

# Supplementary Information for

## Replacement of a Thiourea with an Amidine Group in a Monofunctional Platinum–acridine Antitumor Agent. Effect on DNA Interactions, DNA Adduct Recognition and Repair

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**Table S1.** Cartesian Coordinates for Optimized Structures

<b>9MeA</b>				H	3.46413700	1.15884600	-0.00023600
C	3.09562300	0.55580500	0.00029000	N	1.41780800	1.79788900	0.00012400
N	1.81388200	-0.15611200	-0.00006500	C	0.25103200	1.02471800	0.00008300
C	1.59265800	-1.53621700	-0.00023300	C	-1.13774300	1.41747800	0.00004100
H	2.40657500	-2.24638100	-0.00022900	N	-1.99248500	0.24371700	-0.00010700
N	0.29758800	-1.86305900	-0.00005800	C	-1.56735000	-1.07684400	-0.00011600
C	-0.36952200	-0.62959600	0.00011700	N	-0.28243900	-1.42042100	-0.00011100
C	-1.74606500	-0.28044400	0.00007800	C	0.57489100	-0.34916100	-0.00012000
N	-2.73650100	-1.21981700	0.00008100	H	2.07639100	-2.49233300	-0.00170500
H	-3.70022300	-0.91658100	0.00001800	H	3.39485400	-1.68856100	-0.89214000
H	-2.50153200	-2.20237000	0.00020200	H	3.39157700	-1.68995300	0.89490900
N	-2.08436100	1.04267900	0.00003300	N	-2.52790600	-2.06167400	-0.00001300
C	-1.09209400	1.97660000	0.00025300	H	-2.20913400	-3.01963600	0.00059400
H	-1.41705100	3.01188700	-0.00081800	H	-3.51680900	-1.86460200	0.00075200
N	0.24624500	1.76135000	-0.00032900	O	-1.67338000	2.54727100	0.00015400
C	0.55538900	0.43949400	-0.00015500	H	-2.98397900	0.46870400	-0.00062300
H	2.88065400	1.62757200	-0.00260600				
H	3.67745000	0.31063500	0.89595000	<b>PT-AMD-Cl</b>			
H	3.68022200	0.30609500	-0.89225600	Pt	-0.80304200	0.17425000	-0.11428700
				Cl	-0.23075900	2.37946700	0.61986200
<b>9MeG</b>				N	1.11400600	-0.14352900	-0.71042400
C	2.76062200	-1.64019400	0.00026900	N	3.45501700	-0.09435500	-0.55634800
N	1.95719200	-0.41467900	-0.00033500	N	-1.53066900	-1.71599300	-0.71996800
C	2.41268400	0.91326200	-0.00010400	H	-1.57054800	-1.74027200	-1.74490500

H	-0.89390100	-2.45652800	-0.41017900
N	-2.79552000	0.50662800	0.42468900
H	-2.85549100	0.50173000	1.44906300
H	-3.06239900	1.44544100	0.10787900
C	2.22808700	-0.18374000	0.02855500
C	4.73913100	-0.18430000	0.17521000
H	5.37571700	-0.94510100	-0.29141800
H	4.59063600	-0.46124200	1.21704000
C	2.10467500	-0.36879800	1.53081900
H	1.12271600	0.00740100	1.82403100
H	2.84019300	0.25420500	2.04918800
C	2.24625300	-1.85183200	1.96286100
H	2.12984000	-1.93337500	3.04921000
H	3.22205100	-2.27487100	1.69688800
H	1.47321800	-2.47245300	1.49226000
C	3.57391400	0.15233000	-2.01020700
H	3.02562300	1.05786100	-2.30234900
H	3.20908900	-0.70283900	-2.59652400
H	4.62522700	0.30512800	-2.26033500
C	-2.91435300	-1.90284400	-0.12462400
H	-3.46732000	-2.68407100	-0.65904300
H	-2.78354100	-2.22142100	0.91463700
C	-3.66662300	-0.56613700	-0.18855400
H	-4.62871800	-0.64167900	0.33112200
H	-3.86056500	-0.28055600	-1.22768600
H	5.25973400	0.78053000	0.14092000
H	1.24226400	-0.01766200	-1.71308300

PT-AMD-AQ

Pt	0.83918000	0.13764100	-0.25709600
N	-1.09361500	-0.45621000	-0.52406100
N	-3.39818000	-0.70726800	-0.14844500
N	1.36691100	-1.58780600	0.71319300
H	1.01306100	-1.54541400	1.67787900
H	0.92865400	-2.40226100	0.26582700
N	2.88196800	0.61674700	-0.02040100
H	3.34955400	0.54156700	-0.93280700
H	3.00759100	1.58247400	0.30448600
C	-2.19231700	-0.22806400	0.22833900
C	-4.65646600	-0.53196000	0.62750800
H	-5.37598000	0.04592400	0.03709700
H	-4.48610900	-0.01612600	1.57011500
C	-2.05010100	0.60506200	1.49320400
H	-0.98927400	0.62650400	1.76270500
H	-2.57550400	0.12452500	2.32547400
C	-2.55860100	2.06264800	1.32409900
H	-2.39263700	2.62191900	2.25049300
H	-3.62762100	2.10761200	1.09467600
H	-2.02921400	2.58310300	0.51402700
C	-3.54982200	-1.47744400	-1.40965200
H	-2.96600300	-2.40711600	-1.38211000
H	-3.25528100	-0.87743600	-2.28077900
H	-4.59864900	-1.74837700	-1.53602800

C	2.88900200	-1.73971900	0.71912800
H	3.19036200	-2.45620000	1.49037300
H	3.18347600	-2.13656900	-0.25723900
C	3.50251900	-0.36045000	0.96920800
H	4.59079100	-0.39150900	0.85288800
H	3.27654200	-0.00219400	1.97852100
H	-5.08560200	-1.51595100	0.84394800
H	-1.24037900	-0.98055600	-1.38598600
O	0.45239900	1.96819600	-1.24525400
H	-0.04772100	2.68609100	-0.81146700
H	0.44984100	2.03974900	-2.21958100

PT-AMD-TS-A

Pt	-0.50924200	0.82659500	0.22100200
O	-0.69001200	0.36954500	2.63009000
N	0.63215800	2.56098900	0.53435300
N	-0.96348100	1.78496800	-1.58473000
C	0.76838300	3.33280200	-0.76818200
H	1.56618100	2.86211100	-1.35118200
H	1.04859600	4.37404900	-0.57679100
C	-0.56752900	3.25020100	-1.50788600
H	-0.48521300	3.67670600	-2.51390800
H	-1.35623400	3.78185400	-0.96658600
N	-1.57106400	-0.88802400	-0.10244300
N	-3.35219600	-2.39118900	-0.40349400
C	-3.86332800	0.03450300	-0.12140700
H	-4.60459300	-0.01213500	-0.92675400
C	-2.89046800	-1.12869100	-0.22606500
C	-2.41440000	-3.53915900	-0.45431200
H	-2.98443700	-4.45801900	-0.59709400
H	-1.71355400	-3.44646600	-1.29497300
C	-4.78572200	-2.75113300	-0.56737400
H	-4.91689900	-3.29187400	-1.51083900
H	-5.42656600	-1.87223300	-0.58427900
H	-5.10346900	-3.39848200	0.25774100
C	-4.57669200	0.10139800	1.25718100
H	-5.18325000	-0.78715800	1.45893200
H	-5.24165900	0.97097200	1.28551200
H	-3.84667900	0.20603600	2.06862000
H	-1.85252400	-3.64028700	0.48410200
N	3.37435400	-1.03398700	-2.44035600
N	4.75516200	-1.26389800	-0.46397400
N	1.43064200	-0.55653100	0.75922600
N	3.48914000	-0.97062200	1.62491000
C	4.56426900	-1.22629700	-1.80356500
C	3.62441700	-1.04244100	0.23581900
C	2.33493700	-0.79573300	-0.30278500
C	2.24163500	-0.83891200	-1.72235100
C	2.17119300	-0.67224500	1.88137800
H	1.79134600	-0.52568600	2.88022400
C	4.58036200	-1.20235000	2.59653600
H	4.59768800	-0.40523100	3.34501400
H	5.52223700	-1.20341700	2.04344900

H	4.45536400	-2.17207700	3.08759900
H	-0.87880100	-0.57111800	2.82171200
H	0.17320800	3.14195300	1.24570500
H	-0.37463500	1.29421400	-2.27682500
H	-3.29276600	0.95864700	-0.24987800
H	-0.96488400	-1.70825700	-0.07464000
H	-1.20783400	0.95092400	3.22256600
H	-1.94506500	1.69204400	-1.86396800
H	1.55730900	2.30341300	0.89422600
N	1.06160600	-0.68133000	-2.44796700
H	5.43284600	-1.37403800	-2.43440700
H	0.18928900	-0.96804300	-2.01901800
H	1.16940900	-0.86343800	-3.44372700

PT-AMD-TS-G

Pt	0.96671600	-0.92349900	-0.14060800
O	0.82375500	-1.10705600	2.27588000
N	0.51925100	-2.97899100	-0.32658000
N	1.94427500	-1.21407700	-1.94276800
C	0.86338400	-3.43147000	-1.73441300
H	0.01846700	-3.17215200	-2.38073200
H	1.00506600	-4.51698400	-1.77604700
C	2.13404900	-2.70394300	-2.18387000
H	2.34158600	-2.89659700	-3.24243700
H	2.99982800	-3.02442600	-1.59625700
N	1.42067400	1.05666400	-0.12851800
N	2.65266400	3.04388900	0.06722800
C	3.68923600	0.90749800	0.83620200
H	4.63702100	1.16564800	0.34968300
C	2.54084700	1.69816500	0.22350900
C	1.51652100	3.83032000	-0.47111000
H	1.79924300	4.88379500	-0.49945900
H	1.25482300	3.51130800	-1.48706000
C	3.86457600	3.83473800	0.39194200
H	4.15935600	4.42013200	-0.48610000
H	4.70410900	3.20120000	0.67270600
H	3.65629000	4.52505100	1.21805100
C	3.81672500	1.10971300	2.37006900
H	4.59230700	0.44779900	2.77114800
H	2.86948900	0.88525400	2.87681400
H	4.08993800	2.13600500	2.63368700
H	0.62751000	3.72619700	0.16155100
N	-3.35200200	2.07709400	-1.11566300
N	-4.77472400	0.62454500	0.14838000
N	-1.38868900	-0.50471300	0.75181500
N	-3.49828400	-1.05798600	1.38515000
C	-4.61478400	1.65886800	-0.68704100
C	-3.61788400	0.02549400	0.52557000
C	-2.30435700	0.36732100	0.13803000
C	-2.11521600	1.48776000	-0.73732300
C	-2.14489700	-1.33886600	1.48902300
H	-1.76590200	-2.13175100	2.11604300
C	-4.61982700	-1.73932300	2.06141300

H	-4.23149100	-2.56840700	2.65820700
H	-5.32406200	-2.12215800	1.31790500
H	-5.14410600	-1.03558000	2.71369000
H	1.06469400	-3.49805500	0.37095600
H	1.36673700	-0.79584100	-2.68268700
H	3.50110700	-0.15184600	0.63394600
H	0.61997200	1.58903200	-0.50661500
H	2.84701900	-0.72748700	-1.94487700
H	-0.47354400	-3.14307500	-0.13280900
N	-5.70501600	2.33141800	-1.13624100
H	-6.61353600	2.02157800	-0.81313100
H	-5.65876300	3.12241000	-1.76416000
O	-1.03230200	1.98158400	-1.17015400
H	-3.26276900	2.87664100	-1.73990000
H	1.61779000	-1.14595400	2.84539000
H	0.18907200	-0.42757100	2.58245100

PT-AMD-A

Pt	-1.00029200	-0.69905400	-0.06718900
N	3.51348400	0.04755100	-2.21022100
N	4.50498300	-0.34734100	-0.03414300
N	0.97495300	-0.81248500	0.43851000
N	2.84526600	-0.91488300	1.68724000
N	-3.03362000	-0.67919700	-0.59108100
H	-3.57722700	-0.24981000	0.16721700
H	-3.17771400	-0.10455700	-1.42903200
N	-1.36716900	-2.76097900	0.23045000
H	-0.92029600	-3.27949800	-0.53581200
H	-0.95592600	-3.10675700	1.10442200
C	4.56507200	-0.01877400	-1.34813200
C	3.24864700	-0.58690300	0.38687400
C	2.07453300	-0.53199900	-0.39976400
C	2.25522800	-0.22048200	-1.77849700
C	1.48593700	-1.03234900	1.67233800
H	0.90486800	-1.25378700	2.55372100
C	-3.50876700	-2.10558600	-0.83004500
H	-3.19725600	-2.39619900	-1.83844700
C	-2.86962600	-3.00907500	0.22740000
H	-3.08680500	-4.06267300	0.02155900
H	-3.24740500	-2.77211900	1.22729100
C	-1.03205900	2.38441300	0.19895400
C	-0.07346900	3.76237600	-1.60745500
H	0.09220200	4.82248700	-1.80346700
H	-0.70036800	3.36392300	-2.41616700
C	-0.65473000	2.42951600	2.73038700
H	-0.22757200	3.43725000	2.74250600
C	3.76399300	-1.09240200	2.83411400
H	3.18275600	-1.27386800	3.74145400
H	4.42865800	-1.93917600	2.64368800
H	4.36941100	-0.19074000	2.95555000
H	-1.15659000	2.26996800	3.69071100
H	0.17289100	1.71483100	2.65080400
H	0.90405800	3.26331400	-1.62033000

N	-0.73849200	3.61334200	-0.28896900
C	-1.04751400	4.89284600	0.40166100
H	-0.11742600	5.42976300	0.61920500
H	-1.66993500	5.51559100	-0.25004200
H	-1.58148300	4.73351400	1.33615000
N	-0.74172100	1.27806600	-0.50938600
C	-1.66936400	2.23304800	1.57096500
H	-2.50796900	2.92864400	1.68355900
H	-2.08034200	1.22076500	1.63791300
H	-4.60156600	-2.16179600	-0.78086200
H	-0.23013000	1.41436300	-1.38314500
N	1.23535400	-0.14245000	-2.70300500
H	1.52198900	0.02654800	-3.66325000
H	0.36076300	-0.62847300	-2.54439600
H	5.54262100	0.20555300	-1.75866600

H	4.09961900	-0.67932600	3.28701200
H	-1.85526900	1.77937500	3.81901700
H	-0.43004100	1.49741900	2.79576700
H	0.20372400	3.56306600	-1.33765700
N	-1.50958100	3.50445900	-0.04942400
C	-2.02163700	4.67323300	0.70757500
H	-1.19883500	5.36620600	0.91684100
H	-2.77814100	5.19699500	0.11195300
H	-2.46962500	4.38077000	1.65534100
N	-1.09472500	1.22324500	-0.37904900
C	-2.28234800	1.87581500	1.68126900
H	-3.20360300	2.45470200	1.80474600
H	-2.56585500	0.81917300	1.64687500
H	-4.29276900	-2.59828800	-1.57364300
H	-0.51577900	1.45423400	-1.19442000

PT-AMD-G

Pt	-1.09452700	-0.79374400	-0.13343800
O	1.14204100	0.90869600	-2.14522300
N	3.42276900	0.76495200	-1.69698400
H	3.55898800	1.25533000	-2.57951300
N	4.38064900	-0.17538300	0.28714700
N	0.83318600	-0.72727700	0.55695800
N	2.68249400	-1.11188700	1.77919000
N	5.76155100	0.76007300	-1.33863900
H	5.94381700	1.21518300	-2.22333800
H	6.54858800	0.51929500	-0.74773300
N	-3.02518900	-0.96958800	-0.91716600
H	-3.71987300	-0.75269800	-0.19283500
H	-3.14303200	-0.28570700	-1.67321700
N	-1.17484100	-2.91387000	-0.14957700
H	-0.55194900	-3.23702600	-0.89989200
H	-0.84369800	-3.33299500	0.72539700
C	4.52120300	0.43825300	-0.89803600
C	3.10176100	-0.47677200	0.61272100
C	1.94276700	-0.22314500	-0.14326300
C	2.06008000	0.49795400	-1.38284200
C	1.31502800	-1.24416200	1.70401800
H	0.72304700	-1.68974300	2.48731600
C	-3.22741900	-2.38479700	-1.43385900
H	-2.73172100	-2.45517200	-2.40716200
C	-2.60467900	-3.35551000	-0.42691000
H	-2.62619000	-4.38081300	-0.81185300
H	-3.14746900	-3.33552700	0.52366000
C	-1.60811200	2.21407600	0.36103700
C	-0.86086400	3.82801800	-1.34314600
H	-0.94563000	4.90052300	-1.52458600
H	-1.35100000	3.30207900	-2.17241100
C	-1.34581800	2.09121900	2.90085700
H	-1.05558400	3.14031800	3.02080300
C	3.57183300	-1.54485500	2.87810200
H	2.97441800	-2.01376100	3.66360000
H	4.30567400	-2.26015900	2.49756900

PT-TU-CI

Pt	0.84877600	0.04863100	-0.00647500
S	-0.97092000	-1.46363500	-0.58639300
Cl	-0.56358600	1.80948900	0.82443600
N	2.52712500	1.24045300	0.41726200
H	2.38395100	1.68127500	1.33222900
H	2.56734700	1.98698500	-0.28545600
N	2.28850900	-1.34719900	-0.64605800
H	2.01907000	-1.76344200	-1.54349400
H	2.33432300	-2.09903100	0.05105300
N	-3.17567400	0.21191000	-0.86264500
N	-2.89737000	-0.77185100	1.23393300
H	-3.69714600	-0.23982500	1.56081900
C	3.76123800	0.37012000	0.38513500
H	3.82454000	-0.14977100	1.34658800
H	4.66815500	0.97309700	0.25964200
C	3.62329400	-0.63393400	-0.76729300
H	3.62941800	-0.11642800	-1.73208200
H	4.45027700	-1.35330400	-0.75517500
C	-2.46466200	-0.57227700	-0.02901300
C	-2.72818600	0.58959100	-2.22309700
H	-3.54807500	0.42782600	-2.93073600
H	-1.87253700	-0.01490700	-2.51894600
C	-4.39294200	0.90573300	-0.37554900
H	-4.14138100	1.62608700	0.41493300
H	-4.84006300	1.45539400	-1.20452800
H	-5.13677400	0.18626600	-0.00955900
C	-2.19810600	-1.56514400	2.26444000
H	-2.82484000	-1.57944600	3.16051600
H	-2.03635800	-2.59020500	1.92273600
H	-1.23144300	-1.11204800	2.50710400
H	-2.43925900	1.64735700	-2.22893000

PT-TU-AQ

Pt	-0.93955200	-0.06956800	-0.15643600
S	1.12228200	1.11361100	0.45021600
N	-2.83063400	-0.89291900	-0.61019100

H	-2.83181800	-1.90467900	-0.43487600
H	-3.04036600	-0.74676400	-1.60572500
N	-2.05992400	1.39784300	0.76378700
H	-1.70772400	2.33567800	0.53474400
H	-1.97746900	1.28076600	1.78233400
N	3.69915000	0.53654400	-0.21652800
N	2.38283800	-1.36543300	0.34074300
H	3.18959200	-1.90471100	0.01885700
C	-3.87910300	-0.20345600	0.25305000
H	-3.85950500	-0.67451000	1.24075600
H	-4.87805000	-0.34152000	-0.17400500
C	-3.52185000	1.28064900	0.33561400
H	-3.61776400	1.76818500	-0.63952900
H	-4.16499700	1.80519400	1.04981700
C	2.52503300	0.02913300	0.16720000
C	3.86822900	1.95516600	-0.65658500
H	4.20077700	2.56812000	0.18837600
H	2.92817600	2.35155000	-1.04229900
C	4.96943000	-0.25602000	-0.19940100
H	5.12804500	-0.75786100	-1.16140600
H	5.79741500	0.43503400	-0.02987400
H	4.97534900	-0.98231800	0.61815000
C	1.85556900	-1.90817800	1.65216700
H	1.72751300	-2.98809200	1.54377900
H	2.55510400	-1.70205300	2.46868500
H	0.89153600	-1.45171300	1.87895100
H	4.62556300	1.98267000	-1.44412500
O	0.13169600	-1.62153100	-1.05074000
H	0.01783400	-1.89942000	-1.97818000
H	1.07187800	-1.70880300	-0.66690400

PT-TU-TS-A

Pt	0.66271300	0.98232400	-0.36590500
O	-0.61142900	0.71338300	-2.34064800
N	-0.14384300	2.90890500	-0.24928800
N	2.37569000	1.90401300	0.38336600
C	0.80944200	3.82663200	0.49091000
H	0.61000600	3.72347400	1.56271500
H	0.63929300	4.87242100	0.21273800
C	2.24489900	3.40668600	0.16109100
H	2.96407600	3.94958600	0.78485100
H	2.48088400	3.60130300	-0.88948500
S	1.70804200	-1.17139400	-0.88548600
N	2.33312400	-1.97478800	1.75528200
N	3.77618700	-2.63185100	0.04306200
H	4.21597100	-3.26518000	0.70492000
C	2.66484100	-1.96823200	0.44099200
C	0.98618800	-1.63369400	2.26743900
H	1.07369700	-0.88625000	3.06485400
H	0.35533200	-1.24009700	1.47272500
C	3.24784100	-2.57930600	2.76272900
H	4.27536700	-2.22703900	2.61856500
H	3.22126800	-3.67754300	2.72749500

H	2.92285700	-2.26961100	3.75770200
C	4.35500900	-2.65586800	-1.32189300
H	5.36925600	-3.05697100	-1.25114300
H	4.39679300	-1.64802600	-1.74117000
H	3.76604400	-3.29194800	-1.99088500
H	0.51965300	-2.53478700	2.68512600
N	-1.65002600	-1.71811800	-2.22415600
N	-3.93366700	-2.03749600	-1.66846600
N	-5.00538700	-1.14758300	0.31299900
N	-1.59469400	0.04042900	0.42304600
N	-3.47570800	0.18914300	1.70279400
C	-5.01154600	-1.83627100	-0.85110700
C	-3.80662600	-0.60519100	0.60559000
C	-2.62612100	-0.70975900	-0.17748800
C	-2.74041100	-1.50464600	-1.34267000
C	-2.15495900	0.54493900	1.54253900
H	-1.63883200	1.15594600	2.26843800
C	-4.39849700	0.55325900	2.79734800
H	-3.88157300	1.20460700	3.50685900
H	-4.73966300	-0.35006000	3.31014200
H	-5.26882500	1.07280000	2.38763300
H	-1.08438200	-0.18953300	-2.46387000
H	-1.06509200	2.88284300	0.20052700
H	-0.29122700	3.21476400	-1.21920100
H	3.19822700	1.54192900	-0.11136300
H	2.48798000	1.69618100	1.38188400
H	-0.79902700	-2.07849400	-1.78327200
H	-1.93279000	-2.26584600	-3.03969000
H	-0.16754700	1.00015000	-3.16260500
H	-5.94869700	-2.28055600	-1.16431700

PT-TU-TS-G

Pt	0.64909300	-0.74708700	-0.17202700
O	-0.33255000	-1.06702300	2.03197300
N	-0.36329300	-2.56434100	-0.41831900
N	1.95202700	-1.57592800	-1.57269000
C	0.07704500	-3.20098300	-1.71071200
H	-0.43034500	-2.68542700	-2.53200900
H	-0.20110300	-4.26091800	-1.74420600
C	1.59756300	-3.04039100	-1.81116600
H	1.96821600	-3.36626400	-2.78913000
H	2.10074500	-3.62760400	-1.03594400
S	1.89546100	1.35583700	0.05401400
N	4.60580000	1.80615800	0.03243500
N	3.90519100	0.23697700	1.61085200
H	4.88469900	0.08115100	1.82881900
C	3.60706200	1.08096700	0.59040000
C	4.45318200	2.64058900	-1.18751900
H	5.29566600	2.44415900	-1.85879700
H	3.51972300	2.40762000	-1.69899900
C	5.95484500	1.85462400	0.66119400
H	6.52632500	0.93634500	0.46840300
H	5.87474200	2.02640400	1.74096600

H	6.50923000	2.69055600	0.23224800
C	2.94087500	-0.35656400	2.56136700
H	3.50809700	-0.88573800	3.33166400
H	2.26730700	-1.06011400	2.06541100
H	2.34517300	0.43002900	3.03763700
H	4.45271300	3.70281500	-0.91767700
N	-4.71247500	-0.63183100	0.77891800
H	-5.18023900	-1.44501700	1.17608600
N	-4.87086500	1.58669300	-0.11638400
N	-1.35722400	0.71866600	-0.14860300
N	-2.66805600	2.48231900	-0.72263800
C	-5.45337500	0.49370800	0.39464500
C	-3.52274500	1.50994900	-0.22986600
C	-2.70210000	0.41714300	0.12781000
C	-3.31269400	-0.74173600	0.67784900
C	-1.38242200	1.95839400	-0.65387000
H	-0.51852600	2.51904500	-0.97466800
C	-3.07242800	3.81479300	-1.21238600
H	-2.18792400	4.35129500	-1.56394300
H	-3.54462900	4.38148700	-0.40516700
H	-3.78447000	3.70781900	-2.03514300
H	-0.27263900	-0.41984400	2.75993600
H	-1.26943100	-1.38685300	1.87845900
H	-1.38328000	-2.43213100	-0.33680900
H	-0.08706400	-3.13770400	0.38900000
H	2.92722500	-1.49242400	-1.26935600
H	1.84403700	-1.03389300	-2.43771300
O	-2.72159900	-1.81261900	1.07138700
N	-6.80062500	0.46074100	0.55139700
H	-7.32570600	1.28109900	0.27309900
H	-7.30420400	-0.32850100	0.93356900

PT-TU-A

Pt	-0.26377800	0.62526200	-0.08966500
S	-1.46172700	-1.33263300	0.75783500
N	-4.05403700	-1.63514400	1.44562200
N	-3.80921800	-0.83472700	-0.73964200
N	-1.85933000	1.97565500	0.00361100
N	0.81785700	2.34646600	-0.66391000
C	-3.24811000	-1.23608700	0.43898700
C	-3.08211100	-0.87473300	-2.03671500
C	-3.63883400	-1.98224600	2.82799600
C	-5.29297400	-0.75721500	-0.87268400
C	-1.50103100	3.22470600	-0.79133100
C	-0.04410000	3.58092400	-0.48756500
N	4.68122600	0.64401900	1.13297900
N	4.87292500	-1.44283300	-0.07659000
N	1.38787700	-0.58296600	-0.22695500
N	2.71817900	-2.26170600	-0.92899800
C	5.39208200	-0.39150100	0.60046800
C	3.54061200	-1.36004800	-0.24486800
C	2.70221300	-0.31519700	0.21645100
C	3.33990400	0.69542000	0.98288800

C	1.45189100	-1.75871900	-0.89538200
H	-4.52887800	-1.96842800	3.46211700
H	-2.91564400	-1.25548800	3.20416200
H	-3.18861900	-2.97967700	2.86319500
H	-5.73185800	-0.20641800	-0.03358300
H	-5.53343400	-0.21824800	-1.79109900
H	-3.38127600	-0.01706600	-2.64816200
H	-2.00512200	-0.84398800	-1.87612600
H	-3.33854500	-1.79331300	-2.57975000
H	-5.74788800	-1.75560400	-0.94227800
H	-2.17089000	4.05177300	-0.53078200
H	-1.63475500	2.99008600	-1.85187600
H	0.30117700	4.38857700	-1.14164200
H	0.06711600	3.91883000	0.54850500
H	1.65073100	2.40192200	-0.04006100
H	1.12871600	2.25088200	-1.63695800
H	-2.02223700	2.21692000	0.98886800
H	-2.72311200	1.55432600	-0.35556300
H	0.60716000	-2.24901600	-1.35055000
H	6.46516000	-0.37308200	0.74867800
C	3.18241300	-3.51784400	-1.55959000
H	2.34466100	-3.99662500	-2.07194100
H	3.97562600	-3.29185100	-2.27659500
H	3.57900200	-4.18770600	-0.79218500
H	-5.03195400	-1.81774300	1.23518000
N	2.65936400	1.78020600	1.55956300
H	3.28566700	2.40367100	2.07023900
H	1.79586900	1.56141000	2.05499400

PT-TU-G

Pt	-0.51075600	0.68043300	-0.09352500
S	-1.58782100	-1.37310500	0.73425000
N	-4.15207500	-1.84283400	1.43016400
N	-3.97344200	-0.94194100	-0.72079200
N	-2.14863600	1.91045800	0.31169900
N	0.39533600	2.49953000	-0.60086700
C	-3.37626100	-1.36295700	0.43244800
C	-3.26170500	-0.86732400	-2.02369200
C	-3.70070200	-2.22480300	2.79064500
C	-5.45964300	-0.93021200	-0.83468400
C	-1.93496900	3.28100800	-0.31809700
C	-0.46284500	3.65213800	-0.13465100
N	4.53819300	0.73753700	0.77912300
N	4.62464200	-1.48402900	-0.10016200
N	1.18760300	-0.44417300	-0.43477400
N	2.45400800	-2.24283200	-0.92183300
C	5.22940800	-0.43935000	0.48430100
C	3.30496800	-1.30946100	-0.33896500
C	2.51971500	-0.17666200	-0.04791700
C	3.16823500	0.97175200	0.51631000
C	1.19977200	-1.68698000	-0.95650000
H	-4.58275800	-2.29727800	3.43208200
H	-3.02102300	-1.47101200	3.19426900

H	-3.18611300	-3.19119500	2.77752600	H	-2.21214300	1.99913600	1.33335300
H	-5.91463400	-0.43619800	0.03091300	H	-3.02418700	1.49210000	-0.01965600
H	-5.73620600	-0.36572200	-1.72726300	H	0.33570500	-2.20705400	-1.33333100
H	-3.59320200	0.02165800	-2.57020700	C	2.85754000	-3.58379500	-1.39461200
H	-2.18475900	-0.81034900	-1.87183600	H	1.97831000	-4.11310900	-1.76903600
H	-3.49657100	-1.75430300	-2.62602200	H	3.59652400	-3.48707200	-2.19436000
H	-5.86800500	-1.94539200	-0.94134900	H	3.29941200	-4.14542500	-0.56752700
H	-2.59543900	4.02219700	0.14544000	H	-5.12179800	-2.06485000	1.22191400
H	-2.19122000	3.20078400	-1.37925000	O	2.67701500	2.11669300	0.75975400
H	-0.21894100	4.56366400	-0.69103200	N	6.54562700	-0.51438600	0.79496100
H	-0.23086400	3.82994700	0.92074800	H	7.03457700	-1.37279100	0.57002300
H	1.31978600	2.50439600	-0.09563700	H	7.06227900	0.23299500	1.23953700
H	0.55438300	2.54424800	-1.61297400	H	5.02497200	1.53157000	1.19244400

**Table S2.** Vibrational Frequencies ( $\text{cm}^{-1}$ ) for Optimized Structures**9MeA**

55.7630	116.0871	197.1701	216.1324	254.4594	307.5287
314.0644	526.7769	530.6223	533.0809	550.9364	575.2099
580.6740	664.0541	694.8370	718.6144	735.7323	832.7531
867.8813	881.5982	972.2650	988.6710	1050.6523	1079.5696
1163.4758	1206.4470	1250.3205	1267.7889	1327.4287	1343.2388
1344.6030	1399.6414	1424.7871	1466.9948	1486.5781	1520.9805
1527.5337	1532.7249	1595.2245	1625.2770	1669.9217	3060.1424
3144.6709	3179.2760	3239.9406	3296.0840	3620.8109	3774.0718

**9MeG**

57.6420	109.0291	149.5515	184.4816	214.1818	252.2863
295.0139	326.1955	371.1574	374.8889	482.1665	510.9357
511.9497	597.5805	635.1049	664.0961	664.3341	721.1178
726.4458	734.5391	804.3870	833.1466	838.2566	1008.3058
1049.1676	1051.1918	1095.2814	1124.1758	1163.5391	1236.1969
1294.0953	1333.1846	1353.6301	1385.4976	1418.6439	1469.2605
1500.0990	1524.1684	1527.1138	1539.3740	1578.1702	1630.5271
1672.7826	1728.8008	3059.9465	3142.9974	3181.0811	3298.0033
3599.4121	3640.0001	3787.7257			

**PT-AMD-Cl**

27.6042	41.0543	48.6741	65.3163	87.8270	100.8730
121.9173	125.0702	156.2233	169.0845	174.9748	198.6770
211.9978	234.2373	269.5009	275.1356	300.0904	316.3019
344.5367	402.4788	440.4815	454.2626	499.5160	517.9742
566.3795	663.6362	694.9318	727.0163	740.1606	770.1097
785.9248	823.5492	870.9266	883.2530	940.9100	1000.4634
1017.0549	1025.6005	1071.4606	1081.4800	1094.0083	1114.5260
1116.2414	1126.1986	1163.9395	1173.8779	1198.1495	1204.8406
1264.6299	1291.7093	1299.0659	1321.1272	1347.1231	1368.5751
1388.4787	1415.0378	1433.4958	1441.7858	1480.9806	1489.1860
1510.0074	1515.9591	1519.3953	1522.7735	1524.9473	1528.9688
1531.4128	1534.2052	1539.0254	1559.9025	1627.4789	1691.2093
1696.8850	3036.1639	3051.9454	3061.9080	3087.2669	3093.5169
3105.8179	3113.3462	3132.6138	3136.2915	3148.6316	3152.0556
3164.6800	3166.8454	3185.0795	3223.1669	3452.9968	3456.1743
3533.6085	3544.6703	3571.3335			

**PT-AMD-AQ**

26.2570	46.1271	57.2744	69.3964	102.4970	109.7590
118.4034	138.8381	159.6285	163.8708	170.2511	182.0369
199.2387	211.9160	222.8428	273.7727	278.8082	313.4072
327.8827	390.0037	416.0328	441.0968	455.2464	470.8068
506.6788	541.4310	583.4158	645.9982	695.3181	710.8633
733.5406	757.4819	764.8731	816.7875	820.2711	866.0359
879.4625	935.2533	1001.8218	1020.0139	1024.3286	1072.1715
1072.6648	1090.4754	1106.9551	1120.2287	1130.2546	1173.8152



1203.7179	1205.6113	1250.0786	1250.4000	1284.1864	1301.2484
1338.6025	1351.7905	1357.7428	1391.4396	1419.0733	1442.7199
1443.7056	1479.2852	1489.8760	1495.4116	1511.9153	1516.9399
1521.6479	1524.7833	1525.3410	1528.7444	1530.5298	1538.2051
1552.0183	1632.7232	1663.6077	1686.5665	1694.1506	3045.3651
3049.5742	3076.0262	3085.5996	3101.5094	3104.4455	3125.3849
3127.6290	3146.5753	3157.5026	3164.8915	3171.4671	3179.1798
3197.3553	3229.9337	3432.3460	3440.7671	3511.2833	3522.8742
3562.6521	3701.7110	3833.5025			

PT-AMD-TS-A

-139.2871	20.4616	31.9556	33.8901	43.9737	46.9437
57.6224	71.2897	84.6311	88.0432	94.9480	104.9734
114.3086	126.4854	129.7696	142.1697	152.7819	167.8861
173.9203	189.3398	189.9918	201.4274	208.6729	224.1009
226.0054	237.3087	270.3929	278.9988	292.0203	312.4161
320.1734	326.1866	339.7763	389.1368	419.3307	427.1318
451.6849	458.9389	487.8122	507.2127	519.5939	534.1661
538.4755	571.6377	576.1174	584.2785	648.4249	655.0348
672.6408	707.4929	716.4073	733.1971	735.4208	754.7336
762.5251	792.2276	811.8660	828.9811	832.6432	874.7737
881.5003	882.3361	903.7017	939.1440	986.6885	1006.1808
1009.9072	1019.3342	1026.0665	1061.2244	1073.6112	1075.6825
1090.0364	1093.8343	1113.2893	1121.3985	1140.1067	1162.8909
1173.3449	1187.4532	1194.9763	1204.4381	1225.4228	1247.3841
1253.2857	1259.6966	1292.1530	1309.1778	1311.6995	1326.4041
1333.0473	1351.3098	1354.3465	1357.2258	1377.3864	1381.8939
1394.1369	1418.9490	1442.6617	1443.0693	1460.8496	1470.5811
1479.9790	1487.2971	1501.0407	1515.2471	1515.4150	1518.4321
1519.3482	1525.2999	1525.7845	1525.8993	1529.7036	1530.9897
1534.3444	1537.6192	1550.5568	1594.5465	1612.7754	1615.3057
1623.7705	1662.5713	1692.6947	1700.2100	3040.7110	3063.3075
3073.4188	3080.9226	3090.4429	3095.2597	3100.9484	3118.0682
3138.1281	3152.8092	3157.3113	3158.5285	3167.8799	3174.0312
3178.5975	3194.8015	3198.9538	3230.6721	3269.4227	3317.3114
3366.0451	3449.5536	3518.1122	3534.6172	3547.3362	3549.6871
3670.1686	3693.4938	3824.0144			

PT-AMD-TS-G

-146.1048	20.4564	26.6755	36.4316	56.9585	59.0483
62.6319	73.0284	80.1978	85.2846	92.5875	105.3277
115.7067	124.5498	130.7484	138.5864	152.0322	156.8630
167.2224	185.1506	197.5282	201.9650	204.7620	213.8807
221.0098	227.6368	269.9968	271.1361	279.8711	306.4055
316.8177	319.4825	350.7814	367.5826	384.8439	391.5377
407.3355	438.2427	452.4964	460.5936	486.1448	503.6036
508.7070	525.5337	527.3979	571.3898	613.8652	635.6536
644.1990	671.7634	673.6182	678.4433	718.5031	721.3915
732.9793	738.8235	749.9830	760.2703	792.2856	815.4454
830.3130	846.1196	870.5801	875.4881	879.5800	945.1084
979.9185	1004.8582	1010.1001	1011.1695	1023.7809	1055.6143
1073.0035	1078.8268	1081.9290	1093.6287	1100.8699	1109.1787

1121.9168	1122.4109	1163.9686	1169.4100	1171.4155	1179.9180
1210.7851	1215.5010	1238.2250	1266.6970	1293.2250	1299.1171
1305.5955	1328.3085	1335.3400	1347.5224	1363.3935	1372.1961
1378.3112	1403.8490	1415.7111	1417.8020	1439.1963	1442.2618
1463.8494	1482.5034	1490.6026	1500.5173	1503.9836	1510.2967
1515.6263	1516.7730	1521.1877	1523.7909	1524.7226	1525.2762
1529.1256	1532.1724	1536.4900	1546.7807	1552.9813	1583.0788
1591.4492	1627.7582	1646.4109	1682.8903	1692.5396	1694.8748
1701.5752	3057.1712	3060.1139	3066.5995	3077.7562	3084.6667
3093.5820	3098.0438	3123.8722	3142.1363	3143.1176	3146.7556
3155.2572	3164.1625	3171.0999	3183.5736	3193.6870	3194.8710
3218.8171	3303.4468	3312.4691	3442.1652	3453.8662	3524.9121
3540.6417	3584.4146	3612.0584	3659.9837	3751.8520	3822.0776

PT-AMD-A

23.0335	29.1655	31.9215	55.3376	61.9122	65.7256
65.8699	83.1321	105.1725	106.9359	115.5380	130.4339
153.6154	161.1877	168.1072	186.7619	187.9438	202.0914
210.8731	217.3641	228.7986	247.4440	268.1404	278.5007
285.2912	307.5376	324.0097	347.3615	358.0528	393.3105
436.1628	453.8919	482.4604	508.2227	516.7855	533.1101
549.7769	567.4331	570.1829	588.6856	644.2899	653.7642
669.1581	704.6759	714.8445	716.3876	736.0913	740.7544
768.4584	782.6473	799.4270	828.0671	829.0348	869.2381
879.9983	890.5288	908.8805	941.4252	990.2672	998.2683
1007.3292	1012.9175	1022.2594	1072.8337	1076.4178	1087.7846
1092.6372	1101.0076	1113.7718	1122.4927	1124.0924	1164.0893
1173.7179	1189.0208	1194.6130	1207.9549	1228.7409	1252.6272
1257.5592	1268.3323	1290.3239	1301.8265	1303.5117	1332.9729
1341.7725	1350.5706	1359.3874	1365.1643	1389.6453	1397.9231
1418.1217	1419.8255	1440.8736	1443.9447	1463.8563	1479.1358
1482.0655	1491.8125	1499.5981	1504.8708	1516.6244	1520.4454
1523.4102	1524.5476	1526.6311	1526.7671	1529.0677	1532.6503
1538.2482	1554.2772	1560.4468	1603.8427	1616.2997	1631.6031
1662.4266	1692.7032	1695.3704	3046.2264	3062.5849	3073.0366
3086.7540	3088.4679	3096.5554	3099.3815	3126.0549	3132.7667
3152.3524	3155.5149	3157.8937	3165.8698	3172.0959	3191.0827
3195.5942	3200.5979	3228.7670	3269.9317	3314.7648	3444.7075
3445.7330	3526.3057	3526.8610	3526.9470	3560.8337	3704.0865

PT-AMD-G

20.4678	30.2242	39.8510	50.7163	56.5661	57.3468
67.4847	85.6676	96.3343	99.6249	109.0919	124.1720
143.7147	153.4242	166.8449	180.7260	188.3270	198.7514
207.4302	208.8815	216.2912	227.2064	232.0805	271.8387
278.0054	290.0730	313.8636	319.6551	349.0287	384.3191
390.8948	402.5124	421.9625	436.7686	451.5627	502.8252
505.9571	518.0255	533.2909	567.9941	610.6179	641.2515
649.7942	668.4987	674.8964	677.5874	723.2832	724.7029
734.9301	739.0065	739.8691	761.5285	791.3835	815.0176
826.1349	861.3136	870.9128	881.9508	886.5482	899.0237
944.9270	1009.3473	1012.0085	1013.6891	1022.1294	1072.6052

1075.8900	1078.1981	1090.0220	1093.7398	1104.1541	1113.9702
1122.3834	1125.9293	1164.1222	1172.7216	1174.6560	1183.9890
1209.2171	1222.1515	1238.9641	1262.4260	1291.3443	1303.8077
1311.9979	1331.6140	1348.7959	1351.4257	1357.5687	1379.7993
1386.4875	1400.0872	1418.4225	1424.9634	1440.7107	1441.8904
1477.0564	1480.5361	1488.9293	1501.7731	1506.7219	1508.8933
1515.1265	1520.8564	1524.1555	1525.2345	1525.2703	1525.7677
1527.7429	1531.4116	1535.7308	1551.9785	1562.6494	1596.9953
1628.5572	1646.0668	1684.9997	1689.6869	1694.6255	1702.2007
3051.5718	3059.7954	3068.4008	3087.3130	3087.6044	3095.2966
3099.2600	3130.4914	3132.8720	3144.9349	3154.7881	3156.9950
3161.8963	3171.7923	3188.3392	3193.1354	3199.2915	3223.4885
3319.8116	3446.1082	3446.4819	3446.6865	3529.4280	3532.3384
3579.6089	3607.8118	3746.5814			

PT-TU-CI

10.1621	24.6888	55.4761	72.1849	86.0412	103.6306
107.3549	128.4249	138.6037	146.9388	159.4784	178.6087
210.3045	244.8015	265.6104	282.9753	292.3865	300.1383
327.7757	332.6519	397.4435	438.8839	451.4811	516.3234
523.1435	553.8124	563.4183	614.1126	691.3771	731.2441
774.4806	870.3421	883.3510	889.4259	1000.5151	1016.9985
1046.5050	1073.7941	1080.9183	1116.6769	1122.2565	1151.5896
1156.0600	1166.3845	1179.7905	1200.1042	1208.2402	1276.5587
1297.2798	1320.5953	1345.6768	1403.0377	1415.8989	1435.2012
1439.0106	1475.3536	1494.9260	1500.9661	1508.9834	1515.7919
1519.2442	1520.3898	1526.6549	1529.4861	1536.7494	1554.5659
1637.0168	1692.8512	1696.7552	3043.1419	3066.8385	3074.4935
3087.1870	3093.6067	3125.1733	3148.7156	3151.1838	3165.1654
3168.9397	3186.7601	3195.6974	3216.6576	3453.9321	3457.0838
3539.2365	3541.0603	3620.3169			

PT-TU-AQ

31.8179	48.1091	79.2803	90.8713	99.4247	110.9065
115.7433	141.0023	149.3589	161.2030	170.3116	204.0040
212.8444	236.0696	263.7296	283.0806	314.4665	346.3830
358.5317	374.3353	422.4830	447.2509	448.8203	471.2881
508.4119	535.3048	582.3764	601.0289	670.2490	744.8646
806.9395	830.9342	859.1366	869.9216	879.6853	913.4658
980.8674	1004.1907	1027.8594	1036.1130	1060.9269	1074.3782
1111.6022	1118.2375	1139.7296	1155.6448	1170.1018	1199.8351
1202.3034	1214.8947	1257.0372	1302.4337	1307.9535	1338.8614
1353.8703	1420.0931	1435.0802	1445.5258	1476.9847	1487.0740
1491.0221	1509.8126	1513.9652	1518.7221	1521.9788	1522.4766
1527.6147	1533.7744	1540.1228	1604.9263	1666.3694	1691.7583
1694.7119	2903.4071	3069.4776	3079.3742	3083.2158	3100.7790
3103.9130	3164.0037	3170.0331	3176.9522	3178.2855	3185.0755
3194.5323	3209.0052	3212.1301	3432.2476	3439.5633	3510.1156
3524.5913	3528.2416	3790.5501			

PT-TU-TS-A

-151.8150	23.8058	26.3916	35.8684	44.5076	53.9317
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56.3456	67.8632	81.9362	91.9686	98.9229	101.2027
105.7205	114.7131	120.9060	141.4659	155.1495	164.3216
172.7783	195.1331	199.2030	210.6914	214.0014	225.7874
265.4498	268.6308	273.2631	292.9755	298.4516	306.3515
325.5885	349.5028	375.6602	393.5540	412.9125	439.4859
448.4332	495.6978	524.7011	529.0299	535.2725	542.6670
564.8193	566.4920	574.9698	586.7296	609.6849	650.4355
668.5163	693.1406	705.4725	733.0865	736.3835	751.0538
785.7918	833.4891	866.7234	876.6559	880.1076	884.6381
892.5358	953.5283	984.6520	1003.0689	1006.7960	1023.4292
1033.0641	1070.8194	1074.6409	1079.7617	1090.3749	1118.3499
1121.3436	1138.9063	1149.7153	1152.6790	1163.8970	1175.1425
1180.5924	1200.7331	1204.8147	1213.6528	1247.3489	1251.8470
1265.7552	1294.2605	1304.3207	1319.1204	1325.5330	1344.7985
1351.4711	1380.6981	1390.7077	1395.5967	1415.9007	1435.4731
1437.6463	1463.5709	1471.5143	1482.2916	1499.5779	1501.5622
1505.3317	1508.1155	1519.0746	1522.6567	1523.9002	1526.8615
1528.2672	1531.9275	1537.0481	1538.8698	1552.5548	1591.0687
1619.0973	1622.8958	1675.6506	1690.6323	1695.4584	1707.5022
2795.1093	3046.4814	3055.9529	3078.7656	3084.7445	3093.4770
3098.0567	3132.3734	3138.1437	3155.0328	3171.4817	3172.9532
3185.5474	3188.8306	3194.0979	3195.3130	3218.2105	3272.7977
3294.8051	3448.5690	3449.2809	3470.5019	3530.9243	3531.3761
3593.2814	3605.1781	3761.9770			

PT-TU-TS-G

-149.3696	24.6249	26.0023	30.8374	35.5932	40.2264
49.4326	70.0333	80.0498	81.3640	91.5566	101.8038
115.0407	124.3700	132.2819	139.1068	143.5291	155.3477
163.7922	178.3395	189.5631	204.0856	212.2421	215.6618
219.4321	236.7933	250.6704	269.8759	281.1948	305.8630
315.0354	344.2734	357.7808	364.5790	373.7868	387.8587
405.2948	406.3730	438.6987	449.9195	495.0044	522.5996
526.6775	529.7318	568.4660	576.2448	609.4044	611.1806
628.6975	641.0764	643.7142	675.1712	677.9569	681.5819
723.0881	732.2883	742.5313	764.8444	806.0089	816.4657
842.2475	856.0475	870.7915	878.2091	883.0547	893.2635
1006.7566	1011.2401	1014.4493	1039.6347	1054.4583	1077.3898
1077.5101	1079.5264	1101.5653	1119.3416	1121.5943	1146.2463
1161.7587	1164.3450	1172.7943	1189.3548	1198.7220	1206.6895
1236.0947	1251.6382	1266.7705	1295.4465	1314.7986	1326.2134
1343.4940	1344.1652	1365.5432	1381.0081	1388.1990	1409.0457
1412.9612	1433.1839	1434.4369	1466.9480	1479.2705	1491.3097
1499.4085	1504.3237	1504.9637	1514.6177	1517.1800	1518.2094
1520.8516	1525.4792	1529.4163	1534.8045	1536.8915	1545.8295
1550.9922	1593.0106	1614.4785	1629.6103	1649.8406	1661.2962
1691.2768	1696.5448	1718.9660	3048.0966	3066.2220	3070.0321
3084.9313	3090.7745	3096.2446	3136.2263	3153.1660	3154.8343
3157.0643	3169.3328	3182.1594	3183.3053	3194.4844	3196.4271
3209.5199	3251.3386	3314.5634	3388.4222	3452.9116	3485.1272
3537.5825	3580.4866	3610.1757	3610.4127	3749.3395	3786.4781

**PT-TU-A**

16.6820	30.2962	35.1534	41.4871	52.4127	59.9169
80.2791	90.4137	101.4027	103.1047	111.5643	115.1723
129.3705	159.7506	163.2891	165.6557	185.4185	197.9855
207.7228	220.7450	229.6967	248.7228	262.4883	272.4220
278.4981	294.3798	306.1224	346.8076	351.5381	364.1806
397.0923	433.1730	444.2073	488.1927	528.8481	531.6246
535.8916	551.6278	567.1222	577.8187	583.4000	595.9658
613.5574	650.7837	672.8370	704.6574	713.8269	766.4566
774.3354	821.3971	837.4427	872.1166	875.6713	877.8389
886.5986	901.1818	912.7514	987.0545	1006.8645	1022.5984
1028.6112	1031.6160	1069.9299	1079.0448	1092.6598	1101.7231
1118.0426	1132.1697	1137.7308	1150.8533	1164.0248	1170.9385
1198.9679	1200.5264	1202.8793	1252.0555	1256.3944	1265.1445
1275.4671	1306.3188	1322.1536	1328.9528	1339.2356	1354.9045
1362.2869	1388.0968	1393.2508	1413.1246	1420.0368	1428.0384
1440.7186	1463.2522	1476.6682	1477.6603	1497.9885	1499.8997
1502.1372	1507.6190	1518.5441	1521.4727	1523.0886	1524.9598
1526.3762	1526.5626	1535.7230	1552.6933	1558.9969	1601.7323
1608.5203	1617.6786	1673.6465	1697.6372	1709.6584	3045.9250
3060.3345	3080.5344	3089.3088	3093.0063	3097.4391	3140.0883
3145.0420	3154.3881	3170.0970	3176.1155	3183.1423	3188.3599
3191.7631	3198.6565	3202.2242	3203.3768	3274.0806	3331.5532
3441.3109	3498.8285	3510.5815	3521.7666	3597.9358	3635.1398

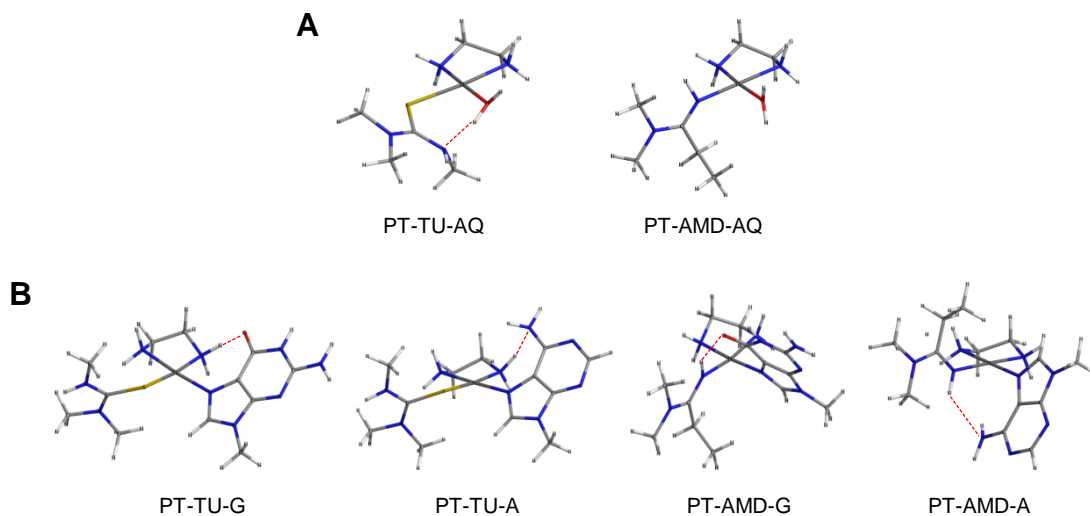
**PT-TU-G**

18.7121	29.2751	35.4678	49.5506	58.0338	65.5764
86.6476	88.0379	99.3498	99.7007	113.5725	123.9357
132.7600	146.5874	162.3666	167.8554	184.1648	197.1917
202.8662	207.7216	218.5151	229.1661	233.4770	262.9032
281.1318	288.0240	294.6595	321.0428	348.0233	369.8293
383.1083	397.4034	409.2819	422.7867	445.7171	453.5889
507.2922	531.3146	539.1255	541.6452	578.1336	584.6518
613.1589	620.5650	639.5242	649.4888	673.9465	680.9033
705.3209	724.1936	733.9447	765.4837	778.7845	817.7667
856.4412	874.7964	877.5484	878.8134	884.8336	893.0633
1011.0443	1014.9493	1030.8580	1037.3681	1071.9411	1077.6871
1083.7942	1093.8810	1107.4232	1119.1204	1133.7886	1143.3260
1151.4351	1164.8637	1171.9811	1190.0337	1200.7853	1202.7600
1246.6665	1258.5371	1289.0501	1312.4250	1327.4804	1352.1535
1354.5408	1363.6220	1383.6074	1387.4574	1391.2190	1420.7179
1423.7029	1427.5601	1448.4412	1476.1369	1477.1330	1498.1383
1502.5985	1502.8237	1505.2848	1505.8724	1519.6788	1521.1594
1521.5973	1522.5532	1525.1935	1527.2684	1536.0029	1552.2300
1565.8725	1597.5869	1606.9491	1650.0451	1676.5433	1696.0890
1699.2796	1727.9814	2975.6694	3044.7810	3060.1453	3079.1033
3088.2187	3092.7478	3096.8058	3138.0382	3144.7888	3153.4530
3169.0500	3174.0122	3187.3563	3188.8730	3196.4651	3200.6526
3205.7117	3340.9623	3442.7980	3498.9602	3527.8181	3578.0304
3603.4068	3607.8238	3746.4666			

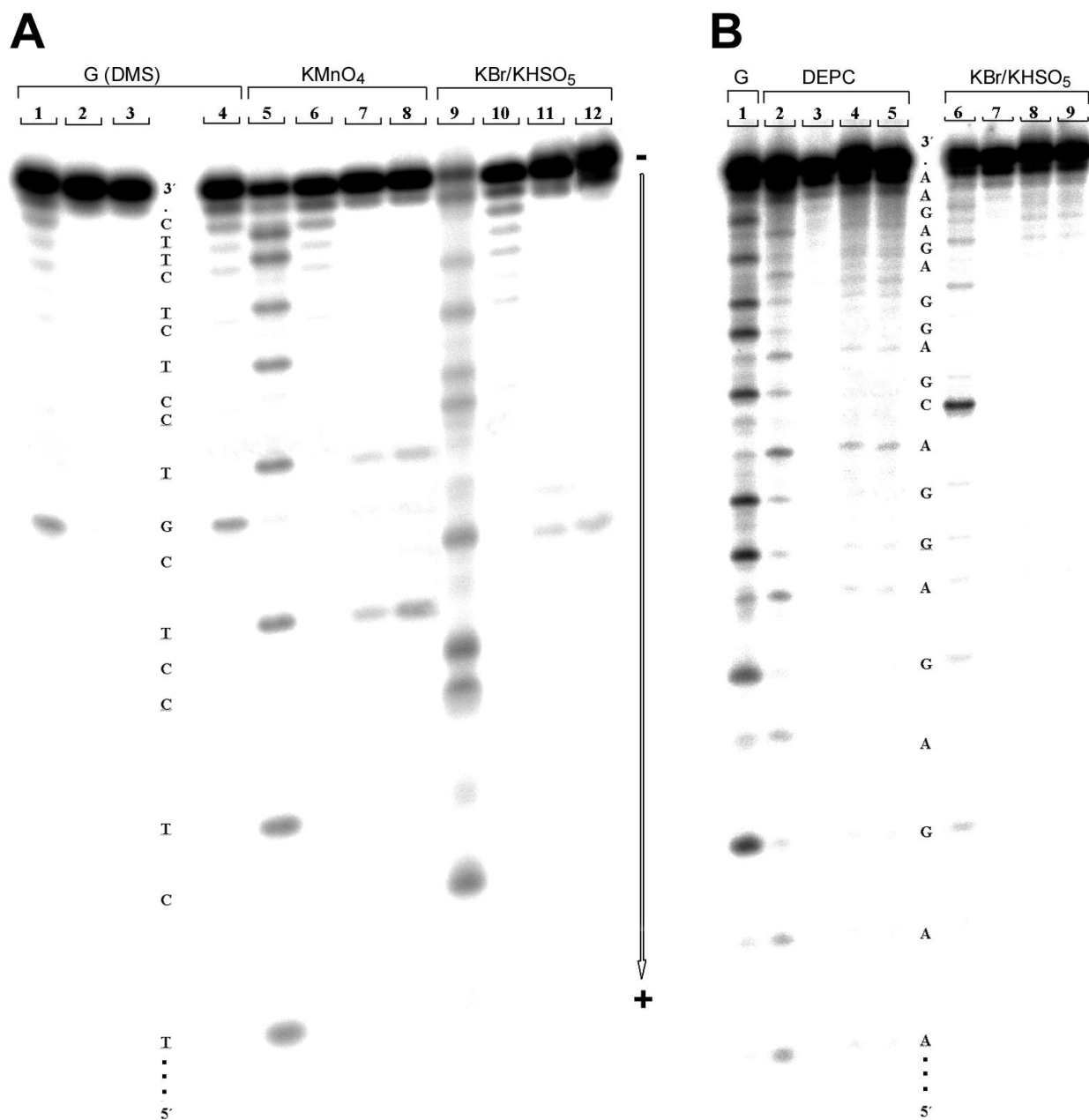
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**Table S3.** Computed Absolute Energies of Optimized Structures (kcal mol<sup>-1</sup>)

	PT-Cl	PT-AQ	PT-TS-A	PT-TS-G	PT-A	PT-G
AMD (NH)	-396337	-434783	-752543	-799777	-704631	-751854
TU (S)	-378027	-416466	-734238	-781466	-686310	-733541



**Figure S1.** Results of the DFT computations. **(A)** Optimized aqua intermediates. (The chloro precursors are not shown.) **(B)** Optimized platinum–nucleobase adducts. Hydrogen bonding interactions are highlighted with dashed red lines.



**Figure S2.** Chemical probes of DNA conformation. Piperidine-induced specific-strand cleavage at  $\text{KMnO}_4$ -modified,  $\text{KBr/KHSO}_5$ -modified, and DEPC-modified bases in the 22-bp duplex (shown in Figure 6) unplatinated or containing a single, site-specific adduct of **1** or **2** at the central G residue in the top strand. The oligomers were 5'-end labeled on either the top (A) or bottom strand (B).

Lanes in Figure S2A (the top strand 5'-end labeled): 1, 4: a Maxam–Gilbert specific reaction for G residues (DMS) in the unplatinated top strand; 2, 3: a Maxam–Gilbert specific reaction for G residues in the strand containing adduct of **1** or **2**, respectively; 5, 9: the unplatinated single strand; 6, 10: the unplatinated duplex; 7, 11: the duplex containing a unique adduct of **1**; 8, 12: the duplex containing a unique adduct of **2**.

Lanes in Figure S2B (the bottom strand 5'-end labeled): 1: a Maxam–Gilbert specific reaction for G residues (DMS) in the unplatinated bottom strand; 2, 6: the unplatinated single strand; 3, 7: the unplatinated duplex; 4, 8: the duplex containing a unique adduct of **1**; 5, 9: the duplex containing a unique adduct of **2**.