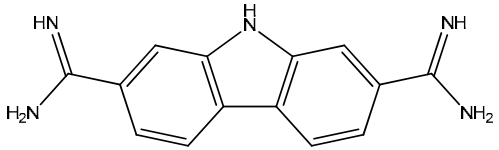
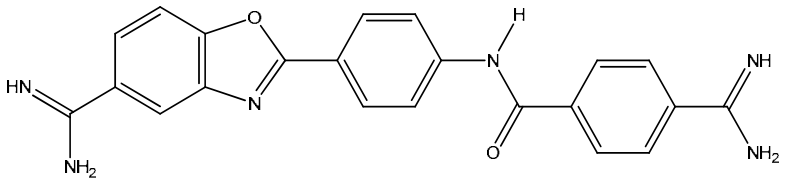
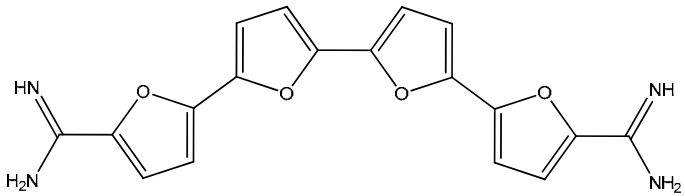
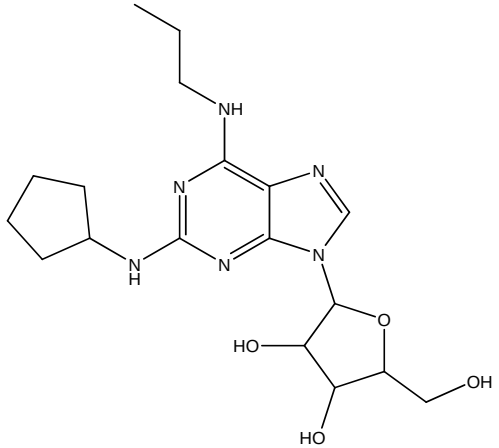
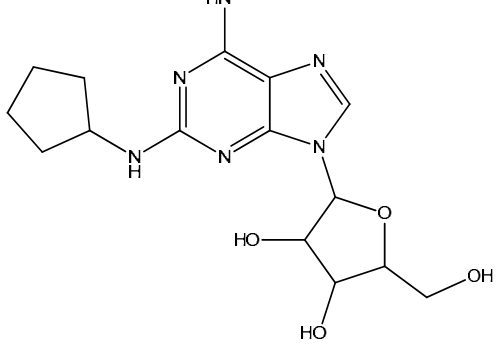
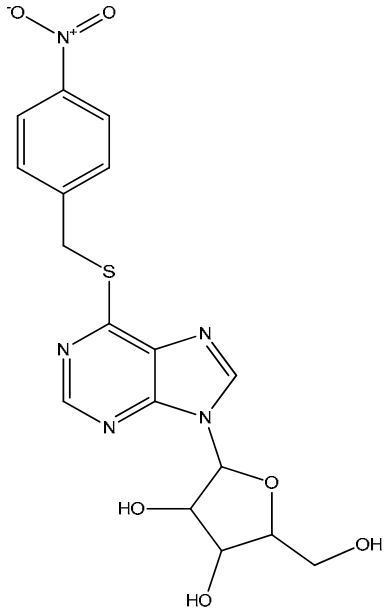
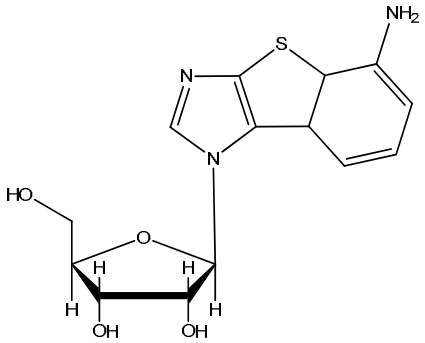
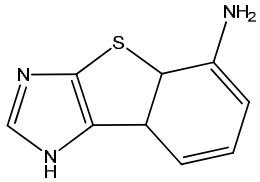
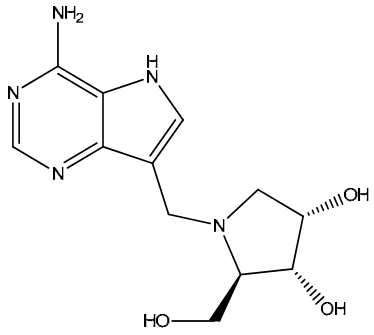
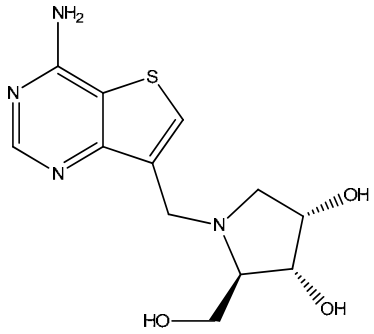
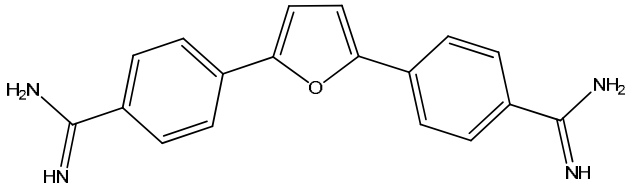
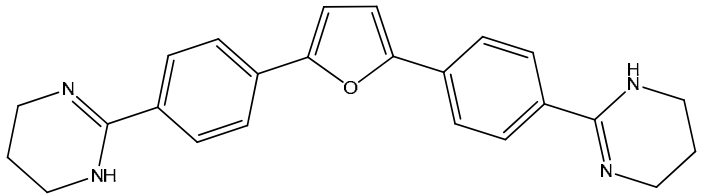
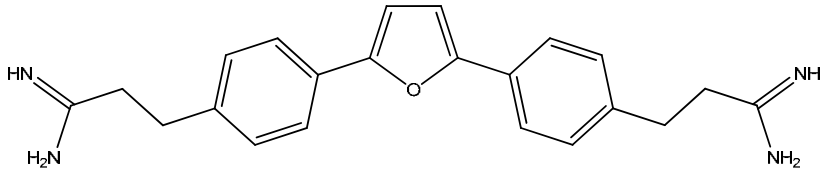
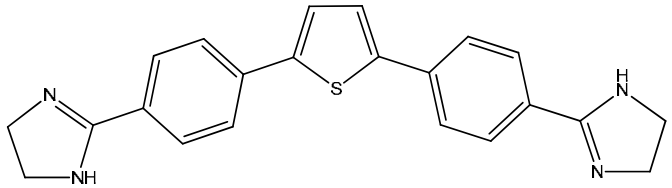
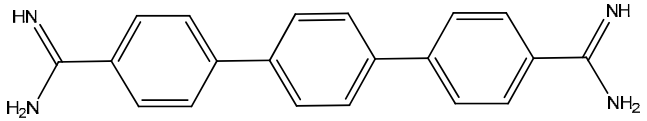
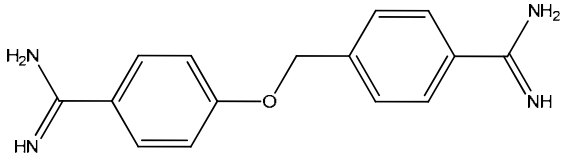
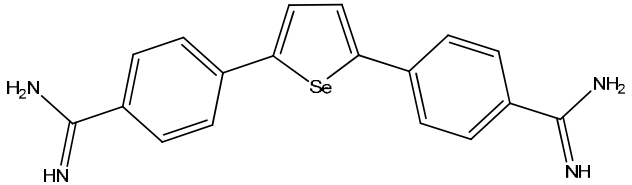
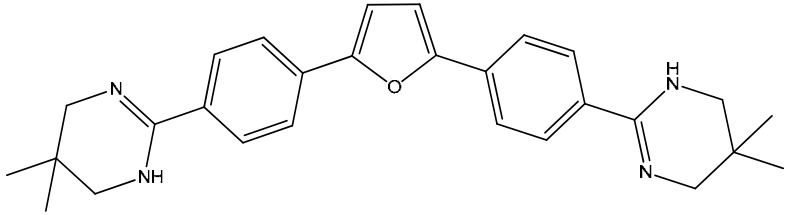
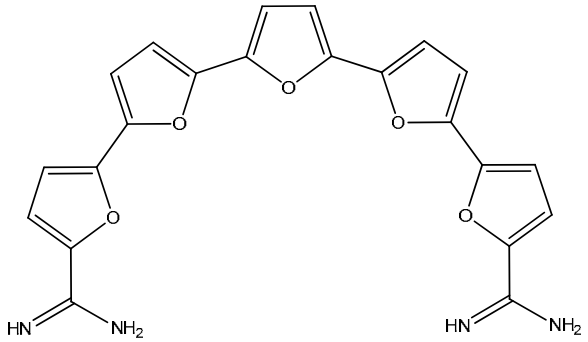
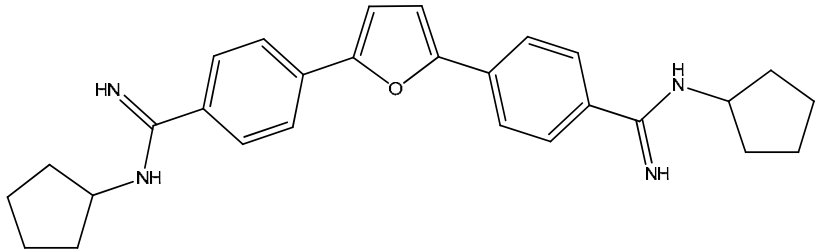
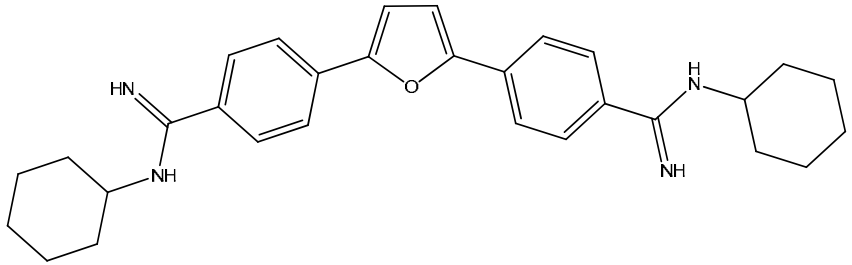
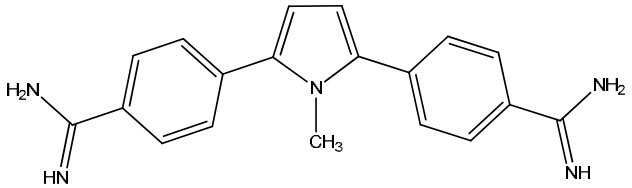
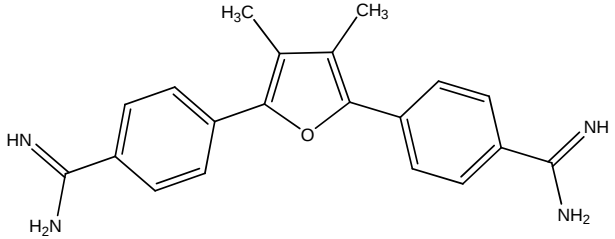
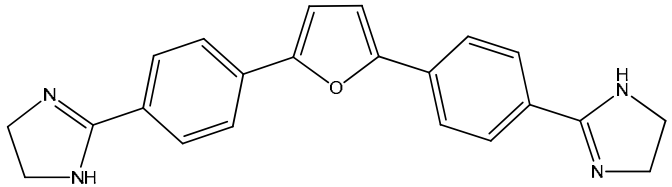
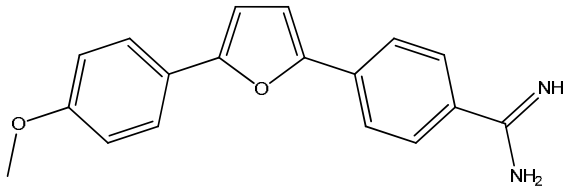
Scaffold	Compound	K_i of P2 (μM)	$\Delta(G^0)$ (kJ/mol)	Source
A	1-deazaadenosine	45.4	-24.8	(1)
A	1-deazapurine	131	-22.2	Aldrich
A	2,6-diaminopurine-2'-d-riboside	4.44	-30.6	MP Biomedicals
A	2-chloro-adenosine	9.65	-28.6	TriLink Biotech
A		7.5	-29.3	(10)
A	2'-deoxyadenosine	0.23	-37.9	Sigma
A	2'-deoxyinosine	165	-21.6	Sigma
A	2-hydroxy-6-aminopurine	9.7	-28.6	Acros
A	2-nitoradenosine	81	-23.4	(1)
A	3-deaza-adenosine	0.29	-37.3	Sigma
A	6-chloropurine riboside	15.4	-27.5	TriLink Biotech
A	8-azidoadenosine	331	-19.9	(8)
A	8-bromoadenosine	37.8	-25.2	Acros
A	9-deazaadenosine	12.2	-28	(7)
A	adenine	0.3	-37.2	Sigma
A	adenosine	0.92	-34.5	Sigma
A	allopurinol	255	-20.5	Sigma
A	DAPI	0.47	-36.1	Fluka
A	DB1208 	0.37	-36.7	(5)
A	DB1464 	0.15	-39	(5)
A	dilazep	150	-21.8	Sigma

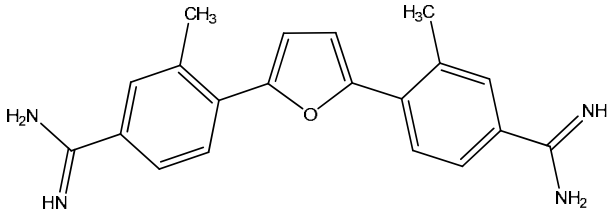
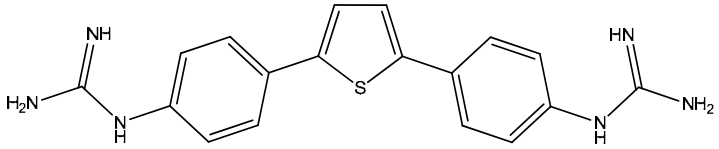
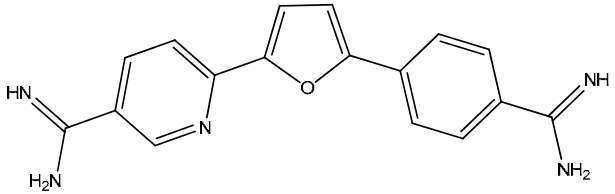
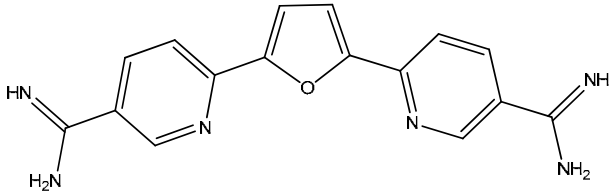
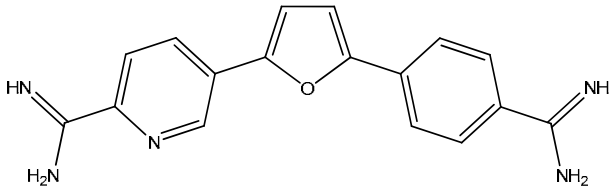
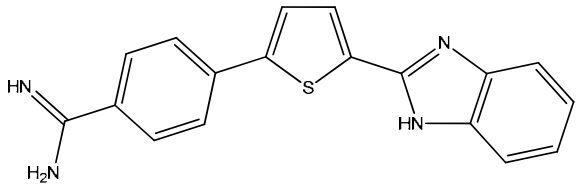
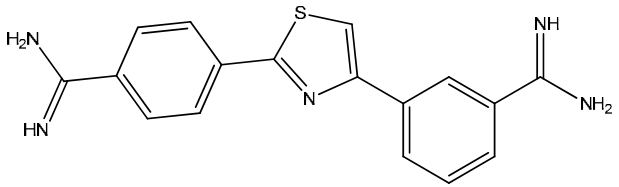
A	dipyridamole	51.6	-24.5	Sigma
A	formycin A	36.5	-25.3	(8)
A	hypoxanthine	500	-18.8	Sigma
A		9	-28.8	(1)
A		19.9	-26.8	(1)

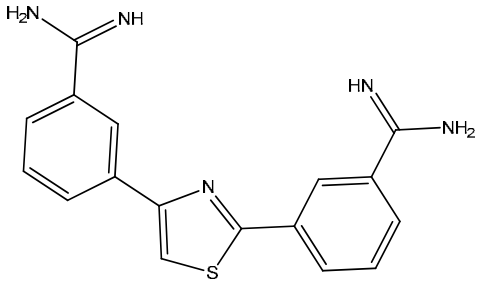
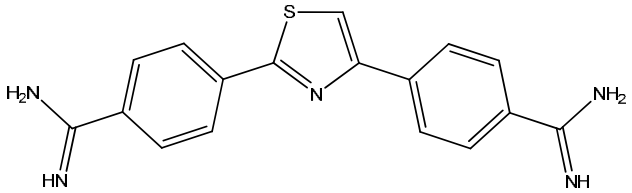
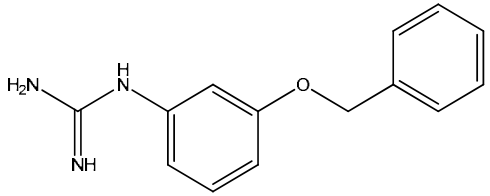
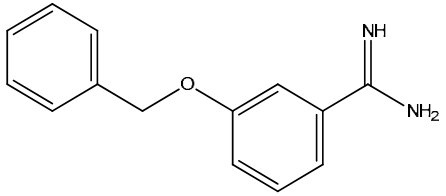
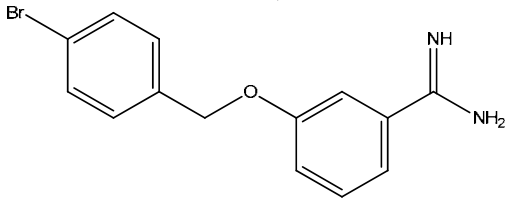
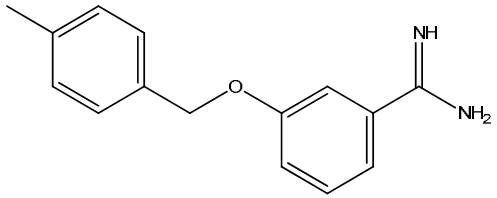
A		74.5	-23.6	Sigma
A	Nebularine (purine riboside)	17.1	-27.2	Sigma
A	oxypurinol	303	-20.1	Sigma
A	purine	18.1	-27.1	Sigma
A		16.2	-27.3	(3)
A		9.7	-28.6	(3)
A	Tubercidin (7-deazaadenosine)	3.81	-30.9	Fluka

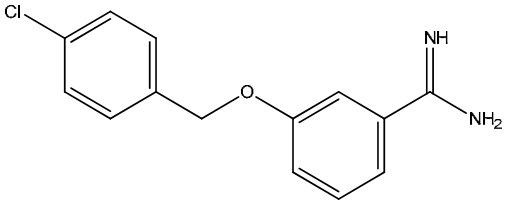
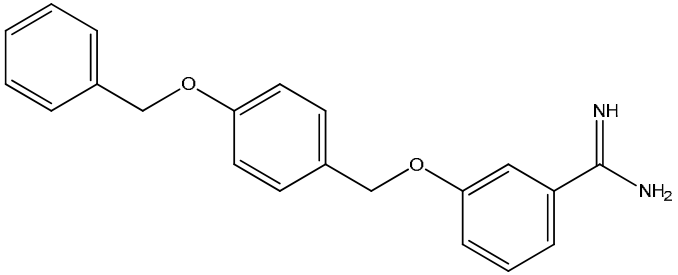
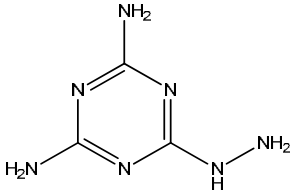
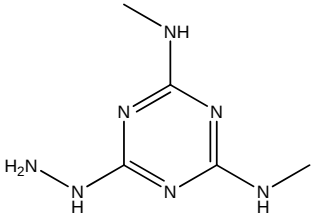
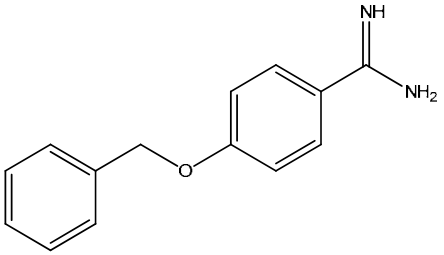
A			8.2	-29	(6)
A			125	-22.3	(6)
A	xanthine		106	-22.7	Sigma
B	2-hydroxybenzamidine		2030	-15.4	Acros
B	3-aminobenzamidine		722	-17.9	Acros
B	4-aminobenzamidine		22.9	-26.5	Acros
B	benzamidine		111	-22.6	Sigma
B	furamidine		1.19	-33.8	(5)
B	DB103		31.4	-25.7	(5)
B	DB1061		7.07	-29.4	(5)

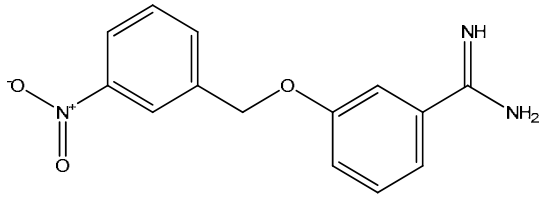
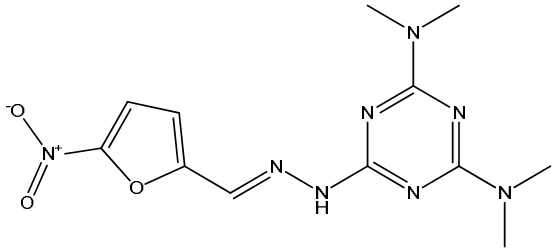
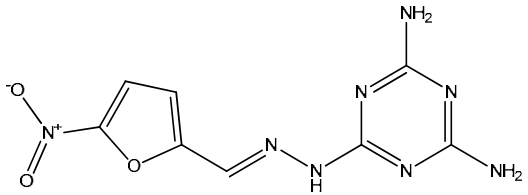
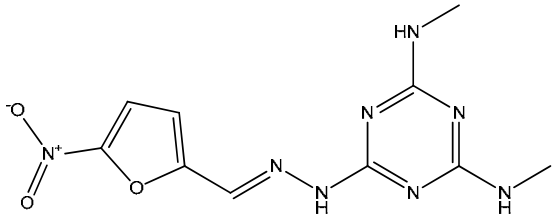
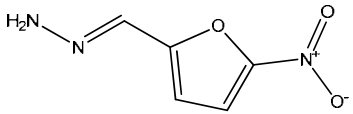
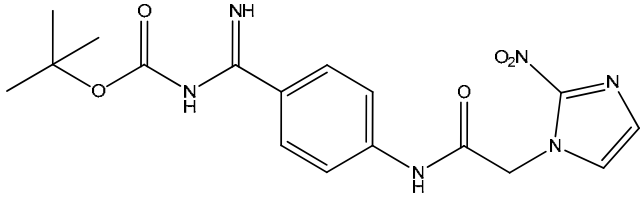
B	DB1064		33.2	-25.6	(5)
B	DB1111		5.5	-30	(5)
B	DB1138		8.1	-29.1	(5)
B	DB1213		1.09	-34	(5)
B	DB1339		25	-26.3	(5)
B	DB1680		0.95	-34.4	(5)

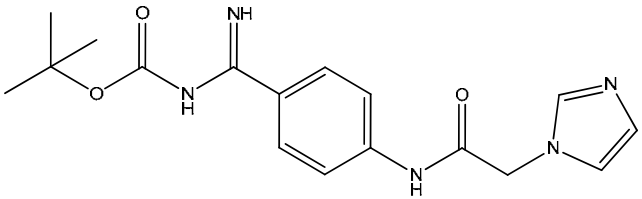
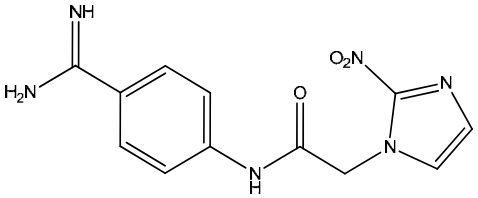
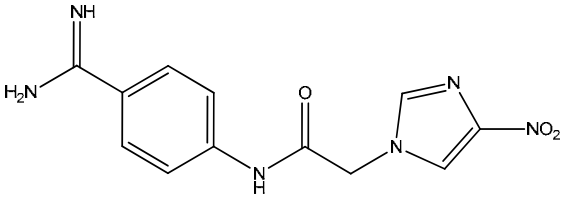
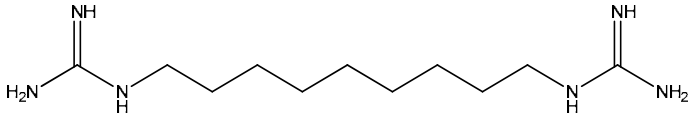
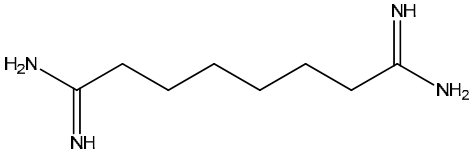
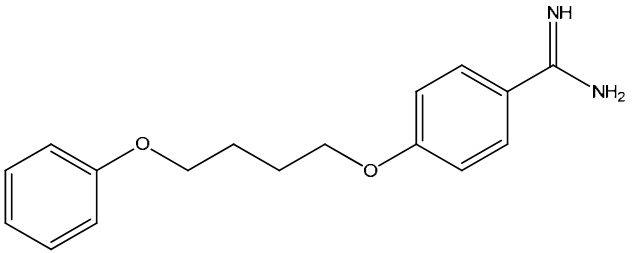
B	DB244		3.23	-31.3	(5)
B	DB249		4.49	-30.5	(5)
B	DB320		0.39	-36.6	(5)
B	DB544		3.02	-31.5	(5)
B	DB60		13.8	-27.7	(5)
B	DB607		4.1	-30.8	(5)

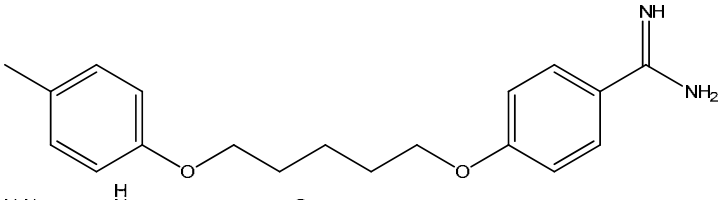
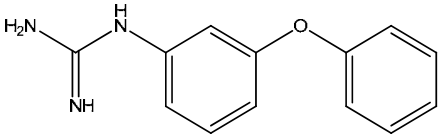
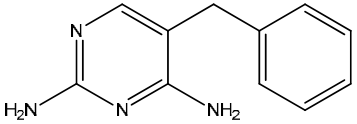
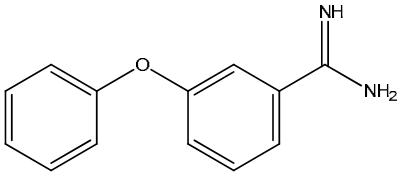
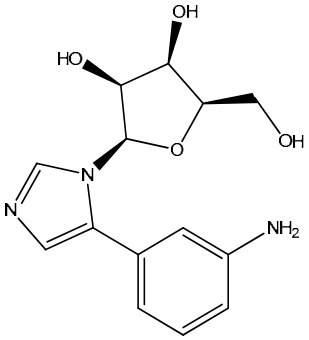
B	DB629		0.88	-34.6	(5)
B	DB686		5.4	-30.1	(5)
B	DB820		1.95	-32.6	(5)
B	DB829		1.4	-33.4	(5)
B	DB867		4	-30.8	(5)
B	DB931		1.23	-33.7	(5)
B	Distamycin A		10.6	-28.4	Sigma
B			1.36	-33.5	(9)

B		0.92	-34.5	(9)
B		3.92	-30.9	(9)
C		8.05	-29.1	(12)
C		0.38	-36.6	(12)
C		0.81	-34.8	(12)
C		0.21	-38.1	(12)

C		1.01	-34.2	(12)
C		1.57	-33.1	(12)
C		11.9	-28.1	(13)
C		59.3	-24.1	(13)
C		5.8	-29.9	(10)
C	2-aminopyridine	14.3	-27.7	Aldrich
C	4,6-diaminopyrimidine	3.22	-31.3	Aldrich
C	4-aminopyridine	145	-21.9	Aldrich
C	4-aminopyrimidine	137	-22.1	Acros
C	4-hydroxybenzamidine	235	-20.7	Aldrich

C	butamidine	1.04	-34.2	(2)
C	stilbamidine	2.42	-32.1	Sanofi-Aventis
D		0.33	-37	(14)
D		129	-22.2	(14)
D		53.4	-24.4	(14)
D		4.6	-30.5	(14)
D		404	-19.4	(14)
D		13.1	-27.9	(14)

D		3.65	-31	(14)
D		1.58	-33.1	(14)
D		2.88	-31.6	(14)
D	heptamidine	0.28	-37.4	(2)
D	hexamidine	0.43	-36.3	(2)
D	iodo-pentamidine	0.27	-37.5	(4)
D	megazol	192	-21.2	(15)
D	octamidine	0.48	-36.1	(2)
D	pentamidine	0.37	-36.7	Sigma
D	propamidine	1.92	-32.6	(11)
E	1,1'-(nonane-1,9-diyl)diguanidine 	45.4	-24.8	Biomol
E		200	-21.1	(9)
E		3.25	-31.3	(9)

E		8.75	-28.9	(9)
F		9.3	-28.7	(12)
F		0.38	-36.6	(13)
F		0.38	-36.6	(12)
F		37.7	-25.3	(3)
F	melarsen oxide	9.7	-28.6	Sanofi-Aventis
F	melarsoprol	0.54	-35.8	Sanofi-Aventis
F	thiamine	364	-19.6	Sigma
G	aminopterin	78.4	-23.4	Sigma
G	diminazene aceturate (berenil)	2.36	-32.1	Sigma
G	ethidium	5.96	-29.8	Sigma
G	isometamidium	0.21	-38.1	May & Baker

(1) Gift of Professor Gerrit-Jan Koomen, University of Amsterdam; Amsterdam, The Netherlands.
(2) Gift of Professor Alan Fairlamb, University of Dundee; Dundee, UK.
(3) Gift of Professor Katherine Radtke-Seley, University of Maryland, Baltimore Co; Baltimore, MA, USA.
(4) Gift of Dr Philip Blower, University of Kent at Canterbury; Canterbury, UK.

(5) Gift of Professor David Boykin, Georgia State University; Atlanta, GE, USA.
(6) Gift of Professor Achiel Haemers, University of Antwerp; Antwerp, Belgium.
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(13) Gift from Professor Ian Gilbert, University of Dundee, UK; see Tye et al (1998) Bioorg Med Chem Lett 8, 811-816 and Klenke et al. (2001) J. Med. Chem. 44, 3440-3352.
(14) Gift from Professor Ian Gilbert, University of Dundee, UK; see Stewart et al (2004) Antimicrob. Ag. Chemother. 48, 1733-1738 and Baliani et al (2005) J. Med. Chem. 48, 5570-5579.
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