

## **SUPPLEMENTARY INFORMATION FOR:**

### **A fragment-based electrophile-first approach to target histidine with aryl-fluorosulfates: application to hMcl-1**

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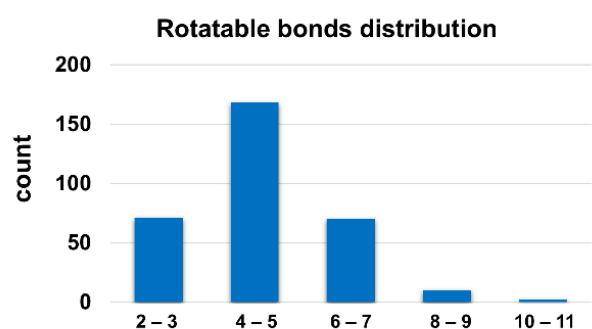
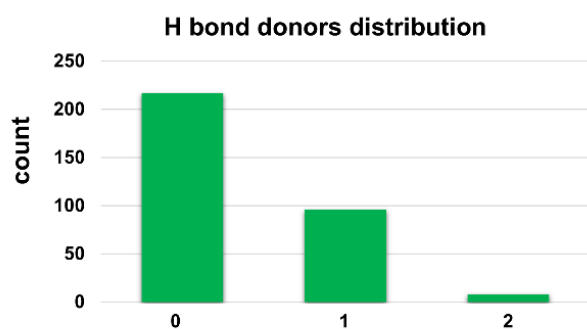
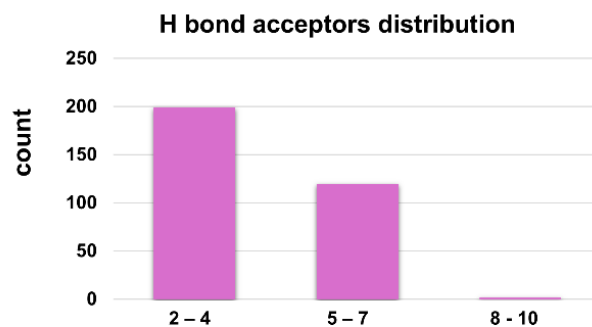
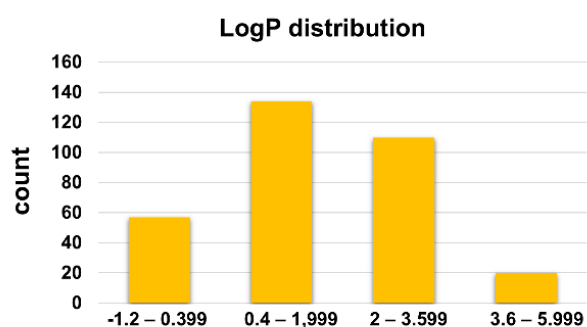
#### **Supplementary information contains:**

Supplementary Figures S1 – S11

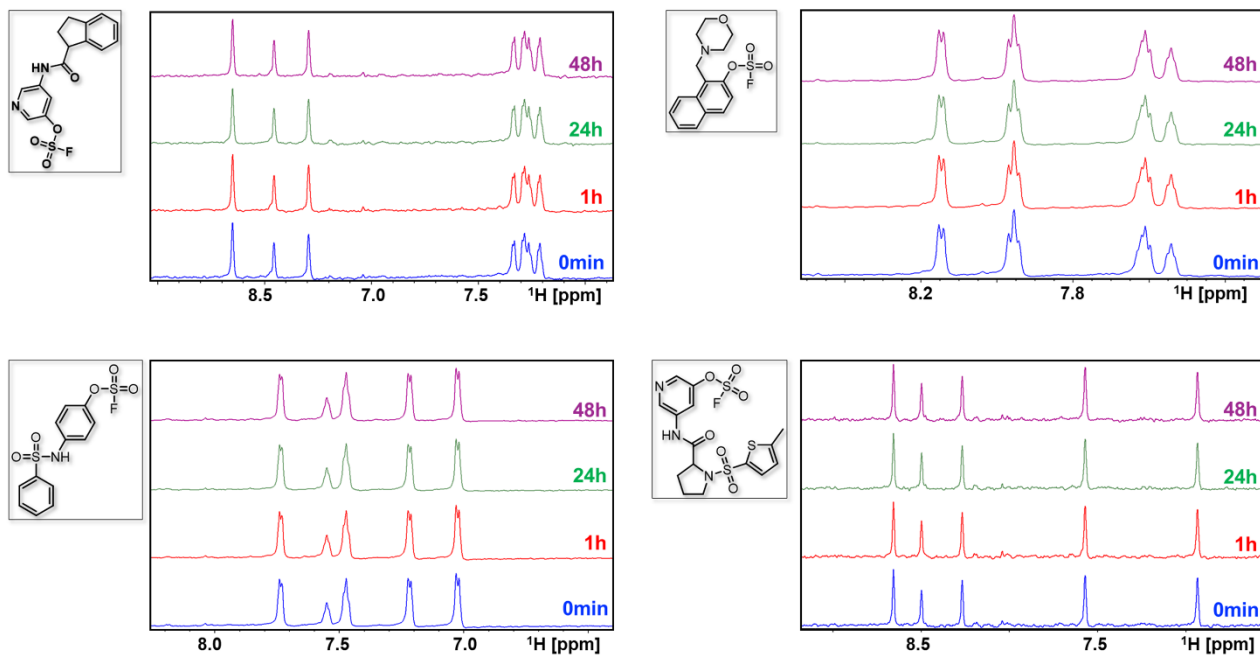
Supplementary Tables S1 – S4

## SUPPLEMENTARY FIGURES

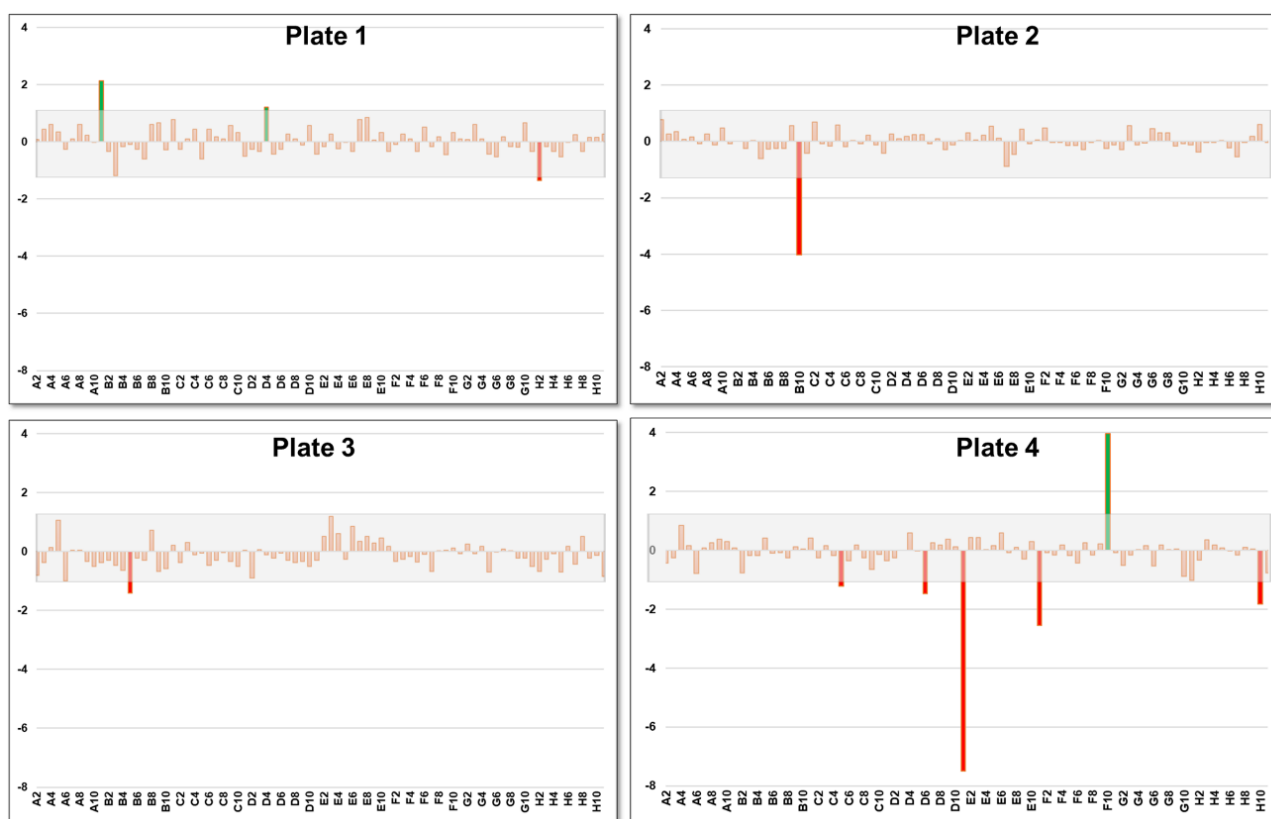
**Supplementary Figure S1:** LogP, number of H-bond acceptors, number of H-bond donors, and number of rotatable bonds distributions of the 320 fragments that compose the library.



**Supplementary Figure S2:** Stability of fluorosulfates tested with 1D  $^1\text{H}$  NMR spectra collected at different time points (0 min, 1 h, 24 h, 48 h).

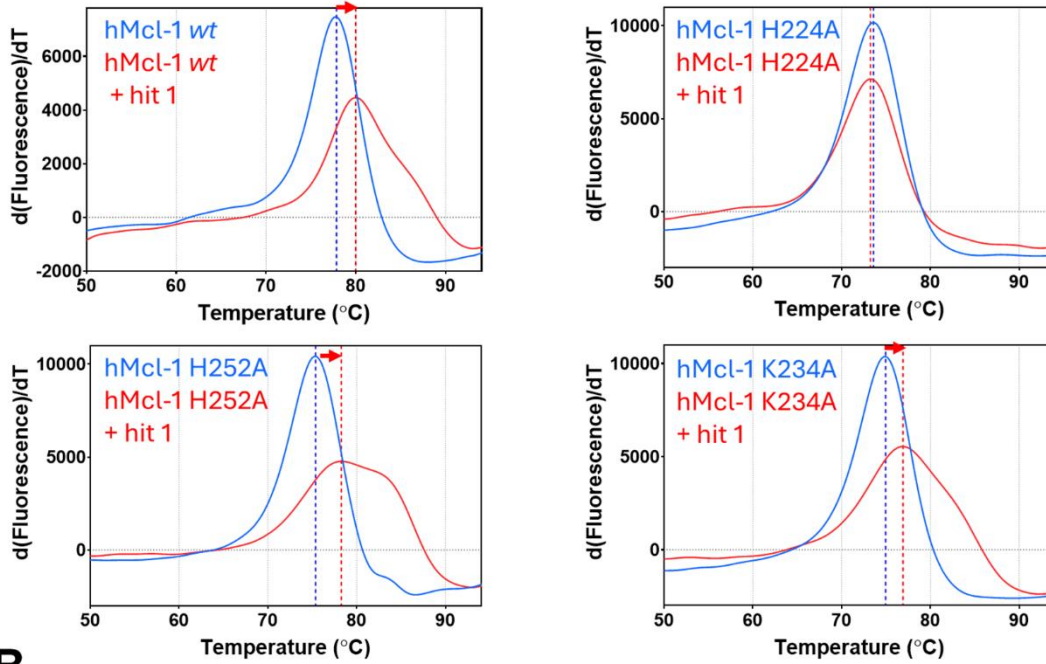


**Supplementary Figure S3:** Primary screening results based on denaturation thermal shift measurements for the 4 plates of 80 compounds each (320 compounds listed in supplementary **Table S1**). In this screening we considered compounds that induced a sizable positive ( $> 1.2$  °C, 3 fragments, green) and negative ( $> -1.2$  °C, 8 fragments, red) for further characterizations.

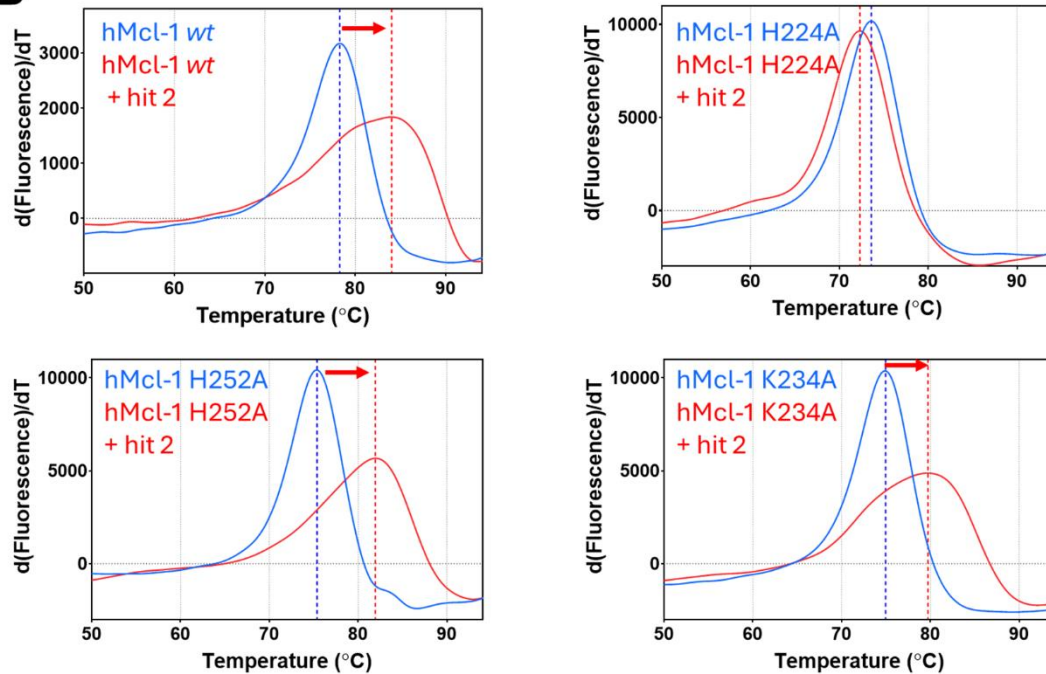


**Supplementary Figure S4:** Thermal denaturation curves for hMcl-1(172-323) or mutant proteins, as indicated, collected in absence and presence of fragment hit 1 (A) or fragment hit 2 (B). **A)**  $\Delta T_m$  (*wt*-hMcl-1) =  $2.11 \pm 0.01$ ;  $\Delta T_m$  (hMcl-1 H224A) =  $-0.34 \pm 0.09$ ;  $\Delta T_m$  (hMcl-1 H252A) =  $2.90 \pm 0.17$ ;  $\Delta T_m$  (hMcl-1 K234A) =  $1.96 \pm 0.17$ . **B)**  $\Delta T_m$  (*wt*-hMcl-1) =  $3.97 \pm 0.17$ ;  $\Delta T_m$  (hMcl-1 H224A) =  $-1.28 \pm 0.17$ ;  $\Delta T_m$  (hMcl-1 H252A) =  $6.57 \pm 0.26$ ;  $\Delta T_m$  (hMcl-1 K234A) =  $4.77 \pm 0.26$ .

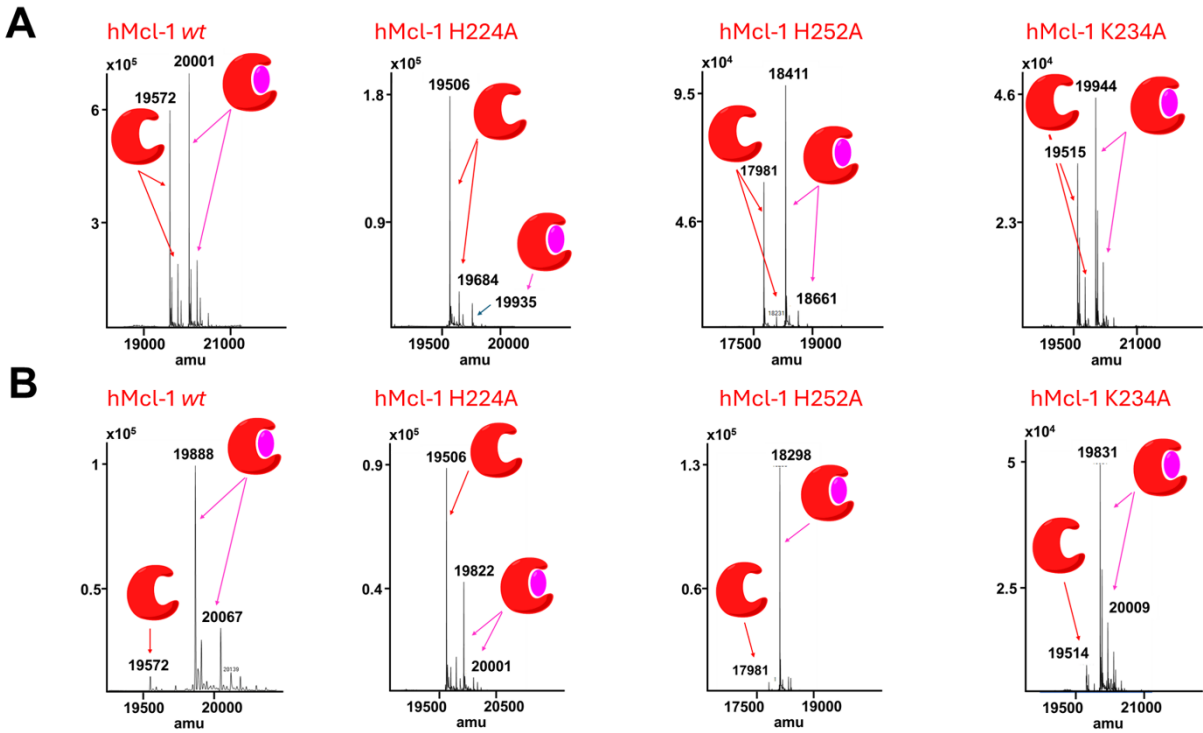
**A**



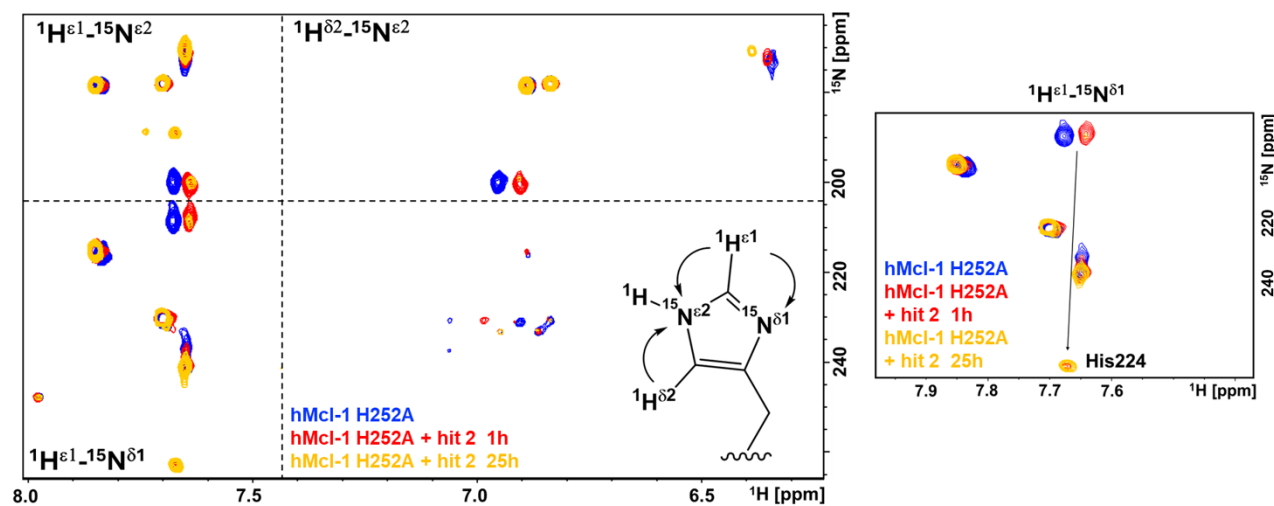
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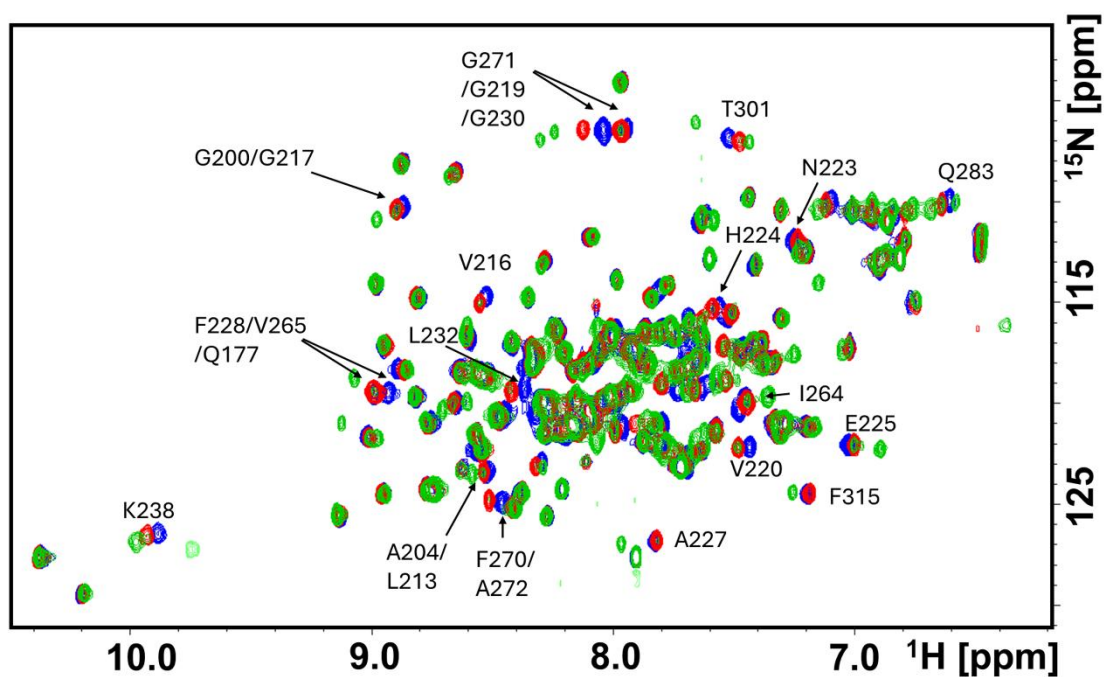
**Supplementary Figure S5:** Mass spectrometry analyses of hMcl-1(171-323) and mutants, as indicated, collected in presence of fragment hit 1 (A) or fragment hit 2 (B).



**Supplementary Figure S6:** Heteronuclear long range [ $^{15}\text{N}$ ,  $^1\text{H}$ ] NMR correlation spectra for His side chains detection. The spectra for hMcl-1(172-323) His252Ala, collected in absence (blue) or presence of fragment hit **2** after various incubation times (red, 1 h; yellow, 25 h) are superimposed. On the right, a zoomed region highlighting the chemical shift perturbations at His 224 is displayed.

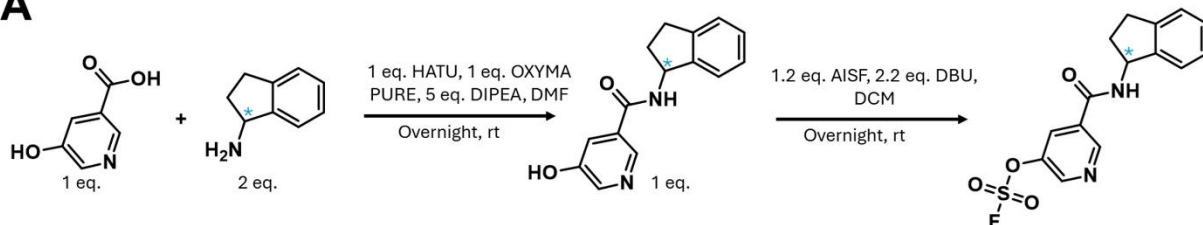


**Supplementary Figure S7:** Backbone 2D [ $^{15}\text{N}$ ,  $^1\text{H}$ ] correlation spectra for  $^{15}\text{N}$ -hMcl-1(172-323) (50  $\mu\text{M}$ ) collected in absence (blue) or presence of fragment hit 2 (1 mM) after various incubation times (red, 1 h; green, 25 h). Resonance assignments are also reported.

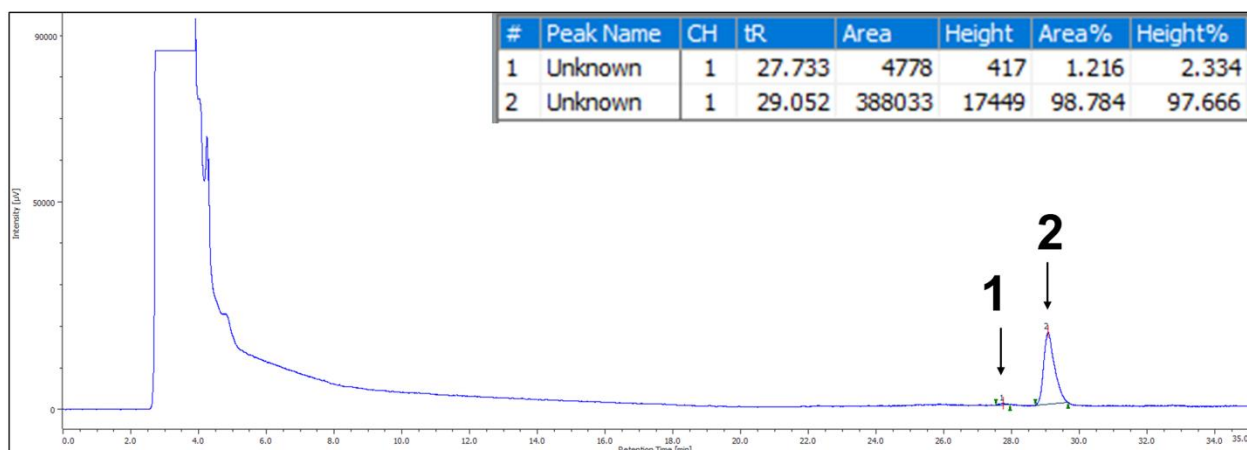
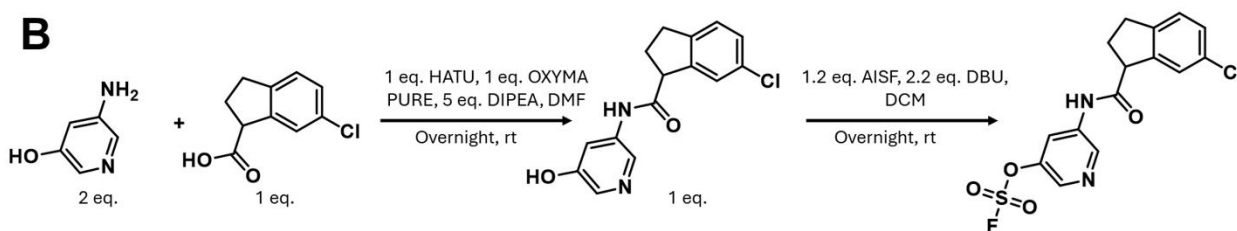


**Supplementary Figure S8:** Synthetic route used to obtain fragment hit **2** and its analogs reported in Figure 6. The purity of **165D9** by HPLC is also reported (purity > 98%).

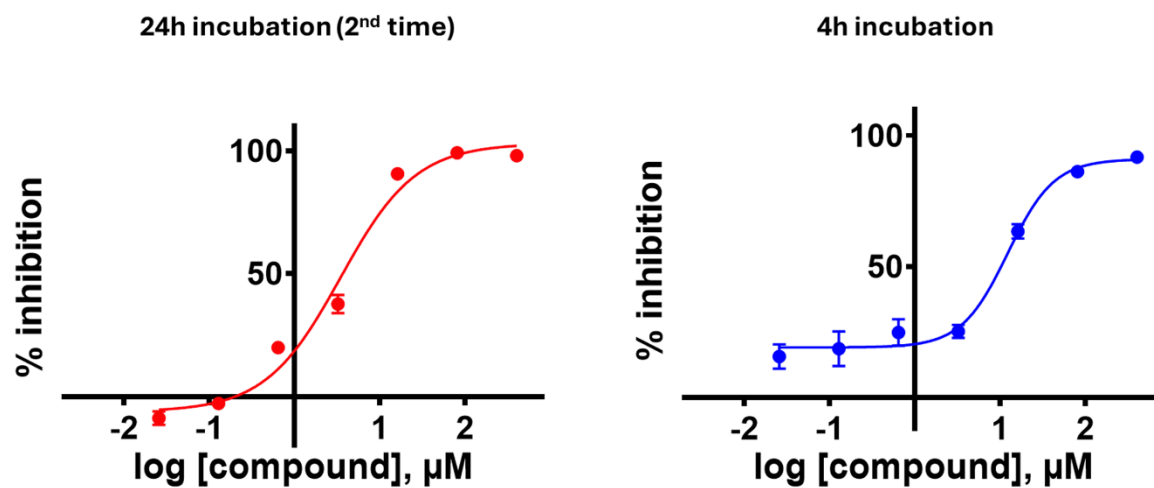
**A**



**B**

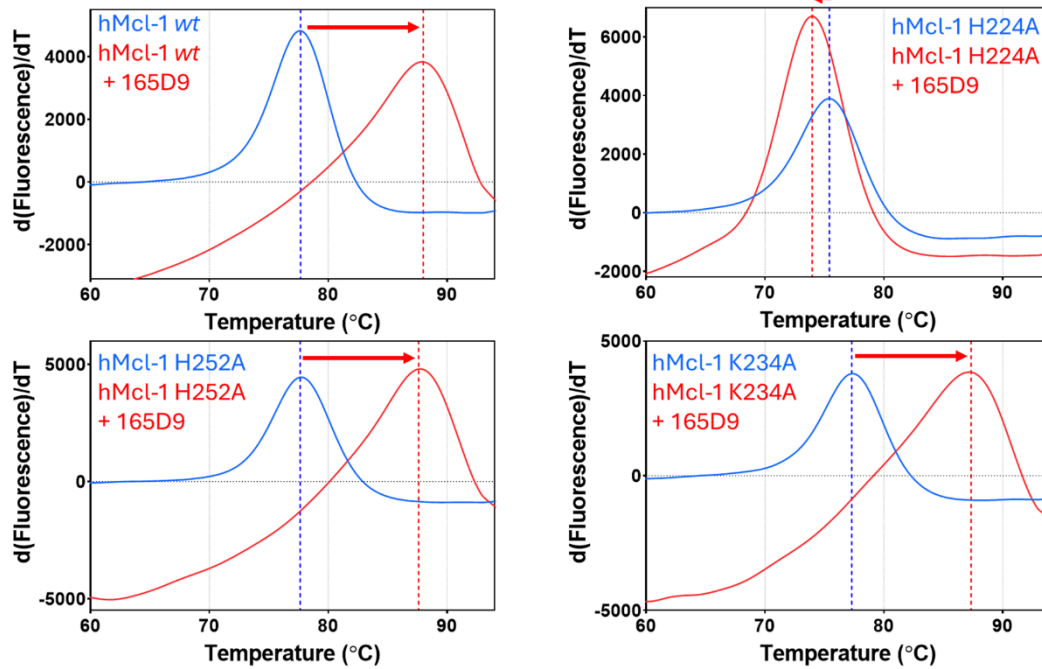


**Supplementary Figure S9:** Dose-response DELFIA inhibition curves with compound **165D9** after 24 h incubation ( $IC_{50} \sim 3.0 \mu M$ ; this experiment is an independent replicate of the data reported in **Figure 6D** that resulted in an  $IC_{50}$  value of  $\sim 2.5 \mu M$ ) or 4 h incubation ( $IC_{50} \sim 12 \mu M$ ).

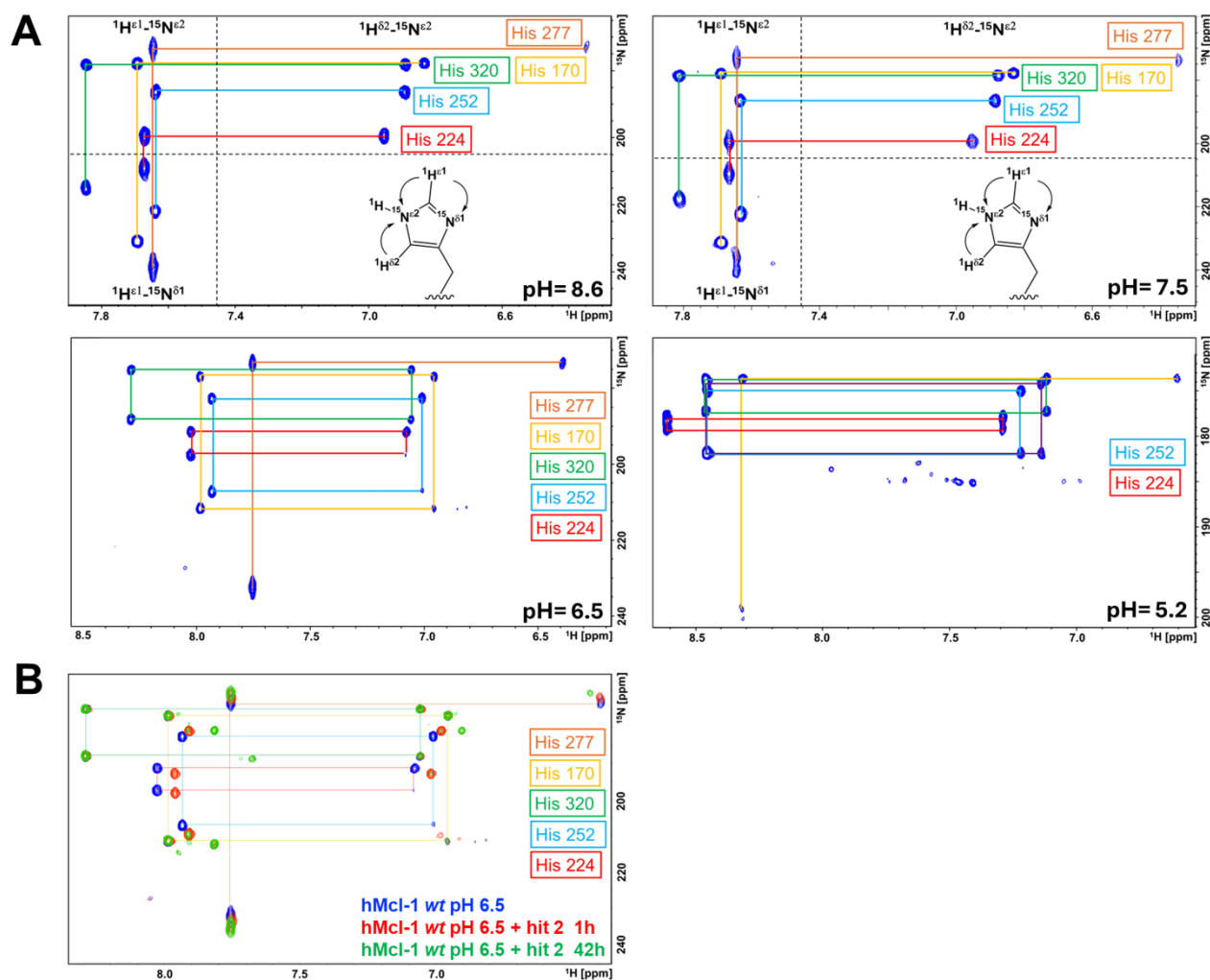


**Supplementary Figure S10: A)** Thermal denaturation curves for hMcl-1(172-323) or its mutants as indicated, collected in absence (blue) or presence of (250  $\mu$ M) **165D9**, after 8 h incubation.  $\Delta T_m$  (*wt*-hMcl-1) =  $10.23 \pm 0.05$ ;  $\Delta T_m$  (hMcl-1 H224A) =  $-1.15 \pm 0.04$ ;  $\Delta T_m$  (hMcl-1 H252A) =  $10.44 \pm 0.06$ ;  $\Delta T_m$  (hMcl-1 K234A) =  $9.96 \pm 0.20$ .

**A**

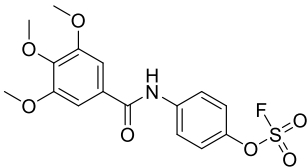
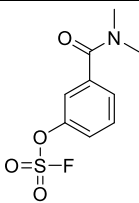
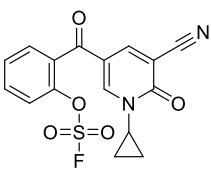
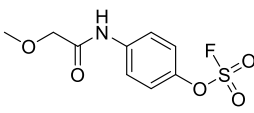
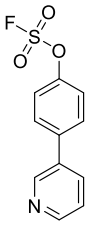


**Supplementary Figure S11:** **A)** 2D long-range [ $^{15}\text{N}$ ,  $^1\text{H}$ ] correlation spectra for His side chains of  $^{15}\text{N}$ -hMcl-1(172-323) (50  $\mu\text{M}$ ) collected at various pH values, as indicated. **B)** 2D long-range [ $^{15}\text{N}$ ,  $^1\text{H}$ ] correlation spectra for His side chains of hMcl-1(172-323) (50  $\mu\text{M}$ ) collected at pH= 6.5 in absence (blue) or presence of fragment hit 2 (1 mM) after various incubation times (red, 1 h; green, 42 h).

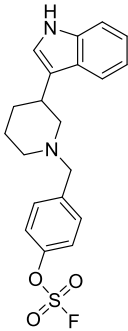
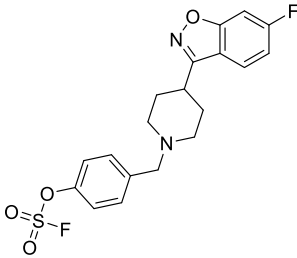
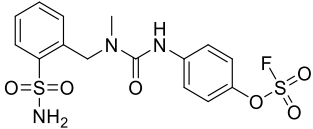
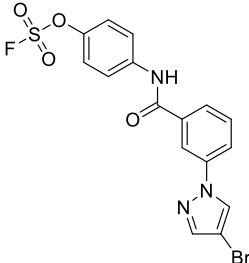
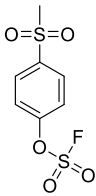
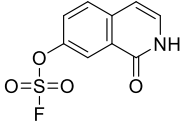


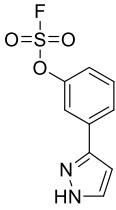
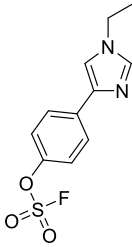
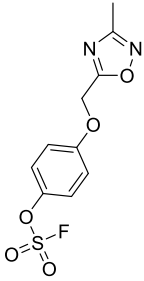
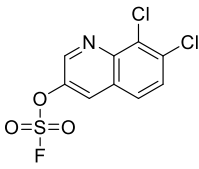
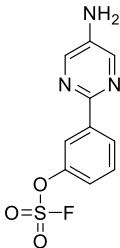
## SUPPLEMENTARY TABLES

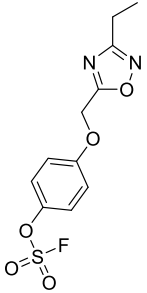
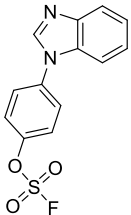
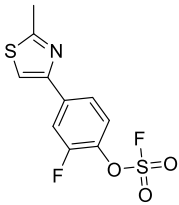
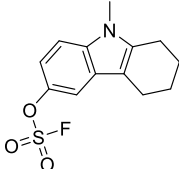
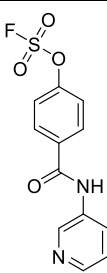
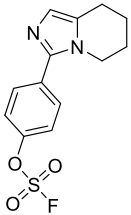
**Supplementary Table S1:** structures and properties of the 320 fragments in the library

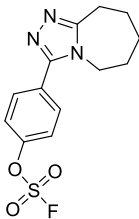
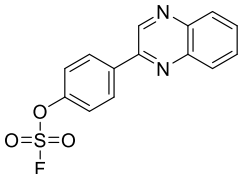
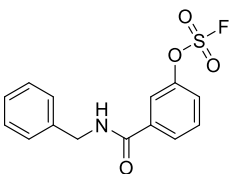
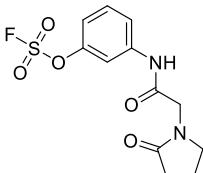
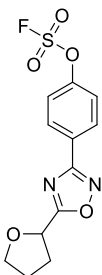
| Structure                                                                                                                                                                                                                           | MW      | LogP  | H bond acceptors | H bond donors | Rotatable bonds |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------|-------|------------------|---------------|-----------------|
| <br><chem>COC1=CC=C(C(=C1)OC)C(=O)Nc2ccc(OS(=O)(=O)F)cc2</chem><br><b>C<sub>16</sub>H<sub>16</sub>FN<sub>2</sub>O<sub>7</sub>S</b>                 | 385.362 | 2.112 | 6                | 1             | 8               |
| <br><chem>CN(C)C(=O)c1ccc(Oc2ccc(OS(=O)(=O)F)cc2)cc1</chem><br><b>C<sub>9</sub>H<sub>10</sub>FN<sub>2</sub>O<sub>4</sub>S</b>                     | 247.24  | 1.063 | 3                | 0             | 4               |
| <br><chem>C1=CC=C(C(=C1)C(=O)Oc2ccc(OS(=O)(=O)F)cc2)C(=O)N3C#CC(=O)NC3</chem><br><b>C<sub>16</sub>H<sub>11</sub>FN<sub>2</sub>O<sub>5</sub>S</b> | 362.331 | 0.926 | 5                | 0             | 6               |
| <br><chem>COC(=O)Nc1ccc(OS(=O)(=O)F)cc1</chem><br><b>C<sub>9</sub>H<sub>10</sub>FN<sub>2</sub>O<sub>5</sub>S</b>                                 | 263.239 | 0.254 | 4                | 1             | 6               |
| <br><chem>C1=CC=C(C(=C1)C(=O)Oc2ccc(OS(=O)(=O)F)cc2)C3=CC=CC=N3</chem><br><b>C<sub>11</sub>H<sub>8</sub>FN<sub>2</sub>O<sub>3</sub>S</b>         | 253.247 | 2.023 | 3                | 0             | 3               |

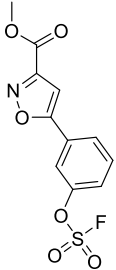
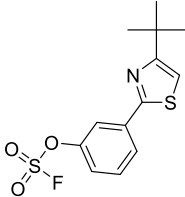
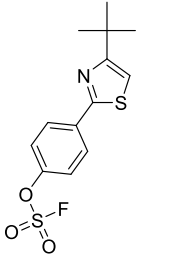
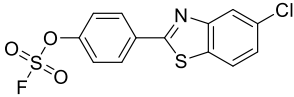
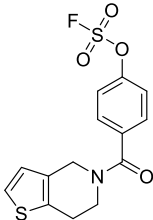
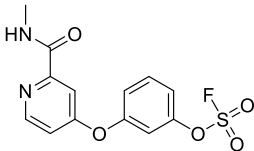


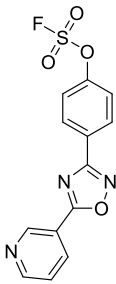
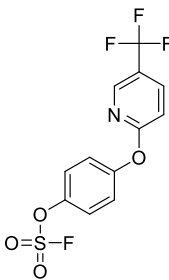
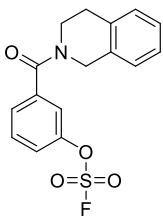
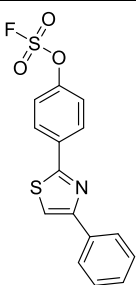
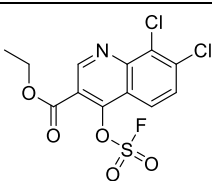
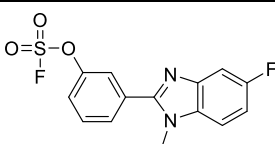
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|-------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------|-------|---|---|---|
| <br><b>C<sub>20</sub>H<sub>21</sub>FN<sub>2</sub>O<sub>3</sub>S</b>              | 388.457 | 3.488 | 4 | 1 | 5 |
| <br><b>C<sub>19</sub>H<sub>18</sub>F<sub>2</sub>N<sub>2</sub>O<sub>4</sub>S</b>  | 408.42  | 3.617 | 6 | 0 | 5 |
| <br><b>C<sub>15</sub>H<sub>16</sub>FN<sub>3</sub>O<sub>6</sub>S<sub>2</sub></b> | 417.426 | 1.214 | 5 | 2 | 8 |
| <br><b>C<sub>16</sub>H<sub>11</sub>BrFN<sub>3</sub>O<sub>4</sub>S</b>          | 440.243 | 3.319 | 5 | 1 | 6 |
| <br><b>C<sub>7</sub>H<sub>7</sub>FO<sub>5</sub>S<sub>2</sub></b>               | 254.246 | 0.391 | 4 | 0 | 3 |
| <br><b>C<sub>9</sub>H<sub>6</sub>FN<sub>2</sub>O<sub>4</sub>S</b>              | 243.208 | 0.934 | 3 | 1 | 2 |

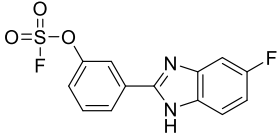
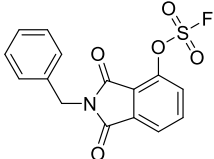
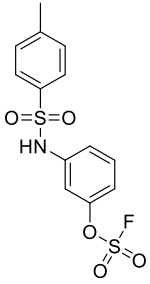
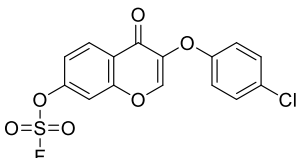
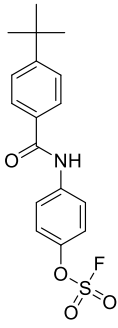
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|------------------------------------------------------------------------------------------------------------------------------------------------------------|---------|-------|---|---|---|
|  <p><b>C<sub>9</sub>H<sub>7</sub>FN<sub>2</sub>O<sub>3</sub>S</b></p>     | 242.224 | 1.885 | 4 | 1 | 3 |
|  <p><b>C<sub>11</sub>H<sub>11</sub>FN<sub>2</sub>O<sub>3</sub>S</b></p>   | 270.278 | 1.658 | 4 | 0 | 4 |
|  <p><b>C<sub>10</sub>H<sub>9</sub>FN<sub>2</sub>O<sub>5</sub>S</b></p>   | 288.249 | 2.578 | 6 | 0 | 5 |
|  <p><b>C<sub>9</sub>H<sub>4</sub>Cl<sub>2</sub>FNO<sub>3</sub>S</b></p> | 296.093 | 2.885 | 3 | 0 | 2 |
|  <p><b>C<sub>10</sub>H<sub>8</sub>FN<sub>3</sub>O<sub>3</sub>S</b></p>  | 269.25  | 1.515 | 5 | 1 | 3 |

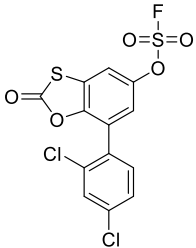
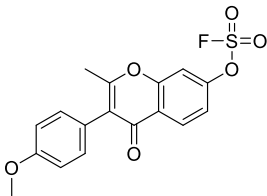
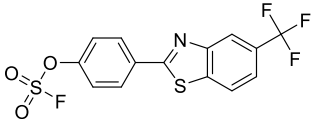
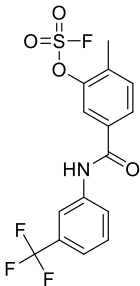
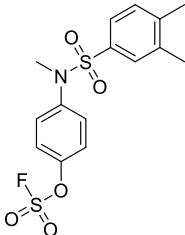
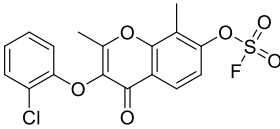
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| <br><b>C<sub>11</sub>H<sub>11</sub>FN<sub>2</sub>O<sub>5</sub>S</b>             | 302.276 | 3.151 | 6 | 0 | 6 |
| <br><b>C<sub>13</sub>H<sub>9</sub>FN<sub>2</sub>O<sub>3</sub>S</b>              | 292.284 | 2.361 | 4 | 0 | 3 |
| <br><b>C<sub>10</sub>H<sub>7</sub>F<sub>2</sub>NO<sub>3</sub>S<sub>2</sub></b> | 291.287 | 3.351 | 4 | 0 | 3 |
| <br><b>C<sub>13</sub>H<sub>14</sub>FN<sub>3</sub>O<sub>3</sub>S</b>           | 283.317 | 2.691 | 3 | 0 | 2 |
| <br><b>C<sub>12</sub>H<sub>9</sub>FN<sub>2</sub>O<sub>4</sub>S</b>            | 296.272 | 1.154 | 4 | 1 | 5 |
| <br><b>C<sub>12</sub>H<sub>9</sub>FN<sub>2</sub>O<sub>4</sub>S</b>            | 296.316 | 2.006 | 4 | 0 | 3 |

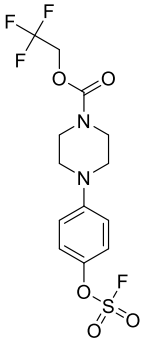
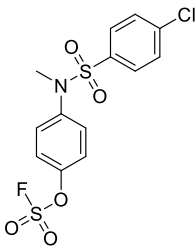
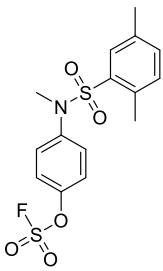
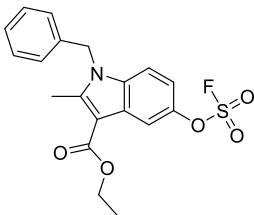
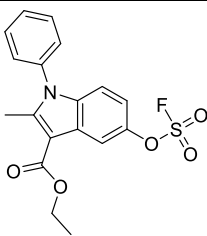
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|    | <b>311.331</b> | <b>2.6</b>    | <b>5</b> | <b>0</b> | <b>3</b> |
| <b>C<sub>13</sub>H<sub>14</sub>FN<sub>3</sub>O<sub>3</sub>S</b>                     |                |               |          |          |          |
|    | <b>304.295</b> | <b>2.954</b>  | <b>4</b> | <b>0</b> | <b>3</b> |
| <b>C<sub>14</sub>H<sub>9</sub>FN<sub>2</sub>O<sub>3</sub>S</b>                      |                |               |          |          |          |
|  | <b>309.311</b> | <b>2.56</b>   | <b>3</b> | <b>1</b> | <b>6</b> |
| <b>C<sub>14</sub>H<sub>12</sub>FNO<sub>4</sub>S</b>                                 |                |               |          |          |          |
|  | <b>316.303</b> | <b>-0.175</b> | <b>4</b> | <b>1</b> | <b>6</b> |
| <b>C<sub>12</sub>H<sub>13</sub>FN<sub>2</sub>O<sub>5</sub>S</b>                     |                |               |          |          |          |
|  | <b>314.287</b> | <b>2.71</b>   | <b>6</b> | <b>0</b> | <b>4</b> |
| <b>C<sub>12</sub>H<sub>11</sub>FN<sub>2</sub>O<sub>5</sub>S</b>                     |                |               |          |          |          |

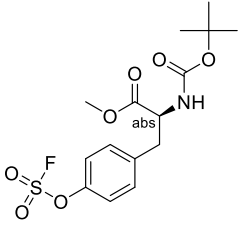
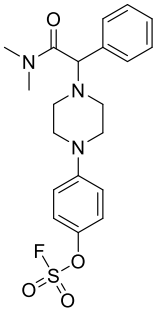
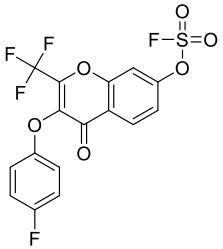
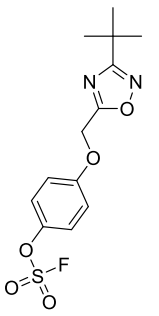
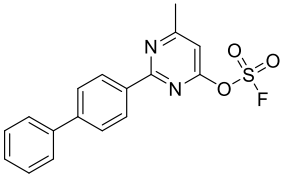
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|-------------------------------------------------------------------------------------|---------|-------|---|---|---|
|    | 301.244 | 1.833 | 5 | 0 | 5 |
| <b>C<sub>11</sub>H<sub>8</sub>FO<sub>6</sub>S</b>                                   |         |       |   |   |   |
|    | 315.377 | 4.605 | 3 | 0 | 4 |
| <b>C<sub>13</sub>H<sub>14</sub>FO<sub>3</sub>S<sub>2</sub></b>                      |         |       |   |   |   |
|   | 315.377 | 4.605 | 3 | 0 | 4 |
| <b>C<sub>13</sub>H<sub>14</sub>FO<sub>3</sub>S<sub>2</sub></b>                      |         |       |   |   |   |
|  | 343.771 | 4.512 | 3 | 0 | 3 |
| <b>C<sub>13</sub>H<sub>7</sub>ClFO<sub>3</sub>S<sub>2</sub></b>                     |         |       |   |   |   |
|  | 341.371 | 2.582 | 3 | 0 | 4 |
| <b>C<sub>14</sub>H<sub>12</sub>FO<sub>4</sub>S<sub>2</sub></b>                      |         |       |   |   |   |
|  | 326.298 | 1.451 | 5 | 1 | 6 |
| <b>C<sub>13</sub>H<sub>11</sub>FN<sub>2</sub>O<sub>5</sub>S</b>                     |         |       |   |   |   |

|                                                                                                                                                                     |         |       |   |   |   |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------|-------|---|---|---|
| <br><b>C<sub>13</sub>H<sub>8</sub>FN<sub>3</sub>O<sub>4</sub>S</b>                 | 321.282 | 2.693 | 6 | 0 | 4 |
| <br><b>C<sub>12</sub>H<sub>7</sub>F<sub>4</sub>NO<sub>4</sub>S</b>                 | 337.245 | 3.522 | 7 | 0 | 5 |
| <br><b>C<sub>16</sub>H<sub>14</sub>FN<sub>2</sub>O<sub>4</sub>S</b>               | 335.349 | 2.774 | 3 | 0 | 4 |
| <br><b>C<sub>15</sub>H<sub>10</sub>FN<sub>3</sub>O<sub>3</sub>S<sub>2</sub></b>  | 335.367 | 4.576 | 3 | 0 | 4 |
| <br><b>C<sub>12</sub>H<sub>8</sub>Cl<sub>2</sub>FN<sub>2</sub>O<sub>5</sub>S</b> | 368.156 | 3.044 | 4 | 0 | 5 |
| <br><b>C<sub>12</sub>H<sub>8</sub>Cl<sub>2</sub>FN<sub>3</sub>O<sub>3</sub>S</b> | 324.302 | 2.909 | 5 | 0 | 3 |

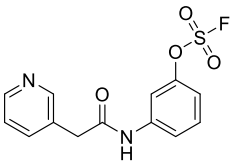
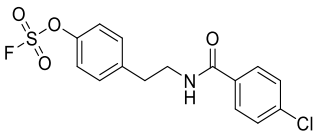
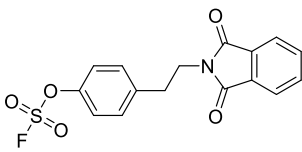
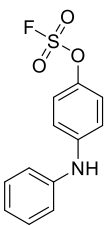
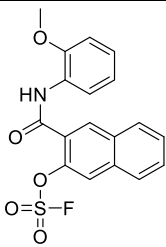
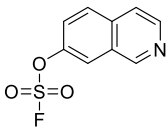
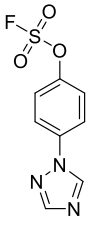
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|-------------------------------------------------------------------------------------|----------------|--------------|----------|----------|----------|
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| <b>C<sub>14</sub>H<sub>10</sub>F<sub>2</sub>N<sub>2</sub>O<sub>3</sub>S</b>         |                |              |          |          |          |
|    | <b>310.275</b> | <b>2.674</b> | <b>5</b> | <b>1</b> | <b>3</b> |
| <b>C<sub>13</sub>H<sub>8</sub>F<sub>2</sub>N<sub>2</sub>O<sub>3</sub>S</b>          |                |              |          |          |          |
|    | <b>335.305</b> | <b>2.372</b> | <b>4</b> | <b>0</b> | <b>4</b> |
| <b>C<sub>15</sub>H<sub>10</sub>FNO<sub>5</sub>S</b>                                 |                |              |          |          |          |
|   | <b>345.359</b> | <b>2.579</b> | <b>4</b> | <b>1</b> | <b>5</b> |
| <b>C<sub>13</sub>H<sub>12</sub>FNO<sub>5</sub>S<sub>2</sub></b>                     |                |              |          |          |          |
|  | <b>370.731</b> | <b>2.601</b> | <b>5</b> | <b>0</b> | <b>4</b> |
| <b>C<sub>15</sub>H<sub>8</sub>ClFO<sub>6</sub>S</b>                                 |                |              |          |          |          |
|  | <b>351.392</b> | <b>4.195</b> | <b>3</b> | <b>1</b> | <b>6</b> |
| <b>C<sub>17</sub>H<sub>18</sub>FNO<sub>4</sub>S</b>                                 |                |              |          |          |          |

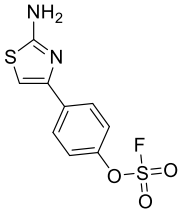
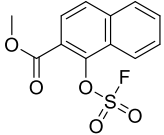
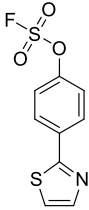
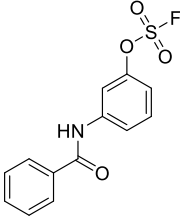
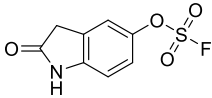
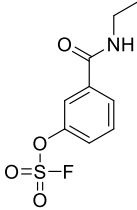
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|------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------|--------------|----------|----------|----------|
| <br><b>C<sub>13</sub>H<sub>5</sub>Cl<sub>2</sub>FO<sub>5</sub>S<sub>2</sub></b> | <b>395.196</b> | <b>4.844</b> | <b>3</b> | <b>0</b> | <b>3</b> |
| <br><b>C<sub>17</sub>H<sub>13</sub>FO<sub>6</sub>S</b>                          | <b>364.343</b> | <b>2.063</b> | <b>5</b> | <b>0</b> | <b>4</b> |
| <br><b>C<sub>14</sub>H<sub>7</sub>F<sub>4</sub>NO<sub>3</sub>S<sub>2</sub></b>  | <b>377.328</b> | <b>4.875</b> | <b>6</b> | <b>0</b> | <b>4</b> |
| <br><b>C<sub>15</sub>H<sub>11</sub>F<sub>4</sub>NO<sub>4</sub>S</b>           | <b>377.31</b>  | <b>3.899</b> | <b>6</b> | <b>1</b> | <b>6</b> |
| <br><b>C<sub>15</sub>H<sub>16</sub>FNO<sub>5</sub>S<sub>2</sub></b>           | <b>373.413</b> | <b>4.332</b> | <b>4</b> | <b>0</b> | <b>5</b> |
| <br><b>C<sub>17</sub>H<sub>12</sub>ClFO<sub>6</sub>S</b>                      | <b>398.785</b> | <b>2.714</b> | <b>5</b> | <b>0</b> | <b>4</b> |

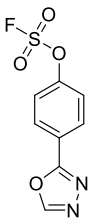
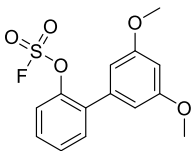
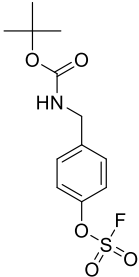
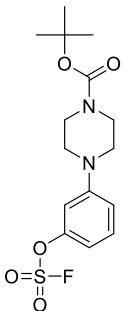
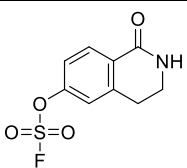
|                                                                                                                                                                      |         |       |   |   |   |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------|-------|---|---|---|
|  <p><b>C<sub>13</sub>H<sub>14</sub>F<sub>4</sub>N<sub>2</sub>O<sub>5</sub>S</b></p> | 386.318 | 2.561 | 7 | 0 | 7 |
|  <p><b>C<sub>13</sub>H<sub>11</sub>ClFNO<sub>5</sub>S<sub>2</sub></b></p>           | 379.801 | 4.121 | 4 | 0 | 5 |
|  <p><b>C<sub>15</sub>H<sub>16</sub>FNO<sub>5</sub>S<sub>2</sub></b></p>            | 373.413 | 4.332 | 4 | 0 | 5 |
|  <p><b>C<sub>19</sub>H<sub>18</sub>FNO<sub>5</sub>S</b></p>                       | 391.413 | 3.689 | 4 | 0 | 7 |
|  <p><b>C<sub>18</sub>H<sub>16</sub>FNO<sub>5</sub>S</b></p>                       | 377.386 | 3.62  | 4 | 0 | 6 |

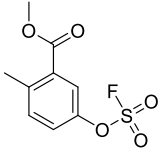
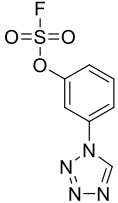
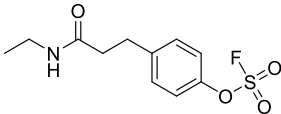
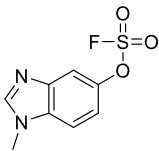
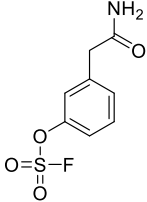
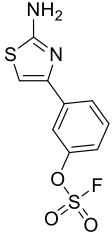
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|--------------------------------------------------------------------------------------------------------------------------------------------------------|---------|-------|---|---|----|
| <br><b>C<sub>15</sub>H<sub>20</sub>FN<sub>2</sub>O<sub>7</sub>S</b>   | 377.383 | 2.086 | 4 | 1 | 10 |
| <br><b>C<sub>20</sub>H<sub>24</sub>FN<sub>3</sub>O<sub>4</sub>S</b>   | 421.487 | 2.7   | 5 | 0 | 7  |
| <br><b>C<sub>16</sub>H<sub>7</sub>F<sub>5</sub>O<sub>6</sub>S</b>    | 422.278 | 2.467 | 9 | 0 | 5  |
| <br><b>C<sub>13</sub>H<sub>15</sub>FN<sub>2</sub>O<sub>5</sub>S</b> | 330.33  | 4.263 | 6 | 0 | 6  |
| <br><b>C<sub>17</sub>H<sub>13</sub>FN<sub>2</sub>O<sub>3</sub>S</b> | 344.36  | 5.413 | 4 | 0 | 4  |

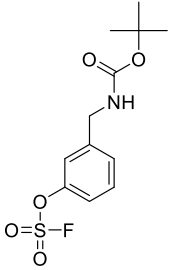
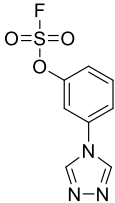
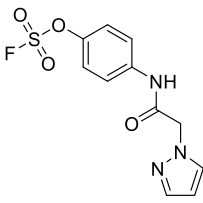
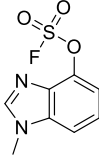
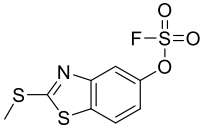
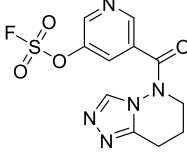


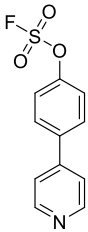
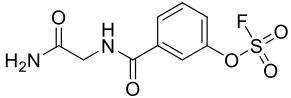
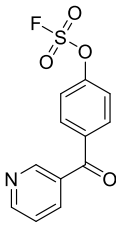
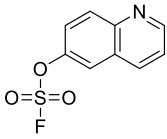
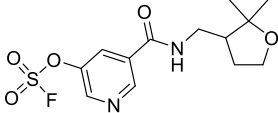
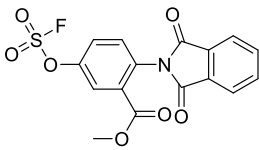
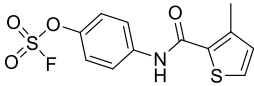
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|------------------------------------------------------------------------------------------------------------------------------------------------------|---------|-------|---|---|---|
| <br><b>C<sub>13</sub>H<sub>11</sub>FN<sub>2</sub>O<sub>4</sub>S</b> | 310.299 | 1.098 | 4 | 1 | 6 |
| <br><b>C<sub>15</sub>H<sub>13</sub>ClFNO<sub>4</sub>S</b>           | 357.78  | 3.398 | 3 | 1 | 7 |
| <br><b>C<sub>16</sub>H<sub>12</sub>FNO<sub>5</sub>S</b>             | 349.332 | 2.651 | 4 | 0 | 5 |
| <br><b>C<sub>12</sub>H<sub>10</sub>FNO<sub>3</sub>S</b>            | 267.274 | 3.15  | 3 | 1 | 4 |
| <br><b>C<sub>18</sub>H<sub>14</sub>FNO<sub>5</sub>S</b>           | 375.37  | 3.362 | 4 | 1 | 6 |
| <br><b>C<sub>9</sub>H<sub>6</sub>FNO<sub>3</sub>S</b>             | 227.209 | 1.345 | 3 | 0 | 2 |
| <br>                                                              | 243.212 | 1.237 | 5 | 0 | 3 |

|                                                                                     |                |              |          |          |          |
|-------------------------------------------------------------------------------------|----------------|--------------|----------|----------|----------|
|                                                                                     |                |              |          |          |          |
| <b>C<sub>8</sub>H<sub>6</sub>FN<sub>3</sub>O<sub>3</sub>S</b>                       |                |              |          |          |          |
|    | <b>274.284</b> | <b>2.701</b> | <b>4</b> | <b>1</b> | <b>3</b> |
| <b>C<sub>9</sub>H<sub>7</sub>FN<sub>2</sub>O<sub>3</sub>S<sub>2</sub></b>           |                |              |          |          |          |
|    | <b>284.257</b> | <b>2.503</b> | <b>3</b> | <b>0</b> | <b>4</b> |
| <b>C<sub>12</sub>H<sub>9</sub>FO<sub>5</sub>S</b>                                   |                |              |          |          |          |
|  | <b>259.269</b> | <b>2.477</b> | <b>3</b> | <b>0</b> | <b>3</b> |
| <b>C<sub>9</sub>H<sub>6</sub>FNO<sub>3</sub>S<sub>2</sub></b>                       |                |              |          |          |          |
|  | <b>295.284</b> | <b>2.491</b> | <b>3</b> | <b>1</b> | <b>5</b> |
| <b>C<sub>13</sub>H<sub>10</sub>FNO<sub>4</sub>S</b>                                 |                |              |          |          |          |
|  | <b>231.197</b> | <b>0.401</b> | <b>3</b> | <b>1</b> | <b>2</b> |
| <b>C<sub>8</sub>H<sub>6</sub>FNO<sub>4</sub>S</b>                                   |                |              |          |          |          |
|  | <b>247.24</b>  | <b>1.165</b> | <b>3</b> | <b>1</b> | <b>5</b> |

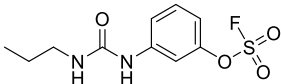
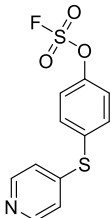
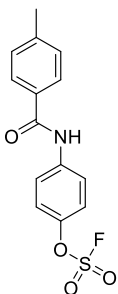
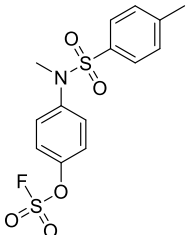
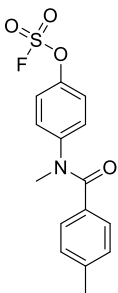
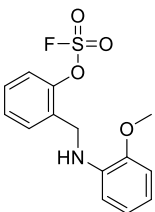
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| <b>C<sub>9</sub>H<sub>10</sub>FN<sub>2</sub>O<sub>4</sub>S</b>                      |                |              |          |          |          |
|    | <b>244.196</b> | <b>0.867</b> | <b>5</b> | <b>0</b> | <b>3</b> |
| <b>C<sub>8</sub>H<sub>5</sub>FN<sub>2</sub>O<sub>4</sub>S</b>                       |                |              |          |          |          |
|    | <b>312.311</b> | <b>3.108</b> | <b>4</b> | <b>0</b> | <b>5</b> |
| <b>C<sub>14</sub>H<sub>13</sub>FO<sub>5</sub>S</b>                                  |                |              |          |          |          |
|  | <b>305.32</b>  | <b>2.122</b> | <b>3</b> | <b>1</b> | <b>7</b> |
| <b>C<sub>12</sub>H<sub>16</sub>FN<sub>2</sub>O<sub>5</sub>S</b>                     |                |              |          |          |          |
|  | <b>360.4</b>   | <b>2.457</b> | <b>4</b> | <b>0</b> | <b>6</b> |
| <b>C<sub>15</sub>H<sub>21</sub>FN<sub>2</sub>O<sub>5</sub>S</b>                     |                |              |          |          |          |
|  | <b>245.224</b> | <b>0.806</b> | <b>3</b> | <b>1</b> | <b>2</b> |
| <b>C<sub>9</sub>H<sub>8</sub>FN<sub>2</sub>O<sub>4</sub>S</b>                       |                |              |          |          |          |

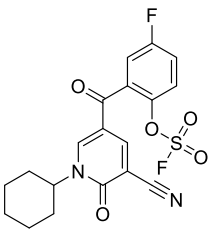
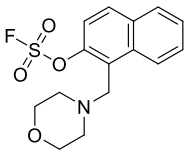
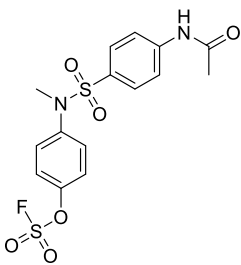
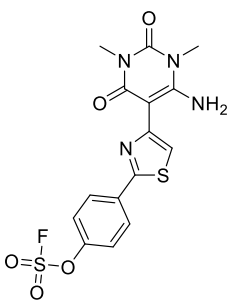
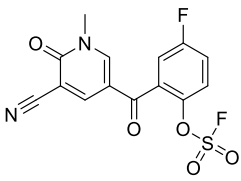
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|------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------|-------|---|---|---|
| <br><b>C<sub>9</sub>H<sub>9</sub>FO<sub>5</sub>S</b>                            | 248.224 | 1.992 | 3 | 0 | 4 |
| <br><b>C<sub>7</sub>H<sub>5</sub>FN<sub>4</sub>O<sub>3</sub>S</b>               | 244.2   | 1.047 | 6 | 0 | 3 |
| <br><b>C<sub>11</sub>H<sub>14</sub>FN<sub>2</sub>O<sub>4</sub>S</b>             | 275.294 | 1.527 | 3 | 1 | 7 |
| <br><b>C<sub>8</sub>H<sub>7</sub>FN<sub>2</sub>O<sub>3</sub>S</b>              | 230.213 | 0.698 | 4 | 0 | 2 |
| <br><b>C<sub>8</sub>H<sub>8</sub>FN<sub>2</sub>O<sub>4</sub>S</b>             | 233.213 | 0.536 | 3 | 1 | 4 |
| <br><b>C<sub>9</sub>H<sub>7</sub>FN<sub>2</sub>O<sub>3</sub>S<sub>2</sub></b> | 274.284 | 2.701 | 4 | 1 | 3 |

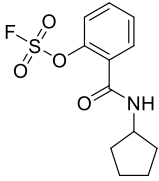
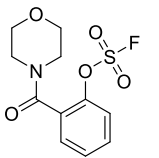
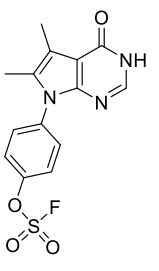
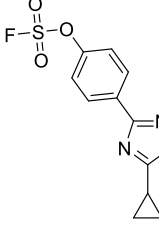
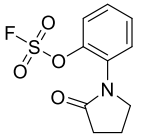
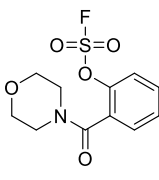
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|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------|--------|---|---|---|
| <br><chem>CC(C)(C)OC(=O)NCc1ccc(OS(=O)(=O)F)cc1</chem><br><b>C<sub>12</sub>H<sub>16</sub>FN<sub>1</sub>O<sub>5</sub>S</b>       | 305.32  | 2.122  | 3 | 1 | 7 |
| <br><chem>FOS(=O)(=O)c1ccc2c(c1)n[nH]2</chem><br><b>C<sub>8</sub>H<sub>6</sub>FN<sub>3</sub>O<sub>3</sub>S</b>                  | 243.212 | 0.641  | 5 | 0 | 3 |
| <br><chem>FOS(=O)(=O)c1ccc(NC(=O)Cn2cc[nH]2)cc1</chem><br><b>C<sub>11</sub>H<sub>10</sub>FN<sub>3</sub>O<sub>4</sub>S</b>      | 299.276 | 0.536  | 5 | 1 | 6 |
| <br><chem>Cn1cc[nH]1c2ccc(OS(=O)(=O)F)cc2</chem><br><b>C<sub>8</sub>H<sub>7</sub>FN<sub>2</sub>O<sub>3</sub>S</b>             | 230.213 | 0.698  | 4 | 0 | 2 |
| <br><chem>Cn1cc[nH]1c2ccc(OS(=O)(=O)F)cc2</chem><br><b>C<sub>8</sub>H<sub>6</sub>FN<sub>3</sub>O<sub>3</sub>S<sub>3</sub></b> | 279.318 | 3.321  | 3 | 0 | 3 |
| <br><chem>Cn1cc[nH]1c2ccc(OS(=O)(=O)F)cc2</chem><br><b>C<sub>11</sub>H<sub>10</sub>FN<sub>5</sub>O<sub>4</sub>S</b>           | 327.29  | -0.263 | 7 | 0 | 4 |

|                                                                                                                                                        |         |        |   |   |   |
|--------------------------------------------------------------------------------------------------------------------------------------------------------|---------|--------|---|---|---|
| <br><b>C<sub>11</sub>H<sub>8</sub>FO<sub>3</sub>S</b>                 | 253.247 | 2.023  | 3 | 0 | 3 |
| <br><b>C<sub>9</sub>H<sub>9</sub>FN<sub>2</sub>O<sub>5</sub>S</b>     | 276.238 | -0.557 | 4 | 2 | 6 |
| <br><b>C<sub>12</sub>H<sub>8</sub>FO<sub>4</sub>S</b>                 | 281.257 | 1.558  | 4 | 0 | 4 |
| <br><b>C<sub>9</sub>H<sub>6</sub>FO<sub>3</sub>S</b>                | 227.209 | 1.769  | 3 | 0 | 2 |
| <br><b>C<sub>13</sub>H<sub>17</sub>FN<sub>2</sub>O<sub>5</sub>S</b> | 332.346 | -0.046 | 5 | 1 | 6 |
| <br><b>C<sub>16</sub>H<sub>10</sub>FO<sub>7</sub>S</b>              | 379.314 | 2.123  | 5 | 0 | 5 |
| <br><b>C<sub>12</sub>H<sub>10</sub>FO<sub>4</sub>S<sub>2</sub></b>  | 315.333 | 2.96   | 3 | 1 | 5 |

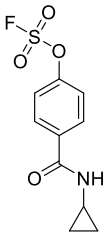
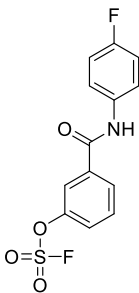
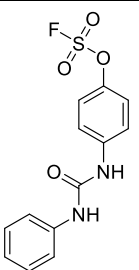
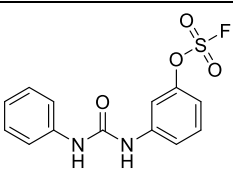
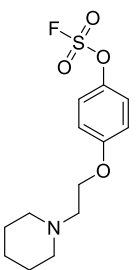


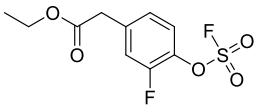
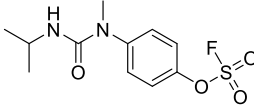
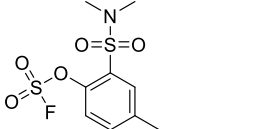
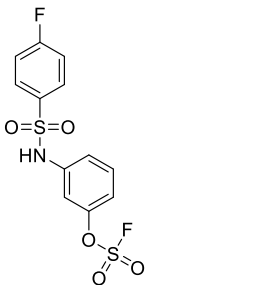
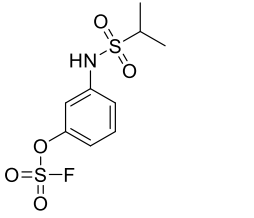
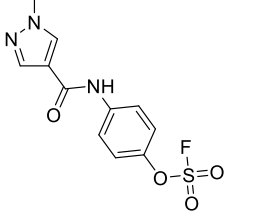
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|--------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------|-------|---|---|---|
| <br><b>C<sub>10</sub>H<sub>13</sub>FN<sub>2</sub>O<sub>4</sub>S</b>               | 276.282 | 1.325 | 3 | 2 | 7 |
| <br><b>C<sub>11</sub>H<sub>8</sub>FN<sub>3</sub>O<sub>3</sub>S<sub>2</sub></b>    | 285.307 | 2.451 | 3 | 0 | 4 |
| <br><b>C<sub>14</sub>H<sub>12</sub>FN<sub>2</sub>O<sub>4</sub>S</b>               | 309.311 | 2.978 | 3 | 1 | 5 |
| <br><b>C<sub>14</sub>H<sub>14</sub>FN<sub>3</sub>O<sub>5</sub>S<sub>2</sub></b> | 359.386 | 3.917 | 4 | 0 | 5 |
| <br><b>C<sub>15</sub>H<sub>14</sub>FN<sub>2</sub>O<sub>4</sub>S</b>             | 323.338 | 3.214 | 3 | 0 | 5 |
| <br><b>C<sub>15</sub>H<sub>14</sub>FN<sub>2</sub>O<sub>4</sub>S</b>             | 311.327 | 2.788 | 4 | 1 | 6 |

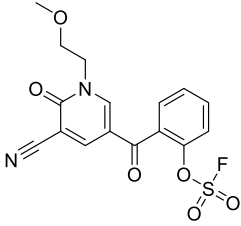
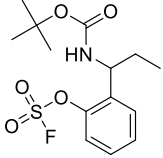
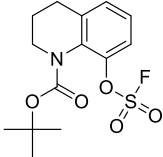
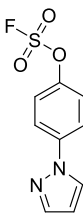
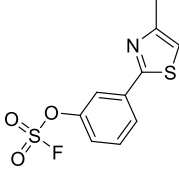
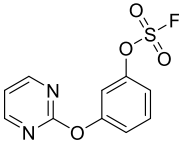
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|                                                                                     |                |              |          |          |          |
| <b>C<sub>14</sub>H<sub>14</sub>FN<sub>2</sub>O<sub>4</sub>S</b>                     |                |              |          |          |          |
|    | <b>422.403</b> | <b>2.336</b> | <b>6</b> | <b>0</b> | <b>6</b> |
| <b>C<sub>19</sub>H<sub>16</sub>F<sub>2</sub>N<sub>2</sub>O<sub>5</sub>S</b>         |                |              |          |          |          |
|    | <b>325.354</b> | <b>2.225</b> | <b>4</b> | <b>0</b> | <b>4</b> |
| <b>C<sub>15</sub>H<sub>16</sub>FN<sub>2</sub>O<sub>4</sub>S</b>                     |                |              |          |          |          |
|  | <b>402.411</b> | <b>2.918</b> | <b>5</b> | <b>1</b> | <b>7</b> |
| <b>C<sub>15</sub>H<sub>15</sub>FN<sub>2</sub>O<sub>6</sub>S<sub>2</sub></b>         |                |              |          |          |          |
|  | <b>412.41</b>  | <b>1.37</b>  | <b>6</b> | <b>1</b> | <b>4</b> |
| <b>C<sub>15</sub>H<sub>13</sub>FN<sub>4</sub>O<sub>5</sub>S<sub>2</sub></b>         |                |              |          |          |          |
|  | <b>354.284</b> | <b>0.788</b> | <b>6</b> | <b>0</b> | <b>5</b> |
| <b>C<sub>14</sub>H<sub>8</sub>F<sub>2</sub>N<sub>2</sub>O<sub>5</sub>S</b>          |                |              |          |          |          |

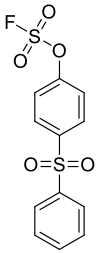
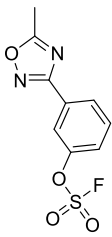
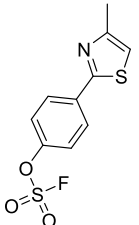
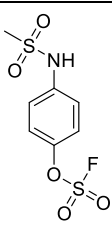
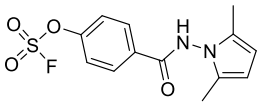
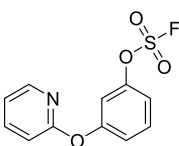
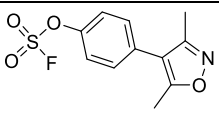
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|--------------------------------------------------------------------------------------------------------------------------------------------------------|---------|-------|---|---|---|
| <br><b>C<sub>12</sub>H<sub>14</sub>FN<sub>2</sub>O<sub>4</sub>S</b>   | 287.305 | 1.958 | 3 | 1 | 5 |
| <br><b>C<sub>11</sub>H<sub>12</sub>FN<sub>2</sub>O<sub>5</sub>S</b>   | 289.277 | 0.664 | 4 | 0 | 4 |
| <br><b>C<sub>14</sub>H<sub>12</sub>FN<sub>3</sub>O<sub>4</sub>S</b>   | 337.325 | 1.911 | 5 | 1 | 3 |
| <br><b>C<sub>11</sub>H<sub>9</sub>FN<sub>2</sub>O<sub>4</sub>S</b>  | 284.261 | 3.208 | 5 | 0 | 4 |
| <br><b>C<sub>10</sub>H<sub>10</sub>FN<sub>2</sub>O<sub>4</sub>S</b> | 259.251 | 0.974 | 3 | 0 | 3 |
| <br><b>C<sub>15</sub>H<sub>14</sub>FN<sub>2</sub>O<sub>5</sub>S</b> | 339.337 | 1.661 | 4 | 0 | 4 |

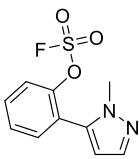
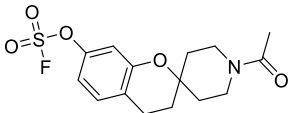
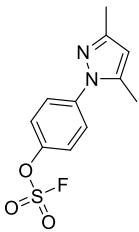
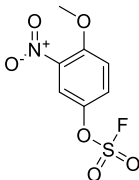
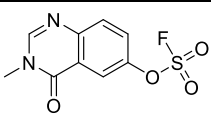
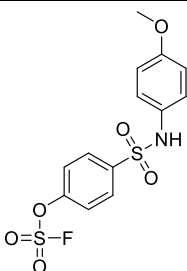


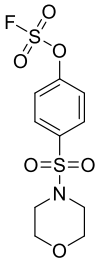
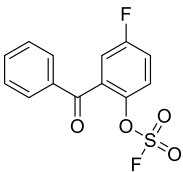
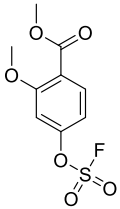
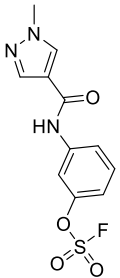
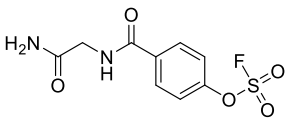
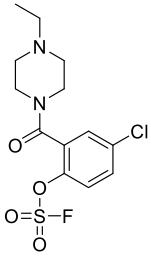
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|    | <b>259.251</b> | <b>1.123</b> | <b>3</b> | <b>1</b> | <b>5</b> |
| <b>C<sub>10</sub>H<sub>10</sub>FN<sub>2</sub>O<sub>4</sub>S</b>                     |                |              |          |          |          |
|    | <b>313.275</b> | <b>2.649</b> | <b>4</b> | <b>1</b> | <b>5</b> |
| <b>C<sub>13</sub>H<sub>9</sub>F<sub>2</sub>N<sub>2</sub>O<sub>4</sub>S</b>          |                |              |          |          |          |
|  | <b>310.299</b> | <b>2.164</b> | <b>3</b> | <b>2</b> | <b>6</b> |
| <b>C<sub>13</sub>H<sub>11</sub>FN<sub>2</sub>O<sub>4</sub>S</b>                     |                |              |          |          |          |
|  | <b>310.299</b> | <b>2.164</b> | <b>3</b> | <b>2</b> | <b>6</b> |
| <b>C<sub>13</sub>H<sub>11</sub>FN<sub>2</sub>O<sub>4</sub>S</b>                     |                |              |          |          |          |
|  | <b>303.348</b> | <b>2.291</b> | <b>4</b> | <b>0</b> | <b>6</b> |
| <b>C<sub>13</sub>H<sub>18</sub>FN<sub>2</sub>O<sub>4</sub>S</b>                     |                |              |          |          |          |

|                                                                                                                                                                   |         |       |   |   |   |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------|-------|---|---|---|
| <br><b>C<sub>10</sub>H<sub>10</sub>F<sub>2</sub>O<sub>5</sub>S</b>               | 280.242 | 1.946 | 4 | 0 | 6 |
| <br><b>C<sub>11</sub>H<sub>15</sub>FN<sub>2</sub>O<sub>4</sub>S</b>              | 290.309 | 1.393 | 3 | 1 | 6 |
| <br><b>C<sub>9</sub>H<sub>12</sub>FN<sub>2</sub>O<sub>5</sub>S<sub>2</sub></b>   | 297.315 | 1.452 | 4 | 0 | 4 |
| <br><b>C<sub>12</sub>H<sub>9</sub>F<sub>2</sub>NO<sub>5</sub>S<sub>2</sub></b>  | 349.323 | 2.25  | 5 | 1 | 5 |
| <br><b>C<sub>9</sub>H<sub>12</sub>FN<sub>2</sub>O<sub>5</sub>S<sub>2</sub></b> | 297.315 | 0.911 | 4 | 1 | 5 |
| <br><b>C<sub>11</sub>H<sub>10</sub>FN<sub>3</sub>O<sub>4</sub>S</b>            | 299.276 | 0.827 | 5 | 1 | 5 |

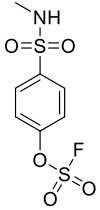
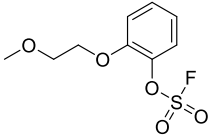
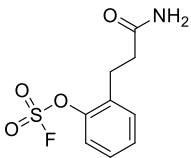
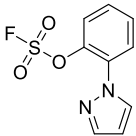
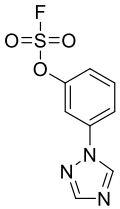
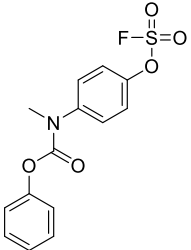
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|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------|-------|---|---|---|
|  <p><b>C<sub>16</sub>H<sub>13</sub>FN<sub>2</sub>O<sub>6</sub>S</b></p>              | 380.346 | 0.475 | 6 | 0 | 8 |
|  <p><b>C<sub>14</sub>H<sub>20</sub>FN<sub>2</sub>O<sub>5</sub>S</b></p>              | 333.374 | 2.927 | 3 | 1 | 8 |
|  <p><b>C<sub>14</sub>H<sub>18</sub>FN<sub>2</sub>O<sub>5</sub>S</b></p>              | 331.358 | 2.685 | 3 | 0 | 5 |
|  <p><b>C<sub>9</sub>H<sub>7</sub>FN<sub>2</sub>O<sub>3</sub>S</b></p>              | 242.224 | 1.685 | 4 | 0 | 3 |
|  <p><b>C<sub>10</sub>H<sub>8</sub>FN<sub>2</sub>O<sub>3</sub>S<sub>2</sub></b></p> | 273.296 | 3.181 | 3 | 0 | 3 |
|  <p><b>C<sub>10</sub>H<sub>7</sub>FN<sub>2</sub>O<sub>4</sub>S</b></p>             | 270.234 | 1.798 | 5 | 0 | 4 |

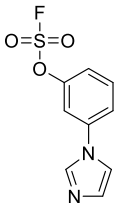
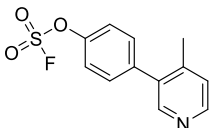
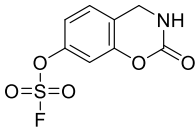
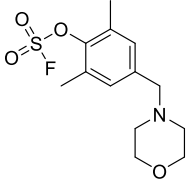
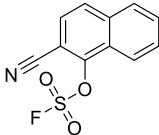
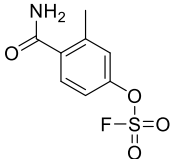
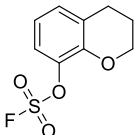
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|--------------------------------------------------------------------------------------------------------------------------------------------------------|---------|--------|---|---|---|
| <br><b>C<sub>12</sub>H<sub>9</sub>FO<sub>5</sub>S<sub>2</sub></b>     | 316.317 | 2.576  | 4 | 0 | 4 |
| <br><b>C<sub>9</sub>H<sub>7</sub>FN<sub>2</sub>O<sub>4</sub>S</b>     | 258.223 | 2.647  | 5 | 0 | 3 |
| <br><b>C<sub>10</sub>H<sub>8</sub>FNO<sub>3</sub>S<sub>2</sub></b>   | 273.296 | 3.181  | 3 | 0 | 3 |
| <br><b>C<sub>7</sub>H<sub>8</sub>FNO<sub>5</sub>S<sub>2</sub></b>   | 269.261 | -0.094 | 4 | 1 | 4 |
| <br><b>C<sub>13</sub>H<sub>13</sub>FN<sub>2</sub>O<sub>4</sub>S</b> | 312.315 | 2.208  | 4 | 1 | 5 |
| <br><b>C<sub>11</sub>H<sub>8</sub>FNO<sub>4</sub>S</b>              | 269.246 | 2.601  | 4 | 0 | 4 |
| <br><b>C<sub>11</sub>H<sub>8</sub>FNO<sub>4</sub>S</b>              | 271.262 | 2.574  | 4 | 0 | 3 |

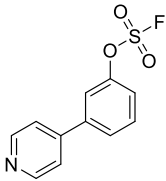
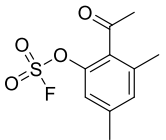
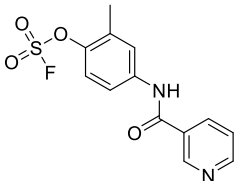
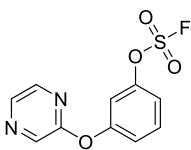
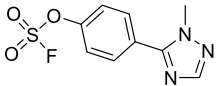
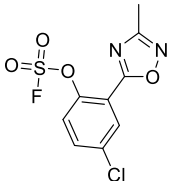
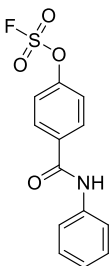
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|-------------------------------------------------------------------------------------|----------------|--------------|----------|----------|----------|
| <b>C<sub>11</sub>H<sub>10</sub>FN<sub>2</sub>O<sub>4</sub>S</b>                     |                |              |          |          |          |
|    | <b>256.251</b> | <b>1.753</b> | <b>4</b> | <b>0</b> | <b>3</b> |
| <b>C<sub>10</sub>H<sub>9</sub>FN<sub>2</sub>O<sub>3</sub>S</b>                      |                |              |          |          |          |
|    | <b>343.369</b> | <b>1.052</b> | <b>4</b> | <b>0</b> | <b>3</b> |
| <b>C<sub>15</sub>H<sub>18</sub>FN<sub>2</sub>O<sub>5</sub>S</b>                     |                |              |          |          |          |
|   | <b>270.278</b> | <b>2.726</b> | <b>4</b> | <b>0</b> | <b>3</b> |
| <b>C<sub>11</sub>H<sub>11</sub>FN<sub>2</sub>O<sub>3</sub>S</b>                     |                |              |          |          |          |
|  | <b>251.184</b> | <b>2.575</b> | <b>4</b> | <b>0</b> | <b>4</b> |
| <b>C<sub>7</sub>H<sub>6</sub>FN<sub>2</sub>O<sub>6</sub>S</b>                       |                |              |          |          |          |
|  | <b>258.223</b> | <b>0.748</b> | <b>4</b> | <b>0</b> | <b>2</b> |
| <b>C<sub>9</sub>H<sub>7</sub>FN<sub>2</sub>O<sub>4</sub>S</b>                       |                |              |          |          |          |
|  | <b>361.358</b> | <b>1.966</b> | <b>5</b> | <b>1</b> | <b>6</b> |
| <b>C<sub>13</sub>H<sub>12</sub>FN<sub>2</sub>O<sub>6</sub>S<sub>2</sub></b>         |                |              |          |          |          |

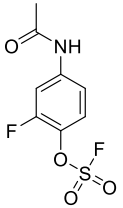
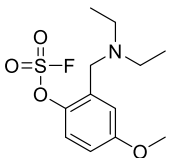
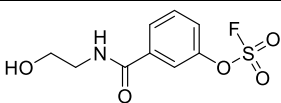
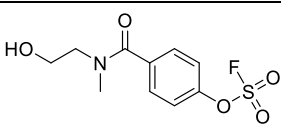
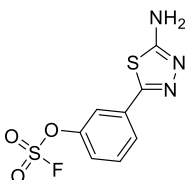
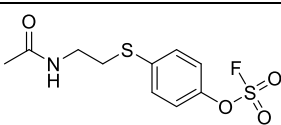
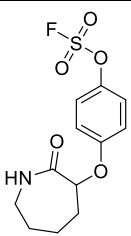
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|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------|--------|---|---|---|
| <br><chem>CN(C)c1ccc(cc1)S(=O)(=O)Oc2ccc(cc2)S(=O)(=O)F</chem><br><b>C<sub>10</sub>H<sub>12</sub>FNO<sub>6</sub>S<sub>2</sub></b>     | 325.325 | 0.565  | 5 | 0 | 4 |
| <br><chem>CN(C)c1ccc(cc1)S(=O)(=O)Oc2ccc(cc2)S(=O)(=O)F</chem><br><b>C<sub>13</sub>H<sub>8</sub>F<sub>2</sub>O<sub>4</sub>S</b>       | 298.26  | 3.053  | 4 | 0 | 4 |
| <br><chem>CN(C)c1ccc(cc1)S(=O)(=O)Oc2ccc(cc2)S(=O)(=O)F</chem><br><b>C<sub>9</sub>H<sub>9</sub>FO<sub>6</sub>S</b>                   | 264.223 | 1.379  | 4 | 0 | 5 |
| <br><chem>CN(C)c1ccc(cc1)S(=O)(=O)Oc2ccc(cc2)S(=O)(=O)F</chem><br><b>C<sub>11</sub>H<sub>10</sub>FN<sub>3</sub>O<sub>4</sub>S</b>   | 299.276 | 0.827  | 5 | 1 | 5 |
| <br><chem>CN(C)c1ccc(cc1)S(=O)(=O)Oc2ccc(cc2)S(=O)(=O)F</chem><br><b>C<sub>9</sub>H<sub>9</sub>FN<sub>2</sub>O<sub>5</sub>S</b>     | 276.238 | -0.557 | 4 | 2 | 6 |
| <br><chem>CN(C)c1ccc(cc1)S(=O)(=O)Oc2ccc(cc2)S(=O)(=O)F</chem><br><b>C<sub>13</sub>H<sub>16</sub>ClFN<sub>2</sub>O<sub>4</sub>S</b> | 350.789 | 1.715  | 4 | 0 | 5 |

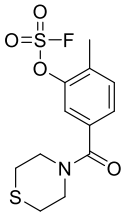
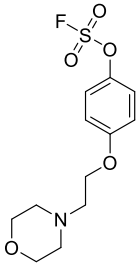
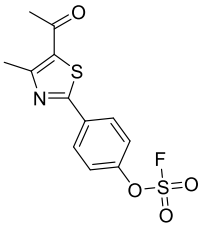
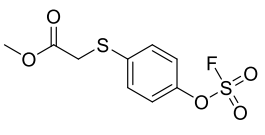
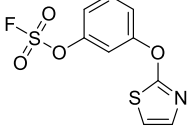
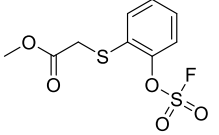


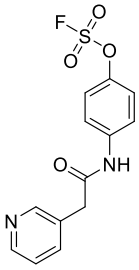
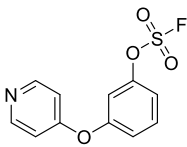
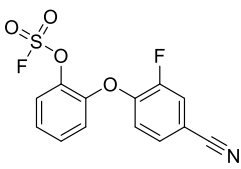
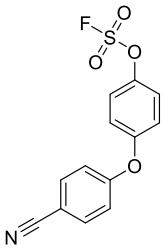
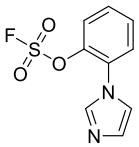
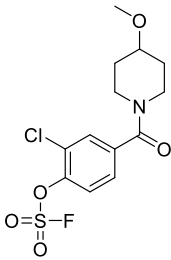
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|----------------------------------------------------------------------------------------------------------------------------------------------------------------|---------|-------|---|---|---|
| <br><b>C<sub>7</sub>H<sub>8</sub>FN<sub>2</sub>O<sub>5</sub>S<sub>2</sub></b> | 269.261 | 2.154 | 4 | 1 | 4 |
| <br><b>C<sub>9</sub>H<sub>11</sub>FO<sub>5</sub>S</b>                         | 250.24  | 1.403 | 4 | 0 | 6 |
| <br><b>C<sub>9</sub>H<sub>10</sub>FN<sub>2</sub>O<sub>4</sub>S</b>            | 247.24  | 0.953 | 3 | 1 | 5 |
| <br><b>C<sub>9</sub>H<sub>7</sub>FN<sub>2</sub>O<sub>3</sub>S</b>            | 242.224 | 1.685 | 4 | 0 | 3 |
| <br><b>C<sub>8</sub>H<sub>6</sub>FN<sub>3</sub>O<sub>3</sub>S</b>           | 243.212 | 1.237 | 5 | 0 | 3 |
| <br><b>C<sub>14</sub>H<sub>12</sub>FN<sub>2</sub>O<sub>5</sub>S</b>         | 325.31  | 3.078 | 3 | 0 | 6 |

|                                                                                                                                                       |         |       |   |   |   |
|-------------------------------------------------------------------------------------------------------------------------------------------------------|---------|-------|---|---|---|
| <br><b>C<sub>9</sub>H<sub>7</sub>FN<sub>2</sub>O<sub>3</sub>S</b>    | 242.224 | 0.885 | 4 | 0 | 3 |
| <br><b>C<sub>12</sub>H<sub>10</sub>FN<sub>2</sub>O<sub>3</sub>S</b>  | 267.274 | 2.511 | 3 | 0 | 3 |
| <br><b>C<sub>8</sub>H<sub>6</sub>FN<sub>2</sub>O<sub>5</sub>S</b>    | 247.196 | 0.877 | 3 | 1 | 2 |
| <br><b>C<sub>13</sub>H<sub>18</sub>FN<sub>2</sub>O<sub>4</sub>S</b> | 303.348 | 2.202 | 4 | 0 | 4 |
| <br><b>C<sub>11</sub>H<sub>6</sub>FN<sub>2</sub>O<sub>3</sub>S</b> | 251.231 | 2.716 | 3 | 0 | 3 |
| <br><b>C<sub>8</sub>H<sub>8</sub>FN<sub>2</sub>O<sub>4</sub>S</b>  | 233.213 | 1.079 | 3 | 1 | 3 |
| <br><b>C<sub>9</sub>H<sub>9</sub>FO<sub>4</sub>S</b>               | 232.225 | 1.954 | 3 | 0 | 2 |

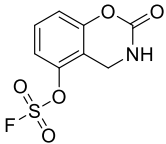
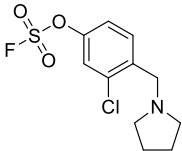
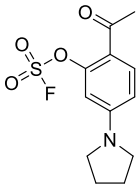
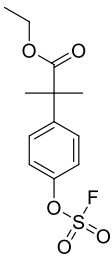
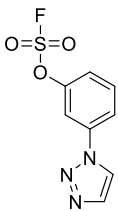
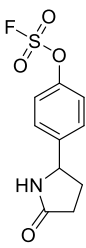
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| <br><b>C<sub>11</sub>H<sub>8</sub>FN<sub>2</sub>O<sub>3</sub>S</b>    | 253.247 | 2.023 | 3 | 0 | 3 |
| <br><b>C<sub>10</sub>H<sub>11</sub>FO<sub>4</sub>S</b>                | 246.252 | 1.972 | 3 | 0 | 3 |
| <br><b>C<sub>13</sub>H<sub>11</sub>FN<sub>2</sub>O<sub>4</sub>S</b>   | 310.299 | 1.641 | 4 | 1 | 5 |
| <br><b>C<sub>10</sub>H<sub>7</sub>FN<sub>2</sub>O<sub>4</sub>S</b>   | 270.234 | 1.264 | 5 | 0 | 4 |
| <br><b>C<sub>9</sub>H<sub>8</sub>FN<sub>3</sub>O<sub>3</sub>S</b>   | 257.239 | 1.627 | 5 | 0 | 3 |
| <br><b>C<sub>9</sub>H<sub>6</sub>ClFN<sub>2</sub>O<sub>4</sub>S</b> | 292.665 | 2.933 | 5 | 0 | 3 |
| <br><b>C<sub>13</sub>H<sub>10</sub>FN<sub>2</sub>O<sub>4</sub>S</b> | 295.284 | 2.491 | 3 | 1 | 5 |

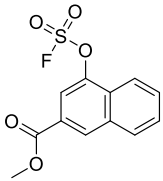
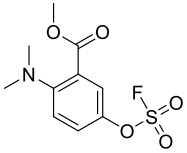
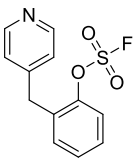
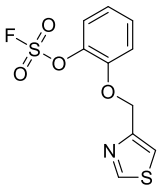
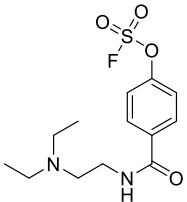
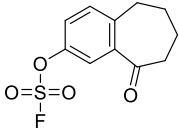
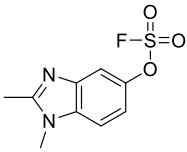
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|------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------|--------------|----------|----------|----------|
| <br><b>C<sub>8</sub>H<sub>7</sub>F<sub>2</sub>NO<sub>4</sub>S</b>               | <b>251.204</b> | <b>0.751</b> | <b>4</b> | <b>1</b> | <b>4</b> |
| <br><b>C<sub>12</sub>H<sub>18</sub>FNO<sub>4</sub>S</b>                         | <b>291.337</b> | <b>2.177</b> | <b>4</b> | <b>0</b> | <b>7</b> |
| <br><b>C<sub>9</sub>H<sub>10</sub>FNO<sub>5</sub>S</b>                          | <b>263.239</b> | <b>0.31</b>  | <b>4</b> | <b>2</b> | <b>6</b> |
| <br><b>C<sub>10</sub>H<sub>12</sub>FNO<sub>5</sub>S</b>                        | <b>277.266</b> | <b>0.546</b> | <b>4</b> | <b>1</b> | <b>6</b> |
| <br><b>C<sub>8</sub>H<sub>6</sub>FN<sub>3</sub>O<sub>3</sub>S<sub>2</sub></b> | <b>275.272</b> | <b>2.411</b> | <b>5</b> | <b>1</b> | <b>3</b> |
| <br><b>C<sub>10</sub>H<sub>12</sub>FNO<sub>4</sub>S<sub>2</sub></b>           | <b>293.327</b> | <b>1.159</b> | <b>3</b> | <b>1</b> | <b>7</b> |
| <br><b>C<sub>12</sub>H<sub>14</sub>FNO<sub>5</sub>S</b>                       | <b>303.304</b> | <b>1.297</b> | <b>4</b> | <b>1</b> | <b>4</b> |

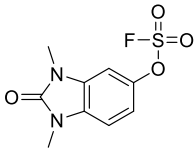
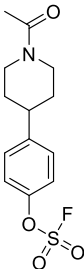
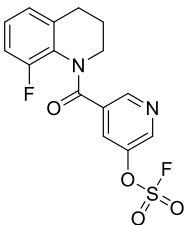
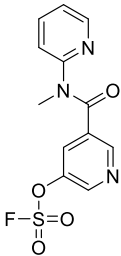
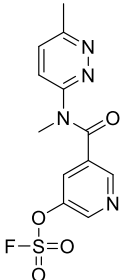
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|-------------------------------------------------------------------------------------------------------------------------------------------------------|---------|-------|---|---|---|
| <br><b>C<sub>12</sub>H<sub>14</sub>FNO<sub>4</sub>S<sub>2</sub></b>  | 319.365 | 1.872 | 3 | 0 | 4 |
| <br><b>C<sub>12</sub>H<sub>16</sub>FNO<sub>5</sub>S</b>              | 305.32  | 1.159 | 5 | 0 | 6 |
| <br><b>C<sub>12</sub>H<sub>10</sub>FNO<sub>4</sub>S<sub>2</sub></b> | 315.333 | 2.549 | 4 | 0 | 4 |
| <br><b>C<sub>9</sub>H<sub>9</sub>FO<sub>5</sub>S<sub>2</sub></b>   | 280.284 | 1.654 | 3 | 0 | 6 |
| <br><b>C<sub>9</sub>H<sub>6</sub>FNO<sub>4</sub>S<sub>2</sub></b>  | 275.268 | 2.942 | 4 | 0 | 4 |
| <br><b>C<sub>9</sub>H<sub>9</sub>FO<sub>5</sub>S<sub>2</sub></b>   | 280.284 | 1.654 | 3 | 0 | 6 |

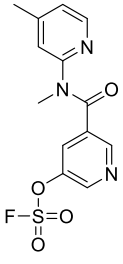
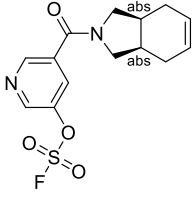
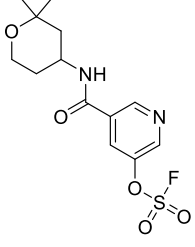
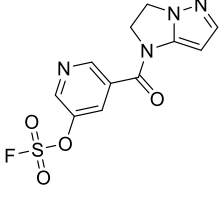
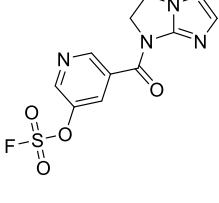
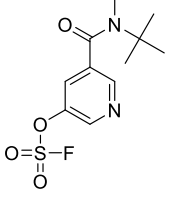
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|-------------------------------------------------------------------------------------------------------------------------------------------------------|---------|-------|---|---|---|
| <br><b>C<sub>13</sub>H<sub>11</sub>FN<sub>2</sub>O<sub>4</sub>S</b>  | 310.299 | 1.098 | 4 | 1 | 6 |
| <br><b>C<sub>11</sub>H<sub>8</sub>FN<sub>2</sub>O<sub>4</sub>S</b>   | 269.246 | 1.885 | 4 | 0 | 4 |
| <br><b>C<sub>13</sub>H<sub>7</sub>F<sub>2</sub>NO<sub>4</sub>S</b>   | 311.259 | 3.414 | 5 | 0 | 5 |
| <br><b>C<sub>13</sub>H<sub>8</sub>FN<sub>2</sub>O<sub>4</sub>S</b> | 293.268 | 3.256 | 4 | 0 | 5 |
| <br><b>C<sub>9</sub>H<sub>7</sub>FN<sub>2</sub>O<sub>3</sub>S</b>  | 242.224 | 0.885 | 4 | 0 | 3 |
| <br><b>C<sub>13</sub>H<sub>15</sub>ClFNO<sub>5</sub>S</b>          | 351.773 | 1.413 | 4 | 0 | 5 |

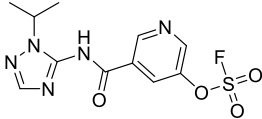
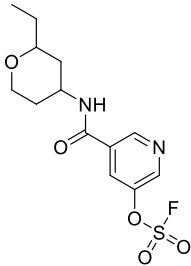
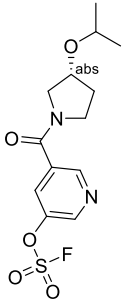
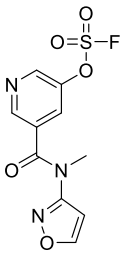
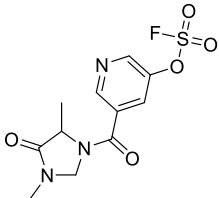


|                                                                                                                                                        |         |       |   |   |   |
|--------------------------------------------------------------------------------------------------------------------------------------------------------|---------|-------|---|---|---|
| <br><b>C<sub>8</sub>H<sub>6</sub>FN<sub>2</sub>O<sub>5</sub>S</b>     | 247.196 | 0.877 | 3 | 1 | 2 |
| <br><b>C<sub>11</sub>H<sub>13</sub>ClFNO<sub>3</sub>S</b>             | 293.737 | 2.501 | 3 | 0 | 4 |
| <br><b>C<sub>12</sub>H<sub>14</sub>FN<sub>2</sub>O<sub>4</sub>S</b>   | 287.305 | 1.598 | 4 | 0 | 4 |
| <br><b>C<sub>12</sub>H<sub>15</sub>FO<sub>5</sub>S</b>               | 290.305 | 3.061 | 3 | 0 | 6 |
| <br><b>C<sub>8</sub>H<sub>6</sub>FN<sub>3</sub>O<sub>3</sub>S</b>   | 243.212 | 1.291 | 5 | 0 | 3 |
| <br><b>C<sub>10</sub>H<sub>10</sub>FN<sub>2</sub>O<sub>4</sub>S</b> | 259.251 | 0.788 | 3 | 1 | 3 |

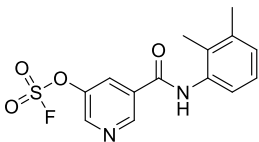
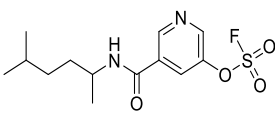
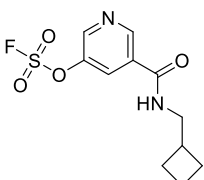
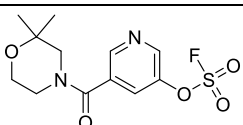
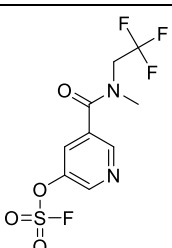
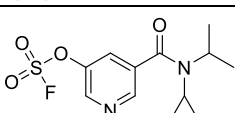
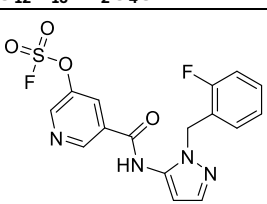
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|------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------|-------|---|---|---|
| <br><b>C<sub>12</sub>H<sub>9</sub>FO<sub>5</sub>S</b>                           | 284.257 | 2.503 | 3 | 0 | 4 |
| <br><b>C<sub>10</sub>H<sub>12</sub>FN<sub>2</sub>O<sub>5</sub>S</b>             | 277.266 | 1.79  | 4 | 0 | 5 |
| <br><b>C<sub>12</sub>H<sub>10</sub>FN<sub>3</sub>O<sub>3</sub>S</b>             | 267.274 | 2.441 | 3 | 0 | 4 |
| <br><b>C<sub>10</sub>H<sub>8</sub>FN<sub>2</sub>O<sub>4</sub>S<sub>2</sub></b> | 289.295 | 2.453 | 4 | 0 | 5 |
| <br><b>C<sub>13</sub>H<sub>19</sub>FN<sub>2</sub>O<sub>4</sub>S</b>           | 318.363 | 1.503 | 4 | 1 | 9 |
| <br><b>C<sub>11</sub>H<sub>11</sub>FO<sub>4</sub>S</b>                        | 258.263 | 2.057 | 3 | 0 | 2 |
| <br><b>C<sub>9</sub>H<sub>9</sub>FN<sub>2</sub>O<sub>3</sub>S</b>             | 244.24  | 1.368 | 4 | 0 | 2 |

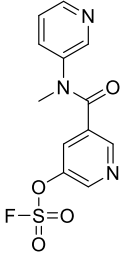
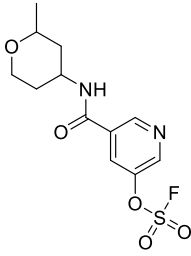
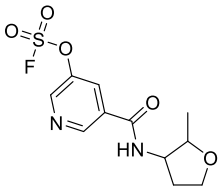
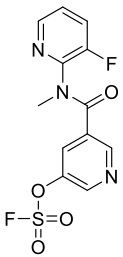
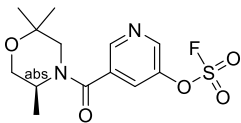
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|-------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------|--------------|----------|----------|----------|
| <br><b>C<sub>9</sub>H<sub>9</sub>FN<sub>2</sub>O<sub>4</sub>S</b>                | <b>260.239</b> | <b>0.602</b> | <b>3</b> | <b>0</b> | <b>2</b> |
| <br><b>C<sub>13</sub>H<sub>16</sub>FNO<sub>4</sub>S</b>                          | <b>301.332</b> | <b>1.416</b> | <b>3</b> | <b>0</b> | <b>4</b> |
| <br><b>C<sub>15</sub>H<sub>12</sub>F<sub>2</sub>N<sub>2</sub>O<sub>4</sub>S</b> | <b>354.328</b> | <b>1.943</b> | <b>5</b> | <b>0</b> | <b>4</b> |
| <br><b>C<sub>12</sub>H<sub>10</sub>FN<sub>3</sub>O<sub>4</sub>S</b>            | <b>311.287</b> | <b>0.768</b> | <b>5</b> | <b>0</b> | <b>5</b> |
| <br><b>C<sub>12</sub>H<sub>11</sub>FN<sub>4</sub>O<sub>4</sub>S</b>            | <b>326.302</b> | <b>1.079</b> | <b>6</b> | <b>0</b> | <b>5</b> |

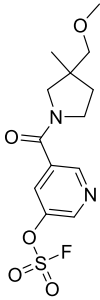
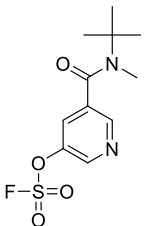
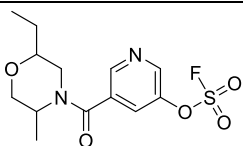
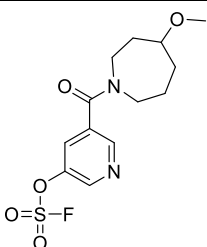
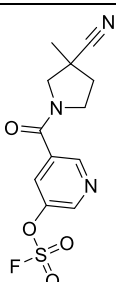
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|--------------------------------------------------------------------------------------------------------------------------------------------------------|---------|--------|---|---|---|
| <br><b>C<sub>13</sub>H<sub>12</sub>FN<sub>3</sub>O<sub>4</sub>S</b>   | 325.314 | 1.255  | 5 | 0 | 5 |
| <br><b>C<sub>14</sub>H<sub>15</sub>FN<sub>2</sub>O<sub>4</sub>S</b>   | 326.342 | 0.856  | 4 | 0 | 4 |
| <br><b>C<sub>13</sub>H<sub>17</sub>FN<sub>2</sub>O<sub>5</sub>S</b>  | 332.346 | -0.181 | 5 | 1 | 5 |
| <br><b>C<sub>11</sub>H<sub>9</sub>FN<sub>4</sub>O<sub>4</sub>S</b>  | 312.275 | -0.33  | 6 | 0 | 4 |
| <br><b>C<sub>11</sub>H<sub>9</sub>FN<sub>4</sub>O<sub>4</sub>S</b>  | 312.275 | -0.337 | 6 | 0 | 4 |
| <br><b>C<sub>12</sub>H<sub>17</sub>FN<sub>2</sub>O<sub>4</sub>S</b> | 304.336 | 0.939  | 4 | 0 | 6 |

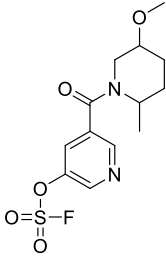
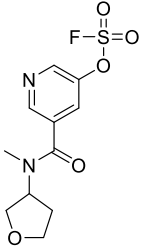
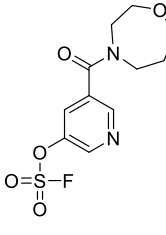
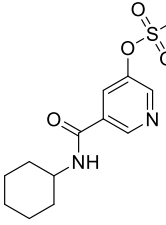
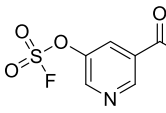
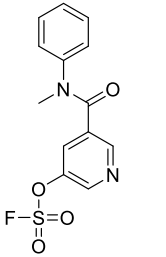
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|--------------------------------------------------------------------------------------------------------------------------------------------------------|---------|--------|---|---|---|
| <br><b>C<sub>11</sub>H<sub>12</sub>FN<sub>5</sub>O<sub>4</sub>S</b>   | 329.306 | 0.679  | 7 | 1 | 6 |
| <br><b>C<sub>13</sub>H<sub>17</sub>FN<sub>2</sub>O<sub>5</sub>S</b>   | 332.346 | 0.087  | 5 | 1 | 6 |
| <br><b>C<sub>13</sub>H<sub>17</sub>FN<sub>2</sub>O<sub>5</sub>S</b>  | 332.346 | 0.069  | 5 | 0 | 6 |
| <br><b>C<sub>10</sub>H<sub>8</sub>FN<sub>3</sub>O<sub>5</sub>S</b>  | 301.248 | 0.278  | 6 | 0 | 5 |
| <br><b>C<sub>11</sub>H<sub>12</sub>FN<sub>3</sub>O<sub>5</sub>S</b> | 317.291 | -0.662 | 5 | 0 | 4 |

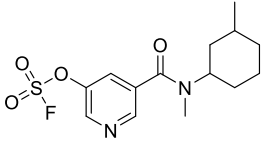
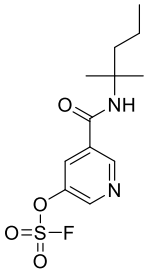
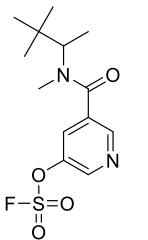
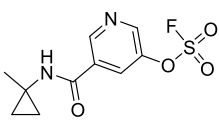
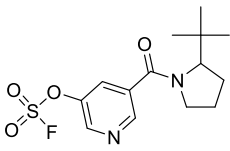
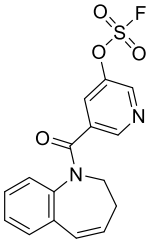


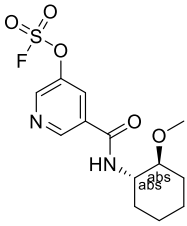
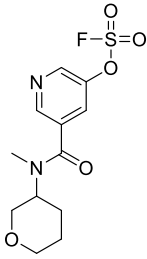
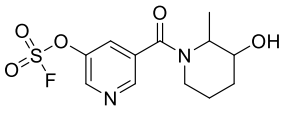
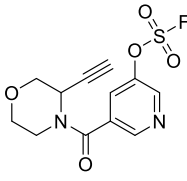
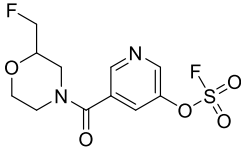
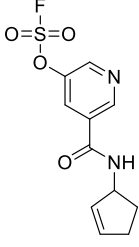
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| <b>C<sub>12</sub>H<sub>15</sub>FN<sub>2</sub>O<sub>5</sub>S</b>                     |                |               |          |          |          |
|    | <b>324.326</b> | <b>2.128</b>  | <b>4</b> | <b>1</b> | <b>5</b> |
| <b>C<sub>14</sub>H<sub>13</sub>FN<sub>2</sub>O<sub>4</sub>S</b>                     |                |               |          |          |          |
|    | <b>318.363</b> | <b>1.797</b>  | <b>4</b> | <b>1</b> | <b>8</b> |
| <b>C<sub>13</sub>H<sub>19</sub>FN<sub>2</sub>O<sub>4</sub>S</b>                     |                |               |          |          |          |
|    | <b>288.293</b> | <b>0.632</b>  | <b>4</b> | <b>1</b> | <b>6</b> |
| <b>C<sub>11</sub>H<sub>13</sub>FN<sub>2</sub>O<sub>4</sub>S</b>                     |                |               |          |          |          |
|  | <b>318.319</b> | <b>-0.137</b> | <b>5</b> | <b>0</b> | <b>4</b> |
| <b>C<sub>12</sub>H<sub>15</sub>FN<sub>2</sub>O<sub>5</sub>S</b>                     |                |               |          |          |          |
|  | <b>316.227</b> | <b>0.705</b>  | <b>7</b> | <b>0</b> | <b>6</b> |
| <b>C<sub>9</sub>H<sub>8</sub>F<sub>4</sub>N<sub>2</sub>O<sub>4</sub>S</b>           |                |               |          |          |          |
|  | <b>302.32</b>  | <b>0.678</b>  | <b>4</b> | <b>0</b> | <b>6</b> |
| <b>C<sub>12</sub>H<sub>15</sub>FN<sub>2</sub>O<sub>4</sub>S</b>                     |                |               |          |          |          |
|  | <b>394.353</b> | <b>1.569</b>  | <b>7</b> | <b>1</b> | <b>7</b> |

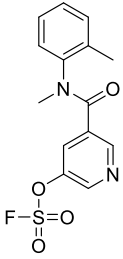
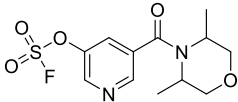
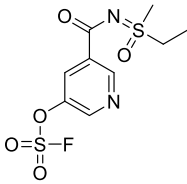
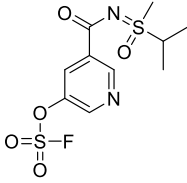
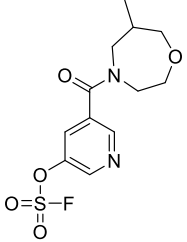
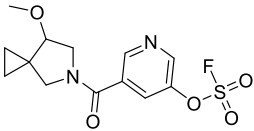
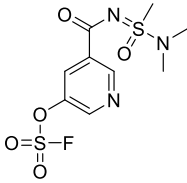
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|-------------------------------------------------------------------------------------|----------------|---------------|----------|----------|----------|
|                                                                                     |                |               |          |          |          |
| <b>C<sub>16</sub>H<sub>12</sub>F<sub>2</sub>N<sub>4</sub>O<sub>4</sub>S</b>         |                |               |          |          |          |
|    | <b>311.287</b> | <b>0.052</b>  | <b>5</b> | <b>0</b> | <b>5</b> |
| <b>C<sub>12</sub>H<sub>10</sub>FN<sub>3</sub>O<sub>4</sub>S</b>                     |                |               |          |          |          |
|   | <b>318.319</b> | <b>-0.399</b> | <b>5</b> | <b>1</b> | <b>5</b> |
| <b>C<sub>12</sub>H<sub>15</sub>FN<sub>2</sub>O<sub>5</sub>S</b>                     |                |               |          |          |          |
|  | <b>304.292</b> | <b>-0.505</b> | <b>5</b> | <b>1</b> | <b>5</b> |
| <b>C<sub>11</sub>H<sub>13</sub>FN<sub>2</sub>O<sub>5</sub>S</b>                     |                |               |          |          |          |
|  | <b>329.278</b> | <b>0.926</b>  | <b>6</b> | <b>0</b> | <b>5</b> |
| <b>C<sub>12</sub>H<sub>9</sub>F<sub>2</sub>N<sub>3</sub>O<sub>4</sub>S</b>          |                |               |          |          |          |
|  | <b>332.346</b> | <b>0.181</b>  | <b>5</b> | <b>0</b> | <b>4</b> |
| <b>C<sub>13</sub>H<sub>17</sub>FN<sub>2</sub>O<sub>5</sub>S</b>                     |                |               |          |          |          |

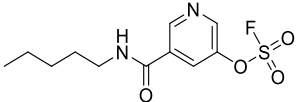
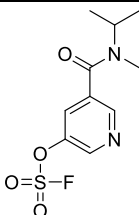
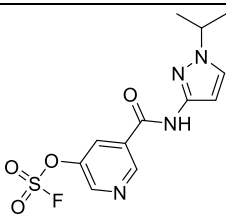
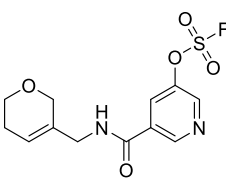
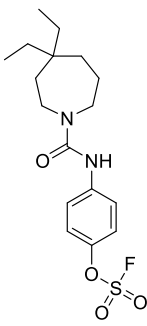
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|--------------------------------------------------------------------------------------------------------------------------------------------------------|---------|--------|---|---|---|
| <br><b>C<sub>13</sub>H<sub>17</sub>FN<sub>2</sub>O<sub>5</sub>S</b>   | 332.346 | 0.279  | 5 | 0 | 6 |
| <br><b>C<sub>11</sub>H<sub>15</sub>FN<sub>2</sub>O<sub>4</sub>S</b>   | 290.309 | 0.6    | 4 | 0 | 5 |
| <br><b>C<sub>13</sub>H<sub>17</sub>FN<sub>2</sub>O<sub>5</sub>S</b>  | 332.346 | 0.449  | 5 | 0 | 5 |
| <br><b>C<sub>13</sub>H<sub>17</sub>FN<sub>2</sub>O<sub>5</sub>S</b> | 332.346 | -0.028 | 5 | 0 | 5 |
| <br><b>C<sub>12</sub>H<sub>12</sub>FN<sub>3</sub>O<sub>4</sub>S</b> | 313.303 | 0.526  | 5 | 0 | 5 |

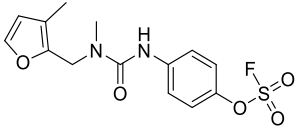
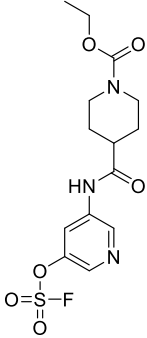
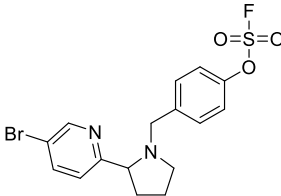
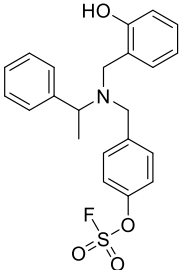
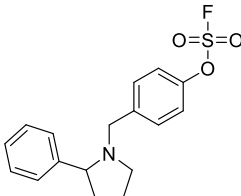
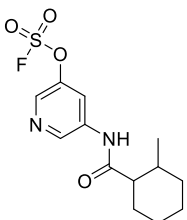
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|--------------------------------------------------------------------------------------------------------------------------------------------------------|---------|--------|---|---|---|
| <br><b>C<sub>13</sub>H<sub>17</sub>FN<sub>2</sub>O<sub>5</sub>S</b>   | 332.346 | 0.185  | 5 | 0 | 5 |
| <br><b>C<sub>11</sub>H<sub>13</sub>FN<sub>2</sub>O<sub>5</sub>S</b>   | 304.292 | -0.588 | 5 | 0 | 5 |
| <br><b>C<sub>13</sub>H<sub>17</sub>FN<sub>2</sub>O<sub>5</sub>S</b>  | 332.346 | 0.237  | 5 | 0 | 5 |
| <br><b>C<sub>12</sub>H<sub>15</sub>FN<sub>2</sub>O<sub>4</sub>S</b> | 302.32  | 1.038  | 4 | 1 | 5 |
| <br><b>C<sub>12</sub>H<sub>15</sub>FN<sub>2</sub>O<sub>4</sub>S</b> | 302.32  | 0.777  | 4 | 0 | 4 |
| <br><b>C<sub>13</sub>H<sub>11</sub>FN<sub>2</sub>O<sub>4</sub>S</b> | 310.299 | 1.389  | 4 | 0 | 5 |

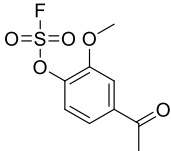
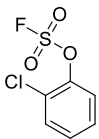
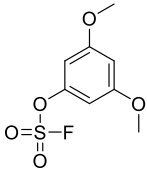
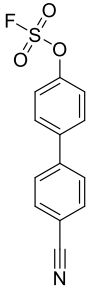
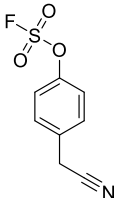
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|--------------------------------------------------------------------------------------------------------------------------------------------------------|----------------|--------------|----------|----------|----------|
| <br><b>C<sub>14</sub>H<sub>19</sub>FN<sub>2</sub>O<sub>4</sub>S</b>   | <b>330.374</b> | <b>1.604</b> | <b>4</b> | <b>0</b> | <b>5</b> |
| <br><b>C<sub>12</sub>H<sub>17</sub>FN<sub>2</sub>O<sub>4</sub>S</b>   | <b>304.336</b> | <b>1.268</b> | <b>4</b> | <b>1</b> | <b>7</b> |
| <br><b>C<sub>13</sub>H<sub>19</sub>FN<sub>2</sub>O<sub>4</sub>S</b>  | <b>318.363</b> | <b>1.807</b> | <b>4</b> | <b>0</b> | <b>6</b> |
| <br><b>C<sub>10</sub>H<sub>11</sub>FN<sub>2</sub>O<sub>4</sub>S</b> | <b>274.266</b> | <b>0.004</b> | <b>4</b> | <b>1</b> | <b>5</b> |
| <br><b>C<sub>14</sub>H<sub>19</sub>FN<sub>2</sub>O<sub>4</sub>S</b> | <b>330.374</b> | <b>1.784</b> | <b>4</b> | <b>0</b> | <b>5</b> |
| <br><b>C<sub>16</sub>H<sub>13</sub>FN<sub>2</sub>O<sub>4</sub>S</b> | <b>348.348</b> | <b>1.883</b> | <b>4</b> | <b>0</b> | <b>4</b> |

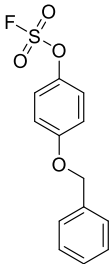
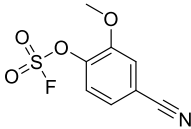
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|--------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------|--------|---|---|---|
| <br><b>C<sub>13</sub>H<sub>17</sub>FN<sub>2</sub>O<sub>5</sub>S</b>               | 332.346 | 0.445  | 5 | 1 | 6 |
| <br><b>C<sub>12</sub>H<sub>15</sub>FN<sub>2</sub>O<sub>5</sub>S</b>               | 318.319 | -0.134 | 5 | 0 | 5 |
| <br><b>C<sub>12</sub>H<sub>15</sub>FN<sub>2</sub>O<sub>5</sub>S</b>               | 318.319 | -0.177 | 5 | 1 | 4 |
| <br><b>C<sub>12</sub>H<sub>11</sub>FN<sub>2</sub>O<sub>5</sub>S</b>             | 314.287 | -0.478 | 5 | 0 | 5 |
| <br><b>C<sub>11</sub>H<sub>12</sub>F<sub>2</sub>N<sub>2</sub>O<sub>5</sub>S</b> | 322.283 | -0.503 | 6 | 0 | 5 |
| <br><b>C<sub>11</sub>H<sub>11</sub>FN<sub>2</sub>O<sub>4</sub>S</b>             | 286.277 | 0.439  | 4 | 1 | 5 |

|                                                                                                                                                                    |         |        |   |   |   |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------|--------|---|---|---|
| <br><b>C<sub>14</sub>H<sub>13</sub>FN<sub>2</sub>O<sub>4</sub>S</b>               | 324.326 | 1.877  | 4 | 0 | 5 |
| <br><b>C<sub>12</sub>H<sub>15</sub>FN<sub>2</sub>O<sub>5</sub>S</b>               | 318.319 | -0.037 | 5 | 0 | 4 |
| <br><b>C<sub>9</sub>H<sub>11</sub>FN<sub>2</sub>O<sub>5</sub>S<sub>2</sub></b>    | 310.314 | 0      | 5 | 0 | 5 |
| <br><b>C<sub>10</sub>H<sub>13</sub>FN<sub>2</sub>O<sub>5</sub>S<sub>2</sub></b> | 324.341 | 0      | 5 | 0 | 5 |
| <br><b>C<sub>12</sub>H<sub>15</sub>FN<sub>2</sub>O<sub>5</sub>S</b>             | 318.319 | -0.082 | 5 | 0 | 4 |
| <br><b>C<sub>13</sub>H<sub>15</sub>FN<sub>2</sub>O<sub>5</sub>S</b>             | 330.33  | 0.026  | 5 | 0 | 5 |
| <br><b>C<sub>13</sub>H<sub>15</sub>FN<sub>2</sub>O<sub>5</sub>S</b>             | 325.329 | 0      | 5 | 0 | 5 |

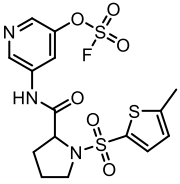
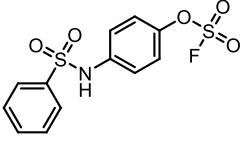
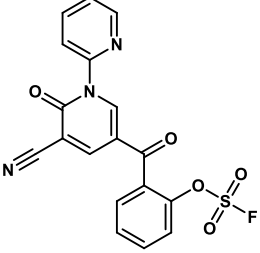
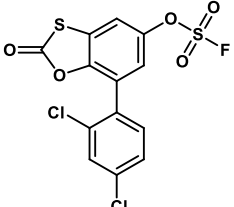
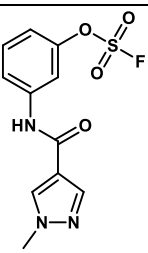
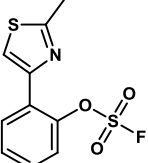
|                                                                                     |                |               |          |          |          |
|-------------------------------------------------------------------------------------|----------------|---------------|----------|----------|----------|
| <b>C<sub>9</sub>H<sub>12</sub>FN<sub>3</sub>O<sub>5</sub>S<sub>2</sub></b>          |                |               |          |          |          |
|    | <b>290.309</b> | <b>1.149</b>  | <b>4</b> | <b>1</b> | <b>8</b> |
| <b>C<sub>11</sub>H<sub>15</sub>FN<sub>2</sub>O<sub>4</sub>S</b>                     |                |               |          |          |          |
|    | <b>276.282</b> | <b>0.383</b>  | <b>4</b> | <b>0</b> | <b>5</b> |
| <b>C<sub>10</sub>H<sub>13</sub>FN<sub>2</sub>O<sub>4</sub>S</b>                     |                |               |          |          |          |
|   | <b>328.318</b> | <b>0.862</b>  | <b>6</b> | <b>1</b> | <b>6</b> |
| <b>C<sub>12</sub>H<sub>13</sub>FN<sub>4</sub>O<sub>4</sub>S</b>                     |                |               |          |          |          |
|  | <b>316.303</b> | <b>-0.483</b> | <b>5</b> | <b>1</b> | <b>6</b> |
| <b>C<sub>12</sub>H<sub>13</sub>FN<sub>2</sub>O<sub>5</sub>S</b>                     |                |               |          |          |          |
|  | <b>372.455</b> | <b>3.521</b>  | <b>3</b> | <b>1</b> | <b>7</b> |
| <b>C<sub>17</sub>H<sub>25</sub>FN<sub>2</sub>O<sub>4</sub>S</b>                     |                |               |          |          |          |

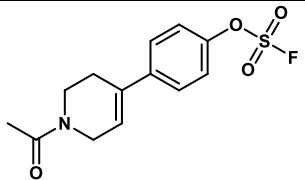
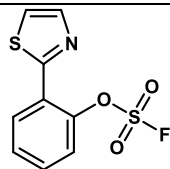
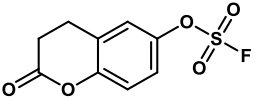
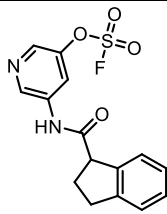
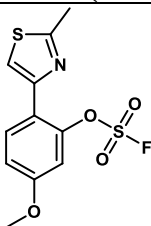
|                                                                                                                                                         |         |        |   |   |   |
|---------------------------------------------------------------------------------------------------------------------------------------------------------|---------|--------|---|---|---|
| <br><b>C<sub>14</sub>H<sub>15</sub>FN<sub>2</sub>O<sub>5</sub>S</b>    | 342.341 | 1.572  | 4 | 1 | 7 |
| <br><b>C<sub>14</sub>H<sub>18</sub>FN<sub>3</sub>O<sub>6</sub>S</b>    | 375.371 | -0.103 | 5 | 1 | 8 |
| <br><b>C<sub>16</sub>H<sub>16</sub>BrFN<sub>2</sub>O<sub>3</sub>S</b> | 415.277 | 3.571  | 4 | 0 | 5 |
| <br><b>C<sub>22</sub>H<sub>22</sub>FNO<sub>4</sub>S</b>              | 415.479 | 5.022  | 4 | 1 | 8 |
| <br><b>C<sub>17</sub>H<sub>18</sub>FNO<sub>3</sub>S</b>              | 335.393 | 3.656  | 3 | 0 | 5 |
| <br><b>C<sub>22</sub>H<sub>22</sub>FNO<sub>4</sub>S</b>              | 316.347 | 1.56   | 4 | 1 | 5 |

|                                                                                     |                |              |          |          |          |
|-------------------------------------------------------------------------------------|----------------|--------------|----------|----------|----------|
| <b>C<sub>13</sub>H<sub>17</sub>FN<sub>2</sub>O<sub>4</sub>S</b>                     |                |              |          |          |          |
|    | <b>248.224</b> | <b>0.871</b> | <b>4</b> | <b>0</b> | <b>4</b> |
| <b>C<sub>9</sub>H<sub>9</sub>FO<sub>5</sub>S</b>                                    |                |              |          |          |          |
|    | <b>210.603</b> | <b>2.244</b> | <b>2</b> | <b>0</b> | <b>2</b> |
| <b>C<sub>6</sub>H<sub>4</sub>ClFO<sub>3</sub>S</b>                                  |                |              |          |          |          |
|   | <b>236.213</b> | <b>1.432</b> | <b>4</b> | <b>0</b> | <b>4</b> |
| <b>C<sub>8</sub>H<sub>9</sub>FO<sub>5</sub>S</b>                                    |                |              |          |          |          |
|  | <b>277.269</b> | <b>3.394</b> | <b>3</b> | <b>0</b> | <b>4</b> |
| <b>C<sub>13</sub>H<sub>8</sub>FNO<sub>3</sub>S</b>                                  |                |              |          |          |          |
|  | <b>215.198</b> | <b>1.663</b> | <b>3</b> | <b>0</b> | <b>4</b> |
| <b>C<sub>8</sub>H<sub>6</sub>FNO<sub>3</sub>S</b>                                   |                |              |          |          |          |

|                                                                                                                                             |                |              |          |          |          |
|---------------------------------------------------------------------------------------------------------------------------------------------|----------------|--------------|----------|----------|----------|
|  <p><b>C<sub>13</sub>H<sub>11</sub>FO<sub>4</sub>S</b></p> | <b>282.285</b> | <b>3.292</b> | <b>3</b> | <b>0</b> | <b>5</b> |
|  <p><b>C<sub>8</sub>H<sub>6</sub>FNO<sub>4</sub>S</b></p>  | <b>231.197</b> | <b>1.592</b> | <b>4</b> | <b>0</b> | <b>4</b> |

**Supplementary Table S2:** Structures and characterization of the positive and negatives hits found with the screening via mass spectrometry analysis (after incubation of hits 250  $\mu$ M with protein 10  $\mu$ M for 48 h) and denaturation thermal shift measurements with hMcl-1(172-323) and its mutants. ND = not detected.

| Structure                                                                                           | $\Delta T_m$<br>Mcl-1 wt | % complex<br>Mcl-1 wt | $\Delta T_m$<br>Mcl-1<br>H224A | $\Delta T_m$<br>Mcl-1<br>H252A | $\Delta T_m$<br>Mcl-1<br>K234A |
|-----------------------------------------------------------------------------------------------------|--------------------------|-----------------------|--------------------------------|--------------------------------|--------------------------------|
| <br>P1 A11 (hit 1) | $2.11 \pm 0.01$          | $\sim 55$             | $-0.34 \pm 0.09$               | $2.90 \pm 0.17$                | $1.96 \pm 0.17$                |
| <br>P1 D4          | $1.2 \pm 0.01$           | $\sim 20$             | $-0.35 \pm 0.01$               | $-0.35 \pm 0.09$               | $-0.27 \pm 0.09$               |
| <br>P1 H2         | $-1.36 \pm 0.01$         | ND                    | -                              | -                              | -                              |
| <br>P2 B10       | $-4.03 \pm 0.01$         | ND                    | -                              | -                              | -                              |
| <br>P3 B5        | $-1.41 \pm 0.08$         | $< 5$                 | $-0.44 \pm 0.09$               | $-0.35 \pm 0.09$               | $0.33 \pm 0.17$                |
| <br>P4 C5        | $-1.21 \pm 0.08$         | ND                    | -                              | -                              | -                              |

|                                                                                                     |                  |      |                  |                  |                  |
|-----------------------------------------------------------------------------------------------------|------------------|------|------------------|------------------|------------------|
| <br>P4 D6          | $-1.46 \pm 0.01$ | < 5  | $-1.89 \pm 0.09$ | $-1.29 \pm 0.26$ | $-0.70 \pm 0.09$ |
| <br>P4 D11         | $-7.5 \pm 0.60$  | ~ 35 | $-3.68 \pm 1.19$ | $-0.10 \pm 0.09$ | $-1.97 \pm 0.01$ |
| <br>P4 E11         | $-2.55 \pm 0.08$ | ND   | -                | -                | -                |
| <br>P4 F10 (hit 2) | $3.97 \pm 0.17$  | ~ 95 | $-1.28 \pm 0.17$ | $6.57 \pm 0.26$  | $4.77 \pm 0.26$  |
| <br>P4 H10        | $-1.82 \pm 0.01$ | ND   | -                | -                | -                |

**Supplementary Table S3:** Mass spectrometry data of hMcl-1(172-323) and its mutants collected in absence or presence of various agents as indicated. Molecular masses are measured and analyzed using an Agilent 6545 QTOF LC/MS mass spectrometer.

| ID                | Calcd [M] | Obs. (m/z)                                                    |
|-------------------|-----------|---------------------------------------------------------------|
| hMcl-1 wt         | 19572.16  | [M] = 19572<br>[M] +178 = 19750                               |
| hMcl-1 wt + hit 1 | 20001.66  | [M] = 20001<br>[M+H] <sup>+</sup> +178 = 20180                |
| hMcl-1 wt + hit 2 | 19888.5   | [M] = 19888<br>[M+H] <sup>+</sup> +178 = 20067                |
| hMcl-1 wt + 165D9 | 19922.2   | [M+H] <sup>+</sup> = 19923<br>[M+H] <sup>+</sup> +178 = 20101 |

| ID                   | Calcd [M] | Obs. (m/z)                                     |
|----------------------|-----------|------------------------------------------------|
| hMcl-1 H224A         | 19506.09  | [M] = 19506<br>[M] +178 = 19684                |
| hMcl-1 H224A + hit 1 | 19935.59  | [M] = 19935                                    |
| hMcl-1 H224A + hit 2 | 19822.4   | [M] = 19822<br>[M+H] <sup>+</sup> +178 = 20001 |
| hMcl-1 H224A + 165D9 | 19856.11  | [M+H] <sup>+</sup> = 19857                     |

| ID                                                | Calcd [M] | Obs. (m/z)                                                    |
|---------------------------------------------------|-----------|---------------------------------------------------------------|
| <sup>15</sup> N hMcl-1 H252A (no His tag)         | 17981     | [M] = 17981<br>[M] +178 = 18159                               |
| <sup>15</sup> N hMcl-1 H252A (no His tag) + hit 1 | 18410.5   | [M+H] <sup>+</sup> = 18411<br>[M+H] <sup>+</sup> +178 = 18661 |
| <sup>15</sup> N hMcl-1 H252A (no His tag) + hit 2 | 18297.34  | [M+H] <sup>+</sup> = 18298<br>[M+H] <sup>+</sup> +178 = 20001 |
| <sup>15</sup> N hMcl-1 H252A (no His tag) + 165D9 | 18331.02  | [M+H] <sup>+</sup> = 18332                                    |

| ID                   | Calcd [M] | Obs. (m/z)                                                    |
|----------------------|-----------|---------------------------------------------------------------|
| hMcl-1 K234A         | 19515.06  | [M] = 19515<br>[M] +178 = 19693                               |
| hMcl-1 K234A + hit 1 | 19944.56  | [M] = 19944<br>[M+H] <sup>+</sup> +178 = 20123                |
| hMcl-1 K234A + hit 2 | 19831.4   | [M] = 19831<br>[M] +178 = 20009                               |
| hMcl-1 K234A + 165D9 | 19865.08  | [M+H] <sup>+</sup> = 19866<br>[M+H] <sup>+</sup> +178 = 20044 |

**Supplementary Table S4:** Data collection and refinement statistics for the complex between hMcl-1(172-323) and fragment hit **2**.

| hMcl-1(172-323)/hit2         |                                          |
|------------------------------|------------------------------------------|
| <b>Data collection</b>       |                                          |
| Beamline                     | DLS I-04                                 |
| Wavelength                   | 0.7460                                   |
| Resolution range (Å)         | 39.03 - 1.82 (1.885 - 1.82)              |
| Space group                  | P 1 21 1                                 |
| Unit cell                    | 41.556, 40.135, 42.052 (90, 111.868, 90) |
| $R_{\text{merge}}^a$         | 0.08596 (4.649)                          |
| Total reflections            | 11680 (834)                              |
| Mean I/sigma(I)              | 12.29 (0.30)                             |
| Completeness (%)             | 96.96 (73.39)                            |
| Wilson B-factor              | 28.06                                    |
| Multiplicity                 | 7.0 (7.3)                                |
| <b>Refinement</b>            |                                          |
| Resolution                   | 39.03 - 1.82 (1.885 - 1.82)              |
| $R_{\text{work}}$            | 0.2536 (0.4440)                          |
| $R_{\text{free}}$            | 0.2869 (0.4703)                          |
| Unique reflections           | 11327 (833)                              |
| Number of non-hydrogen atoms | 1227                                     |
| macromolecules               | 1196                                     |
| ligands                      | 22                                       |
| solvent                      | 9                                        |
| RMS bonds (Å)                | 0.009                                    |
| RMS angles (°)               | 1.25                                     |
| Ramachandran favored (%)     | 92.57                                    |
| Ramachandran allowed (%)     | 7.43                                     |
| Ramachandran outliers (%)    | 0.00                                     |
| Rotamer outliers (%)         | 0.78                                     |
| Clashscore                   | 9.52                                     |

|                  |       |
|------------------|-------|
| Average B-factor | 49.39 |
| macromolecules   | 49.41 |
| ligands          | 46.97 |
| solvent          | 52.37 |

Statistics for the highest-resolution shell are shown in parentheses.