

## SUPPORTING INFORMATION

Unsymmetric mono- and dinuclear platinum(IV)  
complexes featuring an ethylene glycol moiety:  
synthesis, characterization and biological activity

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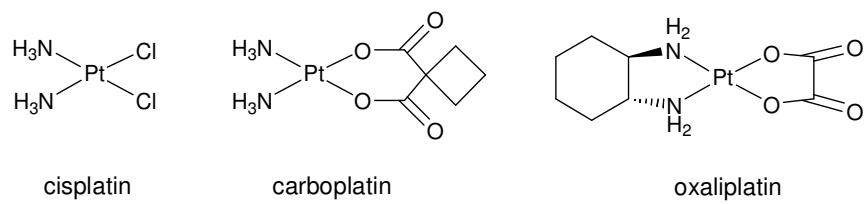
**Table S1.** Crystal data, data collecting parameters, and structure refinement details of **1b<sup>+</sup>·TFA<sup>-</sup>**

<b>1b<sup>+</sup>·TFA<sup>-</sup></b>	
Empirical formula	C <sub>7</sub> H <sub>17</sub> Cl <sub>2</sub> F <sub>3</sub> N <sub>2</sub> O <sub>4</sub> Pt
Fw	516.22
Space group	monoclinic, P-1
<i>a</i> [Å]	6.1836(2)
<i>b</i> [Å]	8.0658(3)
<i>c</i> [Å]	15.5374(7)
$\alpha$ [°]	102.217(3)
$\beta$ [°]	92.750(3)
$\gamma$ [°]	108.655(2)
<i>V</i> [Å <sup>3</sup> ]	711.98(5)
<i>Z</i>	2
$\lambda$ [Å]	0.71073
$\rho_{\text{calcd}}$ [g cm <sup>-3</sup> ]	2.408
crystal size [mm <sup>3</sup> ]	0.20 x 0.20 x 0.08
<i>T</i> [K]	100(2)
$\mu$ [mm <sup>-1</sup> ]	10.273
<i>R</i> <sub>1</sub> <sup>[a]</sup>	0.0228
<i>wR</i> <sub>2</sub> <sup>[b]</sup>	0.0548
GOF <sup>[c]</sup>	1.067

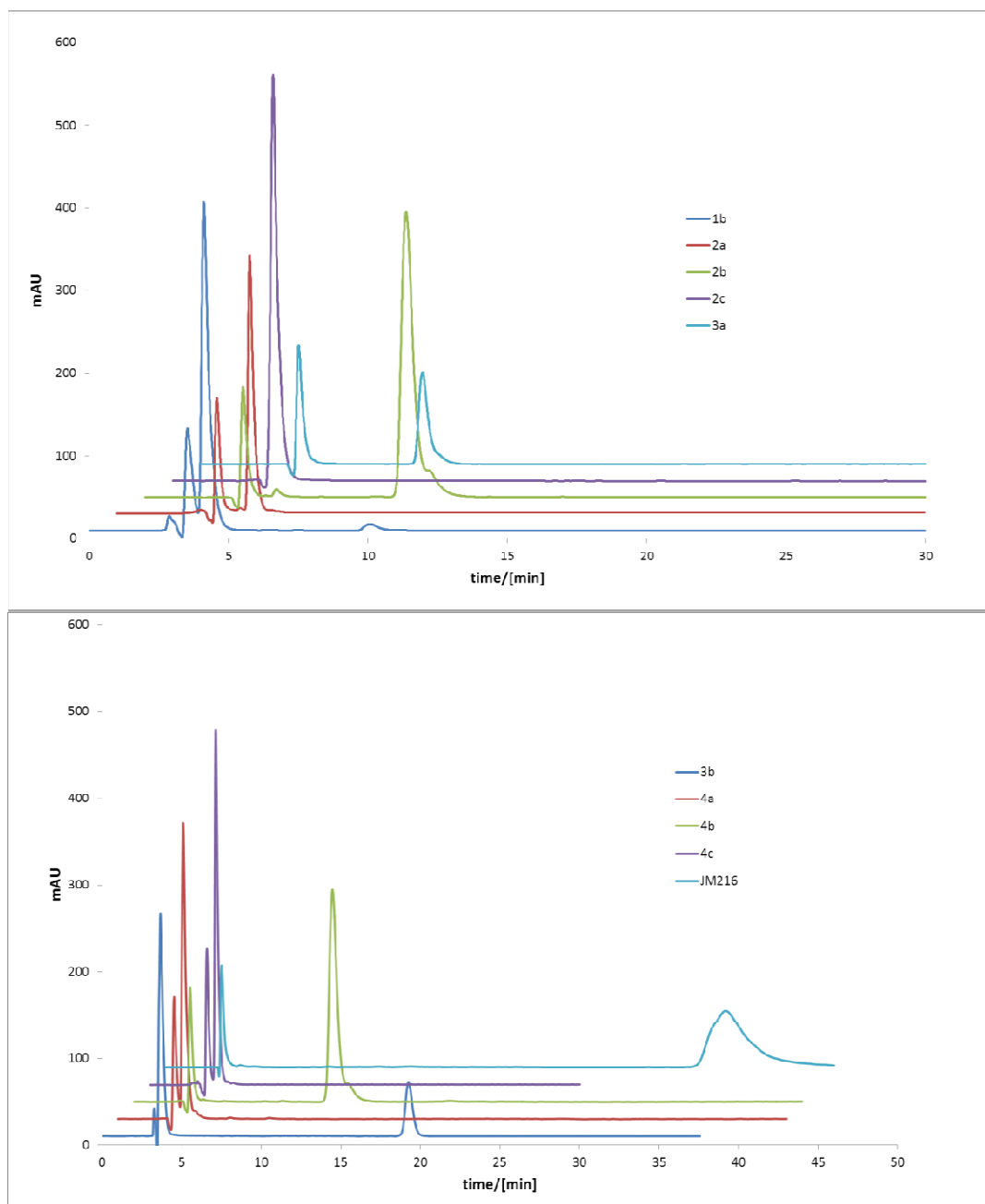
<sup>a</sup>  $R_1 = \sum ||F_o| - |F_c|| / \sum |F_o|$ . <sup>b</sup>  $wR_2 = \{\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]\}^{1/2}$ . <sup>c</sup>  $\text{GOF} = \{\sum [w(F_o^2 - F_c^2)^2] / (n - p)\}^{1/2}$ , where *n* is the number of reflections and *p* is the total number of parameters refined.

**Table S2.** Elemental analysis of novel platinum(IV) compounds

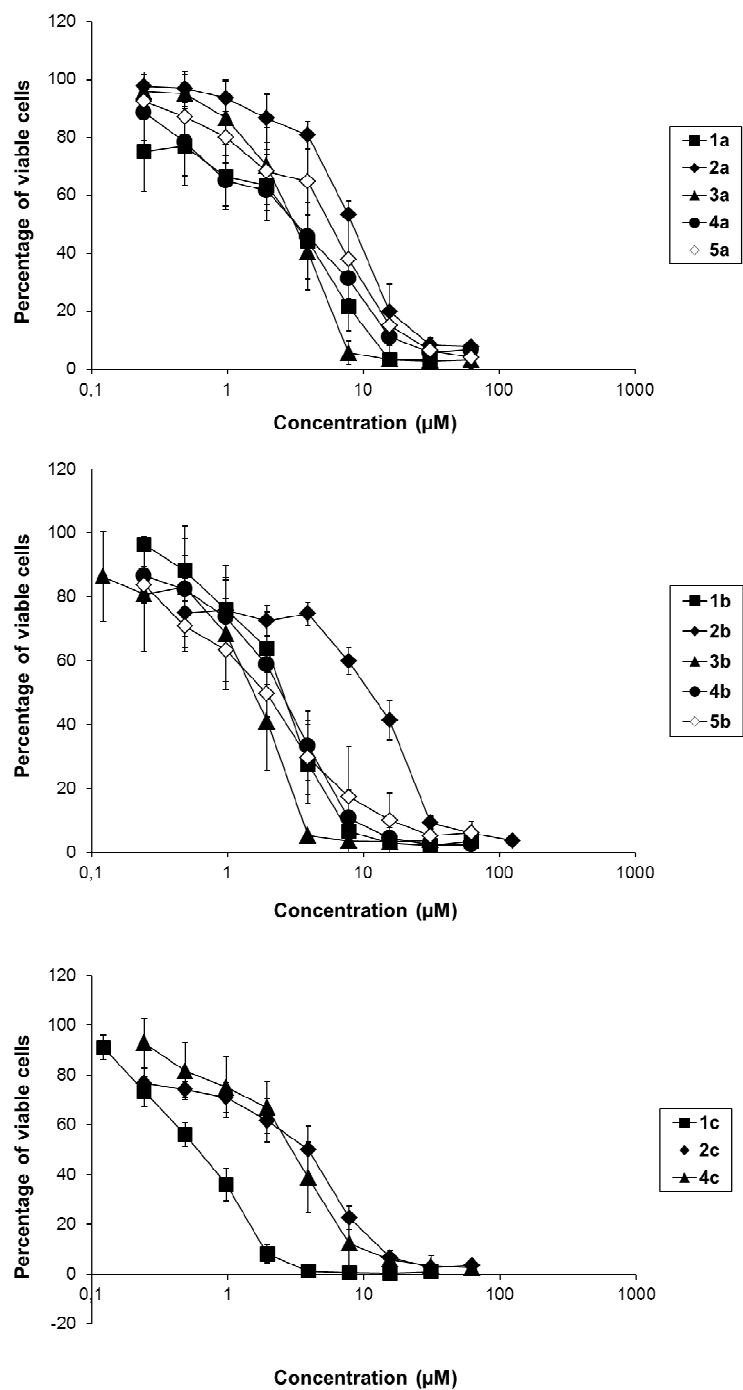
1b	C <sub>5</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub> Cl <sub>2</sub> Pt	calcd	14,93	4,01	6,97
		found	14,73	3,73	6,69
1c	CH <sub>10</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub> Pt·0.5MeOH	calcd	4,95	3,32	7,69
		found	4,94	3,12	7,37
2b	C <sub>9</sub> H <sub>20</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>3</sub> Pt	calcd	21,52	4,10	5,58
		found	21,95	3,93	5,36
2c	C <sub>5</sub> H <sub>14</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>3</sub> Pt	calcd	13,40	3,15	6,25
		found	13,45	2,95	6,00
3b	C <sub>10</sub> H <sub>22</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>5</sub> Pt	calcd	23,26	4,30	5,43
		found	23,34	4,04	5,37
4a	C <sub>10</sub> H <sub>22</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>6</sub> Pt	calcd	22,56	4,17	5,26
		found	22,69	3,96	5,04
4b	C <sub>11</sub> H <sub>24</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>6</sub> Pt·0.5MeOH	calcd	24,56	4,66	4,98
		found	24,80	4,40	4,67
4c	C <sub>7</sub> H <sub>18</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>6</sub> Pt	calcd	17,08	3,69	5,69
		found	17,08	3,45	5,91
5a	C <sub>18</sub> H <sub>38</sub> Cl <sub>4</sub> N <sub>4</sub> O <sub>10</sub> Pt <sub>2</sub> ·MeOH	calcd	22,06	4,09	5,42
		found	21,98	3,74	5,02
5b	C <sub>20</sub> H <sub>42</sub> Cl <sub>4</sub> N <sub>4</sub> O <sub>10</sub> Pt·EtOAc	calcd	24,96	4,55	5,06
		found	24,70	4,48	5,09



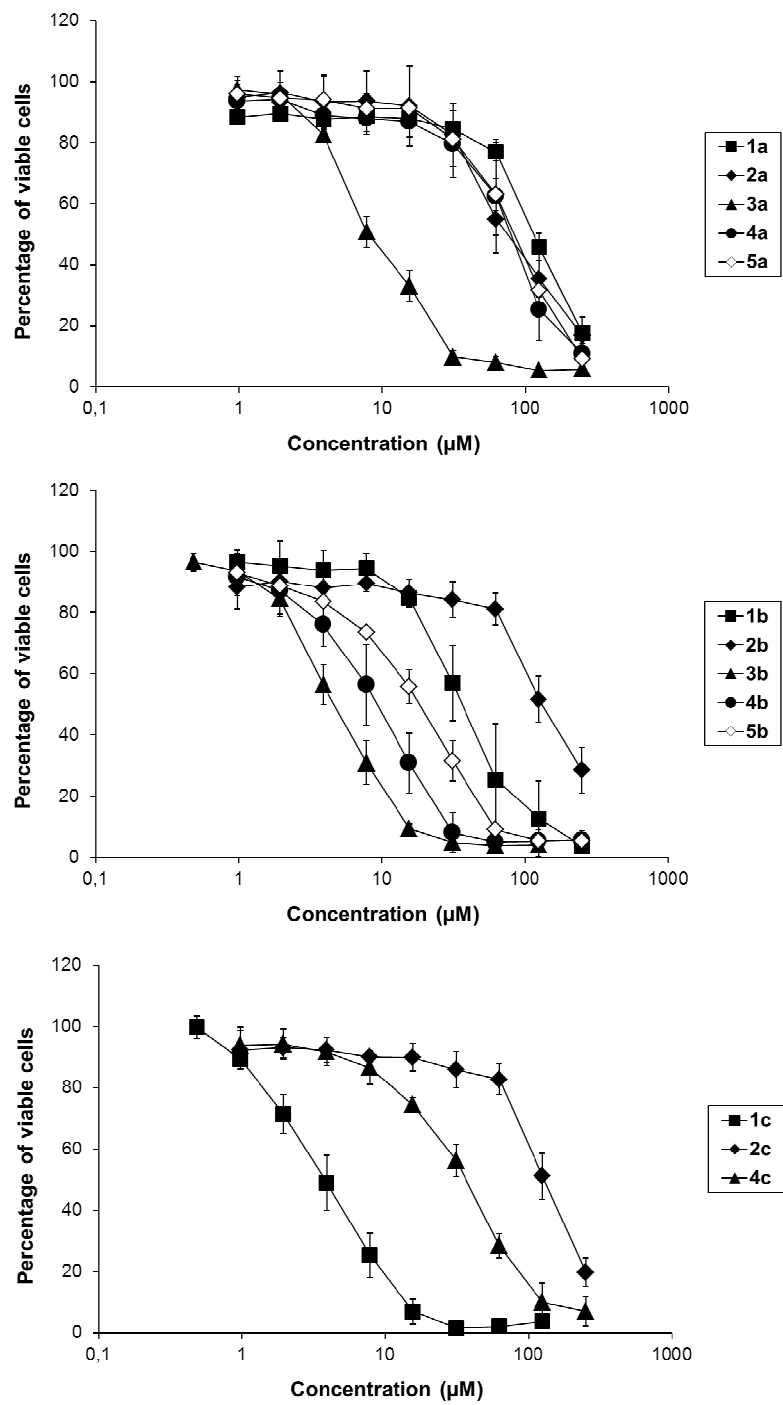
**Figure S1.** Platinum(II) compounds in worldwide clinical application



**Figure S2.** Reversed phase measurements in 20% MeOH/ 80% aqueous formic acid of all synthesized platinum(IV)-compounds, excluding the dimeric species (**5a** and **5b**), which expose retention times higher than 40 min under these conditions.

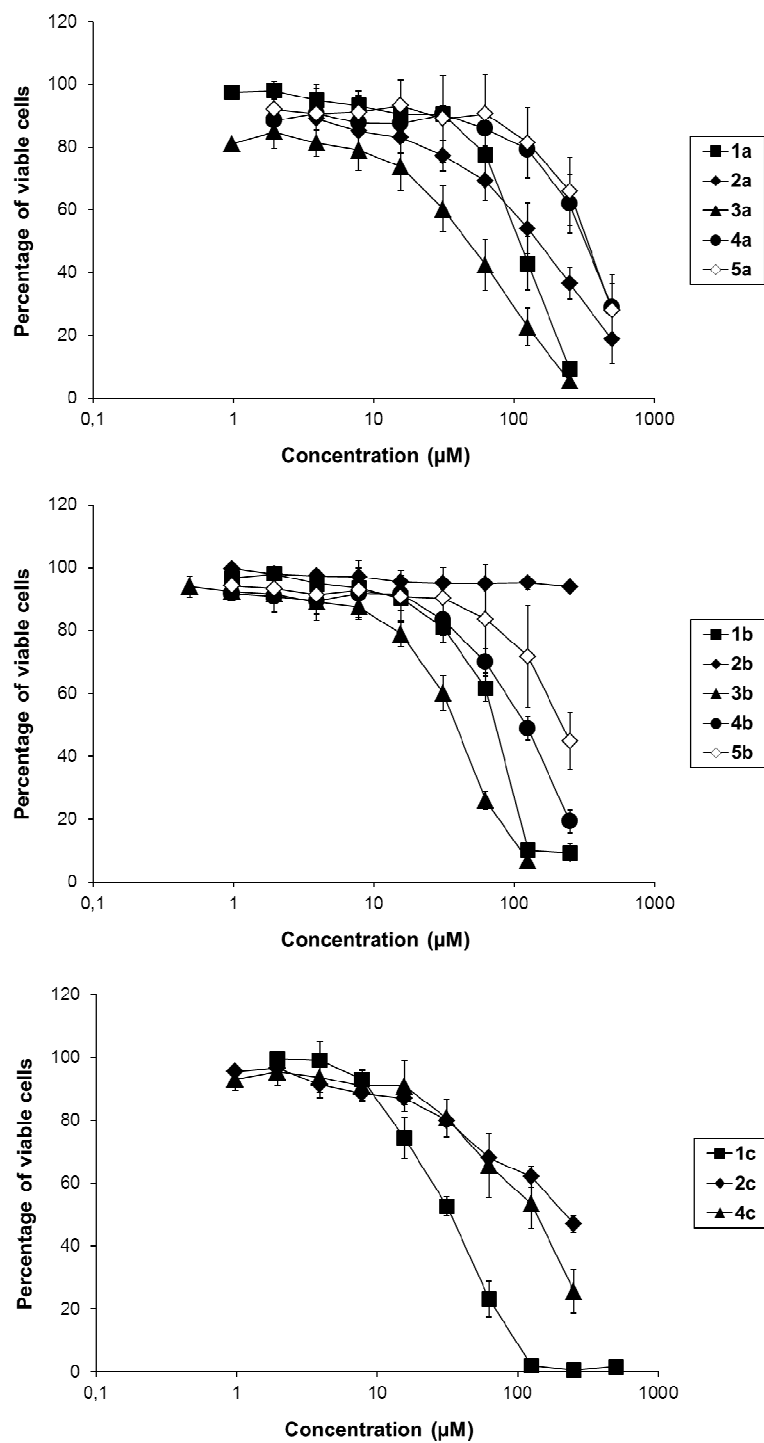


**Figure S3.** Concentration-effect curves in the CH1 cell line obtained by MTT assay (96 h exposure).

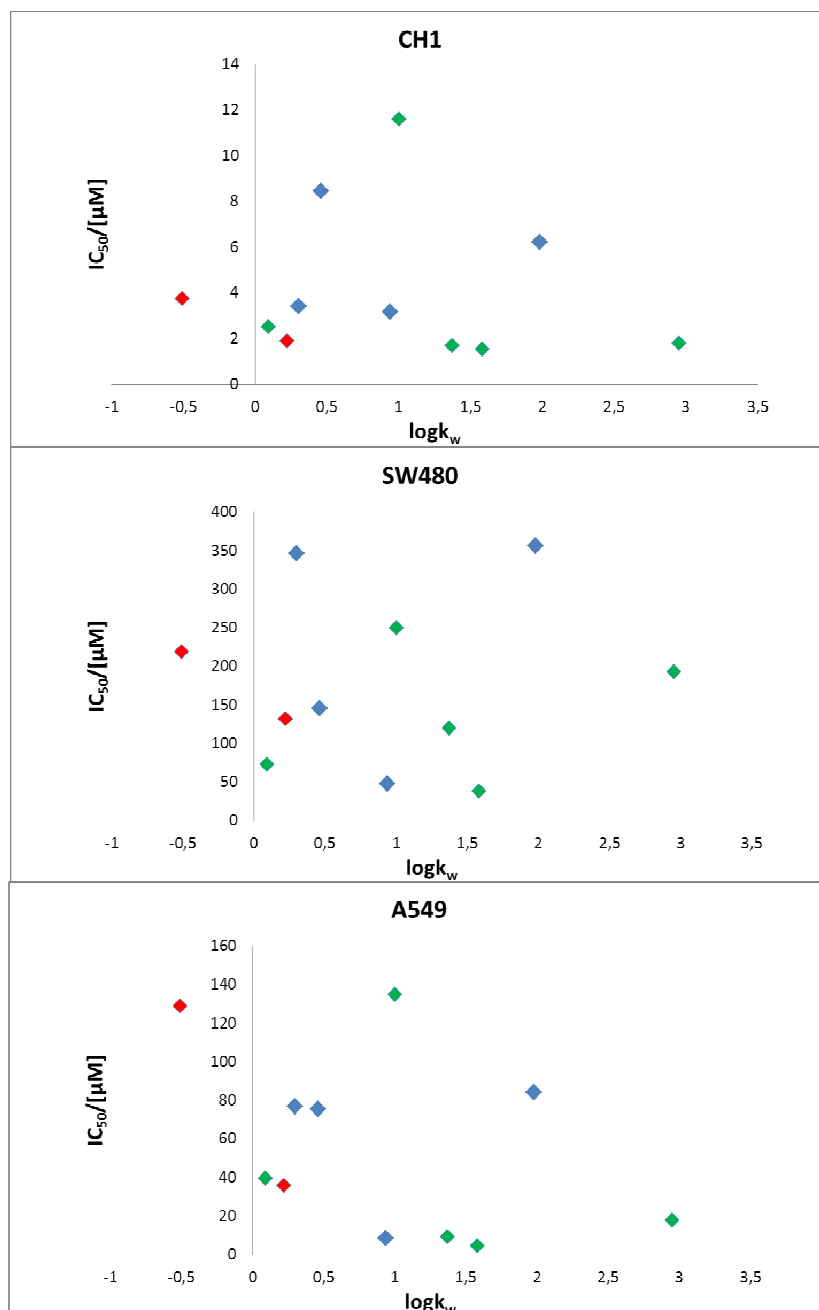


**Figure S4.** Concentration-effect curves in the SW480 cell line obtained by MTT assay (96 h exposure).

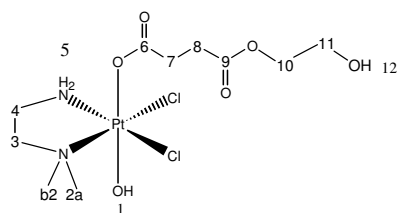




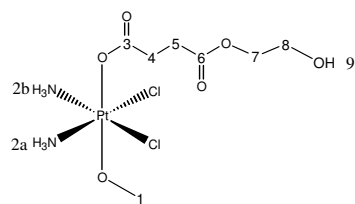
**Figure S5.** Concentration-effect curves in the A549 cell line obtained by MTT assay (96 h exposure).



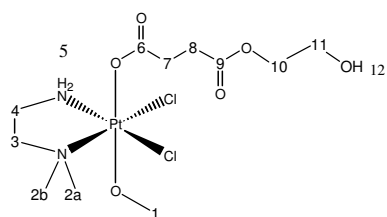
**Figure S6.** Correlation plots between the values  $\log k_w$  and cytotoxicity in three human cancer cell lines. The blue spots show the platinum compounds with the general formular  $Me_2enPtCl_2(OH)(R)$ , the green spots  $Me_2enPtCl_2(OMe)(R)$  and the red spots the complexes with the coordination sphere  $(NH_3)_2PtCl_2(OMe)(R)$ .



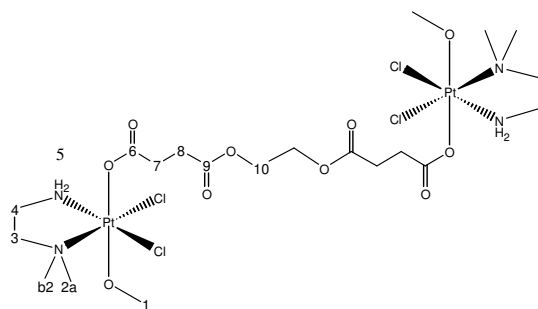
Compound **4a**



Compound **4c**



Compound **4b**



Compound **5b**

Figure S7. NMR-numbering scheme