

# Supporting Information

*for*

Syntheses, Characterization, and Preliminary Comparative  
Cytotoxicity Study of Au(I) and Au(III) Complexes Bearing  
Benzimidazole- and Pyrazole- Derived N-Heterocyclic Carbenes

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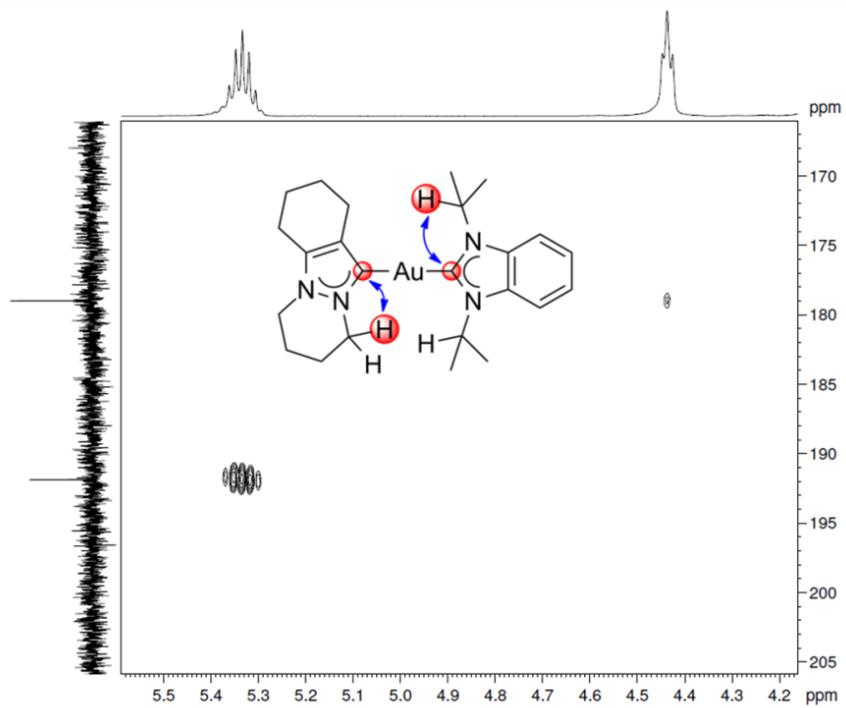
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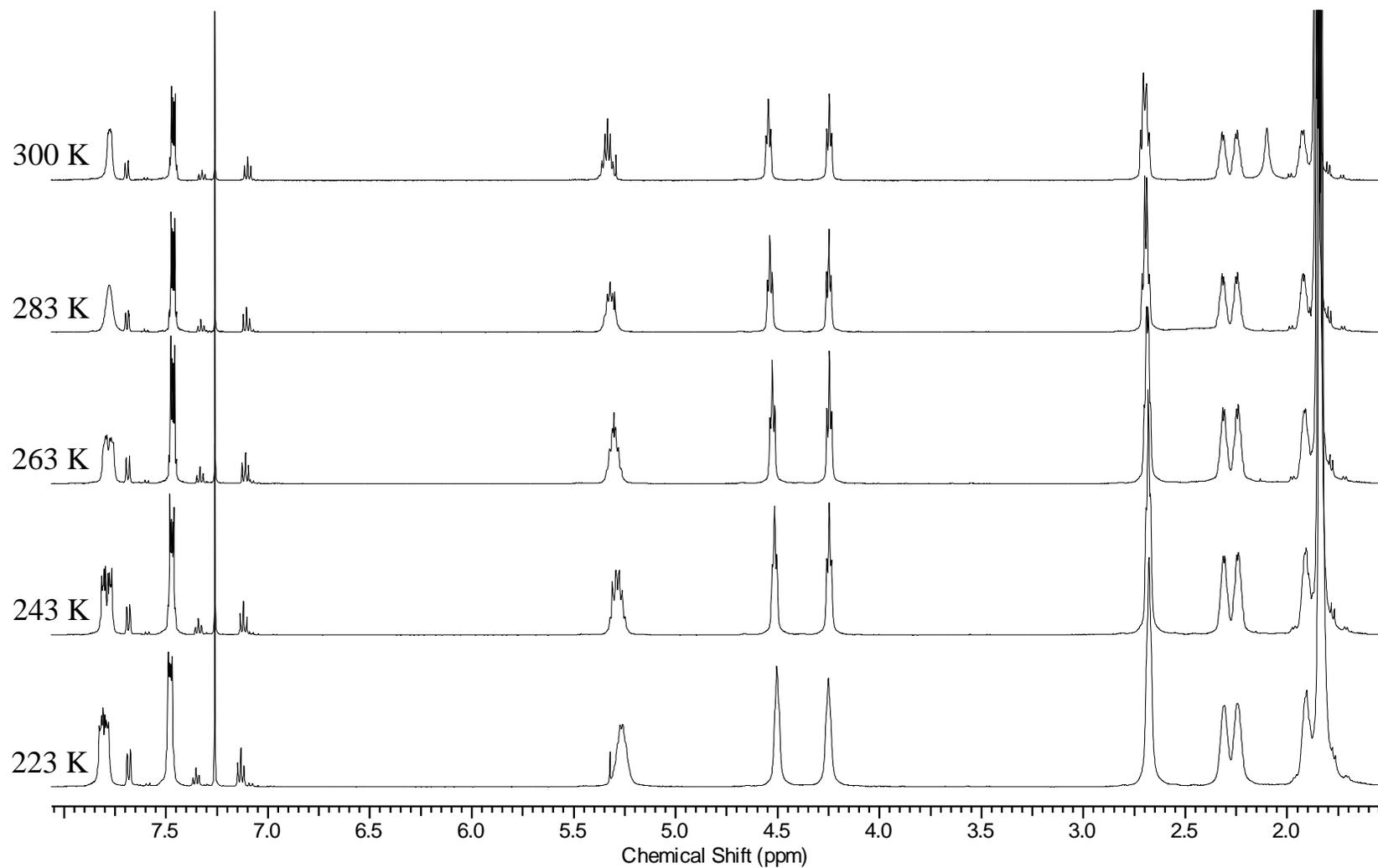
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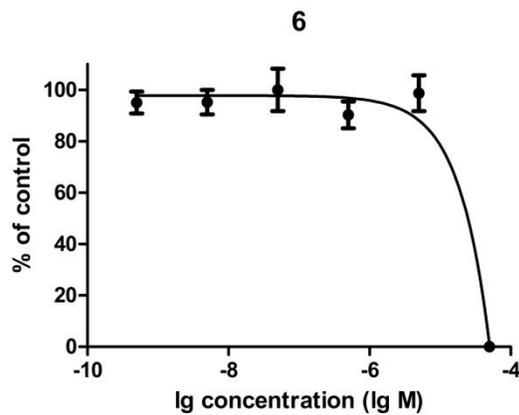
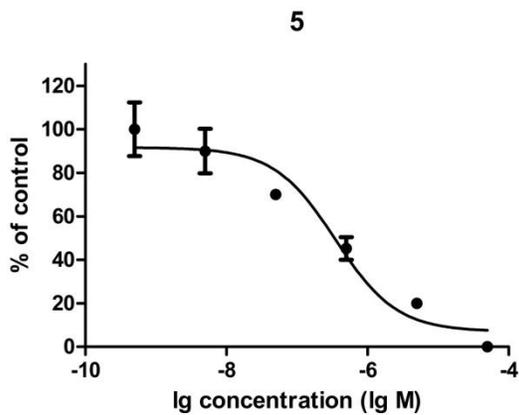
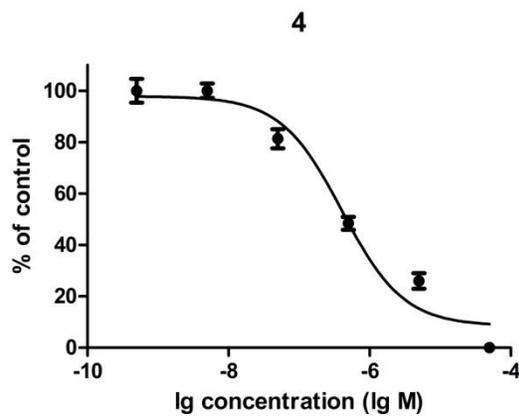
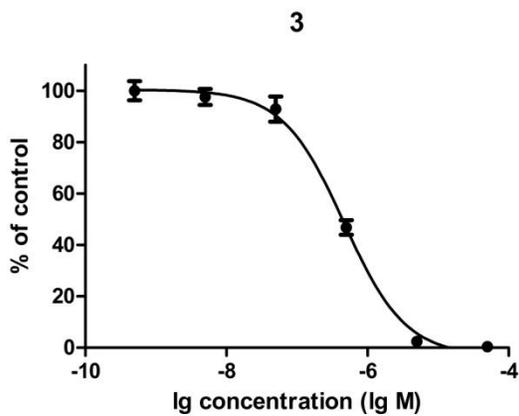
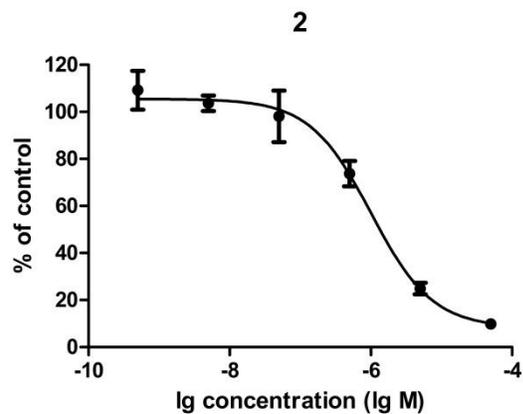
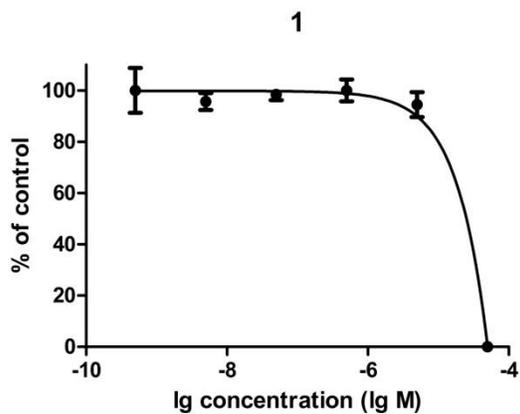
2D-HMBC NMR spectrum of complex 5

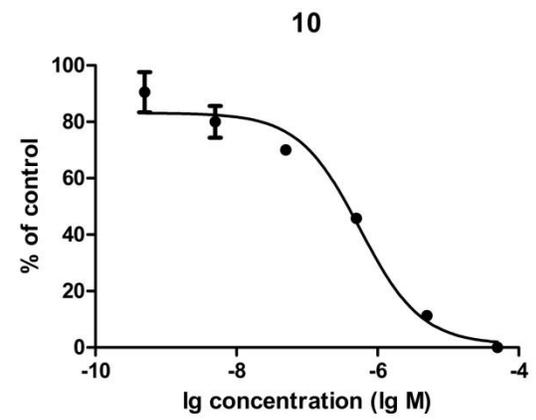
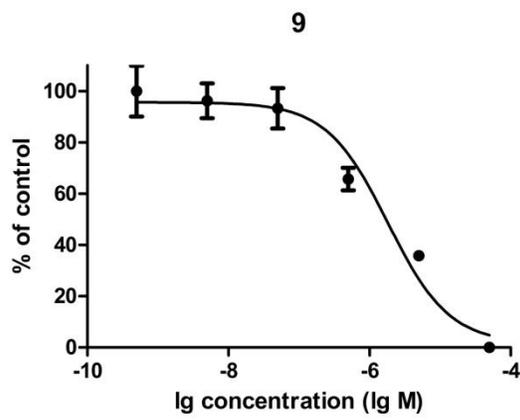
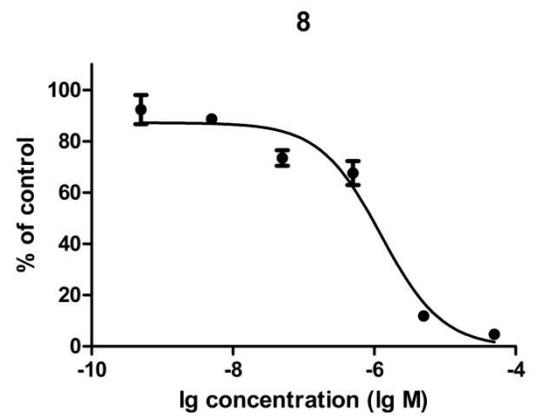
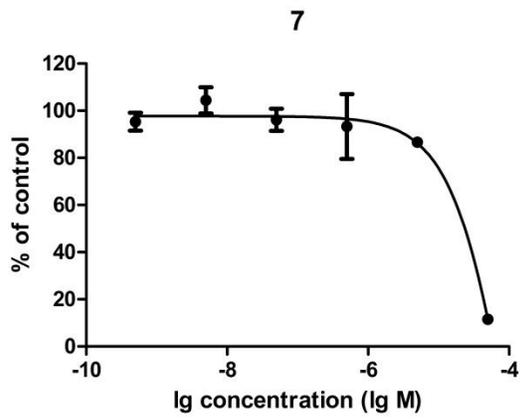


VT  $^1\text{H}$  NMR spectra of complex **10**

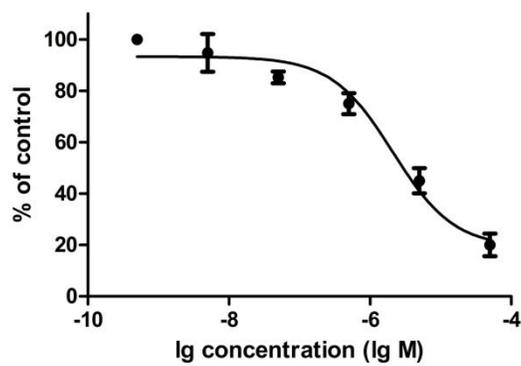


Dose-response curves for complexes 1–10 and cisplatin on the NCI-H1666 cell line.

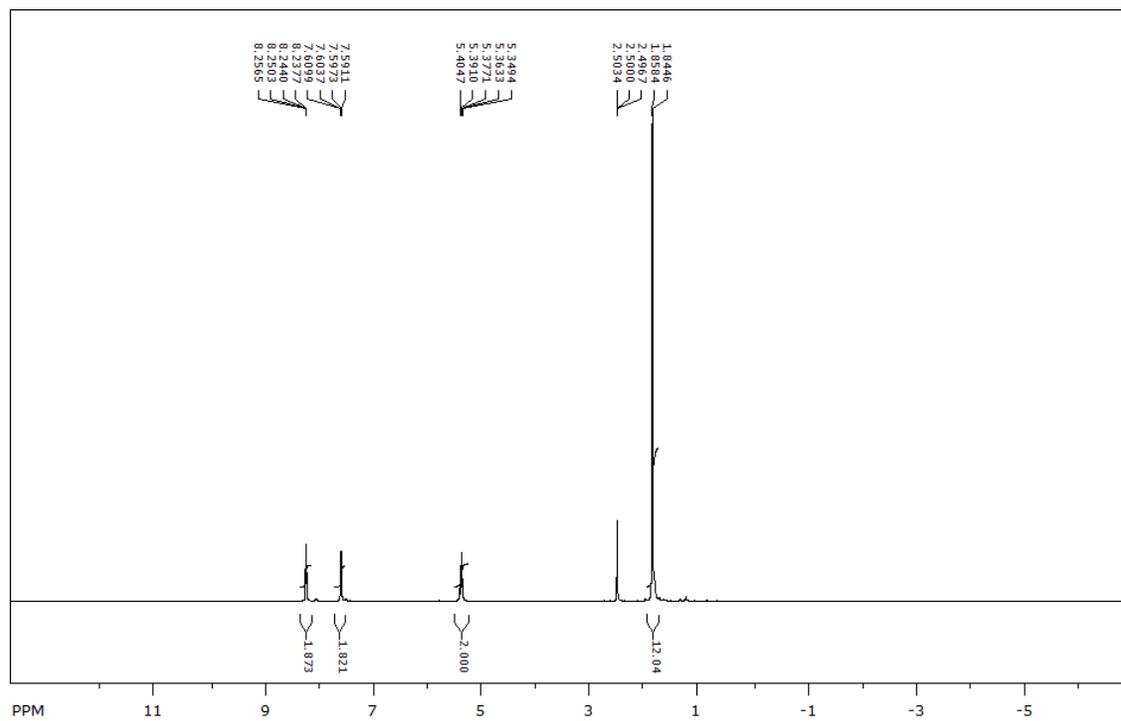




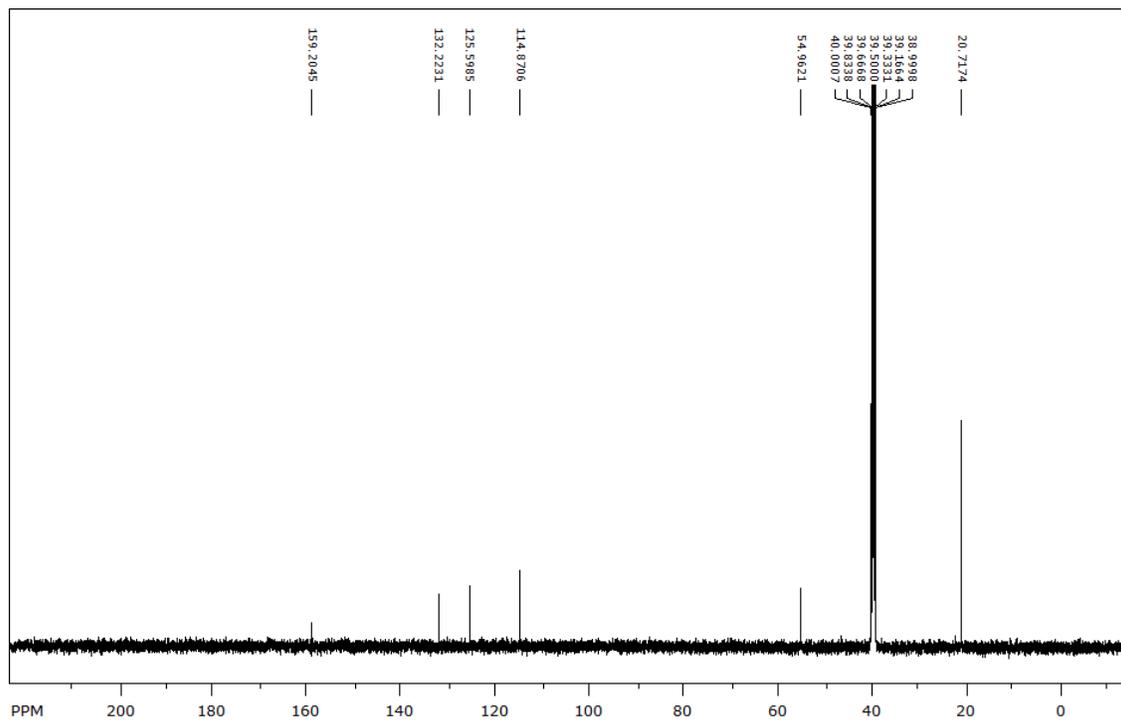
Cisplatin



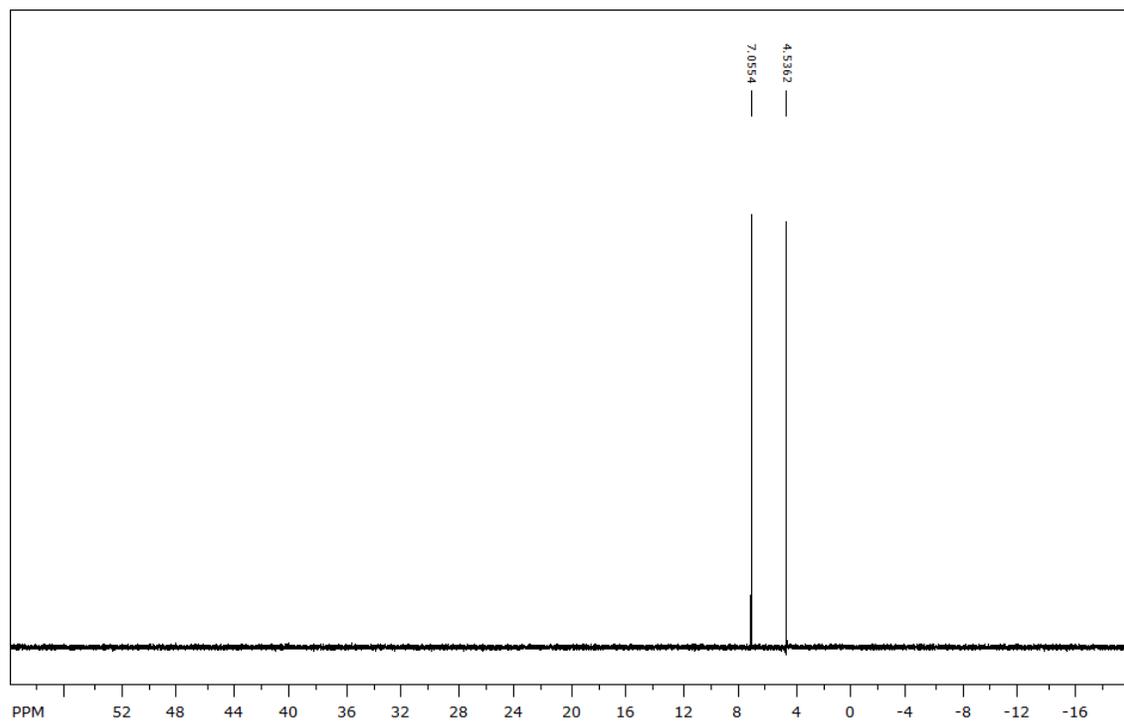
Multi-nuclei NMR spectra of complex **8**  
*<sup>1</sup>H NMR spectrum*



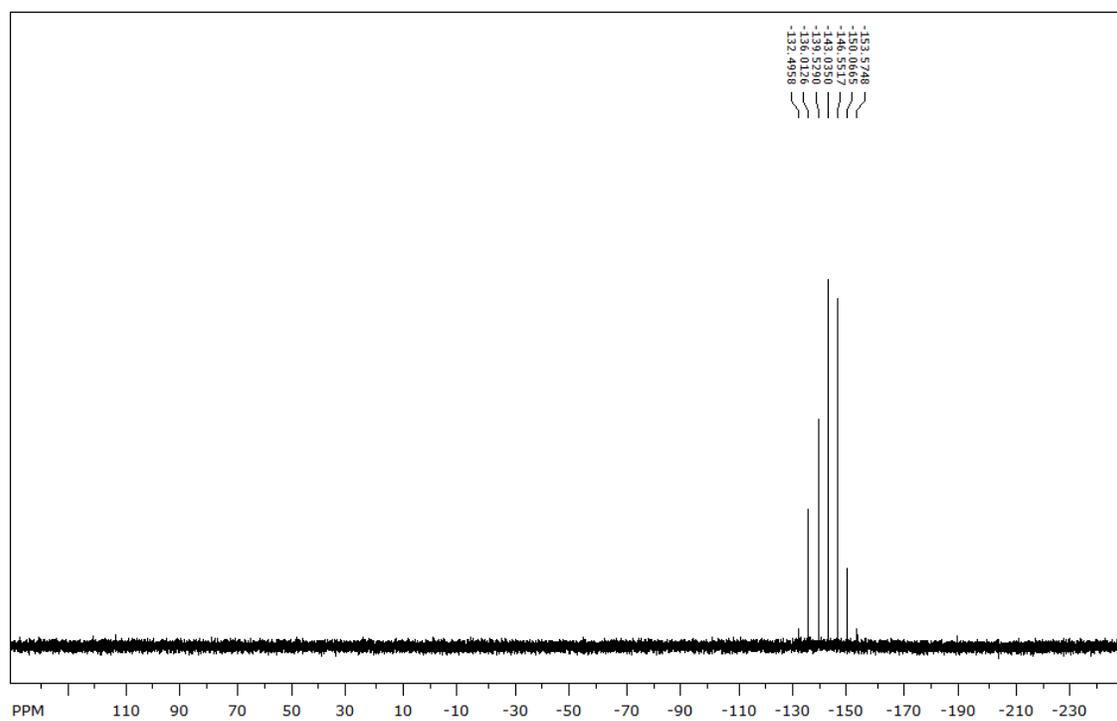
*<sup>13</sup>C NMR spectrum*



$^{19}\text{F}$  NMR spectrum



$^{31}\text{P}$  NMR spectrum



Selected X-ray crystallographic data for complexes 2, 3, 5, 6 and 8

	<b>2</b>	<b>3</b>	<b>5</b>	<b>6</b>	<b>8</b>
formula	C <sub>11</sub> H <sub>16</sub> N <sub>2</sub> AuCl	C <sub>26</sub> H <sub>36</sub> N <sub>4</sub> AuPF <sub>6</sub>	C <sub>24</sub> H <sub>34</sub> N <sub>4</sub> AuPF <sub>6</sub>	C <sub>13</sub> H <sub>18</sub> N <sub>2</sub> AuCl <sub>3</sub>	C <sub>26</sub> H <sub>36</sub> N <sub>4</sub> AuCl <sub>2</sub> PF <sub>6</sub>
fw	408.67	746.52	720.49	505.61	817.42
color, habit	colorless, block	colorless, block	colorless, block	yellow, block	colorless, block
crystal size (mm)	0.52 × 0.30 × 0.30	0.60 × 0.36 × 0.20	0.40 × 0.20 × 0.10	0.60 × 0.48 × 0.28	0.40 × 0.40 × 0.24
temp (K)	223(2)	100(2)	100(2)	100(2)	100(2)
cryst syst	monoclinic	orthorhombic	monoclinic	tetragonal	orthorhombic
space group	<i>P2<sub>1</sub>/n</i>	<i>Fddd</i>	<i>P2<sub>1</sub>/c</i>	<i>P4<sub>1</sub>2<sub>1</sub>2</i>	<i>Fddd</i>
<i>a</i> (Å)	10.5789(8)	11.0460(6)	10.6027(13)	8.7682(7)	12.8544(6)
<i>b</i> (Å)	8.7778(7)	18.0970(11)	13.8516(16)	8.7682(7)	18.6376(8)
<i>c</i> (Å)	12.9485(10)	29.2476(17)	18.185(2)	20.718(3)	24.9384(11)
$\alpha$ (°)	90	90	90	90	90
$\beta$ (°)	91.434(2)	90	102.706(2)	90	90
$\gamma$ (°)	90	90	90	90	90
<i>V</i> (Å <sup>3</sup> )	1202.01(16)	5846.6(6)	2605.3(5)	1592.8(3)	5974.6(5)
<i>Z</i>	4	8	4	4	8
<i>D<sub>c</sub></i> (g cm <sup>-3</sup> )	2.258	1.696	1.837	2.108	1.818
radiation used	Mo K $\alpha$	Mo K $\alpha$	Mo K $\alpha$	Mo K $\alpha$	Mo K $\alpha$
$\mu$ (mm <sup>-1</sup> )	12.430	5.147	5.772	9.727	5.219
$\theta$ (°)	2.46–27.49	2.27–27.49	1.87–27.50	2.52–27.50	2.09–27.49
no. of unique data	8222	9713	18346	11256	10102
max, min transmission	0.1181, 0.0597	0.4258, 0.1482	0.4305, 0.2906	0.1715, 0.0677	0.3673, 0.2293
final <i>R</i> indices	<i>R</i> <sub>1</sub> = 0.0447,	<i>R</i> <sub>1</sub> = 0.0260,	<i>R</i> <sub>1</sub> = 0.0349,	<i>R</i> <sub>1</sub> = 0.0248,	<i>R</i> <sub>1</sub> = 0.0162,
[ <i>I</i> > 2 $\sigma$ ( <i>I</i> )]	w <i>R</i> <sub>2</sub> = 0.1151	w <i>R</i> <sub>2</sub> = 0.0736	w <i>R</i> <sub>2</sub> = 0.0854	w <i>R</i> <sub>2</sub> = 0.0634	w <i>R</i> <sub>2</sub> = 0.0397
<i>R</i> indices (all data)	<i>R</i> <sub>1</sub> = 0.0527,	<i>R</i> <sub>1</sub> = 0.0288	<i>R</i> <sub>1</sub> = 0.0426,	<i>R</i> <sub>1</sub> = 0.0257,	<i>R</i> <sub>1</sub> = 0.0179,
	w <i>R</i> <sub>2</sub> = 0.1194	w <i>R</i> <sub>2</sub> = 0.0749	w <i>R</i> <sub>2</sub> = 0.0999	w <i>R</i> <sub>2</sub> = 0.0636	w <i>R</i> <sub>2</sub> = 0.0407
goodness-of-fit on <i>F</i> <sup>2</sup>	1.052	1.139	1.137	1.162	1.075
peak/hole (e Å <sup>-3</sup> )	2.577/–1.587	1.511/–1.856	1.983/–1.146	2.561/–1.081	0.743/–1.417