

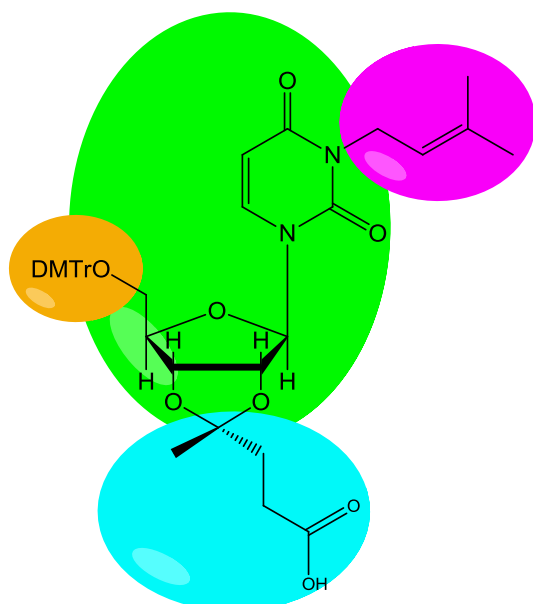
$\log P_{OW}$ -Values of Nucleosides and Nucleolipids

by: **Christine Knies and Helmut Rosemeyer***

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Nomenclature for the Coding of Pyrimidine- and Purine β -D-Ribonucleolipids

NL_1.1.1.1



Nucleolipids are abbreviated by NL. The first number (green) refers to the nucleoside.

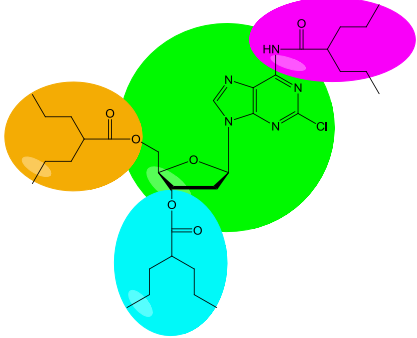
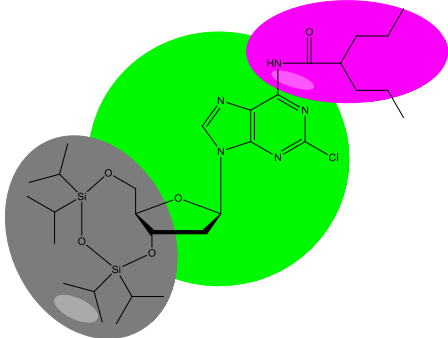
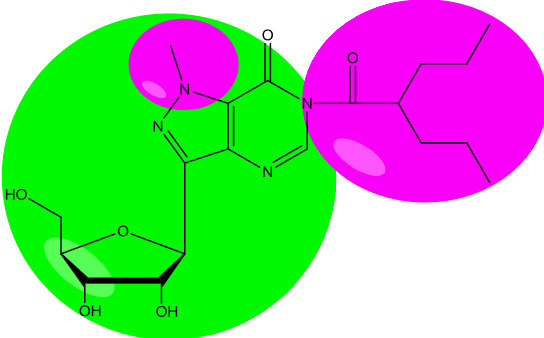
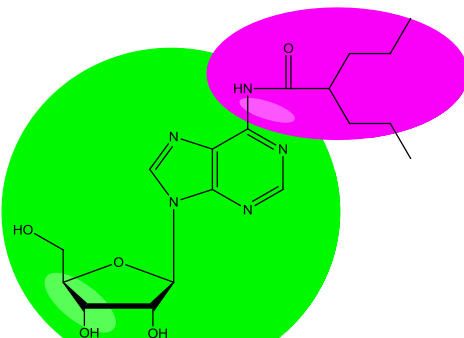
The second number (blue) refers to the moiety at the 2',3'-position at the glyconic ring; cyclic moieties are abbreviated by "cycl" before the number..

The third number (pink) refers to the lipophilic moiety at the base [N(3) for pyrimidines].

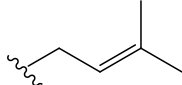
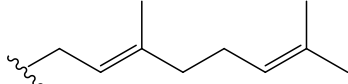
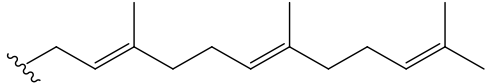

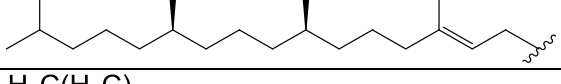
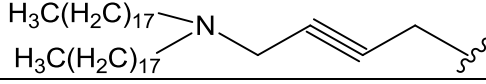
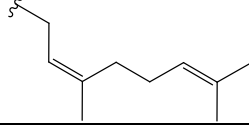
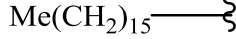
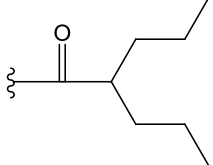
The fourth number (orange) refers to a lipophilic moiety at the 5'-O-position.

Identical residues carry the same number; "0" stands for a molecule without a residue at this position.

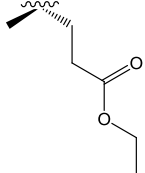
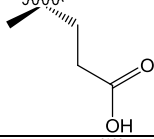
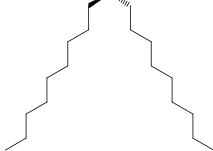
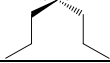
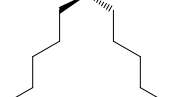
Nomenclature of the Coding for Pyrimidine- and Purine 2'-Deoxy-β-D-ribo- and ribonucleosides

2'-Deoxy-β-D-ribonucleosides	β-D-Ribonucleosides
<p>Example 1 dNL_{7.1.⁶9.3.0}</p>  <p>Example 2 dNL_{7.0.⁶9.0.1}</p> 	<p>Example 1 NL_{9.0.¹4⁶9.0}</p>  <p>Example 2 NL_{6.0.⁶9.0}</p> 
<p>2'-Deoxy-β-D-Nucleolipids are abbreviated by dNL.</p> <p>The first number (green) refers to the nucleoside.</p> <p>The second number (blue) refers to the moiety at the 3'-position at the glyconic ring.</p> <p>The third number (pink) refers to the lipophilic moiety at the base.</p> <p>The fourth number (orange) refers to a lipophilic moiety at the 5'-O-position.</p> <p>2'-Deoxy-Nucleolipids have an additional fifth number (grey), which refers to the moiety at the 3',5'-position at the glyconic ring. "0" stands for a molecule without residue at this position.</p>	<p>The third number (pink) refers to the lipophilic moiety at the base. The exponent refers to the position at the base.</p> <p>¹X or ⁶X for N-Nucleosides/-lipids and additionally ⁷X for C-Nucleosides/-lipids.</p> <p>In case of C-nucleosides a double lipophilisation might occur; in this case the corresponding numbers (pink) are written consecutively (see Example).</p> <p>NL_{9.0.¹4⁶9.0}</p>

Lipophilizing moieties of the base

Coding	Chemical structure
1 (Isopentenyl-)	
2 (Geranyl-)	
3 (Farnesyl-)	
4 (Methyl-)	
5 (Phytyl-)	
6 (4-(Dioctadecylamino)but-2-yn-1-yl)	$\text{H}_3\text{C}(\text{H}_2\text{C})_{17}$ $\text{H}_3\text{C}(\text{H}_2\text{C})_{17}$ 
7 (Neryl-)	
8 (Hexadecyl-)	$\text{Me}(\text{CH}_2)_{15}$ 
9 (Valproyl-)	

Lipophilizing moieties at the O-2'-3'-position of the glycon

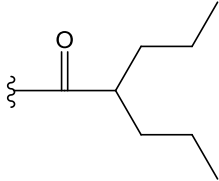
Coding	Chemical structure
1 (Ethyllevulinate)	
2 (Levulinic acid)	
3 (Nonadecyliden-)	
4 (Heptanyliden-)	
5 (Undecanyliden-)	

6	(4-Oxopentyl-4-methylbenzoatyl-)	
Cycl1	(Cyclopentanylidene-)	
Cycl2	(Cyclohexanylidene-)	
Cycl3	(Cycloheptanylidene-)	
Cycl4	(Cyclooctanylidene-)	
Cycl5	(Cyclodecanylidene-)	
Cycl6	(Cyclododecanylidene-)	
Cycl7	(Cyclopentadecanylidene-)	
Cycl8	(Adamantylden-)	

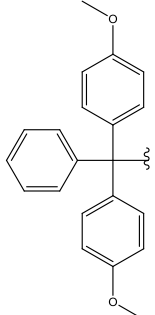
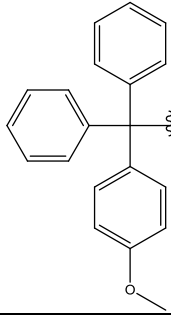
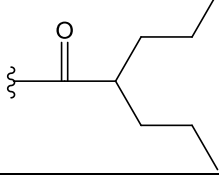
Lipophilizing moieties at the O-3'-5'-position of the glycon

Coding	Chemical structure
1 Markiewicz-Silyl-Clamb	

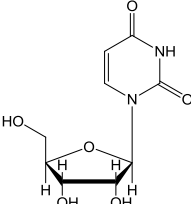
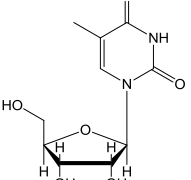
Lipophilizing moieties at the O-3'-position of the glycon

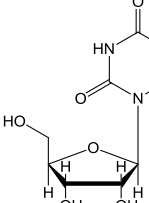
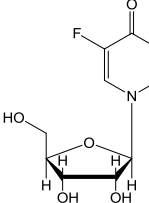
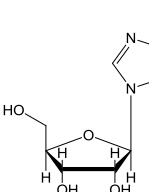
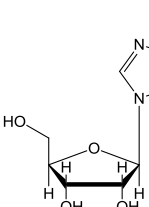
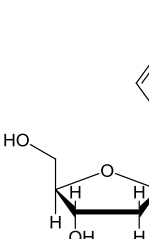
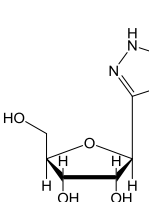
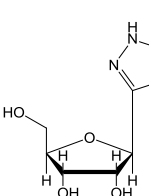
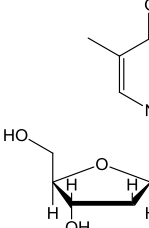
Coding	Chemical structure
1 (Valproyl-)	

Lipophilizing moieties at the O-5'-position of the glycon

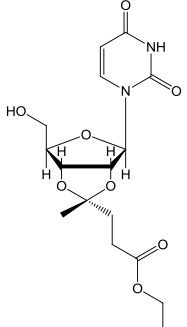
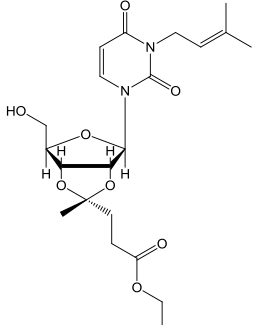
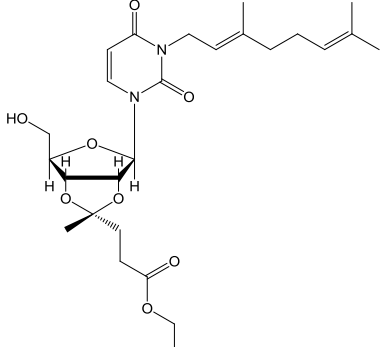
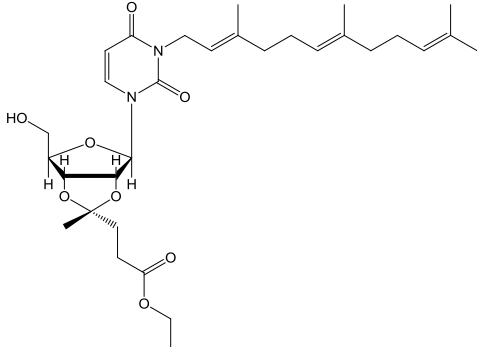
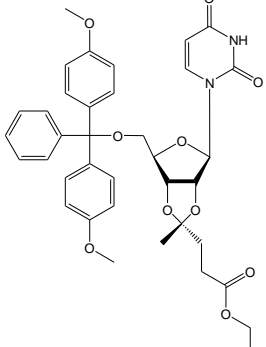
Coding	Chemical structure
1 (Dimethoxytrityl-)	
2 (Monomethoxytrityl-)	
3 (Valproyl-)	

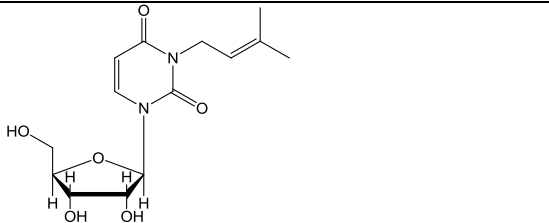
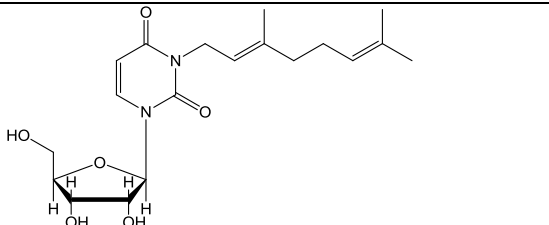
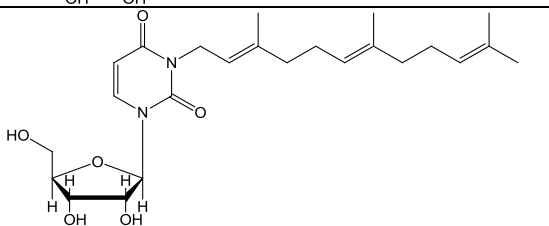
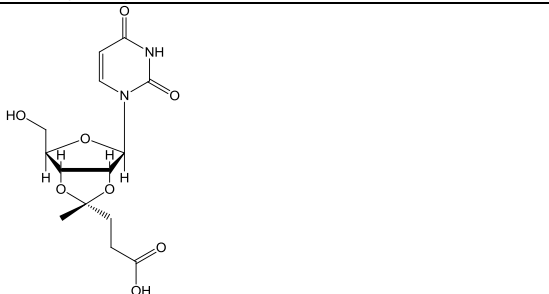
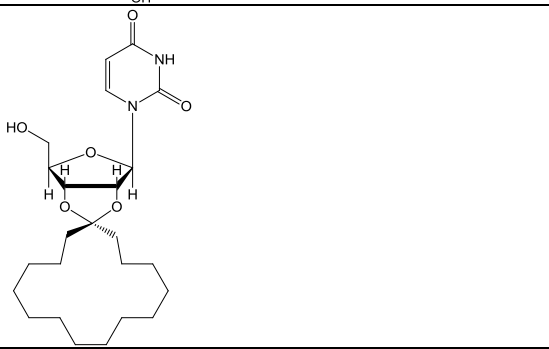
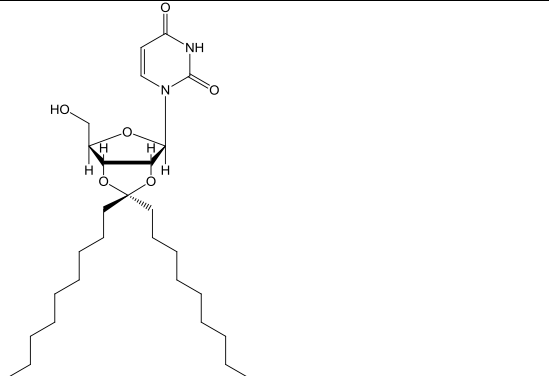
Nucleosides

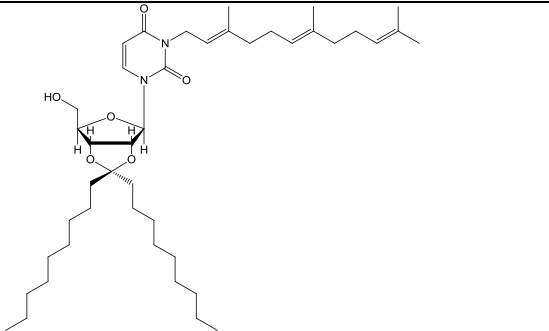
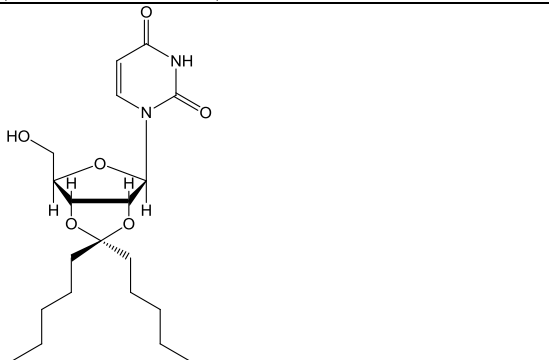
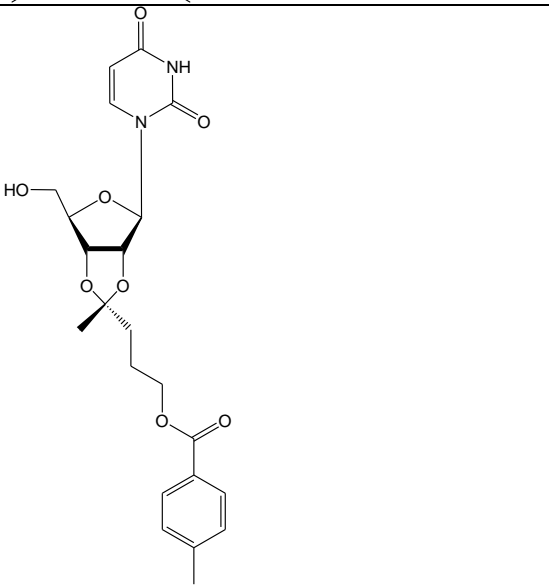
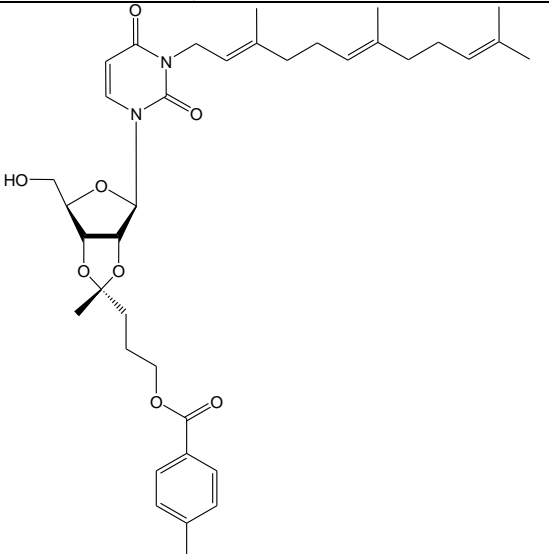
Coding	Chemical structure	logPow
NS_1.0.0.0 (Uridine)		- 1.9 unit ± 0.38
NS_2.0.0.0 (5-Methyluridine)		- 1.19 unit ± 0.38

<p>NS_3.0.0.0 (6-Azauridine)</p>		<p>- 2.14 unit ± 0.74</p>
<p>NS_4.0.0.0 (5-Fluorouridine)</p>		<p>- 1.3 unit ± 0.38</p>
<p>NS_5.0.0.0 (Adenosine)</p>		<p>- 1.05 unit ± 0.38</p>
<p>NS_6.0.0.0 (Inosine)</p>		<p>- 1.73 unit ± 0.38</p>
<p>dNS_7.0.0.0 (Cladribine)</p>		<p>- 0.23 unit ± 0.38</p>
<p>NS_8.0.0.0 (Formycin A)</p>		<p>- 1.25 unit ± 0.74</p>
<p>NS_9.0.0.0 (Formycin B)</p>		<p>- 1.40 unit ± 0.38</p>
<p>dNS_10.0.0.0 (Thymidine)</p>		<p>- 0.96 unit ± 0.38</p>

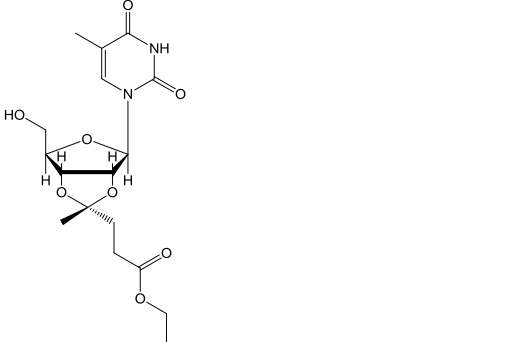
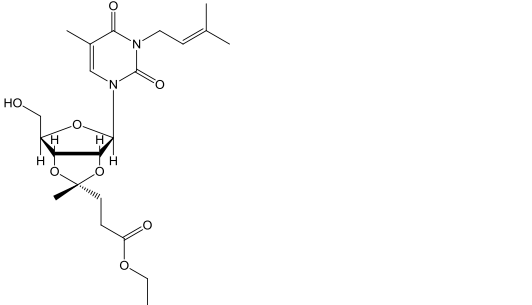
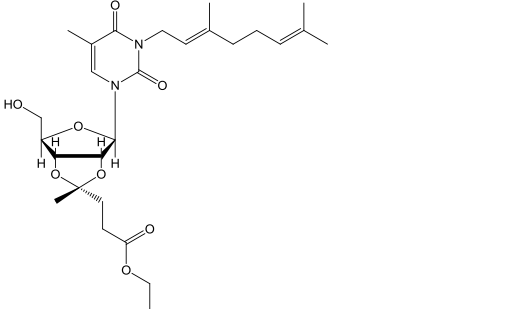
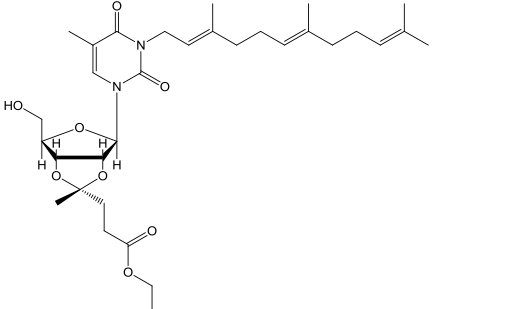
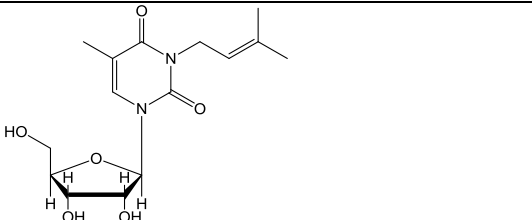
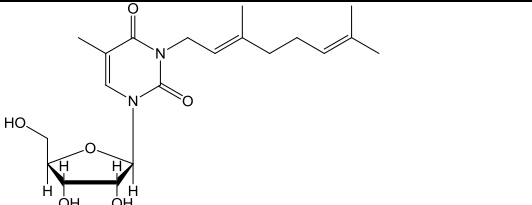
Uridine-Nucleolipides

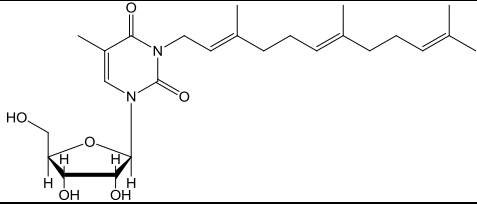
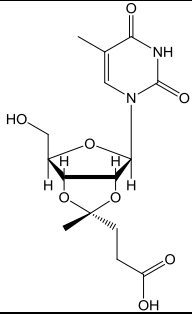
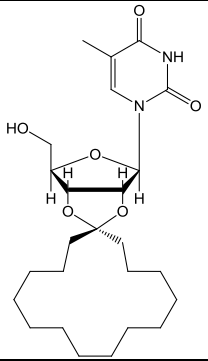
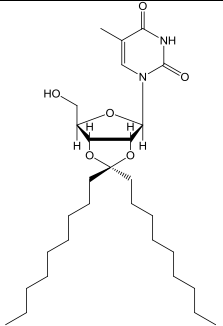
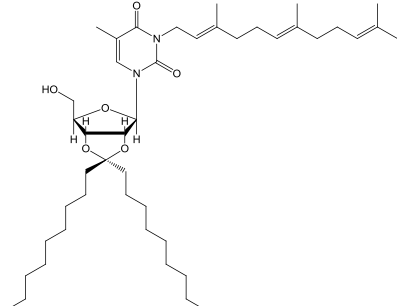
Coding	Chemical Structure	logPow
NL_1.1.0.0		- 0.14 unit ± 0.74
NL_1.1.1.0		0.42 unit ± 0.74
NL_1.1.2.0		2.15 unit ± 0.74
NL_1.1.3.0		3.74 unit ± 0.74
NL_1.1.0.1		3.68 unit ± 0.74

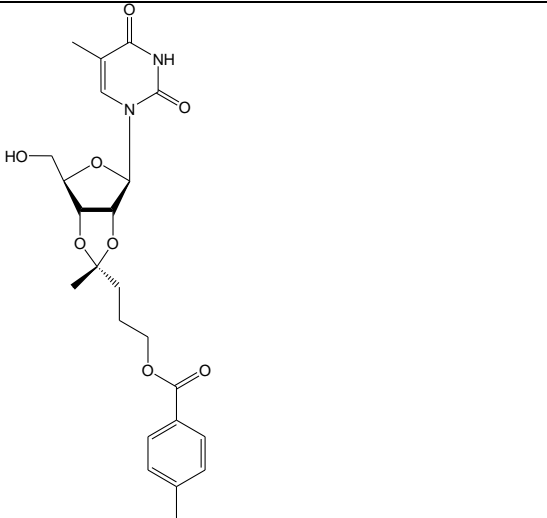
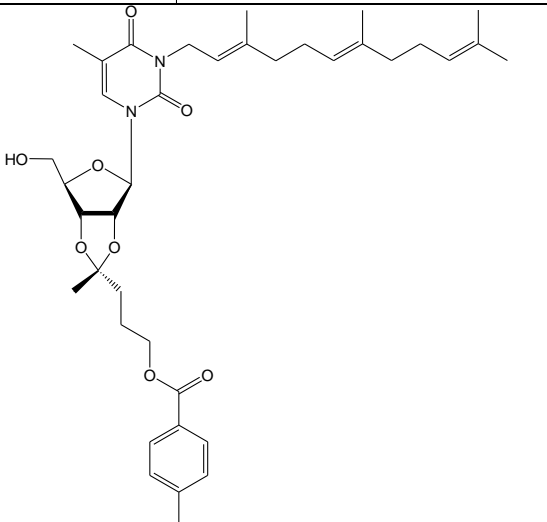
NL_1.0.1.0		- 1.04 unit \pm 0.74
NL_1.0.2.0		0.61 unit \pm 0.74
NL_1.0.3.0		2.0 unit \pm 0.74
NL_1.2.0.0		- 0.71 unit \pm 0.74
NL_1.cycl7.0.0		3.7 unit \pm 0.74
NL_1.3.0.0		5.12 unit \pm 0.74

NL_1.3.3.0		8.48 unit \pm 0.74
NL_1.5.0.0		2.27 unit \pm 0.74
NL_1.6.0.0		1.5 unit \pm 0.74
NL_1.6.3.0		4.18 unit \pm 0.74

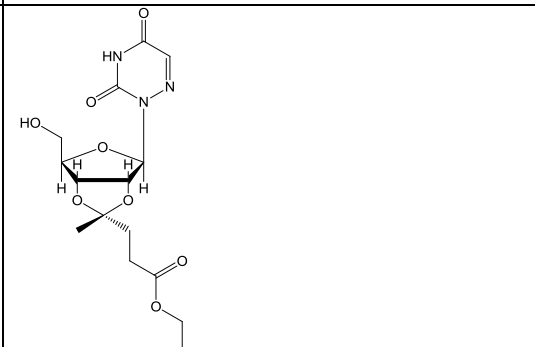
5-Methyluridine-Nucleolipides

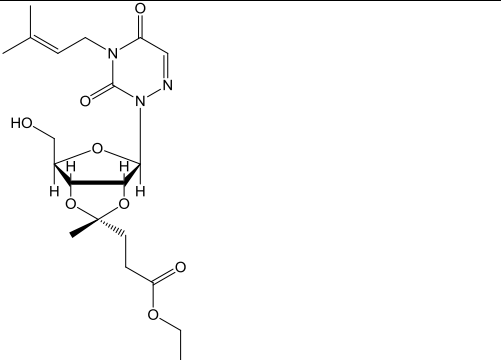
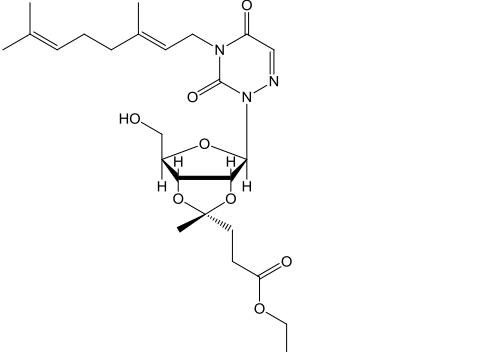
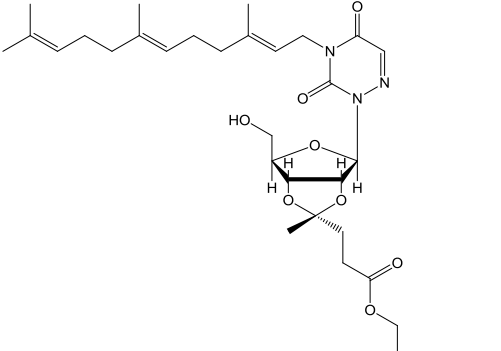
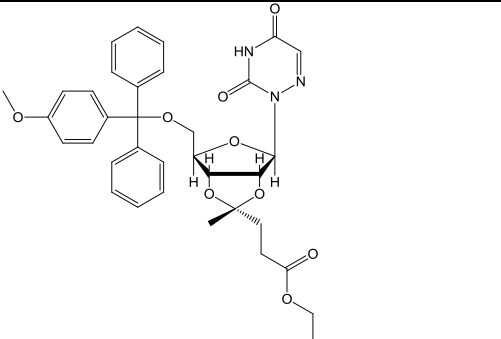
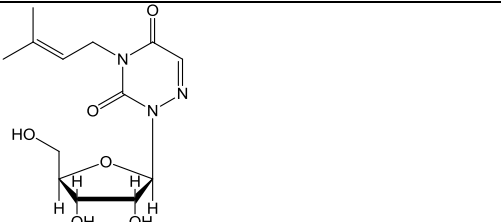
Coding	Chemical structure	logPow
NL_2.1.0.0		0.19 unit ± 0.42
NL_2.1.1.0		0.68 unit ± 0.74
NL_2.1.2.0		2.75 unit ± 0.74
NL_2.1.3.0		4.18 unit ± 0.74
NL_2.0.1.0		- 0.75 unit ± 0.74
NL_2.0.2.0		0.96 unit ± 0.74

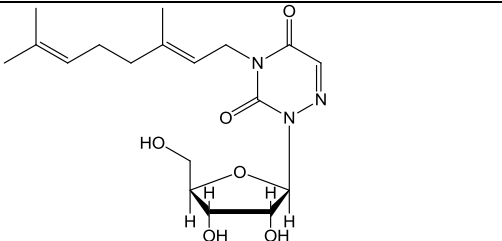
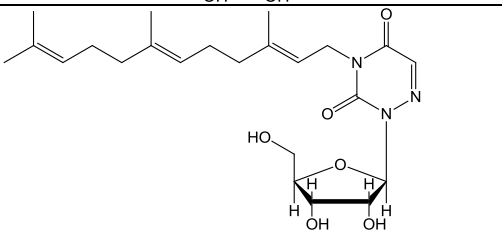
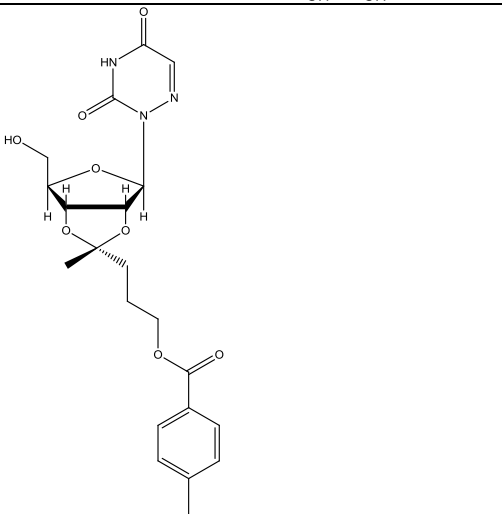
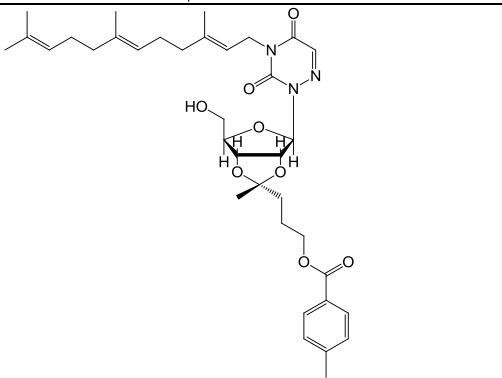
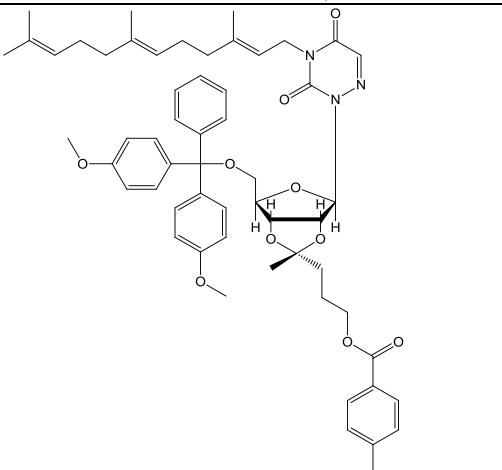
NL_2.0.3.0		2.37 unit \pm 0.74
NL_2.2.0.0		- 0.32 unit \pm 0.74
NL_2.cycl7.0.0		3.99 unit \pm 0.74
NL_2.3.0.0		5.33 unit \pm 0.74
NL_2.3.3.0		8.6 unit \pm 0.74

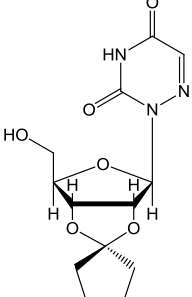
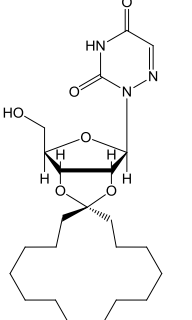
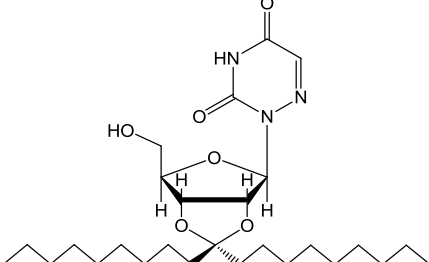
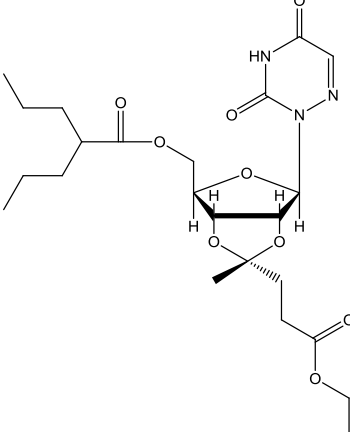
NL_2.6.0.0		1.39 unit \pm 0.38
NL_2.6.3.0		4.83 unit \pm 0.74

6-Azauridine-Nucleolipides

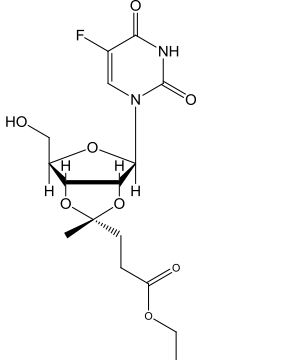
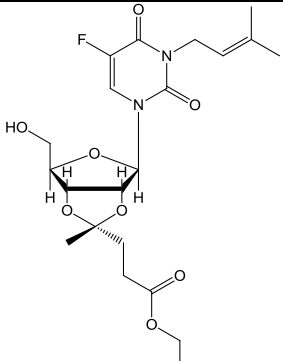
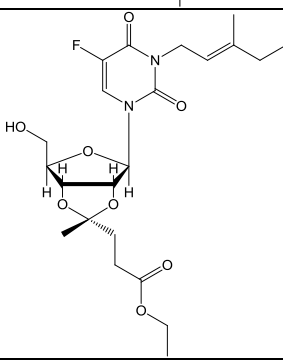
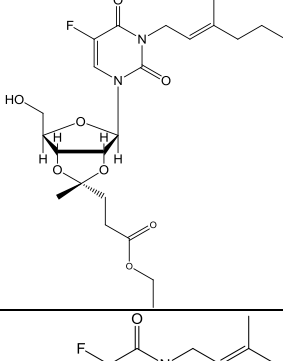
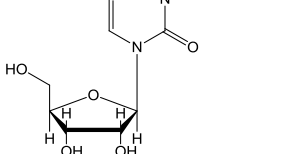
Coding	Chemical structure	logPow
NL_3.1.0.0		0.03 unit \pm 0.74

NL_3.1.1.0		0.34 unit \pm 0.74
NL_3.1.2.0		1.69 unit \pm 0.74
NL_3.1.3.0		3.72 unit \pm 0.74
NL_3.1.0.2		3.77 unit \pm 0.74
NL_3.0.1.0		- 0.74 unit \pm 0.74

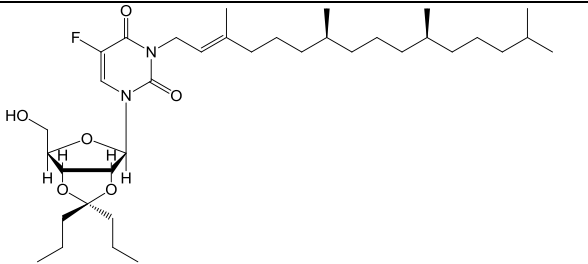
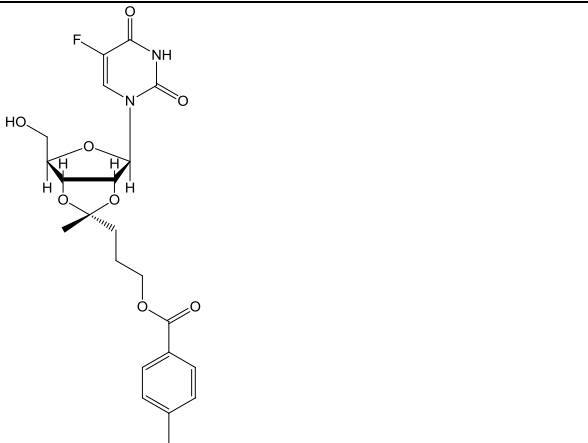
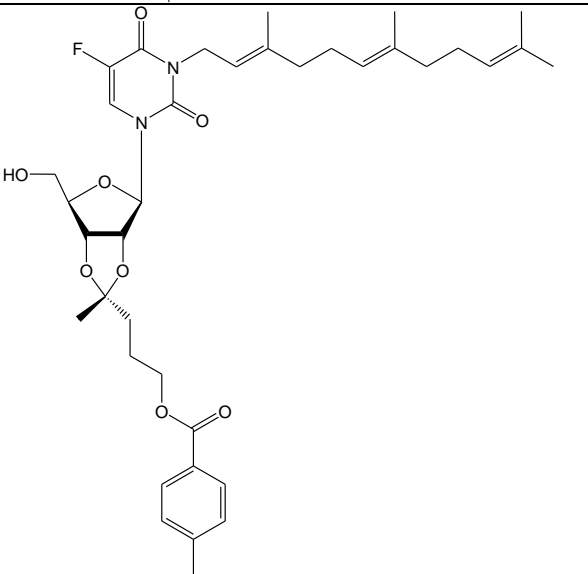
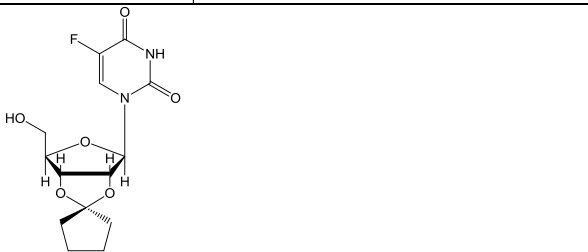
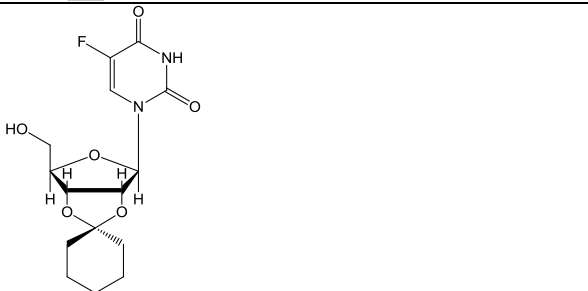
NL_3.0.2.0		0.48 unit \pm 0.74
NL_3.0.3.0		1.9 unit \pm 0.74
NL_3.6.0.0		1.25 unit \pm 0.74
NL_3.6.0.1		4.64 unit \pm 0.74
NL_3.6.3.1		7.40 unit \pm 0.74

NL_3.cycl1.0.0		0.12 unit ± 0.74
NL_3.cycl7.0.0		3.86 unit ± 0.74
NL_3.3.0.0		5.43 unit ± 0.74
NL_3.1.0.3		2.51 unit ± 0.74

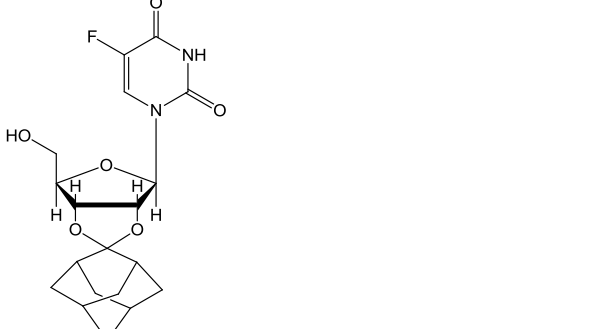
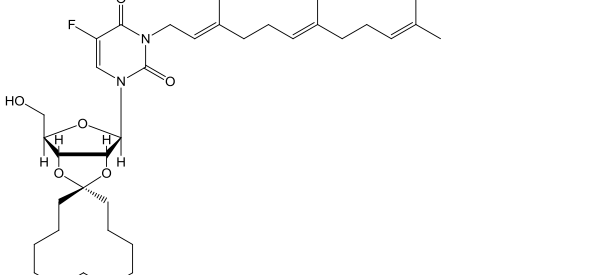
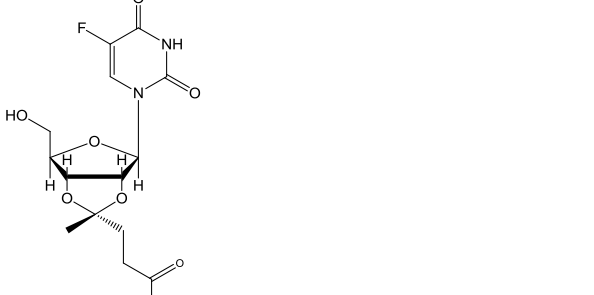
5-Fluorouridine-Nucleolipides

Coding	Chemical structure	logPow
NL_4.1.0.0	 <p>The structure shows a 5-fluorouracil base attached to a ribose sugar at the N1 position. The sugar has a methyl group at the 2' position and is esterified at the 1' position with a 2-ethylhexanoate group.</p>	0.31 unit \pm 0.74
NL_4.1.1.0	 <p>The structure is similar to NL_4.1.0.0, but the methyl group at the 2' position is replaced by an isopentenyl group.</p>	1.02 unit \pm 0.74
NL_4.1.2.0	 <p>The structure is similar to NL_4.1.1.0, but the isopentenyl group at the 2' position is replaced by a geranyl group.</p>	2.37 unit \pm 0.74
NL_4.1.3.0	 <p>The structure is similar to NL_4.1.2.0, but the geranyl group at the 2' position is replaced by a farnesyl group.</p>	4.20 unit \pm 0.74
NL_4.0.1.0	 <p>The structure is similar to NL_4.1.1.0, but the sugar has hydroxyl groups at the 3' and 4' positions instead of a methyl group at the 2' position.</p>	- 0.88 unit \pm 0.74

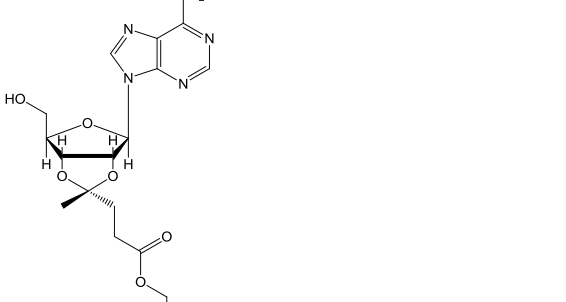
NL_4.0.2.0		0.91 unit \pm 0.74
NL_4.0.3.0		2.16 unit \pm 0.74
NL_4.3.0.0		5.34 unit \pm 0.74
NL_4.4.0.0		1.5 unit \pm 0.74
NL_4.4.7.0		3.52 unit \pm 0.74
NL_4.4.3.0		4.95 unit \pm 0.74

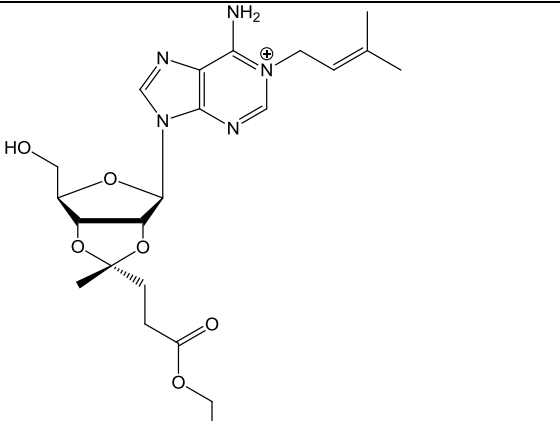
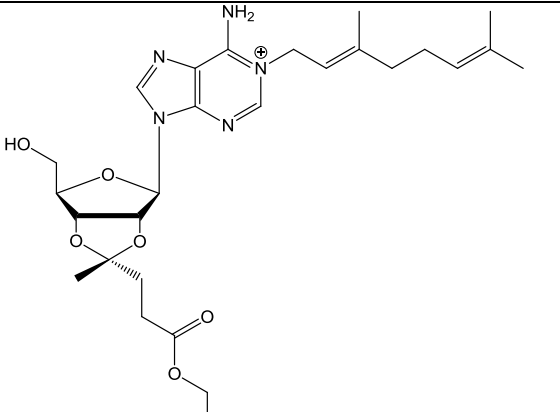
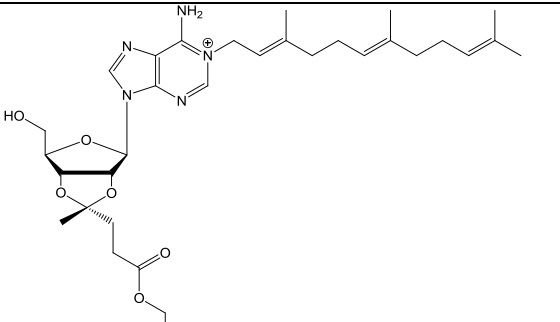
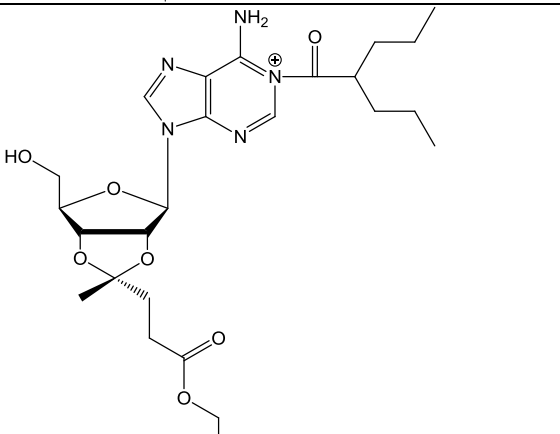
NL_4.4.5.0		6.43 unit \pm 0.74
NL_4.6.0.0		1.89 unit \pm 0.74
NL_4.6.3.0		4.77 unit \pm 0.74
NL_4.cycl1.0.0		0.26 unit \pm 0.74
NL_4.cycl2.0.0		0.67 unit \pm 0.74

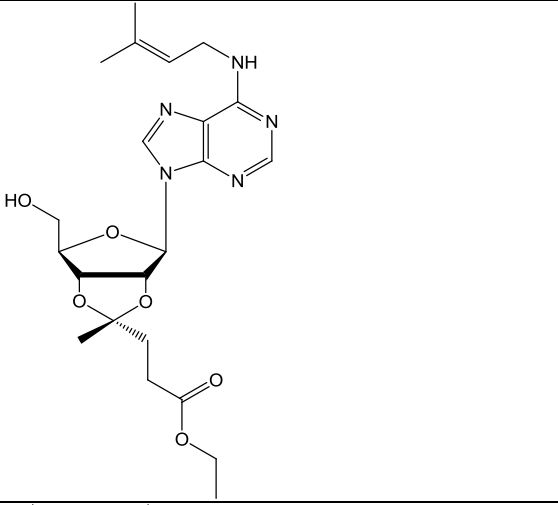
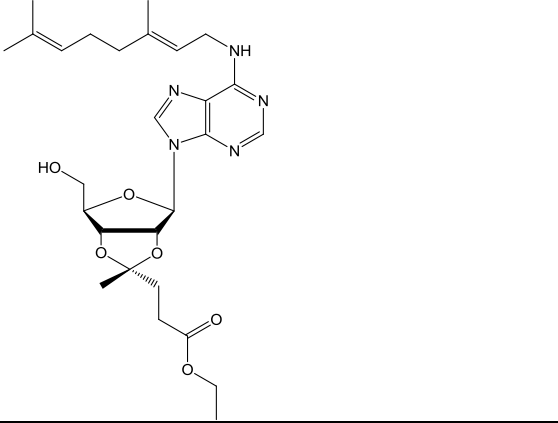
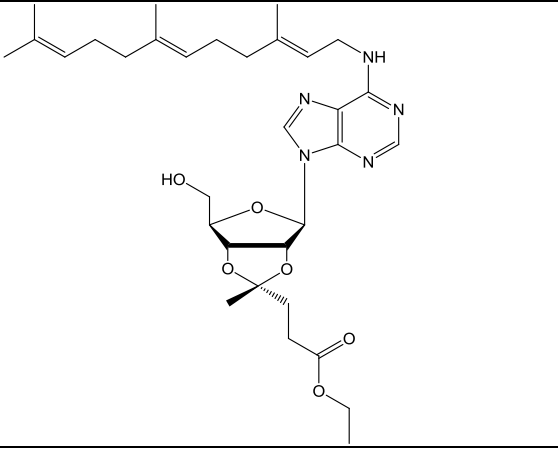
NL_4.cycl3.0.0		1.06 unit \pm 0.74
NL_4.cycl4.0.0		1.6 unit \pm 0.74
NL_4.cycl5.0.0		2.63 unit \pm 0.74
NL_4.cycl6.0.0		3.7 unit \pm 0.74
NL_4.cycl7.0.0		3.99 unit \pm 0.74

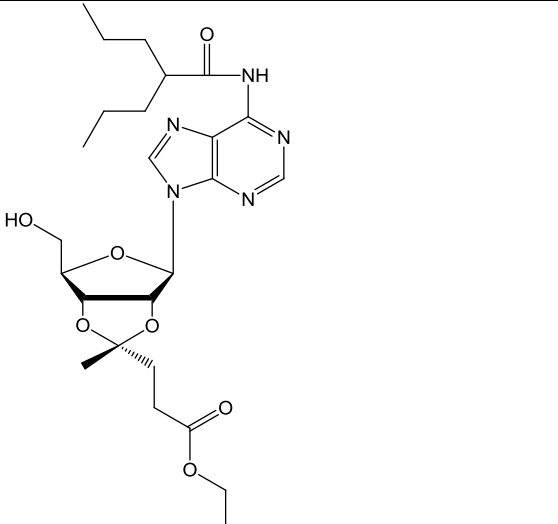
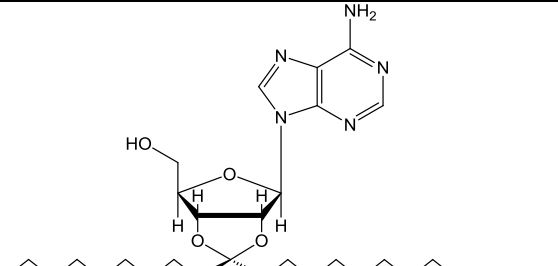
NL_4.cycl8.0.0		1.77 unit \pm 0.74
NL_4.cycl6.3.0		6.39 unit \pm 0.74
NL_4.2.0.0		- 0.61 unit \pm 0.74

Adenosine-Nucleolipides

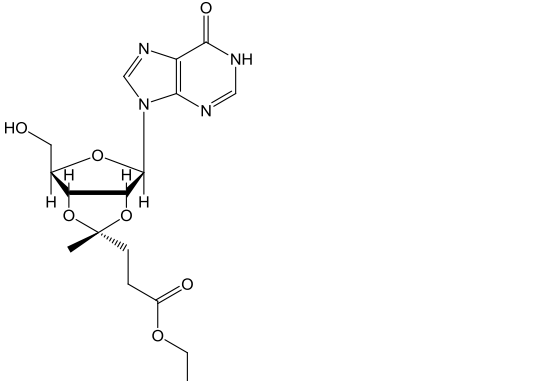
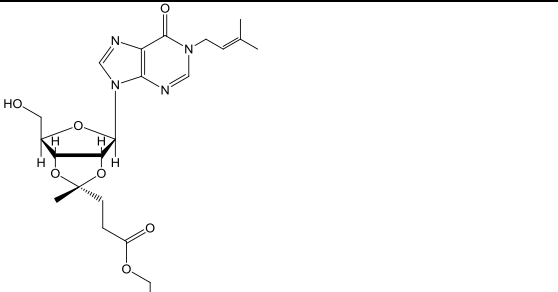
Coding	Chemical structure	logPow
NL_5.1.0.0		0.87 unit \pm 0.74

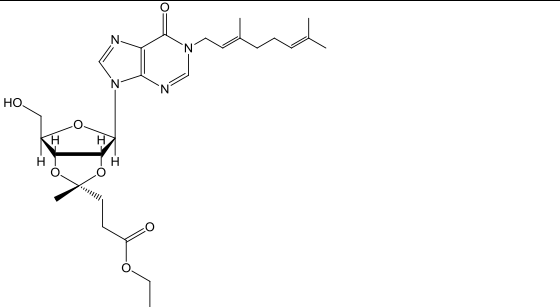
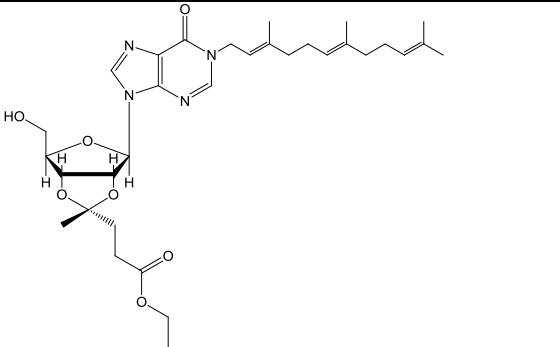
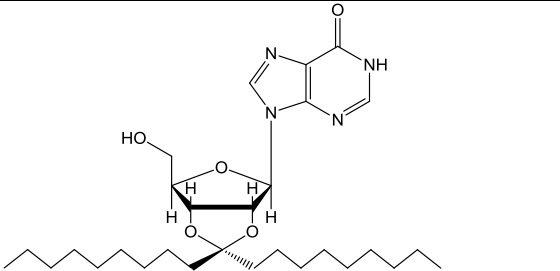
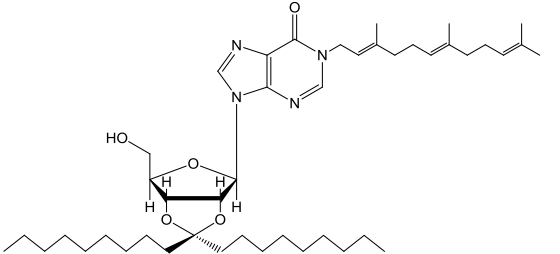
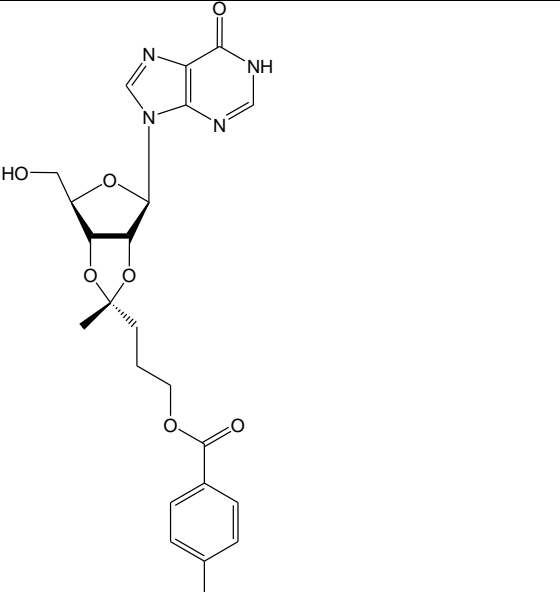
NL_5.1. ¹ 1.0		-2.25 unit ± 0.74
NL_5.1. ¹ 2.0		-1.76 unit ± 0.74
NL_5.1. ¹ 3.0		-0.79 unit ± 0.74
NL_5.1. ¹ 9.0		-0.97 unit ± 0.74

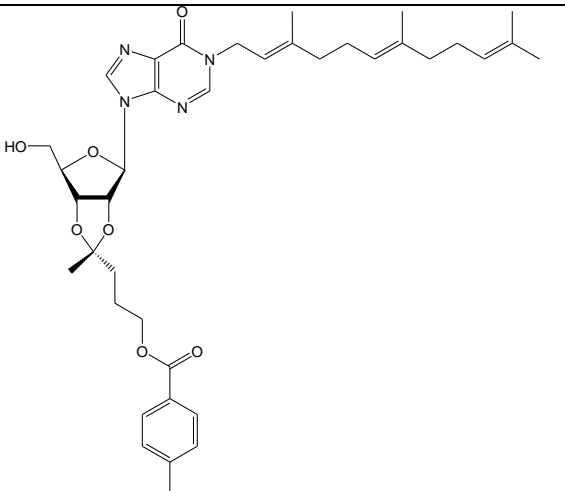
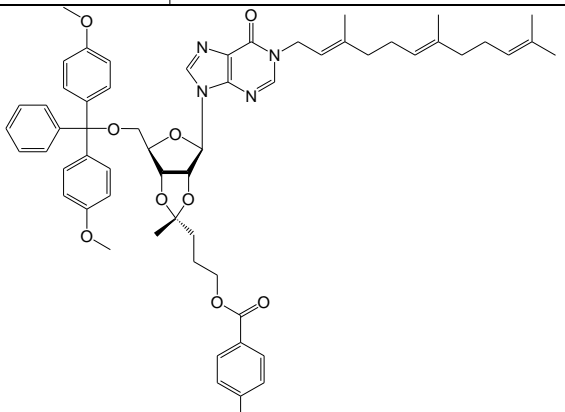
NL_5.1. ⁶ 1.0		2.78 unit ± 0.74
NL_5.1. ⁶ 2.0		3.62 unit ± 0.74
NL_5.1. ⁶ 3.0		4.13 unit ± 0.74

NL_5.1. ⁶ 9.0		3.72 unit ± 0.74
NL_5.3.0.0		5.13 unit ± 0.74

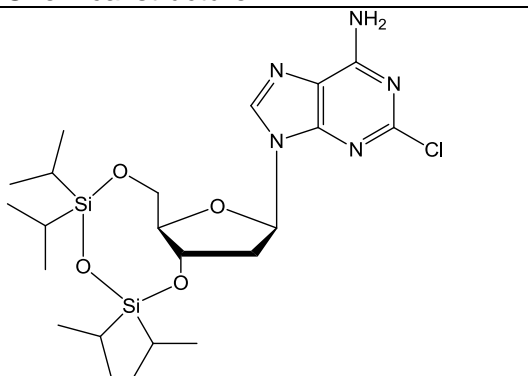
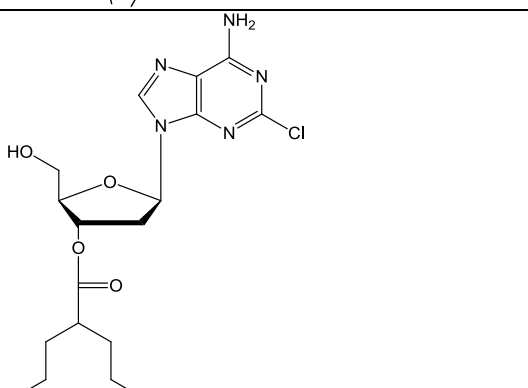
Inosine-Nucleolipides

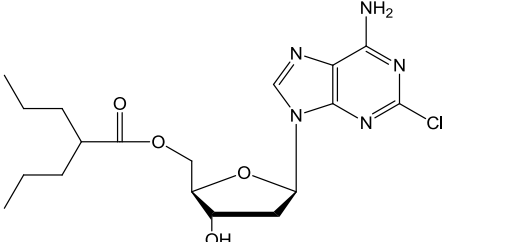
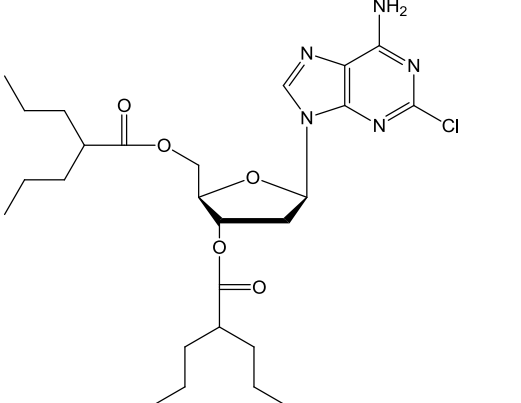
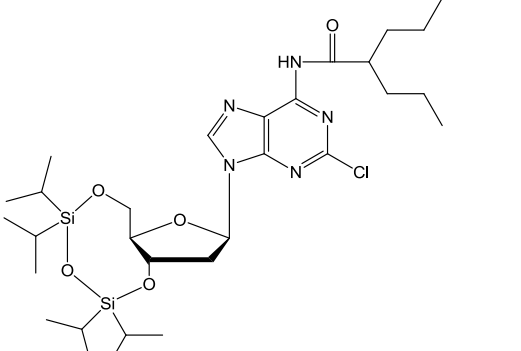
Coding	Chemical structure	logPow
NL_6.1.0.0		- 0.08 unit ± 0.74
NL_6.1. ¹ 1.0		0.72 unit ± 0.74

NL_6.1. ¹ 2.0		2.35 unit ± 0.74
NL_6.1. ¹ 3.0		3.5 unit ± 0.74
NL_6.3.0.0		5.3 unit ± 0.74
NL_6.3. ¹ 3.0		7.73 unit ± 0.74
NL_6.6.0.0		0.97 unit ± 0.74

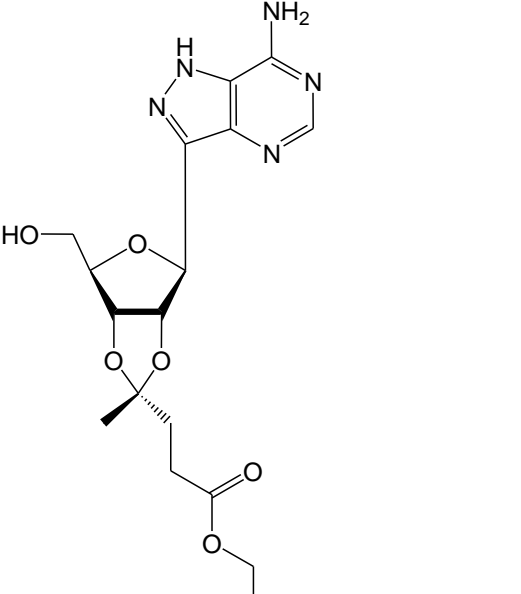
NL_6.6. ¹ 3.0		4.48 unit ± 0.74
NL_6.6. ¹ 3.1		5.91 unit ± 0.74

Cladribin-Nucleolipides

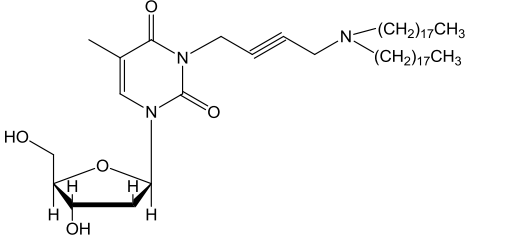
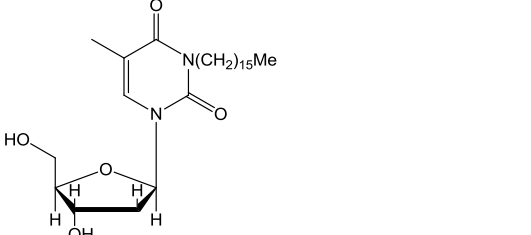
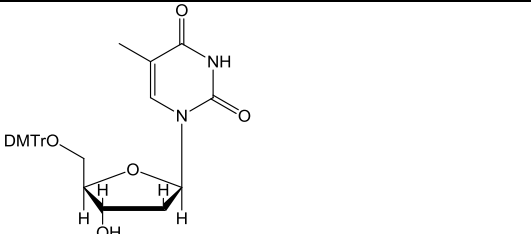
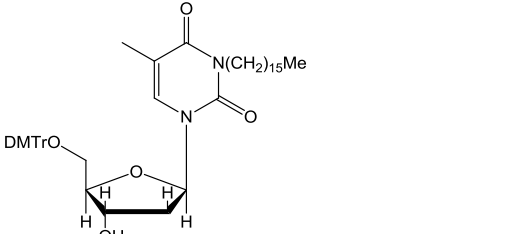
Coding	Chemical structure	logPow
dNL_7.0.0.0.1		3.09 unit ± 0.74
dNL_7.1.0.0.0		3.63 unit ± 0.38

dNL_7.0.0.3.0		3.61 unit ± 0.38
dNL_7.1.0.3.0		4.59 unit ± 0.74
dNL_7.0. ⁶ 9.0.1		5.56 unit ± 0.74

Formycin A-Nucleolipides

Coding	Chemical structure	logPow
NL_8.1.0.0		0.18 unit ± 0.74

Thymidine-Nucleolipides

Coding	Chemical structure	logPow
dNL_10.0.6.0.0		10.02 unit ± 0.74
dNL_10.0.8.0.0		4.79 unit ± 0.74
dNL_10.0.0.1.0		2.91 unit ± 0.74
dNL_10.0.8.1.0		6.91 unit ± 0.74

logP_{ow} Values were calculated using the <http://eadmet.com/de/physprop.php> site with ePhysChem that contains ALOGPS v. 3.01 for logP prediction.

I. V. Tetko, G. I. Poda, C. Ostermann, R. Mannhold, *Chem. Biodiversity* **2009**, 6, 1837.

R. Mannhold, G. I. Poda, C. Ostermann, I. V. Tetko, *Journal of Pharmaceutical Science* **2008**, 3, 861.