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SUPPORTING INFORMATION

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Supporting Information

for

N-Methyl-2,2’-Dipicolylamine Complexes as Potential Models for Metal-Mediated Base Pairs

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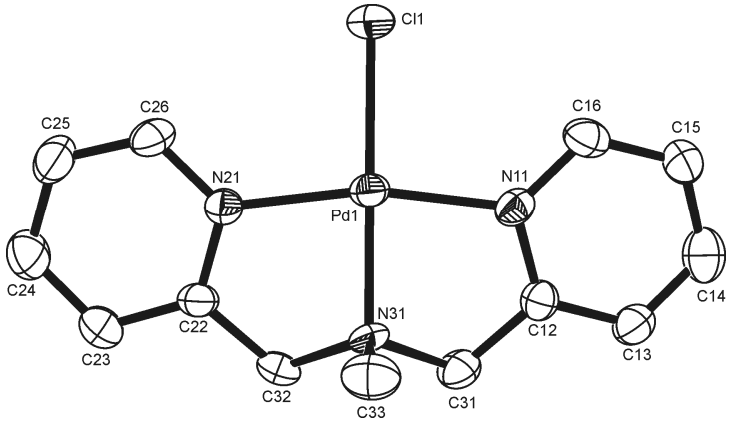


Figure S1: Molecular structure of the cation of [PdCl(dipic)](PF_6) (**1b**). Hydrogen atoms have been omitted for clarity.

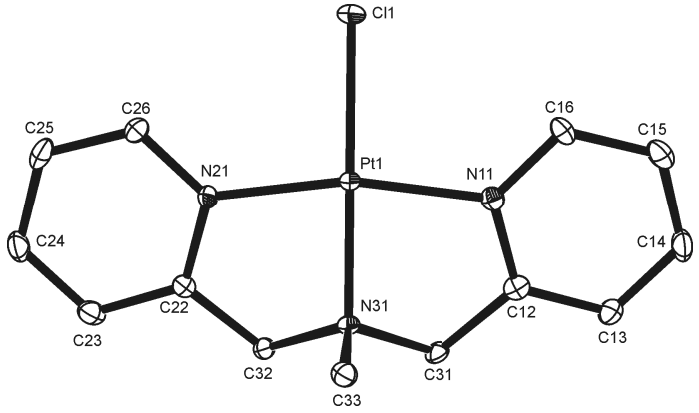


Figure S2: Molecular structure of the cation of [PtCl(dipic)]Cl · H_2O (**2a**). Hydrogen atoms have been omitted for clarity.

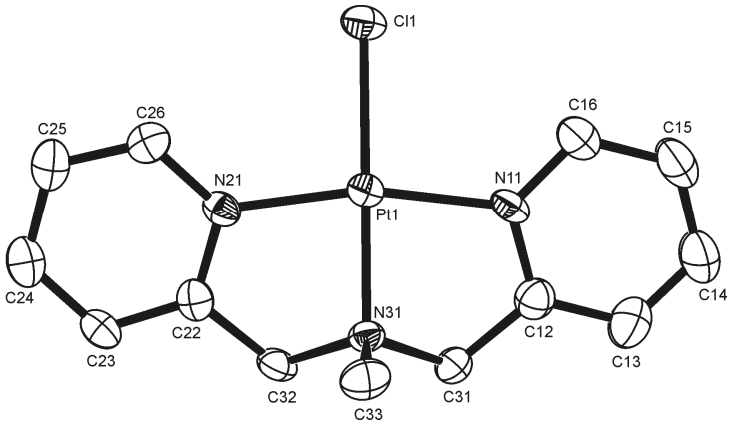
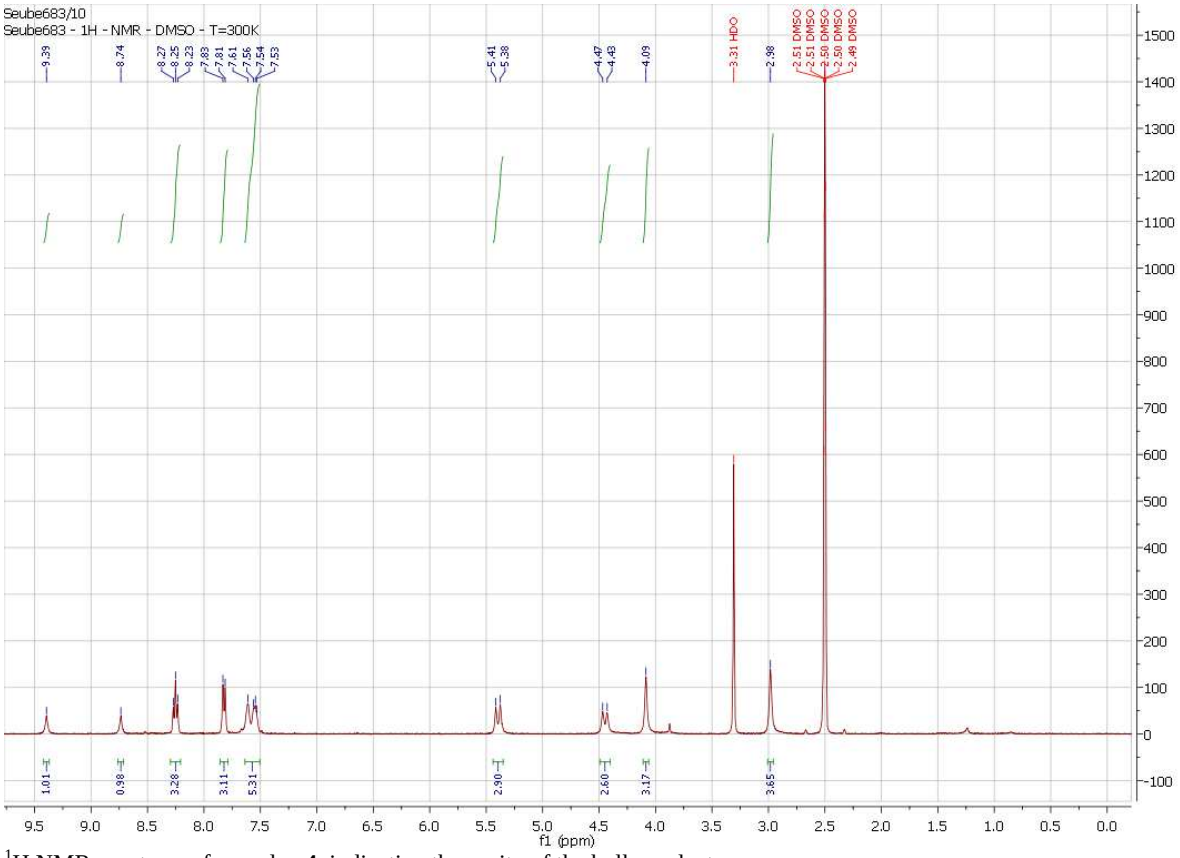


Figure S3: Molecular structure of the cation of [PtCl(dipic)](NO_3) · H_2O (**2b**). Hydrogen atoms have been omitted for clarity.

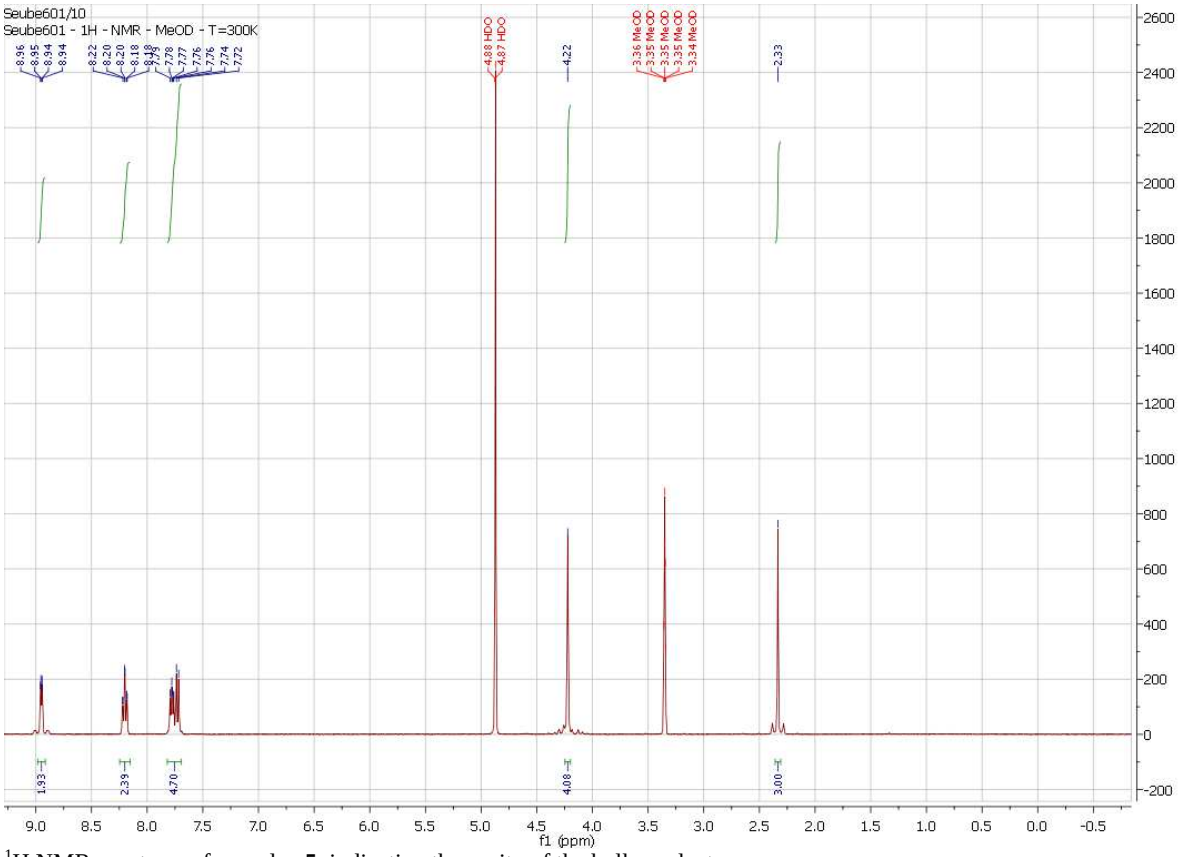
Table S1. Crystallographic data for compounds **1b**, **2a**, and **2b**.

	1b	**2a**	**2b**
empirical formula	$C_{13}H_{15}ClF_6N_3PPd$	$C_{13}H_{17}Cl_2N_3OPt$	$C_{13}H_{15}ClN_4O_4Pt$
formula weight	500.10	497.29	521.83
crystal system	triclinic	monoclinic	triclinic
space group	*P*–1	$P2_1/c$	*P*–1
a, *b*, *c* [Å]	7.3980(15), 10.771(2), 12.338(3)	8.2740(17), 13.025(3), 14.149(3)	7.9150(16), 8.3790(17), 13.273(3)
α, β, γ[°]	110.21(3), 91.61(3), 102.16(3)	90, 93.97(3), 90	81.80(3), 83.76(3), 73.64(3)
V [Å^3]	896.4(3)	1521.2(5)	833.8(3)
Z	2	4	2
ρ_{calcd} [g cm^{-3}]	1.853	2.171	2.078
$\mu(Mo_{K\alpha})$ [mm^{-1}]	1.333	9.574	8.598
crystal size [mm]	0.10 × 0.10 × 0.10	0.20 × 0.20 × 0.18	0.10 × 0.10 × 0.10
temperature [K]	293(2)	150(2)	293(2)
θ_{min}, θ_{max} [°]	2.1, 26.4	3.1, 27.4	2.6, 25.0
dataset	0:9, –13:12, –15:15	–10:10, –16:14, –18:17	0:9, –9:9, –15:15
tot., uniq. data	3604, 3604	23048, 3452	3146, 3146
observed data [$I > 2\sigma(I)$]	1451	2937	2095
N_{ref}, N_{par}	3604, 227	3452, 234	3146, 210
R, wR_2, *S* [$I > 2\sigma(I)$][a]	0.0483, 0.1173, 0.842	0.0234, 0.0463, 1.096	0.0331, 0.0582, 0.805
min. and max. resd. dens. [e Å^{-3}]	0.67, –0.58	1.00, –0.84	0.80, –0.95

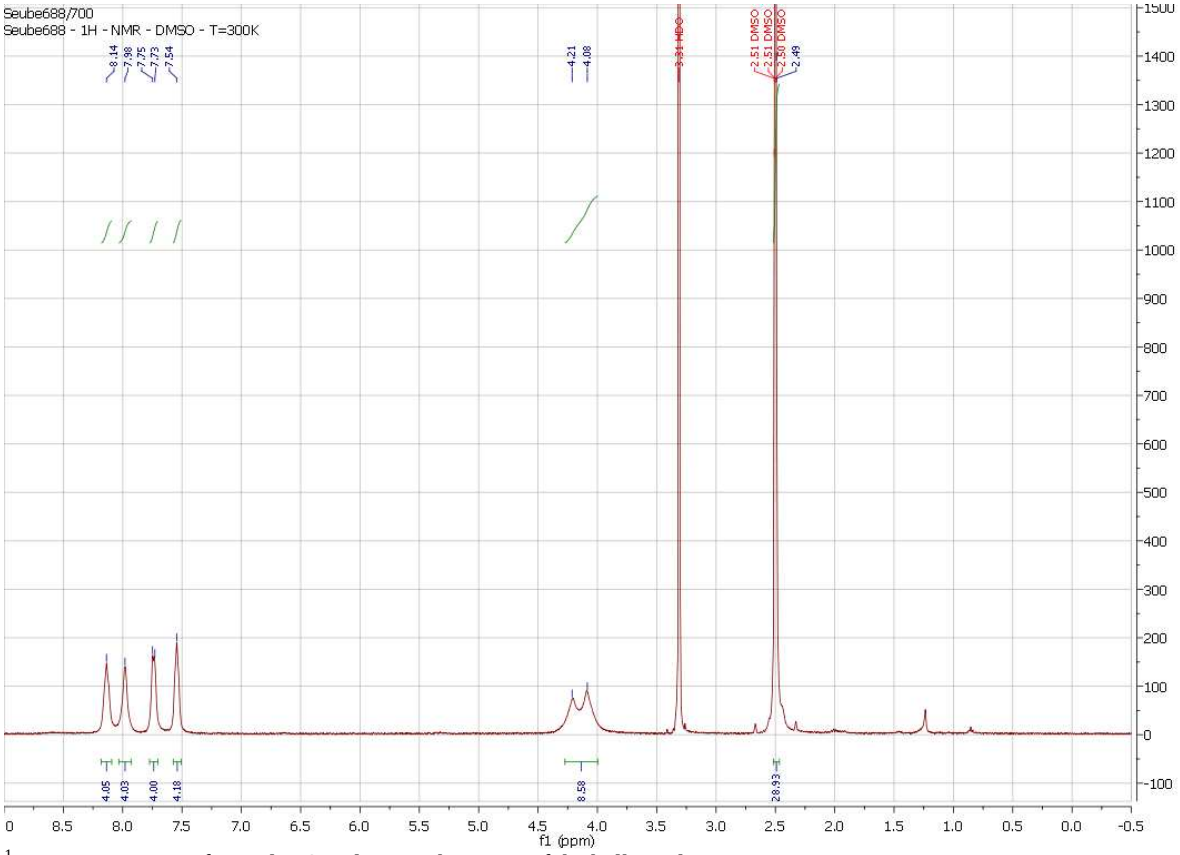
[a] $R_1 = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$, $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2 / \Sigma w(F_o^2)^2]^{1/2}$.



^{1}H NMR spectrum of complex **4**, indicating the purity of the bulk product.



^{1}H NMR spectrum of complex **5**, indicating the purity of the bulk product.



^{1}H NMR spectrum of complex **6**, indicating the purity of the bulk product.