Inhibitors or Toxins? Large Library Target-Specific Screening of Fullerene-based Nanoparticles for Drug Design Purposes

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1. Ligand Collection

All ligand structures collected from literature review.[1-18]

2. Ligand Classification

CheS-Mapper (v2.3.5) program is able to analyze the connection between the structure of chemical compounds, their physico-chemical properties, and biological (or toxic)

effects. At first, Linear Fragments (FP2) were computed by OpenBabel software. Then the structures were clustered using fingerprints by applying SimpleKmean (WEKA) algorithm and employing the Tanimoto similarity measure for the clustering and embedding. Six aligned clusters were selected based on their largest structural fragment that matches the complete cluster. In this circumstance, their orientation in 3D space is adjusted such that the common substructure is superimposed. **Fig. S1** shows six clusters of the ligands considered in this study.

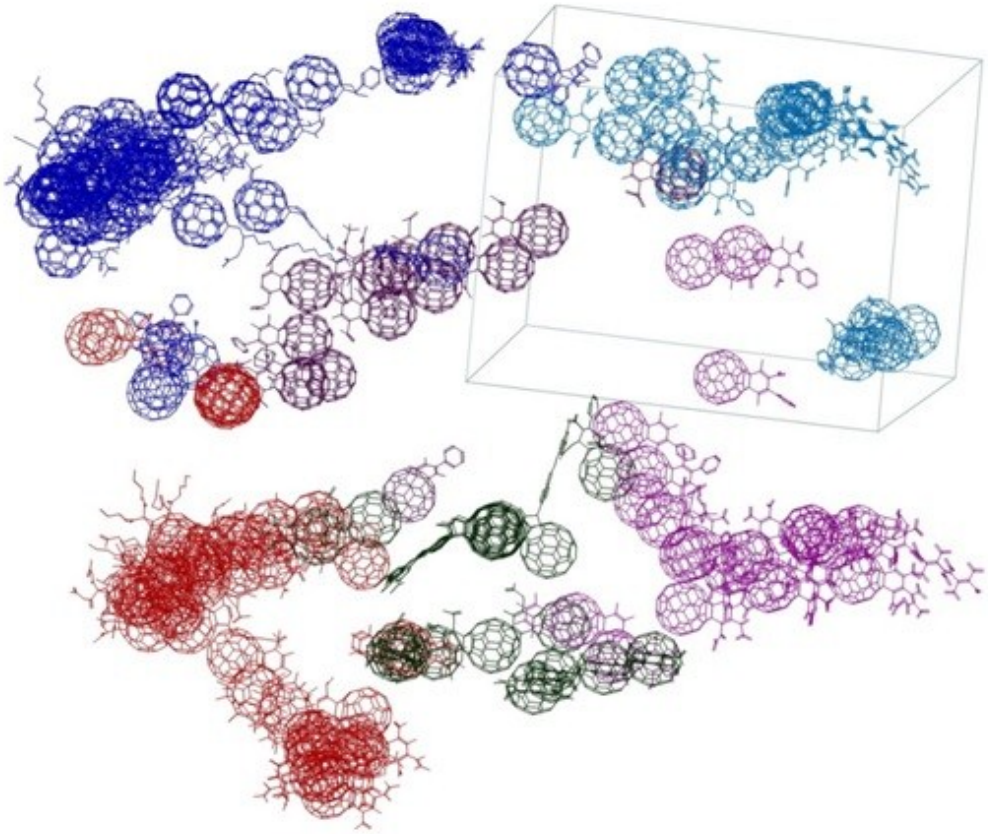


Figure S1 Selection of members for six clusters of FDs from 169 ligands. The compounds are highlighted according to their cluster assignment. Cluster 6 is selected (as indicated by the box).

3. Molecular and Quantum Mechanics

The initial structures were built and optimized by MM^+ molecular mechanics method in HyperChem 8 software package[19] to obtain the basic conformations of the fullerene derivatives. The density functional theory (DFT) with the hybrid meta exchange-correlation functional M06-2X[20] including 6-31G(d,p) basis set[21] has been applied to attain reliable optimal geometries. The calculations were carried out by the Gaussian 09 code. The Berny algorithm using GEDIIS in redundant internal coordinates has been applied to obtain a local minimum.[22] The hybrid meta exchange-correlation functionals, called M06-2X, have been applied to find a stationary point on the potential energy surface. M06-2X functional is parameterized only for nonmetals and design for calculations including main-group thermo-chemistry, kinetics, non-covalent interactions, and electronic excitation energies to valence and Rydberg states.[20] A medium size basis set, 6-31G(d,p), has been used in the DFT calculations This basis set is commonly used for the atoms up to Argon and includes polarization functions added to hydrogen atoms and heavy atoms.[21]

4. Descriptors and Model Preparation

QikProp program is also able to check for Lipinski Rule-of-Five[23] and Jorgensen's Rule-of-Three[24] violations to provide an at-a-glance measure of whether a compound is drug-like. QikProp uses the full 3D molecular structure instead of fragment-based approaches giving consistently correct results in predicting properties for molecules with novel scaffold as for analogs of well-known drugs.

The model performance was assessed by correlation coefficient (R^2) (Eqn.S1) as the measures of goodness-of-fit for developed model:

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i^{obs} - y_i^{pred})^2}{\sum_{i=1}^{n}(y_i^{obs} - \tilde{y}^{obs})^2} \qquad \text{(S1)}$$

where: y_i^{obs} – experimental (observed) value of the property for the i^{th} compound; y_i^{pred} – predicted value for i^{th} compound; $\tilde{y}^{obs}$ – the mean experimental value of the property; n – the number of compounds.

The robustness of the model was assessed by cross-validated coefficient Q^2_{LOO} (leave-one-out method):

$$Q^2_{LOO} = 1 - \frac{\sum_{i=1}^{n}(y_i^{obs} - y_i^{predcv})^2}{\sum_{i=1}^{n}(y_i^{obs} - \tilde{y}^{obs})^2} \qquad \text{(S2)}$$

where: y_i^{obs} – experimental (observed) value of the property for the i^{th} compound; y_i^{predcv} – cross-validated predicted value for i^{th} compound; $\tilde{y}$ – the mean experimental value of the property in the training set; n – the number of compounds in the set.

QSAR assumes that activities (binding score) of a compound are related to its chemical characteristics (descriptors).[25] Thus, selection of appropriate physico-chemical descriptors in activity/toxicity prediction facilitates design of new compounds with enhanced activity.[26] Characteristics of fullerenes significantly influence the obtained biological responses.[27] However, only a few studies have been carried out to develop QSARs in order to correlate molecular structures with activities of FDs.[28,8]

5. Protein-Ligand Docking

First, three-dimensional transformations of each molecule with respect to other is computed, providing the molecular surface of molecules for detecting geometric patches (concave, convex and flat parts). Exclusively, patches with the "hot spot" residues are

kept to match concave with convex and flat parts with any type of patches applying geometric hashing algorithm. A set of complexes of transformations has been computed. In the third stage, complexes with acceptable penetrations are filtered and ranked according to a geometric shape complementarity score pertaining multi-resolution surface data structure. PatchDock implies unbound (rigid) docking where two molecules in their native conformations are given and the docking algorithm considers possible conformational changes upon association. The PatchDock docking algorithm is the fastest technique for large library.[29] The docking calculations were performed keeping the clustering root-mean-square deviation, RMSD (this number indicates the radius of the clustering RMSD in angstroms). This value is used in the final clustering stage of the algorithm. It confirms that the distance between any two output solutions will be at least equal to the specified clustering RMSD value set here as 2 Å.[30]

In AutoDock Vina, the docking is carried out by Lamarckian genetic algorithm (LGA) where the receptors could be either rigid or flexible, depending on demand. The algorithm also includes ligands as flexible molecules if there are any rotatable bonds. The receptor grid was created and centered about the ligand bounded active site of proteins. As an important step for docking, polar hydrogens were added to the receptor. A search space, i.e. "grid box" was chosen with the grid box spacing of 1.0 Å. However, the grid points of x $\times$ y $\times$ z, i.e. size and position of the box vary from protein to protein. In rigid docking, all rotatable bonds of the ligand were set to free by AutoDock Tools but the receptor was set as a rigid entity. In contrast, the closest residues (2-8) around the ligand were set to be rotatable and rest of the part of the protein was fixed as rigid in flexible docking. BINANA software[31] was used to analyze different contributions to

protein-ligand binding and identified the key binding characteristics of investigated fullerene nanoparticles, including contribution of degree of hydrogen bonds, hydrophobic interactions, salt bridges, and pi interactions.

6. Data mining

PDB files of the complexes with the highest score values were considered to view the structure of the compound and to analyze the interactions.

7. Visualization

CheS-Mapper (Chemical Space Mapper), a 3D-viewer for chemical datasets with small compounds was used to view the cluster of the ligand data set. CheS-Mapper embedded a dataset into 3D space, such that compounds that have similar feature values are close to each other. It utilizes Java application, based on the Java libraries Jmol, CDK, WEKA, and utilizes OpenBabel and R (a software environment for statistical computing and graphics). Kohonen's self-organizing map (SOM) was built using MATLAB software. In addition, other useful software, such as Molecular Graphics System- PyMOL[32] and AutoDock Tools[33] were used for visualization and to identify the cavity surface, non-polar interactions and hydrogen bonds. The color coding heatmap was plotted to reflect the corresponding scoring function for protein-ligand docking.

8. Results and Discussion

PatchDock produced acceptable results[29] in the top 1000 solutions in 95.2% of the Antibody-Antigen cases, 85.2% of the Enzyme Inhibitor cases, and 50% of the other cases, suggesting to consider the top most score of the associated docked structure. Docked structures of 1ILH (PDB ID: 1ILH) with ligands 53 and ligand 91 are shown in

Figs. S2b and **S2c** respectively. Complexes of 1D6U with ligand 95 (S**2**d), 96(S**2**e) and 114(S**2**f) are shown in **Figs. S2d-e**.

The crystal structure of elongation factor Tu (EF-Tu, PDB ID: 1HA3) inhibited by an antibiotic-aurodox, holds 3 hydrophobic binding domains (one domain with original ligand, **Fig.** S**2g**) which also are capable to form hydrogen bonds.[34] We found one FD (Ligand **108, Fig. S2h**) containing -$CONH_2$ and -NO_2 groups able to form hydrogen bond with the polar residues in the active site. It is obvious that the spherical hydrophobic fullerene core interacts only with non-polar residues.

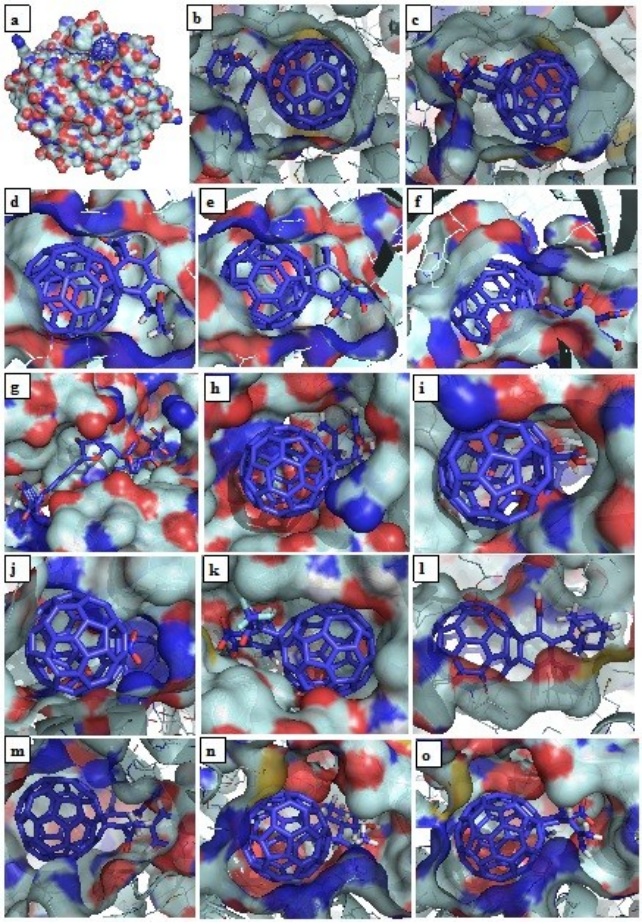


Figure S2 (a) Ligand 6 with blood clotting enzyme thrombin (PDB ID 1A4W). Docked structures of 1ILH with ligand 53(b) and ligand 91(c). Complexes of 1D6U with ligand

95 (d), 96(e) and 114(f). (g) EF-Tu with aurodox. (h) EF-Tu with fullerene derivative. (i) HIV-1 PR bounded with ligand 41. (j) E. coli nitroreductase enzyme with ligand 141. (k) human quinone reductase type 2 with ligand 96. (l) Ligand 46 binds with intestinal fatty acid binding protein (I-FAB PDB ID: 1ICN). (m) L-aminoadipate-semialdehyde dehydrogenase-phosphopantetheinyl transferase (PPT with ligand 136, PDB ID: 2CG5). Ligand 68 (n) and ligand 97 (o) bind with inositol monophosphatases (PDB code: 1LBV). The atom color is defined as pale cyan (protein) and deep blue (fullerene derivative) for carbon, red for oxygen, blue for nitrogen and white for hydrogen in protein.

Interestingly, another three FDs have been found to be different enzyme inhibitors. Ligands **41, 141,** and **96** potentially inhibit the human immunodeficiency virus type 1 protease (HIV-1, PDB ID: 1HOS, **Fig. S2i**), *E.coli* nitroreductase enzyme (NTR, PDB ID 1OOQ, **Fig. S2j**), and the human quinone reductase type 2 (QR2, PDB ID 1QR2, **Fig.** S**2k**), respectively. Previously we and another group reported that FDs might inhibit HIV enzyme.[35, 36] Our current study supports those conclusions. However, for other two enzymes (NTR, PDB ID 1OOQ and QR2, PDB ID 1QR2), no previous study has been performed to reveal their interactions with fullerene derivatives. For another two receptors, we also identified two FDs that are bounded exactly at the same binding sites of the receptors as original, non-fullerene ligands (**Figs.** S**2l** and S**2m**).

We also observed that two ligands significantly hold the active site of inositol monophosphatases[37], a cytosolic enzyme necessary to regenerate the supply of m*yo*-inositol for the synthesis of phosphatidylinositols. For instance, two ligands significantly

hold the active site of inositol monophosphatases. (**Figs. S2n** and S2**o)** bind with inositol monophosphatases (PDB code: 1LBV).

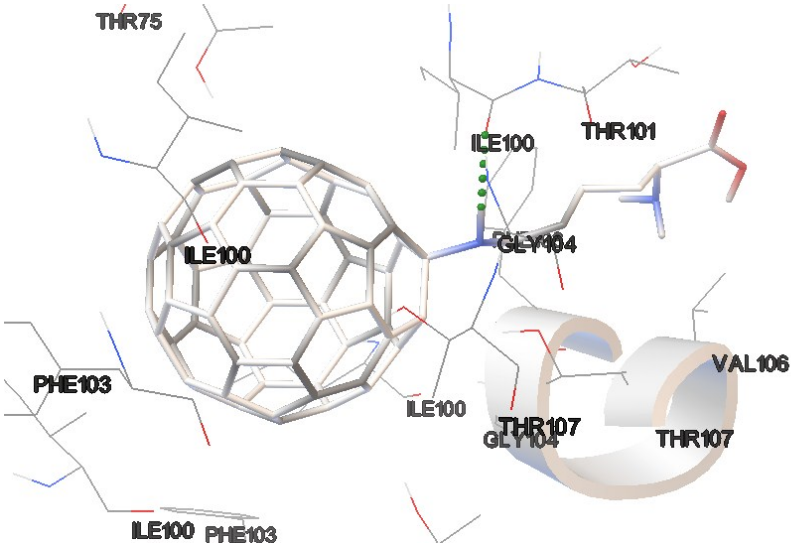
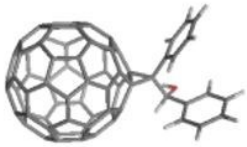
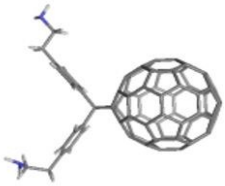
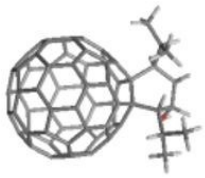
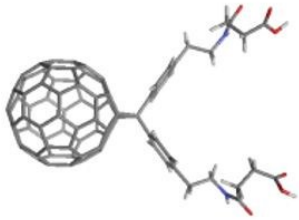
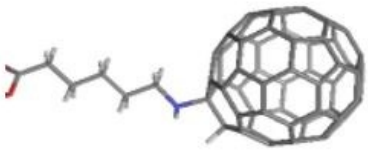
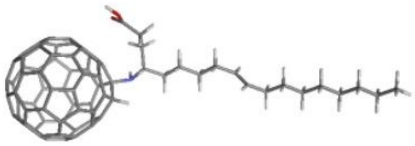
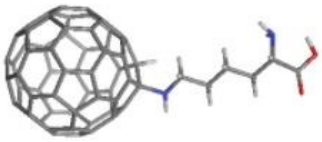
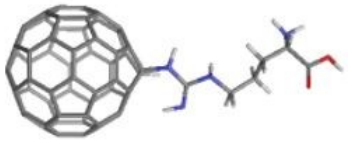
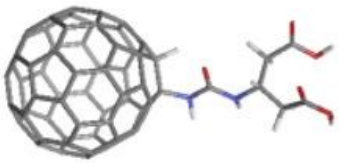
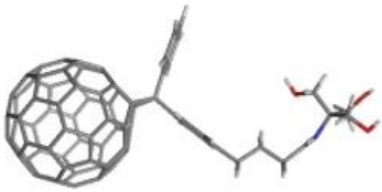
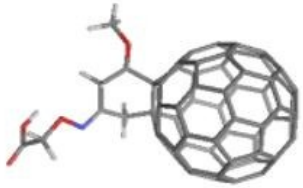
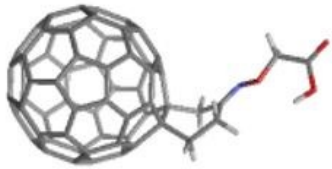


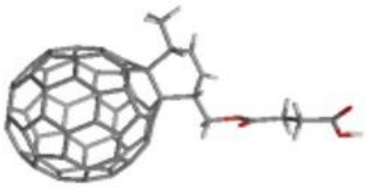
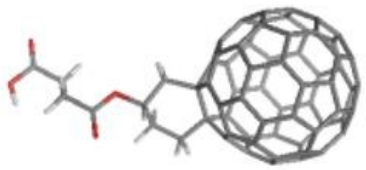
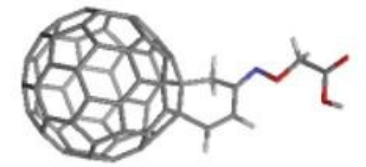
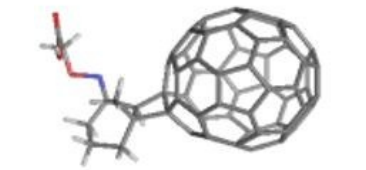
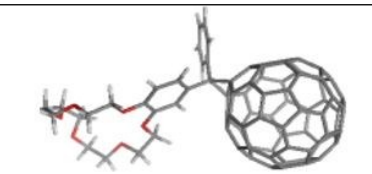
Figure S3 Potassium ion channel (PDB code: 1JVM) with ligand **7** (AutoDock Vina).

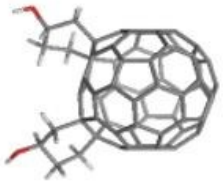
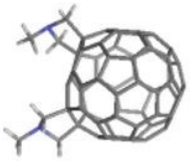
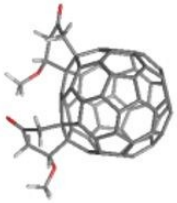
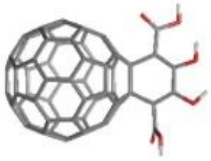
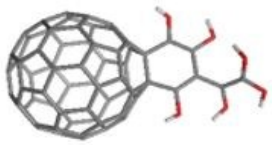
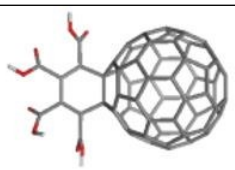
Table S1 All FDs structures with SMILES notation.

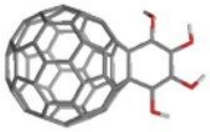
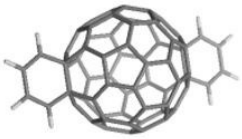
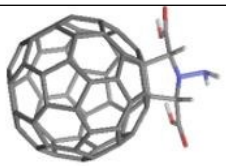
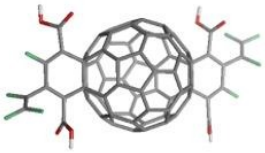
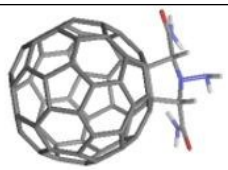
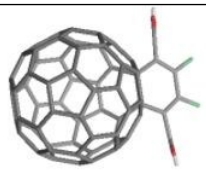
Ligand number	Structure	SMILE notation
1		c1cccc(c1)[C@@]1([C@]23c4c5c6c7c8c9[C@@H]%10[C@@H]%11c%12c%13c%14[C@H]%15[C@H]%16[C@H]%17[C@@H]%13[C@@H]%11[C@H]%11[C@H]%13[C@@H]%10[C@@H]8[C@H]8[C@H]%10[C@@H]7c5c5c7c4c4c3c(c%14c3c%12c9c6[C@]123)c%15c1c4[C@@H]2[C@H]7[C@H]3[C@@H]4[C@@H]6[C@H]([C@@H]%10[C@@H]53)[C@H]8[C@H]%13[C@H]3[C@@H]6[C@@H]5[C@H]([C@@H]%17[C@@H]%113)[C@H]%16[C@H]1[C@H]2[C@H]45)[C@H](c1ccccc1)O
2		c12c3c4[C@H]5[C@H]6[C@H]7[C@@@H]3[C@H]3[C@@H]2[C@H]2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10[C@@H]5[C@@H]4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C%11(c1ccc(cc1)CCN)c1ccc(cc1)CCN

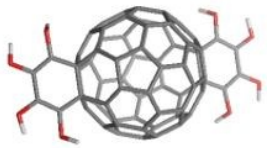
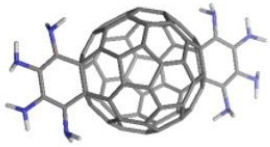
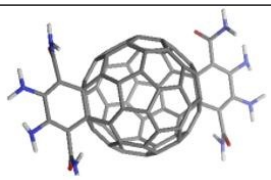
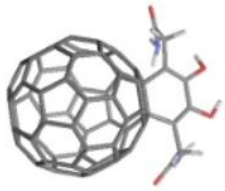
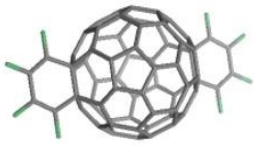
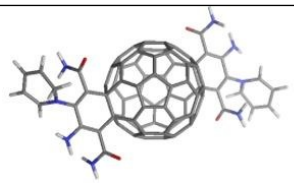
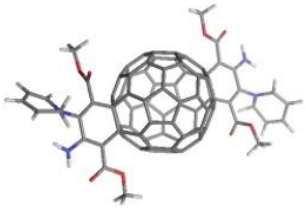
3		c12[C@@H]3[C@H]4[C@H]5[C@H]6[C@H]7[C@@H]3c3c2c2c8c9c1[C@@H]1[C@@H]%10c9c9c%11c8[C@]8%12c2c2c3[C@H]3c%13c2c2[C@@]8(c8c%11c%11[C@@H]9[C@H]9[C@@H]%10[C@H]%10[C@@H]([C@H]41)[C@@H]5[C@@H]1[C@@H]4[C@H]%10[C@H]9[C@@H]5c%11c9c%10[C@@H]5[C@@H]4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1c%13c(c%10[C@@H]41)c2c89)[C@H](C[C@@H]([C@@H]%12C(C)C)O)C(C)C
4		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3[C@@H]2[C@H]2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10[C@@H]5[C@@H]4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C%11(c1ccc(cc1)CCNC(=O)CCC(=O)O)c1ccc(cc1)CCNC(=O)CCC(=O)O
5		[C@H]12[C@@H]3[C@H]4c5c6[C@H]7[C@@H]3[C@H]3[C@@H]2[C@H]2[C@H]8[C@H]9[C@@H]1c1c%10[C@H]9[C@@H]9[C@@H]%11[C@H]8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%12[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%11c%11c9c9c%10c%10c(c41)c5c1[C@@]4([C@H]%10c9c5c%11[C@H]9c%10c5c4c4c1c6c([C@@H]73)c1[C@@H]%12[C@H](c%10c41)[C@@H]2[C@@H]89)NCCCCCC(=O)O
6		[C@H]12[C@@H]3[C@H]4c5c6[C@H]7[C@@H]3[C@H]3[C@@H]2[C@H]2[C@H]8[C@H]9[C@@H]1c1c%10[C@H]9[C@@H]9[C@@H]%11[C@H]8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%12[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%11c%11c9c9c%10c%10c(c41)c5c1[C@@]4([C@H]%10c9c5c%11[C@H]9c%10c5c4c4c1c6[C@@H]([C@@H]73)[C@H]1[C@@H]%12[C@H](c%10c41)[C@@H]2[C@@H]89)N[C@@H](CCCC/C=C/CCCCCCCC)CCC(=O)O
7		[C@H]12[C@@H]3[C@H]4c5c6[C@H]7[C@@H]3[C@H]3[C@@H]2[C@H]2[C@H]8[C@H]9[C@@H]1c1c%10[C@H]9[C@@H]9[C@@H]%11[C@H]8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%12[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%11c%11c9c9c%10c%10c(c41)c5c1[C@@]4([C@H]%10c9c5c%11[C@H]9c%10c5c4c4c1c6c([C@@H]73)c1[C@@H]%12[C@H](c%10c41)[C@@H]2[C@@H]89)NCCCC[C@@H](C(=O)O)N

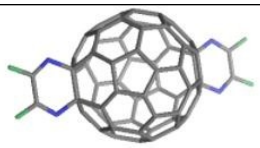
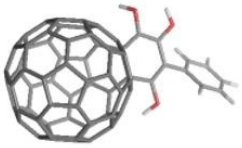
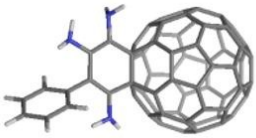
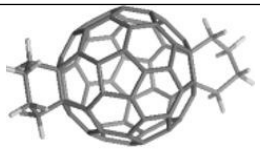
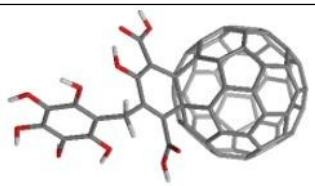
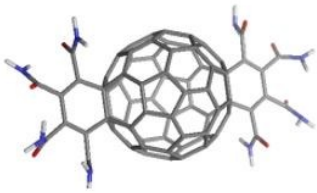
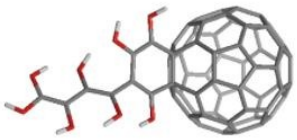
8		C12=C3[C@@H]4[C@@H]5C6=C2[C@@H]2[C@@H]7[C@H]1[C@H]1c8c9[C@@H]7[C@@H]7c%10c%11[C@@H]%12[C@@H]%13c%14c%15c%16c%17c%18c%19c%20c(c4c4[C@@H]%21[C@H]5[C@@H]5[C@H]6[C@@H]6[C@H]2[C@H]7[C@H]%12[C@@H]6[C@H]2[C@@H]5[C@H]5[C@@H]%21c(c%194)c%17[C@@H]%15[C@H]5[C@@H]%132)c3c1c1c%20[C@H]%18[C@]2(c(c81)c(c(c%162)c%11%14)c9%10)NC(=N)NCCC[C@@H](C(=O)O)N
9		OC(=O)CC(NC(=O)N[C@]12[C@H]3c4c5c6c7c8[C@@H]9[C@H]%10[C@@H]%11[C@@H]%12[C@H]%13c%14c%15[C@H]%16[C@@H]%12[C@H]%12[C@@H]%11[C@H]%11[C@@H]9[C@H]9[C@H]%17c8c5c5[C@H]%17[C@@H]8[C@@H]%17[C@H]9[C@H]%11[C@@H]9[C@H]%12[C@H]%11[C@H]%12[C@@H]9[C@@H]%17[C@H]9[C@@H]8[C@H]8c5c4c4c8c5[C@H]9[C@H]%12c8c([C@@H]%16%11)c%15c(c1c%14c(c%13c7%10)c36)c(c24)c58)CC(=O)O
10		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3[C@@H]2[C@H]2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)[C@]%11(c1ccccc1)c1ccc(cc1)CCCC(=O)NC(CO)(CO)CO
11		c12[C@@H]3[C@H]4[C@H]5[C@H]6[C@H]7[C@@H]3c3c2c2c8c9c1[C@@H]1[C@@H]%10c9c9c%11c8[C@]8%12c2c2c3[C@H]3c%13c2c2[C@@]8(c8c%11c%11[C@@H]9[C@H]9[C@@H]%10[C@H]%10[C@@H]([C@H]41)[C@@H]5[C@@H]1[C@@H]4[C@H]%10[C@H]9[C@@H]5c%11c9c%10[C@@H]5[C@@H]4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1c%13c(c%10[C@@H]41)c2c89)[C@@H](C/C(=N\OCC(=O)O)/C%12)OC
12		c12[C@@H]3[C@H]4[C@H]5[C@H]6[C@H]7[C@@H]3c3c2c2c8c9c1[C@@H]1[C@@H]%10c9c9c%11c8[C@]8%12c2c2c3[C@H]3c%13c2c2[C@@]8(c8c%11c%11[C@@H]9[C@H]9[C@@H]%10[C@H]%10[C@@H]([C@H]41)[C@@H]5[C@@H]1[C@@H]4[C@H]%10[C@H]9[C@@H]5c%11c9c%10[C@@H]5[C@@H]4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1c%13c(c%10[C@@H]41)c2c89)CC/C(=N\OCC(=O)O)/C%12

13		c12[C@@H]3[C@H]4[C@H]5[C@H]6[C@H]7[C@@H]3c3c2c2c8c9c1[C@@H]1[C@@H]%10c9c9c%11c8[C@]8%12c2c2c3[C@H]3c%13c2c2[C@@]8(c8c%11c%11[C@@H]9[C@H]9[C@@H]%10[C@H]%10[C@@H]([C@H]41)[C@@H]5[C@@H]1[C@@H]4[C@H]%10[C@H]9[C@@H]5c%11c9c%10[C@@H]5[C@@H]4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1c%13c(c%10[C@@H]41)c2c89)[C@H](C=C[C@H]%12C)COC(=O)CCC(=O)O
14		c12[C@@H]3[C@H]4[C@H]5[C@H]6[C@H]7[C@@H]3c3c2c2c8c9c1[C@@H]1[C@@H]%10c9c9c%11c8[C@]8%12c2c2c3[C@H]3c%13c2c2[C@@]8(c8c%11c%11[C@@H]9[C@H]9[C@@H]%10[C@H]%10[C@@H]([C@H]41)[C@@H]5[C@@H]1[C@@H]4[C@H]%10[C@H]9[C@@H]5c%11c9c%10[C@@H]5[C@@H]4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1c%13c(c%10[C@@H]41)c2c89)C[C@H](CC%12)OC(=O)CCC(=O)O
15		c12[C@@H]3[C@H]4[C@H]5[C@H]6[C@H]7[C@@H]3c3c2c2c8c9c1[C@@H]1[C@@H]%10c9c9c%11c8[C@]8%12c2c2c3[C@H]3c%13c2c2[C@@]8(c8c%11c%11[C@@H]9[C@H]9[C@@H]%10[C@H]%10[C@@H]([C@H]41)[C@@H]5[C@@H]1[C@@H]4[C@H]%10[C@H]9[C@@H]5c%11c9c%10[C@@H]5[C@@H]4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1c%13c(c%10[C@@H]41)c2c89)C=C/C(=N\OCC(=O)O)/C%12
16		N(=C\1/[C@H]2[C@]34[C@]5(c6c7c8c9c%10[C@@H]%11[C@H]%12[C@@H]%13[C@@H]%14[C@H]%15c%16c%17[C@H]%18[C@@H]%14[C@H]%14[C@@H]%13[C@H]%13[C@@H]%11[C@H]%11[C@H]%19c%10c7c7[C@H]%19[C@@H]%10[C@@H]%19[C@H]%11[C@H]%13[C@@H]%11[C@H]%14[C@H]%13[C@H]%14[C@@H]%11[C@@H]%19[C@H]%11[C@@H]%10[C@H]%10c7c6c6c%10c7[C@H]%11[C@H]%14[C@@H]%10[C@H]([C@@H]%18%13)c%17c(c3c%16c(c%15c9%12)c58)c(c46)c7%10)[C@]2(C)CCC1)\OCC(=O)O
17		c12[C@@H]3[C@H]4[C@H]5[C@H]6[C@H]7[C@@H]3c3c2c2c8c9c1[C@@H]1[C@@H]%10c9c9c%11c8[C@]8%12c2c2c3[C@H]3c%13c2c2[C@@]8(c8c%11c%11[C@@H]9[C@H]9[C@@H]%10[C@H]%10[C@@H]([C@H]41)[C@@H]5[C@@H]1[C@@H]4[C@H]%10[C@H]9[C@@H]5c%11c9c%10[C@@H]5[C@@H]4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1c%13c(c%10[C@@H]41)c2c89)[C@@]%12(c1ccccc1)c1ccc2c(c1)OCCOCCOCCOCCOCCO2

18		c12c3c4c5c6c7c3c3c2c2c8c9c1[C@]1%10c%11c9c9[C@@H]%12[C@H]8C8=C%13c%14c%12c%12c9c9c%11c%11c(c5c5[C@]%15%16[C@]%11(c9c9c%12c%11c%12c9c%15c9c5c6[C@H]5c7c6c3[C@@H]([C@@H]28)[C@@H]2C6=C3[C@H](c%12c9[C@@H]53)[C@H](c%14%11)[C@H]%132)C[C@@H](CC%16)O)[C@]41CC[C@@H](C%10)O
19		c12c3c4c5c6c7c3[C@H]3c2c2c8c9c1[C@]1%10c%11c9c9[C@@H]%12[C@H]8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9c%11c%11c(c5c5[C@]%14%15[C@]%11(c9c9c%12[C@H]%11c%12c9c%14c9c5c6[C@@H]([C@@H]73)[C@H]3[C@@H]%13[C@H](c%12c93)[C@@H]2[C@@H]8%11)CN(C%15)C)[C@]41CN(C%10)C
20		c12c3c4c5c6c7c3[C@H]3c2c2c8c9c1[C@]1%10c%11c9c9[C@@H]%12[C@H]8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9c%11c%11c(c5c5[C@]%14%15[C@]%11(c9c9c%12C%11=C8[C@H]2[C@H]2c8c%11c9c%14c9c5c6[C@@H]([C@@H]73)[C@@H]([C@@H]%132)c89)CC(=O)C[C@H]%15OC)[C@]41[C@@H](CC(=O)C%10)OC
21		c12[C@@H]3[C@H]4[C@H]5[C@H]6[C@H]7[C@@H]3c3c2c2c8c9c1[C@@H]1[C@@H]%10c9c9c%11c8[C@]8%12c2c2c3[C@H]3c%13c2c2[C@@]8(c8c%11c%11[C@@H]9[C@H]9[C@@H]%10[C@H]%10[C@@H]([C@H]41)[C@@H]5[C@@H]1[C@@H]4[C@H]%10[C@H]9[C@@H]5c%11c9[C@H]%10[C@@H]5[C@@H]4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1c%13c([C@@H]%10[C@@H]41)c2c89)C(=C(C(=C%12C(=O)O)O)O)C(=O)O
22		c12[C@@H]3[C@H]4C5=C6C7=C3c3c2c2c8c9c1[C@@H]1[C@@H]%10c9c9c%11c8[C@]8%12c2c2c3[C@H]3c%13c2c2[C@@]8(c8c%11c%11[C@@H]9[C@H]9[C@@H]%10[C@H]%10[C@@H]([C@H]41)[C@@H]5[C@@H]1[C@@H]4[C@H]%10[C@H]9[C@@H]5c%11c9c%10[C@@H]5[C@@H]4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1c%13c(c%10[C@@H]41)c2c89)C(=C(C(=C%12O)C(=C(O)O)O)O)O
23		c12[C@@H]3[C@H]4[C@H]5[C@H]6[C@H]7[C@@H]3c3c2c2c8c9c1[C@@H]1[C@@H]%10c9c9c%11c8[C@]8%12c2c2c3[C@H]3c%13c2c2[C@@]8(c8c%11c%11[C@@H]9[C@H]9[C@@H]%10[C@H]%10[C@@H]([C@H]41)[C@@H]5[C@@H]1[C@@H]4[C@H]%10[C@H]9[C@@H]5c%11c9c%10[C@@H]5[C@@H]4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1c%13c(c%10[C@@H]41)c2c89)C(=C(C(=C%12C(=O)O)C(=O)O)C(=O)O)C(=O)O

24		[C@H]12[C@@H]3[C@H]4[C@H]5[C@H]6[C@H]7[C@@H]3c3c2c2c8c9[C@@H]1[C@@H]1[C@@H]%10c9c9c%11c8[C@]8%12c2c2c3[C@H]3c%13c2c2[C@@]8(c8c%11c%11[C@@H]9[C@H]9[C@@H]%10[C@H]%10[C@@H]([C@H]41)[C@@H]5[C@@H]1[C@@H]4[C@H]%10[C@H]9[C@@H]5c%11c9[C@H]%10[C@@H]5[C@@H]4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1c%13c([C@@H]%10[C@@H]41)c2c89)C(=C(C(=C%12O)O)O)O
25		c12c3c4c5c6c7c3c3c2c2c8c9c1c1c%10c9c9c%11c8[C@]8%12c2c2c3[C@H]3c%13c2c2[C@@]8(c8c%11c%11[C@@H]9[C@H]9c%10c%10c(c41)[C@@]15[C@@]4(c5c%10c9c9c%11c%10c%11c9c5c5c4c6c([C@@H]73)c3c%13c(c%11c53)c2c8%10)C=CC=C1)C=CC=C%12
26		c12[C@@H]3[C@H]4[C@H]5[C@H]6[C@H]7[C@@H]3c3c2c2c8c9c1[C@@H]1c%10c9c9[C@]%11%12[C@]8(c8c2c2c3[C@H]3[C@H]%13c2c2c8c8c%11c%11c9c9c%10[C@H]%10[C@@H]([C@H]41)[C@@H]5[C@@H]1[C@@H]4[C@H]%10c9c5c%11c9[C@H]%10[C@@H]5[C@@H]4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2c89)[C@@H](N([C@@H]%12C(=O)O)N)C(=O)O
27		c12c3c4c5c6c7c3c3c2c2c8c9c1c1c%10c9c9c%11c8[C@]8%12c2c2c3[C@H]3c%13c2c2[C@@]8(c8c%11c%11[C@@H]9[C@H]9c%10c%10c(c41)[C@@]15[C@@]4(c5c%10c9c9c%11c%10c%11c9c5c5c4c6c([C@@H]73)c3c%13c(c%11c53)c2c8%10)C(=C(C(=C1C(=O)O)F)C(=C(F)F)F)C(=O)O)C(=C(C(=C%12C(=O)O)C(=C(F)F)F)F)C(=O)O
28		c12[C@@H]3[C@H]4[C@H]5[C@H]6[C@H]7[C@@H]3c3c2c2c8c9c1[C@@H]1c%10c9c9[C@]%11%12[C@]8(c8c2c2c3[C@H]3[C@H]%13c2c2c8c8c%11c%11c9c9c%10[C@H]%10[C@@H]([C@H]41)[C@@H]5[C@@H]1[C@@H]4[C@H]%10c9c5c%11c9[C@H]%10[C@@H]5[C@@H]4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2c89)[C@@H](N([C@@H]%12C(=O)N)N)C(=O)N
29		c12[C@@H]3[C@H]4[C@H]5[C@H]6[C@H]7[C@@H]3c3c2c2c8c9c1[C@@H]1[C@@H]%10c9c9c%11c8[C@]8%12c2c2c3[C@H]3c%13c2c2[C@@]8(c8c%11c%11[C@@H]9[C@H]9[C@@H]%10[C@H]%10[C@@H]([C@H]41)[C@@H]5[C@@H]1[C@@H]4[C@H]%10[C@H]9[C@@H]5c%11c9c%10[C@@H]5[C@@H]4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1c%13c(c%10[C@@H]41)c2c89)C(=C(C(=C%12C(=O)O)F)F)C(=O)O

30		c12c3c4c5c6c7c3c3c2c2c8c9c1c1c%10c9c9c%11c8[C@]8%12c2c2c3[C@H]3c%13c2c2[C@@]8(c8c%11c%11[C@@H]9[C@H]9c%10c%10c(c41)[C@@]15[C@@]4(c5c%10c9c9c%11c%10c%11c9c5c5c4c6c([C@@H]73)c3c%13c(c%11c53)c2c8%10)C(=C(C(=C1O)O)O)O)C(=C(C(=C%12O)O)O)O
31		c12c3c4c5c6c7c3c3c2c2c8c9c1c1c%10c9c9c%11c8[C@]8%12c2c2c3[C@H]3c%13c2c2[C@@]8(c8c%11c%11[C@@H]9[C@H]9c%10c%10c(c41)[C@@]15[C@@]4(c5c%10c9c9c%11c%10c%11c9c5c5c4c6c([C@@H]73)c3c%13c(c%11c53)c2c8%10)C(=C(C(=C1N)N)N)N)C(=C(C(=C%12N)N)N)N
32		c12c3c4c5c6c7c3c3c2c2c8c9c1c1c%10c9c9c%11c8[C@]8%12c2c2c3[C@H]3c%13c2c2[C@@]8(c8c%11c%11[C@@H]9[C@H]9c%10c%10c(c41)[C@@]15[C@@]4(c5c%10c9c9c%11c%10c%11c9c5c5c4c6c([C@@H]73)c3c%13c(c%11c53)c2c8%10)C(=C(C(=C1C(=O)N)N)N)C(=O)N)C(=C(C(=C%12C(=O)N)N)N)C(=O)N
33		c12[C@@H]3[C@H]4[C@H]5[C@H]6[C@H]7[C@@H]3c3c2c2c8c9c1[C@@H]1[C@@H]%10c9c9c%11c8[C@]8%12c2c2c3[C@H]3c%13c2c2[C@@]8(c8c%11c%11[C@@H]9[C@H]9[C@@H]%10[C@H]%10[C@@H]([C@H]41)[C@@H]5[C@@H]1[C@@H]4[C@H]%10[C@H]9[C@@H]5c%11c9c%10[C@@H]5[C@@H]4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1c%13c(c%10[C@@H]41)c2c89)C(=C(C(=C%12CC(=O)N)O)O)CC(=O)N
34		c12c3c4c5c6c7c3c3c2c2c8c9c1c1c%10c9c9c%11c8[C@]8%12c2c2c3[C@H]3c%13c2c2[C@@]8(c8c%11c%11[C@@H]9[C@H]9c%10c%10c(c41)[C@@]15[C@@]4(c5c%10c9c9c%11c%10c%11c9c5c5c4c6c([C@@H]73)c3c%13c(c%11c53)c2c8%10)C(=C(C(=C1F)F)F)F)C(=C(C(=C%12F)F)F)F
35		c12c3c4c5c6c7c3c3c2c2c8c9c1c1c%10c9c9c%11c8[C@]8%12c2c2c3[C@H]3c%13c2c2[C@@]8(c8c%11c%11[C@@H]9[C@H]9c%10c%10c(c41)[C@@]15[C@@]4(c5c%10c9c9c%11c%10c%11c9c5c5c4c6c([C@@H]73)c3c%13c(c%11c53)c2c8%10)C(=C(C(=C1C(=O)N)N)N1CC=CC=C1)C(=O)N)C(=C(C(=C%12C(=O)N)N1C=CC=CC1)N)C(=O)N
36		c12c3c4c5c6c7c3c3c2c2c8c9c1c1c%10c9c9c%11c8[C@]8%12c2c2c3[C@H]3c%13c2c2[C@@]8(c8c%11c%11[C@@H]9[C@H]9c%10c%10c(c41)[C@@]15[C@@]4(c5c%10c9c9c%11c%10c%11c9c5c5c4c6c([C@@H]73)c3c%13c(c%11c53)c2c8%10)C(=C(C(=C1C(=O)OC)N)N1CC=CC=C1)C(=O)OC)C(=C(C(=C%12C(=O)OC)N1C=CC=CC1)N)C(=O)OC

37		c12c3c4c5c6c7c3c3c2c2c8c9c1c1c%10c9c9c%11c8[C@]8%12c2c2c3[C@H]3c%13c2c2[C@@]8(c8c%11c%11[C@@H]9[C@H]9c%10c%10c(c41)[C@@]15[C@@]4(c5c%10c9c9c%11c%10c%11c9c5c5c4c6c([C@@H]73)c3c%13c(c%11c53)c2c8%10)N=C(C(=N1)F)F)N=C(C(=N%12)F)F
38		c12[C@@H]3[C@H]4[C@H]5[C@H]6[C@H]7[C@@H]3c3c2c2c8c9c1[C@@H]1[C@@H]%10c9c9c%11c8[C@]8%12c2c2c3[C@H]3c%13c2c2[C@@]8(c8c%11c%11[C@@H]9[C@H]9[C@@H]%10[C@H]%10[C@@H]([C@H]41)[C@@H]5[C@@H]1C4=C%10C9=C5c%11c9c%10[C@@H]5[C@@H]4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1c%13c(c%10[C@@H]41)c2c89)C(=C(C(=C%12O)c1ccccc1)O)O
39		c12[C@@H]3[C@H]4[C@H]5[C@H]6[C@H]7[C@@H]3c3c2c2c8c9c1[C@@H]1[C@@H]%10c9c9c%11c8[C@]8%12c2c2c3[C@H]3c%13c2c2[C@@]8(c8c%11c%11[C@@H]9[C@H]9[C@@H]%10[C@H]%10[C@@H]([C@H]41)[C@@H]5[C@@H]1[C@@H]4[C@H]%10[C@H]9[C@@H]5c%11c9c%10[C@@H]5[C@@H]4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1c%13c(c%10[C@@H]41)c2c89)C(=C(C(=C%12N)c1ccccc1)N)N
40		c12c3c4c5c6c7c3c3c2c2c8c9c1c1c%10c9c9c%11c8[C@]8%12c2c2c3[C@H]3c%13c2c2[C@@]8(c8c%11c%11[C@@H]9[C@H]9c%10c%10c(c41)[C@@]15[C@@]4(c5c%10c9c9c%11c%10c%11c9c5c5c4c6c([C@@H]73)c3c%13c(c%11c53)c2c8%10)CCCC1)CCCC%12
41		[C@H]12[C@@H]3[C@H]4[C@H]5[C@H]6[C@H]7[C@@H]3c3c2c2c8c9[C@@H]1[C@@H]1[C@@H]%10c9c9c%11c8[C@]8%12c2c2c3[C@H]3c%13c2c2[C@@]8(c8c%11c%11[C@@H]9[C@H]9[C@@H]%10[C@H]%10[C@@H]([C@H]41)[C@@H]5[C@@H]1[C@@H]4[C@H]%10[C@H]9[C@@H]5c%11c9c%10[C@@H]5[C@@H]4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1c%13c(c%10[C@@H]41)c2c89)C(=C(C(=C%12C(=O)O)Cc1c(c(c(c(c1O)O)O)O)O)O)C(=O)O
42		C(=O)(C1=C(C(=C([C@]23[C@@]41c1c5c6c7c8c9c%10c%11c%12c%13c%14c%10c(c59)c5c1c1c9c%10c%15c%16c%17c%18c%19c%20[C@@H]%21c%22c(c7c7c(c46)c4c2c(c%15c31)c%17c%19c4[C@H]%217)c8c%11c1c%22c%20c2[C@@]3([C@]%121C(=C(C(=C3C(=O)N)C(=O)N)C(=O)N)C(=O)N)c1c(c%182)c%16c%10c([C@@H]%14[C@@H]59)c%131)C(=O)N)C(=O)N)C(=O)N)N
43		c12[C@@H]3[C@H]4[C@H]5[C@H]6[C@H]7[C@@H]3c3c2c2c8c9c1[C@@H]1[C@@H]%10c9c9c%11c8[C@]8%12c2c2c3[C@H]3c%13c2c2[C@@]8(c8c%11c%11[C@@H]9[C@H]9[C@@H]%10[C@H]%10[C@

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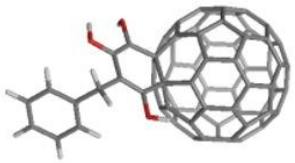
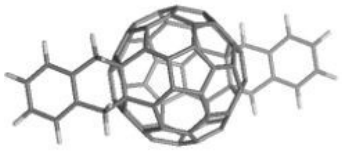
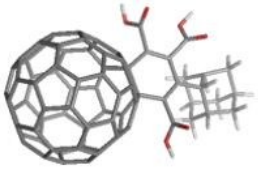
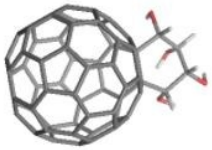
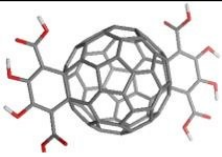
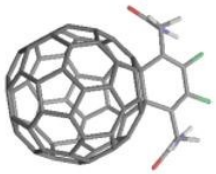
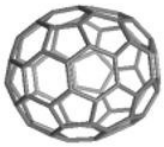
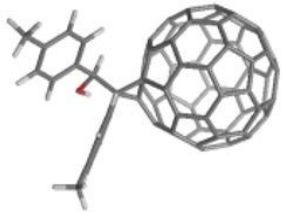
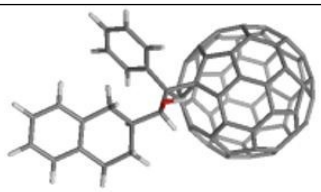
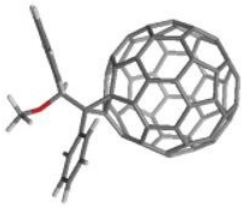
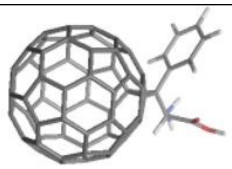
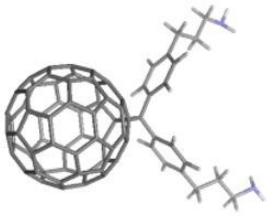
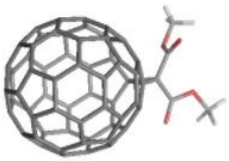
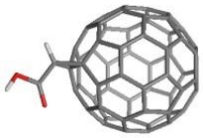
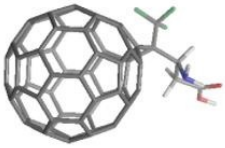
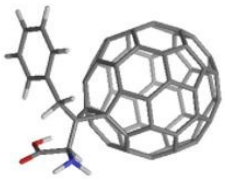
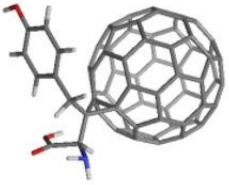
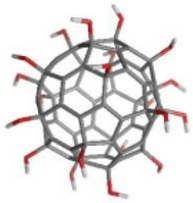
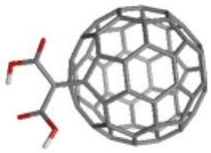
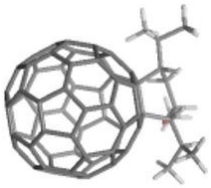
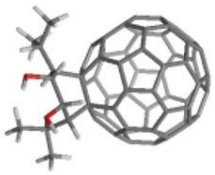
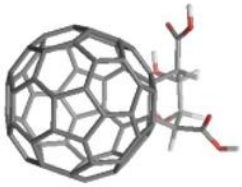
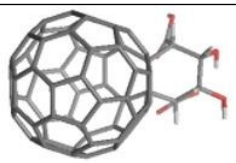
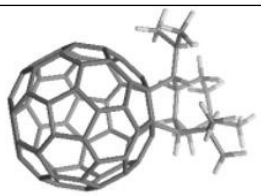
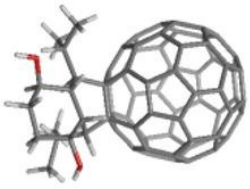
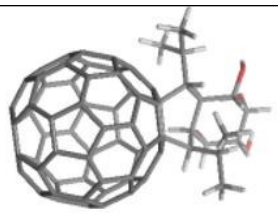
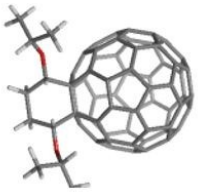
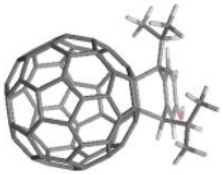
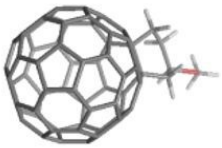
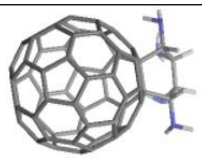
44		c12[C@@H]3[C@H]4[C@H]5[C@H]6[C@H]7[C@@H]3c3c2c2c8c9c1[C@@H]1C%10=C%11[C@@H]%12[C@@H]%13c(c%14c8[C@]8%15c2c2c3[C@H]3c%16c2c2[C@@]8(c8c%14c%13c%13[C@H]%14[C@@H]%12[C@H]%12C%11=C([C@H]41)[C@@H]5[C@@H]1[C@H]%12[C@@H]4[C@H]%14c5c%11c(c2c8c%135)c%16[C@@H]2[C@H]([C@@H]73)[C@H]6[C@H]1[C@H]4[C@H]%112)C(=C(C(=C%15O)Cc1ccccc1)O)O)c9%10
45		c12c3c4c5c6c7c3c3c2c2c8c9c1c1c%10c9c9c%11c8[C@]8%12c2c2c3[C@H]3c%13c2c2[C@@]8(c8c%11c%11[C@@H]9[C@H]9c%10c%10c(c41)[C@@]15[C@@]4(c5c%10c9c9c%11c%10c%11c9c5c5c4c6c([C@@H]73)c3c%13c(c%11c53)c2c8%10)Cc2c(cccc2)C1)Cc1c(C%12)cccc1
46		[C@H]12[C@@H]3[C@H]4[C@H]5[C@H]6[C@H]7[C@@H]3c3c2c2c8c9[C@@H]1[C@@H]1[C@@H]%10c9c9c%11c8[C@]8%12c2c2c3[C@H]3c%13c2c2[C@@]8(c8c%11c%11[C@@H]9[C@H]9[C@@H]%10[C@H]%10[C@@H]([C@H]41)[C@@H]5[C@@H]1[C@@H]4[C@H]%10[C@H]9[C@@H]5c%11c9[C@H]%10[C@@H]5[C@@H]4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1c%13c([C@@H]%10[C@@H]41)c2c89)C(=C(C(=C%12C(=O)O)[C@H]1[C@H]2C[C@H]3C[C@H]1C[C@@H](C2)C3)C(=O)O)C(=O)O
47		c12[C@@H]3[C@H]4[C@H]5[C@H]6[C@H]7[C@@H]3c3c2c2c8c9c1[C@@H]1[C@@H]%10c9c9c%11c8[C@]8%12c2c2c3[C@H]3c%13c2c2[C@@]8(c8c%11c%11[C@@H]9[C@H]9[C@@H]%10[C@H]%10[C@@H]([C@H]41)[C@@H]5[C@@H]1[C@@H]4[C@H]%10[C@H]9[C@@H]5c%11c9c%10[C@@H]5[C@@H]4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1c%13c(c%10[C@@H]41)c2c89)[C@@H]([C@@H]([C@@H]([C@@H]%12O)O)O)O)O
48		c12c3c4c5c6c7c3c3c2c2c8c9c1c1c%10c9c9c%11c8[C@]8%12c2c2c3[C@H]3c%13c2c2[C@@]8(c8c%11c%11[C@@H]9[C@H]9c%10c%10c(c41)[C@@]15[C@@]4(c5c%10c9c9c%11c%10c%11c9c5c5c4c6c([C@@H]73)c3c%13c(c%11c53)c2c8%10)C(=C(C(=C1C(=O)O)O)O)O)C(=O)O)C(=C(C(=C%12C(=O)O)O)O)C(=O)O.[H].[H]

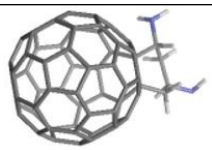
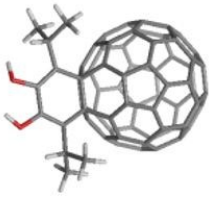
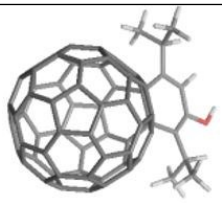
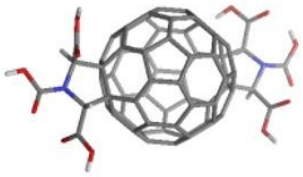
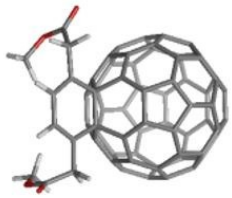
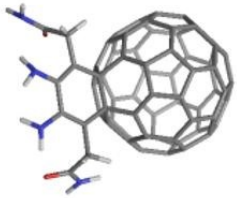
49		c12[C@@H]3[C@H]4[C@H]5[C@H]6[C@H]7[C@@H]3c3c2c2c8c9c1[C@@H]1[C@@H]%10c9c9c%11c8[C@]8%12c2c2c3[C@H]3c%13c2c2[C@@]8(c8c%11c%11[C@@H]9[C@H]9[C@@H]%10[C@H]%10[C@@H]([C@H]41)[C@@H]5[C@@H]1[C@@H]4[C@H]%10[C@H]9[C@@H]5c%11c9c%10[C@@H]5[C@@H]4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1c%13c(c%10[C@@H]41)c2c89)C(=C(C(=C%12CC(=O)N)F)F)CC(=O)N
50		[C@H]12[C@@H]3[C@H]4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3[C@@H]2[C@H]2[C@H]8[C@H]9[C@@H]1[C@@H]1[C@@H]%10[C@H]9[C@@H]9[C@@H]%11[C@H]8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%12[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%11[C@H]%11[C@@H]9[C@H]9[C@@H]%10[C@H]%10[C@@H]([C@H]41)[C@@H]5[C@@H]1[C@@H]4[C@H]%10[C@H]9[C@@H]5[C@H]%11[C@H]9[C@H]%10[C@@H]5[C@@H]4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%12[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89
51		c1c(ccc(c1)[C@@]1([C@]23c4c5c6c7c8c9c%10c%11c%12c%13c%14[C@H]%15[C@H]%16[C@H]%17[C@@H]%13[C@@H]%11[C@H]%11[C@H]%13[C@@H]%10[C@@H]8[C@H]8[C@H]%10[C@@H]7c5c5c7c4c4c3c(c%14c3c%12c9c6[C@]123)c%15c1c4c2c7[C@H]3[C@@H]4[C@@H]6[C@H]([C@@H]%10[C@@H]53)[C@H]8[C@H]%13[C@H]3[C@@H]6[C@@H]5[C@H]([C@@H]%17[C@@H]%113)[C@H]%16[C@H]1[C@H]2[C@H]45)[C@H](c1ccc(cc1)C)O)C
52		c1cccc(c1)[C@@]1([C@]23c4c5c6c7c8c9c%10c%11c%12c%13c%14[C@H]%15[C@H]%16[C@H]%17[C@@H]%13[C@@H]%11[C@H]%11[C@H]%13[C@@H]%10[C@@H]8[C@H]8[C@H]%10[C@@H]7c5c5c7c4c4c3c(c%14c3c%12c9c6[C@]123)c%15c1c4[C@@H]2[C@H]7[C@H]3[C@@H]4[C@@H]6[C@H]([C@@H]%10[C@@H]53)[C@H]8[C@H]%13[C@H]3[C@@H]6[C@@H]5[C@H]([C@@H]%17[C@@H]%113)[C@H]%16[C@H]1[C@H]2[C@H]45)[C@H]([C@H]1CCc2c(C1)cccc2)O
53		c1cccc(c1)[C@@]1([C@]23c4c5c6c7c8c9c%10c%11c%12c%13c%14[C@H]%15[C@H]%16[C@H]%17[C@@H]%13[C@@H]%11[C@H]%11[C@H]%13[C@@H]%10[C@@H]8[C@H]8[C@H]%10[C@@H]7c5c5c7c4c4c3c(c%14c3c%12c9c6[C@]123)c%15c1c4c2c7[C@H]3[C@@H]4[C@@H]6[C@H]([C@@H]%10[C@@H]53)[C@H]8[C@H]%13[C@H]3[C@@H]6[C@@H]5[C@H]([C@@H]%17[C@@H]%113)[C@H]%16[C@H]1[C@H]2[C@H]45)[C@H](c1ccccc1)OC

54		c1cccc(c1)[C@@]1([C@]23c4c5c6c7c8c9[C@@H]%10[C@@H]%11c%12c%13c%14[C@H]%15[C@H]%16[C@H]%17[C@@H]%13[C@@H]%11[C@H]%11[C@H]%13[C@@H]%10[C@@H]8[C@H]8[C@H]%10[C@@H]7c5c5c7c4c4c3c(c%14c3c%12c9c6[C@]123)c%15c1c4[C@@H]2[C@H]7[C@H]3[C@@H]4[C@@H]6[C@H]([C@@H]%10[C@@H]53)[C@H]8[C@H]%13[C@H]3[C@@H]6[C@@H]5[C@H]([C@@H]%17[C@@H]%113)[C@H]%16[C@H]1[C@H]2[C@H]45)[C@@H](N)C(=O)O
55		c1c(ccc(c1)C1([C@]23c4c5c6c7c8c9[C@@H]%10[C@@H]%11c%12c%13c%14[C@H]%15[C@H]%16[C@H]%17[C@@H]%13[C@@H]%11[C@H]%11[C@H]%13[C@@H]%10[C@@H]8[C@H]8[C@H]%10[C@@H]7c5c5c7c4c4c3c(c%14c3c%12c9c6[C@]123)c%15c1c4[C@@H]2[C@H]7[C@H]3[C@@H]4[C@@H]6[C@H]([C@@H]%10[C@@H]53)[C@H]8[C@H]%13[C@H]3[C@@H]6[C@@H]5[C@H]([C@@H]%17[C@@H]%113)[C@H]%16[C@H]1[C@H]2[C@H]45)c1ccc(cc1)CCCN)CCCN
56		C(=O)(C1([C@]23c4c5c6c7c8c9c%10c%11c%12c%13c%14C%15=C%16[C@H]%17[C@@H]%13[C@@H]%11[C@H]%11[C@H]%13[C@@H]%10[C@@H]8[C@H]8[C@H]%10[C@@H]7c5c5c7c4c4c3c(c%14c3c%12c9c6[C@]123)c%15c1c4c2c7[C@H]3[C@@H]4[C@@H]6[C@H]([C@@H]%10[C@@H]53)[C@H]8[C@H]%13[C@H]3[C@@H]6[C@@H]5[C@H]([C@@H]%17[C@@H]%113)[C@H]%16[C@H]1[C@H]2[C@H]45)C(=O)OC)OC
57		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)[C@H]%11C(=O)O
58		c12c3c4C5=C6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8C8=C%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)[C@@]%11([C@@H](N)CC(=O)O)C(F)(F)F

59		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3[C@@H]2[C@H]2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)[C@@]%11(Cc1ccccc1)[C@H](C(=O)O)N
60		[C@H]12[C@@H]3[C@H]4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3[C@@H]2[C@H]2[C@H]8[C@H]9[C@@H]1C1=C4C4=C%10[C@@]%11%12C%13=C%14C(=C9[C@@]1%11[C@]%12(C[C@@H]1CC[C@H](CC1)O)[C@H](C(=O)O)N)[C@@H]1[C@H]8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]9[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]1[C@@H]%14[C@H]1[C@H]%11[C@@H]%13[C@@H]%10[C@H]%10[C@@H]([C@H]54)[C@@H]4[C@@H]5C%10=C%11[C@H]%10[C@@H]%11[C@H]([C@@H]2[C@@H]8[C@@H]1%10)[C@H]9[C@H]([C@H]([C@@H]73)[C@H]64)[C@H]5%11
61		[C@@]12(C3=C4[C@@]5([C@@]6(C7=C8C9=C([C@@]37O)[C@@]3(C1=C1[C@@]7(C%10=C2[C@]4(C2=C4C%11=C%12C%13=C%14[C@]%15(C%16=C%17C(=C7[C@@]7(C%10=C2[C@]%11(C%14=C%1767)O)O)[C@]2(C1=C3[C@@]1(C3=C2[C@]%17(C2=C%15C7=C%10[C@@]2(C3=C([C@]91O)C1=C8[C@@]2(C(=C([C@@]%137O)[C@]%12(C(=C62)[C@@]54O)O)[C@@]%101O)O)O)O)O)O)O)O)O)O)O)O
62		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10[C@@H]5[C@@H]4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C%11(C(=O)O)C(=O)O
63		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@H]%10c9c9c%11c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%12[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%11c%11c9c9[C@@H](c%13c(c41)c5c1c4c%13c9c5c%11[C@H]9[C@H]%11c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%12[C@H]([C@@H]%11[C@@H]41)[C@@H]2[C@@H]89)[C@@H](C[C@@H]([C@@H]%10C(C)C)OC)C(C)C

64		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10[C@@H]5[C@@H]4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)[C@@H]([C@@H]([C@@H]([C@H]%11C(C)C)O)O)C(C)C
65		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8C8=C%13[C@H]%14[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4C1=C6C1=C5[C@@H]6[C@H]([C@@H]%10[C@@H]45)[C@H]([C@@H]%149)C%13=C4[C@H]([C@@H]28)[C@H]3[C@@H]([C@H]64)[C@H]71)[C@@H]([C@@H]([C@@H]([C@H]%11C(=O)O)O)O)C(=O)O
66		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)[C@H]([C@H]([C@H]([C@H]%11C(=O)O)O)O)C(=O)O
67		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)[C@@H]([C@@H]1[C@H]([C@H]%11C(C)C)C[C@@H](CC1)C)C(C)C
68		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)[C@@H]([C@@H]1[C@H]([C@H]%11C(C)C)[C@@H](CC[C@H]1O)O)C(C)C

69		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3[C@@H]2[C@H]2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)[C@@H]([C@@H]1[C@H]([C@H]%11C(C)C)[C@H]([C@H]([C@H]([C@H]1O)O)O)O)C(C)C
70		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3[C@@H]2[C@H]2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10[C@@H]5[C@@H]4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)[C@@H](CC[C@@H]%11OC(C)C)OC(C)C
71		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3[C@@H]2[C@H]2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)[C@@H](c1c([C@H]%11C(C)C)cc(cc1)O)C(C)C
72		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3[C@@H]2[C@H]2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10[C@@H]5[C@@H]4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)CC[C@H](C%11)OC
73		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)[C@@H]([C@@H]([C@@H]([C@@H]%11N)N)N)N

74		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)[C@@H](C[C@H](C%11)N)N
75		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@H]%10c9c9c%11c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%12[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%11c%11c9c9[C@@H](c%13c(c41)c5c1c4c%13c9c5c%11[C@H]9[C@H]%11c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%12[C@H]([C@@H]%11[C@@H]41)[C@@H]2[C@@H]89)/C(=C(\C(=C/%10\C(C)C)\O)/O)/C(C)C
76		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@H]%10c9c9c%11c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%12[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%11c%11c9c9[C@@H](c%13c(c41)c5c1c4c%13c9c5c%11[C@H]9[C@H]%11c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%12[C@H]([C@@H]%11[C@@H]41)[C@@H]2[C@@H]89)/C(=C\C(=C/%10\C(C)C)\O)/C(C)C
77		c12c3c4[C@H]5[C@H]6c7c3c3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8c8c2c2c3c3[C@@]%13%14c2c2c8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12c9c%10c5c4c4c1c6c(c73)c1[C@@]%13(c(c%10c41)c2c89)[C@H](N([C@H]%14C(=O)O)C(=O)O)C(=O)O)[C@@H](N([C@H]%11C(=O)O)C(=O)O)C(=O)O
78		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C(=CC=C%11CC(=O)OC)CC(=O)OC
79		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]

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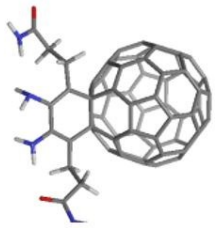
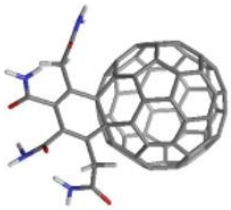
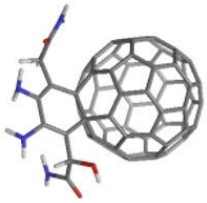
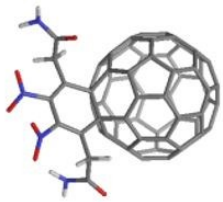
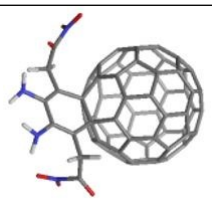
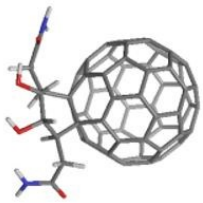
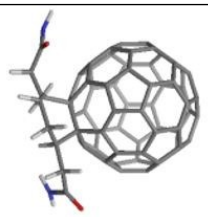
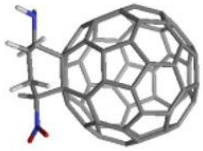
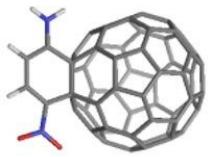
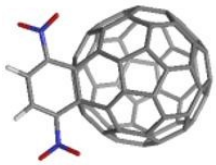
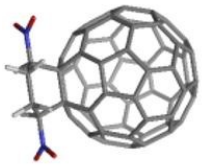
80		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C(=C(C(=C%11CCC(=O)N)N)N)CCC(=O)N
81		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C(=C(C(=C%11CC(=O)N)C(=O)N)C(=O)N)CC(=O)N
82		[C@H]12[C@@H]3[C@H]4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3C2=C2[C@H]8[C@H]9[C@@H]1C1=C4C4=C%10[C@@H]%11C%12=C%13C(=C9[C@H]1/C(=C(\C(=C/%11\[C@@H](C(=O)N)O)\N)/N)/[C@@H](C(=O)N)O)[C@@H]1[C@H]8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]9[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]1[C@@H]%13[C@H]1[C@H]%11[C@@H]%12[C@@H]%10[C@H]%10[C@@H]([C@H]54)[C@@H]4[C@@H]5C%10=C%11[C@H]%10[C@@H]%11[C@H]([C@@H]2[C@@H]8[C@@H]1%10)[C@H]9[C@H]([C@H]([C@@H]73)[C@H]64)[C@H]5%11
83		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C(=C(C(=C%11CC(=O)N)N(=O)=O)N(=O)=O)CC(=O)N
84		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C(=C(C(=C%11CC=O)N)N)CC(=O)N(=O)=O.[N](=O)=O

85		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)[C@H]([C@@H]([C@@H]([C@H]%11CC(=O)N)O)O)CC(=O)N
86		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)[C@H](CC[C@H]%11CC(=O)N)CC(=O)N
87		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3[C@@H]2[C@H]2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10[C@@H]5[C@@H]4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)[C@H](CC[C@H]%11N)N(=O)=O
88		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@H]%10c9c9c%11c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%12[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%11c%11c9c9[C@@H](c%13c(c41)c5c1c4c%13c9c5c%11[C@H]9[C@H]%11c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%12[C@H]([C@@H]%11[C@@H]41)[C@@H]2[C@@H]89)/C(=C\C=C/%10\N)/N(=O)=O
89		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C(=CC=C%11N(=O)=O)N(=O)=O
90		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3[C@@H]2[C@H]2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%1

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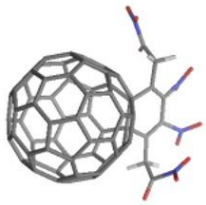
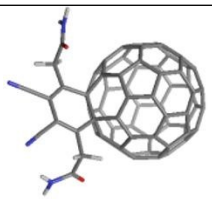
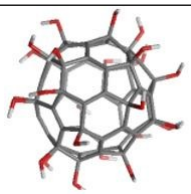
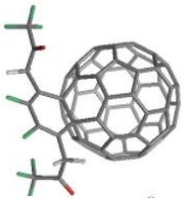
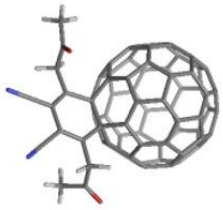
91		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C(=C(C(=C%11CC=O)N(=O)=O)N(=O)=O)CC(=O)N(=O)=O.[N](=O)=O
92		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C(=C(C(=C%11CC(=O)N)C#N)C#N)CC(=O)N
93		C12=C3[C@]4([C@]5([C@]6(C7=C3[C@]3([C@@]2(C2=C8[C@@]9(C3=C3C%10=C%11C%12=C%13[C@]%14(C%15=C([C@@]8(C8=C%16[C@]%17(C%18=C%19[C@@]%20(C%21=C%17[C@]([C@@]%15%16O)(C%15=C%14C%14=C%16[C@@]%15(C%21=C%15[C@@]%20(C(=C4[C@@]%19(C1=C%18[C@]28O)O)C5=C1[C@]%15([C@]%16(C2=C([C@@]%12%14O)[C@]%11(C(=C6[C@]12O)[C@@]73O)O)O)O)O)O)O)O)O)[C@@]%13([C@]9%10O)O)O)O)O)O)O)O)O
94		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C(=C(C(=C%11CC(=O)C(F)(F)F)F)F)CC(=O)C(F)(F)F
95		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]

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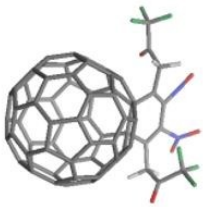
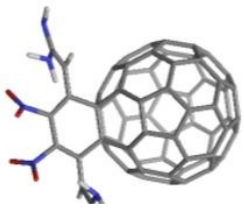
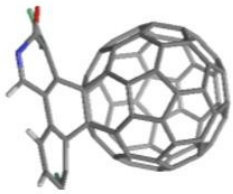
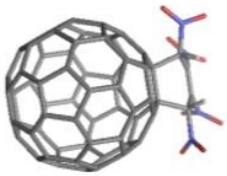
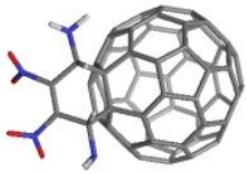
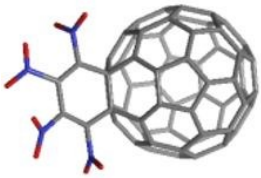
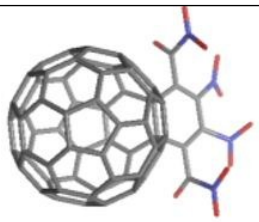
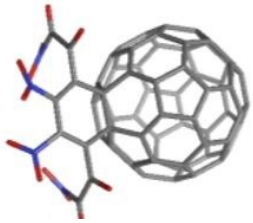
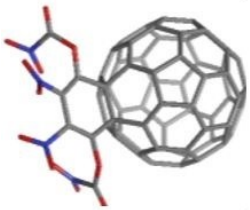
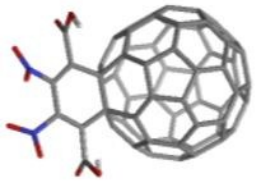
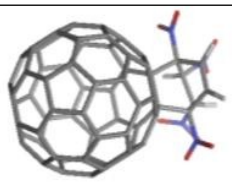
96		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C(=C(C(=C%11CC(=O)C(F)(F)F)N(=O)=O)N(=O)=O)CC(=O)C(F)(F)F
97		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C(=C(C(=C%11C=C(N)N)[N](=O)O)N(=O)=O)C=C(N)N
98		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C1=C(C2=C%11C(=C(F)F)C(=O)N=C2)C=CC(=O)C1=C(F)F
99		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10[C@@H]5[C@@H]4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)[C@H](C(=C([C@H]%11N(=O)=O)N(=O)=O)N(=O)=O)N(=O)=O
100		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)[C@H](C(=C([C@H]%11N)N(=O)=O)N(=O)=O)N

101		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C(=C(C(=C%11N(=O)=O)N(=O)=O)N(=O)=O)N(=O)=O
102		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8c8c%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12c9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13C(=C2c89)[C@@H]%10[C@@H]41)C(=C(C(=C%11C=O)N(=O)=O)N(=O)=O)C(=O)N(=O)=O.[N](=O)=O
103		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8C8=C%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C(=C(C(=C%11C(=O)C(=O)N(=O)=O)N(=O)=O)N(=O)=O)C(=O)C(=O)N(=O)=O
104		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8C8=C%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C(=C(C(=C%11OC(=O)N(=O)=O)N(=O)=O)N(=O)=O)OC(=O)N(=O)=O
105		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C(=C(C(=C%11C(=O)O)N(=O)=O)N(=O)=O)C(=O)O
106		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[

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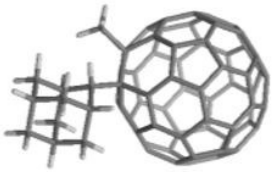
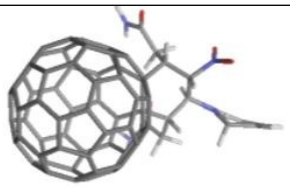
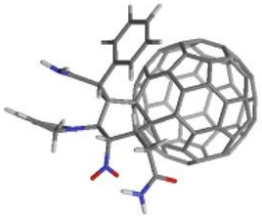
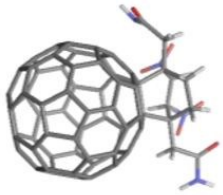
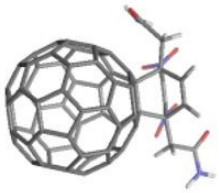
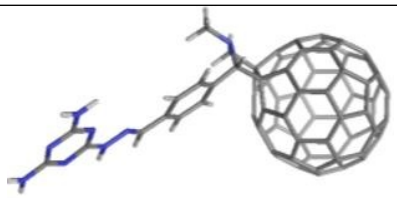
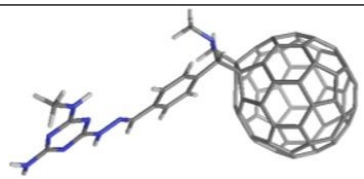
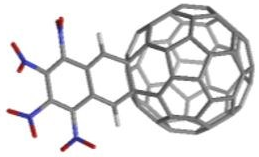
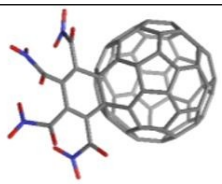
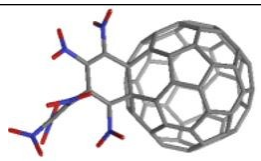
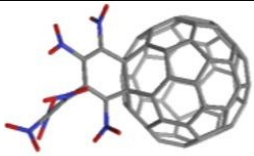
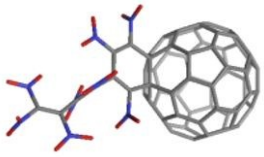
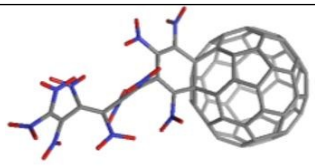
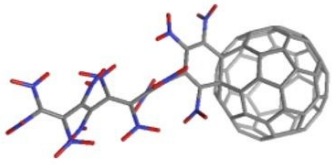
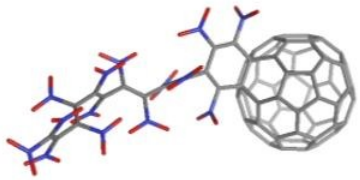
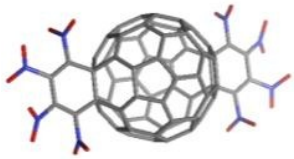
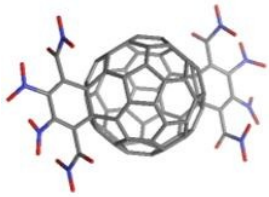
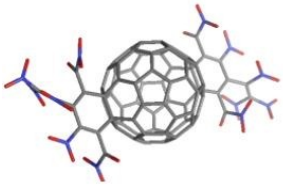
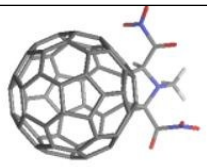
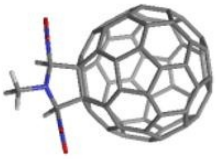
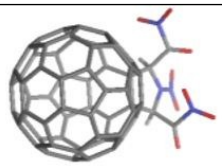
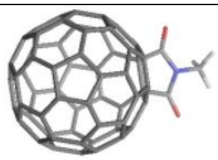
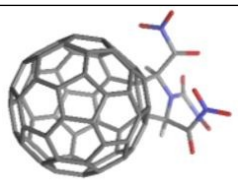
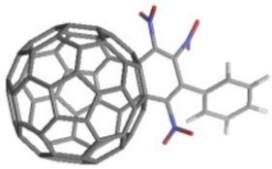
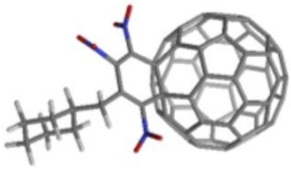
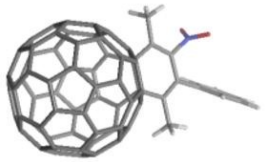
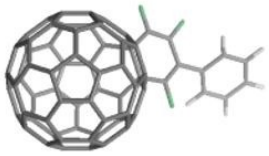
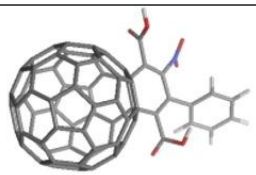
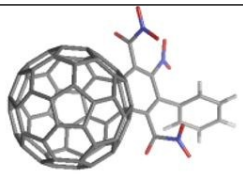
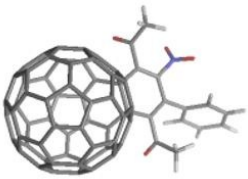
107		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3[C@@H]2[C@H]2c8c9c1c1[C@@]%10(c9c9c%11c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%12[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%11c%11c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%11[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%12[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)[C@@H]1[C@@H]2C[C@@H]3C[C@H]1C[C@@H](C3)C2)C
108		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3[C@@H]2[C@H]2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)[C@H]([C@@H]([C@H]([C@H]%11CC(=O)N)N(=O)=O)N1C=CC=CC1)CC(=O)N
109		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10[C@@H]5[C@@H]4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)[C@@H]([C@@H]([C@H]([C@H]%11CC(=O)N)N(=O)=O)N1C=CC=CC1)[C@H](C(=O)N)c1ccccc1
110		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)[C@]1([C@@H]([C@H]([C@]%11(CC(=O)N)CC1)N(=O)=O)N(=O)=O)CC(=O)N

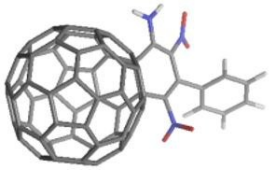
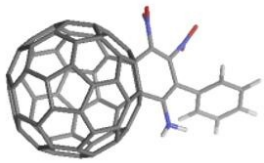
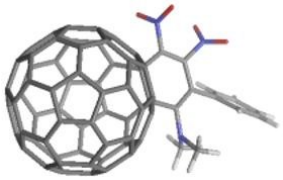
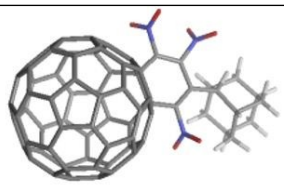
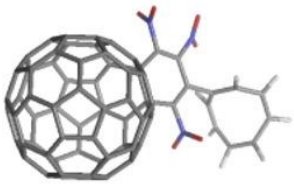
111		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10[C@@H]5[C@@H]4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)[C@]1(C(=C([C@]%11(CC(=O)N)C=C1)N(=O)=O)N(=O)=O)CC(=O)N
112		c1(nc(nc(n1)N)N)N/N=C/c1ccc([C@H]2[C@@]34c5c6c7c8c9c%10[C@H]%11[C@H]%12[C@H]%13[C@@H]9[C@H]9c8c8c6c6c%14c5c5c%15[C@@]3(c3c(c%10c47)c%11c4c7c3c%15c3c%10c5[C@H]%14[C@@H]5[C@@H]%11[C@H]6[C@H]8[C@@H]6[C@H]9[C@H]8[C@H]9[C@@H]6[C@@H]%11[C@H]6[C@@H]5[C@@H]%10[C@H]5[C@@H]3[C@@H]7[C@H]3[C@@H]4[C@@H]%12[C@@H]([C@@H]%138)[C@H]4[C@@H]9[C@@H]6[C@@H]5[C@@H]34)CN2C)cc1
113		c1(nc(nc(n1)NC)N)N/N=C/c1ccc([C@H]2[C@@]34c5c6c7c8c9c%10[C@H]%11[C@H]%12[C@H]%13[C@@H]9[C@H]9c8c8c6c6c%14c5c5c%15[C@@]3(c3c(c%10c47)c%11c4c7c3c%15c3c%10c5[C@H]%14[C@@H]5[C@@H]%11[C@H]6[C@H]8[C@@H]6[C@H]9[C@H]8[C@H]9[C@@H]6[C@@H]%11[C@H]6[C@@H]5[C@@H]%10[C@H]5[C@@H]3[C@@H]7[C@H]3[C@@H]4[C@@H]%12[C@@H]([C@@H]%138)[C@H]4[C@@H]9[C@@H]6[C@@H]5[C@@H]34)CN2C)cc1
114		c12c3c4c5c6c7c3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3C3=C7[C@H]7[C@H]%13[C@@H]%14C%15=C%16c%17c(c%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12c%17[C@H]9c5c4[C@@H]([C@@H]1[C@@H]67)[C@@H]%13[C@@H]%159)C=c1c(=C%11)c(c(c(c1N(=O)=O)N(=O)=O)N(=O)=O)N(=O)=O)[C@H]8[C@@H]%16[C@H]2[C@H]3%14
115		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C(=C(C(=C%11C(=O)N(=O)=O)C(=O)N(=O)=O)C(=O)N(=O)=O)C=O.[N](=O)=O

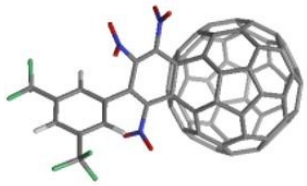
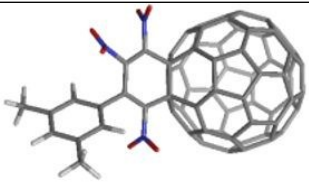
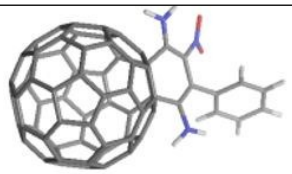
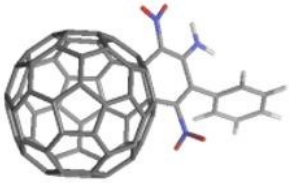
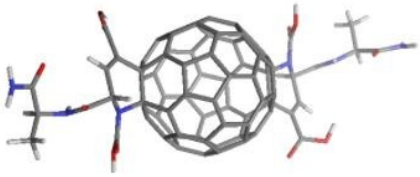
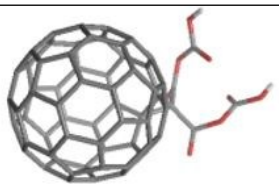
116		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C(=C(C(=C%11N(=O)=O)N(=O)=O)C(=C(N(=O)=O)N(=O)=O)N(=O)=O)N(=O)=O
117		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C(=C(C(=C%11N(=O)=O)C(=C(N(=O)=O)N(=O)=O)N(=O)=O)N(=O)=O)N(=O)=O
118		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3[C@@H]2[C@H]2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C(=C(C(=C%11N(=O)=O)/C(=C(/C(=C(N(=O)=O)N(=O)=O)N(=O)=O)\N(=O)=O)/N(=O)=O)N(=O)=O)N(=O)=O
119		c12c3c4C5=C6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C(=C(C(=C%11N(=O)=O)/C(=C(/C(=C(\N(=O)=O)/C(=C(N(=O)=O)N(=O)=O)N(=O)=O)/N(=O)=O)\N(=O)=O)/N(=O)=O)N(=O)=O)N(=O)=O
120		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3[C@@H]2[C@H]2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C(=C(C(=C%11N(=O)=O)/C(=C(/C(=C(\N(=O)=O)/C(=C(/

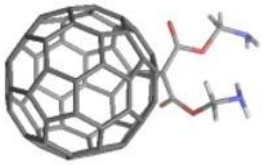
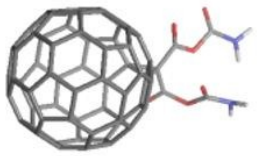
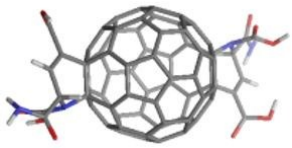
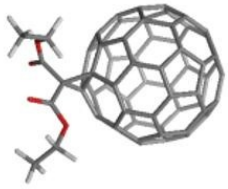
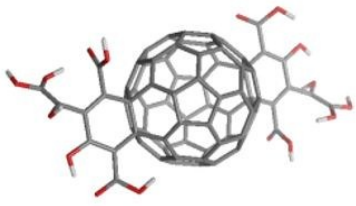
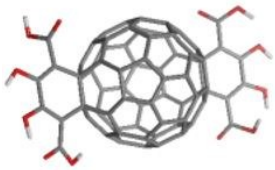
		C(=C(N(=O)=O)N(=O)=O)N(=O)=O)\N(=O)=O)/N(=O)=O)/N(=O)=O)\N(=O)=O)/N(=O)=O)N(=O)=O)N(=O)=O
121		c12c3c4[C@H]5[C@H]6C7=C3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3C3=C7[C@H]7[C@H]%13[C@@H]%14[C@@H]%15[C@H]%16[C@@H]%17c%18c%19c%20c([C@@]%10(c%10c(c41)c5c1c(c%20%10)c%18[C@@H]([C@@H]1[C@@H]67)[C@@H]%13%16)C(=C(C(=C%11N(=O)=O)/C(=C(/C(=C(/C(=C(/C(=C(/C(=C(N(=O)=O)N(=O)=O)N(=O)=O)\N(=O)=O)/N(=O)=O)\N(=O)=O)/N(=O)=O)\N(=O)=O)/N(=O)=O)\N(=O)=O)/N(=O)=O)N(=O)=O)N(=O)=O)c9c1[C@H]%12[C@@H]4[C@H]8[C@@H]([C@H]%15[C@@H]4[C@H]%17c%191)[C@H]2[C@H]3%14
122		c12c3c4[C@H]5[C@H]6c7c3c3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8c8c2c2c3c3[C@@]%13%14c2c2c8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12c9c%10c5c4c4c1c6c(c73)c1[C@@]%13(c(c%10c41)c2c89)C(=C(C(=C%14N(=O)=O)N(=O)=O)N(=O)=O)N(=O)=O)C(=C(C(=C%11N(=O)=O)N(=O)=O)N(=O)=O)N(=O)=O
123		c12c3c4c5c6c7c3c3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8c8c2c2c3c3[C@@]%13%14c2c2c8c8c%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12c9c%10c5c4c4c1c6c(c73)c1[C@@]%13(c(c%10c41)c2c89)C(=C(C(=C%14C(=O)N(=O)=O)N(=O)=O)N(=O)=O)C(=O)N(=O)=O)C(=C(C(=C%11C(=O)N(=O)=O)N(=O)=O)N(=O)=O)C=O.[N](=O)=O
124		c12c3c4[C@H]5[C@H]6c7c3c3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8c8c2c2c3c3[C@@]%13%14c2c2c8c8c%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12c9c%10c5c4c4c1c6c(c73)c1[C@@]%13(c(c%10c41)c2c89)C(=C(C(=C%14C(=O)N(=O)=O)N(=O)=O)C(=C(N(=O)=O)N(=O)=O)N(=O)=O)C(=O)N(=O)=O)C(=C(C(=C%11C(=O)N(=O)=O)C(=C(N(=O)=O)N(=O)=O)N(=O)=O)N(=O)=O)C(=O)N(=O)=O
125		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)[C@H](N([C@H]%11C(=O)N(=O)=O)C)C(=O)N(=O)=O

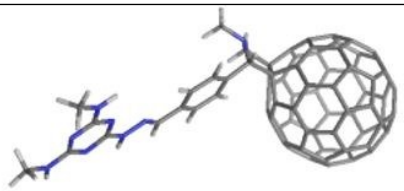
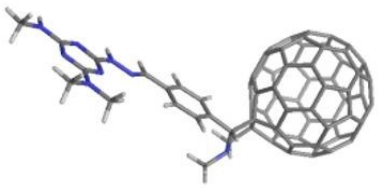
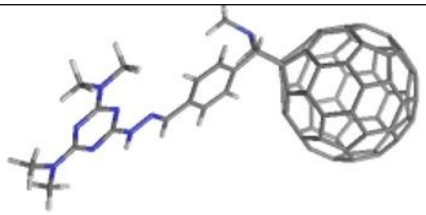
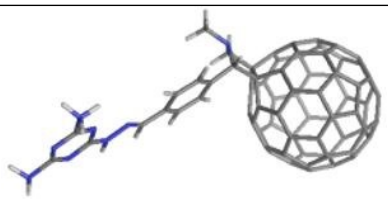
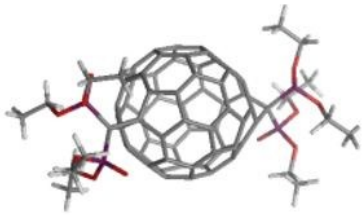
126		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)[C@H](N([C@H]%11N(=O)=O)C)N(=O)=O
127		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8C8=C%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)[C@H](N([C@H]%11C(=O)N(=O)=O)N(=O)=O)C(=O)N(=O)=O
128		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3[C@@H]2[C@H]2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10[C@@H]5[C@@H]4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C(=O)N(C%11=O)C
129		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8C8=C%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)[C@H](N([C@H]%11C(=O)N(=O)=O)C(=O)N(=O)=O)C(=O)N(=O)=O
130		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C(=C(C(=C%11N(=O)=O)c1ccccc1)N(=O)=O)N(=O)=O
131		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[

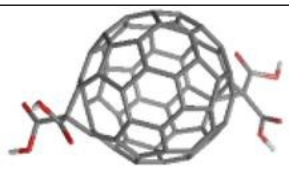
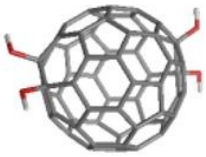
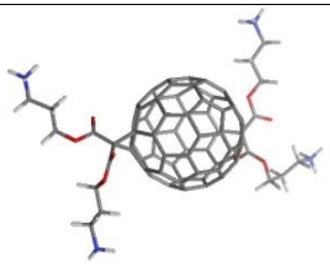
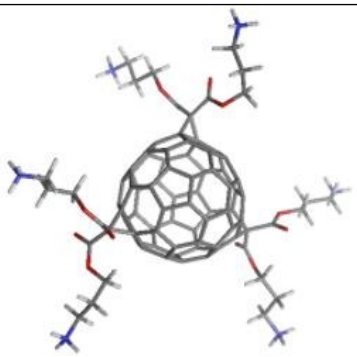
		C@H]%10c5c4[C@H]4C1=C6C(=C1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)[C@@H]73)C(=C(C(=C%11N(=O)=O)CC1CCCCC1)N(=O)=O)N(=O)=O
132		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C(=C(C(=C%11C)c1ccccc1)N(=O)=O)C
133		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12C9=C8C2=C2[C@H]8[C@@H]9c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@@H]([C@@H]%132)[C@@H]84)C(=C(C(=C%11F)c1ccccc1)F)F
134		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C(=C(C(=C%11C(=O)O)c1ccccc1)N(=O)=O)C(=O)O
135		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8C8=C%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C(=C(C(=C%11C=O)c1ccccc1)N(=O)=O)C(=O)N(=O)=O.[N](=O)=O
136		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C(=C(C(=C%11C(=O)C)c1ccccc1)N(=O)=O)C(=O)C

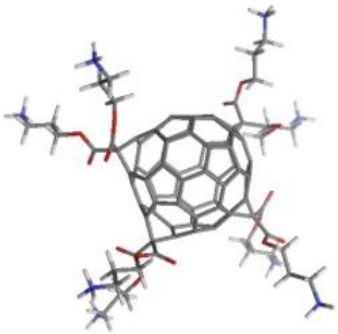
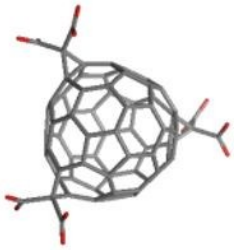
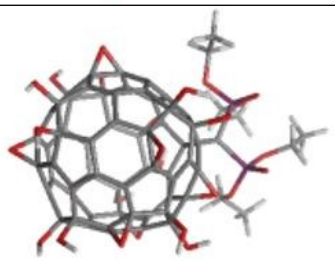
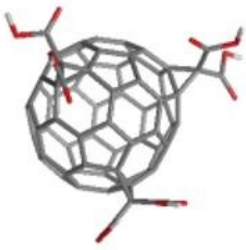
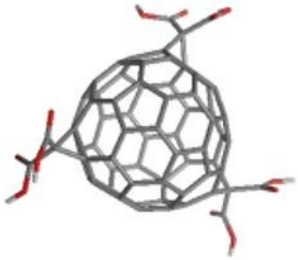
137		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4C1=C6C(=C1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)[C@@H]73)C(=C(C(=C%11N(=O)=O)c1ccccc1)[N](=O)O)N
138		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C(=C(C(=C%11N)c1ccccc1)N(=O)=O)N(=O)=O
139		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C(=C(C(=C%11N(C)C)c1ccccc1)N(=O)=O)N(=O)=O
140		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C(=C(C(=C%11N(=O)=O)[C@H]1[C@@H]2C[C@@H]3C[C@H]1C[C@H](C2)C3)N(=O)=O)N(=O)=O
141		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C(=C(C(=C%11N(=O)=O)C1=CC=CC=CC=C1)N(=O)=O)N(=O)=O

142		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C(=C(C(=C%11N(=O)=O)c1cc(cc(c1)C(F)(F)F)C(F)(F)F)N(=O)=O)N(=O)=O
143		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8C8=C%13[C@H]%14[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@H]1[C@@H]7[C@H]5[C@@H]3[C@@H]([C@@H]28)C2=C%13[C@@H]([C@@H]%149)[C@H]3[C@@H]%10[C@@H]4[C@@H]1[C@H]3[C@@H]52)C(=C(C(=C%11N(=O)=O)c1cc(cc(c1)C)C)N(=O)=O)N(=O)=O
144		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3[C@@H]2[C@H]2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C(=C(C(=C%11N)c1ccccc1)[N](=O)O)N
145		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3[C@@H]2[C@H]2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12[C@H]%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5[C@H]%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C(=C(C(=C%11N(=O)=O)C1CCCCC1)N)[N](=O)O
146		c12c3c4[C@H]5[C@H]6c7c3c3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8c8c2c2c3c3[C@@]%13%14c2c2c8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12c9c%10c5c4c4c1c6c(c73)c1[C@@]%13(c(c%10c41)c2c89)C(=C[C@H](N%14C(=O)O)C(=O)N[C@@H](C)C(=O)N)C(=O)O)N([C@H](C=C%11C(=O)O)C(=O)N[C@H](C(=O)N)C)C(=O)O
147		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[

		C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89C%11(C(=O)OC(=O)O)C(=O)OC(=O)O
148		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8C8=C%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C%11(C(=O)OCN)C(=O)OCN
149		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8C8=C%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10c5c4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C%11(C(=O)OC(=O)N)C(=O)OC(=O)N
150		c12c3c4[C@H]5[C@H]6c7c3c3c2c2c8c9c1c1[C@H]%10c9c9c%11c8c8c2c2c3c3[C@@]%12%13c2c2c8[C@H]8[C@@H]%11c%11c9c9[C@@H](c%14c(c41)c5c1c4c%14c9c5c%11c9c%11c5c4c4c1c6c(c73)c1[C@@]%12(c(c%11c41)c2c89)C(=C[C@H](N%13C(=O)O)C(=O)N)C(=O)O)N([C@H](/C=C\%10/C(=O)O)C(=O)N)C(=O)O
151		c12c3c4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3[C@@H]2[C@H]2c8c9c1c1[C@]%10%11c9c9c%12c8[C@@H]8[C@H]2[C@@H]2[C@H]3[C@H]3[C@H]%13[C@@H]2[C@H]2[C@@H]8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12[C@H]9[C@H]%10[C@@H]5[C@@H]4[C@H]4[C@@H]1[C@@H]6[C@@H]([C@@H]73)[C@H]1[C@@H]%13[C@H]([C@@H]%10[C@@H]41)[C@@H]2[C@@H]89)C%11(C(=O)OCC)C(=O)OCC
152		c12c3c4[C@H]5[C@H]6c7c3c3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8c8c2c2c3c3[C@@]%13%14c2c2c8[C@H]8[C@@H]%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12c9c%10c5c4c4c1c6c(c73)c1[C@@]%13(c(c%10c41)c2c89)C(=C(C(=C%14C(=O)O)O)C(=C(O)O)O)C(=O)O)C(=C(C(=C%11C(=O)O)C(=C(O)O)O)O)C(=O)O
153		c12c3c4[C@H]5[C@H]6c7c3c3c2c2c8c9c1c1[C@H]%10c9c9c%11c8c8c2c2c3c3[C@@]%12%13c2c2c8[C@H]8[C@@H]%11c%11c9c9[C@@H](c%14c(c41)c5c1c4c%14c9c5c%11c9c%11c5c4c4c1c6c(c73)c1[C@@]%12(c(c%11c41)c2c89)C(=C(C(=C%13C(=O)O)O)O)

		C(=O)O)/C(=C(\C(=C/%10\C(=O)O)\O)/O)/C(=O)O.[H]
154		c1(nc(nc(n1)NC)NC)N/N=C/c1ccc([C@H]2[C@@]34c5c6c7c8c9c%10[C@H]%11[C@H]%12[C@H]%13[C@@H]9[C@H]9[C@@H]8[C@H]8c6c6c%14c5c5c%15[C@@]3(c3c(c%10c47)c%11c4c7c3c%15c3c%10c5[C@H]%14[C@@H]5[C@@H]%11[C@H]6[C@H]8[C@@H]6[C@H]9[C@H]8[C@H]9[C@@H]6[C@@H]%11[C@H]6[C@@H]5[C@@H]%10[C@H]5[C@@H]3[C@@H]7[C@H]3[C@@H]4[C@@H]%12[C@@H]([C@@H]%138)[C@H]4[C@@H]9[C@@H]6[C@@H]5[C@@H]34)CN2C)cc1
155		c1(nc(nc(n1)N(C)C)NC)N/N=C/c1ccc([C@H]2[C@@]34c5c6c7c8c9c%10[C@H]%11[C@H]%12[C@H]%13[C@@H]9[C@H]9[C@@H]8[C@H]8c6c6c%14c5c5c%15[C@@]3(c3c(c%10c47)c%11c4c7c3c%15c3c%10c5[C@H]%14[C@@H]5[C@@H]%11[C@H]6[C@H]8[C@@H]6[C@H]9[C@H]8[C@H]9[C@@H]6[C@@H]%11[C@H]6[C@@H]5[C@@H]%10[C@H]5[C@@H]3[C@@H]7[C@H]3[C@@H]4[C@@H]%12[C@@H]([C@@H]%138)[C@H]4[C@@H]9[C@@H]6[C@@H]5[C@@H]34)CN2C)cc1
156		c1(nc(nc(n1)N(C)C)N(C)C)N/N=C/c1ccc([C@H]2[C@@]34c5c6c7c8c9c%10[C@H]%11[C@H]%12[C@H]%13[C@@H]9[C@H]9[C@@H]8[C@H]8c6c6c%14c5c5c%15[C@@]3(c3c(c%10c47)c%11c4c7c3c%15c3c%10c5[C@H]%14[C@@H]5[C@@H]%11[C@H]6[C@H]8[C@@H]6[C@H]9[C@H]8[C@H]9[C@@H]6[C@@H]%11[C@H]6[C@@H]5[C@@H]%10[C@H]5[C@@H]3[C@@H]7[C@H]3[C@@H]4[C@@H]%12[C@@H]([C@@H]%138)[C@H]4[C@@H]9[C@@H]6[C@@H]5[C@@H]34)CN2C)cc1
157		c1(=[NH]/N=C/[C@@H]2C=C[C@@H]([C@H]3[C@@]45c6c7c8c9c%10c%11[C@H]%12[C@H]%13[C@H]%14[C@@H]%10[C@H]%10c9c9c7c7c%15c6c6c%16[C@@]4(c4c(c%11c58)c%12c5c8c4c%16c4c%11c6[C@H]%15[C@@H]6[C@@H]%12[C@H]7[C@H]9[C@@H]7[C@H]%10[C@H]9[C@H]%10[C@@H]7[C@@H]%12[C@H]7[C@@H]6[C@@H]%11[C@H]6c4c8[C@H]4[C@@H]5[C@@H]%13[C@@H]([C@@H]%149)[C@H]5[C@@H]%10[C@@H]7[C@@H]6[C@@H]45)CN3C)C=C2)nc([nH]c(n1)[NH3])[NH3]
158		C12=C3[C@@H]4[C@@H]5C6=C2C2=C7[C@H]8[C@@H]6C6=C9[C@@]%10%11[C@]%12(C(=C56)[C@H]5[C@@H]4C4=C6[C@@H]%13[C@H]5C%12=C5[C@H]%12[C@@H]%13C%13=C%14[C@H]%15[C@@H]%16[C@@H]%17[C@H]%18[C@@H]([C@H]2[C@H]1[C@H]([C@@H]([C@@H]%16[C@H]6%13)[C@H]34)C%17(P(=O)(OCC)OCC)P(=O)(OCC)OCC)C1=C7C2=C3[C@@H]4[C@H]6[C@H](C%12=C%14

		[C@H]7C%15=C%18[C@@H]1[C@@H]3[C@@H]67)C5=C%10[C@@H]4[C@H]9[C@H]82)C%11(P(=O)(OCC)OCC)P(=O)(OCC)OCC
159		c12C3=C4[C@H]5[C@@H]6[C@@H]7C8=C9c%10c(c1[C@@H]59)c1c5c2C2=C9[C@H]%11[C@@H]5C5=C%12[C@@]%13%14[C@]%15(c(c%10[C@H]%10[C@@H]8[C@@H]8[C@@H]%16C(=C%15%10)C%10=C%13[C@H]%13[C@H]%15[C@H]%17[C@@H]%10C%16=C%10C(=C78)[C@H]7[C@@H]6C(=C6[C@@H]([C@@H]32)[C@@H]2C3=C(C%15=C([C@@H]%11[C@@H]%12%13)[C@H]92)[C@@H]%17[C@@H]%10C7=C63)C4(C(=O)O)C(=O)O)c15)C%14(C(=O)O)C(=O)O
160		C12=C3[C@@H]4[C@@H]5[C@@H]6[C@H]2c2c7=C1[C@]1([C@]8(C9=c7c7[C@H]%10[C@H]%11[C@@H]%12[C@@H]%13[C@H]%14[C@@H]%15C%16=C%17[C@H]%18[C@H]%19[C@@H]%20[C@@H]%21[C@H]%22[C@@H]([C@H]4[C@@H]4C%23=C5C5=C%24[C@]%25([C@@]%23(C(=C([C@H]%16%20)C%15=C%25[C@@H]%13[C@H]%24[C@@H]%13[C@H]([C@@H]65)c2c7[C@H]%12%13)[C@H]%214)O)O)C3=C1[C@H]([C@@H]%19%22)C8=C%18C(=C9%10)[C@H]%17[C@@H]%11%14)O)O
161		C(CC[NH3])OC(=O)C1([C@@H]2[C@H]3C4=C5[C@@H]6[C@@H]7C8=C4C4=C9[C@H]%10[C@@H]8C8=C%11[C@@]%12%13[C@]%14(C(=C78)[C@H]7[C@@H]6C6=C8[C@@H]%15[C@H]7C%14=C7[C@H]%14[C@@H]%15C%15=C%16[C@H]%17[C@H]([C@@H]1[C@H]1[C@@H]([C@@H]34)[C@@H]3[C@H]4[C@H]%18C%19=C([C@@H]%10[C@@H]%11[C@H]%10C%12=C7[C@H]7C%14=C%16[C@@H](C%17=C14)[C@@H]%18[C@H]7[C@@H]%19%10)[C@H]93)[C@H]([C@H]2[C@H]56)[C@H]8%15)C%13(C(=O)OCCC[NH3])C(=O)OCCC[NH3])C(=O)OCCC[NH3]
162		[C@H]12[C@@H]3[C@H]4C5=C6[C@H]7[C@@H]3C3=C8[C@@]9%10[C@]%11(C(=C23)[C@H]2[C@H]3[C@@H]1C1=C4C4=C%12[C@@]%13%14C%15=C%16C(=C3[C@@]1%13C%14(C(=O)OCCC[NH3])C(=O)OCCC[NH3])[C@@H]1[C@H]2C%11=C2[C@H]3[C@@H]1[C@@H]%16[C@H]1[C@H]%11[C@@H]%15[C@@H]%12[C@H]%12[C@@H]([C@H]54)[C@@H]4[C@@H]5C%12=C%11[C@H]%11[C@@H]%12[C@@H]%13[C@H](C3=C1%11)C2=C9[C@H]1[C@@H]%13[C@H]([C@H](C7=C81)[C@H]64)C([C@H]5%12)(C(=O)OCCC[NH3])C(=O)OCCC[NH3])C%10(C(=O)OCCC[NH3])C(=O)OCCC[NH3]

163		C12=C3[C@@H]4[C@@H]5[C@@H]6[C@@H]([C@@H]7[C@@H]8[C@H]2C2=C9C%10=C8C8=C%11[C@@]%12%13[C@]%14(C(=C78)[C@@H]6C6=C7[C@@H]5[C@H]5[C@H]8[C@@H]4[C@H]4[C@@H]1[C@@H]2[C@@H]1[C@@H]2[C@@H]([C@H]8[C@@H]8C%15=C5[C@H]7[C@@H]5C(=C%146)C6=C%12C7=C%12[C@@]%14%16[C@@]6(C5=C%15C5=C%14[C@@H]6[C@H]%12[C@H]([C@@H]%10[C@@H]%117)C9=C1[C@@H]6[C@H]2[C@H]85)C%16(C(=O)OCCC[NH3])C(=O)OCCC[NH3])C4(C(=O)OCCC[NH3])C(=O)OCCC[NH3])C%13(C(=O)OCCC[NH3])C(=O)OCCC[NH3])C3(C(=O)OCCC[NH3])C(=O)OCCC[NH3]
164		c12c3c4c5c6c7c3c3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8c8[C@]%132[C@@]2(c3c3[C@H]%14C2=C2c8c8c%12c%12c9c9[C@@]%10(c%10c(c41)c5c1c4c%10c9c5c%12c9[C@H]%10c5c4C4=C5[C@H]%10[C@H]([C@@H]2c89)[C@H]%14C(=C(c73)[C@H]6[C@H]14)C5([C](=O)=O)[C](=O)=O)C%11([C](=O)=O)[C](=O)=O)C%13([C](=O)=O)[C](=O)=O
165		C12=C3[C@@]45[C@]6(C7=C8[C@]9([C@]%10(C7=C3[C@@]37[C@@]2(C2=C%11[C@]%12([C@@]1(C1=C4[C@]4%13[C@@]%14(C%15=C1[C@]1%12[C@@]%12(C%16=C%11C%11=C%17[C@@]%18%19[C@@]%16(C%16=C%20[C@@]%21%22[C@@]([C@]%15([C@]%12%16O)O)(C%14=C%12[C@@]([C@]64O)([C@@]48[C@@]6([C@]8%12[C@]%21(C%12=C%14C%15=C([C@@]%18([C@@]%20%12O)O)C%17=C%12[C@]([C@@]2%11O)(C3=C%10[C@@]2%12[C@@]%15(C9=C6%14)O2)O)C8(P(=O)(OCC)OCC)P(=O)(OCC)OCC)O4)O)O%22)O%19)O1)O%13)O)O)O7)O)O)O5
166		[C@H]12[C@@H]3[C@H]4c5c6c7c3c3c2c2c8c9[C@@H]1[C@@H]1c%10c9c9c%11c8c8c2c2c3c3[C@@]%12%13c2c2c8[C@@]8%14[C@@]%11(c%11c9c9c%10c%10c([C@H]41)c5c1c4c%10c9c5c%11c9c%10[C@@]%115[C@@]4(c4c1c6c(c73)c1[C@@]%12(c(c%10c41)c2c89)C%13(C(=O)O)C(=O)O)C%11(C(=O)O)C(=O)O)C%14(C(=O)O)C(=O)O
167		c12c3c4c5c6c7c3c3c2c2c8c9c1c1[C@]%10%11c9c9c%12c8c8[C@]%132[C@@]2(c3c3[C@H]%14C2=C2c8c8c%12c%12c9c9[C@@]%10(C%10=C(c41)[C@@H]5[C@@H]1[C@@H]4[C@H]%10c9c5c%12c9[C@H]%10C5=C4[C@H]4[C@@H]1[C@@H]6C(=C1[C@@H]%14[C@H]([C@@H]%10[C@@H]4C1(C(=O)O)C(=O)O)[C@@H]2c89)c73)C%11(C(=O)O)C(=O)O)C%13(C(=O)O)C(=O)O

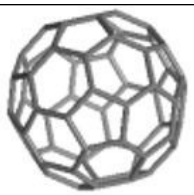
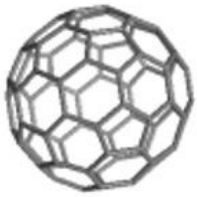
168		c12c3c4c5c6c7c8c9c%10c%11c%12c%13c%14c%15c%16c%17c%18c(c%19c2c2c%20c%21c(c6c32)c2c3c%21c6c%21c%22c(c%18c%19c%20%21)c%18c%17c%15c%15c%17c%18c%18c%19c%17c%17c(c%10c%10c%17c%17c%19c(c6c%22%18)c3c%17c(c8%10)c72)c%15c%11%14)c2c1c(c%13c%162)c4c%12c59
169		[C@@H]12[C@@H]3[C@H]4[C@H]5[C@H]6[C@H]7[C@@H]3[C@H]3[C@H]8[C@@H]1C1=C9[C@@H]%10[C@H]8[C@@H]8C%11=C3[C@H]7[C@@H]3[C@@H]7[C@H]6[C@@H]6[C@@H]%12[C@H]5[C@H]5[C@H]%13[C@H]%14[C@@H]%12[C@H]%12[C@H]%15[C@@H]6[C@@H]7[C@H]6[C@H]7[C@@H]3[C@@H]%11[C@@H]3[C@H]%11[C@@H]%16[C@H]%17[C@H]%18[C@@H]%19[C@@H]%20[C@H]%21[C@@H]%22C%23=C%24[C@@H]([C@H]%13[C@@H]%13[C@H]([C@@H]45)[C@H]2[C@H]1[C@@H]([C@H]%24%13)[C@@H]%22[C@H]9[C@@H]%20[C@H]%10[C@@H]([C@H]%16%19)[C@H]83)[C@H]1[C@@H]%14[C@@H]%12[C@H]2[C@H]3[C@@H]%15[C@@H]6[C@H]([C@@H]%17[C@H]3[C@@H]3[C@H]2[C@H]1[C@H]%23[C@H]%21[C@H]%183)[C@@H]7%11

Table S2 Toxic Ligands in the study

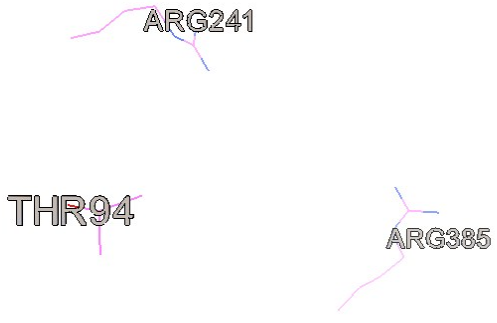
Ligand number											
2	4	6	10	17	27	32	35	36	41	42	43
44	45	46	48	51	52	53	55	67	68	69	70
71	77	80	91	92	94	95	96	97	98	108	109
112	113	114	118	119	120	121	123	124	130	131	132
134	135	136	139	140	141	142	143	146	150	152	154
155	156	157	158	161	162	163	165	167			

Table S3 The corresponding binding affinity (BA, kcal/mol) calculated in Rigid docking in AutoDock Vina

Ligand number	Protein PDB ID										
	1D6	1HA	1HO	1IC	1IL	1JV	1LB	1OO	1QR	1XF	2CG
7						-17.4					
20	12.4										
22										-21.4	
24						-15.2					
41			10.9								
46				17.4							
53					-11.8						
57						-22.4					
61						-6.5					
62						-18.7					
68							-10				
82										-16.4	
84										-20.1	
91					-7.4						
93						-3.9					
95	10.9										
96	8.5								-4.5		
97							-10.2				
10					-8.2						
10										-26.1	
10		-9.5									
11	10.6										
11										-9.5	
12						-19.7					
13											-13.2
14								-9.3			

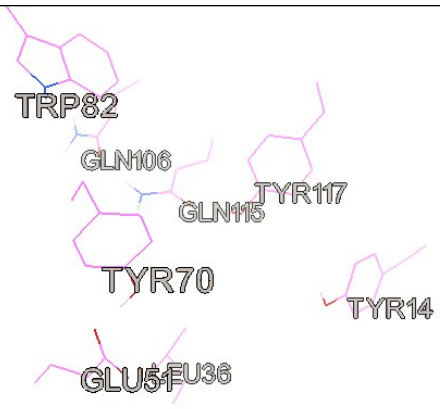
Table S4 Flexible residues for corresponding receptors in AutoDock Vina

PDB code : 1D6U

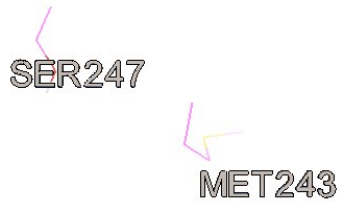


PDB code : 1HA3

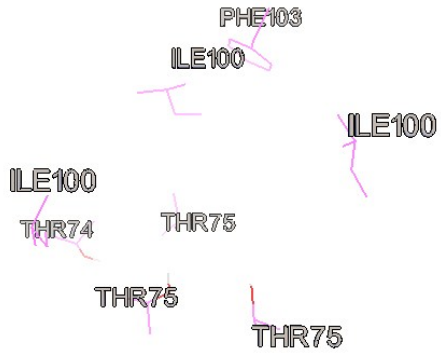
PDB code : 1HOS



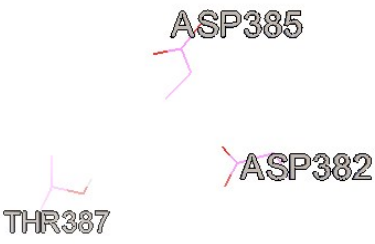
PDB code : 1ICN



PDB code : 1ILH



PDB code : 1JVM

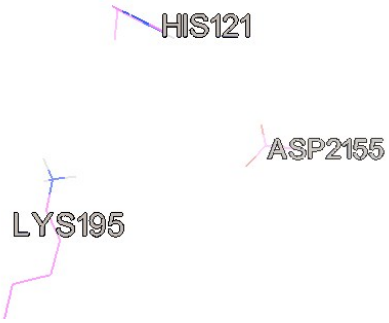


PDB code : 1LBV

PDB code : 1OOQ

PDB code : 1QR2

PDB code : 1XFH



PDB code : 2CG5

Table S5 The corresponding binding affinity calculated in Flexible docking in AutoDock Vina

	1D6U	1HA3	1HOS	1ICN	1ILH	1JVM	1LBV	1OOQ	1QR2	1XFH	2CG5
7						-19.6					
20	-18.7										
22										-20.9	
24						-22.4					
41			-2.2								
46				-14.6							
53					-17.6						

57						-25.3					
61						-12.8					
62						-22.5					
68							-10.5				
82										-19.1	
84										-20	
91					-15.9						
93						-8.4					
95	-18.3										
96	-17								-10.8		
97							-10.2				
104					-15.3						
107										-25.5	
108		-15.4									
114	-16.3										
117										-15	
128						-26.2					
136											-15
141								-13.8			

Table S6 Hydrogen bonds found in AutoDock Rigid Docking:

	1D6U	1HA3	1HOS	1ICN	1ILH	1JVM	1LBV	1OOQ	1QR2	1XFH	2CG5
7						1					
20	-										
22										-	
24						0					
41			1								
46				0							
53					0						
57						0					
61						4					

62						0					
68							0				
82										-	
84										-	
91					0						
93						6					
95	-										
96	-								0		
97							1				
104					1						
107										-	
108		0									
114	-										
117										-	
128						0					
136											0
141								0			

Table S7 Hydrogen bonds found in AutoDock Flexible Docking

	1D6U	1HA3	1HOS	1ICN	1ILH	1JVM	1LBV	1OOQ	1QR2	1XFH	2CG5
7						2					
20	-										
22										-	
24						0					
41			1								
46				0							
53					0						
57						0					
61						4					

62				0					
68					0				
82								-	
84								-	
91			0						
93				6					
95	-								
96	-						0		
97					1				
104			1						
107								-	
108		0							
114	-								
117								-	
128				0					
136									0
141						0			

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