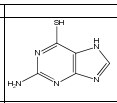
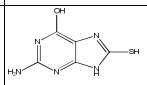
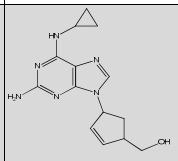
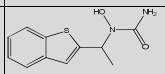
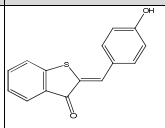
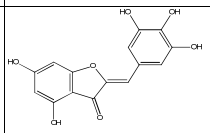
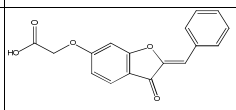
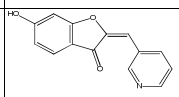
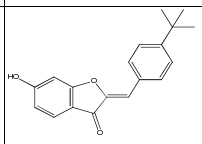
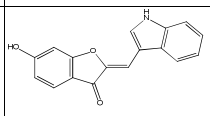
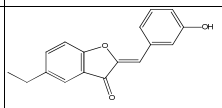
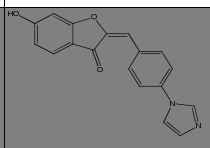
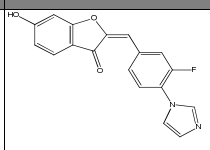
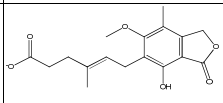
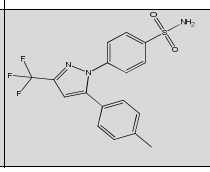
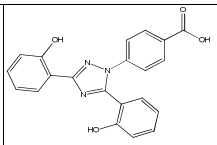
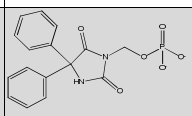
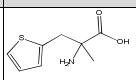
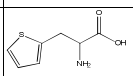
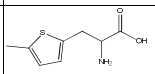
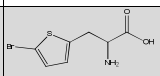
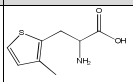
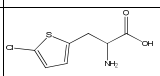
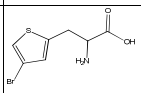
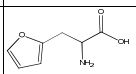
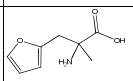
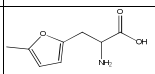
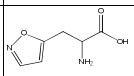
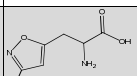
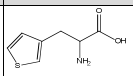
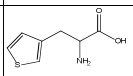
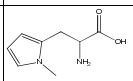
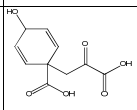
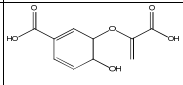
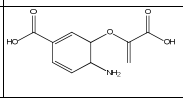
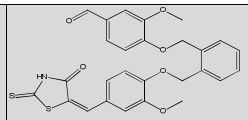
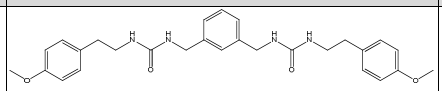
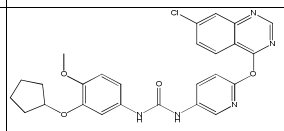
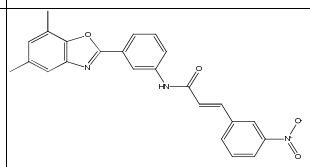
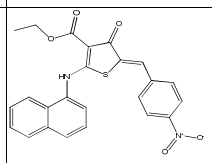
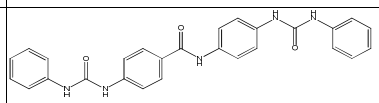
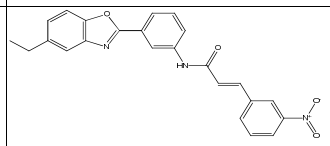
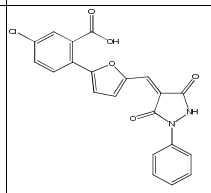
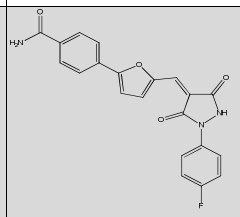
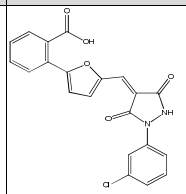
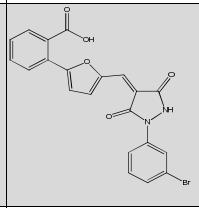
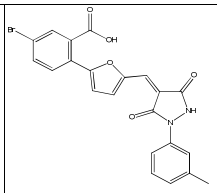
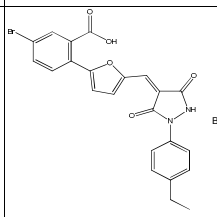
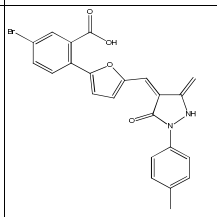
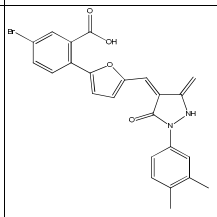
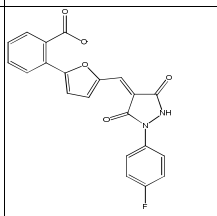
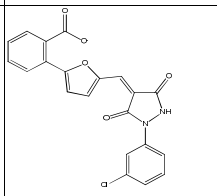
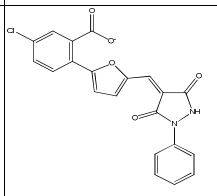
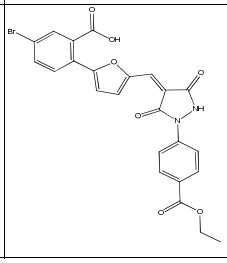
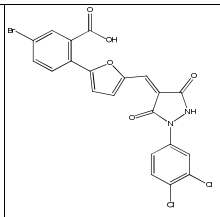
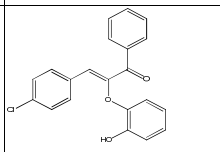
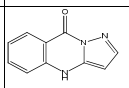
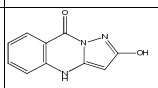
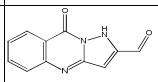
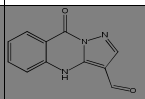
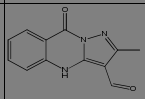
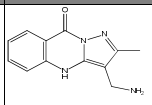
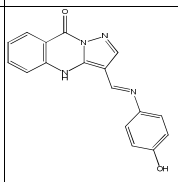
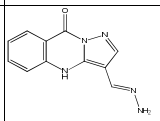
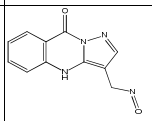
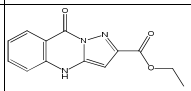
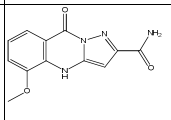
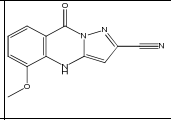
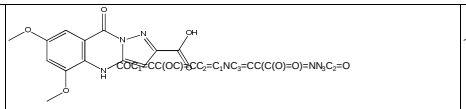
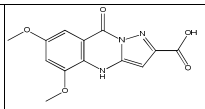
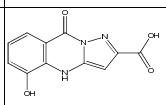
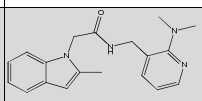
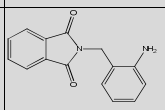
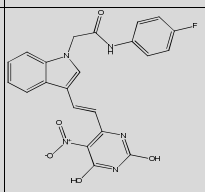
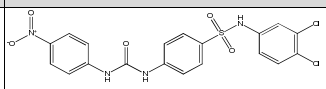
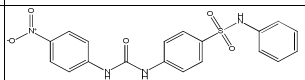
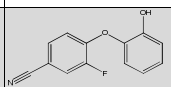
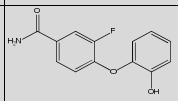
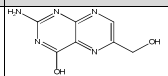
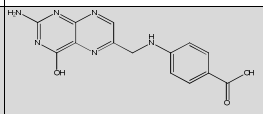
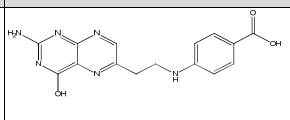
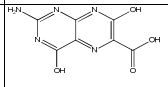
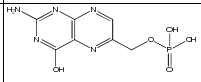
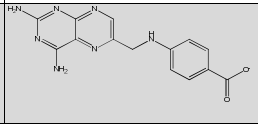
Structure_ID	SMILES	Structure	VD	CL	MRT	T1/2	Target
27928881	SC1=NC(N)=NC2=C1NC=N2		0.61	1.24	8.22	5.69	aroC
28433997	SC1=NC2=C(O)N=C(N)N=C2N1		0.56	1.44	6.44	4.46	aroC
29515579	NC1=NC(N([C@@H]2C[C@H](CO)C=C2)C=N3)=C3C(NC4CC4)=N1		0.75	1.38	9.04	6.26	aroC
28763139	ON(C(N)=O)C(C)C1=CC2=CC=CC=C2S1		2.67	3.16	14.07	9.75	aroC
27144340	O=C1C2=C(S/C1=C\C3=CC=C(O)C=C3)C=CC=C2		3.28	3.71	14.75	10.22	aroC
30013689	OC1=CC(O/C2=C\C3=CC(O)=C(O)C(O)=C3)=C(C2=O)C(O)=C1		2.09	2.81	12.41	8.60	aroC
30979018	O=C(COC1=CC(O/C2=C\C3=CC=CC=C3)=C(C2=O)C=C1)O		0.36	2.59	2.35	1.63	aroC
34736825	OC1=CC(O/C2=C/C3=CC=CN=C3)=C(C2=O)C=C1		1.82	2.73	11.13	7.71	aroC
34775739	OC1=CC(O/C2=C\C3=CC=C(C(C)(C)C)C=C3)=C(C2=O)C=C1		4.90	4.00	20.44	14.16	aroC
38986575	OC1=CC(O/C2=C\C3=CNC4=C3C=CC=C4)=C(C2=O)C=C1		3.25	3.20	16.93	11.73	aroC
87524429	CCC1=CC(C2=O)=C(O/C2=C\C3=CC(O)=CC=C3)C=C1		3.35	4.01	13.93	9.66	aroC
107441709	OC1=CC=C2C(O/C(C2=O)=C/C3=CC=C(C=C3)N4C=NC=C4)=C1		1.17	1.96	9.94	6.89	aroC
126767814	FC1=C(N2C=NC=C2)C=CC(/C=C(C3=O)/OC4=C3C=CC(O)=C4)=C1		1.26	2.09	10.01	6.93	aroC
131479406	[O-]C(CC/C(C)=C/CC1=C(O)C2=C(COC2=O)C(C)=C1OC)=O		0.44	2.50	2.93	2.03	aroC
28850331	FC(F)(C1=NN(C2=CC=C(S(=O)(N)=O)C=C2)C(C3=CC=C(C)C=C3)=C1)F		2.79	3.00	15.49	10.73	aroC

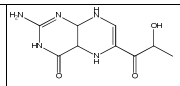
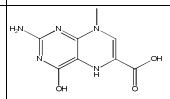
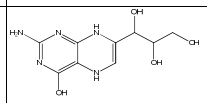
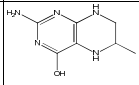
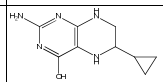
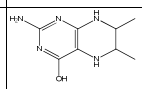
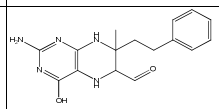
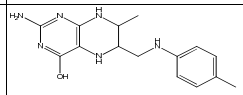
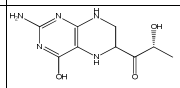
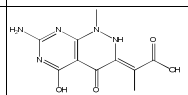
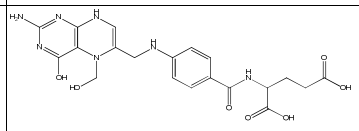
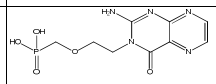
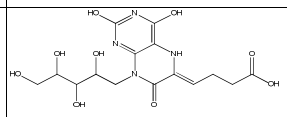
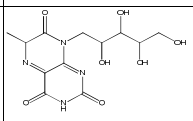
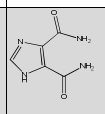
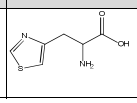
29512152	OC1=C(C2=NC(C3=C(O)C=CC=C3)=NN2C4=CC=C(C(O)=O)C=C4)C=CC=C1		0.84	2.57	5.45	3.78	aroC
180903688	O=P([O-])([O-])OCN(C1=O)C(NC1(C2=CC=CC=C2)C3=CC=CC=C3)=O		0.28	2.41	1.96	1.36	aroC
249758050	NC(C(O)=O)(CC1=CC=CS1)C		0.47	0.99	7.93	5.50	aroG
27644889	N[C@H](CC1=CC=CS1)C(O)=O		0.48	0.87	9.10	6.31	aroG
29254073	CC(S1)=CC=C1CC(N)C(O)=O		0.54	0.67	13.50	9.35	aroG
29254075	NC(C(O)=O)CC1=CC=C(Br)S1		0.58	0.65	14.86	10.30	aroG
29254076	CC1=C(SC=C1)CC(N)C(O)=O		0.51	0.81	10.46	7.25	aroG
152416852	NC(CC(S1)=CC=C1Cl)C(O)=O		0.55	0.68	13.57	9.40	aroG
161743282	BrC1=CSC(CC(N)C(O)=O)=C1		0.55	0.71	12.88	8.93	aroG
30379056	NC(CC1=CC=CO1)C(O)=O		0.47	0.96	8.06	5.59	aroG
249754974	NC(C(O)=O)(CC1=CC=CO1)C		0.45	1.04	7.27	5.04	aroG
129062300	NC(CC(O1)=CC=C1C)C(O)=O		0.50	0.72	11.70	8.10	aroG
187215823	NC(CC1=CC=NO1)C(O)=O		0.46	1.05	7.39	5.12	aroG
39432154	NC(C(O)=O)CC1=CC(C)=NO1		0.49	0.85	9.63	6.67	aroG
28433075	N[C@H](CC1=CSC=C1)C(O)=O		0.46	0.98	7.77	5.38	aroG
29292508	NC(CC1=CSC=C1)C(O)=O		0.46	0.98	7.77	5.38	aroG
161768273	NC(CC1=CC=CN1C)C(O)=O		0.45	1.05	7.19	4.98	aroG
30380340	OC1=CC(C(O)=O)(C=C1)CC(C(O)=O)=O		0.14	1.27	1.80	1.25	aroG
28809758	OC(C1=C[C@@H](OC(C(O)=O)=C)[C@H](O)C=C1)=O		0.14	1.01	2.38	1.65	aroG
61889507	N[C@H]1[C@H](OC(C(O)=O)=C)C=C(C=C2)C(O)=O		0.15	1.02	2.42	1.67	aroG

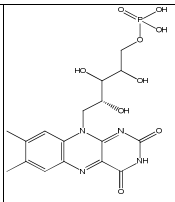
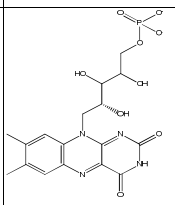
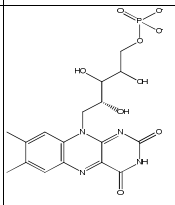
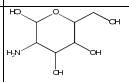
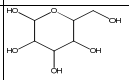
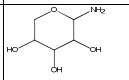
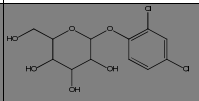
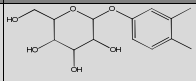
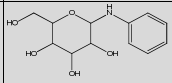
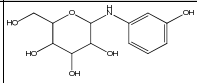
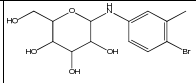
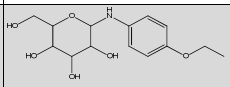
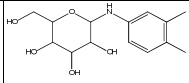
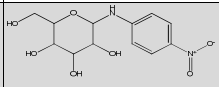
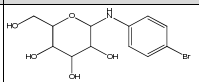
29142037	O=CC1=CC=C(C(OC)=C1)OCC2=CC=CC=C2COC3=CC=C(C=C3OC)/C=C(C(N4)=O)/SC4=S		3.91	3.15	20.67	14.32	aroK
29146142	COC1=CC=C(CCNC(NCC2=CC(CNC(NCCC3=CC=C(OC)C=C3)=O)=CC=C2)=O)C=C1		2.36	2.78	14.16	9.81	aroK
29300286	ClC1=CC2=NC=NC(OC3=NC=C(NC(NC4=CC(OC5CCCC5)=C(OC)C=C4)=O)C=C3)=C2C=C1		3.23	3.67	14.66	10.16	aroK
29720610	O=[N+]([O-])C1=CC(/C=C/C(NC2=CC(C(O3)=NC4=C3C(C)=CC(C)=C4)=CC=C2)=O)=CC=C1		2.74	2.96	15.44	10.70	aroK
29864729	O=[N+](C1=CC=C(/C=C(C2=O)\SC(NC3=CC=CC4=CC=CC=C34)=C2C(OCC)=O)C=C1)[O-]		2.89	3.09	15.61	10.82	aroK
30224149	O=C(NC1=CC=C(NC(NC2=CC=CC=C2)=O)C=C1)C3=CC=C(NC(NC4=CC=CC=C4)=O)C=C3		3.14	3.43	15.26	10.58	aroK
30233573	O=[N+]([O-])C1=CC(/C=C/C(NC2=CC(C(O3)=NC4=C3C=CC(CC)=C4)=CC=C2)=O)=CC=C1		3.00	3.20	15.61	10.82	aroK
30169904	ClC1=CC(C(O)=O)=C(C(O2)=CC=C2/C=C3C(N(NC(6=O)C4=CC=CC=C4)=O)C=C1		0.12	2.80	0.71	0.50	aroK
31629252	FC1=CC=C(N(C(/=O)NC(C2=C\C3=CC=C(C4=CC=C(C(N)=O)C=C4)O3)=O)C=C1		0.66	2.44	4.51	3.12	aroK
30240165	ClC1=CC(N(NC2=O)C(/C2=C\C(O3)=CC=C3C4=C(C(O)=O)C=CC=C4)=O)=CC=C1		0.12	2.80	0.72	0.50	aroK
30240865	BrC1=CC=CC(N(C(/=O)NC(C2=C\C3=CC=C(C4=CC=CC=C4C(O)=O)O3)=O)=O)=C1		0.12	2.80	0.71	0.49	aroK

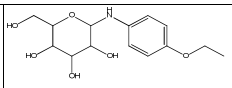
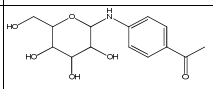
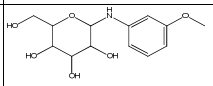
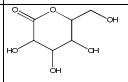
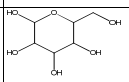
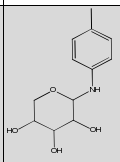
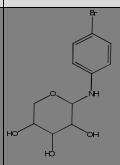
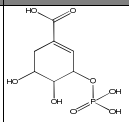
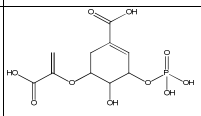
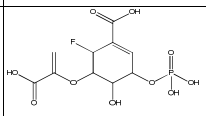
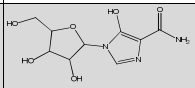
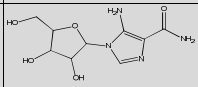
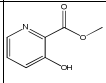
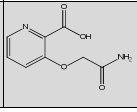
30272448	BrC1=CC(C(O)=O)=C(C(O2)=CC=C2/C=C3C(N(NC\3=O)C4=CC(C)=CC=C4)=O)C=C1		0.11	2.81	0.66	0.46	aroK
35357007	BrC1=CC(C(O)=O)=C(C(O2)=CC=C2/C=C3C(N(NC\3=O)C4=CC=C(CC)C=C4)=O)C=C1	 BrC	0.16	2.81	0.94	0.65	aroK
39446728	BrC1=CC(C(O)=O)=C(C(O2)=CC=C2/C=C3C(N(NC\3=C)C4=CC=C(C)C=C4)=O)C=C1		0.29	2.79	1.75	1.21	aroK
39446743	BrC1=CC(C(O)=O)=C(C(O2)=CC=C2/C=C3C(N(NC\3=C)C4=CC(C)=C(C)C=C4)=O)C=C1		0.37	2.78	2.22	1.54	aroK
75601322	FC1=CC=C(N(NC2=O)C(/C2=C\C(O3)=CC=C3C4=C(C([O-])=O)C=CC=C4)=O)C=C1		0.13	2.78	0.80	0.56	aroK
76152425	ClC1=CC(N(NC2=O)C(/C2=C\C(O3)=CC=C3C4=C(C([O-])=O)C=CC=C4)=O)=CC=C1		0.12	2.80	0.72	0.50	aroK
132064348	ClC1=CC(C([O-])=O)=C(C(O2)=CC=C2/C=C3C(N(NC\3=O)C4=CC=CC=C4)=O)C=C1		0.12	2.80	0.71	0.49	aroK
28877955	BrC1=CC(C(O)=O)=C(C(O2)=CC=C2/C=C3C(N(NC\3=O)C4=CC=C(C(OCC)=O)C=C4)=O)C=C1		0.12	2.80	0.69	0.48	aroK

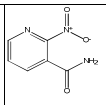
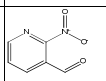
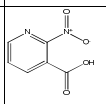
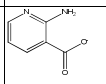
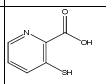
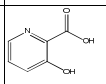
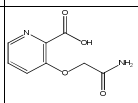
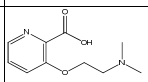
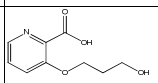
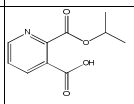
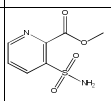
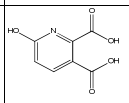
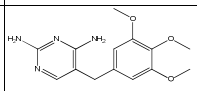
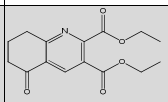
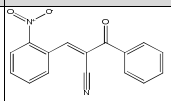
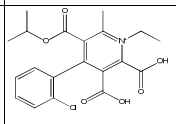
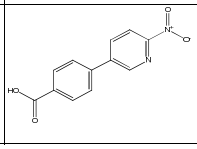
29152838	BrC1=CC(C(O)=O)=C(C(O2)=CC=C2/C=C3C(N(NC\3=O)C4=CC(Cl)=C(Cl)C=C4)=O)C=C1		0.10	2.81	0.61	0.42	aroK
28267724	ClC1=CC=C(/C=C(OC2=C(O)C=CC=C2)/C(C3=CC=CC=C3)=O)C=C1		2.69	2.90	15.43	10.69	aroK
30188195	O=C1N2N=CC=C2NC3=C1C=CC=C3		3.14	4.07	12.88	8.93	coaD
70542065	O=C1N2N=C(C=C2NC3=C1C=CC=C3)O		3.25	4.14	13.08	9.06	coaD
102132334	O=C1N2NC(C=O)=CC2=NC3=C1C=CC=C3		0.86	1.09	13.11	9.09	coaD
27639774	O=C1N2N=CC(C=O)=C2NC3=CC=CC=C31		2.76	3.28	14.06	9.74	coaD
238712227	O=C1N2N=C(C)C(C=O)=C2NC3=CC=CC=C31		2.59	2.94	14.70	10.19	coaD
238713396	O=C1N2N=C(C(CN)=C2NC3=C1C=CC=C3)C		0.73	2.44	5.02	3.48	coaD
147911620	O=C1N2N=CC(/C=N/C3=CC=C(O)C=C3)=C2NC4=C1C=CC=C4		3.38	4.01	14.06	9.74	coaD
148067159	O=C1N2N=CC(/C=N/N)=C2NC3=C1C=CC=C3		2.12	2.61	13.55	9.39	coaD
148227647	O=C1N2N=CC(CN=O)=C2NC3=C1C=CC=C3		2.88	3.94	12.19	8.45	coaD
148936594	O=C1N2N=C(C=C2NC3=C1C=CC=C3)C(OCC)=O		3.14	3.54	14.77	10.24	coaD
187236494	COC1=CC=CC2=C1NC2=CC(C(N)=O)=NN3C2=O		1.86	2.59	11.97	8.30	coaD
187236496	COC1=CC=CC2=C1NC3=CC(C#N)=NN3C2=O		3.05	3.66	13.86	9.61	coaD

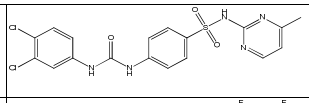
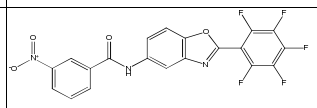
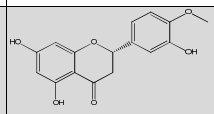
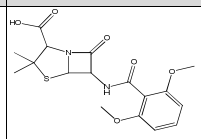
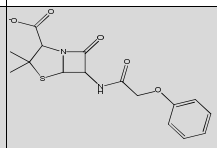
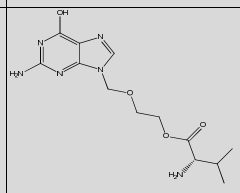
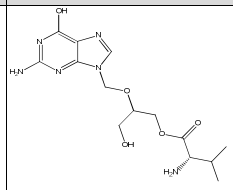
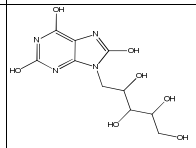
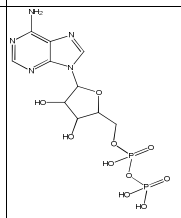
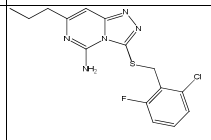
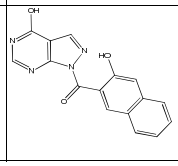
187236497			0.30	2.43	2.06	1.43	coaD
187236498			0.29	2.42	2.03	1.40	coaD
295773423			2.50	3.05	13.65	9.46	fabI
29504564			2.51	3.19	13.10	9.08	fabI
35777990			3.11	3.34	15.48	10.73	fabI
35957082			2.99	2.93	16.97	11.76	fabI
38362581			2.63	2.86	15.34	10.63	fabI
236546277			3.51	4.31	13.56	9.40	fabI
236546278			2.88	3.51	13.67	9.47	fabI
28811136			0.48	1.01	7.86	5.45	folK
27928841			0.37	1.47	4.18	2.90	folK
30385311			0.44	0.81	9.10	6.31	folK
30408296			0.40	1.68	3.99	2.77	folK
68377661			0.21	1.01	3.52	2.44	folK
77912390			0.44	0.81	9.07	6.29	folK

70078879	O=C1NC(N)=NC2NC=C(NC12)C(C(O)C)=O		0.45	1.10	6.90	4.78	folK
30445429	O=C(C1=CN(C2=NC(N)=NC(O)=C2N1)C)O		0.44	1.13	6.47	4.49	folK
313845810	O[C@H](C1=CNC2=C(O)N=C(N)N=C2N1)[C@@H](CO)O		0.45	1.10	6.81	4.72	folK
187140031	C[C@@H]1NC2=C(NC1)N=C(N)N=C2O		0.64	1.27	8.36	5.79	folK
135968811	OC1=NC(N)=NC2=C1NC(CN2)C3CC3		0.85	1.58	8.95	6.20	folK
28775227	OC1=NC(N)=NC2=C1NC(C(N2)C)C		0.86	1.60	8.95	6.20	folK
68371377	OC1=NC(N)=NC2=C1NC([C@@](C)(N2)CCC3=CC=CC=C3)C=O		2.42	3.12	12.94	8.97	folK
129802050	CC1=CC=C(C=C1)NC[C@@H]2NC3=C(NC2C)N=C(N)N=C3O		2.37	3.13	12.61	8.74	folK
129825112	OC1=NC(N)=NC2=C1NC(CN2)C([C@H](C)O)=O		0.48	1.06	7.54	5.22	folK
28918893	C/C(C(O)=O)=C(C1=O)/NN(C2=C1C(O)=NC(N)=N2)C		0.36	0.55	10.94	7.58	folK
313844357	OC1=NC(N)=NC2=C1N(C(CNC3=CC=C(C(N[C@@H](C(O)=O)CCC(O)=O)=O)C=C3)=CN2)CO		0.15	0.56	4.53	3.14	folK
73521837	O=P(COCCN(C(N)=NC1=NC=CN=C21)C2=O)(O)O		0.17	1.04	2.75	1.90	folK
136746903	O=C(CC/C=C(C1=O)\NC2=C(O)N=C(O)N=C2N1C[C@@H]([C@@H]([C@@H](CO)O)O)O)O		0.15	0.99	2.44	1.69	folK
29508912	O=C(CC/C=C(C1=O)\NC2=C(O)N=C(O)N=C2N1C[C@@H]([C@@H]([C@@H](CO)O)O)O)O		0.24	1.10	3.59	2.49	folK
27678823	O=C(N)C1=C(C(N)=O)NC=N1		0.41	1.03	6.60	4.57	folK
30380846	NC(CC1=CSC=N1)C(O)=O		0.46	1.02	7.48	5.18	folK

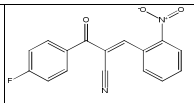
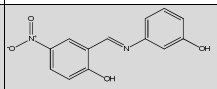
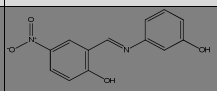
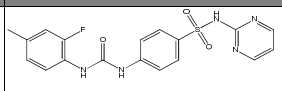
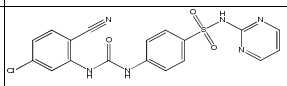
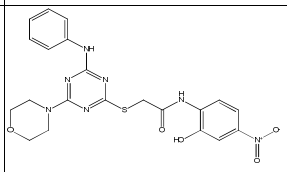
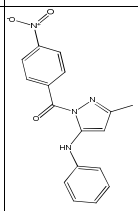
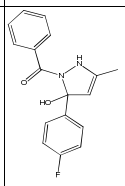
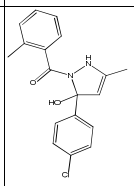
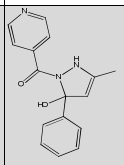
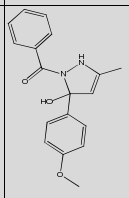
130533128	O=P(O)(OCC(C([C@@H](CN1C2=C(N=C3C1=NC(NC3=O)=O)C=C(C)C(C)=C2)O)O)O)O		0.15	0.52	4.96	3.44	folK
131690280	O=P(OCC(C([C@@H](CN1C2=C(N=C3C1=NC(NC3=O)=O)C=C(C)C(C)=C2)O)O)O)([O-])[O-]		0.15	0.51	5.08	3.52	folK
131690283	O=P(OCC(C([C@@H](CN1C2=C(N=C3C1=NC(NC3=O)=O)C=C(C)C(C)=C2)O)O)O)([O-])[O-]		0.15	0.51	5.08	3.52	folK
153990598	NC(C1O)C(OC(C1O)CO)O		0.42	1.16	5.97	4.14	lpcA
101352797	O[C@@H](C1O)OC([C@H](C1O)O)CO		0.45	1.13	6.68	4.63	lpcA
158582040	N[C@@H](C1O)OC[C@@H](O)C1O		0.52	1.14	7.56	5.24	lpcA
34733326	ClC1=C(OC(C2O)OC(C(C2O)O)CO)C=CC(Cl)=C1		0.90	1.41	10.68	7.40	lpcA
77912390	OCC1OC(OC2=CC=C(C)C(C)=C2)C(O)C(O)C1O		0.80	1.30	10.25	7.10	lpcA
27654666	OC1C(OC(CO)C(O)C1O)NC2=CC=CC=C2		0.49	0.89	9.13	6.32	lpcA
27119828	OC(C1O)C(NC2=CC(O)=CC=C2)OC(C1O)CO		0.47	0.93	8.51	5.89	lpcA
117776378	BrC1=C(C)C=C(NC(C2O)OC(C(C2O)O)CO)C=C1		0.75	1.08	11.66	8.08	lpcA
27654450	OC1C(OC(CO)C(O)C1O)NC2=CC=C(OCC)C=C2		0.50	0.92	9.04	6.26	lpcA
27657439	OC(C1O)C(NC2=CC(C)=C(C)C=C2)OC(C1O)CO		0.65	0.96	11.31	7.84	lpcA
27928841	O=[N+](C1=CC=C(NC2OC(CO)C(O)C(O)C2O)C=C1)[O-]		0.50	0.82	10.20	7.07	lpcA
28116592	BrC1=CC=C(N[C@@H]([C@@H]2O)O[C@H](CO)[C@@H]([O][C@@H]2O)C=C1		0.59	0.84	11.76	8.15	lpcA

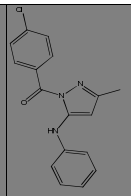
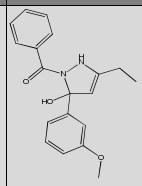
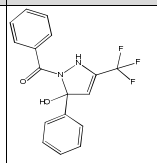
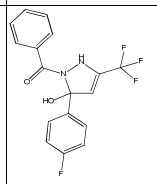
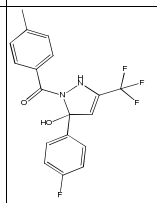
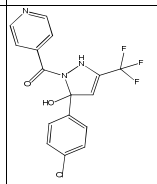
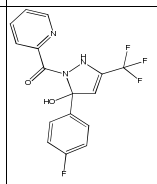
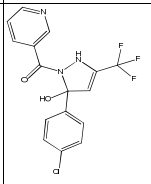
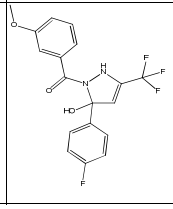
30424932	OC(C1O)C(NC2=CC=C(OCC)C=C2)OC(C1O)CO		0.50	0.92	9.04	6.26	lpcA	
34694328	OC(C1O)C(NC2=CC=C(C(C)=O)C=C2)OC(C1O)CO		0.53	0.60	14.76	10.23	lpcA	
60172860	OC(C1O)C(NC2=CC(OC)=CC=C2)OC(C1O)CO		0.49	0.88	9.18	6.36	lpcA	
28803460	O[C@H]1[C@H](O)[C@@H](O)[C@@H](OC1=O)CO		0.45	1.11	6.72	4.66	lpcA	
30012668	O[C@@H]([C@@H]1O)O[C@@H]([C@@H]([C@@H]1O)O)CO		0.45	1.13	6.68	4.63	lpcA	
27592880	OC1C(OCC(O)C1O)NC2=CC=C(C)C=C2		0.69	1.15	9.98	6.92	lpcA	???
34733326	BrC1=CC=C(N 2OC (O) (O) 2O)C=C1		0.80	1.28	10.43	7.23	lpcA	
28764874	O=P(O)(O[C@H]1[C@@H](O)[C@H](O)CC(C(O)=O)=C1)O		0.15	0.95	2.57	1.78	lpcA	
28780304	O=P(O)(O[C@H]1[C@@H](O)[C@H](OC(C(O)=O)=C)CC(C(O)=O)=C1)O		0.15	0.59	4.36	3.02	lpcA	
70787116	F[C@H]1[C@@H](OC(C(O)=O)=C)[C@H](O)[C@H](OP(O)(O)=O)C=C1C(O)=O		0.15	0.60	4.25	2.94	lpcA	
30424932	OC1=C(C(N)=O)N=CN1[C@@H]2O[C@H](CO)[C@@H](O)[C@H]2O		0.43	1.13	6.43	4.45	lpcA	
27593512	NC1=C(C(N)=O)N=CN1[C@@H]2O[C@H](CO)C(O)C2O		0.44	1.14	6.49	4.50	lpcA	
27737380	O=[N+]([O-])C1=NC=CC=C1O		0.44	2.00	3.66	2.54	nadC	
28665953	O=C(C1=CC=CN=C1)[O-]		0.41	1.02	6.63	4.59	nadC	
28667598	OC1=CC=CN=C1C(OC)=O		2.00	2.82	11.85	8.21	nadC	
30019459	NC(COC1=CC=CN=C1C(O)=O)=O		0.42	0.84	8.32	5.77	nadC	

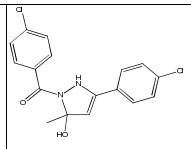
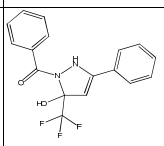
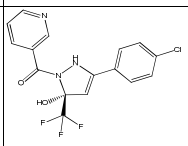
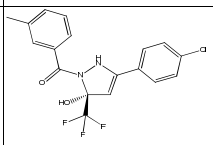
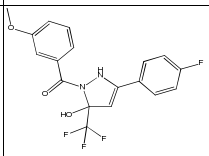
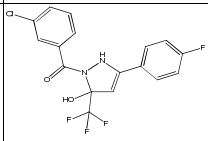
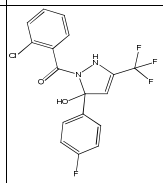
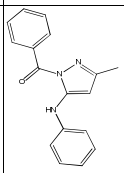
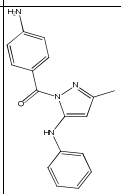
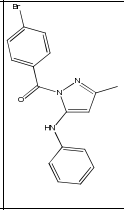
70358905	O=[N+]([O-])C1=NC=CC=C1C(N)=O		0.72	1.30	9.19	6.37	nadC
234796908	O=[N+]([O-])C1=NC=CC=C1C=O		1.56	2.29	11.33	7.85	nadC
30409034	O=[N+]([O-])C1=NC=CC=C1C(O)=O		0.32	1.87	2.87	1.99	nadC
78519792	NC1=NC=CC=C1C([O-])=O		0.41	0.84	8.17	5.66	nadC
70624296	SC1=C(C(O)=O)N=CC=C1		0.46	0.77	9.85	6.83	nadC
131501422	OC1=CC=CN=C1C([O-])=O		0.45	0.63	11.89	8.24	nadC
247608578	NC(COC1=C(C(O)=O)N=CC=C1)=O		0.42	0.84	8.32	5.77	nadC
247608587	O=C(C1=C(OCCCN(C)C)C=CC=N1)O		0.45	1.08	6.95	4.81	nadC
247609672	OCCCOC1=CC=CN=C1C(O)=O		0.45	0.74	10.18	7.06	nadC
161604885	O=C(C1=CC=CN=C1C(OC(C)C)=O)O		0.31	2.15	2.40	1.66	nadC
92156924	O=S(N)(C1=C(C(OC)=O)N=CC=C1)=O		0.58	0.62	15.57	10.79	nadC
30466351	O=C(C1=NC(O)=CC=C1C(O)=O)O		0.22	1.63	2.20	1.52	nadC
183986600	NC1=NC(N)=C(CC2=CC(OC)=C(OC)C(OC)=C2)C=N1		1.21	2.50	8.03	5.56	nadC
29515878	O=C(OCC)C1=C(C(OCC)=O)C=C(C(CC2)=O)C2=N1		2.12	2.66	13.28	9.20	nadC
29716752	O=[N+]([O-])C1=C/C=C(C(C2=CC=CC=C2)=O)\C#N)C=CC=C1		2.45	2.78	14.66	10.16	nadC
68372779	ClC1=C(C2=C(C(OC(C)C)=O)C(C)=[N+](CC)C(C(O)=O)=C2C(O)=O)C=CC=C1		0.18	0.14	21.32	14.78	nadC
154011954	O=[N+]([O-])C1=NC=C(C2=CC=C(C(O)=O)C=C2)C=C1		0.31	2.48	2.07	1.43	nadC

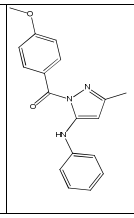
27328604	O=S(NC1=NC(C)=CC=N1)(C2=CC=C(NC(NC3=CC(Cl)=C(Cl)C=C3)=O)C=C2)=O		1.19	2.59	7.65	5.30	nadE
27531718	FC1=C(F)C(F)=C(C(O2)=NC3=C2C=CC(NC(C4=CC([N+]([O-])=O)=CC=C4)=O)=C3)C(F)=C1F		3.12	3.38	15.40	10.67	nadE
28436162	O=C1C[C@@H](C2=CC=C(OC)C(O)=C2)OC3=CC(O)=CC(O)=C13		3.09	3.38	15.24	10.56	nadE
28759193	COC1=CC=CC(OC)=C1C(N[C@H]2[C@H](N3C2=O)SC(C)([C@@H]3C(O)=O)C)=O		0.33	1.76	3.11	2.16	nadE
28759683	CC1([C@@H](N([C@@H]2S1)C([C@H]2NC(COC3=CC=CC=C3)=O)=O)C([O-])=O)C		0.35	1.66	3.53	2.44	nadE
28765426	OC1=C(N=CN2COCCOC([C@H](C(C)C)N)=O)C2=NC(N)=N1		0.95	1.55	10.18	7.06	nadE
70610912	OC1=C(N=CN2COC(COC([C@H](C(C)C)N)=O)CO)C2=NC(N)=N1		0.73	1.18	10.33	7.16	nadE
136822396	OC1=NC2=C(O)N=C(O)N=C2N1CC([C@@H]([C@@H](CO)O)O)O		0.46	0.99	7.74	5.36	nadE
313845526	O=P(O)(OP(O)(O)=O)OC[C@@H]([C@@H]1O)O[C@@H](N2C3=NC=NC(N)=C3N=C2)[C@@H]1O		0.15	0.96	2.55	1.77	nadE
38201847	FC1=C(CSC2=NN=C3N2C(N)=NC(CCC)=C3)C(Cl)=CC=C1		2.74	3.07	14.85	10.29	nadE
27560618	OC1=NC=NC2=C1C=NN2C(C3=CC4=C(C=CC=C4)C=C3O)=O		1.84	2.59	11.88	8.23	nadE

nadE or aroC???

105012384	FC1=CC=C(C(/C(C#N)=C/C2=C([N+]([O-])=O)C=CC=C2)=O)C=C1		2.57	2.85	15.03	10.42	nadE
111735241	O=[N+](C1=CC=C(O)C(/C=N/C2=CC=CC(O)=C2)=C1)[O-]		3.54	3.21	18.33	12.70	nadE
195983203	O= ( )C1=CC(/C=N/C2=CC(O)=CC=C2)=C(O)C=C1		3.54	3.21	18.33	12.70	nadE
206592729	FC1=C(NC(NC2=CC=C(S(=O)(NC3=NC=CC=N3)=O)C=C2)=O)C=CC(C)=C1		1.02	2.51	6.80	4.71	nadE
212465872	O=S(NC1=NC=CC=N1)(C2=CC=C(NC(NC3=C(C#N)C=CC(Cl)=C3)=O)C=C2)=O		1.52	2.60	9.75	6.76	nadE
41513968	O=C(CSC1=NC(N2CCOCC2)=NC(NC3=CC=CC=C3)=N1)NC4=C(O)C=C([N+]([O-])=O)C=C4		2.43	2.75	14.76	10.23	nadE
26883731	O=[N+]([O-])C1=CC=C(C(N2N=C(C=C2NC3=CC=CC=C3)C)=O)C=C1		3.21	3.56	15.04	10.42	ribH
73966975	FC1=CC=C([C@]2(N(NC(C)=C2)C(C3=CC=CC=C3)=O)O)C=C1		3.21	3.88	13.78	9.55	ribH
128161912	ClC1=CC=C([C@]2(N(NC(C)=C2)C(C3=C(C)C=CC=C3)=O)O)C=C1		3.31	3.91	14.09	9.76	ribH
27388010	OC1(C2=CC=CC=C2)N(C(C3=CC=NC=C3)=O)NC(C)=C1		2.12	2.96	11.92	8.26	ribH
27556797	OC1(C2=CC=C(OC)C=C2)N(C(C3=CC=CC=C3)=O)NC(C)=C1		3.02	3.54	14.22	9.86	ribH

27832702	$ClC_1=CC=C(C(N_2N=C(C)C=C_2NC_3=CC=CC=C_3)=O)C=C_1$		3.12	3.36	15.45	10.71	ribH
27907145	$OC_1(C_2=CC=CC(OC)=C_2)N(C(C_3=CC=CC=C_3)=O)NC(CC)=C_1$		3.24	3.91	13.79	9.55	ribH
73921605	$FC(C(N_1)=C[C@@](C_2=CC=CC=C_2)(N_1C(C_3=CC=CC=C_3)=O)O)(F)F$		3.28	3.99	13.71	9.50	ribH
74224504	$FC(C(N_1)=C[C@@](C_2=CC=C(F)C=C_2)(N_1C(C_3=CC=CC=C_3)=O)O)(F)F$		3.30	4.06	13.55	9.39	ribH
74224505	$FC(C(N_1)=C[C@@](C_2=CC=C(F)C=C_2)(N_1C(C_3=CC=C(C)C=C_3)=O)O)(F)F$		3.35	4.19	13.32	9.23	ribH
74235707	$FC(C(N_1)=C[C@@](C_2=CC=C(Cl)C=C_2)(N_1C(C_3=CC=NC=C_3)=O)O)(F)F$		2.99	3.51	14.19	9.83	ribH
74269204	$FC(C(N_1)=C[C@@](C_2=CC=C(F)C=C_2)(N_1C(C_3=NC=CC=C_3)=O)O)(F)F$		2.99	3.54	14.08	9.76	ribH
74357439	$FC(C(N_1)=C[C@@](C_2=CC=C(Cl)C=C_2)(N_1C(C_3=CN=CC=C_3)=O)O)(F)F$		2.99	3.51	14.19	9.83	ribH
74387455	$FC(C(N_1)=C[C@@](C_2=CC=C(F)C=C_2)(N_1C(C_3=CC(OC)=CC=C_3)=O)O)(F)F$		3.22	3.84	13.99	9.69	ribH

28568421	ClC1=CC=C(C(N2)=C[C@@](C)(N3C(C4=CC=C(Cl)C=C4)=O)O)C=C1		3.01	3.23	15.53	10.76	ribH
74035569	FC([C@]1(N(NC(C2=CC=CC=C2)=C1)C(C3=CC=CC=C3)=O)O)(F)F		3.21	3.61	14.83	10.28	ribH
74449206	FC([C@]1(N(NC(C2=CC=C(Cl)C=C2)=C1)C(C3=CN=CC=C3)=O)O)(F)F		2.84	3.20	14.82	10.27	ribH
74742317	FC([C@]1(N(NC(C2=CC=C(Cl)C=C2)=C1)C(C3=CC(C)=CC=C3)=O)O)(F)F		3.28	3.63	15.06	10.43	ribH
75585021	FC([C@]1(N(NC(C2=CC=C(F)C=C2)=C1)C(C3=CC(OC)=CC=C3)=O)O)(F)F		3.12	3.47	15.00	10.40	ribH
75588335	FC([C@]1(N(NC(C2=CC=C(F)C=C2)=C1)C(C3=CC(Cl)=CC=C3)=O)O)(F)F		3.25	3.61	15.03	10.42	ribH
131983591	FC(C(N1)=C[C@@](C2=CC=C(F)C=C2)(N1C(C3=C(Cl)C=CC=C3)=O)O)(F)F		3.31	3.99	13.86	9.60	ribH
29401899	CC1=NN(C(NC2=CC=CC=C2)=C1)C(C3=CC=CC=C3)=O		3.22	3.56	15.04	10.42	ribH
28246698	CC1=NN(C(NC2=CC=CC=C2)=C1)C(C3=CC=C(N)C=C3)=O		3.14	3.48	15.08	10.45	ribH
29365279	BrC1=CC=C(C(N2N=C(C=C2NC3=CC=CC=C3)C)=O)C=C1		3.09	3.33	15.49	10.73	ribH

29401897	$CC_1=NN(C(NC_2=CC=CC=C_2)=C_1)C(C_3=CC=C(OC)C=C_3)=O$		3.20	3.54	15.07	10.45	ribH