**HDAC6 post-ML-screening doking results**

**Preliminary docking results using SAHA as the reference compound:**

* 5-model ensemble: 23/26 compounds scored better than SAHA.
* Multimodal 1: 17/18 compounds scored better than SAHA.

| **No.** | **ID** | **CID** | **SMILES** | **Docking Score (kcal/mol)** | **Docking Pose** |
| --- | --- | --- | --- | --- | --- |
| 1 | 75968780 | 118715730 | C1=CC(=C(C=C1NC2=C3C=C(SC3=NC=N2)NC(=O)CCCCCC(=O)NO)C(F)(F)F)Cl | -8.8 |  |
| 2 | 75968791 | 118715741 | CC1=CC=C(C=C1)NC2=C3C=C(SC3=NC=N2)NC(=O)CCCCCCC(=O)NO | -8.7 |  |
| 3 | 75968781 | 118715731 | C1=CC(=C(C=C1NC2=C3C=C(SC3=NC=N2)NC(=O)CCCCCCC(=O)NO)C(F)(F)F)Cl | -8.6 |  |
| 4 | 75968778 | 118715728 | C1=CC(=C(C=C1NC2=C3C=C(SC3=NC=N2)NC(=O)CCCCCCC(=O)NO)Cl)F | -8.5 |  |
| 5 | 75968792 | 118715742 | CC1=C(C=C(C=C1)NC2=C3C=C(SC3=NC=N2)NC(=O)CCCCCC(=O)NO)C | -8.5 |  |
| 6 | 88541833 | 137633491 | CC(C)C1=CC(=CC=C1)NC2=NC=NC3=C2SC(=C3)NC(=O)CCCCCCC(=O)NO | -8.5 |  |
| 7 | 75179943 | 117829479 | C1=CC2=C(C=CC(=O)N2)C=C1NC(=O)CCCCCCC(=O)NO | -8.5 |  |
| 8 | 75968782 | 118715732 | C1=CC(=C(C=C1F)F)NC2=C3C=C(SC3=NC=N2)NC(=O)CCCCCCC(=O)NO | -8.4 |  |
| 9 | 75968785 | 118715735 | C1=CC(=C(C=C1I)F)NC2=C3C=C(SC3=NC=N2)NC(=O)CCCCCCC(=O)NO | -8.4 |  |
| 10 | 75968777 | 118715727 | C1=CC(=C(C=C1NC2=C3C=C(SC3=NC=N2)NC(=O)CCCCCC(=O)NO)Cl)F | -8.3 |  |
| 11 | 75968783 | 118715733 | C1=CC(=C(C=C1Cl)F)NC2=C3C=C(SC3=NC=N2)NC(=O)CCCCCCC(=O)NO | -8.3 |  |
| 12 | 88545946 | 137638091 | C1=CC(=CC(=C1)NC2=NC=NC3=C2SC(=C3)NC(=O)CCCCCCC(=O)NO)C#N | -8.3 |  |
| 13 | 75968784 | 118715734 | C1=CC(=C(C=C1Br)F)NC2=C3C=C(SC3=NC=N2)NC(=O)CCCCCCC(=O)NO | -8.3 |  |
| 14 | 75968799 | 118715749 | C1CCN(C1)C2=CC=C(C=C2)NC3=C4C=C(SC4=NC=N3)NC(=O)CCCCCCC(=O)NO | -8.3 |  |
| 15 | 88558275 | 137651991 | C1=CC(=CC(=C1)Br)NC2=NC=NC3=C2SC(=C3)NC(=O)CCCCCCC(=O)NO | -8.2 |  |
| 16 | 75968787 | 118715737 | C1=CC(=CC(=C1)Cl)NC2=C3C=C(SC3=NC=N2)NC(=O)CCCCCCC(=O)NO | -8.2 |  |
| 17 | 88549592 | 137642211 | C1=CC(=CC(=C1)F)NC2=NC=NC3=C2SC(=C3)NC(=O)CCCCCCC(=O)NO | -8.2 |  |
| 18 | 88566511 | 137661253 | C1=CC(=C(C=C1F)F)NC2=NC=NC3=C2SC(=C3)NC(=O)CCCCCCC(=O)NO | -8.2 |  |
| 19 | 88565745 | 137660397 | C1=CC(=CC(=C1)Cl)NC2=NC=NC3=C2SC(=C3)NC(=O)CCCCCCC(=O)NO | -8.2 |  |
| 20 | 75968786 | 118715736 | C1=CC(=C(C(=C1)Cl)F)NC2=C3C=C(SC3=NC=N2)NC(=O)CCCCCCC(=O)NO | -8.2 |  |
| 21 | 88559119 | 137652951 | C1=CC(=C(C=C1Cl)F)NC2=NC=NC3=C2SC(=C3)NC(=O)CCCCCCC(=O)NO | -8.2 |  |
| 22 | 88551161 | 137643993 | CCC1=CC(=CC=C1)NC2=NC=NC3=C2SC(=C3)NC(=O)CCCCCCC(=O)NO | -8.1 |  |
| 23 | 43257599 | 71520626 | CC1=CC(=CC(=C1)NC(=O)NOCCCCCC(=O)NO)C | -8.1 |  |
| 24 | 8322105 | 9972242 | C1=CC=C2C(=C1)C=C(N2)C(=O)NCCCCCCC(=O)NO | -8.1 |  |
| 25 | 75968789 | 118715739 | C1=CC=C(C=C1)NC2=C3C=C(SC3=NC=N2)NC(=O)CCCCCCC(=O)NO | -8 |  |
| 26 | 88545829 | 137637958 | C#CC1=CC(=CC=C1)NC2=NC=NC3=C2SC(=C3)NC(=O)CCCCCCC(=O)NO | -8 |  |
| 27 | 88554647 | 137647889 | CC(C)(C)C1=CC(=CC=C1)NC2=NC=NC3=C2SC(=C3)NC(=O)CCCCCCC(=O)NO | -8 |  |
| 28 | 78720782 | 122548362 | CNC1=CC=C(C=C1)C(=O)NCCCCCCC(=O)NO | -7.9 |  |
| 29 | 75968788 | 118715738 | C1=CC=C(C=C1)NC2=C3C=C(SC3=NC=N2)NC(=O)CCCCCC(=O)NO | -7.8 |  |
| SAHA |  |  |  | -7.8 |  |
| 30 | 75968790 | 118715740 | CC1=CC=C(C=C1)NC2=C3C=C(SC3=NC=N2)NC(=O)CCCCCC(=O)NO | -7.6 |  |
| 31 | 43257524 | 71520533 | CC1=CC=C(C=C1)NC(=O)NOCCCCCC(=O)NO | -7.5 |  |
| 32 | 44946060 | 78103379 | C1CC(NC(=O)C1)C(=O)NC(CCCCCS)C(=O)NC2=CC=CC=C2 | -6.8 |  |
| 33 | 54792366 | 91884636 | C1CC(=O)N[C@H]1C(=O)N[C@@H](CCCCCS)C(=O)NC2=CC=CC=C2 | -6.7 |  |