Supporting Material

Theoretical Study of Cisplatin Binding to Purine Bases: Why Does Cisplatin Prefer Guanine Over Adenine?

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Table S1. Cartesian Coordinate of Optimized Geometries

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================================
(NH3)2Pt(Cl)+
================================
  Cl    1.708379294   1.526060058   1.960205485
  Pt    0.032703696  -0.015533050   2.135464597
   N   -1.520536368  -1.505865377   2.005323678
   N   -0.040333066   0.308512803   4.129206607
   H   -0.948595105   0.671330479   4.426860369
   H    0.672209036   1.020424490   4.331205027
   H    0.187361015  -0.533224905   4.662876669
   H   -2.417433753  -1.204126868   2.389178654
   H   -1.269316651  -2.386582841   2.457731565
   H   -1.697789183  -1.731193165   1.022846138
================================
Pt(NH3)2(H2O)2+
================================
  Pt    0.128918792  -0.067933114   1.992515356
   O    2.172483448  -0.558626167   1.854648104
   N   -1.878317153   0.423839084   2.021843467
   N    0.332720167  -0.293927928   3.995131575
   H    0.129656058   0.574041488   4.506362712
   H    1.311745986  -0.548866940   4.184806045
   H   -0.264135649  -1.045065383   4.363322418
   H   -2.083711930   1.291048029   2.531628958
   H   -2.480378129  -0.312892118   2.407489122
   H   -2.212112013   0.580420306   1.059863935
   H    2.421868685  -1.399627459   1.425709199
   H    2.798635138   0.131393548   1.562587061
================================
(NH3)2Pt(Cl)(H2O)+
================================
  Pt    0.098919190  -0.066262847   1.995022279
  Cl    2.347659364  -0.594633473   1.749791417
   N   -1.980860201   0.431474508   2.054579464
   N    0.374964043  -0.315351004   4.015232169
   H    0.227456909   0.541982801   4.550468723
   H    1.357895260  -0.587512692   4.130402130
   H   -0.200728268  -1.055979075   4.418822842
   H   -2.176483091   1.297943997   2.557620052
   H   -2.570814972  -0.300770844   2.451420551
   H   -2.292641855   0.571495185   1.091233816
   O   -0.032684541   0.154750287  -0.118521723
   H    0.619459980   0.827275592  -0.386041814
   H    0.279199448  -0.676343580  -0.520425833
================================
Pt(NH3)2(H2O)(H2O)2+
================================
  Pt    0.123118551  -0.067683757   1.975218119
   O    2.190880750  -0.569714703   1.904844399
   N   -1.875800950   0.415772537   2.075075064
   N    0.344224330  -0.301045515   4.008952221
   H    0.151127613   0.554190484   4.540139856
   H    1.318205617  -0.557039052   4.206084065
   H   -0.240943263  -1.047322030   4.398210526
   H   -2.059250288   1.275520621   2.602429417
   H   -2.455056541  -0.326624312   2.480245973
   H   -2.223227007   0.574212357   1.122584757
   O   -0.137343043   0.179161076  -0.122918691
   H    0.290999038   0.928701928  -0.572239970
   H   -0.080313332  -0.598796427  -0.704881959
   H    2.465019509  -1.417671410   1.514033323
   H    2.839036607   0.109206722   1.648153169
================================
Guanine
================================
   H    0.225591887   1.465873402  -2.842869466
   N    0.148223250   0.804864403  -2.084180486
   C    0.064422732   1.075430279  -0.727658943
   H    0.073956895   2.088440018  -0.349463865
   N   -0.026374016  -0.007422010   0.000716959
   C   -0.002017588  -1.044016340  -0.913223123
   C   -0.065015624  -2.469451847  -0.708263416
   O   -0.150314869  -3.132306834   0.310194515
   N   -0.002794246  -3.142120024  -1.980841125
   H    0.023439220  -4.151837876  -1.899707629
   C    0.093478560  -2.546385596  -3.213053812
   N    0.186809884  -3.381178121  -4.305091945
   H   -0.310462885  -4.259979662  -4.264783939
   H    0.089547626  -2.888805147  -5.182544886
   N    0.145439577  -1.246808141  -3.388809704
   C    0.105964653  -0.559190927  -2.217062974
================================
Adenine
================================
   H    0.234357453   1.508508496  -2.788132212
   N    0.157961578   0.821353272  -2.052948034
   C    0.084597575   1.049248427  -0.692036191
   H    0.104679841   2.051806847  -0.285995559
   N   -0.006135585  -0.050497766   0.016241377
   C    0.008846316  -1.061510720  -0.931774053
   C   -0.055442245  -2.469236236  -0.835441975
   N   -0.021120934  -3.200105798  -1.965107604
   C    0.077974022  -2.556234800  -3.140759046
   H    0.101876311  -3.196640989  -4.020316219
   N    0.149736371  -1.241309562  -3.372809158
   C    0.110227301  -0.545433601  -2.228992922
   N   -0.140560545  -3.112770106   0.353363097
   H   -0.241323473  -2.586910716   1.205627664
   H   -0.252903623  -4.113697738   0.353299303
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1
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   H    0.282067168   1.495829072  -2.752710348
   N    0.157909249   0.821759904  -2.007947779
   C    0.059347097   1.100636372  -0.679399653
   H    0.132762768   2.092653749  -0.262982518
   N   -0.078140327  -0.008431893   0.031737815
   C   -0.065585585  -1.063238315  -0.883660020
   C   -0.200069793  -2.481393290  -0.740181077
   O   -0.423318632  -3.160216538   0.266514828
   N   -0.065903749  -3.130899161  -1.987267302
   H   -0.158961186  -4.139862298  -1.929848445
   C    0.115596674  -2.512307906  -3.207379604
   N    0.199057014  -3.292033627  -4.304136038
   H    0.272369443  -4.295676211  -4.259260244
   H    0.382349438  -2.833948354  -5.184544379
   N    0.186933079  -1.198613950  -3.335098090
   C    0.095832280  -0.543412752  -2.168336016
  Cl    1.655044984   1.669685872   2.023675406
  Pt    0.005924398  -0.007182592   2.091906537
   N   -1.470989700  -1.518731248   2.212141309
   N    0.234745860   0.117406109   4.171012398
   H   -0.620499523   0.347130875   4.677239433
   H    0.901220835   0.882569000   4.315625775
   H    0.641436360  -0.724234314   4.580468602
   H   -2.383427928  -1.171140311   1.917976829
   H   -1.585041883  -1.922228483   3.140300899
   H   -1.169702452  -2.272634109   1.561882762
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   H   -0.389899000   1.382214000  -2.875910000
   N   -0.258466000   0.772222000  -2.079269000
   C   -0.326432000   1.133683000  -0.761444000
   H   -0.557908000   2.128810000  -0.414032000
   N   -0.142031000   0.075545000   0.010759000
   C    0.066721000  -1.004575000  -0.826739000
   C    0.368186000  -2.374240000  -0.523989000
   O    0.553160000  -2.909289000   0.561181000
   N    0.473130000  -3.116889000  -1.736108000
   H    0.640366000  -4.108090000  -1.595527000
   C    0.343686000  -2.605783000  -3.011091000
   N    0.445145000  -3.465999000  -4.045886000
   H    0.728338000  -4.426146000  -3.934753000
   H    0.405381000  -3.077508000  -4.976205000
   N    0.120478000  -1.323571000  -3.262494000
   C   -0.011649000  -0.584710000  -2.148276000
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  Pt   -0.050552000  -0.061951000   2.037634000
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   H   -0.979789000  -0.834138000   4.281997000
   H   -0.125266000   0.522902000   4.658401000
   H    2.585034000  -0.076918000   1.619623000
   H    2.333539000   0.914903000   2.906181000
   H    2.048670000   1.464709000   1.377235000
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2
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   H    0.414276440   1.610832191  -2.706536205
   N    0.336125513   0.919973554  -1.970174261
   C    0.231497634   1.168801631  -0.642953656
   H    0.212527435   2.157632406  -0.210727419
   N    0.137635485   0.042079977   0.055406268
   C    0.153529506  -0.999350057  -0.873424683
   C    0.025623324  -2.402567784  -0.822259012
   N    0.154828339  -3.096027265  -1.953644072
   C    0.350811295  -2.441710300  -3.113374823
   H    0.457450083  -3.063316007  -3.997708886
   N    0.408280679  -1.119586294  -3.298170505
   C    0.303695990  -0.451236120  -2.154827589
  Cl   -1.683725023   1.572818247   2.052169660
  Pt    0.030866457  -0.016522650   2.098488569
   N    1.607407449  -1.460235114   2.127850170
   N   -0.175978008   0.069988150   4.188203199
   H   -0.432402834  -0.814463465   4.627268896
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   H    0.645483102   0.441771912   4.666283134
   H    1.902477930  -1.755148468   3.057701858
   H    2.434987607  -1.092258445   1.657645728
   H    1.291383411  -2.295292914   1.612275347
   N   -0.186564705  -3.104625935   0.356976302
   H   -0.882531552  -2.689341997   0.970643750
   H   -0.369388006  -4.087358884   0.172003815
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4
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   H   -0.328140751   1.416740121  -2.826730084
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   H   -0.446586543   2.074514906  -0.355159567
   N   -0.060633647   0.002602791   0.016959826
   C    0.097702779  -1.073098479  -0.861567427
   C    0.255432205  -2.479007333  -0.733915692
   N    0.462341797  -3.182635897  -1.858478029
   C    0.442721133  -2.564785514  -3.047506553
   H    0.625332614  -3.196566655  -3.912716922
   N    0.204919236  -1.270727538  -3.296501068
   C    0.040701057  -0.582783150  -2.171299305
  Cl   -2.100051932  -1.088867434   2.099883701
  Pt   -0.018030642  -0.031533493   2.059118365
   N    1.918258545   0.874511598   2.012541943
   N   -0.120321646  -0.134123792   4.163194122
   H    0.639059267  -0.652554067   4.605301316
   H   -0.992421574  -0.637050566   4.356862120
   H   -0.191297707   0.778282482   4.614681310
   H    2.636022298   0.242113046   2.368991351
   H    1.977060372   1.743940601   2.543487721
   H    2.173210021   1.091620793   1.048199058
   N    0.226947422  -3.146671810   0.446706169
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   H    0.233454971  -4.155250868   0.354085442
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  Pt    0.219901107   0.037320060   1.942158745
   O   -1.519134910   1.130273999   2.118220564
   N    2.050280149  -0.976620571   1.898473562
   N    0.031251248  -0.103068013   4.032267042
   H   -0.122787563  -1.049984687   4.385929396
   H   -0.803577954   0.444793446   4.264539000
   H    0.805067092   0.305080334   4.561053403
   H    1.943493358  -1.983315127   2.049124224
   H    2.693269380  -0.631978015   2.615578264
   H    2.535630330  -0.852977370   1.007666509
   C   -0.495816536   2.805468301  -0.304151053
   O   -0.919260511   3.116280211   0.833095749
   N   -0.534543697   3.754017837  -1.321780922
   H   -0.897475079   4.660563435  -1.036463358
   C   -0.203244902   3.517792236  -2.650136525
   N   -0.287032156   4.532947035  -3.513615021
   H   -0.554921122   5.471168653  -3.254230100
   H   -0.053261293   4.351610320  -4.481225944
   N    0.176880686   2.317711542  -3.079000808
   C    0.262077540   1.402746045  -2.118760209
   H    0.836176666  -0.366652478  -3.166003244
   N    0.618767030   0.079087361  -2.280166850
   C    0.602781316  -0.520256442  -1.061356331
   H    0.832108682  -1.565687916  -0.916527556
   C    0.016327563   1.554644049  -0.750415737
   N    0.260006084   0.336625296  -0.105241165
   H   -1.318950580   2.054192220   1.596893719
   H   -2.305314465   0.701435794   1.743396493
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7
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  Pt    0.209132303   0.076877797   1.962771787
   O    2.191653764  -0.757518216   1.952901711
   N   -1.636929897   0.948504783   2.060837888
   N    0.336591157  -0.165328878   4.053984928
   H    0.259131575   0.718464482   4.562813626
   H    1.254729742  -0.552755850   4.287419729
   H   -0.360130022  -0.806978471   4.439946679
   H   -1.492065122   1.909846756   1.655871390
   H   -2.023365666   1.034742099   3.001378163
   H   -2.323220599   0.442345396   1.496994968
   C   -0.419002489   2.836984980  -0.344779741
   O   -0.799850913   3.189708256   0.779594634
   N   -0.406639289   3.749459854  -1.409841127
   H   -0.707536736   4.686874509  -1.156174199
   C   -0.099346196   3.446564578  -2.728344943
   N   -0.139867160   4.433091778  -3.629708034
   H   -0.352490913   5.392665441  -3.400650373
   H    0.081487690   4.205888850  -4.590051163
   N    0.218897827   2.215760498  -3.119708444
   C    0.252974978   1.329660375  -2.126906328
   H    0.738140407  -0.502877987  -3.111736736
   N    0.540333985  -0.017798383  -2.242270646
   C    0.485289043  -0.576579475  -1.006464882
   H    0.661874107  -1.625684617  -0.822744701
   C    0.013647614   1.540624332  -0.768972408
   N    0.180209553   0.334027379  -0.085244515
   H    2.326836606  -1.660944266   1.625267131
   H    2.893811399  -0.196345547   1.585352511
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6
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   H    2.213709931   1.131409268  -1.903943182
   N    1.686621420   0.574634071  -1.236812385
   C    1.536491554   0.826379782   0.077341492
   H    1.967850490   1.690093225   0.562759744
   N    0.765302980  -0.087819443   0.675085169
   C    0.376616340  -0.983897834  -0.333204285
   C   -0.465302403  -2.108000445  -0.445669236
   N   -0.650845554  -2.664075099  -1.630123799
   C   -0.018460288  -2.166842547  -2.715917621
   H   -0.204168682  -2.672900947  -3.658294816
   N    0.803544101  -1.116107718  -2.734699365
   C    0.957311221  -0.562208267  -1.542867027
   N   -1.212499744  -2.628181312   0.655440309
   H   -1.884107266  -3.308369413   0.289695196
   H   -0.612209793  -3.122175398   1.320202673
  Pt    0.120710182  -0.053056072   2.634622145
   O   -1.822053114  -0.515739805   2.044867177
   N    2.059145589   0.282422992   3.330969518
   N   -0.715725942  -0.031592775   4.570537438
   H   -0.310589253  -0.699140178   5.230735080
   H   -1.702022421  -0.288604583   4.463813920
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   H    2.278917003  -0.288360182   4.151278624
   H    2.221319954   1.258209340   3.596108677
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   H    2.821852201   0.557297827  -1.553908549
   N    2.085999673   0.128945403  -1.000044437
   C    1.922121618   0.227881104   0.327128940
   H    2.583423290   0.799457258   0.954998637
   N    0.838544226  -0.430581009   0.759208516
   C    0.281561862  -1.030789151  -0.390477752
   C   -0.734478846  -1.954249119  -0.713188380
   N   -1.043385293  -2.160501571  -1.984536594
   C   -0.316754711  -1.584005668  -2.960865612
   H   -0.639988703  -1.761827740  -3.981897439
   N    0.787894969  -0.857169908  -2.781114533
   C    1.037182046  -0.616623657  -1.505779386
   N   -1.442582363  -2.704823989   0.263238351
   H   -2.233169972  -3.161828519  -0.195965881
   H   -0.846917707  -3.443128554   0.645392232
  Pt    0.137775196  -0.056914946   2.688478495
   O    1.914342296   1.143552787   3.020206567
   N   -1.632063648  -1.053612824   2.452596516
   N   -0.420165557   0.311724294   4.703180411
   H   -1.387718581   0.622241495   4.821932074
   H    0.155086194   1.039727277   5.132353227
   H   -0.296761761  -0.524080559   5.281753720
   H   -2.392882859  -0.379116349   2.328338084
   H   -1.860814051  -1.626476369   3.268360089
   H   -1.647132201  -1.706211880   1.605961357
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   H    2.615288041   0.826814079   3.613053885
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1TS
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  Pt   -0.022004272   0.117097420  -0.105765221
   N    0.029583595   0.112188026   2.453326809
   C    2.453240516  -0.010228857   3.296810587
   O    3.149308663  -0.226030227   2.298683269
   N    3.080953458   0.112178730   4.556271376
   H    4.091138279   0.024371223   4.521412062
   C    2.444574241   0.383581065   5.751439830
   N    3.213821434   0.495841306   6.858347477
   H    4.167755859   0.172199551   6.885847769
   H    2.730190916   0.614181223   7.736395270
   N    1.140006515   0.563187329   5.843444481
   C    0.504108806   0.448343299   4.663659049
   H   -1.534099121   0.807146677   5.159822987
   N   -0.846471556   0.586124371   4.450962617
   C   -1.080178948   0.378437092   3.114962157
   H   -2.061819084   0.436973584   2.666071623
   C    1.039770798   0.157427602   3.407915124
   O    0.033442252  -2.175643791   0.756856118
   H   -0.792244550  -2.528299981   0.392129684
   H   -0.156979090  -1.985695052   1.688133401
  Cl   -2.377552792   0.151109507   0.028570347
   N    2.063489064  -0.079072060  -0.259038147
   N   -0.253453700   1.339183030  -1.764193754
   H    0.138057610   2.271549589  -1.630973515
   H   -1.267575322   1.435006479  -1.878865403
   H    0.125704897   0.939160499  -2.622055868
   H    2.475560092  -0.128967138   0.698290104
   H    2.547935225   0.658989700  -0.767055106
   H    2.270136414  -0.963621675  -0.724615577
================================
2TS
================================
   H    2.882292399   0.489002169  -1.949152283
   N    2.171449666   0.073179902  -1.360709204
   C    1.989817596   0.276426691  -0.019873279
   H    2.611338534   0.937200604   0.570311396
   N    0.983767865  -0.428069939   0.471897582
   C    0.499570189  -1.158807719  -0.606864418
   C   -0.470299108  -2.164308164  -0.763361548
   N   -0.744307710  -2.621560041  -1.983641028
   C   -0.033348763  -2.156921312  -3.030946464
   H   -0.310345194  -2.550725447  -4.004712199
   N    0.987471725  -1.295965338  -2.999424938
   C    1.214337209  -0.833943028  -1.772259589
   N   -1.167645232  -2.714409628   0.322834607
   H   -1.746215109  -3.488598161   0.003122726
   H   -0.536796157  -3.021894922   1.059587267
  Pt   -0.028944662   0.132430196   2.794002710
   O   -0.647039143   1.858060001   1.222106464
   H   -0.044907736   1.808177690   0.465523428
   H   -0.414189441   2.672943676   1.692290022
  Cl    2.041794587   1.114913880   3.303914587
   N   -1.952130435  -0.571637944   2.259976592
   N   -0.005476938  -0.556344726   4.752214277
   H   -0.772950804  -0.196615762   5.319438732
   H    0.871194813  -0.197576882   5.145032497
   H    0.010019733  -1.573520675   4.824871194
   H   -2.415627673   0.220917535   1.811206732
   H   -2.553236515  -0.883493931   3.021198106
   H   -1.882076779  -1.334440119   1.560977121
================================
4TS
================================
   H    2.301266547   0.819145996  -2.333417680
   N    1.685064849   0.406522540  -1.645144386
   C    1.296042373   0.945777746  -0.455051051
   H    1.642167671   1.911722169  -0.114088099
   N    0.448435177   0.168165319   0.204177062
   C    0.264829352  -0.944769190  -0.617576545
   C   -0.528916809  -2.120014701  -0.548925522
   N   -0.409656388  -3.019675521  -1.541017089
   C    0.409798306  -2.767589651  -2.571301279
   H    0.458130602  -3.539319734  -3.335443782
   N    1.161579802  -1.679886051  -2.779472073
   C    1.046065427  -0.814098549  -1.774541658
  Cl   -2.326807891   0.076604565   2.570496952
  Pt    0.008172647   0.177682112   2.740779463
   N    2.110812356   0.378493483   2.876203748
   N   -0.208853452  -1.115343103   4.351385176
   H    0.203784509  -2.033320372   4.180126951
   H   -1.220674952  -1.242309951   4.457435825
   H    0.151550069  -0.748610423   5.232526615
   H    2.541030238  -0.071880294   2.067431029
   H    2.552393786  -0.000287277   3.713329577
   H    2.339156685   1.373238611   2.838196595
   N   -1.385926511  -2.406363485   0.463381161
   H   -1.776659459  -1.655597478   1.020934281
   H   -1.980909897  -3.207343642   0.293757793
   O   -0.169683368   2.390758316   1.761590418
   H   -0.707733609   2.139699214   0.993206602
   H   -0.782438814   2.847452651   2.358103631
================================
5TS
================================
  Pt   -0.046401351   0.140960737  -0.061257675
   N   -0.037761765  -0.280692061   2.509659884
   C    2.412103811   0.229441194   3.124516062
   O    3.064180694   0.216482971   2.042991532
   N    3.129627895   0.489745405   4.284462826
   H    4.123519788   0.646051456   4.138782536
   C    2.594695176   0.520201994   5.563751439
   N    3.420753521   0.777748883   6.584425193
   H    4.409211623   0.949455659   6.477868639
   H    3.026552945   0.799203982   7.515012153
   N    1.306182463   0.302754671   5.791867102
   C    0.595888569   0.060909125   4.690212137
   H   -1.373311473  -0.262436219   5.429126240
   N   -0.750210264  -0.206977300   4.631210286
   C   -1.075577008  -0.403442472   3.315466701
   H   -2.084571073  -0.642436417   3.009676000
   C    1.032980947   0.011592314   3.356677975
   O   -0.893369602  -2.056247279   0.519601133
   H   -0.874585146  -2.748950789  -0.159158493
   H   -0.456415943  -2.420825775   1.303291104
   O    1.973670728  -0.189509643  -0.047483312
   N   -2.100383380   0.516116311  -0.123716762
   N    0.495390486   1.561198742  -1.469155603
   H    0.146966569   1.367293790  -2.410001162
   H    1.519138254   1.505843725  -1.502117677
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   H    0.240078117   2.518943388  -1.222054729
   H   -2.573477643  -0.340583047   0.181943028
   H   -2.462393377   0.746188737  -1.047306590
   H   -2.385972352   1.273494249   0.505577737
   H    2.223652473  -1.061721464  -0.387692611
   H    2.474200483  -0.007121119   0.968079739
================================
7TS
================================
  Pt   -0.015946396   0.082873307  -0.069067515
   N   -0.092631831  -0.202906912   2.495297916
   C    2.345449100   0.319809868   3.126171412
   O    2.979346779   0.293178272   2.056110063
   N    3.030582400   0.608088360   4.315552830
   H    4.025717148   0.771189454   4.192838483
   C    2.463246350   0.667312725   5.579055913
   N    3.262460546   0.955056291   6.616109282
   H    4.253008164   1.122592316   6.530089879
   H    2.844982980   0.991709227   7.535725400
   N    1.171449525   0.452055186   5.789219179
   C    0.487589669   0.180792467   4.674828182
   H   -1.505327274  -0.102477799   5.373395178
   N   -0.862811604  -0.075217458   4.589594240
   C   -1.160336387  -0.295050874   3.272514195
   H   -2.165110420  -0.512622069   2.937625592
   C    0.956352038   0.096108377   3.359457392
   O   -0.376216791  -2.196815311   0.498436699
   H   -1.003032009  -2.760984661   0.021619633
   H   -0.541569933  -2.297298566   1.448284723
   O   -2.069484405   0.695030027   0.156477918
   N    1.879432168  -0.623906941  -0.179088197
   N    0.383168162   1.603673701  -1.449842182
   H    1.146666790   2.206879940  -1.133954687
   H   -0.427716662   2.209834837  -1.589446417
   H    0.633242895   1.237321361  -2.371357300
   H    2.385315757  -0.283363281   0.697058994
   H    2.415843761  -0.367292868  -1.008736812
   H    1.816092311  -1.645801182  -0.155203399
   H   -2.276532712   1.507492136   0.642137745
   H   -2.705425067   0.587950338  -0.567137266
================================
6TS
================================
   H    2.596262946   0.473724823  -2.325205969
   N    1.965874059   0.076951590  -1.636251706
   C    1.884614011   0.393765775  -0.316425700
   H    2.515390551   1.156007451   0.119177906
   N    0.968103838  -0.307674203   0.340476039
   C    0.426138371  -1.159332988  -0.627429475
   C   -0.530643481  -2.184472684  -0.657242768
   N   -0.866632196  -2.757357795  -1.800768308
   C   -0.245884112  -2.379202753  -2.939645789
   H   -0.570492808  -2.867665677  -3.853233830
   N    0.734440828  -1.479494821  -3.038122181
   C    1.030126530  -0.908072211  -1.878741387
   N   -1.188920902  -2.670301746   0.531098276
   H   -1.985740497  -3.237236133   0.225366221
   H   -0.564354452  -3.307824768   1.033430315
  Pt    0.031092321   0.165254274   2.804378238
   O   -0.177526522   2.095601234   1.378213700
   H   -0.303322320   1.902394460   0.437662045
   H   -0.850841140   2.748107884   1.625855269
   O   -1.680338291  -0.873439877   2.281425607
   N    1.747763711   1.183437788   3.382276524
   N   -0.300080690  -0.738289102   4.644566233
   H    0.445351398  -1.371714244   4.941844647
   H   -1.154143323  -1.293712926   4.530666295
   H   -0.471553381  -0.072039566   5.401158172
   H    2.598415482   0.668098006   3.143338179
   H    1.806358496   1.415028298   4.376181953
   H    1.766317606   2.070633828   2.870314292
   H   -1.524211782  -1.621417587   1.496136258
   H   -2.441516695  -0.311238659   2.067622839
================================
8TS
================================
   H    2.951601146   0.391098946  -1.990457829
   N    2.251630900   0.003654476  -1.366652524
   C    2.063185088   0.302154723  -0.054022603
   H    2.672294557   1.033290264   0.459737471
   N    1.064138222  -0.379164854   0.496485180
   C    0.579223302  -1.188328241  -0.531476828
   C   -0.417348556  -2.173302817  -0.650602510
   N   -0.693388455  -2.679799231  -1.843850163
   C    0.031555011  -2.293449387  -2.916048228
   H   -0.249447171  -2.730891277  -3.869184644
   N    1.068156176  -1.452381315  -2.914071490
   C    1.296442960  -0.932861885  -1.715504520
   N   -1.158340395  -2.659529522   0.462497652
   H   -1.856313483  -3.315705383   0.106768237
   H   -0.543828414  -3.177371577   1.092313759
  Pt   -0.050516656   0.187263539   2.771249148
   O   -0.742976249   1.785619978   1.200762030
   H   -0.229206178   1.796501911   0.378927173
   H   -0.853258079   2.705293432   1.487945974
   O    1.872214415   1.080544561   3.128478605
   N   -1.875319393  -0.564353592   2.268518506
   N   -0.069546665  -0.701332761   4.671313171
   H   -0.832865180  -0.349073004   5.254319161
   H    0.794222418  -0.505115407   5.181903461
   H   -0.153605959  -1.719650129   4.629731286
   H   -2.375052706   0.183889551   1.777553317
   H   -2.470491444  -0.871483594   3.039777539
   H   -1.737489132  -1.368097987   1.587661268
   H    1.971937348   1.808134053   3.762541671
   H    2.651223506   0.505582720   3.186140904
```

Table S1. Vibrational Frequencies

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================================
(NH3)2Pt(Cl)+
================================
    62.02   118.36   135.88   145.73   159.25   374.44   416.46
   520.25   748.91   766.06   844.82   877.15  1353.72  1367.97
  1631.33  1662.38  1670.87  1677.13  3401.13  3443.70  3502.12
  3534.63  3546.95  3555.87

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(NH3)2Pt(H2O)2+
================================
    72.43   141.60   173.58   177.51   198.21   297.47   426.77
   490.09   516.70   563.13   768.99   861.18   869.49   887.50
   922.83  1409.71  1448.49  1631.55  1647.71  1650.57  1659.31
  1660.67  3373.26  3384.10  3462.63  3470.23  3486.60  3494.96
  3677.22  3765.79

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(NH3)2Pt(Cl)(H2O)+
================================
   103.85   112.22   128.90   166.00   170.40   175.35   185.19
   222.85   353.70   405.22   424.55   507.35   733.30   748.18
   757.08   772.09   845.41   867.23  1340.92  1364.83  1644.24
  1651.38  1669.14  1672.96  1683.79  3410.37  3449.29  3512.65
  3549.24  3555.79  3561.70  3707.67  3789.92

================================
(NH3)2Pt(H2O)(H2O)+
================================
   120.91   142.32   145.49   175.11   194.05   220.07   220.54
   251.98   273.63   393.82   408.17   451.69   498.15   504.21
   564.48   718.52   742.19   847.84   858.22   873.33   898.41
  1408.12  1424.69  1637.84  1647.02  1647.68  1663.65  1667.52
  1678.52  3407.22  3412.14  3499.34  3500.91  3509.40  3513.23
  3714.39  3721.35  3809.58  3813.80

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Guanine
================================
   142.18   161.95   204.70   316.59   333.48   335.18   364.30
   486.65   526.80   534.92   566.55   600.55   628.26   663.82
   669.10   700.49   730.74   779.55   817.30   836.35   946.52
  1047.27  1074.41  1076.68  1145.34  1178.48  1311.70  1336.62
  1368.52  1392.73  1448.76  1522.96  1567.12  1616.73  1623.89
  1673.66  1833.12  3265.29  3579.53  3599.47  3661.78  3696.23

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Adenine
================================
   107.87   168.27   224.18   277.16   304.93   516.82   520.06
   530.72   536.74   579.96   618.27   670.99   688.02   726.35
   812.65   847.02   901.55   943.59   973.61  1013.89  1086.06
  1150.81  1249.32  1273.84  1343.42  1370.01  1375.52  1427.13
  1445.43  1516.63  1530.03  1614.88  1648.08  1674.33  3179.45
  3260.96  3620.83  3664.09  3761.45
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1
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    29.84    49.87    91.05   118.59   139.79   141.24   152.19
   164.28   177.39   195.80   208.11   212.75   242.71   256.37
   310.07   332.83   360.43   369.19   387.40   451.38   463.28
   465.18   506.88   552.33   606.45   630.48   639.64   653.89
   675.82   701.81   724.40   776.20   780.42   789.84   818.66
   840.51   853.02   882.83   999.78  1032.14  1086.90  1143.69
  1167.57  1195.26  1316.48  1327.88  1355.86  1360.79  1371.87
  1437.58  1446.56  1535.93  1574.91  1614.52  1648.06  1648.98
  1655.13  1680.27  1691.00  1713.26  1769.44  3145.99  3314.01
  3420.05  3508.19  3525.64  3567.15  3577.26  3585.35  3615.68
  3638.38  3744.20

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3
================================
    -5.60    33.77    59.60   100.16   116.38   122.32   129.06
   163.22   166.51   171.94   178.94   191.37   202.30   224.29
   251.09   342.48   346.54   365.43   377.23   418.12   456.13
   463.88   497.55   548.18   602.56   625.71   630.18   653.32
   671.99   699.13   726.53   733.21   760.44   780.48   782.67
   807.03   817.52   841.96  1010.27  1029.56  1079.02  1124.06
  1146.98  1192.19  1314.28  1317.65  1329.92  1360.35  1379.37
  1422.63  1454.54  1543.94  1574.68  1610.54  1645.50  1650.76
  1669.51  1678.09  1682.79  1684.65  1796.85  3301.83  3417.74
  3419.14  3524.96  3528.53  3571.71  3572.38  3583.73  3617.06
  3639.58  3746.56

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2
================================
    40.91    59.24    89.44   128.41   136.93   160.47   162.40
   193.40   208.34   222.39   226.30   242.82   275.21   324.60
   339.49   352.13   418.99   455.80   479.88   528.36   549.68
   559.43   617.40   628.32   656.13   662.68   729.47   765.80
   784.11   794.62   815.58   837.81   851.73   877.59   897.62
   986.87  1002.04  1067.96  1128.44  1162.07  1256.43  1275.50
  1328.47  1334.15  1347.80  1357.13  1377.50  1431.24  1457.69
  1513.98  1547.07  1625.51  1644.59  1649.95  1666.11  1669.58
  1680.94  1700.27  3216.72  3305.87  3313.25  3419.68  3507.87
  3512.95  3524.63  3565.85  3570.96  3616.18  3632.62

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4
================================
    39.43    41.73    78.44   104.62   119.95   126.64   136.65
   168.23   178.08   202.36   211.28   231.39   239.88   329.99
   344.49   347.52   419.47   453.06   488.06   526.15   541.58
   551.69   597.32   615.86   629.44   657.79   692.20   729.80
   735.36   755.05   782.68   809.22   815.95   841.15   895.83
   992.19  1003.14  1050.89  1126.25  1165.08  1253.60  1272.37
  1325.35  1330.29  1340.65  1373.28  1374.93  1434.56  1456.53
  1517.48  1554.25  1619.07  1648.25  1650.21  1668.66  1675.60
  1681.25  1685.64  3208.47  3298.10  3420.06  3452.27  3525.11
  3542.22  3555.90  3562.75  3566.76  3635.08  3666.41
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5
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    39.53    57.23    98.28   118.91   122.22   153.05   165.14
   180.58   202.06   207.83   209.75   219.79   237.20   292.24
   336.60   367.21   370.87   407.11   452.51   469.72   495.65
   517.53   529.47   563.73   568.96   620.06   649.51   655.92
   665.43   692.20   713.52   723.17   775.08   787.58   802.86
   805.01   834.82   842.57   850.91   883.17   998.84  1024.72
  1085.17  1150.54  1177.70  1209.69  1269.61  1325.32  1363.18
  1371.79  1379.37  1390.52  1433.04  1439.95  1531.87  1560.97
  1582.62  1616.28  1653.92  1664.64  1667.76  1671.18  1678.24
  1687.18  1712.00  2022.30  3292.73  3426.77  3436.24  3520.19
  3530.45  3537.66  3544.21  3559.61  3590.91  3603.57  3716.09
  3787.84

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7
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    32.98    42.24    88.63   112.17   137.26   154.44   171.17
   182.36   191.21   200.81   207.72   228.44   241.84   256.60
   320.51   344.42   361.59   367.46   377.70   395.65   448.58
   493.55   503.18   510.99   526.39   553.16   619.52   641.78
   651.05   667.34   677.29   703.99   709.26   726.11   779.41
   791.23   807.09   831.67   837.48   896.42   964.12  1002.11
  1024.16  1083.51  1148.92  1172.55  1202.54  1311.44  1358.01
  1376.41  1377.35  1399.52  1434.48  1439.13  1534.00  1572.80
  1614.68  1635.94  1640.00  1662.68  1664.69  1680.99  1696.50
  1708.48  1754.75  2950.63  3296.27  3434.88  3483.98  3530.44
  3538.48  3553.85  3566.38  3595.21  3604.82  3721.28  3745.50
  3844.97

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6
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    47.52    64.99   102.20   125.92   133.69   154.30   180.03
   201.15   206.27   219.09   224.03   239.32   281.97   326.58
   365.81   428.12   448.44   472.50   482.63   527.03   541.58
   553.62   584.99   608.88   632.99   651.86   683.14   719.07
   791.18   805.76   806.46   813.48   845.90   874.26   881.56
   888.56   991.25   993.00  1037.02  1096.55  1123.75  1166.26
  1228.25  1260.38  1277.86  1301.77  1329.95  1364.11  1379.05
  1398.70  1402.98  1462.25  1512.81  1546.98  1609.32  1634.26
  1655.31  1667.53  1671.19  1676.50  1678.28  1686.39  2333.22
  3233.24  3288.10  3427.65  3432.01  3450.44  3520.66  3525.45
  3525.81  3530.97  3537.54  3591.41  3776.35

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8
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   -56.20    43.15   104.19   109.76   158.29   162.28   172.48
   198.98   209.53   220.32   239.37   293.23   304.67   321.12
   346.26   355.26   385.30   418.53   460.80   495.57   532.01
   539.86   544.38   564.69   609.45   636.20   651.94   682.64
   693.57   726.65   784.65   794.66   807.81   878.53   906.61
   914.56   979.97   991.81   998.45  1038.75  1102.98  1129.34
  1178.22  1233.39  1271.10  1310.33  1324.47  1359.58  1391.55
  1405.82  1469.02  1497.45  1513.60  1549.48  1610.41  1626.62
  1638.26  1654.63  1671.87  1673.06  1680.77  1737.57  2650.65
  3232.27  3337.07  3435.17  3450.11  3455.83  3525.64  3528.69
  3533.66  3536.18  3597.63  3739.90  3842.82
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1TS
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  -155.02    -7.59    20.93    73.13    85.12    94.55   122.62
   138.14   144.49   148.52   157.79   178.27   198.47   205.89
   213.24   214.74   221.73   250.83   291.27   326.81   338.56
   360.54   361.78   459.79   464.04   474.33   495.29   510.47
   525.81   541.63   605.57   627.95   641.15   665.50   674.52
   702.40   724.34   777.96   784.54   804.38   830.88   835.68
   881.28   898.96   957.33  1032.48  1088.65  1117.19  1165.64
  1188.55  1315.30  1317.78  1358.36  1372.91  1410.88  1416.71
  1436.81  1519.06  1569.09  1614.22  1639.62  1642.30  1648.53
  1659.40  1674.91  1688.55  1706.18  1767.76  3099.63  3279.41
  3419.19  3497.49  3526.45  3567.47  3571.54  3587.66  3612.11
  3636.99  3738.15  3754.20  3861.88

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2TS
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  -159.86    19.54    30.70    78.47    82.02   108.50   116.24
   137.23   143.11   169.58   187.78   197.30   202.04   219.22
   232.68   242.44   293.78   307.19   334.03   341.37   431.56
   453.26   472.33   481.73   520.00   525.21   535.77   560.42
   605.94   619.31   660.58   673.24   716.32   786.75   795.83
   812.32   837.96   877.49   884.14   901.49   919.91   949.54
   982.04  1078.13  1113.52  1138.52  1251.54  1266.27  1322.13
  1323.56  1347.34  1371.52  1373.36  1416.80  1438.24  1509.09
  1516.45  1623.97  1630.85  1639.06  1647.42  1664.47  1667.03
  1674.13  1714.24  3207.84  3213.84  3268.45  3416.79  3491.43
  3499.26  3525.00  3566.01  3567.43  3597.16  3635.59  3765.42
  3871.61

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4TS
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  -163.00   -12.10    21.25    70.36    83.40   100.21   112.89
   117.97   145.07   153.60   155.62   172.07   177.28   204.90
   212.86   230.78   246.76   306.06   315.13   338.25   436.84
   464.03   516.36   526.23   548.73   554.69   566.45   578.29
   595.50   604.89   617.15   672.28   690.09   726.58   757.74
   765.26   797.86   811.25   835.38   851.98   897.97   953.80
   989.93  1042.89  1119.32  1148.16  1246.03  1270.34  1322.31
  1330.05  1334.12  1369.77  1372.91  1426.52  1444.24  1512.92
  1530.84  1620.31  1634.61  1647.14  1648.86  1661.64  1672.73
  1675.77  1680.36  3202.22  3271.83  3417.57  3452.30  3519.92
  3531.18  3556.93  3560.61  3568.05  3638.69  3665.95  3748.35
  3851.17

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5TS
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  -142.09    10.21    16.06    67.94    87.63   117.37   139.43
   143.39   173.14   182.45   192.80   194.41   204.06   214.81
   222.37   247.67   271.04   293.79   335.85   357.41   401.06
   454.18   466.51   495.32   502.68   535.73   571.50   585.54
   619.33   652.38   657.76   665.44   710.36   718.34   722.55
   778.22   791.38   796.91   810.07   833.03   838.97   855.75
   912.97   956.84   995.05  1023.93  1034.20  1088.22  1131.01
  1148.26  1183.62  1215.68  1241.43  1325.49  1356.84  1369.55
  1381.45  1392.79  1398.52  1421.52  1428.20  1524.36  1568.26
  1615.15  1631.28  1653.29  1664.56  1665.19  1672.12  1679.86
  1686.41  1710.07  1796.32  2063.16  2564.65  3260.69  3416.90
  3421.88  3508.68  3514.38  3526.14  3544.02  3567.44  3598.59
  3614.56  3724.63  3750.90
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7TS
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  -157.39   -29.62    19.89    71.09    80.58   114.03   130.48
   134.57   137.68   158.33   163.25   175.68   208.06   215.43
   229.93   243.79   254.54   258.53   293.80   333.17   353.51
   363.38   370.40   376.55   407.30   440.17   448.91   494.78
   495.42   540.72   546.65   554.16   619.70   645.04   647.75
   667.20   677.80   690.29   707.90   725.36   780.74   791.44
   807.50   833.12   837.27   932.27   958.45   999.07  1024.49
  1085.08  1128.96  1172.51  1197.20  1314.70  1362.12  1370.64
  1371.85  1421.71  1426.51  1439.15  1518.71  1564.69  1598.17
  1613.35  1626.84  1633.04  1656.54  1671.49  1672.60  1695.23
  1706.62  1742.21  2704.49  3273.97  3437.50  3461.07  3533.47
  3540.13  3542.41  3575.08  3603.94  3616.64  3731.35  3751.41
  3763.23  3868.59  3870.38

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6TS
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  -147.09   -10.66    25.18    72.06    93.10   113.03   123.58
   145.91   157.23   181.94   188.98   207.32   218.78   227.05
   235.84   259.55   292.82   302.58   347.23   407.37   452.02
   461.68   479.33   497.92   520.72   523.56   541.43   553.52
   580.82   609.09   633.98   648.17   674.19   711.40   801.46
   813.24   814.57   821.50   861.36   876.52   878.12   933.40
   943.89   986.69  1044.23  1114.71  1138.58  1149.35  1228.61
  1262.15  1299.38  1324.86  1358.38  1359.36  1361.72  1390.08
  1403.61  1447.65  1499.62  1527.94  1595.82  1619.78  1633.98
  1653.07  1664.94  1673.77  1675.37  1681.15  1686.95  1804.97
  3231.09  3270.39  3423.76  3430.73  3440.53  3508.92  3520.16
  3524.52  3538.77  3540.46  3608.17  3758.11  3795.73  3868.03

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8TS
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  -155.62   -17.84    19.51    74.64    82.57   114.50   118.02
   134.97   141.37   172.53   189.29   209.85   220.29   229.57
   255.11   264.98   281.98   300.74   324.57   373.30   386.50
   405.28   451.93   457.12   464.10   525.12   531.64   543.92
   551.67   561.16   605.26   634.42   658.04   676.89   704.02
   715.71   788.92   806.14   814.37   880.00   880.88   925.43
   949.21   986.98  1001.16  1027.23  1096.76  1124.54  1143.69
  1243.13  1263.25  1311.42  1333.54  1364.40  1376.90  1402.63
  1446.73  1462.24  1509.63  1523.32  1612.71  1619.91  1628.33
  1633.69  1647.65  1670.04  1672.60  1674.04  1719.92  2792.28
  3227.88  3272.54  3438.01  3453.74  3462.98  3533.04  3534.22
  3537.58  3543.66  3609.64  3750.44  3754.25  3854.75  3863.98
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Table S3. DFT energy components of platinum complexes, guanine, adenine and sums of appropriate combinations to give the total energies of the fully dissociated reactant side of the platination reaction.

		H(SCF) LACVP**	H(SCF) cc-pVTZ(-f)	Solv LACVP**	H(Sol) cc-pVTZ(-f)	ZPE	H(ZPE-Corr)	S	-TS	G(Gas Phase)	G(Sol)
		eV	eV	kcal/mol	eV	kcal/mol	eV	eu	kcal/mol	eV	eV
(NH3)2Pt(Cl)+		-18838.102	-18840.575	-95.55	-18844.718	50.77	-18842.517	88.949	-26.52	-18839.523	-18843.667
(NH3)2Pt(H2O)2+		-8383.785	-8385.893	-252.36	-8396.836	66.60	-8393.948	87.607	-26.12	-8384.138	-8395.081
(NH3)2Pt(Cl)(H2O)+		-20919.679	-20922.981	-78.67	-20926.392	67.54	-20923.464	97.156	-28.97	-20921.308	-20924.720
(NH3)2Pt(H2O)(H2O)+		-10465.810	-10468.770	-220.59	-10478.336	83.17	-10474.729	96.329	-28.72	-10466.409	-10475.975
G		-14763.655	-14768.538	-26.48	-14769.686	73.43	-14766.502	88.678	-26.44	-14766.500	-14767.649
A		-12716.461	-12720.497	-17.56	-12721.258	70.12	-12718.218	84.197	-25.10	-12718.545	-12719.306
Reactant R=Cl	Pt + G	-33601.757	-33609.113	-122.03	-33614.405	124.20	-33609.019	177.626	-52.96	-33606.024	-33611.315
Reactant R=Cl	Pt + A	-31554.563	-31561.072	-113.11	-31565.977	120.89	-31560.735	173.146	-51.62	-31558.068	-31562.973
Reactant R=H2O	Pt + G	-23147.440	-23154.431	-278.84	-23166.523	140.03	-23160.450	176.284	-52.56	-23150.638	-23162.730
Reactant R=H2O	Pt + A	-21100.246	-21106.390	-269.92	-21118.095	136.72	-21112.166	171.804	-51.22	-21102.683	-21114.387
Reactant R=Cl	Pt + G	-35683.334	-35691.519	-105.15	-35696.079	140.97	-35689.966	185.834	-55.41	-35687.809	-35692.368
Reactant R=Cl	Pt + A	-33636.140	-33643.478	-96.23	-33647.651	137.66	-33641.681	181.354	-54.07	-33639.853	-33644.026
Reactant R=H2O	Pt + G	-25229.465	-25237.308	-247.07	-25248.022	156.60	-25241.231	185.007	-55.16	-25232.909	-25243.623
Reactant R=H2O	Pt + A	-23182.271	-23189.267	-238.15	-23199.594	153.29	-23192.947	180.527	-53.82	-23184.954	-23195.281

Table S4. DFT energy components of the platinated purine bases and transition states.

		H(SCF) LACVP** eV	H(SCF) cc-pVTZ(-f) eV	Solv LACVP** kcal/mol	H(Sol) cc-pVTZ(-f) eV	ZPE kcal/mol	H(ZPE-Corr) eV	S eu	-TS kcal/mol	G(Gas Phase) eV	G(Sol) eV	ΔH(SCF) kcal/mol	G(Solv) kcal/mol	H(Sol) kcal/mol	G(Sol) kcal/mol
Pt-G Pt-NH2-H•••O=C	**1**	-33605.495	-33612.612	-73.00	-33615.778	126.04	-33610.312	131.451	-39.19	-33608.846	-33612.011	-80.69	49.03	-29.82	-16.05
Pt-G	**3**	-33605.000	-33612.140	-81.12	-33615.658	125.35	-33610.222	132.606	-39.54	-33608.419	-33611.936	-69.80	40.91	-27.74	-14.32
Pt-A Pt-NH2-H•••NH2-C	**2**	-31557.607	-31563.911	-73.82	-31567.112	123.62	-31561.751	124.147	-37.01	-31560.155	-31563.357	-65.47	39.29	-23.45	-8.84
Pt-A Pt-Cl•••HNH-C	**4**	-31557.489	-31563.820	-76.82	-31567.151	123.05	-31561.815	128.107	-38.20	-31560.140	-31563.472	-63.37	36.29	-24.92	-11.49
Pt-G Pt-OH-H•••O=C	**5**	-23152.993	-23159.715	-186.76	-23167.814	141.38	-23161.683	128.734	-38.38	-23155.249	-23163.347	-121.85	92.08	-28.42	-14.24
Pt-G Pt-NH2-H•••O=C	**7**	-23152.719	-23159.472	-189.22	-23167.677	141.70	-23161.533	131.895	-39.32	-23155.033	-23163.238	-116.25	89.62	-24.96	-11.72
Pt-A Pt-OH-H•••NH2-C	**6**	-21104.638	-21110.539	-194.55	-21118.975	139.01	-21112.947	122.925	-36.65	-21106.100	-21114.537	-95.68	75.37	-18.02	-3.44
Pt-A Pt-NH2-H•••NH2-C	**8**	-21104.050	-21109.960	-198.40	-21118.563	138.91	-21112.540	121.707	-36.29	-21105.510	-21114.113	-82.33	71.52	-8.62	6.32
Transition States															
Pt-G Pt-NH2-H•••O=C	**1TS**	-35684.405	-35692.393	-73.03	-35695.560	140.86	-35689.452	143.501	-42.78	-35688.140	-35691.307	-20.15	32.12	11.86	24.48
Pt-G (Not possible)															
Pt-A Pt-NH2-H•••NH2-C	**2TS**	-33636.340	-33643.496	-73.89	-33646.700	138.38	-33640.699	140.907	-42.01	-33639.317	-33642.521	-0.42	22.34	22.64	34.70
Pt-A Pt-Cl•••HNH-C	**4TS**	-33636.303	-33643.509	-77.90	-33646.887	138.13	-33640.897	139.317	-41.54	-33639.320	-33642.698	-0.71	18.33	18.09	30.62
Pt-G Pt-OH-H•••O=C	**5TS**	-25232.136	-25239.709	-181.03	-25247.559	154.74	-25240.849	141.418	-42.16	-25234.827	-25242.677	-55.37	66.04	8.81	21.81
Pt-G Pt-NH2-H•••O=C	**7TS**	-25231.683	-25239.305	-187.17	-25247.421	156.14	-25240.651	143.963	-42.92	-25234.395	-25242.512	-46.05	59.9	13.39	25.63
Pt-A Pt-OH-H•••NH2-C	**6TS**	-23183.642	-23190.401	-191.10	-23198.688	153.36	-23192.038	135.246	-40.32	-23185.499	-23193.786	-26.15	47.05	20.97	34.47
Pt-A Pt-NH2-H•••NH2-C	**8TS**	-23183.231	-23190.010	-196.64	-23198.537	153.75	-23191.870	137.845	-41.10	-23185.125	-23193.652	-17.13	41.51	24.84	37.56