Supporting Information

Effect of the Diamine Nonleaving Group in Platinum–Acridinylthiourea Conjugates on DNA Damage and Cytotoxicity

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Table S1. Analytical Data for Target Compounds

Compd	Formula	Calculated (%)			Obtained (%)		
		C	H	N	C	H	N
2	$C_{24}H_{35}ClN_8O_6PtS \cdot H_2O$	35.49	4.59	13.80	35.33	4.65	13.61
3	$C_{21}H_{31}ClN_8O_6PtS$	33.45	4.14	14.86	33.24	3.93	14.61
4	$C_{24}H_{37}ClN_8O_6PtS$	36.20	4.68	14.07	35.81	4.51	13.76
5	$C_{28}H_{29}ClN_8O_6PtS \cdot H_2O$	39.37	3.66	13.12	39.43	3.57	12.61

Table S2. Summary of Crystallographic Data for **2**, **3**, **4**, and **5**

	2	**3**	**4**	**5**
Empirical formula	$C_{24}H_{39.5}ClN_8O_{8.25}PtS$	$C_{21}H_{33}ClN_8O_7PtS$	$C_{24}H_{37}ClN_8O_6PtS$	$C_{28}H_{37}ClN_8O_{10}PtS$
Formula weight	834.74	772.15	796.22	908.26
T/K	193(2)	193(2)	193(2)	193(2)
Crystal system	Monoclinic	Triclinic	Triclinic	Triclinic
Space group	$P2_1$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$
a, Å	10.509(4)	10.646(2)	7.266(1)	14.475(1)
b, Å	31.892(12)	10.981(2)	11.803(1)	18.792(2)
c, Å	10.564(4)	13.126(2)	17.193(2)	19.543(2)
α, °		90.642(2)	95.598(2)	103.440(1)
β, °	117.630(6)	99.622(2)	92.629(2)	98.838(1)
γ, °		113.788(2)	94.082(2)	95.471(1)
V, Å^3	3137(2)	1379.1(3)	1461.7(3)	5061.2(8)
Z	4	2	2	6
μ, mm^{-1}	4.684	5.316	5.016	4.367
Reflections collected	25651	14408	15111	53452
Independ. reflections	12598	7741	8164	28875
R_{int}	0.0672	0.0269	0.0226	0.0386
R_1 [$I > 2\sigma(I)$]	0.0689	0.0344	0.0357	0.0479
wR_2 [$I > 2\sigma(I)$]	0.1168	0.0826	0.0846	0.1125
R_1 (all data)	0.0917	0.0383	0.0403	0.0786
wR_2 (all data)	0.1251	0.0849	0.0868	0.1266

Table S3. Selected Bond Distances (Å) and Bond Angles (°) for **2**, **3**, **4**, and **5**

Compounds	**2**[a]	**3**	**4**	**5**[b]
Pt1-N5	2.011(11)	2.057(3)	2.095(3)	2.010(4)
Pt1-N6	2.034(12)	2.042(3)	2.082(3)	2.035(4)
Pt1-Cl1	2.304(4)	2.301(1)	2.302(1)	2.290(1)
Pt1-S1	2.309(4)	2.294(1)	2.311(1)	2.297(1)
N(6)-Pt(1)-N(5)	82.6(5)	93.5(1)	84.4(1)	80.4(2)
N(6)-Pt(1)-Cl(1)	92.0(3)	178.1(1)	176.5(1)	94.0(1)
N(6)-Pt(1)-S(1)	172.5(3)	87.9(1)	93.8 (1)	173.0(1)
N(5)-Pt(1)-Cl(1)	174.5(4)	86.5(1)	92.1(1)	174.1(1)
N(5)-Pt(1)-S(1)	90.8(4)	178.5(1)	177.4(1)	93.5(1)
Cl(1)-Pt(1)-S(1)	94.5(1)	92.1(1)	89.7(1)	92.2 (1)

[a] Parameters are given for one of the two independent molecules in the asymmetric unit. [b] Parameters are given for one of the three independent molecules in the asymmetric unit.

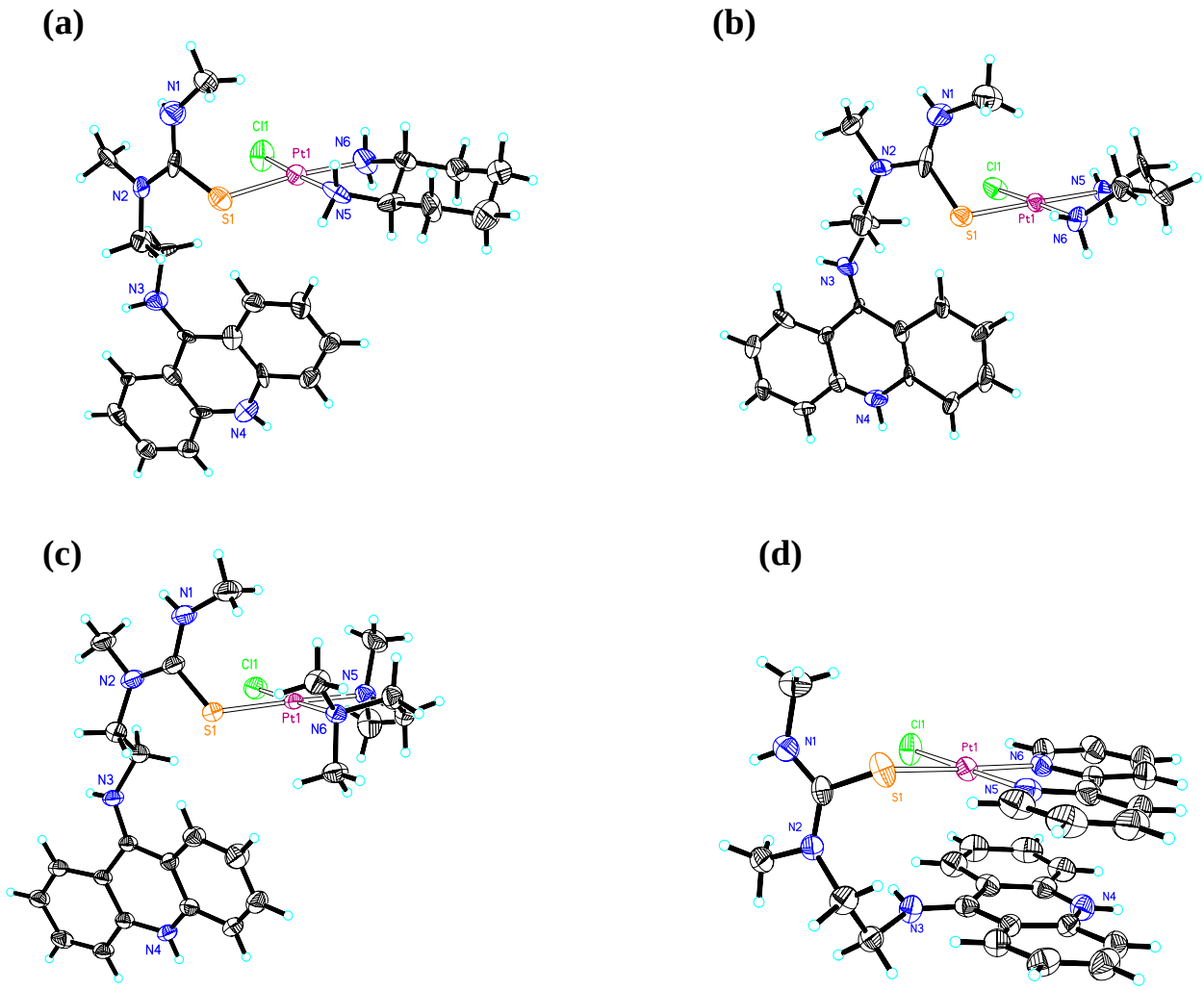

Figure S1. Thermal ellipsoid drawings for the molecular structures of (a) **2**, (b) **3**, (c) **4**, and (d) **5**. Counter ions have been omitted for clarity. Ellipsoids are drawn at the 50% probability level.

Experimental Details

Product Characterization. ^{1}H NMR spectra for the target compounds were recorded on a Bruker Avance 300 instrument operating at 300 MHz. Chemical shifts (δ) are given in parts per million (ppm) relative to the internal standard 3-(trimethylsilyl)-1-propane-sulfonic acid sodium salt (DSS), and coupling constants (J) are in Hz. Elemental analyses were performed by Quantitative Technologies Inc., Madison, NJ. All reagents were used without further purification. Organic solvents were dried and distilled under argon prior to use. Mass spectra of compounds **2**–**5** were recorded in positive-ion mode on an Agilent Technologies 1100LS/MSD Trap instrument. Single crystals of **2**–**5** suitable for X-ray diffraction were grown from saturated aqueous solutions. The X-ray intensity data were measured on a Bruker SMART APEX CCD area detector system. The structures were solved and refined using the Bruker SHELXTL software package (version 6.12). Crystallographic data and additional details of the structure determinations have been deposited in CIF format.

Generation of the Restriction Fragment. The 221-bp restriction fragment (*Nde*I/*Hpa*I) was generated from the 2464-bp plasmid pSP73. Plasmid DNA was isolated using a plasmid purification Mega Kit (Qiagen, Valencia, CA). The fragment was generated by performing PCR with 25-bp primer sequences complementary to the 3′ ends of both the strands, 5′-TATGGACATATTGTCGTTAGAACGC-3′ (P1) and 5′-AACCTGGCTTATCGAAATTAATACG-3′ (P2) (Integrated DNA Technologies, Coralville, IA). PCR products were purified using a PCR purification kit (Qiagen, Valencia, CA) and eluted with 10 mM Tris-HCl (pH 8) buffer. The quality of the PCR products was checked by running 1.5% agarose gels in the presence of a 100-kb DNA ladder (New England Biolabs, Ipswich, MA). DNA concentrations were determined spectrophotometrically.