

**On the role of the arsenic in the hydrolysis and DNA metalation processes in Arsenous Acid–
Platinum(II) Anticancer Complex**

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Table S1: Cartesian coordinates of all the species present on the potential energy surfaces for aquation and DNA purine bases metalation by **1** optimized at B3LYP/*Basis1* and B3LYP/*Basis2* level in water.

Aquation							
<i>Basis1</i>				<i>Basis2</i>			
AsPt-1				AsPt-1			
Pt	0.00018400	0.86059800	-0.00006900	Pt	-0.00000800	0.84931100	-0.00009200
As	-0.00043200	-1.48202700	0.00005600	As	0.00001300	-1.46868700	0.00003900
Cl	0.00052300	3.26608600	0.00027200	Cl	-0.00002200	3.24566100	0.00026200
O	-2.01429800	-1.57367400	-0.00495500	O	2.01658300	-1.56834000	0.00661800
O	2.01390700	-1.57434800	0.00490400	O	-2.01656200	-1.56837100	-0.00650400
O	0.02926800	-2.55697600	1.40456400	O	-0.02796000	-2.54840000	-1.40240500
H	-0.89026400	-2.77749900	1.64885000	H	0.89193000	-2.77181500	-1.64204900
O	-0.03001500	-2.55881600	-1.40298500	O	0.02800400	-2.54804500	1.40275900
H	0.88956600	-2.77997100	-1.64654000	H	-0.89188300	-2.77138800	1.64248300
N	-2.03426800	0.71719600	-0.01821200	N	2.02117400	0.72080600	0.01638100
H	-2.62826100	1.54127200	-0.02662400	H	2.61142200	1.54786000	0.02348300
N	2.03452900	0.71650500	0.01803200	N	-2.02118300	0.72077400	-0.01660400
H	2.62878000	1.54039100	0.02623700	H	-2.61144400	1.54781800	-0.02381900
C	-2.65761900	-0.43437600	-0.01247400	C	2.65379100	-0.42627500	0.01247200
C	-4.15752500	-0.53843400	-0.01442200	C	4.15422800	-0.52008700	0.01427500
H	-4.47944600	-1.10705200	-0.89306500	H	4.48045000	-1.08585700	0.89321600
H	-4.63354000	0.44425000	-0.02539600	H	4.62391200	0.46569500	0.02454500
H	-4.48303500	-1.08832300	0.87485900	H	4.48375500	-1.06833200	-0.87458200
C	2.65751700	-0.43530200	0.01225200	C	-2.65378500	-0.42631600	-0.01254900
C	4.15742300	-0.53966400	0.01316300	C	-4.15422000	-0.52014800	-0.01431900
H	4.47973200	-1.11138900	0.88961300	H	-4.48043500	-1.08624800	-0.89304700
H	4.63366000	0.44287800	0.02714000	H	-4.62391700	0.46562500	-0.02494800
H	4.48231200	-1.08653000	-0.87823700	H	-4.48374000	-1.06806600	0.87474400
AsPt-adduct				AsPt-adduct			
Pt	0.34086400	-0.62922200	0.00386800	Pt	0.32655400	-0.62421800	0.00351800
As	-1.14693600	1.17828300	-0.00083400	As	-1.12526200	1.18153300	-0.00093000
Cl	1.83578600	-2.52474800	0.00236500	Cl	1.79143200	-2.53036700	0.00268900
O	0.31617700	2.53108400	-0.00368200	O	0.35119900	2.52476100	-0.00529400
O	-2.76147400	-0.04141000	-0.00491800	O	-2.76096000	-0.01571700	-0.00363400
O	-1.86949200	1.97401700	1.40492000	O	-1.83913200	1.98834200	1.40447000
H	-1.30701500	2.73215000	1.65517600	H	-1.26966900	2.74230700	1.65075300
O	-1.81894500	2.01201800	-1.40879800	O	-1.79204300	2.02656500	-1.40605700
H	-2.66176500	1.58204600	-1.65075500	H	-2.64263600	1.60984100	-1.64320700
N	1.81416100	0.79034700	-0.01497500	N	1.81602400	0.75831500	-0.01633600
H	2.80630300	0.53162300	-0.02344900	H	2.80435100	0.48546600	-0.02386300
N	-1.31856800	-1.82041300	0.02240200	N	-1.32643900	-1.79910700	0.02323800
H	-1.25111000	-2.83392600	0.03491000	H	-1.26546300	-2.81325300	0.03502300
C	1.54576800	2.06794600	-0.01014500	C	1.57215600	2.04142000	-0.01123200
C	2.62156600	3.11862600	-0.01188500	C	2.66728300	3.07173100	-0.01099200
H	2.49912000	3.76206400	-0.88944600	H	2.55763000	3.71921200	-0.88730100
H	3.61903400	2.67481400	-0.02418600	H	3.65645700	2.60962800	-0.02362900
H	2.51550900	3.74797700	0.87808400	H	2.57299300	3.70153100	0.88005400
C	-2.53273700	-1.32873000	0.00904300	C	-2.53959700	-1.30356500	0.00982100
C	-3.75502400	-2.20498300	0.00881300	C	-3.76506600	-2.17518200	0.00838600
H	-4.36888400	-1.96950100	0.88442100	H	-4.37876600	-1.93848300	0.88382200
H	-3.49578500	-3.26571500	0.02382300	H	-3.51016900	-3.23705400	0.02251500
H	-4.35289600	-1.99134900	-0.88339100	H	-4.36196200	-1.95873400	-0.88384800
O	4.43690100	-0.55792100	-0.11279300	O	4.43395800	-0.61368100	-0.11257300
H	3.88643800	-1.36315000	-0.02771200	H	3.87669800	-1.41339200	-0.02332800
H	4.99227300	-0.53936900	0.68340600	H	4.98873500	-0.59541500	0.68409800
AsPt-TS				AsPt-TS			
Pt	0.71488200	0.04910800	0.20119100	Pt	-0.50776600	0.49015800	-0.20765500
As	-1.58422600	-0.10446000	-0.11829900	As	1.14428900	-1.07119300	0.12073000
Cl	3.09815900	0.16705500	-1.38955900	Cl	-2.31227800	2.01161100	1.40340500

O	-1.55295500	-2.10860600	-0.10816200	O	-0.14303400	-2.60501100	0.10007100
O	-1.81427800	1.88478100	-0.15211900	O	2.59536000	0.31059900	0.16801600
O	-2.45102800	-0.14300900	-1.66103900	O	1.77599200	-1.64933900	1.67134600
H	-2.57149200	-1.07469300	-1.92783800	H	1.27134800	-2.44141500	1.93826400
O	-2.84917700	-0.21045800	1.11657000	O	2.07004900	-1.96035900	-1.10087200
H	-3.16615300	0.69140900	1.31653700	H	2.88950400	-1.46445100	-1.29079200
N	0.71048600	-1.99291500	0.20101500	N	-1.80305600	-1.06923100	-0.22709200
H	1.56417400	-2.53570700	0.29452100	H	-2.80629900	-0.94059300	-0.32431300
N	0.44141200	2.06853800	0.17105300	N	0.96738200	1.87761000	-0.16549200
H	1.21779400	2.71498700	0.27710500	H	0.77651800	2.86937500	-0.27709200
C	-0.38797300	-2.68536900	0.04328200	C	-1.40621300	-2.30511000	-0.06311000
C	-0.40190900	-4.18822000	0.02407800	C	-2.35682800	-3.46888100	-0.04694600
H	-1.06270300	-4.55314000	0.81720500	H	-2.07519400	-4.17665100	-0.83339800
H	0.59687000	-4.60594300	0.16543800	H	-3.39065200	-3.15216000	-0.19881600
H	-0.80740600	-4.53426300	-0.93236500	H	-2.27502300	-3.98909400	0.91320300
C	-0.73624200	2.61098600	0.00337400	C	2.22304900	1.55482900	0.00725900
C	-0.94708300	4.09872000	-0.02821300	C	3.32778900	2.57310900	0.03635300
H	-1.40256600	4.37763800	-0.98410600	H	3.84881500	2.51345300	0.99761200
H	-0.01008600	4.64469300	0.09868700	H	2.94983100	3.58734000	-0.10704500
H	-1.64352500	4.38296400	0.76747300	H	4.05374600	2.34232400	-0.75014900
O	2.64639600	0.31967400	1.56716000	O	-1.82027400	1.94057600	-1.53564900
H	2.78752500	-0.44366000	2.15342600	H	-2.37167500	1.45656500	-2.17473900
H	3.29185700	0.22743500	0.82855100	H	-2.41981800	2.24088400	-0.81417200
AsPt-product				AsPt-product			
Pt	-0.29996200	-0.62593100	-0.03161200	Pt	-0.29138300	-0.61525500	-0.03523200
As	1.31547300	1.04965700	0.01519000	As	1.30408500	1.04400800	0.01653000
Cl	-4.48647200	-0.91078000	0.12874400	Cl	-4.47557700	-0.93869000	0.13718300
O	-0.03837300	2.50473800	-0.00995200	O	-0.04814300	2.50481500	-0.00656900
O	2.82050700	-0.27470800	0.04343400	O	2.81837600	-0.27501600	0.04395300
O	2.10468100	1.77557100	-1.38541800	O	2.09709600	1.77731400	-1.37936200
H	1.59879900	2.56725800	-1.65308400	H	1.59423800	2.57282600	-1.64060300
O	2.00765000	1.82432700	1.44027600	O	1.99571600	1.81863000	1.44331400
H	2.81057700	1.33386300	1.70322800	H	2.80128000	1.33104100	1.70281900
N	-1.66544300	0.89020400	-0.01418100	N	-1.66070000	0.87855300	-0.02307800
H	-2.66962000	0.69434400	-0.00199900	H	-2.66403400	0.67869300	-0.01296600
N	1.25961200	-1.94913100	-0.01867200	N	1.24868200	-1.93855200	-0.01542200
H	1.12715800	-2.95652800	-0.02423600	H	1.11257700	-2.94566200	-0.01892500
C	-1.30160600	2.14427200	-0.01291200	C	-1.30814800	2.13651600	-0.01491900
C	-2.29018900	3.27571600	-0.01829800	C	-2.30606700	3.25957000	-0.01640200
H	-2.11557600	3.91442800	0.85361600	H	-2.14283300	3.89117000	0.86297400
H	-3.31940900	2.91210000	-0.00304600	H	-3.33251500	2.88769200	-0.01127800
H	-2.13445700	3.88624400	-0.91409100	H	-2.14989500	3.88060500	-0.90483700
C	2.50423800	-1.54472800	0.02738900	C	2.49676600	-1.54290000	0.03021800
C	3.66431500	-2.49934700	0.06692100	C	3.65055900	-2.50477000	0.07165300
H	4.31655100	-2.31034700	-0.79191800	H	4.30404800	-2.32194100	-0.78762300
H	3.33560700	-3.54034700	0.04964900	H	3.31550800	-3.54386100	0.05636700
H	4.24918100	-2.31878800	0.97483600	H	4.23701000	-2.32647000	0.97901300
O	-1.78204800	-2.18916700	-0.04831400	O	-1.76117600	-2.17608000	-0.05401300
H	-1.74296200	-2.67802200	-0.89036900	H	-1.72303900	-2.67093300	-0.89277400
H	-2.71844600	-1.80609400	0.00439100	H	-2.70392800	-1.80561100	0.00597100
Guanine platination							
AsPt-H₂O-complex				AsPt-H₂O-complex			
Pt	0.00545300	0.97649500	-0.00128500	Pt	0.00631400	0.96346700	-0.00130400
As	-0.00953800	-1.35252900	0.00070400	As	-0.01141800	-1.33957800	0.00087900
O	-2.00067400	-1.44143200	0.00131700	O	-2.00524900	-1.43369000	-0.00009800
O	1.98381100	-1.46022000	0.00105700	O	1.98460800	-1.45709700	0.00233500
O	0.02441600	-2.39577200	1.41954400	O	0.02013300	-2.38532000	1.41907600
H	-0.89346100	-2.61140200	1.67564800	H	-0.89824900	-2.60106900	1.67260600
O	-0.05130400	-2.40288800	-1.41247400	O	-0.05289000	-2.39371300	-1.41062600
H	0.86486600	-2.62992900	-1.66485200	H	0.86338000	-2.62274200	-1.66018400

N	-2.03371700	0.84590300	-0.02447100	N	-2.01968200	0.85210100	-0.02312500
H	-2.63698300	1.66324500	-0.03903500	H	-2.61867400	1.67284600	-0.03680100
N	2.03752200	0.82537600	0.01920900	N	2.02466900	0.82681700	0.01709200
H	2.63882400	1.64449600	0.02899000	H	2.62255300	1.64870600	0.02545900
C	-2.65308200	-0.30658600	-0.01302100	C	-2.64999700	-0.29526000	-0.01316800
C	-4.15073000	-0.42285800	-0.01390700	C	-4.14836700	-0.39937900	-0.01463600
H	-4.46716100	-1.00532300	-0.88526500	H	-4.46945500	-0.97849900	-0.88656400
H	-4.63418100	0.55573400	-0.03674200	H	-4.62443800	0.58290100	-0.03678400
H	-4.47059500	-0.96444900	0.88242800	H	-4.47326300	-0.93922200	0.88098600
C	2.64738000	-0.33158100	0.01059600	C	2.64315400	-0.32623800	0.00998900
C	4.14398400	-0.46002300	0.01066500	C	4.14032900	-0.44539300	0.00972100
H	4.45700500	-1.03367400	0.88914200	H	4.45753000	-1.01563400	0.88896300
H	4.63473800	0.51515300	0.02075800	H	4.62545600	0.53268900	0.01813700
H	4.45851000	-1.01540100	-0.87902500	H	4.45840400	-1.00021100	-0.87908900
O	0.12186500	3.16068800	0.01030300	O	0.12883600	3.13910900	0.01141300
H	-0.34161500	3.54401500	0.77752100	H	-0.32753800	3.53016000	0.77914800
H	-0.29740400	3.54871500	-0.77971300	H	-0.28058100	3.53659600	-0.77920100
AsPt-G-adduct				AsPt-G-adduct			
Pt	-1.12624000	-0.38568400	0.49757600	Pt	-1.13195900	-0.37248600	0.49981500
As	-2.80762200	0.85037300	-0.53421400	As	-2.79181000	0.84098500	-0.53750400
O	-1.65268300	2.46654800	-0.71117100	O	-1.64431900	2.46427800	-0.72224800
O	-4.11183700	-0.66787100	-0.43791300	O	-4.10133800	-0.67730300	-0.44260000
O	-4.03046500	1.83046900	0.27362700	O	-4.02392600	1.82510900	0.25375800
H	-3.70054800	2.74710000	0.34538300	H	-3.69691100	2.74307700	0.31883800
O	-3.11819100	0.98273900	-2.26457400	O	-3.09580400	0.96309800	-2.27077800
H	-3.76423100	0.29666600	-2.52170400	H	-3.74128400	0.27584400	-2.52546000
N	0.03418100	1.27614800	0.27896800	N	0.02936000	1.27330600	0.28510600
H	1.00242600	1.28874300	0.59790300	H	0.99593300	1.28735600	0.60918400
N	-2.48518500	-1.90781200	0.59081200	N	-2.46902900	-1.89460300	0.59938100
H	-2.26566000	-2.81528400	0.99120300	H	-2.24499500	-2.79851400	1.00579400
C	-0.42428800	2.37415000	-0.26127700	C	-0.42003200	2.37162000	-0.26343100
C	0.41095500	3.61418400	-0.41037900	C	0.42071800	3.60787200	-0.41130000
H	0.45216100	3.89836400	-1.46690600	H	0.47119100	3.88777400	-1.46860000
H	1.42520100	3.46680100	-0.03418200	H	1.43170900	3.45880200	-0.02688700
H	-0.06261700	4.43624500	0.13672300	H	-0.05379400	4.43412200	0.12869000
C	-3.69654300	-1.78156700	0.11056300	C	-3.68080000	-1.78354800	0.11484600
C	-4.70121100	-2.89841500	0.14956200	C	-4.67610700	-2.90835400	0.15986000
H	-5.58828800	-2.56757000	0.69949400	H	-5.56740600	-2.58100600	0.70509500
H	-4.29433400	-3.79403500	0.62354700	H	-4.26337200	-3.79711200	0.64180700
H	-5.01374800	-3.13897100	-0.87195000	H	-4.98428300	-3.15958600	-0.86042900
O	0.43163500	-1.54630900	1.44179000	O	0.41861500	-1.52685600	1.44595500
H	0.22675400	-1.66404800	2.38636700	H	0.21596100	-1.65369800	2.38993000
H	1.30054400	-1.03651800	1.39901300	H	1.29360000	-1.02478000	1.40443900
N	5.25358600	-1.75378800	-1.91214700	N	5.23073600	-1.75822700	-1.91668900
C	4.02910000	-2.39270800	-1.90011700	C	4.00461100	-2.39393900	-1.90039500
H	3.80176000	-3.18660200	-2.59839800	H	3.77199100	-3.18575900	-2.59929300
N	3.22032200	-1.93045700	-0.97600200	N	3.20125700	-1.93159600	-0.97160600
C	3.95236700	-0.93569500	-0.34639700	C	3.93886100	-0.94019300	-0.34322800
C	3.61804500	-0.06684800	0.72251700	C	3.61147300	-0.07195700	0.72805800
O	2.54909300	0.01925300	1.37601900	O	2.54529400	0.01633100	1.38625900
N	4.66637500	0.80316100	1.04318000	N	4.66314500	0.79464200	1.04595000
H	4.48135600	1.43036000	1.82084400	H	4.48285300	1.42104900	1.82537000
C	5.89264400	0.84778000	0.41309000	C	5.88666800	0.83756600	0.41036300
N	6.80645900	1.72826600	0.89469900	N	6.80453800	1.71524700	0.88912300
H	6.51273900	2.51765100	1.45579600	H	6.51540400	2.50401300	1.45347500
H	7.62801500	1.87782200	0.32245500	H	7.62391800	1.86392000	0.31354900
N	6.21106900	0.04684500	-0.58940000	N	6.19865200	0.03751200	-0.59489500
C	5.22590900	-0.81210800	-0.92117800	C	5.21004900	-0.81851800	-0.92369600
H	6.02678500	-1.94347100	-2.53876300	H	6.00057700	-1.94858400	-2.54724900
AsPt- G-TS				AsPt- G-TS			

Pt	-0.64593800	-0.10077500	0.56850100	Pt	-0.64901400	-0.09481900	0.55458700
As	-2.58317000	0.45875500	-0.57766600	As	-2.57034400	0.45177700	-0.56978200
O	-2.00397500	2.36325100	-0.82953500	O	-2.00523700	2.36141600	-0.83042800
O	-3.33378500	-1.39482600	-0.42251000	O	-3.32273500	-1.40531900	-0.41327600
O	-4.11068200	1.03751600	0.10472100	O	-4.10071700	1.02648700	0.11293300
H	-4.09336500	2.01371600	0.12327500	H	-4.08797200	2.00267200	0.12586800
O	-2.86262200	0.40625600	-2.32493700	O	-2.85950700	0.39620200	-2.31631100
H	-3.25650400	-0.45745400	-2.55372400	H	-3.25650900	-0.46714700	-2.54022100
N	-0.07771600	1.83692500	0.28459900	N	-0.07844800	1.82853200	0.27519200
H	0.81839900	2.18198200	0.62137500	H	0.81812100	2.17388700	0.61109000
N	-1.45124100	-1.96893500	0.74120700	N	-1.42979300	-1.95693000	0.73980400
H	-0.97211600	-2.71924600	1.23051900	H	-0.94259600	-2.70171900	1.22991400
C	-0.83614000	2.69793000	-0.34272300	C	-0.83642900	2.69462600	-0.34660800
C	-0.42944100	4.12919200	-0.55542300	C	-0.42868600	4.12625300	-0.55351000
H	-0.40641100	4.34225800	-1.62923100	H	-0.41027800	4.34583600	-1.62610000
H	0.55060700	4.34131900	-0.12327400	H	0.55373000	4.33474400	-0.12480000
H	-1.17623700	4.78909300	-0.10180900	H	-1.17213300	4.78494100	-0.09256400
C	-2.61361200	-2.27474700	0.22464500	C	-2.59307100	-2.27706100	0.23251400
C	-3.20984200	-3.65036600	0.33157900	C	-3.17639600	-3.65717200	0.35064400
H	-4.18636700	-3.58406600	0.82217700	H	-4.14873000	-3.59747200	0.85042000
H	-2.56673100	-4.32914800	0.89541900	H	-2.52241300	-4.32854300	0.91103500
H	-3.36962700	-4.05434700	-0.67361000	H	-3.34257500	-4.06687400	-0.65120000
O	0.67147500	-0.33979600	2.46005100	O	0.66631200	-0.32159200	2.44704400
H	0.20489300	0.07739700	3.20353900	H	0.19614000	0.08816800	3.19246200
H	1.47192900	0.22577800	2.28121100	H	1.46693600	0.24670000	2.27591000
N	2.96796600	-1.98996900	-1.75715100	N	2.94766400	-2.00082800	-1.73246400
C	1.69219100	-1.89892700	-1.25096200	C	1.67380300	-1.90119300	-1.22489700
H	0.87848600	-2.49805400	-1.63410100	H	0.85685500	-2.50031400	-1.60097800
N	1.60163300	-1.01785900	-0.28007900	N	1.58838800	-1.01096600	-0.26132000
C	2.88190100	-0.50288200	-0.14503300	C	2.87093100	-0.49899300	-0.13361000
C	3.40618100	0.47265400	0.74496000	C	3.40009700	0.48311900	0.74589500
O	2.81192100	1.10300200	1.64784400	O	2.80854800	1.12225200	1.64445700
N	4.77022600	0.70014500	0.52179300	N	4.76374900	0.70532000	0.51690300
H	5.20042800	1.38148500	1.14119000	H	5.19760200	1.39136800	1.12855600
C	5.54539100	0.05576800	-0.42187300	C	5.53454600	0.04989700	-0.42295800
N	6.86477300	0.36222100	-0.45451900	N	6.85416600	0.35279100	-0.46297200
H	7.21271500	1.20929800	-0.02508400	H	7.20688000	1.20104800	-0.03992500
H	7.39176600	0.01459800	-1.24553200	H	7.37862200	-0.00454600	-1.25132100
N	5.06219800	-0.86181500	-1.24376800	N	5.04654400	-0.87429900	-1.23475000
C	3.74828700	-1.10185900	-1.06463500	C	3.73270200	-1.10887800	-1.04996200
H	3.27290600	-2.60186100	-2.50530900	H	3.24853800	-2.62004200	-2.47627800
AsPt-G-product				AsPt-G-product			
Pt	0.51459000	-0.00194300	-0.42782200	Pt	0.51993700	0.00005400	-0.42438100
As	2.74455600	-0.00634000	0.30498500	As	2.72926800	-0.00868600	0.30330100
O	2.84803200	1.99855400	0.31140200	O	2.83966100	1.99880500	0.31901800
O	2.82803800	-2.01104900	0.35001000	O	2.81679800	-2.01585700	0.34274600
O	4.17712900	-0.05655500	-0.72271800	O	4.16440600	-0.05544900	-0.72207700
H	4.47127800	0.85799700	-0.89849500	H	4.46025000	0.85959200	-0.89139000
O	3.34053400	0.04095500	1.96451700	O	3.32819300	0.03163300	1.96278800
H	3.47355300	-0.87421900	2.27862900	H	3.46492900	-0.88479900	2.27104300
N	0.66478400	2.03631700	-0.38640700	N	0.65845800	2.02476800	-0.38050100
H	-0.10858400	2.64374700	-0.64043100	H	-0.11645200	2.63053800	-0.63467200
N	0.65670700	-2.04060800	-0.38419200	N	0.64742300	-2.02530600	-0.39258100
H	-0.11617800	-2.64525000	-0.64614400	H	-0.12809900	-2.62522800	-0.65848900
C	1.77046700	2.64989900	-0.04214400	C	1.76027200	2.64569200	-0.03473600
C	1.88715700	4.14840900	-0.02678400	C	1.86835200	4.14468300	-0.01906600
H	2.15323200	4.47921400	0.98255000	H	2.13222600	4.47736000	0.99025100
H	0.95798900	4.63294000	-0.33320400	H	0.93650600	4.62405700	-0.32569100
H	2.69458300	4.45426100	-0.70021600	H	2.67405700	4.45555600	-0.69231000
C	1.75052700	-2.65842200	-0.01085800	C	1.73631300	-2.65469100	-0.02228800

C	1.85222500	-4.15746100	0.03268700	C	1.82696900	-4.15448500	0.01161900
H	2.67536900	-4.48206600	-0.61217800	H	2.64556200	-4.48153600	-0.63786400
H	0.92709000	-4.63830700	-0.29124100	H	0.89730200	-4.62648300	-0.31253800
H	2.08624700	-4.47364100	1.05466000	H	2.06166300	-4.47924800	1.03074500
O	-2.57600100	0.02085000	4.65746700	O	-2.55490200	0.00479100	4.65971600
H	-2.44589600	0.03549300	3.68461100	H	-2.43058200	0.02147300	3.68618500
H	-2.50290100	0.94624500	4.93908500	H	-2.47276200	0.92877700	4.94350400
N	-3.10945300	-0.00056300	-2.65297400	N	-3.09468700	0.01217100	-2.65303900
C	-1.75890200	0.00144900	-2.47722900	C	-1.74478500	0.01338600	-2.47600500
H	-1.05504600	0.00344700	-3.29534200	H	-1.03994600	0.01939200	-3.29333300
N	-1.44669400	0.00060000	-1.19250100	N	-1.43331500	0.00619400	-1.19058000
C	-2.65065400	-0.00194200	-0.49794400	C	-2.63900000	0.00028900	-0.49754500
C	-2.95099000	-0.00611000	0.89897000	C	-2.94064800	-0.01026800	0.89907400
O	-2.16881700	-0.00705100	1.85958500	O	-2.15915200	-0.01563600	1.86012300
N	-4.34273900	-0.00875500	1.11125000	N	-4.33251100	-0.01370600	1.10988800
H	-4.62765800	0.00061100	2.08665600	H	-4.61834900	-0.00878600	2.08508600
C	-5.31221400	-0.00958400	0.12973700	C	-5.30087500	-0.00984400	0.12727500
N	-6.60288900	0.03071000	0.52863400	N	-6.59174800	0.02812200	0.52474800
H	-6.86732300	-0.18594500	1.48049600	H	-6.85770600	-0.18963200	1.47591000
H	-7.30878000	-0.11502000	-0.18163200	H	-7.29743800	-0.11187600	-0.18683400
N	-5.02382500	-0.00972100	-1.16285000	N	-5.01099500	-0.00393600	-1.16515600
C	-3.70244100	-0.00287700	-1.41387500	C	-3.68949300	0.00389800	-1.41460800
H	-3.58897800	-0.00037000	-3.54640200	H	-3.57309200	0.01682300	-3.54708000
Guanine				Guanine			
N	1.74125800	-1.50098300	0.00048500	N	1.74125800	-1.50098300	0.00048500
C	2.71662100	-0.52579200	0.00069100	C	2.71662100	-0.52579200	0.00069100
H	3.76801900	-0.77886600	0.00041200	H	3.76801900	-0.77886600	0.00041200
N	2.21938100	0.68988300	0.00124100	N	2.21938100	0.68988300	0.00124100
C	0.84598400	0.50214500	0.00119000	C	0.84598400	0.50214500	0.00119000
C	-0.22364300	1.45178800	0.00117900	C	-0.22364300	1.45178800	0.00117900
O	-0.17990900	2.68802600	0.00022900	O	-0.17990900	2.68802600	0.00022900
N	-1.47883300	0.79410500	0.00002100	N	-1.47883300	0.79410500	0.00002100
H	-2.28215700	1.41542200	-0.02272300	H	-2.28215700	1.41542200	-0.02272300
C	-1.68045200	-0.56769600	0.00010300	C	-1.68045200	-0.56769600	0.00010300
N	-2.97007100	-1.00570900	-0.06310500	N	-2.97007100	-1.00570900	-0.06310500
H	-3.71731400	-0.40194600	0.25641500	H	-3.71731400	-0.40194600	0.25641500
H	-3.10486000	-1.98902700	0.13816600	H	-3.10486000	-1.98902700	0.13816600
N	-0.69081600	-1.44157400	0.00488900	N	-0.69081600	-1.44157400	0.00488900
C	0.53127100	-0.85993100	0.00037400	C	0.53127100	-0.85993100	0.00037400
H	1.89045800	-2.50291900	-0.00004700	H	1.89045800	-2.50291900	-0.00004700
Adenine platination							
AsPt-A-adduct				AsPt-A-adduct			
Pt	-0.84836400	-0.05591900	-0.62691800	Pt	-0.85456600	-0.04691900	-0.62144100
As	-2.77409000	0.23677700	0.64913300	As	-2.75732400	0.22377300	0.64691800
O	-2.53545200	2.21530700	0.74927500	O	-2.54010500	2.20749600	0.75720800
O	-3.18297300	-1.72108900	0.65791100	O	-3.15807300	-1.73917700	0.65417800
O	-2.89927600	0.17678300	2.40640000	O	-2.87907100	0.15774400	2.40526000
H	-2.80325300	1.08210900	2.76046800	H	-2.79198800	1.06320700	2.76077700
O	-4.39592600	0.55290100	0.03628900	O	-4.38632900	0.52928400	0.04443400
H	-4.86294300	-0.29824500	-0.07154000	H	-4.84734100	-0.32524700	-0.06094800
N	-0.63559700	1.97519500	-0.50671700	N	-0.64600800	1.97095400	-0.50449100
H	0.13686300	2.47686200	-0.93475600	H	0.12337500	2.47623600	-0.93427900
N	-1.29450600	-2.04426200	-0.59273500	N	-1.26915500	-2.02735100	-0.60064600
H	-0.71432600	-2.73379900	-1.06215000	H	-0.68122100	-2.70711400	-1.07504700
C	-1.48979100	2.72247000	0.14623300	C	-1.49895200	2.71830000	0.15116100
C	-1.34246500	4.21348200	0.25975500	C	-1.35434600	4.20961200	0.26245100
H	-2.23747600	4.69624000	-0.14596700	H	-2.24919500	4.69042200	-0.14610100
H	-0.46154300	4.57834300	-0.27214900	H	-0.47304700	4.57533400	-0.26840300
H	-1.26699600	4.48847300	1.31704900	H	-1.28150600	4.48716000	1.31925200

C	-2.35323300	-2.50839500	0.02054600	C	-2.32063900	-2.51188200	0.01057000
C	-2.70112600	-3.96979300	0.04281400	C	-2.64870100	-3.97786100	0.02196300
H	-2.75499800	-4.31193500	1.08147300	H	-2.69314100	-4.32992600	1.05779800
H	-1.96785100	-4.57061300	-0.49882200	H	-1.91017100	-4.56449300	-0.52821700
H	-3.68964600	-4.11263300	-0.40602000	H	-3.63731800	-4.13046400	-0.42346500
O	0.88307700	-0.42495100	-1.86213700	O	0.87067800	-0.39822100	-1.85571400
H	1.75130400	-0.47261500	-1.32535900	H	1.74400400	-0.45283500	-1.32373100
H	1.00104900	0.24318500	-2.55883300	H	0.98805200	0.26429100	-2.55803800
N	4.35822500	-2.24811700	0.77232500	N	4.33488100	-2.24693700	0.76024000
C	3.20454900	-2.04892500	0.07102600	C	3.18217100	-2.04031000	0.06002700
H	2.46688400	-2.82877900	-0.05760000	H	2.44098400	-2.81626400	-0.07181800
N	3.10900000	-0.82461200	-0.41326500	N	3.09177300	-0.81346100	-0.41904700
C	4.27288400	-0.18481800	-0.00323300	C	4.25816800	-0.17983100	-0.00653700
C	4.79064100	1.12007800	-0.18186000	C	4.78157200	1.12353100	-0.18017700
N	4.16778400	2.08363200	-0.90076400	N	4.16283300	2.09288300	-0.89481100
H	4.53542300	3.02532200	-0.85261200	H	4.53471700	3.03270400	-0.84238400
H	3.19747100	1.98392700	-1.16211700	H	3.19178200	1.99908700	-1.15571800
N	5.98934900	1.40946500	0.36782500	N	5.98174700	1.40521500	0.37027500
C	6.64020300	0.45804700	1.05661200	C	6.62850800	0.44823100	1.05516900
H	7.59941100	0.75523400	1.47354400	H	7.58912400	0.73950400	1.47301300
N	6.25802500	-0.80053000	1.29438300	N	6.24079800	-0.80958900	1.28801000
C	5.06607500	-1.06756200	0.74067700	C	5.04766600	-1.06911900	0.73346300
H	4.64004100	-3.10756600	1.22895100	H	4.61313700	-3.10945400	1.21328600
AsPt-A-TS				AsPt-A-TS			
Pt	-0.47364600	-0.17539600	-0.62405800	Pt	-0.47675300	-0.16349900	-0.61209000
As	-2.25598800	0.63438900	0.62651900	As	-2.25050300	0.61792700	0.61964900
O	-1.49520100	2.46953100	0.72610300	O	-1.51041600	2.46319900	0.73615900
O	-3.18845000	-1.13694600	0.62252200	O	-3.17539800	-1.16065400	0.60918500
O	-2.41726000	0.61069400	2.38527600	O	-2.41912300	0.58549200	2.37850700
H	-2.07552100	1.45212000	2.74456600	H	-2.09038700	1.43035300	2.74133100
O	-3.73519300	1.38075100	0.01641600	O	-3.73746100	1.35585800	0.01487500
H	-4.41432400	0.68777400	-0.09576400	H	-4.41091000	0.65775600	-0.09828200
N	0.27319500	1.72172300	-0.51703800	N	0.26295900	1.72159100	-0.49951200
H	1.17719400	1.96388300	-0.92255600	H	1.16825500	1.96889400	-0.89925600
N	-1.44758400	-1.97172500	-0.60140100	N	-1.41987900	-1.96118800	-0.61248800
H	-1.08249400	-2.80100800	-1.06080200	H	-1.04435300	-2.78198600	-1.07921900
C	-0.34421100	2.67182700	0.13280000	C	-0.35765900	2.67070900	0.14973700
C	0.20828300	4.06380800	0.25621500	C	0.19246800	4.06290000	0.27907200
H	-0.51996000	4.77857800	-0.14038000	H	-0.53372600	4.77793700	-0.12088700
H	1.15329800	4.17369300	-0.27907900	H	1.14088100	4.17504300	-0.24985700
H	0.36150300	4.29812300	1.31496800	H	0.33871800	4.29580400	1.33914800
C	-2.60374100	-2.12238600	-0.00700800	C	-2.57764000	-2.13357600	-0.02600600
C	-3.34641800	-3.42879400	-0.00145100	C	-3.30407000	-3.44882100	-0.03760500
H	-4.32516000	-3.28872200	-0.47206800	H	-3.47106200	-3.77943200	0.99266100
H	-3.51683800	-3.74368500	1.03311300	H	-2.74669400	-4.21636800	-0.57831200
H	-2.79869000	-4.20979200	-0.53255400	H	-4.28436600	-3.31523000	-0.50687800
O	0.80017100	-0.70414900	-2.51581200	O	0.79659400	-0.66791200	-2.51103000
H	1.20651300	-1.57409300	-2.34738200	H	1.20147200	-1.54371500	-2.37237400
H	0.26605000	-0.79581400	-3.32478300	H	0.26536300	-0.73103000	-3.32474000
N	3.01679800	-2.05324200	1.77842700	N	3.00896600	-2.06607700	1.75306100
C	1.88267400	-2.11326600	1.01669700	C	1.86610600	-2.10195400	1.00405800
H	1.07951100	-2.80224700	1.23745600	H	1.05773400	-2.78517500	1.22339100
N	1.88700100	-1.24766700	0.02071200	N	1.86890500	-1.22096100	0.02125200
C	3.09980000	-0.57856600	0.14159900	C	3.09096600	-0.56720300	0.13783800
C	3.72289000	0.44728100	-0.60315600	C	3.71945500	0.46103600	-0.59915000
N	3.14197200	1.04139400	-1.68843800	N	3.13769100	1.07317200	-1.67416200
H	3.75933900	1.61664600	-2.25104400	H	3.75726300	1.65237000	-2.23042100
H	2.45776000	0.50127500	-2.21380300	H	2.45370500	0.54025600	-2.20714600
N	4.92588500	0.89373600	-0.19142900	N	4.92964800	0.89027500	-0.19072400
C	5.49186900	0.33847500	0.89422300	C	5.49932400	0.31427400	0.88204300

H	6.46143100	0.74189000	1.17555900	H	6.47469000	0.70478900	1.16145500
N	5.01711800	-0.64732900	1.66211100	N	5.02193500	-0.67904600	1.63844700
C	3.81646100	-1.06957900	1.24151200	C	3.81329200	-1.08255800	1.22282900
H	3.22351000	-2.62264000	2.59072900	H	3.21816000	-2.64997300	2.55440200
As-Pt-A-product				As-Pt-A-product			
Pt	-0.27298100	-0.15659200	-0.25423900	Pt	-0.26886700	-0.16967800	-0.29300700
As	-2.55414200	0.17450300	0.20794900	As	-2.51011000	0.19378900	0.23510200
O	-2.92764700	-1.80964600	0.21905400	O	-2.92611700	-1.78271200	0.23842400
O	-2.36957400	2.15421900	0.23363600	O	-2.28527700	2.17392500	0.28637300
O	-3.84782300	0.38181700	-0.97278600	O	-3.85259400	0.44588200	-0.88085100
H	-4.23272700	-0.49264200	-1.17533400	H	-4.26797300	-0.41656400	-1.07398300
O	-3.32652700	0.23155400	1.79261200	O	-3.20978500	0.24454200	1.85409100
H	-3.36491300	1.16102400	2.09002100	H	-3.22492900	1.17164900	2.16026600
N	-0.70550900	-2.15628400	-0.22504900	N	-0.72316300	-2.15073200	-0.26928400
H	0.00170600	-2.86899000	-0.37819600	H	-0.03122600	-2.87318600	-0.44623900
N	-0.13686600	1.88416400	-0.24488300	N	-0.07991200	1.85125600	-0.27533900
H	0.74660900	2.37091400	-0.42991800	H	0.79665000	2.32344200	-0.51843900
C	-1.91659000	-2.60677700	-0.00155800	C	-1.93293300	-2.59017000	-0.01828600
C	-2.23263000	-4.07669300	0.02002500	C	-2.26665900	-4.05598900	-0.00713000
H	-2.65226700	-4.33998700	0.99658500	H	-2.67337100	-4.32559900	0.97309800
H	-1.34725400	-4.68703700	-0.16931000	H	-1.39248300	-4.67519600	-0.21875500
H	-2.99225900	-4.29482500	-0.73776300	H	-3.04147000	-4.25611500	-0.75457700
C	-1.17433000	2.64268600	-0.00747300	C	-1.09075000	2.63607100	-0.00010300
C	-1.08726800	4.14345500	0.00906000	C	-0.96605100	4.13411200	0.01477300
H	-1.75526600	4.55318000	-0.75604100	H	-1.67786200	4.56474600	-0.69721900
H	-0.06884700	4.49030500	-0.17407600	H	0.04482200	4.45763800	-0.23901800
H	-1.42895800	4.51486800	0.98081400	H	-1.22670600	4.50758600	1.01081900
O	2.50479600	3.09740700	-0.82263000	O	2.45019600	3.10136900	-1.19371000
H	2.57648100	3.96847500	-1.24608800	H	2.46272900	3.97515400	-1.61704100
H	3.08003500	3.15072400	-0.04115900	H	3.24124000	3.08467100	-0.62885300
N	3.56696100	-0.77375000	-1.93945300	N	3.61018200	-0.93019000	-1.82128600
C	2.21632400	-0.66106200	-1.91950300	C	2.26505000	-0.78608200	-1.87943200
H	1.60199800	-0.73756400	-2.80382500	H	1.69430800	-0.90573300	-2.78792300
N	1.76394600	-0.44800300	-0.69204800	N	1.75956800	-0.48711000	-0.69570600
C	2.88500300	-0.41905900	0.13651400	C	2.83490200	-0.43282600	0.18128800
C	3.10088300	-0.24619800	1.52839900	C	2.97413800	-0.15278900	1.55428400
N	2.12373900	-0.03185500	2.43084200	N	1.95008000	0.12379900	2.35798700
H	2.36854700	-0.00884200	3.41228500	H	2.14069600	0.41397300	3.30802000
H	1.14565600	-0.10521900	2.18393300	H	1.02221900	0.28008300	1.98027100
N	4.37652200	-0.28028900	1.97221500	N	4.20502700	-0.18590800	2.07577600
C	5.37481200	-0.47818100	1.09929900	C	5.24233700	-0.47640400	1.28029000
H	6.37476600	-0.49264700	1.52562500	H	6.21410800	-0.48739800	1.76633200
N	5.29380900	-0.66217000	-0.22208200	N	5.23701800	-0.74943400	-0.02521200
C	4.02498900	-0.62341400	-0.64848100	C	4.00438500	-0.71076600	-0.52243500
H	4.13475400	-0.94018100	-2.76282800	H	4.21502800	-1.15604200	-2.60324000
Adenine				Adenine			
N	2.07937000	0.57983000	-0.00001600	N	2.07937000	0.57983000	-0.00001600
C	2.29411600	-0.77833000	0.00008200	C	2.29411600	-0.77833000	0.00008200
H	3.29406400	-1.19084600	0.00025600	H	3.29406400	-1.19084600	0.00025600
N	1.17998000	-1.47972400	-0.00016100	N	1.17998000	-1.47972400	-0.00016100
C	0.17754500	-0.52181800	0.00002000	C	0.17754500	-0.52181800	0.00002000
C	-1.23311400	-0.61125200	0.00009600	C	-1.23311400	-0.61125200	0.00009600
N	-1.89023700	-1.79066000	0.00003900	N	-1.89023700	-1.79066000	0.00003900
H	-2.90077400	-1.80689000	-0.00013600	H	-2.90077400	-1.80689000	-0.00013600
H	-1.38843100	-2.66711500	-0.00026100	H	-1.38843100	-2.66711500	-0.00026100
N	-1.94887500	0.53469200	0.00009000	N	-1.94887500	0.53469200	0.00009000
C	-1.29135000	1.70730400	-0.00004000	C	-1.29135000	1.70730400	-0.00004000
H	-1.92090900	2.59421200	0.00004900	H	-1.92090900	2.59421200	0.00004900
N	0.02779600	1.92366800	-0.00010500	N	0.02779600	1.92366800	-0.00010500
C	0.71769900	0.76992000	-0.00004000	C	0.71769900	0.76992000	-0.00004000

H	2.79043100	1.30105600	0.00044700	H	2.79043100	1.30105600	0.00044700
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Table S2: Cartesian coordinates of all the species present on the potential energy surfaces for aquation and DNA purine bases metallation by cisplatin optimized at B3LYP/*Basis1* and B3LYP/*Basis2* level in water.

Aquation							
<i>Basis1</i>				<i>Basis2</i>			
Cisplatin				Cisplatin			
Pt	0.00000000	0.00000000	0.18669700	Pt	0.00000000	0.00000000	0.18522300
Cl	0.00000000	1.73887400	-1.43746500	Cl	0.00000000	1.72796500	-1.42777800
Cl	0.00000000	-1.73887400	-1.43746500	Cl	0.00000000	-1.72796500	-1.42777800
N	-0.00068400	-1.49141000	1.64048900	N	-0.00035600	-1.48457400	1.62959300
H	0.82403100	-1.45412400	2.24213200	H	0.82355600	-1.44847800	2.23251700
H	-0.82308100	-1.45092300	2.24509000	H	-0.82270600	-1.44671500	2.23453800
N	0.00068400	1.49141000	1.64048900	N	0.00035600	1.48457400	1.62959300
H	-0.82403100	1.45412400	2.24213200	H	-0.82355600	1.44847800	2.23251700
H	0.82308100	1.45092300	2.24509000	H	0.82270600	1.44671500	2.23453800
H	0.00322800	2.40695800	1.18507800	H	0.00181100	2.40033000	1.17430500
H	-0.00322800	-2.40695800	1.18507800	H	-0.00181100	-2.40033000	1.17430500
Cisplatin-H2O				Cisplatin-H2O			
Pt	0.10256400	-0.00021800	-0.10570300	Pt	0.10631300	0.00005400	-0.09876900
Cl	1.68222700	1.73758400	0.29226700	Cl	1.68337400	1.72190700	0.27552500
Cl	1.68722900	-1.73352400	0.29266200	Cl	1.68216400	-1.72289400	0.27540200
N	-1.32264400	-1.47269200	-0.45772500	N	-1.31482100	-1.46582000	-0.42710500
H	-2.22612900	-1.22741100	-0.03328900	H	-2.22400200	-1.21324000	-0.01940200
H	-1.47284200	-1.61253200	-1.45858500	H	-1.45556500	-1.62859300	-1.42602900
N	-1.32612500	1.46842300	-0.45939400	N	-1.31395900	1.46685200	-0.42674500
H	-1.47422600	1.60841500	-1.46053800	H	-1.45699800	1.62779100	-1.42564400
H	-2.22989500	1.22024300	-0.03700700	H	-2.22244600	1.21605800	-0.01647300
H	-1.01929500	2.36247100	-0.07231100	H	-1.00899500	2.35398600	-0.02229100
H	-1.01255100	-2.36615500	-0.07189600	H	-1.01176200	-2.35247900	-0.02019200
O	-3.63065000	-0.00087500	0.72257300	O	-3.66779100	0.00034700	0.67039400
H	-4.54111600	-0.00043800	0.38327000	H	-4.54588700	-0.00013400	0.25450900
H	-3.71809800	0.00029900	1.69068600	H	-3.83709700	-0.00081400	1.62754600
Cisplatin-TS				Cisplatin-TS			
Pt	0.23683500	-0.20378600	0.04473900	Pt	0.23846500	-0.20158300	0.04386300
Cl	-2.35431300	0.54848000	-0.97424200	Cl	-2.35032500	0.53052000	-0.97174000
Cl	1.28109300	1.92088600	-0.10432200	Cl	1.26393200	1.91191900	-0.10845300
N	2.04762000	-1.04243300	-0.47880700	N	2.03786300	-1.02652500	-0.47351000
H	2.34657000	-1.76887100	0.17401700	H	2.34494700	-1.74675000	0.18269800
H	2.02597400	-1.44952900	-1.41553800	H	2.01875400	-1.44079800	-1.40732700
N	-0.69280000	-2.06145900	0.15074100	N	-0.67705900	-2.05460100	0.15899800
H	-0.31688400	-2.75621400	-0.49646900	H	-0.30590300	-2.74967300	-0.49082500
H	-0.64890800	-2.46791600	1.08701200	H	-0.62311400	-2.46169300	1.09459200
H	-1.67793300	-1.92791900	-0.09291400	H	-1.66549200	-1.92759800	-0.07467300
H	2.76344400	-0.31207400	-0.47932400	H	2.75029300	-0.29255600	-0.48140000
O	-1.31988400	0.69351500	1.83715300	O	-1.31735900	0.70021700	1.83199200
H	-1.57762800	-0.00447600	2.46298900	H	-1.57048400	0.00465400	2.46244700
H	-2.06769000	0.78223200	1.20540300	H	-2.06739600	0.78259600	1.20209400
Cisplatin-Product				Cisplatin-Product			
Pt	-0.40463300	0.16101500	0.06674400	Pt	0.40585700	0.15931800	-0.06734600
Cl	3.69054100	-0.34943100	-0.33443600	Cl	-3.68644700	-0.34544800	0.33422300
Cl	-2.02126600	-1.55251900	-0.20616700	Cl	2.00135700	-1.54771200	0.20808600
N	-1.82580700	1.57578900	-0.37547300	N	1.82021800	1.55959500	0.37883200
H	-1.90142100	2.29443700	0.34745600	H	1.89906400	2.28380400	-0.33832500

H	-1.64103000	2.04896000	-1.26251100	H	1.63826100	2.02886100	1.26868600
N	1.06405900	1.62871500	0.28179800	N	-1.04891000	1.62667400	-0.28032200
H	0.95081200	2.40792900	-0.36835500	H	-0.93039700	2.40786000	0.36680300
H	1.06572200	2.02002800	1.22573000	H	-1.05364800	2.01722400	-1.22466900
H	1.99732300	1.22389000	0.10772000	H	-1.98457700	1.22939400	-0.10270200
H	-2.74238300	1.12983500	-0.45803700	H	2.73700800	1.11336500	0.45939300
O	1.01374900	-1.31431400	0.57945600	O	-1.00628000	-1.29750100	-0.58154100
H	0.74097700	-2.16656200	0.19181000	H	-0.73474500	-2.15706700	-0.20932800
H	1.93595700	-1.10154100	0.22046100	H	-1.93021700	-1.09035500	-0.22338300
Guanine platination							
Cisplatin-monoH2O				Cisplatin-monoH2O			
Pt	-0.15112500	-0.01304500	-0.00030200	Pt	-0.14945600	-0.01199400	-0.00003200
Cl	2.21904800	0.05046500	-0.00054400	Cl	2.20286300	0.04024400	-0.00028000
N	-0.07261000	-2.05569700	-0.00017600	N	-0.08580400	-2.04117100	-0.00052600
H	-0.53604500	-2.46135100	0.81561900	H	-0.53928400	-2.44533200	0.82172700
H	-0.50207700	-2.46065500	-0.83478400	H	-0.53156700	-2.44444300	-0.82742900
N	-2.24042600	-0.00575900	0.00233700	N	-2.22688900	0.00437900	0.00117400
H	-2.63532500	-0.39418300	-0.85621500	H	-2.62766800	-0.43796700	-0.82807100
H	-2.64057600	-0.52388200	0.78645000	H	-2.62775500	-0.45976700	0.81832800
H	-2.57630900	0.95693200	0.07714600	H	-2.56179600	0.97040900	0.01401900
H	0.90272600	-2.36387300	0.01938700	H	0.88657800	-2.35960100	0.00374600
O	-0.26883300	2.11204000	0.00903300	O	-0.25336500	2.09682800	0.00413500
H	0.26432100	2.46936200	0.74439300	H	0.24766200	2.45498700	0.76146900
H	0.12917600	2.47113400	-0.80657900	H	0.17846300	2.45604900	-0.79418000
Cisplatin-G-adduct				Cisplatin-G-adduct			
Pt	2.14037900	-0.19544500	0.05672100	Pt	-2.12823200	-0.19625400	-0.06187700
Cl	1.33862800	1.79902700	-0.95819400	Cl	-1.36626800	1.76521000	0.99968200
N	3.12261100	0.94438200	1.45367800	N	-3.09583900	0.95165900	-1.44339400
H	2.79235400	0.76289700	2.40375900	H	-2.76307100	0.78202400	-2.39492500
H	4.13263900	0.78737600	1.44332900	H	-4.10650500	0.79782300	-1.44147200
N	2.77499600	-1.97630500	0.92453500	N	-2.74759000	-1.96123000	-0.95056900
H	3.79199900	-2.06242700	0.96783100	H	-3.76398500	-2.05172200	-1.00064600
H	2.41519000	-2.10025000	1.87277800	H	-2.38353700	-2.07703600	-1.89830500
H	2.43093800	-2.75996600	0.36505900	H	-2.40507600	-2.75074700	-0.39816600
H	2.97079200	1.93848600	1.26690300	H	-2.94519800	1.94428200	-1.24704100
O	1.15050300	-1.40783000	-1.35127500	O	-1.15501700	-1.41063800	1.32954700
H	0.14632300	-1.40162100	-1.18801300	H	-0.14843600	-1.40578400	1.17798700
H	1.29448600	-1.06074000	-2.24973600	H	-1.30835200	-1.07840500	2.23214400
N	-5.52765500	-0.17478000	0.64382600	N	5.51676700	-0.15939500	-0.64199200
C	-5.51872700	-1.53341600	0.39799800	C	5.51667900	-1.51629700	-0.38631200
H	-6.39725500	-2.14178100	0.56438300	H	6.39917200	-2.12015900	-0.54805400
N	-4.35971300	-1.96492400	-0.04166800	N	4.36046800	-1.95216400	0.05632900
C	-3.56495600	-0.82992500	-0.08770600	C	3.55847700	-0.82197600	0.09433000
C	-2.20847800	-0.65601100	-0.47394500	C	2.20114800	-0.65413500	0.47947500
O	-1.40778200	-1.53381000	-0.87433000	O	1.40609500	-1.53476700	0.88521900
N	-1.79910700	0.67754700	-0.36353100	N	1.78321100	0.67608900	0.36139000
H	-0.83153100	0.88429500	-0.62294300	H	0.81545400	0.87864900	0.62342300
C	-2.58779400	1.72267200	0.06959100	C	2.56513000	1.72333600	-0.07882500
N	-2.01909200	2.95608000	0.06244500	N	1.98886900	2.95308600	-0.07859700
H	-1.01006800	3.04447400	0.02626100	H	0.97972800	3.03663300	-0.03681500
H	-2.51606900	3.68652800	0.55585000	H	2.47997800	3.68413200	-0.57695000
N	-3.84874500	1.57256400	0.43694100	N	3.82662400	1.57862200	-0.44665800
C	-4.28028900	0.29731500	0.33823400	C	4.26645000	0.30689000	-0.33954800
H	-6.30937100	0.37132400	0.98579600	H	6.29499700	0.38923800	-0.98781800
Cisplatin-G-TS				Cisplatin-G-TS			
Pt	-1.70281700	0.22256000	-0.10113600	Pt	-1.70360400	0.22052200	-0.10251700
Cl	-2.67737400	-1.62024700	1.02824600	Cl	-2.67262600	-1.60445100	1.02383900
N	-3.35938700	0.26480700	-1.32801600	N	-3.34823300	0.26362400	-1.31690400
H	-3.12443500	0.06408200	-2.30158600	H	-3.11784500	0.05748800	-2.29063900

H	-4.02074700	-0.45128000	-1.01888300	H	-4.01260500	-0.44857900	-1.00444900
N	-0.84674400	1.84054500	-1.10040600	N	-0.84778300	1.82558800	-1.10267200
H	-1.44017900	2.67190100	-1.08362300	H	-1.44103100	2.65732300	-1.09835400
H	0.04552700	2.09157400	-0.65417200	H	0.04155300	2.08415400	-0.65495900
H	-0.64968900	1.62874200	-2.08005600	H	-0.64313200	1.60764500	-2.07953000
H	-3.84622000	1.16216600	-1.30343400	H	-3.83368100	1.16207500	-1.29705100
O	-0.52342000	0.96059300	1.92704900	O	-0.52149800	0.95507700	1.92273200
H	0.26365700	1.45763200	1.59903000	H	0.26376600	1.45666400	1.59719400
H	-1.11276100	1.62572900	2.31967700	H	-1.11317200	1.61620900	2.31866200
N	2.15546800	-2.42088000	-0.48449200	N	2.15191100	-2.41992900	-0.47741100
C	0.82561000	-2.10211800	-0.32756900	C	0.82254600	-2.10010200	-0.31904700
H	0.04041900	-2.83559500	-0.44168700	H	0.03682500	-2.83346400	-0.43047900
N	0.64703900	-0.83544500	-0.02800500	N	0.64468700	-0.83272200	-0.02163500
C	1.92393900	-0.29672000	0.01278500	C	1.92225900	-0.29474700	0.01594200
C	2.36779900	1.02068900	0.29595700	C	2.36735000	1.02287400	0.29641900
O	1.67443800	2.02345700	0.58675100	O	1.67505000	2.02629300	0.58716200
N	3.76082100	1.12943100	0.22506200	N	3.76035900	1.13081600	0.22267600
H	4.13362000	2.04928100	0.44349000	H	4.13401900	2.05086900	0.43875200
C	4.62812800	0.09719600	-0.07545400	C	4.62659800	0.09759400	-0.07739000
N	5.95465200	0.37518500	-0.05226900	N	5.95334900	0.37495900	-0.05710400
H	6.28532900	1.32905200	-0.12100900	H	6.28426600	1.32857100	-0.12834900
H	6.57038900	-0.33456600	-0.42864800	H	6.56795600	-0.33567300	-0.43367300
N	4.21760100	-1.13393000	-0.33425800	N	4.21500500	-1.13382900	-0.33301900
C	2.87907600	-1.27736900	-0.27223500	C	2.87645200	-1.27636700	-0.26860600
H	2.52854200	-3.33459800	-0.71526200	H	2.52413800	-3.33437200	-0.70665600
Cisplatin-G-product				Cisplatin-G-product			
Pt	-1.69050000	0.21599800	-0.11597300	Pt	-1.63253900	0.11811700	-0.14958400
Cl	-2.63637200	-1.39837500	1.35323700	Cl	-2.50425500	-1.33176500	1.49473300
N	-3.44753200	1.31538300	0.08556800	N	-3.41926500	1.15412800	-0.06993300
H	-3.29240500	2.24096700	0.49009600	H	-3.30813800	2.11489300	0.26122300
H	-3.93612300	1.44509100	-0.80266900	H	-3.89703000	1.19572300	-0.97249700
N	-0.87092400	1.64882400	-1.38746400	N	-0.87261500	1.43540100	-1.56303600
H	-1.47328100	2.45485800	-1.55770700	H	-1.50496500	2.19547800	-1.81688200
H	-0.00013200	1.98310500	-0.94988000	H	-0.01971400	1.85262800	-1.16688400
H	-0.64156300	1.25093700	-2.29976600	H	-0.62144400	0.95894300	-2.43099400
H	-4.08783200	0.81916300	0.70939100	H	-4.05456100	0.68780300	0.58182400
O	3.86937900	3.31130100	0.64908100	O	2.60075700	4.32999600	0.85742800
H	2.90173500	3.15721500	0.59044600	H	2.23017000	3.46071600	0.59454500
H	4.03092600	3.66966400	1.53687600	H	2.47208800	4.38250800	1.81749400
N	1.28201000	-2.72778800	-0.53217600	N	1.39898300	-2.76448200	-0.34232700
C	0.02177100	-2.21516600	-0.53693700	C	0.12575600	-2.28362800	-0.36509500
H	-0.86189900	-2.81309400	-0.69311300	H	-0.74434600	-2.91279500	-0.46491700
N	0.03140200	-0.91252400	-0.30624500	N	0.10482400	-0.96742700	-0.23187100
C	1.37230600	-0.55803500	-0.14385200	C	1.43842800	-0.57150900	-0.11968300
C	2.02884700	0.68598100	0.09855800	C	2.05934600	0.70377500	0.02317900
O	1.52749600	1.82558800	0.19735500	O	1.52500600	1.82906200	0.05280100
N	3.41586800	0.52592100	0.21556100	N	3.45321000	0.58727200	0.12075800
H	3.92285200	1.39983200	0.41563800	H	3.95028800	1.46615800	0.23657700
C	4.09835800	-0.65968000	0.07600400	C	4.17156600	-0.58903500	0.05899500
N	5.43895700	-0.63140900	0.25429000	N	5.51178500	-0.51217700	0.20966400
H	5.94956100	0.24112100	0.22149700	H	6.00461400	0.36556800	0.11063200
H	5.95372600	-1.46485700	0.00054000	H	6.04358900	-1.35218000	0.02024600
N	3.49613400	-1.81124900	-0.18647900	N	3.59372900	-1.76915100	-0.10400900
C	2.16048700	-1.70376800	-0.27908200	C	2.25419800	-1.70392400	-0.18192700
H	1.52469700	-3.70068700	-0.68148200	H	1.66336200	-3.74003800	-0.42263600
Adenine platination							
cisPt-A-adduct				Cisplatin-A-adduct			
Pt	1.79928700	-0.22742000	-0.06644300	Pt	1.79944600	-0.22468900	-0.06717100
Cl	3.13941300	1.62384400	0.55831300	Cl	3.13154800	1.60959800	0.55594100
N	3.19051500	-0.74728800	-1.48635200	N	3.18000000	-0.74137900	-1.47944300

H	3.62432000	-1.65367500	-1.29890900	H	3.61316800	-1.64923000	-1.29702600
H	2.79746400	-0.78226500	-2.42907200	H	2.78911200	-0.77301500	-2.42331200
N	0.61238200	-1.87399600	-0.56884700	N	0.61774400	-1.86262700	-0.56715000
H	1.11802800	-2.75343400	-0.44676400	H	1.12385100	-2.74263900	-0.45032600
H	-0.23312900	-1.93400100	0.01328500	H	-0.22600500	-1.92798700	0.01688400
H	0.29944800	-1.83950700	-1.54077900	H	0.29992300	-1.82791100	-1.53764500
H	3.94112600	-0.05272700	-1.49940800	H	3.93329000	-0.04943600	-1.49192600
O	0.40005900	0.32222200	1.40666800	O	0.41197400	0.31830000	1.39677600
H	-0.40409400	0.81726900	0.99330500	H	-0.39802100	0.81091500	0.99201100
H	0.83598100	0.94672900	2.01569600	H	0.84644000	0.94065400	2.00919300
N	-3.53750800	2.19139100	-0.74766000	N	-3.53362000	2.19346600	-0.73808400
C	-2.28110500	2.34691500	-0.23446900	C	-2.27769700	2.34554100	-0.22268200
H	-1.73241100	3.27395400	-0.32455600	H	-1.72785200	3.27230900	-0.30850300
N	-1.83994000	1.25454300	0.35873800	N	-1.83840500	1.25031000	0.36671300
C	-2.86723200	0.33172500	0.22596100	C	-2.86651800	0.32914400	0.22873900
C	-3.02217400	-1.00854500	0.63377800	C	-3.02358900	-1.01238000	0.63132200
N	-4.16183500	-1.64451100	0.31103500	N	-4.16277400	-1.64642100	0.30318900
C	-5.10949200	-0.97655000	-0.37253800	C	-5.10844200	-0.97503900	-0.37977800
N	-5.08547600	0.29120600	-0.79573700	N	-5.08290100	0.29464000	-0.79715300
C	-3.93836200	0.90255500	-0.47185600	C	-3.93600900	0.90380900	-0.46846000
H	-4.06890100	2.89565200	-1.24626900	H	-4.06366400	2.90026400	-1.23452500
N	-2.03870500	-1.70599400	1.29065900	N	-2.04235100	-1.71269700	1.28856800
H	-1.40778000	-1.17176600	1.88108800	H	-1.41481300	-1.18107600	1.88481800
H	-2.34266600	-2.58160400	1.70476400	H	-6.00673000	-1.54006200	-0.61457100
H	-6.00810400	-1.54301100	-0.60257800	H	-2.34795200	-2.59009000	1.69774300
Cisplatin-A-TS				Cisplatin-A-TS			
Pt	1.42094	-0.22181	-0.14141	Pt	1.42100800	-0.21870000	-0.14311900
Cl	2.44845	1.62057	0.93412	Cl	2.44123000	1.60431400	0.93269800
N	2.92885	-0.19263	-1.53526	N	2.91918800	-0.18570600	-1.52390400
H	3.50306	-1.03701	-1.49996	H	3.49489300	-1.02949300	-1.49321700
H	2.57896	-0.09181	-2.48977	H	2.57315400	-0.07993600	-2.47945400
N	0.51469	-1.84267	-1.09669	N	0.51828200	-1.82912500	-1.09883600
H	1.1379	-2.6496	-1.16344	H	1.14070600	-2.63618200	-1.17183700
H	-0.32566	-2.15128	-0.59061	H	-0.32089700	-2.14344600	-0.59440100
H	0.22175	-1.60872	-2.04708	H	0.22207900	-1.59293400	-2.04775100
H	3.54204	0.60368	-1.34618	H	3.53305200	0.60943300	-1.33078900
O	0.45391	-0.93414	2.02681	O	0.45177300	-0.94210400	2.02302000
H	0.20431	-0.08087	2.4251	H	0.20125900	-0.08992400	2.42305900
H	1.17417	-1.28639	2.57818	H	1.17105700	-1.29554900	2.57486500
N	-2.35617	2.36169	-0.41413	N	-2.34997900	2.36178100	-0.40245400
C	-1.08083	2.05121	-0.02986	C	-1.07581900	2.04798300	-0.01737200
H	-0.28287	2.78023	-0.03348	H	-0.27695800	2.77602600	-0.01615900
N	-0.94661	0.78744	0.32594	N	-0.94339400	0.78224700	0.33260300
C	-2.21381	0.23943	0.16405	C	-2.21128900	0.23677500	0.16613300
C	-2.74841	-1.04889	0.37661	C	-2.74799100	-1.05174400	0.37244100
N	-4.04291	-1.2623	0.07547	N	-4.04223700	-1.26219100	0.06781800
C	-4.78062	-0.23815	-0.38981	C	-4.77764000	-0.23513800	-0.39466800
N	-4.40066	1.02601	-0.59978	N	-4.39573200	1.02948200	-0.59829600
C	-3.10576	1.21217	-0.30826	C	-3.10115100	1.21267700	-0.30338400
H	-2.68092	3.26805	-0.73031	H	-2.67294700	3.26999300	-0.71510200
N	-1.98791	-2.09919	0.82098	N	-1.98986400	-2.10441600	0.81440900
H	-1.21388	-1.87064	1.44566	H	-1.21490500	-1.87913200	1.43912000
H	-2.51709	-2.92212	1.0907	H	-2.51993300	-2.92797900	1.08039000
H	-5.818	-0.47186	-0.61558	H	-5.81481000	-0.46659300	-0.62376200
Cisplatin-A-product				Cisplatin-A-product			
Pt	-1.20927100	-0.33686000	-0.18408600	Pt	-1.20422300	-0.33477200	-0.18499600
Cl	-1.55730300	0.36372700	2.06792600	Cl	-1.56949500	0.35390800	2.04854400
N	-3.21610600	0.08819100	-0.55116900	N	-3.19672600	0.08649700	-0.56619200
H	-3.34736900	0.76484400	-1.30543600	H	-3.31506300	0.85685500	-1.22751000
H	-3.75352500	-0.74674700	-0.79259100	H	-3.71194400	-0.71368400	-0.93854300

N	-0.93832800	-0.96873700	-2.16073000	N	-0.91955600	-0.97716500	-2.14496700
H	-0.96531900	-0.18285000	-2.81353200	H	-1.17512400	-0.26566400	-2.83231200
H	-0.03478900	-1.42835100	-2.28522700	H	0.05660200	-1.21963000	-2.32323300
H	-1.65125800	-1.63673100	-2.45917800	H	-1.47209500	-1.81151200	-2.35166800
H	-3.64470800	0.48497000	0.28796500	H	-3.66413200	0.36416400	0.30003600
O	-1.19886500	3.19808400	0.40231800	O	-1.19963600	3.20122600	0.41362700
H	-1.39058100	2.50475200	1.06461700	H	-1.39832200	2.50262300	1.06836600
H	-0.89960800	3.96687100	0.91387500	H	-0.90165400	3.96446100	0.93430300
N	2.47961600	-2.07047200	0.78368900	N	2.46670700	-2.06906500	0.78741200
C	1.13328600	-1.98622900	0.66505700	C	1.12037900	-1.98051700	0.67121900
H	0.46296100	-2.79408700	0.91609300	H	0.44846200	-2.78704000	0.92221800
N	0.75884600	-0.80148200	0.20079100	N	0.74748700	-0.79448600	0.20839800
C	1.93172300	-0.06583700	0.00901200	C	1.92343700	-0.06253500	0.01515200
C	2.24389700	1.24463600	-0.44203900	C	2.23916700	1.24727600	-0.43603000
N	3.55361500	1.57270800	-0.53367600	N	3.54988900	1.57009000	-0.53254700
C	4.49080700	0.68647500	-0.17292600	C	4.48494300	0.68030500	-0.17512100
N	4.31647300	-0.55078500	0.30141800	N	4.30750900	-0.55600400	0.30049300
C	3.01934600	-0.87364300	0.36712700	C	3.00938200	-0.87402700	0.37022300
H	2.99511700	-2.88046800	1.10915200	H	2.98028100	-2.88093500	1.11121100
N	1.34200700	2.17685000	-0.82012100	N	1.34026000	2.18397500	-0.81063600
H	0.38323500	2.17909600	-0.47365100	H	0.38310400	2.19260000	-0.45947800
H	1.72690800	3.09680800	-1.00290700	H	1.72988800	3.10161600	-0.99526200
H	5.51995200	1.02257100	-0.27255700	H	5.51501800	1.01224700	-0.27908900

Table S3: NBO analysis of charge density distribution for all the species of **1** in the aquation process obtained at B3LYP/Basis2 level.

	Complex	Adduct	TS	Product
Pt	0.043	0.049	0.125	0.215
As	2.145	2.154	2.159	2.175
Cl	-0.442	-0.464	-0.668	-0.810
O _w		-1.007	-0.940	-0.923
O ₁	-0.780	-0.797	-0.785	-0.783
O ₁ H	-1.048	-1.048	-1.048	-1.048
C	0.671	0.672	0.673	0.677
N ₁	-0.710	-0.723	-0.718	-0.729

Table S4: NBO analysis of charge density distribution for all the species of **1** in the DNA purine bases metallation process obtained at B3LYP/Basis2 level.

	Adduct-G	TS_G	Product-G
Pt	0.211	0.151	0.161
As	2.180	2.168	2.170
O _w	-0.913	-0.930	-1.009
N ₇	-0.468	-0.471	-0.477
O ₁	-0.772	-0.770	-0.769
O ₁ H	-1.028	-1.030	-1.030
C	0.685	0.684	0.692
N ₁	-0.742	-0.733	-0.742
	Adduct-A	TS_A	Product-A
Pt	0.203	0.203	0.111
As	2.182	2.182	2.174
O _w	-0.934	-0.934	-0.999
N ₇	-0.573	-0.573	-0.493
O ₁	-0.768	-0.768	-0.778
O ₁ H	-1.023	-1.024	-1.029
C	0.692	0.692	0.694
N	-0.757	-0.747	-0.750

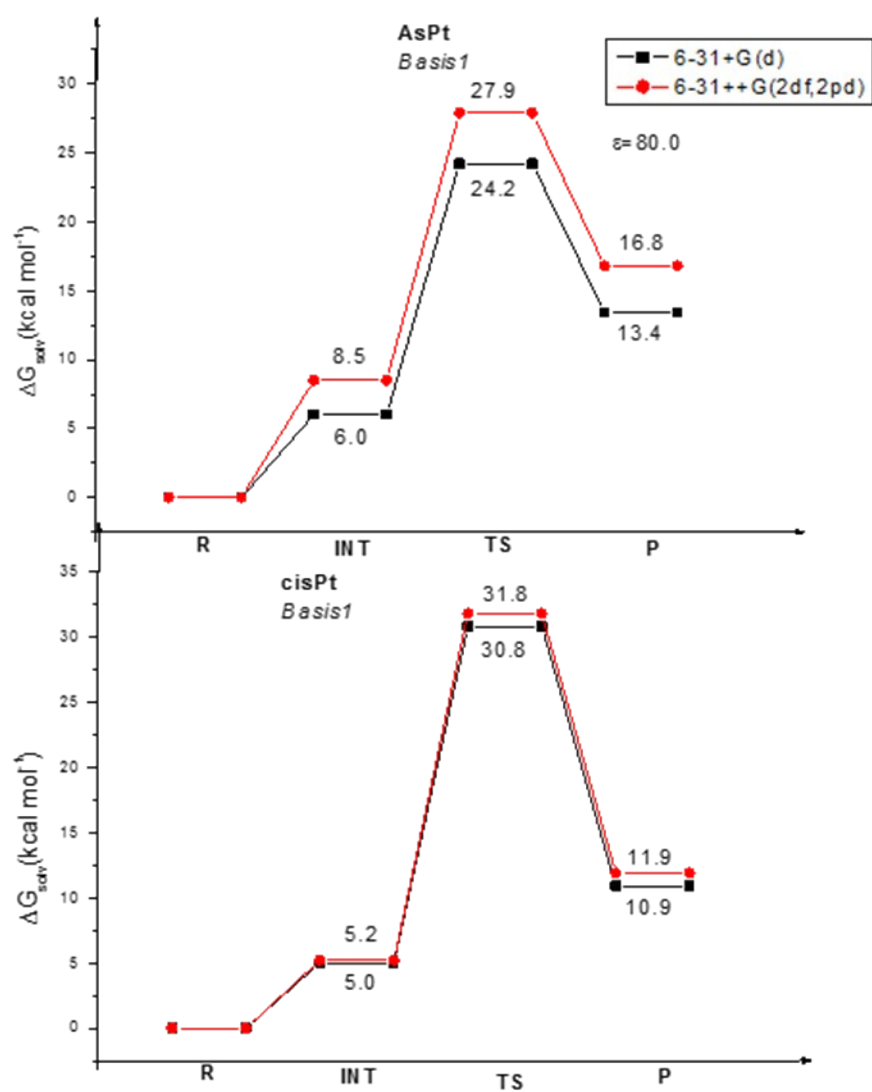


Figure S1. Calculated B3LYP free energy profile for the aquation process of **1** in comparison with cisplatin obtained by *Basis1*. Energies are in kcal mol⁻¹ and relative to reactants' asymptote

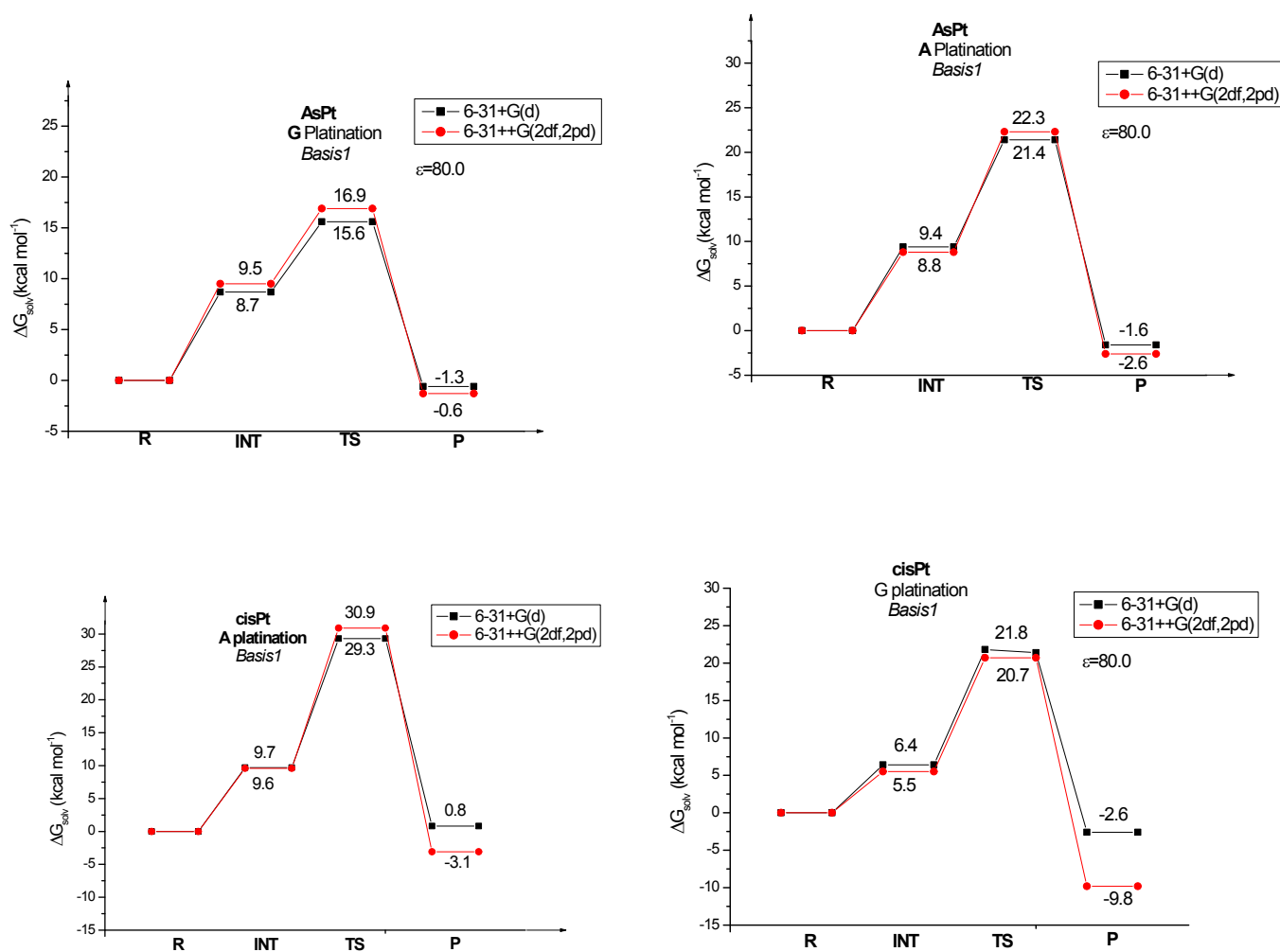


Figure S2. Calculated B3LYP free energy profile for the DNA purine bases metalation process of **1** in comparison with cisplatin obtained by *Basis1*. Energies are in kcal mol⁻¹ and relative to reactants' asymptote.