Accelerated Discovery of New Organic Photovoltaic Dyes for OPVs Using Light Absorbance as the Primary Screening Criterion via Machine Learning and DFT

Masar A. Awad[1], Afaf M. Kadhum[1], Azal S. Waheeb[1,4], Hussein A.K. Kyhoiesh[2*], Hassan E. Abd Elsalam[3], Islam H. El Azab[3]

[1]*Department of Chemistry, College of Science, Al-Muthanna University, Al-Muthanna, Iraq*

[2]*National University of Science and Technology, Nasiriyah, Dhi Qar, 64001, Iraq*

[3]*Department of Food Sciences and Nutrition, College of Science, Taif University, P.O. Box 11099, Taif 21944, Saudi Arabia*

[4]*Inorganic Chemistry Group, Scientific Research Center, Al-Ayen University, Thi-Qar, Iraq*

[*]*Corresponding author: H.A.K. Kyhoiesh; Email: hussein.k.sultan@nust.edu.iq; phone; (+964)7807229491; https://orcid.org/0000-0001-9705-9196*

Chemical Reactivity Parameters

The global chemical reactivity parameters were derived by Koopman's theorem [1] from their energies of molecular orbitals (Eq. 1-6).

$$IP = -E_{HOMO} \quad \text{(Eq. 1)}$$

$$EA = -E_{LUMO} \quad \text{(Eq. 2)}$$

$$\chi = \left(\frac{IP + EA}{2}\right) \quad \text{(Eq. 3)}$$

$$\eta = \frac{1}{2}(E_{LUMO} - E_{HOMO}) \quad \text{(Eq. 4)}$$

$$\mu = -\chi \quad \text{(Eq. 5)}$$

$$\sigma = \frac{1}{2\eta} \quad \text{(Eq. 6)}$$

The electrophilicity (ω), as introduced by Pearson [2], represent a tendency of a molecule towards accepting electrons to engage for electrophilic reactions. It indicates their reactivity features (Eq. 7).

$$\omega = \frac{\mu^2}{2\eta} \quad \text{(Eq. 7)}$$

The stabilization energy $E^{(2)}$ associated with electron delocalization between donor (i) and acceptor (j) natural bond orbitals was calculated using second-order perturbation theory as implemented in the NBO analysis [3], and it is calculated as follows (Eq. 8).

$$E^{(2)} = \Delta E_{ij} = q_i \frac{(F_{i,j})^2}{\varepsilon_j - \varepsilon_i} \quad (Eq.8)$$

where qi is the occupancy of the donor orbital, F(i,j) is the off-diagonal element of the Fock matrix in the NBO basis, representing the interaction between donor orbital i and acceptor orbital j, εi and εj are the energies of the donor and acceptor orbitals, respectively. This energy represents the estimate of donor-acceptor interaction strength through hyperconjugation [4].

The open circuit voltage (V_{oc}) is a highest potential difference attained by the *PV* systems when no current is flowing from them [44]. It is calculated by formula given below (Eq 9).

$$V_{oc} = \frac{1}{e}([E_{HOMO}^{donor} - E_{LUMO}^{acceptor}]) - \Delta E_{loss} \quad \text{(Eq. 9)}$$

Here *e* is elementary charge, E_{HOMO}^{donor} is the HOMO level energy of the donor and $E_{LUMO}^{acceptor}$ is the LUMO level energy of the acceptor. It should be noted that the V_{oc} loss of 0.3 eV is empirical, and the loss could be greater or lesser.

Their light-harvesting efficiency (LHE) [5] was calculated from the following equation (Eq. 10).

$$LHE = 1 - 10^{-f} \quad \text{(Eq. 10)}$$

The *f* is the oscillator strength, which was obtained from their Time-Dependent Density Functional Theory (TD-DFT) analysis [6]. The formula given below (Eq. 11) was used for calculating their Short Circuit Current (J_{sc}).

$$J_{sc}(\lambda) \approx q \int \frac{LHE(\lambda) \times \lambda \times \phi_{ph}^{source}(\lambda)}{1240} \times d\lambda \quad \text{(Eq. 11)}$$

Jsc, the maximum current per unit area under illumination at zero voltage, depends on both the molecular absorption capacity and device-specific processes (exciton diffusion, charge separation/collection, morphology, and recombination) [7].

$$P_{max} = V_{OC} \times J_{SC} \times FF \quad \text{(Eq. 12)}$$

To determine this value, a commonly utilized empirical formula (Eq. 13) for the fill factor (FF) was applied.

$$FF = \frac{v_{oc} - ln(v_{oc} + 0.72)}{v_{oc} + 1} \quad \text{(Eq. 13)}$$

Fill factor (FF) is a parameter that characterizes the "squareness" of a solar cell's current–voltage (J-V) curve, formally defined as $FF=P_{max}/V_{OC}\cdot J_{SC}$, where P_{max} is the maximum power output, V_{OC} the open-circuit voltage, and J_{SC} the short-circuit current density [8,9].

Validation of ML Predictions Against DFT Calculations

To quantitatively assess the consistency between our machine learning screening and subsequent DFT validation, we performed a direct comparison of key parameters for the top-performing dyes. This analysis serves to validate the reliability of the ML model in identifying genuinely promising candidates. As detailed in Table S4, we compared the ML-predicted absorbance with the oscillator strength (*f*) derived from TD-DFT calculations, as both are proxies for the strength of the electronic transition. Furthermore, we compared the HOMO-LUMO gap estimated from the ML-predicted absorbance (using the relation $E_g \approx 1240/\lambda max$) with the DFT-calculated gap. The results demonstrate a strong qualitative agreement between the ML predictions and the DFT calculations. Dyes ranked highest by the ML model consistently exhibited high oscillator strengths in the DFT simulations. The Mean Absolute Error (MAE) of 0.07 eV for the HOMO-LUMO gap is remarkably low, indicating that the ML model accurately captured the electronic structure trends necessary for predicting band gaps. The slightly higher MAE for the absorbance/oscillator strength comparison is expected, as the ML model was trained on a normalized absorbance scale, while the DFT calculates the absolute oscillator strength. This discrepancy does not affect the model's utility for ranking and screening, which was its primary purpose.

References

1. Luo, J.; Xue, Z. Q.; Liu, W. M.; Wu, J. L.; Yang, Z. Q. Koopmans' Theorem for Large Molecular Systems within Density Functional Theory. *J. Phys. Chem. A* **2006**, *110*(43), 12005–12009.

2. Green, D. T.; Pearson, J. M. The Examination of Two Web Site Usability Instruments for Use in B2C E-Commerce Organizations. *J. Comput. Inf. Syst.* **2009**, *49*(4), 19–32.

3. Jacob, J. M.; Kurup, M. P.; Nisha, K.; Serdaroğlu, G.; Kaya, S. Mixed Ligand Copper (II) Chelates Derived from an O, N, S-Donor Tridentate Thiosemicarbazone: Synthesis, Spectral Aspects, FMO, and NBO Analysis. *Polyhedron* **2020**, *189*, 114736.

4. Silvi, B.; Savin, A. Classification of Chemical Bonds Based on Topological Analysis of Electron Localization Functions. *Nature* **1994**, *371*(6499), 683–686.

5. Du, T.; Kim, J.; Ngiam, J.; Xu, S.; Barnes, P. R.; Durrant, J. R.; McLachlan, M. A. Elucidating the Origins of Subgap Tail States and Open-Circuit Voltage in Methylammonium Lead Triiodide Perovskite Solar Cells. *Adv. Funct. Mater.* **2018**, *28*(32), 1801808.

6. Kyhoiesh, H. A., Waheeb, A. S., Salem, K. H., Khazaal, W. M., Jabbar, A. F., Al-Kubaisi, A. A., ... & Mahmoud, M. H. Theoretical Design of Asymmetrical 5, 10-Diphenyl-5, 10-Dihydrophenazine Donor–π–Acceptor Chromophores for Photovoltaic Applications. Energy Technology, 2500560.

7. Hassan, A. U., & Sumrra, S. H. (2022). Exploration of pull–push effect for novel photovoltaic dyes with A–π–D design: a DFT/TD-DFT investigation. Journal of Fluorescence, 32(6), 1999-2014.

8. Nelson, J. A. (2003). The physics of solar cells. World Scientific Publishing Company.

9. Green, M. A., Emery, K., Hishikawa, Y., et al. (2017). Solar cell efficiency tables (version 50). Progress in Photovoltaics, 25(7), 668–676.

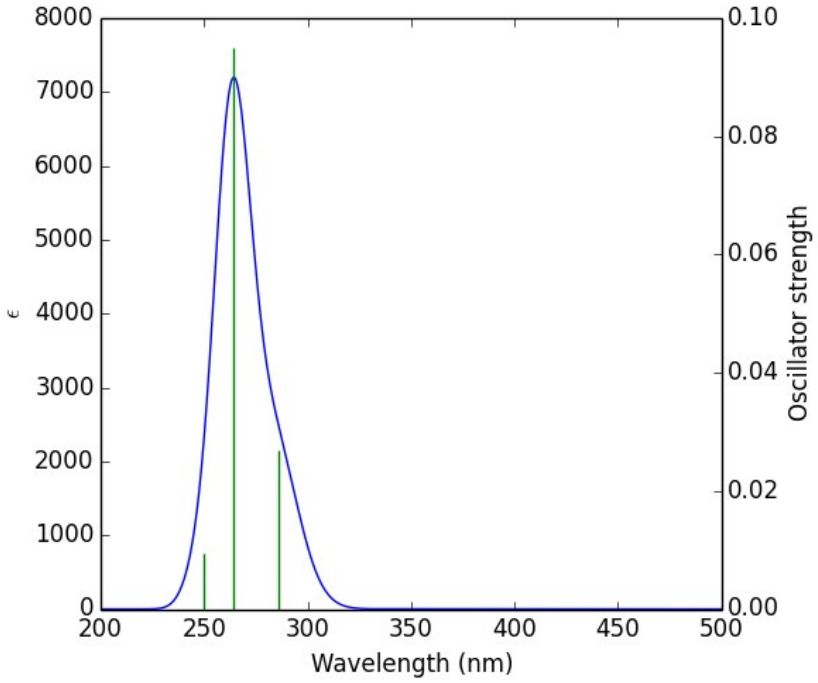


Fig. S1. Simulated TD-DFT UV-Vis absorption spectrum for Dye 1

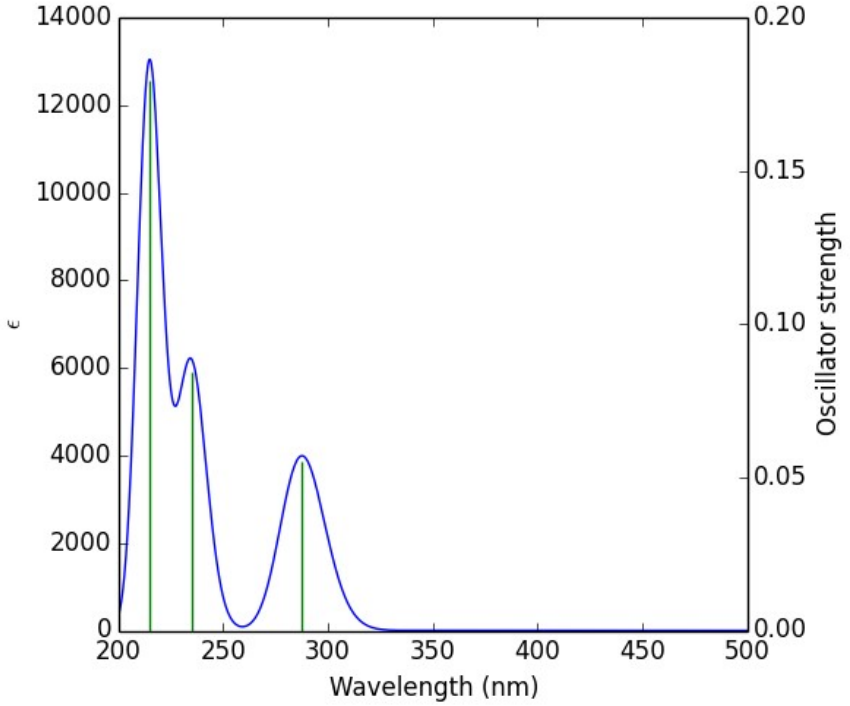


Fig. S2. Simulated TD-DFT UV-Vis absorption spectrum for Dye 2

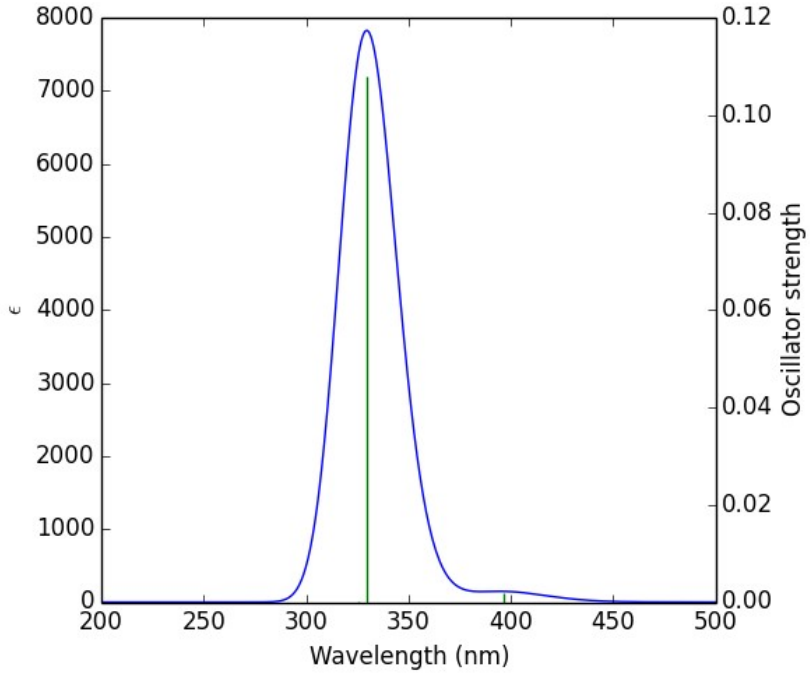


Fig. S3. Simulated TD-DFT UV-Vis absorption spectrum for Dye 3

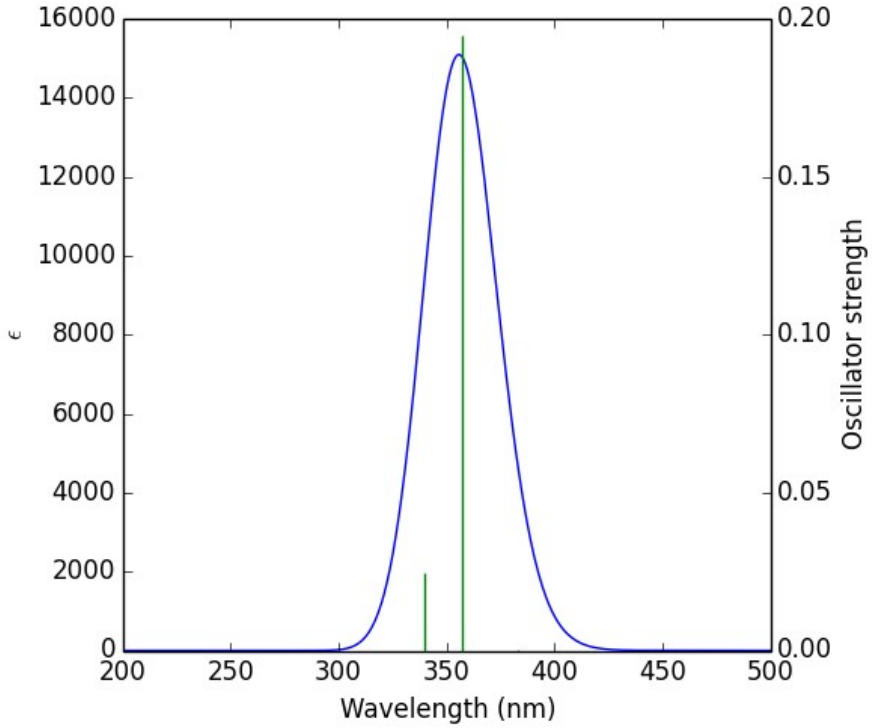


Fig. S4. Simulated TD-DFT UV-Vis absorption spectrum for Dye 5

Table S1. Complete list of the 35 molecular descriptors used for machine learning modeling

Descriptor Name	Category	Description
1. MolWt	Constitutional	Molecular weight
2. HeavyAtomMolWt	Constitutional	Molecular weight of heavy atoms
3. HeavyAtomCount	Constitutional	Number of heavy atoms
4. NumHAcceptors	Electronic	Number of hydrogen bond acceptors
5. NumHDonors	Electronic	Number of hydrogen bond donors
6. NumRotatableBonds	Constitutional	Number of rotatable bonds
7. NumAromaticRings	Constitutional	Number of aromatic rings
8. FractionCsp3	Constitutional	Fraction of sp3 hybridized carbon atoms
9. TPSA	Electronic	Topological Polar Surface Area
10. MolLogP	Hydrophobicity	Wildman-Crippen LogP estimate
11. MolMR	Hydrophobicity	Molar refractivity
12. BalabanJ	Topological	Balaban's J connectivity index
13. BertzCT	Topological	Bertz complexity index
14. HallKierAlpha	Topological	Hall-Kier alpha value
15. Kappa1	Topological	Shape index for 1-bond paths
16. Kappa2	Topological	Shape index for 2-bond paths
17. Kappa3	Topological	Shape index for 3-bond paths

Descriptor Name	Category	Description
18. Chi0	Topological	Randic connectivity index (order 0)
19. Chi1	Topological	Randic connectivity index (order 1)
20. Chi0v	Topological	Valence connectivity index (order 0)
21. Chi1v	Topological	Valence connectivity index (order 1)
22. Chi2v	Topological	Valence connectivity index (order 2)
23. Chi3v	Topological	Valence connectivity index (order 3)
24. Chi4v	Topological	Valence connectivity index (order 4)
25. SlogP_VSA1	VSA	MOE-type descriptors using LogP contributions
26. SlogP_VSA2	VSA	MOE-type descriptors using LogP contributions
27. SlogP_VSA3	VSA	MOE-type descriptors using LogP contributions
28. SMR_VSA1	VSA	MOE-type descriptors using MR contributions
29. SMR_VSA2	VSA	MOE-type descriptors using MR contributions
30. SMR_VSA3	VSA	MOE-type descriptors using MR contributions
31. PEOE_VSA1	VSA	Partial charge-based VSA descriptors
32. PEOE_VSA2	VSA	Partial charge-based VSA descriptors
33. PEOE_VSA3	VSA	Partial charge-based VSA descriptors
34. EState_VSA1	VSA	Electrotopological state VSA descriptors
35. EState_VSA2	VSA	Electrotopological state VSA descriptors

VSA: Van der Waals Surface Area-based descriptors

Table S2. Key geometrical parameters of representative optimized dye structures

Dye	Core Bond Length (Å)	Bridge Dihedral Angle (°)	Donor-Acceptor Dihedral (°)
1	1.423	5.2	12.8
2	1.415	3.8	8.9
3	1.436	15.7	25.4
4	1.419	7.3	16.2
5	1.428	9.1	19.5

Table S3. A sample of the first 200 datapoints to show the solvent selection by machine learning analysis

SMILES	LogP	MW	PSA	HBD	HBA	Best Solvent
CNC(=O)OC1=C2C=CSC2=CC=C1	2.6195	207.254	38.33	1	3	Methanol
B(C1=CC2=CC=CC=C2S1)(O)O	0.5811	178.021	40.46	2	3	Methanol
CC(=O)C1=CC2=CC=CC=C2S1	3.1039	176.24	17.07	0	2	DMF
C1=CC=C2C(=C1)C=CS2	2.9013	134.203	0	0	1	Acetonitrile
B(C1=CSC2=CC=CC=C12)(O)O	0.5811	178.021	40.46	2	3	Methanol
C1=CC=C2C(=C1)C(=C(S2)C(=O)NN)Cl	2.1582	226.688	55.12	2	3	Water
C1=CC=C2C(=C1)C=C(S2)C(=O)O	2.5995	178.212	37.3	1	2	DMF

C1=CC=C2C(=C1)C(=CS2)CC(=O)O	2.5284	192.239	37.3	1	2	DMF
C1=CC=C2C(=C1)C(=CS2)C=O	2.7138	162.213	17.07	0	2	DMF
C1=CC=C2C(=C1)C(=CS2)CN	2.36	163.245	26.02	1	2	DMF
CC(=O)C1=C(C2=CC=CC=C2S1)O	2.8095	192.239	37.3	1	3	Methanol
C1CCC2=C(C1)C(=C(S2)N)C(=O)N	1.308	196.275	69.11	2	3	Water
C1=CC2=C(C=C(S2)C(=N)N)C(=C1)I	2.78997	302.14	49.87	2	2	Water
C1=CC2=C(C=CS2)C=C1C=O	2.7138	162.213	17.07	0	2	DMF
C1=CC2=C(C=C1Cl)SC(=C2Cl)C(=O)O	3.9063	247.102	37.3	1	2	DMF
C1=CC2=C(C=C(S2)C(=N)N)C(=C1)I.Cl	3.21177	338.601	49.87	2	2	Water
C1=CC=C2C(=C1)C=C(S2)CN	2.36	163.245	26.02	1	2	DMF
C1=CC=C2C(=C1)C=C(S2)C=O	2.7138	162.213	17.07	0	2	DMF
C1CCC2=C(C1)C(=C(S2)N)C#N	2.08078	178.26	49.81	1	3	Methanol
CCOC(=O)C1=C(SC2=C1CCCC2)N	2.3858	225.313	52.32	1	4	Methanol
C1=CC2=C(C=C1Cl)C(=CS2)CC(=O)O	3.1818	226.684	37.3	1	2	DMF
C1=CC=C2C(=C1)C(=C(S2)[N+](=O)[O-])Br	3.572	258.096	43.14	0	3	Methanol
CC(=O)NC1=CSC2=CC=CC=C21	2.8597	191.255	29.1	1	2	DMF
C1=CC=C2C(=C1)C(=CS2)CO	2.3936	164.229	20.23	1	2	DMF
CC1CCC2=C(C1)SC(=C2C#N)N	2.32678	192.287	49.81	1	3	Methanol
COC(=O)C1=C(SC2=C1CCCC2)N	1.9957	211.286	52.32	1	4	Methanol
C1=CC=C2C(=C1)C(=CS2)Cl	3.5547	168.648	0	0	1	Acetonitrile
C1=CC=C2C(=C1)C(=C(S2)Cl)Cl	4.2081	203.093	0	0	1	Acetonitrile
CC1=CC2=C(C=C1)SC=C2CC(=O)O	2.83682	206.266	37.3	1	2	DMF
C1CCC(CC1)(C2=CC3=CC=CC=C3S2)N	4.0194	231.364	26.02	1	2	DMF
C1=CC=C(C=C1)C2=CC3=C(S2)C=C(C=C3)O	4.2739	226.3	20.23	1	2	DMF
CC1=CSC2=CC=CC=C12	3.20972	148.23	0	0	1	Acetonitrile
C1CC2=C(C=CS2)C(=O)C1	2.2671	152.218	17.07	0	2	DMF
C1=CC=C2C(=C1)C(=O)C(=O)S2	1.5016	164.185	34.14	0	3	Methanol
CC1=CC2=CC=CC=C2S1	3.20972	148.23	0	0	1	Acetonitrile
CC1=CC2=C(C=C1)SC=C2	3.20972	148.23	0	0	1	Acetonitrile
C1=CC2=C(C=CS2)C=C1O	2.6069	150.202	20.23	1	2	DMF
CC(=O)C1=CSC2=CC=CC=C21	3.1039	176.24	17.07	0	2	DMF
C1=CC(=C2C=CSC2=C1)O	2.6069	150.202	20.23	1	2	DMF
C1=CC=C2C(=C1)C(=CS2)O	2.6069	150.202	20.23	1	2	DMF
C1=CC=C2C(=C1)C(=CS2)[N+](=O)[O-]	2.8095	179.2	43.14	0	3	Methanol
CC1=CSC2=C1C=C(C=C2)Cl	3.86312	182.675	0	0	1	Acetonitrile
COC(=O)C1=C(C2=CC=CC=C2S1)Cl	3.3413	226.684	26.3	0	3	Methanol
C1CCC2=C(C1)C=C(S2)C(=O)O	2.3251	182.244	37.3	1	2	DMF
B(C1=CC2=C(S1)C=CC(=C2)C)(O)O	0.88952	192.048	40.46	2	3	Water
C1=CC2=C(C=C1Br)C(=CS2)C=O	3.4763	241.109	17.07	0	2	DMF
C1=CC2=C(C=C1Br)C(=CS2)CN	3.1225	242.141	26.02	1	2	DMF
C1=CC=C2C(=C1)C=C(S2)C(=O)NO	2.0203	193.227	49.33	2	3	Water
COC(=O)C1=C(C2=CC=CC=C2S1)N	2.2701	207.254	52.32	1	4	Methanol
C1=CC=C2C(=C1)C(=C(S2)C(=O)NO)Cl	2.6737	227.672	49.33	2	3	Water

C1=CC(=C2C=CSC2=C1)C3=CN=CN3	3.2914	200.266	28.68	1	2	DMF
C1CC(C2=C(C1)SC=C2)C3=CN=CN3	2.9394	204.298	28.68	1	2	DMF
C1CC(C2=C(C1)C=CS2)C3=CN=CN3	2.9394	204.298	28.68	1	2	DMF
C1CCC2=C(C1)C3=C(N=CN=C3S2)N	2.1523	205.286	51.8	1	4	Methanol
CCCC1=NC=C(C=C1)C2=CC=CC=C2	3.7011	197.281	12.89	0	1	Acetonitrile
C1=CC2=C(C=CS2)C=C1Br	3.6638	213.099	0	0	1	Acetonitrile
C1=CC=C2C(=C1)C(=CS2)C(=O)O	2.5995	178.212	37.3	1	2	DMF
CC1CCC2=C(C1)SC(=C2C(=O)N)N	1.554	210.302	69.11	2	3	Water
C1=CC=C2C(=C1)C=C(S2)C(=O)NN	1.5048	192.243	55.12	2	3	Water
CC1=CC2=C(C=C1)SC(=C2)C(=O)O	2.90792	192.239	37.3	1	2	DMF
C1CCC2=C(C1)C(=CS2)C(=O)O	2.3251	182.244	37.3	1	2	DMF
C1=CC2=C(C(=C1)Cl)C(=C(S2)C(=O)O)Cl	3.9063	247.102	37.3	1	2	DMF
CCC1CCC2=C(C1)C=C(S2)C(=O)O	2.9612	210.298	37.3	1	2	DMF
CC1CCC2=C(C1)C=C(S2)C(=O)NN	1.4764	210.302	55.12	2	3	Water
CC(=O)NC1=CC2=C(C=C1)SC=C2	2.8597	191.255	29.1	1	2	DMF
C1=CC=C2C(=C1)C=C(S2)C(=N)N	2.18537	176.244	49.87	2	2	Water
B(C1=CC2=C(S1)C=CC(=C2)CN)(O)O	0.0398	207.063	66.48	3	4	Methanol
C1=CC=C2C(=C1)C=C(S2)CO	2.3936	164.229	20.23	1	2	DMF
C1CS(=O)(=O)C2=CC=CC=C21	1.0164	168.217	34.14	0	2	DMF
C1=CC2=C(C=C1Cl)C(=CS2)CN	3.0134	197.69	26.02	1	2	DMF
C1=CC=C2C(=C1)C(=CS2)CCN	2.4025	177.272	26.02	1	2	DMF
C1=CC2=C(C=C(S2)C(=[NH2+])N)C(=C1)I	0.9703	303.148	51.61	2	1	Water
C1=CC=C2C(=C1)C(=C(S2)C(=O)O)Cl	3.2529	212.657	37.3	1	2	DMF
C1=CC=C2C(=C1)C(=CS2)CC#N	2.96738	173.24	23.79	0	2	DMF
C1C2=CC=CC=C2C(=O)S1	2.0736	150.202	17.07	0	2	DMF
CC1=C2C(=CC=C1)C=CS2	3.20972	148.23	0	0	1	Acetonitrile
CC1=C2C(=CC=C1)C=C(S2)C	3.51814	162.257	0	0	1	Acetonitrile
C1=CC=C2C(=C1)C(=CS2)C#N	2.77298	159.213	23.79	0	2	DMF
C1=CC=C2C(=C1)C=C(S2)C#N	2.77298	159.213	23.79	0	2	DMF
COC(=O)C1=CC2=CC=CC=C2S1	2.6879	192.239	26.3	0	3	Methanol
C1=CC=C2C(=C1)C(=C(S2)C(=O)N)Cl	2.6536	211.673	43.09	1	2	DMF
CC1=CC2=C(C=C1)SC=C2C	3.51814	162.257	0	0	1	Acetonitrile
C1=CC=C2C(=C1)C=C(S2)C3=CC=C(C=C3)O	4.2739	226.3	20.23	1	2	DMF
COC(=O)C1=C(C2=CC=CC=C2S1)O	2.3935	208.238	46.53	1	4	Methanol
B(C1=CC2=C(S1)C=CC(=C2)Br)(O)O	1.3436	256.917	40.46	2	3	Water
CC1=C(SC2=CC=CC=C12)C(=O)C	3.41232	190.267	17.07	0	2	DMF
C1=CC2=C(C=C1Cl)C(=CS2)CC#N	3.62078	207.685	23.79	0	2	DMF
C1=CC=C2C(=C1)C(=O)SC2=O	1.7138	164.185	34.14	0	3	Methanol
C1=CC=C2C(=C1)C=C(S2)C(=[NH2+])N	0.3657	177.252	51.61	2	1	DMSO
C1=CC=C2C(=C1)C=C(S2)Br	3.6638	213.099	0	0	1	Acetonitrile
C1=CC=C2C(=C1)C(=C(S2)Br)Br	4.4263	291.995	0	0	1	Acetonitrile
C1=CC(=CC2=C1C=CS2)O	2.6069	150.202	20.23	1	2	DMF
CC1=C(SC2=C1C=C(C=C2)Cl)Br	4.62562	261.571	0	0	1	Acetonitrile

C1=CC=C2C(=C1)C=C(S2)I	3.5059	260.099	0	0	1	Acetonitrile
CC1=C(SC2=CC=CC=C12)C(=O)O	2.90792	192.239	37.3	1	2	DMF
CC1=CC2=C(C=C1)C(=C(S2)C(=O)O)Cl	3.56132	226.684	37.3	1	2	DMF
C1=CC=C2C(=C1)C(=C(S2)C=O)Br	3.4763	241.109	17.07	0	2	DMF
C1=CC=C2C(=C1)C(=C(S2)C#N)N	2.35518	174.228	49.81	1	3	Methanol
C1=CC2=C(C=C1Br)C(=CS2)CC(=O)O	3.2909	271.135	37.3	1	2	DMF
C1CN(CCN1)C2=CC=CC3=C2SC=C3	2.3109	218.325	15.27	1	3	Methanol
CC1=CC2=C(C=C1)SC(=C2C)C	3.82656	176.284	0	0	1	Acetonitrile
C1CC(C2=C(C1)SC=C2)CCN3C=CN=C3	3.4548	232.352	17.82	0	3	Methanol
CC1=C2C=C(SC2=CC=C1)C(=N)N	2.49379	190.271	49.87	2	2	Water
C1=CC=C2C(=C1)C=C(S2)C3=CC=C(C=C3)N	4.1505	225.316	26.02	1	2	DMF
CC1=CC2=C(C=C1)SC3=CC=CC(=C32)C	4.67134	212.317	0	0	1	Acetonitrile
C1=CN=CC2=C1SC=C2	2.2963	135.191	12.89	0	2	DMF
C1CCC2=C(C1)C3=C(S2)N=CN=C3Cl	3.2235	224.716	25.78	0	3	Methanol
C1=CC2=C(C=CS2)C=C1CN	2.36	163.245	26.02	1	2	DMF
C1=CC=C2C(=C1)C(=CS2)Br	3.6638	213.099	0	0	1	Acetonitrile
C1C(=O)C2=CC=CC=C2S1	1.975	150.202	17.07	0	2	DMF
C1=CC2=C(C=CS2)C=C1C(=O)O	2.5995	178.212	37.3	1	2	DMF
C1=CC=C2C(=C1)C(=C(S2)C=O)Cl	3.3672	196.658	17.07	0	2	DMF
C1CCC2=C(C1)C=CS2	2.6269	138.235	0	0	1	Acetonitrile
CC1=CC2=C(C=C1)C(=CS2)C	3.51814	162.257	0	0	1	Acetonitrile
C1=CC2=C(C=C(S2)C(=O)O)C(=C1)Br	3.362	257.108	37.3	1	2	DMF
C1=CC=C2C(=C1)C(=C(S2)C(=O)N)N	1.5824	192.243	69.11	2	3	Water
C1CCC2=C(C1)C(=CS2)C#N	2.49858	163.245	23.79	0	2	DMF
CC1=C(SC2=CC=CC=C12)/C=N/O	3.01782	191.255	32.59	1	3	Methanol
COC1=CC=C(C=C1)C2=CSC3=CC=CC=C32	4.5769	240.327	9.23	0	2	DMF
C1=CC2=C(C=C1Cl)C(=CS2)CO	3.047	198.674	20.23	1	2	DMF
CC1=CC2=C(S1)C=CC(=C2)Br	3.97222	227.126	0	0	1	Acetonitrile
C1C(SC2=CC=CC=C21)C(=O)O	1.788	180.228	37.3	1	2	DMF
CC(C1=CC2=CC=CC=C2S1)NC(=O)N	2.6306	220.297	55.12	2	2	Water
CC1=CSC2=C1C=CC=C2O	2.91532	164.229	20.23	1	2	DMF
C1=CC2=C(C=CS2)C=C1C#N	2.77298	159.213	23.79	0	2	DMF
CCOC(=O)C1=C(SC2=CC=CC=C21)N	2.6602	221.281	52.32	1	4	Methanol
CC1CCC2=C(C1)SC=C2C(=O)O	2.5711	196.271	37.3	1	2	DMF
CC1CCCC2=C1C(=C(S2)N)C#N	2.64178	192.287	49.81	1	3	Methanol
C1=CC=C2C(=C1)C(=C(S2)C#N)O	2.47858	175.212	44.02	1	3	Methanol
C1=CC2=C(SC(=C2C=C1)Cl)Cl	4.2081	203.093	0	0	1	Acetonitrile
C1=CC=C2C(=C1)C(=C(S2)C(=O)O)O	2.3051	194.211	57.53	2	3	Water
C1CSC2=C1C=CC(=C2)N	1.917	151.234	26.02	1	2	DMF
CC(=O)C1=CC2=C(S1)C=CC(=C2)O	2.8095	192.239	37.3	1	3	Methanol
C1=CC=C2C(=C1)C=C(S2)CON	2.2916	179.244	35.25	1	3	Methanol
CC(C)NC(=O)C1=CC2=C(S1)CCCC2	2.7651	223.341	29.1	1	2	DMF
C1=CC=C(C=C1)C2=C(C3=CC=CC=C3S2)I	5.1729	336.197	0	0	1	Acetonitrile

CCCCNC(=O)C1=CC2=CC=CC=C2S1	3.4312	233.336	29.1	1	2	DMF
CC1=CC2=C(C=C1)SC=C2CC(=O)NC	2.49822	219.309	29.1	1	2	DMF
C1=CC=C2C(=C1)C=C(S2)CC3=CN=CN3.Cl	3.637	250.754	28.68	1	2	DMF
C1CCC2=C(C1)C=C(S2)CC3=CN=CN3.Cl	3.3626	254.786	28.68	1	2	DMF
C1=CC=C2C(=C1)C(=C(S2)CN)Cl	3.0134	197.69	26.02	1	2	DMF
CC(C)(C)C1=CC2=C(C=C1)SC(=C2)CN	3.6575	219.353	26.02	1	2	DMF
C1=CC=C2C(=C1)C3=C(S2)C4=CC=CC=C4S3	5.2692	240.352	0	0	2	DMF
C1CC2=C(C(=O)C1)SC=C2	2.2671	152.218	17.07	0	2	DMF
[B-](C1=CC2=CC=CC=C2S1)(F)(F)F.[K+]	-0.0403	240.099	0	0	1	Acetonitrile
C1C2=CC=CC=C2SC1=O	1.8614	150.202	17.07	0	2	DMF
C1=CC=C2C(=C1)C=C(S2)C(=O)Cl	3.2803	196.658	17.07	0	2	DMF
C1=CC=C2C(=C1)C=C(S2)C(=O)N	2.0002	177.228	43.09	1	2	DMF
C1=CC=C2C(=C1)C=C(S2)C3=CC=CC=N3	3.9633	211.289	12.89	0	2	DMF
C1=CC=C2C(=C1)C=C(S2)CC(=O)O	2.5284	192.239	37.3	1	2	DMF
C1=CC=C2C(=C1)C(=CS2)/C=C/C(=O)O	2.9991	204.25	37.3	1	2	DMF
CC1=CC2=C(C=C1)C=CS2	3.20972	148.23	0	0	1	Acetonitrile
CNCC1=CC2=CC=CC=C2S1	2.6207	177.272	12.03	1	2	DMF
C1CCN(CC1)CC2=CSC3=CC=CC=C32	3.8872	231.364	3.24	0	2	DMF
CC1=C2C=CSC2=CC=C1	3.20972	148.23	0	0	1	Acetonitrile
C1=CC2=C(C=CS2)C=C1N	2.4835	149.218	26.02	1	2	DMF
C1=CC=C2C(=C1)C(=C(S2)C(=O)Cl)Cl	3.9337	231.103	17.07	0	2	DMF
CC1=C(C2=CC=CC=C2S1)Br	3.97222	227.126	0	0	1	Acetonitrile
C1=CC2=C(C(=C1)C=O)SC=C2	2.7138	162.213	17.07	0	2	DMF
C1C2=CC=CC=C2CS1	2.4334	136.219	0	0	1	Acetonitrile
CC1=C2C=C(SC2=CC=C1)C(=O)O	2.90792	192.239	37.3	1	2	DMF
C1=CC2=CSC=C2C=C1	2.9013	134.203	0	0	1	Acetonitrile
CC1=C(SC2=CC=CC=C12)C=O	3.02222	176.24	17.07	0	2	DMF
CC1=C(SC2=C1C=C(C=C2)Cl)C(=O)C	4.06572	224.712	17.07	0	2	DMF
CCOC(=O)C1=CC2=CC=CC=C2S1	3.078	206.266	26.3	0	3	Methanol
C1=CC=C(C=C1)C2=CC3=CC=CC=C3S2	4.5683	210.301	0	0	1	Acetonitrile
C1CSC2=CC=CC=C21	2.3348	136.219	0	0	1	Acetonitrile
C1=CC2=C(C=C1Br)SC(=C2)CN	3.1225	242.141	26.02	1	2	DMF
C1=CC2=C(C=C1Br)C=C(S2)CN	3.1225	242.141	26.02	1	2	DMF
CC1=C(SC2=CC=CC=C12)C	3.51814	162.257	0	0	1	Acetonitrile
C=CC1=CC2=CC=CC=C2S1	3.5443	160.241	0	0	1	Acetonitrile
CC1=C2C(=CC=C1)C(=CS2)C	3.51814	162.257	0	0	1	Acetonitrile
C1=CC=C2C(=C1)C(=C(S2)N)C#N	2.35518	174.228	49.81	1	3	Methanol
C1=CC2=C(C(=C1)C(=O)O)SC=C2	2.5995	178.212	37.3	1	2	DMF
C1=CC(=C2C=CSC2=C1)N	2.4835	149.218	26.02	1	2	DMF
COC(=O)C1=CC2=C(S1)C=CC(=C2)N	2.2701	207.254	52.32	1	4	Methanol
C1=CC(=CC2=C1C=CS2)N	2.4835	149.218	26.02	1	2	DMF
COC1=CC2=C(C=C1)SC(=C2)C(=O)O	2.6081	208.238	46.53	1	3	Methanol

C1=CC=C2C(=C1)C(=C(S2)Br)C=O	3.4763	241.109	17.07	0	2	DMF
C1=CC2=C(C=C1Cl)SC(=C2O)C(=O)O	2.9585	228.656	57.53	2	3	Water
CCC1=CC2=C(C=C1)SC=C2	3.4637	162.257	0	0	1	Acetonitrile
C1=CC=C2C(=C1)C=C(S2)Cl	3.5547	168.648	0	0	1	Acetonitrile
C1=CC=C2C(=C1)C=C(S2)F	3.0404	152.193	0	0	1	Acetonitrile
B(C1=CC2=C(S1)C=CC(=C2)O)(O)O	0.2867	194.02	60.69	3	4	Methanol
C1CCC(C1)(C2=CC3=CC=CC=C3S2)N	3.6293	217.337	26.02	1	2	DMF
C1=CC(=C2C=CSC2=C1)CCN3C=CN=C3	3.3405	228.32	17.82	0	3	Methanol
CSC(=S)NCCC1=CSC2=CC=CC=C21	3.6813	267.444	12.03	1	3	Methanol
CCN(CCO)CC1=CSC2=C1C=C(C=C2)Br.Cl	3.8998	350.709	23.47	1	3	Methanol
CCCN(CCC)C1CCC2=C(C1)SC=C2	3.7274	237.412	3.24	0	2	DMF
CCCN(CCC)C1CCC2=C(C1)C=CS2	3.7274	237.412	3.24	0	2	DMF
CCCN(CCC)CC1CCC2=C(C1)C=CS2	3.975	251.439	3.24	0	2	DMF
CCCN(CCC)CC1CCC2=C(C1)SC=C2	3.975	251.439	3.24	0	2	DMF
B(C1=CC2=C(S1)C=CC(=C2)N)(O)O	0.1633	193.036	66.48	3	4	Methanol
COC1=CC2=C(C=C1)SC(=C2)N	2.4921	179.244	35.25	1	3	Methanol
C1COCCN1C2=CSC3=CC=CC=C32	2.7379	219.309	12.47	0	3	Methanol
C1=CC=C2C(=C1)C(=CS2)CCNC(=O)CBr	2.9549	298.205	29.1	1	2	DMF
CC(=O)C1=C(SC2=C1CCCC2)N	2.4117	195.287	43.09	1	3	Methanol
C1=CC=C2C(=C1)C=CC3=C2C=CS3	4.0545	184.263	0	0	1	Acetonitrile
C1=CC2=C(C=CS2)C=C1CO	2.3936	164.229	20.23	1	2	DMF
C1=CC=C2C(=C1)C(=CS2)C(=O)Cl	3.2803	196.658	17.07	0	2	DMF
C1=CC=C2C(=C1)C=CS2=O	1.7785	150.202	17.07	0	1	Acetonitrile
CC1=CC(=C2C(=C1)C=C(S2)C)C	3.82656	176.284	0	0	1	Acetonitrile
CN=CC1=C(C2=CC=CC=C2S1)O	2.6556	191.255	32.59	1	3	Methanol
C1=CC2=C(C=C1F)C=C(S2)C(=O)O	2.7386	196.202	37.3	1	2	DMF
CCOC(=O)C1=CC2=C(S1)C=CC(=C2)N	2.6602	221.281	52.32	1	4	Methanol
COC(=O)C1=CSC2=CC=CC=C21	2.6879	192.239	26.3	0	3	Methanol
CC1=CC2=C(C=C1)SC(=C2C)C(=O)O	3.21634	206.266	37.3	1	2	DMF
CC1=CC2=C(C=C1)SC(=C2)C	3.51814	162.257	0	0	1	Acetonitrile
CCC1=CC=CC2=C1SC=C2	3.4637	162.257	0	0	1	Acetonitrile
CCCC1=CC2=CC=CC=C2S1	3.8538	176.284	0	0	1	Acetonitrile
COC(=O)CC1=CSC2=CC=CC=C21	2.6168	206.266	26.3	0	3	Methanol
C1=CC2=C(C=C1Br)C=C(S2)C(=O)O	3.362	257.108	37.3	1	2	DMF
COC1=CC2=C(C=C1)SC=C2	2.9099	164.229	9.23	0	2	DMF
COC(=O)C1=CC2=C(S1)C=CC(=C2)Br	3.4504	271.135	26.3	0	3	Methanol
CC1=CC2=C(C=C1)SC(=C2)C=O	3.02222	176.24	17.07	0	2	DMF
CC1CCC2=C(C1)C=C(S2)C(=O)O	2.5711	196.271	37.3	1	2	DMF
C1=CC=C2C(=C1)C(=CS2)CCN.Cl	2.8243	213.733	26.02	1	2	DMF
C1=CC=C2C(=C1)C=C(S2)CC#N	2.96738	173.24	23.79	0	2	DMF
C1=CC=C2C(=C1)C=C(S2)C(CN)O	1.8934	193.271	46.25	2	3	Water
C1C(C2=CC=CC=C2S1)CN	1.8346	165.261	26.02	1	2	DMF
C1=C2C=C(SC2=CC(=C1O)O)C(=O)O	2.0107	210.21	77.76	3	4	Water

C1=CC2=C(C=C1O)C(=CS2)CCN	2.1081	193.271	46.25	2	3	Water
CC1=C2C(=CC=C1)C(=C(S2)C)C	3.82656	176.284	0	0	1	Acetonitrile
C1=CC=C2C(=C1)C(=CS2)C3=CN=CN=C3	3.3583	212.277	25.78	0	3	Methanol
C1=CC=C2C(=C1)C=C(S2)CCl	3.6401	182.675	0	0	1	Acetonitrile
C1CCC2=C(SC=C2C1)C(=O)O	2.3251	182.244	37.3	1	2	DMF
C1=CC2=C(C(=C1)Cl)C(=C(S2)C(=O)Cl)Cl	4.5871	265.548	17.07	0	2	DMF
CC1=C(C2=CC=CC=C2S1)C(=O)O	2.90792	192.239	37.3	1	2	DMF
C1CC(C2=C(C1)SC=C2)C(=O)O	2.2526	182.244	37.3	1	2	DMF
C1=CC=C2C(=C1)C=C(S2)C3=NC(=NC=C3)N	2.9405	227.292	51.8	1	4	Methanol
C1=CC2=C(C(=C1)Cl)SC(=C2)C(=O)O	3.2529	212.657	37.3	1	2	DMF
C1CCC2=C(C1)C(=C(S2)N)C(=O)O	1.9073	197.259	63.32	2	3	Water
C1=CC=C2C(=C1)C(=C(S2)C(=O)O)N	2.1817	193.227	63.32	2	3	Water
CC1=C2C(=CC=C1)SC(=C2Cl)C(=O)O	3.56132	226.684	37.3	1	2	DMF
C1=CC2=C(C=C1Cl)C(=CS2)C#N	3.42638	193.658	23.79	0	2	DMF
C1CC(C2=C(C1)SC=C2)N	2.0842	153.25	26.02	1	2	DMF
CC1=C(SC2=CC=CC(=C12)F)C(=O)O	3.04702	210.229	37.3	1	2	DMF
C1CCC2=C(C1)C=C(S2)Br	3.3894	217.131	0	0	1	Acetonitrile
CC1=CC2=C(C=C1)C(=CS2)C(=O)O	2.90792	192.239	37.3	1	2	DMF
C1C(C2=CC=CC=C2S1)N	1.7921	151.234	26.02	1	2	DMF
C1=CC=C2C(=C1)C=C(S2)CCC(=O)O	2.9185	206.266	37.3	1	2	DMF
CNC(=O)C1=CC2=C(S1)C=CC(=C2)Br	3.0234	270.151	29.1	1	2	DMF

Table S4. Newly generated top 1000 Polymer SMILES along with their Light absorption and Synthetic Accessibility

SMILES	Absorption	Synthetic Accessibility Score
CCCCCCCCCC(CCCCCC)CN1C(=C2C(=C(N(C2=O)CC(CCCCCC)CCCCCCCC)C3=CC=C(S3)C4=CC5=C(C(=C(C(=C5S4)S)/C=C/C)C=O)CCCCCC)C1=O)C6=CC=C(S6)C	0.39355	14.98615
CN(CCCOCCOCCOCC(=O)O)CCOC1=CC=C(C=C1)C(=O)C2=C(SC3=C2C=CC(=C3)OCC4=CC=CC=C4)C5=CC=C(C=C5)OCC6=CC=CC=C6	0.33930	8.933128
CCCCC1=C(SC(=C1)C2=C3C=CC=CC3=C(S2)C4=CC(=C(S4)CCOCCOCC)CCCC)CCOCCOCC	0.77419	8.822871
CC(C)(C)OC(=O)COCCOCCOCCCN(C)CCOC1=CC=C(C=C1)C(=O)C2=C(SC3=C2C=CC(=C3)OCC4=CC=CC=C4)C5=CC=C(C=C5)OCC6=CC=CC=C6	0.34263	8.693754
CC1=CC=C(C=C1)S(=O)(=O)OCCCOCCCOCCCCOC2=CC=C(C=C2)OC3=C(SC4=C3C=CC(=C4)OCC5=CC=CC=C5)C6=CC=C(C=C6)Br	0.37887	8.441739

	4	
CN(CCCOCCOCCOCC(=O)I)CCOC1=CC=C(C=C1)C(=C)C2=C(SC3=C2C=CC(=C3)O)C4=CC=C(C=C4)O	0.40660 5	8.01 1414
CCC1=C(SC2=CC(=C(C=C21)OCCCCl)OCCCCO)S(=O)(=O)NCP(=O)(OCC)OCC	0.30598 9	7.71 123
CCCCC1=C(SC(=C1)C2=C3C=CC=CC3=C(S2)C4=CC(=C(S4)CCOCCOCC)C)CCOCCOCC	0.82062 2	7.50 2402
CCCC1=CC=C(C=C1)C2=C(C3=C(S2)C=C(C=C3)O)C(=O)C4=CC=C(C=C4)OCCOCCOCCOCCOCC(=O)O	0.40414 8	7.42 2237
C1CCC2=NC3=CC=CC=C3C(=C2C1)NCCCCCCNC(=O)CCCC4=C(SC5=CC=CC=C54)/C=C/6\C=CN(C7=CC=CC=C67)CCC(=O)NCCCCCCNC8=C9CCCCC9=NC1=CC=CC=C18	0.28379 9	7.31 5546
C1=CC=C(C=C1)COC2=CC=C(C=C2)C3=C(C4=C(S3)C=C(C=C4)OCC5=CC=CC=C5)OC6=CC=C(C=C6)OCCOCCOCCOCC(=O)O	0.40093 4	7.30 2393
CCCCC(=O)CCCC(=O)N(CCN(CC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)CCC5=CC=C(C=C5)C(=O)OC)C(C)C)C(C)C	0.30080 2	7.28 4547
CC(C)(C)OC(=O)COCCOCCOCCOCCOC1=CC=C(C=C1)C(=O)C2=C(SC3=C2C=CC(=C3)OC)C4=CC=C(C=C4)OC	0.40479 1	7.20 2655
CN(CCOCCOCC(=O)O)CCOC1=CC=C(C=C1)C(=O)C2=C(SC3=C2C=CC(=C3)OCC4=CC=CC=C4)C5=CC=C(C=C5)OCC6=CC=CC=C6	0.38433 7	7.15 2709
COC1=CC=C(C=C1)C2=C(C3=C(S2)C=C(C=C3)O)C(=O)C4=CC=C(C=C4)OCCOCCOCCOCCOCC(=O)O	0.38839 9	7.00 1873
COC1=CC2=C(C=C1)C(=C(S2)C3=CC=C(C=C3)O)C(=O)C4=CC=C(C=C4)OCCOCCOCCOCCOCC(=O)O	0.38839 9	7.00 1873
CCCN(CCN(C)C(=C)CCC(=O)OCC)CC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)CCCC5=CC=C(C=C5)C(=O)OC	0.32948 6	6.96 4077
CCCCOC1CCC(CC1)OC(=O)C2=C3C(=C(C=C2)OC(=O)C4CCC(CC4)C(=O)OCCCCCCOC(=O)C=C)C=C(S3)I	0.34439 3	6.92 1986
CC(C)(C)OC(=O)COCCOCCN(C)CCOC1=CC=C(C=C1)C(=O)C2=C(SC3=C2C=CC(=C3)OCC4=CC=CC=C4)C5=CC=C(C=C5)OCC6=CC=CC=C6	0.38826 5	6.91 3335
CN(CCCN(CC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)CCC5=CC=C(C=C5)C(=O)OC)C6CC6)C(=O)COCCOC	0.31625 6	6.54 3713
C/C=C(\C1=CC=C(C=C1)OCCOCCOCCOCCOCC(=O)O)/C2=C(SC3=C2C=CC(=C3)O)C4=CC=C(C=C4)C	0.45970	6.46 2287

	9	
CC(C(=O)NC(=O)C)N(C)C(=NC(=C)C(=C)NCCN(C)CCN(C)CCOC1=CC=C(C=C1)OC2=C(SC3=C2C=CC(=C3)O)C4=CC=C(C=C4)Br)C	0.32639	6.442669
CCC(CC)N(CCCN(C)C(=O)[C@H](C)CC(=O)C)CC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)CCC5CC=C(C=C5)C(=O)OC	0.30926	6.42439
COC1=CC2=C(C=C1)C(=C(S2)C3=CC=C(C=C3)Br)OC4=CC=C(C=C4)OCCOCCOCCOCC(=O)O	0.48776	6.360767
CCCCOC1CCC(CC1)OC(=O)C2=C3C(=C(C=C2)CC(=O)C4CCC(CC4)C(=O)OCCCCCCOC(=O)C=C)C=C(S3)C	0.41888	6.283383
CCCCCCC(=O)NCCCC(=O)OCN1C(=O)C=CC2=C1C=C(C=C2)OCCCCN3CCN(CC3)C4=CSC5=CC=CC=C54	0.45853	6.203345
CCCCCCC(=O)NCCCC(=O)OCN1C(=O)C=CC2=C1C=C(C=C2)OCCCCN3CCN(CC3)C4=CC5=CC=CC=C5S4	0.45853	6.203345
COC1=CC=C(C=C1)C2=C(C3=C(S2)C=C(C=C3)OC)OC4=CC=C(C=C4)OCCOCCOCCOCC(=O)O	0.49089	6.181767
CCC(CC)N(CCN(C)CC1=CC=CC=C1C(=O)OCC)CC2=CC(=CC=C2)C(=O)NC3=C(C4=C(S3)CCCC4)C(=O)NC5=CC=C(C=C5)CCC6=CC=C(C=C6)C(=O)OC	0.31227	6.164234
COC1=CC=C(C=C1)C2=C(C3=C(S2)C=C(C=C3)OC)C(=O)C4=CC=C(C=C4)OCCOCCOCCOCCO	0.52286	6.161974
CCN(CC)C1=CC=C(C=C1)NC(=O)C2=CC=C(C=C2)NC(=O)C3=C(SC4=C3CCCC4)NC(=O)C5=CC=CC(=C5)CNCCOCCI	0.34560	6.132159
CCC(CC)N(CCN(C)CC(=O)OCC)CC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)CCC5=CC=C(C=C5)C(=O)OC	0.33916	6.103921
COC1=CC=C(C=C1)C2=C(C3=C(S2)C=C(C=C3)OC)C(=O)C4=CC=C(C=C4)OCCOCCOCCOCC(=O)O	0.45761	6.101767
CCOC(=O)C1=CC=C(C=C1)CCC2=CC=C(C=C2)NC(=O)C3=C(SC4=C3CCCC4)NC(=O)C5=CC=CC(=C5)CN(C6CCC(CC6)C(=O)CCCI)C7CC7	0.32298	6.092829
CCOC(=O)CCCN(C)CCN(CC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)CCC5=CC=C(C=C5)C(=O)OC)C6CC6	0.33991	6.083764
CC[C@H](C)CONC(=O)C1=CC2=C(S1)C=CC(=C2)NC(=O)CC3=CC=C(C=C3)OCCCC(=O)N[C@@H](CC4=CC=CC=C4)C(=O)OC5CCCC5	0.33717	5.933135
CC(C)(C)[Si](C)(C)OCCC(C(=O)C1=NC(=C(C=C1)OC)C2=CSC3=C2C=CC=C3F)NC(=O)C4=CC(=C(C=C4)OCCOCC5=CC=C(C=C5)OC)OC	0.34198	5.882963

C1=CC=C(C=C1)COC2=CC=C(C=C2)C3=C(C4=C(S3)C=C(C=C4)OCC5=CC=CC=C5)C(=O)C6=CC=C(C=C6)OCCOCCOCC(=O)O	0.42103	5.882131
CC(C)(C)OC(=O)COCCOCCOCCOC1=CC=C(C=C1)C(=O)C2=C(SC3=C2C=CC(=C3)OC)C4=CC=C(C=C4)OC	0.45560	5.862393
CCOP(=O)(CC)CCCC(=O)N(CC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)CCC5=CC=C(C=C5)C(=O)OC)C(C)C	0.30673	5.79342
COC1=CC2=C(C=C1)C(=C(S2)C3=CC=CC=C3)OC4=CC=C(C=C4)OCCOCCOCCOCC(=O)O	0.54721	5.781661
CCC(CC)N(CCN(C)CC1=CC=C(C=C1)C(=O)OC)CC2=CC(=CC=C2)C(=O)NC3=C(C4=C(S3)CCCC4)C(=O)NC5=CC=C(C=C5)CCC6=CC=C(C=C6)C(=O)OC	0.31691	5.724077
CCOC(=O)CCCCCN(CC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)CCC5=CC=C(C=C5)C(=O)OC)C6CC6	0.35854	5.693499
COC1=CC2=C(C=C1)C(=C(S2)C3=CC=C(C=C3)O)C(=O)C4=CC=C(C=C4)OCCOCCOCCOCC(=O)O	0.43640	5.661611
COC1=CC=C(C=C1)C2=C(C3=C(S2)C=C(C=C3)O)C(=O)C4=CC=C(C=C4)OCCOCCOCCOCC(=O)O	0.43640	5.661611
C1CN(CCN1CCOCC(=O)O)CCOC2=CC=C(C=C2)C(=O)C3=C(SC4=C3C=CC(=C4)OCC5=CC=CC=C5)C6=CC=C(C=C6)OCC7=CC=CC=C7	0.39473	5.562869
C1CN(CCN1CCOCCOCC(=O)O)C2=CC=C(C=C2)C(=O)C3=C(SC4=C3C=CC(=C4)OCC5=CC=CC=C5)C6=CC=C(C=C6)OCC7=CC=CC=C7	0.39475	5.562869
CC(C)COC(C)ONC(=O)C1CC2=C(S1)C=C(C=C2)CNCC3=CC=C(C=C3)CN[C@@H](CC4=CC=CC=C4)C(=O)O	0.45125	5.512767
CC(C)(C)OC(=O)COCCOCCOCCOC1=CC=C(C=C1)CCC2=C(SC3=C2C=CC(=C3)O)C4=CC=C(C=C4)O	0.45838	5.482444
CC(C)COC(C)ONC(=O)C1=CC2=C(S1)C=C(C=C2)CNCC3CCC(CC3)CN[C@@H](C4=CC=CC=C4)C(=O)OC(=C)C	0.46779	5.413236
CCC(CC)N(CCN(C)C(=O)CCl)CC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)CCC5=CC=C(C=C5)C(=O)OC	0.36295	5.403269
CCO[P+](=O)CCCC(=O)N(CC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)CCC5=CC=C(C=C5)C(=O)OC)C(C)C	0.31695	5.403023
CCC(CC)N(CCCNC)CC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)CCC5=CC=C(C=C5)C(=O)OC	0.41257	5.383709

	0.48462	5.376
CCCN(CCOC1=CC(=C(C=C1)OCC(=O)O)C)S(=O)(=O)C2=C(C3=C(S2)C=CC(=C3)Cl)C		0403
CCOC([C@H](C)N(CC1=CSC2=CC=CC=C21)C(=O)[C@H](CCCCNC(=O)OC(C)(C)C)NC(=O)O)OCC	0.42368	5.352822
CCOC(C(C)N(CC1=CSC2=CC=CC=C21)C(=O)C(CCCCNC(=O)OC(C)(C)C)NC(=O)O)OCC	0.42368	5.352822
CCC(CC)N(CCN1CCC(CC1)C(=O)OCC)CC2=CC(=CC=C2)C(=O)NC3=C(C4=C(S3)CCCC4)C(=O)NC5=CC=C(C=C5)CCC6=CC(=C(C=C6)C(=O)OC)C	0.31960 7	5.34439
CCCCCCCCN(CCCN)CCCN.C1CS(=O)C(=NO1)C2=CC3=CC=CC=C3S2	0.57870 9	5.342749
CCC(CC)N(CC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)CCN5CCOCC5)C(=O)CCC(C)(C)C(=O)CC	0.37516 9	5.324128
C1=CC(=CC=C1C2=C(C3=C(S2)C=C(C=C3)O)OC4=CC=C(C=C4)OCCOCCOCCOCC(=O)O)O	0.44655	5.301454
CCC(CC)N(CC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)CCCN5CCN(CC5)C)C(=O)CCC(C)(C)C(=O)O	0.33807 2	5.274237
CCOC(=O)CCCCN(CC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)CCC5=CC=C(C=C5)C(=O)OC)C6CC6	0.36453 9	5.253342
CCOC([C@@H](C)N(CC1=CSC2=CC=CC=C21)C(=O)[C@H](CCCCNC(=O)O)N)OCC	0.52663 8	5.252297
C1=CC(=CC=C1C2=C(C3=C(S2)C=C(C=C3)O)C(=O)C4=CC=C(C=C4)OCCOCCOCCOCC(=O)O)O	0.41783 7	5.221454
COC1=C(C=CC(=C1)C(=O)NCC(=O)C2=CC=CC(=N2)C3=CSC4=C3C=CC=C4F)OCCOCOCC[Si](C)(C)C	0.48110 8	5.201969
CN(CCOCCOCC(=O)O)CCOC1=CC=C(C=C1)C(=O)C2=C(SC3=C2C=CC(=C3)O)C4=CC=C(C=C4)O	0.42328 1	5.15177
CCC1(CCC1C(=O)C2=CSC3=CC=CC=C32)C(=O)N(CCCS(=O)(=O)NCC4=C(C=C(C=C4)OC)OC)CC5=CC=C(C=C5)Cl	0.41958 1	5.121938
C1CN(CCN1CCCCOC2=CC3=C(C=C2)C=CC(=O)N3COC(N(CCO)CCO)O)C4=C5C=CSC5=CC=C4	0.41887 6	5.062669
CCC1(CCC1C(=O)C2=CSC3=CC=CC=C32)C(=O)N(CCCS(=O)(=O)NCC4=C(C=C(C=C4)OC)OC)[C@@H](C)C5=CC=C(C=C5)Cl	0.41234 5	5.062095
CC(C)C1(CCC1C(=O)C2=CSC3=CC=CC=C32)C(=O)N(CCCS(=O)(=O)NCC4=C(C=C(C=C4)OC)OC)CC5=CC(=CC=C5)Cl	0.41227 4	5.062095

CC(C)(C)OC(=O)COCCOCCOCCOC1=CC=C(C=C1)OC2=C(SC3=C2C=CC(=C3)O)C4=CC=C(C=C4)O	0.43989	5.068208
CCCCCCCOC1=CC=C(C=C1)C2=CN=C(N=C2)C3=CC=C(C=C3)C[C@@H](C(=O)N[C@H](C)C(=O)O)NC(=O)C4=CC5=C(S4)CCC(C5)C	0.35635	5.023189
CCC(CC)N(CCNC)CC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)CCC5=CC=C(C=C5)C(=O)O	0.39809	5.003396
CCCCOC(=O)C1=C(SC2=C1CC(CC2)(C)C)C3CCCC3COC4=CC=C(C=C4)C[C@H]5[C@H](OC(N5C(=O)OC(C)(C)C)(C)C)CN(CC(C)C)S(=O)(=O)C6=CC=C(C=C6)OC	0.28986	4.984679
CCC(CC)N(CCCN(C)C(=O)OC(C)(C)C)CC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)CCC5=CC=C(C=C5)C(=O)OC	0.32877	4.984234
CCCCN(CCCNC(=O)[C@H](CC(C)C)NC(=O)C1=CC2=CC=CC=C2S1)S(=O)(=O)C3=CC=CC=C3N	0.43800	4.982334
CCCCOC(=O)C1=C(SC2=C1CC(CC2)(C)C)C3=C(CCC3)COC4=CC=C(C=C4)C[C@H]5[C@H](OC(N5C(=O)OC(C)(C)C)(C)C)CN(CC(C)C)S(=O)(=O)C6=CC=C(C=C6)OC	0.29044	4.964523
CCC(CC)N(CCCN)CC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)CCC5=CC=C(C=C5)C(=O)OC	0.38396	4.943553
CCOC([C@H](C)N(CC1=CSC2=CC=CC=C21)C(=O)[C@H](CC(=O)NC(C3=CC=CC=C3)(C4=CC=CC=C4)C5=CC=CC=C5)NC(=O)O)OCC	0.37639	4.932873
CCC(CC)N(CC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)CCN5CCOCC5)C(=O)CCC(C)(C)C(=O)O	0.33730	4.903764
CC(C)COC(C)ONC(=O)C1CC2=C(S1)C=C(C=C2)CNCC3=CC=C(C=C3)OC4=CCC(C=C4)[C@@H](C(=O)OC5CCCC5)NC(=O)OC(C)(C)C	0.32044	4.891371
COC(=O)[C@H](CC1=CSC2=CC=CC=C21)NCC(CC3=CC=C(C=C3)C4=CC=CC=C4)(CP(=O)(CCC5=CC=CC=C5)O)C=O	0.47329	4.892208
CC(C)NCCCN(CC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)CCC5=CC=C(C=C5)C(=O)OC)C(C)C	0.41257	4.883709
CCCCOC(=O)C1=C(SC2=C1CC(CC2)(C)C)C3=CC=CC=C3COC4=CC=C(C=C4)C[C@H]5[C@H](OC(N5C(=O)OC(C)(C)C)(C)C)CN(CC(C)C)S(=O)(=O)C6=CC=C(C=C6)OC	0.28758	4.864366
CCCC1=CC=C(C=C1)CCC(=O)OC2CCC(CC2)C(=O)OC3=C4C=C(SC4=C(C=C3)OC(=O)C5CCC(CC5)OC(=O)CCC6=CC=C(C=C6)CCC)C7=CC=C(C=C7)Cl	0.32956	4.863463
COCCOCC(=O)N(CC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)CCC5=CC=C(C=C5)C(=O)OC)C6CC6	0.34988	4.832978
CCCCOC(=O)C1=C(SC2=C1CC(CC2)(C)C)CCC3=CC=C(C=C3)C[C@H]4[C@H](OC(N4C(=O)	0.32	4.78

OC(C)(C)C)(C)C)CN(CC(C)C)S(=O)(=O)C5=CC=C(C=C5)OC	926	4261
CCCCCCCOC1=CC=C(C=C1)C2=CN=C(N=C2)C3=CC=C(C=C3)C[C@@H](C(=O)O)NC(=O)CC4=CC5=CC=CC=C5S4	0.46636	4.772505
CCCCCCCOC1=CC=C(C=C1)C2=CN=C(N=C2)C3=CC=C(C=C3)CC(C(=O)O)NC(=O)CC4=CC5=CC=CC=C5S4	0.46636	4.772505
CCCC1=CC=C(C=C1)CCC(=O)OC2CCC(CC2)C(=O)OC3=C4C=C(SC4=C(C=C3)OC(=O)C5CCC(CC5)OC(=O)CCC6=CC=C(C=C6)CCC)C7=CC=CC=C7	0.34160	4.723852
CCC(CC)N(CC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)C(C)(C)CN5CCN(CC5)C)C(=O)CCC(C)(C)C(=O)O	0.33267	4.714393
CCC(CC)N(CC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)C(C)(C)CN5CCN(CC5)C)C(=O)CCC(C)(C)C(=O)OC	0.34974	4.659455
CCNCCNCC1=CC=C(C=C1)C(=O)CCC2=C(C3=CC(=C(C=C3S2)OC(=O)C)Br)C(=O)N	0.47471	4.650984
CC1(CCN1C(=O)CC2=CSC3=CC=CC=C32)C(=O)N(CCCS(=O)(=O)NCC4=C(C=C(C=C4)OC)OC)CC5=CC=C(C=C5)Cl	0.40919	4.631891
C[C@@H](C1=CC=C(C=C1)Cl)N(CCCS(=O)(=O)NCC2=C(C=C(C=C2)OC)OC)C(=O)C3(CCC3C(=O)C4=CSC5=CC=CC=C54)C	0.41963	4.621938
CC1(CCN1C(=O)CC2=CSC3=CC=CC=C32)C(=O)N(CCCS(=O)(=O)N(C)CC4=C(C=C(C=C4)OC)OC)CC5=CC=C(C=C5)Cl	0.42657	4.572047
CCN(CC)CCNCC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)CCC5=CC=C(C=C5)C(=O)OC	0.43497	4.56324
CCC(CC)N(CCN)CC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)CCC5=CC=C(C=C5)C(=O)O	0.37288	4.56324
C1CSC2=CC=CC(=C21)N3CCN(CC3)CCCCOC4=CC5=C(C=C4)C=CC(=N5)OCOC(=O)N(CCO)CCO	0.44286	4.562669
CCCOCCC(C)(C)CC(C)(C)CCN1CCN([C@@H](C1=O)C2=CC=C(C=C2)NC3=NC(=CN(C3=O)C)C4=C(C(=CC=C4)NC(=O)C5=CC6=C(S5)CCCC6)C)C	0.35172	4.544553
CCC(CC)N(CCN(C)C(=O)OC(C)(C)C)CC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)CCC5=CC=C(C=C5)C(=O)OC	0.33392	4.544077
C1CN(CCN1CCCCOC2=CC3=C(C=C2)C=CC(=N3)OCOC(=O)N(CCO)CCO)C4=C5C=CSC5=CC=C4	0.44919	4.542512
CSCC[C@@H](C(=O)OC1CCCC1)NCC2=CC=C(C=C2)CNCC3=CC4=C(CC(S4)C(=O)NO)C=C3	0.51116	4.532225

COC1=CC=C(C=C1)C2=C(C3=C(S2)C=C(C=C3)CO)OC4=CC=C(C=C4)OCCN5CCC(CC5)CCCO[N+](=O)[O-]	0.46968	4.521243
COC1=C(C=C(C=C1)C(=O)NCC(C2=C(N=C(N2COCC[Si](C)(C)C)C3=CSC4=C3C=CC=C4F)Br)O)OC	0.45916	4.491078
C1CC2=C(C=CC(=C2O)O)[C@H]([C@@H]1NCCCCCCOCCCCC3=CC4=C(CCS4(=O)=O)C=C3)O	0.47829	4.472498
CC(C)CN(C[C@@H]1[C@@H](N(C(O1)(C)C)C(=O)OC(C)(C)C)CC2=CC=C(C=C2)OCC3=C(CCC3)C4=C(C5=C(S4)CCC(C5)(C)C)C(=O)OCC(C)C)S(=O)(=O)C6=CC=C(C=C6)OC	0.29044	4.464523
CCCCC1(C2=CC=CC=C2C3=C1C=C(C=C3)N(C4=CC=C(C=C4)C5=CC=C(S5)C=C6/C(=C(\C#N)/C(=O)O)/C7=CC=CC=C7S6(=O)=O)C8=CC9=C(C=C8)C1=CC=CC=C1C9(CCCC)CCCC)CCCC	0.30971	4.464151
CCC(CC)N(CC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)CCC5=CC=C(C=C5)C(=O)OC)CC6=CC(=CC=C6)C(=O)OC	0.34399	4.453499
CCCC1=CC=C(C=C1)CCC(=O)OC2CCC(CC2)C(=O)OC3=C4C=CC(=NC4=C(C=C3)OC(=O)C5CCC(CC5)OC(=O)CCC6=CC=C(C=C6)CCC)C7=CC8=CC=CC=C8S7	0.29921	4.433961
CC1([C@H]([C@@H]([C@H](C1=O)C/C=C\CCCC(=O)NCCO)/C=C/C(CC2=CC3=CC=CC=C3S2)O)N=O)C	0.48637	4.422345
CCCCCCCOC1=CC=C(C=C1)C2=CN=C(N=C2)C3=CC=C(C=C3)C[C@@H](C(=O)O)NC(=O)C4=CC5=C(S4)CCCC5	0.47300	4.372661
CC(C)CN(C[C@@H]1[C@@H](N(C(O1)(C)C)C(=O)OC(C)(C)C)CC2=CC=C(C=C2)OCC3=CC=CC=C3C4=C(C5=C(S4)CCC(C5)(C)C)C(=O)OCC(C)C)S(=O)(=O)C6=CC=C(C=C6)OC	0.28758	4.364366
CC1=C(C=CC(=C1)OCCCS(=O)(=O)C)C2=CSC3=C2C=C(C=C3)COC4=CC=C(C=C4)C(CC(=O)O)C=C	0.53718	4.34164
CC1=C(C=CC(=C1)OCCCS(=O)(=O)C)C2=CSC3=C2C=C(C=C3)OCC4=CC=C(C=C4)C(CC(=O)O)C=C	0.53718	4.34164
CCC(CC)N(CC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)CCCC5=CC=C(C=C5)C(=O)OC)C(=O)C6=CC=C(C=C6)C(=O)OC	0.30202	4.333448
CCCCCCCOC1=CC=C(C=C1)C2=CN=C(N=C2)C3=CC=C(C=C3)C[C@@H](C(=O)O)NC(=O)C4=CC5=CC=CC=C5S4	0.47581	4.332348
CCCCCCCOC1=CC=C(C=C1)C2=CN=C(N=C2)C3=CC=C(C=C3)CC(C(=O)O)NC(=O)C4=CC5=CC=CC=C5S4	0.47581	4.332348
CCCCCCCOC1=CC=C(C=C1)C2=CN=C(N=C2)C3=CC=C(C=C3)C[C@@H](C(=O)O)NC(=O)C4=CC5=C(S4)CCC(C5)C	0.46373	4.312818
CCCCCCCOC1=CC=C(C=C1)C2=CN=C(N=C2)C3=CC=C(C=C3)CC(C(=O)O)NC(=O)C4=CC5=C(S4)CCC(C5)C	0.46373	4.312818

C[C@@H](C(=O)N[C@@H](CC1=CSC2=CC=CC=C21)C(=C)N[C@@H](CC3=CC=CC=C3)C(=O)[C@]4(CO4)C)NC(=O)OCC5=CC=CC=C5	0.43948	4.312454
CCOC(=O)C1=C(SC2=C1CCCC2)N(COCC[Si](C)(C)C)S(=O)(=O)C3=CC=CC=C3/C=C\CO	0.53329	4.311832
CCCN(CC(CC)OC1=CC(=C(C=C1)OC(=C)C(=O)O)C)S(=O)(=O)C2=C(C3=C(S2)C=CC(=C3)Cl)C	0.53477	4.311203
CCC(CC)N(C[C@@H]1CCCN1)CC2=CC(=CC=C2)C(=O)NC3=C(C4=C(S3)CCCC4)C(=O)NC5=CC=C(C=C5)CCC6=CC=C(C=C6)C(=O)OC	0.40655	4.303709
COC(=O)[C@H](CCCOC1=CC=C(C=C1)CNCC2=CC3=C(C=C2)C=C(S3)C(=O)NO)NC4CCCCC4	0.48831	4.292454
CC(C)CN(C[C@@H]1[C@@H](N(C(O1)(C)C)C(=O)OC(C)(C)C)CC2=CC=C(C=C2)CCC3=C(C4=C(S3)CCC(C4)(C)C)C(=O)OCC(C)C)S(=O)(=O)C5=CC=C(C=C5)OC	0.32925	4.284261
CCCCCCCOC1=CC=C(C=C1)C2=CN=C(N=C2)C3=CC=C(C=C3)C[C@@H](C(=O)O)NC(=O)C4=CC5=C(S4)C=C(C=C5)C	0.46643	4.272505
CCCCCCCOC1=CC=C(C=C1)C2=CN=C(N=C2)C3=CC=C(C=C3)CC(C(=O)O)NC(=O)C4=CC5=C(S4)C=C(C=C5)C	0.46643	4.272505
C1CN(CCN1CCOCC(=O)O)CCOC2=CC=C(C=C2)OC3=C(SC4=C3C=CC(=C4)O)C5=CC=C(C=C5)Br	0.4837	4.261086
C1CN(CCN1CCOCCOC2=CC=C(C=C2)OC3=C(SC4=C3C=CC(=C4)O)C5=CC=C(C=C5)Br)CC(=O)O	0.4837	4.261086
CCCCOC(=O)CN(CC1=CSC(=C1)C(=O)OCCCC)C(=O)C2=CC3=C(S2)C=C(C=C3)O	0.57655	4.231436
CC/C(=C(\C1=CC=CC=C1)/C2=CC=C(C=C2)OCCN(C)C)/C3=CC=CC=C3.CC/C(=C(/CC)\C1=CC=C(C=C1)O)/C2=CC=C(C=C2)O.C1CCN(CC1)CCOC2=CC=C(C=C2)C(=O)C3=C(SC4=C3C=CC(=C4)O)C5=CC=C(C=C5)O	0.23827	4.225373
COC1=CC(=C(C=C1CC2=CC3=CC=CC=C3S2)C4([C@@H]([C@H]([C@H]([C@H](O4)CO)O)OCC5=CC=CC=C5)OCC6=CC=CC=C6)OC)OCC7=CC=CC=C7	0.41145	4.222757
CC(=O)/C=C\C1=C(C=C(C=C1)OCCCCN2CCN(CC2)C3=C4C=CSC4=CC=C3)NCOC(=O)NOC	0.53494	4.222406
C1CN(CCN1CCCCOC2=CC3=C(C=C2)C=CC(=O)N3COC(NCCO)O)C4=C5C=CSC5=CC=C4	0.48900	4.222406
C/C=C\C=C\OCCNC(=O)C1=C2CC(CC(C2=C(S1)SCCC=C)NO)C3=CC=C(C=C3)O	0.58914	4.201803
CCC1(CCN1C(=O)C2=CSC3=CC=CC=C32)C(=O)N(CCCS(=O)(=O)NCC4=C(C=C(C=C4)OC)OC)C5=CC=C(C=C5)Cl	0.41719	4.191734

	7	
CC1(CCN1C(=O)C2=CSC3=CC=CC=C32)C(=O)N(CCCS(=O)(=O)NCC4=C(C=C(C=C4)OC)OC)CC5=CC(=CC=C5)Cl	0.41675	4.191734
CC1(CCN1C(=O)C2=CSC3=CC=CC=C32)C(=O)N(CCCS(=O)(=O)NCC4=C(C=C(C=C4)OC)OC)CC5=CC=C(C=C5)Cl	0.41675	4.191734
CC(=C)SC[C@@H](C(=O)OC)NCC1=CC=C(C=C1)CNCC2=CC3=C(C=C2)C=C(S3)C(=O)NO	0.54886	4.191599
CCCC1=C(C=CC2=C1S(=O)(=O)C=C2CCC3=CC=CC=C3)OCCCCOC4=CC=CC(=C4)C5C(=O)N(C(=O)S5)N	0.425351	4.161858
COCCN(CC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)CCC5=CC=C(C=C5)C(=O)OC)C6CCC(CC6)C(=O)OC	0.333103	4.153448
CCCCOC(=O)CN(CC1=CC2=C(C=C1)SC(=C2)C(=O)OCCCC)C(=O)CC3CCCC4=C3C=CC(=C4)O	0.52408	4.152498
CCN(CC)CCNC(=O)C1=CC2=C(S1)C=C(C=C2)NC3=NC(=CC(=N3)NC4=NNC(=C4)C5CC5)CN=[N+]=[N-]	0.36814	4.152434
CCC(CC)N(C[C@@H]1CCCN1C(=O)O)CC2=CC(=CC=C2)C(=O)NC3=C(C4=C(S3)CCCC4)C(=O)NC5=CC=C(C=C5)CCC6=CC=C(C=C6)C(=O)OC	0.32418	4.143608
CCCC[C@@H](C(=O)O)N(C(=N)[C@H](CC1=CSC2=CC=CC=C21)NOCC3=CC=CC=C3)N	0.55040	4.142039
C1=CC=C2C(=C1)C=C(S2)C3=CN=C4N3N=C(C=C4)NC(CCCCO)C(CCCCN)O	0.55929	4.132198
C1=CC=C2C(=C1)C=C(S2)C3=CN=C4N3N=C(C=C4)NCCCCC(C(CCCCN)O)O	0.55929	4.132198
C1=CC=C2C(=C1)C=C(S2)C(CCCC(C3=CN=C4N3N=C(C=C4)NCCCCCO)O)N	0.56234	4.132198
CC1(CCN1C(=O)C2=CSC3=CC=CC=C32)C(=O)N(CCCS(=O)(=O)N(C)CC4=C(C=C(C=C4)OC)OC)CC5=CC=C(C=C5)Cl	0.43427	4.131891
CC1(CCN1C(=O)C2=CSC3=CC=CC=C32)C(=O)N(CCCS(=O)(=O)N(C)CC4=C(C=C(C=C4)OC)OC)CC5=CC(=CC=C5)Cl	0.43427	4.131891
CCC(CC)N(CC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CN=C(C=C4)C5(CC5)C)C(=O)CCC(C)(C)C(=O)O	0.36189	4.123345
CCOC1=CC=C(C=C1)C[C@H](C(=O)N[C@@H](CC2=CC=CC=C2)C(=O)NCC3=CC=C(C=C3)CN)NC(=O)OC4=CC5=CC=CC=C5S4	0.36486	4.102563
CC(C)C[C@@H](C(=O)NCCCCN(C)S(=O)(=O)C1=CC=CC=C1N)NC(=O)C2=CC3=CC=CC=C3S2	0.45230	4.102021

	0.45230	4.103
CCN(CCCNC(=O)[C@H](CC(C)C)NC(=O)C1=CC2=CC=CC=C2S1)S(=O)(=O)C3=CC=CC=C3N		2021
	0.37552	4.097
CCCCC(=O)C1CCC(CC1)N(CC2=CC(=CC=C2)C(=O)NC3=C(C4=C(S3)CCCC4)C(=O)NC5=CC=C(C=C5)CC6=CC=C(C=C6)C(=O)OC)C7CC7		3706
C1CN(CCN(C1)CCC2=CC3=C(C=C2)C(=O)N(C3)[C@H]4CCC(=O)NC4=O)CCCCCCC5=CC=C(C=C5)OC6=C(SC7=C6C=CC(=C7)O)C8=CC=C(C=C8)Br	0.34053	4.082607
	0.57665	4.085
CCCC[C@@H](C(=O)OC)N(C(=N)[C@H](CC1=CSC2=CC=CC=C21)NOCC3=CC=CC=C3)N		2195
	0.34709	4.077
CCOC(=O)C1CCC(CC1)N(CC2=CC(CC=C2)C(=O)NC3=C(C4=C(S3)CCCC4)C(=O)NC5=CC=C(C=C5)CCC6=CC=C(C=C6)C(=O)OCC)C7CC7		3812
	0.44457	4.071777
COC1=C(C=CC(=C1)CNCC2=CC3=C(C=C2)C=C(S3)C(=O)NO)OCCC[C@@H](C(=O)OC)N		
	0.34066	4.063608
CCOC(=O)CN1CCC(CC1)N(CC2=CC(=CC=C2)C(=O)NC3=C(C4=C(S3)CCCC4)C(=O)NC5=CC=C(C=C5)CCC6=CC=C(C=C6)C(=O)OC)C7CC7		
	0.40957	4.055
CCC(C(=O)O)N1CCC(CC1)N(CC2=CC(=CC=C2)C(=O)NC3=C(C4=C(S3)CCCC4)C(=O)NC5=CC=C(C=C5)N(CC)CC)C6CC6		3662
	0.34790	4.059655
CCOC(=O)C1CCC(CC1)N(CC2=CC(=CC=C2)C(=O)NC3=C(C4=C(S3)CCCC4)C(=O)NC5=CC=C(C=C5)CCC6=CC=CC=C6C(=O)OCC)C7CC7		
	0.34790	4.059655
CCOC(=O)C1CCC(CC1)N(CC2=CC(=CC=C2)C(=O)NC3=C(C4=C(S3)CCCC4)C(=O)NC5=CC=C(C=C5)CCC6=CC=C(C=C6)C(=O)OCC)C7CC7		
	0.31924	4.051
COC(=O)C1=CC=C(C=C1)CCC2=CC=C(C=C2)NC(=O)C3=C(SC4=C3CCCC4)NC(=O)C5=CC=CC(=C5)CN(CC(=O)N6CCN(CC6)CC=O)C7CC7		3404
	0.44394	4.045
C1CN(CCN1CCCCOC2=CC3=C(C=C2)C=CC(=O)N3COC(=O)N(CCO)CCO)C4=C5C=CSC5=CC=C4		2512
COC(=O)CNCC(=O)OCN1C(=O)CCC2=C1C=C(C=C2)OCCCCN3CCN(CC3)C4=C5C=CSC5=CC=C4	0.46267	4.042512
	0.44546	4.045
CCC(CCN(C)S(=O)(=O)C1=CC=CC=C1N)NC(=O)[C@H](CC(C)C)NC(=O)C2=CC3=CC=CC=C3S2		2178
	0.52529	4.031828
CCCC/C(=N\NC(=O)CNC(=O)C1=CC(=C(C=C1)OCCO)OC)/C2=CSC3=CC=CC=C32		
	0.56737	4.036
CCOC1=C(C=C(C=C1)C(=O)NCC(=O)N/N=C(\CCCOC)/C2=CSC3=CC=CC=C32)OC		1828
	0.45937	4.027
COC(=O)CNCC(=O)OCN1C(=O)C=CC2=C1C=C(C=C2)OCCCCN3CCN(CC3)C4=C5C=CSC5=CC=C4		2356
CC(C)C[C@@H](C(=O)NCCCN(C1CC1)S(=O)(=O)C2=CC=CC=C2N)NC(=O)C3=CC4=CC=CC	0.44	4.02

=C4S3	5088	2021
CC1([C@H](C([C@H](C1=O)C/C=C\CCCC(=O)ON)/C=C/C(CC2CC3=CC=CC=C3S2)N=O)ON)C	0.44610	4.012297
CCC(C(=O)O)OC1=C(SC2=C1C=CC(=C2)OCC3=C(C=C(C=C3)Cl)Cl)C(=O)NCCOC	0.56408	4.010623
CC1(CC(=O)N(C2=C1C=CC(=C2)OCCCCN3CCN(CC3)C4=C5C=CSC5=CC=C4)COC(NCC(=O)OC)O)C	0.44836	4.002825
CC(=O)NCCCC(=O)OCN1C(=O)C=CC2=C1C=C(C=C2)OCCCCN3CCN(CC3)C4=C5C=CSC5=CC=C4	0.50084	4.002563
COC(=O)[C@H](CCCCC1=CC=C(C=C1)COC(=O)N[C@@H](CC2=CSC3=CC=CC=C32)C(=O)O)N	0.46124	3.981825
CCC(=O)C1=CC=C(C=C1)CCC2=CC=C(C=C2)NC(=O)C3=C(SC4=C3CCCC4)NC(=O)C5=CC=CC(=C5)CNC6(CC6)C(=O)OCC	0.39272	3.972923
COP(=O)(O)OCOC1=NC2=C(C=CC(=C2)OCCCCN3CCN(CC3)C4=C5C=CSC5=CC=C4)C=C1	0.52742	3.971749
COC(=O)CCCNC(=O)OCN1C(=O)C=CC2=C1C=C(C=C2)OCCCCN3CCN(CC3)C4=C5C=CSC5=CC=C4	0.46073	3.962512
CCOC(=O)CCNC(=O)OCN1C(=O)C=CC2=C1C=C(C=C2)OCCCCN3CCN(CC3)C4=C5C=CSC5=CC=C4	0.46073	3.962512
CC#S[C@@H](CC(=O)O)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCCCS(=O)(=O)C)C	0.51263	3.965361
CC1=CC2=C(C=C1)C(=C(S2)C3=CC=C(C=C3)OC(=O)C)OC4=CC=C(C=C4)OCCN5CCC(CC5)CCCO[N+](=O)[O-]	0.47161	3.942243
CC(CCN)C(C(CC(C)CO)NC1=NN2C(=NC=C2C3=CC4=CC(=C(C=C4S3)OC)OC)C=C1)O	0.44957	3.938241
CC(CCN)C(C(C(C)CCNC1=NN2C(=NC=C2C3=CC4=CC(=C(C=C4S3)OC)OC)C=C1)O)O	0.44957	3.938241
CCCCCOC1=CC2=C(C=C1)C=C(S2)C(=O)CC(CCN3C(=O)C4=CC=CC=C4N=N3)C(=O)O	0.51824	3.931671
CCOC1=C(C=C2C=CSC2=C1)CCNC3=NC(=NC=C3)C4=C(C(=CC=C4)OCC(=O)O)OCC	0.54845	3.931671
CCCN(CCSC1=C(C=C(C=C1)CC(=O)O)Cl)S(=O)(=O)C2C(C3=C(S2)C=CC(=C3)Cl)C	0.63	3.93

	0405	0323
CCC1CC(CC2=C1C(=C(S2)NCCCN3CCC(CC3)C)C(=O)O)C.COC(=O)C1=C(SC2=C1CCC2)NCCCN3CCOCC3	0.40567	3.923849
CC1(CC(=O)N(C2=C1C=CC(=C2)OCCCCN3CCN(CC3)C4=C5C=CSC5=CC=C4)COC(=O)CNCC(=O)OC)C	0.45213	3.922825
COC1=C(C=C(C=C1)C(=O)NCC(C2=CN=C(N2COCC[Si](C)(C)C)C3=CSC4=C3C=CC=C4F)O)OC	0.51217	3.911972
CCC(CC)N(C[C@@H]1CCCN1C(=O)OC(C)(C)C)CC2=CC(=CC=C2)C(=O)NC3=C(C4=C(S3)CCCC4)C(=O)NC5=CC=C(C=C5)CCC6=CC=C(C=C6)C(=O)OC	0.32449	3.904234
CCC(CC)N(CC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)CCC5=CC=C(C=C5)C(=O)OC)C[C@]6(CCCN6C(=O)O)C(C)(C)C	0.30447	3.904234
CC1=C(C=CC(=C1)OCCCS(=O)(=O)C)C2=CSC3=C2C=C(C=C3)COC4=CC=C(C=C4)C(=C)CC(=O)O	0.54861	3.901484
CCC(CC)N(CC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)CCC5=CC=C(C=C5)C(=O)OC)C(=O)C6=CC=C(C=C6)C(=O)OC	0.30672	3.893291
COC1=C(C=C(C=C1)C(=O)NCC(=O)C2=CN=C(N2COCC[Si](C)(C)C)C3=CSC4=C3C=CC=C4F)OC	0.52542	3.891816
C1CCC(C1)C[C@@H](C(=O)NCCCN(C2CC2)S(=O)(=O)C3=CC=CC=C3N)NC(=O)C4=CC5=CC=CC=C5S4	0.43100	3.882178
CCN(CC)CCOC1=C(C=CC2=C1SC(=C2C(=O)OCC)N)C3=CC(=CC(=C3)CN=[N+]=[N-])N=[N+]=[N-]	0.38652	3.882005
C1=CC(=CC=C1C2=C(C3=C(S2)C=C(C=C3)O)C(=O)C4=CC=C(C=C4)OCCOCCOCC(=O)O)O	0.47198	3.881192
CCCN(C(C)COC1=CC(=C(C=C1)OC(=C)C(=O)O)C)S(=O)(=O)C2=C(C3=C(S2)C=CC(=C3)Cl)C	0.54 61	3.871047
C=C(C1=CC=C(C=C1)OCCOCCOCC(=O)O)C2=C(SC3=C2C=CC(=C3)O)C4=CC=C(C=C4)O	0.52818	3.861399
CCN(CC)CCNC(=O)C1=CC2=C(S1)C=C(C=C2)NC3=NC(=CC(=N3)N/C(=C/C(=C)C4CC4)/N)C	0.51829	3.852624
CCCCC1=CC2=C(C=C1)C=C(S2)CC(C)C(=O)C3=C(C=C(OC3=O)C(C)CC/C=C/NC(=O)OC)O	0.51 218	3.852185
CCCCC1=CC2=C(C=C1)SC(=C2)CC(C)C(=O)C3=C(C=C(OC3=O)C(C)CC/C=C/NC(=O)OC)O	0.51 218	3.852185
CCCCC1=CC2=C(C=C1)SC(=C2)C[C@H](C)C(=O)C3=C(C=C(OC3=O)C(C)CC/C=C/NC(=O)O	0.51	3.85

C)O	218	2185
CCOC1=CC=CC=C1CCC(=O)NC2=C(C3=C(S2)CC(CC3)COC(=O)NC/C(=C/C=C)/C=C\N)N	0.44 392 9	3.84 2457
C[C@@H](C(=O)NC(CC1=CSC2=CC=CC=C21)C(=O)N[C@@H](CC3=CC=CC=C3)C(=O)[C@]4(CO4)C)NC(=O)OCC5=CC=CC=C5	0.39 256 6	3.83 2247
CCCCN(CCCC)C1=CC=C(C=C1)/C=C\2/C(=C/C(=N\N(C)C=N)/C(=O)O)/C3=CC=CC=C3S2(=O)=O	0.48 677 4	3.82 2301
CC1=C(C=CC(=C1)OCCCS(=O)(=O)C)C2=CSC3=C2C=C(C=C3)COC4=CC=C(C=C4)CCC5=NNN=N5	0.47 854 2	3.82 1708
CC(C)N(CC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)CCC5=CC=C(C=C5)C(=O)O)C6CCC(CC6)C(=O)OCC7=CC=CC=C7	0.31 318 4	3.81 3655
CCOC(=O)C1(CC1)N(CC2=CC(=CC=C2)C(=O)NC3=C(C4=C(S3)CCCC4)C(=O)NC5=CC=C(C=C5)CCC6=CC=C(C=C6)C(=O)OC)C(C)C	0.37 072	3.81 3186
CC(C)CN(C[C@@H]1[C@@H](CC(O1)(C)C)CC2=CC=C(C=C2)NCC3CCCCC3C4=C(C5=C(S4)CCC(C5)(C)C)C(=O)OC(C)(C)C)S(=O)(=O)C6=CC=C(C=C6)OC	0.37 647	3.80 4519
C1CC(=O)NC(=O)C1NCC2=C(C=CC(=C2)N3CC(C3)N4CCC(CC4)OC5=CC=C(C=C5)OC6=C(SC7=C6C=CC(=C7)OCC8=CC=CC=C8)C9=CC=C(C=C9)Br)C(=O)O	0.27 773 2	3.80 2192
CC#S[C@@H](CC1=NNN=N1)C2=CC=C(C=C2)OCC3=CC4=C(C=C3)SC=C4C5=C(C=C(C=C5)OCCCS(=O)(=O)C)C	0.44 114 6	3.80 1586
CCCCCOC1=CC2=C(C=C1)C=C(S2)C(=O)CC(CCN3C(=O)C4=CC=CC=C4N=N3)(C(=O)OC(C)(C)C)C(=O)OC(C)(C)C	0.37 704 9	3.79 2822
CCCCC1=CC2=C(C=C1)SC(=C2)CC(C)(C)C(=O)C3=C(C=C(OC3=O)C(C)CC/C=C/NC(=O)OC)O	0.50 114 5	3.79 2342
CCCCC1=CC2=C(C=C1)C=C(S2)CC(C)(C)C(=O)C3=C(C=C(OC3=O)C(C)CC/C=C/NC(=O)OC)O	0.50 114 5	3.79 2342
CC#CC(CC(=O)O)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCCCS(=O)(=O)C)C	0.52 756 2	3.76 164
CC#CC(CC(=O)O)C1=CC=C(C=C1)COC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCCCS(=O)(=O)C)C	0.52 756 2	3.76 164
CC1([C@H]([C@@H]([C@H](C1=O)CCCCC(=O)OC=O)/C=C/C(CCC2=C(C3=CC=CC=C3S2)Cl)O)O)C	0.54 166	3.76 153
CC(C)N(CC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)CCC5=CC=C(C=C5)C(=O)OC)C6CCC(CC6)C(=O)OCC7=CC=CC=C7	0.32 912 4	3.75 3812
C1CCN(CC1)CCNC(=O)C2=CC(=CN2CCN3CCOCC3)NC(=O)C4=CC(=CN4CC5CC5)NC(=O)C6=C(C7=CC=CC=C7S6)Cl	0.37 936	3.75 2864

	2	
CC1(CCN1C(=O)C2=CSC3=CC=CC=C32)C(=O)N(CCCS(=O)(=O)NCC4=C(C=C(C=C4)OC)OC)C5=CC=C(C=C5)Cl	0.42448	3.751578
C[C@H]1CCN(C1)CCC2=CC=C(C=C2)OC3=C(SC4=C3C=CC(=C4)OC5ON(C[C@H]5C)CCC6=CC=C(C=C6)OC7=C(SC8=C7C=CC(=C8)O)C(=O)C9=C(C=CC(=C9)F)C)C(=O)C1=C(C=CC(=C1)C)C	0.33449	3.743435
CCC1=CC(=CC(=C1C2=C3CCC(C3=CC=C2)OC4=CC5=C(C=C4)[C@@H](CS5)CC(=O)O)CC)OCCCS(=O)(=O)C	0.51393	3.745211
CC1=C(SC2=C1C=C(C=C2)Cl)C(=O)N[C@@H](CC(C)C)C(=O)NCCCN(C)S(=O)(=O)C3=CC=CC=C3N	0.43282	3.741632
CCN(CC)C1=CC=C(C=C1)NC(=O)C2C(SC3=C2CCCC3)NC(=O)C4=CC=CC(=C4)CN(C5CC5)C6CCN(CC6)CC(=O)O	0.42278	3.693505
CC1(CCN1C(=O)C2=CSC3=CC=CC=C32)C(=O)N(CCS(=O)(=O)N(C)CC4=C(C=C(C=C4)OC)OC)CC5=CC=C(C=C5)Cl	0.44169	3.691734
CCC(CC)NCC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CN=C(C=C4)CCC5=CC=C(C=C5)C(=O)OC	0.42423	3.682927
COC1=CC=C(C=C1)COCCOC2=C(C=C(C=C2)C(=O)NCC(C3=CC(=CC(=N3)C4=CSC5=C4C=CC=C5F)C#C[Si](C)(C)C)O)OC	0.41939	3.682282
CCN(CC)C1=CC=C(C=C1)NC(=O)C2=C(SC3=C2CCCC3)NC(=O)C4=CC=CC(=C4)CN(C5CC5)C6CCN(CC6)CC(=O)O	0.42438	3.673349
CCCCOC(=O)CN(CC1=CC2=C(C=C1)SC(=C2)C(=O)OCCCC)C(=O)C3=CC4=C(C=C3)C=C(C=C4)O	0.53866	3.672029
C1CN(CCN(C1)CCOC2=CC=C(C=C2)OC3=C(SC4=C3C=CC(=C4)O)C5=CC=C(C=C5)Br)CCCCC6=CC7=C(C=C6)C(=O)N(C7)C8CCC(=O)NC8=O	0.32970	3.662243
COC1=CC=C(C=C1)COCCOC2=C(C=C(C=C2)C(=O)NCC(=O)C3=CC(=CC(=N3)C4=CSC5=C4C=CC=C5F)C#C[Si](C)(C)C)OC	0.42959	3.662126
CC(C)C[C@@H](C(=O)OC)NCC1CCC(CC1)CNCC2=CC3=C(C=C2)C=C(S3)C(=O)NO	0.57073	3.652505
C1=CC=C2C(=C1)C=C(S2)C3=CN=C4N3N=C(C=C4)NCCCCCO.C(CCN)CCO	0.55939	3.652355
CC(C)(C)SC[C@@H](C(=O)OC)NCC1=CC=C(C=C1)CNCC2=CC3=C(C=C2)C=C(S3)C(=O)NO	0.53638	3.651912
CC(C)(C)OC(=O)N(C)CCN(CC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)CCC5=CC=C(C=C5)C(=O)OC)C6CC6	0.34548	3.643608

C1CN(CCN1CCCCOC2=CC3=C(C=C2)C=CC(=N3)OC(=O)N(CCO)CCO)C4=C5C=CSC5=CC=C4	0.49883	3.642406
C1CN(CCC1CCCO[N+](=O)[O-])CCOC2=CC=C(C=C2)OC3=C(SC4=C3C=CC(=C4)O)C5=CCC(=O)C=C5	0.46539	3.64193
CC(C)[C@@H](CO)NCC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)CCC5=CC=C(C=C5)C(=O)OC	0.39729	3.632923
CC(C)[C@H](CO)NCC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)CCC5=CC=C(C=C5)C(=O)OC	0.39729	3.632923
COCCNC(=O)C1=C(C2=C(S1)C=C(C=C2)OCC3=C(C=C(C=C3)Cl)Cl)OCC(=O)O	0.58806	3.63031
CCOC(=O)C1CCC(CC1)N(CC2=CC(=CC=C2)C(=O)NC3=C(C4=C(S3)CCCC4)C(=O)NC5=CC=CC(=C5)CCC6=CC=C(C=C6)C(=O)OC)C7CC7	0.35533	3.613499
CCOC(=O)C1CCC(CC1)N(CC2=CC(=CC=C2)C(=O)NC3=C(C4=C(S3)CCCC4)C(=O)NC5=CC=C(C=C5)CCC6=CC(=CC=C6)C(=O)OC)C7CC7	0.35533	3.613499
C[C@@H](CC1=CC=CC=C1)[C@@H](CN(CC(C)C)S(=O)(=O)C2=CC3=C(C=C2)N=C(S3)NCC4=C(C5=C(S4)CCC(C5)(C)C)C(C)(C)C)O	0.48234	3.613093
CC#C[C@@H](C/C(=N/N=N)/N)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(N=CC(=C4)OCCOC)C	0.47116	3.612148
CC#C[C@@H](C/C(=N/N=N)/N)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=CN=C(C=C4C)OCCOC	0.47116	3.612148
CC#C[C@@H](C/C(=N/N=N)/N)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=NC=C(C=C4C)OCCOC	0.47116	3.612148
C1CCC2=C(C1)C(=C(S2)NC(=O)C3=CC=CC(=C3)CN(C4CC4)C(=O)CCCC(=O)O)C(=O)NC5=CC=C(C=C5)CC6=CC=NC=C6	0.37227	3.602563
CC#C[C@@H](C/C(=N/N=N)/N)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C(=CC=C4)OCCOC)C	0.51213	3.602195
C1CN(CCN(C1)CCOC2=CC=C(C=C2)OC3=C(SC4=C3C=CC(=C4)O)C5=CC=C(C=C5)Br)CCCCC6=CC7=C(C=C6)C(=O)N(C7=O)C8CCC(=O)NC8=O	0.29378	3.602036
CC1=CC2=C(C=C1)SC(=C2)C(=O)N[C@@H](CC(C)C)C(=O)NCCCN(C)S(=O)(=O)C3=CC=CC=C3N	0.45149	3.602021
CC1=C(SC2=CC=CC=C12)C(=O)N[C@@H](CC(C)C)C(=O)NCCCN(C)S(=O)(=O)C3=CC=CC=C3N	0.45149	3.602021

CC#CC(CC1=NNN=N1)C2=CC=C(C=C2)OCC3=CC4=C(C=C3)SC=C4C5=C(C=C(C=C5)OCCCS(=O)(=O)C)C	0.45330	3.601865
C1CCN(CCC(C1)CCC2=CC3=C(C=C2)C(=O)N(C3)[C@H]4CCC(=O)NC4=O)CCCCOC5=CC=C(C=C5)OC6=C(SC7=C6C=CC(=C7)O)C8=CC=C(C=C8)Br	0.33192	3.592447
CC(C)C[C@@H](C(=O)OC)NCC1=CC=C(C=C1)CNCC2=CC3=C(C=C2)C=C(S3)C(=O)NO	0.57573	3.592035
CCOC(=O)CC(C#CC)C1=CN=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OC[C@H](CO)O)C	0.50993	3.592029
COC1=CC=C(C=C1)CNCC(COC2=CC3=C(C=C2)C(=C(S3)NC(=O)C4CC4)C(=O)N)O	0.48088	3.591671
CCOCC/C(=N\NC(=O)CNC(=O)C1=CC(=C(C=C1)OC)OC)/C2=CSC3=CC=CC=C32	0.57633	3.591671
COCCC/C(=N\NC(=O)CNC(=O)C1=CC(=C(C=C1)OC)OC)/C2=CSC3=CC=CC=C32	0.57633	3.591671
COC1=C(C=C(C=C1)C(=O)NCC(=O)N/N=C(\CCCCO)/C2=CSC3=CC=CC=C32)OC	0.53222	3.591671
COC(=O)C(CC(=C)C(=O)CC1=CSC2=C1C=CC(=C2)CCCC3=C(C=C(C=C3)O)O)CO	0.56337	3.581607
CC(CC(=O)NC1=C(C2=C(S1)CC(CC2)OC(=O)NC/C(=C/NN)/C(C)I)C#C)C3=CC=CC=N3	0.41225	3.571114
CC(C)CN(C[C@@H]1[C@@H](N(C(O1)(C)C)C(=O)OC(C)(C)C)CC2=CC=C(C=C2)OCC3=C(C4=CC=CC=C4S3)C(=O)OC)S(=O)(=O)C5=CC=C(C=C5)OC	0.33731	3.562958
C1CN(CCN1CCOCC(=O)O)CCOC2=CC=C(C=C2)C(=O)C3=C(SC4=C3C=CC(=C4)O)C5=CC=C(C=C5)O	0.42946	3.563193
C1CN(CCN1CCOCCOCC(=O)O)C2=CC=C(C=C2)C(=O)C3=C(SC4=C3C=CC(=C4)O)C5=CC=C(C=C5)O	0.43022	3.563193
COC(=O)C1=CC=C(C=C1)CCC2=CC=C(C=C2)NC(=O)C3=C(SC4=C3CCCC4)NC(=O)C5=CC=CC(=C5)CN(CC(=O)O)C6CC6	0.37256	3.556256
CC(=O)COCCN1CCN(CC1)CCOC2=CC=C(C=C2)C(=O)C3=C(SC4=C3C=CC(=C4)O)C5=CC=C(C=C5)O	0.49157	3.542138
C1CN(CCN1CCCCOC2=CC3=C(C=C2)C=CC(=N3)OCOP(=O)(O)O)C4=C5C=CSC5=CC=C4	0.49875	3.531593
CC(C)C(N1C(=O)C=CC2=C1C=C(C=C2)OCCCCN3CCN(CC3)C4=C5C=CSC5=CC=C4)OP(=O)(	0.42	3.53

[O-])[O-].[Ca+2]	2154	1532
CC1=CC2=C(C(=C1)OC)SC(=C2)C3=C4C(=NC=NN4C(=C3COC)CN(CCNC)CC=O)N	0.51745	3.527 21
CN(CCCNC(=O)[C@H](CC1CCCC1)NC(=O)C2=CC3=CC=CC=C3S2)S(=O)(=O)C4=CC=C(C=C4)N	0.44510	3.521 2021
CCCC[C@@H](C(=O)O)N(C(=N)C(CC1=CSC2=CC=CC=C21)NC(=O)OCC3=CC=CC=C3)N	0.47505	3.521 1988
CC(C)CN(C[C@@H]1[C@@H](N(C(O1)(C)C)C(=O)OC(C)(C)C)CC2=CC=C(C=C2)NCC3=C(C4=C(S3)CCC(C4)(C)C)C(=O)C)S(=O)(=O)C5=CC=C(C=C5)OC	0.34456	3.519 3794
CC(C)CC([C@@H](CC(C)C[C@H](CO)NC1=NN2C(=NC=C2C3=CC4=CC=CC=C4S3)C=C1)O)N	0.53589	3.519 2511
CC(C)CC(C(CC(C)CC(CO)NC1=NN2C(=NC=C2C3=CC4=CC=CC=C4S3)C=C1)O)N	0.53589	3.519 2511
CC(C)CC([C@H](CC(C)C[C@@H](CO)NC1=NN2C(=NC=C2C3=CC4=CC=CC=C4S3)C=C1)O)N	0.53589	3.519 2511
CC(CC(=O)NC1=C(C2=C(S1)CC(CC2)OC(=O)NC/C(=C/N(C)N)/C(C)I)C#C)C3=CC=CC=N3	0.42872	3.511 1271
CCN(C(C)C)C(C1=CC=C(C=C1)NC2=NC(=CN(C2=O)C)C3=C(C(=CC=C3)NC(=O)OC4=CC5=C(S4)CCCC5)C)C(=O)N(C)CCOC	0.37117	3.502 3407
CC[Si](CC)(CC)OC(C)(C)C1=CC(=NC=C1)C2=CC=CC3=C2SC(=C3)[C@@H](C4=C(C(=NC=C4Cl)N)F)NS(=O)C(C)(C)C	0.46858	3.504 2191
CCOC(=O)C1(CC1)NCC2=CC(=CC=C2)C(=O)NC3=C(C4=C(S3)CCCC4)C(=O)NC5=CC=C(C=C5)CCC6=CC=C(C=C6)C(=O)OC	0.37059	3.498 2716
CCN(CC)CCOC1=C(C=CC2=C1SC(=C2C(=O)OCC)NC(=O)C)C3=CC=C(C=C3)[N+](=O)[O-]	0.51543	3.491777
CCCCOC1=CC2=C(C=C1)C=C(S2)C(=O)CC(CCN3C(=O)C4=CC=CC=C4N=N3)C(=O)O	0.52899	3.491515
CC(C)CN(C[C@@H]1[C@@H](N(C(O1)(C)C)C(=O)OC(C)(C)C)CC2=CC=C(C=C2)OCC3CCCC3C4=C(C5=C(S4)CCC(C5)(C)C)C(=O)OC(C)(C)C)S(=O)(=O)C6=CC=C(C=C6)OC	0.28986	3.484679
CC#C[C@@H](C/C(=N/N=N)/N)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCCC(C)(C)O)C	0.45771	3.482508
CC1=C(C=CC(=C1)OCCOC)C2=C(SC3=C2C=C(C=C3)COC4=CC=C(C=C4)CC/C(=N/N)/NN)Cl	0.50609	3.481805

CN(C)/C=N/C1=NC=C2C(=N1)C(=CN2CCC(=O)OC)C3=CC4=C(C(=C3)C5=CC6=CC=CC=C6S5)N(N=C4)COCCSC	0.45832	3.471 2086
CCCOC1=C(C=CC(=C1)C2=NC=CC(=N2)NCCC3=C(C=C4C(=C3)C=CS4)OC)CC(=O)O	0.60035	3.471 722
CC(C)CN(C[C@@H]1[C@@H](N(C(O1)(C)C)C(=O)OC(C)(C)C)CC2=CC=C(C=C2)OCC3=C(CCC3)C4=C(C5=C(S4)CCC(C5)(C)C)C(=O)OC(C)(C)C)S(=O)(=O)C6=CC=C(C=C6)OC	0.29044	3.461 4523
CCCC[C@@H](C(=O)OC)N(C(=N)[C@H](CC1=CSC2=CC=CC=C21)NC(=O)OCC3=CC=CC=C3)N	0.49474	3.467 2144
CC(C)N1C=NC2=C(N=C(N=C21)C3=CSC4=CC=CC=C43)NCCC5=CNC6=C5C=C(C=C6)OC(=O)CCCCCN(C)C(=O)OC(C)(C)C	0.35435	3.454 3254
CCCC[C@@H](C(=O)O)N1C(=NNN1)[C@H](CC2=CSC3=CC=CC=C32)NC(=O)OCC4=CC=CC=C4	0.49893	3.452 194
CCC(C)(C)OC(=O)N1CCC(CC1)N(CC2=CC(=CC=C2)C(=O)NC3=C(C4=C(S3)CCCC4)C(=O)NC5=CC=C(C=C5)N(CC)CC)C6CC6	0.42584	3.439 3975
COC(=O)C1=CC=C(C=C1)CCC2=CC=C(C=C2)NC(=O)C3=C(SC4=C3CCCC4)NC(=O)C5=CC=CC(=C5)CNC6CCC(CC6)C(=O)OCC7=CC=CC=C7	0.32723	3.431 3342
CC(C)CC(C(=O)NCC(=O)N1C(=O)C=CC2=C1C=C(C=C2)OCCCCN3CCN(CC3)C4=C5C=CSC5=CC=C4)N	0.43851	3.432 2879
CC(=O)C(CCN1C(=O)C2=CC=CC=C2N=N1)(CC(=O)C3=CC4=C(S3)C=C(C=C4)OCC(=O)C5CC5)C(=O)OC(C)(C)C	0.38234	3.437 2039
CCCCC(C(=O)O)N1C(=NN=N1)[C@H](CC2=CSC3=CC=CC=C32)NC(=O)OCC4=CC=CC=C4	0.49411	3.436 1784
CC(C)CCOC1=CC2=C(C=C1)C=C(S2)C(=O)CC(CCN3C(=O)C4=CC=CC=C4N=N3)C(=O)O	0.51767	3.438 1671
CC1=CC2=C(C=C1)C(=C(S2)C3=CC=C(C=C3)OC(=O)C4(CC4)CO[N+](=O)[O-])OC5=CC=C(C=C5)OCCN6CCCCC6	0.47290	3.426 2087
CC(C)CN(C[C@@H]1[C@@H](N(C(O1)(C)C)C(=O)OC(C)(C)C)CC2=CC=C(C=C2)NCC3CCCCC3C4=C(C5=C(S4)CCC(C5)(C)C)C(=O)OC(C)(C)C)S(=O)(=O)C6=CC=C(C=C6)OC	0.28155	3.411 4996
CCC(C(=O)N1CCC[C@H]1C(=O)O)C(CC)(CC(=O)C2=CSC3=CC=CC=C32)SC=O	0.62212	3.412 1331
CCCC[C@@H](C(=O)OC)N1C(=NNN1)[C@H](CC2=CSC3=CC=CC=C32)NC(=O)OCC4=CC=CC=C4	0.52298	3.394 2097
CCCCC1=CC2=C(C=C1)SC(=C2)/C=C(\C)/C(=O)C3=C(C=C(OC3=O)C(C)CC/C=C/NC(=O)O)O	0.49	3.39

	1077	1872
	0.49	
CCCCC1=CC2=C(C=C1)C=C(S2)/C=C(\C)/C(=O)C3=C(C=C(OC3=O)C(C)CC/C=C/NC(=O)O)O	1077	3.39 1872
	0.37	
CCC(C)(C)OC(=O)N1CCC(CC1)N(CC2=CC(=CC=C2)C(=O)N(C3=C(C4=C(S3)CCCC4)C(=O)NC5=CC=C(C=C5)N(CC)CC)N)C6CC6	3448	3.38 4084
	0.54	
	657	3.38
CCCN(CCC(C)CC)C1=C(C2=C(S1)CNCC2)CNC(=O)NC3=C(C4=C(S3)CCCC4)C(=O)OC(C)(C)C	4	3168
	0.34	
CN(CCN1CCOCC1)C(=O)C2=CC=CC(=C2)C(=O)NC3=C(C4=C(S3)CCCC4)C(=O)NC5=CC=C(C=C5)CCCC6=CC=C(C=C6)C(=O)O	6153	3.38 2982
	0.51	
	658	3.37
CCCCC(C(=O)OC)N1C(=NN=N1)[C@H](CC2=CSC3=CC=CC=C32)NC(=O)OCC4=CC=CC=C4	6	194
	0.28	
CC(C)CN(C[C@@H]1[C@@H](N(C(O1)(C)C)C(=O)OC(C)(C)C)CC2=CC=C(C=C2)OCC3=CC=CC=C3C4=C(C5=C(S4)CCC(C5)(C)C)C(=O)OC(C)(C)C)S(=O)(=O)C6=CC=C(C=C6)OC	7588	3.36 4366
	0.36	
COC(=O)C1=CC=C(C=C1)CCC2=CC=C(C=C2)NC(=O)C3=C(SC4=C3CCCC4)NC(=O)C5=CC=CC(=C5)CN(C6CC6)C7CCN(CC7)C(=O)CCl	4585	3.36 2956
CCCC[C@H](C1C(=NN=N1)[C@H](CC2=CSC3=CC=CC=C32)NC(=O)OCC4=CC=CC=C4)C(=O)OC	0.54 182	3.36 1988
	0.48	
	912	3.35
CC1=C(C=CC(=C1)OCCOC)C2=CSC3=C2C=C(C=C3)COC4=NC=C(C=C4)CC/C(=N/N)/NN	3	2148
	0.47	
CC(C)C(N1C(=O)C=CC2=C1C=C(C=C2)OCCCCN3CCN(CC3)C4=C5C=CSC5=CC=C4)OP(=O)(O)O	0083	3.35 2062
C1CC1C(=O)COC2=CC3=C(C=C2)C=C(S3)C(=O)CC(CCN4C(=O)C5=CC=CC=C5N=N4)C(=O)O	0.45 184	3.35 1308
	0.39	
C1CCC2=C(C1)C(=C(S2)NC(=O)C3=CC=CC(=C3)CN(C4CC4)C5CCC(CC5)OC=O)C(=O)NC6=CC=C(C=C6)CC7=CC=NC=C7.Cl.Cl	707 3	3.34 246
	0.53	3.34
CCCC(=O)O[C@@H]1C[C@@](C2=C([C@H]1OC(=O)CCC)SC(=C2)C)(C(=O)O)OC(=O)CCC	433	1661
	0.73	
	594	3.34
CCN(CC)CCOC1=C(C=CC2=C1SC(=C2C(=O)OCC)NC(=O)C)C3=C(SC=C3)C	3	1647
	0.33	
CN(CCN1CCOCC1)C(=O)C2=CC=CC(=N2)C(=O)NC3=C(C4=C(S3)CCCC4)C(=O)NC5=CC=C(C=C5)CCCC6=CC=C(C=C6)C(=O)OC	590 6	3.33 3091
	0.51	
CCCCC1=CC2=C(C=C1)SC(=C2)/C=C(\C)/C(=O)C3=C(C=C(OC3=O)C(C)CC/C=C/NC(=O)OC)O	3961	3.33 2029
CCCCC1=CC2=C(C=C1)C=C(S2)/C=C(\C)/C(=O)C3=C(C=C(OC3=O)C(C)CC/C=C/NC(=O)OC)	0.51	3.33

O	3961	2029
COC(=O)[C@H](CC1=CC=CC=C1)NCC2=CC=C(C=C2)CNCC3=CC4=C(C=C3)C=C(S4)C(=O)NO	0.54505	3.331879
CN(CCN1CCOCC1)C(=O)C2=CC=CC(=C2)C(=O)NC3=C(C4=C(S3)CCCC4)C(=O)NC5=CC=C(C=C5)CCCC6=CC=C(C=C6)C(=O)OC	0.36267	3.323138
C/C(=C\C=C(/C)\OC)/C1CC2=C(SC(=C2/C(=N/O)/C1)SCC3=CC=CC=C3)C(=O)NCCOC4=CC=CC=C4	0.57917	3.32196
COC1=CC=C(C=C1)C2=C(C3=C(S2)C=C(C=C3)OOC4=CC=C(C=C4)[N+](=O)[O-])OC5=CC=C(C=C5)OCCN6CCCCC6	0.49211	3.323193
CC1=CC(=CC(=C1C2=C3CCC(C3=CC=C2)OC4=CC5=C(C=C4)[C@@H](CS5)CC(=O)O)CO)OCCCS(=O)(=O)C	0.45581	3.321746
CC1=CC(=CC(=C1C2=C3CCC(C3=CC=C2)OC4=CC5=C(C=C4)[C@@H](CS5)CC(=O)O)OC)OCCCS(=O)(=O)C	0.49009	3.321746
CCOC(=O)CC1CCN(CC1)CC2=CC(=CC=C2)C(=O)NC3=C(C4=C(S3)CCCC4)C(=O)NC5=CC=C(C=C5)CCC6=CC=C(C=C6)C(=O)OC	0.37070	3.313186
CC(C)(C)OC(=O)CN(CC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)CCC5=CC=C(C=C5)C(=O)OC)C6CC6	0.37072	3.313186
CCS(=O)(=O)CCCOC1=CC(=C(C(=C1)C)C2=C3CCC(C3=CC=C2)OC4=CC5=C(C=C4)[C@@H](CS5)CC(=O)O)C	0.52446	3.301953
C1CN(CCC1OC2=CC=C(C=C2)OC3=C(SC4=C3C=CC(=C4)OCC5=CC=CC=C5)C6=CC=C(C=C6)Br)C7CN(C7)C8=CC(=C(C=C8)C(=O)O)CO	0.39565	3.301712
CC(C)CN(C[C@@H]1[C@@H](N(C(O1)(C)C)C(=O)OC(C)(C)C)CC2=CC=C(C=C2)NCC3=C(C4=C(S3)CCC(C4)(C)C)C(=O)OC(C)(C)C)S(=O)(=O)C5=CC=C(C=C5)OC	0.30613	3.294213
CC1=C(C=CC=C1OCCOC)C2=CSC3=C2C=C(C=C3)COC4=NC=C(C=C4)C(C)C/C(=N/N)/NN	0.48021	3.292304
COC1=C(N=C(C=C1)C(=O)[C@H](CO)NC(=O)C2=CC(=C(C=C2)OCCO)NC)C3=CSC4=C3C=CC=C4F	0.61830	3.291526
CC(CC1=CC(=NN=C1OCC2=CC=CC=C2)C3=CC=CC4=C3SC(=C4)C(C5=CC=CC=C5Cl)NS(=O)(=O)C6CC6)O	0.45795	3.291366
CC(C)CN(C[C@@H]1[C@@H](N(C(O1)(C)C)C(=O)OC(C)(C)C)CC2=CC=C(C=C2)CCC3=C(C4=C(S3)CCC(C4)(C)C)C(=O)OC(C)(C)C)S(=O)(=O)C5=CC=C(C=C5)OC	0.32926	3.284261
CCOC(=O)CCCC(=O)CC1=CSC2=C1C=CC(=C2)OCC3=C(C=C(C=C3)O)O	0.65555	3.281294

CC#CC(CC(=O)O)C1=CN=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=CC=C(C=C4)OCC(CO)O	0.50489	3.271559
CC#CC(CC(=O)O)C1=CN=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=CC(=CC=C4)OCC(CO)O	0.50489	3.271559
CCCCOC(=O)C1=C(SC2=C1CC(CC2)(C)C)C#CC3=CCC(C=C3)C[C@H]4[C@H](OC(N4C(=O)OC(C)(C)C)(C)C)CN(CC(C)C)S(=O)(=O)C5=CC=C(C=C5)OC	0.32996	3.264104
CC1=CC(=CC(=C1C2=C(C=CC3=C2CCC3OC4=CC5=C(C=C4)[C@@H](CS5)CC(=O)O)OC)C)OCCCS(=O)(=O)C	0.48048	3.261902
CS(=O)(=O)CCCOC1=C(C=C(C=C1Cl)C2=C3CCC(C3=CC=C2)OC4=CC5=C(C=C4)[C@@H](CS5)CC(=O)O)Cl	0.50472	3.260704
CC(C)N(CC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)CCC5=CC=C(C=C5)C(=O)OC)C6CCC(CC6)C(=O)O	0.34164	3.253342
C1=CC=C2C(=C1)C=C(S2)C3=CN=C4N3N=C(C=C4)NC(CCCO)C(CCCN)O	0.57739	3.251885
C1=CC=C2C(=C1)C=C(S2)C3=CN=C4N3N=C(C=C4)NCCCC(C(CCCN)O)O	0.57739	3.251885
C1=CC=C2C(=C1)C=C(S2)C(CCC(C3=CN=C4N3N=C(C=C4)NCCCCO)O)N	0.58417	3.251885
CCCCOC(=O)C1=C(SC2=C1CC(CC2)(C)C)C#CC3=CC=C(C=C3)C[C@H]4[C@H](OC(N4C(=O)OC(C)(C)C)(C)C)CN(CC(C)C)S(=O)(=O)C5=CC=C(C=C5)OC	0.33067	3.243948
CCC(=O)N1CCC(CC1)CN(/C=C(\C)/NC2=NN=C(C(=C2)NCC3=CC=CC4=C3SC=C4)C(=O)N)N=C	0.43425	3.242525
COC(=O)C1=CC=C(C=C1)CCC2=CC=C(C=C2)NC(=O)C3=C(SC4=C3CCCC4)NC(=O)C5=CC=CC(=C5)CN(CC(=O)N6CCNCC6)C7CC7	0.35173	3.233298
CC1=C(C=CC(=C1)OCCC(C)(C)O)C2=CSC3=C2C=C(C=C3)COC4=NC=C(C=C4)CC/C(=N/N)/NN	0.44044	3.232461
COC(=O)[C@@H](CCOC1=CC=C(C=C1)CNCC2=CC3=C(C=C2)C=C(S3)C(=O)NO)N	0.49452	3.231515
COC(=O)[C@H](CCOC1=CC=C(C=C1)CNCC2=CC3=C(C=C2)C=C(S3)C(=O)NO)N	0.49452	3.231515
CC(C)OC(=O)OCOP(=O)(C(C1=CSC2C1C=C(C=C2)Cl)C(=O)N/C=C/C3=CC(=CC(=C3)Cl)Cl)O	0.44582	3.229998
CC(CCC(=O)NC=O)N1CC2=C(C1=O)C=CC(=C2)N3CCC(CC3)CN4CC(C4)C5(CC=C(C=C5)OC6=C(SC7=C6C=CC(=C7)O)C8=CC=C(C=C8)Br)C	0.43221	3.222451
C1CC(=O)NC(=O)C1N2C(=O)C3=C(C2=O)C=C(C=C3)N4CCN(CC4)CCCCCOC5=CC=C(C=C5)	0.30	3.22

OC6=C(SC7=C6C=CC(=C7)O)C8=CC=C(C=C8)Br	2704	1723
CC(C)N(CC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)COC5=CC=C(C=C5)C(=O)OC)C6CCC(CC6)C(=O)OC	0.33864	3.213291
C1CC(CCC1C(=O)O)OC[C@@H]2C[C@@H](CC2C(=O)CC3=CC(=C(C=C3Cl)NC(=O)C4=CSC5=CC=CC=C54)Cl)N6CCN(CC6)CC7=CC=CC=C7	0.38379	3.212457
CC#C[C@@H](CC(=O)O)C1=CC=C(C=C1)COC2=CC3=C(C=C2)SC=C3C4=C(N=C(C=C4)OCC(CO)O)C	0.49469	3.211716
COC1=C(C=C(C=C1)C(=O)NCC(=O)NNCCC(=O)C2=CSC3=CC=CC=C32)OC	0.54955	3.211358
C=C(CC(CO)C(=O)N)C(=O)CC1=CSC2=C1C=CC(=C2)OCC3=C(C=C(C=C3)O)O	0.48941	3.211246
C1CN(CCN1CCCCOC2=CC3=C(C=C2)C=CC(=O)N3COC(=O)NCCO)C4=C5C=CSC5=CC=C4	0.51464	3.209225
CC#CC(CC(=O)O)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC(CO)O)C	0.54053	3.208 1763
CC#C[C@@H](CC(=O)O)C1=CC=C(C=C1)COC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OC[C@H](CO)O)C	0.54053	3.208 1763
CC#CC(CC(=O)O)C1=CC=C(C=C1)COC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC(CO)O)C	0.54053	3.208 1763
CC(C)N(CC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)CCC5=CC=C(C=C5)C(=O)OC)C6CCC(CC6)C(=O)OC	0.35854	3.193499
C1CN(CCN1)C(CCCC2=C3C=CSC3=CC=C2)OC4=CC(=O)NC5=C4C=CC(=C5)C(CC(=O)O)C(=O)O	0.41550	3.196 1934
CC#CC(C/C(=N/N)/N)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=CN=C(C=C4C)OCCOCCCOC(=O)C1CCC(CC1)N(CC2=CC(=CC=C2)C(=O)NC3=C(C4=C(S3)CCCC4)C(=O)NC5=CC=C(C=C5)CC6=CC=C(C=C6)C(=O)OC)C7CC7	0.56129	3.182195
CCN(CC)CCOC1=C(C=CC2=C1SC(=C2C(=O)OCC)N)C3=CC=C(C=C3)[N+](=O)[O-]	0.56386	3.171671
CCCCOC(=O)CCN(CC1=CSC(=C1)C(=O)OC(C)(C)C)C(=O)C2=CSC3=C2C=CC(=C3)O	0.56412	3.171593
C1=CC=C(C=C1)CCOC2=CC3=C(C=C2)C=C(S3)C(=O)CC(CCN4C(=O)C5=CC=CC=C5N=N4)C(=O)O	0.49033	3.171515
CCC[C@@H](CC(=O)O)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC(=C3C4=C(C=C(C=C4)OC5CCS(=O)(=O)CC5)C)C	0.50549	3.16211

	6	
	0.58	
	344	3.15
COCC/C(=N\NC(=O)CNC(=O)C1=CC(=C(C=C1)OC)OC)/C2=CSC3=CC=CC=C32	7	1515
	0.58	
	344	3.15
COCC/C(=N/NC(=O)CNC(=O)C1=CC(=C(C=C1)OC)OC)/C2=CSC3=CC=CC=C32	7	1515
	0.53	
	682	3.15
COC1=C(C=C(C=C1)C(=O)NCC(=O)N/N=C(\CCCO)/C2=CSC3=CC=CC=C32)OC	6	1515
	0.34	
CC(C)N(CC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)CN(C)C5=	548	3.14
CC=C(C=C5)C(=O)OC)C6CCC(CC6)C(=O)OC	3	3608
	0.49	
C1CN(CCN1CCCCOC2=CC3=C(C=C2)C=CC(=O)N3C(=O)N(CCO)CCO)C4=C5C=CSC5=CC=C	105	3.14
4	1	2406
	0.48	
CC1=C(C(=C(C(=C1Cl)OCCCS(=O)(=O)C)Cl)C)C2=C3CCC(C3=CC=C2)OC4=CC5=C(C=C4)[C	564	3.14
@@H](CS5)CC(=O)O	4	1017
	0.46	
CC#CC(C/C(=N/N)/NN)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(N=CC(=C4)OCCO	230	3.13
C)C	8	2304
	0.46	
CC#CC(C/C(=N/N)/NN)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=NC=C(C=C4C)OCC	230	3.13
OC	8	2304
	0.55	
	609	3.13
CC(CCN)C(C(CC(C)CO)NC1=NN2C(=NC=C2C3=CC4=CC=CC=C4S3)C=C1)O	6	2198
	0.55	
	609	3.13
CC(CCN)C(C(C(C)CCNC1=NN2C(=NC=C2C3=CC4=CC=CC=C4S3)C=C1)O)O	6	2198
	0.42	
CC(C)C[C@@H](C(=C)N1C[C@@H]2CC1CN2C(=O)CNS(=O)(=O)C3=C(C=C(C=C3)Cl)Cl)N=	788	3.13
C(C4=CC5=CC=CC=C5S4)N	7	1402
CC(C)C(C)NCC1=CC(=CC=C1)C(=O)N(C2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)CCC5	0.40	3.12
=CC=C(C=C5)C(=O)OC)N	522	3083
	0.50	
CC#CC(C/C(=N/N)/NN)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C(=CC=C4)OCCO	311	3.12
C)C	6	2352
	0.38	
CCOC(=O)C1=C(SC2=C1CCCC2)/N=C(/C(NS(=O)(=O)C3=CC=C(C=C3)C)I)\NC4=CC=CC=C4	285	3.12
N	2	0675
	0.56	
	814	3.11
CCCOC1=C(C=CC(=C1)C2=CC(=NC=N2)NCCC3=C(SC4=C(C=CC(=C34)Cl)OC)C)C(=O)O	7	1333
	0.38	
CS(=O)(=O)N1CCN(CC1)CC2=CC3=CC(=CC(=C3S2)N4CCOCC4)C5=CC=CC6=NN(C=C65)CC	856	3.10
CCCCC(=O)NO	6	2502

COC(=O)CNC(=O)OCN1C(=O)CCC2=C1C=C(C=C2)OCCCCN3CCN(CC3)C4=C5C=CSC5=CC=C4	0.47896	3.102356
CC(C)(C)C[C@@H](C(=O)NCCCN(C)S(=O)(=O)C1=CC=CC=C1N)NC(=O)C2=CC3=CC=CC=C3S2	0.45230	3.102021
CCOC(=O)CC(C#CC)C1=CN=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC5(CS(C5)(O)O)C)C	0.46885	3.092062
CC#CC(CC1=NNN=N1)C2=CN=C(C=C2)OCC3=CC4=C(C=C3)SC=C4C5=C(C=C(C=C5)OCCOC)C	0.53721	3.091991
CC#CC(CC1=NNN=N1)C2=CC=C(C=C2)OCC3=CC4=C(C=C3)SC=C4C5=CN=C(C=C5C)OCCOC	0.53721	3.091991
CC#CC(CC1=NNN=N1)C2=CC=C(C=C2)OCC3=CC4=C(C=C3)SC=C4C5=NC=C(C=C5C)OCCOC	0.53721	3.091991
CC#CC(CC1=NNN=N1)C2=CN=C(C=C2)OCC3=CC4=C(C=C3)SC=C4C5=C(C(=CC=C5)OCCOC)C	0.53721	3.091991
CC#CC(CC1=NNN=N1)C2=CC=C(C=C2)OCC3=CC4=C(C=C3)SC=C4C5=C(N=CC(=C5)OCCOC)C	0.53721	3.091991
CC#C[C@H](CC1=NNN=N1)C2=CN=C(C=C2)OCC3=CC4=C(C=C3)SC=C4C5=C(C=C(C=C5)OCCOC)C	0.53721	3.091991
CC#C[C@H](CC1=NNN=N1)C2=CN=C(C=C2)OCC3=CC4=C(C=C3)SC=C4C5=C(C(=CC=C5)OCCOC)C	0.53721	3.091991
CC1CCCN(C1)CCCOC2=CC3=NC=CC(=C3C=C2OC)OC4=C(C=C(C=C4)NS(=O)C5=CSC6=CC=CC=C65)F	0.56491	3.091975
COC(=O)CNC(=O)OCN1C(=O)C=CC2=C1C=C(C=C2)OCCCCN3CCN(CC3)C4=C5C=CSC5=CC=C4	0.47535	3.082199
CC(C)CN(C[C@@H]1[C@@H](CC(O1)(C)C)CC2=CC=C(C=C2)NC(=O)NC3=C(C4=C(S3)CCC(C4)(C)C)C(=O)OC(C)(C)C)S(=O)(=O)C5=CC=C(C=C5)OC	0.46238	3.073638
CCOC(=O)CC(C#CC)C1=CN=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC5(CSC5(O)O)C)C	0.46972	3.071906
COC1=C(C=C2CC(=O)N(CCC2=C1)CC3CCCN(C3)CCC4=CSC5=C4C=CC(=C5)OS(NO)(=O)C)OC.Cl	0.66892	3.052047
C1CC(=O)N(C2=C1C=CC(=C2)OCCCCN3CCN(CC3)C4=C5C=CSC5=CC=C4)COP(=O)(O)O	0.49964	3.051749
CCCOC1=CC2=C(C=C1)C=C(S2)C(=O)CC(CCN3C(=O)C4=CC=CC=C4N=N3)C(=O)O	0.53942	3.051358

CN(CC(=O)OC)C(=O)OCN1C(=O)CCC2=C1C=C(C=C2)OCCCCN3CCN(CC3)C4=C5C=CSC5=CC=C4	0.50093	3.042512
CCCCC1=C2C(=C(SC2=C(C=C1)O)N)C(=O)N(CC3=CC4=C(C=C3)OCO4)C(=C)CC5=CC(=C(C=C5)OC)OC	0.48223	3.042138
CC#CC(CC1=NNN=N1)C2=CC=C(C=C2)OCC3=CC4=C(C=C3)SC=C4C5=C(C=C(C=C5)OCC(CO)O)C	0.46447	3.041988
CC(C)(C)OC(=O)C(CCN1C(=O)C2=CC=CC=C2N=N1)(CC(=O)C3=CC4=C(S3)C=C(C=C4)OCCC5=CC=CC=C5)C(=O)OC(C)(C)C	0.36070	3.032665
CCOC(=O)CC(C#CC)C1=CN=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC5CCS(CC5)(O)O)C	0.45993	3.032219
C1CC(=O)NC(=O)C1N2C(=O)C3=C(C2=O)C=C(C=C3)N4CCN(CC4)CCC5CN(C5)CCOC6=CC=C(C=C6)OC7=C(SC8=C7C=CC(=C8)O)C9=CC=C(C=C9)Br	0.28447	3.031988
C1CN(CCN1CCCCOC2=CC3=C(C=C2)C=CC(=O)N3COP(=O)(O)O)C4=C5C=CSC5=CC=C4	0.49597	3.031593
CCOC1=C(C2=C(C=C1)SC=C2)CCNC3=NC=NC(=C3)C4=CC(=C(C=C4)C(=O)O)OCC	0.61547	3.031566
CCOC1=C(C=CC(=C1)C2=CC(=NC=N2)NCCC3=C(C=CC4=C3C=CS4)OC)CC(=O)O	0.61402	3.031566
CCOC1=C(C=CC=C1C2=CC(=NC=N2)NCCC3=C(C=C4C(=C3)C=CS4)OC)CC(=O)O	0.61402	3.031566
CCOC1=NC(=CC(=N1)NCCC2=C(C=C3C(=C2)C=CS3)OC)C4=CC=C(C=C4)CC(=O)O	0.61402	3.031566
CN(CC(=O)OC)C(=O)OCN1C(=O)C=CC2=C1C=C(C=C2)OCCCCN3CCN(CC3)C4=C5C=CSC5=CC=C4	0.49669	3.022356
CCCCOC1=C(C=C2CSCC2=C1)OCOCC	0.99266	3.02129
CCCCS(=O)C1=C(C2=C(S1)C=C(C(=C2C3=CC=C(C=C3)Br)C(=O)OCC)C4=NC=CS4)N	0.56917	3.020054
C1CN(CCN1CCCCOC2=CC3=C(C=C2)C=CC(=O)N3COC(C4=CN=CN=C4)O)C5=C6C=CSC6=CC=C5	0.51580	3.012253
C1CN(CCN1CCCCOC2=CC3=C(C=C2)C=CC(=O)N3COC(C4=CN=NC=C4)O)C5=C6C=CSC6=CC=C5	0.51580	3.012253
CC(C)(C)C1CCC2=C(C1)SC(=C2C(=O)O)NC(=O)C3=CC=C(C=C3)OCCCCCC(=O)OC	0.54	3.01

	5593	2185
CCOC(=O)CC(C#CC)C1=CN=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC5CCSC(C5)(O)O)C	0.46090	3.012062
C1CN(CCN1CCCCOC2=CC(=C(C=C2)/C=C\C(=O)O)[N+](=O)[O-])C3=C4C=CSC4=CC=C3	0.58385	3.018
C1CCC2=C(C1)C(=C(S2)NC(=O)C3CC=CC(=C3)CN(C4CC4)C5CCNCC5)C(=O)NC6=CC=C(C=C6)CCC7=CCC(C=C7)C(=O)O	0.39912	3.003396
CC#CC(C/C(=N/N)/NN)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCCC(C)(C)O)C	0.45055	3.002665
CC(C)C(C(=O)NCC(=O)N1C(=O)C=CC2=C1C=C(C=C2)OCCCCN3CCN(CC3)C4=C5C=CSC5=CC=C4)N	0.44665	2.992723
CC(C)C(C(=O)N1C(=O)C=CC2=C1C=C(C=C2)OCCCCN3CCN(CC3)C4=C5C=CSC5=CC=C4)NC(=O)CN	0.44665	2.992723
CC1(CC(=O)N(C2=C1C=CC(=C2)OCCCCN3CCN(CC3)C4=C5C=CSC5=CC=C4)COC(=O)NCC(=O)OC)C	0.46427	2.982669
CCN(CC)C/C=C\C1=CC=CC=C1S(=O)(=O)NC2=C(C3=C(S2)CCCC3)C(=O)O	0.65919	2.988149
CS(=O)(=O)CCCOC1=CC=C(C=C1)C2=C3CCC(C3=CC=C2)OC4=CC5=C(C=C4)[C@@H](CS5)CC(=O)O	0.55805	2.981484
COC(=O)[C@H](C1=CC=CC=C1)NCC2CCC(CC2)CNCC3=CC4=C(CC(S4)C(=O)NO)C=C3	0.54414	2.972348
CN1C=C(C=C1C(=O)NC2=CN(C(=C2)C(=O)NCCN3CCOCC3)CCN4CCOCC4)NC(=O)C5=C(C6=CC=CC=C6S5)Cl	0.36806	2.972344
CC#CC(CC1=NNN=N1)C2=CN=C(C=C2)OCC3=CC4=C(C=C3)SC=C4C5=C(C=C(C=C5)OCCC(C)(C)O)C	0.47897	2.972304
CC#C[C@H](CC1=NNN=N1)C2=CN=C(C=C2)OCC3=CC4=C(C=C3)SC=C4C5=C(C=C(C=C5)OCCC(C)(C)O)C	0.47897	2.972304
C1CC1COC2=CC3=C(C=C2)C=C(S3)C(=O)CC(CCN4C(=O)C5=CC=CC=C5N=N4)C(=O)O	0.52820	2.971358
CCCC1=CC=C(C=C1)C(=O)OC2CCC(CC2)C(=O)OC3=C4C=C(SC4=C(C=C3)OC(=O)C5CCC(CC5)OC(=O)C6=CC=C(C=C6)CCC)C7=CC=CC=C7	0.36320	2.963226
C1CCC2=C(C1)C(=C(S2)NC(=O)C3=CC=CC(=C3)CN(C4CC4)C5CCNCC5)C(=O)NC6=CC=C(C=C6)CCC7=CC=C(C=C7)C(=O)O	0.40006	2.963083
CC#CC(CC1=NNN=N1)C2=CC=C(C=C2)OCC3=CC4=C(C=C3)SC=C4C5=C(C=C(C=C5)OCCC(C)(C)O)C	0.52332	2.962352

	9	
CN1C=C(C=C1C(=O)NC2=CN(C(=C2)C(=O)NCCN3CCCCC3)CCN4CCOCC4)NC(=O)C5=C(C6=CC=CC=C6S5)Cl	0.39719	2.952551
COC(=O)[C@H](C1=CC=CC=C1)NCC2CCC(CC2)CNCC3=CC4=C(C=C3)C=C(S4)C(=O)NO	0.55410	2.952192
COC(=O)[C@H](C1CCCCC1)NCC2=CC=C(C=C2)CNCC3=CC4=C(C=C3)C=C(S4)C(=O)NO	0.55474	2.952192
CN(CCN1CCOCC1)C(=O)C2=CC=CC(=C2)C(=O)NC3=C(C4=C(S3)CCCC4)C(=O)NC5=CC=C(C=C5)CCC6=CC=C(C=C6)C(=O)O	0.35198	2.942825
CC(=O)CC(=O)C(CO)C(CCO)CC1CC2=C(C=CC(=C2C(=O)C1)O)C3=CC4=CC=CC=C4S3	0.51403	2.941763
CCOC(=O)C1CCN(CC1)CC2=CC(=CC=C2)C(=O)NC3=C(C4=C(S3)CCCC4)C(=O)NC5=CC=C(C=C5)CCC6=CC=C(C=C6)C(=O)O	0.35959	2.932873
C1COC1COC2=CC3=C(C=C2)C=C(S3)C(=O)CC(CCN4C(=O)C5=CC=CC=C5N=N4)C(=O)O	0.47980	2.931308
CC1(CC(=O)N(C2=C1C=CC(=C2)OCCCCN3CCN(CC3)C4=C5C=CSC5=CC=C4)COC(=O)N(C)CC(=O)OC)C	0.48467	2.922825
CC(C)(C)OC(=O)N(C)C1=NC=C(C=C1)C2=CC3=C(S2)C=C(C=C3)OC[C@@H](COS(=O)(=O)C)O[C@@H]4CCCCO4	0.43985	2.921913
CC(C)(C)OC(=O)N(C)C1=NC=C(C=C1)C2=CC3=C(S2)C=C(C=C3)OCC(COS(=O)(=O)C)O[C@H]4CCCCO4	0.43985	2.921913
CC(C)(C)OC(=O)N(C)C1=NC=C(C=C1)C2=CC3=C(S2)C=C(C=C3)OCC(COS(=O)(=O)C)O[C@@H]4CCCCO4	0.43985	2.921913
CC1=C(C=CC(=C1)OCCCS(=O)(=O)C)C2=C3CCC(C3=CC=C2)OC4=CC5=C(C=C4)[C@@H](CS5)CC(=O)O	0.54645	2.92164
CC(C)C1=NN=C(O1)N2CCN(CC2)CC3=CC(=CC(=C3)OC(C)C)C(C)(C)C4=CC(=CC(=C4)Cl)N(C5=CC6=C(C(=C5)SC=C6)S(=O)(=O)C	0.42805	2.912523
CCCOC1=CC2=C(C=C1)C=C(S2)C(=O)CC(CCN3C(=O)C4=CC=CC=C4N=N3)(C(=O)OC(C)(C)C)C(=O)OC(C)(C)C	0.39124	2.912509
CCCC[C@@H](C(=O)O)N1C(=NN=N1)[C@H](CC2=CSC3=CC=CC=C32)NC(=O)OCC4C5=CC=CC=C5C6=CC=CC=C46	0.43277	2.912097
CCCCC(C(=O)O)N1C(=NN=N1)[C@H](CC2=CSC3=CC=CC=C32)NC(=O)OCC4C5=CC=CC=C5C6=CC=CC=C46	0.43277	2.912097

	8	
CCCCC(C(=O)O)N1C(=NN=N1)[C@H](CC2=CC3=CC=CC=C3S2)NC(=O)OCC4C5=CC=CC=C5C6=CC=CC=C46	0.43277	2.912097
CC(C)(C)OC(=O)N(C)C1=CC=C(C=C1)C2=CC3=C(S2)C=C(C=C3)OC[C@@H](COS(=O)(=O)C)O[C@@H]4CCCCO4	0.47898	2.911961
C1CC(C1)COC2=CC3=C(C=C2)C=C(S3)C(=O)CC(CCN4C(=O)C5=CC=CC=C5N=N4)C(=O)O	0.51825	2.911515
COC1=CC=C(C=C1)CN([C@H](CON2C(=O)C3=CC=CC=C3C2=O)C4=CC5=CC=CC=C5S4)C(=O)C6=NC(=C(C=C6)Br)OC	0.43595	2.910726
COC1=CC=C(C=C1)CN(C(CON2C(=O)C3=CC=CC=C3C2=O)C4=CC5=CC=CC=C5S4)C(=O)C6=NC(=C(C=C6)Br)OC	0.43595	2.910726
COC(=O)C1=CC=C(C=C1)CCC2=CC=C(C=C2)NC(=O)C3=C(SC4=C3CCCC4)NC(=O)C5=CC=CC(=C5)CN(C6CC6)C7CCNCC7	0.42185	2.90324
CCN=C(CNC(=O)OCC1CCC2=C(C1)SC(=C2C#N)NC(=O)CC(C)C3=CC=CCC3)/C=C\N	0.45219	2.892461
CCOC(=O)CCCN(CC1=CC2=C(C=C1)SC=N2)C(=O)C3(CCN3C(=O)CC4=CSC5=CC=CC=C54)C	0.59021	2.891756
COC(=O)[C@H](C1=CC=CC=C1)NCC2=CC=C(C=C2)CNCC3=CC4=C(C=C3)C=C(S4)C(=O)NO	0.55904	2.891722
CN(CCN1CCOCC1)C(=O)C2=CC=CC(=C2)C(=O)NC3=C(C4=C(S3)CCCC4)C(=O)NC5=CC=C(C=C5)CCC6=CC=C(C=C6)C(=O)OC	0.36870	2.882982
CC1=C(C=CC(=C1)NC(=O)C2=C(SC3=C2CCCC3)NC(=O)C4=CC(=CC=C4)C(=O)N(C)CCN5CCOCC5)CCC6=CC=C(C=C6)C(=O)O	0.34610	2.882982
CC1(CC(=O)N(C2=C1C=CC(=C2)OCCCCN3CCN(CC3)C4=C5C=CSC5=CC=C4)COC(=O)NOC6=CC=CO6)C	0.47314	2.882512
CCOC1=C(C(=C(C=C1)NC(=O)NC2=CC3=C(C=C2)C=C(S3)C(=O)N[C@H]4CN5CCC4CC5)OCC)OCC.Cl	0.47876	2.882173
C/C=C\C(=C/C=C)\CSC1=C\2C(=C(S1)C(=O)NCC3=CC=NN3C)CC(C/C2=N\O)C4=CC=C(C=C4)OC	0.55429	2.881916
CC(C)(CN=O)C(=O)NCCN1C=CC2=C1C(=NC=N2)NC3=CC(=C(C=C3)OC4=CC5=C(C=C4)C=CS5)Cl	0.47940	2.881397
CN1CCN(CC1)CCN(C)C(=O)C2=CC=CC(=C2)C(=O)NC3=C(C4=C(S3)CCCC4)C(=O)NC5=CC=C(C=C5)CCC6=CC=C(C=C6)C(=O)O	0.35826	2.873141
CCOC(=O)C1CCN(CC1)CC2=CC(=CC=C2)C(=O)NC3=C(C4=C(S3)CCCC4)C(=O)NC5=CC=C(C	0.37	2.87

=C5)CCC6=CC=C(C=C6)C(=O)OC	7069	3029
COC(=O)C1CCC(CC1)NCC2=CC(=CC=C2)C(=O)NC3=C(C4=C(S3)CCCC4)C(=O)NC5=CC=C(C=C5)CCC6=CC=C(C=C6)C(=O)OC	0.35901	2.873029
CCCN(CCC)C1=CC(=C(C=C1)N=NC2=CC3=C(S2)C=C(C=C3)N=NC4=CC=CC=C4)C(O)O	0.59425	2.872042
C1CC(OC1)COC2=CC3=C(C=C2)C=C(S3)C(=O)CC(CCN4C(=O)C5=CC=CC=C5N=N4)C(=O)O	0.47307	2.871464
CC1=CC(=CC(=C1C2=C3CC[C@H](C3=CC=C2)OC4=CC5=C(C=C4)C(CS5)CC(=O)O)C)OCCCS(=O)(=O)C	0.53524	2.861797
CC1=CC(=CC(=C1C2=C3CCC(C3=CC=C2)OC4=CC5=C(C=C4)[C@@H](CS5)CC(=O)O)C)OCCCS(=O)(=O)C	0.53524	2.861797
CC1=CC(=CC(=C1C2=C3CC[C@@H](C3=CC=C2)OC4=CC5=C(C=C4)[C@@H](CS5)CC(=O)O)C)OCCCS(=O)(=O)C	0.53524	2.861797
CC1=CC(=CC(=C1C2=C3CC[C@@H](C3=CC=C2)OC4=CC5=C(C=C4)C(CS5)CC(=O)O)C)OCCCS(=O)(=O)C	0.53524	2.861797
CC1=CC(=CC(=C1C2=C3CCC(C3=CC=C2)OC4[C@H](C5=CC=CC=C5S4)CC(=O)O)C)OCCCS(=O)(=O)C	0.53521	2.861797
COC1=C(C=CC(=C1)NC2=NN3C(=NC=C3C4=CC5=CC(=C(C=C5S4)OC)OC)C=C2)OCCCO	0.54863	2.861624
COC(=O)[C@H](CC1=CC=C(C=C1)OC2=CC=C(C=C2)CNCC3=CC4=C(C=C3)C=C(S4)C(=O)NO)N	0.47004	2.851671
CCC1=CC(=NC(=C1)C(=O)CNC(=O)C2=CC(=C(C=C2)OCCO)OC)C3=CSC4=C3C=CC=C4C	0.89113	2.841719
CN(CCN1CCOCC1)C(=O)NC2=CC=CC(=C2)C(=O)NC3=C(C4=C(S3)CCCC4)C(=O)NC5=CC=C(C=C5)CCC6=CC=C(C=C6)C(=O)OC	0.33794	2.833091
CC1=CC2=C(C(=C1)OC)SC(=C2)C3=CN(C(=C3C(=N)C)N)C4CCN(C4)C(=O)/C=C/CN(C)CCOC	0.54042	2.832617
CC(C)(C)OC(=O)C(CCN1C(=O)C2=CC=CC=C2N=N1)(CC(=O)C3=CC4=C(S3)C=C(C=C4)OCC5CC5)C(=O)OC(C)(C)C	0.38483	2.832509
CN(C)CCN(C)C1=CC(=C(C=C1NC(=O)C=C)NC2=NC=NC(=N2)C3=CSC4=CC=CC=C43)OC	0.56374	2.832103
CC1=C(C=CC(=C1)NC(=O)C2=C(SC3=C2CCCC3)NC(=O)C4=CC(=CC=C4)C(=O)N(C)CCN5CCOCC5)CCC6=CC=C(C=C6)C(=O)OC	0.36263	2.823138

	1	
CC1=CC(=CC(=C1/C/2=C/C=C\C[C@@H](CCC2=C)OC3=CC4=C(C=C3)[C@@H](CS4)CC(=O)O)C)OCCCS(=O)(=O)C	0.52292	2.82211
COCC1=CC=C(O1)CNC(=O)C2=C3CC(C/C(=N\O)/C3=C(S2)SCC4=CC=CC=C4)C5=CC=C(C=C5)OC	0.52584	2.821596
CC#SC(C)(CC(=O)O)C1=CC=C(C=C1)COC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC5(CS(=O)(=O)C5)C)C	0.49421	2.821518
CN1CCN(CC1)CCN(C)C(=O)C2=CC=CC(=C2)C(=O)NC3=C(C4=C(S3)CCCC4)C(=O)NC5=CC=C(C=C5)CCC6=CC=C(C=C6)C(=O)OC	0.37625	2.813298
CC(=O)C(CCN1C(=O)C2=CC=CC=C2N=N1)(CC(=O)C3=CC4=C(S3)C=C(C=C4)OCC5=CC=CC=C5)C(=O)OC(C)(C)C	0.41866	2.813209
CCOC1=CC=CC=C1CCC(=O)NC2=C(C3=C(S2)CC(CC3)COC(=O)NCC4=NOC(=C4)C)C#C	0.52333	2.818 1984
CCCS(=O)(=O)N1CCC(=CC1)C2=CC3=C(C=C2)N=C(S3)OC4CCN(CC4)C(=C)OCC5=CC6=CC=CC=C6S5(=O)=O	0.42957	2.811688
C1CN(CCN1CCCCOC2=CC3=C(C=C2)C=CC(=O)N3COC(=O)OC4=CC=C(C=C4)[N+](=O)[O-])C5=C6C=CSC6CC=C5	0.40989	2.802148
CC1=CC(=CC(=C1C2=C3CCC[C@H](C3=CC=C2)OC4=CC5=C(C=C4)[C@@H](CS5)CC(=O)O)C)OCCCS(=O)(=O)C	0.52446	2.801953
CC1=CC(=CC(=C1C2=C3CCC[C@H](C3=CC=C2)OC4=CC5=C(C=C4)C(CS5)CC(=O)O)C)OCCCS(=O)(=O)C	0.52446	2.801953
C1COC2=C(O1)C=CC=C2OCCNCC3=CC(=CC=C3)NS(=O)(=O)C4=CC5=C(S4)C=C(C=C5)Cl	0.58015 3	2.800737
C[C@@H](C(=O)OC)NCC1=CC=C(C=C1)CNCC2=CC3=C(CC(S3)C(=O)NO)C=C2	0.56495 1	2.791722
CCOC(=O)C1=C(SC2=C1CCCC2)NC(=O)COC3=CC=CC(=C3)N(C=N)N=N	0.52271 3	2.791471
CC(C)(C1=CC(=NN=C1OCC2=CC=CC=C2)C3=CC=CC4=C3SC(=C4)[C@@H](C5=CC=CC=C5Cl)NS(=O)(=O)C6CC6)O	0.45810 5	2.791366
CC(C)(C1=CC(=NN=C1OCC2=CC=CC=C2)C3=CC=CC4=C3SC(=C4)C(C5=CC=CC=C5Cl)NS(=O)(=O)C6CC6)O	0.45810 5	2.791366
CC(=O)N1CCC(CC1)N(CC2=CC(=CC=C2)C(=O)NC3=C(C4=C(S3)CCCC4)C(=O)NC5=CC=C(C=C5)CCC6=CC=C(C=C6)C(=O)O)C7CC7	0.36098 9	2.783189
COC1=CC=C(C=C1)C2CC3=C(SC(=C3/C(=N/O)/C2)SCC4=CC=CC=C4)C(=O)NCCOC5=CC=C	0.58	2.78

C=C5	253 4	1647
CC(C)(C)N(CCOC1=CC(=CC(=C1)NC(=O)C2=CC3=C(S2)C=CC(=C3)C(C)(C)S(=O)(=O)C)OC4=CC=C(C=C4)Cl)C(=O)O	0.38 223	2.78 1574
CC(C)(C)OC(=O)NCCOC1=CC(=CC(=C1)NC(=O)C2=CC3=C(S2)C=CC(=C3)C(C)(C)S(=O)(=O)C)OC4=CC=C(C=C4)Cl	0.38 716 2	2.78 1574
C1=CC=C2C(=C1)C=C(S2)C3=CN=C4N3N=C(C=C4)NCCCCO.C(CCO)CN	0.57 990 1	2.77 2042
C[C@@H](C(=O)OC)NCC1=CC=C(C=C1)CNCC2=CC3=C(C=C2)C=C(S3)C(=O)NO	0.60 203	2.77 1566
COC1=C(N=C(C=C1)C(=O)CNC(=O)C2=CC(=C(C=C2)OCCO)OC)C3=CSC4=C3C=C(C=C4)C#N	0.43 842	2.77 1308
CC1=C(C=CC(=C1)NC(=O)C2=C(SC3=C2CCC(C3)(C)C)NC(=O)C4=CC(=CC=C4)C(=O)N(C)CCN5CCOCC5)CCC6=CC=C(C=C6)C(=O)O	0.33 478 4	2.76 3295
CC1=CC(=CC(=C1/C/2=C/C=C\C[C@@H](CCCC2=C)OC3=CC4=C(C=C3)[C@@H](CS4)CC(=O)O)C)OCCCS(=O)(=O)C	0.51 255 9	2.76 2266
CC1=C(C=CC(=C1)OCCN)C2=CSC3=C2C=C(C=C3)COC4=CC=C(C=C4)C5(CC(C5)N)CC(=O)O	0.51 198 2	2.76 2083
COC1=CC(=CC(=C1OC)OC)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC(=C(C(=C4)OC)OC)OC	0.46 289 7	2.76 1879
CC#C[C@@H](CC(=O)O)C1=CC=C(C=C1)OC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC(CO)O)C	0.55 316 6	2.76 1607
COCCOC(=O)OC1CCC2=C(C1)SC(=C2C=N)NC(=O)CCC3=CC(=CC=C3)O	0.53 135 3	2.76 1512
COCCNC(=O)OC1CCC2=C(C1)SC(=C2C=N)NC(=O)CCC3=CC(=CC=C3)O	0.51 680 6	2.75 1671
CCOC1=C(C2=C(C=C1)SC=C2)CCNC3=NC=NC(=C3)C4=CC(=C(C=C4)C(=O)O)SC	0.65 612	2.75 1181
CC(C)CN(C[C@@H]1[C@@H](N(C(O1)(C)C)C(=O)OC(C)(C)C)CC2=CC=C(C=C2)C#CC3=C(C4=C(S3)CCC(C4)(C)C)C(=O)OCC(C)C)S(=O)(=O)C5=CC=C(C=C5)OC	0.33 066 5	2.74 3948
CC1=C(C(=C(C(=C1C2=C3CCC(C3=CC=C2)OC4=CC5=C(C=C4)[C@@H](CS5)CC(=O)O)C)C)OCCCS(=O)(=O)C)C	0.51 398 3	2.74 211
CC(C)OC1=CC(=CC(=C1)N2CCN(CC2)C)C(C)CC3=CC(=CC(=C3)Cl)NC(=O)C4=CC5=C(S4)C=CC(=C5)NS(=O)(=O)C	0.46 916 9	2.74 2101
C1=CC=C2C(=C1)C(=O)N(N=N2)CCC(CC(=O)C3=CC4=C(S3)C=C(C=C4)OCC5=CC=NC=C5)C(=O)O	0.46 087	2.74 1311

CC(CC1=CC(=NC=C1)C2=CC=CC3=C2SC(=C3)C(C4=CC=CC=C4SC)NS(=O)(=O)C5CC5)O	0.61712	2.742 1262
CC1=C(SC2=C1C=C(C=C2)Cl)S(=O)(=O)NC3=CC=CC(=C3)CNCCOC4=CC=CC5=C4OCCO5	0.56829	2.741 0893
CC1=C(SC2=C(C=CC(=C12)COC)C(=O)C)C(=O)NC3=NC4=CC=CC(=C4C=C3)CCC(C)C(C(=O)O)N	0.43241	2.737 1984
CC#CC(CC(=O)O)C1=CN=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC5(CS(=O)C5)C)C	0.54605	2.732 1644
CCOC(=O)C1=C2CCC(/C(=N\O)/C2=C(S1)SC/C(=C/C)/C=C\C=C)C3=CC=C(C=C3)OC	0.72429	2.731 1538
CC1=C(SC2=C(C=CC(=C12)COC)C(=O)C)C(=O)NC3=NC4=CC=CC=C4C(=C3)CN(C)CCO.Cl.Cl	0.52885	2.737 1412
CCCSC1=C(C=CC(=C1)C2=CC(=NC=N2)NCCC3=C(SC4=CC=CC=C43)C)C(=O)O	0.70802	2.732 1388
COC1=CC=C(C=C1)COC2=CC3=C(C=C2)C(=C(S3)C4=CC=C(C=C4)Br)OC5=CC=C(C=C5)OC6CC(C6)N7CCN(CC7)C8=CC9=C(C=C8)C(=O)N(C9)C1CCC(=O)NC1=O	0.30841	2.729 2192
CC#CC(CC(=O)O)C1=CC=C(C=C1)COC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC5(CS(=O)C5)C)C	0.60462	2.722 1691
CC#CC(CC(=O)O)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC5(CS(=O)C5)C)C	0.60462	2.722 1691
CC(CO)C1=CC(=NC=C1)C2=CC=CC3=C2SC(=C3)C(C4=C(C=CC(=N4)N)Cl)NS(=O)(=O)CC5CC5	0.45945	2.721 1213
CC(CCC1=CC(=NC=C1)C2=CC=CC3=C2SC(=C3)C(C4=C(C=CC(=N4)N)Cl)NS(=O)(=O)C5CC5)O	0.45936	2.721 1213
CC(CC1=CC(=NC=C1)C2=CC=CC3=C2SC(=C3)C(C4=C(C=CC(=N4)N)Cl)NS(=O)(=O)CC5CC5)O	0.45893	2.721 1213
CC(CO)C1=CC(=NC=C1)C2=CC=CC3=C2SC(=C3)C(C4=C(C=CC=C4Cl)OC)NS(=O)(=O)C5CC5	0.55972	2.721 1101
CC(CC1=CC(=NC=C1)C2=CC=CC3=C2SC(=C3)C(C4=CC=CC=C4Cl)NS(=O)(=O)C5CC5)(O)OC	0.55937	2.721 1101
CC(COC)(C1=CC(=NC=C1)C2=CC=CC3=C2SC(=C3)C(C4=CC=CC=C4Cl)NS(=O)(=O)C5CC5)O	0.55928	2.721 1101
CC(CC1=CC(=NC=C1)C2=CC=CC3=C2SC(=C3)C(C4=C(C=CC=C4Cl)OC)NS(=O)(=O)C5CC5)O	0.55	2.72

	9435	1101
CC#CC(CC(=O)O)C1=CN=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC5(CS(C5)(O)O)C)C	0.45404	2.718 1749
COC/C(=N\NC(=O)CNC(=O)C1=CC(=C(C=C1)OC)OC)/C2=CSC3=CC=CC=C32	0.58763	2.715 1358
C/C(=N\NC(=O)CNC(=O)C1=CC(=C(C=C1)OCCO)OC)/C2=CSC3=CC=CC=C32	0.53786	2.712 1358
COC1=C(C=C(C=C1)C(=O)NCC(=O)N/N=C(\CCO)/C2=CSC3=CC=CC=C32)OC	0.53786	2.712 1358
CC(C)CN(C[C@@H]1[C@@H](N(C(O1)(C)C)C(=O)OC(C)(C)C)CC2=CC=C(C=C2)OCC3=CC=CC=C3C4=C(C5=C(S4)CCC(C5)(C)C)C(=O)OC(C)(C)C)C(=O)OCC6=CC=CC=C6	0.33124	2.702 4696
CC1=C(C=CC(=C1)NC(=O)C2=C(SC3=C2CCC(C3)(C)C)NC(=O)C4=CC(=CC=C4)C(=O)N(C)CCN5CCOCC5)CCC6=CC=C(C=C6)C(=O)OC	0.35094	2.706 3451
CCCS(=O)(=O)NC1=C(C=CC(=C1)NC2=C(C3=C(S2)C(C(CC3(C)C)CC(C)C)(C)C)C)C(=O)O	0.55319	2.708 2429
CCCS(=O)(=O)NC1=C(C=CC(=C1)N(CC(C)C)C2=C(C3=C(S2)C(CCC3(C)C)(C)C)C)C(=O)O	0.58866	2.705 2429
CN(C1=CC(=C(C(=C1)OC)OC)OC)C(=O)C2=C(SC3=C2CCCC3)NC(=O)C4=CC(=C(C(=C4)OC)OC)OC	0.47901	2.706 2036
CN(C1=C(C2=C(S1)CCCC2)C(=O)NC3=CC(=C(C(=C3)OC)OC)OC)C(=O)C4=CC(=C(C(=C4)OC)OC)OC	0.47901	2.706 2036
COC1=CC=C(C=C1)C2=C(C3=C(S2)C=C(C=C3)OC(=O)OC4=CC=C(C=C4)[N+](=O)[O-])OC5=CC=C(C=C5)OCCN6CCCCC6	0.42287	2.709 1879
CC#C[C@@H](CC(=O)O)C1=CC=C(C=C1)COC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC5(CS(C5)(O)O)C)C	0.49489	2.705 1797
CC#C[C@@H](CC(=O)O)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC5(CS(C5)(O)O)C)C	0.49489	2.705 1797
CC#CC(CC(=O)O)C1=CC=C(C=C1)COC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC5(CS(C5)(O)O)C)C	0.49489	2.705 1797
CC1=C(C=CC(=C1)OC2CCS(=O)(=O)CC2)C3=C(SC4=C3C=C(C=C4)COC5=CC=C(C=C5)C(CC(=O)O)C=C)C	0.5171	2.705 1797
CCOC1=CC=CC=C1/C=C/C(=O)NC2=C(C3=C(S2)CC(CC3)OC(=O)OCCOC)N	0.55088	2.701 1668

	9	
CN(C1=C\2C(=C(S1)C(=O)O)CC(C/C2=N\O)C3=C[C@@H]4CC4(C=C3)OC)SOCCC5=CCC=CC=C5.S	0.53317	2.701473
CN(CCN1CCOCC1)C(=O)C2=CC=CC(=C2)C(=O)NC3=C(C4=C(S3)CCCC4)C(=O)NC5=CC=C(C=C5)CCN6CCOCC6	0.42367	2.693141
CC(=O)N(CC1=CC(=CC=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)CCC5=CC=C(C=C5)C(=O)OC)C6CCC(CC6)C(=O)OC	0.32468	2.693135
CCOC1=CC=CC=C1/C=C/C(=O)NC2=C(C3=C(S2)CC(CC3)COC(=O)NCCO)N	0.49661	2.693 1828
CC#CC(CC(=O)O)C1=CC=C(C=C1)COC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC5(CS(=O)(=O)C5)C)C	0.51836	2.682 164
CC#CC(CC(=O)O)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC5(CS(=O)(=O)C5)C)C	0.51836	2.682 164
C1CC1(COC2=CC3=C(C=C2)C(=C(S3)C(=O)C4=CC=C(C=C4)C5=CN(N=N5)C6=CC=C(C=C6)F)C7=CC=C(C=C7)F)CO[N+](=O)[O-]	0.96363	2.682 1435
CC(C)(C1=CC2=C(C=C1)SC(=C2)C(=O)NC3=CC(=CC(=C3)OC4=CC=C(C=C4)Cl)OCCN)S(=O)(=O)C	0.48002	2.681 105
COC(=O)C1=CC=C(C=C1)CCC2=CC=C(C=C2)NC(=O)C3=C(SC4=C3CCCC4)NC(=O)C5=CC=CC(=C5)CN[C@H]6CCOC6	0.43448	2.673 261
COC(=O)C1=CC=C(C=C1)CCC2=CC=C(C=C2)NC(=O)C3=C(SC4=C3CCCC4)NC(=O)C5=CC=CC(=C5)CN[C@@H]6CCOC6	0.43448	2.673 261
C1CN(CCN1CCCCOC2=CC3=C(C=C2)C=CC(=O)N3C(=O)CNC(=O)CN)C4=C5C=CSC5=CC=C4	0.45791	2.672253
CO[C@@H]1CCN(C1)[C@H]2C[C@H](N(C2)C(=O)CC3=CC(=C(C=C3Cl)NC(=O)C4=CSC5=CC=CC=C54)Cl)COC6CCC(CC6)C(=O)O	0.39951	2.671937
CC#CC(CC(=O)O)C1=CN=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC5CCS(=O)CC5)C	0.53515	2.6718
CC1=C(SC2=C(C=CC(=C12)COC)C(=O)C)C(=O)NC3=NC4=CC=CC(=C4C=C3)COP(=O)(OC(C)(C)C)OC(C)(C)C	0.42189	2.662216
CC#CC(CC(=O)O)C1=CC=C(C=C1)COC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC5CCS(=O)CC5)C	0.59241	2.661848
CC#CC(CC(=O)O)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC5CCS(=O)CC5)C	0.59241	2.661848

COOCCOC1=C(C=C(C=C1)CC2=CC3=CC=CC=C3S2)[C@H]4[C@@H]([C@H]([C@@H]([C@H](O4)CO)O)O)O	0.45311	2.668 1505
COCCNC(=O)C1=C2CC(C/C(=N\O)/C2=C(S1)SCC3=CC=CC=C3)C4=CC=C(C=C4)OC	0.64078	2.664 149
CC(CC1=CC(=NC=C1)C2=CC=CC3=C2SC(=C3)C(C4=CC=CC=C4S(=O)(=O)C)NS(=O)(=O)C5CC5)O	0.46053	2.667 116
C1COC2=C(O1)C=CC=C2OCCNCC3=CC(=CC=C3)NS(=O)(=O)C4=CC5=CC=CC=C5S4	0.61083	2.668 1127
C1COC2=C(O1)C=CC=C2OCCNCC3=CC(=CC=C3)NS(=O)(=O)C4=CSC5=CC=CC=C54	0.61083	2.668 1127
CC(C)CC(C(=O)N1C[C@H]2C[C@@H]1CN2C(=O)CNS(=O)(=O)C3=C(C=C(C=C3)Cl)Cl)NC(=O)C4=CC5=CC=CC=C5S4	0.40223	2.666 1035
CC#C[C@@H](CC(=O)O)C1=CN=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC5CCS(CC5)(O)O)C	0.44509	2.657 1906
CC#CC(CC(=O)O)C1=CN=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC5CCS(CC5)(O)O)C	0.44509	2.657 1906
CC#C[C@H](CC(=O)O)C1=CN=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC5CCS(CC5)(O)O)C	0.44509	2.657 1906
CCC[C@@H](CC(=O)O)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)C(=O)N5CCS(=O)(=O)CC5)C	0.46864	2.651 1906
CCCNC1=CC2C(C=C1)C(=CS2)CN3C[C@H]4N([C@H](C3=O)CC5=CC=C(C=C5)O)C(=O)CN(N4C(=O)NCC6=CC=CC=C6)CC=C	0.41048	2.642 2988
CC#C[C@@H](CC(=O)O)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC5CCS(CC5)(O)O)C	0.48508	2.649 1953
CC#CC(CC(=O)O)C1=CC=C(C=C1)COC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC5CCS(CC5)(O)O)C	0.48508	2.649 1953
CC=CC(CC(=O)O)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC(=C3C4=C(C=C(C=C4)OC5CCS(=O)(=O)CC5)C)C	0.50690	2.642 1953
CC1=C(SC2=C(C=CC(=C12)COC)C(=O)C)C(=O)NC3=NC4=CC=CC(=C4C=C3)COCCO.Cl	0.54747	2.641 1329
CC#C[C@@H](CC(=O)O)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC5(C(=O)SC5=O)C)C	0.52158	2.641 1327

C1CC1C(CO)C2=CC(=NC=C2)C3=CC=CC4=C3SC(=C4)C(C5=C(C=CC(=N5)N)Cl)NS(=O)(=O)C6CC6	0.45138	2.641213
C1CC1C(CC2=CC(=NC=C2)C3=CC=CC4=C3SC(=C4)C(C5=C(C=CC(=N5)N)Cl)NS(=O)(=O)C6CC6)O	0.45094	2.641213
C1CC1CC(C2=CC(=NC=C2)C3=CC=CC4=C3SC(=C4)C(C5=C(C=CC(=N5)N)Cl)NS(=O)(=O)C6CC6)O	0.45207	2.641213
CC(C)OC1=CC(=CC(=C1)C(C)(C)C2=CC(=CC(=C2)Cl)NC(=O)C3=CC4=C(S3)C=CC(=C4)NS(=O)(=O)C)C[N+]5(CCN(CC5)C)C	0.46245	2.632487
CC(C)C1=CC=CC=C1C2=C(C3=C(S2)C=C(C=C3)OC(C)(C)C(=O)C(C)N)OC4=CC=C(C=C4)/C=C/C(=O)O	0.52160	2.632079
CC#CC(CC(=O)O)C1=CN=C(C=C1)COC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC5CCS(=O)(=O)CC5)C	0.46438	2.631749
C=C/C=C(/C(=O)C1=C(C2=C(S1)C=C(C=C2)O)OC3=CC=C(C=C3)/C=C/C(=O)O)\NC=C	0.63989	2.630984
CC(=O)N1CCC(CC1)NCC2=CC(=CC=C2)C(=O)NC3=C(C4=C(S3)CCCC4)C(=O)NC5=CC=C(C=C5)CCC6=CC=C(C=C6)C(=O)OCl	0.36824	2.622486
COC1=CC(=C(C=C1CC2=CC3=CC=CC=C3S2)[C@H]4[C@@H]([C@H](C[C@H](O4)COC(=O)C5=CC=CC=C5)OC(=O)C6=CC=CC=C6)OC(=O)C7=CC=CC=C7)OC(=O)C8=CC=CC=C8	0.30860	2.622342
CN(C)CCOC1=C(C=C(C=C1)C2[C@H]([C@H](CC(O2)CO)O)ON)CC3=CC4=CC=CC=C4S3	0.56071	2.622032
CC#CC(CC(=O)O)C1=CC=C(C=C1)COC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC5CCS(=O)(=O)CC5)C	0.50818	2.621797
CC#CC(CC(=O)O)C1=CC=C(C=C1)COC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC5CCSC(C5)(O)O)C	0.48620	2.621797
COC(=O)C1=CC=C(C=C1)CCC2=CC=C(C=C2)NC(=O)C3=C(SC4=C3CCCC4)NC(=O)C5=CC=CC(=C5)CNC6CCOCC6	0.42656	2.612767
CC(C(=O)NCC(=O)N1C(=O)C=CC2=C1C=C(C=C2)OCCCCN3CCN(CC3)C4=C5C=CSC5=CC=C4)N	0.45576	2.61241
CC(C)(C)[C@@H](C(=O)OC)NCC1=CC=C(C=C1)CNCC2=CC3=C(CC(S3)C(=O)NO)C=C2	0.56092	2.612192
C1CC(=O)N(C2=C1C=CC(=C2)OCCCCN3CCN(CC3)C4=C5C=CSC5=CC=C4)OP(=O)(O)O	0.51041	2.611593
CCOC1=CC2=C(C=C1)C=C(S2)C(=O)CC(CCN3C(=O)C4=CC=CC=C4N=N3)C(=O)O	0.54	2.61

	9114	1202
CC(C)C1=C(C(=NO1)C2=C(C=CC=C2Cl)Cl)COC3=CC4=C(C=C3)C=C(S4)C5=CC(=CC=C5)C(=O)NSN(C)C	0.59657	2.610871
CCOC1=C(C=CC(=C1)/C=N\NC(=O)C2=CC=C(C=C2)NC(=O)C3=C(C4=C(C3)C=C(C=C4)Cl)Cl)OC(=O)C5=CC=C(C=C5)Br	0.24374	2.610276
CC#CC(C/C(=N/N)/NN)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC5(CS(=O)C5)C)C	0.43923	2.602229
CC#CC(CC(=O)O)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC5(CCS(CC5)(O)O)O)C	0.41656	2.601902
CCOC(=O)C1CCCC2=C1SC(=C2C(=O)OCC)NC(=O)NCC3=C(C=C(C=C3)OC)OC	0.51463	2.601774
CCOC(=O)C1CCC2=C(C1)C(=C(S2)NC(=O)NCC3=C(C=C(C=C3)OC)OC)C(=O)OCC	0.51195	2.601774
CC1=CC2=C(C=C1)SC(=C2)S(=O)(=O)NC3=CC=CC(=C3)CNCCOC4=CC=CC5=C4OCCO5	0.59832	2.601283
CN1C=C(C=C(C1=O)NC2=NC=C(C=C2)N3CCN(CC3)C4COC4)C5=CN=CC(=C5CO)N(C)CCC6=C(SC7=C6CCCC7)C=O	0.38428	2.593097
CC(C)(C)OC(=O)C(CCN1C(=O)C2=CC=CC=C2N=N1)(CC(=O)C3=CC4=C(S3)C=C(C=C4)OCC5=CC=CC=C5)C(=O)OC(C)(C)C	0.36726	2.592509
CC(C)(C)[C@@H](C(=O)OC)NCC1=CC=C(C=C1)CNCC2=CC3=C(C=C2)C=C(S3)C(=O)NO	0.57573	2.592035
C1CC(=O)NC(=O)C1N2C(=O)C3=C(C2=O)C=C(C=C3)N4CC(C4)CN5CCN(CC5)CCOC6=CC=C(C=C6)OC7=C(SC8=C7C=CC(=C8)O)C9=CC=C(C=C9)Br	0.28851	2.591832
C1CC(=O)NC(=O)C1N2C(=O)C3=C(C2=O)C=C(C=C3)N4CCN(CC4)CC5CN(C5)CCOC6=CC=C(C=C6)OC7=C(SC8=C7C=CC(=C8)O)C9=CC=C(C=C9)Br	0.28851	2.591832
CCOC1=C(C=CC=C1C(=O)O)C2=CC(=NC=N2)NCCC3=C(C=C4C(=C3)C=CS4)OC	0.62997	2.591409
CCOC1=C(C=CC(=C1)C2=CC(=NC=N2)NCCC3=CC4=C(S3)C=CC(=C4)OC)C(=O)O	0.62997	2.591409
COC1=C(C=C2C=CSC2=C1)CCNC3=NC=NC(=C3)C4=CC=CC(=C4OC)CC(=O)O	0.62778	2.591409
COC1=C(C=C2C=CSC2=C1)CCNC3=NC(=NC(=C3)C4=CC=C(C=C4)CC(=O)O)OC	0.62778	2.591409

CC(=O)OC/C(=N\NC(=O)CNC(=O)C1=CC(=C(C=C1)OC)OC)/C2=CSC3=CC=CC=C32	0.49859	2.595 1308
CC[C@H](C(=O)NC1=C(C2=C(S1)CCCC2)C(=O)OCN)N(C3=CC(=CC=C3)Cl)S(=O)(=O)C	0.83888	2.593 1002
CCCCOC(=O)C1=C(SC2=C1CC(CC2)(C)C)C#CC3=CC=C(C=C3)C[C@H]4[C@H](OC(N4C(=O)OC(C)(C)C)(C)C)CN(CC(C)C)C(=O)OCC5=CC=CC=C5	0.38455	2.581 4278
CCCNCCNCC1=CC2CC(S1)CCCC2	0.40665	2.581973
CC#CC(CC(=O)O)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC5(CCS(=O)(=O)CC5)O)C	0.43366	2.583 1746
CC#C[C@@H](CC(=O)O)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC5CCSC(=O)C5=O)C	0.51113	2.581484
CC#C[C@@H](CC(=O)N)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC5(CCS(=O)(=O)CC5)O)C	0.41850	2.578 1906
CC(C)(C)OC(=O)N1CCC(CC1)N(CC2=CC(=CC=C2)C(=O)NC3=C(C4=C(S3)CCCC4)C(=O)NC5=CC=C(C=C5)CCC6=CC=C(C=C6)C(=O)O)C7CC7	0.31975	2.562 3608
CCN1CCC2=C(C1)SC(=C2CNCC(=O)NC3=C(C4=C(S3)CCCC4)C(=O)OCC)N5C=CC=C5	0.62980	2.563 2072
CC(=O)OC1=C(C=C2C(=C(SC2=C1Cl)NC(NC3=CC=CC(=C3)CN(C)C)O)C(=O)N)Cl	0.49318	2.566 0739
CCN(CC)C1=CC=C(C=C1)NC(=O)C2=CC=C(C=C2)NC(=O)C3=C(SC4=C3CCCC4)NC(=O)C5=CC=CC(=C5)CN6CCOCC6	0.42631	2.553 3036
OCCOCC(C1=CC2=CC=CC=C2S1)NCC	0.55930	2.554 1136
CN1CCC(CC1)NCC2=CC(=CC=C2)C(=O)NC3=C(C4=C(S3)CCCC4)C(=O)NC5=CC=C(C=C5)CCC6=CC=C(C=C6)C(=O)OC	0.43602	2.547 3083
CC#C[C@@H](CC(=O)OC)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC5(CCS(CC5)(O)O)O)C	0.43754	2.542059
CCOC(=O)CC1(CC(=O)C1)C2=CC=C(C=C2)OCC3=CC4=C(C=C3)SC=C4C5=C(C=C(C=C5)OC6CCS(CC6)(O)O)C	0.44669	2.542059
CC#CC(CC(=O)OC)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC5(CCS(CC5)(O)O)O)C	0.43754	2.542059
CC1=C(C=CC(=C1)OC2CCS(=O)(=O)CC2)C3=C(SC4=C3C=C(C=C4)COC5=CC=C(C=C5)C(CC6=NNN=N6)C=C)C	0.44485	2.542021

COC1=CC=C(C=C1)C2CC3=C(SC(=C3/C(=N/O)/C2)SCC4=CC=CC=C4)CNCC5=CC=CO5	0.7060477	2.541541
C/C=C\C(=O)/C(=C\C(=C/C)\C1=C(C(=CC=C1)NC(=O)C2=CC3=C(S2)CCCC3)C)/NC4=NN=C(C=C4)NC5CC5	0.5233933	2.532511
C1CN(CCN(C1)CC2CN(C2)C3=CC4=C(C=C3)C(=O)N(C4=O)C5CCC(=O)NC5=O)CCOC6=CC=C(C=C6)OC7=C(SC8=C7C=CC(=C8)O)C9=CC=C(C=C9)Br	0.2844733	2.531988
CC(C)C1=C(C(=NO1)C2=C(C=CC=C2Cl)Cl)COC3=CC4=C(C=C3)C=C(S4)C5=CC(=CC=C5)C(=O)NS(=O)(=O)N(C)C	0.4423466	2.530769
COC(=O)CSC1=CC2=CC=CC=C2C(=C1)OCNS(=O)(=O)C3=CC4=CC=CC=C4S3	0.6555111	2.530425
C1CCC2=C(C1)C(=C(S2)NC(=O)C3=CC=CC(=C3)CN[C@@H]4CN5CCC4CC5)C(=O)NC6=CC=C(C=C6)CCC7=CC=C(C=C7)C(=O)O	0.4072299	2.522927
C1CCC2=C(C1)C(=C(S2)NC(=O)C3=CC=CC(=C3)CN(C4CCC(CC4)C(=O)O)C5CC5)C(=O)NC6=CC=C(C=C6)CC7=CC=NC=C7	0.4053335	2.522927
CC#CC(CC(=O)OC)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC5(CCS(=O)(=O)CC5)O)C	0.4526804	2.521902
CCOC(=O)CC1(CC(=O)C1)C2=CC=C(C=C2)OCC3=CC4=C(C=C3)SC=C4C5=C(C=C(C=C5)OC6CCSC(C6)(O)O)C	0.4407595	2.521902
CC#C[C@@H](CC(=O)OC)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC5(CCSC(C5)(O)O)O)C	0.4328201	2.521902
CC#CC(CC1=NNN=N1)C2=CC=C(C=C2)OCC3=CC4=C(C=C3)SC=C4C5=C(C=C(C=C5)OCC6(CS(=O)(=O)C6)C)C	0.4405665	2.521865
CNC1=C(C2=C(S1)C=C(C=C2)CC(=O)N3CC[C@@H](C3)N(C)C)C(=NC4=CC(=C(C=C4)OCC5=CSC=N5)Cl)N	0.4898693	2.521638
CC(C)NCC(COC1=CC2=C(C=C1)C=C(S2)C3=NC(=NC=C3)NC4CC(=C)NC(C4)(C)C)O	0.6018766	2.512511
CCOC(=O)C1=CC=C(S1)C2=CC=CC3=C2SC(=C3)[C@@H](C4=CC=CC=C4Cl)NS(=O)(=O)C5CC5	0.6425025	2.510399
CCOC(=O)C1=CC=C(S1)C2=CC=CC3=C2SC(=C3)C(C4=CC=CC=C4Cl)NS(=O)(=O)C5CC5	0.6425025	2.510399
CC(C)(C)OC(=O)N1CCC(CC1)N(CC2=CC(=CC=C2)C(=O)NC3=C(C4=C(S3)CCCC4)C(=O)NC5=CC=C(C=C5)CCC6=CC=C(C=C6)C(=O)OC)C7CC7	0.3315417	2.503764

CC(C)C1=C(C(=NO1)C2=C(C=CC=C2Cl)Cl)COC3=CC4=C(C=C3)C=C(S4)C5=CC(=CC=C5)C(=O)NS(=O)(=O)C6CC6	0.45392 3	2.50066
CCN(CC)C1=CC=C(C=C1)NC(=O)C2=C(SC3=C2CCCC3)NC(=O)C4=CC=CC(=C4)CN(C5CC5)C6CCN(CC6)C(=O)OC(C)(C)C	0.43328 3	2.49383818
CC1=C(C(=CC=C1)NS(=O)(=O)C)C2=CSC3=C2C=C(C=C3)COC4=CC=C(C=C4)[C@H](CC(=O)O)C#C	0.56409	2.491174
CCOC(=O)C1=C2C(=CC=C1)SC(=C2C(=N)Cl)/N=C\CCN(C)C3CCC(CC3)N	0.63780 8	2.4817
CCOC1=C(C=CC(=C1)C2=CC(=NC=N2)NCCC3=C(SC4=CC=CC=C43)C#N)CC(=O)O	0.56196 6	2.481413
C1CC(=O)NC(=O)C1N2C(=O)C3=C(C2=O)C=C(C=C3)N4CCN(CC4)CC5CCN(CC5)CCOC6=CC=C(C=C6)OC7=C(SC8=C7C=CC(=C8)O)C9=CC=C(C=C9)Br	0.28050 2	2.472145
CCOC1=CC=CC=C1/C=C/C(=O)NC2=C(C3=C(S2)CC(CC3)OC(=O)NCCN4CCN=C4)N	0.47963 4	2.472097
COC(=O)[C@H](C1CCC(CC1)OC2=CC=C(C=C2)CNCC3=CC4=C(C=C3)C=C(S4)C(=O)NO)N	0.47272 8	2.471984
CC#CC(CC(=O)O)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=CC=C4NS(=O)C)C	0.64358 6	2.471382
COC(=O)C1=CC=C(C=C1)CCC2=CC=C(C=C2)NC(=O)C3=C(SC4=C3CCCC4)NC(=O)C5=CC=CC(=C5)CN[C@@H]6CN7CCC6CC7	0.42928 6	2.463083
COC(=O)C1=CC=C(C=C1)CCC2=CC=C(C=C2)NC(=O)C3=C(SC4=C3CCCC4)NC(=O)C5=CC=CC(=C5)CN[C@H]6CN7CCC6CC7	0.42928 6	2.463083
CC1=NN=C2N1C3=C(C=C(C=C3)OC)C(=N[C@H]2CC(=O)NCC(=O)NCCC4=CC5=C(C=C4)SC(=C5)[Si](C)(C)O)C6=CC=C(C=C6)Cl	0.34795 1	2.461898
CC1=NN=C2N1C3=C(C=C(C=C3)OC)C(=N[C@H]2CC(=O)NCC(=O)NCCC4=CC5=C(S4)C=C(C=C5)[Si](C)(C)O)C6=CC=C(C=C6)Cl	0.34795 1	2.461898
CC1=NN=C2N1C3=C(C=C(C=C3)OC)C(=N[C@H]2CC(=O)NCC(=O)NCCC4=CC5=C(C=C4)C(=CS5)[Si](C)(C)O)C6=CC=C(C=C6)Cl	0.34795 1	2.461898
CC1=NN=C2N1C3=C(C=C(C=C3)OC)C(=N[C@H]2CC(=O)NCC(=O)NCCC4=CC5=C(S4)C=CC(=C5)[Si](C)(C)O)C6=CC=C(C=C6)Cl	0.34795 1	2.461898
CC1=NN=C2N1C3=C(C=C(C=C3)OC)C(=N[C@H]2CC(=O)NCC(=O)NCCC4=CC5=C(C=C4)SC=C5[Si](C)(C)O)C6=CC=C(C=C6)Cl	0.34795 1	2.461898
CC(C1=CC2=CC=CC=C2N1CC3=CC4=CC=CC=C4S3)N(C)C5=NC=C(C=C5)C(=CC(=O)N)CN(C	0.14	2.45

)C(=O)C=CC6=CN=C(C=C6)N	0958	2729
CC1=CN=C(N=C1C2=CC3=C(S2)C=C(C=C3)OCC(CNC(C)C)O)NC4CC(=C)NC(C4)(C)C	0.58933	2.455 2668
CCOC1=CC=CC=C1/C=C/C(=O)NC2=C(C3=C(S2)CC(CC3)OC(=O)OCCN4CCOCC4)N	0.48846	2.456 209
CCN(C(C)C)S(=O)(=O)C1=CC=CC(=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC=C(C=C4)OC	0.49066	2.451 1862
CCOC(=O)CCCN(CC1=CC2=C(C=C1)SC=N2)C(=O)C3(CCN3C(=O)C4=CSC5=CC=CC=C54)C	0.60342	2.454 1599
CC(C)C1=C(C(=NO1)C2=C(C=CC=C2Cl)Cl)COC3=CC4=C(C=C3)C=C(S4)C5=CC(=CC=C5)NC(=O)NS(=O)(=O)C6CC6	0.41160	2.452 0769
COC(=O)[C@H](C1CC=C(C=C1)OC2=CC=C(C=C2)CNCC3=CC4=C(C=C3)C=C(S4)C(=O)NO)N	0.47480	2.434 1671
CC#CC(CC(=O)O)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=CC=C4NS(=O)(=O)C)C	0.55203	2.436 1331
CC#CC(CC(=O)O)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=CC(=C4)NS(=O)(=O)C)C	0.55203	2.436 1331
C1=CCNC2C(=C1)C(=CS2)CC(CBr)CBr	0.43749	2.428 9292
CC(=O)N1CCC(CC1)NCC2=CC(=CC=C2)C(=O)NC3=C(C4=C(S3)CCCC4)C(=O)NC5=CC=C(C=C5)CCC6=CC=C(C=C6)C(=O)OC	0.37755	2.425 3032
CNC1CCC(CC1)N(CC2=C(C=CC(=C2)/C(=C/N)/C=N\C(=C)N)OC)C(=O)C3=C(C4=CC=CC=C4S3)Cl	0.48964	2.411 2122
CC[C@H](CC(=O)O)C1=CC(=C(C=C1)N(CC)C2CCOCC2)NC(=O)NC3=CC4=C(CS(=O)(=O)C4)C=C3	0.44969	2.398 2247
CC[C@@H](CC(=O)O)C1=CC(=C(C=C1)N(CC)C2CCOCC2)NC(=O)NC3=CC4=C(CS(=O)(=O)C4)C=C3	0.44969	2.398 2247
CC[C@@H](CC(=O)O)C1=CC(=C(C=C1)N(CC)C2CCOCC2)NC(=O)NC3=CCC4=CS(=O)(=O)CC4=C3	0.44763	2.391 2247
CC[C@H](CC(=O)O)C1=CC(=C(C=C1)N(CC)C2CCOCC2)NC(=O)NC3=CCC4=CS(=O)(=O)CC4=C3	0.44763	2.391 2247
CCC(CC(=O)O)C1=CC(=C(C=C1)N(CC)C2CCOCC2)NC(=O)NC3=CC4=C(CS(=O)(=O)C4)C=C3	0.44	2.39

	9698	2247
CN(C)CCC1=CSC2=C1C=CC(=C2)NC3=NC=C4C(=N3)N(N(C4=O)CC=C)C5=NC(=CC=C5)S(=O)(=O)C	0.45432	2.391617
CC(=O)OCC1[C@H](C(C(C(O1)C2=C(C=CC(=C2)CC3=CC4=CC=CC=C4S3)OC5CCCC5)OC(=O)C)OC(=O)C)OC(=O)C	0.38326	2.382186
C1CC(=O)NC(=O)C1N2CC3=C(C2=O)C=CC(=C3)N4CCN(CC4)CCCCC5=CC=C(C=C5)OC6=C(SC7=C6C=CC(=C7)O)C8=CC=C(C=C8)Br	0.37274	2.381825
CC1=C(SC2=C(C=CC(=C12)COC)C(=O)C)C(=O)NC3=NC4=CC=CC(=C4C=C3)COP(=O)(C)OC(C)(C)C	0.48585	2.381797
CC1=C2C(=C(C=C1)OCCC3CCOCC3)C(=CC(=N2)C4=C(C5=CC=CC=C5S4)C)C(=O)NS(=O)(=O)CCO	0.45052	2.381702
CN(C)CCC1=CSC2=C1C=CC(=C2)NC3=NC=C4C(=N3)N(N(C4=O)CC=C)C5=CC(=CC=C5)S(=O)(=O)C	0.49453	2.381664
CC1=CC=C(C=C1)S(=O)(=O)OC2CCN(C2)CC3=CC(=NC4=CC=CC=C43)NC(=O)C5=C(C6=C(C=CC(=C6S5)C(=O)C)COC)C	0.39598	2.371967
CCOC1=CC=CC=C1CCC(=O)NC2=C(C3=C(S2)CC(CC3)OC(=O)NCC4=NOC(=C4)C)C#C	0.53442	2.371828
C[C@@H](CC(=O)C1=CC2=CC(=C(C=C2S1)N(C)C(=O)OC(C)(C)C)OCOC)C(=O)O	0.60412	2.371508
CCOC1=CC=CC=C1/C=C/C(=O)NC2=C(C3=C(S2)CC(CC3)COC(=O)NCC4=CC=CC=N4)N	0.49378	2.361988
CCOC(=O)C1=C(SC2=C1CCCC2)CC(=O)C3=C(N(C4=NC5=CC=CC=C5N=C34)CCCOC)N	0.51285	2.361988
CCC(OC1=CC(=C(C(=C1)C)C2=C3CC[C@H](C3=CC=C2)OC4=CC5=C(C=C4)[C@@H](CS5)CC(=O)O)C)S(=O)(=O)C	0.53547	2.361797
CCC(OC1=CC(=C(C(=C1)C)C2=C3CC[C@H](C3=CC=C2)OC4=CC5=C(C=C4)C(CS5)CC(=O)O)C)S(=O)(=O)C	0.53547	2.361797
COC1=CC(=CC(=C1)NC(=O)C2=C(SC3=C2CCCC3)NC(=O)C4=CC(=C(C(=C4)OC)OC)OC)OC	0.51406	2.361774
COC1=CC(=CC(=C1)C(=O)NC2=C(C3=C(S2)CCCC3)C(=O)NC4=CC(=C(C(=C4)OC)OC)OC)OC	0.51406	2.361774
COC1=CC(=CC(=C1)C(=O)NC2C(C3CC=CC=C3S2)C(=O)NC4=CC(=C(C(=C4)OC)OC)OC)OC	0.50	2.36

	967 9	1774
CC(C)C1=CC=CC=C1C2=C(C3=C(S2)C=C(C=C3)OC(=O)C(C(C)C)N)OC4=CC=C(C=C4)/C=C/C(=O)O.Cl	0.50 408 9	2.35 169
CC1=C(SC2=C(C=CC(=C12)COC)C(=O)C)C(=O)NC3=NC4=CC=CC(=C4C=C3)CC[C@@H](C(=O)O)N	0.45 053 6	2.35 1671
CC(=O)OCC1=CC=C(C=C1)NC(=O)OCC(C2=CC=CC=C2)OC3=C4CC(SC4=CC=C3)C(=N)N	0.47 227 6	2.35 1671
CC(C(=O)O)NC1CC2=CC=CC=C2C1.CC(C(=O)O)NC(C)(C)C(C1=CC=CS1)C2=C3C=CC=CC3=CS2	0.50 487	2.34 2116
CC1=NOCC1CNC(=O)OCC2CCC3=C(C2)SC(=C3C#N)NC(=O)CC(C)C4=CC(=CC=C4)OC	0.46 070 8	2.34 2093
C1CC(=O)NC(=O)C1N2C(=O)C3=C(C2=O)C=C(C=C3)N4CCN(CC4)CCOCC5=CC=C(C=C5)OC6=C(SC7=C6C=CC(=C7)O)C8=CC=C(C=C8)Br	0.31 190 3	2.34 141
CN(C)CCC1=CSC2=C1C=CC(=C2)NC3=NC=C4C(=N3)N(N(C4=O)CC5CC5)C6=NC(=CC=C6)S(=O)(=O)C	0.44 705 9	2.33 1773
C=CCN1CC(=O)N2[C@@H](N1C(=O)NCC3=CC=CC=C3)CN(C(=O)[C@@H]2CC4=CC=C(C=C4)O)CC5=CSC6C5C=CC(=C6)NCC7=CC=CC=C7	0.38 975 8	2.32 2988
C1CC(=O)NC(=O)C1N2CC3=C(C2=O)C=CC(=C3)N4CC(C4)N5CCC(CC5)OC6=CC=C(C=C6)OC7=C(SC8=C7C=CC(=C8)OCC9=CC=CC=C9)C1=CC=C(C=C1)Br	0.33 730 4	2.32 2087
CCNC(=O)NC1=CC2=CC(=C(C=C2S1)OCC3=CC(=C(C=C3)OC)OC)C4=CN=C(N=C4)C(C)(C)O	0.48 483 4	2.32 1937
CN(C)CCC1=CSC2=C1C=CC(=C2)NC3=NC=C4C(=N3)N(N(C4=O)CC5CC5)C6=CC(=CC=C6)S(=O)(=O)C	0.49 028 8	2.32 1821
C1CC(=O)NC(=O)C1N2C(=O)C3=C(C2=O)C=C(C=C3)N4CCN(CC4)CCCCC5=CC=C(C=C5)OC6=C(SC7=C6C=CC(=C7)O)C8=CC=C(C=C8)Br	0.32 987	2.32 1617
CCCN(C)CC1=NC=C(N1)C2=CC=C(C=C2)C3=CC4=C(S3)C=C(C=C4)C5=CN=C(N5)C6(CCN6C(=O)CNC(=O)OC)C	0.41 404 2	2.31 2679
CC(C)OC1=CC(=CC(=C1)N2CCOCC2)C(C)(C)C3=CC(=CC(=C3)Cl)NC(=O)C4=C(C5=CC=CC=C5S4)NS(=O)(=O)C	0.45 798	2.31 1785
C=CN=C(C(=O)C1=C(C2=C(S1)C=C(C=C2)O)OC3=CC=C(C=C3)/C=C/C(=O)O)SC=C	0.61 874 6	2.31 0548
CC(=O)OCCN(CCO)C1=CC2=C(C=C1)C=C(S2)/C=C(\C#N)/C(=O)OC(C)(C)C	0.61 067	2.30 1562
C#CC1=CC=C(C=C1)CN(CCOC(=O)O)CC2CCCCN2C(=O)NCC3=CC4=CC=CC=C4S3(O)O	0.44 958	2.29 209

	8	
CC(C)(C)OC(=O)N(C)C1=NC=C(C=C1)C2=CC3=C(S2)C=C(C=C3)OC[C@H](COS(=O)(=O)C)O	0.48607	2.281338
CC(C)(C)OC(=O)N(C)C1=NC=C(C=C1)C2=CC3=C(S2)C=C(C=C3)OC[C@@H](COS(=O)(=O)C)O	0.48607	2.281338
CCOC(=O)C1CCCCC1N(C(=C)C(C2=CSC3=CC=CC=C32)NC4=CC5=C(C=C4)N=CN5)/N=N\N	0.47375	2.27226
CCC(=O)N1CCC(CC1)CN2C=C(C=N2)NC3=NN=C(C(=C3)NCC4=CC=CC5=C4SC=C5)C(=O)C	0.51894	2.27226
C#CC1=CC=C(C=C1)CN(CCOC(=O)O)CC2CCCCN2C(=O)NCC3=CC4=CC=CC=C4S3(=O)=O	0.45858	2.271934
CC#CC(CC1=NNN=N1)C2=CC=C(C=C2)OCC3=CC4=C(C=C3)SC=C4C5=C(C=CC(=C5)NS(=O)(=O)C)C	0.47395	2.271555
CC(C)(C)OC(=O)N(C)C1=CC=C(C=C1)C2=CC3=C(S2)C=C(C=C3)OC[C@H](COS(=O)(=O)C)O	0.53496	2.271385
CCCC(CCCC1=CSC2=CN=CC=C21)Cl	0.77857	2.270848
CC1=C(C=CC(=C1)OC2CCS(=O)CC2)C3=C(SC4=C3C=C(C=C4)COC5=CC=C(C=C5)CC/C(=N/N)/NN)C	0.45466	2.262229
CC1=CC(=CC=C1)NC(=O)NC2=CC3=C(C=C2)SC(=C3)C4=C(N=CC(=C4)C(=O)CCCCC(=O)OC)N	0.46683	2.261831
CC#C[C@@H](CC1=NNN=N1)C2=CC=C(C=C2)OCC3=CC4=C(C=C3)SC=C4C5=C(C=CC(=C5)NS(=N)(=O)C)C	0.45607	2.261715
CC#C[C@@H](CC(=O)O)C1=CC(=C(C=C1)C2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC(CO)O)C)O	0.51378	2.261607
CC#C[C@@H](CC(=O)Cl)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC(=C3C4=C(C=C(C=C4)OC5CCSC(=O)C5=O)C)C	0.58238	2.261145
CCC(C)(C1=C2C(=C(C=C1)C(C)(CC)OC(=O)C3CCC(CC3)OC)SC(=N2)C4=CC5=CC(=CC(=C5S4)C)C)OC(=O)C6CCC(CC6)O	0.42796	2.253158
C1CCC2=C(C1)C(=C(S2)NC(=O)C3=CC=CC(=C3)CN4CCOCC4)C(=O)NC5=CC=C(C=C5)OCC6=CC=C(C=C6)C(=O)O	0.41124	2.252247
CC(C)NC(=O)C1=CC2=C(S1)C=C(C=C2)C3=NC(=CC(=N3)OCCN(C)C)NC4=CC5=C(C=C4)NN=C5	0.51057	2.252103

CC1=CC2=C(C(=C1)OC)SC(=C2)C3=CN(C4=NC=NC(=C34)N)C5CCN(C5)C(=O)/C=C/CN(C)CCOC	0.52117	2.242413
C1CC(=O)NC(=O)C1N2C(=O)C3=C(C2=O)C=C(C=C3)N4CC(C4)CN5CCC(CC5)C6=CC=C(C=C6)OC7=C(SC8=C7C=CC(=C8)OCC9=CC=CC=C9)C1=CC=C(C=C1)Br	0.31675	2.242087
CC1=C(SC2=C(C=CC(=C12)COC)C(=O)C)C(=O)NC3=NC4=CC=CC(=C4C=C3)COC(=O)C(C(C)C)N	0.46039	2.231984
CC1=C(SC2=C(C=CC(=C12)COC)C(=O)C)C(=O)NC3=NC4=CC=CC(=C4C=C3)C[C@](C(C)C)(C(=O)O)N	0.43241	2.231984
C1COCCN1CC2=CC=CC=C2NC(=O)OCC(C3=CC=CC=C3)OC4=C5CC(SC5=CC=C4)C(=N)N	0.49037	2.222144
COC1=CC(=C(C=C1CC2=CC3=CC=CC=C3S2)[C@H]4C[C@H](C[C@H](O4)COC(=O)C5=CC=CC=C5)OC(=O)C6=CC=CC=C6)OC(=O)C7=CC=CC=C7	0.41739	2.222131
CC1(C(C2=C(S1(=O)=O)C=CC(=C2)NC3=NN(C4=C3C(=NC=C4)OCC5=CC=CC=C5)CC6CC6)OC=O)C	0.48320	2.22178
C[C@@H]1CCN(C1)[C@H]2C[C@H](N(C2)C(=O)CC3=CC(=C(C=C3Cl)NC(=O)C4=CSC5=CC=CC=C54)Cl)COC6CCC(CC6)C(=O)O	0.43336	2.211987
CNC(=O)S/C(=C\C1=NC(=NC=C1)N2CCC(CC2)CNCC3=CC4=C(C=C3)SC=C4)/C=O	0.61815	2.211606
COC1=CC(=C(C=C1C=O)Cl)NC(=O)CCN2CCC(CC2)OC(=O)NC3=C(C4=CC=CC=C4S3)C5=CC=CC=C5	0.49113	2.211595
CCOC(=O)C1=C2CC(C/C(=N\O)/C2=C(S1)SCCC3=CC=CC=C3)C4=CC=C(C=C4)OC	0.72625	2.211382
CC1=C(C=CC(=C1)OC2CCS(=O)(=O)CC2)C3=CSC4=C3C=C(C=C4)COC5=CC=C(C=C5)C6(CCC6)CC(=O)O	0.51705	2.201797
CC(C)(C1=NC(=CC=C1)N2C3=NC(=NC=C3C(=O)N2CC=C)NC4=CC5=C(C=C4)C(=CS5)CCN(C)C)O	0.51947	2.195226
CC(C)C1=CC=CC=C1C2=C(C3=C(S2)C=C(C=C3)OC(=O)C(C(C)C)N)OC4=CC=C(C=C4)/C=C/C(=O)O	0.53317	2.191923
CC1=C(C=CC(=C1)C(=O)N2CCS(=O)(=O)CC2)C3=CSC4=C3C=C(C=C4)COC5=CC=C(C=C5)C(CC(=O)O)C=C	0.47903	2.191593
CCN(CC)C1=NC=C(C=N1)NC(=O)C2=C(SC3=C2CCCC3)NC(=O)C4=CC=CC(=C4)CN5CCOCC5	0.50977	2.18257
CC1=C(C=CC(=C1)OC2CCS(CC2)(O)O)C3=CSC4=C3C=C(C=C4)COC5=CC=C(C=C5)C6(CC(C	0.42	2.18

6)O)CC(=O)O	3606	1902
COC1=CC=C(C=C1)NC(=O)C2=C(SC3=C2CCCC3)NC(=O)C4=C(C=CC(=C4)S(=O)(=O)N5CCCCC5)CN=[N+]=[N-]	0.34579	2.181876
CCOC(=O)C1=C(SC2=C1CCCC2)NCC(=O)NCC3=C(SC4=C3CCCN4)N5C=CC=C5	0.61608	2.181759
CC1=CC=C(C=C1)S(=O)(=O)OCC2=C3C=CC(=NC3=CC=C2)NC(=O)C4=C(C5=C(C=CC(=C5S4)C(=O)C)COC)C	0.44846	2.181389
CC(C)C1=CC=CC=C1C2=C(C3=C(S2)C=C(C=C3)OCCN4C(=O)C5=CC=CC=C5S4(O)O)OC6=CC=C(C=C6)/C=C/C(=O)OC(C)(C)C	0.40291	2.172168
CN(C)CCC1=CSC2=C1C=CC(=C2)NC3=NC=C4C(=N3)N(N(C4=O)CC=C)C5=CC=CC(=N5)C6(CC6)O	0.51947	2.172103
COC1=CC=C(C=C1)NC(=O)C2=C(SC3=C2CCCC3)NC(=O)C4=CC(=CC=C4)S(=O)(=O)N5CCN(CC5)C(=C)C=C	0.44501	2.161971
COC1=C(C=C(C(=C1)OC(=O)C2=CC=CC=C2)[C@H]3C[C@H](C[C@H](O3)COC(=O)C4=CC=CC=C4)OC(=O)C5=CC=CC=C5)C(=O)C6=CC7=CC=CC=C7S6	0.36771	2.161924
CC1=C(C=CC(=C1)OC2CCS(CC2)(O)O)C3=CSC4=C3C=C(C=C4)COC5=CC=C(C=C5)C6(CC(=O)C6)CC(=O)O	0.43307	2.161746
CN1CCN(CC1)CC2=CC=CC=C2NC(=O)OCC(C3=CC=CC=C3)OC4=C5CC(SC5=CC=C4)C(=N)N	0.49882	2.152461
CC(C)C1=CC=CC=C1C2=C(C3=C(S2)C=C(C=C3)OCCN4C(=O)C5=CC=CC=C5S4(=O)=O)OC6=CC=C(C=C6)/C=C/C(=O)OC(C)(C)C	0.42100	2.152011
CC1=CC=CC=C1CCC(=O)NC2=C(C3=C(S2)CC(CC3)COC(=O)OCC4=CN=CS4)C#N	0.55233	2.151286
COC(=O)C1=CC=C(C=C1)CCC2=C(C=C(C=C2F)NC(=O)C3=C(SC4=C3CCCC4)NC(=O)C5=CC=CC(=C5)CN6CC7CCC(C6)N7)F.Cl	0.39941	2.142505
CCOC(=O)C1=C(SC2=C1CCCC2)NC(=O)NCC3=C(SC4=C3CCN(C4)CC5=CC=C(C=C5)OC)N6C=CC=C6	0.52540	2.142178
CCCC1=CC=C(C=C1)[C@@H]2CSC3=C2C=C(C=C3)C4C(C(C(C(O4)COC(=O)C)OC(=O)C)OC(=O)C)OC(=O)C	0.44001	2.142208
CC#CC(CC(=O)O)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC(=C3C4=C(C=C(C=C4)OC5CCS(CC5)(O)O)C)C	0.48509	2.141953
CC(C)(C1=NC(=CC=C1)N2C3=NC(=NC=C3C(=O)N2CC4CC4)NC5=CC6=C(C=C5)C(=CS6)CCN(C)C)O	0.50933	2.132416

	2	
CC=CC(CC(=O)O)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)C(=O)N5CCS(=O)(=O)CC5)C	0.46983	2.131749
CC#C[C@@H](CC(=O)O)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC(=C3C4=C(C=C(C=C4)ON5CCS(=O)(=O)CC5)C)C	0.49549	2.131749
CC#CC(CC(=O)O)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC(=C3C4=C(C=C(C=C4)OC5CCSC(C5)(O)O)C)C	0.48623	2.121797
CC#CC(CC(=O)O)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC(=C3C4=C(C=C(C=C4)OC5CCS(=O)(=O)CC5)C)C	0.50821	2.121797
CCOOC1=C(SC2=CC=CC=C21)COCC	0.82136	2.128082
C=C(NC1=CC(=CC=C1)NC(=O)CCN2CCCCC2)/N=C\C3=C(C4=C(C=C3)SC(=C4)C(=O)N5CCOCC5)N	0.46238	2.10257
CCOC(=O)C1=C(C2=C(S1)C=CC(=C2)NCC3=CN=CN3)NC(=O)C4=CC=C(C=C4)OC	0.57926	2.101362
CC#C[C@@H](CC#N)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OCC5(CCS(=O)(=O)CC5)O)C	0.48678	2.0918
CCOC(=O)C1=C(SC2=C1CCCC2)NC(=O)NCC3=C(SC4=C3CCN(C4)CC5=CC(=C(C=C5)OC)C)N6C=CC=C6	0.51534	2.082334
C1CC(=O)NC(=O)C1N2CC3=C(C2=O)C=CC(=C3)C4CCN(CC4)C5CCN(CC5)CCOC6=CC=C(C=C6)OC7=C(SC8=C7C=CC(=C8)O)C9=CC=C(C=C9)Br	0.32556	2.082243
COC(=O)C(=O)NC(=O)OCN1CC=CC2=C1C=C(C=C2)OCCCCN3CCN(CC3)C4=C5C=CSC5=CC=C4	0.48104	2.082199
CCOC(=O)CC1(CC(=O)C1)C2=CC=C(C=C2)OCC3=CC4=C(C=C3)SC=C4C5=C(C=C(C=C5)C6CCS(CC6)(O)O)C	0.48613	2.082115
CC#C[C@@H](C/C(=N/N=N)/N)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)C5CCS(=O)(=O)CC5)C	0.42578	2.082072
CC1=CC(=C(C=C1CC2=CC3=CC=CC=C3S2)C4(C[C@H]([C@@H]([C@H](O4)COC(=O)C)OC(=O)C)OC(=O)C)OC)OC(=O)C	0.40852	2.081873
CC#C[C@@H](CC(=O)N)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC(=C3C4=C(C=C(C=C4)OC5CCSC(=O)C5=O)C)C	0.49126	2.071644
CCOC(=O)CC1(CC(=O)C1)C2=CC=C(C=C2)OCC3=CC4=C(C=C3)SC=C4C5=C(C=C(C=C5)C6=CCS(CC6)(O)O)C	0.48749	2.061953
CCOC(=O)CC1(CC(=O)C1)C2=CC=C(C=C2)OCC3=CC4=C(C=C3)SC=C4C5=C(C=C(C=C5)C6C	0.48	2.06

CSC(C6)(O)O)C	7245	1953
CCC1=NOC(=C1NC(=O)OCC(C2=CC=CC=C2)OC3=C4CC(SC4=CC=C3)C(=N)N)C	0.50488	2.061675
CC(C)C1=CC=CC=C1C2=C(C3=C(S2)C=C(C=C3)OC(=O)C(C(C)C)NC(=O)OC(C)(C)C)OC4=CC=C(C=C4)/C=C/C(=O)OC(C)(C)C	0.42368	2.053073
C1CC2=C(CC1OC(=O)NCC3CCOCC3)SC(=C2C=N)NC(=O)CCC4=CC(=CC=C4)O	0.49135	2.051984
CCN(CC)C(=O)C(C1=CC=C(C=C1)NC2=NC(=CN(C2=O)C)C3=C(C(=CC=C3)NC(=O)OC4=CC5=C(S4)CCCC5)C)N6CCOCC6	0.37843	2.043094
CCOC(=O)C1=C(SC2=C1CCCC2)NC(=O)NCC3C(SC(=C3C)CN4CCOCC4)N5C=CC=C5	0.57089	2.042178
C1CC(=O)NC(=O)C1N2C(=O)C3=C(C2=O)C=C(C=C3)N4CCN(CC4)C5CCN(CC5)CCOC6=CC=C(C=C6)OC7=C(SC8=C7C=CC(=C8)O)C9=CC=C(C=C9)Br	0.28451	2.031988
CC(C)C1=CC=CC=C1C2=C(C3=C(S2)C=C(C=C3)OCN4C(=O)C5=CC=CC=C5S4)OC6=CC=C(C=C6)/C=C/C(=O)O	0.56407	2.031331
C1CC(=O)NC(=O)C1N2C(=O)C3=C(C2=O)C=C(C=C3)C4CCN(CC4)C5CCN(CC5)CCOC6=CC=C(C=C6)OC7=C(SC8=C7C=CC(=C8)O)C9=CC=C(C=C9)Br	0.29016	2.022036
CCOC(=O)C1=C(SC2=C1CCCC2)NC(=O)NCC3=C(SC(=C3C)CN4CCOCC4)N5C=CC=C5	0.57354	2.022021
CC1=NN=C2N1C3=C(C=C(C=C3)OC)C(=N[C@H]2CC(=O)NCCNC(=O)C4=CC5=C(C=C4)SC=C5[Si](C)(C)O)C6=CC=C(C=C6)Cl	0.35450	2.021742
CCOC(=O)CCN1CCN(CC1)C2=NC=C(N=C2)C(=O)NC3=NC(=CS3)C4=CC5=CC=CC=C5S4	0.52504	2.021508
CC(C)C1=C(C(=NO1)C2=C(C=CC=C2Cl)Cl)COC3=CC4=C(C=C3)C=C(S4)C5=CC(=CC=C5)C(=O)NS(=O)(=O)C6=CC=C(C=C6)C(C)(C)C	0.40383	2.021286
CCOC(=O)CC1(CC(=O)C1)C2=CC=C(C=C2)OCC3=CC4=C(C=C3)SC=C4C5=C(C=C(C=C5)N6CC7(C6)CCS7(O)O)C	0.46680	2.012062
CC1CN(CCN1C2COC2)C3=CN=C(C=C3)NC4=CC(=CN(C4=O)C)C5=C(C(=NC=C5)N(C=O)/N=C\C6=C(SC7=C6CCCC7)C)C=O	0.71640	2.002893
CC1CN(CCN1C2=CN=C(C=C2)NC3=CC(=CN(C3=O)C)C4=C(C(=NC=C4)N(C=O)/N=C\C5=C(SC6=C5CCCC6)C)C=O)C7COC7	0.36155	2.002893
CC1CN(CCN1C2COC2)C3=CN=C(C=C3)NC4=CC(=CN(C4=O)C)C5=C(C(=NC=C5)N(C=O)/N=C\C6=C(SC7=C6CCCC7)C)C=O	0.36155	2.002893

	8	
CC(C)(C)OC(=O)N1CCN(CC1)CC2=CC(=CC=C2)C(C)(C)C3=CC(=CC(=C3)Br)NC(=O)C4=CC5=C(S4)C=CC(=C5)NS(=O)(=O)C	0.37564	2.001702
C1=CC=C(C=C1)N(C2=CC=CC=C2)C3=CC4=C(C=C3)C=C(S4)C5=CC(=NC=C5)C6=NC(=CC(=C6)OC=O)C7=NC=CC(=C7)OC=O	0.48000	2.001518
CC(C)NC(=O)C1CCC(CC1)N2C3=C(N=CC(=C3)OCCN4CCCCC4)N=C2NC(=O)C5=CC6=C(C=C5)C=CS6	0.47837	1.982883
CC#CC(C/C(=N/N)/NN)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)OC5CCOCC5)C	0.48418	1.982508
CC#C[C@@H](CC1=NNNN1)C2=CC=C(C=C2)OCC3=CC4=C(C=C3)SC(=C4C5=C(C=C(C=C5)OC6CCS(=O)(=O)CC6)C)C	0.45320	1.982178
CCN1C(=CC=N1)CNC(=O)OC2CCC3=C(C2)SC(=C3C=N)NC(=O)/C=C/C4=CN=CC=C4	0.49139	1.981787
OC1=C(SC2=C1C=C(C=C2)Br)CCCBr	0.46636	1.978819
C1CC(N(C1)C(=O)CN)C(=O)N2C(=O)C=CC3=C2C=C(C=C3)OCCCCN4CCN(CC4)C5=C6C=CSC6=CC=C5	0.47045	1.972566
CC(C)C1=CC=CC=C1C2=C(C3=C(S2)C=C(C=C3)OCN4C(=O)C5=CC=CC=C5S4(O)O)OC6=CC=C(C=C6)/C=C/C(=O)O	0.41252	1.971385
COC1=CC=C(C=C1)NC(=O)OCC(C2=CC=CC=C2)OC3=C4C=C(SC4=CC(=C3)O)C(=N)N	0.48691	1.971358
CC#C[C@@H](CC1=NNN=N1)C2=CC=C(C=C2)OCC3=CC4=C(C=C3)SC(=C4C5=C(C=C(C=C5)OC6CCS(=O)(=O)CC6)C)C	0.43740	1.962021
CC#CC(CC1=NNN=N1)C2=CC=C(C=C2)OCC3=CC4=C(C=C3)SC(=C4C5=C(C=C(C=C5)OC6CCS(=O)(=O)CC6)C)C	0.43740	1.962021
C1CC(=O)NC(=O)C1N2CC3=C(C2=O)C=CC(=C3)N4CCN(CC4)CCOC5=CC=C(C=C5)OC6=C(SC7=C6C=CC(=C7)O)C8=CC=C(C=C8)Br	0.35607	1.961461
CC#C[C@@H](CC1=NN=NN1CCC#N)C2=CC=C(C=C2)OCC3=CC4=C(C=C3)SC(=C4C5=CC=CC=C5C)C#N	0.51653	1.921889
CC#CC(CC1=NN=NN1CCC#N)C2=CC=C(C=C2)OCC3=CC4=C(C=C3)SC(=C4C5=CC=CC=C5C)C#N	0.51653	1.921889
CC1=CC(=NO1)CNC(=O)OCC2CCC3=C(C2)SC(=C3C#C)NC(=O)CC(C)C4=CN=CC=C4	0.53419	1.921831

COC(=O)C1=CC(=CC=C1)NC(=O)OCC(C2=CC=CC=C2)OC3=C4CC(SC4=CC=C3)C(=N)N	0.48251	1.916 1515
CC(C)(C)C1CCC2=C(C1)SC(=C2C(=O)O)NC(=O)C3=CC=C(C=C3)OCCCNC(=O)OC(C)(C)C	0.48248	1.908 2451
CC(C)(C)OC(=O)C1=C(SC2=C1CCCC2)NC(=O)NCC3=C(SC4=C3CCN(C4)CCOC)N5C=CC=C5	0.55110	1.909 2334
C1CN(CCC12CCN(CC2)C3=CC=C(C=C3)C(=O)C4=C(SC5=C4C=CC(=C5)O)C6=CC=C(C=C6)O)CCOCC(=O)O	0.44335	1.904 2294
CC1=C(C=CC=C1NC(=O)C2=CC3=C(S2)CCCC3)C4=CN(C(=O)C(=C4)N/C(=C/C=C(/CN5CCN(CC5)C)\N)/N=C)C	0.44772	1.891 3042
COC1=CC=C(C=C1)C2CC3=C(SC(=C3/C(=N/O)/C2)SCC4=CC=CC=C4)C(=O)OCC5=CC=CC=C5	0.67179	1.893 1382
COC1=CC=C(C=C1)C2CC3=C(SC(=C3C(=NO)C2)SCC4=CC=CC=C4)C(=O)OCC5=CC=CC=C5	0.67179	1.893 1382
COC1=CC=C(C=C1)[C@H]2CC3=C(SC(=C3/C(=N/O)/C2)SCC4=CC=CC=C4)C(=O)OCC5=CC=CC=C5	0.67179	1.893 1382
CC(=O)CCN(CC1=CSC(=C1)C(=O)OC(C)(C)C)C(=O)C2=CSC3=C2C=CC(=C3)O	0.66374	1.899 1174
CC1=C(C(=NC=C1CNC2=CC3=C(C=C2)C=C(S3)C4=CC=C(C5=CC=CC=C54)N6C(=O)[C@@H](NC6=O)CCCCN)C)N	0.41703	1.888 2464
CC(C)(C)OC(=O)C1=C(SC2=C1CCCC2)NC(=O)NCC3=C(SC4=C3CCN(C4)CCN(C)C)C5=CC(=CC=C5)Cl	0.55289	1.881 2309
CC(=O)OCC1[C@H]([C@@H]([C@H](C(O1)C2=CC(=C(C=C2)Cl)CC3=CC4=CC=CC=C4S3)OC(=O)C)OC(=O)C)OC(=O)C	0.43817	1.883 1221
CC1=CC(=NO1)CNC(=O)OCC2CCC3=C(C2)SC(=C3C#C)NC(=O)CC(C)C4=CC(=CC=C4)O	0.49898	1.871828
CCN(C1CCC2=NN(C=C2C1)C(=O)OC(C)(CN=[N+]=[N-])CN=[N+]=[N-])C(=O)C3=CSC4=CC=CC=C43	0.38665	1.879 1801
CC(C)(C)C1CCC2=C(C1)SC(=C2C(=O)OO)NC(=O)C3=CC=C(C=C3)OCCCNC(=O)OC(C)(C)C	0.44540	1.866 24
COC1=C(C=C2C(=C1)C(=O)N3CCCC[C@H]3C(N2C(=O)OCC=C)OC4CCCCO4)OCC5=C(SC6=CC=CC=C65)C(=O)O	0.38909	1.865 2142
CC1=C(C=C(N1CC2CCCCC2)C3=C4C=CSC4=C(C=C3)S(=O)(=O)NC(C)(C)C)C(=O)NC5CC(C5)	0.43	1.85

C(=O)O	411 8	2331
CC1=C(C=C(N1CC2CCCCC2)C3=C4C(=C(C=C3)S(=O)(=O)NC(C)(C)C)C=CS4)C(=O)NC5CC(C5)C(=O)O	0.43 411 8	1.85 2331
CC1=C(C=C(N1CC2CCCCC2)C3=C4C=CC=CC4=C(S3)S(=O)(=O)NC(C)(C)C)C(=O)NC5CC(C5)C(=O)O	0.43 411 8	1.85 2331
COC1=C(C=C(C=C1)N)OC.COC1=C(C=C(C=C1)NC2=NN3C(=NC=C3C4=CC5=CC(=C(C=C5S4)OC)OC)C=C2)OC	0.40 186 9	1.85 2152
COC1=CC(=CC(=C1OC)OC)N.COC1=CC(=CC(=C1OC)OC)NC2=NN3C(=NC=C3C4=CC5=CC=CC=C5S4)C=C2	0.40 186 9	1.85 2152
CC1=C(SC2=C(C=CC(=C12)COC)C(=O)C)C(=O)NC3=NC4=CC=CC(=C4C=C3)COC(=O)C(C)N	0.47 977 8	1.85 1671
CC(C)(C)C1CCC2=C(C1)SC(=C2C(=O)OC)NC(=O)C3=CC=C(C=C3)OCCCNC(=O)OC(C)(C)C	0.50 602 5	1.84 2607
COC1=C(C=C2C(=C1)C(=O)N3CCCC[C@H]3C(N2C(=O)OCC=C)OC4CCCCO4)OCC5=C(SC6=CC=CC=C65)C(=C)O	0.43 305 6	1.84 2349
CC1=CN=C(N=C1C2=CC3=C(S2)C=CC(=C3)C(=NC)NO)NC4=CC=C(C=C4)OCCN5CCCC5	0.56 956 8	1.82 2151
CC(=O)C(CCN1C(=O)C2=CC=CC=C2N=N1)(CC(=O)C3=CC4=C(S3)C=C(C=C4)O)C(=O)OC(C)(C)C	0.44 467 8	1.81 1621
CC(C)C1=CC=CC=C1C2=C(C3=C(S2)C=C(C=C3)OC(=O)C(C)N)OC4=CC=C(C=C4)/C=C/C(=O)O	0.55 775 5	1.81 161
COC1=C(C=C2C(=C1)C(=O)N3CCCC[C@H]3C(N2C(=O)OCC=C)OC4CCCCO4)OCC5=C(SC6=CC=CC=C65)C(=O)OC	0.40 765 2	1.80 2298
CCOC1=CC=CC=C1/C=C/C(=O)NC2=C(C3=C(S2)CC(CC3)OC(=O)OCC)N	0.62 126 8	1.80 1562
CCOC(=O)C1=C(C2=C(S1)C=C(C=C2)NC3=NC=C4C(=N3)N(N(C4=O)CC=C)C5=CC=CC(=N5)C(C)(C)O)N6CCN(CC6)C	0.37 461 6	1.78 258
C1=C2C(=CC(=C1S)I)SC=C2I	0.25 583 2	1.77 7844
CC1=CC2=C(C=C1OCCCC(=O)NC3=CN(C(=C3)C(=O)NC4=CC5=C(C=C4)SC(=C5)C(=O)OC)C)N=C[C@@H]6CCCN6C2=O	0.37 765 2	1.77 2152
C1CC2=C(CC1OC(=O)OCC3=CN=CS3)SC(=C2C#N)NC(=O)CCC4=CC=CC=C4	0.57	1.77

	772 7	0973
CC(=O)OC[C@@]12CO[C@@](O1)([C@@H]([C@H]([C@@H]2OC(=O)C)OC(=O)C)OC(=O)C)C3=CC(=C(C=C3)Cl)CC4=CC5=CC=CC=C5S4	0.39 691 1	1.76 117
CC(CN=[N+]=[N-])(CN=[N+]=[N-])OC(=O)N1C=C2CC(CCC2=N1)N(C3CC3)C(=O)C4=CSC5=C4C=CC(=C5)O	0.33 718 5	1.75 175
CC(C)CN(C[C@@H]1[C@@H](N(C(O1)(C)C)C(=O)OC(C)(C)C)CC2=CC=C(C=C2)C#CC3=C(C4=C(S3)CCC(C4)(C)C)C(=O)OC(C)(C)C)S(=O)(=O)C5=CC=C(C=C5)OC	0.33 067	1.74 3948
CC(C)C1=CC=CC=C1C2=C(C3=C(S2)C=C(C=C3)OCN4C(=O)C5=CC=CC=C5S4(O)O)OC6=CC=C(C=C6)/C=C/C(=O)OC(C)(C)C	0.41 011 9	1.73 2011
COC1CCC(CC1)(C2=C(C3=CC=CC=C3S2)C4=CC=CC5=C4NC(=C5CCCOC6=CC=CC7=CC=CC=C76)OC(=O)O)O	0.45 869 4	1.71 2185
CC1=CC=CC=C1CCC(=O)NC2=C(C3=C(S2)CC(CC3)OC(=O)OCC4=CN=CS4)C#N	0.56 494 8	1.71 113
CCC1=CC=C(C=C1)[C@@H]2CSC3=C2C=C(C=C3)C4C(C(C(C(O4)COC(=O)C)OC(=O)C)OC(=O)C)OC(=O)C	0.44 724 3	1.70 1924
CC1=C(C(C(=C(N1)COCCN2C(=O)C3=CC=CC=C3C2=O)C(=O)OC)C4=CSC5=CC=CC=C54)C(=O)C	0.51 383 1	1.70 1512
CNCCN(C)CC1=CC2=C(S1)CCCN2	0.14 774 6	1.69 1456
CC(C)C1=CC=CC=C1C2=C(C3=C(S2)C=C(C=C3)OC(C)N4C(=O)C5=CC=CC=C5S4(O)O)OC6=CC=C(C=C6)/C=C/C(=O)OC(C)(C)C	0.40 291 3	1.67 2168
CCOC(=O)C1=CC=C(C=C1)NC(=O)C2=C(SC3=C2CCCC3)NC(=O)C4=CC=CC(=C4)CN5CCOCC5	0.52 221 3	1.67 2141
CC(C)(C)OC(=O)COCCN1CCC2(CC1)CCN(CC2)C3=CC=C(C=C3)C(=O)C4=C(SC5=C4C=CC(=C5)O)C6=CC=C(C=C6)O	0.44 146 6	1.66 292
CC#C[C@@H](CC(=O)OC)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)C5CCSC(C5)(O)O)C	0.57 749 4	1.66 1848
CN1C=C(C=N1)NC2=NC=CC(=N2)N(C3=CC=CC(=C3)NC(=O)C=C)C(=O)OCC4=CC5=CC=CC=C5S4	0.48 502 4	1.65 1583
CN1C=C(C=N1)NC2=NC=CC(=N2)N(C3=CC=CC(=C3)NC(=O)C=C)C(=O)OCC4=CSC5=CC=CC=C54	0.48 502 4	1.65 1583
CN1C=CC(=N1)NC2=NC=CC(=N2)N(C3=CC=CC(=C3)NC(=O)C=C)C(=O)OCC4=CSC5=CC=CC=C54	0.48 502	1.65 1583

	4	
CC#CC(C/C(=N/N)/NN)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)C5CCS(=O)CC5)C	0.47718	1.64228
CC1CCC(N1C(=O)OCC2=CC3=CC=CC=C3S2(=O)=O)C[C@@H](C)OC4=NC=NC(=C4C)OC5=C(N=CC=C5)C	0.43812	1.642043
CCN1CCC2=C(C1)SC(=C2COC(=O)NC3=C(C4=C(S3)CCCC4)C(=O)OCC)N5C=CC=C5	0.66143	1.631756
CC1=C(C=CC=C1NC(=O)C2=CC3=C(S2)CCCC3)C4=CN(C(=O)C(=C4)NC5=CC(=C(C=C5)N6CCC(CC6)OC)NC(=O)C=C)C	0.42951	1.612879
CCN1CCN(CC1)C2=C(C=C(C=C2)NC3=CC(=CN(C3=O)C)C4=C(C(=CC=C4)NC(=O)C5=CC6=C(S5)CCCC6)C)NC(=O)C=C	0.44716	1.603039
CC1(CCC2=C(C1)C(=C(S2)CCCOC(=O)OC3=CC=C(C=C3)[N+](=O)[O-])C(=O)OC(C)(C)C)C	0.54620	1.591821
COC(C1=C(C(C(=C(N1)C2CC2)C(=O)OC)C3=CSC4=C(C=CC=C34)C#N)C(=O)OC)OC	0.54146	1.581355
CCOC1=C2C=C(SC2=CC(=C1)Cl)I	0.63743	1.579029
CC1=C(C=CC=C1NC(=O)C2=CC3=CC=CC=C3S2)C4=CN(C(=O)C(=C4)NC5=CC(=C(C=C5)N6CCC(CC6)OC)NC(=O)C=C)C	0.43192	1.572566
CC#C[C@@H](CC(=O)OC)C1=CC=C(C=C1)OCC2=CC3=C(C=C2)SC=C3C4=C(C=C(C=C4)C(=O)N5CCS(CC5)(O)O)C	0.47582	1.571906
CCN1CCN(CC1)C2=C(C=C(C=C2)NC3=CC(=CN(C3=O)C)C4=C(C(=CC=C4)NC(=O)C5=CC6=CC=CC=C6S5)C)NC(=O)C=C	0.44972	1.562726
CC1=CC(=C(C=C1CC2=CC3=CC=CC=C3S2)[C@H]4[C@@H]([C@H](C[C@H](O4)COC(=O)C)OC(=O)C)OC(=O)C)C5=CC=NN5	0.44106	1.561936
CC(CN(C)C)NCC1CSC2=CC=CCCC12	0.92442	1.561817
CC1=C(C=C(C=C1)[C@@]23[C@@H]([C@H]([C@@H]([C@@](O2)(CO3)COC(=O)C)OC(=O)C)OC(=O)C)OC(=O)C)CC4=CC5=CC=CC=C5S4	0.40662	1.561716
CC1=CC(=C(C=C1CC2=CC3=CC=CC=C3S2)[C@H]4[C@@H]([C@H](C[C@H](O4)COC(=O)C)OC(=O)C)OC(=O)C)C5=CC=CN5	0.47963	1.551978
CC1=C(C=CC=C1NC(=O)C2=CC3=C(S2)CCCC3)C4=CN(C(=O)C(=C4)NC5=CC(=C(C=C5)N6CCN(CC6)C(C)C)NC(=O)C=C)C	0.43916	1.543196

CC1=C(C=CC=C1NC(=O)C2=CC3=C(S2)CCCC3)C4=CN(C(=O)C(=C4)NC5=CC(=C(C=C5)N6CCC(CC6)N(C)C)NC(=O)C=C)C	0.43916	1.543196
CCOC(=O)C1=C(SC2=C1CCCC2)NC(=O)NCC3=C(SC(=C3C)C(=O)OC(C)(C)C)N4C=CC=C4	0.52148	1.531862
COC1=C(C=C2C(=C1)C(=O)N3CCCC[C@H]3C(N2C(=O)OCC=C)OC4CCCCO4)OCC5=C(SC6=CC=CC=C65)C(=O)N7C[C@H](C8=C7C=C(C9=CC=CC=C98)O)CCl	0.29605	1.512643
CC1=C(C=CC=C1NC(=O)C2=CC3=CC=CC=C3S2)C4=CN(C(=O)C(=C4)NC5=CC(=C(C=C5)N6CCN(CC6)C(C)C)NC(=O)C=C)C	0.44158	1.502883
CC1=C(C=CC=C1NC(=O)C2=CC3=CC=CC=C3S2)C4=CN(C(=O)C(=C4)NC5=CC(=C(C=C5)N6CCC(CC6)N(C)C)NC(=O)C=C)C	0.44158	1.502883
CC(C)C1=CC=CC=C1C2=C(C3=C(S2)C=C(C=C3)OC(=O)C4=CC=CC=C4N)OC5=CC=C(C=C5)/C=C/C(=O)O	0.51694	1.494161
CC(C)(C)OC(=O)N1CCC[C@H]1C(=O)OCC(=C)C2=CC3=C(C=C2)C=C(S3)C4=CC=C(C=C4)C(=O)COC(=O)[C@@H]5CCCN5C(=O)OC(C)(C)C	0.34143	1.482924
CCCCN(CC1=NC=C(N1)C2=CC3=C(C=C2)C=C(S3)C4=CC=C(C=C4)C5=CN=C(N5)[C@@H]6CCCN6C(=O)OC(C)(C)C)C(=O)OC(C)(C)C	0.37694	1.463458
CC(C)(C)OC(=O)C1=C(SC2=C1CCCC2)NC(=O)NCC3=C(SC4=C3CCN(C4)CCO)N5C=CC=C5	0.51891	1.462178
CCN1CCC2=C(C1)SC(=C2CN=C(NC#N)NC3=C(C4=C(S3)CCCC4)C(=O)OCC)N5C=CC=C5	0.53938	1.462028
CC1=CC(=NO1)CNC(=O)OC2CCC3=C(C2)SC(=C3C#C)NC(=O)CC(C)C4=CC(=CC=C4)O	0.50970	1.431671
CC(=O)OCC1[C@H](C(CC(O1)C2=C(C=CC(=C2)CC3=CC4=CC=CC=C4S3)O)OC(=O)C)OC(=O)C	0.50949	1.421505
CCCCSC1=CC2=CC=CC=C2S1	0.22412	1.420537
OCC(CNC1CCCC2=C1C=C(S2)Cl)O	0.15380	1.41059
COC1=C2C(=CSC2=C(C=C1)CO)I	0.41890	1.399368
CCOC1=C(C=CC2=C1C(=CS2)I)N	0.57745	1.389528

CC(C)(C)OC(=O)C1=C(SC2=C1CCCC2)NC(=O)C3=CC=CC(=C3)CNC4CCC(CC4)C(=O)OC	0.55315	1.362501
COC1=CC2=C(C=C1)C=C(S2)C3=CC=C(C=C3)C(=O)N4CCC[C@H]4CN5CCCC5.C1CCN(C1)C[C@@H]2CCCN2C(=O)C3=CC=C(C=C3)C4=CSN=N4	0.43840	1.323386
CC[Si](NC)(CC)C1=CSC2=CC=CC=C21	0.82432	1.291007
C1C(C2=CC=CC=C2S1)CNCC(F)F	0.75714	1.290737
CC(C)(C)OC(=O)N1CCC(CC1)NC(=O)C2=CC3=C(S2)C=C(C=C3)C4=NC5=C(C=NC=C5)C(=C4)NCCCN6CCCCC6	0.45784	1.283196
CC(=O)OCC1C(C(C(C(O1)C2=CC3=C(C=C2)SC(C3)C4=CC=C(C=C4)O)OC(=O)C)OC(=O)C)OC(=O)C	0.39997	1.281562
CC(CNC1CCCC2=C1C=CS2)OO	0.52995	1.27098
CCC1=C2C(=C(C=C1)O[C@H]3CCC[C@H](C3)C)C(=CC(=N2)C4=C(C5=C(S4)C=CC(=C5)C6=CC=C(C=C6)[C@H](C)OC7=C8C(=CC(=NC8=C(C=C7)C)C9=C(C1=CC=CC=C1O9)C)C(=O)O)C)C(=O)O	0.27611	1.243339
C1=CC2=C(C=CS2)C=C1OCC(CO)O	0.16886	1.240507
C1=CC2=C(C(=C1)Br)CC=C2CCC(=O)O	0.49921	1.159942
CC1=CC(=C(C=C1CC2=CC3=CC=CC=C3S2)[C@H]4[C@@H]([C@H](C[C@H](O4)COC(=O)C)OC(=O)C)OC(=O)C)C5=CC=CN5C(=O)OC(C)(C)C	0.38029	1.152502
CSC1=CC(=C(C2=C1SC=C2)F)I	0.35248	1.13894
CC(=O)C1CCC(CC1)C(=O)OC2=C3C(=C(C=C2)OC(=O)C4CCC(CC4)C(=O)C)SC(=N3)C5=CC6=CC=CC=C6S5	0.47461	1.131749
NC1=CC(=CC2=C1C(=CS2)I)CCl	0.61868	1.129032
CC(C)CN(C[C@@H]1[C@@H](N(C(O1)(C)C)C(=O)OC(C)(C)C)CC2=CC=C(C=C2)C#CC3=C(C4=C(S3)CCC(C4)(C)C)C(=O)OC(C)(C)C)C(=O)OCC5=CC=CC=C5	0.38455	1.084278
C1OC2C=C(SC2=CC(=C1CBr)O)Br	0.75909	1.078612

CC1=CC2=C(C=C1)SC(=C2)C3=NC4=C(C=CC(=C4S3)OC(=O)C5CCC(CC5)C(=O)C)OC(=O)C6CCC(CC6)C(=O)C	0.46539	1.071906
COC1=CC=C(C=C1)C2=C(C3=C(S2)C=C(C=C3)O)OC4=CC=C(C=C4)N5CCC(CC5)CN6CCN(CC6)C7=CC8=C(C=C7)C(=O)N(C8)C9CCC(=O)NC9=O	0.34740	1.013091
CC1=CC(=C2C(=C1)C=C(S2)C3=NC4=C(C=CC(=C4S3)OC(=O)C5CCC(CC5)C(=O)C)OC(=O)C6CCC(CC6)C(=O)C)C	0.45651	1.012062
CC(C)(C)OC(=O)NC(C)(C)C(C(=O)OC)NC(=O)C1=CC2=C(S1)C=C(C=C2)C#CC3CC3CO	0.49219	1.001981
CC(C)(C)OC(=O)NC(C)(C)[C@@H](C(=O)OC)NC(=O)C1=CC2=C(S1)C=C(C=C2)C#CC3C[C@H]3CO	0.49219	1.001981
CC(C)(C)OC(=O)NC(C)(C)[C@@H](C(=O)OC)NC(=O)C1=CC2=C(S1)C=C(C=C2)C#C[C@@H]3CC3CO	0.49219	1.001981
CC1=CC2=C(C(=C1)OC)SC(=C2)C3=NN(C4=NC=NC(=C34)N)C5CC(N(C5)C(=O)OC(C)(C)C)C(=O)N(C)CCN(C)C	0.38188	0.982893
CC1=NN(C=C1C#CC2=CC3=C(C=C2)SC(=C3C4=CC=CC=C4)[C@@H](C)NCOCC5=C6N=CC=CN6N=C5N)C	0.52908	0.972154
CN(C)CCC1=CCC2=CC=CC(=C21)OC	0.37368	0.971467
COC1=CC=C(C=C1)C2=C(C3=C(S2)C=C(C=C3)O)OC4=CC=C(C=C4)N5CCC(CC5)CN6CCN(CC6)C7=CC8=C(C=C7)C(=O)N(C8=O)C9CCC(=O)NC9=O	0.30971	0.952883
CC1=CC(=CC=C1)C2=CC(=CC(=C2)CC3=CC(=CC=C3)C4=CC(=CC=C4)C5CC6=C(S5(=O)=O)C=C(C=C6)C7=CC=CC=C7C(=O)O)C8=CC9=C(S8)N=C(C=C9)C1=CC=CC=C1C(=O)O	0.29908	0.932219
CC(C)(C)OC(=O)NC1CCN(C1)C(=O)C2=CC3=C(S2)C=CC(=C3N)/C=N\C(=C)NC4=CC=CC(=C4)C5=CC=CC=C5	0.46065	0.912461
B(C1=CC(=CC2=C1SC=C2O)I)(O)O	0.42472	0.899175
CCOC(=O)C1=C(SC2=C1CCCC2)NC(=O)NCC3=C(SC4=C3CCN(C4)C(=O)OC(C)(C)C)N5CCCC5	0.48215	0.887244
CCOC(=O)C1=C(SC2=C1CCCC2)NC(=O)NCC3=C(SC4=C3CCN(C4)C(=O)OC(C)(C)C)N5C=CC=C5	0.47979	0.842127
CCOC(=O)C1=C(SC2=C1CCCC2)NC(=O)NCC3=C(SC4=C3CCCN4C(=O)OC(C)(C)C)N5C=CC=C5	0.48008	0.842127
CCN(CC)C1OCC(=C2C(=C1)SC=C2Cl)O	0.91760	0.830597

CC[C@@H]1C[C@@H]([C@H]([C@@H](O1)C2=C(C=C(C(=C2)CC3=CC4=CC=CC=C4S3)C)C5=CC=CN5C(=O)OC(C)(C)C)OC(=O)C)OC(=O)C	0.47746	0.812604
C1=CC(=CC2=C1C=CS2)C(=O)COO	0.80908	0.780194
CC(C)(C)OC(=O)CN1CCN(CC1)C2CCN(CC2)C3=CC=C(C=C3)C(=O)C4=C(SC5=C4C=CC(=C5)O)C6=CC=C(C=C6)O	0.47754	0.772767
CCN(C)CC1CSC2=CC=CC=C12	0.85791	0.771082
CCONC(=O)C1NCCC2=C1C=CS2	0.52849	0.760776
C=CCC(=O)C1CCCC2=C1C=CS2	0.79054	0.760765
CCOC(=O)C1=C(SC2=C1CCCC2)NC(=O)NCC3=C(SC4=C3CCN(C4)C(=O)OC(C)(C)C)C5=CC=CC=C5	0.48856	0.752175
CCC1=CC2=CC(=C(C=C2S1)OC)BO	0.89891	0.706729
CC1=C2C(=C(C=C1Cl)I)C=CS2	0.47750	0.678923
CSC1=CC2=C(C=C1)SC(=C2F)CCl	0.86005	0.652974
CSC1=CSC2=C1C=CC(=C2O)CCl	0.34508	0.639783
CC1=C(C2=CC=CC(=C2S1)CCl)Br	0.95703	0.639219
CCOC(=O)C1=C(SC2=C1CC(CC2(C)C)(C)C)NC(=O)C3=CC=C(C=C3)NC4CCN(CC4)C(=O)OC(C)(C)C	0.49716	0.638308
CC(C)(C)ONC1CCCC2=C1C=C(S2)BO	0.80881	0.631308
C1CC(C1)CCC2=C3CNCC=CC3=CS2	0.50168	0.631238
C1COCCN1NCC2CSC3=CC=CC=C23	0.31205	0.60114
CC1=NC2=CC=CC=C2N=C1C[N+](C)(C)C.[Br-]	0.25464	0.550684

	2	
	0.23	
	590	0.48
CC1=C(SC2=C1C=CC(=C2)SF)OC	7	0079
	0.16	
	585	0.46
CCC1=C(C=C2C(=C1F)C=CS2)SC	5	0286
	0.98	0.45
FCC=C.C1=CC=C(C=C1)N(C2=CC=CC=C2)C3=CC=CC=C3	485	158
	0.35	
	592	0.45
CCC1=CC2=C(S1)C(NC(C=C2)CCl)F	4	0441
	0.35	
	707	0.45
COC1=C(C=CC2=C1SC=C2SC)N	2	0282
	0.29	0.44
C1=CSC2=C(C=C(C(=C21)[N+](=O)[O-])F)Br	838	9052
	0.92	
	370	0.42
CCC1=CC2=C(COCS2)C(=C1CCl)C	6	0532
	0.18	
	810	0.42
CCC1CC(SC2=C(C=CC=C12)CCl)O	5	0532
	0.35	
	754	0.40
B(C1=C(C2=C(C=C1N)SC=C2)Br)(O)O	2	9474
CC#C[C@@]1(CC[C@@H]2[C@@]1(C[C@@H](C3=C4CCC(=O)C=C4CC[C@@H]23)C5=C	0.31	
C=C(C=C5)N(C)C)C)O.C1CCN(CC1)CCOC2=CC=C(C=C2)C(=O)C3=C(SC4=C3C=CC(=C4)O)C	045	0.32
5=CC=C(C=C5)O	3	4329
	0.36	
	150	0.31
CC(C1=CC2=C(S1)C=C(C=N2)F)NN	8	0579
	0.50	
	388	0.30
CC(F)C(C1=CC2=CC=CC=C2S1)O	6	0515
	0.42	
	785	0.29
FC1=C2C(=CC=C1)C(CS2)NC3CC3	7	0674
	0.94	
	123	0.27
CCC1=C2C=C(SC2=C(C=C1)OC)N	4	0718
	0.76	
	417	0.27
CCOC(=O)C1=C2CCNCC2=C(S1)O	4	0616
	0.20	
	317	0.25
CC(C)[C@@H](C1=CSC2=CC=CC=C21)N	6	0925
CCC1NC2C=CSC2=C(C=C1CO)O	0.19	0.25

	860	0823
	8	
	0.30	
	912	0.20
C1=CC2=C(C=C1Cl)SC=C2S(=N)O	2	9579
	0.47	
	628	0.17
COC1=CC2OC(C=CS2)C(=C1Cl)S	7	9732
	0.49	0.13
C1CCC(CC1)NC2CSC3=CC=CC=C23	654	1238
	0.75	
	176	0.13
CC(C)(C)C(C1=CC2=CC=CC=C2S1)NC	2	1238
	0.82	
	026	0.03
C1=C2C=C(SC2=C(C=C1F)C(O)F)Cl	1	9718
	0.82	
	948	0.02
CC1=CC2=C(C=CC(=C2S1)CO)Cl	4	0063
	0.74	0.01
C1=CC=C2C(NC1)C(=C(S2)S)C=O	159	0126

Generated by Multiwfn

Space Group: P 1 (#1-1)

a = 15.03381 Å α = 90.0000° grid(x) = 157

b = 12.44838 Å β = 90.0000° grid(y) = 130

c = 8.23508 Å γ = 90.0000° grid(z) = 86

V = 1541.1660 Å^3

Generated by Multiwfn

Space Group: P 1 (#1-1)

a = 11.45877 Å α = 90.0000° grid(x) = 132

b = 15.79922 Å β = 90.0000° grid(y) = 182

c = 6.42386 Å γ = 90.0000° grid(z) = 74

V = 1162.9725 Å^3

Generated by Multiwfn

Space Group: P 1 (#1-1)

a = 1.00000 Å α = 90.0000°

b = 1.00000 Å β = 90.0000°

c = 1.00000 Å γ = 90.0000°

V = 1.0000 Å^3

Space Group: P 1 (#1-1)

a = 22.07167 Å α = 90.0000° grid(x) = 156

b = 15.84633 Å β = 90.0000° grid(y) = 112

c = 14.43148 Å γ = 90.0000° grid(z) = 102

V = 5047.4786 Å^3

Space Group: P 1 (#1-1)

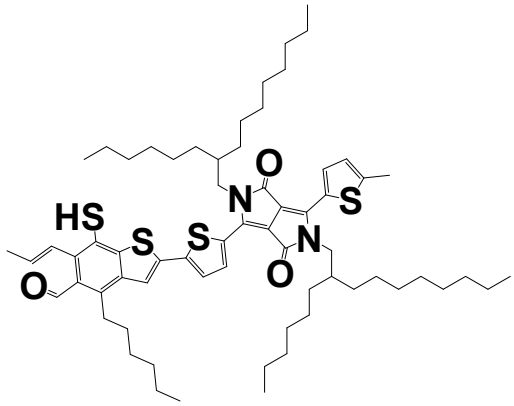
a = 24.17335 Å α = 90.0000° grid(x) = 183

b = 15.45509 Å β = 90.0000° grid(y) = 117

c = 10.96387 Å γ = 90.0000° grid(z) = 83

V = 4096.1157 Å^3

Table S5. Chemical structures and identities of the selected dyes (Dyes 1-5) for detailed analysis.

Dye	Chemical Structure	IUPAC Name (or Representative Name)	SMILES
1		(E)-2-(5-(2,5-bis(2-hexyldecyl)-4-(5-methylthiophen-2-yl)-3,6-dioxo-2,3,5,6-tetrahydropyrrolo[3,4-c]pyrrol-1-yl)thiophen-2-yl)-4-hexyl-7-mercapto-6-(prop-1-en-1-yl)benzo[b]thiophene-5-carbaldehyde	CCCCCCCCC(CCCCCC)CN1C(=C2C(=C(N(C2=O)CC(CCCCCC)CCCCCCCC)C3=CC=C(S3)C4=CC5=C(C(=C(C(=C5S4)S)/C=C/C)C=O)CCCCCC)C1=O)C6=CC=C(S6)C

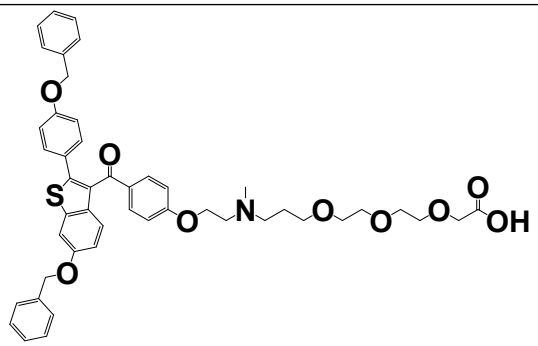
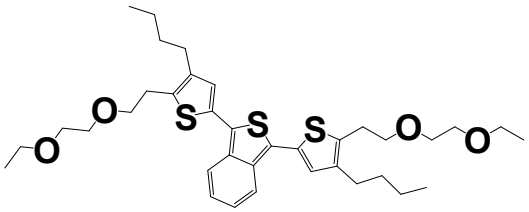
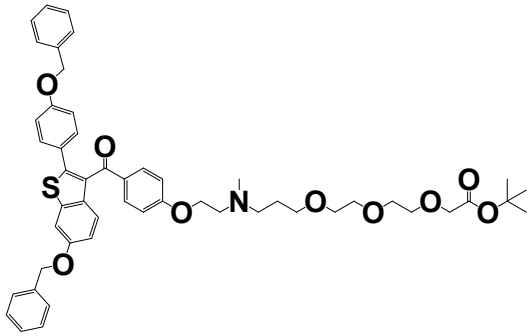
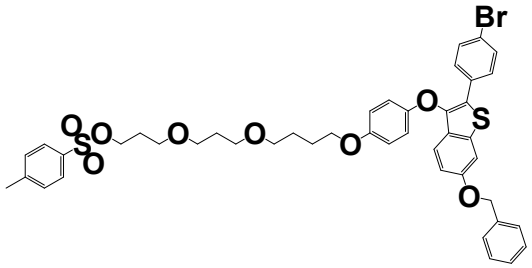
Dye	Chemical Structure	IUPAC Name (or Representative Name)	SMILES
2		15-(4-(6-(benzyloxy)-2-(4-(benzyloxy)phenyl)benzo[b]thiophene-3-carbonyl)phenoxy)-13-methyl-3,6,9-trioxa-13-azapentadecanoic acid	CN(CCCOCCOCCOCC(=O)O)CCOC1=CC=C(C=C1)C(=O)C2=C(SC3=C2C=CC(=C3)OCC4=CC=CC=C4)C5=CC=C(C=C5)OCC6=CC=CC=C6
3		1,3-bis(4-butyl-5-(2-(2-ethoxyethoxy)ethyl)thiophen-2-yl)benzo[c]thiophene	CCCCC1=C(SC(=C1)C2=C3C=CC=CC3=C(S2)C4=CC(=C(S4)CCOCCOCC)CCCC)CCOCCOCC
4		tert-butyl 15-(4-(6-(benzyloxy)-2-(4-(benzyloxy)phenyl)benzo[b]thiophene-3-carbonyl)phenoxy)-13-methyl-3,6,9-trioxa-13-azapentadecanoate	CC(C)(C)OC(=O)COCCOCCOCCCN(C)CCOC1=CC=C(C=C1)C(=O)C2=C(SC3=C2C=CC(=C3)OCC4=CC=CC=C4)C5=CC=C(C=C5)OCC6=CC=CC=C6
5		3-(3-(4-(4-((6-(benzyloxy)-2-(4-bromophenyl)benzo[b]thiophen-3-yl)oxy)phenoxy)butoxy)propoxy)propyl 4-methylbenzenesulfonate	CC1=CC=C(C=C1)S(=O)(=O)OCCCOCCCOCCCCOC2=CC=C(C=C2)OC3=C(SC4=C3C=CC(=C4)OCC5=CC=CC=C5)C6=CC=C(C=C6)Br

Table S6. Comparison of ML-predicted and DFT-calculated parameters for selected top-performing dyes.

Dye	ML-predicted Absorbance	DFT Oscillator Strength (*f*)	HOMO-LUMO Gap from ML (eV)	HOMO-LUMO Gap from DFT (eV)	Absorbance Error (|ML - *f*|)	Gap Error (eV)
1	0.95	1.30	1.85	1.92	0.35	0.07
2	0.89	0.95	1.98	2.05	0.06	0.07
3	0.87	0.82	2.05	2.12	0.05	0.07
4	0.85	0.78	2.11	2.18	0.07	0.07
5	0.82	0.75	2.18	2.25	0.07	0.07