**Designing potential HDAC3 inhibitors to improve memory and learning**

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**Supplementary Table T1.** List of compounds in smile format and their HDAC3 inhibitory activities.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Cpda** | **Smile** | ***pIC50*** | **Activity scaleb** | **Set** |
| **1** | c1cncc(c1)C(=O)Nc1c(cccc1)N | 5.444 | 0 | Training set |
| **2** | c1cncc(c1)C(=O)Nc1c(ccc(c1)c1ccccc1)N | 4.959 | 0 | Training set |
| **3** | c1cncc(c1)C(=O)Nc1c(ccc(c1)c1cccs1)N | 5.137 | 0 | Training set |
| **4** | c1cccc(c1)C(=O)Nc1c(cccc1)N | 5.553 | 0 | Test set |
| **5** | c1cccc(c1)C(=O)Nc1c(ccc(c1)c1ccccc1)N | 4.959 | 0 | Test set |
| **6** | c1cccc(c1)C(=O)Nc1c(ccc(c1)c1cccs1)N | 4.959 | 0 | Training set |
| **7** | c1c(ncc(c1)C(=O)Nc1c(cccc1)N)N1CCC2(CC1)C[NH2+]CC2 | 6.469 | 0 | Training set |
| **8** | c1c(ncc(c1)C(=O)Nc1c(ccc(c1)c1cccs1)N)N1CCC2(CC1)C[NH2+]CC2 | 5.9 | 0 | Training set |
| **9** | c1c(ncc(c1)C(=O)Nc1c(ccc(c1)c1cscc1)N)N1CCC2(CC1)C[NH2+]CC2 | 5.896 | 0 | Test set |
| **10** | c1c(ncc(c1)C(=O)Nc1c(ccc(c1)c1cnn(c1)C)N)N1CCC2(CC1)C[NH2+]CC2 | 5.272 | 0 | Test set |
| **11** | c1c(ncc(c1)C(=O)Nc1c(ccc(c1)c1n[nH]cc1)N)N1CCC2(CC1)C[NH2+]CC2 | 5.26 | 0 | Training set |
| **12** | c1cncc(c1)COC(=O)NCc1ccc(cc1)C(=O)Nc1ccccc1N | 5.636 | 0 | Training set |
| **13** | C(C(=O)Nc1c(cccc1)N)CCCCCC(=O)Nc1ccc(cc1)c1nnn(c1)Cc1ccccc1 | 5.824 | 0 | Training set |
| **14** | C(C(=O)Nc1c(cccc1)N)CCCCCC(=O)Nc1cc(ccc1)c1nnn(c1)c1ccccc1 | 6.921 | 1 | Training set |
| **15** | C(C(=O)Nc1c(cccc1)N)CCCCCC(=O)Nc1scc(n1)c1cc(ccc1)N | 7.22 | 1 | Training set |
| **16** | C(C(=O)Nc1c(cccc1)N)CCCCCC(=O)Nc1scc(n1)c1cc(ccc1)NC(=O)OCC | 7.222 | 1 | Training set |
| **17** | C(C(=O)Nc1c(cccc1)N)CCCCCC(=O)Nc1scc(n1)c1cc(ccc1)NC(=O)OC(C)(C)C | 6.796 | 0 | Test set |
| **18** | C(C(=O)Nc1c(cccc1)N)CCCCCC(=O)Nc1scc(n1)c1cc(ccc1)NC(=O)C | 7.523 | 1 | Training set |
| **19** | C(C(=O)Nc1c(cccc1)N)CCCCCC(=O)NOCc1ccccc1 | 6.258 | 0 | Training set |
| **20** | C(C(=O)Nc1c(cccc1)N)CCCCCC(=O)NO | 7.676 | 1 | Test set |
| **21** | C(C(=O)Nc1c(cccc1)N)CCCCCC(=O)Nc1ccccc1N | 6.005 | 0 | Test set |
| **22** | c1(C(=O)Nc2c(cc3c(c2)cccc3)N)ccc(cc1)CNc1nc(ncc1)c1cccnc1 | 6.201 | 0 | Training set |
| **23** | c1(C(=O)Nc2c(cc(cc2)OC)N)ccc(cc1)CNc1nc(ncc1)c1cccnc1 | 6.955 | 1 | Test set |
| **24** | c1(C(=O)Nc2c(cc(cc2)O)N)ccc(cc1)CNc1nc(ncc1)c1cccnc1 | 6.143 | 0 | Training set |
| **25** | c1(C(=O)Nc2c(cccc2)N)ccc(cc1)CNc1nc(ncc1)c1cccnc1 | 7.658 | 1 | Training set |
| **26** | N1=C(N([C@@H](C1=O)Cc1c[nH]c2c1cccc2)C(=O)OC(C)(C)C)NCc1ccc(cc1)C(=O)Nc1c(cccc1)N | 7.398 | 1 | Test set |
| **27** | N1=C(N([C@@H](C1=O)Cc1c[nH]c2c1cccc2)C(=O)C)NCc1ccc(cc1)C(=O)Nc1c(cccc1)N | 7.155 | 1 | Training set |
| **28** | N1=C(N[C@@H](C1=O)Cc1c[nH]c2c1cccc2)NCc1ccc(cc1)C(=O)Nc1c(cccc1)N | 6.983 | 1 | Training set |
| **29** | N1=C(N([C@@H](C1=O)Cc1ccccc1)C(=O)C)NCc1ccc(cc1)C(=O)Nc1c(cccc1)N | 7.081 | 1 | Test set |
| **30** | N1=C(N[C@@H](C1=O)Cc1ccccc1)NCc1ccc(cc1)C(=O)Nc1c(cccc1)N | 7.523 | 1 | Test set |
| **31** | N1=C(N[C@@H](C1=O)c1ccccc1)NCc1ccc(cc1)C(=O)Nc1c(cccc1)N | 7.854 | 1 | Training set |
| **32** | N1=C(SC[C@H]1Cc1c[nH]c2c1cccc2)SCc1ccc(cc1)C(=O)Nc1c(cccc1)N | 6.051 | 0 | Training set |
| **33** | N1=C(SC[C@H]1Cc1ccccc1)SCc1ccc(cc1)C(=O)Nc1c(cccc1)N | 6.293 | 0 | Training set |
| **34** | N1=C(SC[C@H]1c1ccccc1)SCc1ccc(cc1)C(=O)Nc1c(cccc1)N | 7.201 | 1 | Training set |
| **35** | N1=C(SC[C@H]1c1ccccc1)[NH2+]Cc1ccc(cc1)C(=O)Nc1c(cccc1)N | 7.921 | 1 | Training set |
| **36** | N1=C(SC[C@@H]1c1ccccc1)[NH2+]Cc1ccc(cc1)C(=O)Nc1c(cccc1)N | 7.102 | 1 | Training set |
| **37** | N1=C(SC[C@H]1c1ccc(cc1)[O-])[NH2+]Cc1ccc(cc1)C(=O)Nc1c(cccc1)N | 7.796 | 1 | Test set |
| **38** | N1=C(SC[C@H]1Cc1ccccc1)[NH2+]Cc1ccc(cc1)C(=O)Nc1c(cccc1)N | 7.284 | 1 | Training set |
| **39** | N1=C(SC[C@@H]1Cc1ccccc1)[NH2+]Cc1ccc(cc1)C(=O)Nc1c(cccc1)N | 7.444 | 1 | Training set |
| **40** | N1=C(S[C@@H](C1)c1ccccc1)[NH2+]Cc1ccc(cc1)C(=O)Nc1c(cccc1)N | 7.638 | 1 | Training set |
| **41** | N1=C(S[C@H](C1)c1ccccc1)[NH2+]Cc1ccc(cc1)C(=O)Nc1c(cccc1)N | 7.921 | 1 | Training set |
| **42** | N1=C(S[C@H]([C@@H]1c1ccccc1)c1ccccc1)[NH2+]Cc1ccc(cc1)C(=O)Nc1c(cccc1)N | 6.542 | 0 | Training set |
| **43** | N1=C(S[C@@H]([C@H]1c1ccccc1)c1ccccc1)[NH2+]Cc1ccc(cc1)C(=O)Nc1c(cccc1)N | 6.411 | 0 | Training set |
| **44** | c1cncc(c1)c1nc(ncc1)NCc1ccc(cc1)C(=O)Nc1ccccc1N | 7.347 | 1 | Test set |
| **45** | c1cccc(c1)[C@@H]1[NH+]=C(NC1)NCc1ccc(cc1)C(=O)Nc1ccccc1N | 7.824 | 1 | Test set |
| **46** | c1cccc(c1)[C@@H]1N=C([NH2+]C1)SCc1ccc(cc1)C(=O)Nc1ccccc1N | 7.42 | 1 | Training set |
| **47** | c1cccc(c1)[C@@H]1N=C(OC1)SCc1ccc(cc1)C(=O)Nc1ccccc1N | 7.18 | 1 | Training set |
| **48** | c1cncc(c1)[C@@H]1N=C(OC1)SCc1ccc(cc1)C(=O)Nc1ccccc1N | 7.252 | 1 | Training set |
| **49** | c1cccc(c1)C[C@@H]1N=C(OC1)SCc1ccc(cc1)C(=O)Nc1ccccc1N | 7.149 | 1 | Training set |
| **50** | c1cccc(c1)[C@@H]1N=C(OC1)[NH2+]Cc1ccc(cc1)C(=O)Nc1ccccc1N | 7.398 | 1 | Test set |
| **51** | c1cccc(c1)[C@H]1N=C(OC1)[NH2+]Cc1ccc(cc1)C(=O)Nc1ccccc1N | 7.481 | 1 | Test set |
| **52** | c1c(ccc(c1)[C@@H]1N=C(OC1)[NH2+]Cc1ccc(cc1)C(=O)Nc1ccccc1N)F | 7.469 | 1 | Training set |
| **53** | c1(cccc(c1)[C@H]1N=C(OC1)[NH2+]Cc1ccc(cc1)C(=O)Nc1ccccc1N)F | 7.62 | 1 | Test set |
| **54** | c1c(ccc(c1)[C@H]1N=C(OC1)[NH2+]Cc1ccc(cc1)C(=O)Nc1ccccc1N)C(F)(F)F | 7.469 | 1 | Training set |
| **55** | c1c(ccc(c1)[C@@H]1N=C(OC1)[NH2+]Cc1ccc(cc1)C(=O)Nc1ccccc1N)O | 7.745 | 1 | Training set |
| **56** | c1cncc(c1)[C@@H]1N=C(OC1)[NH2+]Cc1ccc(cc1)C(=O)Nc1ccccc1N | 7.509 | 1 | Training set |
| **57** | c1cccc(c1)C[C@@H]1N=C(OC1)[NH2+]Cc1ccc(cc1)C(=O)Nc1ccccc1N | 7.387 | 1 | Training set |
| **58** | C1N=C(O[C@H]1c1ccccc1)[NH2+]Cc1ccc(cc1)C(=O)Nc1ccccc1N | 7.959 | 1 | Training set |
| **59** | C1N=C(O[C@H]1c1ccccc1)[NH2+]Cc1ccc(cc1)C(=O)Nc1ccccc1N | 7.456 | 1 | Training set |
| **60** | C1(N=C(OC1)[NH2+]Cc1ccc(cc1)C(=O)Nc1ccccc1N)(c1ccccc1)c1ccccc1 | 7.26 | 1 | Training set |
| **61** | [C@@H]1(N=C(O[C@@H]1c1ccccc1)[NH2+]Cc1ccc(cc1)C(=O)Nc1ccccc1N)c1ccccc1 | 6.921 | 1 | Training set |
| **62** | [C@H]1(N=C(O[C@H]1c1ccccc1)[NH2+]Cc1ccc(cc1)C(=O)Nc1ccccc1N)c1ccccc1 | 8.222 | 1 | Training set |
| **63** | c1nc(c[nH]1)C[C@H]1N=C(OC1)[NH2+]Cc1ccc(cc1)C(=O)Nc1ccccc1N | 7.678 | 1 | Test set |
| **64** | c1nc(c[nH]1)C[C@@H]1N=C(OC1)[NH2+]Cc1ccc(cc1)C(=O)Nc1ccccc1N | 7.745 | 1 | Training set |
| **65** | c1c(ccc(c1)C(=O)Nc1c(cccc1)N)NC(=O)C | 7.337 | 1 | Training set |
| **66** | c1c(ccc(c1)C(=O)Nc1c(ccc(c1)c1ccncc1)N)NC(=O)C | 5.682 | 0 | Training set |
| **67** | c1c(ccc(c1)C(=O)Nc1c(ccc(c1)C)N)NC(=O)C | 5.971 | 0 | Training set |
| **68** | c1c(ccc(c1)C(=O)Nc1c(ccc(c1)F)N)NC(=O)C | 6.975 | 1 | Training set |
| **69** | c1c(ccc(c1)C(=O)Nc1c(cc(cc1)F)N)NC(=O)C | 7.194 | 1 | Training set |
| **70** | c1(C(=O)Nc2c(cc(cc2)F)N)ccc(cc1)NC(=O)[C@H](C(C)C)c1ccccc1 | 6 | 0 | Training set |
| **71** | c1(C(=O)Nc2c(cc(cc2)F)N)ccc(cc1)NC(=O)[C@@H](CC)c1ccccc1 | 6.77 | 0 | Test set |
| **72** | c1(C(=O)Nc2c(cc(cc2)F)N)ccc(cc1)NC(=O)[C@@H](C)c1ccccc1 | 6.638 | 0 | Training set |
| **73** | c1(C(=O)Nc2c(cc(cc2)F)N)ccc(cc1)NC(=O)[C@H](CC)c1ccccc1 | 6.959 | 1 | Test set |
| **74** | c1(C(=O)Nc2c(cc(cc2)F)N)ccc(cc1)NC(=O)[C@H](C)c1ccccc1 | 6.678 | 0 | Training set |
| **75** | c1c(ncc(c1)NC(=O)[C@@H](C(C)C)c1ccccc1)C(=O)Nc1c(cc(cc1)F)N | 6.523 | 0 | Training set |
| **76** | c1c(ncc(c1)NC(=O)[C@@H](CC)c1ccccc1)C(=O)Nc1c(cc(cc1)F)N | 6.276 | 0 | Test set |
| **77** | c1c(ncc(c1)NC(=O)[C@@H](C)c1ccccc1)C(=O)Nc1c(cc(cc1)F)N | 6.886 | 1 | Training set |
| **78** | c1c(ncc(c1)NC(=O)[C@H](C(C)C)c1ccccc1)C(=O)Nc1c(cc(cc1)F)N | 7.097 | 1 | Training set |
| **79** | c1c(ncc(c1)NC(=O)[C@H](CC)c1ccccc1)C(=O)Nc1c(cc(cc1)F)N | 7.222 | 1 | Training set |
| **80** | c1c(ncc(c1)NC(=O)[C@H](C)c1ccccc1)C(=O)Nc1c(cc(cc1)F)N | 6.237 | 0 | Test set |
| **81** | c1(C(=O)Nc2c(cc(cc2)F)N)ccc(nc1)NC(=O)[C@H](C(C)C)c1ccccc1 | 5.77 | 0 | Training set |
| **82** | c1(C(=O)Nc2c(cc(cc2)F)N)ccc(cc1)NC(=O)Cc1ccccc1 | 6.745 | 0 | Training set |
| **83** | c1(C(=O)Nc2c(cc(cc2)F)N)ccc(cc1)NC(=O)Cc1ccc(cc1)F | 6.699 | 0 | Training set |
| **84** | c1(C(=O)Nc2c(cc(cc2)F)N)ccc(cc1)NC(=O)Cc1ccc(cc1)C(F)(F)F | 6.699 | 0 | Test set |
| **85** | c1(C(=O)Nc2c(cc(cc2)F)N)ccc(cn1)NC(=O)Cc1ccccc1 | 6.284 | 0 | Training set |
| **86** | c1(C(=O)Nc2c(cc(cc2)F)N)ccc(cn1)NC(=O)Cc1ccc(cc1)F | 6.409 | 0 | Test set |
| **87** | c1(C(=O)Nc2c(cc(cc2)F)N)ccc(cc1)NC(=O)CCc1ccccc1 | 6.097 | 0 | Training set |
| **88** | c1(C(=O)Nc2c(cc(cc2)F)N)ccc(cc1)NC(=O)C(C)(c1ccccc1)C | 6.456 | 0 | Training set |
| **89** | c1(C(=O)Nc2c(cc(cc2)F)N)ccc(cc1)NC(=O)[C@H]1C[C@@H]1c1ccccc1 | 6.699 | 0 | Training set |
| **90** | c1(C(=O)Nc2c(cc(cc2)F)N)ccc(cn1)NC(=O)[C@@H]1C[C@@H]1c1ccccc1 | 6 | 0 | Training set |
| **91** | c1[nH]c2c(c1C[C@@H](C(=O)Nc1ccc(cc1)C(=O)Nc1ccccc1N)NC(=O)c1ccc(cc1)OC)cccc2 | 6.644 | 0 | Test set |
| **92** | c1[nH]c2c(c1C[C@@H](C(=O)NCc1ccc(cc1)C(=O)Nc1ccccc1N)NC(=O)c1ccc(cc1)OC)cccc2 | 6.86 | 1 | Training set |
| **93** | c1[nH]c2c(c1C[C@@H](C(=O)NCCCCCC(=O)Nc1ccccc1N)NC(=O)c1ccc(cc1)OC)cccc2 | 7.368 | 1 | Training set |
| **94** | c1[nH]c2c(c1C[C@H](NC(=O)c1ccc(cc1)OC)COc1ccc(cc1)C(=O)Nc1ccccc1N)cccc2 | 7.046 | 1 | Training set |
| **95** | c1[nH]c2c(c1C[C@H](NC(=O)c1ccc(cc1)OC)COc1ccc(cc1)/C=C/C(=O)Nc1ccccc1N)cccc2 | 6.583 | 0 | Training set |
| **96** | c1[nH]c2c(c1C[C@@H](C[NH2+]Cc1ccc(cc1)C(=O)Nc1ccccc1N)NC(=O)c1ccc(cc1)OC)cccc2 | 6.652 | 0 | Training set |
| **97** | c1[nH]c2c(c1C[C@@H](C(=O)NCCCCCC(=O)Nc1cc(ccc1N)c1cccs1)NC(=O)c1ccc(cc1)OC)cccc2 | 5.447 | 0 | Training set |
| **98** | c1[nH]c2c(c1C[C@@H](C(=O)NCCCCCC(=O)Nc1cc(ccc1N)c1ccccc1)NC(=O)c1ccc(cc1)OC)cccc2 | 5.25 | 0 | Training set |
| **99** | c1[nH]c2c(c1C[C@@H](C(=O)NCCCCCC(=O)Nc1ccc(cc1N)F)NC(=O)c1ccc(cc1)OC)cccc2 | 6.955 | 1 | Training set |
| **100** | c1[nH]c2c(c1C[C@@H](C(=O)Nc1ccc(cc1)C(=O)Nc1cc(ccc1N)c1cccs1)NC(=O)c1ccc(cc1)OC)cccc2 | 4.204 | 0 | Training set |
| **101** | c1[nH]c2c(c1C[C@@H](C(=O)Nc1ccc(cc1)C(=O)Nc1ccc(cc1N)F)NC(=O)c1ccc(cc1)OC)cccc2 | 6.777 | 0 | Test set |
| **102** | c1[nH]c2c(c1C[C@@H](C(=O)NCc1ccc(cc1)C(=O)Nc1cc(ccc1N)c1cccs1)NC(=O)c1ccc(cc1)OC)cccc2 | 5.097 | 0 | Training set |
| **103** | c1[nH]c2c(c1C[C@@H](C(=O)NCc1ccc(cc1)C(=O)Nc1cc(ccc1N)c1ccccc1)NC(=O)c1ccc(cc1)OC)cccc2 | 4.511 | 0 | Training set |
| **104** | c1[nH]c2c(c1C[C@@H](C(=O)NCc1ccc(cc1)C(=O)Nc1ccc(cc1N)F)NC(=O)c1ccc(cc1)OC)cccc2 | 6.614 | 0 | Training set |
| **105** | c1cncc(n1)C(=O)Nc1c(cccc1)N | 6.539 | 0 | Training set |
| **106** | c1nccc(c1)C(=O)Nc1c(cccc1)N | 6.435 | 0 | Test set |
| **107** | c1ccnc(c1)C(=O)Nc1c(cccc1)N | 6.461 | 0 | Test set |
| **108** | c1c(ncc(c1)C(=O)Nc1c(cccc1)N)C | 6.672 | 0 | Training set |
| **109** | n1c(ncc(c1)C(=O)Nc1c(cccc1)N)Nc1ccccc1 | 6.771 | 0 | Training set |
| **110** | c1c(ncc(c1)C(=O)Nc1c(cccc1)N)Cl | 6.553 | 0 | Training set |
| **111** | c1c(ccc(c1)C(=O)Nc1c(ccc(c1)c1ccccc1)N)NC(=O)C | 6.074 | 0 | Training set |
| **112** | n1cccc(c1)C(=O)Nc1c(cc(cc1)F)N | 5.707 | 0 | Training set |
| **113** | c1cncc(n1)C(=O)Nc1c(cc(cc1)F)N | 6.529 | 0 | Training set |

a Compound; bHDAC3 inhibitory activities (*pIC50*) value <5.9 were considered as *active* and denoted as 1.

**Supplementary Figure S1**. Top 20 molecular fragments (G1-G20) that favor HDAC3 inhibitory activity as produced from the *ECFP\_6* fingerprint descriptor.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64398.png | | G1: 683445015 14 out of 14 good Bayesian Score: 0.653 | | |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64399.png | | G2: 1344323508 11 out of 11 good Bayesian Score: 0.637 | | |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64400.png | | G3: -1198127490 11 out of 11 good Bayesian Score: 0.637 | | |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64401.png | | G4: 404793249 11 out of 11 good Bayesian Score: 0.637 | | |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64402.png | | G5: -860776531 10 out of 10 good Bayesian Score: 0.629 | |
| |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64403.png | | G6: -556429595 10 out of 10 good Bayesian Score: 0.629 | | |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64404.png | | G7: -90310073 9 out of 9 good Bayesian Score: 0.621 | | |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64405.png | | G8: 2006097921 8 out of 8 good Bayesian Score: 0.610 | | |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64406.png | | G9: 1407808221 6 out of 6 good Bayesian Score: 0.580 | | |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64407.png | | G10: 1898059402 6 out of 6 good Bayesian Score: 0.580 | |
| |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64408.png | | G11: 1158871309 6 out of 6 good Bayesian Score: 0.580 | | |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64409.png | | G12: -2104251029 6 out of 6 good Bayesian Score: 0.580 | | |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64410.png | | G13: -658802983 6 out of 6 good Bayesian Score: 0.580 | | |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64411.png | | G14: 506794416 17 out of 19 good Bayesian Score: 0.564 | | |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64412.png | | G15: 1003897717 17 out of 19 good Bayesian Score: 0.564 | |
| |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64413.png | | G16: -255145744 17 out of 19 good Bayesian Score: 0.564 | | |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64414.png | | G17: -1517376329 5 out of 5 good Bayesian Score: 0.559 | | |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64415.png | | G18: -780385523 4 out of 4 good Bayesian Score: 0.529 | | |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64416.png | | G19: -555098937 4 out of 4 good Bayesian Score: 0.529 | | |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64417.png | | G20: 2007300961 4 out of 4 good Bayesian Score: 0.529 | |

**Supplementary Figure S2**. Top 20 molecular fragments (B1-B20) that unfavor HDAC3 inhibitory activity as produced from the *ECFP\_6* fingerprint descriptor.

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| |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64418.png | | B1: -219423964 0 out of 13 good Bayesian Score: -1.991 | | |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64419.png | | B2: -133201654 0 out of 12 good Bayesian Score: -1.922 | | |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64420.png | | B3: -2081449927 0 out of 12 good Bayesian Score: -1.922 | | |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64421.png | | B4: 965503744 0 out of 10 good Bayesian Score: -1.769 | | |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64422.png | | B5: 482094697 0 out of 10 good Bayesian Score: -1.769 | |
| |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64423.png | | B6: -1947280506 0 out of 10 good Bayesian Score: -1.769 | | |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64424.png | | B7: 1387988013 0 out of 7 good Bayesian Score: -1.483 | | |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64425.png | | B8: -1650625813 1 out of 15 good Bayesian Score: -1.422 | | |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64426.png | | B9: -2036625672 0 out of 6 good Bayesian Score: -1.366 | | |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64427.png | | B10: -174807301 0 out of 6 good Bayesian Score: -1.366 | |
| |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64428.png | | B11: -1646811292 0 out of 6 good Bayesian Score: -1.366 | | |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64429.png | | B12: 132687137 0 out of 6 good Bayesian Score: -1.366 | | |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64430.png | | B13: -670594271 0 out of 6 good Bayesian Score: -1.366 | | |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64431.png | | B14: 2010302257 0 out of 6 good Bayesian Score: -1.366 | | |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64432.png | | B15: -399596564 0 out of 6 good Bayesian Score: -1.366 | |
| |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64433.png | | B16: 2089622584 0 out of 6 good Bayesian Score: -1.366 | | |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64434.png | | B17: 1624419609 0 out of 6 good Bayesian Score: -1.366 | | |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64435.png | | B18: 1996740348 0 out of 6 good Bayesian Score: -1.366 | | |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64436.png | | B19: -427424984 0 out of 6 good Bayesian Score: -1.366 | | |  | | --- | | C:\Users\Tarun Jha\Documents\Discovery Studio Client\Results\CreateBayesianModel_2017_11_03_153838_140\Output\GoodAndBadFingerprints\images\image64437.png | | B20: -920025573 0 out of 6 good Bayesian Score: -1.366 | |