Quantum chemical profiling of the electronic structure and hydrolytic stability of modified ribonucleosides

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Table S1. Calculated HOMO−LUMO Energy Gap (eV) for Me-pNp-Me Ribonucleotides. Nucleosides are grouped by canonical base and ordered by decreasing $E_{HOMO-LUMO}$. Yellow highlight: N contains sulfur; orange highlight: N contains selenium. Boxed pyrimidine nucleosides have ≥2 non-hydrogen atoms attached to the 5 position.

Adenosine		Guanosine		Uridine		Cytidine	
Name	$E_{HOMO-LUMO}$	Name	$E_{HOMO-LUMO}$	Name	$E_{HOMO-LUMO}$	Name	$E_{HOMO-LUMO}$
9A	7.84	None4	7.63	58U	8.97	cytidine	7.87
09A	7.83	guanosine	7.56	8U	8.97	0C	7.86
19A	7.78	0G	7.55	308U	8.86	4C	7.79
019A	7.78	1G	7.54	3U	7.93	04C	7.78
2A	7.66	00G	7.54	03U	7.92	51C	7.77
28A	7.65	01G	7.50	0U	7.91	None3	7.77
0A	7.60	2G	7.45	30U	7.90	3C	7.73
adenosine	7.60	02G	7.42	uridine	7.89	5C	7.62
8A	7.59	22G	7.35	39U	7.83	05C	7.61
69A	7.59	022G	7.33	522U	7.83	50C	7.60
00A	7.58	7G	7.31	531U	7.81	44C	7.58
68A	7.55	101G	7.25	0522U	7.80	044C	7.57
65A	7.49	027G	7.24	9U	7.80	71C	7.52
2165A	7.48	102G	7.24	309U	7.80	071C	7.52
62A	7.47	27G	7.22	051U	7.78	21C	7.48
63A	7.47	105G	7.21	54U	7.77	20C	7.47
06A	7.44	10G	7.19	510U	7.77	42C	7.39
6A	7.44	104G	7.18	51U	7.76	042C	7.38
662A	7.42	106G	7.12	09U	7.76	None2	7.12
60A	7.41	227G	7.06	520U	7.75	2C	6.97
64A	7.41	4G	6.97	053U	7.71		
61A	7.40	100G	6.96	0521U	7.70		
67A	7.39	34G	6.90	511U	7.70		
01Am	7.28	42G	6.81	521U	7.69		
01A	7.28	47G	6.78	583U	7.68		
066A	7.24	34832G	6.73	53U	7.67		
66A	7.23	342G	6.72	52U	7.67		
None1	7.12	3480G	6.71	5U	7.66		
621A	7.09	348G	6.71	05U	7.64		
2160A	7.07	34830G	6.70	1309U	7.63		
2161A	7.07	347G	6.70	19U	7.63		
2162A	6.99	3470G	6.69	501U	7.60		
2163A	6.99	3483G	6.68	0503U	7.60		
2164A	6.62	103G	6.56	502U	7.56		
				503U	7.56		
				0583U	7.56		
				55U	7.55		
				50U	7.26		

21U	7.14
21511U	7.13
21510U	7.13
2U	7.10
02U	7.09
25U	7.04
2.510U	7.04
2.511U	7.03
2540U	7.03
251U	7.03
253U	7.03
2583U	7.03
2521U	7.02
2151U	6.99
254U	6.98
20U	6.72
20510U	6.70
20.511U	6.67
None5	6.64
2051U	6.59
74U	6.45

Table S2. Calculated WBI of the Glycosidic Bond in Me-pNp-Me Ribonucleotides. Nucleosides are grouped by canonical base and ordered by decreasing $E_{HOMO-LUMO}$. Yellow highlight: N contains sulfur; orange highlight: N contains selenium. Boxed pyrimidine nucleosides have ≥2 non-hydrogen atoms attached to the 5 position.

Adenosine		Guanosine		Uridine		Cytidine	
Name	WBI	Name	WBI	Name	WBI	Name	WBI
621A	0.9380	1G	0.9381	39U	0.9897	None2	0.9542
2A	0.9377	105G	0.9377	9U	0.9896	21C	0.9111
28A	0.9324	2G	0.9368	09U	0.9896	20C	0.9105
662A	0.9324	00G	0.9364	309U	0.9895	4C	0.8946
01Am	0.9314	101G	0.9362	19U	0.9889	04C	0.8945
8A	0.9313	guanosine	0.9358	1309U	0.9883	044C	0.8939
19A	0.9299	0G	0.9315	58U	0.9491	44C	0.8937
2161A	0.9292	10G	0.9281	21U	0.9456	5C	0.8932
61A	0.9283	None4	0.9258	2151U	0.9419	cytidine	0.8925
6A	0.9282	102G	0.9258	21510U	0.9390	50C	0.8905
66A	0.9279	22G	0.9223	21511U	0.9383	3C	0.8902
60A	0.9279	02G	0.9208	8U	0.9260	51C	0.8902
01A	0.9274	022G	0.9192	308U	0.9237	05C	0.8844
066A	0.9258	01G	0.9186	0U	0.9096	2C	0.8834
06A	0.9253	34G	0.9177	0521U	0.9088	0C	0.8832
68A	0.9231	104G	0.9175	0503U	0.9047	None3	0.8820
019A	0.9231	100G	0.9146	503U	0.9028	042C	0.8764
None1	0.9225	103G	0.9127	583U	0.8943	42C	0.8762
0A	0.9202	106G	0.9028	5U	0.8840	071C	0.8746
2160A	0.9198	348G	0.8919	50U	0.8825	71C	0.8736
2165A	0.9164	342G	0.8916	uridine	0.8821		
64A	0.9146	3483G	0.8915	3U	0.8819		
63A	0.9144	347G	0.8913	30U	0.8818		
67A	0.9142	34830G	0.8910	053U	0.8818		
65A	0.9141	34832G	0.8903	502U	0.8809		
62A	0.9141	3480G	0.8903	501U	0.8802		
2162A	0.9134	3470G	0.8903	0583U	0.8792		
2163A	0.9132	47G	0.8858	51U	0.8790		
9A	0.9116	42G	0.8853	74U	0.8790		
09A	0.9110	4G	0.8844	520U	0.8780		
69A	0.9100	7G	0.8764	53U	0.8773		
2164A	0.9075	27G	0.8723	05U	0.8768		
adenosine	0.9001	227G	0.8707	511U	0.8762		
00A	0.8899	027G	0.8679	25U	0.8747		
				02U	0.8746		
				2U	0.8744		
				2540U	0.8738		

03U	0.8722
521U	0.8716
2.511U	0.8713
2.510U	0.8710
0522U	0.8705
52U	0.8705
510U	0.8695
522U	0.8694
54U	0.8688
251U	0.8678
051U	0.8674
531U	0.8664
253U	0.8656
20U	0.8651
2583U	0.8650
2521U	0.8649
None5	0.8635
254U	0.8629
20.511U	0.8608
55U	0.8599
20510U	0.8515
2051U	0.8495