Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

SUPPLYMENTARY INFORMATION

Tolerance of N^2-heteroaryl modifications on guanine bases in a DNA G-quadruplex

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Contents

Table S1. Calculated ΔE_{conf} energies.

	ΔE_{conf} [kcal/mol]	T_m [°C]
G^{Py}	-4.0	54.0
$G^{2\text{-}Pym}$	-9.9	44.5
G^{Pyra}	-3.5	63.2
$G^{4\text{-}Pym}$	-3.5	62.4
G^{Pyda}	-2.6	66.2

Energies were calculated from the structure optimized using Gaussian09, *in vacuo* at ωB97X-D/6-31+Gd level. The optimized structures were confirmed not to have imaginary frequencies. The ΔE_{conf} energies were calculated from the subtraction of energy of open-type conformation from that of closed-type conformation.

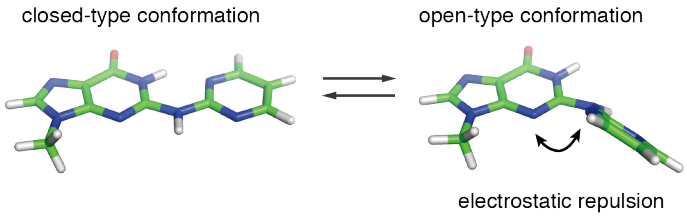
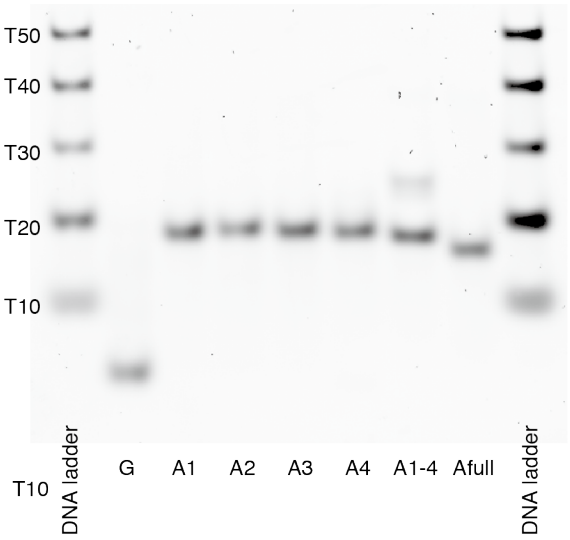


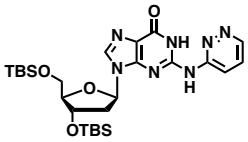
Figure S1. Optimized structure of $G^{2\text{-}Pym}$ base. Only $G^{2\text{-}Pym}$ base has electrostatic repulsion in open-type conformation.

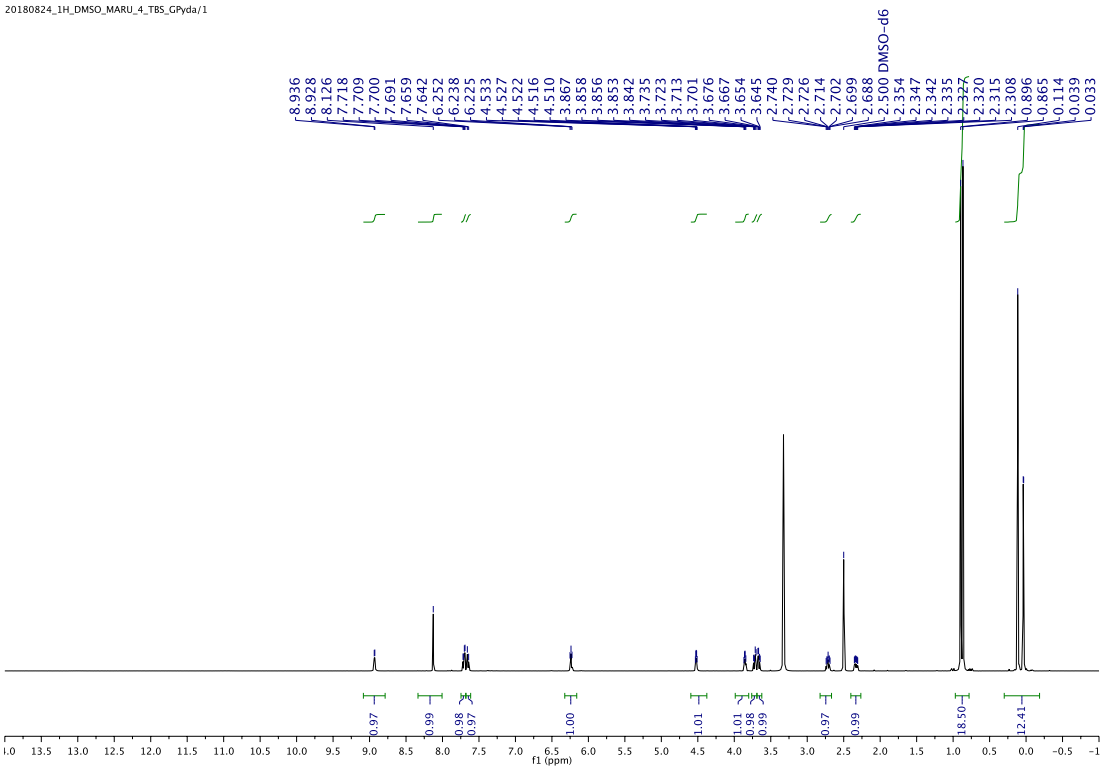


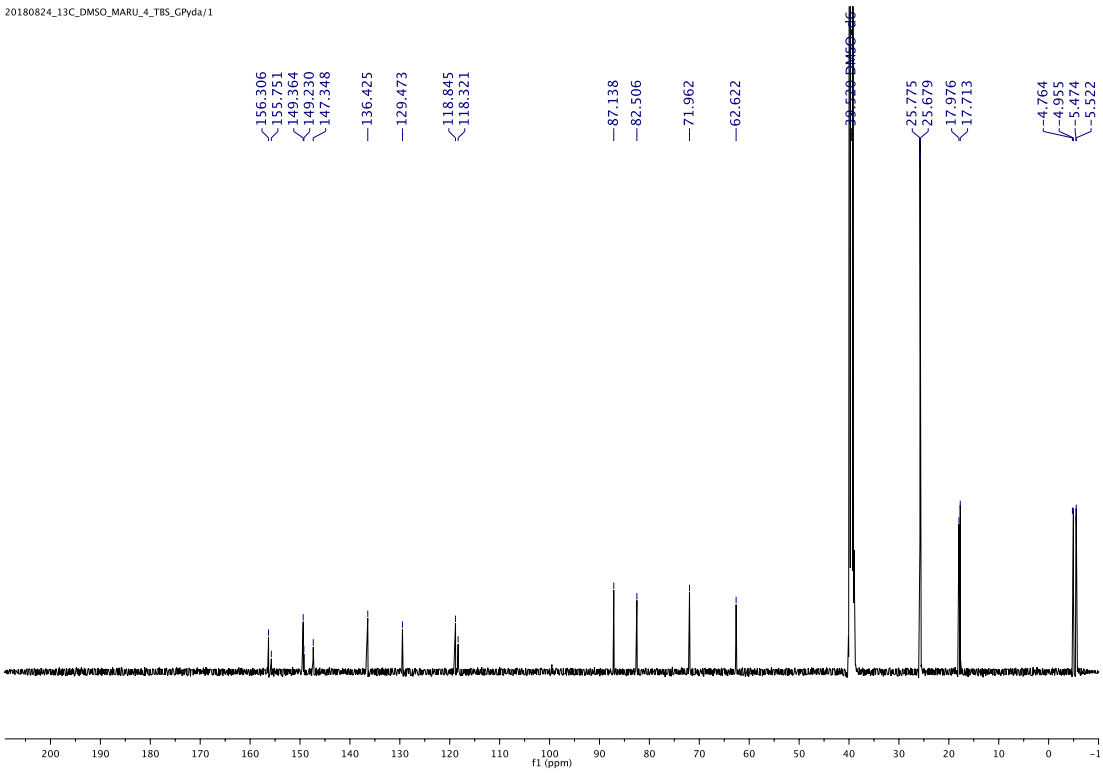
G 5´-d(AGGGTTAGGGTTAGGGTTAGGG)
A1 5´-d(AG**A**GTTAGGGTTAGGGTTAGGG)
A2 5´-d(AGGGTTAG**A**GTTAGGGTTAGGG)
A3 5´-d(AGGGTTAGGGTTAG**A**GTTAGGG)
A4 5´-d(AGGGTTAGGGTTAGGGTTAG**A**G)
A1-4 5´-d(AG**A**GTTAG**A**GTTAG**A**GTTAG**A**G)
Afull 5´-d(A**AAA**TTA**AAA**TTA**AAA**TTA**AAA**)

Figure S2. Gel electrophoresis of oligonucleotides. These oligonucleotides are expected not to form G4 structure.

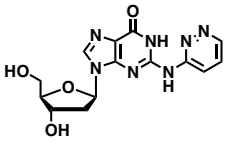
^{1}H-NMR and ^{13}C-NMR spectra of compound **1**

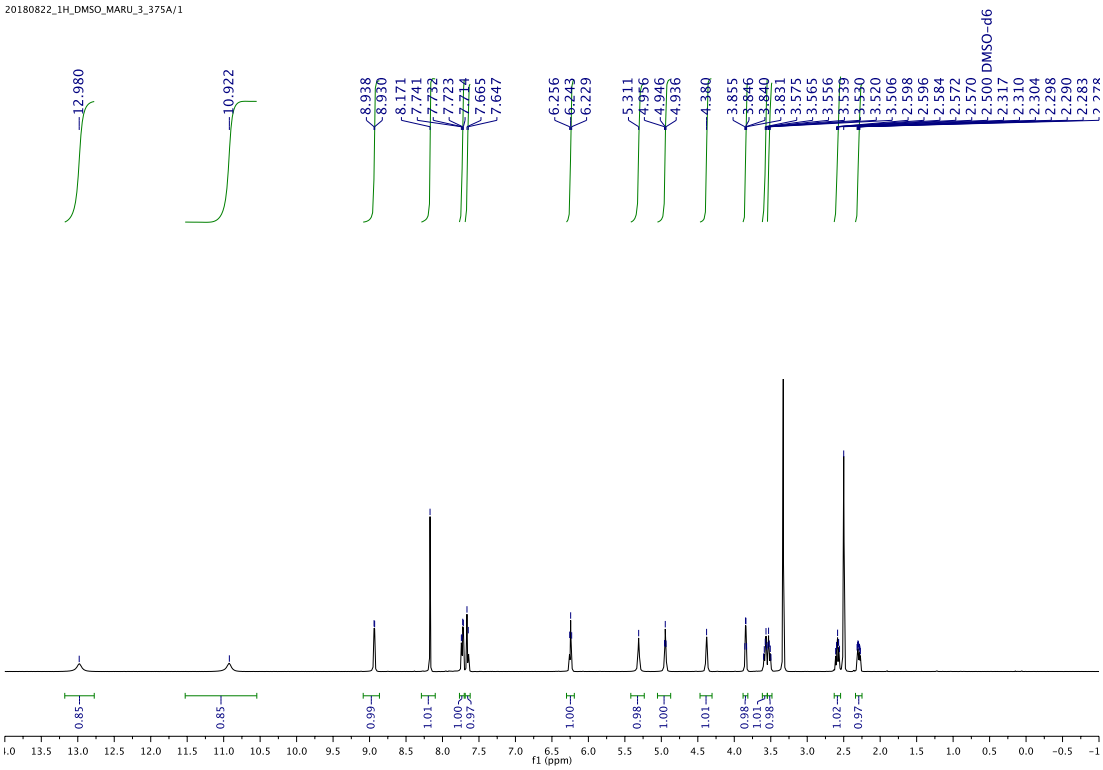


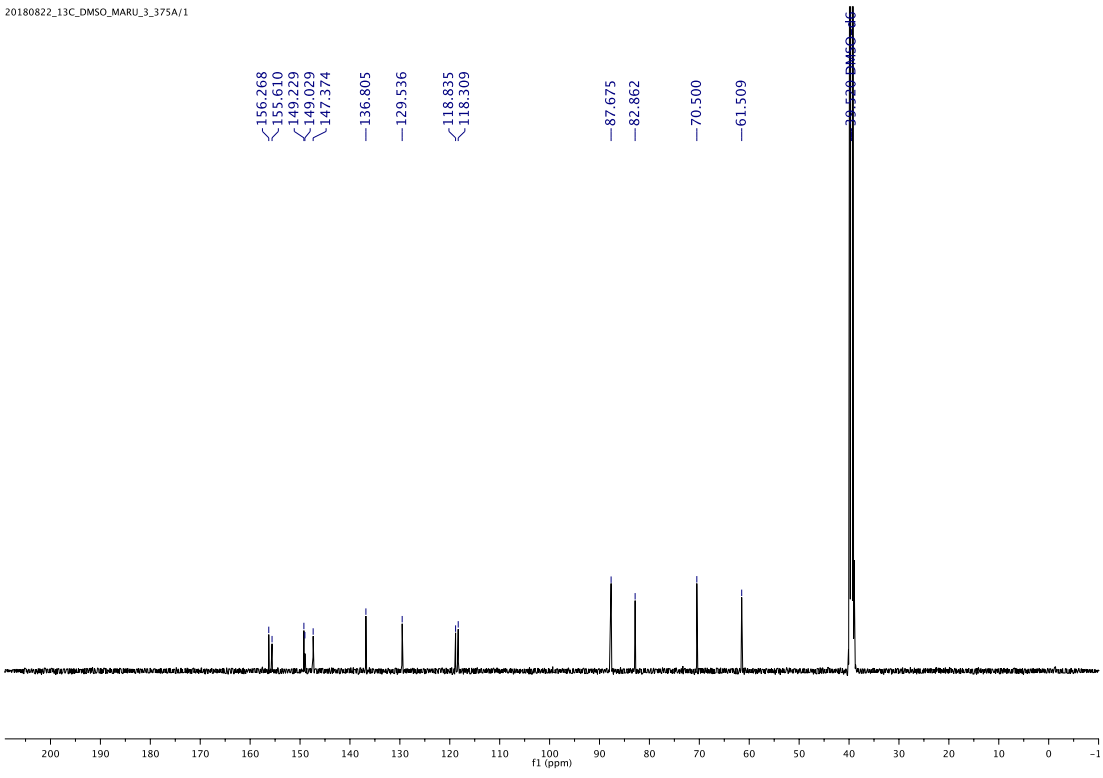




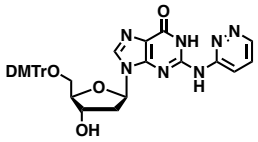
^{1}H-NMR and ^{13}C-NMR spectra of compound **2**

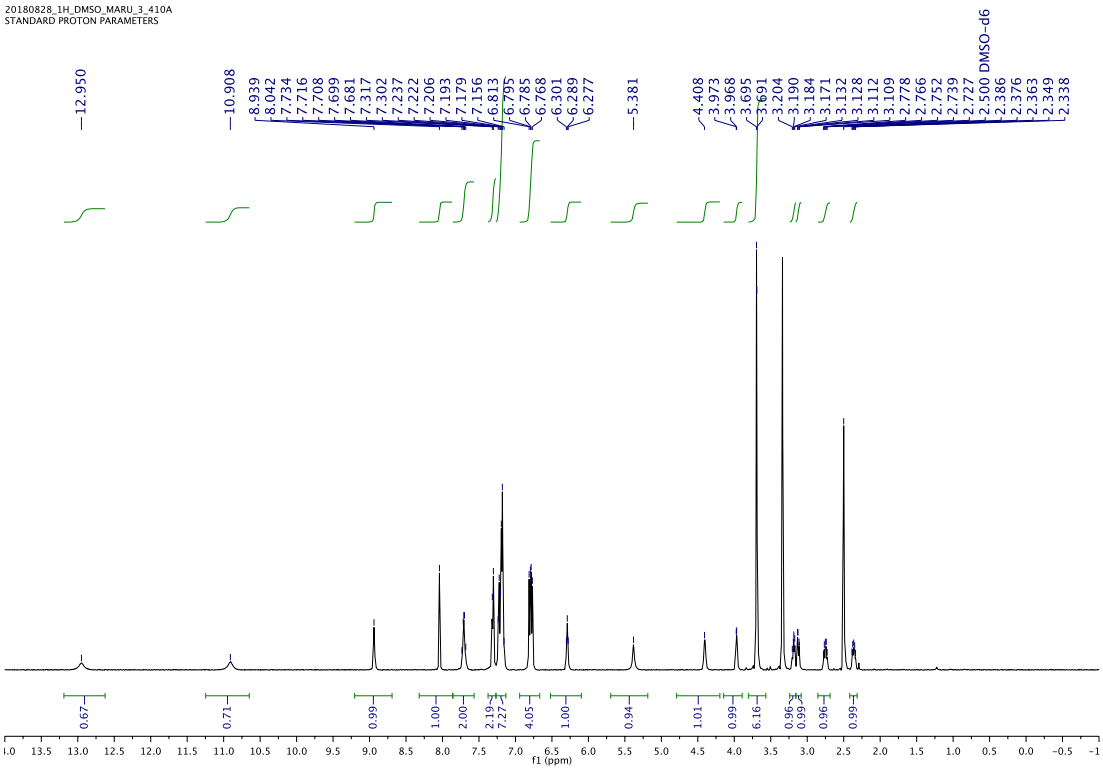


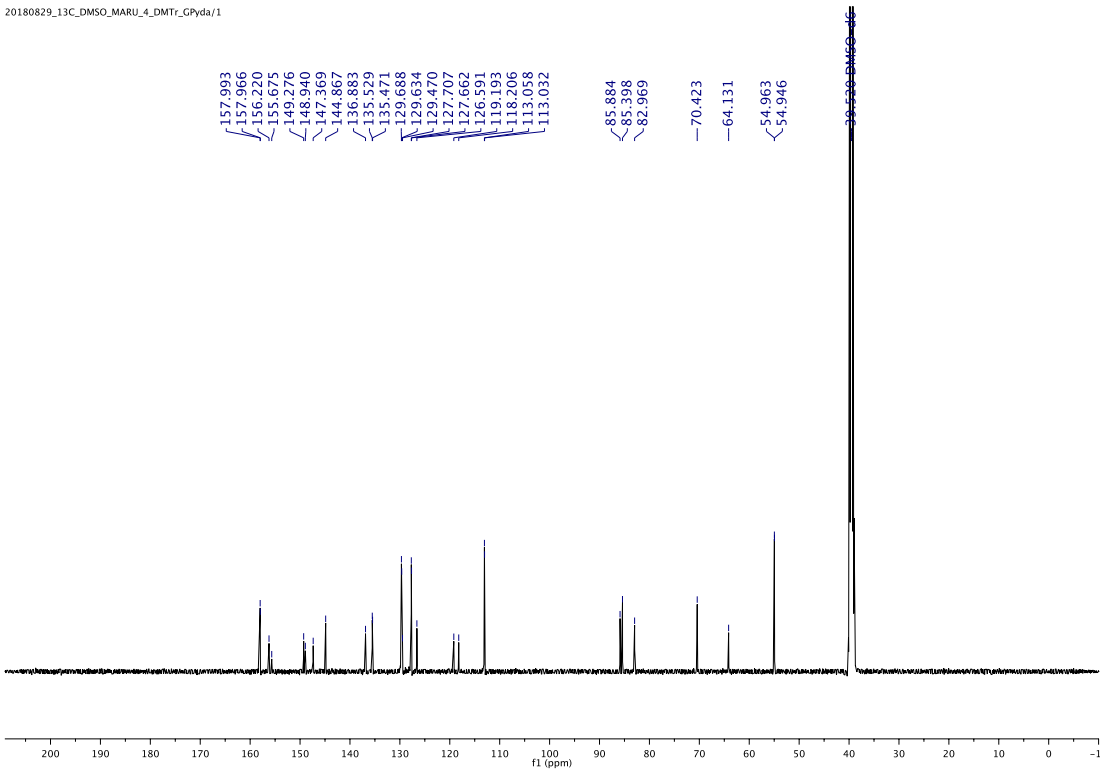




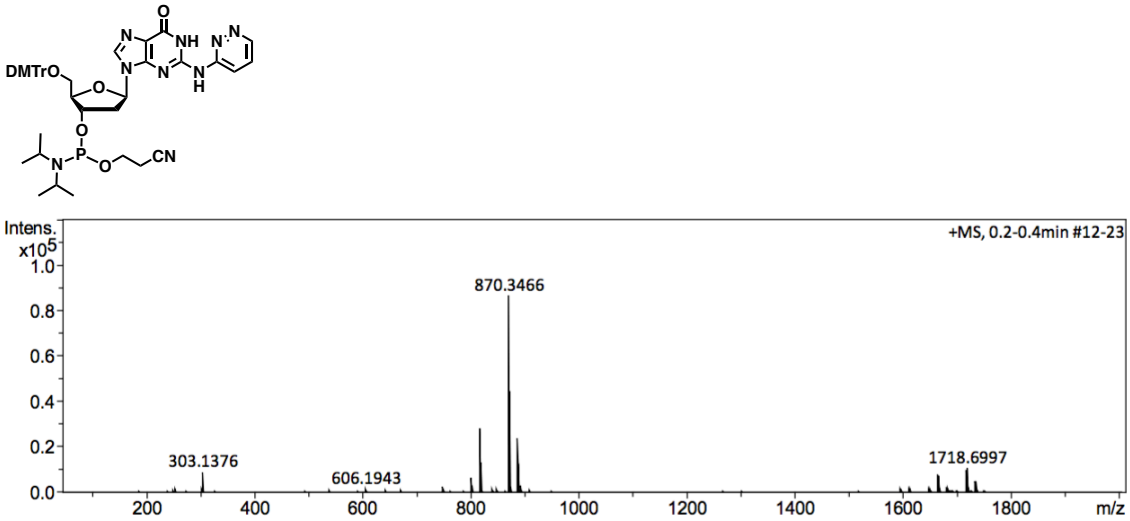
^{1}H-NMR and ^{13}C-NMR spectra of compound **3**





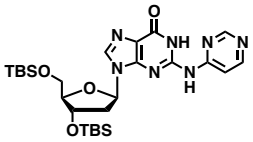


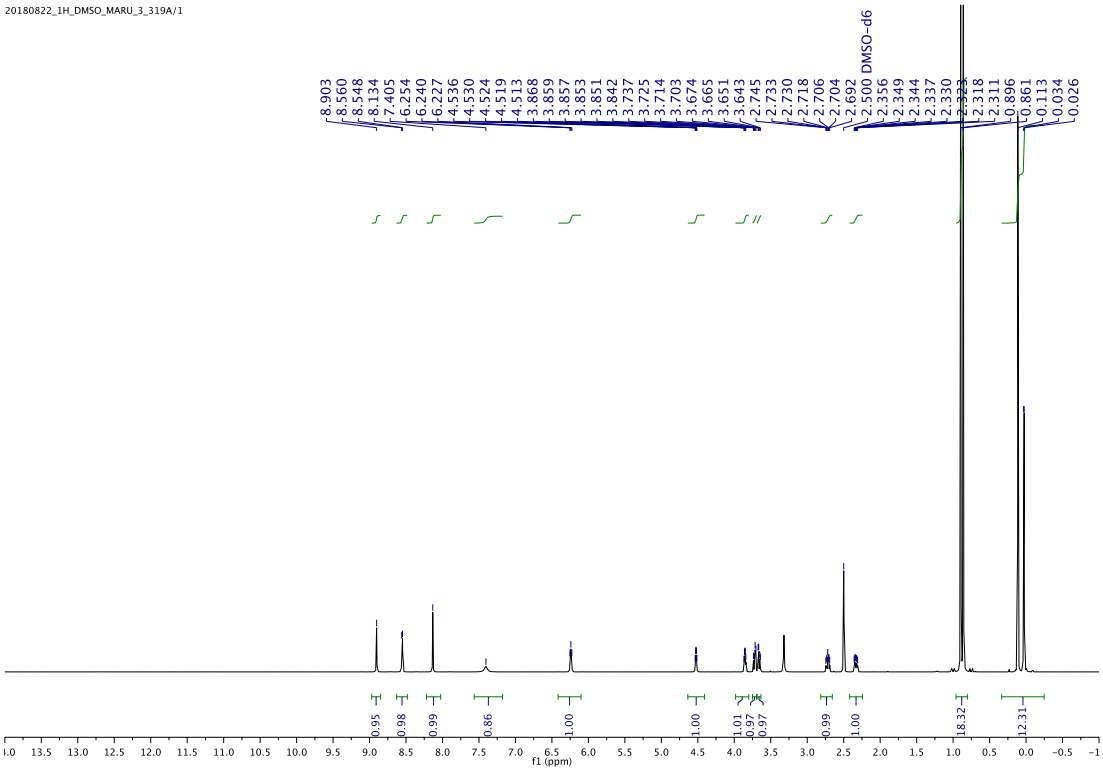
ESI Mass spectrum of compound **4**

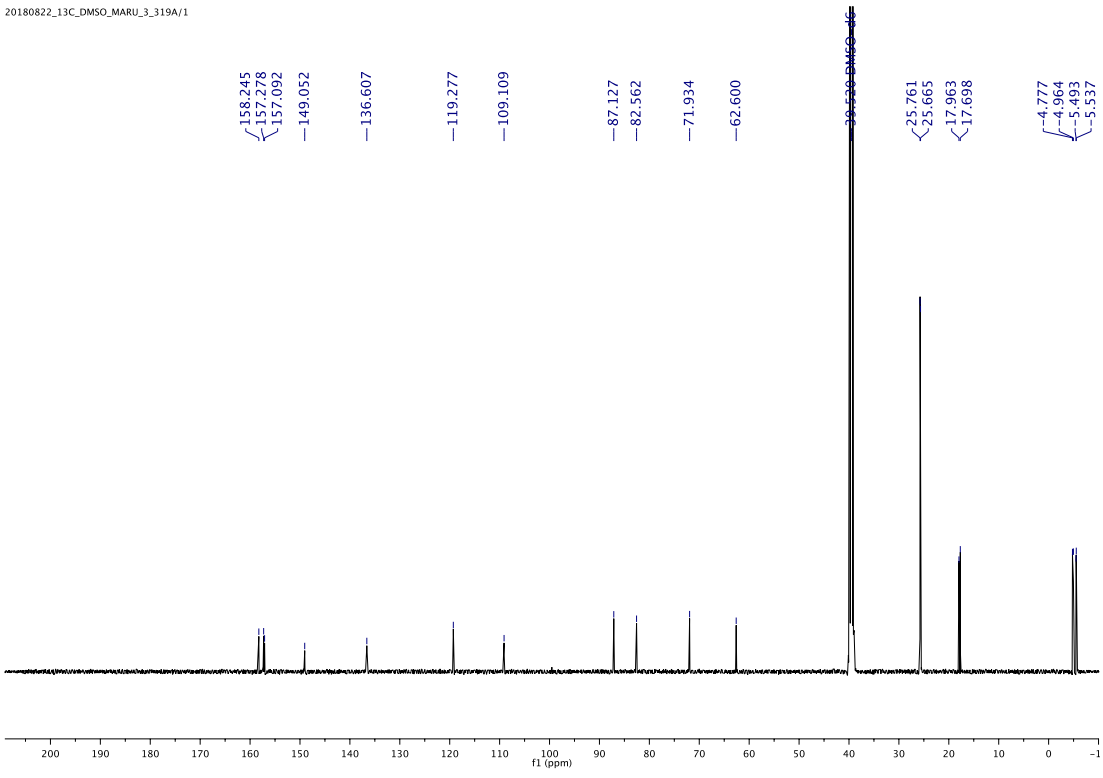


HRMS(ESI) calcd for **[**$C_{44}H_{50}N_9O_7P$+Na]$^+$ 870.3463, found 870.3466.

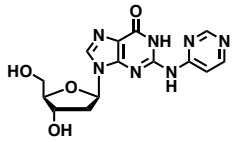
^{1}H-NMR and ^{13}C-NMR spectra of compound **5**

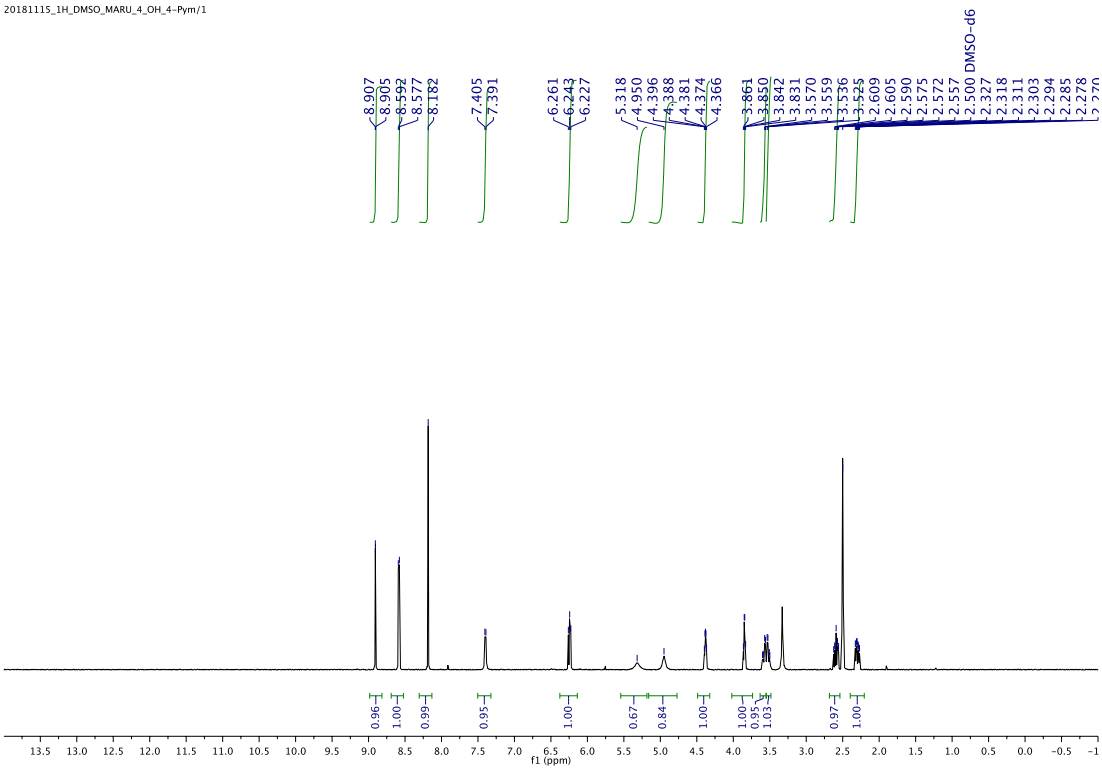


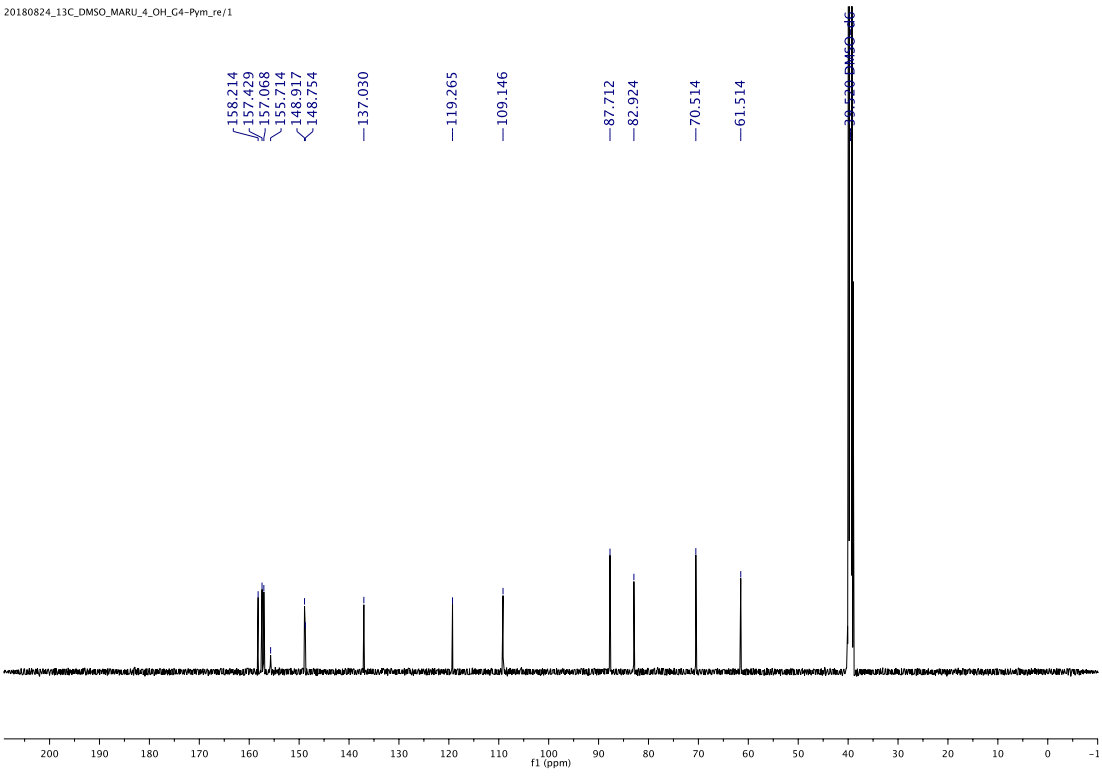




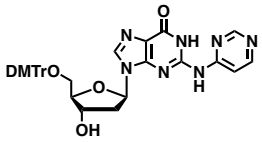
^{1}H-NMR and ^{13}C-NMR spectra of compound **6**

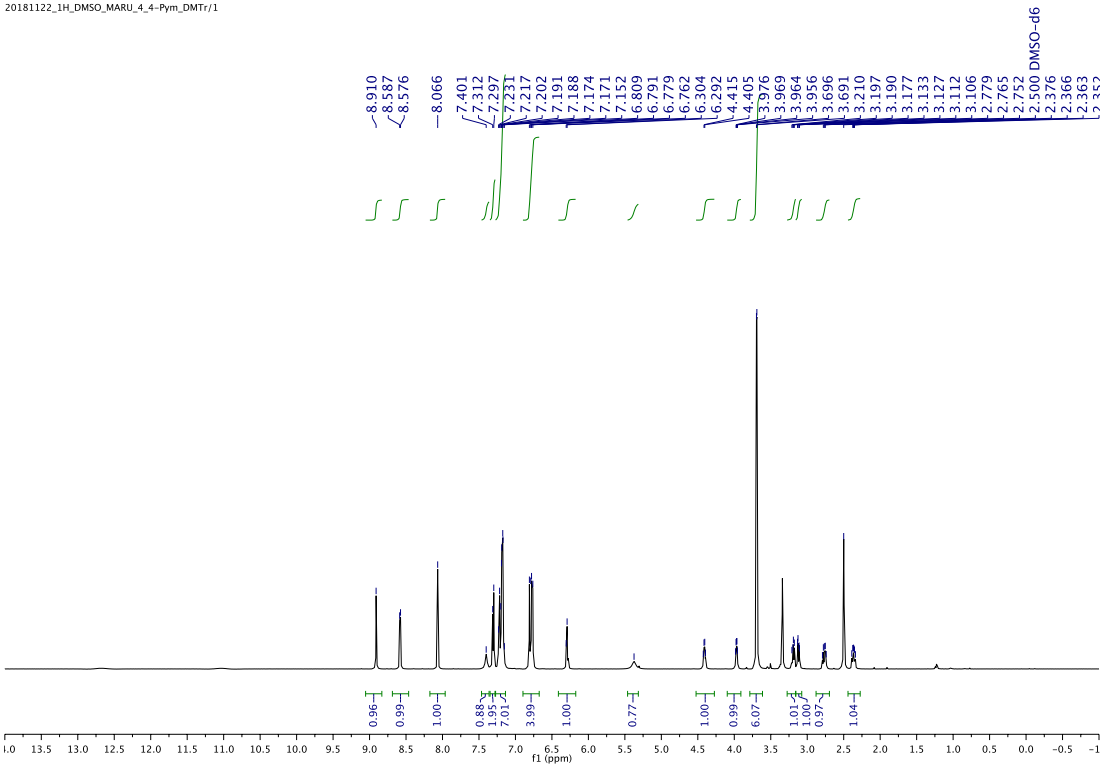


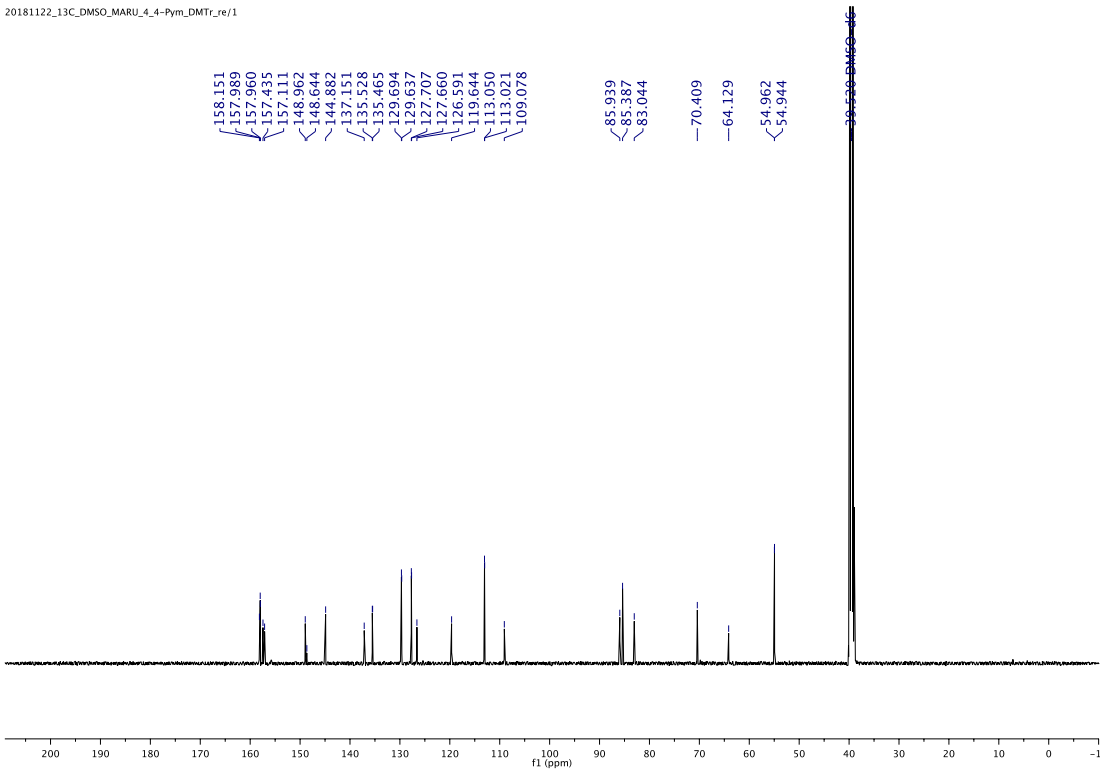




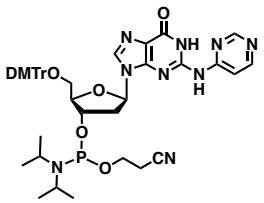
^{1}H-NMR and ^{13}C-NMR spectra of compound **7**

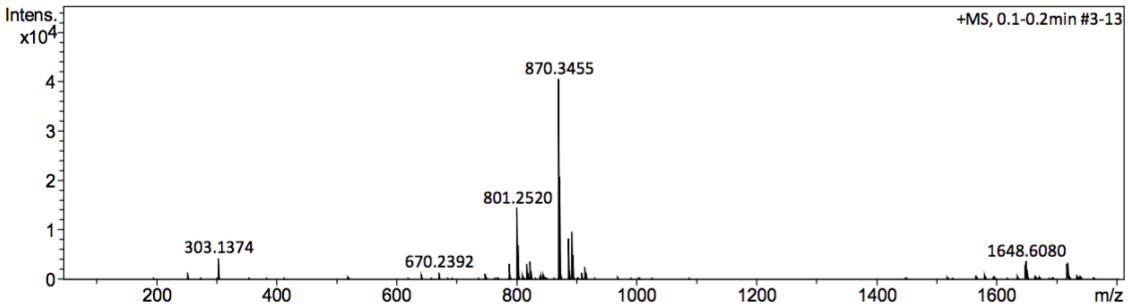






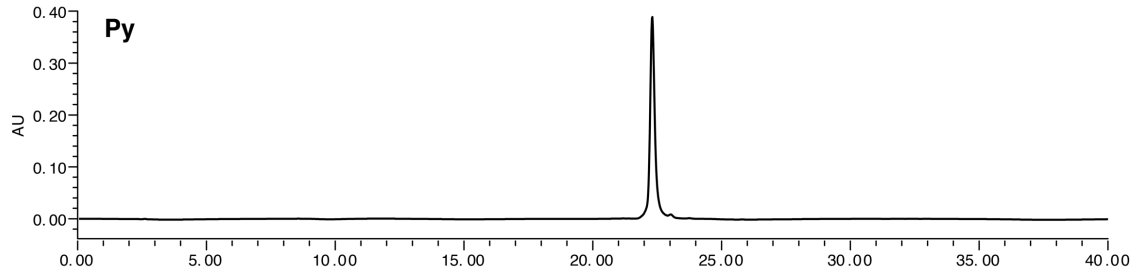
ESI Mass spectrum of compound **8**

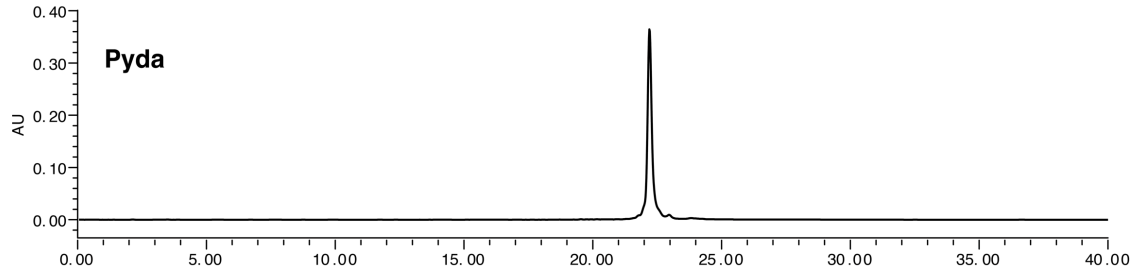


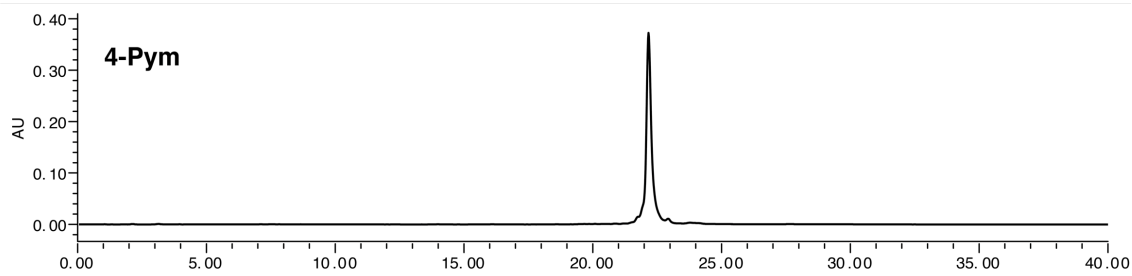


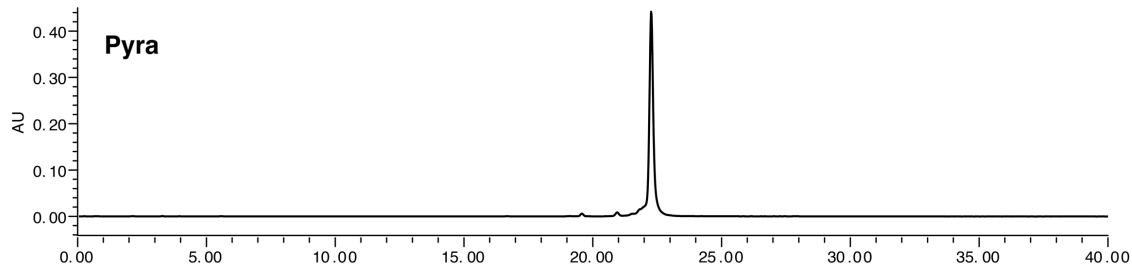
HRMS(ESI) calcd for **[**$C_{44}H_{50}N_9O_7P$+Na]$^+$ 870.3463, found 870.3455.

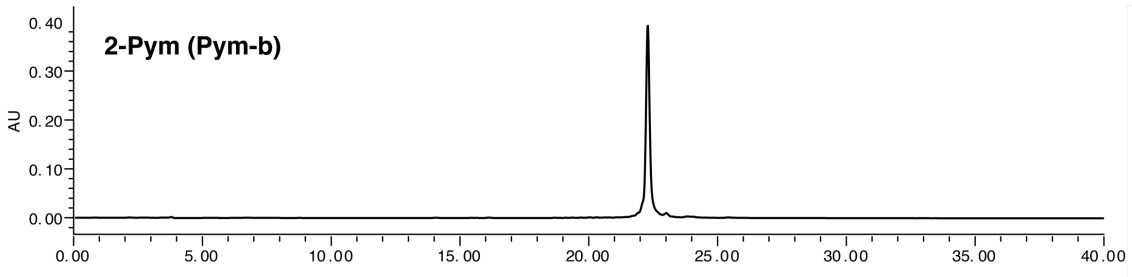
HPLC chart of oligonucleotides

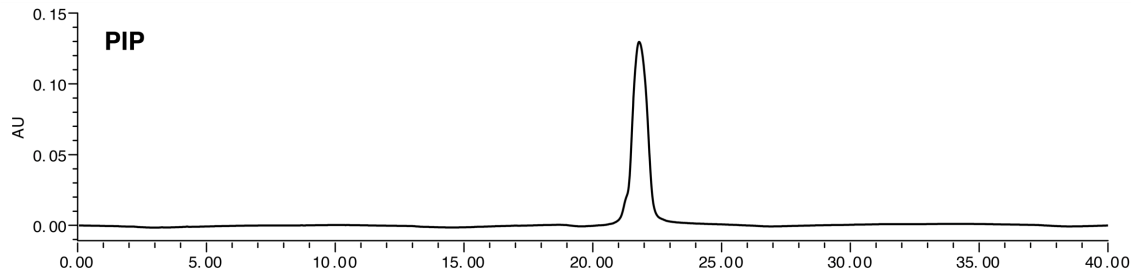


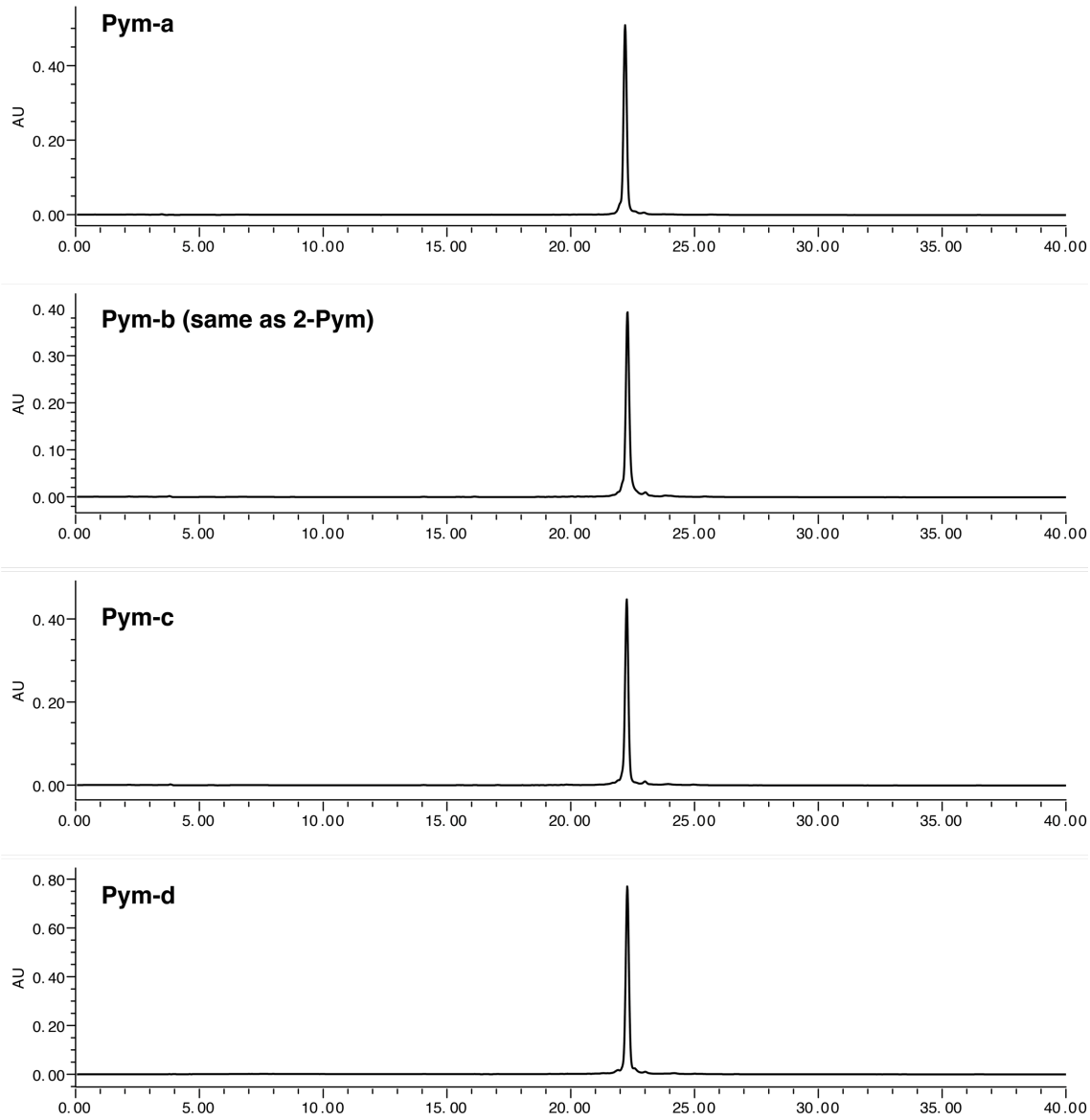




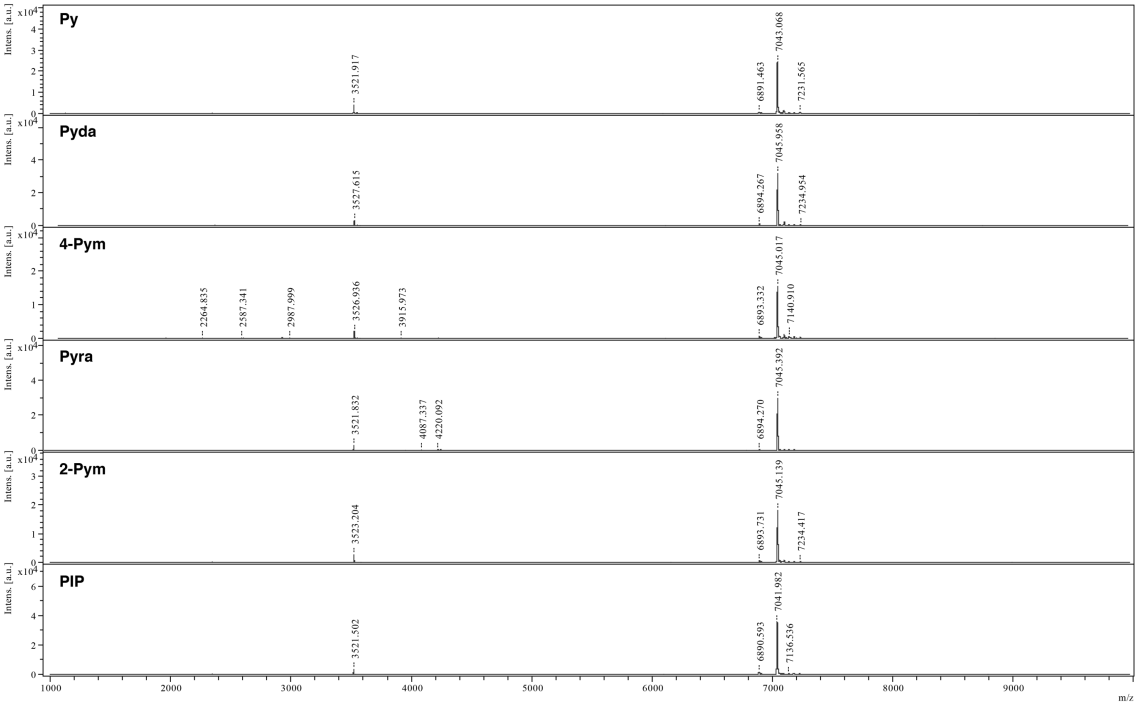


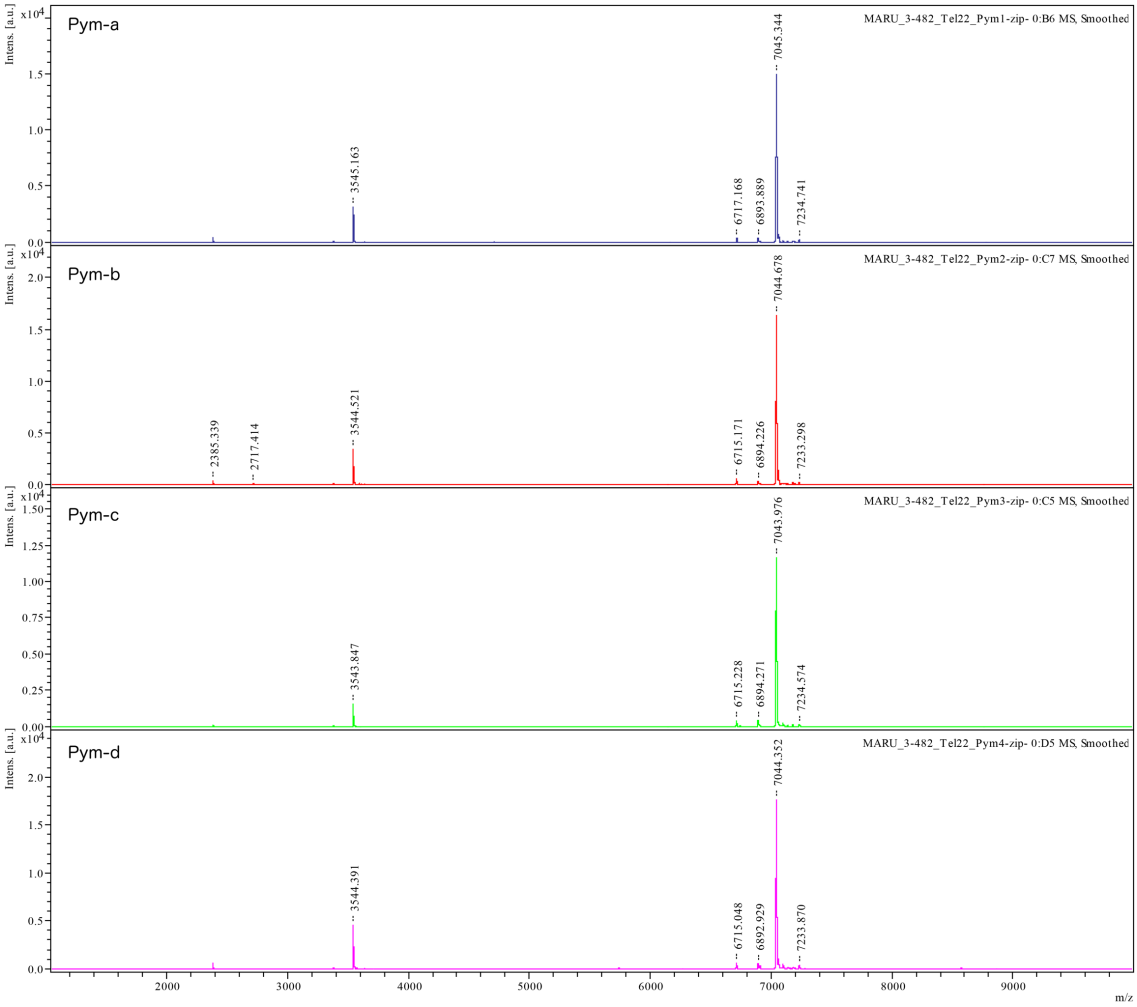





Pym-a
AU
0.40
0.20
0.00
0.00
5.00
10.00
15.00
20.00
25.00
30.00
35.00
40.00
Pym-b (same as 2-Pym)
AU
0.40
0.30
0.20
0.10
0.00
0.00
5.00
10.00
15.00
20.00
25.00
30.00
35.00
40.00
Pym-c
AU
0.40
0.20
0.00
0.00
5.00
10.00
15.00
20.00
25.00
30.00
35.00
40.00
Pym-d
AU
0.80
0.60
0.40
0.20
0.00
0.00
5.00
10.00
15.00
20.00
25.00
30.00
35.00
40.00

MALDI-TOF-Mass chart of oligonucleotides.





Results of frequency analysis of optimized structures.

G^{Py}

closed-type conformation			open-type conformation		
34.9901	51.4280	66.1062	31.5480	35.8740	58.6726
100.8992	110.0178	138.3738	88.5045	106.6565	138.1534
187.4550	191.5723	228.0792	173.1271	213.0751	239.1112
255.4811	283.9896	310.3323	247.5833	269.3261	304.8609
365.8632	371.6614	419.1989	370.1028	375.4173	425.9473
528.4932	530.6437	543.2107	468.0876	520.6839	545.6928
559.4588	621.1462	638.7173	546.4557	594.5876	625.0554
657.2790	663.0754	694.4045	640.9578	660.6475	684.4156
729.4916	743.7136	755.4396	701.4280	736.1998	736.4338
761.1432	777.8515	796.6855	757.3448	768.2488	775.1758
839.3800	849.3604	853.0502	804.1819	840.5588	882.6581
888.6392	928.4701	1000.2386	907.4336	919.0272	1000.1548
1022.7922	1023.0671	1059.3369	1019.8643	1032.1315	1067.9378
1084.0518	1093.2779	1111.4824	1085.6141	1091.9304	1107.0609
1149.7796	1167.5077	1171.3573	1143.0297	1167.0617	1168.3071
1197.0566	1265.7004	1278.1403	1194.6767	1269.4384	1274.2247
1320.5753	1332.9749	1361.2841	1297.1873	1335.3947	1349.3592
1380.9282	1402.5830	1428.0862	1370.6900	1404.1199	1422.1559
1462.6852	1483.0813	1505.2473	1476.8493	1488.4139	1503.5948
1511.0796	1536.4303	1548.1821	1511.9682	1515.3298	1538.0913
1549.3930	1577.8468	1621.6225	1546.3336	1593.5677	1631.8314
1640.1730	1664.6714	1693.7183	1639.1215	1664.1480	1679.7258
1695.5681	1838.7436	3087.0662	1698.1771	1846.5929	3087.0799
3166.5155	3185.3720	3216.9114	3165.9061	3188.2091	3208.2430
3220.6671	3233.6121	3253.6045	3222.5263	3247.7990	3281.8281
3277.5311	3488.1804	3668.0800	3302.1327	3632.9280	3647.9817

G^{Pyda}

closed-type conformation			open-type conformation		
34.8866	51.5612	66.5909	28.7539	35.2205	62.9104
101.9157	109.7593	138.2187	88.6501	106.7874	137.9720
188.6888	190.4091	226.4412	173.1254	213.5431	234.6684
256.0357	281.8596	310.6058	247.8544	270.1653	302.0632
366.7996	370.9805	390.2985	370.4786	375.8732	397.7482
528.7351	531.7558	545.3119	471.6882	519.9136	546.1834
559.8905	624.0526	648.4559	559.7200	606.0228	629.2804
657.1969	659.5015	693.2702	646.4020	660.9140	690.4488
727.8614	743.4663	762.4174	700.4128	736.3035	737.1088
765.4622	777.1925	828.5188	757.2814	772.3762	774.6268
841.3039	848.7341	855.5578	839.2144	842.3844	884.8994
921.2457	949.9720	1022.6312	904.0259	966.0688	1033.1295
1046.2994	1057.8591	1082.3778	1046.1860	1066.5748	1084.0989
1091.6579	1107.5524	1160.5805	1091.6145	1107.1257	1156.7304
1167.5305	1169.8555	1235.5058	1167.1247	1167.3836	1226.4712
1254.9940	1266.6603	1313.5558	1241.9401	1270.9478	1285.8176
1335.5055	1355.2459	1403.7151	1332.0002	1353.0772	1404.9518
1429.3101	1450.6792	1482.4296	1418.2388	1440.2493	1479.9978
1497.7238	1508.4511	1511.3400	1496.1237	1507.3709	1512.3961
1536.3360	1549.5004	1577.4582	1535.6128	1542.9926	1592.3674
1617.8230	1640.1185	1649.3922	1630.7062	1639.4055	1650.6470
1684.8757	1693.6953	1845.2310	1662.8234	1691.5718	1850.2933
3087.3015	3166.8507	3185.8770	3086.8808	3165.5046	3188.8186
3221.8138	3237.5469	3250.5913	3231.0978	3246.8599	3282.8129
3278.3369	3478.4423	3664.1648	3298.9402	3629.0977	3637.0633

$G^{4\text{-}Pym}$

closed-type conformation			open-type conformation		
36.2008	55.1132	66.8054	31.5561	39.3866	60.8173
99.9098	110.5150	138.8842	86.4864	107.1517	140.2826
186.4528	190.6684	224.1220	172.5637	212.3878	234.4651
256.3855	284.4641	309.1100	248.7905	267.9601	306.6018
369.6411	371.6122	385.8760	373.1231	375.2809	393.9508
529.4245	541.8892	553.7702	481.5745	520.2118	545.9833
584.0257	620.8924	645.6070	568.6928	592.3946	630.1322
657.2857	692.8068	703.4321	661.2733	682.7799	690.9683
725.8862	744.6506	762.7432	700.8743	736.9784	738.1553
777.1282	788.1298	838.1412	760.4328	774.6143	801.2743
845.3789	847.4604	857.2157	844.7558	879.5365	890.0634
941.2045	997.2925	1025.6011	916.9261	1001.6641	1023.9232
1037.0454	1061.8553	1088.3797	1038.5113	1068.2493	1091.7071
1105.8614	1123.1224	1166.7863	1106.2040	1109.6340	1165.9566
1167.5362	1223.1475	1264.1593	1166.9944	1218.2985	1258.3357
1267.0439	1316.6833	1335.4516	1269.8354	1289.2613	1333.2117
1360.1730	1385.2963	1404.9953	1359.9001	1372.7722	1406.2667
1429.4034	1445.2907	1481.5667	1424.9406	1453.1063	1478.2075
1500.6378	1511.4945	1521.7809	1491.8737	1511.1430	1512.3475
1539.0887	1553.5405	1576.4474	1537.2916	1545.3678	1589.8426
1617.9841	1637.4098	1661.2967	1625.3487	1636.1093	1657.4214
1681.4922	1698.2980	1843.9101	1675.6506	1700.6422	1850.6329
3088.3356	3168.4324	3187.0782	3088.1488	3167.5413	3189.8804
3213.8178	3232.5848	3238.2280	3211.1849	3227.4268	3283.2388
3279.1079	3503.8961	3661.2568	3306.1607	3631.1214	3643.7623

G^{Pyra}

closed-type conformation			open-type conformation		
33.7355	51.4253	66.3463	27.2787	34.0014	55.0747
98.9036	110.2724	137.7282	87.0788	107.0809	136.9815
186.1174	191.2868	219.8021	171.9759	212.6467	231.1415
255.8522	279.3965	309.4175	248.7893	269.7729	304.3257
366.5362	371.6620	432.0465	370.4728	375.7100	434.3673
529.2553	538.8831	543.0866	458.1263	520.3678	547.7073
559.9558	618.8795	636.7498	555.0720	596.2621	619.6330
657.1496	683.0265	692.7251	642.0518	660.8681	691.7416
724.3515	743.8656	769.2124	700.4245	735.5311	739.6186
769.9525	776.8935	829.3650	762.2372	774.8360	778.7412
844.1464	856.9887	864.3766	844.0294	872.5355	886.9030
932.6929	943.1429	998.6188	911.6894	970.0505	998.2366
1037.0925	1058.7934	1086.3920	1034.8390	1068.2334	1091.8193
1104.8659	1120.2965	1166.7843	1093.2799	1119.6431	1165.5298
1167.5315	1211.4535	1257.1405	1166.1006	1211.6470	1255.1882
1265.7005	1313.3836	1323.8113	1269.5104	1288.2378	1314.4142
1360.5784	1376.2584	1404.1260	1345.2837	1352.1303	1406.0054
1424.7855	1446.6125	1482.4749	1423.0922	1476.4425	1481.1097
1504.3345	1511.4097	1535.4256	1491.5197	1511.4445	1512.2708
1544.8887	1549.0732	1577.3217	1537.3585	1546.1720	1594.1204
1619.2633	1637.4120	1650.5436	1631.4607	1639.5718	1641.5463
1674.6227	1694.9795	1842.4965	1669.1448	1692.7187	1848.6408
3088.1655	3168.2517	3186.7548	3089.2851	3169.2615	3190.3489
3193.3301	3228.1295	3246.4067	3218.2813	3237.1074	3282.7325
3278.9143	3513.3687	3659.8567	3298.8144	3632.4500	3646.1370

$G^{2\text{-}Pym}$

closed-type conformation			open-type conformation		
37.1672	55.7294	64.8494	27.5505	34.1009	65.6471
101.3300	110.7388	136.8158	68.5294	110.5569	161.2342
186.6737	191.4408	219.9760	169.1319	182.4689	231.3149
256.4929	287.9114	313.7846	255.2545	273.4259	337.1714
370.8980	371.7723	416.3914	370.6272	394.2154	417.0478
529.2708	529.6628	549.0768	476.1555	519.7296	546.7874
628.8295	637.0854	653.4014	548.0934	607.4741	634.5401
657.4158	670.3661	695.6448	647.4109	662.2644	679.1334
726.1645	743.8884	773.5581	714.7179	720.1306	745.3069
778.2868	810.0423	821.7871	772.7492	783.0467	817.6444
838.9790	844.3997	856.3288	829.6558	847.6299	901.5665
940.9723	1019.3361	1023.7966	927.1619	1018.7076	1020.7191
1024.5939	1062.6729	1088.2203	1022.7046	1066.0248	1092.9710
1104.8885	1121.0426	1140.5956	1099.6570	1120.6735	1136.6420
1167.5650	1170.8665	1264.4561	1168.2328	1172.7014	1266.0858
1281.8073	1299.4637	1323.4639	1269.7657	1296.5927	1311.2455
1355.0020	1387.5007	1404.2047	1340.4657	1387.3308	1409.6038
1431.0808	1453.9593	1482.5998	1425.2796	1463.9351	1481.0530
1504.2424	1510.6343	1511.2395	1494.8746	1504.4415	1511.7910
1537.3979	1555.9700	1577.5714	1532.3208	1542.5027	1577.8318
1622.4259	1639.7739	1660.5942	1611.8911	1631.0299	1665.6533
1681.1831	1694.8000	1840.5140	1670.6470	1703.1498	1844.4078
3088.2095	3168.5715	3186.3551	3090.3550	3172.5738	3189.6563
3215.6648	3222.3403	3265.6974	3208.3984	3212.1513	3260.4199
3278.5257	3508.4479	3658.7901	3281.1632	3641.5175	3647.0730

Coordination of optimized structures (ωB97XB/6-31+G(p) level of theory)

$G^{2\text{-Pym}}$ closed-type

H	−3.44969	−2.84235	−0.89177
H	−4.93728	−2.43583	0.00147
C	−3.84883	−2.35124	−0.00057
N	−0.03078	0.94334	−0.00000
C	−0.01568	−0.41351	−0.00014
N	1.19777	−1.07778	−0.00045
N	−1.08483	−1.17004	−0.00002
C	−2.22764	−0.43691	0.00015
C	−2.37759	0.94288	0.00012
C	−1.19590	1.76562	−0.00001
O	−1.07369	2.97535	−0.00011
N	−3.71034	1.28700	0.00031
C	−4.33717	0.14261	0.00041
N	−3.49377	−0.94796	0.00044
H	0.87361	1.41868	−0.00025
H	1.07331	−2.08065	−0.00010
C	2.50130	−0.59849	−0.00020
H	−5.41233	0.01582	0.00066
H	−3.44617	−2.84425	0.88794
N	3.55936	−1.52510	0.00036
C	4.85291	−1.03815	0.00056
C	5.07087	0.34278	0.00022
C	3.96056	1.17045	−0.00032
N	2.69996	0.71835	−0.00055
H	5.69053	−1.72934	0.00099
H	6.07149	0.75991	0.00039
H	4.06621	2.25193	−0.00060

$G^{2\text{-Pym}}$ open-type

H	1.35464	3.24584	−0.96441
H	2.60918	3.78696	0.18324
C	1.82694	3.04773	0.00068
N	0.87833	−1.88136	−0.00001
C	0.00990	−0.81382	0.00040
N	−1.32176	−1.18272	0.00073
N	0.39925	0.42370	0.00054
C	1.75243	0.54332	0.00019
C	2.72699	−0.44385	−0.00018
C	2.30444	−1.81856	−0.00028
O	2.94232	−2.85362	−0.00064
N	3.98490	0.11177	−0.00041
C	3.76408	1.39925	−0.00019
N	2.42729	1.72906	0.00018
H	0.52850	−2.83216	−0.00025
H	−1.53305	−2.17126	0.00108
C	−2.48197	−0.41928	0.00027
H	4.52857	2.16567	−0.00029
H	1.06954	3.11543	0.78521
N	−2.50683	0.78503	0.56073
C	−3.67689	1.42335	0.49809
C	−4.80491	0.88476	−0.10673
C	−4.65054	−0.38425	−0.65746
N	−3.49917	−1.04623	−0.61182
H	−3.70021	2.40975	0.95622
H	−5.74686	1.41847	−0.14778
H	−5.47367	−0.89313	−1.15348

$G^{4\text{-Pym}}$ closed-type

H	−3.44969	−2.84235	−0.89177
H	−4.93728	−2.43583	0.00147
C	−3.84883	−2.35124	−0.00057
N	−0.03078	0.94334	−0.00000
C	−0.01568	−0.41351	−0.00014
N	1.19777	−1.07778	−0.00045
N	−1.08483	−1.17004	−0.00002
C	−2.22764	−0.43691	0.00015
C	−2.37759	0.94288	0.00012
C	−1.19590	1.76562	−0.00001
O	−1.07369	2.97535	−0.00011
N	−3.71034	1.28700	0.00031
C	−4.33717	0.14261	0.00041
N	−3.49377	−0.94796	0.00044
H	0.87361	1.41868	−0.00025
H	1.07331	−2.08065	−0.00010
C	2.50130	−0.59849	−0.00020
H	−5.41233	0.01582	0.00066
H	−3.44617	−2.84425	0.88794
C	3.55936	−1.52510	0.00036
C	4.85291	−1.03815	0.00056
N	5.07087	0.34278	0.00022
C	3.96056	1.17045	−0.00032
N	2.69996	0.71835	−0.00055
H	4.06621	2.25193	−0.00060

H	3.37499	−2.54050	0.00062
H	5.65299	−1.68999	0.00096

$G^{4\text{-Pym}}$ open-type

H	−1.16835	3.17737	0.88959
H	−2.57751	3.80697	−0.00003
C	−1.78989	3.05120	−0.00069
N	−0.91447	−1.89983	−0.00008
C	−0.02494	−0.85283	−0.00046
N	1.29439	−1.22040	−0.00097
N	−0.39698	0.39833	−0.00047
C	−1.74871	0.54441	−0.00002
C	−2.73779	−0.42726	0.00033
C	−2.33955	−1.80954	0.00028
O	−2.99699	−2.83137	0.00045
N	−3.98731	0.14797	0.00056
C	−3.74850	1.43095	0.00030
N	−2.40505	1.74049	0.00000
H	−0.57939	−2.85597	0.00003
H	1.51594	−2.20762	−0.00137
C	2.45832	−0.44089	−0.00035
H	−4.50073	2.20937	0.00038
H	−1.16979	3.17737	−0.89201
C	2.48728	0.95816	0.00008
C	3.73479	1.56912	0.00067
N	4.89232	0.79517	0.00074
C	4.74290	−0.58709	0.00019
N	3.55861	−1.19868	−0.00034
H	5.60982	−1.24320	0.00019
H	1.61735	1.51336	−0.00004
H	3.80385	2.59881	0.00106

G^{Py} closed-type

H	−3.44969	−2.84235	−0.89177
H	−4.93728	−2.43583	0.00147
C	−3.84883	−2.35124	−0.00057
N	−0.03078	0.94334	−0.00000
C	−0.01568	−0.41351	−0.00014
N	1.19777	−1.07778	−0.00045
N	−1.08483	−1.17004	−0.00002
C	−2.22764	−0.43691	0.00015
C	−2.37759	0.94288	0.00012
C	−1.19590	1.76562	−0.00001
O	−1.07369	2.97535	−0.00011
N	−3.71034	1.28700	0.00031
C	−4.33717	0.14261	0.00041
N	−3.49377	−0.94796	0.00044
H	0.87361	1.41868	−0.00025
H	1.07331	−2.08065	−0.00010
C	2.50130	−0.59849	−0.00020
H	−5.41233	0.01582	0.00066
H	−3.44617	−2.84425	0.88794
C	3.55936	−1.52510	0.00036
C	4.85291	−1.03815	0.00056
C	5.07087	0.34278	0.00022
C	3.96056	1.17045	−0.00032
N	2.69996	0.71835	−0.00055
H	3.36065	−2.59273	0.00065
H	5.69053	−1.72934	0.00099
H	6.07149	0.75991	0.00039
H	4.06621	2.25193	−0.00060

G^{Py} open-type

H	−1.16835	3.17737	0.88959
H	−2.57751	3.80697	−0.00003
C	−1.78989	3.05120	−0.00069
N	−0.91447	−1.89983	−0.00008
C	−0.02494	−0.85283	−0.00046
N	1.29439	−1.22040	−0.00097
N	−0.39698	0.39833	−0.00047
C	−1.74871	0.54441	−0.00002
C	−2.73779	−0.42726	0.00033
C	−2.33955	−1.80954	0.00028
O	−2.99699	−2.83137	0.00045
N	−3.98731	0.14797	0.00056
C	−3.74850	1.43095	0.00030
N	−2.40505	1.74049	0.00000
H	−0.57939	−2.85597	0.00003
H	1.51594	−2.20762	−0.00137
C	2.45832	−0.44089	−0.00035
H	−4.50073	2.20937	0.00038
H	−1.16979	3.17737	−0.89201
C	2.48728	0.95816	0.00008
C	3.73479	1.56912	0.00067
C	4.89232	0.79517	0.00074
C	4.74290	−0.58709	0.00019
N	3.55861	−1.19868	−0.00034
H	1.56741	1.52456	−0.00010

H	3.79759	2.65360	0.00105
H	5.87927	1.24480	0.00118
H	5.60982	−1.24320	0.00019

G^{Pyda} closed-type

H	−3.44969	−2.84235	−0.89177
H	−4.93728	−2.43583	0.00147
C	−3.84883	−2.35124	−0.00057
N	−0.03078	0.94334	−0.00000
C	−0.01568	−0.41351	−0.00014
N	1.19777	−1.07778	−0.00045
N	−1.08483	−1.17004	−0.00002
C	−2.22764	−0.43691	0.00015
C	−2.37759	0.94288	0.00012
C	−1.19590	1.76562	−0.00001
O	−1.07369	2.97535	−0.00011
N	−3.71034	1.28700	0.00031
C	−4.33717	0.14261	0.00041
N	−3.49377	−0.94796	0.00044
H	0.87361	1.41868	−0.00025
H	1.07331	−2.08065	−0.00010
C	2.50130	−0.59849	−0.00020
H	−5.41233	0.01582	0.00066
H	−3.44617	−2.84425	0.88794
C	3.55936	−1.52510	0.00036
C	4.85291	−1.03815	0.00056
C	5.07087	0.34278	0.00022
N	3.96056	1.17045	−0.00032
N	2.69996	0.71835	−0.00055
H	3.37499	−2.54050	0.00062
H	5.65299	−1.68999	0.00096
H	6.02661	0.73211	0.00037

G^{Pyda} open-type

H	−1.16835	3.17737	0.88959
H	−2.57751	3.80697	−0.00003
C	−1.78989	3.05120	−0.00069
N	−0.91447	−1.89983	−0.00008
C	−0.02494	−0.85283	−0.00046
N	1.29439	−1.22040	−0.00097
N	−0.39698	0.39833	−0.00047
C	−1.74871	0.54441	−0.00002
C	−2.73779	−0.42726	0.00033
C	−2.33955	−1.80954	0.00028
O	−2.99699	−2.83137	0.00045
N	−3.98731	0.14797	0.00056
C	−3.74850	1.43095	0.00030
N	−2.40505	1.74049	0.00000
H	−0.57939	−2.85597	0.00003
H	1.51594	−2.20762	−0.00137
C	2.45832	−0.44089	−0.00035
H	−4.50073	2.20937	0.00038
H	−1.16979	3.17737	−0.89201
C	2.48728	0.95816	0.00008
C	3.73479	1.56912	0.00067
C	4.89232	0.79517	0.00074
N	4.74290	−0.58709	0.00019
N	3.55861	−1.19868	−0.00034
H	1.61735	1.51336	−0.00004
H	3.80385	2.59881	0.00106
H	5.82739	1.23182	0.00119

G^{Pyra} closed-type

H	−3.44969	−2.84235	−0.89177
H	−4.93728	−2.43583	0.00147
C	−3.84883	−2.35124	−0.00057
N	−0.03078	0.94334	−0.00000
C	−0.01568	−0.41351	−0.00014
N	1.19777	−1.07778	−0.00045
N	−1.08483	−1.17004	−0.00002
C	−2.22764	−0.43691	0.00015
C	−2.37759	0.94288	0.00012
C	−1.19590	1.76562	−0.00001
O	−1.07369	2.97535	−0.00011
N	−3.71034	1.28700	0.00031
C	−4.33717	0.14261	0.00041
N	−3.49377	−0.94796	0.00044
H	0.87361	1.41868	−0.00025
H	1.07331	−2.08065	−0.00010
C	2.50130	−0.59849	−0.00020
H	−5.41233	0.01582	0.00066
H	−3.44617	−2.84425	0.88794
C	3.55936	−1.52510	0.00036
N	4.85291	−1.03815	0.00056
C	5.07087	0.34278	0.00022
C	3.96056	1.17045	−0.00032
N	2.69996	0.71835	−0.00055
H	6.07149	0.75991	0.00039

H	4.06621	2.25193	−0.00060
H	3.37499	−2.54050	0.00062

G^{Pyra} open-type

H	−1.16835	3.17737	0.88959
H	−2.57751	3.80697	−0.00003
C	−1.78989	3.05120	−0.00069
N	−0.91447	−1.89983	−0.00008
C	−0.02494	−0.85283	−0.00046
N	1.29439	−1.22040	−0.00097
N	−0.39698	0.39833	−0.00047
C	−1.74871	0.54441	−0.00002
C	−2.73779	−0.42726	0.00033
C	−2.33955	−1.80954	0.00028
O	−2.99699	−2.83137	0.00045
N	−3.98731	0.14797	0.00056
C	−3.74850	1.43095	0.00030
N	−2.40505	1.74049	0.00000
H	−0.57939	−2.85597	0.00003
H	1.51594	−2.20762	−0.00137
C	2.45832	−0.44089	−0.00035
H	−4.50073	2.20937	0.00038
H	−1.16979	3.17737	−0.89201
C	2.48728	0.95816	0.00008
N	3.73479	1.56912	0.00067
C	4.89232	0.79517	0.00074
C	4.74290	−0.58709	0.00019
N	3.55861	−1.19868	−0.00034
H	5.87927	1.24480	0.00118
H	5.60982	−1.24320	0.00019
H	1.61735	1.51336	−0.00004