

## Electronic Supplementary Information for

### **A versatile gold synthon for acetylene C-H bond activation**

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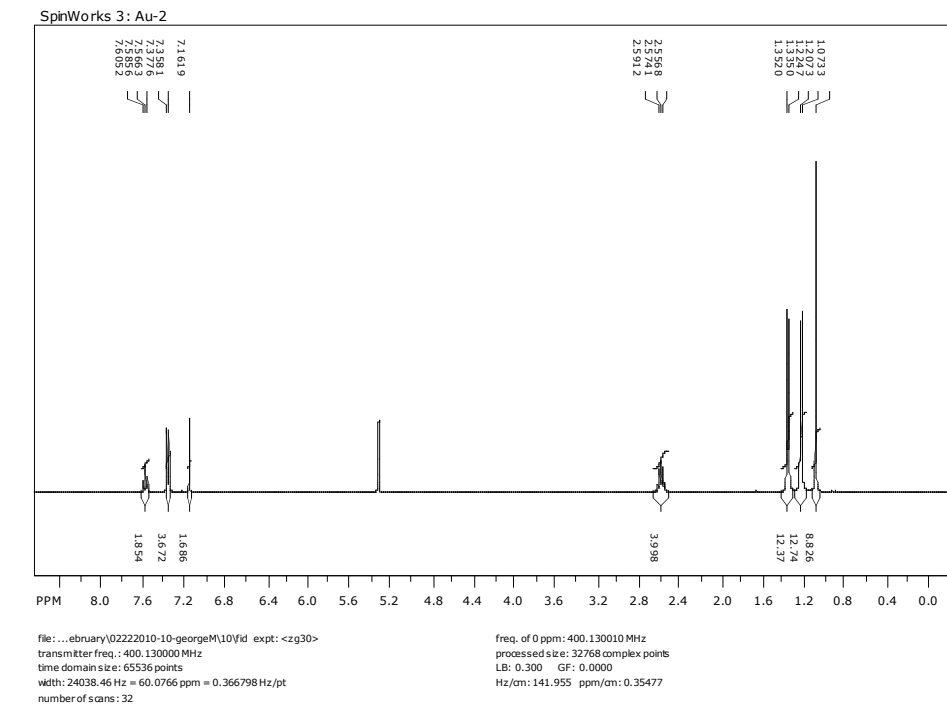
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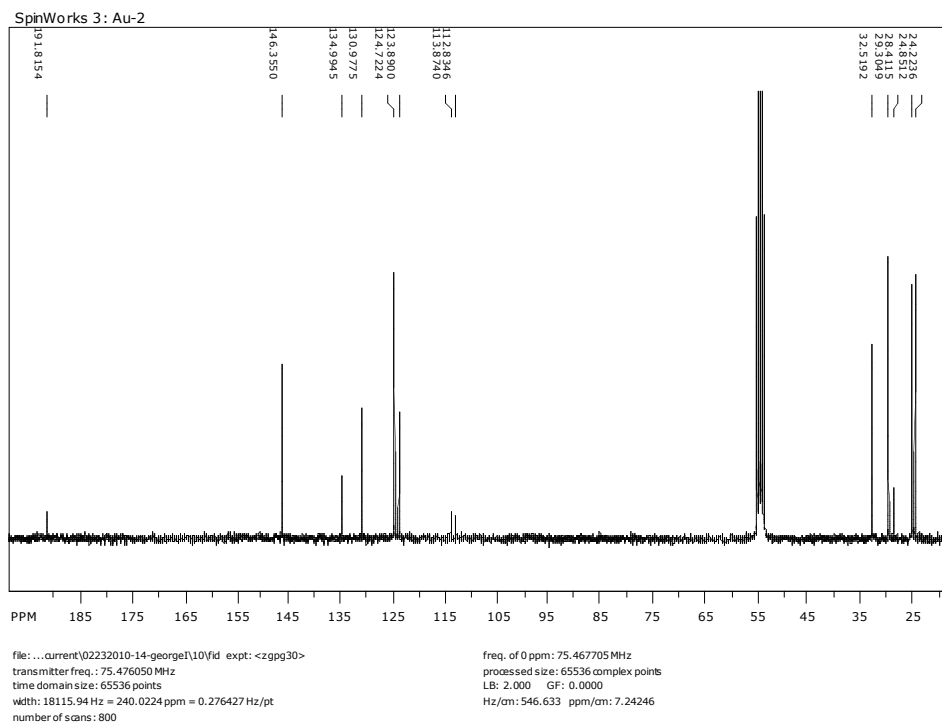
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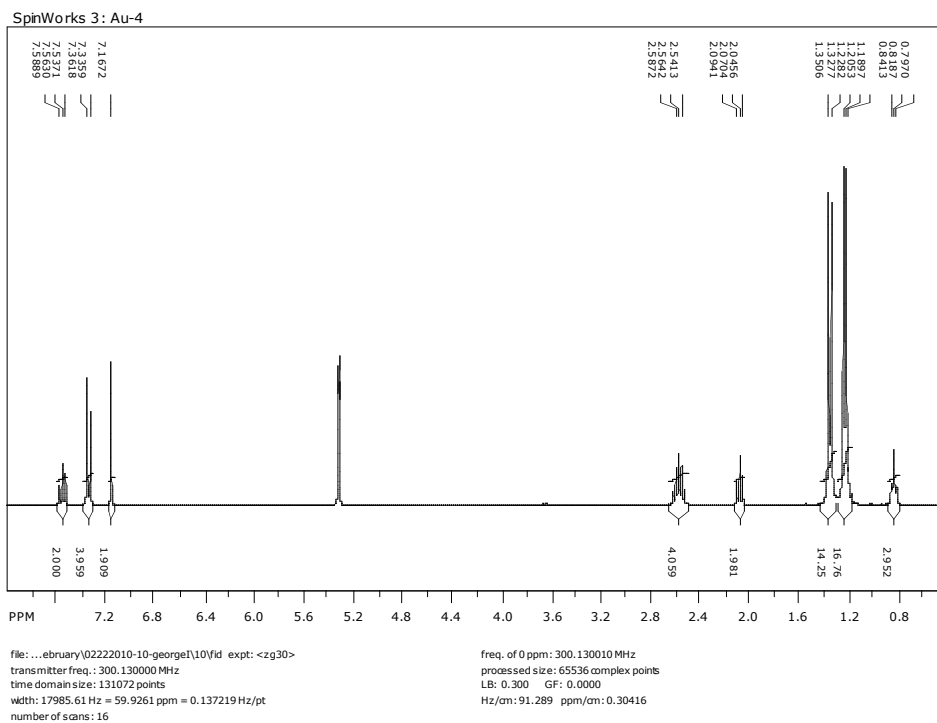
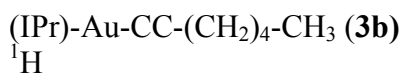
## Au-NMRs

### (IPr)-Au-CC-<sup>t</sup>Bu (**3a**) <sup>1</sup>H

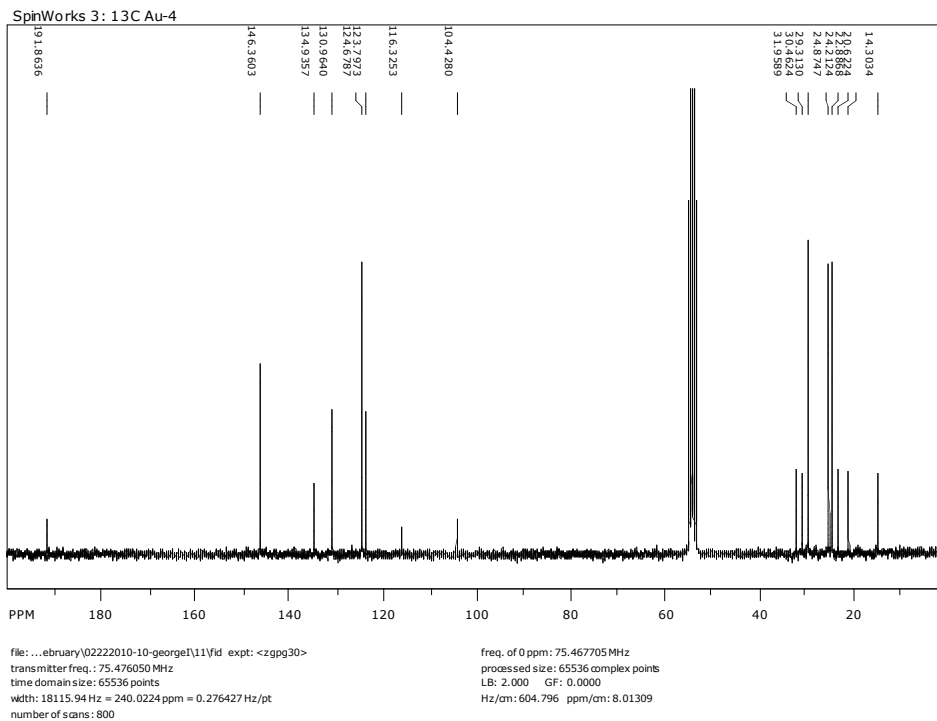


### <sup>13</sup>C

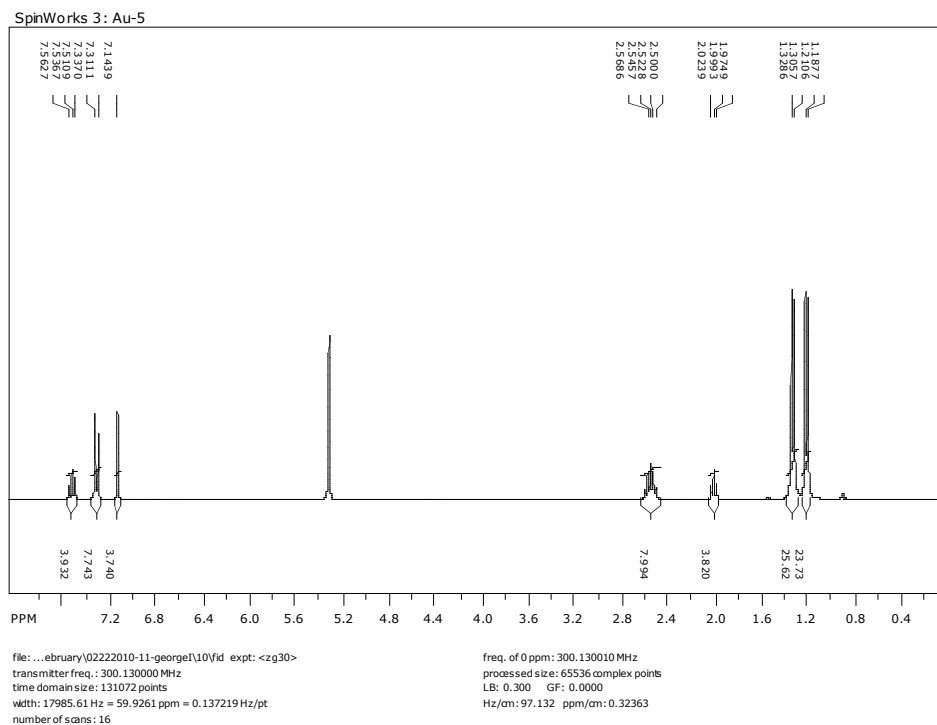




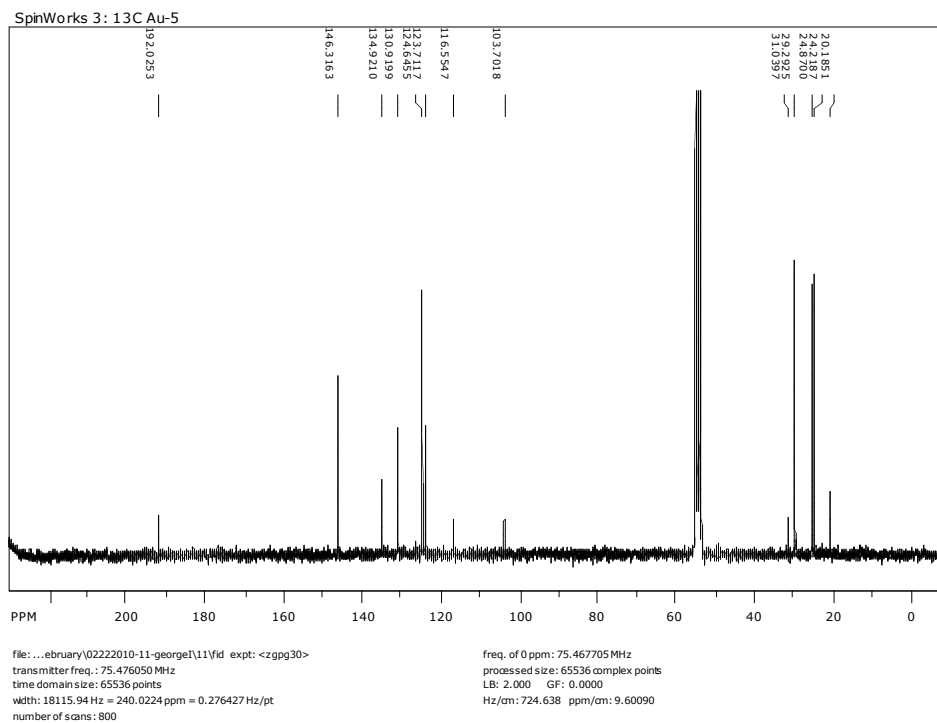
<sup>13</sup>C



(IPr)-Au-CC-(CH<sub>2</sub>)<sub>3</sub>-CC-Au-(IPr) (**3c**)  
<sup>1</sup>H

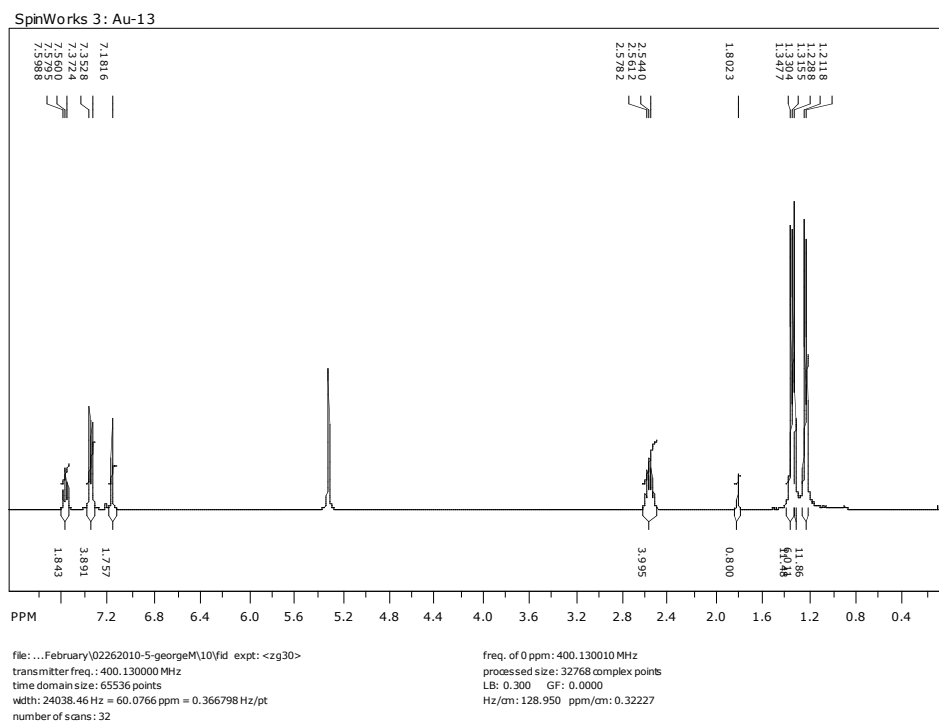


<sup>13</sup>C

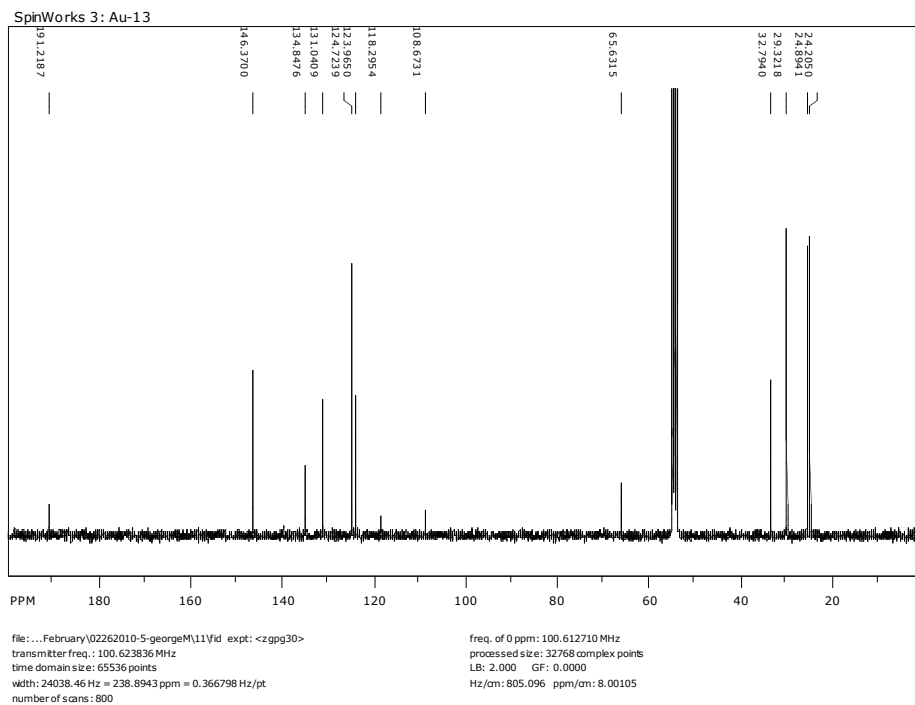


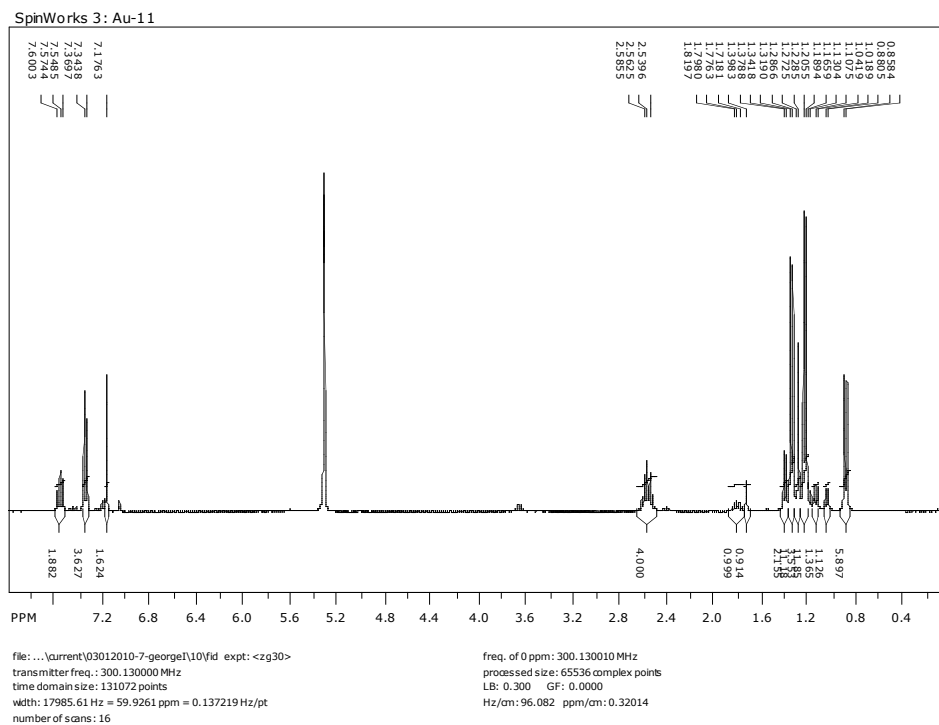
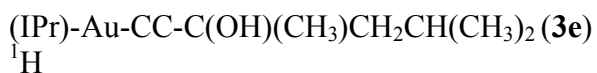
(IPr)-Au-CC-C(OH)(CH<sub>3</sub>)<sub>2</sub> (**3d**)

<sup>1</sup>H

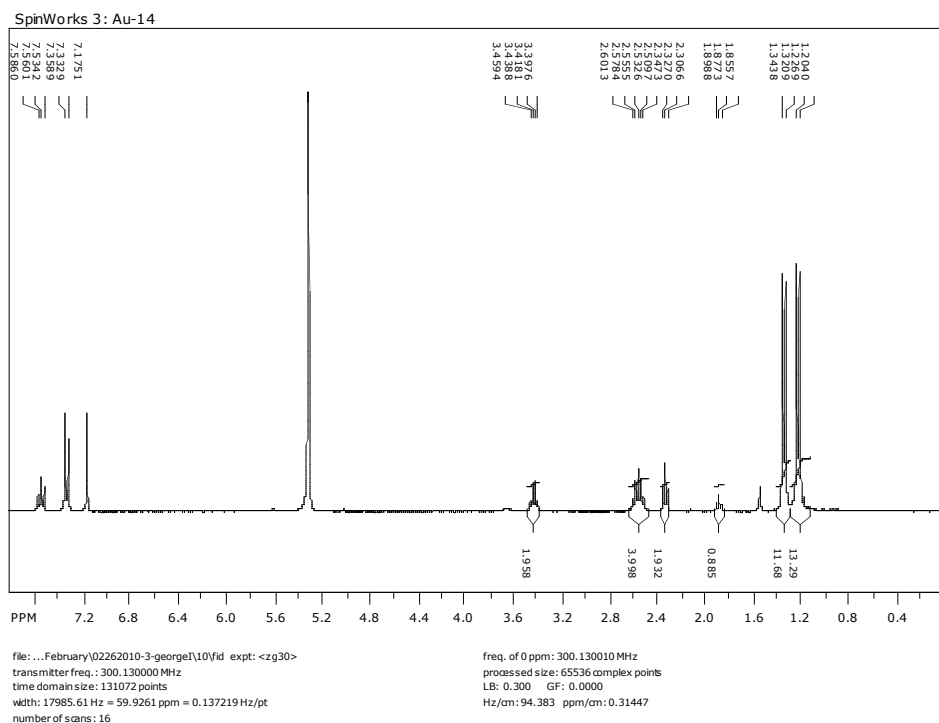


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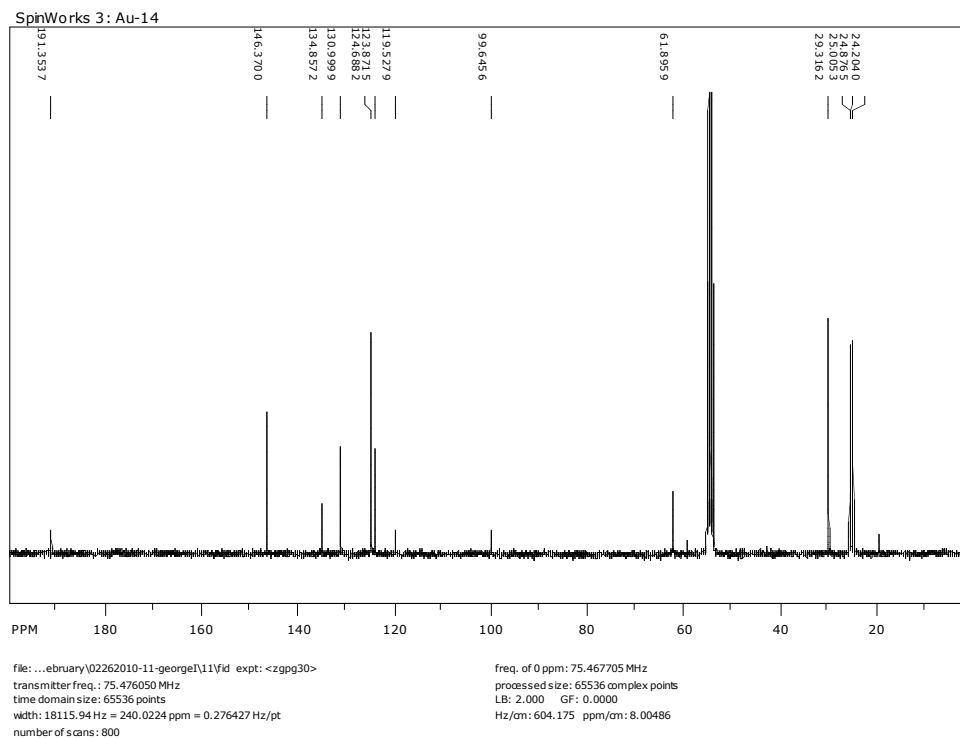


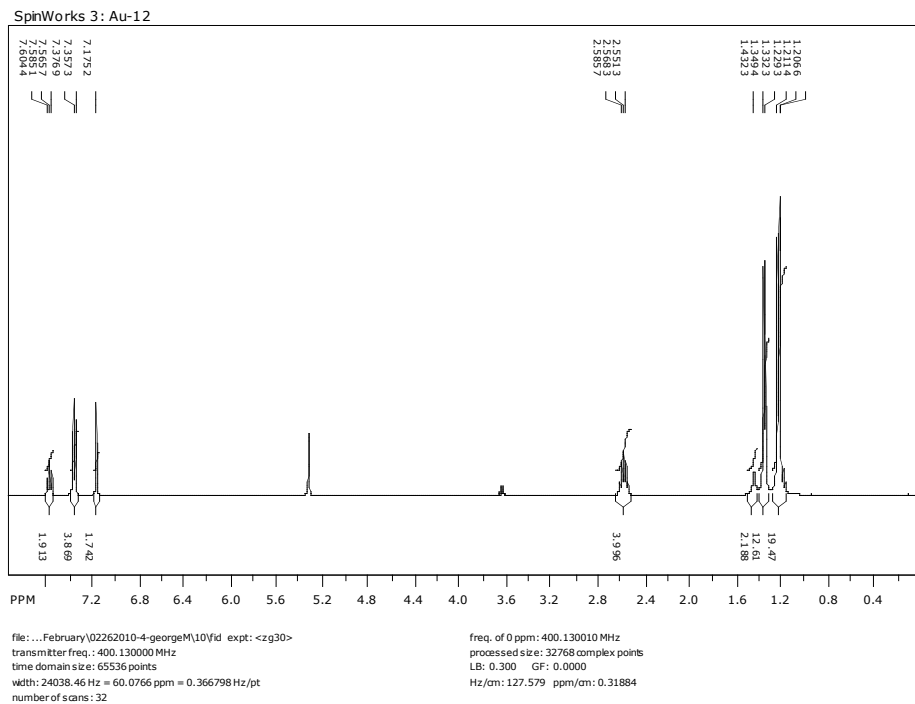


(IPr)-Au-CC-CH<sub>2</sub>CH<sub>2</sub>OH (**3f**)  
<sup>1</sup>H

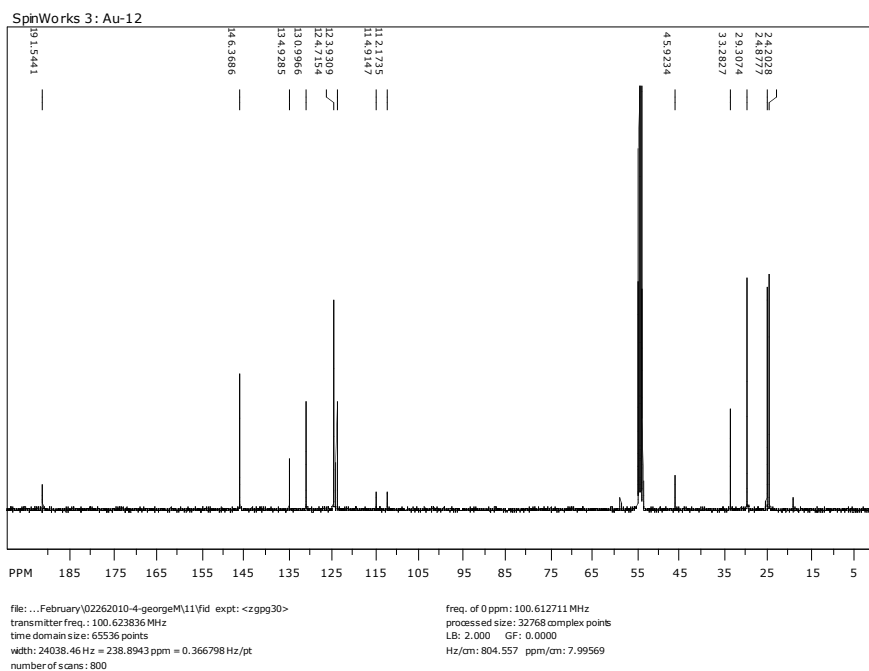


<sup>13</sup>C



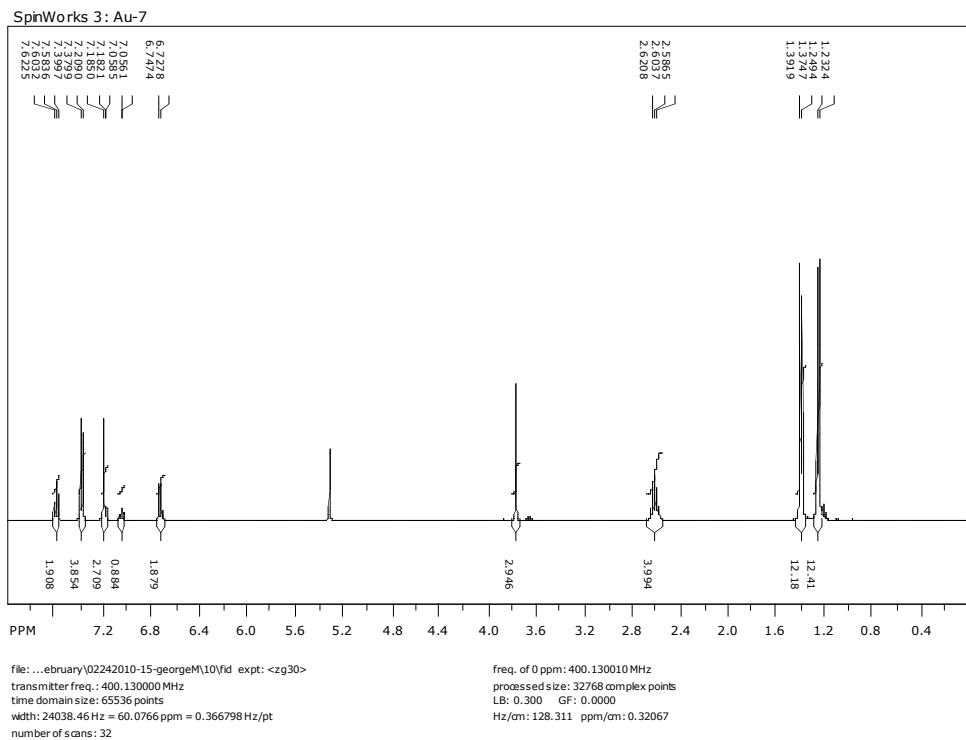


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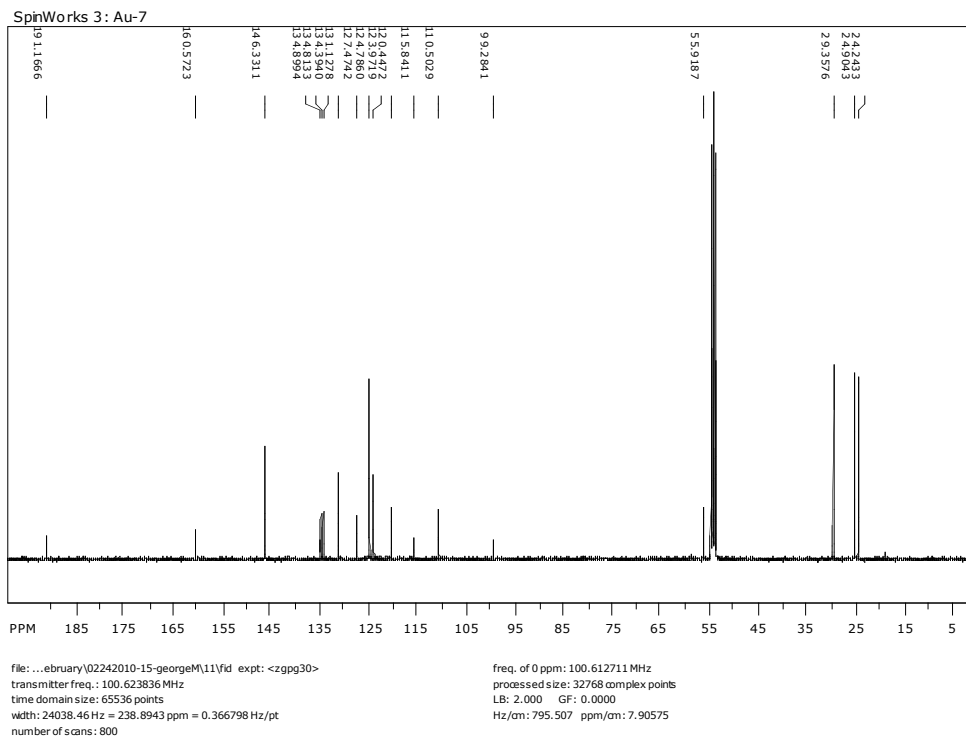




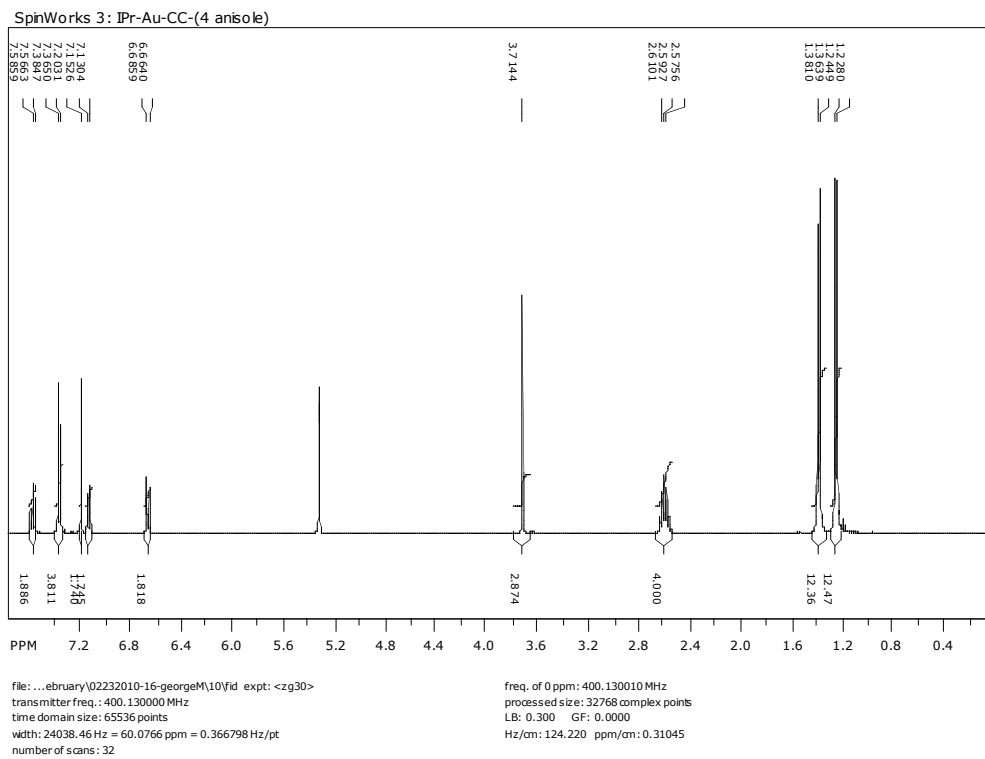
# 2-[(IPr)-Au-CC]-anisole <sup>1</sup>H



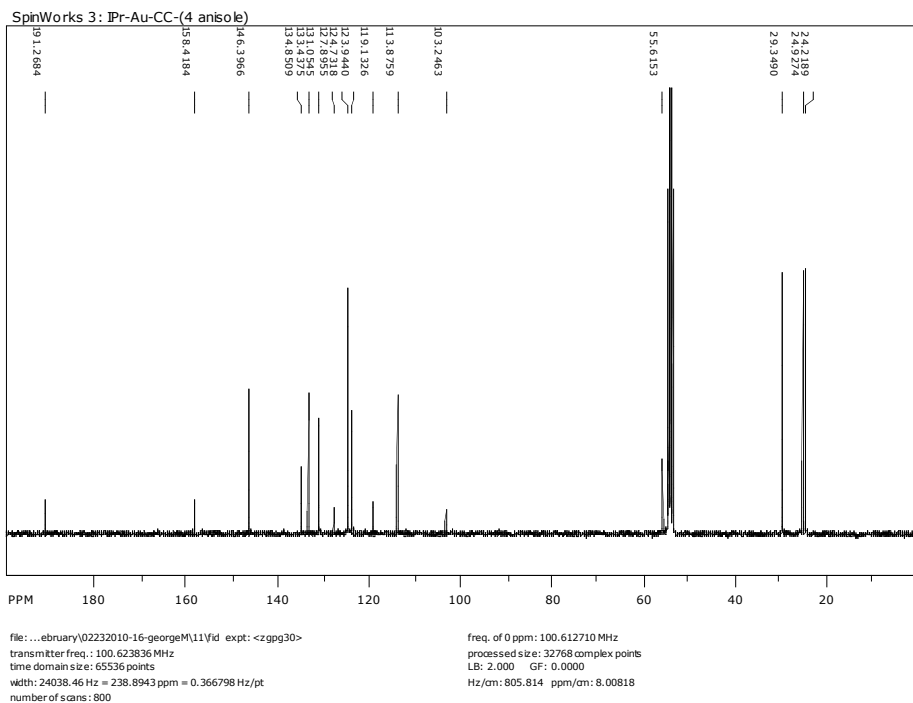
# <sup>13</sup>C



# 4-[(IPr)-Au-CC]-anisole <sup>1</sup>H

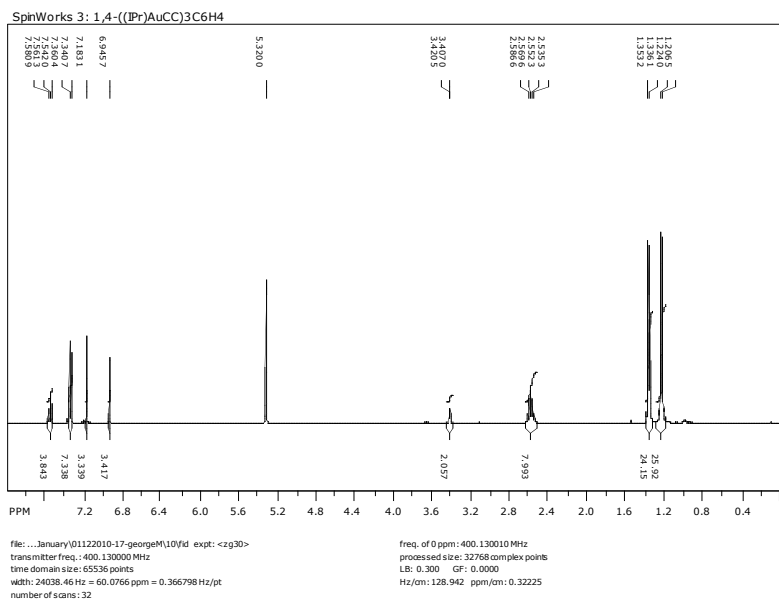
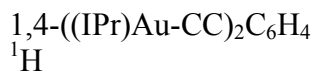


# <sup>13</sup>C

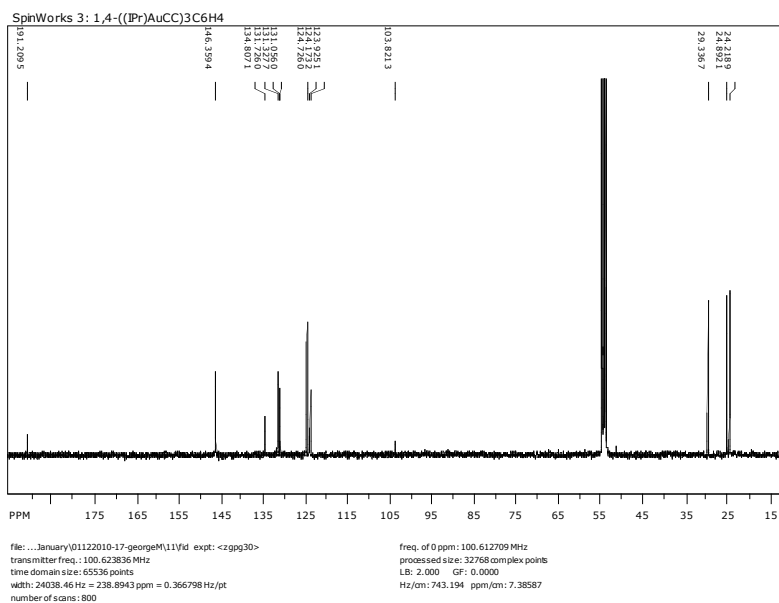




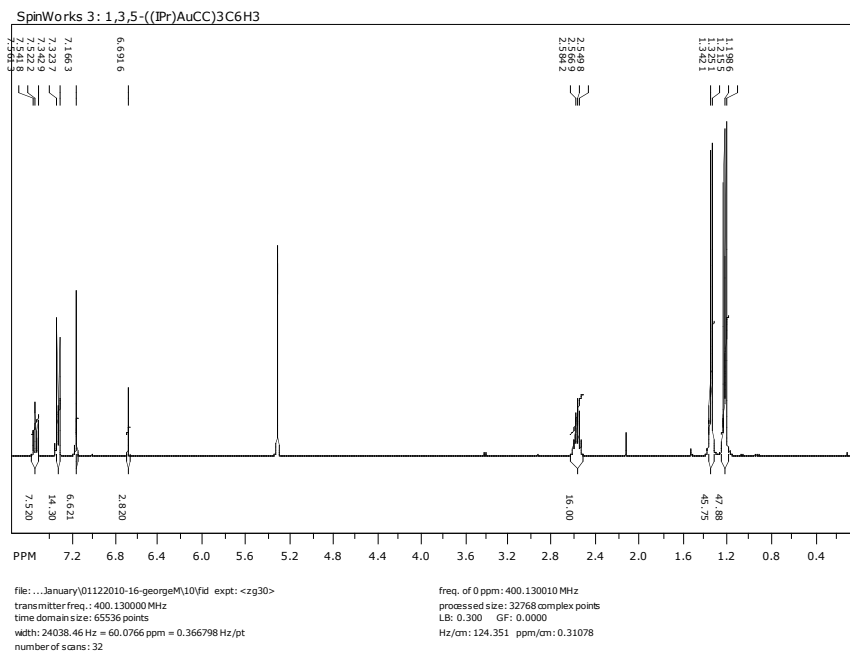
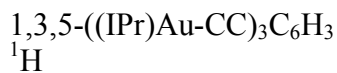




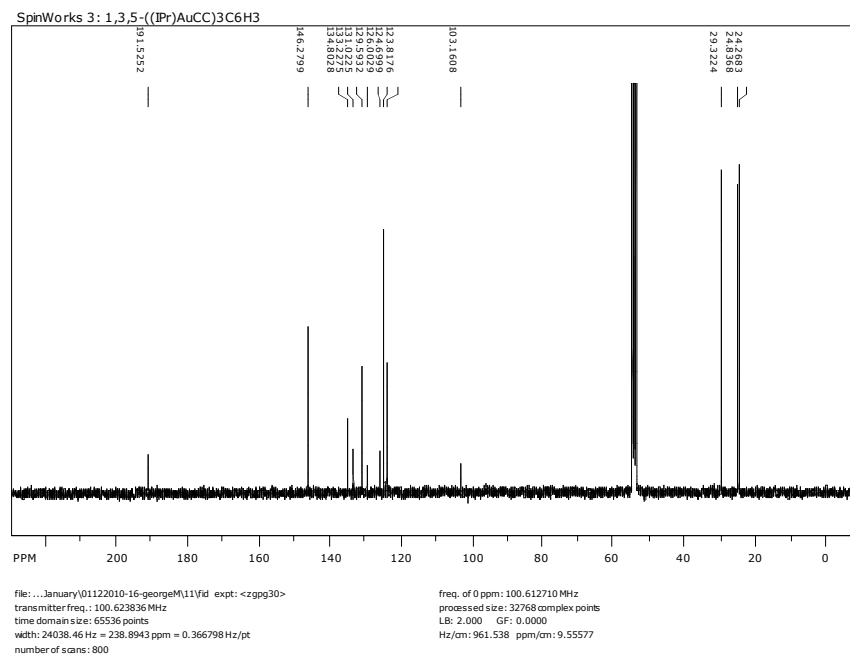
<sup>13</sup>C







<sup>13</sup>C



**Table S1.** Crystallographic data for complexes **3p-3r**.

Compound reference	<b>3p</b>	<b>3q</b>	<b>3r</b>
Chemical formula	C <sub>64</sub> H <sub>76</sub> Au <sub>2</sub> N <sub>4</sub> •C <sub>4</sub> H <sub>8</sub> O	C <sub>64</sub> H <sub>76</sub> Au <sub>2</sub> N <sub>4</sub> •3(C <sub>4</sub> H <sub>8</sub> O)	C <sub>93</sub> H <sub>111</sub> Au <sub>3</sub> N <sub>6</sub> •C <sub>4</sub> H <sub>8</sub> O
Formula Mass	1367.32	1511.53	1975.88
Crystal system	Monoclinic	Monoclinic	Monoclinic
<i>a</i> /Å	20.969(7)	26.957(7)	16.191(10)
<i>b</i> /Å	14.209(4)	15.707(4)	24.037(13)
<i>c</i> /Å	23.049(11)	16.660(4)	26.30(2)
$\alpha$ /°	90.00	90.00	90.00
$\beta$ /°	112.490(7)	96.742(8)	92.389(7)
$\gamma$ /°	90.00	90.00	90.00
Unit cell volume/Å <sup>3</sup>	6345(4)	7005(3)	10228(12)
Temperature/K	93(2)	93(2)	93(2)
Space group	<i>I</i> 2/ <i>a</i>	<i>C</i> <i>c</i>	<i>I</i> <i>a</i>
No. of formula units per unit cell, <i>Z</i>	4	4	4
No. of reflections measured	19195	21968	50965
No. of independent reflections	5687	9476	17329
<i>R</i> <sub>int</sub>	0.0527	0.0373	0.1330
Final <i>R</i> <sub><i>I</i></sub> values ( <i>I</i> > 2σ( <i>I</i> ))	0.0386	0.0457	0.1526
Final <i>wR</i> ( <i>F</i> <sup>2</sup> ) values ( <i>I</i> > 2σ( <i>I</i> ))	0.0943	0.1165	0.3784
Final <i>R</i> <sub><i>I</i></sub> values (all data)	0.0450	0.0471	0.1693
Final <i>wR</i> ( <i>F</i> <sup>2</sup> ) values (all data)	0.1006	0.1180	0.4153
CCDC number	771218	771219	771220