

# **Collective Synthesis of 3-Acylindoles, Indole-3-carboxylic esters, Indole-3-sulfinic acids and 3-Methylsulfonyl indoles from Free (N-H) Indoles via Common *N*-Indolyltriethylborate**

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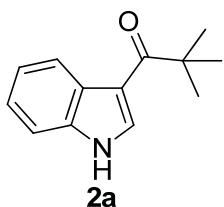
## I. General Information

Chemicals were purchased from commercial sources without further purification. The solvents were dried using standard conditions. Glassware was dried in oven and cooled before use. Acyl chlorides were purchased or prepared under standard conditions ( $\text{SOCl}_2$ , 80 °C,  $\text{N}_2$ ).  $^1\text{H}$  NMR (500MHz) and  $^{13}\text{C}$  NMR (125 MHz) spectra are recorded on a Bruker AV-500 spectrometer in  $\text{DMSO-d}_6$  or  $\text{CDCl}_3$ . For  $^1\text{H}$  NMR (500MHz),  $\text{DMSO-d}_6$  ( $\delta = 2.5$  ppm) and  $\text{CDCl}_3$  ( $\delta = 7.26$  ppm) served as internal standard. The chemical shift ( $\delta$ ) of each signal is reported in parts per million (ppm) and all coupling constants ( $J$ ) are reported in Hertz (Hz). The multiplicities of the signals are described using the following abbreviation s: s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, m = multiplet, br = broad. For  $^{13}\text{C}$  NMR (125 MHz),  $\text{DMSO-d}_6$  ( $\delta = 39.46$  ppm) and  $\text{CDCl}_3$  ( $\delta = 7.25$  ppm) served as internal standard. High-resolution Mass spectral (HRMS) data were measured on a Bruker Apex II. Column chromatography was carried out on silica gel (200-300 mesh).

## II. Experimental Procedures

Indole (58.6 mg, 0.50 mmol) was dissolved in THF (10.0 mL) under N<sub>2</sub> at rt. To this solution was added *t*-BuOK (62.0 mg, 0.55 mmol). The mixture was stirred at rt for 30 minutes. A solution of Et<sub>3</sub>B (in hexanes, 1.0 M, 0.55 mL, 0.55 mmol) was then added dropwise and the reaction was stirred for another 30 minutes. Acid chloride (or chloroformate, thiophenyl chloride, methylsulfonyl chloride) (0.55 mmol) was added and the reaction was stirred at -15 °C for 24 hours. The reaction was quenched with the careful addition of saturated aqueous ammonium chloride (3.0 mL) and the mixture was diluted with water (10 mL). The aqueous phase was extracted with EtOAc (3x10 mL) and the organic phases were combined, dried (Na<sub>2</sub>SO<sub>4</sub>), filtered. The filtrate was evaporated under reduced pressure to give a residue, which was purified by flash column chromatography eluting with petroleum ether/EtOAc to give the corresponding product.

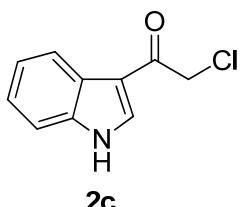
### III. Compound Characterization



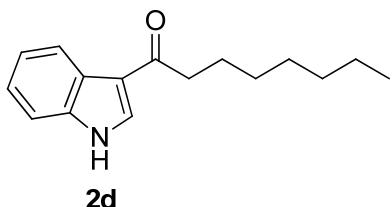
**1-(1*H*-indol-3-yl)-2,2-dimethylpropan-1-one (2a):** Isolated as white amorphous solid (91.5 mg, 0.455 mmol, 91% yield);  $R_f = 0.5$  (petroleum ether/EtOAc = 2:1);  $^1\text{H}$  NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  11.84 (1H, br), 8.34 (1H, d,  $J = 1.5$  Hz), 8.28 (1H, d,  $J = 4.0$  Hz), 7.44 (1H, d,  $J = 4.0$  Hz), 7.20-7.13 (2H, m), 1.34 (9H, s) ppm;  $^{13}\text{C}$  NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  201.11, 135.62, 132.39, 127.17, 122.46, 122.04, 121.41, 112.23, 111.70, 43.38, 28.26 ppm; HRMS (ESI) m/z: [M + H]<sup>+</sup> found for 202.1230, calcd for C<sub>13</sub>H<sub>16</sub>NO 202.1226.



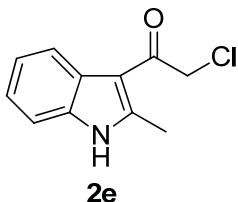
**1-(1*H*-indol-3-yl)ethanone (2b):** Isolated as white amorphous solid (69.2 mg, 0.435 mmol, 87% yield);  $R_f = 0.4$  (petroleum ether/Et-OAc = 2:1);  $^1\text{H}$  NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  11.90 (1H, br), 8.29 (1H, d,  $J = 1.5$  Hz), 8.17 (1H, d,  $J = 4.0$  Hz), 7.46 (1H, d,  $J = 4.0$  Hz), 7.22-7.15 (2H, m), 2.44 (3H, s) ppm;  $^{13}\text{C}$  NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  192.60, 136.62, 134.31, 125.25, 122.67, 121.60, 121.28, 113.77, 112.03, 27.22 ppm; HRMS (ESI) m/z: [M + Na]<sup>+</sup> found for 182.0579, calcd for C<sub>10</sub>H<sub>9</sub>NONa 182.0578.



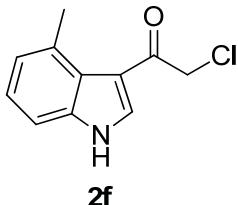
**2-chloro-1-(1*H*-indol-3-yl)ethanone (2c):** Isolated as white amorphous solid (77.2 mg, 0.400 mmol, 80% yield);  $R_f = 0.4$  (petroleu-m ether/EtOAc = 2:1);  $^1\text{H}$  NMR (500MHz, DMSO-d<sub>6</sub>):  $\delta$  12.12 (1H, br), 8.43 (1H, d,  $J = 1.5$  Hz), 8.17-8.15 (1H, m), 7.51-7.49 (1H, m), 7.26-7.20 (2H, m), 4.87 (2H, s) ppm;  $^{13}\text{C}$  NMR (125MHz, DMSO-d<sub>6</sub>):  $\delta$  186.12, 136.59, 134.73, 125.37, 123.16, 122.11, 121.12, 113.59, 112.30, 46.37 ppm; HRMS (ESI) m/z: [M + H]<sup>+</sup> found for 194.0370, calcd for C<sub>10</sub>H<sub>9</sub>ClNO 194.6367.



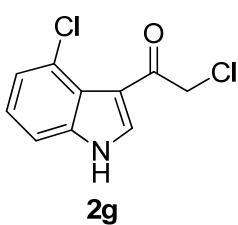
**1-(1*H*-indol-3-yl)octan-1-one (**2d**):** Isolated as white amorphous solid (62.0 mg, 0.255 mm ol, 51% yield);  $R_f = 0.2$  (petroleum ether/EtOAc = 6:1);  $^1\text{H}$  NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  11.87 (1H, br), 8.30 (1H, d,  $J = 1.5$  Hz), 8.18 (1H, d,  $J = 4.0$  Hz), 7.46-7.44 (1H, m), 7.21-7.14 (2H, m), 2.82 (2H, t,  $J = 7.0$  Hz), 1.65-1.61 (2H, m), 1.32-1.31 (4H, m), 1.27-1.23 (4H, m), 0.86 (3H, t,  $J = 7.0$  Hz) ppm;  $^{13}\text{C}$  NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  195.46, 136.61, 133.66, 125.40, 122.63, 121.55, 121.36, 116.42, 112.00, 38.74, 31.21, 28.85, 28.61, 24.94, 22.05, 13.93 ppm; HRMS (ESI) m/z: [M + H]<sup>+</sup> found for 244.1693, calcd for C<sub>16</sub>H<sub>22</sub>NO 244.1696.



**2-chloro-1-(2-methyl-1*H*-indol-3-yl)ethanone (**2e**):** Isolated as white amorphous solid (85.9 mg, 0.415 mmol, 83% yield);  $R_f = 0.4$  (petroleum ether/EtOAc = 2:1);  $^1\text{H}$  NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  12.01 (1H, br), 8.01-7.98 (1H, m), 7.40-7.36 (1H, m), 7.18-7.15 (2H, m), 4.92 (2H, s), 2.71 (3H, s) ppm;  $^{13}\text{C}$  NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  186.06, 145.26, 134.79, 126.51, 122.09, 121.66, 120.64, 111.34, 110.86, 49.50, 15.01 ppm; HRMS (ESI) m/z: [M + H]<sup>+</sup> found for 208.0526, calcd for C<sub>11</sub>H<sub>11</sub>ClNO 208.0528.

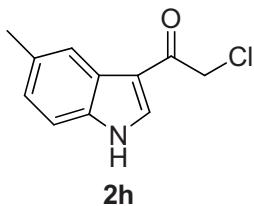


**2-chloro-1-(4-methyl-1*H*-indol-3-yl)ethanone (**2f**):** Isolated as white amorphous solid (83.9 mg, 0.405 mmol, 81% yield);  $R_f = 0.4$  (petroleum ether/EtOAc = 2:1);  $^1\text{H}$  NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  12.08 (1H, br), 8.41 (1H, d,  $J = 1.5$  Hz), 7.29 (1H, d,  $J = 4.0$  Hz), 7.12 (1H, t,  $J = 7.5$  Hz), 6.94 (1H, d,  $J = 3.5$  Hz), 4.93 (2H, s), 2.70 (3H, s);  $^{13}\text{C}$  NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  185.51, 137.53, 135.24, 131.57, 124.00, 123.70, 123.30, 115.15, 109.84, 47.83, 22.49 ppm; HRMS (ESI) m/z: [M + H]<sup>+</sup> found for 208.0522, calcd for C<sub>11</sub>H<sub>11</sub>ClNO 208.0524.

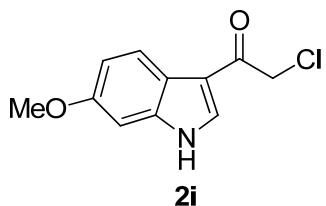


**2-chloro-1-(4-chloro-1*H*-indol-3-yl)ethanone (**2g**):** Isolated as pale red solid (89.7 mg, 0.395 mmol, 79% yield);  $R_f = 0.4$  (petroleum ether/EtOAc = 2:1);  $^1\text{H}$  NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  12.36 (1H, br), 8.47 (1H, d,  $J = 1.5$  Hz), 7.48-7.46 (1H, m), 7.25-7.21 (2H, m), 4.96 (2H, s) ppm;  $^{13}\text{C}$  NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  184.73, 138.70, 135.42, 125.49, 124.00, 123.19, 122.45, 113.96, 111.37, 48.29 ppm; HRMS (ESI) m/z: [M + H]<sup>+</sup> found fo

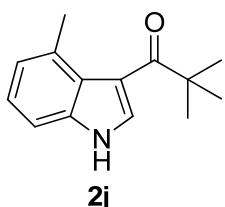
r 227.9982, calcd for C<sub>10</sub>H<sub>8</sub>Cl<sub>2</sub>NO 227.9977.



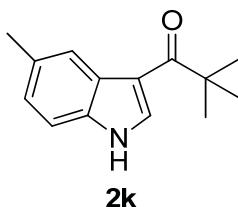
**2-chloro-1-(5-methyl-1*H*-indol-3-yl)ethanone (2h):** Isolated as white amorphous solid (93.2 mg, 0.450 mmol, 90% yield);  $R_f$  = 0.4 (petroleum ether/EtOAc = 2:1); <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  12.01 (1H, br), 8.36 (1H, d,  $J$  = 1.5 Hz), 7.97 (1H, s), 7.37 (1H, d,  $J$  = 4.0 Hz), 7.08-7.06 (1H, m), 4.84 (2H, s), 2.41 (3H, s) ppm; <sup>13</sup>C NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  186.00, 134.90, 134.67, 130.99, 125.65, 124.61, 120.85, 113.23, 111.92, 46.30, 21.27 ppm; HRMS (ESI) m/z: [M + H]<sup>+</sup> found for 208.0525, calcd for C<sub>11</sub>H<sub>11</sub>ClNO 208.0524.



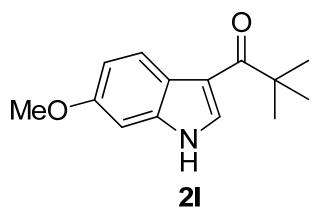
**2-chloro-1-(6-methoxy-1*H*-indol-3-yl)ethanone (2i):** Isolated as white amorphous solid (81.4 mg, 0.365 mmol, 73% yield);  $R_f$  = 0.5 (petroleum ether/EtOAc = 2:1); <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  11.92 (1H, br), 8.30 (1H, d,  $J$  = 2.0 Hz), 8.00 (1H, d,  $J$  = 5.0 Hz), 6.97 (1H, d,  $J$  = 1.0 Hz), 6.87-6.85 (1H, m), 4.84 (2H, s), 3.79 (3H, s) ppm; <sup>13</sup>C NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  185.99, 156.58, 137.54, 133.79, 121.74, 119.28, 113.76, 111.87, 95.33, 55.23, 46.19 ppm; HRMS (ESI) m/z: [M + H]<sup>+</sup> found for 224.0476, calcd for C<sub>11</sub>H<sub>11</sub>ClNO 224.0473.



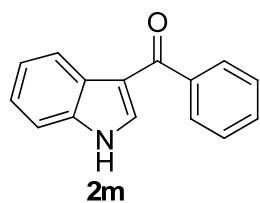
**2,2-dimethyl-1-(4-methyl-1*H*-indol-3-yl)propan-1-one (2j):** Isolated as white amorphous solid (74.2 mg, 0.345 mmol, 69% yield);  $R_f$  = 0.4 (petroleum ether/EtOAc = 2:1); <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  11.59 (1H, br), 7.93 (1H, d,  $J$  = 1.5 Hz), 7.27 (1H, d,  $J$  = 4.0 Hz), 7.06 (1H, t,  $J$  = 7.5 Hz), 6.85 (1H, d,  $J$  = 3.5 Hz), 2.37 (3H, s), 1.31 (9H, s); <sup>13</sup>C NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  204.44, 136.06, 130.63, 128.22, 125.29, 122.30, 122.28, 115.41, 109.49, 43.99, 28.13, 21.28 ppm; HRMS (ESI) m/z: [M + H]<sup>+</sup> found for 216.1380, calcd for C<sub>14</sub>H<sub>18</sub>NO 216.1383.



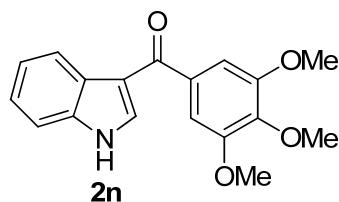
**2,2-dimethyl-1-(5-methyl-1*H*-indol-3-yl)propan-1-one (2k):** Isolated as white amorphous solid (91.4 mg, 0.425 mmol, 85% yield);  $R_f = 0.3$  (petroleum ether/EtOAc = 6:1);  $^1\text{H}$  NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  11.72 (1H, br), 8.27 (1H, d,  $J = 1.5$  Hz), 8.10 (1H, s), 7.32 (1H, d,  $J = 4.0$  Hz), 7.01 (1H, d,  $J = 4.0$  Hz), 3.32 (3H, s), 1.33 (9H, s) ppm;  $^{13}\text{C}$  NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  201.05, 133.95, 132.31, 130.08, 127.4.6, 123.91, 121.81, 111.88, 111.31, 43.33, 28.62, 21.36 ppm; HRMS (ESI) m/z: [M + H]<sup>+</sup> found for 216.1335, calcd for C<sub>14</sub>H<sub>18</sub>NO 216.1333.



**1-(6-methoxy-1*H*-indol-3-yl)-2,2-dimethylpropan-1-one (2l):** Isolated as white amorphous solid 99.4 mg, 0.430 mmol, (86% yield);  $R_f = 0.3$  (petroleum ether/EtOAc = 4:1);  $^1\text{H}$  NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  11.63 (1H, br), 8.20 (1H, d,  $J = 1.5$  Hz), 8.13 (1H, d,  $J = 4.5$  Hz), 6.92 (1H, d,  $J = 1.0$  Hz), 6.81-6.78 (1H, m), 3.77 (3H, s), 1.33 (9H, s) ppm;  $^{13}\text{C}$  NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  201.06, 156.16, 136.48, 131.35, 122.72, 121.20, 112.32, 111.25, 94.72, 55.15, 43.35, 28.68 ppm; HRMS (ESI) m/z: [M + H]<sup>+</sup> found for 232.1330, calcd for C<sub>14</sub>H<sub>18</sub>NO<sub>2</sub> 232.1332.

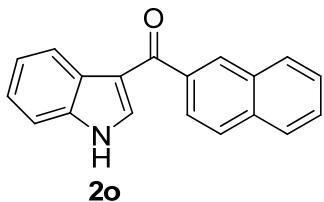


**(1*H*-indol-3-yl)(phenyl)methanone (2m):** The reaction was conducted at 0 °C, product was isolated as white amorphous solid (59.7 mg, 0.270 mmol, 54% yield);  $R_f = 0.3$  (petroleum ether/EtOAc = 4:1);  $^1\text{H}$  NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  12.09 (1H, br), 8.29-8.28 (1H, m), 7.95 (1H, d,  $J = 1.5$  Hz), 7.82-7.80 (2H, m), 7.62-7.61 (1H, m), 7.57-7.54 (3H, m), 7.30-7.26 (2H, m) ppm;  $^{13}\text{C}$  NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  189.96, 140.53, 136.71, 135.77, 131.03, 128.38, 128.36, 126.24, 123.12, 121.89, 121.46, 114.99, 112.24 ppm; HRMS (ESI) m/z: [M + H]<sup>+</sup> found for 222.0917, calcd for C<sub>15</sub>H<sub>12</sub>NO 222.0913.

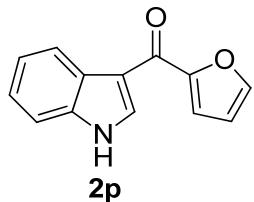


**(1*H*-indol-3-yl)(3,4,5-trimethoxyphenyl)methanone (2n):** The reaction was conducted at 0

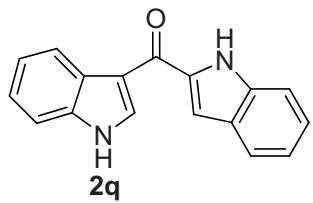
<sup>0</sup>C, product was isolated as white amorphous solid (127.6 mg, 0.410 mmol, 82% yield);  $R_f$  = 0.3 (petroleum ether/EtOAc = 2:1); <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  12.04 (1H, br), 8.27-8.26 (1H, m), 8.11 (1H, d,  $J$  = 3.0 Hz), 7.54-7.53 (1H, m), 7.29-7.23 (2H, m), 7.11 (2H, s), 3.88 (6H, s), 3.78 (3H, s) ppm; <sup>13</sup>C NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  188.95, 152.60, 140.02, 136.70, 135.78, 135.58, 126.40, 123.06, 121.80, 121.44, 114.84, 112.17, 106.04, 60.09, 55.96 ppm; HRMS (ESI) m/z: [M + Na]<sup>+</sup> found for 334.1055, calcd for C<sub>18</sub>H<sub>14</sub>NO Na 334.1050.



**(1H-indol-3-yl)(naphthalen-2-yl)methanone (2o):** The reaction was conducted at 0 °C, product was isolated as white amorphous solid (94.9 mg, 0.350 mmol, 70% yield);  $R_f$  = 0.4 (petroleum ether/EtOAc = 2:1); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  8.63 (1H, br), 8.52-8.50 (1H, m), 8.18 (1H, d,  $J$  = 4.0 Hz), 7.96 (1H, d,  $J$  = 4.0 Hz), 7.90 (1H, d,  $J$  = 4.0 Hz), 7.68-7.66 (1H, m), 7.53-7.43 (5H, m), 7.38-7.35 (2H, m) ppm; <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  192.64, 138.82, 136.51, 134.75, 133.77, 130.77, 130.16, 128.21, 126.86, 126.34, 126.02, 125.96, 125.92, 124.52, 124.15, 123.05, 122.74, 119.32, 111.40 ppm; HRMS (ESI) m/z: [M + H]<sup>+</sup> found for 272.1075, calcd for C<sub>19</sub>H<sub>14</sub>NO 272.1070.

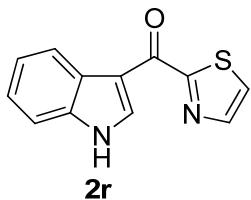


**Furan-2-yl(1H-indol-3-yl)methanone (2p):** The reaction was conducted at 0 °C, product was isolated as white amorphous solid (78.1 mg, 0.370 mmol, 74% yield);  $R_f$  = 0.4 (petroleum ether/EtOAc = 2:1); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  9.12 (1H, br), 8.56-8.54 (1H, m), 8.39 (1H, d,  $J$  = 1.5 Hz), 7.61 (1H, s), 7.45-7.43 (1H, m), 7.34-7.29 (3H, m), 6.58-6.57 (1H, m) ppm; <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  176.97, 154.50, 145.10, 136.06, 133.38, 126.85, 124.04, 122.93, 122.81, 116.70, 115.76, 112.23, 111.54 ppm; HRMS (ESI) m/z: [M + H]<sup>+</sup> found for 212.0710, calcd for C<sub>13</sub>H<sub>12</sub>NO<sub>2</sub> 212.0707.

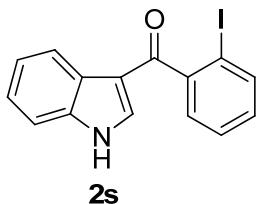


**(1H-indol-2-yl)(1H-indol-3-yl)methanone (2q):** The reaction was conducted at 0 °C, product was isolated as white amorphous solid (97.5 mg, 0.375 mmol, 75% yield);  $R_f$  = 0.4 (petroleum ether/EtOAc = 2:1); <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  12.11 (1H, br), 11.78 (1H, s), 8.47 (1H, d,  $J$  = 1.5 Hz), 8.34-8.32 (1H, m), 7.72 (1H, d,  $J$  = 4.0 Hz), 7.56-7.51 (2H, m), 7.36 (1H, d,  $J$  = 1.0 Hz), 7.28-7.25 (3H, m), 7.11-7.05 (1H, m) ppm; <sup>13</sup>C NMR

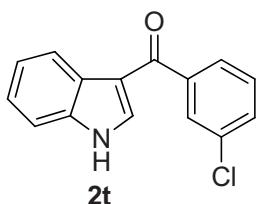
(125 MHz, DMSO-d<sub>6</sub>): δ 180.45, 137.09, 136.53, 136.27, 133.77, 127.34, 126.44, 124.29, 123.01, 122.24, 121.69, 121.49, 119.91, 115.07, 112.48, 112.20, 107.19 ppm; HRMS (ESI) m/z: [M + H]<sup>+</sup> found for 261.1027, calcd for C<sub>17</sub>H<sub>13</sub>N<sub>2</sub>O 261.1022.



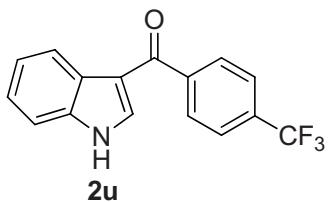
**(1*H*-indol-3-yl)(thiazol-2-yl)methanone (2r):** The reaction was conducted at 0 °C, product was isolated as pale yellow solid (37.6 mg, 0.165 mmol, 33% yield); R<sub>f</sub> = 0.4 (petroleum ether/EtOAc = 2:1); <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>): δ 12.28 (1H, br), 9.10 (1H, d, J = 1.5 Hz), 8.34-8.30 (1H, m), 8.18-8.16 (1H, m), 8.15-8.14 (1H, m), 7.58-7.56 (1H, m), 7.30-7.26 (2H, m) ppm; <sup>13</sup>C NMR (125 MHz, DMSO-d<sub>6</sub>): δ 177.22, 169.56, 144.62, 137.71, 136.31, 126.47, 126.10, 123.39, 122.44, 121.42, 112.56, 112.44 ppm; HRMS (ESI) m/z: [M + Na]<sup>+</sup> found for 251.0256, calcd for C<sub>12</sub>H<sub>8</sub>N<sub>2</sub>OSNa 251.0250.



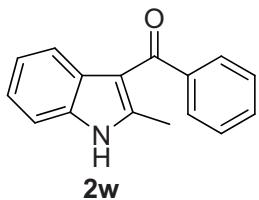
**(1*H*-indol-3-yl)(2-iodophenyl)methanone (2s):** The reaction was conducted at 0 °C, product was isolated as white amorphous solid (135.3 mg, 0.390 mmol, 78% yield); R<sub>f</sub> = 0.5 (petroleum ether/EtOAc = 2:1); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ 9.0 (1H, br), 8.37-8.36 (1H, m), 7.92 (1H, d, J = 4.0 Hz), 7.46-7.38 (4H, m), 7.36-7.31 (2H, m), 7.17-7.13 (1H, m) ppm; <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>): δ 192.06, 146.15, 139.72, 136.67, 135.20, 130.64, 128.10, 127.72, 125.76, 124.23, 123.15, 122.59, 117.16, 111.57, 92.56 ppm; HRMS (ESI) m/z: [M + H]<sup>+</sup> found for 347.9886, calcd for C<sub>15</sub>H<sub>11</sub>NIO 347.9880.



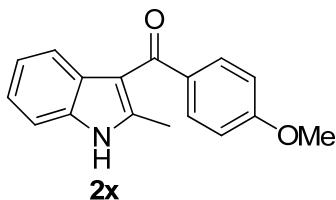
**(3-chlorophenyl)(1*H*-indol-3-yl)methanone (2t):** The reaction was conducted at 0 °C, product was isolated as white amorphous solid (103.3 mg, 0.405 mmol, 81% yield); R<sub>f</sub> = 0.5 (petroleum ether/EtOAc = 2:1); <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>): δ 12.13 (1H, br), 8.25-8.23 (1H, m), 7.98 (1H, d, J = 3.0 Hz), 7.76-7.73 (2H, m), 7.68-7.66 (1H, m), 7.59-7.52 (2H, m), 7.29-7.23 (2H, m) ppm; <sup>13</sup>C NMR (125 MHz, DMSO-d<sub>6</sub>): δ 188.26, 142.44, 136.78, 136.31, 133.25, 130.79, 130.39, 127.87, 127.04, 126.10, 123.29, 122.09, 121.40, 114.69, 112.33 ppm; HRMS (ESI) m/z: [M + Na]<sup>+</sup> found for 278.0341, calcd for C<sub>15</sub>H<sub>10</sub>ClN<sub>2</sub>O 278.0343.



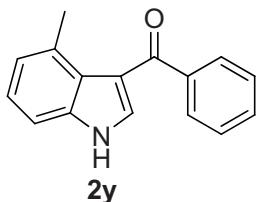
**(1*H*-indol-3-yl)(4-(trifluoromethyl)phenyl)methanone (2u):** The reaction was conducted at 0 °C, product was isolated as white amorphous solid (120.0 mg, 0.415 mmol, 83% yield);  $R_f$  = 0.3 (petroleum ether/EtOAc = 4:1);  $^1\text{H}$  NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  12.19 (1H, br), 8.28-8.26 (1H, m), 7.99-7.98 (2H, m), 7.96 (1H, s), 7.91 (1H, s), 7.89 (1H, s), 7.54-7.53 (1H, m), 7.30-7.25 (2H, m) ppm;  $^{13}\text{C}$  NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  188.74, 144.08, 136.80, 136.63, 130.85, 126.04, 125.40 (q,  $J$  = 3.75 Hz), 125.12, 123.38, 122.95, 122.20, 121.42, 114.79, 112.35 ppm; HRMS (ESI) m/z: [M + H]<sup>+</sup> found for 290.0793, calcd for C<sub>16</sub>H<sub>13</sub>F<sub>3</sub>NO 290.0787.



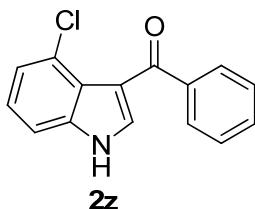
**(2-methyl-1*H*-indol-3-yl)(phenyl)methanone (2w):** The reaction was conducted at 0 °C, product was isolated as white amorphous solid (104.6 mg, 0.445 mmol, 89% yield);  $R_f$  = 0.4 (petroleum ether/EtOAc = 2:1);  $^1\text{H}$  NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  8.78 (1H, br), 7.77-7.75 (2H, m), 7.57-7.54 (1H, m), 7.48-7.45 (2H, m), 7.40 (1H, d,  $J$  = 4.0 Hz), 7.30 (1H, d,  $J$  = 4.0 Hz), 7.18-7.15 (1H, m), 7.09-7.06 (1H, m), 2.53 (3H, s) ppm;  $^{13}\text{C}$  NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  193.30, 143.66, 141.31, 134.73, 131.53, 128.90, 128.33, 127.63, 122.48, 121.59, 121.01, 114.03, 110.66, 14.52 ppm; HRMS (ESI) m/z: [M + H]<sup>+</sup> found for 236.1073, calcd for C<sub>16</sub>H<sub>14</sub>NO 236.1070.



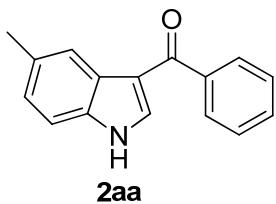
**(4-methoxyphenyl)(2-methyl-1*H*-indol-3-yl)methanone (2x):** The reaction was conducted at 0 °C, product was isolated as white amorphous solid (107.4 mg, 0.405 mmol, 81% yield);  $R_f$  = 0.4 (petroleum ether/EtOAc = 2:1);  $^1\text{H}$  NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  11.83 (1H, br), 7.63-7.60 (2H, m), 7.35 (1H, d,  $J$  = 4.0 Hz), 7.31 (1H, d,  $J$  = 4.0 Hz), 7.10-7.07 (1H, m), 7.03-6.97 (3H, m), 3.83 (3H, s), 2.40 (3H, s) ppm;  $^{13}\text{C}$  NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  190.49, 161.85, 143.29, 134.88, 133.61, 130.69, 127.29, 121.57, 120.64, 119.89, 113.52, 112.64, 111.16, 55.36, 13.99 ppm; HRMS (ESI) m/z: [M + H]<sup>+</sup> found for 266.1179, calcd for C<sub>17</sub>H<sub>16</sub>NO<sub>2</sub> 266.1176.



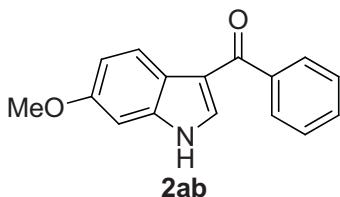
**(4-methyl-1*H*-indol-3-yl)(phenyl)methanone (**2y**):** The reaction was conducted at 0 °C, product was isolated as white amorphous solid (89.3 mg, 0.380 mmol, 76% yield);  $R_f = 0.4$  (petroleum ether/EtOAc = 2:1);  $^1\text{H}$  NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  8.53(1H, br), 7.92-7.90 (2H, m), 7.59-7.56 (1H, m), 7.50 (1H, d,  $J = 1.5$  Hz), 7.49-7.46 (2H, m), 7.28 (1H, d,  $J = 4.0$  Hz), 7.25-7.22 (1H, m), 7.08 (1H, d,  $J = 3.5$  Hz), 2.71 (3H, s) ppm;  $^{13}\text{C}$  NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  191.09, 140.55, 137.02, 133.34, 133.16, 131.93, 129.85, 128.21, 125.21, 124.20, 124.10, 119.00, 108.97, 22.14 ppm; HRMS (ESI) m/z: [M + H]<sup>+</sup> found for 236.1074, calcd for C<sub>16</sub>H<sub>14</sub>NO 236.1070.



**(4-chloro-1*H*-indol-3-yl)(phenyl)methanone (**2z**):** The reaction was conducted at 0 °C, product was isolated as white amorphous solid (82.9 mg, 0.325 mmol, 65% yield);  $R_f = 0.4$  (petroleum ether/EtOAc = 2:1);  $^1\text{H}$  NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  12.20 (1H, br), 7.85-7.81 (3H, m), 7.65-7.62 (1H, m), 7.54-7.50 (3H, m), 7.25-7.19 (2H, m) ppm;  $^{13}\text{C}$  NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  188.91, 139.73, 138.30, 134.33, 132.18, 129.38, 128.38, 125.32, 123.64, 123.43, 122.28, 115.70, 111.35 ppm; HRMS (ESI) m/z: [M + H]<sup>+</sup> found for 256.0527, calcd for C<sub>15</sub>H<sub>11</sub>ClNO 256.0524.

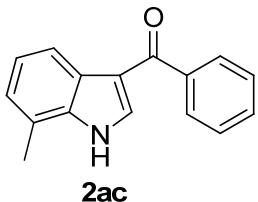


**(5-methyl-1*H*-indol-3-yl)(phenyl)methanone (**2aa**):** The reaction was conducted at 0 °C, product was isolated as white amorphous solid (68.2 mg, 0.290 mmol, 58% yield);  $R_f = 0.4$  (petroleum ether/EtOAc = 4:1);  $^1\text{H}$  NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  11.95 (1H, br), 8.08 (1H, s), 7.86 (1H, d,  $J = 1.5$  Hz), 7.78-7.76 (2H, m), 7.61-7.58 (1H, m), 7.55-7.52 (2H, m), 7.40 (1H, d,  $J = 4.0$  Hz), 7.10-7.08 (1H, m), 2.44 (3H, s) ppm;  $^{13}\text{C}$  NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  189.90, 140.65, 135.75, 135.02, 130.93, 130.72, 128.35, 128.31, 126.51, 124.59, 121.19, 114.62, 111.85, 21.35 ppm; HRMS (ESI) m/z: [M + H]<sup>+</sup> found for 236.1074, calcd for C<sub>16</sub>H<sub>14</sub>NO 236.1070.

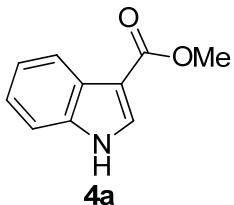


**(6-methoxy-1*H*-indol-3-yl)(phenyl)methanone (**2ab**):** The reaction was conducted at 0 °C, product was isolated as white amorphous solid (82.9 mg, 0.330 mmol, 66% yield);  $R_f = 0.5$  (petroleum ether/EtOAc = 2:1);  $^1\text{H}$  NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  11.86 (1H, br), 8.11 (1H, d,  $J = 8.5$  Hz), 7.80-7.76 (3H, m), 7.61-7.58 (1H, m), 7.54-7.51 (2H, m), 7.00 (1H,

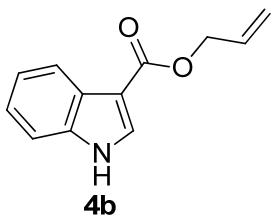
d,  $J = 2.0$  Hz), 6.89-6.87 (1H, m), 3.80 (3H, s) ppm;  $^{13}\text{C}$  NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  190.31, 157.06, 141.01, 138.11, 135.35, 131.47, 128.84, 128.80, 122.60, 120.68, 115.56, 112.17, 95.71, 55.73 ppm; HRMS (ESI) m/z: [M + H]<sup>+</sup> found for 252.1022, calcd for C<sub>16</sub>H<sub>14</sub>NO<sub>2</sub> 252.1019.



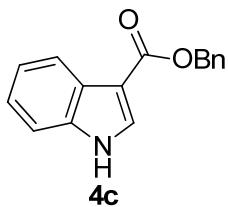
**(7-methyl-1*H*-indol-3-yl)(phenyl)methanone (2ac):** The reaction was conducted at 0 °C, product was isolated as white amorphous solid (96.4 mg, 0.410 mmol, 82% yield);  $R_f = 0.5$  (petroleum ether/EtOAc = 2:1);  $^1\text{H}$  NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  12.08 (1H, br), 8.08 (1H, d,  $J = 8.0$  Hz), 7.87 (1H, d,  $J = 3.0$  Hz), 7.79-7.78 (2H, m), 7.62-7.599 (1H, m), 7.56-7.53 (2H, m), 7.16-7.13 (1H, m), 7.07-7.06 (1H, m), 2.53 (3H, s) ppm;  $^{13}\text{C}$  NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  190.02, 140.58, 136.16, 135.25, 131.02, 128.38, 126.05, 123.71, 122.10, 121.52, 119.02, 115.39, 16.70 ppm; HRMS (ESI) m/z: [M + H]<sup>+</sup> found for 236.1075, calcd for C<sub>16</sub>H<sub>14</sub>NO 236.1070.



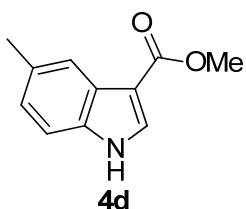
**Methyl-1*H*-indole-3-carboxylate (4a):** Isolated as white amorphous solid (79.6 mg, 0.455 mmol, 91% yield);  $R_f = 0.5$  (petroleum ether/EtOAc = 2:1);  $^1\text{H}$  NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  11.94 (1H, br), 8.10 (1H, d,  $J = 3.0$  Hz), 8.03-8.01 (1H, m), 7.51-7.49 (1H, m), 7.24-7.18 (2H, m), 3.82 (3H, s) ppm;  $^{13}\text{C}$  NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  164.75, 136.34, 132.40, 125.62, 122.35, 121.23, 120.39, 112.32, 106.30, 50.60 ppm; HRMS (ESI) m/z: [M + Na]<sup>+</sup> found for 198.0529, calcd for C<sub>10</sub>H<sub>9</sub>NO<sub>2</sub>Na 198.0525.



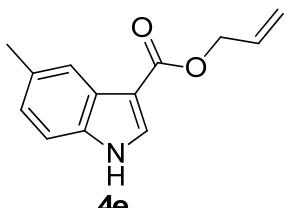
**Allyl-1*H*-indole-3-carboxylate (4b):** Isolated as white amorphous solid (90.5 mg, 0.450 mmol, 90% yield);  $R_f = 0.4$  (petroleum ether/EtOAc = 4:1);  $^1\text{H}$  NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  11.96 (1H, br), 8.11 (1H, d,  $J = 3.0$  Hz), 8.01-7.99 (1H, m), 7.50-7.48 (1H, m), 7.22-7.17 (2H, m), 6.11-6.03 (1H, m), 5.43-5.39 (1H, m), 5.27-5.25 (1H, m), 4.78-4.77 (2H, m) ppm;  $^{13}\text{C}$  NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  163.94, 136.39, 133.45, 132.62, 125.63, 122.38, 121.29, 120.38, 117.25, 112.38, 106.20, 63.50 ppm; HRMS (ESI) m/z: [M + Na]<sup>+</sup> found for 224.0686, calcd for C<sub>12</sub>H<sub>11</sub>NO<sub>2</sub>Na 224.0682.



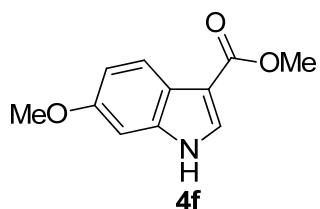
**Benzyl-1*H*-indole-3-carboxylate (4c):** Isolated as white amorphous solid (116.7 mg, 0.465 mmol, 93% yield);  $R_f = 0.5$  (petroleum ether/EtOAc = 2:1);  $^1\text{H}$  NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  11.98 (1H, br), 8.14 (1H, d,  $J = 3.0$  Hz), 8.01-7.99 (1H, m), 7.50-7.47 (3H, m), 7.42-7.39 (2H, m), 7.36-7.32 (1H, m), 7.22-7.16 (2H, m), 5.34 (2H, s) ppm;  $^{13}\text{C}$  NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  164.13, 137.04, 136.42, 132.76, 128.47, 127.82, 127.77, 125.64, 122.40, 121.33, 120.37, 112.40, 106.22, 64.50 ppm; HRMS (ESI) m/z: [M + Na]<sup>+</sup> found for 274.0842, calcd for C<sub>16</sub>H<sub>13</sub>NO<sub>2</sub>Na 274.0838.



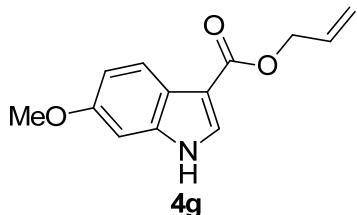
**Methyl-5-methyl-1*H*-indole-3-carboxylate (4d):** Isolated as white amorphous solid (80.4 mg, 0.425 mmol, 85% yield);  $R_f = 0.4$  (petroleum ether/EtOAc = 2:1);  $^1\text{H}$  NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  11.80 (1H, br), 8.01 (1H, s), 7.79 (1H, s), 7.35 (1H, d,  $J = 4.0$  Hz), 7.03-7.01 (1H, m), 3.79 (3H, s), 2.41 (3H, s) ppm;  $^{13}\text{C}$  NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  164.81, 134.69, 132.33, 129.98, 125.89, 123.88, 120.05, 111.97, 105.82, 50.53, 21.31 ppm; HRMS (ESI) m/z: [M + Na]<sup>+</sup> found for 212.0684, calcd for C<sub>11</sub>H<sub>11</sub>NO<sub>2</sub>Na 212.0682.



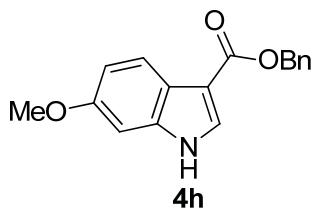
**Allyl-5-methyl-1*H*-indole-3-carboxylate (4e):** Isolated as white amorphous solid (89.3 mg, 0.415 mmol, 83% yield);  $R_f = 0.4$  (petroleum ether/EtOAc = 5:1);  $^1\text{H}$  NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  11.83 (1H, br), 8.04 (1H, d,  $J = 1.5$  Hz), 7.79 (1H, s), 7.36 (1H, d,  $J = 4.0$  Hz), 7.04-7.02 (1H, m), 6.10-6.03 (1H, m), 5.42-5.38 (1H, m), 5.27-5.24 (1H, m), 4.77-4.78 (2H, s), 2.41 (3H, s) ppm;  $^{13}\text{C}$  NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  163.95, 134.71, 133.50, 132.49, 130.01, 125.91, 123.89, 120.03, 117.14, 112.00, 105.68, 63.39, 21.32 ppm; HRMS (ESI) m/z: [M + H]<sup>+</sup> found for 216.1023, calcd for C<sub>13</sub>H<sub>14</sub>NO<sub>2</sub> 216.1019.



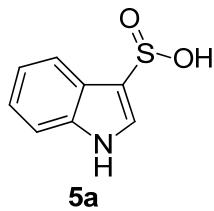
**Methyl-6-methoxy-1*H*-indole-3-carboxylate (4f):** The reaction was conducted at 0 °C, product was isolated as white amorphous solid (91.3 mg, 0.445 mmol, 89% yield);  $R_f$  = 0.4 (petroleum ether/EtOAc = 6:1);  $^1\text{H}$  NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  11.70 (1H, br), 7.93 (1H, d,  $J$  = 1.5 Hz), 7.84 (1H, d,  $J$  = 3.5 Hz), 6.95 (1H, d,  $J$  = 1.0 Hz), 6.83 (1H, d,  $J$  = 1.0 Hz), 3.78-3.77 (6H, m) ppm;  $^{13}\text{C}$  NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  164.75, 156.10, 137.13, 131.20, 120.99, 119.64, 111.33, 106.34, 95.16, 55.19, 50.54 ppm; HRMS (ESI) m/z: [M + Na]<sup>+</sup> found for 228.0634, calcd for C<sub>11</sub>H<sub>11</sub>NO<sub>3</sub>Na 228.0631.



**Allyl-6-methoxy-1*H*-indole-3-carboxylate (4g):** The reaction was conducted at 0 °C, product was isolated as white amorphous solid (89.0 mg, 0.385 mmol, 77% yield);  $R_f$  = 0.4 (petroleum ether/EtOAc = 4:1);  $^1\text{H}$  NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  11.75 (1H, br), 7.97 (1H, d,  $J$  = 1.5 Hz), 7.84 (1H, d,  $J$  = 4.5 Hz), 6.96 (1H, d,  $J$  = 1.0 Hz), 6.85-6.82 (1H, m), 6.10-6.02 (1H, m), 5.42-5.37 (1H, m), 5.28-5.24 (1H, m), 6.76-4.75 (2H, m), 3.78 (3H, s) ppm;  $^{13}\text{C}$  NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  163.95, 156.12, 137.19, 133.46, 131.44, 120.98, 119.65, 117.25, 111.41, 106.24, 95.22, 63.46, 55.20 ppm; HRMS (ESI) m/z: [M + Na]<sup>+</sup> found for 254.0785, calcd for C<sub>13</sub>H<sub>13</sub>NO<sub>3</sub>Na 254.0788

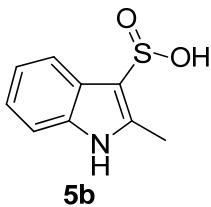


**Benzyl-6-methoxy-1*H*-indole-3-carboxylate (4h):** The reaction was conducted at 0 °C, product was isolated as white amorphous solid (113.8 mg, 0.405 mmol, 81% yield);  $R_f$  = 0.4 (petroleum ether/EtOAc = 4:1);  $^1\text{H}$  NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  11.76 (1H, br), 8.00 (1H, s), 7.82 (1H, d,  $J$  = 4.0 Hz), 7.47-7.46 (2H, m), 7.41-7.38 (2H, m), 7.35-7.33 (1H, m), 6.96 (1H, d,  $J$  = 1.0 Hz), 6.83-6.81 (1H, m), 5.31 (2H, s), 3.78 (3H, s) ppm;  $^{13}\text{C}$  NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  164.13, 156.13, 137.21, 137.03, 131.58, 128.46, 128.31, 127.77, 127.67, 120.96, 111.42, 106.24, 95.25, 64.46, 55.20 ppm; HRMS (ESI) m/z: [M + Na]<sup>+</sup> found for 304.0946, calcd for C<sub>17</sub>H<sub>15</sub>NO<sub>3</sub>Na 304.0944.

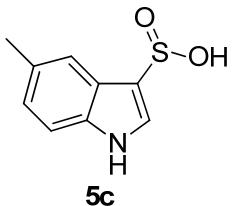


**1*H*-indole-3-sulfonic acid (5a):** Isolated as yellow gum (72.4 mg, 0.400 mmol, 80% yield);  $R_f$  = 0.4 (petroleum ether/EtOAc = 2:1);  $^1\text{H}$  NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  11.25 (1H, br), 7.71 (1H, d,  $J$  = 4.0 Hz), 7.63 (1H, d,  $J$  = 1.5 Hz), 7.37-7.33 (1H, m), 7.09-7.01 (2H,

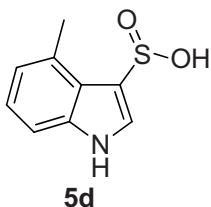
m), 3.62 (1H, br) ppm;  $^{13}\text{C}$  NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  136.14, 129.59, 128.44, 121.50, 119.33, 118.54, 111.86, 105.30 ppm; HRMS (ESI) m/z: [M + Na]<sup>+</sup> found for 204.0093, calcd for C<sub>8</sub>H<sub>7</sub>NO<sub>2</sub>SNa 204.0089.



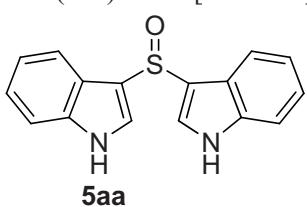
**2-methyl-1*H*-indole-3-sulfinic acid (5b):** Isolated as yellow gum (80.0 mg, 0.410 mmol, 82% yield);  $R_f$  = 0.4 (petroleum ether/EtOAc = 2:1);  $^1\text{H}$  NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  11.18 (1H, br), 7.53 (1H, d,  $J$  = 3.5 Hz), 7.23-7.21 (1H, m), 7.00-6.94 (2H, m), 2.59 (3H, s) ppm;  $^{13}\text{C}$  NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  138.91, 135.02, 129.65, 120.7, 119.14, 117.93, 110.83, 102.36, 12.14 ppm; HRMS (ESI) m/z: [M + Na]<sup>+</sup> found for 218.0249, calcd for C<sub>9</sub>H<sub>9</sub>NO<sub>2</sub>SNa 218.0246.



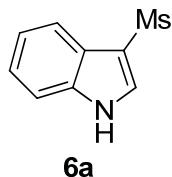
**5-methyl-1*H*-indole-3-sulfinic acid (5c):** Isolated as yellow gum (69.2 mg, 0.355 mmol, 71% yield);  $R_f$  = 0.4 (petroleum ether/EtOAc = 2:1);  $^1\text{H}$  NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  11.11 (1H, br), 7.55 (1H, d,  $J$  = 1.5 Hz), 7.51 (1H, s), 7.22 (1H, d,  $J$  = 4.0 Hz), 6.91-6.89 (1H, m), 3.92 (2H, br), 2.37 (3H, s) ppm;  $^{13}\text{C}$  NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  134.51, 129.52, 128.67, 127.85, 123.10, 118.20, 111.55, 104.78, 21.23 ppm; HRMS (ESI) m/z: [M + Na]<sup>+</sup> found for 218.0249, calcd for C<sub>9</sub>H<sub>9</sub>NO<sub>2</sub>SNa 218.0246.



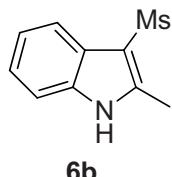
**4-methyl-1*H*-indole-3-sulfinic acid (5d):** Isolated as yellow gum (73.1 mg, 0.375 mmol, 75% yield);  $R_f$  = 0.4 (petroleum ether/EtOAc = 2:1);  $^1\text{H}$  NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  11.18 (1H, br), 7.21 (1H, d,  $J$  = 4.0 Hz), 7.03 (1H, d,  $J$  = 1.0 Hz), 6.98 (1H, t,  $J$  = 7.0 Hz), 6.74 (1H, d,  $J$  = 3.5 Hz), 3.39 (3H, br), 2.72 (3H, s) ppm;  $^{13}\text{C}$  NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  136.91, 129.92, 127.49, 125.22, 121.73, 120.68, 109.91, 107.44, 19.33 ppm; HRMS (ESI) m/z: [M + Na]<sup>+</sup> found for 218.0250, calcd for C<sub>9</sub>H<sub>9</sub>NO<sub>2</sub>SNa 218.0246.



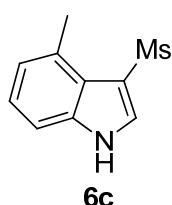
**3,3'-sulfinylbis(1*H*-indole) (**5aa**):** 0.5 equiv of  $\text{SOCl}_2$  was used to react with **1a**. Product **5aa** was isolated as yellow solid (48.2 mg, 0.173 mmol, 69% yield);  $R_f = 0.5$  (petroleum ether/EtOAc = 2:1);  $^1\text{H}$  NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  11.25 (2H, br), 7.71 (2H, d,  $J = 4.0$  Hz), 7.63 (2H, d,  $J = 1.5$  Hz), 7.36-7.33 (2H, m), 7.09-7.00 (4H, m) ppm;  $^{13}\text{C}$  NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  136.15, 129.62, 128.45, 121.52, 119.35, 118.55, 111.87, 105.31 ppm; HRMS (ESI) m/z: [M + H]<sup>+</sup> found for 281.0744, calcd for C<sub>16</sub>H<sub>13</sub>N<sub>2</sub>OS 281.0743.



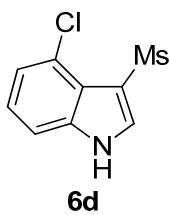
**3-(methylsulfonyl)-1*H*-indole (**6a**):** Isolated as white amorphous solid (85.8 mg, 0.44 mmol, 88% yield);  $R_f = 0.3$  (petroleum ether/EtOAc = 2:1);  $^1\text{H}$  NMR (500MHz, DMSO-d<sub>6</sub>):  $\delta$  12.18 (1H, br), 8.04 (1H, d,  $J = 2.5$  Hz), 7.82 (1H, d,  $J = 8.0$  Hz), 7.56 (1H, d,  $J = 8.0$  Hz), 7.32-7.24 (2H, m), 3.20 (3H, s) ppm;  $^{13}\text{C}$  NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  136.22, 130.76, 123.36, 123.03, 121.54, 118.69, 114.96, 112.72, 45.19 ppm; HRMS (ESI) m/z: [M + Na]<sup>+</sup> found for 218.0249, calcd for C<sub>9</sub>H<sub>9</sub>NO<sub>2</sub>SNa 218.0246.



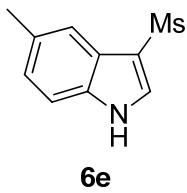
**2-methyl-3-(methylsulfonyl)-1*H*-indole (**6b**):** Isolated as white amorphous solid (87.8 mg, 0.420 mmol, 84% yield);  $R_f = 0.2$  (petroleum ether/EtOAc = 2:1);  $^1\text{H}$  NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  12.05 (1H, br), 7.75 (1H, d,  $J = 4.0$  Hz), 7.41 (1H, d,  $J = 4.0$  Hz), 7.21-7.14 (2H, m), 3.15 (3H, s), 3.10 (3H, s) ppm;  $^{13}\text{C}$  NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  141.56, 134.32, 125.11, 122.27, 121.21, 118.43, 111.55, 109.86, 45.29, 12.29 ppm; HRMS (ESI) m/z: [M + Na]<sup>+</sup> found for 232.0406, calcd for C<sub>10</sub>H<sub>11</sub>NO<sub>2</sub>SNa 232.0403.



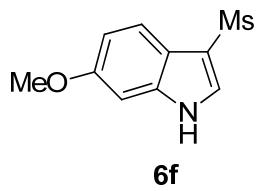
**4-methyl-3-(methylsulfonyl)-1*H*-indole (**6c**):** Isolated as white amorphous solid (89.9 mg, 0.430 mmol, 86% yield);  $R_f = 0.2$  (petroleum ether/EtOAc = 2:1);  $^1\text{H}$  NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  12.12 (1H, br), 7.99 (1H, d,  $J = 1.5$  Hz), 7.36 (1H, d,  $J = 4.5$  Hz), 7.16 (1H, t,  $J = 7.5$  Hz), 7.00 (1H, d,  $J = 3.5$  Hz), 3.26 (3H, s), 2.75 (3H, s) ppm;  $^{13}\text{C}$  NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  137.37, 132.56, 129.39, 123.34, 123.26, 121.91, 116.53, 110.46, 46.30, 20.74 ppm; HRMS (ESI) m/z: [M + Na]<sup>+</sup> found for 232.0406, calcd for C<sub>10</sub>H<sub>11</sub>NO<sub>2</sub>SNa 232.0403.



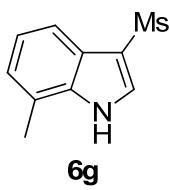
**4-chloro-3-(methylsulfonyl)-1*H*-indole (6d):** Isolated as white amorphous solid (91.6 mg, 0.400 mmol, 80% yield);  $R_f$  = 0.4 (petroleum ether/EtOAc = 2:1);  $^1\text{H}$  NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  12.47 (1H, br), 8.12 (1H, d,  $J$  = 1.5 Hz), 7.54-7.53 (1H, m), 7.31-7.26 (2H, m), 3.49 (3H, s) ppm;  $^{13}\text{C}$  NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  138.64, 134.13, 124.14, 123.49, 122.71, 120.48, 115.79, 112.11, 46.04 ppm; HRMS (ESI) m/z: [M + Na]<sup>+</sup> found for 251.9861, calcd for C<sub>9</sub>H<sub>8</sub>ClNO<sub>2</sub>SNa 251.9856.



**5-methyl-3-(methylsulfonyl)-1*H*-indole (6e):** Isolated as white amorphous solid (94.1 mg, 0.450 mmol, 90% yield);  $R_f$  = 0.2 (petroleum ether/EtOAc = 2:1);  $^1\text{H}$  NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  12.03 (1H, br), 7.94 (1H, d,  $J$  = 1.5 Hz), 7.58 (1H, s), 7.41 (1H, d,  $J$  = 5.0 Hz), 7.11-7.09 (1H, m), 3.16 (3H, s), 2.42 (3H, s) ppm;  $^{13}\text{C}$  NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  134.56, 130.61, 130.48, 124.62, 123.61, 118.21, 114.38, 112.40, 45.16, 21.21 ppm; HRMS (ESI) m/z: [M + H]<sup>+</sup> found for 210.0586, calcd for C<sub>10</sub>H<sub>12</sub>NO<sub>2</sub>S 210.0583.



**6-methoxy-3-(methylsulfonyl)-1*H*-indole (6f):** Isolated as white amorphous solid (103.5 mg, 0.460 mmol, 92% yield);  $R_f$  = 0.3 (petroleum ether/EtOAc = 2:1);  $^1\text{H}$  NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  11.93 (1H, br), 7.86 (1H, d,  $J$  = 1.5 Hz), 7.64 (1H, d,  $J$  = 4.5 Hz), 7.00 (1H, d,  $J$  = 1.0 Hz), 6.89-6.87 (1H, m), 3.79 (3H, s), 3.15 (3H, s) ppm;  $^{13}\text{C}$  NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  156.57, 137.13, 129.51, 119.36, 117.41, 114.99, 111.85, 95.35, 55.31, 45.20 ppm; HRMS (ESI) m/z: [M + Na]<sup>+</sup> found for 248.0355, calcd for C<sub>10</sub>H<sub>11</sub>NO<sub>3</sub>SNa 248.0353.



**7-methyl-3-(methylsulfonyl)-1*H*-indole (6g):** Isolated as white amorphous solid (90.9 mg, 0.435 mmol, 87% yield);  $R_f$  = 0.2 (petroleum ether/EtOAc = 2:1);  $^1\text{H}$  NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  12.19 (1H, br), 7.99 (1H, d,  $J$  = 1.5 Hz), 7.61 (1H, d,  $J$  = 4.0 Hz), 7.15-7.12 (1H, t,  $J$  = 7.5 Hz), 7.07 (1H, d,  $J$  = 3.5 Hz), 3.15 (3H, s), 2.49 (3H, s) ppm;  $^{13}\text{C}$  N

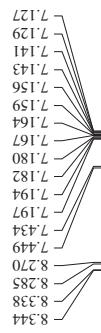
MR (125 MHz, DMSO-d<sub>6</sub>): δ 135.75, 130.32, 123.47, 123.16, 122.20, 121.76, 116.20, 115.36, 45.15, 16.65 ppm; HRMS (ESI) m/z: [M + Na]<sup>+</sup> found for 232.0406, calcd for C<sub>10</sub>H<sub>11</sub>NO<sub>2</sub>SNa 232.0403.

# IV. $^1\text{H}$ and $^{13}\text{C}$ NMR

liushouxin-xh-tewu



— 11.837 —



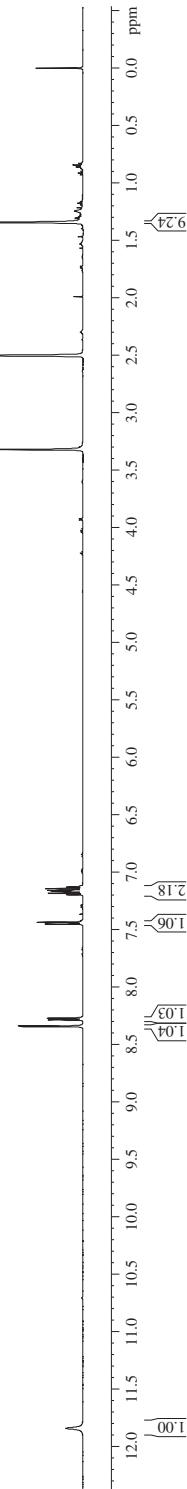
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PC

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Bruker Avance III-500  
500MHz,DMSO-d<sub>6</sub>



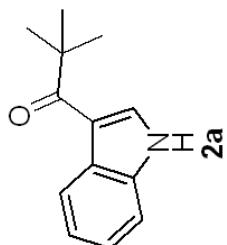
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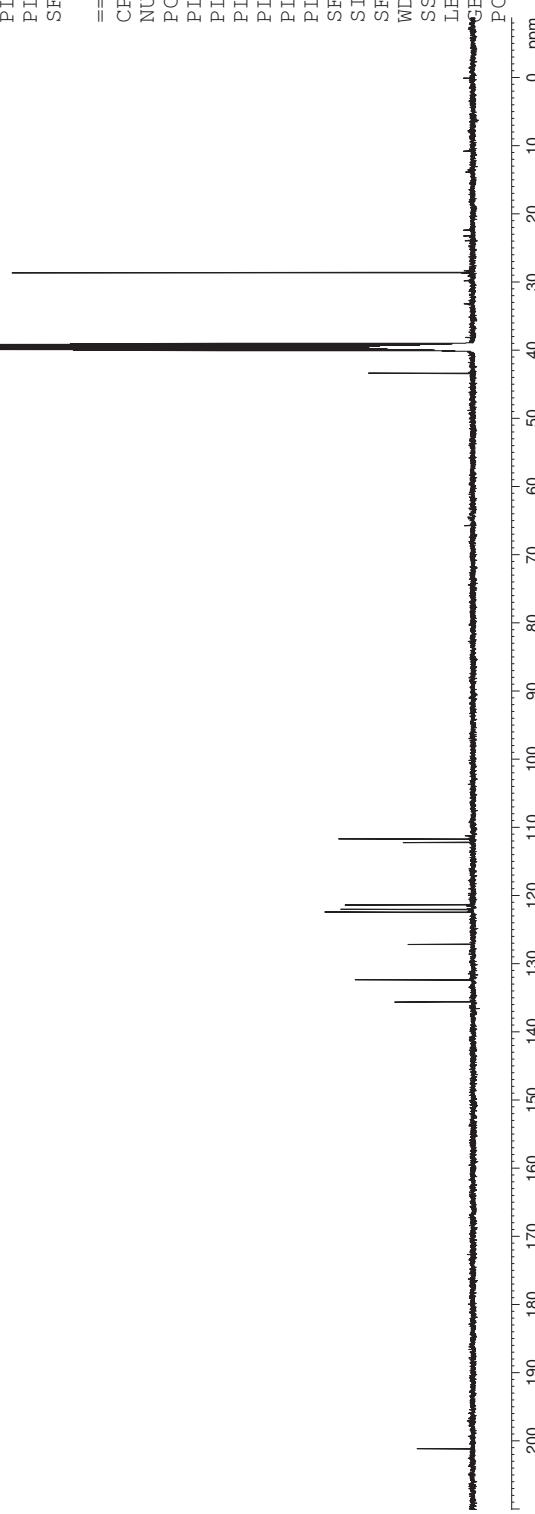
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PCPD2         80.00 usec
PL12          2.00 dB
PL12W         17.78 dB
PL13          17.78 dB
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PL12W         0.44392112 W
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Bruker Avance III-500  
125MHz,DMSO-d<sub>6</sub>



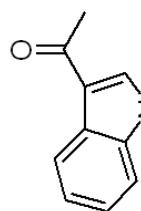


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11.897

**2b**

Bruker Avance III-500  
500MHz,DMSO-d<sub>6</sub>

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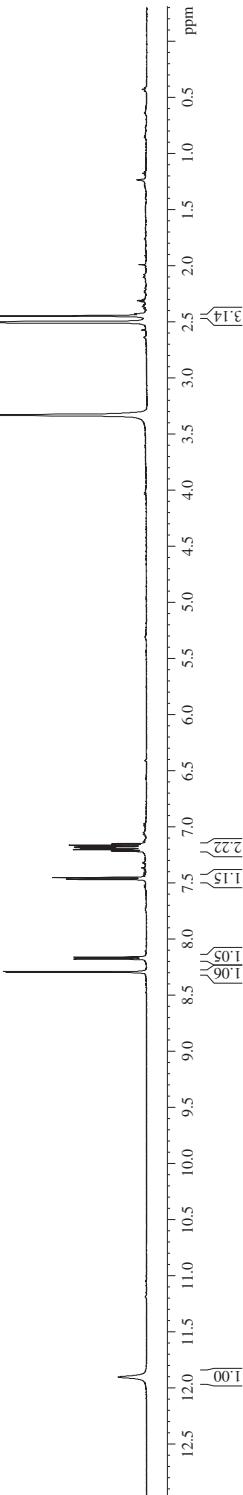
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192.66  
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|| 134.31  
|| 122.67  
|| 121.60  
|| 116.77  
|| 112.03  
/ / 112.28  
\\ \\ 121.28  
/ / 122.67  
\\ \\ 125.25  
/ / 121.60  
\\ \\ 122.67  
/ / 116.77  
\\ \\ 112.03

40.02  
39.85  
39.69  
39.52  
39.35  
39.19  
39.02  
39.02  
39.02  
27.22



```

=====
NAME          2016.05.10
EXPNO         10
PROCNO        1
Date_         20160510
Time          20.34
INSTRUM      spect
PROBHD       5 mm PABBO BB-
PULPROG      zgpp30
TD            32768
SOLVENT       DMSO
NS            1501
DS            0
SWH          29761.904 Hz
FIDRES       0.908261 Hz
AQ            0.5505524 sec
RG            2050
DW            16.800 usec
DE            6.500 usec
TE            299.6 K
D1            2.0000000 sec
D11           0.03000000 sec
TD0            1

=====
```

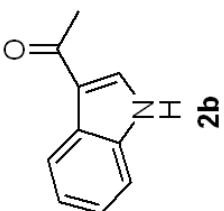
```

=====
CHANNEL f1
NUC1          13C
P1            12.30 usec
PL1           4.50 dB
PL1W          33.60015869 W
SF01          125.7703643 MHz

=====
```

```

=====
CHANNEL f2
Waltz16
NUC2          1H
PCPD2         80.00 usec
PL12          2.00 dB
PL12          17.78 dB
PL13          17.78 dB
PL2W          16.79986763 W
PL12W         0.44392112 W
PL13W         0.44392112 W
SF02          500.1320005 MHz
SI             32768
SF             125.7578514 MHz
WDW           0
SSB           1.00 Hz
LB            0
PC            1.40
```



*Bruker Avance III-500*  
*125MHz,DMSO-d<sub>6</sub>*

liushouxin-xh-lyyixian



```

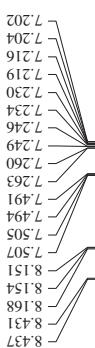
NAME          2016.05.10
EXPRO        7
PROCNO       1
Date         20160510
Time         19.38
INSTRUM     spect
PROBHD      PABBO BB-
PULPROG    2930
TD          65536
SOLVENT     DMSO
NS          8
DS          0
SWH         10330.578 Hz
FIDRES     0.157532 Hz
AQ          3.1719923 sec
RG          362
DW          48.400 usec
DE          6.50  usec
TE          298.3  K
D1          1.00000000 sec
TDDO        1

=====
CHANNEL f1 =====
NUC1        1H
P1          13.00 usec
PL1         2.00  dB
PL1W        16.79986763 W
SF01        500.1330085 MHz
SI          322768
SF          500.1300097 MHz
MWDW       EM
SSSB        0
LB          0.30  Hz
GB          0
PC          1.00

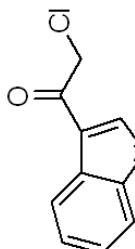
```



3.329 —

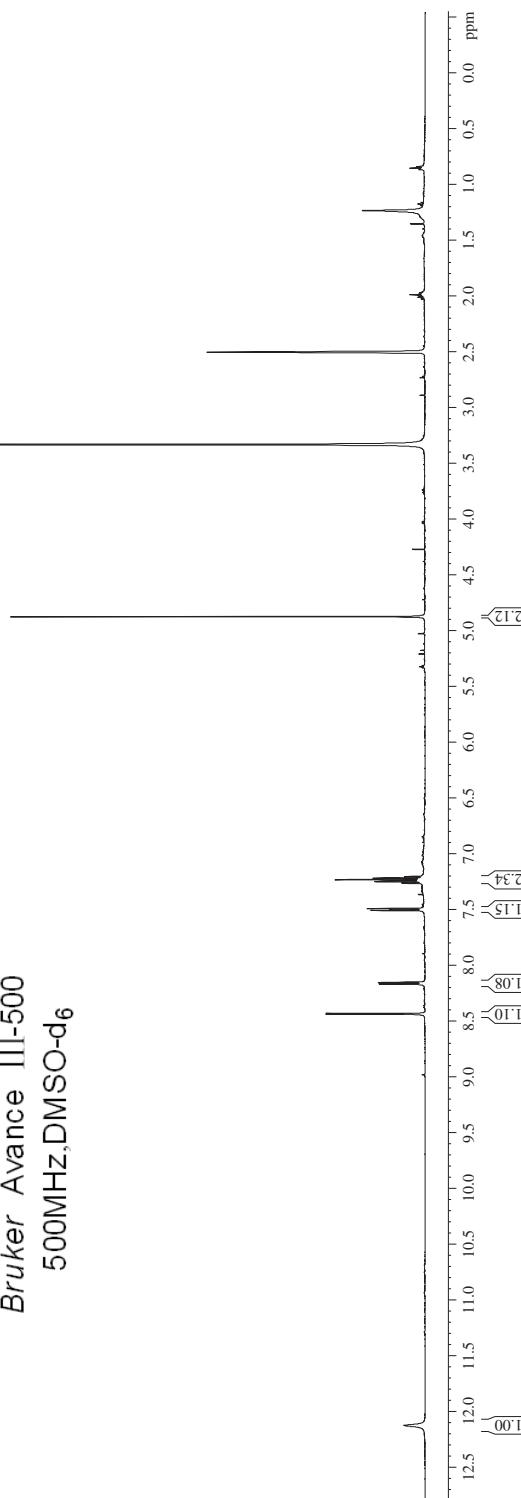


— 12.120



2c

*Bruker Avance III-500*  
500MHz,DMSO-d<sub>6</sub>



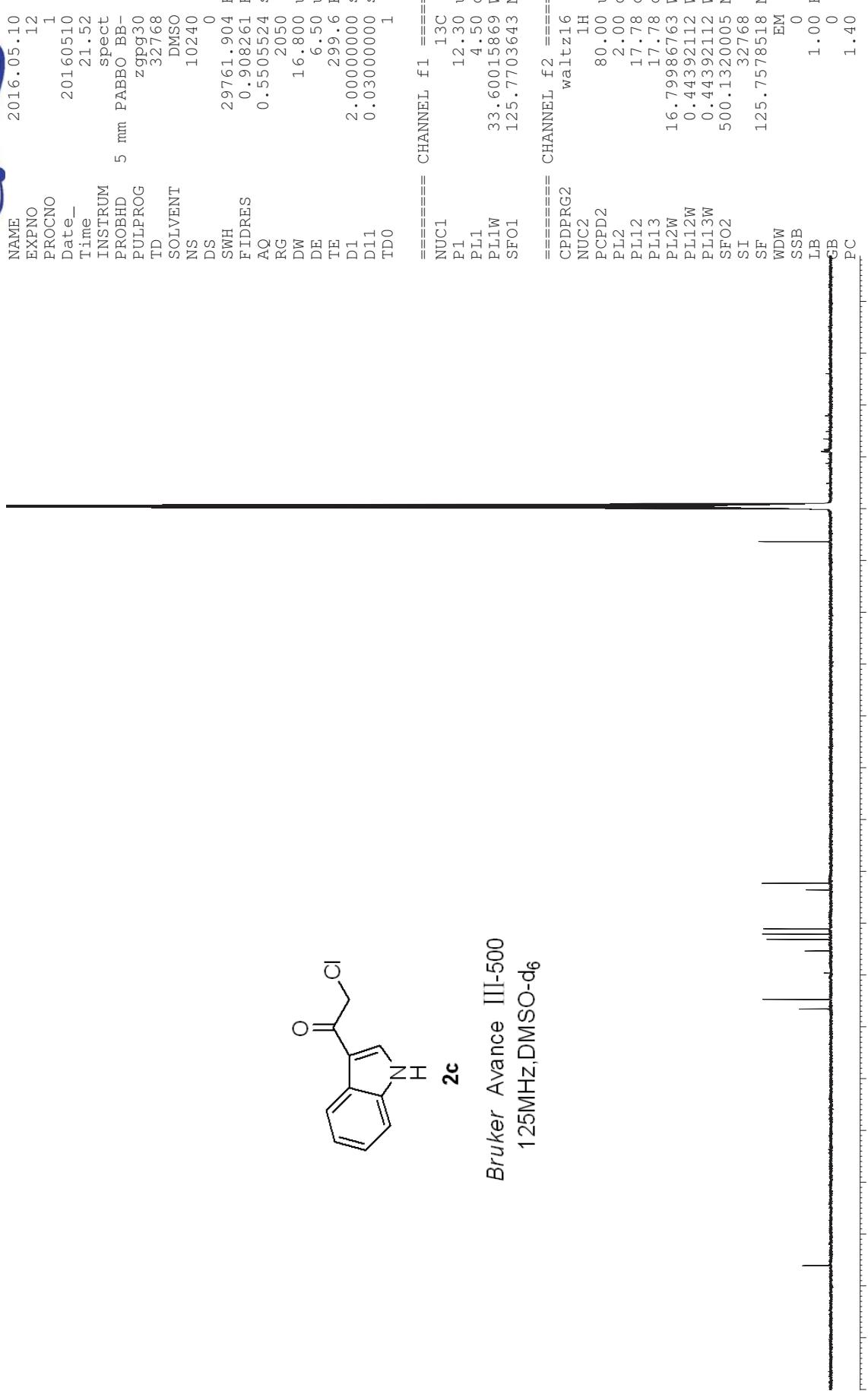
186.12

```

    / \
   / \ \
  / \ \ \
 / \ \ \ \
/ \ \ \ \ \
136.59
134.73
125.37
123.16
121.12
113.59
112.30
  
```

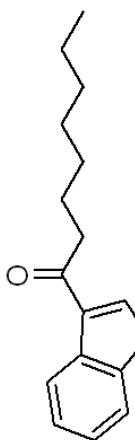
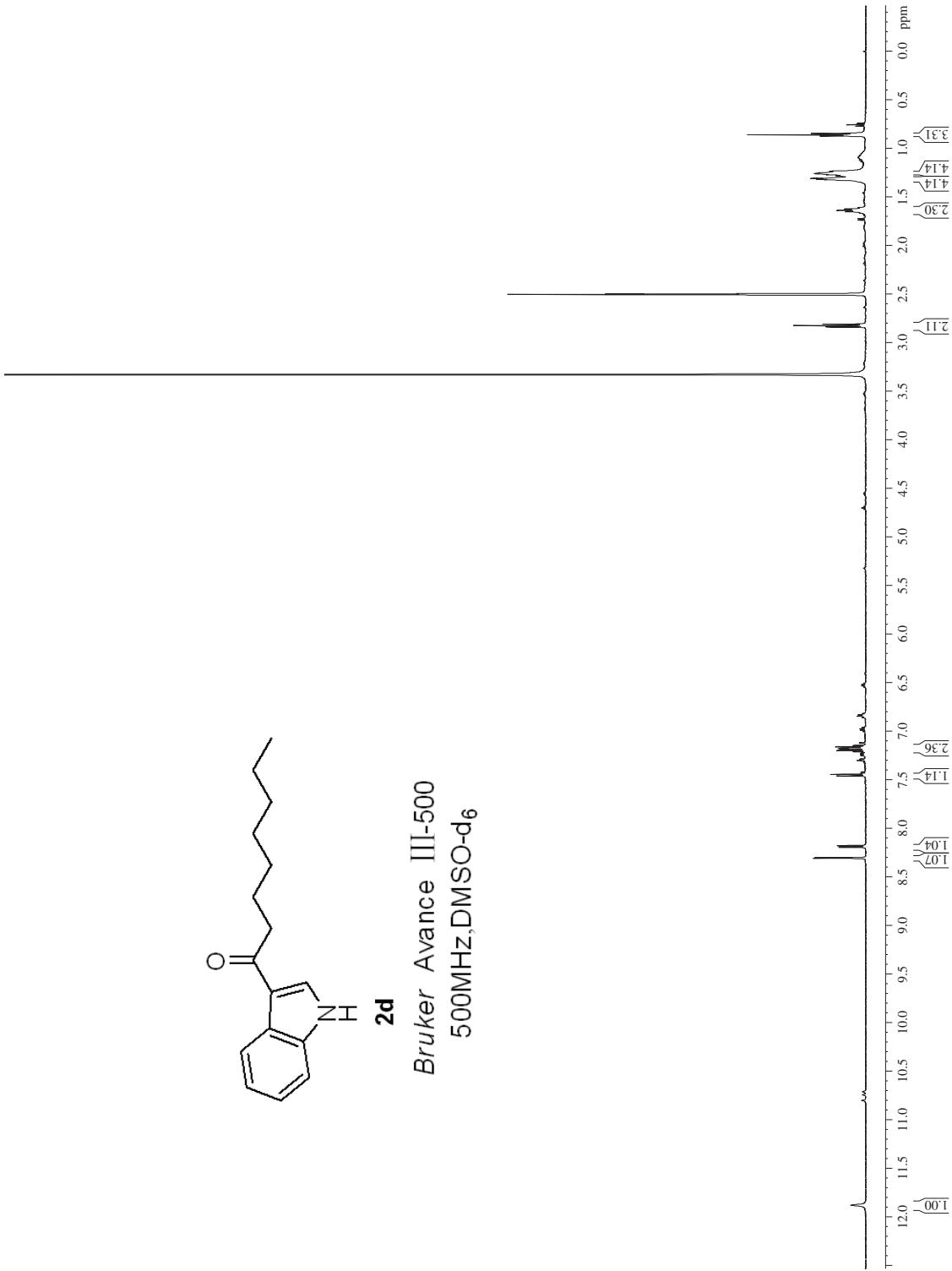
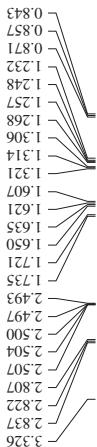
```

  46.37
  40.02
  39.85
  39.68
  39.52
  39.35
  39.18
  39.02
  
```





NAME	2016-06-22
EXPNO	6
PROCNO	1
Date_	20160622
Time	13.15
INSTRUM	5 mm PABBO BB-
PROBHD	spec
PULPROG	Zg30
TD	65536
SOLVENT	DMSO
NS	4
DS	0
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.171923 sec
RG	362
DW	48.400 usec
DE	6.50 usec
TE	298.1 K
TE	1.0000000 sec
D1	1
TDDO	
===== CHANNEL f1 =====	
NUC1	1H
P1	13.00 usec
P1L	2.00 dB
P1LW	16.79986763 W
SEFO1	500.1330885 MHz
SI	1.32768
SF	500.1300101 MHz
WDW	EM
SSB	0
LB	0.30 Hz
CB	0
PC	0
BC	1.00

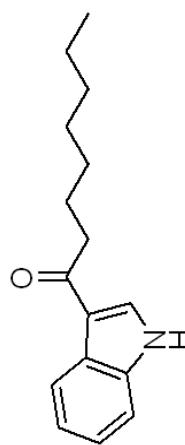


*Bruker Avance III-500*  
500MHz,DMSO-d<sub>6</sub>

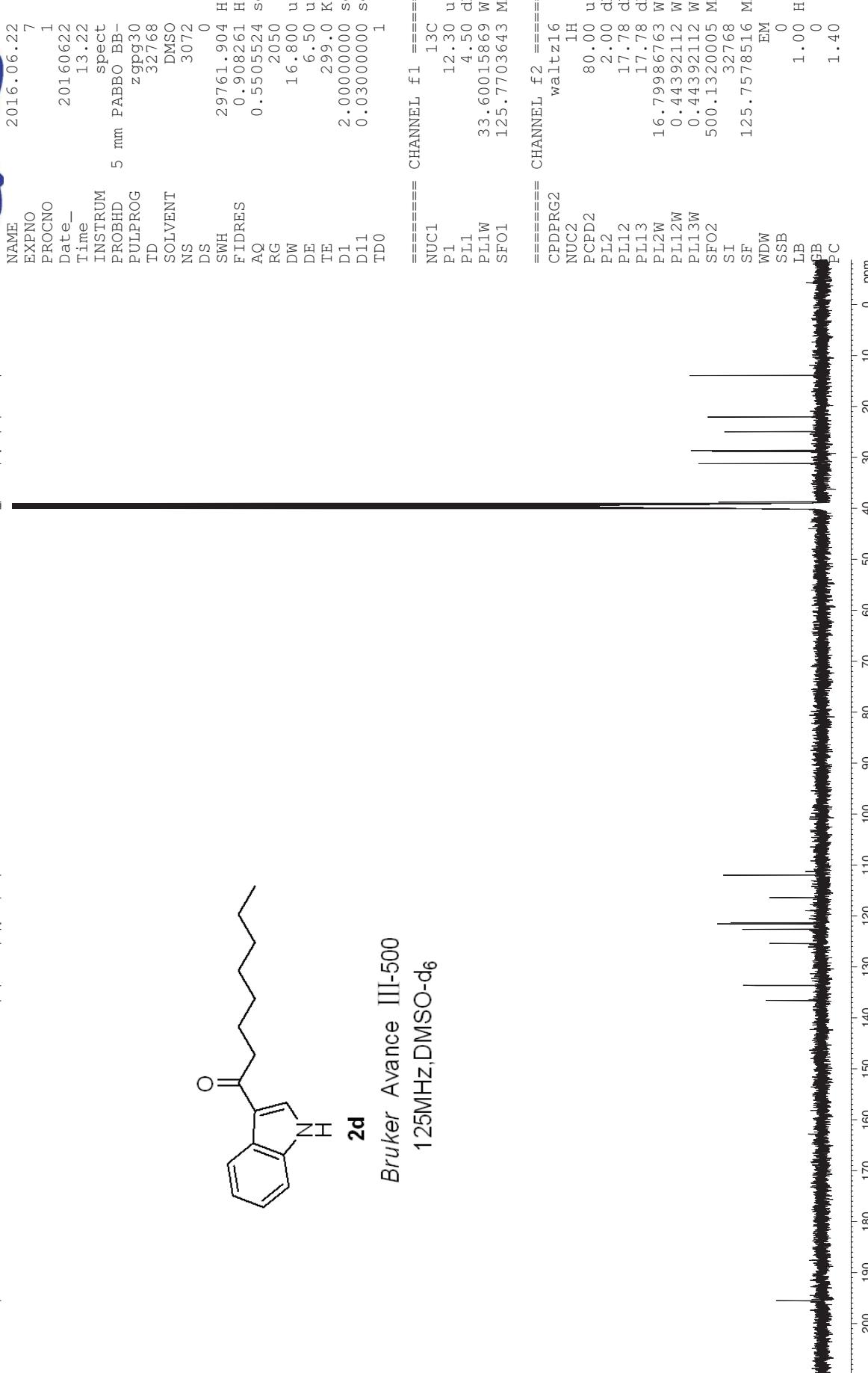


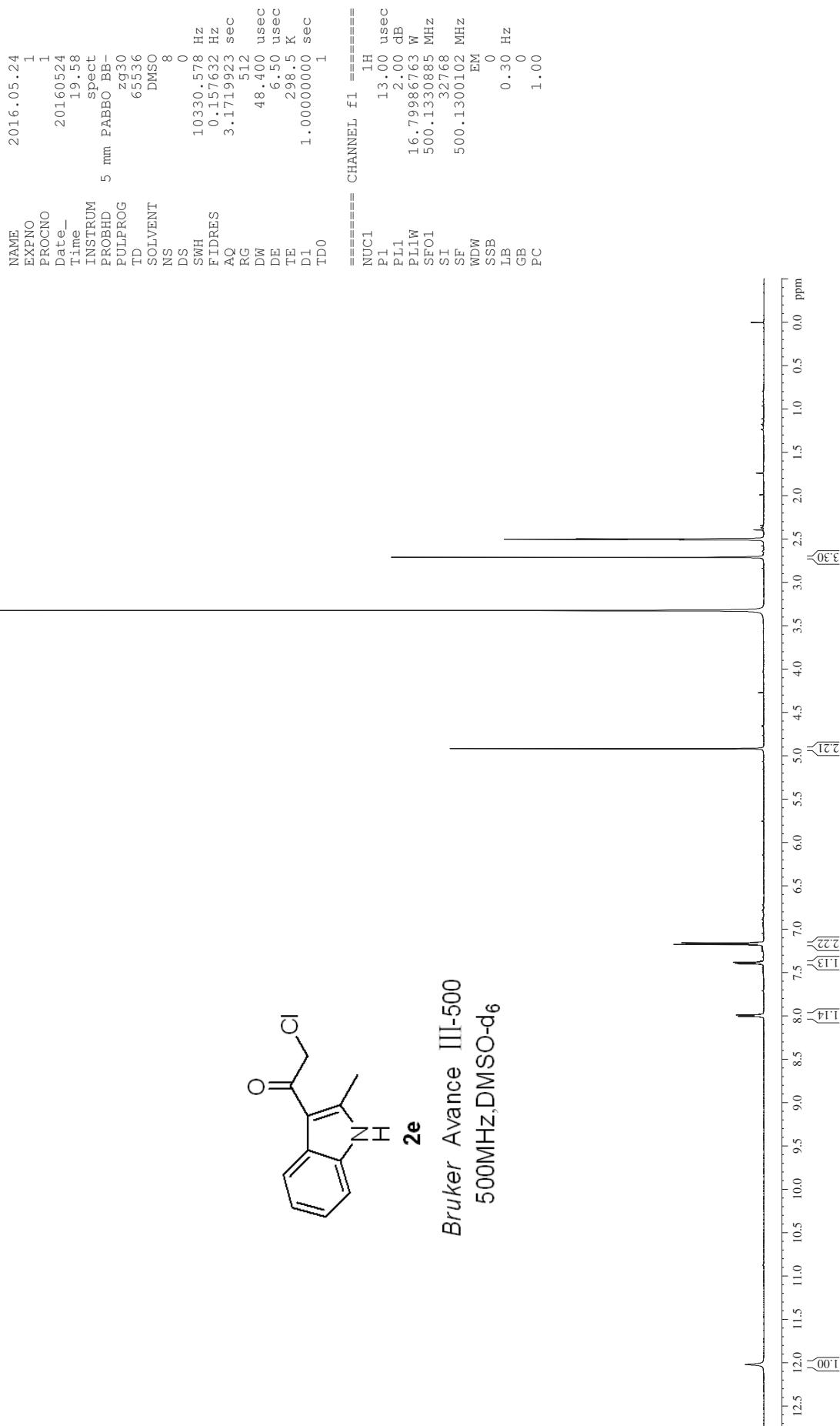
40.02  
 39.85  
 39.69  
 39.52  
 39.35  
 39.19  
 39.02  
 38.74  
 31.21  
 28.85  
 28.61  
 24.94  
 22.05  
 13.93

136.61  
 133.66  
 125.40  
 122.63  
 121.55  
 121.36  
 116.42  
 112.00



Bruker Avance III-500  
125MHz,DMSO-d<sub>6</sub>





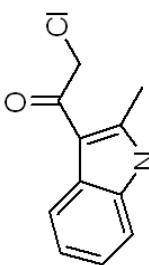
186.06

145.26

134.79  
 126.51  
 122.09  
 121.66  
 120.64  
 111.34  
 110.86

15.01

39.02  
 39.19  
 39.36  
 39.52  
 39.69  
 39.86  
 39.93  
 40.02  
 49.50

**2e**

Bruker Avance III-500  
 125MHz, DMSO-d<sub>6</sub>

**BRUKER**

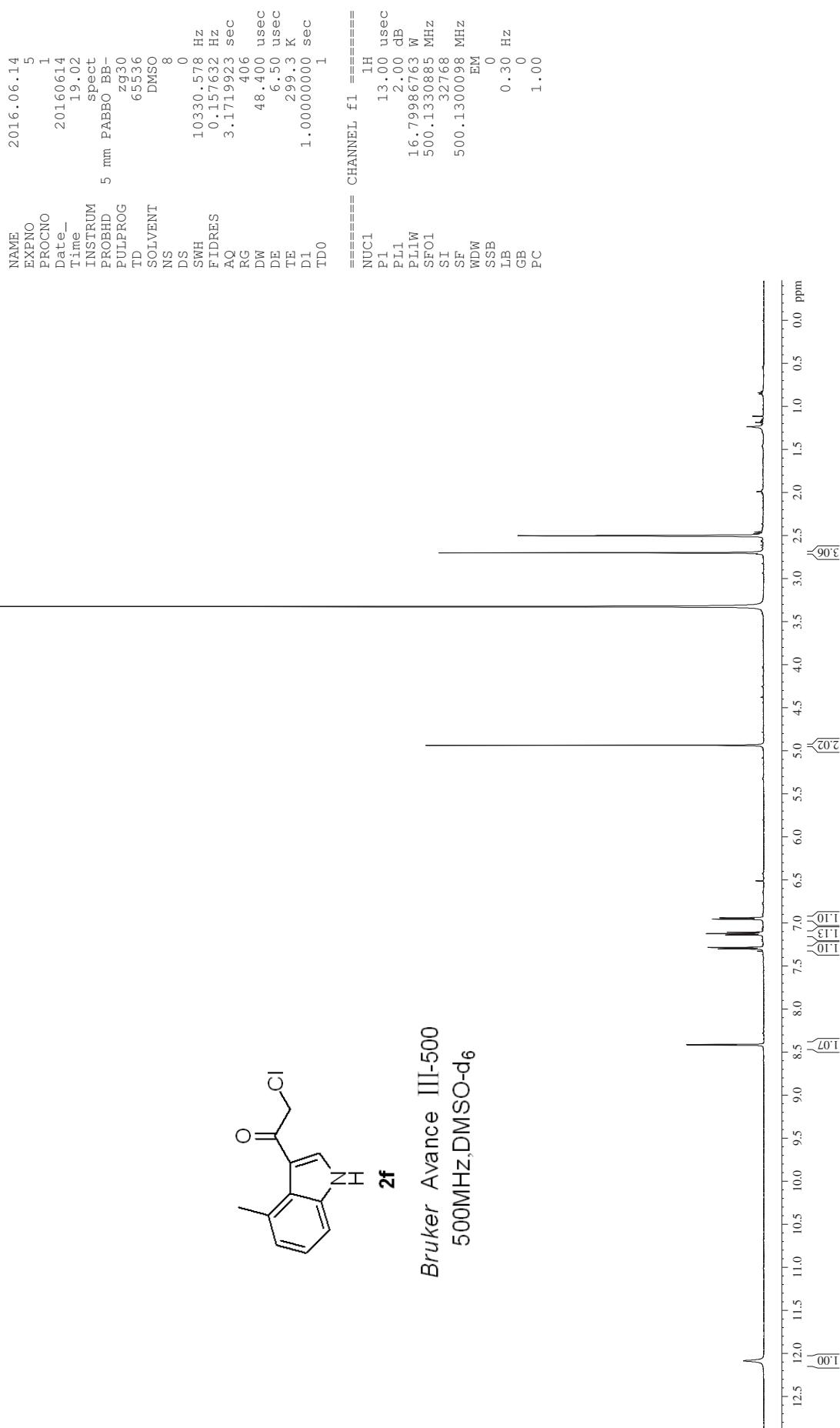
2016.05.24  
 5  
 EXPNO  
 PROCNO  
 Date\_ 1  
 Time 20160524  
 INSTRUM 7.52  
 spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zppg30  
 TD 32768  
 SOLVENT DMSO  
 NS 1024

DS 0  
 SWH 29761.904 Hz  
 FIDRES 0.908261 Hz  
 AQ 0.5505524 sec  
 RG 2050  
 DW 16.800 usec  
 DE 6.50 usec  
 TE 299.8 K  
 D1 2.0000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 ======  
 NUC1 13C  
 P1 12.30 usec  
 PLL 4.50 dB  
 PLLW 33.60015869 W  
 SFO1 125.7703643 MHz

===== CHANNEL f2 ======  
 CPDPRG2 Waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL12 2.00 dB  
 PL12 17.78 dB  
 PL13 17.78 dB  
 PL2W 16.79986763 W  
 PL12W 0.44392112 W  
 PL13W 0.44392112 W  
 SFO2 500.1320005 MHz  
 SI 32768  
 SF 125.7578524 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40





— 185.55  
 — 137.53  
 — 131.57  
 — 124.00  
 — 123.70  
 — 115.15  
 — 109.84  
 — 47.83  
 — 40.02  
 — 39.85  
 — 39.69  
 — 39.52  
 — 39.35  
 — 39.19  
 — 39.02  
 — 39.02  
 — 39.02  
 — 39.02  
 — 39.02  
 — 39.02  
 — 22.49



```

=====
NAME          2016.06.14
EXPNO         9
PROCNO        1
Date_         20160614
Time          20.50
INSTRUM       spect
PROBHD       5 mm PABBO BB-
PULPROG      zgpp930
TD            32768
SOLVENT       DMSO
NS            1507
DS            0
SWH           29761.904 Hz
FIDRES       0.908261 Hz
AQ            0.5505524 sec
RG            2050
DW            16.800 usec
DE            6.500 usec
TE            301.2 K
D1            2.0000000 sec
D11           0.03000000 sec
TD0            1

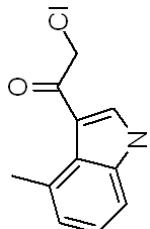
=====
```

```

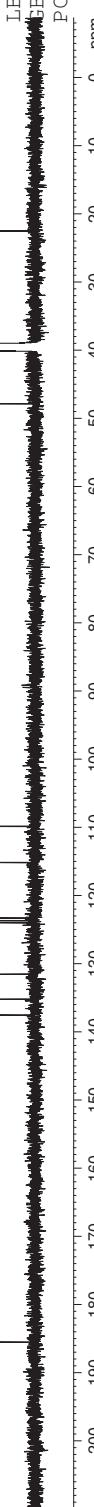
===== CHANNEL f1 =====
NUC1          13C
P1            12.30 usec
PL1           4.50 dB
PLLW          33.60015869 W
SFO1          125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2      Waltz16
NUC2          1H
PCPD2         80.00 usec
PL12          2.00 dB
PL12          17.78 dB
PL13          17.78 dB
PL2W          16.79986763 W
PL12W         0.44392112 W
PL13W         0.44392112 W
SFO2          500.1320005 MHz
SI             32768
SF            125.7578535 MHz
WDW           0
SSB           1.00 Hz
LB            0
PC            1.40

=====
```

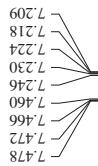


**2f**  
*Bruker Avance III-500*  
*125MHz, DMSO-d<sub>6</sub>*





— 4.957 —

8.480  
8.474

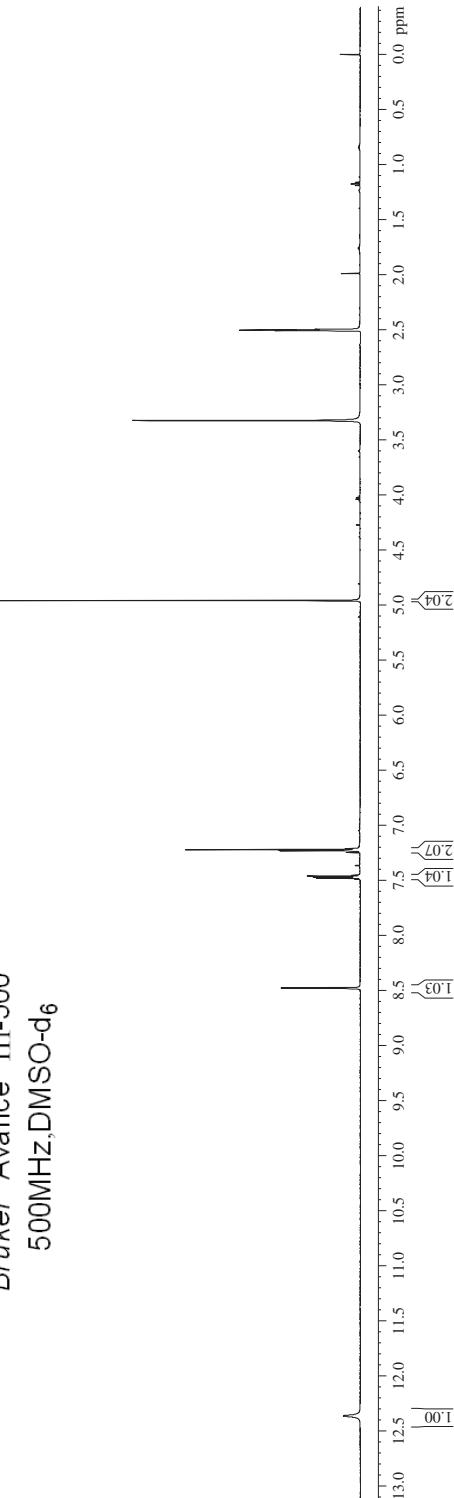
— 12.357 —

```

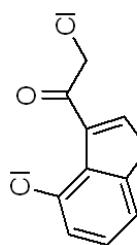
NAME          2016.05.27
EXNO          27
PROCNO        1
Date_-
Time         21.49
INSTRUM      spect
PROBHD      5 mm PABBO BB-
PULPROG     zg30
TD           65536
SOLVENT      DMSO
NS            4
DS            0
SWH          10330.578 Hz
FIDRES       0.157632 Hz
AQ           3.1719923 sec
RG           322
DW           48.400 usec
DE           6.50 usec
TE           298.5 K
D1           1.00000000 sec
TDO          1

===== CHANNEL f1 =====
NUC1          1H
P1           13.00 usec
PL1          2.00 CB
PL1W        16.79386763 W
SF01        500.1330885 MHz
SI           32768
SF           500.1300104 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00

```



Bruker Avance III-500  
500MHz,DMSO-d<sub>6</sub>

**2g**

liushouxin-xh-4-cl-Cl

— 184.73 —

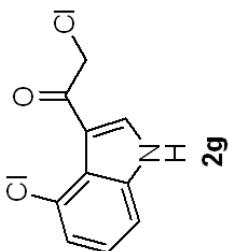
— 138.70 —  
/ \ 125.49  
|| 124.00  
/ \ 123.19  
|| 122.45  
/ \ 113.96  
|| 111.37

— 48.29 —  
/ \ 39.02  
|| 39.19  
/ \ 39.35  
|| 39.52  
/ \ 39.69  
|| 39.85  
/ \ 39.96  
|| 40.02

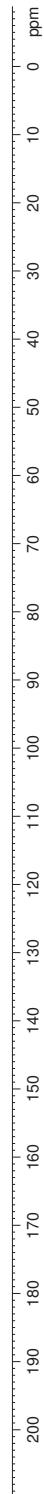


NAME 2016.05.27  
EXPNO 28  
PROCNO 1  
Date\_ 20160527  
Time 21.58  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgppg30  
TD 32768  
SOLVENT DMSO  
NS 266  
DS 0  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 0.5505524 sec  
RG 2050  
DW 16.800 usec  
DE 6.50 usec  
TE 299.9 K  
D1 2.0000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 12.30 usec  
PL1 4.50 dB  
PL1W 33.60015869 W  
SFO1 125.7703643 MHz  
===== CHANNEL f2 =====  
CPDPRG2 Waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL1 2.00 dB  
PL1.2 17.78 dB  
PL1.3 17.78 dB  
PL2W 16.79986763 W  
PL1.2W 0.44392112 W  
PL1.3W 0.44392112 W  
SFO2 500.1320005 MHz  
SI 32768  
SF 125.7578527 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



Bruker Avance III-500  
125MHz,DMSO-d<sub>6</sub>



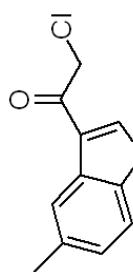
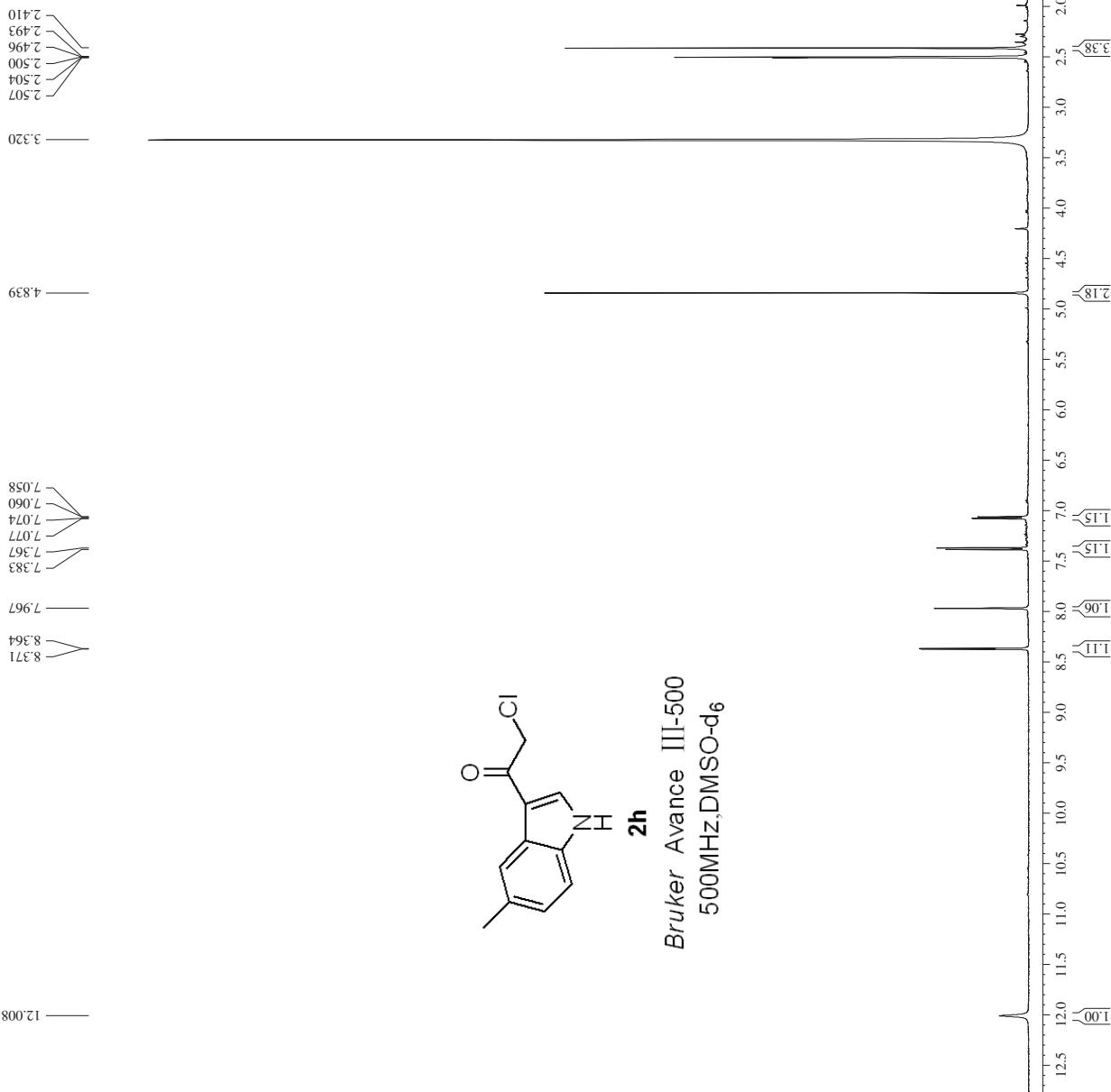
 BRUKER

```

EXPTIME 2016.06.14
EXPNO 7
PROCNO 1
Date 20160614
Time 19.28
INSTRUM spect
PAPBOD 5 mm
PAPLPROG 65536
DSOLVENT DMSO
NS 8
DS 0
SWH 10330.578
SFIDRES Hz
AQ 0.157632
RG 3.1719923
TD 406
DW 48.400
DE 6.50
TE 299.4
D1 1.00000000
TDDO 1

=====
CHANNEL f1 =====
NUC1 1H
P1 13.00 usec
PL1 2.00 dB
PPL1 16.79986763
P1W SF01 500.1330885 MHz
SI ST 32768
SF WWDW 500.1300098 MHz
SSB LB EM
GB PC
PC

```



**2h**  
*Bruker Avance III-500*  
500MHz,DMSO-d<sub>6</sub>

186.00  
134.90  
130.67  
125.65  
124.61  
120.85  
113.23  
111.92

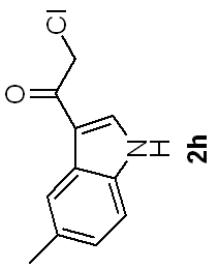
134.90  
130.67  
125.65  
124.61  
120.85  
113.23  
111.92

46.30  
40.02  
39.85  
39.69  
39.52  
39.35  
39.19  
39.02  
39.02

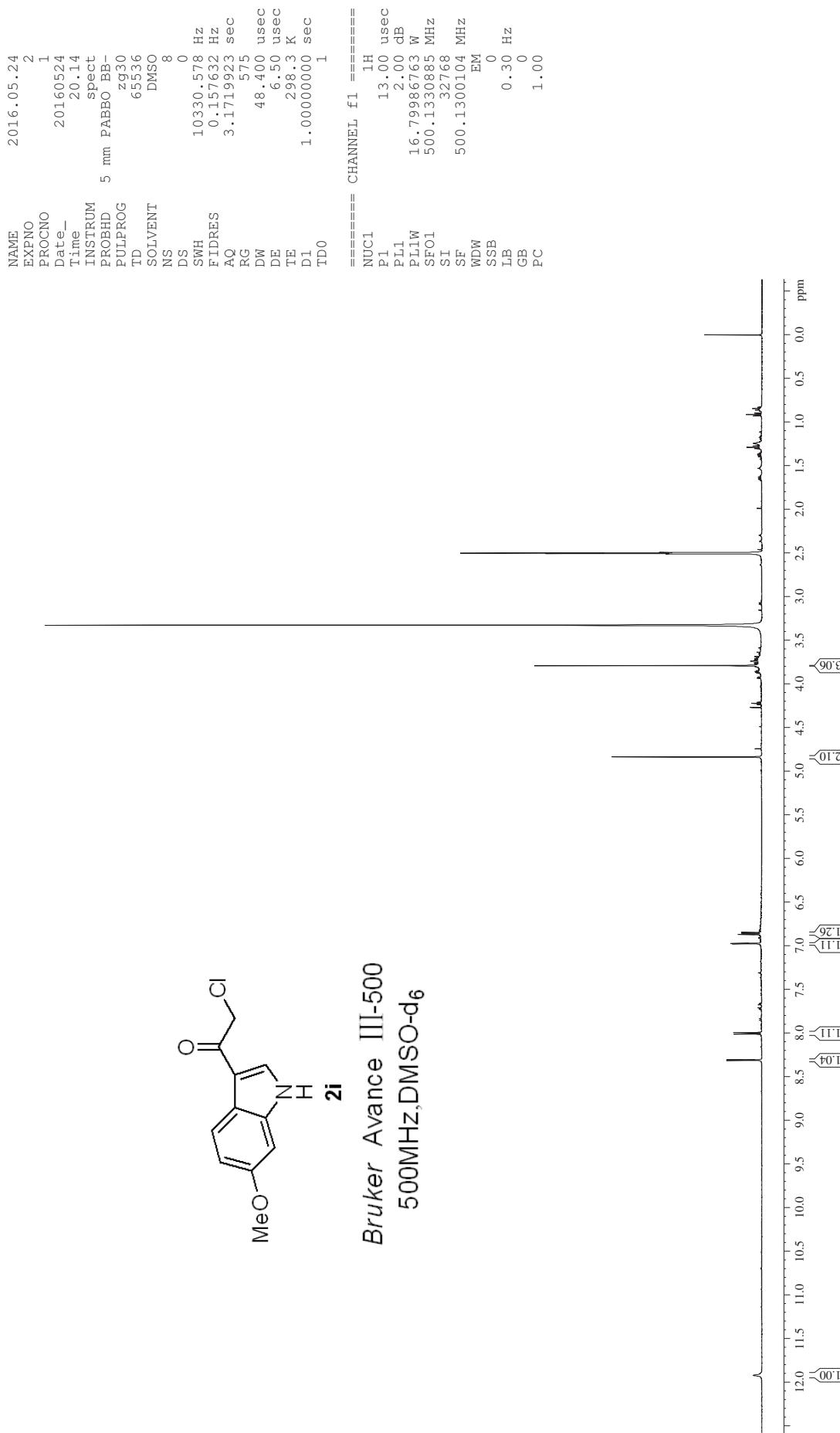


NAME 2016.06.14  
EXPNO 8  
PROCNO 1  
Date\_ 20160614  
Time 19.33  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgppg30  
TD 32768  
SOLVENT DMSO  
NS 1689  
DS 0  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 0.5505524 sec  
RG 2050  
DW 16.800 usec  
DE 6.50 usec  
TE 300.7 K  
D1 2.0000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 12.30 usec  
PL1 4.50 dB  
PL1W 33.60015869 W  
SFO1 125.7703643 MHz  
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL1 2.00 dB  
PL1.2 17.78 dB  
PL1.3 17.78 dB  
PL2W 16.79986763 W  
PL1.2W 0.44392112 W  
PL1.3W 0.44392112 W  
SFO2 500.1320005 MHz  
SI 32768  
SF 125.7578533 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
PC 0  
1.40



Bruker Avance III-500  
125MHz,DMSO-d<sub>6</sub>



liushouxin-xh-6

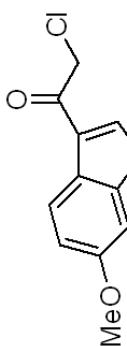
— 156.58 —  
— 137.54 —  
— 133.79 —  
— 121.74 —  
— 119.28 —  
— 111.87 —  
— 95.33 —

55.23  
46.19  
40.02  
39.85  
39.69  
39.52  
39.35  
39.19  
39.02  
39.02

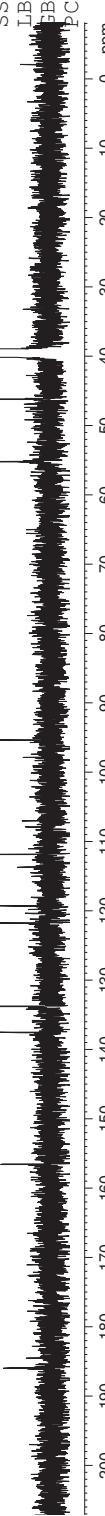


NAME 2016.05.24  
EXPNO 21  
PROCNO 1  
Date\_ 20160524  
Time 20.46  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpp930  
TD 32768  
SOLVENT DMSO  
NS 8192  
DS 0  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 0.5505524 sec  
RG 2050  
DW 16.800 usec  
DE 6.50 usec  
TE 300.1 K  
D1 2.0000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 12.30 usec  
PL1 4.50 dB  
PL1W 33.60015869 W  
SFO1 125.7703643 MHz  
===== CHANNEL f2 =====  
CPDPRG2 Waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL1 2.00 dB  
PL1.2 17.78 dB  
PL1.3 17.78 dB  
PL2W 16.79986763 W  
PL1.2W 0.44392112 W  
PL1.3W 0.44392112 W  
SFO2 500.1320005 MHz  
SI 32768  
SF 125.7578528 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
QB 0  
PC 1.40



**2i**  
*Bruker Avance III-500*  
**125MHz,DMSO-d<sub>6</sub>**





1306

2.371  
2.497  
2.500  
2.503

3.327

6.842  
6.856  
7.046  
7.062  
7.076  
7.263  
7.279  
7.928  
7.933

11.591

```

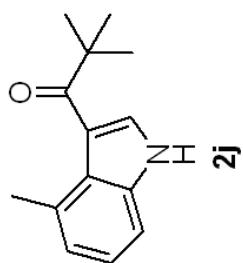
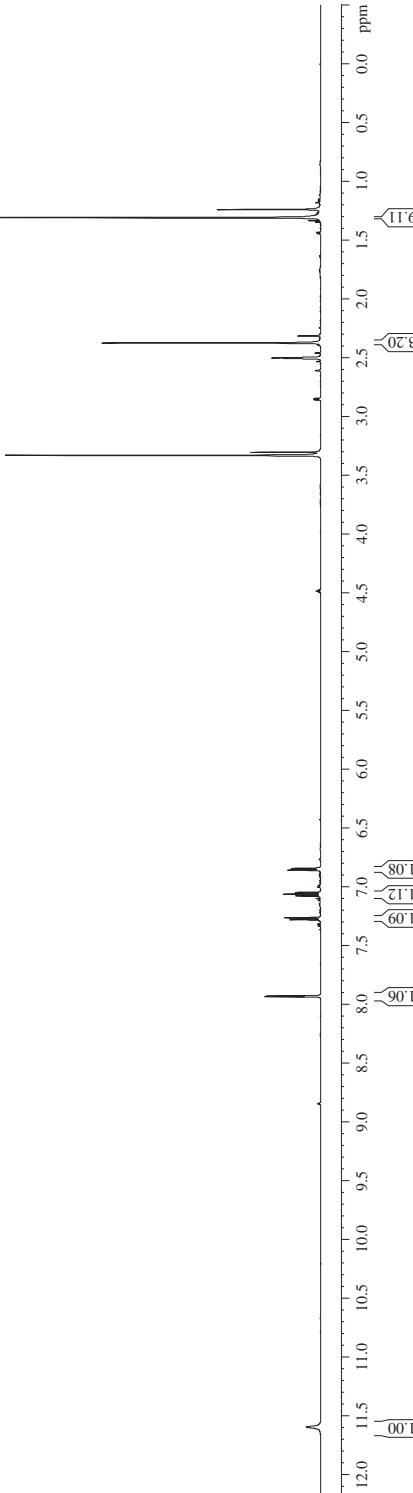
NAME          2016.06.14
EXN0          1
PROCNO       1
Date_        20160614
Time         22.06
INSTRUM     spect
PROBHD      5 mm PABBO BB-
PULPROG    zg30
TD           65536
SOLVENT      DMSO
NS            2
DS            0
SWH          10330.578 Hz
FIDRES     0.157632 Hz
AQ           3.1719923 sec
RG           203
DW           48.400 usec
DE           6.50 usec
TE           299.7 K
D1          1.00000000 sec
TDO          1

```

```

===== CHANNEL f1 =====
NUC1          1H
P1            13.00 usec
PL1           2.00 CB
PL1W        16.79386763 W
SF01         500.1330885 MHz
SI            322768
SF           500.1300096 MHz
WDW           EM
SSB           0
LB           0.30 Hz
GB           0
PC           1.00

```



Bruker Avance III-500  
500MHz,DMSO-d<sub>6</sub>

lijushouxin-xh-4-ch3

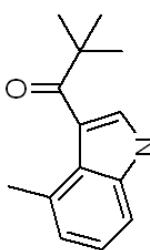
204.44  
136.07  
130.64  
128.23  
125.29  
122.30  
122.28  
115.41  
109.49

40.00  
39.85  
39.69  
39.52  
39.35  
39.19  
39.02  
39.00  
28.14  
21.29

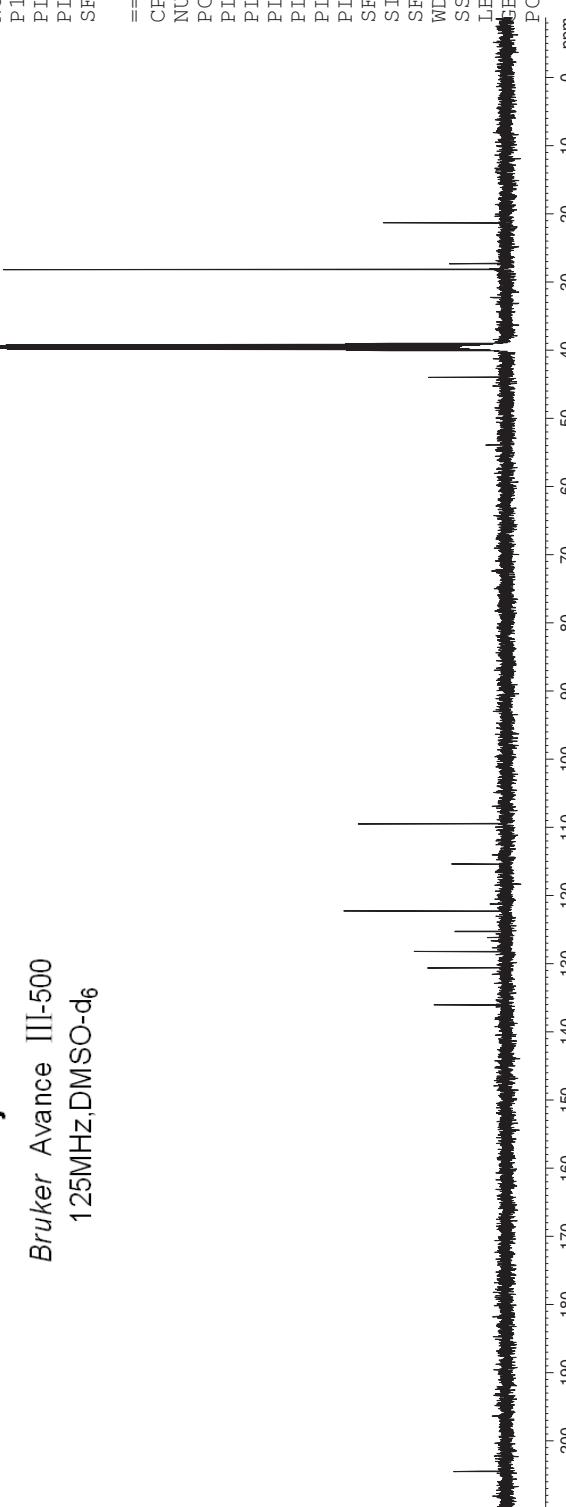


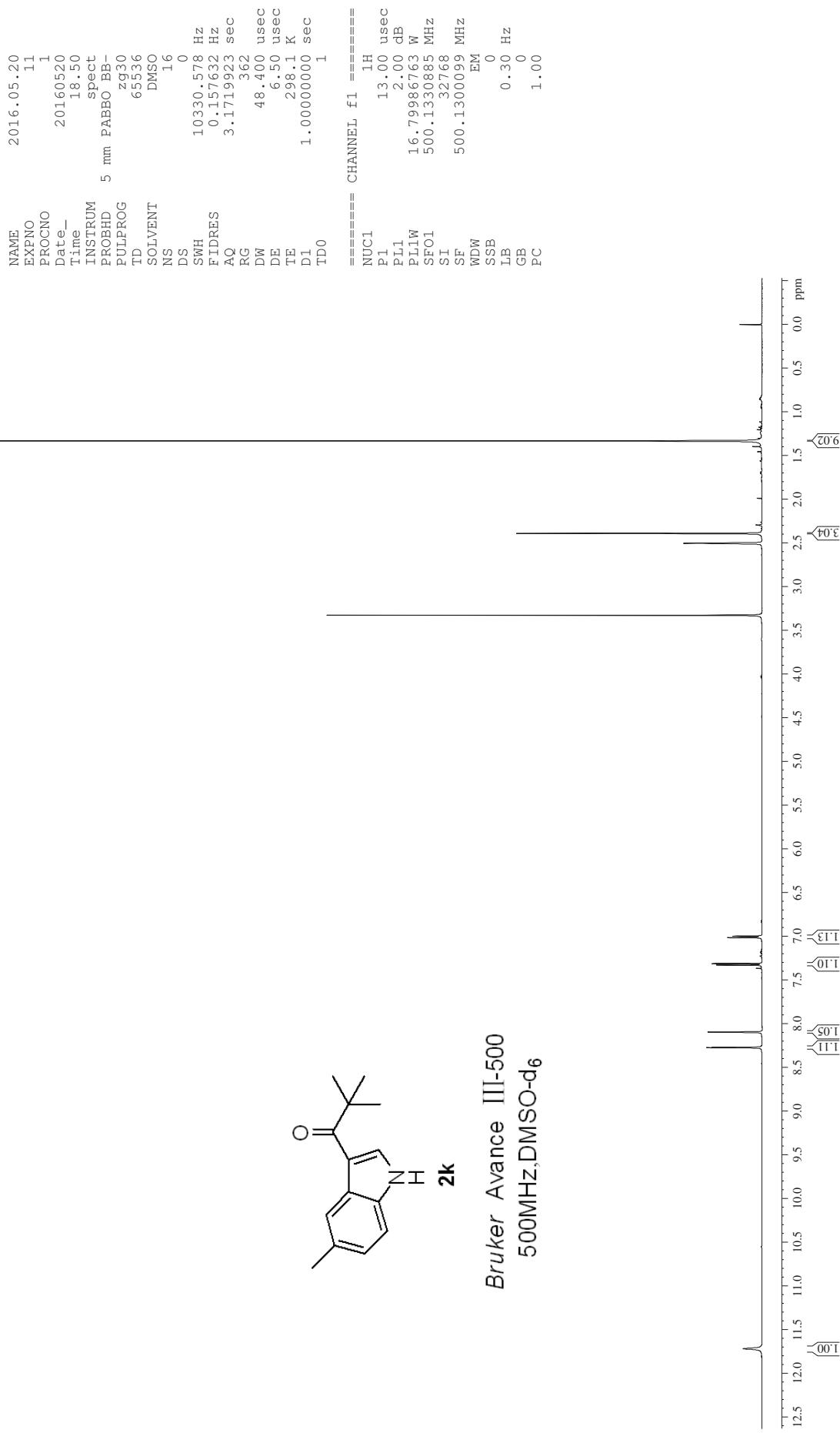
NAME 2016.06.14  
EXPNO 11  
PROCNO 1  
Date\_ 20160614  
Time 22.13  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgppg30  
TD 32768  
SOLVENT DMSO  
NS 100  
DS 0  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 0.5505524 sec  
RG 2050  
DW 16.800 usec  
DE 6.50 usec  
TE 301.2 K  
D1 2.0000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 12.30 usec  
PL1 4.50 dB  
PL1W 33.60015869 W  
SFO1 125.7703643 MHz  
===== CHANNEL f2 =====  
CPDPRG2 Waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL1 2.00 dB  
PL1.2 17.78 dB  
PL1.3 17.78 dB  
PL2W 16.79986763 W  
PL1.2W 0.44392112 W  
PL1.3W 0.44392112 W  
SFO2 500.1320005 MHz  
SI 32768  
SF 125.7578525 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
SB 0  
PC 1.40



**2j**  
*Bruker Avance III-500*  
125MHz,DMSO-d<sub>6</sub>





liushouxin-xh-5-te

201.05  
133.95  
132.31  
130.08  
127.46  
123.91  
121.81  
111.31  
111.88

43.33  
40.02  
39.52  
39.69  
39.52  
39.19  
39.22  
28.62  
21.36



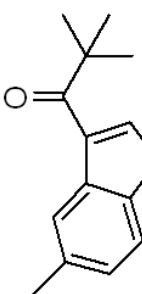
2016.05.20  
12  
1  
20160520  
18.58  
spect  
spec

INSTRUM  
PROBHD  
PULPROG  
TD  
SOLVENT  
NS  
DS  
SWH  
FIDRES  
AQ  
RG  
DW  
DE  
TE  
D1  
D11  
TD0

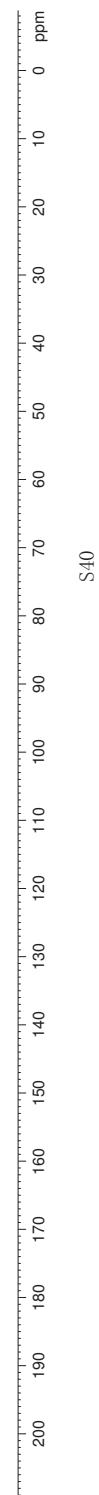
5 mm PABBO BB-  
zgpp30  
32768  
DMSO  
1225  
0  
29761.904 Hz  
0.908261 Hz  
0.5505524 sec  
2050  
16.800 usec  
6.50 usec  
299.6 K  
2.0000000 sec  
0.03000000 sec  
1

===== CHANNEL f1 ======  
NUC1  
P1  
PLL  
PLLW  
SFO1  
===== CHANNEL f2 ======  
Waltz16  
1H  
80.00 usec  
2.00 dB  
17.78 dB  
17.78 dB  
16.79986763 W  
0.44392112 W  
0.44392112 W  
500.1320005 MHz  
32768  
125.7578532 MHz  
EM

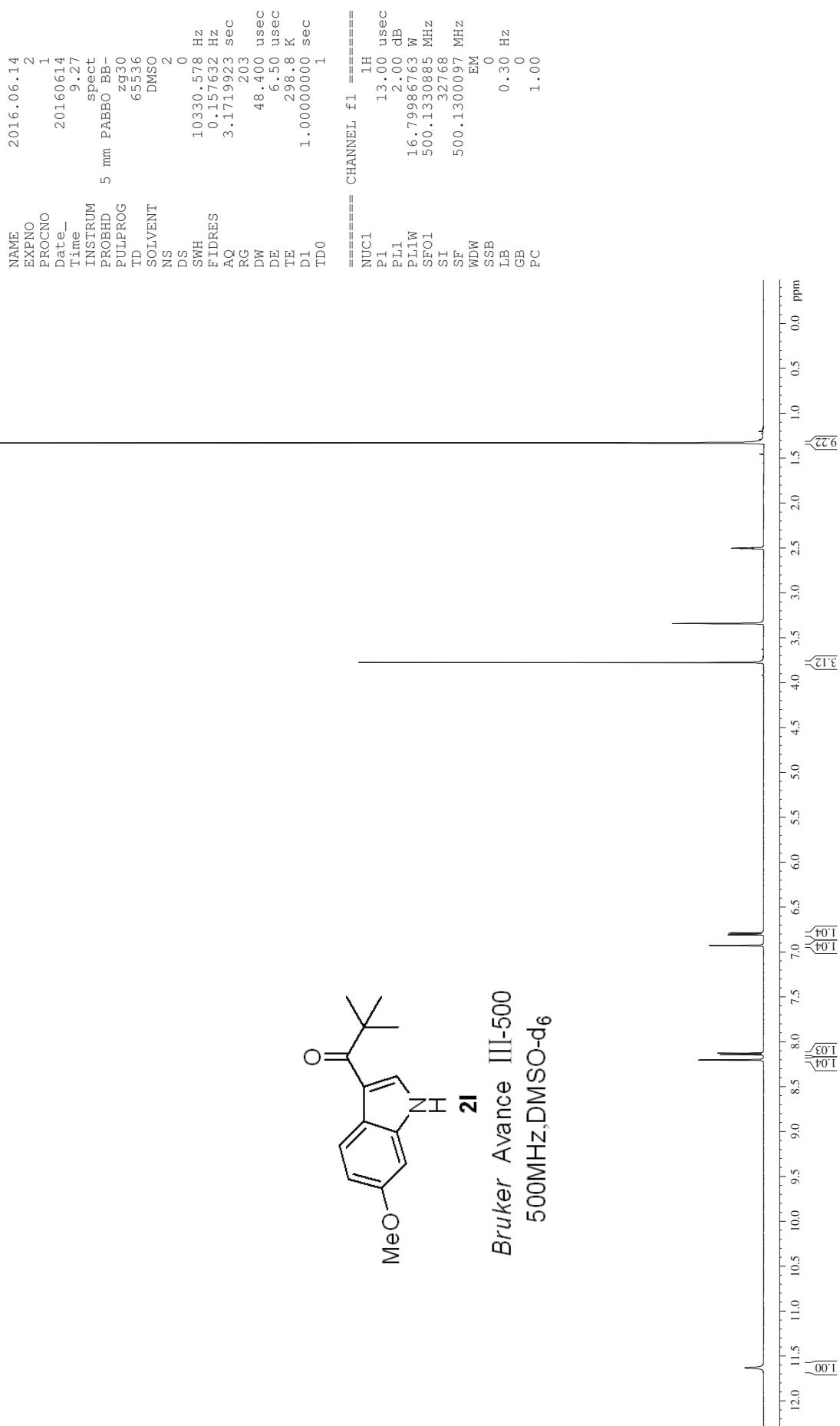
Bruker Avance III-500  
125MHz,DMSO-d<sub>6</sub>



**2k**

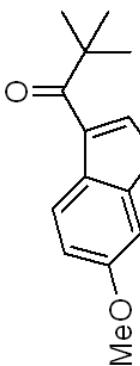
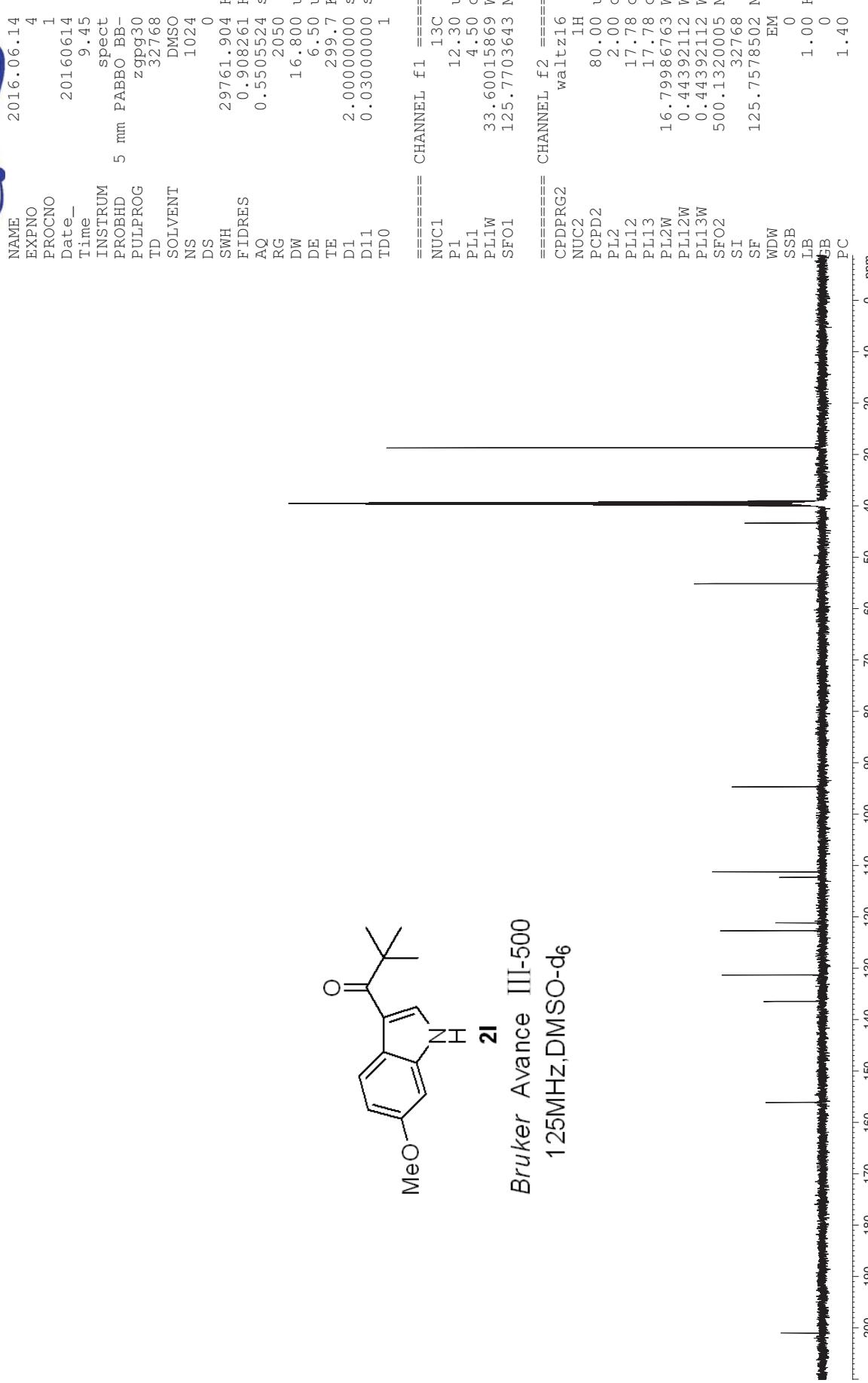


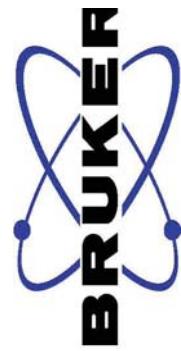
S40





liushouxin-xh-6-ome  
201.06  
156.16  
136.48  
131.35  
122.72  
121.20  
112.32  
111.25  
94.72





2.527  
2.524  
2.520  
2.517  
2.513

8.292  
8.279  
8.276  
7.957  
7.950  
7.895  
7.891  
7.802  
7.623  
7.619  
7.611  
7.608  
7.606  
7.574  
7.559  
7.545  
7.543  
7.304  
7.301  
7.290  
7.287  
7.275  
7.272  
7.266  
7.258

12.089

```

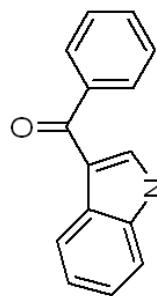
NAME          2016.04.14
EXNO          19
PROCNO        1
Date_-
Time          20.52
INSTRUM      spect
PROBHD       5 mm PABBO BB-
PULPROG      zg30
TD           65536
SOLVENT       DMSO
NS            16
DS             0
SWH          10330.578 Hz
FIDRES       0.157632 Hz
AQ            3.1719923 sec
RG            161
DW           48.400 usec
DE            6.50 usec
TE            298.0 K
D1           1.00000000 sec
TDO          1

```

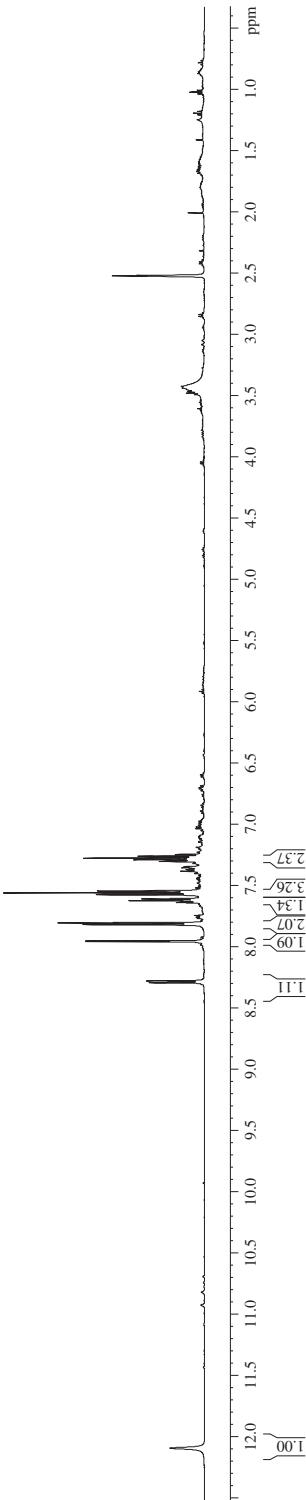
```

===== CHANNEL f1 =====
NUC1          1H
P1            13.00 usec
PL1           2.00 CB
PL1W          16.79386763 W
SF01          500.1330885 MHz
SI             32768
SF            500.1300001 MHz
WDW           EM
SSB            0
LB            0.30 Hz
GB            0
PC            1.00

```

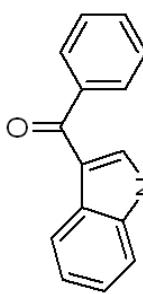


**2m**  
*Bruker Avance III-500*  
 500MHz,DMSO-d<sub>6</sub>



liu shou xin-xh-c  
189.69

140.53  
136.71  
135.77  
131.03  
128.38  
128.36  
126.24  
123.12  
121.46  
121.49  
114.99  
112.24



Bruker Avance III-500  
125MHz, DMSO-d<sub>6</sub>



```

=====
NAME          2016.03.09
EXPNO
PROCNO        1
Date_         20160309
Time         19.59
INSTRUM
PROBHD      5 mm PABBO BB-
PULPROG    zgppg30
TD           36864
SOLVENT      DMSO
NS            410
DS             0
SWH         29761.904 Hz
FIDRES     0.807343 Hz
AQ           0.6193652 sec
RG            2050
RGD
DW           16.800 usec
DE           6.500 usec
TE           298.0 K
D1           2.0000000 sec
D11          0.03000000 sec
TD0            1

=====
CHANNEL f1
NUC1          13C
P1            12.30 usec
PL1
PLL          33.60015869 W
SFO1        125.7703643 MHz

=====
CHANNEL f2
OPDPRG2      Waltz16
NUC2          1H
PCPD2
PL2           80.00 usec
PL1.2        2.00 dB
PL1.3        17.78 dB
PL1.2W       17.78 dB
PL1.3W       16.79986763 W
PL1.2W       0.44392112 W
PL1.3W       0.44392112 W
SFO2        500.1320005 MHz
SI            32768
SF           125.7578508 MHz
WDW
SSB
LB           0.0 Hz
QB
PC

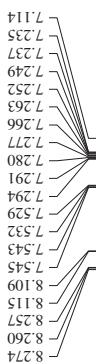
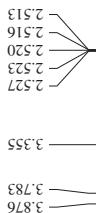
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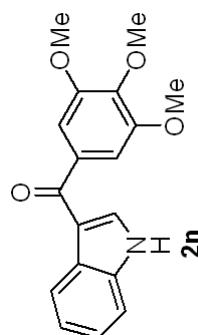
```

NAME          2016.04.13
EXNO          13
PROCNO        1
Date_-
Time         20160413
19.15
INSTRUM      spect
PROBHD       5 mm PABBO BB-
PULPROG     zg30
TD           65536
SOLVENT      DMSO
NS            8
DS            0
SWH          10330.578 Hz
FIDRES       0.157632 Hz
AQ           3.1719923 sec
RG            228
DW           48.400 usec
DE           6.50 usec
TE           298.0 K
D1          1.00000000 sec
TDO0
===== CHANNEL f1 =====
NUC1          1H
P1            13.00 usec
PL1           2.00 CB
PL1W          16.79386763 W
SF01          500.1330885 MHz
SI             322768
SF            500.1300004 MHz
WDW
SSB
LB            0.30 Hz
GB            0
PC            1.00

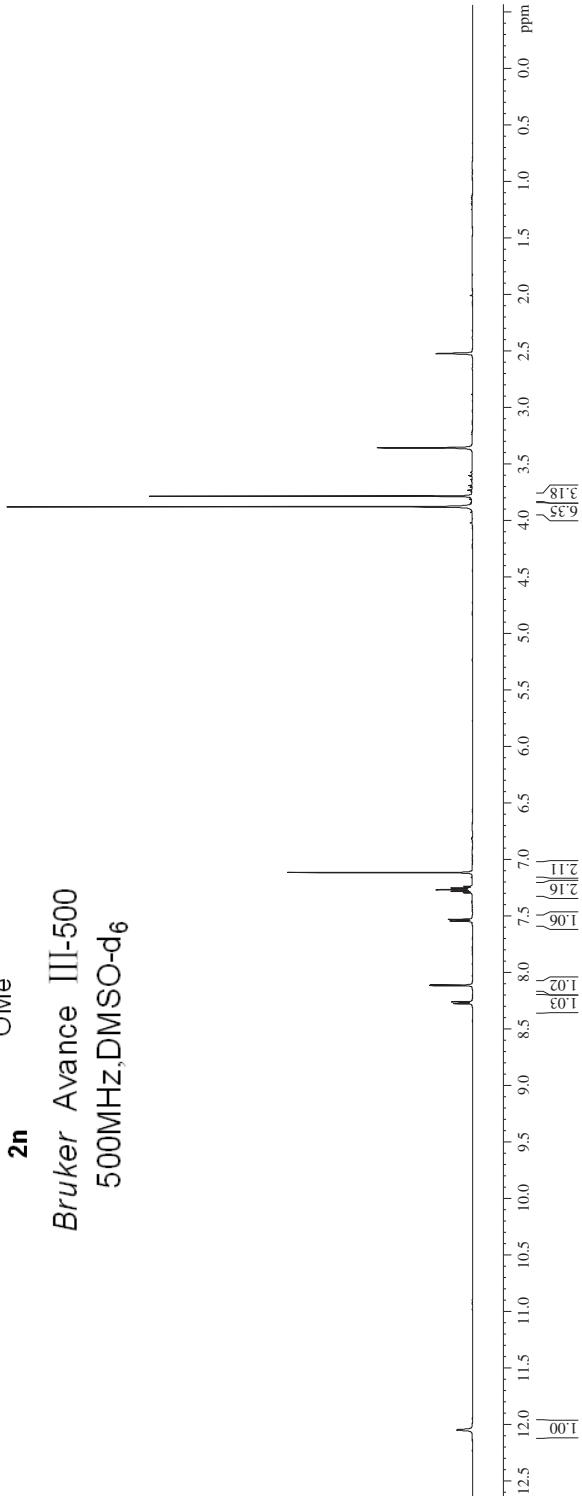
```



12.041



*Bruker Avance III-500*  
*500MHz,DMSO-d<sub>6</sub>*



liushouxin-xh-1-c

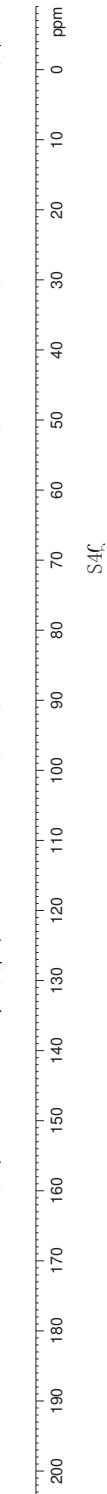


140.02  
136.70  
135.78  
135.58  
126.40  
123.06  
121.80  
121.44  
114.84  
112.17  
106.04

60.09  
55.96  
40.02  
39.85  
39.69  
39.52  
39.35  
39.19  
39.02

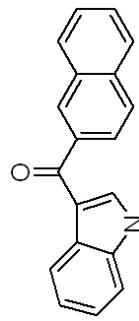
**BRUKER**

NAME 2016.04.13  
EXPNO 14  
PROCNO 1  
Date\_ 20160413  
Time 19.23  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgppg30  
TD 32768  
SOLVENT DMSO  
NS 135  
DS 0  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 0.5505524 sec  
RG 2050  
DW 16.800 usec  
DE 6.50 usec  
TE 298.0 K  
D1 2.0000000 sec  
D11 0.03000000 sec  
TD0 1  
===== CHANNEL f1 =====  
NUC1 13C  
P1 12.30 usec  
PL1 4.50 dB  
PL1W 33.60015869 W  
SF01 125.7703643 MHz  
===== CHANNEL f2 =====  
CPDPRG2 1H  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.00 dB  
PL1.2 17.78 dB  
PL1.3 17.78 dB  
PL2W 16.79986763 W  
PL1.2W 0.44392112 W  
PL1.3W 0.44392112 W  
SF02 500.1320005 MHz  
SI 32768  
SF 125.7578502 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





7.676  
7.662  
7.609  
7.533  
7.518  
7.516  
7.513  
7.502  
7.499  
7.497  
7.486  
7.483  
7.469  
7.452  
7.446  
7.440  
7.434  
7.364  
7.362  
7.360  
7.349  
7.346  
7.344  
7.373  
7.376  
7.379  
7.362  
7.349  
7.346  
7.260

**2o**

*Bruker Avance III-500*  
500MHz, CDCl<sub>3</sub>

```

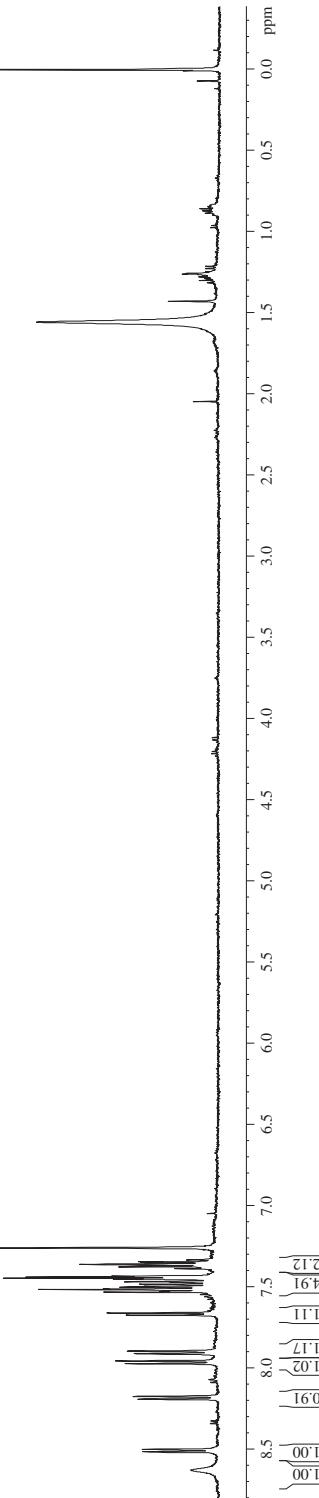
=====
NAME          2016.04.01
EXNO          12
PROCNO        1
Date_-
Time         16.53
INSTRUM      spect
PROBHD      5 mm PABBO BB-
PULPROG     zg30
TD           36864
SOLVENT      CDCl3
NS            8
DS           0
SWH          10330.578 Hz
FIDRES       0.28035 Hz
AQ           1.7842675 sec
RG           645
DW           48.400 usec
DE           6.50 usec
TE           298.0 K
D1           1.0000000 sec
TDO          1

```

```

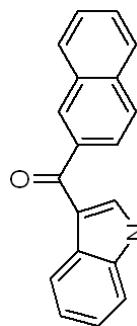
===== CHANNEL f1 =====
NUC1          1H
P1           13.00 usec
PL1          2.00 CB
PL1W        16.79386763 W
SF01        500.1323506 MHz
SI           32768
SF          500.1300231 MHz
WDW          EM
SSB          0
LB          0.30 Hz
GB          0
PC          1.00

```



138.82  
134.75  
136.51  
133.77  
134.77  
136.51  
130.77  
133.77  
130.77  
128.21  
126.86  
126.34  
126.02  
125.96  
124.52  
123.05  
124.15  
122.74  
121.40

77.28  
77.03  
76.78



**2o**  
*Bruker Avance III-500*  
125MHz, CDCl<sub>3</sub>



0.02

```

=====
NAME          2016.04.01
EXPNO         13
PROCNO        1
Date_        20160401
Time       20.29
INSTRUM      spect
PROBHD      5 mm PABBO BB-
PULPROG    zgpp930
TD        32768
SOLVENT      CDC13
NS         12288
DS           0
SWH       29761.904 Hz
FIDRES     0.508261 Hz
AQ        0.5505524 sec
RG          2050
DW        16.800 usec
DE        6.500 usec
TE        298.0 K
D1        2.0000000 sec
D11       0.03000000 sec
TD0          1

=====
CHANNEL f1
NUC1            13C
P1             12.30 usec
PL1           4.50 dB
PLL1          33.60015869 W
PLL1W         125.7703643 MHz

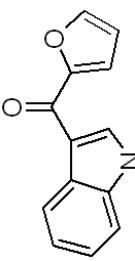
=====
CHANNEL f2
NUC2            1H
PCPD2          80.00 usec
PL12          2.00 dB
PLL12         17.78 dB
PLL13         17.78 dB
PLL2W         16.79986763 W
PLL12W        0.44392112 W
PLL13W        0.44392112 W
SFO2          500.1320005 MHz
SI              32768
SF          125.7577890 MHz
WDW           EM
SSB           0
LB           1.00 Hz
PC           0

```



liushouxin-xh

9.122  
8.555  
8.547  
8.539  
8.398  
8.392  
7.908  
7.449  
7.436  
7.432  
7.340  
7.325  
7.301  
7.287  
7.260  
7.257  
6.975  
6.978  
6.982



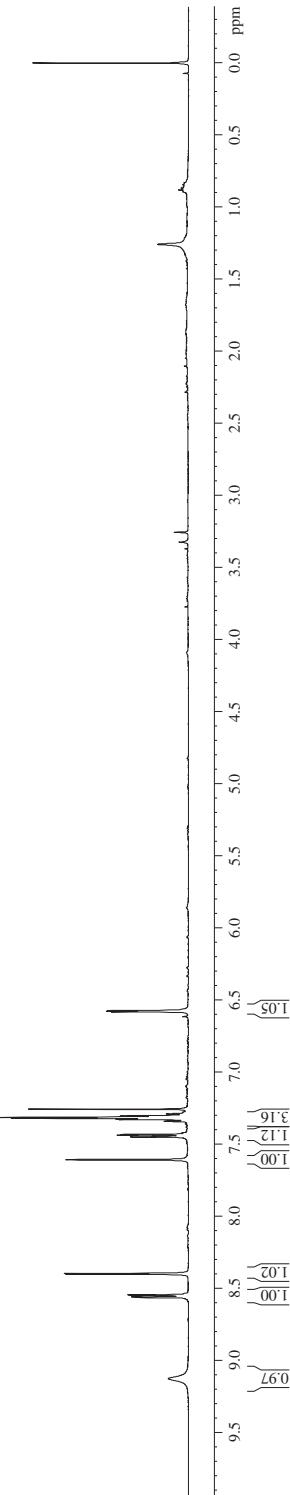
20

*Bruker Avance III-500*  
500MHz, CDCl<sub>3</sub>



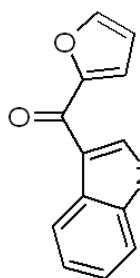
0.000 —

NAME	2016-03-12
EXPNO	1
PROCNO	1
Date_	20160312
Time	15.43
INSTRUM	spec
PROBHD	5 mm PABBO BB-
PULPROG	Zg30
TD	36864
SOLVENT	CDC13
NS	8
DS	0
SWH	10330.578 Hz
FIDRES	0.280235 Hz
AQ	1.7842675 sec
RG	362
DW	48.400 usec
DE	6.50 usec
TE	29.80 K
DD1	1.0000000 sec
TD0	1
===== CHANNEL f1 =====	
NUC1	1H
P1	13.00 usec
PL1	2.00 dB
PL1W	16.79986763 W
SFO1	500.1335009 MHz
ST1	32768
SF01	500.1300249 MHz
WDW	EM
SSB	0
LB	0.30 Hz
PC	0

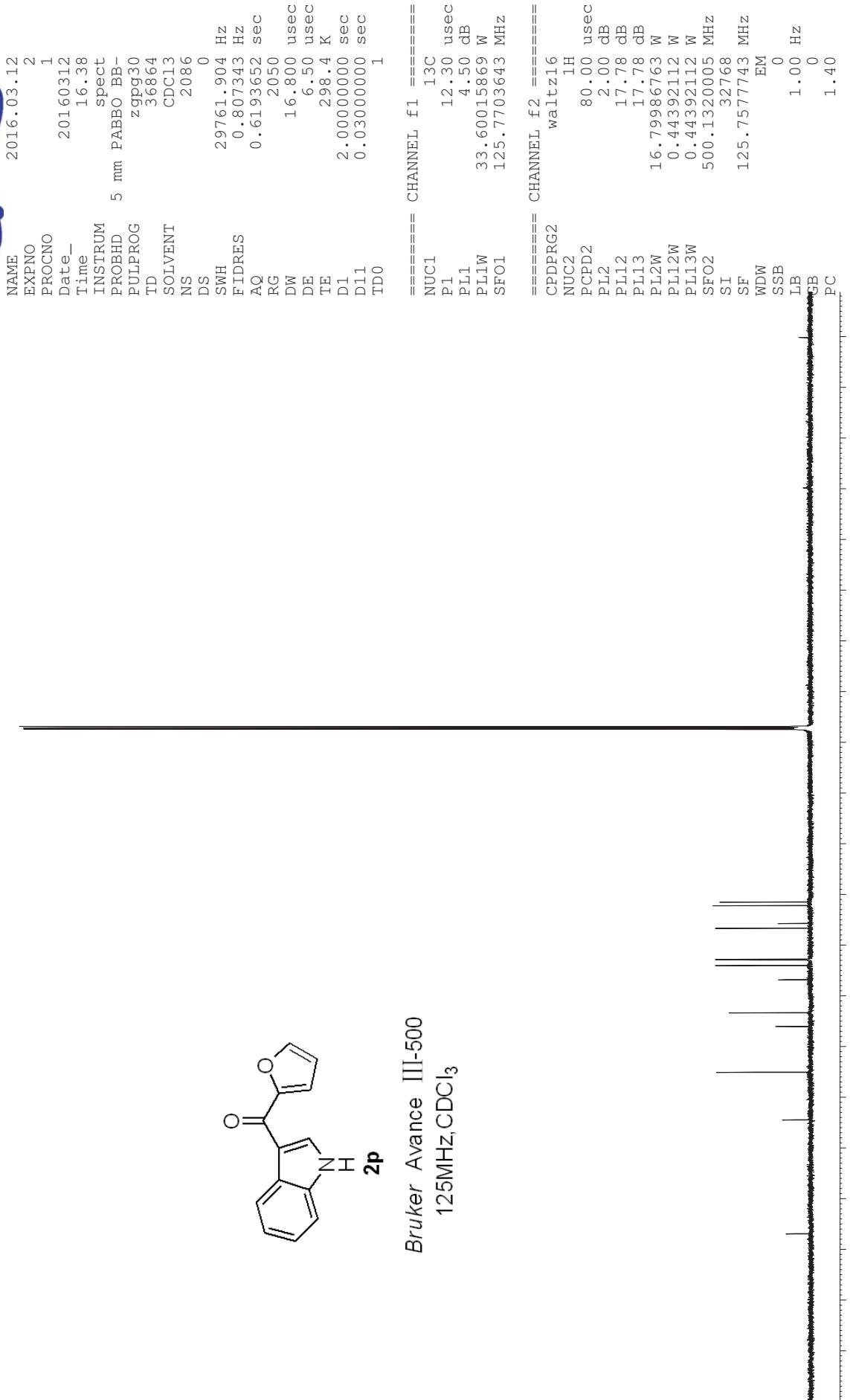




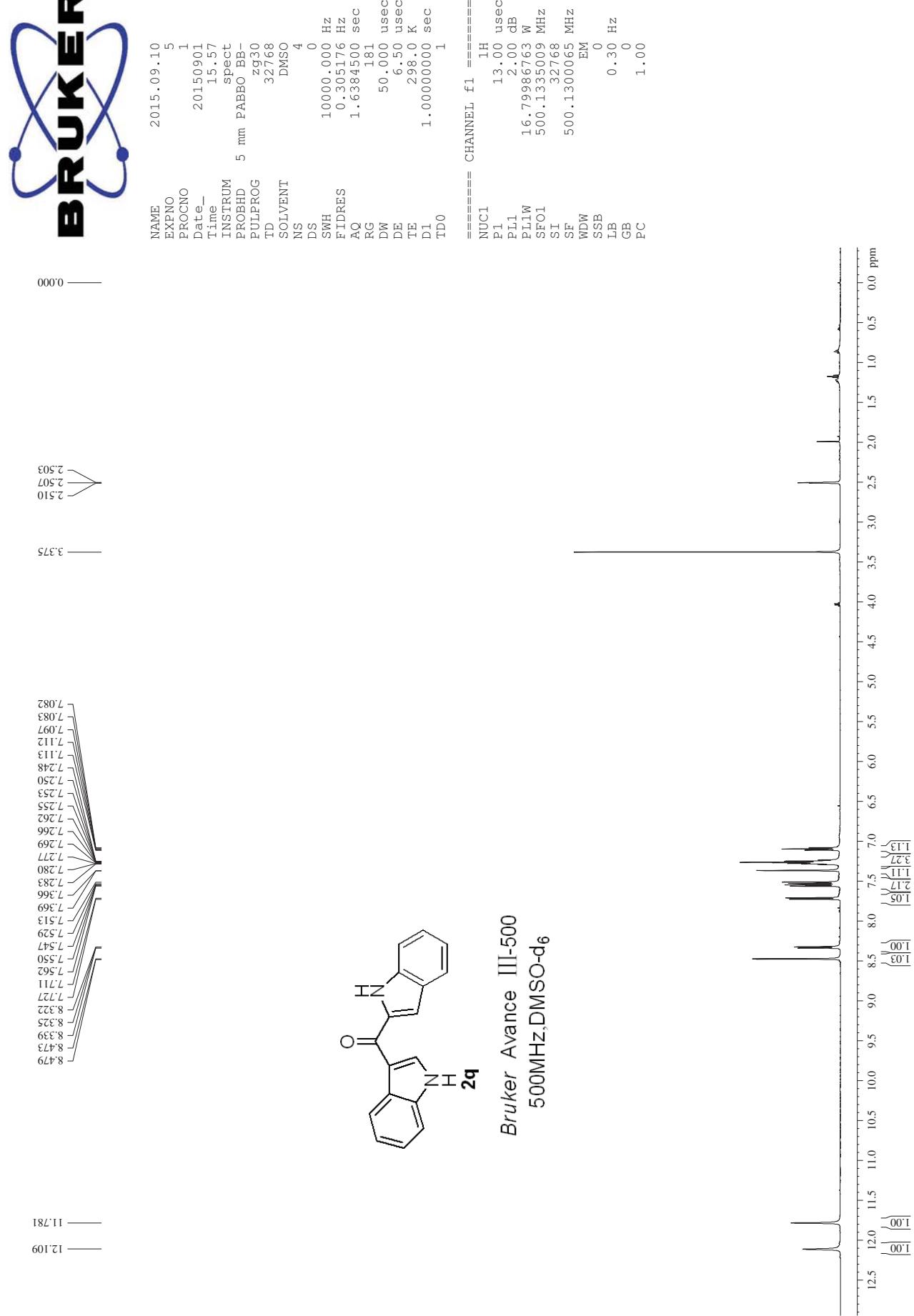
liushouxin-xh  
176.97  
154.50  
145.10  
136.06  
133.38  
126.85  
124.04  
122.93  
122.81  
116.70  
115.76  
112.23  
111.54  
77.41  
77.16  
76.91



**2p**  
Bruker Avance III-500  
125MHz, CDCl<sub>3</sub>



liushouxin-1h1-1



lishouxin-1h1-1

— 180.45 —

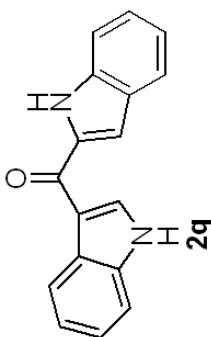
137.09  
136.27  
133.77  
127.34  
126.44  
124.29  
123.01  
122.24  
121.49  
119.91  
115.07  
112.48  
112.20  
107.19

39.85  
39.62  
39.52  
39.35  
39.19



NAME 2015.09.10  
EXPNO 1  
PROCNO 1  
Date\_ 20150901  
Time 19.02  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgppg30  
TD 16384  
SOLVENT DMSO  
NS 522  
DS 4  
SWH 29761.904 Hz  
FIDRES 1.816522 Hz  
AQ 0.2753012 sec  
RG 2050  
DW 16.800 usec  
DE 6.50 usec  
TE 298.7 K  
D1 2.0000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 12.30 usec  
PL1 4.50 dB  
PL1W 33.60015869 W  
SF01 125.7703643 MHz  
===== CHANNEL f2 =====  
CPDPRG2 Waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.00 dB  
PL1.2 17.78 dB  
PL1.3 17.78 dB  
PL2W 16.79986763 W  
PL1.2W 0.44392112 W  
PL1.3W 0.44392112 W  
SF02 500.1320005 MHz  
SI 32768  
SF 125.7578503 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



Bruker Avance III-500  
125MHz,DMSO-d<sub>6</sub>



**BRUKER**

```

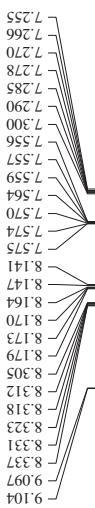
EXPTIME 2016.05.30
EXPNO 27
PROCNO 1
Date 20160530
Time 17.51
INSTRUM spect
PAPEROBJ BB-
PAPLPROG 5 mm PABBO
TD 2930
SOLVENT DMSO
NS 8
DS 0
SWH 10330.578 Hz
SFIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 362
DW 48.400 usec
DE 6.50 usec
TE 298.3 K
D1 1.00000000 sec
TDDO 1

=====
CHANNEL f1 =====
NUC1 1H
P1 13.00 usec
PL1 2.00 dB
PPL1 16.79986763 W
PL1W 500.1330885 MHz
SF01 SI 32768
SF02 SF 500.1300120 MHz
SF03 WDDW EM
SF04 SSSB 0 0.30 Hz
SF05 LB GB
SF06 PC
SF07 PC
SF08 PC

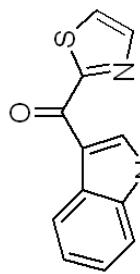
```



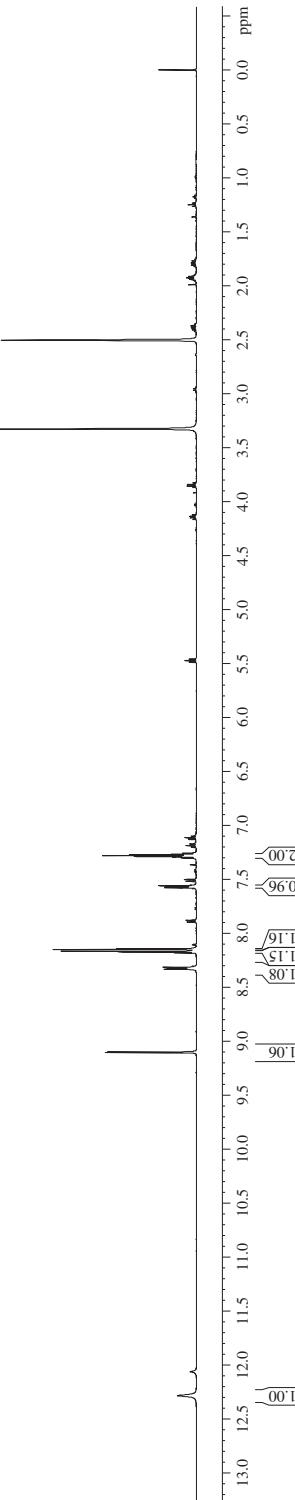
524



— 12.278

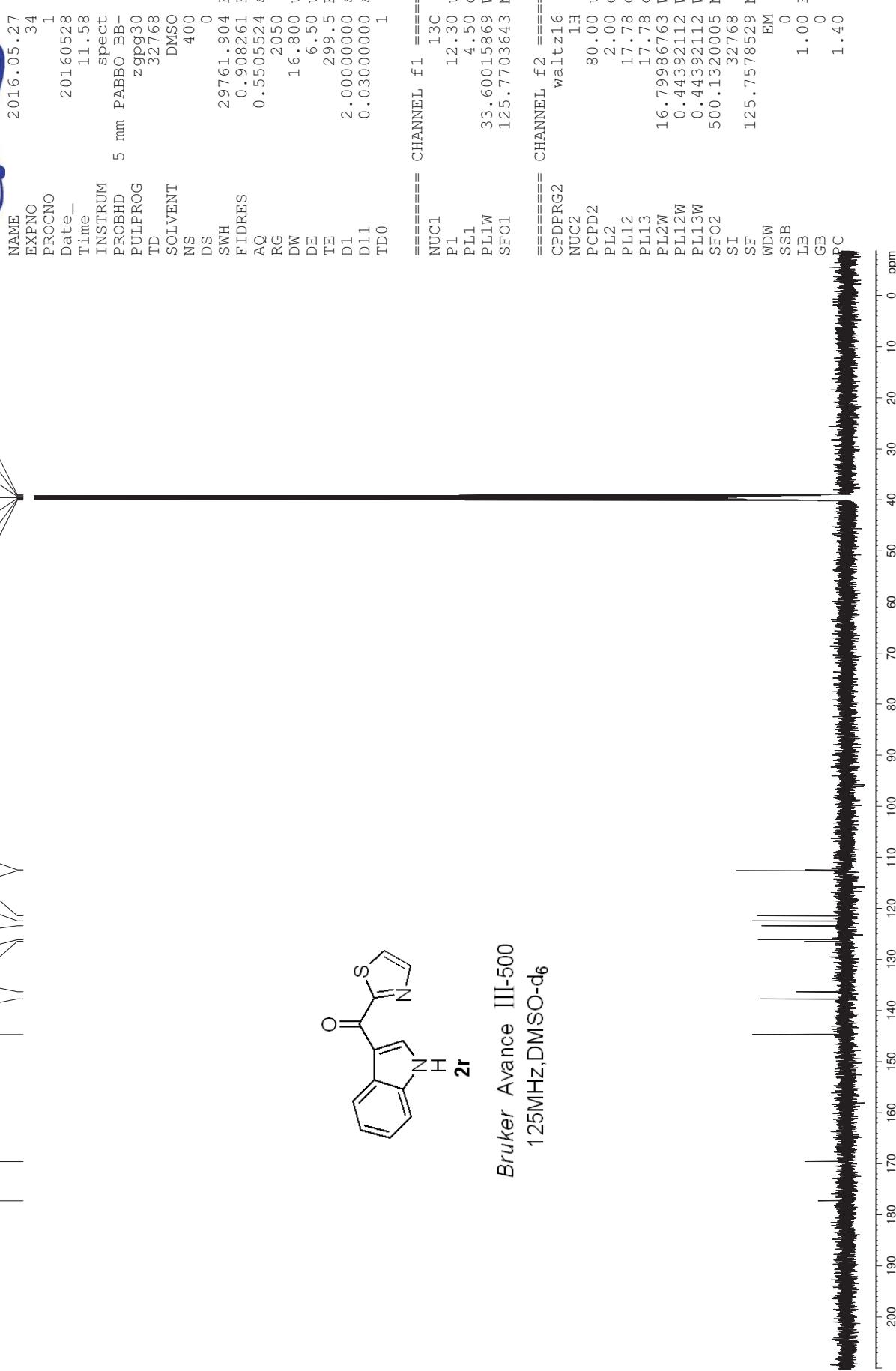


*Bruker Avance III-500*  
500MHz,DMSO-d<sub>6</sub>



liushouxin-xh-sai zuo

39.02  
39.19  
39.35  
39.52  
39.69  
39.85  
40.02



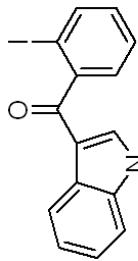
liushouxin-xh-2



NAME	2016.03.16
EXPRO	3
PROCNO	1
Date_	20160316
Time_	10.07
INSTRMD	
PABBO	
PROBID	5 mm
PULPROG	
TD	2930
SOLVENT	368864
INS	CDCL3
DS	8
SWH	0
FIDRES	10330.578 Hz
AQ	0.280235 Hz
RG	1.7842615 sec
DW	512
DE	48 - 400 usec
TE	6.50 usec
DI	298.0 K
TDDO	1.00000000 sec
	1
===== CHANNEL f1 =====	
NUC1	1H
P1	13.00 usec
PPL1	2.00 dB
PL1W	16.79986763 W
SFO1	500.1335009 MHz
SI	32768
SF	500.1300244 MHz
MWDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

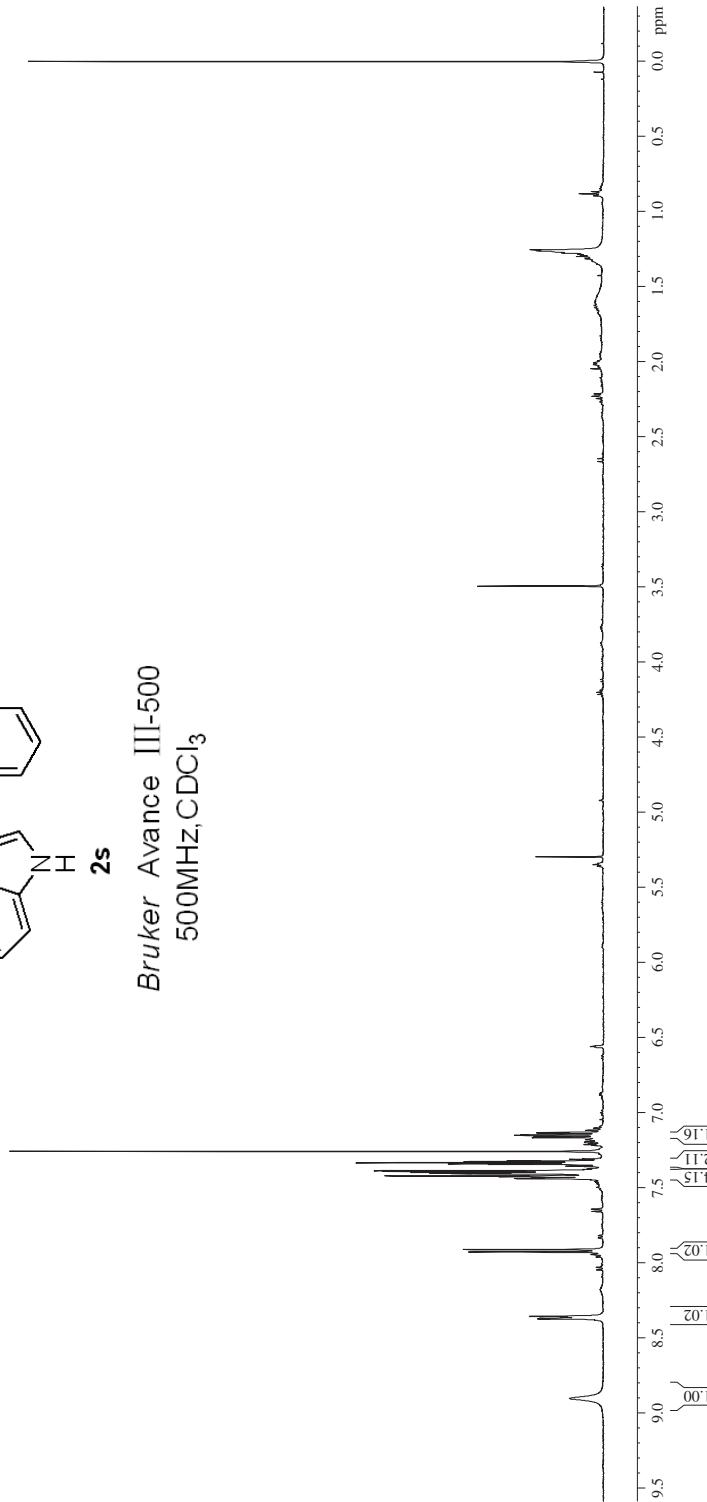
— 3.493 —

7,131  
7,136  
7,146  
7,147  
7,150  
7,151  
7,161  
7,166  
7,258  
7,261  
7,262  
7,265  
7,266  
7,333  
7,340  
7,345  
7,346  
7,349  
7,352  
7,358  
7,389  
7,392  
7,395  
7,396  
7,405  
7,407  
7,413  
7,421  
7,424  
7,426  
7,433  
7,439  
7,447  
7,459  
7,461  
7,472  
7,493  
7,527  
8,352



25

*Bruker Avance III-500*  
500MHz, CDCl<sub>3</sub>



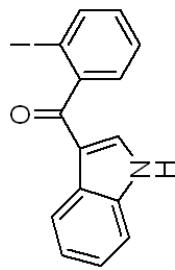
52

liu shou xin -xh-2

192.0<sup>o</sup>

146.15  
139.72  
136.67  
135.20  
130.64  
128.10  
127.72  
125.76  
124.23  
123.15  
122.59  
121.16  
111.57

92.56  
77.30  
77.04  
76.79

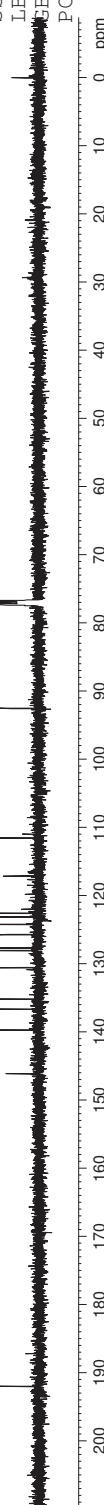


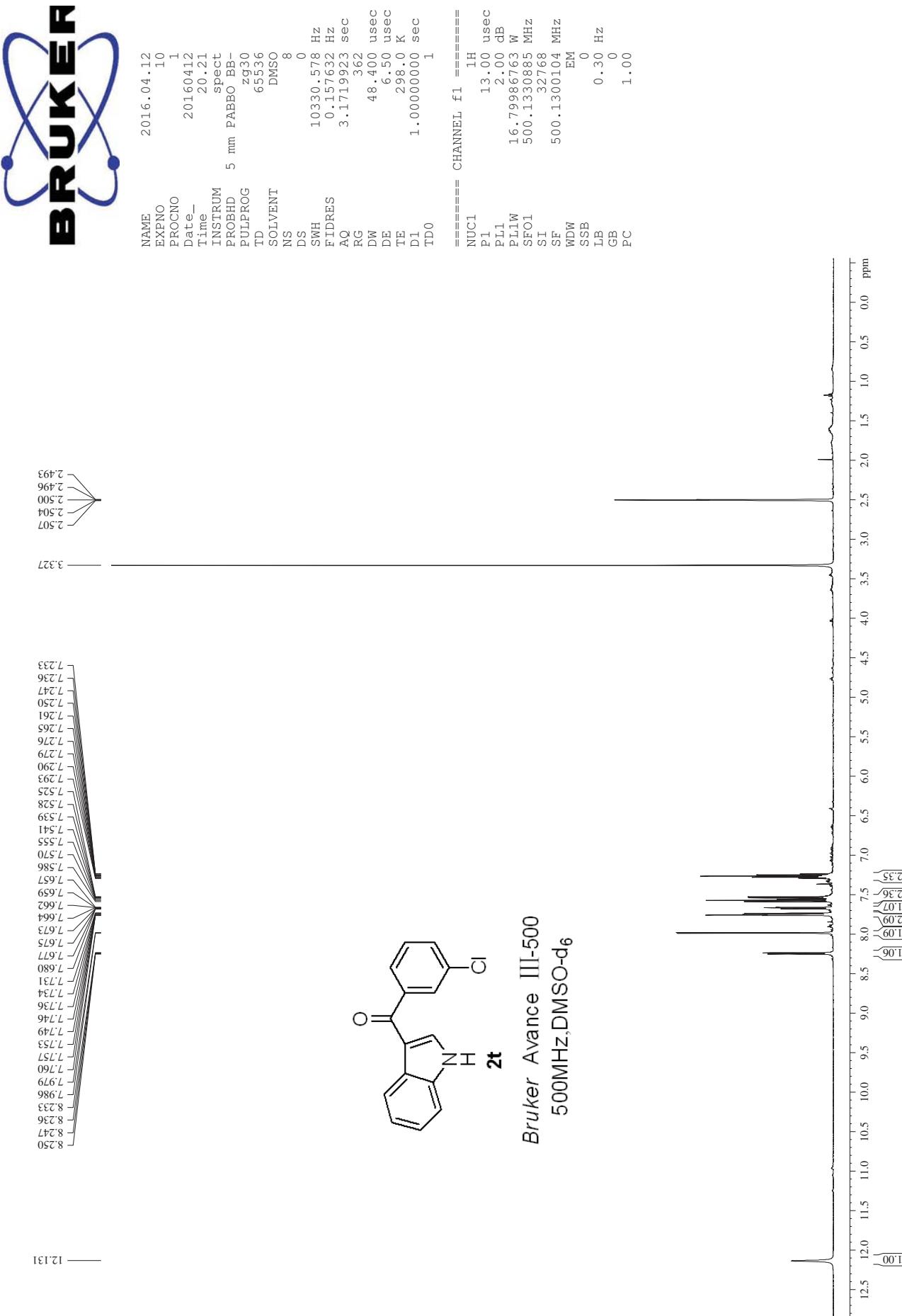
**2s**

Bruker Avance III-500  
125MHz, CDCl<sub>3</sub>

===== NAME 2016.03.18  
EXPNO 10  
PROCNO 1  
Date\_ 20160318  
Time 15.08  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgppg30  
TD 32768  
SOLVENT CDCl<sub>3</sub>  
NS 705  
DS 0  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 0.5505524 sec  
RG 2050  
DW 16.800 usec  
DE 6.50 usec  
TE 298.3 K  
D1 2.0000000 sec  
D11 0.03000000 sec  
TD0 1  
===== CHANNEL f1 ======  
NUC1 13C  
P1 12.30 usec  
PL1 4.50 dB  
PL1W 33.60015869 W  
SFO1 125.7703643 MHz  
===== CHANNEL f2 ======  
CPDPRG2 Waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.00 dB  
PL1.2 17.78 dB  
PL1.3 17.78 dB  
PL2W 16.79986763 W  
PL1.2W 0.44392112 W  
PL1.3W 0.44392112 W  
SFO2 500.1320005 MHz  
SI 32768  
SF 125.7577890 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
SB 0  
PC 1.40

STC





142.44  
136.31  
136.78  
133.25  
130.79  
130.39  
127.87  
127.04  
126.10  
123.29  
122.09  
121.40  
114.69  
112.33  
40.02  
39.86  
39.69  
39.52  
39.35  
39.19  
39.02  
39.02

142.44  
136.31  
136.78  
133.25  
130.79  
130.39  
127.87  
127.04  
126.10  
123.29  
122.09  
121.40  
114.69  
112.33  
40.02  
39.86  
39.69  
39.52  
39.35  
39.19  
39.02  
39.02

**BRUKER**

```

=====
NAME          2016.04.12
EXPNO         11
PROCNO        1
Date_        20160412
Time       20.40
INSTRUM     spect
PROBHD      5 mm PABBO BB-
PULPROG    zgpp30
TD        32768
SOLVENT      DMSO
NS           272
DS            0
SWH        29761.904 Hz
FIDRES     0.908261 Hz
AQ        0.5505524 sec
RG          2050
DW        16.800 usec
DE        6.500 usec
TE        298.1 K
D1        2.0000000 sec
D11       0.03000000 sec
TD0          1

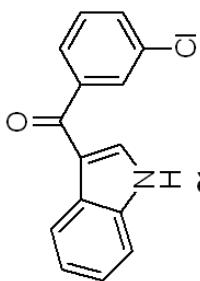
=====
```

```

=====
CHANNEL f1 =====
NUC1          13C
P1             12.30 usec
PL1           4.50 dB
PLLW          33.60015869 W
SFO1        125.7703643 MHz

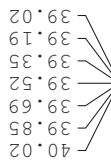
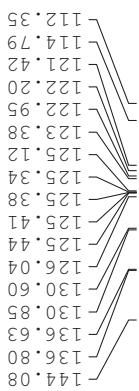
===== CHANNEL f2 =====
CPDPRG2      Waltz16
NUC2          1H
PCPD2        80.00 usec
PL12          2.00 dB
PL12          17.78 dB
PL13          17.78 dB
PL2W          16.79986763 W
PL12W         0.44392112 W
PL13W         0.44392112 W
SFO2        500.1320005 MHz
SI             32768
SF          125.7578507 MHz
WDW           EM
SSB           0
LB           1.00 Hz
SB           0
PC           1.40
```

*Bruker Avance III-500*  
125MHz,DMSO-d<sub>6</sub>

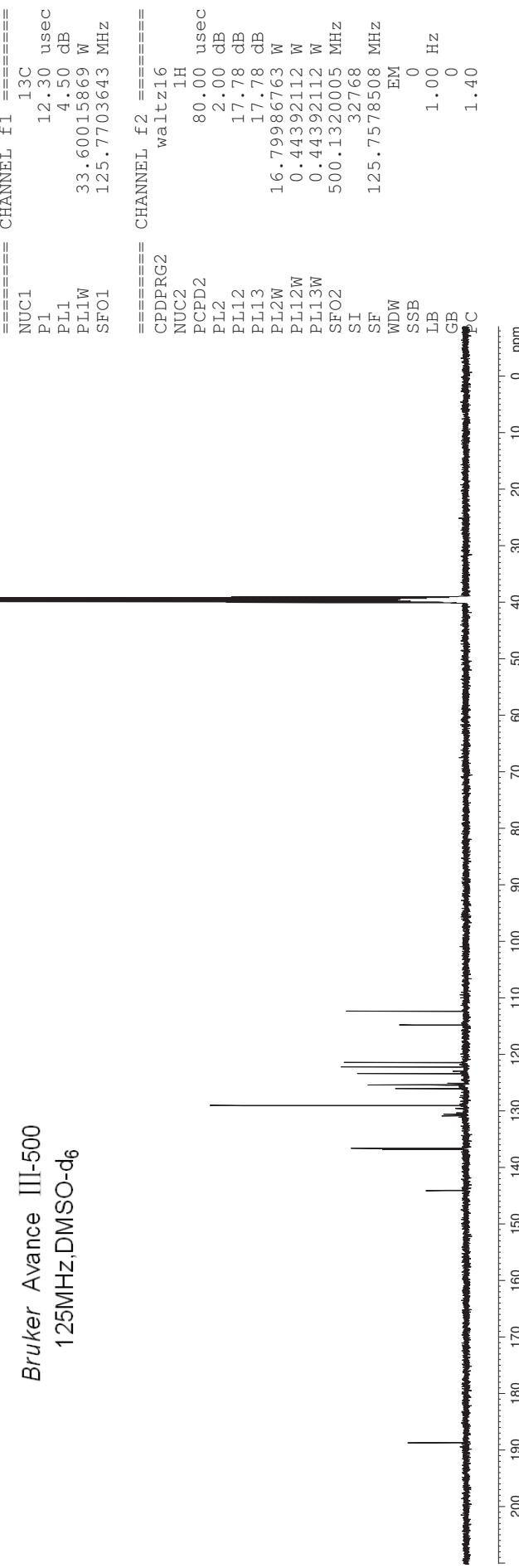


liushouxin-xh-CF3-C

188.74

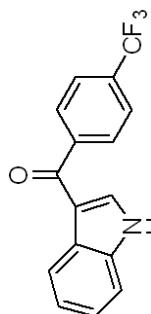
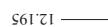


NAME 2016.04.09  
EXPNO 3  
PROCNO 1  
Date\_ 20160409  
Time 17.49  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgppg30  
TD 32768  
SOLVENT DMSO  
NS 1038  
DS 0  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 0.5505524 sec  
RG 2050  
DW 16.800 usec  
DE 6.50 usec  
TE 298.0 K  
D1 2.0000000 sec  
D11 0.03000000 sec  
TD0 1

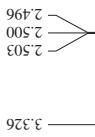


Bruker Avance III-500  
125MHz,DMSO-d<sub>6</sub>

liushouxin-xh-CF3



*Bruker Avance III-500*  
500MHz,DMSO-d<sub>6</sub>



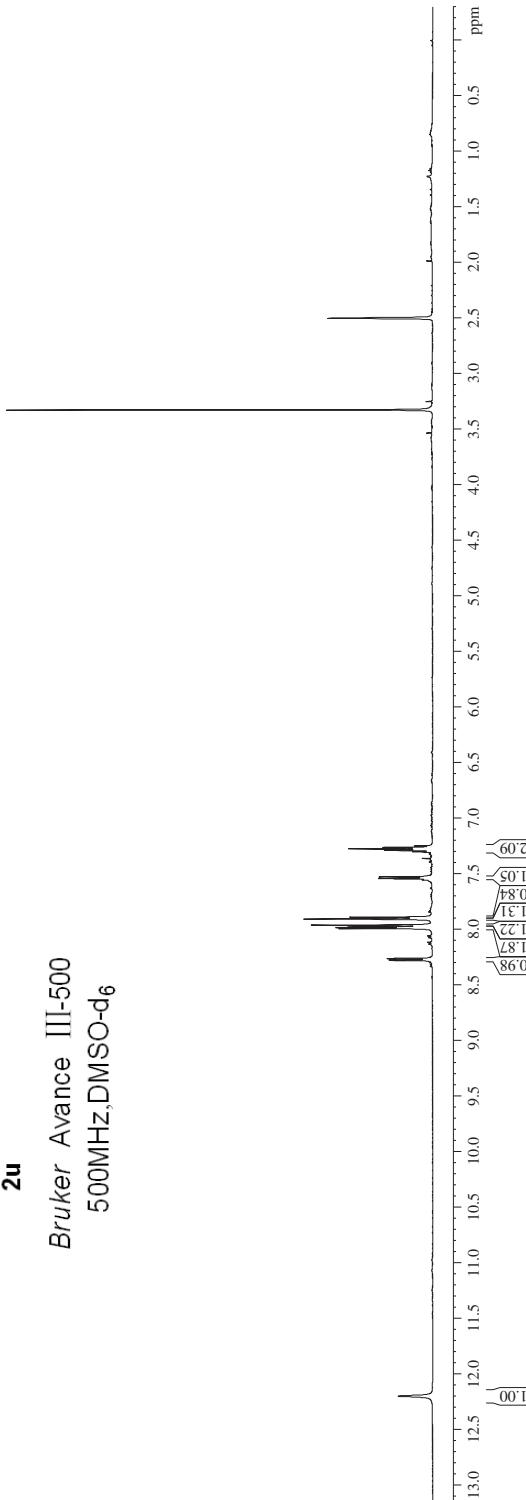
— 3.326 —

— 3.326 —

NAME	2016.04.09
EXPNO	2
PROCNO	1
Date—	20160409
Time—	17.00
INSTRUM	spec
PROMBDH	PABB0
PULPROG	BB- 930
TD	36864
SOLVENT	DMSO
NS	32
DS	0
SWH	10330.578
FIDRES	Hz 0.280235
AQ	sec 1.7842675
RG	256
DW	48.400
DE	usec 6.50
TE	usec 50.00
TM	K 29.8.0
D1	sec 1.00000000
TDO	1

===== CHANNEL f1 =====

NUC1	1H
P1	13.00
PL1	usec 2.00
PL1W	dB -67.63
SFO1	W 500.1323506 MHz
S1	132768
SE	500.1300103 MHz
WW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



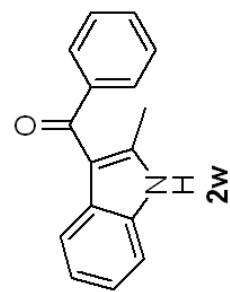
50



0.005

-2.534

8.778  
7.755  
7.755  
7.769  
7.753  
7.753  
7.569  
7.554  
7.539  
7.476  
7.460  
7.445  
7.413  
7.397  
7.314  
7.298  
7.260  
7.182  
7.180  
7.152  
7.150  
7.093  
7.092  
7.078  
7.063  
7.062

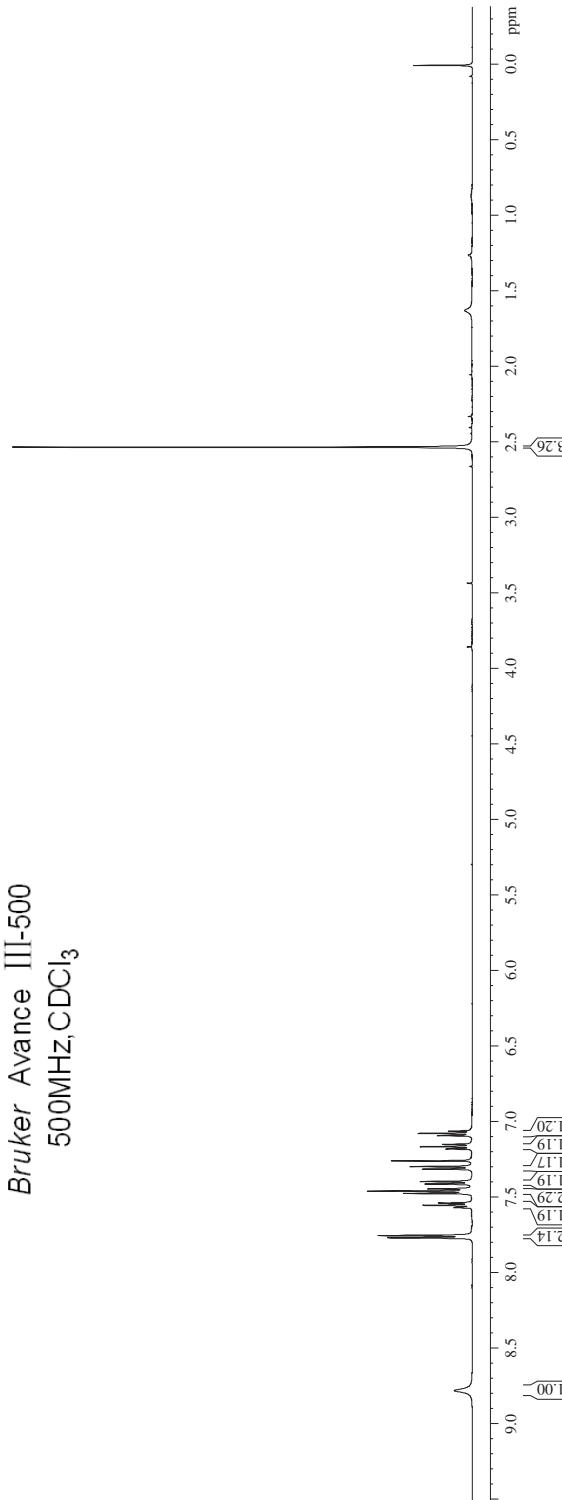


Bruker Avance III-500  
500MHz, CDCl<sub>3</sub>

```

NAME          2016.03.22
EXNO           6
PROCNO        1
Date_      20160322
Time       20.44
INSTRUM     spect
PROBHD      5 mm PABBO BB-
PULPROG    zg30
TD        36864
SOLVENT    CDCl3
NS           8
DS            0
SWH       10330.578 Hz
FIDRES    0.28035 Hz
AQ        1.7842675 sec
RG          362
DW        48.400 usec
DE         6.50 usec
TE        298.0 K
D1       1.00000000 sec
TDO0
===== CHANNEL f1 =====
NUC1          1H
P1        13.00 usec
PL1          2.00 QB
PL1W      16.79386763 W
SF01      500.1335009 MHz
SI          322768 EM
SF      500.1300233 MHz
WDW
SSB
LB          0.30 Hz
GB          0
PC         1.00

```

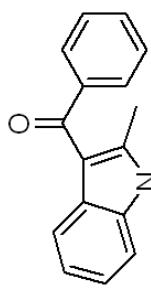


liu shou xin -xh

193.30

143.66  
141.31  
134.73  
131.53  
128.90  
128.33  
127.63  
122.48  
121.59  
121.01  
114.03  
110.66

77.30  
122.48  
121.59  
121.01  
114.03  
110.66



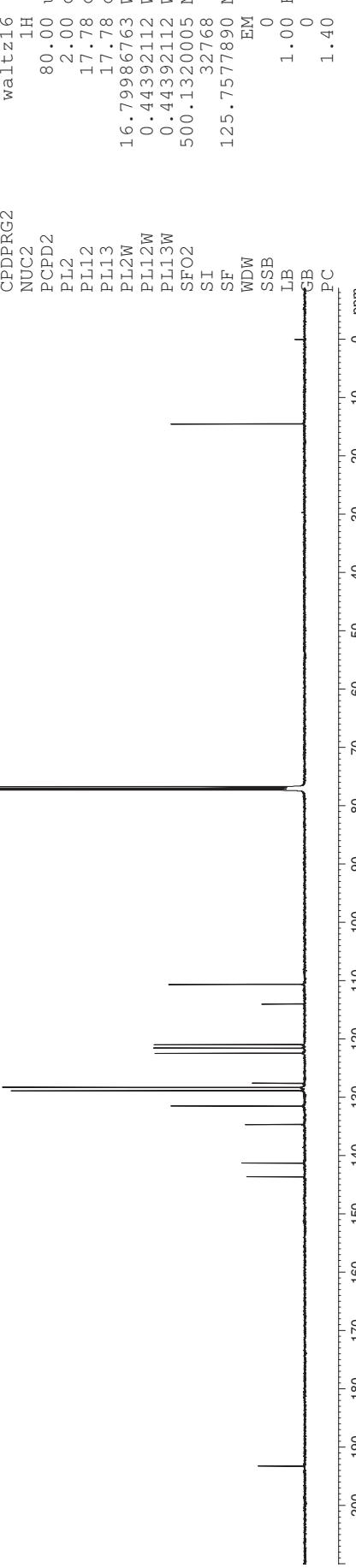
*Bruker Avance III-500*  
125MHz, CDCl<sub>3</sub>

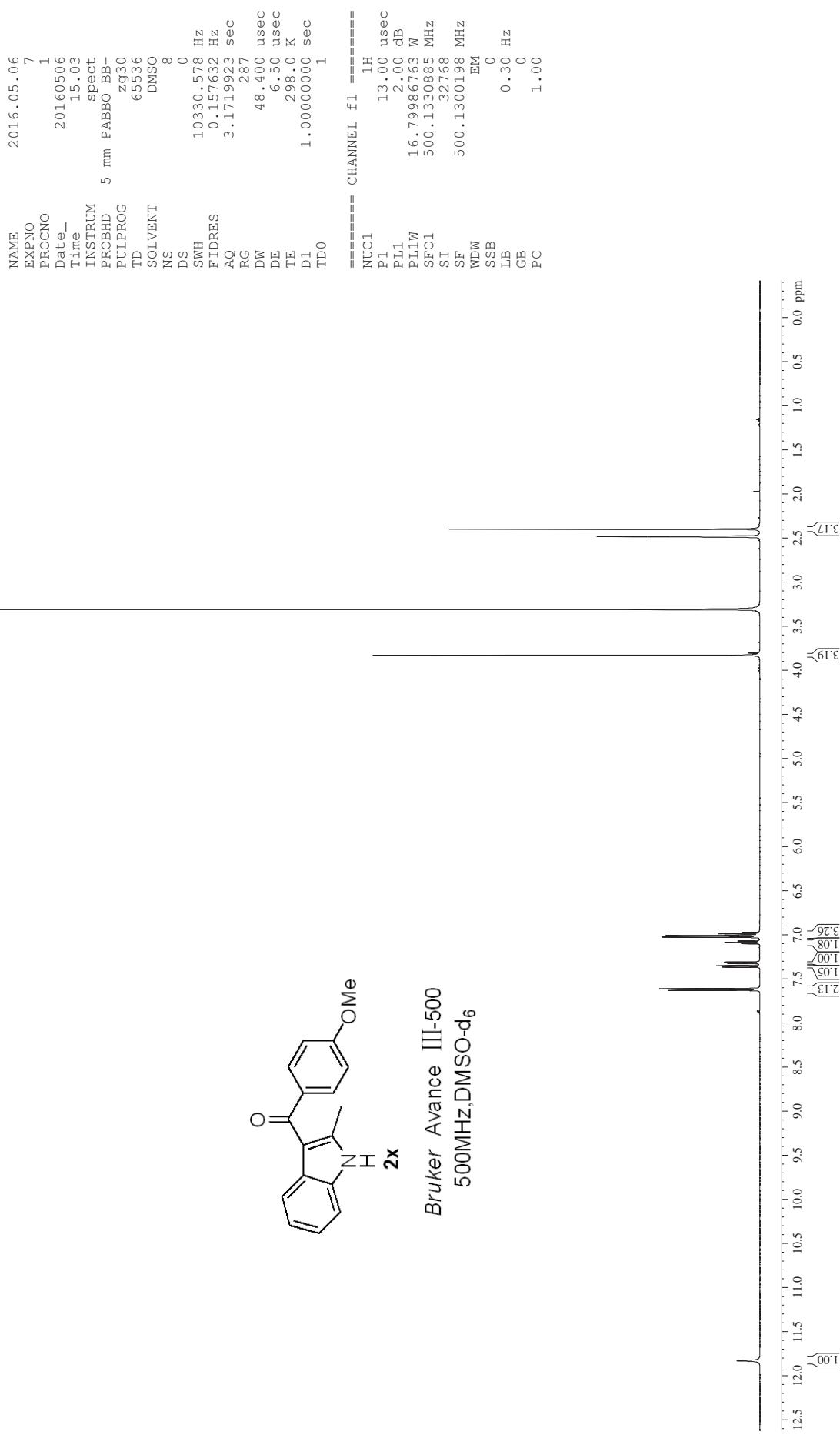


NAME 2016.03.22  
EXPNO 7  
PROCNO 1  
Date\_ 20160322  
Time 21.30  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zppg30  
TD 32768  
SOLVENT CDC13  
NS 14664  
DS 0  
SWH 29761.904 Hz  
FIDRES 0.508261 Hz  
AQ 0.5505524 sec  
RG 2050  
DW 16.800 usec  
DE 6.50 usec  
TE 298.5 K  
D1 2.0000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 12.30 usec  
PL1 4.50 dB  
PL1W 33.60015869 W  
SFO1 125.7703643 MHz

===== CHANNEL f2 =====  
CPDPRG2 Waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.00 dB  
PL1.2 17.78 dB  
PL1.3 17.78 dB  
PL2W 16.79986763 W  
PL1.2W 0.44392112 W  
PL1.3W 0.44392112 W  
SFO2 500.1320005 MHz  
SI 32768  
SF 125.7577890 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





liushouxin-xh

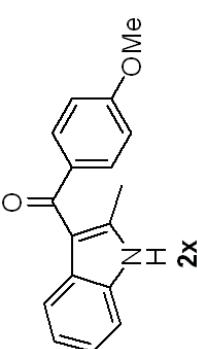
190.49

161.85

143.29

134.88  
133.61  
130.69  
127.29  
121.57  
120.64  
119.89  
113.52  
112.64  
111.16

55.36  
40.02  
39.85  
39.69  
39.52  
39.35  
39.19  
39.02  
39.02



Bruker Avance III-500  
125MHz,DMSO-d<sub>6</sub>

13.99

NAME  
EXPNO  
PROCNO  
Date\_—  
Time\_—  
INSTRUM  
PROBHD  
PULPROG  
TD  
SOLVENT  
NS

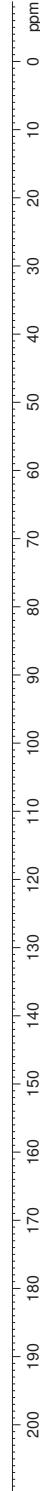
2016.05.07  
1  
20160507  
1  
9.40  
spect  
5 mm PABBO BB-  
zppg30  
32768  
DMSO  
8444  
DS 0  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 0.5505524 sec  
RG 2050  
DW 16.800 usec  
DE 6.50 usec  
TE 298.3 K  
D1 2.0000000 sec  
D11 0.03000000 sec  
TD0 1

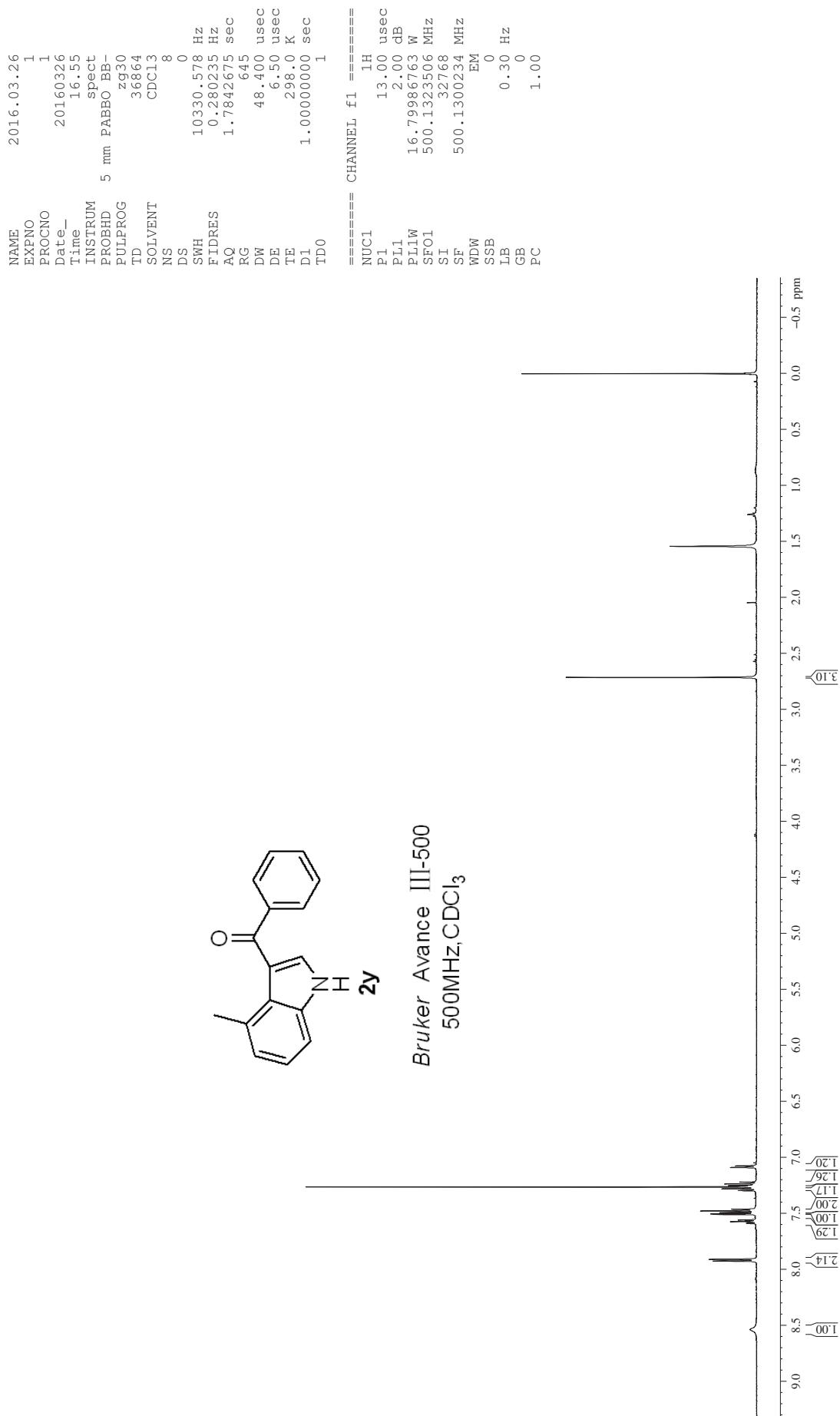
===== CHANNEL f1 =====

NUC1 13C  
P1 12.30 usec  
PL1 4.50 dB  
PL1W 33.60015869 W  
SF01 125.7703643 MHz

===== CHANNEL f2 =====

OPDPRG2 Waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL1 2.00 dB  
PL1.2 17.78 dB  
PL1.3 17.78 dB  
PL2W 16.79986763 W  
PL1.2W 0.44392112 W  
PL1.3W 0.44392112 W  
SF02 500.1320005 MHz  
SI 32768  
SF 125.7578518 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





liu shou xin -xh

191.09  
137.02  
133.34  
131.93  
129.85  
128.21  
125.21  
124.10  
124.20  
119.00  
108.97

77.28  
77.03  
76.77

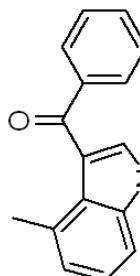
— 0.01 —

— 22.14 —



NAME 2016.03.26  
EXPNO 5  
PROCNO 1  
Date\_ 20160327  
Time 10.55  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zppg30  
TD 32768  
SOLVENT CDCl3  
NS 18432  
DS 0  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 0.5505524 sec  
RG 2050  
DW 16.800 usec  
DE 6.50 usec  
TE 298.0 K  
D1 2.0000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 12.30 usec  
PL1 4.50 dB  
PL1W 33.60015869 W  
SFO1 125.7703643 MHz  
===== CHANNEL f2 =====  
CPDPRG2 Waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL1 2.00 dB  
PL1.2 17.78 dB  
PL1.3 17.78 dB  
PL2W 16.79986763 W  
PL1.2W 0.44392112 W  
PL1.3W 0.44392112 W  
SFO2 500.1320005 MHz  
SI 32768  
SF 125.7577890 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
PC 0  
PC 1.40



**2y**  
Bruker Avance III-500  
125MHz, CDCl<sub>3</sub>

SFC

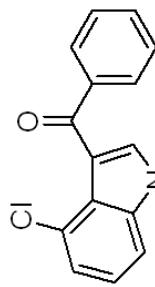


2.493  
2.497  
2.500  
2.504  
2.507

—3.453—

7.185  
7.187  
7.200  
7.202  
7.222  
7.238  
7.253  
7.499  
7.501  
7.511  
7.515  
7.517  
7.526  
7.542  
7.561  
7.617  
7.622  
7.631  
7.634  
7.646  
7.649  
7.651  
7.801  
7.813  
7.816  
7.827  
7.847  
7.853  
7.937  
7.939

—12.200—

**2z**

*Bruker Avance III-500*  
500MHz,DMSO-d<sub>6</sub>

```

NAME          2016.04.19
EXNO          10
PROCNO        1
Date_-
Time         18.12
INSTRUM      spect
PROBHD       5 mm PABBO BB-
PULPROG      zg30
TD           65536
SOLVENT      DMSO
NS            32
DS            0
SWH          10330.578 Hz
FIDRES       0.157632 Hz
AQ            3.1719923 sec
RG            406
DW           48.400 usec
DE            6.50 usec
TE            298.0 K
D1           1.00000000 sec
TDO          1

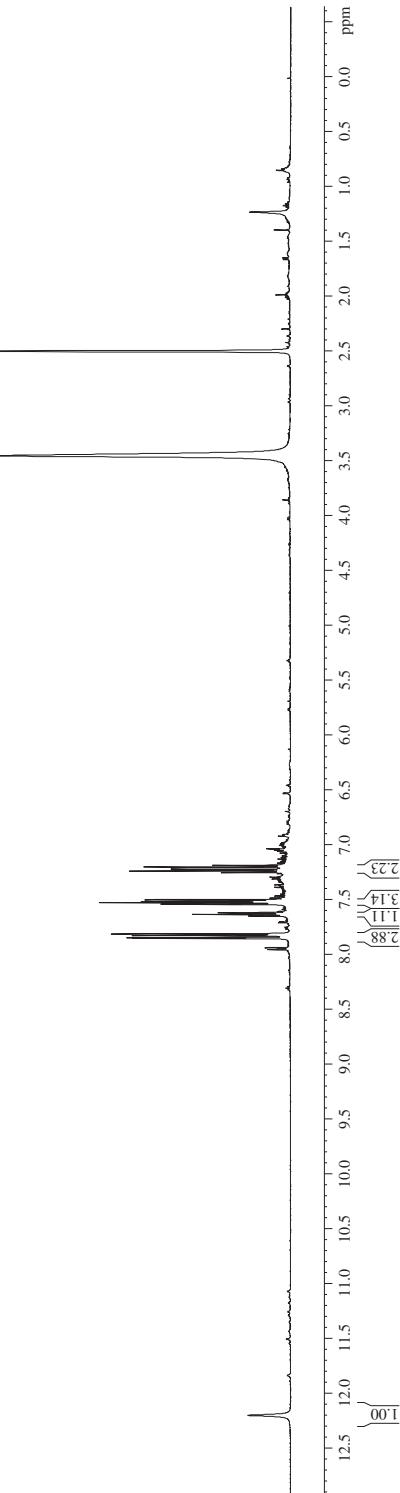
```

===== CHANNEL f1 =====

```

NUC1          1H
P1            13.00 usec
PL1          2.00 CB
PL1W        16.79386763 W
SFO1        500.1330885 MHz
SI             32768
SF           500.1300101 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00

```

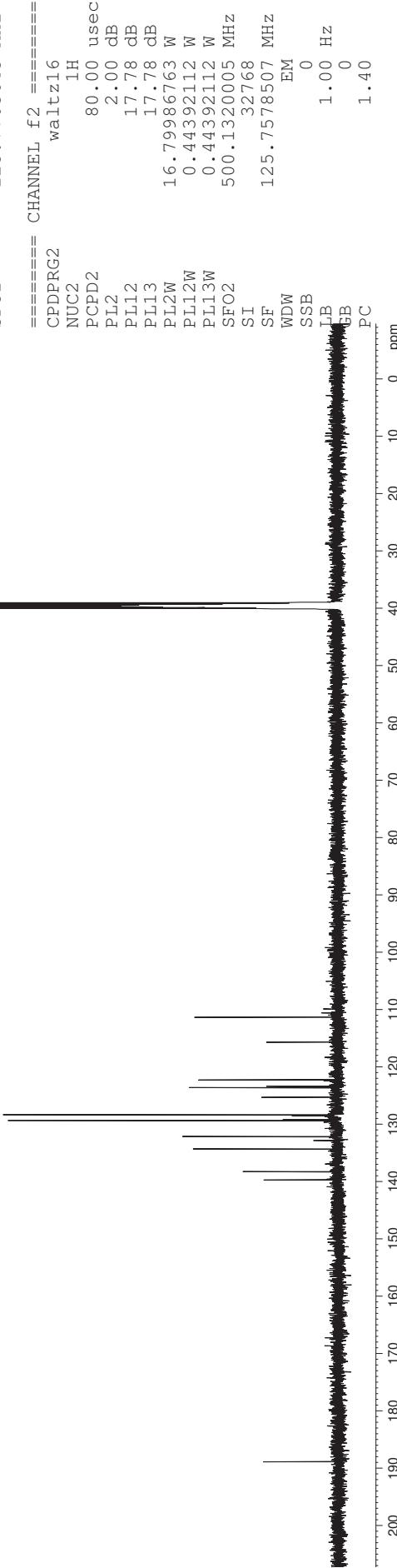
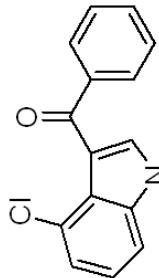


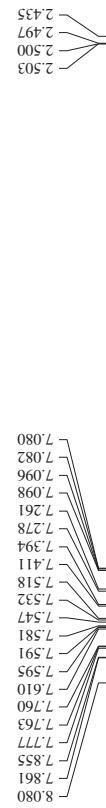
liushouxin-xh-c

139.73  
 138.30  
 134.21  
 129.38  
 128.38  
 125.32  
 123.36  
 122.28  
 115.70  
 111.36

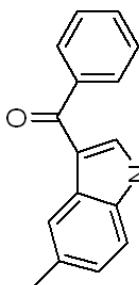
NAME	2016.04.19
EXPNO	11
PROCNO	1
Date _	20160419
Date _	20.26
INSTRUM	spect
PROBHD	5 mm PAEBO BB-
PULP,PROG	zpgq30
TD	32768
SOLVENT	DMSO
NS	3003
DS	4
SWH	29761.904
FIDRES	0.908261
AQ	0.5505524
RG	2050
DW	1.6.800
DE	6.50
TE	298.0
D1	2.00000000
D11	0.03000000
TDO	1

125MHz, DMSO-d<sub>6</sub>

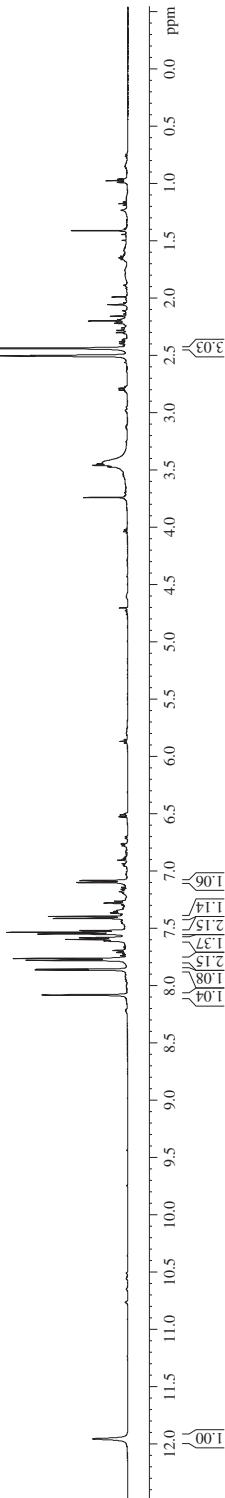




=====  
NAME 2016.04.11  
EXNO 10  
PROCNO 1  
Date\_ 20160411  
Time 17.56  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 36864  
SOLVENT DMSO  
NS 8  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.280235 Hz  
AQ 1.7842675 sec  
RG 287  
DW 48.400 usec  
DE 6.50 usec  
TE 298.0 K  
D1 1.00000000 sec  
TDO 1  
=====  
===== CHANNEL f1 ======  
NUC1 1H  
P1 13.00 usec  
PL1 2.00 CB  
PL1W 16.79386763 W  
SF01 500.1323506 MHz  
SI 32768 EM  
SF 500.1300103 MHz  
WDW 0  
SSB 0.30 Hz  
LB 0  
GB 0  
PC 1.00



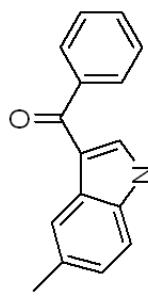
*Bruker Avance III-500*  
500MHz,DMSO-d<sub>6</sub>



liushouxin-xh-5-Me

189.69

140.65  
135.75  
130.93  
130.72  
128.35  
126.51  
124.59  
121.19  
114.62  
111.85



**2aa**

Bruker Avance III-500  
125MHz,DMSO-d<sub>6</sub>

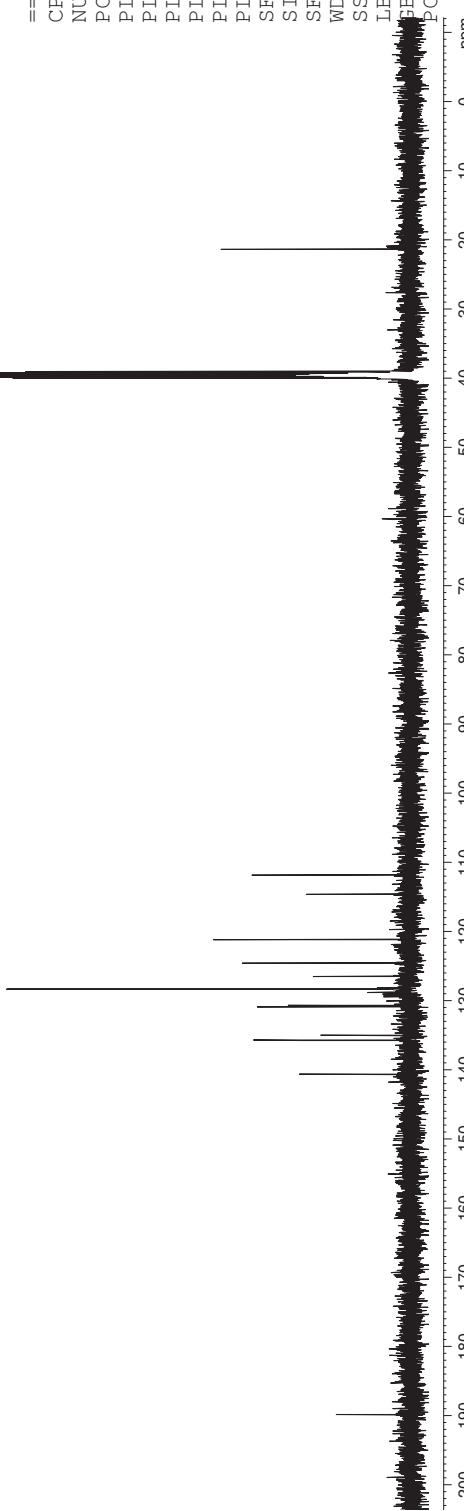
40.02  
39.85  
39.69  
39.52  
39.35  
39.19  
39.02  
39.02

21.35



NAME 2016.04.11  
EXPNO 11  
PROCNO 1  
Date\_ 20160411  
Time 18.09  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgppg30  
TD 32768  
SOLVENT DMSO  
NS 201  
DS 0  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 0.5505524 sec  
RG 2050  
DW 16.800 usec  
DE 6.50 usec  
TE 298.0 K  
D1 2.0000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 12.30 usec  
PL1 4.50 dB  
PL1W 33.60015869 W  
SFO1 125.7703643 MHz  
===== CHANNEL f2 =====  
CPDPRG2 Waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.00 dB  
PL1.2 17.78 dB  
PL1.3 17.78 dB  
PL2W 16.79986763 W  
PL1.2W 0.44392112 W  
PL1.3W 0.44392112 W  
SFO2 500.1320005 MHz  
SI 32768  
SF 125.7578512 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
PB 0  
PC 1.40 ppm





2.492  
2.495  
2.499  
2.503  
2.506  
3.357  
3.701  
3.804

6.870  
6.875  
6.888  
6.892  
6.898  
7.000  
7.005  
7.319  
7.323  
7.513  
7.514  
7.517  
7.529  
7.534  
7.537  
7.538  
7.539  
7.540  
7.544  
7.549  
7.550  
7.559  
7.560  
7.569  
7.576  
7.579  
7.582  
7.585  
7.590  
7.594  
7.599  
7.609  
7.611  
7.616  
7.639  
7.649  
7.659  
7.669  
7.676  
7.689  
7.716  
7.735  
7.749  
7.759  
7.769  
7.776  
7.789  
8.069  
8.116

11.859

```

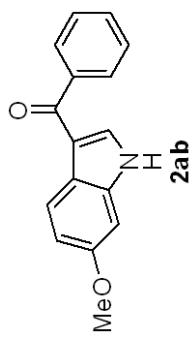
NAME          2016.04.14
EXNO          10
PROCNO        1
Date_-
Time         20160414 10.09
INSTRUM      spect
PROBHD       5 mm PABBO BB-
PULPROG      zg30
TD           65536
SOLVENT      DMSO
NS            8
DS            0
SWH          10330.578 Hz
FIDRES       0.157632 Hz
AQ            3.1719923 sec
RG            287
DW            48.400 usec
DE            6.50 usec
TE            298.0 K
D1           1.00000000 sec
TDO          1

```

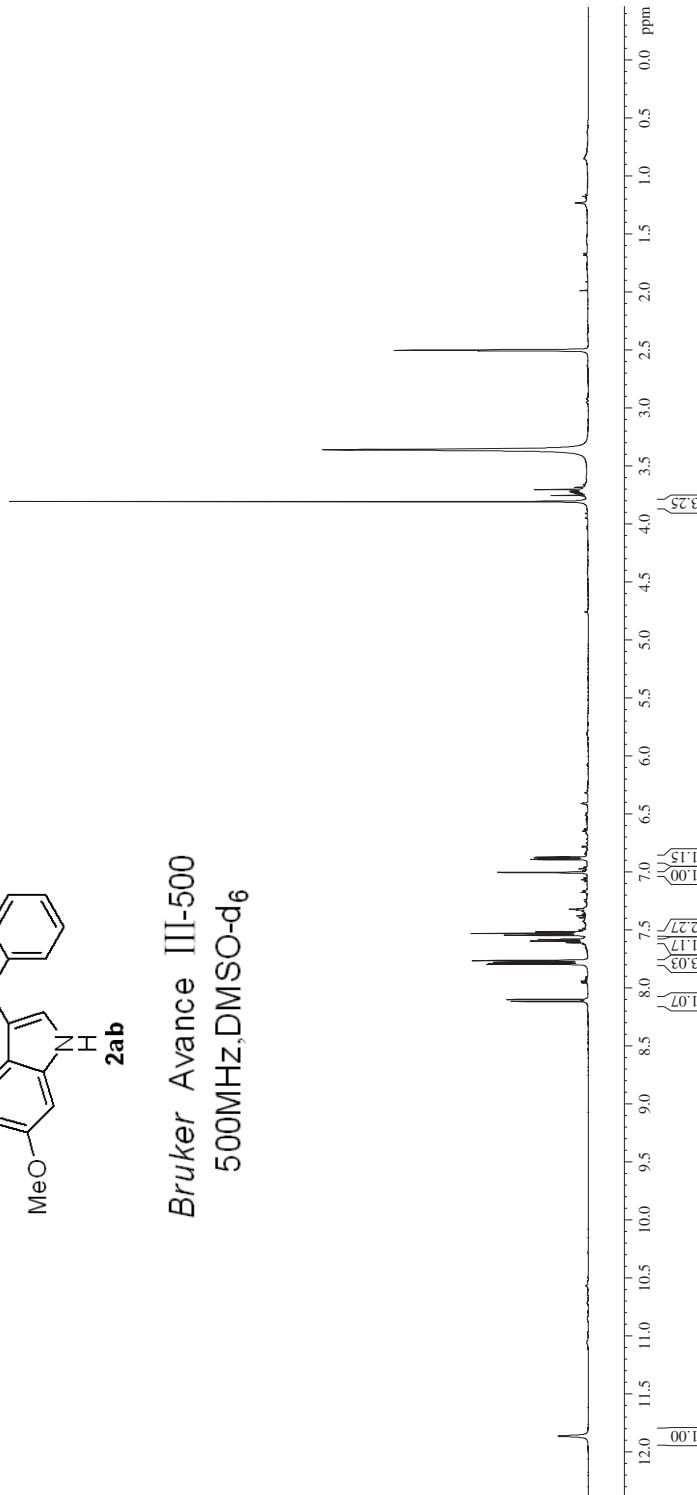
```

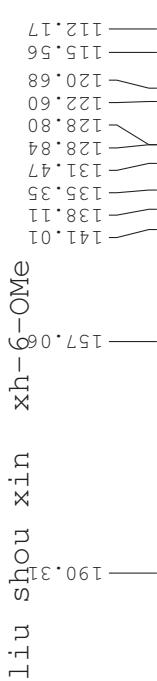
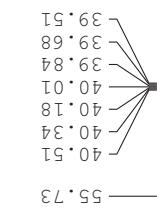
===== CHANNEL f1 =====
NUC1          1H
P1            13.00 usec
PL1           2.00 CB
PL1W          PL1W
SF01          16.79386763 W
SI             500.1330885 MHz
SF             500.1300109 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

```



Bruker Avance III-500  
500MHz,DMSO-d<sub>6</sub>





```

=====
NAME          2016.04.14
EXPNO         11
PROCNO        1
Date_         20160414
Time          10.12
INSTRUM       spect
PROBHD       5 mm PABBO BB-
PULPROG      zppg30
TD           32768
SOLVENT       DMSO
NS            342
DS            4
SWH          29761.904 Hz
FIDRES       0.908261 Hz
AQ            0.505524 sec
RG            2050
DW           16.800 usec
DE            6.500 usec
TE            298.1 K
D1           2.0000000 sec
D11           0.03000000 sec
TD0            1

=====
```

```

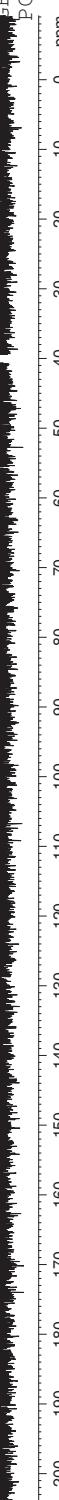
===== CHANNEL f1 =====
NUC1          13C
P1            12.30 usec
PL1           4.50 dB
PLL1          33.60015869 W
PLL1W         125.7703643 MHz
SFO1          125.7577890 MHz
EM            0
WALTZ16       1H
NUC2          80.00 usec
PCPD2         2.00 dB
PL12          17.78 dB
PL13          17.78 dB
PL2W          16.79986763 W
PL12W         0.44392112 W
PLL13W        0.44392112 W
SFO2          500.1320005 MHz
SI             32768
SF            125.7577890 MHz
WDW           EM
SSB           1.00 Hz
LB            0
PC            1.40

===== CHANNEL f2 =====
WALTZ16       1H
NUC2          80.00 usec
PCPD2         2.00 dB
PL12          17.78 dB
PL13          17.78 dB
PL2W          16.79986763 W
PL12W         0.44392112 W
PLL13W        0.44392112 W
SFO2          500.1320005 MHz
SI             32768
SF            125.7577890 MHz
WDW           EM
SSB           1.00 Hz
LB            0
PC            1.40
```

*Bruker Avance III-500*  
125MHz,DMSO-d<sub>6</sub>

**2ab**

**2ab**



12.082

8.092  
7.876  
7.870  
7.792  
7.778  
7.75  
7.720  
7.620  
7.605  
7.601  
7.593  
7.590  
7.588  
7.557  
7.542  
7.528  
7.523  
7.512  
7.500  
7.493  
7.42  
7.388  
7.357  
7.342  
7.328  
7.323  
7.312  
7.26  
7.157  
7.142  
7.126  
7.120  
7.070  
7.056

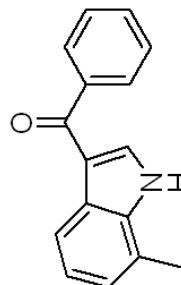
3.347  
—  
2.525  
2.502  
2.499  
2.495  
—



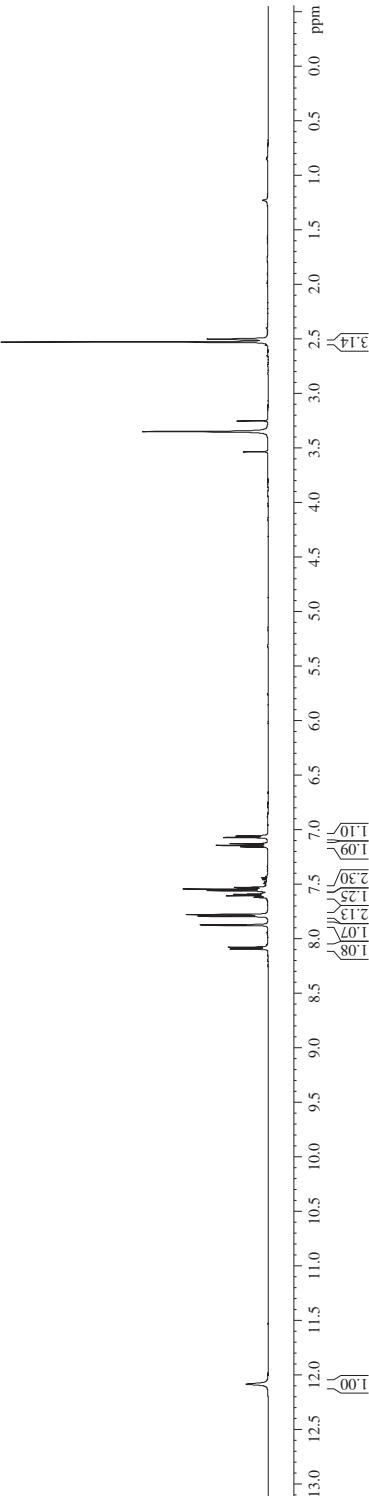
```

NAME          2016.04.21
EXN0          1
PROCNO        1
Date_-
Time         10.16
INSTRUM      spect
PROBHD       5 mm PABBO BB-
PULPROG      zg30
TD           65536
SOLVENT      DMSO
NS            8
DS            0
SWH          10330.578 Hz
FIDRES       0.157632 Hz
AQ           3.1719923 sec
RG           228
DW           48.400 usec
DE           6.50 usec
TE           298.0 K
D1           1.00000000 sec
TDO          1
===== CHANNEL f1 =====
NUC1          1H
P1            13.00 usec
PL1           2.00 CB
PL1W          16.79386763 W
SF01          500.1330885 MHz
SI             32768
SF            500.1300108 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

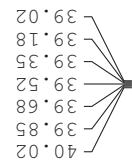
```

**2ac**

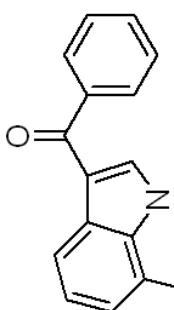
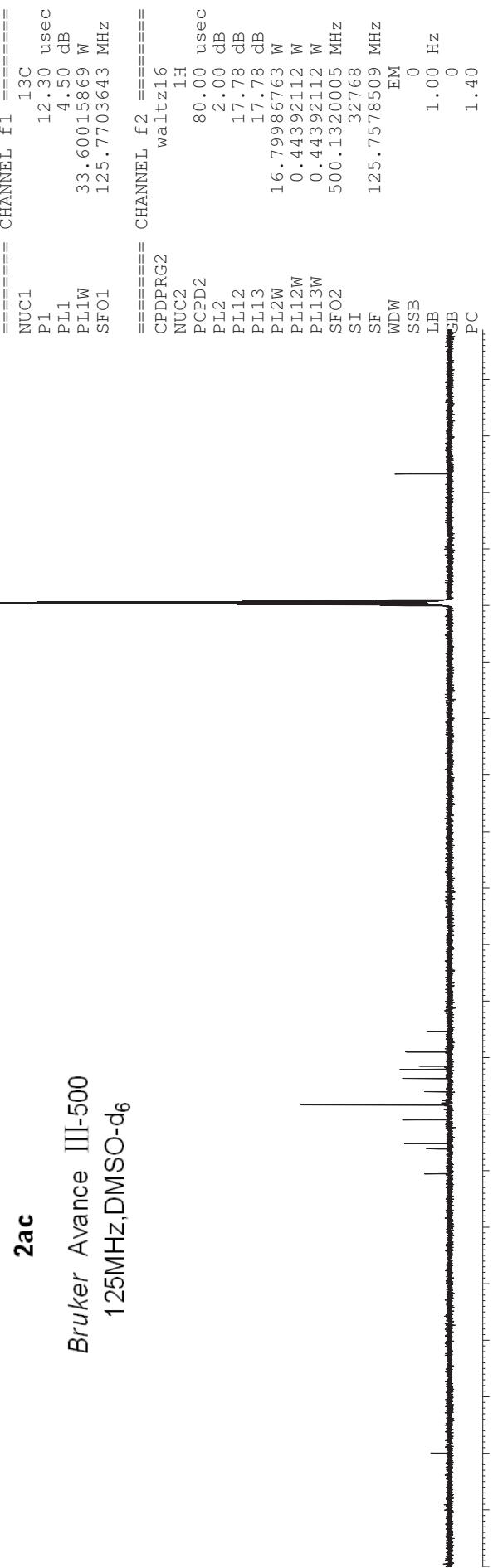
*Bruker Avance III-500*  
500MHz,DMSO-d<sub>6</sub>



liushouxin-xh-7-ch3-C



NAME 2016.04.21  
EXPNO 26  
PROCNO 1  
Date\_ 20160421  
Time 21.18  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpp30  
TD 32768  
SOLVENT DMSO  
NS 125  
DS 0  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 0.505524 sec  
RG 2050  
DW 16.800 usec  
DE 6.50 usec  
TE 298.0 K  
D1 2.0000000 sec  
D11 0.03000000 sec  
TD0 1



**2ac**

Bruker Avance III-500  
125MHz,DMSO-d<sub>6</sub>

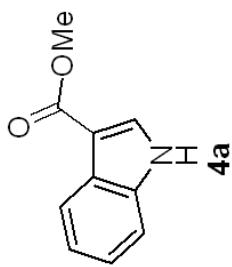
liushouxin-xh-cl



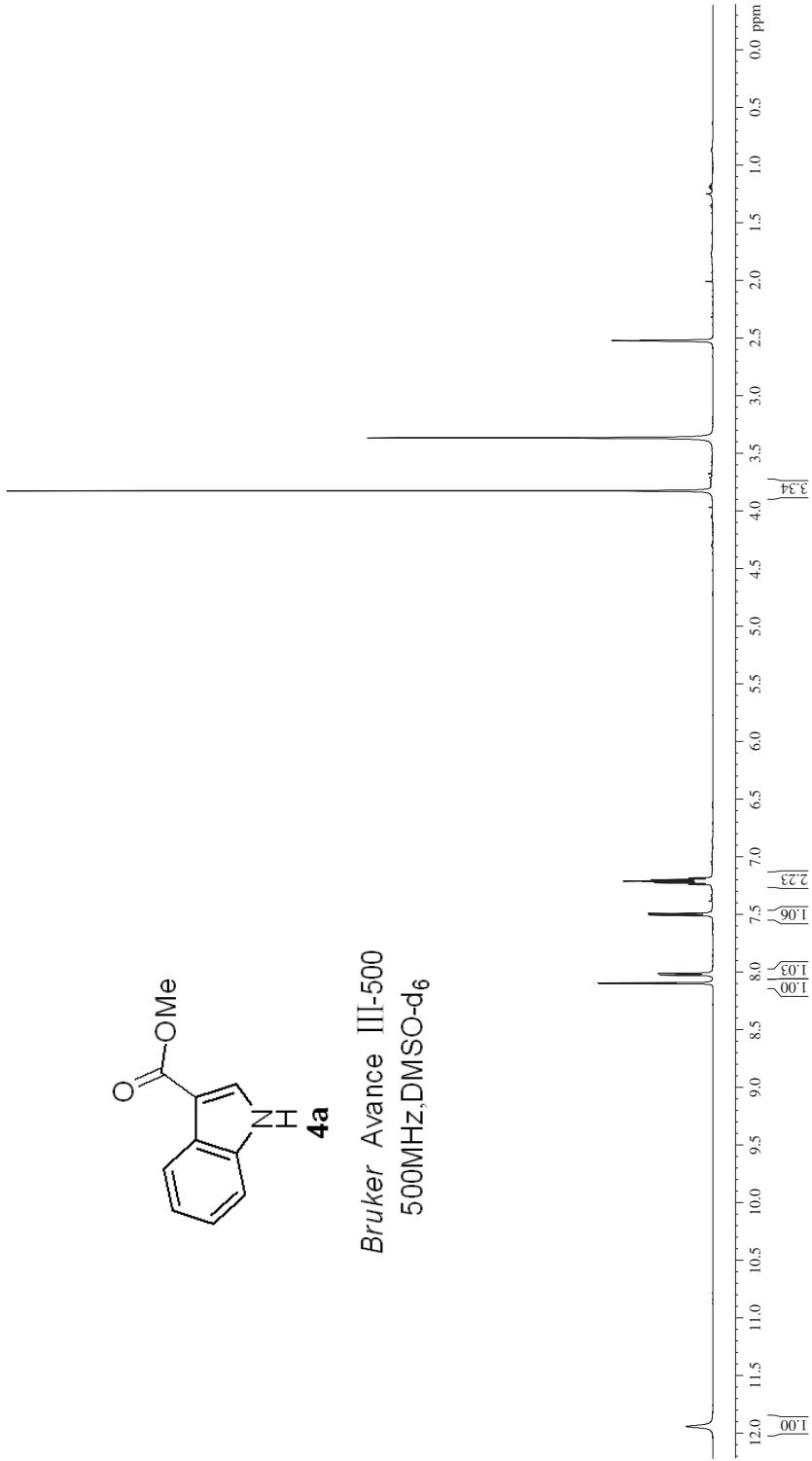
NAME	2016-05-3
EXPNO	12
PROCNO	1
Date_	20160503
Time	22.11
INSTRUM	spec
PROBHD	5 mm
PULPROG	PABBO BB-
	ZG30
TD	65536
SOLVENT	DMSO
NS	8
DS	0
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	322
DW	48.400 usec
DE	6.50 usec
TE	298.0 K
D1	1.0000000 sec
TD0	1
===== CHANNEL f1 =====	
NUC1	1H
P1	13.00 usec
PL1	2.00 dB
PL1W	16.79986763 W
SFO1	500.1330885 MHz
ST	32768
SF	500.1300002 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	1.00 GB



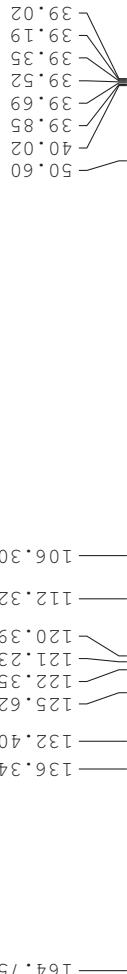
3.363  
—  
3.822  
—



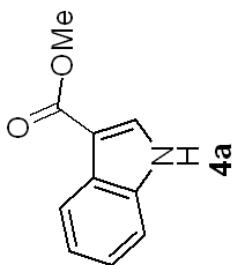
*Bruker Avance III-500*  
500MHz,DMSO-d<sub>6</sub>



liushouxin-xh-g1-c

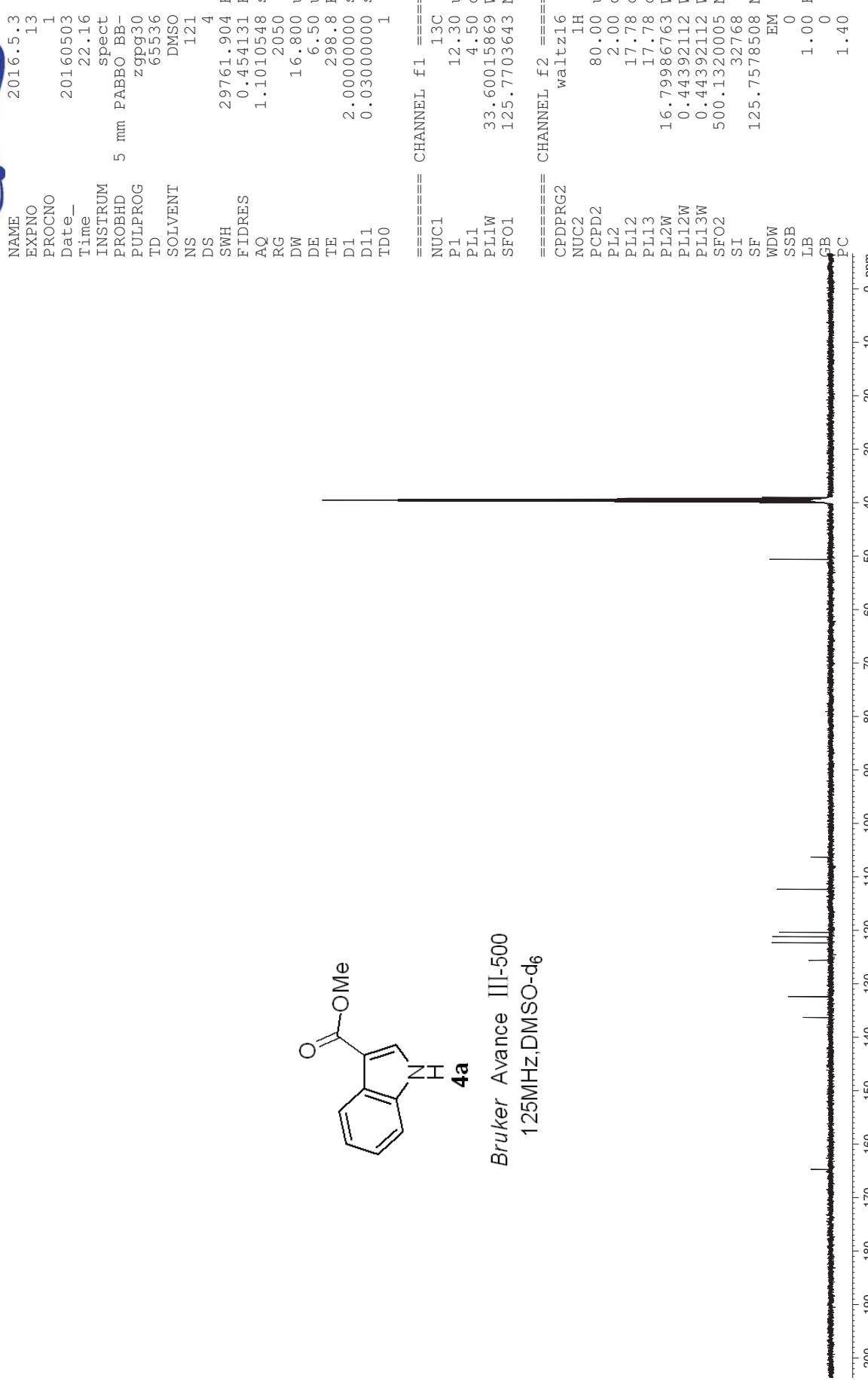


164.751-C  
136.34  
132.40  
125.62  
122.35  
121.23  
120.39  
112.32  
106.30  
=====



Bruker Avance III-500  
125MHz,DMSO-d<sub>6</sub>

136.34  
132.40  
125.62  
122.35  
121.23  
120.39  
112.32  
106.30  
=====



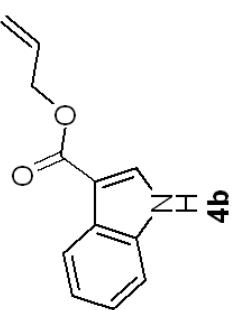


2.507  
2.500  
2.503  
2.496  
2.493

—3.491—

8.117  
8.010  
8.009  
8.005  
8.003  
8.001  
8.111  
7.996  
7.992  
7.496  
7.493  
7.484  
7.479  
6.109  
6.099  
6.088  
6.078  
6.075  
6.067  
6.054  
6.043  
6.033  
5.392  
5.389  
5.368  
5.270  
5.267  
5.248  
5.245  
4.781  
4.771

—11.963—

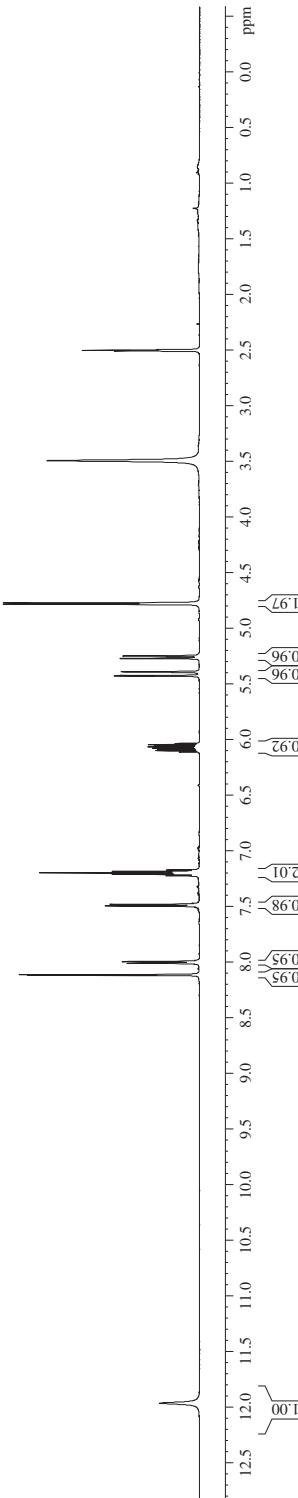


Bruker Avance III-500  
500MHz, DMSO-d<sub>6</sub>

```

=====
NAME          2016.04.29
EXNO          13
PROCNO        1
Date_-
Time         15.25
INSTRUM      spect
PROBHD       5 mm PABBO BB-
PULPROG      zg30
TD           65536
SOLVENT       DMSO
NS            8
DS            0
SWH          10330.578 Hz
FIDRES       0.157632 Hz
AQ            3.1719923 sec
RG            203
DW           48.400 usec
DE            6.50 usec
TE            298.0 K
D1           1.00000000 sec
TDO          1
===== CHANNEL f1 =====
NUC1          1H
P1            13.00 usec
PL1           2.00 CB
PL1W          16.79386763 W
SF01          500.1330885 MHz
SI             32768
SF            500.1300104 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

```



136.39  
133.45  
132.62  
125.63  
122.38  
121.29  
120.38  
117.25  
112.38  
106.20

— 63.50 —

40.02  
39.85  
39.68  
39.66  
39.52  
39.35  
39.18  
39.02



```

=====
NAME          2016.04.29
EXPNO         14
PROCNO        1
Date_         20160429
Time          15.35
INSTRUM       spect
PROBHD       5 mm PABBO BB-
PULPROG      zppg30
TD           65536
SOLVENT       DMSO
NS            75
DS            4
SWH          29761.904 Hz
FIDRES       0.454131 Hz
AQ            1.1010548 sec
RG            2050
DW            16.800 usec
DE            6.500 usec
TE            298.5 K
D1           2.0000000 sec
D11          0.03000000 sec
TD0           1

```

```

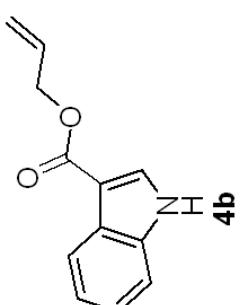
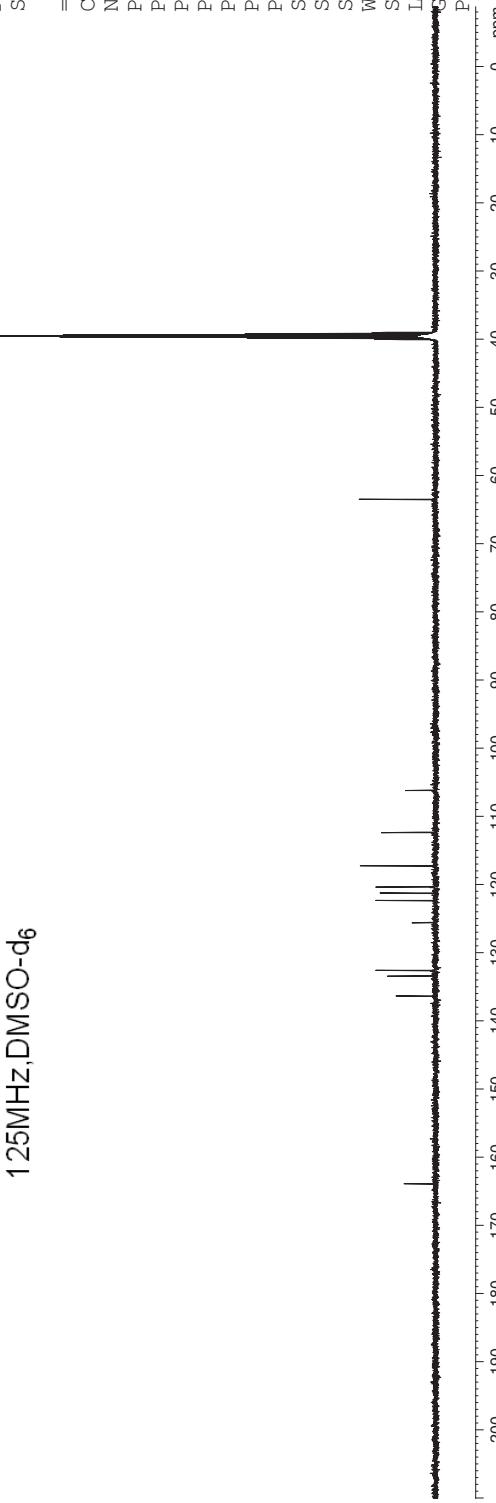
=====
CHANNEL f1 =====
NUC1          13C
P1            12.30 usec
PL1          4.50 dB
PL1W         33.60015869 W
SF01         125.7703643 MHz

```

```

=====
CHANNEL f2 =====
OPDPRG2      Waltz16
NUC2          1H
PCPD2         80.00 usec
PL12          2.00 dB
PL12          17.78 dB
PL13          17.78 dB
PL2W          16.79986763 W
PL12W         0.44392112 W
PL13W         0.44392112 W
SF02         500.1320005 MHz
SI            32768
SF           125.7578507 MHz
WDW          EM
SSB           0
LB            1.00 Hz
QB           0
PC           1.40

```



Bruker Avance III-500  
125MHz,DMSO-d<sub>6</sub>

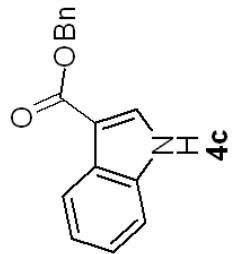


2.493  
2.496  
2.500  
2.503  
2.507

3.347

5.338  
7.159  
7.162  
7.173  
7.176  
7.179  
7.191  
7.205  
7.208  
7.219  
7.222  
7.320  
7.335  
7.339  
7.349  
7.361  
7.386  
7.401  
7.416  
7.473  
7.483  
7.487  
7.497  
7.990  
7.993  
8.007  
8.136

11.976



Bruker Avance III-500  
500MHz,DMSO-d<sub>6</sub>

```

NAME          2016.04.27
EXNO          13
PROCNO        1
Date_-
Time         13.56
INSTRUM      spect
PROBHD      5 mm PABBO BB-
PULPROG    zg30
TD           65536
SOLVENT      DMSO
NS            8
DS            4
SWH          10330.578 Hz
FIDRES       0.157632 Hz
AQ            3.1719923 sec
RG           181
DW           48.400 usec
DE            6.50 usec
TE            298.0 K
D1           1.00000000 sec
TDO          1

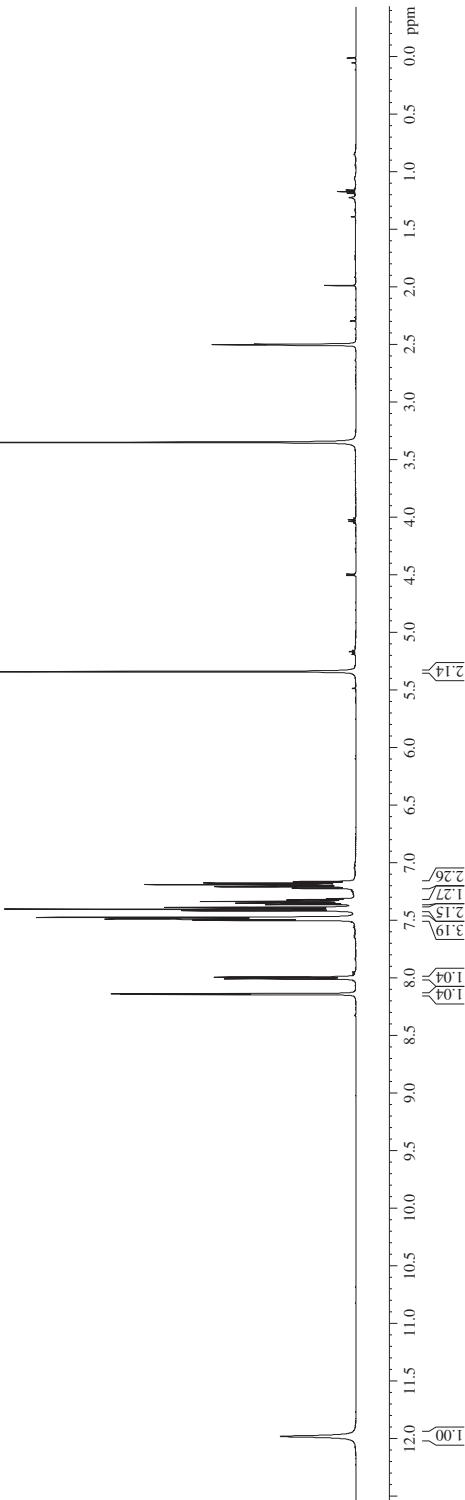
```

===== CHANNEL f1 =====

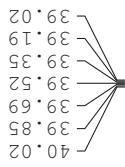
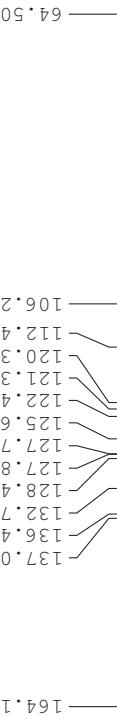
```

NUC1          1H
P1            13.00 usec
PL1           2.00 CB
PL1W        16.79386763 W
SFO1        500.1330885 MHz
SI             32768
SF           500.1300104 MHz
WDW           EM
SSB            0
LB            0.30 Hz
GB            0
PC           1.00

```

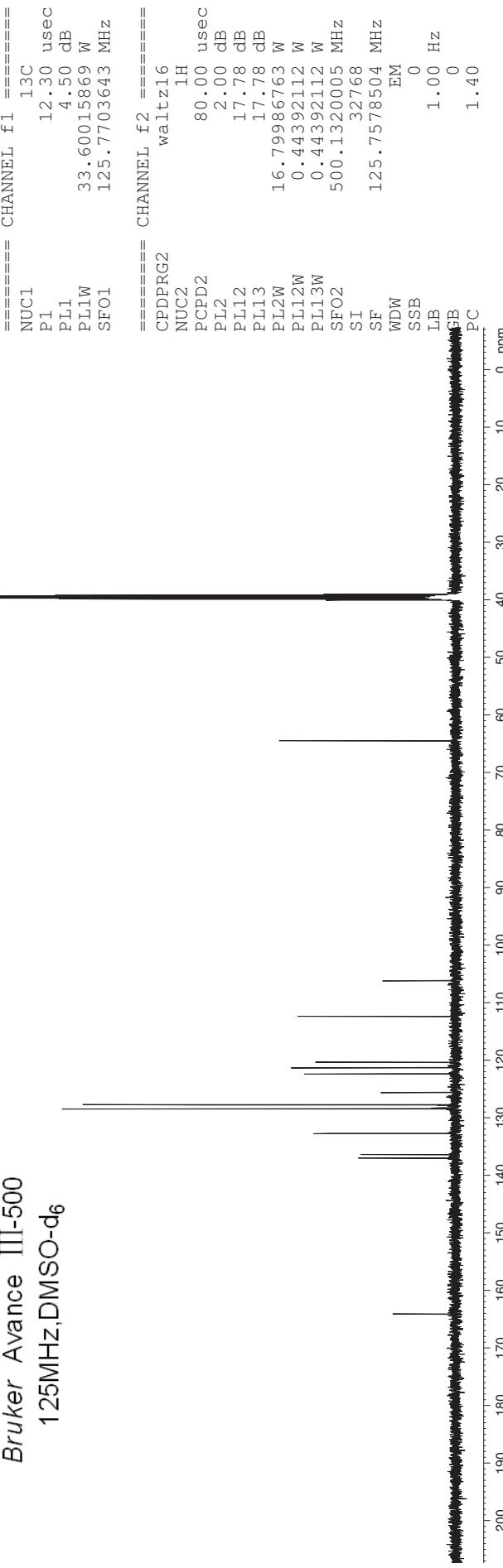
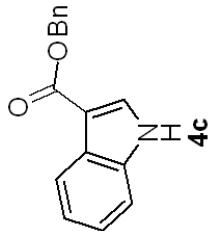


liushouxin-xh-cbz-cl-C



NAME 2016.04.27  
EXPNO 14  
PROCNO 1  
Date\_ 20160427  
Time 14.06  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgppg30  
TD 32768  
SOLVENT DMSO  
NS 142  
DS 0  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 0.5505524 sec  
RG 2050  
DW 16.800 usec  
DE 6.50 usec  
TE 298.3 K  
D1 2.0000000 sec  
D11 0.03000000 sec  
TD0 1

Bruker Avance III-500  
125MHz, DMSO-d<sub>6</sub>





```

NAME          2016.06.16
EXNO           8
PROCNO          1
Date_        20160616
Time         20.18
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD        65536
SOLVENT    DMSO
NS            4
DS             0
SWH       10330.578 Hz
FIDRES   0.157632 Hz
AQ        3.1719923 sec
RG          256
DW        48.400 usec
DE          6.50 usec
TE        297.4 K
D1     1.00000000 sec
TDO0
===== CHANNEL f1 =====
NUC1          1H
P1        13.00 usec
PL1          2.00 CB
PL1W      16.79386763 W
SFO1      500.1330885 MHz
SI          32768
SF        500.1300098 MHz
WDW
SSB
LB          0.30 Hz
GB          0
PC        1.00

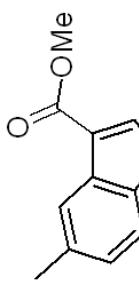
```

2.507  
2.503  
2.500  
2.496  
2.493  
2.407

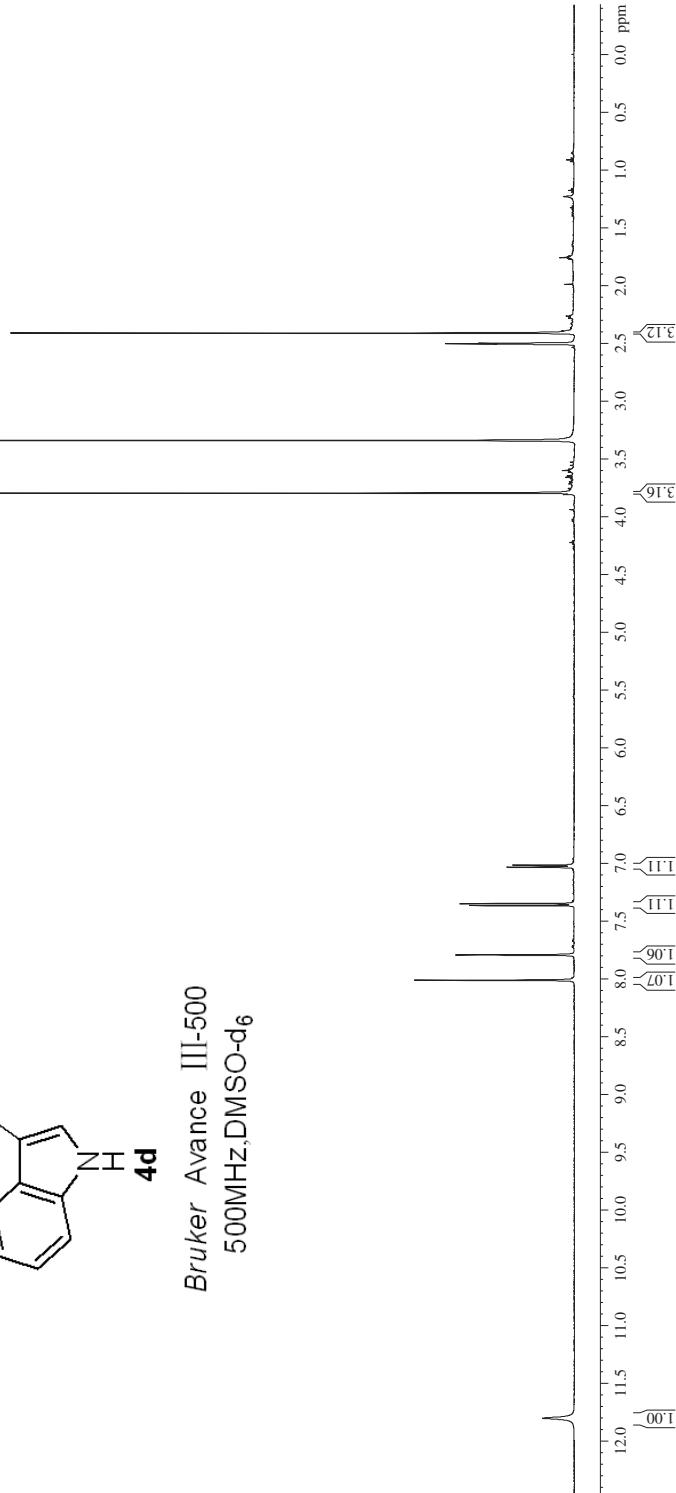
3.337  
3.792

7.013  
7.016  
7.016  
7.029  
7.032  
7.346  
7.363  
7.790

11.800



**4d**  
*Bruker Avance III-500*  
500MHz,DMSO-d<sub>6</sub>





```

=====
NAME          2016.06.16
EXPNO         9
PROCNO        1
Date_         20160616
Time          20.23
INSTRUM      spect
PROBHD       5 mm PABBO BB-
PULPROG      zgpp30
TD            32768
SOLVENT       DMSO
NS            630
DS            0
SWH          29761.904 Hz
FIDRES       0.908261 Hz
AQ            0.5505524 sec
RG            2050
DW            16.800 usec
DE            6.500 usec
TE            298.7 K
D1            2.0000000 sec
D11           0.03000000 sec
TD0            1

=====
CHANNEL f1
=====
NUC1          13C
P1            12.30 usec
PL1           4.50 dB
PLL1          33.60015869 W
PLL1W         125.7703643 MHz
SFO1          EM

=====
CHANNEL f2
=====
CPDPRG2      Waltz16
NUC2          1H
PCPD2         80.00 usec
PL12          2.00 dB
PL12W         17.78 dB
PL13          17.78 dB
PL13W         16.79986763 W
PL12W         0.44392112 W
PLL13W        0.44392112 W
SFO2          500.1320005 MHz
SI             32768
SF             125.7578507 MHz
WDW           EM
SSB           0
LB             1.00 Hz
PC             0
PC             1.40

```

Bruker Avance III-500  
125MHz,DMSO-d<sub>6</sub>

**4d**



2.406  
2.493  
2.497  
2.500  
2.504  
2.507  
3.322  
4.757  
4.760  
4.763  
4.767  
4.770  
4.773  
5.229  
5.242  
5.245  
5.248  
5.260  
5.263  
5.266  
5.269  
5.377  
5.381  
5.384  
5.388  
5.412  
5.415  
5.419  
5.422  
6.026  
6.037  
6.048  
6.058  
6.061  
6.069  
6.071  
6.082  
6.092  
6.103  
7.019  
7.022  
7.035  
7.038  
7.352  
7.369  
7.792  
7.793  
8.040  
8.046

— 11.829 —

```

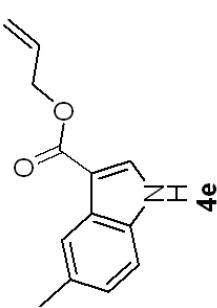
NAME          2016.05.20
EXNO          9
PROCNO        1
Date_-
Time         18.44
INSTRUM      spect
PROBHD       5 mm PABBO BB-
PULPROG      zg30
TD           65536
SOLVENT      DMSO
NS            16
DS            0
SWH          10330.578 Hz
FIDRES       0.157632 Hz
AQ            3.1719923 sec
RG            362
DW            48.400 usec
DE            6.50 usec
TE            298.3 K
D1           1.00000000 sec
TDO          1

```

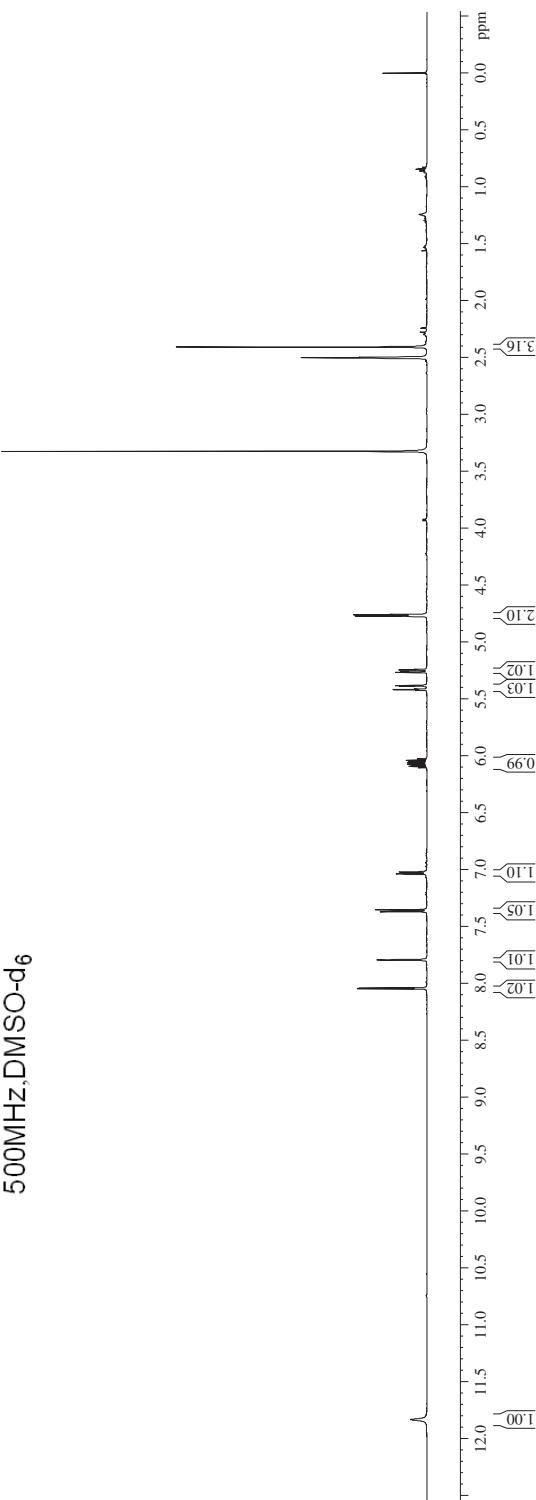
```

===== CHANNEL f1 =====
NUC1          1H
P1            13.00 usec
PL1           2.00 CB
PL1W          16.79386763 W
SF01          500.1330885 MHz
SI             32768
SF            500.1300102 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB           0
PC            1.00

```



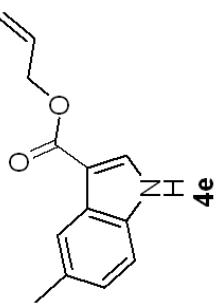
Bruker Avance III-500  
500MHz,DMSO-d<sub>6</sub>



liushouxin-xh-5- $\chi_1$

163.98

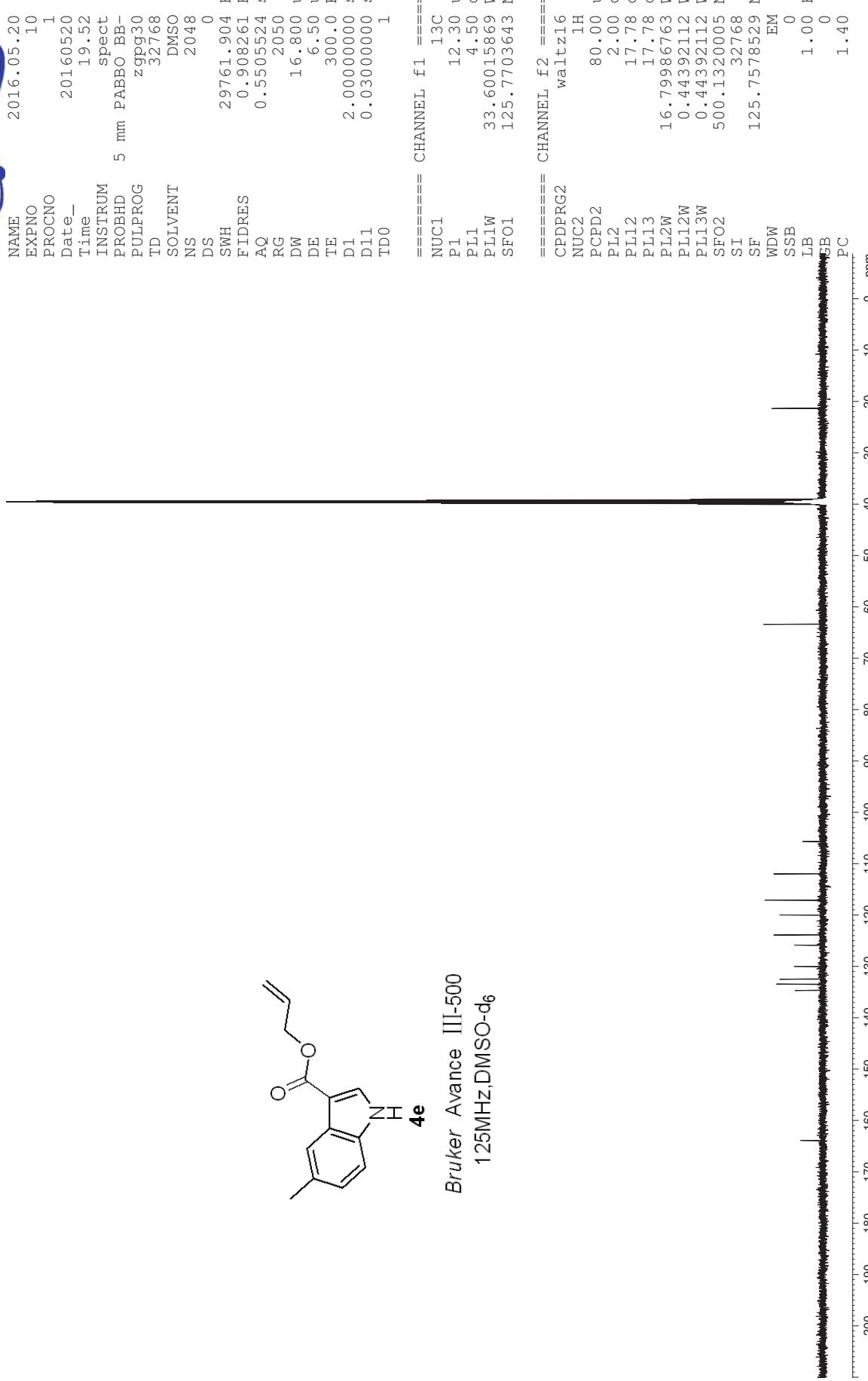
134.71  
133.50  
132.49  
130.01  
125.91  
123.89  
120.03  
117.14  
112.00  
105.68



Bruker Avance III-500  
125MHz,DMSO-d<sub>6</sub>

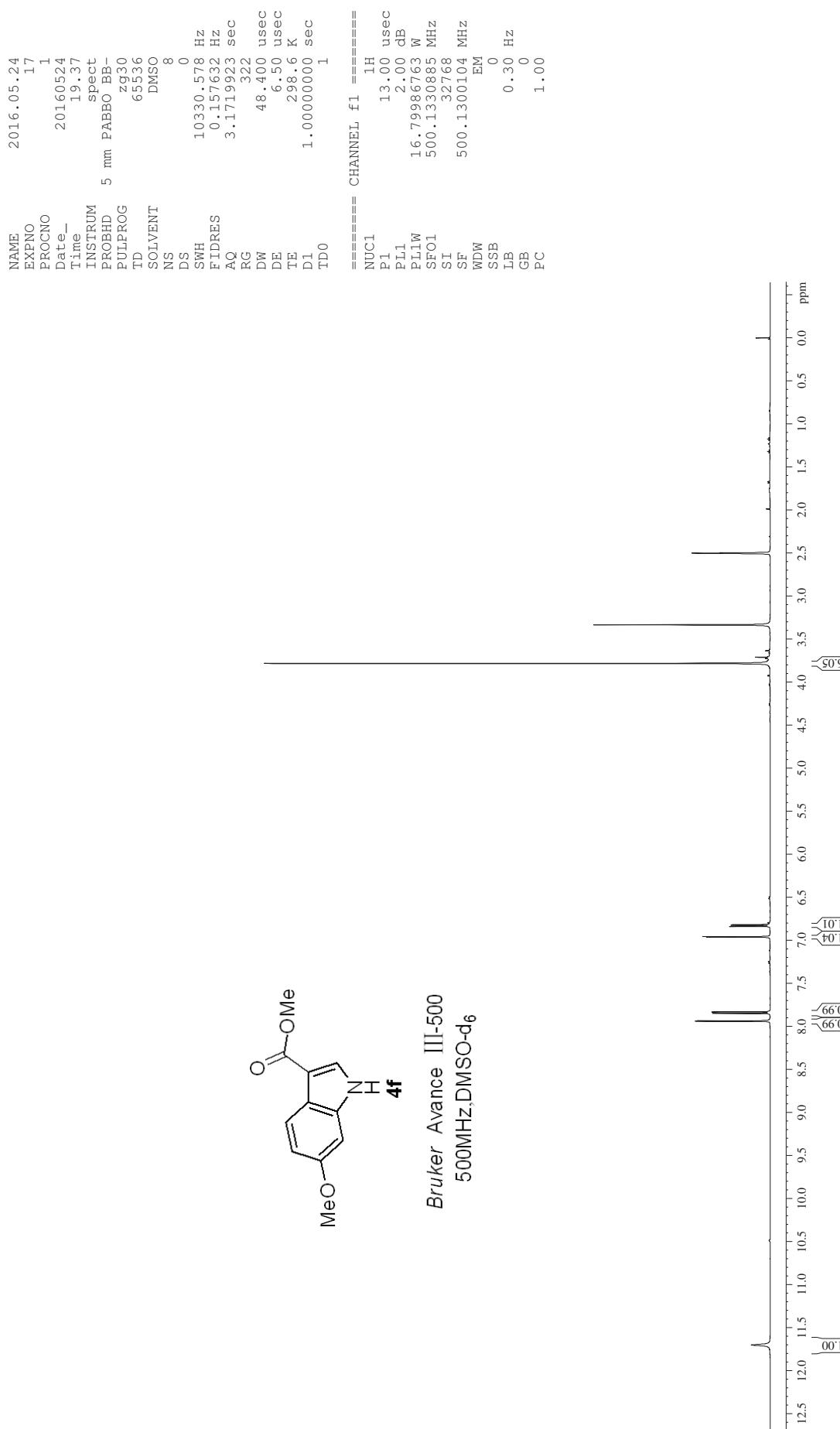
— 21.32 —

— 63.39 —





11.696  
 11.696  
 3.782  
 3.782  
 V  
 3.780  
 3.780  
 —  
 3.333  
 —  
 2.507  
 2.507  
 2.504  
 2.504  
 2.500  
 2.500  
 2.496  
 2.496  
 2.493  
 2.493



39.02  
39.19  
39.35  
39.52  
39.69  
39.85  
40.02  
40.54  
50.19  
55.02

95.16  
106.34  
111.33  
119.64  
120.99  
131.20  
137.13  
156.10  
164.75



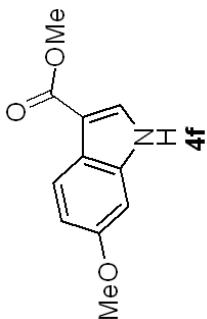
```

=====
NAME          2016.05.24
EXPNO         18
PROCNO        1
Date_         20160524
Time         19.49
INSTRUM      spect
PROBHD      5 mm PABBO BB-
PULPROG    zgppg30
TD           32768
SOLVENT      DMSO
NS            301
DS            0
SWH         29761.904 Hz
FIDRES       0.908261 Hz
AQ            0.5005524 sec
RG            2050
DW           16.800 usec
DE            6.500 usec
TE           300.1 K
D1           2.0000000 sec
D11          0.03000000 sec
TD0            1

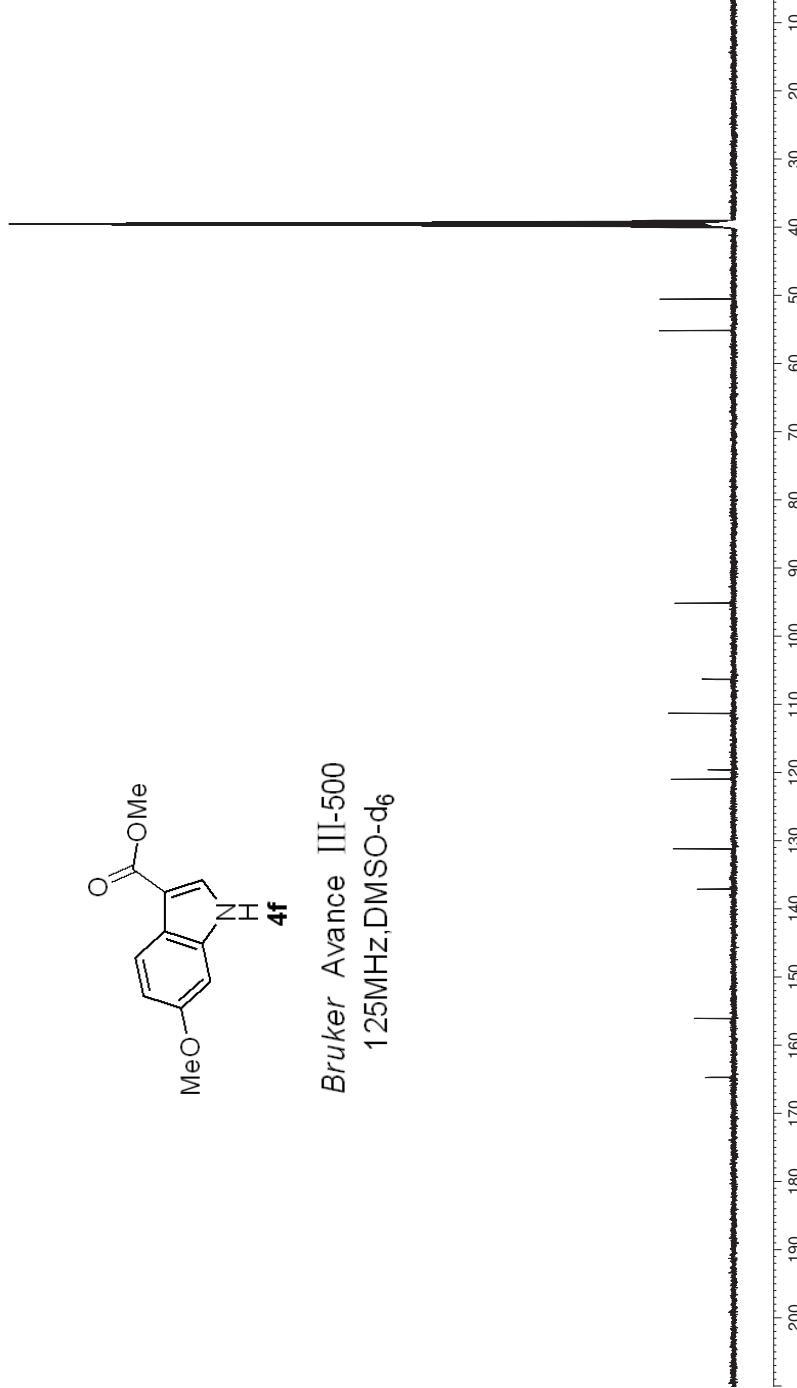
=====
```

```

===== CHANNEL f1 =====
NUC1          13C
P1            12.30 usec
PL1          4.50 dB
PL1W         33.60015869 MHz
SFO1        125.7703643 MHz
===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2          1H
PCPD2         80.00 usec
PL12          2.00 dB
PL12          17.78 dB
PL13          17.78 dB
PL2W         16.79986763 W
PL12W        0.44392112 W
PL13W        0.44392112 W
SFO2        500.1320005 MHz
SI             32768 MHz
SF           125.7578525 MHz
WDW          EM
SSB           0 Hz
LB            0
PC           1.40
```

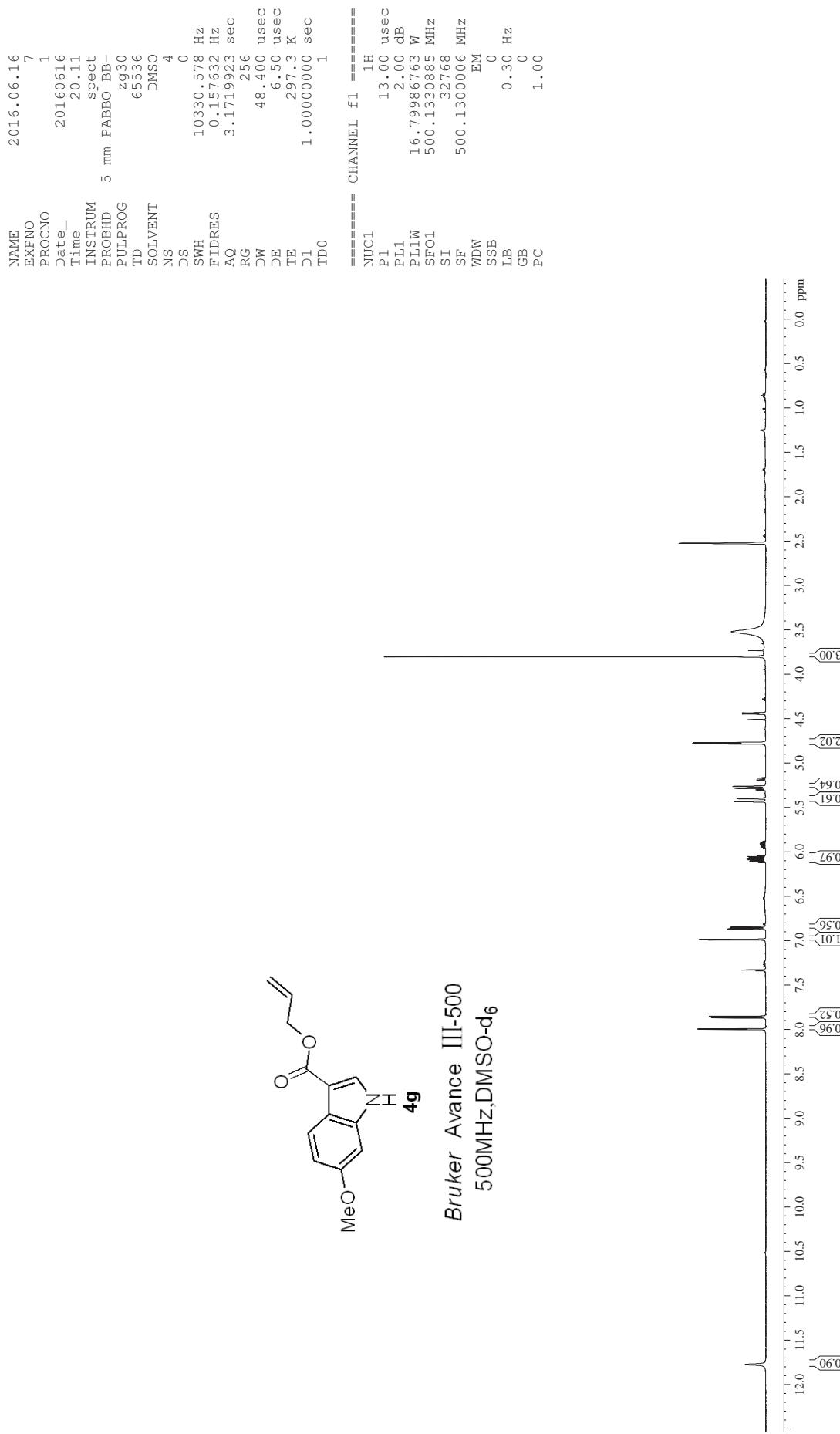


Bruker Avance III-500  
125MHz,DMSO-d<sub>6</sub>

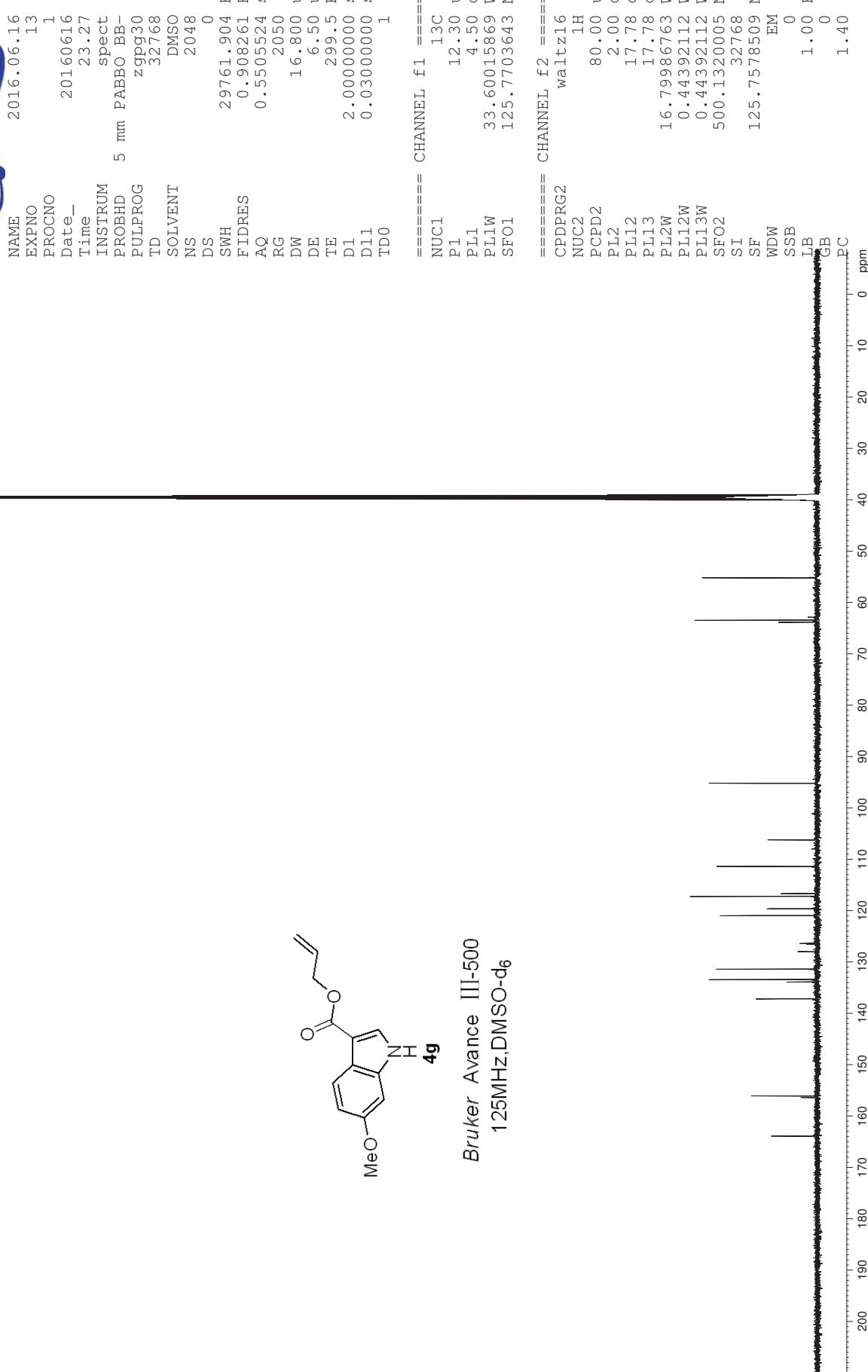
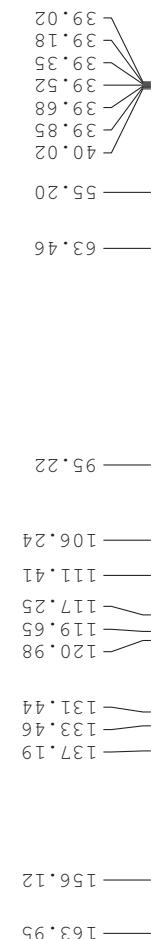




11.748  
7.978 7.972 7.848 7.830 6.986 6.984 6.823 6.828 6.976 6.978 6.041 6.031 6.020 5.416 5.413 5.410 5.407 5.379 5.375 5.372 5.274 5.277 5.281 5.262 5.249 5.241 5.249 5.239 4.756 4.758 4.748 4.730 4.736 4.739 4.749 4.750 4.753 4.756 4.758 4.761 3.780 3.498 3.497 2.503 2.500 2.497 2.420 2.403



liushouxin-xh





2.507  
2.504  
2.500  
2.497  
2.493

3.334  
3.775

5.312

6.996  
6.961  
6.929  
6.893  
6.861  
6.834  
6.811  
6.816

11.756

```

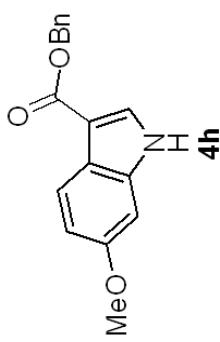
NAME          2016.06.16
EXNO           6
PROCNO        1
Date_        20160616
Time         20.05
INSTRUM     spect
PROBHD      5 mm PABBO BB-
PULPROG    zg30
TD        65536
SOLVENT      DMSO
NS            4
DS            0
SWH       10330.578 Hz
FIDRES    0.157632 Hz
AQ        3.1719923 sec
RG            256
DW        48.400 usec
DE        6.50 usec
TE        297.4 K
D1      1.00000000 sec
TDO          1

```

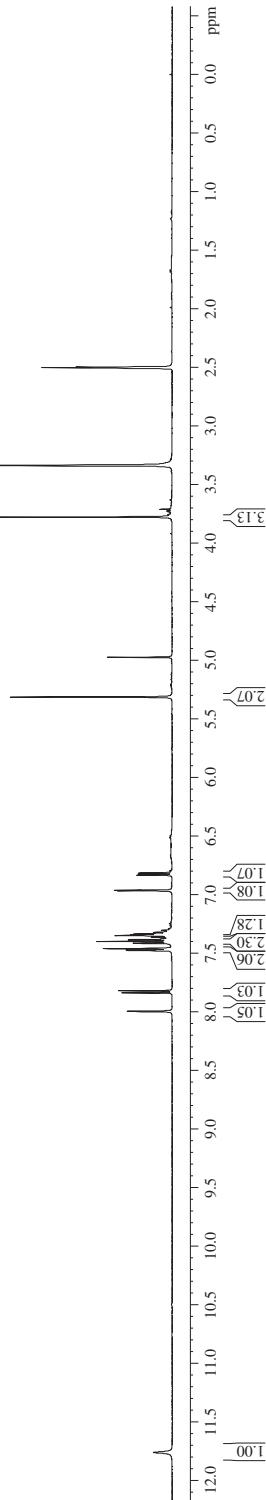
```

===== CHANNEL f1 =====
NUC1          1H
P1        13.00 usec
PL1          2.00 CB
PL1W      16.79386763 W
SF01      500.1330885 MHz
SI            32768
SF      500.1300098 MHz
WDW          EM
SSB            0
LB        0.30 Hz
GB            0
PC        1.00

```



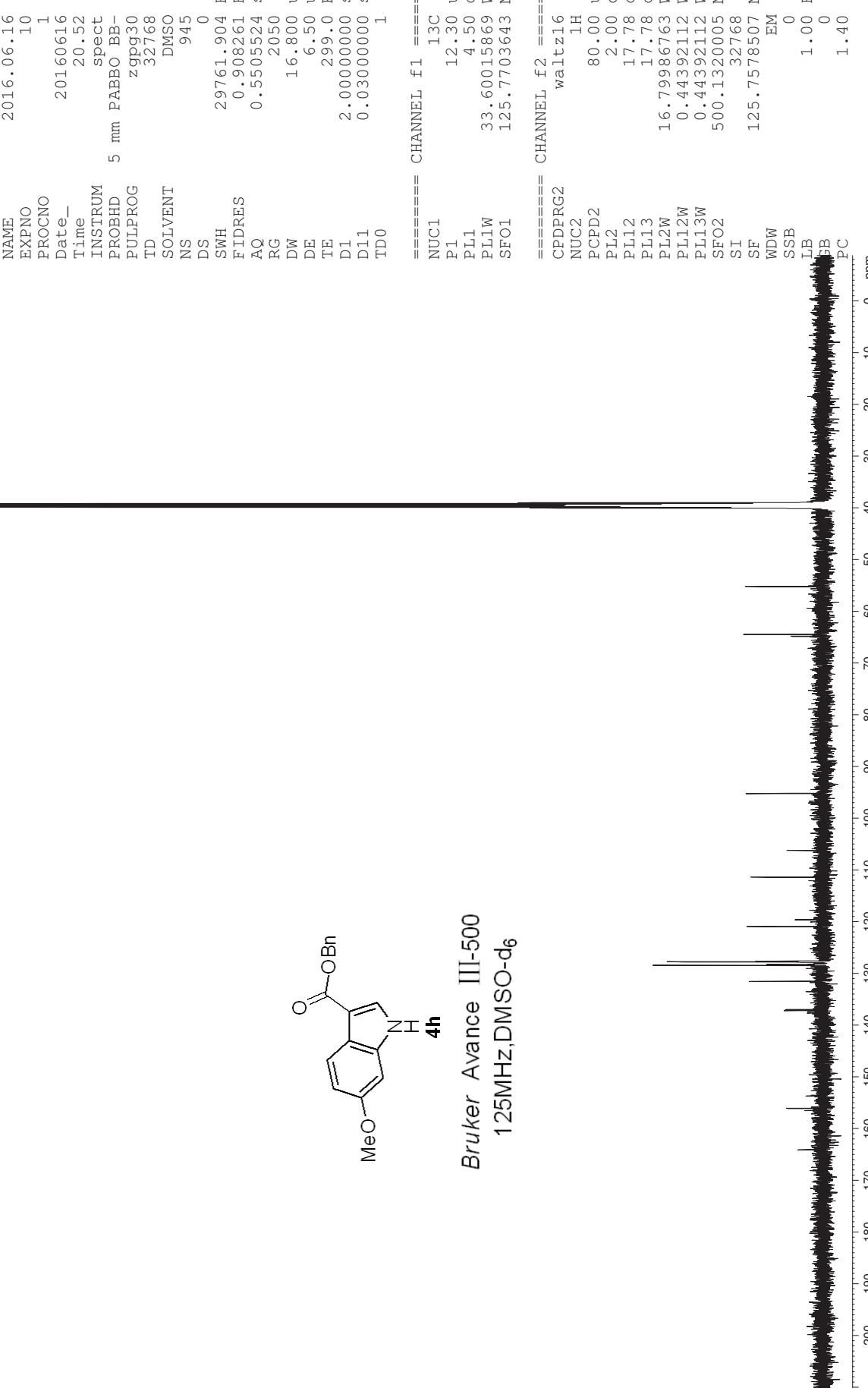
Bruker Avance III-500  
500MHz,DMSO-d<sub>6</sub>



liushouxin-6-cbz



137.21  
131.03  
128.31  
128.46  
128.58  
127.77  
127.67  
120.96  
111.42  
106.24  
95.25  
64.46  
55.20  
40.02  
39.85  
39.69  
39.66  
39.52  
39.19  
39.02  
39.02





2.507  
2.504  
2.500  
2.497  
2.493

3.621

7.007  
7.009  
7.022  
7.036  
7.038  
7.059  
7.073  
7.075  
7.087  
7.089  
7.132  
7.1347  
7.1365  
7.1633  
7.1705  
7.1721

11.252

```

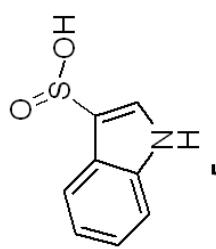
NAME          2016.05.27
EXNO           31
PROCNO        1
Date_-
Time         20160528
INSTRUM      spect
PROBHD      5 mm PABBO BB-
PULPROG    zg30
TD        65536
SOLVENT      DMSO
NS            4
DS            0
SWH       10330.578 Hz
FIDRES     0.157632 Hz
AQ        3.1719923 sec
RG            322
DW        48.400 usec
DE        6.50 usec
TE        298.1 K
D1      1.00000000 sec
TDO0          1

```

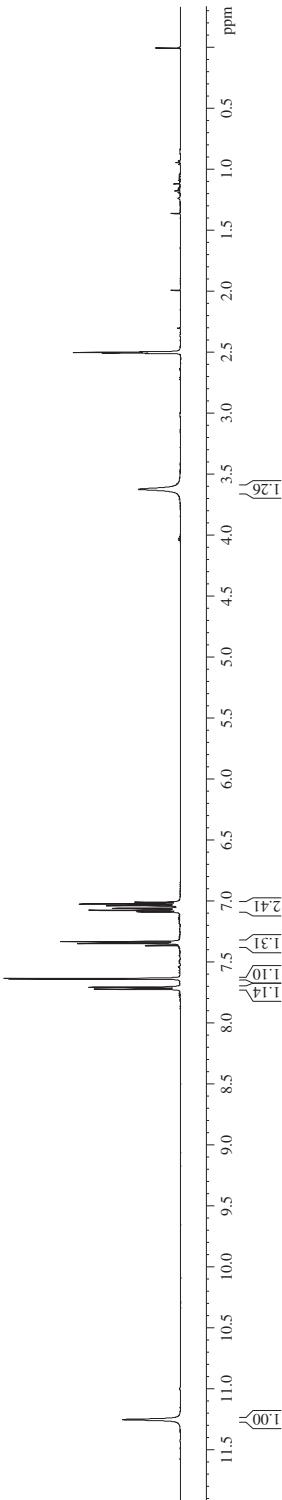
```

===== CHANNEL f1 =====
NUC1           1H
P1            13.00 usec
PL1           2.00 CB
PL1W        16.79386763 W
SF01        500.1330885 MHz
SI             32768
SF           500.1300103 MHz
WDW           EM
SSB            0
LB            0.30 Hz
GB            0
PC           1.00

```



Bruker Avance III-500  
500MHz,DMSO-d<sub>6</sub>



40.02  
39.85  
39.69  
39.52  
39.35  
39.19  
39.02  
39.00



```

=====
NAME          2016.05.27
EXPNO         32
PROCNO        1
Date_         20160528
Time          8.55
INSTRUM      spect
PROBHD       5 mm PABBO BB-
PULPROG      zppg30
TD           32768
SOLVENT      DMSO
NS            1024
DS            0
SWH          29761.904 Hz
FIDRES       0.908261 Hz
AQ            0.5505524 sec
RG            2050
DW           16.800 usec
DE           6.500 usec
TE           298.7 K
D1           2.0000000 sec
D11          0.03000000 sec
TD0           1

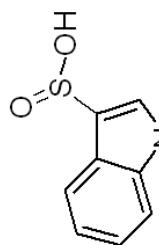
=====
```

```

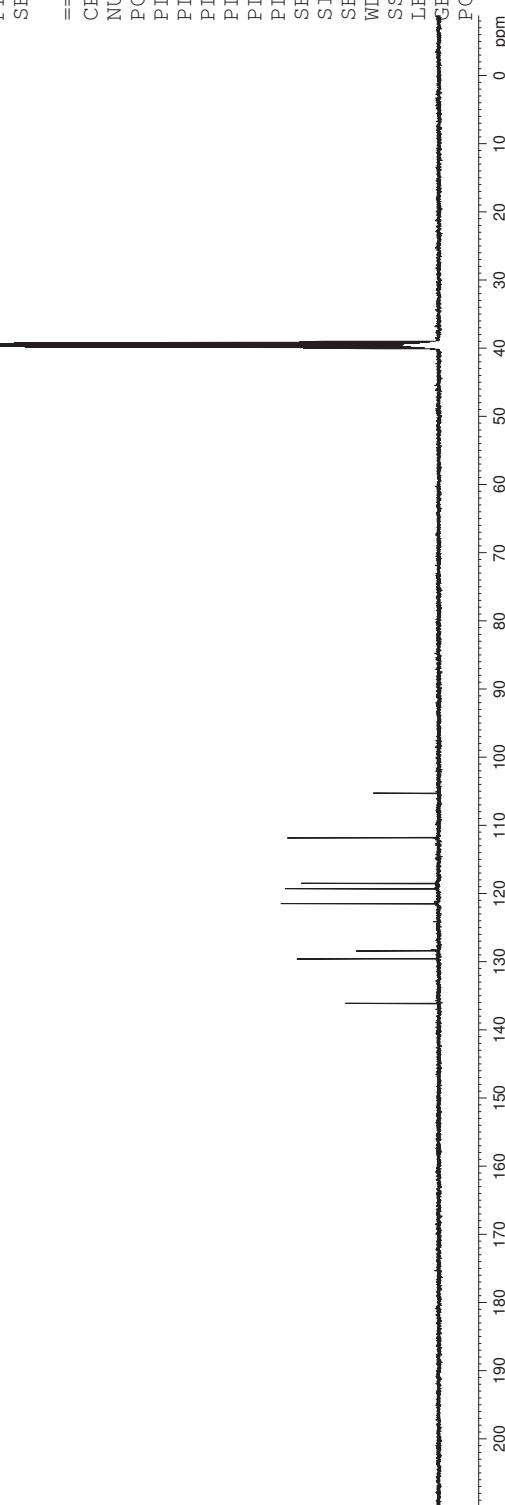
===== CHANNEL f1 =====
NUC1          13C
P1            12.30 usec
PL1          4.50 dB
PL1W         33.60015869 W
SFO1         125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2          1H
PCPD2         80.00 usec
PL12          2.00 dB
PL12          17.78 dB
PL13          17.78 dB
PL2W          16.79986763 W
PL12W         0.44392112 W
PL13W         0.44392112 W
SFO2         500.1320005 MHz
SI            32768
SF           125.7578530 MHz
WDW          0
SSB          1.00 Hz
LB            0
PC           1.40

=====
```



**5a**  
*Bruker Avance III-500*  
125MHz,DMSO-d<sub>6</sub>





3.329  
2.588  
2.507  
2.504  
2.500  
2.496  
2.493

11.177  
7.327  
7.225  
7.213  
7.211  
6.996  
6.984  
6.981  
6.969  
6.953  
6.950  
6.938  
6.936

```

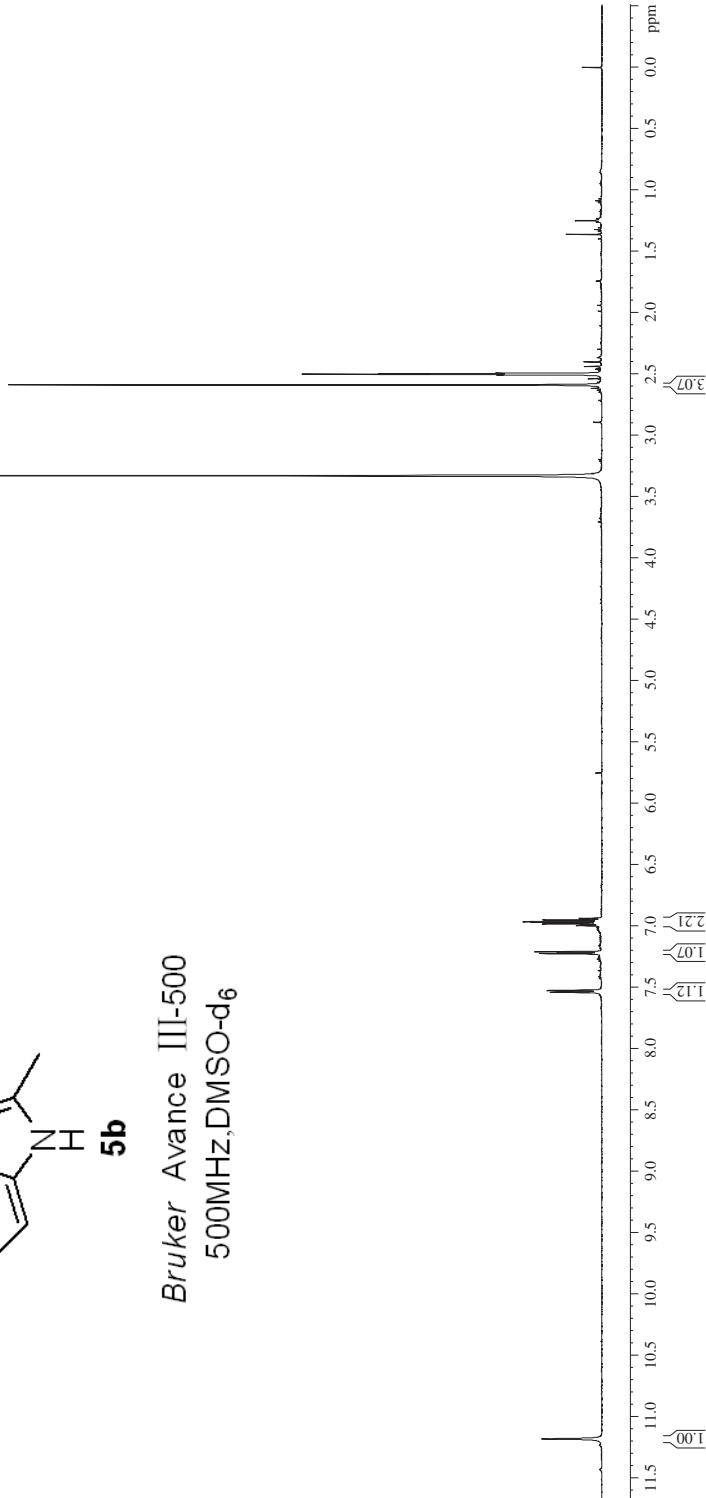
NAME          2016.06.02
EXNO          14
PROCNO        1
Date_-
Time         16.49
INSTRUM      spect
PROBHD      5 mm PABBO BB-
PULPROG     zg30
TD           65536
SOLVENT      DMSO
NS            4
DS            0
SWH          10330.578 Hz
FIDRES       0.157632 Hz
AQ           3.1719923 sec
RG           406
DW           48.400 usec
DE           6.50  usec
TE           298.0 K
D1           1.00000000 sec
TDO          1

```

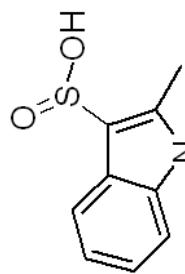
```

===== CHANNEL f1 =====
NUC1          1H
P1           13.00 usec
PL1          2.00  CB
PL1W        16.79386763 W
SFO1        500.1330885 MHz
SI            32768
SF           500.1300103 MHz
WDW          0
SSB          0.30  Hz
LB           0
GB           0
PC           1.00

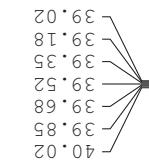
```



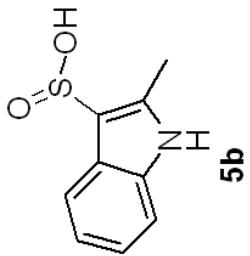
**5b**  
*Bruker Avance III-500*  
 500MHz,DMSO-d<sub>6</sub>



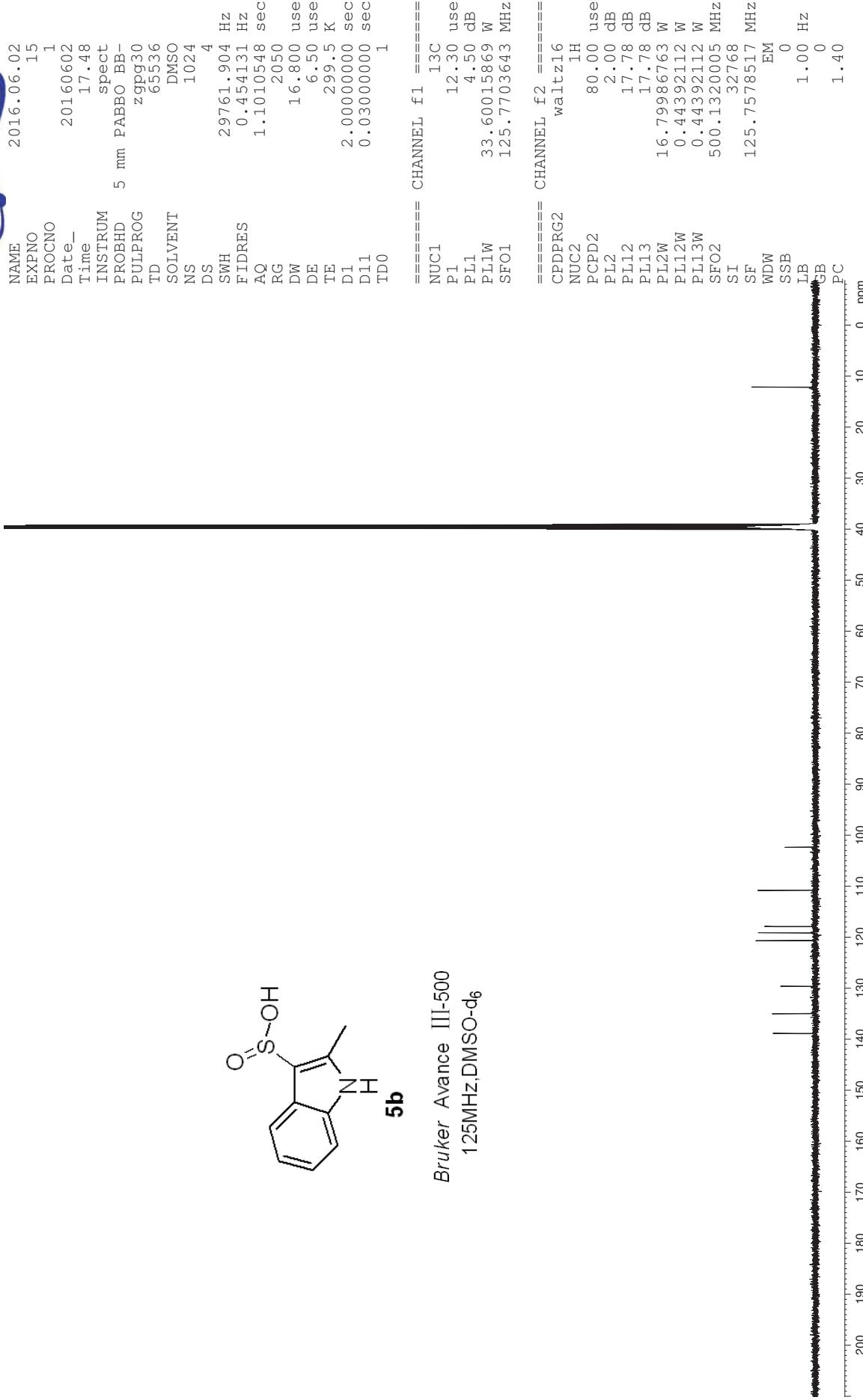
— 12.14 —



— 102.36 —  
 110.83  
 117.93  
 119.14  
 120.70  
 129.65  
 135.02  
 138.91



Bruker Avance III-500  
 125MHz,DMSO-d<sub>6</sub>



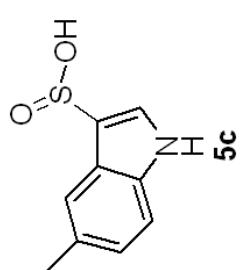


2.504  
2.500  
2.497  
2.369

—3.917—

7.553  
7.548  
7.509  
7.232  
7.216  
6.906  
6.909  
6.892  
6.890

—11.107—



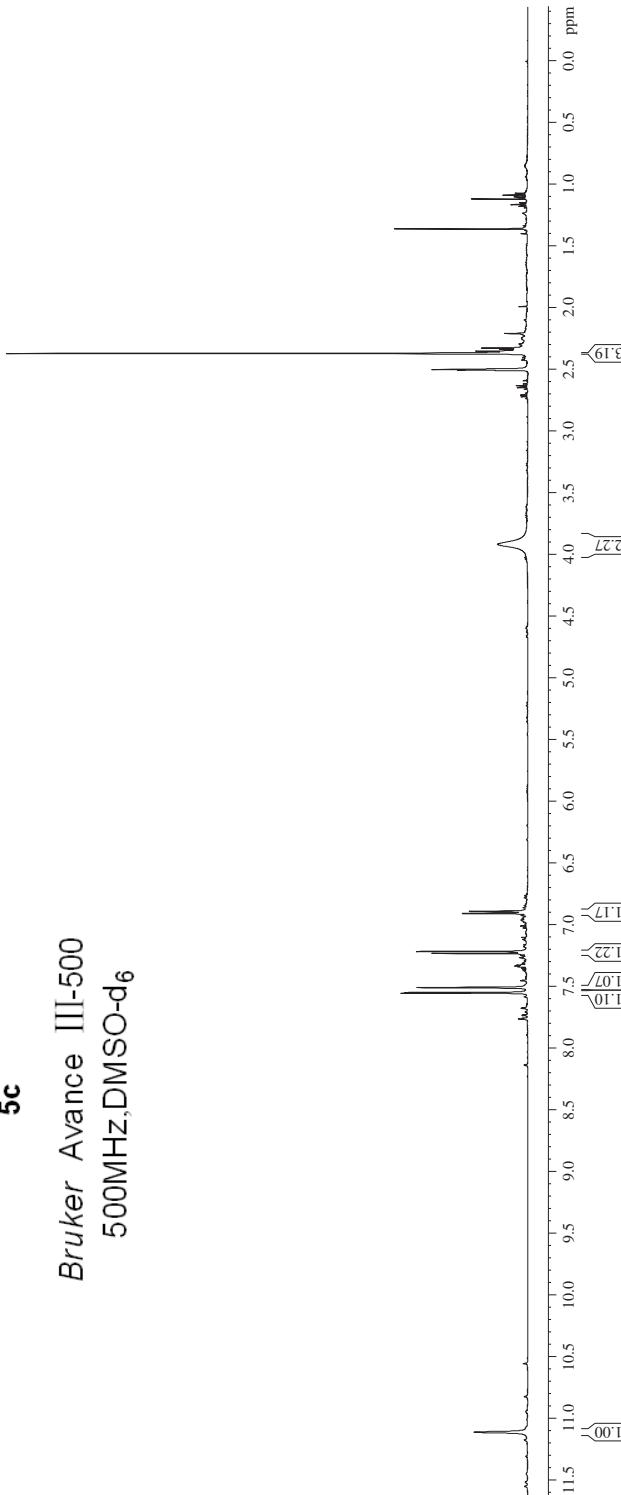
Bruker Avance III-500  
500MHz,DMSO-d<sub>6</sub>

```

NAME          2016.06.02
EXNO          13
PROCNO        1
Date_-
Time         16.44
INSTRUM      spect
PROBHD      5 mm PABBO BB-
PULPROG     zg30
TD           65536
SOLVENT      DMSO
NS            4
DS            0
SWH          10330.578 Hz
FIDRES       0.157632 Hz
AQ           3.1719923 sec
RG           228
DW           48.400 usec
DE           6.50 usec
TE           298.0 K
D1           1.00000000 sec
TDO          1

===== CHANNEL f1 =====
NUC1          1H
P1           13.00 usec
PL1          2.00 CB
PL1W        16.79386763 W
SF01        500.1330885 MHz
SI           32768
SF          500.1300102 MHz
WDW          EM
SSB          0
LB          0.30 Hz
GB          0
PC          1.00

```







2.724  
2.507  
2.503  
2.500  
2.496

3.388

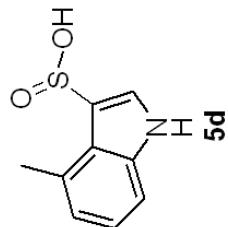
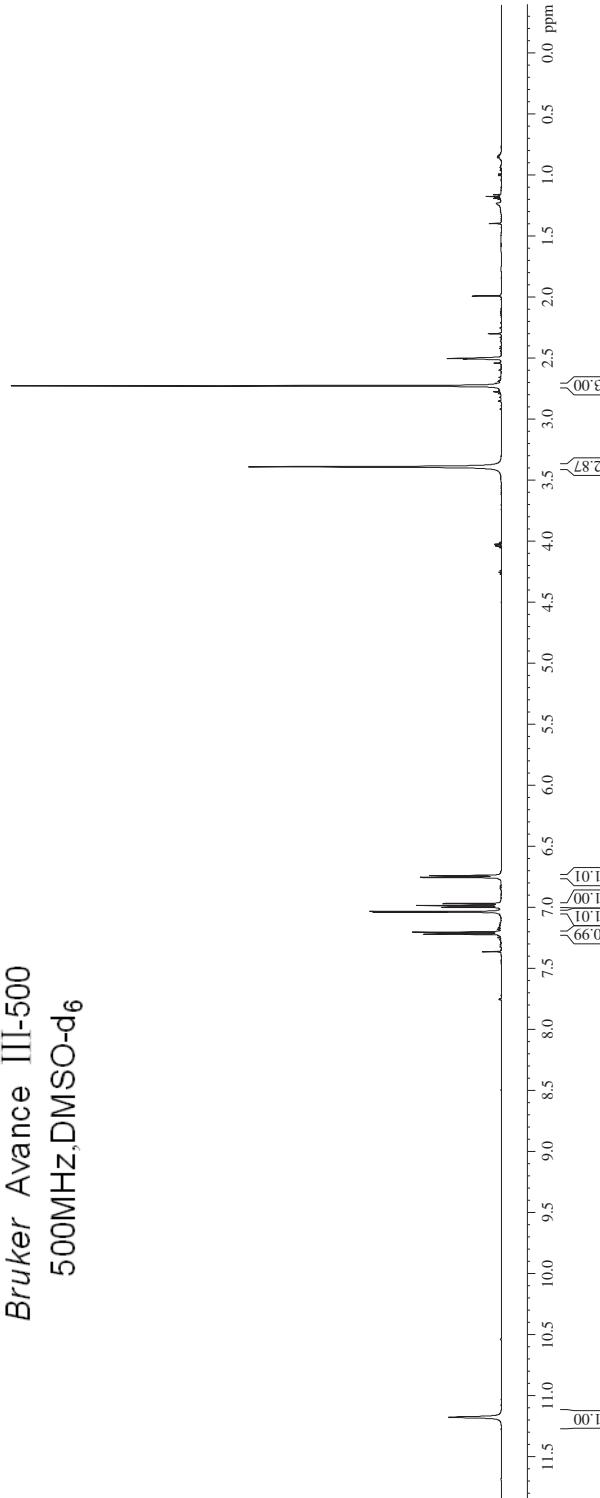
7.217  
7.201  
7.193  
7.032  
6.997  
6.983  
6.967  
6.753  
6.738

11.176

```

NAME          2016.06.03
EXNO           5
PROCNO        1
Date_-
Time         20160603
21.45
INSTRUM      spect
PROBHD      5 mm PABBO BB-
PULPROG    zg30
TD        65536
SOLVENT      DMSO
NS            8
DS            0
SWH       10330.578 Hz
FIDRES     0.157632 Hz
AQ        3.1719923 sec
RG          181
DW        48.400 usec
DE          6.50 usec
TE        298.0 K
D1        1.00000000 sec
TDO        1

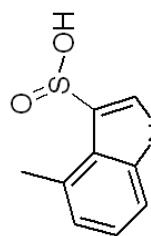
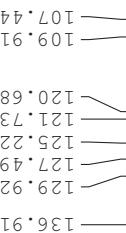
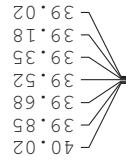
```



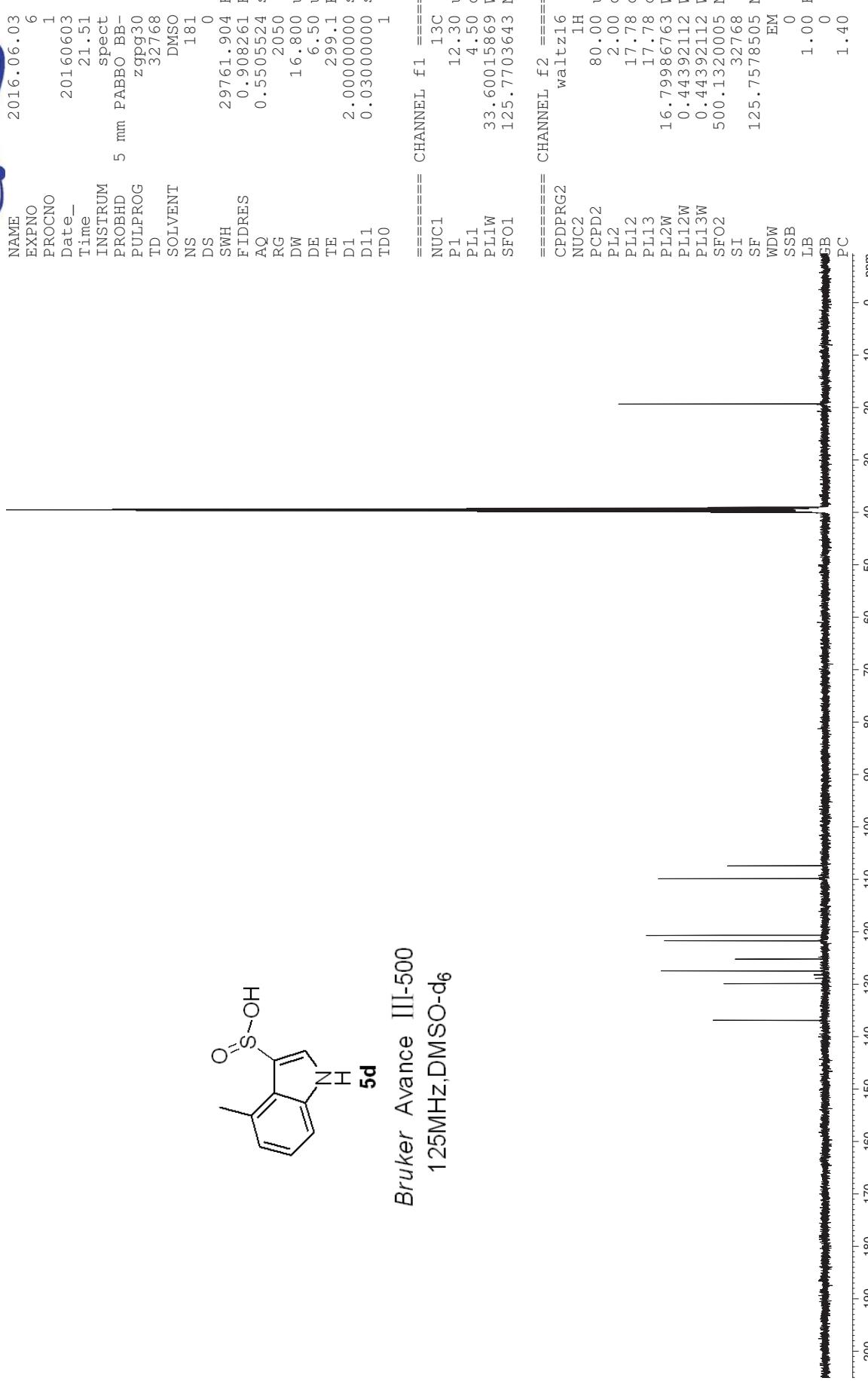
Bruker Avance III-500  
500MHz,DMSO-d<sub>6</sub>



19.33



Bruker Avance III-500  
125MHz, DMSO-d<sub>6</sub>





2.507  
2.504  
2.500  
2.496  
2.493

3.337

7.005  
7.007  
7.019  
7.020  
7.034  
7.036  
7.055  
7.057  
7.071  
7.073  
7.083  
7.087  
7.329  
7.345  
7.356  
7.631  
7.636  
7.702  
7.717

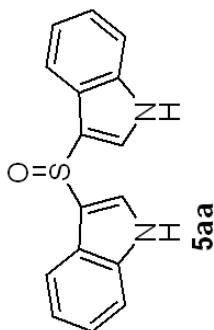
11.246

```

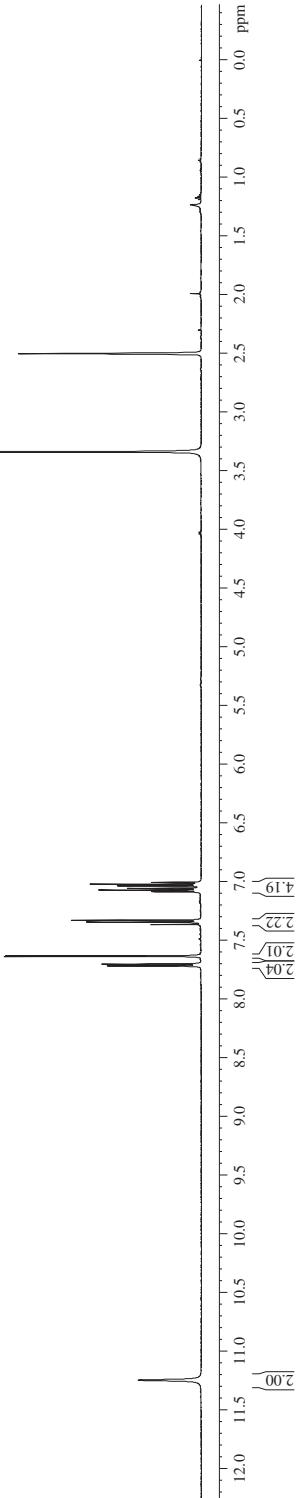
NAME          2016.06.22
EXNO           4
PROCNO        1
Date_-
Time         12.56
INSTRUM     spect
PROBHD      5 mm PABBO BB-
PULPROG    zg30
TD        65536
SOLVENT      DMSO
NS            4
DS            0
SWH       10330.578 Hz
FIDRES     0.157632 Hz
AQ        3.1719923 sec
RG            362
DW        48.400 usec
DE          6.50 usec
TE        297.7 K
D1       1.00000000 sec
TDO          1

===== CHANNEL f1 =====
NUC1           1H
P1            13.00 usec
PL1           2.00 CB
PL1W        16.79386763 W
SF01        500.1330885 MHz
SI            322768
SF        500.1300093 MHz
WDW           EM
SSB            0
LB          0.30 Hz
GB            0
PC          1.00

```



Bruker Avance III-500  
500MHz,DMSO-d<sub>6</sub>



39.02  
39.19  
39.35  
39.52  
39.69  
39.85  
39.92  
40.02

105.31  
111.87  
118.55  
119.35  
121.52  
128.45  
129.62  
136.15



```

=====
NAME          2016.06.22
EXPNO         5
PROCNO        1
Date_         20160622
Time          13.00
INSTRUM       spect
PROBHD       5 mm PABBO BB-
PULPROG      zgppg30
TD            32768
SOLVENT       DMSO
NS             301
DS             0
SWH           29761.904 Hz
FIDRES       0.908261 Hz
AQ            0.5505524 sec
RG            2050
DW            16.800 usec
DE            6.500 usec
TE            298.8 K
D1            2.0000000 sec
D11           0.03000000 sec
TD0            1

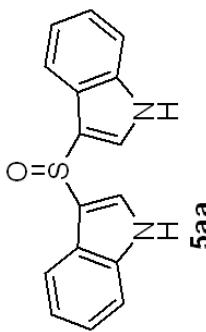
=====
```

```

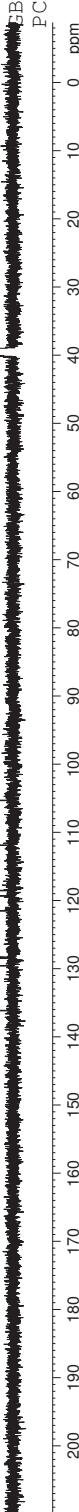
===== CHANNEL f1 =====
NUC1          13C
P1            12.30 usec
PL1           4.50 dB
PL1W          33.60015869 W
SFO1          125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2          1H
PCPD2         80.00 usec
PL12          2.00 dB
PL12          17.78 dB
PL13          17.78 dB
PL2W          16.79986763 W
PL12W         0.44392112 W
PL13W         0.44392112 W
SFO2          500.1320005 MHz
SI             32768
SF             125.7578509 MHz
WDW           0
SSB           1.00 Hz
LB            0
JB             1.40 PC

=====
```



Bruker Avance II-500  
125MHz,DMSO-d<sub>6</sub>



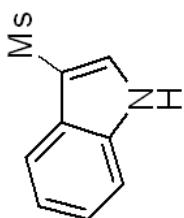


```

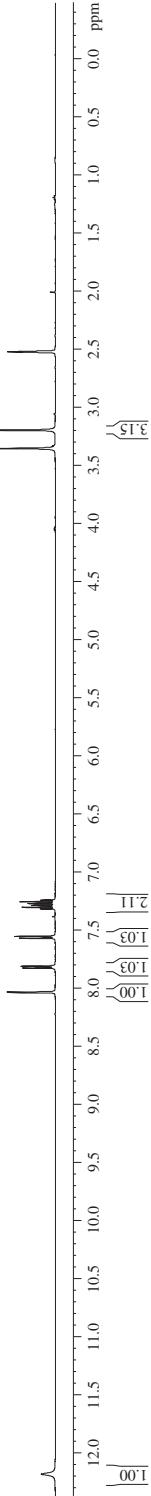
NAME          2016.05.3
EXNO          10
PROCNO        1
Date_-
Time         20160503
21.58
INSTRUM      spect
PROBHD      5 mm PABBO BB-
PULPROG    zg30
TD        65536
SOLVENT      DMSO
NS           8
DS
SWH       10330.578 Hz
FIDRES     0.157632 Hz
AQ        3.1719923 sec
RG           322
DW        48.400 usec
DE        6.50 usec
TE        298.0 K
D1      1.00000000 sec
TDO
===== CHANNEL f1 =====
NUC1          1H
P1            13.00 usec
PL1           2.00 CB
PL1W        16.79386763 W
SF01        500.1330885 MHz
SI            32768
SF           500.1300004 MHz
WDW
SSB
LB           0.30 Hz
GB           0
PC           1.00

```

12.178 ——————  
8.032 ——————  
7.890 ——————  
7.868 ——————  
7.562 ——————  
7.317 ——————  
7.315 ——————  
7.301 ——————  
7.287 ——————  
7.285 ——————  
7.271 ——————  
7.269 ——————  
7.255 ——————  
7.241 ——————  
7.240 ——————  
2.523 ——————  
3.195 ——————  
3.353 ——————  
2.520 ——————  
2.516 ——————

**6a**

Bruker Avance III-500  
500MHz,DMSO-d<sub>6</sub>



**6a**

Bruker Avance II-500  
125MHz,DMSO-d<sub>6</sub>



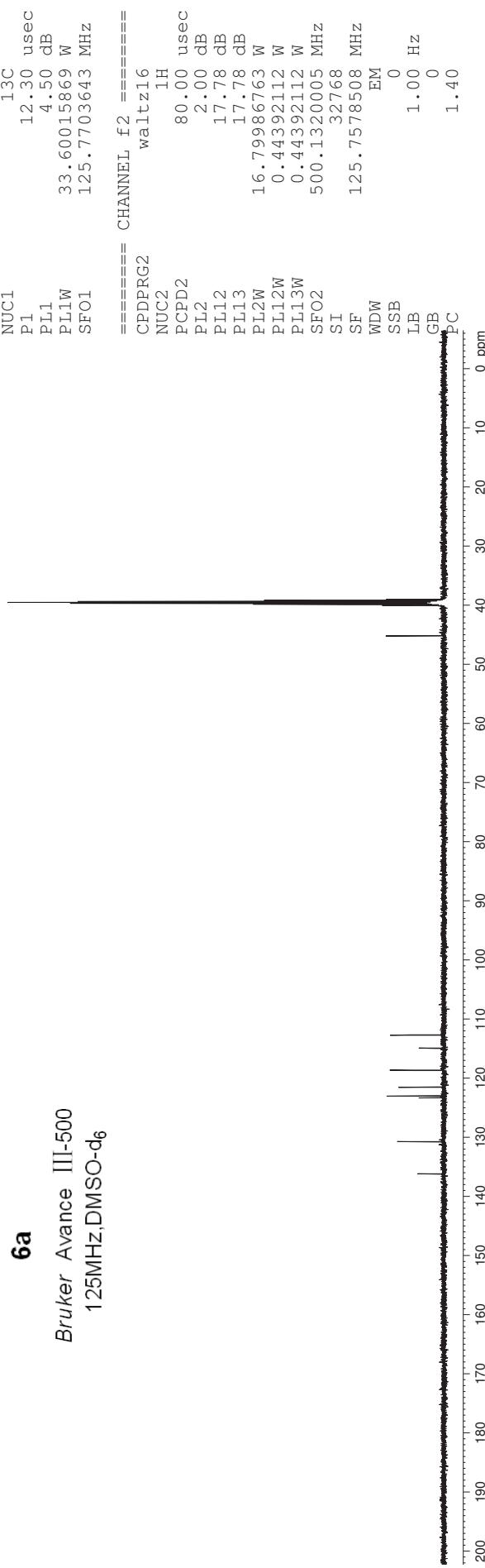
```

=====
NAME          2016.5.3
EXPNO         11
PROCNO        1
Date_        20160503
Time       22.05
INSTRUM      spect
PROBHD      5 mm PABBO BB-
PULPROG    zgppg30
TD        65536
SOLVENT      DMSO
NS           96
DS            4
SWH       29761.904 Hz
FIDRES     0.454131 Hz
AQ        1.1010548 sec
RG          2050
DW        16.800 usec
DE          6.50  usec
TE        298.9 K
D1        2.0000000 sec
D11       0.03000000 sec
TD0          1

===== CHANNEL f1 =====
NUC1        13C
P1        12.30 usec
PL1        4.50 dB
PLL1W     33.60015869 W
SFO1      125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2        1H
PCPD2      80.00 usec
PL12       2.00 dB
PL12        17.78 dB
PL13       17.78 dB
PL2W      16.79986763 W
PL12W     0.44392112 W
PL13W     0.44392112 W
SFO2      500.1320005 MHz
SI          32768
SF        125.7578508 MHz
WDW        EM
SSB          0
LB        1.00 Hz
GB          0
PC        1.40

```

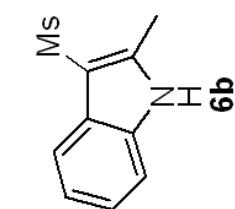




3357  
3102  
2624  
2503  
2500  
2496  
2493

7.749  
7.743  
7.423  
7.408  
7.206  
7.208  
7.194  
7.192  
7.175  
7.173  
7.170  
7.156  
7.143  
7.141

12.050



Bruker Avance III-500  
500MHz,DMSO-d<sub>6</sub>

```

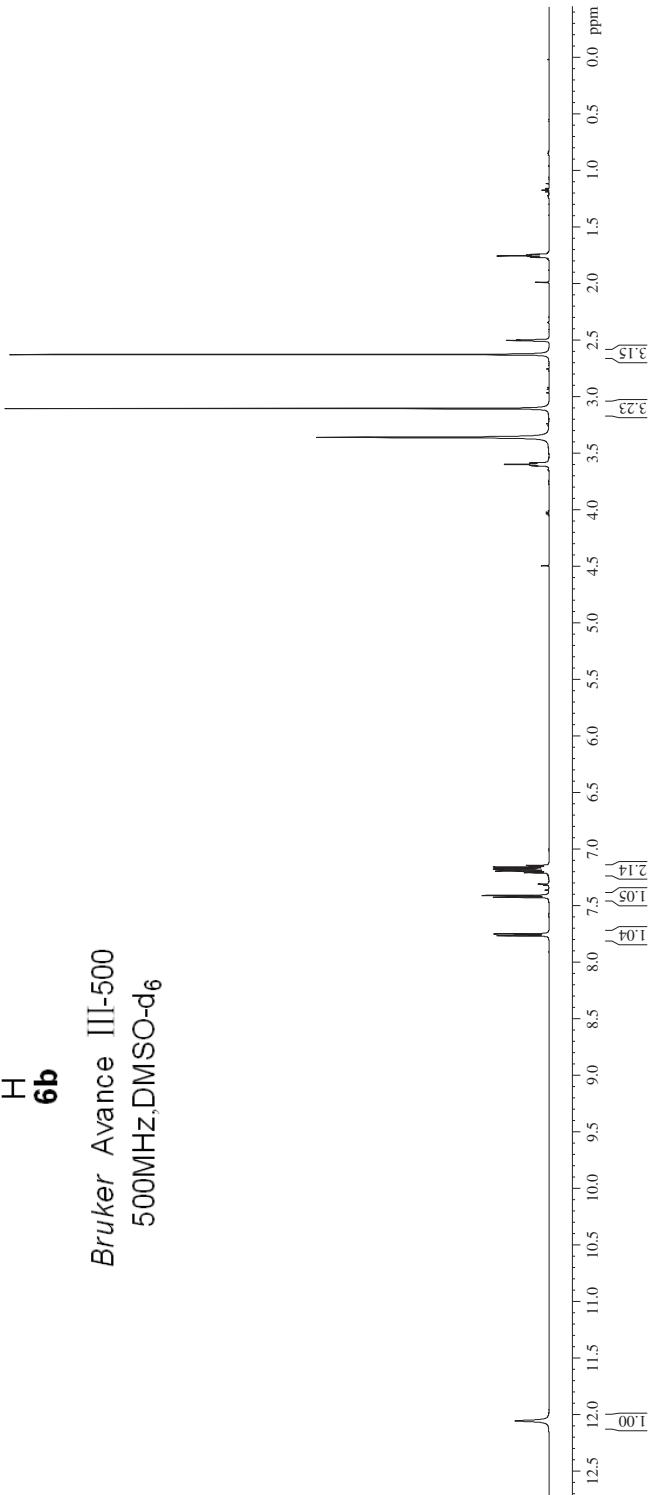
NAME          2016.05.13
EXNO          19
PROCNO        1
Date_-
Time         20.29
INSTRUM      spect
PROBHD      5 mm PABBO BB-
PULPROG     zg30
TD           65536
SOLVENT      DMSO
NS            6
DS            0
SWH          10330.578 Hz
FIDRES       0.157632 Hz
AQ           3.1719923 sec
RG           144
DW           48.400 usec
DE           6.50 usec
TE           298.1 K
D1           1.00000000 sec
TDO          1

```

```

===== CHANNEL f1 =====
NUC1          1H
P1            13.00 usec
PL1           2.00 CB
PL1W          16.79386763 W
SF01          500.1330885 MHz
SI             32768
SF            500.1300104 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

```

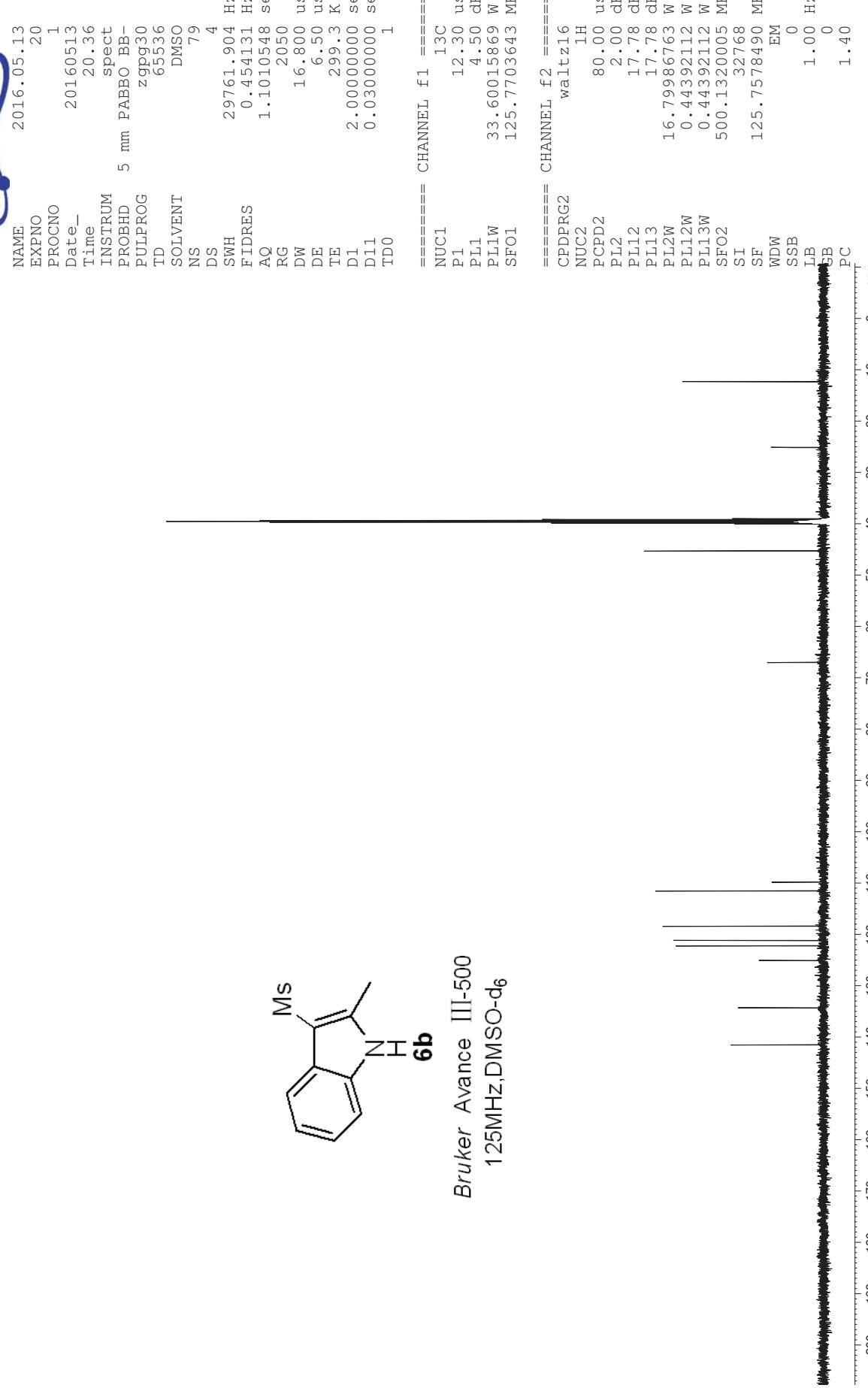


— 12.29 —

25.12  
39.02  
39.19  
39.35  
39.52  
39.69  
39.86  
40.02  
45.29

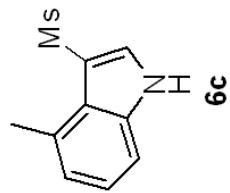
— 67.02 —

109.86  
111.55  
118.43  
121.21  
122.27  
125.11  
134.32  
141.56

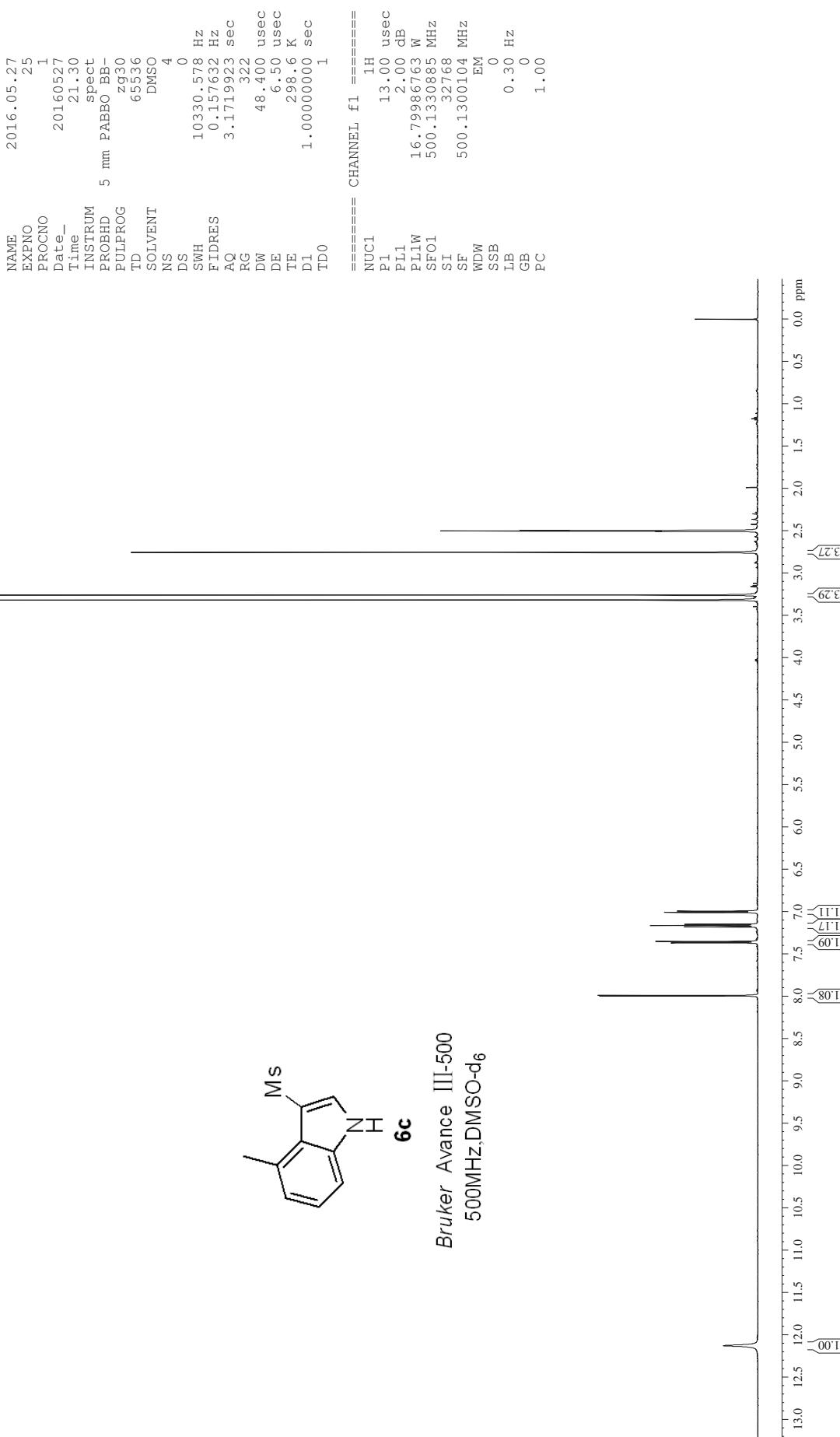




12.123



Bruker Avance III-500  
500MHz,DMSO-d<sub>6</sub>



20.74



```

=====
NAME          2016.05.27
EXPNO         26
PROCNO        1
Date_         20160527
Time          21.39
INSTRUM      spect
PROBHD       5 mm PABBO BB-
PULPROG      zppg30
TD           32768
SOLVENT      DMSO
NS            286
DS            0
SWH          29761.904 Hz
FIDRES       0.908261 Hz
AQ            0.5505524 sec
RG            2050
DW           16.800 usec
DE            6.500 usec
TE            299.9 K
D1           2.0000000 sec
D11          0.03000000 sec
TD0           1

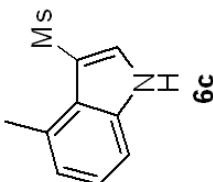
```

```

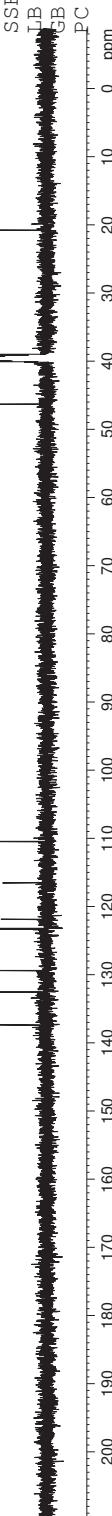
=====
CHANNEL f1 =====
NUC1          13C
P1            12.30 usec
PL1          4.50 dB
PL1W         33.60015869 W
SF01         125.7703643 MHz

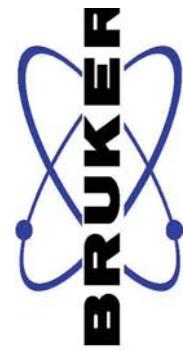
=====
CHANNEL f2 =====
CPDPRG2      waltz16
NUC2          1H
PCPD2        80.00 usec
PL2           2.00 dB
PL1.2        17.78 dB
PL1.3        17.78 dB
PL2W         16.79986763 W
PL1.2W       0.44392112 W
PL1.3W       0.44392112 W
SF02         500.1320005 MHz
SI            32768
SF           125.7578527 MHz
WDW          EM
SSB           0
LB           1.00 Hz
QB           0
PC           1.40

```



Bruker Avance III-500  
125MHz,DMSO-d<sub>6</sub>



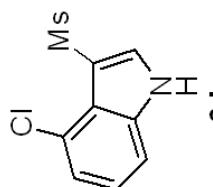


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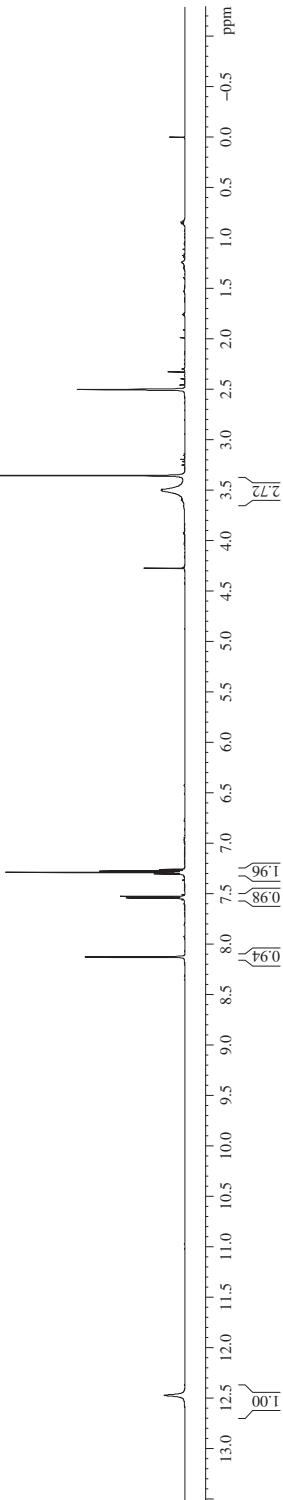
NAME          2016.05.30
EXNO          29
PROCNO        1
Date_-
Time         18.28
INSTRUM      spect
PROBHD      5 mm PABBO BB-
PULPROG     zg30
TD           65536
SOLVENT      DMSO
NS            8
DS
SWH          10330.578 Hz
FIDRES       0.157632 Hz
AQ           3.1719923 sec
RG           362
DW           48.400 usec
DE           6.50 usec
TE           298.0 K
D1           1.00000000 sec
TDO0

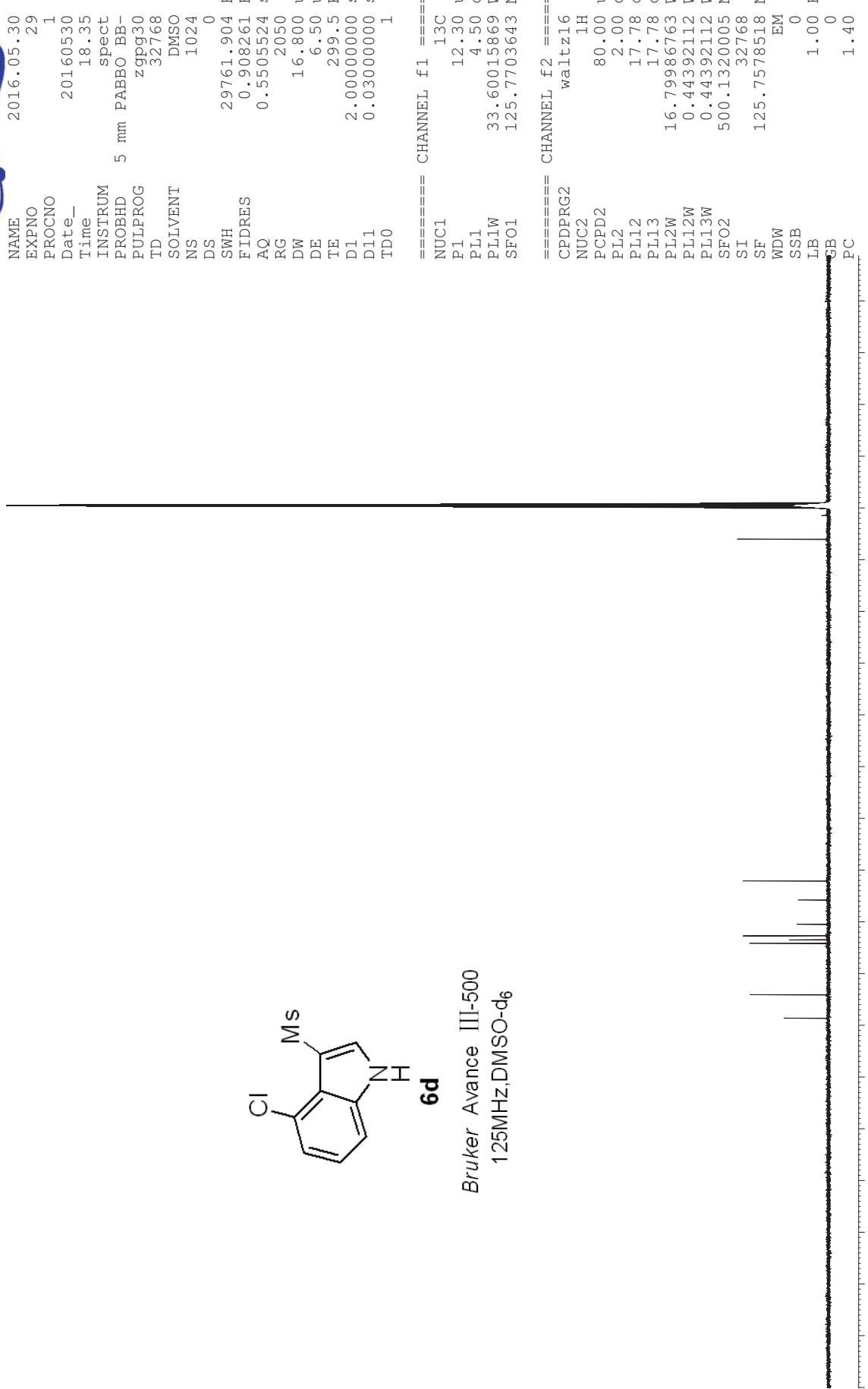
===== CHANNEL f1 =====
NUC1          1H
P1           13.00 usec
PL1          2.00 CB
PL1W        16.79386763 W
SFO1        500.1330885 MHz
SI
SF           500.1300102 MHz
WDW
SSB
LB
GB
PC

```



Bruker Avance III-500  
500MHz,DMSO-d<sub>6</sub>





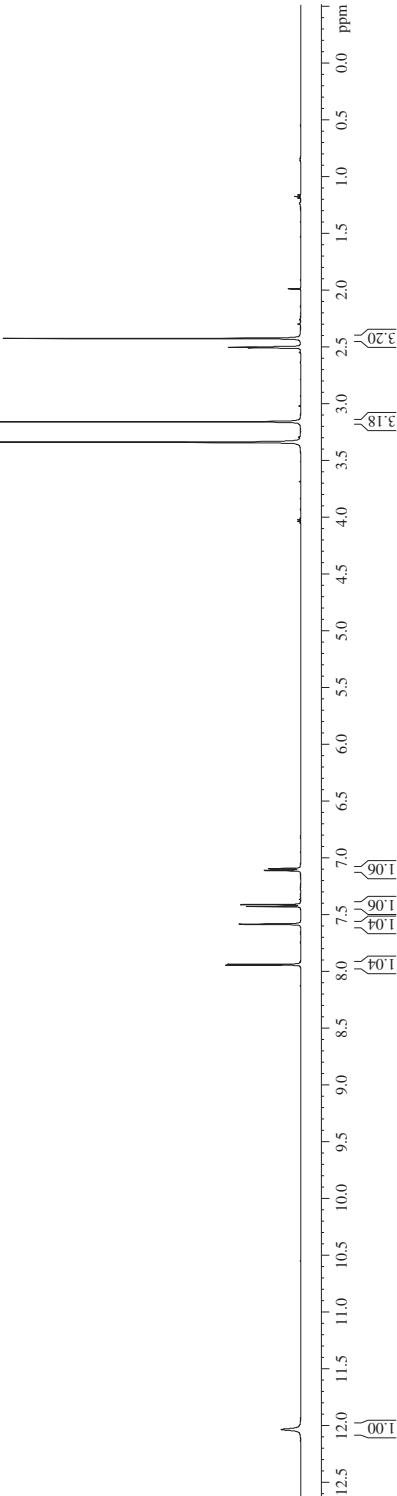


3.336  
3.157  
2.507  
2.504  
2.500  
2.496  
2.493  
2.422

```

NAME          2016.05.13
EXN0           8
PROCNO        1
Date_-
Time         13.00
INSTRUM      spect
PROBHD       5 mm PABBO BB-
PULPROG      zg30
TD            65536
SOLVENT      DMSO
NS             8
DS
SWH          10330.578 Hz
FIDRES       0.157632 Hz
AQ            3.1719923 sec
RG            256
DW            48.400 usec
DE            6.50 usec
TE            298.0 K
D1           1.00000000 sec
TDO0          1
===== CHANNEL f1 =====
NUC1          1H
P1            13.00 usec
PL1           2.00 CB
PL1W          16.79386763 W
SF01          500.1330885 MHz
SI             322768
SF             500.1300101 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

```



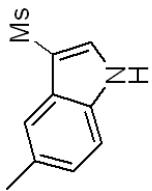
**6e**  
*Bruker Avance III-500*  
500MHz,DMSO-d<sub>6</sub>



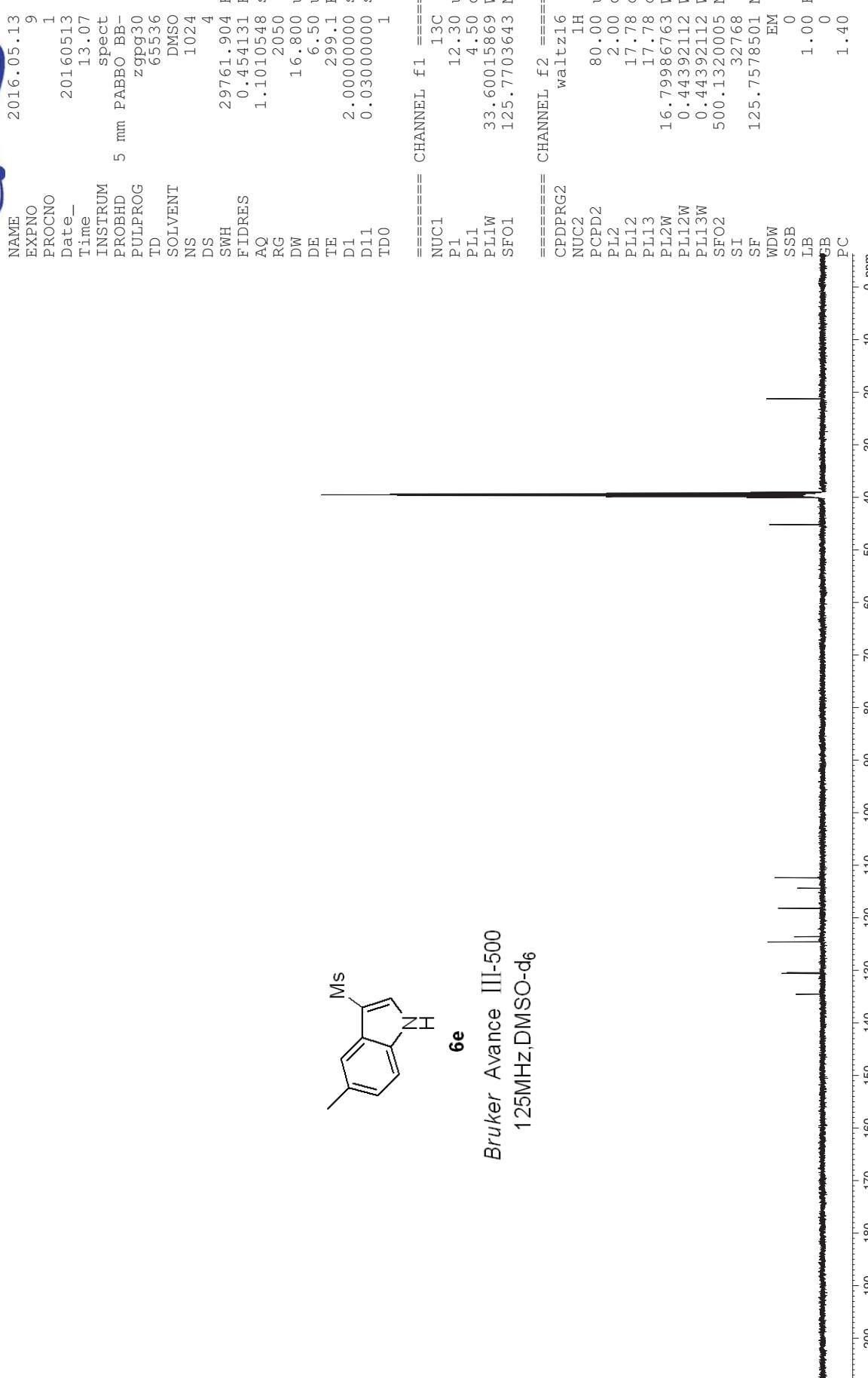
21.21

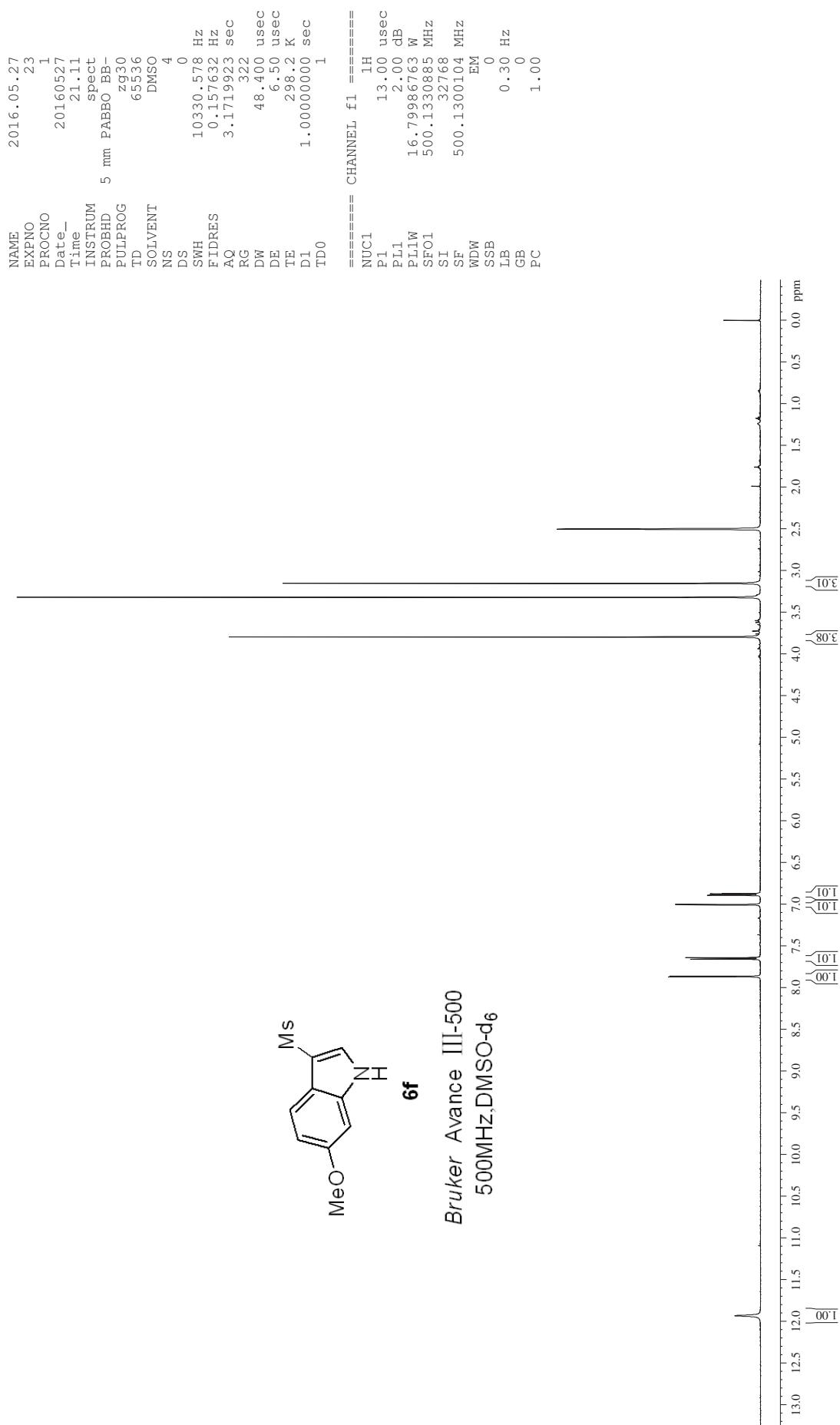
39.02  
39.35  
39.52  
39.69  
39.85  
40.02  
45.16

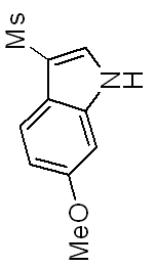
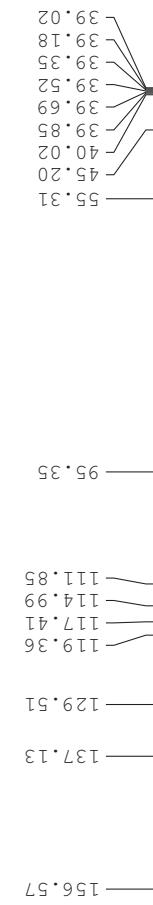
112.40  
114.38  
118.21  
123.61  
124.62  
130.48  
130.61  
134.56

**6e**

*Bruker Avance III-500*  
125MHz,DMSO-d<sub>6</sub>

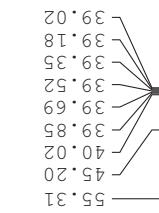


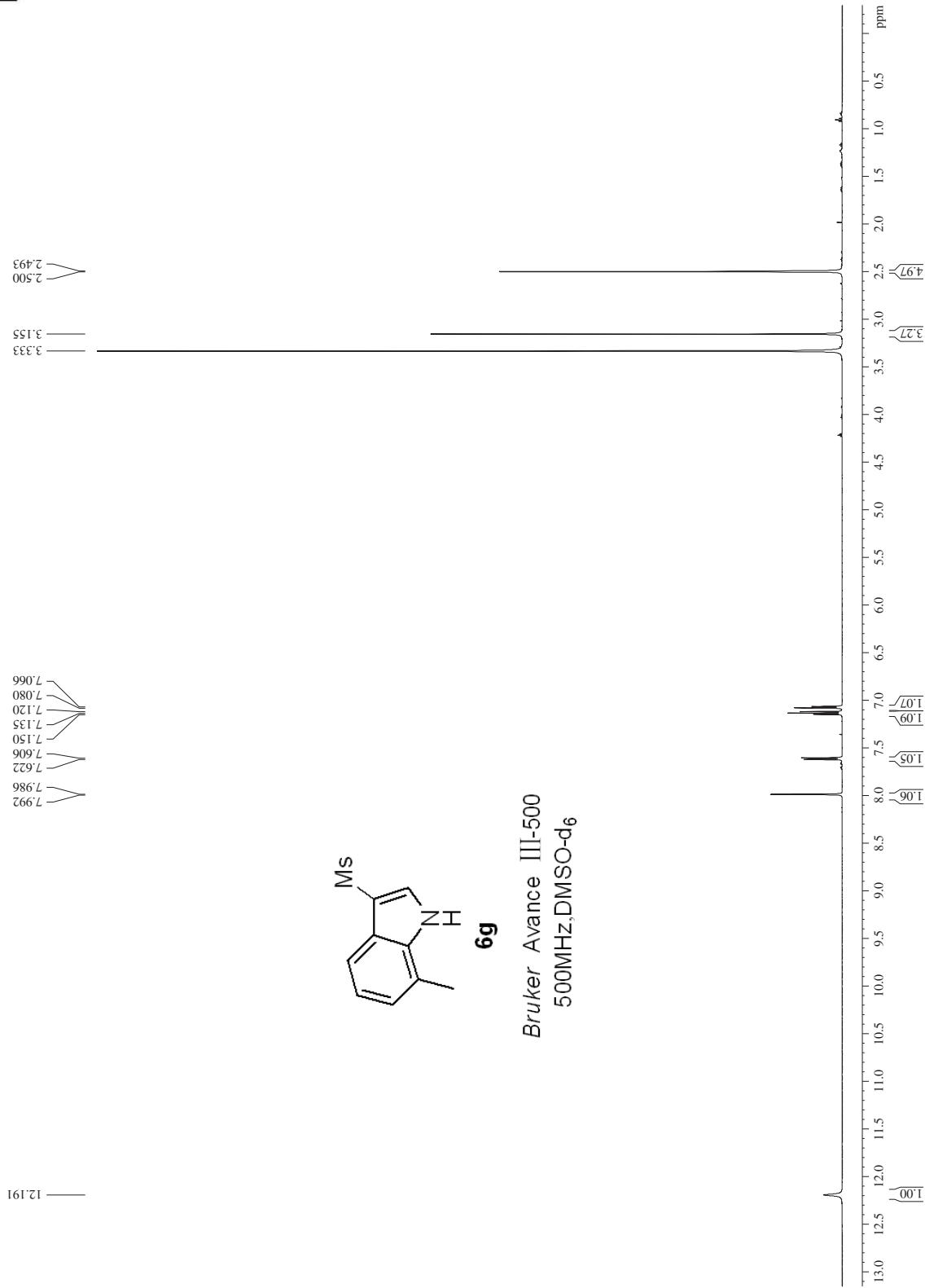




**6f**

Bruker Avance III-500  
125MHz,DMSO-d<sub>6</sub>



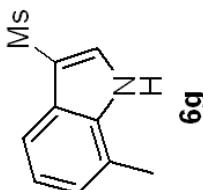




16.65

39.02  
39.19  
39.52  
39.69  
39.85  
40.02  
45.15

115.36  
116.20  
116.76  
121.20  
123.16  
123.47  
130.32  
135.75



Bruker Avance III-500  
125MHz, DMSO-d<sub>6</sub>

