

Supplementary Information

Transformer neural network for protein-specific de novo drug generation as a
machine translation problem

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SMILES representation for generated compounds.

- O=C(N[C@@H]1C[C@@H]1c1ccc(C(F)(F)F)cc1)N1CCN(S(=O)(=O)c2ccc(C(F)(F)F)cc2)CC1
- COc1ccc(CN(Cc2ccc(-c3ccc(C(=O)O)cc3)cc2)Cc2ccc(C(C)(C)C)cc2)cc1
- COc1ccc(CN(Cc2ccc(-c3ccc(C(=O)O)cc3)cc2)c2ccc(C(=O)O)cc2)cc1
- O=C(N[C@@H]1C[C@H]1c1ccc(O)cc1)Nc1ccc(Cl)cc1
- Cc1cccc1NC(=O)Nc1ccc(S(=O)(=O)Nc2ccc(N3CCN(C)CC3)cc2)cc1
- CC(C)[C@H](CC(=O)NO)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](Cc1cccc1)C(=O)N[C@@H](Cc1cccc1)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](CC(C)C)C(=O)O
- O=C(O)c1ccc(NC(=O)c2nc3cccc3[nH]2)cc1
- Cc1cc(C(=O)Nc2ccc(F)cc2)cc(-c2ccc(C(=O)O)cc2)c1
- O=C(c1cccc1)c1ccc(O)c(O)c1
- COc1ccc(-c2nc(Nc3ccc(F)c(Cl)c3)c3c(n2)CCNC3)cc1
- COc1ccc(-c2cc(=O)oc3cccc23)cc1
- O=C(O)c1ccc(Oc2ccc(Cl)cc2)c(Cl)c1
- O=C(N[C@@H]1C[C@@H]1c1cccc1)c1ccc(Cl)cc1
- O=C(O)c1ccc(N2CCN(c3ccc4c(c3)OCO4)CC2)cc1
- CN[C@@H]1C[C@H]2O[C@@]1(C)[C@@H]1OC)n1c3cccc3c3c4c(c5c6cccc6n2c5c31)C(=O)NC4
- CN(C)C(=O)Nc1ccc2c(c1)S(=O)(=O)c1cccc1N2
- C[C@@H](NC(=O)[C@H](Cc1cccc1)NC(=O)[C@H](Cc1c[nH]c2cccc12)NC(=O)[C@H](Cc1cccc1)NC(=O)[C@H](Cc1cccc1)NC(=O)[C@H](Cc1cccc1)NC(=O)[C@H](C)C(N)=O)C(N)=O
- COc1cc2c(cc1OC)C(=O)c1c(-c3cccc3)n[nH]c1-2
- COc1ccc([C@H]2C[C@H]3[C@@H](O)CC[C@H]3C2)cc1
- CNC(=O)c1ccc2c(c1)[nH]c1cccc12
- O=C(N[C@@H]1C[C@@H]1c1cccc1)N1CC[C@@H](c2ccc(Cl)cc2)[C@@H]1C(F)(F)F
- COc1ccc(C(=O)Nc2ccc(Cl)cc2)cc1Cl
- COC(=O)C(=O)N1CCN(C(=O)c2ccc(-c3ccc4c(c3)CC(=O)O4)cc2)CC1
- COc1ccc2c(c1)nc(Nc1ccc(C(=O)O)cc1)c1cccc1C2
- CN(C)C(=O)c1ccc2c(c1)[C@]1(C)CC[C@@H](C2)[C@@H]1C(=O)O
- CNC(=O)Oc1ccc2c(c1)[C@]1(C)CCN(C)[C@@H]1N2C
- COc1ccc2[nH]cc(C)c2c1
- COc1cc2c(cc1OC)C(c1cccc1)N(C)C(=O)C2
- O=C(c1cccc1)N1CCC2(CC1)OC(=O)c1cc(O)ccc1O2
- COc1ccc(C(=O)Nc2ccc(Cl)c(Cl)c2)cc1
- COc1cc2c(cc1OC)C(=O)N(CC(=O)O)C2=O
- C[C@]12O[C@H](C[C@]1(O)CO)n1c3cccc3c3c4c(c5c6cccc6n2c5c31)CNC4=O
- CC(C)[C@H](NC(=O)[C@H](Cc1cccc1)NC(=O)c1ccc(-c2cccc2)cc1)C(=O)O
- COc1ccc(C(=O)N2CCN(c3ccc4c(c3)OCO4)CC2)cc1
- COc1ccc(S(=O)(=O)NC(=O)c2c(Cl)cc(Cl)cc2Cl)cc1
- COc1cccc1N1CCN(CCCNC(=O)c2cc(OC)c(OC)c(OC)c2)CC1
- CNC[C@@H](O)[C@H](c1cccc1)N(C)C
- NC(=O)c1ccc(Oc2cccc2)cc1
- CN(C)C(=O)c1ccc(S(=O)(=O)N2CCN(Cc3ccc4c(c3)OCO4)CC2)cc1

40. O=C(Nc1ccc2ccccc2c1)S(=O)(=O)c1ccc2ccccc2c1
41. O=C(O)c1ccc(O)c(O)c1
42. CN(C)C(=O)c1ccc2c(c1)[nH]c1ccc(C#N)cc12
43. CC(=O)N[C@@H]1CC[C@H](C(=O)O)CC1
44. CC(=O)N1CCN(c2ccc([N+](=O)[O-])cc2)CC1
45. CC(C)(C)c1ccc(S(=O)(=O)Nc2ccc3c(c2)OCO3)cc1
46. O=C(O)c1ccc(-c2ccccc2)cc1
47. COc1cc2c(cc1OC)C(=O)c1c(-c3cnc[nH]3)c[nH]c1-2
48. CC(C)(C)c1ccc2c(c1)OCO2
49. O=C(O)c1ccc(-c2ccc(O)cc2)cc1
50. O=C(N[C@@H]1C[C@@H]1c1ccc(OCc2ccccc2)cc1)N1Cc2ccccc2C1
51. CC(C)(C)NC(=O)c1ccc(Oc2ccccc2)cc1
52. COc1ccc(-n2c(=O)n(-c3ccc(Cl)cc3)c3cc(C(=O)NS(C)(=O)=O)ccc32)cc1
53. CO[C@@H]1[C@H](N(C)C(=O)c2ccccc2)C[C@H]2O[C@]1(C)n1c3ccccc3c3c4c(c5c6ccccc6n2c5c31)
)C(=O)NC4
54. Cc1cc(C(=O)Nc2ccc(-c3ccccc3)cc2)nc2ccccc12
55. NC(=O)c1ccc(Oc2cn(Cc3ccc4c(c3)OCO4)nc2)cc1
56. C[C@@H]1NC(C)(C)CO[C@@]1(O)c1ccc(Cl)c(Cl)c1
57. COc1ccc(NC(=O)Nc2ccc(Cl)c(Cl)c2)c(Cl)c1
58. CC(=O)N[C@@H]1C[C@H]2O[C@@](C)([C@@H]1OC)n1c3ccccc3c3c4c(c5c6ccccc6n2c5c31)C(=O)
)NC4
59. O=C(O)c1ccc(Oc2ccc(-c3ccc(C(F)(F)F)cc3)cc2)cc1
60. CC(C)C[C@H](NS(=O)(=O)c1ccccc1)C(=O)O
61. COc1ccccc(NC(=S)Nc2ccc(Cl)c2)c1
62. COc1ccccc(N2CCN(Cc3ccccc3)CC2)c1
63. CC(=O)N[C@@H](CC(=O)O)C(=O)N[C@H](Cc1ccccc1)C(=O)N[C@H](Cc1ccccc1)C(=O)O
64. O=C(O)c1ccc(Oc2ccc(Oc3ccccc3)cc2)cc1
65. COc1ccc2c(c1)C=Cc1ccc(C(=O)O)cc1)C(=O)N2C
66. COC(=O)c1ccc2c(c1)NC(=O)/C2=C(\Nc1ccc(F)cc1)c1ccccc1
67. O=C(Nc1nc(-c2ccc(OC(F)(F)F)cc2)cs1)c1nc(C(F)(F)F)nc(N2CCOCC2)c1Cl
68. COc1cc2c(cc1OC)CN(Cc1ccccc1)C2
69. COc1ccc(S(=O)(=O)c2ccccc2)cc1
70. O=C(O)c1ccc2c(c1)C(=O)N(Cc1ccccc1)C2
71. COc1cc(Nc2nc(Sc3ccc(NC(=O)CN4CCOCC4)cc3)nc(N3CCNCC3)n2)cc(OC)c1OC
72. O=C(O)c1ccc(OC(F)(F)F)cc1
73. COc1ccc(-c2ccc(CSc3nc(-c4ccccc4)c[nH]3)cc2)cc1
74. O=C(N[C@@H]1C[C@H]1c1ccccc1)c1ccc2c(c1)OCO2
75. COc1ccccc(CNC(=O)Nc2ccc(Cl)cc2)c1
76. CCCCCCCCCCCCCCCCCC
77. O=C(NCc1ccccc1)c1ccc(C(F)(F)F)cc1
78. CCN(CC)C(=O)[C@H]1CC[C@H]2[C@@H]3C[C@@H]4C[C@@](O)(C4)[C@H]3CC[C@@]21C
79. COc1ccc2oc(=O)c(O)c(O)c2c1
80. O=c1[nH]c(=O)n([C@H]2C[C@@H](c3ccc4c(c3)OCO4)O2)c2ccccc12
81. N#Cc1ccc(-c2noc(-c3ccc4c(c3)OCO4)n2)cc1

82. O=C(N[C@@H](Cc1cccc1)C(=O)N1CCC[C@H]1c1cccc1)c1cccc1
83. COc1ccc2nc(N3CCN(Cc4ccc(Cl)c(Cl)c4)CC3)[nH]c2c1
84. O=C(Nc1ccc(Cl)cc1)c1ccc(Cl)c(Cl)c1
85. O=C(O)c1ccc2c(c1)[nH]c1ccc(Cl)cc12
86. CC[C@H](C)[C@H](NC(=O)[C@H](Cc1c[nH]c2cccc12)NC(=O)[C@@H]1CCCN1C(=O)[C@@H](N)C
CCN=C(N)N)C(=O)N[C@@H](Cc1c[nH]c2cccc12)C(N)=O
87. CC(C)(C)NC(=O)c1ccc(OCCSc2nc(-c3cccc3)no2)cc1
88. NC(=O)c1sc(-c2cccs2)nc1-c1ccc2c(c1)OCO2
89. CN(C)c1ccc(C2CCN(Cc3ccc(Cl)cc3)CC2)cc1
90. O=C(c1cccc1)N1CCC(Nc2ncnc3cccc23)CC1
91. COc1cc2c(cc1OC)/C=C/c1ccc(Nc3cccc3)cc1)C(=O)NC2
92. Cc1ccc(C(=O)Nc2cccc(CNC(=O)c3cccc3)c2)cc1
93. COc1cc2c(cc1OC)-c1[nH]c3cccc3c1C2
94. COc1ccc2c(c1)C(=O)Nc1ccc(-c3cccc3)cc1C2
95. COc1ccc(CNC(=O)c2ccc3c(c2)c(C)c(C)n3C)cc1
96. O=C(N[C@@H](Cc1cccc1)C(=O)c1nc(-c2cccc2)c(-c2cccc2)[nH]1)c1cccc1
97. C[C@H]1NC(C)(C)CO[C@@]1(O)c1ccc(Cl)c(Cl)c1
98. COc1cc2c(cc1OC)-c1nc(Nc3ccc(F)cc3)ncc1CC2
99. COC(=O)c1cccc(NS(=O)(=O)c2ccc(Cl)cc2)c1
100. NC(=O)c1cc2c(Oc3ccc([N+](=O)[O-])cc3)cncc2s1
101. COc1cc2c(cc1OC)C(=O)N(CC(=O)Nc1cccc1)C2=O
102. O=c1n(CCN2CCN(Cc3ccc(Cl)cc3)CC2)n(C2CCN(C(=O)c3cccc3)CC2)n1C(Cl)c1ccc(Cl)cc1
103. Cc1ccc(-c2noc(C)n2)c(-c2ccc(NS(C)(=O)=O)cc2)n1
104. C[C@@H](NC(=O)c1ccc(C(F)(F)F)cc1)C(=O)N[C@H]1CCC(=O)N(c2ccc(C(F)(F)F)cc2)C1
105. CC(C)c1nc(C(=O)Nc2ccc(C(F)(F)F)cc2)oc1C(C)(C)C
106. COC(=O)c1cccc(CNC(=O)c2cc(-c3cccc3)ccc2C(=O)Nc2ccc(Cl)cc2)c1
107. Cc1c(C#N)cccc1-c1noc(-c2ccc(C(F)(F)F)cc2)n1
108. CC(C)c1cc(NC(=O)[C@H]2CCN(c3ccc(C(F)(F)F)cc3)CC2)nc2cccc12
109. Cc1cccc(NC(=O)c2ccc(N3CCOCC3)cc2)c1
110. C[C@]12CC[C@@H](C[C@@H]1OC)n1c3cccc3c3c4c(c5c6cccc6n2c5c31)CNC4=O
111. Cc1cccc1NC(=O)c1ccc(N2CCCC2)cc1
112. Cc1ccc(-c2ccc(C(F)(F)F)cc2)nc1
113. COc1ccc(NC(=O)[C@@H]2CCCN2C(=O)[C@@H](c2cccc2)c2cccc2)cc1
114. O=C(N[C@@H]1CC[C@H](O)CC1)c1ccc2c(c1)C(=O)CCC2
115. C[C@]12CC[C@@H]3c4ccc(O)cc4CC[C@H]3[C@@H]1CC[C@@H]2O
116. CN1CCN(c2ccc(Nc3ncnc4cc(-c5ccc(F)cc5)ncc34)cc2)CC1
117. Nc1ncc(-c2ccc3c(c2)OCO3)nc1-c1ccc2c(c1)OCO2
118. CC(C)(C)c1ccc(NC(=O)Nc2ccc(C(=O)O)cc2)cc1
119. CC(C)NC(=O)c1ccc2c(c1)[C@@]1(C)CC[C@H](O)[C@@H]1N2C
120. COc1cc(NC(=O)C(C)(C)C)ccc1C(=O)Nc1ccc(Cl)cc1
121. NC(=O)c1cccc(OC[C@H]2CN3CCC[C@@H]3C2)c1
122. NC(=O)c1ccc(-c2cccc2Cl)cc1
123. COc1ccc([C@H]2C[C@H](O)[C@@H](O)[C@H]2O)cc1
124. O=C1NC(=O)C(c2ccc3cccc3c2)C1=O

125. NC(=O)c1ccc(Nc2nccc(-c3ccc4c(c3)NC(=O)C4=O)n2)cc1
126. COc1ccc(-c2ccc(CC(=O)O)cc2)cc1
127. O=C(Nc1ccc(Oc2ccccc2)cc1)c1cnc2ccccc2c1
128. CN(C)C(=O)c1ccc(Oc2ccccc2Cl)c(Cl)c1
129. COc1cc2c(cc1OC)C(O)C(=O)N(C)C(=O)c1ccc(C(F)(F)F)cc1S2(=O)=O
130. Nc1ncc(C(=O)Nc2ccc(S(N)(=O)=O)cc2)s1
131. CN(C)C(=O)c1ccc2c(=O)n(Cc3ccccc3)c(=O)c2c1
132. C[C@@H]1N(C)CCN1c1ccccc1Cl
133. COc1ccc(-c2c(-c3ccccc3)nc(C)n2-c2ccc(Cl)cc2)cc1
134. COC(=O)c1ccc2c(c1)[C@@]1(C)CCN(C(=O)c3ccccc3)[C@@H]1C2
135. COc1ccc2c(c1)C(C(=O)Nc1ccc(Cl)cc1)C(=O)N2
136. NS(=O)(=O)c1ccc(-c2ccc(N3CCNCC3)cc2)cc1
137. CC(C)(C)C(=O)N[C@@H](Cc1c[nH]c2ccccc12)C(=O)N[C@@H](Cc1ccccc1)C(=O)O
138. COc1ccc(-c2n[nH]c3c2C(=O)c2ccc(-c4ccccc4)cc2-3)cc1
139. COc1ccc(C2=C(c3ccc(F)cc3)c3ccccc3N(C)C2=O)cc1
140. CC(C)(C)c1nn(-c2ccc(F)cc2Cl)c2c1C(=O)CCC2
141. CC(C)[C@H](NC(=O)[C@H](Cc1c[nH]c2ccccc12)NC(=O)OCc1ccccc1)C(=O)O
142. O=C(Nc1nc2ccccc2s1)c1ccccc1
143. CC(C)[C@H](NC(=O)[C@H](Cc1ccccc1)NC(=O)[C@H](Cc1ccccc1)NC(=O)[C@H](Cc1ccccc1)NC(=O)OCc1ccccc1)C(=O)O
144. COc1ccc(S(=O)(=O)N2CCN(C(=O)c3ccc4c(c3)OCO4)CC2)cc1
145. CC(C)[C@H](NC(=O)c1ccccc1)C(=O)N[C@H]1C[C@H]2O[C@](C)([C@@H]1OC)n1c3ccccc3c3c4c(c5c6ccccc6n2c5c31)C(=O)NC4
146. O=C(Nc1ccccc1)N1CCC(N2CCCC2)CC1
147. Cc1ccc(-c2sc(C(F)(F)F)nc2C(=O)c2ccc(Cl)cc2)cc1
148. CC(C)(C)c1cnc(N2CCN(c3ccc(C(F)(F)F)cc3)CC2)s1
149. COC(=O)c1ccc2[nH]ncc2c1
150. O=C(Nc1nc(-c2ccccc2)ns1)c1ccc(N2CCCC2)cc1
151. O=C(O)c1ccc(OCCN2CCN(c3ccccc(Cl)c3)CC2)cc1
152. COc1cc(NC(=O)C(C)(C)C)ccc1C(=O)Nc1ccc(Cl)c(Cl)c1
153. NC(=O)c1ccc2c(c1)C(=Nc1ccc(S(N)(=O)=O)cc1)C(=O)N2
154. C[C@H]1CC[C@@H](NC(=O)Nc2ccc(C(F)(F)F)c2Cl)CC1
155. Nc1ncnc(N2CCC(Nc3ncnc4[nH]cc(-c5ccc(C(F)(F)F)cc5)c34)CC2)n1
156. C[C@]12CC[C@H]3[C@@H](CC[C@H]4CCCC[C@@]43C)[C@@H]1CC[C@@H]2O
157. Nc1nc2ccccc2c(=O)[nH]1
158. COc1ccc(Nc2nccc(-c3ccc4c(c3)NC(=O)C4=O)n2)cc1
159. COC(=O)c1ccccc(-c2nc(NC(C)=O)c(NC(C)=O)o2)c1
160. COc1ccc(-c2c(C)noc2-c2ccc3nc(N)n(C)c3c2)cc1
161. COc1ccc(CNC(=O)c2cc(-c3ccc4c(c3)OCO4)n[nH]2)cc1
162. COc1cc2c(cc1OC)-c1[nH]nc(-c3ccc(N4CCOCC4)cc3)c1C2
163. Cc1ccc(-c2cc(C(F)(F)F)ccc2C(=O)Nc2ccc(-c3ccccc3)cc2)cc1
164. NC(=O)c1ccc2nc(-c3ccc(NC(=O)c4ccc5c(c4)OCO5)cc3)[nH]c2c1
165. C[C@@H](NC(=O)[C@H](Cc1ccccc1)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C(C)C

166. C[C@@H]1C[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@@H]3CC[C@@]21C
167. COc1ccc(C(=O)Nc2ccc(-c3ccccc3)cc2)cc1
168. COc1ccc(-n2nnnc2C(=O)c2ccc(-n3cnc4ccccc43)cc2)cc1
169. COc1ccc(S(=O)(=O)N2CCN(C(=O)N3CCN(C)CC3)CC2)cc1
170. Cc1ccccc1Oc1ccc(-c2ccccc2)nc1
171. COc1ccc(S(=O)(=O)N2C[C@@H](OC)[C@@H](OC)C2)cc1
172. O=C(Nc1ccc(Cl)cc1)N1CCN(Cc2ccccc2)CC1
173. O=C(Nc1nc2ccccc2s1)c1ccc2c(c1)NC(=O)C2
174. CC(C)[C@H](NC(=O)[C@H](Cc1ccccc1)NC(=O)OCc1ccccc1)C(=O)O
175. Cc1ccccc1S(=O)(=O)N1CCN(C2CCCC2)CC1
176. CC(C)[C@H](NC(=O)c1ccc(-c2ccccc2)cc1)C(=O)O
177. O=C(Nc1nnc(-c2ccccc2)s1)c1ccccc1
178. NC(=O)c1ccc(Nc2nccc(-c3ccc4c(c3)OCO4)n2)cc1
179. COc1ccc(CNC(=O)c2cc3c(cc2OC)C(=O)N(C)C3=O)cc1
180. CC(C)(C)NC(=O)c1ccc(NS(=O)(=O)c2ccc(C(F)(F)F)cc2)cc1
181. CN1CCN(c2ccc(-c3cnc4[nH]c5c(F)cccc5c4c3)cc2)CC1
182. NC(=O)c1ccc2c(c1)nc(NCc1ccc(Cl)cc1)c1cc(C(N)=O)ccc1C2
183. COc1ccc2c(c1)[C@H]1CC[C@H](C2)N1C
184. O=C(O)c1ccc(Nc2nccc(-c3ccccc3)n2)cc1
185. O=C(Nc1ccc(-c2ccccc2)cc1)N1CCC(Oc2ccc(Cl)cc2)CC1
186. NC(=O)c1cnc(-c2ccc3c(c2)CNC3=O)[nH]1
187. CNC(=O)[C@@H]1C[C@H]2O[C@@](C)([C@@H]1OC)n1c3ccccc3c3c4c(c5c6ccccc6n2c5c31)C(=O)NC4
188. C[C@]12CC[C@H]3[C@@H](CC[C@H]4CCC(=O)CC[C@@]43C)[C@@H]1CC[C@@H]2O
189. COc1cc(Nc2ncc3ccc(F)cc3n2)ccc1F
190. COc1ccc(Cl)c(Cl)c1C1c2c(c(OC)c1OC)n(C)n2C(=O)c1ccc(F)cc1
191. COc1cc2c(cc1OC)C(=O)C(C(=O)Nc1ccccc1)C(=O)N2
192. COc1ccc2c(c1)C(=O)C(CC1CCN(Cc3ccccc3)CC1)C2
193. COc1cc2c(cc1OC)C(=O)C(C)(C)CCC2NC(=O)c1ccc(-c2ccc(C(=O)O)cc2)cc1
194. O=C(O)c1cccc(Nc2nc3ccccc(C(F)(F)F)c3c(=O)[nH]2)c1
195. CCCCCCCCCC(=O)NCCCCCCCC(=O)OC(C)C
196. CCCCCCCCCCCCCCCCCCCCCCCCCC(=O)O
197. COc1ccc(C[C@]2(c3ccccc3)[C@@H](c3ccccc3)N[C@@H](C)C2)cc1
198. COc1cccc(C(=O)Nc2cccc(C(F)(F)F)c2)c1
199. COc1ccc(NC(=O)NCCc2ccccc2)cc1
200. COc1ccc(CN(C(=O)c2ccc(N(C)C(F)(F)F)cc2)C(C)(C)C(=O)O)cc1
201. COc1ccc2c(c1)C(=O)C(C)(C)N2c1ccc(S(N)(=O)=O)cc1
202. COc1cc(NC(=O)[C@@H](C)NC(=O)c2ccccc2Cl)ccc1C(F)(F)F
203. COc1cc(N2CCN(C(=O)OC(C)(C)C)CC2)ccc1S(C)(=O)=O
204. Cc1cc(C(=O)Nc2cccc(C(F)(F)F)c2)cc(N2CCC(N3CCOCC3)CC2)n1
205. COc1ccc2c(c1)C(=O)/C2=C\c1ccc(C(=O)O)cc1
206. COc1cc2c(cc1OC)C(=O)N(Cc1ccccc1)CC2
207. O=C(O)c1ccccc1-c1ccc2c3[nH]ncc3c(=O)n(CC(F)(F)F)c2c1
208. COc1ccc2c(c1)C(=O)/C(=C/c1ccc(S(N)(=O)=O)cc1)O2

209. O=C(Nc1ccc(N2CCN(C(=O)c3ccc(Cl)c(Cl)c3)CC2)cc1)N1CCOCC1
210. O=C(Nc1ccc(Cl)c(Cl)c1)c1ccc(NS(=O)(=O)c2cccs2)cc1
211. O=C(Nc1ccc(Cl)c(Cl)c1)c1ccc(Cl)c(Cl)c1
212. Cc1cc(-c2ccc3c(c2)OC[C@@H](c2ccccc2C(F)(F)F)[C@@H](O)[C@@H]3O)ccc1C(F)(F)F
213. COc1ccc(NC(=O)/C=C2\C(=O)Nc3ccccc32)cc1
214. COc1cc2c(cc1C(=O)Nc1ccccc1)C(=O)N2
215. O=C(NC1CCN(Cc2ccc(C(F)(F)F)cc2)CC1)c1ccc(F)cc1
216. COc1ccccc1N1CCN(C(=O)c2c(-c3ccccc3)[nH]c3ccccc23)CC1
217. COc1ccccc1N1CCN(CCCNC(=O)c2nc(C)n(-c3ccccc3)c2C)CC1
218. O=C(O)c1ccc(C(=O)OCc2ccccc2)cc1
219. CC(C)(C)c1ccc(NC(=O)Nc2ccc(C(F)(F)F)c2)c1
220. O=C(O)c1ccc(C(F)(F)F)cc1-c1ccc2c(c1)OCO2
221. COc1ccc(C(=O)N2CCC(CNC(=O)c3c(Cl)cc(Cl)cc3Cl)CC2)cc1
222. COc1ccc(S(=O)(=O)Nc2ccc(Cl)c(Cl)c2)cc1
223. CC(C)(C)c1ccc(NC(=O)Nc2ccc(C(F)(F)F)cc2)cc1
224. O=C(N[C@@H]1CC[C@H](N2CCCC2)C1)c1ccc(-c2nc3ccccc3s2)cc1
225. O=C(N[C@@H]1COCC[N+]1)c1ccc(F)cc1
226. COc1ccc(-c2nc(NC(=O)c3ccc(N(C)C)cc3)c3ccc(F)cc3n2)cc1
227. N#Cc1ccc(C(=O)Nc2ccccc2-c2ccccc2)cc1
228. CC(C)(C)c1ccccc1NC(=O)C1CC1
229. O=C(NC1CCCCC1)c1ccc(-c2ccccc2)cc1
230. COc1ccc(NC(=O)Nc2ccc(C(F)(F)F)cc2)cc1
231. COc1ccc2c(c1)C(=O)C(CC1CCCCC1)C2
232. O=C(Nc1ccc(Cl)cc1)N1CCC(C(O)(c2ccc(Cl)cc2)c2ccc(Cl)cc2)CC1
233. O=C(O)c1cc(-c2cncc2)cc(NC2CCN(CCO)CC2)n1
234. Cc1ccccc1N1CCC(CNC(=O)c2ccccc2Cl)CC1
235. O=C(Nc1ccc(Cl)cc1)N1CCC(Nc2nccc(-c3ccccc3)n2)CC1
236. COc1cc(Nc2ncc3c(n2)C(=O)/C3=C\C2ccccc2)cc(OC)c1OC
237. CC(=O)N1CCN(C(=O)N2CCCC2)CC1c1ccc(Cl)cc1Cl
238. O=C(O)C1=C(c2ccccc2)C(=O)N(Cc2ccccc2)C1=O
239. O=C(Nc1ccc(-c2ccccc2)cc1)[C@H]1CCCN(Cc2ccccc2)C1
240. COc1ccccc1C(=O)Nc1ccccc1
241. COc1cc(N2CCN(C)CC2)cc(Nc2ncc(Br)c(N[C@H](C)C(=O)O)n2)c1
242. O=C(Nc1ccc(C(F)(F)F)cc1)[C@H]1C[C@@H]2[C@@H](O)[C@@H](O)[C@H]2O1
243. COc1ccc(NC(=O)Nc2ccc(C(F)(F)F)c2)cc1
244. COc1cc(Nc2nc(Nc3ccc(Cl)c(Cl)c3)nc(Nc3ccc(N4CCN(C)CC4)cc3)n2)ccn1
245. O=C(Nc1ccccc1)N1CCN(Cc2ccccc2)CC1
246. COc1ccc(S(=O)(=O)N2CCN(C(=O)C3CC3)CC2)cc1
247. C[C@]12CC[C@H]3[C@@H](C[C@@H](O)C4CC4)C[C@@H]3[C@@H]1CCC2=O
248. COc1ccc2c(c1)C(C)(C)C2
249. COc1ccccc1NC(=O)CN1CCN(c2nc3ccccc3s2)CC1
250. COc1cc2c(cc1OC)C(=O)C(C(=O)O)C(=O)N2
251. N#Cc1ccc(NC(=O)Nc2ccc(C(F)(F)F)cc2)cc1
252. COc1ccc2c(c1)NC(=O)/C(=C/c1ccc(N(C)C)cc1)C(=O)N2

253. COc1ccc(-c2cc3c(c(=O)n2-c2ccc(F)cc2)CNC3)cc1
254. O=C1NC(=O)c2cc(-c3ccc(O)cc3)ccc2N1c1ccc(Cl)cc1
255. CC(C)(C)OC(=O)N[C@@H]1CCC[C@H]1NC(=O)OCc1ccccc1C(F)(F)F
256. COc1cc(Nc2ncc(C(=O)Nc3cccc(C(F)(F)F)c3)s2)ccc1N1CCN(C)CC1
257. COc1cccc(C(=O)Nc2cccc2C(=O)Nc2ccc(C(=O)O)cc2)c1
258. COc1ccc(Nc2ncc3c(c2)NC(=O)/C3=C\c2ccc(OC)cc2)cc1
259. COc1ccc(C[C@H](C)NC(=O)c2ccccc2)cc1
260. COc1ccc(-c2nn(CC(=O)O)c3ccc(F)cc23)cc1OC
261. NS(=O)(=O)c1ccc(C(=O)NCc2ccc(C(F)(F)F)cc2)cc1
262. COc1ccccc1N1CCN(C(=O)c2cc3ccccc3[nH]2)CC1
263. COc1cc(C(=O)N[C@@H]2CC[C@H](C(=O)O)CC2)ccc1OC
264. CC(C)(C)c1nc(C(=O)Nc2nc(C(F)(F)F)cs2)cs1
265. CC(C)C[C@H](NC(=O)[C@H](Cc1ccccc1)NC(=O)[C@@H]1CCCN1C(=O)[C@H](CCCNC(=N)N)NC(=O)[C@H](CCCN)NC(=O)[C@@H](N)Cc1ccccc1)C(N)=O
266. O=C(O)c1ccc(Cl)cc1S(=O)(=O)Nc1ccc(Cl)cc1
267. O=C(O)C1=C(c2ccc(Oc3ccc(Cl)cc3)cc2)CCC1
268. COc1ccc2c(c1)C(=O)C(C)(C)C(=O)N2c1ccccc1
269. O=S(=O)(c1ccc(Cl)cc1)C1CCN(S(=O)(=O)c2ccccc2)CC1
270. O=C(O)c1ccc(C(=O)Nc2ccc(C(F)(F)F)cc2)cc1
271. O=C(Nc1ccc(Cl)c(Cl)c1)N1CCCC1
272. CCCS(=O)(=O)c1ccc(CN(Cc2ccc(OC)c(OC)c2)CC2CCCC2)cc1
273. O=C(O)c1ccc(NC(=O)Nc2ccc(C(F)(F)F)cc2)cc1
274. O=C(N[C@@H]1C[C@H]2O[C@H](n3cnc4ccccc43)[C@@H](O)[C@@H]2[C@@H]1O)c1ccccc1
275. COc1cc(Nc2ncc(Br)c(Nc3ccc(C(=O)O)cc3)n2)ccc1N1CCN(C)CC1
276. O=C(N[C@H]1CC[C@H](N2CCCC2)[C@H](O)C1)c1ccc(F)cc1
277. COc1ccc2c(c1)C(=O)N(C)/C2=C\c1ccc(/C=C/C(=O)O)cc1
278. COc1ccc(C(=O)Nc2ccc(-c3ccc(OC)cc3)cc2)cc1
279. COc1cccc(C(=O)Nc2cccc2C(=O)Nc2cccc(C(=O)O)c2)c1
280. Cc1cc(C(F)(F)F)ccc1-c1cnc2c(c1)OCO2
281. O=C(O)c1ccc(Nc2nc3cc(Cl)ccc3s2)cc1
282. COc1cc(Nc2ncc3c(n2)C(c2cccc2C(F)(F)F)CC3)ccc1C(N)=O
283. COc1ccc2c(c1)[C@]1(C)CCN(C(=O)OC(C)(C)C)[C@@H]1N2C
284. O=C(N[C@@H](Cc1ccccc1)C(=O)N1CCC[C@H]1c1ccccc1)C(=O)N1CCC[C@H]1c1ccccc1
285. COc1cc(-c2cnc(N)s2)cc(C(=O)O)c1
286. CC(C)(C)c1ccc(NC(=O)c2ccccc2)cc1
287. CC(C)(C)c1ccc(NC(=O)Nc2ccc(-c3cnc(N)nc3)cc2)cc1
288. COc1cc(-c2ccc(OC)cc2)cc(-c2ccccc2)c1
289. COc1ccc(-c2ccc(C(=O)O)c(C)c2)cc1
290. O=C(O)c1cc(-c2ccccc2)cc(-c2ccccc2)c1
291. CCCCCCCCCCCCCCNC(=O)[C@@H]1O[C@@H](C(=O)N[C@H]2CCC(C)(C)C2)[C@H](O)[C@H]1O
292. NS(=O)(=O)c1ccc(NC(=O)c2ccccc2)cc1
293. COC(=O)c1cccc(NC(=O)C2(N)CCN(c3cccc(Cl)c3)CC2)c1
294. CC(C)(C)OC(=O)Nc1ccc(S(=O)(=O)Nc2cccc(Cl)c2)cc1

295. CC(C)C[C@H]1NC(=O)[C@H](Cc2ccccc2)NC(=O)[C@H](Cc2ccccc2)NC(=O)[C@H](Cc2ccccc2)NC(=O)[C@H](Cc2ccccc2)NC1=O
296. C[C@@H]1C[C@H]2O[C@@](C)([C@@H]1OC)n1c3ccccc3c3c4c(c5c6ccccc6n2c5c31)C(=O)NC4
297. Cc1ccc(-c2ccc(C(=O)Nc3ccc(C(=O)N(C)C)cc3)cc2)cc1
298. COC(=O)c1ccc(Sc2cnc(C(=O)N3CCN(c4ccccc4)CC3)o2)cc1
299. O=c1[nH]c2ccccc2[nH]1
300. O=C(Nc1cc(-c2ccc3c(c2)OCO3)ccc1O)c1ccc(F)cc1
301. O=C(NO)c1ccc2c(Nc3ccc(Cl)cc3)ncnc2c1
302. C[C@]12CC[C@H]3c4cc(Cl)ccc4CC[C@H]3[C@@H]1CC[C@@H]2NS(=O)(=O)c1ccccc1
303. CC(C)C[C@H]1O[C@@H](O)[C@@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H]1O
304. COc1ccc(-c2nc3nc(-c4ccc(OC)cc4)oc3n3ccnc23)cc1
305. COc1ccc2[nH]cc(CCN3CCC(c4ccccc4)CC3)c2c1
306. O=C(O)C[C@H]1[C@@H](O)CO[C@H]1[C@@H](O)CC[C@@]1(O)CC[C@@H](O)[C@H]1O
307. COc1ccc(C(=O)N[C@@H]2C[C@@H](O)[C@@H](O)[C@@H]2O)cc1
308. Cc1cc(-c2cc(C(F)(F)F)nc(-c3ccc4c(c3)OCO4)n2)nc(-c2ccc(Cl)c(Cl)c2)n1
309. COc1ccc(-n2nnnc2C)cc1-c1ccc(S(=O)(=O)N2CCCCC2)cc1
310. CC(C)(C)c1ccc(S(=O)(=O)N2CCN(c3ccccc3)CC2)cc1
311. CC(C)(C)c1cnc(C2CC2)nc1
312. COc1ccc(-c2nc(C(=O)Nc3ccc(OC)cc3)[nH]c2-c2ccc(OC)cc2)cc1
313. O=C1NC(=O)/C(=C/c2cnn3c(N4CCNCC4)cc(-c4ccc(C(F)(F)F)cc4)cc23)N1
314. CS(=O)(=O)c1ccc(NC(=O)NC2CCCC2)cc1
315. CC(C)(C)OC(=O)N1CCC(c2cc(-c3ccc4nc(-c5nnc(N)o5)[nH]c4c3)ccc2C#N)CC1
316. COc1ccc(S(=O)(=O)N2CCN(C(=O)c3ccc(C(F)(F)F)cc3)CC2)cc1
317. CN1C(=O)[C@]2(C)Oc3ccccc3N(C)C12
318. O=C(Nc1ccc(-c2ccccc2)cc1)c1ccc(O)cc1
319. CC(C)(C)OC(=O)N1CC=C(c2c[nH]c3ncc(Cl)cc23)CC1
320. O=C(Nc1cc(-c2ccccc2)ncn1)c1ccccc1
321. COc1cc(-c2ccncc2)cc(C(=O)O)c1
322. O=C(O)c1ccc(Nc2nccc(-c3cccc(N4CCOCC4)c3)n2)cc1
323. COc1ccc(C(=O)Nc2ccc(C(=O)O)cc2)c(Oc2ccc(Cl)cc2)c1
324. O=C(O)c1ccc(-c2ccc(-c3ccc(F)cc3)cc2)cc1
325. COc1ccc(NC(=O)N[C@@H]2Cc3ccccc3O2)cc1
326. COc1cc2c(cc1OC)C(=O)C1=C(C(=O)O)C(C(=O)N(C)C)CC1C2
327. O=C(O)c1ccc(C2CC2)cc1-c1ccc2c(c1)CCCC2
328. O=C(O)c1ccc(-c2ccc3c(-c4ccccc4)c[nH]c3c2)cc1
329. CN1CCN(c2ccc(-c3c(-c4ccccc4)c[nH]c3-c3ccccc3)cc2)CC1
330. O=C(N[C@@H]1C[C@@H](O)[C@H]1OCc1ccc(F)cc1)c1ccc(Cl)cc1
331. O=C(N[C@@H]1CC[C@H]1OCc1ccccc1)c1ccccc1
332. O=C(N[C@@H]1C[C@H](O)CC[C@@H]1OCc1ccccc1)c1ccccc1
333. O=C(Nc1ccc(F)cc1)Nc1ncc(Cl)c(Nc2ncnc3ccccc23)n1
334. O=C(NCC#Cc1ccc2ncnc(Nc3ccccc3)c2c1)c1ccc(F)c1
335. O=C(N[C@@H]1CNC[C@H]1O)c1ccc2c(c1)[nH]c1ccccc12
336. O=C(N[C@@H](Cc1ccccc1)C(=O)Nc1ccccc1)c1ccccc1
337. COc1ccc(-c2nc([C@H]3CC[C@H](NC(=O)C4CCCC4)CC3)c(C(F)(F)F)[nH]2)cc1

338. O=C(O)c1ccc2c(c1)C(c1ccccc1)CCC2
339. CC(C)(C)c1ccc(C(=O)NCCCN2CCN(c3nc4ccccc4s3)CC2)cc1
340. CC(C)(C)OC(=O)c1ccc(-c2ccc(C(F)(F)F)nc2)cc1
341. O=C(N[C@@H]1C[C@H](O)CN1)c1cc(F)c(F)c(F)c1
342. Cc1cc(-c2ccc(F)c(F)c2)c(-c2ccc(F)c(C(F)(F)F)c2)o1
343. COc1cc2c(cc1OC)C(=O)N(C)C(=O)N2
344. O=c1[nH]c(=O)[nH]c2ccccc12
345. CN1CCN(c2ccc(C(=O)Nc3ccc(Cl)cc3Cl)cc2)CC1
346. CC(C)(C)c1ccc(S(=O)(=O)N2CCN(c3nc4ccccc4[nH]3)CC2)cc1
347. COc1cc(C(=O)Nc2ncc(-c3ccc(C(=O)O)cc3)s2)ccc1Cl
348. CN1CCN(c2ccc(C(F)(F)F)cc2)CC1
349. CCCCCCCCCCCCCCCCCCP(=O)([O-])O[N-]
350. COc1cc2c(cc1OC)C(=O)N(C)c1ccc(-c3ccc(C(F)(F)F)cc3)cc1C2
351. O=C1CC2(CCCC2)[C@@H](O)[C@@H]1O
352. CC(C)[C@H]1NC(=O)[C@H](CC(=O)O)NC(=O)[C@H](Cc2ccccc2)NC(=O)[C@H](Cc2ccccc2)NC(=O)[C@H](Cc2ccccc2)NC(=O)[C@H](Cc2ccccc2)NC1=O
353. COc1ccc(-c2cc(C(=O)O)ccc2Cl)cc1
354. CC(C)(C)c1ccc(NC(=O)c2ccc(-c3ccccc3C(=O)O)cc2)cc1
355. CC(C)C[C@H](NC(=O)[C@H](Cc1ccccc1)NC(=O)[C@H](CC(=O)O)NC(=O)[C@H](Cc1ccccc1)NC(=O)OCc1ccccc1)C(=O)O
356. CC(C)(C)c1ccc(-c2ccccc2C(=O)O)cc1
357. O=C(NC1CC1)c1ccc(Nc2ncc3ccc(Cl)cc3n2)cc1
358. COc1ccc(C(=O)Nc2ccc(C(F)(F)F)cc2)cc1C(=O)Nc1ccc(C(F)(F)F)cc1
359. Cc1cc(C(F)(F)F)cc(C(F)(F)F)c1C(=O)N[C@@H]1CCCC[C@H]1Nc1ccccc1
360. CC(C)(C)OC(=O)N[C@H](Cc1ccccc1)C(=O)N[C@@H](CCN=C(N)N)C(=O)O
361. CC(C)C[C@@H]1O[C@@H](c2ccccc2)[C@H](O)[C@@H]1O
362. Cc1cc(Cl)cc(Cl)c1C(=O)N[C@H]1CC[C@@H](CO)O1
363. O=C(N[C@@H]1CC[C@H](O)[C@H]1OC(=O)[C@H](Cc1ccccc1)NC(=O)OCc1ccccc1)C(F)(F)F
364. O=C(O)c1ccc(-c2ccc3c(c2)OCO3)cc1
365. COc1cc2c(cc1O)CCC2=O
366. CC(C)(C)OC(=O)N[C@@H]1C[C@H](Oc2ccc(-c3ccccc3C(=O)O)cc2)C[C@H]1O
367. CC(C)(C)OC(=O)c1ccc(NC(=O)[C@H]2CC[C@H](NC(=O)[C@H]3C[C@@H](N)CC3)CC2)cc1
368. O=C(Nc1ccc(Oc2ccc(O)cc2)cc1)c1ccccc1
369. O=C(c1ccc(Cl)cc1)N1CCN(C2CCCC2)CC1
370. CCCCCCCCCCCCCCCCCCP(=O)(O)O
371. O=C(O)c1ccc(Cc2cc(Cc3ccccc3)[nH]n2)cc1
372. COc1cc(NC(=O)[C@@H](Cc2ccc(OC)cc2)NC(=O)c2ccccc2)ccn1
373. COc1cc(N2CCC(N(C)C)CC2)ccc1Nc1ncc(Cl)c(Cl)c1Cl
374. COc1ccc(S(=O)(=O)Nc2ccc(C(F)(F)F)cc2)cc1
375. COc1cc(Nc2c(C#N)cnc3cc(OC)c(O)cc23)cc(OC)c1OC
376. COc1cc(COc2ccc([C@@H](O)C(=O)O)cc2)cc(C(=O)O)c1O
377. CC(C)(C)OC(=O)N[C@@H](Cc1c[nH]c2ccccc12)C(=O)N[C@@H](C(=O)O)C(C)C
378. COc1ccc(NC(=O)c2cncc(N)n2)cc1Cl
379. c1ccc2c(N3CCNCC3)nccc2c1

380. CC(=O)N[C@@H]1CC[C@H]2O[C@@](C)([C@@H]1OC)n1c3cccc3c3c4c(c5c6cccc6n2c5c31)C(=O)NC4

381. O=C(N[C@H]1CC[C@H](c2cccc2)CC1)c1ccc(N2CCOCC2)nc1

382. COc1cc(C(=O)Nc2ccc([N+](=O)[O-])c([N+](=O)[O-])c2)c(OC)c(OC)c1OC

383. Cc1cnc(C(=O)Nc2cc(C(F)(F)F)cc(C(F)(F)F)c2)c(C)c1

384. CC(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](Cc1cccc1)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C(C)C)C(=O)O

385. COc1ccc(S(=O)(=O)N2CCN(C(=O)OCc3ccc(Cl)cc3)CC2)cc1

386. COc1ccc(S(=O)(=O)N2CCC(Oc3ccc(Cl)cc3)CC2)cc1

387. O=C(O)[C@H](Cc1cccc1)[C@H](O)C(=O)N(Cc1ccc(Cl)cc1)C1CC1

388. O=C(Nc1cc(-c2ccc(O)cc2)nc2cccc12)c1cccc1

389. CC(=O)N[C@@H](Cc1cccc1)C(=O)N[C@@H](Cc1cccc1)C(=O)N[C@@H](CC(C)C)C(=O)O

390. COC(=O)[C@H](Cc1cccc1)NC(=O)[C@H](Cc1c[nH]c2cccc12)NC(=O)[C@H](Cc1c[nH]c2cccc12)NC(=O)OC(C)C

391. CC(C)(C)c1cc(C(=O)N[C@@H](CC(=O)O)C(=O)N[C@@H](CC2CCCC2)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](CC(C)C)C(=O)O)ccc1Cl

392. O=C(O)c1c(-c2cccc2)c2cccc2n1C1CC1

393. COc1ccc2c(c1)C(c1cccc1)=NCCN2

394. COC(=O)c1ccc(NC(=O)Nc2ccc([N+](=O)[O-])cc2)cc1

395. COc1ccc(S(=O)(=O)Nc2cccc(C(=O)O)c2)cc1OC

396. COc1cc(N2CCOCC2)cc(C)c1-n1c(C)nnc1C

397. CCOC(=O)c1ccc(NC(=O)N[C@@H](CC2CCCC2)C(=O)O)cc1

398. CCN(C)C/C=C/C(C)=C/C(=O)OC(C)C

399. COc1ccc(S(=O)(=O)N2CCC[C@H]2C(=O)N(C)C)cc1OC

400. COc1ccc(S(=O)(=O)N(Cc2cccc2)c2cccc2)cc1

401. Cc1ccc(NC(=O)C(C)(C)C)cc1-c1ccc(S(=O)(=O)Nc2cccc2C(F)(F)F)cc1

402. COc1cc(NC(=O)c2ccc(OC(F)(F)F)cc2)cc2c1O[C@@H]1O[C@@H](C(F)(F)F)[C@@H](O)[C@]12C

403. COc1ccc(-c2cc(C(=O)O)cc(C(=O)O)c2)cc1C(=O)O

404. C[C@@H]1C[C@H]2C[C@H](CC[C@@H]3[C@@H](O)CC[C@@H]32)[C@H]2C[C@@H]1CC[C@]2(C)C

405. CN(C)C(=O)c1ccc2c(c1)Nc1cccc1C2=O

406. CC(=O)N[C@@H](Cc1cccc1)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](Cc1cccc1)C(=O)O

407. C[C@]12O[C@H](C[C@]1(O)CO)n1c3cccc3c3c4c(c5c6cccc6n2c5c31)C(=O)NC4

408. COc1cc(Nc2ncnc3cc(-c4ccc(OC)cc4)[nH]c23)cc(OC)c1OC

409. O=C(O)c1ccc(C(=O)N2CCC(CCc3cccc3)CC2)cc1

410. CCCCCCCCCCCC(=O)C(F)(F)F

411. N#Cc1ccc2c(C3CC3)n[nH]c2c1

412. Cc1cc(NC(=O)c2ccc(Cl)cc2)c2cccc2n1

413. CC(C)[C@H](NC(=O)[C@@H](Cc1cccc1)NC(=O)OCc1cccc1)C(=O)N[C@@H](CC1CCCC1)C(=O)O

414. Cc1nc2cccc2c2c(=O)[nH]c12

415. COc1ccc(-c2ccc(N3CCC(C(=O)O)CC3)cc2)cc1

416. O=C1c2cccc2C(=O)N1CC1CCN(Cc2ccc(C(F)(F)F)cc2)CC1

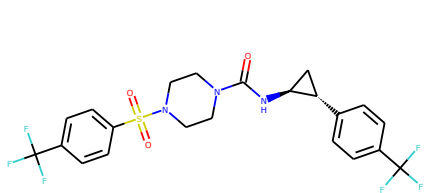
417. COc1cccc(-c2cc(COc3ccc4c(c3)OCO4)c(CO)c(OC)c2OC)c1

418. Cc1nnc(N2CCC(N3CCN(C)CC3)CC2)c(N2CCN(C(=O)Nc3cccc(Cl)c3Cl)CC2)n1

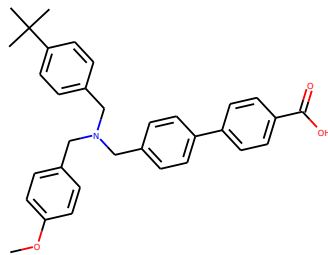
419. COc1ccc(-c2nc(N3CCN(C)CC3)c(C(=O)O)[nH]2)cc1
 420. COc1ccc(C=C(N3CCN(C(=O)OC)CC3)C(=O)OC2c2ccccc2C(=O)O)cc1
 421. C[C@@H]1OC(=O)n2c(C#N)cnc2Nc2ccc(Cl)cc2S(=O)(=O)N1C
 422. C[C@H]1C[C@@H](NC(=O)c2ccc(OC(F)(F)F)c(C(F)(F)F)c2)[C@H](c2ccc(Cl)cc2)C1
 423. COc1cccc(NC(=O)[C@H](Cc2ccccc2)NC(=O)[C@H](Cc2ccccc2)NC(=O)OCc2ccccc2)c1
 424. O=C(O)c1ccc2c(O)cccc2c1O
 425. CC(C)[C@@H](Oc1ccccc1)C(=O)N1CCCCC1
 426. Cc1cc(C(=O)N[C@@H](Cc2ccccc2)C(=O)N[C@H](Cc2ccccc2)C(=O)N[C@H](C(=O)O)C(C)C)cc(O)c1O
 427. COc1cc(NC(=O)c2ccccc(-c3ccc4c(c3)OCO4)c2)cc(OC)c1OC
 428. COc1cc(-c2cc(N3CCN(C)CC3)ccc2O)ccc1OCCO
 429. O=C1Nc2c(Cl)cccc2C(=O)Nc2ccc(Cl)c(Cl)c21
 430. Cc1ccc(NC(=O)c2ccc(C(C)C)cc2C(=O)Nc2ccccc2C(C)C)cc1
 431. COc1ccc(C(=O)Nc2cccc(C(=O)Nc3cccc(C(=O)O)c3)c2)cc1
 432. COC(=O)c1cc(Cn2c(=O)n(Cc3ccccc3)c3ccccc3c2=O)ccn1
 433. CC(C)[C@H](O)[C@H](C)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](Cc1ccccc1)NC(=O)OC(C)C
 434. C[C@]12CC[C@@H]3c4ccc(O)cc4CC[C@H]3[C@@H]1CCC2=O
 435. COc1ccc(C[C@H]2CC[C@H](NC(=O)c3ccc(C(C)(C)C)cc3)CC2)cc1
 436. COc1cc(N2CCN(C3CCCCC3)CC2)c2ncn(C3CCCCC3)c2c1
 437. CCCN(CCC)C(=O)C(C)(C)NC(=O)OCc1ccccc1
 438. CC(=O)N1CCC(NC(=O)C2(NC(=O)[C@@H](Cc3ccccc3)NC(=O)c3ccccc3Cl)CC2)CC1
 439. CCCNC(=O)c1ccc(C(=O)Nc2cccc([N+](=O)[O-])c2)cc1
 440. COc1c(N)ncnc1N1CCC(c2nc(-c3ccc(F)c(C(F)(F)F)c3)cn2CCN2CCCC2)CC1
 441. CN(C)C(=O)C1CCN(Cc2ccc(OC(=O)Nc3ccccc3)cc2)CC1
 442. Cc1cc(N2CCOCC2)ccc1-c1nc2ccccc2[nH]1
 443. CN(C)C(=O)c1cccc(-c2ccc(N3CCN(c4ncnc5ccccc45)CC3)nc2)c1
 444. COc1cc(-c2ccc(NC(=O)C3CC3)cc2)ccc1OCCN1CCOCC1
 445. CC(=O)N[C@@H](Cc1ccccc1)C(=O)N[C@H](Cc1ccccc1)CP(=O)(O)O
 446. COc1ccc(Cc2c(O)c(O)c(O)c2O)cc1
 447. CC(=O)N[C@@H](Cc1ccccc1)C(=O)N[C@H](Cc1ccccc1)C(=O)O
 448. CC(C)[C@@H](O)[C@H](Cc1ccc(Cl)c(Cl)c1)c1ccc(C2CC2)cc1
 449. CCN(CC)CCNC(=O)c1c(C)[nH]c(/C=C\C(=O)Nc3ccc(F)cc32)c1C
 450. N[C@@H]1C[C@H]2O[C@@](C)([C@@H]1OC)n1c3ccccc3c3c4c(c5c6ccccc6n2c5c31)C(=O)NC4
 451. COc1ccc(S(=O)(=O)N2CCN(Cc3ccccc3)CC2)cc1
 452. COc1cc(C(=O)N2CCC(C(=O)O)CC2)ccc1-c1ccc(OC)cc1
 453. CN(C)CCCNC(=O)c1cc(-c2ccc(Oc3ccccc3)cc2)[nH]n1
 454. CN1CCN(c2ccc(-c3c[nH]c4ccccc34)cc2)CC1
 455. CNC(=O)c1c(C)c2ccccc2n1CC(=O)NC1CCN(CCCc2c[nH]c3ccccc23)CC1

Supplementary Table S1. SMILES representation for generated compounds.

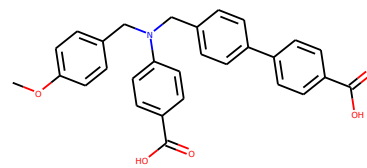
Graph representation of all the generated molecules



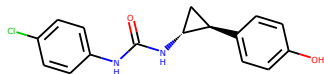
Generated molecule 1



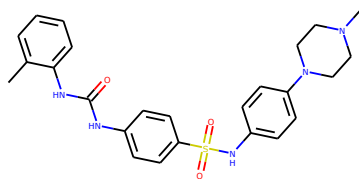
Generated molecule 2



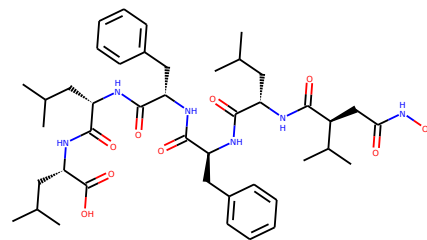
Generated molecule 3



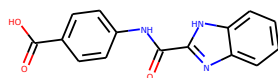
Generated molecule 4



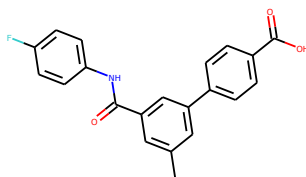
Generated molecule 5



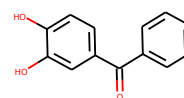
Generated molecule 6



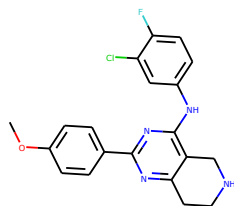
Generated molecule 7



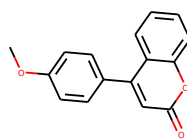
Generated molecule 8



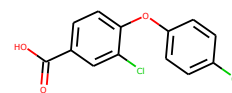
Generated molecule 9



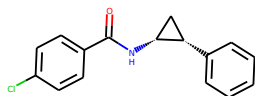
Generated molecule 10



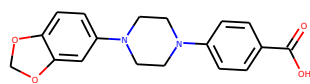
Generated molecule 11



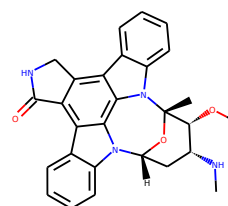
Generated molecule 12



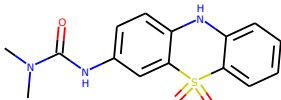
Generated molecule 13



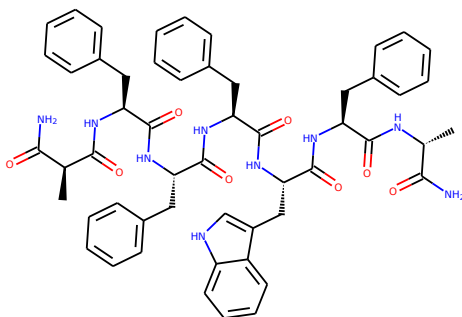
Generated molecule 14



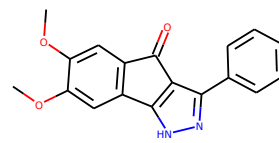
Generated molecule 15



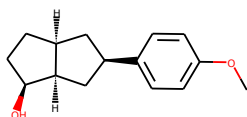
Generated molecule 16



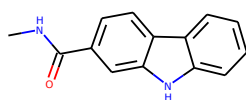
Generated molecule 17



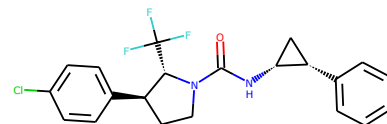
Generated molecule 18



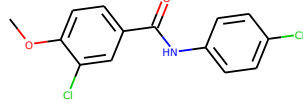
Generated molecule 19



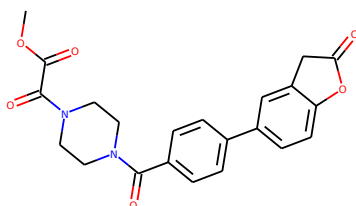
Generated molecule 20



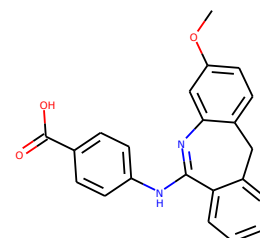
Generated molecule 21



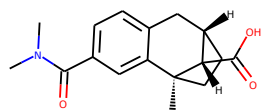
Generated molecule 22



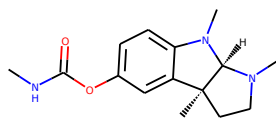
Generated molecule 23



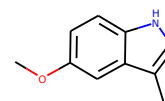
Generated molecule 24



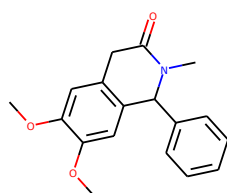
Generated molecule 25



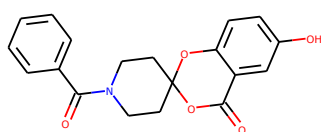
Generated molecule 26



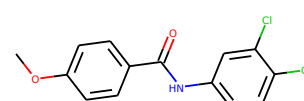
Generated molecule 27



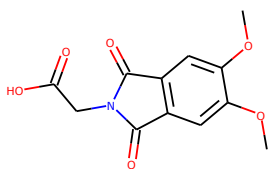
Generated molecule 28



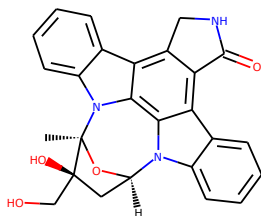
Generated molecule 29



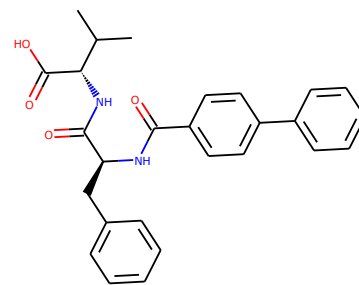
Generated molecule 30



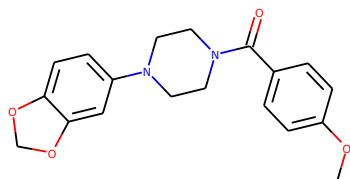
Generated molecule 31



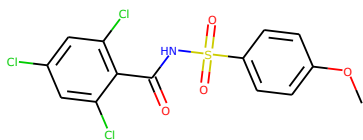
Generated molecule 32



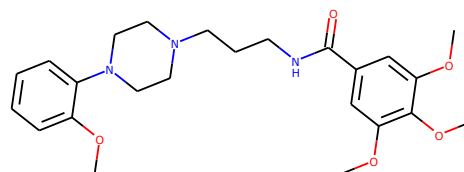
Generated molecule 33



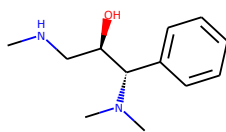
Generated molecule 34



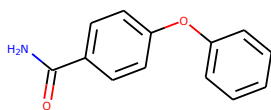
Generated molecule 35



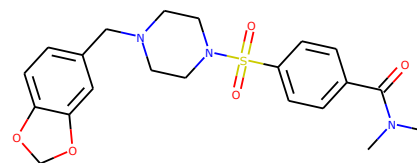
Generated molecule 36



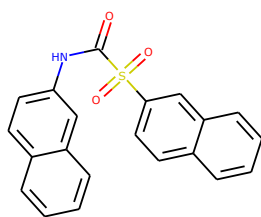
Generated molecule 37



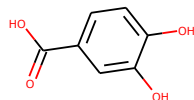
Generated molecule 38



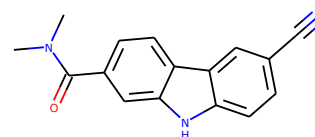
Generated molecule 39



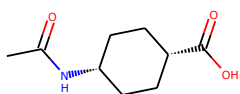
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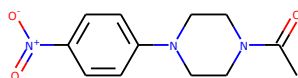
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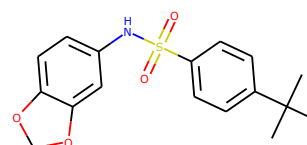
Generated molecule 42



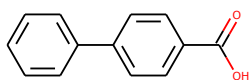
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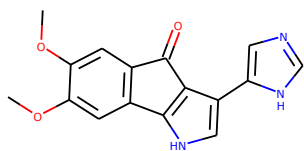
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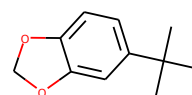
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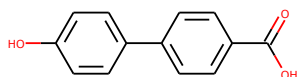
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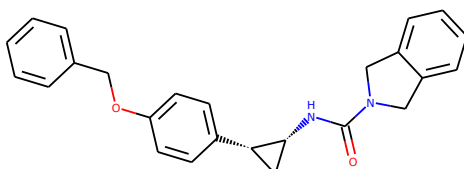
Generated molecule 47



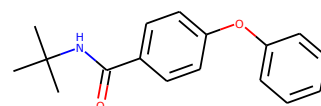
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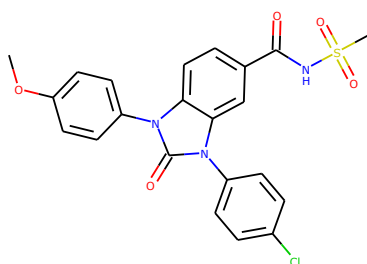
Generated molecule 49



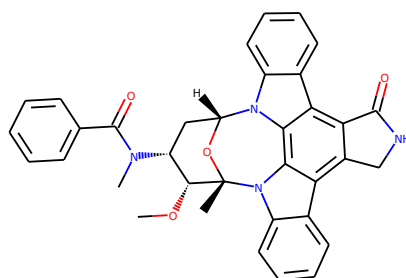
Generated molecule 50



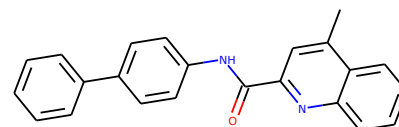
Generated molecule 51



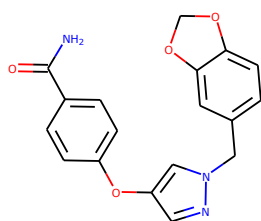
Generated molecule 52



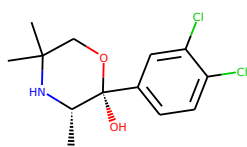
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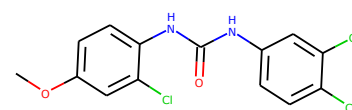
Generated molecule 54



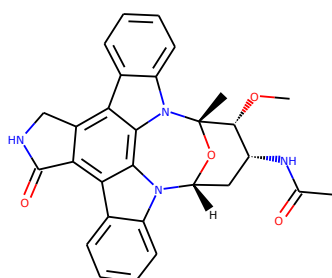
Generated molecule 55



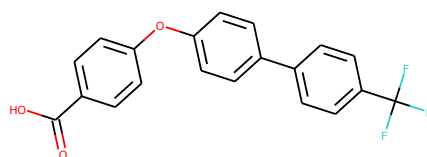
Generated molecule 56



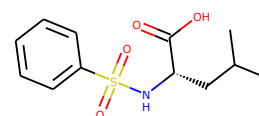
Generated molecule 57



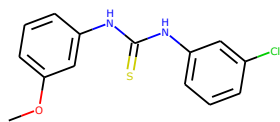
Generated molecule 58



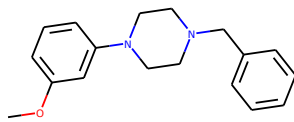
Generated molecule 59



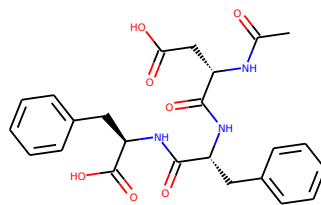
Generated molecule 60



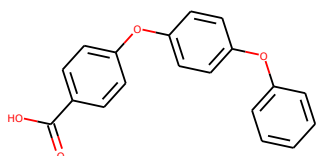
Generated molecule 61



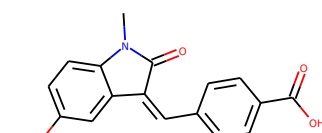
Generated molecule 62



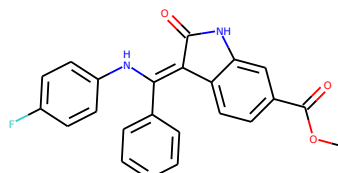
Generated molecule 63



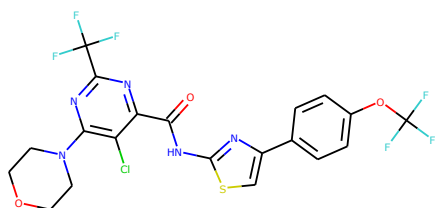
Generated molecule 64



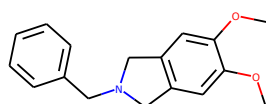
Generated molecule 65



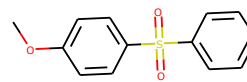
Generated molecule 66



Generated molecule 67



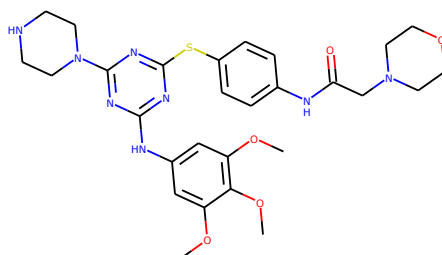
Generated molecule 68



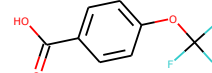
Generated molecule 69



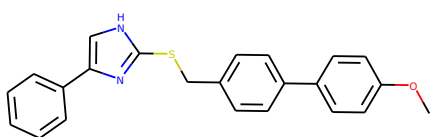
Generated molecule 70



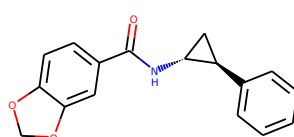
Generated molecule 71



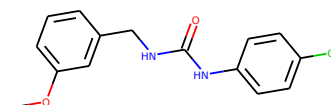
Generated molecule 72



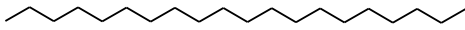
Generated molecule 73



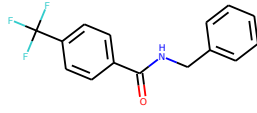
Generated molecule 74



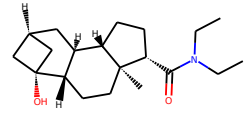
Generated molecule 75



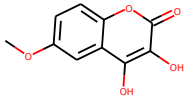
Generated molecule 76



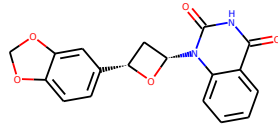
Generated molecule 77



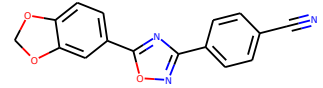
Generated molecule 78



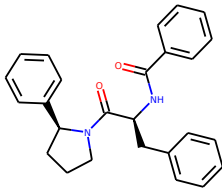
Generated molecule 79



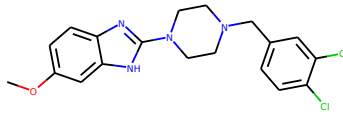
Generated molecule 80



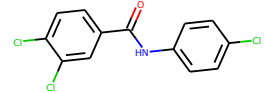
Generated molecule 81



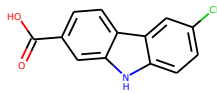
Generated molecule 82



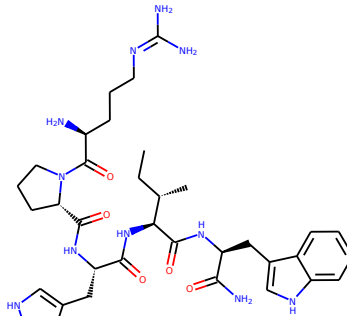
Generated molecule 83



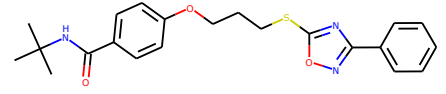
Generated molecule 84



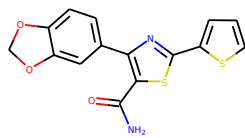
Generated molecule 85



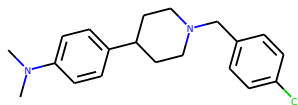
Generated molecule 86



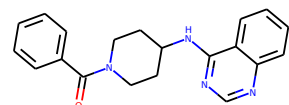
Generated molecule 87



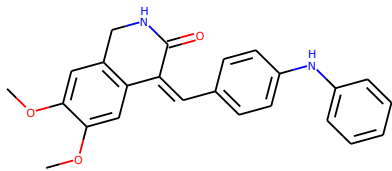
Generated molecule 88



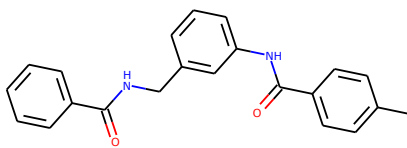
Generated molecule 89



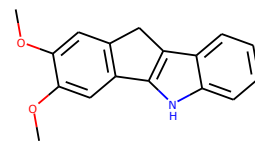
Generated molecule 90



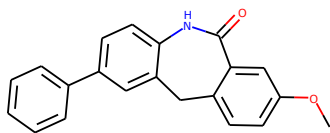
Generated molecule 91



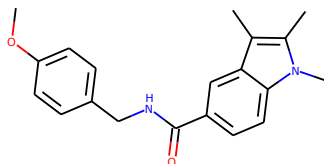
Generated molecule 92



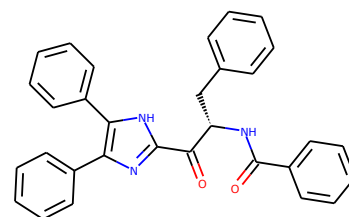
Generated molecule 93



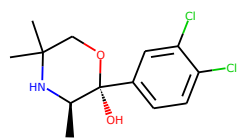
Generated molecule 94



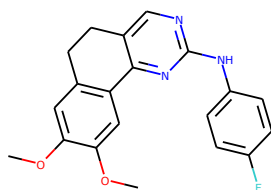
Generated molecule 95



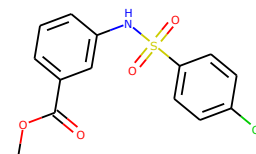
Generated molecule 96



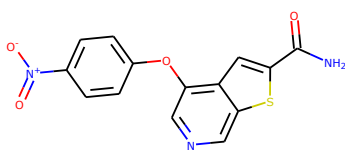
Generated molecule 97



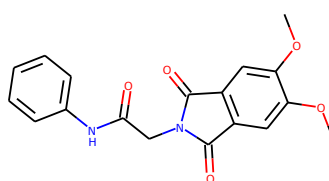
Generated molecule 98



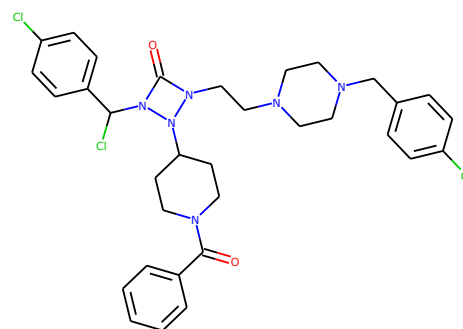
Generated molecule 99



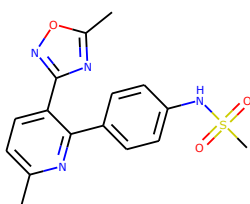
Generated molecule 100



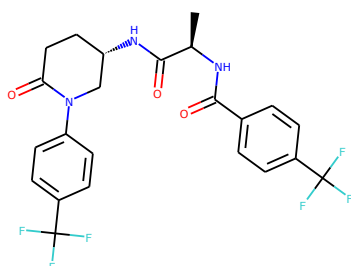
Generated molecule 101



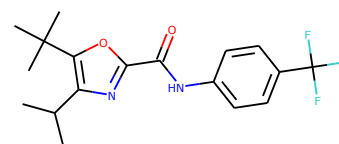
Generated molecule 102



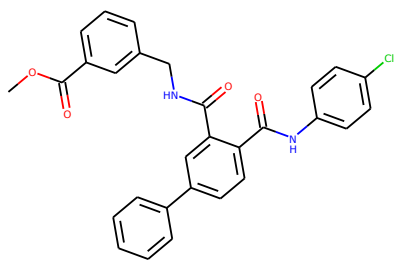
Generated molecule 103



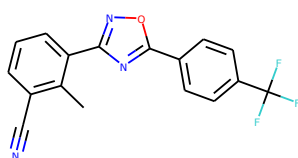
Generated molecule 104



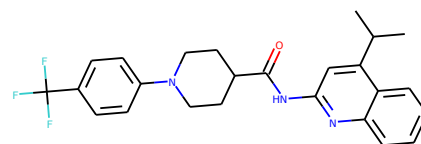
Generated molecule 105



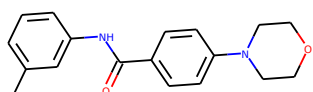
Generated molecule 106



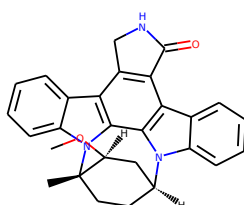
Generated molecule 107



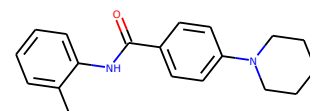
Generated molecule 108



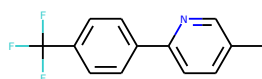
Generated molecule 109



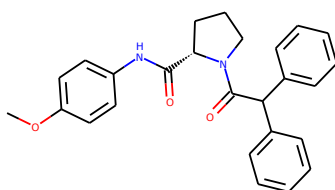
Generated molecule 110



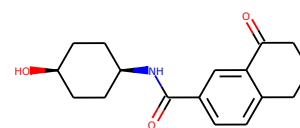
Generated molecule 111



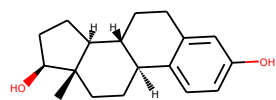
Generated molecule 112



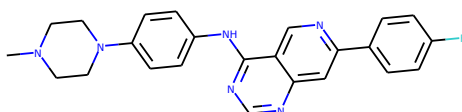
Generated molecule 113



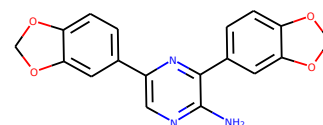
Generated molecule 114



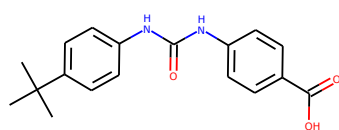
Generated molecule 115



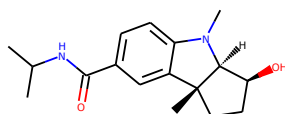
Generated molecule 116



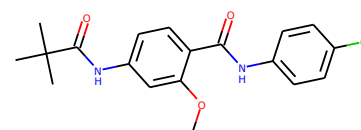
Generated molecule 117



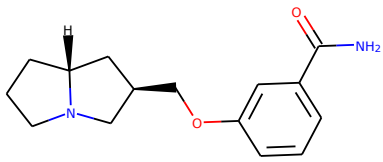
Generated molecule 118



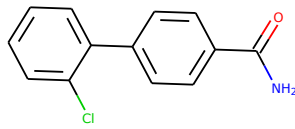
Generated molecule 119



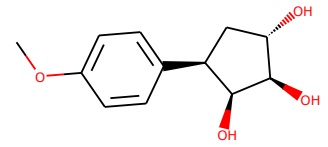
Generated molecule 120



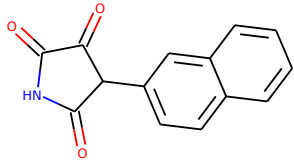
Generated molecule 121



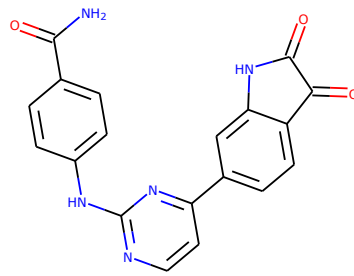
Generated molecule 122



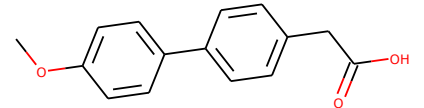
Generated molecule 123



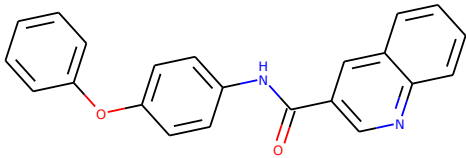
Generated molecule 124



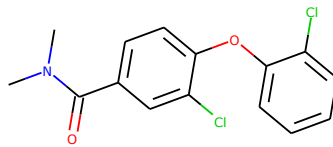
Generated molecule 125



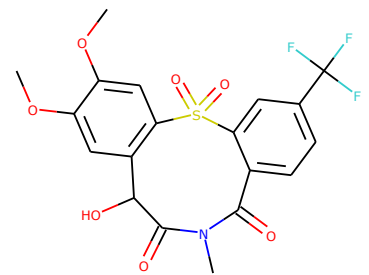
Generated molecule 126



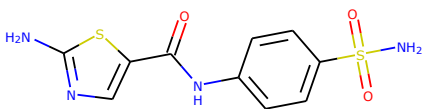
Generated molecule 127



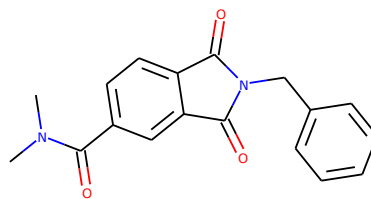
Generated molecule 128



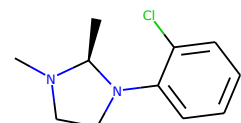
Generated molecule 129



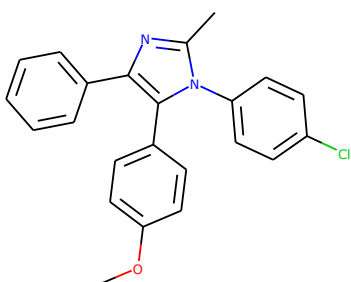
Generated molecule 130



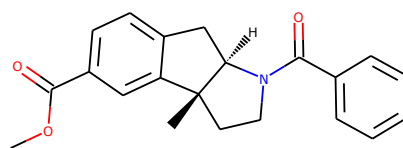
Generated molecule 131



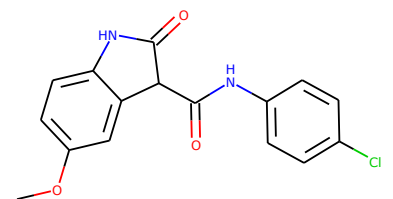
Generated molecule 132



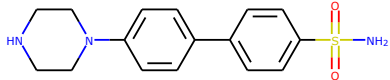
Generated molecule 133



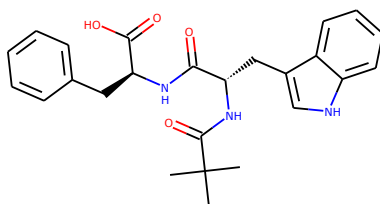
Generated molecule 134



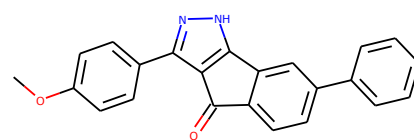
Generated molecule 135



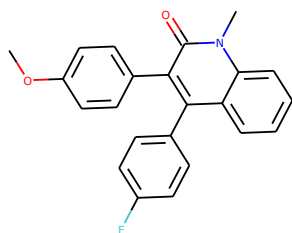
Generated molecule 136



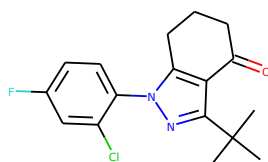
Generated molecule 137



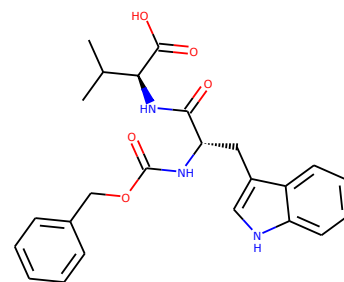
Generated molecule 138



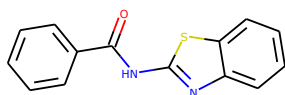
Generated molecule 139



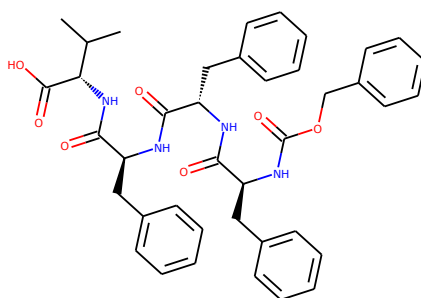
Generated molecule 140



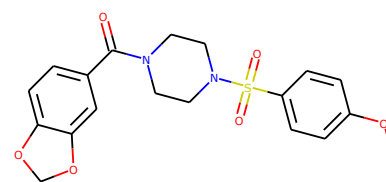
Generated molecule 141



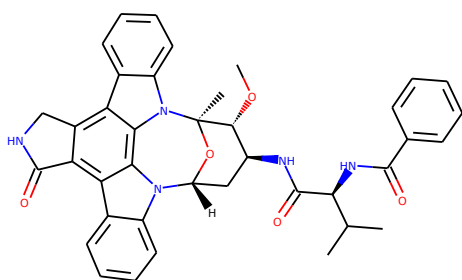
Generated molecule 142



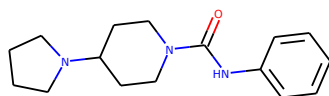
Generated molecule 143



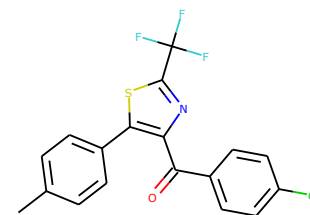
Generated molecule 144



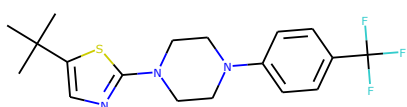
Generated molecule 145



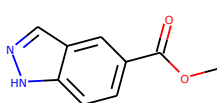
Generated molecule 146



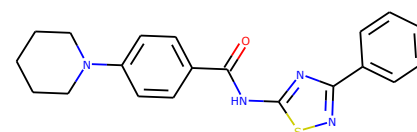
Generated molecule 147



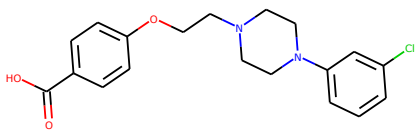
Generated molecule 148



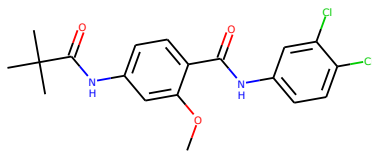
Generated molecule 149



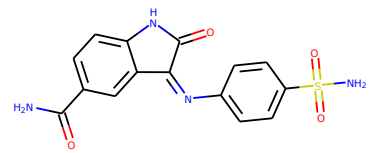
Generated molecule 150



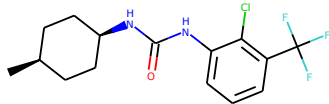
Generated molecule 151



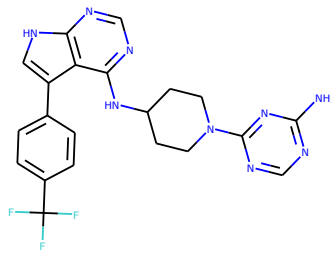
Generated molecule 152



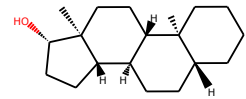
Generated molecule 153



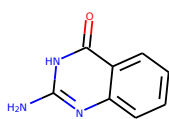
Generated molecule 154



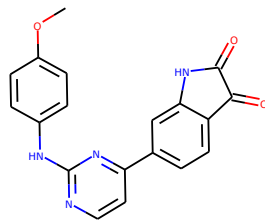
Generated molecule 155



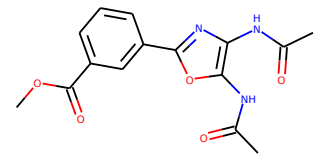
Generated molecule 156



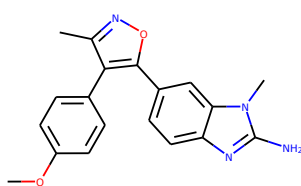
Generated molecule 157



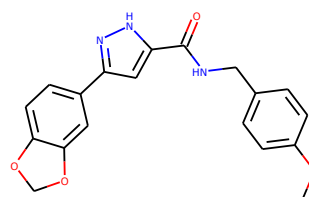
Generated molecule 158



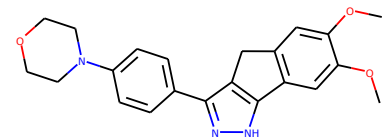
Generated molecule 159



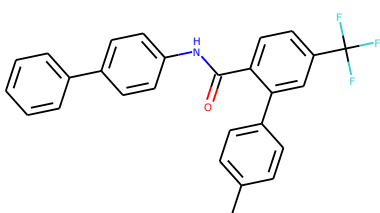
Generated molecule 160



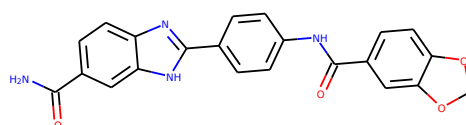
Generated molecule 161



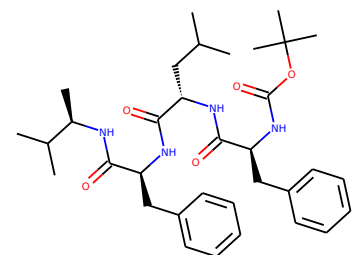
Generated molecule 162



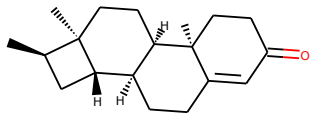
Generated molecule 163



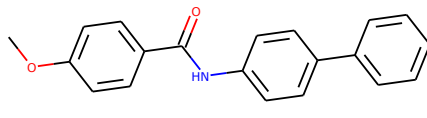
Generated molecule 164



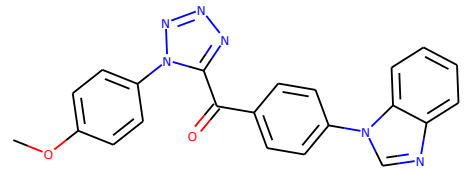
Generated molecule 165



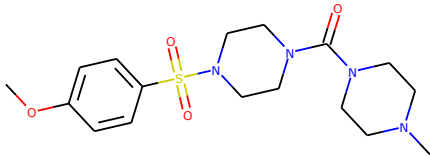
Generated molecule 166



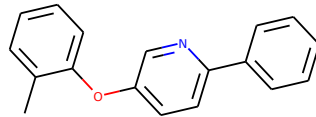
Generated molecule 167



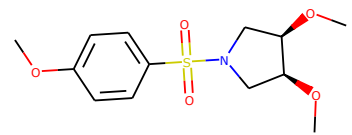
Generated molecule 168



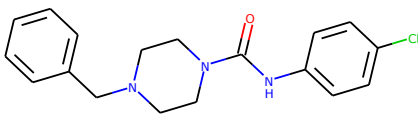
Generated molecule 169



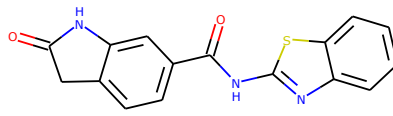
Generated molecule 170



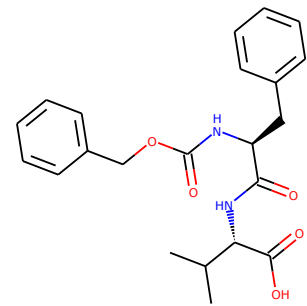
Generated molecule 171



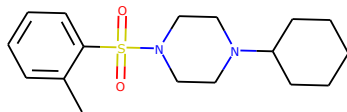
Generated molecule 172



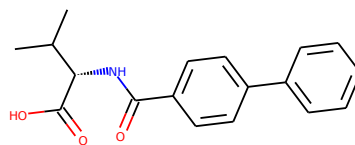
Generated molecule 173



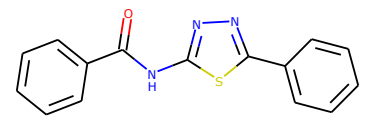
Generated molecule 174



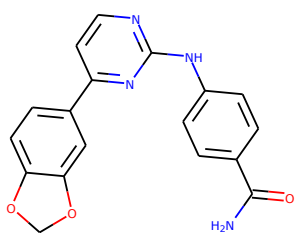
Generated molecule 175



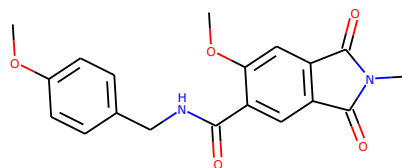
Generated molecule 176



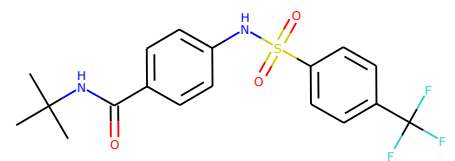
Generated molecule 177



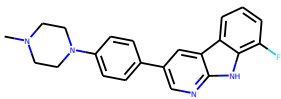
Generated molecule 178



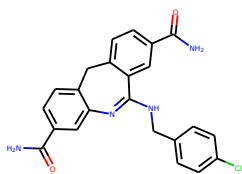
Generated molecule 179



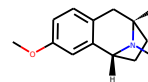
Generated molecule 180



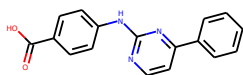
Generated molecule 181



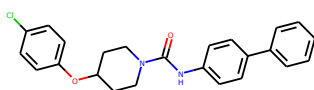
Generated molecule 182



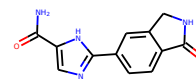
Generated molecule 183



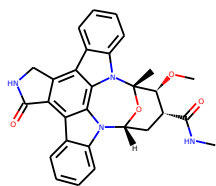
Generated molecule 184



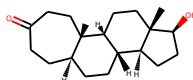
Generated molecule 185



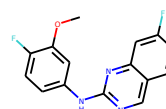
Generated molecule 186



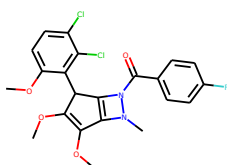
Generated molecule 187



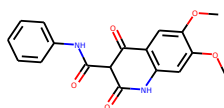
Generated molecule 188



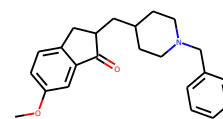
Generated molecule 189



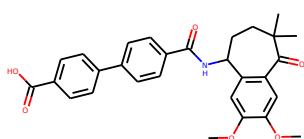
Generated molecule 190



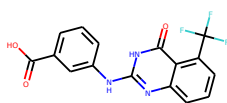
Generated molecule 191



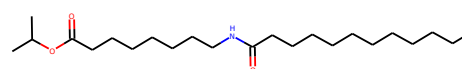
Generated molecule 192



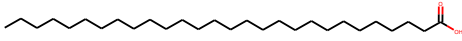
Generated molecule 193



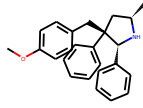
Generated molecule 194



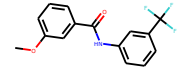
Generated molecule 195



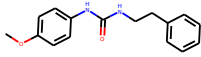
Generated molecule 196



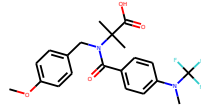
Generated molecule 197



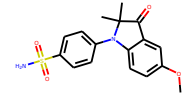
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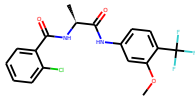
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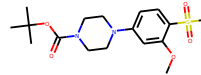
Generated molecule 200



Generated molecule 201



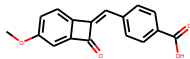
Generated molecule 202



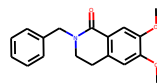
Generated molecule 203



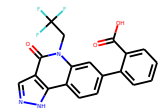
Generated molecule 204



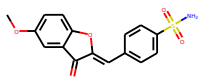
Generated molecule 205



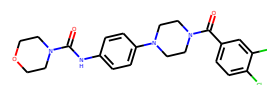
Generated molecule 206



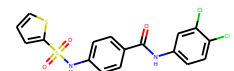
Generated molecule 207



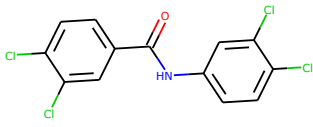
Generated molecule 208



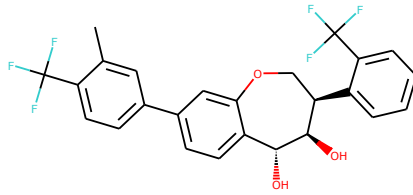
Generated molecule 209



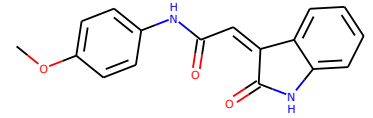
Generated molecule 210



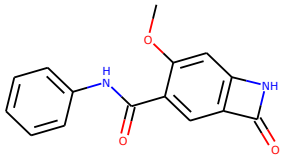
Generated molecule 211



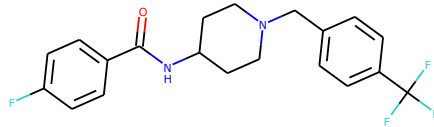
Generated molecule 212



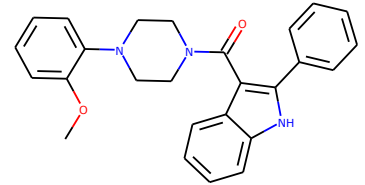
Generated molecule 213



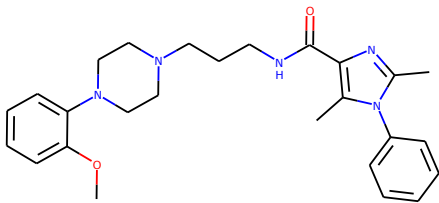
Generated molecule 214



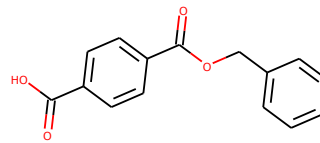
Generated molecule 215



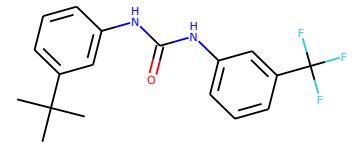
Generated molecule 216



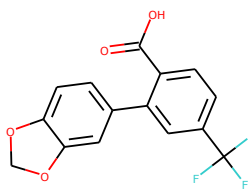
Generated molecule 217



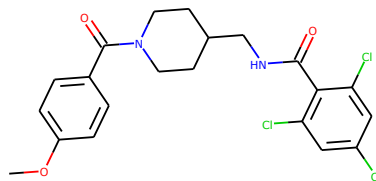
Generated molecule 218



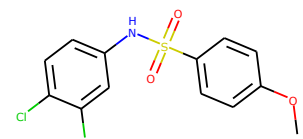
Generated molecule 219



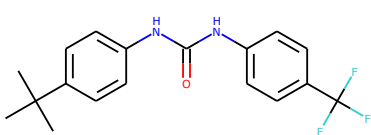
Generated molecule 220



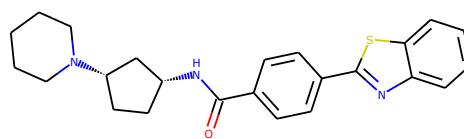
Generated molecule 221



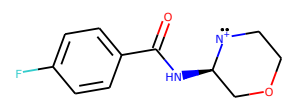
Generated molecule 222



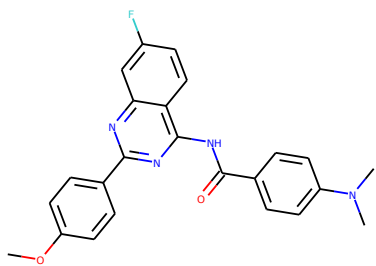
Generated molecule 223



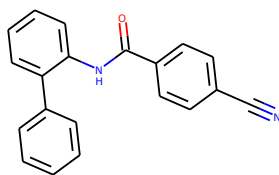
Generated molecule 224



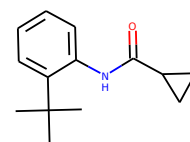
Generated molecule 225



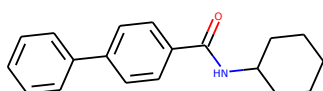
Generated molecule 226



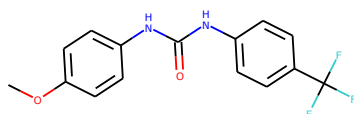
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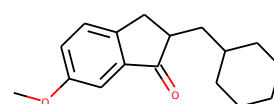
Generated molecule 228



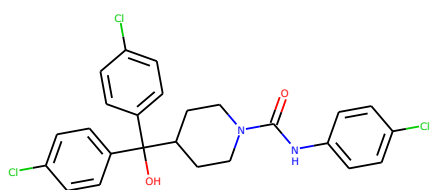
Generated molecule 229



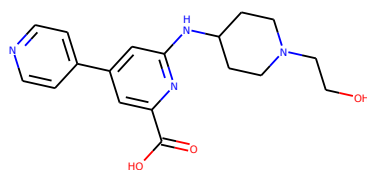
Generated molecule 230



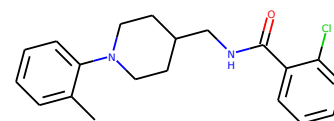
Generated molecule 231



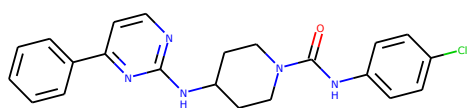
Generated molecule 232



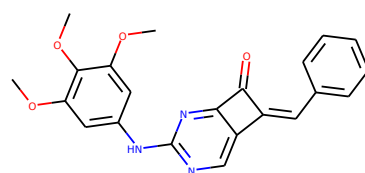
Generated molecule 233



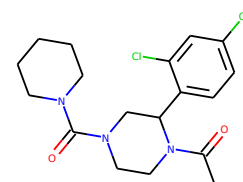
Generated molecule 234



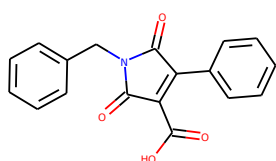
Generated molecule 235



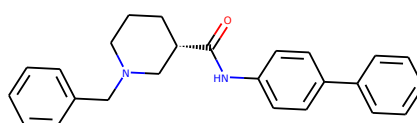
Generated molecule 236



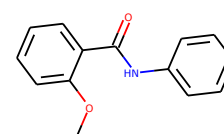
Generated molecule 237



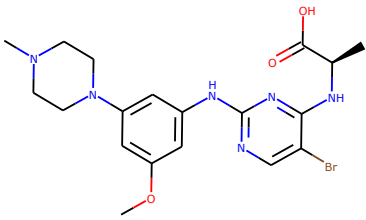
Generated molecule 238



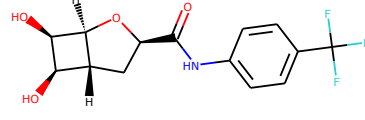
Generated molecule 239



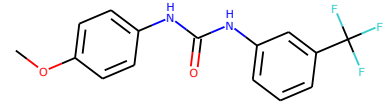
Generated molecule 240



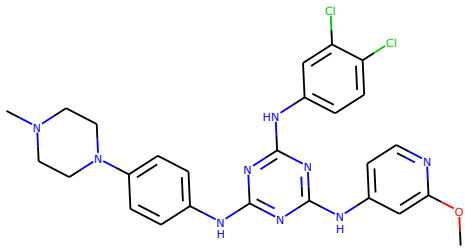
Generated molecule 241



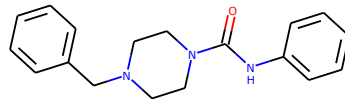
Generated molecule 242



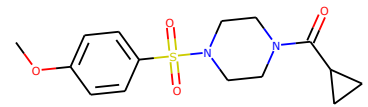
Generated molecule 243



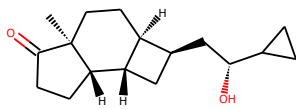
Generated molecule 244



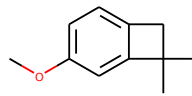
Generated molecule 245



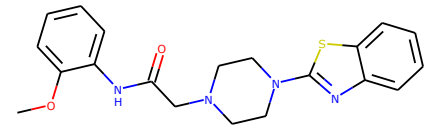
Generated molecule 246



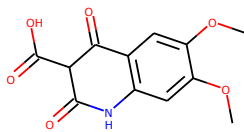
Generated molecule 247



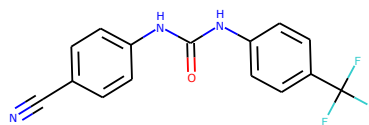
Generated molecule 248



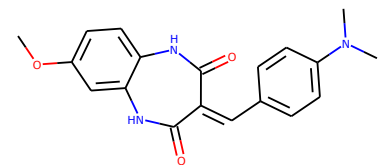
Generated molecule 249



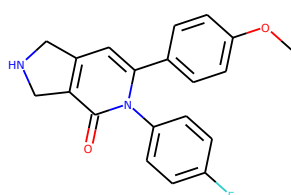
Generated molecule 250



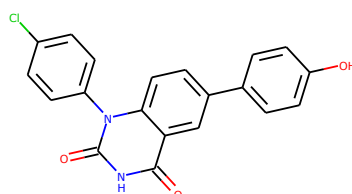
Generated molecule 251



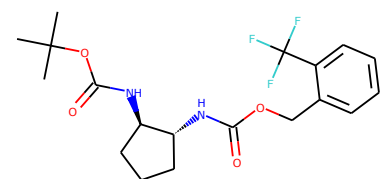
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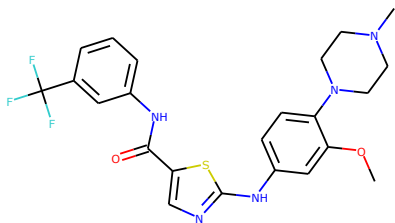
Generated molecule 253



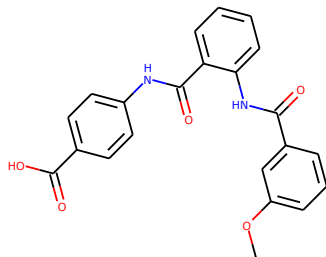
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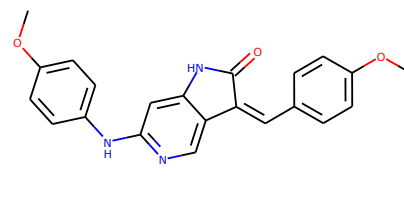
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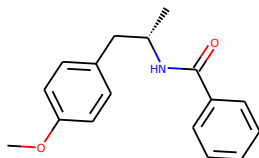
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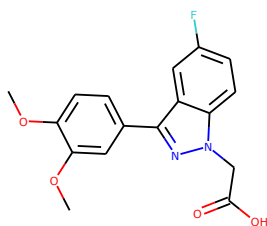
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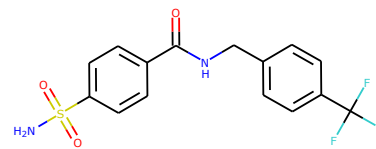
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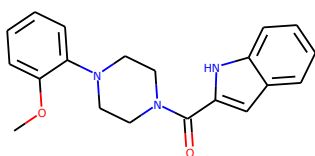
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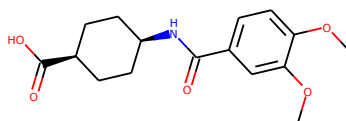
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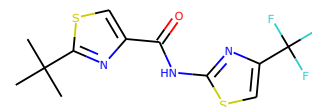
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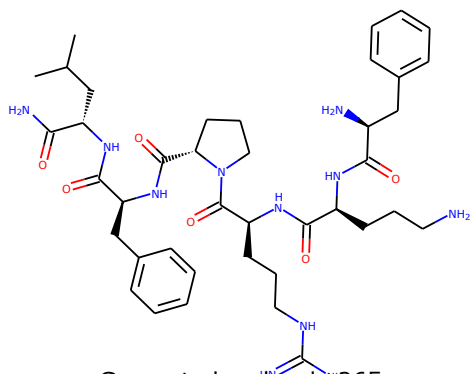
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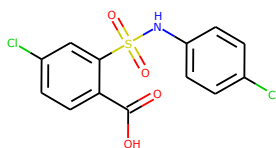
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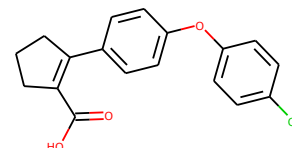
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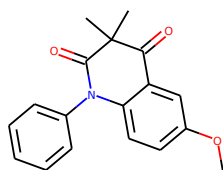
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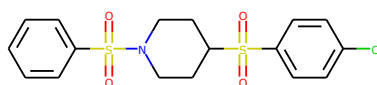
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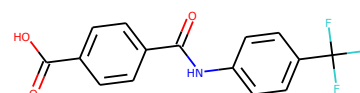
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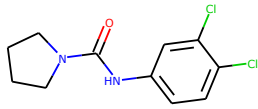
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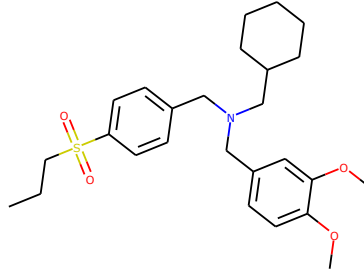
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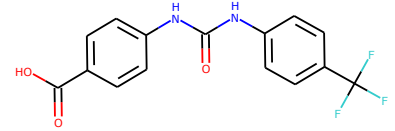
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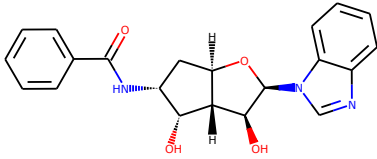
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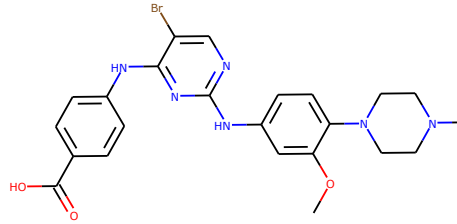
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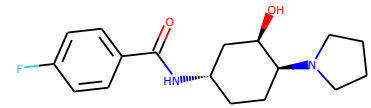
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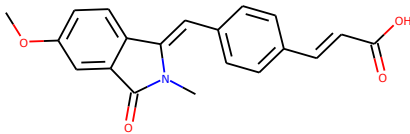
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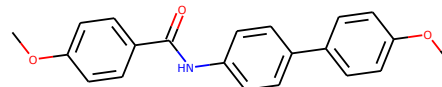
Generated molecule 275



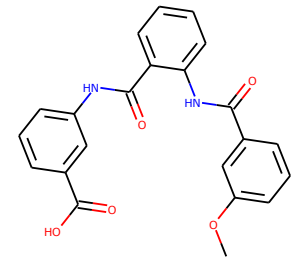
Generated molecule 276



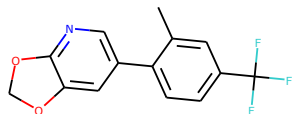
Generated molecule 277



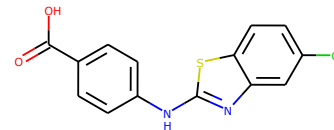
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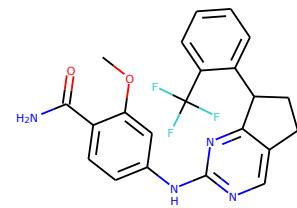
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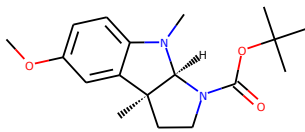
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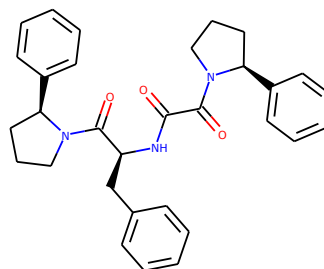
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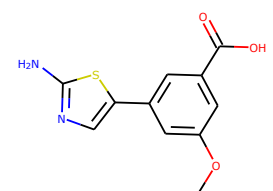
Generated molecule 282



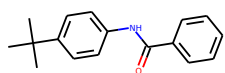
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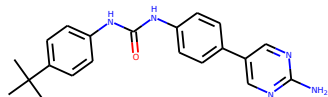
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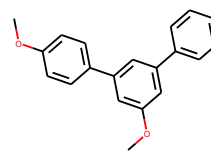
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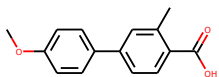
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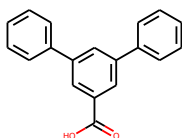
Generated molecule 287



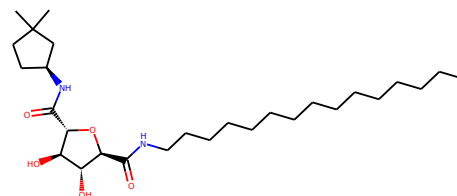
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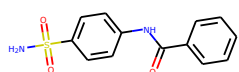
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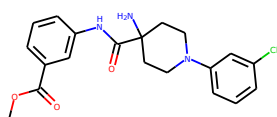
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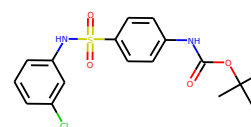
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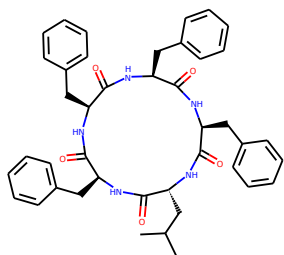
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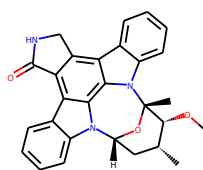
Generated molecule 293



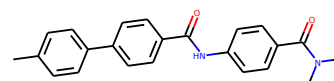
Generated molecule 294



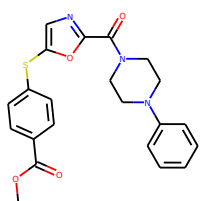
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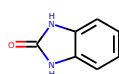
Generated molecule 296



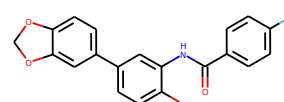
Generated molecule 297



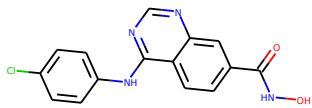
Generated molecule 298



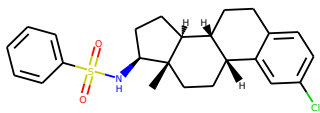
Generated molecule 299



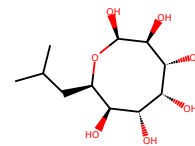
Generated molecule 300



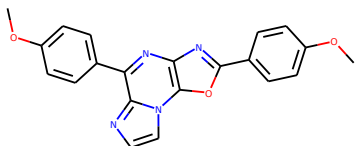
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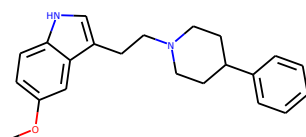
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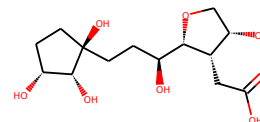
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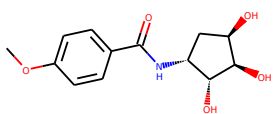
Generated molecule 304



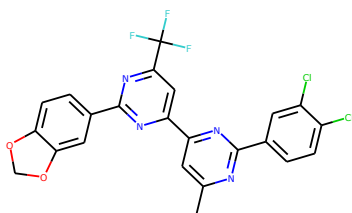
Generated molecule 305



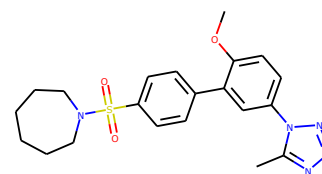
Generated molecule 306



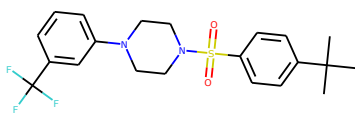
Generated molecule 307



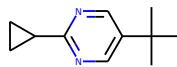
Generated molecule 308



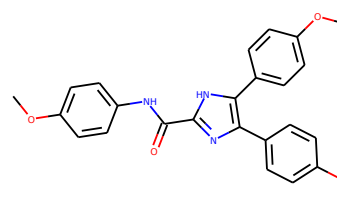
Generated molecule 309



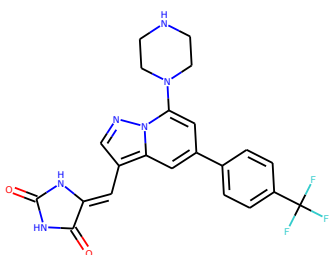
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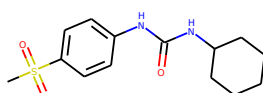
Generated molecule 311



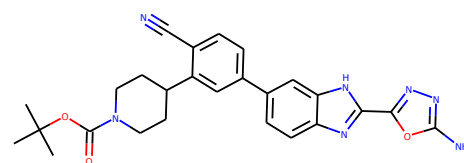
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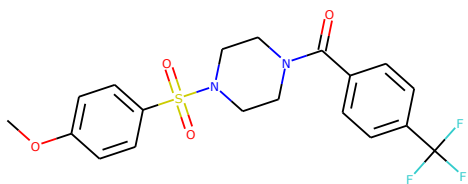
Generated molecule 313



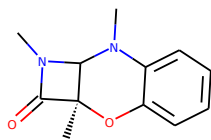
Generated molecule 314



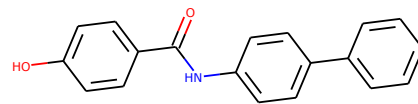
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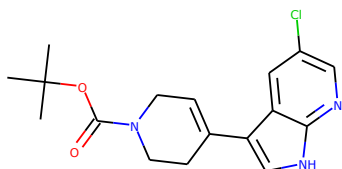
Generated molecule 316



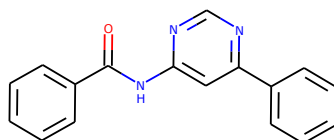
Generated molecule 317



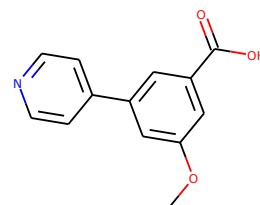
Generated molecule 318



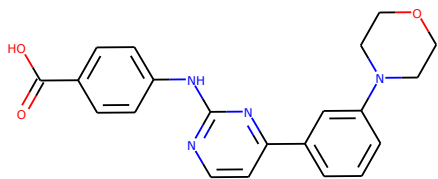
Generated molecule 319



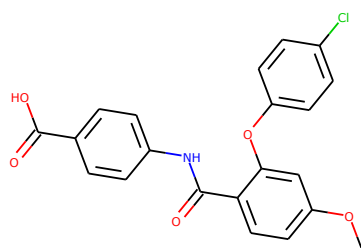
Generated molecule 320



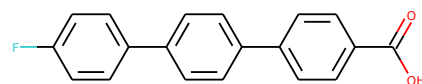
Generated molecule 321



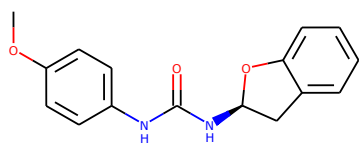
Generated molecule 322



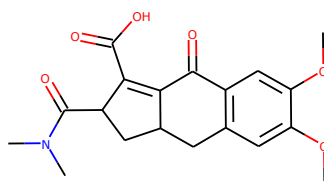
Generated molecule 323



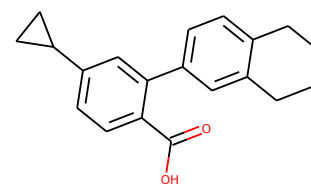
Generated molecule 324



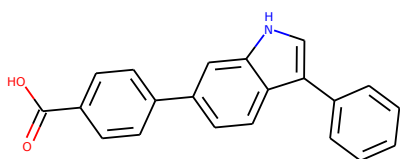
Generated molecule 325



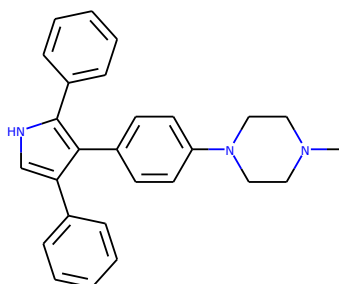
Generated molecule 326



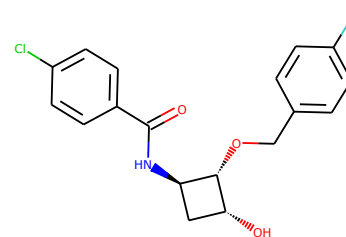
Generated molecule 327



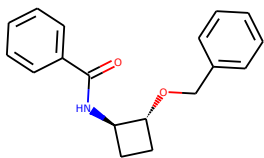
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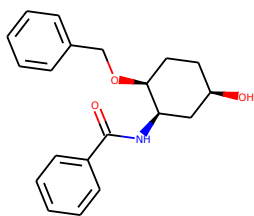
Generated molecule 329



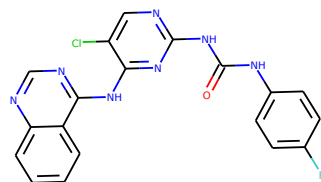
Generated molecule 330



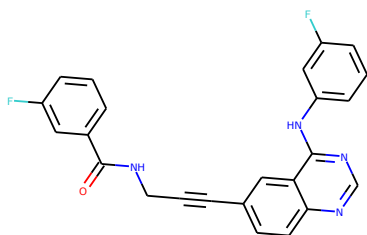
Generated molecule 331



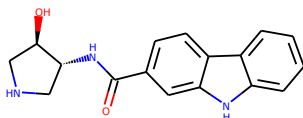
Generated molecule 332



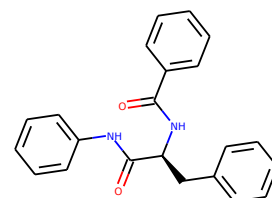
Generated molecule 333



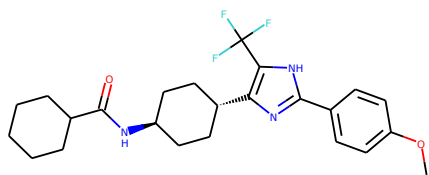
Generated molecule 334



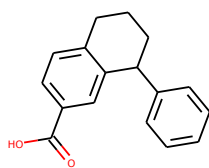
Generated molecule 335



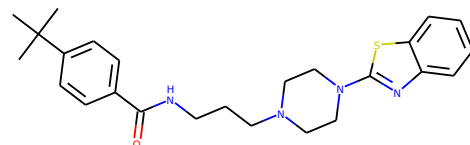
Generated molecule 336



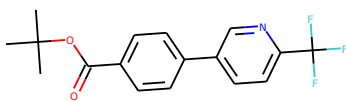
Generated molecule 337



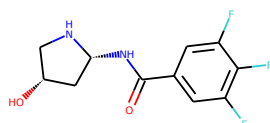
Generated molecule 338



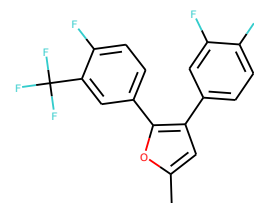
Generated molecule 339



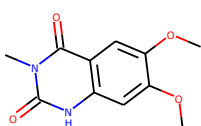
Generated molecule 340



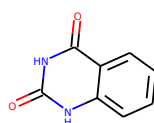
Generated molecule 341



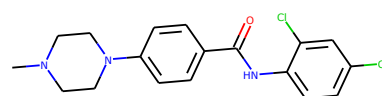
Generated molecule 342



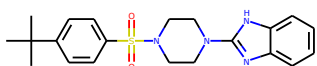
Generated molecule 343



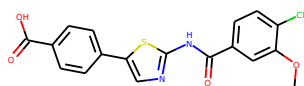
Generated molecule 344



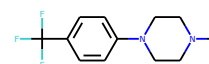
Generated molecule 345



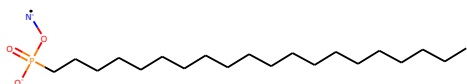
Generated molecule 346



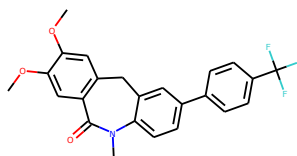
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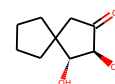
Generated molecule 348



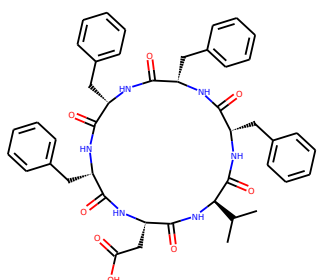
Generated molecule 349



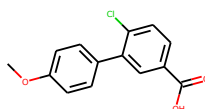
Generated molecule 350



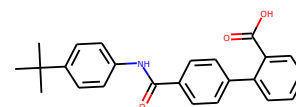
Generated molecule 351



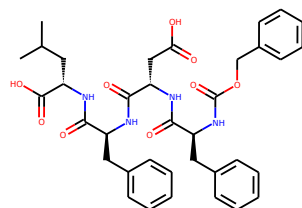
Generated molecule 352



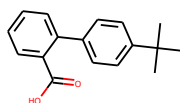
Generated molecule 353



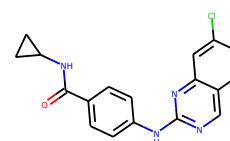
Generated molecule 354



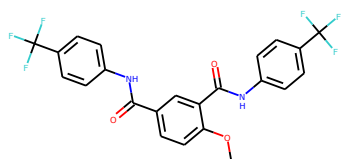
Generated molecule 355



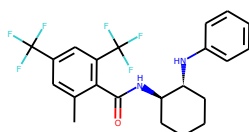
Generated molecule 356



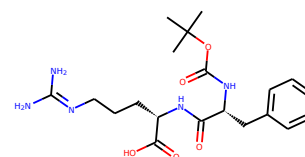
Generated molecule 357



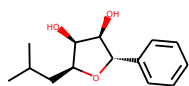
Generated molecule 358



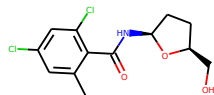
Generated molecule 359



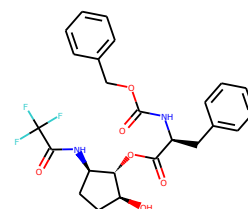
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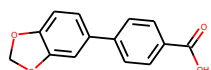
Generated molecule 361



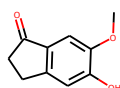
Generated molecule 362



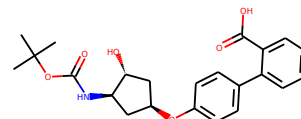
Generated molecule 363



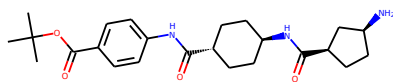
Generated molecule 364



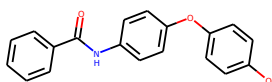
Generated molecule 365



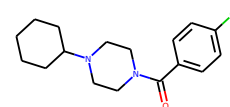
Generated molecule 366



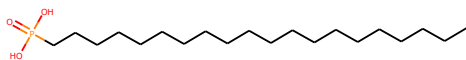
Generated molecule 367



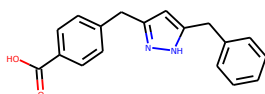
Generated molecule 368



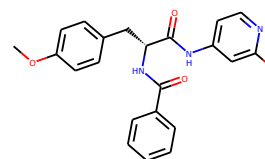
Generated molecule 369



Generated molecule 370



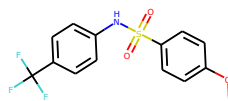
Generated molecule 371



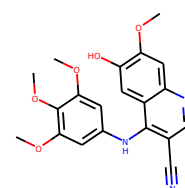
Generated molecule 372



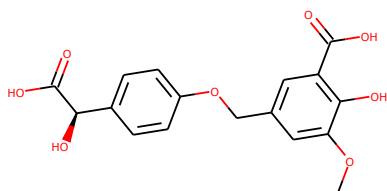
Generated molecule 373



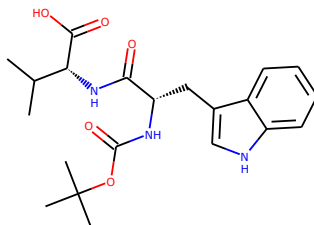
Generated molecule 374



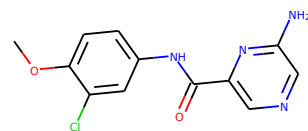
Generated molecule 375



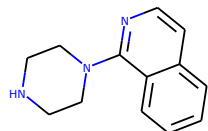
Generated molecule 376



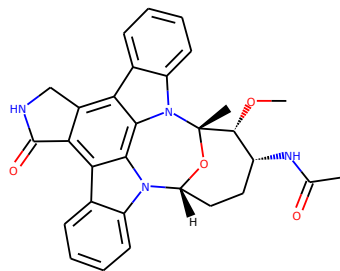
Generated molecule 377



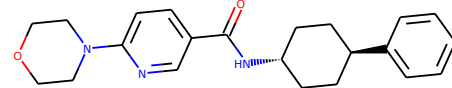
Generated molecule 378



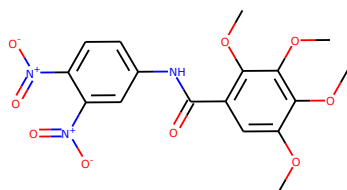
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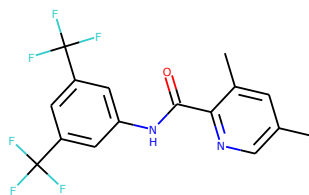
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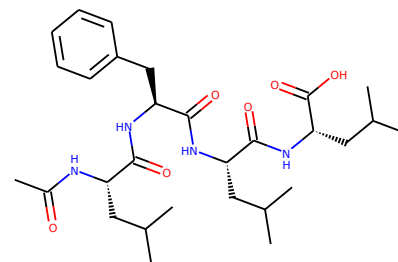
Generated molecule 381



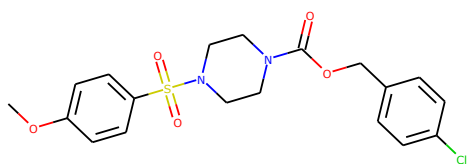
Generated molecule 382



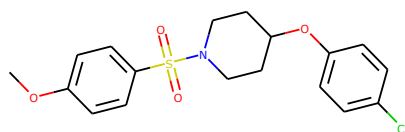
Generated molecule 383



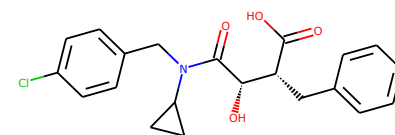
Generated molecule 384



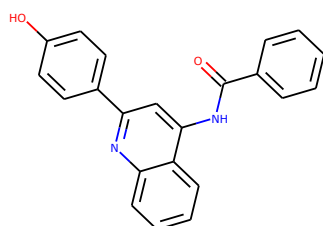
Generated molecule 385



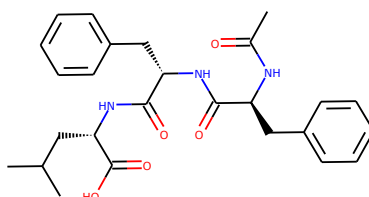
Generated molecule 386



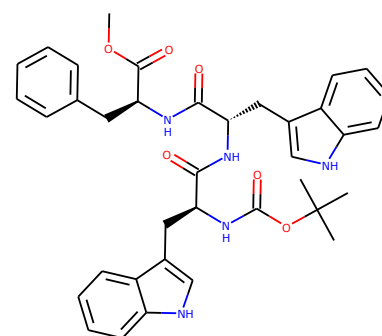
Generated molecule 387



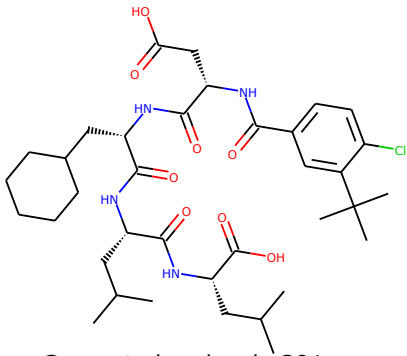
Generated molecule 388



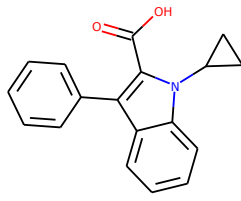
Generated molecule 389



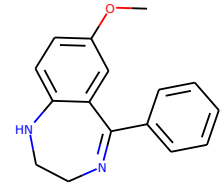
Generated molecule 390



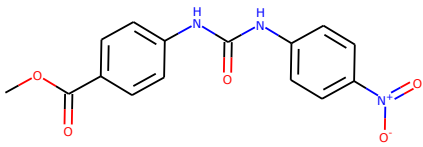
Generated molecule 391



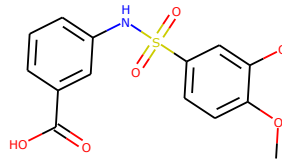
Generated molecule 392



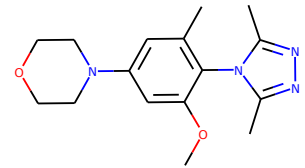
Generated molecule 393



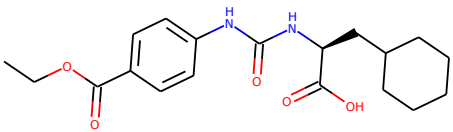
Generated molecule 394



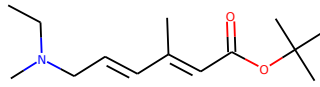
Generated molecule 395



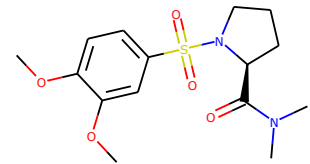
Generated molecule 396



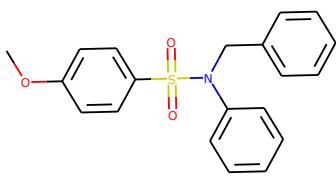
Generated molecule 397



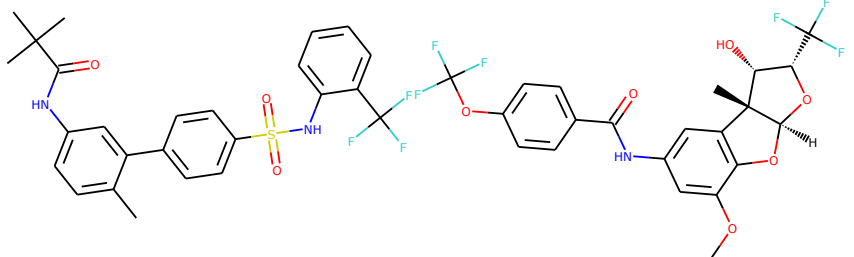
Generated molecule 398



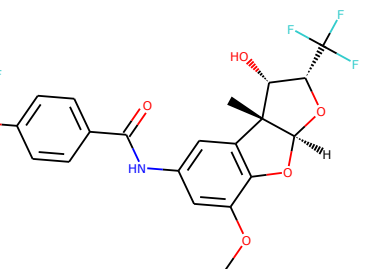
Generated molecule 399



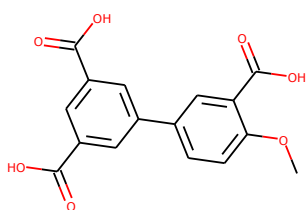
Generated molecule 400



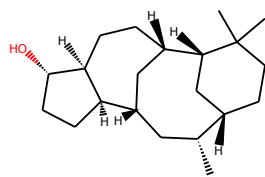
Generated molecule 401



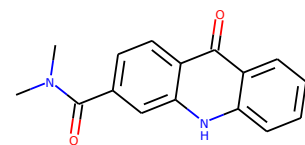
Generated molecule 402



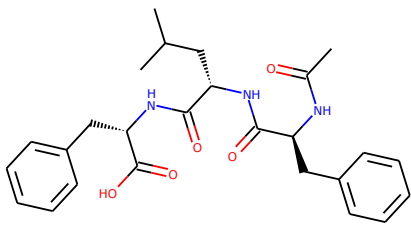
Generated molecule 403



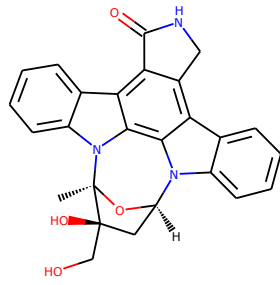
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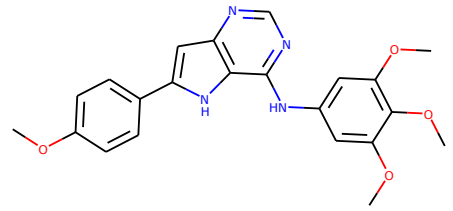
Generated molecule 405



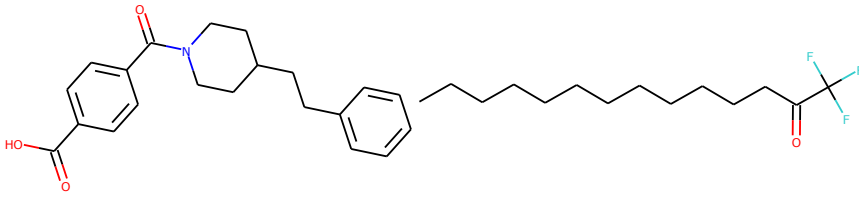
Generated molecule 406



Generated molecule 407

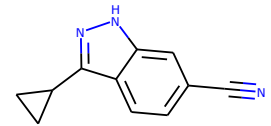


Generated molecule 408

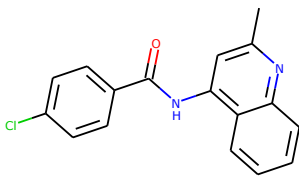


Generated molecule 409

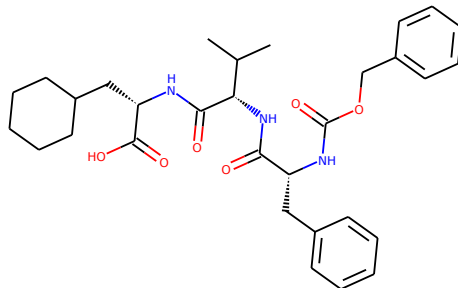
Generated molecule 410



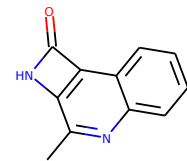
Generated molecule 411



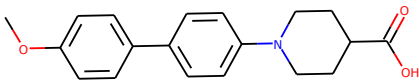
Generated molecule 412



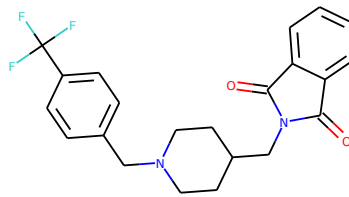
Generated molecule 413



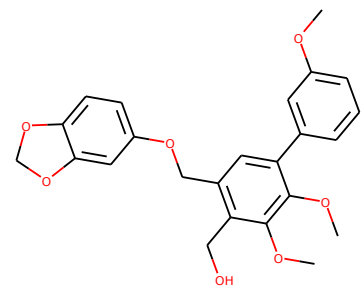
Generated molecule 414



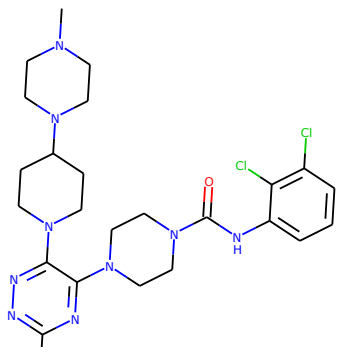
Generated molecule 415



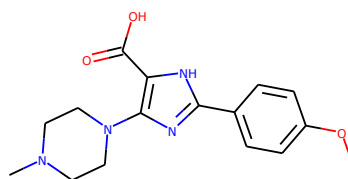
Generated molecule 416



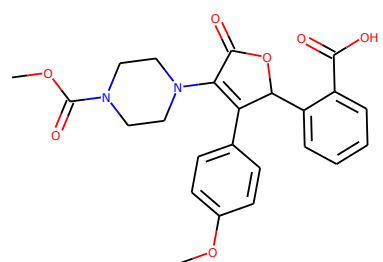
Generated molecule 417



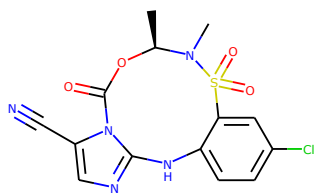
Generated molecule 418



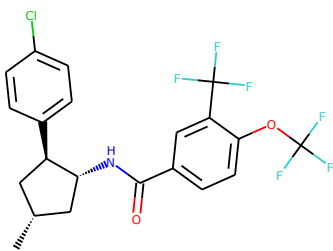
Generated molecule 419



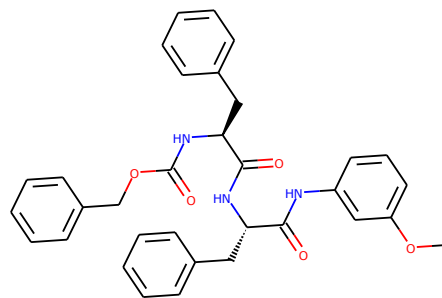
Generated molecule 420



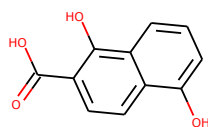
Generated molecule 421



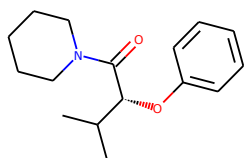
Generated molecule 422



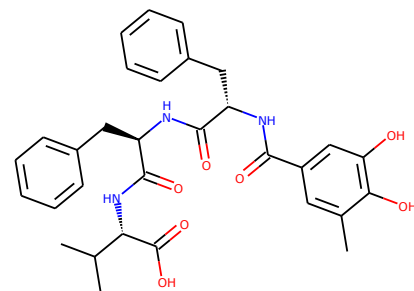
Generated molecule 423



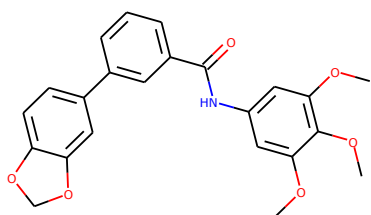
Generated molecule 424



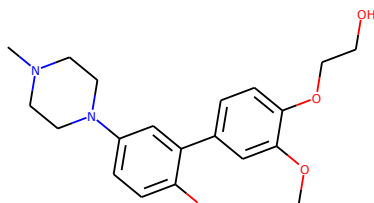
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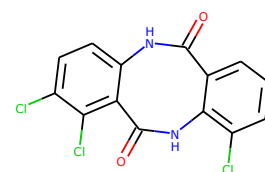
Generated molecule 426



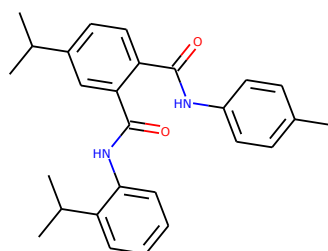
Generated molecule 427



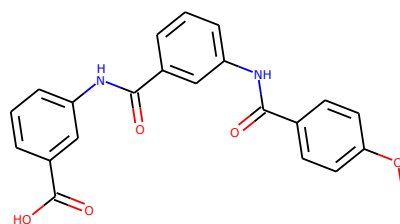
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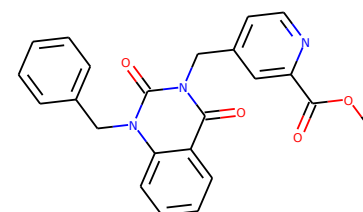
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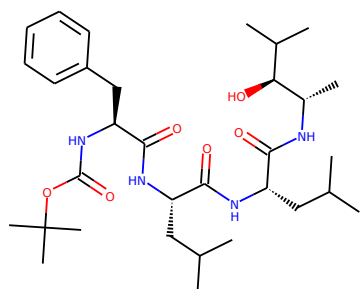
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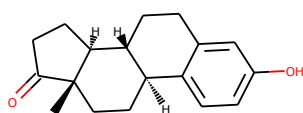
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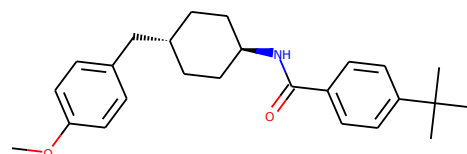
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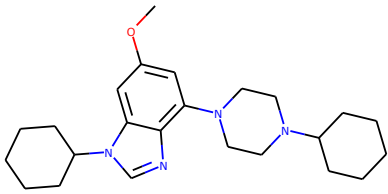
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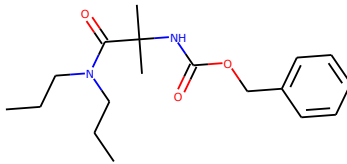
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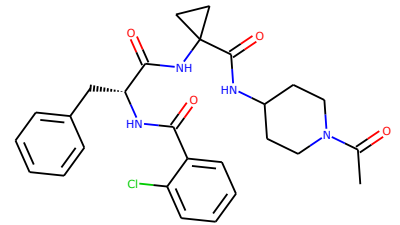
Generated molecule 435



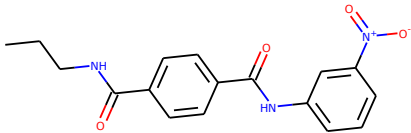
Generated molecule 436



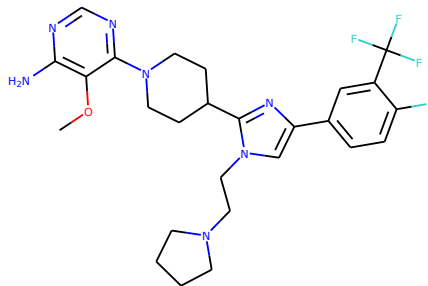
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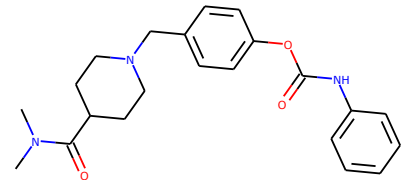
Generated molecule 438



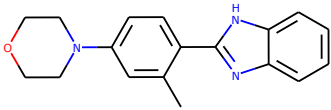
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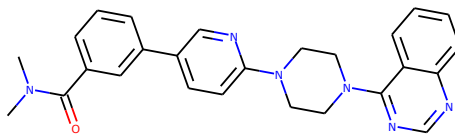
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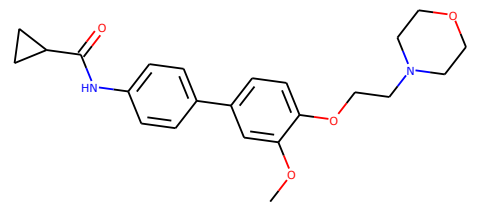
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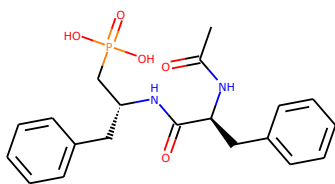
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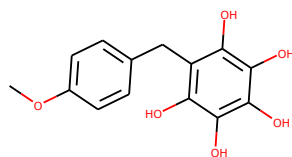
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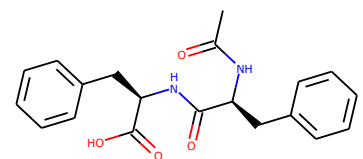
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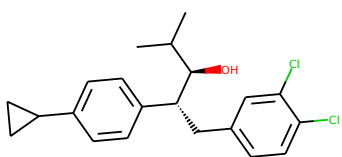
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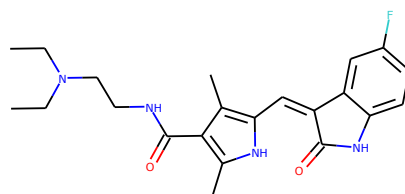
Generated molecule 446



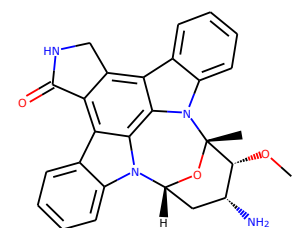
Generated molecule 447



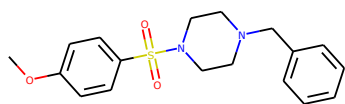
Generated molecule 448



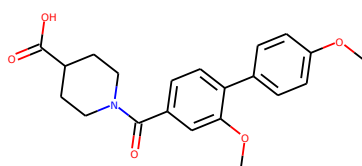
Generated molecule 449



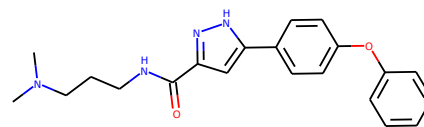
Generated molecule 450



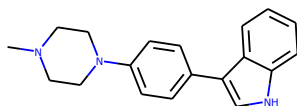
Generated molecule 451



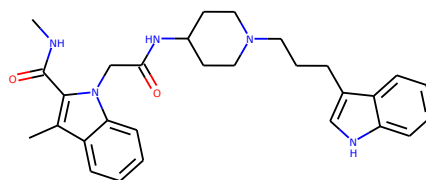
Generated molecule 452



Generated molecule 453



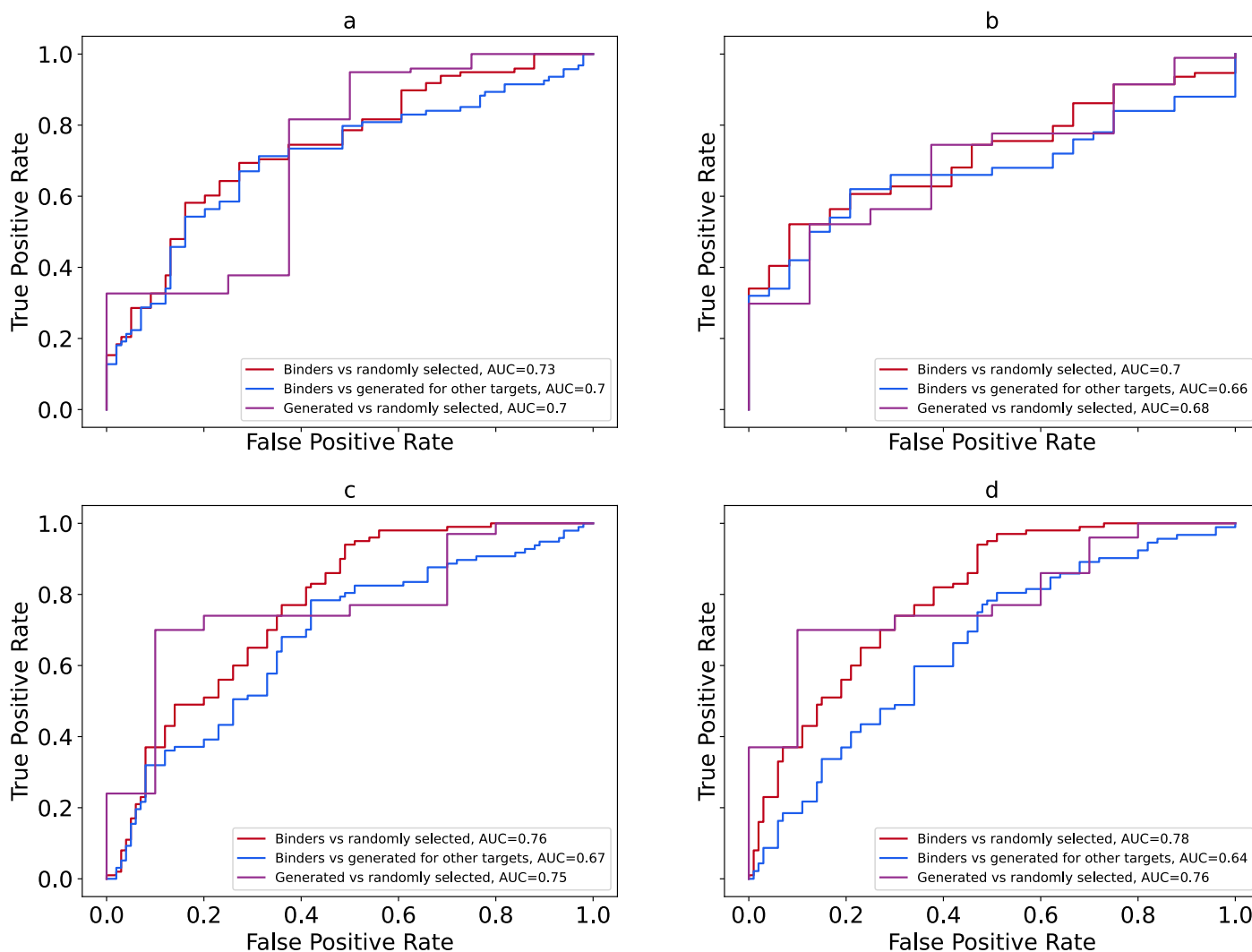
Generated molecule 454



Generated molecule 455

Supplementary Figure S2. Graph representation for generated compounds.

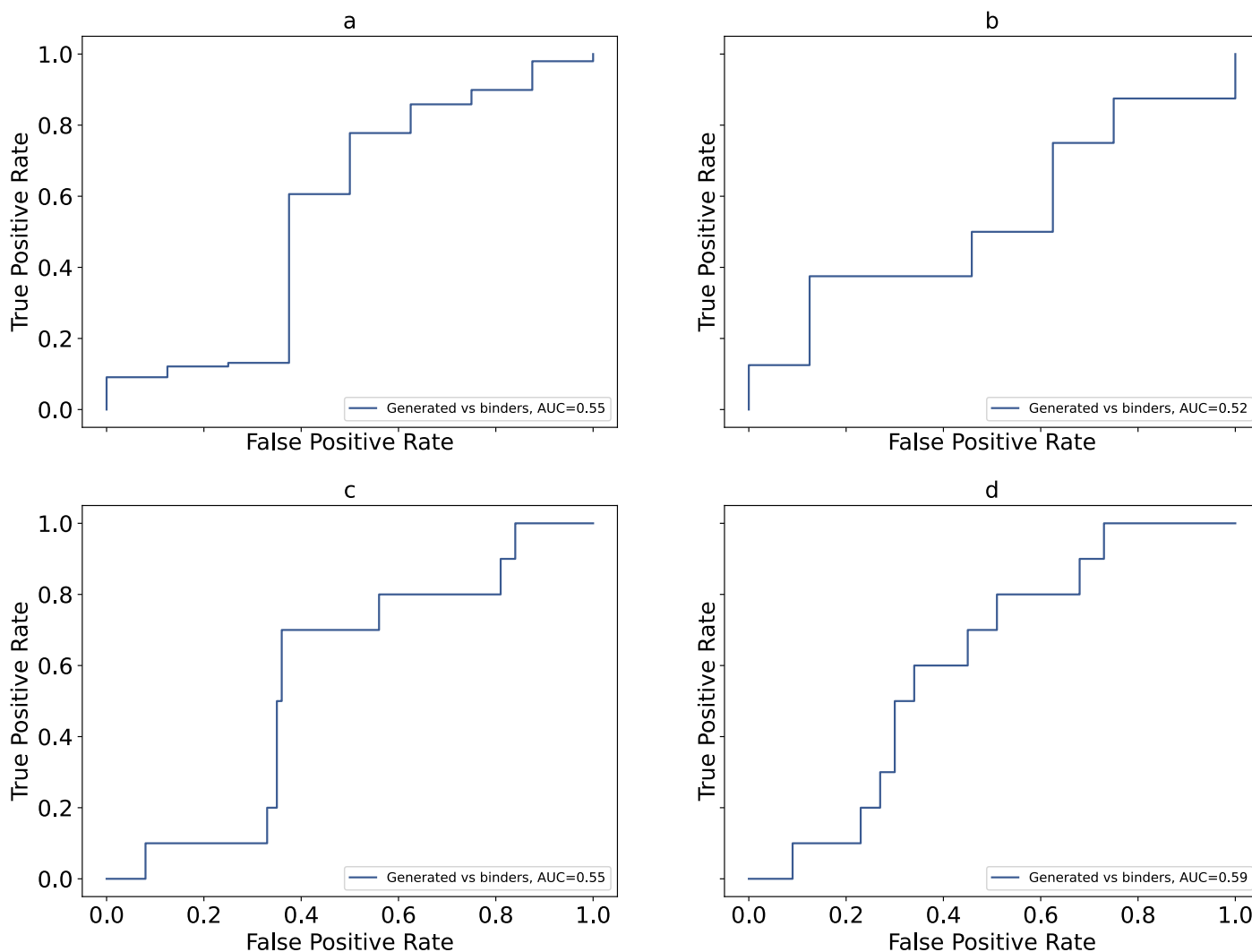
ROC curves and corresponding AUC for the structures of Insulin-like growth factor 1 receptor (IGF-1R) and Vascular endothelial growth factor receptor 2 (VEGFR2).



Supplementary Figure S3. ROC curves and corresponding AUC for the following structures:

- (a) structure of IGF-1R with PDB code 4D2R
- (b) structure of IGF-1R with PDB code 2OJ9
- (c) structure of VEGFR2 with PDB code 4ASE
- (d) structure of VEGFR2 with PDB code 2P2H

ROC comparison of known binders versus generated molecules and corresponding AUC for the structures of Insulin-like growth factor 1 receptor (IGF-1R) and Vascular endothelial growth factor receptor 2 (VEGFR2).



Supplementary Figure S4. ROC comparison of known binders versus molecules generated for IGF-1R and VEGFR2 and corresponding AUC for the following structures:

- (a) structure of IGF-1R with PDB code 4D2R
- (b) structure of IGF-1R with PDB code 2OJ9
- (c) structure of VEGFR2 with PDB code 4ASE
- (d) structure of VEGFR2 with PDB code 2P2H