



**New Journal of Chemistry**

**Photophysical properties of homobimetallic Cu(I)-Cu(I) and heterobimetallic Cu(I)-Ag(I) complexes of 2-(6-bromo-2-pyridyl)-1*H*-imidazo[4,5-*f*][1,10]phenanthroline**

Zhan Wu, Shu Cui, Zhenqin Zhao, Bingling He, Xiu-Ling Li\*

School of Chemistry and Materials Science, Jiangsu Normal University, Xuzhou, Jiangsu 221116, China

Table S1. Crystallographic data and select refinement details for complexes **1a**·4CH<sub>2</sub>Cl<sub>2</sub>, **2b**·2CH<sub>2</sub>Cl<sub>2</sub>·2CH<sub>3</sub>OH·2H<sub>2</sub>O, **1c**·4H<sub>2</sub>O and **2c**·4CH<sub>2</sub>Cl<sub>2</sub>

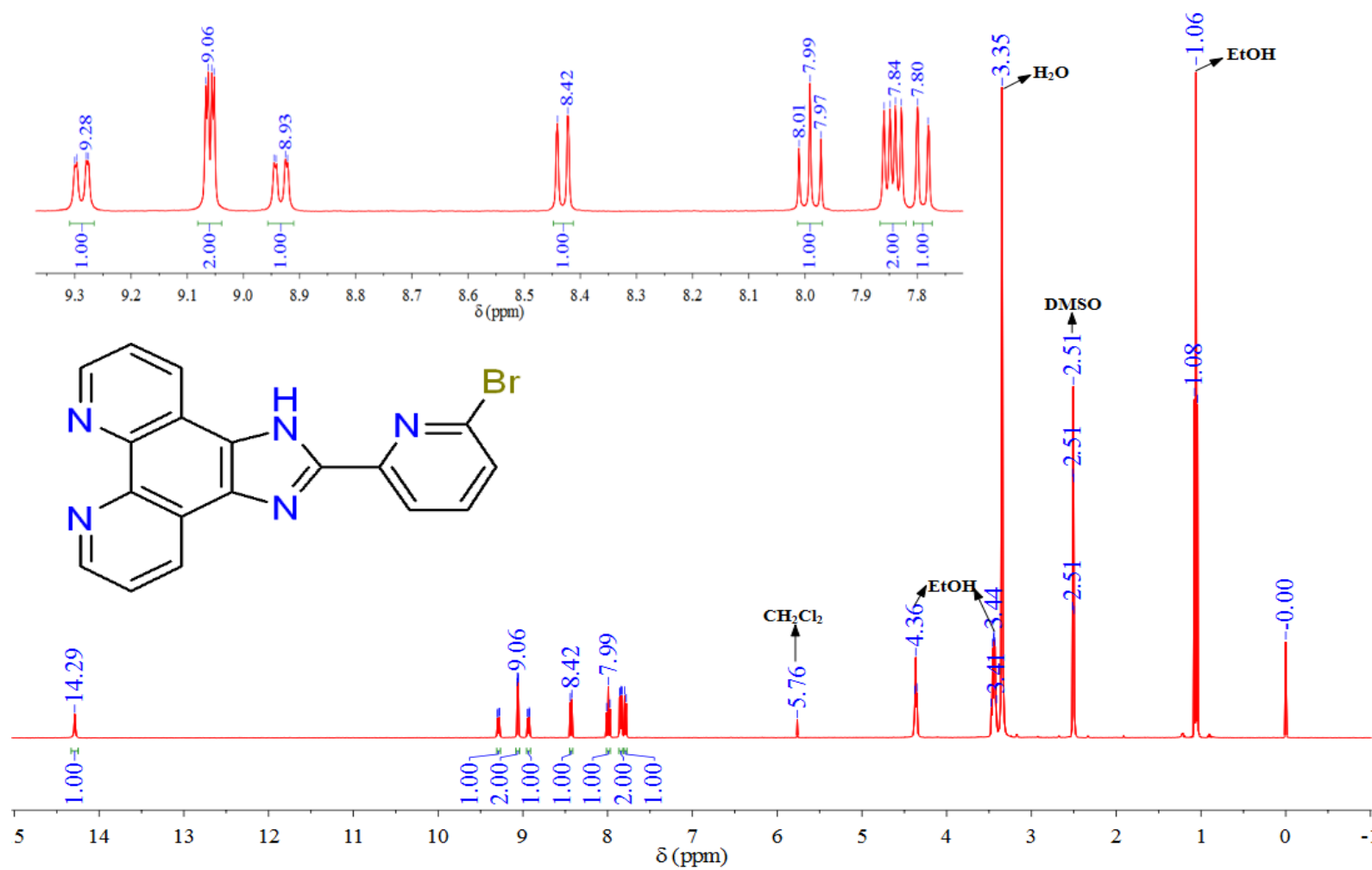
	<b>1a</b> ·4CH <sub>2</sub> Cl <sub>2</sub>	<b>2b</b> ·2CH <sub>2</sub> Cl <sub>2</sub> ·2CH <sub>3</sub> OH·2H <sub>2</sub> O	<b>1c</b> ·4H <sub>2</sub> O	<b>2c</b> ·4CH <sub>2</sub> Cl <sub>2</sub>
Formula weight	C <sub>94</sub> H <sub>74</sub> BrCl <sub>10</sub> Cu <sub>2</sub> N <sub>5</sub> O <sub>10</sub> P <sub>4</sub>	C <sub>100</sub> H <sub>89</sub> BrCl <sub>5</sub> Cu <sub>2</sub> N <sub>5</sub> O <sub>10</sub> P <sub>4</sub>	C <sub>90</sub> H <sub>73</sub> AgBrClCuN <sub>5</sub> O <sub>10</sub> P <sub>4</sub>	C <sub>100</sub> H <sub>81</sub> AgBrCl <sub>9</sub> CuN <sub>5</sub> O <sub>6</sub> P <sub>4</sub>
T (K)	150(2)	150(2)	150(2)	150(2)
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073
Crystal system	triclinic	monoclinic	orthorhombic	monoclinic
Space group	<i>P</i> -1	<i>Pc</i>	<i>P</i> 2 <sub>1</sub> 2 <sub>1</sub>	<i>P</i> 2 <sub>1</sub> / <i>c</i>
Unit cell dimensions				
a (Å)	15.5719(15)	13.8873(11)	13.8637(12)	18.887(4)
b (Å)	15.9403(15)	10.6708(8)	24.798(2)	18.800(4)
c (Å)	20.762(2)	31.655(2)	26.122(2)	27.414(6)
α (°)	82.0390(10)	90.00	90.00	90.00
β (°)	70.3860(10)	96.5600(10)	90.00	100.064(3)
γ (°)	83.2990(10)	90.00	90.00	90.00
V (Å <sup>3</sup> )	4794.2(8)	4660.2(6)	8980.5(13)	9584(4)
Z	2	2	4	4
D <sub>calc</sub> (Mg·m <sup>-3</sup> )	1.468	1.397	1.274	1.485
μ (mm <sup>-1</sup> )	1.265	1.155	1.052	1.218
F(000)	2152	2008	3504	3680
Reflections collected	24403	22894	36196	39931
Independent reflections	16608	12211	11582	13468
Reflections with I > 2σ(I)	13598	11457	10739	9549
Data/restraints/parameters	16608/0/1054	12211/2/1109	11582/0/983	13468/0/1036
Goodness-of-fit (GOF) on F <sup>2</sup>	1.044	1.053	1.038	1.007
Final R indices [I > 2σ(I)]	0.0451	0.0275	0.0315	0.0440
wR <sub>2</sub> [I > 2σ(I)]	0.1194	0.0693	0.0707	0.0970
R indices (all data)	0.0568	0.0304	0.0361	0.0714
wR <sub>2</sub> (all data)	0.1263	0.0703	0.0725	0.1071

**Table S2.** Main bond lengths (Å) and angles (°) for complexes **1a** 4CH<sub>2</sub>Cl<sub>2</sub>, **2b** 2CH<sub>2</sub>Cl<sub>2</sub>·2CH<sub>3</sub>OH·2H<sub>2</sub>O, **1c**·4H<sub>2</sub>O and **2c** 4CH<sub>2</sub>Cl<sub>2</sub>

<b>1a</b> 4CH <sub>2</sub> Cl <sub>2</sub>							
Cu1–N1	2.078(3)	Cu1–N2	2.045(3)	Cu1–P1	2.288(1)	Cu1–P2	2.210 (1)
C13–N3	1.363(4)	C13–N4	1.324(4)	Cu2–N4	2.061(3)	Cu2–N5	2.213(3)
Cu2–P3	2.287 (1)	Cu2–P4	2.245(1)	N1–Cu1–N2	81.25(10)	N1–Cu1–P1	99.95(7)
N1–Cu1–P2	133.74(8)	N2–Cu1–P1	100.95(7)	N2–Cu1–P2	118.20(7)	P1–Cu1–P2	114.87(3)
N4–Cu2–N5	79.06(10)	N4–Cu2–P3	102.29(7)	N4–Cu2–P4	118.51(8)	N5–Cu2–P3	104.06(8)
N5–Cu2–P4	123.26(8)	P3–Cu2–P4	120.90(3)				
<b>2b</b> 2CH <sub>2</sub> Cl <sub>2</sub> ·2CH <sub>3</sub> OH·2H <sub>2</sub> O							
Cu1–N1	2.069(3)	Cu1–N2	2.067(3)	Cu1–P1	2.222(1)	Cu1–P2	2.256(1)
C13–N3	1.361(5)	C13–N4	1.348(5)	Cu2–N4	2.044(3)	Cu2–N5	2.178(3)
Cu2–P3	2.247(1)	Cu2–P4	2.278(1)	N1–Cu1–N2	80.87(12)	N1–Cu1–P1	113.64(9)
N1–Cu1–P2	109.95(9)	N2–Cu1–P1	125.80(10)	N2–Cu1–P2	103.00(9)	P1–Cu1–P2	117.61(4)
N4–Cu2–N5	79.79(12)	N4–Cu2–P3	123.50(9)	N4–Cu2–P4	106.77(10)	N5–Cu2–P3	114.65(9)
N5–Cu2–P4	103.17(9)	P3–Cu2–P4	120.33(4)				
<b>1c</b> ·4H <sub>2</sub> O							
Cu1–N1	2.081(4)	Cu1–N2	2.046(4)	Cu1–P1	2.208(2)	Cu1–P2	2.283(2)
C13–N3	1.366(7)	C13–N4	1.346(6)	Ag1–N4	2.265(4)	Ag1–N5	2.491(4)
Ag1–P3	2.524(2)	Ag1–P4	2.404(2)	N1–Cu1–N2	80.98(16)	N1–Cu1–P1	129.86(13)
N1–Cu1–P2	98.57(13)	N2–Cu1–P1	120.66(14)	N2–Cu1–P2	105.36(14)	P1–Cu1–P2	114.96(6)
N4–Ag1–N5	71.00(14)	N4–Ag1–P3	103.28(12)	N4–Ag1–P4	128.78(12)	N5–Ag1–P3	93.96(11)
N5–Ag1–P4	139.57(11)	P3–Ag1–P4	110.87(5)				
<b>2c</b> 4CH <sub>2</sub> Cl <sub>2</sub>							
Cu1–N1	2.039(3)	Cu1–N2	2.102(3)	Cu1–P1	2.244(1)	Cu1–P2	2.237(1)
C13–N3	1.341(5)	C13–N4	1.358(5)	Ag1–N4	2.264(3)	Ag1–N5	2.477(3)

Ag1-P3	2.469(1)	Ag1-P4	2.443(1)	N1-Cu1-N2	80.57(13)	N1-Cu1-P1	119.06(10)
N1-Cu1-P2	118.32(10)	N2-Cu1-P1	107.43(10)	N2-Cu1-P2	111.60(10)	P1-Cu1-P2	113.90(5)
N4-Ag1-N5	71.42(11)	N4-Ag1-P3	117.29(8)	N4-Ag1-P4	125.43(8)	N5-Ag1-P3	106.74(8)
N5-Ag1-P4	114.51(8)	P3-Ag1-P4	112.28(4)				

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Figure S1.  $^1\text{H}$  NMR of bippH in  $\text{DMSO-}d_6$

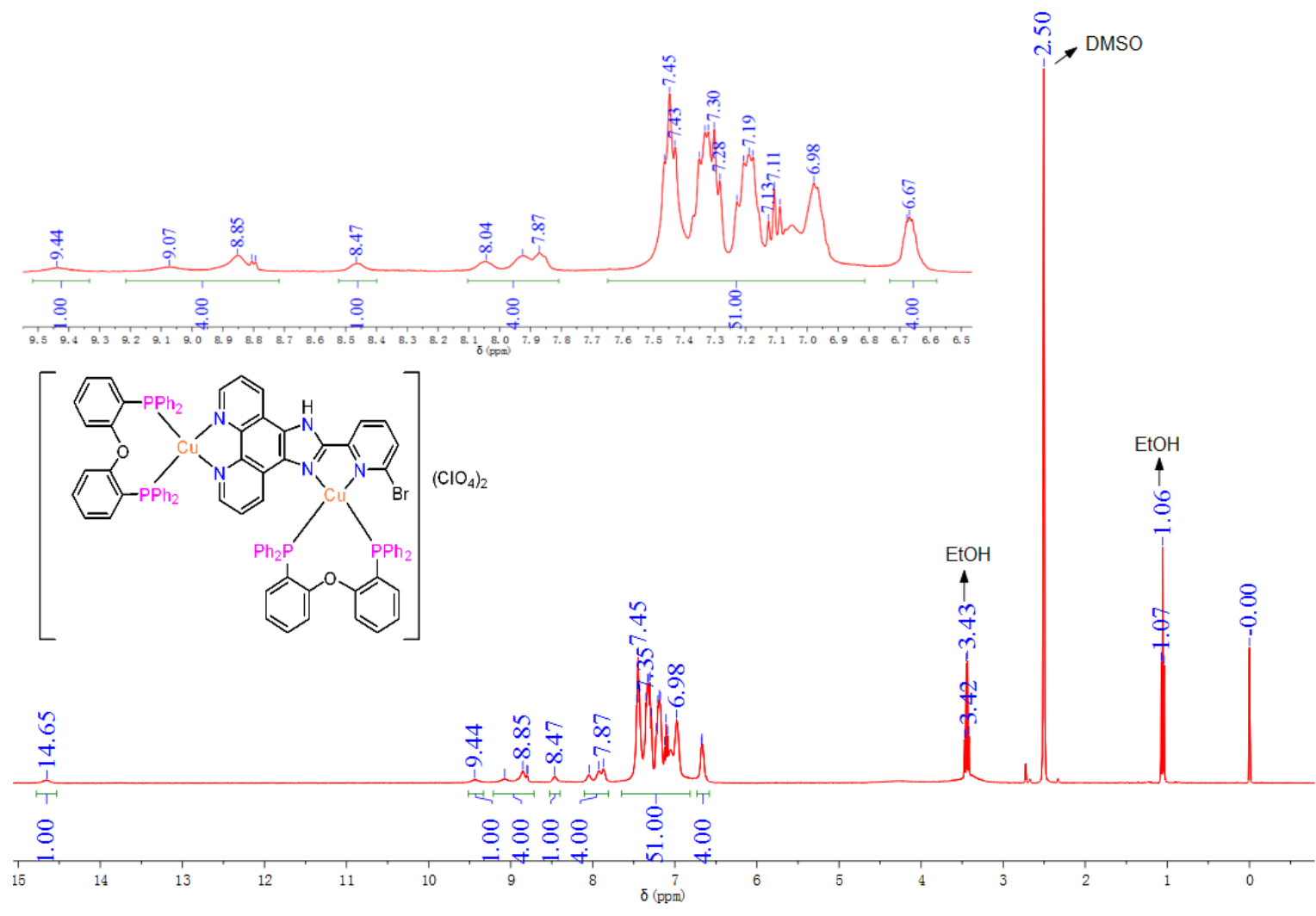
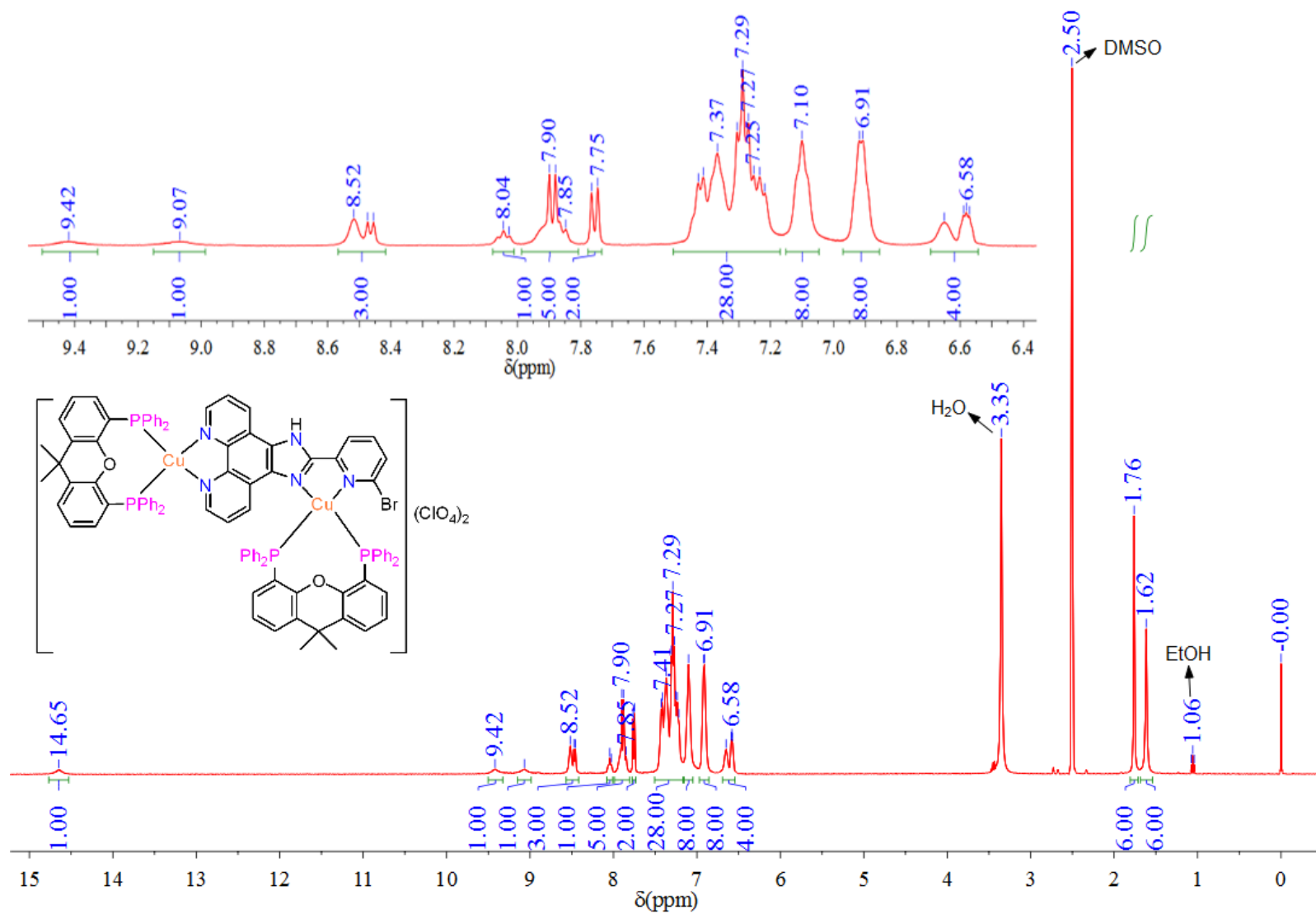


Figure S2. <sup>1</sup>H NMR of complex **1a** in DMSO-*d*<sub>6</sub>

Figure S3.  $^1\text{H}$  NMR of complex **2a** in  $\text{DMSO-}d_6$

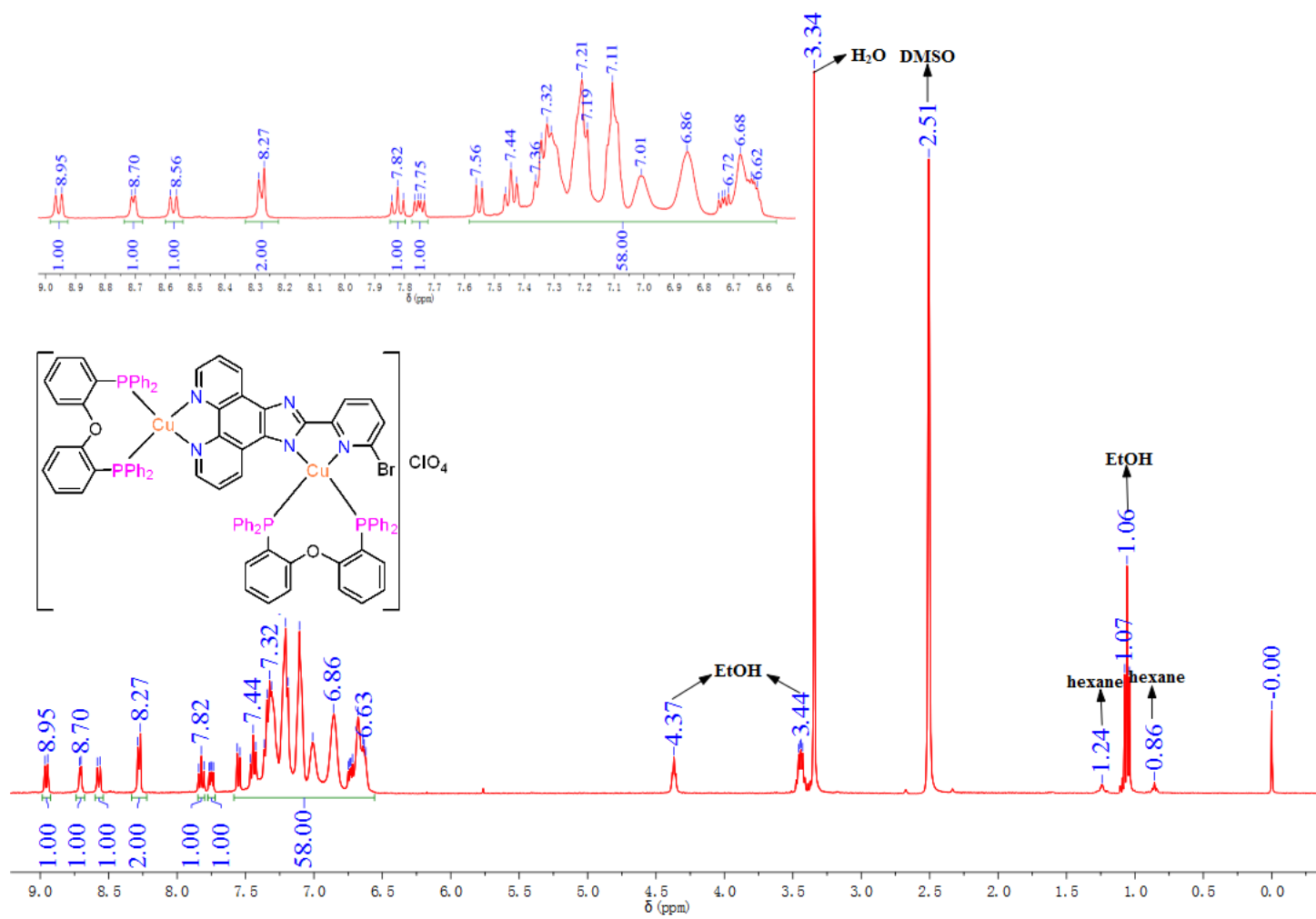
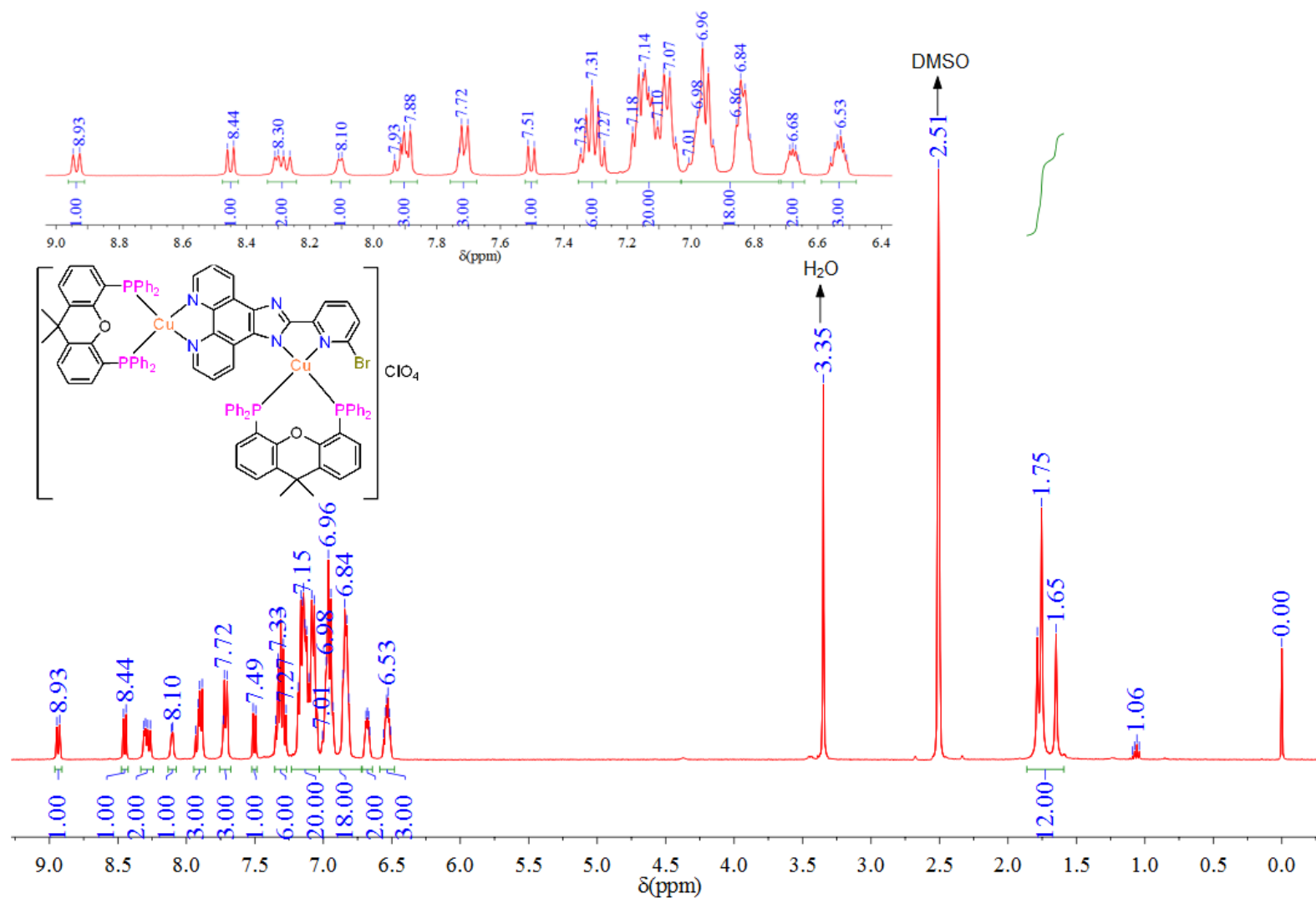


Figure S4.  $^1\text{H}$  NMR of complex **1b** in  $\text{DMSO-}d_6$



Figure S5.  $^1\text{H}$  NMR of complex **2b** in  $\text{DMSO-}d_6$

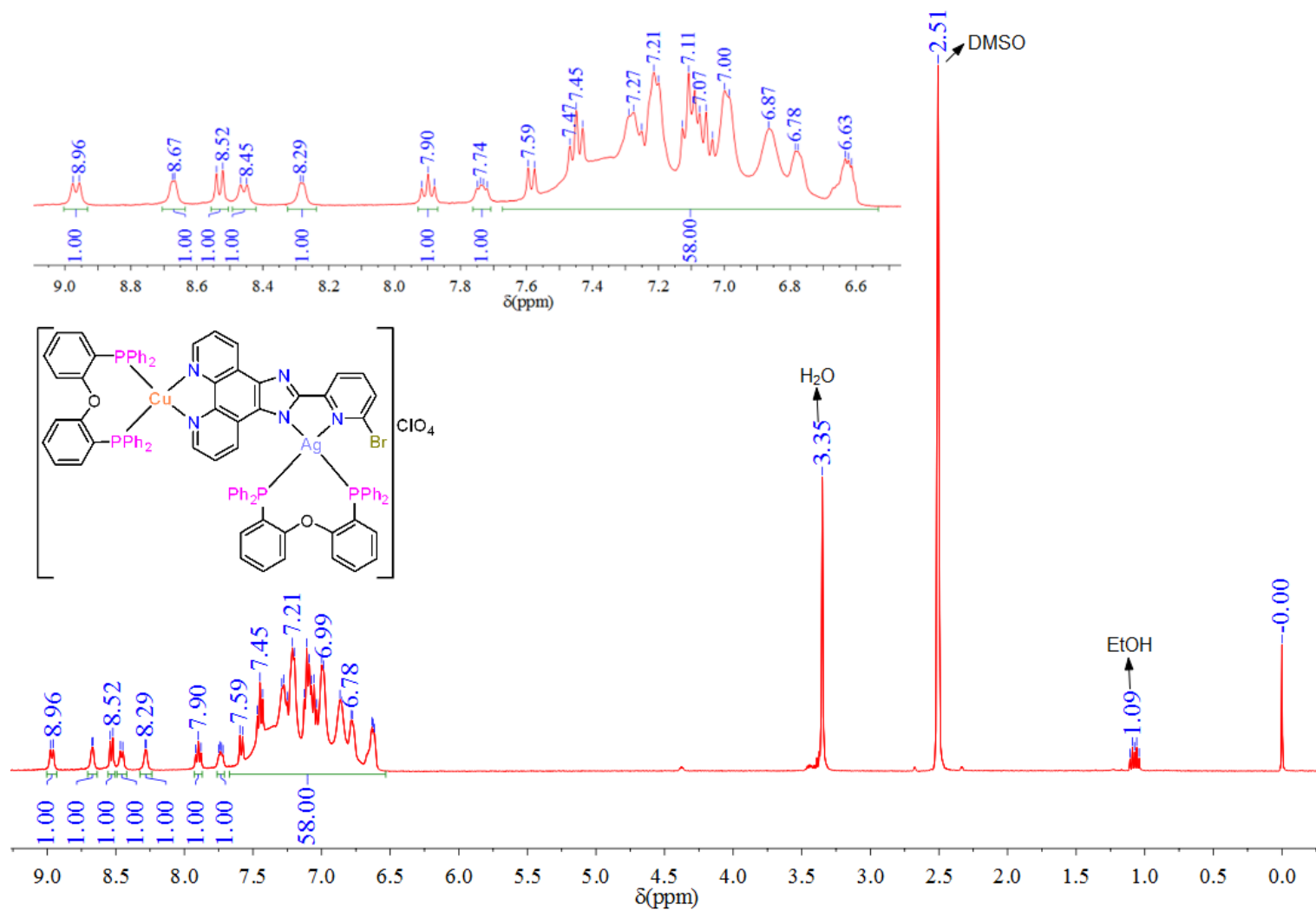
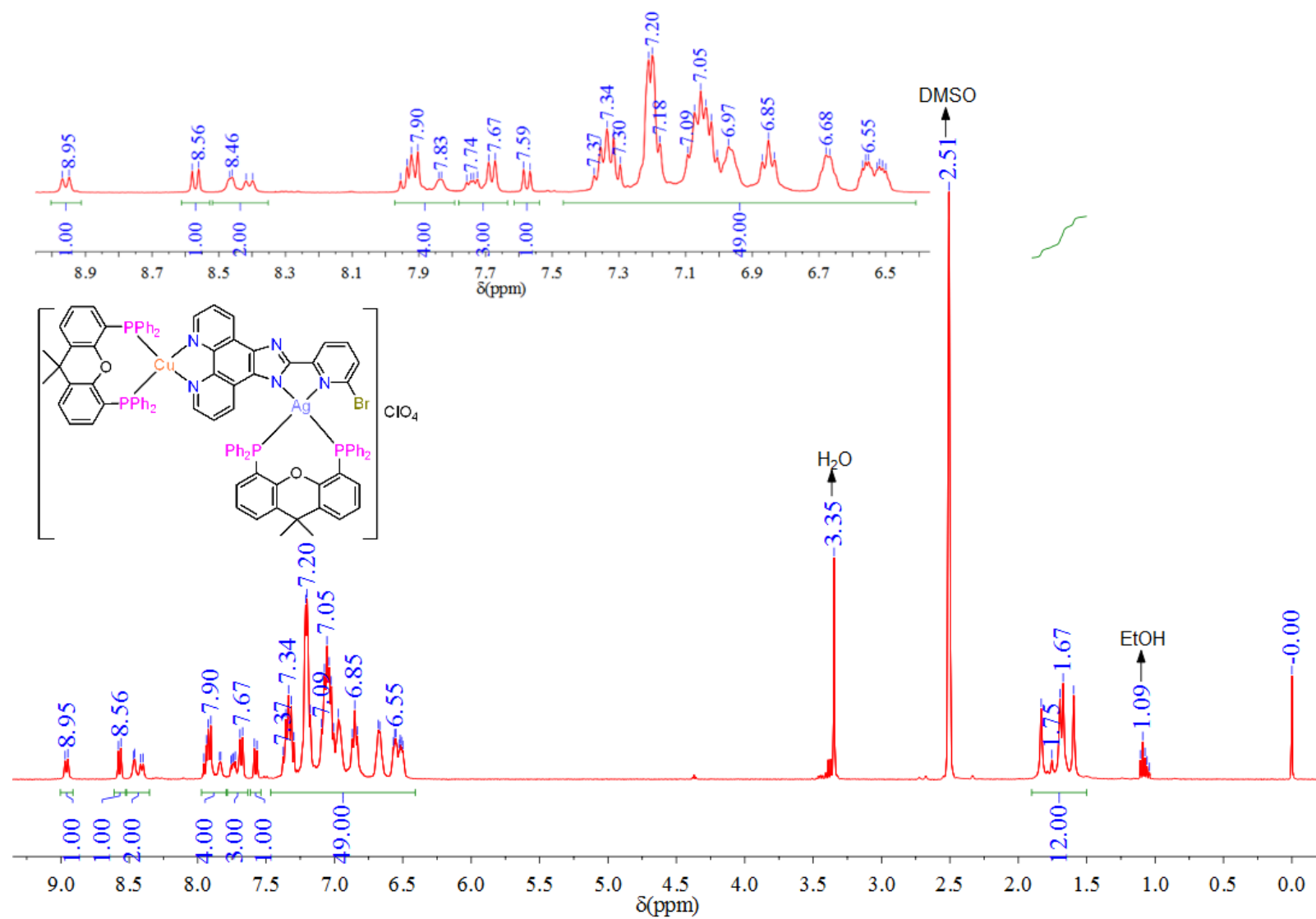


Figure S6.  $^1\text{H}$  NMR of complex **1c** in  $\text{DMSO-}d_6$

Figure S7.  $^1\text{H}$  NMR of complex **2c** in  $\text{DMSO-}d_6$

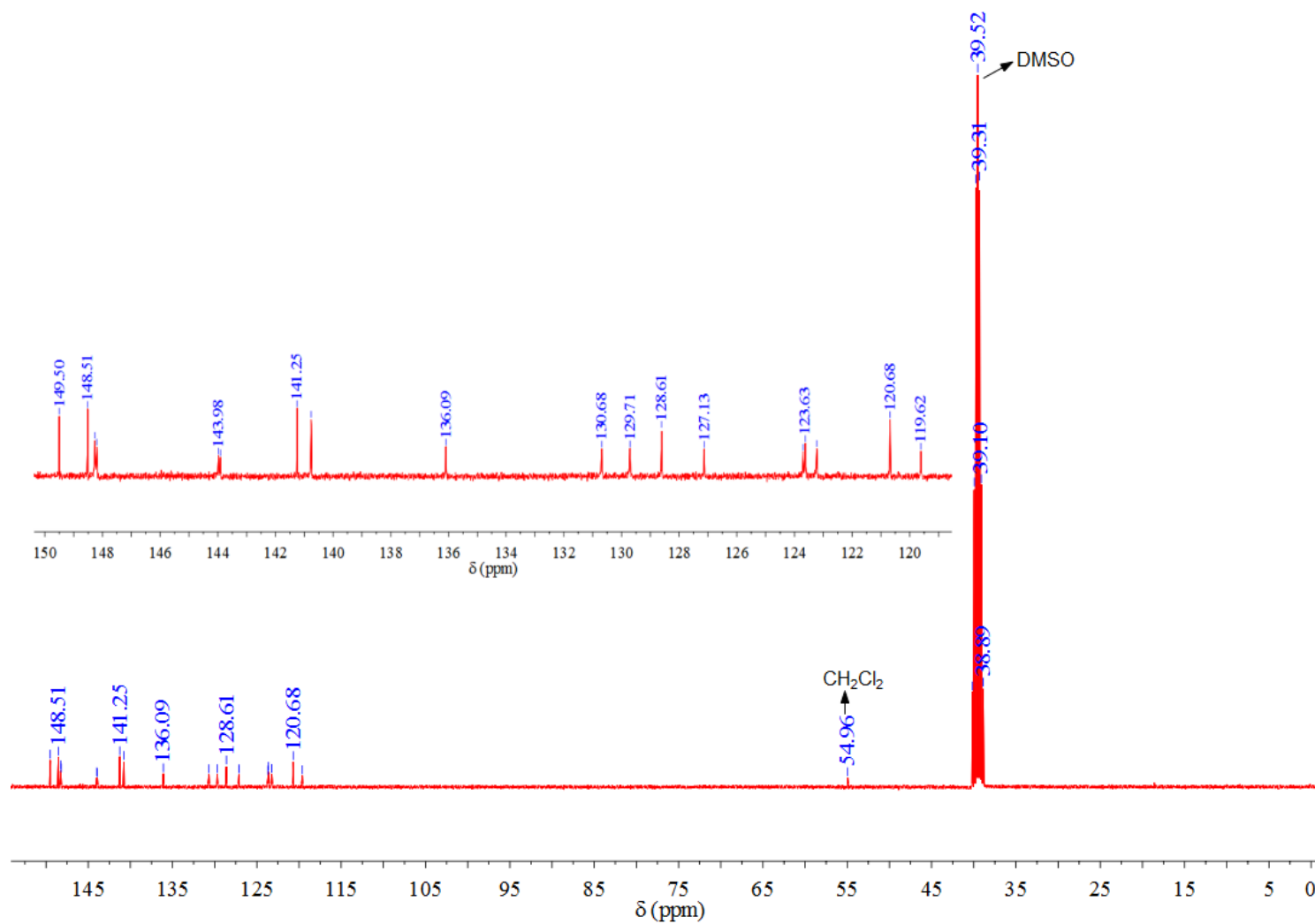


Figure S8.  $^{13}\text{C}$  NMR of bpiPH in  $\text{DMSO-}d_6$

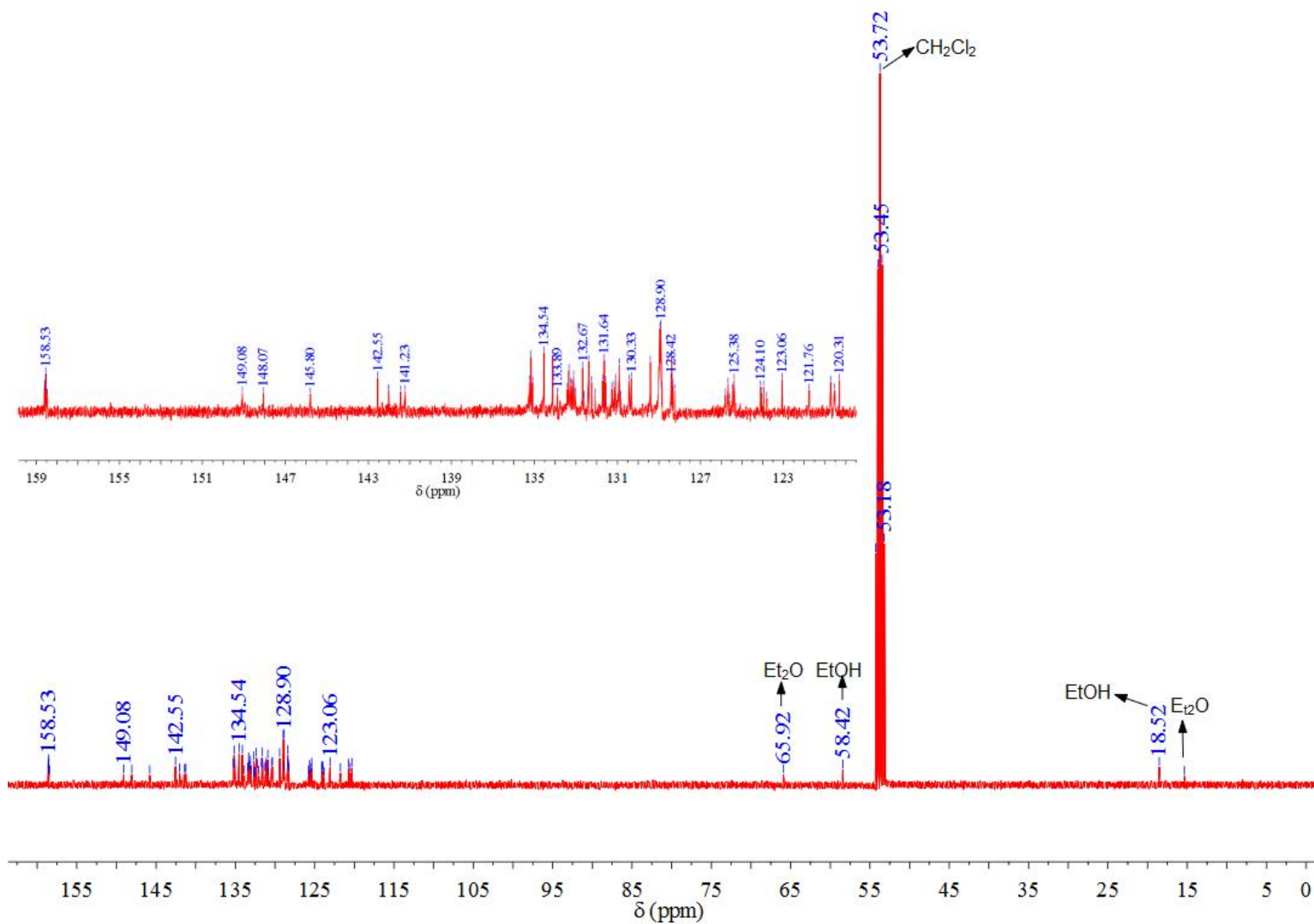


Figure S9. <sup>13</sup>C NMR of complex **1a** in CD<sub>2</sub>Cl<sub>2</sub>

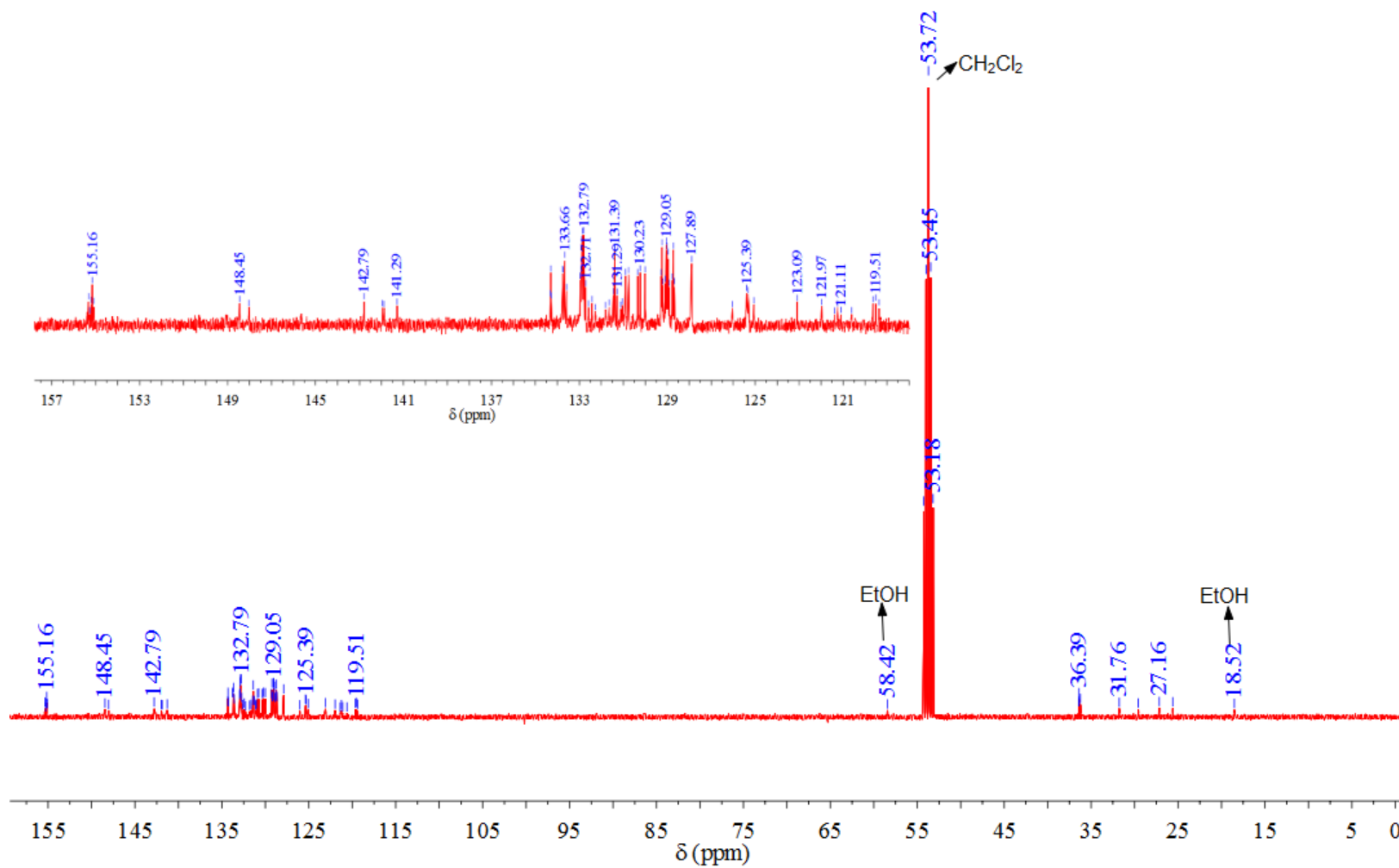
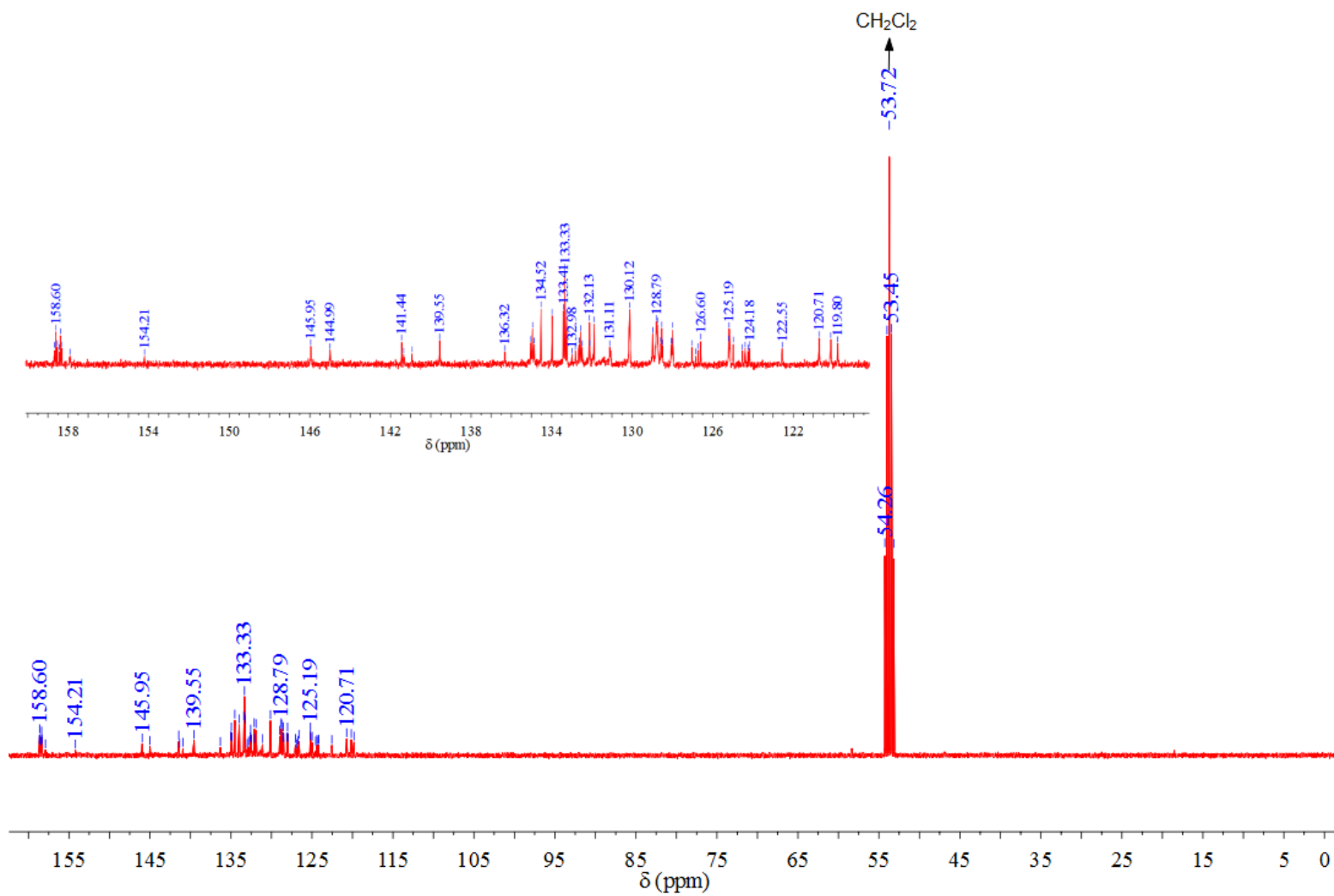


Figure S10.  $^{13}\text{C}$  NMR of complex **2a** in  $\text{CD}_2\text{Cl}_2$

Figure S11.  $^{13}\text{C}$  NMR of complex **1b** in  $\text{CD}_2\text{Cl}_2$

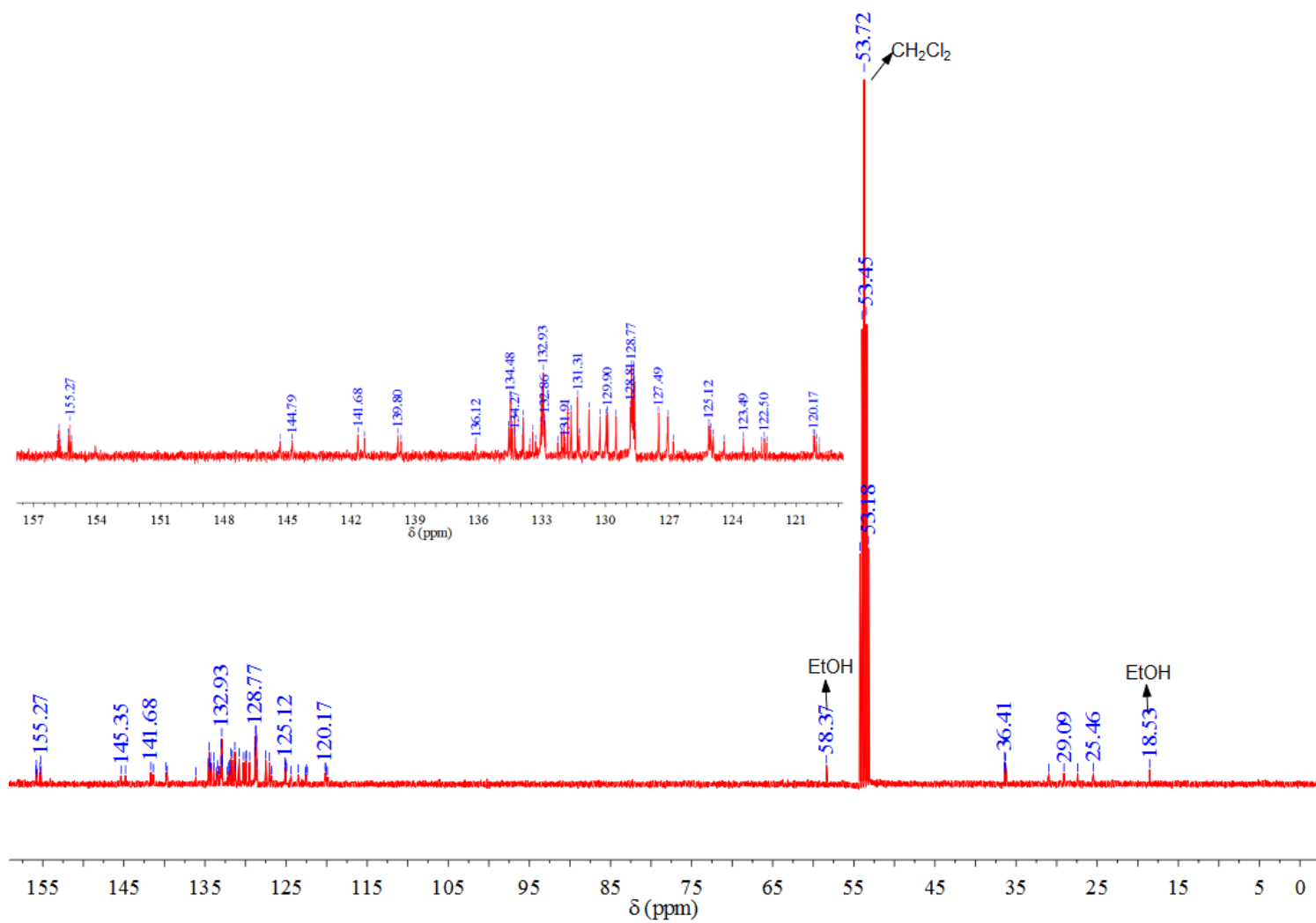
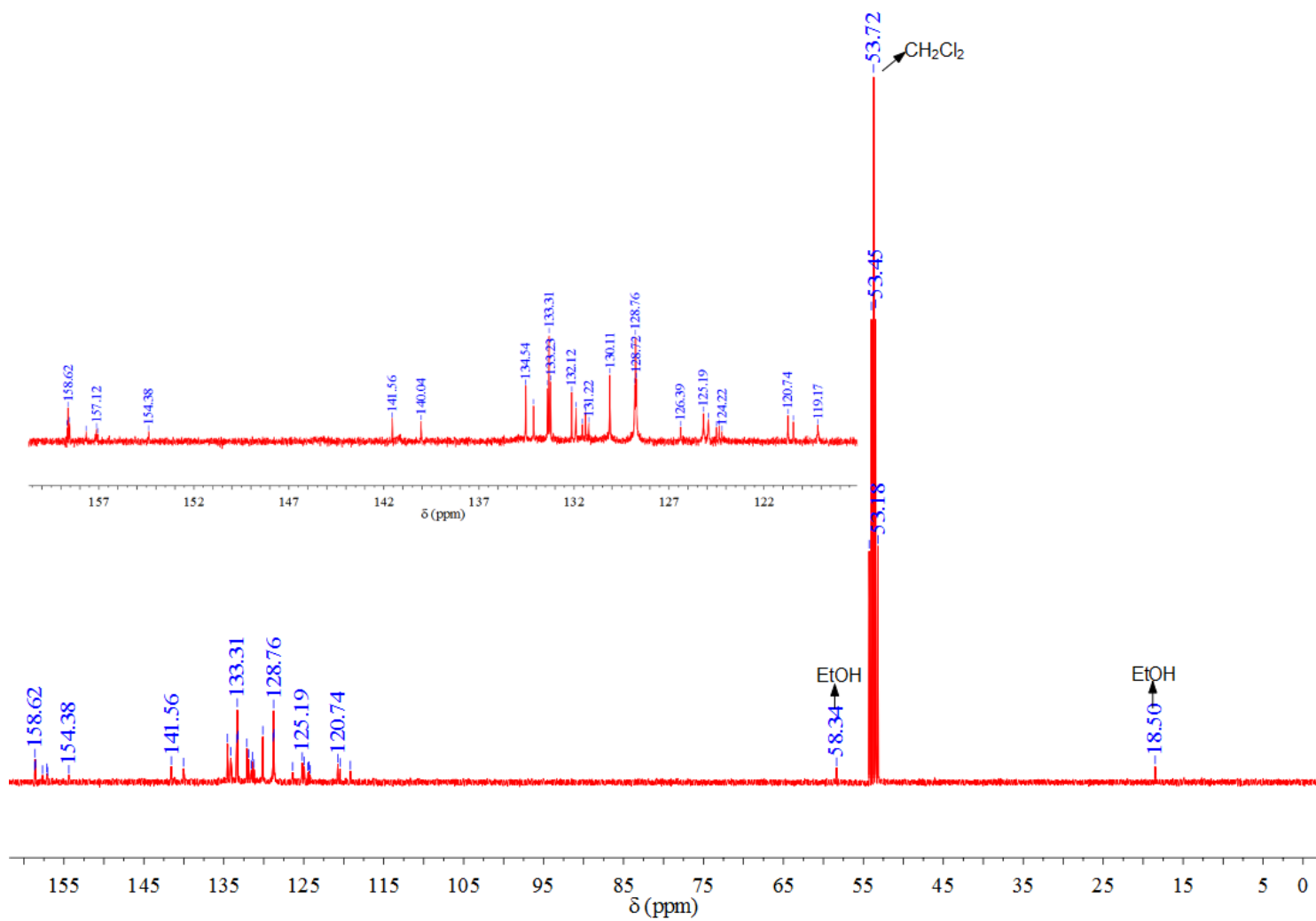


Figure S12.  $^{13}\text{C}$  NMR of complex **2b** in  $\text{CD}_2\text{Cl}_2$



Figure S13.  $^{13}\text{C}$  NMR of complex **1c** in  $\text{CD}_2\text{Cl}_2$

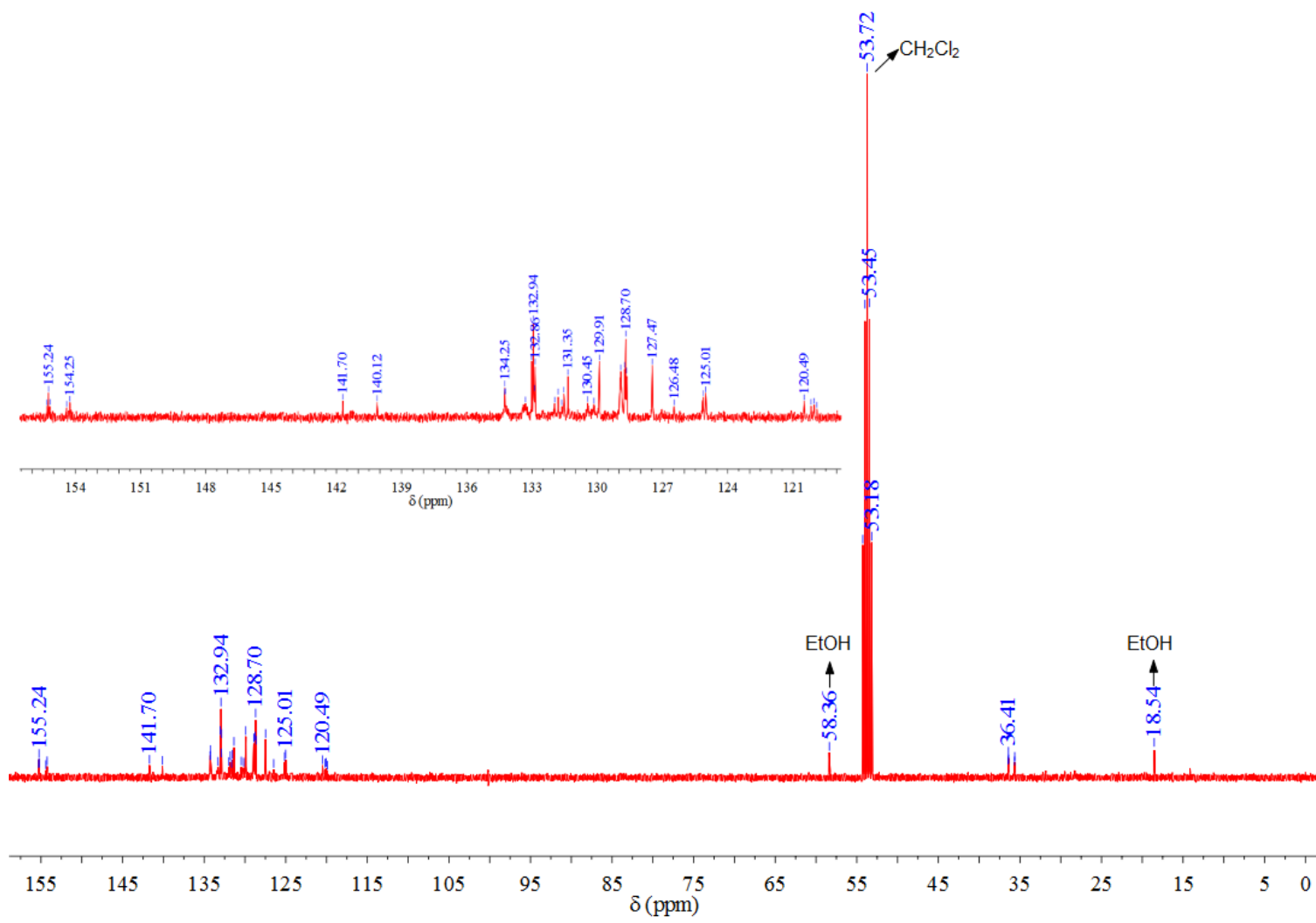


Figure S14.  $^{13}\text{C}$  NMR of complex **2c** in  $\text{CD}_2\text{Cl}_2$

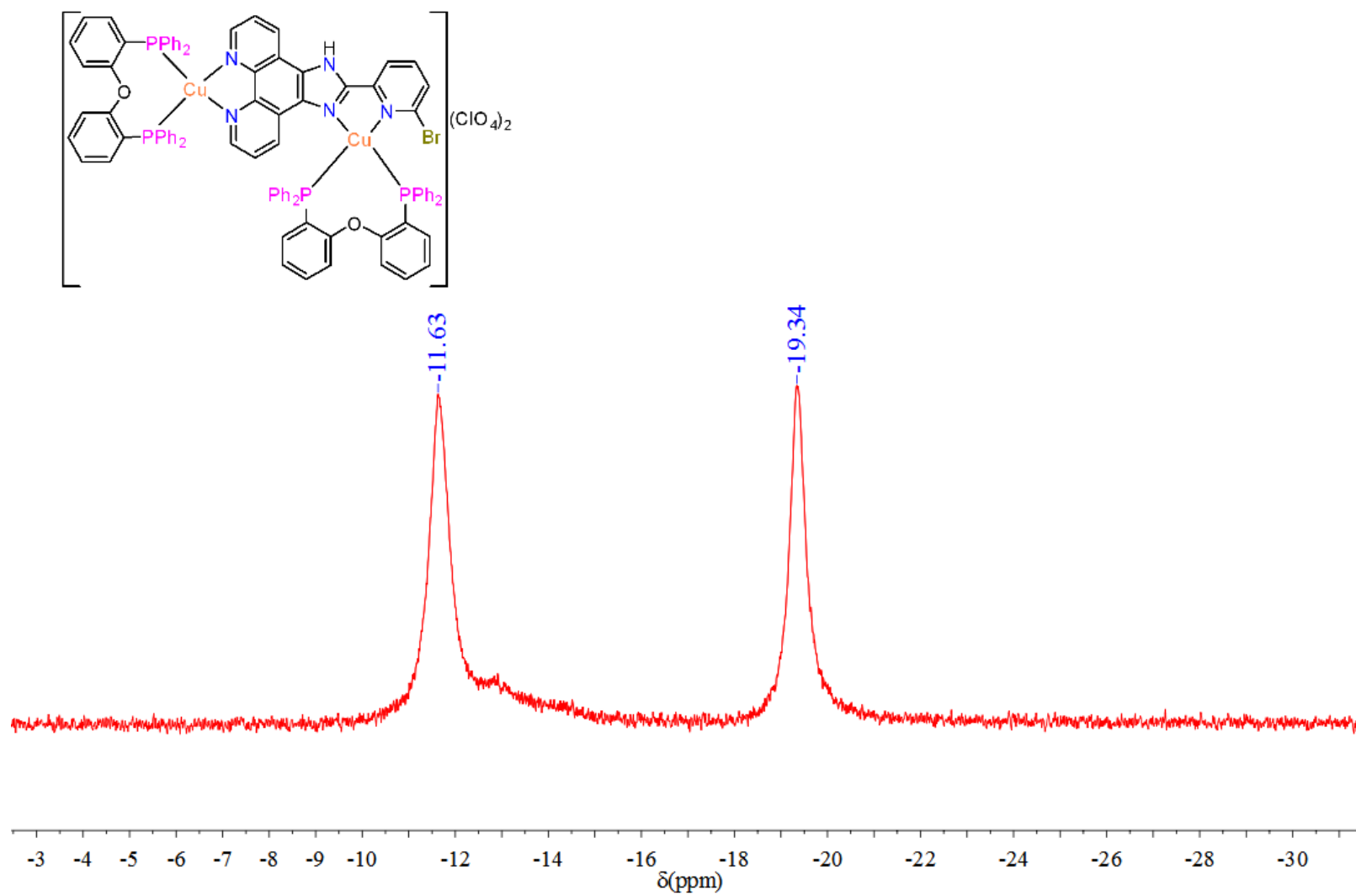


Figure S15.  $^{31}\text{P}$   $\{^1\text{H}\}$  NMR of complex **1a** in DMSO-*d*<sub>6</sub>

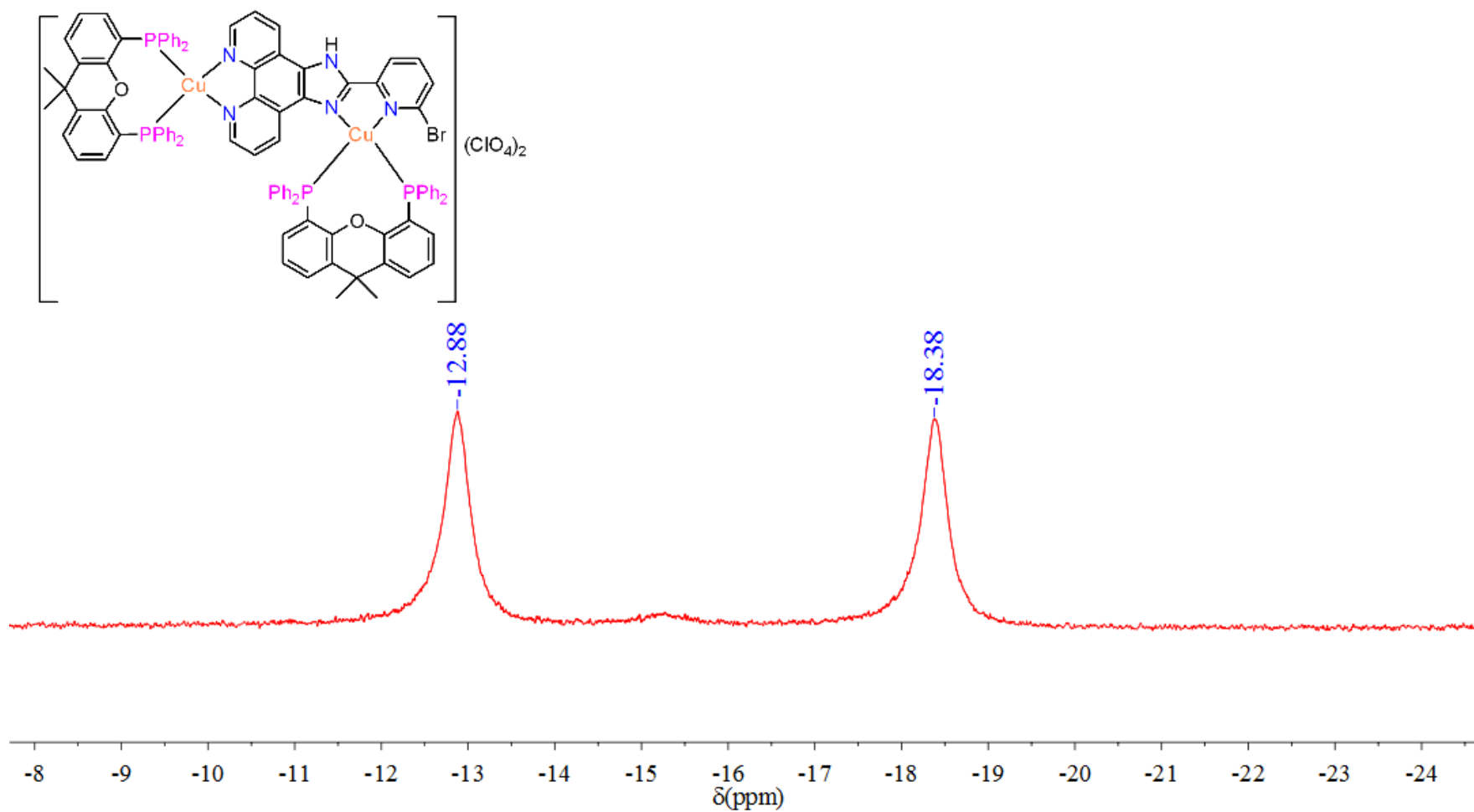


Figure S16.  $^{31}\text{P}$   $\{^1\text{H}\}$  NMR of complex **2a** in  $\text{DMSO-}d_6$

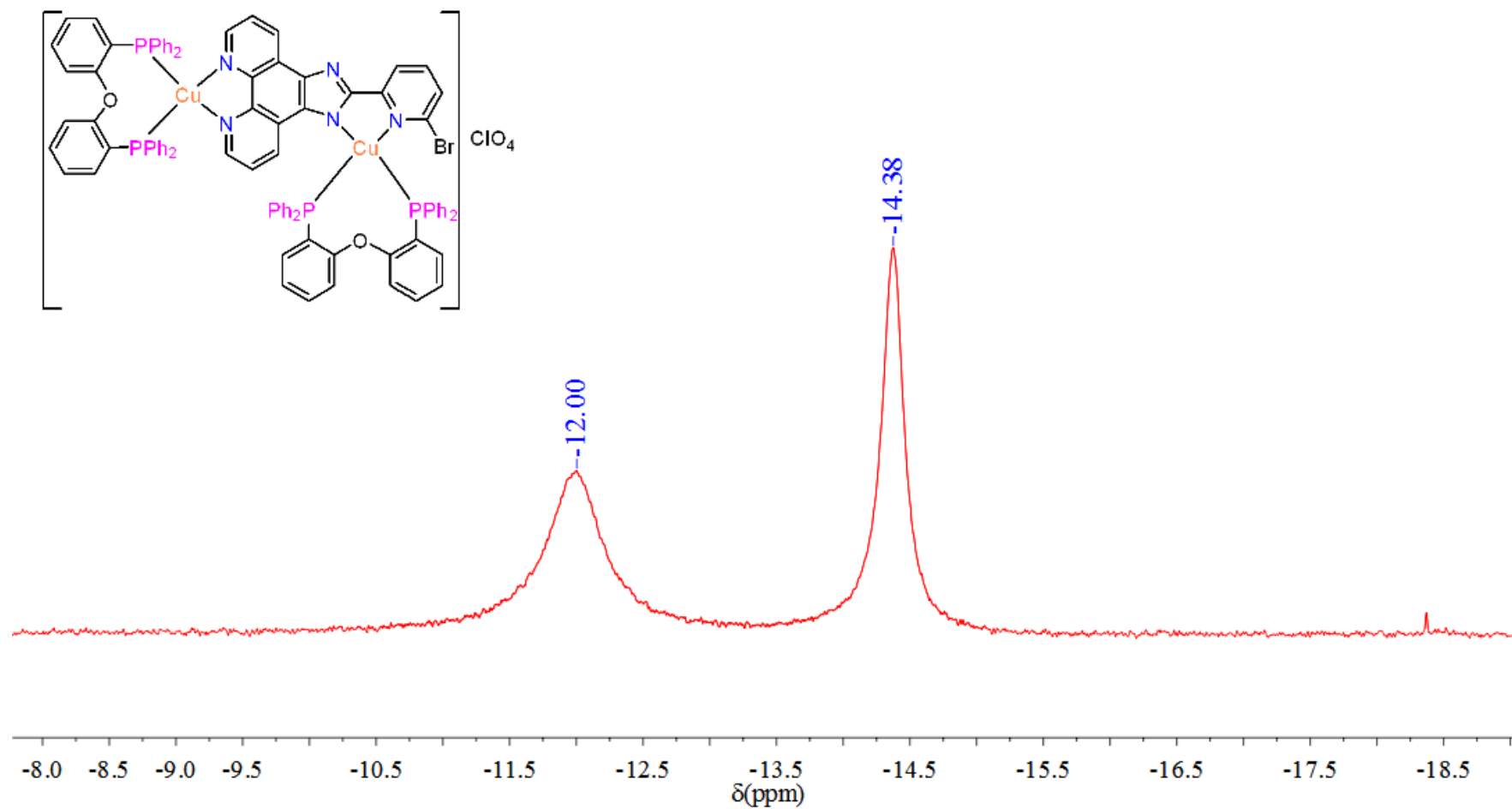


Figure S17.  $^{31}\text{P}$  { $^1\text{H}$ } NMR of complex **1b** in  $\text{DMSO-}d_6$

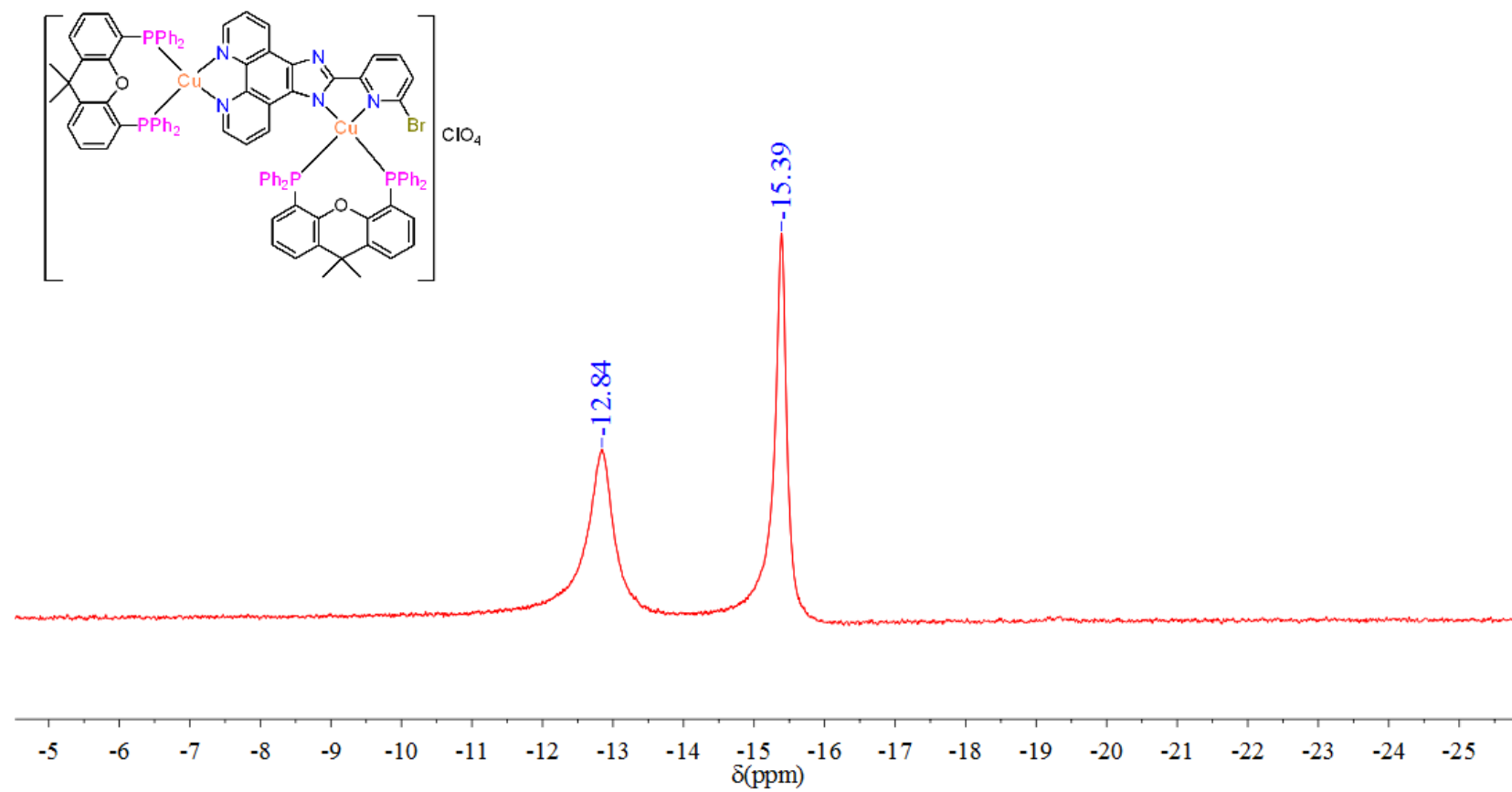


Figure S18.  $^{31}\text{P}$   $\{^1\text{H}\}$  NMR of complex **2b** in  $\text{DMSO-}d_6$

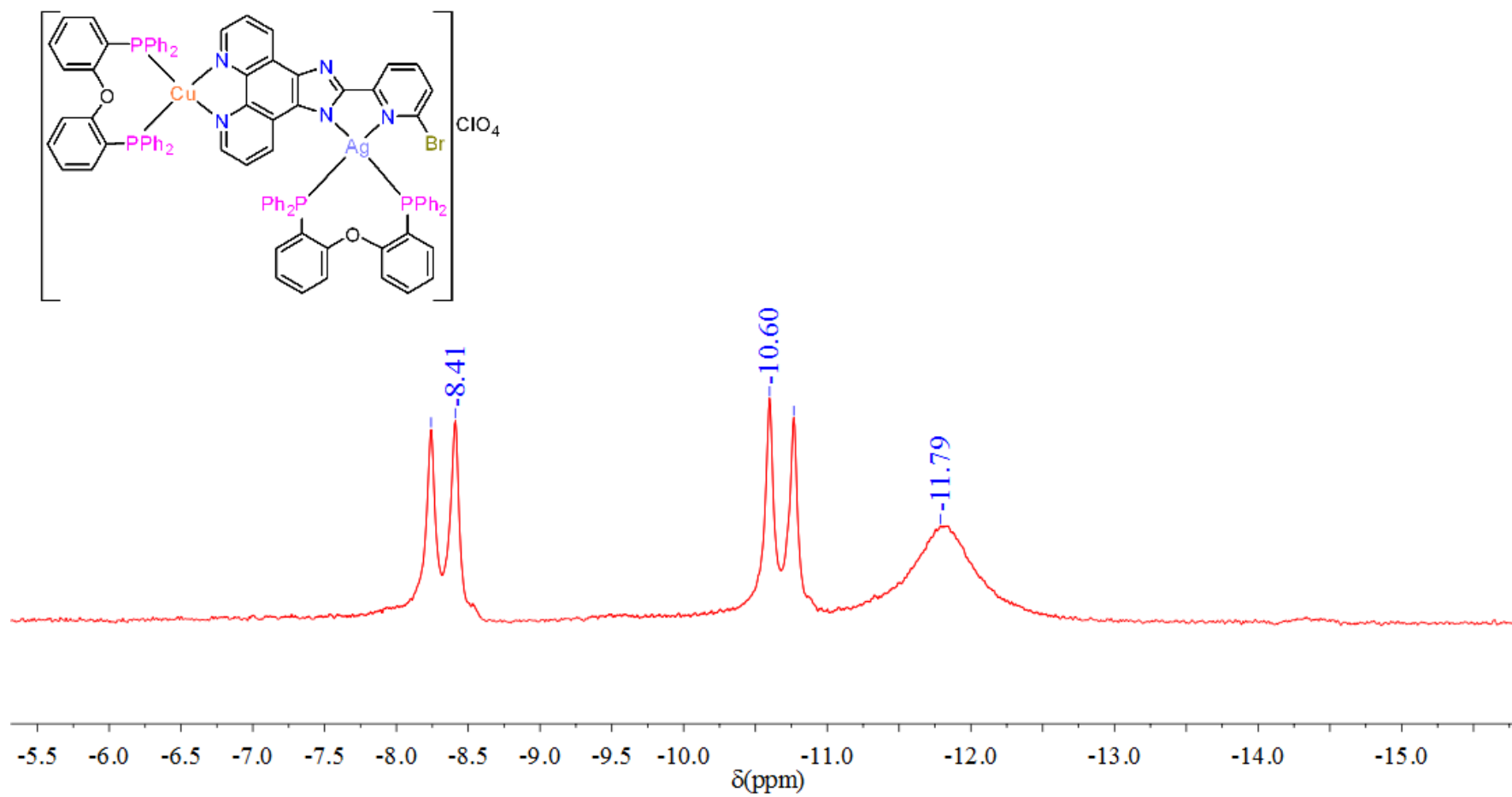


Figure S19.  $^{31}\text{P}$   $\{^1\text{H}\}$  NMR of complex **1c** in DMSO-*d*<sub>6</sub>

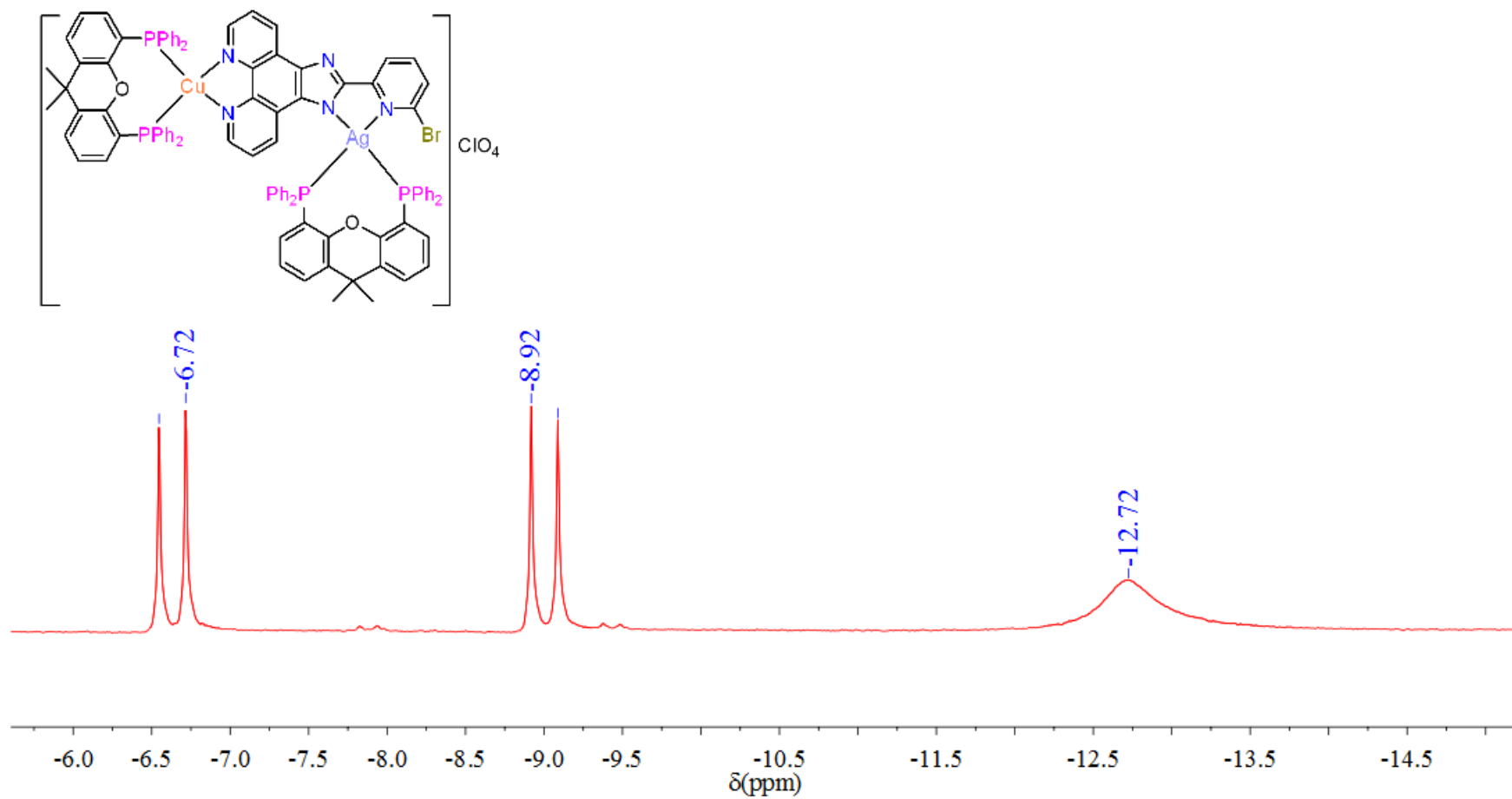


Figure S20.  $^{31}\text{P}$   $\{^1\text{H}\}$  NMR of complex **2c** in  $\text{DMSO-}d_6$



● Spectrum from Data20220318-02-P-1+2-1.wiff (sample 1) - Sample001, Experiment 1, +TOF MS (80 - 5000) from 0.094 to 0.113 min  
 ● C18H11BrN5

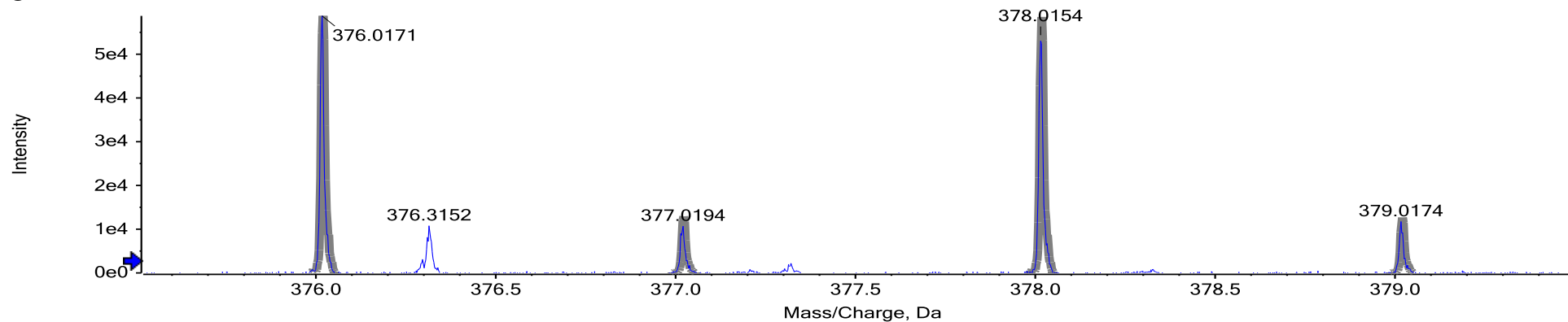
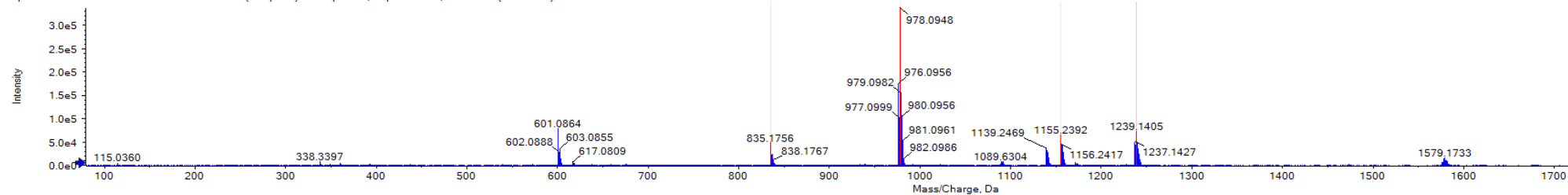
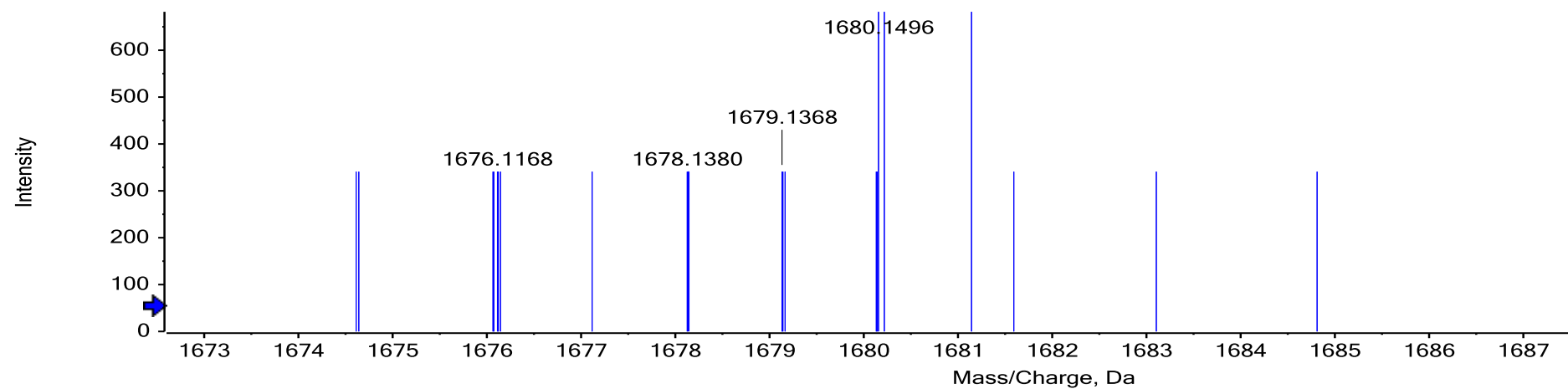


Figure S21. MS spectra of bpipH

Spectrum from Data20220318-02-P-1+2-2.wiff (sample 1) - Sample002, Experiment 1, +TOF MS (80 - 5000) from 0.103 min



Spectrum from Data20220318-02-P-1+2-2.wiff (sample 1) - Sample002, Experiment 1, +TOF MS (80 - 5000) from 0.103 min



Spectrum from Data20220318-02-P-1+2-2.wiff (sample 1) - Sample002, Experiment 1, +TOF MS (80 - 5000) from 0.122 min

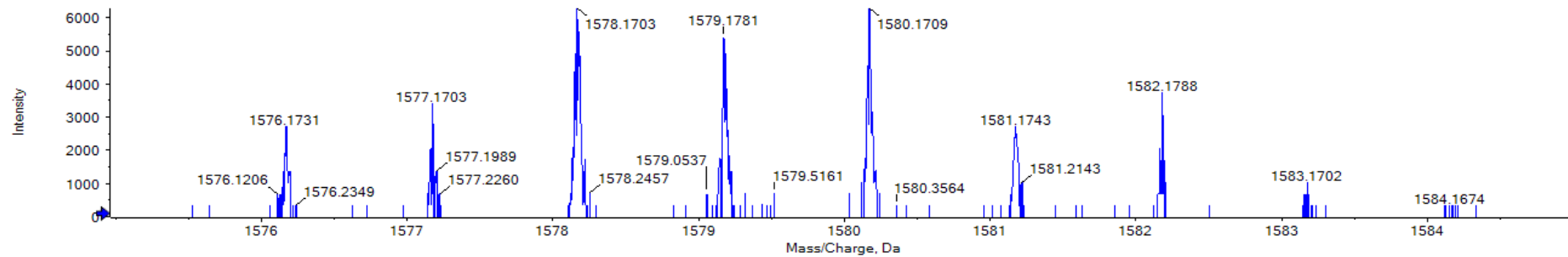
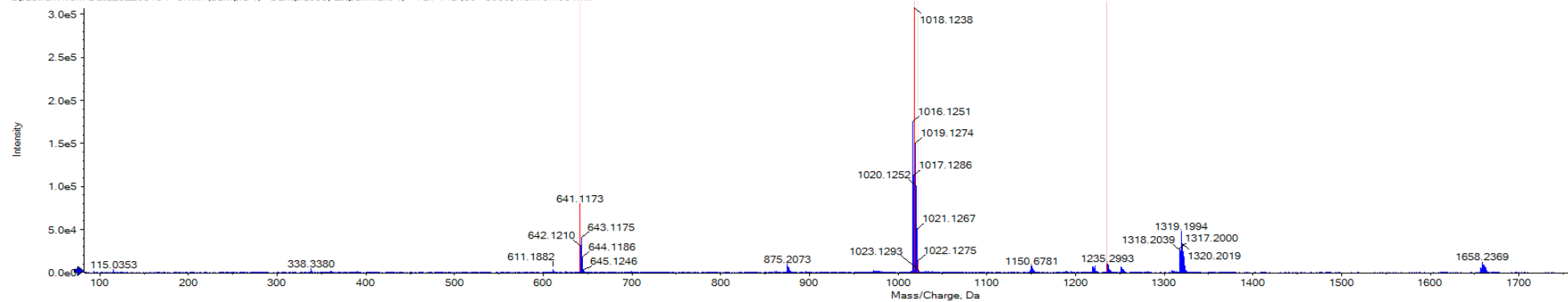
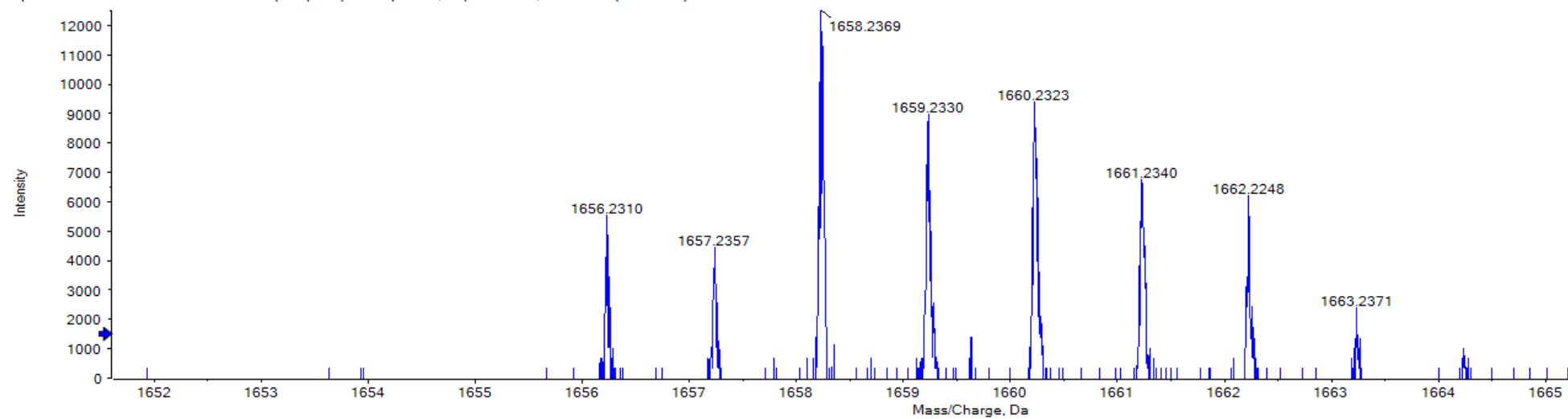


Figure S22. MS spectra of complex **1a**

Spectrum from Data20220318-P-3.wiff (sample 1) - Sample003, Experiment 1, -TOF MS (80 - 5000) from 0.103 min



Spectrum from Data20220318-P-3.wiff (sample 1) - Sample003, Experiment 1, +TOF MS (80 - 5000) from 0.103 min



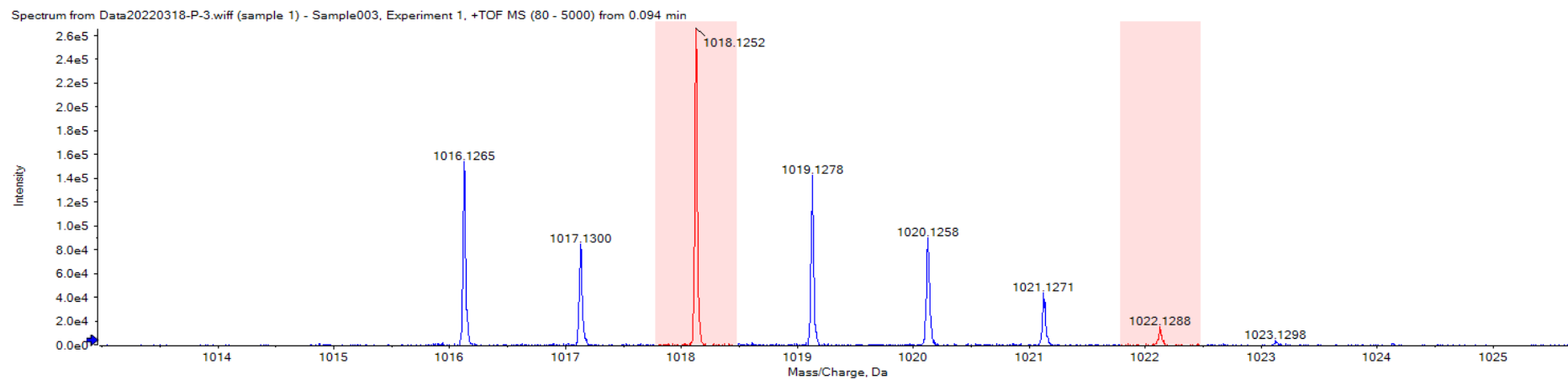


Figure S23. MS spectra of complex **2a**

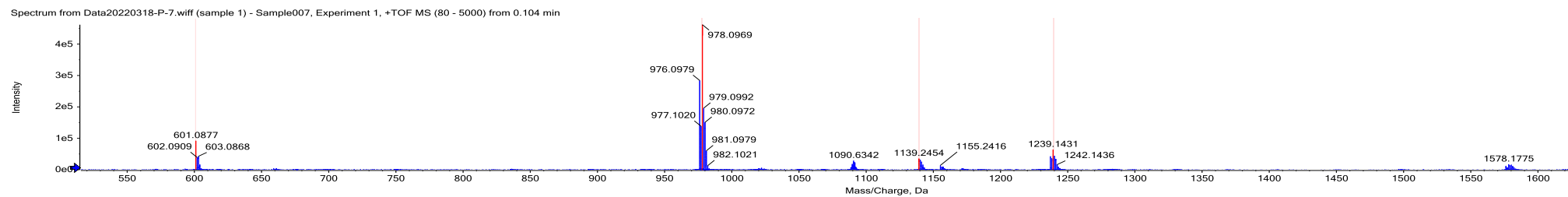


Figure S24. MS spectra of complex **1b**

Spectrum from Data20220318-P-6.wiff (sample 1) - Sample006, Experiment 1, +TOF MS (80 - 5000) from 0.094 min

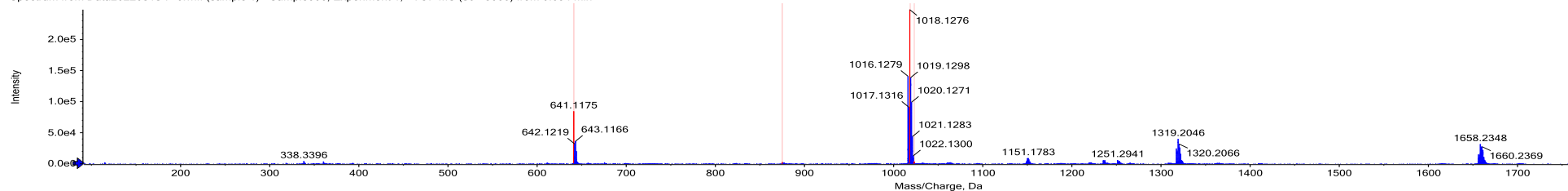


Figure S25. MS spectra of complex **2b**

Spectrum from Data20220318-P-8~13-5.wiff (sample 1) - Sample005, Experiment 1, +TOF MS (80 - 5000) from 0.103 min

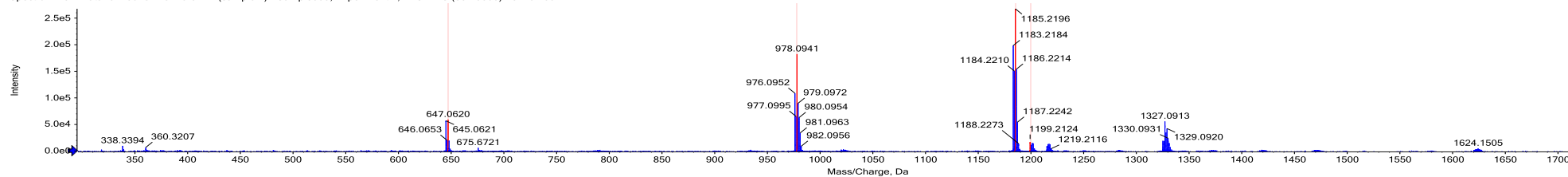


Figure S26. MS spectra of complex **1c**

Spectrum from Data20220318-P-8~13-6.wiff (sample 1) - Sample006, Experiment 1, +TOF MS (80 - 5000) from 0.063 min

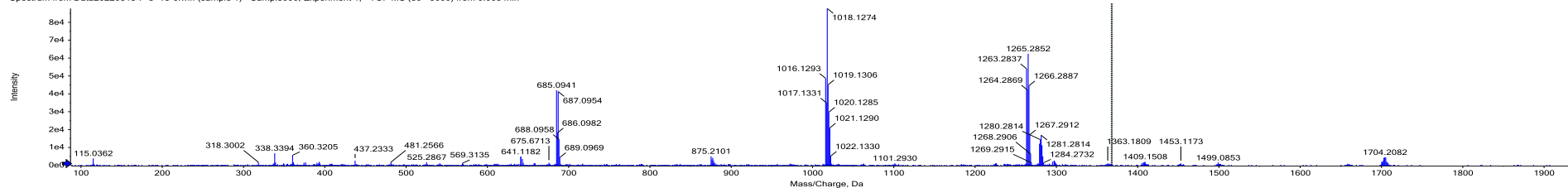


Figure S27. MS spectra of complex **2c**