Structure	Name	CAS #	SMILES
HO O N N N N N N N N N N N N N N N N N N	2'-O-Acetyl-3'-deoxyadenosine	96436-88-3	OC[COH]10[COOH](N2C(N=CN=C3N)=C3N= C2)[COH](OC(C)=O)C1
H ₃ CO NH ₂	2-Amino-N-(5-chloropyridin-2-yl)-5- methoxybenzamide	280773-17-3	NC1=CC=C(OC)C=C1C(NC2=NC=C{CI})C=C2}= O
HO NH ₂	9-beta-D-Arabinofuranosyladenine	58-61-7	O[COOH]1[COOH](CO)O[COOH](N2C(N=CN =C3N)=C3N=C2)[COOH]1O
HN NH H COOH	(+)-Biotin	58-85-5	O=C1N[CO](CS[COH]2CCCCC(O)=O)([H]))[CO]2([H])N1
HN NH H H COOCH ₃	(+)-Biotin methyl ester	608-16-2	O=C1N[CO](CS[COH]2CCCCC(OC)=O)([H])[C O]2([H])N1
H H CH ₃ CH ₃ CH ₃	Borane - t-Butylamine Complex	7337-45-3	[H]B([H])[H].NC(C)(C)C
Br NCH ₃	4-Bromo-12-(8-fluoro-1-oxophthalazin-2-yl)- 9-hydroxy-6-methyl-6-azatricyclo- [9.4.0.0 ^{2.7}]-pentadeca-1(15),2(7),3,11,13- pentaen-5-one	NA	FC1=CC=CC2=C1C(N(C3=C(CC(O)CC(N5C)=C4 C=C(Br)C5=O)C4=CC=C3)N=C2)=O

F O CH ₃	2-(2-(Bromomethyl)-3-(6-methoxy-2- methylpyridin-3-yl)phenyl)-8- fluorophthalazin-1(2H)-one	NA	FC1=CC=CC2=C1C(N(C3=C(CBr)C(C4=CC=C(O C)N=C4C)=CC=C3)N=C2)=O
Br COOCH ₃	(3S)-3-(4-Bromothiophen-2-yl)-3-[(2- methylpropane-2- sulfinyl)amino]butanoate	NA	BrC1=CSC([COO](CC(OC)=O)(C)NS(C(C)(C)C) =O)=C1
$\begin{array}{c c} H_3C \\ \hline \\ O \\ \hline \\ H_3C \\ \end{array} \begin{array}{c} N \\ O \\ \hline \\ CH_3 \\ \end{array} \begin{array}{c} CH_3 \\ CH_3 \\ \end{array}$	4(5)-(4-t-Butyl cyclopropyl(2,5- dimethyloxazol-4-yl)methylcarbamate	NA	CC1=NC(CN(C2CC2)C(OC(C)(C)C)=O)=C(C)O1
H ₃ C NH NH	6-t-Butyl-8-fluoro-2H-phthalazin-1-one	NA	FC1=CC(C(C)(C)C)=CC(C=NN2)=C1C2=O
H ₃ C CH ₃	6-t-Butyl-8-fluorophthalazin-1(2H)-one	NA	FC1=C2C(C=NNC2=O)=CC(C(C)(C)C)=C1
O CH ₃ CH ₃ CH ₃ CH ₃ CH ₃ CH ₃	t-Butyl-N-[(2E,4S)-4-(4-bromothiophen-2- yl)-4-methyl-6-oxo-1,3-diazepan-2- ylidene]carbamate	NA	BrC1=CSC([CO](N/C2=N/C(OC(C)(C)C)=O)(C) CC(N2C)=O)=C1
F N N CI	6-[(2-Chloranyl-5-fluoranyl-pyrimidin-4- yl)amino]-2,2-bis(fluoranyl)-4H-1,4- benzoxazin-3-one	NA	FC3=C(N=C(Cl)N=C3)NC1=CC2=C(OC(F)(F)C(N2)=O)C=C1
F O CI OAc	2-(3-(2-Chloro-6-(8-fluoro-1-oxophthalazin- 2(1H)-yl)phenyl)methyl acetate	NA	FC1=CC=CC2=C1C(N(C3=C(COC(C)=O)C(CI)= CC=C3)N=C2)=O

F O CI OH	2-(3-Chloro-2-(hydroxymethyl)phenyl)-8- fluorophthalazin-1(2H)-one	NA	FC1=CC=CC2=C1C(N(C3=C(CO)C(CI)=CC=C3) N=C2)=O
N O CH ₂ OH	6-Chloropurine Riboside	2004-06-0	O[COOH]([COH]([COH](N2C=NC3=C2N=CN= C3CI)O1)O)[COH]1CO
F O OH	2-(3-Cyclopropyl-2-(hydroxymethyl)phenyl)- 8-fluorophthalazin-1(2H)-one	NA	FC1=CC=CC2=C1C(N(C3=C(CO)C(C4CC4)=CC =C3)N=C2)=O
F O N OAG	(2-Cyclopropyl-6-(8-fluoro-1-oxophthalazin- 2(1H)-yl)phenyl)methyl acetate	NA	FC1=CC=CC2=C1C(N(C3=C(COC(C)=O)C(C4C C4)=CC=C3)N=C2)=O
HO NH2	3'-Deoxyadenosine	73-03-0	O[COOH]1C[COOH](CO)O[COH]1N2C(N=CN =C3N)=C3N=C2
OCH ₅	Dicyclohexyl(2',6'-dimethoxybiphenyl-2- yl)phosphine	657408-07-6	COC(C=CC=C4OC)=C4C1=CC=CC=C1P(C3CCC CC3)C2CCCCC2
H ₃ C CH ₃	1,2-Dihydro-2,2,4,7-tetramethylquinoline	1810-62-4	CC2=CC(C)(C)NC1=CC(C)=CC=C12
H ₃ C CH ₃	1-(3-Dimethylaminopropyl)-3- ethylcarbodiimide	25952-53-8	CCN=C=NCCCN(C)C

O CH ₃	5,5-Dimethylpyrrolidin-2-one	5165-28-6	O=C1CCC(C)(C)N1
NH ₂ H ₃ C H ₃ OH OH CH ₅ H ₅ C CH ₅ CH ₅ CH ₅ OMC	9(S)-Erythromycylamine	26116-56-3	O[CO]([COH](O)[COOH](C)[COOH](N)[COH] (C)C[CO](O)(C)[COH](OC3OC(C)CC(N(C)C)C3 O)[COOH](C)[COH](OC2OC(C)C(O)C(C)(OC) C2)[COH]1C)(C)[COOH](CC)OC1=O
F O OCH6 N N N N N N N N N N N N N N N N N N N	(2-{8-Fluoro-1-oxophthalazin-2(1H)-yl)-6-(2- methoxy-4-methylpyridin-3- yl)phenyl)methyl acetate	NA	FC1=CC=CC2=C1C(N(C3=C(COC(C)=O)C(C4=C (C)C=CN=C4OC)=CC=C3)N=C2)=O
F O N OAc	(2-(8-Fluoro-1-oxophthalazin-2(1H)-yl)-6- (pyridin-2-yl)phenyl)methyl acetate	NA	FC1=CC=CC2=C1C(N(C3=C(COC(C)=O)C(C4=C C=CC=N4)=CC=C3)N=C2)=O
F O CH ₃	(2-(8-Fluoro-1-oxophthalazin-2(1H)-yl)-6- methylphenyl)methyl acetate	NA	FC1=CC=CC2=C1C(N(C3=C(COC(C)=O)C(C)=C C=C3)N=C2)=O
F O OCH ₅	12-{8-Fluoro-1-oxophthalazin-2-yl)-5- methoxy-6-azatricyclo[9.4.0.0 ^{2,7}]pentadeca- 1(15),2(7),3,5,11,13-hexaene-9-one	NA	FC1=CC=CC2=C1C(N(C3=C(CC(CC5=C4C=CC(OC)=N5)=O)C4=CC=C3)N=C2)=O
	12-{8-Fluoro-1-oxophthalazin-2-yl)-6- azatricyclo-[9.4.0.0 ^{2,7}]-pentadeca- 1(15),2(7),3,11,13-pentaene-5,9-dione	NA	FC1=CC=CC2=C1C(N(C3=C(CC(CC(N5)=C4C=C C5=O)=O)C4=CC=C3)N=C2)=O
F O N N N N N N N N N N N N N N N N N N	12-{8-Fluoro-1-oxophthalazin-2-yl)-9- hydroxy-6-azatricyclo-[9.4.0.0 ^{2,7}]- pentadeca-1(15),2(7),3,11,13-pentaen-5- one	NA	FC1=CC=CC2=C1C(N(C3=C(CC(O)CC(N5)=C4C =CC5=O)C4=CC=C3)N=C2)=O

F O NCH ₅	12-(8-Fluoro-1-oxophthalazin-2-yl)-9- hydroxy-6-methyl-6-azatricyclo-[9.4.0.0 ^{2,7}]- pentadeca-1(15),2(7),3,11,13-pentaen-5- one	NA	FC1=CC=CC2=C1C(N(C3=C(CC(O)CC(N5C)=C4 C=CC5=O)C4=CC=C3)N=C2)=O
F O CH ₃	8-Fluoro-2-(2-(hydroxymethyl)-3-(6- methoxy-2-methylpyridin-3- yl)phenyl)phthalazin-1(2H)-one	NA	FC1=CC=CC2=C1C(N(C3=C(CO)C(C4=CC=C(O C)N=C4C)=CC=C3)N=C2)=O
F O N N OH	8-Fluoro-2-(2-(hydroxymethyl)-3-(pyridin-2- yl)phenyl)phthalazin-1(2H)-one	NA	FC1=CC=CC2=C1C(N(C3=C(CO)C(C4=CC=CC= N4)=CC=C3)N=C2)=O
F O CH ₃	8-Fluoro-2-(2-(hydroxymethyl)-3- methylphenyl)phthalazin-1(2H)-one	NA	FC1=CC=CC2=C1C(N(C3=C(CO)C(C)=CC=C3)N =C2)=O
N H ₃ C PF6-N+-CH ₃	нвти	94790-37-1	FC1=CC=CC2=C1N(O/C(N(C)C)=[N+](C)/C)N =N2.F[P-](F)(F)(F)(F)F
NH NCH _b	(7S)-2-Imino-7-methyl-7-{4-[5-{prop-1-yn-1- yl)pyridin-3-yl]thiphen-2-yl}-1,3-diazepan-5- one	NA	O=C(N3C)C[COO](NC3=N)(C)C1=CC(C2=CN= CC(C#CC)=C2)=CS1
H ₃ CH ₂ C	(Methoxycarbonylsulfamoyl)triethylammo nium Hydroxide Inner Salt	29684-56-8	O=S([N+](CC)(CC)CC)([N-]C(OC)=O)=O
N OCH3	4(5)-(4-Methoxyphenyl)-2-phenyl-1H- imidazole	NA	COC(C=C3)=CC=C3C1=CN=C(C2=CC=CC=C2) N1

H ₃ C COOCH ₃	Methyl 6-((4R,5S)-5-methyl-2- oxoimidazolidin-4-yl)hexanoate	NA	O=C1N[COOH](C)[COOH](CCCCCC(OC)=O)N 1
HN NH COOH	6-((4R,5S)-5-Methyl-2-oxoimidazolidin-4- yl)hexanoic acid	NA	O=C1N[COOH](C)[COOH](CCCCCC(O)=O)N1
H ₃ C	N-{(2,5-Dimethyloxazol-4- yl)methyl)cyclopropanamine	NA	CC1=NC(CNC2CC2)=C(C)O1
H ₃ C OCH ₃	N,N-Dimethyformamide Dimethylacetal	4637-24-5	cn(c)c(oc)oc
H ₃ C CH ₃ CH ₃ CH ₃ CH ₃ CH ₃	N,O-Bis(trimethylsilyl)acetamide	10416-59-8	c/c(o[si](c)(c)c)=n\[si](c)(c)c