

## Supporting Information for:

### Development of a Comprehensive, Validated Pharmacophore Hypothesis for Anthrax Toxin Lethal Factor (LF) Inhibitors Using Genetic Algorithms, Pareto Scoring, and Structural Biology

Ting-Lan Chiu and Elizabeth A. Amin

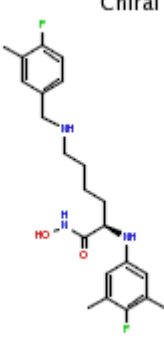
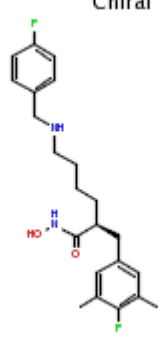
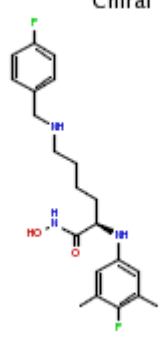
To be published in *J. Chem. Inf. Model.*

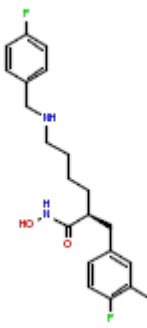
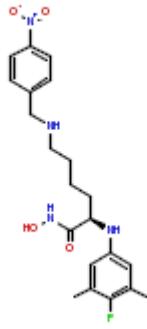
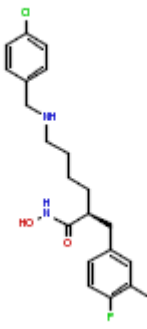
This supporting information was prepared on June 2, 2012 and consists of 203 pages.

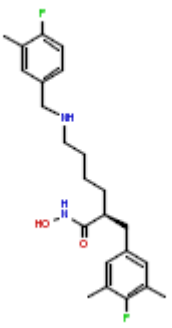
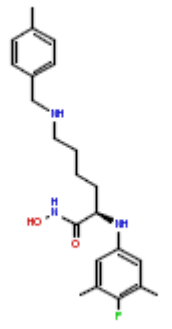
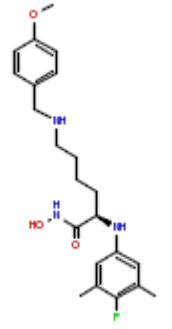
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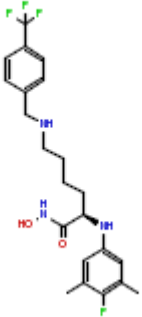
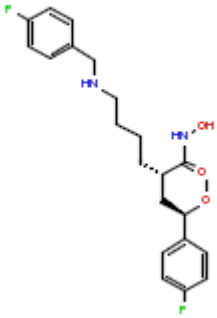
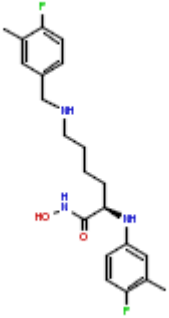
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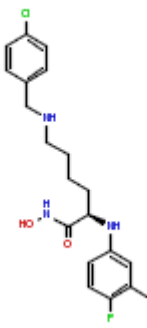
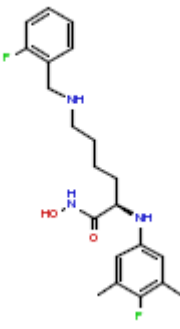
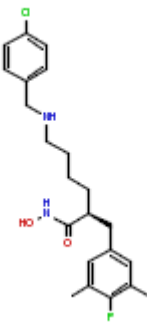
Table S1. Structures, LF biological activities, references, compound designators, and docking scores for screening set compounds in dataset **DB1A**. Asterisk next to biological activity value denotes inclusion in training set **DB1A\_Training**.

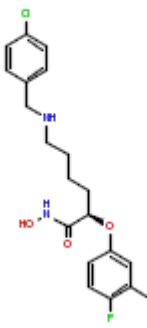
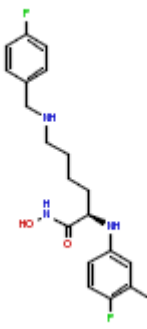
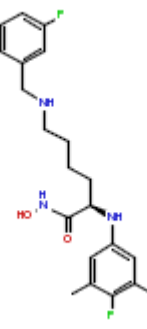
| Structure   | LF IC <sub>50</sub> or K <sub>i</sub> (μM) | Reference | Compound Designator | Docking Score (Surflex-Dock) |
|---|--|-----------|---------------------|------------------------------|
| <p>Chiral</p>    | 0.00005                                    | 1         | 1a                  | 12.69                        |
| <p>Chiral</p>   | 0.00013                                    | 1         | 5b                  | 11.16                        |
| <p>Chiral</p>  | 0.00024                                    | 1         | 1b                  | 12.11                        |

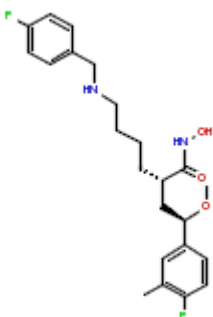
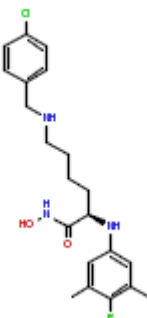
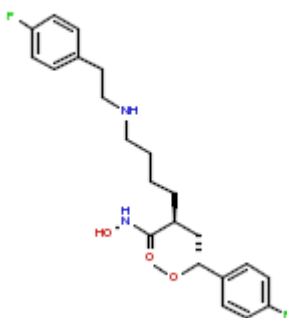
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|---|---------|---|----|-------|
| <p>Chiral</p>  <chem>O=C(O)C(Cc1ccc(F)cc1)CCCNCCc2ccc(F)cc2</chem>             | 0.00025 | 1 | 9b | 11.93 |
| <p>Chiral</p>  <chem>O=C(O)C(Cc1ccc(F)cc1)CCCNCCc2ccc([N+](=O)[O-])cc2</chem> | 0.00030 | 2 | 25 | 12.63 |
| <p>Chiral</p>  <chem>O=C(O)C(Cc1ccc(F)cc1)CCCNCCc2ccc(Cl)cc2</chem>          | 0.00036 | 1 | 9c | 10.36 |

|   |         |   |    |       |
|---|---------|---|----|-------|
| <p>Chiral</p>    | 0.00039 | 1 | 5a | 11.31 |
| <p>Chiral</p>   | 0.00041 | 2 | 22 | 11.53 |
| <p>Chiral</p>  | 0.00044 | 2 | 23 | 13.45 |

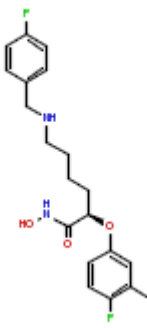
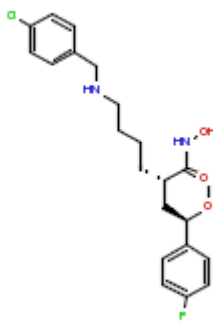
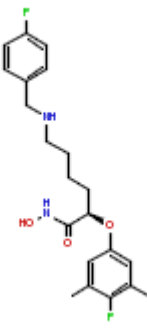
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|--|---------|---|----|-------|
| <p>Chiral</p>  <chem>Cc1cc(F)c(NC(=O)O)cc1CNCNCCNCc1ccc(C(F)(F)F)cc1</chem> | 0.00047 | 2 | 24 | 12.53 |
| <p>Chiral</p>  <chem>Oc1cc(O)cc(NC(=O)O)c1CNCNCCNCc1ccc(F)cc1</chem>       | 0.00058 | 1 | 3b | 12.69 |
| <p>Chiral</p>  <chem>Cc1cc(F)c(NC(=O)O)cc1CNCNCCNCc1ccc(F)cc1</chem>      | 0.00062 | 1 | 6a | 12.20 |

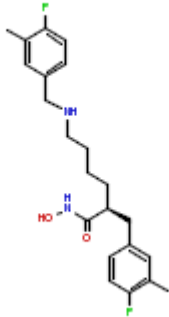
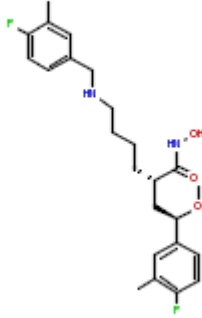
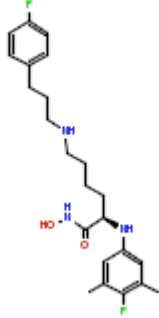
|   |         |   |    |       |
|---|---------|---|----|-------|
| <p>Chiral</p>  <p>Chemical structure of a chiral molecule. It features a 4-chlorophenyl group connected via a methylene bridge to a secondary amine. This secondary amine is part of a 4-aminobutyl chain, which is further connected to a chiral center. The chiral center is bonded to a hydroxamic acid group (-NHOH) and a 4-fluorophenyl group.</p>   | 0.00068 | 1 | 6c | 11.98 |
| <p>Chiral</p>  <p>Chemical structure of a chiral molecule. It features a 3-fluorophenyl group connected via a methylene bridge to a secondary amine. This secondary amine is part of a 4-aminobutyl chain, which is further connected to a chiral center. The chiral center is bonded to a hydroxamic acid group (-NHOH) and a 4-fluorophenyl group.</p>  | 0.00069 | 2 | 18 | 11.43 |
| <p>Chiral</p>  <p>Chemical structure of a chiral molecule. It features a 4-chlorophenyl group connected via a methylene bridge to a secondary amine. This secondary amine is part of a 4-aminobutyl chain, which is further connected to a chiral center. The chiral center is bonded to a hydroxamic acid group (-NHOH) and a 4-fluorophenyl group.</p> | 0.00071 | 1 | 5c | 11.20 |

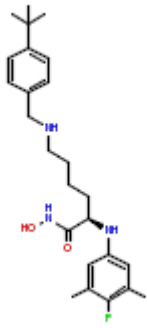
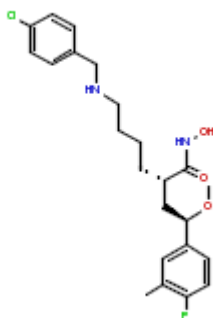
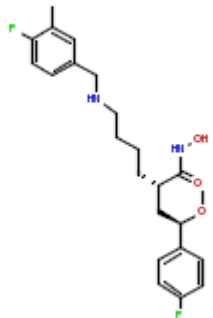
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|--|---------|---|----|-------|
| <p>Chiral</p>  <p>The structure shows a chiral center (C*) bonded to a hydroxyl group (HO), a hydrogen atom (H), a 4-chlorobenzylamino group (-NH-CH2-C6H4-Cl), and a 3-fluorophenyl group (-NH-C6H4-F).</p>      | 0.00075 | 1 | 8c | 11.04 |
| <p>Chiral</p>  <p>The structure shows a chiral center (C*) bonded to a hydroxyl group (HO), a hydrogen atom (H), a 4-fluorobenzylamino group (-NH-CH2-C6H4-F), and a 3-fluorophenyl group (-NH-C6H4-F).</p>      | 0.00081 | 1 | 6b | 11.94 |
| <p>Chiral</p>  <p>The structure shows a chiral center (C*) bonded to a hydroxyl group (HO), a hydrogen atom (H), a 4-fluorobenzylamino group (-NH-CH2-C6H4-F), and a 2,6-difluorophenyl group (-NH-C6H3F2).</p> | 0.00085 | 2 | 19 | 11.92 |

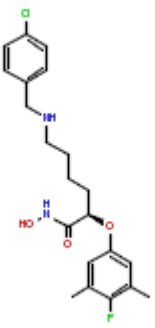
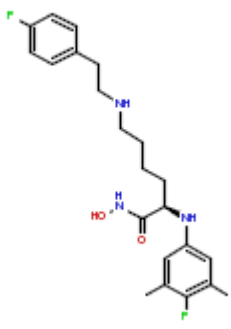
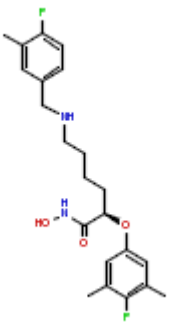
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|---|---------|---|----|-------|
| <p>Chiral</p>    | 0.00093 | 1 | 7b | 12.61 |
| <p>Chiral</p>   | 0.00100 | 1 | 1c | 11.15 |
| <p>Chiral</p>  | 0.00110 | 1 | 3d | 12.20 |

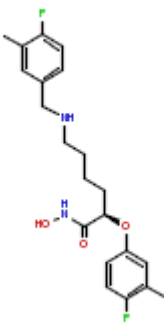
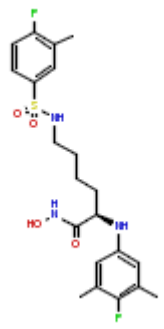
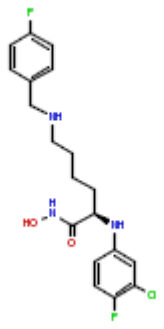


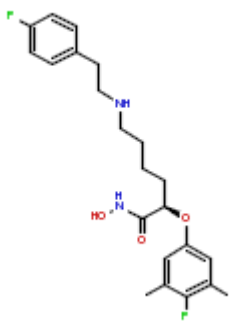
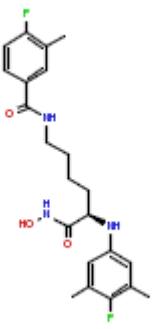
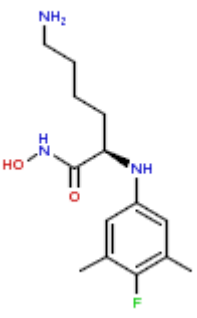
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|---|---------|---|----|-------|
| <p>Chiral</p>    | 0.00110 | 1 | 8b | 12.78 |
| <p>Chiral</p>   | 0.00120 | 1 | 3c | 11.60 |
| <p>Chiral</p>  | 0.00120 | 1 | 4b | 11.79 |

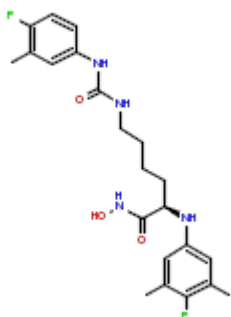
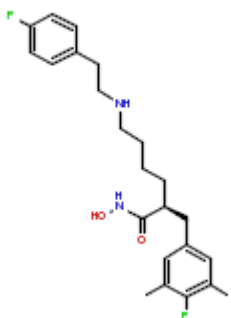
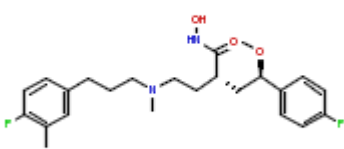
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| <p>Chiral</p>    | 0.00120 | 1 | 9a | 11.20 |
| <p>Chiral</p>   | 0.00130 | 1 | 7a | 12.77 |
| <p>Chiral</p>  | 0.00130 | 2 | 28 | 11.27 |

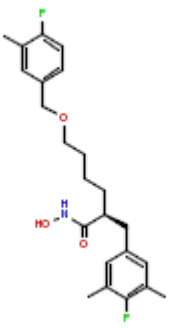
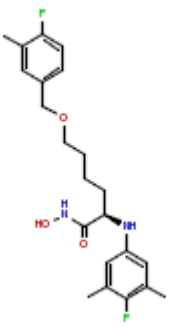
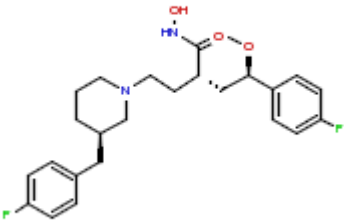
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| <p>Chiral</p>    | 0.00140 | 2 | 26 | 12.78 |
| <p>Chiral</p>   | 0.00140 | 1 | 7c | 11.97 |
| <p>Chiral</p>  | 0.00150 | 1 | 3a | 12.67 |

|   |         |   |    |       |
|---|---------|---|----|-------|
| <p>Chiral</p>    | 0.00200 | 1 | 4c | 11.79 |
| <p>Chiral</p>   | 0.00210 | 1 | 1d | 13.05 |
| <p>Chiral</p>  | 0.00240 | 1 | 4a | 11.55 |

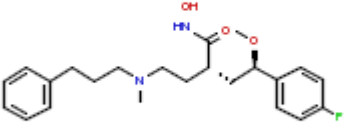
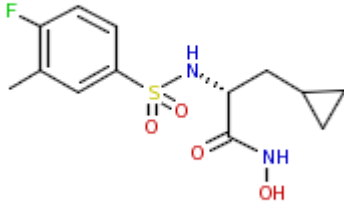
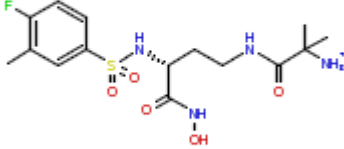
|   |         |   |    |       |
|---|---------|---|----|-------|
| <p>Chiral</p>  <p>Chemical structure of a chiral molecule. It features a central chiral carbon atom bonded to a hydroxyl group (HO), a hydrogen atom (H), a 4-fluorophenyl group, and a 4-fluorophenyl group. The 4-fluorophenyl group is connected to a 4-fluorophenyl group via a 4-aminobenzyl chain.</p>   | 0.00300 | 1 | 8a | 11.79 |
| <p>Chiral</p>  <p>Chemical structure of a chiral molecule. It features a central chiral carbon atom bonded to a hydroxyl group (HO), a hydrogen atom (H), a 4-fluorophenyl group, and a 4-fluorophenyl group. The 4-fluorophenyl group is connected to a 4-fluorophenyl group via a 4-aminobenzyl chain.</p>  | 0.00310 | 2 | 15 | 12.41 |
| <p>Chiral</p>  <p>Chemical structure of a chiral molecule. It features a central chiral carbon atom bonded to a hydroxyl group (HO), a hydrogen atom (H), a 4-fluorophenyl group, and a 4-fluorophenyl group. The 4-fluorophenyl group is connected to a 4-fluorophenyl group via a 4-aminobenzyl chain.</p> | 0.00380 | 1 | 17 | 11.90 |

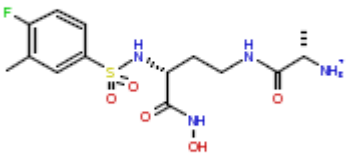
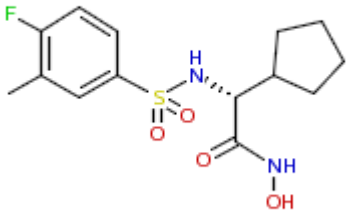
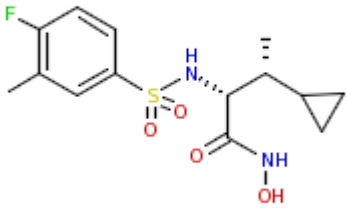
|  |         |   |    |       |
|--|---------|---|----|-------|
| <p>Chiral</p>  <chem>O=C(O)N[C@@H](CCCCNCc1ccc(F)cc1)Oc2cc(F)c(F)c(F)c2</chem>      | 0.00460 | 1 | 4d | 11.50 |
| <p>Chiral</p>  <chem>O=C(O)N[C@@H](CCCCNC(=O)c1ccc(F)cc1)Nc2cc(F)c(F)c(F)c2</chem> | 0.00730 | 2 | 14 | 11.30 |
| <p>Chiral</p>  <chem>O=C(O)N[C@@H](CCCCN)Nc1cc(F)c(F)c(F)c1</chem>                | 0.00820 | 2 | 13 | 10.61 |

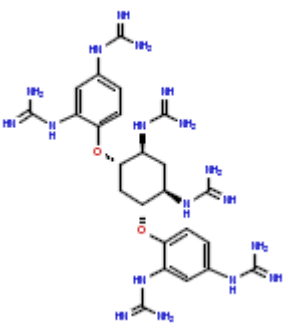
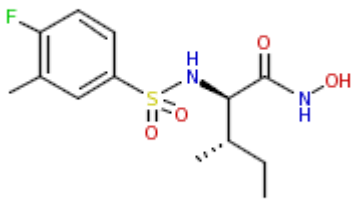
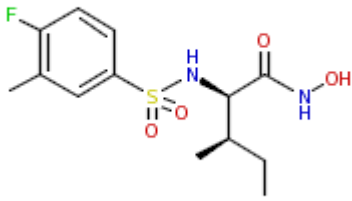
|   |         |   |    |       |
|---|---------|---|----|-------|
| <p>Chiral</p>  <chem>O=C(O)C(NC1=CC=C(C=C1)F)NCCCCNC2=CC=C(C=C2)F</chem>   | 0.00930 | 2 | 17 | 10.79 |
| <p>Chiral</p>  <chem>O=C(O)C(NC1=CC=C(C=C1)F)NCCCCNC2=CC=C(C=C2)F</chem>  | 0.00950 | 1 | 5d | 12.18 |
| <p>Chiral</p>  <chem>O=C(O)C(NC1=CC=C(C=C1)F)NCCCCNC2=CC=C(C=C2)F</chem> | 0.01100 | 2 | 40 | 13.02 |

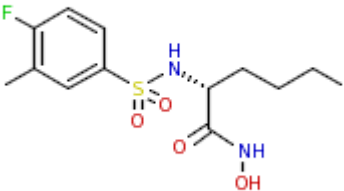
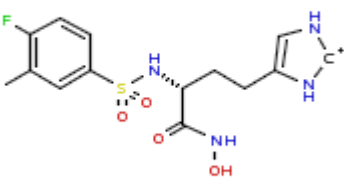
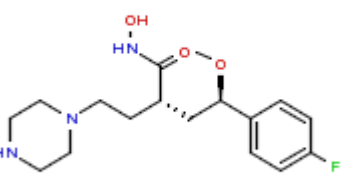
|  |         |   |    |       |
|--|---------|---|----|-------|
| <p>Chiral</p>  <chem>O=C(O)C[C@H](N)CCCCOCC1=CC=C(F)C=C1</chem>         | 0.02500 | 1 | 15 | 12.09 |
| <p>Chiral</p>  <chem>O=C(O)C[C@@H](N)CCCCOCC1=CC=C(F)C=C1</chem>       | 0.03040 | 1 | 13 | 12.14 |
| <p>Chiral</p>  <chem>O=C(O)C[C@H](N)CCCCN1CCN(CC1)Cc2ccc(F)cc2</chem> | 0.03300 | 2 | 34 | 11.34 |

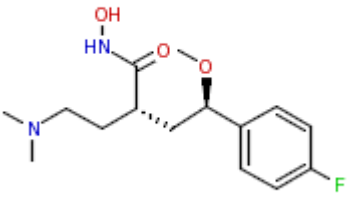
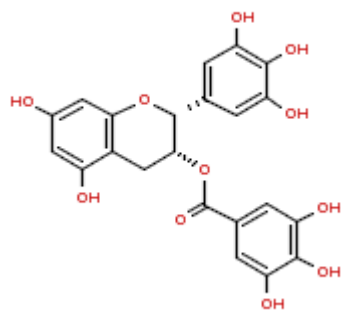
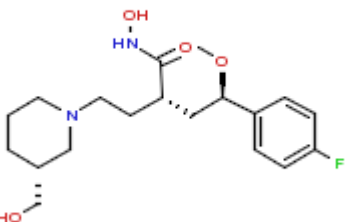


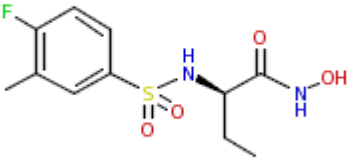
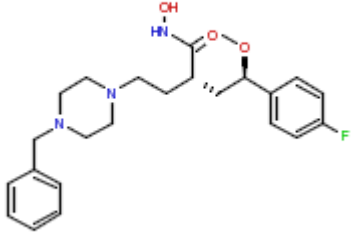
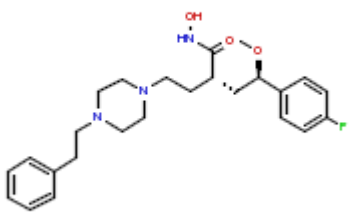
|  |          |   |    |       |
|--|----------|---|----|-------|
| <p>Chiral</p>  <chem>CN(C)CCc1ccccc1C(O)C(=O)NS(=O)(=O)c2ccc(F)cc2</chem>                       | 0.04200  | 2 | 39 | 11.19 |
| <p>Chiral</p>  <chem>Cc1ccc(F)c(S(=O)(=O)N[C@@H](C1CC1)C(=O)N[C@@H](C1CC1)O)c1</chem>           | 0.05100* | 3 | 44 | 10.35 |
| <p>Chiral</p>  <chem>CN(C)C(=O)NCC[C@@H](C(=O)N[C@@H](C1CC1)O)NS(=O)(=O)c2ccc(F)c(C)c2</chem> | 0.05700* | 3 | 48 | 11.69 |

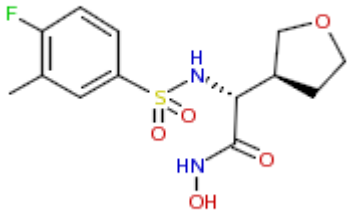
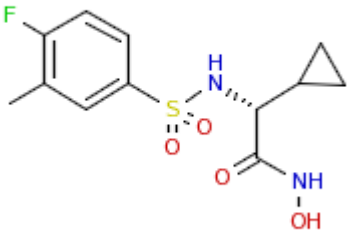
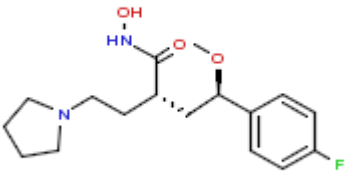
|   |          |   |    |       |
|---|----------|---|----|-------|
| <p>Chiral</p>  <chem>Cc1ccc(F)c(c1)S(=O)(=O)N[C@@H](C(=O)N[OH])CCN[C@@H](C)C(=O)N</chem> | 0.05900* | 3 | 47 | 11.64 |
| <p>Chiral</p>  <chem>Cc1ccc(F)c(c1)S(=O)(=O)N[C@@H](C(=O)N[OH])C2CCCC2</chem>            | 0.06400* | 3 | 37 | 10.29 |
| <p>Chiral</p>  <chem>Cc1ccc(F)c(c1)S(=O)(=O)N[C@@H](C(=O)N[OH])C[C@H]2CC2</chem>       | 0.06500* | 3 | 45 | 10.51 |

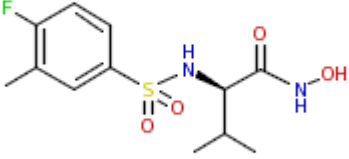
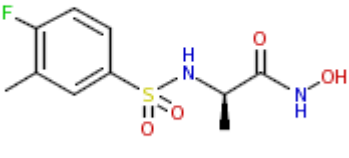
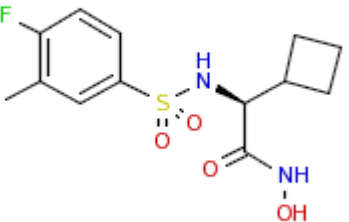
|   |          |   |    |       |
|---|----------|---|----|-------|
| <p>Chiral</p>    | 0.06500  | 4 | 14 | 4.80  |
| <p>Chiral</p>    | 0.06700* | 3 | 42 | 10.55 |
| <p>Chiral</p>  | 0.06700* | 3 | 43 | 10.09 |

|  |          |   |    |       |
|--|----------|---|----|-------|
| <p>Chiral</p>  <chem>CCCC[C@@H](NS(=O)(=O)c1ccc(F)c(C)c1)C(=O)NO</chem>               | 0.07000* | 3 | 33 | 11.23 |
| <p>Chiral</p>  <chem>CCCC[C@@H](NS(=O)(=O)c1ccc(F)c(C)c1)C(=O)NOCC1=CN=C[NH+]1</chem> | 0.07500* | 3 | 51 | 11.33 |
| <p>Chiral</p>  <chem>OC(=O)N[C@@H](CCN1CCNCC1)C(=O)OC[C@H](c1ccc(F)cc1)O</chem>     | 0.09000  | 2 | 35 | 11.51 |

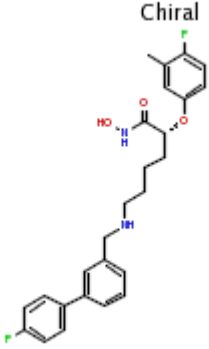
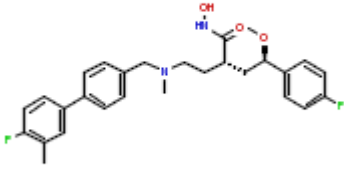
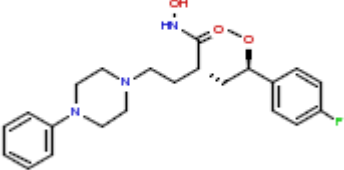
|   |         |   |      |       |
|---|---------|---|------|-------|
| <p>Chiral</p>  <chem>CN(C)CC[C@@H](O)C(=O)O[C@H](c1ccc(F)cc1)C2CCN(C2)O</chem>       | 0.09600 | 2 | 29   | 10.21 |
| <p>Chiral</p>  <chem>O=C(Oc1ccc(O)c(O)c1)[C@@H]2[C@@H](O)[C@H](O)[C@H](O)O2</chem>  | 0.09700 | 5 | EGCG | 2.78  |
| <p>Chiral</p>  <chem>C1CCN(C1)CC[C@@H](O)C(=O)O[C@H](c1ccc(F)cc1)C2CCN(C2)O</chem> | 0.09900 | 2 | 33   | 12.53 |

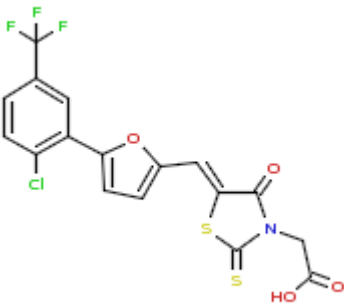
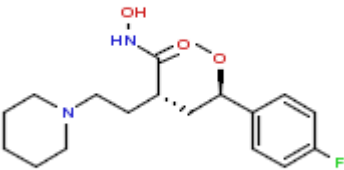
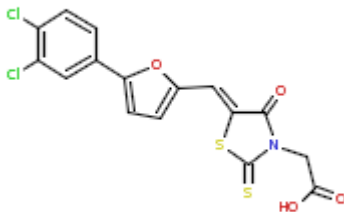
|   |          |   |    |       |
|---|----------|---|----|-------|
| <p>Chiral</p>    | 0.10000* | 3 | 32 | 9.40  |
| <p>Chiral</p>    | 0.11500  | 2 | 37 | 10.56 |
| <p>Chiral</p>  | 0.11800  | 2 | 38 | 10.92 |

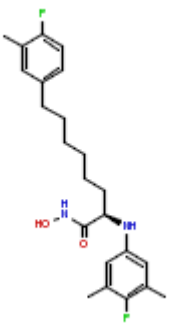
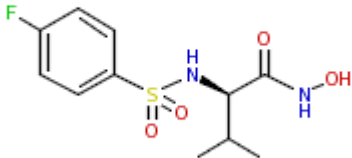
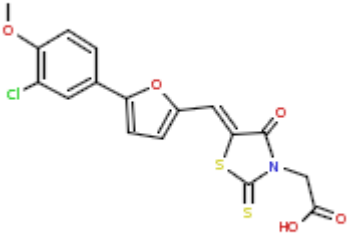
|  |          |   |    |       |
|--|----------|---|----|-------|
| <p>Chiral</p>  <chem>O=C(O)C(S(=O)(=O)Nc1ccc(F)c(C)c1)C1OCCO1</chem>    | 0.12000* | 3 | 41 | 9.81  |
| <p>Chiral</p>  <chem>O=C(O)C(S(=O)(=O)Nc1ccc(F)c(C)c1)C2CC2</chem>      | 0.12000* | 3 | 35 | 10.16 |
| <p>Chiral</p>  <chem>O=C(O)C(S(=O)(=O)Nc1ccc(F)c(C)c1)C2CCNCC2</chem> | 0.12200  | 2 | 30 | 10.50 |

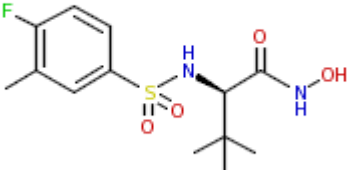
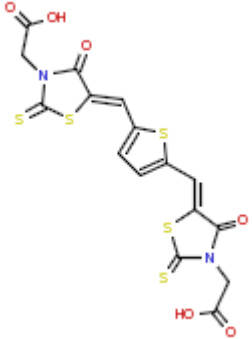
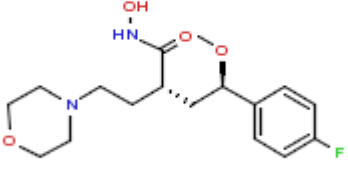
|   |          |   |    |       |
|---|----------|---|----|-------|
| <p>Chiral</p>  <p>The structure shows a central chiral carbon atom bonded to a hydrogen atom (wedge), an isopropyl group (dash), a sulfonamide group (-NH-SO<sub>2</sub>-) attached to a 4-fluorophenyl ring, and a hydrazide group (-C(=O)-NH-OH).</p>  | 0.13000* | 3 | 16 | 10.20 |
| <p>Chiral</p>  <p>The structure is identical to the one above, but the chiral carbon atom has the isopropyl group on a wedge and the hydrogen atom on a dash, representing the (R) enantiomer.</p>   | 0.13000* | 3 | 31 | 8.79  |
| <p>Chiral</p>  <p>The structure shows a central chiral carbon atom bonded to a hydrogen atom (wedge), a cyclobutyl ring (dash), a sulfonamide group (-NH-SO<sub>2</sub>-) attached to a 4-fluorophenyl ring, and a hydrazide group (-C(=O)-NH-OH).</p> | 0.13000* | 3 | 36 | 9.92  |

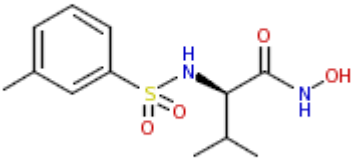
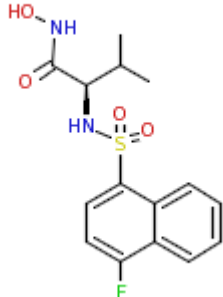
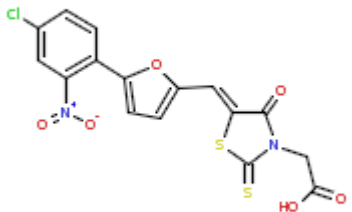


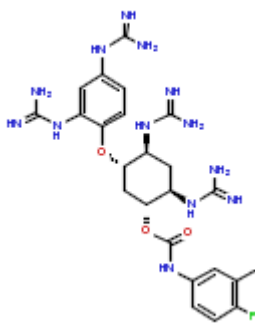
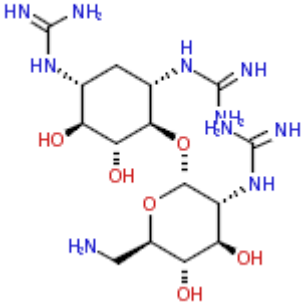
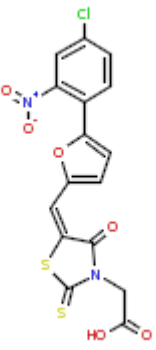
|  |         |   |    |       |
|--|---------|---|----|-------|
| <p>Chiral</p>  <p>Chemical structure of a chiral molecule. It features a piperazine ring connected to a biphenyl system. The piperazine ring is also connected to a chiral auxiliary containing a hydroxyl group and a fluorinated phenyl ring.</p>   | 0.13000 | 6 | 18 | 12.68 |
| <p>Chiral</p>  <p>Chemical structure of a chiral molecule. It features a piperazine ring connected to a biphenyl system. The piperazine ring is also connected to a chiral auxiliary containing a hydroxyl group and a fluorinated phenyl ring.</p>   | 0.13500 | 2 | 41 | 12.25 |
| <p>Chiral</p>  <p>Chemical structure of a chiral molecule. It features a piperazine ring connected to a biphenyl system. The piperazine ring is also connected to a chiral auxiliary containing a hydroxyl group and a fluorinated phenyl ring.</p> | 0.15100 | 2 | 36 | 10.81 |

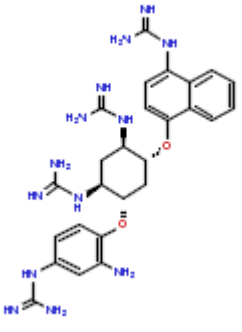
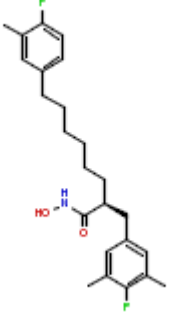
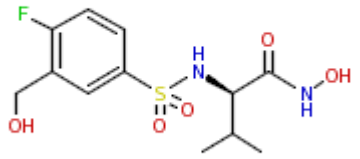
|  |          |   |    |       |
|--|----------|---|----|-------|
|  <chem>CC(=O)N1C(=O)C(S1)=C/C=C/c2cc(Oc3ccc(C(F)(F)F)c(Cl)c3)cc2</chem> | 0.19000* | 7 | 65 | 6.14  |
| Chiral<br> <chem>OC(=O)N[C@@H](C)C[C@H](C1CCNCC1)CC2CCNCC2</chem>       | 0.23000  | 2 | 31 | 10.93 |
|  <chem>CC(=O)N1C(=O)C(S1)=C/C=C/c2cc(Oc3ccc(Cl)c(Cl)c3)cc2</chem>     | 0.26000* | 7 | 64 | 5.85  |

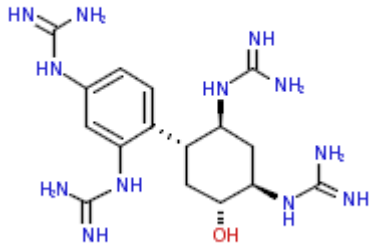
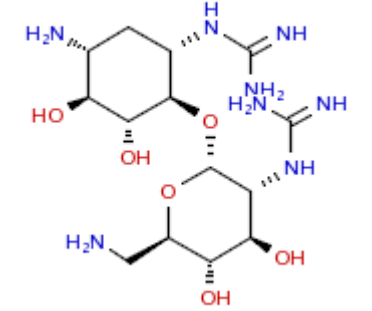
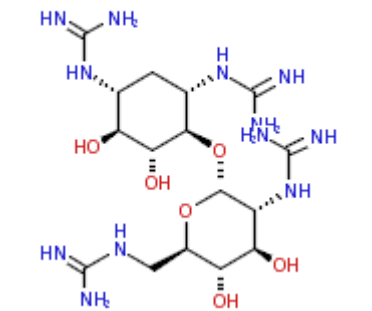
|   |          |   |         |       |
|---|----------|---|---------|-------|
| <p>Chiral</p>  | 0.27300  | 1 | 14      | 11.98 |
| <p>Chiral</p>  | 0.29000* | 3 | 13      | 9.00  |
|              | 0.29800* | 8 | BI-11B1 | 5.94  |

|   |          |   |    |       |
|---|----------|---|----|-------|
| <p>Chiral</p>  <chem>CC(C)(C)C(NS(=O)(=O)c1ccc(F)cc1)C(=O)NO</chem>            | 0.30000* | 3 | 34 | 10.23 |
|  <chem>OC(=O)CN1C(=O)SC(=S)C1=C/C=C2C=CC=C2S/C=C3C(=O)N(CCC(=O)O)C3=S</chem>  | 0.32000* | 7 | 67 | 6.53  |
| <p>Chiral</p>  <chem>OC(=O)N[C@@H](C[C@H](O)C1=CC=C(F)C=C1)CCN2CCOCC2</chem> | 0.35000  | 2 | 32 | 10.60 |

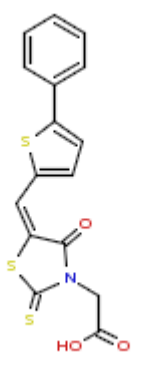
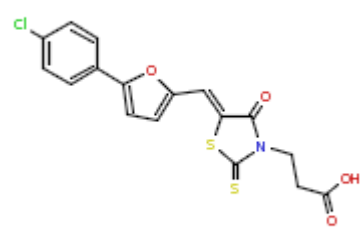
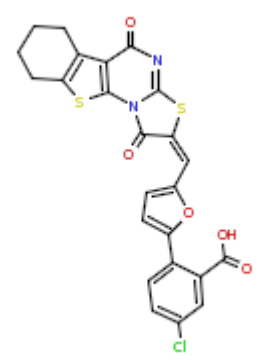
|  |          |   |          |       |
|--|----------|---|----------|-------|
| <p>Chiral</p>  <chem>CC(C)[C@H](NS(=O)(=O)c1cccc(C)c1)C(=O)NO</chem>            | 0.40000* | 3 | 15       | 9.73  |
| <p>Chiral</p>  <chem>CC(C)[C@H](NS(=O)(=O)c1ccc2ccccc2c1F)C(=O)NO</chem>       | 0.46000* | 3 | 25       | 10.48 |
|  <chem>CC(=O)O[C@@H]1CN(C1=S)C=Cc2cc(O)c(cc2Oc3ccc(cc3)[N+](=O)[O-])Cl</chem> | 0.50000* | 8 | BI-11A11 | 6.50  |

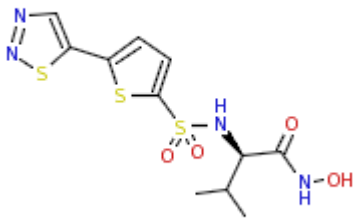
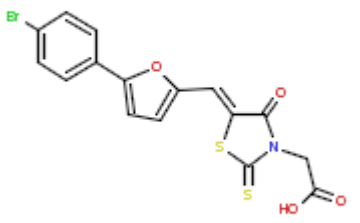
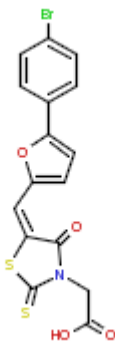
|  |          |    |    |      |
|--|----------|----|----|------|
| <p>Chiral</p>   | 0.50000  | 4  | 12 | 9.28 |
| <p>Chiral</p>  | 0.50000  | 9  | 23 | 8.51 |
|               | 0.50000* | 10 | 30 | 5.87 |

|   |          |    |    |       |
|---|----------|----|----|-------|
| <p>Chiral</p>    | 0.56000  | 11 | 1d | 7.56  |
| <p>Chiral</p>   | 0.57700  | 1  | 16 | 11.37 |
| <p>Chiral</p>  | 0.60000* | 3  | 27 | 10.76 |

|   |         |   |    |      |
|---|---------|---|----|------|
| <p style="text-align: center;">Chiral</p>    | 0.60000 | 4 | 8c | 7.55 |
| <p style="text-align: center;">Chiral</p>   | 0.70000 | 9 | 21 | 8.69 |
| <p style="text-align: center;">Chiral</p>  | 0.70000 | 9 | 4  | 7.14 |



|  |          |    |         |      |
|--|----------|----|---------|------|
|  <chem>CC(=O)OCCN1C(=O)C(S1)C=Cc2cc(C3=CC=CC=C3)cs2</chem>  | 0.74000* | 10 | 9       | 6.52 |
|  <chem>CC(=O)OCCN1C(=O)C(S1)C=Cc2cc(C3=CC=C(C=C3)Cl)oc2</chem>  | 0.80000* | 8  | BI-MFM3 | 5.57 |
|  <chem>CC(=O)OCCN1C(=O)C(S1)C=Cc2cc(C3=CC=C(C=C3)Cl)oc2C4=CC5=C(C=C4)N(C(=O)N5C6CCCCC6)C7=CC=CC=C7</chem> | 0.80000  | 12 | 1       | 6.67 |

|   |          |    |          |      |
|---|----------|----|----------|------|
| <p>Chiral</p>  <chem>CC(C)[C@@H](NS(=O)(=O)c1cc2c(s1)scn2)C(=O)NO</chem> | 0.81000* | 3  | 30       | 8.31 |
|  <chem>BrC1=CC=C(C=C1)C2=CC=CO2C=C3C(=O)NC(CS3)C(=O)O</chem>             | 0.85000* | 8  | BI-11A10 | 6.04 |
|  <chem>BrC1=CC=C(C=C1)C2=CC=CO2C=C3C(=O)NC(CS3)C(=O)O</chem>           | 0.85000* | 10 | 4        | 6.12 |

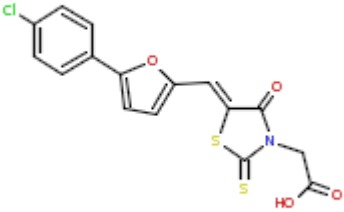
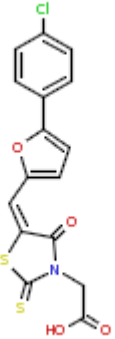
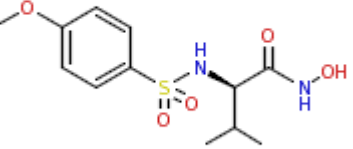
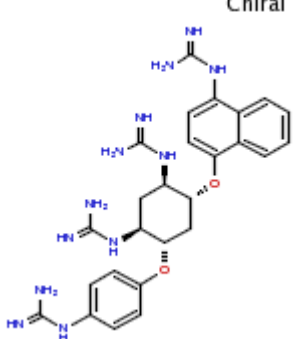
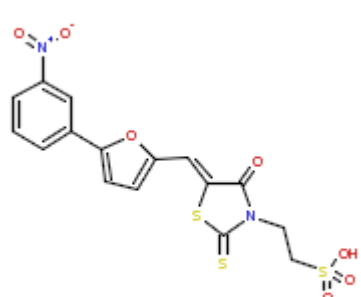
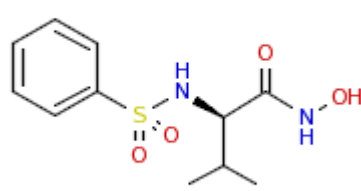
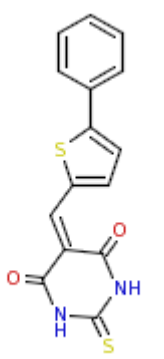
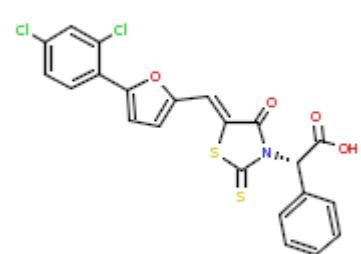
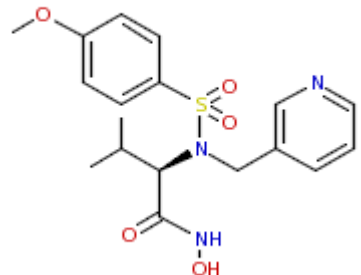
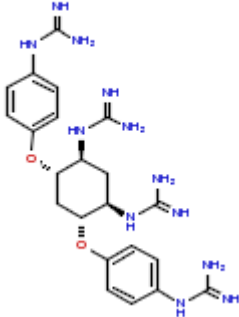
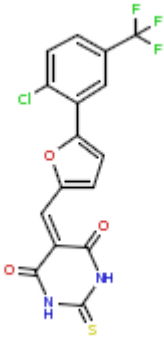
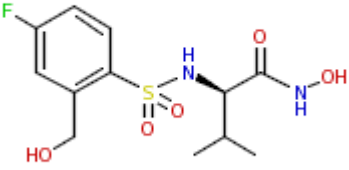
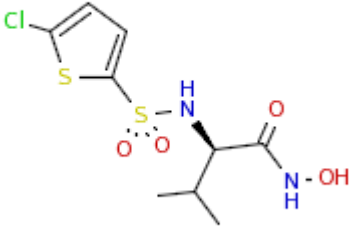
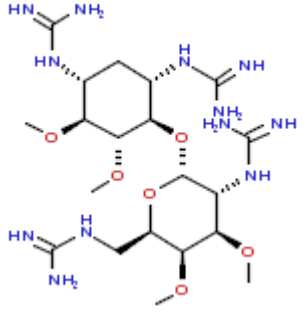
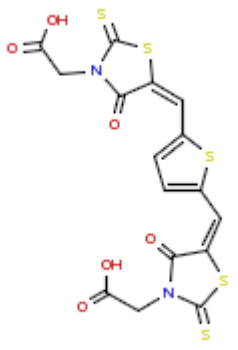
|   |          |    |         |      |
|---|----------|----|---------|------|
|              | 0.90000* | 8  | BI-11A9 | 6.05 |
|             | 0.90000* | 10 | 3       | 5.63 |
| Chiral<br> | 0.90000* | 3  | 2       | 9.65 |

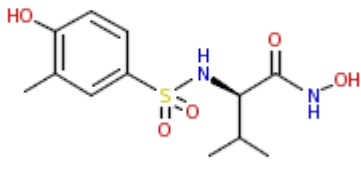
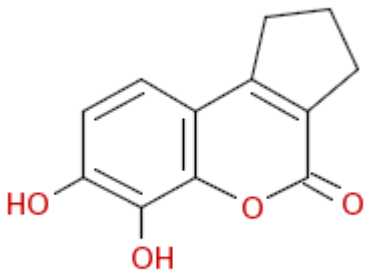
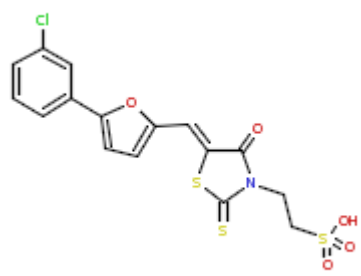
Table S2. Structures, LF biological activities, references, compound designators, and docking scores for screening set compounds in dataset **DB1B**.

| Structure   | LF IC <sub>50</sub><br>or K <sub>i</sub><br>( $\mu$ M) | Reference | Compound<br>Designator | Docking Score<br>(Surflex-Dock) |
|---|--|-----------|------------------------|---------------------------------|
| <p style="text-align: center;">Chiral</p>    | 1.002  | 4         | 1e                     | 8.63                            |
|   | 1.090  | 7         | 9                      | 5.95                            |
| <p style="text-align: center;">Chiral</p>  | 1.100  | 3         | 10                     | 8.36                            |

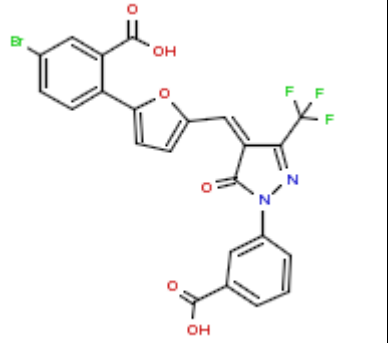
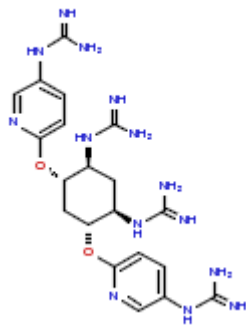
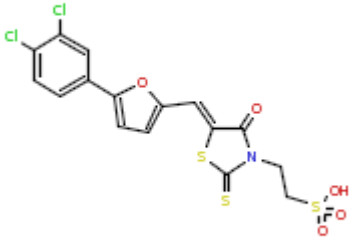
|   |       |    |    |  |      |
|---|-------|----|----|--|------|
|              |       |    |    |  |      |
|   | 1.200 | 10 | 23 |  | 4.36 |
| Chiral<br>   |       |    |    |  |      |
|   | 1.200 | 7  | 13 |  | 6.16 |
| Chiral<br> |       |    |    |  |      |
|   | 1.200 | 3  | 1  |  | 9.57 |

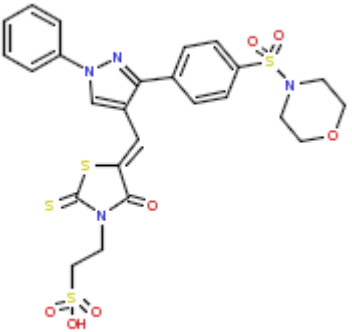
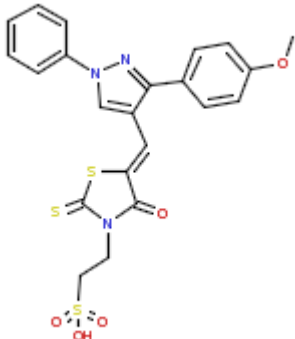
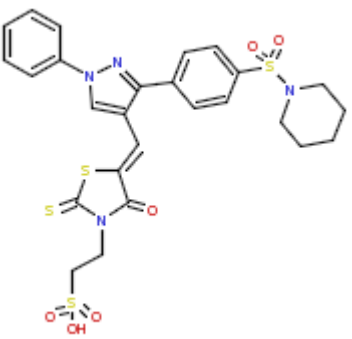
|   |       |    |    |       |
|---|-------|----|----|-------|
| <p>Chiral</p>    | 1.241 | 4  | 1g | 9.81  |
|                 | 1.300 | 10 | 21 | 5.05  |
| <p>Chiral</p>  | 1.310 | 3  | 28 | 10.18 |

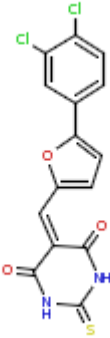
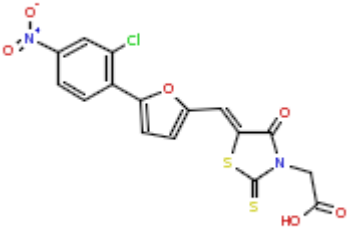
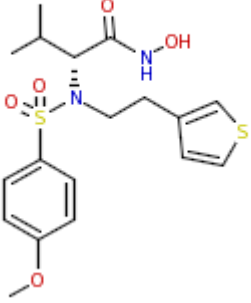
|  |       |    |    |      |
|--|-------|----|----|------|
| <p>Chiral</p>  <chem>CC(C)[C@H](NS(=O)(=O)c1ccc(Cl)cc1)C(=O)NO</chem>                                 | 1.310 | 3  | 29 | 7.65 |
| <p>Chiral</p>  <chem>COC1[C@@H](CNC(=N)N)[C@H](OC)[C@@H](CNC(=N)N)[C@H](OC)[C@@H](CNC(=N)N)O1</chem> | 1.500 | 9  | 29 | 7.05 |
|  <chem>O=C(O)CN1C(=O)S=C1C=C2C=CC=C2S2C(=O)N(C2)C(=O)O</chem>                                       | 1.600 | 10 | 12 | 4.99 |

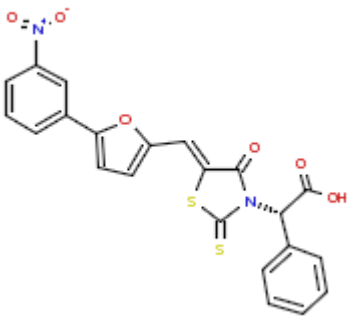
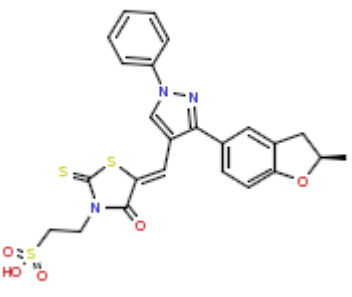
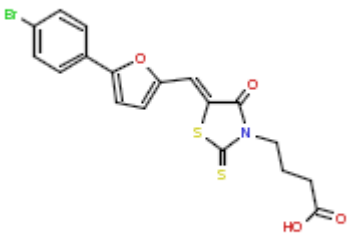
|   |       |    |    |      |
|---|-------|----|----|------|
| <p>Chiral</p>  | 1.640 | 3  | 26 | 9.41 |
|                | 1.700 | 13 | 6  | 7.03 |
|              | 1.700 | 7  | 10 | 6.07 |

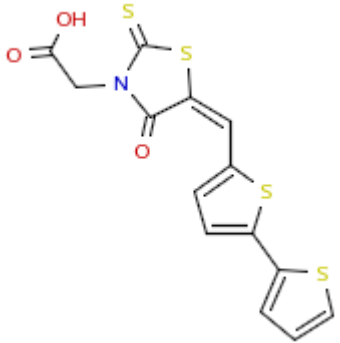
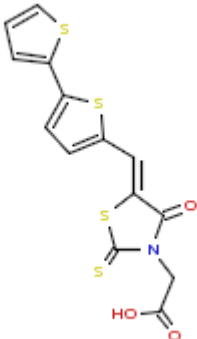
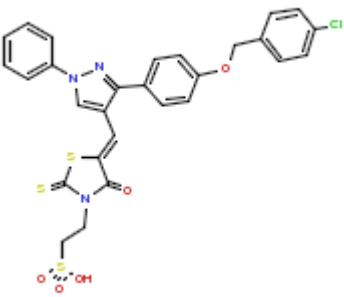


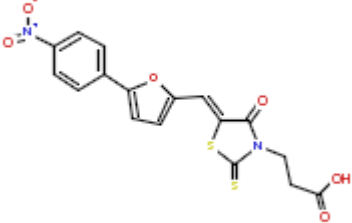
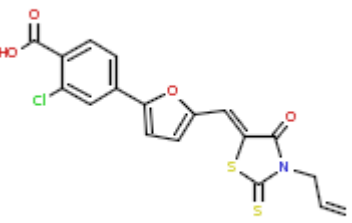
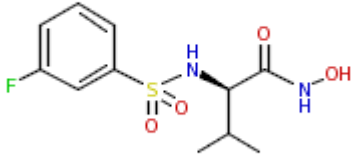
|  |       |    |    |      |
|--|-------|----|----|------|
|                 | 1.700 | 12 | 2  | 6.97 |
| <p>Chiral</p>  | 1.716 | 4  | 1i | 9.88 |
|               | 1.780 | 7  | 11 | 5.64 |

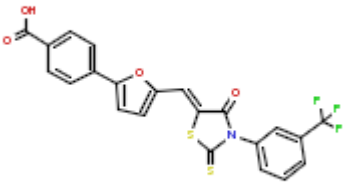
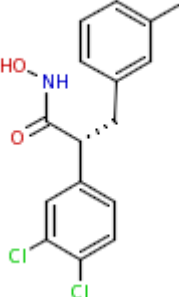
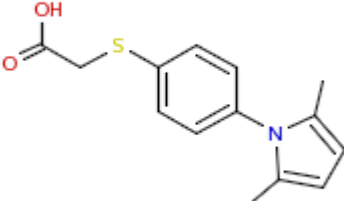
|  |       |   |    |      |
|--|-------|---|----|------|
|  <p>The structure shows a thiazolidine ring with a sulfur atom at the top and a nitrogen atom at the bottom. The nitrogen is substituted with a propyl chain ending in a sulfonic acid group (-SO<sub>3</sub>H). The 2-position of the thiazolidine ring is connected via a double bond to a 1-phenyl-1H-imidazole ring. The 4-position of the imidazole ring is substituted with a 4-(morpholin-4-yl)phenyl group.</p>   | 1.860 | 7 | 42 | 7.33 |
|  <p>The structure shows a thiazolidine ring with a sulfur atom at the top and a nitrogen atom at the bottom. The nitrogen is substituted with a propyl chain ending in a sulfonic acid group (-SO<sub>3</sub>H). The 2-position of the thiazolidine ring is connected via a double bond to a 1-phenyl-1H-imidazole ring. The 4-position of the imidazole ring is substituted with a 4-methoxyphenyl group.</p>           | 2.040 | 7 | 40 | 6.90 |
|  <p>The structure shows a thiazolidine ring with a sulfur atom at the top and a nitrogen atom at the bottom. The nitrogen is substituted with a propyl chain ending in a sulfonic acid group (-SO<sub>3</sub>H). The 2-position of the thiazolidine ring is connected via a double bond to a 1-phenyl-1H-imidazole ring. The 4-position of the imidazole ring is substituted with a 4-(piperidin-2-yl)phenyl group.</p> | 2.070 | 7 | 43 | 6.80 |

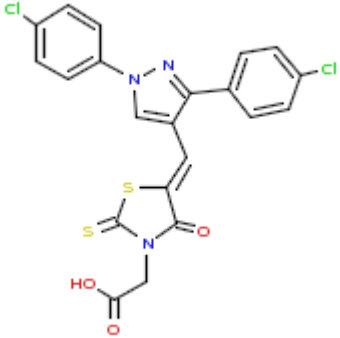
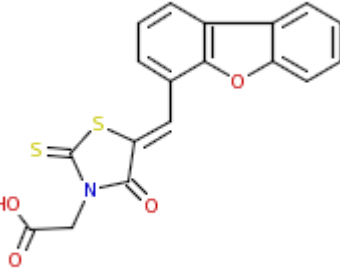
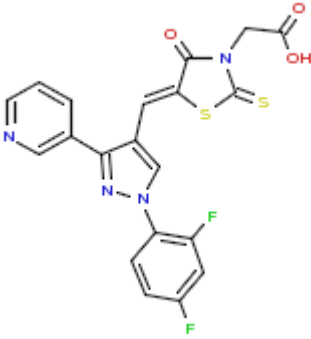
|   |       |    |    |      |
|---|-------|----|----|------|
| <br><chem>Clc1ccc(cc1)Oc2ccoc2C=C3C(=O)NC(=O)S3</chem>                       | 2.100 | 10 | 22 | 4.45 |
| <br><chem>O=[N+]([O-])c1ccc(Cl)c(c1)Oc2ccoc2C=C3C(=O)NC(=O)S3CC(=O)O</chem>  | 2.100 | 7  | 4  | 5.87 |
| Chiral<br><br><chem>COc1ccc(cc1)S(=O)(=O)N[C@@H](CC2=CC=CS2)C(=O)NO</chem> | 2.100 | 3  | 8  | 8.38 |

|  |       |   |    |      |
|--|-------|---|----|------|
| <p>Chiral</p>  <chem>O=C(O)[C@H](c1ccccc1)N1C(=O)C(S1)=C2C=C(C=C2OC3=CC=C(C=C3)[N+](=O)[O-])</chem>                               | 2.180 | 7 | 7  | 5.94 |
| <p>Chiral</p>  <chem>O=C(O)CCNS(=O)(=O)N1C(=O)C(S1)=C2C=C(C=C2OC3=CC=C(C=C3)O4=CC=CC=C4O5C=C(C=C5)N6=CC=CC=C6)N7=CC=CC=C7</chem> | 2.290 | 7 | 39 | 6.80 |
|  <chem>O=C(O)CCN1C(=O)C(S1)=C2C=C(C=C2OC3=CC=C(C=C3)Br)</chem>  | 2.300 | 8 | 21 | 6.59 |

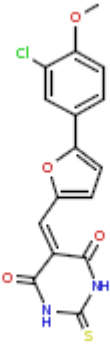
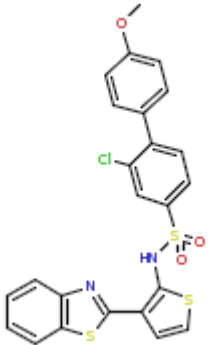
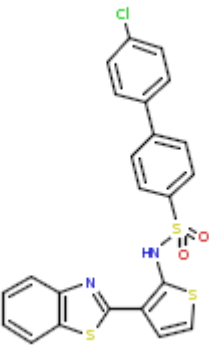
|   |       |    |    |      |
|---|-------|----|----|------|
|    | 2.300 | 10 | 24 | 6.83 |
|   | 2.300 | 7  | 66 | 5.52 |
|  | 2.450 | 7  | 38 | 6.63 |

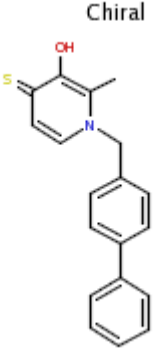
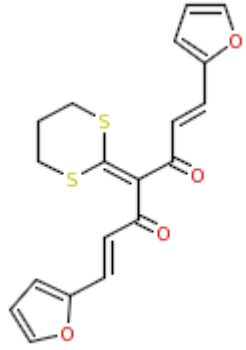
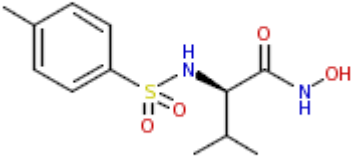
|  |       |   |    |      |
|--|-------|---|----|------|
| <br><chem>CC(=O)OCCN1C(=O)C(S1)=C/C=C/c2cc(O)cc2[N+](=O)[O-]</chem> | 2.700 | 8 | 19 | 6.13 |
| <br><chem>C=CCN1C(=O)C(S1)=C/C=C/c2cc(O)c(Cl)cc2</chem>             | 2.700 | 8 | 20 | 5.90 |
| Chiral<br><br><chem>CC(C)C(NC(=O)NO)S(=O)(=O)c1ccc(F)cc1</chem>   | 2.800 | 3 | 12 | 9.24 |

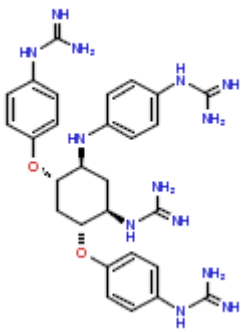
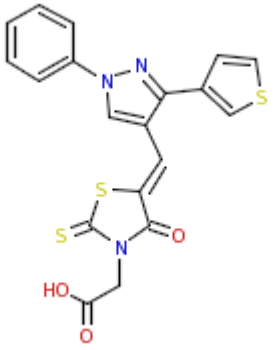
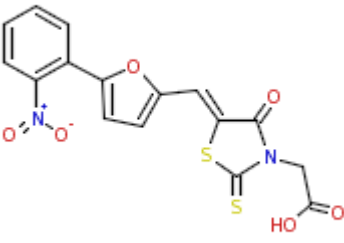
|  |       |    |    |       |
|--|-------|----|----|-------|
|                 | 2.900 | 8  | 18 | 4.15  |
| <p>Chiral</p>  | 2.900 | 6  | 22 | 10.59 |
|               | 2.900 | 12 | 56 | 5.27  |

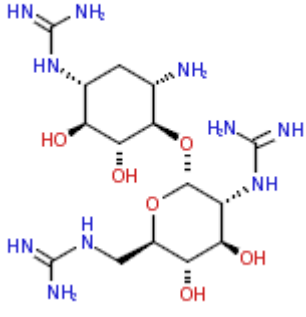
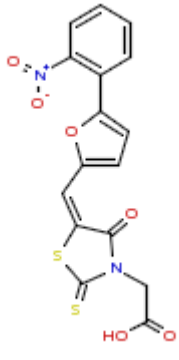
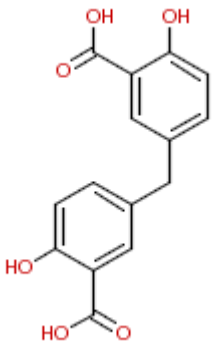
|   |       |   |    |      |
|---|-------|---|----|------|
|  <chem>CC(=O)OCCN1C(=O)C(S1)=C/C=C/c2cn(c2)c3ccc(Cl)cc3</chem>     | 2.950 | 7 | 34 | 6.17 |
|  <chem>CC(=O)OCCN1C(=O)C(S1)=C/C=C/c2ccc3c(c2)oc4ccccc34</chem>    | 2.960 | 7 | 55 | 6.00 |
|  <chem>CC(=O)OCCN1C(=O)C(S1)=C/C=C/c2cn(c2)c3ccc(F)c(F)c3</chem> | 2.990 | 7 | 32 | 8.05 |

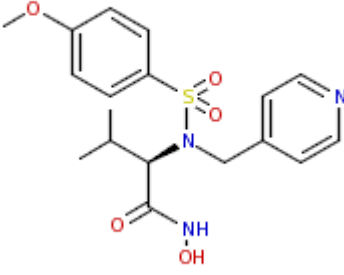
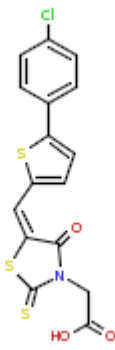
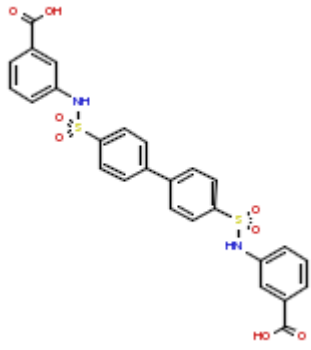


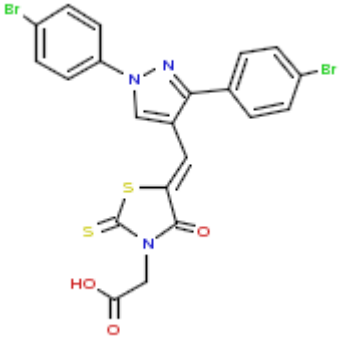
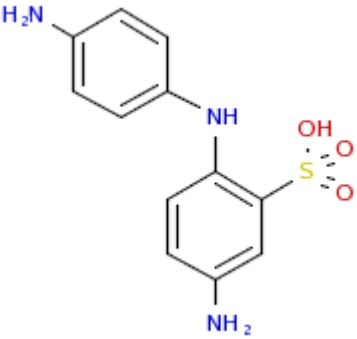
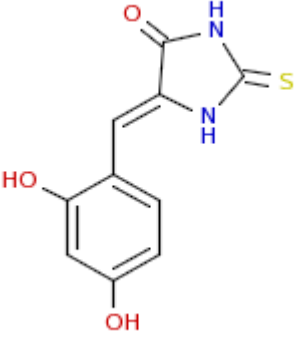
|   |  |       |    |     |      |
|---|--|-------|----|-----|------|
|    |  | 3.000 | 10 | 29  | 4.89 |
|   |  | 3.000 | 14 | 124 | 6.21 |
|  |  | 3.000 | 14 | 71  | 7.24 |

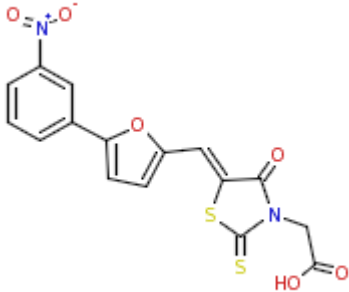
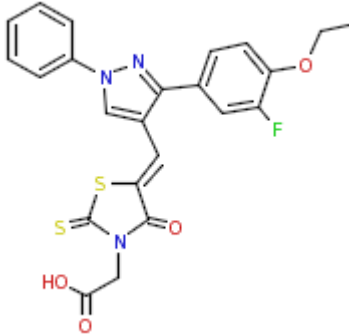
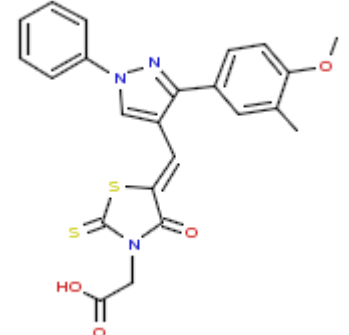
|   |       |    |    |      |
|---|-------|----|----|------|
| <p>Chiral</p>    | 3.000 | 6  | 11 | 7.92 |
|                 | 3.000 | 12 | 3  | 5.95 |
| <p>Chiral</p>  | 3.000 | 3  | 14 | 8.96 |

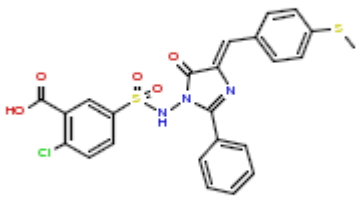
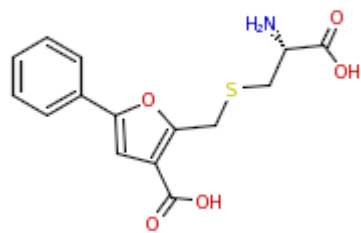
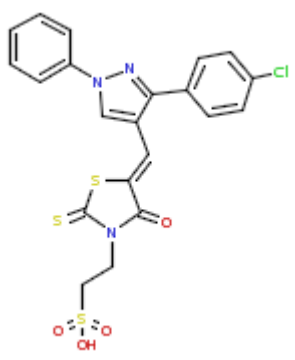
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|---|-------|---|----------|------|
| <p>Chiral</p>  | 3.053 | 4 | 1n       | 8.56 |
|               | 3.070 | 7 | 29       | 7.34 |
|              | 3.100 | 8 | BI-11A12 | 6.22 |

|   |       |    |    |      |
|---|-------|----|----|------|
| <p>Chiral</p>  <p>The structure shows a complex molecule with two pyranose-like rings. The top ring has a guanidino group (HN=NH) at the top, a hydroxyl group (HO) at the bottom, and another guanidino group (HN=NH) on the right. The bottom ring has a hydroxyl group (HO) at the bottom, a guanidino group (HN=NH) on the left, and a hydroxyl group (HO) on the right. The two rings are connected via an oxygen atom and a methylene group.</p> | 3.100 | 9  | 17 | 8.44 |
|  <p>The structure features a thiazolidine ring system. It has a nitro group (NO<sub>2</sub>) attached to a benzene ring, which is further connected to a furan ring. The thiazolidine ring has a sulfur atom (S) and a nitrogen atom (N) with a carbonyl group (C=O) and a carboxylic acid group (HO-C=O) attached to it.</p>   | 3.100 | 10 | 5  | 7.57 |
|  <p>The structure consists of two benzene rings connected by a methylene group (-CH<sub>2</sub>-). The top benzene ring has a carboxylic acid group (HO-C=O) and a hydroxyl group (OH) at the top, and another hydroxyl group (OH) at the bottom. The bottom benzene ring has a hydroxyl group (HO) and a carboxylic acid group (HO-C=O) at the bottom.</p>  | 3.100 | 12 | 4  | 9.72 |

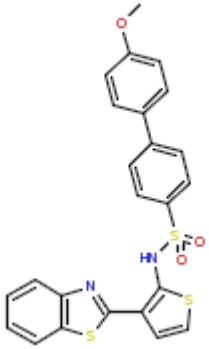
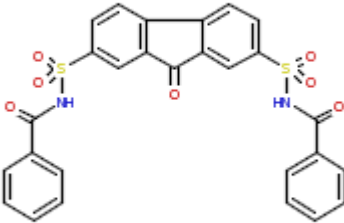
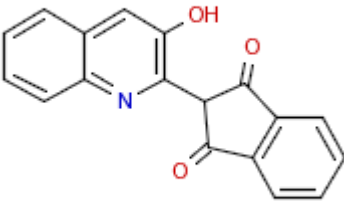
|  |       |    |    |       |
|--|-------|----|----|-------|
| <p>Chiral</p>  <chem>CC(C)[C@H](NS(=O)(=O)c1ccc(OC)cc1)C(=O)NO</chem>                     | 3.100 | 3  | 7  | 10.64 |
|  <chem>OC(=O)CN1C(=O)C=C2C=C(C=C2S)C3=CC=C(Cl)C=C3S1</chem>                              | 3.200 | 10 | 11 | 5.89  |
|  <chem>OC(=O)c1ccc(NS(=O)(=O)c2ccc(cc2)NS(=O)(=O)c3ccc(cc3)Nc4ccc(cc4)C(=O)O)cc1</chem> | 3.200 | 15 | 9  | 7.96  |

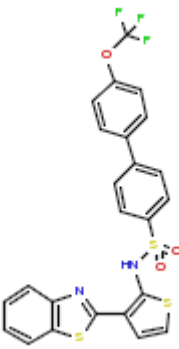
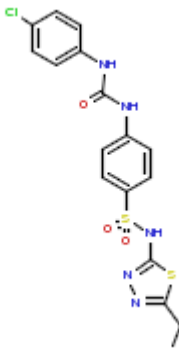
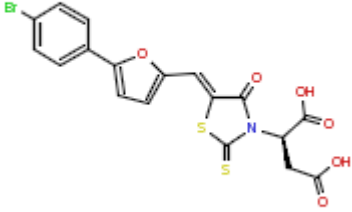
|  |       |    |    |      |
|--|-------|----|----|------|
|  <chem>CC(=O)OCCN1C(=O)C(S1)=C(C=C2C=CC(=C2)Br)N3C=CC(=C3)Br</chem> | 3.350 | 7  | 35 | 3.94 |
|  <chem>NC1=CC=C(NC1=CC=C(N)S(=O)(=O)O</chem>                       | 3.400 | 14 | 1  | 7.17 |
|  <chem>Oc1cc(O)ccc1C=C2NC(=O)NC(=S2)</chem>                       | 3.400 | 12 | 5  | 6.96 |

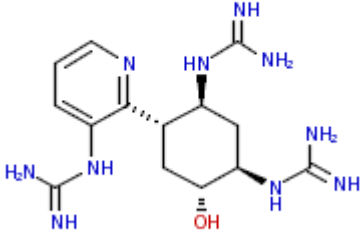
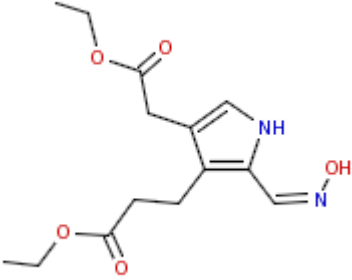
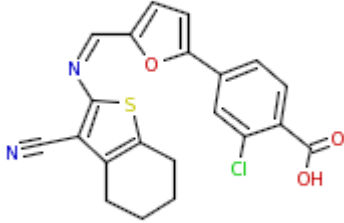
|   |       |   |    |      |
|---|-------|---|----|------|
|  <chem>O=C(O)CN1C(=O)S=C1C=Cc2cc(Oc3ccc([N+](=O)[O-])cc3)co2</chem>    | 3.450 | 7 | 3  | 6.28 |
|  <chem>O=C(O)CN1C(=O)S=C1C=Cc2cc(Nc3ccccc3)nn2C4=CC=C(C=C4)OCC</chem> | 3.450 | 7 | 46 | 4.86 |
|  <chem>O=C(O)CN1C(=O)S=C1C=Cc2cc(Nc3ccccc3)nn2C4=CC=C(C=C4)OC</chem> | 3.580 | 7 | 36 | 4.81 |

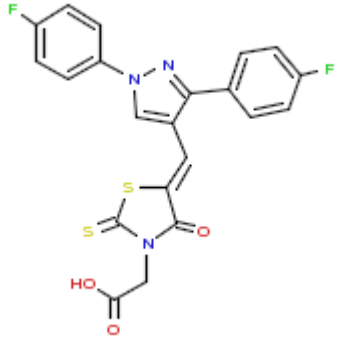
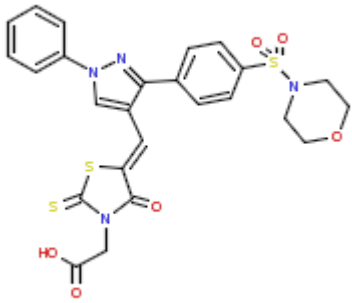
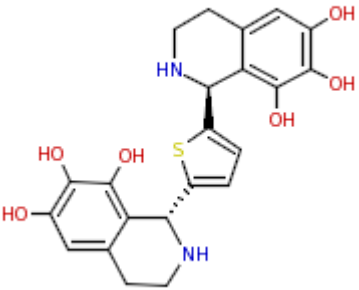
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|---|-------|----|----|--|------|
|            |       |    |    |  |      |
|   | 3.600 | 12 | 6  |  | 6.98 |
| Chiral<br> |       |    |    |  |      |
|   | 3.600 | 12 | 7  |  | 6.61 |
|          |       |    |    |  |      |
|   | 3.660 | 7  | 41 |  | 5.47 |

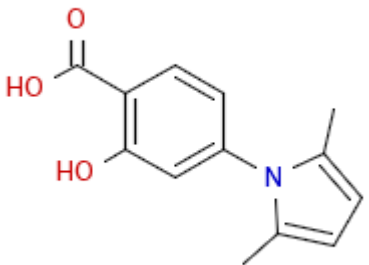
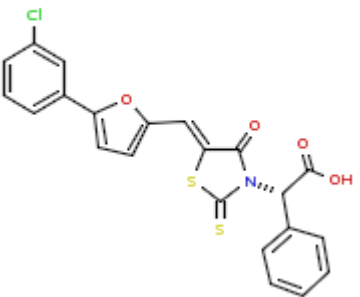
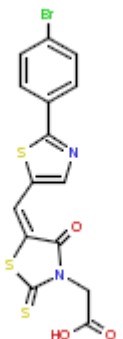


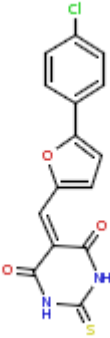
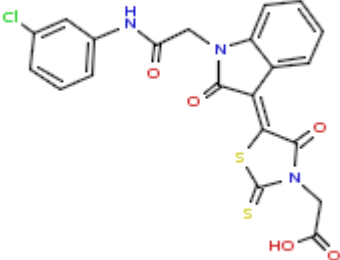
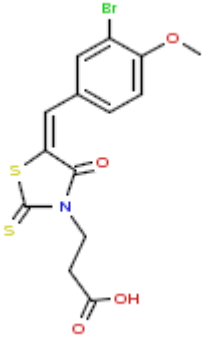
|   |       |    |    |      |
|---|-------|----|----|------|
|  <chem>COc1ccc(cc1)-c2ccc(cc2)NS(=O)(=O)c3sc4c(s3)cnc45</chem> | 3.800 | 14 | 70 | 8.01 |
|  <chem>O=C1C(=O)c2ccc(cc2C1=O)S(=O)(=O)NC(=O)c3ccccc3</chem>   | 3.800 | 15 | 18 | 8.34 |
|  <chem>Oc1c2ccccc2n(c1)C3C(=O)c4ccccc4C3=O</chem>            | 3.890 | 13 | 5  | 7.43 |

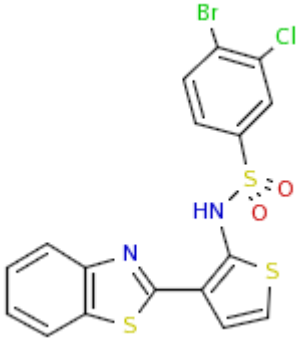
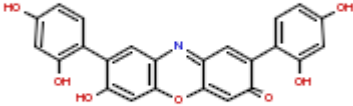
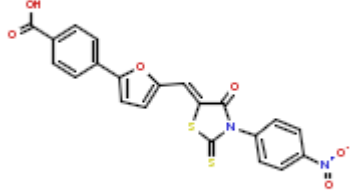
|   |       |    |    |      |
|---|-------|----|----|------|
| <br><chem>C1=CC=C(C=C1)C2=NC(=S)C=C2C3=NC(=S)C=C3N(S(=O)(=O)OC4=CC=C(C=C4)OC(F)(F)F)C5=CC=CC=C5</chem> | 3.900 | 14 | 72 | 7.91 |
| <br><chem>CCC1=CN=C(S1)N(S(=O)(=O)NC2=CC=C(C=C2)NC(=O)NC3=CC=C(C=C3)Cl)C4=CC=CC=C4</chem>             | 3.900 | 12 | 8  | 7.14 |
| Chiral<br><br><chem>OC(CC(=O)O)N1C(=O)C(S1)C(=C2C=CC(OC2)c3ccc(Br)cc3)C4=CC=CC=C4</chem>             | 3.980 | 7  | 5  | 6.08 |

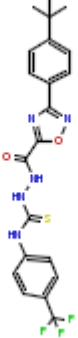
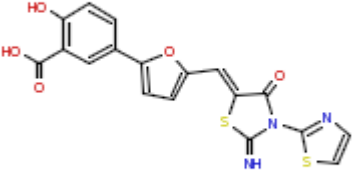
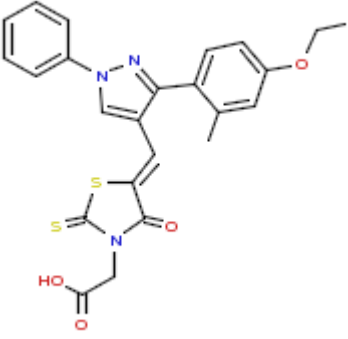
|  |       |    |    |       |
|--|-------|----|----|-------|
| <p>Chiral</p>  <chem>Nc1ncnc1[C@H]2CC[C@@H](C(=O)O)[C@H](NC(=N)N)C2NC(=N)N</chem> | 4.100 | 4  | 8e | 7.76  |
|  <chem>CCOC(=O)CCc1c[nH]c1C(=O)OCC</chem>   | 4.200 | 14 | 2  | 10.76 |
|  <chem>O=C(O)c1cc(Cl)ccc1Oc2oc3c(nc3s2)C4CCCCC4</chem>                          | 4.200 | 12 | 9  | 4.91  |

|   |       |    |    |      |
|---|-------|----|----|------|
|                  | 4.220 | 7  | 33 | 7.92 |
|                 | 4.260 | 7  | 31 | 6.20 |
| <p>Chiral</p>  | 4.300 | 16 | 5a | 5.63 |

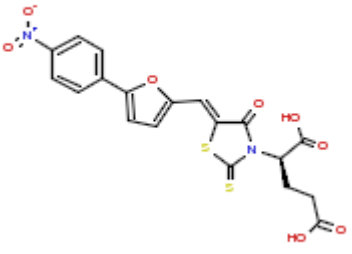
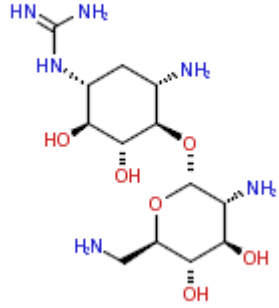
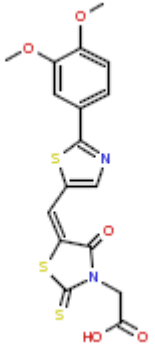
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|--|-------|----|----|------|
|             |       |    |    |      |
|  | 4.300 | 12 | 10 | 5.18 |
| Chiral<br> |       |    |    |      |
|  | 4.340 | 7  | 8  | 6.19 |
|           |       |    |    |      |
|  | 4.400 | 10 | 16 | 5.40 |

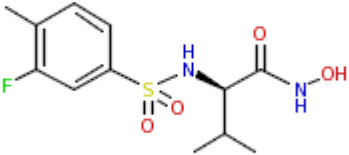
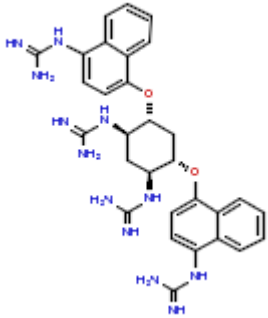
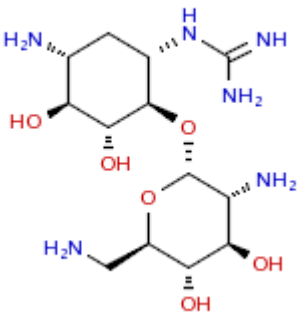
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|---|-------|----|----|------|
|    | 4.400 | 10 | 25 | 4.73 |
|    | 4.400 | 7  | 62 | 5.47 |
|  | 4.400 | 12 | 11 | 6.50 |

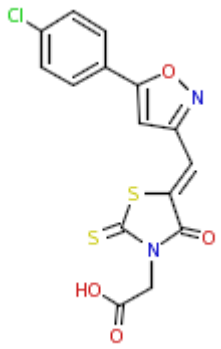
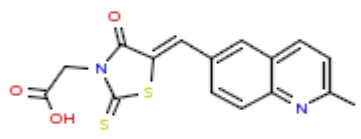
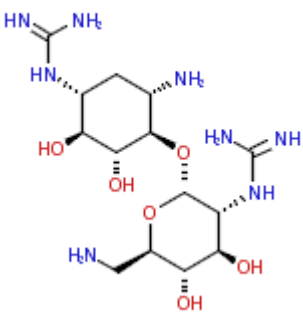
|   |  |       |    |     |      |
|---|--|-------|----|-----|------|
|    |  | 4.500 | 14 | 123 | 6.50 |
|    |  | 4.500 | 16 | 2   | 6.63 |
|  |  | 4.800 | 8  | 16  | 4.68 |

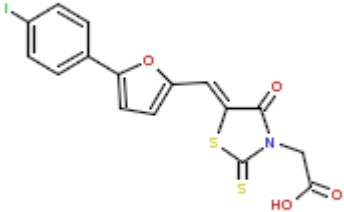
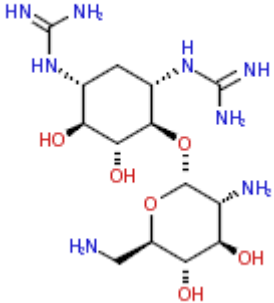
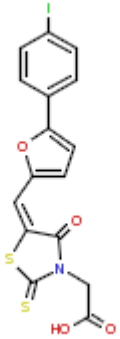
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|---|--|-------|----|----|------|
|    |  | 4.800 | 14 | 3  | 7.08 |
|    |  | 4.800 | 12 | 12 | 4.29 |
|  |  | 4.870 | 7  | 37 | 6.46 |

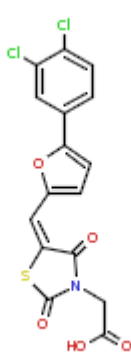
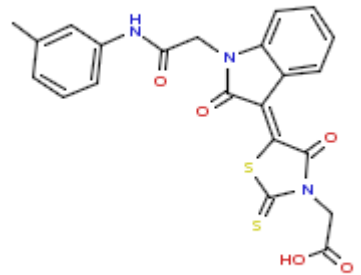
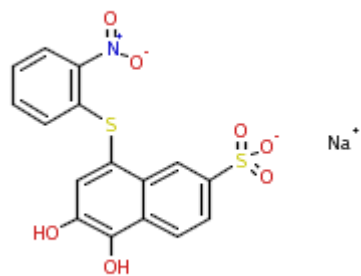


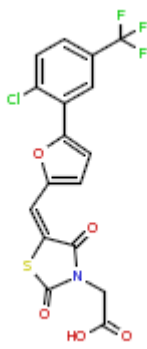
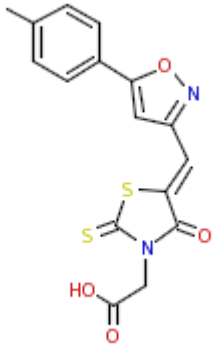
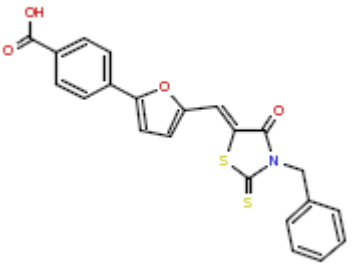
|  |       |    |    |      |
|--|-------|----|----|------|
| <p>Chiral</p>  <chem>O=C(O)CC[C@@H]1C(=O)N(C2=CC=C(C=C2)OC3=CC=C(C=C3)[N+](=O)[O-])S1</chem>          | 4.910 | 7  | 6  | 6.36 |
| <p>Chiral</p>  <chem>NC(=O)N[C@@H]1[C@H](O)[C@@H](O[C@@H]2[C@H](O)[C@@H](CO)O[C@H]2N)O[C@H]1O</chem> | 5.000 | 9  | 9  | 5.83 |
|  <chem>O=C(O)CCN1C(=O)C=C(C2=CN=C(S2)C3=CC=C(C=C3)OC)S1</chem>                                      | 5.000 | 10 | 15 | 6.59 |

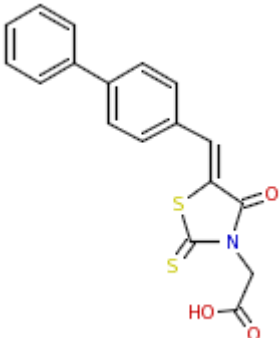
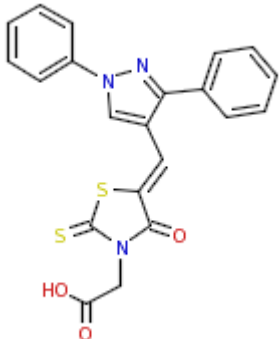
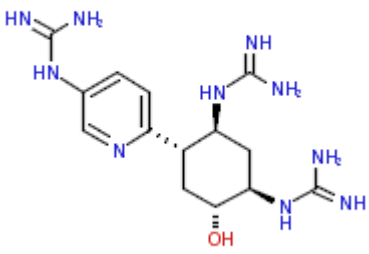
|  |       |   |    |      |
|--|-------|---|----|------|
| <p>Chiral</p>  <chem>CC(C)C(S(=O)(=O)c1ccc(C)c(F)c1)C(=O)NO</chem>  | 5.180 | 3 | 18 | 9.42 |
| <p>Chiral</p>  <chem>NC(=O)Nc1ccc2c(c1)oc3c2N(C(=O)Nc4ccc(NC(=O)N)cc4)C(=O)Nc5ccc(NC(=O)N)cc5</chem>         | 5.188 | 4 | 1f | 5.74 |
| <p>Chiral</p>  <chem>NC(=O)N[C@@H]1C[C@@H](O)[C@H](O)[C@@H](N)O1[C@@H]2C[C@@H](O)[C@H](O)[C@@H](N)O2</chem> | 5.200 | 9 | 11 | 8.36 |

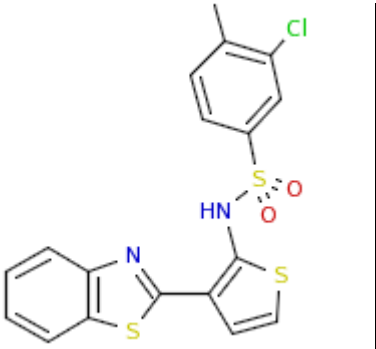
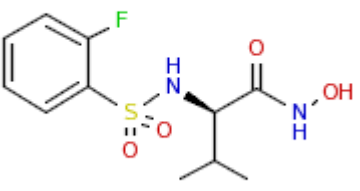
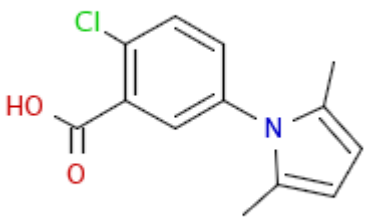
|   |       |   |    |      |
|---|-------|---|----|------|
|              | 5.200 | 7 | 24 | 6.40 |
|              | 5.260 | 7 | 54 | 4.92 |
| Chiral<br> | 5.300 | 9 | 20 | 8.92 |

|  |       |    |    |      |
|--|-------|----|----|------|
|                 |       |    |    |      |
|  | 5.500 | 8  | 15 | 6.01 |
| <p>Chiral</p>  |       |    |    |      |
|  | 5.600 | 9  | 19 | 7.11 |
|               |       |    |    |      |
|  | 5.600 | 10 | 2  | 5.76 |

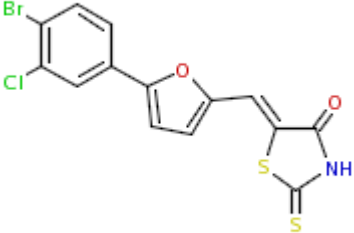
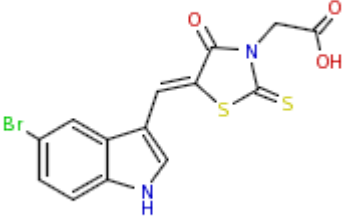
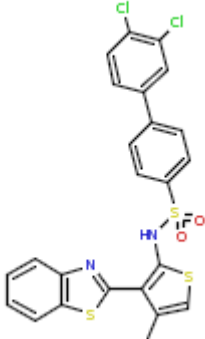
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|--|-------|----|----|------|
|  <chem>O=C(O)CN1C(=O)S1C=Cc2cc(Cl)c(Cl)cc2</chem>                                     | 5.600 | 10 | 28 | 6.22 |
|  <chem>O=C(O)CN1C(=O)S1C(=O)c2c3ccccc3n2C(=O)Nc4ccc(C)cc4</chem>                      | 5.710 | 7  | 63 | 6.28 |
|  <chem>[Na+].[O-]S(=O)(=O)c1ccc(O)c2c(O)c(S(=O)(=O)c3ccccc3[N+](=O)[O-])cc12</chem> | 5.890 | 13 | 4  | 8.06 |

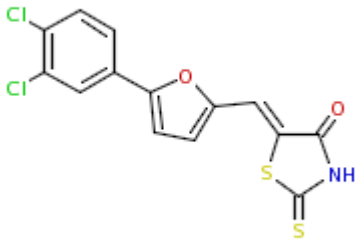
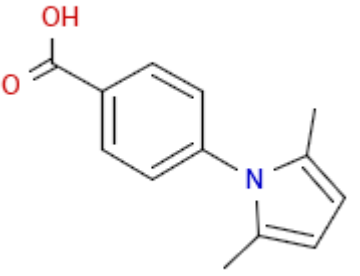
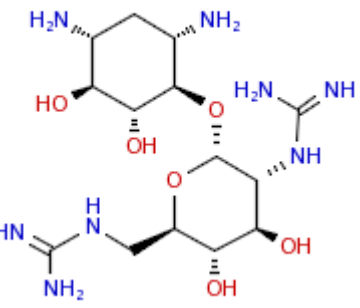
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|---|-------|----|----|------|
|  <chem>CC(=O)N1C(=O)SC1=C/C=C/c2cc(Oc3ccc(Cl)c(C(F)(F)F)c3)co2</chem>      | 5.900 | 10 | 17 | 6.97 |
|  <chem>CC(=O)N1C(=O)SC1=C/C=C/c2cc(Oc3ccc(C)cc3)no2</chem>                | 5.900 | 7  | 22 | 6.63 |
|  <chem>CC(=O)N1C(=O)SC1=C/C=C/c2cc(Oc3ccc(C(=O)O)cc3)co2Cc4ccccc4</chem> | 6.000 | 8  | 14 | 5.51 |

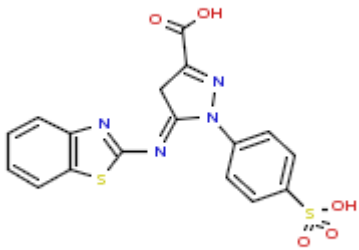
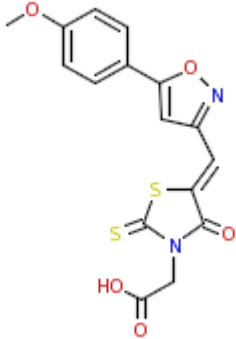
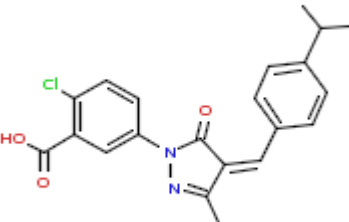
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|---|-------|---|----|-------|
| <br><chem>O=C(O)CN1C(=O)S=C1C=Cc2ccc(cc2)c3ccccc3</chem>                         | 6.200 | 7 | 49 | 5.62  |
| <br><chem>O=C(O)CN1C(=O)S=C1C=Cc2c3c(ncn3c2)c4ccccc4</chem>                     | 6.250 | 7 | 30 | 8.36  |
| Chiral<br><br><chem>O[C@@H]1CC[C@H](NC(=N)N)C[C@H]1C2=CN=C(NC(=N)N)C=C2</chem> | 6.600 | 4 | 8d | 10.03 |

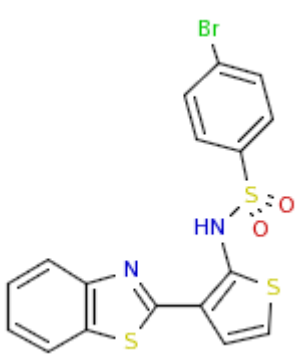
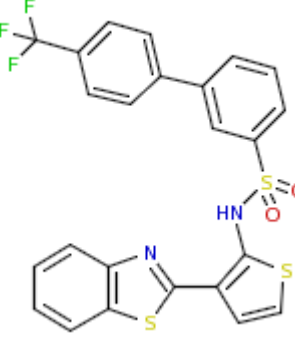
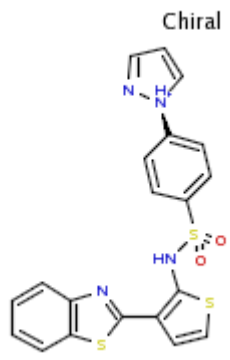
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|--|-------|----|----|------|
| <br><chem>Cc1ccc(S(=O)(=O)Nc2sc3c(c2)nc4ccccc43)c1</chem>           | 6.600 | 14 | 55 | 6.47 |
| Chiral<br><br><chem>CC(C)C[C@@H](NS(=O)(=O)c1ccccc1F)C(=O)NO</chem> | 6.600 | 3  | 11 | 8.62 |
| <br><chem>CC1=C(C)N(c2ccc(Cl)cc2C(=O)O)C=C1</chem>                | 6.800 | 12 | 57 | 4.60 |

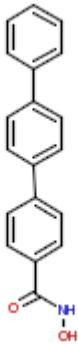
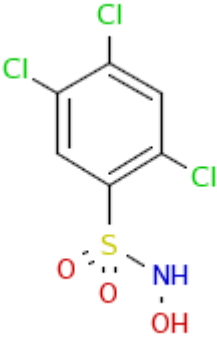
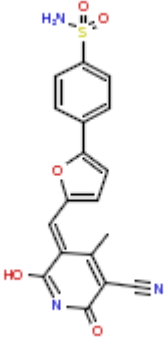


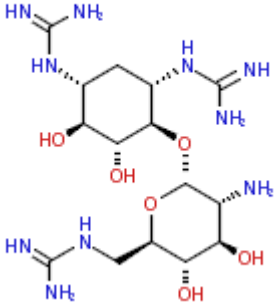
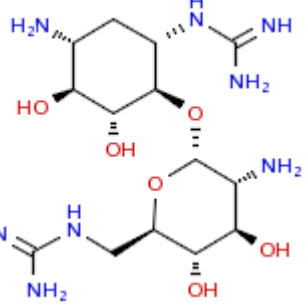
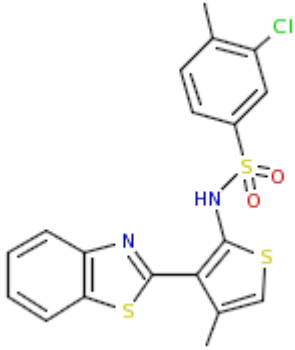
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|---|-------|----|----|------|
|  <chem>O=C1NC(=S)C=C1C2=CC=CO2C3=CC=C(C=C3)BrC4=CC=C(C=C4)Br</chem>  | 7.000 | 8  | 13 | 4.01 |
|  <chem>OC(=O)CN1C(=O)C=C1C2=CC=C3C=CNC3=C2Br</chem>  | 7.040 | 7  | 61 | 6.80 |
|  <chem>CC1=CC=C2C(S1)=NC3=CC=CC=C3N2C4=CC=CC=C4C5=CC=C(C=C5)C6=CC=C(C=C6)C7=CC=C(C=C7)ClC8=CC=C(C=C8)Cl</chem> | 7.200 | 14 | 75 | 7.05 |

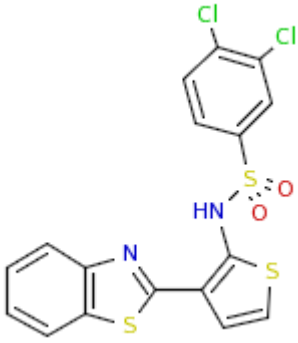
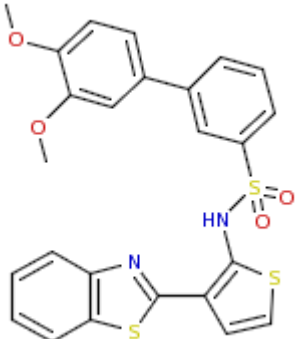
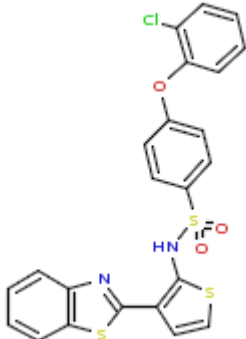
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|--|-------|----|----|------|
|  <chem>O=C1NC(=S)C=C1C2=CC=C(C=C2)C3=CC=C(Cl)C(Cl)=C3</chem>  | 7.400 | 8  | 12 | 4.09 |
|  <chem>CC1=C(C)N(C1)C2=CC=C(C=C2)C(=O)O</chem>  | 7.600 | 12 | 58 | 5.40 |
| Chiral<br> <chem>NC(=N)N[C@@H]1[C@@H](O)[C@H](O)[C@@H](O)[C@H](O)[C@H]1O[C@@H]2[C@@H](O)[C@H](O)[C@@H](O)[C@H](O)[C@H]2O</chem> | 7.700 | 9  | 22 | 8.63 |

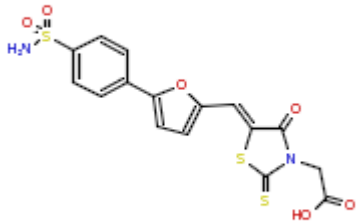
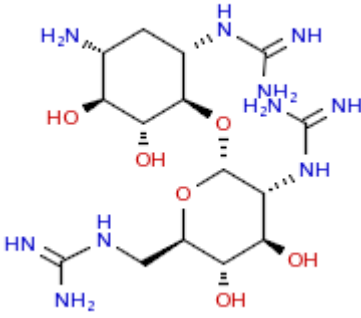
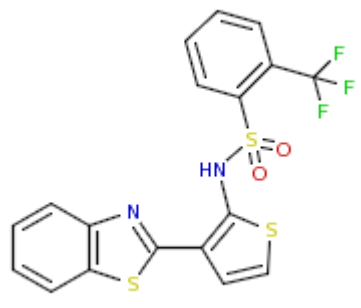
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|--|-------|----|----|------|
|  <chem>OS(=O)(=O)c1ccc(cc1)N2C(=O)C(=N2)C(=O)O</chem> | 7.700 | 12 | 13 | 5.34 |
|  <chem>CC1(C)S(=O)C(=O)N1C(=O)O</chem>               | 7.800 | 7  | 23 | 7.58 |
|  <chem>CC1(C)S(=O)C(=O)N1C(=O)O</chem>              | 7.900 | 12 | 14 | 6.96 |

|   |       |    |    |      |
|---|-------|----|----|------|
| <br><chem>BrC1=CC=C(S(=O)(=O)NC2=C(C=C3C=CC=C3S2)C4=CN=C5C=CC=C45)C1</chem>                        | 8.000 | 14 | 68 | 6.49 |
| <br><chem>FC(F)(F)C1=CC=C(S(=O)(=O)NC2=C(C=C3C=CC=C3S2)C4=CN=C5C=CC=C45)C1</chem>                 | 8.000 | 14 | 77 | 6.76 |
| <p>Chiral</p> <br><chem>C1=CN=C2C=CC=C12C3=CC=C(S(=O)(=O)NC4=C(C=C5C=CC=C5N4)C6=CN=CN6)C3</chem> | 8.000 | 14 | 85 | 6.54 |

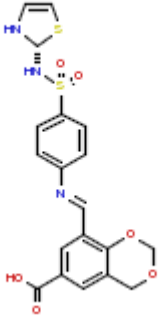
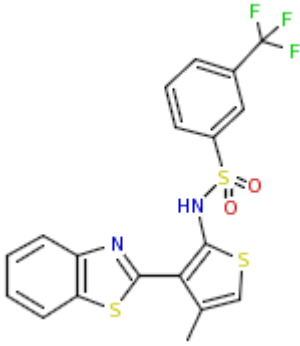
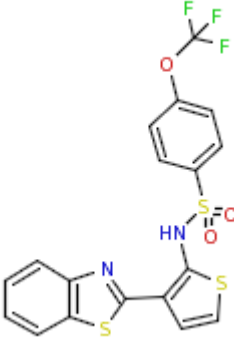
|   |       |    |    |      |
|---|-------|----|----|------|
| <br><chem>CC(=O)Nc1ccc(cc1)-c2ccc(cc2)c3ccccc3</chem>                    | 8.000 | 6  | 1  | 6.63 |
| <br><chem>Clc1cc(Cl)c(Cl)cc1S(=O)(=O)NHO</chem>                         | 8.300 | 6  | 2  | 5.34 |
| <br><chem>Cc1c(C#N)c(=O)n(c1O)/C=C/c2cc(O)c3ccc(cc32)S(=O)(=O)N</chem> | 8.300 | 12 | 15 | 7.73 |

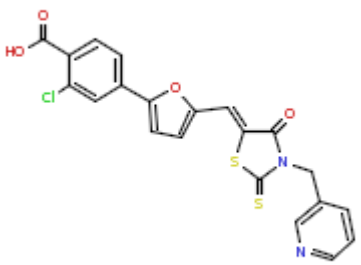
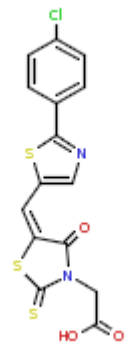
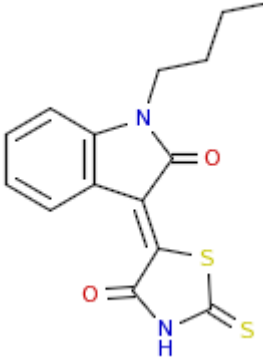
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|--|-------|----|----|------|
| <p>Chiral</p>   | 8.700 | 9  | 16 | 8.60 |
| <p>Chiral</p>  | 8.800 | 9  | 15 | 7.64 |
|               | 8.900 | 14 | 21 | 6.24 |

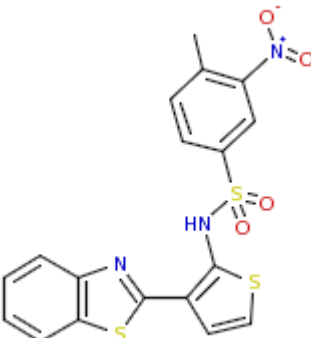
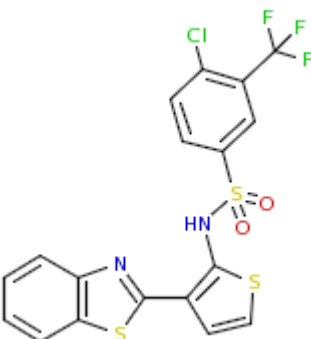
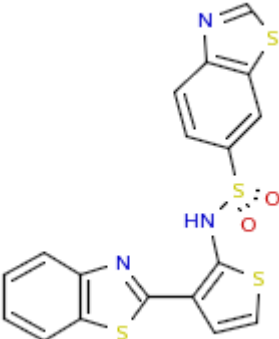
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|---|-------|----|----|------|
| <br><chem>Clc1ccc(cc1S(=O)(=O)N)C2=CN=C3C=CSC32</chem>     | 9.000 | 14 | 60 | 6.61 |
| <br><chem>COc1cc(OC)ccc1S(=O)(=O)N)C2=CN=C3C=CSC32</chem> | 9.000 | 14 | 78 | 6.57 |
| <br><chem>Clc1ccccc1O)C2=CN=C3C=CSC32</chem>             | 9.000 | 14 | 79 | 6.91 |

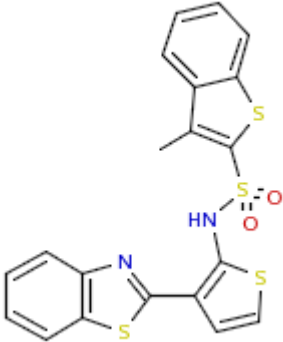
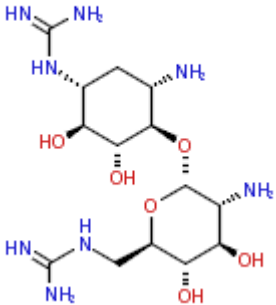
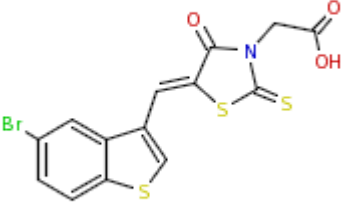
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|---|-------|----|----|------|
|  <p>Chemical structure of a sulfonamide derivative. It features a benzene ring with a sulfonamide group (-SO<sub>2</sub>NH<sub>2</sub>) at the para position, connected to a furan ring, which is further linked to a thiazolidine ring system containing a carboxylic acid group (-COOH).</p>   | 9.100 | 8  | 11 | 7.45 |
| <p>Chiral</p>  <p>Chemical structure of a chiral molecule. It consists of a central cyclohexane ring with a hydroxyl group (-OH) and an amino group (-NH<sub>2</sub>) on one side, and a complex side chain containing multiple amide and imine groups on the other. The side chain includes a furan ring and a thiazolidine ring system.</p> | 9.200 | 9  | 25 | 8.81 |
|  <p>Chemical structure of a thiazole derivative. It features a benzothiazole ring system connected to a thiazole ring, which is further linked to a sulfonamide group (-SO<sub>2</sub>NH<sub>2</sub>) and a trifluoromethyl group (-CF<sub>3</sub>) on a benzene ring.</p>   | 9.300 | 14 | 45 | 5.58 |

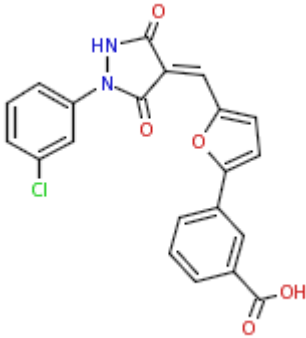
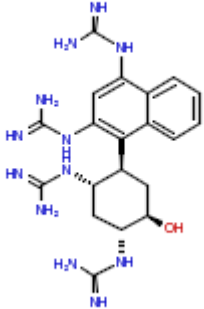
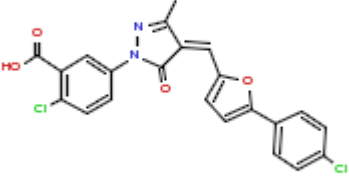


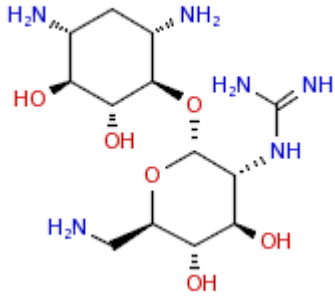
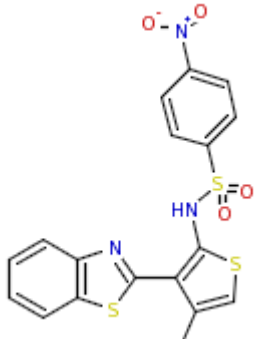
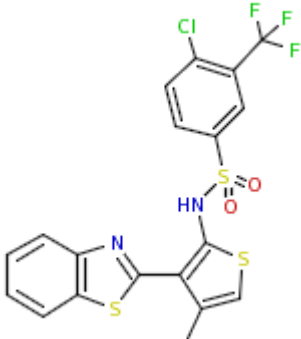
|   |       |    |    |      |
|---|-------|----|----|------|
| <p>Chiral</p>  | 9.300 | 12 | 16 | 6.45 |
|               | 9.400 | 14 | 10 | 6.48 |
|              | 9.600 | 14 | 46 | 6.53 |

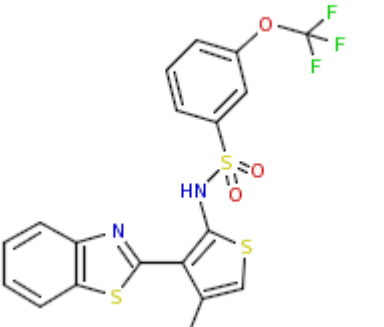
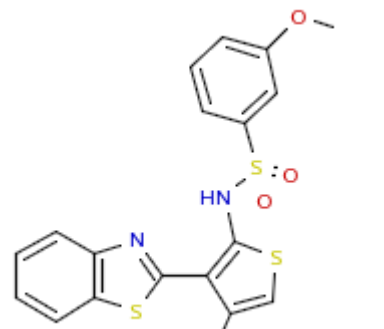
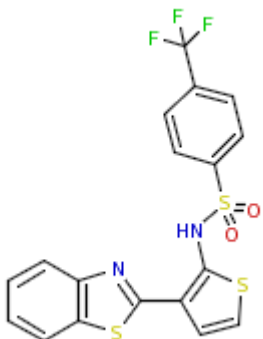
|   |        |    |    |      |
|---|--------|----|----|------|
|    | 9.900  | 8  | 10 | 6.27 |
|   | 10.000 | 10 | 14 | 5.64 |
|  | 10.000 | 13 | 3  | 4.02 |

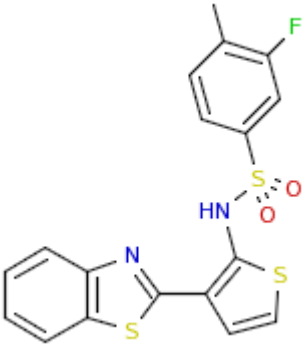
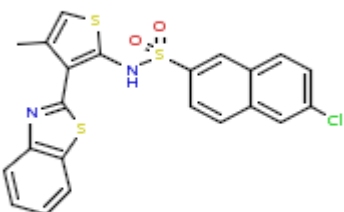
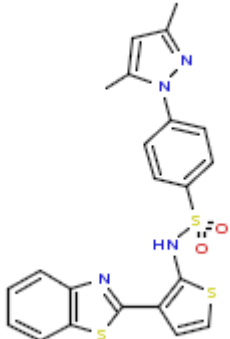
|  |        |    |    |      |
|--|--------|----|----|------|
| <br><chem>Cc1ccc(cc1)S(=O)(=O)Nc2sc3ccccc3n2</chem>           | 10.000 | 14 | 63 | 5.86 |
| <br><chem>Clc1ccc(cc1C(F)(F)F)S(=O)(=O)Nc2sc3ccccc3n2</chem> | 10.000 | 14 | 64 | 6.52 |
| <br><chem>C1=NC=C(S1)c2ccccc2S(=O)(=O)Nc3sc4ccccc4n3</chem> | 10.000 | 14 | 92 | 6.86 |

|  |        |    |    |      |
|--|--------|----|----|------|
|             | 10.000 | 14 | 96 | 6.83 |
| Chiral<br> | 10.200 | 9  | 14 | 7.56 |
|           | 10.400 | 7  | 58 | 4.49 |

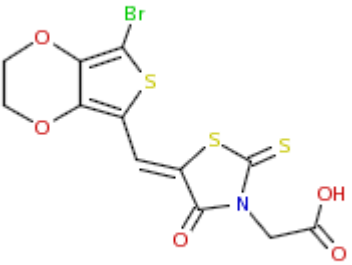
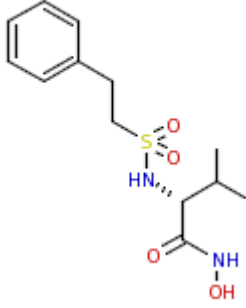
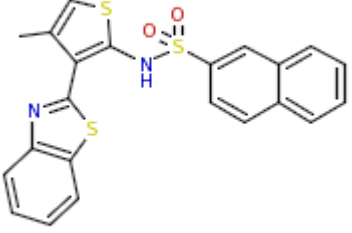
|  |        |    |    |      |
|--|--------|----|----|------|
|                 | 10.500 | 12 | 17 | 7.59 |
| <p>Chiral</p>  | 10.700 | 4  | 8g | 3.55 |
|               | 10.700 | 12 | 18 | 6.73 |

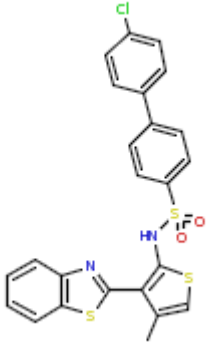
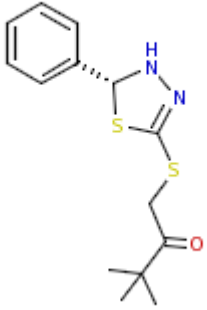
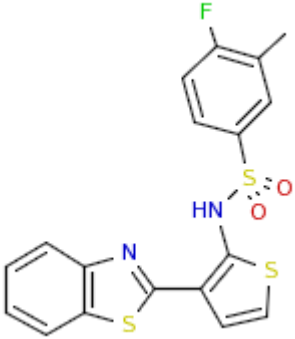
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|---|--------|----|----|------|
| <p>Chiral</p>  | 10.900 | 9  | 13 | 8.04 |
|               | 11.000 | 14 | 17 | 7.79 |
|              | 11.000 | 14 | 30 | 6.25 |

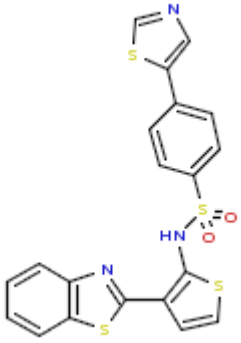
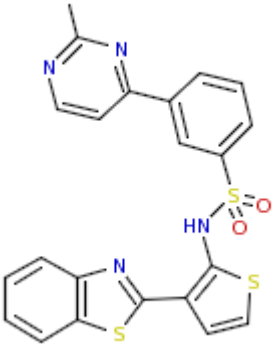
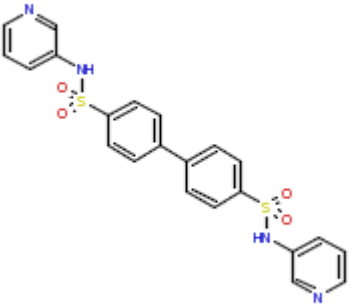
|   |        |    |    |      |
|---|--------|----|----|------|
|  <p>The structure shows a benzothiazole core (a benzene ring fused to a five-membered ring containing one sulfur and one nitrogen atom). The nitrogen atom is bonded to a sulfur atom, which is double-bonded to an oxygen atom and single-bonded to a hydrogen atom. This sulfur atom is also bonded to a phenyl ring. The para position of this phenyl ring is substituted with a trifluoromethoxy group (-OCF<sub>3</sub>).</p> | 11.000 | 14 | 32 | 7.08 |
|  <p>The structure is similar to the first one, but the trifluoromethoxy group is replaced by a methoxy group (-OCH<sub>3</sub>).</p>  | 11.000 | 14 | 33 | 6.50 |
|  <p>The structure is similar to the first one, but the trifluoromethoxy group is replaced by a trifluoromethyl group (-CF<sub>3</sub>).</p>  | 11.000 | 14 | 51 | 6.43 |

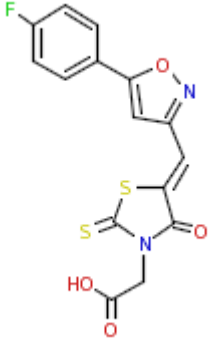
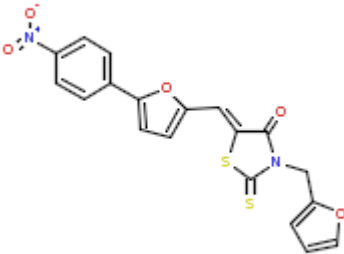
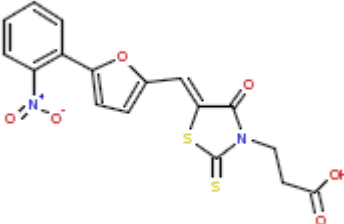
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|---|--------|----|----|------|
| <br><chem>C1=CC=C2C(S1)=NC(=C2)C3=CC=CC=C3S3NS(=O)(=O)c4ccc(F)cc4</chem>                       | 11.000 | 14 | 53 | 6.37 |
| <br><chem>C1=CC=C2C(S1)=NC(=C2)C3=CC=CC=C3S3NS(=O)(=O)c4ccc(Cl)cc4C5=CC=CC=C5S5</chem>         | 11.000 | 14 | 67 | 7.04 |
| <br><chem>C1=CC=C2C(S1)=NC(=C2)C3=CC=CC=C3S3NS(=O)(=O)c4ccc(cc4N5C=CN5C)C6=CC=CC=C6S6</chem> | 11.000 | 14 | 89 | 6.22 |

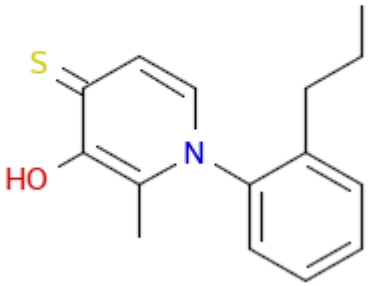
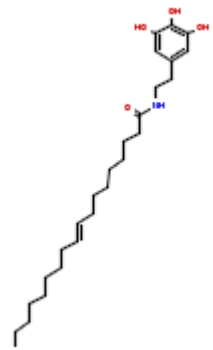
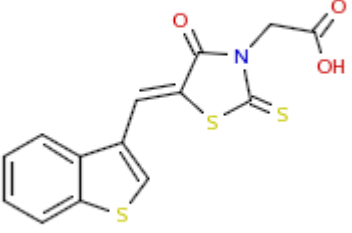


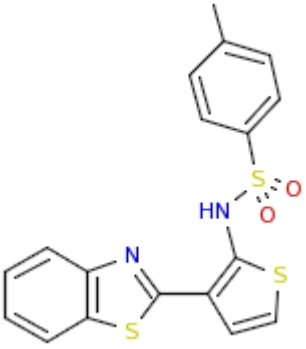
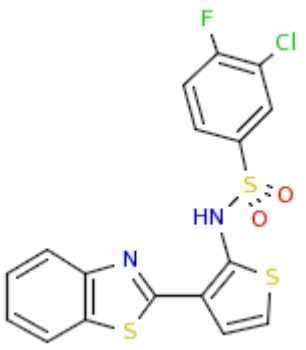
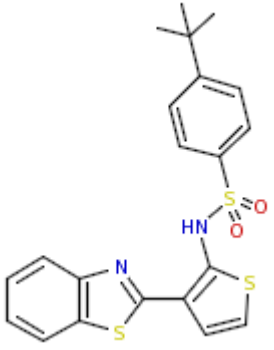
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|--|--------|----|----|-------|
| <br><chem>O=C(O)CN1C(=S)S(=S)C1/C=C/c2sc3c(c2)OCCO3Br</chem>  | 11.400 | 7  | 47 | 4.87  |
| Chiral<br><br><chem>CC(C)C(=O)N(O)S(=O)(=O)CCc1ccccc1</chem> | 11.880 | 3  | 19 | 11.05 |
| <br><chem>O=S(=O)(Nc1sc2ccccc12)c3ccc4ccccc34</chem>        | 12.000 | 14 | 34 | 7.22  |

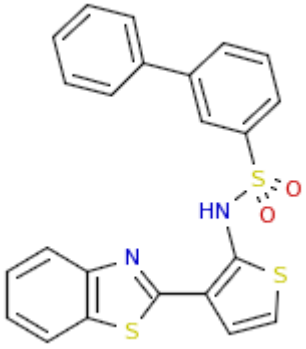
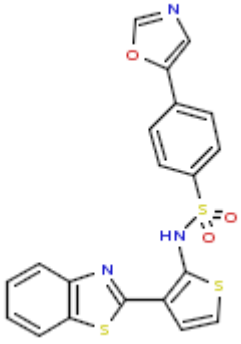
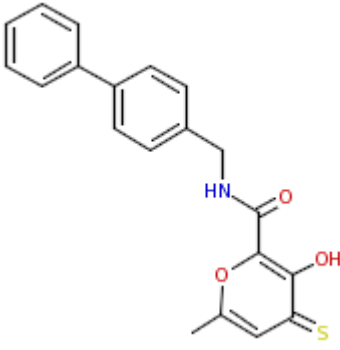
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|--|--------|----|----|------|
|             | 12.000 | 14 | 37 | 7.29 |
| Chiral<br> | 12.000 | 14 | 4  | 5.95 |
|           | 12.000 | 14 | 54 | 6.83 |

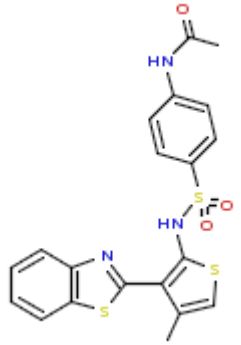
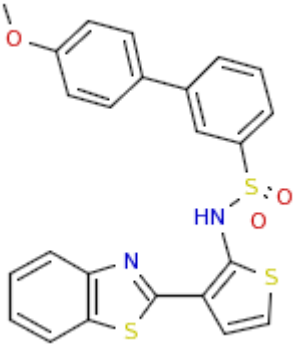
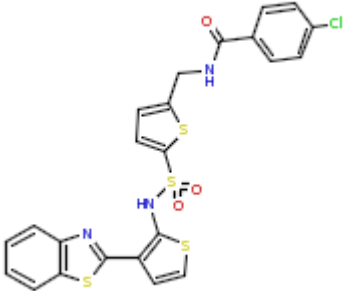
|   |        |    |    |      |
|---|--------|----|----|------|
|    | 12.000 | 14 | 82 | 7.17 |
|   | 12.000 | 14 | 88 | 7.42 |
|  | 12.000 | 15 | 8  | 8.19 |

|  |        |   |    |      |
|--|--------|---|----|------|
|  <chem>CC(=O)N1C(=O)S=C1C=Cc2cc(O)c(C3=CC=C(F)C=C3)c2</chem>                    | 12.400 | 7 | 25 | 6.48 |
|  <chem>C1=CC=C(C=C1)OC1=CC=C(C=C1)C=Cc2cc(O)c3c(S)nc(C4=CC=C(C=C4)O)c3=O</chem> | 12.600 | 8 | 9  | 5.42 |
|  <chem>CC(=O)CN1C(=O)S=C1C=Cc2cc(O)c(C3=CC=C(C=C3)N(=O)[O-])c2</chem>         | 12.800 | 8 | 8  | 7.02 |

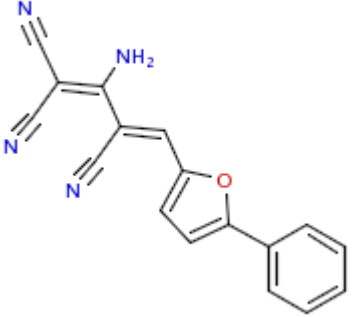
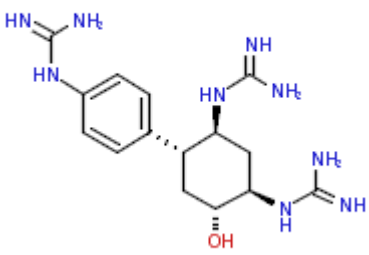
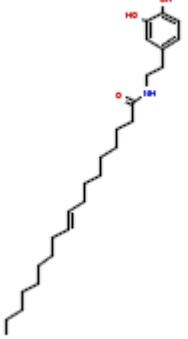
|   |        |    |      |       |
|---|--------|----|------|-------|
| <p>Chiral</p>  | 13.000 | 17 | 94F8 | 6.72  |
|               | 13.000 | 18 | 4    | 10.75 |
|              | 13.000 | 7  | 57   | 4.82  |

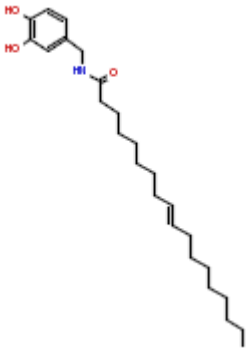
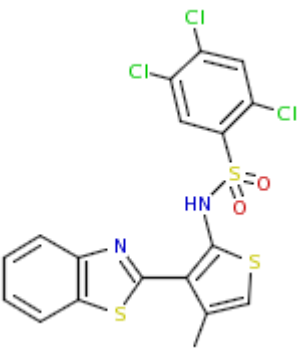
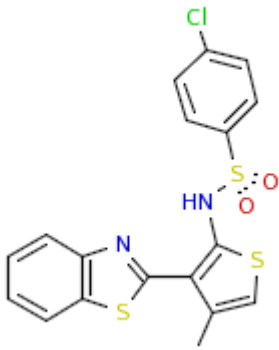
|   |        |    |    |      |
|---|--------|----|----|------|
| <br><chem>Cc1ccc(cc1)S(=O)(=O)Nc2sc3ccccc3n2</chem>          | 13.000 | 14 | 48 | 6.56 |
| <br><chem>Fc1cc(Cl)ccc1S(=O)(=O)Nc2sc3ccccc3n2</chem>       | 13.000 | 14 | 57 | 6.51 |
| <br><chem>CC(C)(C)c1ccc(cc1)S(=O)(=O)Nc2sc3ccccc3n2</chem> | 13.000 | 14 | 59 | 7.37 |

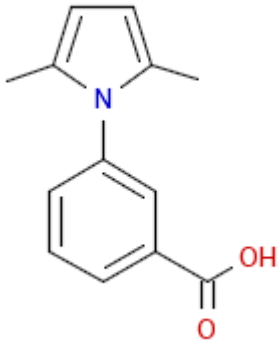
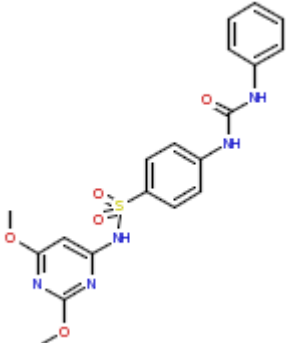
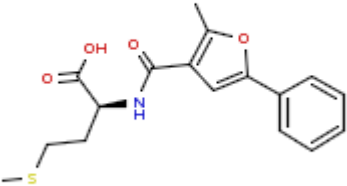
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|---|--------|----|-------|------|
| <br><chem>O=S(=O)(c1ccc(cc1)-c2ccccc2)c3nc4ccccc4s3</chem>       | 13.000 | 14 | 76    | 7.81 |
| <br><chem>O=S(=O)(c1ccc(cc1)-c2nc3ccccc3o2)c3nc4ccccc4s3</chem> | 13.000 | 14 | 83    | 6.27 |
| <br><chem>O=C(NCc1ccc(cc1)-c2ccccc2)c3c(O)c(=S)cc(O)c3</chem>  | 13.900 | 19 | AM-2S | 6.28 |

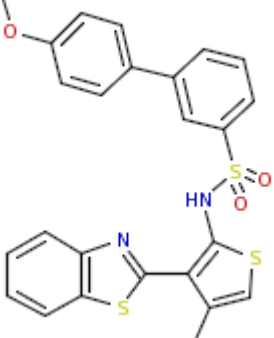
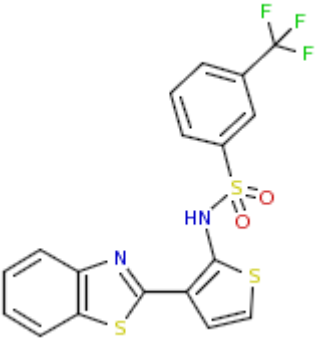
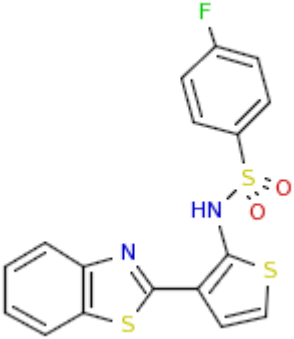
|   |        |    |    |      |
|---|--------|----|----|------|
|    | 14.000 | 14 | 16 | 8.00 |
|   | 14.000 | 14 | 73 | 6.92 |
|  | 14.000 | 14 | 98 | 7.40 |

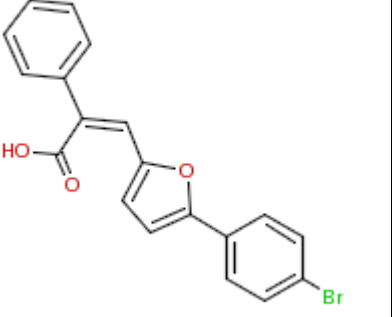
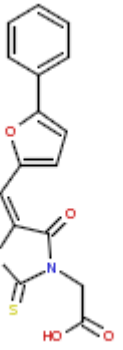
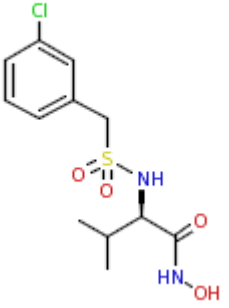


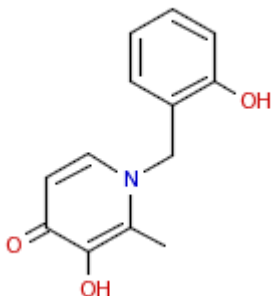
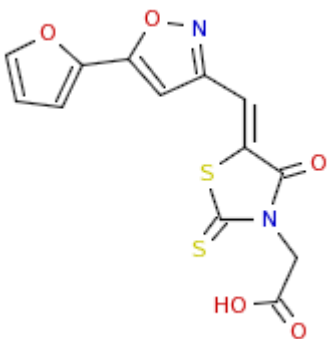
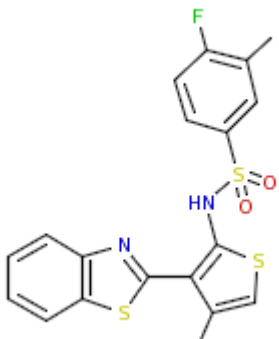
|  |        |    |    |      |
|--|--------|----|----|------|
|  <chem>N#CC1=NC(=C(N)C=C1)/C=C/C2=CC(=C(O2))C3=CC=CC=C3</chem>              | 14.800 | 12 | 19 | 5.27 |
| Chiral<br> <chem>NC(=N)N[C@@H]1C[C@H](NC(=N)N)[C@@H](O)[C@H]1NC(=N)N</chem> | 14.900 | 4  | 8a | 9.38 |
|  <chem>CCCCCCCCC/C=C\CCCCCCCC(=O)NCC1=CC=C(O)C=C1</chem>                  | 15.000 | 18 | 1  | 9.78 |

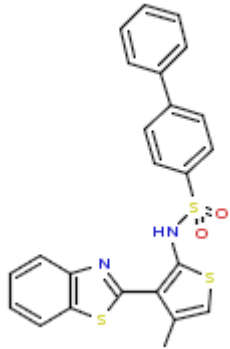
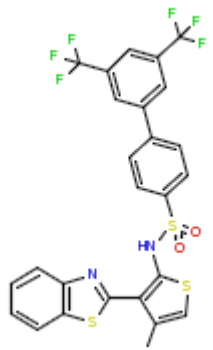
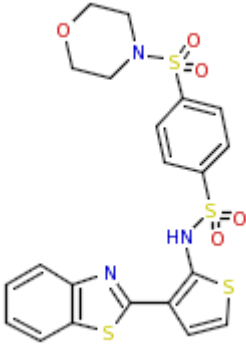
|   |        |    |    |       |
|---|--------|----|----|-------|
|  <chem>Oc1ccc(O)cc1NC(=O)CCCCCCCC/C=C\CCCCCCCC</chem>            | 15.000 | 20 | 5  | 11.56 |
|  <chem>Clc1cc(Cl)c(Cl)cc1NS(=O)(=O)c2sc3c(c2)sc4ccccc4n3</chem> | 15.000 | 14 | 22 | 5.92  |
|  <chem>Clc1ccc(cc1)NS(=O)(=O)c2sc3c(c2)sc4ccccc4n3</chem>      | 15.000 | 14 | 5  | 6.46  |

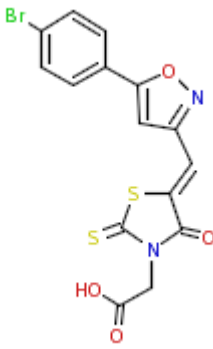
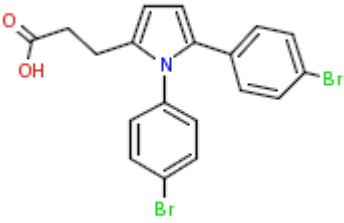
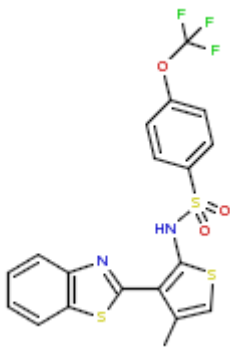
|  |        |    |          |      |
|--|--------|----|----------|------|
| <br><chem>Cc1cc(C)n(c1)C(=O)O</chem>  | 15.000 | 12 | 59       | 5.13 |
| <br><chem>COC1=CC=C(C=C1N)NS(=O)(=O)Nc2ccc(NC(=O)c3ccccc3)cc2</chem>       | 15.300 | 12 | Table2_6 | 8.24 |
| Chiral<br><br><chem>CSCC[C@H](C(=O)O)NC(=O)c1cc2oc(C)c2cc1c3ccccc3</chem> | 15.900 | 12 | 20       | 6.51 |

|   |        |    |    |      |
|---|--------|----|----|------|
| <br><chem>COc1ccc(cc1)-c2ccc(cc2)NS(=O)(=O)c3sc4c(c3)sc5ccccc45</chem> | 16.000 | 14 | 38 | 7.09 |
| <br><chem>Cc1ccc(cc1)S(=O)(=O)Nc2sc3c(c2)sc4ccccc34</chem>            | 16.000 | 14 | 44 | 7.10 |
| <br><chem>Fc1ccc(cc1)NS(=O)(=O)c2sc3c(c2)sc4ccccc34</chem>           | 16.000 | 14 | 49 | 6.56 |

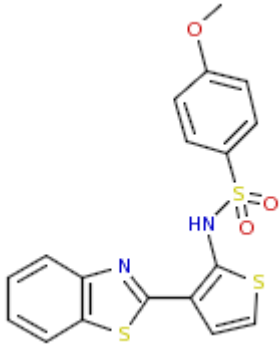
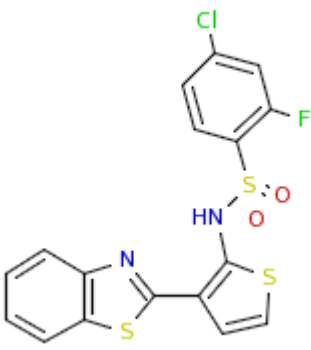
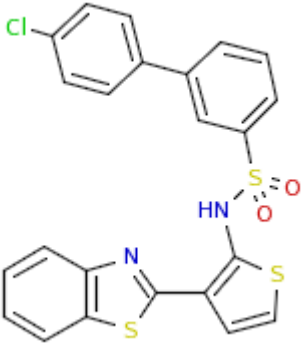
|  |        |    |    |      |
|--|--------|----|----|------|
| <br><chem>O=C(O)C=C1C=C(C=C1)Oc2ccc(Br)cc2</chem>                     | 16.500 | 12 | 21 | 6.54 |
| <br><chem>O=C(O)CN1C(=O)C=C1S2C=CC(=C2)C3=CC=CC=C3</chem>            | 16.600 | 10 | 26 | 7.80 |
| Chiral<br><br><chem>CC(C)C(C(=O)O)N(S(=O)(=O)Cc1ccc(Cl)cc1)N</chem> | 16.600 | 3  | 20 | 9.67 |

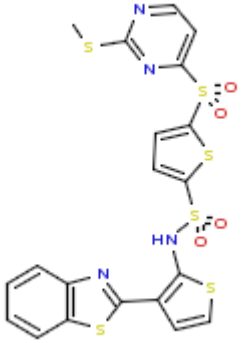
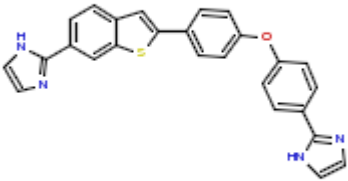
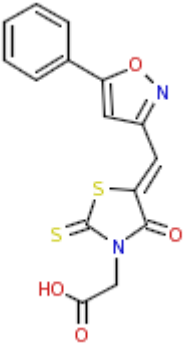
|   |        |    |      |      |
|---|--------|----|------|------|
| <p>Chiral</p>  | 17.000 | 17 | 94D8 | 6.81 |
|               | 17.000 | 7  | 20   | 6.27 |
|              | 17.000 | 14 | 20   | 6.51 |

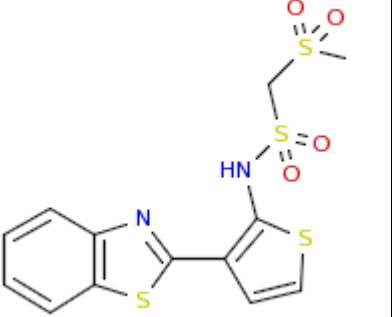
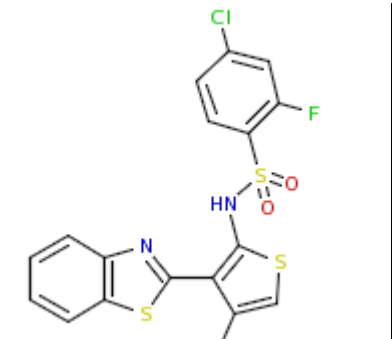
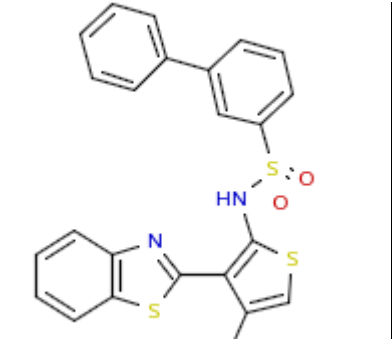
|   |        |    |    |      |
|---|--------|----|----|------|
|    | 17.000 | 14 | 35 | 7.53 |
|   | 17.000 | 14 | 40 | 6.92 |
|  | 17.000 | 14 | 87 | 7.81 |

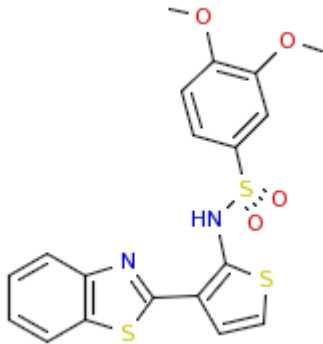
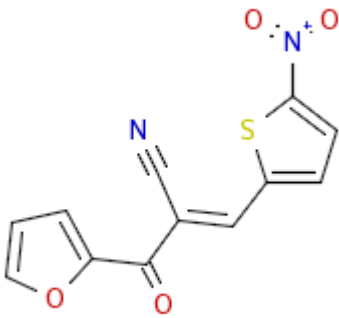
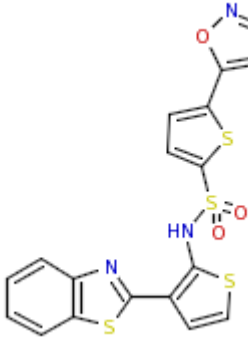
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|--|--------|----|----|------|
|  <chem>CC(=O)N1C(=O)S(=S)C1=C/C=C/C2=CC(=C(C=C2)Br)OC3=CN=C3</chem>             | 17.300 | 7  | 26 | 6.43 |
|  <chem>CC(=O)OCC1=C(C=C2C(=CN1)C=C2C3=CC=CC=C3Br)C4=CC=CC=C4Br</chem>           | 17.700 | 12 | 60 | 6.79 |
|  <chem>COc1ccc(cc1)S(=O)(=O)NC2=C(C=C3SC=C3)SC2c4c5ccccc45n6c7ccccc7s6</chem> | 18.000 | 14 | 12 | 7.12 |

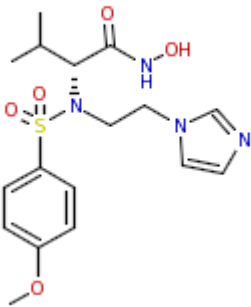
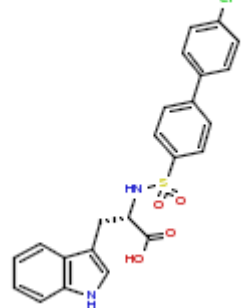
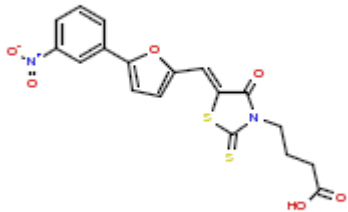


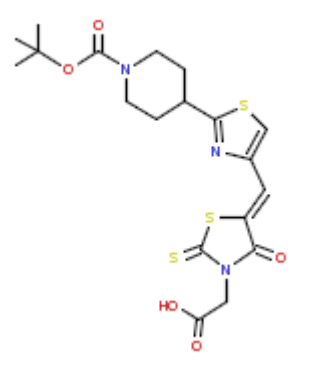
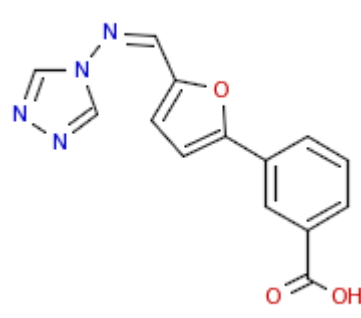
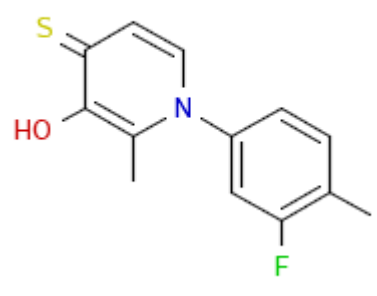
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|---|--------|----|----|------|
| <br><chem>COc1ccc(cc1)S(=O)(=O)Nc2sc(C3=NC4=CC=CC=C4S3)c5ccsc5</chem>              | 18.000 | 14 | 47 | 6.23 |
| <br><chem>Fc1cc(Cl)ccc1S(=O)(=O)Nc2sc(C3=NC4=CC=CC=C4S3)c5ccsc5</chem>            | 18.000 | 14 | 52 | 6.40 |
| <br><chem>Clc1ccc(cc1)-c2ccc(cc2)S(=O)(=O)Nc3sc(C4=NC5=CC=CC=C5S4)c6ccsc6</chem> | 18.000 | 14 | 74 | 7.93 |

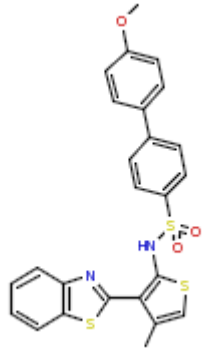
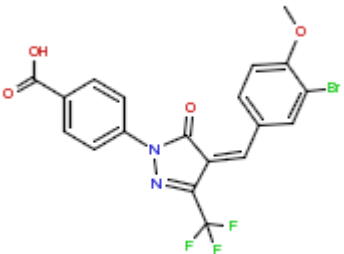
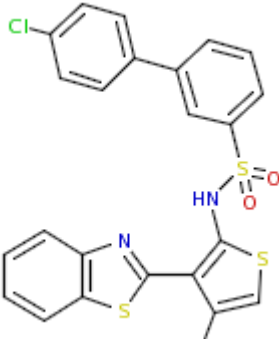
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|---|--------|----|-----|------|
|    | 18.000 | 14 | 99  | 8.80 |
|    | 18.000 | 21 | 25a | 6.95 |
|  | 18.700 | 7  | 21  | 6.48 |

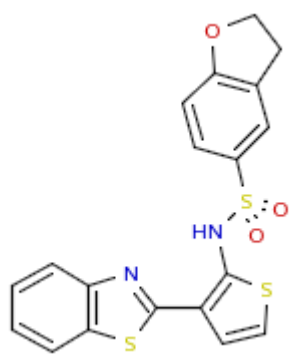
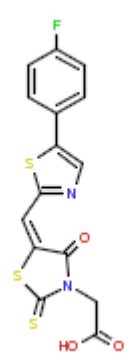
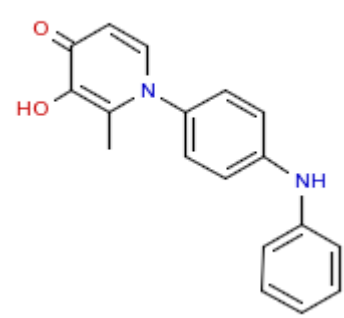
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|--|--------|----|-----|------|
|  <chem>CS(=O)NC1=CC=C2C=C(C1)S=C2c3sc4ccccc4n3</chem>                     | 19.000 | 14 | 101 | 6.57 |
|  <chem>Fc1ccc(Cl)cc1S(=O)(=O)Nc2cc3c(csc23)c4sc5ccccc5n4</chem>          | 19.000 | 14 | 18  | 6.30 |
|  <chem>c1ccc(cc1)-c2ccc(cc2)S(=O)(=O)Nc3cc4c(csc34)c5sc6ccccc6n5</chem> | 19.000 | 14 | 41  | 8.31 |

|   |        |    |    |      |
|---|--------|----|----|------|
|    | 19.000 | 14 | 58 | 6.37 |
|   | 19.000 | 14 | 6  | 5.15 |
|  | 19.000 | 14 | 97 | 8.22 |

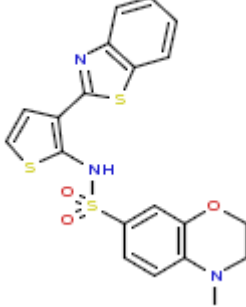
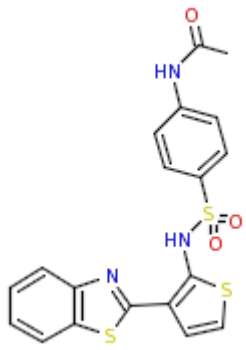
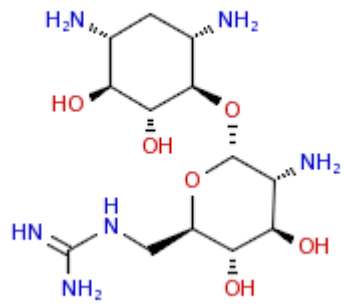
|   |        |   |    |      |
|---|--------|---|----|------|
| <p>Chiral</p>  <chem>CC(C)CC(=O)NO.NC1=CC=CC=C1C1=CC=C(C=C1)S(=O)(=O)N1CCN2C=CN=C21</chem> | 19.100 | 3 | 9  | 8.08 |
| <p>Chiral</p>  <chem>Clc1ccc(cc1)C1=CC=C(C=C1)S(=O)(=O)N1CCN2C=CC=C21</chem>              | 19.700 | 6 | 16 | 7.98 |
|  <chem>O=C(O)CCN1C=NC(=O)C1=Cc2cc(O)cc(Oc3ccc([N+](=O)[O-])cc3)c2</chem>                 | 20.000 | 8 | 7  | 6.89 |

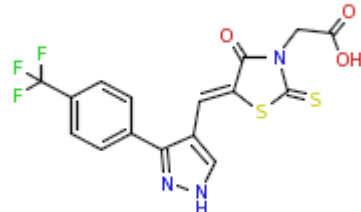
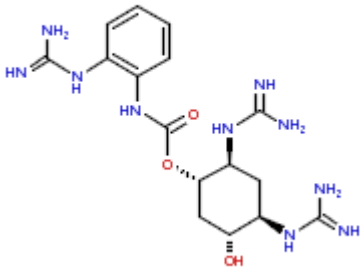
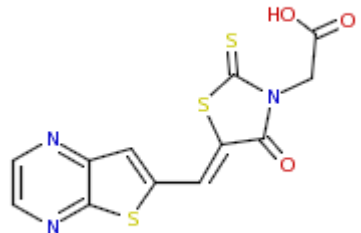
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|---|--------|----|-------|------|
|              | 20.000 | 7  | 18    | 4.40 |
|             | 20.900 | 12 | 22    | 5.77 |
| Chiral<br> | 21.000 | 17 | 94G10 | 6.78 |

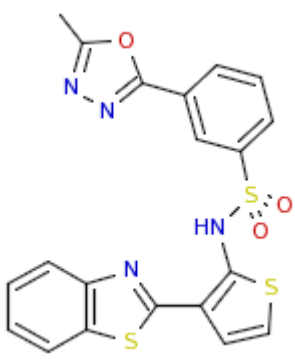
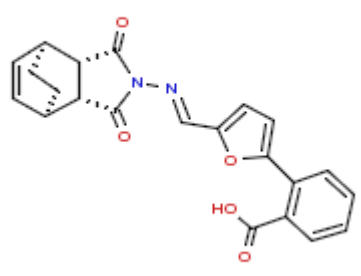
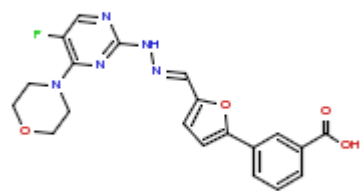
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|---|--------|----|----|------|
|    | 21.000 | 14 | 36 | 8.29 |
|    | 21.300 | 12 | 45 | 5.59 |
|  | 22.000 | 14 | 39 | 8.50 |

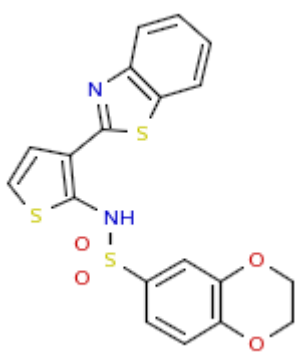
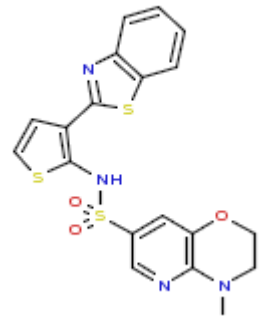
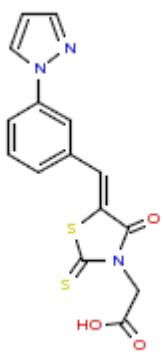
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|---|--------|----|-------|------|
|              | 22.000 | 14 | 90    | 6.49 |
|             | 22.400 | 10 | 27    | 5.82 |
| Chiral<br> | 23.000 | 17 | 94F10 | 8.18 |

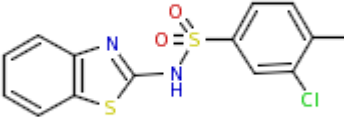
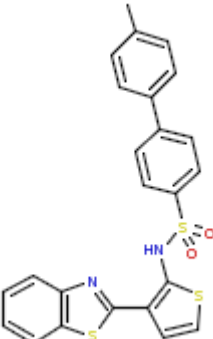
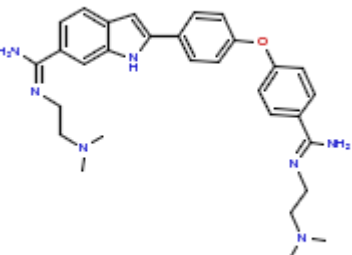


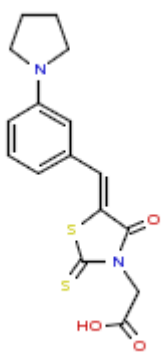
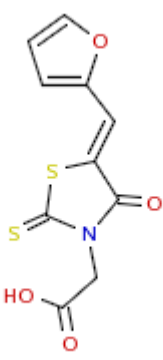
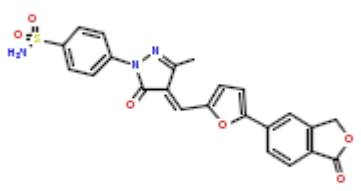
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|---|--------|----|----|------|
| <p>Chiral</p>    | 23.000 | 14 | 95 | 6.02 |
|                 | 24.000 | 14 | 50 | 7.68 |
| <p>Chiral</p>  | 24.300 | 9  | 7  | 7.58 |

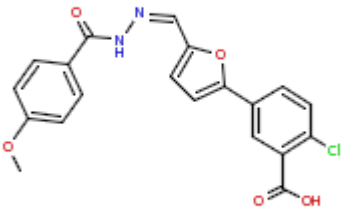
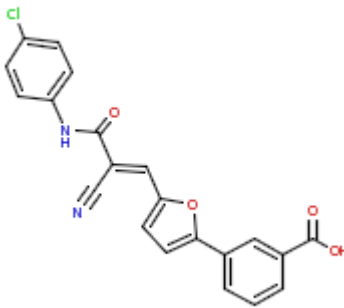
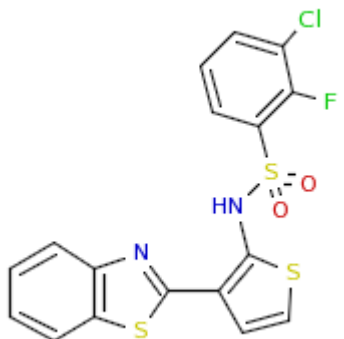
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|---|--------|---|----|------|
| <br><chem>COC(=O)N1C(=O)S=C1C=C2C=CN2c3ccc(C(F)(F)F)cc3</chem>                                   | 24.600 | 7 | 27 | 6.99 |
| Chiral<br><br><chem>NC(=N)N[C@@H]1C[C@@H](O)[C@H](NC(=O)Nc2ccc(NC(=N)N)cc2)[C@H]1NC(=N)N</chem> | 24.800 | 4 | 10 | 8.57 |
| <br><chem>COC(=O)N1C(=O)S=C1C=C2C=C3SC4=CN=CN=C4S3</chem>                                      | 24.900 | 7 | 59 | 5.40 |

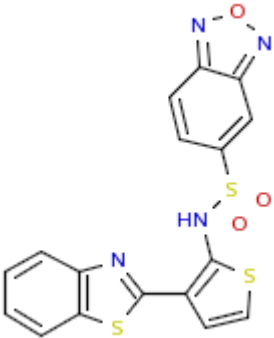
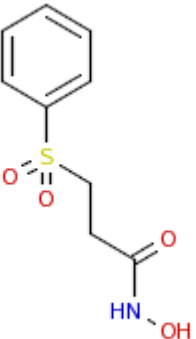
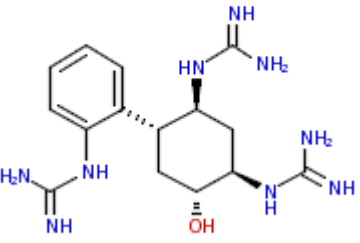
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|--|--------|----|----|------|
|             | 25.000 | 14 | 84 | 6.06 |
| Chiral<br> | 25.600 | 12 | 23 | 6.71 |
|           | 26.600 | 12 | 24 | 6.12 |

|  |        |    |    |      |
|--|--------|----|----|------|
| <br><chem>C1=CC=C2C(=N1)S=C2C3=CC=CC=C3NC(=O)S(=O)(=O)c4ccc5c(c4)OCCO5</chem>               | 27.000 | 14 | 93 | 6.93 |
| Chiral<br><br><chem>C1=CC=C2C(=N1)S=C2C3=CC=CC=C3NC(=O)S(=O)(=O)c4cnc5c(c4)N(C)CCO5</chem> | 27.000 | 14 | 94 | 7.63 |
| <br><chem>OC(=O)CN1C(=O)S=C1S=C2C(=N1)S=C2C3=CC=C(C=C3)C4=CC=CC=C4N5C=CN=C5</chem>        | 27.900 | 7  | 52 | 6.44 |

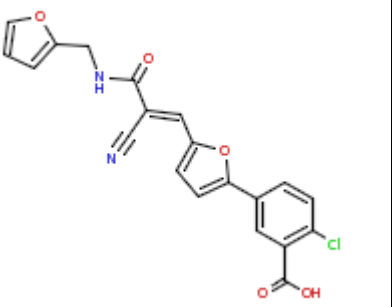
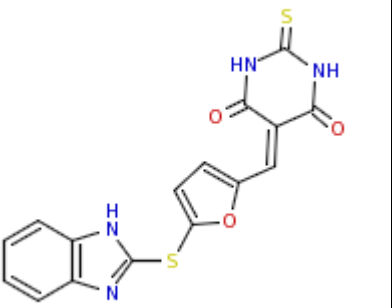
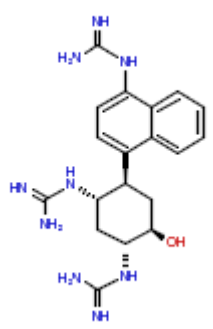
|   |        |    |     |      |
|---|--------|----|-----|------|
| <br><chem>Cc1ccc(Cl)cc1S(=O)(=O)Nc2sc3ccccc3n2</chem>                            | 28.000 | 14 | 102 | 6.52 |
| <br><chem>Cc1ccc(cc1)S(=O)(=O)Nc2sc3ccccc3n2</chem>                             | 28.000 | 14 | 69  | 7.84 |
| <br><chem>CN(C)CCN=Cc1ccc2c(c1)c[nH]2c3ccc(Oc4ccc(NC(=O)CCN(C)C)cc4)cc3</chem> | 28.000 | 21 | 12  | 8.30 |

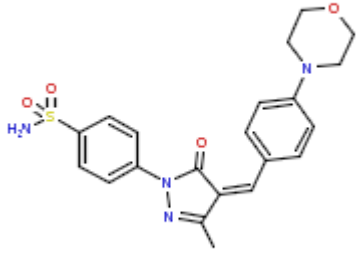
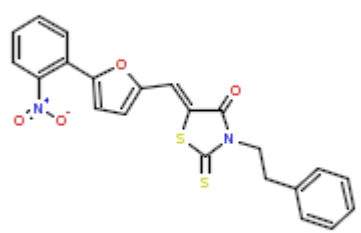
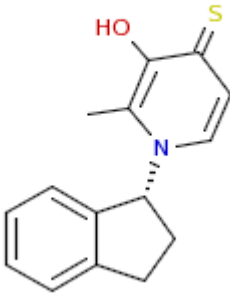
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|---|--------|----|----------|------|
|    | 28.100 | 7  | 50       | 5.27 |
|   | 28.300 | 12 | Table2_3 | 4.78 |
|  | 29.600 | 12 | 52       | 5.19 |


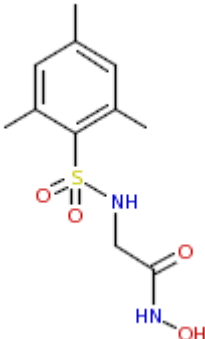
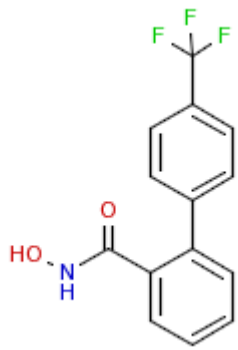
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|---|--------|----|----|------|
|    | 29.700 | 12 | 25 | 6.16 |
|   | 29.900 | 12 | 26 | 5.39 |
|  | 30.000 | 14 | 61 | 6.49 |


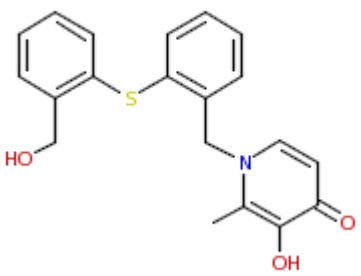
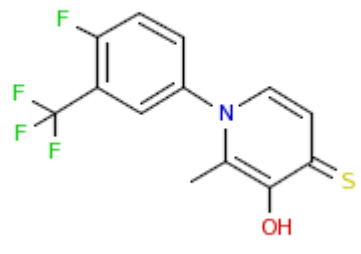
|   |        |    |    |      |
|---|--------|----|----|------|
|              | 30.000 | 14 | 91 | 6.52 |
|             | 30.000 | 6  | 7  | 8.54 |
| Chiral<br> | 30.600 | 4  | 8b | 6.56 |

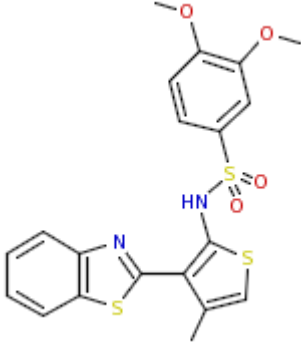
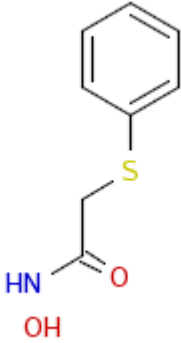
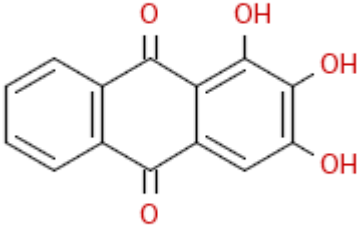


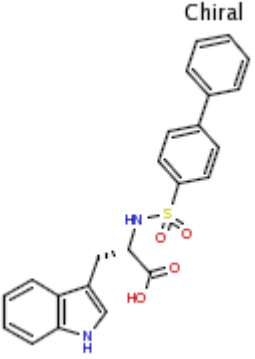
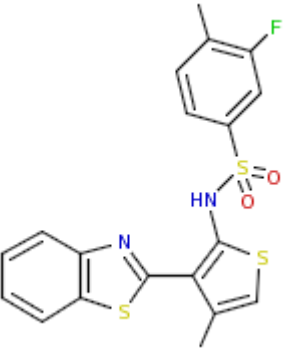
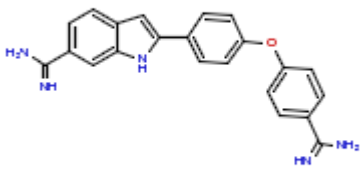
|   |        |    |          |      |
|---|--------|----|----------|------|
|  <chem>Nc1ccoc1C(=O)C(C#N)=Cc2ccoc2-c3ccc(Cl)c(C(=O)O)c3</chem>                      | 30.700 | 12 | 27       | 6.79 |
|  <chem>C1=CN2C(=N1)C=C2Sc3ccoc3C=C4NC(=S)NC4=O</chem>                               | 30.900 | 12 | Table2_5 | 6.55 |
| <p>Chiral</p>  <chem>Nc1cc2c(c1)ccc3ccccc23[C@@H]4C[C@H](O)[C@@H](C(=N)N)C4</chem> | 31.400 | 4  | 8f       | 8.00 |

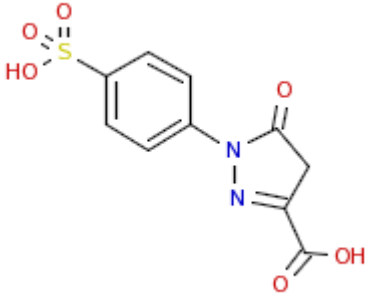
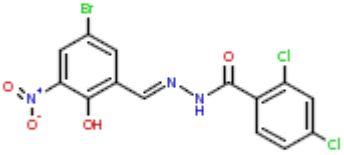
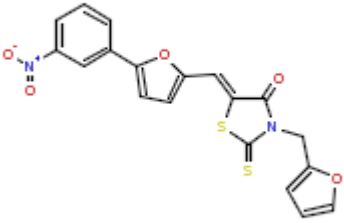
|   |        |    |       |      |
|---|--------|----|-------|------|
|              | 31.700 | 12 | 53    | 5.53 |
|              | 31.900 | 8  | 6     | 5.97 |
| Chiral<br> | 32.000 | 17 | 94F12 | 6.08 |

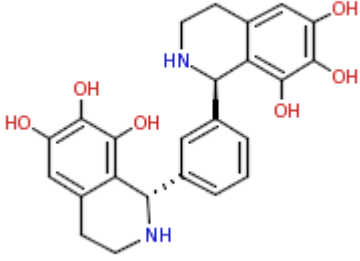
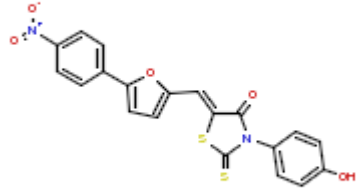
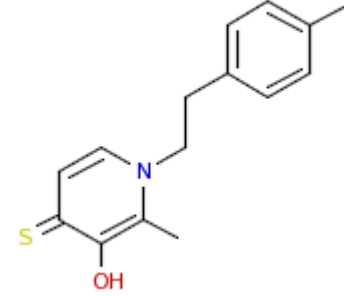
|   |        |    |   |      |
|---|--------|----|---|------|
|    | 32.000 | 18 | 6 | 9.07 |
|   | 32.000 | 6  | 5 | 9.41 |
|  | 32.000 | 6  | 6 | 9.08 |

|   |        |    |          |  |      |
|---|--------|----|----------|--|------|
|              |        |    |          |  |      |
|   | 32.500 | 7  | 48       |  | 5.76 |
| Chiral<br>  |        |    |          |  |      |
|   | 34.000 | 17 | 94B11    |  | 7.93 |
| Chiral<br> |        |    |          |  |      |
|   | 34.000 | 17 | 9.40E+13 |  | 6.38 |

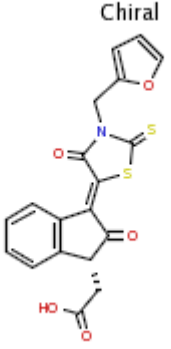
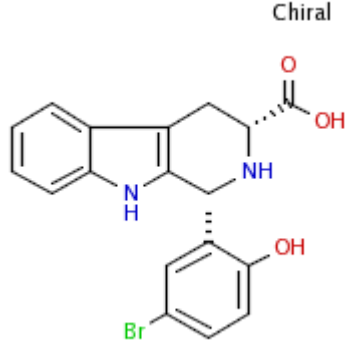
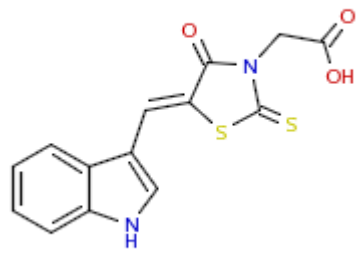
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|---|--------|----|----|------|
|    | 34.000 | 14 | 24 | 7.41 |
|   | 34.000 | 6  | 4  | 7.03 |
|  | 34.000 | 16 | 1  | 6.65 |

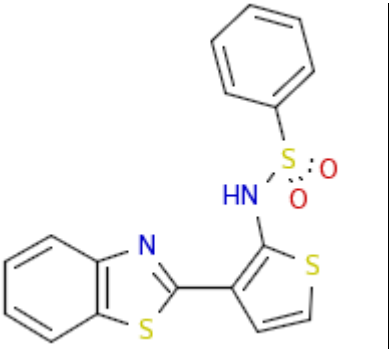
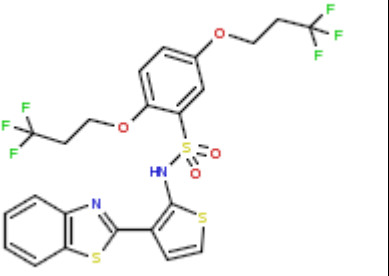
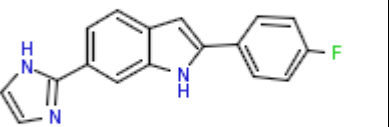
|   |        |    |    |      |
|---|--------|----|----|------|
| <p>Chiral</p>  <chem>O=C(O)CNS(=O)(=O)c1ccc(cc1)-c2ccccc2</chem>     | 34.900 | 6  | 15 | 8.82 |
|  <chem>Cc1cc(C)sc1C2=NC3=CC=CC=C3S2NS(=O)(=O)c4ccc(F)cc4</chem>     | 35.000 | 14 | 19 | 6.62 |
|  <chem>NC(=O)c1ccc2c(c1)c[nH]2-c3ccc(Oc4ccc(NC(=O)N)cc4)cc3</chem> | 35.000 | 21 | 5  | 6.56 |

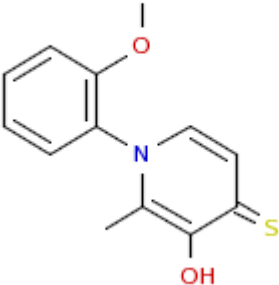
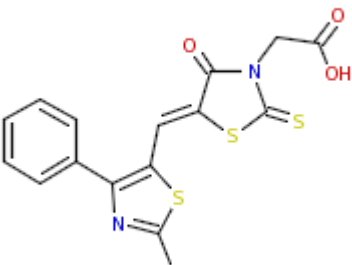
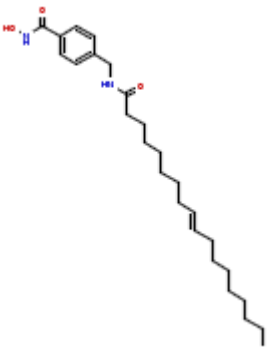
|   |        |    |          |      |
|---|--------|----|----------|------|
|    | 35.200 | 12 | 46       | 6.14 |
|    | 35.500 | 12 | Table2_1 | 5.91 |
|  | 36.300 | 8  | 5        | 6.69 |

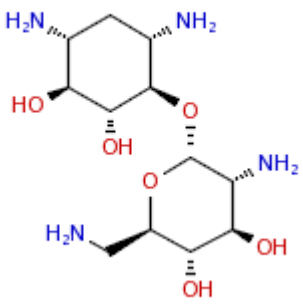
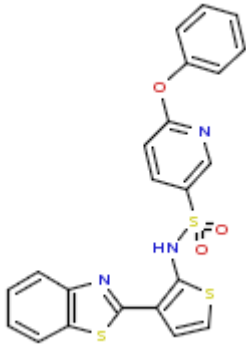
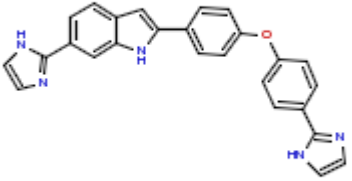
|  |        |    |      |      |
|--|--------|----|------|------|
| <p>Chiral</p>  <p>The structure shows a piperidine ring (blue NH) attached to a 1,2,3,4-tetrahydroquinoline system. The quinoline system has two hydroxyl groups (red OH) at the 6 and 7 positions. The piperidine ring is also substituted with a phenyl ring (dotted bond) and a 2,3,4-trihydroxyphenyl group (solid bond).</p> | 36.700 | 16 | 6a   | 5.72 |
|  <p>The structure features a furan ring connected to a thiophene ring. The thiophene ring is further substituted with a nitro group (red NO2) and a 4-hydroxyphenyl group (red OH).</p>   | 37.700 | 8  | 4    | 5.09 |
| <p>Chiral</p>  <p>The structure shows a thiophene ring (yellow S) substituted with a hydroxyl group (red OH) and a methyl group. It is connected via a piperidine ring (blue N) to a 4-methylphenyl group.</p>  | 38.000 | 17 | 94G8 | 7.23 |

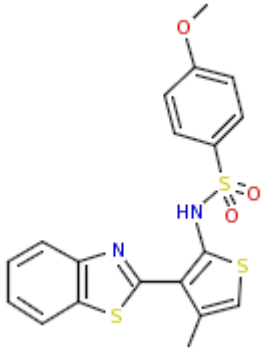
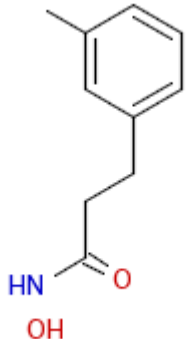
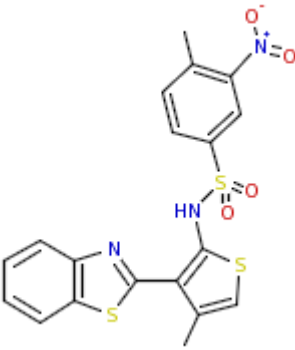


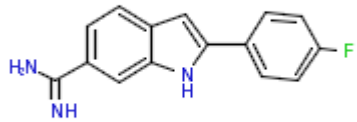
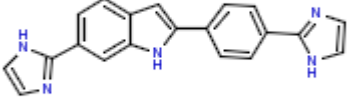
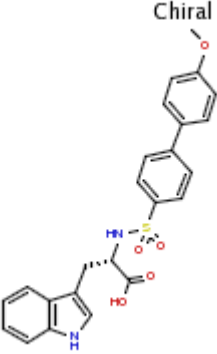
|  |        |    |    |      |
|--|--------|----|----|------|
| <p>Chiral</p>   | 38.000 | 13 | 2  | 5.58 |
| <p>Chiral</p>  | 38.200 | 13 | 1  | 5.80 |
|               | 38.700 | 7  | 60 | 5.19 |

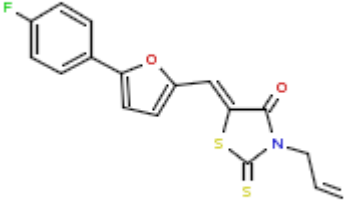
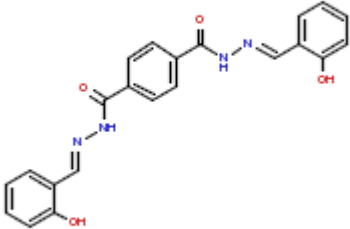
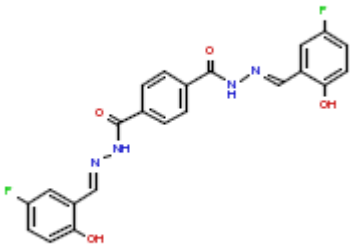
|  |        |    |     |      |
|--|--------|----|-----|------|
|  <chem>O=S(=O)(c1ccccc1)Nc2sc3ccccc3n2-c4ccsc4</chem>               | 39.000 | 14 | 43  | 6.71 |
|  <chem>COc1ccc(OCC(F)(F)F)cc1S(=O)(=O)Nc2sc3ccccc3n2-c4ccsc4</chem> | 39.000 | 14 | 56  | 7.70 |
|  <chem>Fc1ccc(cc1)-c2c[nH]c3ccccc23-c4c[nH]n4</chem>              | 40.000 | 21 | 40c | 7.06 |

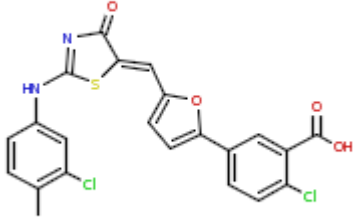
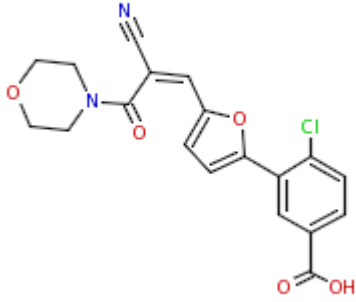
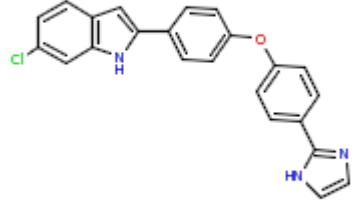
|   |        |    |          |      |
|---|--------|----|----------|------|
| <p>Chiral</p>  | 41.000 | 17 | 9.40E+10 | 4.86 |
|                | 41.000 | 7  | 19       | 7.73 |
|              | 42.000 | 20 | 6        | 9.04 |

|   |        |    |           |      |
|---|--------|----|-----------|------|
| <p>Chiral</p>  <p>The structure shows a complex molecule with two six-membered rings. The top ring is a cyclohexane with two amino groups (H<sub>2</sub>N) and two hydroxyl groups (OH). The bottom ring is a pyranose-like ring with two hydroxyl groups (OH) and one amino group (NH<sub>2</sub>). The rings are connected via an oxygen atom.</p> | 42.900 | 9  | 2_neamine | 8.78 |
|  <p>The structure features a benzothiazole core connected to a thiophene ring. This thiophene ring is further linked to a pyridine ring, which is substituted with a phenoxy group and a sulfonamide group (NH-SO<sub>2</sub>-O-Ph).</p>  | 43.000 | 14 | 81        | 7.67 |
|  <p>The structure features a benzimidazole core connected to a thiophene ring. This thiophene ring is further linked to a pyridine ring, which is substituted with a phenoxy group and another pyridine ring.</p>  | 43.000 | 21 | 13        | 6.26 |

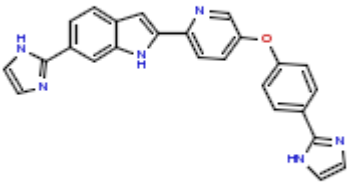
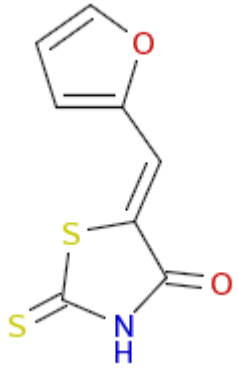
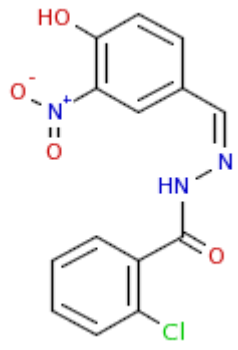
|  |        |    |    |      |
|--|--------|----|----|------|
| <br><chem>COc1ccc(cc1)S(=O)(=O)NC2=C(C)SC=C2C3=NC4=CC=CC=C4S3</chem>              | 46.000 | 14 | 13 | 7.00 |
| <br><chem>CC1=CC=C(C=C1)CCC(=O)N</chem>  | 47.000 | 6  | 3  | 7.30 |
| <br><chem>Cc1ccc(cc1)[N+](=O)[O-]S(=O)(=O)NC2=C(C)SC=C2C3=NC4=CC=CC=C4S3</chem> | 48.000 | 14 | 29 | 7.12 |

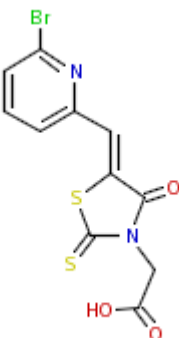
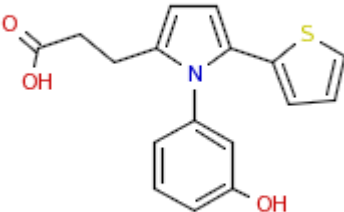
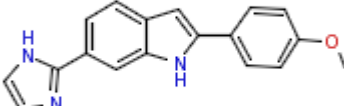
|   |        |    |     |      |
|---|--------|----|-----|------|
| <br><chem>NC(=O)c1ccc2c(c1)c(c[nH]2)C3=CC=C(C=C3)F</chem>                            | 48.000 | 21 | 40b | 6.29 |
| <br><chem>NC(=O)c1ccc2c(c1)c(c[nH]2)C3=CN=CN3</chem>                                 | 49.000 | 21 | 44a | 5.75 |
| <br><chem>COC1=CC=C(C=C1)S(=O)(=O)N[C@@H](C(=O)O)c2c[nH]c3ccccc23</chem><br>Chiral | 49.100 | 6  | 17  | 9.27 |

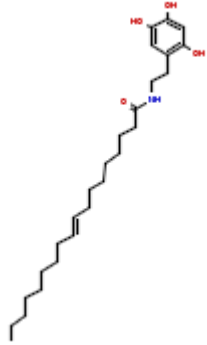
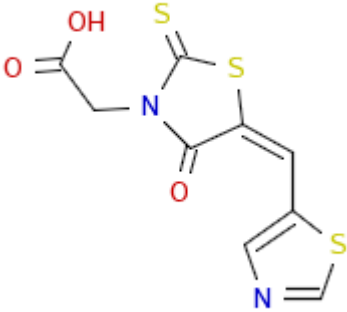
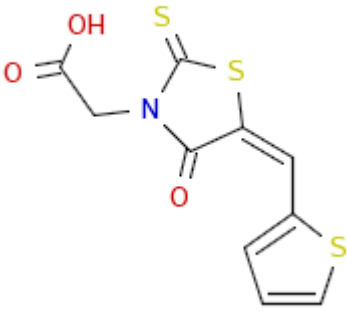
|   |        |    |    |      |
|---|--------|----|----|------|
|    | 50.000 | 8  | 3  | 4.48 |
|    | 50.000 | 22 | 3h | 8.25 |
|  | 50.000 | 22 | 7h | 7.98 |

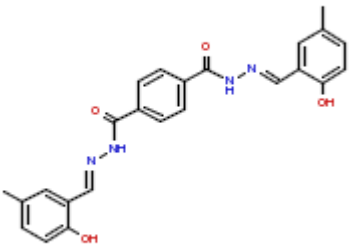
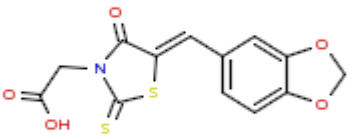
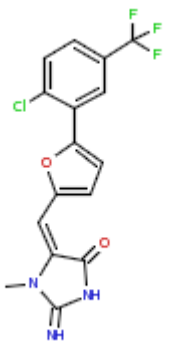
|   |        |    |    |      |
|---|--------|----|----|------|
|    | 50.000 | 12 | 29 | 6.71 |
|   | 50.000 | 12 | 30 | 4.89 |
|  | 51.000 | 21 | 32 | 6.41 |

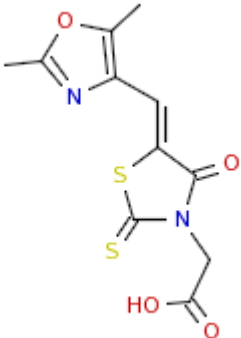
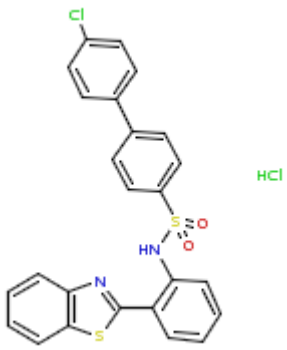
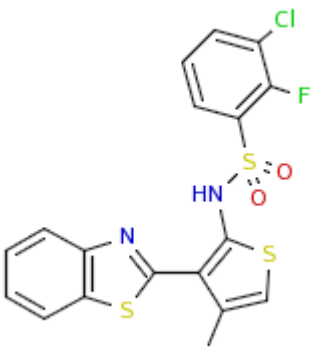


|   |        |    |          |      |
|---|--------|----|----------|------|
|    | 55.000 | 21 | 24a      | 5.45 |
|   | 56.400 | 12 | Table2_4 | 3.23 |
|  | 56.900 | 12 | Table2_2 | 6.09 |

|   |        |    |     |      |
|---|--------|----|-----|------|
|  <p>Chemical structure of a brominated thiazolidine derivative. It features a thiazolidine ring with a carbonyl group at the 2-position and a carboxylic acid group at the 4-position. The 5-position is substituted with a vinyl group, which is further substituted with a 4-bromophenyl ring.</p>               | 58.000 | 7  | 56  | 5.58 |
|  <p>Chemical structure of a thiazolidine derivative. It features a thiazolidine ring with a carbonyl group at the 2-position and a carboxylic acid group at the 4-position. The 5-position is substituted with a vinyl group, which is further substituted with a 4-hydroxyphenyl ring and a thiophene ring.</p>   | 60.000 | 12 | 61  | 8.62 |
|  <p>Chemical structure of a thiazolidine derivative. It features a thiazolidine ring with a carbonyl group at the 2-position and a carboxylic acid group at the 4-position. The 5-position is substituted with a vinyl group, which is further substituted with a 4-methoxyphenyl ring and a thiophene ring.</p> | 61.000 | 21 | 43c | 7.38 |

|   |        |    |    |      |
|---|--------|----|----|------|
|    | 70.000 | 17 | 5  | 9.55 |
|   | 72.400 | 10 | 13 | 6.05 |
|  | 79.400 | 10 | 10 | 5.75 |

|  |         |    |    |      |
|--|---------|----|----|------|
|  <p>The structure shows a central benzene ring with a carbonyl group at the top. This carbonyl is linked via a hydrazone bridge (-NH-N=) to a phenol ring (with an -OH group at the para position). The other side of the carbonyl is linked via another hydrazone bridge (-NH-N=) to another phenol ring (with an -OH group at the para position).</p> | 80.000  | 22 | 2h | 8.63 |
|  <p>The structure features a thiazolidine ring system. One nitrogen atom is substituted with a propionic acid chain (-CH2-CH2-COOH). The sulfur atom is double-bonded to a carbon atom, which is also double-bonded to a phenyl ring. This phenyl ring is further substituted with a 1,3-dioxolane ring.</p>  | 83.300  | 7  | 53 | 5.67 |
|  <p>The structure shows a thiazolidine ring system with a methyl group on one nitrogen and a carbonyl group on the other. It is connected via a double bond to a furan ring. The furan ring is further connected to a benzene ring that has a chlorine atom and a trifluoromethyl group (-CF3) at the para position.</p>                              | 100.000 | 10 | 19 | 5.95 |

|   |         |    |     |      |
|---|---------|----|-----|------|
|    | 100.000 | 7  | 17  | 6.01 |
|   | 100.000 | 14 | 112 | 8.03 |
|  | 100.000 | 14 | 27  | 6.33 |

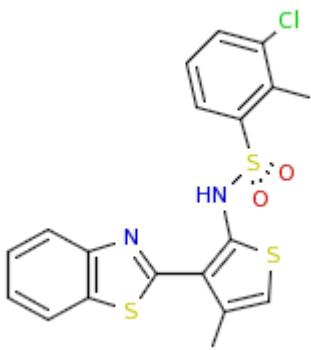
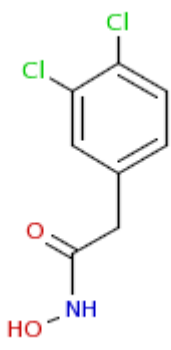
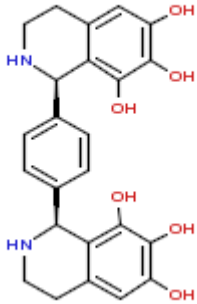
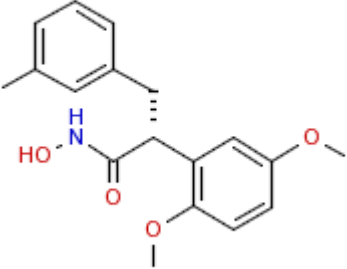
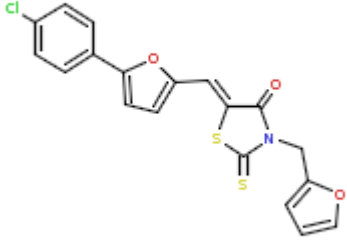
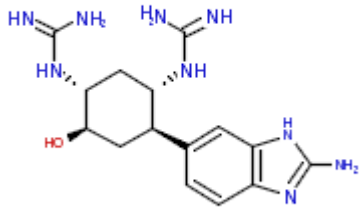
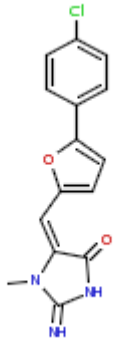
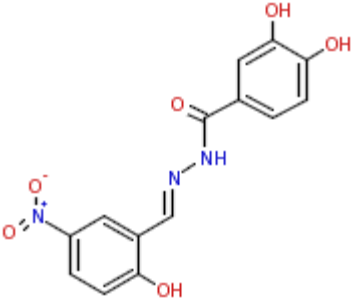
|   |         |    |    |      |
|---|---------|----|----|------|
| <br><chem>Cc1cc(C2=NC3=CC=CC=C3S2)sc1NS(=O)(=O)c4cc(Cl)cc(Cl)c4</chem> | 100.000 | 14 | 28 | 6.85 |
| <br><chem>NC(=O)Cc1cc(Cl)cc(Cl)c1</chem>                              | 100.000 | 6  | 20 | 6.29 |

Table S3. Structures, LF biological activities, references, compound designators, and docking scores for screening set compounds in dataset **DB1C**.

| Structure  | LF IC <sub>50</sub><br>or K <sub>i</sub><br>(μM) | Reference | Compound<br>Designator | Docking Score<br>(Surflex-Dock) |
|--|--|-----------|------------------------|---------------------------------|
| <p style="text-align: center;">Chiral</p>   | 123.8  | 16        | 7a                     | 5.95                            |
| <p style="text-align: center;">Chiral</p>  | 130.0  | 6         | 23                     | 9.83                            |
|   | 150.0  | 8         | 2                      | 4.91                            |

|  |       |    |    |      |
|--|-------|----|----|------|
| <p>Chiral</p>  <chem>NC(=N)N[C@H]1CC[C@@H](C2=CC=C3N=C(N)N=C32)C[C@@H]1O</chem> | 153.7 | 4  | 8h | 8.09 |
|  <chem>CN1C=NC2=C1NC(=O)N2C=C3OC=CC3c4ccc(Cl)cc4</chem>                        | 200.0 | 10 | 18 | 5.08 |
|  <chem>O=C(NC(=O)c1ccc(O)c(O)c1)N=NC=C2C=CC(=C2)[N+](=O)[O-]</chem>           | 200.0 | 22 | 1a | 7.69 |



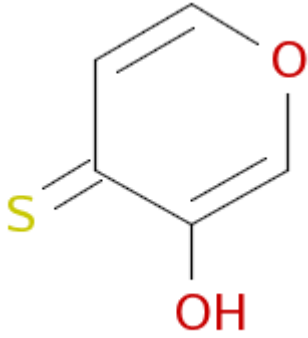
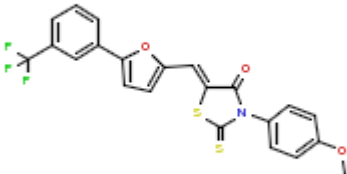
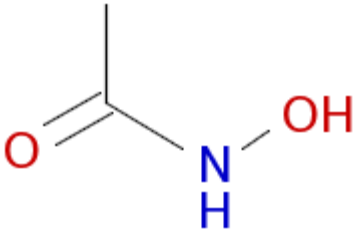
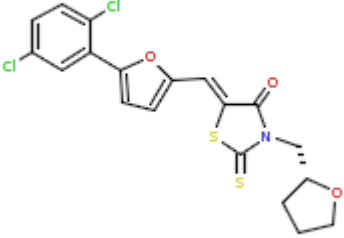
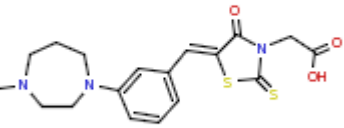
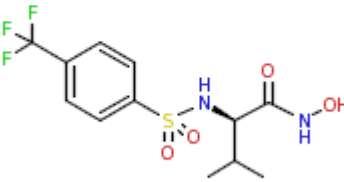
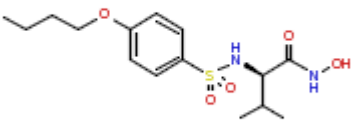
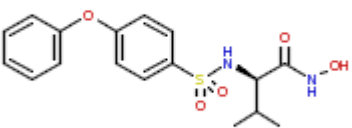
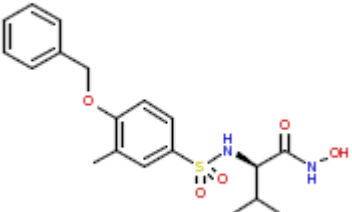
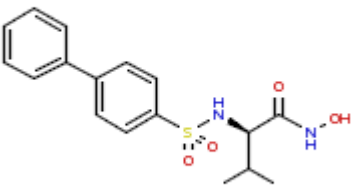
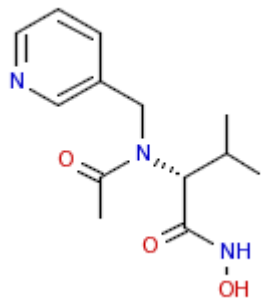
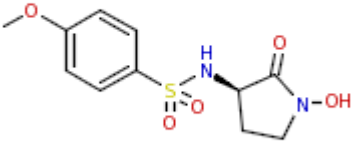
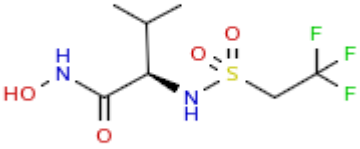
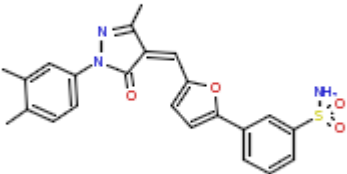
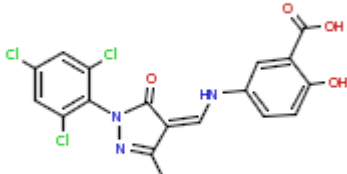
|   |         |    |    |      |
|---|---------|----|----|------|
|  <chem>O=C1C=CC(O)O1=S</chem>  | 204.0   | 23 | 2d | 4.65 |
|  <chem>COc1ccc(N2C(=O)C(=S)N2C=C3C=C(O4C=CC(=C4)C(F)(F)F)O3)cc1</chem> | 300.0   | 8  | 1  | 5.29 |
|  <chem>CC(=O)NO</chem>   | 11400.0 | 23 | 1g | 4.72 |

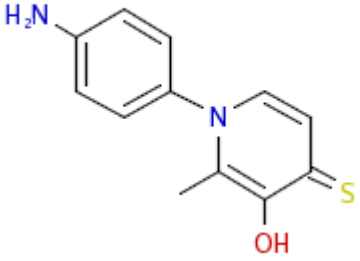
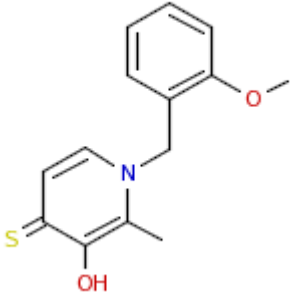
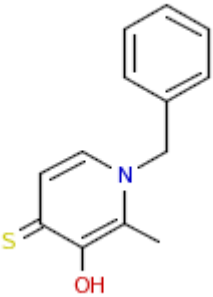
Table S4. Structures, LF biological activities, references, compound designators, and docking scores for screening set compounds in dataset **DB1D**.

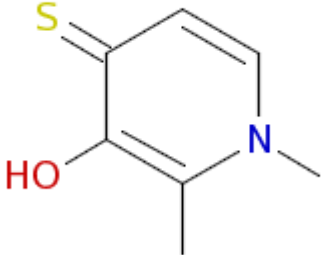
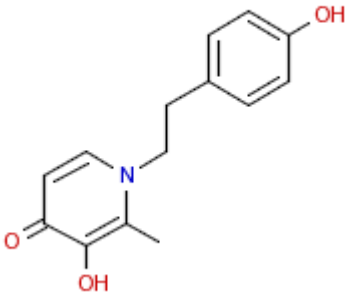
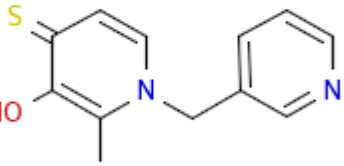
| Structure   | LF IC <sub>50</sub><br>or K <sub>i</sub><br>( $\mu$ M) | Reference | Compound<br>Designator | Docking Score<br>(Surflex-Dock) |
|---|--|-----------|------------------------|---------------------------------|
| <p>Chiral</p>    | >25  | 7         | 16                     | 5.55                            |
| <p>Chiral</p>  | >25  | 7         | 51                     | 7.45                            |
| <p>Chiral</p>  | >40  | 3         | 17                     | 9.92                            |

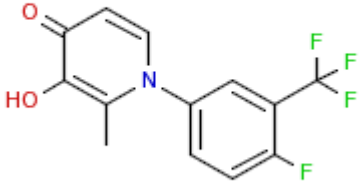
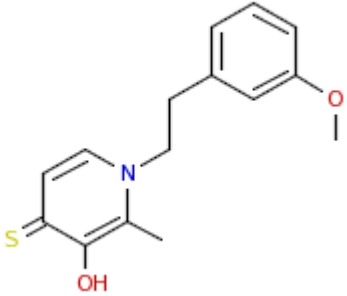
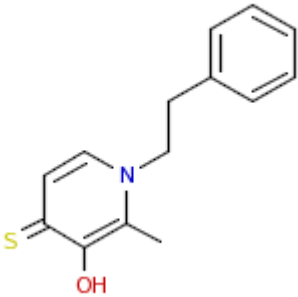
|  |     |   |    |       |
|--|-----|---|----|-------|
| <p>Chiral</p>  <p>The structure shows a central chiral carbon atom bonded to a hydrogen atom (wedge), an isopropyl group (dash), a sulfonamide group (-SO<sub>2</sub>NH-), and a carbonyl group (-C(=O)NH-OH). The sulfonamide group is attached to a benzene ring with a propyl ether group (-OCH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>) at the para position.</p> | >40 | 3 | 21 | 11.68 |
| <p>Chiral</p>  <p>The structure is similar to the first one, but the benzene ring is substituted with a phenoxy group (-O-C<sub>6</sub>H<sub>5</sub>) at the para position.</p>   | >40 | 3 | 22 | 9.27  |
| <p>Chiral</p>  <p>The structure is similar to the first one, but the benzene ring is substituted with a benzyl ether group (-OCH<sub>2</sub>-C<sub>6</sub>H<sub>5</sub>) at the para position.</p>  | >40 | 3 | 23 | 10.25 |

|   |     |   |    |      |
|---|-----|---|----|------|
| <p>Chiral</p>  <chem>CC(C)[C@H](NS(=O)(=O)c1ccc(cc1)-c2ccccc2)C(=O)NO</chem> | >40 | 3 | 24 | 9.96 |
| <p>Chiral</p>  <chem>CC(C)[C@H](NC(=O)C)C(=O)NO</chem>                      | >40 | 3 | 3  | 9.35 |
| <p>Chiral</p>  <chem>COc1ccc(cc1)S(=O)(=O)N[C@H]2CCCN2=O</chem>            | >40 | 3 | 5  | 7.42 |

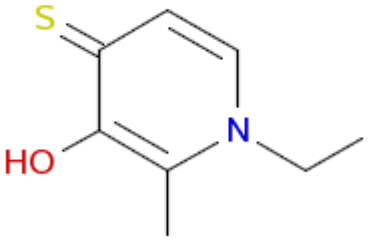
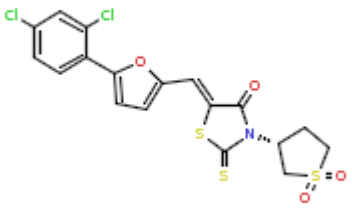
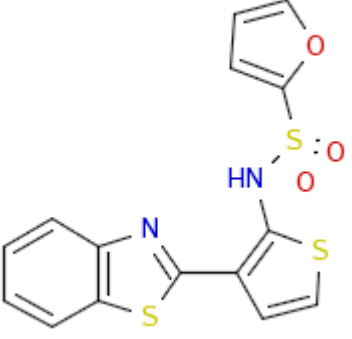
|   |     |    |    |      |
|---|-----|----|----|------|
| <p>Chiral</p>  <chem>CC(C)C(C(=O)O)NS(=O)(=O)CC(F)(F)F</chem>                    | >40 | 3  | 6  | 8.26 |
|  <chem>CC1=CN2C(=O)N(C1)c3ccc(C)cc3C=C4OC(=C4)c5ccc(S(=O)(=O)N)cc5</chem>        | >45 | 12 | 38 | 5.84 |
|  <chem>CC1=CN2C(=O)N(C1)c3ccc(Cl)c(Cl)c3C=C4OC(=C4)Nc5ccc(O)c(C(=O)O)c5</chem> | >45 | 12 | 47 | 6.23 |

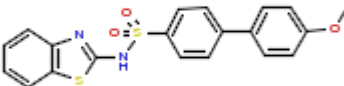
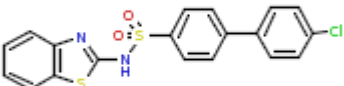
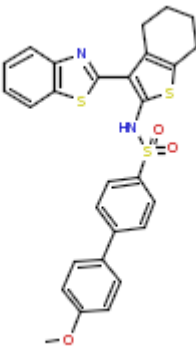
|   |     |    |      |      |
|---|-----|----|------|------|
| <p>Chiral</p>  <chem>Nc1ccc(cc1)N2C=CC(=S)C(O)=C2C</chem>    | >50 | 17 | 94C7 | 6.34 |
| <p>Chiral</p>  <chem>COc1cccc(c1)CN2C=CC(=S)C(O)=C2C</chem> | >50 | 17 | 94F5 | 6.01 |
| <p>Chiral</p>  <chem>c1ccccc1CN2C=CC(=S)C(O)=C2C</chem>    | >50 | 17 | 94F9 | 6.21 |

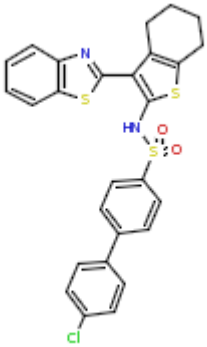
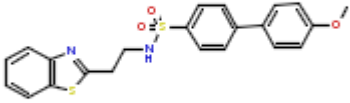
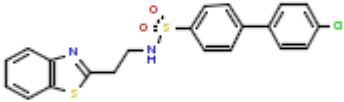
|   |     |    |       |      |
|---|-----|----|-------|------|
| <p>Chiral</p>    | >50 | 17 | 94G11 | 5.52 |
| <p>Chiral</p>   | >50 | 17 | 94G12 | 7.31 |
| <p>Chiral</p>  | >50 | 17 | 94G4  | 6.25 |

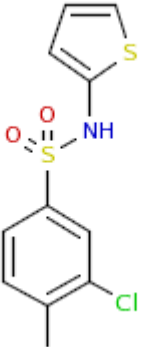
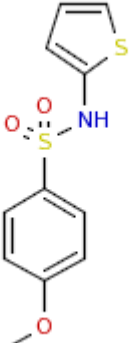
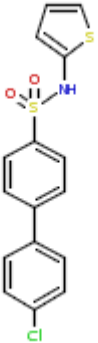
|   |     |    |      |      |
|---|-----|----|------|------|
| <p>Chiral</p>    | >50 | 17 | 94G6 | 6.06 |
| <p>Chiral</p>   | >50 | 17 | 94G7 | 8.84 |
| <p>Chiral</p>  | >50 | 17 | 94H2 | 7.18 |

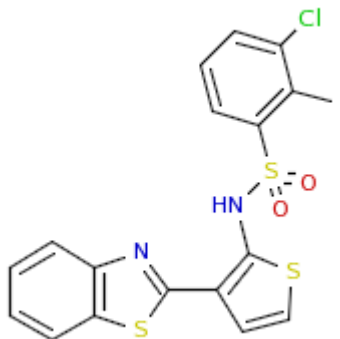
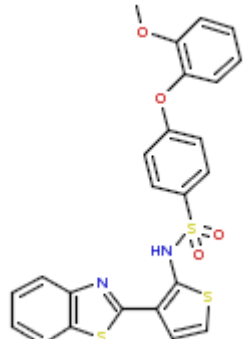
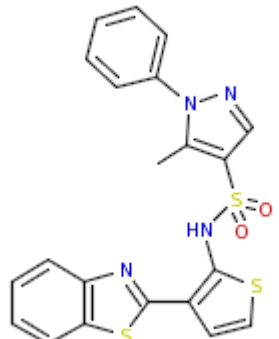


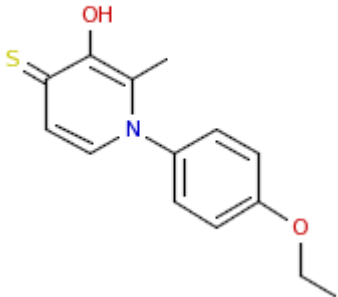
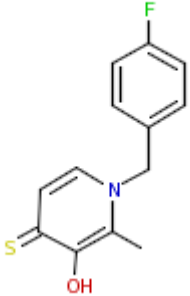
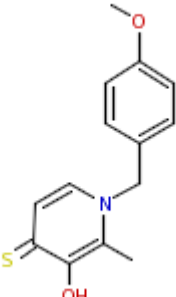
|   |     |    |      |      |
|---|-----|----|------|------|
| <p>Chiral</p>  | >50 | 17 | 94H3 | 5.56 |
| <p>Chiral</p>  | >50 | 7  | 15   | 4.31 |
|              | >50 | 14 | 100  | 7.55 |

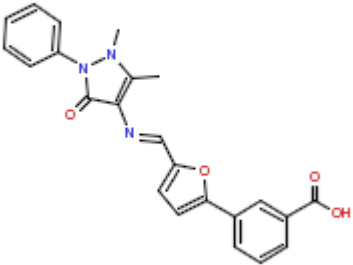
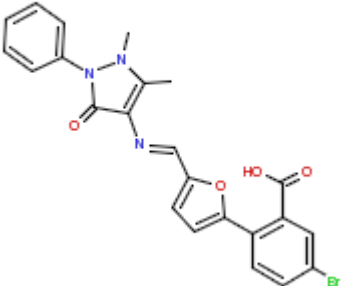
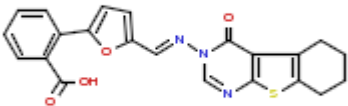
|  |     |    |     |      |
|--|-----|----|-----|------|
| <br><chem>COc1ccc(cc1)-c2ccc(cc2)NS(=O)(=O)c3nc4ccccc4s3</chem>                   | >50 | 14 | 103 | 7.83 |
| <br><chem>Clc1ccc(cc1)-c2ccc(cc2)NS(=O)(=O)c3nc4ccccc4s3</chem>                   | >50 | 14 | 104 | 7.52 |
| <br><chem>COc1ccc(cc1)-c2ccc(cc2)NS(=O)(=O)c3c4c(s3)C5CCCCC5c4n6ccccc6s6</chem> | >50 | 14 | 105 | 8.25 |

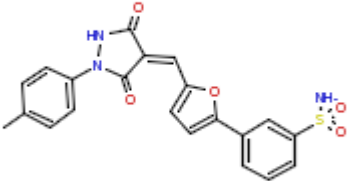
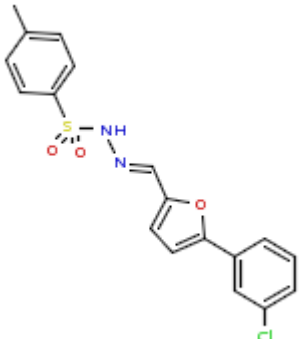
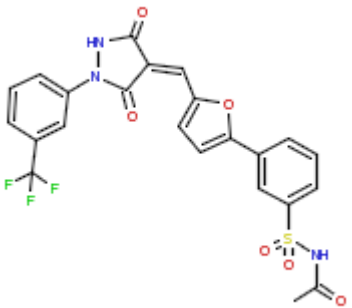
|   |     |    |     |      |
|---|-----|----|-----|------|
| <br><chem>C1=CC=C2C(S1)=NC(=C2)C3=CC=C(C=C3)S(=O)(=O)NCC4=CC=C(C=C4)C5=CC=C(C=C5)Cl</chem> | >50 | 14 | 106 | 7.44 |
| <br><chem>C1=CC=C2C(S1)=NC(=C2)CCN(S(=O)(=O)c3ccc(O)cc3)c4ccc(O)cc4</chem>                 | >50 | 14 | 109 | 7.66 |
| <br><chem>C1=CC=C2C(S1)=NC(=C2)CCN(S(=O)(=O)c3ccc(Cl)cc3)c4ccc(O)cc4</chem>              | >50 | 14 | 110 | 7.87 |

|   |     |    |     |      |
|---|-----|----|-----|------|
| <br><chem>Clc1ccc(cc1)S(=O)(=O)N=C2C=CC=S2</chem>                | >50 | 14 | 113 | 6.09 |
| <br><chem>COC1=CC=C(C=C1)S(=O)(=O)N=C2C=CC=S2</chem>            | >50 | 14 | 114 | 4.97 |
| <br><chem>Clc1ccc(cc1)C2=CC=C(C=C2)S(=O)(=O)N=C3C=CC=S3</chem> | >50 | 14 | 115 | 6.37 |

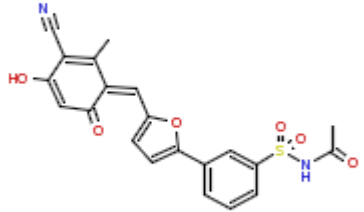
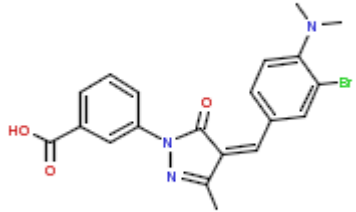
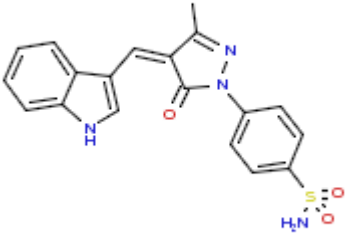
|   |     |    |    |      |
|---|-----|----|----|------|
|  <chem>Cc1ccc(Cl)cc1S(=O)(=O)Nc2sc3ccccc3n2</chem>               | >50 | 14 | 62 | 6.68 |
|  <chem>COC1=CC=C(OC)C=C1S(=O)(=O)Nc2sc3ccccc3n2</chem>          | >50 | 14 | 80 | 8.45 |
|  <chem>Cc1cc2c(c1)nn(C2)c3ccccc3S(=O)(=O)Nc4sc5ccccc5n4</chem> | >50 | 14 | 86 | 7.11 |

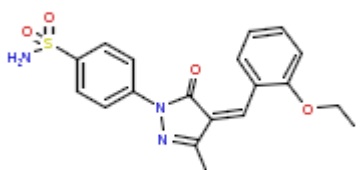
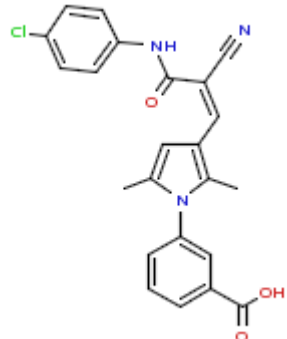
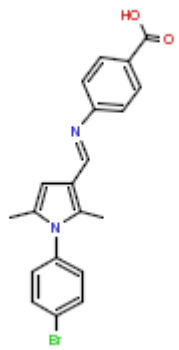
|   |     |   |    |      |
|---|-----|---|----|------|
| <p>Chiral</p>  <chem>CCOC1=CC=C(C=C1)N2C=CC(=O)N(C)C2=O</chem>   | >50 | 6 | 12 | 6.70 |
| <p>Chiral</p>  <chem>Fc1ccc(cc1)CN2C=CC(=O)N(C)C2=O</chem>      | >50 | 6 | 13 | 6.62 |
| <p>Chiral</p>  <chem>COC1=CC=C(C=C1)CN2C=CC(=O)N(C)C2=O</chem> | >50 | 6 | 14 | 6.94 |

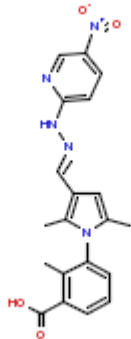
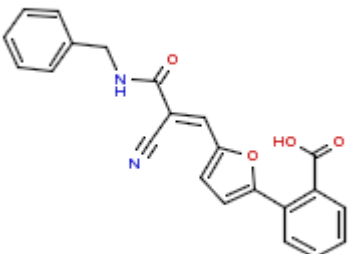
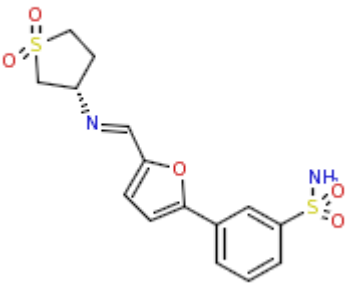
|  |     |    |    |      |
|--|-----|----|----|------|
| <p>Chiral</p>   | >50 | 12 | 31 | 6.68 |
| <p>Chiral</p>  | >50 | 12 | 32 | 6.88 |
|               | >50 | 12 | 33 | 7.75 |

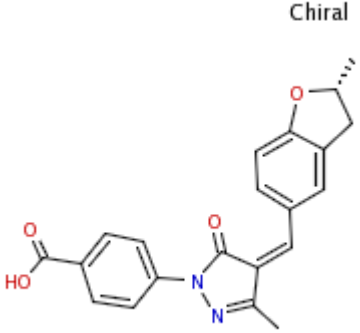
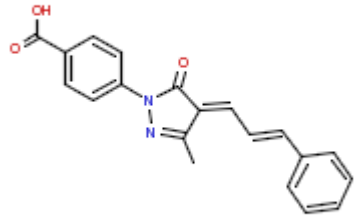
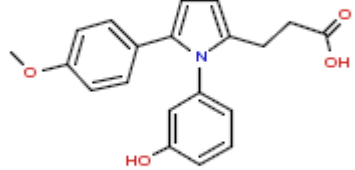
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|---|-----|----|----|------|
|    | >50 | 12 | 39 | 7.10 |
|   | >50 | 12 | 40 | 6.83 |
|  | >50 | 12 | 41 | 7.90 |

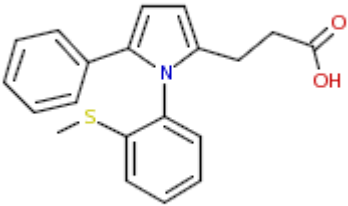
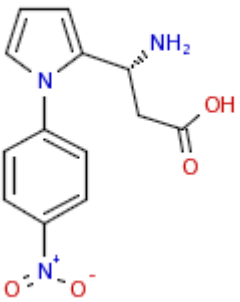
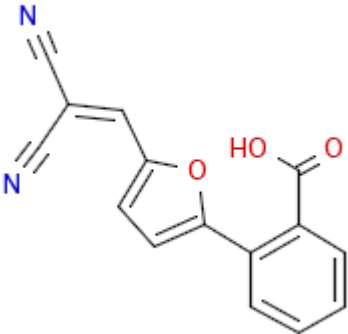


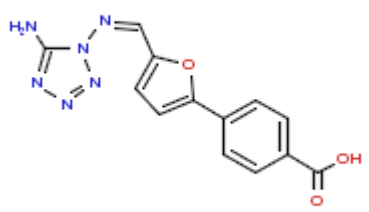
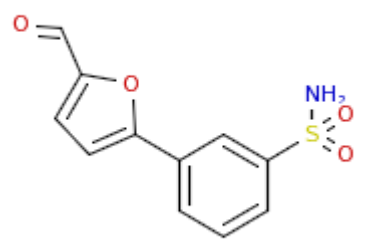
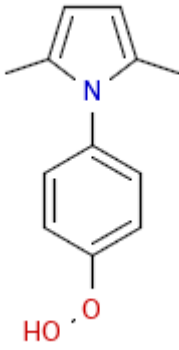
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|---|-----|----|----|------|
|    | >50 | 12 | 42 | 7.80 |
|    | >50 | 12 | 48 | 5.68 |
|  | >50 | 12 | 54 | 8.83 |

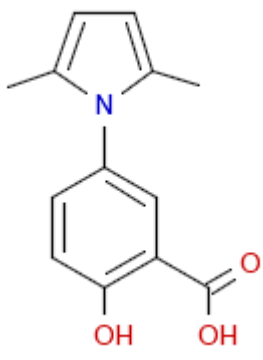
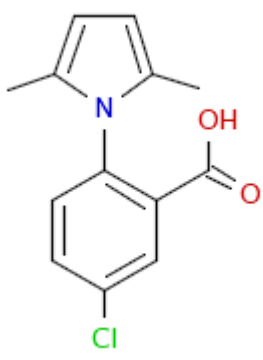
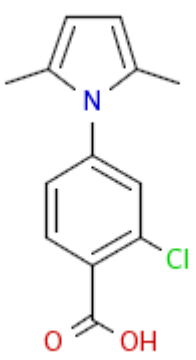
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|---|-----|----|----|------|
|  <p>Chemical structure of a sulfonamide derivative. It features a central imidazole ring substituted with a methyl group, a carbonyl group, and a 4-(sulfamoyl)phenyl group. The imidazole ring is also substituted with a 2-ethoxyphenyl group.</p> | >50 | 12 | 55 | 6.68 |
|  <p>Chemical structure of a nitrile derivative. It features a central imidazole ring substituted with two methyl groups and a 4-(4-chlorophenyl)phenyl group. The imidazole ring is also substituted with a 2-cyanoethyl group.</p>                 | >50 | 12 | 62 | 5.80 |
|  <p>Chemical structure of a bromophenyl derivative. It features a central imidazole ring substituted with two methyl groups and a 4-(4-bromophenyl)phenyl group. The imidazole ring is also substituted with a 2-(4-carboxyphenyl)ethyl group.</p> | >50 | 12 | 63 | 5.61 |

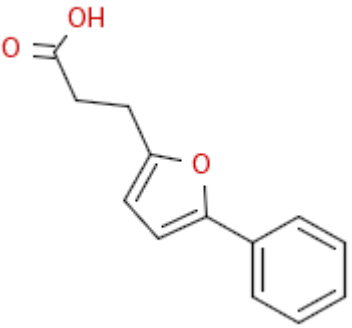
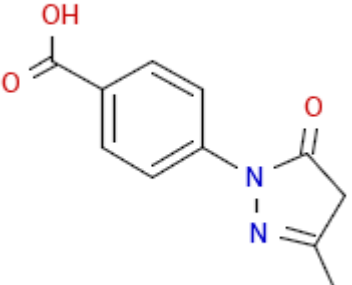
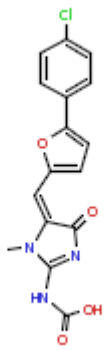
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|---|-----|----|----|------|
|              | >50 | 12 | 64 | 6.98 |
|              | >55 | 12 | 34 | 7.78 |
| Chiral<br> | >55 | 12 | 43 | 5.94 |

|   |     |    |    |      |
|---|-----|----|----|------|
| <p>Chiral</p>  | >55 | 12 | 49 | 6.53 |
|                | >60 | 12 | 50 | 5.35 |
|              | >60 | 12 | 65 | 8.17 |

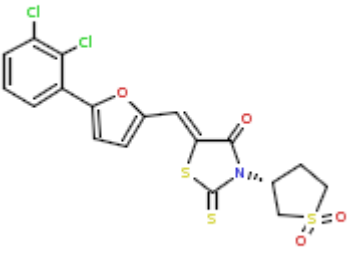
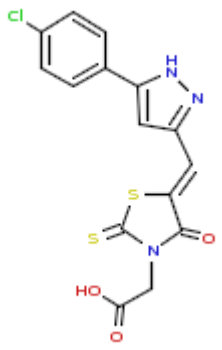
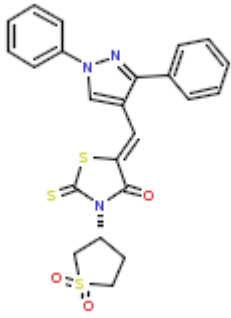
|  |     |    |    |      |
|--|-----|----|----|------|
|                 | >60 | 12 | 66 | 7.20 |
| <p>Chiral</p>  | >70 | 12 | 67 | 7.24 |
|               | >75 | 12 | 35 | 6.13 |

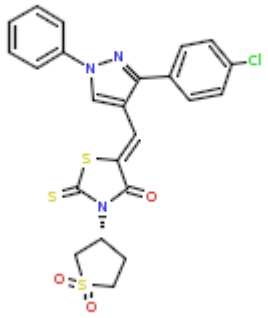
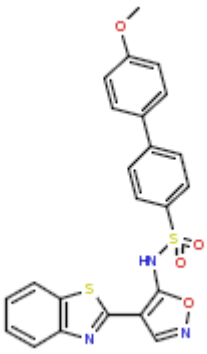
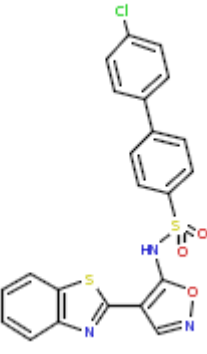
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|---|-----|----|----|------|
| <br><chem>Nc1ncnc2n1c2/C=C/c3cc(O)ccc3</chem>      | >80 | 12 | 36 | 6.22 |
| <br><chem>NC(=O)S(=O)(=O)c1ccc(cc1)/C=C/C=O</chem> | >80 | 12 | 44 | 4.14 |
| <br><chem>Cc1c(C)cn(c1)C2=CC=C(O)C=C2</chem>     | >85 | 12 | 68 | 7.29 |

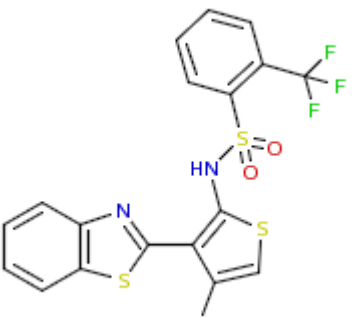
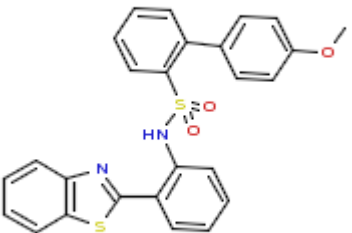
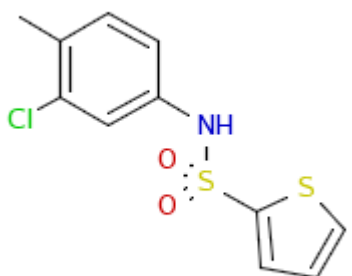
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|--|-----|----|----|------|
| <br><chem>Cc1cc(C)n(c1-c1ccc(O)c(C(=O)O)c1)C(=O)O</chem>    | >85 | 12 | 69 | 6.31 |
| <br><chem>Cc1cc(C)n(c1-c1ccc(Cl)c(C(=O)O)c1)C(=O)O</chem>  | >85 | 12 | 70 | 3.29 |
| <br><chem>Cc1cc(C)n(c1-c1ccc(Cl)c(C(=O)O)c1)C(=O)O</chem> | >85 | 12 | 71 | 4.94 |

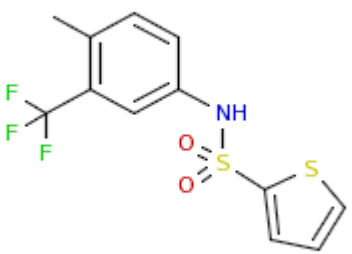
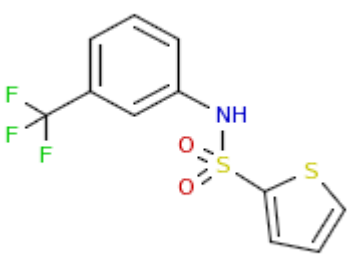
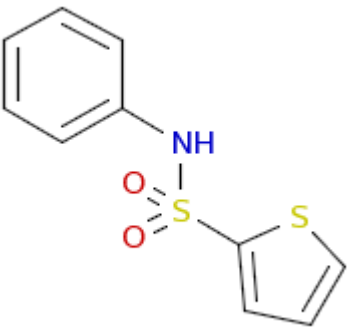
|   |      |    |    |      |
|---|------|----|----|------|
|  <chem>CC(=O)CCc1cc(O)c(c1)c2ccccc2</chem>               | >90  | 12 | 37 | 6.60 |
|  <chem>CC1=CNC(=O)N1c2ccc(cc2)C(=O)O</chem>              | >90  | 12 | 51 | 4.45 |
|  <chem>CC1=CNC(=O)N1C=Cc2cc(O)c(c2)c3ccc(Cl)cc3</chem> | >100 | 10 | 20 | 4.86 |

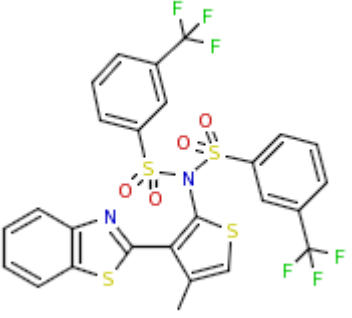
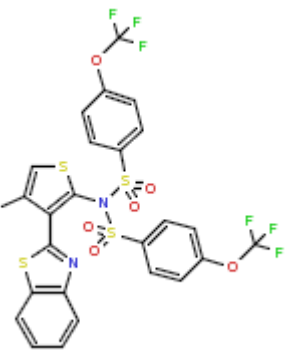
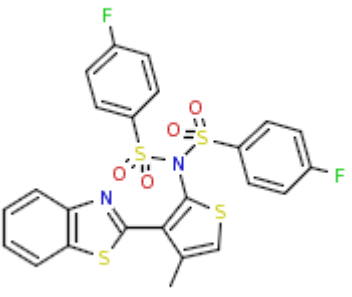


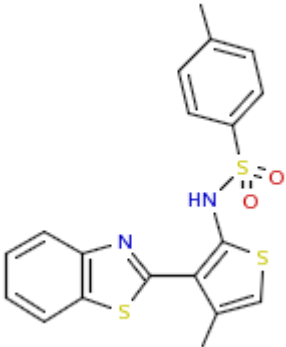
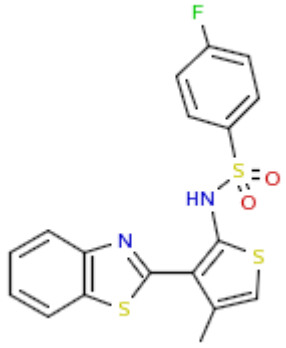
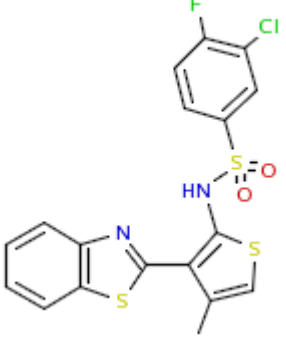
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|---|------|---|----|------|
| <p>Chiral</p>  <chem>Clc1cc(Cl)ccc1-c1ccoc1/C=C2\N(C(=O)S2)S(=O)(=O)C3CCCC3</chem> | >100 | 7 | 14 | 4.98 |
|  <chem>Clc1ccc(cc1)/C=C2\N(C(=O)S2)CC(=O)O</chem>                                 | >100 | 7 | 28 | 6.56 |
| <p>Chiral</p>  <chem>c1ccc(cc1)/C=C2\N(C(=O)S2)S(=O)(=O)C3CCCC3</chem>           | >100 | 7 | 44 | 4.84 |

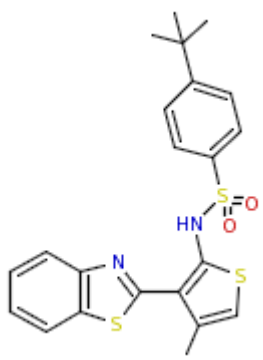
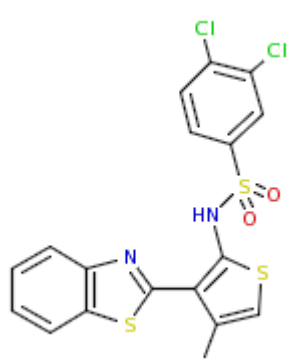
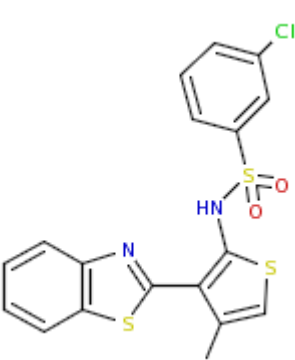
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|---|------|----|-----|------|
| <p>Chiral</p>  <chem>O=C1NC(S1)C=C2C=CN(C2)c3ccccc3c4ccc(Cl)cc4</chem>                   | >100 | 7  | 45  | 4.76 |
|  <chem>COc1ccc(cc1)-c2ccc(cc2)NS(=O)(=O)c3cc4c(c3)nc5c4cnc56c7ccccc7n8c(=O)sc68</chem>  | >100 | 14 | 107 | 8.58 |
|  <chem>Clc1ccc(cc1)-c2ccc(cc2)NS(=O)(=O)c3cc4c(c3)nc5c4cnc56c7ccccc7n8c(=O)sc68</chem> | >100 | 14 | 108 | 7.11 |

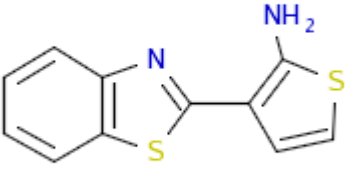
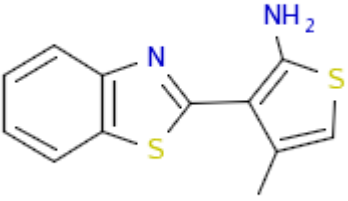
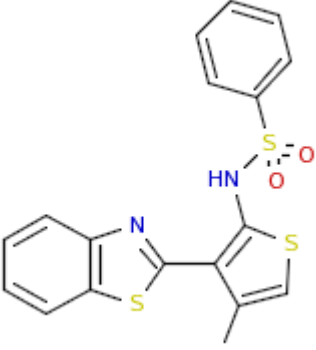
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|---|------|----|-----|------|
| <br><chem>Cc1sc(C2=NC3=CC=CC=C3S2)nc1NS(=O)(=O)c4ccc(C(F)(F)F)cc4</chem> | >100 | 14 | 11  | 6.06 |
| <br><chem>Cc1sc(C2=NC3=CC=CC=C3S2)nc1NS(=O)(=O)c4ccc(OC)cc4</chem>       | >100 | 14 | 111 | 7.32 |
| <br><chem>Cc1sc(C2=NC3=CC=C(C=C3)C=C2)nc1NS(=O)(=O)c4ccc(Cl)cc4</chem> | >100 | 14 | 116 | 5.30 |

|  |      |    |     |      |
|--|------|----|-----|------|
| <br><chem>Cc1ccc(cc1C(F)(F)F)NS(=O)(=O)c2ccsc2</chem> | >100 | 14 | 117 | 5.70 |
| <br><chem>Cc1ccc(cc1C(F)(F)F)NS(=O)(=O)c2ccsc2</chem> | >100 | 14 | 118 | 5.53 |
| <br><chem>c1ccc(cc1)NS(=O)(=O)c2ccsc2</chem>        | >100 | 14 | 119 | 5.22 |

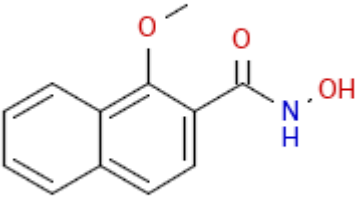
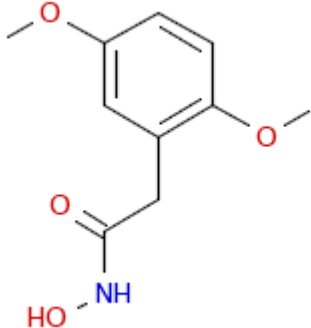
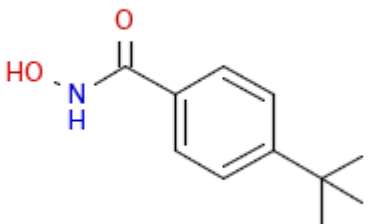
|  |      |    |     |      |
|--|------|----|-----|------|
|  <p>The structure shows a central nitrogen atom bonded to two sulfur atoms, each part of a sulfonamide group. The sulfonamide groups are further substituted with two trifluoromethylphenyl rings. The central nitrogen is also bonded to a benzothiazole ring system.</p>                  | >100 | 14 | 120 | 5.45 |
|  <p>The structure shows a central nitrogen atom bonded to two sulfur atoms, each part of a sulfonamide group. The sulfonamide groups are further substituted with two (4-(trifluoromethoxy)phenyl)sulfonyl groups. The central nitrogen is also bonded to a benzothiazole ring system.</p> | >100 | 14 | 121 | 4.45 |
|  <p>The structure shows a central nitrogen atom bonded to two sulfur atoms, each part of a sulfonamide group. The sulfonamide groups are further substituted with two (4-fluorophenyl)sulfonyl groups. The central nitrogen is also bonded to a benzothiazole ring system.</p>            | >100 | 14 | 122 | 4.29 |

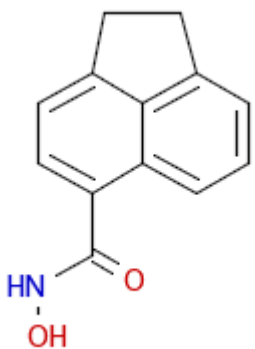
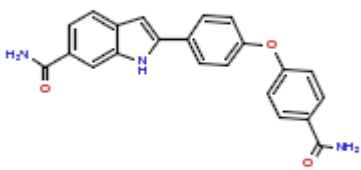
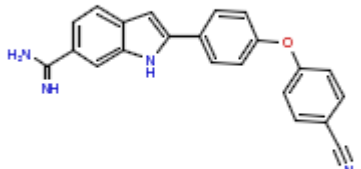
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|---|------|----|----|------|
| <br><chem>Cc1cc(C)sc1C2=NC3=CC=CC=C3S2NS(=O)(=O)c4ccc(C)cc4</chem>       | >100 | 14 | 14 | 6.83 |
| <br><chem>Cc1cc(C)sc1C2=NC3=CC=CC=C3S2NS(=O)(=O)c4ccc(F)cc4</chem>      | >100 | 14 | 15 | 6.21 |
| <br><chem>Cc1cc(C)sc1C2=NC3=CC=CC=C3S2NS(=O)(=O)c4cc(F)c(Cl)cc4</chem> | >100 | 14 | 23 | 6.43 |

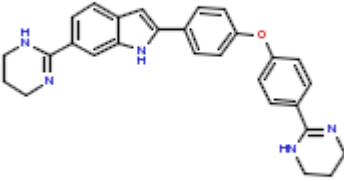
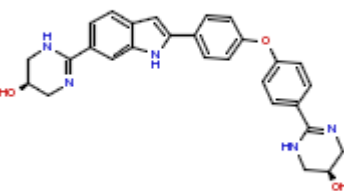
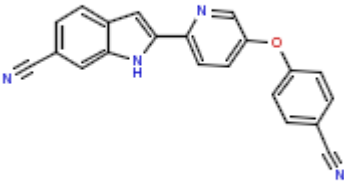
|   |      |    |    |      |
|---|------|----|----|------|
| <br>Chemical structure of a thienothiopyran derivative. It features a benzothiazole ring system connected to a thiophene ring. The thiophene ring is substituted with a methyl group and a sulfonamide group (-NH-SO <sub>2</sub> -). The sulfonamide group is further substituted with a tert-butyl group.          | >100 | 14 | 25 | 7.22 |
| <br>Chemical structure of a thienothiopyran derivative. It features a benzothiazole ring system connected to a thiophene ring. The thiophene ring is substituted with a methyl group and a sulfonamide group (-NH-SO <sub>2</sub> -). The sulfonamide group is further substituted with a 2,4-dichlorophenyl group. | >100 | 14 | 26 | 6.16 |
| <br>Chemical structure of a thienothiopyran derivative. It features a benzothiazole ring system connected to a thiophene ring. The thiophene ring is substituted with a methyl group and a sulfonamide group (-NH-SO <sub>2</sub> -). The sulfonamide group is further substituted with a 4-chlorophenyl group.    | >100 | 14 | 31 | 6.13 |

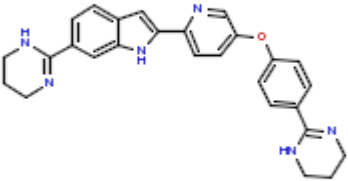
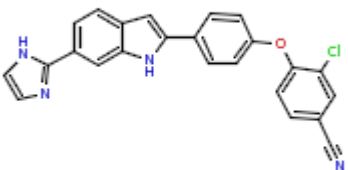
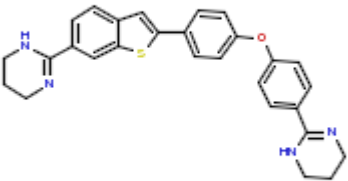
|   |      |    |    |      |
|---|------|----|----|------|
| <br><chem>Nc1ccc(s1)-c2ccccc2N</chem>                      | >100 | 14 | 42 | 4.00 |
| <br><chem>Cc1c(N)cc(s1)-c2ccccc2N</chem>                   | >100 | 14 | 8  | 4.14 |
| <br><chem>NS(=O)(=O)c1ccc(Nc2cc(s2)-c3ccccc3N)cc1</chem> | >100 | 14 | 9  | 5.94 |

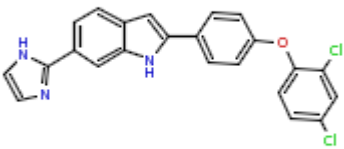
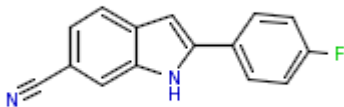
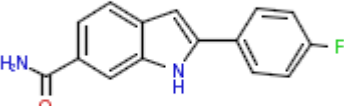


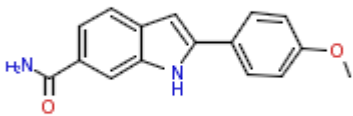
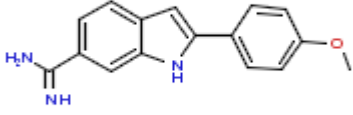
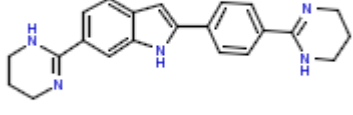
|  |      |   |    |      |
|--|------|---|----|------|
|  <chem>COc1cccc2ccccc12C(=O)NO</chem>     | >100 | 6 | 10 | 5.26 |
|  <chem>COc1cc(OC)ccc1CC(=O)NO</chem>     | >100 | 6 | 21 | 6.94 |
|  <chem>CC(C)(C)c1ccc(cc1)C(=O)NO</chem> | >100 | 6 | 8  | 5.15 |

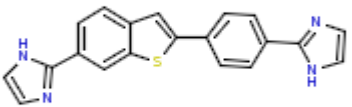
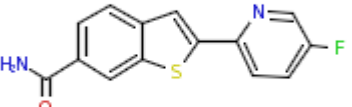
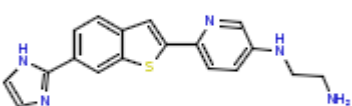
|   |      |    |    |      |
|---|------|----|----|------|
|    | >100 | 6  | 9  | 7.23 |
|    | >100 | 21 | 10 | 6.79 |
|  | >100 | 21 | 11 | 6.27 |

|   |      |    |     |      |
|---|------|----|-----|------|
|                | >100 | 21 | 14  | 7.65 |
| <p>Chiral</p>  | >100 | 21 | 15  | 5.41 |
|              | >100 | 21 | 23a | 7.02 |

|   |      |    |     |      |
|---|------|----|-----|------|
|    | >100 | 21 | 24b | 5.50 |
|    | >100 | 21 | 24c | 6.21 |
|  | >100 | 21 | 25b | 7.20 |

|   |      |    |     |      |
|---|------|----|-----|------|
|    | >100 | 21 | 29  | 6.38 |
|    | >100 | 21 | 39  | 6.37 |
|  | >100 | 21 | 40a | 5.66 |

|   |      |    |     |      |
|---|------|----|-----|------|
|    | >100 | 21 | 43a | 6.48 |
|    | >100 | 21 | 43b | 6.19 |
|  | >100 | 21 | 44b | 6.98 |

|   |      |    |     |      |
|---|------|----|-----|------|
| <br><chem>C1=CN=C(N1)c2ccc(cc2)c3sc4ccccc43</chem> | >100 | 21 | 46a | 5.97 |
| <br><chem>CC(=O)Nc1ccc2c(c1)sc3ccccc32</chem>      | >100 | 21 | 49  | 5.46 |
| <br><chem>CCNc1ccc2c(c1)sc3ccccc32</chem>        | >100 | 21 | 50  | 7.72 |

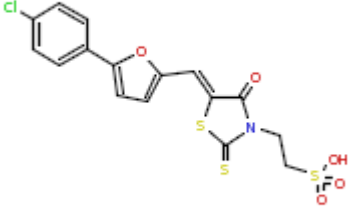
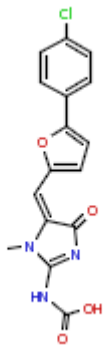
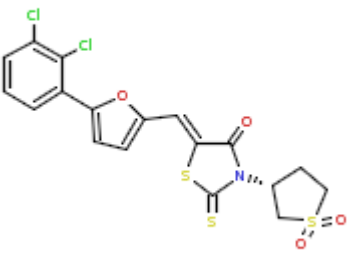
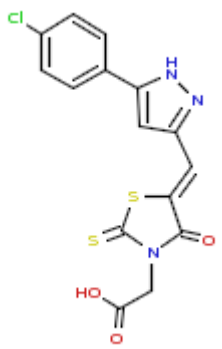
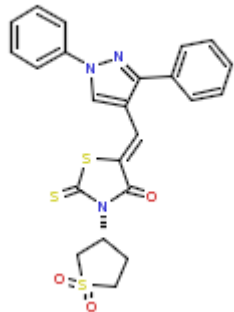
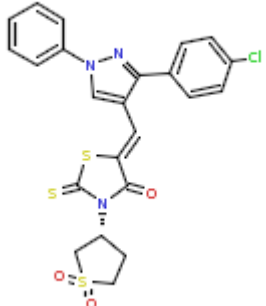
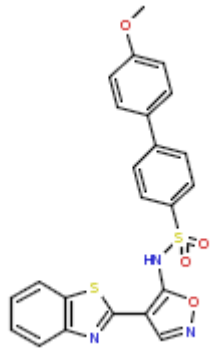
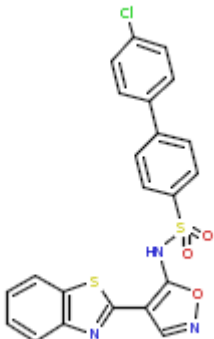
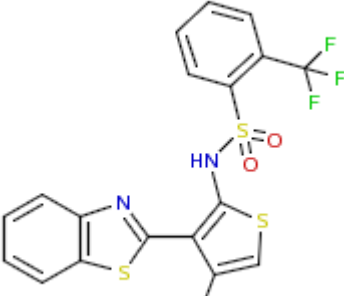
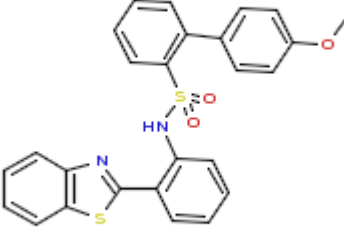
|   |      |   |    |      |
|---|------|---|----|------|
|  | >200 | 7 | 12 | 5.77 |
|---|------|---|----|------|

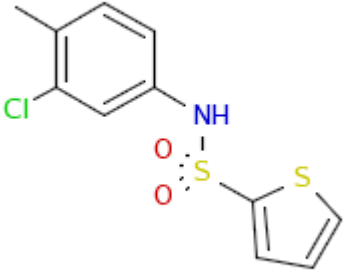
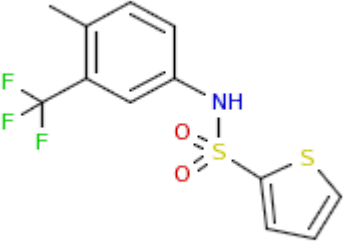
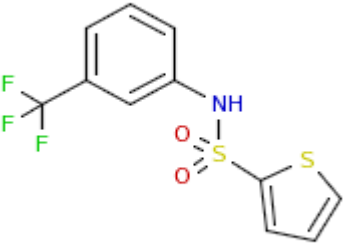


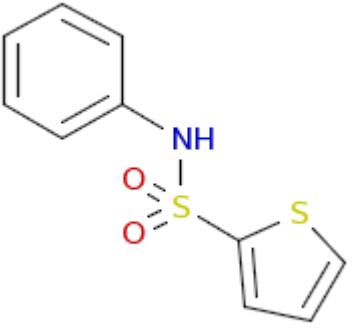
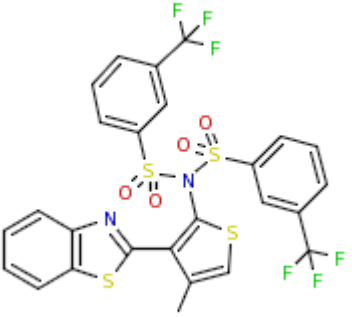
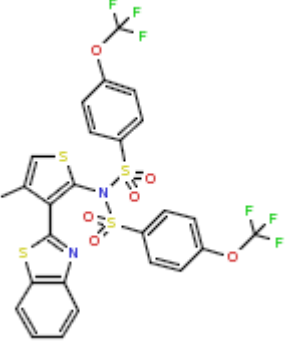
Table S5. Structures, LF biological activities, references, compound designators, and docking scores for screening set compounds in dataset **DB1E**.

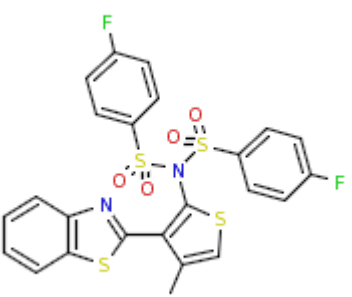
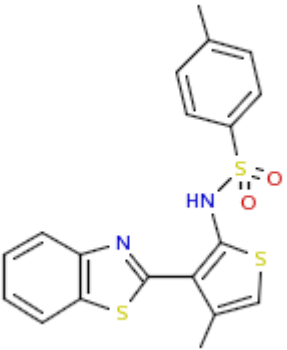
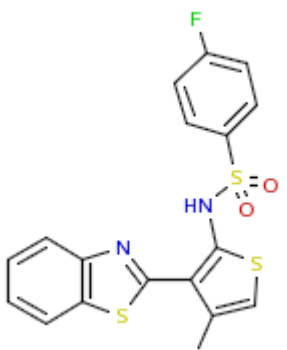
| Structure   | LF IC <sub>50</sub><br>or K <sub>i</sub><br>( $\mu$ M) | Reference | Compound<br>Designator | Docking Score<br>(Surflex-Dock) |
|---|--|-----------|------------------------|---------------------------------|
|              | >100   | 10        | 20                     | 4.86                            |
| Chiral<br> | >100   | 7         | 14                     | 4.98                            |
|            | >100   | 7         | 28                     | 6.56                            |

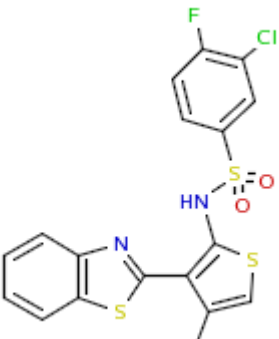
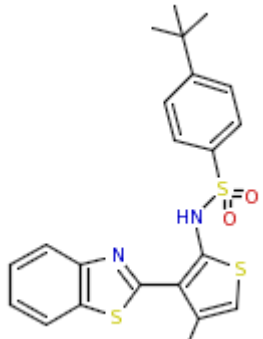
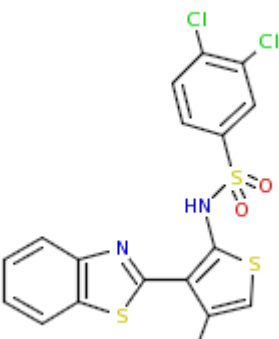
|  |      |    |     |      |
|--|------|----|-----|------|
| <p>Chiral</p>  <chem>O=C1NC(S1)C(=O)C2=CN(C2)N3=CC=CC=C3</chem>                                 | >100 | 7  | 44  | 4.84 |
| <p>Chiral</p>  <chem>O=C1NC(S1)C(=O)C2=CN(C2)N3=CC=C(Cl)C=C3</chem>                            | >100 | 7  | 45  | 4.76 |
|  <chem>COc1ccc(cc1)-c2ccc(cc2)S(=O)(=O)Nc3cc4nc5ccccc5s4c3C(=O)N1C(S1)C(=O)N2=CC=CC=C2</chem> | >100 | 14 | 107 | 8.58 |

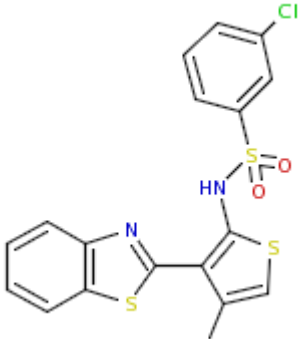
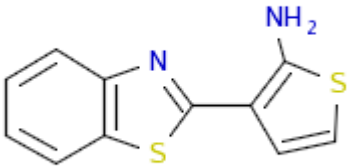
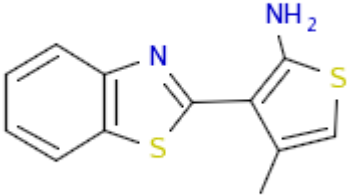
|   |      |    |     |      |
|---|------|----|-----|------|
| <br><chem>Clc1ccc(cc1)-c2ccc(cc2)NS(=O)(=O)c3nc4c(s4)c5ccccc5n3</chem> | >100 | 14 | 108 | 7.11 |
| <br><chem>Cc1cc2c(s1)c3ccccc3n2C4=CN(C4)C(F)(F)F</chem>                | >100 | 14 | 11  | 6.06 |
| <br><chem>COc1ccc(cc1)-c2ccccc2NS(=O)(=O)c3c4c(s3)c5ccccc5n4</chem>  | >100 | 14 | 111 | 7.32 |

|   |      |    |     |      |
|---|------|----|-----|------|
| <br><chem>Clc1ccc(NC(=O)S1=CC=CS1)cc1</chem>       | >100 | 14 | 116 | 5.30 |
| <br><chem>C(F)(F)Fc1ccc(NC(=O)S1=CC=CS1)cc1</chem> | >100 | 14 | 117 | 5.70 |
| <br><chem>c1ccc(NC(=O)S1=CC=CS1)cc1</chem>       | >100 | 14 | 118 | 5.53 |

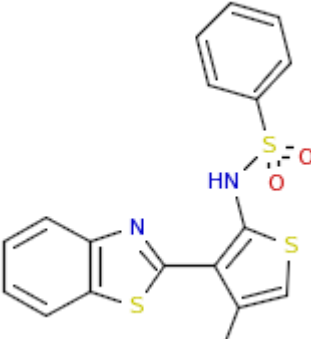
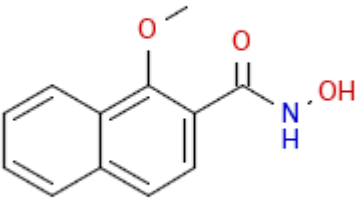
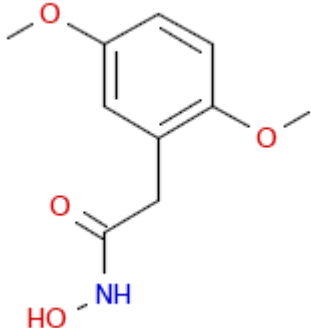
|  |      |    |     |      |
|--|------|----|-----|------|
|  <chem>Nc1ccccc1S(=O)(=O)c2ccsc2</chem>                                   | >100 | 14 | 119 | 5.22 |
|  <chem>Cc1csc2c1nc3ccccc3s2N(S(=O)(=O)c4ccc(F)(F)F)c5ccc(F)(F)F5</chem>  | >100 | 14 | 120 | 5.45 |
|  <chem>Cc1csc2c1nc3ccccc3s2N(S(=O)(=O)c4ccc(F)(F)F)c5ccc(F)(F)F5</chem> | >100 | 14 | 121 | 4.45 |

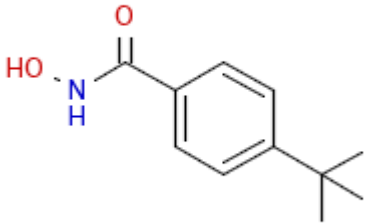
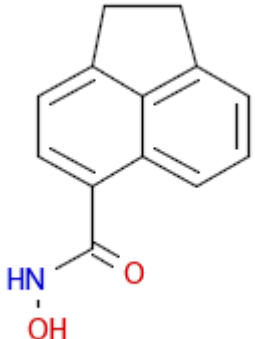
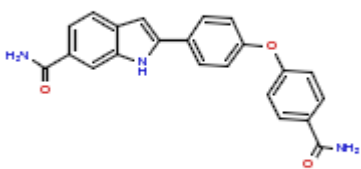
|   |      |    |     |      |
|---|------|----|-----|------|
|    | >100 | 14 | 122 | 4.29 |
|   | >100 | 14 | 14  | 6.83 |
|  | >100 | 14 | 15  | 6.21 |

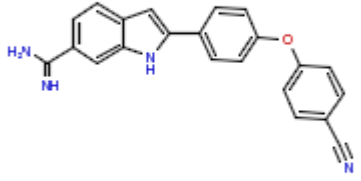
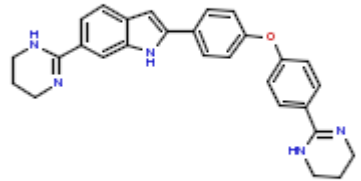
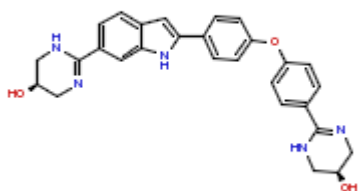
|  |      |    |    |      |
|--|------|----|----|------|
|  <chem>Cc1sc(C2=NC3=CC=CC=C3S2)sc1NS(=O)(=O)c4cc(F)c(Cl)cc4</chem>    | >100 | 14 | 23 | 6.43 |
|  <chem>CC(C)(C)c1ccc(cc1)S(=O)(=O)Nc2sc(C3=NC4=CC=CC=C4S3)c2</chem>  | >100 | 14 | 25 | 7.22 |
|  <chem>Cc1sc(C2=NC3=CC=CC=C3S2)sc1NS(=O)(=O)c4cc(Cl)c(Cl)cc4</chem> | >100 | 14 | 26 | 6.16 |

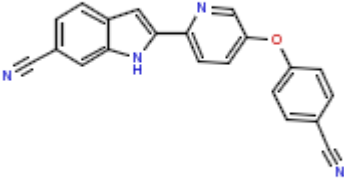
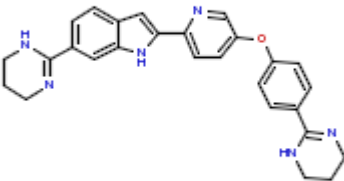
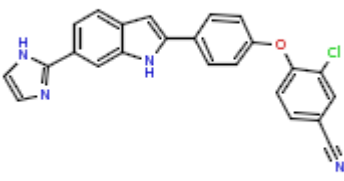
|  |      |    |    |      |
|--|------|----|----|------|
| <br><chem>CC1=CC=C(C=C1)S=C(NC(=O)S(=O)(=O)c2ccc(Cl)cc2)C2=CC=CC=C2S</chem> | >100 | 14 | 31 | 6.13 |
| <br><chem>CC1=CC=C(C=C1)S=C(N)C2=CC=CC=C2S</chem>                           | >100 | 14 | 42 | 4.00 |
| <br><chem>CC1=CC=C(C=C1)S=C(N)C2=C(C)C=CC=C2S</chem>                      | >100 | 14 | 8  | 4.14 |

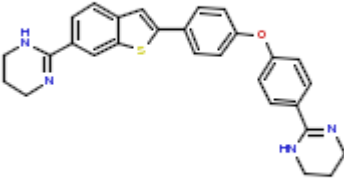
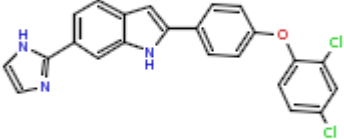
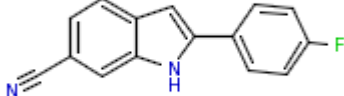


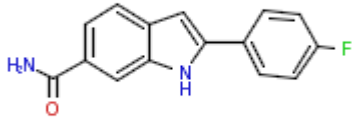
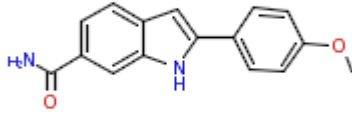
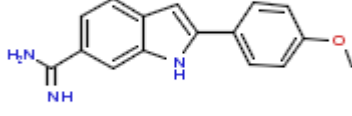
|  |      |    |    |      |
|--|------|----|----|------|
| <br><chem>Cc1csc2c(c1)nc3ccccc32NS(=O)(=O)c4ccccc4</chem> | >100 | 14 | 9  | 5.94 |
| <br><chem>COc1ccc2ccccc2c1C(=O)NO</chem>                  | >100 | 6  | 10 | 5.26 |
| <br><chem>COc1ccc(cc1OC)CC(=O)NO</chem>                 | >100 | 6  | 21 | 6.94 |

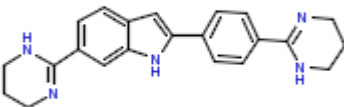
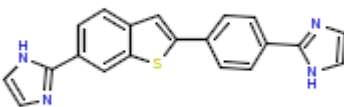
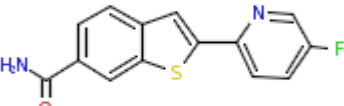
|   |      |    |    |      |
|---|------|----|----|------|
| <br><chem>CC(C)(C)c1ccc(cc1)C(=O)N</chem>                | >100 | 6  | 8  | 5.15 |
| <br><chem>O=C(O)C1=CC=C2C3=CC=CC=C3C4=CC=CC=C142</chem> | >100 | 6  | 9  | 7.23 |
| <br><chem>NC(=O)c1ccc(cc1)COc2ccc(N)cc2</chem>         | >100 | 21 | 10 | 6.79 |

|  |      |    |    |      |
|--|------|----|----|------|
| <br><chem>Nc1nc2ccccc2n1-c1ccc(Oc2ccc(C#N)cc2)cc1</chem>                            | >100 | 21 | 11 | 6.27 |
| <br><chem>C1CCNCC1c1nc2ccccc2n1-c1ccc(Oc2ccc(C3CCNCC3)cc2)cc1</chem>                | >100 | 21 | 14 | 7.65 |
| Chiral<br><br><chem>Oc1ccncc1c1nc2ccccc2n1-c1ccc(Oc2ccc(C3CC(O)CN3)cc2)cc1</chem> | >100 | 21 | 15 | 5.41 |

|   |      |    |     |      |
|---|------|----|-----|------|
|    | >100 | 21 | 23a | 7.02 |
|    | >100 | 21 | 24b | 5.50 |
|  | >100 | 21 | 24c | 6.21 |

|  |      |    |     |      |
|--|------|----|-----|------|
| <br><chem>C1CCN(C1)c2ccc3c(c2)sc(c3)C4=CC=C(C=C4)Oc5ccc(cc5)N6CCNCC6</chem> | >100 | 21 | 25b | 7.20 |
| <br><chem>C1CCN(C1)c2ccc3c(c2)sc(c3)C4=CC=C(C=C4)Oc5ccc(Cl)c(Cl)c5</chem>   | >100 | 21 | 29  | 6.38 |
| <br><chem>N#Cc1ccc2c(c1)c(c[nH]2)C3=CC=C(F)C=C3</chem>                    | >100 | 21 | 39  | 6.37 |

|  |      |    |     |      |
|--|------|----|-----|------|
| <br><chem>NC(=O)c1ccc2c(c1)c(c[nH]2)C3=CC=C(C=C3)F</chem>     | >100 | 21 | 40a | 5.66 |
| <br><chem>COc1ccc(cc1)C2=Cc3c(c[nH]3)C(=O)N</chem>            | >100 | 21 | 43a | 6.48 |
| <br><chem>NC(=N)C1=CC=C2C(=C1)C=C(C2)C3=CC=C(C=C3)OC</chem> | >100 | 21 | 43b | 6.19 |

|   |      |    |     |      |
|---|------|----|-----|------|
|    | >100 | 21 | 44b | 6.98 |
|    | >100 | 21 | 46a | 5.97 |
|  | >100 | 21 | 49  | 5.46 |

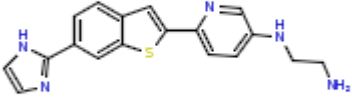
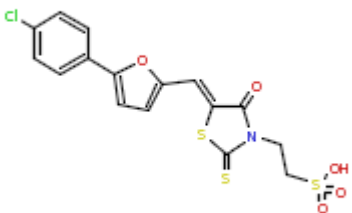
|   |      |    |    |      |
|---|------|----|----|------|
|  | >100 | 21 | 50 | 7.72 |
|  | >200 | 7  | 12 | 5.77 |



Table S6. Pairwise distances (Å) between features in final pharmacophore hypothesis **UM1**.

| Pairwise Distance (Å) | F6 Hyd | F7 Hyd | F8 Hyd | F13 Acc | F20 Hyd | F21 Acc | F22 Acc | F23 Don |
|-----------------------|--------|--------|--------|---------|---------|---------|---------|---------|
| F6 Hyd <sup>a</sup>   |        | 4.63   | 8.45   | 1.69    | 6.06    | 1.55    | 5.03    | 1.12    |
| F7 Hyd                |        |        | 3.89   | 4.43    | 10.53   | 5.86    | 9.20    | 5.36    |
| F8 Hyd                |        |        |        | 8.03    | 14.42   | 9.75    | 12.78   | 9.06    |
| F13 Acc               |        |        |        |         | 6.96    | 2.78    | 6.26    | 1.48    |
| F20 Hyd               |        |        |        |         |         | 4.67    | 4.32    | 5.81    |
| F21 Acc               |        |        |        |         |         |         | 4.53    | 1.92    |
| F22 Acc               |        |        |        |         |         |         |         | 4.79    |
| F23 Don               |        |        |        |         |         |         |         |         |

<sup>a</sup>Hyd = hydrophobic; Aro = aromatic; Acc = hydrogen-bond acceptor; Don = hydrogen-bond donor

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