

## Cisplatin Cytotoxicity: a Theoretical Study of Induced Mutations

José P. Cerón-Carrasco<sup>a</sup>, Denis Jacquemin<sup>a\*</sup> and Emilie Cauët<sup>b</sup>

<sup>a</sup> CEISAM, UMR CNRS 6230, BP 92208, Université de Nantes, 2, Rue de la Houssinière, 44322 Nantes, Cedex 3, France, <sup>b</sup>Service de Chimie Quantique et Photophysique, Université Libre de Bruxelles, 50 Avenue F. D. Roosevelt, B-1050 Bruxelles, Belgium.

*\*e-mail: denis.jacquemin@univ-nantes.fr*

### **Supporting Information Material:**

- **Optimised high-layer geometries: p. S2**
- **Atomic charges used during the MD simulations: p. S25**

**Method 1 – canonical structure**

N	-5.05093200	-1.07252200	-0.36308900
C	-5.05649800	-0.45714600	-1.57332500
N	-3.85586300	-0.50425100	-2.11661800
C	-3.05673300	-1.22667200	-1.25166700
C	-1.67481800	-1.59073400	-1.33565600
O	-0.91756300	-1.33600900	-2.26543200
N	-1.27888600	-2.29086500	-0.20618400
C	-2.10351100	-2.64232800	0.84426800
N	-1.57017000	-3.33973900	1.83402800
N	-3.38949100	-2.30484600	0.90617000
C	-3.78808700	-1.60163200	-0.14522600
H	-5.91625900	0.02434600	-2.01079600
H	-0.27361200	-2.56968900	-0.21013600
H	-0.57273000	-3.56458900	1.84821100
H	-2.19216800	-3.72736200	2.52317200
N	-2.54841800	2.38021200	0.75953500
C	-3.28234900	1.99238400	-0.31724800
N	-2.51190600	1.80526100	-1.37099900
C	-1.20465100	2.04274700	-0.96112300
C	0.06779600	1.85261900	-1.60153300
O	0.28605800	1.54283600	-2.77593700
N	1.11166100	2.06546000	-0.71765400
C	0.98383500	2.54222800	0.57025300
N	2.09085100	2.85549100	1.22891400
N	-0.19111800	2.70691400	1.15826200
C	-1.21834300	2.40878500	0.37513500
H	-4.34948400	1.84935100	-0.30128500
H	2.04100000	1.85788300	-1.11596700

H	3.00039600	2.57035300	0.87565100
H	1.98163900	3.24326000	2.15233300
N	5.77071200	0.54098700	-1.25731000
C	4.46233500	1.01503100	-1.00329600
O	4.15248800	1.43002900	0.10592500
N	3.56558100	1.01397600	-2.01957200
C	3.88088400	0.55428800	-3.21367200
N	2.91105200	0.57279600	-4.14798500
C	5.17376100	0.00721700	-3.49587500
C	6.08079700	0.04348900	-2.49192000
H	2.03697000	1.02293000	-3.88172600
H	3.13628200	0.46832900	-5.12307800
H	5.43695600	-0.38344700	-4.46720800
H	7.09692400	-0.30807200	-2.63790900
N	3.33421600	-2.88537300	1.23468800
C	1.95694000	-2.93613700	0.93395800
O	1.14729300	-3.23003000	1.80427300
N	1.55876100	-2.64241300	-0.32611900
C	2.42909900	-2.34601900	-1.27890800
N	1.94073400	-2.03333000	-2.47993500
C	3.84003600	-2.35695800	-1.02636400
C	4.22987700	-2.60475000	0.24227400
H	0.93278500	-1.92242900	-2.56989400
H	2.53928500	-1.72248700	-3.22460100
H	4.55977000	-2.17380100	-1.80965300
H	5.27362300	-2.59579700	0.52468600
Pt	-2.95976700	0.98778400	-3.19439800
N	-3.29607000	-0.07554700	-4.96746300
N	-1.94144000	2.57201300	-4.10455800

H	-2.70634600	-0.90832300	-4.90518000
H	-4.25651400	-0.40649700	-5.02896000
H	-2.18212000	3.46254700	-3.67266300
H	-0.94762500	2.39104700	-3.88556000
H	-3.07782000	0.38671900	-5.84628600
H	-2.04203700	2.69549700	-5.10802700

**Method 1 – G6C rare tautomer**

N	-5.04703000	-1.07019300	-0.36095500
C	-5.04881800	-0.46222500	-1.57477900
N	-3.85115100	-0.52469700	-2.12219900
C	-3.05566300	-1.24952400	-1.25488900
C	-1.68054600	-1.64384700	-1.34426400
O	-0.92030500	-1.43937500	-2.28205900
N	-1.29340500	-2.32793800	-0.19771800
C	-2.11723700	-2.65360300	0.85926200
N	-1.59053000	-3.34363100	1.86140200
N	-3.39731700	-2.30561800	0.91624200
C	-3.78824700	-1.60684000	-0.14327100
H	-5.90361000	0.02923200	-2.01071100
H	-0.29618600	-2.60650100	-0.19362700
H	-0.59988200	-3.57764000	1.88072500
H	-2.21664700	-3.71474300	2.55533100
N	-2.53825200	2.38370000	0.75431700
C	-3.26361800	1.97699500	-0.31952500
N	-2.48592400	1.78049000	-1.36837000
C	-1.17648500	2.03325700	-0.96273600
C	0.11669400	1.85123200	-1.56998800
O	0.28974300	1.50644700	-2.77796600

N	1.17384600	2.07311500	-0.75789700
C	0.99592900	2.55434300	0.50605000
N	2.08600000	2.92081100	1.19462100
N	-0.17313200	2.71874400	1.13451600
C	-1.20315500	2.41503300	0.36937100
H	-4.33036100	1.83213500	-0.30822500
H	2.52643700	1.41105300	-1.43979900
H	2.99987000	2.62978400	0.89273900
H	1.94856800	3.28458800	2.12262200
N	5.72015800	0.55150100	-1.22276300
C	4.41002000	0.88487000	-0.80924600
O	4.11554900	1.10607800	0.33916700
N	3.46620500	0.98275500	-1.80435900
C	3.67766900	0.65426200	-3.08973700
N	2.68043400	0.80931000	-3.93269800
C	4.96783100	0.14518600	-3.44689500
C	5.94161600	0.13542700	-2.50292100
H	1.75303700	1.12752200	-3.56817300
H	2.81889300	0.64030800	-4.91553300
H	5.17560900	-0.17376000	-4.45669100
H	6.94745400	-0.19741500	-2.73636200
N	3.34450400	-2.87863800	1.22418300
C	1.96424100	-2.88862000	0.92391300
O	1.14455500	-3.14092700	1.79296600
N	1.58073400	-2.61267400	-0.34765700
C	2.45879500	-2.39643000	-1.30585000
N	1.98163400	-2.07559100	-2.51946700
C	3.86887800	-2.44449800	-1.05312000
C	4.24838000	-2.65367700	0.22804000

H	0.96806700	-2.04560800	-2.62493400
H	2.56289900	-2.17224600	-3.33354000
H	4.59750100	-2.30676100	-1.83811300
H	5.29248900	-2.65309100	0.51142700
Pt	-2.93996200	0.97681600	-3.18542400
N	-3.29654800	-0.06007800	-4.97833100
N	-1.89174500	2.55543500	-4.05262200
H	-4.26252300	-0.37348300	-5.04146100
H	-3.07338800	0.41334400	-5.84961100
H	-2.13900900	3.44431800	-3.62183000
H	-0.90778300	2.34714800	-3.78214700
H	-2.72120900	-0.90305500	-4.92975900
H	-1.94783300	2.68590200	-5.05803400

**Method 1 – G7C rare tautomer**

N	-5.05179200	-1.06350300	-0.36884800
C	-5.04367700	-0.44515400	-1.57681200
N	-3.83591700	-0.50225200	-2.10941800
C	-3.04462800	-1.23385500	-1.24138400
C	-1.66180000	-1.60535700	-1.27282400
O	-0.90843600	-1.29045800	-2.22678900
N	-1.23889700	-2.31119000	-0.19414500
C	-2.10064700	-2.64085600	0.81221500
N	-1.62305400	-3.34541400	1.84592800
N	-3.39872800	-2.30697200	0.89675600
C	-3.79331100	-1.60269900	-0.14525900
H	-5.89504300	0.04430000	-2.02119800
H	0.39747900	-2.56233000	-0.29466200
H	-0.67727500	-3.69876600	1.83283700

H	-2.29471800	-3.76858800	2.46279400
N	-2.53955800	2.38308800	0.75887700
C	-3.26853500	1.98955800	-0.31939400
N	-2.49487100	1.80440000	-1.37015000
C	-1.18966400	2.04430800	-0.95662300
C	0.08529500	1.85574500	-1.59068900
O	0.32050500	1.54162200	-2.76075300
N	1.12457100	2.07879600	-0.69969900
C	0.98981600	2.55779800	0.58582000
N	2.09570100	2.87681500	1.24934200
N	-0.18538200	2.71738800	1.16728600
C	-1.20986500	2.41314800	0.37873700
H	-4.33448800	1.83730300	-0.30485700
H	2.05494900	1.89315900	-1.09624300
H	3.00820100	2.61052500	0.89661900
H	1.98252200	3.28215900	2.16459900
N	5.77549900	0.53134300	-1.26157500
C	4.46886100	1.01355700	-1.01092200
O	4.15172700	1.41731600	0.09906900
N	3.57852200	1.01944500	-2.03386900
C	3.89550200	0.55713800	-3.22491200
N	2.91383400	0.55886800	-4.15229800
C	5.18602600	0.00454400	-3.50507100
C	6.08962600	0.03660900	-2.49728700
H	2.05745900	1.04634500	-3.88778500
H	3.13906100	0.46624900	-5.12951200
H	5.45039400	-0.38712600	-4.47563300
H	7.10540000	-0.31742900	-2.64018700
N	3.29910300	-2.89668000	1.23723700

C	1.92061600	-3.00562800	1.00121900
O	1.15010500	-3.41016800	1.83398600
N	1.48279000	-2.60435000	-0.23762400
C	2.28166200	-2.19518600	-1.24248900
N	1.71547500	-1.78052200	-2.34893500
C	3.69649000	-2.23552900	-1.01953300
C	4.14053900	-2.54708600	0.21928000
H	0.67011500	-1.65366500	-2.37661300
H	2.27928600	-1.41323500	-3.10058200
H	4.38258800	-1.99193400	-1.81611400
H	5.19449100	-2.53514000	0.45977100
Pt	-2.93540100	0.97183400	-3.18838600
N	-3.26421400	-0.12124600	-4.94129700
N	-1.91595900	2.55587200	-4.11654100
H	-2.68392200	-0.95749100	-4.84480700
H	-4.22748900	-0.44349300	-5.00184700
H	-2.16226000	3.44887000	-3.69339700
H	-0.92250300	2.38395400	-3.89688500
H	-3.03126000	0.31409200	-5.82963600
H	-2.01761200	2.66928000	-5.12092000

**Model A – canonical structure**

N	4.64004100	2.99303700	-5.79003800
C	5.28789400	2.38642900	-4.73716900
N	4.45213700	1.91156300	-3.84458500
C	3.17685700	2.20226700	-4.30545700
C	1.88376900	1.98274700	-3.73198800
O	1.61724500	1.25278000	-2.77096900
C	1.12069500	3.45094000	-5.53596100



N	0.09072200	4.12851100	-6.01884200
N	2.29292600	3.50032300	-6.15777800
C	3.27483600	2.90845900	-5.48980500
N	6.34887500	5.10885100	-0.89142900
C	6.45402900	3.90538200	-1.53147400
N	5.47933600	3.08455000	-1.19921700
C	4.65946900	3.79928000	-0.32379200
C	3.46237900	3.44463900	0.38070200
O	2.96988200	2.31591000	0.49516400
N	2.87361100	4.53792700	0.98661800
C	3.39435300	5.81311100	0.98810500
N	2.66028800	6.75859100	1.56194500
N	4.56955500	6.10484600	0.44979700
C	5.14957000	5.08615500	-0.17741500
N	-1.95961500	5.22215900	2.90801200
C	-2.49418400	3.96778800	2.82945300
C	-1.78310000	2.89616700	2.43682800
C	-0.41674900	3.12512800	2.09137300
N	0.34017600	2.07527100	1.72668600
N	0.11662700	4.33349900	2.10497600
C	-0.60682200	5.43330900	2.52002100
O	-0.10347500	6.54212700	2.55801000
N	-3.08608400	4.78189300	-2.28526400
C	-3.45109400	4.11025700	-1.15630700
C	-2.85221100	2.95253400	-0.80434800
C	-1.75939600	2.51451400	-1.62140800
N	-1.02655600	1.44769900	-1.26989100
N	-1.43205700	3.13419500	-2.74289900
C	-2.12503900	4.22638500	-3.16150700

O	-1.92375400	4.72741700	-4.26249100
Pt	4.84524900	1.24151800	-1.93330200
N	5.13126300	0.56798700	0.02141900
N	3.93200700	-0.50988600	-2.58843600
N	0.90675400	2.69638400	-4.39907400
H	6.35073800	2.24357000	-4.65571400
H	-0.75036200	4.28961300	-5.44922000
H	0.27708800	4.71426400	-6.81786100
H	7.23953700	3.69517800	-2.23842000
H	1.95009600	4.40629200	1.44484500
H	1.73666000	6.59180100	1.97385900
H	3.05319200	7.68477400	1.59622200
H	-3.53255500	3.86305700	3.10639400
H	-2.22689200	1.91307500	2.41154500
H	1.30025300	2.18788300	1.40860800
H	-0.00267900	1.14172700	1.87354300
H	-4.23518600	4.56184800	-0.56030000
H	-3.15773200	2.41317800	0.07661700
H	-0.16407300	1.27094600	-1.77819900
H	-1.14192700	1.05115700	-0.35501600
H	4.32274300	0.94599700	0.53650900
H	5.18062300	-0.43716500	0.16262500
H	2.94030200	-0.23260000	-2.64560300
H	4.24109200	-0.76934700	-3.52313200
H	5.97376100	0.97098800	0.42669700
H	4.01337800	-1.33310600	-1.99837700
H	-0.02239200	2.73106600	-3.92539900

**Model A – G6C rare tautomer**

N	4.63583600	2.99451600	-5.78799900
C	5.27279000	2.39204300	-4.72509300
N	4.42895800	1.90962000	-3.84482300
C	3.15782500	2.19538800	-4.32115800
C	1.85393200	1.96357800	-3.76690800
O	1.55561900	1.21479500	-2.83627000
C	1.11963700	3.45749500	-5.57238900
N	0.09070200	4.13339500	-6.07595600
N	2.29337300	3.50257800	-6.18028100
C	3.26928700	2.90444800	-5.50145300
N	6.34633000	5.11177600	-0.88729900
C	6.40383600	3.91431200	-1.54133900
N	5.40769200	3.12015500	-1.19899400
C	4.61623300	3.84479300	-0.29944700
C	3.40411400	3.56631700	0.42448800
O	2.89249400	2.40564600	0.49864100
N	2.82847500	4.61350200	1.05159600
C	3.42332200	5.83313900	1.02553000
N	2.75289400	6.85828900	1.58743500
N	4.60598900	6.12967700	0.48078900
C	5.15361500	5.11098900	-0.15711100
N	-1.93321600	5.24162500	2.91619300
C	-2.45440100	3.99051000	2.70988200
C	-1.74551700	2.96169600	2.20709300
C	-0.37357000	3.18406300	1.87505600
N	0.39197400	2.26454700	1.34665000
N	0.13618100	4.40532200	2.14688500
C	-0.57225400	5.49522500	2.65703500

O	-0.03183100	6.55437100	2.83761800
N	-3.10393800	4.77805800	-2.25682800
C	-3.63623400	4.05520700	-1.23086500
C	-3.13903700	2.84597700	-0.88480600
C	-1.98479200	2.39858200	-1.60182300
N	-1.34833800	1.24808700	-1.22685900
N	-1.46106500	3.08518100	-2.59068400
C	-2.03939600	4.24589200	-3.02162000
O	-1.66073800	4.80089900	-4.04176300
Pt	4.78517200	1.28111200	-1.90161900
N	5.00035600	0.68782600	0.07798100
N	3.90870900	-0.50663300	-2.53627800
N	0.89128100	2.70472200	-4.43872500
H	6.33585300	2.26367000	-4.62472100
H	-0.71069800	4.34256600	-5.48063900
H	0.29727600	4.73262900	-6.85960800
H	7.17553500	3.68118700	-2.25582800
H	1.12909000	4.57868300	1.85301000
H	1.94882200	6.70528900	2.17986500
H	3.24425900	7.73208300	1.66217000
H	-3.49148100	3.85652400	2.98275800
H	-2.18810700	1.98638600	2.08293300
H	1.40662000	2.40783700	1.05606800
H	-0.05913500	1.42178800	1.02107900
H	-4.46782500	4.51067000	-0.70583000
H	-3.58015600	2.27028700	-0.08728200
H	-0.59281900	0.98278100	-1.85415700
H	-1.93927400	0.49416700	-0.90844500
H	4.18615800	1.14541800	0.53313200

H	4.99204700	-0.30803900	0.27694700
H	2.91613600	-0.24905900	-2.63181300
H	4.25093000	-0.78905000	-3.45217800
H	5.84824800	1.07477300	0.48665800
H	3.98619400	-1.30954600	-1.91887800
H	-0.03379500	2.72337800	-3.98253600

**Model A – G7C rare tautomer**

N	4.64603900	2.99161900	-5.79356400
C	5.27455700	2.41318300	-4.71444700
N	4.41936300	1.94742200	-3.83400400
C	3.14889600	2.21629700	-4.32659700
C	1.83256100	2.03953800	-3.79239900
O	1.60070800	1.29535800	-2.79126200
C	1.12639900	3.42240900	-5.56194600
N	0.12845100	4.12149400	-6.11561800
N	2.30229800	3.47661000	-6.20058900
C	3.27497200	2.90032500	-5.51983500
N	6.34950000	5.10800600	-0.89036600
C	6.44915600	3.90184600	-1.52890000
N	5.47751900	3.08175800	-1.18855000
C	4.66398600	3.79887300	-0.30927400
C	3.46696400	3.45220800	0.39927200
O	2.95804500	2.33200800	0.52428800
N	2.88687500	4.55367900	1.00343900
C	3.41053900	5.82662000	0.99735600
N	2.67980300	6.77925100	1.56871800
N	4.58129900	6.11128100	0.45412700
C	5.15660000	5.08595400	-0.17020900

N	-1.96695700	5.21641700	2.90915400
C	-2.50082100	3.96083700	2.86456600
C	-1.79284900	2.88129200	2.48724200
C	-0.43994700	3.10962400	2.09762000
N	0.28935300	2.04947800	1.66600200
N	0.09680600	4.31098900	2.09126700
C	-0.61554300	5.41997900	2.51476600
O	-0.10606700	6.52318000	2.54798300
N	-3.06311400	4.78541900	-2.31495200
C	-3.23274500	4.16463800	-1.11126300
C	-2.50802700	3.08369900	-0.75321300
C	-1.47020200	2.63802800	-1.63149500
N	-0.59388300	1.71590500	-1.31215100
N	-1.38930100	3.21110100	-2.84702300
C	-2.17791100	4.26010900	-3.27372600
O	-2.08089700	4.69840200	-4.39443000
Pt	4.79840300	1.25287400	-1.94507600
N	5.09044500	0.53294800	0.00138400
N	3.82330400	-0.44633100	-2.62895600
N	0.85284400	2.71884900	-4.42508000
H	6.33554200	2.27527600	-4.60585400
H	-0.75667100	4.24218300	-5.64337400
H	0.35016700	4.67564000	-6.92561400
H	7.22879500	3.69081900	-2.24211100
H	1.96778800	4.41967100	1.45944800
H	1.76222100	6.61311100	1.98721400
H	3.07751300	7.70320300	1.60166500
H	-3.53725900	3.85988400	3.14928300
H	-2.23698500	1.89779700	2.47857200

H	1.27159700	2.17559200	1.41732100
H	0.01656700	1.13188500	1.98185600
H	-3.98382500	4.58941000	-0.45666400
H	-2.67222300	2.59470400	0.19046700
H	0.22645300	1.50753300	-1.93871700
H	-0.54358000	1.43745000	-0.34286400
H	4.29903700	0.91440600	0.53638300
H	5.11915100	-0.47602200	0.11779500
H	2.84732300	-0.10032500	-2.70891300
H	4.14214300	-0.71444100	-3.55770700
H	5.94719000	0.90686900	0.40401000
H	3.84377700	-1.27524900	-2.04233200
H	-0.60282400	2.93582400	-3.51855100

**Model B – canonical structure**

N	4.64597600	2.98820900	-5.78883400
C	5.29467500	2.38821500	-4.73068600
N	4.45698100	1.91014900	-3.84343300
C	3.18058300	2.18068600	-4.31290300
C	1.88737300	1.97227100	-3.73511400
O	1.61514400	1.25796400	-2.76474300
C	1.12524900	3.41515400	-5.57259000
N	0.08729000	4.05878500	-6.06350800
N	2.30704900	3.47084900	-6.18076600
C	3.27989900	2.88609800	-5.49974600
N	6.35071600	5.10599200	-0.88929100
C	6.44526100	3.90721800	-1.54248100
N	5.46689700	3.09171200	-1.21309200
C	4.65684100	3.79751400	-0.32101300

C	3.44039000	3.45767600	0.35549500
O	2.91349800	2.34058100	0.42762200
N	2.87311900	4.55121200	0.97672500
C	3.41736200	5.82193300	1.01459800
N	2.70457000	6.76404800	1.60523500
N	4.59817600	6.09919300	0.47110800
C	5.15799200	5.08017900	-0.16247200
N	-1.96284200	5.21661100	2.90978800
C	-2.51898100	3.96553200	2.81772700
C	-1.82714900	2.89437400	2.40284000
C	-0.45566500	3.10669500	2.05569300
N	0.27109600	2.05756000	1.67604700
N	0.09851700	4.31504100	2.10997400
C	-0.61309900	5.39880200	2.53348900
O	-0.10068600	6.51671300	2.58292600
N	-3.08331800	4.78025200	-2.27461400
C	-3.50342200	4.08391200	-1.17203700
C	-2.93966800	2.90687900	-0.82777500
C	-1.83240000	2.45325900	-1.62430700
N	-1.14592200	1.36401100	-1.29006900
N	-1.44344000	3.11717700	-2.70889100
C	-2.07192200	4.24474700	-3.09471800
O	-1.76882500	4.81454000	-4.14763000
Pt	4.82744300	1.24688000	-1.92590000
N	5.07603200	0.59512500	0.04184900
N	3.89995000	-0.50316700	-2.56700300
N	0.91905200	2.68476600	-4.41185000
H	6.35780100	2.24579100	-4.63877500
H	-0.76710900	4.12304500	-5.51469200



H	0.12366400	4.56819000	-6.94711000
H	7.22875900	3.68827400	-2.25000000
H	1.95876800	4.41247600	1.44571200
H	1.79698000	6.56426100	2.02731200
H	3.11208100	7.69058700	1.75476600
H	-3.55468300	3.86351200	3.10895200
H	-2.27157700	1.91234000	2.37741200
H	1.22111600	2.16369100	1.32886100
H	-0.18960300	1.15887300	1.60603300
H	-4.29977700	4.53082600	-0.58628600
H	-3.28014700	2.36100700	0.03815600
H	-0.31528000	1.14594800	-1.83142000
H	-1.39504100	0.80301600	-0.48268300
H	4.24554700	0.96042700	0.53239200
H	5.13968600	-0.40759400	0.19643400
H	2.90850200	-0.21961900	-2.61855600
H	4.19659300	-0.77666300	-3.50166600
H	5.89551600	1.01608100	0.47530000
H	3.97830800	-1.32234800	-1.97046900
H	-0.01317800	2.69933200	-3.95542400
O	-0.90679900	5.71375500	-8.09218900
H	-1.32228400	6.29649600	-7.43391100
H	-1.62697600	5.42035100	-8.65729200
H	-1.56563700	6.37149700	-5.15271000
O	-1.61438500	7.11052100	-5.77525100
H	-0.88545300	7.69775300	-5.56294400
O	-4.32756800	0.21481000	1.94951600
H	-4.91186000	-0.53535700	2.08835200
H	-4.86860900	0.89471800	1.51068200

O	-5.92916900	2.29180500	0.90708900
H	-6.51062400	2.18825100	0.14880200
H	-6.50449700	2.57928800	1.62537900
O	-1.73016400	-0.17368300	1.16580600
H	-1.49404400	-1.10221100	1.23425300
H	-2.66914300	-0.10546200	1.43336100
H	-0.60327700	8.36851700	2.47195100
O	-0.89908000	9.07060500	3.06708000
H	-0.66934300	9.90468700	2.64966100
H	0.58797600	8.49724500	4.18813300
O	1.50971500	8.39065600	4.46935200
H	1.67178500	7.44403600	4.53069900
O	3.17003200	9.37057400	2.55904300
H	2.63975800	9.15839800	3.35315700
H	3.74334700	10.10360100	2.78960300

**Model B – G6C rare tautomer**

N	4.64583900	2.98791700	-5.78877400
C	5.28912200	2.38917100	-4.72537700
N	4.44824000	1.90263700	-3.84718500
C	3.17408000	2.16818600	-4.32633700
C	1.87631300	1.95220500	-3.76013100
O	1.58710300	1.23149400	-2.80001000
C	1.12786800	3.41050700	-5.59403800
N	0.09139500	4.06050100	-6.08470400
N	2.31027800	3.46897100	-6.19475300
C	3.27983600	2.87965100	-5.50894600
N	6.33964600	5.10727200	-0.88631100
C	6.40020500	3.91054600	-1.54574600

N	5.40434800	3.11435500	-1.21095200
C	4.60550800	3.82436300	-0.30485200
C	3.36958500	3.54480300	0.39003300
O	2.83882300	2.39019500	0.44235900
N	2.79260300	4.59289400	1.01059300
C	3.39881600	5.81444000	1.00979500
N	2.72620200	6.82616000	1.56852600
N	4.59336600	6.10897100	0.47854800
C	5.14240000	5.09395100	-0.15494900
N	-1.94576700	5.22518000	2.90898000
C	-2.47057000	3.95753600	2.78778000
C	-1.76881900	2.90098800	2.34327000
C	-0.40657200	3.10302300	1.95415000
N	0.35164600	2.14057200	1.50351300
N	0.08649000	4.36062800	2.07070700
C	-0.61269000	5.45338500	2.56075400
O	-0.07593300	6.53386500	2.66039900
N	-3.08322300	4.78003200	-2.27487800
C	-3.52983500	4.06506100	-1.19740100
C	-2.97458100	2.88040700	-0.85952600
C	-1.85354300	2.43544100	-1.64453500
N	-1.16645700	1.34333600	-1.31206400
N	-1.44476000	3.11365800	-2.70873300
C	-2.06274000	4.24847900	-3.09204700
O	-1.74430300	4.82910200	-4.13063500
Pt	4.78755700	1.27336600	-1.90439600
N	4.96804200	0.69599400	0.08399900
N	3.90031400	-0.51089000	-2.53641300
N	0.91419300	2.67145500	-4.44191600

H	6.35252900	2.25847500	-4.62132000
H	-0.76560300	4.11610400	-5.54330700
H	0.12840200	4.57256400	-6.96589400
H	7.17591300	3.67141300	-2.25488700
H	1.08543000	4.52420800	1.75550500
H	1.89901600	6.63837900	2.11301300
H	3.18995600	7.71826800	1.72218600
H	-3.50437900	3.83822800	3.07985900
H	-2.20634500	1.91683500	2.29536200
H	1.33461800	2.28768800	1.13879600
H	-0.08603700	1.22822300	1.41168000
H	-4.34355800	4.50092400	-0.62718800
H	-3.34907200	2.31186700	-0.02267900
H	-0.34769600	1.11788500	-1.87102400
H	-1.45595400	0.74025100	-0.55132400
H	4.13389200	1.14604700	0.51363200
H	4.96687600	-0.29805000	0.29331800
H	2.90611900	-0.24960200	-2.61175000
H	4.22056600	-0.79221400	-3.46057300
H	5.79644900	1.09700500	0.51830000
H	3.98568900	-1.31840600	-1.92575600
H	-0.01933500	2.67899700	-3.99701100
O	-0.90679900	5.71375400	-8.09219200
H	-1.32228400	6.29649600	-7.43391100
H	-1.62697600	5.42035200	-8.65729200
H	-1.56566600	6.37151800	-5.15268100
O	-1.61436100	7.11050600	-5.77527000
H	-0.88545300	7.69775300	-5.56294400
O	-4.32756400	0.21480600	1.94953300

H	-4.91186000	-0.53535700	2.08835200
H	-4.86860900	0.89471800	1.51068200
O	-5.92916900	2.29180500	0.90708900
H	-6.51062400	2.18825100	0.14880200
H	-6.50449700	2.57928800	1.62537900
O	-1.73013000	-0.17369000	1.16582100
H	-1.49406400	-1.10221500	1.23426500
H	-2.66915500	-0.10545000	1.43331600
H	-0.60329000	8.36851200	2.47195100
O	-0.89907200	9.07061000	3.06707800
H	-0.66934200	9.90468700	2.64966200
H	0.58797500	8.49724400	4.18813400
O	1.50973700	8.39063800	4.46936200
H	1.67178500	7.44403600	4.53069900
O	3.17007700	9.37053900	2.55906400
H	2.63969400	9.15845000	3.35312800
H	3.74334800	10.10360100	2.78960200

**Model B – G7C rare tautomer**

N	4.63965900	2.99201900	-5.78056100
C	5.27270600	2.41691800	-4.69846100
N	4.42078500	1.95940400	-3.81094600
C	3.14271900	2.21827700	-4.29172300
C	1.82351200	2.05756200	-3.73567700
O	1.57758700	1.34274700	-2.71864000
C	1.11576600	3.40768800	-5.54079800
N	0.11450200	4.07888800	-6.10043700
N	2.29781800	3.46831500	-6.17469400
C	3.26720600	2.89835500	-5.49211600

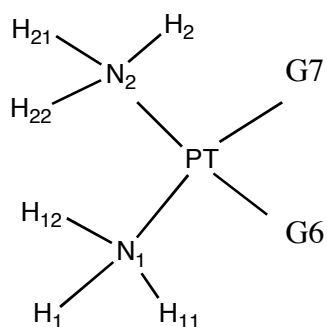
N	6.35243800	5.10600500	-0.88677400
C	6.44817400	3.90213000	-1.53152300
N	5.47895000	3.08362600	-1.18637400
C	4.67287000	3.79212300	-0.29298000
C	3.46334400	3.45470200	0.39683600
O	2.93347400	2.34093900	0.49356400
N	2.89642700	4.55613800	1.00743100
C	3.43208900	5.82959500	1.02406500
N	2.71260300	6.77690400	1.60243800
N	4.60630100	6.10536300	0.47309700
C	5.16776900	5.07924100	-0.15145500
N	-1.96471900	5.21583700	2.90958800
C	-2.51494600	3.96194600	2.83426200
C	-1.81966100	2.88857100	2.42821400
C	-0.44951500	3.10447400	2.07327700
N	0.28002900	2.05656100	1.69174600
N	0.09686200	4.31522200	2.10824200
C	-0.61542300	5.40042800	2.52803400
O	-0.10876900	6.51907400	2.56806300
N	-3.06024400	4.78143700	-2.29170600
C	-3.39060200	4.07601800	-1.16271700
C	-2.76624100	2.92381500	-0.82941600
C	-1.65393900	2.48605500	-1.62521800
N	-0.89612800	1.46231800	-1.31824400
N	-1.36585800	3.19643200	-2.73871100
C	-2.08932100	4.28243900	-3.16453700
O	-1.87368200	4.78493000	-4.24579200
Pt	4.78800200	1.25984600	-1.92348600
N	5.05567600	0.54954900	0.03121500

N	3.77394600	-0.42319200	-2.59375100
N	0.84747100	2.73281900	-4.37887700
H	6.33381000	2.26902900	-4.59262200
H	-0.79531700	4.05750200	-5.67463800
H	0.20697200	4.54613700	-6.99570500
H	7.22376300	3.68418400	-2.24798400
H	1.98730600	4.41742300	1.47922700
H	1.81258000	6.57339100	2.03439200
H	3.11859900	7.70409200	1.74937300
H	-3.54865400	3.85862300	3.13242000
H	-2.25776900	1.90289400	2.42316300
H	1.24468700	2.15925000	1.37974300
H	-0.15512700	1.14292000	1.69603700
H	-4.17705100	4.49393200	-0.54389400
H	-3.04773600	2.37868500	0.05751600
H	-0.02737500	1.29156500	-1.85996900
H	-1.12471200	0.90024100	-0.50015600
H	4.24910600	0.92435500	0.55051200
H	5.09169800	-0.45848700	0.15560300
H	2.80123500	-0.05784000	-2.64248500
H	4.05693800	-0.69532200	-3.53281200
H	5.89758400	0.93236000	0.45616100
H	3.79601900	-1.25495600	-2.01084000
H	-0.55466400	2.91927900	-3.40550900
O	-0.90681200	5.71374500	-8.09219600
H	-1.32227100	6.29650400	-7.43391000
H	-1.62697500	5.42035400	-8.65729400
H	-1.56569100	6.37153900	-5.15265800
O	-1.61434600	7.11049100	-5.77528400

H	-0.88545100	7.69775100	-5.56294600
O	-4.32755800	0.21480300	1.94951500
H	-4.91186600	-0.53535100	2.08835900
H	-4.86861500	0.89471400	1.51068400
O	-5.92916800	2.29180600	0.90708900
H	-6.51062400	2.18825100	0.14880200
H	-6.50449700	2.57928800	1.62537900
O	-1.73009500	-0.17372100	1.16579200
H	-1.49409100	-1.10222100	1.23427800
H	-2.66914600	-0.10542500	1.43334000
H	-0.60327700	8.36852100	2.47195000
O	-0.89908000	9.07060400	3.06708100
H	-0.66934400	9.90468700	2.64966100
H	0.58797600	8.49724500	4.18813300
O	1.50969600	8.39067200	4.46934400
H	1.67178500	7.44403600	4.53069900
O	3.16999100	9.37060400	2.55902100
H	2.63981300	9.15835500	3.35318200
H	3.74334800	10.10359900	2.78960600



Table S1: Partial Charges on cisplatin and bound guanines.



Atom Name	Cisplatin Charges	Atom Name	G6 charges	G7 charges
PT	0.870	N1	-0.279	-0.253
N1	-0.381	H1	0.318	0.322
H1	0.281	C2	0.306	0.391
H11	-0.011	N2	-0.434	-0.428
H12	0.274	H21	0.274	0.272
N2	-0.432	H22	0.349	0.353
H2	0.154	N3	-0.115	-0.114
H21	-0.014	C4	-0.156	-0.163
H22	0.180	C5	0.156	0.269
		C6	-0.125	-0.165
		O6	-0.323	0.293
		N7	-0.106	-0.002
		C8	-0.016	-0.245
		H8	0.000	-0.327
		N9	-0.018	-0.036
		H9	-0.167	-0.166