

SUPPLEMENTARY MATERIAL of the manuscript

Binding free energy predictions of Farnesoid X receptor (FXR) agonists using a Linear Interaction Energy (LIE) approach with reliability estimation: application to the D3R Grand Challenge 2

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Table S1. Dataset of 46 FXR ligands obtained from literature for training of LIE models for the benzimidazole, isoxazole and sulfonamide classes of compounds. Listed are the ligand ID used throughout the current work; ChEMBL IDs of the ligands; literature references (Ref.) from which IC50 values were retrieved to obtain the experimentally observed FXR binding free energy ΔG_{obs} (in kJ mol^{-1}), calculated as $\Delta G_{\text{obs}} = RT \ln (\text{IC}_{50}/2)$; the predicted binding free energy (ΔG_{pred}) in kJ mol^{-1} ; and differences $\Delta G_{\text{obs}} - \Delta G_{\text{pred}}$ (Diff., in kJ mol^{-1}).

Compound class	ID	ChEMBL ID	Ref.	ΔG_{obs}	ΔG_{pred}	Diff.
Benzimidazoles	1	CHEMBL1642356	[5]	-33.1	-35.1	2.0
	2	CHEMBL1642359	[5]	-32.2	-37.7	5.5
	3	CHEMBL1642358	[5]	-38.3	-42.6	4.3
	4	CHEMBL1642346	[5]	-42.9	-37.6	-5.3
	5	CHEMBL1642350	[5]	-36.5	-41.1	4.6
	6	CHEMBL1642354	[5]	-41.0	-39.2	-1.8
	7	CHEMBL1642347	[5]	-35.7	-35.4	-0.3
	8	CHEMBL1668262	[15]	-39.4	-40.3	0.9
	9	CHEMBL1668242	[15]	-35.6	-38.1	2.5
	10	CHEMBL1668247	[15]	-43.3	-39.0	-4.3
	11	CHEMBL1668256	[15]	-33.4	-38.9	5.5

	12	CHEMBL1668254	[15]	-40.3	-38.6	-1.7
	13	CHEMBL1668253	[15]	-42.3	-42.0	-0.3
	14	CHEMBL1668240	[15]	-37.5	-36.3	-1.2
	15	CHEMBL1668244	[15]	-48.3	-41.5	-6.8
	16	CHEMBL1668259	[15]	-47.8	-43.8	-4.0
	17	CHEMBL1668258	[15]	-44.3	-41.7	-2.7
	18	CHEMBL1615154	[15]	-50.1	-45.5	-4.6
	19	CHEMBL1668248	[15]	-47.1	-48.5	1.4
	20	CHEMBL1668245	[15]	-37.0	-44.1	7.0
	21	CHEMBL1668260	[15]	-35.0	-34.1	-0.9
	22	CHEMBL1668261	[15]	-40.2	-40.3	0.2
Isoxazoles	1	CHEMBL511389	[16]	-39.9	-36.3	-3.6
	2	CHEMBL511559	[16]	-32.7	-34.6	1.9
	3	CHEMBL466880	[16]	-33.7	-37.1	3.3
	4	CHEMBL466471	[16]	-34.9	-39.2	4.3
	5	CHEMBL513149	[16]	-36.0	-37.6	1.6
	6	CHEMBL466523	[16]	-44.0	-39.4	-4.7
	7	CHEMBL466323	[16]	-42.2	-41.4	-0.8
	8	CHEMBL466887	[16]	-39.2	-40.8	1.6
	9	CHEMBL466318	[16]	-40.7	-38.0	-2.7
	10	CHEMBL469135	[16]	-37.2	-38.8	1.6
	11	CHEMBL466315	[16]	-39.7	-37.2	-2.5
Sulfonamides	1	CHEMBL1367639	[17]	-43.9	-41.6	-2.3
	2	CHEMBL3264627	[17]	-36.3	-40.6	4.3
	3	CHEMBL3264635	[17]	-45.6	-40.9	-4.7
	4	CHEMBL3264639	[17]	-46.4	-45.4	-1.0
	5	CHEMBL3264640	[17]	-43.8	-42.6	-1.2
	6	CHEMBL3264642	[17]	-47.7	-45.4	-2.4
	7	CHEMBL3264644	[17]	-48.5	-46.4	-2.1
	8	CHEMBL3264645	[17]	-46.3	-45.2	-1.0
	9	CHEMBL3264646	[17]	-41.4	-42.8	1.5
	10	CHEMBL3264648	[17]	-40.9	-44.9	4.0
	11	CHEMBL3264650	[17]	-42.7	-43.7	1.0
	12	CHEMBL3264651	[17]	-45.0	-43.3	-1.7
	13	CHEMBL3264987	[17]	-38.6	-44.2	5.6

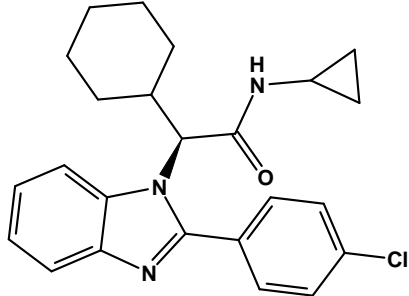
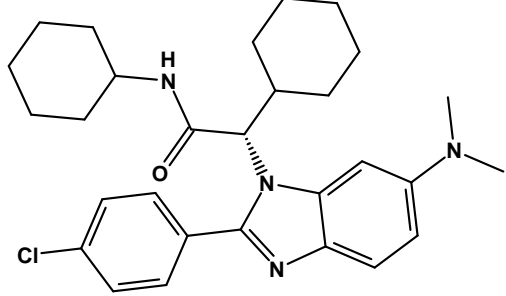
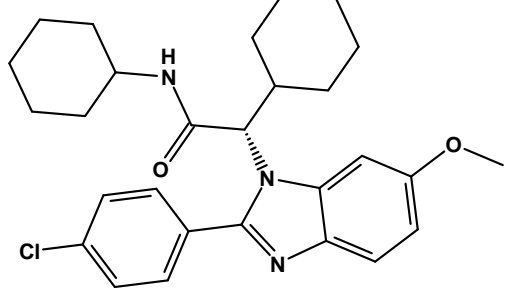
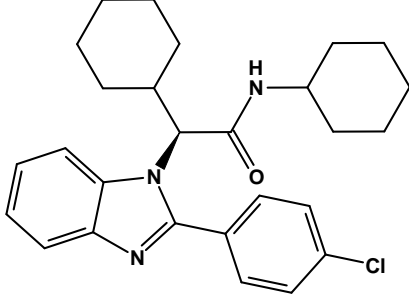
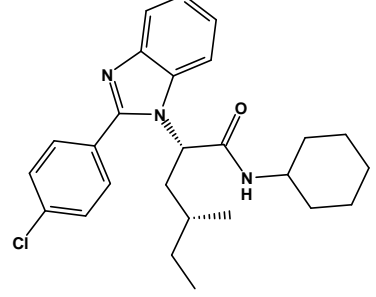
Table S2. Dataset of 30 FXR ligands obtained from literature for testing the LIE models for the benzimidazole, isoxazole and sulfonamide classes of compounds, and of 60 FXR ligands of the D3R GC2 ligand set. Listed are the ligand ID used throughout the current work; ChEMBL or D3R (FXR) IDs of the ligands; literature references (Ref.) from which IC₅₀ values were retrieved to obtain the experimentally observed FXR binding free energy ΔG_{obs} (in kJ mol⁻¹), calculated as $\Delta G_{\text{obs}} = RT \ln (\text{IC}_{50}/2)$; the predicted binding free energy (ΔG_{pred}) in kJ mol⁻¹; differences $\Delta G_{\text{obs}} - \Delta G_{\text{pred}}$ (Diff., in kJ mol⁻¹); the violations for each of the 5 AD criteria (1 for violated and 0 for non-violated); and the total CI score per prediction.

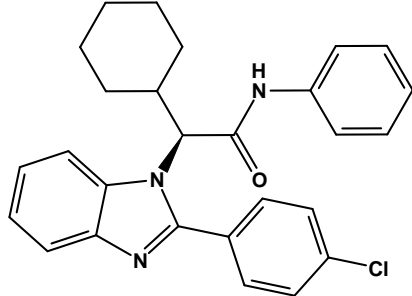
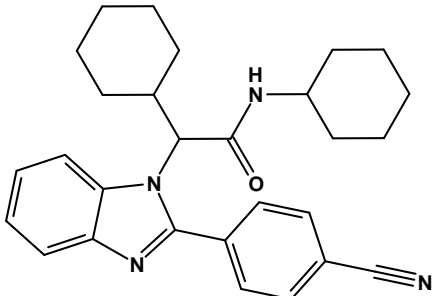
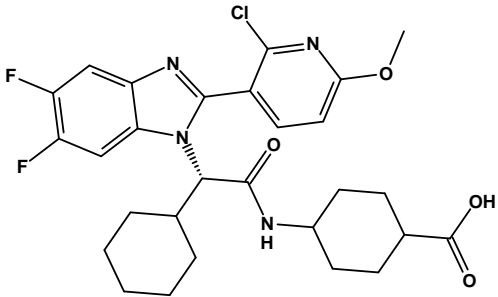
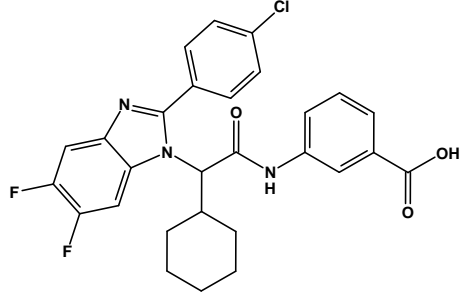
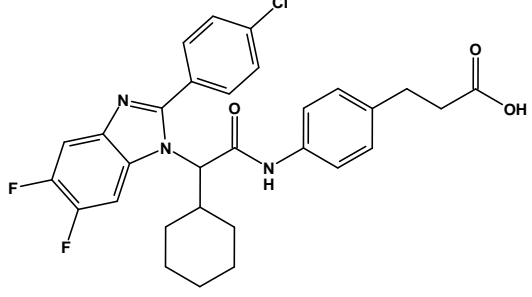
Compound class	ID	ChEMBL/FXR ID	Ref.	ΔG_{obs}	ΔG_{pred}	Diff.	AD criteria					CI score
							1	2	3	4	5	
Literature test												
Benzimidazole	1	CHEMBL1642355	[5]	-33.8	-33.8	0.0	0	0	0	0	0	0
	2	CHEMBL1642360	[5]	-31.9	-43.1	11.2	0	0	0	0	1	1
	3	CHEMBL1642361	[5]	-31.7	-38.6	6.9	0	0	0	1	0	1
	4	CHEMBL1642351	[5]	-32.9	-37.5	4.5	0	0	0	0	0	0
	5	CHEMBL1642353	[5]	-28.2	-37.0	8.8	0	0	0	0	0	0
	6	CHEMBL1642357	[5]	-33.0	-38.9	6.0	0	0	0	0	0	0
	7	CHEMBL1642349	[5]	-27.7	-36.1	8.4	0	0	0	1	0	1
	8	CHEMBL1642348	[5]	-30.0	-38.5	8.6	0	1	0	1	0	2
	9	CHEMBL1642362	[15]	-47.1	-43.1	-4.0	0	0	0	0	0	0
	10	CHEMBL1668243	[15]	-48.1	-44.2	-3.8	0	0	0	1	0	1
	11	CHEMBL1668241	[15]	-39.1	-37.2	-2.0	0	0	0	0	0	0
	12	CHEMBL1668246	[15]	-35.4	-38.8	3.4	0	0	0	1	1	2
	13	CHEMBL1668255	[15]	-40.3	-37.0	-3.3	0	0	0	1	1	2
	14	CHEMBL1668251	[15]	-37.5	-37.9	0.4	0	0	0	1	0	1
	15	CHEMBL1668239	[15]	-44.3	-40.5	-3.8	0	0	0	0	0	0

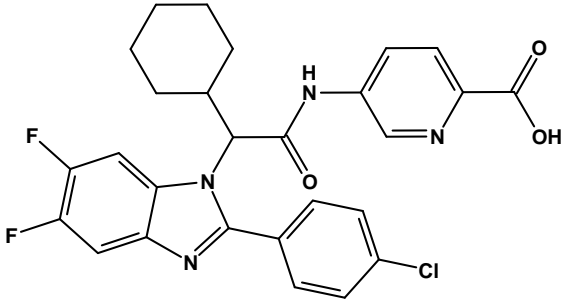
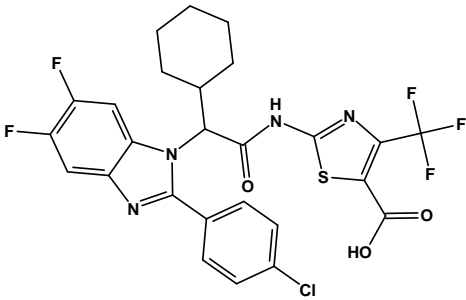
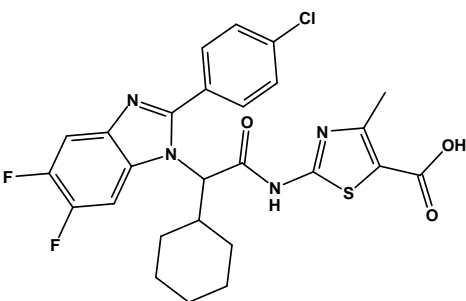
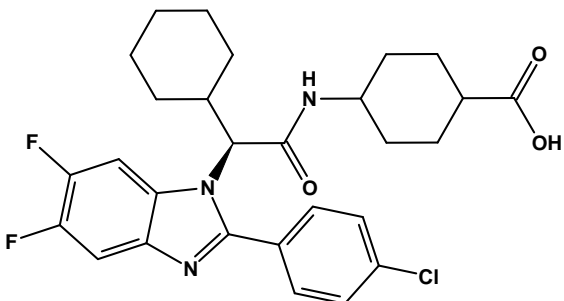
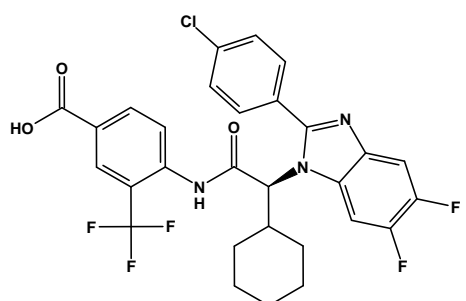
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	17	CHEMBL1668250	[15]	-32.9	-39.2	6.3	0	0	0	1	1	2
	18	CHEMBL1615150	[15]	-46.1	-36.5	-9.5	0	0	0	1	1	2
	19	CHEMBL1668257	[15]	-48.3	-45.1	-3.2	0	0	0	1	1	2
	20	CHEMBL1615152	[15]	-44.5	-40.1	-4.5	0	0	0	1	0	1
	21	CHEMBL1668249	[15]	-53.5	-44.2	-9.4	0	0	0	1	1	2
	22	CHEMBL1615153	[15]	-43.8	-41.5	-2.2	0	0	0	1	1	2
	23	CHEMBL1668252	[15]	-36.7	-36.6	-0.1	0	0	0	1	1	2
Sulfonamide	1	CHEMBL3264637	[17]	-46.9	-45.4	-1.5	0	0	0	1	0	1
	2	CHEMBL3264638	[17]	-45.6	-38.8	-6.8	0	0	1	1	1	3
	3	CHEMBL3264641	[17]	-43.6	-44.5	0.9	0	0	0	1	1	2
	4	CHEMBL3264643	[17]	-42.7	-43.5	0.9	0	0	0	1	0	1
	5	CHEMBL3264647	[17]	-40.3	-44.9	4.6	0	0	0	1	1	2
	6	CHEMBL3264649	[17]	-44.2	-43.7	-0.5	0	0	0	1	0	1
	7	CHEMBL3264988	[17]	-38.1	-43.8	5.8	0	0	0	1	1	2
D3R predictions												
Benzimidazole	1	FXR_19		-42.3	-37.5	-4.8	0	0	0	0	0	0
	2	FXR_27		-48.1	-36.3	-11.8	0	0	0	1	0	1
	3	FXR_62		-40.7	-41.9	1.1	0	0	0	1	1	2
	4	FXR_60		-47.0	-46.8	-0.2	0	1	0	1	1	3
	5	FXR_52		-40.7	-42.4	1.7	0	0	0	1	0	1
	6	FXR_20		-48.8	-40.8	-7.9	0	0	0	0	0	0
	7	FXR_50		-32.2	-36.7	4.5	0	0	0	0	0	0
	8	FXR_25		-45.0	-42.1	-2.9	0	0	0	0	0	0
	9	FXR_58		-46.3	-40.9	-5.5	0	0	0	1	1	2
	10	FXR_72		-47.4	-43.7	-3.7	0	0	0	1	1	2
	11	FXR_24		-46.0	-38.5	-7.5	0	0	0	1	1	2
	12	FXR_56		-30.5	-47.5	17.0	0	0	0	1	1	2
	13	FXR_53		-40.9	-38.1	-2.8	0	0	0	1	0	1

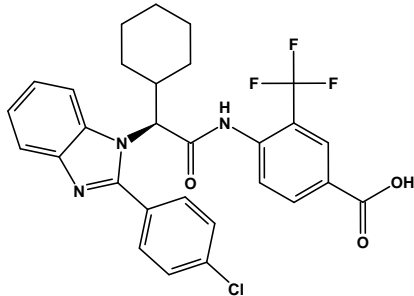
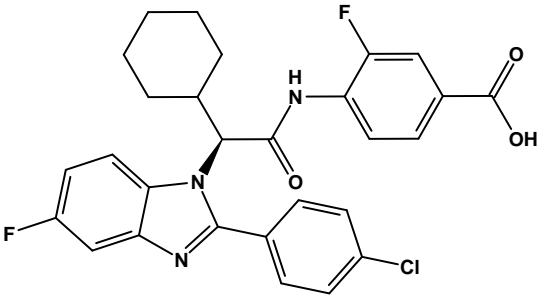
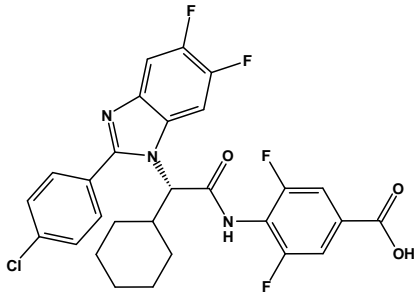
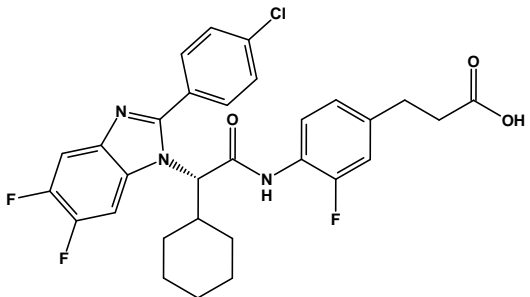
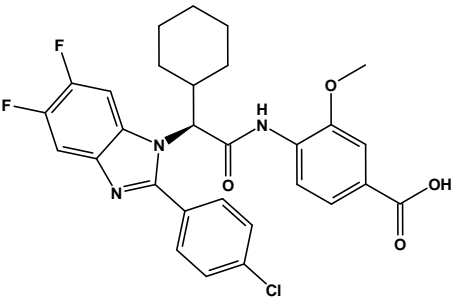
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15	FXR_21	-37.0	-42.2	5.3	0	0	0	0	0	0
16	FXR_54	-36.8	-39.3	2.5	0	0	0	0	0	0
17	FXR_61	-47.5	-37.5	-10.0	0	1	0	1	0	2
18	FXR_28	-45.9	-40.7	-5.3	0	1	0	0	1	2
19	FXR_29	-44.4	-42.7	-1.7	0	1	0	1	0	2
20	FXR_71	-45.0	-43.5	-1.5	0	1	0	1	1	3
21	FXR_42	-45.8	-34.4	-11.3	0	0	0	1	0	1
22	FXR_32	-43.0	-33.6	-9.4	0	0	0	1	0	1
23	FXR_22	-49.8	-45.4	-4.5	0	0	0	1	0	1
24	FXR_64	-40.9	-32.7	-8.2	0	0	0	1	0	1
25	FXR_68	-26.3	-36.0	9.8	0	0	0	1	1	2
26	FXR_69	-34.6	-51.4	16.7	1	0	1	1	1	4
27	FXR_66	-30.4	-39.0	8.6	0	0	0	1	1	2
28	FXR_67	-29.3	-40.8	11.5	0	0	0	1	1	2
29	FXR_31	-50.0	-34.1	-15.9	0	0	0	1	0	1
30	FXR_57	-49.8	-35.8	-14.0	0	0	0	1	0	1
31	FXR_55	-58.3	-38.4	-19.9	0	0	0	1	0	1
32	FXR_26	-34.7	-41.9	7.2	0	0	0	1	0	1
33	FXR_70	-38.2	-40.2	2.0	0	0	0	1	0	1
34	FXR_36	-45.6	-43.2	-2.4	0	0	0	1	0	1
35	FXR_63	-27.9	-43.5	15.6	0	0	0	1	1	2
36	FXR_51	-41.5	-36.4	-5.0	0	0	0	1	0	1
37	FXR_30	-42.8	-41.3	-1.5	0	0	0	1	1	2
38	FXR_37	-30.0	-35.0	5.0	0	0	0	0	0	0
39	FXR_6	-45.1	-35.5	-9.6	0	0	0	1	1	2
40	FXR_9	-33.4	-37.3	3.8	0	0	0	1	0	1
41	FXR_13	-47.3	-49.6	2.3	0	0	0	1	1	2
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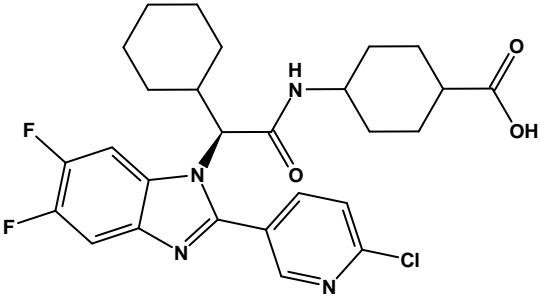
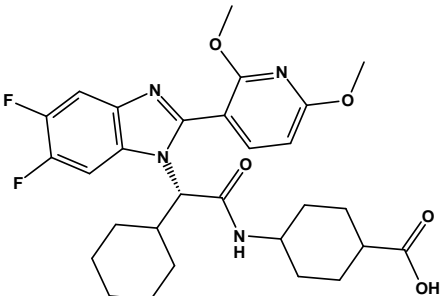
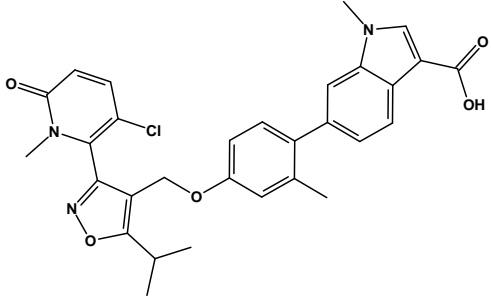
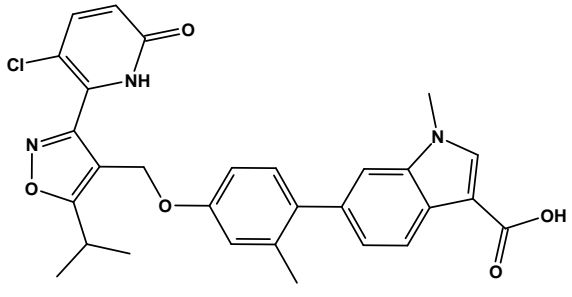
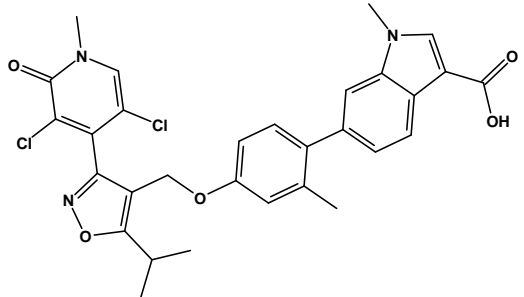
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	44	FXR_8	-33.9	-42.1	8.2	0	0	0	1	0	1
	45	FXR_7	-41.6	-43.1	1.5	0	0	0	0	0	0
	46	FXR_14	-47.9	-37.4	-10.5	0	0	0	1	0	1
Isoxazole	1	FXR_4	-31.3	-35.3	3.9	0	1	1	1	1	4
	2	FXR_23	-37.7	-36.2	-1.5	0	1	0	1	1	3
	3	FXR_33	-44.0	-39.2	-4.9	0	0	0	1	0	1
	4	FXR_65	-42.2	-37.2	-5.0	0	0	0	1	0	1
Sulfonamide	1	FXR_90	-24.8	-43.2	18.4	0	1	0	1	0	2
	2	FXR_102	-27.8	-43.6	15.8	0	0	0	1	1	2
	3	FXR_15	-28.0	-43.5	15.4	0	1	0	0	1	2
Spiro	1	FXR_81	-33.8	-42.0	8.3	0	1	0	1	0	2
Miscellaneous	1	FXR_1	-26.2	-41.5	15.3	0	1	0	1	0	2
	2	FXR_2	-36.6	-36.6	0.0	0	1	1	1	1	4
	3	FXR_3	-22.3	-34.3	12.0	0	1	1	1	1	4
	4	FXR_5	-35.4	-37.6	2.2	0	1	0	1	0	2
	5	FXR_18	-33.4	-33.0	-0.4	0	1	0	1	1	3
	6	FXR_34	-48.4	-37.0	-11.4	0	1	0	0	1	2

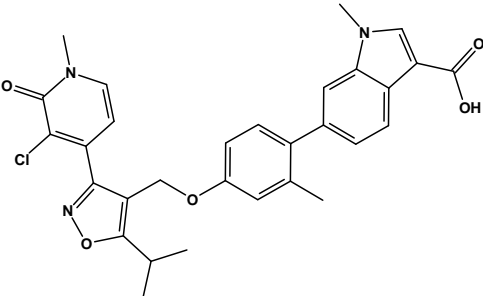
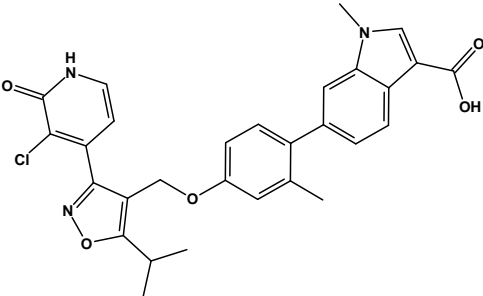
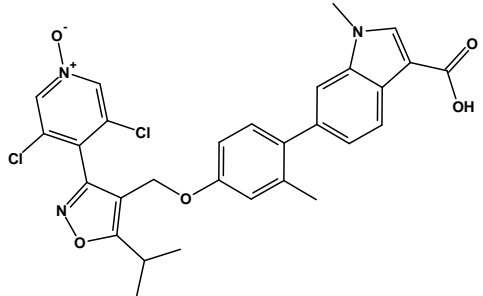
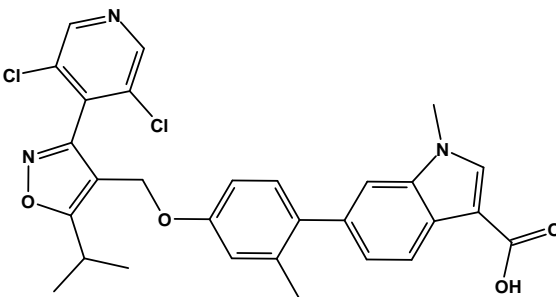
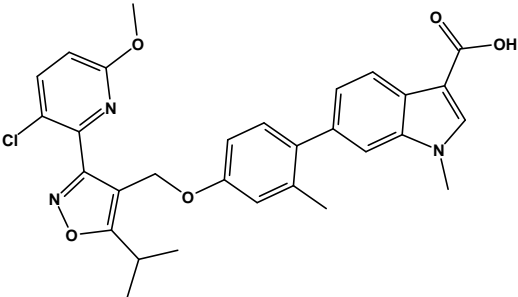
	Compound class	ID	ChEMBL ID	Structure
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2	Benzimidazole	2	CHEMBL1642359	
3	Benzimidazole	3	CHEMBL1642358	
4	Benzimidazole	4	CHEMBL1642346	
5	Benzimidazole	5	CHEMBL1642350	

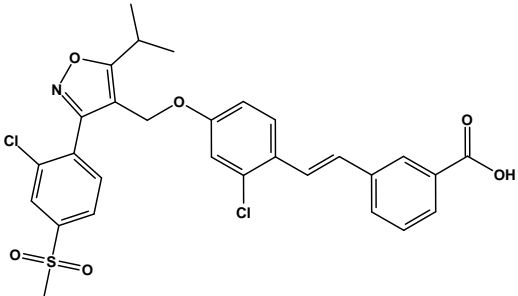
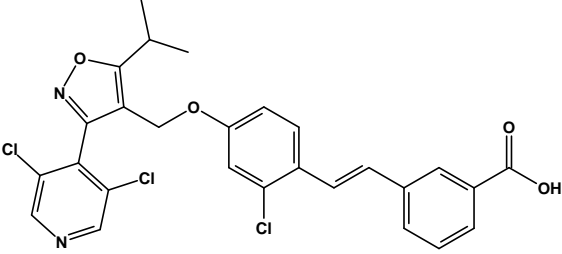
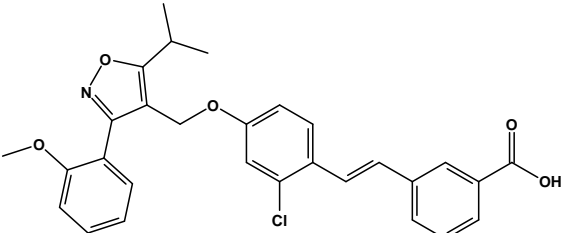
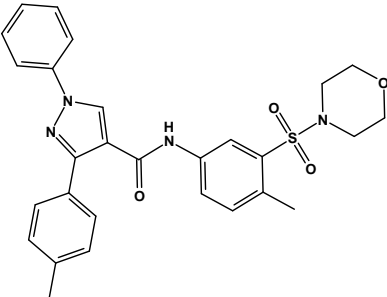
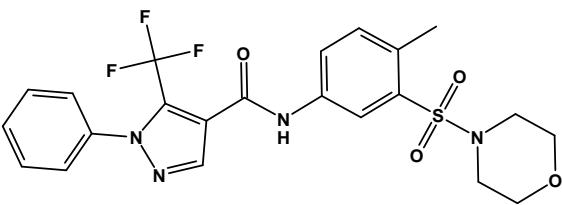
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6	Benzimidazole	6	CHEMBL1642354	
7	Benzimidazole	7	CHEMBL1642347	
8	Benzimidazole	8	CHEMBL1668262	
9	Benzimidazole	9	CHEMBL1668242	
10	Benzimidazole	10	CHEMBL1668247	

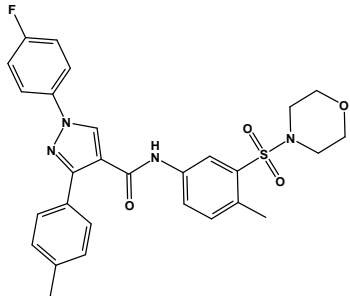
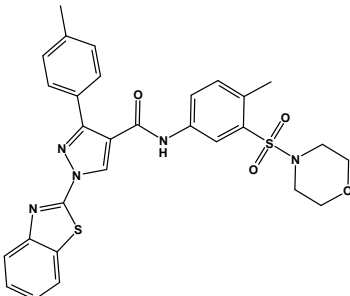
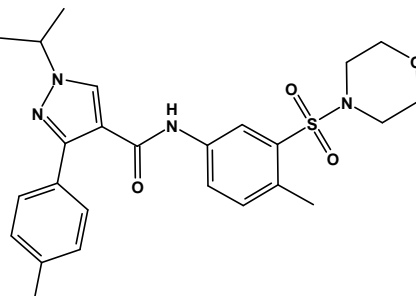
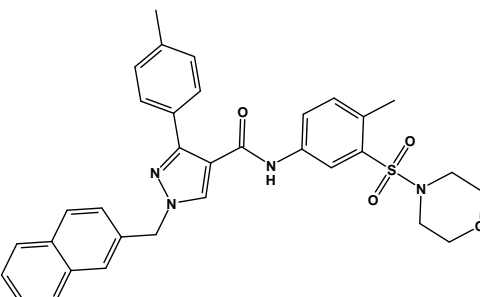
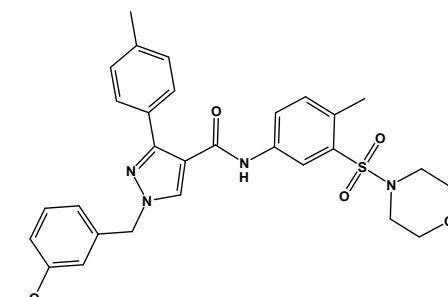
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11	Benzimidazole	11	CHEMBL1668256	
12	Benzimidazole	12	CHEMBL1668254	
13	Benzimidazole	13	CHEMBL1668253	
14	Benzimidazole	14	CHEMBL1668240	
15	Benzimidazole	15	CHEMBL1668244	

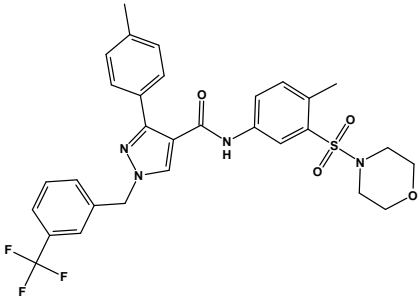
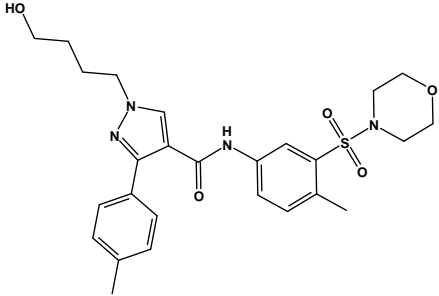
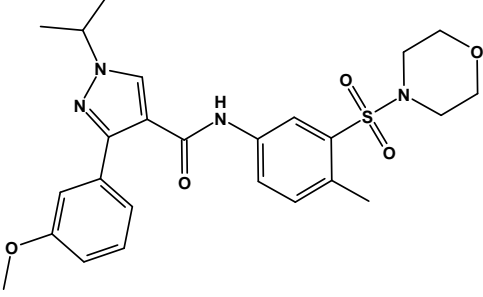
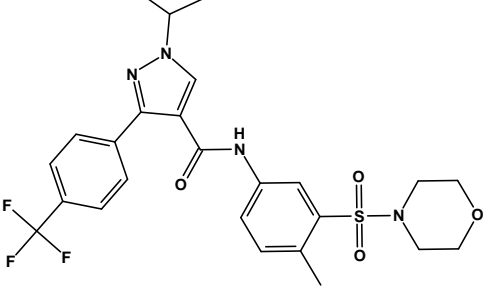
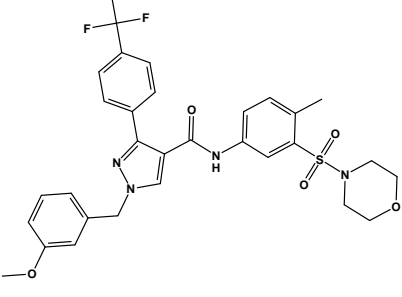
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16	Benzimidazole	16	CHEMBL1668259	
17	Benzimidazole	17	CHEMBL1668258	
18	Benzimidazole	18	CHEMBL1615154	
19	Benzimidazole	19	CHEMBL1668248	
20	Benzimidazole	20	CHEMBL1668245	

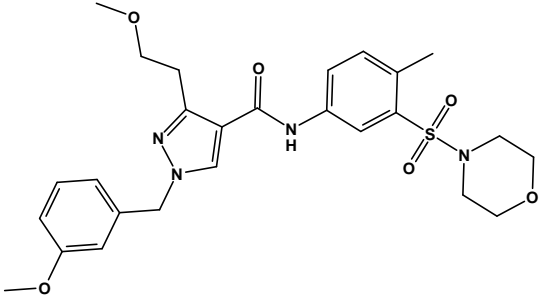
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21	Benzimidazole	21	CHEMBL1668260	
22	Benzimidazole	22	CHEMBL1668261	
23	Isoxazole	1	CHEMBL511389	
24	Isoxazole	2	CHEMBL511559	
25	Isoxazole	3	CHEMBL466880	

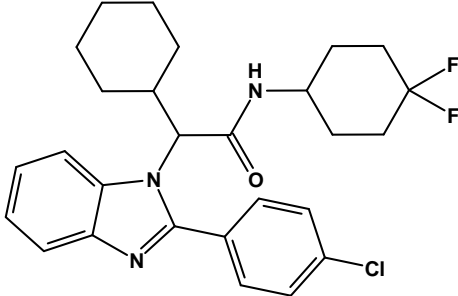
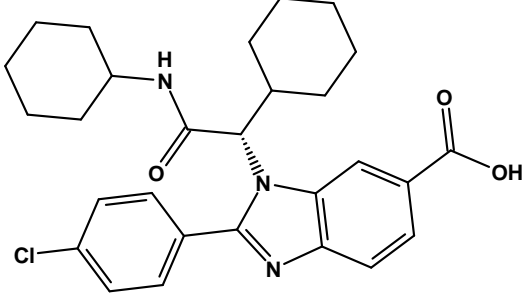
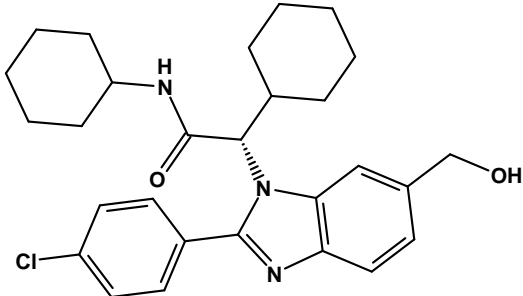
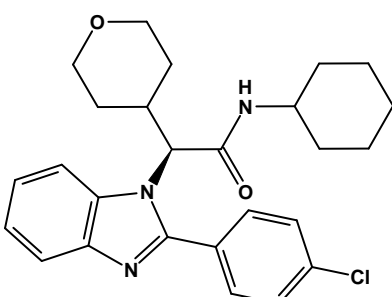
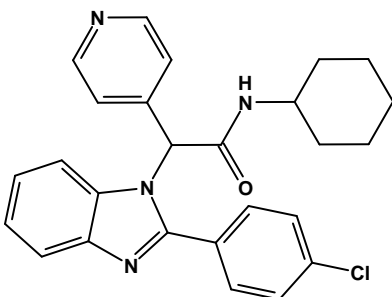
	Compound class	ID	ChEMBL ID	Structure
26	Isoxazole	4	CHEMBL466471	
27	Isoxazole	5	CHEMBL513149	
28	Isoxazole	6	CHEMBL466523	
29	Isoxazole	7	CHEMBL466323	
30	Isoxazole	8	CHEMBL466887	

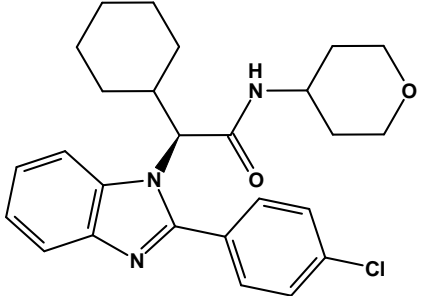
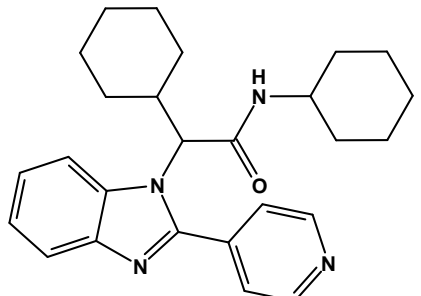
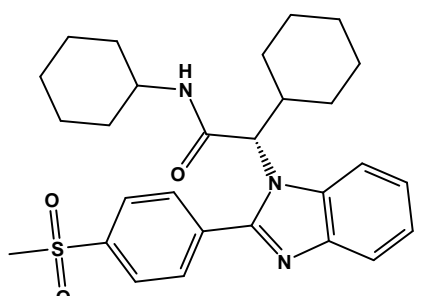
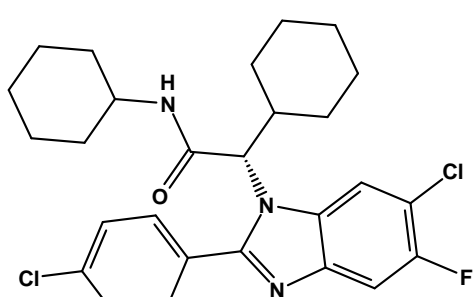
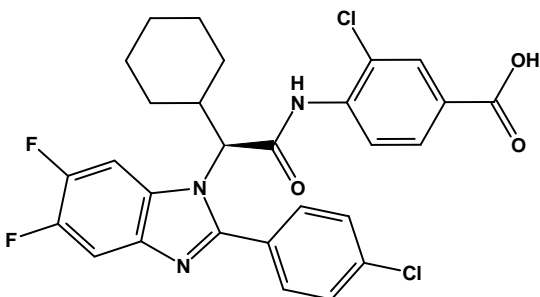
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31	Isoxazole	9	CHEMBL466318	
32	Isoxazole	10	CHEMBL469135	
33	Isoxazole	11	CHEMBL466315	
34	Sulfonamide	1	CHEMBL1367639	
35	Sulfonamide	2	CHEMBL3264627	

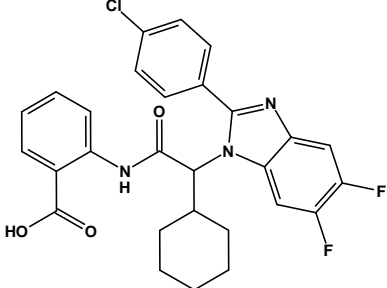
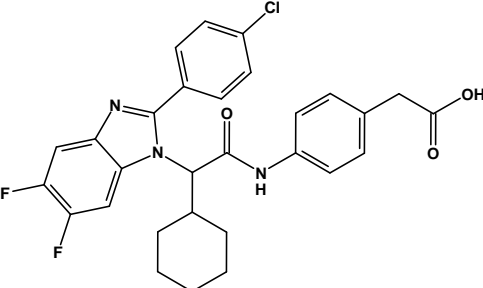
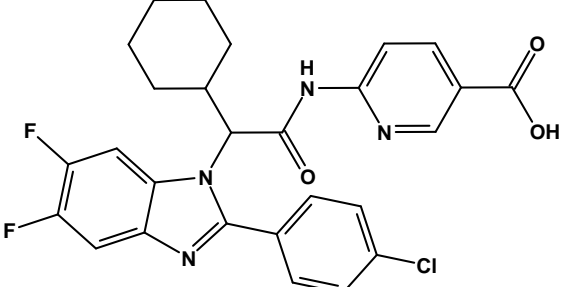
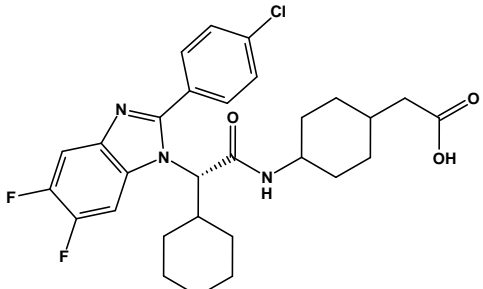
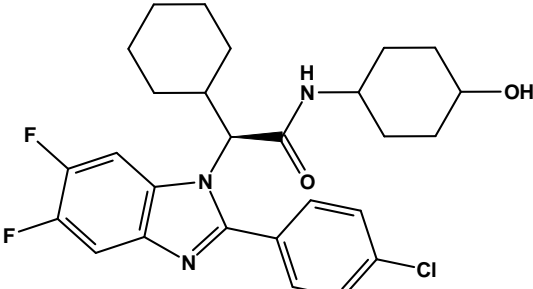
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36	Sulfonamide	3	CHEMBL3264635	
37	Sulfonamide	4	CHEMBL3264639	
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39	Sulfonamide	6	CHEMBL3264642	
40	Sulfonamide	7	CHEMBL3264644	

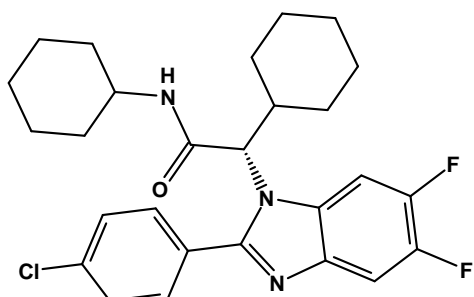
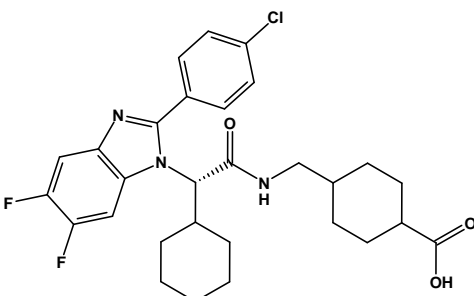
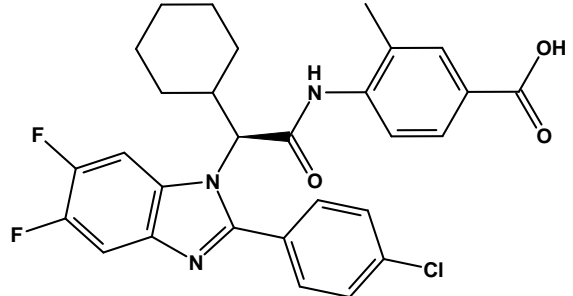
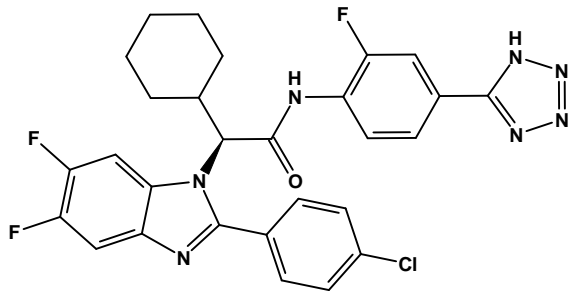
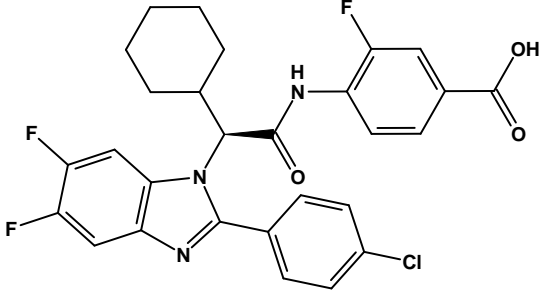
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41	Sulfonamide	8	CHEMBL3264645	
42	Sulfonamide	9	CHEMBL3264646	
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44	Sulfonamide	11	CHEMBL3264650	
45	Sulfonamide	12	CHEMBL3264651	

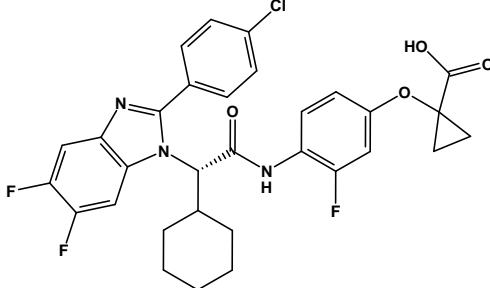
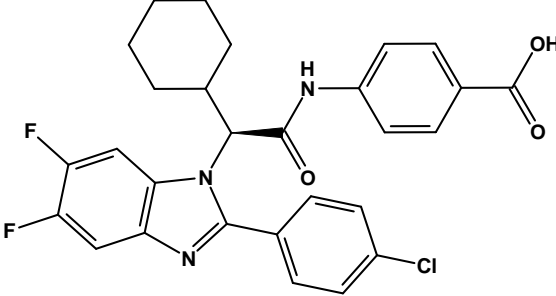
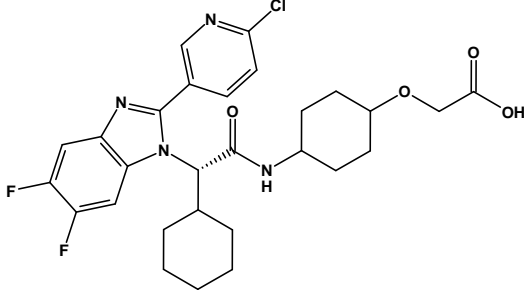
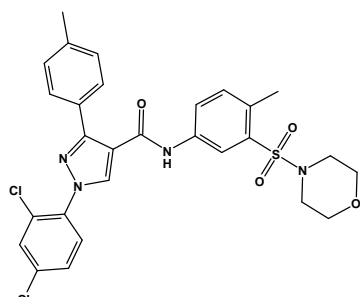
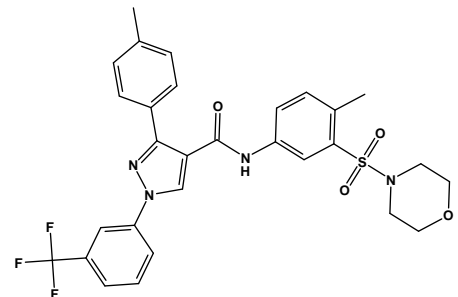
	Compound class	ID	ChEMBL ID	Structure
46	Sulfonamide	13	CHEMBL3264987	 <p>The chemical structure of CHEMBL3264987 is a sulfonamide derivative. It features a central imidazole ring. One nitrogen of the imidazole is substituted with a (4-methoxyphenyl)methyl group. The other nitrogen is substituted with a (2-methoxyethyl) group. The 2-position of the imidazole ring is substituted with a sulfonamide group (-NH-C(=O)-). The sulfonamide nitrogen is further substituted with a 4-methylphenyl group. The sulfonamide sulfur atom is double-bonded to two oxygen atoms and is also bonded to a morpholine ring.</p>

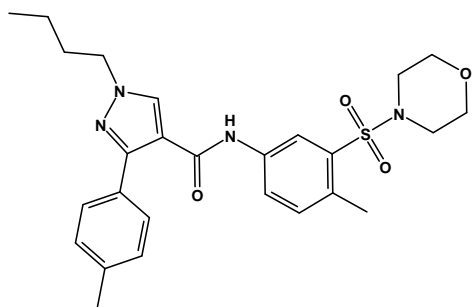
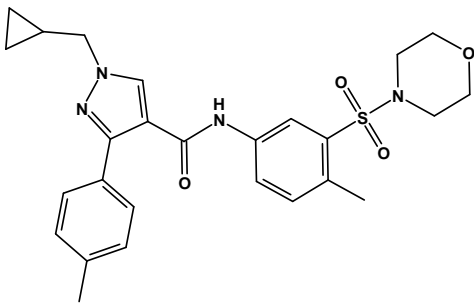
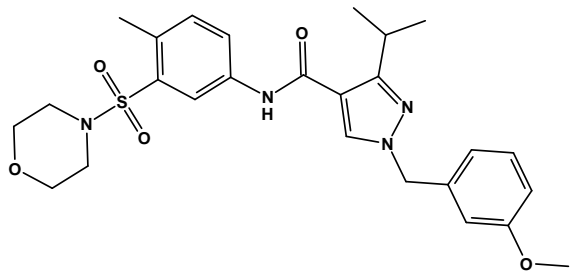
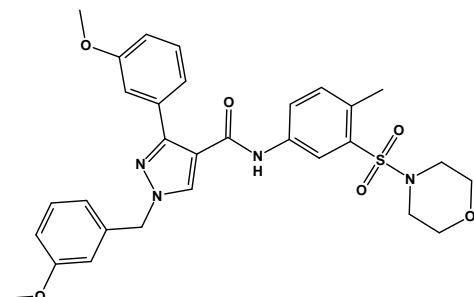
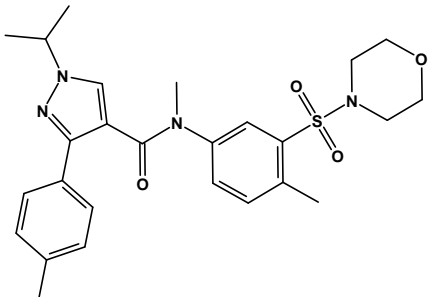
	Compound class	ID	ChEMBLID	Structure
1	Benzimidazole	1	CHEMBL1642355	
2	Benzimidazole	2	CHEMBL1642360	
3	Benzimidazole	3	CHEMBL1642361	
4	Benzimidazole	4	CHEMBL1642351	
5	Benzimidazole	5	CHEMBL1642353	

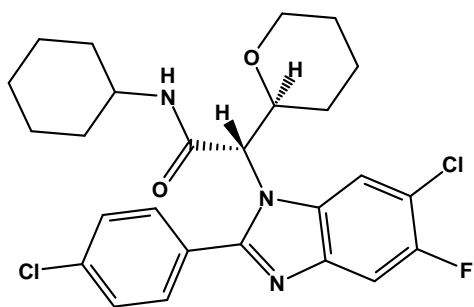
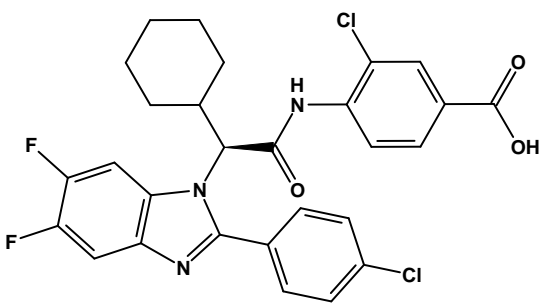
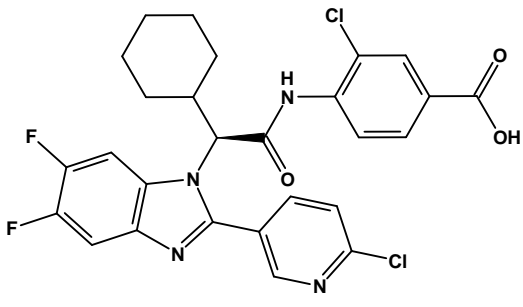
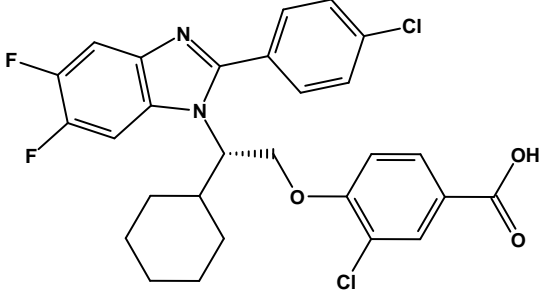
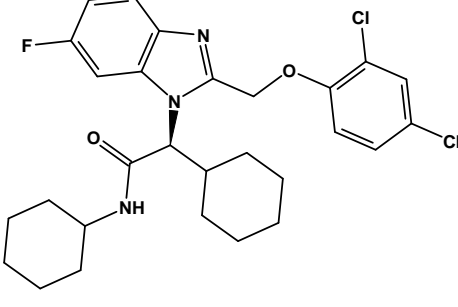
	Compound class	ID	ChEMBLID	Structure
6	Benzimidazole	6	CHEMBL1642357	
7	Benzimidazole	7	CHEMBL1642349	
8	Benzimidazole	8	CHEMBL1642348	
9	Benzimidazole	9	CHEMBL1642362	
10	Benzimidazole	10	CHEMBL1668243	

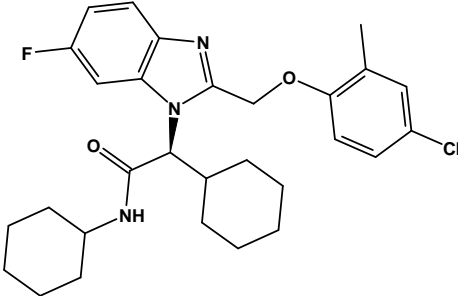
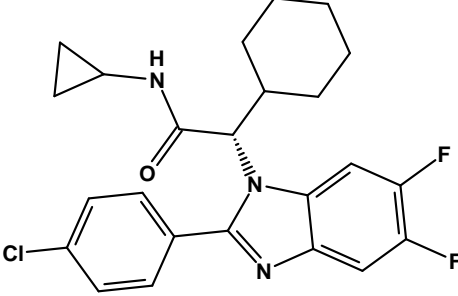
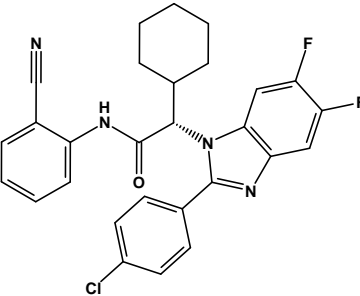
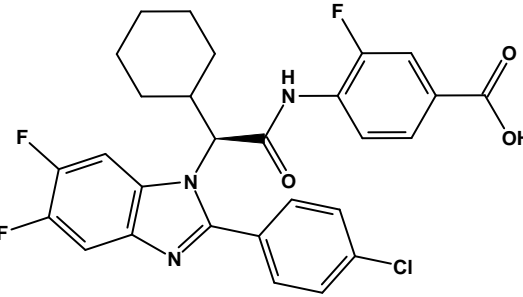
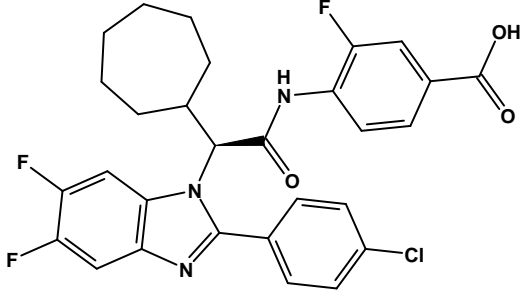
	Compound class	ID	ChEMBLID	Structure
11	Benzimidazole	11	CHEMBL1668241	
12	Benzimidazole	12	CHEMBL1668246	
13	Benzimidazole	13	CHEMBL1668255	
14	Benzimidazole	14	CHEMBL1668251	
15	Benzimidazole	15	CHEMBL1668239	

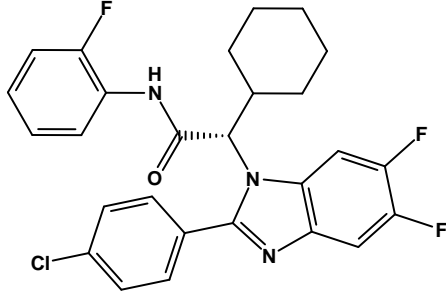
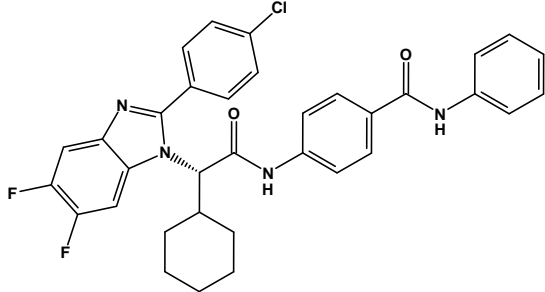
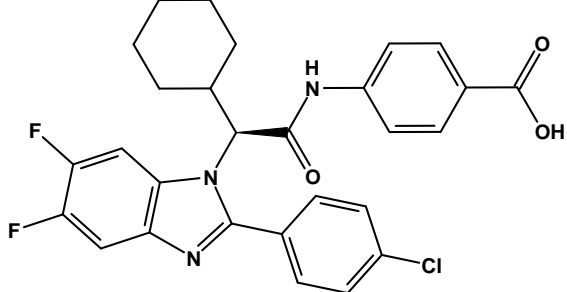
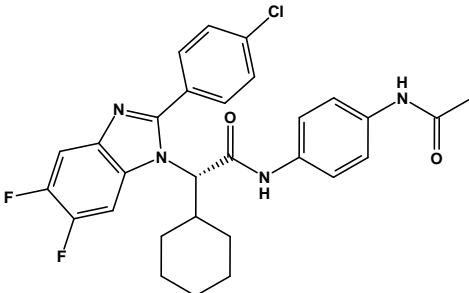
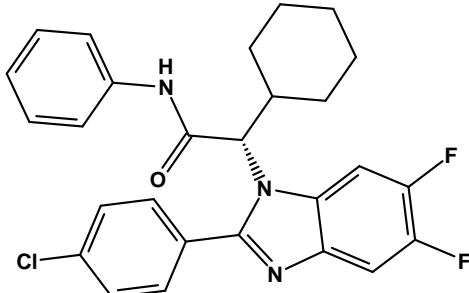
	Compound class	ID	ChEMBLID	Structure
16	Benzimidazole	16	CHEMBL1668238	
17	Benzimidazole	17	CHEMBL1668250	
18	Benzimidazole	18	CHEMBL1615150	
19	Benzimidazole	19	CHEMBL1668257	
20	Benzimidazole	20	CHEMBL1615152	

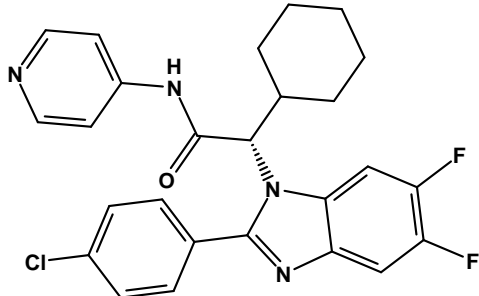
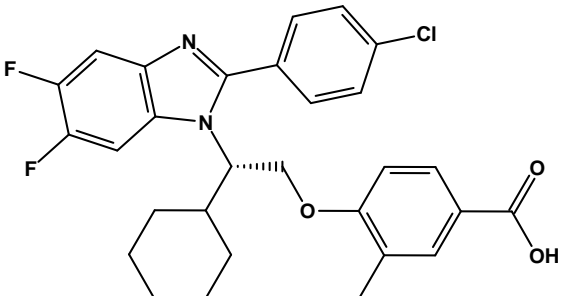
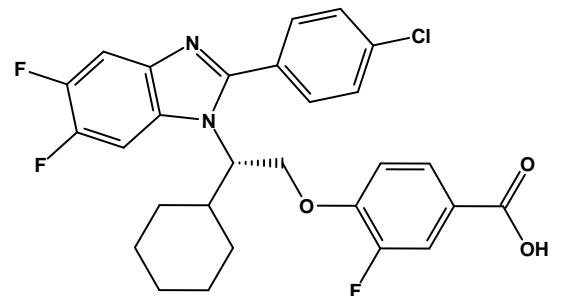
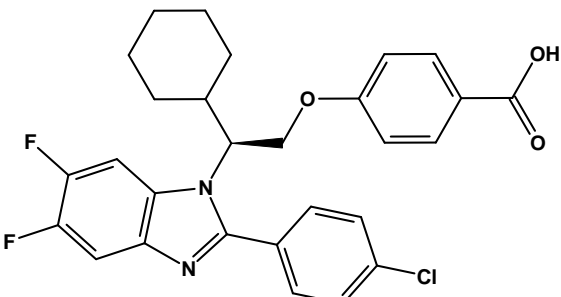
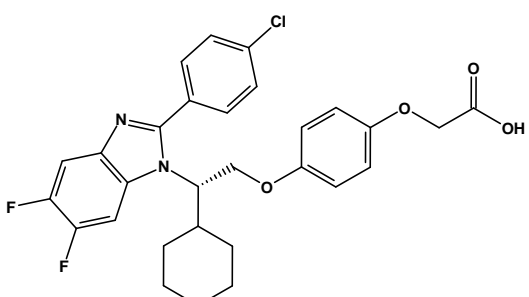
	Compound class	ID	ChEMBLID	Structure
21	Benzimidazole	21	CHEMBL1668249	
22	Benzimidazole	22	CHEMBL1615153	
23	Benzimidazole	23	CHEMBL1668252	
24	Sulfonamide	1	CHEMBL3264637	
25	Sulfonamide	2	CHEMBL3264638	

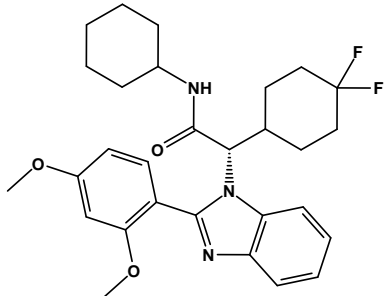
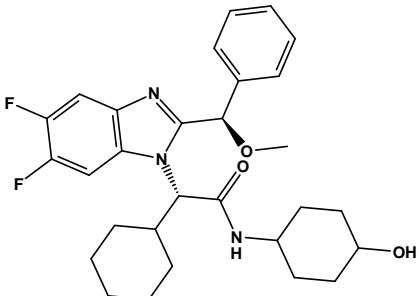
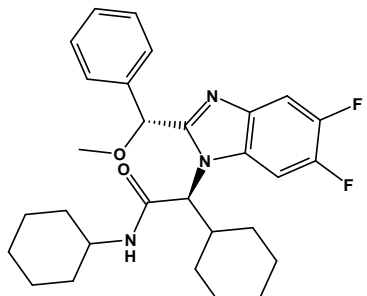
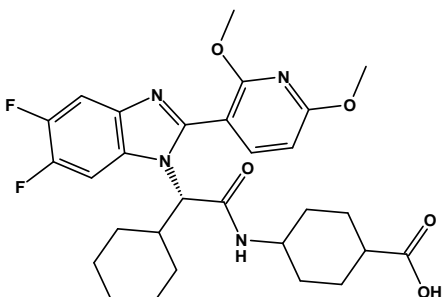
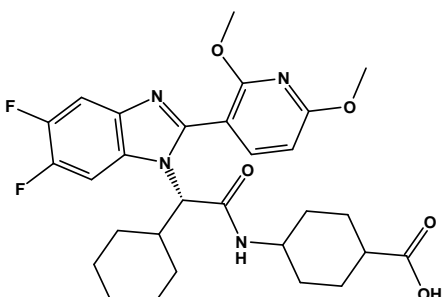
	Compound class	ID	ChEMBLID	Structure
26	Sulfonamide	3	CHEMBL3264641	 <chem>CCCCN1C=CC(C1)C(=O)Nc2ccc(C)c(S(=O)(=O)N3CCOCC3)c2</chem>
27	Sulfonamide	4	CHEMBL3264643	 <chem>CC1CC1CN(C1=CC=C(C=C1)C)C(=O)Nc2ccc(C)c(S(=O)(=O)N3CCOCC3)c2</chem>
28	Sulfonamide	5	CHEMBL3264647	 <chem>CC(C)C1=CN(C1)CN(C1=CC=C(C=C1)C)C(=O)Nc2ccc(C)c(S(=O)(=O)N3CCOCC3)c2</chem>
29	Sulfonamide	6	CHEMBL3264649	 <chem>COc1ccc(cc1)CN(C1=CC=C(C=C1)C)C(=O)Nc2ccc(C)c(S(=O)(=O)N3CCOCC3)c2</chem>
30	Sulfonamide	7	CHEMBL3264988	 <chem>CC(C)N1C=CC(C1)C(=O)Nc2ccc(C)c(S(=O)(=O)N3CCOCC3)c2</chem>

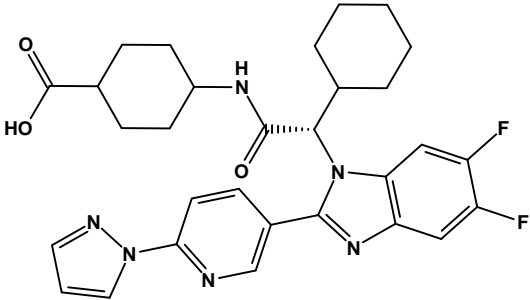
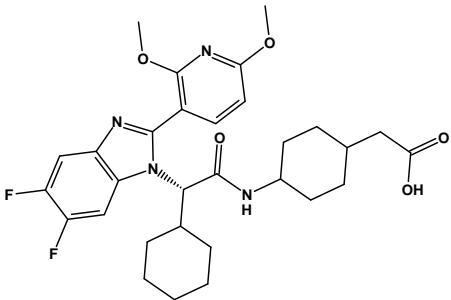
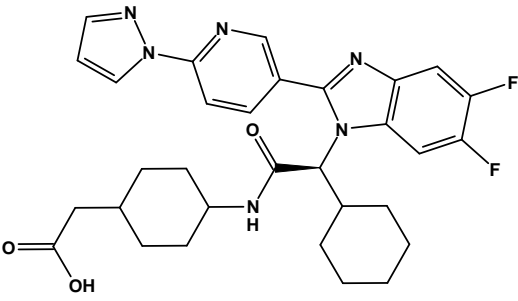
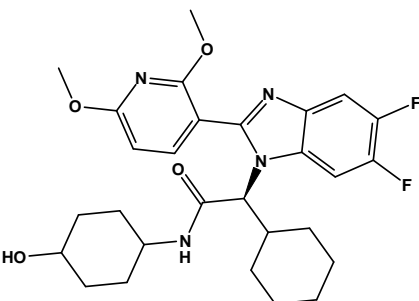
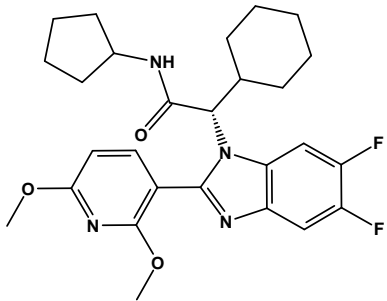
	Compound class	ID	FXR ID	Structure
1	Benzimidazole	1	FXR_19	
2	Benzimidazole	2	FXR_27	
3	Benzimidazole	3	FXR_62	
4	Benzimidazole	4	FXR_60	
5	Benzimidazole	5	FXR_52	

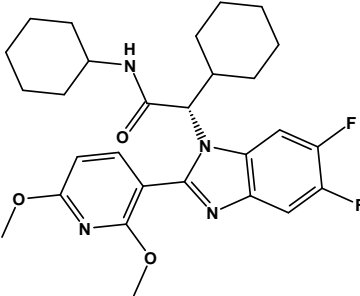
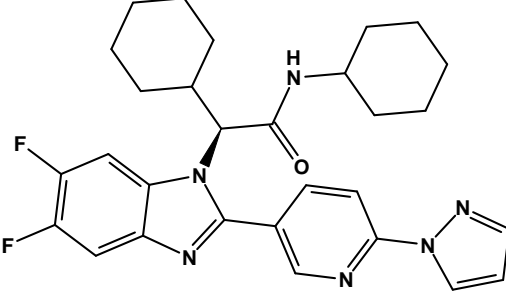
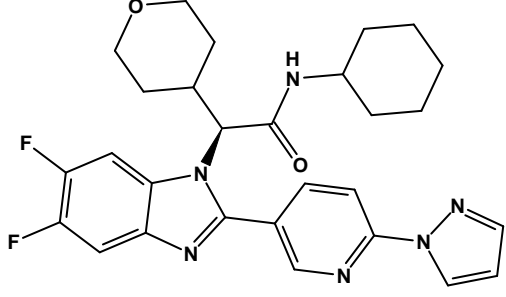
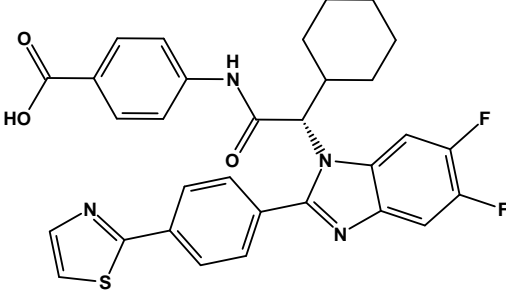
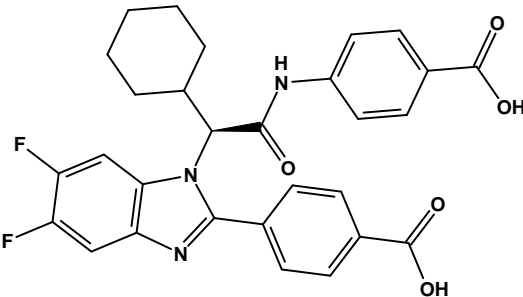
	Compound class	ID	FXR ID	Structure
6	Benzimidazole	6	FXR_20	
7	Benzimidazole	7	FXR_50	
8	Benzimidazole	8	FXR_25	
9	Benzimidazole	9	FXR_58	
10	Benzimidazole	10	FXR_72	

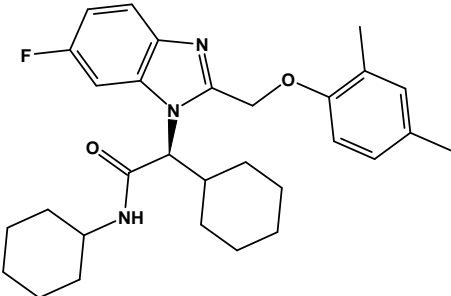
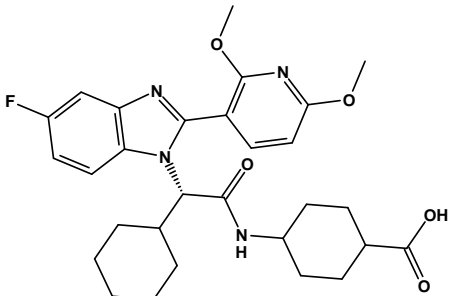
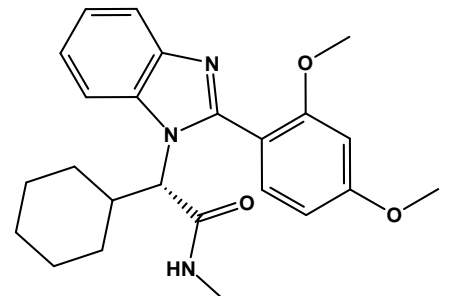
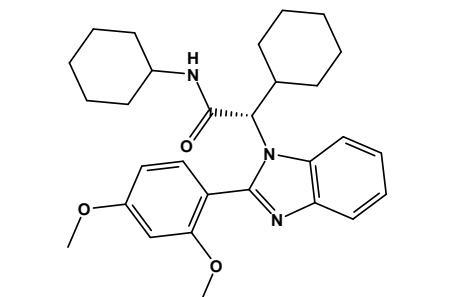
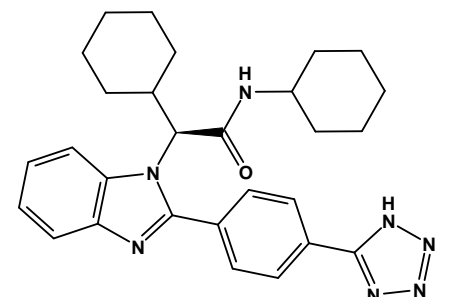
	Compound class	ID	FXR ID	Structure
11	Benzimidazole	11	FXR_24	
12	Benzimidazole	12	FXR_56	
13	Benzimidazole	13	FXR_53	
14	Benzimidazole	14	FXR_59	
15	Benzimidazole	15	FXR_21	

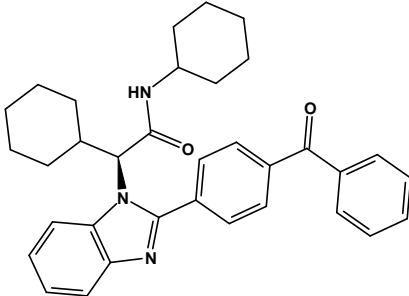
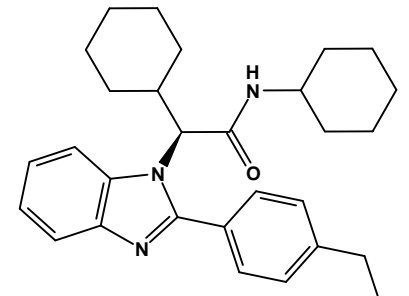
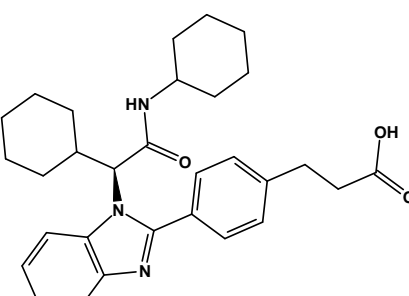
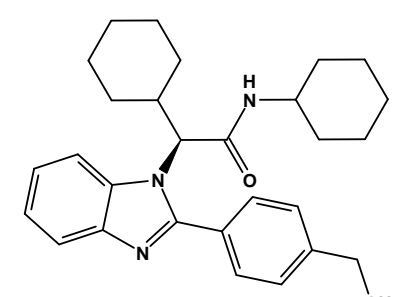
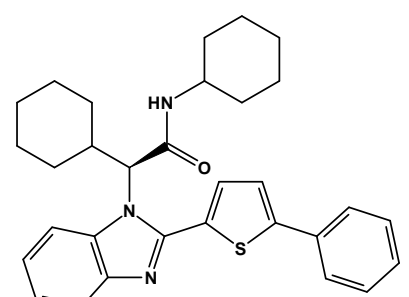
	Compound class	ID	FXR ID	Structure
16	Benzimidazole	16	FXR_54	
17	Benzimidazole	17	FXR_61	
18	Benzimidazole	18	FXR_28	
19	Benzimidazole	19	FXR_29	
20	Benzimidazole	20	FXR_71	

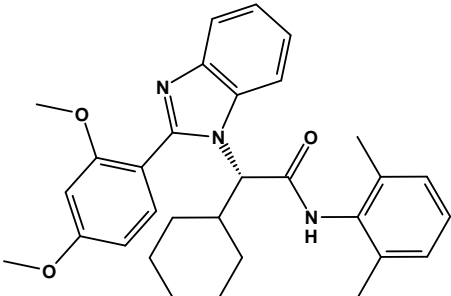
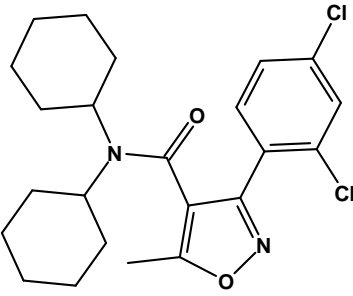
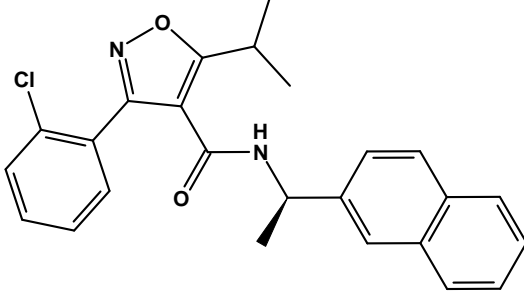
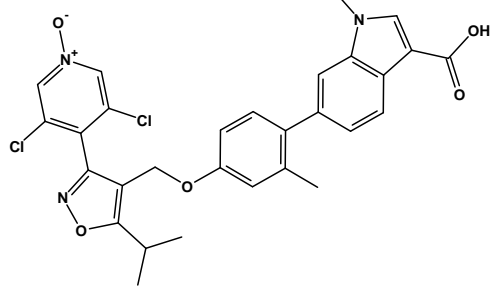
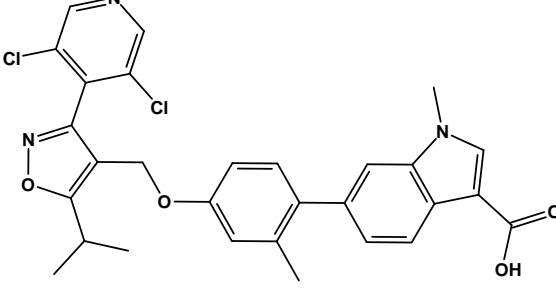
	Compound class	ID	FXR ID	Structure
21	Benzimidazole	21	FXR_42	
22	Benzimidazole	22	FXR_32	
23	Benzimidazole	23	FXR_22	
24	Benzimidazole	24	FXR_64	
25	Benzimidazole	25	FXR_68	

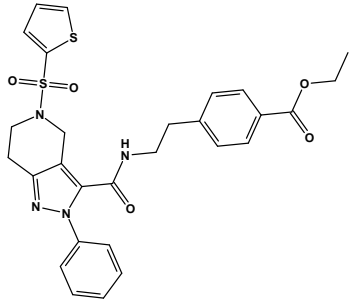
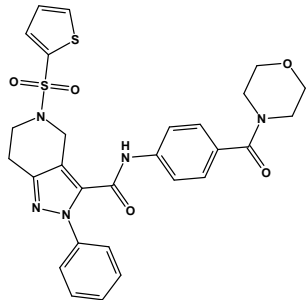
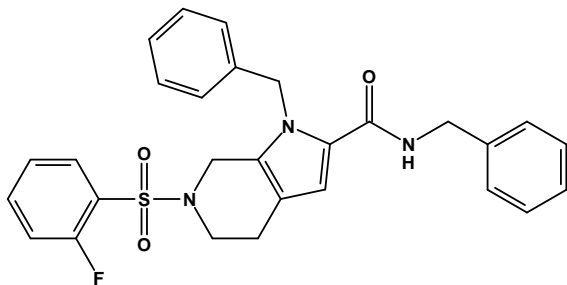
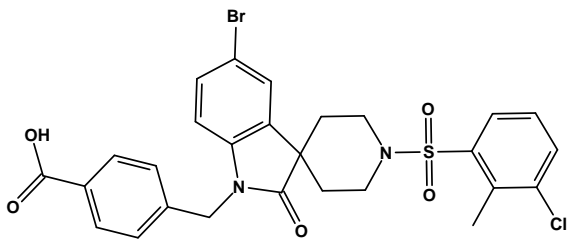
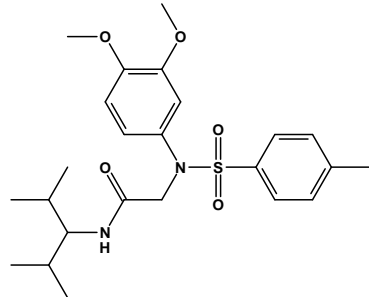
	Compound class	ID	FXR ID	Structure
26	Benzimidazole	26	FXR_69	
27	Benzimidazole	27	FXR_66	
28	Benzimidazole	28	FXR_67	
29	Benzimidazole	29	FXR_31	
30	Benzimidazole	30	FXR_57	

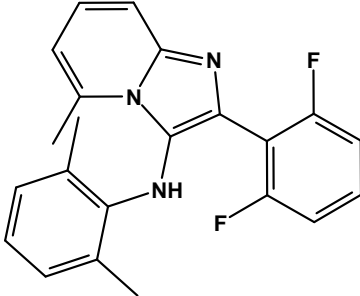
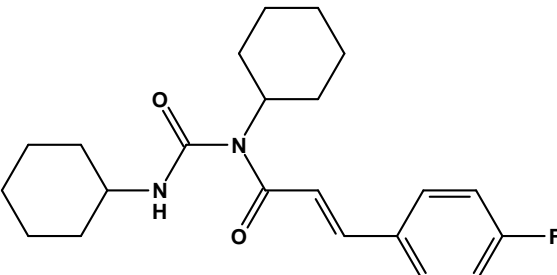
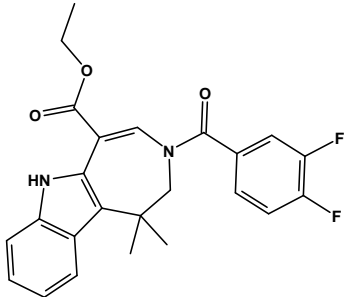
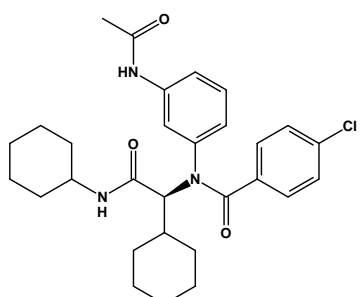
	Compound class	ID	FXR ID	Structure
31	Benzimidazole	31	FXR_55	
32	Benzimidazole	32	FXR_26	
33	Benzimidazole	33	FXR_70	
34	Benzimidazole	34	FXR_36	
35	Benzimidazole	35	FXR_63	

	Compound class	ID	FXR ID	Structure
36	Benzimidazole	36	FXR_51	
37	Benzimidazole	37	FXR_30	
38	Benzimidazole	38	FXR_37	
39	Benzimidazole	39	FXR_6	
40	Benzimidazole	40	FXR_9	

	Compound class	ID	FXR ID	Structure
41	Benzimidazole	41	FXR_13	 <chem>O=C(c1ccccc1)c2ccc(cc2)C3=C(N4CCCCC4)C5=CC=CC=C5N3C6CCCCC6</chem>
42	Benzimidazole	42	FXR_39	 <chem>CCc1ccc(cc1)C2=C(N3CCCCC3)C4=CC=CC=C4N2C5CCCCC5</chem>
43	Benzimidazole	43	FXR_40	 <chem>OC(=O)CCc1ccc(cc1)C2=C(N3CCCCC3)C4=CC=CC=C4N2C5CCCCC5</chem>
44	Benzimidazole	44	FXR_8	 <chem>OCc1ccc(cc1)C2=C(N3CCCCC3)C4=CC=CC=C4N2C5CCCCC5</chem>
45	Benzimidazole	45	FXR_7	 <chem>c1ccc(cc1)c2sc(C3=C(N4CCCCC4)C5=CC=CC=C5N3)cc2</chem>

	Compound class	ID	FXR ID	Structure
46	Benzimidazole	46	FXR_14	
47	Isoxazole	1	FXR_4	
48	Isoxazole	2	FXR_23	
49	Isoxazole	3	FXR_33	
50	Isoxazole	4	FXR_65	

	Compound class	ID	FXR ID	Structure
51	Sulfonamide	1	FXR_90	
52	Sulfonamide	2	FXR_102	
53	Sulfonamide	3	FXR_15	
54	Spiro	1	FXR_81	
55	Miscellaneous	1	FXR_1	

	Compound class	ID	FXR ID	Structure
56	Miscellaneous	2	FXR_2	
57	Miscellaneous	3	FXR_3	
58	Miscellaneous	4	FXR_5	
59	Miscellaneous	5	FXR_18	
60	Miscellaneous	6	FXR_34	