Supporting Information

Quantitative structure-activity relationships for structurally diverse chemotypes having anti-*Trypanosoma cruzi* activity

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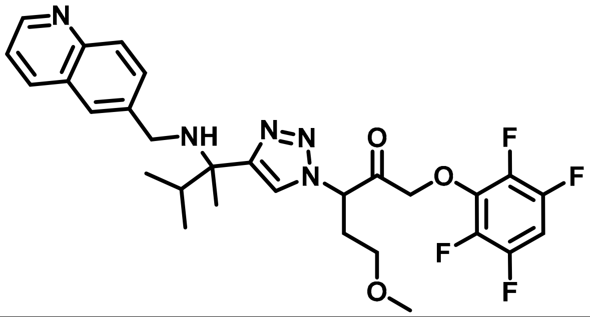
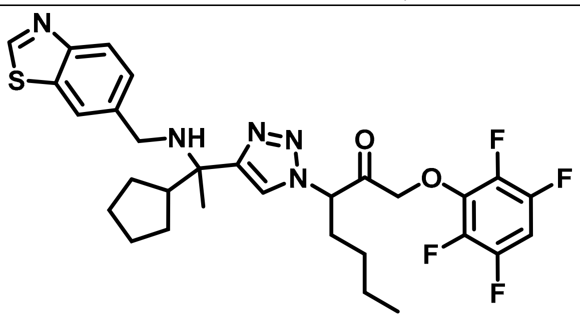
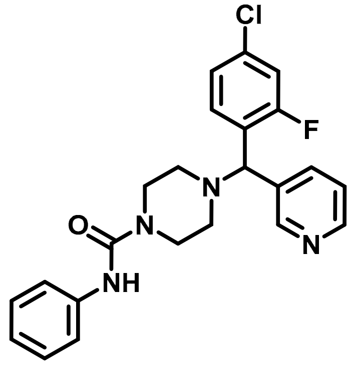
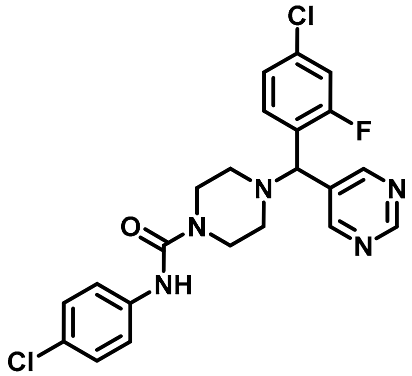
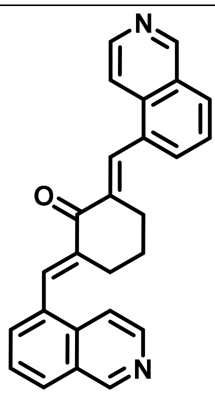
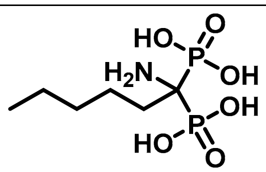
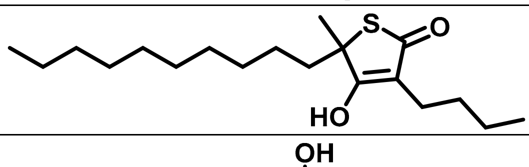
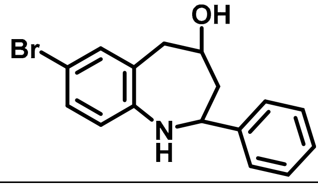
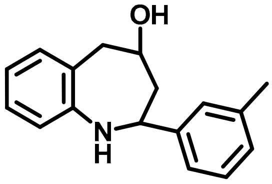
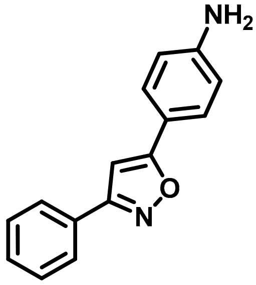
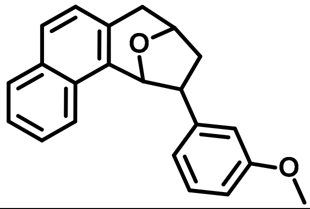
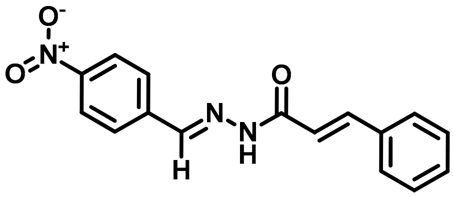
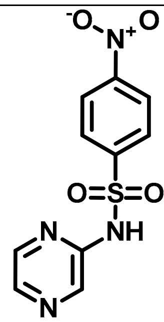
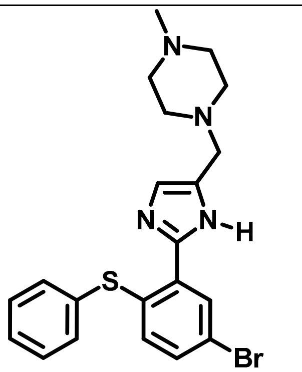
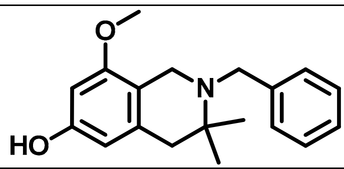
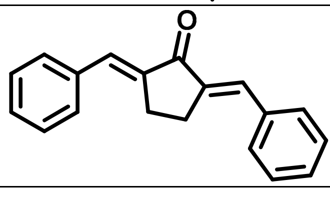
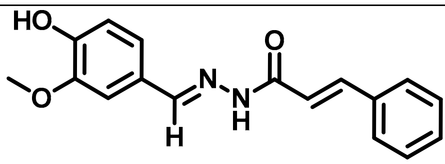
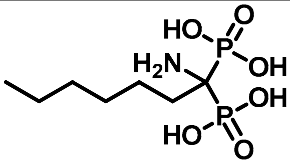
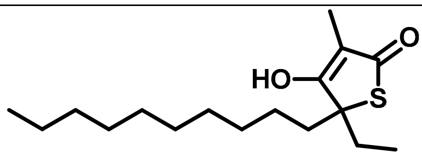
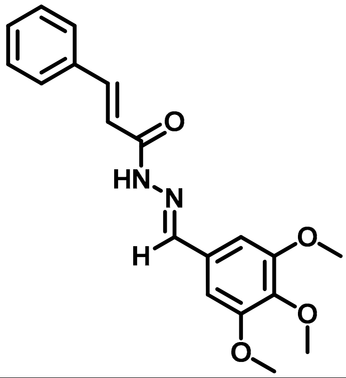
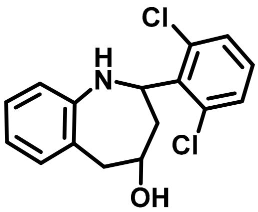
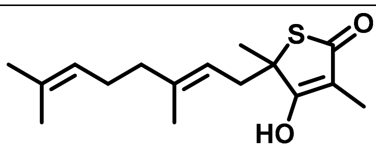
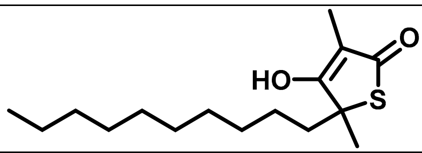
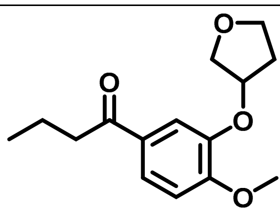
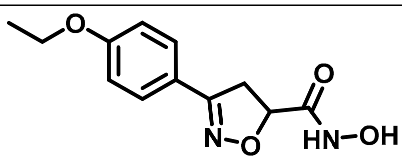
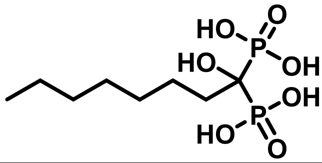
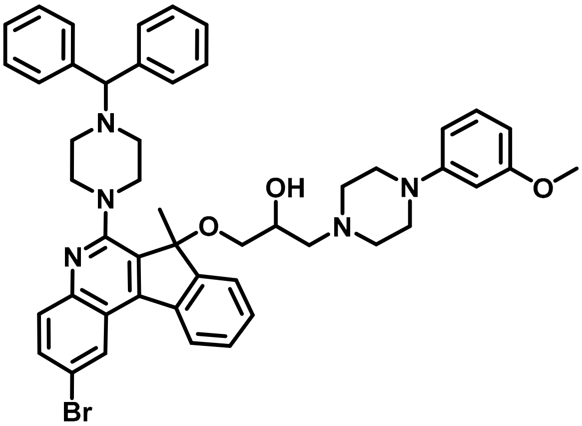
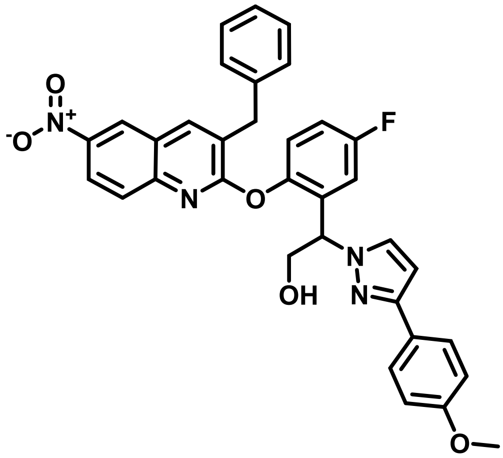
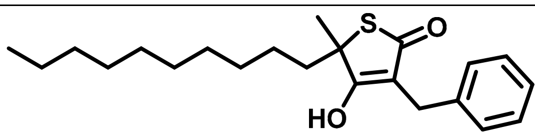
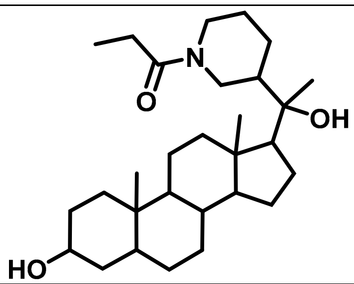
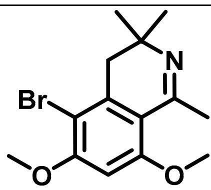
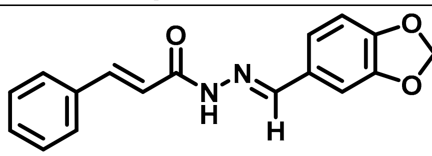
Table S1. Dataset used to build the artificial neural networks and the kernel-based partial least squares models.

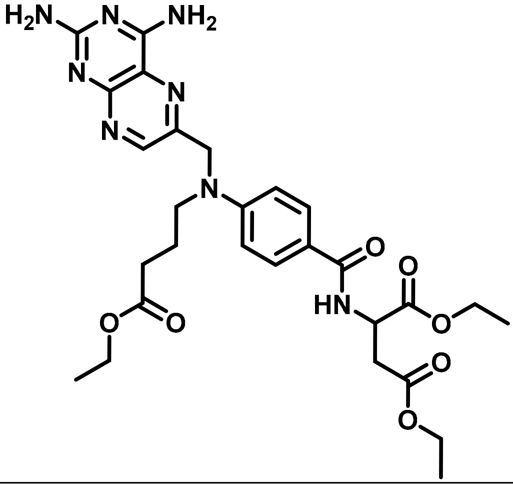
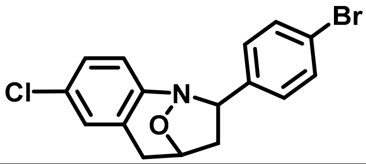
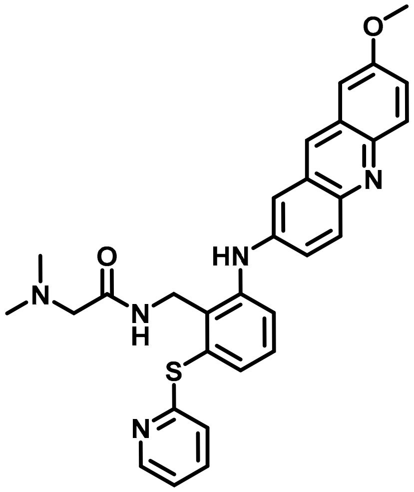
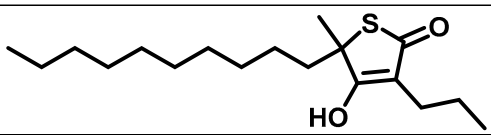
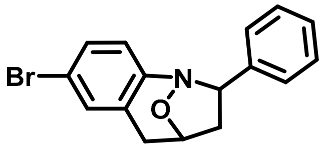
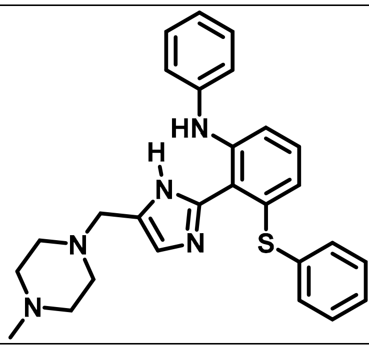
Molecule	Structure	pIC_{50}	Reference
3		8.70	1
4		8.52	1

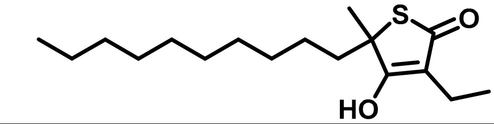
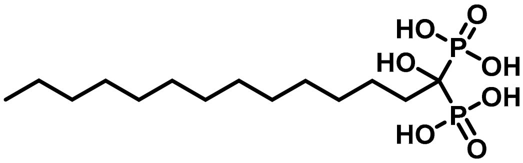
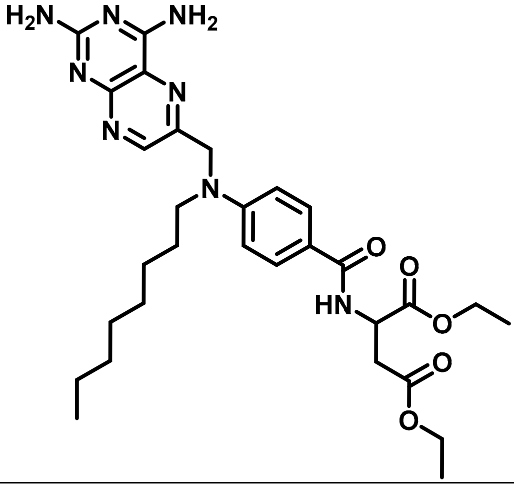
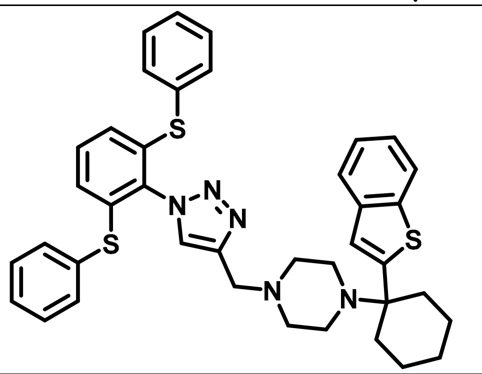
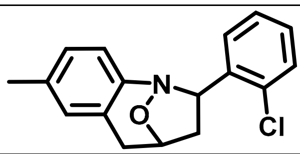
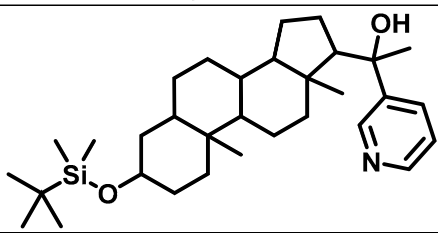
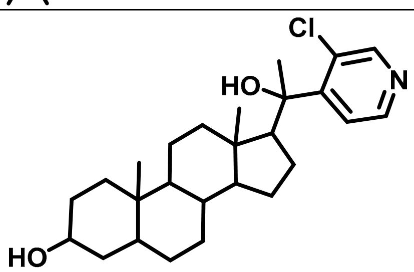
5		8.22	2
6		8.00	2
7		4.16	3
8		4.11	4
9		4.11	5
10		4.01	6
46		4.01	6

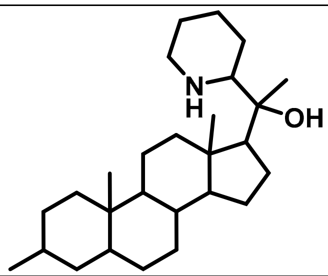
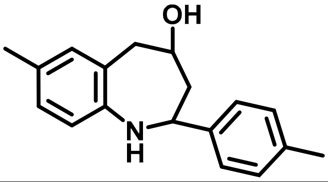
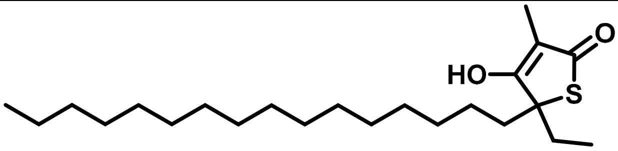
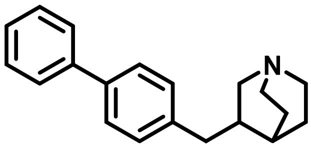
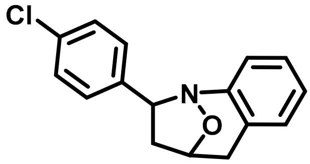
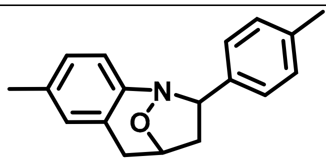
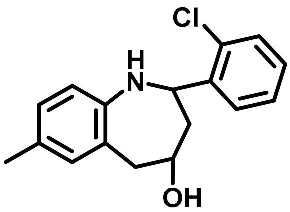
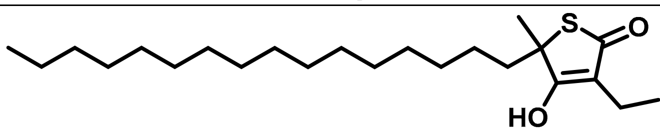
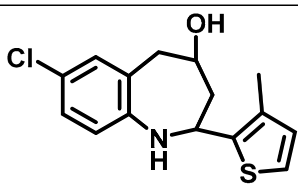
47		4.04	7
48		4.05	8
49*		4.09	9
50		4.12	10
51		4.12	11
52		4.12	12
53*		4.14	3

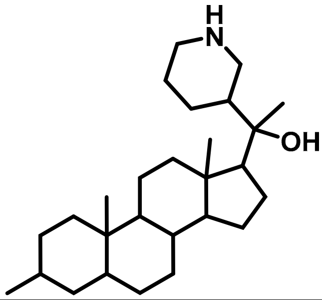
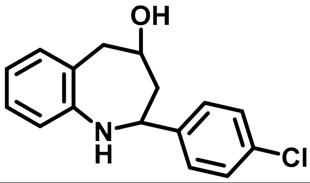
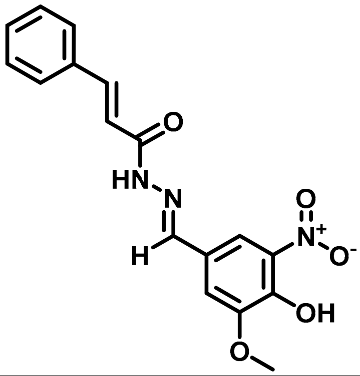
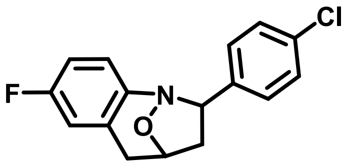
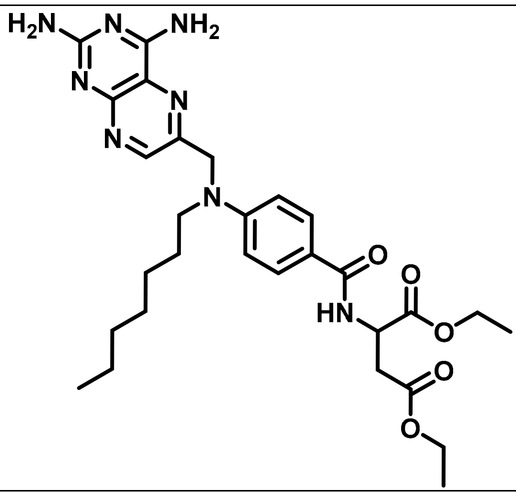
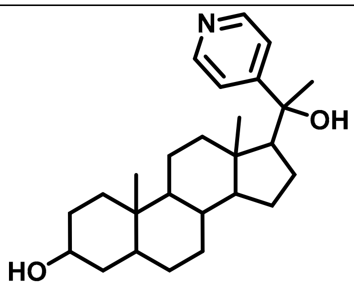
54		4.14	9
55		4.14	4
56*		4.14	5
57		4.15	9
58		4.16	6
59		4.17	5
60		4.17	5
61*		4.17	13
62		4.18	14

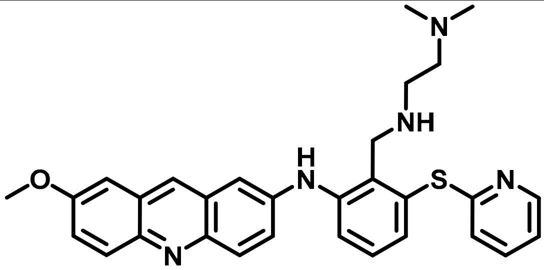
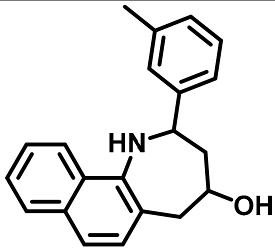
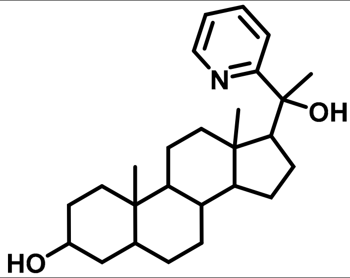
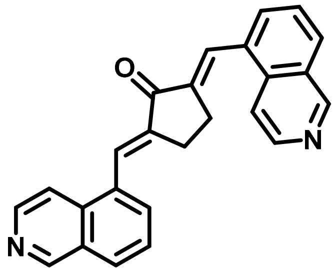
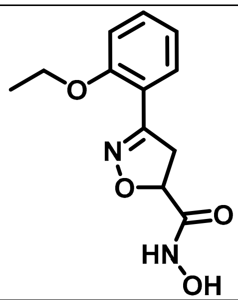
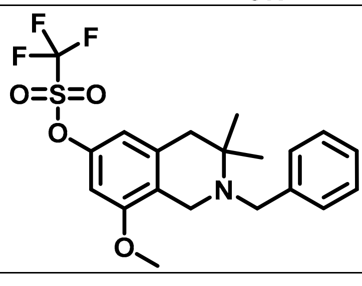
63*		4.18	15
64		4.19	16
65		4.19	16
66		4.19	5
67		4.19	17
68		4.20	12
69		4.21	9

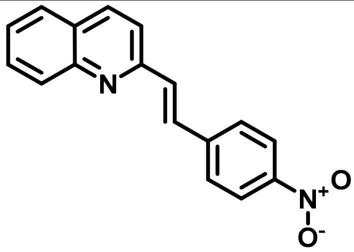
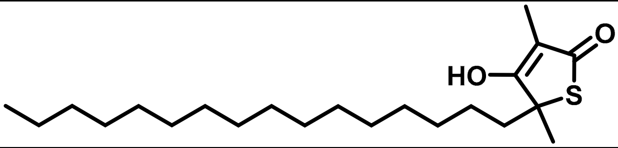
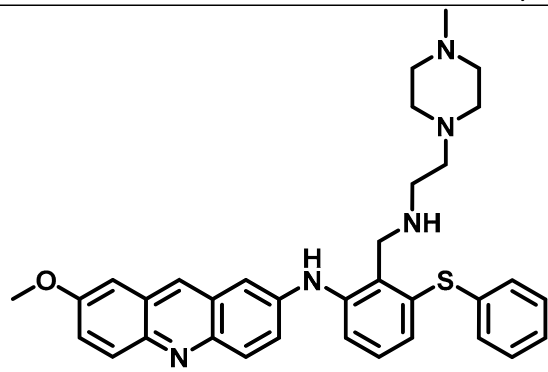
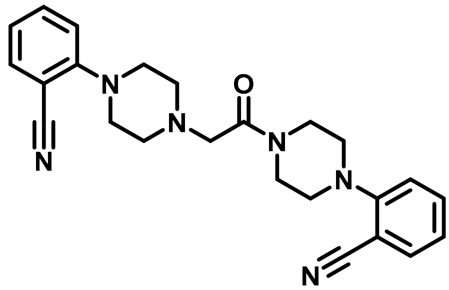
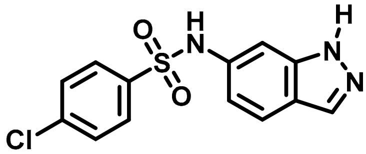
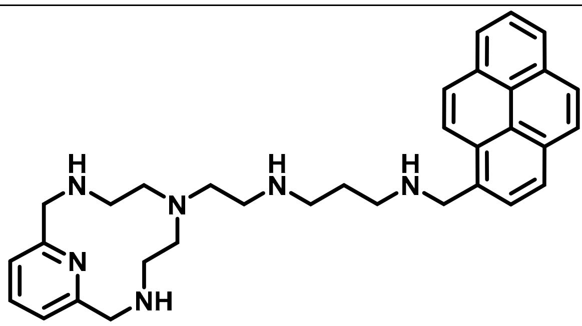
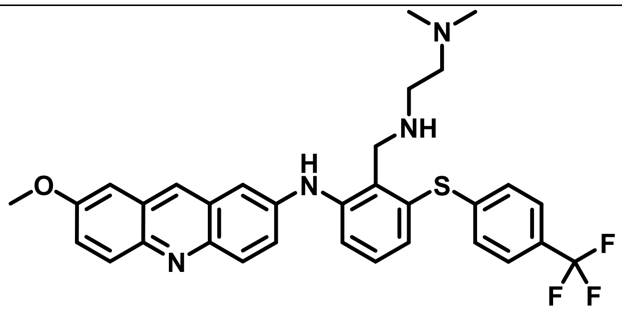
70*		4.21	18
71		4.22	6
72		4.24	19
73		4.25	5
74		4.25	6
75*		4.27	11

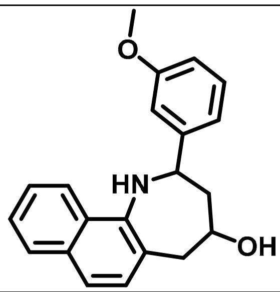
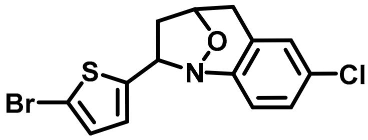
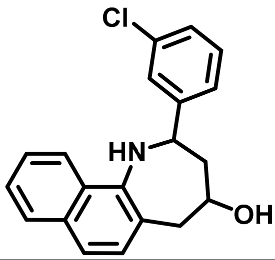
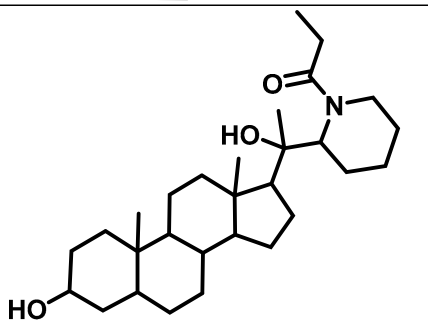
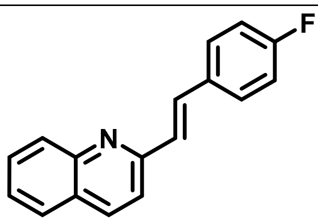
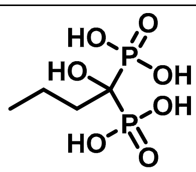
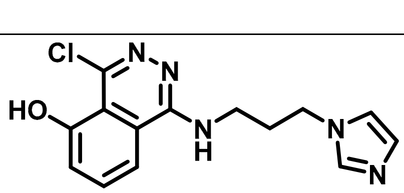
76		4.27	5
77*		4.27	15
78		4.27	18
79		4.28	11
80		4.28	6
81		4.29	17
82		4.30	17

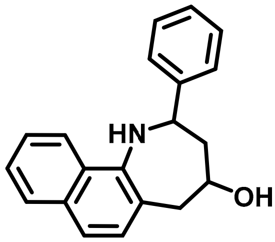
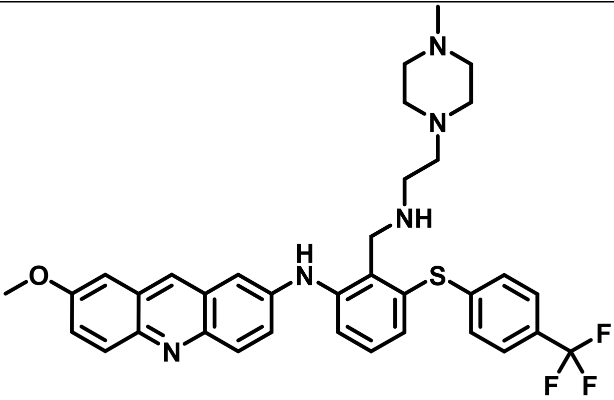
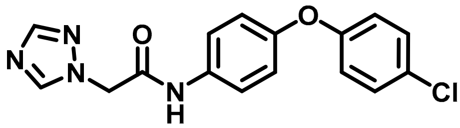
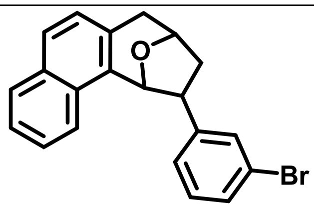
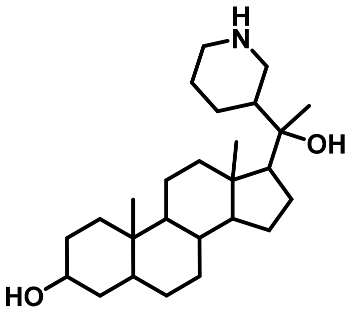
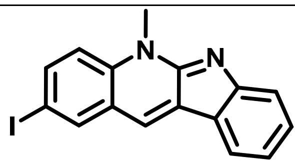
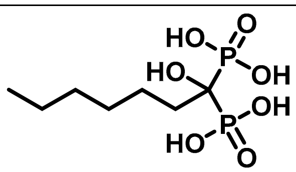
83		4.30	17
84*		4.30	6
85		4.31	5
86		4.33	20
87*		4.34	6
88		4.34	6
89		4.34	6
90*		4.37	5
91		4.38	21

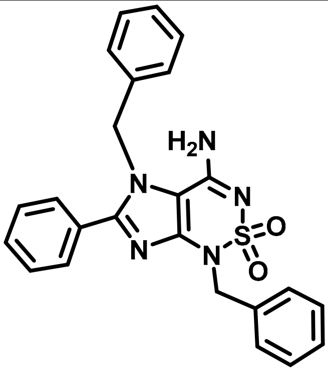
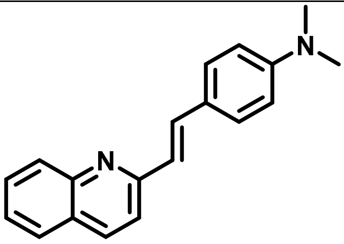
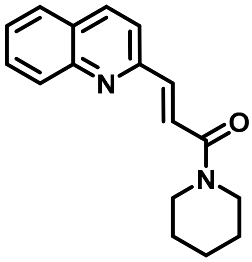
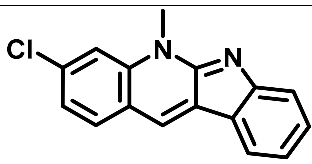
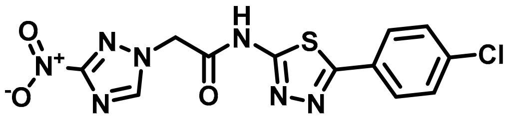
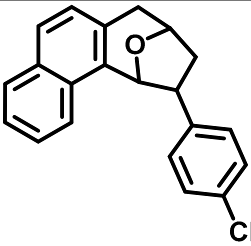
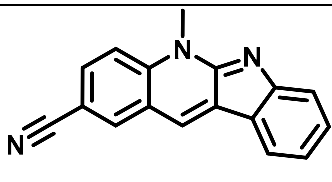
92		4.38	17
93		4.38	6
94		4.40	9
95		4.40	6
96*		4.41	18
97		4.46	17

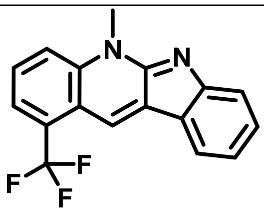
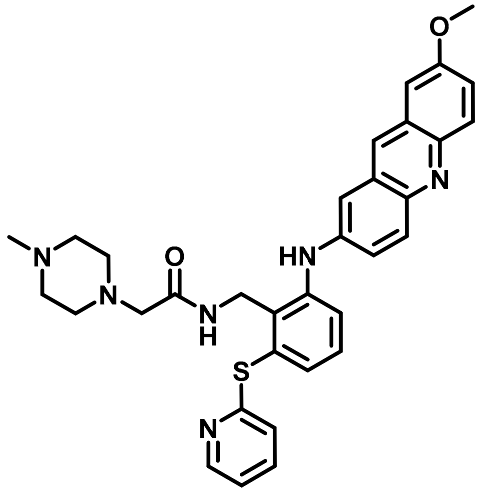
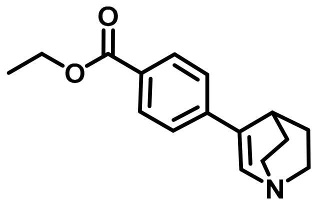
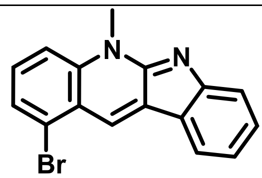
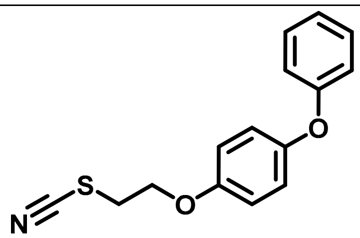
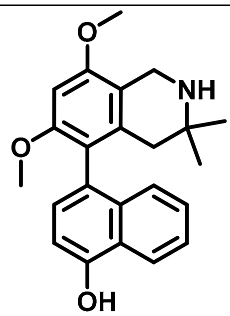
98*		4.47	19
99		4.48	8
100		4.48	17
101		4.50	3
102		4.52	14
103		4.55	12

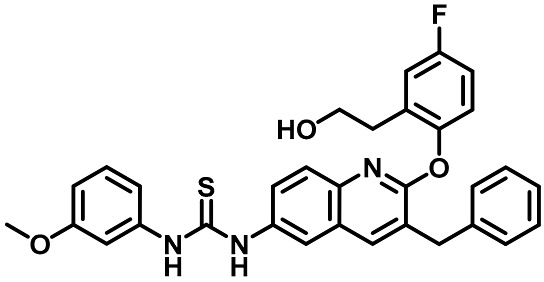
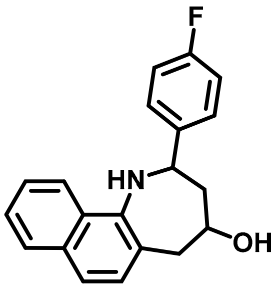
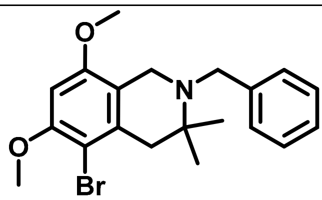
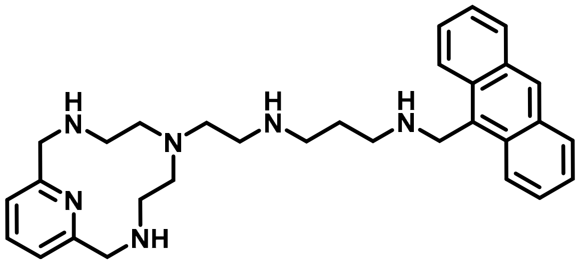
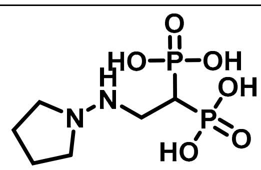
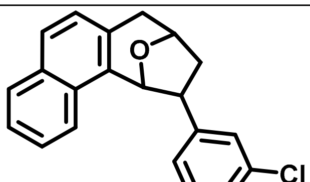
104*		4.55	22
105		4.55	5
106		4.56	19
107		4.59	23
108		4.59	10
109*		4.60	24
110		4.61	19

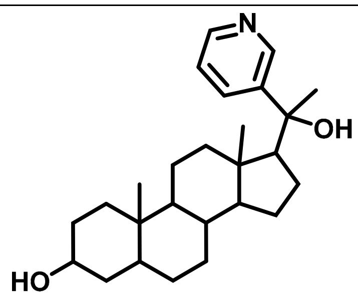
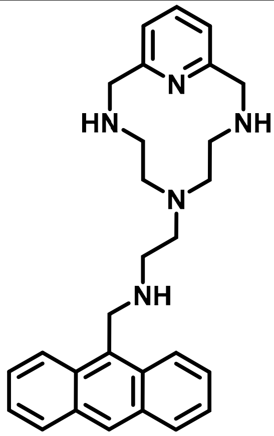
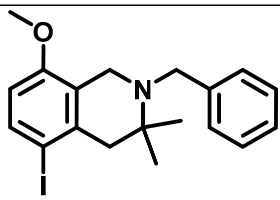
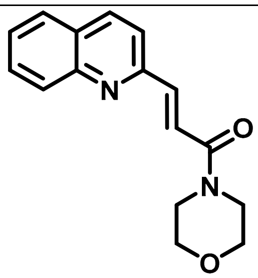
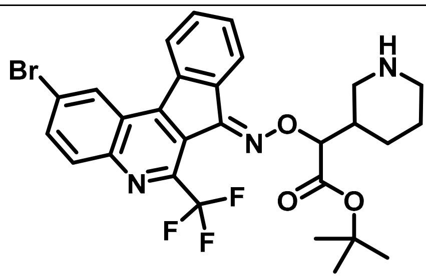
111		4.61	8
112*		4.62	21
113		4.63	8
114		4.64	17
115		4.66	22
116*		4.67	15
117		4.68	25

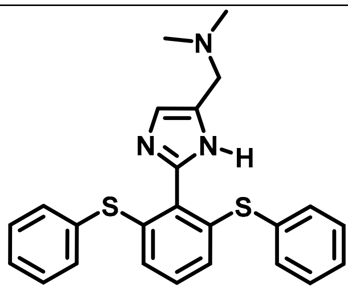
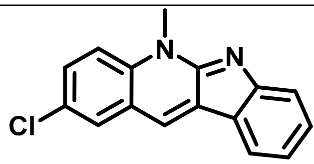
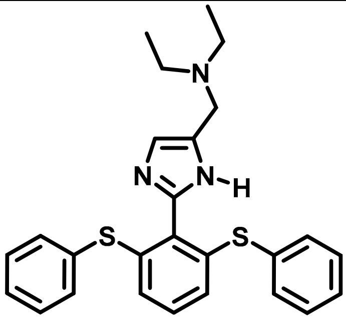
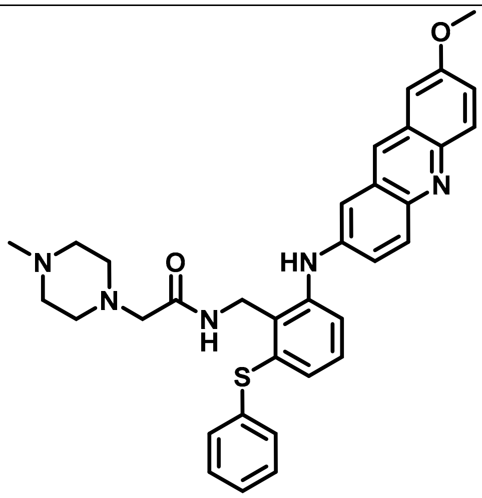
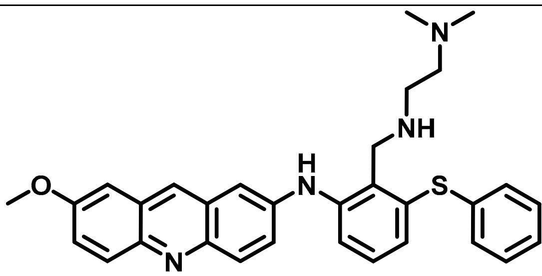
118		4.71	8
119		4.72	19
120		4.74	26
121		4.74	8
122*		4.74	17
123		4.74	27
124		4.74	15

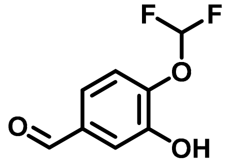
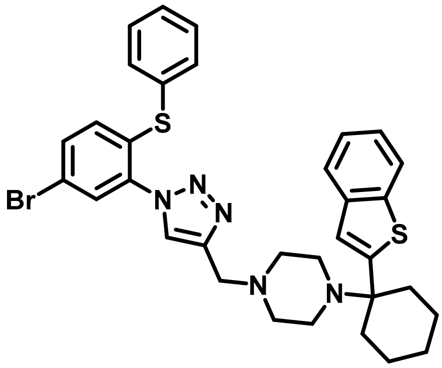
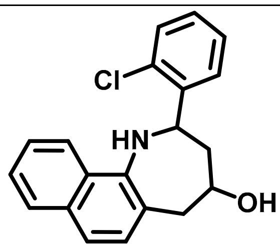
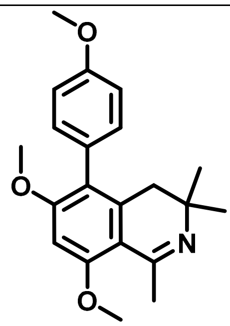
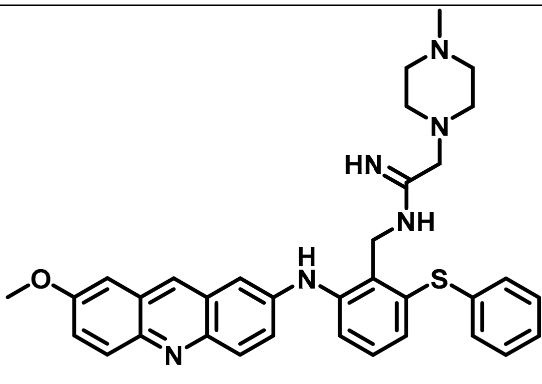
125		4.77	28
126		4.77	22
127*		4.77	22
128		4.77	27
129		4.78	29
130		4.79	8
131*		4.79	27

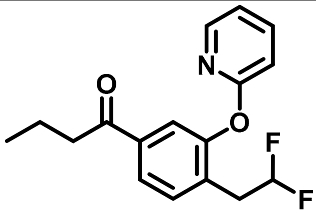
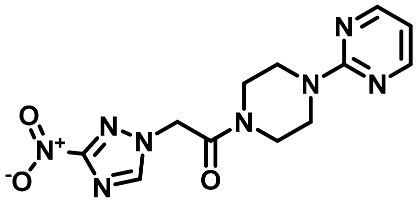
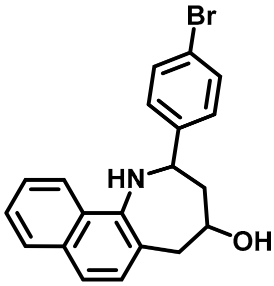
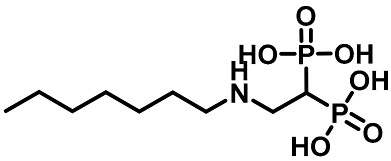
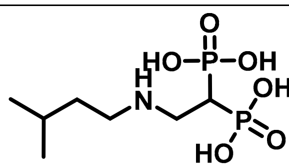
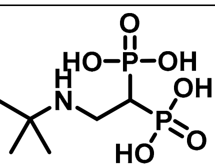
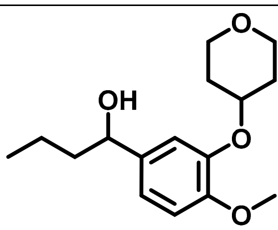
132		4.79	27
133		4.80	19
134		4.80	20
135*		4.80	27
136		4.80	15
137		4.82	12

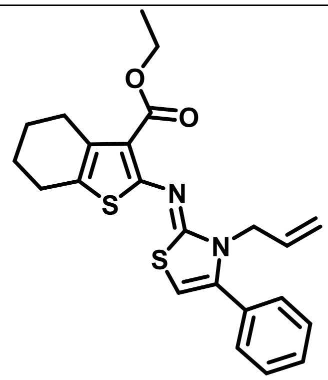
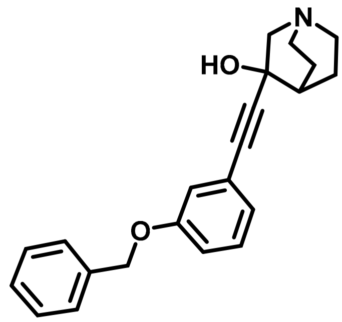
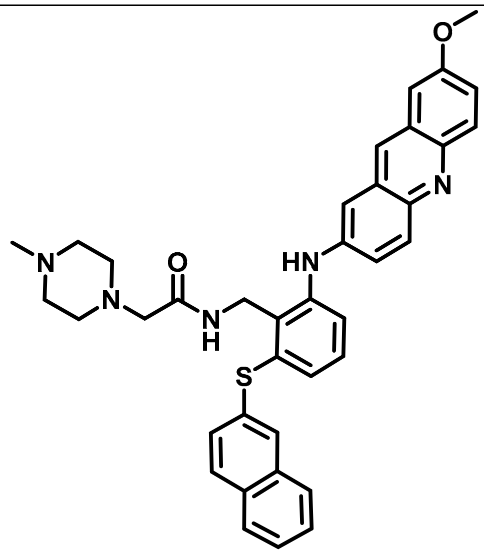
138*		4.83	16
139		4.83	8
140		4.83	12
141		4.85	24
142		4.85	30
143		4.88	8

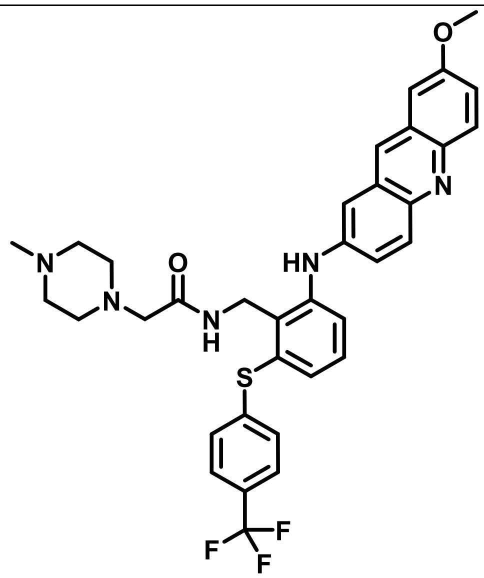
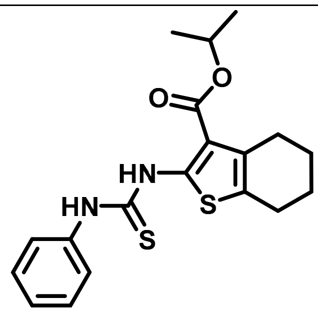
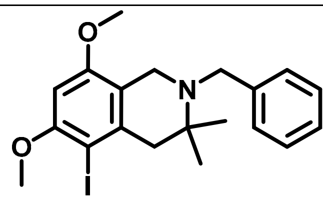
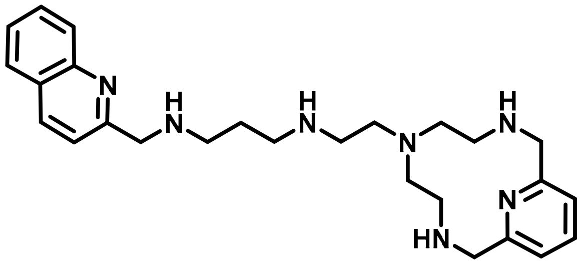
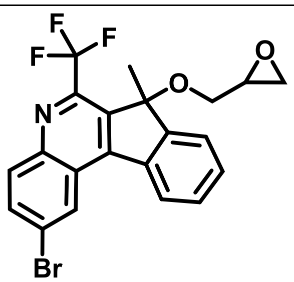
144*		4.88	17
145		4.89	24
146		4.89	12
147		4.89	22
148		4.91	16

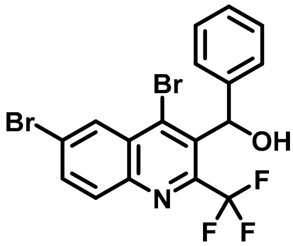
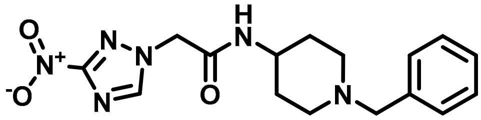
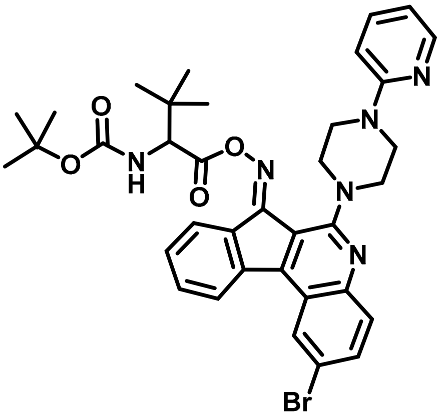
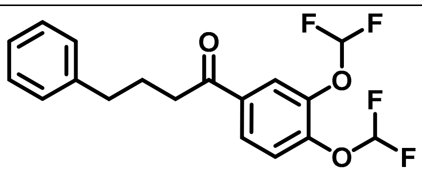
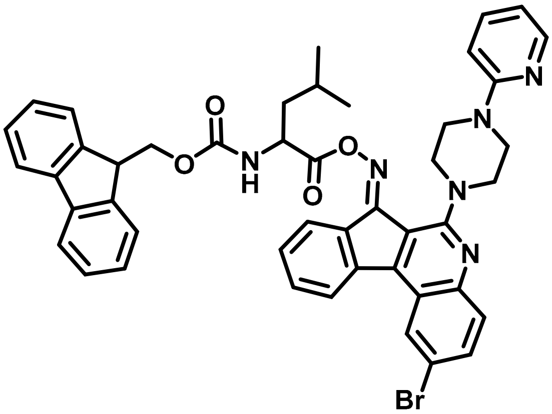
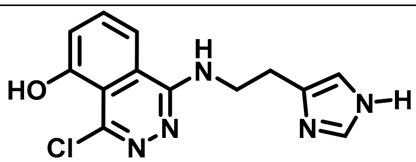
149		4.91	11
150*		4.92	27
151*		4.94	11
152		4.95	19
153		4.95	19

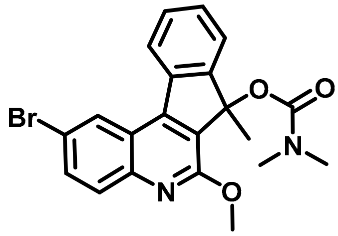
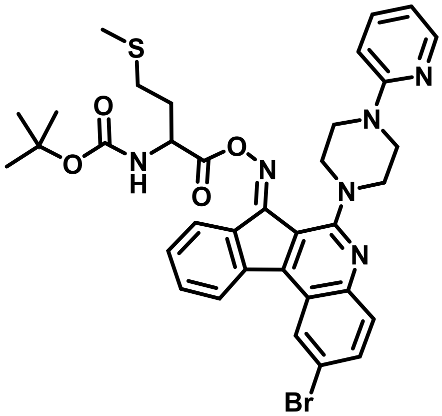
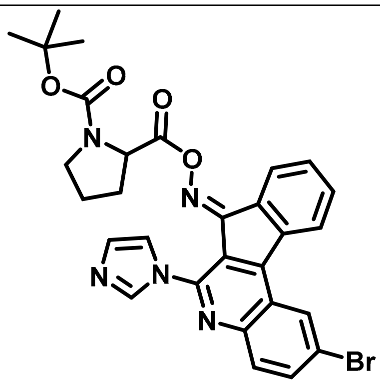
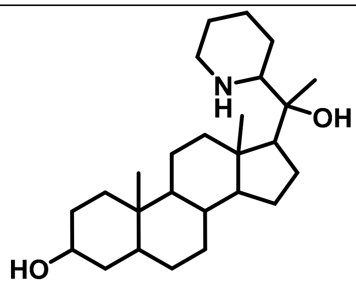
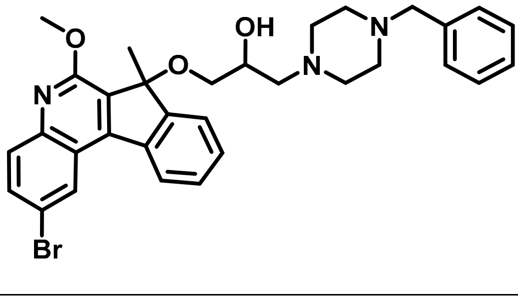
154		4.96	13
155*		4.97	11
156		4.97	8
157		4.97	12
158		4.99	19

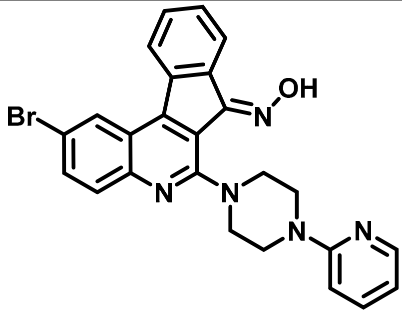
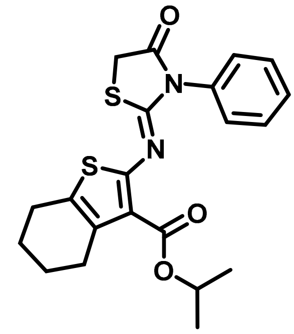
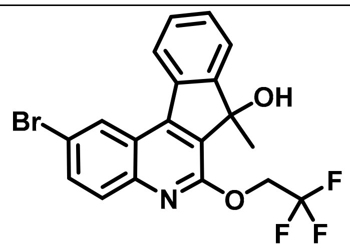
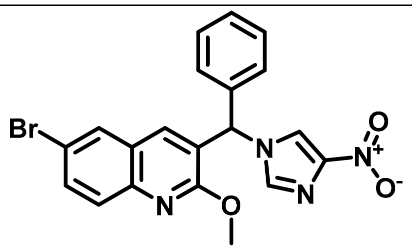
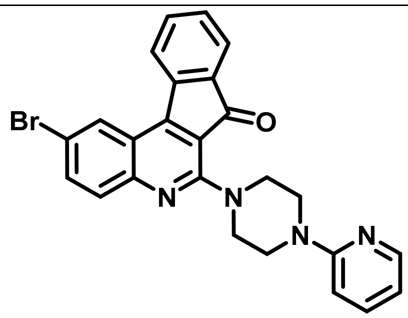
159		4.99	13
160		5.00	23
161		5.00	8
162		5.00	30
163*		5.00	30
164		5.00	30
165		5.00	13

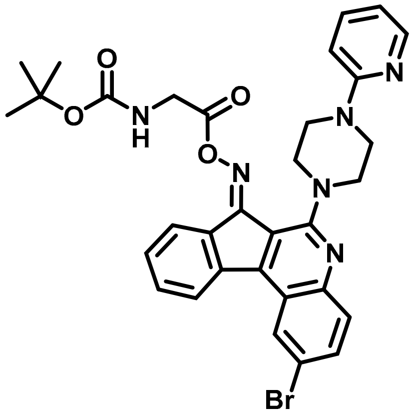
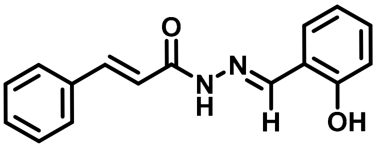
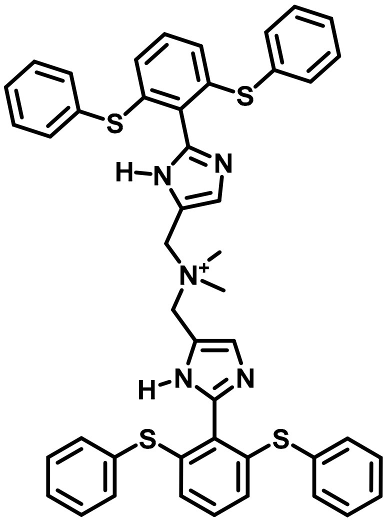
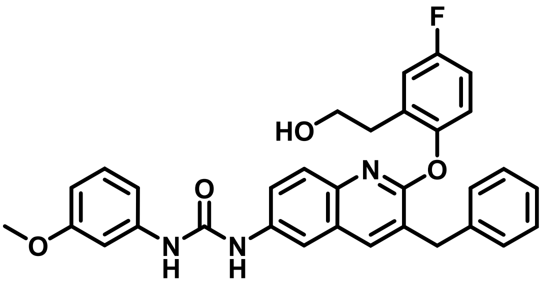
166*		5.01	31
167		5.02	20
168		5.03	19

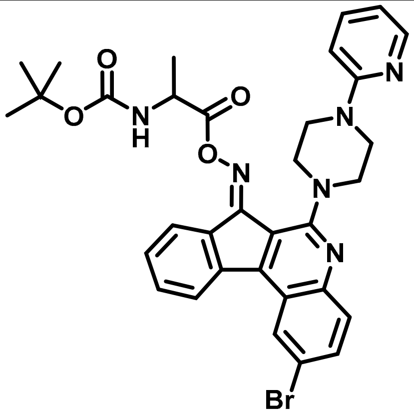
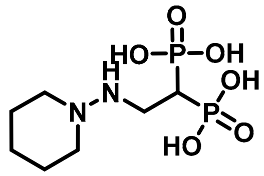
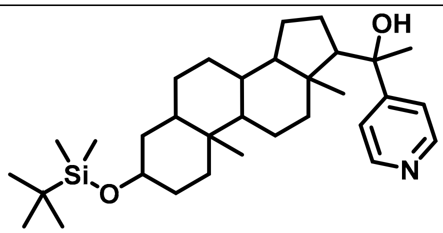
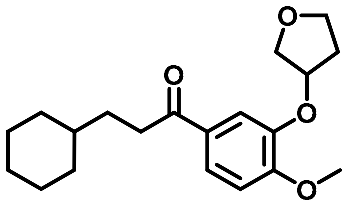
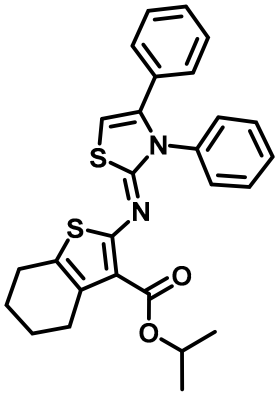
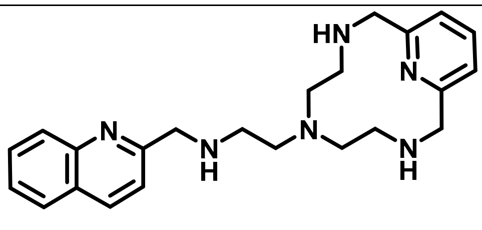
169		5.03	19
170*		5.06	31
171		5.07	12
172		5.08	24
173		5.08	16

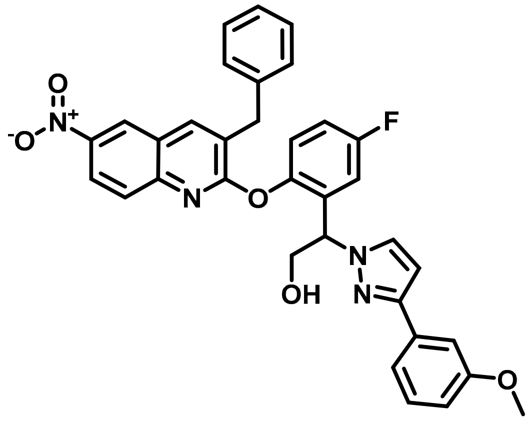
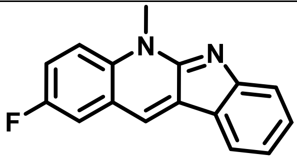
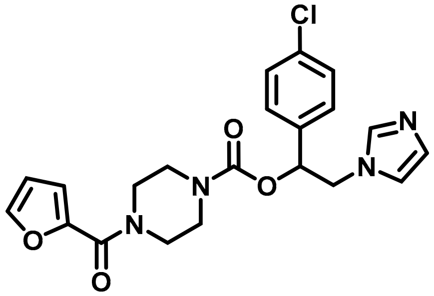
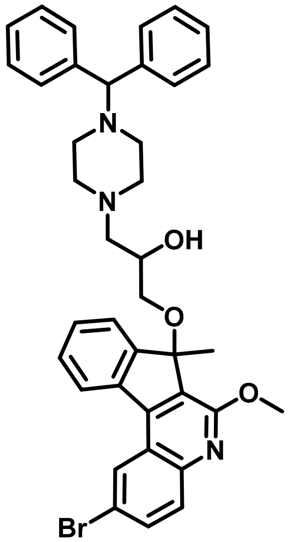
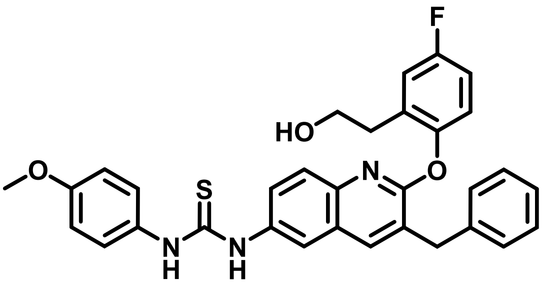
174*		5.09	16
175		5.10	26
176		5.10	16
177		5.11	13
178*		5.12	16
179		5.13	25

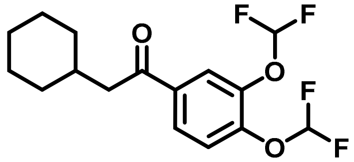
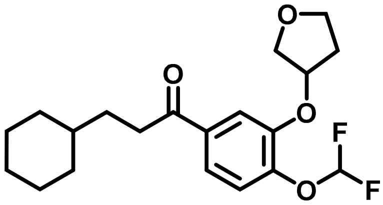
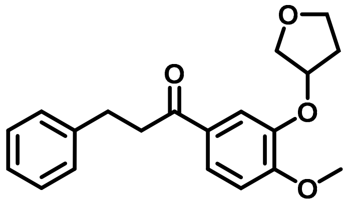
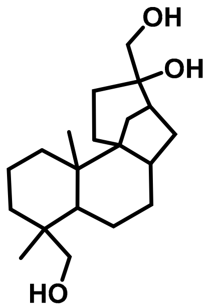
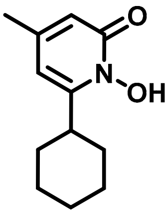
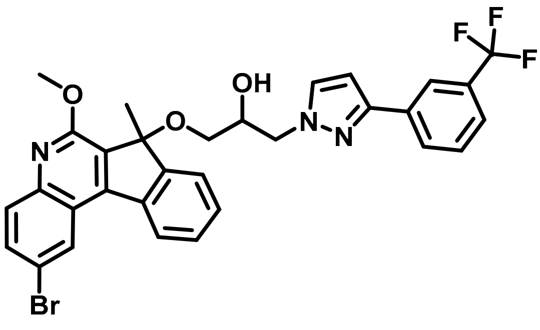
180		5.13	16
181		5.13	16
182		5.13	16
183		5.13	17
184*		5.14	16

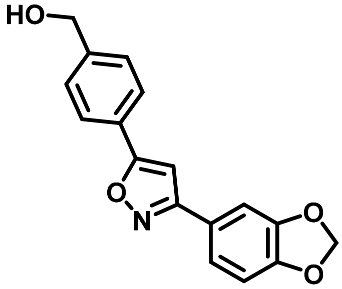
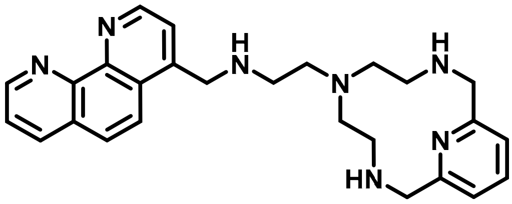
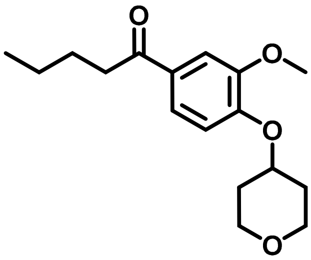
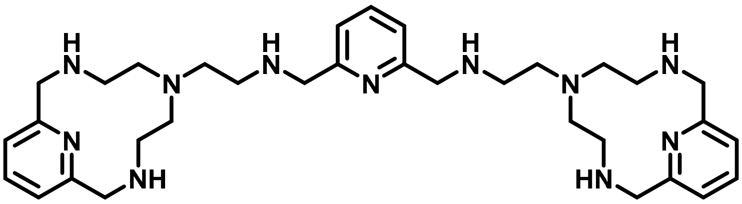
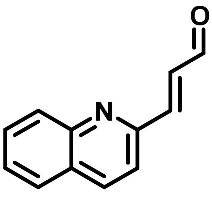
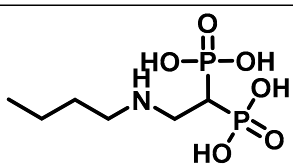
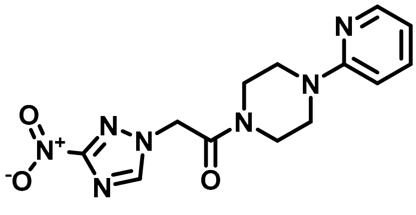
185		5.15	16
186		5.16	31
187*		5.16	16
188		5.16	16
189		5.16	16

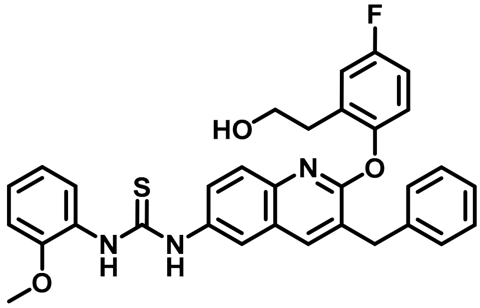
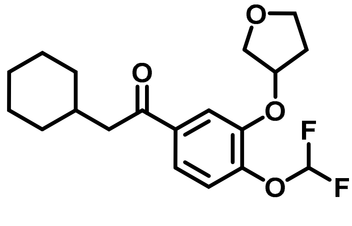
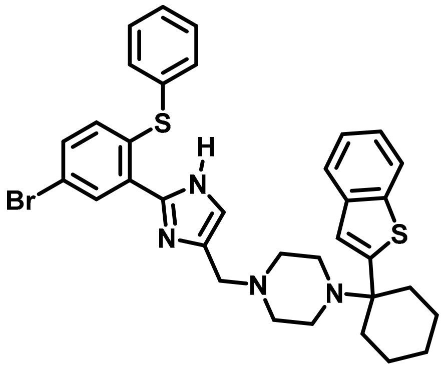
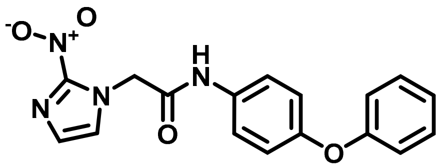
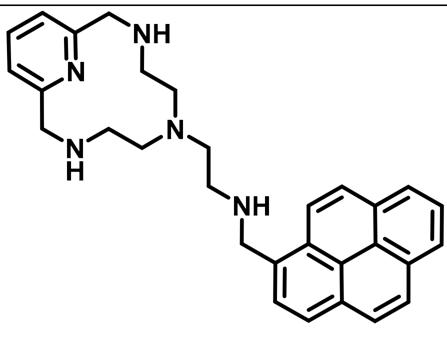
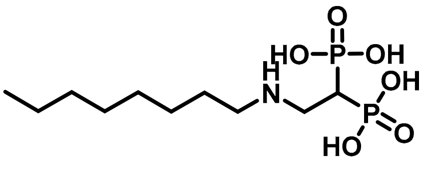
190*		5.17	16
191		5.18	9
192		5.20	11
193		5.21	16

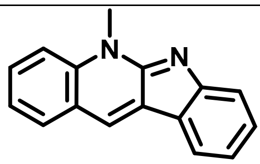
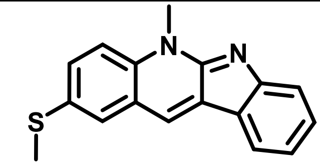
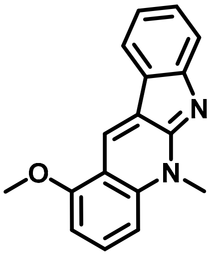
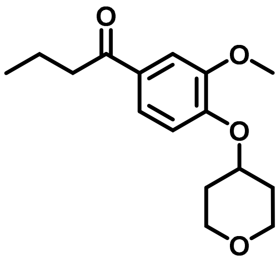
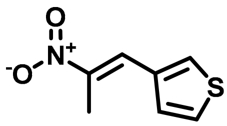
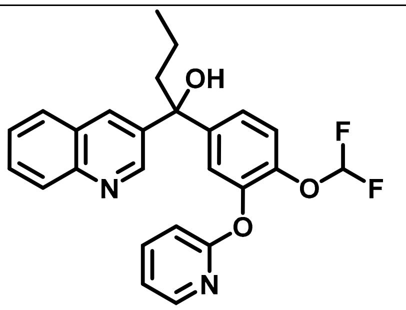
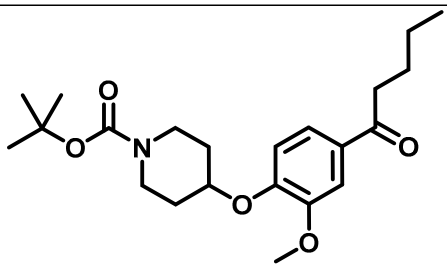
194		5.21	16
195*		5.21	30
196		5.21	17
197		5.21	13
198		5.22	31
199		5.22	24

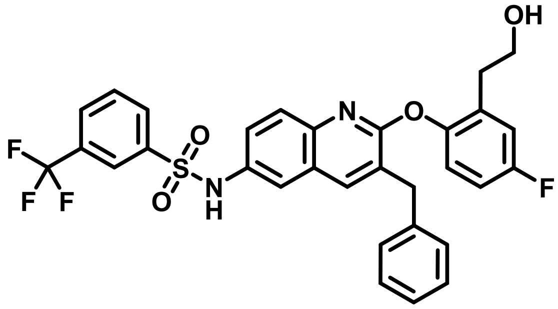
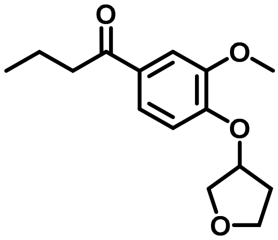
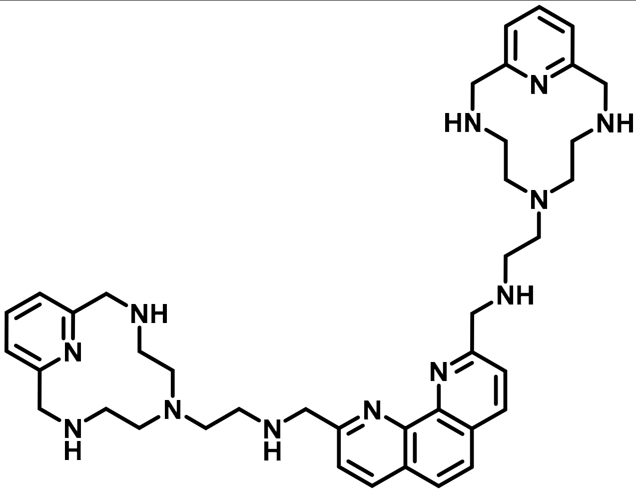
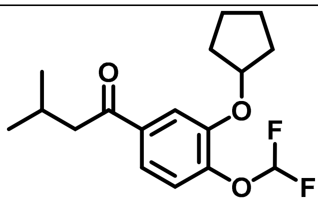
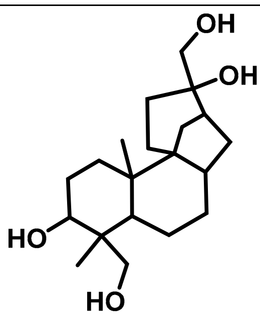
200		5.22	16
201*		5.22	27
202		5.23	32
203		5.23	16
204		5.24	16

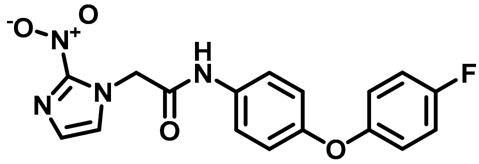
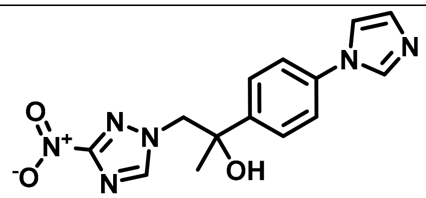
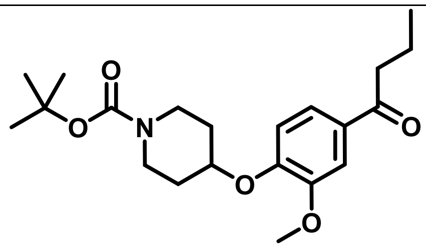
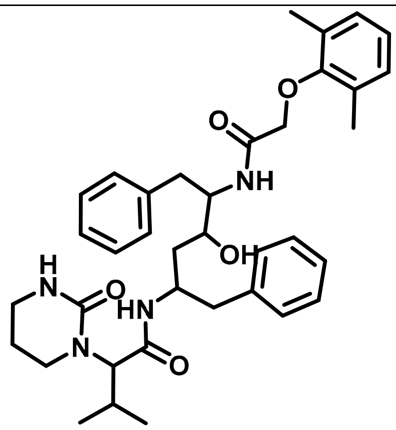
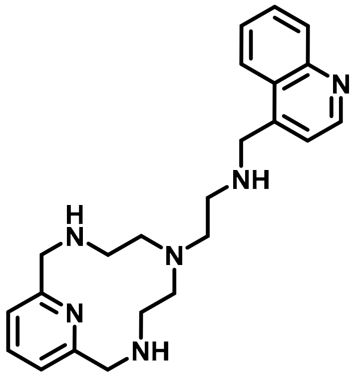
205		5.24	13
206		5.24	13
207*		5.25	13
208		5.26	33
209		5.27	7
210*		5.27	16

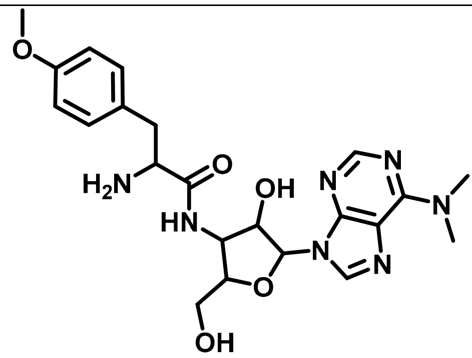
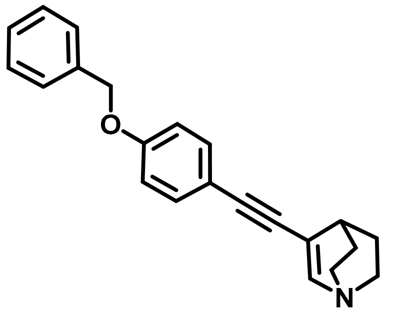
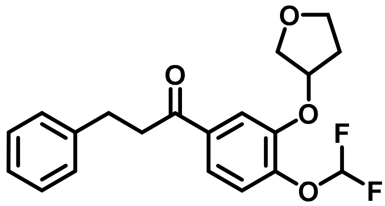
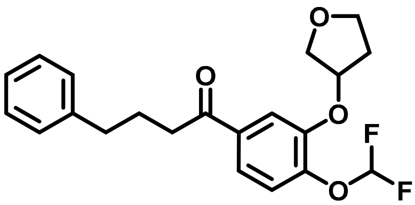
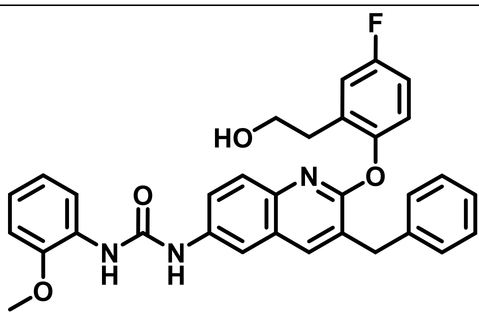
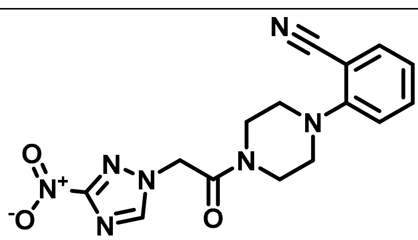
211		5.28	7
212		5.28	24
213*		5.28	13
214		5.29	24
215		5.30	22
216		5.32	30
217		5.33	23

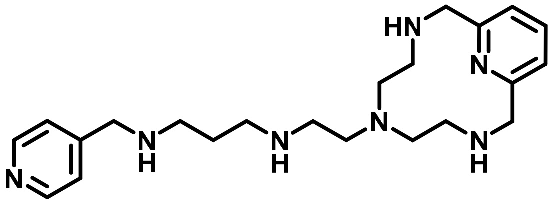
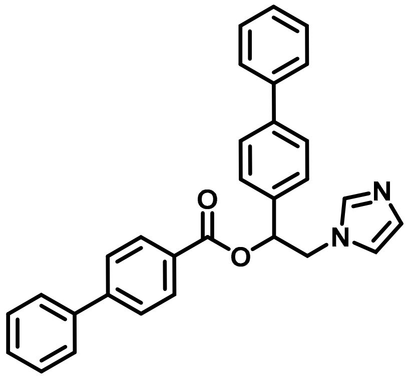
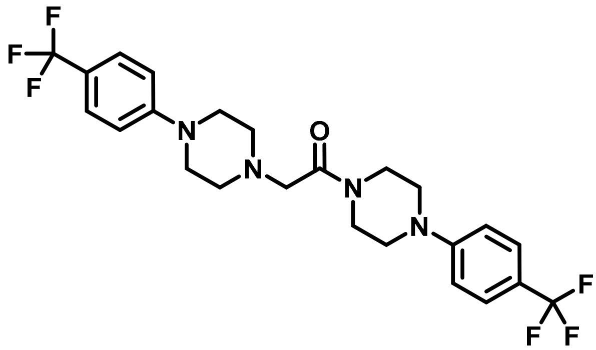
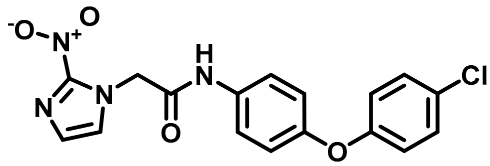
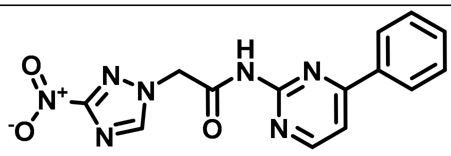
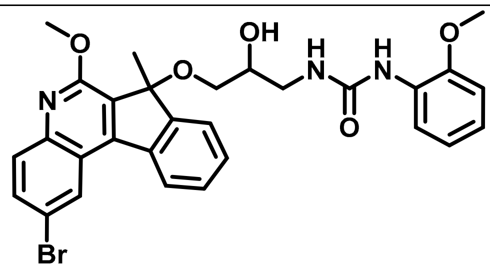
218*		5.36	15
219		5.36	13
220		5.37	11
221		5.38	26
222		5.38	24
223		5.39	30

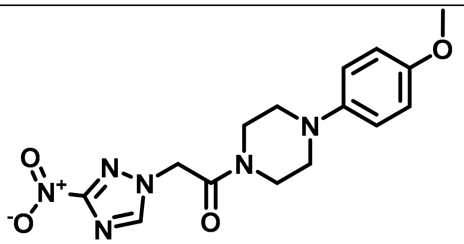
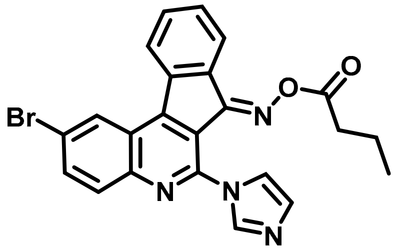
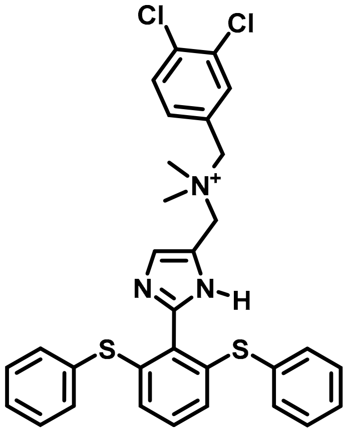
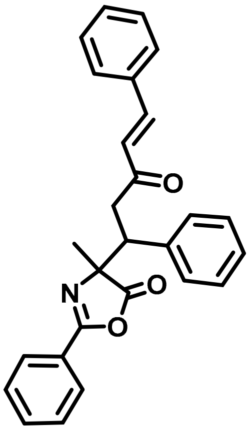
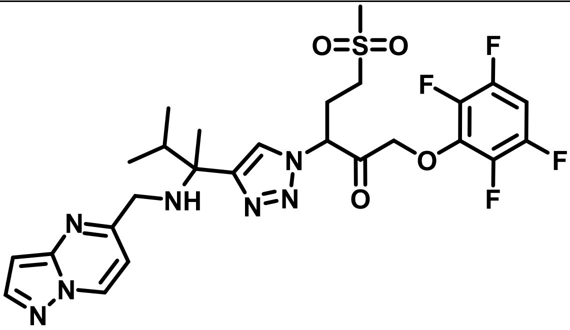
224*		5.40	27
225		5.40	27
226*		5.40	27
227		5.40	13
228		5.41	34
229		5.42	13
230		5.42	13

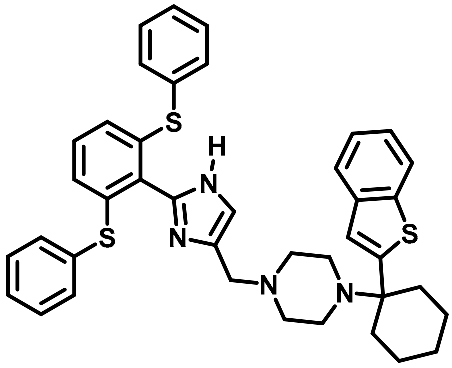
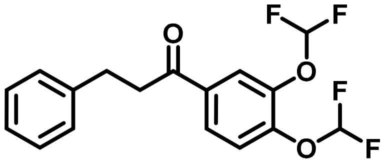
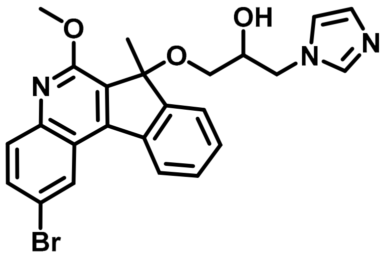
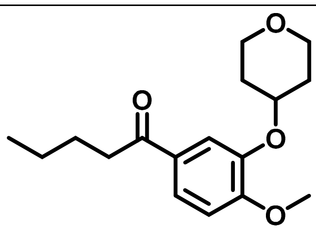
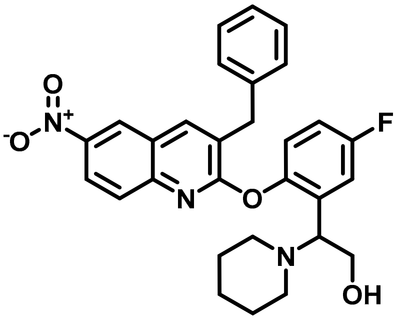
231		5.43	16
232*		5.43	13
233		5.44	24
234		5.44	13
235		5.46	33

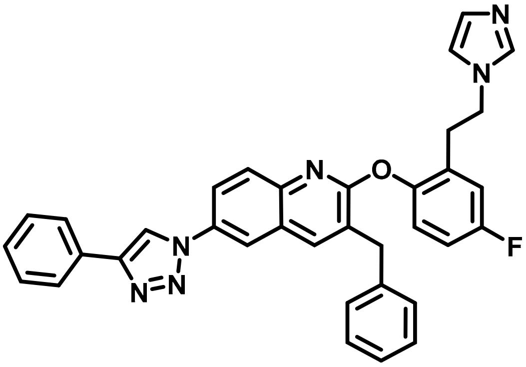
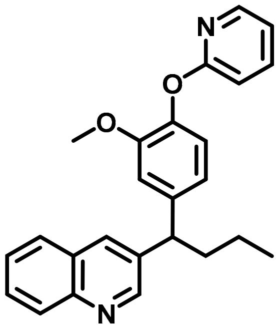
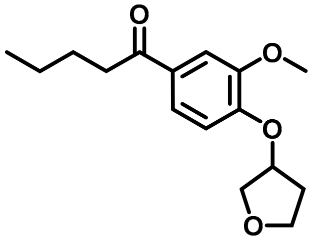
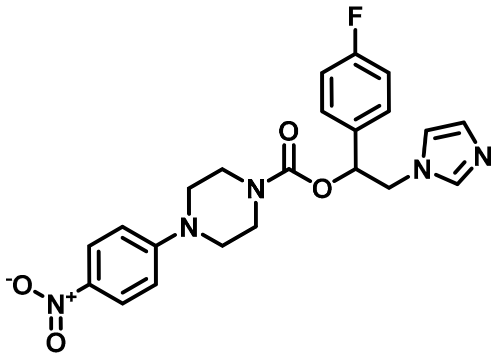
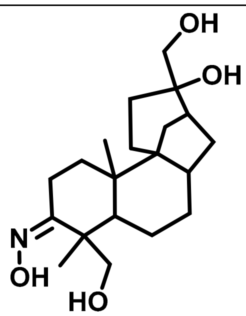
236*		5.48	26
237		5.48	29
238		5.48	13
239		5.49	35
240		5.49	24

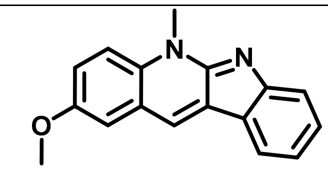
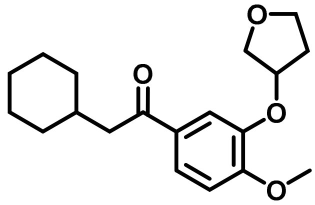
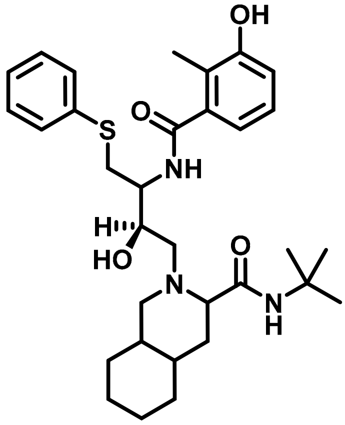
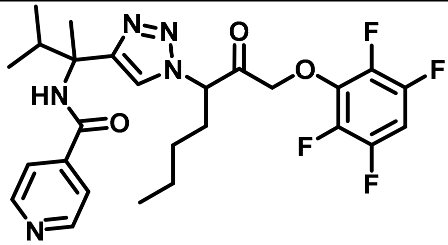
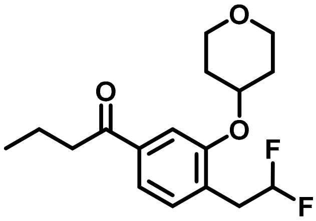
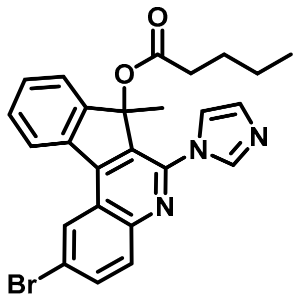
241*		5.50	36
242		5.51	20
243		5.51	13
244		5.51	13
245*		5.54	16
246		5.55	23

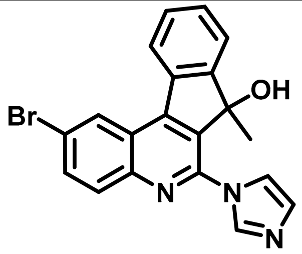
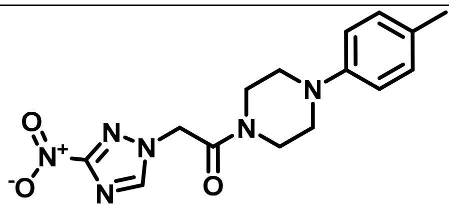
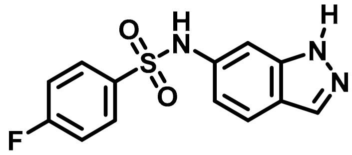
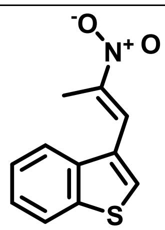
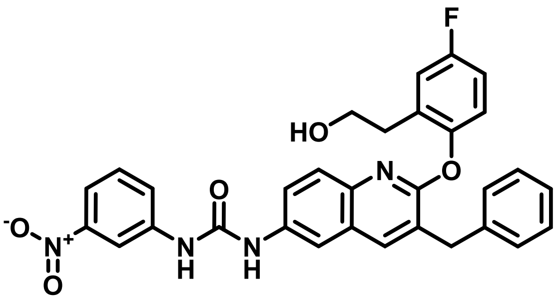
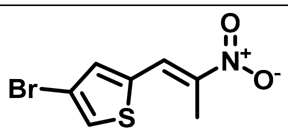
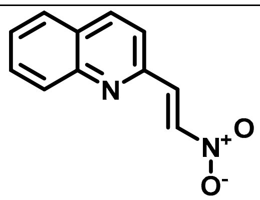
247*		5.55	24
248		5.57	32
249		5.57	23
250		5.59	26
251*		5.60	26
252		5.60	16

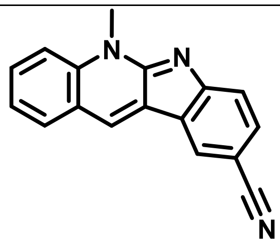
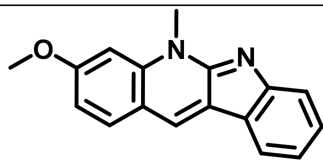
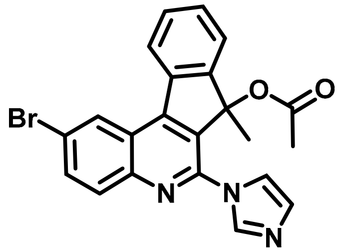
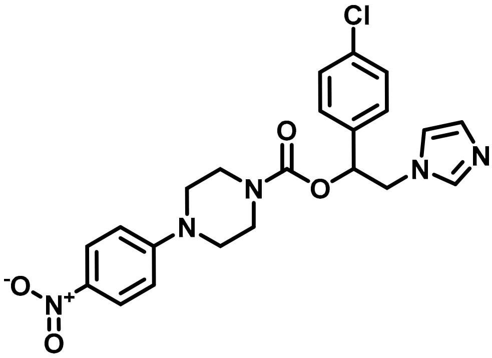
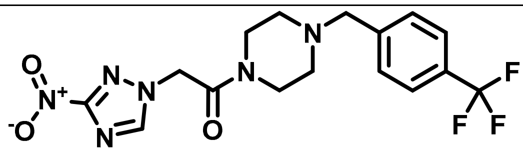
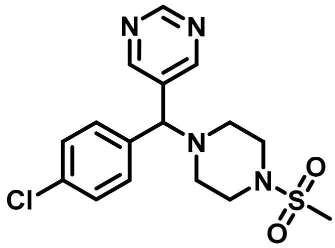
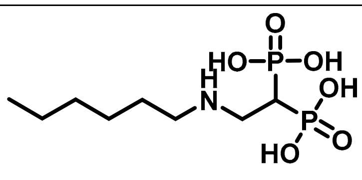
253		5.62	23
254		5.62	16
255		5.62	11
256		5.63	37
257		5.63	1

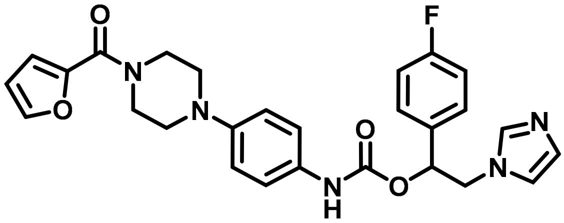
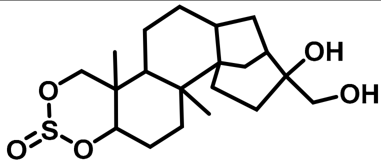
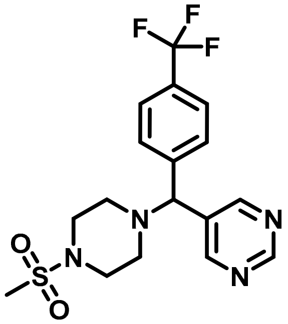
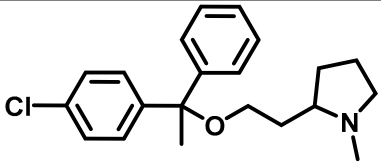
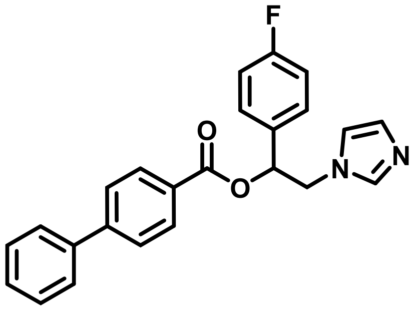
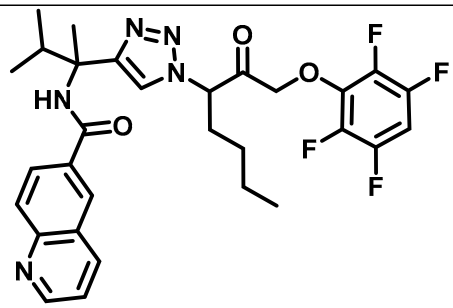
258*		5.63	11
259		5.64	13
260		5.67	16
261		5.68	13
262		5.70	16

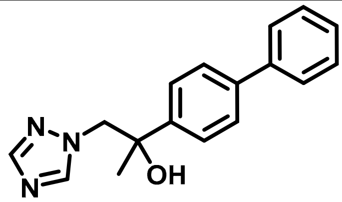
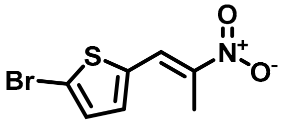
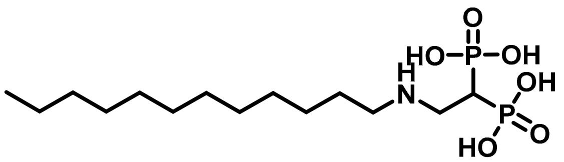
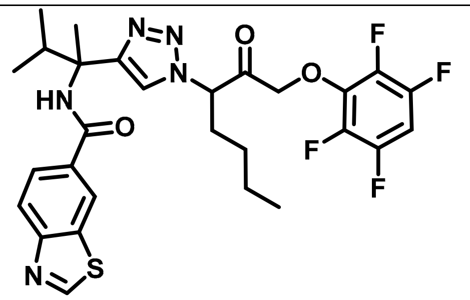
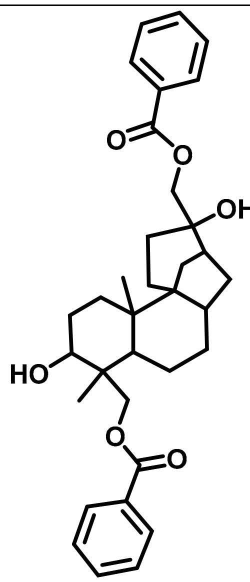
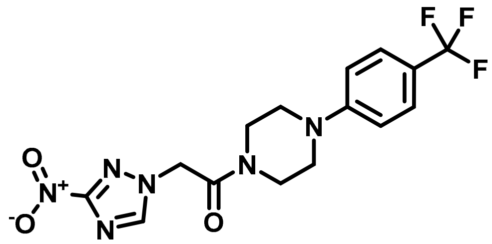
263*		5.71	16
264		5.72	13
265		5.74	13
266*		5.77	32
267		5.77	33

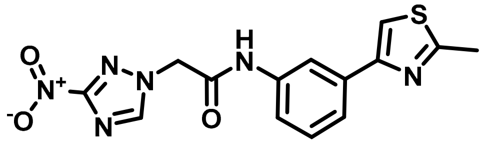
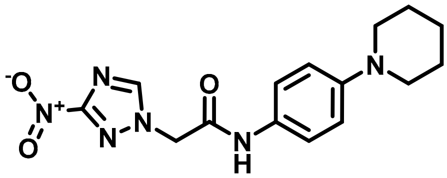
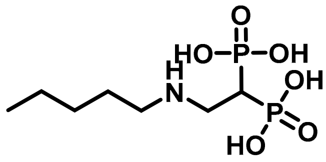
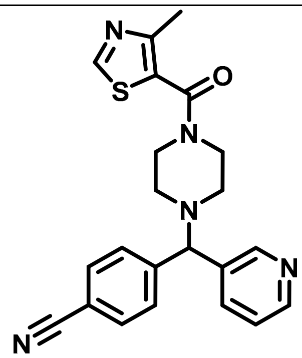
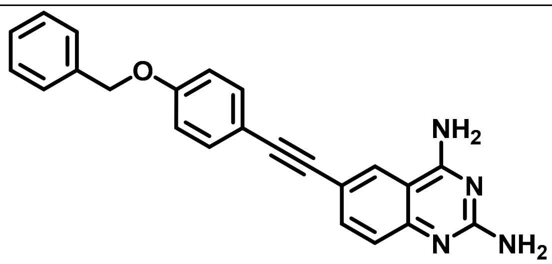
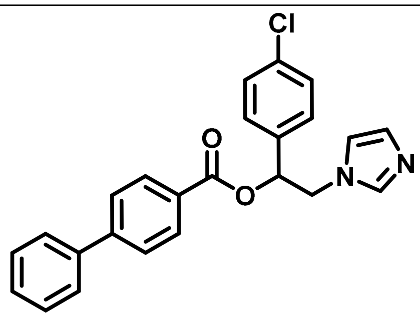
268		5.77	27
269*		5.77	13
270		5.80	35
271		5.80	1
272		5.80	13
273*		5.84	16

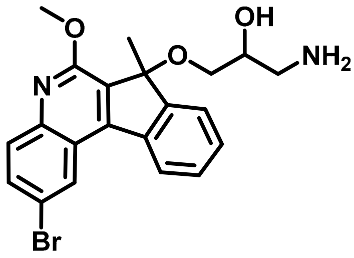
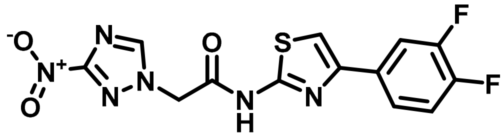
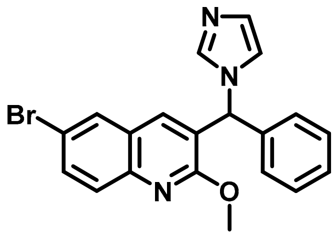
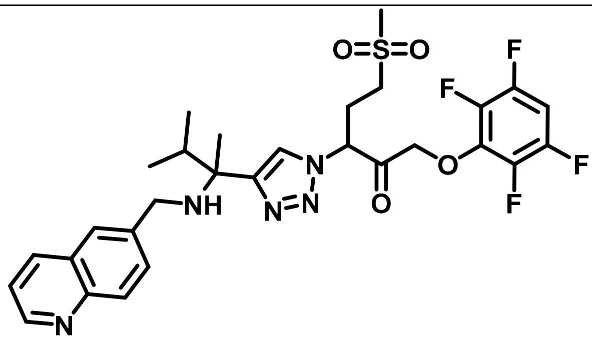
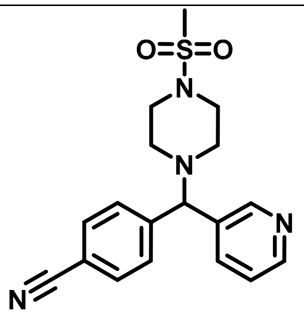
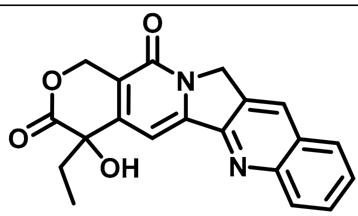
274		5.86	16
275		5.88	23
276		5.89	10
277		5.89	34
278		6.00	16
279		6.00	34
280		6.00	22

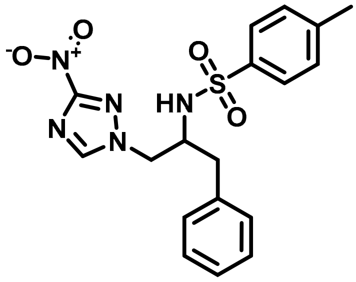
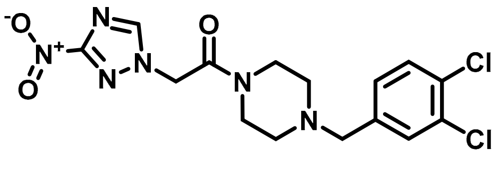
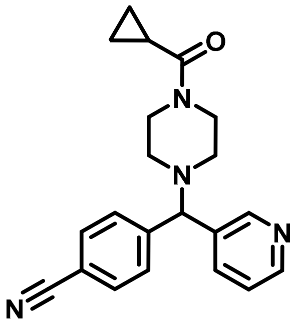
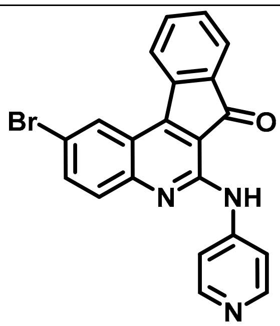
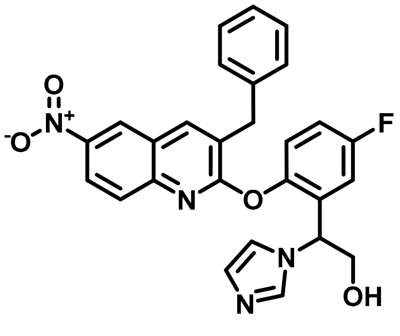
281*		6.00	27
282		6.00	27
283*		6.03	16
284		6.06	32
285**		6.06	23
286		6.06	2
287		6.08	30

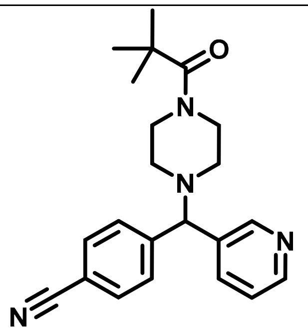
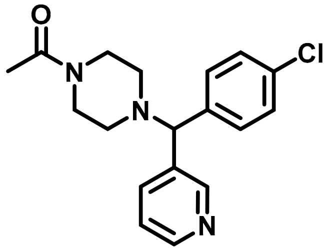
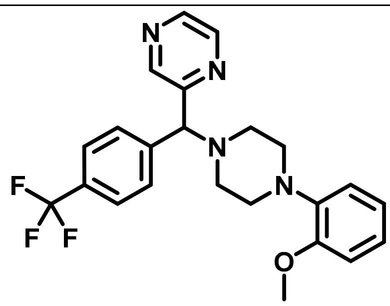
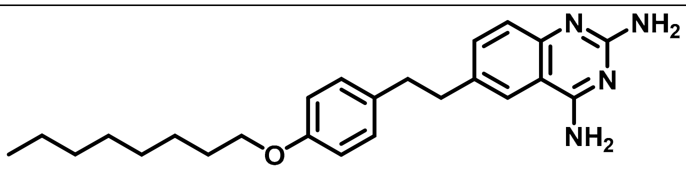
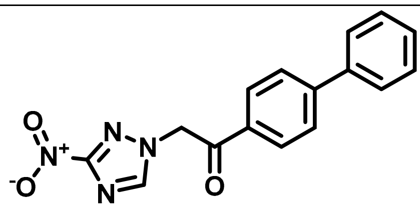
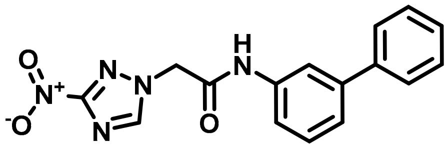
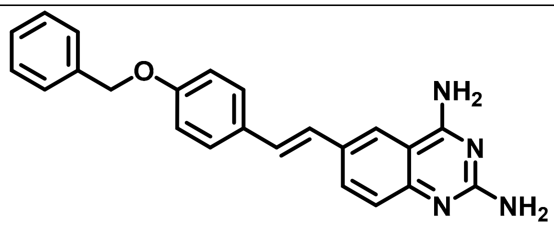
288*		6.10	32
289		6.11	33
290		6.11	2
291		6.12	36
292*		6.15	32
293		6.15	1

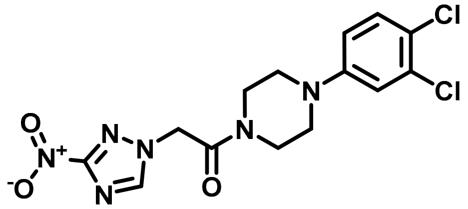
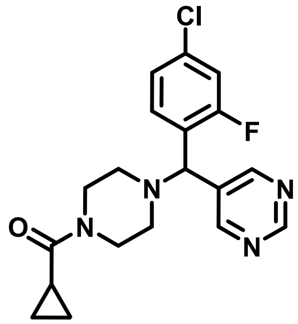
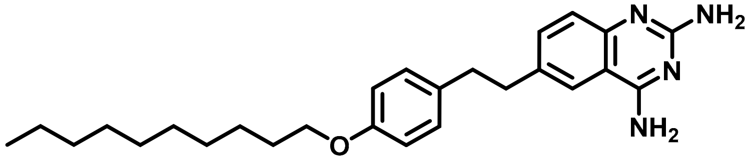
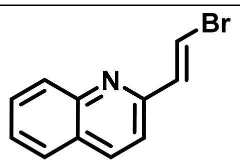
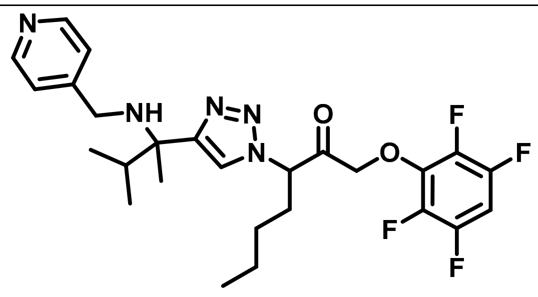
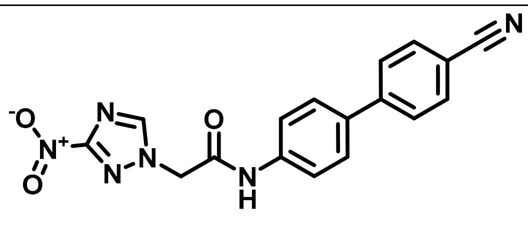
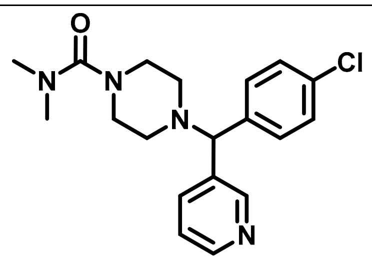
294		6.15	29
295		6.15	34
296*		6.17	38
297		6.19	1
298		6.22	33
299		6.22	23

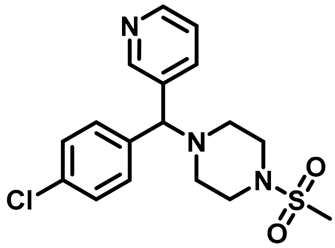
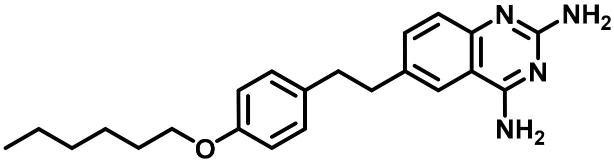
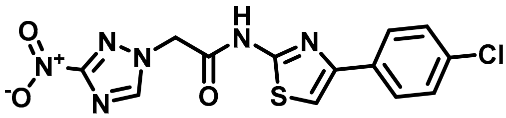
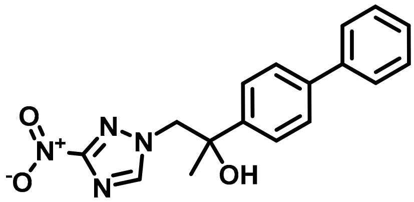
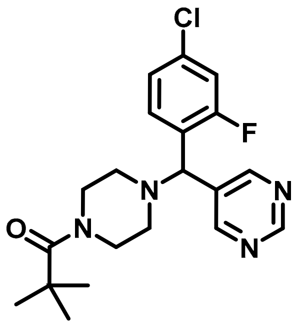
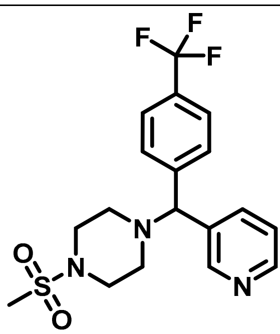
300		6.26	29
301*		6.26	29
302		6.27	30
303		6.29	2
304		6.30	39
305		6.32	32

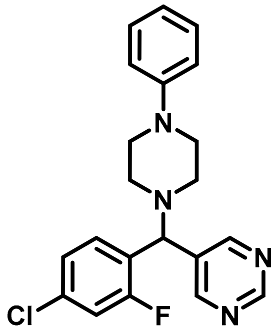
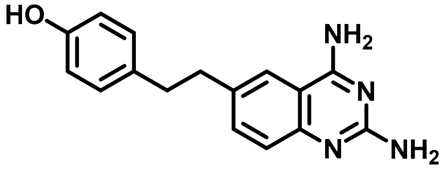
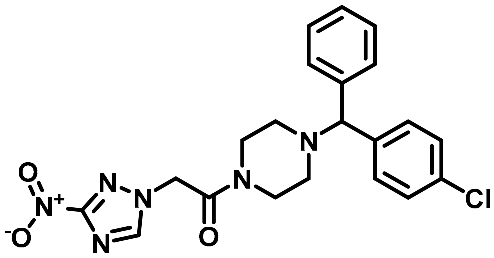
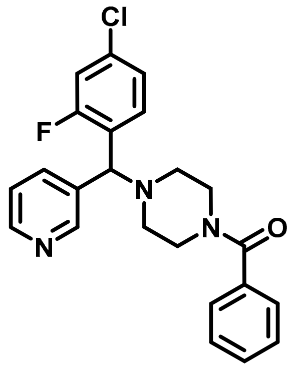
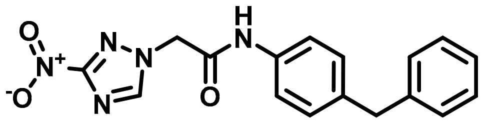
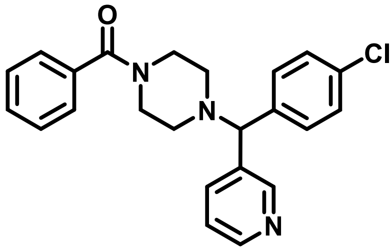
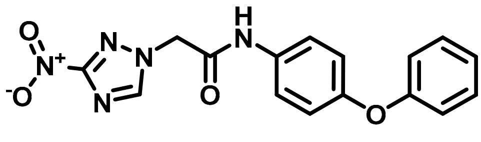
306		6.33	16
307*		6.34	29
308		6.34	16
309*		6.42	1
310		6.44	2
311		6.47	36

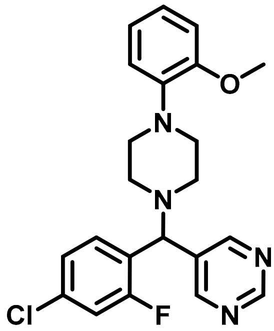
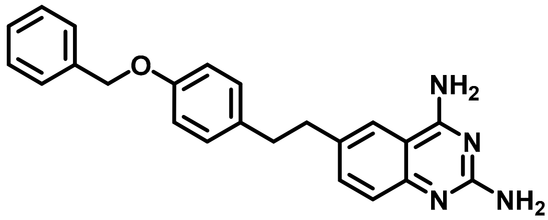
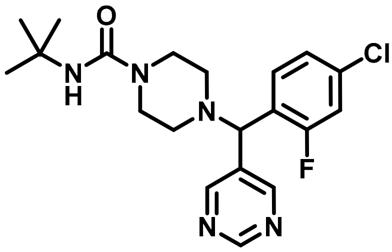
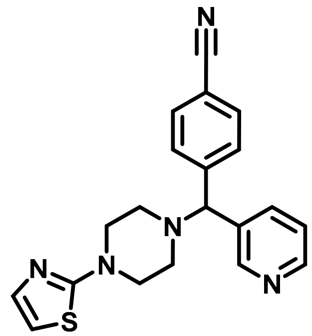
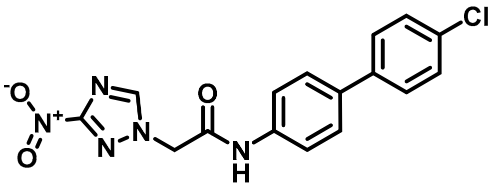
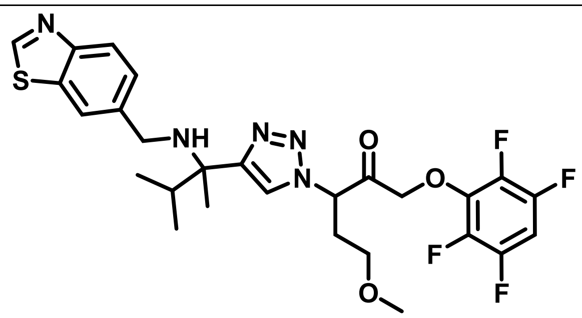
312		6.47	29
313*		6.53	23
314		6.55	2
315		6.60	16
316		6.60	16

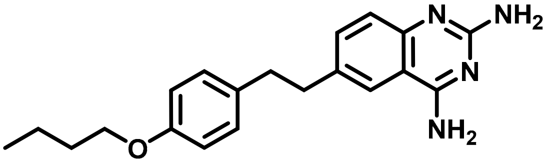
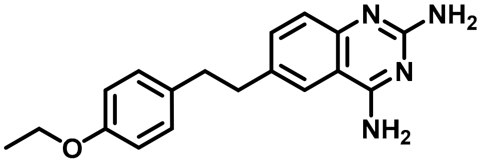
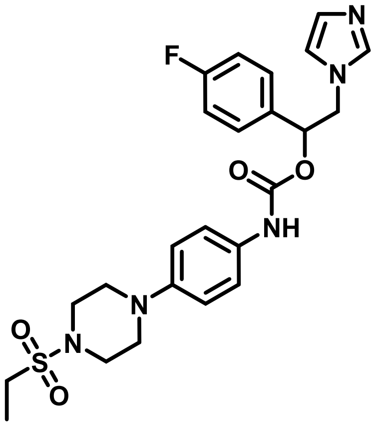
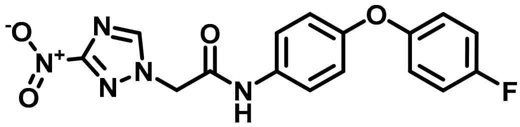
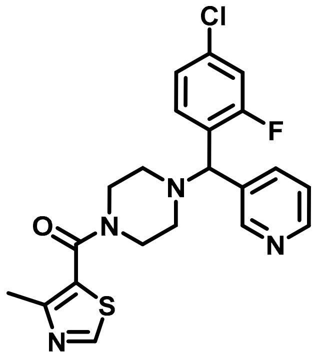
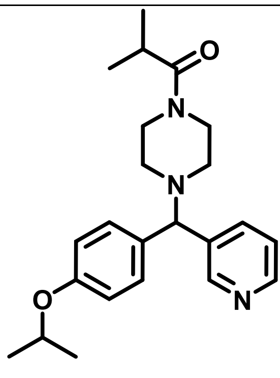
317*		6.60	2
318		6.62	2
319		6.62	2
320		6.66	39
321*		6.73	29
322		6.74	26
323		6.74	39

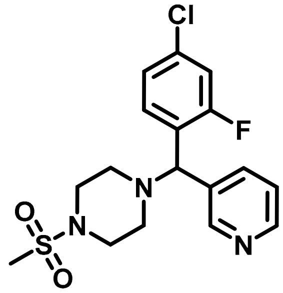
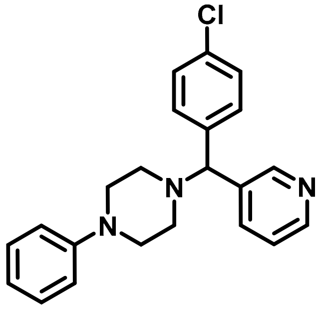
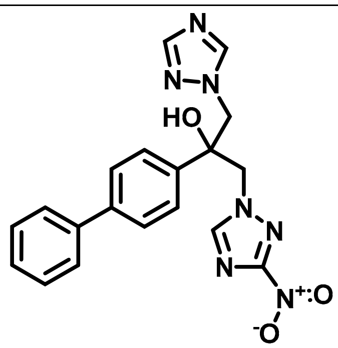
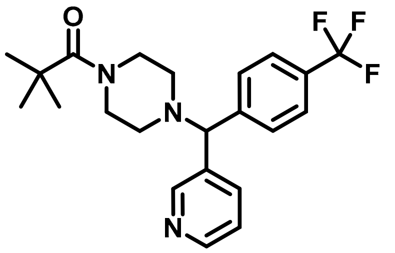
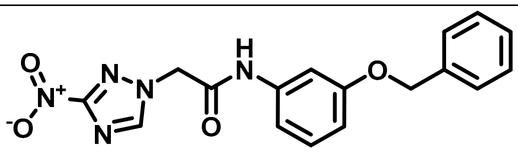
324		6.77	23
325		6.77	2
326*		6.82	39
327		6.82	22
328		6.84	1
329		6.86	29
330		6.92	2

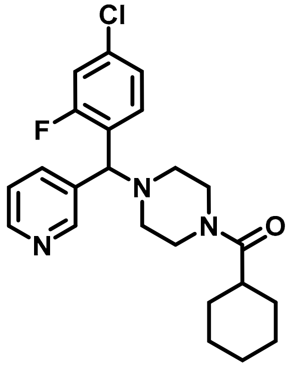
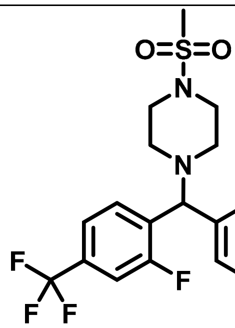
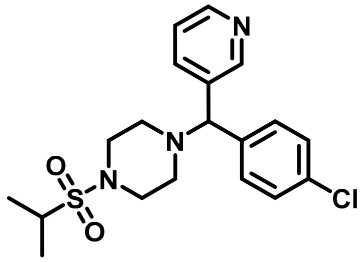
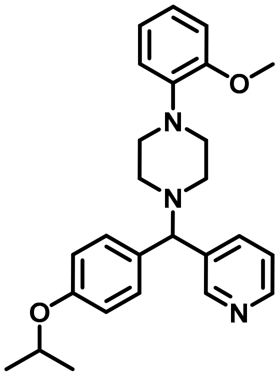
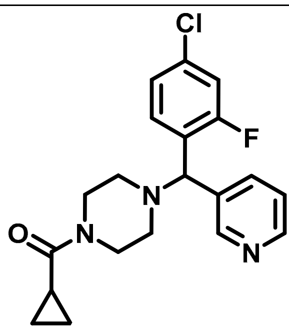
331*		6.96	2
332		6.96	39
333		6.99	29
334		6.99	29
335		7.09	2
336		7.11	2

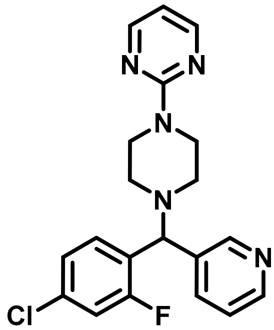
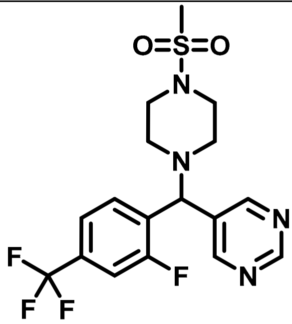
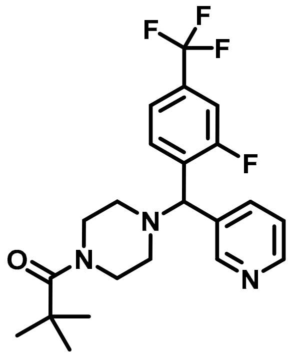
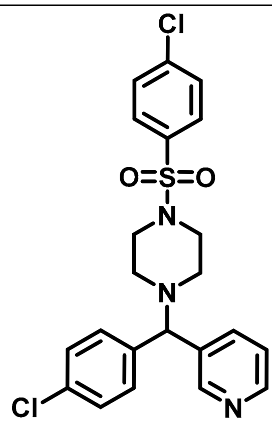
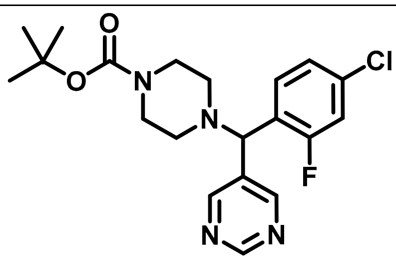
337*		7.11	2
338		7.11	39
339		7.14	23
340		7.15	2
341*		7.17	26
342		7.17	2
343**		7.19	26

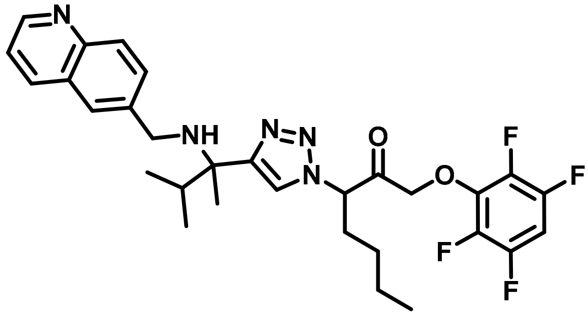
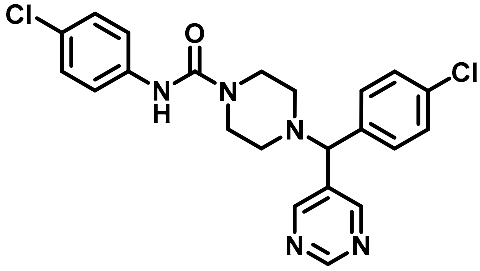
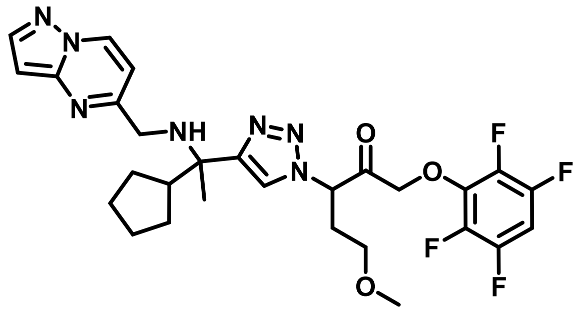
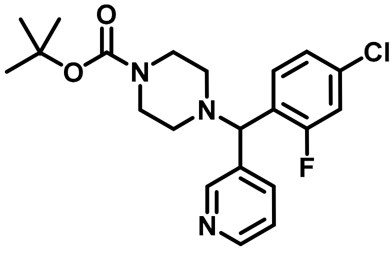
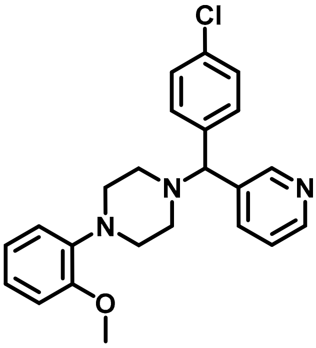
344**		7.19	2
345**		7.23	39
346*		7.27	2
347		7.30	2
348*		7.35	29
349**		7.36	1

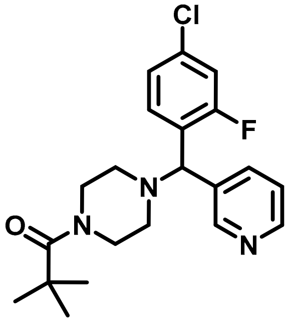
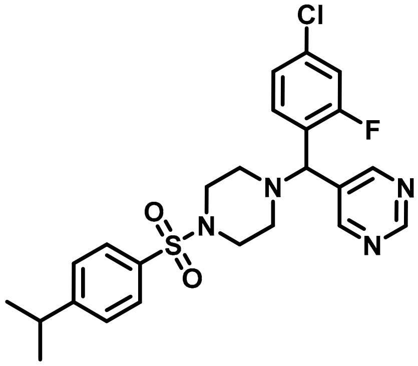
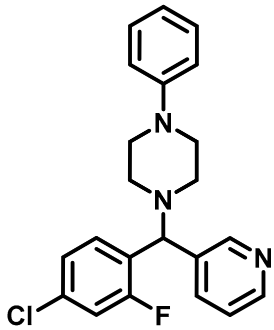
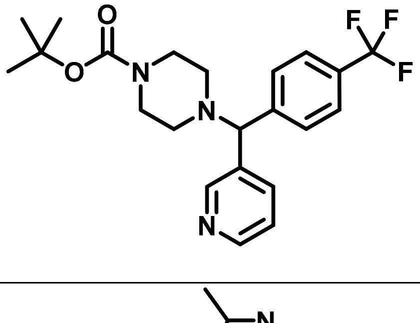
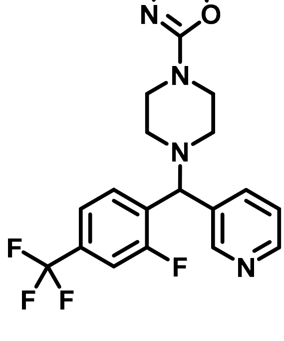
350**		7.38	39
351		7.39	39
352**		7.40	32
353*		7.44	26
354**		7.44	2
355		7.46	2

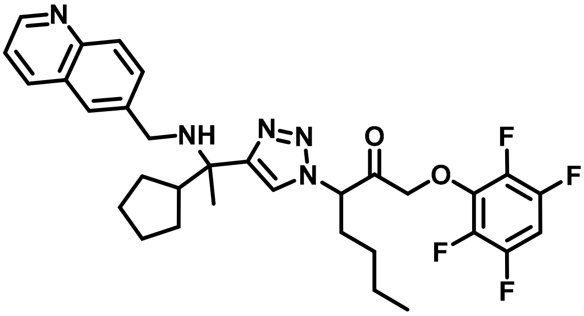
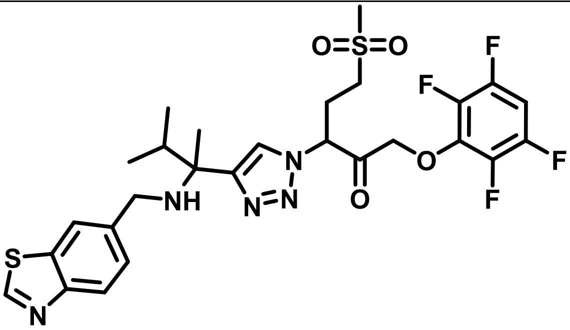
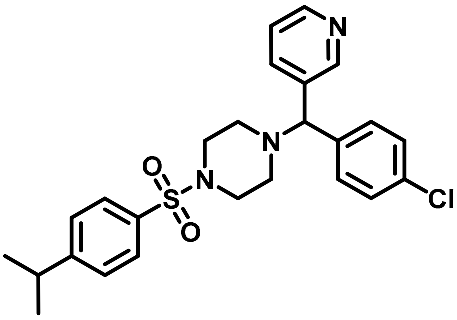
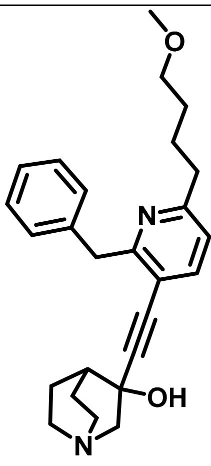
356		7.46	2
357		7.47	2
358*		7.48	29
359		7.52	2
360**		7.55	26

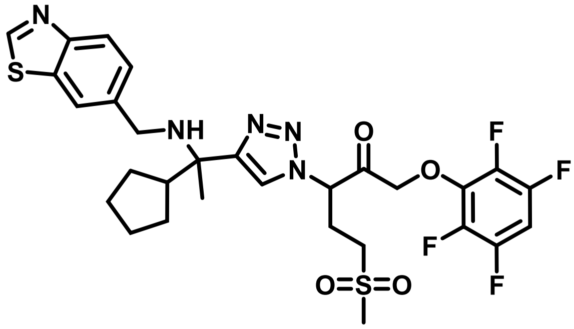
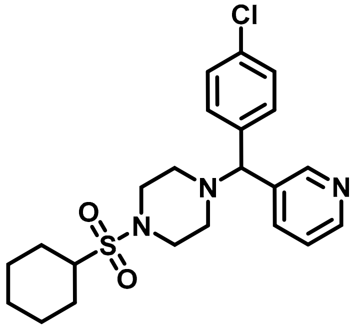
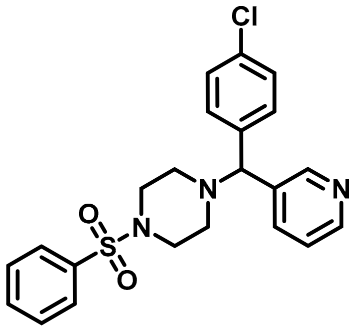
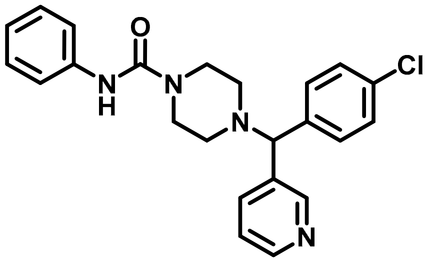
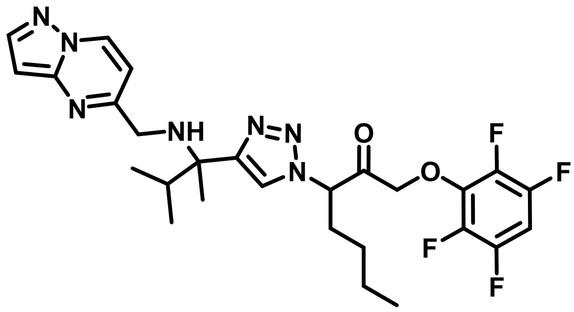
361**		7.55	2
362*		7.55	2
363		7.55	2
364		7.55	2
365		7.59	2

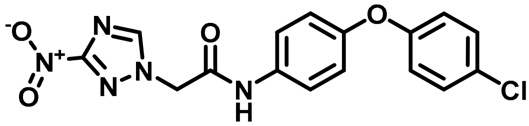
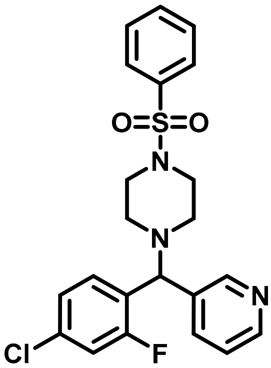
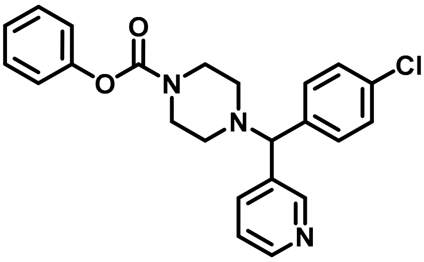
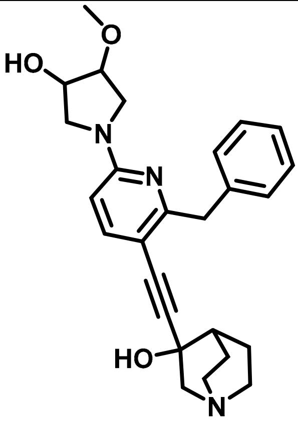
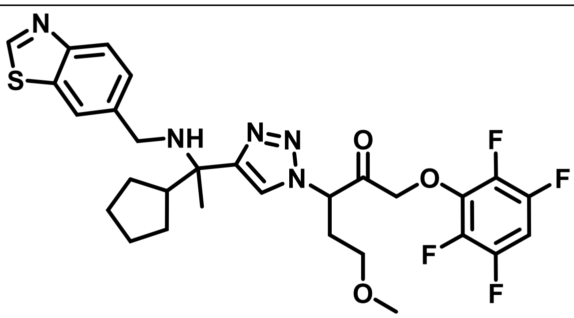
366*		7.59	2
367		7.60	2
368		7.62	2
369		7.62	2
370**		7.62	2

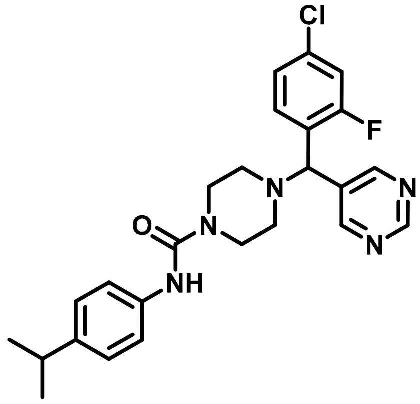
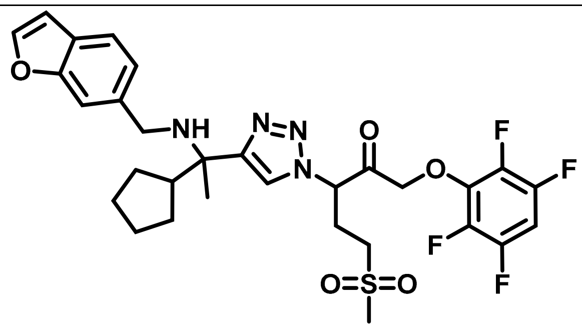
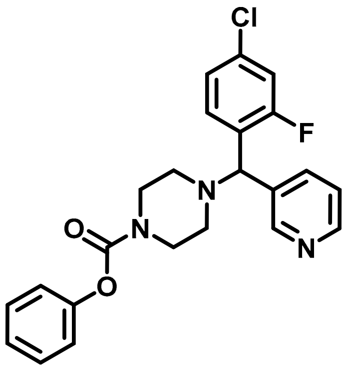
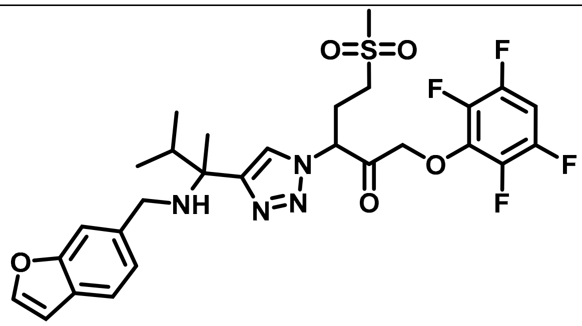
371*		7.66	1
372		7.66	2
373**		7.70	1
374		7.70	2
375		7.70	2

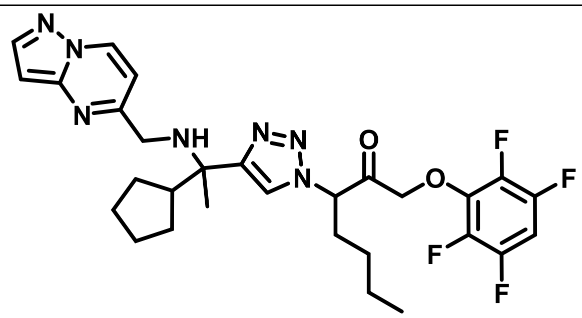
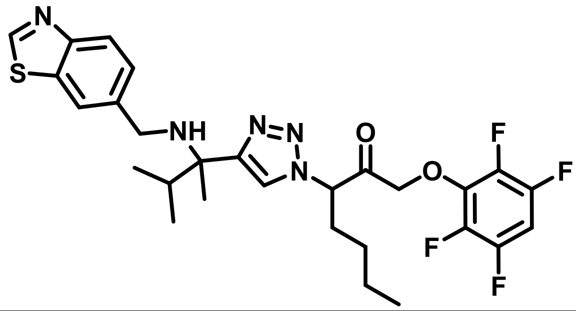
376*		7.72	2
377**		7.74	2
378**		7.74	2
379**		7.77	2
380**		7.77	2

381*		7.82	1
382		7.92	1
383**		7.92	2
384		7.96	20

385**		8.00	1
386*		8.00	2
387		8.05	2
388**		8.05	2
389*		8.10	1

390**		8.10	26
391**		8.10	2
392**		8.10	2
393**		8.10	20
394*		8.15	1

395**		8.15	2
396**		8.30	1
397*		8.30	2
398*		8.52	1

399**		8.52	1
400*		8.70	1

* Test set compounds; **Compounds used in the construction of the fragment collection.

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