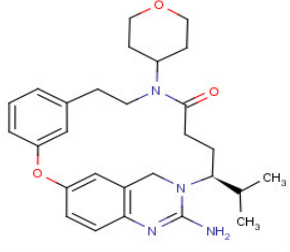
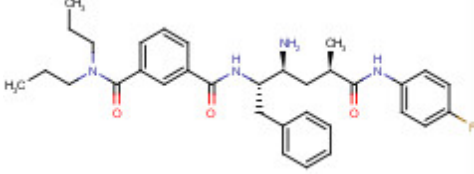
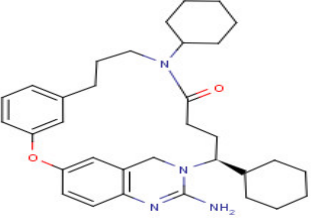
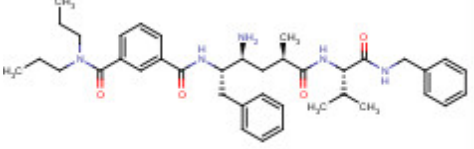
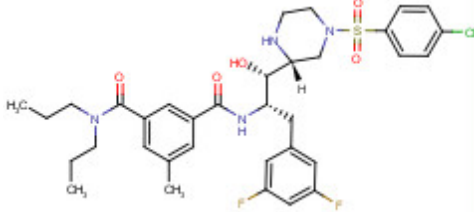
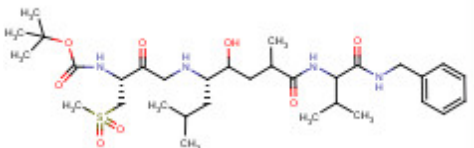
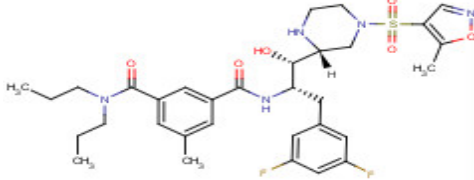
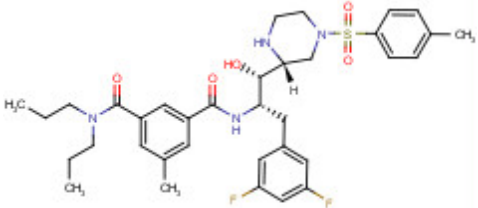
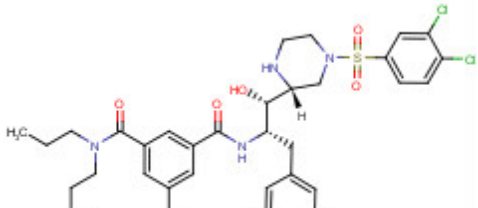
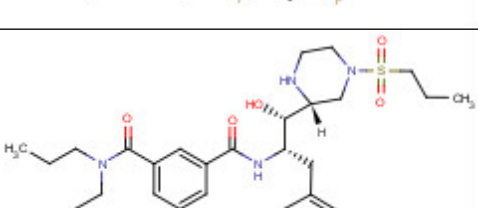
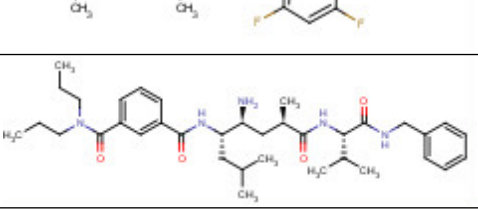
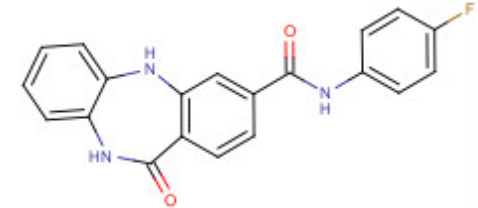
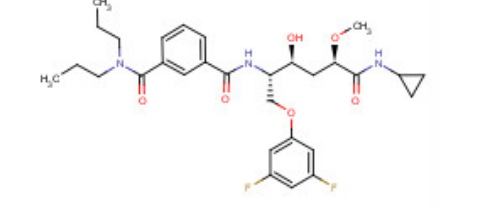
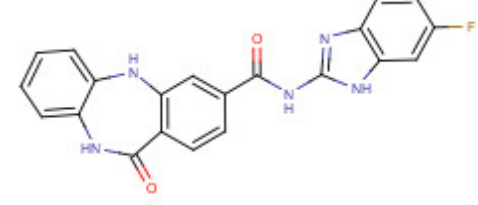


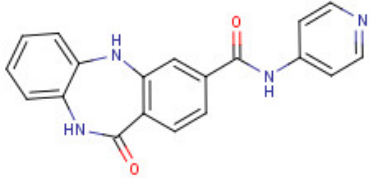
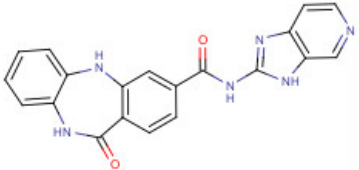
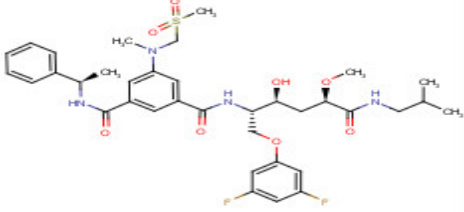
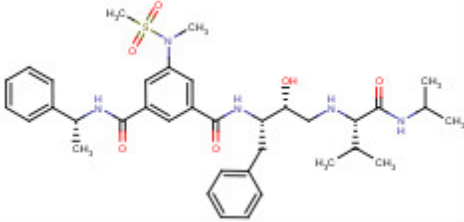
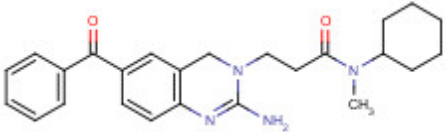
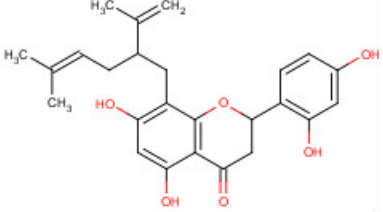
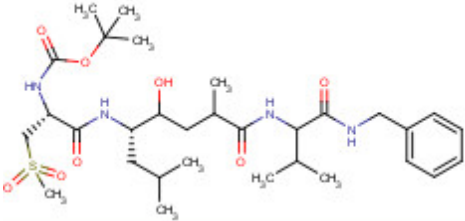
### List of training and test set compounds

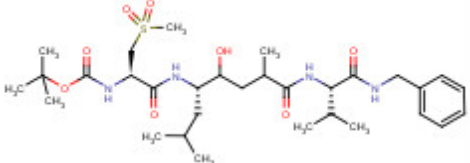
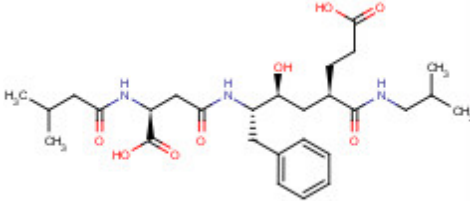
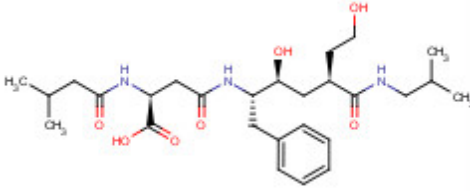
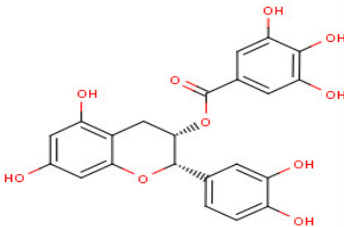
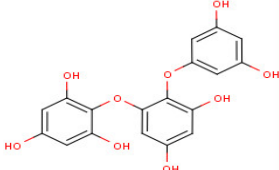
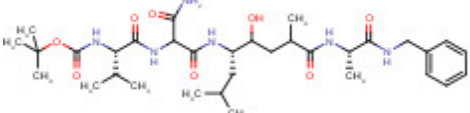
#### Training set:

Name	K <sub>i</sub> (nM)	Structure
ChEBI_726077	5	
ChEBI_726223	5	
ChEBI_726222	12	
ChEBI_726152	17	
ChEBI_726154	20	

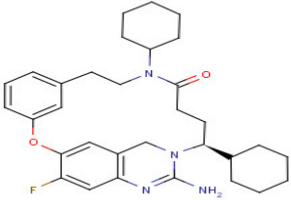
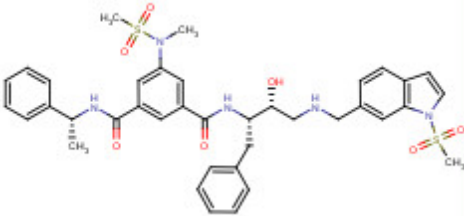
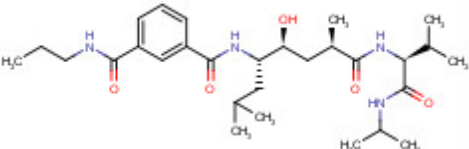
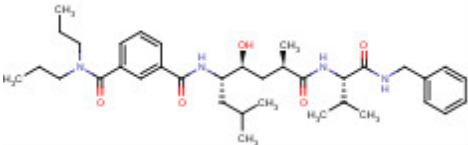
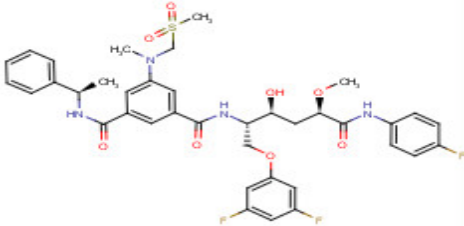
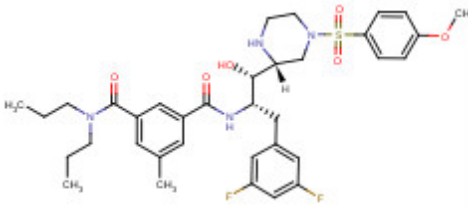
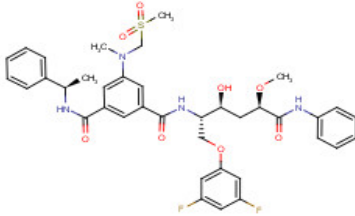
ChEBI_726153	22	
Aminoethylene (AE) compound 7	26	
ChEBI_726078	31	
Aminoethylene (AE) compound 6	33	
ChEBI_729023	42	
ChEBI_409428	1129	
ChEBI_729033	53	

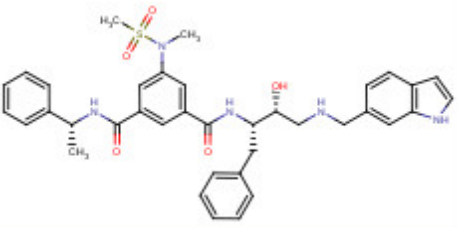
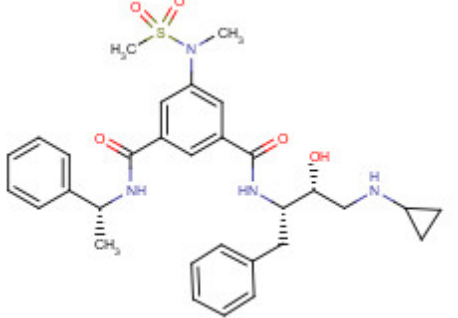
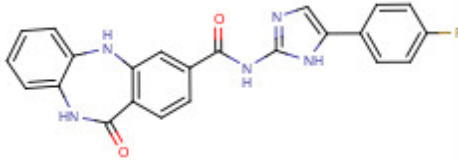
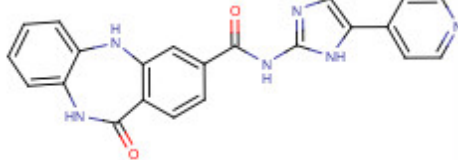
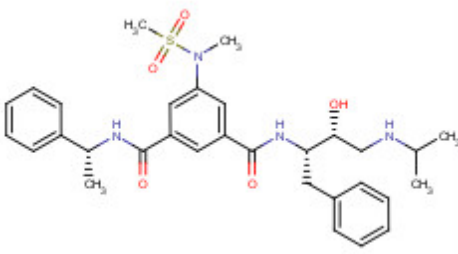
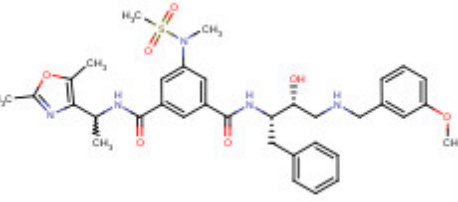
<b>ChEBI_729020</b>	60	
<b>ChEBI_729027</b>	73	
<b>ChEBI_729039</b>	95	
<b>Aminoethylene (AE) compound 2</b>	120	
<b>ChEBI_672067</b>	211	
<b>ChEBI_703982</b>	220	
<b>ChEBI_672014</b>	244	

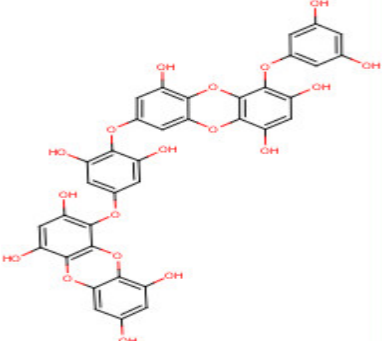
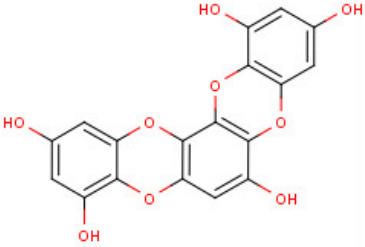
<b>ChEBI_672046</b>	295	
<b>ChEBI_672170</b>	309	
<b>ChEBI_703977</b>	400	
<b>ChEBI_522501</b>	564	
<b>2-aminoquinazoline, 1</b>	900	
<b>ChEBI_568666</b>	1100	
<b>ChEBI_200522</b>	1129	

<b>ChEBI_414615</b>	1129	
<b>ChEBI_359523</b>	1700	
<b>ChEBI_359878</b>	1900	
<b>ChEBI_310228</b>	5300	
<b>ChEBI_732204</b>	12100	
<b>ChEBI_414661</b>	61.4	

## Test set

Name	$K_i$ (nM)	Structure
<b>ChEBI_726221</b>	8	
<b>ChEBI_522503</b>	27	
<b>Isophthalamide Derivative 22</b>	788	
<b>Hydroxyethylene (HE) compound 1</b>	71	
<b>ChEBI_703980</b>	100	
<b>ChEBI_729025</b>	120	
<b>ChEBI_703979</b>	200	

<b>ChEBI_522502</b>	230	
<b>L-000384950</b>	233	
<b>ChEBI_672131</b>	293	
<b>ChEBI_672112</b>	348	
<b>ChEBI_522508</b>	425	
<b>ChEBI_522510</b>	894	

<p><b>ChEBI_582815</b></p>	<p>1500</p>	
<p><b>ChEBI_655277</b></p>	<p>8000</p>	
<p><b>Quercetin</b></p>	<p>14000</p>	