

# **NMR studies of group 8 metallodrugs: $^{187}\text{Os}$ -enriched organo-osmium half-sandwich anticancer complex**

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## **Supporting Information**

**Tables S1-S2**

**p S2**

**Figures S1-S2**

**p S3, S4**

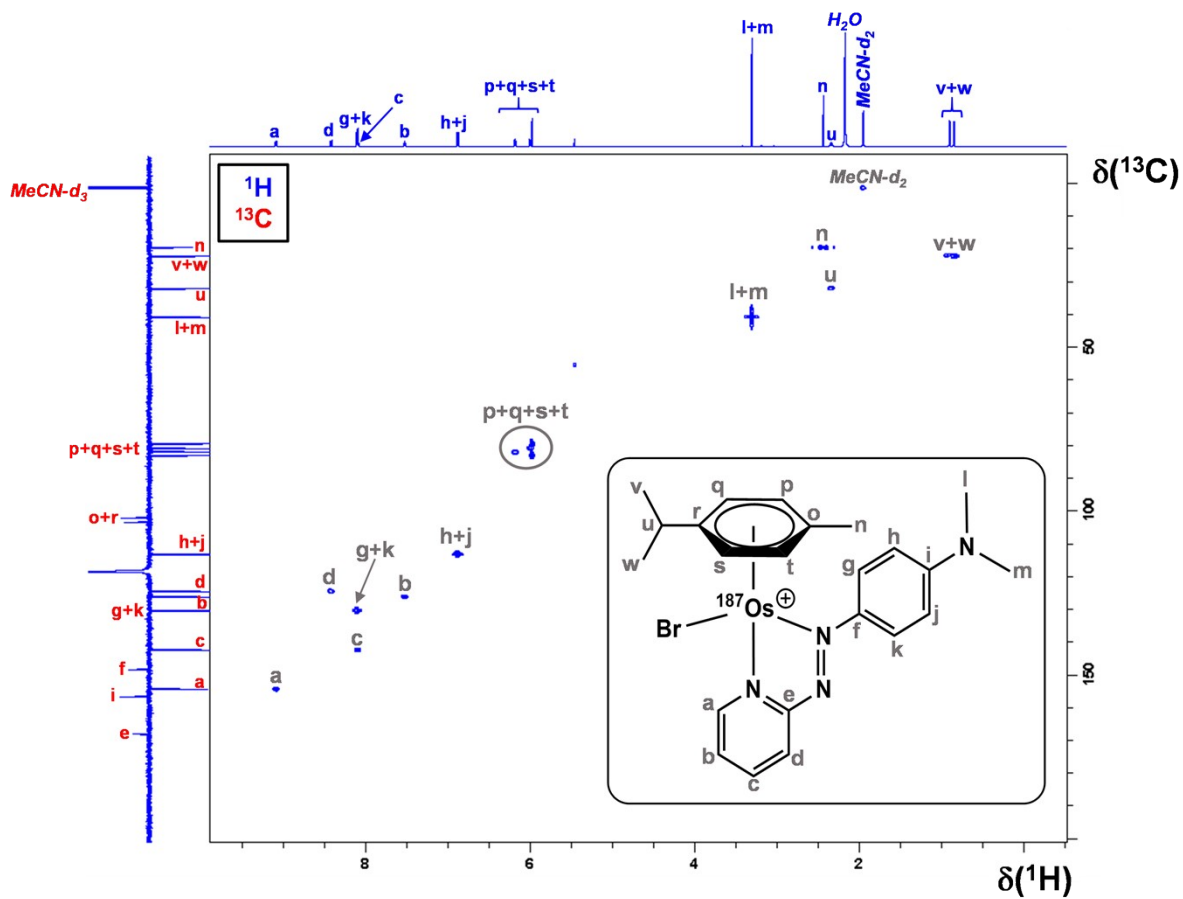
**Table S1:** X-ray crystal structure parameters

Parameter	Complex 1
Formula	C <sub>23</sub> H <sub>28</sub> BrF <sub>6</sub> N <sub>4</sub> OsP
Molar mass /g mol <sup>-1</sup>	775.57
Density /mg m <sup>-3</sup>	1.998
Crystal system	Triclinic
Crystal dimensions /mm	0.60 x 0.40 x 0.14
Space group	P-1
Crystal character	Purple block
<i>a</i> /Å	8.3424(2)
<i>b</i> /Å	12.5262(4)
<i>c</i> /Å	12.6754(3)
<i>a</i> /deg	85.480(2)
<i>β</i> /deg	79.486(2)
<i>γ</i> /deg	82.407(2)
<i>T</i> /K	100(2)
<i>Z</i>	2
<i>R</i> [ <i>F</i> > 4σ( <i>F</i> )]	0.0358
R <sub>w</sub>	0.0886
GOF	1.038
Δρ max and min /eÅ <sup>-3</sup>	2.816 & -2.520

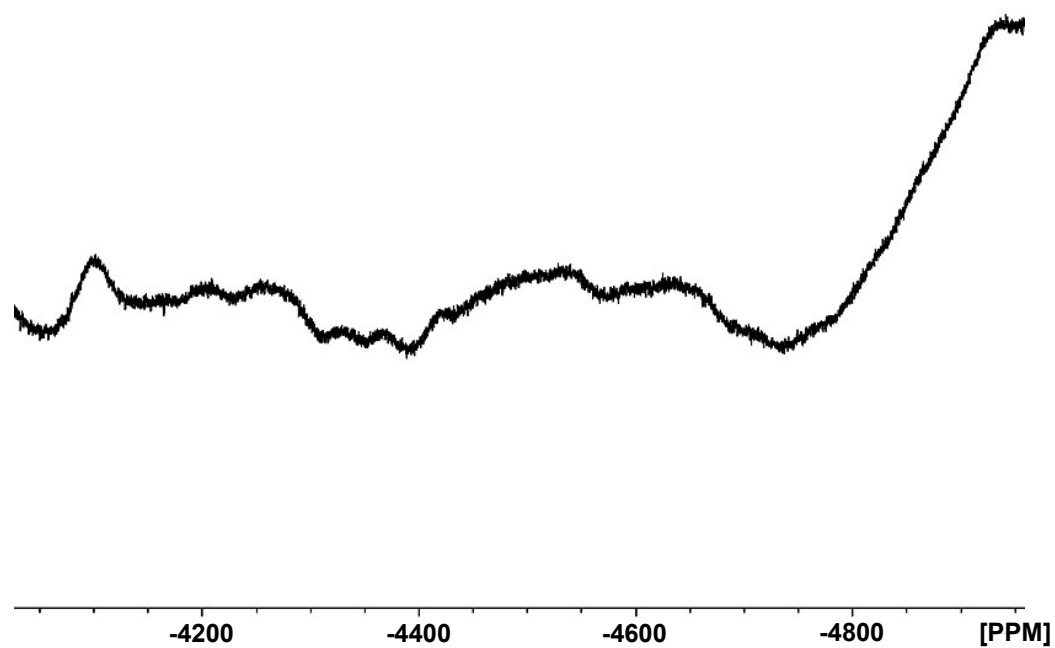
**Table S2:** A2780 human ovarian cancer cytotoxicity of complexes [Os(η<sup>6</sup>-*p*-cym)(*N,N*-Azpy-NMe<sub>2</sub>)X]PF<sub>6</sub> for a 24 h drug exposure with 72 h recovery time. X = Cl, Br, I.

Complex	IC <sub>50</sub> (μM)
1-Cl <sup>a</sup>	1.8±0.1
1-Br	0.40±0.01
1-I <sup>a</sup>	0.18±0.01

<sup>a</sup>Taken from reference<sup>29</sup>



**Figure S1:**  $^{13}\text{C}$  –  $^1\text{H}$  HMQC 2D NMR spectrum of complex 1 in  $\text{MeCN-}d_3$ . Channel F1  $^1\text{H}$ , 600 MHz, channel F2  $^{13}\text{C}$ , 150 MHz.



**Figure S2:** Attempt on direct  $^{187}\text{Os}$  NMR detection for  $[\text{}^{187}\text{Os}]\text{-1}$  (13.69 MHz). Only baseline noise is present.