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基于分子描述符和机器学习方法预测和虚拟筛选 MMP-13 对 MMP-1 的选择性抑制剂

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Predicting and Virtually Screening the Selective Inhibitors of MMP-13 over MMP-1 by Molecular Descriptors and Machine Learning Methods

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表S1　MMP-1和MMP-13抑制剂的IC_{50}值，MMP-1/MMP-13的IC_{50}值的比率以及化合物的来源

Table S1　The IC_{50} values of MMP-1, MMP-13 inhibitors, the ratios of MMP-1/MMP-13 for IC_{50} values, and the source of compounds

No.	ID	MMP-1 IC_{50} (nmol/L)	MMP-13 IC_{50} (nmol/L)	$IC_{50\ (MMP-1)}$ / $IC_{50\ (MMP-13)}$	来源
1	5-5	10000	50	200.00	[1]
2	5-7	1700	1	1700.00	[1]
3	5-8	10000	0.4	25000.00	[1]
4	5-9	1500	0.5	3000.00	[1]
5	5-10	10000	2	5000.00	[1]
6	6-43	175	1.7	102.94	[2]
7	8-3	119	0.3	396.67	[3]
8	8-17	109	0.4	272.50	[3]
9	8-20	81	0.2	405.00	[3]
10	8-23	74	0.4	185.00	[3]
11	8-25	24	0.2	120.00	[3]
12	8-26	75	0.1	750.00	[3]
13	8-28	127	0.1	1270.00	[3]
14	8-29	184	1	184.00	[3]
15	8-6	293	1	293.00	[3]
16	8-30	155	1	155.00	[3]
17	8-31	329	0.7	470.00	[3]
18	8-32	1548	11	140.73	[3]
19	8-7	790	2	395.00	[3]
20	8-35	4235	8	529.38	[3]
21	8-36	86	0.4	215.00	[3]
22	10-22	560	1	560.00	[4]
23	10-23	260	2	130.00	[4]
24	10-24	1300	0.7	1857.14	[4]
25	10-25	450	0.8	562.50	[4]
26	10-29	350	2	175.00	[4]
27	10-32	3100	27	114.81	[4]
28	10-34	500	3	166.67	[4]
29	10-35	1200	0.7	1714.29	[4]
30	10-37	240	2	120.00	[4]
31	10-39	260	0.5	520.00	[4]
32	10-40	140	1	140.00	[4]
33	10-41	1200	0.9	1333.33	[4]
34	10-42	270	0.8	337.50	[4]

35	10-43	440	0.9	488.89	[4]
36	10-44	280	1	280.00	[4]
37	10-45	210	0.4	525.00	[4]
38	10-46	2000	0.9	2222.22	[4]
39	10-49	490	1	490.00	[4]
40	10-50	920	0.6	1533.33	[4]
41	10-51	2000	0.7	2857.14	[4]
42	10-53	300	1	300.00	[4]
43	10-54	1000	0.9	1111.11	[4]
44	10-55	310	1	310.00	[4]
45	10-58	42	0.4	105.00	[4]
46	10-59	100	0.4	250.00	[4]
47	10-60	230	0.4	575.00	[4]
48	10-61	200	0.5	400.00	[4]
49	10-62	580	4	145.00	[4]
50	10-63	260	0.3	866.67	[4]
51	10-64	920	0.3	3066.67	[4]
52	10-65	300	2.8	107.14	[4]
53	10-66	1800	4.4	409.09	[4]
54	10-68	600	0.7	857.14	[4]
55	10-69	750	0.5	1500.00	[4]
56	10-70	780	0.5	1560.00	[4]
57	10-71	350	0.4	875.00	[4]
58	10-72	480	0.4	1200.00	[4]
59	10-73	2900	2	1450.00	[4]
60	10-74	570	0.3	1900.00	[4]
61	10-75	2500	2	1250.00	[4]
62	11-10	175	1.7	102.94	[5]
63	11-12	996	4.2	237.14	[5]
64	11-25	219	1.5	146.00	[5]
65	11-26	227	1	227.00	[5]
66	11-42	322	1.8	178.89	[5]
67	11-45	493	1.1	448.18	[5]
68	12-11c	6000	8	750.00	[6]
69	12-11d	100000	710	140.85	[6]
70	12-11e	6500	48	135.42	[6]
71	12-11f	3600	7	514.29	[6]
72	12-11g	2200	11	200.00	[6]
73	12-11h	1500	6	250.00	[6]
74	12-11i	26000	105	247.62	[6]
75	12-11j	4200	23	182.61	[6]

76	12-11k	18000	37	486.49	[6]
77	12-11l	3200	16	200.00	[6]
78	12-11m	12000	102	117.65	[6]
79	12-11n	50000	26	1923.08	[6]
80	12-11o	13000	10	1300.00	[6]
81	12-11p	7000	5	1400.00	[6]
82	12-11q	56000	21	2666.67	[6]
83	12-11r	40000	13	3076.92	[6]
84	12-11s	15000	4	3750.00	[6]
85	12-11t	41000	7	5857.14	[6]
86	12-11u	56000	36	1555.56	[6]
87	12-11v	27000	12	2250.00	[6]
88	13-4a	768	7	109.71	[7]
89	13-4e	100000	42	2380.95	[7]
90	13-4h	74	0.016	4625.00	[7]
91	13-4i	116	0.6	193.33	[7]
92	13-13	9500	67	141.79	[7]
93	15-6h	10000	28	357.14	[8]
94	15-6i	10000	33	303.03	[8]
95	15-7h	10000	12.2	819.67	[8]
96	15-RS130830	800	0.6	1333.33	[8]
97	16-10	4350	43	101.16	[9]
98	16-12	4999	36	138.86	[9]
99	16-13	4183	17	246.06	[9]
100	16-14	9829	22	446.77	[9]
101	16-15	8270	26	318.08	[9]
102	16-16	6728	21	320.38	[9]
103	16-17	284	0.8	355.00	[9]
104	16-18	4785	1	4785.00	[9]
105	16-19	22927	64	358.23	[9]
106	16-21	3780	13	290.77	[9]
107	16-22	2190	8	273.75	[9]
108	16-23	7960	67	118.81	[9]
109	16-24	7910	32	247.19	[9]
110	16-25	5350	16	334.38	[9]
111	16-26	4660	29	160.69	[9]
112	16-27	4730	11	430.00	[9]
113	16-28	4130	21	196.67	[9]
114	16-29	4110	7	587.14	[9]
115	16-30	5960	11	541.82	[9]
116	17-4a	2200	7.9	278.48	[10]

117	17-4b	643	2.9	221.72	[10]
118	17-4c	465	0.75	620.00	[10]
119	17-4d	320	0.34	941.18	[10]
120	17-9c	346	2.4	144.17	[10]
121	19-28	3660	24	152.50	[11]
122	19-32	3400	33	103.03	[11]
123	19-33	10000	14	714.29	[11]
124	19-34	10000	50	200.00	[11]
125	19-38	10000	59	169.49	[11]
126	19-39	10000	89	112.36	[11]
127	19-40	10000	35	285.71	[11]
128	19-47	3340	22	151.82	[11]
129	19-49	24800	147	168.71	[11]
130	19-62	11500	103	111.65	[11]
131	22-13a	5210	29.5	176.61	[12]
132	22-13b	2760	5.4	511.11	[12]
133	22-13c	1400	1	1400.00	[12]
134	22-13d	1420	0.7	2028.57	[12]
135	22-13e	1370	0.4	3425.00	[12]
136	22-13f	3490	6.9	505.80	[12]
137	22-13g	4900	13.9	352.52	[12]
138	22-13h	1760	1.8	977.78	[12]
139	22-13i	2590	3.5	740.00	[12]
140	22-13m	1080	1	1080.00	[12]
141	22-13n	6050	55.3	109.40	[12]
142	22-13l	1850	2.4	770.83	[12]
143	22-13m	3310	3	1103.33	[12]
144	22-13n	1220	1	1220.00	[12]
145	22-2	8710	24.2	359.92	[12]
146	24-94	10000	100	100.00	[13]
147	24-95	10000	10	1000.00	[13]
148	24-96	10000	20	500.00	[13]
149	25-6	8900	3.3	2696.97	[14]
150	30-39	10000	64	156.25	[15]
151	30-50	238	1	238.00	[15]
152	30-54	593	4	148.25	[15]
153	30-57	761	2	380.50	[15]
154	31-1	10000	1.2	8333.33	[16]
155	31-2d	45000	162	277.78	[16]
156	31-2f	50000	129	387.60	[16]
157	31-2g	70000	391	179.03	[16]

158	31-2h	10000	13	769.23	[16]
159	31-2i	10000	11	909.09	[16]
160	31-2j	36000	275	130.91	[16]
161	31-2p	10000	32	312.50	[16]
162	31-2q	10000	27	370.37	[16]
163	31-2u	63000	195	323.08	[16]
164	32-19	492	2	246.00	[17]
165	32-20	519	2	259.50	[17]
166	32-21	450	2	225.00	[17]
167	32-22	494	2	247.00	[17]
168	32-23	368	2	184.00	[17]
169	32-24	1330	3	443.33	[17]
170	32-25	1390	7	198.57	[17]
171	32-26	598	2	299.00	[17]
172	32-27	1930	11	175.45	[17]
173	32-31	3680	33	111.52	[17]
174	32-32	4440	34	130.59	[17]
175	32-33	5110	44	116.14	[17]
176	32-34	2380	1	2380.00	[17]
177	32-35	656	2	328.00	[17]
178	32-36	4730	5	946.00	[17]
179	32-37	642	2	321.00	[17]
180	32-38	662	2	331.00	[17]
181	32-39	1310	9	145.56	[17]
182	32-40	2610	1	2610.00	[17]
183	32-41	1210	4	302.50	[17]
184	32-42	3790	1	3790.00	[17]
185	32-43	629	3	209.67	[17]
186	32-44	2900	2	1450.00	[17]
187	32-45	393	3	131.00	[17]
188	32-46	1950	1	1950.00	[17]
189	32-47	2180	2	1090.00	[17]
190	32-48	3420	2	1710.00	[17]
191	32-49	7060	2	3530.00	[17]
192	32-50	10000	2	5000.00	[17]
193	32-51	10000	16	625.00	[17]
194	32-52	1410	2	705.00	[17]
195	32-53	1720	1	1720.00	[17]
196	32-54	1070	1	1070.00	[17]
197	32-55	801	1	801.00	[17]
198	32-56	1260	2	630.00	[17]

199	32-57	2560	2	1280.00	[17]
200	32-58	3160	5	632.00	[17]
201	32-59	1500	1	1500.00	[17]
202	32-60	531	3	177.00	[17]
203	32-61	422	2	211.00	[17]
204	32-62	3670	5	734.00	[17]
205	32-64	4750	6	791.67	[17]
206	32-66	490	1	490.00	[17]
207	32-RS130830	233	2	116.50	[17]
208	35-1	170	1.7	100.00	[18]
209	35-5	1200	0.9	1333.33	[18]
210	35-6	500	0.93	537.63	[18]
211	35-7	280	0.53	528.30	[18]
212	35-9	330	0.97	340.21	[18]
213	35-10	420	0.75	560.00	[18]
214	35-11	490	1.5	326.67	[18]
215	35-12	180	0.64	281.25	[18]
216	35-13	1100	0.56	1964.29	[18]
217	35-14	1700	9.7	175.26	[18]
218	35-15	3900	4.6	847.83	[18]
219	35-16	320	1.2	266.67	[18]
220	35-17	780	0.87	896.55	[18]
221	35-18	4800	1.7	2823.53	[18]
222	35-20	3900	5	780.00	[18]
223	35-21	5400	6.5	830.77	[18]
224	35-22	9600	19	505.26	[18]
225	35-23	8800	24	366.67	[18]
226	35-24	6500	11	590.91	[18]
227	35-25	12000	13	923.08	[18]
228	35-27	12000	5.7	2105.26	[18]
229	35-28	3800	14	271.43	[18]
230	35-29	1400	1.5	933.33	[18]
231	35-30	5900	4.6	1282.61	[18]
232	35-32	750	1.5	500.00	[18]
233	35-33	550	2	275.00	[18]
234	35-34	290	0.56	517.86	[18]
235	35-35	350	1	350.00	[18]
236	35-36	59	0.35	168.57	[18]
237	35-37	1200	1.3	923.08	[18]
238	35-38	740	0.77	961.04	[18]
239	35-39	870	0.93	935.48	[18]

240	35-40	260	0.37	702.70	[18]
241	35-41	150	0.5	300.00	[18]
242	35-42	180	0.65	276.92	[18]
243	35-43	1500	3.3	454.55	[18]
244	41-B3	1530	1.6	956.25	[19]
245	47-14b	450	1.1	409.09	[20]
246	47-14c	600	4.2	142.86	[20]
247	47-16a	100000	820	121.95	[20]
248	47-16b	100000	480	208.33	[20]
249	47-17a	1500	6	250.00	[20]
250	47-17e	6500	48	135.42	[20]
251	47-17f	2200	11	200.00	[20]
252	47-17m	6000	8	750.00	[20]
253	54-9a	268	0.1	2680.00	[21]
254	54-9b	1800	0.45	4000.00	[21]
255	54-9c	435	0.15	2900.00	[21]
256	54-9d	3600	0.8	4500.00	[21]
257	54-9e	400	0.3	1333.33	[21]
258	54-9f	300	0.1	3000.00	[21]
259	54-9g	1400	0.25	5600.00	[21]
260	54-9h	10000	0.8	12500.00	[21]
261	54-9i	8000	0.4	20000.00	[21]
262	54-9j	1140	0.1	11400.00	[21]
263	54-9k	2500	0.1	25000.00	[21]
264	54-9l	5000	0.25	20000.00	[21]
265	54-9m	5000	1	5000.00	[21]
266	54-6	8660	0.4	21650.00	[21]
267	54-19a	3600	0.4	9000.00	[21]
268	54-19b	4500	0.3	15000.00	[21]
269	54-19c	1000	0.25	4000.00	[21]
270	54-19d	10000	0.25	40000.00	[21]
271	54-19e	10000	0.2	50000.00	[21]
272	54-19f	10000	2.7	3703.70	[21]
273	54-19g	2000	0.5	4000.00	[21]
274	54-19h	770	0.1	7700.00	[21]
275	54-19i	10000	2.9	3448.28	[21]
276	54-19j	4400	1.9	2315.79	[21]
277	54-19k	2000	0.6	3333.33	[21]
278	54-19l	2400	0.2	12000.00	[21]
279	54-19m	1000	0.3	3333.33	[21]
280	54-19n	6000	0.5	12000.00	[21]

281	54-19o	10000	0.2	50000.00	[21]
282	54-19p	10000	1.2	8333.33	[21]
283	54-19q	10000	0.35	28571.43	[21]
284	54-19r	10000	5.5	1818.18	[21]
285	54-19s	10000	0.6	16666.67	[21]
286	54-19t	10000	0.2	50000.00	[21]
287	54-19u	10000	0.1	100000.00	[21]
288	54-19v	10000	0.1	100000.00	[21]
289	54-19w	4000	0.1	40000.00	[21]
290	54-19x	6000	0.1	60000.00	[21]
291	54-19y	4600	0.2	23000.00	[21]
292	54-19z	5900	0.1	59000.00	[21]
293	54-19aa	4500	0.1	45000.00	[21]
294	54-19bb	3600	0.2	18000.00	[21]
295	54-19cc	2600	0.2	13000.00	[21]
296	54-19dd	10000	0.6	16666.67	[21]
297	54-19ee	10000	0.1	100000.00	[21]
298	56-25	30000	30	1000.00	[22]
299	69-2-1	100000	76	1315.79	[23]
300	69-2-2	10000	1.2	8333.33	[23]
301	69-2-3	10000	13	769.23	[23]
302	69-2-7	1000	8.7	114.94	[23]
303	69-2-28	1000	9	111.11	[23]
304	69-2-35	10000	45	222.22	[23]
305	74-3c	1000	2.5	400.00	[24]
306	74-3l	1000	4	250.00	[24]
307	74-3q	1000	6.8	147.06	[24]
308	75-14c	1000	7.3	136.99	[25]
309	79-3	800	0.6	1333.33	[26]
310	79-4a	10000	27	370.37	[26]
311	79-4b	10000	33	303.03	[26]
312	79-4c	10000	2.7	3703.70	[26]
313	79-4d	10000	3.7	2702.70	[26]
314	79-4g	10000	14	714.29	[26]
315	79-4h	10000	6.7	1492.54	[26]
316	79-4i	10000	1.5	6666.67	[26]
317	79-4j	10000	13	769.23	[26]
318	79-4k	10000	18	555.56	[26]
319	79-4l	10000	19	526.32	[26]
320	79-4m	10000	7.7	1298.70	[26]
321	79-4n	10000	12	833.33	[26]

322	79-4o	10000	14.8	675.68	[26]
323	79-4p	10000	4.3	2325.58	[26]
324	79-4q	10000	2.2	4545.45	[26]
325	80-5a	10000	41.5	240.96	[27]
326	80-5b	170	0.2	850.00	[27]
327	80-5c	10000	24	416.67	[27]
328	80-5d	1600	1.6	1000.00	[27]
329	80-5e	1200	0.3	4000.00	[27]
330	80-5f	2400	2.4	1000.00	[27]
331	80-5g	2350	1.1	2136.36	[27]
332	80-5h	10000	1.4	7142.86	[27]
333	80-5i	700	0.6	1166.67	[27]
334	80-7b	4400	2.4	1833.33	[27]
335	80-15b	130	0.4	325.00	[27]
336	81-19	100000	6.3	15873.02	[28]
337	81-20	100000	15	6666.67	[28]
338	81-21	100000	1.1	90909.09	[28]
339	81-24	100000	2.2	45454.55	[28]
340	84-5	51000	73	698.63	[29]
341	91-1	10000	25	400.00	[30]
342	91-2	10000	25	400.00	[30]
343	92-4n	1000	0.8	1250.00	[31]
344	92-4r	1000	1.4	714.29	[31]
345	94-4q	444	3	148.00	[32]
346	94-4r	674	6	112.33	[32]
347	94-4s	745	4	186.25	[32]
348	94-4t	343	3	114.33	[32]
349	94-4u	155	0.8	193.75	[32]
350	94-4v	82	0.7	117.14	[32]
351	101-6c	98000	970	101.03	[33]
352	102-7	28000	260	107.69	[34]
353	102-1a	490	4.1	119.51	[34]
354	102-9	3500	4.1	853.66	[34]
355	102-10	29000	62	467.74	[34]
356	102-11	8300	25	332.00	[34]
357	102-12	12000	74	162.16	[34]
358	102-13	10000	12	833.33	[34]
359	104-27	5460	46	118.70	[35]
360	105-3a	10000	50	200.00	[36]
361	105-3e	600	4	150.00	[36]
362	105-3f	1500	6	250.00	[36]

363	105-3i	8000	32	250.00	[36]
364	105-3j	10000	45	222.22	[36]
365	105-3l	4000	18	222.22	[36]
366	105-3m	1500	0.5	3000.00	[36]
367	105-3n	10000	2	5000.00	[36]
368	106-6b	1560	7	222.86	[37]
369	107-18	1500	15	100.00	[38]
370	107-21	10000	5.9	1694.92	[38]
371	107-22	10000	3.7	2702.70	[38]
372	107-23	600	0.4	1500.00	[38]
373	107-24	10000	24	416.67	[38]
374	107-25	10000	0.8	12500.00	[38]
375	107-26	770	1.1	700.00	[38]
376	107-27	1400	1.1	1272.73	[38]
377	107-28	400	0.6	666.67	[38]
378	107-29	10000	4	2500.00	[38]
379	107-30	10000	2.9	3448.28	[38]
380	107-31	8000	0.4	20000.00	[38]
381	107-32	500	0.3	1666.67	[38]
382	107-33	900	0.8	1125.00	[38]
383	107-34	350	0.4	875.00	[38]
384	107-35	440	0.4	1100.00	[38]
385	107-36	90	0.2	450.00	[38]
386	107-37	1600	0.3	5333.33	[38]
387	107-38	258	2	129.00	[38]
388	107-39	475	0.2	2375.00	[38]
389	109-11	1100	8.3	132.53	[39]
390	109-12	1400	9.4	148.94	[39]
391	109-13	1600	7.7	207.79	[39]
392	109-21	770	7	110.00	[39]
393	109-28	1200	4.5	266.67	[39]
394	110-16	400000	1.8	222222.22	[40]
395	112-2	16000	1.3	12307.69	[41]
396	114-4	30000	2.3	13043.48	[42]
397	114-13	60000	2.1	28571.43	[42]
398	114-14	34000	1.9	17894.74	[42]
399	114-16	37100	4.9	7571.43	[42]
400	114-18	28000	3.8	7368.42	[42]
401	114-20	23400	7.1	3295.77	[42]
402	114-23	37100	11	3372.73	[42]
403	118-7	100000	23	4347.83	[43]

404	120-5	6300	63	100.00	[44]
405	120-6	5700	57	100.00	[44]
406	120-7	3100	31	100.00	[44]
407	120-8	18000	180	100.00	[44]
408	120-9	8800	88	100.00	[44]
409	120-10	17000	17	1000.00	[44]
410	121-30	12000	13	923.08	[45]
411	121-36	24000	3.7	6486.49	[45]
412	123-2	356	0.3	1186.67	[46]
413	123-9	3350	0.3	11166.67	[46]
414	123-23	10000	11	909.09	[46]
415	123-22a	10000	0.75	13333.33	[46]
416	123-22b	3600	6.8	529.41	[46]
417	123-22e	10000	90	111.11	[46]
418	123-22f	10000	18	555.56	[46]
419	123-22g	10000	50	200.00	[46]
420	123-24a	10000	1.3	7692.31	[46]
421	123-24b	3230	12.1	266.94	[46]
422	123-24c	680	3.3	206.06	[46]
423	123-24d	950	0.6	1583.33	[46]
424	123-24f	4540	0.5	9080.00	[46]
425	123-24g	10000	0.8	12500.00	[46]
426	123-24h	10000	4	2500.00	[46]
427	123-24i	10000	0.9	11111.11	[46]
428	123-24j	2020	1.3	1553.85	[46]
429	123-24k	6370	3.9	1633.33	[46]
430	123-24l	10000	3.5	2857.14	[46]
431	123-24m	10000	2	5000.00	[46]
432	123-24n	9330	1	9330.00	[46]
433	123-24o	10000	0.8	12500.00	[46]
434	123-24p	10000	0.6	16666.67	[46]
435	123-24q	10000	0.4	25000.00	[46]
436	123-24r	10000	0.9	11111.11	[46]
437	123-24s	10000	0.6	16666.67	[46]
438	123-24t	7050	0.5	14100.00	[46]
439	123-24u	1740	0.4	4350.00	[46]
440	123-25a	1290	1.4	921.43	[46]
441	123-25b	770	1.6	481.25	[46]
442	123-25c	6560	0.8	8200.00	[46]
443	123-25d	2300	2.8	821.43	[46]
444	123-26a	4180	16	261.25	[46]

445	123-26b	10000	8	1250.00	[46]
446	123-26c	10000	3.6	2777.78	[46]
447	123-26d	10000	0.9	11111.11	[46]
448	123-26e	10000	1.7	5882.35	[46]
449	123-27a	4300	1.4	3071.43	[46]
450	123-27b	650	1.2	541.67	[46]
451	123-27c	12900	0.7	18428.57	[46]
452	123-27d	10000	0.7	14285.71	[46]
453	123-27e	10000	5.5	1818.18	[46]
454	123-27f	10000	4	2500.00	[46]
455	123-27g	10000	4.7	2127.66	[46]
456	123-27h	10000	6.9	1449.28	[46]
457	123-27i	10000	12.7	787.40	[46]
458	123-28a	10000	7.6	1315.79	[46]
459	123-28b	10000	28	357.14	[46]
460	123-28c	10000	49	204.08	[46]
461	124-1a	12000	45	266.67	[47]
462	124-2	4800	39	123.08	[47]
463	124-3	610	2.8	217.86	[47]
464	124-4a	3300	7.2	458.33	[47]
465	124-4b	13000	10	1300.00	[47]
466	124-4c	11000	15	733.33	[47]
467	124-4d	13000	19	684.21	[47]
468	124-4e	5600	41	136.59	[47]
469	124-4f	59000	63	936.51	[47]
470	124-4i	10000	91	109.89	[47]
471	124-4l	10000	25	400.00	[47]
472	124-1b	490	4.1	119.51	[47]
473	124-5	48000	3	16000.00	[47]
474	126-4x	10000	4	2500.00	[48]
475	126-4y	10000	27.7	361.01	[48]
476	126-4z	10000	70	142.86	[48]
477	126-4aa	10000	9	1111.11	[48]
478	127-2l	10000	0.6	16666.67	[49]
479	127-2m	10000	1	10000.00	[49]
480	127-8c	10000	0.42	23809.52	[49]
481	127-SC-276	8660	0.4	21650.00	[49]
482	133-4d	542	2	271.00	[50]
483	133-4e	745	1	745.00	[50]
484	133-4o	10000	44	227.27	[50]
485	133-4p	3245	4	811.25	[50]

486	133-4q	10000	38	263.16	[50]
487	133-4r	1314	3	438.00	[50]
488	133-4s	2268	18	126.00	[50]
489	133-4t	10000	26	384.62	[50]
490	135-8r	3100	16	193.75	[51]
491	135-8u	1012	1	1012.00	[51]
492	135-9g	1922	3	640.67	[51]
493	135-9i	1805	1	1805.00	[51]
494	137-14	1310	12	109.17	[52]
495	137-71	3963	10	396.30	[52]
496	148-5	400000	1.8	222222.22	[53]
497	148-27	1000	2.5	400.00	[53]
498	148-34	100000	30	3333.33	[53]
499	148-35	100000	270	370.37	[53]
500	148-37	30000	0.67	44776.12	[53]
501	153-24	1548	11	140.73	[54]
502	153-28	4235	8	529.38	[54]
503	153-36	1300	0.7	1857.14	[54]
504	153-44	3100	27	114.81	[54]
505	153-47	1200	0.7	1714.29	[54]
506	153-53	1200	0.9	1333.33	[54]
507	153-58	2000	0.9	2222.22	[54]
508	153-63	2000	0.7	2857.14	[54]
509	153-66	1000	0.9	1111.11	[54]
510	153-78	1800	4.4	409.09	[54]
511	153-85	2900	2	1450.00	[54]
512	153-87	2500	2	1250.00	[54]
513	156-1	1100	1.7	647.06	[55]
514	156-2	9700	1.6	6062.50	[55]
515	156-8a	100000	260	384.62	[55]
516	156-8q	70000	350	200.00	[55]
517	163-18	10000	50	200.00	[56]
518	163-19	1700	1	1700.00	[56]
519	163-20	10000	0.4	25000.00	[56]
520	163-30	3245	4	811.25	[56]
521	163-32	16000	1.3	12307.69	[56]
522	163-34	400000	1.8	222222.22	[56]
523	163-36	1560	7	222.86	[56]
524	163-37	5450	3	1816.67	[56]
525	163-38	1600	3	533.33	[56]
526	163-46	13000	10	1300.00	[56]

527	163-1	100000	30	3333.33	[56]
528	163-9	30000	0.67	44776.12	[56]
529	163-49	100000	9.8	10204.08	[56]
530	163-11	100000	30.5	3278.69	[56]
531	163-52	10000	12.2	819.67	[56]
532	165-16b	30000	30	1000.00	[57]
533	165-16c	1200	4.5	266.67	[57]
534	167-7a	3857	8	482.13	[58]
535	167-7c	25000	8.2	3048.78	[58]
536	168-1c	1600	9.5	168.42	[59]
537	172-XXVI	5000	1	5000.00	[60]
538	172-XXVII4	1400	0.25	5600.00	[60]
539	172-XXVIII	1000	0.25	4000.00	[60]
540	172-XXIX	6000	0.5	12000.00	[60]
541	172-XXXVIII	3300	7.2	458.33	[60]
542	178-5	400000	1.8	222222.22	[61]
543	178-27	1000	2.5	400.00	[61]
544	178-34	100000	30	3333.33	[61]
545	178-35	100000	270	370.37	[61]
546	178-37	30000	0.67	44776.12	[61]

表S2　训练集中化合物的类别和来源(I: MMP-13对MMP-1的选择性抑制剂, N: MMP-13非抑制剂)

Table S2　The compounds in the training set for MMP-13, true class and the source of compounds (I: MMP-13 selective inhibitor over MMP-1, N: MMP-13 non-inhibitor)

No.	ID	类别	来源	No.	ID	类别	来源
1	54-19ee	I	[21]	228	62858	N	MDDR
2	109-11	I	[39]	229	51002	N	MDDR
3	123-24s	I	[46]	230	91528	N	MDDR
4	123-24f	I	[46]	231	2759	N	MDDR
5	114-14	I	[42]	232	71941	N	MDDR
6	123-24o	I	[46]	233	117716	N	MDDR
7	54-19o	I	[21]	234	112512	N	MDDR
8	123-24n	I	[46]	235	150892	N	MDDR
9	54-19x	I	[21]	236	126915	N	MDDR
10	123-24q	I	[46]	237	141920	N	MDDR

11	123-24l	I	[46]	238	94487	N	MDDR
12	120-7	I	[44]	239	87431	N	MDDR
13	123-24g	I	[46]	240	138071	N	MDDR
14	54-19t	I	[21]	241	139640	N	MDDR
15	107-22	I	[38]	242	35740	N	MDDR
16	120-6	I	[44]	243	59136	N	MDDR
17	123-24m	I	[46]	244	26358	N	MDDR
18	54-9j	I	[21]	245	150606	N	MDDR
19	79-4c	I	[26]	246	44780	N	MDDR
20	123-22e	I	[46]	247	150503	N	MDDR
21	123-27a	I	[46]	248	154193	N	MDDR
22	123-24r	I	[46]	249	86177	N	MDDR
23	32-57	I	[17]	250	112703	N	MDDR
24	123-26b	I	[46]	251	128182	N	MDDR
25	16-26	I	[9]	252	122764	N	MDDR
26	15-7h	I	[8]	253	84237	N	MDDR
27	123-22b	I	[46]	254	54228	N	MDDR
28	123-25d	I	[46]	255	99741	N	MDDR
29	123-9	I	[46]	256	125263	N	MDDR
30	16-12	I	[9]	257	107403	N	MDDR
31	22-13g	I	[12]	258	19345	N	MDDR
32	107-37	I	[38]	259	6057	N	MDDR
33	13-4e	I	[7]	260	14418	N	MDDR
34	137-71	I	[52]	261	380	N	MDDR
35	110-16	I	[40]	262	73972	N	MDDR
36	32-52	I	[17]	263	74741	N	MDDR
37	12-11c	I	[6]	264	120261	N	MDDR
38	114-16	I	[42]	265	156416	N	MDDR
39	19-32	I	[11]	266	10837	N	MDDR
40	35-23	I	[18]	267	21478	N	MDDR
41	35-28	I	[18]	268	62068	N	MDDR
42	16-14	I	[9]	269	149870	N	MDDR
43	24-94	I	[13]	270	74544	N	MDDR
44	54-19bb	I	[21]	271	59024	N	MDDR
45	124-4c	I	[47]	272	103462	N	MDDR

46	123-24k	I	[46]	273	27339	N	MDDR
47	79-4l	I	[26]	274	93314	N	MDDR
48	123-24i	I	[46]	275	4451	N	MDDR
49	32-58	I	[17]	276	40174	N	MDDR
50	32-64	I	[17]	277	127666	N	MDDR
51	123-26e	I	[46]	278	115093	N	MDDR
52	32-40	I	[17]	279	50829	N	MDDR
53	35-25	I	[18]	280	59232	N	MDDR
54	5-7	I	[1]	281	130010	N	MDDR
55	123-25a	I	[46]	282	11282	N	MDDR
56	123-25c	I	[46]	283	37653	N	MDDR
57	16-28	I	[9]	284	2717	N	MDDR
58	148-35	I	[53]	285	104809	N	MDDR
59	123-24j	I	[46]	286	159314	N	MDDR
60	19-39	I	[11]	287	154534	N	MDDR
61	123-24h	I	[46]	288	84939	N	MDDR
62	35-13	I	[18]	289	132525	N	MDDR
63	16-22	I	[9]	290	148205	N	MDDR
64	16-21	I	[9]	291	121496	N	MDDR
65	133-4o	I	[50]	292	17861	N	MDDR
66	54-19k	I	[21]	293	109817	N	MDDR
67	19-38	I	[11]	294	62302	N	MDDR
68	80-5a	I	[27]	295	94303	N	MDDR
69	32-34	I	[17]	296	64011	N	MDDR
70	102-7	I	[34]	297	101783	N	MDDR
71	32-54	I	[17]	298	155946	N	MDDR
72	123-26c	I	[46]	299	128043	N	MDDR
73	102-9	I	[34]	300	45438	N	MDDR
74	102-11	I	[34]	301	91179	N	MDDR
75	124-5	I	[47]	302	155602	N	MDDR
76	123-24b	I	[46]	303	10478	N	MDDR
77	54-19dd	I	[21]	304	117843	N	MDDR
78	102-13	I	[34]	305	22552	N	MDDR
79	12-11k	I	[6]	306	121184	N	MDDR
80	135-9g	I	[51]	307	26416	N	MDDR

81	109-28	I	[39]	308	20063	N	MDDR
82	105-3m	I	[36]	309	3135	N	MDDR
83	69-1	I	[23]	310	33112	N	MDDR
84	148-37	I	[53]	311	2019	N	MDDR
85	32-41	I	[17]	312	75759	N	MDDR
86	104-27	I	[35]	313	67015	N	MDDR
87	167-7c	I	[58]	314	122179	N	MDDR
88	12-11s	I	[6]	315	128992	N	MDDR
89	35-18	I	[18]	316	10556	N	MDDR
90	124-4i	I	[47]	317	128435	N	MDDR
91	54-19b	I	[21]	318	106931	N	MDDR
92	31-2u	I	[16]	319	148432	N	MDDR
93	124-4a	I	[47]	320	95468	N	MDDR
94	118-7	I	[43]	321	83895	N	MDDR
95	16-24	I	[9]	322	27143	N	MDDR
96	123-24u	I	[46]	323	11865	N	MDDR
97	123-24a	I	[46]	324	112113	N	MDDR
98	16-16	I	[9]	325	13489	N	MDDR
99	32-51	I	[17]	326	53251	N	MDDR
100	12-11l	I	[6]	327	50925	N	MDDR
101	133-4p	I	[50]	328	81691	N	MDDR
102	32-48	I	[17]	329	26422	N	MDDR
103	32-62	I	[17]	330	25724	N	MDDR
104	22-13i	I	[12]	331	87505	N	MDDR
105	120-10	I	[44]	332	88748	N	MDDR
106	31-2q	I	[16]	333	89025	N	MDDR
107	80-5g	I	[27]	334	37044	N	MDDR
108	127-2m	I	[49]	335	52640	N	MDDR
109	121-36	I	[45]	336	127210	N	MDDR
110	109-13	I	[39]	337	69946	N	MDDR
111	10-66	I	[4]	338	144175	N	MDDR
112	79-4j	I	[26]	339	15388	N	MDDR
113	15-6i	I	[8]	340	44283	N	MDDR
114	10-35	I	[4]	341	6025	N	MDDR
115	54-19aa	I	[21]	342	131793	N	MDDR

116	127-2l	I	[49]	343	80602	N	MDDR
117	54-19m	I	[21]	344	153699	N	MDDR
118	124-4e	I	[47]	345	12415	N	MDDR
119	12-11p	I	[6]	346	140388	N	MDDR
120	19-34	I	[11]	347	37522	N	MDDR
121	32-27	I	[17]	348	156358	N	MDDR
122	32-50	I	[17]	349	131154	N	MDDR
123	22-13a	I	[12]	350	113424	N	MDDR
124	135-9i	I	[51]	351	4468	N	MDDR
125	54-19p	I	[21]	352	107553	N	MDDR
126	15-6h	I	[8]	353	14906	N	MDDR
127	32-49	I	[17]	354	8320	N	MDDR
128	123-23	I	[46]	355	6701	N	MDDR
129	102-12	I	[34]	356	4166	N	MDDR
130	80-5d	I	[27]	357	23422	N	MDDR
131	124-4d	I	[47]	358	140405	N	MDDR
132	107-21	I	[38]	359	8833	N	MDDR
133	24-96	I	[13]	360	71186	N	MDDR
134	10-75	I	[4]	361	108193	N	MDDR
135	123-28a	I	[46]	362	10772	N	MDDR
136	41-B3	I	[19]	363	39757	N	MDDR
137	16-27	I	[9]	364	149513	N	MDDR
138	16-19	I	[9]	365	84151	N	MDDR
139	106-6b	I	[37]	366	13920	N	MDDR
140	22-13f	I	[12]	367	157791	N	MDDR
141	54-19l	I	[21]	368	63276	N	MDDR
142	12-11t	I	[6]	369	17437	N	MDDR
143	79-4q	I	[26]	370	19318	N	MDDR
144	31-2f	I	[16]	371	46114	N	MDDR
145	123-28c	I	[46]	372	50835	N	MDDR
146	54-19c	I	[21]	373	91294	N	MDDR
147	10-54	I	[4]	374	638	N	MDDR
148	10-24	I	[4]	375	73774	N	MDDR
149	124-4f	I	[47]	376	75450	N	MDDR
150	165-16b	I	[57]	377	55038	N	MDDR

151	16-25	I	[9]	378	138720	N	MDDR
152	12-11q	I	[6]	379	153912	N	MDDR
153	17-4a	I	[10]	380	32524	N	MDDR
154	12-11j	I	[6]	381	115482	N	MDDR
155	32-32	I	[17]	382	147932	N	MDDR
156	79-4d	I	[26]	383	111901	N	MDDR
157	12-11g	I	[6]	384	107919	N	MDDR
158	32-46	I	[17]	385	71844	N	MDDR
159	107-24	I	[38]	386	58917	N	MDDR
160	12-11u	I	[6]	387	108603	N	MDDR
161	12-11i	I	[6]	388	122540	N	MDDR
162	102-10	I	[34]	389	50594	N	MDDR
163	107-29	I	[38]	390	85410	N	MDDR
164	133-4t	I	[50]	391	8754	N	MDDR
165	12-11h	I	[6]	392	51258	N	MDDR
166	10-51	I	[4]	393	95069	N	MDDR
167	107-18	I	[38]	394	62059	N	MDDR
168	167-7a	I	[58]	395	16610	N	MDDR
169	12-11d	I	[6]	396	69816	N	MDDR
170	126-4x	I	[48]	397	60755	N	MDDR
171	135-8u	I	[51]	398	6141	N	MDDR
172	101-6c	I	[33]	399	70295	N	MDDR
173	19-49	I	[11]	400	72111	N	MDDR
174	10-46	I	[4]	401	113655	N	MDDR
175	32-39	I	[17]	402	7990	N	MDDR
176	79-4g	I	[26]	403	82457	N	MDDR
177	10-32	I	[4]	404	17459	N	MDDR
178	105-3l	I	[36]	405	41020	N	MDDR
179	133-4s	I	[50]	406	37551	N	MDDR
180	47-16a	I	[20]	407	159615	N	MDDR
181	19-33	I	[11]	408	114904	N	MDDR
182	12-11v	I	[6]	409	41224	N	MDDR
183	121-30	I	[45]	410	57775	N	MDDR
184	112-2	I	[41]	411	53680	N	MDDR
185	10-73	I	[4]	412	86601	N	MDDR

186	35-21	I	[18]	413	129758	N	MDDR
187	133-4q	I	[50]	414	58188	N	MDDR
188	12-11r	I	[6]	415	5685	N	MDDR
189	30-39	I	[15]	416	38521	N	MDDR
190	32-33	I	[17]	417	77289	N	MDDR
191	32-31	I	[17]	418	43999	N	MDDR
192	126-4aa	I	[48]	419	92386	N	MDDR
193	123-22g	I	[46]	420	124472	N	MDDR
194	114-18	I	[42]	421	56413	N	MDDR
195	105-3i	I	[36]	422	37268	N	MDDR
196	22-13m	I	[12]	423	29367	N	MDDR
197	12-11f	I	[6]	424	98869	N	MDDR
198	32-42	I	[17]	425	86596	N	MDDR
199	165-16c	I	[57]	426	17655	N	MDDR
200	124-4l	I	[47]	427	132998	N	MDDR
201	123-22a	I	[46]	428	73175	N	MDDR
202	12-11n	I	[6]	429	58260	N	MDDR
203	19-40	I	[11]	430	109676	N	MDDR
204	133-4r	I	[50]	431	155479	N	MDDR
205	123-28b	I	[46]	432	22933	N	MDDR
206	126-4y	I	[48]	433	111911	N	MDDR
207	105-3j	I	[36]	434	142114	N	MDDR
208	74-3l	I	[24]	435	89007	N	MDDR
209	81-20	I	[28]	436	149752	N	MDDR
210	135-8r	I	[51]	437	76783	N	MDDR
211	137-14	I	[52]	438	152439	N	MDDR
212	81-21	I	[28]	439	61796	N	MDDR
213	114-13	I	[42]	440	54211	N	MDDR
214	56-25	I	[22]	441	96369	N	MDDR
215	47-16b	I	[20]	442	129073	N	MDDR
216	69-28	I	[23]	443	65205	N	MDDR
217	105-3f	I	[36]	444	61668	N	MDDR
218	105-3a	I	[36]	445	96065	N	MDDR
219	12-11o	I	[6]	446	123945	N	MDDR
220	126-4z	I	[48]	447	79073	N	MDDR

221	92-4r	I	[31]	448	47092	N	MDDR
222	107712	N	MDDR	449	74169	N	MDDR
223	121621	N	MDDR	450	22534	N	MDDR
224	44884	N	MDDR	451	64177	N	MDDR
225	26413	N	MDDR	452	73428	N	MDDR
226	99029	N	MDDR	453	51648	N	MDDR
227	124178	N	MDDR	454	12644	N	MDDR

表S3　测试集中化合物的类别和来源(I：MMP-13对MMP-1的选择性抑制剂，N：MMP-13非抑制剂)

Table S3　The compounds in the testing set for MMP-13, true class and the source of compounds (I: MMP-13 selective inhibitor over MMP-1, N: MMP-13 non-inhibitor)

No.	ID	类别	来源	No.	ID	类别	来源
1	54-19w	I	[21]	119	54-9d	I	[21]
2	109-12	I	[39]	120	127-8c	I	[49]
3	123-27e	I	[46]	121	81-19	I	[28]
4	123-27g	I	[46]	122	153-28	I	[54]
5	114-4	I	[42]	123	25-6	I	[14]
6	123-27f	I	[46]	124	54-9h	I	[21]
7	54-19r	I	[21]	125	121623	N	MDDR
8	123-27h	I	[46]	126	47880	N	MDDR
9	54-19y	I	[21]	127	77964	N	MDDR
10	123-24t	I	[46]	128	118245	N	MDDR
11	123-27i	I	[46]	129	25184	N	MDDR
12	120-8	I	[44]	130	158352	N	MDDR
13	123-24p	I	[46]	131	144071	N	MDDR
14	54-19v	I	[21]	132	53430	N	MDDR
15	107-27	I	[38]	133	37106	N	MDDR
16	120-9	I	[44]	134	156811	N	MDDR
17	22-13b	I	[12]	135	82379	N	MDDR
18	54-9l	I	[21]	136	64809	N	MDDR
19	79-4m	I	[26]	137	19170	N	MDDR
20	123-22f	I	[46]	138	83857	N	MDDR
21	123-27c	I	[46]	139	46347	N	MDDR
22	123-26d	I	[46]	140	155173	N	MDDR
23	54-19f	I	[21]	141	149343	N	MDDR

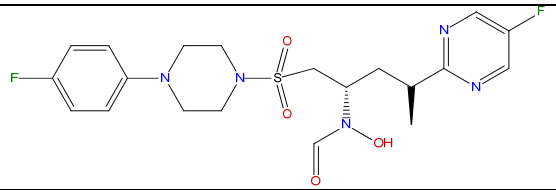
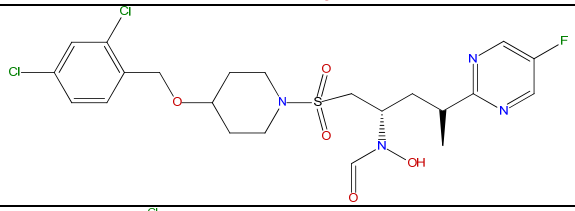
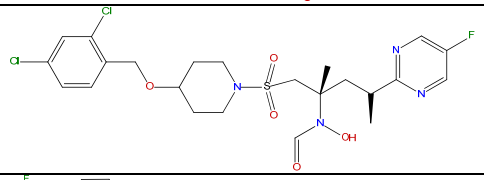
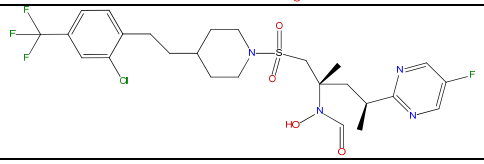
24	16-29	I	[9]	142	104806	N	MDDR
25	16-30	I	[9]	143	79648	N	MDDR
26	79-4o	I	[26]	144	5106	N	MDDR
27	54-19d	I	[21]	145	101059	N	MDDR
28	16-18	I	[9]	146	19363	N	MDDR
29	22-13d	I	[12]	147	72150	N	MDDR
30	22-13h	I	[12]	148	94137	N	MDDR
31	80-5e	I	[27]	149	102244	N	MDDR
32	31-2j	I	[16]	150	152138	N	MDDR
33	32-36	I	[17]	151	82544	N	MDDR
34	123-27d	I	[46]	152	105641	N	MDDR
35	35-14	I	[18]	153	97240	N	MDDR
36	12-11e	I	[6]	154	1273	N	MDDR
37	114-20	I	[42]	155	7473	N	MDDR
38	31-2p	I	[16]	156	151219	N	MDDR
39	35-24	I	[18]	157	139810	N	MDDR
40	35-29	I	[18]	158	15444	N	MDDR
41	19-28	I	[11]	159	95361	N	MDDR
42	35-20	I	[18]	160	79392	N	MDDR
43	54-19cc	I	[21]	161	102653	N	MDDR
44	31-2i	I	[16]	162	359	N	MDDR
45	91-2	I	[30]	163	121143	N	MDDR
46	16-13	I	[9]	164	101516	N	MDDR
47	54-19e	I	[21]	165	149687	N	MDDR
48	16-23	I	[9]	166	37694	N	MDDR
49	35-27	I	[18]	167	130137	N	MDDR
50	5-8	I	[1]	168	22952	N	MDDR
51	22-13c	I	[12]	169	90574	N	MDDR
52	54-19g	I	[21]	170	79216	N	MDDR
53	69-3	I	[23]	171	33355	N	MDDR
54	123-26a	I	[46]	172	68425	N	MDDR
55	19-47	I	[11]	173	44385	N	MDDR
56	16-15	I	[9]	174	42034	N	MDDR
57	35-15	I	[18]	175	601	N	MDDR
58	32-59	I	[17]	176	8245	N	MDDR
59	32-24	I	[17]	177	64235	N	MDDR
60	54-19s	I	[21]	178	42943	N	MDDR
61	31-2d	I	[16]	179	128011	N	MDDR
62	32-56	I	[17]	180	141027	N	MDDR
63	24-95	I	[13]	181	91809	N	MDDR
64	35-22	I	[18]	182	88467	N	MDDR

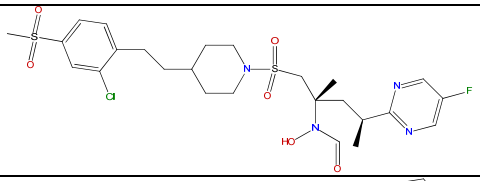
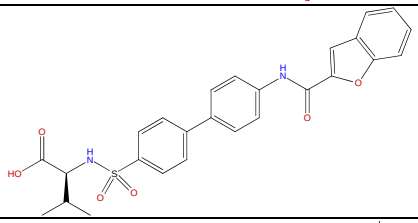
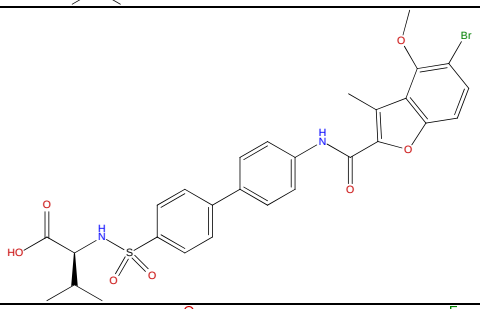
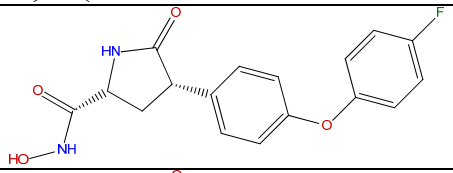
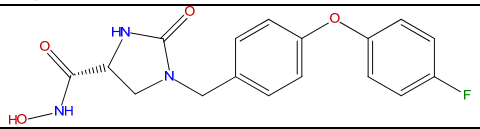
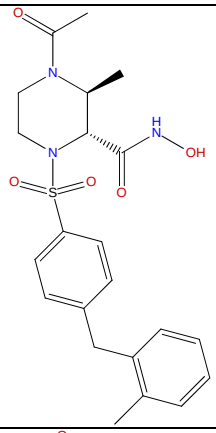
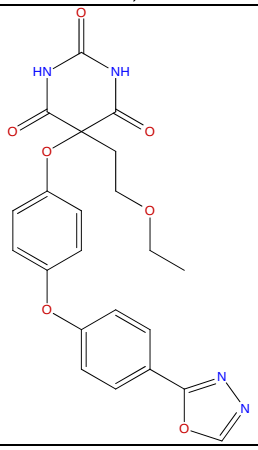
65	35-30	I	[18]	183	36590	N	MDDR
66	32-53	I	[17]	184	90460	N	MDDR
67	35-5	I	[18]	185	154504	N	MDDR
68	105-3n	I	[36]	186	128333	N	MDDR
69	80-5f	I	[27]	187	126201	N	MDDR
70	79-4h	I	[26]	188	108248	N	MDDR
71	81-24	I	[28]	189	32883	N	MDDR
72	54-19j	I	[21]	190	132989	N	MDDR
73	80-5c	I	[27]	191	33677	N	MDDR
74	80-5h	I	[27]	192	122250	N	MDDR
75	54-19z	I	[21]	193	44834	N	MDDR
76	124-4b	I	[47]	194	15642	N	MDDR
77	54-9k	I	[21]	195	95749	N	MDDR
78	22-13n	I	[12]	196	21164	N	MDDR
79	124-2	I	[47]	197	57952	N	MDDR
80	69-7	I	[23]	198	93980	N	MDDR
81	120-5	I	[44]	199	146877	N	MDDR
82	79-4p	I	[26]	200	116634	N	MDDR
83	54-9g	I	[21]	201	14872	N	MDDR
84	54-19q	I	[21]	202	58212	N	MDDR
85	114-23	I	[42]	203	148485	N	MDDR
86	79-4i	I	[26]	204	9122	N	MDDR
87	54-19u	I	[21]	205	96183	N	MDDR
88	10-41	I	[4]	206	59319	N	MDDR
89	32-44	I	[17]	207	117573	N	MDDR
90	124-1a	I	[47]	208	111806	N	MDDR
91	22-13e	I	[12]	209	65740	N	MDDR
92	54-9i	I	[21]	210	68999	N	MDDR
93	75-14c	I	[25]	211	17188	N	MDDR
94	16-10	I	[9]	212	3394	N	MDDR
95	148-27	I	[53]	213	1036	N	MDDR
96	69-35	I	[23]	214	65978	N	MDDR
97	12-11m	I	[6]	215	156986	N	MDDR
98	54-19a	I	[21]	216	87865	N	MDDR
99	54-19i	I	[21]	217	6155	N	MDDR
100	19-62	I	[11]	218	95848	N	MDDR
101	54-9m	I	[21]	219	45505	N	MDDR
102	31-2h	I	[16]	220	158045	N	MDDR
103	80-7b	I	[27]	221	97948	N	MDDR
104	22-13l	I	[12]	222	68512	N	MDDR
105	54-19n	I	[21]	223	24279	N	MDDR

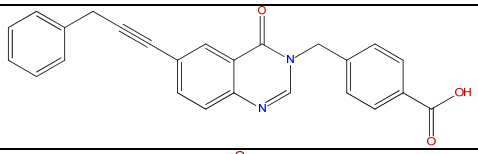
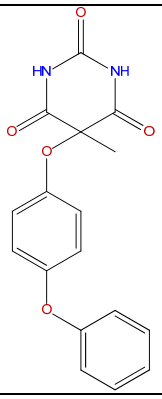
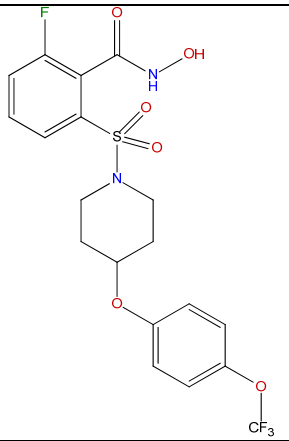
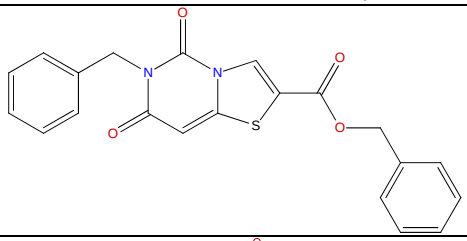
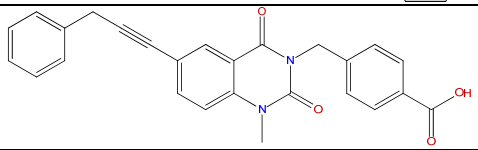
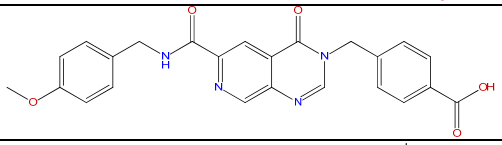
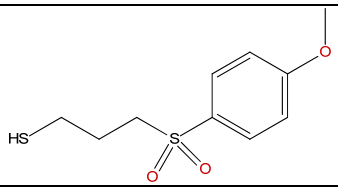
106	13-13	I	[7]	224	47414	N	MDDR
107	91-1	I	[30]	225	114637	N	MDDR
108	31-2g	I	[16]	226	12101	N	MDDR
109	74-3q	I	[24]	227	80033	N	MDDR
110	54-6	I	[21]	228	13804	N	MDDR
111	32-47	I	[17]	229	48981	N	MDDR
112	153-24	I	[54]	230	62915	N	MDDR
113	32-25	I	[17]	231	33224	N	MDDR
114	54-9b	I	[21]	232	29831	N	MDDR
115	92-4n	I	[31]	233	48851	N	MDDR
116	31-1	I	[16]	234	137235	N	MDDR
117	84-5	I	[29]	/235	123934	N	MDDR
118	79-4k	I	[26]	236	7332	N	MDDR

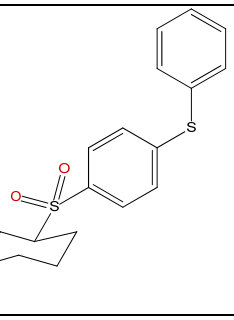
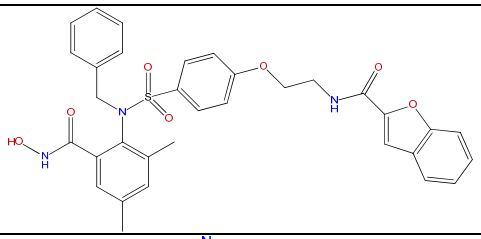
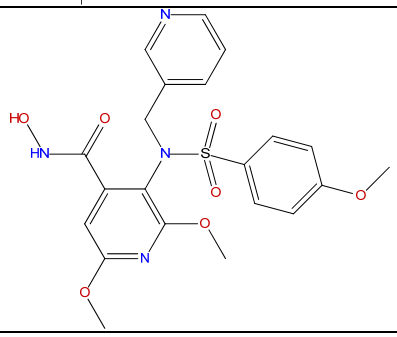
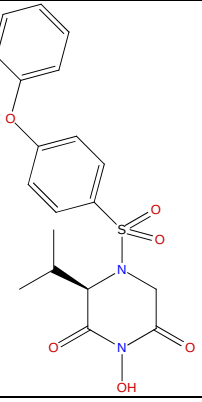
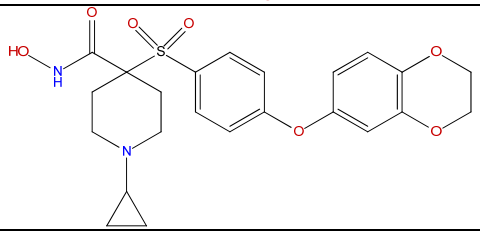
表S4　外部验证集中化合物的结构、类别和来源(I：MMP-13对MMP-1的选择性抑制剂，N：MMP-13非抑制剂)

Table S4　The compounds in the external independent validation set for MMP-13, structures, true class and the source of compounds (I: MMP-13 selective inhibitor over MMP-1, N: MMP-13 non-inhibitor)

No.	ID	结构	类别	来源
1	156-1		I	[55]
2	156-2		I	[55]
3	156-4		I	[55]
4	156-8a		I	[55]

5	/156-8q		I	[55]
6	163-32		I	[56]
7	/163-34		I	[56]
8	163-36		I	[56]
9	163-37		I	[56]
10	163-38		I	[56]
11	163-46		I	[56]

12	/163-49		I	[56]
13	163-50		I	[56]
14	163-51	/	I	[56]
15	163-52		I	[56]
16	163-1		I	[56]
17	163-9		I	[56]
18	163-11		I	[56]
19	163-18		I	[56]
20	163-19	/	I	[56]

21	163-20		I	[56]
22	163-26		I	[56]
23	163-29		I	[56]
24	163-30	/	I	[56]
25	168-1c		I	[59]
26	172-XXIX		I	[60]
27	172-XXVI	/	I	[60]

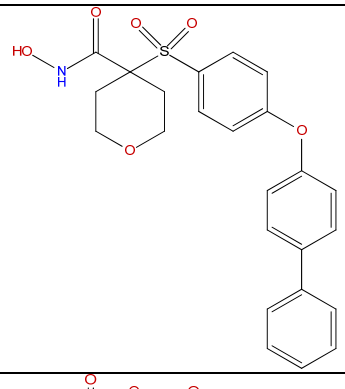
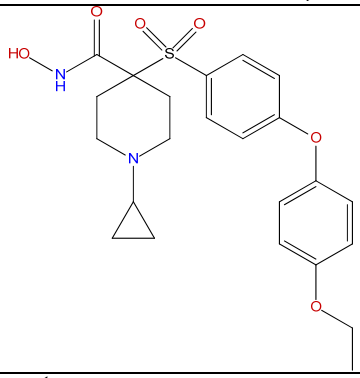
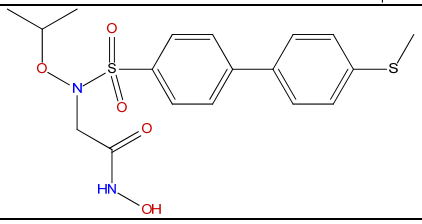
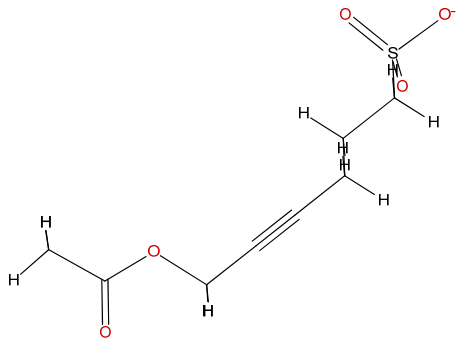
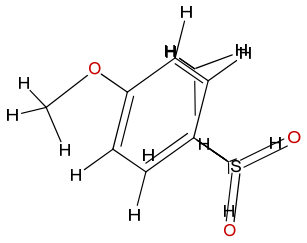
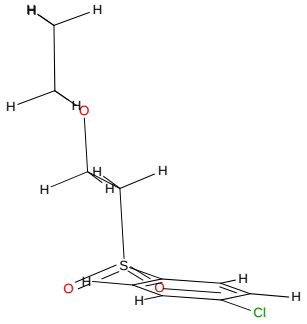
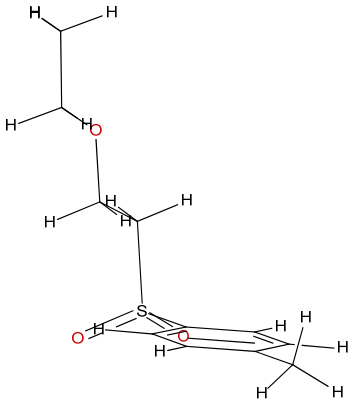
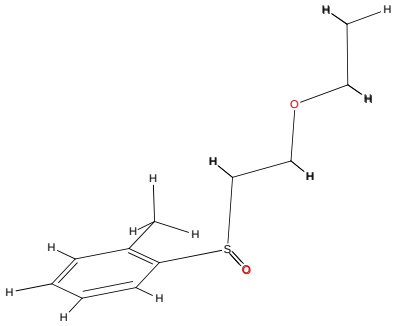
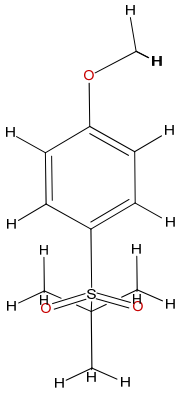
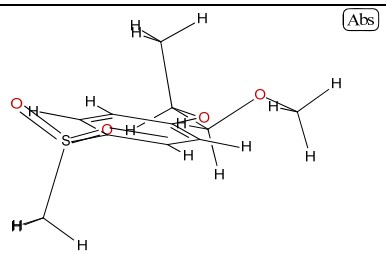
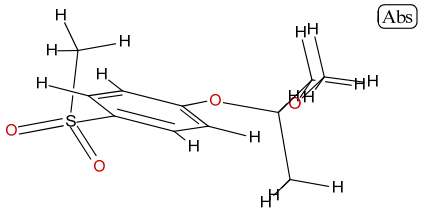
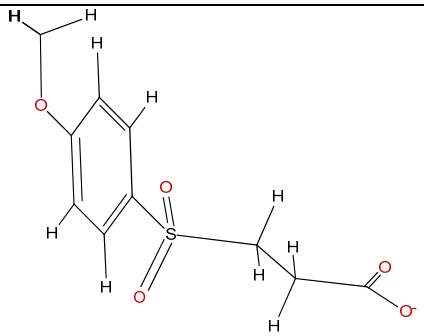
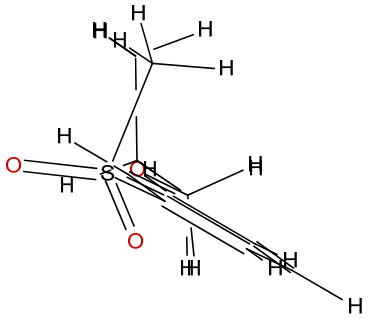
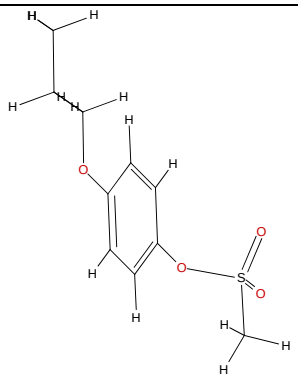
28	172-XXVI I4		I	[60]
29	172-XXVI II		I	[60]
30	172-XXX VIII		I	[60]

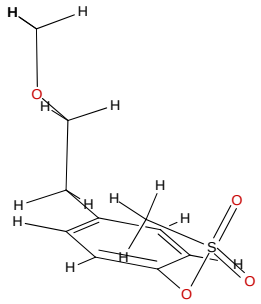
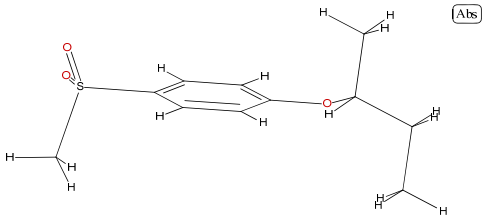
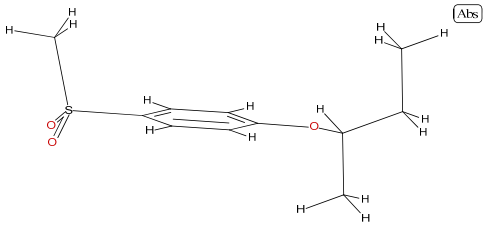
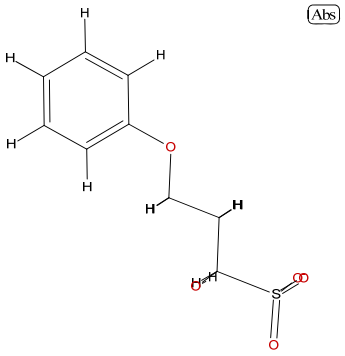
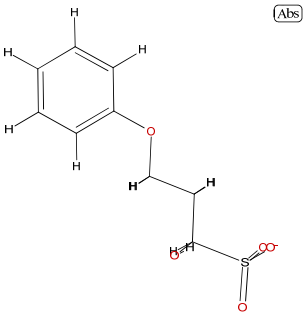
表 S5　28个经过虚拟筛选命中的潜在的对MMP-13有选择性抑制作用的化合物

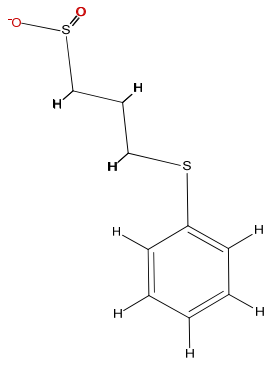
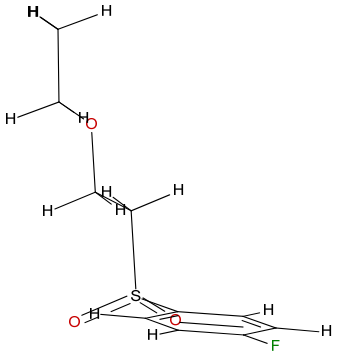
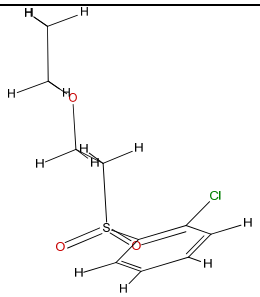
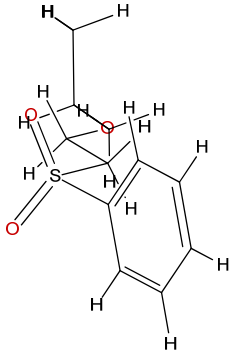
Table S5　28 potential hits which may be selective inhibitors for MMP-13 by virtual screening

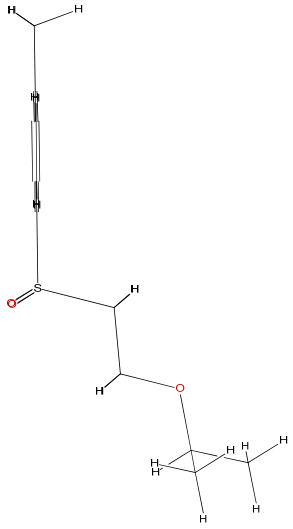
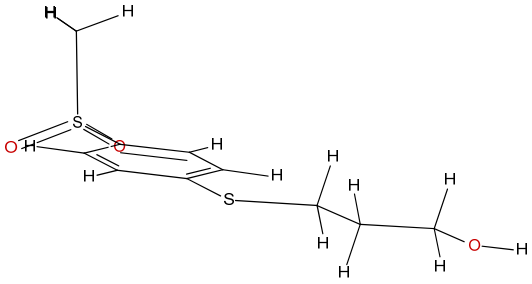
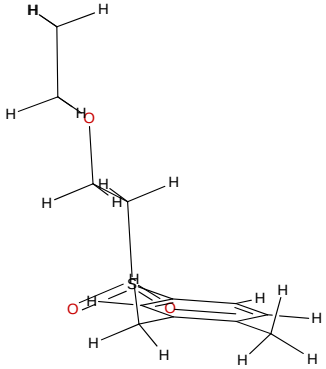
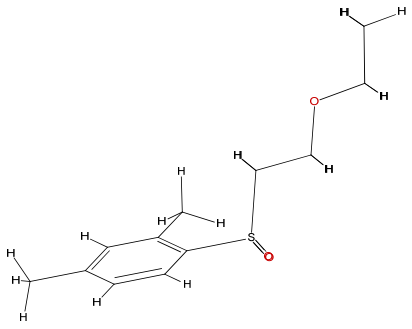
No.	ID	Structure
1	ZINC05378696	

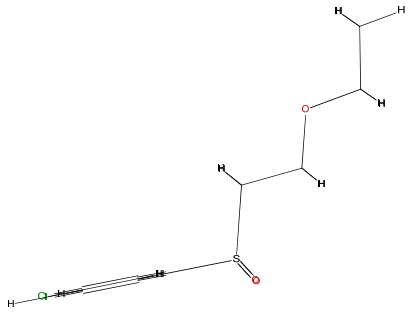
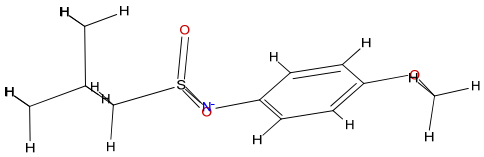
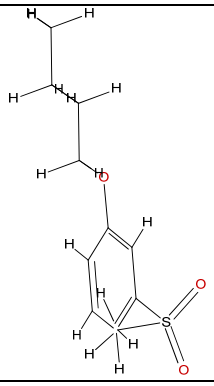
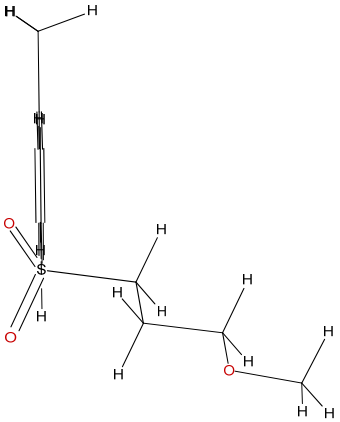
2	ZINC34569283	
3	ZINC60423558	
4	ZIN/C60423570	
5	ZIN/C57878759	
6	ZINC00270963	

7	ZINC78940872	
8	ZINC78940878	
9	ZIN/C00266945	
10	ZIN/C60815089	
11	ZINC70828337	

12	ZINC70828764	
13	ZINC78837195	
14	ZIN/C78837203	
15	ZINC71776975	
16	ZINC71776977	

17	ZINC05604176	
18	ZINC57874921	
19	ZINC57875173	
20	ZINC78873700	

21	ZINC78873703	
22	ZINC60393921	
23	ZINC57875908	
24	ZINC57875966	

25	ZINC78978756	
26	ZINC66574967	
27	ZINC71912419	
28	ZINC67746866	

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