','Iophendylate',-6.1), (794,'DB06707','Levonordefrin',-6.1),(795,'DB00233','Aminosalicylic acid',-6.1), (796,'DB00423','Methocarbamol',-6.1),(797,'DB06691','Mepyramine',-6.1), (798,'DB00244','Mesalazine',-6.1),(799,'DB08946','Iopanoic acid',-6.1),(800,'DB00575','Clonidine',-6.1),(801,'DB00379','Mexiletine',-6.1),(802,'DB00135','Tyrosine',-6),(803,'DB00629','Guanabenz',-6), (804,'DB00585','Nizatidine',-6),(805,'DB00369','Cidofovir',-6), (806,'DB06218','Lacosamide',-6),(807,'DB00419','Miglustat',-6), (808,'DB01783','Pantothenic acid',-6),(809,'DB00299','Penciclovir',-6), (810,'DB00181','Baclofen',-6),(811,'DB00634','Sulfacetamide',-6), (812,'DB06795','Mafenide',-6),(813,'DB00373','Timolol',-5.9), (814,'DB00593','Ethosuximide',-5.9),(815,'DB04564','Gluconolactone',-5.9), (816,'DB06704','Iobenguane',-5.9),(817,'DB00302','Tranexamic acid',-5.9), (818,'DB00184','Nicotine',-5.9),(819,'DB06788','Histrelin',-5.9), (820,'DB00191','Phentermine',-5.9),(821,'DB01197','Captopril',-5.9),(822,'DB00300','Tenofovir disoproxil',-5.9),(823,'DB04173','Fructose',-5.9), (824,'DB00126','Ascorbic acid',-5.9),(825,'DB01296','Glucosamine',-5.9), (826,'DB03209','Oteracil',-5.8),(827,'DB00198','Oseltamivir',-5.8), (828,'DB00211','Midodrine',-5.8),(829,'DB02362','Aminobenzoic acid',-5.8), (830,'DB08958','Hexetidine',-5.8),(831,'DB00413','Pramipexole',-5.8), (832,'DB01189','Desflurane',-5.8),(833,'DB05541','Brivaracetam',-5.8),(834,'DB00291','Chlorambucil',-5.8),(835,'DB00610','Metaraminol',-5.8), (836,'DB00120','Phenylalanine',-5.8),(837,'DB00491','Miglitol',-5.8),(838,'DB00368','Norepinephrine',-5.8), (839,'DB00201','Caffeine',-5.7), (840,'DB00144','Phosphatidyl serine',-5.7), (841,'DB00388','Phenylephrine',-5.7), (842,'DB00617','Paramethadione',-5.7), (843,'DB00544','Fluorouracil',-5.7), (844,'DB00106','Abarelix',-5.7),(845,'DB00316','Acetaminophen',-5.7),(846,'DB01626','Pargyline',-5.6),(847,'DB06785','Ganirelix',-5.6),(848,'DB08797','Salicylamide',-5.6),(849,'DB03793','Benzoic acid',-5.6),(850,'DB01580','Oxprenolol',-5.6), (851,'DB08826','Deferiprone',-5.5), (852,'DB00182','Amphetamine',-5.5), (853,'DB00159','Icosapent',-5.5), (854,'DB00290','Bleomycin',-5.5), (855,'DB00501','Cimetidine',-5.5), (856,'DB08887','Icosapent ethyl',-5.5),

(857,'DB03756','Doconexent',-5.5), (858,'DB06714','Propylhexedrine',-5.5),(859,'DB00352','Tioguanine',-5.5),(860,'DB00397','Phenylpropanolamine',-5.5),(861,'DB00165','Pyridoxine',-5.5),(862,'DB06797','Mebutamate',-5.5), (863,'DB01914','D-glucose',-5.5), (864,'DB00399','Zoledronic acid',-5.5), (865,'DB01577','Metamfetamine',-5.5),(866,'DB01576','Dextroamphetamine',-5.5),(867,'DB03088','Pidolic acid',-5.4),(868,'DB04224','Oleic Acid',-5.4),(869,'DB05246','Methsuximide',-5.4), (870,'DB06689','Ethanolamine oleate',-5.4),(871,'DB00395','Carisoprodol',-5.4), (872,'DB00550','Propylthiouracil',-5.4),(873,'DB00326','Calcium glucoheptonate',-5.4), (874,'DB00437','Allopurinol',-5.4),(875,'DB05057','Erdosteine',-5.4), (876,'DB05018','Migalastat',-5.4),(877,'DB00236','Pipobroman',-5.4), (878,'DB03796','Palmitic Acid',-5.4),(879,'DB00050','Cetrorelix',-5.3), (880,'DB00632','Docosanol',-5.3),(881,'DB00166','Lipoic acid',-5.3), (882,'DB00627','Niacin',-5.3), (883,'DB01956','Taurine',-5.3), (884,'DB00155','Citrulline',-5.3), (885,'DB06699','Degarelix',-5.3),(886,'DB00545','Pyridostigmine',-5.3), (887,'DB01718','Cetrimonium',-5.3),(888,'DB06243','Eflornithine',-5.3),(889,'DB01638','Sorbitol',-5.3),(890,'DB03193','Stearic acid',-5.3),(891,'DB00132','alpha-Linolenic acid',-5.3),(892,'DB00403','Ceruletide',-5.2),(893,'DB00548','Azelaic acid',-5.2),(894,'DB00202','Succinylcholine',-5.2), (895,'DB06261','Hexaminolevulinate',-5.2),(896,'DB04931','Afamelanotide',-5.2),(897,'DB00262','Carmustine',-5.2),(898,'DB00347','Trimethadione',-5.2),(899,'DB03017','Lauric acid',-5.2),(900,'DB00609','Ethionamide',-5.2),(901,'DB00282','Pamidronic acid',-5.2),(902,'DB06804','Nonoxynol-9',-5.1), (903,'DB00259','Sulfanilamide',-5.1), (904,'DB01613','Erythrityl tetranitrate',-5.1), (905,'DB00371','Meprobamate',-5.1), (906,'DB06770','Benzyl alcohol',-5.1), (907,'DB06799','Methenamine',-5.1), (908,'DB04221','Didecyldimethylammonium',-5), (909,'DB01563','Chloral hydrate',-5), (910,'DB00138','Cystine',-5), (911,'DB00142','Glutamic acid',-5), (912,'DB00130','L-Glutamine',-5),(913,'DB00173','Adenine',-4.9),(914,'DB01181','Ifosfamide',-4.9),(915,'DB06154','Pentaerythritol tetranitrate',-4.9), (916,'DB02701','Nicotinamide',-4.9),(917,'DB04272','Citric acid',-4.9), (918,'DB00630','Alendronic acid',-4.9),(919,'DB00583','Levocarnitine',-4.9), (920,'DB00141','N-Acetylglucosamine',-4.8),(921,'DB00027','Gramicidin D',-4.8), (922,'DB00006','Bivalirudin',-4.8),(923,'DB06823','Tiopronin',-4.8),(924,'DB00330','Ethambutol',-4.8),(925,'DB03255','Phenol',-4.8), (926,'DB06753','Triclofos',-

4.8),(927,'DB06775','Carglumic acid',-4.8), (928,'DB00529','Foscarnet',-4.8),(929,'DB00313','Valproic acid',-4.8), (930,'DB00128','Aspartic acid',-4.7),(931,'DB00389','Carbimazole',-4.7), (932,'DB04339','Carbocisteine',-4.7),(933,'DB00531','Cyclophosphamide',-4.7), (934,'DB00123','L-Lysine',-4.6),(935,'DB00148','Creatine',-4.6), (936,'DB06698','Betahistine',-4.6),(937,'DB00228','Enflurane',-4.6),(938,'DB00230','Pregabalin',-4.6),(939,'DB06815','Pyrithione',-4.6), (940,'DB04160','Pyrophosphoric acid',-4.6),(941,'DB00339','Pyrazinamide',-4.6), (942,'DB00119','Pyruvic acid',-4.6),(943,'DB00161','Valine',-4.6),(944,'DB00174','Asparagine',-4.6),(945,'DB00488','Altretamine',-4.5), (946,'DB00129','Ornithine',-4.5),(947,'DB06811','Polidocanol',-4.5), (948,'DB00189','Ethchlorvynol',-4.5),(949,'DB00134','Methionine',-4.4), (950,'DB06706','Isometheptene',-4.4),(951,'DB02893','D-Methionine',-4.4),(952,'DB00513','Aminocaproic acid',-4.4),(953,'DB00156','Threonine',-4.4), (954,'DB00272','Betazole',-4.4),(955,'DB00260','Cycloserine',-4.4),(956,'DB00139','Succinic acid',-4.4), (957,'DB08908','Dimethyl fumarate',-4.3), (958,'DB04398','Lactic acid',-4.3), (959,'DB01612','Amyl Nitrite',-4.3), (960,'DB06637','Dalfampridine',-4.3), (961,'DB08842','Acetylcarnitine',-4.3), (962,'DB01213','Fomepizole',-4.2), (963,'DB00551','Acetohydroxamic acid',-4.2),(964,'DB00566','Succimer',-4.2), (965,'DB03929','D-Serine',-4.1), (966,'DB08809','Dichloroacetic acid',-4.1),(967,'DB06756','Glycine betaine',-4.1),(968,'DB00331','Metformin',-4.1), (969,'DB02530','gamma-Aminobutyric acid',-4),(970,'DB06151','Acetylcysteine',-4), (971,'DB01440','gamma-Hydroxybutyric acid',-4),(972,'DB00151','Cysteine',-4), (973,'DB01839','Propylene glycol',-4),(974,'DB00411','Carbamoylcholine',-3.9), (975,'DB06709','Methacholine',-3.9),(976,'DB03766','Propanoic acid',-3.8),(977,'DB03085','Glycolic acid',-3.8),(978,'DB03754','Tromethamine',-3.7), (979,'DB04572','Thiotepa',-3.7), (980,'DB00145','Glycine',-3.6), (981,'DB04827','Urethane',-3.5), (982,'DB02325','Isopropyl alcohol',-3.5), (983,'DB05381','Histamine',-3.4), (984,'DB01401','Choline magnesium trisalicylate',-3.4), (985,'DB03166','Acetic acid',-3.4), (986,'DB03175','Propyl alcohol',-3.4),(987,'DB06824','Triethylenetetramine',-3.3),(988,'DB03904','Urea',-3.1),(989,'DB00122','Choline',-3.1), (990,'DB00592','Piperazine',-3.1),(991,'DB06782','Dimercaprol',-3),(992,'DB00536','Guanidine',-2.5),(993,'DB00435','Nitric Oxide',-1.9),(994,'DB03843','Formaldehyde',-1.8),(995,'DB11588','Carbon monoxide',-1.8), (996,'DB00653','Magnesium sulfate',-

1.1),(997,'DB00258','Calcium acetate',-1.1), (998,'DB00416','Metocurine iodide',-0.9), (999,'DB00462','Methscopolamine bromide',-0.9),(1000,'DB05109','Trabectedin',12.2);

- This created a database by the name of FDA and inside it a table named docking is formed, inside which we get three columns; Index, DrugBankID, Ligand and Binding_affinity. It contains 1000 entries of ligands.

13) Concluding this work, a website was created which fetches the information stored in the FDA database. The website was created using HTML, CSS and PHP.

- Following is the code for the design of a new website for the database GUI:

CODE FOR INDEX PAGE:

```
<?php
  include 'cbh.php';
?>
<html>
<head>
<meta name="viewport" content="width=device-width, initial-scale=1">
<title>CDBD (COVID-19 POTENTIAL DRUG BINDING ENERGY  DATABASE)
</title>
<style>
input[type=text] {
width: 130px;
  box-sizing: border-box;
  border: 2px solid #ccc;
  border-radius: 4px;
  font-size: 16px;
  background-color: white;
  background-image: url('searchicon.png');
  background-position: 10px 10px;
  background-repeat: no-repeat;
  padding: 12px 20px 12px 40px;
  -webkit-transition: width 0.4s ease-in-out;
  transition: width 0.4s ease-in-out;
}
```

```
input[type=text]:focus {
  width: 100%;
}
body {background-image: url("xx.jpg");}
h1 {color: #8B1C62;}
h1 {font-size:400%;}
h1 {text-align:center;}
h2 {color: #8B1C62;}
h2 {font-size:300%;}
h2 {text-align:center;}
h3 {color: Black;}
h3 {font-size:100%;}
h3  {text-align:left;}
{
  margin: 0;
  font-family: Arial, Helvetica, sans-serif;
}

.topnav {
  overflow: hidden;
  background-color: #e9e9e9;
}

.topnav a {
  float: left;
  display: block;
  color: black;
  text-align: center;
  padding: 14px 16px;
  text-decoration: none;
  font-size: 17px;
}

.topnav a:hover {
```

```
  background-color: #ddd;
  color: black;
}

.topnav a.active {
  background-color: #2196F3;
  color: white;
}

.topnav input[type=text] {
  float: right;
  padding: 6px;
  margin-top: 8px;
  margin-right: 16px;
  border: none;
  font-size: 17px;
}

@media screen and (max-width: 600px) {
  .topnav a, .topnav input[type=text] {
    float: none;
    display: block;
    text-align: left;
    width: 100%;
    margin:        0;
    padding: 14px;
  }

}
</style>

</head>
<body>
<div class="topnav">
```

```
  <a class="active" href="#home">Home</a>
  <a href="about.php">About</a>
  <a href="search.php">Search</a>
  <a href="credits.html">Credits & Citations</a>
  <a href="contact.php">Contact</a>
</div>
<h1> CDBD </h1>
<h2> (COVID-19 POTENTIAL DRUG BINDING ENERGY DATABASE) </h2>
<marquee id='scroll_news' style="font-family:Book Antiqua; color: #FFFFFF" bgcolor="#FAF0E6" >
<div onMouseOver="document.getElementById('scroll_news').stop();" onMouseOut="document.getElementById('scroll_news').start();">

<a href="structures.html"><img src="structure.jpg" title="Structure" width="300" height="200" /></a> <a href="symptoms.html"><img src="symptoms.jpg" title="Symptoms" width="300" height="200" /></a> <a href="countries.html"><img src="countries.jpg" title="Countries" width="300" height="200" /></a> <a href="updates.html"><img src="updates.png" title="Updates" width="300" height="200" /></a>

</div>
</marquee>
<h3>Click on the images to know more about them</h3>
</body>
</html>
```

CODE FOR STRUCTURES INSIDE THE INDEX PAGE:

```
<!DOCTYPE html>
<html>
<head>
<style>
body {
  background-color: coral;
h1 {color: Black;}
h1 {font-size:400%;}
```

```
h1  {text-align:center;}
}
</style>
</head>
<body>

<h1>STRUCTURE OF CORONA VIRUS</h1>
<img src="Sars_structure.png" alt="structure">

<p>Corona Viruse is a large family containing many viruses, where Covid-19 is the newest member.It causes respiratory disease, among the other many other symptoms.</p>
<p>Coronaviruses contains a genetic blueprint called RNA (beige), similar to DNA. The RNA is single-stranded and acts as a molecular message that is used to produce proteins required for other elements of virus.</p>
<p>The nucleoproteins— (dark blue discs)—proteins are bound to the string of RNA, it give the virus a structure and also enables in its replication.</p>
<p>The projections that are seen on outside of the coronavirus are the spike proteins (red-orange). These spikes of proteins gives the virus a crown-like appearance when viewed under the microscope, this is the reason its given the Latin name corona. The spikes of the proteins acts as grappling hooks that will help the virus to latch to host and get them the infection. Like various other viruses, coronaviruses are not able to reproduce outside of a living host.</p>


</body>
</html>
```

CODE FOR THE SYMPTOMS PAGE INSIDE THE INDEX PAGE:

```
<!DOCTYPE html>
<html>
<head>
<style>
body {
  background-color: coral;
```

```
h1  {color:  Black;}
h1   {font-size:400%;}
h1   {text-align:center;}
}
</style>
</head>
<body>
<h1>SYMPTOMS OF COVID 19</H1>
<img src="COVID-symptoms.jpg" alt="SYMPTOMS"width="1000" height="500">
<H2> Common Symptoms</H2>
<p>Common Symptoms of patients hospitalized:</p>
<ul>
<li>Fever: 99% </li>
<li>Fatigue:70%</Li>
<li>A dry cough: 59%</li>
<li>Loss of appetite: 40%</li>
<li>Body aches: 35%</li>
<li>Shortness of breath: 31%</li>
<li>Mucus or phlegm: 27%</li>
</ul>
<p>Symptoms begin within 2 to 14 days after you are contact with the virus.</p>

<p>Other symptoms may include:</p>
<ul>
<li>Sore throat</li>
<li>Headache</li>
<li>Chills, sometimes with shaking</li>
<li>Loss of smell or taste</li>
<li>Congestion or runny nose</li>
<li>Nausea or vomiting</li>
<li>Diarrhea</li>
</ul>
<body>
<HTML>
```

CODE FOR THE PAGE CONTAINING THE AFFECTED COUNTRIES INFORMATION INSIDE THE INDEX PAGE:

```
<!DOCTYPE html>
<html>
<head>
<style>
body {
  background-color: coral;
h1 {color: Black;}
h1 {font-size:400%;}
h1 {text-align:center;}
table, th, td {
  border: 1px solid black;
  padding: 5px;

}
</style>
<BODY>
<h2>COUNTRIES MOST AFFECTED</h2>
<DIV>
<table style="width:50%">
<tr>
<th>COUNTRIES</TH>
<th>CASES</th>
<th>DEATHS</th>
</tr>
<tr>
<td>United States</td>
<td>33,418,826          </td>
<td>594,911</td>
</tr>
<tr>
<td>India</td>
<td>21,892,676</td>
```

```
<td>238,270</td>
</tr>
<tr>
<td>Brazil</td>
<td>15,087,360</td>
<td>419,393</td>
</tr>
<tr>
<td>France</td>
<td>5,747,214</td>
<td>106,101</td>
</tr>
<tr>
<td>Turkey</td>
<td>4,998,089</td>
<td>42,465</td>
</tr>
<tr>
<td>Russia</td>
<td>4,863,514</td>
<td>112,622</td>
</tr>
<tr>
<td>United Kingdom</td>
<td>4,431,043</td>
<td>127,598</td>
</tr>
<tr>
<td>Italy</td>
<td>4,092,747</td>
<td>122,470</td>
</tr>
<tr>
<td>Spain</td>
```

```
<td>3,567,408</td>
<td>78,792</td>
</tr>
<tr>
<td>Germany</td>
<td>3,504,012</td>
<td>85,056</td>
</tr>
<tr>
<td>Argentina</td>
<td>3,118,134</td>
<td>66,872</td>
</tr>
</table>
</DIV>
<BR><BR><BR>
</table>
<P>
<h2> VACCINATIONS AROUND THE WORLD</h2>
</P>
<table style="width:50%">
<tr>
<th>COUNTRIES</TH>
<th>VACCINATED</th>
<th>FULLY VACCINATED</th>
</tr>
<tr>
<td>Seychelles</td>
<td>70%</td>
<td>61%</td>
</tr>
<tr>
<td>Israel</td>
<td>60%</td>
```

```
<td>56%</td>
</tr>
<tr>
<td>San Marino</td>
<td>63%</td>
<td>32%</td>
</tr>
<tr>
<td>Bahrain</td>
<td>47%</td>
<td>34%</td>
</tr>
<tr>
<td>Chile</td>
<td>44%</td>
<td>37%</td>
</tr>
<tr>
<td>Maldives</td>
<td>57%</td>
<td>23%</td>
</tr>
<tr>
<td>U.K.</td>
<td>52%</td>
<td>24%</td>
</tr>
<tr>
<td>United States</td>
<td>45%</td>
<td>33%</td>
</tr>
<tr>
<td>Malta</td>
```

```
<td>49%</td>
<td>22%</td>
</tr>
<tr>
<td>Hungary</td>
<td>43%</td>
<td>24%</td>
</tr>
<tr>
<td>Bhutan</td>
<td>63%</td>
<td>-</td>
</tr>
<tr>
<td>Monaco</td>
<td>33%</td>
<td>30%</td>
</tr>
<tr>
<td>Qatar</td>
<td>38%</td>
<td>23%</td>
</tr>
<tr>
<td>India</td>
<td>9.6%</td>
<td>2.3%</td>
</tr>
</table>
</BODY>
</HTML>
```

CODE FOR THE UPDATES PAGE INSIDE THE INDEX PAGE:

```
<!DOCTYPE html>
```

```
<html>
<head>
<style>
body {
  background-color: coral;
h1 {color: Black;}
h1 {font-size:400%;}
h1 {text-align:center;}
}
</style>
</head>
<body>
<h1>LATEST UPDATES ON COVID19!!!</H1>
<img src="up1.webp" alt="updates"width="500" height="300">
<img src="up2.jpg" alt="updates"width="500" height="300">
<h2>Total number of cases so far:</h2>
<h2>Number of people dead:</h2>
</body>
</html>
```

CODE FOR LINKING THE WEBSITE TO THE DATABASE:

```
<?php
$server= "localhost";
$username= "root";
$password= "";
$dbname= "fda";
$conn= mysqli_connect($server, $username, $password, $dbname);
?>
```

CODE FOR ABOUT PAGE:

```
<html>
<head>
<style>
.topnav {
  overflow: hidden;
```

```
  background-color: #e9e9e9;
}

.topnav a {
  float: left;
  display: block;
  color: black;
  text-align: center;
  padding: 14px 16px;
  text-decoration: none;
  font-size: 17px;
}

.topnav a:hover {
  background-color: #ddd;
  color: black;
}

.topnav a.active {
  background-color: #2196F3;
  color: white;
}

.topnav input[type=text] {
  float: right;
  padding: 6px;
  margin-top: 8px;
  margin-right: 16px;
  border: none;
  font-size: 17px;
}

@media screen and (max-width: 600px) {
  .topnav a, .topnav input[type=text] {
```

```
    float: none;
    display: block;
    text-align: left;
    width: 100%;
    margin: 0;
    padding: 14px;
  }

}
body
{
  background-image: url('gi.gif');
  background-repeat: no-repeat;
  background-attachment: fixed;
  background-size: cover;
}
h2  {color: White;}
h2  {font-size:400%;}

</style>
</head>
<body>
<div class="topnav">
  <a href="index.html">Home</a>
  <a class="active" href="#about">About</a>
  <a href="search.php">Search</a>
  <a href="credits.html">Credits & Citations</a>
  <a href="contact.php">Contact</a>
</div>
<h2>ABOUT</h2>
<p  style="color:white";font-size:100px;"><b>  Coronavirus disease 2019 (COVID-19), also known as the coronavirus or COVID, is a contagious disease caused by severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2). The first known case was identified in Wuhan, China, in December 2019.The
```

disease has since spread worldwide, leading to an ongoing pandemic. </p>
<p style="color:white";"font-size:100px;"> There is no specific, effective treatment or cure for coronavirus disease 2019 (COVID-19), the disease caused by the SARS-CoV-2 virus.Thus, the cornerstone of management of COVID-19 is supportive care, which includes treatment to relieve symptoms, fluid therapy, oxygen support and prone positioning as needed, and medications or devices to support other affected vital organs. </p>
<p style="color:white";"font-size:100px;"> Therefore, this website named CDBD has tried to give its contribution in finding the cure of this deadly disease. It was founded by Garima Sharma and Purvanshi Sharma with the great help of their mentor Dr. Tiratha Raj Singh of JUIT (Jaypee University of Information Technology) Waknaghat on 1st May 2021. </p>
<p style="color:white";"font-size:100x;"> This website contains the database of binding energy of FDA approved drugs. Wherein, the binding energies were calculated by docking these FDA approved drugs with the N-protein of SARS-CoV-2 by AutoVina software. The N protein plays an important role in the transcription and replication of viral RNA, packaging the encapsidated genome into virions and inhibits the cell cycle process of the host cells. The N protein is abundantly expressed during infections and also has high immunogenic activity. Therefore, N protein could be potential targets for finding the cure of SARS-CoV-2. </p>
<p style="color:white";"font-size:100px;"> The binding energies of the drugs against N proteins will give an insight on how effectively the drug will bind at the target protein site to block its action and hence could aid in stoppping its replication. Further, work on these drugs could be done and they can be selected as a potential cure. You can search the binding energy database by typing its Drugbank ID </p>
</body>
</html>

CODE FOR CREDITS & CITATIONS PAGE:

<html>
<head>
<style>
.topnav {

```
  overflow: hidden;
  background-color: #e9e9e9;
}

.topnav a {
  float: left;
  display: block;
  color: black;
  text-align: center;
  padding: 14px 16px;
  text-decoration: none;
  font-size: 17px;
}

.topnav a:hover {
  background-color: #ddd;
  color: black;
}

.topnav a.active {
  background-color: #2196F3;
  color: white;
}

.topnav input[type=text] {
  float: right;
  padding: 6px;
  margin-top: 8px;
  margin-right: 16px;
  border: none;
  font-size: 17px;
}

@media screen and (max-width: 600px) {
```

```
  .topnav a, .topnav input[type=text] {
    float: none;
    display: block;
    text-align: left;
    width: 100%;
    margin:      0;
    padding: 14px;
  }

}
</style>
</head>
<body>
<div class="topnav">
  <a href="index.html">Home</a>
  <a href="about.php">About</a>
  <a href="search.php">Search</a>
  <a class="active" href="#Credits & Citations">Credits & Citations</a>
  <a href="contact.php">Contact</a>
</div>
<h2>Credits & Citations</h2>
<h3><b> We would like to acknowledge the following sources: </b></h3>
 <a          href="https://www.covid19hg.org/blog/2021-02-19-layperson-lit-review/">Image for Structure of SARS-CoV-2 </a><br><br>
 <a  href="https://images.app.goo.gl/aGquDsPXcKeC2nw28">Second  Image for Structure of SARS-CoV-2 </a><br><br>
 <a      href="https://www.gograph.com/clipart/coronavirus-cov-infographics-elements-human-are-gg124201329.html">Image  for  symptoms  of  COVID-19</a><br><br>
 <a          href="https://www.meritushealth.com/patients-visitors/public-notice/covid-19-frequently-asked-questions/?hcb=1">Second  Image  for symptoms of COVID-19 </a><br><br>
 <a          href="https://www.google.com/amp/s/blog.ipleaders.in/the-recent-situation-of-covid-19-worldwide-and-how-they-are-dealing-with-
```

```
it/amp/">Image for worldwide cases of COVID-19</a><br><br>
 <a    href="https://tradesmartonline.in/blog/following-are-the-features-which-will-enrich-your-trading-experience-along-with-online-trading/">UPDATES Image</a><br><br>
</body>
</html>
```

CODE FOR THE CSS PAGE TO LINK WITH THE PHP FILES:

```
.topnav {
  overflow: hidden;
  background-color: #e9e9e9;
}

.topnav a {
  float: left;
  display: block;
  color: black;
  text-align: center;
  padding: 14px 16px;
  text-decoration: none;
  font-size: 17px;
}

.topnav a:hover {
  background-color: #ddd;
  color: black;
}

.topnav a.active {
  background-color: #2196F3;
  color: white;
}

.topnav input[type=text] {
  float: right;
```

```
  padding: 6px;
  margin-top: 8px;
  margin-right: 16px;
  border: none;
  font-size: 17px;
}

@media screen and (max-width: 600px) {
  .topnav a, .topnav input[type=text] {
    float: none;
    display: block;
    text-align: left;
    width: 100%;
    margin:        0;
    padding: 14px;
  }
}
#home .home a,
#about .about a,
#Contact.contact a,
#Search .Search a,

}
```

CODE FOR CONTACT PAGE:

```
<html>
<head>
<meta charset="utf-8">
    <meta http-equiv="X-UA-Compatible" content="IE=edge">
    <link rel="stylesheet" href="./mycss.css" type="text/css">
<style>
body {
  background-image: url('amt.jpg');
  background-repeat: no-repeat;
  background-attachment: fixed;
```

```
  background-size: cover;
h6 {color: Tomato;}
h6 {font-size:400%;}
h6 {text-align:center;}
}
.my{
   color:  turquoise;
   font-size:400%;
   text-align:center;
 }
</style>
</head>
<body>
<div class="topnav">
  <a href="index.html">Home</a>
  <a href="about.php">About</a>
  <a href="search.php">Search</a>
  <a href="credits.html">Credits & Citations</a>
  <a class="active" href="#contact">Contact</a>
</div>
<div class="my">
<h6>HI, THERE!</h6>
</div>
<H1><center><b>We would love your feedback</b></center></H1>
<p style="font-size:100%;"><b><br><br>Please give your feedback below
</br></br></b> </p>
<?php
$Suggestions= "";
if ($_SERVER["REQUEST_METHOD"] == "POST") {
 if (empty($_POST["Suggestions"])) {
    $Suggestions = "";
  } else {
    $Suggestions = test_input($_POST["Suggestions"]);
  }
```

```
}
function test_input($data) {
  $data = trim($data);
  $data = stripslashes($data);
  $data = htmlspecialchars($data);
  return $data;
}
?>
<form
action="mailto:171504@juitsolan.in;171507@juitsolan.in;tiratharaj.singh@ju
itsolan.in" method="post" enctype="text/plain">
Suggestions: <textarea name="Suggestions" rows="6" cols="40"><?php echo
$Suggestions;?>
</textarea>
<input type="submit" style="font-face: 'Comic Sans MS'; font-size: larger;
color: White; background-color: Black; border: 3pt ridge lightgrey"
value="Send Me!" >
  <br><br>
</form>
<?php
echo "<br>";
echo $Suggestions;
?>
<H1><center>This would reach directly to our mailbox. Thank you for your
suggestions</center></H1>
</div>
</body>
</html>
```

CODE FOR SEARCH PAGE:

```
<html>
<head>
<meta charset="UTF-8">
<meta name="viewport" content="user-scalable=0, width=device-width,
initial-scale=1.0
```

```
<meta charset="utf-8">
   <meta http-equiv="X-UA-Compatible" content="IE=edge">
   <link rel="stylesheet" href="./mycss.css" type="text/css">
<title>CDBD (COVID-19 POTENTIAL DRUG BINDING ENERGY DATABASE)</title>
</head>
<body>
<div class="topnav">
  <a href="index.html">Home</a>
  <a href="about.php">About</a>
  <a class="active" href="#search">Search</a>
  <a href="credits.html">Credits & Citations</a>
  <a href="contact.php">Contact</a>
</div>
<h2>SEARCH</h2>
          <div class="container">


                  <h2>Search by DrugBankID </h2>
                   <form action="" method="POST">
                      <input type="text" name="DrugBankID" placeholder="Eg. ID:DB00558"/> <br/>
                       <input type="submit" name="search" value="Search">

                   </form>
                   <table  border="1">
                   <tr>
                         <th>Index</th>
                          <th>DrugBankID </th>
                           <th>Ligand</th>
                          <th>Binding_affinity</th>

                    <tr><br>
```

```
<?php
$connection =mysqli_connect("localhost","root","");
$db=mysqli_select_db($connection,'fda');
if(isset($_POST['search']))
{
   $id=$_POST['DrugBankID'];
   $queryResult="SELECT * FROM docking where DrugBankID='$id' ";
   $Run=mysqli_query($connection,$queryResult)                    or
die(mysqli_error($connection));
   while($row = mysqli_fetch_array($Run))
   {
    ?>

                        <tr>
                            <td> <?php echo $row['Index']; ?></td>
                            <td> <?php echo $row['DrugBankID']; ?> </td>
                            <td> <?php echo $row['Ligand']; ?> </td>
                            <td> <?php echo $row['Binding_affinity']; ?> </td>

                        </tr>

                    <?php
                }
            }
            ?>

        </table>

    </div>


</body>
</html>
```

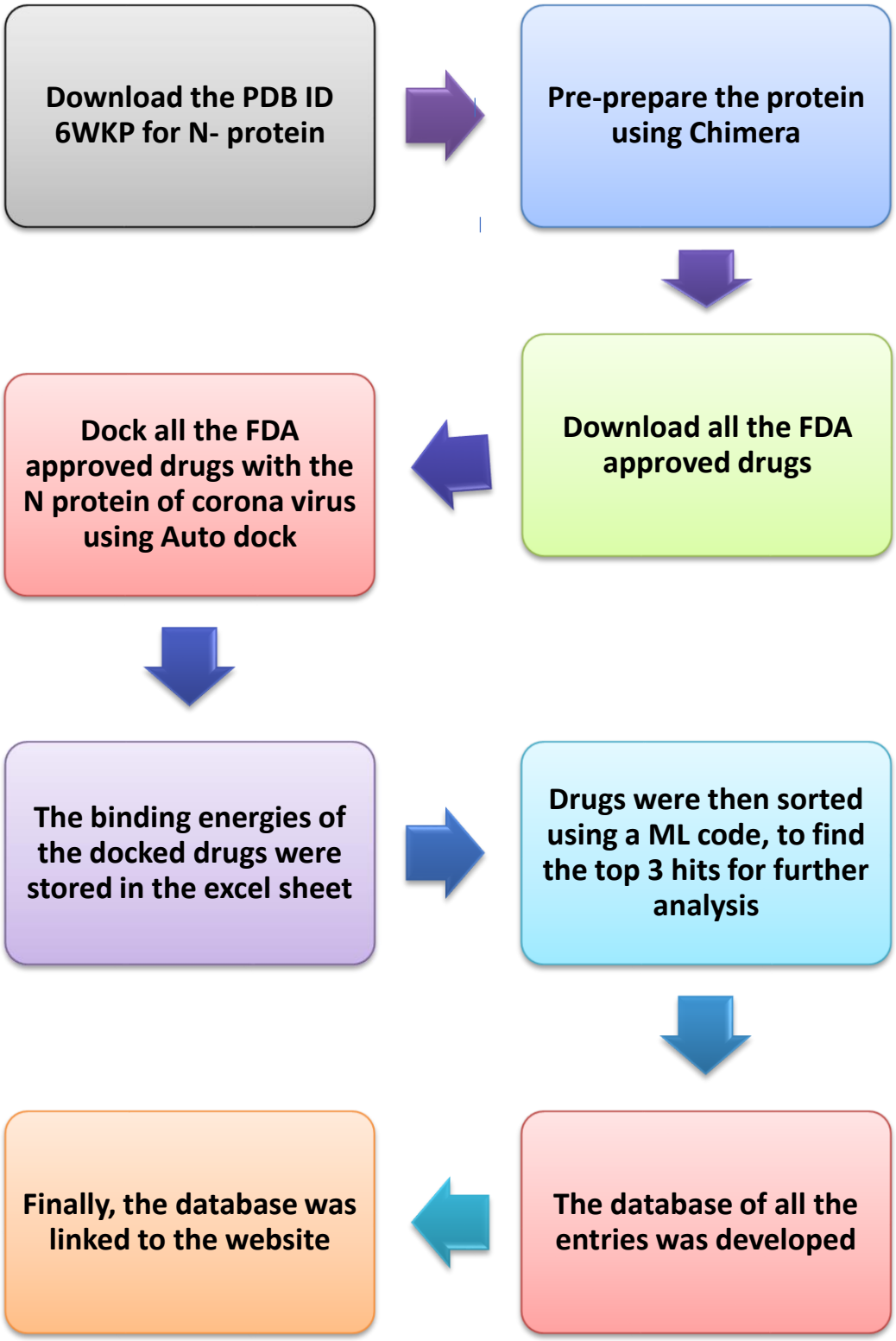


Figure 8. Flow chart of the methodology

CHAPTER 3.

RESULTS AND DISCUSSIONS

1) The above proteins were prepared using UCSF Chimera and saved as protein.pdb. There were 4 chains in total, out of which chain B was selected since it is the chain containing the ligand. The ligand was deleted for starting the docking studies along with the chain and the pre-preparation of the protein is completed and it is saved as protein.pdb. Also, all 1000 of the ligands were pre-prepared and minimized using UCSF chimera. In the end they were stored as ligand.mol2 files in different folders.

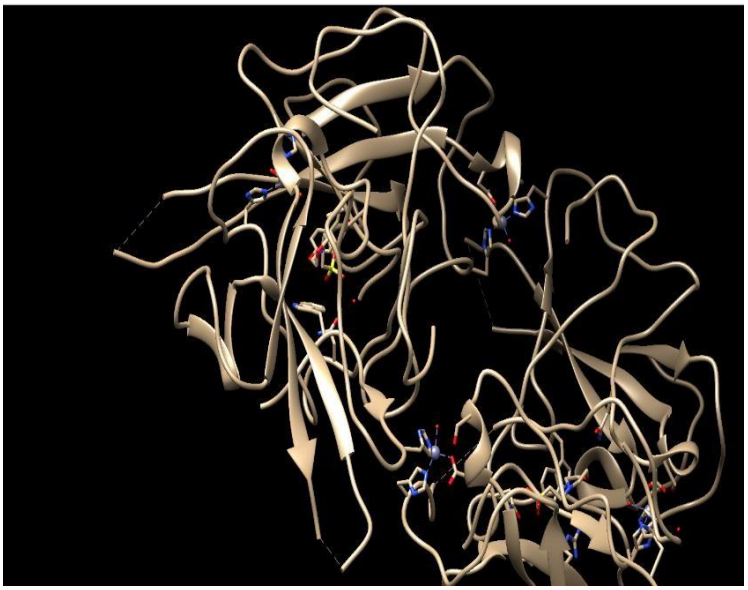


Figure 9. Unprepared structure of 6WKP

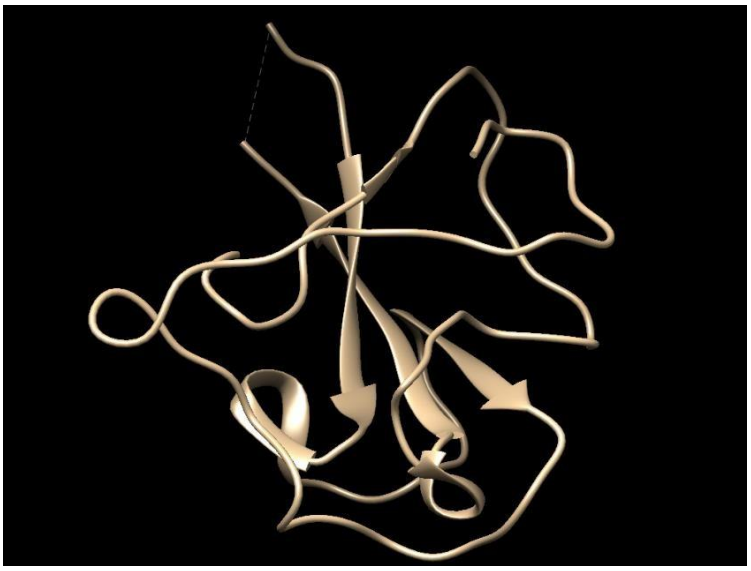


Figure 10. Prepared structure of N-protein in Chimera

2) After this step the preparation of the ligand.mol2 and the protein.pdb file is done using mgltools AutoDock software. The protein was stored as protein.pdbqt file and the ligand was saved as ligand.pdbqt file, ready to be docked. Also, here the grid parameters were defined and set for the actual docking process. This is done for all the 1000 inhibitor molecules. Also a config.txt file was created containing the parameters for the docking process.

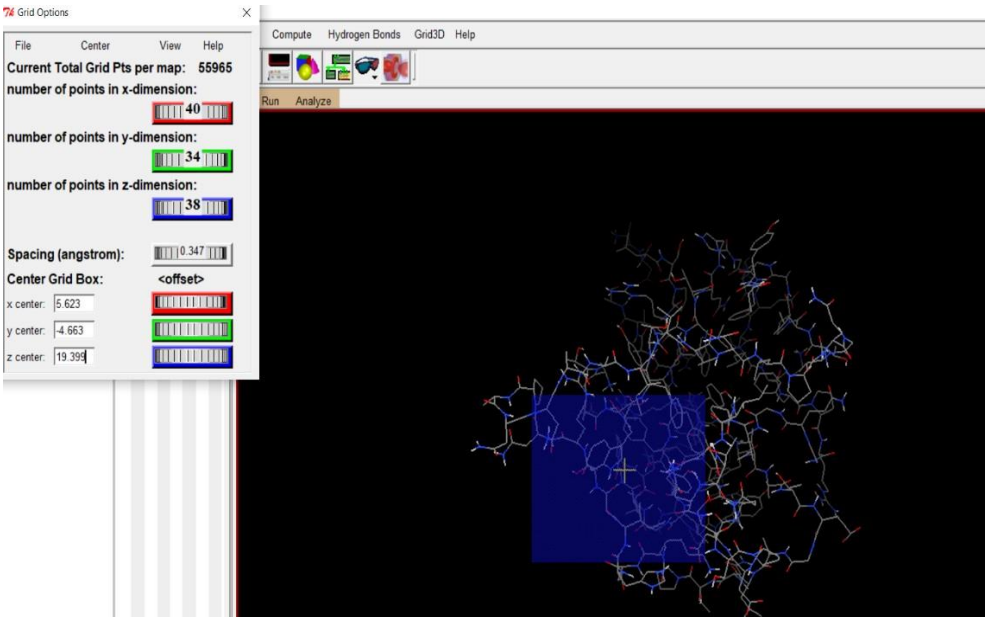


Figure 11. Preparation of Grid Box for docking

```
receptor= protein.pdbqt
ligand= ligand.pdbqt

center_x= 5.623
center_y= -4.663
center_z= 19.399

size_x= 40
size_y= 34
size_z= 38

energy_range= 4
exhaustiveness= 8
```

Figure 12. config.txt file

14) Now, the actual docking process commences for 1000 inhibitors and various folders were made, in which a config.txt, grid.txt, ligand.pdbqt, protein.pdbqt, ligand.mol2 and protein.pdb files are present in each folder, after the preparation step from the mgltools AutoDock software. The docking takes place through AutoDock Vina version 1.1.2. The commands for docking work in the command prompt (cmd). This gives us the binding affinities of all the 1000 inhibitors. The output is given in log.txt files.

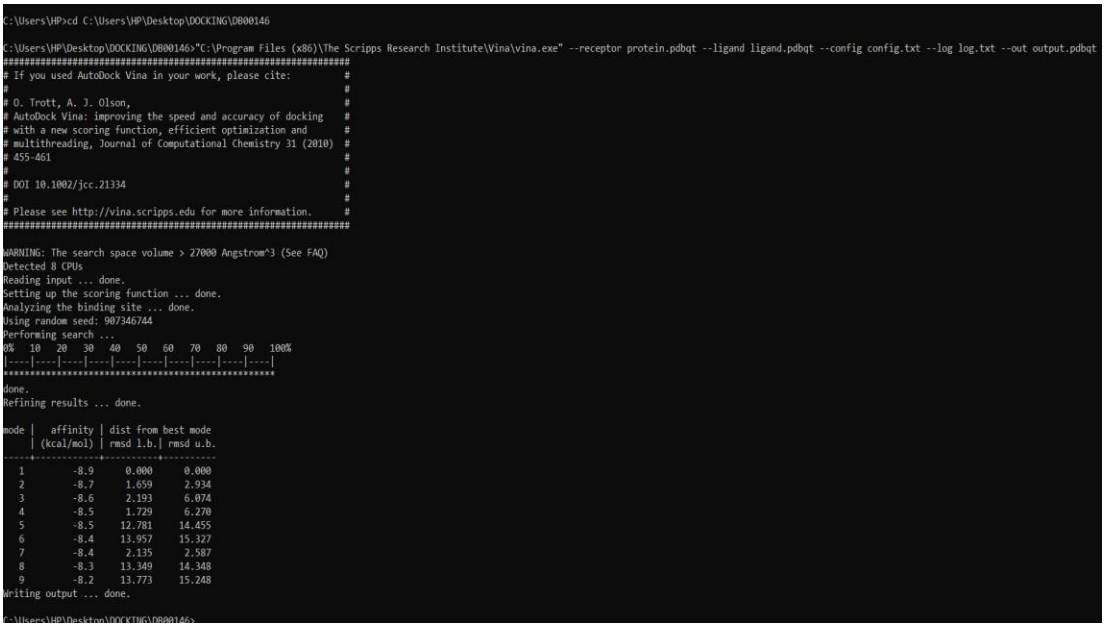


Figure 13. cmd bar for Autovina Docking of an inhibitor

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

WARNING: The search space volume > 27000 Angstrom^3 (See FAQ)
Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 670208672
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1        -13.6      0.000      0.000
   2        -13.4      2.173      5.750
   3        -13.3      1.736      5.826
   4        -13.3      2.189      5.610
   5        -13.2      2.438      5.121
   6        -12.7     16.523     19.766
   7        -12.7     16.680     19.994
   8        -12.6      2.075      3.833
   9        -12.6     16.185     19.528
Writing output ... done.
```

Figure 14. Log file generated for Rifabutin

```
mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1        -13.6      0.000      0.000
   2        -13.1      1.580      3.124
   3        -13.1      0.652      3.912
   4        -12.2     13.067     15.324
   5        -11.7      1.455      4.016
   6        -11.4     14.417     16.966
   7        -11.3      1.846      3.170
   8        -11.2     12.581     13.820
   9        -11.1     13.857     16.048
Writing output ... done.
```

Figure 15. Log file generated for Drospirenone

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

WARNING: The search space volume > 27000 Angstrom^3 (See FAQ)
Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 184582372
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -13.2       0.000       0.000
   2         -13.1      14.748      17.605
   3         -12.7       0.759       1.950
   4         -12.6       2.221       5.770
   5         -12.3      15.011      17.760
   6         -12.3       1.358       5.863
   7         -11.5      12.176      14.641
   8         -11.4      13.182      15.529
   9         -11.3       1.698       6.427
Writing output ... done.
```

Figure 16. Log file generated for Dihydroergotamine

15) The results were stored in an excel sheet (Appendix 1). The excel sheet was sorted based on the ascending order of the Binding affinities. This was done by a python code on Spyder.

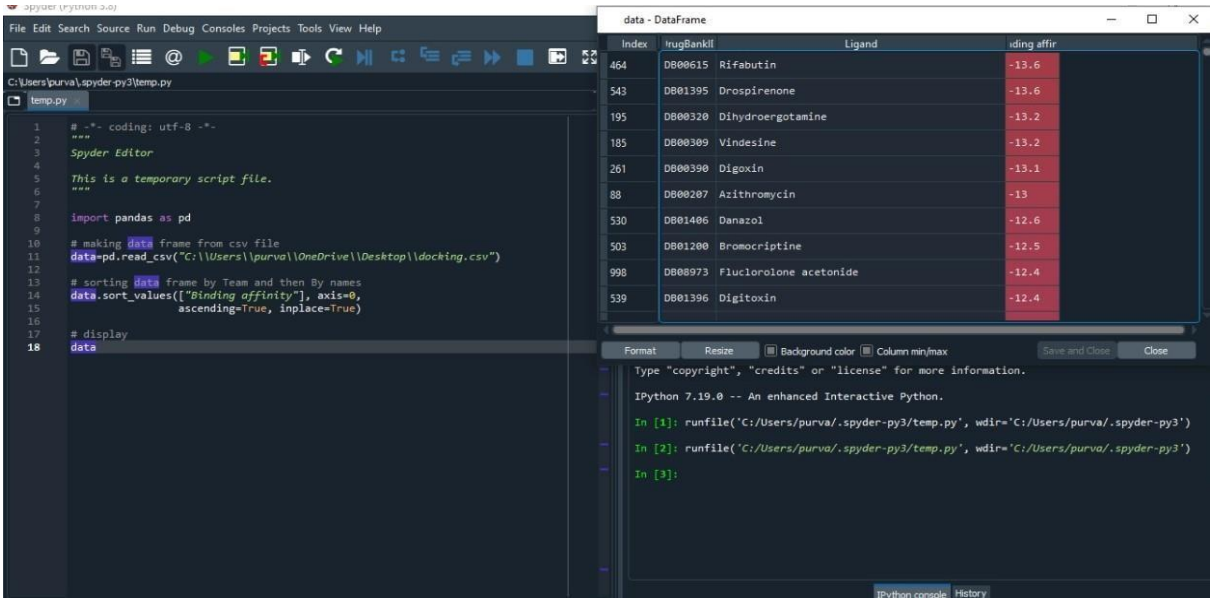


Figure 17. The panel of the python code in Spyder showing the sorted binding affinities

Table1. Data for Top 3 hits for binding affinities

S.No	DrugBankID	Ligand	Binding Affinity
1.	DB00615	Rifabutin	-13.6
2.	DB01395	Drospirenone	-13.6
3.	DB00320	Dihydroergotamine	-13.2

16) SQL queries were applied to the XAMPP software to create a Database named fda. The database had 1000 entries. Inside the database a table named docking was created.

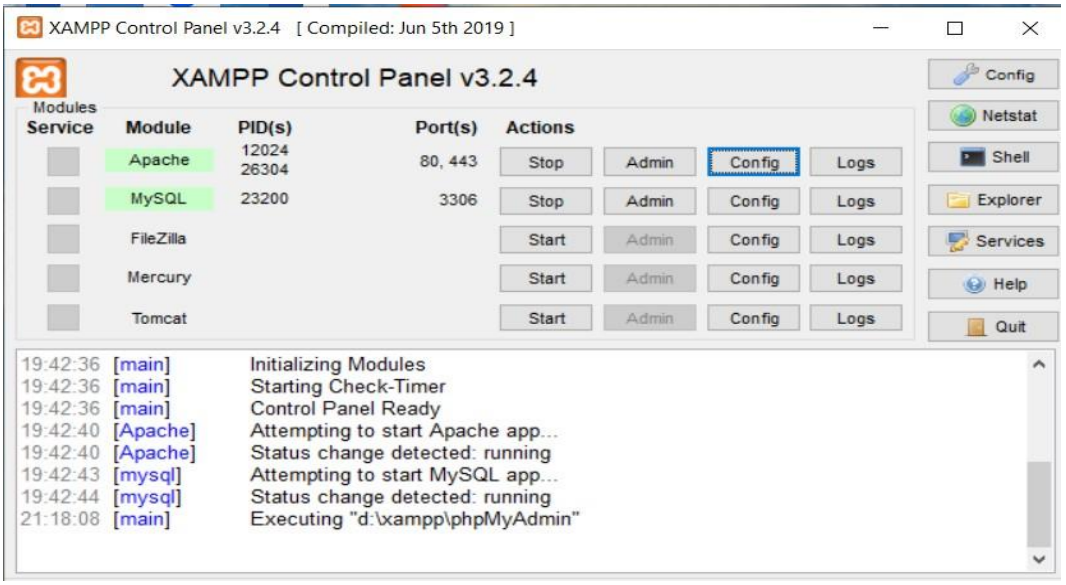
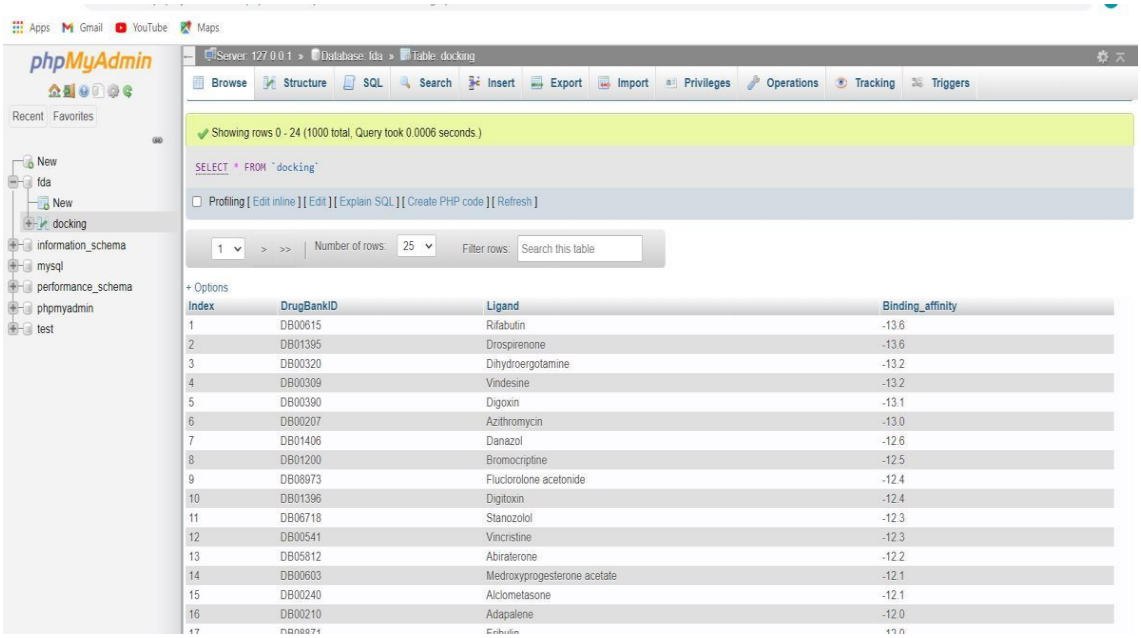


Figure 18. XAMPP control Panel



Index	DrugBankID	Ligand	Binding_affinity
1	DB00615	Rifabutin	-13.6
2	DB01395	Drospirenone	-13.6
3	DB00320	Dihydroergotamine	-13.2
4	DB00309	Vindesine	-13.2
5	DB00390	Digoxin	-13.1
6	DB00207	Azithromycin	-13.0
7	DB01406	Danazol	-12.6
8	DB01200	Bromocriptine	-12.5
9	DB08973	Fluclorolone acetonide	-12.4
10	DB01396	Digitoxin	-12.4
11	DB06718	Stanozolol	-12.3
12	DB00541	Vincristine	-12.3
13	DB05812	Abiraterone	-12.2
14	DB00603	Medroxyprogesterone acetate	-12.1
15	DB00240	Alclometasone	-12.1
16	DB00210	Adapalene	-12.0

Figure 19. FDA database created using phpMyAdmin of XAMPP

17) The creation of a website was done using HTML, CSS and PHP. The website was linked to the Database created in phpMyAdmin of XAMPP and the contact page of the website was linked to the email addresses. It was operable by the localhost of the XAMPP software having the IP address of 127.0.0.1. The website was named CDBD (COVID-19 Potential Drug Binding Energy Database).

Figure 20. Home Page of the Website

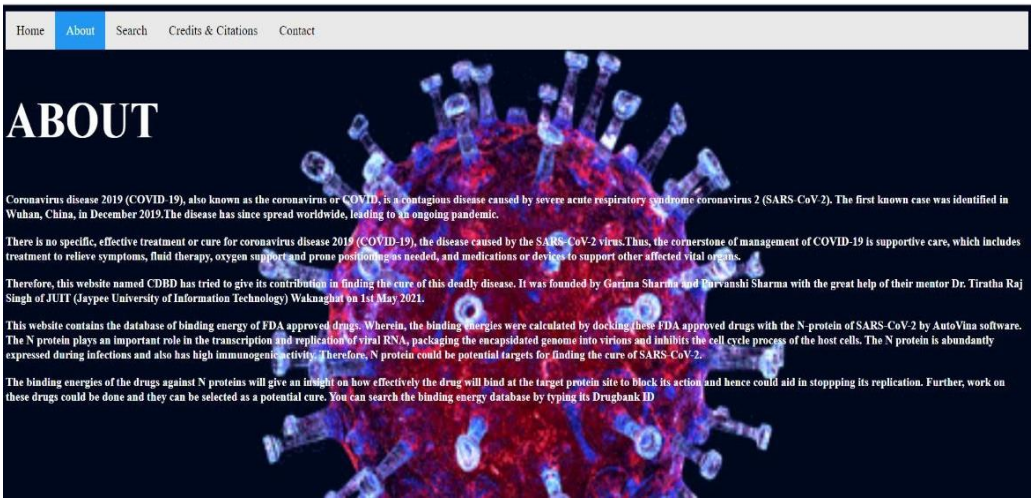


Figure 21. About Page of the website

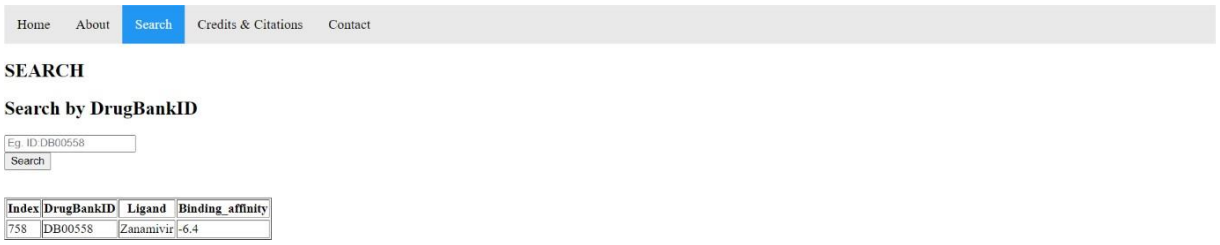


Figure 22. Search page of the website which is connected to the Database

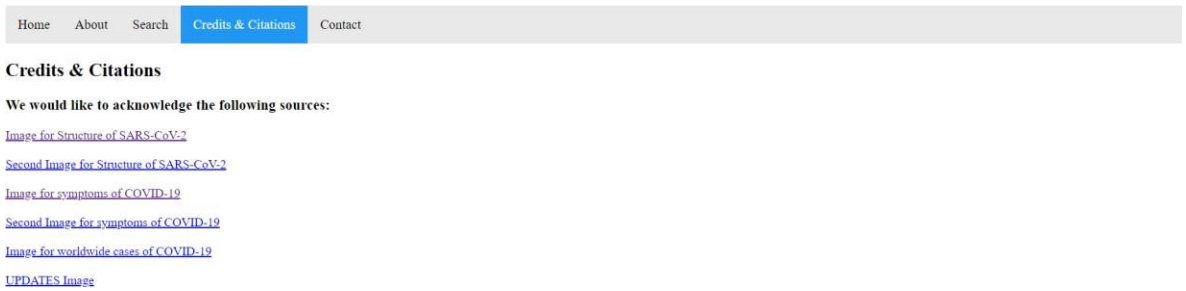


Figure23. Credits and citation page of the website

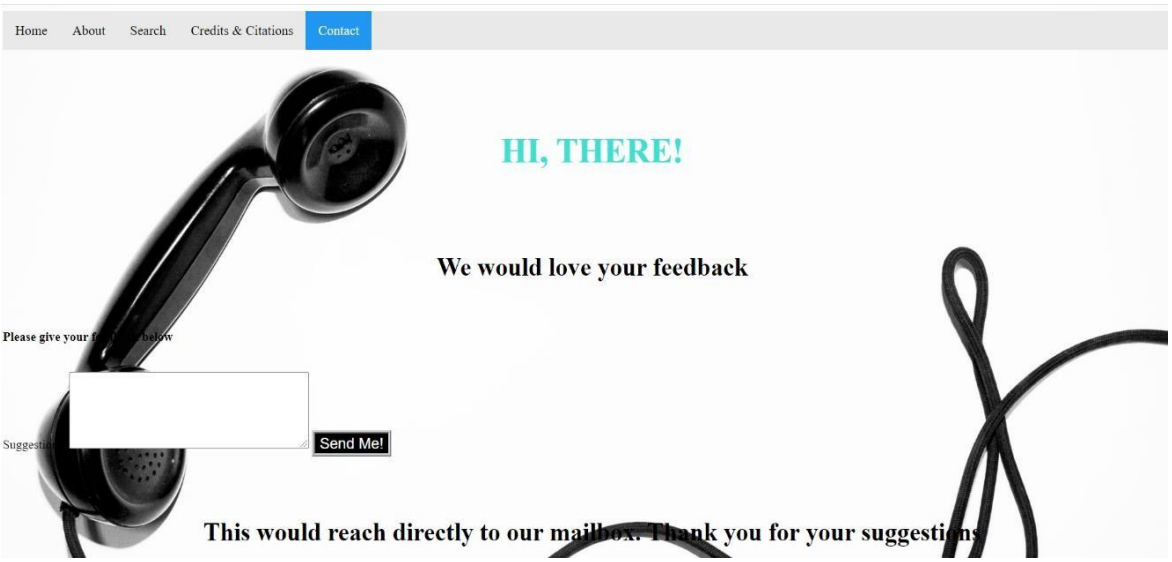


Figure 24. Contact page of the website linked to email IDs

CHAPTER 4.

CONCLUSION

COVID-19 is a highly contagious disease and has caused a pandemic worldwide. So, it becomes necessary to find the cure for this disease. Worldwide, many scientists have been working to find the cure for this pandemic so that we can live our normal lives. By sequence analysis, it can be seen that the structure of SARS-Cov-2 is very much similar to the structure of SARS-CoV, homologically and it shows less similarity to the MERS CoV virus. No similarity is seen to other human coronaviruses. Analyzing the structure of SARS-CoV-2, a major protein called the N or the Nucleocapsid protein is said to play an important role in the replication process of the virus. Also, it can be seen that the structure of the N protein is available in the RCSB site. Therefore, this protein can be considered an important drug target for the treatment of COVID-19 disease. Identification of potential inhibitors for N-protein of Corona virus was a challenge, We have used a simple protocol to identify potent inhibitors through virtual screening process. Finally a unique database named CDBD was developed for the identified FDA approved compounds. Hence, creating a database based on the docking studies between N protein and the FDA-approved drugs can provide us with the binding affinities, thereby giving us a clear picture about the potential drugs for blocking the N-protein and hence, it can help the experimental scientists for the management and the treatment of the COVID-19 disease. We believe that this database will serve as an accompaniment for the researchers and medical professionals working globally for the management of Covid-19 and will be a special supplement of information for the mankind.

CDBD is a unique and first of its kind database. We will update it as per the availability of new data in near future. CDBD is freely available for the academic and research purpose to provide important information to the scientific community at: http://www.bioinfoindia.org/cdbd

REFERENCES

1.https://www.ncbi.nlm.nih.gov/pmc/articles/PMC6222344/

2. WHO | World Health Organization

3. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC6222344/

4. Crystal structure of SARS-CoV-2 main protease provides a basis for design of improved alpha- ketoamide inhibitors Rolf HilgenfeldLinlin Zhang, Daizong Lin, Xinyuanyuan Sun, Ute Curth, Christian Drosten, Lucie Sauerhering, Stephan Becker, Katharina Rox and Rolf Hilgenfeld published online March 20, 2020 originally published online March 20,2020

5.http://science.sciencemag.org/content/suppl/2020/03/19/science.abb3405.DC1

6. SARS death leads to China dispute". CNN. 10 April 2003. Archived from the original on 28 November 2007. *Retrieved 3 April 2007*.

7. "Mechanisms of Coronavirus cell entry mediated by the viral spike protein" Sandrine Belouzard, Jean K.Millet, Beth N. Licitra, Gary R. Whittaker Accepted on 14 June 2012, published on 20 June2012.

8. "Mechanisms of Coronavirus cell entry mediated by the viral spike protein" Sandrine Belouzard, Jean K.Millet, Beth N. Licitra, Gary R. Whittaker Accepted on 14 June 2012, published on 20 June2012.

9. : Cascarina SM, Ross ED. A proposed role for the SARS-CoV-2 nucleocapsid protein in the formation and regulation of biomolecular condensates. The FASEB Journal. 2020;34:9832–9842. https://doi.org/10.1096/fj.202001351

10. : Cascarina SM, Ross ED. A proposed role for the SARS-CoV-2 nucleocapsid protein in the formation and regulation of biomolecular condensates. The FASEB Journal. 2020;34:9832–9842. https://doi.org/10.1096/fj.202001351

11. : Crystal structure of SARS-CoV-2 nucleocapsid protein RNA binding domain reveals potential unique drug targeting sites Sisi Kanga , Mei Yanga , Zhongsi Hongb , Liping Zhangc , Zhaoxia Huanga , Xiaoxue Chena , Suhua Hea , Ziliang Zhoua , Zhechong Zhoua , Qiuyue Chena , Yan Yana , Changsheng Zhangc , Hong Shana,d,e, *, Shoudeng Chen, Received 4 March 2020; received in revised form 19 March 2020; accepted 31 March 2020, https://doi.org/10.1016/j.apsb.2020.04.009 2

12. . Zhu N, Zhang D, Wang W, et al. A novel coronavirus from patients with pneumonia in China, 2019. N Engl J Med. 2020;382:727-733.

13. DRUG DESIGNING : A REVIEW

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14. Drug Designing, Discovery and Development Techniques Elvis A. Martis1 and Rakesh R. Somani2 1Department of Pharmaceutical Chemistry, Bombay College of Pharmacy, Santacruz [E], Mumbai, 2Department of Pharmaceutical Chemistry, V.E.S. College of Pharmacy, Chembur [E], Mumbai, India

InTech-Drug_designing_discovery_and_development_techniques.pdf (intechopen.com)

15. Arvind Kumar Yadav, Rohit Shukla, Harish Changotra, Tiratha Raj Singh (2021). Recent challenges and progress of potential vaccines for Coronavirus disease 2019 (COVID-19). International Journal for Computational Biology, 9 (), 7-

REFERENCES FOR FIGURES

1. "What are the long-term health risks following COVID-19?". NewsGP. Royal Australian College of General Practitioners (RACGP). 24 June 2020. *Retrieved 8 September 2020*
2. *"*Mechanisms of Coronavirus cell entry mediated by the viral spike protein" Sandrine Belouzard, Jean K.Millet, Beth N. Licitra, Gary R. Whittaker Accepted on 14 June 2012, published on 20 June2012.
3. Cascarina SM, Ross ED. A proposed role for the SARS-CoV-2 nucleocapsid protein in the formation and regulation of biomolecular condensates. The FASEB Journal. 2020;34:9832–9842. https://doi.org/10.1096/fj.202001351
4. "Definition of Coronavirus by Merriam-Webster". Merriam-Webster. Archived from the original on 2020-03-23. Retrieved 2020-03-24.
5. www.rcsb.org
6. https://go.drugbank.com/releases/latest

APPENDIX 1

Index		DrugBankID	Ligand	Binding affinity
1		DB00615	Rifabutin	-13.6
2		DB01395	Drospirenone	-13.6
3		DB00320	Dihydroergotamine	-13.2

4		DB00309	Vindesine	-13.2
5		DB00390	Digoxin	-13.1
6		DB00207	Azithromycin	-13
7		DB01406	Danazol	-12.6
8		DB01200	Bromocriptine	-12.5
9		DB08973	Fluclorolone acetonide	-12.4
10		DB01396	Digitoxin	-12.4
11		DB06718	Stanozolol	-12.3
12		DB00541	Vincristine	-12.3
13		DB05812	Abiraterone	-12.2
14		DB00603	Medroxyprogesterone acetate	-12.1
15		DB00240	Alclometasone	-12.1
16		DB00210	Adapalene	-12
17		DB08871	Eribulin	-12
18		DB06786	Halcinonide	-12
19		DB06710	Methyltestosterone	-11.9
20		DB01234	Dexamethasone	-11.9
21		DB01260	Desonide	-11.9
22		DB00611	Butorphanol	-11.9
23		DB00443	Betamethasone	-11.9
24		DB00602	Ivermectin	-11.9
25		DB00180	Flunisolide	-11.8
26		DB00591	Fluocinolone acetonide	-11.8
27		DB00621	Oxandrolone	-11.8
28		DB01185	Fluoxymesterone	-11.8
29		DB00511	Acetyldigitoxin	-11.8
30		DB00421	Spironolactone	-11.8
31		DB00304	Desogestrel	-11.7
32		DB00596	Ulobetasol	-11.7
33		DB01708	Prasterone	-11.6
34		DB04839	Cyproterone acetate	-11.6
35		DB02789	Pregnenolone	-11.6
36		DB06595	Midostaurin	-11.5
37		DB06212	Tolvaptan	-11.5
38		DB00337	Pimecrolimus	-11.5

39		DB08906	Fluticasone furoate	-11.5
40		DB00367	Levonorgestrel	-11.5
41		DB00444	Teniposide	-11.5
42		DB00378	Dydrogesterone	-11.4
43		DB01211	Clarithromycin	-11.4
44		DB00396	Progesterone	-11.4
45		DB00324	Fluorometholone	-11.4
46		DB01590	Everolimus	-11.4
47		DB06713	Norelgestromin	-11.3
48		DB00504	Levallorphan	-11.3
49		DB06412	Oxymetholone	-11.3
50		DB00253	Medrysone	-11.3
51		DB06287	Temsirolimus	-11.3
52		DB00223	Diflorasone	-11.2
53		DB06230	Nalmefene	-11.2
54		DB05990	Obeticholic acid	-11.2
55		DB08971	Fluocortolone	-11.2
56		DB01216	Finasteride	-11.2
57		DB06290	Simeprevir	-11.2
58		DB08905	Formestane	-11.2
59		DB00294	Etonogestrel	-11.2
60		DB06777	Chenodeoxycholic acid	-11.2
61		DB08827	Lomitapide	-11.2
62		DB08867	Ulipristal	-11.1
63		DB00361	Vinorelbine	-11.1
64		DB04845	Ixabepilone	-11.1
65		DB04573	Estriol	-11.1
66		DB00512	Vancomycin	-11.1
67		DB06800	Methylnaltrexone	-11
68		DB06780	Desoxycorticosterone acetate	-11
69		DB00655	Estrone	-11
70		DB01177	Idarubicin	-11
71		DB00351	Megestrol acetate	-11
72		DB00254	Doxycycline	-10.9
73		DB08930	Dolutegravir	-10.9

74		DB00618	Demeclocycline	-10.9
75		DB02659	Cholic Acid	-10.9
76		DB03619	Deoxycholic acid	-10.9
77		DB00588	Fluticasone propionate	-10.8
78		DB01238	Budesonide	-10.8
79		DB01586	Ursodeoxycholic acid	-10.8
80		DB00547	Desoximetasone	-10.8
81		DB04038	Ergosterol	-10.7
82		DB00307	Bexarotene	-10.7
83		DB00327	Hydromorphone	-10.7
84		DB00295	Morphine	-10.7
85		DB04574	Estrone sulfate	-10.7
86		DB04540	Cholesterol	-10.7
87		DB04575	Quinestrol	-10.7
88		DB06809	Plerixafor	-10.7
89		DB00288	Amcinonide	-10.6
90		DB00377	Palonosetron	-10.6
91		DB01419	Antrafenine	-10.6
92		DB00199	Erythromycin	-10.6
93		DB01410	Ciclesonide	-10.6
94		DB05013	Ingenol mebutate	-10.5
95		DB04348	Taurocholic acid	-10.5
96		DB00497	Oxycodone	-10.4
97		DB00620	Triamcinolone	-10.4
98		DB08901	Ponatinib	-10.4
99		DB01420	Testosterone propionate	-10.3
100		DB02703	Fusidic acid	-10.3
101		DB04868	Nilotinib	-10.3
102		DB00434	Cyproheptadine	-10.3
103		DB06335	Saxagliptin	-10.2
104		DB00318	Codeine	-10.2
105		DB08815	Lurasidone	-10.2
106		DB06148	Mianserin	-10.2
107		DB01380	Cortisone acetate	-10.2
108		DB01251	Gliquidone	-10.2

109		DB01248	Docetaxel	-10.1
110		DB00514	Dextromethorphan	-10.1
111		DB06210	Eltrombopag	-10.1
112		DB00635	Prednisone	-10.1
113		DB01764	Dalfopristin	-10.1
114		DB01619	Phenindamine	-10
115		DB06810	Plicamycin	-10
116		DB04834	Rapacuronium	-10
117		DB06589	Pazopanib	-10
118		DB00266	Dicoumarol	-10
119		DB04824	Phenolphthalein	-9.9
120		DB00340	Metixene	-9.9
121		DB00370	Mirtazapine	-9.9
122		DB01209	Dezocine	-9.9
123		DB00362	Anidulafungin	-9.9
124		DB00256	Lymecycline	-9.9
125		DB00398	Sorafenib	-9.9
126		DB00430	Cefpiramide	-9.9
127		DB08907	Canagliflozin	-9.9
128		DB00186	Lorazepam	-9.9
129		DB08899	Enzalutamide	-9.9
130		DB00590	Doxazosin	-9.9
131		DB06717	Fosaprepitant	-9.8
132		DB00606	Cyclothiazide	-9.8
133		DB06789	Hydroxyprogesterone caproate	-9.8
134		DB00560	Tigecycline	-9.8
135		DB01184	Domperidone	-9.8
136		DB00549	Zafirlukast	-9.8
137		DB08875	Cabozantinib	-9.8
138		DB08896	Regorafenib	-9.8
139		DB00394	Beclomethasone dipropionate	-9.8
140		DB00445	Epirubicin	-9.8
141		DB04911	Oritavancin	-9.7
142		DB00652	Pentazocine	-9.7
143		DB00619	Imatinib	-9.7

144		DB05039	Indacaterol	-9.7
145		DB00197	Troglitazone	-9.7
146		DB00628	Clorazepic acid	-9.7
147		DB06216	Asenapine	-9.6
148		DB06077	Lumateperone	-9.6
149		DB06781	Difluprednate	-9.6
150		DB04703	Hesperidin	-9.6
151		DB01551	Dihydrocodeine	-9.6
152		DB08912	Dabrafenib	-9.6
153		DB04842	Fluspirilene	-9.6
154		DB00222	Glimepiride	-9.6
155		DB04861	Nebivolol	-9.6
156		DB01196	Estramustine	-9.5
157		DB06153	Pizotifen	-9.5
158		DB01544	Flunitrazepam	-9.5
159		DB08874	Fidaxomicin	-9.5
160		DB04115	Berberine	-9.5
161		DB01587	Ketazolam	-9.5
162		DB04864	Huperzine A	-9.5
163		DB00481	Raloxifene	-9.4
164		DB00579	Mazindol	-9.4
165		DB04816	Dantron	-9.4
166		DB00455	Loratadine	-9.4
167		DB08864	Rilpivirine	-9.4
168		DB06772	Cabazitaxel	-9.4
169		DB05239	Cobimetinib	-9.4
170		DB08903	Bedaquiline	-9.4
171		DB00301	Flucloxacillin	-9.4
172		DB00404	Alprazolam	-9.4
173		DB00436	Bendroflumethiazide	-9.4
174		DB06816	Pyrvinium	-9.4
175		DB00605	Sulindac	-9.4
176		DB06147	Sulfathiazole	-9.4
177		DB06401	Bazedoxifene	-9.4
178		DB06697	Artemether	-9.4

179		DB06145	Spiramycin	-9.4
180		DB01599	Probucol	-9.4
181		DB06201	Rufinamide	-9.4
182		DB06202	Lasofoxifene	-9.4
183		DB06176	Romidepsin	-9.3
184		DB06605	Apixaban	-9.3
185		DB01452	Diamorphine	-9.3
186		DB00358	Mefloquine	-9.3
187		DB06813	Pralatrexate	-9.3
188		DB00231	Temazepam	-9.3
189		DB00319	Piperacillin	-9.3
190		DB04918	Ceftobiprole	-9.3
191		DB06174	Noscapine	-9.3
192		DB01591	Solifenacin	-9.3
193		DB00342	Terfenadine	-9.2
194		DB03147	Flavin adenine dinucleotide	-9.2
195		DB06817	Raltegravir	-9.2
196		DB06684	Vilazodone	-9.2
197		DB00220	Nelfinavir	-9.2
198		DB00157	NADH	-9.2
199		DB08942	Isoxicam	-9.2
200		DB00485	Dicloxacillin	-9.2
201		DB04876	Vildagliptin	-9.2
202		DB01426	Ajmaline	-9.2
203		DB06144	Sertindole	-9.2
204		DB04908	Flibanserin	-9.2
205		DB00310	Chlorthalidone	-9.2
206		DB08882	Linagliptin	-9.2
207		DB08911	Trametinib	-9.2
208		DB08820	Ivacaftor	-9.2
209		DB00218	Moxifloxacin	-9.1
210		DB01329	Cefoperazone	-9.1
211		DB00470	Dronabinol	-9.1
212		DB00209	Trospium	-9.1
213		DB00438	Ceftazidime	-9.1

214		DB00450	Droperidol	-9.1
215		DB00303	Ertapenem	-9.1
216		DB05016	Ataluren	-9.1
217		DB00247	Methysergide	-9.1
218		DB06410	Doxercalciferol	-9.1
219		DB01327	Cefazolin	-9
220		DB00136	Calcitriol	-9
221		DB00524	Metolazone	-9
222		DB08828	Vismodegib	-9
223		DB00224	Indinavir	-9
224		DB00460	Verteporfin	-9
225		DB00158	Folic acid	-9
226		DB00246	Ziprasidone	-9
227		DB06708	Lumefantrine	-9
228		DB01595	Nitrazepam	-9
229		DB00554	Piroxicam	-9
230		DB06827	Viomycin	-9
231		DB00496	Darifenacin	-9
232		DB00328	Indomethacin	-9
233		DB00486	Nabilone	-9
234		DB00385	Valrubicin	-8.9
235		DB00146	Calcifediol	-8.9
236		DB00625	Efavirenz	-8.9
237		DB06766	Alcaftadine	-8.9
238		DB06274	Alvimopan	-8.9
239		DB06626	Axitinib	-8.9
240		DB00153	Ergocalciferol	-8.9
241		DB08881	Vemurafenib	-8.9
242		DB00321	Amitriptyline	-8.9
243		DB04209	Dequalinium	-8.9
244		DB00414	Acetohexamide	-8.9
245		DB00482	Celecoxib	-8.9
246		DB04835	Maraviroc	-8.9
247		DB06155	Rimonabant	-8.9
248		DB00169	Cholecalciferol	-8.9

249		DB01436	Alfacalcidol	-8.9
250		DB00642	Pemetrexed	-8.9
251		DB01254	Dasatinib	-8.9
252		DB00408	Loxapine	-8.8
253		DB08883	Perampanel	-8.8
254		DB00543	Amoxapine	-8.8
255		DB08965	Fusafungine	-8.8
256		DB03247	Flavin mononucleotide	-8.8
257		DB00607	Nafcillin	-8.8
258		DB00206	Reserpine	-8.8
259		DB00562	Benzthiazide	-8.8
260		DB06791	Lanreotide	-8.8
261		DB06771	Besifloxacin	-8.8
262		DB08804	Nandrolone decanoate	-8.8
263		DB01237	Bromodiphenhydramine	-8.8
264		DB00349	Clobazam	-8.8
265		DB00564	Carbamazepine	-8.8
266		DB01327	Cefamandole	-8.8
267		DB00365	Grepafloxacin	-8.8
268		DB00490	Buspirone	-8.8
269		DB00471	Montelukast	-8.8
270		DB00641	Simvastatin	-8.8
271		DB00363	Clozapine	-8.8
272		DB00578	Carbenicillin	-8.7
273		DB00344	Protriptyline	-8.7
274		DB00468	Quinine	-8.7
275		DB00252	Phenytoin	-8.7
276		DB00354	Buclizine	-8.7
277		DB00163	Vitamin E	-8.7
278		DB00540	Nortriptyline	-8.7
279		DB00533	Rofecoxib	-8.7
280		DB01394	Colchicine	-8.7
281		DB06414	Etravirine	-8.7
282		DB00589	Lisuride	-8.7
283		DB08816	Ticagrelor	-8.7

284		DB01609	Deferasirox	-8.7
285		DB00563	Methotrexate	-8.7
286		DB08950	Indoramin	-8.7
287		DB01624	Zuclopenthixol	-8.7
288		DB01559	Clotiazepam	-8.6
289		DB01588	Prazepam	-8.6
290		DB00520	Caspofungin	-8.6
291		DB00580	Valdecoxib	-8.6
292		DB01328	Cefonicid	-8.6
293		DB01501	Difenoxin	-8.6
294		DB00457	Prazosin	-8.6
295		DB01589	Quazepam	-8.6
296		DB01330	Cefotetan	-8.6
297		DB00656	Trazodone	-8.6
298		DB04946	Iloperidone	-8.6
299		DB06268	Sitaxentan	-8.6
300		DB08954	Ifenprodil	-8.6
301		DB04571	Trioxsalen	-8.6
302		DB04821	Nomifensine	-8.6
303		DB06814	Protokylol	-8.6
304		DB00115	Cyanocobalamin	-8.6
305		DB01623	Thiothixene	-8.6
306		DB06249	Arzoxifene	-8.6
307		DB08865	Crizotinib	-8.6
308		DB08439	Parecoxib	-8.6
309		DB01212	Ceftriaxone	-8.5
310		DB01242	Clomipramine	-8.5
311		DB06228	Rivaroxaban	-8.5
312		DB00276	Amsacrine	-8.5
313		DB01253	Ergometrine	-8.5
314		DB01175	Escitalopram	-8.5
315		DB01418	Acenocoumarol	-8.5
316		DB00475	Chlordiazepoxide	-8.5
317		DB05316	Pimavanserin	-8.5
318		DB01558	Bromazepam	-8.5

319		DB05294	Vandetanib	-8.5
320		DB00293	Raltitrexed	-8.5
321		DB06292	Dapagliflozin	-8.5
322		DB06725	Lornoxicam	-8.5
323		DB00104	Octreotide	-8.5
324		DB00067	Vasopressin	-8.4
325		DB08931	Riociguat	-8.4
326		DB01608	Periciazine	-8.4
327		DB00433	Prochlorperazine	-8.4
328		DB00502	Haloperidol	-8.4
329		DB06603	Panobinostat	-8.4
330		DB02266	Flufenamic acid	-8.4
331		DB04794	Bifonazole	-8.4
332		DB01340	Cilazapril	-8.4
333		DB00400	Griseofulvin	-8.4
334		DB00637	Astemizole	-8.4
335		DB00248	Cabergoline	-8.4
336		DB00216	Eletriptan	-8.4
337		DB00227	Lovastatin	-8.4
338		DB07776	Flavone	-8.4
339		DB08893	Mirabegron	-8.3
340		DB06211	Doripenem	-8.3
341		DB00275	Olmesartan	-8.3
342		DB00537	Ciprofloxacin	-8.3
343		DB00298	Dapiprazole	-8.3
344		DB00542	Benazepril	-8.3
345		DB00091	Cyclosporine	-8.3
346		DB00498	Phenindione	-8.3
347		DB06213	Regadenoson	-8.3
348		DB00353	Methylergometrine	-8.3
349		DB04841	Flunarizine	-8.3
350		DB00458	Imipramine	-8.3
351		DB04812	Benoxaprofen	-8.3
352		DB00469	Tenoxicam	-8.3
353		DB00480	Lenalidomide	-8.3

354		DB01628	Etoricoxib	-8.3
355		DB04570	Latamoxef	-8.3
356		DB00257	Clotrimazole	-8.2
357		DB06203	Alogliptin	-8.2
358		DB06590	Ceftaroline fosamil	-8.2
359		DB06636	Isavuconazonium	-8.2
360		DB01605	Pivmecillinam	-8.2
361		DB06711	Naphazoline	-8.2
362		DB00192	Indecainide	-8.2
363		DB01413	Cefepime	-8.2
364		DB04854	Febuxostat	-8.2
365		DB05154	Pretomanid	-8.2
366		DB01603	Meticillin	-8.2
367		DB01218	Halofantrine	-8.2
368		DB00417	Phenoxymethylpenicillin	-8.2
369		DB00415	Ampicillin	-8.2
370		DB00479	Amikacin	-8.2
371		DB00622	Nicardipine	-8.1
372		DB08822	Azilsartan medoxomil	-8.1
373		DB00357	Aminoglutethimide	-8.1
374		DB00613	Amodiaquine	-8.1
375		DB04820	Nialamide	-8.1
376		DB08910	Pomalidomide	-8.1
377		DB01621	Pipotiazine	-8.1
378		DB08897	Aclidinium	-8.1
379		DB00567	Cephalexin	-8.1
380		DB06787	Hexocyclium	-8.1
381		DB06608	Tafenoquine	-8.1
382		DB00179	Masoprocol	-8.1
383		DB06237	Avanafil	-8.1
384		DB00447	Loracarbef	-8.1
385		DB08860	Pitavastatin	-8.1
386		DB00203	Sildenafil	-8.1
387		DB00382	Tacrine	-8.1
388		DB00650	Leucovorin	-8.1

389		DB00332	Ipratropium	-8.1
390		DB01332	Cefradine	-8.1
391		DB01604	Pivampicillin	-8.1
392		DB00338	Omeprazole	-8.1
393		DB00334	Olanzapine	-8.1
394		DB04843	Mepenzolate	-8.1
395		DB01320	Fosphenytoin	-8.1
396		DB05015	Belinostat	-8.1
397		DB04898	Ximelagatran	-8.1
398		DB04896	Milnacipran	-8.1
399		DB08895	Tofacitinib	-8
400		DB01228	Encainide	-8
401		DB04844	Tetrabenazine	-8
402		DB00568	Cinnarizine	-8
403		DB00425	Zolpidem	-8
404		DB06803	Niclosamide	-8
405		DB00478	Rimantadine	-8
406		DB00442	Entecavir	-8
407		DB00412	Rosiglitazone	-8
408		DB08801	Dimetindene	-8
409		DB00561	Doxapram	-8
410		DB00584	Enalapril	-8
411		DB00314	Capreomycin	-8
412		DB00323	Tolcapone	-8
413		DB00317	Gefitinib	-8
414		DB00509	Dextrothyroxine	-8
415		DB00503	Ritonavir	-8
416		DB00278	Argatroban	-8
417		DB01393	Bezafibrate	-8
418		DB00245	Benzatropine	-8
419		DB05521	Telaprevir	-8
420		DB00348	Nitisinone	-8
421		DB01421	Paromomycin	-8
422		DB00451	Levothyroxine	-8
423		DB00374	Treprostinil	-8

424		DB04711	Iodipamide	-8
425		DB04813	Bithionol	-7.9
426		DB00251	Terconazole	-7.9
427		DB00492	Fosinopril	-7.9
428		DB00487	Pefloxacin	-7.9
429		DB00270	Isradipine	-7.9
430		DB01188	Ciclopirox	-7.9
431		DB01607	Ticarcillin	-7.9
432		DB04838	Cyclandelate	-7.9
433		DB04890	Bepotastine	-7.9
434		DB00140	Riboflavin	-7.9
435		DB00623	Fluphenazine	-7.9
436		DB01437	Glutethimide	-7.9
437		DB00402	Eszopiclone	-7.9
438		DB00238	Nevirapine	-7.9
439		DB00284	Acarbose	-7.9
440		DB04865	Omacetaxine mepesuccinate	-7.9
441		DB00296	Ropivacaine	-7.9
442		DB05351	Dexlansoprazole	-7.9
443		DB00448	Lansoprazole	-7.9
444		DB00215	Citalopram	-7.9
445		DB00528	Lercanidipine	-7.9
446		DB06616	Bosutinib	-7.9
447		DB06764	Tetryzoline	-7.9
448		DB01205	Flumazenil	-7.8
449		DB01602	Bacampicillin	-7.8
450		DB06016	Cariprazine	-7.8
451		DB06207	Silodosin	-7.8
452		DB00643	Mebendazole	-7.8
453		DB06267	Udenafil	-7.8
454		DB08916	Afatinib	-7.8
455		DB06694	Xylometazoline	-7.8
456		DB08976	Floctafenine	-7.8
457		DB00467	Enoxacin	-7.8
458		DB00604	Cisapride	-7.8

459		DB00229	Cefotiam	-7.8
460		DB00507	Nitazoxanide	-7.8
461		DB00508	Triflupromazine	-7.8
462		DB00297	Bupivacaine	-7.8
463		DB00525	Tolnaftate	-7.8
464		DB01430	Almitrine	-7.7
465		DB01409	Tiotropium	-7.7
466		DB00452	Framycetin	-7.7
467		DB00170	Menadione	-7.7
468		DB00519	Trandolapril	-7.7
469		DB08909	Glycerol phenylbutyrate	-7.7
470		DB06282	Levocetirizine	-7.7
471		DB00424	Hyoscyamine	-7.7
472		DB08873	Boceprevir	-7.7
473		DB00601	Linezolid	-7.7
474		DB01656	Roflumilast	-7.7
475		DB08934	Sofosbuvir	-7.7
476		DB01698	Rutin	-7.7
477		DB05676	Apremilast	-7.7
478		DB00305	Mitomycin	-7.7
479		DB01264	Darunavir	-7.7
480		DB00177	Valsartan	-7.7
481		DB04871	Lorcaserin	-7.7
482		DB00535	Cefdinir	-7.7
483		DB00343	Diltiazem	-7.7
484		DB00572	Atropine	-7.7
485		DB00582	Voriconazole	-7.7
486		DB06794	Lodoxamide	-7.6
487		DB00208	Ticlopidine	-7.6
488			Ceftizoxime	-7.6
489		DB00235	Milrinone	-7.6
490		DB00213	Pantoprazole	-7.6
491		DB00214	Torasemide	-7.6
492		DB06480	Prucalopride	-7.6
493		DB00441	Gemcitabine	-7.6

494		DB00243	Ranolazine	-7.6
495		DB00261	Anagrelide	-7.6
496		DB00267	Cefmenoxime	-7.6
497		DB00279	Liothyronine	-7.6
498		DB02638	Terlipressin	-7.6
499		DB04938	Ospemifene	-7.6
500		DB00341	Cetirizine	-7.6
501		DB00372	Thiethylperazine	-7.6
502		DB00384	Triamterene	-7.6
503		DB08818	Hyaluronic acid	-7.6
504		DB00465	Ketorolac	-7.6
505		DB00035	Desmopressin	-7.6
506		DB08932	Macitentan	-7.6
507		DB00648	Mitotane	-7.6
508		DB08967	Dimetotiazine	-7.6
509		DB00598	Labetalol	-7.6
510		DB00387	Procyclidine	-7.5
511		DB06802	Nepafenac	-7.5
512		DB06594	Agomelatine	-7.5
513		DB06654	Safinamide	-7.5
514		DB06209	Prasugrel	-7.5
515		DB00586	Diclofenac	-7.5
516		DB01744	Camphor	-7.5
517		DB00472	Fluoxetine	-7.5
518		DB01231	Diphenidol	-7.5
519		DB01178	Chlormezanone	-7.5
520		DB00406	Gentian violet cation	-7.5
521		DB00477	Chlorpromazine	-7.5
522		DB01221	Ketamine	-7.5
523		DB03585	Oxyphenbutazone	-7.5
524		DB01247	Isocarboxazid	-7.5
525		DB04825	Prenylamine	-7.5
526		DB00392	Profenamine	-7.5
527		DB00376	Trihexyphenidyl	-7.5
528		DB01415	Ceftibuten	-7.4

529		DB01428	Oxybenzone	-7.4
530		DB06712	Nilvadipine	-7.4
531		DB06729	Sulfaphenazole	-7.4
532		DB00439	Cerivastatin	-7.4
533		DB06413	Armodafinil	-7.4
534		DB00420	Promazine	-7.4
535		DB06402	Telavancin	-7.4
536		DB01601	Lopinavir	-7.4
537		DB00427	Triprolidine	-7.4
538		DB06742	Ambroxol	-7.4
539		DB06193	Pixantrone	-7.4
540		DB06152	Nylidrin	-7.4
541		DB00118	Ademetionine	-7.4
542		DB00315	Zolmitriptan	-7.4
543		DB02925	Piretanide	-7.4
544		DB04920	Clevidipine	-7.4
545		DB03615	Ribostamycin	-7.4
546		DB00346	Alfuzosin	-7.4
547		DB04837	Clofedanol	-7.4
548		DB04743	Nimesulide	-7.4
549		DB06403	Ambrisentan	-7.4
550		DB01195	Flecainide	-7.4
551		DB00555	Lamotrigine	-7.4
552		DB00553	Methoxsalen	-7.4
553		DB08604	Triclosan	-7.4
554		DB00530	Erlotinib	-7.4
555		DB00559	Bosentan	-7.4
556		DB01274	Arformoterol	-7.4
557		DB08877	Ruxolitinib	-7.4
558		DB00539	Toremifene	-7.4
559		DB00162	Vitamin A	-7.4
560		DB00523	Alitretinoin	-7.4
561		DB00401	Nisoldipine	-7.3
562		DB00456	Cefalotin	-7.3
563		DB00576	Sulfamethizole	-7.3

564		DB02772	Sucrose	-7.3
565		DB01618	Molindone	-7.3
566		DB04953	Ezogabine	-7.3
567		DB06820	Sulconazole	-7.3
568		DB00242	Cladribine	-7.3
569		DB00131	Adenosine phosphate	-7.3
570		DB08936	Chlorcyclizine	-7.3
571		DB00273	Topiramate	-7.3
572		DB06441	Cangrelor	-7.3
573		DB00474	Methohexital	-7.3
574		DB04930	Permethrin	-7.3
575		DB06751	Drotaverine	-7.3
576		DB00500	Tolmetin	-7.3
577		DB00205	Pyrimethamine	-7.3
578		DB00552	Pentostatin	-7.3
579		DB00383	Oxyphencyclimine	-7.3
580		DB00432	Trifluridine	-7.2
581		DB05271	Rotigotine	-7.2
582		DB06736	Aceclofenac	-7.2
583		DB01581	Sulfamerazine	-7.2
584		DB01176	Cyclizine	-7.2
585		DB06807	Phenyl aminosalicylate	-7.2
586		DB01282	Carbetocin	-7.2
587		DB01322	Kava	-7.2
588		DB02959	Oxitriptan	-7.2
589		DB08943	Isoconazole	-7.2
590		DB00193	Tramadol	-7.2
591		DB00274	Cefmetazole	-7.2
592		DB00263	Sulfisoxazole	-7.2
593		DB00185	Cevimeline	-7.2
594		DB06217	Vernakalant	-7.2
595		DB06695	Dabigatran etexilate	-7.2
596		DB00178	Ramipril	-7.2
597		DB00495	Zidovudine	-7.2
598		DB00459	Acitretin	-7.2

599		DB08872	Gabapentin enacarbil	-7.2
600		DB00255	Diethylstilbestrol	-7.2
601		DB04465	Lactose	-7.2
602		DB00322	Floxuridine	-7.2
603		DB00532	Mephenytoin	-7.2
604		DB00175	Pravastatin	-7.1
605		DB00499	Flutamide	-7.1
606		DB00285	Venlafaxine	-7.1
607		DB00493	Cefotaxime	-7.1
608		DB00517	Anisotropine methylbromide	-7.1
609		DB01243	Chloroxine	-7.1
610		DB00473	Hexylcaine	-7.1
611		DB00573	Fenoprofen	-7.1
612		DB00150	Tryptophan	-7.1
613		DB04846	Celiprolol	-7.1
614		DB08880	Teriflunomide	-7.1
615		DB01331	Cefoxitin	-7.1
616		DB00461	Nabumetone	-7.1
617		DB00196	Fluconazole	-7.1
618		DB00581	Lactulose	-7.1
619		DB06700	Desvenlafaxine	-7.1
620		DB04817	Metamizole	-7.1
621		DB04951	Pirfenidone	-7.1
622		DB00633	Dexmedetomidine	-7.1
623		DB01416	Cefpodoxime	-7.1
624		DB01627	Lincomycin	-7
625		DB00283	Clemastine	-7
626		DB04880	Enoximone	-7
627		DB00557	Hydroxyzine	-7
628		DB00393	Nimodipine	-7
629		DB04840	Debrisoquine	-7
630		DB01987	Cocarboxylase	-7
631		DB00410	Mupirocin	-7
632		DB04826	Thenalidine	-7
633		DB00440	Trimethoprim	-7

634		DB00556	Perflutren	-7
635		DB00521	Carteolol	-7
636		DB06701	Dexmethylphenidate	-7
637		DB01240	Epoprostenol	-7
638		DB08889	Carfilzomib	-7
639		DB00239	Oxiconazole	-7
640		DB00454	Meperidine	-7
641		DB06614	Peramivir	-7
642		DB00631	Clofarabine	-7
643		DB01582	Sulfamethazine	-7
644		DB00137	Lutein	-7
645		DB06288	Amisulpride	-7
646		DB00204	Dofetilide	-7
647		DB00250	Dapsone	-7
648		DB00640	Adenosine	-7
649		DB06762	Pinacidil	-7
650		DB00483	Gallamine triethiodide	-7
651		DB00080	Daptomycin	-7
652		DB00333	Methadone	-6.9
653		DB01190	Clindamycin	-6.9
654		DB00639	Butoconazole	-6.9
655		DB00345	Aminohippuric acid	-6.9
656		DB03312	Brivudine	-6.9
657		DB00571	Propranolol	-6.9
658		DB01579	Phendimetrazine	-6.9
659		DB00494	Entacapone	-6.9
660		DB02546	Vorinostat	-6.9
661		DB00418	Secobarbital	-6.9
662		DB00194	Vidarabine	-6.9
663		DB08933	Luliconazole	-6.9
664		DB00380	Dexrazoxane	-6.9
665		DB08918	Levomilnacipran	-6.9
666		DB00287	Travoprost	-6.9
667		DB01606	Tazobactam	-6.9
668		DB08941	Isoxsuprine	-6.9

669		DB00654	Latanoprost	-6.9
670		DB01262	Decitabine	-6.9
671		DB00476	Duloxetine	-6.9
672		DB00187	Esmolol	-6.8
673		DB01353	Butobarbital	-6.8
674		DB00649	Stavudine	-6.8
675		DB00360	Sapropterin	-6.8
676		DB00600	Monobenzone	-6.8
677		DB00391	Sulpiride	-6.8
678		DB04815	Clioquinol	-6.8
679		DB00647	Dextropropoxyphene	-6.8
680		DB00608	Chloroquine	-6.8
681		DB08819	Tafluprost	-6.8
682		DB00268	Ropinirole	-6.8
683		DB00574	Fenfluramine	-6.8
684		DB01616	Alverine	-6.8
685		DB01611	Hydroxychloroquine	-6.8
686		DB01610	Valganciclovir	-6.8
687		DB08868	Fingolimod	-6.8
688		DB00308	Ibutilide	-6.8
689		DB00234	Reboxetine	-6.8
690		DB01600	Tiaprofenic acid	-6.8
691		DB06821	Sulfameter	-6.8
692		DB01427	Amrinone	-6.8
693		DB01191	Dexfenfluramine	-6.8
694		DB00312	Pentobarbital	-6.7
695		DB04822	Oxeladin	-6.7
696		DB00355	Aztreonam	-6.7
697		DB00249	Idoxuridine	-6.7
698		DB08964	Gemeprost	-6.7
699		DB04657	Carboxin	-6.7
700		DB00007	Leuprolide	-6.7
701		DB00381	Amlodipine	-6.7
702		DB00271	Diatrizoate	-6.7
703		DB08944	Isoaminile	-6.7

704		DB00359	Sulfadiazine	-6.7
705		DB01249	Iodixanol	-6.7
706		DB01632	5-O-phosphono-alpha-D-ribofuranosyl diphosphate	-6.7
707		DB01275	Hydralazine	-6.7
708		DB01625	Isopropamide	-6.7
709		DB01424	Aminophenazone	-6.6
710		DB01241	Gemfibrozil	-6.6
711		DB00449	Dipivefrin	-6.6
712		DB01597	Cilastatin	-6.6
713		DB01319	Fosamprenavir	-6.6
714		DB00405	Dexbrompheniramine	-6.6
715		DB00484	Brimonidine	-6.6
716		DB00428	Streptozocin	-6.6
717		DB00422	Methylphenidate	-6.6
718		DB01620	Pheniramine	-6.6
719		DB08814	Triflusal	-6.6
720		DB00183	Pentagastrin	-6.6
721		DB08799	Antazoline	-6.6
722		DB00409	Remoxipride	-6.6
723		DB00289	Atomoxetine	-6.6
724		DB07565	Chloramphenicol succinate	-6.6
725		DB00325	Nitroprusside	-6.6
726		DB06150	Sulfadimethoxine	-6.5
727		DB00336	Nitrofural	-6.5
728		DB00014	Goserelin	-6.5
729		DB01438	Phenazopyridine	-6.5
730		DB00241	Butalbital	-6.5
731		DB00577	Valaciclovir	-6.5
732		DB04855	Dronedarone	-6.5
733		DB00429	Carboprost tromethamine	-6.5
734		DB00306	Talbutal	-6.5
735		DB06204	Tapentadol	-6.5
736		DB00280	Disopyramide	-6.5
737		DB00645	Dyclonine	-6.5

738		DB06702	Fesoterodine	-6.5
739		DB01435	Antipyrine	-6.5
740		DB00366	Doxylamine	-6.5
741		DB00518	Albendazole	-6.5
742		DB00350	Minoxidil	-6.5
743		DB06774	Capsaicin	-6.5
744		DB06769	Bendamustine	-6.5
745		DB00612	Bisoprolol	-6.5
746		DB00599	Thiopental	-6.5
747		DB08947	Iopamidol	-6.5
748		DB04832	Zimelidine	-6.5
749		DB06755	Beta carotene	-6.5
750		DB01407	Clenbuterol	-6.4
751		DB00264	Metoprolol	-6.4
752		DB00121	Biotin	-6.4
753		DB00190	Carbidopa	-6.4
754		DB08966	Fursultiamine	-6.4
755		DB01194	Brinzolamide	-6.4
756		DB00431	Lindane	-6.4
757		DB00446	Chloramphenicol	-6.4
758		DB00558	Zanamivir	-6.4
759		DB00237	Butabarbital	-6.4
760		DB00651	Dyphylline	-6.4
761		DB00219	Oxyphenonium	-6.4
762		DB01362	Iohexol	-6.4
763		DB06119	Cenobamate	-6.4
764		DB00221	Isoetharine	-6.4
765		DB01598	Imipenem	-6.3
766		DB02513	Thymol	-6.3
767		DB00195	Betaxolol	-6.3
768		DB00527	Cinchocaine	-6.3
769		DB04948	Lofexidine	-6.3
770		DB00176	Fluvoxamine	-6.3
771		DB06262	Droxidopa	-6.3
772		DB06716	Fospropofol	-6.3

773		DB00335	Atenolol	-6.3
774		DB00226	Guanadrel	-6.3
775		DB00265	Crotamiton	-6.3
776		DB02300	Calcipotriol	-6.3
777		DB00594	Amiloride	-6.3
778		DB00356	Chlorzoxazone	-6.3
779		DB06819	Phenylbutyric acid	-6.2
780		DB00277	Theophylline	-6.2
781		DB00143	Glutathione	-6.2
782		DB00152	Thiamine	-6.2
783		DB00426	Famciclovir	-6.2
784		DB00489	Sotalol	-6.2
785		DB00114	Pyridoxal phosphate	-6.2
786		DB00281	Lidocaine	-6.2
787		DB06826	Unoprostone	-6.2
788		DB03310	Glutathione disulfide	-6.2
789		DB00292	Etomidate	-6.2
790		DB08949	Inositol nicotinate	-6.2
791		DB00217	Bethanidine	-6.1
792		DB00636	Clofibrate	-6.1
793		DB01187	Iophendylate	-6.1
794		DB06707	Levonordefrin	-6.1
795		DB00233	Aminosalicylic acid	-6.1
796		DB00423	Methocarbamol	-6.1
797		DB06691	Mepyramine	-6.1
798		DB00244	Mesalazine	-6.1
799		DB08946	Iopanoic acid	-6.1
800		DB00575	Clonidine	-6.1
801		DB00379	Mexiletine	-6.1
802		DB00135	Tyrosine	-6
803		DB00629	Guanabenz	-6
804		DB00585	Nizatidine	-6
805		DB00369	Cidofovir	-6
806		DB06218	Lacosamide	-6
807		DB00419	Miglustat	-6

808		DB01783	Pantothenic acid	-6
809		DB00299	Penciclovir	-6
810		DB00181	Baclofen	-6
811		DB00634	Sulfacetamide	-6
812		DB06795	Mafenide	-6
813		DB00373	Timolol	-5.9
814		DB00593	Ethosuximide	-5.9
815		DB04564	Gluconolactone	-5.9
816		DB06704	Iobenguane	-5.9
817		DB00302	Tranexamic acid	-5.9
818		DB00184	Nicotine	-5.9
819		DB06788	Histrelin	-5.9
820		DB00191	Phentermine	-5.9
821		DB01197	Captopril	-5.9
822		DB00300	Tenofovir disoproxil	-5.9
823		DB04173	Fructose	-5.9
824		DB00126	Ascorbic acid	-5.9
825		DB01296	Glucosamine	-5.9
826		DB03209	Oteracil	-5.8
827		DB00198	Oseltamivir	-5.8
828		DB00211	Midodrine	-5.8
829		DB02362	Aminobenzoic acid	-5.8
830		DB08958	Hexetidine	-5.8
831		DB00413	Pramipexole	-5.8
832		DB01189	Desflurane	-5.8
833		DB05541	Brivaracetam	-5.8
834		DB00291	Chlorambucil	-5.8
835		DB00610	Metaraminol	-5.8
836		DB00120	Phenylalanine	-5.8
837		DB00491	Miglitol	-5.8
838		DB00368	Norepinephrine	-5.8
839		DB00201	Caffeine	-5.7
840		DB00144	Phosphatidyl serine	-5.7
841		DB00388	Phenylephrine	-5.7
842		DB00617	Paramethadione	-5.7

843		DB00544	Fluorouracil	-5.7
844		DB00106	Abarelix	-5.7
845		DB00316	Acetaminophen	-5.7
846		DB01626	Pargyline	-5.6
847		DB06785	Ganirelix	-5.6
848		DB08797	Salicylamide	-5.6
849		DB03793	Benzoic acid	-5.6
850		DB01580	Oxprenolol	-5.6
851		DB08826	Deferiprone	-5.5
852		DB00182	Amphetamine	-5.5
853		DB00159	Icosapent	-5.5
854		DB00290	Bleomycin	-5.5
855		DB00501	Cimetidine	-5.5
856		DB08887	Icosapent ethyl	-5.5
857		DB03756	Doconexent	-5.5
858		DB06714	Propylhexedrine	-5.5
859		DB00352	Tioguanine	-5.5
860		DB00397	Phenylpropanolamine	-5.5
861		DB00165	Pyridoxine	-5.5
862		DB06797	Mebutamate	-5.5
863		DB01914	D-glucose	-5.5
864		DB00399	Zoledronic acid	-5.5
865		DB01577	Metamfetamine	-5.5
866		DB01576	Dextroamphetamine	-5.5
867		DB03088	Pidolic acid	-5.4
868		DB04224	Oleic Acid	-5.4
869		DB05246	Methsuximide	-5.4
870		DB06689	Ethanolamine oleate	-5.4
871		DB00395	Carisoprodol	-5.4
872		DB00550	Propylthiouracil	-5.4
873		DB00326	Calcium glucoheptonate	-5.4
874		DB00437	Allopurinol	-5.4
875		DB05057	Erdosteine	-5.4
876		DB05018	Migalastat	-5.4
877		DB00236	Pipobroman	-5.4

878		DB03796	Palmitic Acid	-5.4
879		DB00050	Cetrorelix	-5.3
880		DB00632	Docosanol	-5.3
881		DB00166	Lipoic acid	-5.3
882		DB00627	Niacin	-5.3
883		DB01956	Taurine	-5.3
884		DB00155	Citrulline	-5.3
885		DB06699	Degarelix	-5.3
886		DB00545	Pyridostigmine	-5.3
887		DB01718	Cetrimonium	-5.3
888		DB06243	Eflornithine	-5.3
889		DB01638	Sorbitol	-5.3
890		DB03193	Stearic acid	-5.3
891		DB00132	alpha-Linolenic acid	-5.3
892		DB00403	Ceruletide	-5.2
893		DB00548	Azelaic acid	-5.2
894		DB00202	Succinylcholine	-5.2
895		DB06261	Hexaminolevulinate	-5.2
896		DB04931	Afamelanotide	-5.2
897		DB00262	Carmustine	-5.2
898		DB00347	Trimethadione	-5.2
899		DB03017	Lauric acid	-5.2
900		DB00609	Ethionamide	-5.2
901		DB00282	Pamidronic acid	-5.2
902		DB06804	Nonoxynol-9	-5.1
903		DB00259	Sulfanilamide	-5.1
904		DB01613	Erythrityl tetranitrate	-5.1
905		DB00371	Meprobamate	-5.1
906		DB06770	Benzyl alcohol	-5.1
907		DB06799	Methenamine	-5.1
908		DB04221	Didecyldimethylammonium	-5
909		DB01563	Chloral hydrate	-5
910		DB00138	Cystine	-5
911		DB00142	Glutamic acid	-5
912		DB00130	L-Glutamine	-5

913		DB00173	Adenine	-4.9
914		DB01181	Ifosfamide	-4.9
915		DB06154	Pentaerythritol tetranitrate	-4.9
916		DB02701	Nicotinamide	-4.9
917		DB04272	Citric acid	-4.9
918		DB00630	Alendronic acid	-4.9
919		DB00583	Levocarnitine	-4.9
920		DB00141	N-Acetylglucosamine	-4.8
921		DB00027	Gramicidin D	-4.8
922		DB00006	Bivalirudin	-4.8
923		DB06823	Tiopronin	-4.8
924		DB00330	Ethambutol	-4.8
925		DB03255	Phenol	-4.8
926		DB06753	Triclofos	-4.8
927		DB06775	Carglumic acid	-4.8
928		DB00529	Foscarnet	-4.8
929		DB00313	Valproic acid	-4.8
930		DB00128	Aspartic acid	-4.7
931		DB00389	Carbimazole	-4.7
932		DB04339	Carbocisteine	-4.7
933		DB00531	Cyclophosphamide	-4.7
934		DB00123	L-Lysine	-4.6
935		DB00148	Creatine	-4.6
936		DB06698	Betahistine	-4.6
937		DB00228	Enflurane	-4.6
938		DB00230	Pregabalin	-4.6
939		DB06815	Pyrithione	-4.6
940		DB04160	Pyrophosphoric acid	-4.6
941		DB00339	Pyrazinamide	-4.6
942		DB00119	Pyruvic acid	-4.6
943		DB00161	Valine	-4.6
944		DB00174	Asparagine	-4.6
945		DB00488	Altretamine	-4.5
946		DB00129	Ornithine	-4.5
947		DB06811	Polidocanol	-4.5

948		DB00189	Ethchlorvynol	-4.5
949		DB00134	Methionine	-4.4
950		DB06706	Isometheptene	-4.4
951		DB02893	D-Methionine	-4.4
952		DB00513	Aminocaproic acid	-4.4
953		DB00156	Threonine	-4.4
954		DB00272	Betazole	-4.4
955		DB00260	Cycloserine	-4.4
956		DB00139	Succinic acid	-4.4
957		DB08908	Dimethyl fumarate	-4.3
958		DB04398	Lactic acid	-4.3
959		DB01612	Amyl Nitrite	-4.3
960		DB06637	Dalfampridine	-4.3
961		DB08842	Acetylcarnitine	-4.3
962		DB01213	Fomepizole	-4.2
963		DB00551	Acetohydroxamic acid	-4.2
964		DB00566	Succimer	-4.2
965		DB03929	D-Serine	-4.1
966		DB08809	Dichloroacetic acid	-4.1
967		DB06756	Glycine betaine	-4.1
968		DB00331	Metformin	-4.1
969		DB02530	gamma-Aminobutyric acid	-4
970		DB06151	Acetylcysteine	-4
971		DB01440	gamma-Hydroxybutyric acid	-4
972		DB00151	Cysteine	-4
973		DB01839	Propylene glycol	-4
974		DB00411	Carbamoylcholine	-3.9
975		DB06709	Methacholine	-3.9
976		DB03766	Propanoic acid	-3.8
977		DB03085	Glycolic acid	-3.8
978		DB03754	Tromethamine	-3.7
979		DB04572	Thiotepa	-3.7
980		DB00145	Glycine	-3.6
981		DB04827	Urethane	-3.5
982		DB02325	Isopropyl alcohol	-3.5

983		DB05381	Histamine	-3.4
984		DB01401	Choline magnesium trisalicylate	-3.4
985		DB03166	Acetic acid	-3.4
986		DB03175	Propyl alcohol	-3.4
987		DB06824	Triethylenetetramine	-3.3
988		DB03904	Urea	-3.1
989		DB00122	Choline	-3.1
990		DB00592	Piperazine	-3.1
991		DB06782	Dimercaprol	-3
992		DB00536	Guanidine	-2.5
993		DB00435	Nitric Oxide	-1.9
994		DB03843	Formaldehyde	-1.8
995		DB11588	Carbon monoxide	-1.8
996		DB00653	Magnesium sulfate	-1.1
997		DB00258	Calcium acetate	-1.1
998		DB00416	Metocurine iodide	-0.9
999		DB00462	Methscopolamine bromide	-0.9
1000		DB05109	Trabectedin	12.2