Electronic Supplementary Information for Dalton Transactions

Supporting Information to the Dalton Transactions paper:

Quinoxaline-2-carboxamide as a carrier ligand in two new platinum(II) compounds: Synthesis, crystal structure, cytotoxic activity and DNA studies.

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List of contents:

X-ray Crystallographic Analysis and Data collection. The molecular structure of complexes **1** and **2** were determined by single-crystal X-ray diffraction methods. Single crystals of *cis*-[Pt(qnxca)(MeCN)Cl_2] (**1**) were obtained by slow evaporation of its acetonitrile solution, while a single crystal of [Pt(qnxca$_{-H}$)(dmso)Cl] (**2**) was obtained by slow diffusion of dimethylsulfoxide into the aqueous solution of the alkaline reaction mixture. Crystal data, data collection parameters, and structure refinement details are given in Table S1. Cif files are available as supporting information.

X-ray intensities were collected on a Nonius KappaCCD diffractometer with sealed tube (Mo-Kα, graphite monochromator, λ = 0.71073 Å, compound **1**) or on a Nonius KappaCCD diffractometer with rotating anode (Mo-Kα, graphite monochromator, λ = 0.71073 Å, compound **2**). A suitable crystal was greased to the end of a glass thread (compound **1**) or oil mounted on top of a Lindemann capillary (compound **2**). The data were integrated using DENZO[1] (compound **1**) or EvalCCD[2] (compound **2**). The structures were solved by direct methods implemented in SHELXS-97[3] (compound **1**) or automated Patterson methods with DIRDIF-99[4] (compound **2**) and refined by a full-matrix least-squares procedure based on F^2 with SHELXL-97[3]. All non-hydrogen atoms were refined anisotropically. The *C*-bound H atoms were positioned geometrically (C – H = 0.96 Å and 0.93 Å for methyl and aromatic carbon atom respectively) and refined as ridding, with U_{iso} (H) = 1.2 or 1.5 times U_{eq}(C). The *N*-bound hydrogen atoms were located in a difference map and refined using distance restraints (DFIX) with N – H = 0.86 Å and with U_{iso}(H) = 1.2 U_{eq}(N) (compound **1**) or refined freely with isotropic displacement parameters (compound **2**).

Table S1. Crystal data and structure refinement details for **1** and **2**.

	1	**2**
Chemical formula	$C_{11}H_{10}N_4OPtCl_2$	$C_{11}H_{12}ClN_3O_2PtS$
Formula weight [g/mol]	480.21	480.84
T [K]	293(2)	150(2)
Crystal system	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/c$
a [Å]	8.2756(2)	10.3211(3)
b [Å]	8.8185(2)	18.9564(7)
c [Å]	19.8387(5)	7.0183(2)
β [deg]	99.4107(8)	105.028(1)
V [Å^3]	1428.31(6)	1326.17(7)
Z	4	4
D_{calc} [g/cm^3]	2.233	2.408
μ [mm^{-1}]	10.194	10.939
Crystal size [mm^3]	0.13 x 0.25 x 0.38	0.03 x 0.04 x 0.36
Crystal colour	yellow	red
abs.corr. method	multi-scan	analytical
abs.corr. range	0.11-0.35	0.13-0.60
$\sin(\theta/\lambda)_{max}$ [Å^{-1}]	0.65	0.61
Refl. (measured/unique)	6124/3255	20861/2484
R_{int}	0.029	0.066
Parameters/restraints	180/2	178/0
R1/wR2 ($I/\sigma(I) > 2$)	0.0337/0.0786	0.0323/0.0774
R1/wR2 (all data)	0.0481/0.0849	0.0431/0.0824
S	1.01	1.10
Residual density [e/Å^3]	-1.43, 1.25	-1.47, 2.18

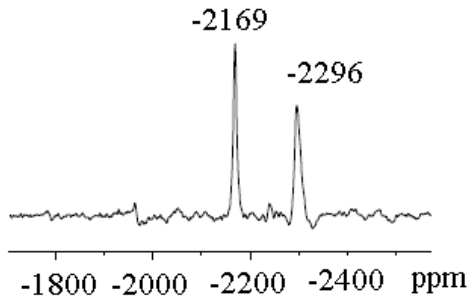

Figure S1. ^{195}Pt NMR spectrum (300 MHz) of **1** in DMF-d_7 at 37 °C reacted with 1 equiv. 9-EtG in D_2O 24 h after mixing.

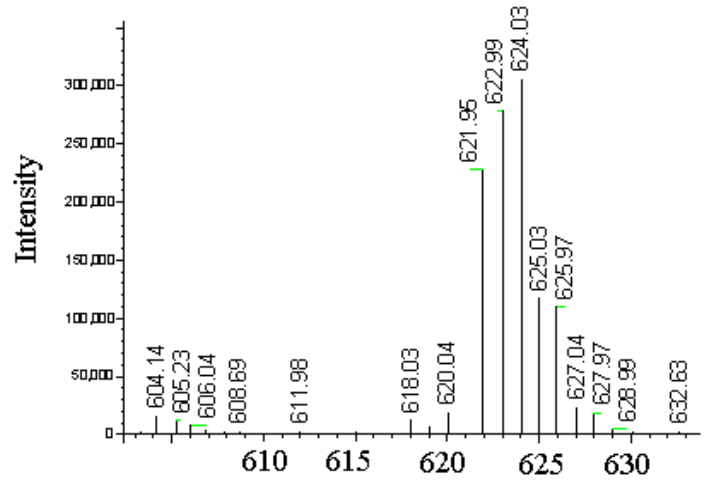

Figure S2. ESI-MS spectrum of **1** in DMF 24 h after mixing with 1 equiv. of 9EtG in H_2O. Peak at m/z = 624 corresponding to $[Pt(qnxca)(9EtG)(MeCN)Cl]^+$ species.

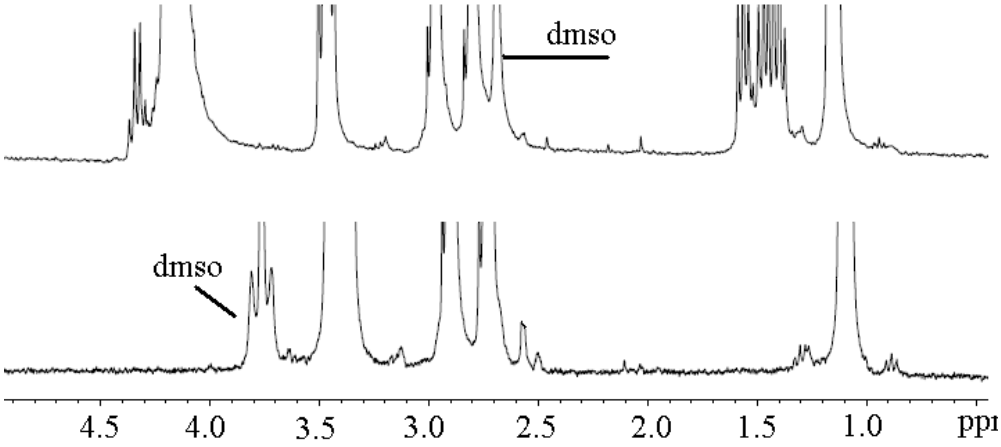

Figure S3. ^{1}H NMR spectrum (300 MHz) of **2** in DMF-d_7 at 37 °C reacted with 1 equiv. 9-EtG in D_2O fresh (bottom spectrum) and 24 h after mixing (top spectrum).

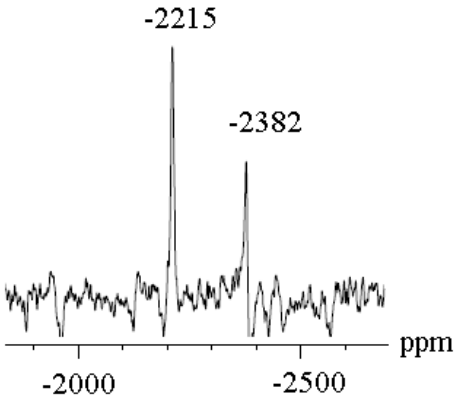

Figure S4. ^{195}Pt NMR spectrum (300 MHz) of **2** in DMF-d_7 at 37 °C reacted with 1 equiv. 9-EtG in D_2O 24 h after mixing.

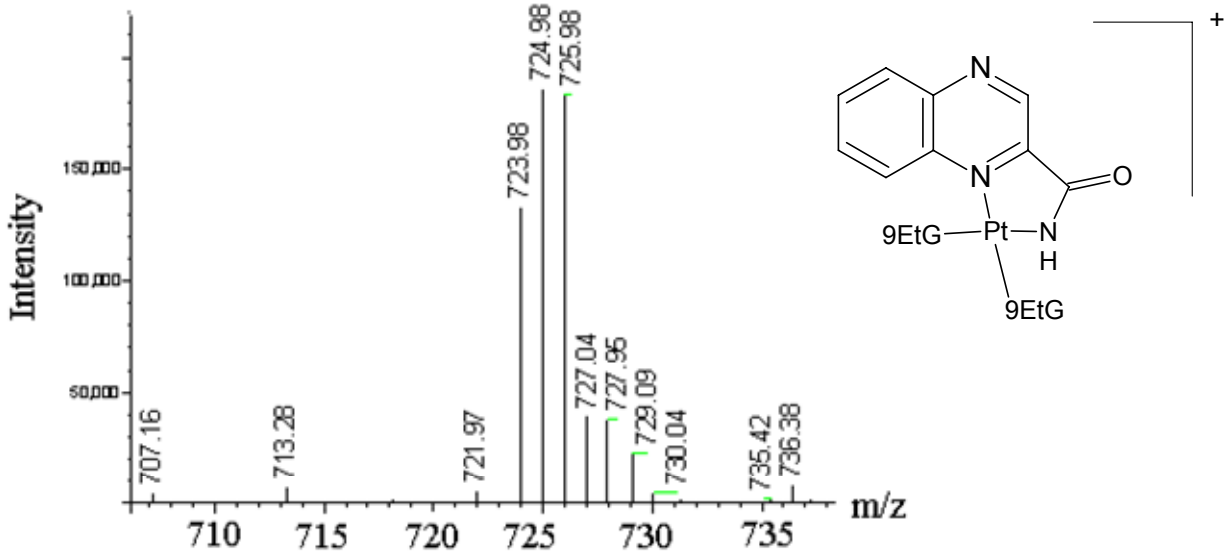

Figure S5. ESI-MS spectrum of **2** in DMF 24 h after mixing with 1 equiv. of 9EtG in H_2O. Peak at m/z = 724 corresponding to $[Pt(qnxca_{-H})(9EtG)_2]^+$ species.

References

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