Supporting Information

A New Class of Antitumor *trans*-amine-amidine-Pt(II) Cationic Complexes: Influence of Chemical Structure and Solvent on *in vitro* and *in vivo* Tumor Cell Proliferation

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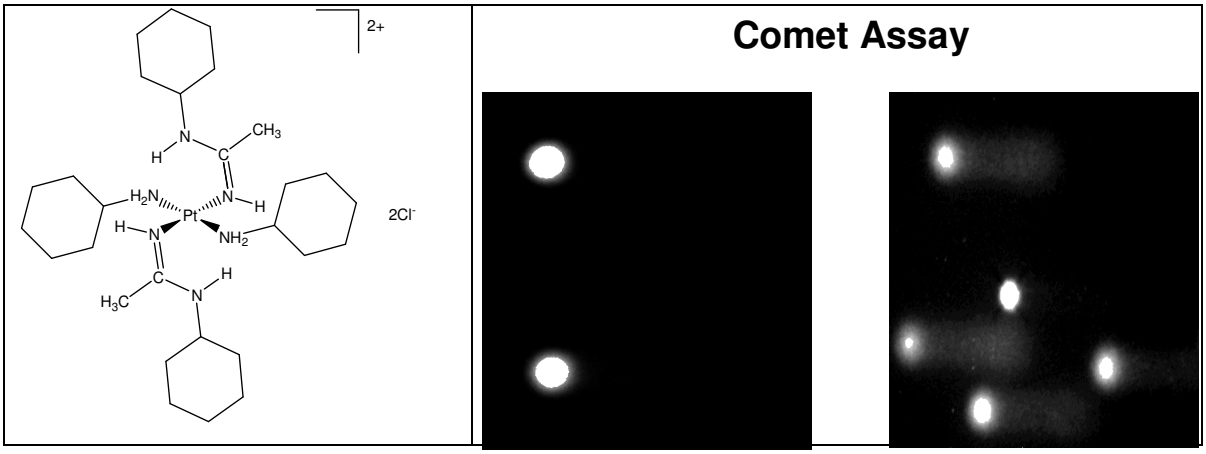
Table of Contents Graphic

A New Class of Antitumor *trans*-Amine-Amidine-Pt(II) Cationic Complexes: Influence of Chemical Structure and Solvent on *in vitro* and *in vivo* Tumor Cell Proliferation



Content :

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S1

Elemental analyses

Compound **1** :

trans-[Pt($NH_2\overbrace{CHCH_2CH_2}$)$_2${N(H)=C($CH_3$)N(H)$\overbrace{CHCH_2CH_2}$}$_2$]$^{2+}$[$Cl^-$]$_2$

Anal. Calc. for $C_{16}H_{38}N_6Cl_2O_2Pt$ (MW 612.51) : C, 31.38; H, 6.25; N, 13.72. Found: C, 31.40; H, 6.27; N, 13.74.

Compound **2**

trans-[Pt($NH_2\overbrace{CH(CH_2)_3CH_2}$)$_2${N(H)=C($CH_3$)N(H)$\overbrace{CH(CH_2)_3CH_2}$}$_2$]$^{2+}$[$Cl^-$]$_2$

Anal.Calc. for $C_{24}H_{54}N_6Cl_2O_2Pt$ (MW 724.71) : C, 39.79; H, 7.51; N, 11.60. Found: C, 39.82; H, 7.50; N, 11.62.

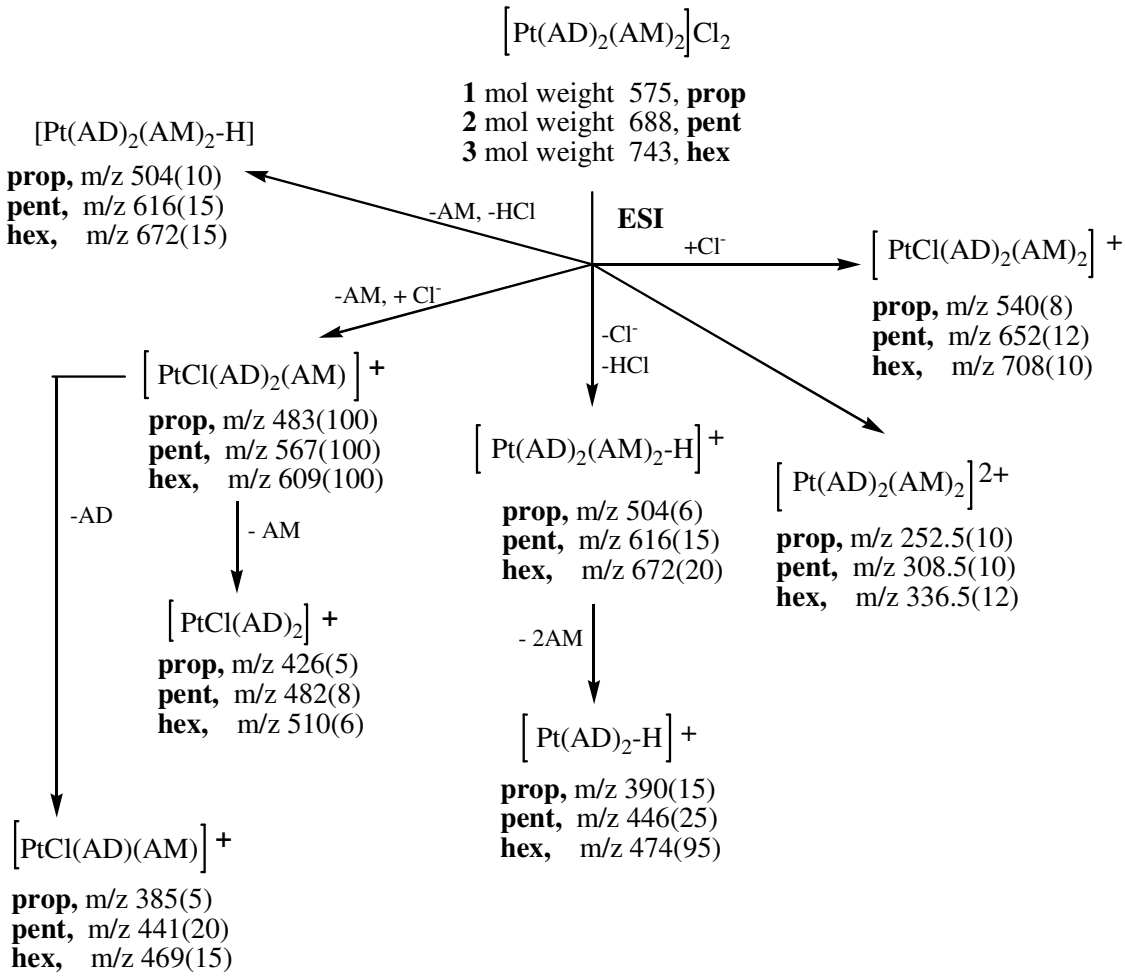
Compound **3**

trans-[Pt($NH_2\overbrace{CH(CH_2)_4CH_2}$)$_2${N(H)=C($CH_3$)N(H)$\overbrace{CH(CH_2)_4CH_2}$}$_2$]$^{2+}$[$Cl^-$]$_2$

Anal.Calc. for $C_{28}H_{62}N_6Cl_2O_2Pt$ (MW 780.81): C, 43.07; H, 8.00; N, 10.76. Found: C, 43.08; H, 7.99; N, 10.79.

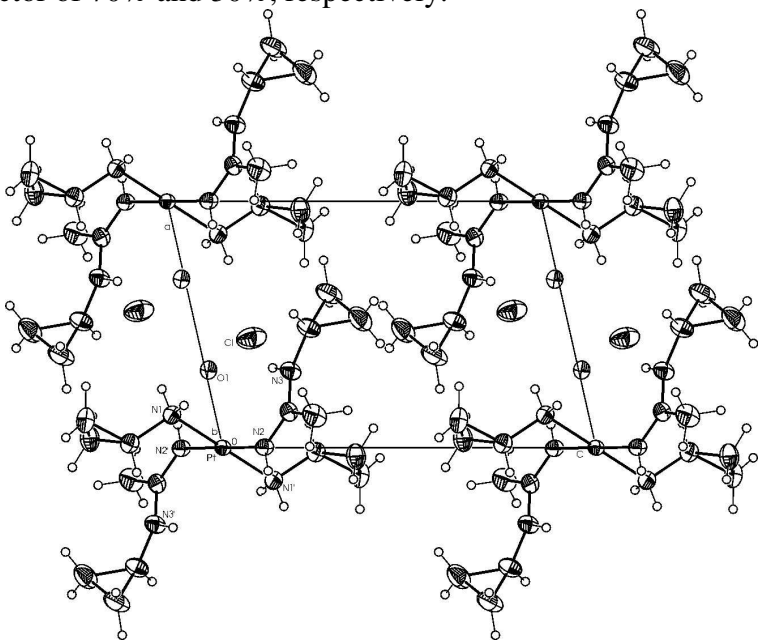
S2

Scheme SI 1 : The fragmentation pathways of compounds 1, 2 and 3 dissolved in CH_3CN under ESI conditions



S3

Figure SI 1. Crystal packing viewed down *b* axis of *trans*-[Pt($NH_2\overline{CHCH_2CH_2}$)$_2${N(H)=C($CH_3$)N(H)$\overline{CHCH_2CH_2}$}$_2$]$^{2+}$[$Cl^-$]$_2$. 2H_2O (**1**). The two Cl anions and the two water molecules were in disordered position, with an occupancy factor of 70% and 30%, respectively.



S4

Table SI 1. Crystal Data and Structure Refinement Parameters for Compound **1**

compound	**1**
empirical formula	$C_{16}H_{38}N_6O_2Cl_2Pt$
fw	612.52
T,K	293(2)
λ (Å)	0.71073
crystal system	triclinic
space group	$P\bar{1}$
a (Å)	7.336(2)
b (Å)	8.228(2)
c (Å)	10.622(3)
α (deg)	83.82(2)
β (deg)	103.76(2)
γ (deg)	103.21(2)
V (Å^3)	605.3(3)
Z	1
ρ_{calc}, g cm^{-3}	1.680
F(000)	304
θ range/°	3-28
μ (Mo Kα), mm^{-1}	6.038
No. reflections collected	3053
No. observed [I≥2σ(I)]	2888
R (F^2)[a]	0.030
Rw (F^2)[b]	0.077
GOF	1.107

[a]$R = \sum(|Fo| - |Fc|)/\sum|Fo|$, [b]$R_W = [\sum\{w(|Fo|^2 - |Fc|^2)^2\}/\sum\{w(|Fo|^2)^2\}]^{1/2}$

Table SI 2. Selected bond lengths (Å) and angles (°) for compound **1**

Pt-N(1)	2.055(4)	N(1)-Pt-N(2)	87.7(2)
Pt-N(2)	2.006(4)	N(1)-Pt-N(2)'	92.3(2)
N(1)-C(1)	1.458(7)	C(1)-N(1)-Pt	114.5(3)
N(2-C(4)	1.297(6)	C(4)-N(3)-C(6)	123.7(5)
N(3)-C(4)	1.341(7)	C(4)-N(2)-Pt	127.1(3)
N(3)-C(6)	1.434(7)	N(1)-C(1)-C(2)	119.1(5)
C(1)-C(2)	1.462(8)	N(1)-C(1)-C(3)	119.9(5)
C(1)-C(3)	1.486(8)	N(2)-C(4)-N(3)	120.3(4)
C(2)-C(3)	1.490(9)	N(2)-C(4)-C(5)	120.8(5)
C(4)-C(5)	1.498(7)	N(3)-C(4)-C(5)	119.0(5)
C(6)-C(8)	1.473(9)	N(3)-C(6)-C(8)	119.3(7)
C(6)-C(7)	1.485(9)	N(3)-C(6)-C(7)	116.4(6)
C(8)-C(7)	1.467(9)		

' at –x,-y,-z