**Table S1.** Internal dataset compounds used for QSAR modeling (Sp: Split, Tr=Training, ITr=Invisible training set, Cl=Calibration set)

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Cpd** | **SMILES** | **pIC50** | **Sp 1** | **Sp 2** | **Sp 3** | **Reference** |
| **1** | O[C@@H](C(=O)N1COC2([C@H]1C(=O)NCc1c(C)nsc1C)CCCC2)C[C@H](C(=O)N[C@H]1[C@@H](O)COc2c1cccc2)Cc1ccccc1 | 10.000 | Tr | Tr | Tr | 1 |
| **2** | O[C@@H](C(=O)N1COC2([C@H]1C(=O)NCc1c(C)noc1C)CCCC2)C[C@H](C(=O)N[C@H]1[C@@H](O)COc2c1cccc2)Cc1ccccc1 | 9.699 | Tr | Tr | Tr | 1 |
| **3** | O[C@@H](C(=O)N1COC2([C@H]1C(=O)NCc1c(C)cccc1C)CCCC2)C[C@H](C(=O)N[C@H]1[C@@H](O)COc2c1cccc2)Cc1ccccc1 | 10.000 | Cl | Cl | Cl | 1 |
| **4** | O[C@@H](C(=O)N1COC2([C@@H]1C(=O)NCc1c(Cl)cccc1Cl)CCCC2)C[C@@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccccc1 | 9.959 | Tr | Cl | Cl | 1 |
| **5** | O[C@@H](C(=O)N1COC([C@@H]1C(=O)NCc1c(C)cccc1C)(C)C)C[C@H](C(=O)N[C@H]1CCOc2c1cccc2)Cc1ccccc1 | 9.769 | Tr | Tr | Tr | 1 |
| **6** | O[C@@H](C(=O)N1CCCC[C@@H]1C(=O)NCc1c(C)cccc1C)C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccccc1 | 7.377 | Cl | Cl | Cl | 1 |
| **7** | O[C@@H](C(=O)N1CCC[C@@H]1C(=O)NCc1c(C)cccc1C)C[C@H](C(=O)N[C@H]1[C@@H](O)COc2c1cccc2)Cc1ccccc1 | 7.854 | ITr | Itr | Itr | 1 |
| **8** | O[C@@H](C(=O)N1CCC([C@@H]1C(=O)NCc1c(C)cccc1C)(C)C)C[C@H](C(=O)N[C@@H]1CCOc2c1cccc2)Cc1ccccc1 | 9.854 | Tr | Tr | Tr | 1 |
| **9** | O[C@@H](C(=O)N1CC[C@H]1C(=O)NCc1c(C)cccc1C)C[C@H](C(=O)N[C@H]1[C@@H](O)COc2c1cccc2)Cc1ccccc1 | 7.046 | Tr | Cl | Cl | 1 |
| **10** | O[C@H](CN1CCN(C[C@H]1C(=O)NC(C)(C)C)S(=O)(=O)c1nc(sc1C)C)C[C@H](C(=O)N[C@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1 | 9.796 | Tr | Cl | Cl | 2 |
| **11** | O[C@H](CN1CCN(C[C@H]1C(=O)NC(C)(C)C)S(=O)(=O)c1cccc2c1nccc2)C[C@H](C(=O)N[C@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1 | 10.886 | Tr | Tr | Tr | 2 |
| **12** | O[C@H](CN1CCN(C[C@H]1C(=O)NC(C)(C)C)Cc1ccncc1)C[C@H](C(=O)N[C@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1 | 9.409 | Tr | Tr | Tr | 2 |
| **13** | O[C@H](CN1CCN(C[C@H]1C(=O)NC(C)(C)C)Cc1cccnc1)C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1 | 9.252 | Tr | Tr | Itr | 2 |
| **14** | O[C@H](CN1CCN(C[C@H]1C(=O)NC(C)(C)C)CC(=O)OC(C)(C)C)C[C@H](C(=O)N[C@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1 | 9.092 | Tr | Cl | Cl | 2 |
| **15** | O[C@H](CN1CCN(C[C@H]1C(=O)NC(C)(C)C)C(=O)c1cc2ccccc2oc1=O)C[C@H](C(=O)N[C@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1 | 9.886 | Cl | Tr | Tr | 2 |
| **16** | O[C@@H](C[C@H](C(=O)N[C@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)CN1CCNC[C@H]1C(=O)NC(C)(C)C | 7.420 | Cl | Cl | Cl | 2 |
| **17** | O[C@@H](C[C@H](C(=O)N[C@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)CN1CCN(C[C@H]1C(=O)NC(C)(C)C)CCOCc1ccccc1 | 9.000 | Tr | Tr | Cl | 2 |
| **18** | O[C@@H](C[C@H](C(=O)N[C@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)CN1CCN(C[C@H]1C(=O)NC(C)(C)C)Cc1ccccc1S | 9.268 | Cl | Cl | Cl | 2 |
| **19** | O[C@@H](C[C@H](C(=O)N[C@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)CN1CCN(C[C@H]1C(=O)NC(C)(C)C)Cc1ccccc1 | 9.523 | Tr | Tr | Tr | 2 |
| **20** | O[C@@H](C[C@H](C(=O)N[C@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)CN1CCN(C[C@H]1C(=O)NC(C)(C)C)Cc1ccc(cc1F)F | 9.509 | Cl | Tr | Tr | 2 |
| **21** | O[C@@H](C[C@H](C(=O)N[C@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)CN1CCN(C[C@H]1C(=O)NC(C)(C)C)Cc1ccc(cc1[S-])Br | 10.222 | Tr | Tr | Tr | 2 |
| **22** | CCN1CCN([C@@H](C1)C(=O)NC(C)(C)C)C[C@H](C[C@H](C(=O)N[C@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)O | 8.215 | Cl | Itr | Cl | 2 |
| **23** | O[C@H](CN1CCN(C[C@H]1C(=O)NC(C)(C)C)S(=O)(=O)c1cccnc1)C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1 | 9.523 | Tr | Tr | Tr | 2 |
| **24** | O[C@H](CN1C[C@H](C[C@H]1C(=O)NC(C)(C)C)Oc1ccc2c(c1)cccc2)C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1 | 7.824 | Cl | Itr | Tr | 2 |
| **25** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)CN1CCN(C[C@H]1C(=O)NC(C)(C)C)C(=O)OCc1ccccc1 | 9.456 | Tr | Tr | Tr | 2 |
| **26** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)C[N@@H+]1CCCC[C@H]1C(=O)NC(C)(C)C | 7.097 | ITr | Itr | Itr | 2 |
| **27** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)C[N@@H+]1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C | 8.108 | ITr | Cl | Tr | 2 |
| **28** | O=C(O[C@H]1CO[C@@H]2[C@H]1CCO2)N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1 | 6.879 | Tr | Itr | Itr | 3 |
| **29** | O=C(O[C@@H]1CO[C@H]2[C@@H]1CCO2)N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1 | 8.194 | Tr | Itr | Itr | 3 |
| **30** | NC(=O)C[C@H](C(=O)N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1)NC(=O)c1ccc2c(n1)cccc2 | 9.638 | Tr | Tr | Tr | 3 |
| **31** | CCOc1ccc(cn1)CN1CCN([C@@H](C1)C(=O)NC(C)(C)C)C[C@H](C[C@H](C(=O)N[C@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)O | 8.469 | Tr | Itr | Itr | 3 |
| **32** | O=C(O[C@H]1CS(=O)(=O)C[C@H]1C)N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1 | 6.666 | Tr | Tr | Tr | 4 |
| **33** | O=C(O[C@H]1CCS(=O)(=O)[C@H]1C)N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1 | 7.943 | Cl | Cl | Tr | 4 |
| **34** | O=C(O[C@H]1CCS(=O)(=O)[C@H]1C)N[C@H]([C@@H](CN1C[C@H]2CCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1 | 7.900 | Cl | Tr | Tr | 4 |
| **35** | O=C(O[C@@H]1CCS(=O)(=O)[C@@H]1C1CCCC1)N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1 | 7.646 | Cl | Tr | Tr | 4 |
| **36** | O=C(O[C@@H]1CCS(=O)(=O)[C@@H]1C)N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1 | 7.652 | Cl | Tr | Itr | 4 |
| **37** | O=C(O[C@@H]1CCS(=O)(=O)[C@@H]1C(C)C)N[C@H]([C@@H](CN1CC[N@H+](C[C@H]1C(=O)NC(C)(C)C)C1CCCCCC1)O)Cc1ccccc1 | 7.039 | Tr | Tr | Cl | 4 |
| **38** | O=C(N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1)OC1CS(=O)(=O)C1 | 6.983 | Tr | Cl | Cl | 4 |
| **39** | O=C(N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1)O[C@H]1CCSC1 | 6.879 | Cl | Cl | Tr | 4 |
| **40** | O=C(N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1)O[C@H]1C[C@H](S(=O)(=O)C1)C | 7.086 | Tr | Tr | Tr | 4 |
| **41** | O=C(N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1)O[C@@H]1CCSC1 | 6.658 | Tr | Itr | Itr | 4 |
| **42** | O=C(N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1)O[C@@H]1CCCS(=O)(=O)C1 | 5.684 | Tr | Tr | Tr | 4 |
| **43** | O=C(N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1)O[C@@H]1C[C@@H](S(=O)(=O)C1)C | 5.796 | Cl | Itr | Cl | 4 |
| **44** | O=C(N[C@H]([C@@H](CN1C[C@H]2CCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1)O[C@@H]1COCC1 | 7.215 | ITr | Cl | Cl | 4 |
| **45** | CCCC[C@H]1[C@H](CCS1(=O)=O)OC(=O)N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1 | 7.827 | ITr | Tr | Cl | 4 |
| **46** | CCCC[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1 | 7.339 | Cl | Tr | Itr | 4 |
| **47** | CCC[C@H]1[C@H](CCS1(=O)=O)OC(=O)N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1 | 8.208 | Tr | Tr | Tr | 4 |
| **48** | CC(C[C@@H](C(=O)N[C@H](C(=O)N)Cc1ccccc1)NC(=O)[C@@H](C[C@@H]([C@@H](NC(=O)[C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)Cc1ccccc1)O)Cc1ccccc1)C | 7.699 | Tr | Itr | Cl | 4 |
| **49** | O=C(O[C@H]1CCS(=O)(=O)[C@H]1C1CCCC1)N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1 | 8.208 | Tr | Tr | Tr | 4 |
| **50** | O=C(O[C@@H]1CS(=O)(=O)C[C@@H]1C)N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1 | 7.155 | Tr | Itr | Tr | 4 |
| **51** | O=C(O[C@@H]1CCS(=O)(=O)[C@@H]1C(C)C)N[C@H]([C@@H](CN1C[C@H]2CCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1 | 8.523 | Tr | Tr | Tr | 4 |
| **52** | O=C(N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1)O[C@H]1CCCS(=O)(=O)C1 | 5.758 | Tr | Tr | Tr | 4 |
| **53** | O=C(N[C@H]([C@@H](CN1C[C@H]2CCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1)O[C@H]1CCS(=O)(=O)C1 | 7.947 | ITr | Tr | Tr | 4 |
| **54** | CCC[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1 | 7.697 | Tr | Tr | Tr | 4 |
| **55** | O=C(O[C@H]1COCC=C1)N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1 | 7.311 | Tr | Tr | Tr | 5 |
| **56** | O=C(O[C@@H]1COCC=C1)N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1 | 6.503 | ITr | Cl | Itr | 5 |
| **57** | O=C(N[C@H]([C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)O)Cc1ccccc1)OC1CCOCC1 | 8.914 | ITr | Itr | Tr | 5 |
| **58** | O=C(N[C@H]([C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)O)Cc1ccccc1)OC1CCCC1 | 9.481 | Tr | Cl | Cl | 5 |
| **59** | O=C(N[C@H]([C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)O)Cc1ccccc1)O[C@H]1COCC1 | 10.523 | Cl | Cl | Cl | 5 |
| **60** | O=C(N[C@H]([C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)O)Cc1ccccc1)O[C@@H]1COCC1 | 10.222 | Cl | Cl | Tr | 5 |
| **61** | O=C(N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1)O[C@H]1CCCOC1 | 6.407 | Tr | Tr | Tr | 5 |
| **62** | O=C(N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1)O[C@@H]1CCOC1 | 6.159 | Tr | Tr | Tr | 5 |
| **63** | O=C(N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1)O[C@@H]1CCCOC1 | 6.511 | Tr | Tr | Tr | 5 |
| **64** | Ic1ccc(cc1)C[C@@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O | 9.143 | Tr | Cl | Cl | 8 |
| **65** | O[C@@H]([C@H](Cc1ccccc1)NC(=O)[C@H](C1CCOCC1)NC(=O)c1ccc2c(n1)cccc2)CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C | 7.168 | ITr | Tr | Tr | 6 |
| **66** | O[C@@H]([C@H](Cc1ccccc1)NC(=O)[C@H](C1CCCC1)NC(=O)c1ccc2c(n1)cccc2)CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C | 8.585 | Tr | Cl | Cl | 6 |
| **67** | O[C@@H]([C@H](Cc1ccccc1)NC(=O)[C@H]([C@H]1CCS(=O)(=O)C1)NC(=O)c1ccc2c(n1)cccc2)CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C | 9.301 | Tr | Tr | Tr | 6 |
| **68** | O[C@@H]([C@H](Cc1ccccc1)NC(=O)[C@H]([C@@H]1CSCC1)NC(=O)c1ccc2c(n1)cccc2)CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C | 9.222 | Tr | Cl | Cl | 6 |
| **69** | O[C@@H]([C@H](Cc1ccccc1)NC(=O)[C@H]([C@@H]1COCC1)NC(=O)c1nc(Cl)c(nc1N)N(C)C)CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C | 9.620 | Tr | Tr | Tr | 6 |
| **70** | O[C@@H]([C@H](Cc1ccccc1)NC(=O)[C@H]([C@@H]1COCC1)NC(=O)c1cnc(c(n1)Cl)N(C)C)CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C | 10.222 | Tr | Itr | Itr | 6 |
| **71** | O[C@@H]([C@H](Cc1ccccc1)NC(=O)[C@H]([C@@H]1CCS(=O)(=O)C1)NC(=O)c1ccc2c(n1)cccc2)CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C | 7.409 | Cl | Itr | Itr | 6 |
| **72** | COC(=O)c1nc(Cl)c(nc1N)N[C@H](C(=O)N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1)[C@@H]1COCC1 | 9.796 | Tr | Cl | Cl | 6 |
| **73** | CC([C@@H](C(=O)N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1)NC(=O)c1cnc2c(n1)cccc2)C | 9.409 | Tr | Tr | Tr | 6 |
| **74** | CC([C@@H](C(=O)N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1)NC(=O)c1ccc2c(n1)cccc2)C | 9.155 | Tr | Cl | Itr | 6 |
| **75** | O[C@@H]([C@H](Cc1ccccc1)NC(=O)[C@H]([C@H]1CSCC1)NC(=O)c1ccc2c(n1)cccc2)CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C | 8.481 | Cl | Cl | Tr | 6 |
| **76** | O[C@@H]([C@H](Cc1ccccc1)NC(=O)[C@H]([C@@H]1COCC1)NC(=O)c1cnccn1)CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C | 8.548 | Tr | Tr | Tr | 6 |
| **77** | O[C@@H]([C@H](Cc1ccccc1)NC(=O)[C@H]([C@@H]1COCC1)NC(=O)c1cnc2c(n1)cccc2)CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C | 9.921 | ITr | Itr | Tr | 6 |
| **78** | O[C@@H]([C@H](Cc1ccccc1)NC(=O)[C@H]([C@@H]1COCC1)NC(=O)c1cc(=O)c2c(o1)cccc2)CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C | 9.959 | Tr | Tr | Cl | 6 |
| **79** | CC([C@@H](C(=O)N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1)NC(=O)c1cc(=O)c2c(o1)cccc2)C | 9.824 | Cl | Tr | Tr | 6 |
| **80** | C[N@@H+]1CCN(CC1)c1ncc(nc1Cl)C(=O)N[C@H](C(=O)N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1)[C@@H]1COCC1 | 10.149 | ITr | Cl | Cl | 6 |
| **81** | O=C(O[C@H]1CCS(=O)(=O)[C@H]1C(C)C)N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1 | 7.959 | Tr | Itr | Itr | 7 |
| **82** | O=C(O[C@@H]1CCS(=O)(=O)[C@@H]1C)N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1 | 7.652 | Tr | Tr | Tr | 7 |
| **83** | O=C(O[C@@H]1CCS(=O)(=O)[C@@H]1C(C)C)N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1 | 8.523 | Tr | Tr | Tr | 7 |
| **84** | O=C(O[C@@H]1CCO[C@@H]1C)N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1 | 6.772 | Cl | Cl | Tr | 7 |
| **85** | CC[C@H]1[C@H](CCS1(=O)=O)OC(=O)N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1 | 8.268 | Tr | Tr | Tr | 7 |
| **86** | CC[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1 | 7.883 | Tr | Tr | Tr | 7 |
| **87** | CC(C[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1)C | 7.523 | Tr | Tr | Tr | 7 |
| **88** | O=C(O[C@H]1CCS(=O)(=O)[C@H]1C)N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1 | 7.943 | Cl | Itr | Tr | 7 |
| **89** | O=C(O[C@H]1CCO[C@H]1C)N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1 | 7.281 | Tr | Tr | Tr | 7 |
| **90** | O=C(O[C@H]1CCO[C@H]1C)N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1 | 7.281 | Tr | Tr | Tr | 7 |
| **91** | O=C(O[C@@H]1CCO[C@@H]1C)N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1 | 6.772 | Tr | Cl | Tr | 7 |
| **92** | O=C(N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1)OCCS(=O)(=O)C | 5.987 | Tr | Cl | Tr | 7 |
| **93** | O=C(N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1)O[C@H]1CCS(=O)(=O)C1 | 7.125 | Tr | Tr | Tr | 7 |
| **94** | O=C(N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1)O[C@H]1CCOC1 | 6.796 | Tr | Tr | Tr | 7 |
| **95** | CC(C[C@H]1[C@H](CCS1(=O)=O)OC(=O)N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1)C | 7.921 | Tr | Tr | Tr | 7 |
| **96** | OCCCc1ccc(cc1)C[C@@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)C[C@@H]([C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)O | 10.000 | Tr | Cl | Cl | 8 |
| **97** | OCCc1ccc(cc1)C[C@@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)C[C@@H]([C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)O | 9.796 | Tr | Tr | Tr | 8 |
| **98** | Oc1cccc(c1)C[C@@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O | 9.678 | Tr | Tr | Tr | 8 |
| **99** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)O)Cc1ccccc1 | 9.638 | Tr | Tr | Tr | 8 |
| **100** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccc(cc1)S(=O)(=O)C)O)Cc1ccccc1 | 9.770 | Tr | Cl | Tr | 8 |
| **101** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccc(cc1)CCCN1CCOCC1)O)Cc1ccccc1 | 9.367 | Tr | Tr | Tr | 8 |
| **102** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccc(cc1)C(F)(F)F)O)Cc1ccccc1 | 9.585 | Tr | Itr | Itr | 8 |
| **103** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccc(cc1)[S@@](=O)C)O)Cc1ccccc1 | 9.292 | Tr | Tr | Tr | 8 |
| **104** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccc(cc1)[N+](=O)[O-])O)Cc1ccccc1 | 9.569 | Tr | Tr | Cl | 8 |
| **105** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)C/C=C/c1ccc(cc1)CCN1CCOCC1)O)Cc1ccccc1 | 9.538 | Cl | Cl | Tr | 8 |
| **106** | Nc1ccc(cc1)C[C@@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O | 9.509 | Tr | Tr | Tr | 8 |
| **107** | CSc1ccc(cc1)C[C@@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O | 9.658 | Tr | Cl | Itr | 8 |
| **108** | COCCOCOCCCc1ccc(cc1)C[C@@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O | 10.155 | Tr | Tr | Cl | 8 |
| **109** | COC(CCc1ccc(cc1)C[C@@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)C[C@@H]([C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)O)OC | 10.097 | Cl | Cl | Cl | 8 |
| **110** | Cc1ccc(cc1)C[C@@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O | 9.538 | Tr | Tr | Tr | 8 |
| **111** | CC(C[C@@H](C(=O)N[C@H](C(=O)N)Cc1ccccc1)NC(=O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)CCCc1ccccc1)C | 9.444 | Tr | Cl | Itr | 8 |
| **112** | CC(C[C@@H](C(=O)N[C@H](C(=O)N)Cc1ccccc1)NC(=O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)Cc1ccccc1)C | 9.377 | Tr | Tr | Tr | 8 |
| **113** | CC(C[C@@H](C(=O)N[C@H](C(=O)N)Cc1ccccc1)NC(=O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)Cc1ccc(cc1)c1ccccc1)C | 9.367 | Tr | Tr | Cl | 8 |
| **114** | CC(C[C@@H](C(=O)N[C@H](C(=O)N)Cc1ccccc1)NC(=O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)C)C | 8.222 | Tr | Cl | Cl | 8 |
| **115** | OCc1ccc(cc1)C[C@@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O | 9.770 | Tr | Tr | Tr | 8 |
| **116** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccc(cc1)C(C)(C)C)O)Cc1ccccc1 | 9.569 | Tr | Tr | Tr | 8 |
| **117** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)C/C=C/c1ccc(cc1)O)O)Cc1ccccc1 | 9.770 | Cl | Cl | Tr | 8 |
| **118** | Fc1ccc(cc1)C[C@@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O | 9.357 | Tr | Cl | Tr | 8 |
| **119** | COCCOCOCCc1ccc(cc1)C[C@@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)C[C@@H]([C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)O | 9.886 | Tr | Tr | Tr | 8 |
| **120** | CC(C[C@@H](C(=O)N[C@H](C(=O)N)Cc1ccccc1)NC(=O)[C@H](Cc1cccc2c1cccc2)C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)C | 8.921 | Tr | Tr | Tr | 8 |
| **121** | OC[C@@H](c1ccccc1)NC(=O)[C@H](Cc1ccccc1)NC[C@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O | 4.420 | Cl | Cl | Cl | 9 |
| **122** | O=C(OC(C)(C)C)N[C@H]([C@@H](CN[C@@H]([C@@H](c1ccccc1)O)C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)O)Cc1ccccc1 | 5.071 | ITr | Itr | Itr | 9 |
| **123** | NC(=O)C[C@H](C(=O)N[C@H]([C@@H](CN[C@H](C(=O)N[C@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)O)Cc1ccccc1)NC(=O)c1ccc2c(n1)cccc2 | 8.268 | ITr | Cl | Cl | 9 |
| **124** | NC(=O)C[C@H](C(=O)N[C@H]([C@@H](CN[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)O)Cc1ccccc1)[NH3+] | 5.959 | Cl | Cl | Cl | 9 |
| **125** | NC(=O)C[C@@H](C(=O)N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1)NC(=O)c1ccc2c(n1)cccc2 | 9.638 | Tr | Tr | Tr | 9 |
| **126** | NC(=O)C[C@@H](C(=O)N[C@H]([C@@H](CN[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)O)Cc1ccccc1)NC(=O)OC(C)(C)C | 6.530 | Tr | Tr | Cl | 9 |
| **127** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)NCc1ccccc1)Cc1ccccc1)O)Cc1ccccc1 | 6.955 | Tr | Cl | Tr | 10 |
| **128** | CC[C@@H]([C@H](C(=O)NCc1nc2c([nH]1)cccc2)NC(=O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)Cc1ccccc1)C | 10.155 | Cl | Cl | Cl | 10 |
| **129** | CC[C@@H]([C@H](C(=O)NC[C@@H](CO)O)NC(=O)[C@H](Cc1ccccc1)C[C@@H]([C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)O)C | 9.824 | Tr | Cl | Cl | 10 |
| **130** | CC(CCNC(=O)[C@H](Cc1ccccc1)C[C@@H]([C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)O)C | 6.328 | Tr | Tr | Itr | 10 |
| **131** | CC(C[C@H](C(=O)NCc1ccccc1)NC(=O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)Cc1ccccc1)C | 8.854 | Cl | Cl | Cl | 10 |
| **132** | CC(C[C@@H](C(=O)N[C@H](C(=O)N)Cc1ccccc1)NC(=O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)C/C=C/c1ccccc1)C | 9.824 | Tr | Tr | Tr | 10 |
| **133** | CC(C[C@@H](C(=O)N[C@H](C(=O)N)Cc1ccccc1)NC(=O)[C@@H](C[C@@H]([C@@H](NC(=O)CC(C)(C)C)Cc1ccccc1)O)Cc1ccccc1)C | 8.222 | Tr | Cl | Cl | 10 |
| **134** | CC(C[C@@H](C(=O)N[C@H](C(=O)N)Cc1ccccc1)NC(=O)[C@@H](C[C@@H]([C@@H](NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)Cc1ccccc1)Cc1ccccc1)O)Cc1ccccc1)C | 9.000 | ITr | Itr | Itr | 10 |
| **135** | CC[C@@H]([C@H](C(=O)NCc1ccccc1)NC(=O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)Cc1ccccc1)C | 9.149 | Cl | Itr | Tr | 10 |
| **136** | CC(C[C@H](C(=O)NCCc1ccccc1)NC(=O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)Cc1ccccc1)C | 7.921 | Cl | Tr | Tr | 10 |
| **137** | CC(C[C@H](C(=O)N)NC(=O)[C@H](Cc1ccccc1)C[C@@H]([C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)O)C | 7.921 | Tr | Tr | Tr | 10 |
| **138** | OCc1cnc2c(c1)cc(o2)CN1CCN([C@H](C1)C(=O)NC(C)(C)C)C[C@@H](C[C@H](C(=O)N[C@H]1[C@@H](O)Cc2c1cccc2)Cc1ccccc1)O | 9.745 | Tr | Tr | Tr | 11 |
| **139** | O[C@H](CN1CCN(C[C@H]1C(=O)NC(C)(C)C)Cc1cnc2c(c1)cccc2)C[C@H](C(=O)N[C@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1 | 9.854 | Tr | Tr | Tr | 11 |
| **140** | O[C@H](CN1CCN(C[C@H]1C(=O)NC(C)(C)C)Cc1cnc2c(c1)c(C)nn2C)C[C@H](C(=O)N[C@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1 | 9.456 | Tr | Tr | Tr | 11 |
| **141** | O[C@H](C[C@H](C(=O)N[C@@H]1[C@@H](O)Cc2c1cccc2)Cc1ccccc1)CN1CCN(C[C@H]1C(=O)NC(C)(C)C)Cc1oc2c(c1C)cccc2 | 9.959 | Cl | Tr | Tr | 11 |
| **142** | O[C@H](C[C@H](C(=O)N[C@@H]1[C@@H](O)Cc2c1cccc2)Cc1ccccc1)CN1CCN(C[C@H]1C(=O)NC(C)(C)C)Cc1ccc2c(c1)cco2 | 8.770 | ITr | Itr | Itr | 11 |
| **143** | O[C@H](C[C@H](C(=O)N[C@@H]1[C@@H](O)Cc2c1cccc2)Cc1ccccc1)CN1CCN(C[C@@H]1C(=O)NC(C)(C)C)Cc1cc2c(s1)nccc2 | 9.959 | Cl | Tr | Tr | 11 |
| **144** | O[C@H](C[C@H](C(=O)N[C@@H]1[C@@H](O)Cc2c1cccc2)Cc1ccccc1)CN1CCN(C[C@@H]1C(=O)NC(C)(C)C)Cc1cc2c(o1)nccc2 | 9.495 | ITr | Tr | Tr | 11 |
| **145** | O[C@@H](CN1CCN(C[C@@H]1C(=O)NC(C)(C)C)Cc1csc2c1cccn2)C[C@H](C(=O)N[C@@H]1[C@@H](O)Cc2c1cccc2)Cc1ccccc1 | 9.699 | Tr | Cl | Tr | 11 |
| **146** | O[C@@H](CN1CCN(C[C@@H]1C(=O)NC(C)(C)C)Cc1c[nH]c2c1cccc2)C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1 | 8.770 | Cl | Tr | Cl | 11 |
| **147** | O[C@@H](C[C@H](C(=O)N[C@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)CN1CCN(C[C@H]1C(=O)NC(C)(C)C)Cc1cnc2c(c1)CCO2 | 9.167 | ITr | Itr | Itr | 11 |
| **148** | O[C@@H](C[C@H](C(=O)N[C@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)CN1CCN(C[C@H]1C(=O)NC(C)(C)C)Cc1ccc(nc1)Cl | 9.310 | Tr | Tr | Tr | 11 |
| **149** | O[C@@H](C[C@H](C(=O)N[C@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)CN1CCN(C[C@H]1C(=O)NC(C)(C)C)Cc1cc2c(o1)cc([nH+]c2)C | 9.721 | Tr | Tr | Tr | 11 |
| **150** | O[C@@H](C[C@H](C(=O)N[C@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)CN1CCN(C[C@H]1C(=O)NC(C)(C)C)C(=O)c1cnc2c(c1)cco2 | 8.770 | Cl | Tr | Tr | 11 |
| **151** | O[C@@H](C[C@H](C(=O)N[C@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)C[N@@H+]1CCN(C[C@H]1C(=O)NC(C)(C)C)Cc1nc2c([nH]1)cccc2 | 9.328 | Tr | Tr | Cl | 11 |
| **152** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1cccnc1)CN1CCN(C[C@H]1C(=O)NC(C)(C)C)Cc1cc2c(s1)scc2 | 9.921 | ITr | Tr | Cl | 11 |
| **153** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)CN1CCN(C[C@H]1C(=O)NC(C)(C)C)Cc1cnc2c(c1Cl)cco2 | 9.602 | Tr | Tr | Tr | 11 |
| **154** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)CN1CCN(C[C@H]1C(=O)NC(C)(C)C)Cc1cnc2c(c1Cl)c(C)nn2C | 9.854 | Cl | Tr | Tr | 11 |
| **155** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)CN1CCN(C[C@H]1C(=O)NC(C)(C)C)Cc1cnc2c(c1)occ2 | 9.770 | Tr | Tr | Tr | 11 |
| **156** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)CN1CCN(C[C@H]1C(=O)NC(C)(C)C)Cc1cnc2c(c1)cco2 | 9.456 | ITr | Tr | Tr | 11 |
| **157** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)CN1CCN(C[C@H]1C(=O)NC(C)(C)C)Cc1ccc(nc1)C | 9.208 | Tr | Itr | Tr | 11 |
| **158** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)CN1CCN(C[C@H]1C(=O)NC(C)(C)C)Cc1cc2c(o1)cncc2 | 9.409 | Cl | Tr | Cl | 11 |
| **159** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)CN1CCN(C[C@H]1C(=O)NC(C)(C)C)Cc1cc2c(o1)cccc2 | 9.745 | Tr | Tr | Tr | 11 |
| **160** | CSc1ncccc1CN1CCN([C@@H](C1)C(=O)NC(C)(C)C)C[C@H](C[C@H](C(=O)N[C@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)O | 9.585 | ITr | Cl | Cl | 11 |
| **161** | COc1ncccc1CN1CCN([C@@H](C1)C(=O)NC(C)(C)C)C[C@H](C[C@H](C(=O)N[C@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)O | 8.959 | Tr | Tr | Tr | 11 |
| **162** | CCOC(=O)c1cnc2c(c1)cc(o2)CN1CCN([C@H](C1)C(=O)NC(C)(C)C)C[C@@H](C[C@H](C(=O)N[C@@H]1[C@@H](O)Cc2c1cccc2)Cc1ccccc1)O | 9.569 | ITr | Cl | Itr | 11 |
| **163** | OC[C@H](c1ccccc1)NC(=O)[C@@H](C[C@@H]([C@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)Cc1ccccc1 | 7.413 | ITr | Tr | Cl | 12 |
| **164** | OC[C@@H](NC(=O)[C@@H](C[C@@H]([C@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)Cc1ccccc1)Cc1ccccc1 | 6.161 | Tr | Tr | Tr | 12 |
| **165** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)NCC1CCCCC1)Cc1ccccc1)O)Cc1ccccc1 | 4.523 | Cl | Tr | Cl | 12 |
| **166** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)NC1Cc2c(C1)cccc2)Cc1ccccc1)O)Cc1ccccc1 | 6.886 | Tr | Tr | Tr | 12 |
| **167** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@H]1CCCC[C@H]1O)Cc1ccccc1)O)Cc1ccccc1 | 6.914 | Cl | Cl | Tr | 12 |
| **168** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@H]1c2ccccc2[C@H]([C@H]1O)O)CCCc1ccccc1)O)Cc1ccccc1 | 9.721 | Tr | Itr | Tr | 12 |
| **169** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@H]1C=CC[C@H]1O)Cc1ccccc1)O)Cc1ccccc1 | 8.021 | Tr | Tr | Tr | 12 |
| **170** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@H]1[C@@H](O)COc2c1cccc2)Cc1ccccc1)O)Cc1ccccc1 | 7.393 | Tr | Tr | Tr | 12 |
| **171** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@H](C(=O)[O-])C(C)C)Cc1ccccc1)O)Cc1ccccc1 | 6.793 | Tr | Tr | Cl | 12 |
| **172** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@]1(C)[C@H](O)Cc2c1cccc2)Cc1ccccc1)O)Cc1ccccc1 | 6.673 | ITr | Itr | Itr | 12 |
| **173** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@@H]1CCc2c1cccc2)Cc1ccccc1)O)Cc1ccccc1 | 7.465 | Cl | Cl | Tr | 12 |
| **174** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccccc1)O)Cc1ccccc1 | 9.745 | Cl | Tr | Tr | 12 |
| **175** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)CCc2c1cccc2)Cc1ccccc1)O)Cc1ccccc1 | 9.155 | Cl | Cl | Itr | 12 |
| **176** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)CSc1ccccc1)O)Cc1ccccc1 | 9.602 | Tr | Cl | Tr | 12 |
| **177** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1cc[nH+]cc1)O)Cc1ccccc1 | 9.276 | ITr | Tr | Cl | 12 |
| **178** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1c(F)c(F)c(c(c1F)F)F)O)Cc1ccccc1 | 9.222 | Tr | Tr | Tr | 12 |
| **179** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)CC(=O)c1ccccc1)O)Cc1ccccc1 | 8.266 | Tr | Tr | Tr | 12 |
| **180** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)C/C=C/c1ccccc1)O)Cc1ccccc1 | 9.638 | Tr | Tr | Tr | 12 |
| **181** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@@H](C1CCCCC1)C)Cc1ccccc1)O)Cc1ccccc1 | 6.836 | Cl | Cl | Cl | 12 |
| **182** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)(Cc1ccccc1)C)O)Cc1ccccc1 | 8.114 | Tr | Tr | Tr | 12 |
| **183** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@@]1(CCCN(C1=O)[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)O)Cc1ccccc1 | 5.897 | Tr | Tr | Tr | 12 |
| **184** | O=C(OC(C)(C)C)N[C@H]([C@H]([C@@H]1CCC[C@H]1C(=O)NCc1ccccc1)O)Cc1ccc(cc1)O | 6.230 | Tr | Cl | Tr | 12 |
| **185** | O=C(OC(C)(C)C)N[C@H]([C@H](/C=C(\C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)/Cc1ccccc1)O)Cc1ccccc1 | 8.886 | Tr | Tr | Tr | 12 |
| **186** | O=C(OC(C)(C)C)N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1 | 5.520 | Cl | Tr | Cl | 12 |
| **187** | O=C(OC(C)(C)C)N[C@H]([C@@H](CN[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)O)Cc1ccccc1 | 6.640 | Tr | Cl | Tr | 12 |
| **188** | O=C(OC(C)(C)C)CN(C[C@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)Cc1ccccc1 | 5.330 | Tr | Itr | Cl | 12 |
| **189** | O=C(N[C@H]1[C@H](O)Cc2c1cccc2)C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O | 6.246 | ITr | Itr | Itr | 12 |
| **190** | O=C(N[C@@H]1[C@H](O)Cc2c1cccc2)CC[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O | 5.533 | Cl | Cl | Cl | 12 |
| **191** | O[C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1 | 9.161 | Tr | Cl | Tr | 12 |
| **192** | O[C@@H](CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C | 5.170 | ITr | Tr | Cl | 12 |
| **193** | O[C@@H](C[C@H](C(=O)N[C@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)CN1CCC[C@H]1C(=O)NC(C)(C)C | 6.460 | Cl | Tr | Tr | 12 |
| **194** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)C[N@@H+]1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C | 8.119 | Tr | Cl | Cl | 12 |
| **195** | O[C@@H]([C@H](Cc1ccccc1)NC(=O)[C@H]([C@H]1COCC1)NC(=O)c1ccc2c(n1)cccc2)CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C | 8.268 | Cl | Cl | Tr | 12 |
| **196** | O[C@@H]([C@H](Cc1ccccc1)NC(=O)[C@H]([C@@H]1COCC1)NC(=O)c1ccc2c(n1)cccc2)CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C | 10.268 | ITr | Itr | Itr | 12 |
| **197** | O[C@@H]([C@@H]([C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C | 5.862 | ITr | Itr | Cl | 12 |
| **198** | COC(=O)[C@@H]1Cc2c([C@@H]1NC(=O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)Cc1ccccc1)cccc2 | 7.178 | Tr | Tr | Cl | 12 |
| **199** | C=CC[C@@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O | 7.561 | Tr | Tr | Tr | 12 |
| **200** | O=C(OC(C)(C)C)N[C@H]([C@H](CN[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)O)Cc1ccccc1 | 5.328 | ITr | Itr | Itr | 9 |
| **201** | O=C(OC(C)(C)C)N[C@H]([C@H](CN[C@@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)O)Cc1ccccc1 | 4.631 | Tr | Tr | Itr | 9 |
| **202** | O=C(OC(C)(C)C)N[C@H]([C@@H](CN[C@@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)O)Cc1ccccc1 | 5.137 | ITr | Itr | Itr | 9 |
| **203** | Oc1ccc(cc1)C[C@@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O | 9.796 | Tr | Itr | Itr | 13 |
| **204** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)O)Cc1ccc(cc1)OCCN1CCOCC1 | 9.260 | Tr | Cl | Tr | 13 |
| **205** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)O)Cc1ccc(cc1)O | 9.456 | Tr | Tr | Tr | 13 |
| **206** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccc(cc1)OCCN1CCSCC1)O)Cc1ccccc1 | 9.328 | Cl | Cl | Itr | 13 |
| **207** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccc(cc1)OCCN1CCS(=O)(=O)CC1)O)Cc1ccccc1 | 10.097 | Tr | Tr | Tr | 13 |
| **208** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccc(cc1)OCCN1CCOCC1)O)Cc1ccccc1 | 9.347 | Cl | Tr | Tr | 13 |
| **209** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccc(cc1)OCCN1CCOCC1)O)Cc1ccc(cc1)OCCN1CCOCC1 | 8.721 | Tr | Tr | Cl | 13 |
| **210** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccc(cc1)OCCN1CC[S@@](=O)CC1)O)Cc1ccccc1 | 10.155 | Cl | Cl | Cl | 13 |
| **211** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccc(cc1)OCCN1CC[N@H+](CC1)C)O)Cc1ccccc1 | 9.699 | Tr | Tr | Tr | 13 |
| **212** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccc(cc1)OCCCN1CCOCC1)O)Cc1ccccc1 | 8.699 | Tr | Tr | Tr | 13 |
| **213** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccc(cc1)OCc1ccccc1)O)Cc1ccccc1 | 9.745 | ITr | Tr | Tr | 13 |
| **214** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccc(cc1)OCC[NH+]1CCCCC1)O)Cc1ccccc1 | 8.796 | Tr | Tr | Tr | 13 |
| **215** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccc(cc1)OCC[NH+]1CCCC1)O)Cc1ccccc1 | 8.745 | Tr | Itr | Tr | 13 |
| **216** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccc(cc1)OCC[NH+](C)C)O)Cc1ccccc1 | 8.678 | Tr | Cl | Cl | 13 |
| **217** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccc(cc1)OCC[N+]1([O-])CCOCC1)O)Cc1ccccc1 | 9.699 | ITr | Itr | Itr | 13 |
| **218** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccc(cc1)OCC(=O)N1CCOCC1)O)Cc1ccccc1 | 9.699 | ITr | Itr | Itr | 13 |
| **219** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccc(cc1)O)O)Cc1ccc(cc1)O | 9.824 | Cl | Tr | Cl | 13 |
| **220** | COCC[NH+](CCOC)CCOc1ccc(cc1)C[C@@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)C[C@@H]([C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)O | 9.046 | Tr | Cl | Cl | 13 |
| **221** | [O-]C(=O)COc1ccc(cc1)C[C@@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)C[C@@H]([C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)O | 10.398 | Tr | Cl | Cl | 13 |
| **222** | OCCOc1ccc(cc1)C[C@@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)C[C@@H]([C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)O | 10.046 | Cl | Tr | Tr | 13 |
| **223** | O=C(OC(C)(C)C)N[C@H]([C@H](C[C@H](C(=O)N[C@H]1c2ccccc2[C@H]([C@H]1O)O)Cc1ccccc1)O)Cc1ccccc1 | 10.000 | Cl | Tr | Tr | 14 |
| **224** | O=C(N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1)O[C@@H]1CCS(=O)(=O)C1 | 6.854 | Cl | Cl | Tr | 15 |
| **225** | O[C@H](CN1CC[N@H+](C[C@H]1C(=O)NCC(F)(F)F)Cc1ncc(o1)c1ccc(cc1)Cl)C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccc(o1)c1cnccc1C | 10.523 | Cl | Tr | Tr | 16 |
| **226** | O[C@H](CN1CC[N@H+](C[C@H]1C(=O)NCC(F)(F)F)Cc1csc(n1)c1ccc(cc1)F)C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccc(o1)c1cnccc1C | 9.959 | Tr | Tr | Tr | 16 |
| **227** | O[C@H](CN1CC[N@H+](C[C@H]1C(=O)NCC(F)(F)F)Cc1ccc(s1)c1ccc(cc1)Cl)C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccc(o1)c1cnccc1C | 10.398 | Tr | Cl | Tr | 16 |
| **228** | O[C@H](CN1CC[N@H+](C[C@H]1C(=O)NCC(F)(F)F)C(c1ncc(s1)c1ccc(cc1)Cl)(C)C)C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccc(o1)c1cnccc1C | 10.523 | ITr | Cl | Cl | 16 |
| **229** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1cc2c(s1)ccnc2)CN1CC[N@H+](C[C@H]1C(=O)NCC(F)(F)F)Cc1ccc(s1)c1ccc(cc1)Cl | 10.301 | Tr | Tr | Tr | 16 |
| **230** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1cc2c(s1)ccnc2)CN1CC[N@H+](C[C@H]1C(=O)NCC(F)(F)F)Cc1ccc(o1)c1ccc(cc1)Cl | 10.523 | Tr | Tr | Tr | 16 |
| **231** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1cc2c(s1)ccnc2)CN1CC[N@@H+](C[C@H]1C(=O)NCC(F)(F)F)Cc1csc(n1)c1ccc(cc1)C(F)(F)F | 10.155 | Tr | Tr | Tr | 16 |
| **232** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1cc2c(o1)cncc2)CN1CC[N@H+](C[C@H]1C(=O)NCC(F)(F)F)Cc1ccc(o1)c1ccc(cc1)Cl | 10.301 | Cl | Cl | Tr | 16 |
| **233** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1cc2c(o1)cncc2)CN1CC[N@H+](C[C@H]1C(=O)NCC(F)(F)F)C(c1ncc(o1)c1ccc(cc1)Cl)(C)C | 10.699 | Tr | Tr | Cl | 16 |
| **234** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1cc2c(s1)ccnc2)CN1CC[N@H+](C[C@H]1C(=O)NCC(F)(F)F)C(c1ncc(s1)c1ccc(cc1)Cl)(C)C | 10.398 | Tr | Tr | Tr | 16 |
| **235** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1cc2c(s1)ccnc2)CN1CC[N@H+](C[C@H]1C(=O)NCC(F)(F)F)C(c1ncc(o1)c1ccc(cc1)Cl)(C)C | 10.699 | Cl | Tr | Tr | 16 |
| **236** | O[C@H](CN1CC[N@H+](C[C@H]1C(=O)NCC(F)(F)F)Cc1ccc(o1)c1ccc(cc1)Cl)C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1nnc(o1)c1ccccc1 | 10.721 | Cl | Itr | Itr | 17 |
| **237** | O[C@H](CN1CC[N@H+](C[C@H]1C(=O)NCC(F)(F)F)C(c1ncc(o1)c1ccc(cc1)F)(C)C)C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1nnc(o1)c1ccccc1 | 10.699 | ITr | Tr | Itr | 17 |
| **238** | O[C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1nnco1)CN1CC[N@H+](C[C@H]1C(=O)NCC(F)(F)F)Cc1ccc(o1)c1ccc(cc1)Cl | 10.824 | ITr | Itr | Cl | 17 |
| **239** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1nnc(o1)C)CN1CC[N@H+](C[C@H]1C(=O)NCC(F)(F)F)C(c1ncc(o1)c1ccc(cc1)Cl)(C)C | 10.796 | Cl | Cl | Itr | 17 |
| **240** | COc1cncc(c1)c1cnc(o1)C([N@@H+]1CCN([C@@H](C1)C(=O)NCC(F)(F)F)C[C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1nnc(o1)c1ccccc1)O)(C)C | 9.319 | Cl | Itr | Cl | 17 |
| **241** | COc1cncc(c1)c1cnc(o1)C([N@@H+]1CCN([C@@H](C1)C(=O)NCC(F)(F)F)C[C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1nnc(o1)C)O)(C)C | 9.398 | ITr | Cl | Cl | 17 |
| **242** | CCCc1nnc(o1)C[C@@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)C[C@@H](CN1CC[N@H+](C[C@H]1C(=O)NCC(F)(F)F)C(c1ncc(o1)c1cncc(c1)OC)(C)C)O | 9.495 | ITr | Itr | Itr | 17 |
| **243** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1nnco1)CN1CC[N@H+](C[C@H]1C(=O)NCC(F)(F)F)C(c1ncc(o1)c1ccc(cc1)F)(C)C | 10.620 | Tr | Tr | Tr | 17 |
| **244** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1nnc(o1)C)CN1CC[N@H+](C[C@H]1C(=O)NCC(F)(F)F)C(c1ncc(o1)c1ccc(cc1)F)(C)C | 10.569 | Tr | Tr | Tr | 17 |
| **245** | COc1cncc(c1)c1cnc(o1)C([N@@H+]1CCN([C@@H](C1)C(=O)NCC(F)(F)F)C[C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1nnco1)O)(C)C | 9.620 | Tr | Tr | Tr | 17 |
| **246** | CCCc1nnc(o1)C[C@@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)C[C@@H](CN1CC[N@H+](C[C@H]1C(=O)NCC(F)(F)F)C(c1ncc(o1)c1ccc(cc1)F)(C)C)O | 10.796 | Cl | Tr | Cl | 17 |
| **247** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1cccnc1)CN1CCN(C[C@H]1C(=O)NCC(F)(F)F)Cc1cc2c(s1)scc2 | 10.523 | Tr | Tr | Tr | 18 |
| **248** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1cccnc1)CN1CCN(C[C@H]1C(=O)NCC(F)(F)F)Cc1cc2c(o1)c(Cl)ccc2 | 10.699 | Tr | Tr | Tr | 18 |
| **249** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1cc[nH+]cc1)CN1CCN(C[C@H]1C(=O)NCC(F)(F)F)Cc1cc2c(s1)scc2 | 10.155 | ITr | Itr | Cl | 18 |
| **250** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1cc[nH+]cc1)CN1CCN(C[C@H]1C(=O)NCC(F)(F)F)Cc1cc2c(o1)cccc2 | 10.000 | Cl | Tr | Cl | 18 |
| **251** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1cc[nH+]cc1)CN1CCN(C[C@H]1C(=O)NCC(F)(F)F)Cc1cc2c(o1)c(Cl)ccc2 | 10.523 | Cl | Cl | Cl | 18 |
| **252** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1cc[nH+]cc1)CN1CC[N@H+](C[C@H]1C(=O)NCC(F)(F)F)Cc1ccc(o1)c1ccccc1 | 10.398 | Cl | Tr | Tr | 18 |
| **253** | CC[C@@H]([C@H](C(=O)NCc1nc2c([nH]1)cccc2)NC(=O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)C/C=C/c1ccccc1)C | 10.523 | ITr | Itr | Itr | 10 |
| **254** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1cccnc1)CN1CCN(C[C@H]1C(=O)NCC(F)(F)F)Cc1cc2c(o1)cccc2 | 10.398 | Cl | Cl | Tr | 19 |
| **255** | O[C@H](CN1CCN(C[C@H]1C(=O)NCC(F)(F)F)Cc1ccn(c1)c1cccc(c1)F)C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1cccnc1 | 10.301 | Tr | Tr | Tr | 19 |
| **256** | O[C@H](CN1CCN(C[C@H]1C(=O)NCC(F)(F)F)Cc1ccn(c1)c1cccc(c1)Cl)C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1cccnc1 | 10.301 | Tr | Tr | Tr | 19 |
| **257** | O[C@H](CN1CCN(C[C@H]1C(=O)NCC(F)(F)F)Cc1ccn(c1)c1cccc(c1)C)C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1cccnc1 | 10.000 | Tr | Cl | Tr | 19 |
| **258** | O[C@H](CN1CCN(C[C@H]1C(=O)NCC(F)(F)F)Cc1ccn(c1)c1ccc(cc1)C(F)(F)F)C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1cccnc1 | 10.398 | Tr | Tr | Tr | 19 |
| **259** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1cccnc1)CN1CCN(C[C@H]1C(=O)NCC(F)(F)F)Cc1ccn(c1)c1ccccc1Cl | 9.745 | Tr | Tr | Tr | 19 |
| **260** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1cccnc1)CN1CCN(C[C@H]1C(=O)NCC(F)(F)F)Cc1ccn(c1)c1ccccc1C | 9.796 | Cl | Tr | Tr | 19 |
| **261** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1cccnc1)CN1CCN(C[C@H]1C(=O)NCC(F)(F)F)Cc1ccn(c1)c1cccc(c1)C(F)(F)F | 10.301 | Tr | Tr | Tr | 19 |
| **262** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1cccnc1)CN1CCN(C[C@H]1C(=O)NCC(F)(F)F)Cc1ccn(c1)c1ccc(cc1)Cl | 10.523 | ITr | Itr | Tr | 19 |
| **263** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1cccnc1)CN1CCN(C[C@H]1C(=O)NCC(F)(F)F)Cc1ccn(c1)c1ccc(c(c1F)F)F | 10.301 | Tr | Tr | Tr | 19 |
| **264** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1cccnc1)CN1CCN(C[C@H]1C(=O)NCC(F)(F)F)Cc1ccn(c1)c1ccc(c(c1)Cl)Cl | 10.699 | Cl | Cl | Cl | 19 |
| **265** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1cccnc1)CN1CCN(C[C@H]1C(=O)NCC(F)(F)F)Cc1ccn(c1)c1cc(Cl)c(c(c1)Cl)Cl | 10.699 | Tr | Tr | Tr | 19 |
| **266** | N#Cc1cccc(c1)n1ccc(c1)CN1CCN([C@@H](C1)C(=O)NCC(F)(F)F)C[C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1cccnc1)O | 9.824 | Cl | Tr | Tr | 19 |
| **267** | N#Cc1ccc(cc1)n1ccc(c1)CN1CCN([C@@H](C1)C(=O)NCC(F)(F)F)C[C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1cccnc1)O | 10.000 | Cl | Tr | Tr | 19 |
| **268** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1cccnc1)CN1CCN(C[C@H]1C(=O)NCC(F)(F)F)Cc1ccn(c1)c1ccccc1F | 9.796 | ITr | Tr | Tr | 19 |
| **269** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1cccnc1)CN1CCN(C[C@H]1C(=O)NCC(F)(F)F)Cc1ccn(c1)c1ccccc1C(F)(F)F | 8.879 | Tr | Tr | Tr | 19 |
| **270** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1cccnc1)CN1CCN(C[C@H]1C(=O)NCC(F)(F)F)Cc1ccn(c1)c1ccccc1 | 9.959 | ITr | Cl | Tr | 19 |
| **271** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1cccnc1)CN1CCN(C[C@H]1C(=O)NCC(F)(F)F)Cc1ccn(c1)c1ccc(cc1)F | 10.301 | Tr | Tr | Tr | 19 |
| **272** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1cccnc1)CN1CCN(C[C@H]1C(=O)NCC(F)(F)F)Cc1ccn(c1)c1ccc(cc1)C | 10.222 | Tr | Tr | Tr | 19 |
| **273** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1cccnc1)CN1CC[N@H+](C[C@H]1C(=O)NCC(F)(F)F)Cc1ccc(o1)c1ccccc1 | 10.699 | Cl | Tr | Tr | 19 |
| **274** | N#Cc1ccccc1n1ccc(c1)CN1CCN([C@@H](C1)C(=O)NCC(F)(F)F)C[C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1cccnc1)O | 9.337 | Tr | Tr | Tr | 19 |
| **275** | O[C@H](CN1CCN(C[C@H]1C(=O)NCC(F)(F)F)Cc1ncc(o1)c1cccnc1)C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccccc1 | 9.854 | ITr | Cl | Cl | 20 |
| **276** | O[C@H](CN1CCN(C[C@H]1C(=O)NCC(F)(F)F)C(c1ncc(o1)c1cccnc1)(C)C)C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccccc1 | 10.398 | Tr | Tr | Tr | 20 |
| **277** | O[C@H](CN1CC[N@H+](C[C@H]1C(=O)NCC(F)(F)F)Cc1ccc(o1)c1ccncc1)C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccccc1 | 10.097 | Tr | Tr | Itr | 20 |
| **278** | O[C@H](CN1CC[N@H+](C[C@H]1C(=O)NCC(F)(F)F)Cc1ccc(o1)c1cccnc1)C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccccc1 | 10.523 | Tr | Tr | Tr | 20 |
| **279** | O[C@H](CN1CC[N@@H+](C[C@H]1C(=O)NCC(F)(F)F)C(c1ccc(o1)c1ccncc1)(C)C)C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccccc1 | 10.301 | ITr | Itr | Itr | 20 |
| **280** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccccc1)CN1CCN(C[C@H]1C(=O)NCC(F)(F)F)Cc1ncc(o1)c1ccccn1 | 9.886 | ITr | Itr | Itr | 20 |
| **281** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccccc1)CN1CCN(C[C@H]1C(=O)NCC(F)(F)F)C(c1ncc(o1)c1cncc(c1)Cl)(C)C | 10.699 | Tr | Tr | Tr | 20 |
| **282** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccccc1)CN1CCN(C[C@H]1C(=O)NCC(F)(F)F)C(c1ncc(o1)c1ccccn1)(C)C | 10.398 | Tr | Tr | Tr | 20 |
| **283** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccccc1)CN1CC[N@H+](C[C@H]1C(=O)NCC(C(F)(F)F)(F)F)C(c1cc2c(o1)ccnc2)(C)C | 9.854 | ITr | Cl | Tr | 20 |
| **284** | COc1cncc(c1)c1cnc(o1)C(N1CCN([C@@H](C1)C(=O)NCC(F)(F)F)C[C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccccc1)O)(C)C | 10.699 | Tr | Tr | Tr | 20 |
| **285** | O[C@H](CN1CCN(C[C@H]1C(=O)NCC(F)(F)F)Cc1ncc(o1)c1ccncc1)C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccccc1 | 10.000 | Tr | Tr | Tr | 20 |
| **286** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccccc1)CN1CC[N@H+](C[C@H]1C(=O)NCC(F)(F)F)C(c1cc2c(o1)ccnc2)(C)C | 10.155 | ITr | Cl | Tr | 20 |
| **287** | O[C@@H](C[C@H](C(=O)N[C@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)CN1CCN(C[C@H]1C(=O)NC(C)(C)C)Cc1cc2c(o1)cccc2 | 9.310 | Tr | Tr | Tr | 21 |
| **288** | O[C@H](CN1CCN(C[C@H]1C(=O)NC(C)(C)C)CCCC(F)(F)F)C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1 | 7.824 | Cl | Cl | Cl | 21 |
| **289** | O[C@H](CN1CCN(C[C@H]1C(=O)NC(C)(C)C)Cc1noc2c1cccc2)C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1 | 8.932 | ITr | Tr | Tr | 21 |
| **290** | O[C@H](CN1CCN(C[C@H]1C(=O)NC(C)(C)C)Cc1cn(c2c1cccc2)C)C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1 | 8.174 | Tr | Cl | Tr | 21 |
| **291** | O[C@@H](C[C@H](C(=O)N[C@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)CN1CCN(C[C@H]1C(=O)NC(C)(C)C)S(=O)(=O)c1ccc2c(c1)[nH+]c(cc2)N(C)C | 9.658 | ITr | Itr | Itr | 21 |
| **292** | O[C@@H](C[C@H](C(=O)N[C@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)CN1CCN(C[C@H]1C(=O)NC(C)(C)C)Cc1ncc(s1)c1ccccc1 | 9.585 | Tr | Itr | Itr | 21 |
| **293** | O[C@@H](C[C@H](C(=O)N[C@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)CN1CCN(C[C@H]1C(=O)NC(C)(C)C)Cc1cc2c(o1)ccc(c2)F | 9.027 | Tr | Cl | Tr | 21 |
| **294** | O[C@@H](C[C@H](C(=O)N[C@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)CN1CC[N@@H+](C[C@H]1C(=O)NC(C)(C)C)Cc1ccc(s1)c1cc(nn1C)C(F)(F)F | 9.886 | ITr | Itr | Cl | 21 |
| **295** | O[C@@H](C[C@H](C(=O)N[C@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)C[N@@H+]1CCN(C[C@H]1C(=O)NC(C)(C)C)Cc1nc2c(s1)cccc2 | 8.921 | Tr | Tr | Tr | 21 |
| **296** | O[C@@H](C[C@H](C(=O)N[C@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)C[N@@H+]1CCN(C[C@H]1C(=O)NC(C)(C)C)Cc1nc2c(o1)cccc2 | 8.921 | Cl | Itr | Itr | 21 |
| **297** | O[C@@H](C[C@H](C(=O)N[C@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)C[N@@H+]1CCN(C[C@H]1C(=O)NC(C)(C)C)CC1(CC1)c1ccccc1 | 8.114 | Cl | Tr | Cl | 21 |
| **298** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)CN1CCN(C[C@H]1C(=O)NC(C)(C)C)Cc1cccc(c1)C(NC(=O)OC(C)(C)C)(C)C | 7.553 | ITr | Itr | Itr | 21 |
| **299** | O=C(O[C@@H]1CCS(=O)(=O)[C@@H]1C(C)C)N[C@H]([C@@H](CN1CCN(C[C@H]1C(=O)NC(C)(C)C)CC(C)(C)C)O)Cc1ccccc1 | 7.319 | Tr | Tr | Tr | 22 |
| **300** | O=C(O[C@@H]1CCS(=O)(=O)[C@@H]1C(C)C)N[C@H]([C@@H](CN1CCN(C[C@H]1C(=O)NC(C)(C)C)C1CCSCC1)O)Cc1ccccc1 | 6.623 | ITr | Itr | Itr | 22 |
| **301** | O=C(O[C@@H]1CCS(=O)(=O)[C@@H]1C(C)C)N[C@H]([C@@H](CN1CCN(C[C@H]1C(=O)NC(C)(C)C)C1CCOCC1)O)Cc1ccccc1 | 7.461 | Tr | Tr | Tr | 22 |
| **302** | O=C(O[C@@H]1CCS(=O)(=O)[C@@H]1C(C)C)N[C@H]([C@@H](CN1CCN(C[C@H]1C(=O)NC(C)(C)C)C1CCC1)O)Cc1ccccc1 | 7.762 | Tr | Tr | Tr | 22 |
| **303** | O=C(O[C@@H]1CCS(=O)(=O)[C@@H]1C(C)C)N[C@H]([C@@H](CN1CCN(C[C@H]1C(=O)NC(C)(C)C)C1Cc2c(C1)cccc2)O)Cc1ccccc1 | 8.276 | Cl | Tr | Tr | 22 |
| **304** | O=C(O[C@@H]1CCS(=O)(=O)[C@@H]1C(C)C)N[C@H]([C@@H](CN1CCN(C[C@H]1C(=O)NC(C)(C)C)C1CC1)O)Cc1ccccc1 | 8.319 | Tr | Tr | Tr | 22 |
| **305** | O=C(O[C@@H]1CCS(=O)(=O)[C@@H]1C(C)C)N[C@H]([C@@H](CN1CCN(C[C@H]1C(=O)NC(C)(C)C)C(C)C)O)Cc1ccccc1 | 7.244 | Tr | Itr | Itr | 22 |
| **306** | O=C(O[C@@H]1CCS(=O)(=O)[C@@H]1C(C)C)N[C@H]([C@@H](CN1CCN(C[C@H]1C(=O)NC(C)(C)C)[C@H]1CSCC1)O)Cc1ccccc1 | 8.081 | Tr | Tr | Cl | 22 |
| **307** | O=C(O[C@@H]1CCS(=O)(=O)[C@@H]1C(C)C)N[C@H]([C@@H](CN1CCN(C[C@H]1C(=O)NC(C)(C)C)[C@@H]1C[C@@H](C1)c1ccccc1)O)Cc1ccccc1 | 8.420 | ITr | Tr | Cl | 22 |
| **308** | O=C(O[C@@H]1CCS(=O)(=O)[C@@H]1C(C)C)N[C@H]([C@@H](CN1CC[N@H+](C[C@H]1C(=O)NC(C)(C)C)C1CCCCC1)O)Cc1ccccc1 | 7.873 | Cl | Itr | Tr | 22 |
| **309** | O=C(O[C@@H]1CCS(=O)(=O)[C@@H]1C(C)C)N[C@H]([C@@H](CN1CC[N@H+](C[C@H]1C(=O)NC(C)(C)C)C1CCCC1)O)Cc1ccccc1 | 7.733 | ITr | Tr | Tr | 22 |
| **310** | CCCN1CCN([C@@H](C1)C(=O)NC(C)(C)C)C[C@H]([C@H](Cc1ccccc1)NC(=O)O[C@@H]1CCS(=O)(=O)[C@@H]1C(C)C)O | 7.863 | Cl | Cl | Cl | 22 |
| **311** | CCCCCCCCN1CCN([C@@H](C1)C(=O)NC(C)(C)C)C[C@H]([C@H](Cc1ccccc1)NC(=O)O[C@@H]1CCS(=O)(=O)[C@@H]1C(C)C)O | 8.076 | Tr | Itr | Cl | 22 |
| **312** | CCC(N1CCN([C@@H](C1)C(=O)NC(C)(C)C)C[C@H]([C@H](Cc1ccccc1)NC(=O)O[C@@H]1CCS(=O)(=O)[C@@H]1C(C)C)O)CC | 7.006 | Tr | Cl | Tr | 22 |
| **313** | CC(CN1CCN([C@@H](C1)C(=O)NC(C)(C)C)C[C@H]([C@H](Cc1ccccc1)NC(=O)O[C@@H]1CCS(=O)(=O)[C@@H]1C(C)C)O)C | 7.567 | Tr | Cl | Itr | 22 |
| **314** | O=C([C@@H](C[C@@H](C(=O)N1CSC([C@H]1C(=O)NCc1ccccc1C)(C)C)O)Cc1ccccc1)N[C@@H]1[C@H](O)COc2c1cccc2 | 10.155 | Cl | Tr | Cl | 23 |
| **315** | O[C@H](CN1CSC([C@H]1C(=O)NCc1ccccc1C)(C)C)C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccccc1 | 9.284 | Tr | Cl | Tr | 23 |
| **316** | O[C@H](C(=O)N1CSC([C@H]1C(=O)NCc1ncccc1C)(C)C)C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccccc1 | 9.886 | Tr | Tr | Itr | 23 |
| **317** | O[C@H](C(=O)N1CSC([C@H]1C(=O)NCc1c(F)cccc1F)(C)C)C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccccc1 | 9.620 | Tr | Tr | Tr | 23 |
| **318** | O[C@H](C(=O)N1CSC([C@H]1C(=O)NCc1c(Cl)cccc1Cl)(C)C)C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccccc1 | 10.398 | Tr | Tr | Tr | 23 |
| **319** | O[C@H](C(=O)N1CSC([C@H]1C(=O)NCc1c(C)nsc1C)(C)C)C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccccc1 | 10.301 | Tr | Cl | Tr | 23 |
| **320** | O[C@H](C(=O)N1CSC([C@H]1C(=O)NCc1c(C)noc1C)(C)C)C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccccc1 | 10.155 | Tr | Tr | Tr | 23 |
| **321** | O[C@H](C(=O)N1CSC([C@H]1C(=O)NCc1c(C)ccnc1C)(C)C)C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccccc1 | 9.796 | ITr | Cl | Itr | 23 |
| **322** | O[C@H](C(=O)N1CSC([C@H]1C(=O)NCc1c(C)cccc1C)(C)C)C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccccc1 | 9.553 | Cl | Tr | Tr | 23 |
| **323** | O[C@H](C(=O)N1CSC([C@H]1C(=O)NCc1c(C)cccc1C)(C)C)C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1 | 10.398 | Tr | Itr | Itr | 23 |
| **324** | O[C@@H](C(=O)N1CSC([C@H]1C(=O)NCc1c(C)cccc1C)(C)C)C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccccc1 | 10.523 | ITr | Tr | Itr | 23 |
| **325** | O[C@H](C(=O)N1CSC([C@H]1C(=O)NCc1c(C)cccc1C)(C)C)C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccccc1 | 9.553 | ITr | Tr | Tr | 23 |
| **326** | O[C@H](C[C@H](C(=O)NCc1c(C)cc(cc1C)O)Cc1ccccc1)CN1CCN(C[C@@H]1C(=O)NC(C)(C)C)S(=O)(=O)c1cccs1 | 9.328 | Tr | Tr | Cl | 24 |
| **327** | O[C@H](C[C@H](C(=O)NCc1c(C)cc(cc1C)O)Cc1ccccc1)CN1CCN(C[C@@H]1C(=O)NC(C)(C)C)S(=O)(=O)c1ccc2c(c1)CCN2c1ncccn1 | 9.699 | Cl | Cl | Cl | 24 |
| **328** | O[C@@H](CN1CCN(C[C@@H]1C(=O)NC(C)(C)C)S(=O)(=O)c1cccs1)C[C@H](C(=O)N[C@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1 | 10.000 | Tr | Tr | Tr | 24 |
| **329** | O[C@H](CN1CC[N@H+](C[C@H]1C(=O)Nc1ccccc1)C(c1oc2c(c1)cncc2)(C)C)C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccccc1 | 7.860 | Tr | Tr | Tr | 25 |
| **330** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccccc1)CN1CC[N@H+](C[C@H]1C(=O)NCCC(F)(F)F)C(c1cc2c(o1)ccnc2)(C)C | 8.796 | Tr | Tr | Tr | 25 |
| **331** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccccc1)CN1CC[N@H+](C[C@H]1C(=O)NCc1ccccc1)C(c1cc2c(o1)ccnc2)(C)C | 8.660 | Cl | Tr | Cl | 25 |
| **332** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccccc1)CN1CC[N@H+](C[C@H]1C(=O)NCC1CC1)C(c1cc2c(o1)ccnc2)(C)C | 9.301 | Tr | Tr | Tr | 25 |
| **333** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccccc1)CN1CC[N@H+](C[C@H]1C(=O)NCC(F)(F)F)Cc1ccc(o1)c1ccccn1 | 10.301 | Cl | Itr | Tr | 20 |
| **334** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccccc1)CN1CC[N@H+](C[C@H]1C(=O)NC1CCCC1)C(c1cc2c(o1)ccnc2)(C)C | 9.432 | Tr | Tr | Itr | 25 |
| **335** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccccc1)CN1CC[N@H+](C[C@H]1C(=O)NC1CC1)C(c1cc2c(o1)ccnc2)(C)C | 9.222 | Tr | Tr | Tr | 25 |
| **336** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccccc1)CN1CC[N@@H+](C[C@H]1C(=O)NCc1cccs1)C(c1cc2c(o1)ccnc2)(C)C | 9.187 | Cl | Itr | Itr | 25 |
| **337** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccccc1)CN1CC[N@@H+](C[C@H]1C(=O)NCC(C)C)C(c1cc2c(o1)ccnc2)(C)C | 9.398 | Tr | Itr | Itr | 25 |
| **338** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccccc1)CN1CC[N@@H+](C[C@H]1C(=O)NCC(C)(C)C)C(c1cc2c(o1)ccnc2)(C)C | 8.936 | Tr | Tr | Tr | 25 |
| **339** | CCNC(=O)[C@@H]1C[N@@H+](CCN1C[C@H](C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccccc1)O)C(c1cc2c(o1)ccnc2)(C)C | 9.215 | ITr | Cl | Cl | 25 |
| **340** | O[C@H](CN1CC[N@@H+](C[C@H]1C(=O)NC(C)(C)C)C(c1oc2c(c1)cncc2)(C)C)C[C@H](C(=O)N[C@@H]1[C@H](O)COc2c1cccc2)Cc1ccccc1 | 10.125 | Tr | Cl | Tr | 26 |
| **341** | O[C@H](CN1CC[N@@H+](C[C@H]1C(=O)NC(C)(C)C)C(c1oc2c(c1)cncc2)(C)C)C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1 | 9.824 | Cl | Cl | Cl | 26 |
| **342** | O[C@H](CN1CC[N@@H+](C[C@H]1C(=O)NC(C)(C)C)C(c1cccnc1)(C)C)C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1 | 8.936 | Cl | Tr | Cl | 26 |
| **343** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)CN1CCN(C[C@H]1C(=O)NC(C)(C)C)Cc1cc2c(o1)ccnc2 | 9.658 | Tr | Tr | Tr | 27 |
| **344** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)CN1CCN(C[C@H]1C(=O)NC(C)(C)C)Cc1cc2c(o1)ccnc2 | 9.638 | Tr | Tr | Tr | 26 |
| **345** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)CN1CCN(C[C@H]1C(=O)NC(C)(C)C)S(=O)(=O)C | 8.796 | ITr | Cl | Cl | 27 |
| **346** | O[C@@H](C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1)CN1CCN(C[C@H]1C(=O)NC(C)(C)C)Cc1ccc(c(c1)Cl)Cl | 8.959 | Cl | Tr | Tr | 27 |

**Table S2** Test set compounds

|  |  |  |  |
| --- | --- | --- | --- |
| **Cpd** | **SMILES** | **pIC50** | **Reference** |
| **347** | [C@]1(C(=O)[C-](C(=O)O1)[C@H](CCC=C(C)C)C)(C(=O)NC(C)(C)C)CCc1ccccc1 | 5.886 | 28 |
| **348** | [C@@]1(C(=O)[C-](C(=O)O1)[C@@H](c1ccccc1)C)(C(=O)NC(C)(C)C)CCc1ccccc1 | 5.699 | 28 |
| **349** | [C@@]1(C(=O)[C-](C(=O)O1)CCc1ccccc1)(C(=O)NC(C)(C)C)CCc1ccccc1 | 5.523 | 28 |
| **350** | [C@@]1(C(=O)[C-](C(=O)O1)[C@@H](c1ccccc1)C)(C(=O)NC(C)(C)C)CCc1ccccc1 | 5.398 | 28 |
| **351** | [C@]1(C(=O)[C-](C(=O)O1)Cc1ccccc1)(C(=O)NC(C)(C)C)CCc1ccccc1 | 4.959 | 28 |
| **352** | [C@]1(C(=O)[C-](C(=O)O1)c1ccc(C(C)(C)C)cc1)(C(=O)NC(C)(C)C)CCc1ccccc1 | 4.770 | 28 |
| **353** | [C@]1(C(=O)[C-](C(=O)O1)c1ccc(cc1)c1ccccc1)(C(=O)NC(C)(C)C)CCc1ccccc1 | 4.569 | 28 |
| **354** | [C@@]1(C(=O)[C-](C(=O)O1)[C@H](c1ccccc1)C)(C(=O)NCCc1ccc(Cl)cc1)C(C)C | 4.509 | 28 |
| **355** | [C@@]1(C(=O)[C-](C(=O)O1)N(C(=O)OC(C)(C)C)C)(C(=O)NC(C)(C)C)CCc1ccccc1 | 4.328 | 28 |
| **356** | [C@@]1(C(=O)[C-](C(=O)O1)CCc1ccccc1)(C(=O)NC(C)(C)C)C | 4.155 | 28 |
| **357** | [C@]1(C(=O)[C-](C(=O)O1)[C@@H](c1ccccc1)C)(C(=O)NC(C)(C)C)C | 3.979 | 28 |
| **358** | [C@@]1(C(=O)[C-](C(=O)O1)[C@H](CCC=C(C)C)C)(C(=O)NC(C)(C)C)C | 3.821 | 28 |
| **359** | [C@@]1(C(=O)[C-](C(=O)O1)N(C(=O)OC(C)(C)C)C)(C(=O)NC[C@@H]1OCCC1)CCc1ccccc1 | 3.714 | 28 |
| **360** | [C@@]1(C(=O)[C-](C(=O)O1)CCc1ccccc1)(C(=O)NC1CC1)C | 3.532 | 28 |
| **361** | C(=O)(N[C@H]([C@H]([C@@H]([C@@H](NC(=O)[C@H](N[C@H](C(=O)OCc1ccccc1)C)C(C)C)Cc1ccccc1)O)O)Cc1ccccc1)[C@@H](NC(=O)[C@@H](NC(=O)OCc1ccccc1)C)C(C)C | 8.398 | 29 |
| **362** | N1C(=O)[C@@H](NC(=O)[C@@H]([C@@H](NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)C)Cc2ccc(cc2)O)C(C)C)Cc2ccccc2)O)Cc2ccc(OCCCNC(=O)[C@H]1C(C)C)cc2 | 8.222 | 29 |
| **363** | N1C(=O)[C@@H](NC(=O)[C@@H]([C@@H](NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)C)Cc2ccccc2)C(C)C)Cc2ccccc2)O)Cc2ccc(OCCCNC(=O)[C@H]1C(C)C)cc2 | 8.155 | 29 |
| **364** | N1C(=O)[C@@H](NC(=O)[C@@H]([C@@H](NC(=O)[C@@H](NC(=O)[C@H](Cc2c[nH]c3c2cccc3)NC(=O)C)C(C)C)Cc2ccccc2)O)Cc2ccc(OCCCNC(=O)[C@H]1C(C)C)cc2 | 8.000 | 29 |
| **365** | S(=O)(=O)([C@@H](NC(=O)N[C@H](C(=O)N[C@H]([C@H](C(=O)N[C@@H]1C(=O)N[C@H](C(=O)NCCCOc2ccc(C1)cc2)C(C)C)O)Cc1ccccc1)C(C)C)C)c1ccc(cc1)C | 7.886 | 29 |
| **366** | N1C(=O)[C@@H](NC(=O)C(=O)[C@@H](NC(=O)OC(C)(C)C)Cc2ccccc2)Cc2ccc(OCCCNC(=O)[C@H]1C(C)C)cc2 | 7.886 | 29 |
| **367** | N1C(=O)[C@@H](NC(=O)[C@H]([C@@H](NC(=O)OC(C)(C)C)Cc2ccccc2)O)Cc2ccc(OCCCNC(=O)[C@H]1C(C)C)cc2 | 7.000 | 29 |
| **368** | C(=O)([C@@H]([C@@H](NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)C)Cc1ccc(cc1)O)C(C)C)Cc1ccccc1)O)N[C@H](C(=O)N[C@H](C(=O)N)C(C)C)Cc1ccc(cc1)O | 6.674 | 29 |
| **369** | N1C(=O)[C@@H](NC(=O)[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc2ccccc2)O)Cc2ccc(OCCCNC(=O)[C@H]1C(C)C)cc2 | 6.201 | 29 |
| **370** | C(=O)(N[C@H]([C@H](C(=O)OC)O)Cc1ccccc1)[C@@H](NC(=O)[C@H](Cc1c[nH]c2c1cccc2)NC(=O)C)C(C)C | 4.854 | 29 |
| **371** | C(=O)(N[C@H]([C@H](C(=O)OC)O)Cc1ccccc1)[C@@H](NC(=O)[C@@H](NC(=O)C)Cc1ccc(cc1)O)C(C)C | 4.149 | 29 |
| **372** | C(=O)(N[C@H]([C@H](C(=O)OC)O)Cc1ccccc1)[C@@H](NC(=O)[C@@H](NC(=O)C)Cc1ccccc1)C(C)C | 3.947 | 29 |
| **373** | C1C[C@@H]2CN(C[C@H]([C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)c3ccc4c(cccc4)n3)[C@H]3CCOC3)O)[C@@H](C[C@H]2CC1)C(=O)NC(C)(C)C | 10.301 | 30 |
| **374** | C(OC(=O)N[C@H]([C@H](C[C@H](C(=O)N[C@@H]1[C@@H]([C@@H](c2c1cccc2)O)O)Cc1ccccc1)O)Cc1ccccc1)(C)(C)C | 10.000 | 30 |
| **375** | C(OC(=O)N[C@H]([C@H](C[C@H](C(=O)N[C@H]1c2c(cccc2)C[C@@H]1O)Cc1ccc(cc1)O)O)Cc1ccccc1)(C)(C)C | 9.796 | 30 |
| **376** | C(OC(=O)N[C@H]([C@H](C[C@H](C(=O)N[C@H]1c2c(cccc2)C[C@@H]1O)Cc1ccc(cc1)C(C)(C)C)O)Cc1ccccc1)(C)(C)C | 9.770 | 30 |
| **377** | N([C@H]1c2c(OC[C@@H]1O)cccc2)C(=O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)Cc1ccccc1 | 9.745 | 30 |
| **378** | [C@@H]1([C@@H]([C@@H](c2c1cccc2)O)O)NC(=O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)CCCc1ccccc1 | 9.721 | 30 |
| **379** | C(OC(=O)N[C@H]([C@H](C[C@H](C(=O)N[C@H]1c2c(cccc2)C[C@@H]1O)C/C=C\c1ccccc1)O)Cc1ccccc1)(C)(C)C | 9.638 | 30 |
| **380** | C(=O)(N[C@H](C(=O)N[C@@H](Cc1ccccc1)[C@@H](CN1[C@@H](C[C@H]2[C@@H](C1)CCCC2)C(=O)NC(C)(C)C)O)CC(=O)N)c1ccc2c(cccc2)n1 | 9.638 | 30 |
| **381** | C(OC(=O)N[C@H]([C@H](C[C@H](C(=O)N[C@H]1c2c(cccc2)C[C@@H]1O)Cc1ccccc1)O)Cc1ccccc1)(C)(C)C | 9.602 | 30 |
| **382** | N([C@H]1c2c(C[C@@H]1O)cccc2)C(=O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)CSc1ccccc1 | 9.602 | 30 |
| **383** | C(OC(=O)N[C@H]([C@H](C[C@H](C(=O)N[C@H]1c2c(cccc2)C[C@@H]1O)Cc1ccc(cc1)C(F)(F)F)O)Cc1ccccc1)(C)(C)C | 9.585 | 30 |
| **384** | C(OC(=O)N[C@H]([C@H](C[C@H](C(=O)N[C@H]1c2c(cccc2)C[C@@H]1O)Cc1ccc(cc1)[N+](=O)[O-])O)Cc1ccccc1)(C)(C)C | 9.569 | 30 |
| **385** | C(OC(=O)N[C@H]([C@H](C[C@H](C(=O)N[C@H]1c2c(cccc2)C[C@@H]1O)Cc1ccc(cc1)C)O)Cc1ccccc1)(C)(C)C | 9.538 | 30 |
| **386** | C(OC(=O)N[C@H]([C@H](C[C@H](C(=O)N[C@H]1c2c(cccc2)C[C@@H]1O)Cc1ccc(cc1)N)O)Cc1ccccc1)(C)(C)C | 9.509 | 30 |
| **387** | N([C@H]1c2c(C[C@@H]1O)cccc2)C(=O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)Cc1cc[nH+]cc1 | 9.284 | 30 |
| **388** | C(OC(=O)N[C@H]([C@H](C[C@H](C(=O)N[C@H]1c2c(cccc2)C[C@@H]1O)Cc1c(c(c(c(c1F)F)F)F)F)O)Cc1ccccc1)(C)(C)C | 9.222 | 30 |
| **389** | N([C@H]1c2c(CC[C@@H]1O)cccc2)C(=O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)Cc1ccccc1 | 9.161 | 30 |
| **390** | C(OC(=O)N[C@H]([C@H](C[C@H](C(=O)N[C@H]1c2c(cccc2)C[C@@H]1O)Cc1ccc(cc1)I)O)Cc1ccccc1)(C)(C)C | 9.143 | 30 |
| **391** | N([C@H]1c2c(C[C@@H]1O)cccc2)C(=O)/C(=C\[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)/Cc1ccccc1 | 8.886 | 30 |
| **392** | C1C[C@@H]2CN(C[C@H]([C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)c3ccc4c(cccc4)n3)[C@@H]3CCOC3)O)[C@@H](C[C@H]2CC1)C(=O)NC(C)(C)C | 8.268 | 30 |
| **393** | N([C@H]1c2c(C[C@@H]1O)cccc2)C(=O)[C@H](CC(=O)c1ccccc1)C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O | 8.268 | 30 |
| **394** | N1([C@H](C(=O)NC(C)(C)C)C[C@H]2[C@@H](C1)CCCC2)C[C@H](C[C@H](C(=O)N[C@H]1c2c(C[C@@H]1O)cccc2)Cc1ccccc1)O | 8.119 | 30 |
| **395** | N([C@H]1c2c(C[C@@H]1O)cccc2)C(=O)[C@@](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)(Cc1ccccc1)C | 8.108 | 30 |
| **396** | N([C@H]1c2c(C[C@@H]1O)cccc2)C(=O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)CC=C | 7.553 | 30 |
| **397** | C(OC(=O)N[C@H]([C@H](C[C@H](C(=O)N[C@H]1CCc2c1cccc2)Cc1ccccc1)O)Cc1ccccc1)(C)(C)C | 7.469 | 30 |
| **398** | C(=O)(N[C@@H](c1ccccc1)CO)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)Cc1ccccc1 | 7.409 | 30 |
| **399** | N([C@@H]1c2c(OC[C@H]1O)cccc2)C(=O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)Cc1ccccc1 | 7.387 | 30 |
| **400** | N1([C@H](C(=O)NC(C)(C)C)C[C@H]2[C@@H](C1)CCCC2)C[C@H](C[C@H](C(=O)N[C@@H](C(=O)Nc1nc2c(cc1)cccc2)C(C)C)Cc1ccccc1)O | 7.284 | 30 |
| **401** | [C@H]1([C@@H](NC(=O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc2ccccc2)O)Cc2ccccc2)c2c(C1)cccc2)C(=O)OC | 7.180 | 30 |
| **402** | [C@H]([C@H](C[C@H](C(=O)NCc1ccccc1)Cc1ccccc1)O)(Cc1ccccc1)NC(=O)OC(C)(C)C | 6.939 | 30 |
| **403** | C(=O)(N[C@@H]1[C@H](O)CCCC1)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)Cc1ccccc1 | 6.910 | 30 |
| **404** | C(=O)(N[C@@H](c1ccccc1)C)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)Cc1ccccc1 | 6.839 | 30 |
| **405** | [C@@]1(NC(=O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc2ccccc2)O)Cc2ccccc2)(c2c(C[C@@H]1O)cccc2)C | 6.670 | 30 |
| **406** | N([C@H]1c2c(C[C@@H]1O)cccc2)C(=O)[C@@H](NC[C@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)Cc1ccccc1 | 6.640 | 30 |
| **407** | [C@H]1(c2c(C[C@@H]1O)cccc2)NC(=O)C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O | 6.250 | 30 |
| **408** | C(=O)(N[C@H]([C@H]([C@H]1[C@H](C(=O)NCc2ccccc2)CCC1)O)Cc1ccc(cc1)O)OC(C)(C)C | 6.230 | 30 |
| **409** | C(=O)(N[C@H]([C@H](C[C@H](C(=O)N[C@@H](Cc1ccccc1)CO)Cc1ccccc1)O)Cc1ccccc1)OC(C)(C)C | 6.160 | 30 |
| **410** | C1CC[C@](C(=O)N1[C@H]1c2c(C[C@@H]1O)cccc2)(C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)Cc1ccccc1 | 5.900 | 30 |
| **411** | [C@H]1(c2c(C[C@@H]1O)cccc2)NC(=O)CC[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O | 5.530 | 30 |
| **412** | N1([C@H](C(=O)NC(C)(C)C)C[C@H]2[C@@H](C1)CCCC2)C[C@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O | 5.520 | 30 |
| **413** | [N@H+]1([C@H](C(=O)NC(C)(C)C)C[C@H]2[C@@H](C1)CCCC2)C[C@H](CN1[C@H](C(=O)NC(C)(C)C)C[C@H]2[C@H](C1)CCCC2)O | 5.170 | 30 |
| **414** | [C@@H]1([C@H]([C@@H](c2c1cccc2)O)O)NC(=O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)Cc1ccccc1 | 10.000 | 31 |
| **415** | [C@@H]1([C@H]([C@H](c2c1cccc2)O)O)NC(=O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)CCCc1ccccc1 | 9.721 | 31 |
| **416** | N([C@H]1c2c(C[C@H]1O)cccc2)C(=O)[C@H](C[C@@H]([C@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)CSc1ccccc1 | 9.602 | 31 |
| **417** | [N+](=O)(c1ccc(C[C@H](C(=O)N[C@H]2c3c(C[C@H]2O)cccc3)C[C@@H]([C@H](NC(=O)OC(C)(C)C)Cc2ccccc2)O)cc1)[O-] | 9.569 | 31 |
| **418** | N([C@@H]1c2c(C[C@H]1O)cccc2)C(=O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)Cc1ccc(N)cc1 | 9.509 | 31 |
| **419** | N([C@H]1c2c(C[C@H]1O)cccc2)C(=O)[C@@H](C[C@@H](C[C@H](C(=O)N[C@@H]1c2c(C[C@H]1O)cccc2)Cc1ccccc1)O)Cc1ccccc1 | 9.161 | 31 |
| **420** | N([C@H]1c2c(C[C@H]1O)cccc2)C(=O)/C(=C\[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)/Cc1ccccc1 | 8.886 | 31 |
| **421** | [C@H](C(=O)N[C@@H]1c2c(C[C@H]1O)cccc2)(C(=O)c1ccccc1)C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O | 8.268 | 31 |
| **422** | C(=O)(N[C@H]1C=CC[C@H]1O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)Cc1ccccc1 | 8.022 | 31 |
| **423** | C(=O)(N[C@H](c1ccccc1)C)[C@@H](C[C@@H]([C@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)Cc1ccccc1 | 6.839 | 31 |
| **424** | N(C(=O)[C@@H](C[C@@H]([C@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)Cc1ccccc1)[C@H](C(=O)[O-])C(C)C | 6.790 | 31 |
| **425** | [C@]1(NC(=O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc2ccccc2)O)Cc2ccccc2)(c2c(C[C@H]1O)cccc2)C | 6.670 | 31 |
| **426** | [C@@H]1(c2c(C[C@H]1O)cccc2)NC(=O)C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O | 6.250 | 31 |
| **427** | N1(C(=O)[C@](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc2ccccc2)O)(Cc2ccccc2)CCC1)[C@H]1[C@H](Cc2c1cccc2)O | 5.900 | 31 |
| **428** | [C@H]1(c2c(C[C@H]1O)cccc2)NC(=O)CC[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O | 5.530 | 31 |
| **429** | N([C@@H]1c2c(C[C@@H]1O)cccc2)C(=O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)Cc1ccc(cc1)O | 9.796 | 32 |
| **430** | N([C@@H]1c2c(C[C@@H]1O)cccc2)C(=O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)Cc1ccc(C(C)(C)C)cc1 | 9.770 | 32 |
| **431** | [C@H]1([C@@H]([C@@H](c2c1cccc2)O)O)NC(=O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)CCCc1ccccc1 | 9.721 | 32 |
| **432** | N([C@@H]1c2c(C[C@@H]1O)cccc2)C(=O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)C/C=C\c1ccccc1 | 9.638 | 32 |
| **433** | N([C@@H]1c2c(C[C@@H]1O)cccc2)C(=O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)CSc1ccccc1 | 9.602 | 32 |
| **434** | N([C@@H]1c2c(C[C@@H]1O)cccc2)C(=O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)Cc1ccccc1 | 9.602 | 32 |
| **435** | N([C@@H]1c2c(C[C@@H]1O)cccc2)C(=O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)Cc1ccc(C(F)(F)F)cc1 | 9.585 | 32 |
| **436** | [N+](=O)(c1ccc(C[C@@H](C(=O)N[C@@H]2c3c(C[C@@H]2O)cccc3)C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc2ccccc2)O)cc1)[O-] | 9.569 | 32 |
| **437** | N([C@@H]1c2c(C[C@@H]1O)cccc2)C(=O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)Cc1ccc(cc1)C | 9.538 | 32 |
| **438** | N([C@@H]1c2c(C[C@@H]1O)cccc2)C(=O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)Cc1ccc(N)cc1 | 9.509 | 32 |
| **439** | N([C@@H]1c2c(C[C@@H]1O)cccc2)C(=O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)Cc1cc[nH+]cc1 | 9.276 | 32 |
| **440** | c1(c(c(c(c(c1F)F)F)F)F)C[C@@H](C(=O)N[C@@H]1c2c(C[C@@H]1O)cccc2)C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O | 9.222 | 32 |
| **441** | N([C@@H]1c2c(CC[C@@H]1O)cccc2)C(=O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)Cc1ccccc1 | 9.155 | 32 |
| **442** | N([C@@H]1c2c(C[C@@H]1O)cccc2)C(=O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)Cc1ccc(I)cc1 | 9.143 | 32 |
| **443** | N([C@@H]1c2c(C[C@@H]1O)cccc2)C(=O)[C@H](CC(=O)c1ccccc1)C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O | 8.268 | 32 |
| **444** | N([C@@H]1c2c(C[C@@H]1O)cccc2)C(=O)[C@@](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)(Cc1ccccc1)C | 8.114 | 32 |
| **445** | C(=O)(N[C@@H]1C=CC[C@@H]1O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)Cc1ccccc1 | 8.022 | 32 |
| **446** | N([C@@H]1c2c(C[C@@H]1O)cccc2)C(=O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)CC=C | 7.569 | 32 |
| **447** | C(=O)(N[C@@H]1c2c(CC1)cccc2)[C@@H](C[C@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)Cc1ccccc1 | 7.469 | 32 |
| **448** | [C@H]1([C@H](NC(=O)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc2ccccc2)O)Cc2ccccc2)c2c(C1)cccc2)C(=O)OC | 7.180 | 32 |
| **449** | C(=O)(N[C@H]1[C@H](O)CCCC1)[C@@H](C[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O)Cc1ccccc1 | 6.914 | 32 |
| **450** | [C@@H]1(c2c(C[C@@H]1O)cccc2)NC(=O)CC[C@@H]([C@@H](NC(=O)OC(C)(C)C)Cc1ccccc1)O | 5.532 | 32 |

**Table S3.** Important optimized parameter settings of the OCHEM QSAR machine learning methods

|  |  |
| --- | --- |
| Method | Parameter settings |
| ASNN | Training method: SuperSAB  Number of neurons in hidden layer: 8  Learning iterations:1000  Ensemble:64 |
| KNN | Distance: Euclidean Distance  KNN neighbour: Models were optimized with number of neighbours 1-100, no improvement was observed with neighbours > 100 |
| RF | OCHEM options  Maximum number of trees: 512  Maximum tree depth: Unlimited, models were optimized with increasing number of tree depth until the best model is obtained by bootstrap replica of training set using randomly selected subsets of descriptors  Weka options  Sub-sample proportion: 0.33  Minimum number of cases: 1  Bag-size sample: 100  Batch size: 100  Attribute importance: Mean impurity decrease method  Number of iterations:100  Number of attributes to consider: log2(N), where N is number of descriptors  Node counts: Unlimited  Number of decimal places: 2  Minimum number in child node: 1  Maximum number of nodes: Unlimited  Maximum number of levels: Unlimited |
| XGBoost | Maximum depth of a tree: 8  ETA - Step size shrinkage: 0.2  Lambda - L2 regularization term on weights: 1  Rounds - The number of rounds for boosting:1024  Objective: Linear regression |
| FSMLR | Shrinkage:1  Nfolds: 10  Descriptor Num Factor: 1  Descriptor Extra Factor: 5 |
| MLNN | Batch size: 1024  Epochs: 1000  Training/internal validation set ratio: 0.8  Model: Seven layers (Dense7) network |

**Table S4.** Favorable attributes of Model 4

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Attributes | Probe 1 | Probe 2 | Probe 3 | Average | NTra | NTsb | SDc |
| VS3-N...12.. | 7.000 | 7.001 | 7.003 | 7.001 | 12 | 5 | 0.001 |
| C6...A..3... | 6.997 | 7.002 | 7.000 | 7.000 | 49 | 16 | 0.000 |
| S...C...(... | 7.002 | 6.999 | 6.997 | 6.999 | 11 | 2 | 0.001 |
| EC0-S...2... | 6.996 | 6.997 | 7.001 | 6.998 | 18 | 6 | 0.000 |
| VS3-o...19.. | 6.903 | 6.998 | 6.902 | 6.934 | 12 | 7 | 0.002 |
| C5...A..1... | 6.805 | 6.904 | 6.725 | 6.811 | 76 | 22 | 0.000 |
| O...C...1... | 6.704 | 6.703 | 6.998 | 6.802 | 24 | 4 | 0.002 |
| C5....H.2... | 6.396 | 6.703 | 6.701 | 6.600 | 9 | 3 | 0.000 |
| O...(...O... | 6.400 | 6.404 | 6.097 | 6.300 | 48 | 13 | 0.001 |
| PT3-C...14.. | 6.696 | 5.796 | 5.995 | 6.162 | 13 | 4 | 0.000 |
| C6...AH.2... | 6.101 | 6.099 | 6.099 | 6.100 | 11 | 2 | 0.001 |
| VS2-S...17.. | 6.100 | 6.149 | 5.846 | 6.032 | 10 | 2 | 0.001 |
| VS3-N...22.. | 6.146 | 5.950 | 5.996 | 6.031 | 162 | 60 | 0.000 |
| PT3-S...11.. | 6.154 | 6.054 | 5.803 | 6.004 | 10 | 2 | 0.001 |
| [...C...(... | 5.700 | 5.899 | 6.051 | 5.884 | 208 | 68 | 0.000 |
| PT3-N...7... | 5.800 | 5.796 | 5.800 | 5.799 | 147 | 41 | 0.000 |
| O...(...N... | 5.497 | 5.997 | 5.802 | 5.765 | 253 | 83 | 0.000 |
| VS3-H...17.. | 5.654 | 5.653 | 5.795 | 5.701 | 238 | 80 | 0.000 |
| C5....H.1... | 5.397 | 5.498 | 5.698 | 5.531 | 51 | 15 | 0.000 |
| n...c...2... | 5.503 | 5.499 | 5.586 | 5.529 | 28 | 7 | 0.001 |
| BOND10100000 | 5.554 | 5.795 | 5.223 | 5.524 | 260 | 83 | 0.000 |
| VS2-O...6... | 5.524 | 5.371 | 5.574 | 5.489 | 32 | 11 | 0.000 |
| VS3-C...9... | 5.547 | 5.505 | 5.401 | 5.484 | 187 | 57 | 0.000 |
| VS2-N...12.. | 5.503 | 5.497 | 5.277 | 5.426 | 142 | 43 | 0.000 |
| VS3-H...22.. | 5.553 | 5.505 | 5.202 | 5.420 | 18 | 4 | 0.001 |
| VS3-N...14.. | 5.504 | 5.202 | 5.245 | 5.317 | 32 | 13 | 0.001 |
| [...N...(... | 5.497 | 5.045 | 5.052 | 5.198 | 237 | 75 | 0.000 |
| [...(...[... | 5.201 | 5.096 | 5.105 | 5.134 | 141 | 42 | 0.000 |
| PT3-S...9... | 4.701 | 5.403 | 5.105 | 5.070 | 29 | 10 | 0.000 |
| 1...n...(... | 5.096 | 5.503 | 4.439 | 5.013 | 14 | 5 | 0.000 |
| C...=....... | 4.903 | 4.905 | 4.896 | 4.901 | 84 | 29 | 0.000 |
| VS2-N...13.. | 4.924 | 4.800 | 4.849 | 4.858 | 187 | 63 | 0.000 |
| VS3-S...22.. | 4.498 | 4.624 | 5.198 | 4.773 | 17 | 4 | 0.001 |
| VS3-N...8... | 4.600 | 4.903 | 4.796 | 4.767 | 21 | 4 | 0.001 |
| VS3-C...29.. | 5.104 | 4.548 | 4.446 | 4.699 | 55 | 15 | 0.001 |
| VS2-C...5... | 4.878 | 4.749 | 4.249 | 4.625 | 59 | 20 | 0.000 |
| C5...AH.1... | 4.598 | 4.605 | 4.595 | 4.599 | 37 | 12 | 0.000 |
| C6...AH.5... | 4.503 | 4.597 | 4.421 | 4.507 | 40 | 15 | 0.000 |
| VS3-C...13.. | 4.514 | 4.374 | 4.603 | 4.497 | 169 | 58 | 0.000 |
| VS3-N...15.. | 4.623 | 4.649 | 4.045 | 4.439 | 19 | 8 | 0.001 |
| VS3-C...25.. | 4.574 | 4.340 | 4.327 | 4.413 | 170 | 49 | 0.000 |
| VS3-N...11.. | 4.605 | 4.299 | 4.302 | 4.402 | 51 | 18 | 0.000 |
| VS3-O...17.. | 4.598 | 4.124 | 4.301 | 4.341 | 12 | 2 | 0.002 |
| C...O...(... | 4.121 | 4.204 | 4.600 | 4.308 | 89 | 23 | 0.001 |
| S........... | 4.202 | 4.296 | 4.351 | 4.283 | 61 | 20 | 0.000 |
| n...(....... | 4.297 | 4.120 | 4.348 | 4.255 | 41 | 9 | 0.001 |
| EC1-N...5... | 4.285 | 4.550 | 3.827 | 4.221 | 35 | 10 | 0.000 |
| VS3-F...8... | 4.429 | 3.604 | 4.386 | 4.140 | 11 | 2 | 0.001 |
| VS3-O...15.. | 4.288 | 4.103 | 3.926 | 4.106 | 59 | 18 | 0.000 |
| C4......0... | 3.996 | 4.304 | 4.003 | 4.101 | 257 | 85 | 0.000 |
| C...[...C... | 3.450 | 4.489 | 4.347 | 4.096 | 254 | 85 | 0.000 |
| VS2-C...7... | 4.230 | 3.773 | 4.117 | 4.040 | 86 | 27 | 0.000 |
| N...(...1... | 3.926 | 3.949 | 4.199 | 4.025 | 41 | 13 | 0.000 |
| PT3-o...9... | 4.003 | 4.000 | 4.004 | 4.002 | 27 | 14 | 0.002 |
| VS3-C...16.. | 3.924 | 3.902 | 4.053 | 3.960 | 261 | 85 | 0.000 |
| o...1...(... | 4.022 | 4.017 | 3.798 | 3.946 | 40 | 18 | 0.001 |
| VS3-F...5... | 3.777 | 3.988 | 4.005 | 3.923 | 45 | 17 | 0.000 |
| VS3-O...14.. | 3.896 | 3.953 | 3.753 | 3.867 | 196 | 67 | 0.000 |
| VS2-o...13.. | 3.999 | 3.697 | 3.899 | 3.865 | 27 | 14 | 0.002 |
| N...C...C... | 4.004 | 3.604 | 3.602 | 3.737 | 113 | 41 | 0.000 |
| C...C...(... | 3.902 | 3.697 | 3.604 | 3.734 | 89 | 30 | 0.000 |
| C...[...(... | 3.213 | 4.065 | 3.874 | 3.717 | 166 | 49 | 0.000 |
| VS2-N...18.. | 3.404 | 3.701 | 3.997 | 3.701 | 12 | 8 | 0.002 |
| c...(...O... | 3.601 | 3.703 | 3.551 | 3.618 | 24 | 7 | 0.000 |
| EC1-C...12.. | 3.703 | 3.398 | 3.697 | 3.600 | 260 | 85 | 0.000 |
| PT2-C...8... | 3.699 | 3.698 | 3.401 | 3.599 | 260 | 85 | 0.000 |
| PT3-H...8... | 3.697 | 3.398 | 3.698 | 3.598 | 260 | 85 | 0.000 |
| s...(....... | 3.399 | 3.398 | 3.901 | 3.566 | 13 | 2 | 0.002 |
| VS3-C...18.. | 3.679 | 3.402 | 3.523 | 3.535 | 246 | 82 | 0.000 |
| VS2-H...11.. | 3.702 | 3.449 | 3.403 | 3.518 | 260 | 85 | 0.000 |
| =...C...(... | 3.403 | 3.403 | 3.697 | 3.501 | 81 | 29 | 0.000 |
| EC1-O...8... | 3.626 | 3.410 | 3.435 | 3.490 | 37 | 8 | 0.001 |
| VS2-C...14.. | 3.299 | 3.696 | 3.473 | 3.489 | 260 | 85 | 0.000 |
| H...[...1... | 3.675 | 3.196 | 3.555 | 3.475 | 241 | 79 | 0.000 |
| N...1...C... | 3.296 | 3.797 | 3.086 | 3.393 | 182 | 62 | 0.000 |
| VS3-N...26.. | 3.952 | 3.084 | 3.102 | 3.379 | 51 | 15 | 0.000 |
| c...c...(... | 3.687 | 3.176 | 3.271 | 3.378 | 130 | 42 | 0.000 |
| [...(...C... | 3.397 | 3.048 | 3.302 | 3.249 | 257 | 84 | 0.000 |
| VS3-N...19.. | 3.404 | 3.098 | 3.096 | 3.200 | 41 | 11 | 0.001 |
| VS3-H...15.. | 3.255 | 3.396 | 2.900 | 3.183 | 253 | 83 | 0.000 |
| PT2-O...6... | 2.573 | 3.673 | 3.251 | 3.166 | 37 | 8 | 0.001 |
| PT3-O...8... | 2.772 | 3.199 | 3.426 | 3.132 | 46 | 15 | 0.000 |
| PT3-C...9... | 3.103 | 3.101 | 3.105 | 3.103 | 261 | 85 | 0.000 |
| C7....H.1... | 2.805 | 3.396 | 3.098 | 3.100 | 30 | 13 | 0.001 |
| F...(...(... | 3.402 | 2.653 | 3.200 | 3.085 | 49 | 18 | 0.000 |
| S...C....... | 2.846 | 3.246 | 3.099 | 3.063 | 50 | 16 | 0.000 |
| n...(...c... | 2.852 | 3.398 | 2.796 | 3.015 | 35 | 5 | 0.002 |
| C7......0... | 2.791 | 3.228 | 3.028 | 3.015 | 226 | 69 | 0.000 |
| VS3-N...20.. | 3.147 | 2.747 | 3.103 | 2.999 | 30 | 8 | 0.001 |
| 2...(...(... | 2.796 | 3.097 | 3.096 | 2.997 | 12 | 3 | 0.001 |
| VS3-C...6... | 3.199 | 2.899 | 2.797 | 2.965 | 20 | 4 | 0.001 |
| VS2-N...5... | 2.851 | 3.005 | 3.002 | 2.953 | 16 | 1 | 0.003 |
| VS3-C...19.. | 2.955 | 3.103 | 2.795 | 2.951 | 260 | 85 | 0.000 |
| ++++N---B2== | 2.799 | 3.108 | 2.940 | 2.949 | 261 | 85 | 0.000 |
| HALO10000000 | 2.902 | 3.249 | 2.586 | 2.912 | 39 | 12 | 0.000 |
| VS3-o...25.. | 3.105 | 2.799 | 2.802 | 2.902 | 12 | 3 | 0.001 |
| o...c....... | 2.698 | 2.747 | 3.249 | 2.898 | 12 | 4 | 0.000 |
| s...1...(... | 2.799 | 2.904 | 2.804 | 2.836 | 13 | 3 | 0.001 |
| ++++O---B2== | 3.026 | 2.761 | 2.697 | 2.828 | 261 | 85 | 0.000 |
| NOSP11000000 | 2.954 | 3.076 | 2.445 | 2.825 | 203 | 65 | 0.000 |
| VS2-H...3... | 2.800 | 2.802 | 2.800 | 2.801 | 9 | 4 | 0.001 |
| VS2-C...15.. | 2.802 | 2.796 | 2.801 | 2.800 | 253 | 83 | 0.000 |
| ++++N---O=== | 2.597 | 2.825 | 2.976 | 2.800 | 261 | 85 | 0.000 |
| c...c...1... | 2.677 | 2.877 | 2.822 | 2.792 | 260 | 85 | 0.000 |
| VS3-C...10.. | 2.828 | 2.597 | 2.796 | 2.740 | 171 | 59 | 0.000 |
| O...=...C... | 2.998 | 2.450 | 2.571 | 2.673 | 81 | 29 | 0.000 |
| VS3-C...12.. | 2.802 | 2.696 | 2.501 | 2.667 | 130 | 42 | 0.000 |
| PT3-O...4... | 2.947 | 2.497 | 2.501 | 2.648 | 39 | 11 | 0.000 |
| o...(....... | 2.604 | 2.499 | 2.834 | 2.646 | 43 | 18 | 0.001 |
| c...c...2... | 2.746 | 2.651 | 2.501 | 2.632 | 188 | 65 | 0.000 |
| s........... | 2.848 | 2.329 | 2.602 | 2.593 | 19 | 3 | 0.002 |
| VS3-H...11.. | 2.316 | 3.046 | 2.392 | 2.585 | 261 | 85 | 0.000 |
| VS2-S...15.. | 2.476 | 2.628 | 2.600 | 2.568 | 26 | 10 | 0.001 |
| VS3-o...23.. | 1.998 | 2.955 | 2.700 | 2.551 | 10 | 4 | 0.001 |
| VS3-O...12.. | 2.603 | 2.400 | 2.573 | 2.525 | 112 | 33 | 0.000 |
| s...1....... | 2.291 | 2.551 | 2.546 | 2.463 | 14 | 3 | 0.001 |
| VS2-C...17.. | 2.504 | 2.705 | 2.149 | 2.453 | 243 | 81 | 0.000 |
| PT2-N...5... | 2.501 | 2.596 | 2.249 | 2.448 | 261 | 85 | 0.000 |
| VS2-C...11.. | 2.591 | 2.170 | 2.574 | 2.445 | 261 | 85 | 0.000 |
| PT3-F...3... | 2.174 | 2.974 | 2.170 | 2.439 | 46 | 18 | 0.001 |
| n...c...1... | 2.298 | 2.570 | 2.398 | 2.422 | 50 | 11 | 0.001 |
| VS3-H...5... | 2.248 | 2.453 | 2.528 | 2.410 | 37 | 4 | 0.002 |
| c...n...c... | 2.198 | 2.197 | 2.796 | 2.397 | 66 | 17 | 0.001 |
| PT2-N...2... | 2.590 | 2.099 | 2.499 | 2.396 | 17 | 1 | 0.003 |
| C...N...1... | 2.404 | 2.650 | 2.117 | 2.390 | 164 | 58 | 0.000 |
| O...c...1... | 2.703 | 2.202 | 2.199 | 2.368 | 9 | 3 | 0.000 |
| EC1-N...8... | 2.146 | 2.599 | 2.322 | 2.355 | 261 | 85 | 0.000 |
| VS2-C...16.. | 2.564 | 2.217 | 2.221 | 2.334 | 156 | 49 | 0.000 |
| PT3-C...13.. | 2.726 | 2.004 | 2.183 | 2.304 | 22 | 6 | 0.001 |
| ...[...(... | 2.254 | 2.402 | 2.246 | 2.300 | 34 | 14 | 0.001 |
| VS2-N...20.. | 2.152 | 2.925 | 1.795 | 2.291 | 160 | 55 | 0.000 |
| VS2-H...12.. | 2.454 | 1.971 | 2.434 | 2.286 | 83 | 24 | 0.000 |
| C...C...1... | 2.627 | 2.302 | 1.925 | 2.285 | 160 | 63 | 0.001 |
| VS2-H...9... | 2.440 | 2.409 | 1.953 | 2.267 | 252 | 83 | 0.000 |
| PT2-N...3... | 2.414 | 2.078 | 2.213 | 2.235 | 19 | 9 | 0.001 |
| PT3-H...9... | 2.578 | 2.242 | 1.875 | 2.232 | 83 | 24 | 0.000 |
| VS2-C...10.. | 2.120 | 2.399 | 2.120 | 2.213 | 213 | 63 | 0.000 |
| EC1-H...2... | 2.196 | 2.204 | 2.203 | 2.201 | 261 | 85 | 0.000 |
| PT2-C...9... | 1.929 | 2.598 | 2.042 | 2.190 | 83 | 24 | 0.000 |
| C...c...2... | 2.251 | 2.096 | 2.201 | 2.183 | 103 | 34 | 0.000 |
| PT2-H...1... | 2.199 | 2.199 | 2.101 | 2.166 | 261 | 85 | 0.000 |
| n...n....... | 2.329 | 2.330 | 1.778 | 2.145 | 9 | 5 | 0.002 |
| PT3-C...8... | 2.103 | 2.002 | 2.247 | 2.117 | 261 | 85 | 0.000 |
| c...(...c... | 2.397 | 2.023 | 1.851 | 2.090 | 81 | 26 | 0.000 |
| EC1-C...13.. | 1.964 | 1.792 | 2.458 | 2.071 | 83 | 24 | 0.000 |
| EC0-s...2... | 1.909 | 2.322 | 1.849 | 2.027 | 19 | 3 | 0.002 |
| PT3-C...2... | 1.905 | 1.895 | 2.254 | 2.018 | 236 | 76 | 0.000 |
| PT3-C...3... | 1.899 | 2.198 | 1.902 | 2.000 | 93 | 26 | 0.000 |
| VS2-N...22.. | 1.905 | 1.900 | 2.101 | 1.969 | 19 | 7 | 0.000 |
| c...n...1... | 1.900 | 2.051 | 1.904 | 1.951 | 27 | 8 | 0.000 |
| o...1....... | 1.891 | 2.154 | 1.796 | 1.947 | 42 | 20 | 0.001 |
| N...@@..H... | 1.999 | 1.614 | 2.223 | 1.945 | 15 | 6 | 0.001 |
| VS3-C...14.. | 1.950 | 1.796 | 2.088 | 1.944 | 259 | 84 | 0.000 |
| PT3-H...3... | 2.038 | 2.001 | 1.697 | 1.912 | 261 | 85 | 0.000 |
| VS3-H...16.. | 2.072 | 1.866 | 1.779 | 1.906 | 153 | 45 | 0.000 |
| VS2-N...10.. | 1.900 | 1.903 | 1.899 | 1.901 | 51 | 18 | 0.000 |
| VS3-H...7... | 1.652 | 2.236 | 1.811 | 1.900 | 86 | 27 | 0.000 |
| =........... | 2.152 | 2.151 | 1.298 | 1.867 | 261 | 85 | 0.000 |
| VS2-N...17.. | 1.849 | 1.698 | 2.020 | 1.856 | 152 | 49 | 0.000 |
| PT2-C...11.. | 2.248 | 1.149 | 2.123 | 1.840 | 115 | 38 | 0.000 |
| n...1....... | 1.805 | 1.748 | 1.949 | 1.834 | 47 | 15 | 0.000 |
| VS3-N...25.. | 2.003 | 1.697 | 1.798 | 1.833 | 20 | 5 | 0.001 |
| NOSP11100000 | 2.021 | 1.777 | 1.634 | 1.811 | 58 | 20 | 0.000 |
| N...@@...... | 1.902 | 1.804 | 1.720 | 1.809 | 15 | 6 | 0.001 |
| PT3-N...14.. | 2.023 | 1.672 | 1.704 | 1.800 | 25 | 8 | 0.000 |
| PT2-N...9... | 1.826 | 1.537 | 1.995 | 1.786 | 170 | 61 | 0.000 |
| EC1-O...5... | 1.692 | 1.924 | 1.690 | 1.769 | 261 | 85 | 0.000 |
| ++++Cl--B2== | 1.599 | 1.903 | 1.699 | 1.734 | 21 | 9 | 0.001 |
| c...(...C... | 2.250 | 1.587 | 1.276 | 1.704 | 37 | 14 | 0.000 |
| ++++CL--O=== | 1.599 | 1.902 | 1.597 | 1.699 | 21 | 9 | 0.001 |
| ++++CL--N=== | 1.901 | 1.596 | 1.595 | 1.697 | 21 | 9 | 0.001 |
| C6...AH.3... | 1.502 | 1.424 | 2.109 | 1.678 | 45 | 19 | 0.001 |
| VS3-C...24.. | 1.600 | 1.797 | 1.602 | 1.666 | 115 | 44 | 0.001 |
| VS2-O...5... | 1.846 | 1.647 | 1.495 | 1.663 | 128 | 38 | 0.000 |
| PT3-H...2... | 1.603 | 1.771 | 1.549 | 1.641 | 66 | 14 | 0.001 |
| @@..H...... | 2.105 | 1.197 | 1.552 | 1.618 | 15 | 6 | 0.001 |
| C...S...C... | 1.602 | 1.600 | 1.604 | 1.602 | 14 | 5 | 0.000 |
| PT2-Cl..2... | 1.603 | 1.598 | 1.603 | 1.602 | 21 | 9 | 0.001 |
| Cl.......... | 1.597 | 1.600 | 1.601 | 1.599 | 21 | 9 | 0.001 |
| [...N...@@.. | 1.500 | 2.097 | 1.104 | 1.567 | 15 | 6 | 0.001 |
| VS3-H...21.. | 1.250 | 2.104 | 1.324 | 1.559 | 67 | 18 | 0.001 |
| PT2-C...3... | 1.392 | 1.698 | 1.490 | 1.527 | 257 | 83 | 0.000 |
| s...(...c... | 1.550 | 1.601 | 1.403 | 1.518 | 13 | 2 | 0.002 |
| S...C...1... | 1.604 | 1.299 | 1.596 | 1.500 | 16 | 4 | 0.001 |
| PT2-C...2... | 1.497 | 1.903 | 1.097 | 1.499 | 48 | 12 | 0.001 |
| EC0-Cl..1... | 1.596 | 1.598 | 1.300 | 1.498 | 21 | 9 | 0.001 |
| c...n...(... | 1.433 | 1.097 | 1.947 | 1.492 | 21 | 3 | 0.002 |
| [...1....... | 1.598 | 1.401 | 1.463 | 1.487 | 242 | 79 | 0.000 |
| VS3-H...13.. | 1.199 | 1.751 | 1.500 | 1.483 | 246 | 81 | 0.000 |
| 1...o...(... | 0.950 | 1.988 | 1.497 | 1.478 | 40 | 18 | 0.001 |
| [...C...1... | 1.549 | 1.752 | 1.085 | 1.462 | 55 | 16 | 0.000 |
| VS2-C...21.. | 1.496 | 1.351 | 1.495 | 1.447 | 68 | 18 | 0.001 |
| c...C...N... | 1.605 | 1.305 | 1.399 | 1.436 | 21 | 10 | 0.001 |
| PT3-F...4... | 1.401 | 1.596 | 1.297 | 1.431 | 12 | 2 | 0.002 |
| EC1-N...12.. | 1.458 | 1.204 | 1.602 | 1.421 | 170 | 61 | 0.000 |
| C...O...C... | 1.462 | 1.051 | 1.751 | 1.421 | 34 | 7 | 0.001 |
| VS3-S...20.. | 1.605 | 1.300 | 1.302 | 1.402 | 10 | 3 | 0.000 |
| EC1-S...8... | 1.599 | 1.303 | 1.303 | 1.402 | 21 | 6 | 0.000 |
| EC1-Cl..3... | 1.600 | 1.301 | 1.304 | 1.401 | 21 | 9 | 0.001 |
| Cl..(....... | 1.599 | 1.302 | 1.302 | 1.401 | 20 | 9 | 0.001 |
| O...c...2... | 1.402 | 1.100 | 1.699 | 1.400 | 71 | 24 | 0.000 |
| PT2-F...2... | 1.597 | 1.301 | 1.299 | 1.399 | 12 | 2 | 0.002 |
| C5...AH.2... | 1.745 | 1.429 | 0.996 | 1.390 | 44 | 20 | 0.001 |
| C...N...(... | 1.450 | 1.122 | 1.598 | 1.390 | 220 | 70 | 0.000 |
| VS2-C...4... | 1.329 | 1.352 | 1.396 | 1.359 | 10 | 2 | 0.001 |
| VS3-O...13.. | 1.302 | 1.255 | 1.497 | 1.351 | 211 | 74 | 0.000 |
| VS3-H...6... | 1.325 | 1.359 | 1.365 | 1.350 | 45 | 21 | 0.001 |
| PT3-O...11.. | 1.147 | 1.701 | 1.178 | 1.342 | 79 | 23 | 0.000 |
| C...(...=... | 1.497 | 1.100 | 1.400 | 1.332 | 260 | 85 | 0.000 |
| EC1-F...3... | 1.389 | 1.299 | 1.297 | 1.328 | 12 | 2 | 0.002 |
| VS3-C...5... | 1.421 | 1.225 | 1.325 | 1.324 | 164 | 55 | 0.000 |
| s...c....... | 1.297 | 1.296 | 1.297 | 1.297 | 11 | 1 | 0.003 |
| VS3-H...12.. | 1.037 | 1.496 | 1.305 | 1.279 | 258 | 85 | 0.000 |
| PT3-N...3... | 1.298 | 0.685 | 1.804 | 1.262 | 22 | 1 | 0.003 |
| VS3-H...4... | 1.141 | 1.261 | 1.348 | 1.250 | 11 | 2 | 0.001 |
| PT3-N...5... | 1.100 | 1.052 | 1.553 | 1.235 | 33 | 16 | 0.001 |
| VS2-C...19.. | 1.346 | 1.003 | 1.298 | 1.216 | 122 | 41 | 0.000 |
| PT2-O...3... | 0.998 | 1.303 | 1.302 | 1.201 | 261 | 85 | 0.000 |
| VS2-Cl..6... | 1.299 | 1.297 | 1.000 | 1.199 | 16 | 9 | 0.002 |
| 1...N...(... | 0.997 | 1.297 | 1.298 | 1.197 | 21 | 4 | 0.001 |
| EC1-C...10.. | 0.864 | 1.333 | 1.366 | 1.187 | 261 | 85 | 0.000 |
| EC1-N...11.. | 0.902 | 1.148 | 1.503 | 1.184 | 65 | 23 | 0.000 |
| C...S...(... | 0.999 | 1.298 | 1.252 | 1.183 | 28 | 10 | 0.000 |
| F...(...C... | 1.646 | 1.240 | 0.645 | 1.177 | 48 | 18 | 0.000 |
| PT3-C...10.. | 1.046 | 1.286 | 1.175 | 1.169 | 253 | 81 | 0.000 |
| O...(...C... | 1.148 | 1.401 | 0.930 | 1.160 | 249 | 82 | 0.000 |
| C...[...1... | 1.097 | 0.803 | 1.571 | 1.157 | 176 | 57 | 0.000 |
| [...O...(... | 1.496 | 1.101 | 0.851 | 1.149 | 38 | 14 | 0.000 |
| VS3-S...19.. | 0.827 | 1.303 | 1.303 | 1.144 | 10 | 1 | 0.002 |
| n...1...(... | 0.701 | 1.426 | 1.304 | 1.144 | 17 | 3 | 0.002 |
| ﯯ--S=== | 0.998 | 1.049 | 1.354 | 1.134 | 73 | 23 | 0.000 |
| EC0-N...2... | 1.000 | 1.299 | 1.096 | 1.131 | 108 | 32 | 0.000 |
| c...O....... | 0.745 | 1.102 | 1.528 | 1.125 | 77 | 26 | 0.000 |
| [...1...[... | 1.388 | 1.139 | 0.755 | 1.094 | 176 | 57 | 0.000 |
| O...C....... | 1.197 | 1.201 | 0.847 | 1.082 | 186 | 50 | 0.001 |
| PT2-N...8... | 1.203 | 1.028 | 0.998 | 1.077 | 65 | 23 | 0.000 |
| [...H...@@.. | 1.128 | 1.048 | 1.049 | 1.075 | 249 | 81 | 0.000 |
| H...@@..C... | 0.954 | 1.067 | 1.174 | 1.065 | 249 | 81 | 0.000 |
| EC0-O...2... | 1.000 | 1.053 | 1.138 | 1.064 | 261 | 85 | 0.000 |
| PT2-F...3... | 1.234 | 1.195 | 0.751 | 1.060 | 48 | 18 | 0.000 |
| C...1...C... | 0.754 | 1.297 | 1.049 | 1.033 | 16 | 5 | 0.000 |
| (...S...(... | 1.002 | 1.003 | 1.004 | 1.003 | 9 | 2 | 0.001 |
| ﯯ--B2== | 1.047 | 1.000 | 0.952 | 1.000 | 73 | 23 | 0.000 |
| (...Cl..(... | 1.002 | 0.996 | 0.998 | 0.999 | 13 | 7 | 0.002 |
| PT3-Cl..4... | 0.997 | 0.995 | 1.002 | 0.998 | 16 | 9 | 0.002 |
| VS2-O...8... | 0.998 | 0.996 | 0.996 | 0.997 | 23 | 6 | 0.001 |
| EC1-C...15.. | 1.347 | 1.005 | 0.637 | 0.996 | 115 | 38 | 0.000 |
| (...C...(... | 0.728 | 0.823 | 1.392 | 0.981 | 261 | 85 | 0.000 |
| N...1....... | 1.046 | 1.278 | 0.571 | 0.965 | 183 | 62 | 0.000 |
| VS3-H...9... | 1.015 | 1.079 | 0.752 | 0.949 | 261 | 85 | 0.000 |
| o........... | 1.297 | 0.704 | 0.736 | 0.912 | 51 | 22 | 0.001 |
| VS3-N...24.. | 0.496 | 0.851 | 1.375 | 0.908 | 19 | 4 | 0.001 |
| C...(...2... | 0.999 | 1.002 | 0.703 | 0.901 | 180 | 60 | 0.000 |
| PT3-H...5... | 0.788 | 0.842 | 1.074 | 0.901 | 261 | 85 | 0.000 |
| VS2-C...22.. | 0.700 | 0.995 | 0.997 | 0.897 | 19 | 4 | 0.001 |
| EC1-O...3... | 0.339 | 1.450 | 0.902 | 0.897 | 261 | 85 | 0.000 |
| [...2....... | 0.128 | 1.017 | 1.527 | 0.890 | 54 | 16 | 0.000 |
| C...(...(... | 1.189 | 0.688 | 0.752 | 0.876 | 223 | 67 | 0.000 |
| N...[...C... | 0.553 | 0.952 | 1.083 | 0.863 | 237 | 75 | 0.000 |
| VS2-H...5... | 1.046 | 0.486 | 0.978 | 0.837 | 111 | 31 | 0.000 |
| VS2-C...8... | 0.780 | 1.116 | 0.573 | 0.823 | 260 | 85 | 0.000 |
| VS2-H...7... | 1.042 | 0.762 | 0.655 | 0.819 | 261 | 85 | 0.000 |
| N...@...H... | 1.095 | 1.054 | 0.271 | 0.807 | 24 | 11 | 0.001 |
| PT3-C...12.. | 1.021 | 0.097 | 1.295 | 0.804 | 192 | 59 | 0.000 |
| 2...c...1... | 0.997 | 0.702 | 0.699 | 0.799 | 174 | 59 | 0.000 |
| EC1-F...4... | 0.789 | 0.646 | 0.923 | 0.786 | 48 | 18 | 0.000 |
| EC1-N...6... | 1.073 | 0.824 | 0.405 | 0.767 | 99 | 27 | 0.001 |
| C...C....... | 0.842 | 0.347 | 1.064 | 0.751 | 209 | 76 | 0.000 |
| ﯯ--S=== | 0.753 | 0.802 | 0.698 | 0.751 | 73 | 23 | 0.000 |
| VS3-O...10.. | 0.772 | 0.701 | 0.752 | 0.742 | 54 | 11 | 0.001 |
| 1...s...(... | 0.983 | 0.625 | 0.602 | 0.737 | 12 | 2 | 0.002 |
| n...1...c... | 0.703 | 0.696 | 0.798 | 0.732 | 30 | 11 | 0.000 |
| PT2-o...4... | 0.396 | 0.525 | 1.233 | 0.718 | 48 | 22 | 0.001 |
| PT3-C...4... | 0.417 | 1.121 | 0.600 | 0.713 | 261 | 85 | 0.000 |
| PT2-C...5... | 0.547 | 0.750 | 0.833 | 0.710 | 261 | 85 | 0.000 |
| [...C....... | 0.842 | 0.427 | 0.841 | 0.703 | 261 | 85 | 0.000 |
| VS2-H...10.. | 0.895 | 0.750 | 0.401 | 0.682 | 261 | 85 | 0.000 |
| C6...AH.4... | 0.399 | 0.695 | 0.899 | 0.664 | 93 | 28 | 0.000 |
| 2........... | 0.603 | 0.596 | 0.792 | 0.664 | 228 | 76 | 0.000 |
| (...F...(... | 0.442 | 0.641 | 0.871 | 0.651 | 50 | 18 | 0.000 |
| c...2...c... | 0.701 | 0.748 | 0.496 | 0.648 | 188 | 65 | 0.000 |
| EC1-s...6... | 0.304 | 0.804 | 0.824 | 0.644 | 17 | 3 | 0.002 |
| VS3-C...23.. | 0.701 | 0.503 | 0.703 | 0.635 | 235 | 76 | 0.000 |
| VS2-N...16.. | 0.397 | 0.503 | 0.999 | 0.633 | 11 | 9 | 0.003 |
| H...@...C... | 0.653 | 0.559 | 0.652 | 0.621 | 260 | 85 | 0.000 |
| VS3-H...8... | 0.771 | 0.142 | 0.938 | 0.617 | 260 | 85 | 0.000 |
| VS3-H...3... | 0.703 | 0.404 | 0.720 | 0.609 | 9 | 1 | 0.002 |
| EC1-S...10.. | 0.697 | 0.398 | 0.700 | 0.599 | 36 | 12 | 0.000 |
| c...2....... | 0.530 | 0.802 | 0.453 | 0.595 | 188 | 65 | 0.000 |
| VS3-Cl..8... | 0.598 | 0.399 | 0.784 | 0.594 | 14 | 7 | 0.001 |
| [...H...@... | 0.578 | 0.452 | 0.747 | 0.592 | 260 | 85 | 0.000 |
| EC1-o...6... | 0.896 | 0.517 | 0.347 | 0.587 | 48 | 22 | 0.001 |
| c...(....... | 0.600 | 0.696 | 0.405 | 0.567 | 161 | 51 | 0.000 |
| VS3-H...14.. | 0.649 | 0.474 | 0.548 | 0.557 | 260 | 85 | 0.000 |
| VS3-C...26.. | 0.488 | 0.528 | 0.653 | 0.556 | 60 | 19 | 0.000 |
| VS2-H...6... | 0.486 | 0.280 | 0.798 | 0.521 | 261 | 85 | 0.000 |
| C6...A..2... | 0.299 | 0.452 | 0.800 | 0.517 | 13 | 3 | 0.001 |
| PT2-s...4... | 0.500 | 0.440 | 0.599 | 0.513 | 17 | 3 | 0.002 |
| EC1-C...11.. | 0.423 | 0.504 | 0.602 | 0.510 | 261 | 85 | 0.000 |
| [...N...@... | 0.704 | 0.574 | 0.247 | 0.508 | 24 | 11 | 0.001 |
| VS3-C...15.. | 0.615 | 0.498 | 0.385 | 0.499 | 225 | 77 | 0.000 |
| o...(...c... | 0.702 | 0.047 | 0.736 | 0.495 | 42 | 18 | 0.001 |
| [...2...C... | 0.758 | 0.249 | 0.422 | 0.476 | 53 | 15 | 0.000 |
| EC1-O...4... | 0.102 | 0.448 | 0.698 | 0.416 | 51 | 15 | 0.000 |
| VS3-O...11.. | 0.398 | 0.672 | 0.166 | 0.412 | 120 | 45 | 0.000 |
| PT2-C...7... | 0.598 | 0.292 | 0.336 | 0.409 | 261 | 85 | 0.000 |
| =...(....... | 0.474 | 0.449 | 0.275 | 0.399 | 260 | 85 | 0.000 |
| VS3-C...22.. | 0.398 | 0.396 | 0.403 | 0.399 | 205 | 65 | 0.000 |
| @...H...... | 0.602 | 0.051 | 0.495 | 0.383 | 24 | 11 | 0.001 |
| [...H....... | 0.704 | 0.201 | 0.199 | 0.368 | 261 | 85 | 0.000 |
| EC1-O...7... | 0.226 | 0.272 | 0.600 | 0.366 | 201 | 61 | 0.000 |
| PT2-O...5... | 0.099 | 0.351 | 0.599 | 0.350 | 201 | 61 | 0.000 |
| C...C...C... | 0.388 | 0.247 | 0.397 | 0.344 | 78 | 25 | 0.000 |
| ﯯ--B2== | 0.205 | 0.303 | 0.492 | 0.333 | 52 | 19 | 0.000 |
| VS2-H...4... | 0.275 | 0.199 | 0.499 | 0.324 | 261 | 85 | 0.000 |
| VS2-C...9... | 0.147 | 0.283 | 0.533 | 0.321 | 231 | 76 | 0.000 |
| 2...(....... | 0.151 | 0.400 | 0.400 | 0.317 | 186 | 62 | 0.000 |
| [...N....... | 0.342 | 0.465 | 0.137 | 0.314 | 237 | 75 | 0.000 |
| EC1-C...7... | 0.491 | 0.199 | 0.238 | 0.309 | 261 | 85 | 0.000 |
| VS2-O...9... | 0.151 | 0.451 | 0.323 | 0.309 | 259 | 85 | 0.000 |
| O...=...(... | 0.351 | 0.171 | 0.396 | 0.306 | 260 | 85 | 0.000 |
| VS2-C...6... | 0.401 | 0.402 | 0.104 | 0.302 | 44 | 19 | 0.001 |
| PT2-S...6... | 0.099 | 0.398 | 0.399 | 0.299 | 48 | 18 | 0.000 |
| EC1-H...3... | 0.348 | 0.050 | 0.490 | 0.296 | 261 | 85 | 0.000 |
| c...1...C... | 0.248 | 0.100 | 0.397 | 0.248 | 22 | 8 | 0.000 |
| VS3-C...21.. | 0.103 | 0.200 | 0.437 | 0.247 | 239 | 79 | 0.000 |
| c...1....... | 0.196 | 0.279 | 0.250 | 0.242 | 260 | 85 | 0.000 |
| PT3-C...5... | 0.146 | 0.148 | 0.383 | 0.226 | 192 | 62 | 0.000 |
| EC1-C...8... | 0.135 | 0.328 | 0.148 | 0.204 | 260 | 85 | 0.000 |
| PT3-O...3... | 0.396 | 0.105 | 0.104 | 0.201 | 128 | 38 | 0.000 |
| PT2-O...2... | 0.296 | 0.074 | 0.195 | 0.188 | 261 | 85 | 0.000 |
| VS3-N...16.. | 0.148 | 0.203 | 0.097 | 0.149 | 151 | 46 | 0.000 |
| PT2-H...2... | 0.073 | 0.252 | 0.039 | 0.122 | 261 | 85 | 0.000 |
| VS3-O...8... | 0.103 | 0.102 | 0.100 | 0.101 | 13 | 4 | 0.000 |
| PT3-O...5... | 0.097 | 0.096 | 0.099 | 0.098 | 259 | 85 | 0.000 |
| VS2-O...7... | 0.096 | 0.096 | 0.096 | 0.096 | 258 | 85 | 0.000 |

a: Number of SMILES which contain structural attribute in the training set, b: Number of SMILES which contain structural attribute in the test set, c: SMILES-Defect

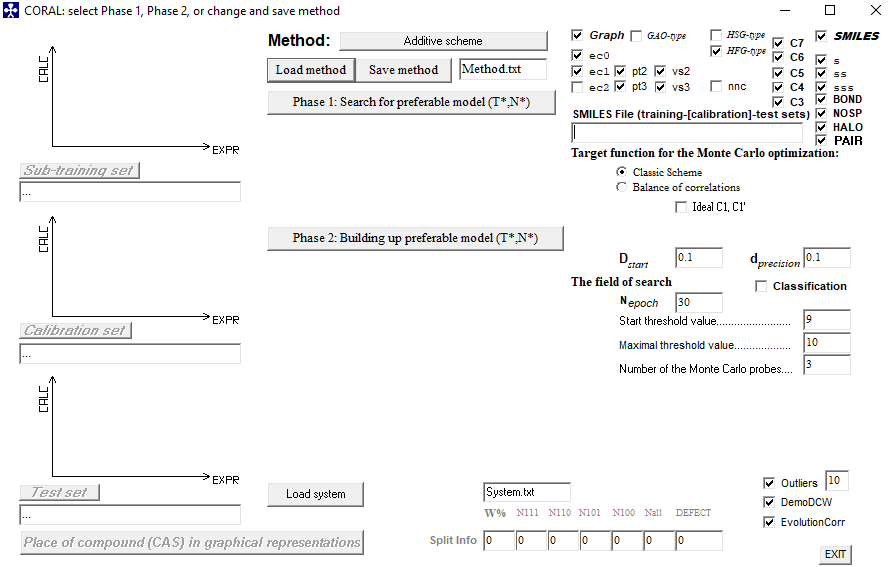
**Table S5.** Unfavorable attributes of Model 4

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Attributes | Probe 1 | Probe 2 | Probe 3 | Average | NTra | NTsb | SDc |
| VS3-H...19.. | -2.002 | -2.000 | -2.003 | -2.002 | 15 | 5 | 0.000 |
| H........... | -2.005 | -2.004 | -1.995 | -2.001 | 261 | 85 | 0.000 |
| VS3-N...13.. | -2.003 | -2.002 | -1.999 | -2.001 | 14 | 7 | 0.001 |
| S...C...C... | -1.996 | -2.004 | -2.004 | -2.001 | 34 | 14 | 0.001 |
| PT3-S...6... | -1.999 | -2.001 | -2.002 | -2.001 | 14 | 6 | 0.001 |
| VS3-N...17.. | -2.000 | -1.999 | -2.003 | -2.000 | 133 | 42 | 0.000 |
| VS3-N...23.. | -1.996 | -2.004 | -2.000 | -2.000 | 12 | 7 | 0.002 |
| VS2-S...12.. | -1.997 | -2.000 | -2.003 | -2.000 | 14 | 6 | 0.001 |
| O...C...C... | -2.002 | -1.997 | -2.000 | -2.000 | 46 | 9 | 0.001 |
| C5......0... | -1.999 | -2.004 | -1.995 | -2.000 | 35 | 13 | 0.000 |
| VS2-N...14.. | -1.996 | -1.999 | -2.003 | -2.000 | 85 | 29 | 0.000 |
| VS3-H...18.. | -2.003 | -1.999 | -1.995 | -1.999 | 68 | 20 | 0.000 |
| PT3-C...11.. | -2.001 | -1.996 | -1.999 | -1.999 | 78 | 24 | 0.000 |
| VS2-C...20.. | -1.998 | -1.998 | -1.998 | -1.998 | 63 | 17 | 0.001 |
| [........... | -1.996 | -1.954 | -1.998 | -1.982 | 261 | 85 | 0.000 |
| [...(...N... | -1.804 | -1.998 | -2.003 | -1.935 | 37 | 11 | 0.000 |
| (...N...(... | -1.702 | -2.004 | -2.001 | -1.902 | 13 | 0 | 1.000 |
| PT3-N...11.. | -1.997 | -1.697 | -2.001 | -1.898 | 170 | 58 | 0.000 |
| H.......... | -1.602 | -2.003 | -2.001 | -1.869 | 47 | 19 | 0.001 |
| [......H... | -1.699 | -1.996 | -1.905 | -1.867 | 47 | 19 | 0.001 |
| VS3-C...8... | -1.870 | -1.751 | -1.873 | -1.832 | 256 | 83 | 0.000 |
| PT3-O...6... | -1.800 | -1.905 | -1.701 | -1.802 | 259 | 85 | 0.000 |
| VS3-C...20.. | -1.602 | -1.998 | -1.803 | -1.801 | 121 | 41 | 0.000 |
| VS3-N...10.. | -1.700 | -1.701 | -2.002 | -1.801 | 26 | 5 | 0.001 |
| VS2-N...19.. | -1.801 | -1.699 | -1.802 | -1.768 | 12 | 4 | 0.000 |
| VS3-C...27.. | -1.700 | -1.596 | -1.998 | -1.765 | 60 | 16 | 0.001 |
| PT2-N...6... | -1.699 | -1.703 | -1.852 | -1.752 | 24 | 8 | 0.000 |
| (........... | -2.001 | -1.699 | -1.550 | -1.750 | 261 | 85 | 0.000 |
| c...C...(... | -1.700 | -1.704 | -1.700 | -1.701 | 259 | 84 | 0.000 |
| VS3-N...21.. | -1.696 | -1.699 | -1.578 | -1.658 | 124 | 43 | 0.000 |
| EC1-N...9... | -1.615 | -1.801 | -1.550 | -1.655 | 24 | 8 | 0.000 |
| 1...C...(... | -1.872 | -1.647 | -1.373 | -1.631 | 184 | 62 | 0.000 |
| O...(...1... | -1.452 | -1.750 | -1.647 | -1.617 | 93 | 30 | 0.000 |
| N...C...(... | -1.450 | -1.712 | -1.452 | -1.538 | 204 | 65 | 0.000 |
| N........... | -1.699 | -1.655 | -1.230 | -1.528 | 261 | 85 | 0.000 |
| 1...(....... | -1.554 | -1.548 | -1.450 | -1.518 | 223 | 73 | 0.000 |
| VS2-N...11.. | -1.403 | -1.699 | -1.403 | -1.501 | 65 | 20 | 0.000 |
| PT2-C...6... | -1.458 | -1.730 | -1.239 | -1.475 | 253 | 83 | 0.000 |
| C...1...(... | -1.496 | -1.401 | -1.364 | -1.420 | 48 | 19 | 0.001 |
| EC0-C...4... | -1.498 | -1.398 | -1.345 | -1.414 | 261 | 85 | 0.000 |
| 2...c...(... | -1.397 | -1.398 | -1.400 | -1.399 | 55 | 22 | 0.001 |
| VS3-H...20.. | -1.362 | -1.604 | -1.230 | -1.398 | 61 | 16 | 0.001 |
| [...C...C... | -1.202 | -1.399 | -1.525 | -1.375 | 96 | 36 | 0.000 |
| EC1-C...9... | -1.347 | -1.553 | -1.222 | -1.374 | 261 | 85 | 0.000 |
| C...(....... | -1.236 | -1.304 | -1.555 | -1.365 | 261 | 85 | 0.000 |
| EC1-C...14.. | -1.049 | -1.700 | -1.345 | -1.365 | 115 | 33 | 0.000 |
| EC0-H...1... | -1.339 | -1.405 | -1.301 | -1.348 | 261 | 85 | 0.000 |
| H...[...(... | -1.401 | -1.349 | -1.054 | -1.268 | 261 | 85 | 0.000 |
| @@.......... | -1.095 | -1.280 | -1.409 | -1.262 | 249 | 81 | 0.000 |
| PT2-C...10.. | -1.117 | -1.297 | -1.345 | -1.253 | 115 | 33 | 0.000 |
| PT3-C...6... | -1.347 | -1.155 | -1.159 | -1.220 | 261 | 85 | 0.000 |
| VS2-o...12.. | -1.399 | -1.101 | -1.099 | -1.200 | 18 | 7 | 0.001 |
| PT2-H...3... | -1.064 | -1.191 | -1.160 | -1.138 | 261 | 85 | 0.000 |
| c...(...1... | -1.191 | -0.896 | -1.299 | -1.129 | 85 | 29 | 0.000 |
| PT3-o...8... | -1.096 | -1.102 | -1.105 | -1.101 | 18 | 7 | 0.001 |
| ++++F---S=== | -1.102 | -1.095 | -1.102 | -1.100 | 11 | 1 | 0.003 |
| EC1-H...4... | -1.099 | -1.000 | -1.196 | -1.098 | 261 | 85 | 0.000 |
| [...(...O... | -1.098 | -1.096 | -1.101 | -1.098 | 216 | 72 | 0.000 |
| C...1....... | -1.100 | -1.252 | -0.853 | -1.069 | 199 | 71 | 0.000 |
| [.......... | -1.502 | -0.878 | -0.798 | -1.059 | 49 | 20 | 0.001 |
| n...c...(... | -0.874 | -0.973 | -1.196 | -1.014 | 14 | 7 | 0.001 |
| VS2-H...8... | -0.886 | -1.066 | -1.088 | -1.013 | 261 | 85 | 0.000 |
| C3......0... | -1.102 | -1.103 | -0.796 | -1.000 | 258 | 84 | 0.000 |
| @........... | -1.247 | -0.876 | -0.839 | -0.987 | 260 | 85 | 0.000 |
| F...(...F... | -1.051 | -0.804 | -1.099 | -0.985 | 49 | 19 | 0.001 |
| VS3-N...6... | -1.097 | -0.795 | -1.052 | -0.981 | 9 | 3 | 0.000 |
| C...c...1... | -0.847 | -1.095 | -0.996 | -0.979 | 260 | 85 | 0.000 |
| PT3-O...7... | -0.974 | -0.797 | -1.097 | -0.956 | 85 | 28 | 0.000 |
| O...C...(... | -1.001 | -1.098 | -0.602 | -0.901 | 154 | 46 | 0.000 |
| PT3-H...1... | -0.937 | -0.739 | -0.849 | -0.841 | 12 | 2 | 0.002 |
| (...O...(... | -0.903 | -0.847 | -0.764 | -0.838 | 247 | 80 | 0.000 |
| VS2-O...12.. | -1.096 | -0.899 | -0.501 | -0.832 | 101 | 32 | 0.000 |
| PT2-C...1... | -0.428 | -1.072 | -0.961 | -0.820 | 12 | 2 | 0.002 |
| c...c...c... | -0.833 | -0.604 | -1.001 | -0.813 | 260 | 85 | 0.000 |
| O...=....... | -0.827 | -0.972 | -0.612 | -0.804 | 261 | 85 | 0.000 |
| n...c...c... | -0.805 | -0.799 | -0.798 | -0.801 | 68 | 20 | 0.000 |
| VS2-N...9... | -0.799 | -0.801 | -0.801 | -0.800 | 20 | 9 | 0.001 |
| 1...c...(... | -0.797 | -0.804 | -0.796 | -0.799 | 108 | 34 | 0.000 |
| N...(...C... | -0.799 | -1.135 | -0.396 | -0.777 | 151 | 46 | 0.000 |
| C...(...1... | -0.849 | -0.772 | -0.661 | -0.761 | 121 | 40 | 0.000 |
| ........... | -0.797 | -0.700 | -0.747 | -0.748 | 49 | 20 | 0.001 |
| EC0-N...3... | -0.408 | -0.674 | -1.109 | -0.730 | 261 | 85 | 0.000 |
| N...C....... | -0.827 | -0.716 | -0.645 | -0.729 | 233 | 75 | 0.000 |
| EC0-O...1... | -0.471 | -0.955 | -0.755 | -0.727 | 261 | 85 | 0.000 |
| 1........... | -0.601 | -0.670 | -0.850 | -0.707 | 261 | 85 | 0.000 |
| H...[...2... | -0.537 | -1.073 | -0.451 | -0.687 | 53 | 15 | 0.000 |
| EC0-F...1... | -0.445 | -0.947 | -0.654 | -0.682 | 52 | 19 | 0.000 |
| O...(....... | -0.523 | -0.450 | -1.051 | -0.675 | 261 | 85 | 0.000 |
| VS3-N...18.. | -0.672 | -0.472 | -0.879 | -0.674 | 68 | 25 | 0.000 |
| c...C....... | -0.801 | -0.801 | -0.415 | -0.672 | 260 | 85 | 0.000 |
| H...@....... | -0.383 | -0.651 | -0.752 | -0.596 | 260 | 85 | 0.000 |
| F........... | -0.450 | -0.485 | -0.748 | -0.561 | 52 | 19 | 0.000 |
| 1...[...... | -0.499 | -0.413 | -0.748 | -0.554 | 11 | 3 | 0.001 |
| VS3-H...10.. | -0.680 | -0.489 | -0.484 | -0.551 | 209 | 64 | 0.000 |
| C...@@...... | -0.639 | -0.267 | -0.702 | -0.536 | 249 | 81 | 0.000 |
| C...2....... | -0.755 | -0.403 | -0.388 | -0.515 | 57 | 17 | 0.000 |
| PT3-N...6... | -0.352 | -0.747 | -0.412 | -0.504 | 73 | 23 | 0.000 |
| O...[...C... | -0.500 | -0.446 | -0.500 | -0.482 | 158 | 54 | 0.000 |
| C........... | -0.612 | -0.321 | -0.414 | -0.449 | 261 | 85 | 0.000 |
| PT3-C...7... | -0.534 | -0.297 | -0.476 | -0.436 | 260 | 85 | 0.000 |
| HALO11000000 | -0.205 | -0.495 | -0.501 | -0.400 | 13 | 7 | 0.002 |
| ++++F---Cl== | -0.202 | -0.499 | -0.500 | -0.400 | 13 | 7 | 0.002 |
| c...c....... | -0.229 | -0.374 | -0.526 | -0.376 | 260 | 85 | 0.000 |
| VS2-C...12.. | -0.208 | -0.388 | -0.517 | -0.371 | 257 | 83 | 0.000 |
| PT3-H...6... | -0.301 | -0.375 | -0.379 | -0.352 | 258 | 85 | 0.000 |
| VS3-C...17.. | -0.273 | -0.374 | -0.403 | -0.350 | 260 | 85 | 0.000 |
| VS2-C...13.. | -0.247 | -0.326 | -0.447 | -0.340 | 254 | 80 | 0.000 |
| VS3-C...4... | -0.327 | -0.303 | -0.353 | -0.328 | 127 | 39 | 0.000 |
| EC1-C...6... | -0.203 | -0.503 | -0.204 | -0.303 | 230 | 69 | 0.000 |
| PT2-N...4... | -0.198 | -0.501 | -0.202 | -0.300 | 98 | 27 | 0.001 |
| VS3-O...20.. | -0.197 | -0.498 | -0.201 | -0.299 | 31 | 9 | 0.000 |
| c........... | -0.350 | -0.199 | -0.301 | -0.283 | 260 | 85 | 0.000 |
| PT3-H...4... | -0.087 | -0.242 | -0.511 | -0.280 | 260 | 85 | 0.000 |
| VS3-C...11.. | -0.041 | -0.229 | -0.513 | -0.261 | 260 | 85 | 0.000 |
| n...c....... | -0.360 | -0.116 | -0.270 | -0.249 | 90 | 25 | 0.000 |
| VS2-F...6... | -0.403 | -0.222 | -0.099 | -0.242 | 50 | 19 | 0.001 |
| PT3-N...8... | -0.165 | -0.252 | -0.252 | -0.223 | 199 | 67 | 0.000 |
| O........... | -0.203 | -0.051 | -0.401 | -0.219 | 261 | 85 | 0.000 |
| C...@....... | -0.203 | -0.251 | -0.198 | -0.217 | 260 | 85 | 0.000 |
| n........... | -0.203 | -0.202 | -0.199 | -0.201 | 109 | 32 | 0.000 |
| [...O....... | -0.196 | -0.197 | -0.204 | -0.199 | 162 | 54 | 0.000 |
| S...(...=... | -0.071 | -0.200 | -0.099 | -0.123 | 37 | 12 | 0.000 |
| c...1...(... | -0.146 | -0.114 | -0.078 | -0.113 | 207 | 69 | 0.000 |
| EC0-C...3... | -0.128 | -0.047 | -0.138 | -0.104 | 261 | 85 | 0.000 |

a: Number of SMILES which contain structural attribute in the training set, b: Number of SMILES which contain structural attribute in the test set, c: SMILES-Defect



**Figure S1.** Applicability domain of Model 1 (left) and Model 2 (right)

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**Figure S2.** Screenshot of the setup file of Coral package used for generating the QSAR Model 3.

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