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Supporting Information

Alternative role of cisplatin in DNA damage – Theoretical studies on influence of excess electrons on the cisplatin-DNA complex

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Content

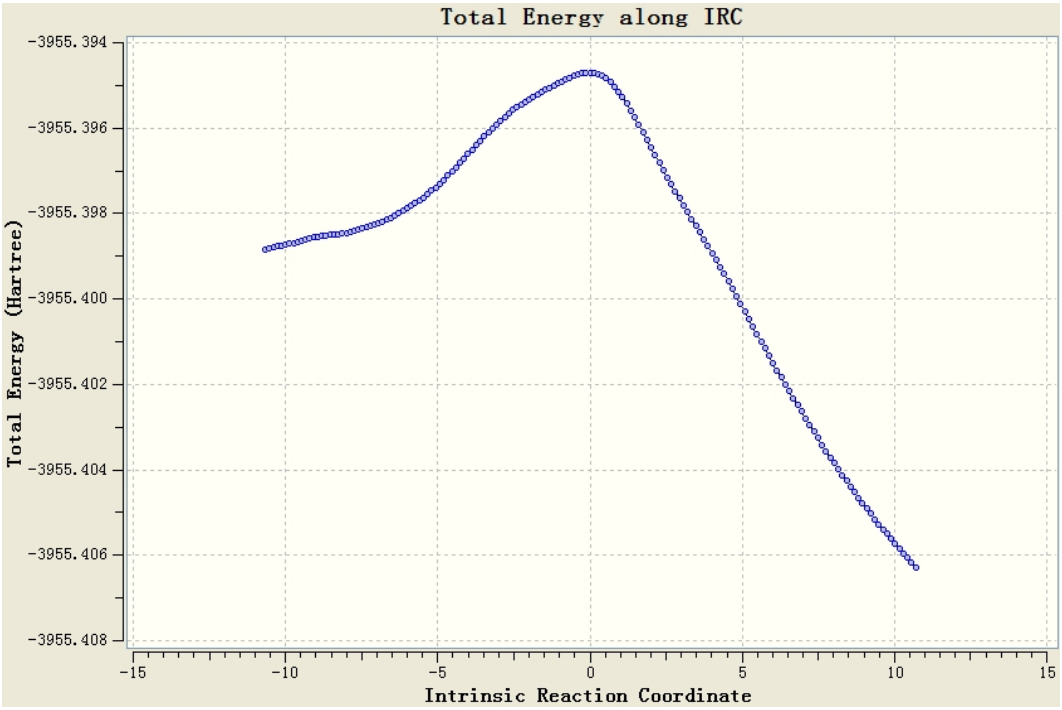

Fig. S1 The total energy along IRC of the transition state of Pt-N7$_b$ scission in water solution.

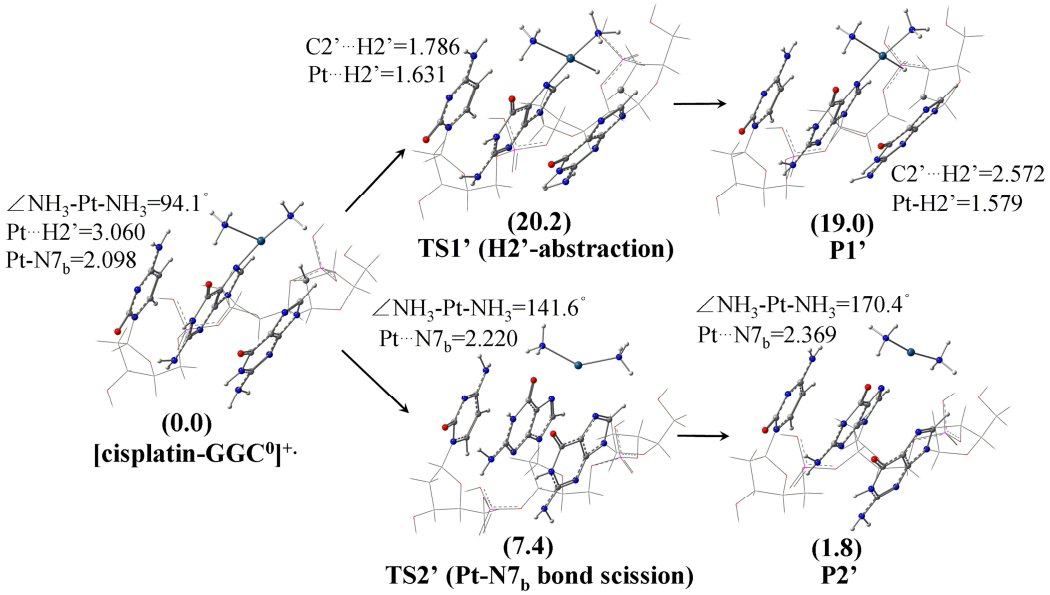

Fig. S2 Stationary structures and the selected geometrical parameters along the H abstraction and Pt-N7$_b$ bond scission reactions of the protonated reactant [cisplatin-GGC^0]$^{+\bullet}$ in water solution (bond length in Å and energies in kcal mol^{-1}).

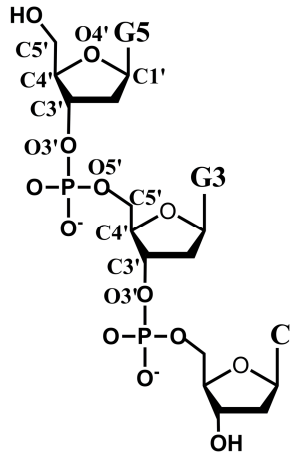

Fig. S3 The structure and atomic labeling of the sugar backbone model considered in the present study.

According to the atomic labeling in Fig.S1, the torsion angles are defined as below. The δ-1 torsion angle is defined as C5'$_{G5}$-C4'$_{G5}$-C3'$_{G5}$-O3', ε-1 as C4'$_{G5}$-C3'$_{G5}$- O3'-P, ζ-1 as C3'$_{G5}$-O3'-P-O5', α as O3'-P-O5'-C5'$_{G3}$, β as P-O5'-C5'$_{G3}$-C4'$_{G3}$, γ as O5'-C5'$_{G3}$-C4'$_{G3}$-C3'$_{G3}$, δ as C5'$_{G3}$-C4'$_{G3}$-C3'$_{G3}$-O3', and χ-1 as O4'-C1'-N1-C4 in G5.

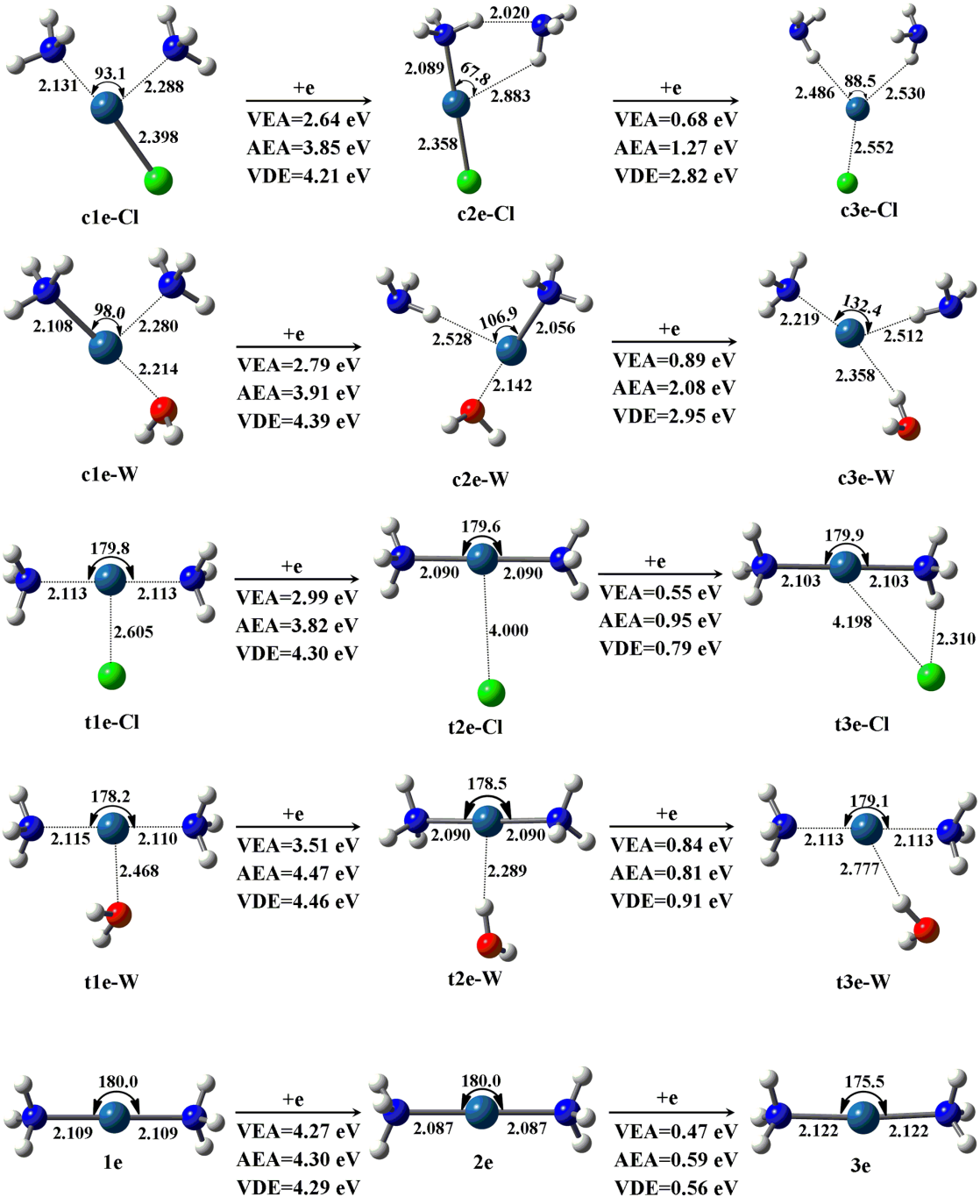

Fig. S4 Optimized geometries and the electron affinities of Pt-containing species from injection of one, two and three electrons at M06, SDD/6-31++G(d,p) method in water solution.

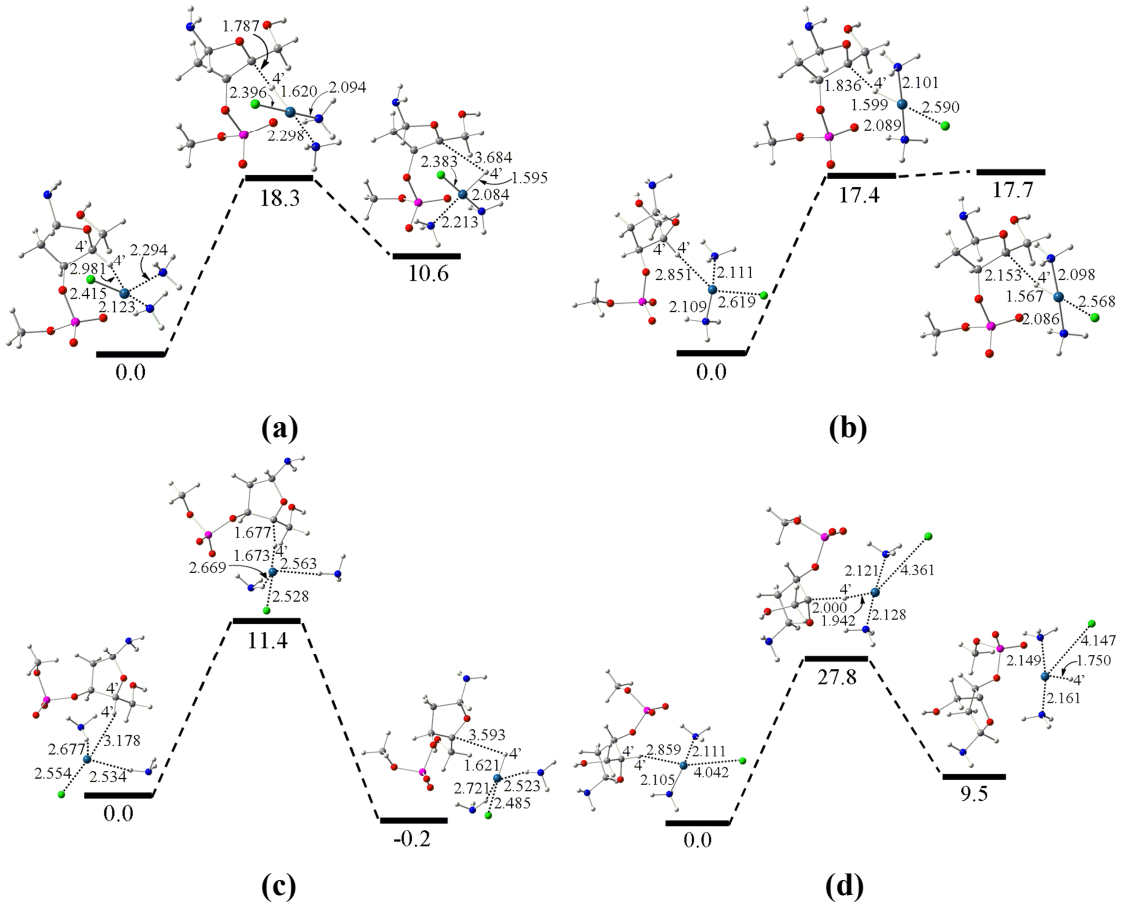

Fig. S5 M06/SDD, 6-31++G(d,p) free energy profile (in kcal/mol) for H4' abstraction from nucleotide by (a) *cis*-$[Pt(NH_3)_2Cl]^{\bullet}$, (b) *trans*-$[Pt(NH_3)_2Cl]^{\bullet}$, (c) *cis*-$[Pt(NH_3)_2Cl]^{2-\bullet}$ and (d) *trans*-$[Pt(NH_3)_2Cl]^{2-\bullet}$ in water solution.

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Table S1 Coordinates of optimized structures of the neutral [cisplatin-GGC]^0 and it's single-electron adduct [cisplatin-GGC]$^{\cdot-}$ in water solution.

[cisplatin-GGC]^0

Atom	Coordinates (Angstroms)		
	X	Y	Z
O	-5.853518	0.771432	-1.745339
C	-6.644733	1.816292	-1.200576
C	-5.794235	2.623568	-0.238431
O	-5.423725	1.793020	0.874062
C	-4.478576	3.138407	-0.839953
O	-4.118490	4.341204	-0.172036
C	-3.509325	2.024528	-0.478418
C	-4.033234	1.600695	0.892352
N	-3.717605	0.199822	1.164414
C	-3.893466	-0.816128	0.280467
N	-3.230938	-1.894538	0.650132
C	-2.609926	-1.573674	1.844787
C	-1.710058	-2.323327	2.673608
O	-1.310678	-3.469489	2.540314
N	-1.280090	-1.528394	3.752013
C	-1.652776	-0.229126	4.003786
N	-1.104021	0.368026	5.078005
N	-2.476931	0.449223	3.230647
C	-2.900793	-0.262199	2.172056
H	-7.504097	1.411391	-0.651659
H	-7.017800	2.482485	-1.989251
H	-6.383115	3.464612	0.140635
H	-4.555029	3.312415	-1.917059
H	-3.628498	1.210523	-1.195644
H	-2.469454	2.345183	-0.444783
H	-3.574914	2.161727	1.713067
H	-4.489615	-0.706318	-0.618003
H	-0.621628	-1.986234	4.375150
H	-0.671127	-0.172234	5.813801
H	-1.484367	1.268109	5.336532
P	-2.954482	5.282088	-0.874058
O	-2.882621	6.517773	-0.040975
O	-3.151563	5.285903	-2.353837
O	-1.601812	4.368811	-0.613050
C	-1.083522	4.337735	0.705613
C	0.120538	3.422226	0.772744
O	-0.283125	2.042132	0.856931
C	1.097194	3.527189	-0.436229
O	2.354921	3.949274	0.082900
C	1.066451	2.103373	-0.999152
C	0.783708	1.321633	0.270603
N	0.411024	-0.072360	0.104833
C	-0.691685	-0.581111	-0.505159
N	-0.684119	-1.900526	-0.489413
C	0.483710	-2.274584	0.142214
C	1.060743	-3.563086	0.395368
O	0.663238	-4.671128	0.049228
N	2.239594	-3.426533	1.132204
C	2.860477	-2.243085	1.456931
N	4.024995	-2.324429	2.144573
N	2.353098	-1.062852	1.164788
C	1.173729	-1.140647	0.526376
H	-1.845029	3.987110	1.416514
H	-0.776755	5.345431	1.005647
H	0.692614	3.664189	1.676746
H	0.754640	4.260503	-1.168944
H	0.210082	2.005080	-1.676277
H	1.978640	1.822897	-1.516905
H	1.668214	1.308205	0.919294
H	-1.481901	0.036622	-0.910298
H	2.719492	-4.300316	1.326557
H	4.558977	-3.172311	1.986613
H	4.603016	-1.496568	1.988907
P	3.813356	3.467287	-0.498053
O	4.817596	4.386152	0.116952
O	3.748616	3.201798	-1.972537
O	3.925283	1.973571	0.187297
C	4.530850	1.815357	1.461344
C	5.842144	1.065142	1.312880
O	5.600613	-0.269133	0.860135
C	6.809783	1.652855	0.277398
O	8.144568	1.256553	0.549320
C	6.395517	0.952791	-1.015163
C	5.873407	-0.405171	-0.526868
N	4.693375	-0.937856	-1.224685
C	4.481646	-2.336346	-1.095740
O	5.260541	-2.999385	-0.414921
N	3.417925	-2.894623	-1.743491
C	2.583256	-2.136591	-2.426678
N	1.553979	-2.763354	-3.070541
C	2.701804	-0.715907	-2.488830
C	3.783659	-0.165960	-1.876763
H	3.853066	1.222807	2.084737
H	4.711088	2.786959	1.931216
H	6.323556	0.991643	2.295235
H	6.712290	2.742244	0.208226
H	5.646415	1.550847	-1.531216
H	7.257030	0.824998	-1.672985
H	6.629302	-1.182013	-0.631576
H	1.706370	-3.752149	-3.235276
H	1.130815	-2.267418	-3.845386
H	1.992627	-0.104598	-3.032485
H	3.955209	0.904365	-1.900182
Pt	-2.322990	-3.137745	-0.743549
N	-4.001591	-4.348114	-0.918763
N	-1.242954	-4.282490	-2.086897
H	-3.807662	-5.318989	-0.668003
H	-4.745953	-4.027976	-0.297088
H	-0.809774	-3.688041	-2.795154
H	-0.485593	-4.715867	-1.541981
H	-4.384968	-4.348304	-1.865403
H	-1.762317	-5.014677	-2.571454
H	8.427901	1.692296	1.367052
H	-6.408338	0.250862	-2.344093

[cisplatin-GGC]$^{-}$

Atom	Coordinates (Angstroms)		
	X	Y	Z
O	-6.119734	0.395522	0.805395
C	-6.365660	1.583672	1.533265
C	-5.099313	2.402068	1.625148
O	-4.151743	1.762399	2.485331
C	-4.397706	2.616680	0.285340
O	-3.840851	3.922289	0.279430
C	-3.327916	1.540069	0.294283
C	-2.999608	1.371005	1.772323
N	-2.658317	0.002266	2.130334
C	-3.462091	-1.107929	1.951406
N	-2.919795	-2.215769	2.384391
C	-1.694747	-1.821125	2.880706
C	-0.637466	-2.605848	3.433524
O	-0.559366	-3.817353	3.593996
N	0.450509	-1.771897	3.796349
C	0.504597	-0.408003	3.659050
N	1.660734	0.197644	4.031180
N	-0.473619	0.306047	3.149748
C	-1.519902	-0.446608	2.751905
H	-6.712224	1.359606	2.554704
H	-7.138940	2.197143	1.040849
H	-5.355646	3.377396	2.063951
H	-5.087924	2.505493	-0.561035
H	-3.732401	0.603935	-0.117908
H	-2.446171	1.847191	-0.273177
H	-2.130722	1.980099	2.068127
H	-4.452600	-0.997924	1.515857
H	1.268577	-2.268436	4.141786
H	2.254283	-0.243608	4.721655
H	1.616568	1.207604	4.082496
P	-3.159454	4.486552	-1.119089
O	-3.177741	5.975036	-1.000033
O	-3.712617	3.739731	-2.289326
O	-1.603481	3.949134	-0.950749
C	-0.889174	4.434465	0.165354
C	0.404305	3.679907	0.330266
O	0.115601	2.301702	0.592058
C	1.370986	3.707831	-0.869864
O	2.669881	3.950006	-0.339889
C	1.165789	2.327435	-1.472231
C	0.950342	1.506377	-0.220259
N	0.329247	0.215936	-0.423376
C	-0.822759	-0.076724	-1.090130
N	-1.144539	-1.349039	-0.988561
C	-0.136075	-1.932693	-0.236690
C	0.106738	-3.284293	0.158566
O	-0.539814	-4.302847	-0.073157
N	1.284373	-3.362488	0.927138
C	2.128026	-2.323428	1.231632
N	3.203475	-2.588558	2.014069
N	1.903875	-1.087713	0.841282
C	0.780641	-0.958378	0.124985
H	-1.487118	4.311157	1.083381
H	-0.669276	5.508307	0.050979
H	0.934702	4.107571	1.195409
H	1.120104	4.509141	-1.579332
H	0.240654	2.347320	-2.064422
H	1.999082	1.997298	-2.098072
H	1.905018	1.284875	0.278210
H	-1.397953	0.668175	-1.626163
H	1.497370	-4.295237	1.271612
H	3.599096	-3.520089	1.933819
H	3.914318	-1.856274	1.930161
P	4.091031	3.330065	-0.895644
O	5.159448	4.187983	-0.300520
O	4.016898	3.007147	-2.355280
O	4.091305	1.860118	-0.149160
C	4.461665	1.725817	1.206215
C	5.580975	0.714842	1.333752
O	5.137819	-0.591833	0.963888
C	6.786926	0.989180	0.432810
O	7.963674	0.406241	0.958409
C	6.443181	0.222442	-0.832866
C	5.657209	-0.973616	-0.303358
N	4.575724	-1.463433	-1.158714
C	4.254689	-2.852981	-1.063196
O	4.921641	-3.569003	-0.319479
N	3.212526	-3.321227	-1.798521
C	2.481915	-2.495275	-2.532205
N	1.445296	-3.020768	-3.219447
C	2.723664	-1.090425	-2.589614
C	3.777786	-0.624365	-1.876265
H	3.590495	1.371971	1.781487
H	4.793777	2.690286	1.617875
H	5.891892	0.672865	2.389347
H	6.911266	2.068623	0.248545
H	5.852753	0.858910	-1.497734
H	7.348985	-0.093387	-1.360429
H	6.304598	-1.842052	-0.151588
H	1.365862	-4.028337	-3.267038
H	0.961894	-2.473910	-3.918424
H	2.098290	-0.423544	-3.177857
H	4.017644	0.435514	-1.845033
Pt	-3.057563	-2.070071	-1.430098
N	-5.086473	-2.586336	-1.767147
N	-2.253422	-3.947156	-2.455019
H	-5.413835	-2.233565	-2.667164
H	-5.241534	-3.594731	-1.771189
H	-1.734465	-3.726976	-3.303086
H	-1.605331	-4.326469	-1.757152
H	-5.707890	-2.199464	-1.056861
H	-2.942443	-4.660277	-2.688253
H	8.173288	0.847441	1.794399
H	-6.924425	-0.140653	0.829496

Table S2 The torsion angles (δ-1, ε-1, ζ-1, α, β, γ and δ) and glycosyl angles (χ-1) (°) along the H-abstraction reaction in water solution. All the angles are defined as shown in Fig. S1.

complexes	δ-1	ε-1	ζ-1	α	β	γ	δ	χ-1
[cisplatin-GGC]^{0}	151.5	-165.3	-71.6	-74.1	178.1	41.1	118.7	-125.3
[cisplatin-GGC]$^{-\cdot}$	143.7	-173.4	-88.6	-60.9	169.7	57.8	135.5	-116.9
TS1	99.1	-167.6	-79.3	-66.2	-168.6	59.9	153.9	179.5
P1	86.7	-156.7	-71.1	-64.7	-174.4	62.3	152.5	170.6

Table S3 Coordinates of optimized structures in Fig. 2

TS1

Atom	Coordinates (Angstroms)		
	X	Y	Z
O	-6.566295	1.056345	-0.495490
C	-6.572970	2.116353	0.441539
C	-5.254268	2.169558	1.160989
O	-5.091675	0.986838	1.948776
C	-4.014426	2.257842	0.253950
O	-3.569074	3.607323	0.170934
C	-3.058841	1.347559	0.947285
C	-3.716789	0.862936	2.194138
N	-3.401327	-0.523590	2.510883
C	-4.156808	-1.662993	2.341016
N	-3.473095	-2.765377	2.518506
C	-2.192275	-2.331734	2.797078
C	-0.983375	-3.064700	3.015557
O	-0.784266	-4.271892	3.030949
N	0.102242	-2.168143	3.218910
C	0.051569	-0.797207	3.147003
N	1.212940	-0.113687	3.330413
N	-1.063460	-0.133519	2.939992
C	-2.130195	-0.943666	2.785289
H	-7.383994	1.990869	1.175585
H	-6.714555	3.086950	-0.060838
H	-5.250473	3.054498	1.822426
H	-4.251539	1.911155	-0.762747
H	-3.310437	-0.072881	-0.106799
H	-1.979717	1.473524	0.890881
H	-3.421429	1.467657	3.076017
H	-5.214089	-1.598688	2.110639
H	0.998325	-2.627094	3.376466
H	2.068577	-0.600108	3.082339
H	1.166539	0.833842	2.954637
P	-2.451894	3.950137	-0.997217
O	-2.424726	5.436727	-1.110998
O	-2.633071	3.021311	-2.159674
O	-1.055111	3.412494	-0.307294
C	-0.507439	4.018483	0.839063
C	0.896758	3.492585	1.060469
O	0.870869	2.063201	1.212938
C	1.905319	3.733590	-0.065072
O	3.184862	3.742959	0.557679
C	1.661787	2.529240	-0.959455
C	1.437442	1.441884	0.070000
N	0.589537	0.346630	-0.367046
C	-0.619773	0.376428	-0.997810
N	-1.138107	-0.832137	-1.103216
C	-0.218794	-1.700416	-0.535458
C	-0.207525	-3.120424	-0.370569
O	-1.016437	-3.962175	-0.750773
N	0.938424	-3.518905	0.349777
C	1.941883	-2.696034	0.789837
N	2.943735	-3.236646	1.530157
N	1.939310	-1.397217	0.588944
C	0.850046	-0.965578	-0.058175
H	-1.119256	3.772844	1.724517
H	-0.482059	5.114620	0.733562
H	1.284117	3.921044	1.994588
H	1.736450	4.687258	-0.586567
H	0.755333	2.703618	-1.549134
H	2.502114	2.327454	-1.627967
H	2.383687	0.961718	0.346487
H	-1.109596	1.297009	-1.312003
H	0.987089	-4.515247	0.547746
H	3.180565	-4.205126	1.340783
H	3.764944	-2.626105	1.546197
P	4.603364	3.292875	-0.156076
O	5.679828	3.936603	0.654249
O	4.519132	3.394018	-1.645007
O	4.594668	1.668862	0.155285
C	4.843288	1.200011	1.462980
C	5.742816	-0.015742	1.413262
O	5.095588	-1.131771	0.800792
C	7.024919	0.195540	0.603923
O	8.062640	-0.652759	1.051981
C	6.634181	-0.283012	-0.783903
C	5.625704	-1.389439	-0.493219
N	4.528829	-1.530261	-1.449812
C	3.962970	-2.834718	-1.595216
O	4.499937	-3.782812	-1.027470
N	2.838158	-2.966813	-2.345768
C	2.258324	-1.903341	-2.882582
N	1.125514	-2.096757	-3.583760
C	2.771026	-0.579843	-2.724734
C	3.894054	-0.447920	-1.979013
H	3.888218	0.936177	1.950492
H	5.332156	1.981329	2.063726
H	5.987244	-0.300477	2.448566
H	7.328056	1.255916	0.610554
H	6.206114	0.546223	-1.353397
H	7.504499	-0.664997	-1.327001
H	6.104286	-2.372829	-0.474202
H	0.759484	-3.034586	-3.683437
H	0.633975	-1.332479	-4.024962
H	2.274383	0.283166	-3.160513
H	4.323419	0.528272	-1.766684
Pt	-3.165923	-1.199322	-1.270475
N	-5.238211	-1.477906	-1.254710
N	-2.810002	-2.791390	-2.827285
H	-5.724806	-0.659811	-0.863655
H	-5.613754	-1.636231	-2.190762
H	-2.379763	-2.419758	-3.673016
H	-2.142338	-3.427943	-2.378865
H	-5.492872	-2.291221	-0.692561
H	-3.620845	-3.337181	-3.116030
H	8.293779	-0.398407	1.957117
H	-7.389891	1.094361	-1.001692

P1

Atom	Coordinates (Angstroms)		
	X	Y	Z
O	-6.307445	0.950047	-0.720575
C	-6.463357	2.096304	0.095214
C	-5.273650	2.282027	0.994816
O	-5.177781	1.201058	1.922767
C	-3.912048	2.340895	0.297611
O	-3.624675	3.667088	-0.112380
C	-3.021259	1.805074	1.355814
C	-3.854769	1.138418	2.392145
N	-3.495290	-0.275000	2.573678
C	-4.251959	-1.406411	2.366463
N	-3.567977	-2.515805	2.495026
C	-2.287132	-2.093545	2.787117
C	-1.083456	-2.837972	2.992770
O	-0.889691	-4.046067	2.970392
N	0.001048	-1.953749	3.245544
C	-0.049991	-0.581401	3.242072
N	1.113735	0.090980	3.464319
N	-1.161347	0.092028	3.061657
C	-2.226692	-0.706192	2.841082
H	-7.375461	2.025106	0.708502
H	-6.539176	3.007505	-0.519894
H	-5.412995	3.231717	1.543367
H	-3.923235	1.687208	-0.591542
H	-3.503726	-0.316311	-0.136523
H	-1.941713	1.897180	1.420032
H	-3.768886	1.619917	3.384566
H	-5.306140	-1.332576	2.125066
H	0.882523	-2.418612	3.451415
H	1.966785	-0.375352	3.170213
H	1.061941	1.059224	3.151391
P	-2.550125	3.848561	-1.353621
O	-2.548689	5.303366	-1.677947
O	-2.754577	2.763243	-2.365878
O	-1.134068	3.426365	-0.621356
C	-0.607803	4.199733	0.432786
C	0.756750	3.666446	0.822400
O	0.672949	2.274524	1.181924
C	1.832254	3.724361	-0.264204
O	3.077850	3.817410	0.415492
C	1.621446	2.398114	-0.970974
C	1.316700	1.484836	0.197174
N	0.497420	0.334122	-0.147411
C	-0.722911	0.298109	-0.758568
N	-1.174552	-0.937159	-0.858008
C	-0.206947	-1.752932	-0.290347
C	-0.098049	-3.172154	-0.160166
O	-0.865180	-4.058757	-0.524188
N	1.108438	-3.511963	0.483686
C	2.082563	-2.639800	0.895743
N	3.171240	-3.141444	1.524083
N	1.973305	-1.334243	0.759280
C	0.833123	-0.960455	0.162955
H	-1.279003	4.151460	1.306436
H	-0.516961	5.257108	0.136740
H	1.101919	4.221064	1.705358
H	1.705159	4.584688	-0.937647
H	0.752595	2.477421	-1.633033
H	2.491900	2.085180	-1.551867
H	2.240070	1.053173	0.606645
H	-1.253229	1.192722	-1.079725
H	1.233872	-4.509619	0.635850
H	3.450522	-4.088722	1.293304
H	3.949802	-2.477562	1.534626
P	4.516011	3.328451	-0.233014
O	5.573214	4.035771	0.549108
O	4.452355	3.327319	-1.726363
O	4.506568	1.728777	0.188565
C	4.880522	1.325415	1.487956
C	5.839919	0.158024	1.407459
O	5.201031	-0.994754	0.854613
C	7.056019	0.411700	0.511339
O	8.163022	-0.371408	0.910496
C	6.602658	-0.122824	-0.834994
C	5.706647	-1.291112	-0.441453
N	4.591343	-1.574114	-1.339351
C	4.200089	-2.938795	-1.503906
O	4.867576	-3.819390	-0.966814
N	3.089745	-3.197699	-2.241936
C	2.380012	-2.207131	-2.762353
N	1.275485	-2.532272	-3.462380
C	2.713231	-0.830842	-2.577707
C	3.817807	-0.569893	-1.838322
H	3.982535	1.022960	2.052835
H	5.365390	2.154262	2.024096
H	6.163601	-0.093863	2.429417
H	7.306135	1.484772	0.475066
H	6.065167	0.658400	-1.380655
H	7.454947	-0.451801	-1.438121
H	6.270566	-2.227363	-0.390123
H	1.086192	-3.508664	-3.647524
H	0.756537	-1.835123	-3.977545
H	2.101405	-0.033350	-2.991344
H	4.125130	0.446603	-1.597968
Pt	-3.151217	-1.421279	-1.200932
N	-5.200403	-1.779853	-1.339264
N	-2.619294	-3.028942	-2.656018
H	-5.708647	-0.962201	-0.982062
H	-5.521840	-1.954909	-2.292140
H	-2.146074	-2.679104	-3.487631
H	-1.968312	-3.634041	-2.144558
H	-5.471947	-2.587092	-0.775935
H	-3.396876	-3.604553	-2.976583
H	8.438006	-0.082287	1.792686
H	-7.010094	0.971108	-1.385683

TS2

Atom	Coordinates (Angstroms) X	Y	Z
O	-6.358956	0.322401	-0.622516
C	-6.572991	1.642789	-0.172871
C	-5.532790	2.117454	0.811548
O	-5.495867	1.225640	1.932923
C	-4.093266	2.173902	0.329016
O	-3.880664	3.347447	-0.421141
C	-3.356024	2.161704	1.658997
C	-4.201712	1.207886	2.487603
N	-3.688615	-0.170855	2.432011
C	-4.377050	-1.324508	2.135871
N	-3.652947	-2.408195	2.258239
C	-2.419841	-1.948145	2.667559
C	-1.211296	-2.661729	2.938830
O	-0.967473	-3.857122	2.844312
N	-0.196896	-1.762416	3.358637
C	-0.295334	-0.393170	3.394651
N	0.820059	0.309363	3.719568
N	-1.412805	0.251511	3.147530
C	-2.424303	-0.565223	2.791119
H	-7.575802	1.745944	0.269591
H	-6.528960	2.293017	-1.056433
H	-5.814502	3.131345	1.149375
H	-3.860892	1.274628	-0.270942
H	-2.300571	1.877338	1.608230
H	-3.425743	3.168733	2.094881
H	-4.251458	1.489765	3.548160
H	-5.423393	-1.295527	1.859497
H	0.687988	-2.207773	3.589251
H	1.722567	-0.127857	3.570103
H	0.772305	1.287950	3.447509
P	-2.691134	3.365619	-1.559016
O	-2.691586	4.739046	-2.132300
O	-2.782667	2.119884	-2.394006
O	-1.345985	3.112111	-0.646977
C	-0.867578	4.088134	0.254967
C	0.500073	3.677407	0.769944
O	0.452096	2.350828	1.328050
C	1.611065	3.628940	-0.279621
O	2.830793	3.873007	0.406946
C	1.490055	2.202404	-0.773819
C	1.200670	1.465949	0.520111
N	0.476914	0.220188	0.311784
C	-0.725072	0.059329	-0.320896
N	-1.022328	-1.206781	-0.514470
C	0.047915	-1.922713	0.001935
C	0.375527	-3.312584	-0.020455
O	-0.242789	-4.262611	-0.496064
N	1.623712	-3.539099	0.590058
C	2.481125	-2.582243	1.071004
N	3.665779	-2.986382	1.580263
N	2.175666	-1.299436	1.079610
C	0.985927	-1.036807	0.518943
H	-1.556495	4.188450	1.107830
H	-0.794175	5.071320	-0.235342
H	0.786669	4.371978	1.571332
H	1.467031	4.369932	-1.079290
H	0.633262	2.125845	-1.453329
H	2.387249	1.849221	-1.282696
H	2.128340	1.177690	1.034385
H	-1.332148	0.907990	-0.625904
H	1.916665	-4.512764	0.581429
H	4.053827	-3.862022	1.244908
H	4.349553	-2.227677	1.637302
P	4.292248	3.506654	-0.275114
O	5.304459	4.317226	0.464952
O	4.171801	3.481942	-1.764042
O	4.440950	1.919747	0.166682
C	4.952405	1.563401	1.433492
C	5.986986	0.471805	1.280904
O	5.377154	-0.735783	0.815064
C	7.094697	0.782586	0.269348
O	8.294293	0.109711	0.596400
C	6.573950	0.152985	-1.009202
C	5.825435	-1.070222	-0.492269
N	4.684991	-1.502076	-1.294583
C	4.470538	-2.901499	-1.482851
O	5.291536	-3.698589	-1.034584
N	3.341860	-3.286855	-2.132327
C	2.454748	-2.389760	-2.539549
N	1.345390	-2.844855	-3.153815
C	2.621464	-0.984931	-2.339410
C	3.743812	-0.599124	-1.687167
H	4.134388	1.194579	2.074964
H	5.412978	2.434635	1.921241
H	6.424239	0.269322	2.271113
H	7.250429	1.869896	0.171573
H	5.916880	0.858395	-1.528903
H	7.393721	-0.125685	-1.679063
H	6.478880	-1.946307	-0.435334
H	1.174571	-3.842095	-3.161552
H	0.569073	-2.229564	-3.357230
H	1.874058	-0.267620	-2.669766
H	3.941534	0.438902	-1.423056
Pt	-3.011539	-1.510196	-1.463736
N	-4.340928	-0.276552	-2.645774
N	-3.021040	-3.479467	-0.527347
H	-3.878587	0.648634	-2.686879
H	-4.524647	-0.598284	-3.593871
H	-2.083429	-3.901872	-0.526450
H	-3.337313	-3.378042	0.443867
H	-5.228366	-0.149991	-2.149250
H	-3.658287	-4.118874	-0.998138
H	8.618918	0.456821	1.439936
H	-6.440304	-0.269002	0.138656

P2

Atom	Coordinates (Angstroms)		
	X	Y	Z
O	-5.593161	-0.016908	1.540635
C	-5.911683	1.171620	2.250911
C	-4.678538	2.044011	2.332676
O	-3.741904	1.474356	3.249654
C	-3.981186	2.170377	0.978030
O	-3.605298	3.511771	0.712315
C	-2.787073	1.241509	1.113583
C	-2.536241	1.138799	2.609206
N	-2.136319	-0.204438	2.997996
C	-2.899876	-1.350533	2.880723
N	-2.250772	-2.437863	3.202144
C	-0.991279	-1.990709	3.545446
C	0.166554	-2.724468	3.943218
O	0.331393	-3.932114	4.063786
N	1.242690	-1.836908	4.191182
C	1.240426	-0.483595	3.981940
N	2.431130	0.156959	4.113316
N	0.170244	0.189742	3.622580
C	-0.896543	-0.608388	3.415199
H	-6.254853	0.938228	3.269543
H	-6.708838	1.733022	1.737446
H	-4.972162	3.037373	2.701923
H	-4.661355	1.847307	0.185501
H	-3.022590	0.247987	0.711769
H	-1.905895	1.630904	0.597860
H	-1.720358	1.799205	2.942670
H	-3.936544	-1.283907	2.561275
H	2.127842	-2.307339	4.358750
H	3.143623	-0.244727	4.709644
H	2.368785	1.167094	4.142673
P	-3.099853	3.834808	-0.829844
O	-3.397699	5.273135	-1.080919
O	-3.548830	2.728516	-1.745034
O	-1.476135	3.607872	-0.702963
C	-0.761639	4.337041	0.273115
C	0.638371	3.781374	0.398952
O	0.581069	2.399056	0.766751
C	1.510963	3.822970	-0.858129
O	2.850882	3.946031	-0.395795
C	1.177121	2.489754	-1.506653
C	1.055874	1.592474	-0.292867
N	0.198586	0.431419	-0.470087
C	-0.955666	0.261548	-1.193933
N	-1.410659	-0.966070	-1.116598
C	-0.514944	-1.653395	-0.313845
C	-0.426704	-3.024843	0.084268
O	-1.195361	-3.961570	-0.124414
N	0.757125	-3.251704	0.814129
C	1.721653	-2.320811	1.110655
N	2.821932	-2.741289	1.785213
N	1.597141	-1.050079	0.798173
C	0.490317	-0.786980	0.089933
H	-1.262358	4.241560	1.250471
H	-0.719187	5.407042	0.012484
H	1.150050	4.329790	1.202765
H	1.267914	4.675148	-1.509717
H	0.212340	2.592824	-2.014892
H	1.935784	2.161424	-2.221605
H	2.029575	1.166480	-0.018960
H	-1.465542	1.078508	-1.701444
H	0.869408	-4.205026	1.151270
H	3.131009	-3.687094	1.581628
H	3.580886	-2.058501	1.710419
P	4.194552	3.332920	-1.125995
O	5.341764	4.117554	-0.580172
O	3.969990	3.107571	-2.586460
O	4.221900	1.816225	-0.468706
C	4.554462	1.636512	0.891373
C	5.441228	0.419915	1.035511
O	4.737557	-0.779320	0.704800
C	6.666056	0.430182	0.116089
O	7.730253	-0.319368	0.666452
C	6.181325	-0.328766	-1.107318
C	5.196686	-1.334005	-0.518288
N	4.053029	-1.671733	-1.368793
C	3.578370	-3.017319	-1.356830
O	4.150957	-3.851916	-0.660833
N	2.500478	-3.316712	-2.132376
C	1.881577	-2.372277	-2.817714
N	0.819234	-2.746645	-3.587689
C	2.250957	-0.998365	-2.753114
C	3.347376	-0.701588	-2.012274
H	3.634448	1.498562	1.484935
H	5.089267	2.518110	1.275861
H	5.750928	0.342883	2.089417
H	6.970685	1.462078	-0.125779
H	5.707027	0.361733	-1.810694
H	7.012380	-0.828445	-1.615399
H	5.677598	-2.294304	-0.307753
H	0.790784	-3.735037	-3.816625
H	0.562828	-2.129784	-4.350250
H	1.702477	-0.228253	-3.288448
H	3.705522	0.320058	-1.896752
Pt	-3.398392	-1.650973	-2.063398
N	-4.630381	-0.004199	-1.551653
N	-2.337520	-3.366173	-2.699952
H	-4.174797	0.919062	-1.651625
H	-5.453183	0.012099	-2.155125
H	-1.479531	-3.094336	-3.185561
H	-2.043760	-3.882358	-1.861489
H	-4.980629	-0.070861	-0.589104
H	-2.855915	-3.994200	-3.311820
H	8.019413	0.115903	1.481606
H	-6.357226	-0.609810	1.580718