Supporting Information for:

Influence of Chlorine Substitution on the Hydrolytic Stability of Biaryl Ether Nucleoside Adducts Produced by Phenolic Toxins

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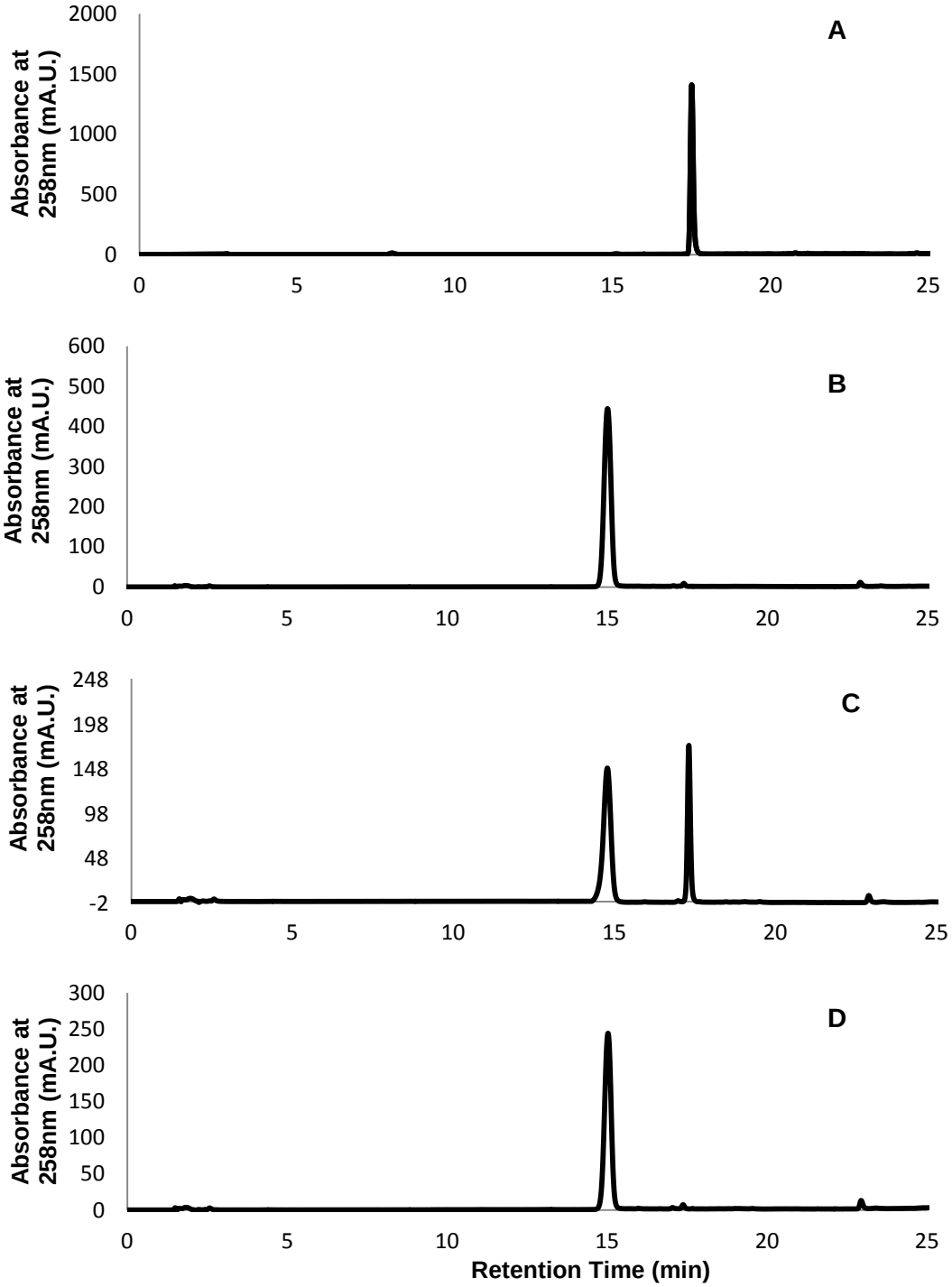


Figure S1: Reverse-phase HPLC chromatograms resulting from A) Ph-O-dG in purified water, (5% DMSO) B) Ph-O-G in purified water (5% DMSO), C) Ph-O-dG in 0.1M HCl for 5 minutes, D) Ph-O-dG in 0.1M HCl for 10 minutes.

Table S1: Temperature dependence on k_{obs} at pH 1 (0.2 M HCl/KCl).

	Rate, k_{obs} (min^{-1}) at Temperature (°C) in pH 1				
Adduct	**25**	**35**	**45**	**55**	**65**
PCP-dG	0.033	0.145	0.355	1.00	2.8
Ph-O-dG	0.288	1.11	2.5	6.7	17
4-Cl-Ph-O-dG	0.235	0.81	1.95	5.6	14.5
2-Cl-Ph-O-dG	0.220	0.871	1.9	5.44	13.3
DCP-dG	0.1404	0.51	1.19	3.2	8.1
TCP-dG	0.075	0.260	0.68	1.76	4.5
4-Me-Ph-O-dG	0.304	1.178	2.62	7.0	18.0
4-MeO-Ph-O-dG	0.318	1.152	2.83	7.4	18.5

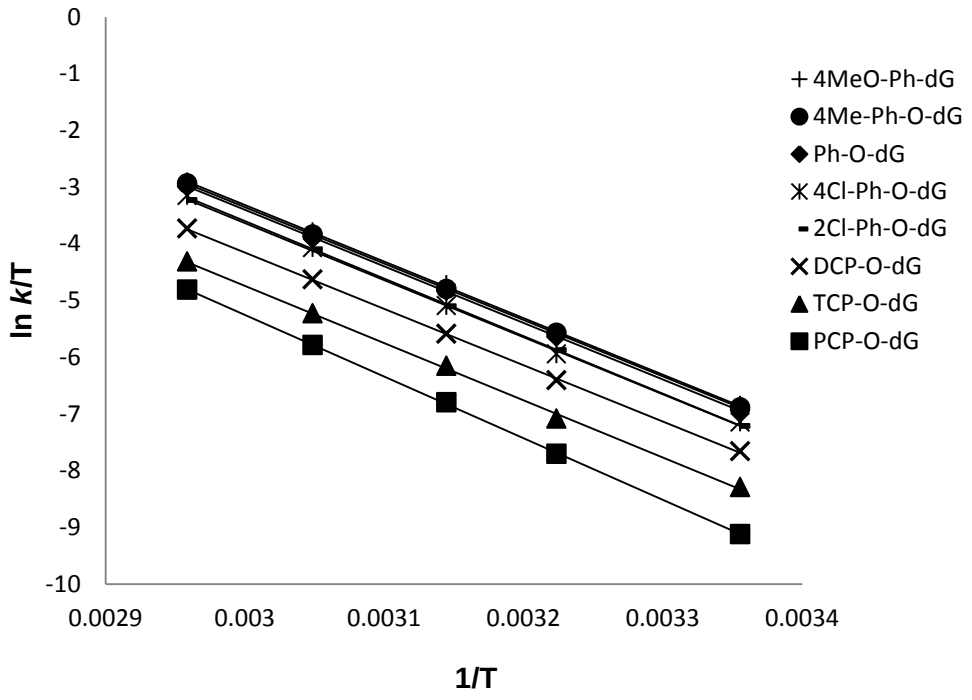


Figure S2: Eyring plots for rate data at pH 1.

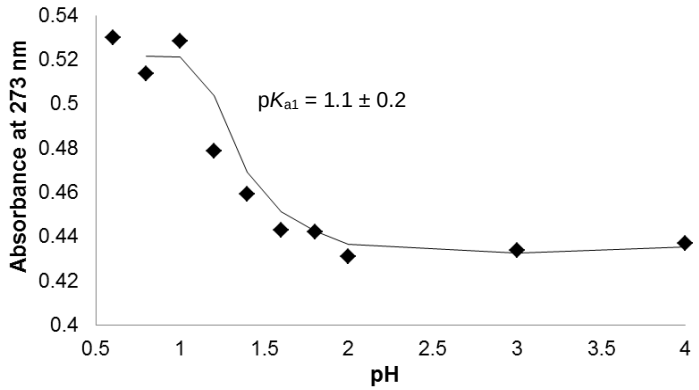


Figure S3. Plot of absorbance at 273 nm vs pH for Ph-O-dG at 25°C.

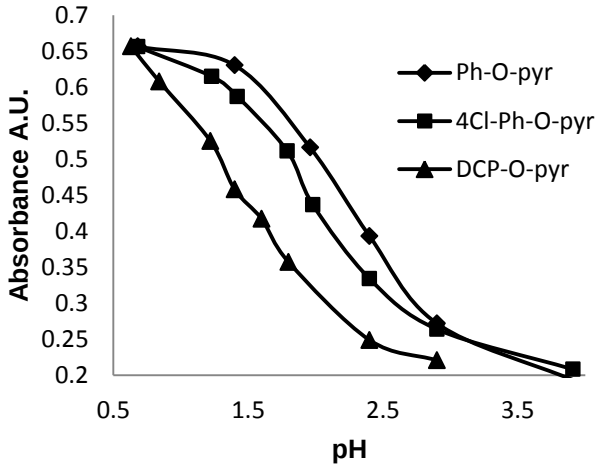


Figure S4: Plot of normalized absorbance at 280 nm (Ph-O-pyr, 4-Cl-Ph-O-pyr) and 275 nm (DCP-O-pyr) vs pH at 25^{o}C.

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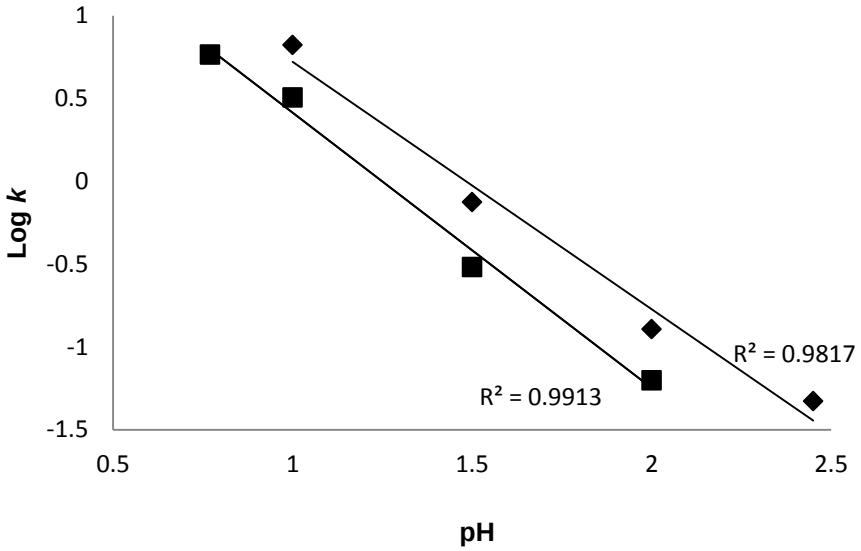


Figure S5: pH rate profile for Ph-O-dG (♦), and DCP-O-dG (■) obtained in pH 0.8, 1, 1.5, 2 (0.2M KCl/HCl) and 2.5 (0.05M Citrate, 0.31M NaCl) at 55^{o}C.

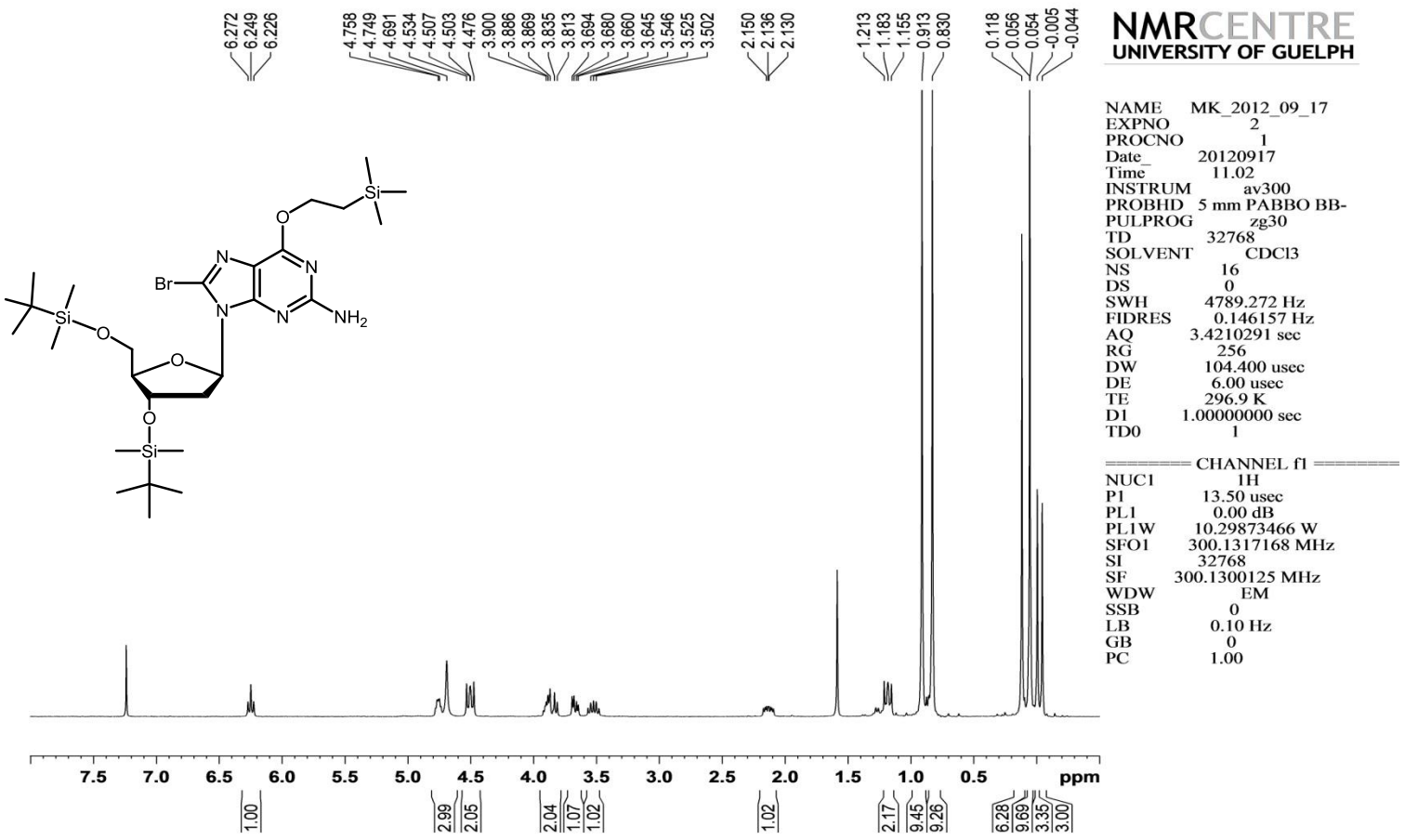


Figure S6: ^{1}H spectrum of **2**.

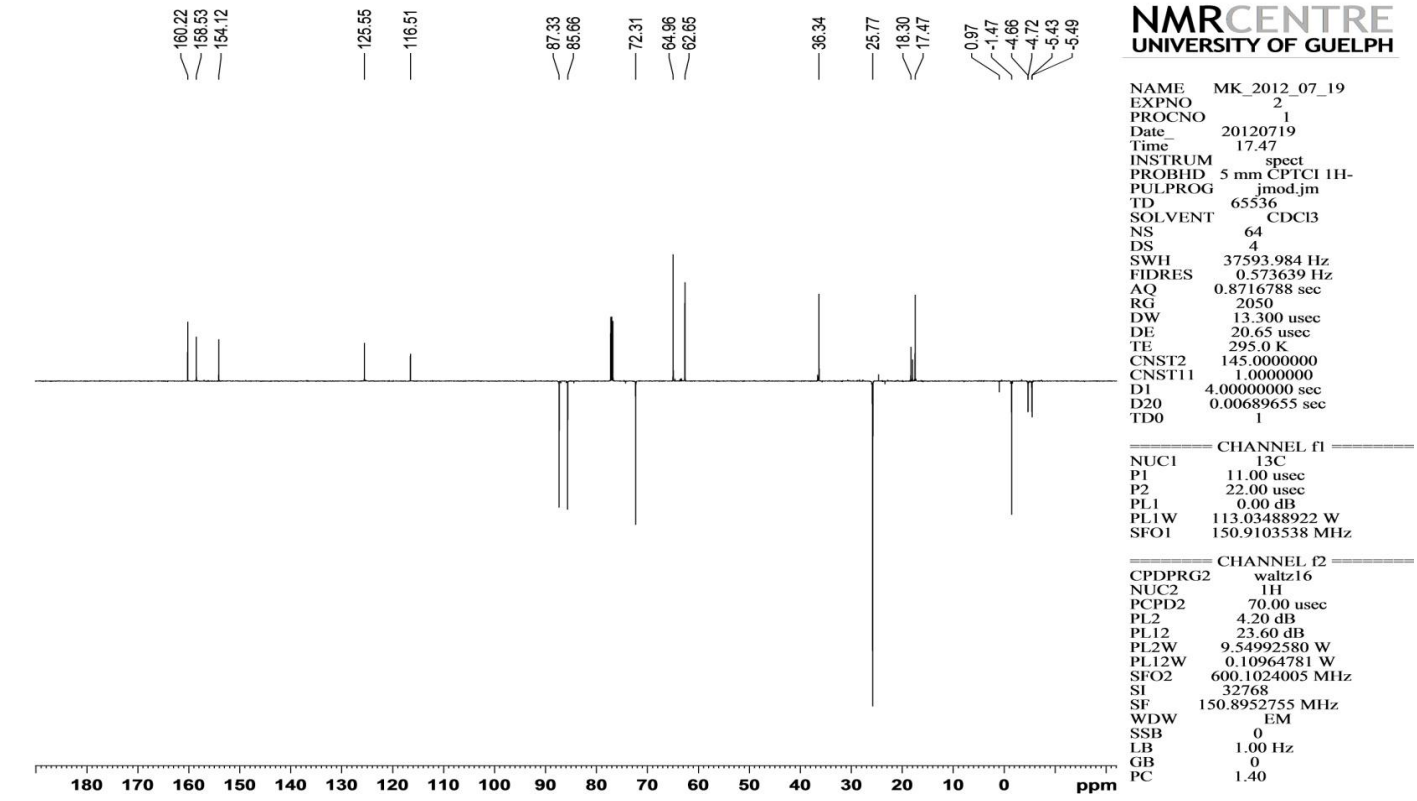


Figure S7: ^{13}C spectrum of **2**.

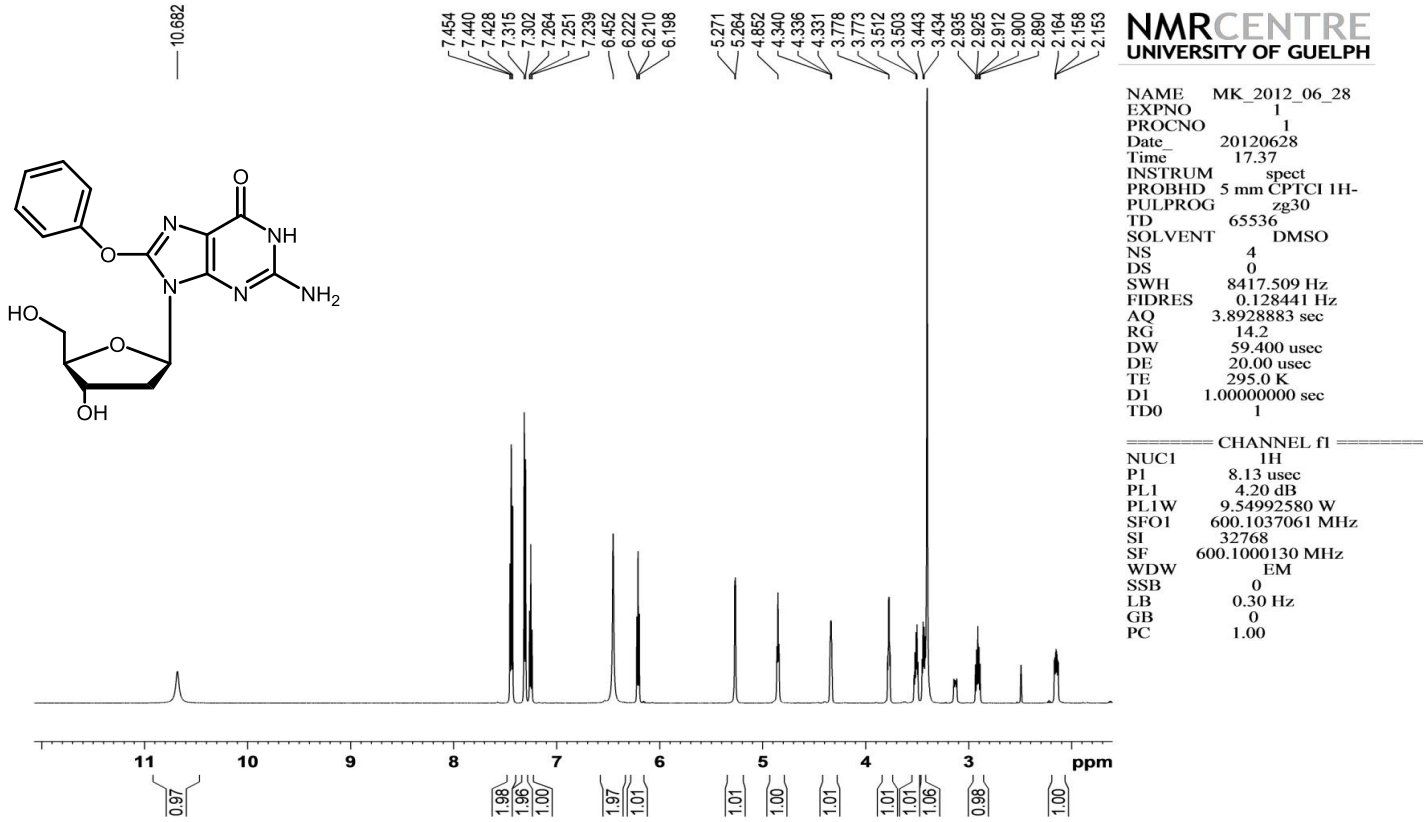


Figure S8: ^{1}H spectrum of Ph-O-dG.

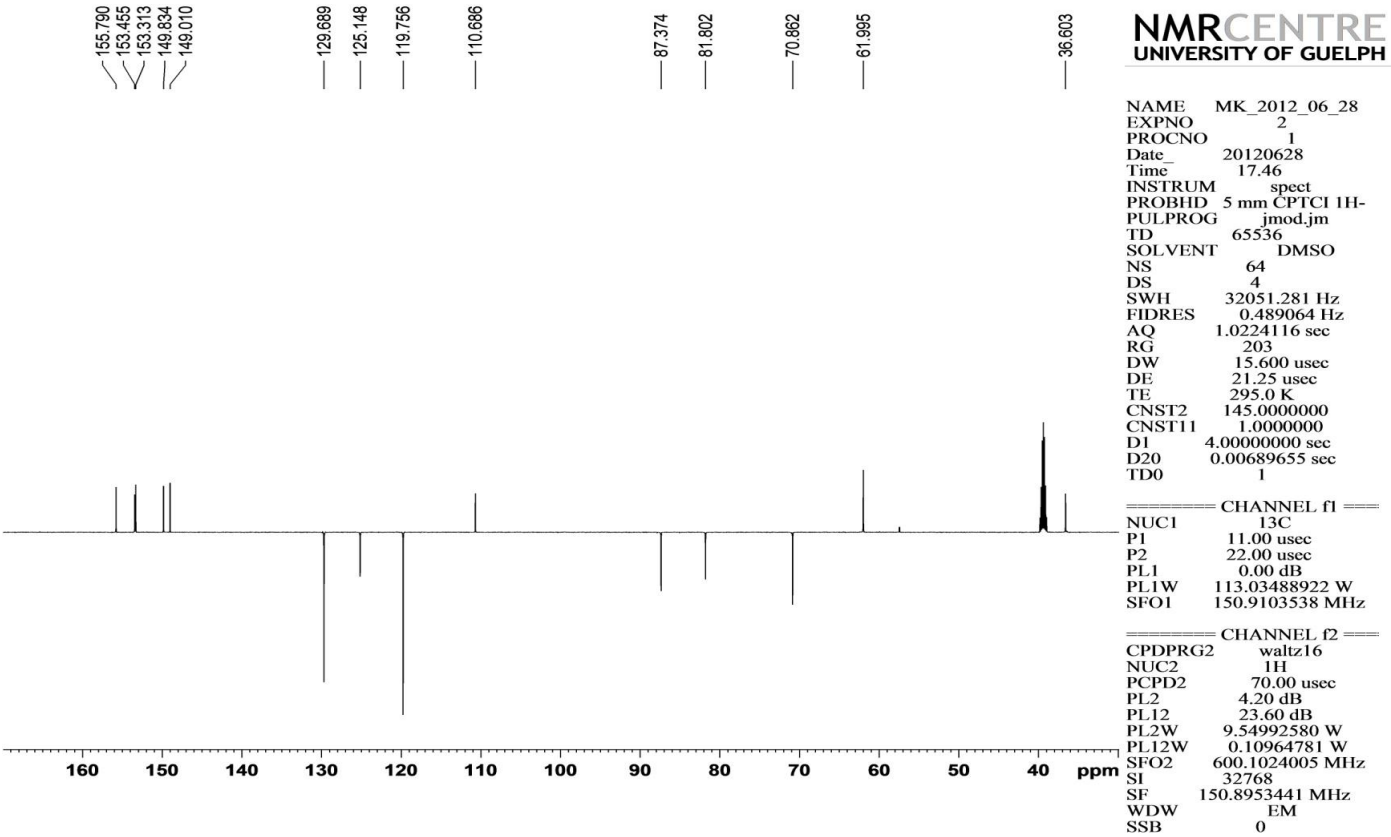


Figure S9: ^{13}C spectrum of Ph-O-dG.

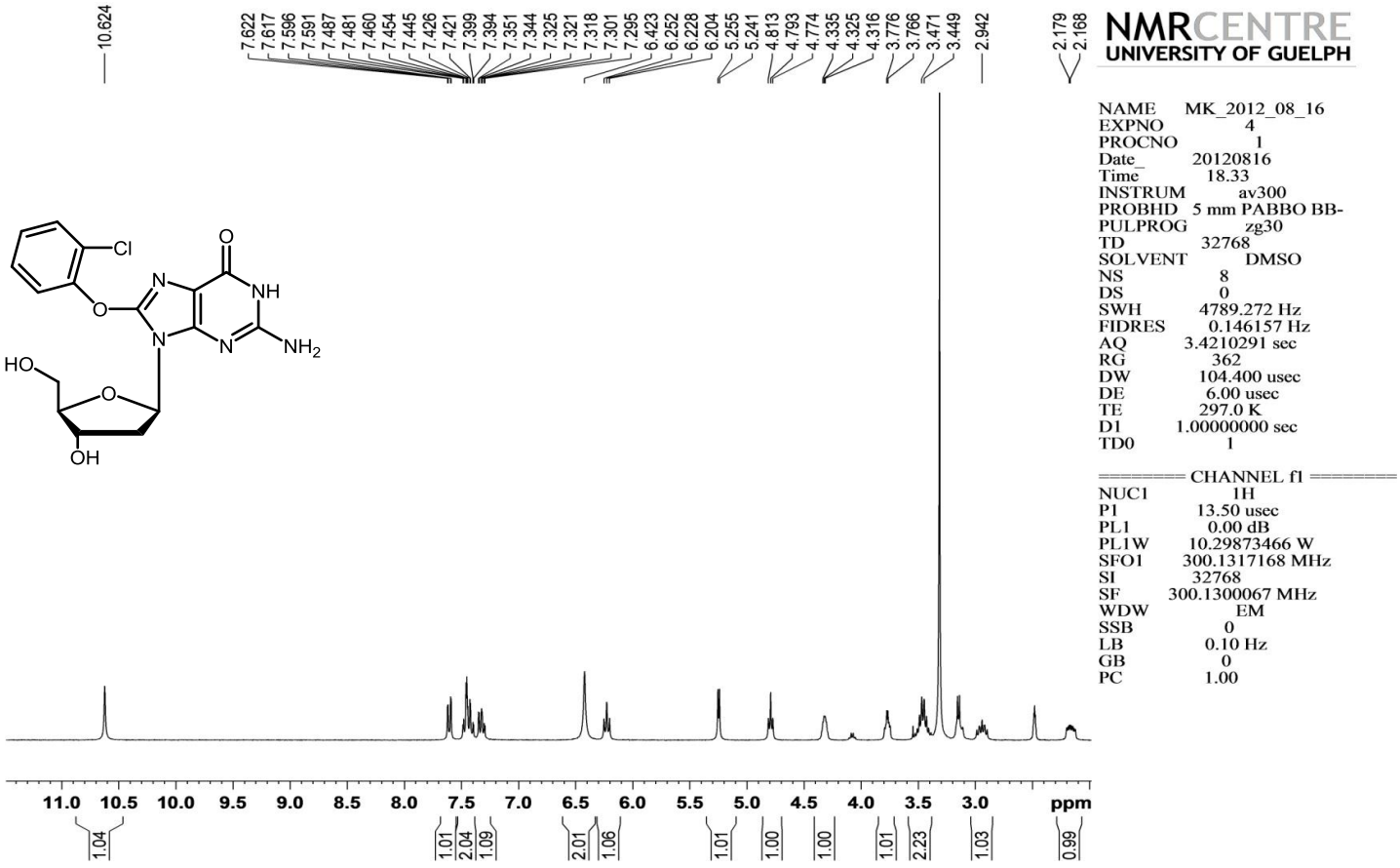


Figure S10: ^{1}H spectrum of 2Cl-Ph-O-dG.

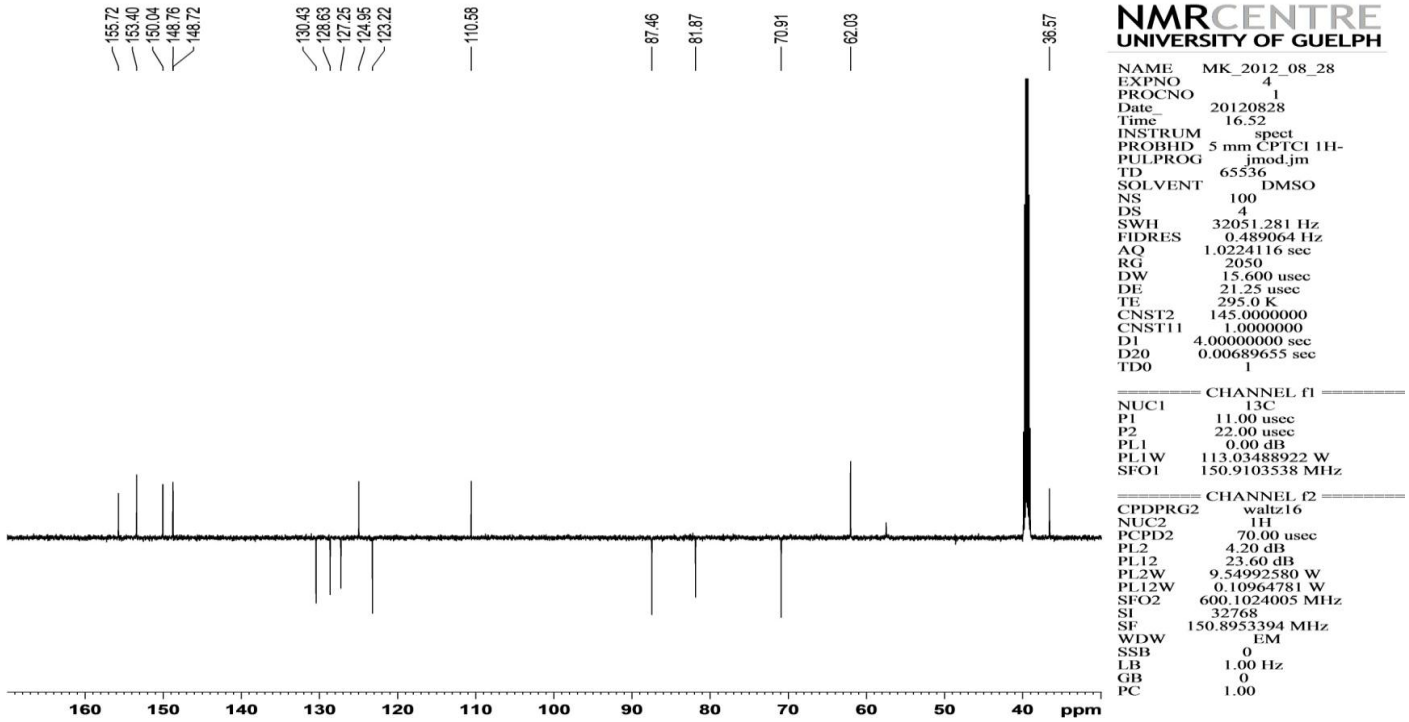


Figure S11: ^{13}C spectrum of 2Cl-Ph-O-dG.

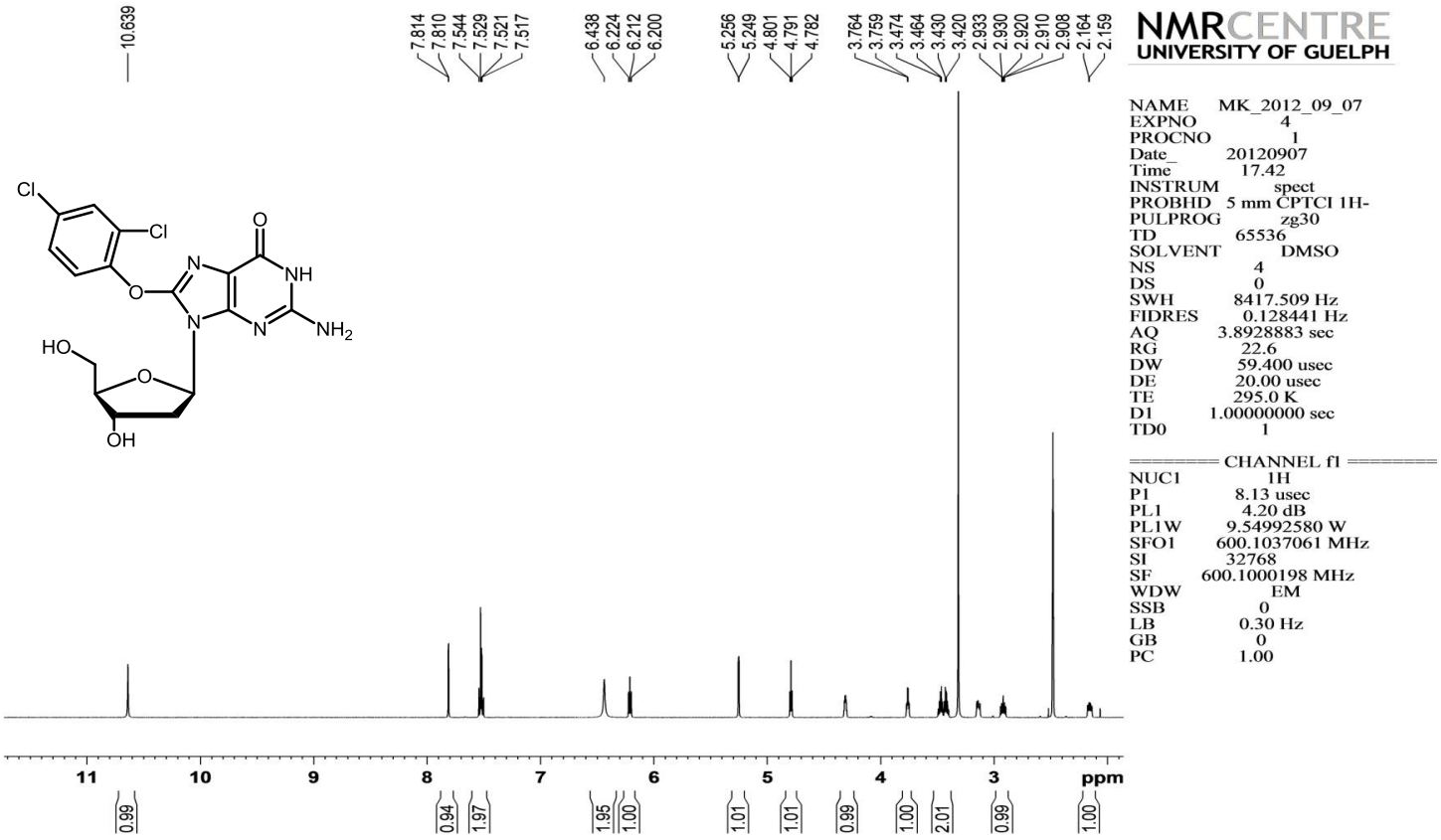


Figure S12: ^{1}H spectrum of DCP-O-dG.

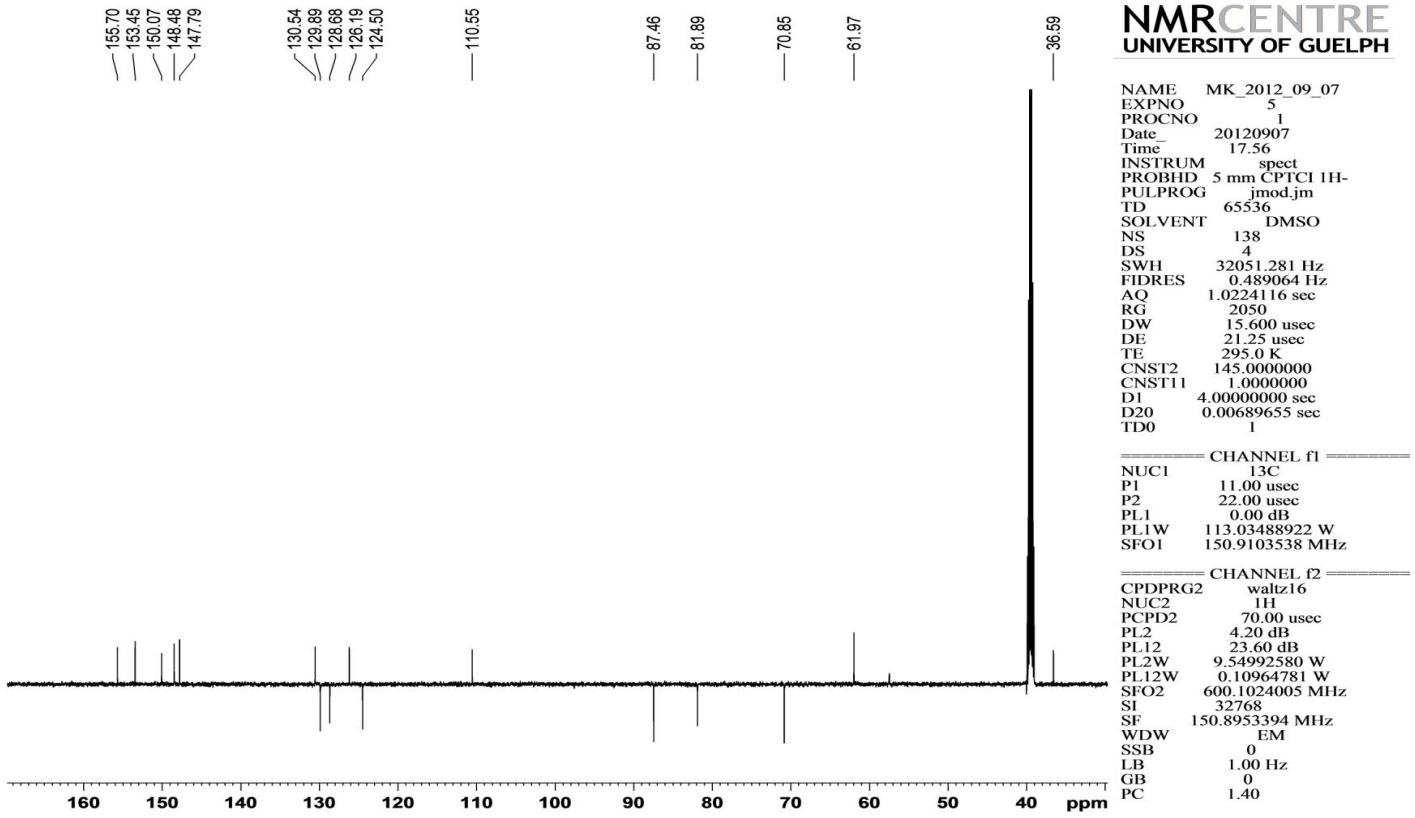


Figure S13: ^{1}C spectrum of DCP-O-dG.

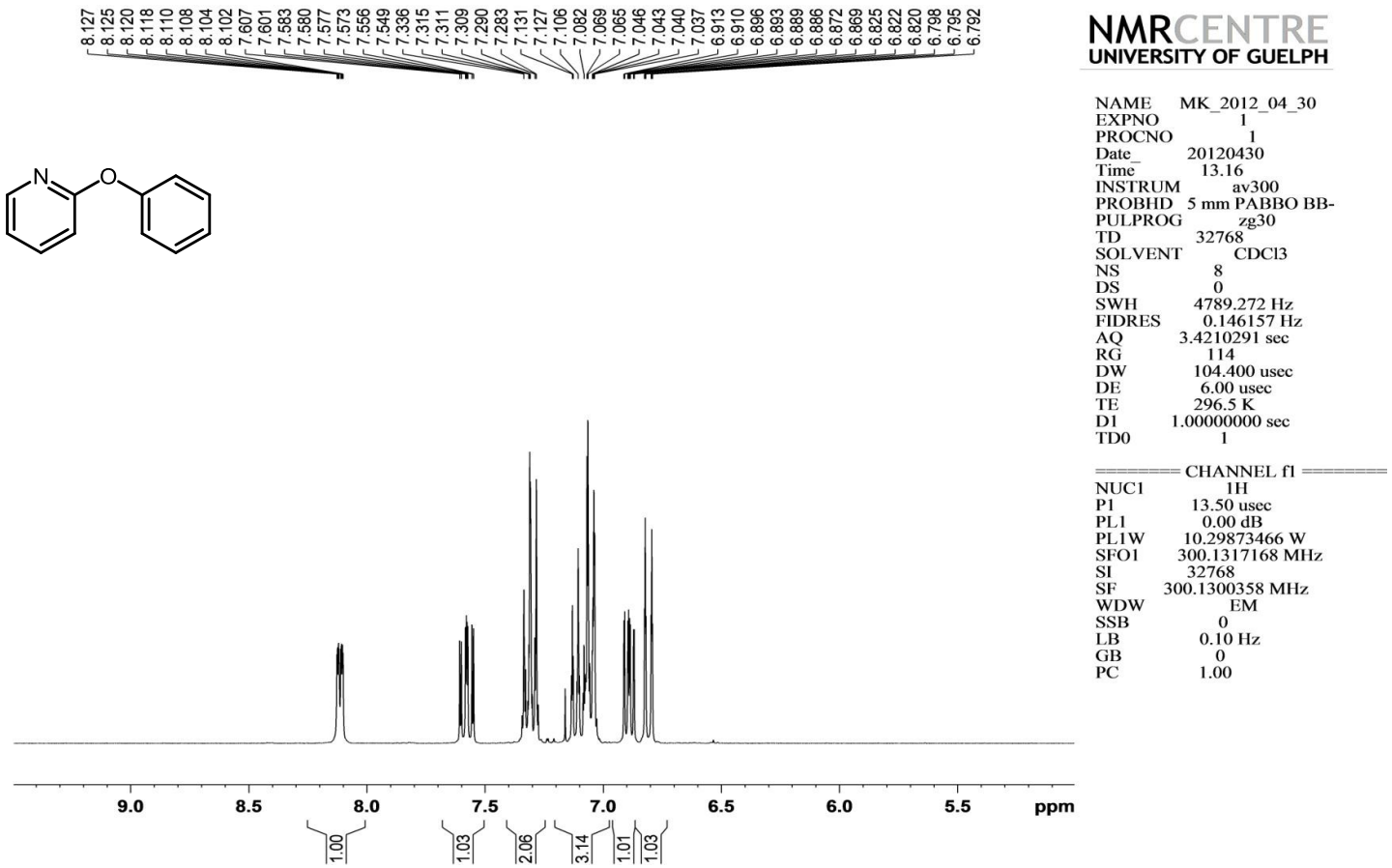


Figure S14: ^{1}H spectrum of Ph-O-pyr.

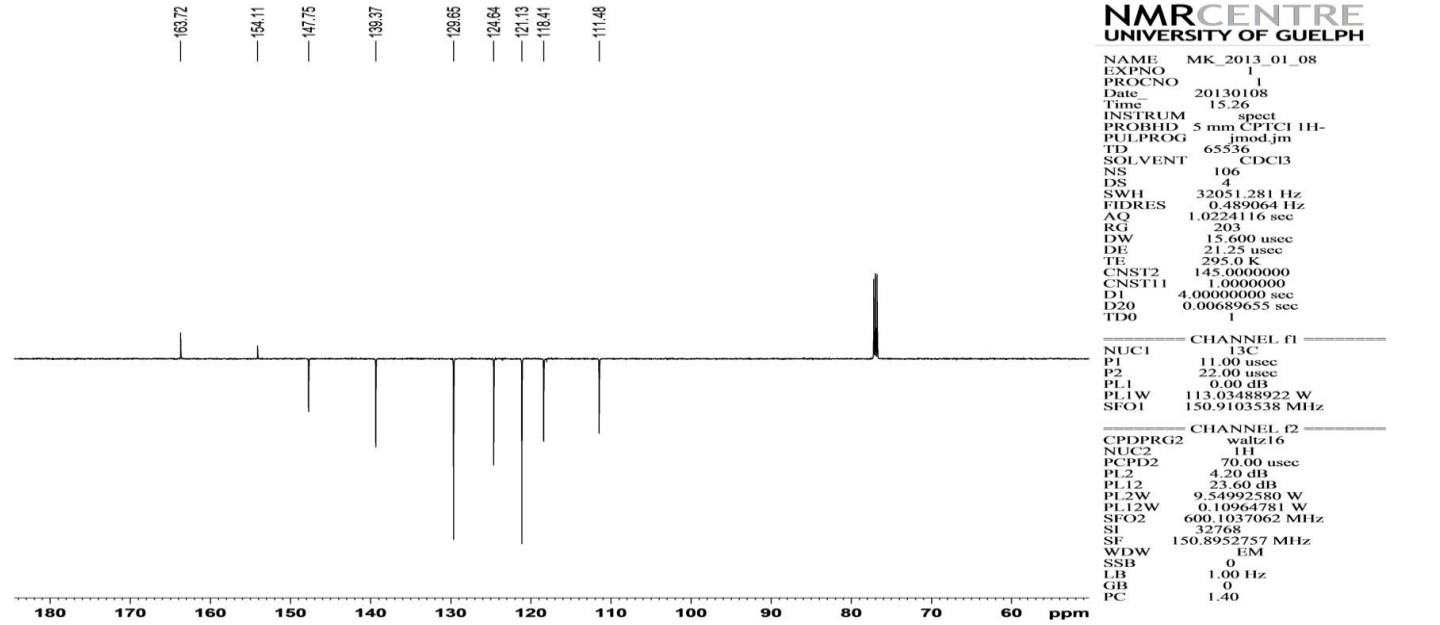


Figure S15: ^{13}C spectrum of Ph-O-pyr.

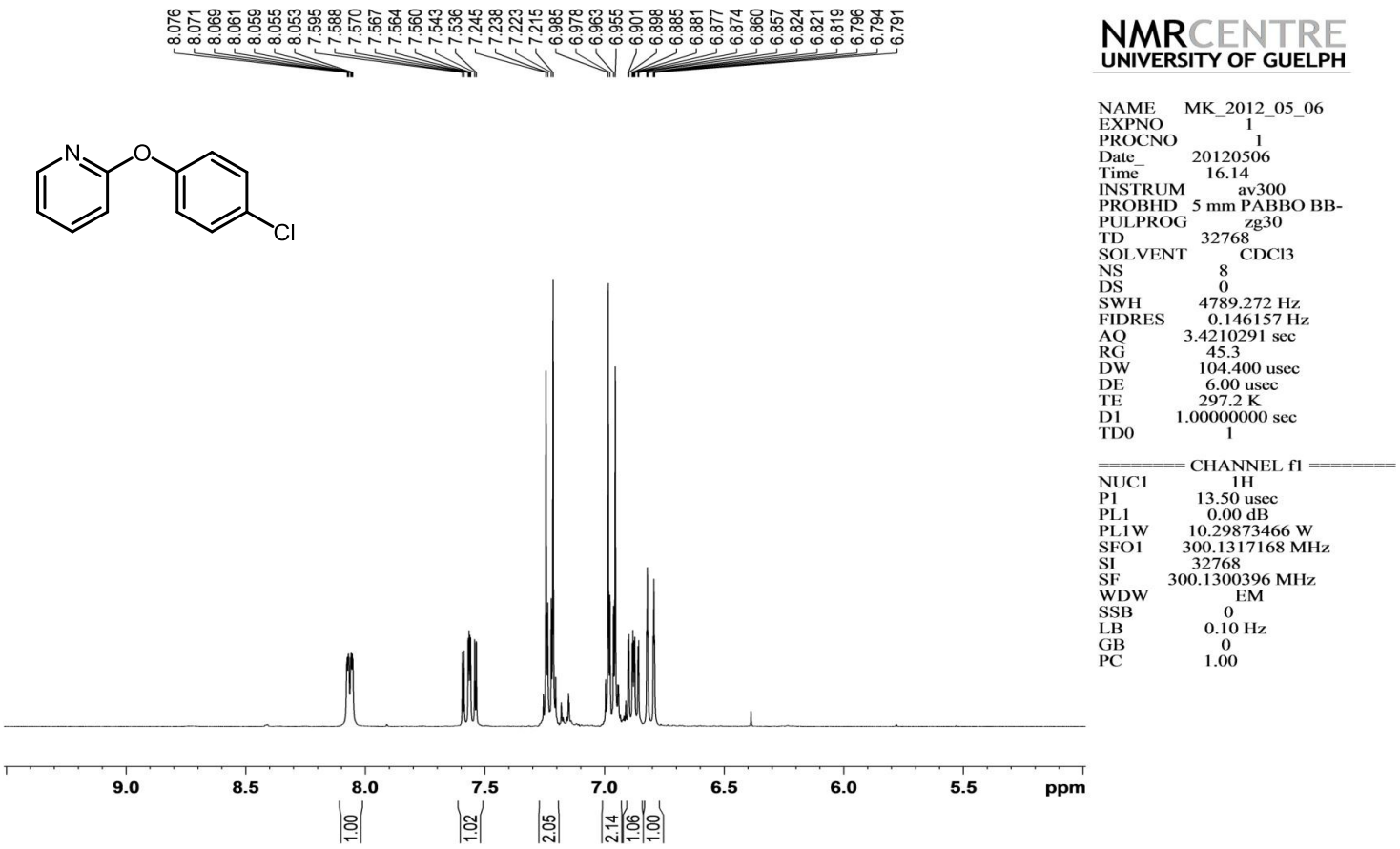


Figure S16: ^{13}H spectrum of 4Cl-Ph-O-pyr.

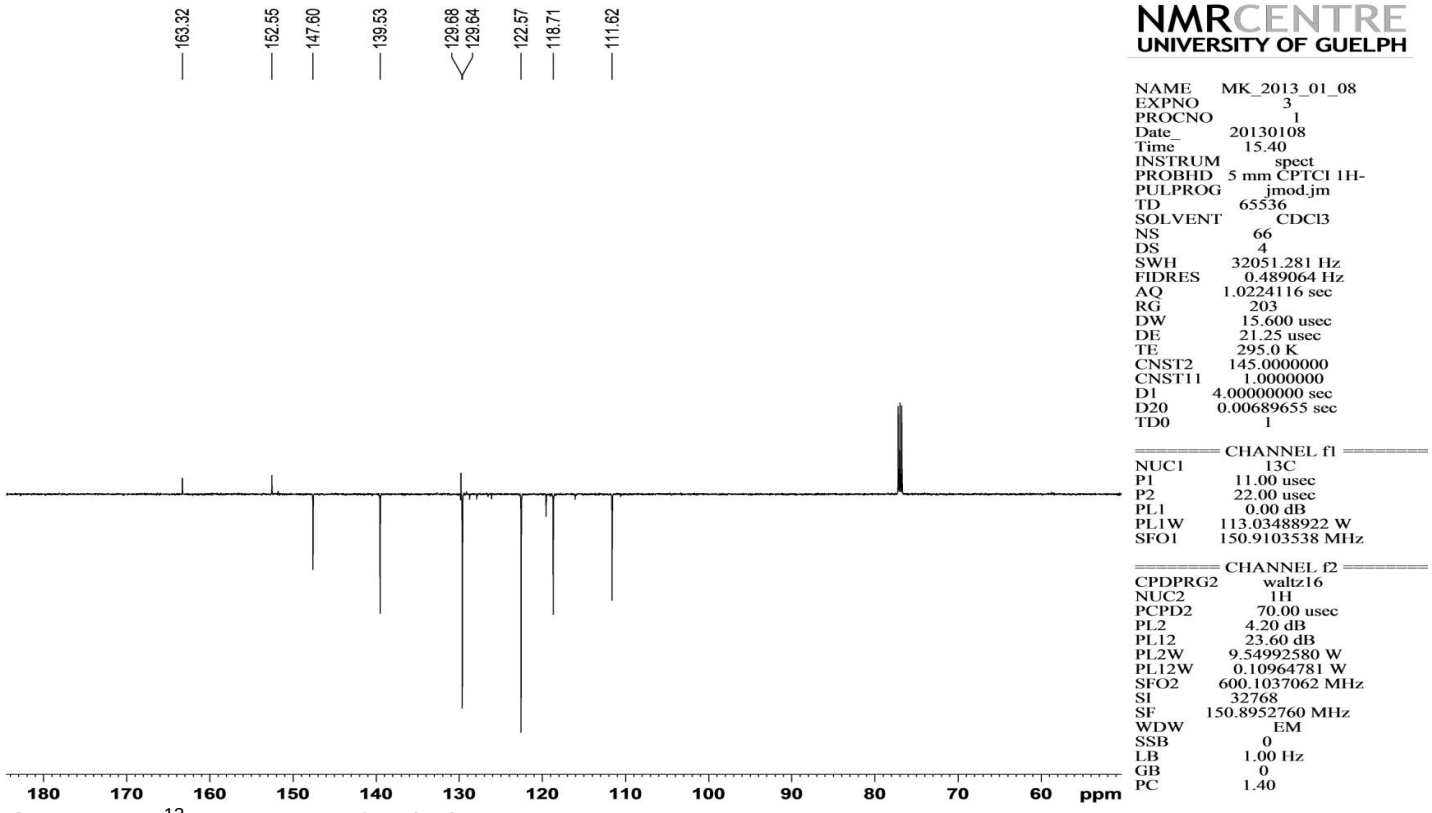


Figure S17: ^{13}C spectrum of 4Cl-Ph-O-pyr.

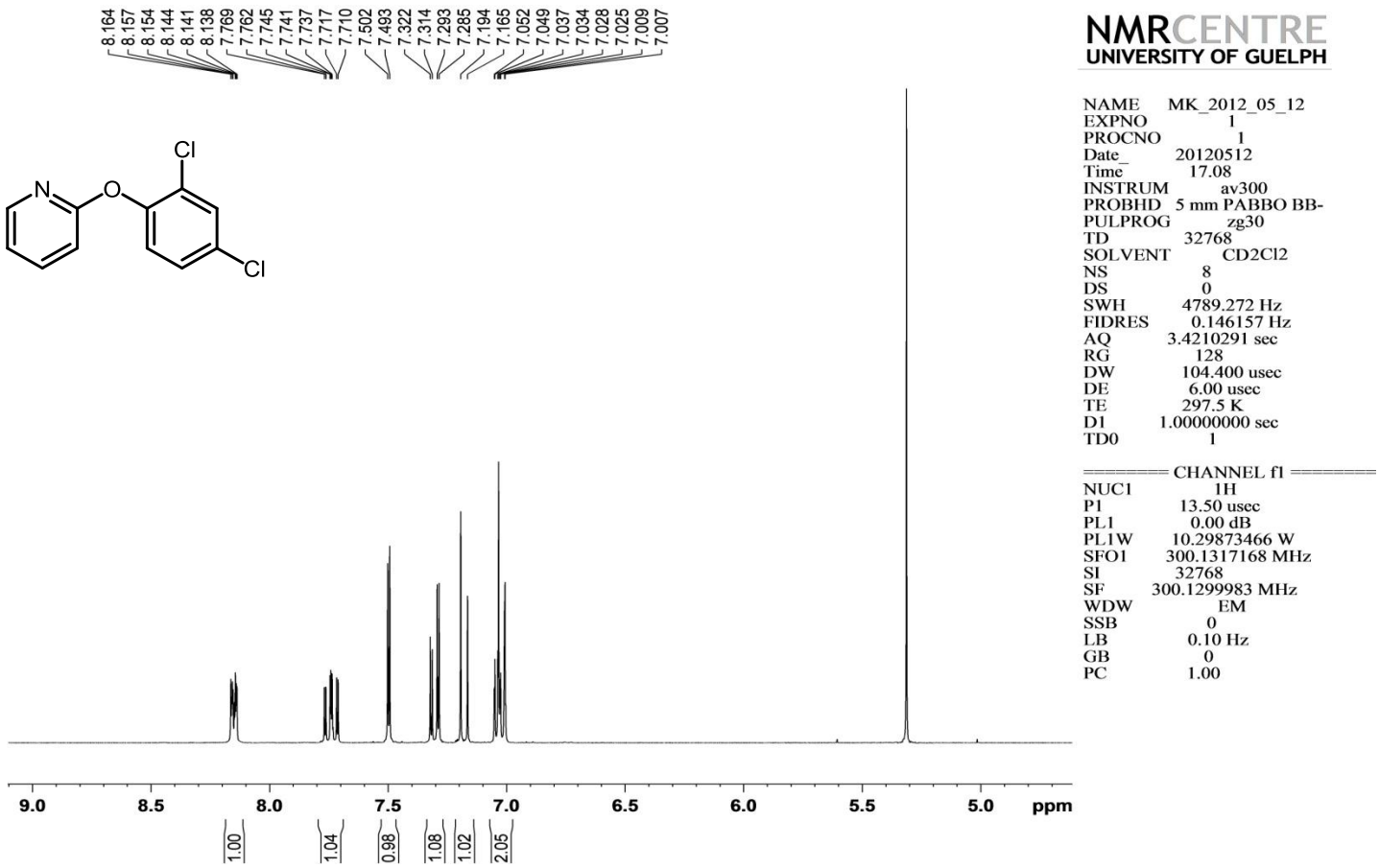


Figure S18: ^{1}H spectrum of DCP-O-pyr.

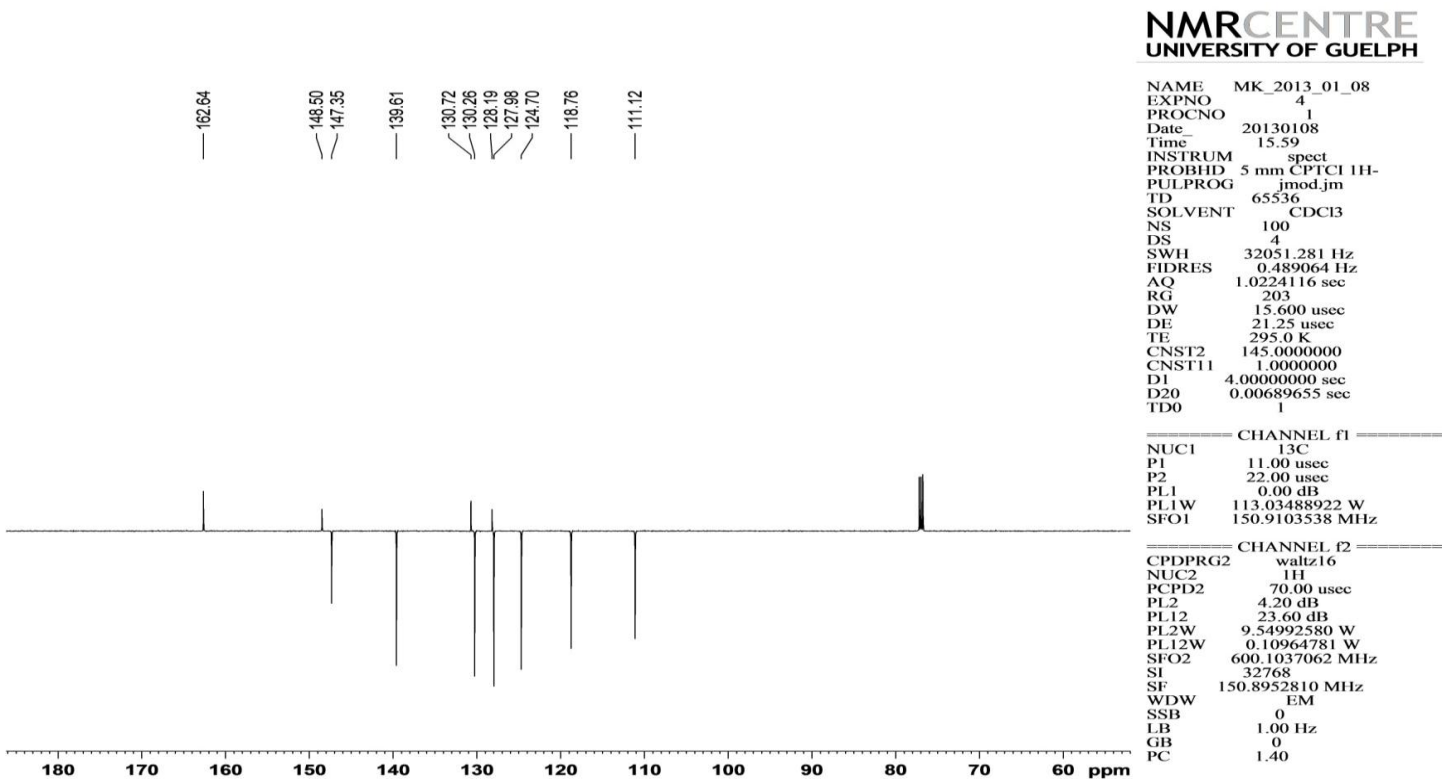


Figure S19: ^{13}C spectrum of DCP-O-pyr.

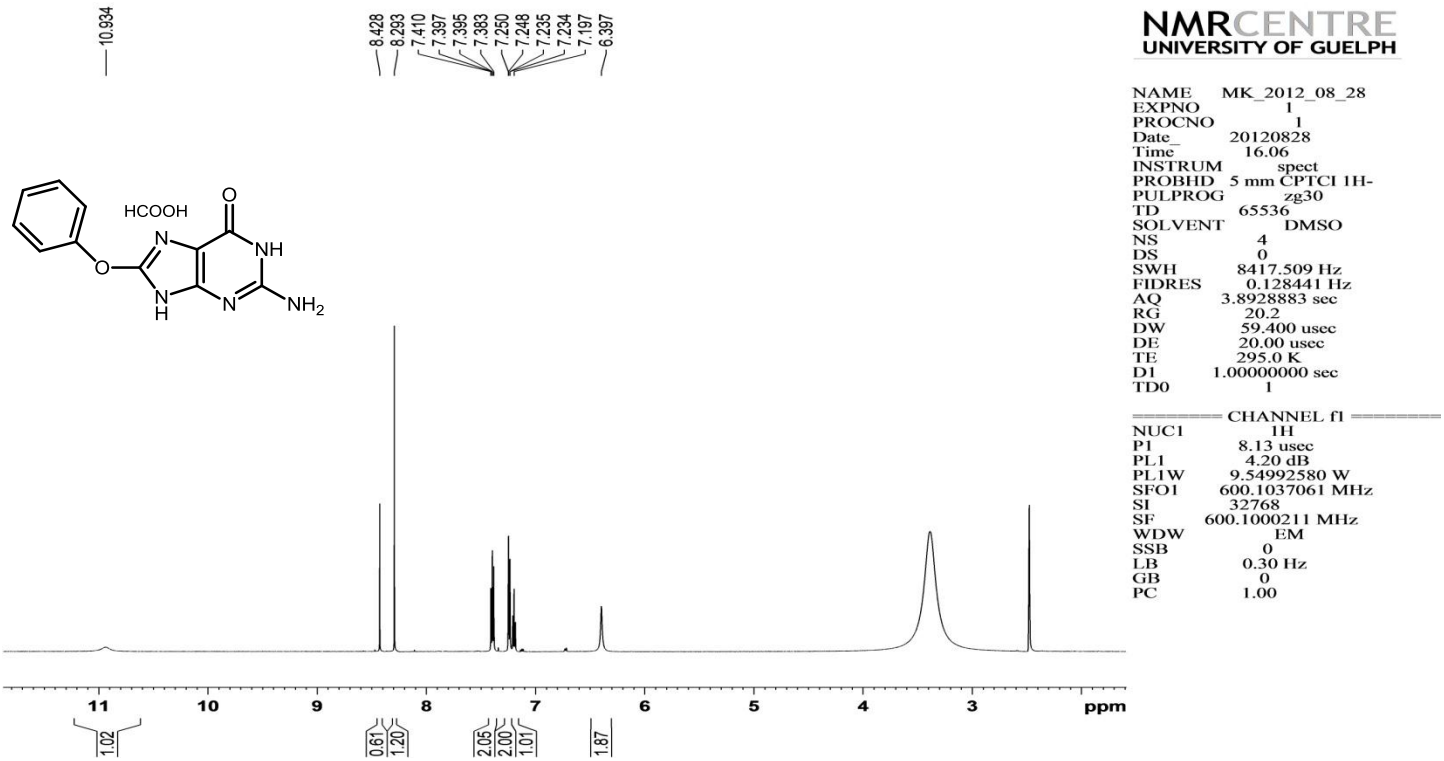


Figure S20: ^{1}H spectrum of Ph-O-G (HCOOH).

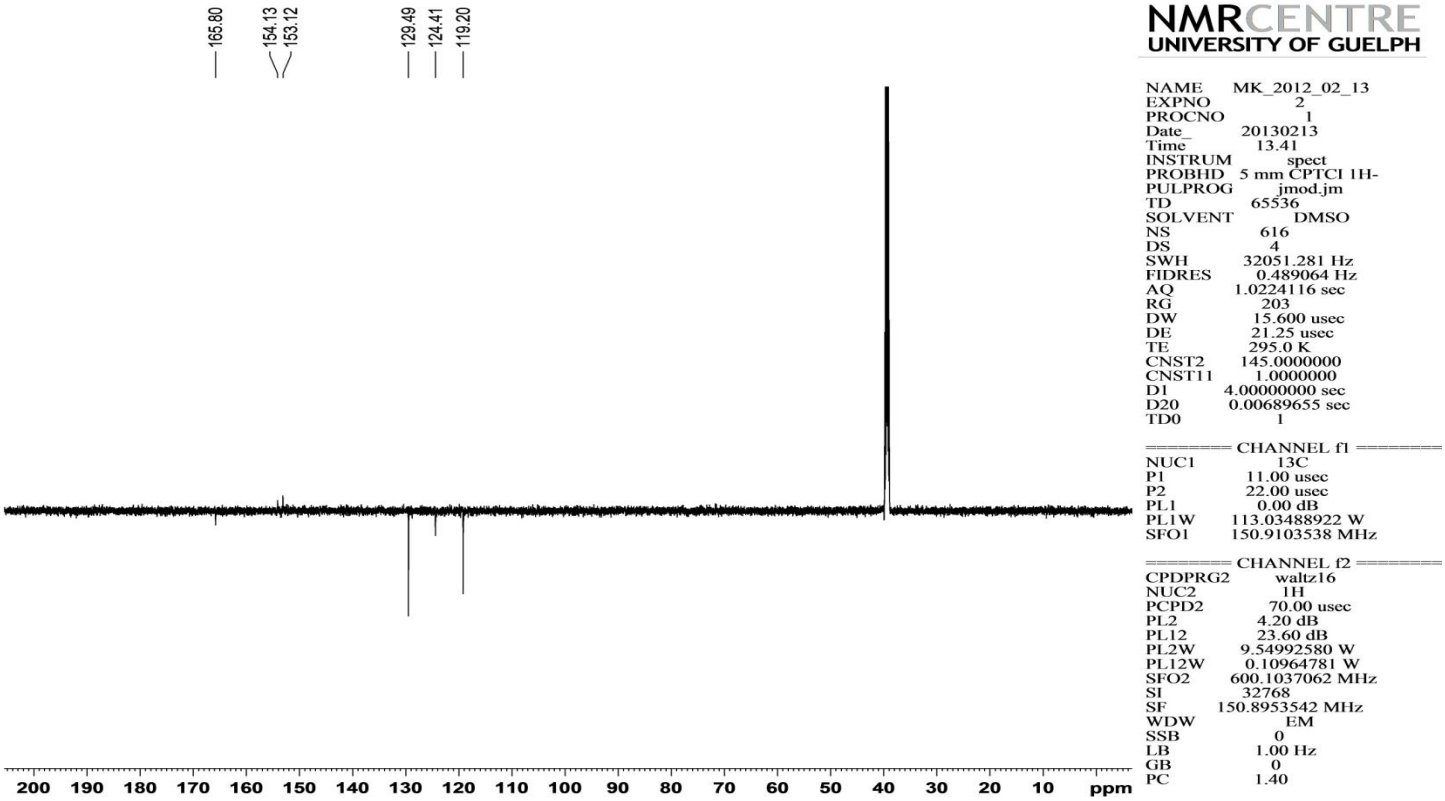


Figure S21: ^{13}C spectrum of Ph-O-G (HCOOH).

Tables S2-S37. Cartesian coordinates of global minimum structures of neutral, N^7H^+ and N^3H^+ *O*-linked C^8-dG adducts and dG, calculated at the B3LYP/6-31G(d) level in gas and solvent (Water) phase

Table S2. dG Netural (gas)

Calculated energy (in Hartrees)= -963.54037136

Atom	Coordinates (Angstroms) X	Y	Z
C	1.10967400	0.45552900	0.22426300
O	1.83592600	0.08817300	-0.95160800
H	0.75419000	1.48779900	0.14286500
C	2.12325100	0.30128500	1.36330500
C	3.22758300	0.42370100	-0.77852300
C	3.41100400	0.81036100	0.70771700
H	2.23861700	-0.75386500	1.62836200
H	1.84210400	0.86296900	2.25949900
C	4.04045500	-0.78597200	-1.23300000
H	3.47616400	1.29906200	-1.39262700
H	4.30527700	0.34129200	1.13796200
H	5.10597800	-0.60830300	-1.05397800
H	3.89908500	-0.93025200	-2.31456300
O	3.68795700	-1.95594100	-0.50927400
H	2.76089600	-2.12995700	-0.74109100
O	3.51406200	2.23386400	0.74747200
H	3.64714100	2.49593100	1.67203600
N	-0.06993100	-0.37094200	0.32942600
C	-0.14511700	-1.74181500	0.55032000
C	-1.36629500	0.04084800	0.10907500
N	-1.36345800	-2.21018400	0.50436400
C	-2.14809700	-1.10577400	0.23143500
N	-1.75436200	1.31771300	-0.14068600
C	-3.57384200	-0.99956600	0.05354900
C	-3.05002400	1.42817300	-0.31482700
O	-4.45563300	-1.83835700	0.09486100
N	-3.91833100	0.37090300	-0.22708800
N	-3.58804900	2.65068400	-0.65492100
H	-4.90070900	0.50259000	-0.44095100
H	-4.51274300	2.86407300	-0.30287200
H	-2.92744400	3.41043300	-0.54882900
H	0.74031400	-2.33152300	0.74502900

Table S3. Ph-O-dG Neutral (gas)

Calculated energy (in Hartrees)= -1269.81916645

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	0.61582000	-1.47235000	-0.07125500
O	1.45511300	-1.60719100	1.06644200
H	-0.27010900	-2.10577800	0.02792200
C	1.47437100	-1.90628200	-1.26895300
C	2.52291100	-2.54443100	0.80149800
C	2.33601600	-3.01550700	-0.65450800
H	2.10669800	-1.07917100	-1.60022900
H	0.86869200	-2.25182000	-2.11280700
C	3.86005600	-1.86008400	1.08631000
H	2.40161000	-3.40636700	1.46948000
H	3.29961300	-3.12199100	-1.16804400
H	4.66020300	-2.60905700	1.04529800
H	3.82736100	-1.46336900	2.11394400
O	4.18085900	-0.85377600	0.14347800
H	3.42402600	-0.22235200	0.11983100
O	1.64243400	-4.26332300	-0.59578500
H	1.51777200	-4.57497400	-1.50600600
N	0.12475100	-0.10120200	-0.12932800
C	-1.20228300	0.32318400	-0.09217900
C	0.86743300	1.06429600	-0.11652700
N	-1.35029400	1.61704400	-0.08092900
C	-0.05069600	2.10360400	-0.08912000
N	2.22248600	1.14412000	-0.11030500
C	0.42369200	3.46039100	-0.07143500
C	2.68695900	2.37514700	-0.08902000
O	-0.17474300	4.52129800	-0.06020900
N	1.86840200	3.46872700	-0.07377100
N	4.04455300	2.57526200	-0.13323800
H	2.26342000	4.40173600	-0.11550700
H	4.41508600	3.39990300	0.32020200
H	4.58485100	1.73096600	0.02744700
O	-2.12167900	-0.65349100	-0.09757700
C	-3.50029500	-0.46761800	0.01134800
C	-4.21434500	-1.66703700	0.07451700
C	-4.14928200	0.76698100	0.04709100
C	-5.60199000	-1.63356600	0.17674400
H	-3.67122600	-2.60647100	0.04549500
C	-5.54396000	0.77624400	0.15156000
H	-3.58106400	1.68505600	-0.00292500
C	-6.27457400	-0.40914800	0.21604000
H	-6.15633200	-2.56667800	0.22732200
H	-6.05729200	1.73352400	0.18147500
H	-7.35745700	-0.38191300	0.29664900

Table S4. 4Cl-Ph-O-dG Neutral (gas)

Calculated energy (in Hartrees)= -1729.41462828

Atom	Coordinates (Angstroms) X	Y	Z
C	1.22052000	-1.47557500	-0.08857900
O	2.03117600	-1.62807200	1.06655300
H	0.32073200	-2.09245700	-0.01098800
C	2.09652400	-1.92217600	-1.26860000
C	3.08708700	-2.58516500	0.82285200
C	2.92320700	-3.04940000	-0.63809600
H	2.75179000	-1.10644800	-1.58293600
H	1.50339700	-2.25429900	-2.12654800
C	4.43017500	-1.92669500	1.13838600
H	2.93440200	-3.44572200	1.48598800
H	3.89560600	-3.17294700	-1.13061200
H	5.21656000	-2.69071600	1.11433500
H	4.38222200	-1.52999500	2.16536100
O	4.79114500	-0.92613500	0.20378200
H	4.04778100	-0.28003000	0.16421900
O	2.20445900	-4.28344300	-0.59784600
H	2.10230800	-4.59606600	-1.51053400
N	0.75661800	-0.09448200	-0.15349300
C	-0.56064700	0.35634600	-0.13970600
C	1.52150300	1.05682300	-0.12416100
N	-0.68505100	1.65217300	-0.12898200
C	0.62360000	2.11381800	-0.11214600
N	2.87698400	1.11008900	-0.09135900
C	1.12347200	3.46139800	-0.08222200
C	3.36493100	2.33219000	-0.05763400
O	0.54456300	4.53280400	-0.08011300
N	2.56761200	3.44166000	-0.05623600
N	4.72584400	2.50503000	-0.07313600
H	2.98145000	4.36697900	-0.08643900
H	5.10534900	3.32560200	0.37993300
H	5.24807900	1.65123700	0.09635300
O	-1.50283700	-0.60105500	-0.16343300
C	-2.87337000	-0.38026900	-0.06877700
C	-3.62265800	-1.55865400	-0.01855100
C	-3.49369300	0.86939600	-0.03377200
C	-5.00920000	-1.49704900	0.06909500
H	-3.10950900	-2.51450700	-0.04575800
C	-4.88721500	0.92375600	0.05601000
H	-2.90407700	1.77458600	-0.07346500
C	-5.63408400	-0.24970100	0.10610000
H	-5.59845900	-2.40663300	0.11013300
H	-5.38564400	1.88677500	0.08558600
Cl	-7.38794100	-0.16374700	0.21735700

Table S5. DCP-O-dG Neutral (gas)

Calculated energy (in Hartrees)= -2189.00576382

Atom	Coordinates (Angstroms) X	Y	Z
C	1.33191900	-1.35395500	-0.04176300
O	2.15626500	-1.53957800	1.09800900
H	0.39066800	-1.90009600	0.06842300
C	2.14598500	-1.88386300	-1.23100400
C	3.13595800	-2.57489600	0.85237400
C	2.90733300	-3.05395300	-0.59523000
H	2.84986400	-1.12321700	-1.57755200
H	1.51019700	-2.18976000	-2.06780100
C	4.52897400	-2.00956200	1.12898800
H	2.93567100	-3.40954600	1.53551700
H	3.85728000	-3.25326500	-1.10684800
H	4.53090800	-1.59238100	2.14894100
H	5.25758300	-2.82878600	1.10433600
O	4.94178800	-1.05405100	0.16894000
H	4.24491800	-0.35809600	0.13199500
O	2.10769600	-4.23404900	-0.51277500
H	1.94409400	-4.54587200	-1.41674100
N	0.97105400	0.05969900	-0.12603700
C	-0.30681700	0.60636000	-0.11318900
C	1.81741000	1.15265300	-0.11970900
N	-0.33952300	1.90723900	-0.11907400
C	0.99913600	2.27306600	-0.11653300
N	3.17277900	1.10867000	-0.10099600
C	1.59530000	3.58131800	-0.10820500
C	3.74852200	2.29248800	-0.08899100
O	1.09442500	4.69122900	-0.11499700
N	3.03394100	3.45733400	-0.09417200
N	5.11724500	2.36442000	-0.12061500
H	3.51374900	4.34962700	-0.13963300
H	5.56335600	3.16291200	0.31036300
H	5.57856200	1.47685300	0.05247300
O	-1.31692400	-0.28326500	-0.12533400
C	-2.65719000	0.02937200	-0.03929100
C	-3.18683200	1.31922200	0.04365200
C	-3.52410100	-1.07629700	-0.04031700
C	-4.56778100	1.49919400	0.12880400
H	-2.51582100	2.16736600	0.03781900
C	-4.90149900	-0.89955200	0.04362800
C	-5.41347800	0.39424200	0.12859400
H	-4.97745900	2.50097200	0.19352700
H	-5.55852400	-1.76078100	0.04320400
Cl	-2.88321500	-2.70208900	-0.14567500
Cl	-7.15187600	0.62004300	0.23430100

Table S6. TCP-O-dG Neutral (gas)

Calculated energy (in Hartrees)= -2648.59270457

Atom	Coordinates (Angstroms) X	Y	Z
C	-1.73977400	-1.45184200	0.05087300
O	-2.60377300	-1.48963400	-1.07341200
H	-0.91978900	-2.16668100	-0.06896200
C	-2.61708400	-1.81165600	1.25916300
C	-3.76097300	-2.31236700	-0.79918500
C	-3.59944400	-2.81835500	0.64819200
H	-3.15560900	-0.92869000	1.61165300
H	-2.03519100	-2.22811200	2.08743200
C	-5.02323100	-1.48765800	-1.05331600
H	-3.74105400	-3.17373400	-1.47837300
H	-4.56000400	-2.82965100	1.17803200
H	-4.96435800	-1.08233900	-2.07638900
H	-5.89628900	-2.14999200	-1.00898500
O	-5.22323500	-0.46731700	-0.09308600
H	-4.40782500	0.08714300	-0.08057900
O	-3.04086500	-4.13012000	0.56315300
H	-2.93112400	-4.46461300	1.46716200
N	-1.11695600	-0.13322100	0.11412300
C	0.23384800	0.16194300	0.07494200
C	-1.73610100	1.10635000	0.11203000
N	0.52939500	1.42383800	0.06785000
C	-0.71377700	2.04469700	0.08522000
N	-3.07512800	1.32379100	0.11626900
C	-1.04718200	3.44370500	0.07498800
C	-3.41104100	2.59615300	0.10383900
O	-0.34481600	4.43797100	0.06361700
N	-2.48411600	3.59944800	0.08605200
N	-4.74009300	2.93366400	0.16059900
H	-2.78077900	4.56809500	0.13215300
H	-5.02944800	3.79586200	-0.28165100
H	-5.36626000	2.15013900	0.00416600
O	1.09883600	-0.88657600	0.06944200
C	2.44356300	-0.58286000	0.00709500
C	3.09449000	-0.48696600	-1.22791500
C	3.19622000	-0.45713900	1.17965900
C	4.46774400	-0.26193200	-1.29913900
C	4.57028800	-0.23225000	1.13110800
C	5.18770200	-0.13468900	-0.11360000
H	4.95932100	-0.18744100	-2.26121500
H	5.14058500	-0.13444800	2.04640900
Cl	2.40781700	-0.59508800	2.72974800
Cl	6.91526800	0.14703100	-0.18958300

Cl	2.17900100	-0.66333000	-2.70054900

Table S7. PCP-O-dG Neutral (gas)

Calculated energy (in Hartrees)= -3567.76004024

Atom	Coordinates (Angstroms) X	Y	Z
C	2.36715900	-1.44837200	-0.11497000
O	3.21049700	-1.52009500	1.02249900
H	1.54293100	-2.16348700	-0.02959200
C	3.26408800	-1.77689800	-1.31758300
C	4.37062300	-2.33870400	0.74554400
C	4.23249800	-2.80383300	-0.71776000
H	3.81131800	-0.88623800	-1.63589600
H	2.69575600	-2.16842900	-2.16711500
C	5.63027200	-1.52546100	1.04480900
H	4.33599300	-3.21832600	1.40012800
H	5.20185500	-2.80421500	-1.23138100
H	5.55425500	-1.14816500	2.07739000
H	6.50213700	-2.18907500	0.99785900
O	5.85032900	-0.47977000	0.11662700
H	5.03706100	0.07736400	0.10463600
O	3.66773900	-4.11500300	-0.67855900
H	3.57815500	-4.42696800	-1.59279000
N	1.74884900	-0.12589100	-0.15194000
C	0.39992300	0.17363700	-0.11848900
C	2.37162000	1.11166800	-0.10854100
N	0.10692700	1.43495900	-0.08037500
C	1.35202500	2.05236000	-0.06726000
N	3.71093100	1.32446300	-0.09131800
C	1.68923000	3.44981900	-0.01600000
C	4.05057300	2.59525200	-0.04016600
O	0.98912400	4.44489300	0.01389900
N	3.12650400	3.60091100	-0.00671200
N	5.38058700	2.92890000	-0.07025000
H	3.42660200	4.56951400	-0.02256500
H	5.66802400	3.78188000	0.39049300
H	6.00364500	2.14062200	0.07372200
O	-0.47223700	-0.87124900	-0.15125000
C	-1.81176200	-0.56147700	-0.06136900
C	-2.56025100	-0.39689200	-1.22988700
C	-2.42613400	-0.50389000	1.19291100
C	-3.94039400	-0.16227100	-1.14781600
C	-3.80571700	-0.26882100	1.28323200
C	-4.56168200	-0.09530800	0.11105900
Cl	-1.45413500	-0.73830100	2.60858400
Cl	-6.26915400	0.19479100	0.21824900

Cl	-1.75103800	-0.49825600	-2.76063000
Cl	-4.57046000	-0.19850400	2.83812900
Cl	-4.87111600	0.04127500	-2.59684600

Table S8. dG N^7H^+ (gas)

Calculated energy (in Hartrees)= -963.94179434

Atom	Coordinates (Angstroms) X	Y	Z
C	1.16274000	0.68038900	-0.20529800
O	2.03165400	0.10715200	-1.14661000
H	0.73648600	1.61670500	-0.57603400
C	1.95213600	0.85384800	1.10189200
C	3.40247900	0.13982500	-0.67794100
C	3.39009200	1.01828200	0.58692400
H	1.87541300	-0.05019100	1.71192300
H	1.60798700	1.71121200	1.68615100
C	3.91526600	-1.28134000	-0.50388000
H	4.00242500	0.63632400	-1.44680400
H	4.12907400	0.68128500	1.32499800
H	4.97163900	-1.24096100	-0.20666100
H	3.84884200	-1.80432900	-1.46726300
O	3.12910700	-1.95321500	0.49044400
H	3.59340600	-2.76534200	0.74582800
O	3.65159000	2.34291000	0.14850900
H	3.75158400	2.91513600	0.92563600
N	-0.00010900	-0.23673600	-0.06339800
C	0.09199200	-1.57842000	0.01054700
C	-1.34491600	0.11963400	-0.04780400
N	-1.13593700	-2.09342900	0.08312100
C	-2.05833100	-1.06223500	0.04930600
N	-1.83248400	1.36657400	-0.11686700
C	-3.49548200	-1.06014700	0.08645600
C	-3.15858200	1.41212700	-0.08831400
O	-4.25931600	-2.00021100	0.17022200
N	-3.95198800	0.28862700	0.00968400
N	-3.77004700	2.61013800	-0.13956800
H	-4.96322600	0.37818200	0.04243600
H	-4.76997100	2.71506600	-0.22284500
H	-3.19098900	3.42825900	-0.26662700
H	1.03598700	-2.11267700	0.02372600
H	-1.36333600	-3.07974900	0.14288400

Table S9. Ph-O-dG N^7H^+ (gas)

Calculated energy (in Hartrees)= -1270.21137139

Atom	Coordinates (Angstroms) X	Y	Z
C	0.88724000	-1.53655800	-0.02942200
O	1.74975100	-1.47884700	1.07756800
H	0.10823100	-2.29336500	0.10720400
C	1.76060800	-1.84094900	-1.25095800
C	2.96793000	-2.23314600	0.79827900
C	2.78548300	-2.79520500	-0.63461700
H	2.25768000	-0.93717600	-1.60854000
H	1.20775900	-2.31292000	-2.06557400
C	4.17809800	-1.32322300	1.00294000
H	3.00899300	-3.05798900	1.52053500
H	3.72997700	-2.79976900	-1.19126700
H	4.12749500	-0.90056300	2.01828500
H	5.09034900	-1.92708500	0.94200600
O	4.28112500	-0.31200100	0.01505900
H	3.43943500	0.18875200	0.03449100
O	2.16838600	-4.07687800	-0.62322800
H	2.80038000	-4.72863000	-0.28090000
N	0.15946300	-0.23922900	-0.09711200
C	-1.18901400	-0.10270100	-0.06323200
C	0.70672400	1.05038400	-0.10118200
N	-1.52062500	1.19382400	-0.06591000
C	-0.34162100	1.94102300	-0.08780300
N	2.01114800	1.35329500	-0.11533200
C	-0.11995900	3.35742500	-0.08420700
C	2.27803700	2.65615100	-0.10421400
O	-0.93261500	4.26012900	-0.07188900
N	1.28965800	3.60869400	-0.09601300
N	3.56549400	3.04054000	-0.10233400
H	1.52738100	4.59617300	-0.08910700
H	3.85473800	4.00625900	-0.06546400
H	4.27586300	2.31744200	-0.06765700
O	-1.99155700	-1.14003600	-0.04510800
C	-3.40124700	-0.89752000	0.03491800
C	-4.12428400	-0.83942600	-1.15010200
C	-3.98281200	-0.79541200	1.29287800
C	-5.50679000	-0.65773600	-1.06204200
H	-3.62551300	-0.95207700	-2.10746400
C	-5.36636700	-0.61369200	1.35805200
H	-3.37705600	-0.87504300	2.19001100
C	-6.12362600	-0.54337800	0.18608300
H	-6.09806700	-0.61368900	-1.97115600
H	-5.84908800	-0.53562100	2.32704100
H	-7.19871700	-0.40661500	0.24597500
H	-2.46693400	1.55689700	-0.05295800

Table S10. 4Cl-Ph-O-dG N^7H^+ (gas)

Calculated energy (in Hartrees)= -1729.80152569

Atom	Coordinates (Angstroms) X	Y	Z
C	1.46625900	-1.54166600	-0.03837500
O	2.31265700	-1.50564200	1.08140000
H	0.66634600	-2.27854600	0.08596000
C	2.34987600	-1.86803600	-1.24686100
C	3.51573600	-2.29105700	0.82007300
C	3.33856900	-2.84971700	-0.61475700
H	2.87657800	-0.97782000	-1.59592700
H	1.79751200	-2.32499900	-2.07031800
C	4.74553100	-1.41168600	1.04082500
H	3.52515100	-3.11567200	1.54360500
H	4.29045400	-2.88145900	-1.15770000
H	4.69218400	-0.98747800	2.05535300
H	5.64294900	-2.03841700	0.99203400
O	4.88687300	-0.40392000	0.05429800
H	4.05888000	0.11925100	0.06421500
O	2.68513700	-4.11319300	-0.61109800
H	3.29400000	-4.78300400	-0.26176900
N	0.77199100	-0.22569300	-0.11535400
C	-0.57223200	-0.05513900	-0.09976300
C	1.35144500	1.05017200	-0.10728800
N	-0.87212100	1.24882600	-0.10223000
C	0.32530000	1.96639300	-0.10518500
N	2.66269900	1.32094500	-0.10234800
C	0.58131600	3.37717600	-0.09289800
C	2.96129700	2.61709100	-0.08283300
O	-0.20976400	4.29866300	-0.08818700
N	1.99653400	3.59374900	-0.08451100
N	4.25742200	2.96943100	-0.06226300
H	2.25844100	4.57508000	-0.07068700
H	4.57007000	3.92755500	-0.01727900
H	4.94931100	2.22891500	-0.02106600
O	-1.40079100	-1.07429600	-0.09676700
C	-2.80214700	-0.80359300	-0.03008200
C	-3.51662700	-0.72170500	-1.21936800
C	-3.40157000	-0.70611700	1.22024300
C	-4.89494500	-0.51741500	-1.15205500
H	-3.01553700	-0.83309300	-2.17557900
C	-4.77996500	-0.50162400	1.28001700
H	-2.81286400	-0.80555900	2.12658600
C	-5.51632800	-0.40598000	0.09528700
H	-5.48327400	-0.45290000	-2.06052100
H	-5.28033800	-0.42520300	2.23890600
H	-1.80840900	1.63715400	-0.10165700

Cl	-7.23759500	-0.15118200	0.17492500

Table S11. DCP-O-dG N^7H^+ (gas)

Calculated energy (in Hartrees)= -2189.38985431

Atom	Coordinates (Angstroms) X	Y	Z
C	1.58465000	-1.50490600	-0.27917400
O	2.33094900	-1.54095700	0.90906200
H	0.75209300	-2.21490500	-0.25255100
C	2.55891400	-1.81934100	-1.41944500
C	3.52231400	-2.36443800	0.72189900
C	3.45246800	-2.86151800	-0.74431800
H	3.14525600	-0.93749100	-1.68509400
H	2.06561600	-2.22373100	-2.30550800
C	4.75879600	-1.54444200	1.08632400
H	3.43633600	-3.21529600	1.40905700
H	4.44661100	-2.91068000	-1.20394100
H	4.63231900	-1.16103200	2.11054500
H	5.63436900	-2.20313600	1.08624700
O	5.02053200	-0.50238400	0.16178800
H	4.21170200	0.04819500	0.12159300
O	2.75629900	-4.09765100	-0.84905100
H	3.30649300	-4.80312900	-0.47359300
N	0.94494500	-0.16119900	-0.36242500
C	-0.38784400	0.05980600	-0.44064300
C	1.56517800	1.09051000	-0.25202700
N	-0.64326900	1.37169300	-0.41159500
C	0.57344500	2.04338400	-0.28667700
N	2.88013700	1.31149600	-0.13247200
C	0.87516900	3.44207900	-0.18840000
C	3.21959000	2.59340000	-0.02806000
O	0.11737700	4.39089900	-0.20304500
N	2.29146500	3.60474000	-0.05994600
N	4.52096600	2.89613900	0.11034400
H	2.58474700	4.57405600	0.01916000
H	4.85924400	3.83814400	0.23686000
H	5.18077800	2.12881200	0.17872400
O	-1.24729800	-0.93017400	-0.56811500
C	-2.62971600	-0.65201900	-0.43733500
C	-3.40527500	-0.60869100	-1.59014100
C	-3.19987600	-0.52450500	0.83374900
C	-4.78093100	-0.41654100	-1.48242800
H	-2.93439700	-0.74170800	-2.55887300
C	-4.57600800	-0.32989500	0.94360200
C	-5.35445000	-0.27637300	-0.21550500
H	-5.40214600	-0.38259300	-2.36991500

H	-5.03198200	-0.23023400	1.92168000
H	-1.56191900	1.79743200	-0.45692900
Cl	-7.07122700	-0.03600200	-0.07024300
Cl	-2.20914100	-0.61339300	2.26327600

Table S12. TCP-O-dG N^7H^+ (gas)

Calculated energy (in Hartrees)= -2648.97729750

Atom	Coordinates (Angstroms) X	Y	Z
C	-1.73653200	-1.48668900	0.04218900
O	-2.60335400	-1.50137400	-1.06113400
H	-0.89828300	-2.17703700	-0.09459300
C	-2.57802800	-1.85582300	1.26816900
C	-3.75501800	-2.35338000	-0.77643700
C	-3.52225200	-2.89344300	0.65764800
H	-3.14642500	-0.99411100	1.62350100
H	-1.98610100	-2.27724800	2.08296300
C	-5.03663100	-1.54732800	-0.98148700
H	-3.72776900	-3.18098300	-1.49603100
H	-4.46112000	-2.97420300	1.21802900
H	-5.02481800	-1.12801500	-1.99936000
H	-5.89562300	-2.22408900	-0.91328100
O	-5.21860900	-0.54229500	0.00111300
H	-4.42125800	0.02554100	-0.02652900
O	-2.80103900	-4.11929000	0.64778300
H	-3.37793600	-4.82284100	0.31077900
N	-1.11677900	-0.13100300	0.10316500
C	0.21199600	0.11722700	0.08121000
C	-1.76766200	1.11016700	0.08952100
N	0.44096500	1.43322100	0.07157200
C	-0.79437500	2.08237200	0.07474700
N	-3.09161300	1.30746800	0.09232700
C	-1.12838700	3.47701600	0.05498000
C	-3.46194700	2.58488000	0.06632700
O	-0.38893400	4.44011300	0.03966400
N	-2.55305200	3.61408900	0.05362800
N	-4.77556300	2.86395700	0.05287200
H	-2.86971300	4.57909600	0.03410500
H	-5.14221200	3.80291900	0.01161800
H	-5.42512200	2.08531300	0.02693700
O	1.09548800	-0.86236700	0.08583500
C	2.46412100	-0.54949900	0.01529100
C	3.09665600	-0.48576900	-1.23151700
C	3.20466600	-0.41763200	1.19528700
C	4.47210600	-0.27645300	-1.30235800
C	4.58051500	-0.20832900	1.13299300

C	5.19917600	-0.14085000	-0.11743800
H	4.96553200	-0.22666100	-2.26559000
H	5.15698900	-0.10634400	2.04449500
Cl	2.40476500	-0.51569200	2.73738100
Cl	6.91529400	0.11759600	-0.20080200
Cl	2.16325000	-0.66847600	-2.68728900
H	1.35105700	1.87916200	0.06924900

Table S13. PCP-O-dG N^7H^+ (gas)

Calculated energy (in Hartrees)= -3568.14074218

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	2.35370200	-1.48253200	-0.11501100
O	3.20536600	-1.54565400	0.99779000
H	1.50680700	-2.16856400	-0.01398700
C	3.20712800	-1.81518800	-1.34312000
C	4.35345200	-2.39753400	0.69674000
C	4.13444500	-2.88296300	-0.75888400
H	3.78729200	-0.94644400	-1.66051000
H	2.62181100	-2.20186500	-2.17962500
C	5.63953300	-1.61195800	0.94750100
H	4.30894000	-3.25027600	1.38535500
H	5.07980300	-2.95145100	-1.30981500
H	5.61757000	-1.22839800	1.97919800
H	6.49281900	-2.29456300	0.86736100
O	5.84489900	-0.57509500	0.00325400
H	5.05312700	-0.00030000	0.04057200
O	3.40258900	-4.10153600	-0.80288100
H	3.96990700	-4.82291300	-0.48800800
N	1.74749800	-0.11877200	-0.13510200
C	0.42156800	0.14211200	-0.11732800
C	2.41031600	1.11480100	-0.07167000
N	0.20467700	1.45894000	-0.06407900
C	1.44617500	2.09539600	-0.03292200
N	3.73579900	1.29884500	-0.05305700
C	1.79307300	3.48542300	0.04058900
C	4.11797300	2.57105100	0.02253500
O	1.06215600	4.45397400	0.08275300
N	3.21874200	3.60816200	0.06156500
N	5.43365100	2.83640100	0.06162600
H	3.54439500	4.56869600	0.11911600
H	5.80886000	3.76995900	0.13616600
H	6.07579900	2.05118800	0.06560200
O	-0.47067100	-0.82997800	-0.16739300
C	-1.83562500	-0.51602700	-0.06976100
C	-2.56924900	-0.33481200	-1.24433500

C	-2.43579500	-0.50213000	1.19153000
C	-3.95481800	-0.12327900	-1.15603300
C	-3.82093300	-0.29044500	1.28347300
C	-4.57703100	-0.10167500	0.10867000
Cl	-1.45384700	-0.75204100	2.59568100
Cl	-6.27821700	0.15812500	0.21973800
Cl	-1.74825200	-0.38308700	-2.76918300
Cl	-4.58198400	-0.26652300	2.83138900
Cl	-4.87934700	0.10580400	-2.59407700
H	-0.69989800	1.91602500	-0.05844800

Table S14. dG N^3H^+ (gas)

Calculated energy (in Hartrees)= -963.91468945

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	-1.38863800	-0.65089600	-0.85844800
O	-1.49648800	0.74612500	-0.62346900
H	-1.42545200	-0.82422700	-1.93917400
C	-2.54557200	-1.32709000	-0.11554200
C	-2.73210800	1.06237300	0.08546800
C	-3.59213000	-0.20133300	-0.05656900
H	-2.23406400	-1.59449000	0.89628000
H	-2.91907600	-2.21148300	-0.63846300
C	-2.43030300	1.50201200	1.51009200
H	-3.20646800	1.88539800	-0.45626900
H	-4.27160400	-0.32453200	0.79579500
H	-3.37811600	1.79865200	1.98344200
H	-1.78523700	2.39484500	1.47749100
O	-1.79861400	0.43323900	2.19880900
H	-1.76013500	0.64903700	3.14296300
O	-4.29753100	-0.06217500	-1.28020800
H	-4.93582100	-0.78873000	-1.35896600
N	-0.05931900	-1.09129500	-0.37894600
C	0.35606400	-2.37879900	-0.04518300
C	1.06581200	-0.33614300	-0.29420600
N	1.63016800	-2.45453300	0.23731000
C	2.09982800	-1.17222900	0.08620600
N	1.18753800	1.02088800	-0.53997100
C	3.43147000	-0.64455400	0.25337500
C	2.40172900	1.58715800	-0.41089800
O	4.47313800	-1.15183900	0.57124900
N	3.43570100	0.80540600	-0.05837500
N	2.55593900	2.90498600	-0.61619000
H	4.36313400	1.21269000	0.02157100
H	3.46705000	3.33815800	-0.55711300
H	1.81088900	3.46397700	-1.00879600

H	-0.33948400	-3.20625700	-0.03302400
H	0.32324200	1.54301000	-0.68934100

Table S15. Ph-O-dG N^3H^+ (gas)

Calculated energy (in Hartrees)= -1270.20029499

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	-0.65156000	-1.52991900	-0.37488700
O	-1.95286000	-1.39192800	-0.93053100
H	0.01309800	-2.03683100	-1.07970700
C	-0.83349400	-2.33760100	0.91696100
C	-2.86327700	-2.35346400	-0.35183400
C	-2.00701900	-3.26372900	0.54673300
H	-1.10303900	-1.67075400	1.74402900
H	0.06800000	-2.88658800	1.19898300
C	-3.96926900	-1.60450900	0.40259700
H	-3.28432500	-2.94137200	-1.17396900
H	-2.56193800	-3.60385600	1.43278300
H	-4.80656900	-2.27822100	0.62031600
H	-3.60133000	-1.20491600	1.35246500
O	-4.42563400	-0.45189300	-0.33114100
H	-4.81155800	-0.75138100	-1.17199900
O	-1.59789400	-4.34990800	-0.26395100
H	-1.10522700	-4.98404800	0.28119900
N	-0.12327700	-0.17247200	-0.18574900
C	1.22096700	0.18492500	-0.05232000
C	-0.79945800	1.01356600	-0.07809800
N	1.41592500	1.46047200	0.12822700
C	0.14530100	2.00151700	0.11408700
N	-2.16163400	1.22468000	-0.13965000
C	-0.26766400	3.37160400	0.28577400
C	-2.62582300	2.47380800	0.03960400
O	0.35746100	4.38601600	0.46091300
N	-1.74186700	3.46462700	0.24706800
N	-3.95164100	2.67967400	-0.00496700
H	-2.07535300	4.41200500	0.39861400
H	-4.35063700	3.59434500	0.14810700
H	-4.57398700	1.87862300	-0.02433600
O	2.09269300	-0.82132500	-0.10218900
C	3.48457300	-0.54633500	-0.08432700
C	4.22976900	-1.19679100	0.89037500
C	4.06596500	0.26284400	-1.05382800
C	5.61509400	-1.02340600	0.89714200
H	3.73297800	-1.82432800	1.62316200
C	5.45100000	0.43039200	-1.02917800
H	3.45583800	0.75674800	-1.80155800

C	6.22522400	-0.20988600	-0.05890300
H	6.21325100	-1.52435200	1.65222700
H	5.92353900	1.06269200	-1.77464900
H	7.30243900	-0.07516800	-0.04922400
H	-2.80981600	0.47273900	-0.41514300

Table S16. 4Cl-Ph-O-dG N^3H^+ (gas)

Calculated energy (in Hartrees)= -1729.79258747

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	-1.23830800	-1.52387300	-0.38231700
O	-2.54467400	-1.42223600	-0.93291700
H	-0.56287100	-2.01370900	-1.08890200
C	-1.39350600	-2.33295700	0.91227900
C	-3.42634600	-2.40811400	-0.34952500
C	-2.54181400	-3.29249500	0.54741000
H	-1.67848900	-1.67198300	1.73890100
H	-0.47679000	-2.85695600	1.19274400
C	-4.54987900	-1.68954500	0.40835900
H	-3.83333400	-3.00842300	-1.16968100
H	-3.08386900	-3.64643500	1.43589200
H	-4.18997000	-1.27971700	1.35691800
H	-5.36753200	-2.38599600	0.62888700
O	-5.04019100	-0.54992300	-0.32395100
H	-5.42346400	-0.85975600	-1.16230300
O	-2.10423900	-4.36784400	-0.26264500
H	-1.60305400	-4.99349900	0.28450200
N	-0.74651200	-0.15120800	-0.19862600
C	0.58735500	0.24642400	-0.07462700
C	-1.45705500	1.01388700	-0.08358500
N	0.74429300	1.52713300	0.10622800
C	-0.54214800	2.02969400	0.10421200
N	-2.82502100	1.18494700	-0.13565300
C	-0.99390800	3.38728100	0.27897600
C	-3.32481600	2.41998300	0.04897900
O	-0.39591100	4.41874200	0.44845100
N	-2.46950900	3.43666000	0.25226800
N	-4.65590600	2.58591000	0.01459500
H	-2.83034600	4.37349600	0.40716600
H	-5.08161500	3.48846600	0.16815600
H	-5.25428700	1.76666500	-0.00660000
O	1.48559900	-0.73605100	-0.13499100
C	2.87293200	-0.46904300	-0.09503900
C	3.45943000	0.56035400	-0.82455800
C	3.62882800	-1.36224400	0.65572200
C	4.84626200	0.70107500	-0.78500000

H	2.85716900	1.25222600	-1.39925000
C	5.01497800	-1.22181400	0.68828000
H	3.13777900	-2.15815600	1.20578500
C	5.61466000	-0.18781500	-0.03190500
H	5.32692800	1.49903100	-1.33991600
H	5.62289400	-1.90708400	1.26835100
Cl	7.35399300	-0.00380500	0.00952800
H	-3.45311400	0.41612300	-0.41182600

Table S17. DCP-O-dG N^3H^+ (gas)

Calculated energy (in Hartrees)= -2189.38277914

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	-1.51251400	-1.43530100	-0.44399000
O	-2.69356600	-1.28615200	-1.22111800
H	-0.78298100	-2.07895700	-0.94311300
C	-1.98388100	-2.03459600	0.88825300
C	-3.66839400	-2.27585700	-0.83530800
C	-3.11364600	-2.97354000	0.43384700
H	-1.18447800	-2.55228400	1.42425500
H	-2.37312800	-1.24092500	1.53654900
C	-5.01508200	-1.57171100	-0.71326900
H	-3.74685400	-3.03475300	-1.62300100
H	-3.88430300	-3.09480700	1.21042700
H	-5.80781900	-2.28914300	-0.47520200
H	-5.25892900	-1.09466800	-1.66523500
O	-5.00155900	-0.50132100	0.26179800
H	-5.16013900	-0.87481700	1.14359900
O	-2.62988300	-4.23114200	-0.00208300
H	-2.31762900	-4.73620700	0.76593900
N	-0.90534800	-0.11118500	-0.34248000
C	0.44304700	0.22740800	-0.45309000
C	-1.53100500	1.08589400	-0.11871600
N	0.68929300	1.49689600	-0.31435400
C	-0.55512800	2.05967100	-0.10194100
N	-2.88122500	1.30749700	0.05006500
C	-0.91904800	3.43975900	0.09953200
C	-3.29979900	2.57118800	0.23646600
O	-0.26398900	4.44813800	0.15286800
N	-2.38425500	3.55494500	0.26102100
N	-4.61175600	2.80221000	0.41014400
H	-2.68333800	4.51492900	0.40559100
H	-4.97934000	3.74127800	0.46362600
H	-5.27140600	2.04037400	0.30448300
O	1.29371300	-0.77793900	-0.68834400
C	2.66567800	-0.51543900	-0.54666600

C	3.41945500	-0.20894900	-1.67222400
C	3.27140000	-0.64602600	0.70444100
C	4.79507600	-0.02341200	-1.55555000
H	2.92500900	-0.11904700	-2.63358100
C	4.64616800	-0.46208500	0.83356700
C	5.39546200	-0.15024000	-0.30183000
H	5.39441400	0.21730300	-2.42595700
H	5.12146700	-0.56290800	1.80190300
H	-3.56879100	0.53607600	0.02626000
Cl	7.11927200	0.07917200	-0.14227600
Cl	2.31407000	-1.04724600	2.11207500

Table S18. TCP-O-dG N^3H^+ (gas)

Calculated energy (in Hartrees)= -2648.97173575

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	1.69598300	-1.45501900	0.14007500
O	2.77070400	-1.32261600	1.06072800
H	0.92260100	-2.12720700	0.52214000
C	2.33682800	-1.99261600	-1.14725200
C	3.80553600	-2.27904000	0.75608400
C	3.41896600	-2.93517100	-0.59433400
H	2.78701200	-1.16759800	-1.71209400
H	1.61966400	-2.50013600	-1.79733700
C	5.14147600	-1.54670000	0.81655200
H	3.80867100	-3.06591300	1.51975100
H	4.27935600	-3.01756000	-1.27597500
H	5.26103400	-1.09857100	1.80555300
H	5.97261500	-2.24055100	0.65065800
O	5.21799500	-0.44370300	-0.11836800
H	5.48984700	-0.78163900	-0.98670700
O	2.90538000	-4.21333500	-0.26637800
H	2.69898600	-4.69379700	-1.08432600
N	1.08138200	-0.13502300	0.01784800
C	-0.27442900	0.18419500	0.00821300
C	1.70664300	1.08206000	-0.05028400
N	-0.52849400	1.45587800	-0.06825300
C	0.72151900	2.04502400	-0.10193900
N	3.06284600	1.32926800	-0.05852100
C	1.07963800	3.43970900	-0.16575900
C	3.47599700	2.60763300	-0.10363800
O	0.41547100	4.44198600	-0.21919300
N	2.55115800	3.58144000	-0.15817500
N	4.79448900	2.86423800	-0.11117000
H	2.84690200	4.55249500	-0.19756200
H	5.14870000	3.80852300	-0.05903300

H	5.45271600	2.10371000	0.01121800
O	-1.13053900	-0.84583800	0.06094800
C	-2.49307100	-0.54975800	0.05108200
C	-3.18931000	-0.50382200	-1.15922800
C	-3.18442900	-0.38360700	1.25392700
C	-4.56462600	-0.28711400	-1.17808400
C	-4.56021700	-0.16621800	1.25417100
C	-5.23407800	-0.11840000	0.03397900
H	-5.09950200	-0.25089100	-2.11917000
H	-5.09197700	-0.03719800	2.18887100
H	3.75809100	0.56588600	-0.00762400
Cl	-6.95665600	0.15366300	0.02316200
Cl	-2.32007200	-0.45611200	2.76546100
Cl	-2.32980200	-0.72690700	-2.66119600

Table S19. PCP-O-dG N^3H^+ (gas)

Calculated energy (in Hartrees)= -3568.13687235

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	2.32817900	-1.45094500	0.16474200
O	3.39240700	-1.29515700	1.09291600
H	1.54933300	-2.11155200	0.55604200
C	2.98171900	-2.02417500	-1.10073400
C	4.42948800	-2.26075100	0.82519500
C	4.05444500	-2.95433800	-0.50969800
H	3.44087800	-1.21586500	-1.68213900
H	2.27091400	-2.54763500	-1.74514200
C	5.76535600	-1.52790900	0.87729700
H	4.42447800	-3.02540400	1.61101900
H	4.92143200	-3.05933100	-1.17956800
H	5.87563700	-1.05110300	1.85389000
H	6.59739600	-2.22688600	0.74007800
O	5.85214100	-0.45301300	-0.08900700
H	6.13741200	-0.81537000	-0.94307000
O	3.53176700	-4.22015800	-0.15042100
H	3.33743600	-4.72591100	-0.95599000
N	1.71657100	-0.13337400	0.00109100
C	0.36255200	0.18917200	-0.02114200
C	2.34463700	1.08099600	-0.09308200
N	0.11061700	1.45833300	-0.12976400
C	1.36191700	2.04436400	-0.17234000
N	3.70124900	1.32590000	-0.09897600
C	1.72257000	3.43695900	-0.26717000
C	4.11661500	2.60267500	-0.17017900
O	1.05967700	4.43799900	-0.34758400
N	3.19389500	3.57644300	-0.25435300

N	5.43515200	2.85722300	-0.17205800
H	3.49164400	4.54596100	-0.31320800
H	5.79080200	3.80202400	-0.14360200
H	6.09165600	2.09891400	-0.02832600
O	-0.49903900	-0.83697400	0.05419300
C	-1.85798200	-0.53296400	0.04712800
C	-2.54363900	-0.51118700	-1.16748400
C	-2.52103600	-0.33965900	1.25936700
C	-3.92752300	-0.28283200	-1.17646700
C	-3.90522000	-0.11055700	1.25994400
C	-4.60632400	-0.08023400	0.03980500
H	4.39556400	0.56343000	-0.02391800
Cl	-6.31222000	0.20270800	0.03510000
Cl	-1.60912200	-0.39577500	2.73322900
Cl	-1.65840800	-0.77531300	-2.63694600
Cl	-4.78645500	-0.25370300	-2.67720700
Cl	-4.73715400	0.13054200	2.75644000

Table S20. dG Neutral (Water)

Calculated energy (in Hartrees)= -963.57030955

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	1.09819900	0.37228600	0.30400300
O	1.80226200	0.06074200	-0.90179800
H	0.76453300	1.41524900	0.28806700
C	2.12832500	0.14246000	1.41085400
C	3.17165800	0.49402200	-0.74762400
C	3.40085500	0.71388100	0.76921800
H	2.25478500	-0.92838300	1.59680800
H	1.86585800	0.63662700	2.34985600
C	4.06514000	-0.55823100	-1.39216400
H	3.31239800	1.45690800	-1.25672300
H	4.30007500	0.19444100	1.11964500
H	5.11196000	-0.25499500	-1.29097200
H	3.83349100	-0.62187600	-2.46536000
O	3.94012000	-1.82893000	-0.76457400
H	3.01967100	-2.10596900	-0.90385200
O	3.52370800	2.12326200	0.96568000
H	3.72121000	2.27146900	1.90484400
N	-0.10344900	-0.42989600	0.37076800
C	-0.22077700	-1.79510200	0.59348000
C	-1.38208200	0.02273100	0.12124400
N	-1.45364000	-2.22907400	0.52084500
C	-2.20069600	-1.09968300	0.22668700
N	-1.73034100	1.30083600	-0.14913200
C	-3.61262800	-0.94722700	0.02652900

C	-3.02776900	1.45145300	-0.33979700
O	-4.51019600	-1.78590600	0.06702700
N	-3.92430300	0.41185000	-0.25958400
N	-3.51928600	2.67406300	-0.68910800
H	-4.90785800	0.58700900	-0.43876700
H	-4.48858000	2.88695600	-0.49275500
H	-2.88063000	3.44486500	-0.54102400
H	0.64171300	-2.40964400	0.80843800

Table S21. Ph-O-dG Neutral (Water)

Calculated energy (in Hartrees)= -1269.84509303

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	-0.59884900	-1.47374400	0.04723500
O	-1.44913700	-1.62697100	-1.08319700
H	0.30007100	-2.08479200	-0.06676100
C	-1.42482100	-1.93215700	1.25525100
C	-2.50447300	-2.57790000	-0.79435900
C	-2.26217600	-3.06269500	0.64735000
H	-2.07511500	-1.12495300	1.60018400
H	-0.79813700	-2.26471100	2.08732900
C	-3.85797000	-1.91052400	-1.03203800
H	-2.39779400	-3.42635600	-1.48133400
H	-3.20377800	-3.21753400	1.18703800
H	-4.64140800	-2.67576900	-0.98497700
H	-3.86130100	-1.49446000	-2.05181000
O	-4.17861300	-0.92418100	-0.06422300
H	-3.45619400	-0.25297300	-0.07421100
O	-1.52177000	-4.28234700	0.55377300
H	-1.34281000	-4.58495200	1.45903800
N	-0.13624400	-0.09015900	0.09759400
C	1.18608700	0.34679700	0.08323400
C	-0.89491600	1.06587800	0.09647600
N	1.32320200	1.64357400	0.09027700
C	0.01447000	2.11515900	0.09331900
N	-2.24647600	1.14135200	0.08229200
C	-0.47062000	3.46164000	0.08490200
C	-2.71643800	2.37894700	0.07443200
O	0.14959200	4.52241800	0.08350100
N	-1.89725300	3.47593300	0.07877800
N	-4.06116400	2.57818400	0.11425500
H	-2.30581400	4.40511300	0.08910300
H	-4.44294800	3.45384000	-0.21810400
H	-4.62543900	1.76097800	-0.08609300
O	2.11312300	-0.62164200	0.08626800
C	3.49126800	-0.43714500	-0.01410900
C	4.20763400	-1.63759500	-0.03631200
C	4.14092700	0.79608000	-0.08478200
C	5.59645900	-1.60482100	-0.13235600

H	3.66729500	-2.57724300	0.02045500
C	5.53708900	0.80604200	-0.18192100
H	3.57340100	1.71507000	-0.06352200
C	6.26907300	-0.38075800	-0.20604200
H	6.15168200	-2.53825000	-0.15026400
H	6.04965700	1.76243700	-0.23802700
H	7.35214000	-0.35507900	-0.28107800

Table S22. 4Cl-Ph-O-dG Neutral $_{(Water)}$

Calculated energy (in Hartrees)= -1729.44065355

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	1.20469800	-1.47671900	-0.05276500
O	2.04029900	-1.64599900	1.08569000
H	0.29417100	-2.07235000	0.05063500
C	2.03482600	-1.94641200	-1.25339700
C	3.08181300	-2.61505600	0.80601900
C	2.84610300	-3.09274600	-0.63915200
H	2.70273800	-1.14988400	-1.58930800
H	1.41113100	-2.26607200	-2.09268300
C	4.44416600	-1.97207000	1.05911500
H	2.95280200	-3.46260900	1.49019800
H	3.79039200	-3.26277900	-1.16941800
H	5.21432100	-2.75107800	1.01919100
H	4.44407200	-1.55740200	2.07943700
O	4.79257400	-0.99035100	0.09612300
H	4.08232400	-0.30638100	0.09925400
O	2.08370000	-4.29942000	-0.55556300
H	1.91023700	-4.59842600	-1.46308500
N	0.76680900	-0.08458700	-0.10488200
C	-0.54592700	0.37650200	-0.10120100
C	1.54575600	1.05826500	-0.09506400
N	-0.66144900	1.67471500	-0.10688400
C	0.65506100	2.12346600	-0.09815100
N	2.89789800	1.10983600	-0.06967800
C	1.16316400	3.46152700	-0.08350100
C	3.38936700	2.33930800	-0.05612900
O	0.56077500	4.53219600	-0.08584500
N	2.58959100	3.45073800	-0.06477900
N	4.73701900	2.51469700	-0.08482000
H	3.01466500	4.37258100	-0.06896500
H	5.13259400	3.38509700	0.24487100
H	5.28687700	1.68824300	0.11739700
O	-1.49336900	-0.57481900	-0.11147900
C	-2.86333900	-0.35768200	-0.04139700
C	-3.61132700	-1.53867500	-0.01599000

C	-3.48750200	0.89024300	-0.00261000
C	-4.99951500	-1.48026600	0.05042800
H	-3.09850200	-2.49424900	-0.04732600
C	-4.88285000	0.94409500	0.06512400
H	-2.90142000	1.79751200	-0.02495900
C	-5.62464700	-0.23298700	0.09086700
H	-5.58475100	-2.39293900	0.07115800
H	-5.38119400	1.90701800	0.09632300
Cl	-7.38532000	-0.15010000	0.17529500

Table S23. DCP-O-dG Neutral (Water)

Calculated energy (in Hartrees)= -2189.03100933

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	1.32153800	-1.35336100	-0.03514200
O	2.15090700	-1.57141300	1.09892900
H	0.37174100	-1.88246900	0.07834900
C	2.10834400	-1.88761700	-1.23770200
C	3.12161200	-2.61225000	0.81970300
C	2.84112300	-3.08409500	-0.61933300
H	2.82956900	-1.14324200	-1.58319500
H	1.45795100	-2.16772900	-2.07077000
C	4.52693800	-2.06240100	1.05676500
H	2.94011600	-3.44299300	1.51243100
H	3.76650800	-3.32473700	-1.15542000
H	4.56304100	-1.63914200	2.07286600
H	5.24083900	-2.89337200	1.01916600
O	4.93499600	-1.11631600	0.08181700
H	4.27468300	-0.38399700	0.08484900
O	1.99610000	-4.23292800	-0.51909500
H	1.79438400	-4.52697100	-1.42236600
N	0.98266700	0.06731300	-0.09433500
C	-0.29203100	0.62020100	-0.08783500
C	1.83947200	1.15341300	-0.09374800
N	-0.31880500	1.92201800	-0.09888900
C	1.02523900	2.27843900	-0.09782600
N	3.19153300	1.11085100	-0.07707200
C	1.62464100	3.57868500	-0.09041900
C	3.76711100	2.30369900	-0.07207700
O	1.09736800	4.68786500	-0.09270900
N	3.04652100	3.46826100	-0.07932100
N	5.12234400	2.38533400	-0.11049000
H	3.53597100	4.35745900	-0.08695900
H	5.58031900	3.23169400	0.19999700
H	5.61797000	1.52511800	0.09045300
O	-1.30610700	-0.26518200	-0.09134700

C	-2.64630200	0.04528800	-0.02648700
C	-3.18238500	1.33419900	0.01987400
C	-3.51140000	-1.06235900	-0.01016900
C	-4.56484300	1.51365200	0.08400400
H	-2.51653000	2.18519200	0.00422600
C	-4.89040100	-0.89000600	0.05284400
C	-5.40473500	0.40479000	0.09992800
H	-4.97597400	2.51608500	0.12003300
H	-5.54464200	-1.75324300	0.06522800
Cl	-2.86308200	-2.68895400	-0.06786800
Cl	-7.14841200	0.62825000	0.17944500

Table S24. TCP-O-dG Neutral (Water)

Calculated energy (in Hartrees)= -2648.62029275

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	1.72664800	-1.45517300	-0.02695300
O	2.60132600	-1.51188100	1.09129300
H	0.89248300	-2.15022800	0.10465700
C	2.57611400	-1.84037200	-1.24396200
C	3.74871500	-2.34787200	0.79256400
C	3.53187600	-2.87441000	-0.63832400
H	3.13785400	-0.97584700	-1.60503900
H	1.97403900	-2.24185600	-2.06350000
C	5.02726400	-1.53591500	0.99471100
H	3.74536700	-3.19273100	1.49188500
H	4.47496500	-2.94070200	-1.19307500
H	5.00438100	-1.10610400	2.00839800
H	5.88612300	-2.21500600	0.94285100
O	5.22423000	-0.53704600	0.00759100
H	4.44234000	0.06331000	0.03217200
O	2.91840300	-4.15979000	-0.51682100
H	2.75607800	-4.49204700	-1.41479300
N	1.12850200	-0.12251700	-0.08161900
C	-0.21986800	0.18041400	-0.06015500
C	1.76141700	1.11137800	-0.09139200
N	-0.50781200	1.44634700	-0.06991500
C	0.74405100	2.05708900	-0.08554300
N	3.09651200	1.32882200	-0.09063000
C	1.08302600	3.44795900	-0.08550600
C	3.43200300	2.60994700	-0.09252700
O	0.35302300	4.43566600	-0.08136400
N	2.49999200	3.61322900	-0.09194600
N	4.74601200	2.95130400	-0.14722800
H	2.80859000	4.58011800	-0.10569100
H	5.03620300	3.86977700	0.16076400

H	5.39977300	2.20259900	0.04779900
O	-1.08999000	-0.86146400	-0.04676900
C	-2.43692600	-0.56087700	0.00171000
C	-3.09858200	-0.45945300	1.23051800
C	-3.18141000	-0.44984800	-1.17784700
C	-4.47375100	-0.24461500	1.29143700
C	-4.55753600	-0.23532500	-1.14262200
C	-5.18341900	-0.13350200	0.09778200
H	-4.97369000	-0.16821100	2.24899200
H	-5.12192700	-0.15172000	-2.06297200
Cl	-2.37529900	-0.59045100	-2.71997000
Cl	-6.91487700	0.13665100	0.15832200
Cl	-2.18857100	-0.61338200	2.71236300

Table S25. PCP-O-dG Neutral (Water)

Calculated energy (in Hartrees)= -3567.78712517

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	2.35394600	-1.45420600	-0.06240400
O	3.21508700	-1.52475500	1.06481800
H	1.51621600	-2.14811400	0.05223100
C	3.21590000	-1.82858000	-1.27393800
C	4.36436500	-2.36012300	0.77049100
C	4.16285100	-2.87083700	-0.66833800
H	3.78307400	-0.96150500	-1.62012300
H	2.62208400	-2.22055400	-2.10403000
C	5.64227700	-1.55355100	0.99650700
H	4.35058200	-3.21232500	1.46062900
H	5.11210200	-2.93288500	-1.21291600
H	5.60817400	-1.13400900	2.01415300
H	6.49995200	-2.23436700	0.94816900
O	5.85383100	-0.54524200	0.02205100
H	5.07352900	0.05707000	0.04373300
O	3.54549200	-4.15601200	-0.56744200
H	3.39308000	-4.47862900	-1.47063400
N	1.76006400	-0.11866500	-0.10958100
C	0.41400100	0.18930400	-0.09744000
C	2.39634500	1.11397000	-0.09786600
N	0.12815100	1.45489000	-0.09460300
C	1.38156000	2.06256300	-0.09044900
N	3.73162400	1.32745600	-0.08108700
C	1.72411700	3.45267100	-0.07025800
C	4.07062900	2.60779900	-0.06354500
O	0.99654200	4.44181700	-0.06196600
N	3.14134400	3.61371200	-0.05992100
N	5.38559700	2.94548800	-0.09964500

H	3.45272000	4.57979600	-0.05828900
H	5.67633500	3.86058500	0.21752000
H	6.03597200	2.19277500	0.09102200
O	-0.46349000	-0.84998200	-0.10632000
C	-1.80429300	-0.54203200	-0.03835400
C	-2.54247300	-0.41195900	-1.21795200
C	-2.43233700	-0.45598800	1.20741800
C	-3.92476600	-0.18601500	-1.15473200
C	-3.81400800	-0.22944400	1.27826600
C	-4.55918700	-0.09210400	0.09520200
Cl	-1.47172600	-0.64397000	2.63958700
Cl	-6.27047900	0.18917300	0.17820400
Cl	-1.71584000	-0.54370700	-2.73736300
Cl	-4.59490600	-0.12381100	2.82435100
Cl	-4.84261000	-0.02494600	-2.61844900

Table S26. dG N^7H^+ (Water)

Calculated energy (in Hartrees)= -964.01654963

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	1.10813600	0.40215800	0.12797300
O	1.90202000	-0.07137300	-0.94450300
H	0.73586800	1.41377300	-0.06235100
C	2.02888600	0.36261200	1.34694200
C	3.25208800	0.42191500	-0.74451900
C	3.34139500	0.87626300	0.73394000
H	2.15505400	-0.66797900	1.69346200
H	1.67350100	0.97804500	2.17659700
C	4.23151100	-0.67244600	-1.14595600
H	3.40702100	1.30112600	-1.38261900
H	4.21436100	0.44462900	1.23533700
H	5.24806000	-0.27362900	-1.06797000
H	4.05809600	-0.94931100	-2.19485100
O	4.17101600	-1.81020600	-0.29399900
H	3.35562500	-2.28621300	-0.51506900
O	3.41150800	2.30068900	0.72219600
H	3.53384200	2.59673400	1.63903800
N	-0.09558200	-0.43240000	0.20973300
C	-0.14262100	-1.76738700	0.40431200
C	-1.40071300	0.02877000	0.04496300
N	-1.40654500	-2.17059500	0.38137900
C	-2.22529900	-1.07770400	0.16180400
N	-1.75868400	1.29796400	-0.17631800
C	-3.64977400	-0.94179400	0.04866700
C	-3.07414000	1.45966000	-0.29228300
O	-4.51202800	-1.80460800	0.12653200

N	-3.97054000	0.41765800	-0.18179900
N	-3.56127800	2.68295200	-0.54785400
H	-4.96517000	0.60136900	-0.27607100
H	-4.54900900	2.89103400	-0.54179200
H	-2.91366300	3.45837200	-0.55302700
H	0.70653300	-2.41359700	0.55368600
H	-1.70865000	-3.13171100	0.50277500

Table S27. Ph-O-dG N^7H^+ (Water)

Calculated energy (in Hartrees)= -1270.28818343

Atom	Coordinates (Angstroms) X	Y	Z
C	0.84996700	-1.52901800	0.00268700
O	1.74038600	-1.49917700	1.09565000
H	0.05566400	-2.26364800	0.16178200
C	1.68872300	-1.86661700	-1.23394100
C	2.93764800	-2.26743800	0.78491700
C	2.72002000	-2.82697200	-0.64216700
H	2.18492900	-0.97329400	-1.61766900
H	1.10010200	-2.32848900	-2.02878400
C	4.16699200	-1.37754500	0.95339300
H	2.99395600	-3.09128700	1.50699900
H	3.65371300	-2.83621500	-1.21565700
H	4.13757600	-0.92988400	1.95854600
H	5.06249100	-2.00657000	0.89684600
O	4.28784500	-0.38841300	-0.05701700
H	3.47479900	0.16334200	-0.02132500
O	2.11568500	-4.11921200	-0.61832200
H	2.75289700	-4.74191100	-0.23182200
N	0.16056400	-0.22138700	-0.05913600
C	-1.18757000	-0.06434900	-0.04361800
C	0.72847300	1.05785300	-0.07445400
N	-1.49950100	1.23171200	-0.06058000
C	-0.31141700	1.96212900	-0.07768000
N	2.03846400	1.34352500	-0.07948300
C	-0.06756800	3.37123900	-0.08789800
C	2.31352100	2.64828900	-0.08697500
O	-0.87272700	4.29183100	-0.09151300
N	1.33236600	3.60708800	-0.09316700
N	3.59625100	3.03979200	-0.10783200
H	1.59424400	4.58846800	-0.10248900
H	3.86785200	4.00573100	0.00653000
H	4.31223900	2.33144400	-0.00976000
O	-1.99623300	-1.09693500	-0.02519400
C	-3.40316100	-0.86282900	0.03839100
C	-4.11396300	-0.80826600	-1.15419900

C	-4.00056100	-0.77310800	1.28978200
C	-5.49909100	-0.64184900	-1.08102200
H	-3.60018600	-0.89981800	-2.10519500
C	-5.38646700	-0.60690400	1.34059200
H	-3.40074600	-0.83791300	2.19138800
C	-6.13189900	-0.54070500	0.16055100
H	-6.07936700	-0.59549700	-1.99706400
H	-5.87924100	-0.53356300	2.30488000
H	-7.20891000	-0.41336200	0.20886200
H	-2.44054400	1.60912000	-0.06367600

Table S28. 4Cl-Ph-O-dG N^7H^+ (Water)

Calculated energy (in Hartrees)= -1729.88146464

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	1.42108000	-1.53375900	-0.00624500
O	2.29545400	-1.52761800	1.09955200
H	0.60258200	-2.24343900	0.14280500
C	2.26718800	-1.89996200	-1.22971600
C	3.47480600	-2.33090300	0.80749600
C	3.25886400	-2.89009500	-0.61980800
H	2.79668400	-1.02350200	-1.60770000
H	1.67653700	-2.34548200	-2.03231100
C	4.72713000	-1.47580800	0.98811900
H	3.49793000	-3.15251400	1.53389600
H	4.19937700	-2.93202600	-1.18056900
H	4.69718100	-1.02222200	1.99055400
H	5.60458300	-2.13084900	0.94670800
O	4.89023900	-0.49600400	-0.02530400
H	4.09481200	0.08133600	-0.00034600
O	2.61259300	-4.16185100	-0.59859300
H	3.22439800	-4.80346300	-0.20211700
N	0.77223400	-0.20533300	-0.08111100
C	-0.56971400	-0.00743400	-0.08878800
C	1.37837100	1.05647100	-0.08487100
N	-0.84340100	1.29674300	-0.10972100
C	0.36604700	1.99125700	-0.10524100
N	2.69583000	1.30300400	-0.06477300
C	0.65159600	3.39279800	-0.10412900
C	3.00976200	2.59915300	-0.06079700
O	-0.12619100	4.33629100	-0.11839700
N	2.05768800	3.58697100	-0.08117300
N	4.30346300	2.95102400	-0.05223900
H	2.34839400	4.56026700	-0.07777700
H	4.60425200	3.90878600	0.05661700
H	4.99653700	2.22055600	0.04808300

O	-1.40803400	-1.01892400	-0.08759900
C	-2.80444900	-0.75629800	-0.02608200
C	-3.51729300	-0.69769000	-1.21720900
C	-3.40623800	-0.65112300	1.22217600
C	-4.89831100	-0.50900000	-1.15556100
H	-3.01009600	-0.80247300	-2.17000600
C	-4.78707800	-0.46208600	1.27922800
H	-2.81486400	-0.72144300	2.12853300
C	-5.51532300	-0.39205600	0.09065900
H	-5.48293600	-0.45796800	-2.06681900
H	-5.28623200	-0.37582100	2.23750300
H	-1.77137800	1.70469200	-0.13198700
Cl	-7.25468000	-0.15572000	0.16561100

Table S29. DCP-O-dG N^7H^+ (Water)

Calculated energy (in Hartrees)= -2189.46908688

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	1.57502100	-1.48899700	-0.18928000
O	2.44060100	-1.57795400	0.91891200
H	0.73378600	-2.18026100	-0.08857900
C	2.41769400	-1.80351600	-1.42909800
C	3.59779300	-2.39749100	0.58343000
C	3.37438100	-2.85975400	-0.87715900
H	2.97542800	-0.92143400	-1.74935200
H	1.81935200	-2.18020100	-2.26072900
C	4.87394300	-1.59414200	0.82541500
H	3.59011300	-3.26321900	1.25687700
H	4.31678400	-2.89638600	-1.43508000
H	4.84965700	-1.20425300	1.85442400
H	5.73158600	-2.27168500	0.74805400
O	5.07431100	-0.55759800	-0.12262900
H	4.29799800	0.04232500	-0.06262200
O	2.68770700	-4.10870400	-0.93859100
H	3.27601600	-4.79413200	-0.58223500
N	0.96765200	-0.13757100	-0.18808800
C	-0.36517400	0.10420200	-0.21012100
C	1.61235700	1.10362400	-0.11938900
N	-0.60020000	1.41434900	-0.17240200
C	0.62928200	2.06944000	-0.11169100
N	2.93557300	1.30746600	-0.06689200
C	0.95730500	3.46033900	-0.04126100
C	3.28901000	2.59196300	0.00291400
O	0.20854500	4.42656600	-0.02586600
N	2.36769600	3.60886400	0.01509500
N	4.59191000	2.90032500	0.05122600

H	2.68679000	4.57183700	0.06622800
H	4.92531300	3.84380200	0.18613300
H	5.26147100	2.14373100	0.10834900
O	-1.23539200	-0.88389500	-0.27271200
C	-2.61440600	-0.59022500	-0.30398500
C	-3.22602100	-0.35433200	-1.52974600
C	-3.35190100	-0.64025800	0.88202600
C	-4.60230300	-0.14260100	-1.57923600
H	-2.62899200	-0.34514500	-2.43520800
C	-4.72974700	-0.43264500	0.83825000
C	-5.33575300	-0.18415100	-0.39326000
H	-5.09298800	0.04412300	-2.52699500
H	-5.31294700	-0.46699200	1.75028600
H	-1.51401900	1.85398400	-0.18561700
Cl	-7.06789400	0.07636500	-0.44319300
Cl	-2.56556600	-0.96261000	2.40341200

Table S30. TCP-O-dG N^7H^+ (Water)

Calculated energy (in Hartrees)= -2649.05536218

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	-1.69582500	-1.47696800	-0.00195100
O	-2.57591300	-1.51624300	-1.10107600
H	-0.83976700	-2.13899400	-0.15813200
C	-2.51125900	-1.89169800	1.22654100
C	-3.70488100	-2.38883000	-0.80325900
C	-3.44252100	-2.93998700	0.61925200
H	-3.09130800	-1.04856300	1.60616900
H	-1.89098500	-2.30048200	2.02624200
C	-5.00610800	-1.60694100	-0.96955400
H	-3.68576300	-3.20693500	-1.53365700
H	-4.37350900	-3.04620200	1.18747700
H	-5.01200100	-1.15009900	-1.97088000
H	-5.84382200	-2.31157600	-0.92160600
O	-5.21525000	-0.64052400	0.04815200
H	-4.45698800	-0.01641700	0.01347300
O	-2.71419800	-4.16620300	0.58583300
H	-3.28387000	-4.84411600	0.18736500
N	-1.12166000	-0.11219300	0.07433700
C	0.20346600	0.16248600	0.08899300
C	-1.79796700	1.11417700	0.08884300
N	0.40730000	1.47713700	0.12381100
C	-0.83841800	2.10289500	0.12172200
N	-3.12620300	1.28769100	0.06891200
C	-1.20020300	3.48750600	0.13722000
C	-3.51100800	2.56531700	0.07978000

O	-0.47415200	4.47028000	0.16536300
N	-2.61403200	3.60374200	0.11322500
N	-4.82099800	2.84441800	0.06826200
H	-2.95616300	4.56006600	0.12035100
H	-5.17960500	3.78586800	-0.00018800
H	-5.47412300	2.07678000	-0.02118500
O	1.09600600	-0.81324200	0.08279200
C	2.46187400	-0.51439300	0.01007200
C	3.08586500	-0.40002900	-1.23704300
C	3.21910300	-0.45598000	1.18467700
C	4.46130000	-0.19539600	-1.31462500
C	4.59574600	-0.25318600	1.12023000
C	5.19529800	-0.12261300	-0.13150400
H	4.94406700	-0.10136000	-2.27927300
H	5.18160000	-0.20270400	2.02935100
Cl	2.43973800	-0.64165800	2.72985600
Cl	6.92229200	0.13353900	-0.22085500
Cl	2.14178100	-0.52096500	-2.69431000
H	1.30787600	1.94290600	0.16002200

Table S31. PCP-O-dG N^7H^+ (Water)

Calculated energy (in Hartrees)= -3568.22006039

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	2.31420400	-1.47129900	-0.10621200
O	3.17931300	-1.58234600	0.99894200
H	1.45049300	-2.13334500	0.00029300
C	3.14098200	-1.81913400	-1.34780300
C	4.30698300	-2.44321000	0.66406700
C	4.06239800	-2.90504400	-0.79304900
H	3.72767800	-0.95825700	-1.67376500
H	2.52718900	-2.17868300	-2.17566000
C	5.61058100	-1.68333000	0.89836900
H	4.27069900	-3.30447300	1.34209300
H	5.00080500	-2.97752300	-1.35424000
H	5.60258200	-1.28682300	1.92504200
H	6.44400900	-2.39060200	0.82283500
O	5.84420500	-0.65990500	-0.05651400
H	5.08998300	-0.03291300	0.00278400
O	3.33263700	-4.12956200	-0.84444500
H	3.89725800	-4.83191700	-0.48268500
N	1.75179700	-0.09831600	-0.10833400
C	0.43023000	0.18976100	-0.11727500
C	2.43900100	1.12058700	-0.04403400
N	0.23738600	1.50561400	-0.07658800
C	1.48837500	2.11822900	-0.02624800

N	3.76795100	1.28028300	0.00017800
C	1.86210600	3.49825800	0.04687600
C	4.16396800	2.55271600	0.07268100
O	1.14431000	4.48691600	0.07100600
N	3.27628000	3.59954400	0.09323200
N	5.47589500	2.81698000	0.11834800
H	3.62626700	4.55155900	0.14644000
H	5.84408700	3.74920000	0.24130800
H	6.12064900	2.03828000	0.16272400
O	-0.47055200	-0.77980900	-0.18043200
C	-1.83186200	-0.48635000	-0.07642300
C	-2.57328300	-0.30392100	-1.24557300
C	-2.43417500	-0.50253400	1.18394300
C	-3.95736800	-0.09668500	-1.14940400
C	-3.81775600	-0.29495400	1.28025400
C	-4.57501000	-0.08759200	0.11357500
Cl	-1.45462300	-0.78440300	2.58256900
Cl	-6.28285400	0.17517700	0.23299700
Cl	-1.76240400	-0.34836800	-2.77417000
Cl	-4.58050500	-0.29945000	2.83439300
Cl	-4.89167900	0.14218700	-2.58683500
H	-0.65728700	1.98398600	-0.08814900

Table S32. dG N^3H^+ (Water)

Calculated energy (in Hartrees)= -964.01886449

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	-1.31569800	-0.72312400	-0.71434200
O	-1.45415700	0.66822900	-0.46727000
H	-1.36114300	-0.91869600	-1.79136900
C	-2.46324300	-1.39156100	0.03836200
C	-2.84063900	0.98581700	-0.14264200
C	-3.58563400	-0.36089000	-0.15937400
H	-2.21515300	-1.46805700	1.10065200
H	-2.72470800	-2.37780500	-0.35229400
C	-2.86839100	1.73284800	1.18582900
H	-3.23738800	1.62888300	-0.93511800
H	-4.33184800	-0.41915000	0.64086000
H	-3.90200700	2.01804400	1.40609400
H	-2.27815300	2.65479000	1.09214100
O	-2.41935600	0.94094100	2.27883200
H	-1.46076000	0.82901100	2.17444800
O	-4.19601200	-0.47561200	-1.44257300
H	-4.68969100	-1.31172600	-1.46257200
N	0.02454800	-1.10898100	-0.24026500
C	0.46331000	-2.37351600	0.13563200

C	1.14012700	-0.33113700	-0.22548700
N	1.74770500	-2.42107100	0.38604900
C	2.19439200	-1.13510900	0.16314500
N	1.24787300	1.00797100	-0.52395800
C	3.51677000	-0.57860100	0.27239300
C	2.46289000	1.59069200	-0.43755600
O	4.56414500	-1.10743300	0.59146700
N	3.51582500	0.82315000	-0.07318600
N	2.61537400	2.88263400	-0.70362800
H	4.43192000	1.25866200	-0.01733200
H	3.51955500	3.33070300	-0.63657000
H	1.83773600	3.45954100	-0.99721300
H	-0.22399700	-3.20471900	0.20142700
H	0.39609600	1.53308500	-0.71764800

Table S33. Ph-O-dG N^3H^+ (Water)

Calculated energy (in Hartrees)= -1270.28747073

Atom	Coordinates (Angstroms) X	Y	Z
C	0.68419400	-1.54875300	0.35795000
O	1.96482600	-1.40061400	0.94547200
H	0.00675400	-2.06567300	1.04321800
C	0.89736200	-2.33776900	-0.93940500
C	2.91415800	-2.31700300	0.34274300
C	2.08637300	-3.23860000	-0.56379400
H	1.16536900	-1.66003800	-1.75640400
H	0.01303400	-2.90530000	-1.23752300
C	3.99176400	-1.52627400	-0.41118600
H	3.36358200	-2.89036800	1.15872900
H	2.65253800	-3.56391300	-1.44581800
H	4.85404700	-2.17297300	-0.60893600
H	3.61725000	-1.15564500	-1.36913700
O	4.39375900	-0.35226000	0.31169200
H	4.78471600	-0.61885800	1.16160700
O	1.68637500	-4.34914900	0.23086400
H	1.15629800	-4.94003400	-0.32860300
N	0.13352500	-0.19387900	0.17294400
C	-1.20976600	0.13297900	0.02958500
C	0.78542500	1.00602500	0.08526000
N	-1.44178700	1.40384000	-0.14378300
C	-0.17810000	1.97598800	-0.10887100
N	2.13116100	1.25821400	0.16431400
C	0.20706700	3.35011300	-0.26512600
C	2.55825900	2.52465000	-0.00767200
O	-0.48213200	4.33951600	-0.44272800
N	1.64170400	3.49756700	-0.20618800

N	3.86408600	2.77816600	0.03331800
H	1.96579800	4.45071000	-0.34003300
H	4.22969700	3.70862000	-0.11447100
H	4.52013300	2.00528400	0.07696000
O	-2.07288000	-0.89046600	0.06212300
C	-3.45283900	-0.60561400	0.06795100
C	-4.19196700	-0.98690000	-1.04594700
C	-4.04534900	-0.04467300	1.19590000
C	-5.57568800	-0.79352400	-1.02951500
H	-3.68984900	-1.42800500	-1.90077500
C	-5.42795600	0.14761100	1.19575900
H	-3.43839400	0.23172100	2.05170600
C	-6.19335600	-0.22536900	0.08690600
H	-6.16685100	-1.08784100	-1.89159300
H	-5.90603400	0.58483600	2.06732600
H	-7.26893100	-0.07603300	0.09532200
H	2.82293800	0.52263300	0.39157200

Table S34. 4Cl-Ph-O-dG N^3H^+ (Water)

Calculated energy (in Hartrees)= -1729.88219869

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	-1.27582300	-1.54677700	-0.35001600
O	-2.54684200	-1.41532800	-0.96083700
H	-0.57717500	-2.04814600	-1.02543300
C	-1.50038200	-2.34586300	0.93925600
C	-3.49456200	-2.34630900	-0.37747400
C	-2.66977300	-3.26125000	0.53826600
H	-1.79177600	-1.67638000	1.75505300
H	-0.61355800	-2.90267600	1.24979600
C	-4.59428300	-1.57203600	0.36096800
H	-3.92341900	-2.92121600	-1.20333400
H	-3.24631000	-3.59941600	1.40863100
H	-4.23960500	-1.19568500	1.32429300
H	-5.44991500	-2.23116200	0.54590300
O	-5.00234700	-0.40430900	-0.36885100
H	-5.37425500	-0.67713300	-1.22532800
O	-2.24004300	-4.36123700	-0.25541700
H	-1.71123700	-4.94778300	0.30981900
N	-0.75024900	-0.18360700	-0.14633500
C	0.58318300	0.16408700	0.02881400
C	-1.42264800	1.00563000	-0.06627700
N	0.79179300	1.43656200	0.21484900
C	-0.47897600	1.98940000	0.15447900
N	-2.76980000	1.23821800	-0.17394100
C	-0.88820800	3.35705800	0.31020800

C	-3.21970600	2.49740200	-0.00570600
O	-0.21761700	4.35492400	0.50848500
N	-2.32294400	3.48271000	0.22094000
N	-4.52753700	2.73201000	-0.07867700
H	-2.66474400	4.42995600	0.35193500
H	-4.91099600	3.65575700	0.06713400
H	-5.17046700	1.94948900	-0.14231200
O	1.46266200	-0.84858500	0.01647800
C	2.83591400	-0.56661000	-0.01350100
C	3.39637800	0.18910100	-1.04068100
C	3.61819200	-1.15398300	0.97472400
C	4.77846300	0.37030300	-1.06962900
H	2.76930500	0.63190400	-1.80601200
C	5.00239800	-0.97948700	0.94266100
H	3.14952000	-1.74210800	1.75632800
C	5.56619400	-0.21593700	-0.07814400
H	5.23504500	0.95615200	-1.85949900
H	5.62836400	-1.43055800	1.70436300
Cl	7.31314400	0.01188200	-0.12095200
H	-3.44573900	0.49368000	-0.41954800

Table S35. DCP-O-dG N^3H^+ (Water)

Calculated energy (in Hartrees)= -2189.47296990

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	-1.56109800	-1.48865400	-0.26653000
O	-2.59679100	-1.36867900	-1.23025500
H	-0.77370000	-2.16325300	-0.61285700
C	-2.23854300	-2.01008500	1.00601900
C	-3.68359700	-2.27018900	-0.91092800
C	-3.31087600	-2.94431800	0.42841200
H	-1.54203000	-2.52262100	1.67340400
H	-2.69839900	-1.18515600	1.55959100
C	-4.98681300	-1.47939900	-0.94593100
H	-3.73670600	-3.04543600	-1.68402000
H	-4.17527100	-3.04544600	1.09690300
H	-5.84007900	-2.14770900	-0.79385800
H	-5.08926400	-1.00505600	-1.92452700
O	-5.02039800	-0.40440500	0.01256300
H	-5.30934000	-0.73947700	0.87720600
O	-2.77892000	-4.22341200	0.09593700
H	-2.54268300	-4.67197800	0.92451700
N	-0.93745700	-0.16863800	-0.13833600
C	0.41731000	0.13703200	-0.16175700
C	-1.55171700	1.05141400	-0.03176600
N	0.69099800	1.40560400	-0.07126300

C	-0.55845300	2.00601700	0.00961200
N	-2.89429600	1.31954200	0.01747000
C	-0.90415200	3.39652400	0.11173800
C	-3.28329600	2.60703900	0.11320600
O	-0.18561200	4.37866900	0.15926100
N	-2.33595900	3.57044800	0.15804600
N	-4.58115600	2.89314200	0.16262300
H	-2.63294100	4.53991200	0.22203600
H	-4.91588800	3.84500100	0.21891200
H	-5.26764500	2.15060500	0.09537000
O	1.27106800	-0.89696700	-0.26151400
C	2.63267100	-0.60327600	-0.33740200
C	3.22291800	-0.42572900	-1.58427900
C	3.40923200	-0.57715500	0.82393000
C	4.59654100	-0.21388700	-1.68316200
H	2.60174000	-0.45981900	-2.47284100
C	4.78524400	-0.36742100	0.74023800
C	5.36016700	-0.18634100	-0.51663400
H	5.06261600	-0.07571500	-2.65172700
H	5.38944500	-0.34797000	1.63900800
H	-3.62030400	0.57449200	-0.01273400
Cl	7.09381100	0.07812900	-0.62475300
Cl	2.66545600	-0.81413700	2.38765300

Table S36. TCP-O-dG N^3H^+ (Water)

Calculated energy (in Hartrees)= -2649.06135449

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	1.70209000	-1.47409300	0.12261100
O	2.73298100	-1.38165700	1.09350500
H	0.90523900	-2.14554200	0.45323100
C	2.38036400	-1.98085000	-1.15511400
C	3.81264900	-2.28886000	0.76336200
C	3.43721700	-2.93813100	-0.58706400
H	2.85447500	-1.15166100	-1.68966200
H	1.68186600	-2.47239900	-1.83602600
C	5.12407300	-1.51211700	0.81594700
H	3.85493700	-3.07639200	1.52449600
H	4.30317400	-3.04187400	-1.25311500
H	5.23350300	-1.06562300	1.80683700
H	5.97008400	-2.18486100	0.64425800
O	5.16636600	-0.41147200	-0.11227600
H	5.45334000	-0.72234800	-0.98639600
O	2.88596800	-4.21426000	-0.27497500
H	2.64596200	-4.64742500	-1.11063900
N	1.09289100	-0.14394100	0.01317900

C	-0.25722300	0.17336900	0.00276500
C	1.71829300	1.07403800	-0.04894100
N	-0.52176800	1.44363600	-0.06650600
C	0.73333700	2.03703800	-0.09680000
N	3.06304800	1.33349300	-0.05540700
C	1.09114500	3.42731700	-0.15455200
C	3.46380500	2.62011400	-0.10642700
O	0.38058600	4.41501900	-0.19996200
N	2.52466400	3.59170100	-0.15048200
N	4.76457200	2.89647800	-0.11278500
H	2.82967800	4.56036300	-0.17829000
H	5.10849900	3.84630600	-0.14233800
H	5.44355400	2.14691500	-0.04639400
O	-1.12628200	-0.85723200	0.05371200
C	-2.47789200	-0.55279500	0.04602700
C	-3.18210000	-0.50172300	-1.16132500
C	-3.17253500	-0.38642600	1.24845600
C	-4.55762200	-0.28180600	-1.17839300
C	-4.54804100	-0.16517800	1.25505900
C	-5.22025100	-0.11436100	0.03572800
H	-5.09366900	-0.24393900	-2.11851500
H	-5.07663600	-0.03769700	2.19149800
H	3.78233100	0.58124100	-0.04389500
Cl	-6.95065900	0.16314200	0.02891300
Cl	-2.30697900	-0.46396100	2.76134100
Cl	-2.32830300	-0.72335900	-2.66667300

Table S37. PCP-O-dG N^3H^+ (Water)

Calculated energy (in Hartrees)= -3568.22777177

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	2.33100000	-1.47353600	0.10691700
O	3.33392500	-1.37088200	1.10493500
H	1.52390900	-2.13985200	0.42287400
C	3.04332900	-1.99662100	-1.14549000
C	4.42211800	-2.28186300	0.81502100
C	4.08142400	-2.94890000	-0.53585400
H	3.53422500	-1.17532400	-1.67694700
H	2.36309700	-2.49529800	-1.83961000
C	5.73124000	-1.50348100	0.89052800
H	4.44475200	-3.05874900	1.58778300
H	4.96462600	-3.06406500	-1.17676300
H	5.81242700	-1.03862300	1.87566100
H	6.58185700	-2.17859500	0.75487400
O	5.79968000	-0.42065500	-0.05702400
H	6.11417200	-0.74742400	-0.91584800

O	3.51751800	-4.21886500	-0.22178200
H	3.30311300	-4.66445800	-1.05787900
N	1.72670100	-0.14361500	-0.03395300
C	0.37908700	0.17836400	-0.05889200
C	2.35566500	1.07295700	-0.09735400
N	0.11711000	1.44759400	-0.14048000
C	1.37370800	2.03793900	-0.16214800
N	3.70094700	1.32966200	-0.09068500
C	1.73479800	3.42763700	-0.22346800
C	4.10462200	2.61548200	-0.14239600
O	1.02625000	4.41571600	-0.28209600
N	3.16817500	3.58890600	-0.20328000
N	5.40554400	2.88970600	-0.13287900
H	3.47574700	4.55679400	-0.23133300
H	5.75136500	3.83892200	-0.16118600
H	6.08254700	2.13945000	-0.05518000
O	-0.49719000	-0.84947300	-0.00893000
C	-1.84308500	-0.53636500	0.01368700
C	-2.55576600	-0.48662800	-1.18663000
C	-2.49014800	-0.36556300	1.23991700
C	-3.93874200	-0.25645800	-1.16387600
C	-3.87265500	-0.13381800	1.26911900
C	-4.59542800	-0.07786600	0.06540600
H	4.41918800	0.57673500	-0.05568200
Cl	-6.30677000	0.20815700	0.09746100
Cl	-1.55525000	-0.45521900	2.69741100
Cl	-1.70014100	-0.72025300	-2.67657100
Cl	-4.82833300	-0.19458700	-2.65143200
Cl	-4.68061400	0.07897800	2.78903900
