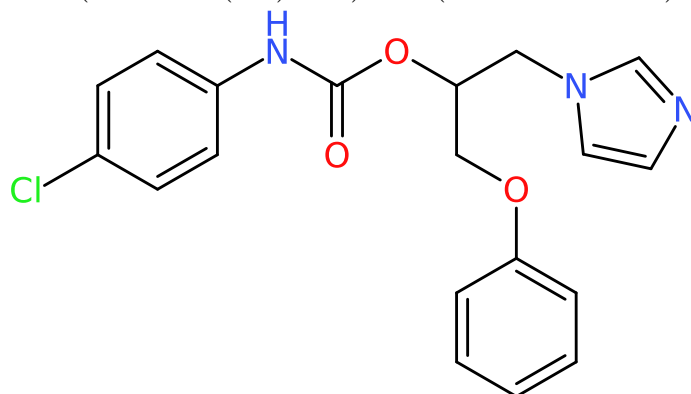


target fishing

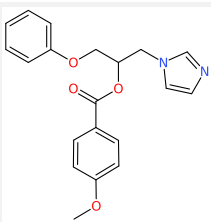
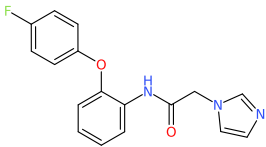
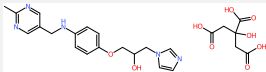
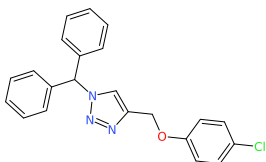
smiles: O=C(Nc1ccc(Cl)cc1)OC(COc2ccccc2)Cn3ccnc3



Target	score	reliable
Cytochrome P450 19A1:Homo sapiens	4.22	no
Mitochondrial complex V; ATP synthase:Bos taurus	3.19	no
Thromboxane-A synthase:Homo sapiens	2.96	no
Cytochrome P450 1A2:Homo sapiens	2.60	no
Cytochrome P450 2C19:Homo sapiens	2.60	no
Cytochrome P450 2C9:Homo sapiens	2.60	no
Beta-1 adrenergic receptor:Homo sapiens	2.30	no
Cytochrome P450 2D6:Homo sapiens	2.30	no
Heme oxygenase 1:Rattus norvegicus	2.26	no
Vascular endothelial growth factor receptor 2:Homo sapiens	1.83	no
Beta-2 adrenergic receptor:Canis lupus familiaris	1.75	no
15-cis-phytoene desaturase:Synechococcus elongatus (strain PCC 7942) (Anacystis nidulans R2)	1.70	no
Prostanoid EP1 receptor:Homo sapiens	1.47	no
Cytochrome P450 3A4:Homo sapiens	1.42	no
Beta-3 adrenergic receptor:Homo sapiens	1.38	no
Neuronal acetylcholine receptor protein alpha-7 sub-unit:Rattus norvegicus	1.21	no
Metabotropic glutamate receptor 5:Homo sapiens	1.20	no
Histamine H2 receptor:Cavia porcellus	1.10	no
Histamine H3 receptor:Rattus norvegicus	1.10	no
Histamine H1 receptor:Cavia porcellus	1.10	no
Sterol 14-alpha demethylase:Trypanosoma cruzi (strain CL Brener)	1.06	no
Vascular endothelial growth factor receptor 1:Homo sapiens	1.00	no
Anandamide amidohydrolase:Rattus norvegicus	0.93	no
1-acylglycerol-3-phosphate O-acyltransferase beta:Homo sapiens	0.87	no
M18 aspartyl aminopeptidase:Plasmodium falciparum 3D7	0.87	no
Galanin receptor 3:Homo sapiens	0.87	no
Lysophosphatidic acid receptor Edg-2:Homo sapiens	0.87	no
P2X purinoceptor 7:Homo sapiens	0.86	no
P2X purinoceptor 7:Rattus norvegicus	0.86	no
Lysine-specific histone demethylase 1:Homo sapiens	0.86	no

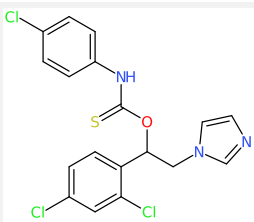
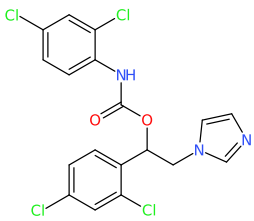
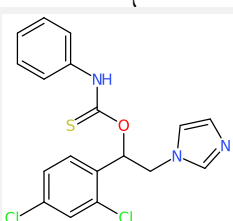
tid: 65
chembl id: [CHEMBL1978](#)
name: Cytochrome P450 19A1:Homo sapiens

similarity analysis

structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 CHEMBL1485809 IC50:16.5nM	0.66		0.55		0.53	0.61	0.54			0.64		0.62	0.52
 CHEMBL1784798 IC50:248nM	0.72							0.84	0.73				
 CHEMBL1784796 IC50:3.50μM				0.87									
 CHEMBL1824763 IC50:13.4μM											0.79		

tid: 100264
chembl id: [CHEMBL612444](#)
name: Mitochondrial complex V; ATP synthase:Bos taurus

similarity analysis

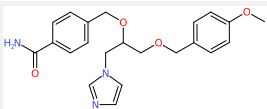
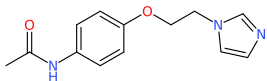
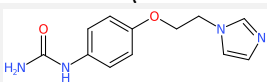
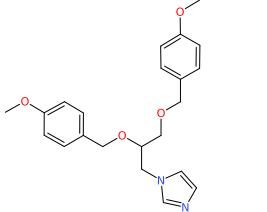
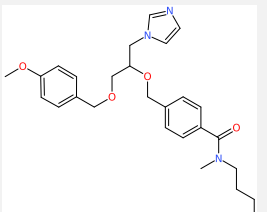
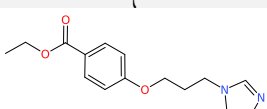
structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 CHEMBL8376 IC50:430nM					0.46								
 CHEMBL416142 IC50:6.77μM	0.69	0.76	0.43				0.57	0.82	0.82	0.60	0.93	0.56	0.51
 CHEMBL8244 IC50:3.60μM				0.80		0.45							

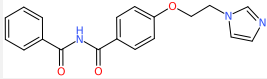
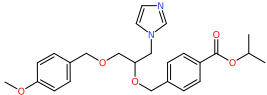
tid: 248

chembl id: [CHEMBL1835](#)

name: Thromboxane-A synthase:Homo sapiens

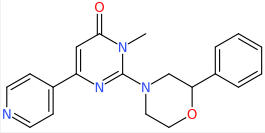
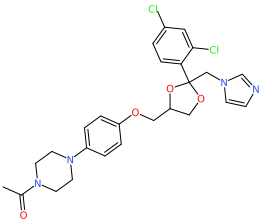
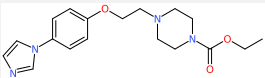
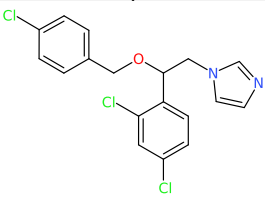
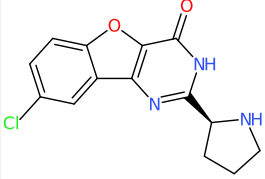
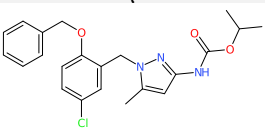
similarity analysis

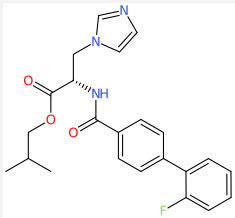
structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 CHEMBL290637 IC50:6.00μM					0.47								
 CHEMBL33690 IC50:4.00μM							0.54						
 CHEMBL33151 IC50:840nM	0.57	0.68					0.48		0.86		0.80		
 CHEMBL41441 IC50:9.90μM					0.46	0.85							
 CHEMBL40983 IC50:5.40μM										0.62			
 CHEMBL30604 IC50:3.00μM												0.50	

structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 <p>CHEMBL33874 IC50:180nM</p>									0.71				
 <p>CHEMBL38988 IC50:1.61μM</p>													0.42

tid: 12594
chembl id: [CHEMBL3356](#)
name: Cytochrome P450 1A2:Homo sapiens

similarity analysis

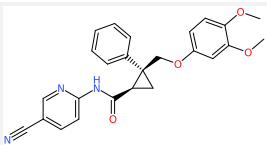
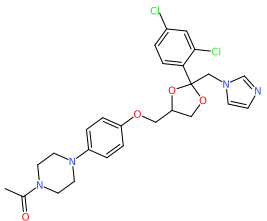
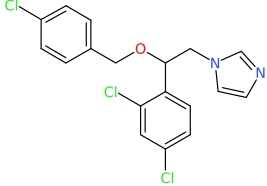
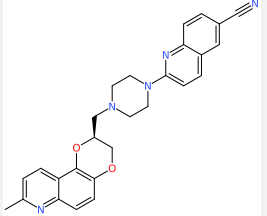
structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 CHEMBL3091546 IC50:23.1μM					0.41								
 CHEMBL157101 IC50:26.0μM	0.63	0.36					0.46					0.37	
 CHEMBL114555 IC50:2.24μM				0.89				0.84					
 CHEMBL808 IC50:300nM					0.32								
 CHEMBL2030402 IC50:6.90μM										0.58			
 CHEMBL256092 IC50:7.80μM									0.73		0.88		0.53

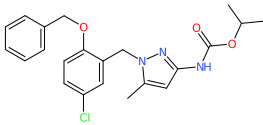
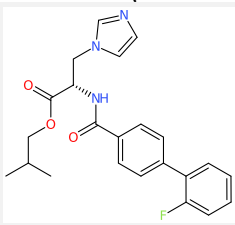
structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 <p>CHEMBL3984743 IC50:21.0μM</p>													

0.47

tid: 12912
chembl id: [CHEMBL3622](#)
name: Cytochrome P450 2C19:Homo sapiens

similarity analysis

structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 CHEMBL3343259 IC50:8.60μM					0.41								
 CHEMBL157101 IC50:15.4μM	0.63	0.36					0.46			0.54			
 CHEMBL114555 IC50:469nM				0.89				0.84					
 CHEMBL808 IC50:40.0nM					0.32								
 CHEMBL551964 IC50:98.0μM												0.38	

structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 <p>CHEMBL256092 IC50:69.0μM</p>									0.73		0.88		0.53
 <p>CHEMBL3984743 IC50:1.16μM</p>													0.47

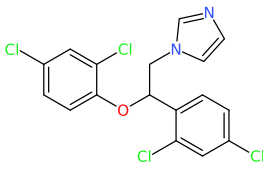
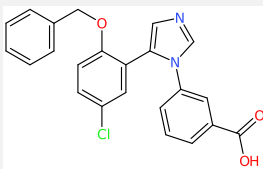
tid: 12911

chembl id: [CHEMBL3397](#)

name: Cytochrome P450 2C9:Homo sapiens

similarity analysis

structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 CHEMBL256092 IC50:17.0μM					0.41						0.88		0.53
 CHEMBL157101 IC50:24.3μM			0.63	0.36			0.46					0.37	
 CHEMBL114555 IC50:1.44μM					0.89			0.84					
 CHEMBL808 IC50:200nM						0.32							
 CHEMBL1090211 IC50:3.40μM											0.55		

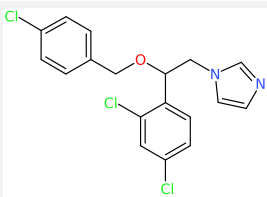
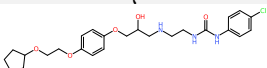
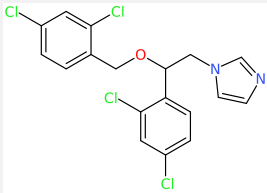
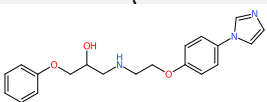
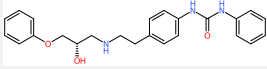
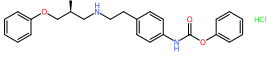
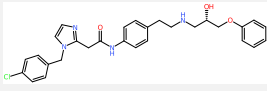
structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 CHEMBL270902 IC50:10.00μM	0.47												
 CHEMBL207293 IC50:1.90μM	0.74												

tid: 50

chembl id: [CHEMBL213](#)

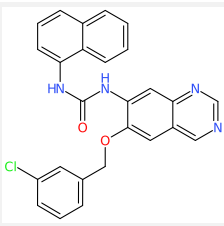
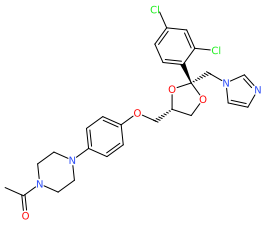
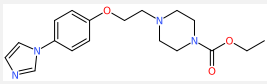
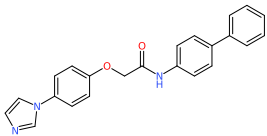
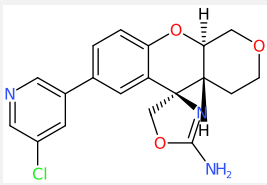
name: Beta-1 adrenergic receptor:Homo sapiens

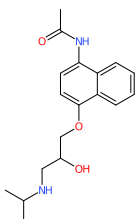
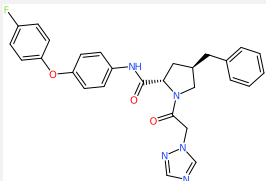
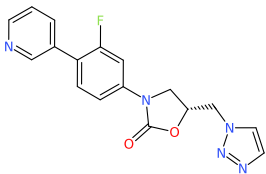
similarity analysis

structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 CHEMBL808 IC50:12.8µM					0.39								
 CHEMBL2348202 Kd:11.2nM			0.38				0.44			0.61			
 CHEMBL91 IC50:12.6µM				0.54							0.67		
 CHEMBL98975 IC50:40.0nM				0.89				0.86					
 CHEMBL434524 EC50:3.60nM					0.38								
 CHEMBL1203992 EC50:40.0nM											0.47	0.39	
 CHEMBL467502 EC50:270nM		0.55							0.72				

tid: 11365
chembl id: [CHEMBL289](#)
name: Cytochrome P450 2D6:Homo sapiens

similarity analysis

structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 CHEMBL3634101 IC50:5.10μM					0.41						0.75		
 CHEMBL75 IC50:10.0nM			0.63	0.36			0.46						
 CHEMBL114555 IC50:3.20μM					0.89			0.84					
 CHEMBL4097104 IC50:100.0nM			0.57				0.40						
 CHEMBL3265335 IC50:1.10μM											0.54		

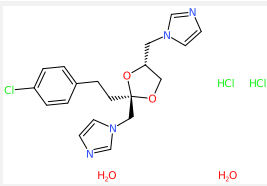
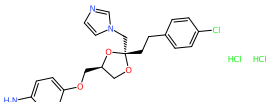
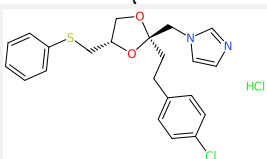
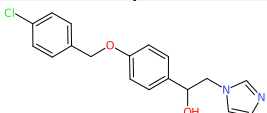
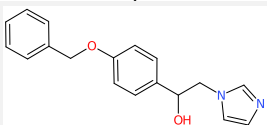
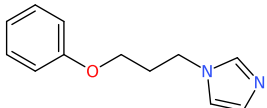
structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 <p>CHEMBL359496 IC50:100.0μM</p>												0.42	
 <p>CHEMBL2018484 IC50:392nM</p>												0.72	
 <p>CHEMBL394864 IC50:6.60μM</p>												0.40	

tid: 20059

chembl id: [CHEMBL5035](#)

name: Heme oxygenase 1:Rattus norvegicus

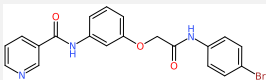
similarity analysis

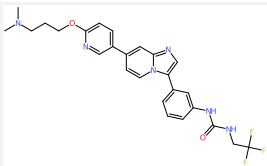
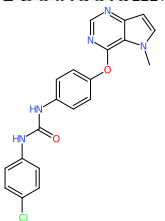
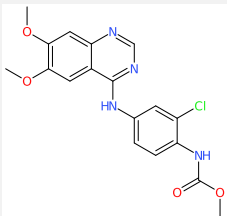
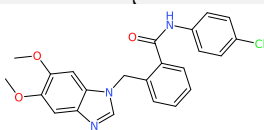
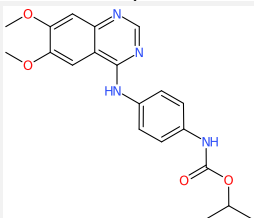
structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 CHEMBL459907 IC50:10.00μM					0.46					0.64			
 CHEMBL473177 IC50:1.40μM			0.45				0.47	0.84	0.77				
 CHEMBL475163 IC50:1.03μM			0.67										
 CHEMBL4176027 IC50:13.1μM			0.57		0.85								
 CHEMBL4161217 IC50:500nM						0.42							
 CHEMBL1363752 IC50:31.0μM												0.52	

structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 <p>CHEMBL284827 IC50:28.0μM</p>											0.71		
 <p>CHEMBL472792 IC50:590nM</p>													0.42

tid: 10980
chembl id: [CHEMBL279](#)
name: Vascular endothelial growth factor receptor 2:Homo sapiens

similarity analysis

structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 CHEMBL203003 IC50:92.0nM					0.48								
 CHEMBL3221547 IC50:500nM			0.34				0.46						
 CHEMBL1290247 IC50:5.00nM		0.65											
 CHEMBL234202 IC50:708nM	0.53			0.78									
 CHEMBL2206661 IC50:5.20μM					0.33								
 CHEMBL1162958 IC50:766nM									0.65				

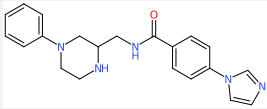
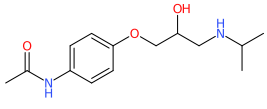
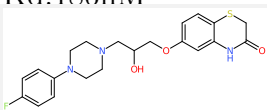
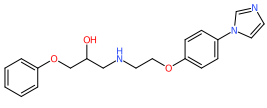
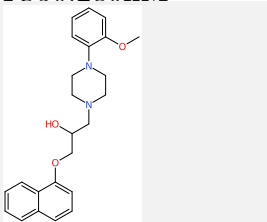
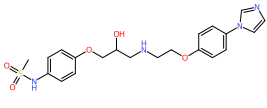
structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 <p>CHEMBL3690500 IC50:35.3nM</p>													0.42
 <p>CHEMBL1254752 IC50:32.0nM</p>							0.83						
 <p>CHEMBL2018751 IC50:5.05μM</p>													0.81
 <p>CHEMBL206567 IC50:3.55μM</p>								0.77					
 <p>CHEMBL2018750 IC50:5.05μM</p>													0.49

tid: 12887

chembl id: [CHEMBL2289](#)

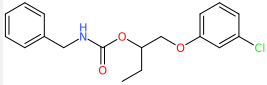
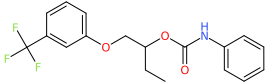
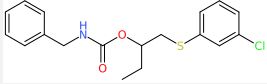
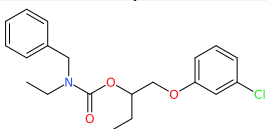
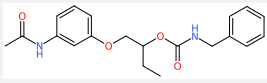
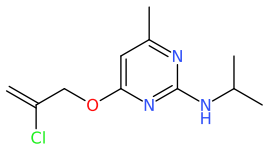
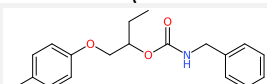
name: Beta-2 adrenergic receptor:Canis lupus familiaris

similarity analysis

structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 CHEMBL350847 IC50:4.30μM					0.37								
 CHEMBL6995 Kd:186nM			0.33				0.41					0.43	
 CHEMBL143608 Ki:5.30μM			0.47										
 CHEMBL98975 IC50:280nM	0.47			0.89		0.36		0.86	0.66				0.29
 CHEMBL142635 Ki:1.00μM										0.51			
 CHEMBL99585 IC50:46.5μM											0.48		

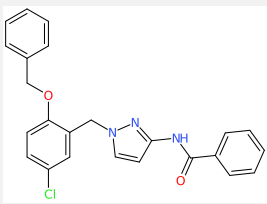
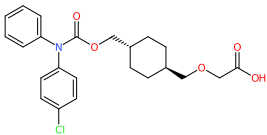
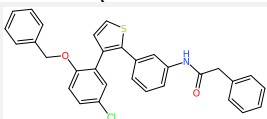
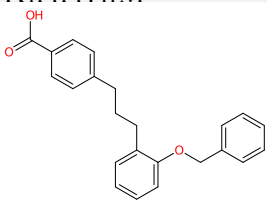
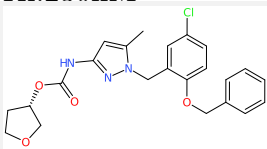
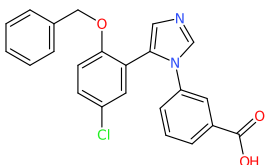
tid: 106616
chembl id: [CHEMBL2366472](#)
name: 15-cis-phytoene desaturase:Synechococcus elongatus
(strain PCC 7942) (Anacystis nidulans R2)

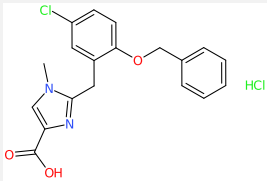
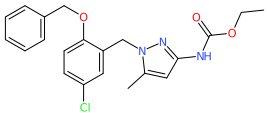
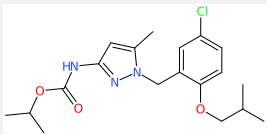
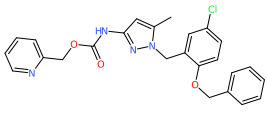
similarity analysis

structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 CHEMBL2272986 IC50:50.1nM					0.49								
 CHEMBL2272975 IC50:50.1nM			0.47			0.46	0.51					0.50	
 CHEMBL2272700 IC50:5.20μM			0.54										
 CHEMBL2272703 IC50:63.1nM				0.81					0.64				
 CHEMBL2272713 IC50:3.98μM								0.62		0.58			
 CHEMBL2272974 IC50:7.94μM												0.59	
 CHEMBL2272987 IC50:3.16μM	0.56												0.65

tid: 261
 · chembl id: [CHEMBL1811](#)
 name: Prostanoid EP1 receptor:Homo sapiens

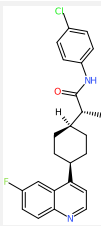
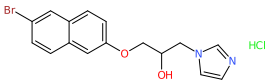
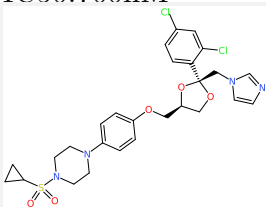
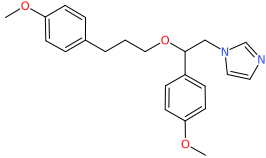
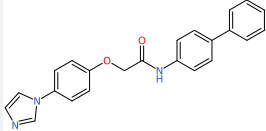
similarity analysis

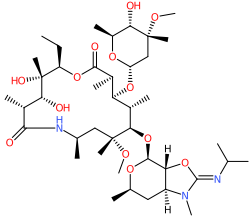
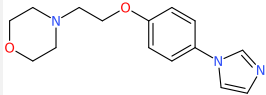
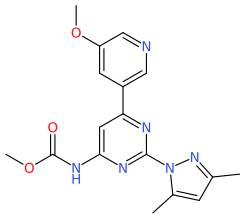
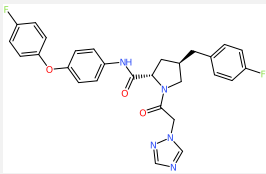
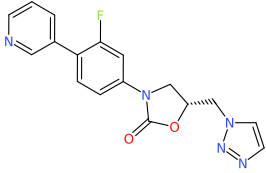
structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 CHEMBL255485 IC50:251nM					0.46								
 CHEMBL3301604 Ki:9.60μM			0.36				0.46					0.36	
 CHEMBL180046 Ki:4.47nM		0.55											
 CHEMBL124199 Ki:230nM					0.71								
 CHEMBL429321 IC50:79.4nM						0.27							0.60
 CHEMBL207293 IC50:126nM											0.53		

structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 <p>CHEMBL535640 IC50:316nM</p>								0.73					
 <p>CHEMBL258226 IC50:79.4nM</p>											0.88		
 <p>CHEMBL258183 IC50:50.1nM</p>								0.47					
 <p>CHEMBL253538 IC50:79.4nM</p>								0.76					

tid: 17045
chembl id: [CHEMBL340](#)
name: Cytochrome P450 3A4:Homo sapiens

similarity analysis

structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 CHEMBL4161733 IC50:5.10μM							0.41						
 CHEMBL2448692 IC50:700nM					0.50		0.53					0.56	
 CHEMBL3922888 IC50:185nM											0.66		
 CHEMBL258502 IC50:45.0nM						0.85							
 CHEMBL4097104 IC50:20.0nM					0.57		0.40						

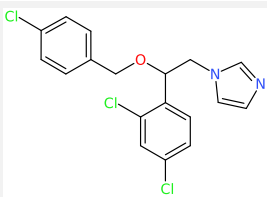
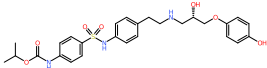
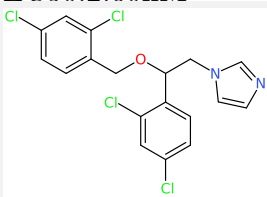
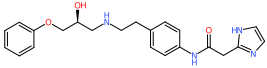
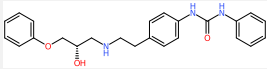
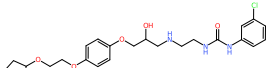
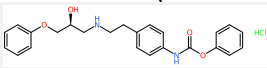
structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 <p>CHEMBL2159133 IC50:1.00μM</p>										0.58			
 <p>CHEMBL113018 IC50:5.67μM</p>								0.82					
 <p>CHEMBL519549 IC50:16.0μM</p>											0.81		
 <p>CHEMBL2018485 IC50:12.6μM</p>								0.72					
 <p>CHEMBL394864 IC50:6.80μM</p>												0.40	

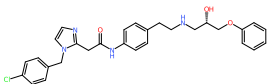
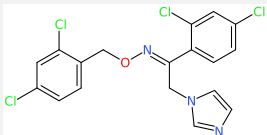
tid: 226

chembl id: [CHEMBL246](#)

name: Beta-3 adrenergic receptor:Homo sapiens

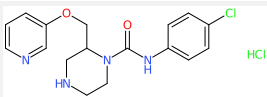
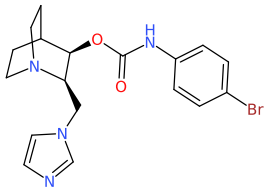
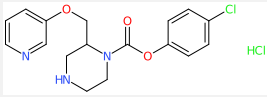
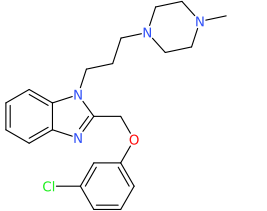
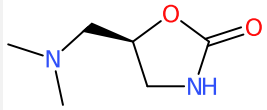
similarity analysis

structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 <p>CHEMBL808 IC50:6.15μM</p>					0.39								
 <p>CHEMBL13106 EC50:2.60nM</p>			0.37				0.44						
 <p>CHEMBL91 IC50:5.48μM</p>			0.54										
 <p>CHEMBL466879 EC50:510nM</p>				0.82									
 <p>CHEMBL434524 EC50:1.60nM</p>					0.38								
 <p>CHEMBL2348201 EC50:10.00μM</p>										0.57			
 <p>CHEMBL1203992 EC50:2.30μM</p>												0.47	0.39

structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 CHEMBL467502 EC50:74.0nM	0.55							0.83	0.72				
 CHEMBL1262 IC50:4.74μM											0.69		

tid: 12167
chembl id: [CHEMBL4980](#)
name: Neuronal acetylcholine receptor protein alpha-7 sub-unit:Rattus norvegicus

similarity analysis

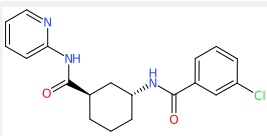
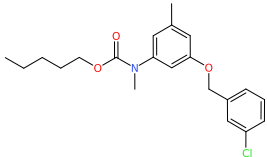
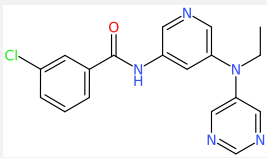
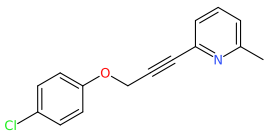
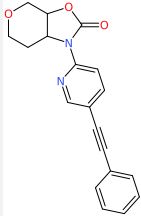
structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 CHEMBL3262153 IC50:70.0nM	0.50				0.52					0.56			
 CHEMBL193743 Ki:10.0nM		0.69	0.38			0.34	0.47					0.48	
 CHEMBL3262155 IC50:9.50nM				0.77					0.73		0.69		
 CHEMBL403376 EC50:10.00μM								0.78					
 CHEMBL2441754 Ki:94.0μM													0.40

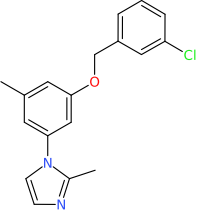
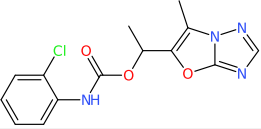
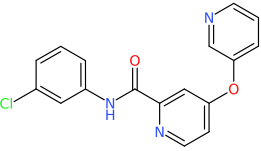
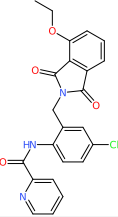
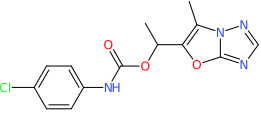
tid: 11280

chembl id: [CHEMBL3227](#)

name: Metabotropic glutamate receptor 5:Homo sapiens

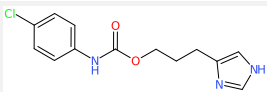
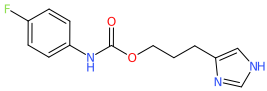
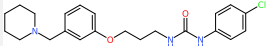
similarity analysis

structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 CHEMBL2338561 IC50:5.00µM					0.43								
 CHEMBL206998 Ki:33.0nM			0.37	0.79			0.43					0.35	
 CHEMBL3655656 IC50:260nM				0.63									
 CHEMBL212129 IC50:102nM							0.25						
 CHEMBL3983913 EC50:60.0nM										0.58			

structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 <p>CHEMBL207733 Ki:27.0nM</p>								0.78					
 <p>CHEMBL1630060 IC50:501nM</p>											0.76		
 <p>CHEMBL3660209 IC50:390nM</p>							0.54						
 <p>CHEMBL395644 EC50:280nM</p>										0.71			
 <p>CHEMBL1630062 IC50:2.51μM</p>												0.66	

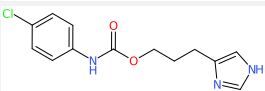
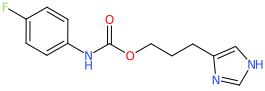
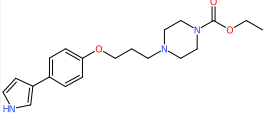
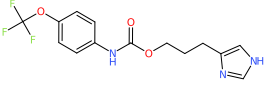
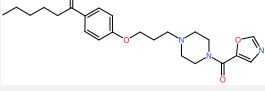
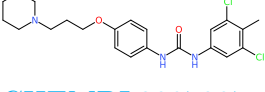
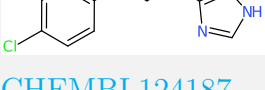
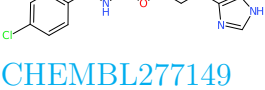
tid: 10116
chembl id: [CHEMBL2882](#)
name: Histamine H2 receptor:Cavia porcellus

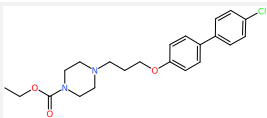
similarity analysis

structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 CHEMBL16231 Ki:79.4μM	0.44		0.39		0.49		0.44	0.74				0.39	0.60
 CHEMBL274989 Ki:63.1μM		0.53											
 CHEMBL81520 Kd:631nM				0.76		0.30				0.51			
 CHEMBL277149 Ki:79.4μM											0.69		
 CHEMBL309659 Kd:316nM									0.65				

tid: 11300
chembl id: [CHEMBL4124](#)
name: Histamine H3 receptor:Rattus norvegicus

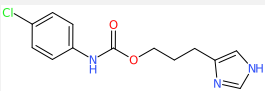
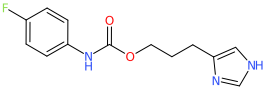
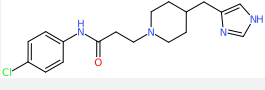
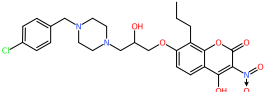
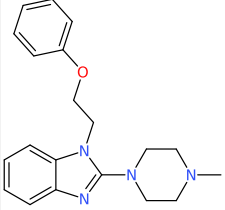
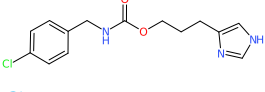
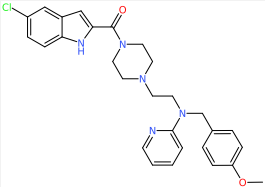
similarity analysis

structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 CHEMBL16231 Ki:4.09nM	0.44				0.49	0.27	0.44						0.60
 CHEMBL274989 Ki:24.6nM	0.53												
 CHEMBL101692 Ki:56.2nM				0.83									
 CHEMBL16640 Ki:26.0nM	0.39												
 CHEMBL60509 Ki:44.7nM									0.52				
 CHEMBL2387307 Ki:135nM												0.42	
 CHEMBL124187 Ki:21.0nM							0.78						
 CHEMBL277149 Ki:13.3nM												0.69	

structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 <p>CHEMBL105385 Ki:191nM</p>									0.68				

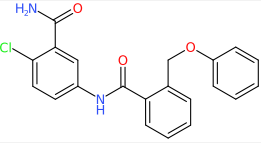
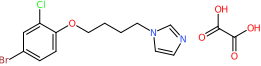
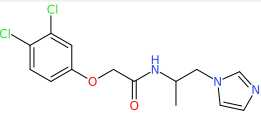
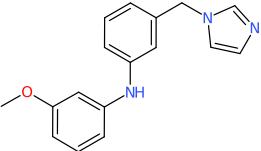
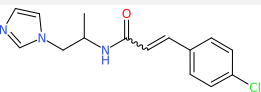
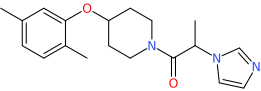
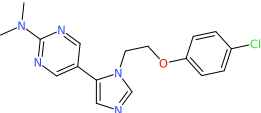
tid: 17074
chembl id: [CHEMBL3943](#)
name: Histamine H1 receptor:Cavia porcellus

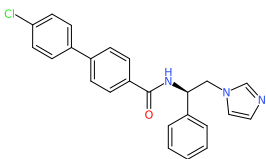
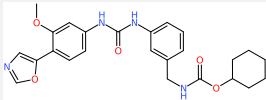
similarity analysis

structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 CHEMBL16231 Ki:63.1μM	0.44		0.39		0.49	0.27	0.44					0.39	0.60
 CHEMBL274989 Ki:79.4μM	0.53												
 CHEMBL371730 Ki:290nM				0.78									
 CHEMBL286017 Kd:3.98nM									0.47				
 CHEMBL276735 IC50:6.90nM								0.76					
 CHEMBL277149 Ki:15.8μM											0.69		
 CHEMBL1910379 Kd:20.4nM									0.69				

tid: 103036
chembl id: [CHEMBL1075110](#)
name: Sterol 14-alpha demethylase:Trypanosoma cruzi (strain CL Brener)

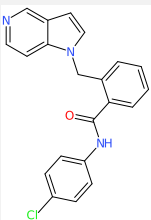
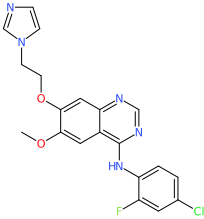
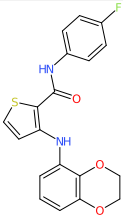
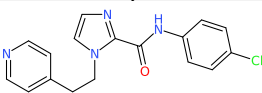
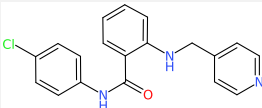
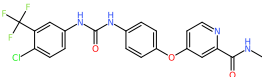
similarity analysis

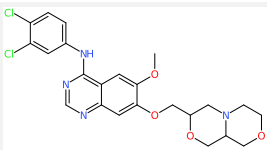
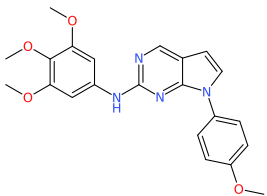
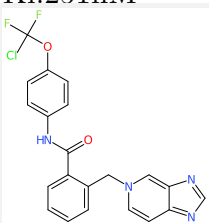
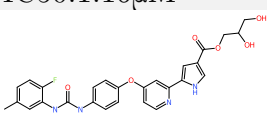
structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 CHEMBL3431227 IC50:79.4µM					0.48								
 CHEMBL3431397 IC50:63.1nM			0.38				0.45					0.40	
 CHEMBL3431305 IC50:63.1nM			0.67						0.69				
 CHEMBL2326052 Kd:210nM				0.78									
 CHEMBL3431250 IC50:158nM					0.36								
 CHEMBL3431307 IC50:100.0nM										0.49			
 CHEMBL3431242 IC50:50.1nM								0.79			0.79		

structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 <p>CHEMBL1236676 Kd:70.0nM</p>	0.58												
 <p>CHEMBL3431205 IC50:25.1μM</p>													0.40

tid: 10979
chembl id: [CHEMBL1868](#)
name: Vascular endothelial growth factor receptor 1:Homo sapiens

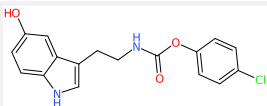
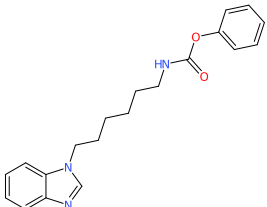
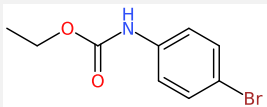
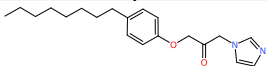
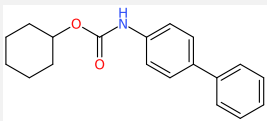
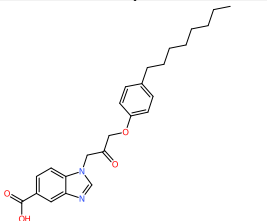
similarity analysis

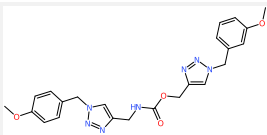
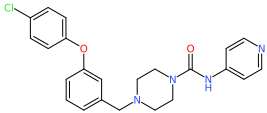
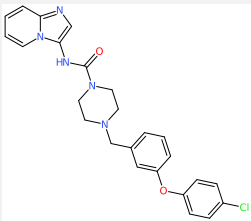
structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 CHEMBL203003 IC50:220nM					0.48								
 CHEMBL147192 IC50:100.0nM			0.32				0.44	0.75					
 CHEMBL4286029 IC50:1.90μM			0.61										
 CHEMBL234202 IC50:940nM	0.53			0.78									
 CHEMBL101683 IC50:180nM						0.27							
 CHEMBL1336 IC50:45.2nM										0.53			

structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 <p>CHEMBL3943570 IC50:50.0nM</p>												0.36	
 <p>CHEMBL1975927 Ki:251nM</p>												0.73	
 <p>CHEMBL205413 IC50:1.16μM</p>											0.70		
 <p>CHEMBL3660290 IC50:16.0nM</p>												0.41	

tid: 11289
chembl id: [CHEMBL3229](#)
name: Anandamide amidohydrolase:Rattus norvegicus

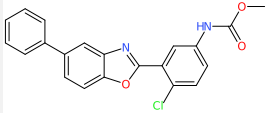
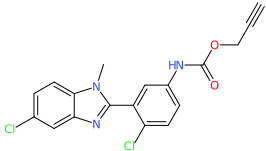
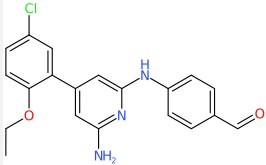
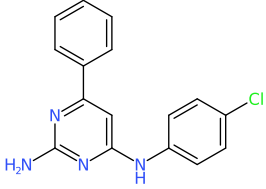
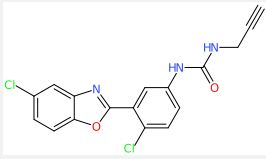
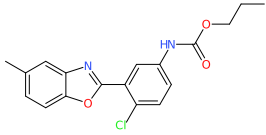
similarity analysis

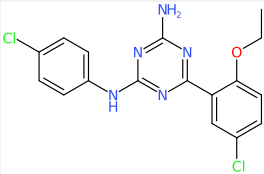
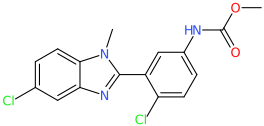
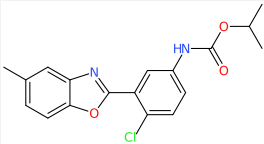
structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 CHEMBL241137 IC50:6.80μM					0.45								
 CHEMBL3585522 IC50:290nM				0.80			0.38	0.80					
 CHEMBL3683934 IC50:4.00μM			0.58										
 CHEMBL598974 IC50:558nM			0.36									0.42	
 CHEMBL541244 IC50:17.0μM					0.37								0.53
 CHEMBL482959 IC50:610nM										0.56			

structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 CHEMBL4218592 IC50:5.80nM											0.93		
 CHEMBL2164601 IC50:520nM	0.51												
 CHEMBL2207351 IC50:119nM									0.72				

tid:	12608	
chembl id:	CHEMBL4772	
name:	1-acylglycerol-3-phosphate	O-acyltransferase
	beta:Homo sapiens	

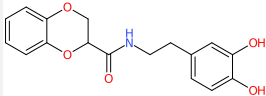
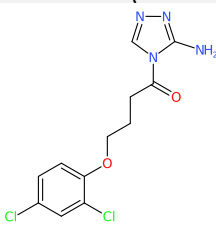
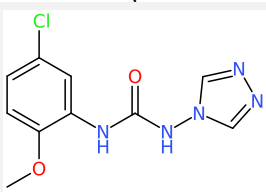
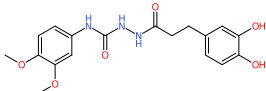
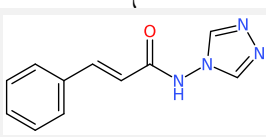
similarity analysis

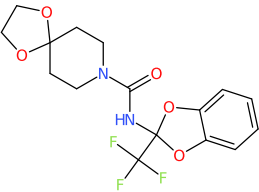
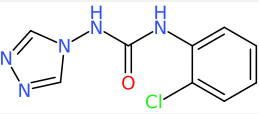
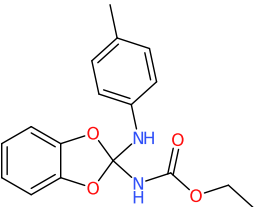
structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 <p>CHEMBL36197 IC50:64.0μM</p>							0.34						
 <p>CHEMBL418604 IC50:60.0nM</p>			0.59	0.35			0.41		0.66				
 <p>CHEMBL193911 IC50:50.0nM</p>							0.67						
 <p>CHEMBL75791 IC50:1.10μM</p>							0.28						
 <p>CHEMBL35967 IC50:100.0nM</p>										0.46			
 <p>CHEMBL35615 IC50:12.0μM</p>												0.38	

structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 <p>CHEMBL193589 IC50:191nM</p>							0.70						
 <p>CHEMBL290583 IC50:650nM</p>	0.39										0.87		
 <p>CHEMBL34893 IC50:16.0μM</p>													0.55

tid: 103696
chembl id: [CHEMBL1293263](#)
name: M18 aspartyl aminopeptidase:Plasmodium falciparum 3D7

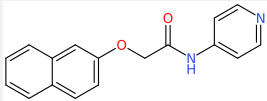
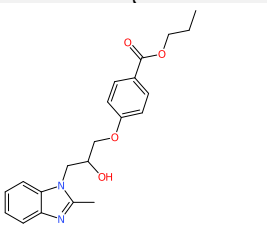
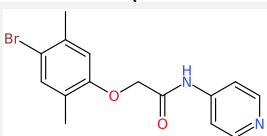
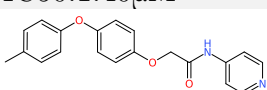
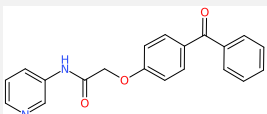
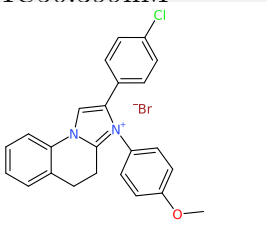
similarity analysis

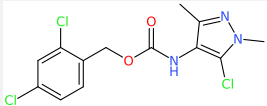
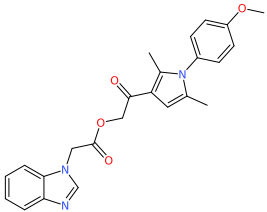
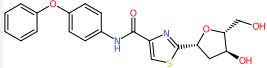
structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 CHEMBL1417867 IC50:2.11μM					0.35								
 CHEMBL1503953 IC50:2.60μM							0.36		0.68				
 CHEMBL1491018 IC50:832nM			0.54	0.30				0.71			0.87	0.29	
 CHEMBL1413985 IC50:2.51μM					0.68								
 CHEMBL1378749 IC50:1.76μM						0.22							

structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 <p>CHEMBL1462474 IC50:2.78μM</p>										0.44			
 <p>CHEMBL1488151 IC50:1.47μM</p>										0.39			
 <p>CHEMBL1612425 IC50:5.07μM</p>													0.40

tid: 12886
chembl id: [CHEMBL2731](#)
name: Galanin receptor 3:Homo sapiens

similarity analysis

structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 CHEMBL1603921 IC50:1.77μM	0.50				0.44								
 CHEMBL1510261 IC50:1.57μM			0.40				0.48			0.56		0.50	
 CHEMBL1417355 IC50:1.40μM	0.65												
 CHEMBL1705098 IC50:158nM				0.77									
 CHEMBL1424583 IC50:399nM					0.32								
 CHEMBL1457690 IC50:5.02μM							0.74						

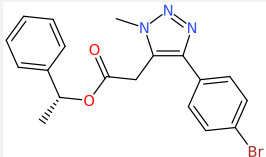
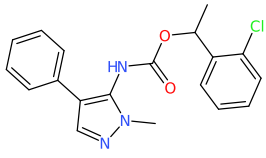
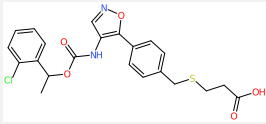
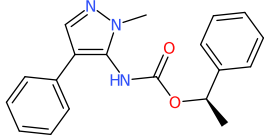
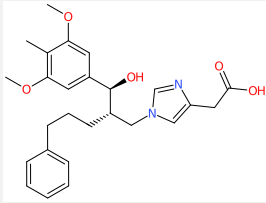
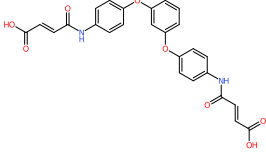
structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 <p>CHEMBL1478769 IC50:2.13μM</p>											0.87		
 <p>CHEMBL1376266 IC50:762nM</p>									0.66				
 <p>CHEMBL2355112 IC50:400nM</p>													0.40

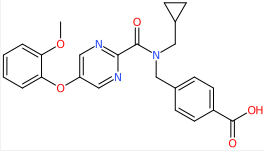
tid: 10808

chembl id: [CHEMBL3819](#)

name: Lysophosphatidic acid receptor Edg-2:Homo sapiens

similarity analysis

structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 <p>CHEMBL4111515 IC50:21.9µM</p>					0.39								
 <p>CHEMBL2182056 IC50:3.59µM</p>	0.44						0.30		0.61		0.87	0.29	0.46
 <p>CHEMBL246928 IC50:260nM</p>			0.52										
 <p>CHEMBL2182053 IC50:17.5µM</p>					0.69								
 <p>CHEMBL4176330 IC50:180nM</p>				0.32				0.65					
 <p>CHEMBL482498 IC50:27.4µM</p>						0.26							

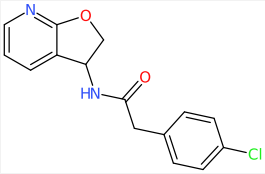
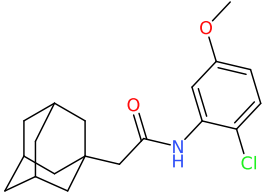
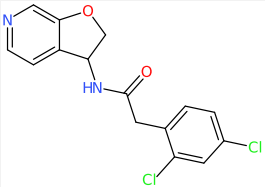
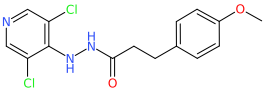
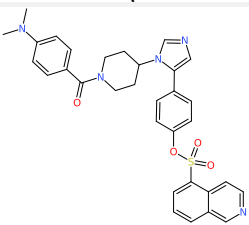
structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 <p>CHEMBL3897650 IC50:170nM</p>										0.47			

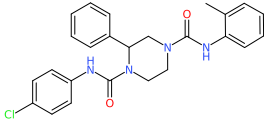
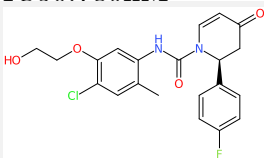
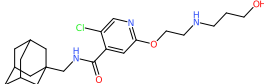
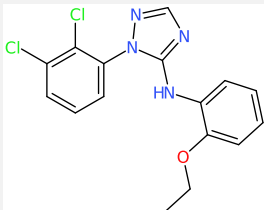
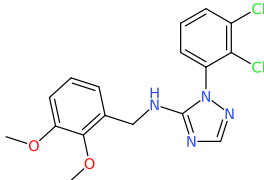
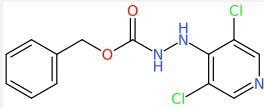
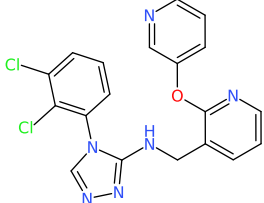
tid: 10417

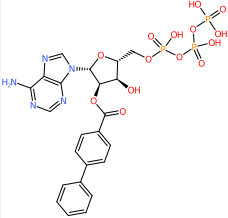
chembl id: [CHEMBL4805](#)

name: P2X purinoceptor 7:Homo sapiens

similarity analysis

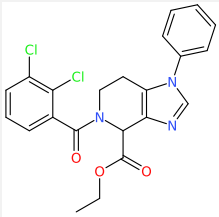
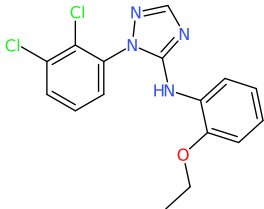
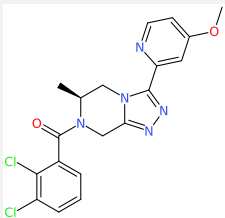
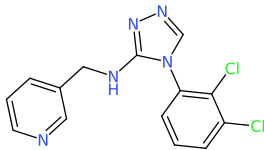
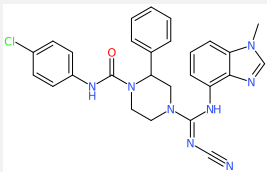
structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 <p>CHEMBL3946649 IC50:1.41μM</p>							0.44						
 <p>CHEMBL131241 IC50:63.1nM</p>							0.33						
 <p>CHEMBL3969023 IC50:15.0nM</p>							0.54						
 <p>CHEMBL2048264 IC50:1.50μM</p>							0.71						
 <p>CHEMBL4165149 IC50:0.30nM</p>							0.31						

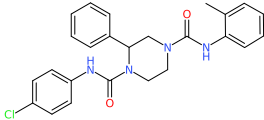
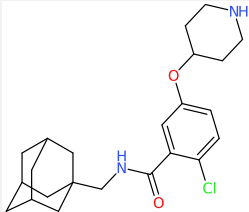
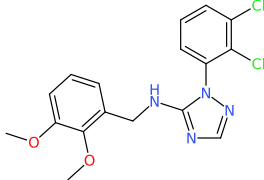
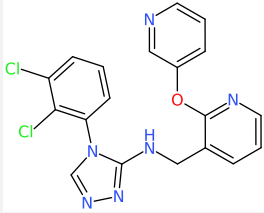
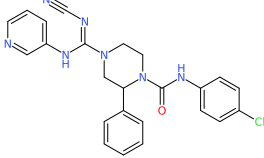
structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 CHEMBL21149 IC50:780nM							0.23						
 CHEMBL3741412 IC50:9.00nM											0.51		
 CHEMBL560167 IC50:79.4nM												0.33	
 CHEMBL403105 IC50:1.86μM								0.73					
 CHEMBL271030 IC50:30.9nM											0.86		
 CHEMBL2048274 IC50:370nM							0.41						
 CHEMBL255614 IC50:30.9nM								0.67					

structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 <p>CHEMBL339386 EC50:52.0μM</p>													0.37

tid: 10540
 · chembl id: [CHEMBL2496](#)
 name: P2X purinoceptor 7:Rattus norvegicus

similarity analysis

structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 CHEMBL3950348 IC50:1.89µM					0.43					0.47			
 CHEMBL403105 IC50:11.0µM							0.30	0.73					
 CHEMBL3604426 IC50:10.0nM					0.45								
 CHEMBL404091 IC50:1.12µM					0.68								
 CHEMBL479578 IC50:5.19µM					0.29								

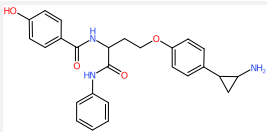
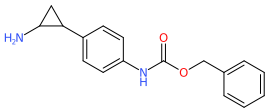
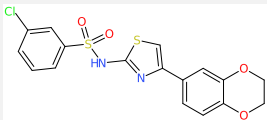
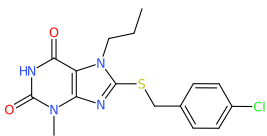
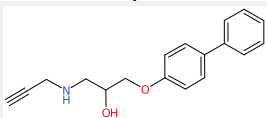
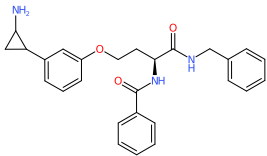
structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 CHEMBL21149 IC50:620nM							0.23						
 CHEMBL393384 IC50:631nM												0.32	
 CHEMBL271030 IC50:135nM											0.86		
 CHEMBL255614 IC50:35.5nM							0.37		0.67				
 CHEMBL481481 IC50:2.04μM													0.28

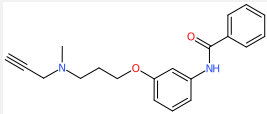
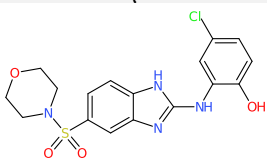
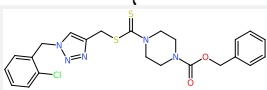
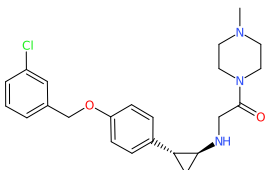
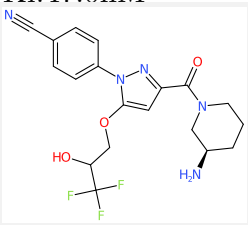
tid: 102439

chembl id: [CHEMBL6136](#)

name: Lysine-specific histone demethylase 1:Homo sapiens

similarity analysis

structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 CHEMBL3104339 IC50:1.90μM							0.43						
 CHEMBL1795981 Ki:1.56μM					0.74		0.34						0.38
 CHEMBL3134368 IC50:29.5μM									0.54				
 CHEMBL1581095 IC50:25.7μM					0.28								
 CHEMBL2426048 IC50:38.7μM							0.32						
 CHEMBL1797639 IC50:2.42μM										0.43			

structure	mfp1	featmfp1	rdkit7	pattern	ap_bits	tt_bits	fp2	pubchem	cdk_maccs	graph	substructure	hybridization	klekota_roth
 CHEMBL2426047 IC50:93.1µM													0.36
 CHEMBL3786908 IC50:90.0µM								0.66					
 CHEMBL2334486 IC50:53.2µM												0.86	
 CHEMBL3651589 Ki:47.0nM												0.34	
 CHEMBL4066743 IC50:155nM													0.63