

## Electronic Supplementary Material

### **A new amido-phosphane as ligand for copper and silver complexes. Synthesis, characterization and catalytic application for azide-alkyne cycloaddition in glycerol**

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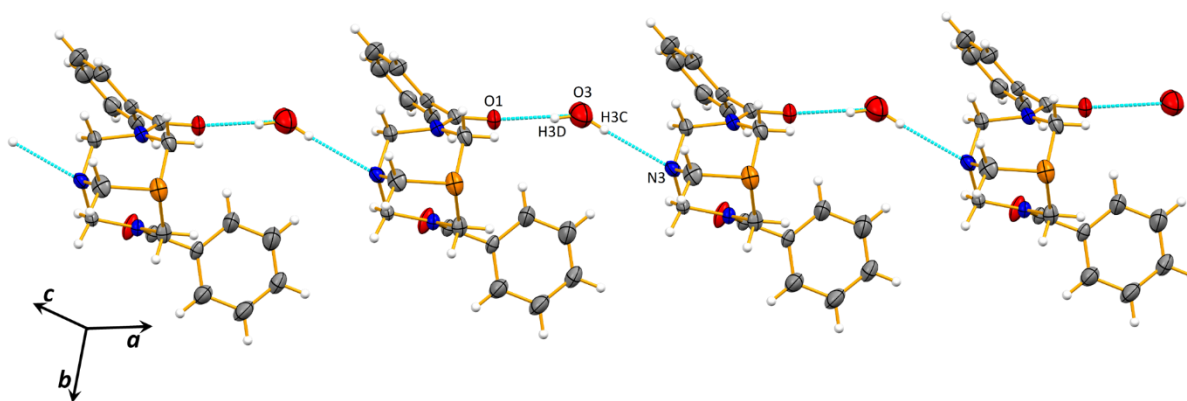
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## 1. X-ray data



**Figure S1.** The H-bond 1D chain of compound **1** spreading along the crystallographic *a* axis.

**Table S1.** Crystallographic data and structure refinement details for **1**.

Empirical formula	C <sub>38</sub> H <sub>42</sub> N <sub>6</sub> O <sub>5</sub> P
Formula Weight	724.71
Crystal system	monoclinic
Space group	P 21/n
Temperature/K	298(2)
<i>a</i> /Å	9.5691(5)
<i>b</i> /Å	21.4898(12)
<i>c</i> /Å	10.0298(5)
$\beta$ /°	116.955(2)
<i>V</i> (Å <sup>3</sup> )	1819.0(5)
<i>Z</i>	2
<i>D</i> <sub>calc</sub> (g cm <sup>-3</sup> )	1.309
<i>F</i> 000	764
$\mu$ (Mo K $\alpha$ ) (mm <sup>-1</sup> )	0.170
Rfls. collected/unique/observed	26254 / 4024 / 2779
<i>R</i> <sub>int</sub>	0.0533
Final <i>R</i> 1 <sup>a</sup> , <i>wR</i> 2 <sup>b</sup> ( <i>I</i> ≥ 2σ)	0.1226, 0.3516
Goodness-of-fit on <i>F</i> <sup>2</sup>	1.209

$$^a R = \sum ||F_o| - |F_c|| / \sum |F_o|; ^b wR(F^2) = [\sum w(|F_o|^2 - |F_c|^2)^2 / \sum w|F_o|^4]^{1/2}.$$

## 2. NMR spectra of DBPTA (1) and its complexes 2-12.

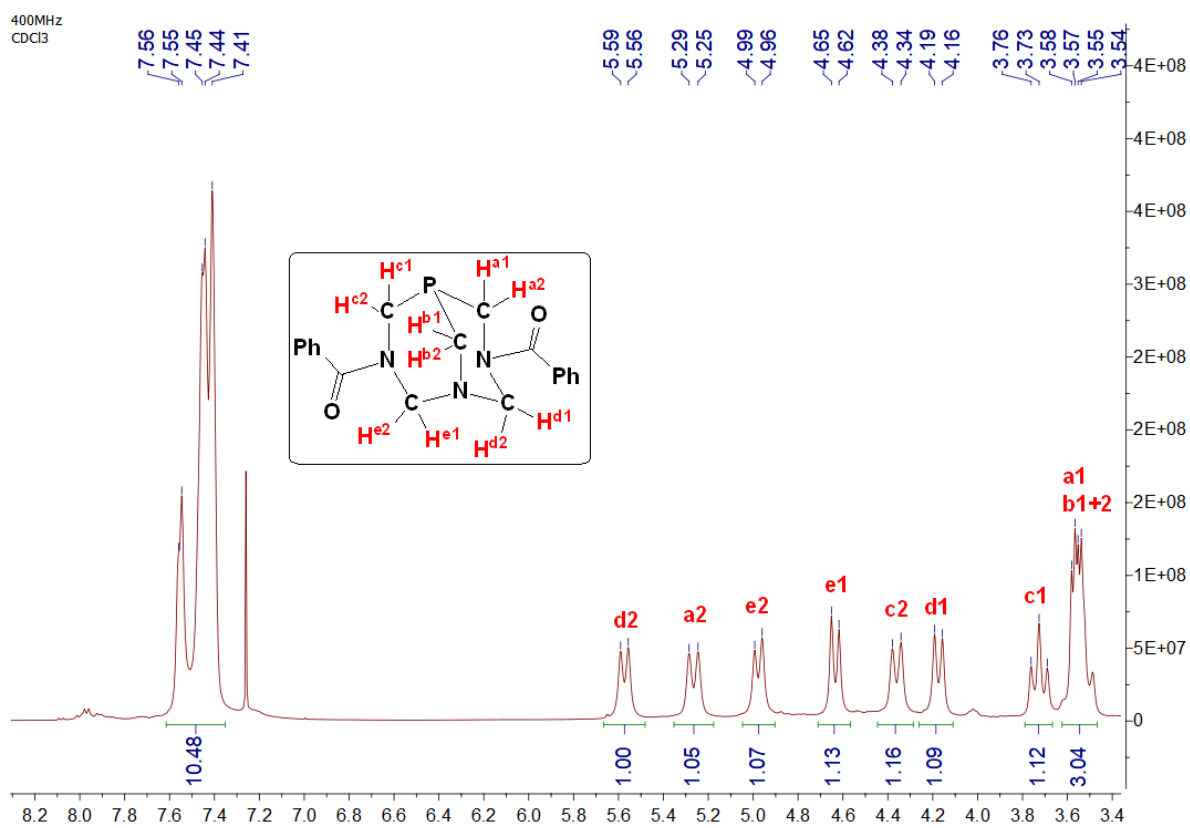


Figure S2. <sup>1</sup>H NMR spectrum of DBPTA (1) in CDCl<sub>3</sub> (400 MHz).

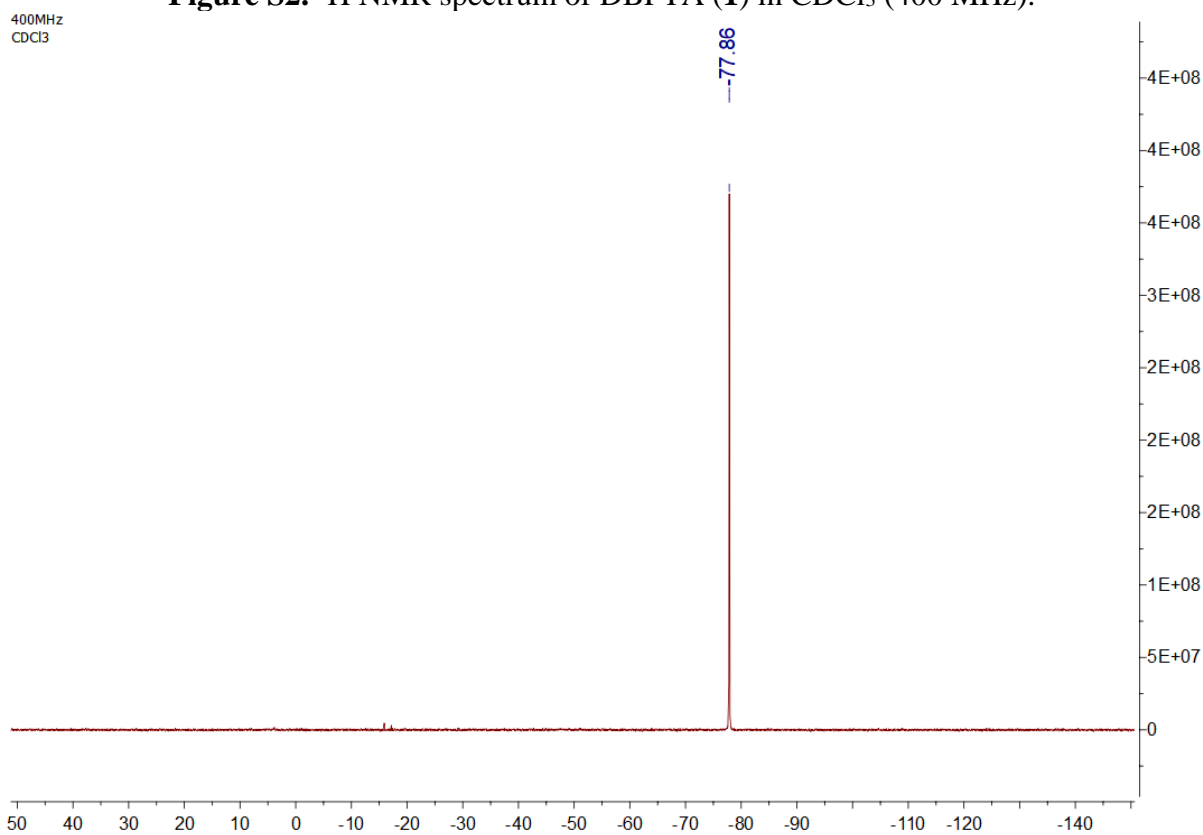
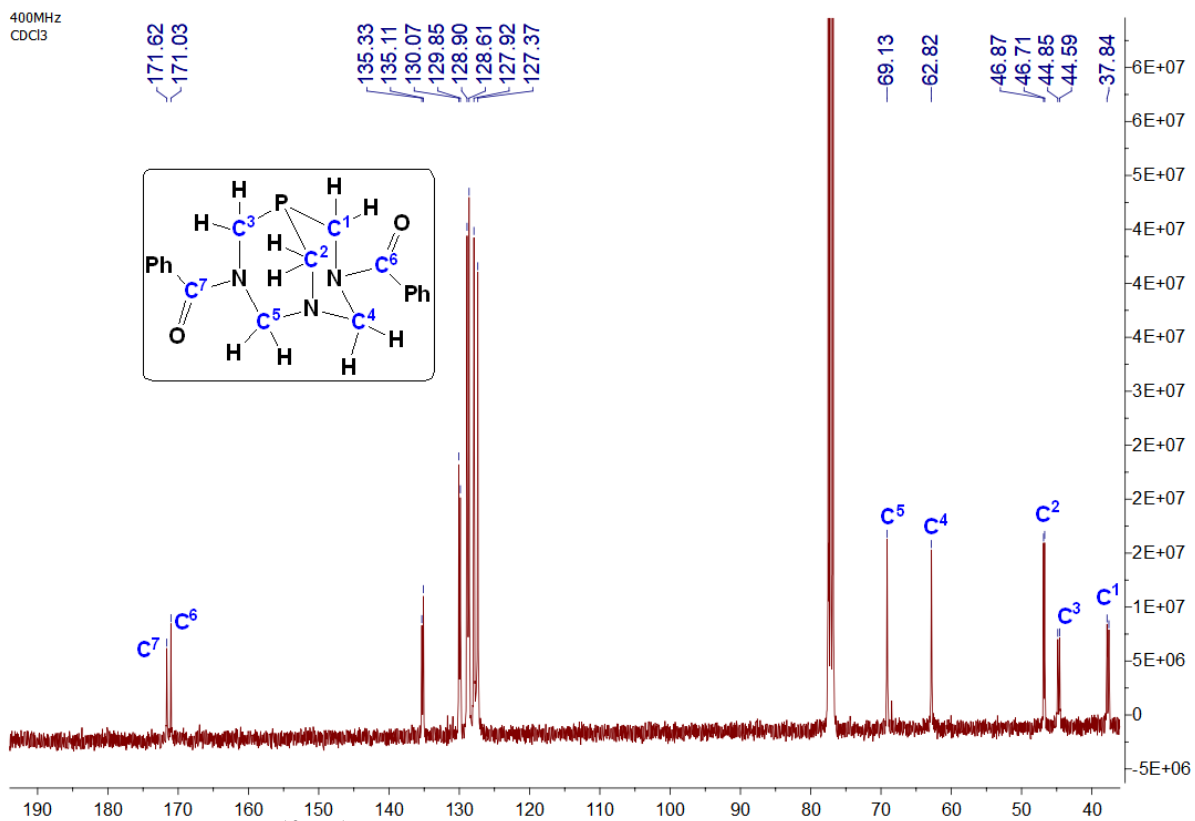
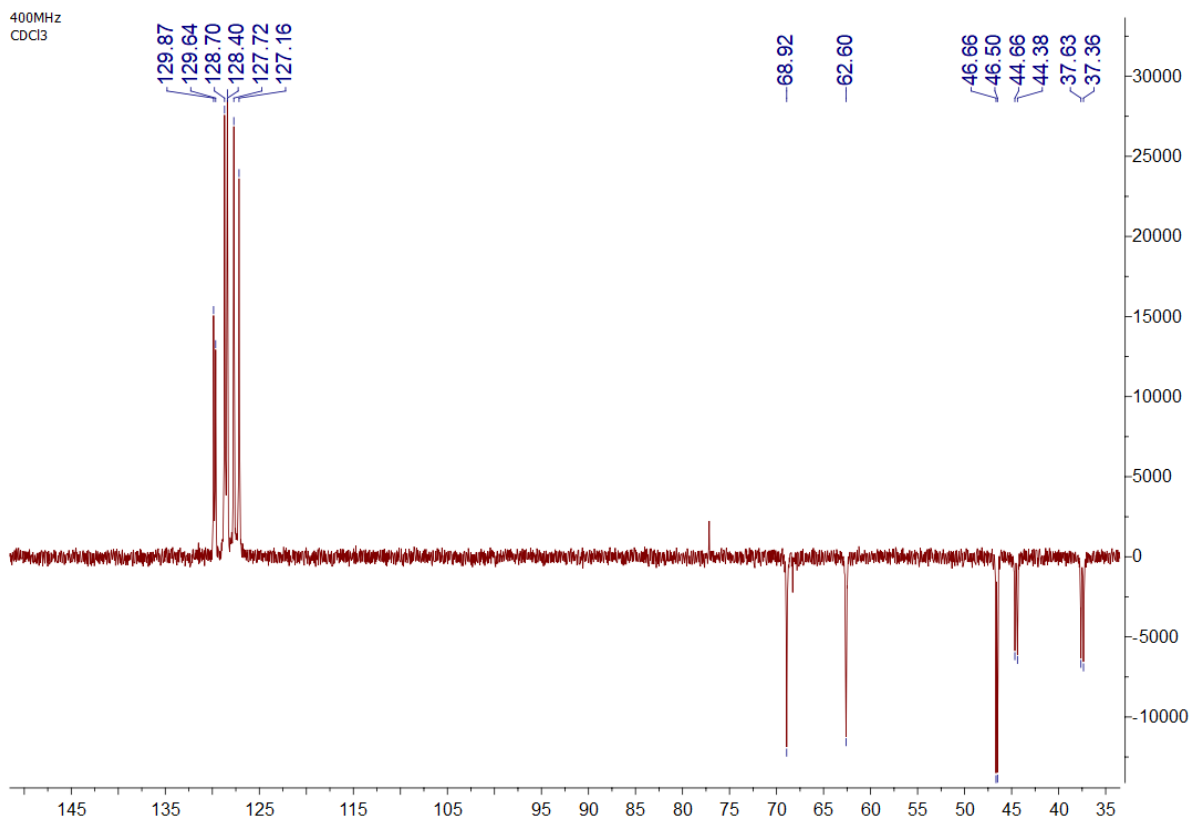


Figure S3. <sup>31</sup>P NMR spectrum of DBPTA (1) in CDCl<sub>3</sub> (400 MHz).



**Figure S4.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of DBPTA (**1**) in  $\text{CDCl}_3$  (400 MHz).



**Figure S5.** DEPT NMR spectrum of DBPTA (**1**) in  $\text{CDCl}_3$  (400 MHz).

400MHz  
CDCl<sub>3</sub>

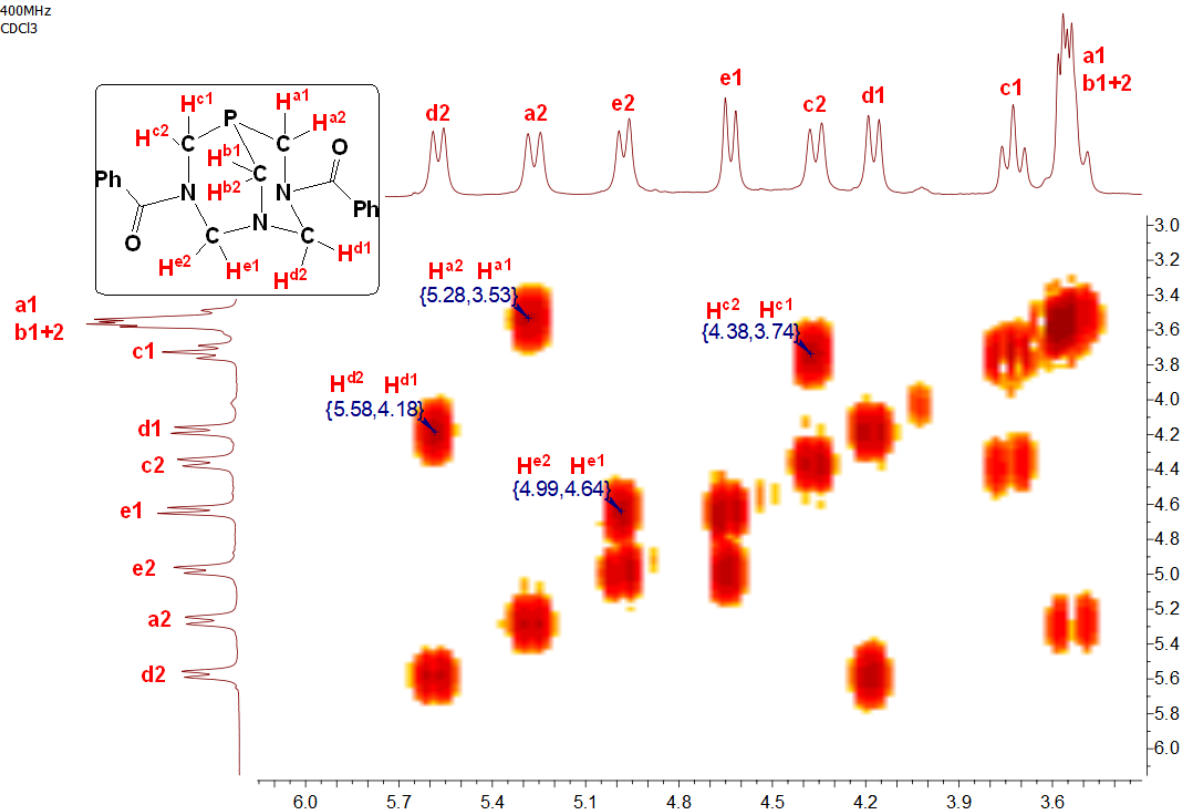


Figure S6. COSY spectrum of DBPTA (1) in CDCl<sub>3</sub> (400 MHz).

400MHz  
CDCl<sub>3</sub>

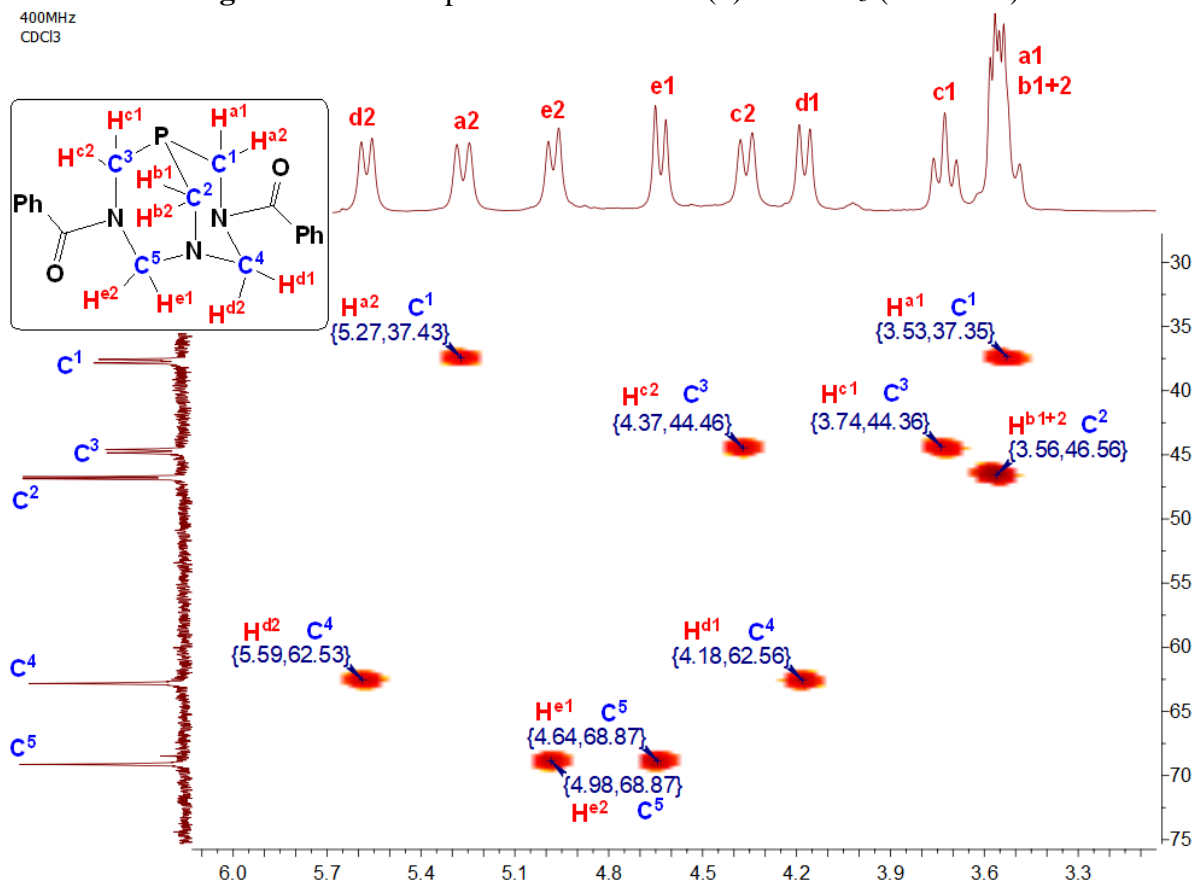
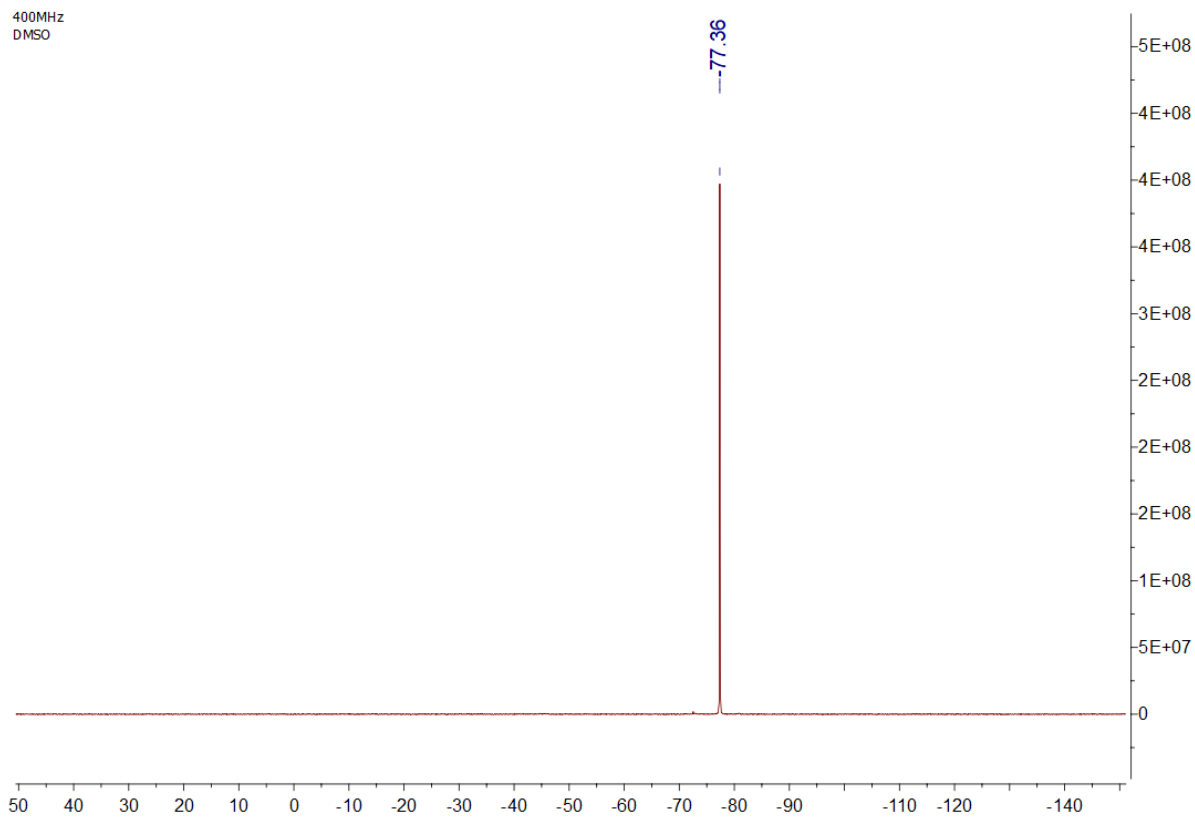
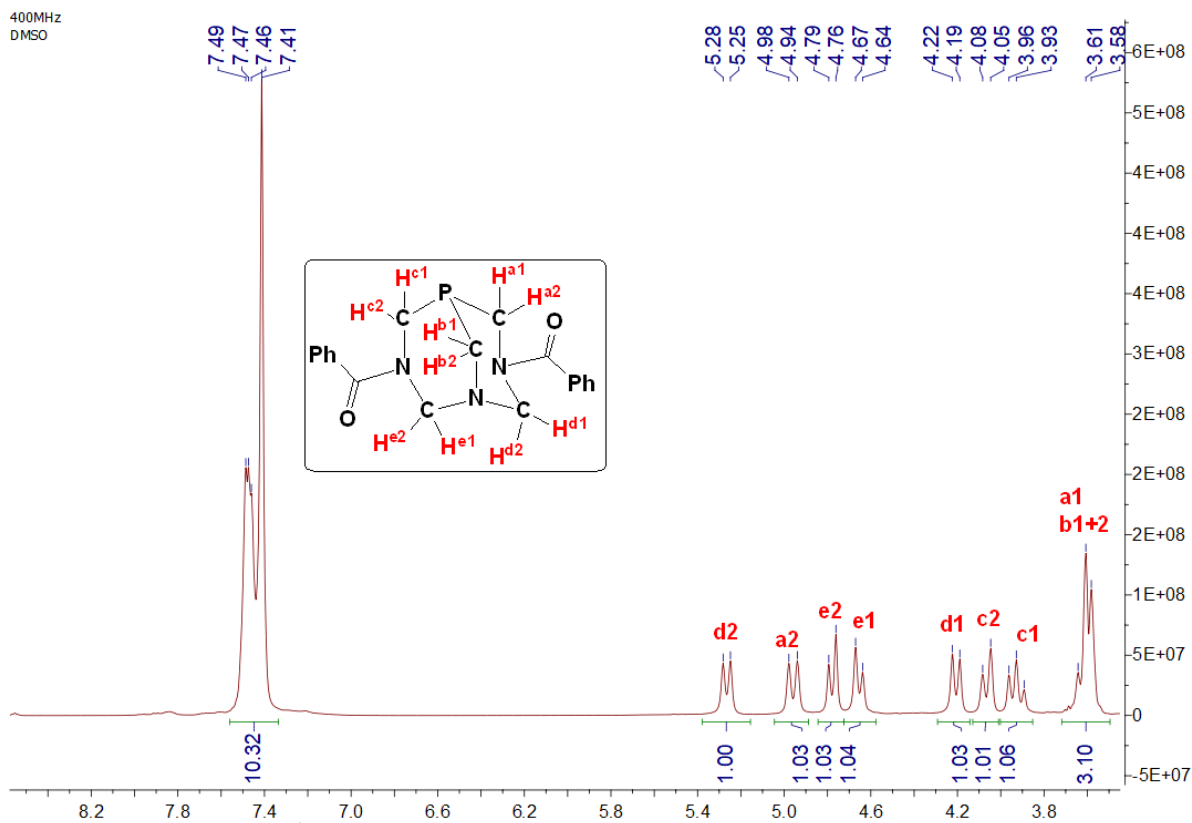
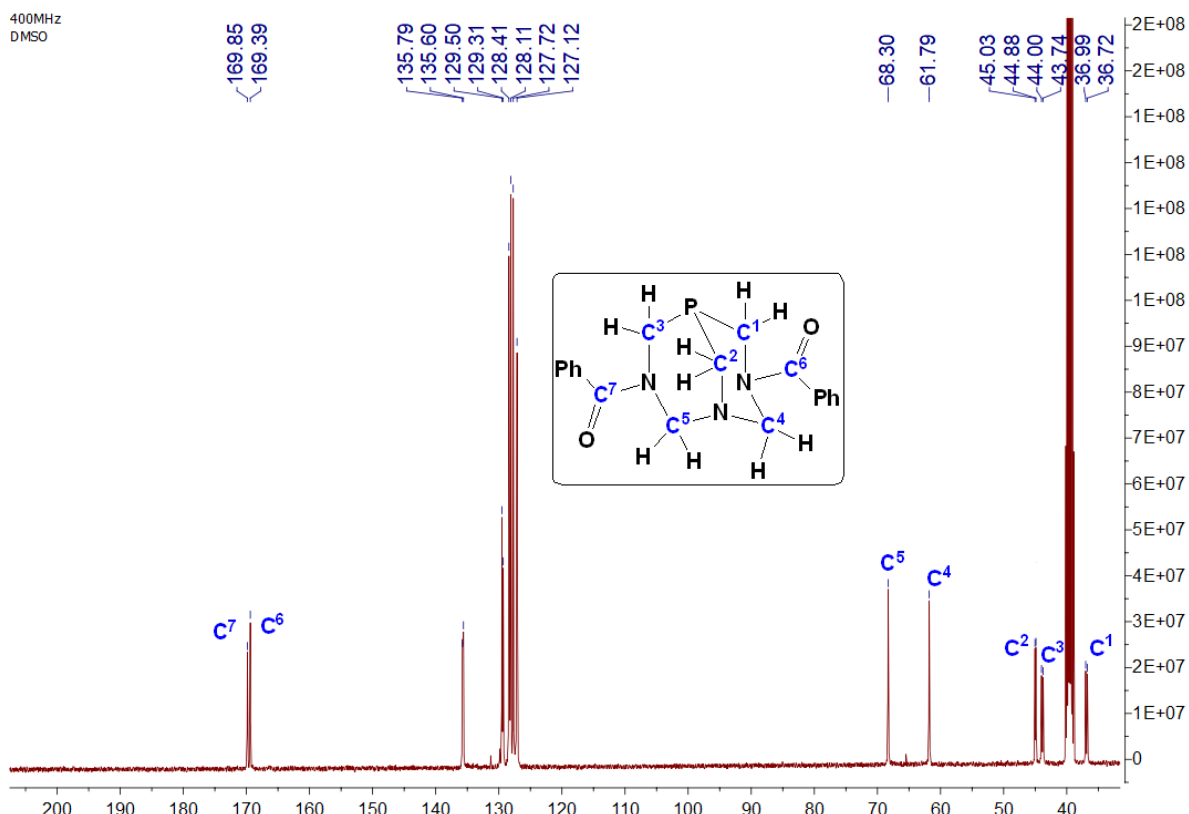
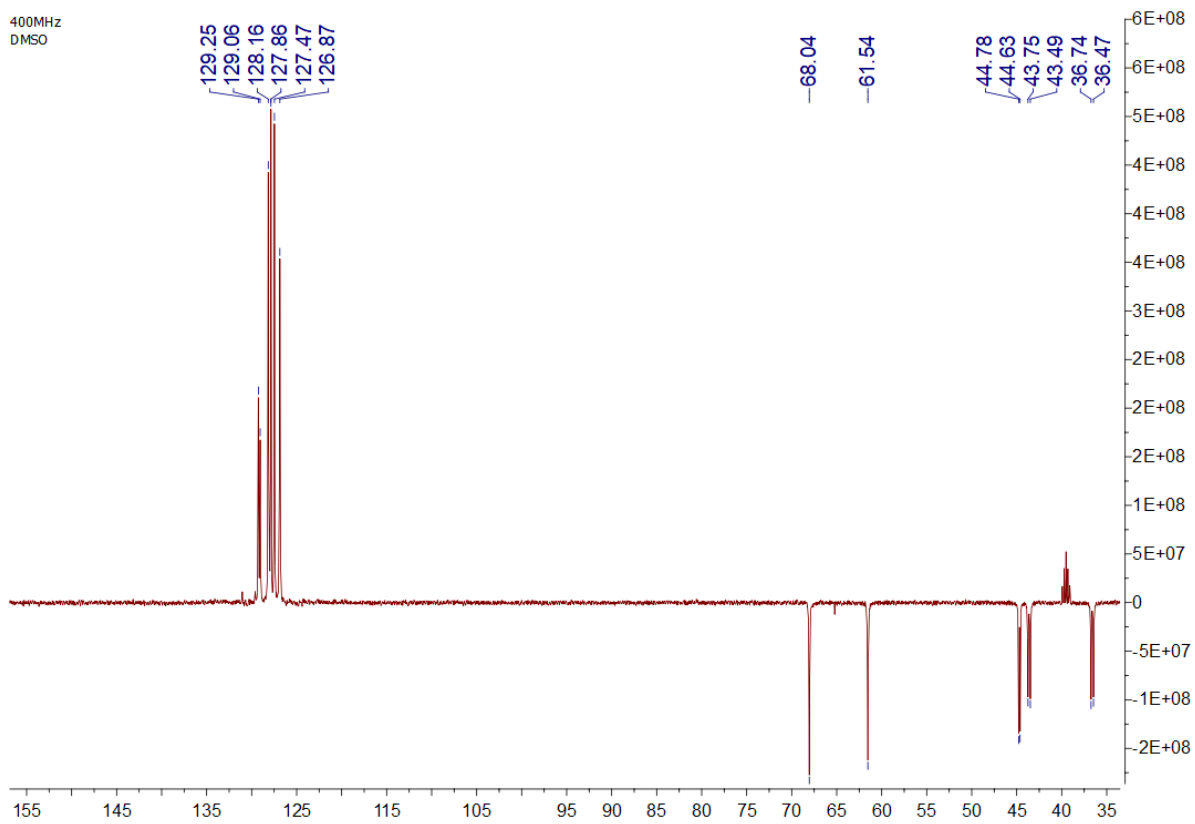


Figure S7. HSQC spectrum of DBPTA (1) in CDCl<sub>3</sub> (400 MHz).

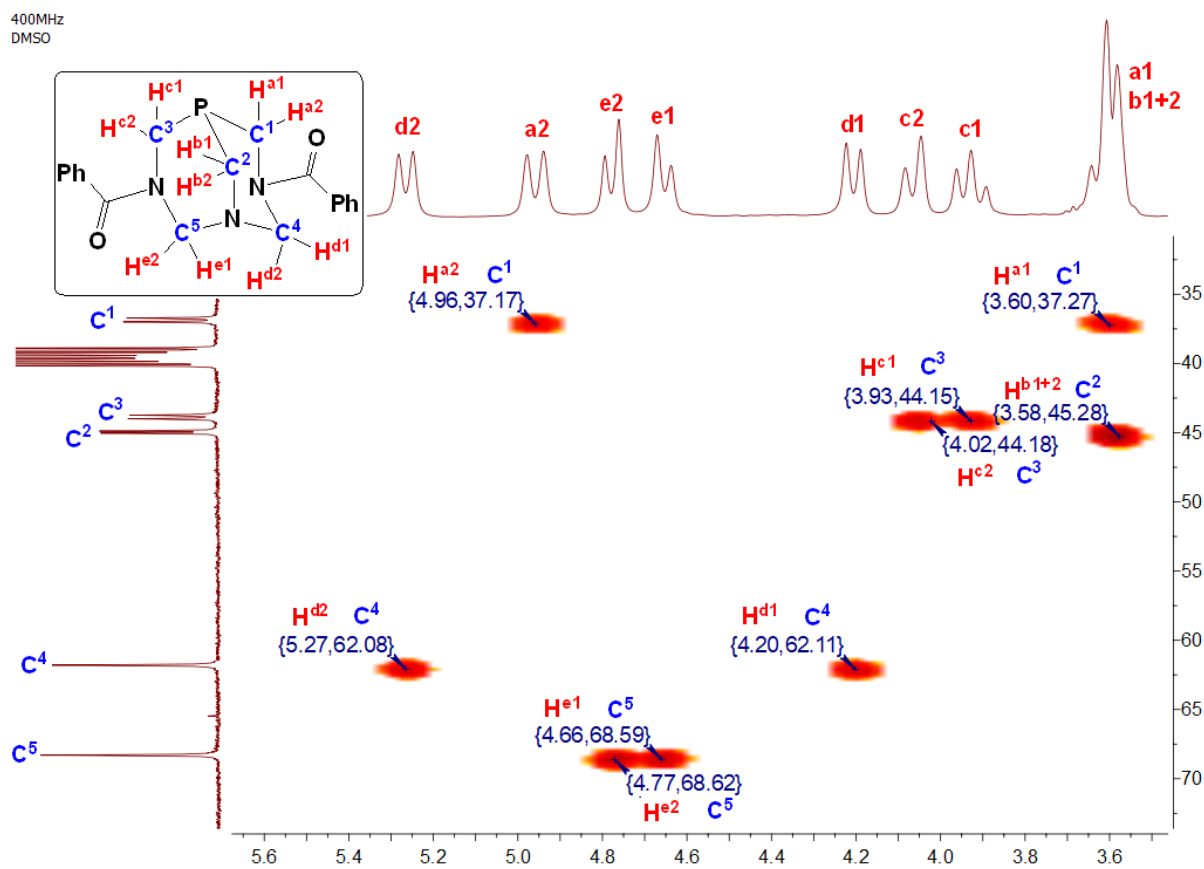
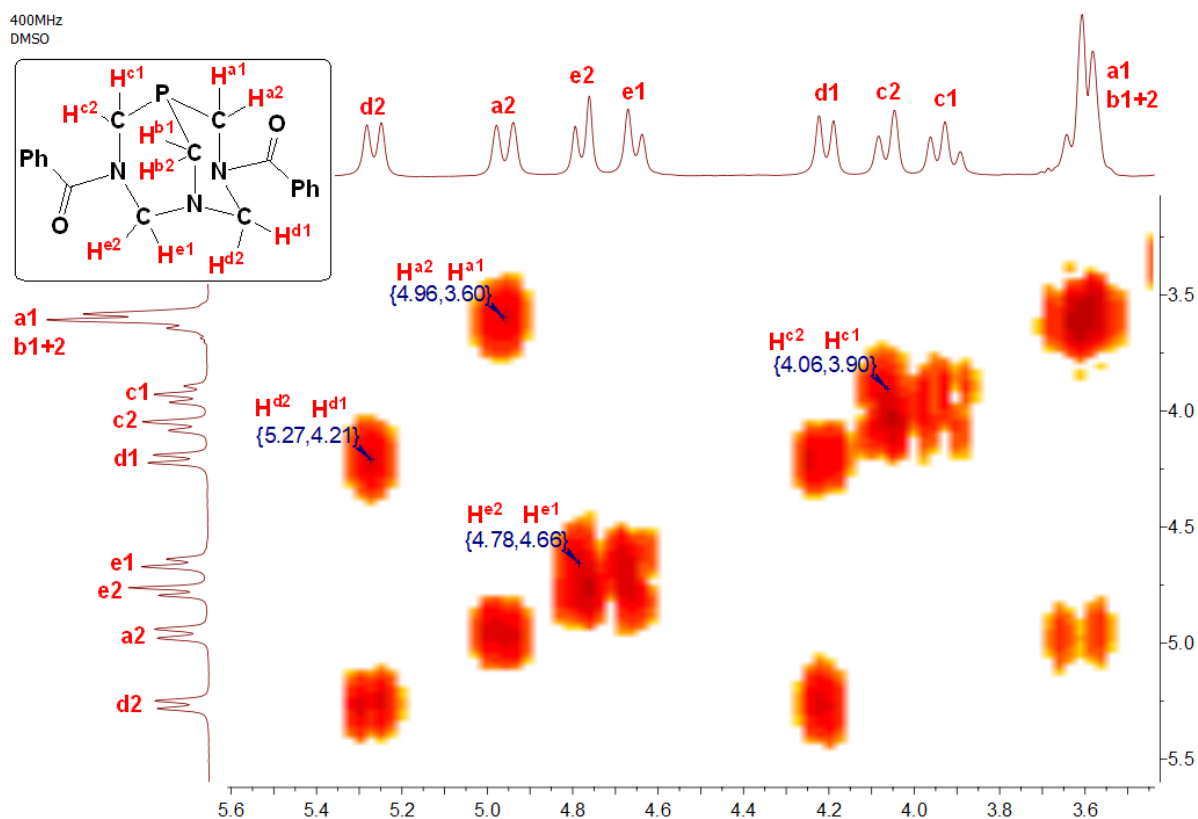




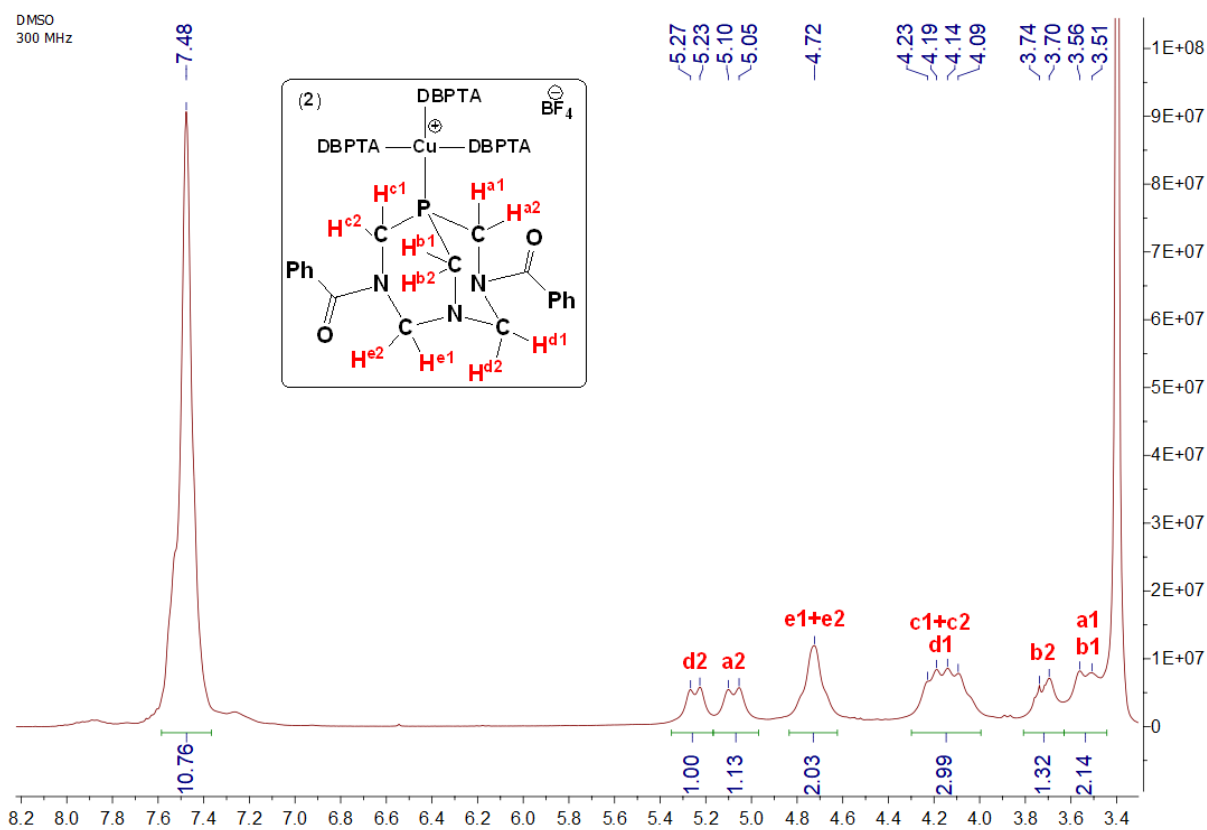
**Figure S10.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of DBPTA (**1**) in  $\text{DMSO-}d_6$  (400 MHz).



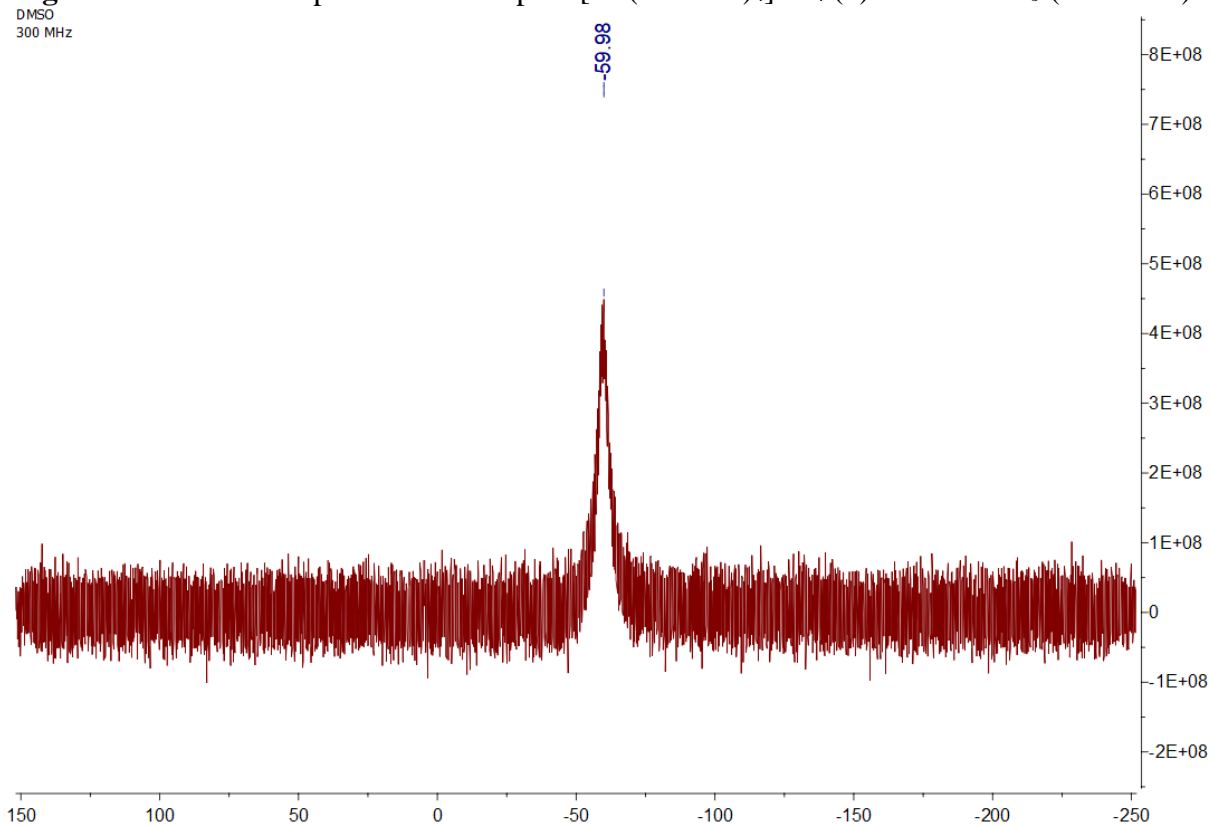
**Figure S11.** DEPT NMR spectrum of DBPTA (**1**) in  $\text{DMSO-}d_6$  (400 MHz).







**Figure S14.**  $^1\text{H}$  NMR spectrum of complex  $[\text{Cu}(\text{DBPTA})_4]\text{BF}_4$  (**2**) in  $\text{DMSO-}d_6$  (300 MHz).



**Figure S15.**  $^{31}\text{P}$  NMR spectrum of complex  $[\text{Cu}(\text{DBPTA})_4]\text{BF}_4$  (**2**) in  $\text{DMSO-}d_6$  (300 MHz).



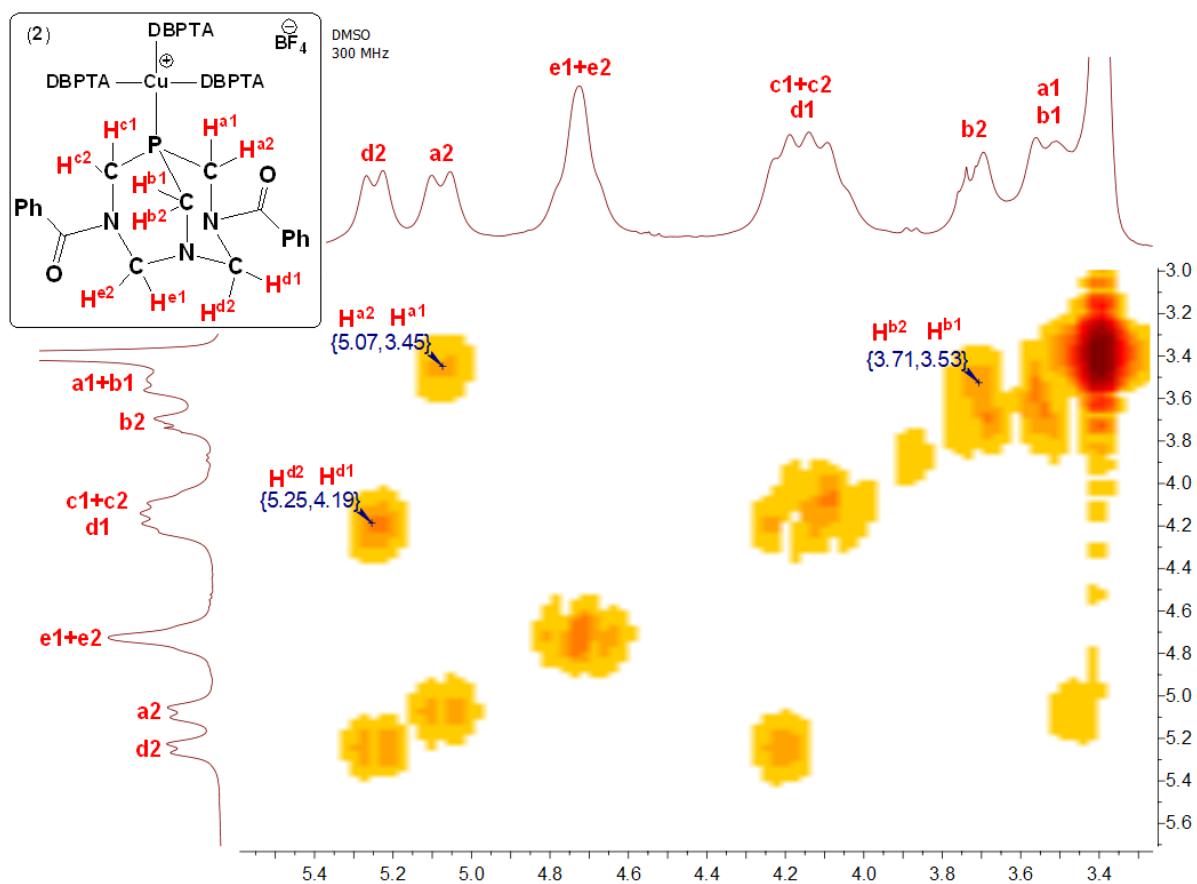


Figure S18. COSY spectrum of complex  $[\text{Cu}(\text{DBPTA})_4]\text{BF}_4$  (2) in  $\text{DMSO-}d_6$  (300 MHz).

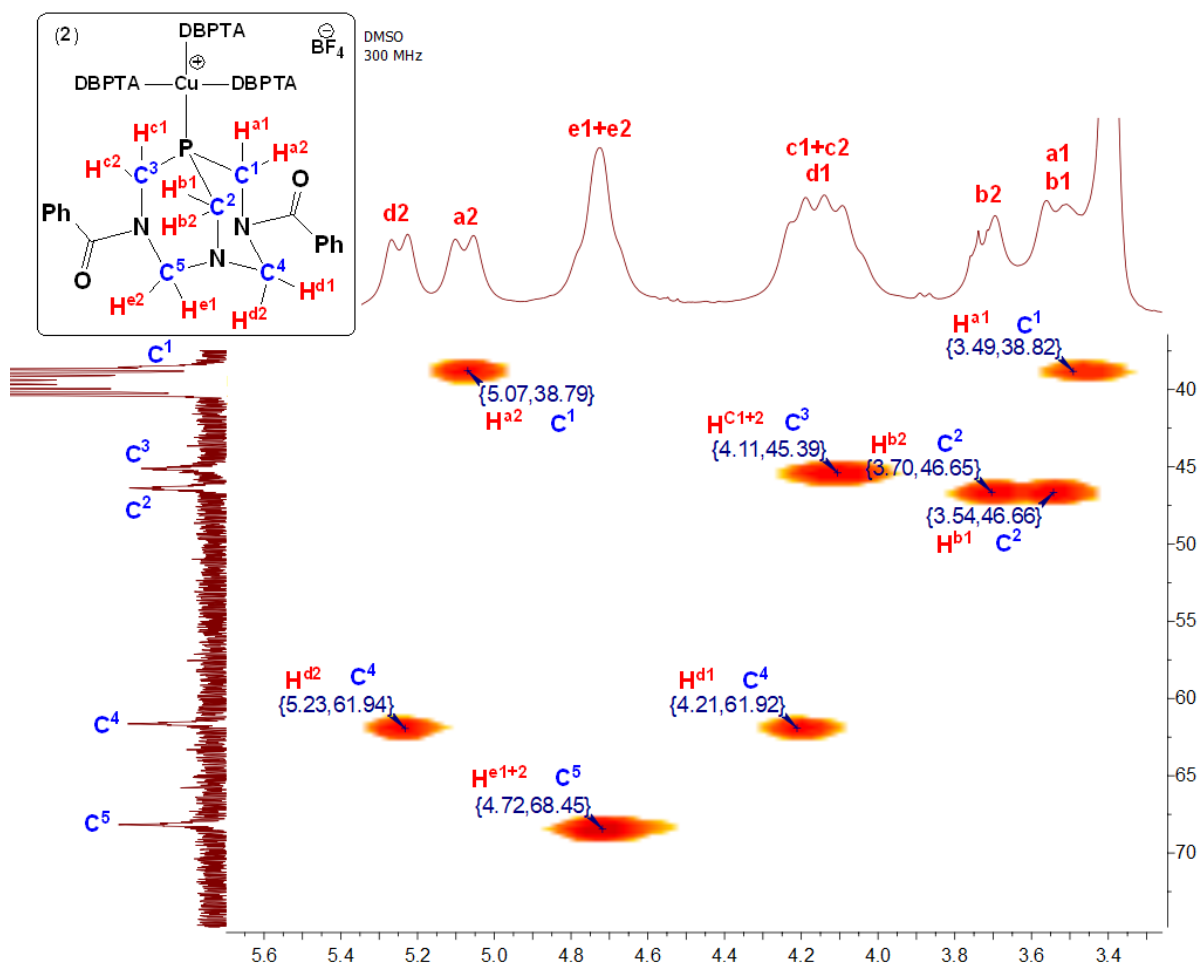


Figure S19. HSQC spectrum of complex  $[\text{Cu}(\text{DBPTA})_4]\text{BF}_4$  (2) in  $\text{DMSO}-d_6$  (300 MHz).

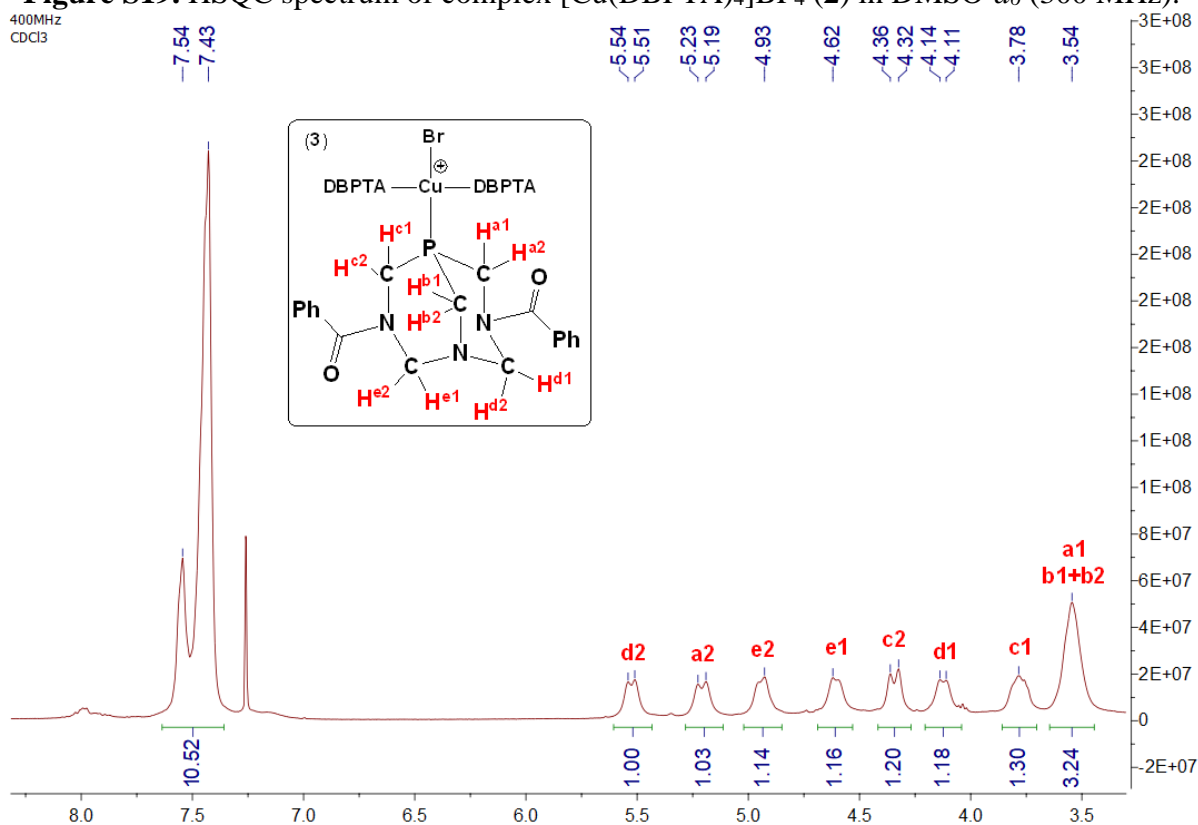
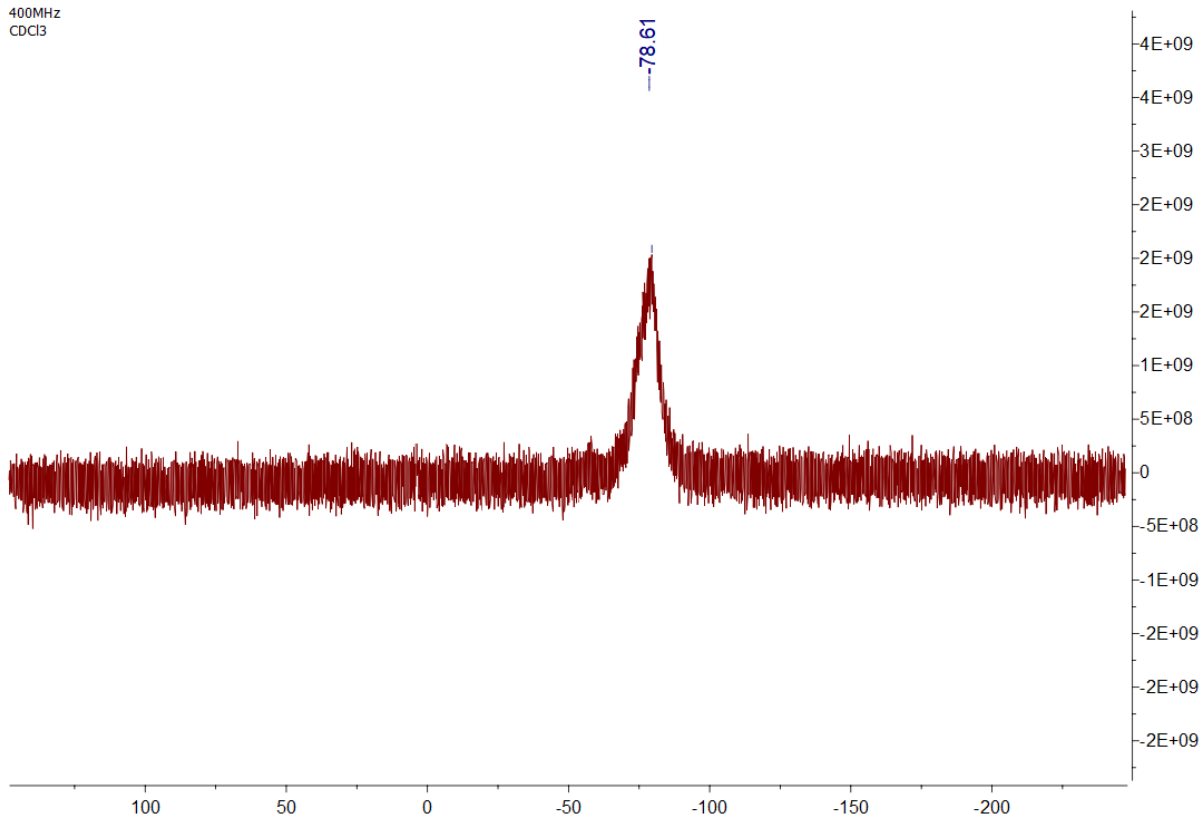
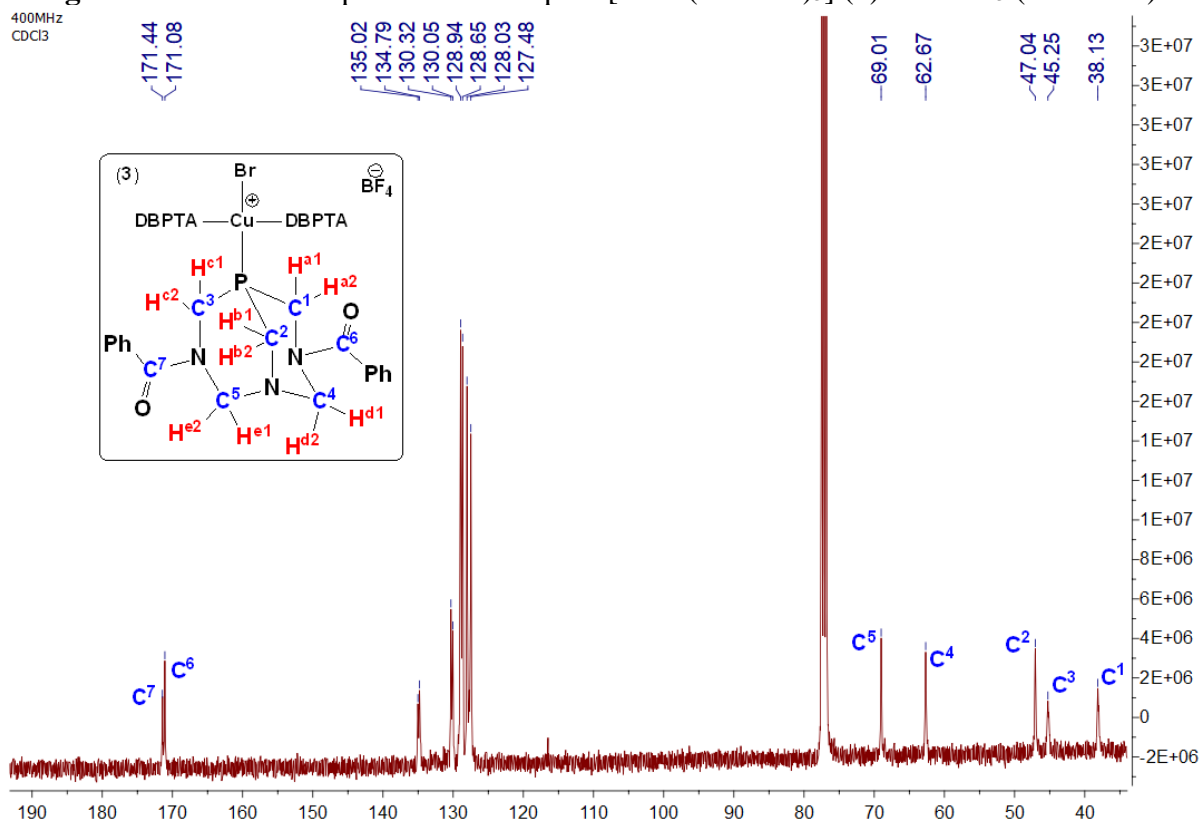


Figure S20.  $^1\text{H}$  NMR spectrum of complex  $[\text{CuBr}(\text{DBPTA})_3]$  (3) in  $\text{CDCl}_3$  (400 MHz).

400MHz  
CDCl<sub>3</sub>



**Figure S21.** <sup>31</sup>P NMR spectrum of complex [CuBr(DBPTA)<sub>3</sub>] (**3**) in CDCl<sub>3</sub> (400 MHz).



**Figure S22.** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of complex [CuBr(DBPTA)<sub>3</sub>] (**3**) in CDCl<sub>3</sub> (400 MHz).

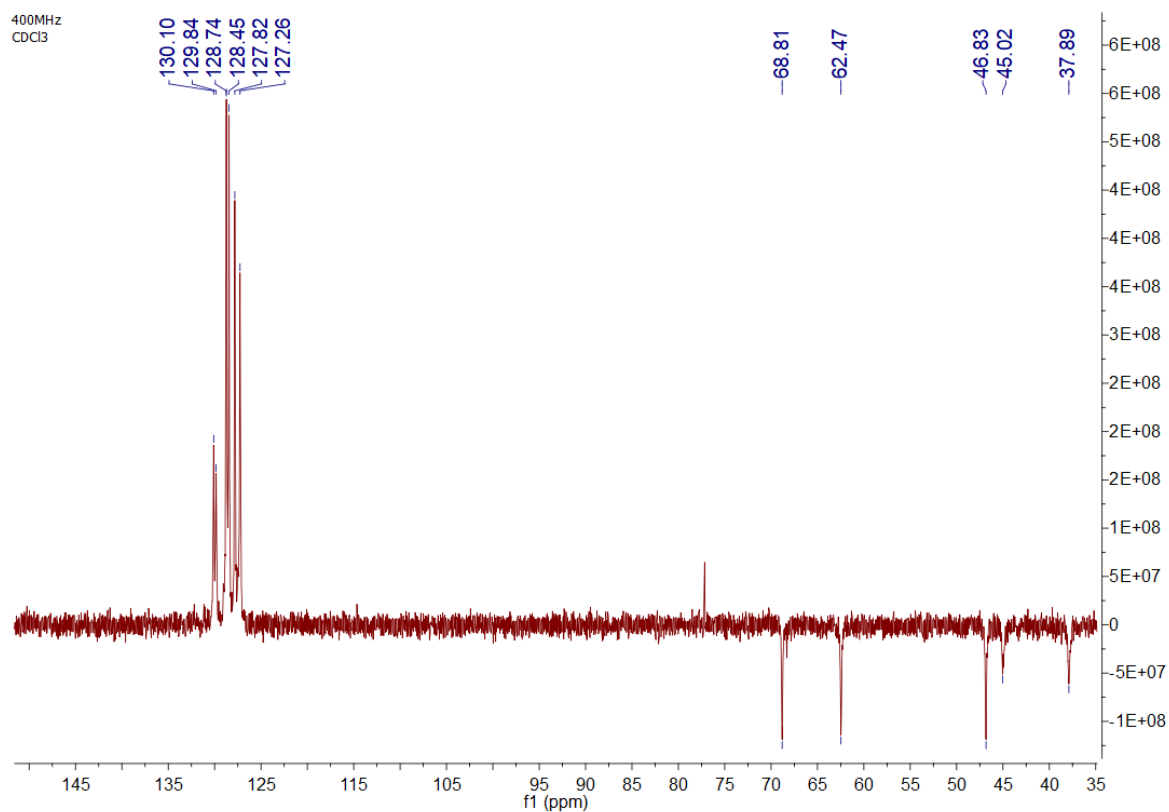


Figure S23. DEPT NMR spectrum of complex  $[\text{CuBr}(\text{DBPTA})_3]$  (**3**) in  $\text{CDCl}_3$  (400 MHz).

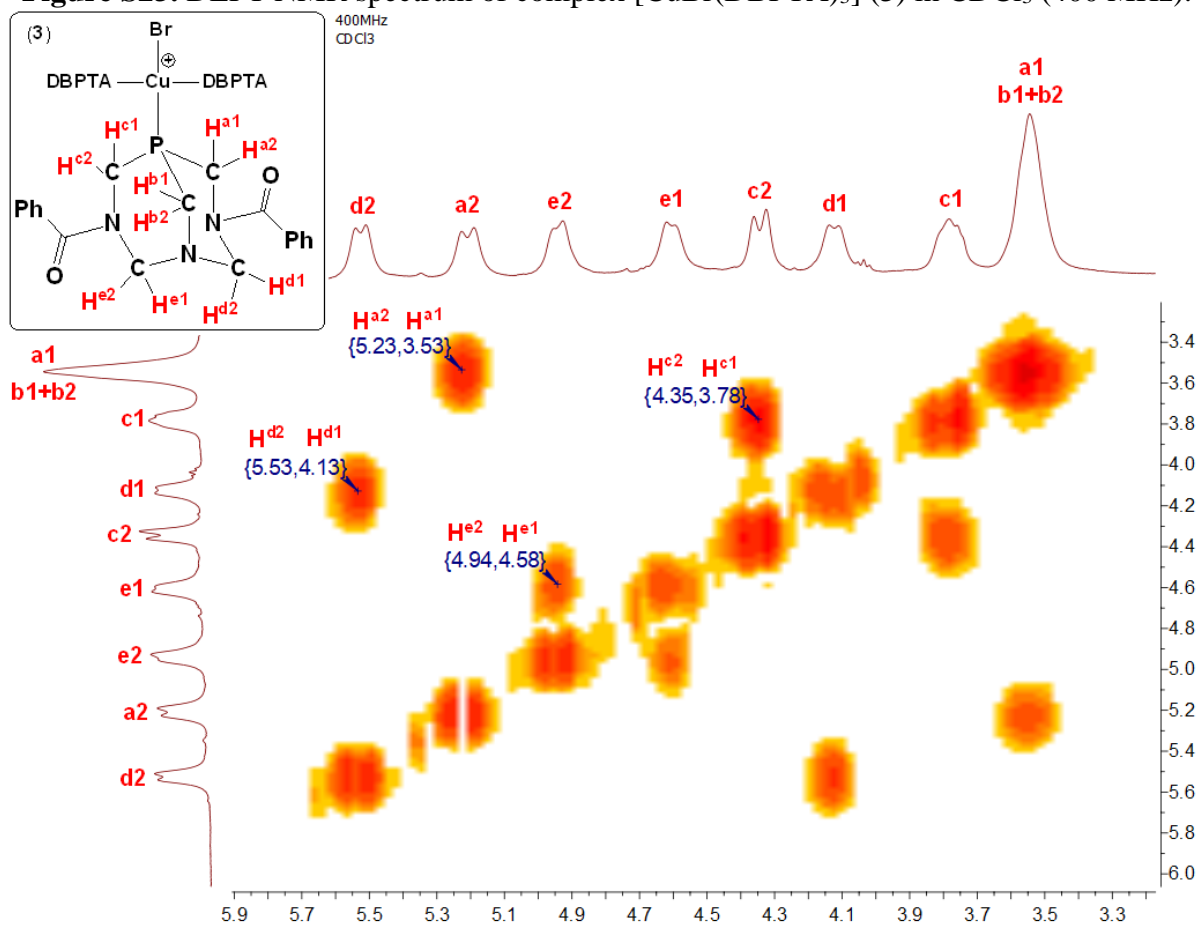


Figure S24. COSY spectrum of complex  $[\text{CuBr}(\text{DBPTA})_3]$  (**3**) in  $\text{CDCl}_3$  (400 MHz).

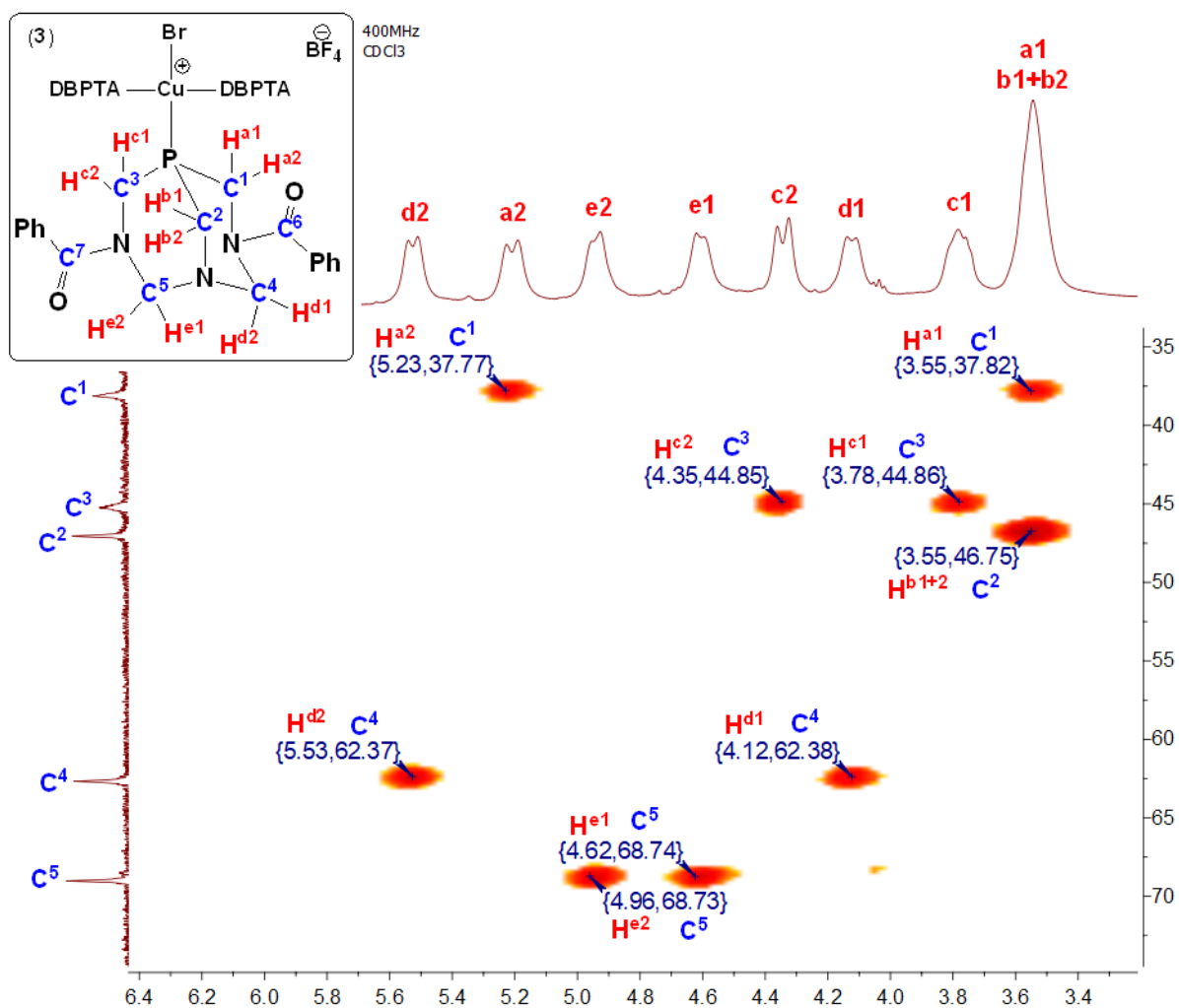
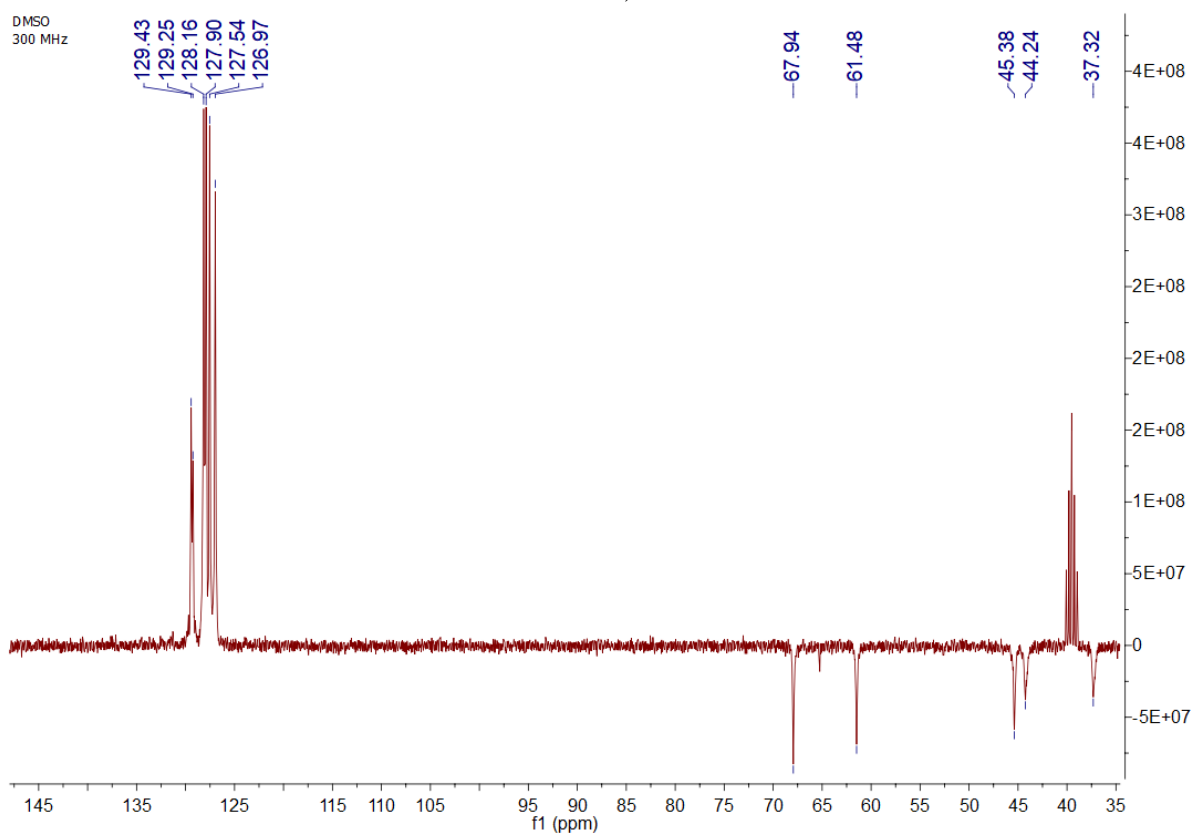
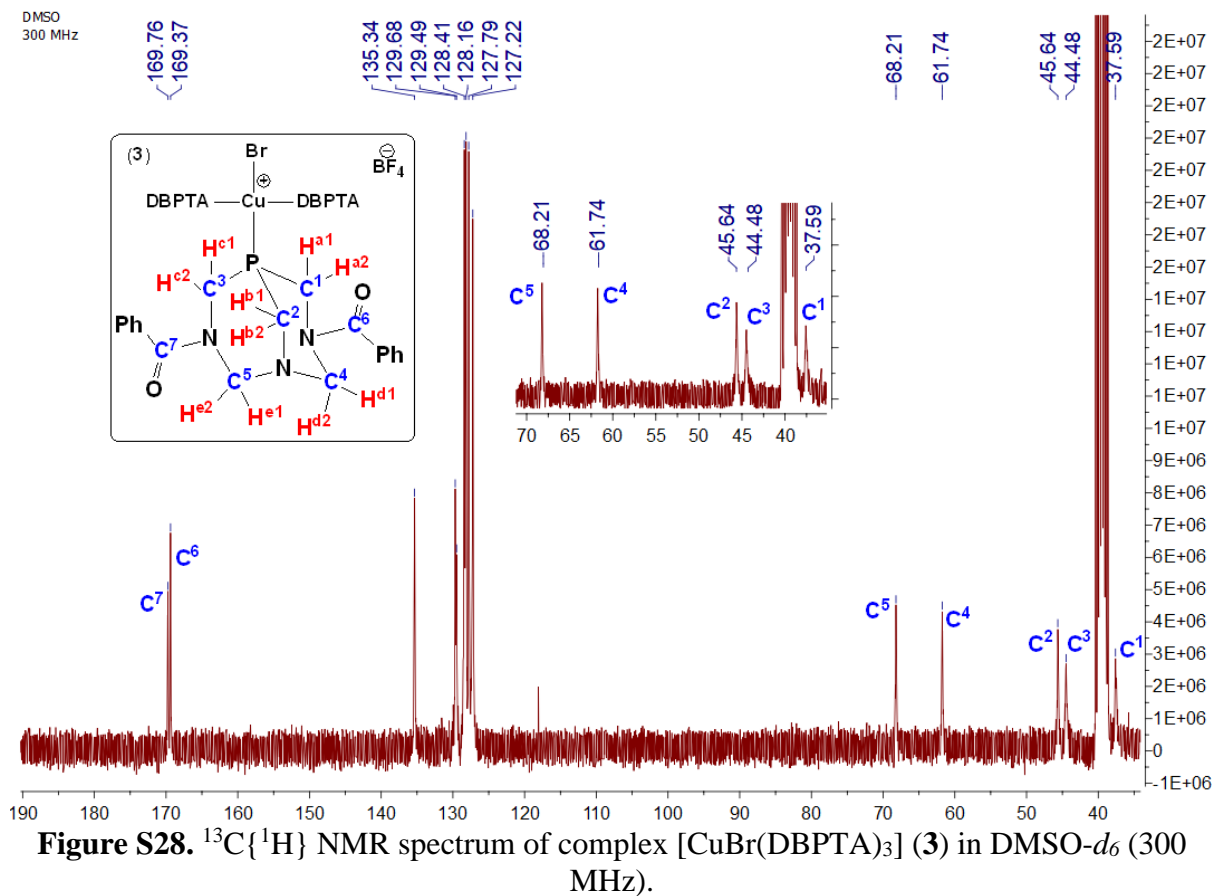
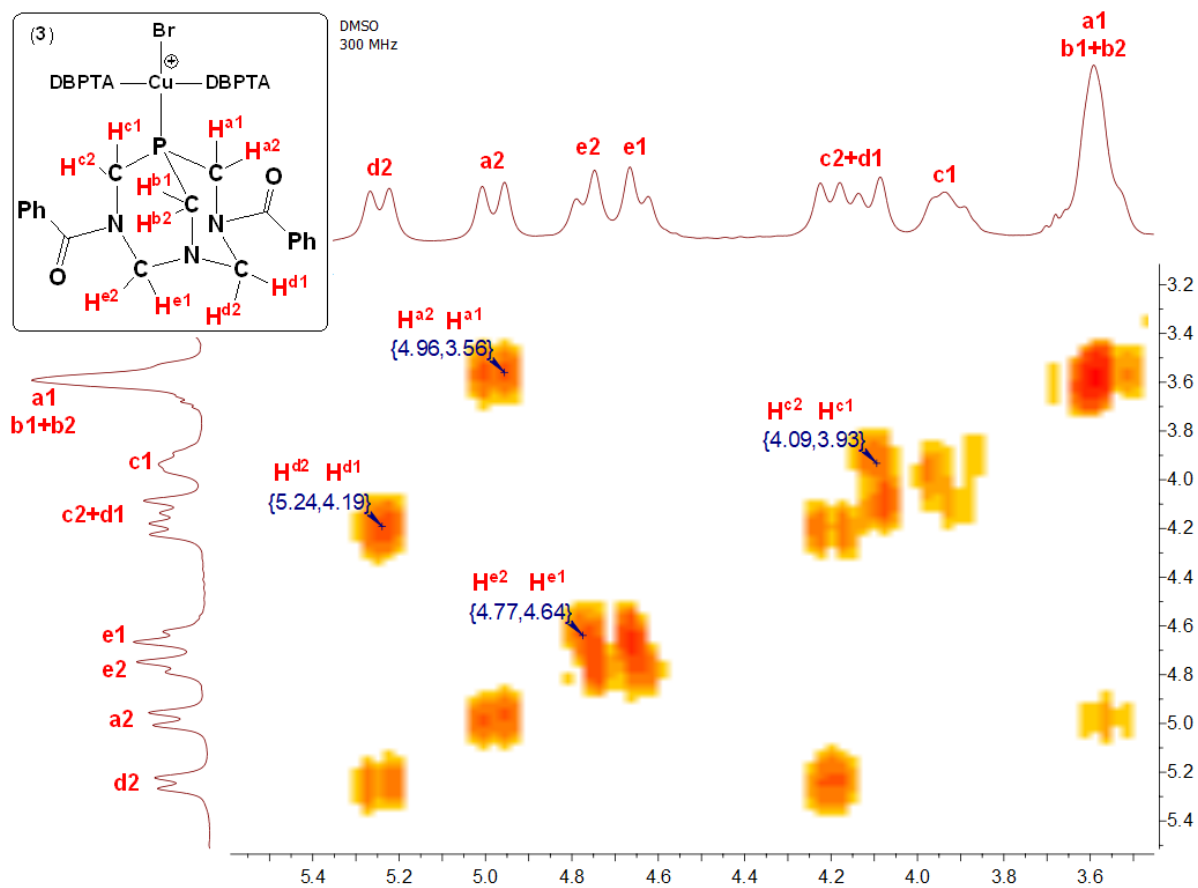


Figure S25. HSQC spectrum of complex  $[\text{CuBr}(\text{DBPTA})_3]$  (3) in  $\text{CDCl}_3$  (400 MHz).



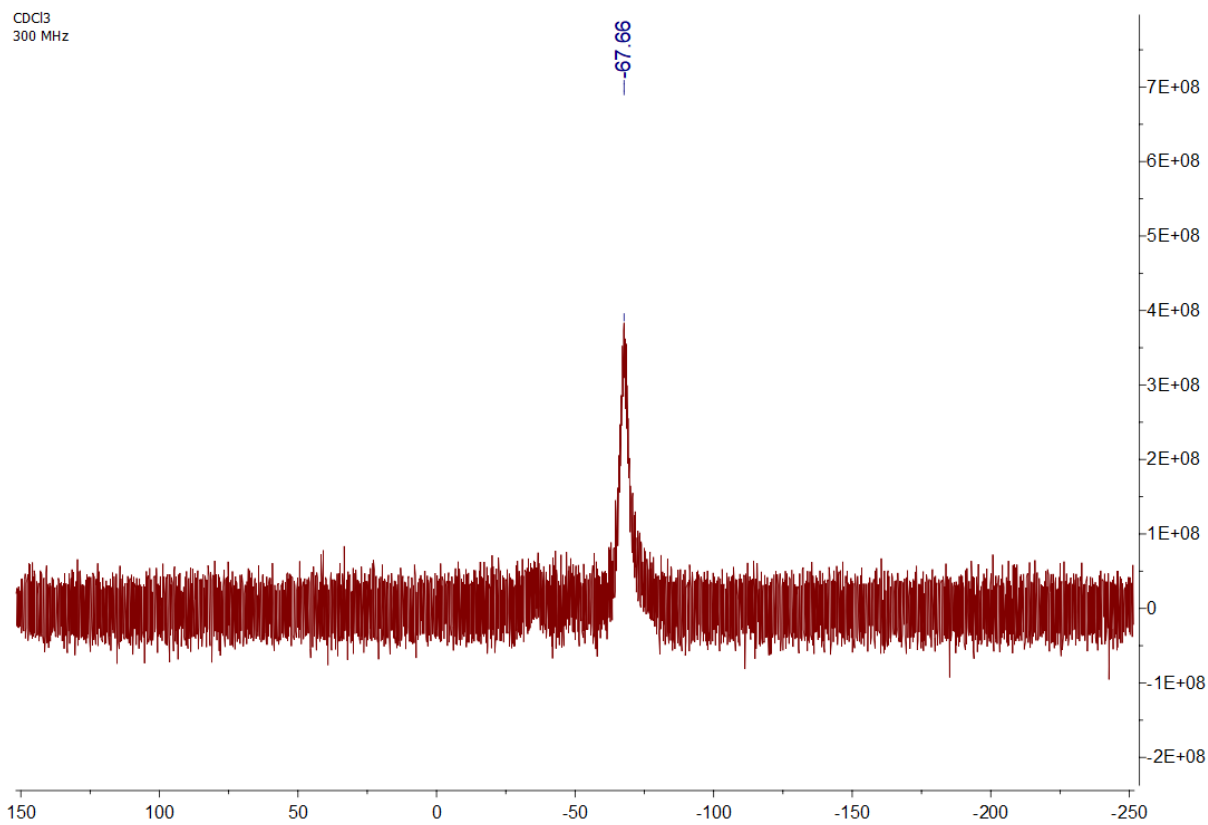




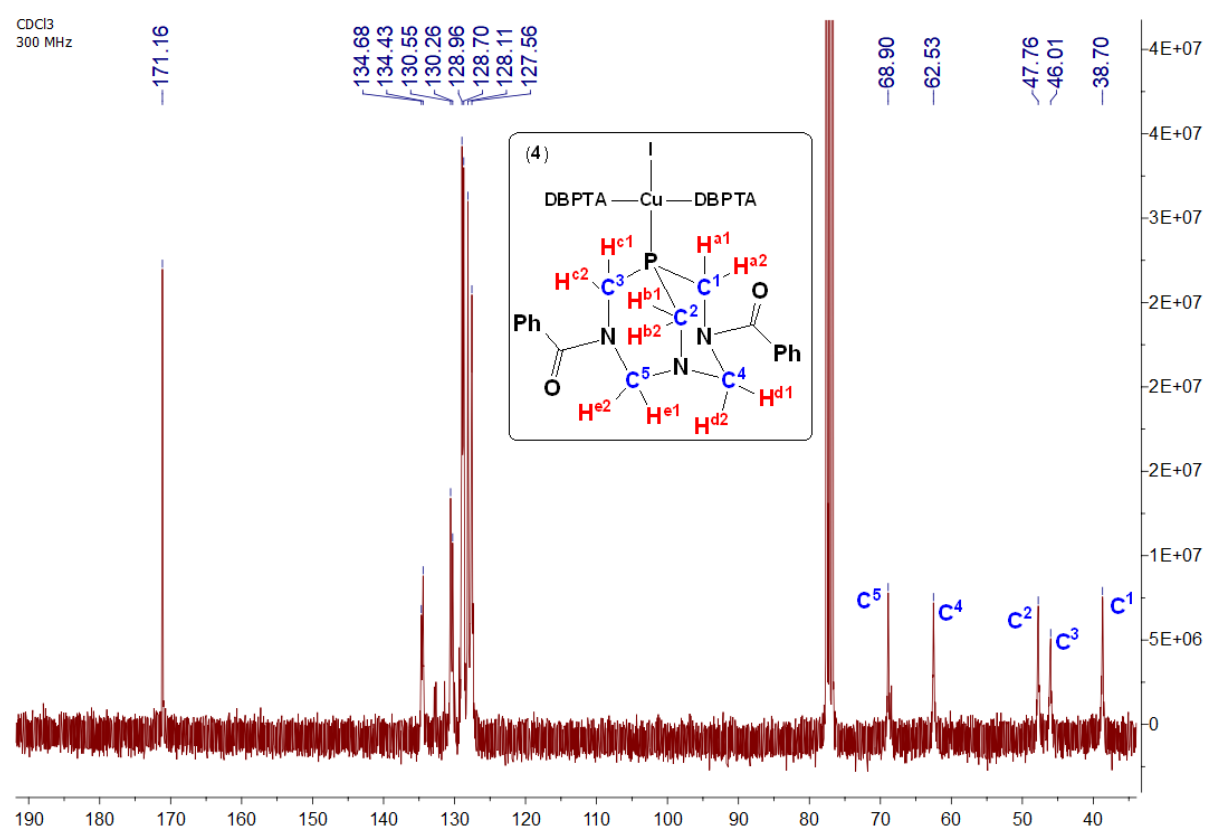


**Figure S30.** COSY spectrum of complex [CuBr(DBPTA)<sub>3</sub>] (**3**) in DMSO-*d*<sub>6</sub> (300 MHz).

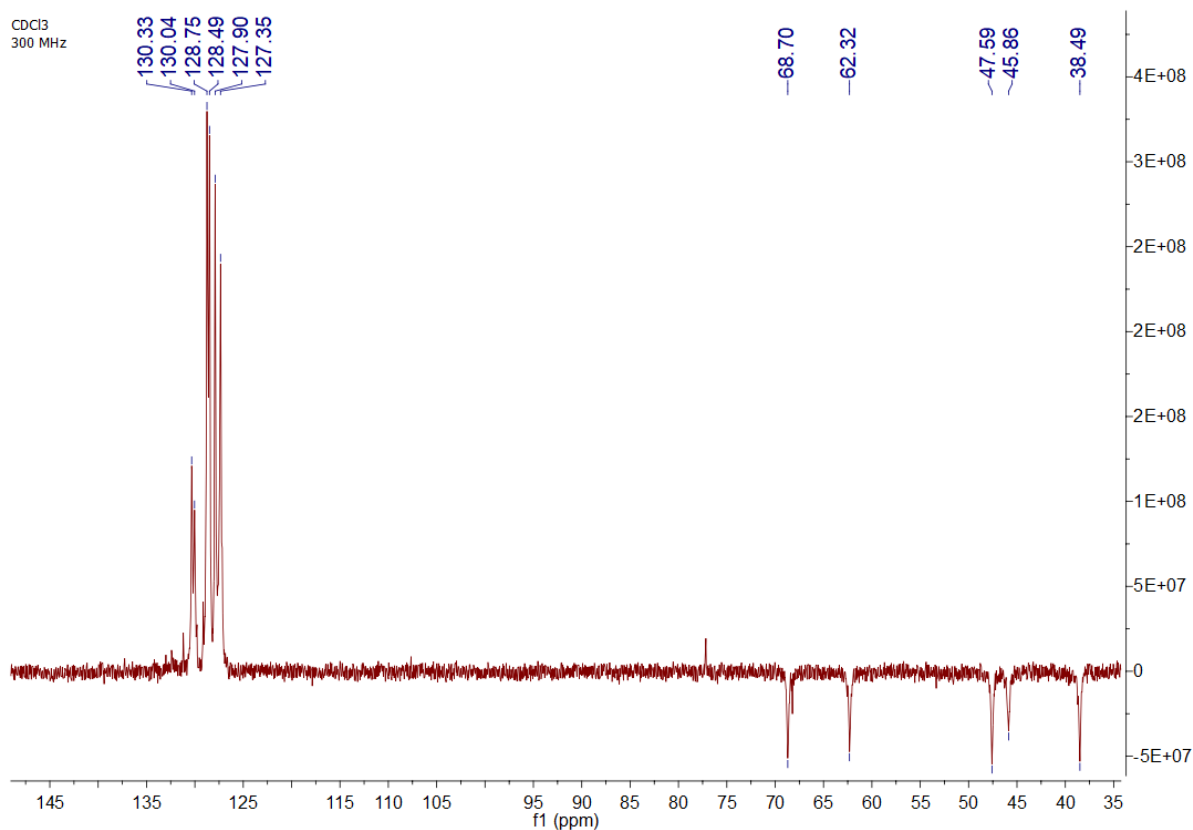




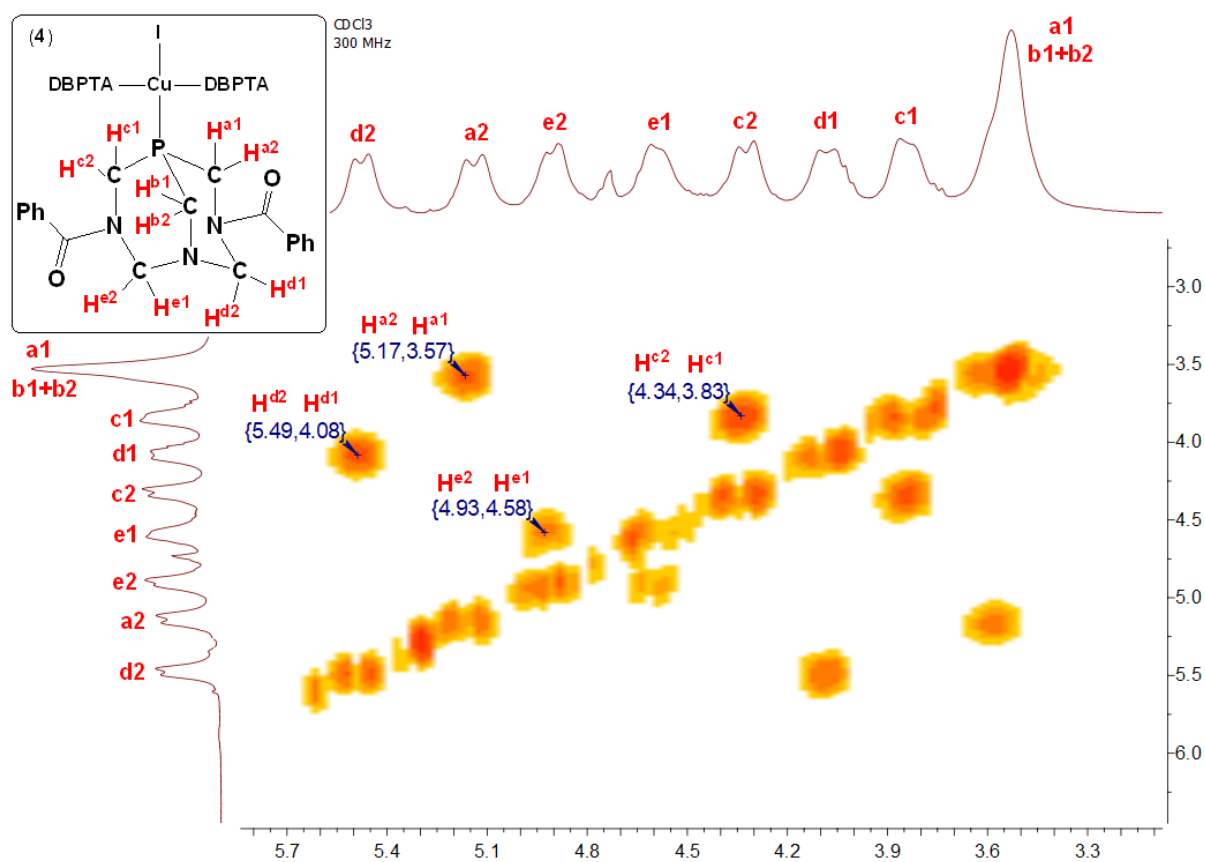
**Figure S33.** <sup>31</sup>P NMR spectrum of complex [CuI(DBPTA)<sub>3</sub>] (**4**) in CDCl<sub>3</sub> (300 MHz).



**Figure S34.** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of complex [CuI(DBPTA)<sub>3</sub>] (**4**) in CDCl<sub>3</sub> (300 MHz).



**Figure S35.** DEPT NMR spectrum of complex  $[\text{CuI}(\text{DBPTA})_3]$  (**4**) in  $\text{CDCl}_3$  (300 MHz).



**Figure S36.** COSY spectrum of complex  $[\text{CuI}(\text{DBPTA})_3]$  (**4**) in  $\text{CDCl}_3$  (300 MHz).

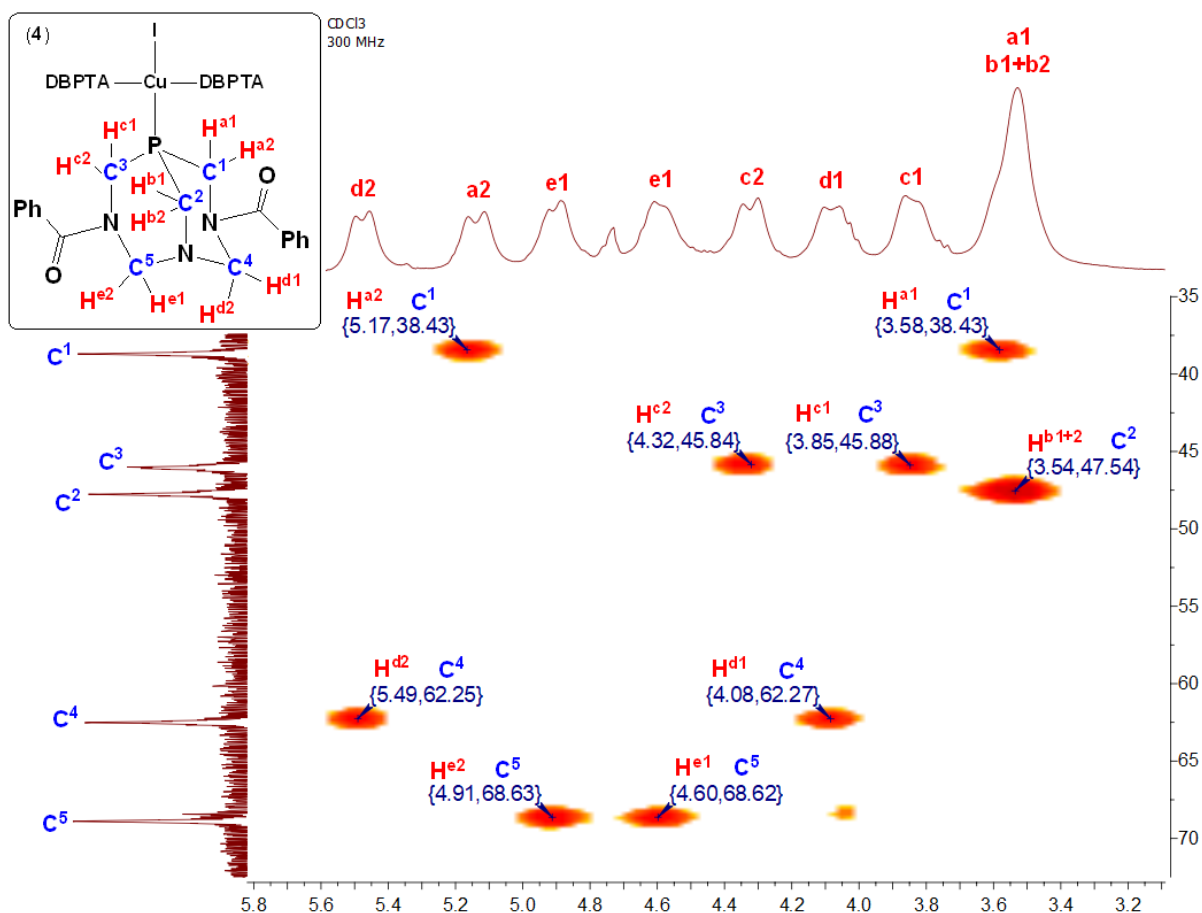


Figure S37. HSQC spectrum of complex  $[\text{CuI}(\text{DBPTA})_3]$  (**4**) in  $\text{CDCl}_3$  (300 MHz).

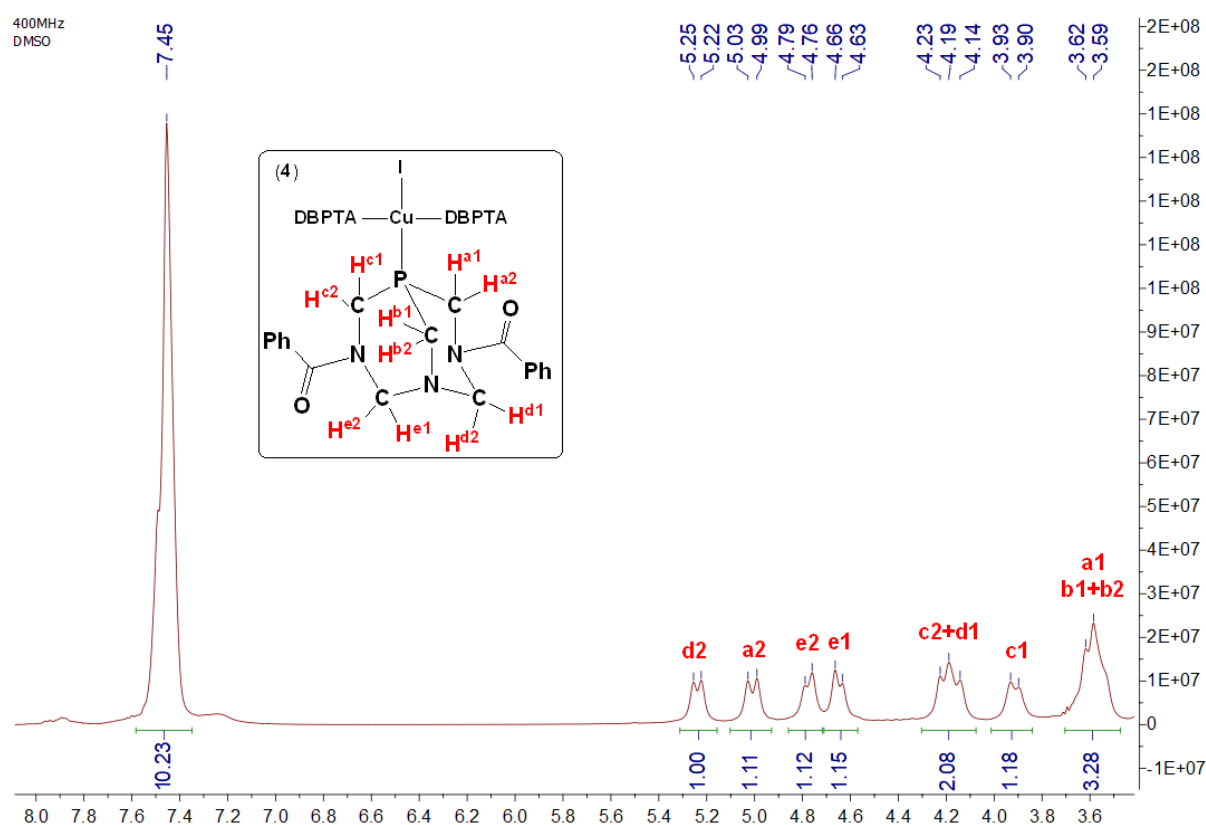


Figure S38.  $^1\text{H}$  NMR spectrum of complex  $[\text{CuI}(\text{DBPTA})_3]$  (**4**) in  $\text{DMSO-}d_6$  (400 MHz).

400MHz  
DMSO

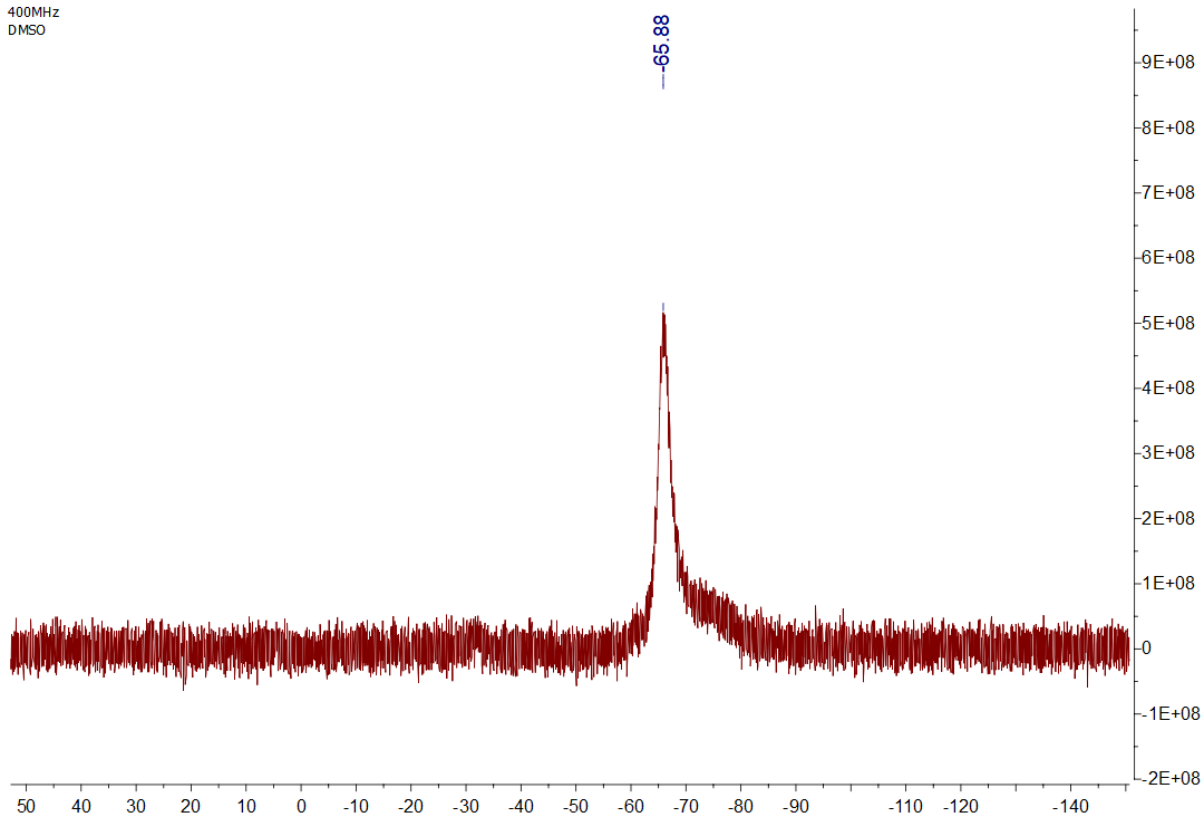


Figure S39.  $^{31}\text{P}$  NMR spectrum of complex  $[\text{CuI}(\text{DBPTA})_3]$  (**4**) in  $\text{DMSO-}d_6$  (400 MHz).

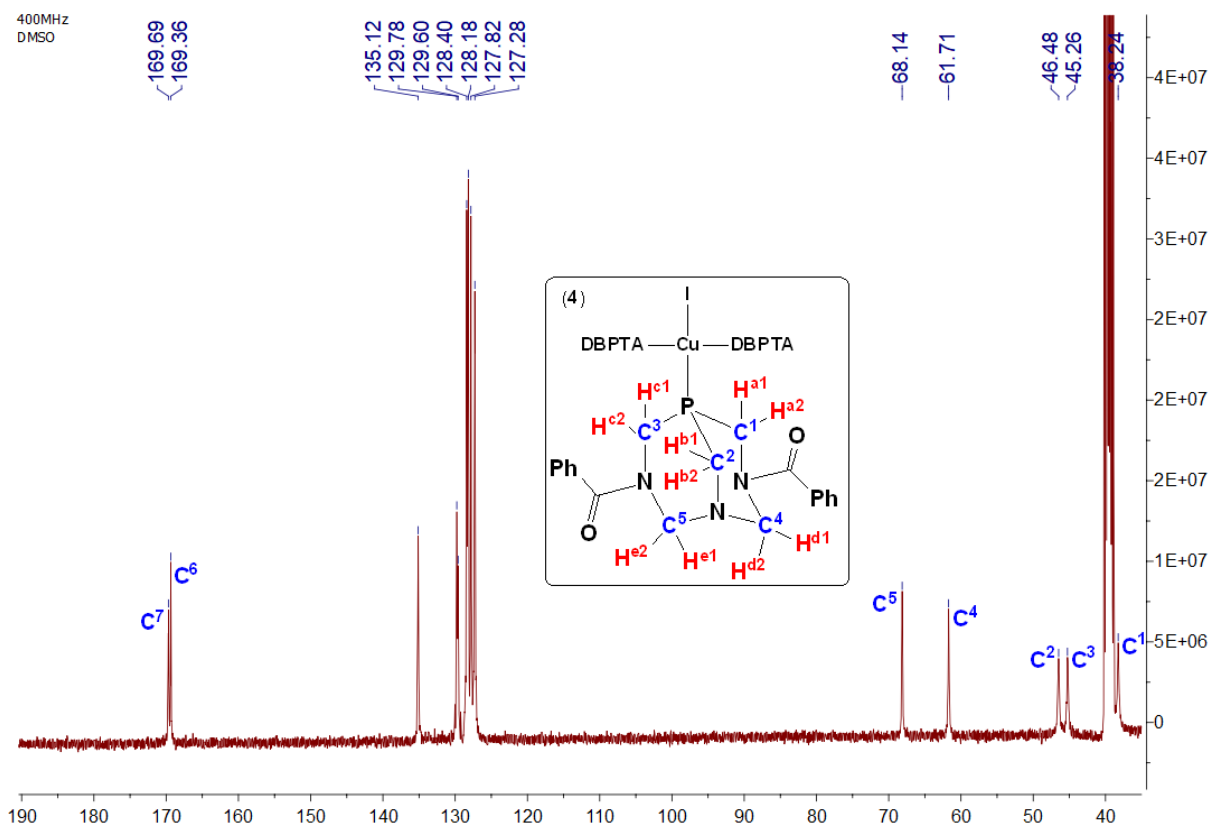
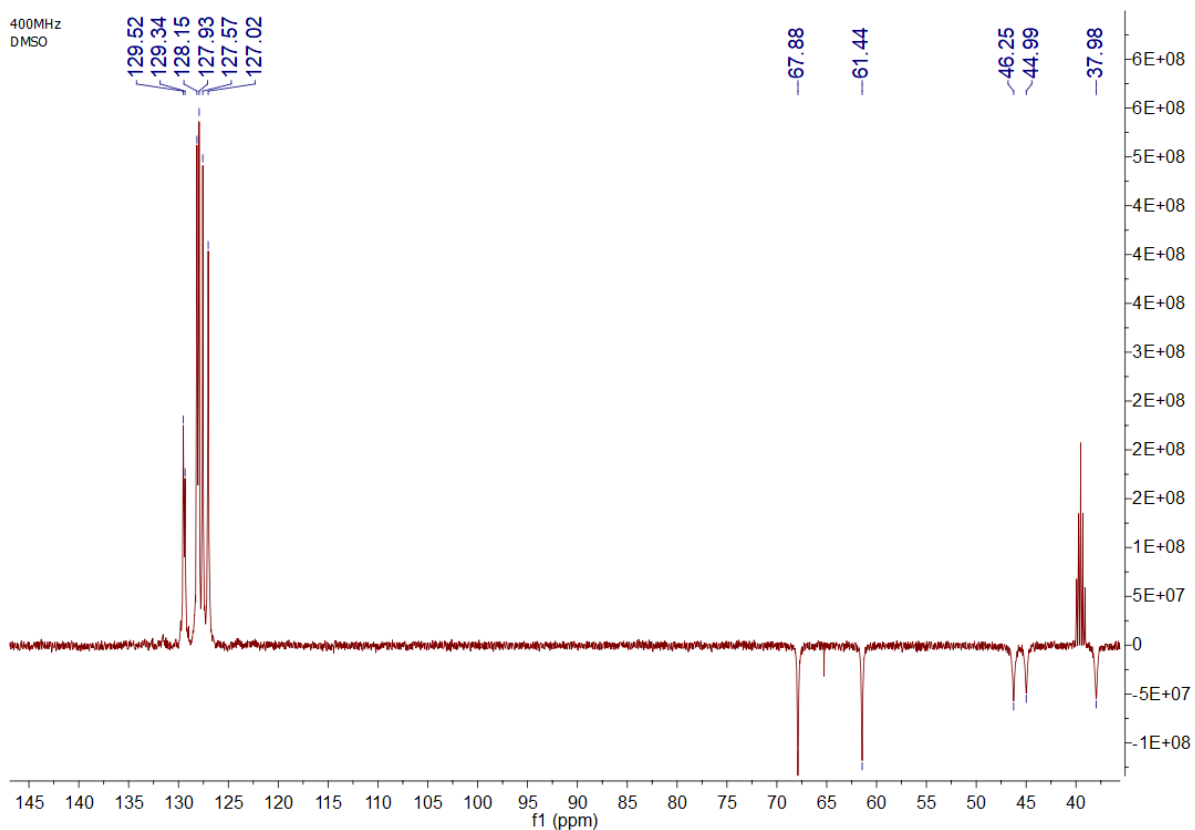
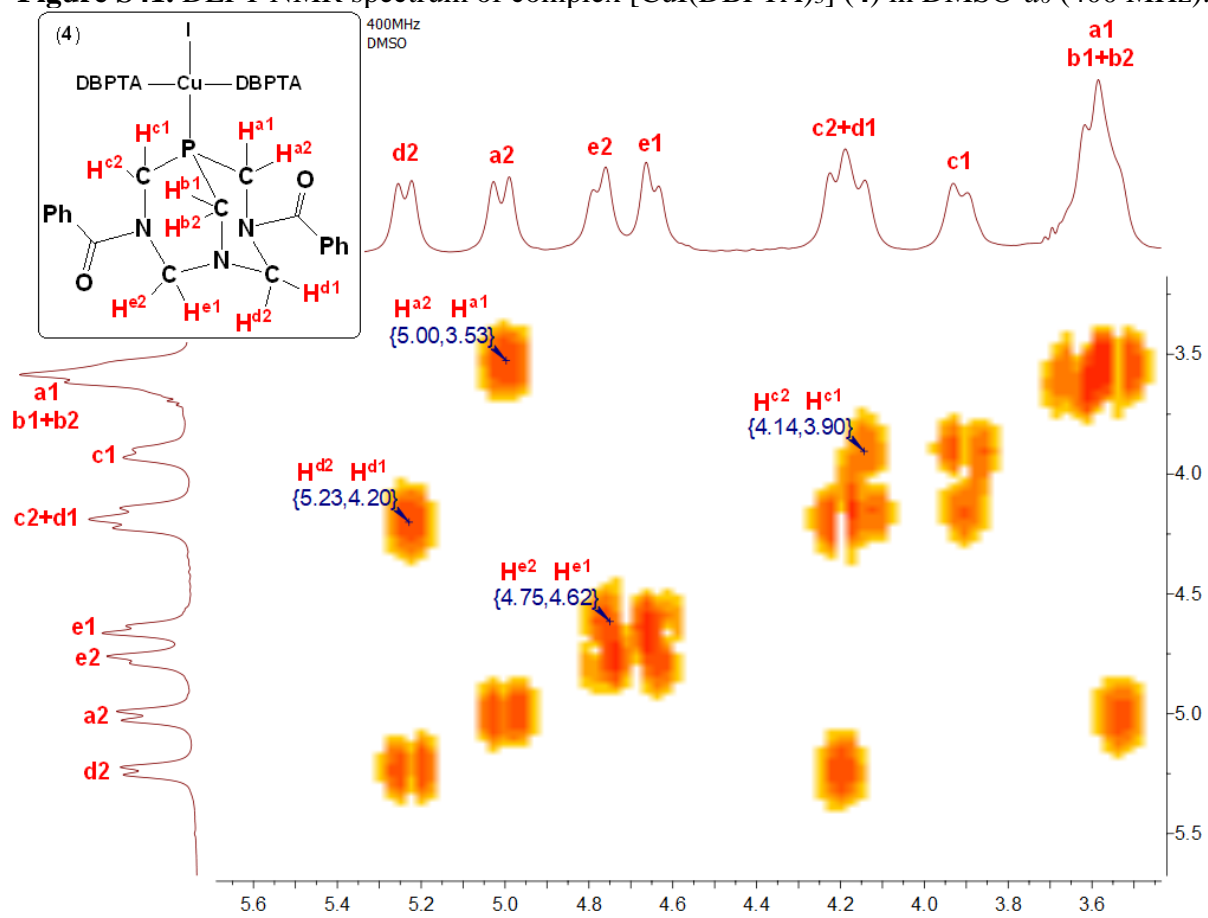


Figure S40.  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of complex  $[\text{CuI}(\text{DBPTA})_3]$  (**4**) in  $\text{DMSO-}d_6$  (400 MHz).



**Figure S41.** DEPT NMR spectrum of complex  $[\text{CuI}(\text{DBPTA})_3]$  (**4**) in  $\text{DMSO-}d_6$  (400 MHz).



**Figure S42.** COSY spectrum of complex  $[\text{CuI}(\text{DBPTA})_3]$  (**4**) in  $\text{DMSO-}d_6$  (400 MHz).



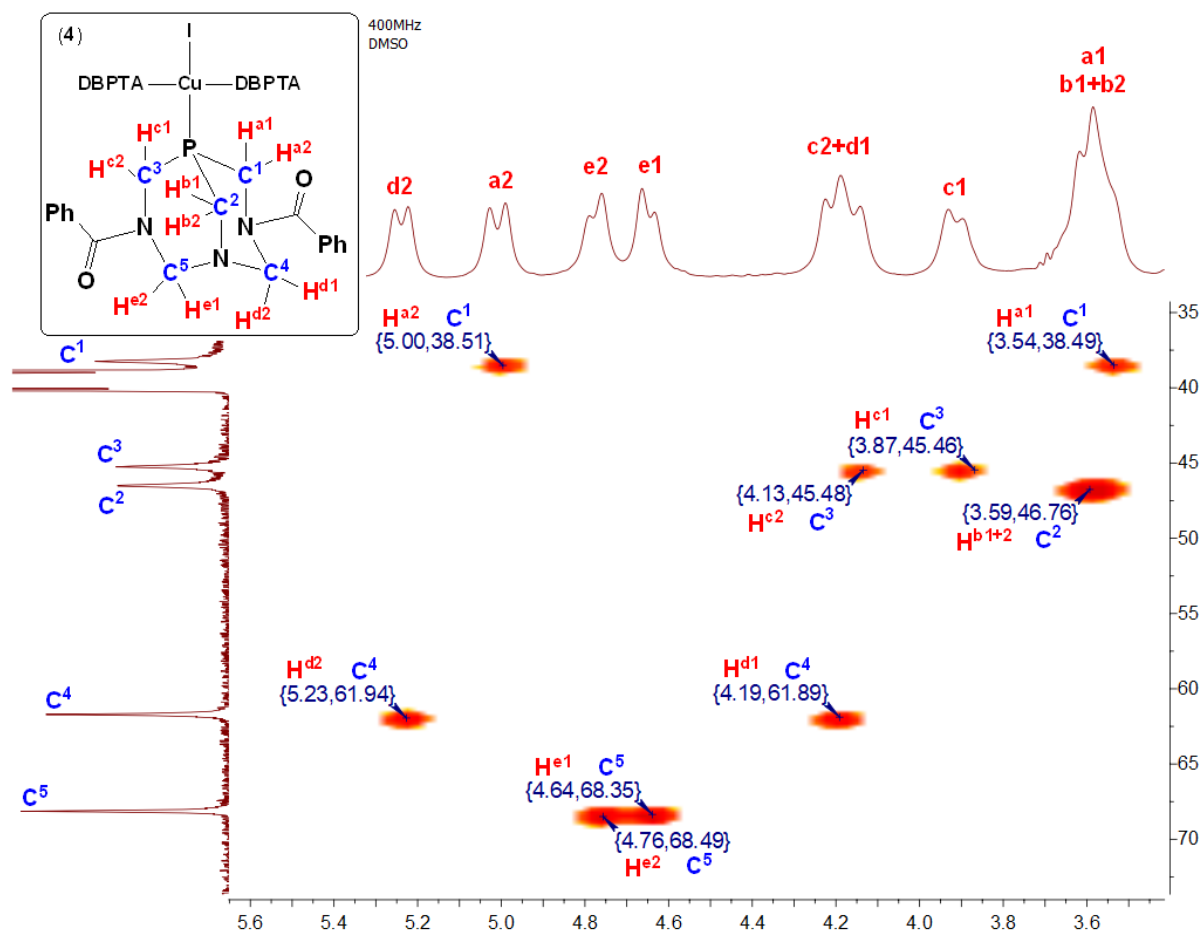


Figure S43. HSQC spectrum of complex  $[\text{Cu}(\text{DBPTA})_3]$  (4) in  $\text{DMSO-}d_6$  (400 MHz).

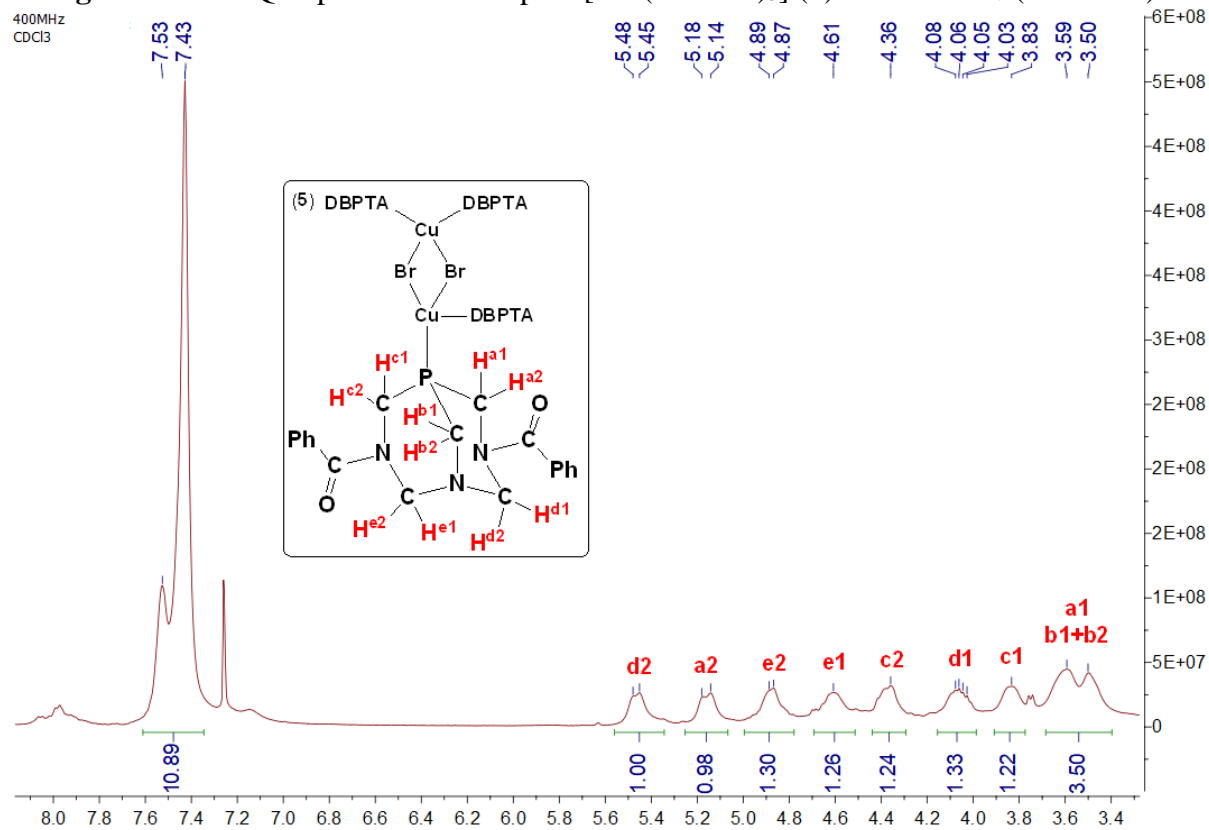
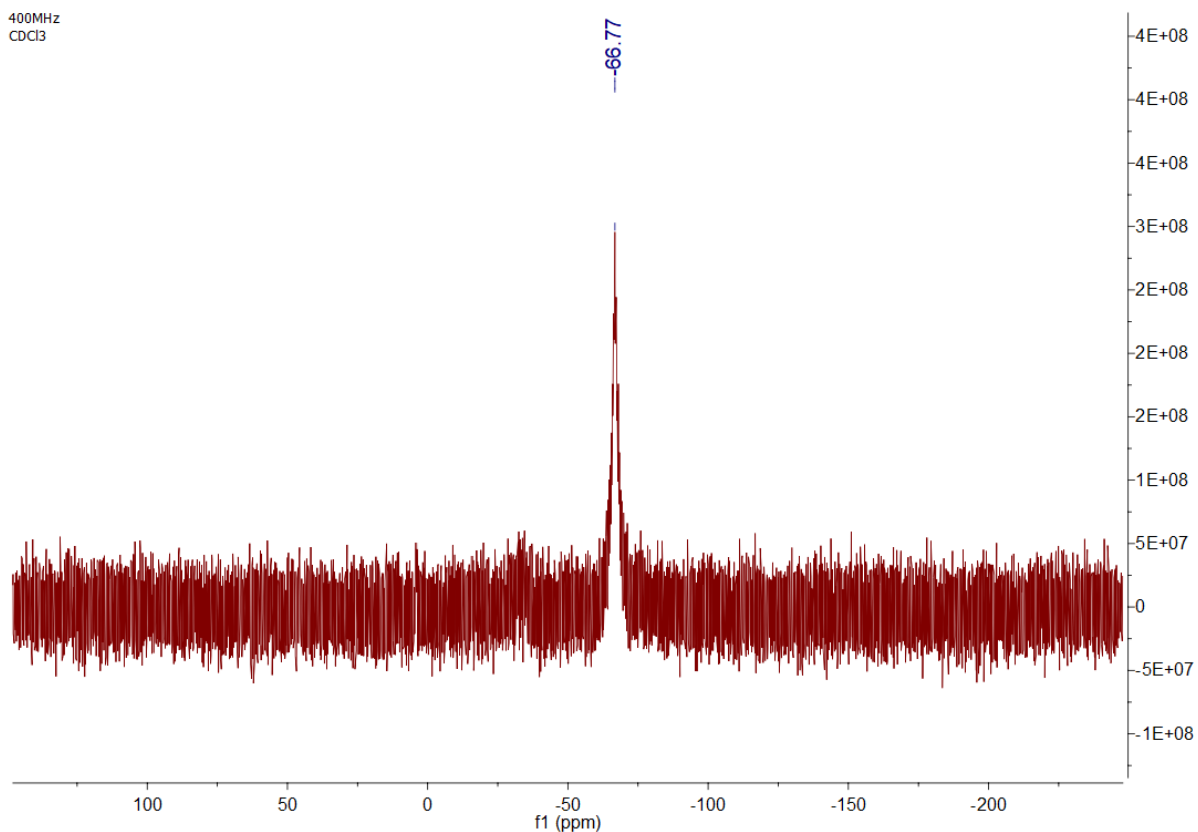
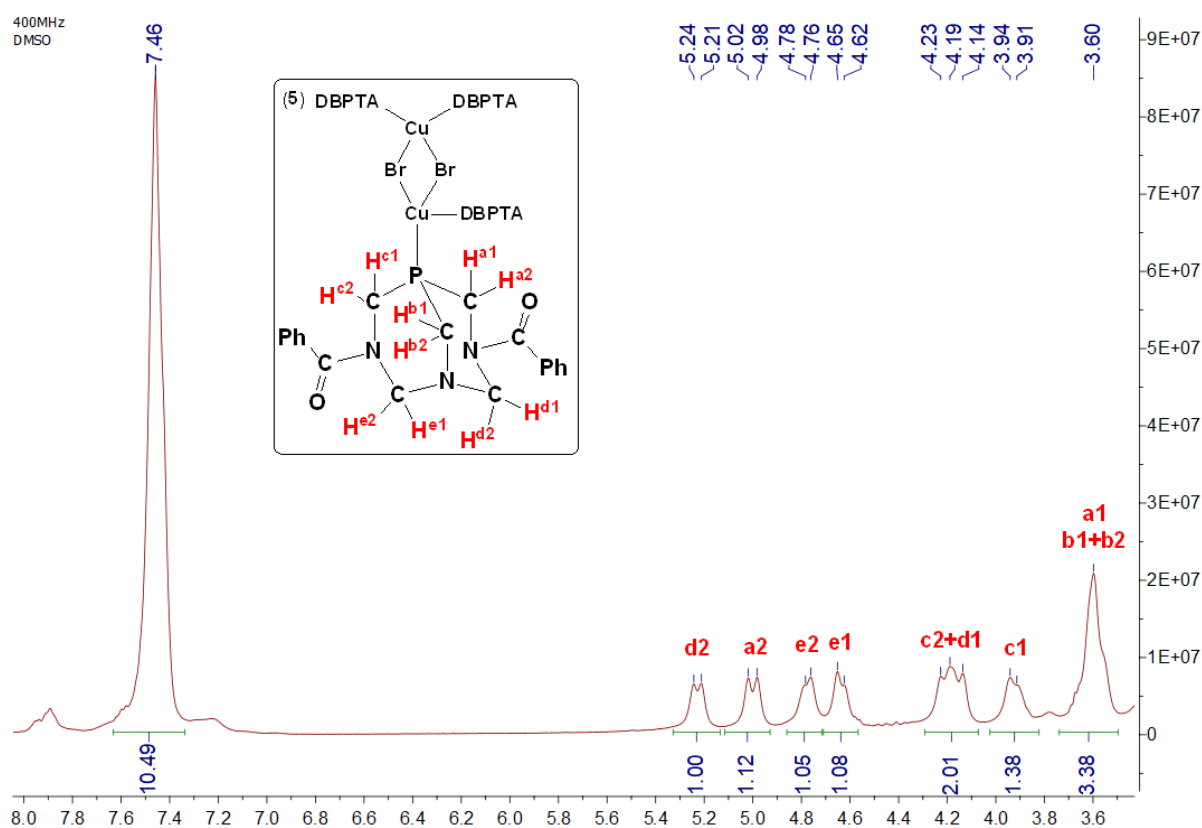


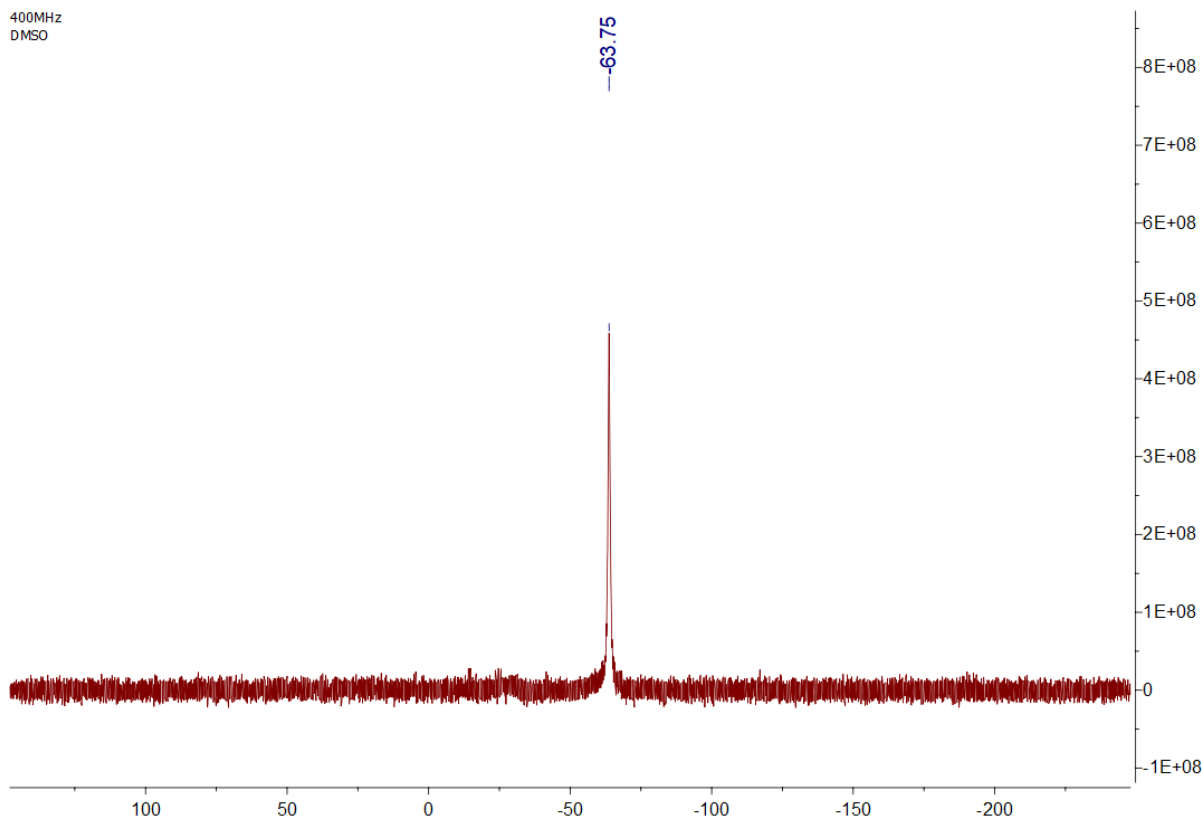
Figure S44.  $^1\text{H}$  NMR spectrum of complex  $[\text{Cu}(\mu\text{-Br})(\text{DBPTA})_2]_2$  (5) in  $\text{CDCl}_3$  (400 MHz).



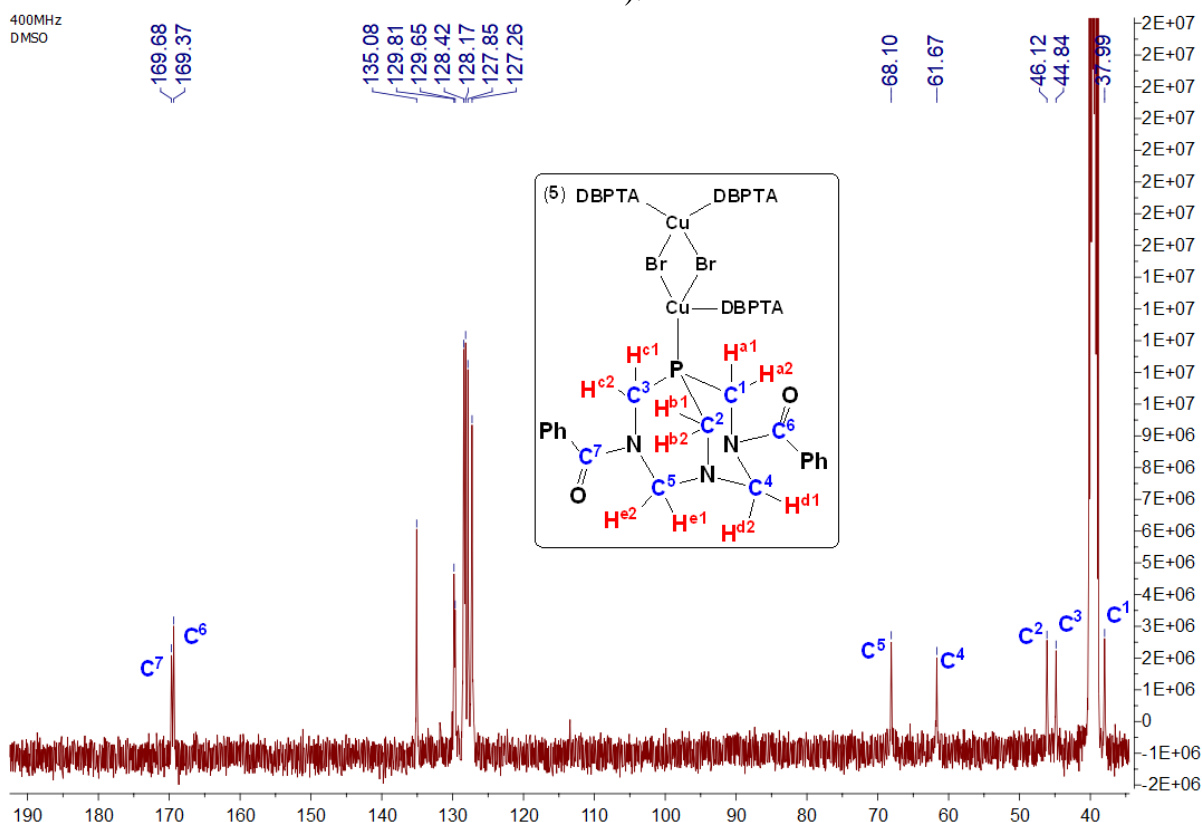
**Figure S45.** <sup>31</sup>P NMR spectrum of complex [Cu(μ-Br)(DBPTA)<sub>2</sub>]<sub>2</sub> (**5**) in CDCl<sub>3</sub> (400 MHz).



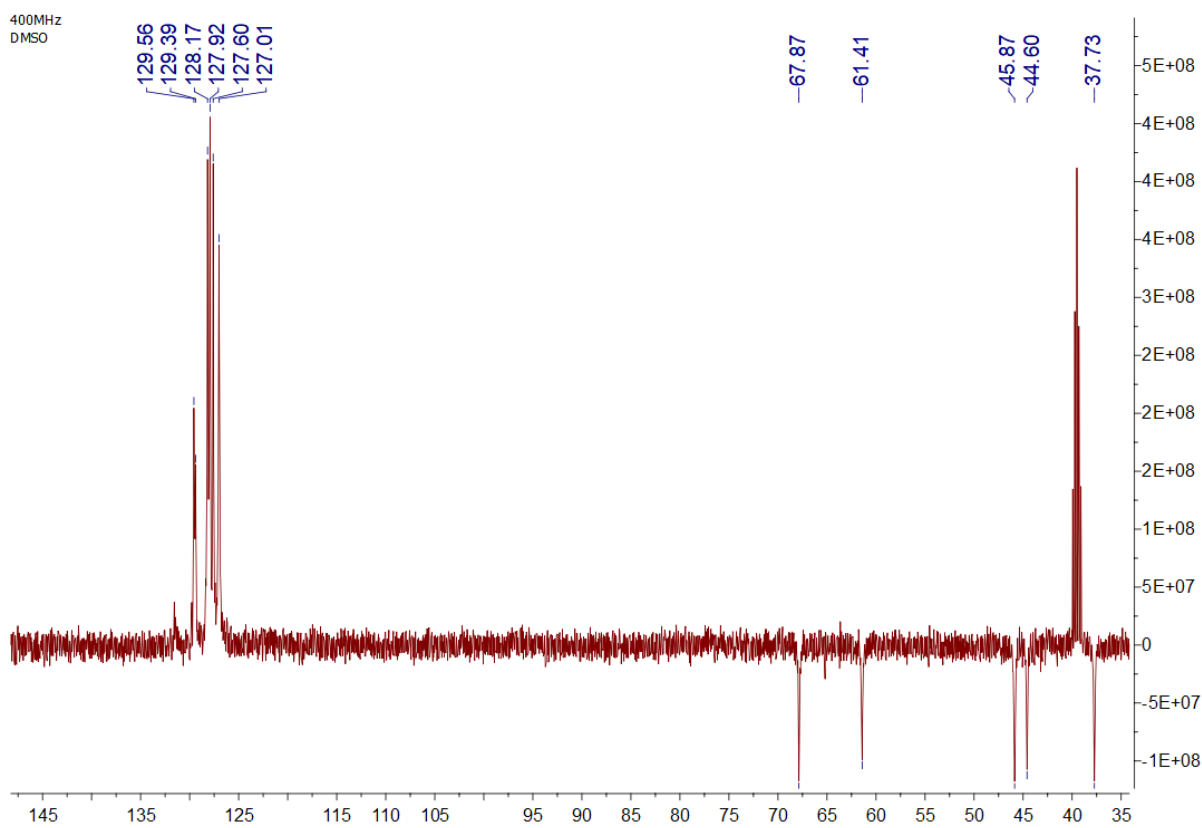
**Figure S46.** <sup>1</sup>H NMR spectrum of complex [Cu(μ-Br)(DBPTA)<sub>2</sub>]<sub>2</sub> (**5**) in DMSO-*d*<sub>6</sub> (400 MHz).



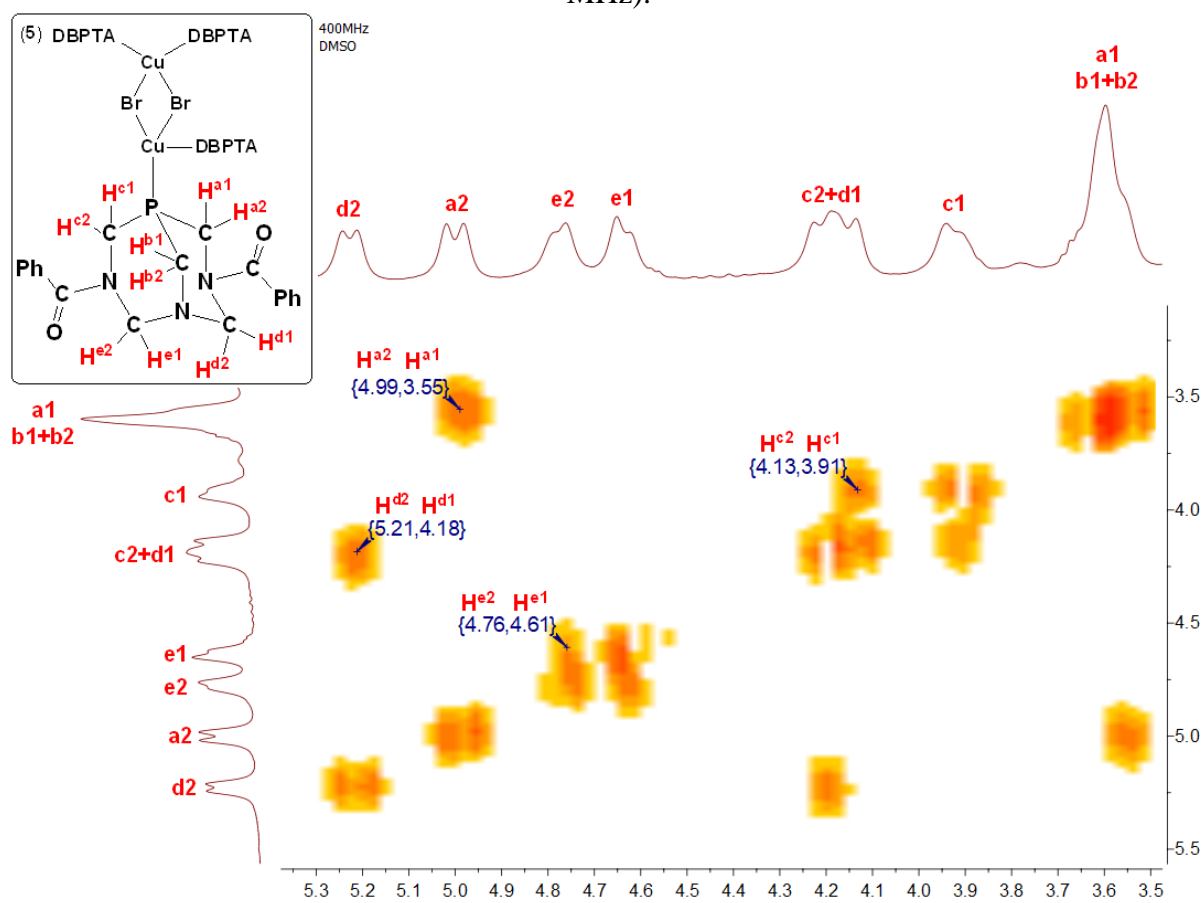
**Figure S47.**  $^{31}\text{P}$  NMR spectrum of complex  $[\text{Cu}(\mu\text{-Br})(\text{DBPTA})_2]_2$  (**5**) in  $\text{DMSO-}d_6$  (400 MHz).



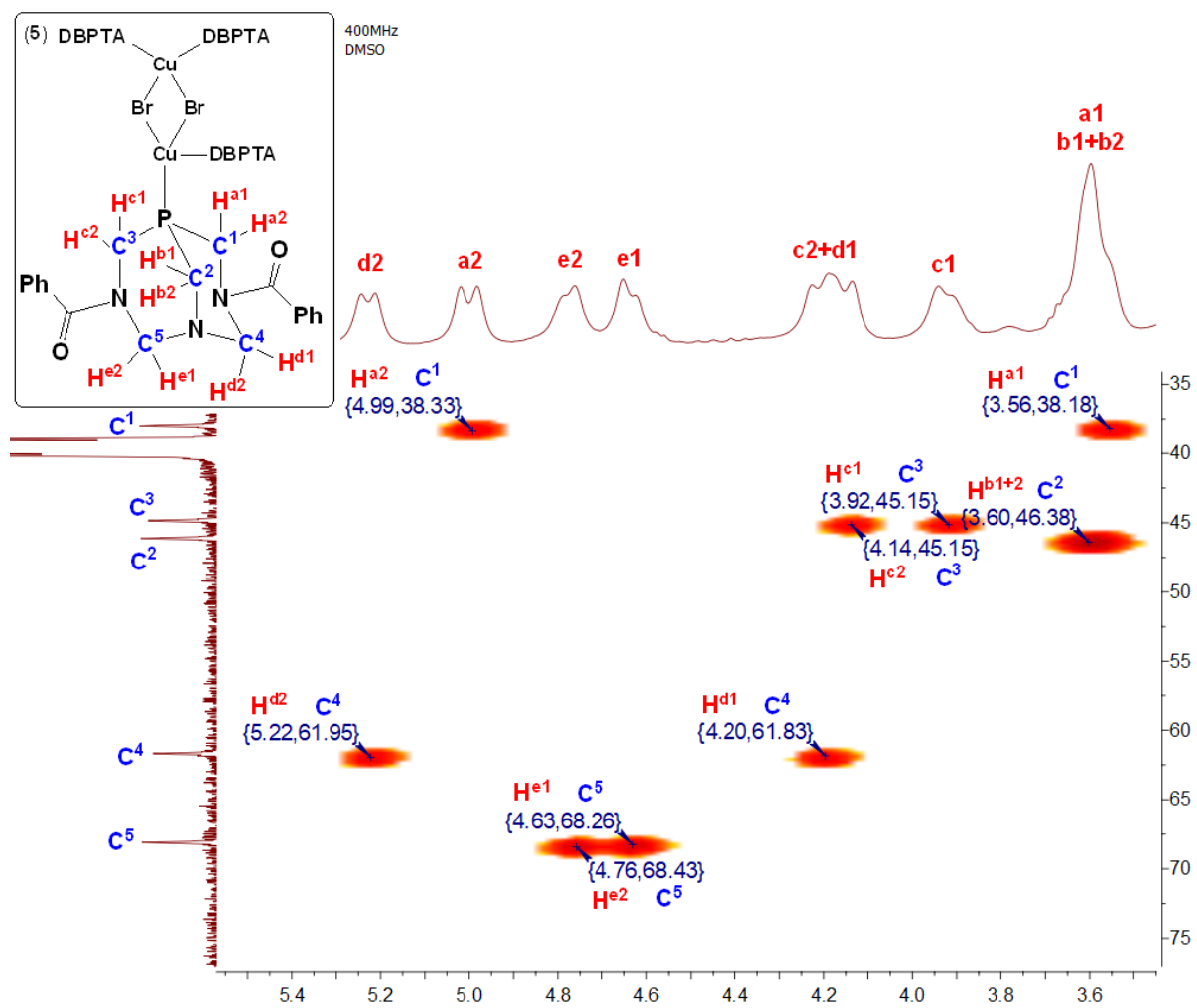
**Figure S48.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of complex  $[\text{Cu}(\mu\text{-Br})(\text{DBPTA})_2]_2$  (**5**) in  $\text{DMSO-}d_6$  (400 MHz).



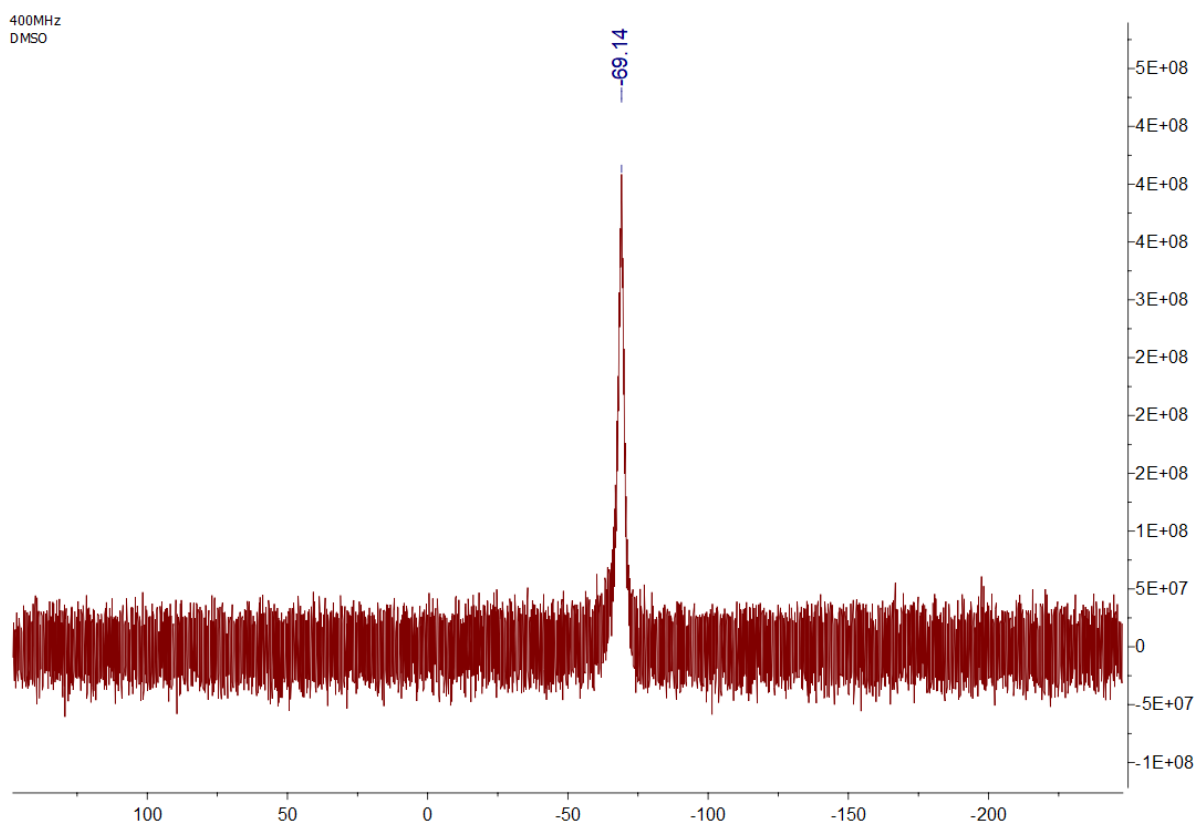
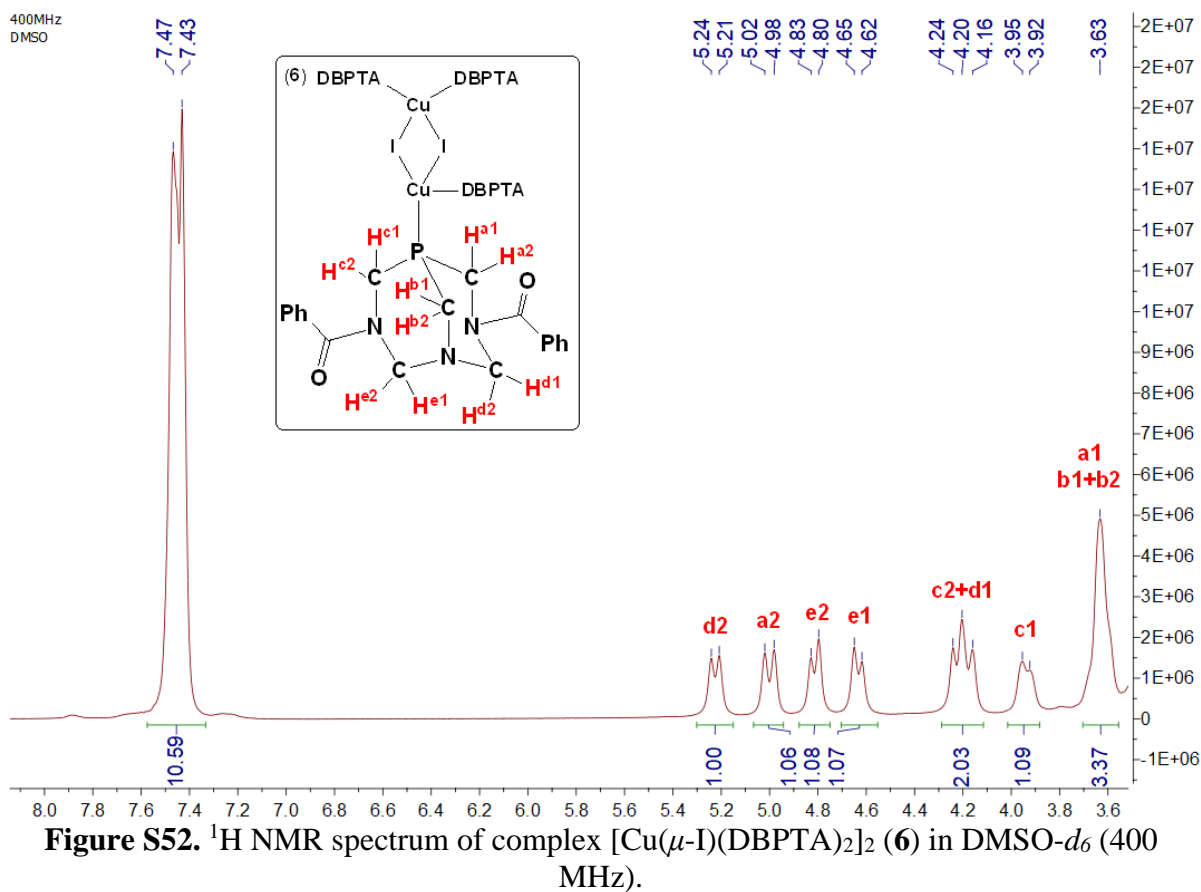
**Figure S49.** DEPT NMR spectrum of complex  $[\text{Cu}(\mu\text{-Br})(\text{DBPTA})_2]_2$  (**5**) in  $\text{DMSO-}d_6$  (400 MHz).

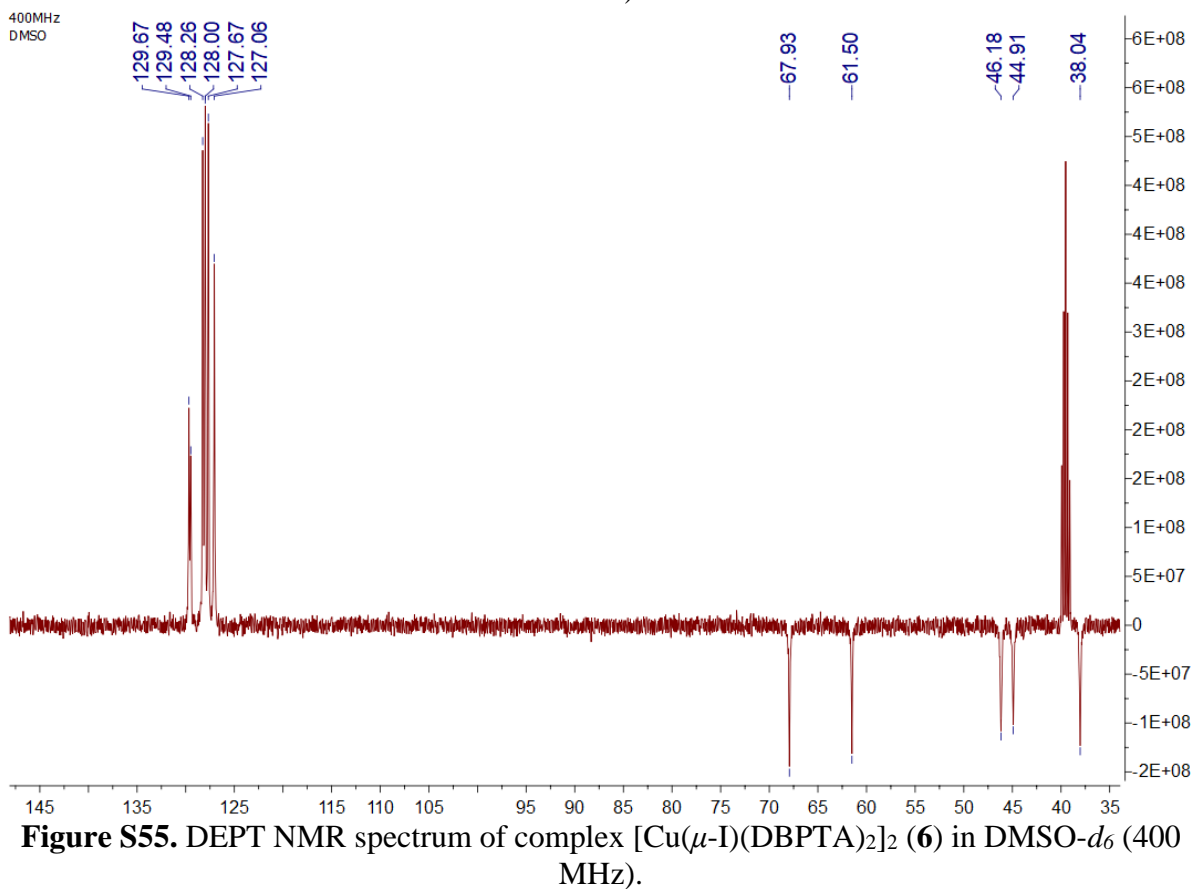
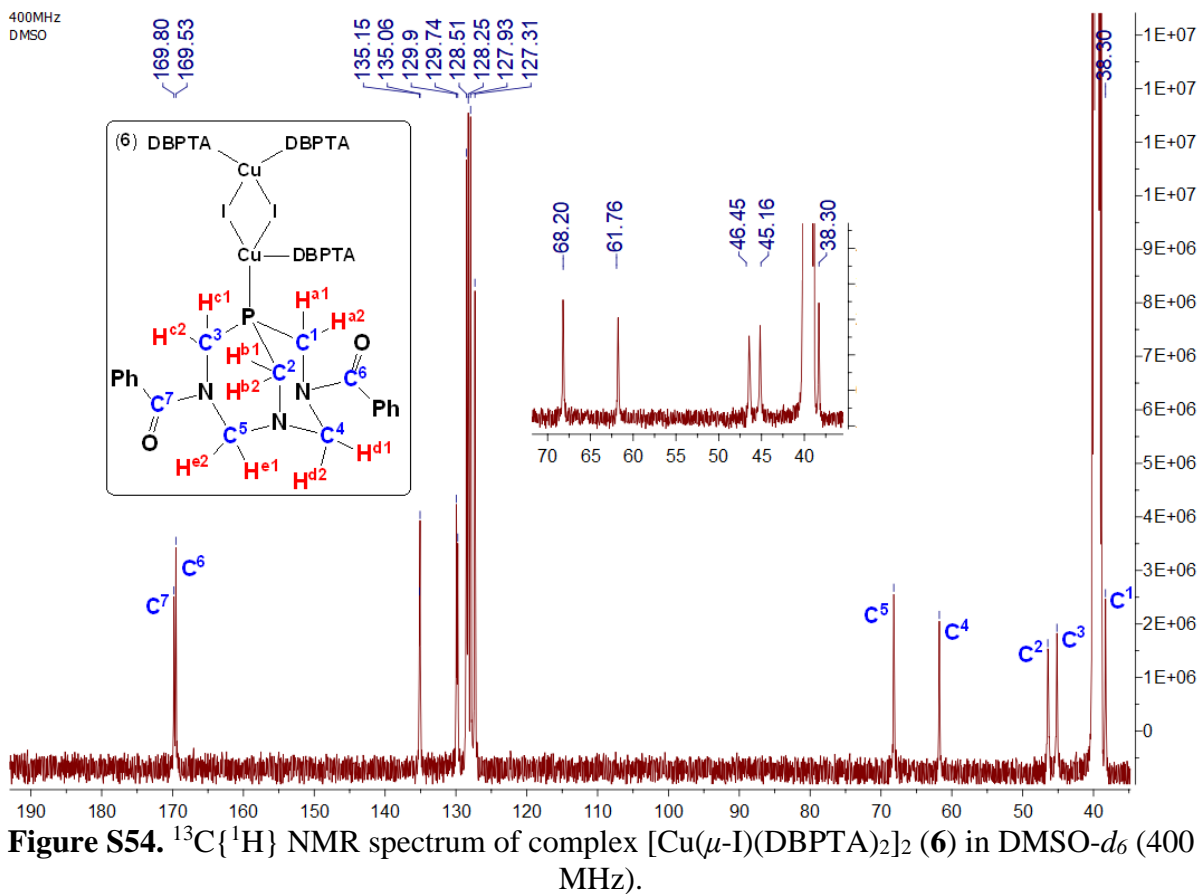


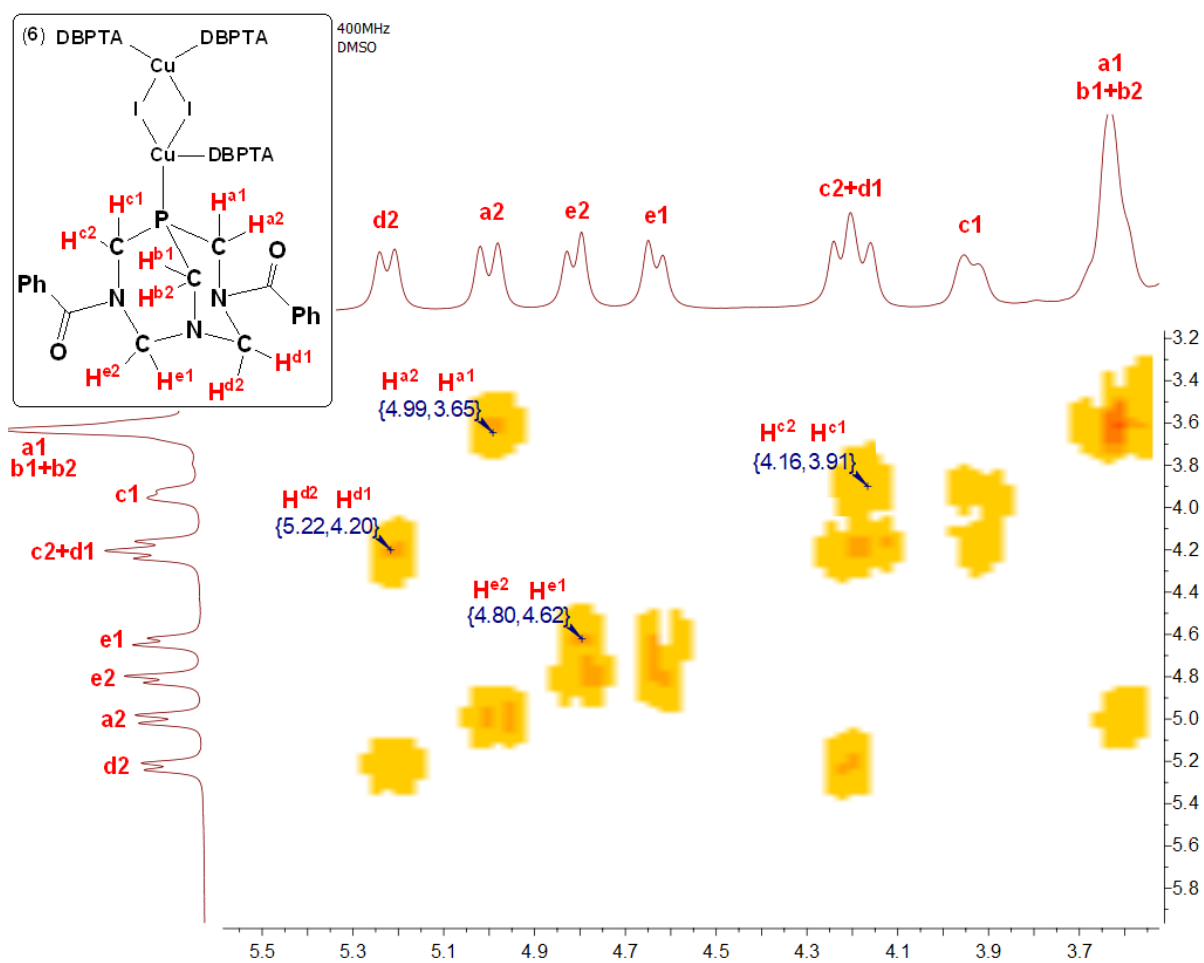
**Figure S50.** COSY spectrum of complex  $[\text{Cu}(\mu\text{-Br})(\text{DBPTA})_2]_2$  (**5**) in  $\text{DMSO-}d_6$  (400 MHz).



**Figure S51.** HSQC spectrum of complex  $[Cu(\mu\text{-Br})(DBPTA)_2]_2$  (5) in DMSO- $d_6$  (400 MHz).







**Figure S56.** COSY spectrum of complex  $[Cu(\mu-I)(DBPTA)_2]_2$  (**6**) in  $DMSO-d_6$  (400 MHz).



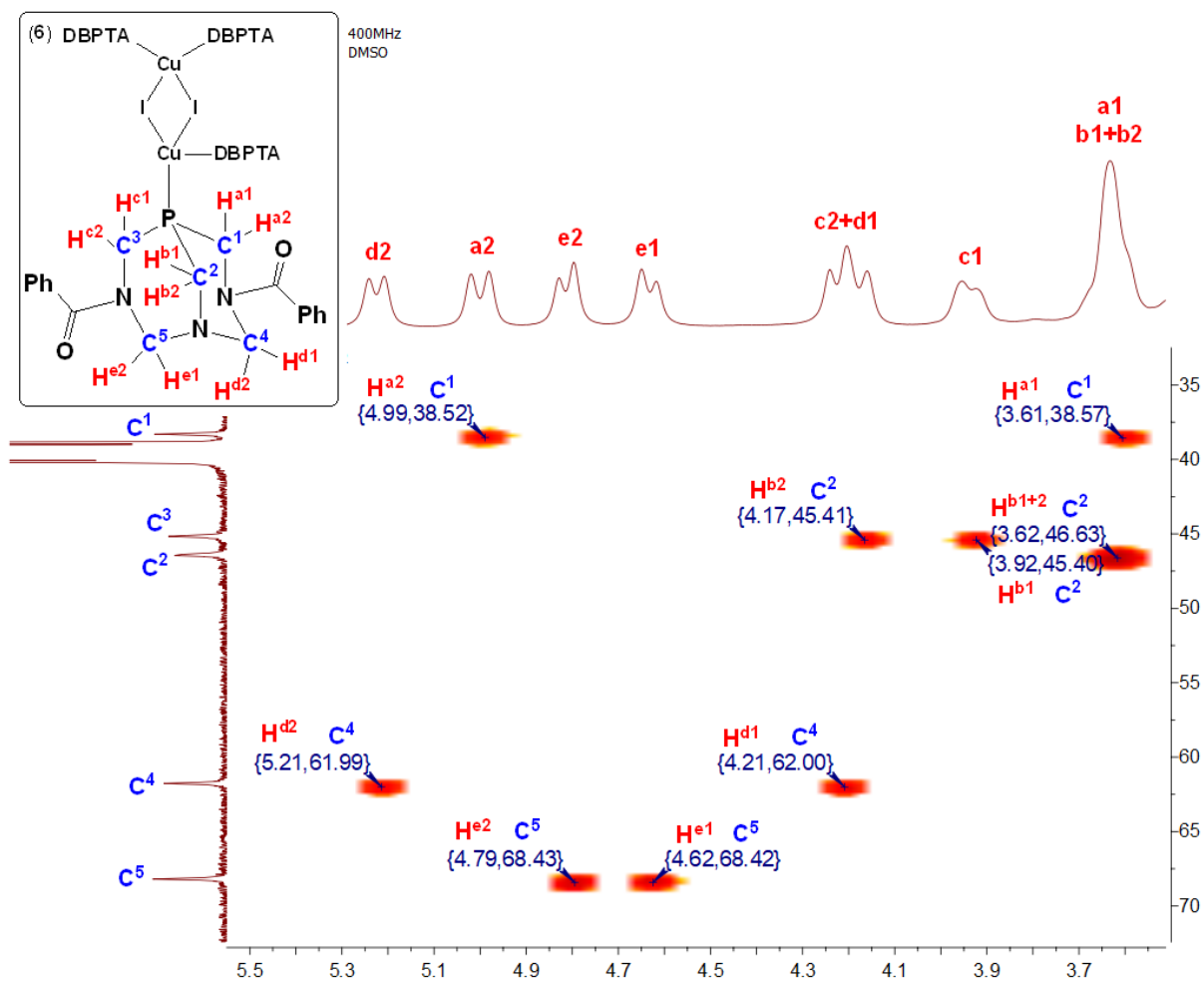
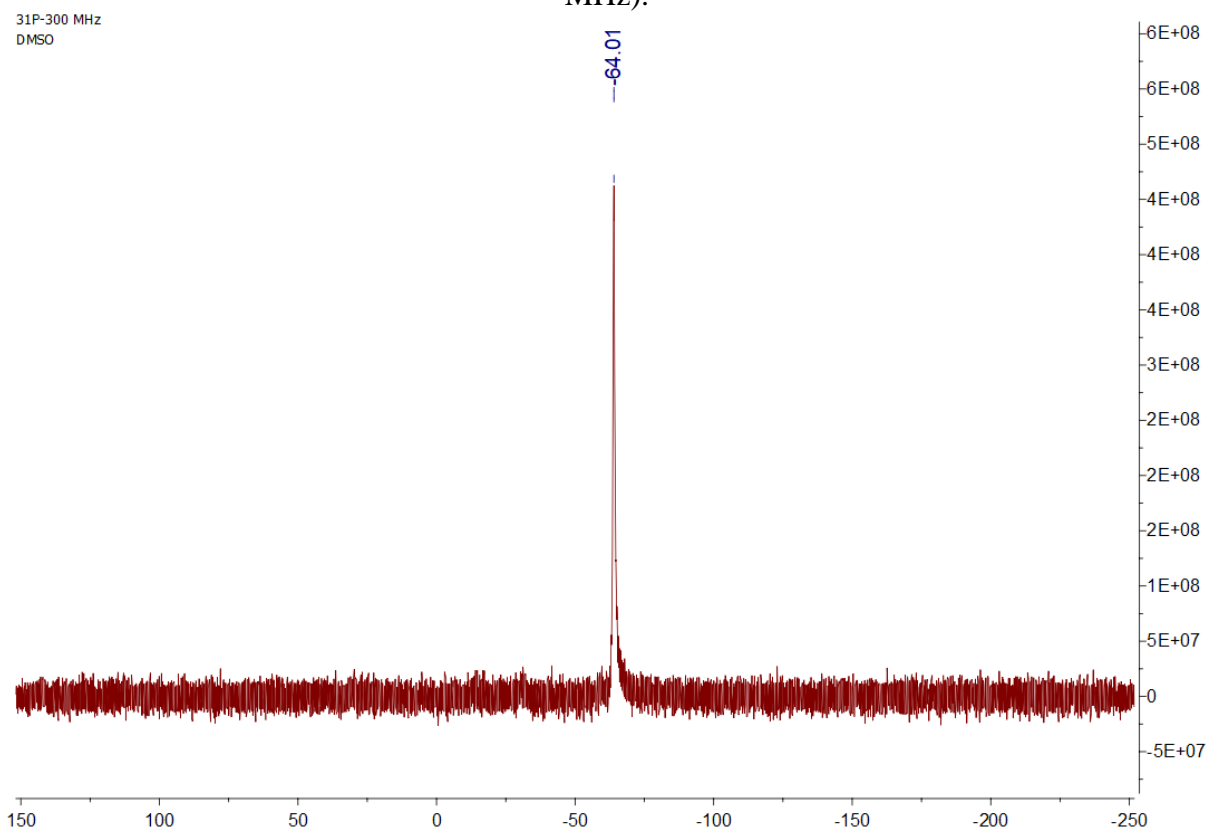
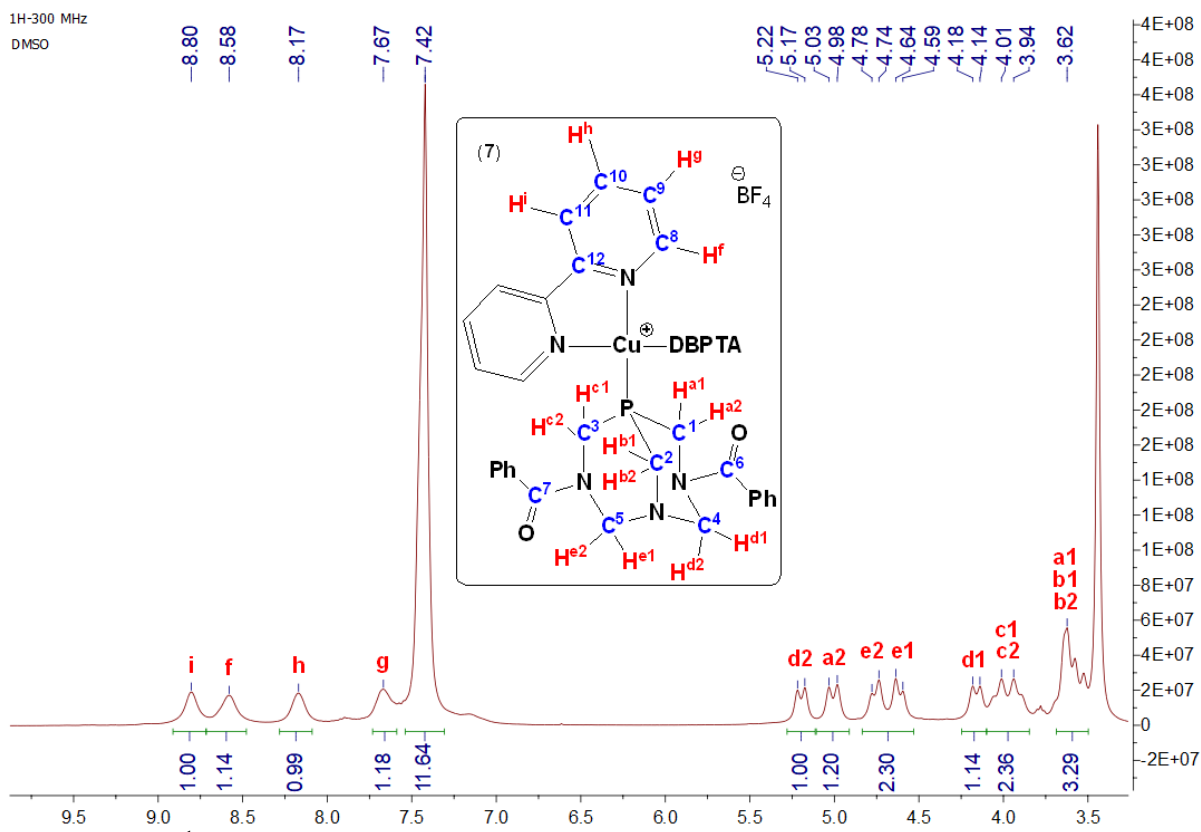
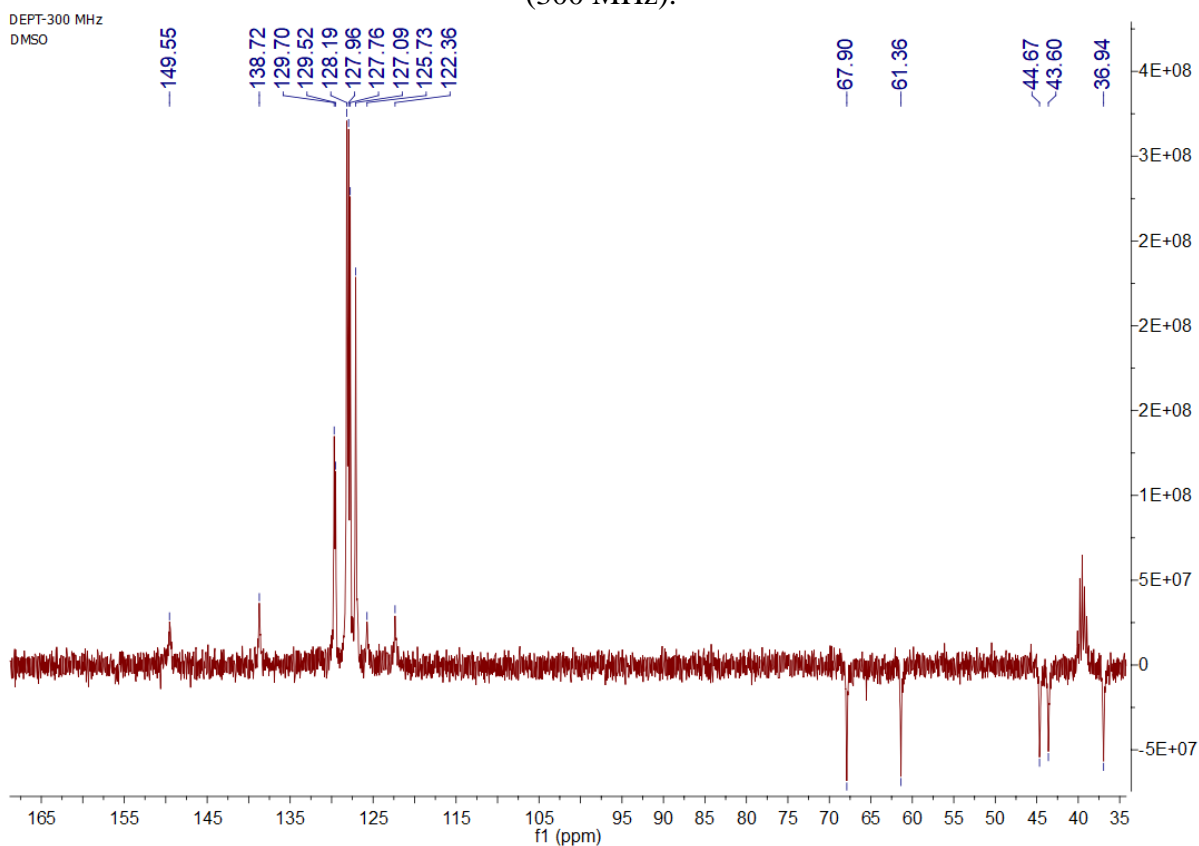
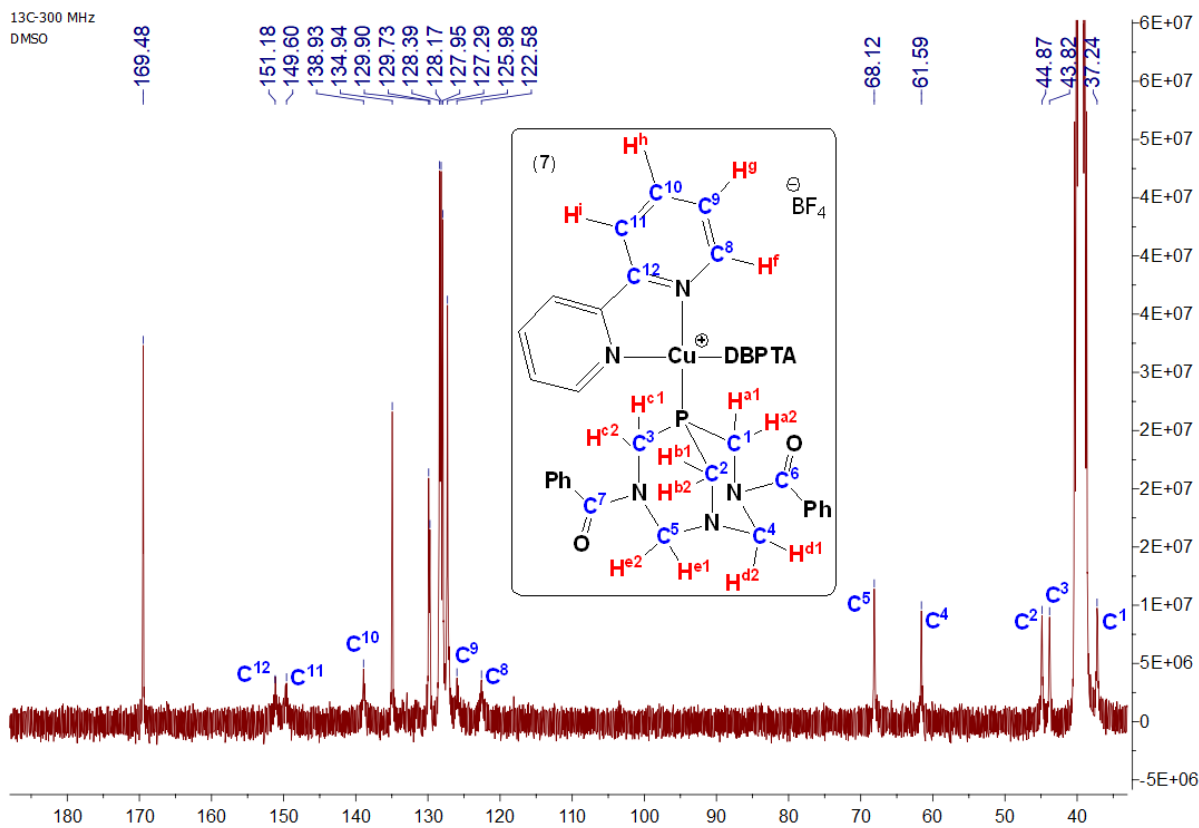
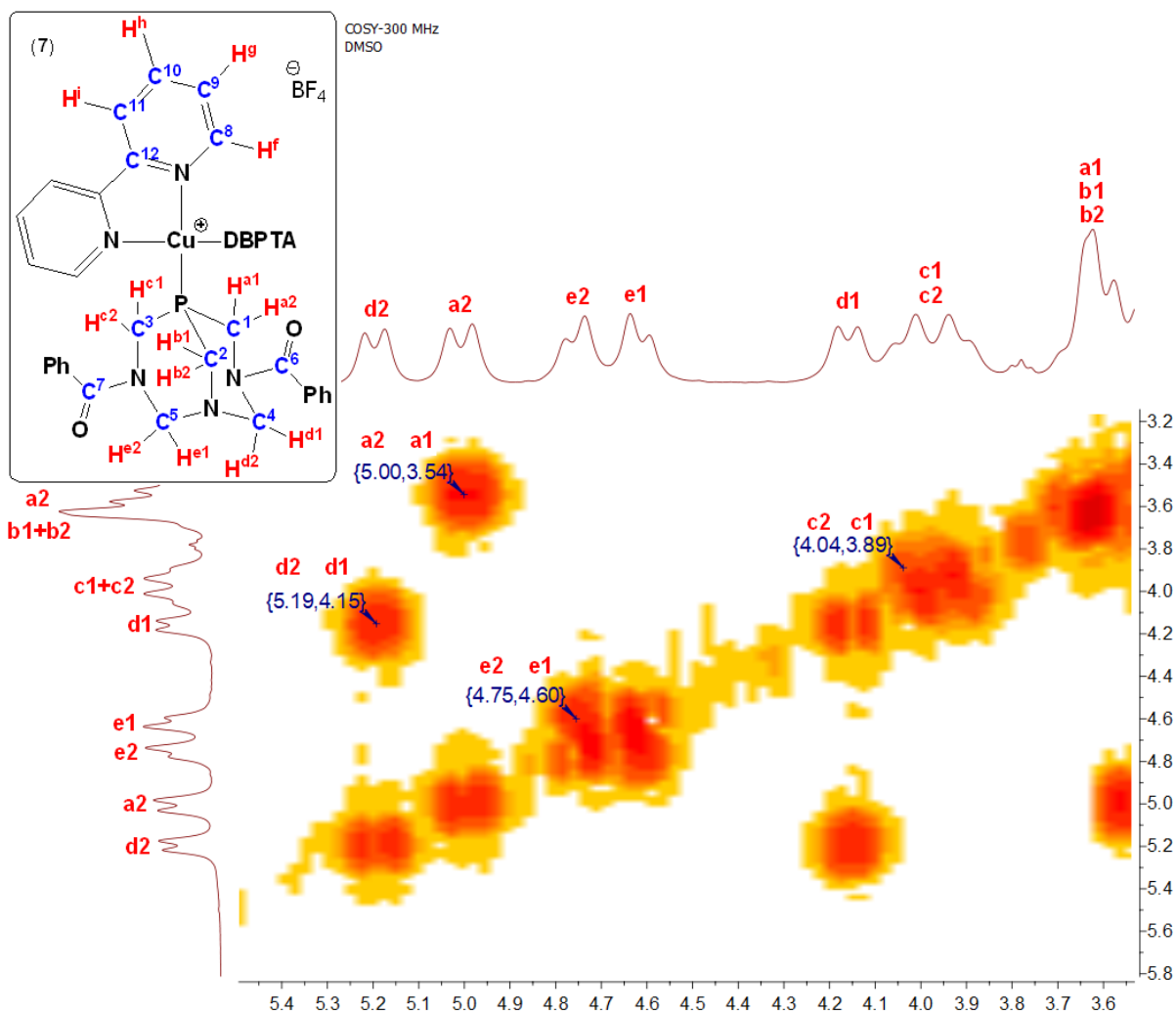


Figure S57. HSQC spectrum of complex  $[\text{Cu}(\mu\text{-I})(\text{DBPTA})_2]_2$  (6) in  $\text{DMSO-}d_6$  (400 MHz).







**Figure S62.** COSY spectrum of complex [Cu(bpy)(DBPTA)<sub>2</sub>BF<sub>4</sub>] (7) in DMSO-*d*<sub>6</sub> (300 MHz).

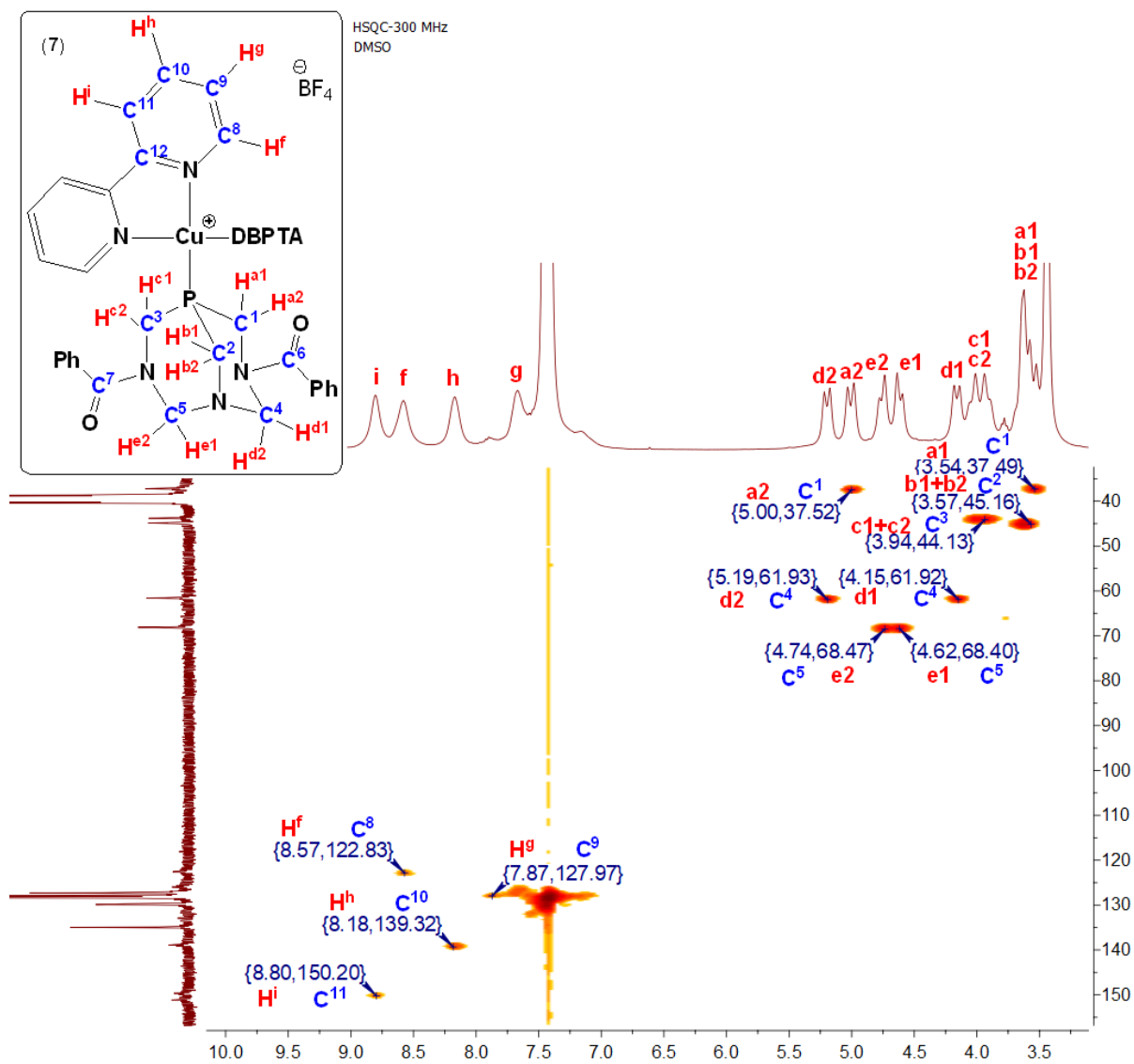
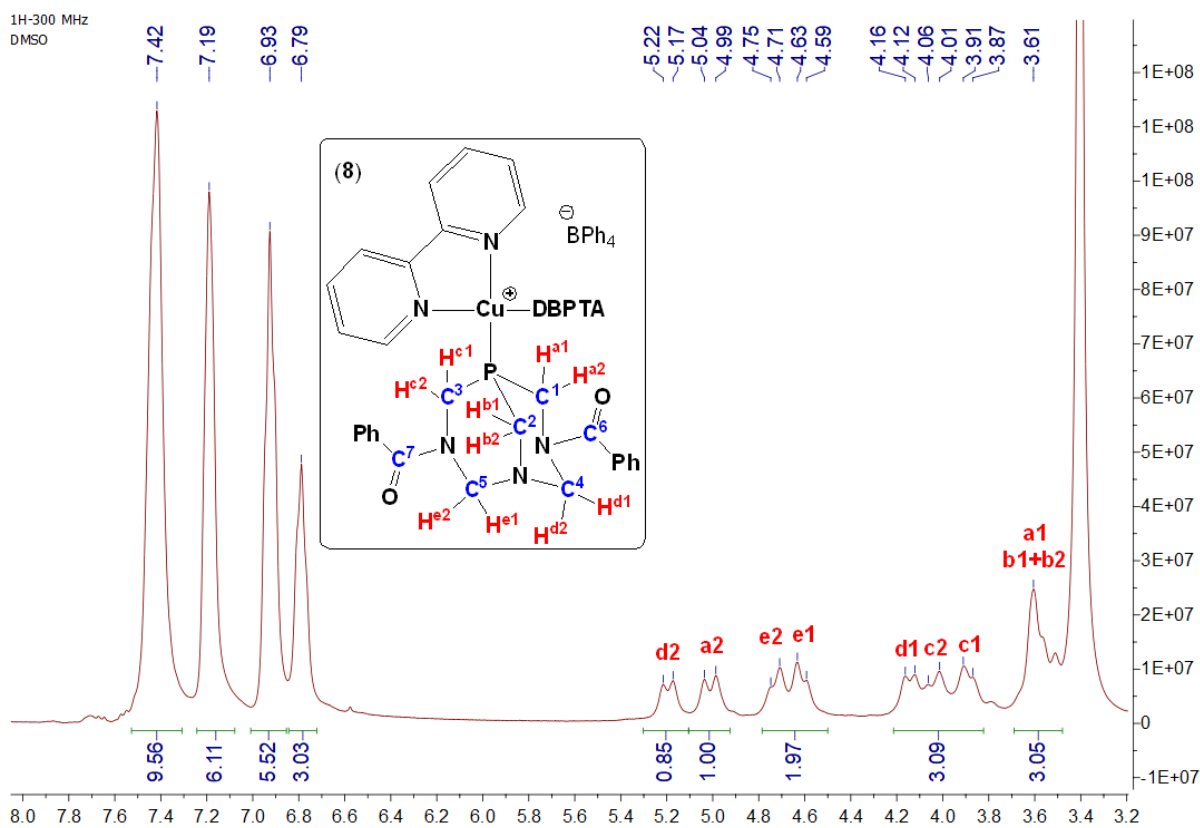
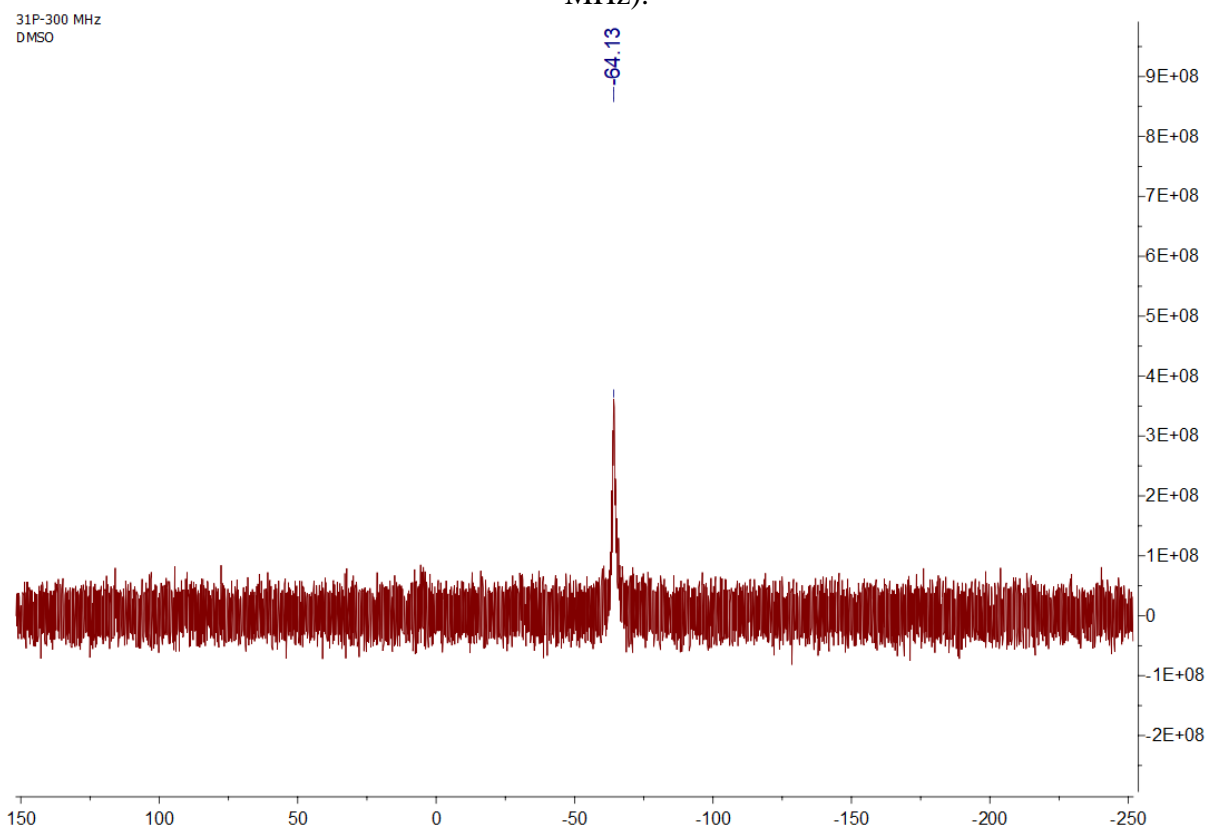


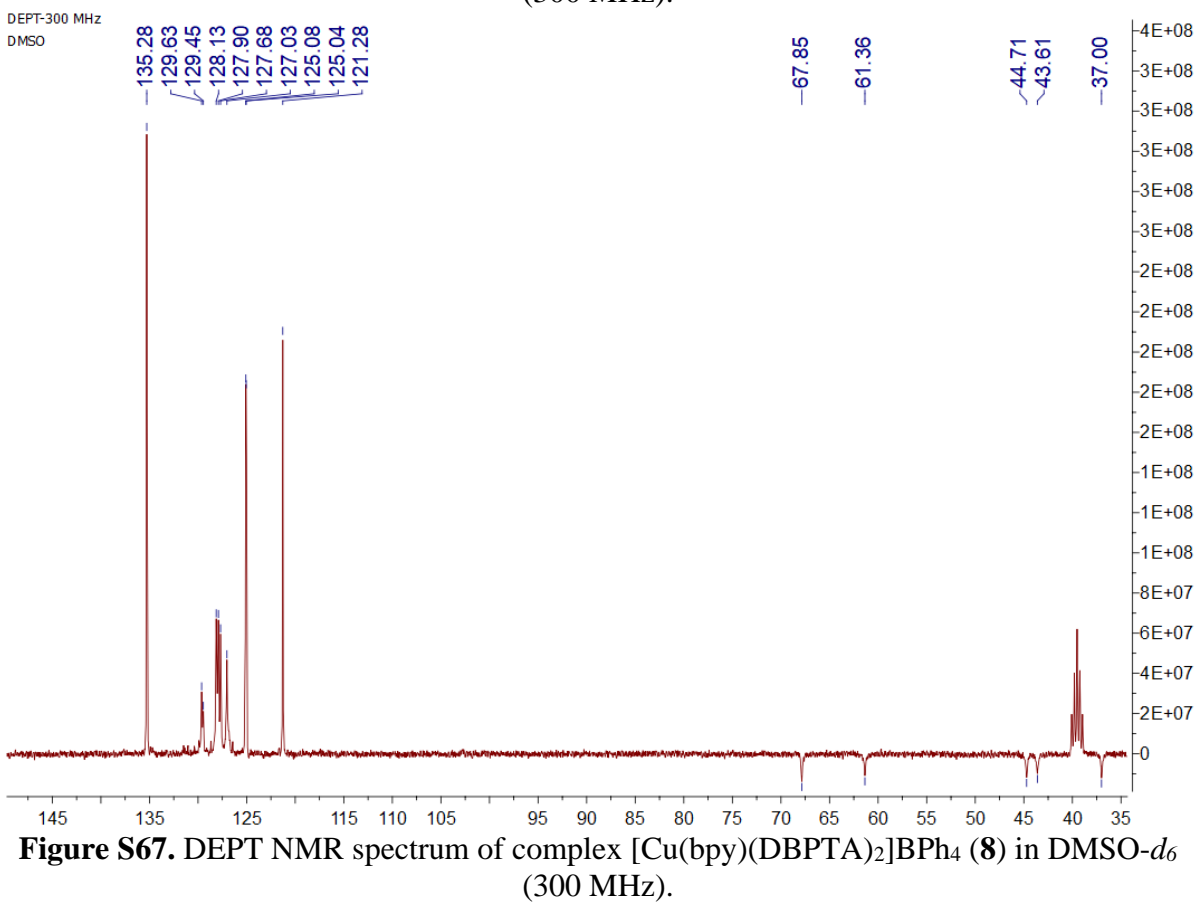
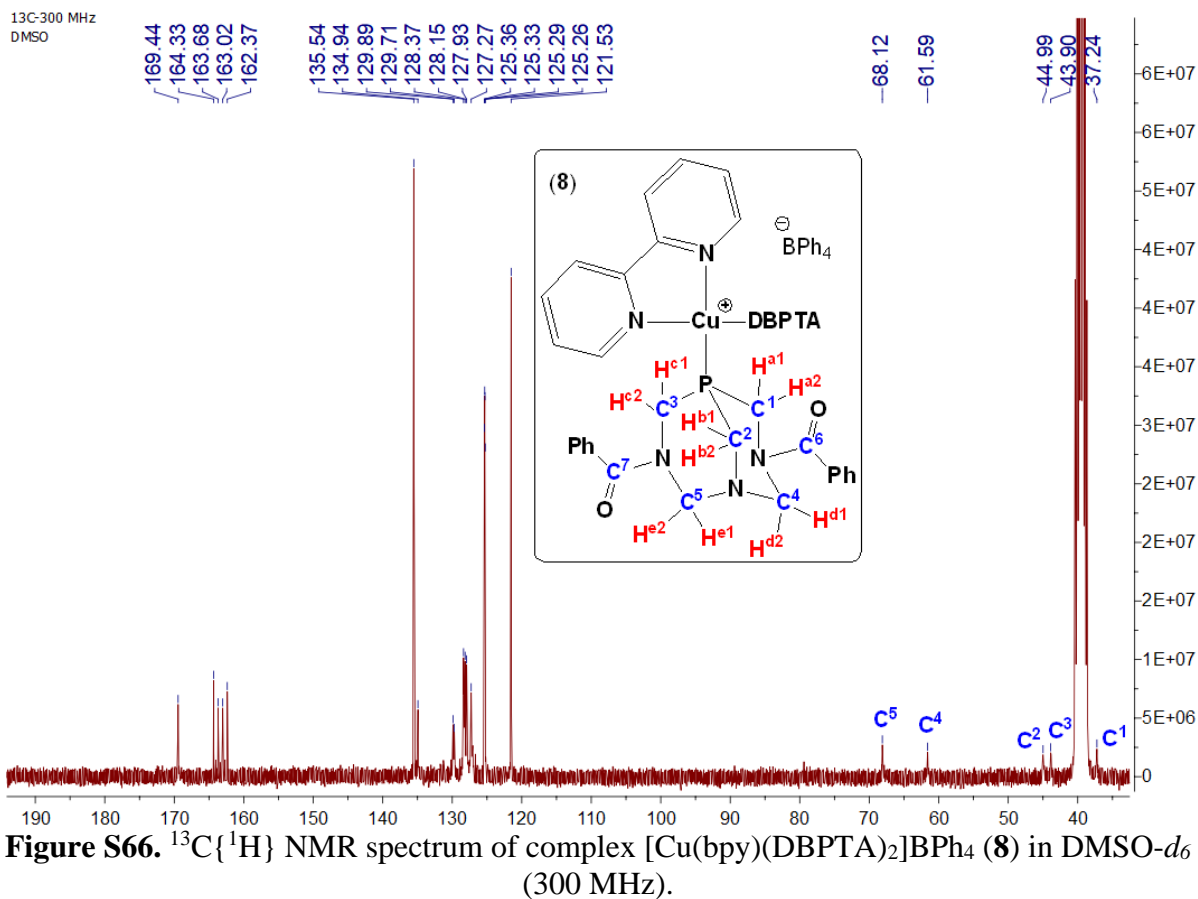
Figure S63. HSQC spectrum of complex  $[\text{Cu}(\text{bpy})(\text{DBPTA})_2]\text{BF}_4$  (7) in  $\text{DMSO}-d_6$  (300 MHz).

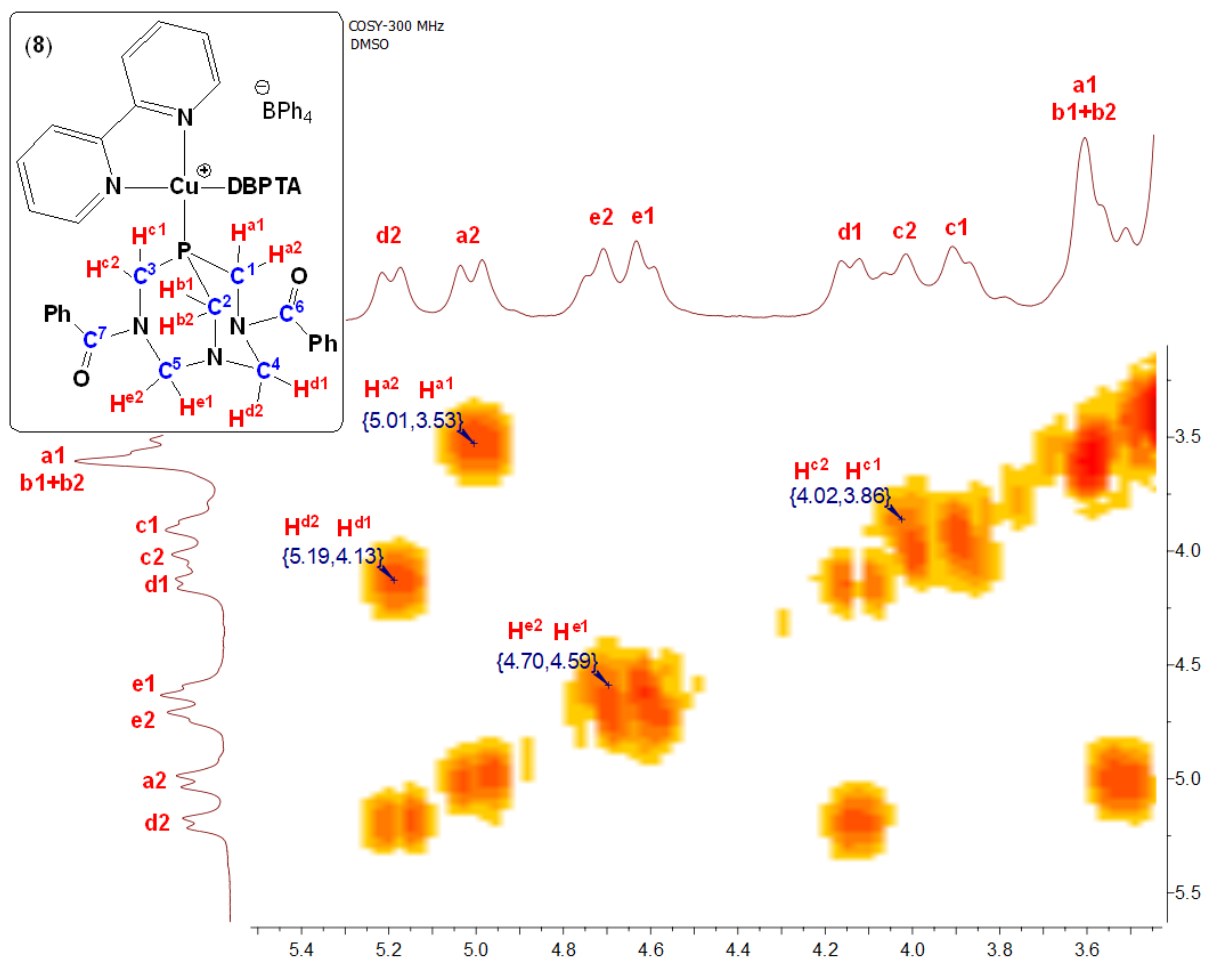


**Figure S64.**  $^1\text{H}$  NMR spectrum of complex  $[\text{Cu}(\text{bpy})(\text{DBPTA})_2]\text{BPh}_4$  (**8**) in  $\text{DMSO-}d_6$  (300 MHz).



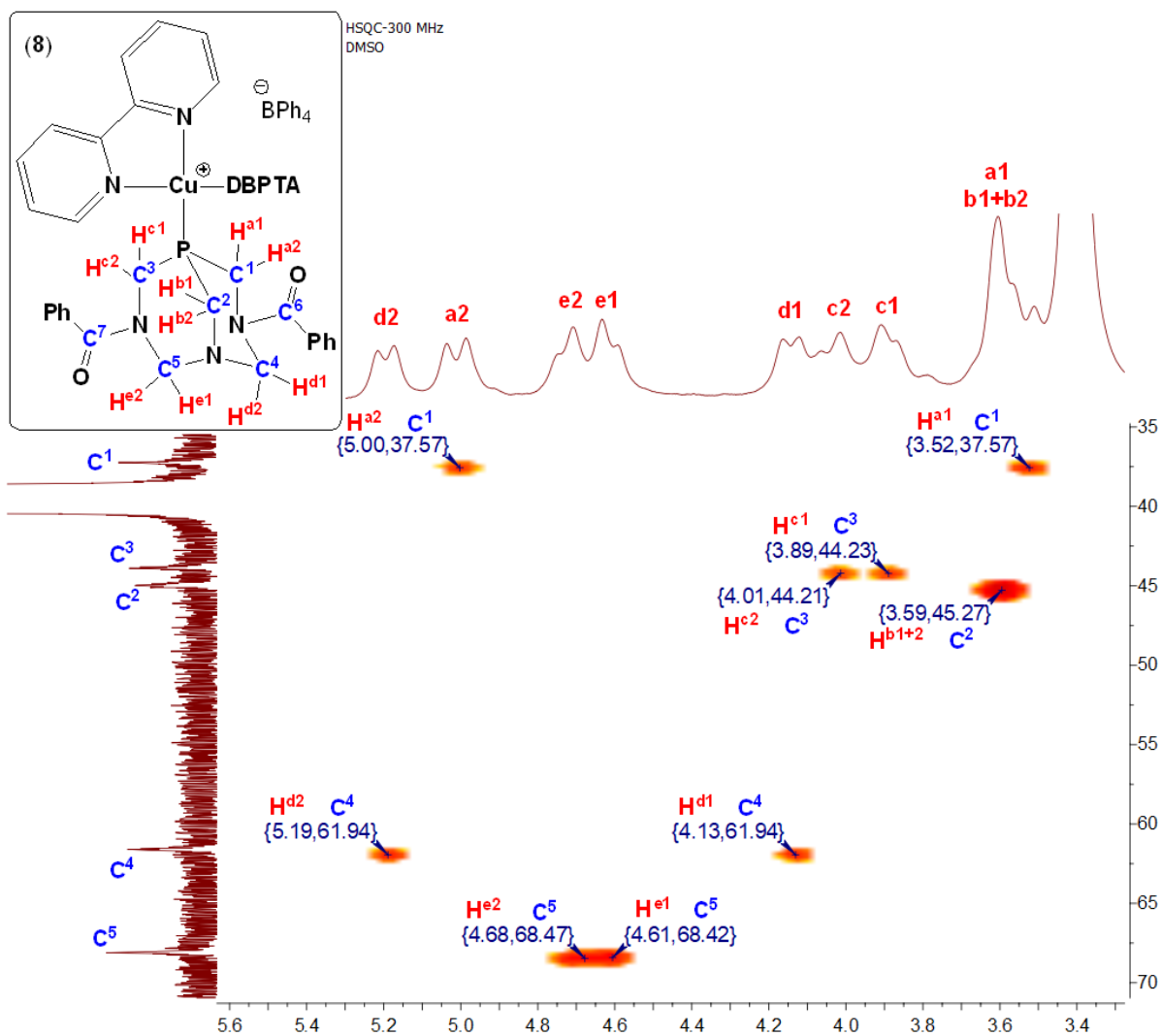
**Figure S65.**  $^{31}\text{P}$  NMR spectrum of complex  $[\text{Cu}(\text{bpy})(\text{DBPTA})_2]\text{BPh}_4$  (**8**) in  $\text{DMSO-}d_6$  (300 MHz).



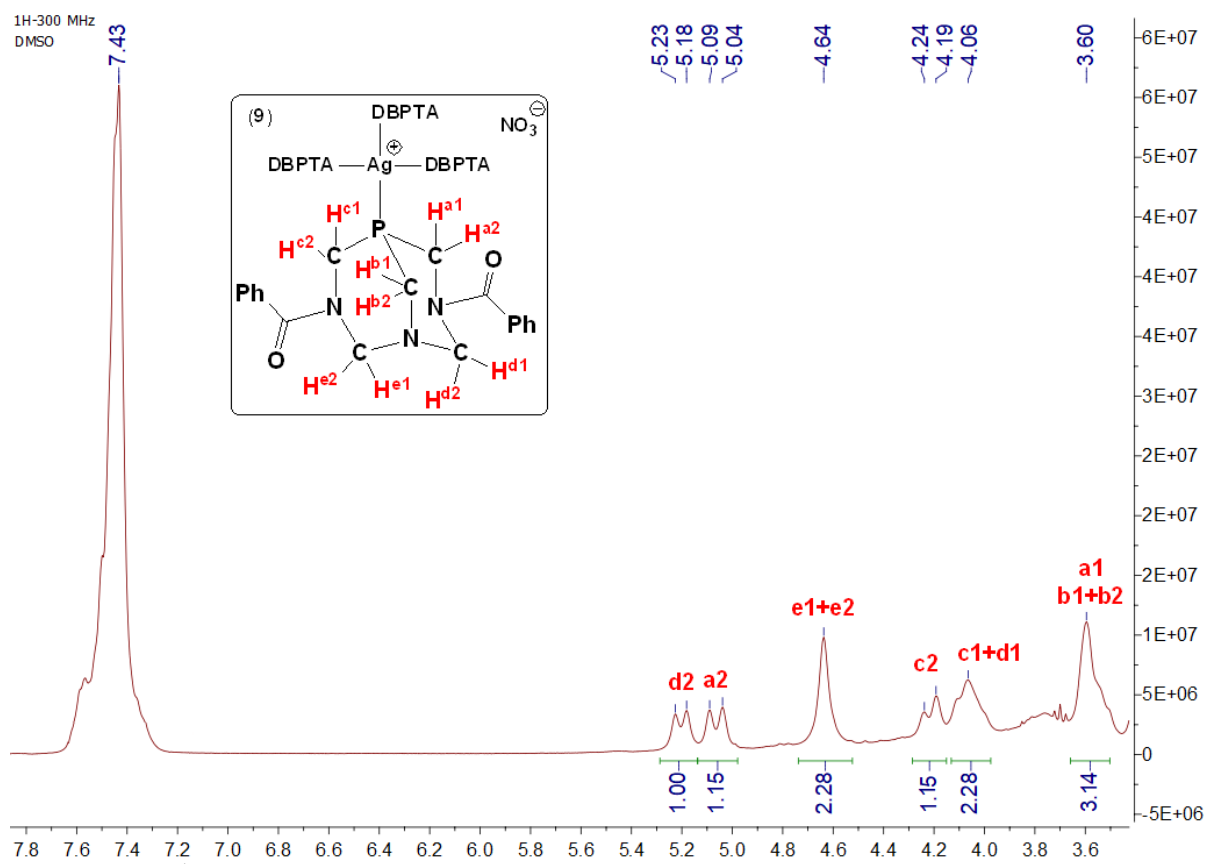


**Figure S68.** COSY spectrum of complex [Cu(bpy)(DBPTA)<sub>2</sub>]BPh<sub>4</sub> (**8**) in DMSO-*d*<sub>6</sub> (300 MHz).

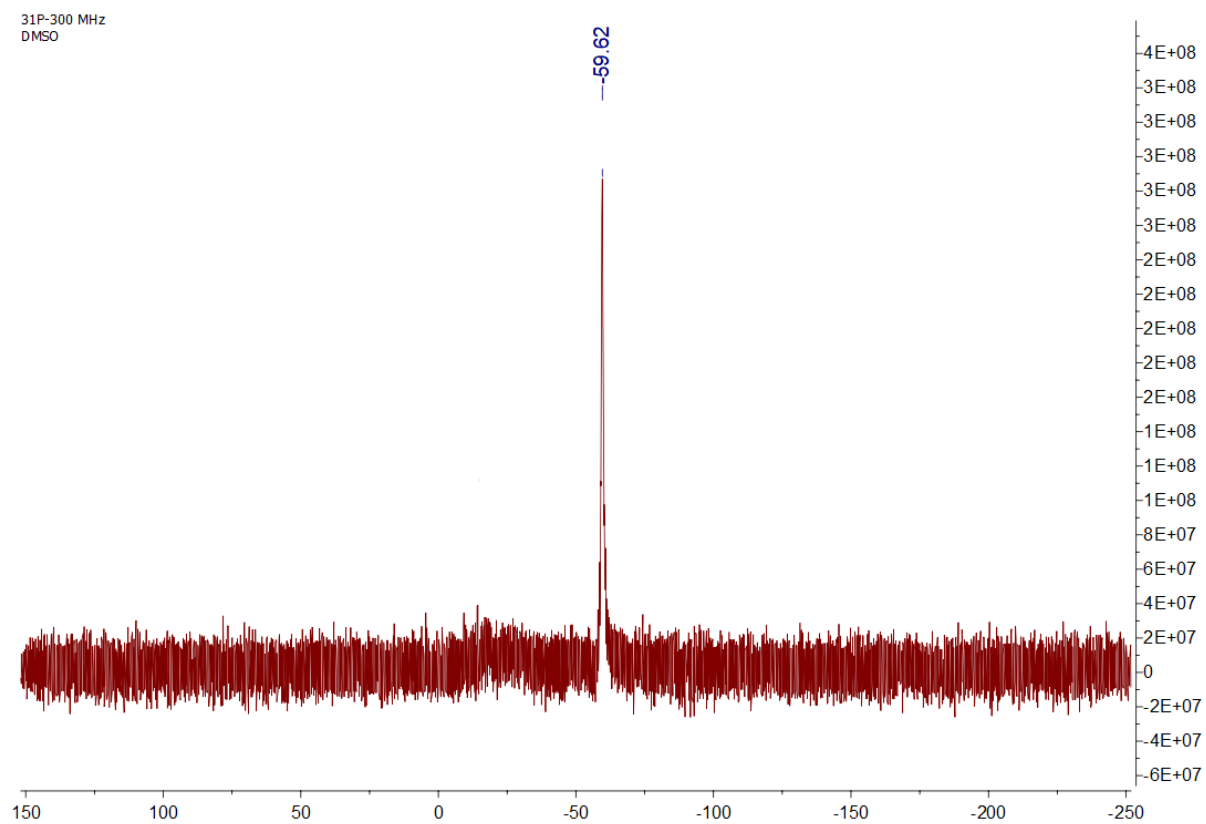




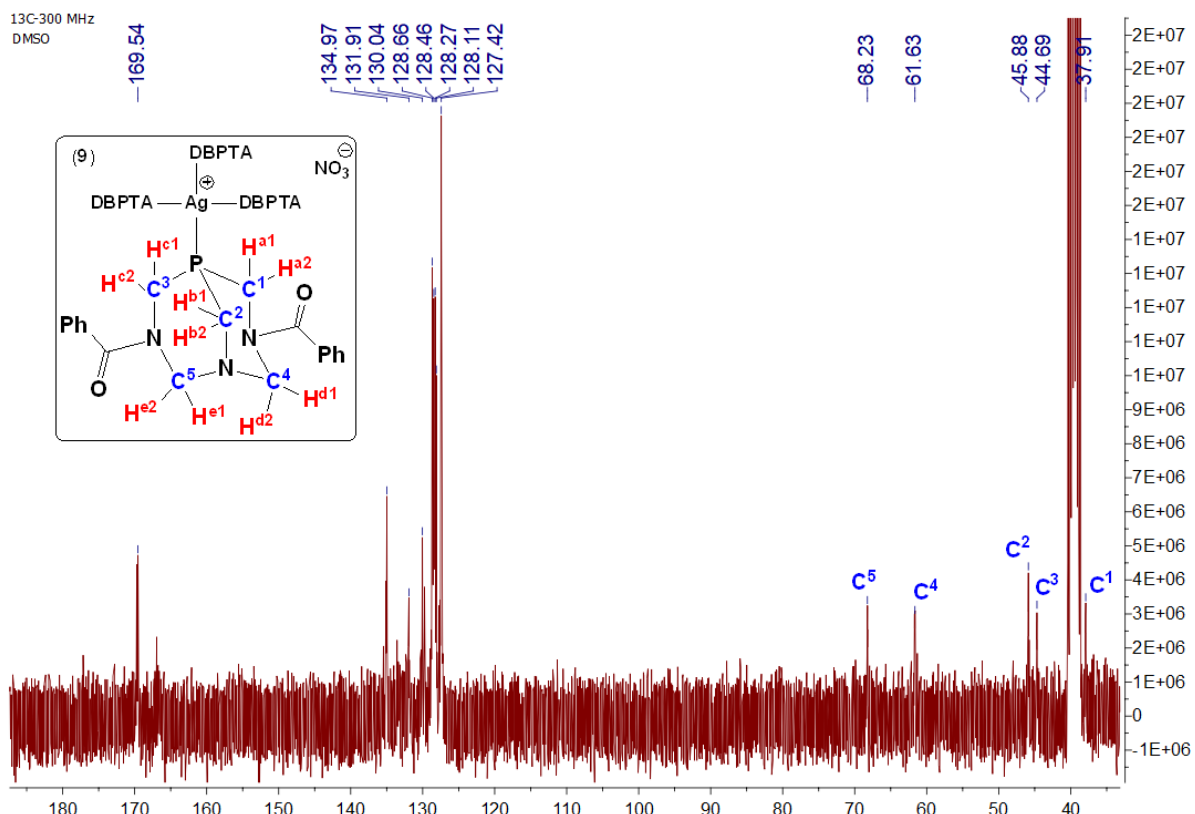
**Figure S69.** HSQC spectrum of complex [Cu(bpy)(DBPTA)<sub>2</sub>]BPh<sub>4</sub> (8) in DMSO-*d*<sub>6</sub> (300 MHz).



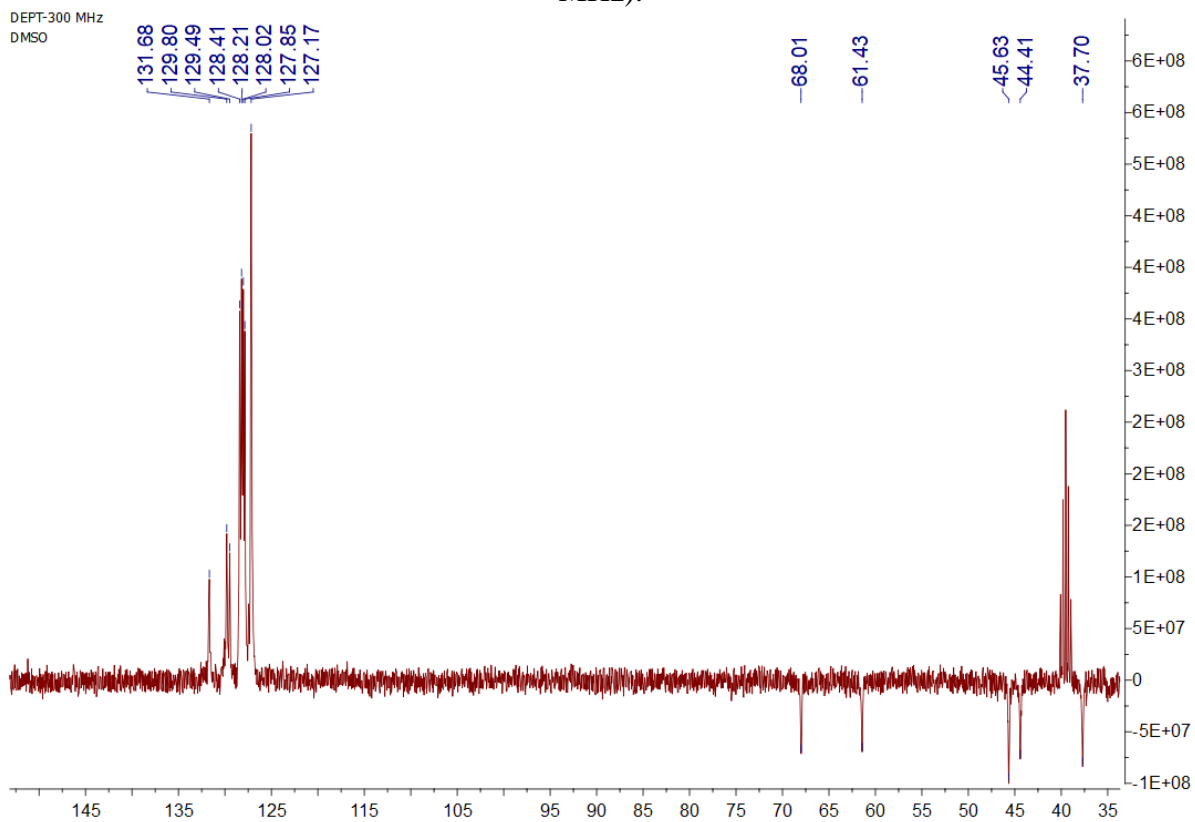
**Figure S70.** <sup>1</sup>H NMR spectrum of complex [Ag(DBPTA)<sub>4</sub>]NO<sub>3</sub> (**9**) in DMSO-*d*<sub>6</sub> (300 MHz).



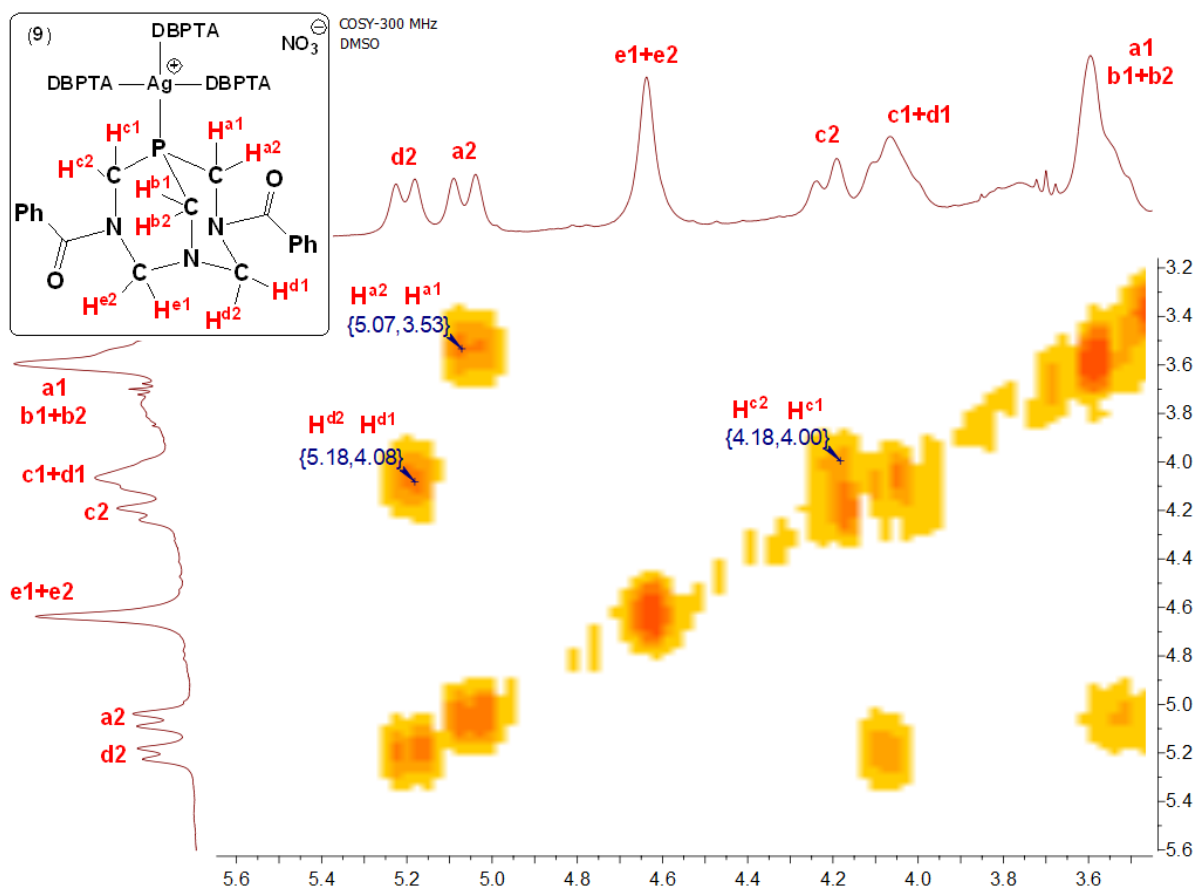
**Figure S71.** <sup>31</sup>P NMR spectrum of complex [Ag(DBPTA)<sub>4</sub>]NO<sub>3</sub> (**9**) in DMSO-*d*<sub>6</sub> (300 MHz).



**Figure S72.**  $^{13}C\{^1H\}$  NMR spectrum of complex  $[Ag(DBPTA)_4]NO_3$  (9) in DMSO- $d_6$  (300 MHz).



**Figure S73.** DEPT NMR spectrum of complex  $[Ag(DBPTA)_4]NO_3$  (9) in DMSO- $d_6$  (300 MHz).



**Figure S74.** COSY spectrum of complex  $[\text{Ag}(\text{DBPTA})_4]\text{NO}_3$  (**9**) in  $\text{DMSO-}d_6$  (300 MHz).

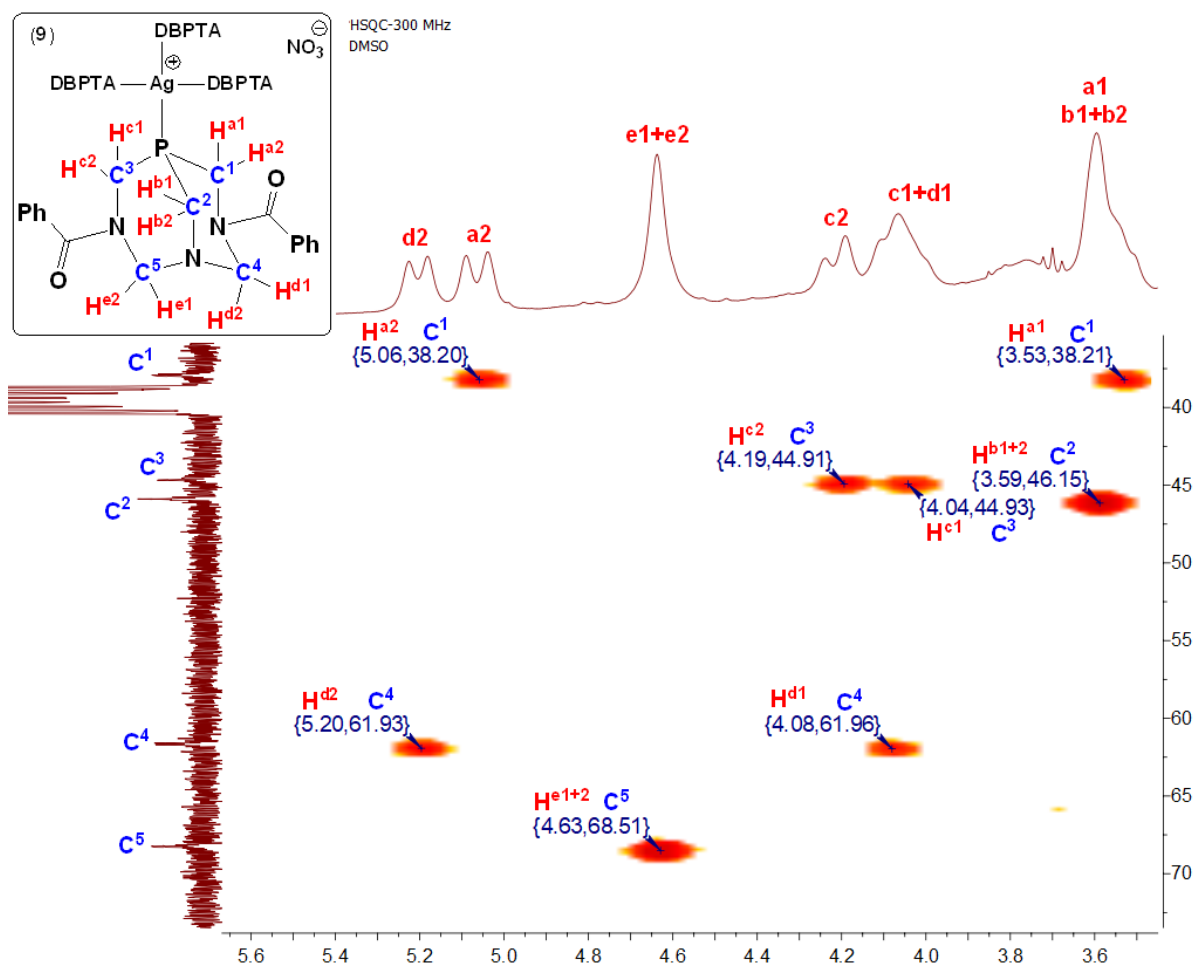


Figure S75. HSQC spectrum of complex [Ag(DBPTA)<sub>4</sub>]<sup>+</sup>NO<sub>3</sub><sup>-</sup> (**9**) in DMSO-*d*<sub>6</sub> (300 MHz).

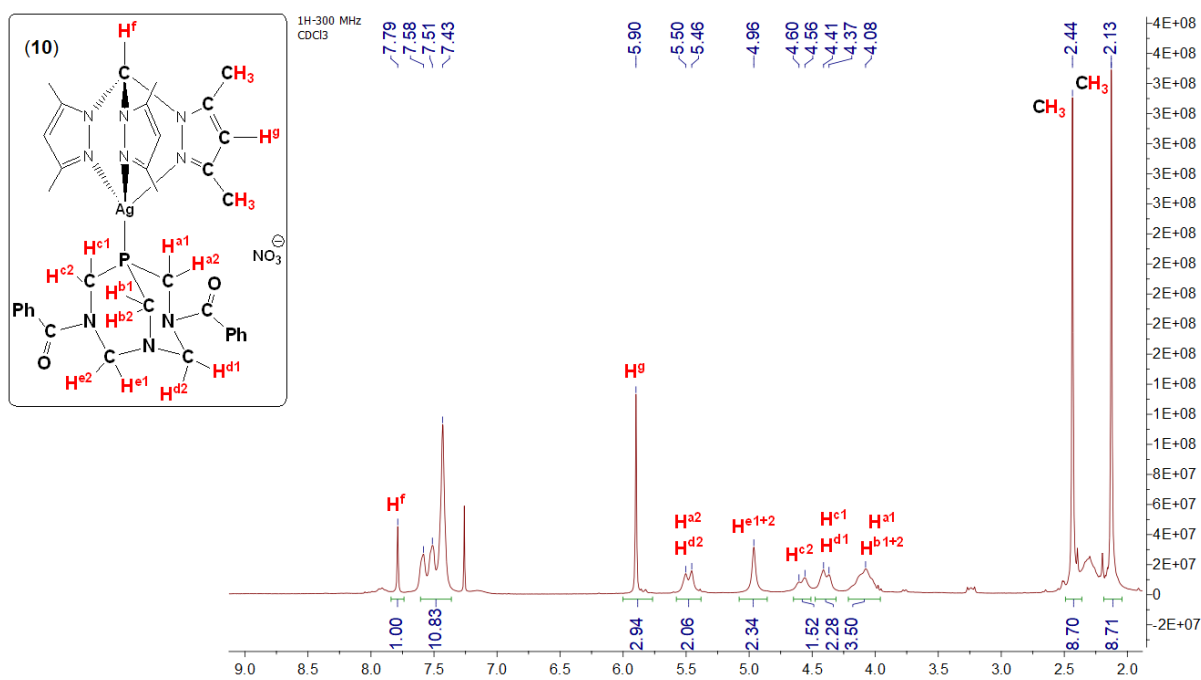
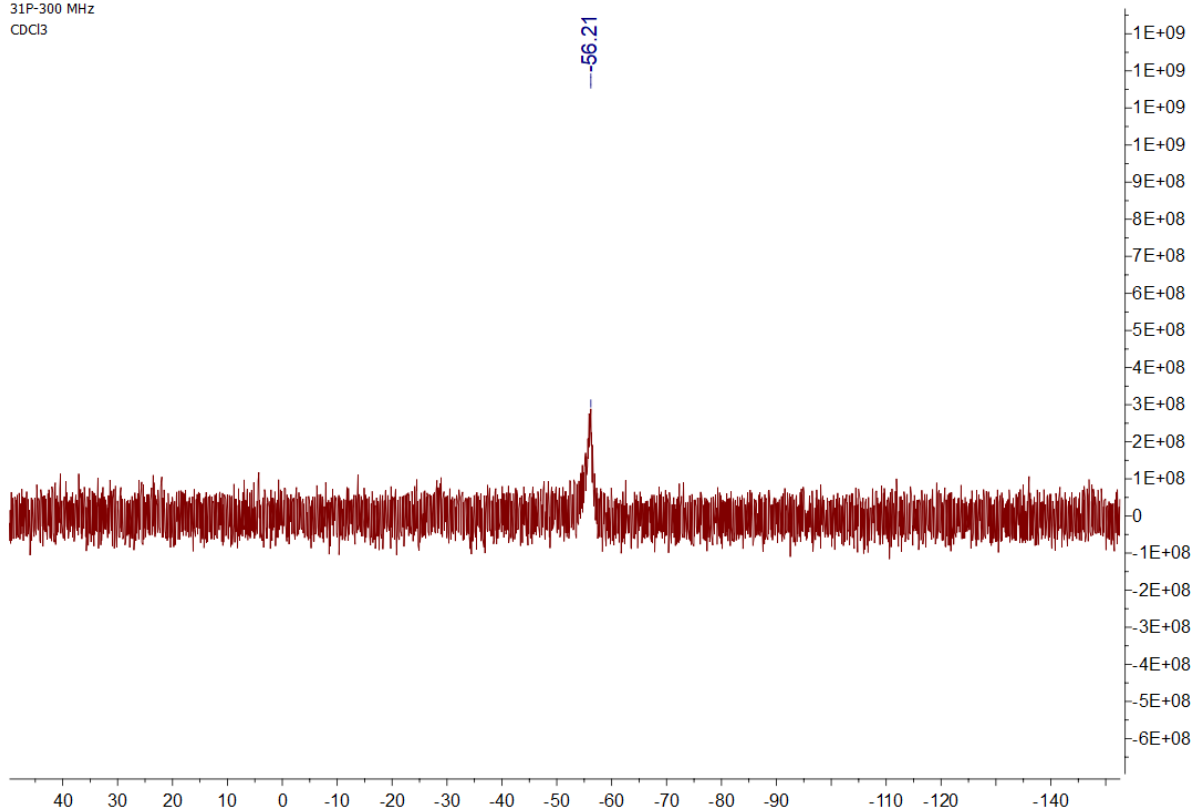
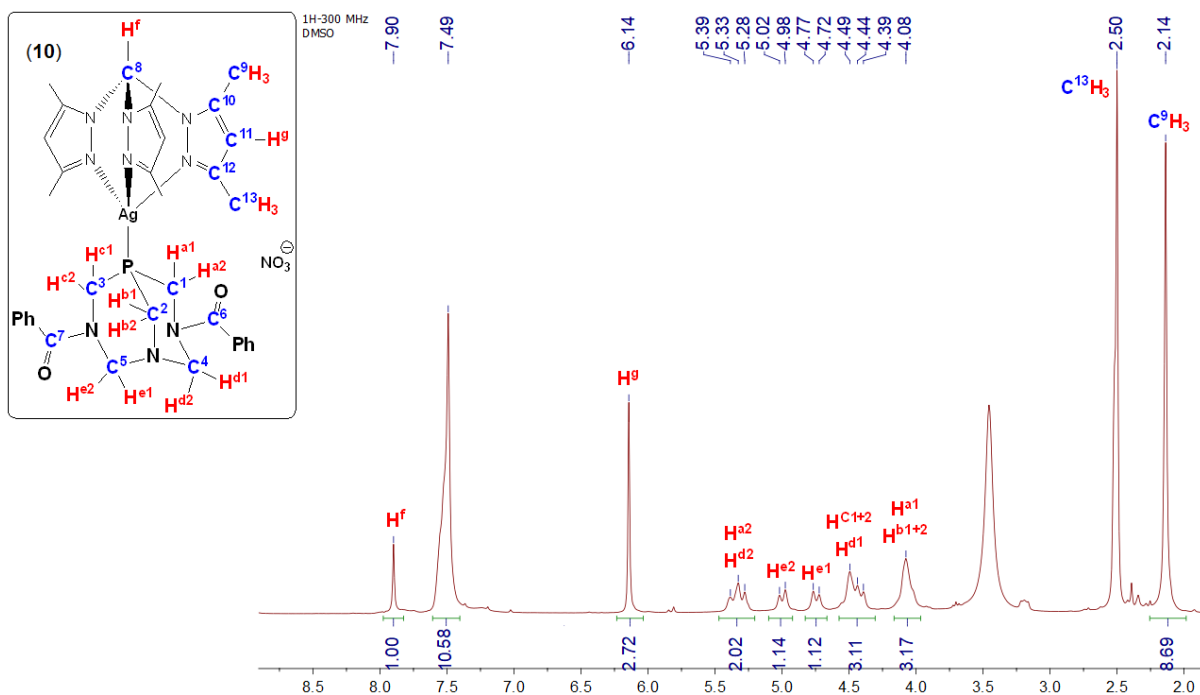


Figure S76. <sup>1</sup>H NMR spectrum of complex [Ag(TPM\*)(DBPTA)]<sup>+</sup>NO<sub>3</sub><sup>-</sup> (**10**) in CDCl<sub>3</sub> (300 MHz).

31P-300 MHz  
CDCl3

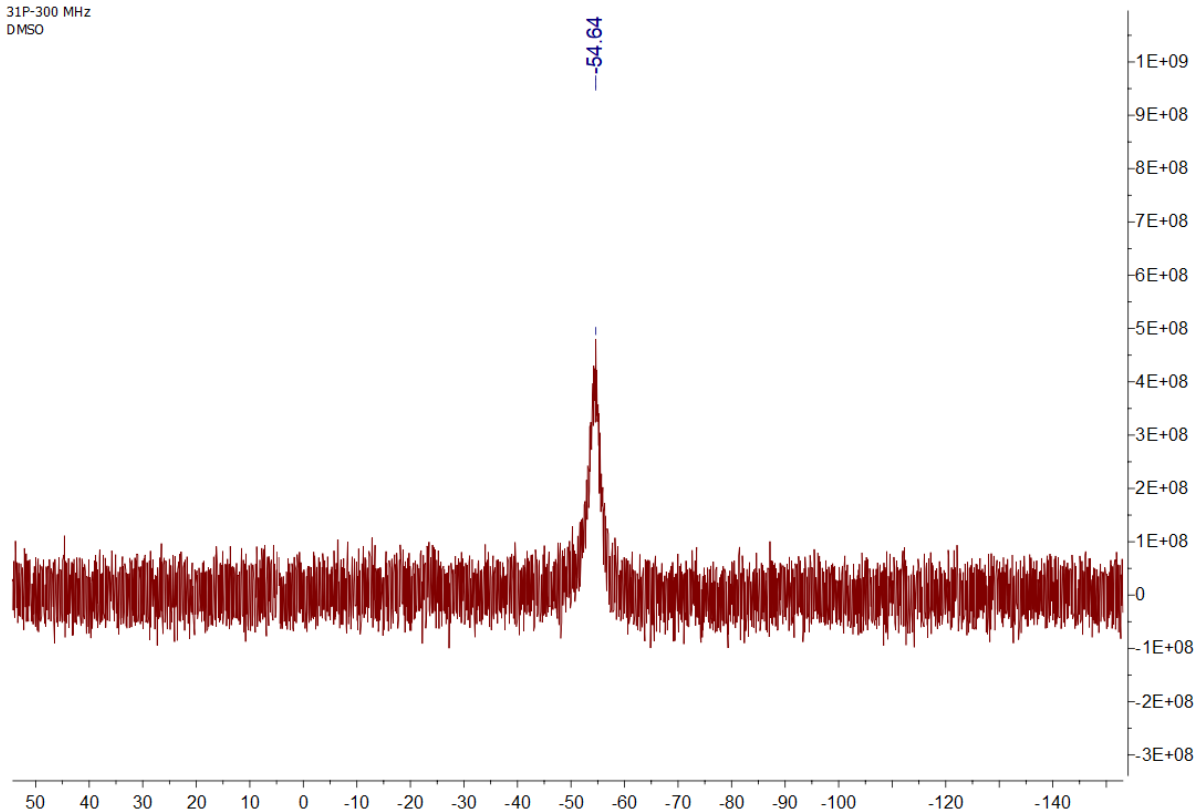


**Figure S77.**  $^{31}\text{P}$  NMR spectrum of complex  $[\text{Ag}(\text{TPM}^*)(\text{DBPTA})]\text{NO}_3$  (**10**) in  $\text{CDCl}_3$  (300 MHz).

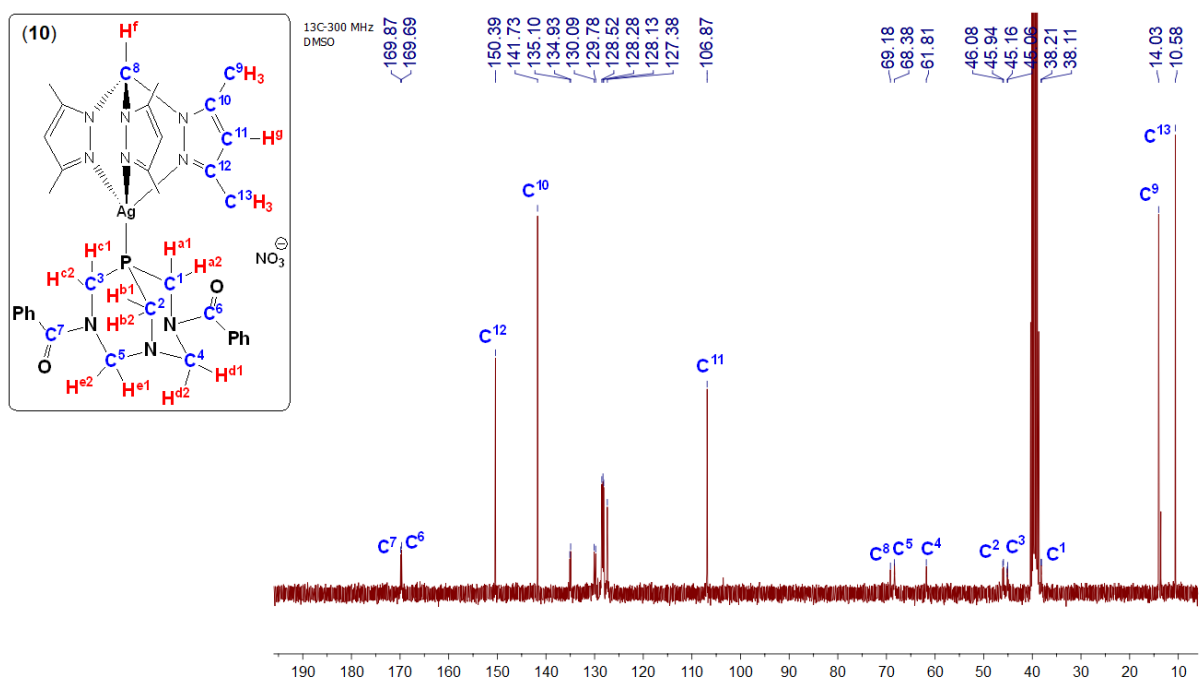


**Figure S78.**  $^1\text{H}$  NMR spectrum of complex  $[\text{Ag}(\text{TPM}^*)(\text{DBPTA})]\text{NO}_3$  (**10**) in  $\text{DMSO}-d_6$  (300 MHz).

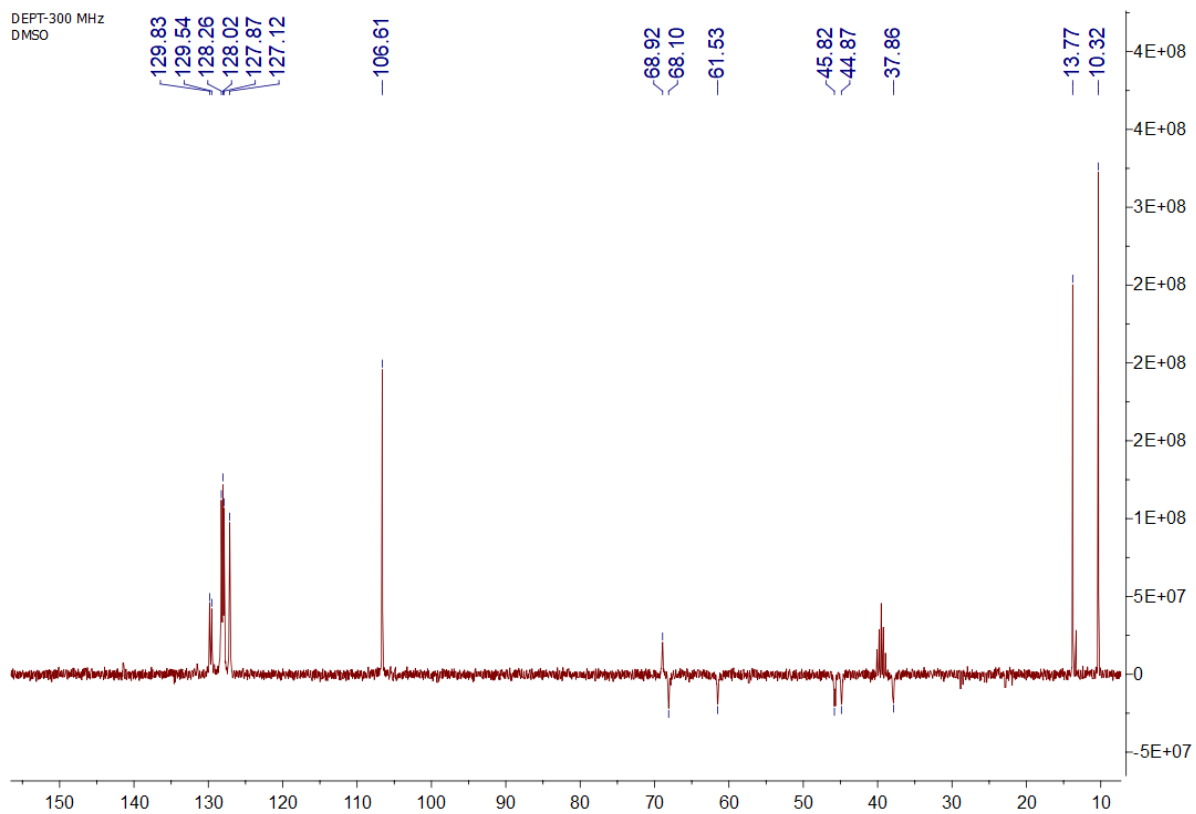
31P-300 MHz  
DMSO



**Figure S79.** <sup>31</sup>P NMR spectrum of complex [Ag(TPM\*)(DBPTA)]NO<sub>3</sub> (10) in DMSO-*d*<sub>6</sub> (300 MHz).

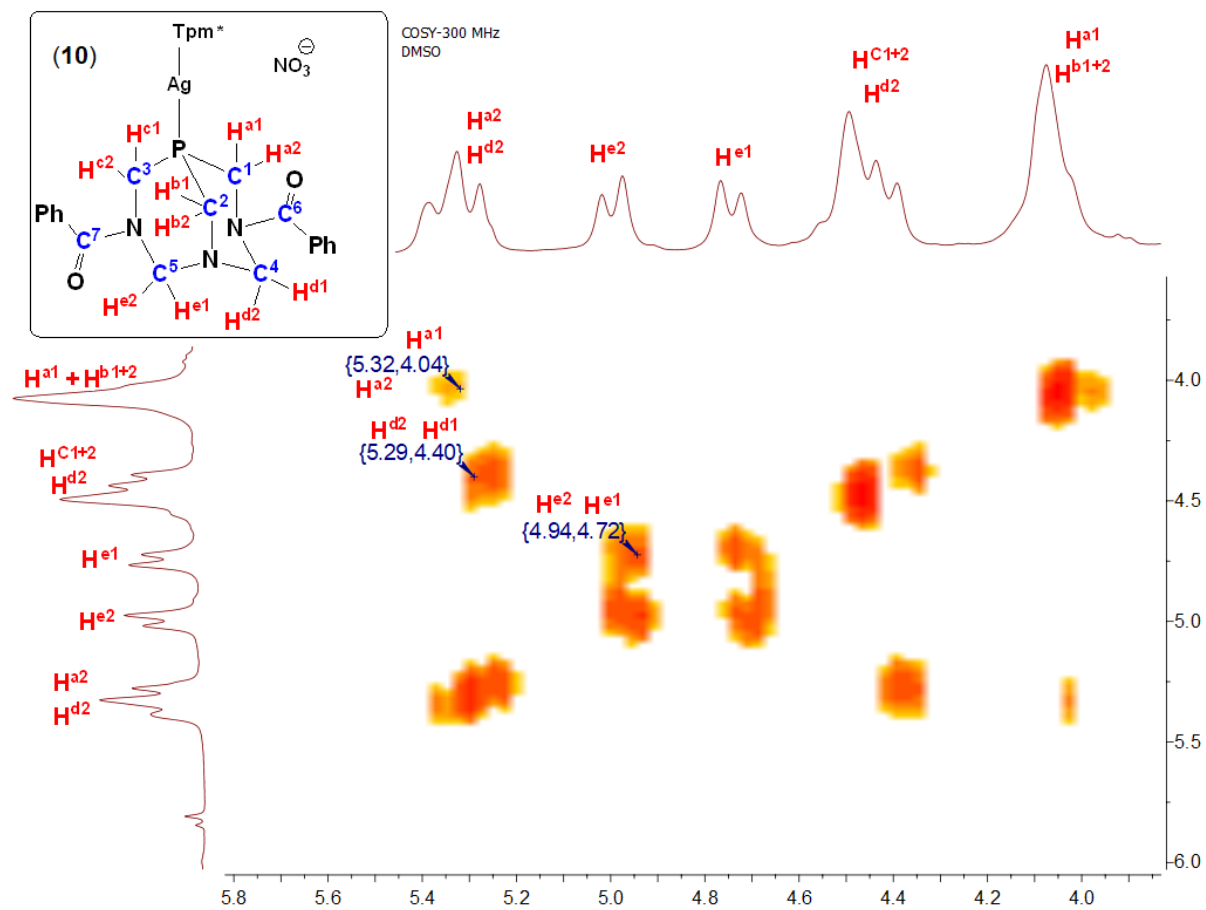


**Figure S80.** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of complex [Ag(TPM\*)(DBPTA)]NO<sub>3</sub> (10) in DMSO-*d*<sub>6</sub> (300 MHz).

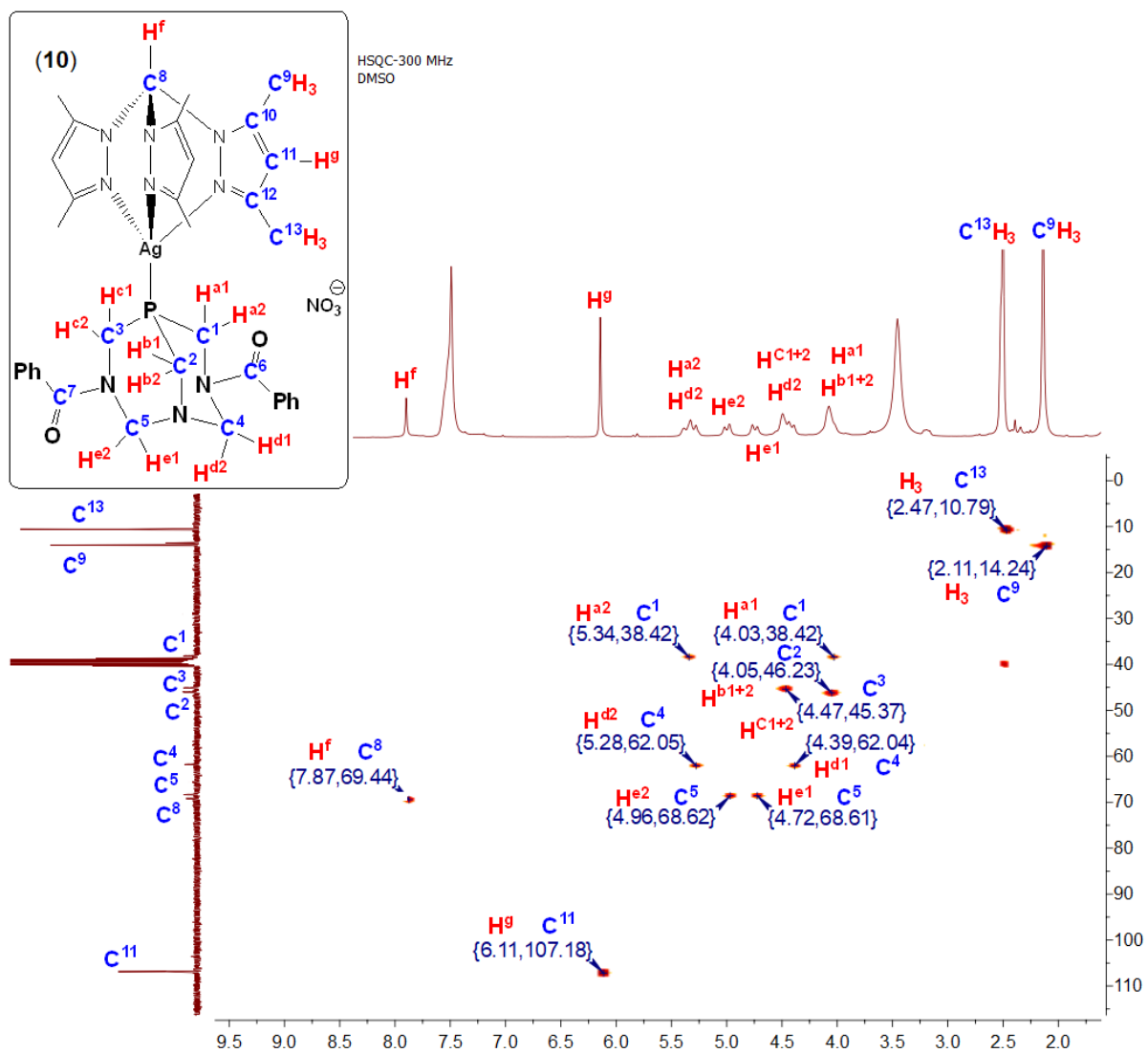


**Figure S81.** DEPT NMR spectrum of complex  $[\text{Ag}(\text{TPM}^*)(\text{DBPTA})]\text{NO}_3$  (**10**) in  $\text{DMSO-}d_6$  (300 MHz).

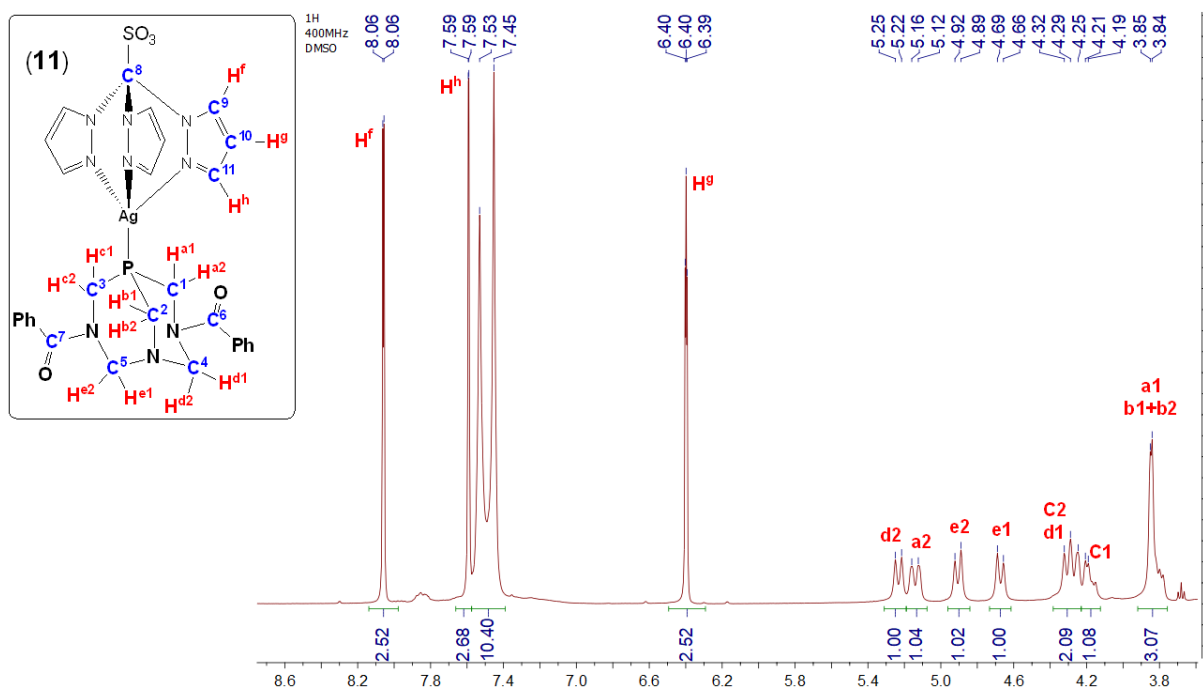




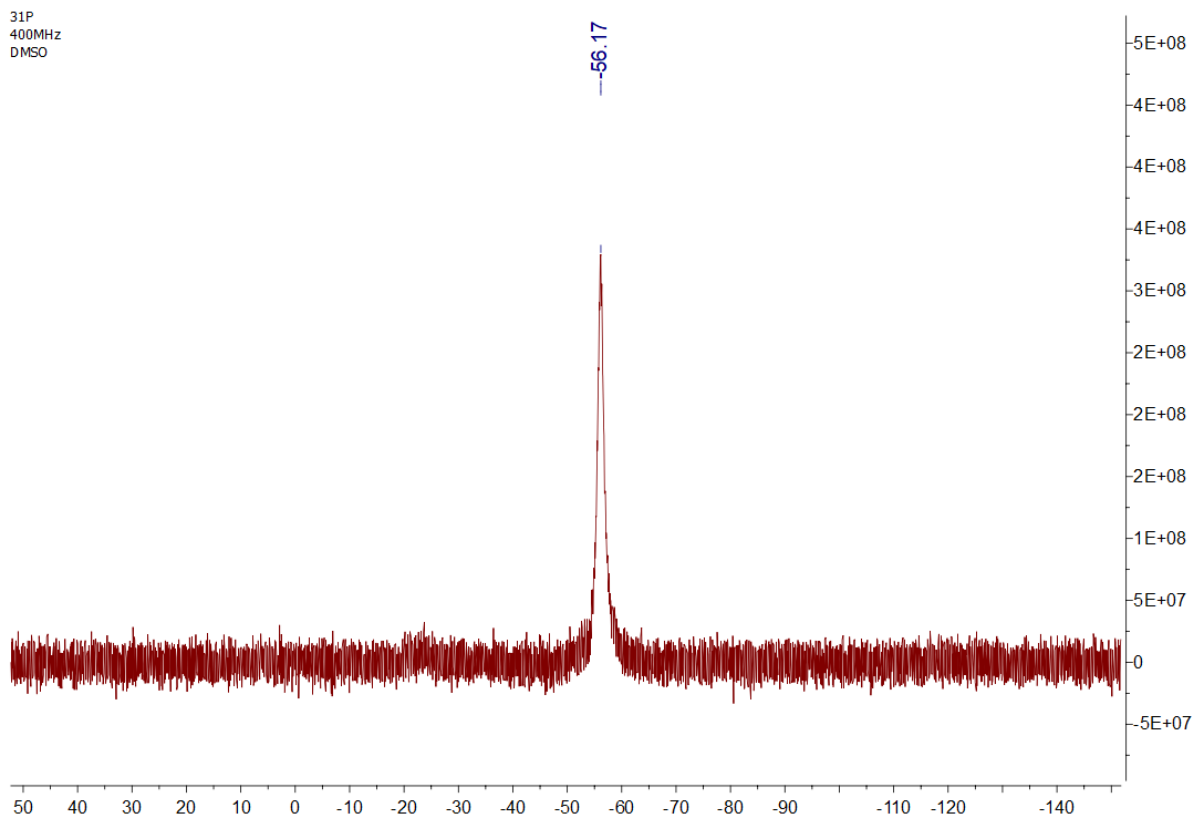
**Figure S82.** COSY spectrum of complex [Ag(TPM\*)(DBPTA)]NO<sub>3</sub> (**10**) in DMSO-*d*<sub>6</sub> (300 MHz).



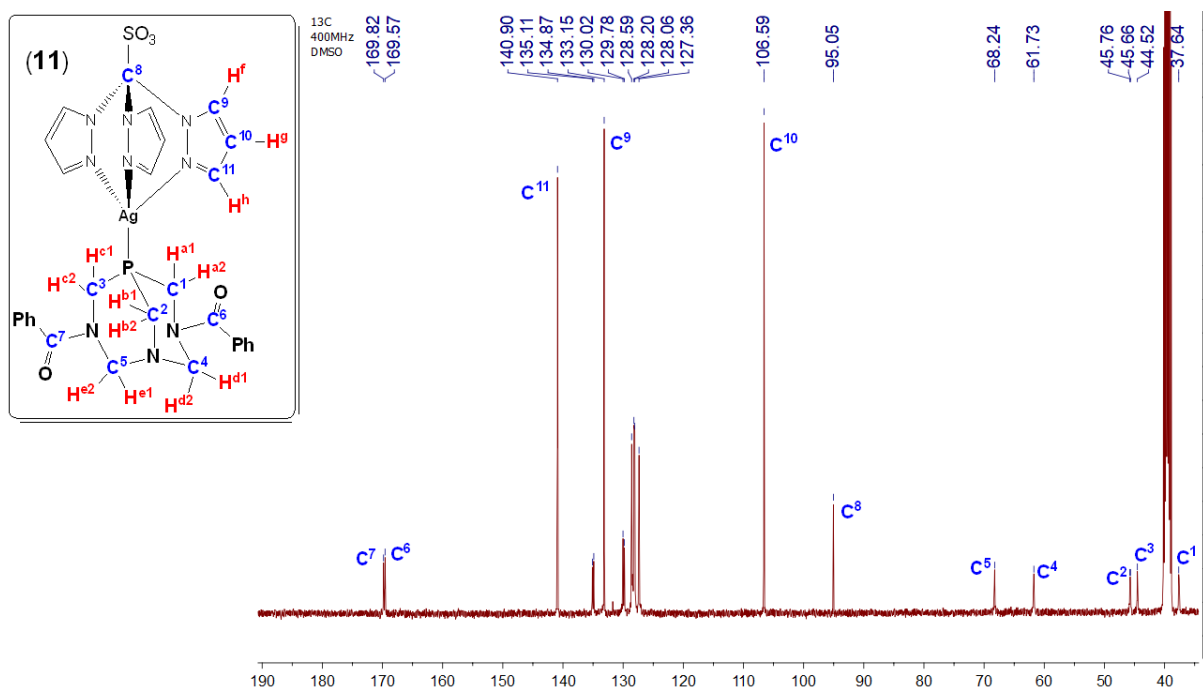
**Figure S83.** HSQC spectrum of complex  $[\text{Ag}(\text{TPM}^*)(\text{DBPTA})]\text{NO}_3$  (**10**) in  $\text{DMSO-}d_6$  (300 MHz).



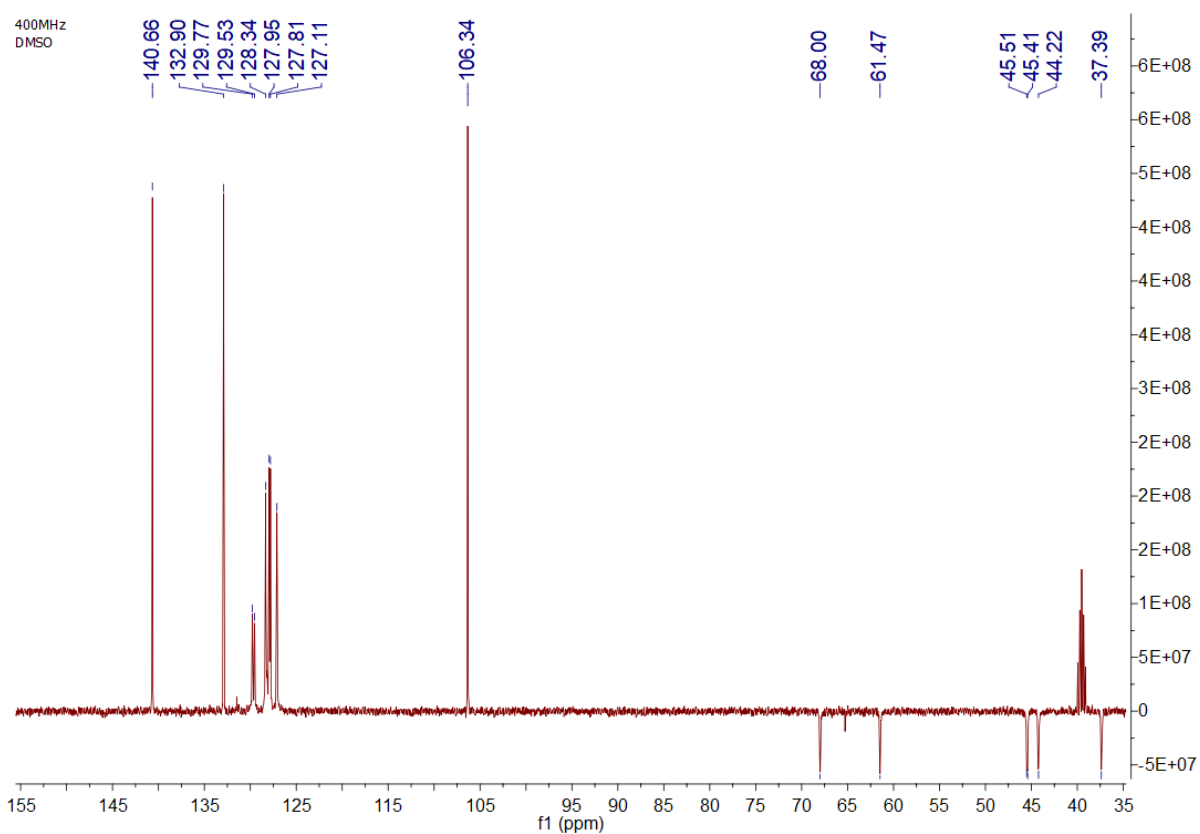
**Figure S84.**  $^1\text{H}$  NMR spectrum of complex  $[\text{Ag}(\text{Tpms})(\text{DBPTA})]$  (**11**) in  $\text{DMSO-}d_6$  (400 MHz).



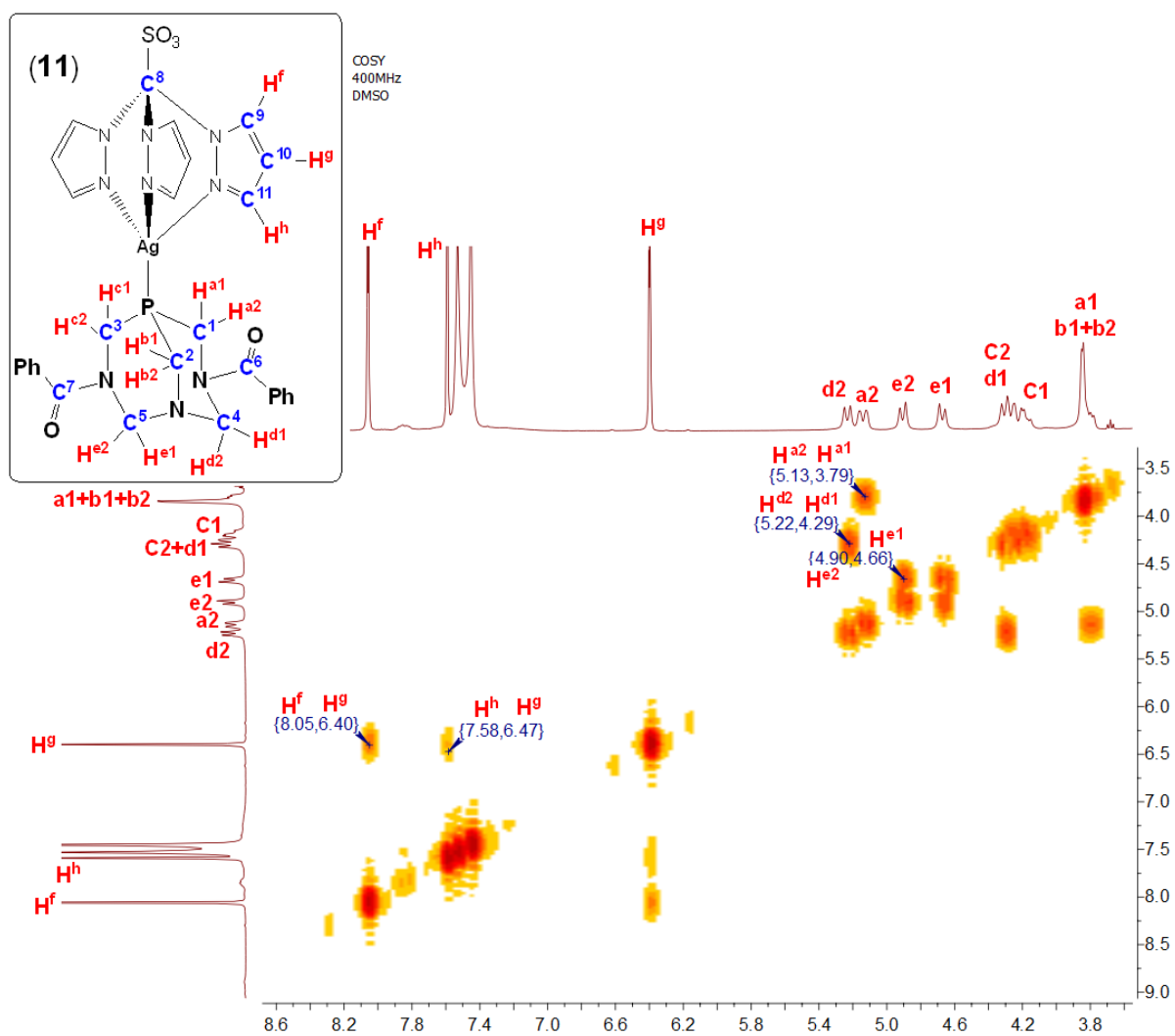
**Figure S85.**  $^{31}\text{P}$  NMR spectrum of complex  $[\text{Ag}(\text{Tpms})(\text{DBPTA})]$  (**11**) in  $\text{DMSO-}d_6$  (400 MHz).



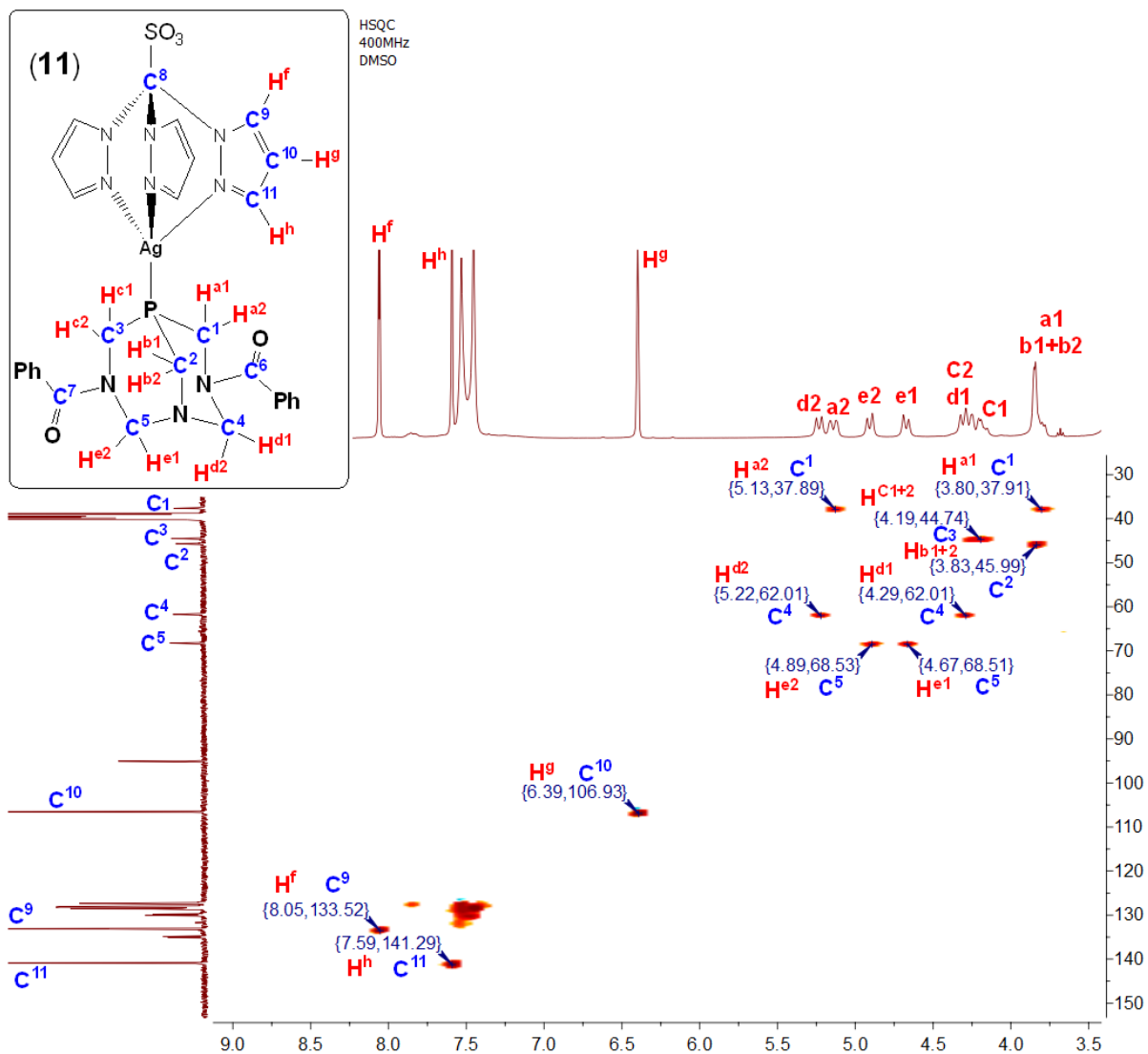
**Figure S86.** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of complex [Ag(Tpms)(DBPTA)] (**11**) in DMSO-*d*<sub>6</sub> (400 MHz).



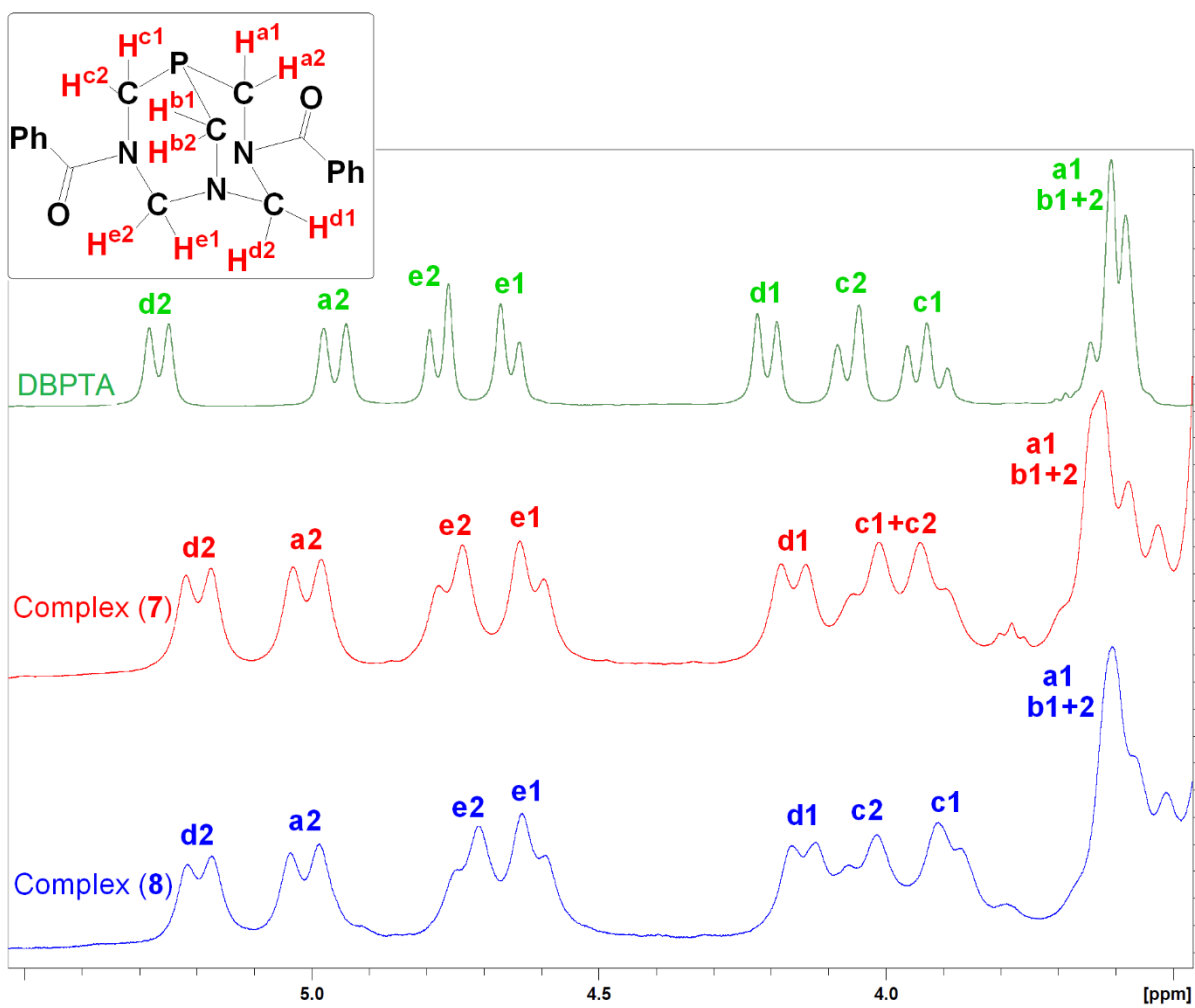
**Figure S87.** DEPT NMR spectrum of complex [Ag(Tpms)(DBPTA)] (**11**) in DMSO-*d*<sub>6</sub> (400 MHz).



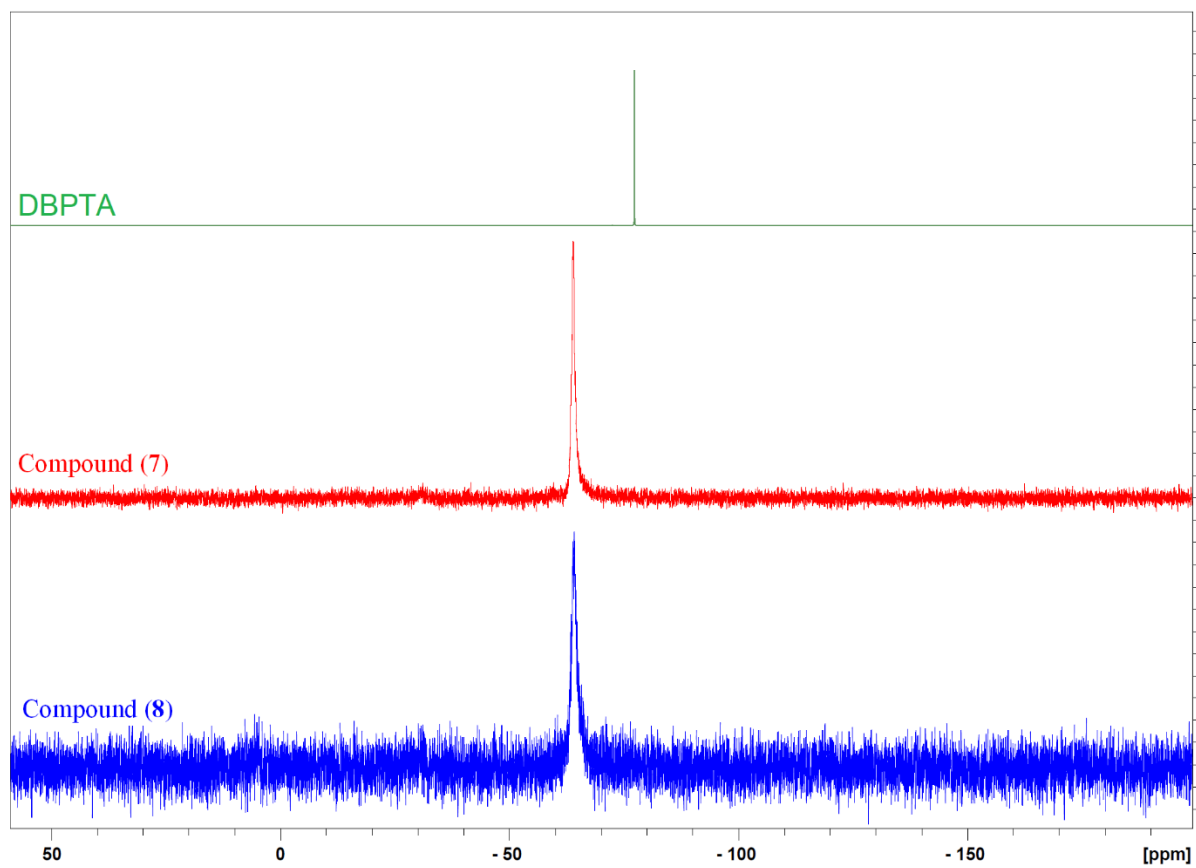
**Figure S88.** COSY spectrum of complex [Ag(Tpms)(DBPTA)] (**11**) in DMSO-*d*<sub>6</sub> (400 MHz).



**Figure S89.** HSQC spectrum of complex [Ag(Tpms)(DBPTA)] (11) in DMSO-*d*<sub>6</sub> (400 MHz).

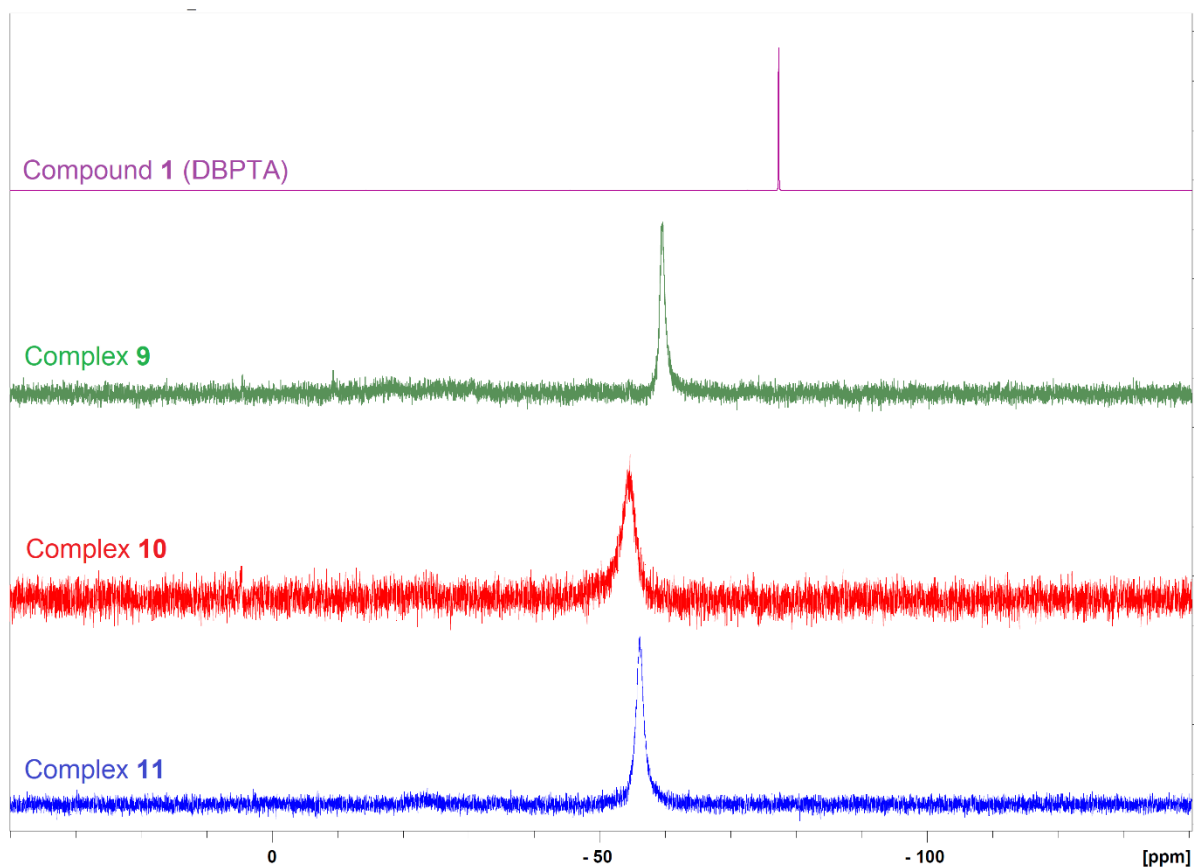


**Figure S90.** <sup>1</sup>H NMR spectra of DBPTA (1) and the copper complexes 7 and 8 in DMSO-*d*<sub>6</sub>.

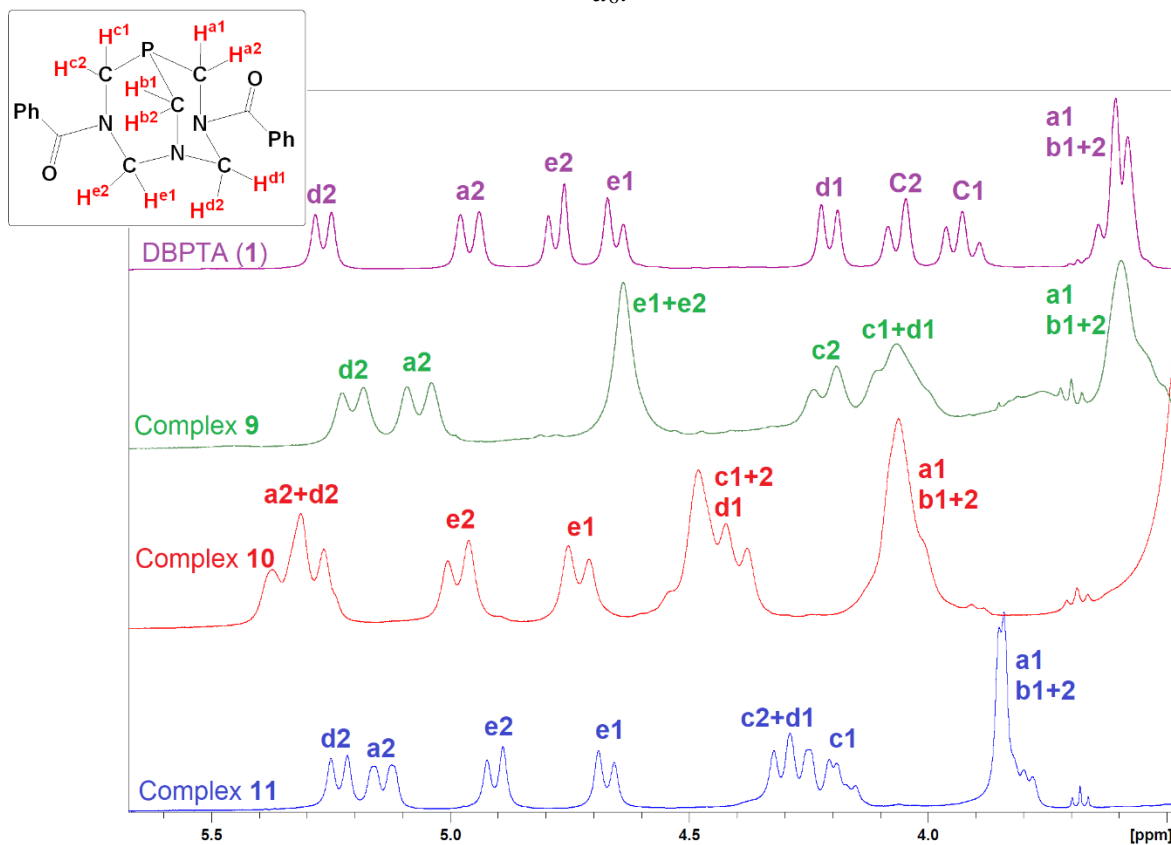


**Figure S91.**  $^{31}\text{P}\{^1\text{H}\}$  NMR spectra of DBPTA (**1**) and the copper complexes **7** and **8** in  $\text{DMSO-}d_6$ .

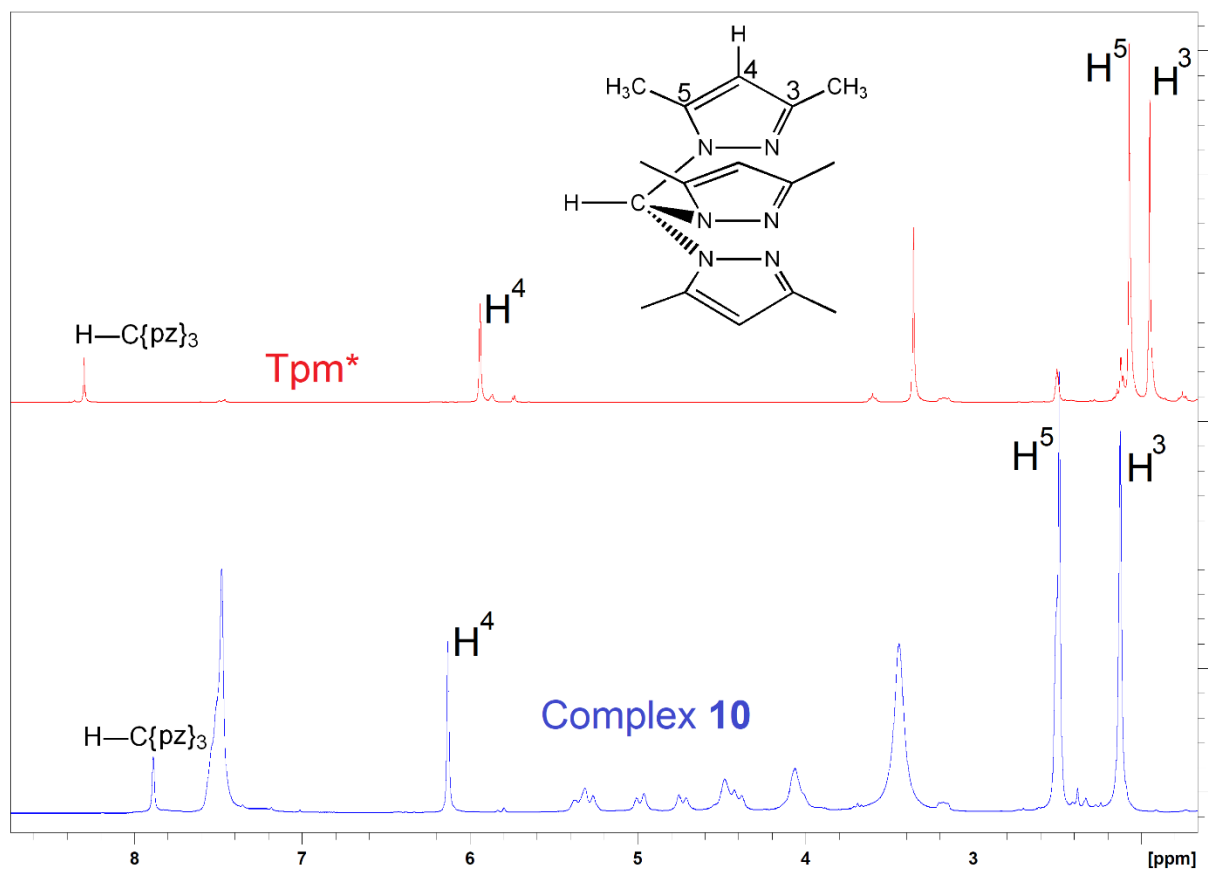




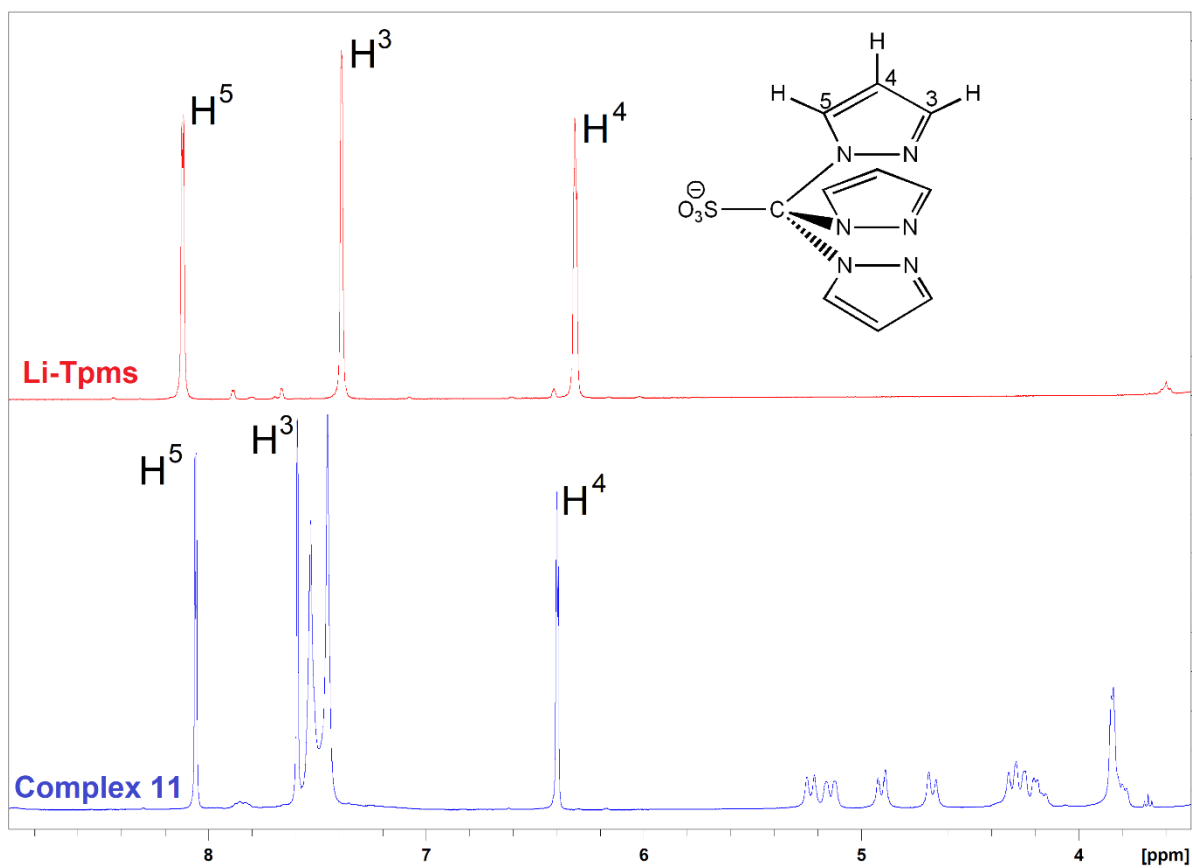
**Figure S92.**  $^{31}\text{P}\{^1\text{H}\}$  NMR spectra of DBPTA (**1**) and the silver complexes **9-11** in  $\text{DMSO-}d_6$ .



**Figure S93.**  $^1\text{H}$  NMR spectra of DBPTA (**1**) and the silver complexes **9-11** in  $\text{DMSO-}d_6$ .

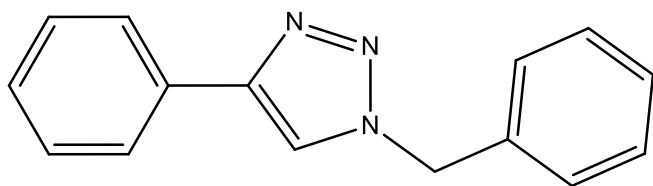


**Figure S94.** <sup>1</sup>H NMR spectra of Tpm\* (Top) and the silver complexes **10** (Bottom) in DMSO-*d*<sub>6</sub>.

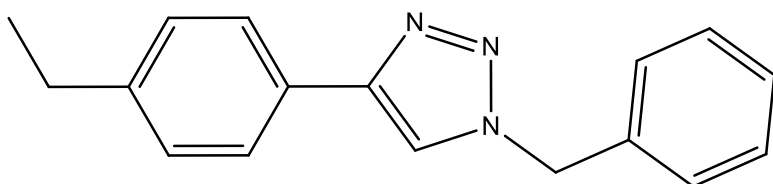


**Figure S95.** <sup>1</sup>H NMR spectra of Li-Tpms (Top) and the silver complexes **11** (Bottom) in DMSO-*d*<sub>6</sub>.

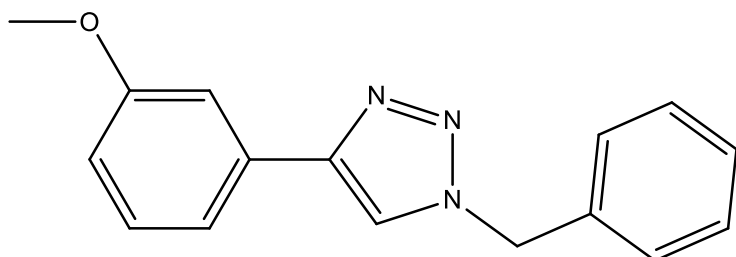
### 3. Characterization data of triazoles



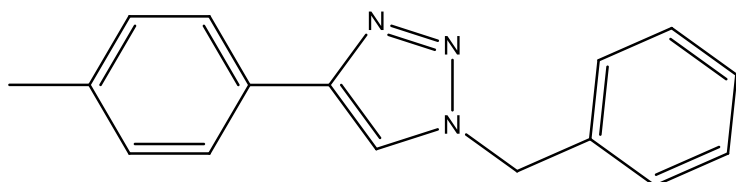
1-benzyl-4-phenyl-1*H*-1,2,3-triazole: Elemental analysis calcd (%) for C<sub>15</sub>H<sub>13</sub>N<sub>3</sub>: C 76.57, H 5.57, N 17.86; found: C 76.77, H 5.49, N 17.92. <sup>1</sup>H NMR (300 MHz, DMSO-d<sub>6</sub>, δ): 8.63 (s, 1H), 7.85 (d, *J* = 7.6 Hz, 2H), 7.45-7.32 (m, 8H), 5.65 (s, 2H).



1-benzyl-4-(4-ethylphenyl)-1*H*-1,2,3-triazole: Elemental analysis calcd (%) for C<sub>17</sub>H<sub>17</sub>N<sub>3</sub>: C 77.54, H 6.51, N 15.96; found: C 77.35, H 6.42, N 16.05. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>, δ): 7.68 (m, 2H, Ar-H), 7.61 (s, 1H, Ar-H), 7.40-7.34 (m, 3H, Ar-H), 7.31-7.25 (m, 4H, Ar-H), 5.49 (s, 2H, PhCH<sub>2</sub>N), 2.61 (q, *J* = 7.9 Hz, 2H, CH<sub>2</sub>CH<sub>3</sub>), 1.28 (t, *J* = 7.9 Hz, 3H, CH<sub>2</sub>CH<sub>3</sub>).

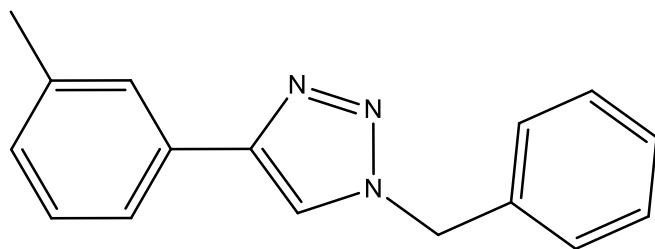


1-benzyl-4-(3-methoxyphenyl)-1*H*-1,2,3-triazole: Elemental analysis calcd (%) for C<sub>16</sub>H<sub>15</sub>N<sub>3</sub>O: C 72.43, H 5.70, N 15.84; found: C 72.25, H 5.64, N 15.72. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>, δ): 7.60 (s, 1H, Ar-H), 7.41-7.22 (m, 8H, Ar-H), 7.74 (m, 1H, Ar-H), 5.48 (s, 2H, PhCH<sub>2</sub>N), 3.81 (s, 3H, CH<sub>3</sub>).

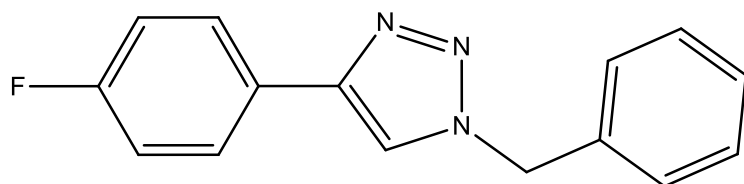


1-benzyl-4-(p-tolyl)-1*H*-1,2,3-triazole: Elemental analysis calcd (%) for C<sub>16</sub>H<sub>15</sub>N<sub>3</sub>: C 77.08, H 6.06, N 16.85; found: C 77.13, H 6.11, N 16.77. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>, δ): 7.63 (d, *J* =

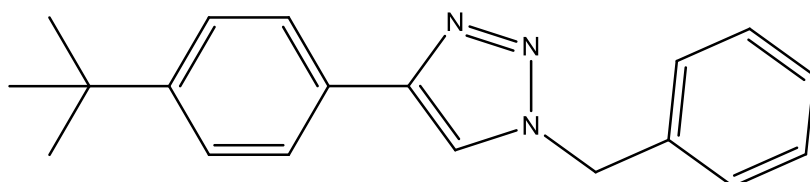
7.9, 2H, Ar-H), 7.54 (s, 1H, Ar-H), 7.30–7.15 (m, 7H, Ar-H), 5.48 (s, 2H, PhCH<sub>2</sub>N), 2.31 (s, 3H, CH<sub>3</sub>).



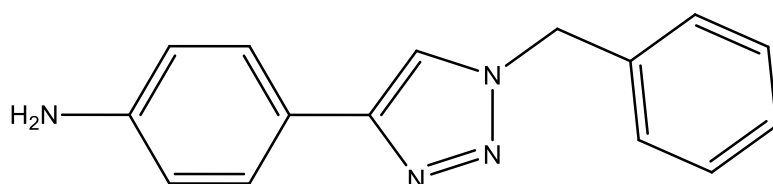
1-benzyl-4-(m-tolyl)-1H-1,2,3-triazole: Elemental analysis calcd (%) for C<sub>16</sub>H<sub>15</sub>N<sub>3</sub>: C 77.08, H 6.06, N 16.85; found: C 76.91, H 6.01, N 16.67. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>, δ): 7.61 (br s, 2H, Ar-H), 7.52–7.49 (m, 1H, Ar-H), 7.43–7.27 (m, 6H, Ar-H), 7.14 (m, 1H, Ar-H), 5.49 (s, 2H, PhCH<sub>2</sub>N), 2.34 (s, 3H, CH<sub>3</sub>).



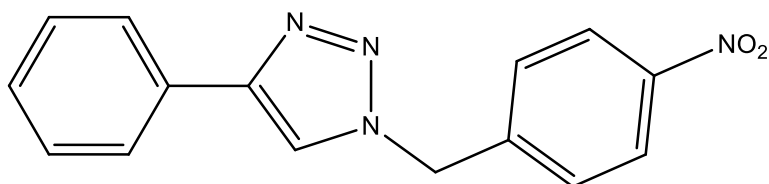
1-benzyl-4-(4-fluorophenyl)-1H-1,2,3-triazole: Elemental analysis calcd (%) for C<sub>15</sub>H<sub>12</sub>FN<sub>3</sub>: C 71.13, H 4.78, N 16.59; found: C 70.98, H 4.66, N 16.43. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>, δ): 7.78–7.69 (m, 2H, Ar-H), 7.61 (s, 1H, Ar-H), 7.39–7.22 (m, 5H, Ar-H), 7.16–7.07 (m, 2H, Ar-H), 5.43 (s, 2H, PhCH<sub>2</sub>N).



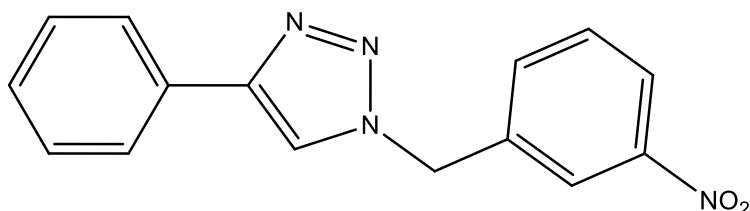
1-benzyl-4-(4-(tert-butyl)phenyl)-1H-1,2,3-triazole: Elemental analysis calcd (%) for C<sub>19</sub>H<sub>21</sub>N<sub>3</sub>: C 78.32, H 7.26, N 14.42; found: C 78.25, H 7.22, N 14.37. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>, δ): 7.71 (d, *J* = 7.9 Hz, 2H, Ar-H), 7.63 (m, 1H, Ar-H), 7.40 (d, *J* = 7.9 Hz, 2H, Ar-H), 7.34–7.28 (m, 4H, Ar-H), 5.52 (s, 2H, PhCH<sub>2</sub>N), 1.35 (s, 9H, CH<sub>3</sub>).



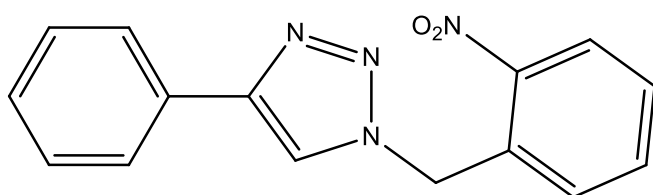
4-(1-benzyl-1*H*-1,2,3-triazol-4-yl)aniline: Elemental analysis calcd (%) for C<sub>15</sub>H<sub>14</sub>N<sub>4</sub>: C 71.98, H 5.64, N 22.38; found: C 72.09, H 5.57, N 22.52. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>, δ): 7.63–7.55 (m, 3H, Ar-H), 7.39–7.25 (m, 5H, Ar-H), 6.81–6.74 (m, 2H, Ar-H), 5.58 (s, 2H, PhCH<sub>2</sub>N), 3.67 (br s, 2H, NH<sub>2</sub>).



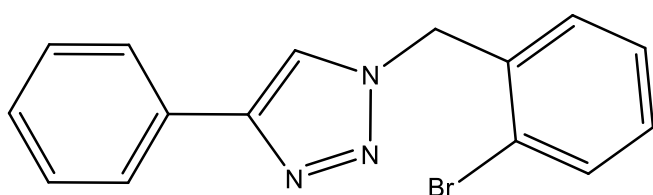
1-(4-nitrobenzyl)-4-phenyl-1*H*-1,2,3-triazole: Elemental analysis calcd (%) for C<sub>15</sub>H<sub>12</sub>N<sub>4</sub>O<sub>2</sub>: C 64.28, H 4.32, N 19.99; found: C 64.16, H 4.28, N 20.05. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>, δ): 8.70 (s, 1H), 8.25 (d, *J* = 8.4 Hz, 2H), 7.85 (d, *J* = 7.6 Hz, 2H), 7.57 (d, *J* = 8.4 Hz, 2H), 7.45 (t, *J* = 7.6 Hz, 2H), 7.34 (m, 1H), 5.85 (s, 2H).



1-(3-nitrobenzyl)-4-phenyl-1*H*-1,2,3-triazole: Elemental analysis calcd (%) for C<sub>15</sub>H<sub>12</sub>N<sub>4</sub>O<sub>2</sub>: C 64.28, H 4.32, N 19.99; found: C 64.34, H 4.26, N 20.09. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>, δ): 8.70 (s, 1H), 8.27 (s, 1H), 8.21 (d, *J* = 8 Hz, 1H), 7.79–7.86 (m, 3H), 7.69 (t, *J* = 8 Hz, 1H), 7.43 (t, *J* = 7.6 Hz, 2H), 7.32 (m, 1H), 5.84 (s, 2H).



1-(2-nitrobenzyl)-4-phenyl-1*H*-1,2,3-triazole: Elemental analysis calcd (%) for C<sub>15</sub>H<sub>12</sub>N<sub>4</sub>O<sub>2</sub>: C 64.28, H 4.32, N 19.99; found: C 64.21, H 4.38, N 20.15. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>, δ): 8.62 (s, 1H), 8.17 (d, *J* = 8 Hz, 1H), 7.86 (d, *J* = 7.6 Hz, 2H), 7.77 (t, *J* = 7.6 Hz, 1H), 7.65 (t, *J* = 8 Hz, 1H), 7.45 (t, *J* = 7.6 Hz, 2H), 7.34 (m, 1H), 7.15 (d, *J* = 7.6 Hz, 1H), 6.02 (s, 2H).



1-(2-bromobenzyl)-4-phenyl-1H-1,2,3-triazole: Elemental analysis calcd (%) for C<sub>15</sub>H<sub>12</sub>BrN<sub>3</sub>: C 57.34, H 3.85, N 13.37; found: C 57.15, H 3.66, N 13.19. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>,  $\delta$ ): 8.61 (s, 1H), 7.86 (d, *J* = 7.6 Hz, 2H), 7.70 (d, *J* = 8 Hz, 1H), 7.46-7.33 (m, 5H), 7.22 (d, *J* = 7.6 Hz, 1H), 5.73 (s, 2H).