

## Electronic Supporting Information

### Functionalized hypercrosslinked polymers with knitted *N*-heterocyclic carbene–copper complexes as efficient and recyclable catalysts for organic transformations

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## 1. General remarks

Indole, 2-methylindole, 5-bromoindole and 1,2-dimethylindole were purchased from Energy Chemical Company. Ethyl-indole-2-carboxylate, 2-phenylindole, 1-iododecane, 4-iodoanisole, and 1-(*tert*-butyl)-4-ethynylbenzene were purchased from Alfa Aesar Chemical Company. 6-Methylindole, 5-methoxyindole, 4-nitroindole, 1,3-cyclohexanedione, and 1,3-cyclopentanedione were purchased from Accela ChemBio Co. Ltd. Benzyl chloride, dimedone, benzimidazole, and formaldehyde dimethyl acetal (FDA, 98%) were purchased from Sinopharm Chemical Reagent Co. Ltd. Pyruvic aldehyde, 5-methoxy-7-methylindole, 5-fluoro-2-methylindole, 7-ethyl-1*H*-indole, 4-chloroindole, and 6-bromoindole were purchased from Adamas Reagent Co. Ltd. 6-Nitroindole, 5-methylindole, 7-azaindole, 5-methoxy-1*H*-pyrrolo[3,2-*b*]pyridine, 3,4-(methylenedioxy) phenylglyoxal hydrate, 5-bromo-2-thiopheneglyoxal hydrate, and 4-bromophenylglyoxal hydrate were purchased from BePharm Co. Ltd. 2-Chlorobenzaldehyde, iodoethane, sodium azide, and 1-ethyl-2-phenylindole were purchased from Aladdin Industrial Corporation. <sup>1</sup>H and <sup>13</sup>C NMR spectra were recorded on a Bruker AV-400. IR spectra were recorded on a FT-IR Bruker (EQUINOX 55) using KBr technology. High-resolution mass spectra (HRMS) were obtained on Bruker Compass Data Analysis 4.0.

## 2. Synthesis of *N,N'*-dibenzylbenzimidazolium chloride (NHC)

NHC was synthesized according to a reported procedure.<sup>1</sup> 1-Benzyl-1*H*-benzimidazole (2.08 g, 10.0 mmol) was suspended in toluene (100 mL). Then, benzyl chloride (1.40 mL, 12.0 mmol) was added and the mixture refluxed for 20 h. The solids were filtered and washed with Et<sub>2</sub>O to give target compound as a white solid (1.90 g, 57%). mp: 210–211 °C. <sup>1</sup>H NMR (400 MHz, DMSO, 25 °C): δ = 10.23 (s, 1H), 7.98 (dd, *J*<sub>a</sub> = 3.2 Hz, *J*<sub>b</sub> = 6.4 Hz, 2H), 7.64 (dd, *J*<sub>a</sub> = 3.2 Hz, *J*<sub>b</sub> = 6.4 Hz, 2H), 7.54 (d, *J* = 4.0 Hz, 4H), 7.45–7.38 (m, 6H), 5.81 ppm (s, 4H); <sup>13</sup>C NMR (100 MHz, DMSO, 25 °C): δ = 143.4, 134.5, 131.5, 129.5, 129.2, 128.8, 127.2, 114.6, 50.5 ppm.

## 3. General procedure for the synthesis of HCP–NHC

HCP-NHC was synthesized according to a reported procedure.<sup>2</sup> NHC (2.01g, 6.0 mmol), benzene (1.40 g, 18 mmol), formaldehyde dimethyl acetal (4.10 g, 54 mmol), FeCl<sub>3</sub> (8.75 g, 54 mmol) and 1,2-dichloroethane (40 mL) were used in this polymerization at 80 °C for 24 h.

## 4. Spectroscopic data of the obtained compounds

**5,5-Dimethyl-2-(1-(2-methyl-1*H*-indol-3-yl)-2-oxo-2-phenylethylidene)cyclohexane-1,3-dione (4a):** Red solid; mp: 128–130 °C. <sup>1</sup>H NMR (400 MHz, DMSO, 25 °C): δ = 12.26 (s, 1H), 7.64 (s, 2H), 7.45 (d, *J* = 4.0 Hz, 2H), 7.36 (t, *J* = 7.6 Hz, 1H), 7.27 (t, *J* = 7.6 Hz, 2H), 7.09–7.05 (m, 1H), 6.99 (t, *J* = 8.0 Hz, 1H), 2.62–2.49 (m, 4H), 2.34 (s, 3H), 1.05 ppm (s, 6H); <sup>13</sup>C NMR (100 MHz,

DMSO, 25 °C):  $\delta$  = 197.7, 194.6, 160.8, 157.7, 136.2, 135.8, 144.8, 132.5, 129.4, 128.4, 128.1, 127.2, 126.2, 122.4, 121.1, 120.1, 111.7, 53.2, 51.7, 29.8, 28.2, 28.1, 14.7 ppm; IR (KBr)  $\nu$  = 3339, 2957, 2927, 2870, 1735, 1670, 1601, 1448, 1334, 1243, 1178, 1023, 749, 695  $\text{cm}^{-1}$ ; HRMS (ESI):  $m/z$ : calcd for  $\text{C}_{25}\text{H}_{23}\text{NNaO}_3$ : 408.1576  $[\text{M} + \text{Na}]^+$ ; found: 408.1569.

**5,5-Dimethyl-2-(2-oxo-2-phenyl-1-(2-phenyl-1*H*-indol-3-yl)ethylidene)cyclohexane-1,3-dione (4b)**: Red solid; mp: 240–242 °C.  $^1\text{H}$  NMR (400 MHz, DMSO, 25 °C):  $\delta$  = 12.22 (s, 1H), 7.68 (d,  $J$  = 8.0 Hz, 2H), 7.54 (d,  $J$  = 2.0 Hz, 2H), 7.49–7.35 (m, 7H), 7.22 (d,  $J$  = 8.0 Hz, 1H), 7.16 (t,  $J$  = 8.0 Hz, 1H), 7.05 (t,  $J$  = 8.0 Hz, 1H), 2.58–2.50 (m, 2H), 2.43–2.40 (m, 1H), 2.09–2.00 (m, 1H), 1.02 (s, 3H), 0.89 ppm (s, 3H);  $^{13}\text{C}$  NMR (100 MHz, DMSO, 25 °C):  $\delta$  = 198.3, 195.4, 154.5, 157.2, 144.7, 137.1, 136.6, 133.1, 132.2, 131.8, 129.5, 129.4, 129.0, 128.9, 128.4, 127.2, 123.1, 121.8, 120.5, 112.8, 109.3, 53.3, 52.5, 29.9, 28.9, 28.4 ppm; IR (KBr)  $\nu$  = 3248, 3061, 2956, 1734, 1663, 1447, 1321, 1241, 1026, 753, 698  $\text{cm}^{-1}$ ; HRMS (ESI):  $m/z$ : calcd for  $\text{C}_{30}\text{H}_{25}\text{NNaO}_3$ : 470.1732  $[\text{M} + \text{Na}]^+$ ; found: 470.1727.

**2-(1-(1*H*-Indol-3-yl)-2-oxo-2-phenylethylidene)-5,5-dimethylcyclohexane-1,3-dione (4c)**: Red solid; mp: 206–208 °C.  $^1\text{H}$  NMR (400 MHz, DMSO, 25 °C):  $\delta$  = 12.25 (s, 1H), 7.91 (s, 1H), 7.69 (t,  $J$  = 4.0 Hz, 2H), 7.50–7.44 (m, 2H), 7.39 (t,  $J$  = 8.0 Hz, 2H), 7.19 (t,  $J$  = 8.0 Hz, 2H), 7.13 (t,  $J$  = 8.0 Hz, 1H), 2.83 (s, 1H), 2.55–2.50 (m, 3H), 1.07 ppm (s, 6H);  $^{13}\text{C}$  NMR (100 MHz, DMSO, 25 °C):  $\delta$  = 198.0, 196.5, 195.8, 156.7, 137.7, 136.6, 136.4, 133.1, 129.1, 128.4, 127.0, 124.7, 123.3, 122.1, 122.0, 113.4, 111.3, 53.8, 52.3, 30.5, 28.8, 28.2 ppm; IR (KBr)  $\nu$  = 3307, 2954, 2926, 1652, 1472, 1424, 1369, 1235, 1138, 1024, 1004, 749, 695  $\text{cm}^{-1}$ ; HRMS (ESI):  $m/z$ : calcd for  $\text{C}_{24}\text{H}_{21}\text{NNaO}_3$ : 394.1419  $[\text{M} + \text{Na}]^+$ ; found: 394.1410.

**Ethyl 3-(1-(4,4-dimethyl-2,6-dioxocyclohexylidene)-2-oxo-2-phenylethyl)-1*H*-indole-2-carboxylate (4d)**: Red solid; mp: 178–179 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , 25 °C, TMS):  $\delta$  = 9.65 (s, 1H), 8.07 (t,  $J$  = 4.0 Hz, 2H), 7.91 (d,  $J$  = 8.0 Hz, 1H), 7.40 (t,  $J$  = 8.0 Hz, 1H), 7.30 (t,  $J$  = 7.6 Hz, 2H), 7.19 (d,  $J$  = 4.0 Hz, 2H), 7.15–7.09 (m, 1H), 4.29–4.18 (m, 2H), 2.71 (d,  $J$  = 16.0 Hz, 1H), 2.60–2.54 (m, 3H), 1.29 (t,  $J$  = 8.0 Hz, 3H), 1.13 (s, 3H), 1.09 ppm (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , 25 °C):  $\delta$  = 198.4, 196.3, 194.4, 161.0, 154.9, 136.0, 135.4, 135.2, 133.1, 129.0, 128.4, 126.7, 126.2, 125.6, 123.0, 122.1, 112.9, 112.1, 61.33, 53.9, 53.4, 30.0, 28.7, 28.6, 14.2 ppm; IR (KBr)  $\nu$  = 3327, 2958, 1709, 1669, 1531, 1431, 1376, 1326, 1244, 1102, 749, 695  $\text{cm}^{-1}$ ; HRMS (ESI):  $m/z$ : calcd for  $\text{C}_{27}\text{H}_{25}\text{NNaO}_5$ : 466.1630  $[\text{M} + \text{Na}]^+$ ; found: 466.1623.

**2-(1-(6-Methoxy-4-methyl-1*H*-indol-3-yl)-2-oxo-2-phenylethylidene)-5,5-dimethylcyclohexane-1,3-dione (4e)**: Red solid; mp: 251–252 °C.  $^1\text{H}$  NMR (400 MHz, DMSO, 25 °C):  $\delta$  = 12.17 (s, 1H), 7.67 (d,  $J$  = 8.0 Hz, 2H), 7.47 (t,  $J$  = 8.0 Hz, 1H), 7.40–7.37 (m, 2H), 7.20 (d,  $J$  = 8.0 Hz, 1H), 6.72 (dd,  $J_a$  = 4.0 Hz,  $J_b$  = 8.0 Hz, 1H), 3.63 (s, 3H), 2.55–2.50 (m, 4H), 2.30 (s, 3H), 1.07 ppm (s, 6H);  $^{13}\text{C}$  NMR (100 MHz, DMSO, 25 °C):  $\delta$  = 197.8, 195.0, 157.6,

155.0, 136.4, 132.5, 130.6, 128.5, 128.0, 127.1, 126.3, 112.3, 111.2, 103.5, 55.1, 29.8, 28.1, 14.8 ppm; IR (KBr)  $\nu$  = 3249, 2954, 1663, 1633, 1432, 1334, 1261, 1201, 1026, 1007, 811, 697  $\text{cm}^{-1}$ ; HRMS (ESI):  $m/z$ : calcd for  $\text{C}_{26}\text{H}_{25}\text{NNaO}_4$ : 438.1681  $[\text{M} + \text{Na}]^+$ ; found: 438.1675.

**2-(1-(2,5-Dimethyl-1*H*-indol-3-yl)-2-oxo-2-phenylethylidene)-5,5-dimethylcyclohexane-1,3-dione (4f)**: Red solid; mp: 179–181 °C.  $^1\text{H}$  NMR (400 MHz, DMSO, 25 °C):  $\delta$  = 12.15 (s, 1H), 7.65 (d,  $J$  = 2.0 Hz, 2H), 7.47–7.44 (m, 1H), 7.37 (t,  $J$  = 8.0 Hz, 1H), 7.18 (d,  $J$  = 8.0 Hz, 1H), 7.04 (s, 1H), 6.90 (d,  $J$  = 8.0 Hz, 1H), 2.55–2.50 (m, 4H), 2.31 (s, 3H), 2.26 (s, 3H), 1.07 ppm (s, 6H);  $^{13}\text{C}$  NMR (100 MHz, DMSO, 25 °C):  $\delta$  = 197.9, 195.2, 158.3, 136.8, 134.5, 132.9, 130.7, 128.9, 128.5, 127.3, 127.0, 124.2, 120.7, 111.8, 53.5, 52.3, 30.3, 28.6, 21.9, 15.2 ppm; IR (KBr)  $\nu$  = 3228, 2955, 2869, 1663, 1638, 1436, 1332, 1247, 1024, 1004, 759, 696  $\text{cm}^{-1}$ ; HRMS (ESI):  $m/z$ : calcd for  $\text{C}_{26}\text{H}_{25}\text{NNaO}_3$ : 422.1732  $[\text{M} + \text{Na}]^+$ ; found: 422.1724.

**2-(1-(5-Fluoro-2-methyl-1*H*-indol-3-yl)-2-oxo-2-phenylethylidene)-5,5-dimethylcyclohexane-1,3-dione (4g)**: Red solid; mp: 202–203 °C.  $^1\text{H}$  NMR (400 MHz, DMSO, 25 °C):  $\delta$  = 12.27 (s, 1H), 7.66 (d,  $J$  = 4.0 Hz, 2H), 7.47 (t,  $J$  = 7.6 Hz, 1H), 7.38 (t,  $J$  = 8.0 Hz, 2H), 7.30 (dd,  $J_a$  = 4.0 Hz,  $J_b$  = 8.0 Hz, 1H), 6.95–6.92 (m, 2H), 2.58 (s, 4H), 2.34 (s, 3H), 1.06 ppm (s, 6H);  $^{13}\text{C}$  NMR (100 MHz, DMSO, 25 °C):  $\delta$  = 197.0, 194.8, 159.6, 157.3, 136.4, 133.1, 132.8, 129.0, 128.5, 128.2, 127.4 (d,  $J$  = 10.0 Hz), 113.15 (d,  $J$  = 5.0 Hz), 110.6, 110.3, 106.0, 105.7, 53.4, 30.2, 28.5, 15.1 ppm;  $^{19}\text{F}$  NMR (377 MHz, DMSO, 25 °C):  $\delta$  = -121.4 ppm (s, 1F); IR (KBr)  $\nu$  = 2956, 2871, 1660, 1441, 1334, 1251, 1183, 1025, 1006  $\text{cm}^{-1}$ ; HRMS (ESI)  $m/z$ : calcd for  $\text{C}_{25}\text{H}_{22}\text{FNNaO}_3$ : 426.1481  $[\text{M} + \text{Na}]^+$ ; found: 426.1484.

**5,5-Dimethyl-2-(1-(1-methyl-2-phenyl-1*H*-indol-3-yl)-2-oxo-2-phenylethylidene)cyclohexane-1,3-dione (4h)**: Red solid; mp: 113–115 °C.  $^1\text{H}$  NMR (400 MHz, DMSO, 25 °C):  $\delta$  = 7.60 (d,  $J$  = 4.0 Hz, 2H), 7.54 (d,  $J$  = 8.0 Hz, 1H), 7.50–7.43 (m, 4H), 7.35 (t,  $J$  = 8.0 Hz, 2H), 7.29–7.23 (m, 4H), 7.12 (d,  $J$  = 7.6 Hz, 1H), 3.52 (s, 3H), 2.55–2.46 (m, 2H), 2.31–2.24 (m, 1H), 2.03–1.98 (m, 1H), 0.98 (s, 3H), 0.81 ppm (s, 3H);  $^{13}\text{C}$  NMR (100 MHz, DMSO, 25 °C):  $\delta$  = 197.8, 195.9, 194.5, 156.8, 145.7, 138.0, 136.5, 133.1, 131.4, 130.5, 129.6, 128.9, 128.8, 128.3, 126.1, 123.2, 122.2, 120.6, 111.7, 110.1, 53.4, 52.4, 31.8, 29.8, 28.8, 28.4 ppm; IR (KBr)  $\nu$  = 3058, 2954, 2870, 1734, 1666, 1466, 1394, 1367, 1249, 1056, 1028, 749, 699  $\text{cm}^{-1}$ ; HRMS (ESI):  $m/z$ : calcd for  $\text{C}_{31}\text{H}_{27}\text{NNaO}_3$ : 484.1889  $[\text{M} + \text{Na}]^+$ ; found: 484.1891.

**2-(1-(1-Ethyl-2-phenyl-1*H*-indol-3-yl)-2-oxo-2-phenylethylidene)-5,5-dimethylcyclohexane-1,3-dione (4i)**: Red solid; mp: 167–168 °C.  $^1\text{H}$  NMR (400 MHz, DMSO, 25 °C):  $\delta$  = 7.60 (t,  $J$  = 8.0 Hz, 3H), 7.49 (t,  $J$  = 7.6 Hz, 1H), 7.34–7.33 (m, 3H), 7.37 (t,  $J$  = 8.0 Hz, 2H), 7.26–7.22 (m, 4H), 7.11 (t,  $J$  = 8.0 Hz, 1H), 4.06–3.98 (m, 2H), 2.59–2.46 (m, 2H), 2.29–2.25 (m, 1H), 2.04 (s, 1H), 1.08 (t,  $J$  = 8.0 Hz, 3H), 0.98 (s, 3H), 0.78 (s, 3H) ppm;  $^{13}\text{C}$  NMR (100 MHz, DMSO, 25 °C):  $\delta$  = 197.7, 196.0, 194.7, 156.7, 145.1, 136.7, 136.4, 133.1, 131.2, 130.6, 129.7, 129.0, 128.9, 128.3,

126.3, 123.3, 122.2, 120.8, 111.8, 111.5, 53.4, 52.3, 39.3, 29.7, 28.8, 28.3, 15.3 ppm; IR (KBr)  $\nu$  = 3445, 3059, 2956, 1734, 1665, 1462, 1407, 1356, 1232, 1055, 1027, 761, 699  $\text{cm}^{-1}$ ; HRMS (ESI):  $m/z$ : calcd for  $\text{C}_{32}\text{H}_{29}\text{NO}_3$ : 498.2045  $[\text{M} + \text{Na}]^+$ ; found: 498.2040.

**2-(1-(4-Ethyl-1*H*-indol-3-yl)-2-oxo-2-phenylethylidene)-5,5-dimethylcyclohexane-1,3-dione**

**(4j)**: Red solid; mp: 123–125 °C.  $^1\text{H}$  NMR (400 MHz, DMSO, 25 °C):  $\delta$  = 12.27 (s, 1H), 7.86 (s, 1H), 7.70 (d,  $J$  = 8.0 Hz, 2H), 7.48 (t,  $J$  = 8.0 Hz, 1H), 7.38 (t,  $J$  = 7.6 Hz, 2H), 7.07–7.04 (m, 2H), 7.10–7.03 (m, 1H), 2.84 (quint,  $J$  = 8.0 Hz, 2H), 2.58–2.50 (m, 4H), 1.23 (t,  $J$  = 8.0 Hz, 3H), 1.07 ppm (s, 6H);  $^{13}\text{C}$  NMR (100 MHz, DMSO, 25 °C):  $\delta$  = 194.8, 156.6, 136.4, 135.9, 133.1, 129.1, 129.0, 128.4, 127.2, 124.7, 122.2, 119.8, 111.6, 53.8, 52.3, 30.5, 28.6, 23.9, 15.0 ppm; IR (KBr)  $\nu$  = 3162, 3102, 2959, 2873, 1657, 1488, 1427, 1368, 1229, 1144, 1052, 1026, 1005, 752, 698  $\text{cm}^{-1}$ ; HRMS (ESI):  $m/z$ : calcd for  $\text{C}_{26}\text{H}_{25}\text{NNaO}_3$ : 422.1732  $[\text{M} + \text{Na}]^+$ ; found: 422.1728.

**5,5-Dimethyl-2-(1-(5-methyl-1*H*-indol-3-yl)-2-oxo-2-phenylethylidene)cyclohexane-1,3-dione**

**(4k)**: Red solid; mp: 212–213 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , 25 °C, TMS):  $\delta$  = 9.98 (s, 1H), 7.73 (d,  $J$  = 8.0 Hz, 2H), 7.38 (t,  $J$  = 6.8 Hz, 1H), 7.30–7.25 (m, 3H), 6.94 (d,  $J$  = 8.0 Hz, 1H), 6.90–6.86 (m, 2H), 2.68 (d,  $J$  = 16.0 Hz, 2H), 2.49 (s, 2H), 2.37 (s, 3H), 1.15 ppm (d,  $J$  = 8.0 Hz, 6H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , 25 °C):  $\delta$  = 197.6, 196.6, 195.7, 159.0, 136.9, 136.5, 135.7, 132.7, 131.8, 128.6, 128.4, 125.4, 125.2, 124.2, 122.3, 112.7, 112.4, 54.1, 52.5, 30.4, 28.7, 21.9 ppm; IR (KBr)  $\nu$  = 3296, 2956, 1734, 1648, 1421, 1366, 1238, 1139, 802, 694  $\text{cm}^{-1}$ ; HRMS (ESI):  $m/z$ : calcd for  $\text{C}_{25}\text{H}_{23}\text{NNaO}_3$ : 408.1576  $[\text{M} + \text{Na}]^+$ ; found: 408.1577.

**2-(1-(5-Methoxy-1*H*-indol-3-yl)-2-oxo-2-phenylethylidene)-5,5-dimethylcyclohexane-1,3-dione**

**(4l)**: Red solid; mp: 145–147 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , 25 °C, TMS):  $\delta$  = 10.08 (s, 1H), 7.75 (d,  $J$  = 8.0 Hz, 2H), 7.42–7.38 (m, 2H), 7.31–7.28 (m, 2H), 6.95 (d,  $J$  = 8.0 Hz, 1H), 6.70 (d,  $J$  = 12.0 Hz, 1H), 6.52 (s, 1H), 3.73 (s, 3H), 2.67 (s, 2H), 2.49 (s, 2H), 1.14 ppm (s, 6H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , 25 °C):  $\delta$  = 197.7, 196.4, 195.9, 159.0, 155.9, 137.5, 136.5, 132.8, 132.1, 128.6, 128.3, 125.1, 113.7, 112.9, 112.7, 105.4, 55.6, 54.1, 52.4, 30.3, 28.7 ppm; IR (KBr)  $\nu$  = 3305, 2955, 1735, 1663, 1633, 1466, 1367, 1247, 1204, 1140, 1039, 803, 695  $\text{cm}^{-1}$ ; HRMS (ESI):  $m/z$ : calcd for  $\text{C}_{25}\text{H}_{23}\text{NNaO}_4$ : 424.1525  $[\text{M} + \text{Na}]^+$ ; found: 424.1517.

**2-(1-(5-Fluoro-1*H*-indol-3-yl)-2-oxo-2-phenylethylidene)-5,5-dimethylcyclohexane-1,3-dione**

**(4m)**: Red solid; mp: 120–122 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , 25 °C, TMS):  $\delta$  = 10.99 (d,  $J$  = 12.0 Hz, 1H), 7.74 (d,  $J$  = 8.0 Hz, 2H), 7.56 (s, 1H), 7.41 (t,  $J$  = 7.6 Hz, 1H), 7.30 (t,  $J$  = 8.0 Hz, 2H), 7.09–7.06 (m, 1H), 6.910–6.86 (m, 1H), 2.70 (s, 2H), 2.51 (s, 2H), 1.15 ppm (s, 6H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , 25 °C):  $\delta$  = 197.9, 196.9, 195.7, 161.3, 158.9, 158.1, 137.4, 136.2, 133.0, 128.7, 128.3, 122.7 (d,  $J$  = 11.0 Hz), 120.5, 112.0, 110.7 (d,  $J$  = 24.0 Hz), 99.4, 99.1, 54.2, 52.6, 30.4, 28.6 ppm.  $^{19}\text{F}$  NMR (377 MHz,  $\text{CDCl}_3$ , 25 °C):  $\delta$  = -118.4 ppm (sext,  $J$  = 6.4 Hz, 1F); IR (KBr)  $\nu$  = 3301, 3067, 2960, 1732, 1671, 1622, 1524, 1450, 1375, 1242, 1141, 1043, 955, 844,

694  $\text{cm}^{-1}$ ; HRMS (ESI):  $m/z$ : calcd for  $\text{C}_{24}\text{H}_{20}\text{FNNaO}_3$ : 412.1325  $[\text{M} + \text{Na}]^+$ ; found: 412.1320.

**2-(1-(6-Methoxy-4-methyl-1*H*-indol-3-yl)-2-oxo-2-phenylethylidene)-5,5-**

**dimethylcyclohexane-1,3-dione (4n):** Red solid; mp: 125–126 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , 25 °C, TMS):  $\delta$  = 10.04 (s, 1H), 7.70 (d,  $J$  = 8.0 Hz, 2H), 7.37 (t,  $J$  = 8.0 Hz, 1H), 7.27 (t,  $J$  = 8.0 Hz, 3H), 6.58 (s, 1H), 6.36 (s, 1H), 3.75 (s, 3H), 2.71–2.60 (m, 2H), 2.50 (s, 2H), 2.12 (s, 3H), 1.15 ppm (d,  $J$  = 8.0 Hz, 6H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , 25 °C):  $\delta$  = 197.3, 196.8, 195.4, 159.4, 156.0, 136.9, 136.4, 132.7, 132.0, 128.6, 128.3, 125.1, 124.4, 123.8, 113.7, 113.1, 102.8, 55.6, 54.1, 52.4, 30.4, 28.5, 16.2 ppm; IR (KBr)  $\nu$  = 3297, 2953, 1732, 1664, 1640, 1465, 1427, 1366, 1211, 1136, 1047, 844, 800, 697  $\text{cm}^{-1}$ ; HRMS (ESI):  $m/z$ : calcd for  $\text{C}_{26}\text{H}_{25}\text{NNaO}_4$ : 438.1681  $[\text{M} + \text{Na}]^+$ ; found: 438.1676.

**5,5-Dimethyl-2-(1-(6-nitro-1*H*-indol-3-yl)-2-oxo-2-phenylethylidene)cyclohexane-1,3-dione**

**(4o):** Red solid; mp: 125–126 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , 25 °C, TMS):  $\delta$  = 10.39 (s, 1H), 8.00–7.94 (m, 2H), 7.90 (d,  $J$  = 3.2 Hz, 1H), 7.76 (d,  $J$  = 8.0 Hz, 2H), 7.43 (t,  $J$  = 8.0 Hz, 1H), 7.32 (t,  $J$  = 8.0 Hz, 2H), 7.27 (d,  $J$  = 2.0 Hz, 1H), 2.76 (s, 2H), 2.60 (s, 2H), 1.18 ppm (s, 6H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , 25 °C):  $\delta$  = 198.2, 197.2, 195.6, 156.4, 143.6, 138.4, 135.6, 133.4, 128.8, 128.4, 121.4, 117.0, 111.4, 109.2, 54.3, 53.8, 31.0, 30.4, 28.6  $\text{cm}^{-1}$ ; IR (KBr)  $\nu$  = 3329, 2958, 2929, 1734, 1664, 1512, 1448, 1339, 1241, 1115, 1044, 699  $\text{cm}^{-1}$ ; HRMS (ESI):  $m/z$ : calcd for  $\text{C}_{24}\text{H}_{20}\text{N}_2\text{NaO}_5$ : 439.1270  $[\text{M} + \text{Na}]^+$ ; found: 439.1259.

**2-(1-(4-Hydroxy-1*H*-indol-3-yl)-2-oxo-2-phenylethylidene)-5,5-dimethylcyclohexane-1,3-**

**dione (4p):** Red solid; mp: 147–149 °C.  $^1\text{H}$  NMR (400 MHz, DMSO, 25 °C):  $\delta$  = 11.74 (s, 1H), 9.80 (s, 1H), 7.80 (d,  $J$  = 8.0 Hz, 2H), 7.48 (t,  $J$  = 7.6 Hz, 1H), 7.40 (t,  $J$  = 8.0 Hz, 2H), 7.29 (d,  $J$  = 4.0 Hz, 1H), 7.00 (t,  $J$  = 8.0 Hz, 1H), 6.88 (d,  $J$  = 8.0 Hz, 1H), 6.52 (d,  $J$  = 8.0 Hz, 1H), 2.72 (s, 1H), 2.43 (s, 3H), 1.11 ppm (s, 6H);  $^{13}\text{C}$  NMR (100 MHz, DMSO, 25 °C):  $\delta$  = 197.0, 195.5, 156.1, 151.8, 139.7, 136.1, 133.0, 131.3, 129.0, 128.5, 124.5, 113.6, 107.3, 104.4, 53.1, 52.5, 30.2, 28.9 ppm; IR (KBr)  $\nu$  = 3301, 2954, 2871, 1658, 1594, 1526, 1494, 1451, 1426, 1307, 1241, 1130, 1024, 782, 744, 700  $\text{cm}^{-1}$ ; HRMS (ESI):  $m/z$ : calcd for  $\text{C}_{24}\text{H}_{21}\text{NNaO}_4$ : 410.1368  $[\text{M} + \text{Na}]^+$ ; found: 410.1362.

**2-(1-(5-Methoxy-1*H*-pyrrolo[3,2-*b*]pyridin-3-yl)-2-oxo-2-phenylethylidene)-5,5-**

**dimethylcyclohexane-1,3-dione (4q):** Red solid; mp: 122–124 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , 25 °C, TMS):  $\delta$  = 9.96 (s, 1H), 7.82 (d,  $J$  = 8.0 Hz, 2H), 7.45–7.41 (m, 2H), 7.32 (t,  $J$  = 7.6 Hz, 2H), 7.24 (d,  $J$  = 8.0 Hz, 1H), 6.43 (d,  $J$  = 8.0 Hz, 1H), 3.72 (s, 3H), 2.84–2.68 (m, 2H), 2.48 (s, 2H), 1.16–1.10 ppm (m, 6H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 198.0, 197.5, 196.1, 160.5, 154.6, 139.2, 136.2, 134.3, 132.8, 129.9, 128.6, 125.9, 123.1, 111.3, 106.9, 54.3, 53.4, 53.0, 31.6, 30.4, 29.1 ppm; IR (KBr)  $\nu$  = 3269, 2955, 2927, 2870, 1652, 1583, 1452, 1407, 1296, 1241, 1145, 1024, 938, 813, 694, 667, 582  $\text{cm}^{-1}$ ; HRMS (ESI):  $m/z$ : calcd for  $\text{C}_{24}\text{H}_{22}\text{N}_2\text{NaO}_4$ : 425.1477  $[\text{M} + \text{Na}]^+$ ;

found: 425.1474.

**2-(2-Cyclopropyl-1-(2-methyl-1*H*-indol-3-yl)-2-oxoethylidene)-5,5-dimethylcyclohexane-1,3-dione (4r):** Orange solid; mp: 123–125 °C. <sup>1</sup>H NMR (400 MHz, DMSO, 25 °C):  $\delta$  = 12.22 (s, 1H), 7.35 (d, *J* = 8.0 Hz, 1H), 7.19 (d, *J* = 8.0 Hz, 1H), 7.13 (t, *J* = 8.0 Hz, 1H), 7.06 (t, *J* = 7.6 Hz, 1H), 2.55–2.50 (m, 4H), 2.27 (s, 3H), 2.01–1.93 (m, 1H), 1.05–0.98 (m, 8H), 0.86–0.81 ppm (m, 2H); <sup>13</sup>C NMR (100 MHz, DMSO, 25 °C):  $\delta$  = 205.8, 195.3, 147.8, 136.2, 127.2, 122.8, 121.6, 120.3, 111.2, 109.4, 53.7, 52.4, 32.2, 30.1, 28.9, 14.8 ppm; IR (KBr)  $\nu$  = 3323, 2959, 2930, 1729, 1675, 1627, 1456, 1373, 1334, 1242, 1051, 1025, 746 cm<sup>-1</sup>; HRMS (ESI): *m/z*: calcd for C<sub>22</sub>H<sub>23</sub>NNaO<sub>3</sub>: 372.1576 [M + Na]<sup>+</sup>; found: 372.1572.

**5,5-Dimethyl-2-(1-(2-methyl-1*H*-indol-3-yl)-2-oxopropylidene)cyclohexane-1,3-dione (4s):** Red solid; mp: 147–149 °C. <sup>1</sup>H NMR (400 MHz, DMSO, 25 °C):  $\delta$  = 12.29 (s, 1H), 7.38 (d, *J* = 8.0 Hz, 1H), 7.23 (d, *J* = 8.0 Hz, 2H), 7.16 (t, *J* = 8.0 Hz, 1H), 7.07 (t, *J* = 7.6 Hz, 1H), 2.54–2.50 (m, 4H), 2.25 (s, 3H), 2.15 (s, 3H), 1.05 ppm (s, 3H); <sup>13</sup>C NMR (100 MHz, DMSO, 25 °C):  $\delta$  = 203.2, 160.0, 148.2, 136.3, 128.7, 128.2, 126.7, 123.0, 122.0, 120.1, 112.2, 109.0, 56.3, 31.2, 30.2, 30.0, 28.6, 14.9 ppm; IR (KBr)  $\nu$  = 3298, 2961, 2922, 1720, 1673, 1603, 1460, 1261, 1197, 1023, 804, 749, 537 cm<sup>-1</sup>; HRMS (ESI): *m/z*: calcd for C<sub>20</sub>H<sub>21</sub>NNaO<sub>3</sub>: 346.1419 [M + Na]<sup>+</sup>; found: 346.1412.

**2-(2-(4-Bromophenyl)-1-(2-methyl-1*H*-indol-3-yl)-2-oxoethylidene)-5,5-dimethylcyclohexane-1,3-dione (4t):** Red solid; mp: 185–186 °C. <sup>1</sup>H NMR (400 MHz, DMSO, 25 °C):  $\delta$  = 12.34 (s, 1H), 7.57 (s, 4H), 7.31 (d, *J* = 8.0 Hz, 2H), 7.09 (t, *J* = 8.0 Hz, 1H), 7.01 (t, *J* = 7.6 Hz, 1H), 2.60–2.50 (m, 4H), 2.34 (s, 3H), 1.06 ppm (s, 6H); <sup>13</sup>C NMR (100 MHz, DMSO, 25 °C):  $\delta$  = 197.9, 194.4, 193.7, 156.9, 156.8, 135.8, 135.3, 131.6, 129.9, 127.0, 126.5, 126.1, 122.5, 121.5, 120.0, 111.7, 53.1, 51.5, 29.8, 28.0, 14.1 ppm; IR (KBr)  $\nu$  = 3180, 2955, 1667, 1639, 1585, 1439, 1332, 1243, 1174, 1005, 802, 751 cm<sup>-1</sup>; HRMS (ESI): *m/z*: calcd for C<sub>25</sub>H<sub>22</sub>BrNNaO<sub>3</sub>: 486.0681 [M + Na]<sup>+</sup>; found: 486.0672.

**2-(2-(Benzo[*d*][1,3]dioxol-5-yl)-1-(2-methyl-1*H*-indol-3-yl)-2-oxoethylidene)-5,5-dimethylcyclohexane-1,3-dione (4u):** Red solid; mp: 126–128 °C. <sup>1</sup>H NMR (400 MHz, DMSO, 25 °C):  $\delta$  = 12.25 (s, 1H), 7.30 (d, *J* = 8.0 Hz, 1H), 7.16–7.06 (m, 4H), 6.99 (t, *J* = 7.6 Hz, 1H), 6.86 (t, *J* = 7.6 Hz, 1H), 6.04 (s, 2H), 2.50 (s, 4H), 2.32 (s, 3H), 1.05 ppm (s, 6H); <sup>13</sup>C NMR (100 MHz, DMSO, 25 °C):  $\delta$  = 195.0, 159.7, 151.6, 148.1, 136.1, 131.8, 128.3, 127.9, 126.4, 125.0, 123.3, 122.4, 121.0, 112.0, 108.1, 108.0, 101.8, 53.7, 52.6, 30.1, 29.0, 28.4, 14.8 ppm; IR (KBr)  $\nu$  = 3274, 2955, 2924, 1736, 1702, 1615, 1544, 1458, 1423, 1331, 1226, 1103, 1044, 981, 746 cm<sup>-1</sup>; HRMS (ESI): *m/z*: calcd for C<sub>26</sub>H<sub>23</sub>NNaO<sub>5</sub>: 452.1474 [M + Na]<sup>+</sup>; found: 452.1470.

**2-(2-(Benzofuran-2-yl)-1-(2-methyl-1*H*-indol-3-yl)-2-oxoethylidene)-5,5-dimethylcyclohexane-1,3-dione (4v):** Red solid; mp: 128–130 °C. <sup>1</sup>H NMR (400 MHz, DMSO,

25 °C):  $\delta$  = 12.38 (s, 1H), 7.71 (d,  $J$  = 8.0 Hz, 1H), 7.63 (d,  $J$  = 8.0 Hz, 1H), 7.49–7.46 (m, 1H), 7.34–7.28 (m, 3H), 7.22–7.15 (m, 1H), 7.09 (t,  $J$  = 8.0 Hz, 1H), 6.99 (t,  $J$  = 8.0 Hz, 1H), 2.62 (s, 2H), 2.52–2.50 (m, 2H), 2.35 (s, 3H), 1.07 ppm (s, 6H);  $^{13}\text{C}$  NMR (100 MHz, DMSO, 25 °C):  $\delta$  = 198.7, 194.8, 185.5, 155.1, 152.8, 136.3, 128.6, 127.2, 127.0, 124.5, 124.0, 123.1, 122.1, 120.4, 113.0, 112.6, 112.3, 53.6, 52.3, 52.2, 30.2, 29.5, 28.5, 15.2 ppm; IR (KBr)  $\nu$  = 2955, 2923, 2853, 1661, 1556, 1444, 1332, 1240, 1022, 1006, 816, 750  $\text{cm}^{-1}$ ; HRMS (ESI):  $m/z$ : calcd for  $\text{C}_{27}\text{H}_{23}\text{NNaO}_4$ : 448.1525  $[\text{M} + \text{Na}]^+$ ; found: 448.1522.

**2-(2-(5-Bromothiophen-2-yl)-1-(2-methyl-1H-indol-3-yl)-2-oxoethylidene)-5,5-**

**dimethylcyclohexane-1,3-dione (4w):** Red solid; mp: 123–125 °C.  $^1\text{H}$  NMR (400 MHz, DMSO, 25 °C):  $\delta$  = 12.39 (s, 1H), 7.34 (d,  $J$  = 8.0 Hz, 1H), 7.19 (d,  $J$  = 4.0 Hz, 2H), 7.13–7.10 (m, 2H), 7.02 (t,  $J$  = 8.0 Hz, 1H), 2.61–2.58 (m, 2H), 2.52–2.50 (m, 2H), 2.31 (s, 3H), 1.05 ppm (s, 6H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , 25 °C):  $\delta$  = 198.7, 183.6, 156.5, 149.2, 145.2, 143.9, 136.0, 132.4, 131.2, 128.0, 126.5, 123.6, 122.6, 120.9, 111.9, 53.7, 52.7, 30.1, 29.1, 28.2, 14.7 ppm; IR (KBr)  $\nu$  = 3284, 2964, 2927, 1663, 1432, 1330, 1248, 1104, 1025, 748, 694  $\text{cm}^{-1}$ ; HRMS (ESI):  $m/z$ : calcd for  $\text{C}_{23}\text{H}_{20}\text{BrNNaO}_3\text{S}$ : 492.0245  $[\text{M} + \text{Na}]^+$ ; found: 492.0239.

**2-(1-(2-Methyl-1H-indol-3-yl)-2-oxo-2-phenylethylidene)cycloheptane-1,3-dione (4x):** Red solid; mp: 70–72 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , 25 °C, TMS):  $\delta$  = 8.73 (d,  $J$  = 12.0 Hz 1H), 7.83 (d,  $J$  = 4.0 Hz, 2H), 7.41 (t,  $J$  = 8.0 Hz, 1H), 7.32–7.29 (m, 3H), 7.12–7.06 (m, 3H), 2.76–2.73 (m, 2H), 2.63–2.60 (m, 2H), 2.06–2.05 (m, 5H), 2.02–1.98 ppm (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , 25 °C):  $\delta$  = 204.4, 200.0, 195.6, 151.1, 137.5, 136.2, 135.6, 135.3, 132.9, 128.7, 128.5, 126.2, 122.2, 120.9, 119.0, 111.2, 107.2, 43.0, 41.7, 24.8, 24.2, 13.5 ppm; IR (KBr)  $\nu$  = 3336, 2930, 2864, 1665, 1596, 1453, 1251, 1130, 1044, 1009, 842, 747  $\text{cm}^{-1}$ ; HRMS (ESI):  $m/z$ : calcd for  $\text{C}_{24}\text{H}_{21}\text{NNaO}_3$ : 394.1419  $[\text{M} + \text{Na}]^+$ ; found: 394.1414.

**4,4-Dimethyl-2-(1-(2-methyl-1H-indol-3-yl)-2-oxo-2-phenylethylidene)cyclohexane-1,3-dione (4y):** Red solid (*Z/E* isomer mixture); mp: 127–129 °C.  $^1\text{H}$  NMR (400 MHz, DMSO, 25 °C):  $\delta$  = 12.21 (s, 1H), 7.66 (d,  $J$  = 4.0 Hz, 2H), 7.45 (t,  $J$  = 8.0 Hz, 1H), 7.37 (t,  $J$  = 8.0 Hz, 2H), 7.30 (t,  $J$  = 8.0 Hz, 1H), 7.22 (s, 1H), 7.07 (t,  $J$  = 8.0 Hz, 1H), 6.99 (t,  $J$  = 8.0 Hz, 1H), 2.68 (t,  $J$  = 7.6 Hz, 1H), 2.58 (s, 1H), 2.35 (s, 3H), 1.89 (t,  $J$  = 7.6 Hz, 2H), 1.25–1.22 (m, 3H), 1.07 ppm (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , 25 °C):  $\delta$  = 202.7, 198.4, 195.5, 158.8, 146.8, 136.7, 136.3, 133.0, 128.9, 128.6, 126.7, 122.8, 121.8, 120.5, 112.1, 43.2, 42.1, 36.5, 35.1, 31.7, 31.3, 25.3, 25.0, 15.2 ppm; IR (KBr)  $\nu$  = 3247, 2955, 2924, 1649, 1486, 1440, 1332, 1251, 1101, 1132, 1005, 932, 798, 751  $\text{cm}^{-1}$ ; HRMS (ESI):  $m/z$ : calcd for  $\text{C}_{25}\text{H}_{23}\text{NNaO}_3$ : 408.1576  $[\text{M} + \text{Na}]^+$ ; found: 408.1578.

**2-(1-(1H-Indol-3-yl)-2-oxo-2-phenylethylidene)-5,5-dimethylcyclohexane-1,3-dione (5a):** Yellow solid; mp: 92–93 °C.  $^1\text{H}$  NMR (400 MHz, DMSO, 25 °C):  $\delta$  = 10.90 (s, 1H), 10.64 (s, 1H), 7.77 (d,  $J$  = 8.0 Hz, 2H), 7.49 (t,  $J$  = 7.6 Hz, 1H), 7.42 (q,  $J$  = 8.0 Hz, 3H), 7.18 (d,  $J$  = 8.0 Hz, 1H),



6.91 (t,  $J = 8.0$  Hz, 1H), 6.81 (t,  $J = 7.6$  Hz, 1H), 5.81 (s, 1H), 2.30 (s, 3H), 2.24–1.99 (m, 4H), 0.83 ppm (s, 6H);  $^{13}\text{C}$  NMR (100 MHz, DMSO, 25 °C):  $\delta = 198.7, 196.1, 171.0, 138.3, 135.5, 133.3, 132.1, 129.0, 128.5, 127.8, 120.1, 119.8, 118.1, 114.8, 110.4, 109.0, 50.3, 43.3, 41.0, 32.3, 28.2, 12.5$  ppm; IR (KBr)  $\nu = 3348, 3060, 2959, 2872, 2652, 1735, 1691, 1638, 1455, 1421, 1372, 1251, 1147, 1100, 1046, 1007, 930, 847, 786, 744, 693$   $\text{cm}^{-1}$ ; HRMS (ESI)  $m/z$ : calcd for  $\text{C}_{25}\text{H}_{25}\text{NNaO}_3$ : 410.1732  $[\text{M} + \text{Na}]^+$ ; found: 410.1728.

**3-Acetyl-2-(1H-indol-3-yl)-1-phenylpentane-1,4-dione (5b)**: Brown viscous liquid;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , TMS, 25 °C):  $\delta = 8.80$  (s, 1H), 7.94 (d,  $J = 7.2$  Hz, 2H), 7.73–7.01 (m, 1H), 7.36 (t,  $J = 7.2$  Hz, 1H), 7.27–7.23 (m, 3H), 7.14–7.12 (m, 2H), 7.01 (d,  $J = 2.8$  Hz, 1H), 5.67 (d,  $J = 11.2$  Hz, 1H), 5.06 (d,  $J = 11.2$  Hz, 1H), 2.28 (s, 3H), 1.86 ppm (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , 25 °C):  $\delta = 204.0, 202.3, 197.8, 136.5, 135.8, 133.0, 128.7, 128.4, 125.7, 124.2, 122.5, 120.3, 118.9, 111.7, 109.0, 70.2, 45.5, 31.5, 30.3$  ppm; IR (KBr)  $\nu = 3398, 2934, 1725, 2696, 1597, 1355, 1264, 744, 691, 560, 504, 427$   $\text{cm}^{-1}$ ; HRMS (ESI):  $m/z$ : calcd for  $\text{C}_{21}\text{H}_{19}\text{NNaO}_3$ : 356.1263  $[\text{M} + \text{Na}]^+$ ; found: 356.1257.

**2-((2-Chlorophenyl)(2-methyl-1H-indol-3-yl)methylene)-5,5-dimethylcyclohexane-1,3-dione (7a)**: Orange solid; mp: 179–180 °C.  $^1\text{H}$  NMR (400 MHz, DMSO, 25 °C):  $\delta = 12.06$  (s, 1H), 7.38–7.29 (m, 5H), 7.01 (t,  $J = 8.0$  Hz, 1H), 6.80 (t,  $J = 8.0$  Hz, 1H), 6.41 (d,  $J = 8.0$  Hz, 1H), 2.70–2.59 (m, 2H), 2.43 (d,  $J = 8.0$  Hz, 2H), 2.19 (s, 3H), 1.09–1.01 ppm (m, 6H);  $^{13}\text{C}$  NMR (100 MHz, DMSO, 25 °C):  $\delta = 180.6, 136.1, 130.1, 128.2, 127.2, 122.2, 121.3, 119.9, 115.8, 111.9, 54.1, 29.9, 29.4, 27.9, 14.5$  ppm; IR (KBr)  $\nu = 3390, 2959, 2924, 2872, 2648, 1762, 1608, 1463, 1373, 1252, 1041, 909, 735$   $\text{cm}^{-1}$ ; HRMS (ESI):  $m/z$ : calcd for  $\text{C}_{24}\text{H}_{22}\text{ClNNaO}_2$ : 414.1237  $[\text{M} + \text{Na}]^+$ ; found: 414.1231.

**1-Denzyl-4-phenyl-1H-1,2,3-triazole (8a)**:<sup>3</sup> White solid; mp: 128–130 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , 25 °C, TMS):  $\delta = 7.80$  (d,  $J = 4.0$  Hz, 2H), 7.66 (s, 1H), 7.42–7.36 (m, 5H), 7.33–7.30 (m, 3H), 5.58 ppm (s, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , 25 °C):  $\delta = 148.3, 134.7, 130.6, 129.2, 128.8, 128.2, 128.1, 125.7, 119.5, 54.3$  ppm.

**1-Benzyl-4-(4-fluorophenyl)-1H-1,2,3-triazole (8b)**:<sup>4</sup> White solid; mp: 109–110 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , 25 °C, TMS):  $\delta = 7.75$  (q,  $J = 4.0$  Hz, 2H), 7.64 (s, 1H), 7.35 (s, 3H), 7.29 (d,  $J = 4.0$  Hz, 2H), 7.05 (d,  $J = 8.4$  Hz, 2H), 5.53 ppm (s, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , 25 °C):  $\delta = 162.7$  (d,  $J = 246.0$  Hz), 147.3, 134.7, 129.2, 128.8, 128.1, 127.45 (d,  $J = 9.0$  Hz), 119.4, 115.8 (d,  $J = 21.0$  Hz), 54.2 ppm;  $^{19}\text{F}$  NMR (377 MHz,  $\text{CDCl}_3$ , 25 °C):  $\delta = -113.5$  ppm (heptet,  $J = 5.6$  Hz, 1F).

**1-Benzyl-4-(4-methoxyphenyl)-1H-1,2,3-triazole (8c)**:<sup>4</sup> White solid; mp: 138–139 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , 25 °C, TMS):  $\delta = 7.71$  (d,  $J = 8.0$  Hz, 2H), 7.58 (s, 1H), 7.37–7.35 (m, 3H), 7.29–7.27 (m, 2H), 6.92 (d,  $J = 12.0$  Hz, 2H), 5.52 (s, 2H), 3.80 ppm (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,

CDCl<sub>3</sub>, 25 °C):  $\delta$  = 159.6, 148.1, 134.8, 129.1, 128.7, 128.0, 127.0, 123.3, 118.8, 114.2, 55.3, 54.2 ppm.

**1-Benzyl-4-(4-(*tert*-butyl)phenyl)-1*H*-1,2,3-triazole (8d):**<sup>4</sup> White solid; mp: 112–113 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, 25 °C, TMS):  $\delta$  = 7.72 (d, *J* = 8.0 Hz, 2H), 7.64 (s, 1H), 7.41 (d, *J* = 8.0 Hz, 2H), 7.35–7.34 (m, 3H), 7.28–7.26 (m, 2H), 5.52 (s, 2H), 1.23 ppm (s, 9H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, 25 °C):  $\delta$  = 151.3, 148.2, 134.9, 129.1, 128.7, 128.0, 127.8, 125.8, 125.5, 119.4, 54.2, 34.7, 31.3 ppm.

**1-Benzyl-4-(4-ethylphenyl)-1*H*-1,2,3-triazole (8e):**<sup>3</sup> White solid; mp: 147–148 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, 25 °C, TMS):  $\delta$  = 7.70 (d, *J* = 8.0 Hz, 2H), 7.63 (s, 1H), 7.35–7.33 (m, 3H), 7.28–7.26 (m, 2H), 7.21 (d, *J* = 8.0 Hz, 2H), 5.51 (s, 2H), 2.64 (q, *J* = 8.0 Hz, 2H), 1.23 ppm (t, *J* = 8.0 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, 25 °C):  $\delta$  = 148.3, 144.4, 134.8, 129.1, 128.7, 128.3, 128.0, 125.7, 119.3, 54.2, 28.7, 15.5 ppm.

**1-Benzyl-4-(4-pentylphenyl)-1*H*-1,2,3-triazole (8f):**<sup>5</sup> White solid; mp: 103–104 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, 25 °C, TMS):  $\delta$  = 7.70 (d, *J* = 8.0 Hz, 2H), 7.62 (s, 1H), 7.37–7.35 (m, 3H), 7.29–7.27 (m, 2H), 7.20 (d, *J* = 8.0 Hz, 2H), 5.53 (s, 2H), 2.60 (t, *J* = 8.0 Hz, 2H), 1.61 (quint, *J* = 8.0 Hz, 2H), 1.35–1.26 (m, 4H), 0.88 ppm (t, *J* = 8.0 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, 25 °C):  $\delta$  = 148.3, 143.1, 134.8, 129.1, 128.9, 128.7, 128.0, 125.6, 119.3, 54.2, 35.7, 31.5, 31.1, 22.6, 14.1 ppm.

**1-Benzyl-4-(4-propylphenyl)-1*H*-1,2,3-triazole (8g):**<sup>6</sup> White solid; mp: 113–115 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, 25 °C, TMS):  $\delta$  = 7.70 (d, *J* = 8.0 Hz, 2H), 7.62 (s, 1H), 7.38–7.34 (m, 3H), 7.29–7.27 (m, 2H), 7.20 (d, *J* = 8.0 Hz, 2H), 5.54 (s, 2H), 2.59 (d, *J* = 7.6 Hz, 2H), 1.68–1.59 (m, 2H), 0.93 ppm (t, *J* = 8.0 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, 25 °C):  $\delta$  = 148.3, 142.9, 134.8, 129.1, 128.9, 128.7, 128.0, 125.6, 119.2, 54.2, 37.8, 24.5, 13.8 ppm.

**1-Phenethyl-4-phenyl-1*H*-1,2,3-triazole (8h):**<sup>6</sup> White solid; mp: 124–125 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, 25 °C, TMS):  $\delta$  = 7.77–7.75 (m, 2H), 7.47 (s, 1H), 7.38 (t, *J* = 8.0 Hz, 2H), 7.31–7.21 (m, 4H), 7.10 (d, *J* = 4.0 Hz, 2H), 4.59 (t, *J* = 7.6 Hz, 2H), 3.21 ppm (t, *J* = 8.0 Hz, 2H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, 25 °C):  $\delta$  = 147.5, 137.1, 130.7, 128.9, 128.8, 128.1, 127.1, 125.7, 120.0, 51.7, 36.8 ppm.

**1-Ethyl-4-phenyl-1*H*-1,2,3-triazole (8i):**<sup>6</sup> White solid; mp: 55–57 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, 25 °C, TMS):  $\delta$  = 7.83–7.81 (m, 2H), 7.76 (s, 1H), 7.41 (t, *J* = 8.0 Hz, 2H), 7.32 (m, 1H), 4.43 (q, *J* = 8.0 Hz, 2H), 1.58 ppm (t, *J* = 7.6 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, 25 °C):  $\delta$  = 147.8, 130.8, 128.8, 128.1, 125.7, 119.0, 45.4, 15.5 ppm.

**1-Ethyl-4-(4-fluorophenyl)-1*H*-1,2,3-triazole (8j):**<sup>4</sup> White solid; mp: 114–115 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, 25 °C, TMS):  $\delta$  = 7.81–7.77 (m, 2H), 7.74 (s, 1H), 7.10 (t, *J* = 8.0 Hz, 2H), 4.44 (q, *J* = 8.0 Hz, 2H), 1.58 ppm (t, *J* = 7.6 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, 25 °C):  $\delta$  = 163.8,

161.4, 146.9, 127.38 (d,  $J = 12.0$  Hz), 118.8, 115.7 (d,  $J = 22.0$  Hz), 45.4, 15.5 ppm.  $^{19}\text{F}$  NMR (377 MHz,  $\text{CDCl}_3$ , 25 °C):  $\delta = -113.8$  ppm (heptet,  $J = 5.7$  Hz, 1F).

**4-Phenyl-1-propyl-1H-1,2,3-triazole (8k):**<sup>7</sup> White solid; mp: 102–103 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , 25 °C, TMS):  $\delta = 7.83$  (d,  $J = 8.0$  Hz, 2H), 7.75 (s, 1H), 7.41 (t,  $J = 8.0$  Hz, 2H), 7.31 (t,  $J = 8.0$  Hz, 1H), 4.36 (t,  $J = 8.0$  Hz, 2H), 1.94–1.90 (m, 2H), 1.33–1.25 (m, 14H), 0.87 ppm (t,  $J = 8.0$  Hz, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , 25 °C):  $\delta = 147.7$ , 130.8, 128.8, 128.0, 125.7, 119.5, 50.4, 31.9, 30.4, 29.5, 29.4, 29.3, 29.0, 26.5, 22.7, 14.1 ppm.

**4-((4-Phenyl-1H-1,2,3-triazol-1-yl)methyl)benzoic acid (8l):**<sup>8</sup> White solid; mp: 114–116 °C.  $^1\text{H}$  NMR (400 MHz, DMSO, 25 °C):  $\delta = 8.66$  (s, 1H), 7.96 (d,  $J = 8.0$  Hz, 2H), 7.86 (d,  $J = 8.0$  Hz, 2H), 7.46–7.42 (m, 4H), 7.34–7.31 (m, 1H), 5.75 ppm (s, 2H);  $^{13}\text{C}$  NMR (100 MHz, DMSO, 25 °C):  $\delta = 167.5$ , 147.2, 141.1, 131.2, 131.0, 130.3, 129.4, 128.4, 125.7, 122.3, 53.1 ppm.

**1-(4-Nitrobenzyl)-4-phenyl-1H-1,2,3-triazole (8m):**<sup>6</sup> White solid; mp: 140–141 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , 25 °C, TMS):  $\delta = 8.20$  (d,  $J = 8.0$  Hz, 2H), 7.80 (d,  $J = 8.0$  Hz, 3H), 7.43–7.39 (m, 4H), 7.35–7.31 (m, 1H), 5.68 ppm (s, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , 25 °C):  $\delta = 148.7$ , 148.1, 141.8, 130.1, 128.9, 128.6, 128.5, 125.8, 124.3, 119.9, 53.2 ppm.

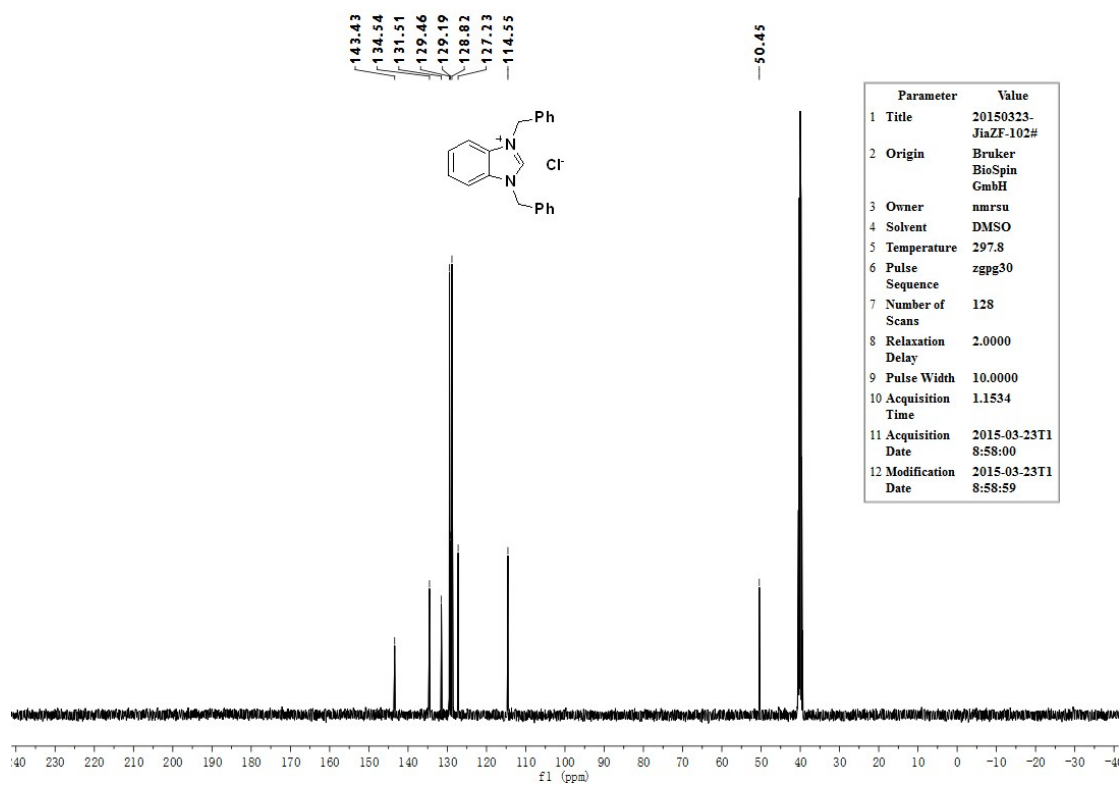
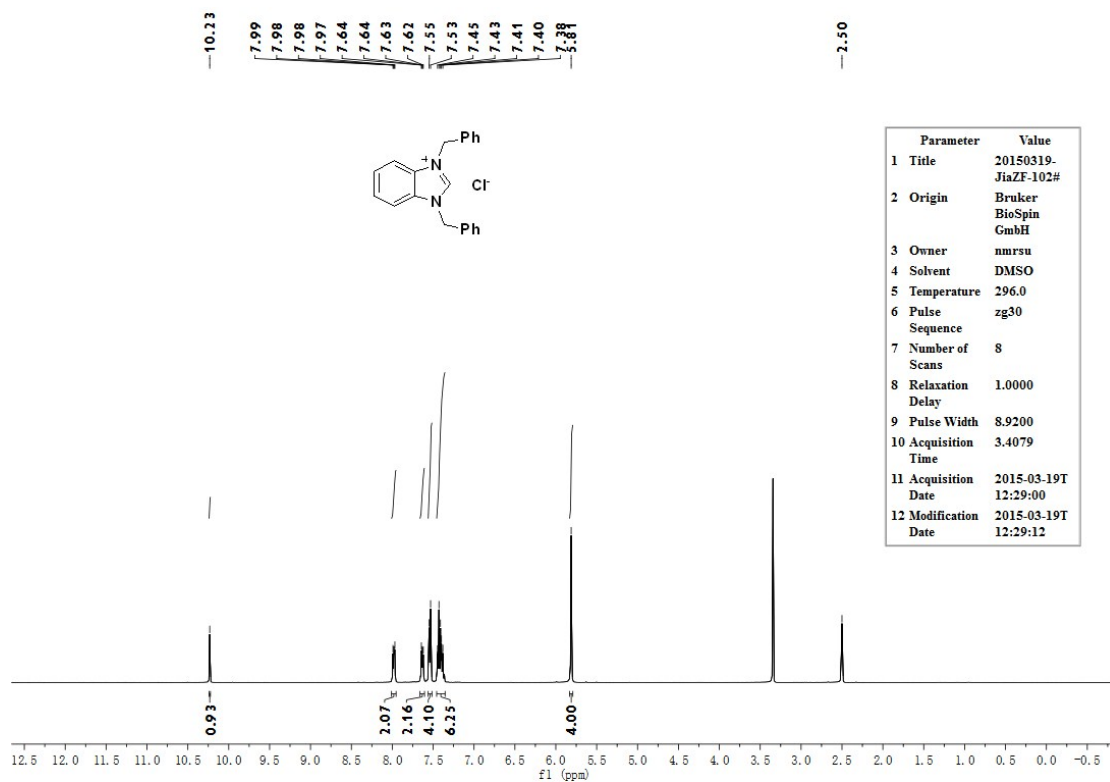
**1-Benzyl-4-(phoxymethyl)-1H-1,2,3-triazole (8n):**<sup>3</sup> White solid; mp: 102–104 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , 25 °C, TMS):  $\delta = 7.52$  (s, 2H), 7.37–7.33 (m, 3H), 7.28–7.24 (m, 4H), 6.96–6.93 (m, 3H), 5.50 (s, 2H), 5.16 ppm (s, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , 25 °C):  $\delta = 158.2$ , 144.7, 134.5, 129.6, 129.2, 128.8, 128.1, 122.7, 121.3, 114.8, 62.1, 54.2 ppm.

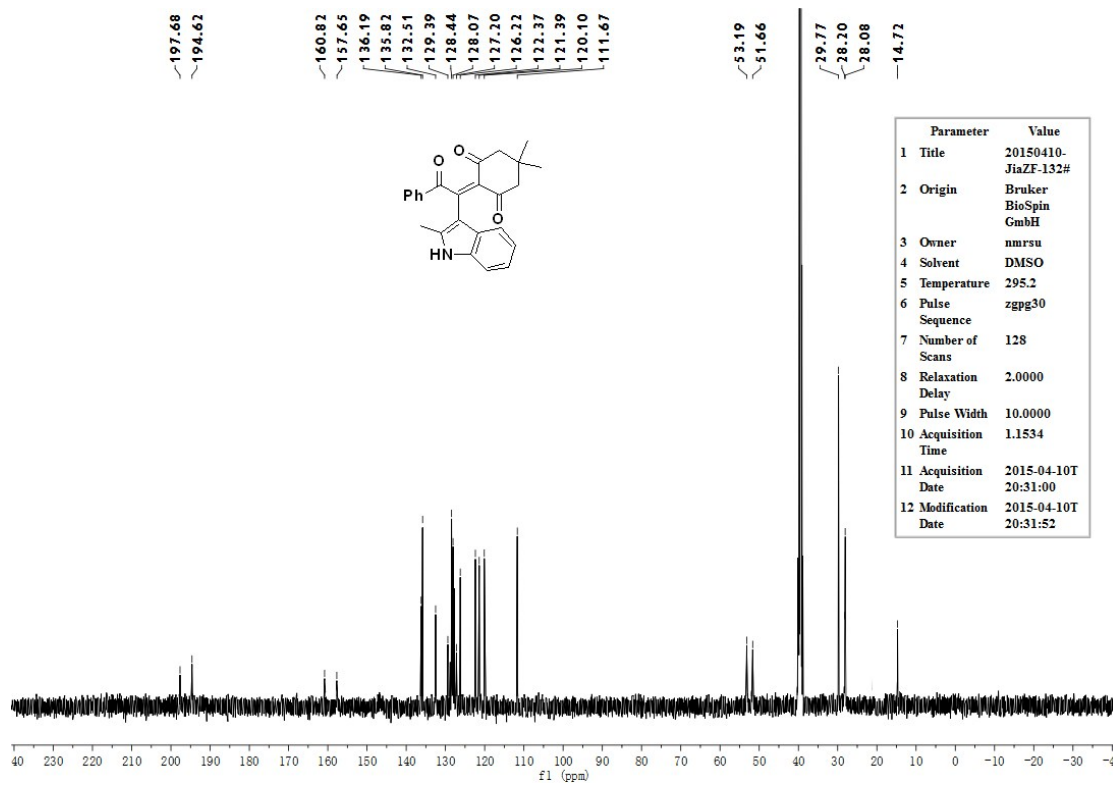
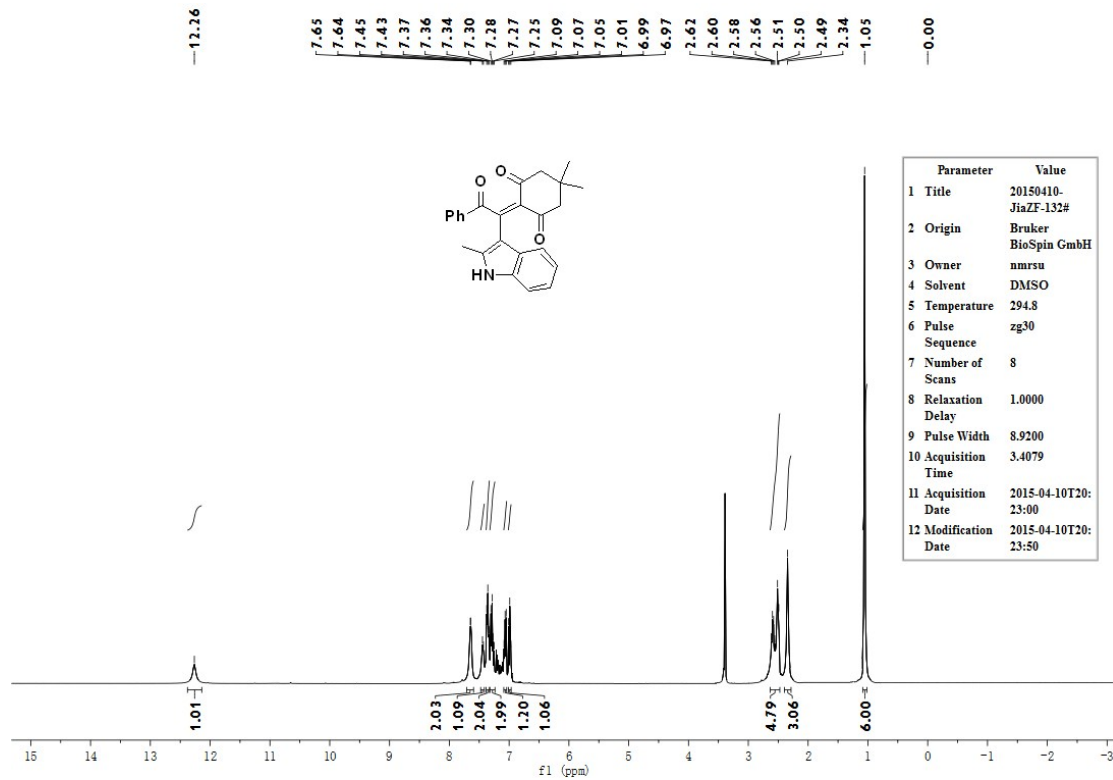
**1-Hexyl-4-phenyl-1H-1,2,3-triazole (8o):**<sup>4</sup> White solid; mp: 63–64 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , 25 °C, TMS):  $\delta = 7.84$ –7.82 (m, 2H), 7.75 (s, 1H), 7.41 (t,  $J = 8.0$  Hz, 2H), 7.32 (t,  $J = 8.0$  Hz, 1H), 4.37 (t,  $J = 8.0$  Hz, 2H), 1.96–1.89 (m, 2H), 1.36–1.29 (m, 6H), 0.88 ppm (t,  $J = 8.0$  Hz, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , 25 °C):  $\delta = 147.7$ , 130.8, 128.8, 128.1, 125.7, 119.5, 50.4, 31.2, 30.3, 26.2, 22.4, 13.9 ppm.

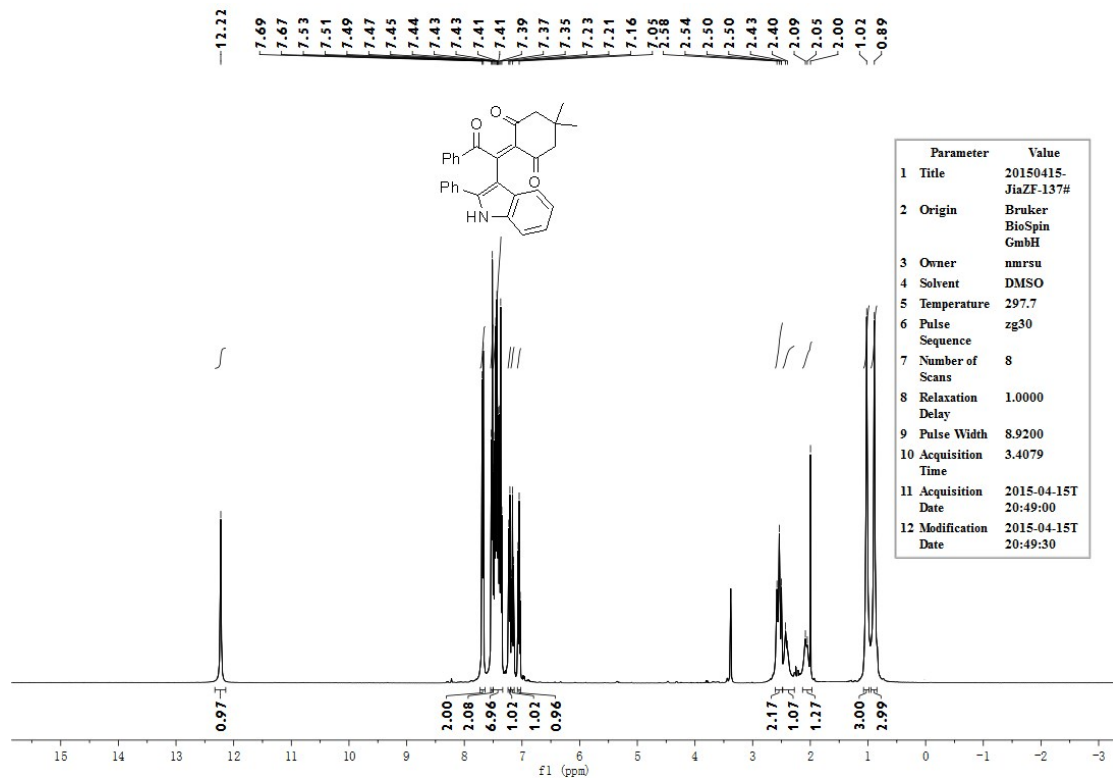
**1,4-Diphenylbuta-1,3-diyne (9a):**<sup>5</sup> White solid; mp: 83–85 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , 25 °C, TMS):  $\delta = 7.51$ –7.52 (m, 5H), 7.33–7.31 ppm (m, 5H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , 25 °C):  $\delta = 132.6$ , 129.3, 128.5, 121.9, 81.7, 74.1 ppm.

**1-(4-Methoxyphenyl)-1H-indole (10a):**<sup>9</sup> White solid; mp: 70–72 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , 25 °C, TMS):  $\delta = 7.68$  (d,  $J = 8.0$  Hz, 1H), 7.46 (d,  $J = 8.0$  Hz, 1H), 7.40 (d,  $J = 8.0$  Hz, 2H), 7.28 (d,  $J = 4.0$  Hz, 1H), 7.22–7.13 (m, 2H), 7.03 (d,  $J = 8.0$  Hz, 2H), 6.65 (d,  $J = 4.0$  Hz, 1H), 3.87 ppm (d, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , 25 °C):  $\delta = 158.3$ , 138.2, 136.3, 132.9, 129.0, 128.3, 126.0, 122.2, 121.0, 120.1, 114.7, 110.4, 102.9, 55.6 ppm.

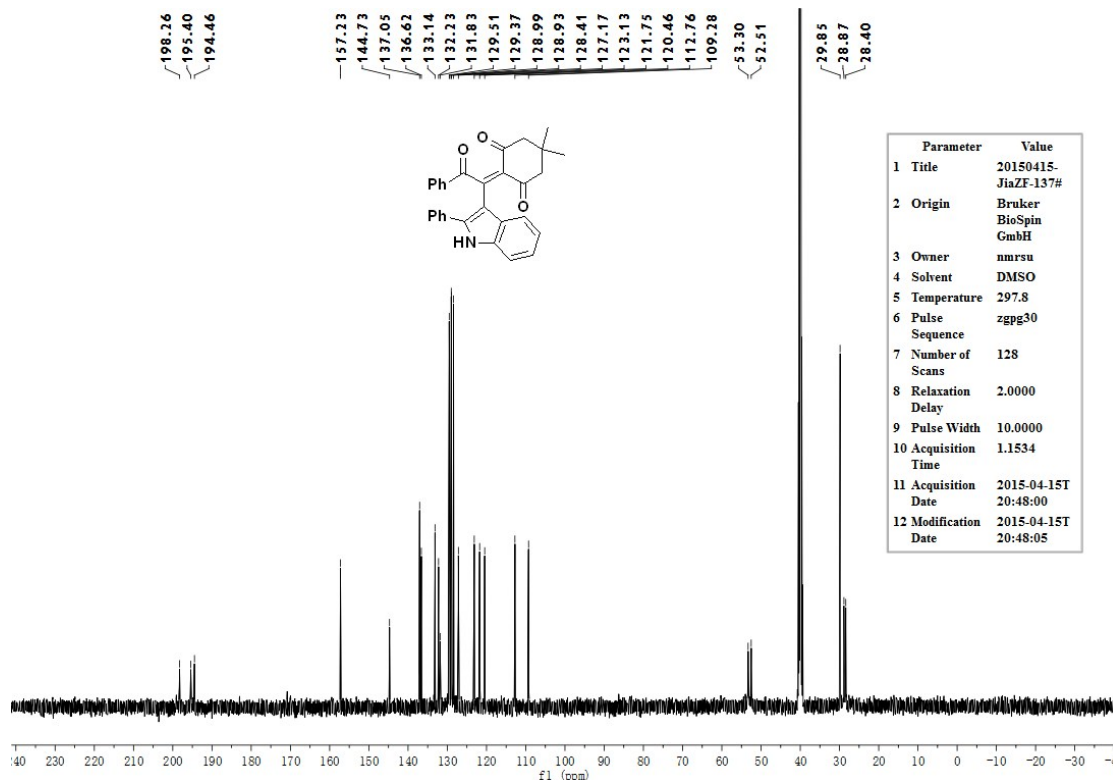
## 5. <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra



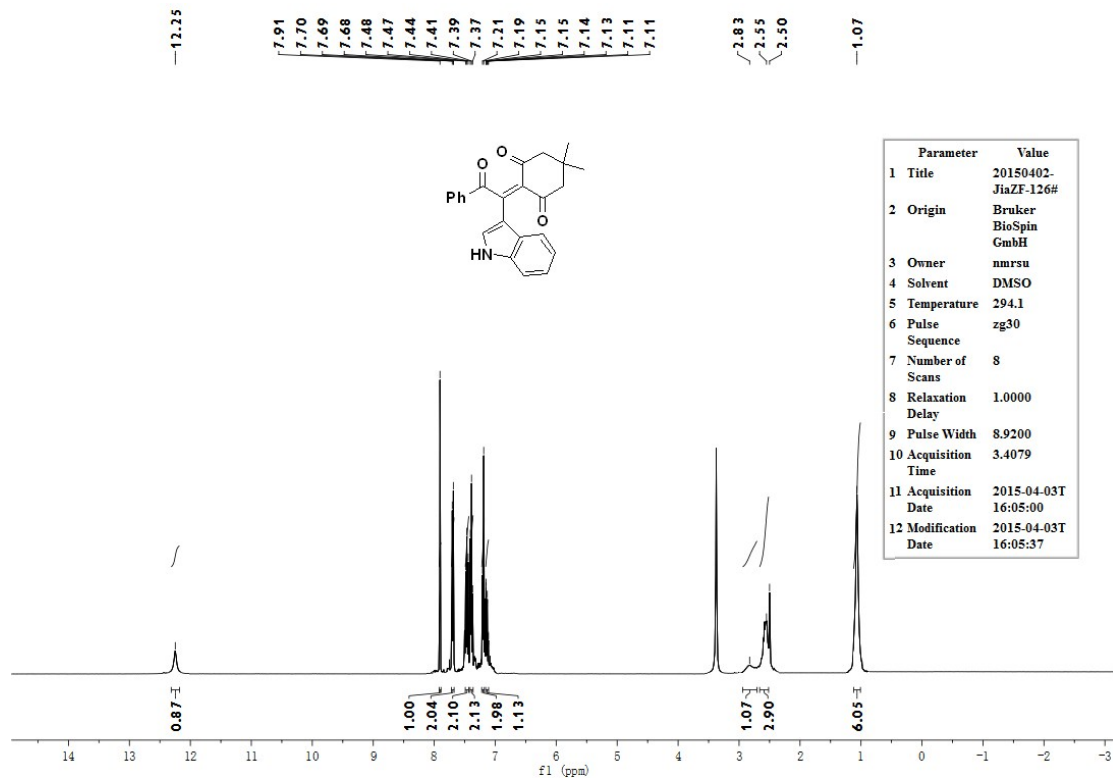




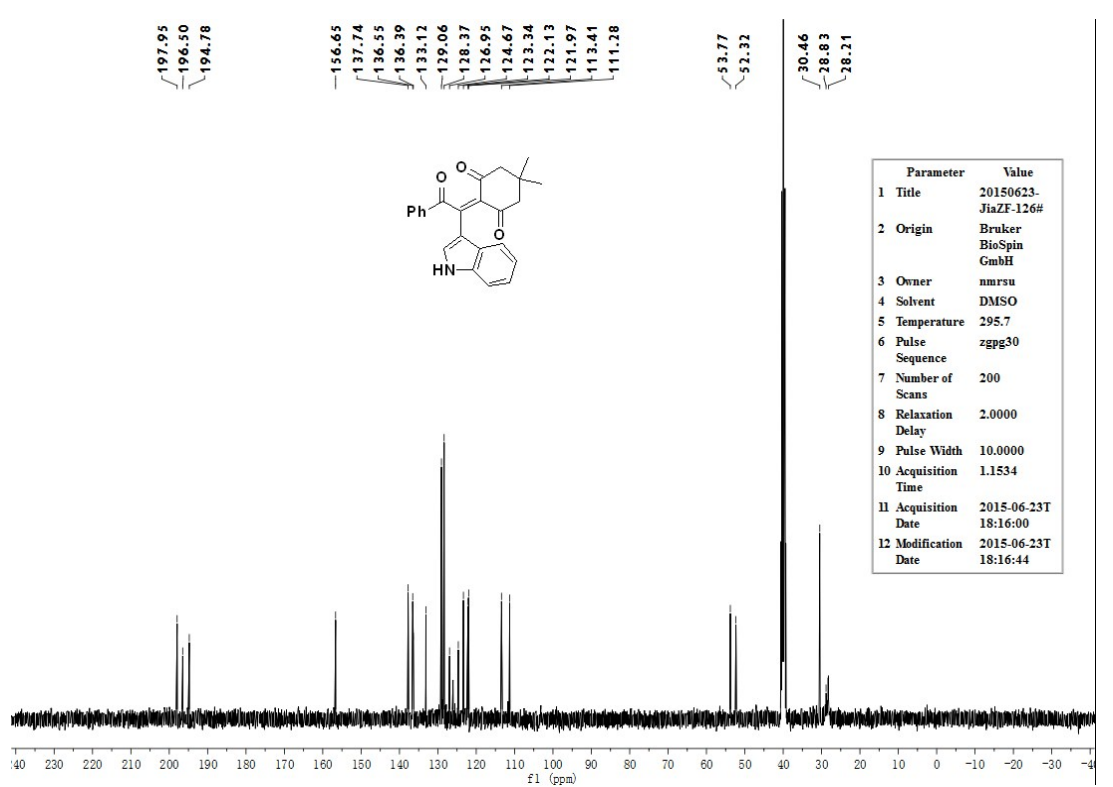
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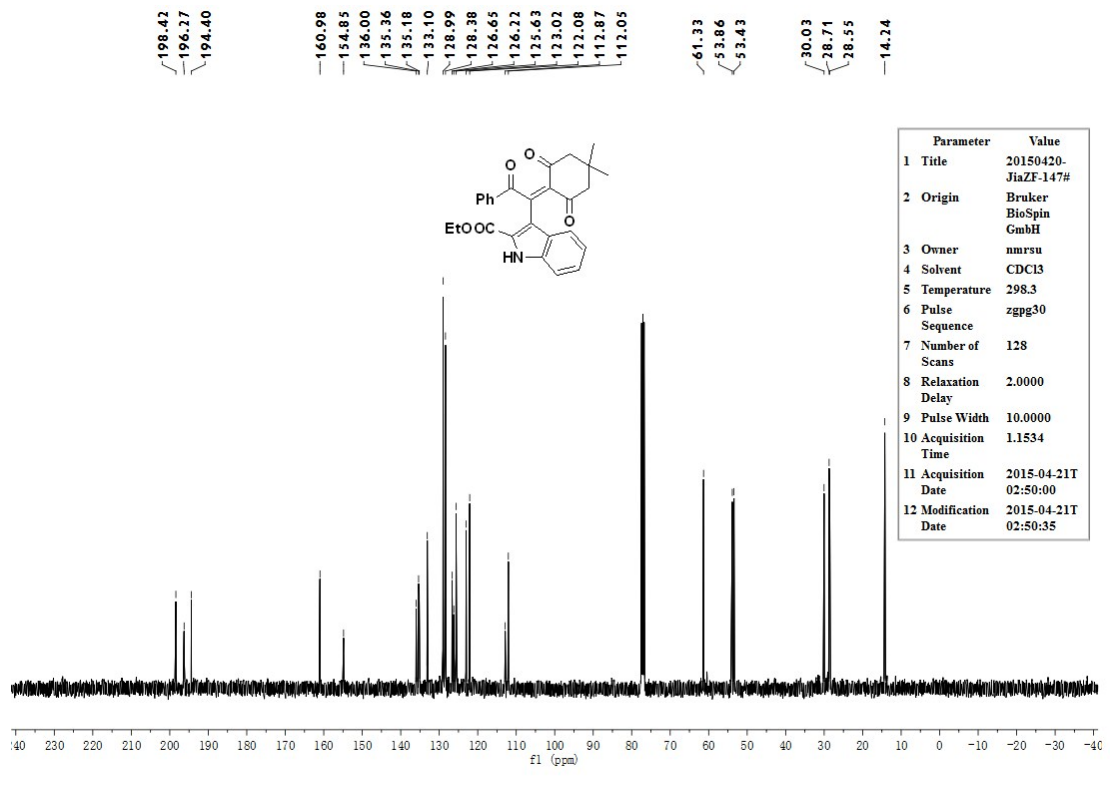
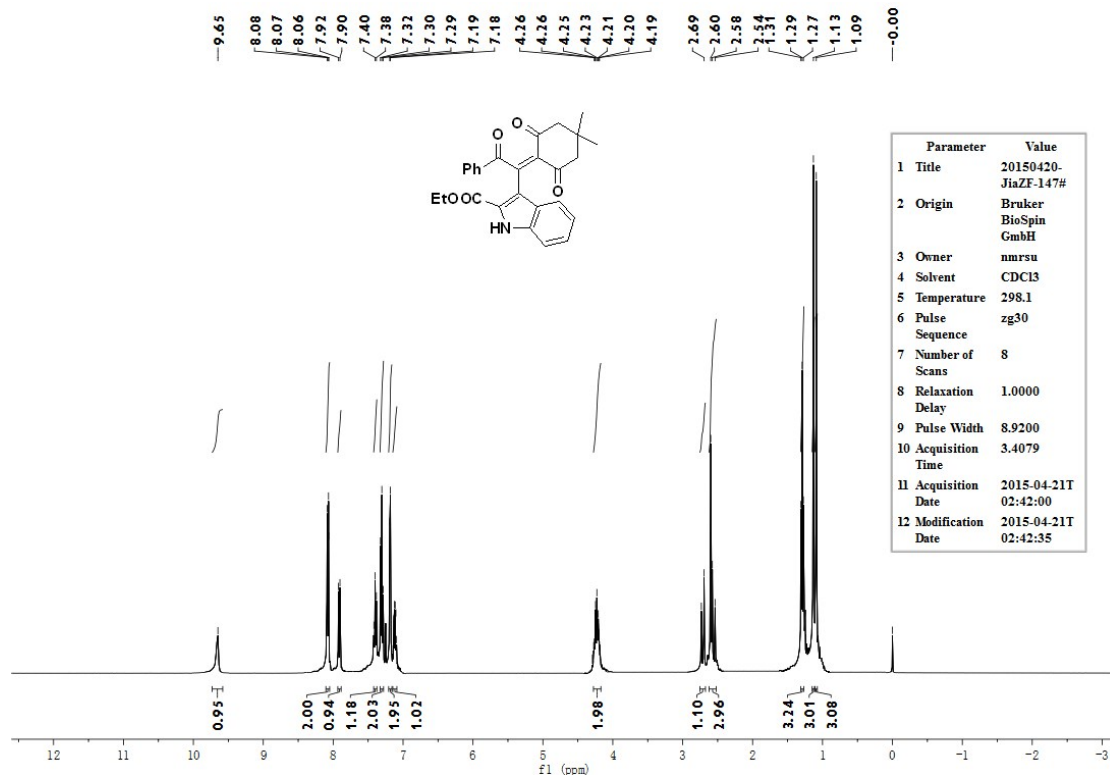
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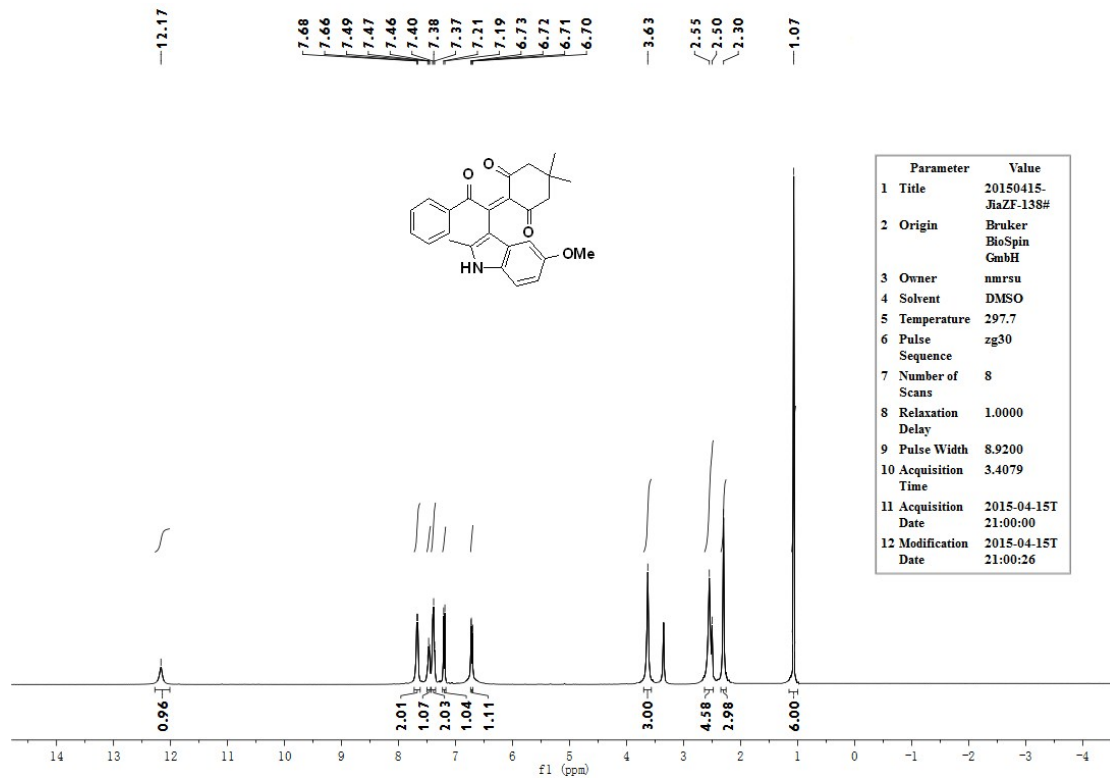
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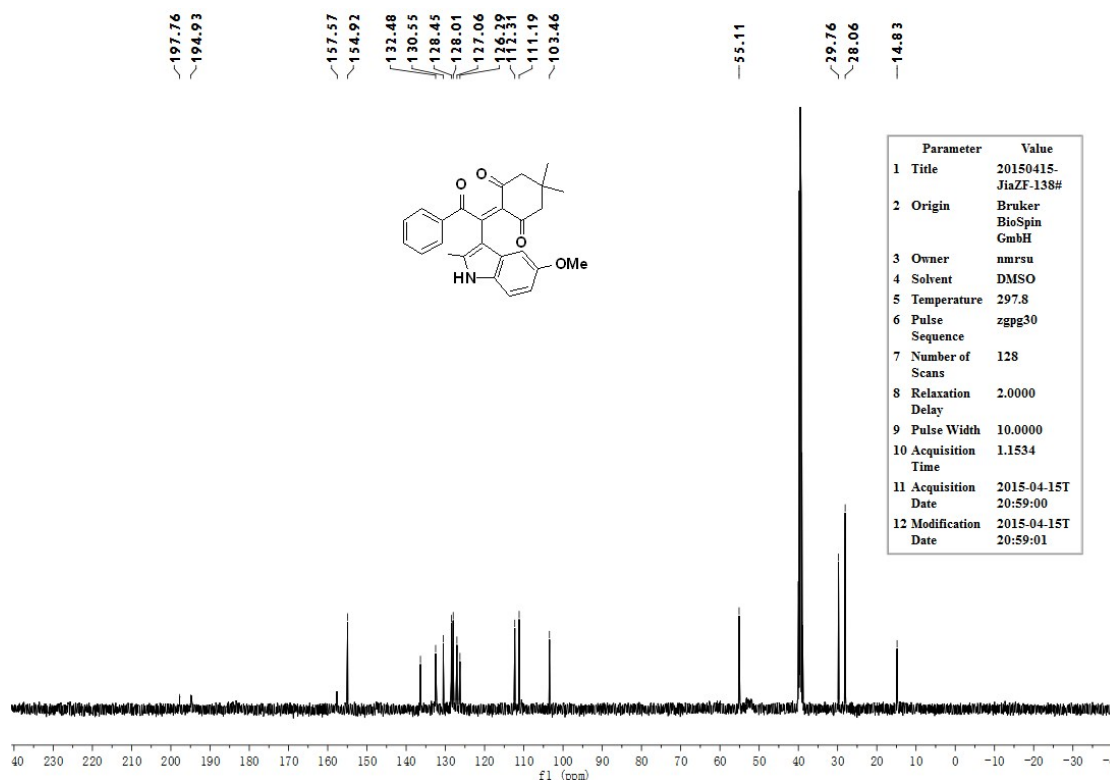
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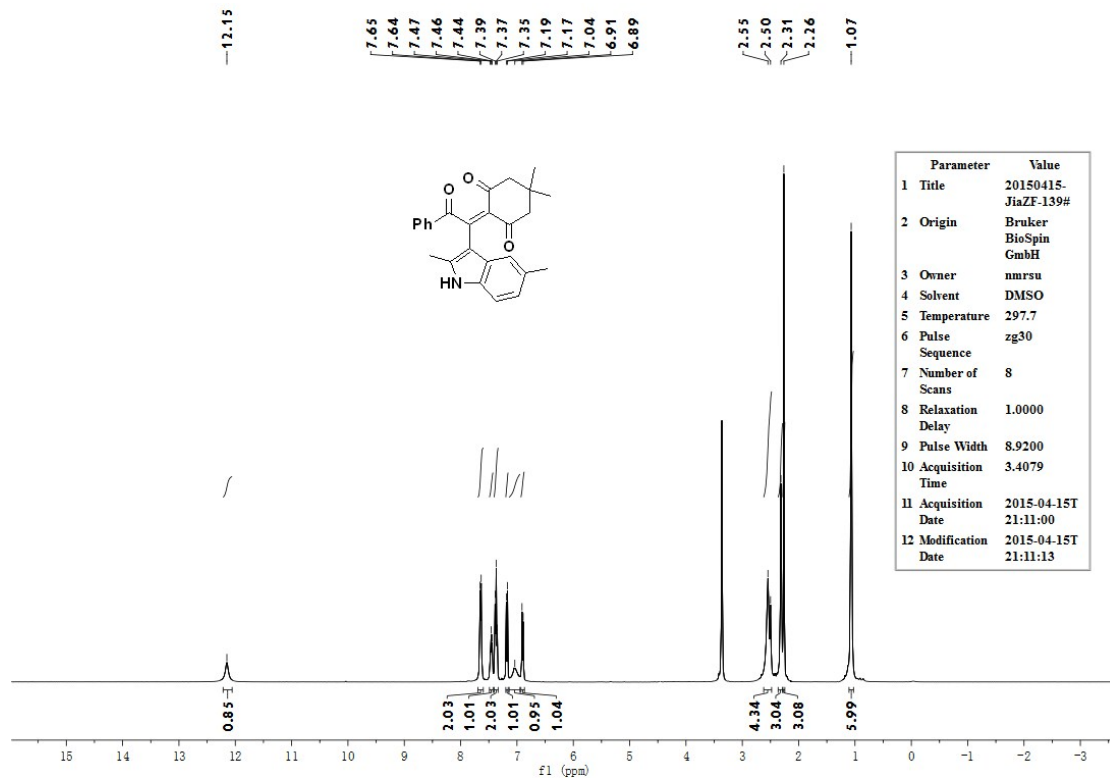




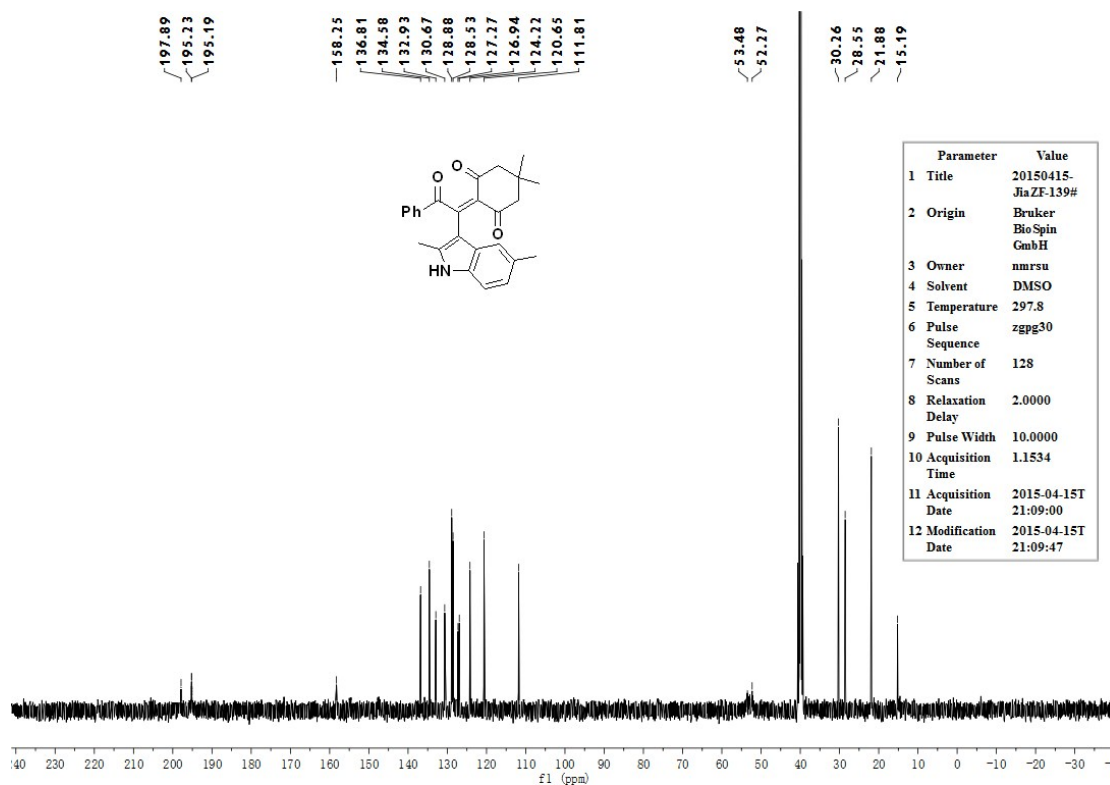
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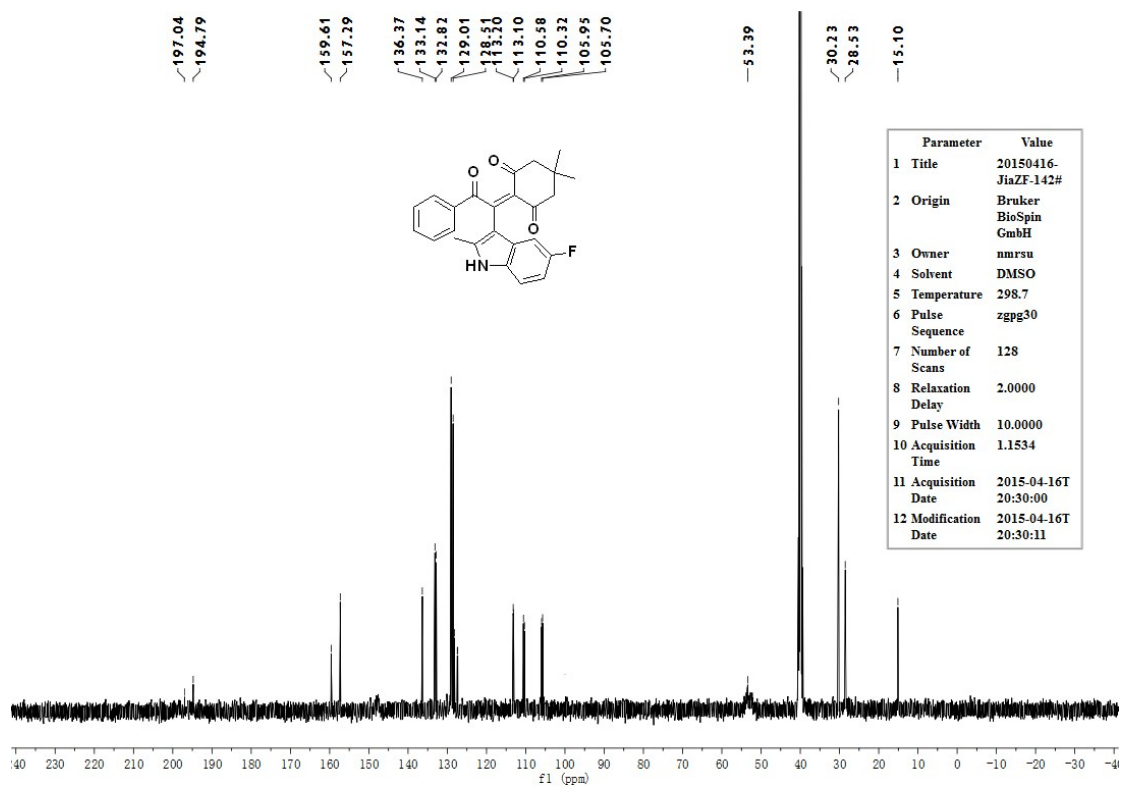
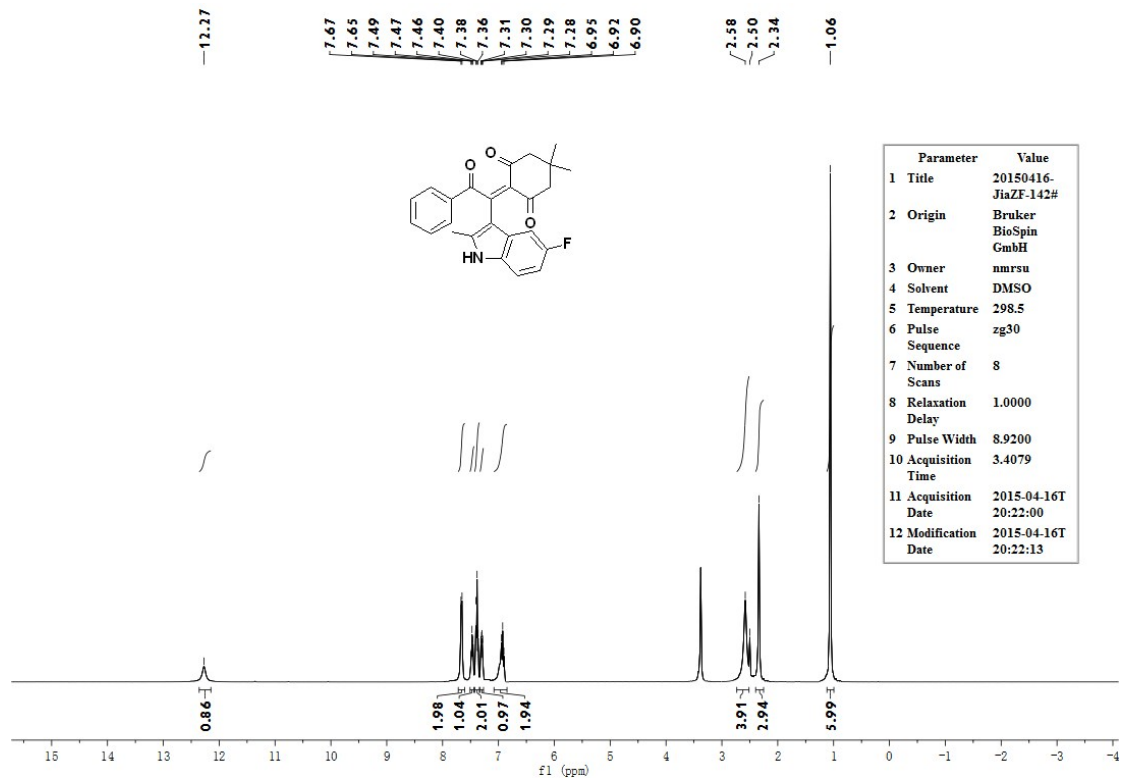
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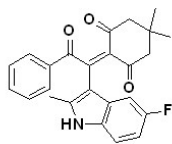


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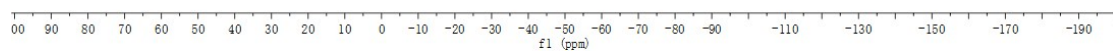
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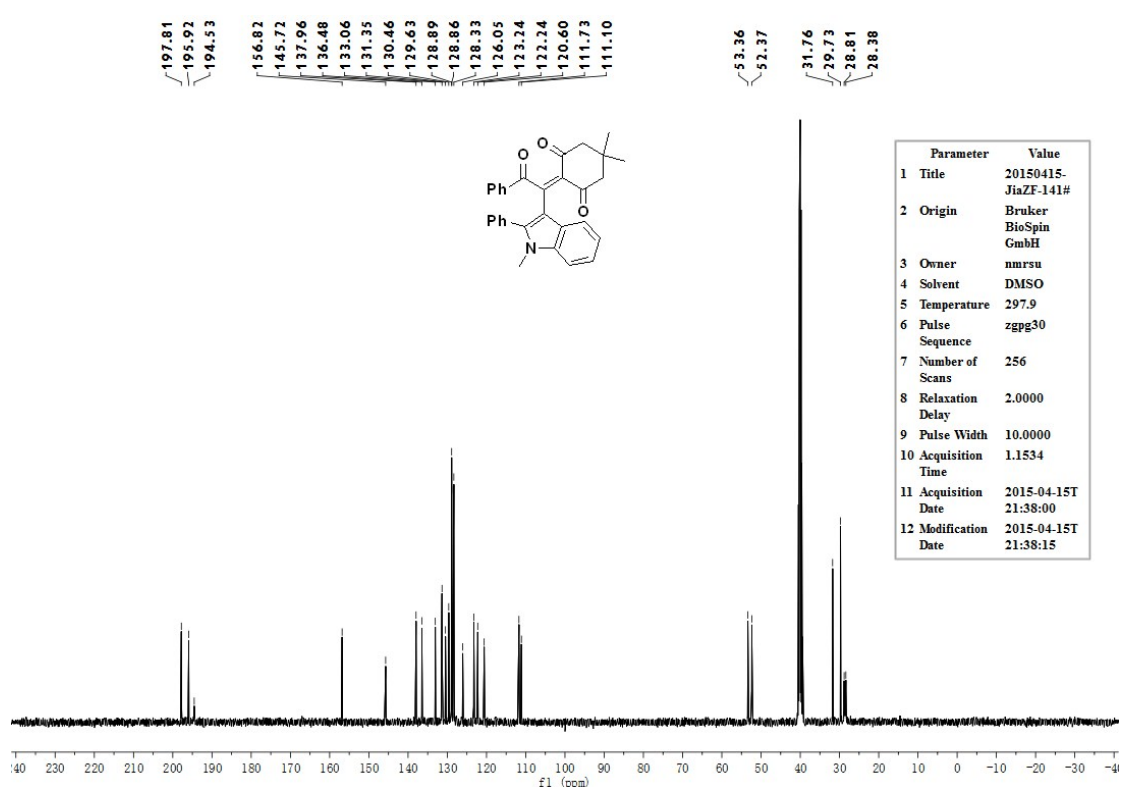
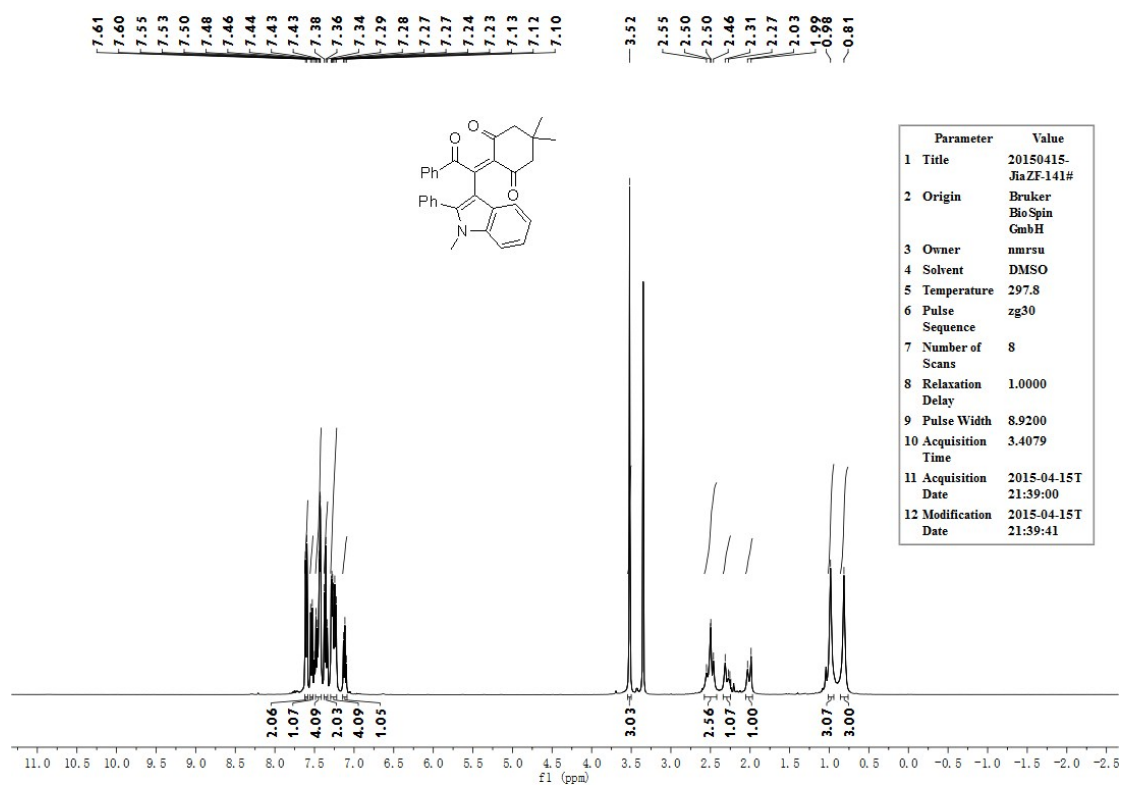


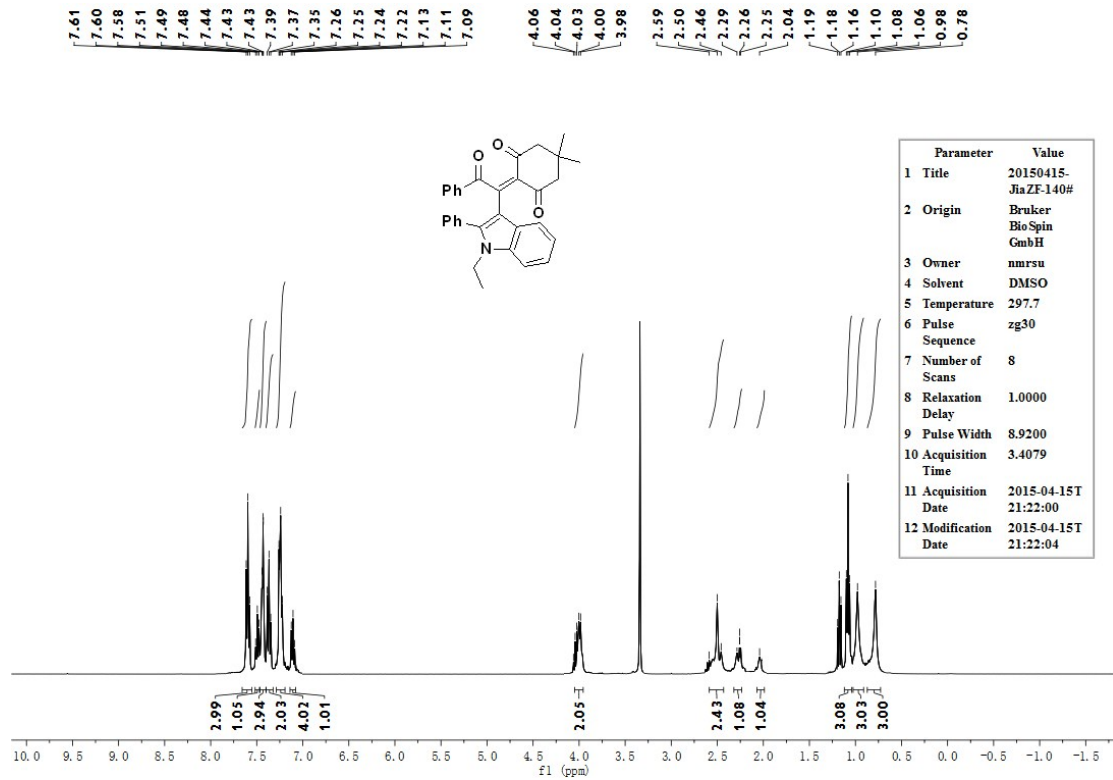


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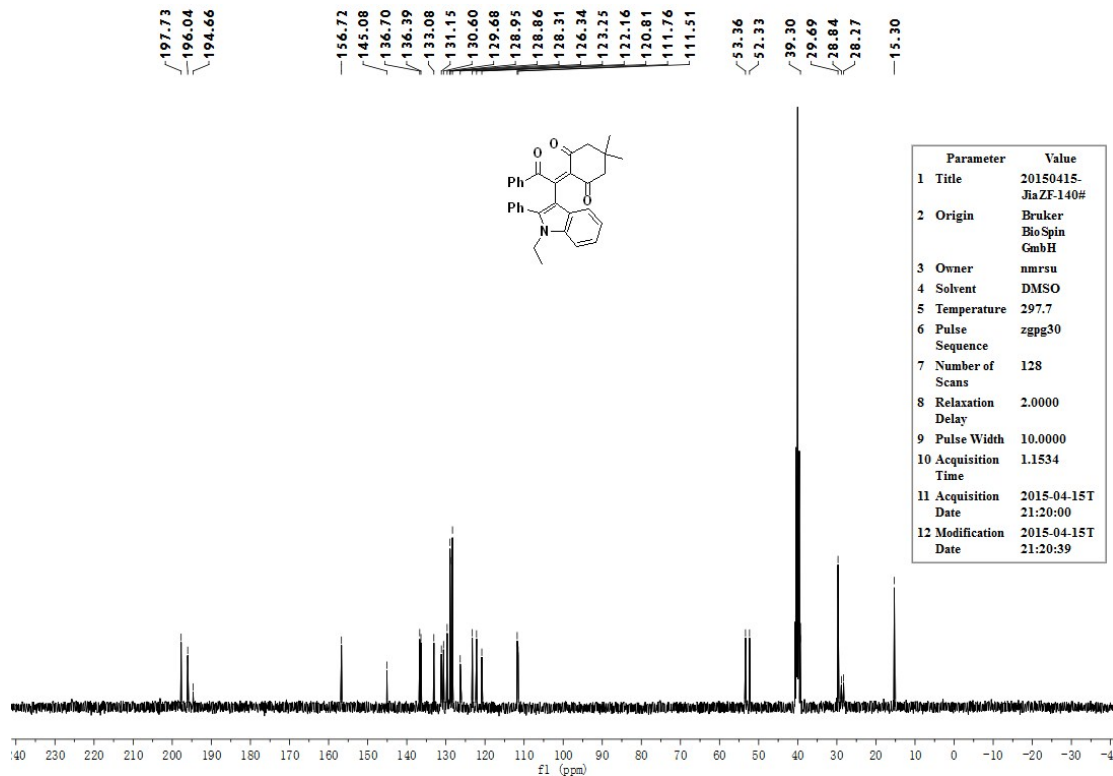
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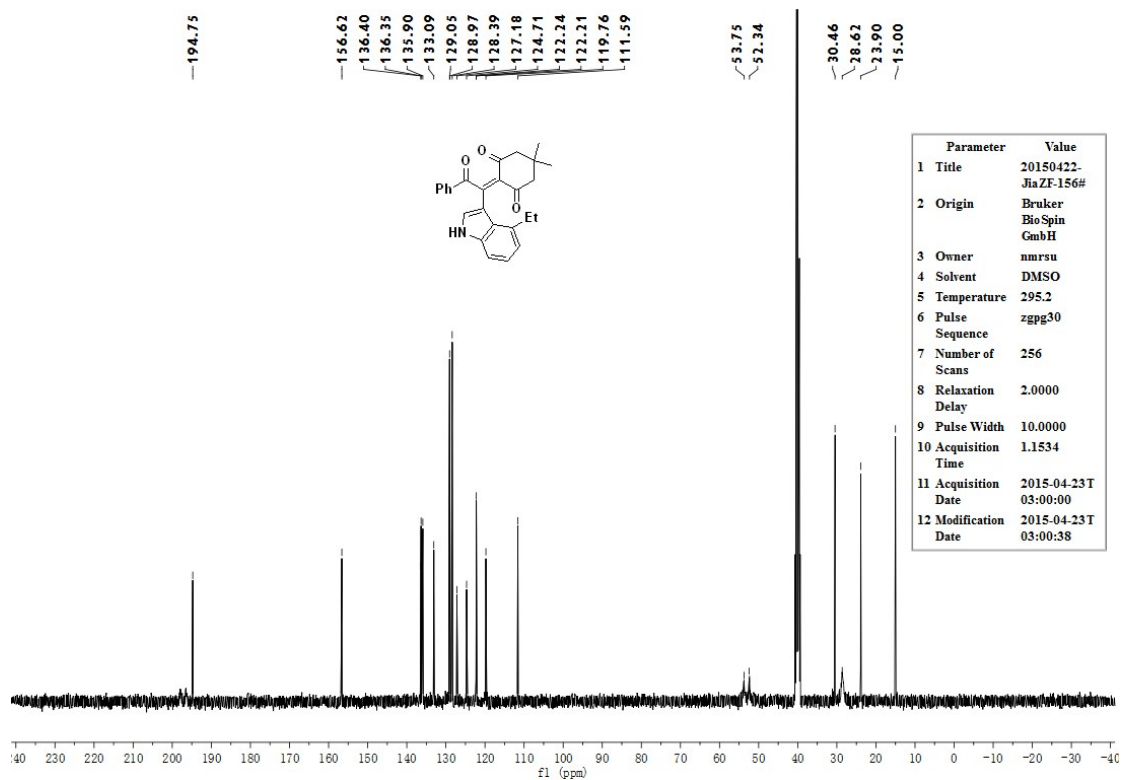
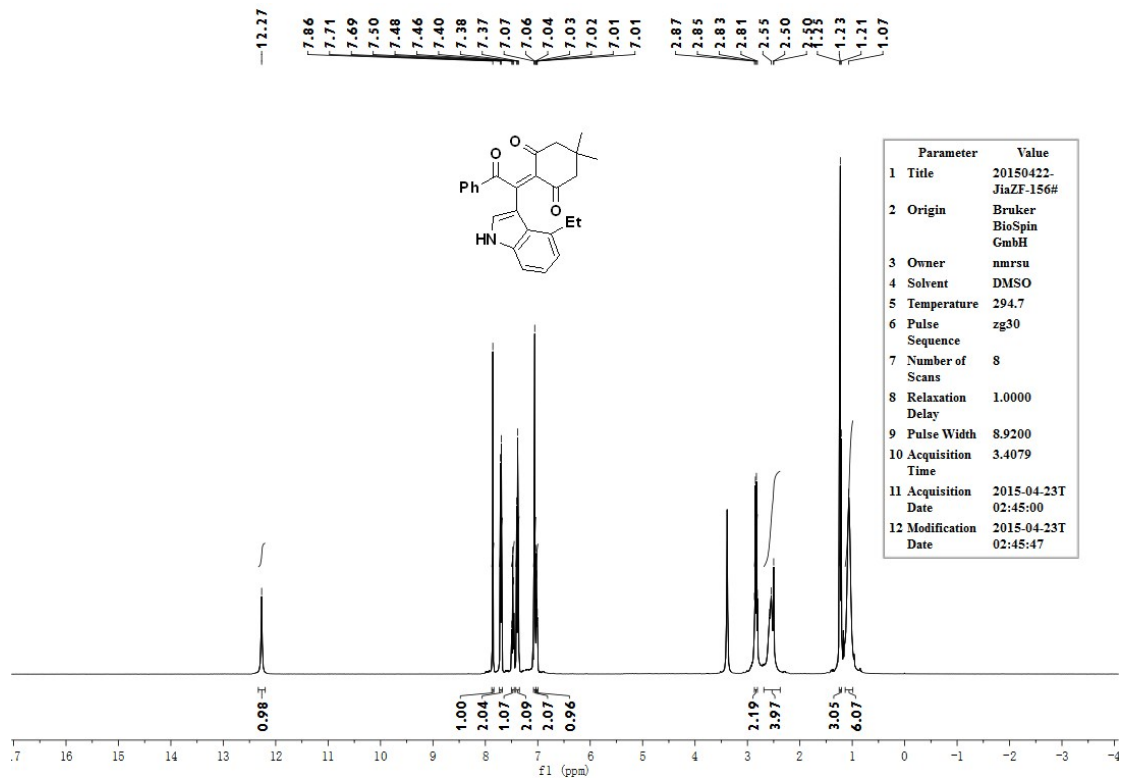


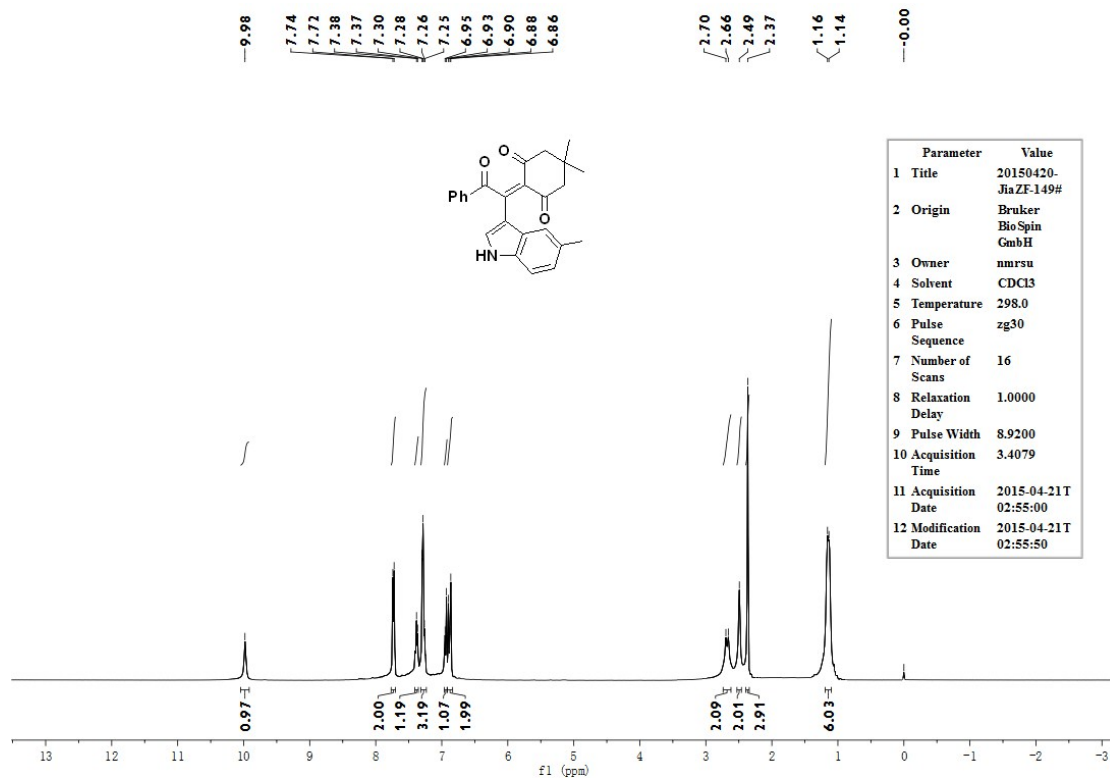


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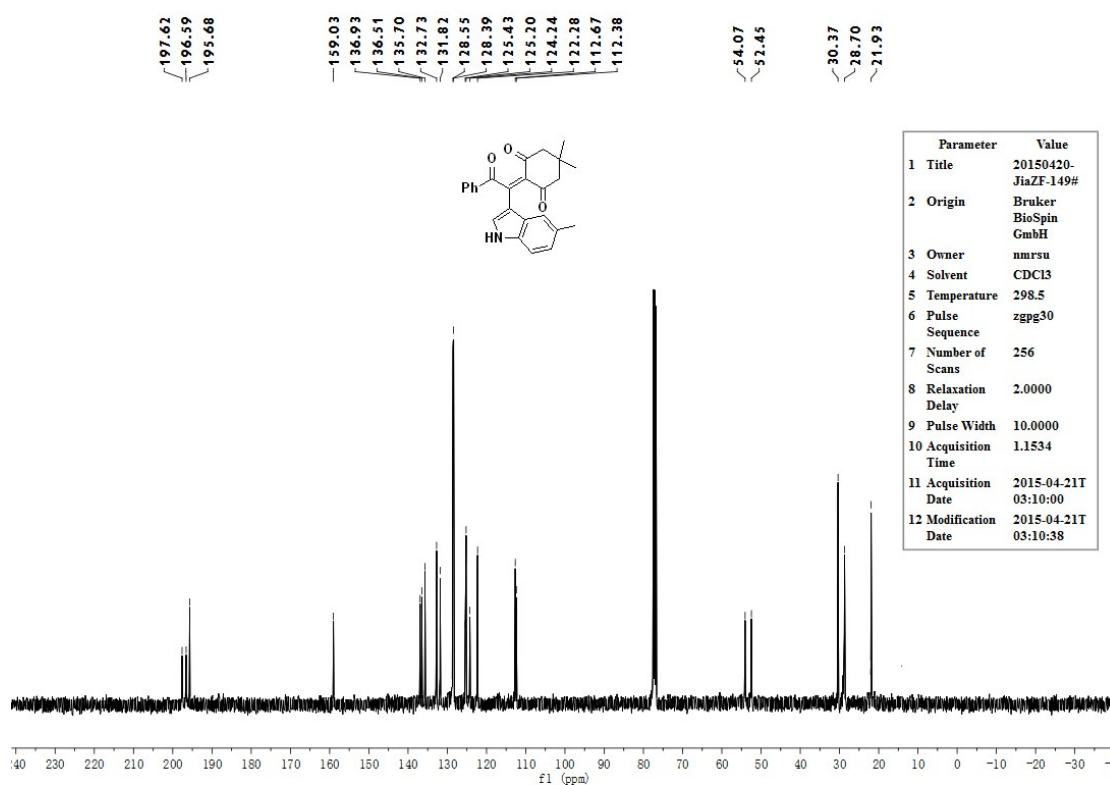


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11 Acquisition Date	2015-04-15T 21:20:00
12 Modification Date	2015-04-15T 21:20:39



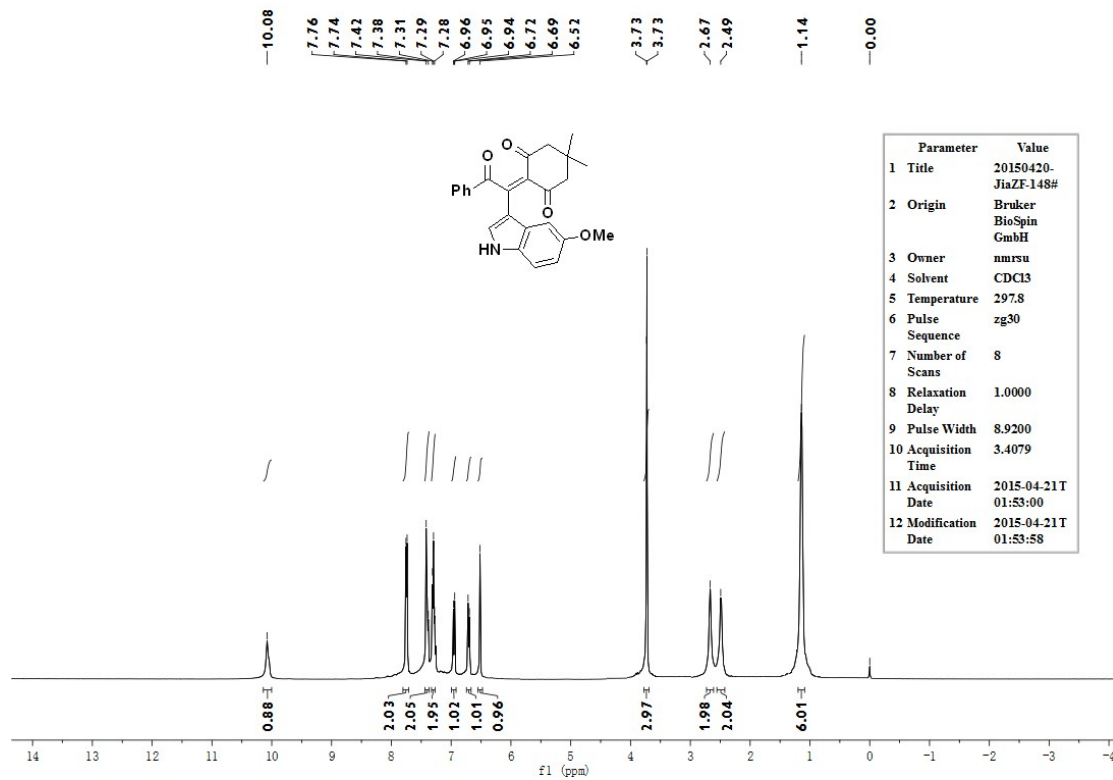


Parameter	Value
1 Title	20150420-JiaZF-149#
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Solvent	CDCl3
5 Temperature	298.0
6 Pulse Sequence	zg30
7 Number of Scans	16
8 Relaxation Delay	1.0000
9 Pulse Width	8.9200
10 Acquisition Time	3.4079
11 Acquisition Date	2015-04-21T 02:55:00
12 Modification Date	2015-04-21T 02:55:50

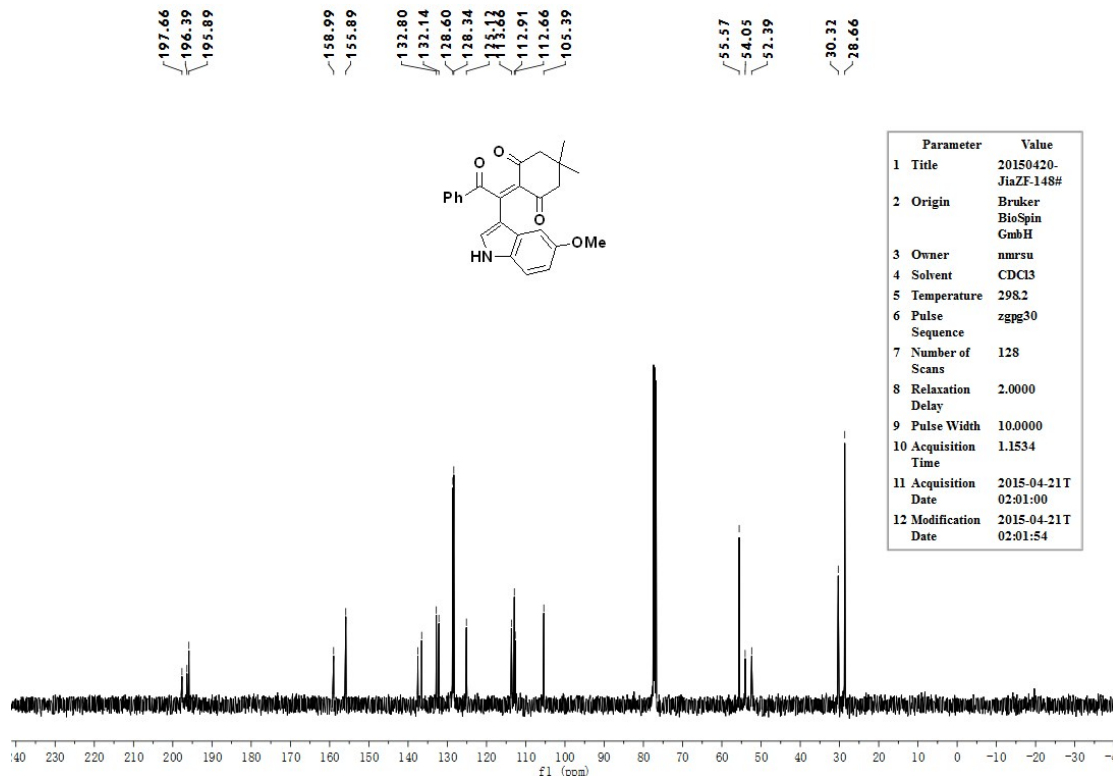


Parameter	Value
1 Title	20150420-JiaZF-149#
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Solvent	CDCl3
5 Temperature	298.5
6 Pulse Sequence	zgpg30
7 Number of Scans	256
8 Relaxation Delay	2.0000
9 Pulse Width	10.0000
10 Acquisition Time	1.1534
11 Acquisition Date	2015-04-21T 03:10:00
12 Modification Date	2015-04-21T 03:10:38

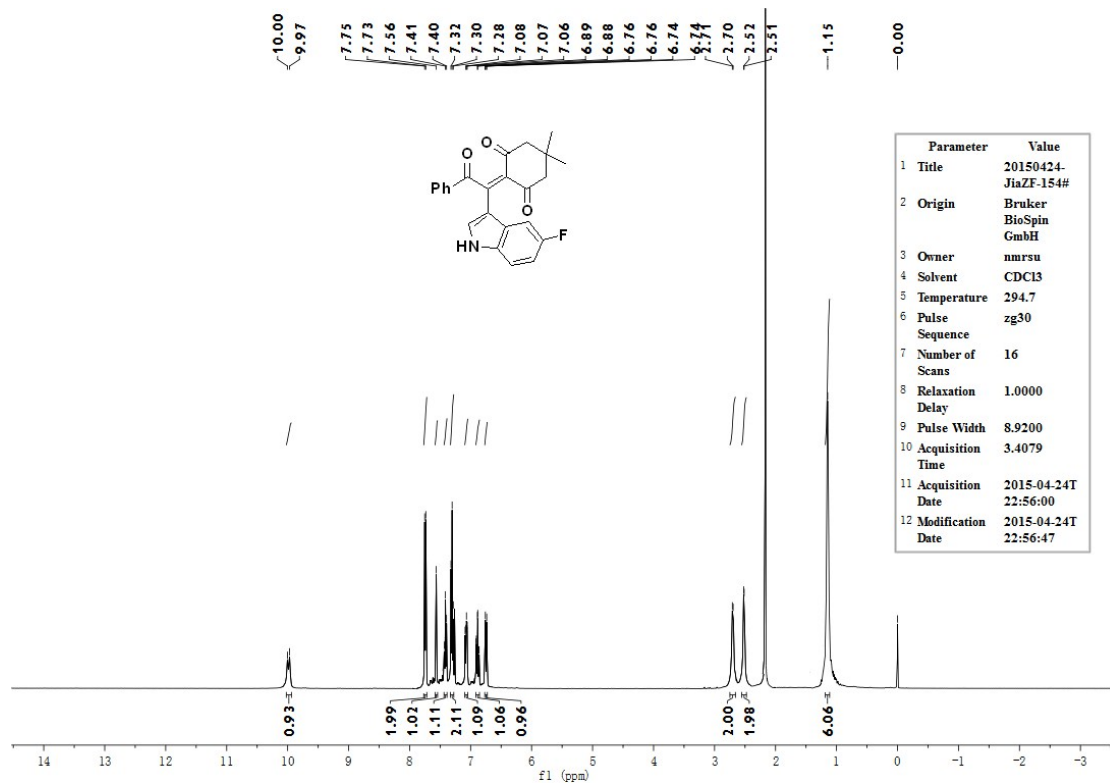




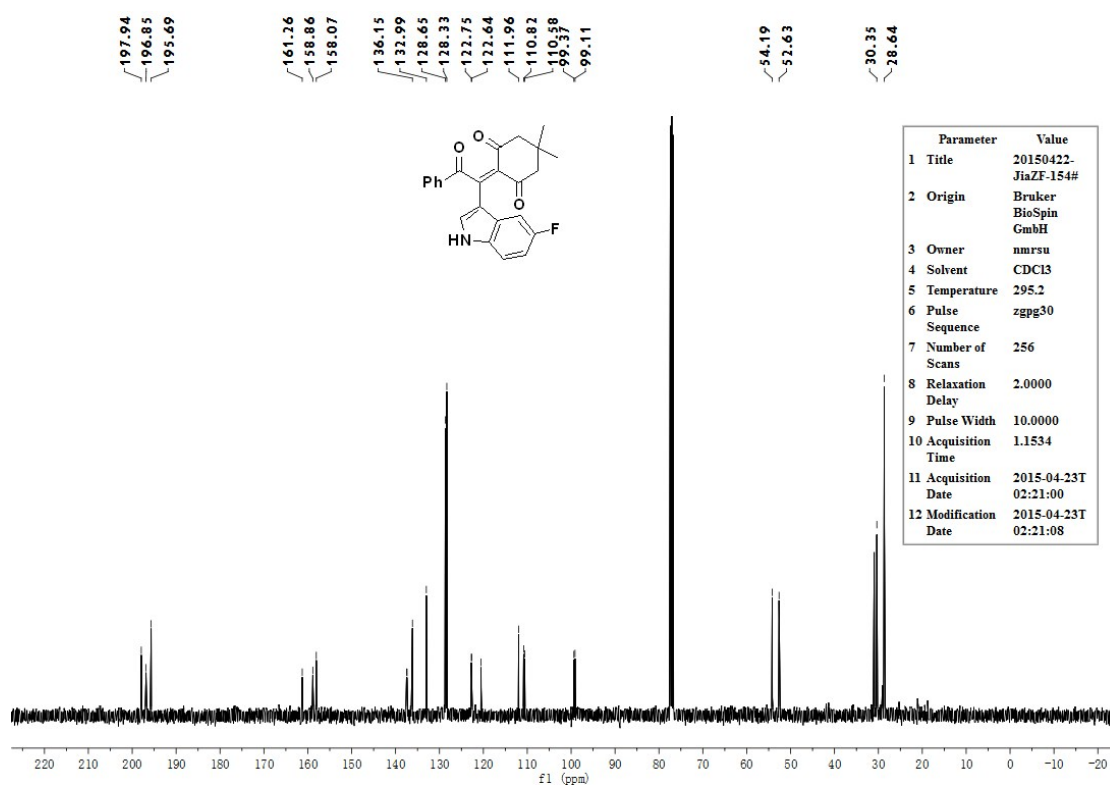
Parameter	Value
1 Title	20150420-JiaZF-148#
2 Origin	Bruker BioSpin GmbH
3 Owner	nmsu
4 Solvent	CDCl3
5 Temperature	297.8
6 Pulse Sequence	zg30
7 Number of Scans	8
8 Relaxation Delay	1.0000
9 Pulse Width	8.9200
10 Acquisition Time	3.4079
11 Acquisition Date	2015-04-21T 01:53:00
12 Modification Date	2015-04-21T 01:53:58



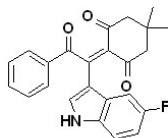
Parameter	Value
1 Title	20150420-JiaZF-148#
2 Origin	Bruker BioSpin GmbH
3 Owner	nmsu
4 Solvent	CDCl3
5 Temperature	298.2
6 Pulse Sequence	zpgg30
7 Number of Scans	128
8 Relaxation Delay	2.0000
9 Pulse Width	10.0000
10 Acquisition Time	1.1534
11 Acquisition Date	2015-04-21T 02:01:00
12 Modification Date	2015-04-21T 02:01:54



Parameter	Value
1 Title	20150424-JiaZF-154#
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Solvent	CDCl3
5 Temperature	294.7
6 Pulse Sequence	zg30
7 Number of Scans	16
8 Relaxation Delay	1.0000
9 Pulse Width	8.9200
10 Acquisition Time	3.4079
11 Acquisition Date	2015-04-24T 22:56:00
12 Modification Date	2015-04-24T 22:56:47

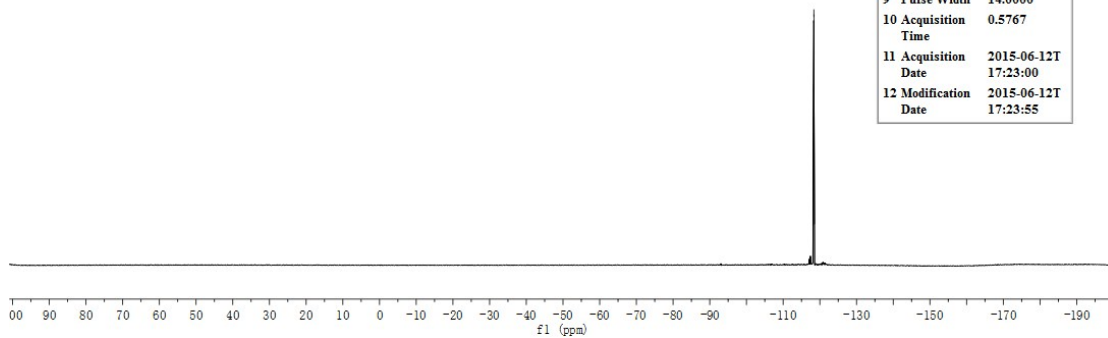


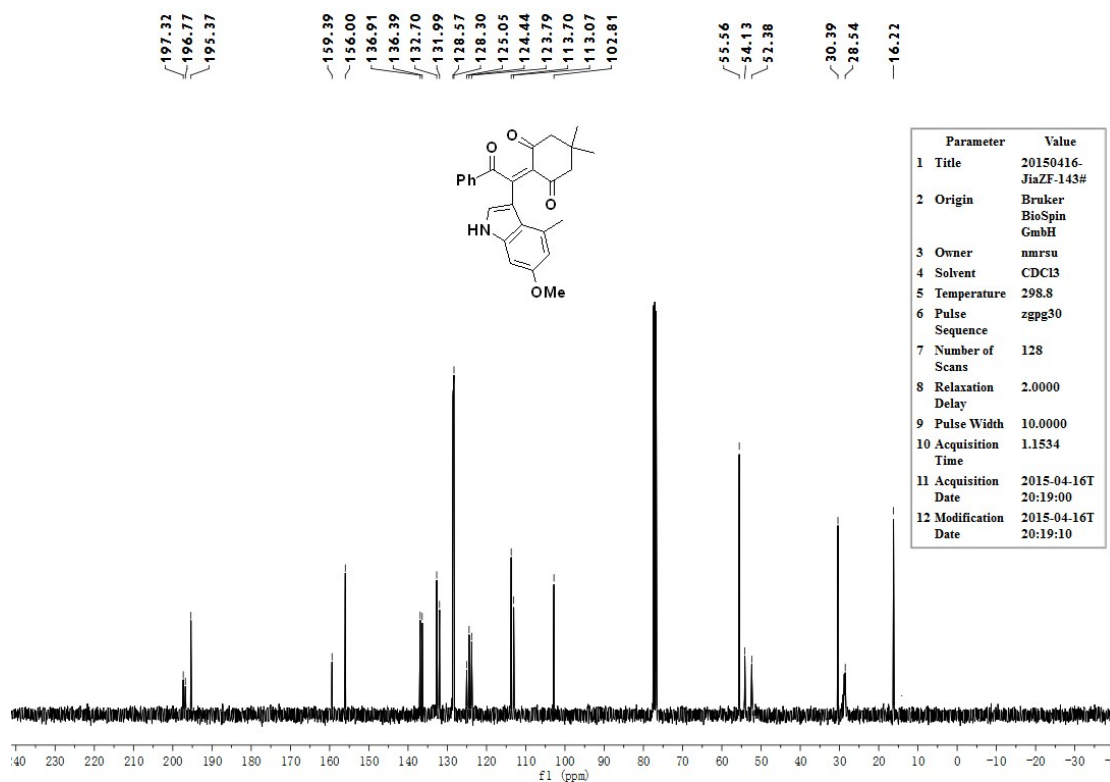
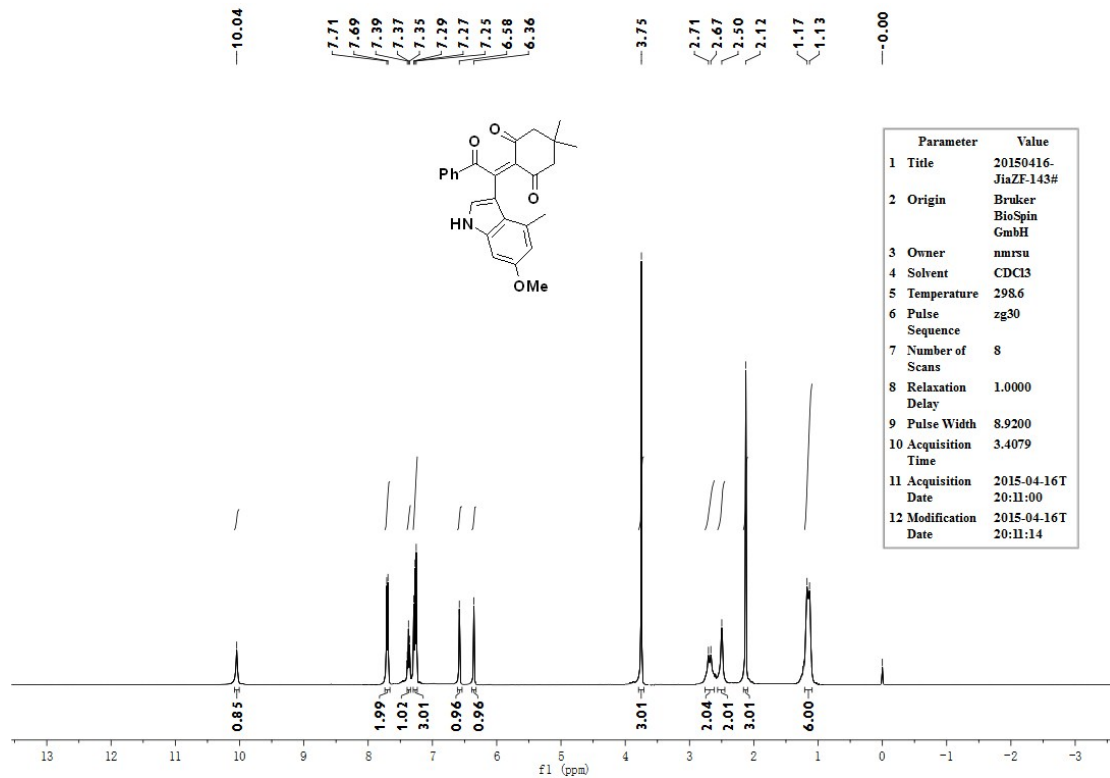
Parameter	Value
1 Title	20150422-JiaZF-154#
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Solvent	CDCl3
5 Temperature	295.2
6 Pulse Sequence	zgpg30
7 Number of Scans	256
8 Relaxation Delay	2.0000
9 Pulse Width	10.0000
10 Acquisition Time	1.1534
11 Acquisition Date	2015-04-23T 02:21:00
12 Modification Date	2015-04-23T 02:21:08

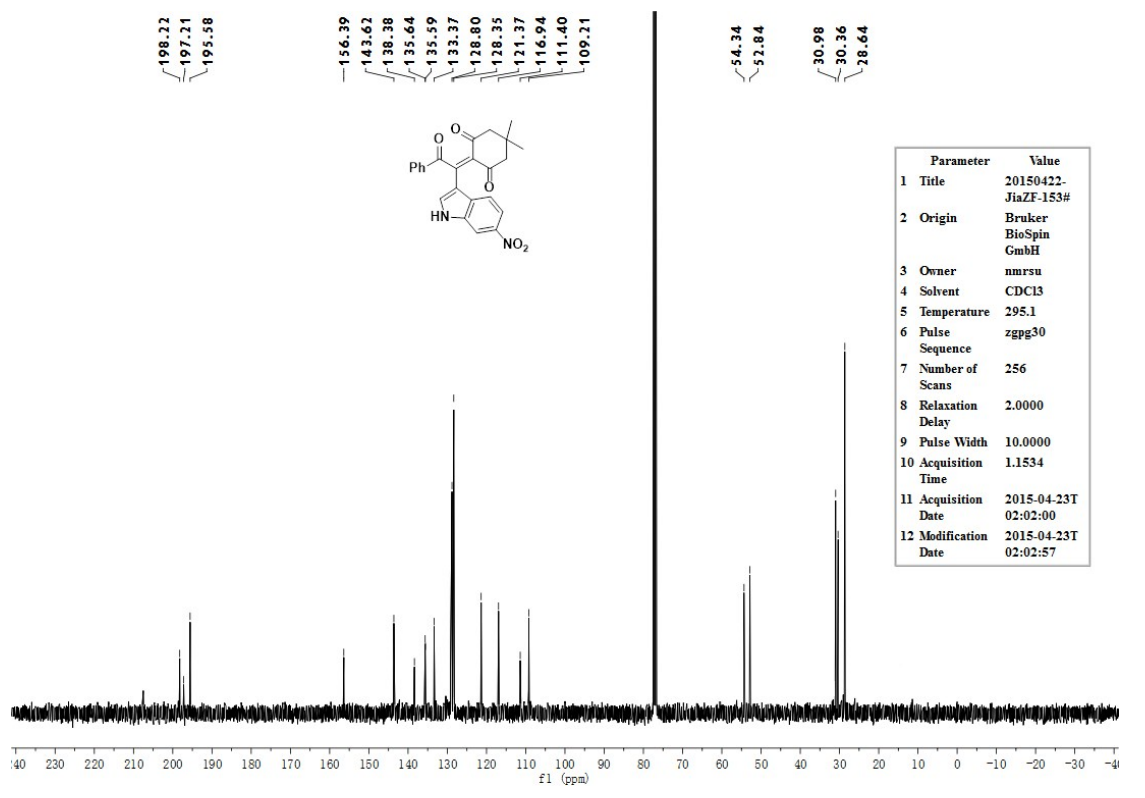
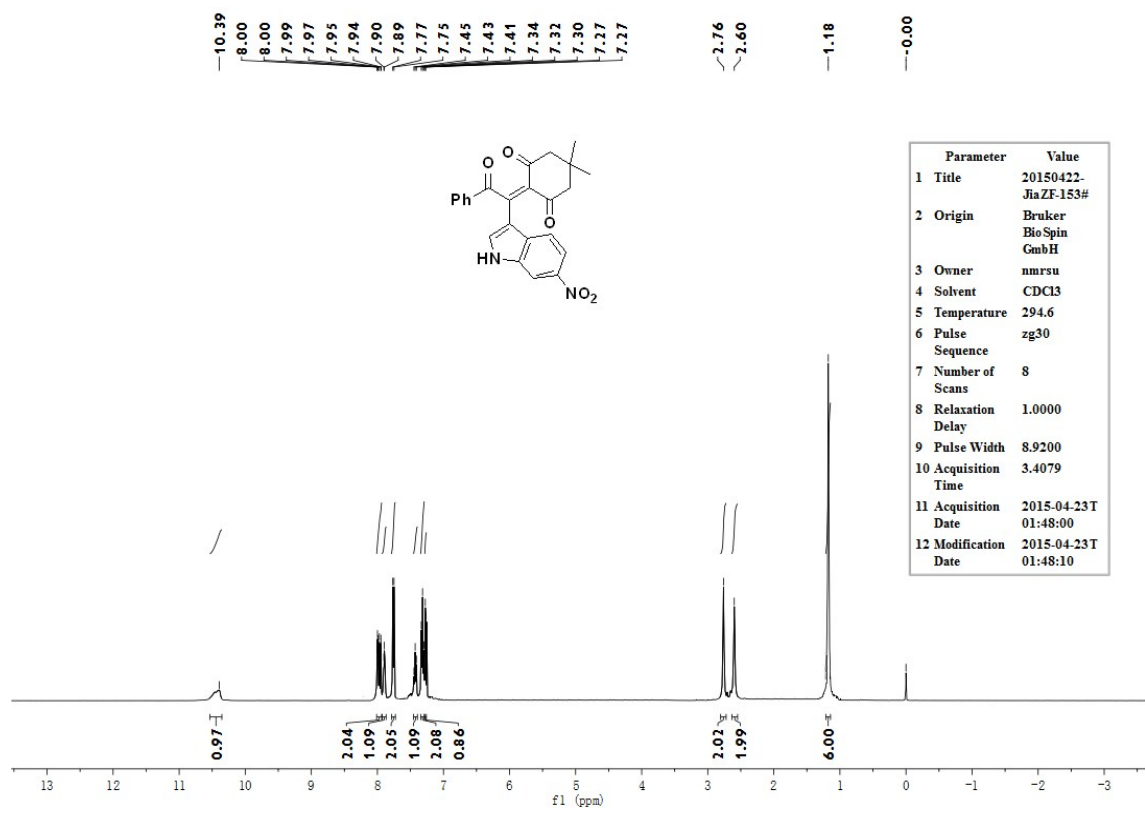


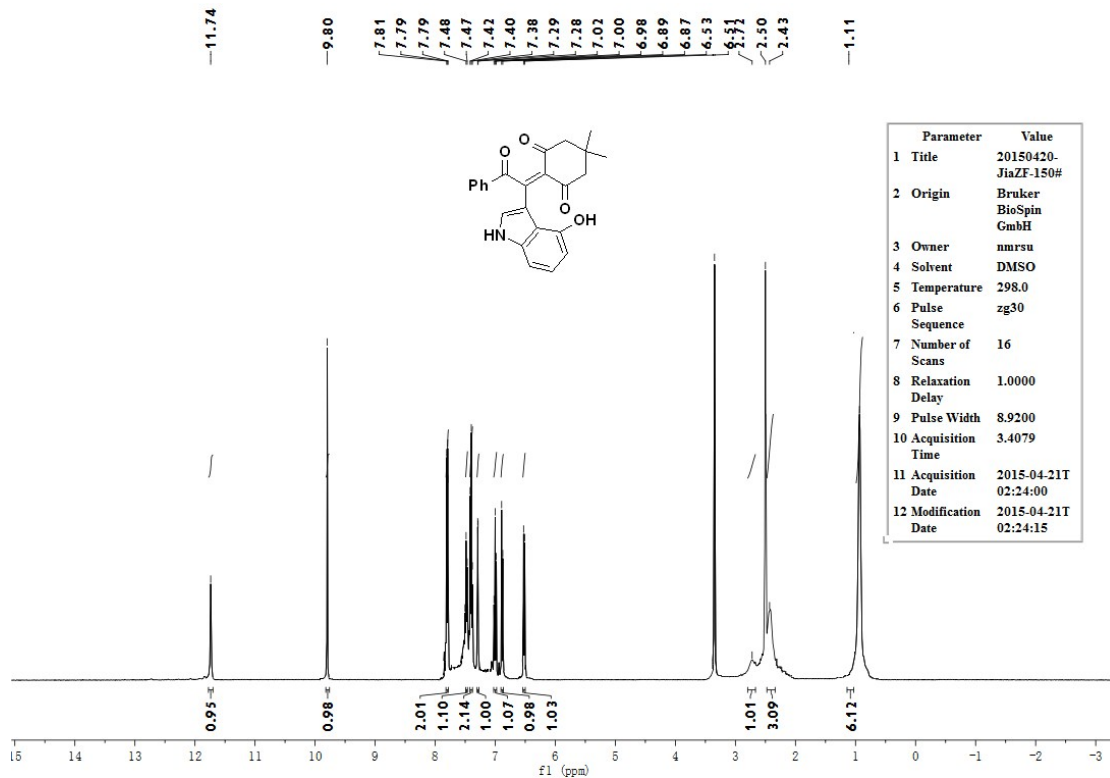
-118.34  
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-118.36  
-118.38  
-118.40

Parameter	Value
1 Title	20150612-JiaZF-178#
2 Origin	Bruker BioSpin GmbH
3 Owner	nmsru
4 Solvent	CDC13
5 Temperature	294.7
6 Pulse Sequence	zgfgq
7 Number of Scans	64
8 Relaxation Delay	1.5000
9 Pulse Width	14.0000
10 Acquisition Time	0.5767
11 Acquisition Date	2015-06-12T 17:23:00
12 Modification Date	2015-06-12T 17:23:55

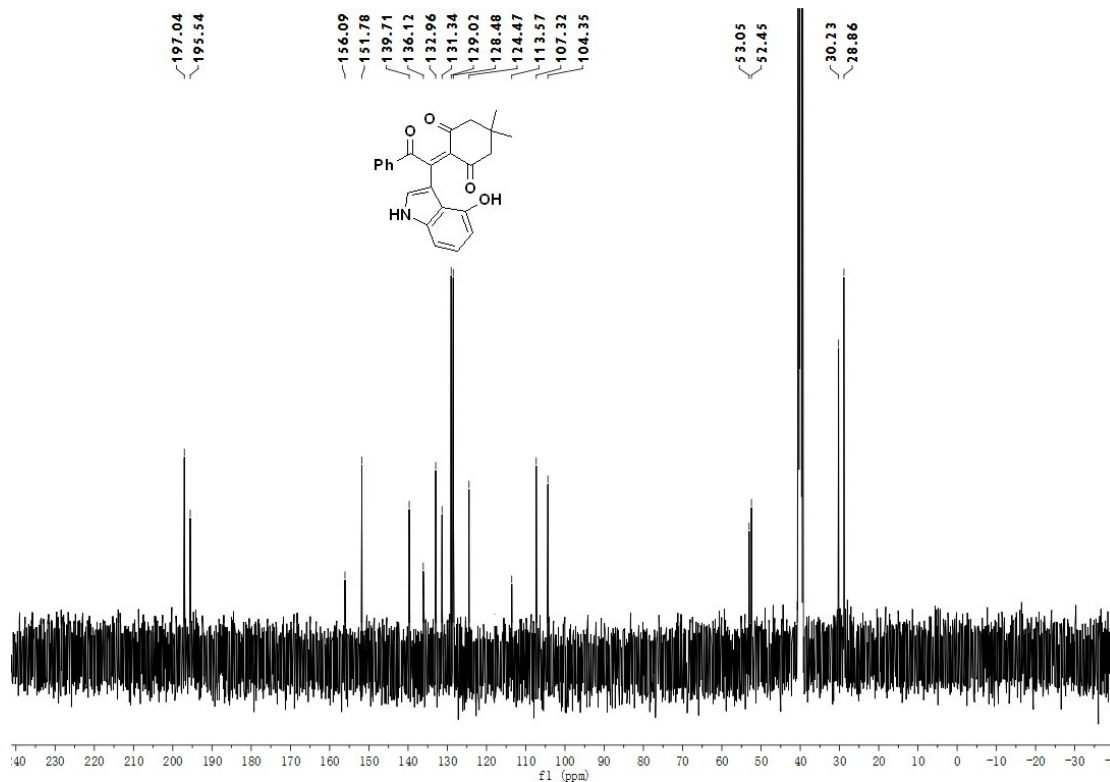


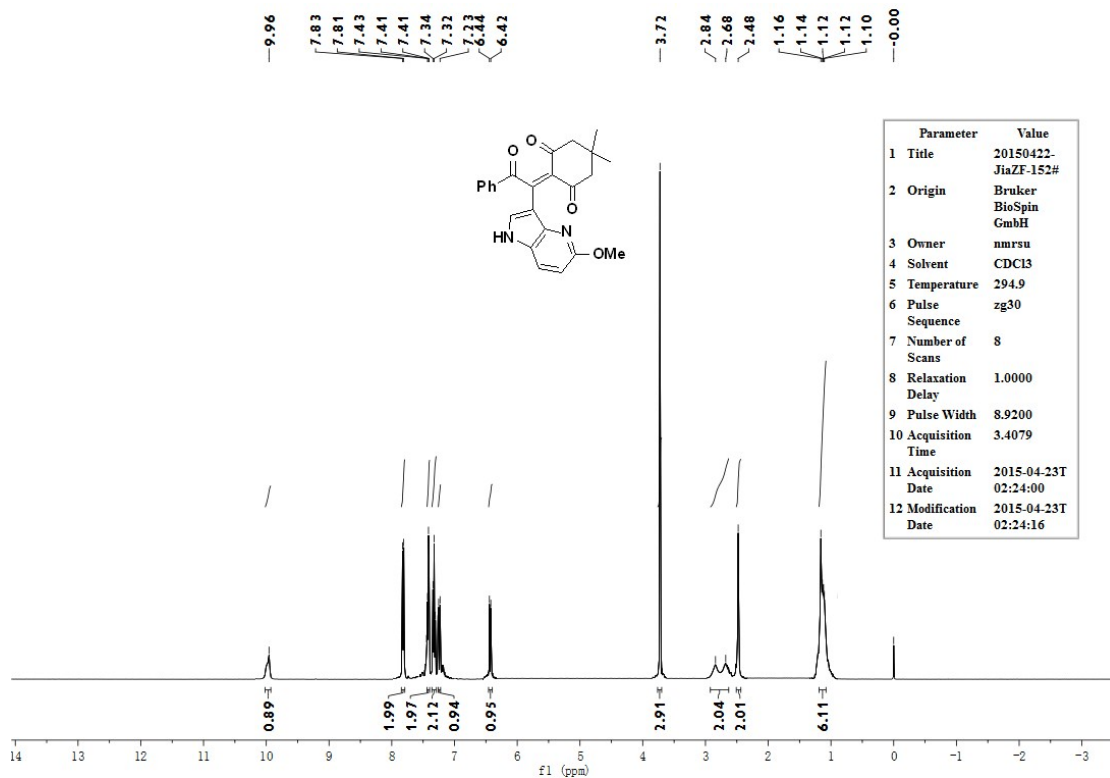




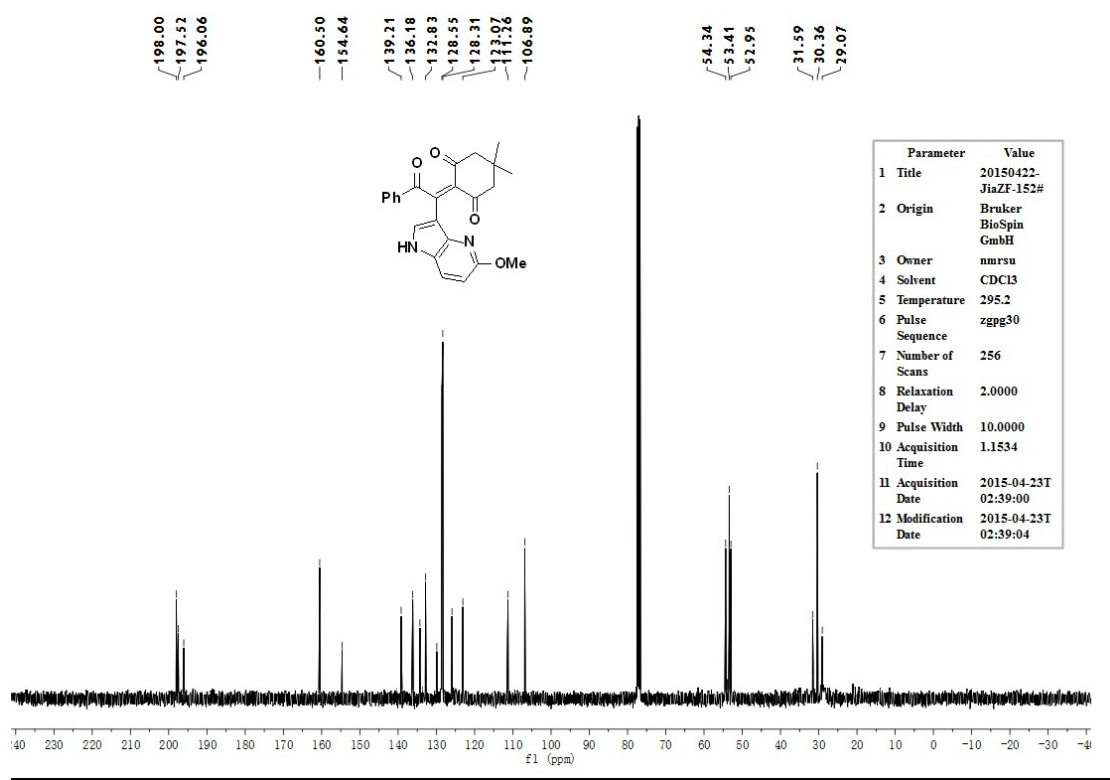


Parameter	Value
1 Title	20150420-JiaZF-150#
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Solvent	DMSO
5 Temperature	298.0
6 Pulse Sequence	zg30
7 Number of Scans	16
8 Relaxation Delay	1.0000
9 Pulse Width	8.9200
10 Acquisition Time	3.4079
11 Acquisition Date	2015-04-21T02:24:00
12 Modification Date	2015-04-21T02:24:15

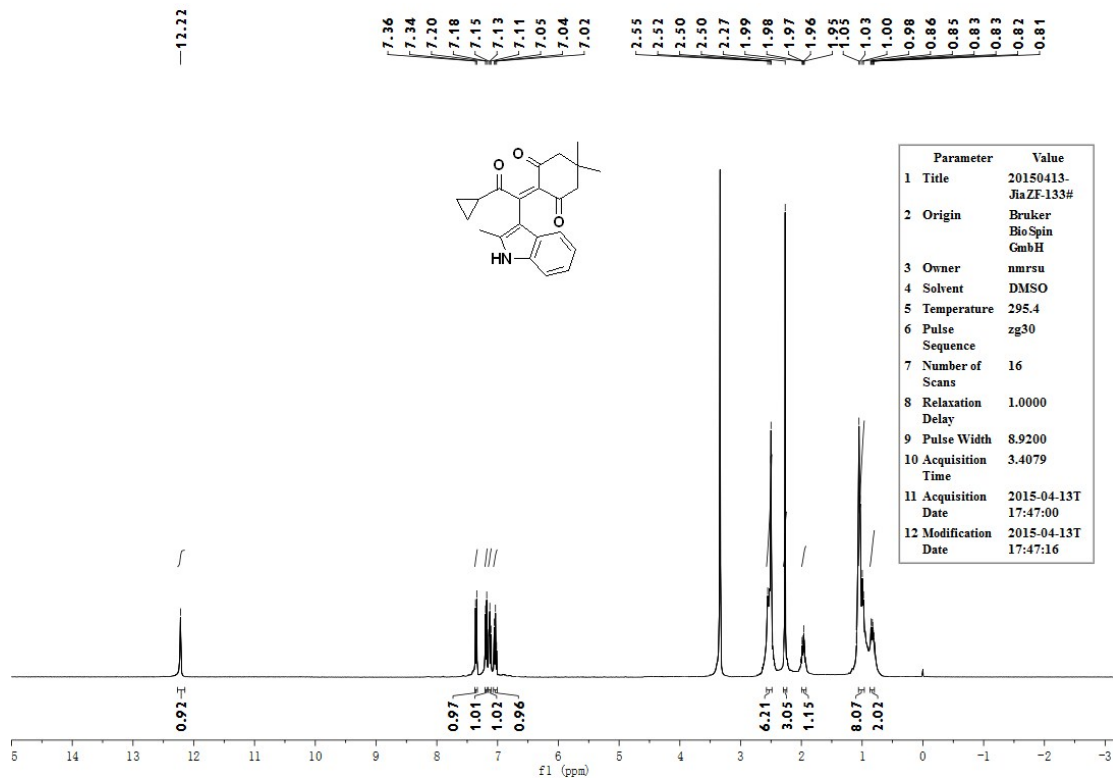




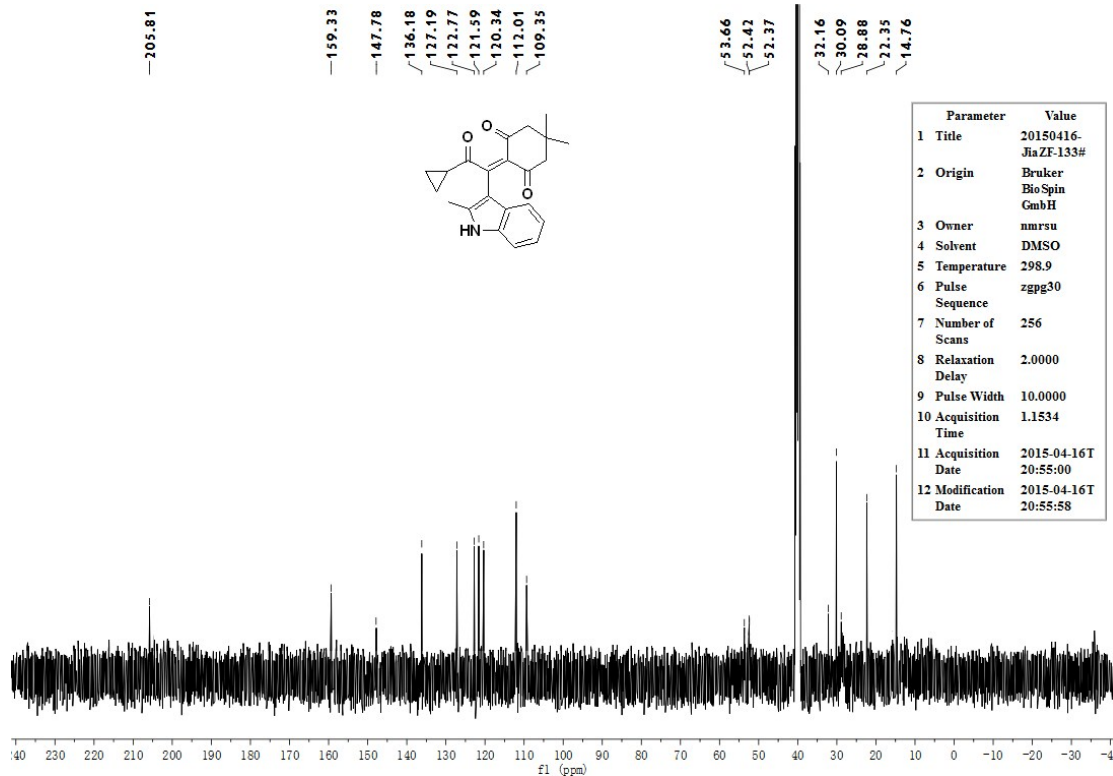
Parameter	Value
1 Title	20150422-JiaZF-152#
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Solvent	CDCl3
5 Temperature	294.9
6 Pulse Sequence	zg30
7 Number of Scans	8
8 Relaxation Delay	1.0000
9 Pulse Width	8.9200
10 Acquisition Time	3.4079
11 Acquisition Date	2015-04-23T02:24:00
12 Modification Date	2015-04-23T02:24:16



Parameter	Value
1 Title	20150422-JiaZF-152#
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Solvent	CDCl3
5 Temperature	295.2
6 Pulse Sequence	zgpg30
7 Number of Scans	256
8 Relaxation Delay	2.0000
9 Pulse Width	10.0000
10 Acquisition Time	1.1534
11 Acquisition Date	2015-04-23T02:39:00
12 Modification Date	2015-04-23T02:39:04

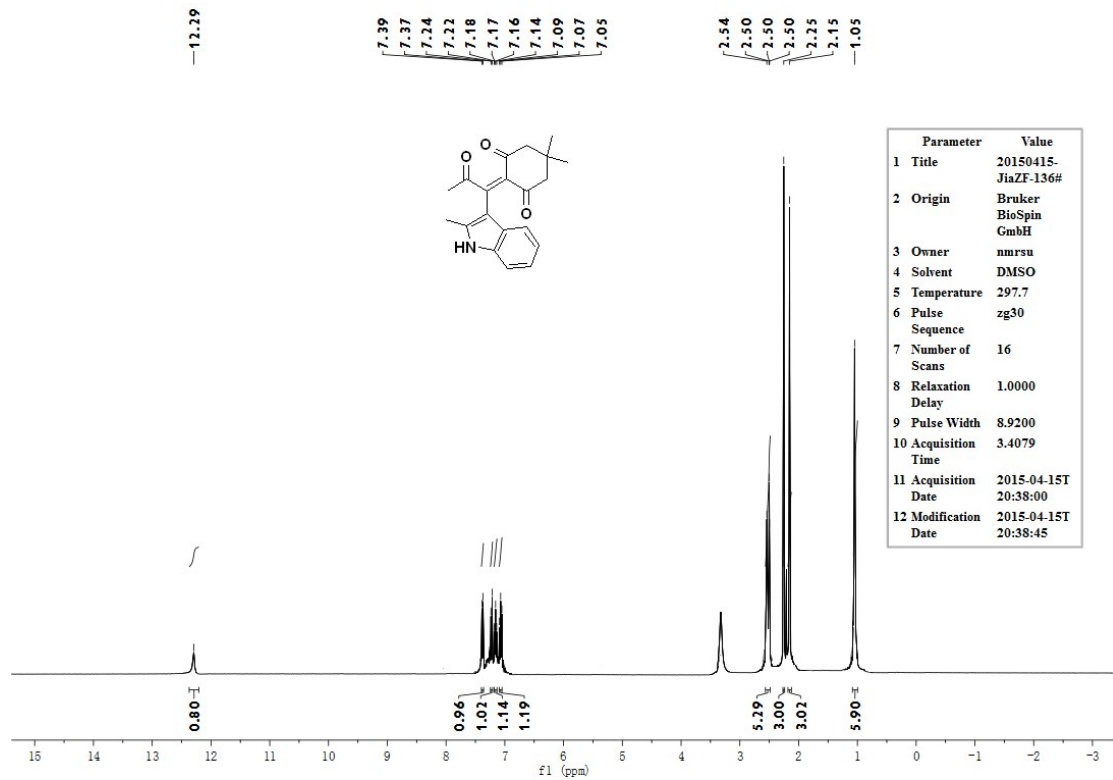


Parameter	Value
1 Title	20150413-JiaZF-133#
2 Origin	Bruker BioSpin GmbH
3 Owner	nmsru
4 Solvent	DMSO
5 Temperature	295.4
6 Pulse Sequence	zg30
7 Number of Scans	16
8 Relaxation Delay	1.0000
9 Pulse Width	8.9200
10 Acquisition Time	3.4079
11 Acquisition Date	2015-04-13T 17:47:00
12 Modification Date	2015-04-13T 17:47:16

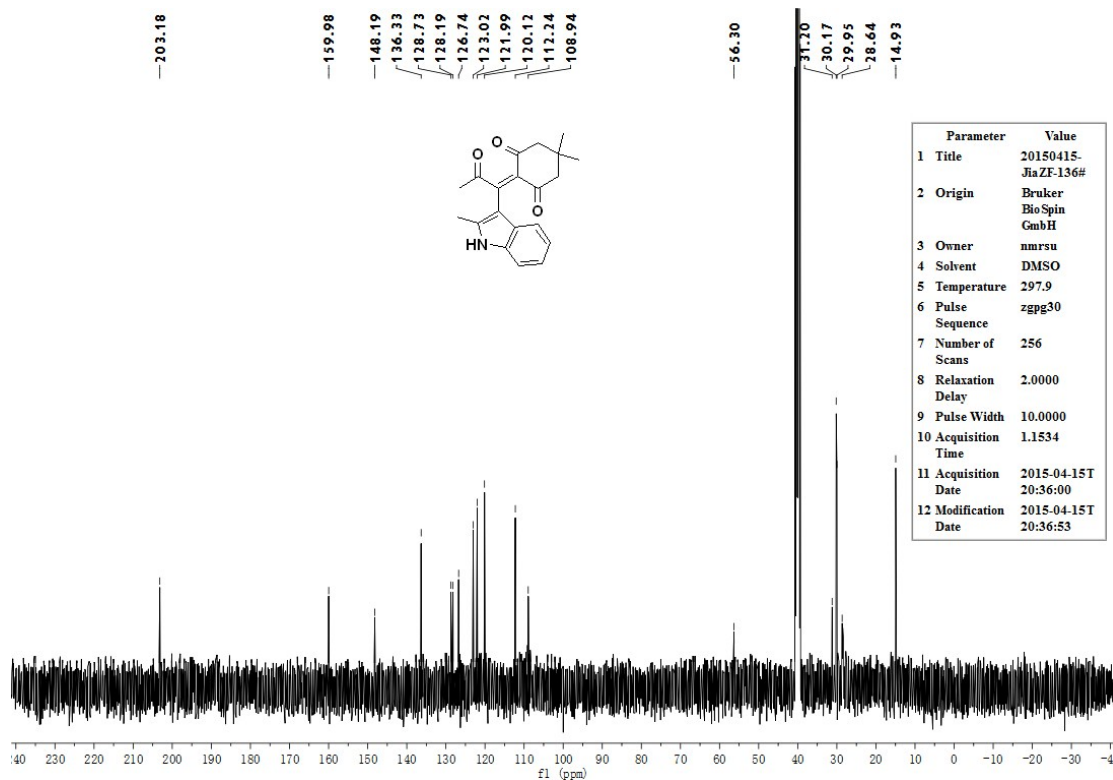


Parameter	Value
1 Title	20150416-JiaZF-133#
2 Origin	Bruker BioSpin GmbH
3 Owner	nmsru
4 Solvent	DMSO
5 Temperature	298.9
6 Pulse Sequence	zgpg30
7 Number of Scans	256
8 Relaxation Delay	2.0000
9 Pulse Width	10.0000
10 Acquisition Time	1.1534
11 Acquisition Date	2015-04-16T 20:55:00
12 Modification Date	2015-04-16T 20:55:58

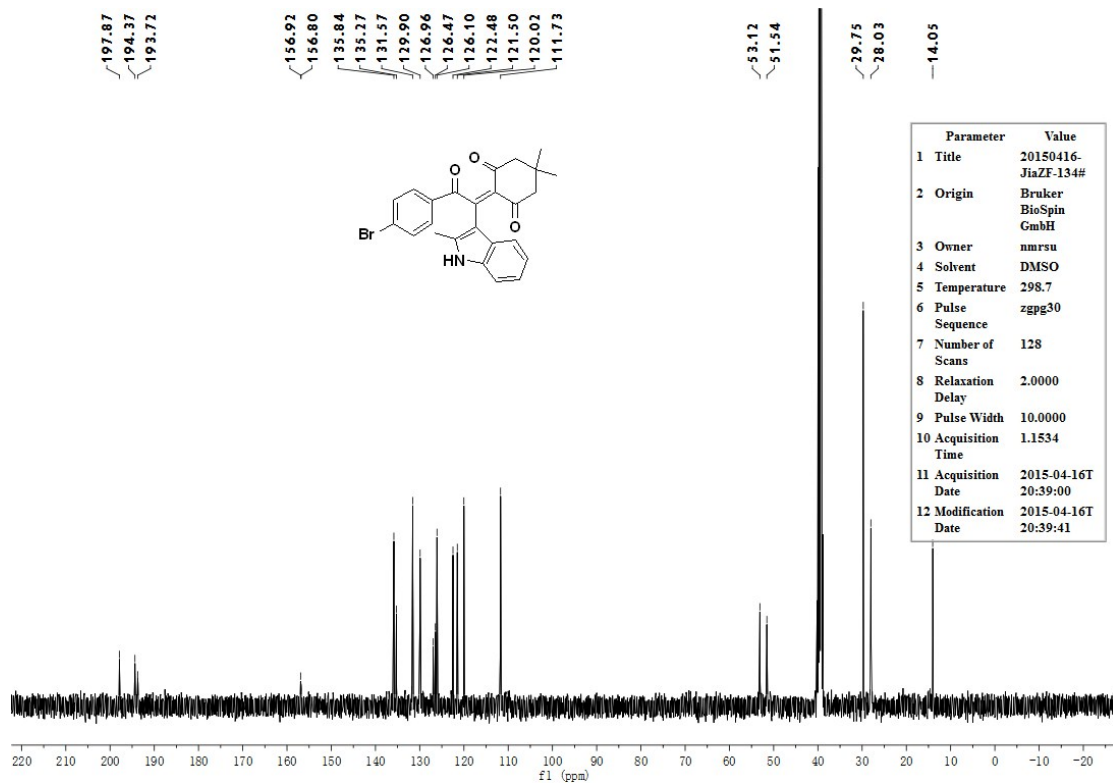
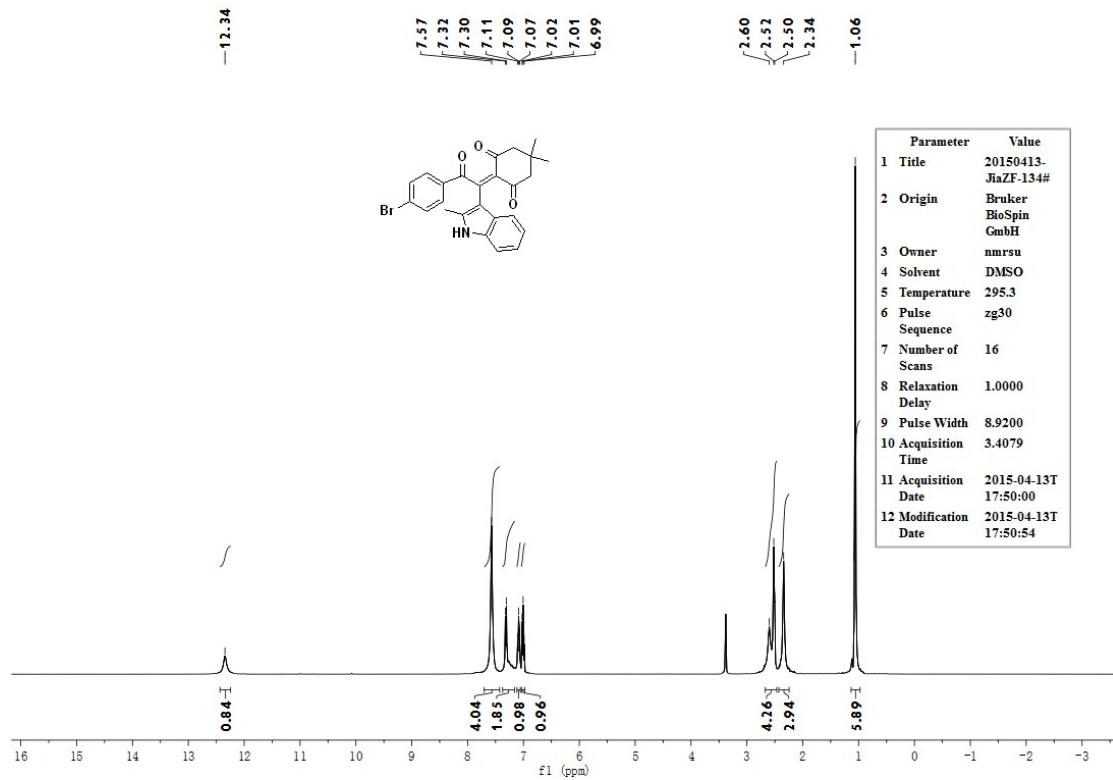


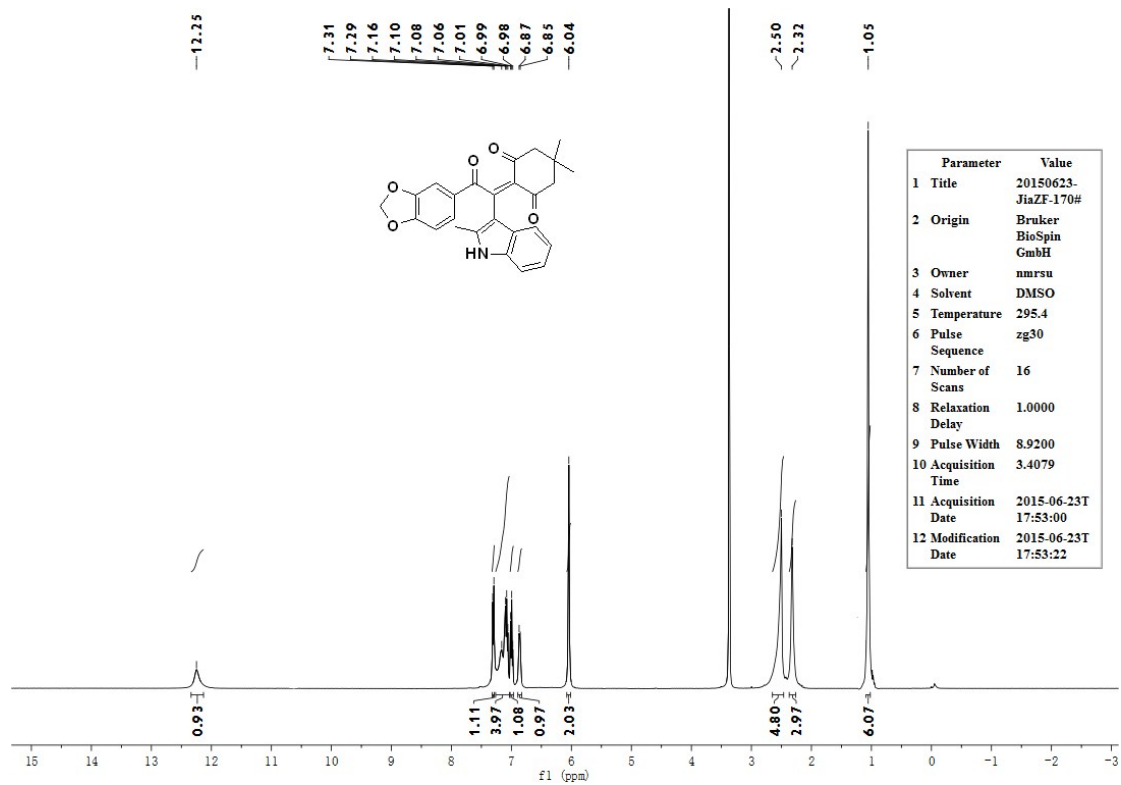


Parameter	Value
1 Title	20150415-JiaZF-136#
2 Origin	Bruker BioSpin GmbH
3 Owner	nrrsu
4 Solvent	DMSO
5 Temperature	297.7
6 Pulse Sequence	zg30
7 Number of Scans	16
8 Relaxation Delay	1.0000
9 Pulse Width	8.9200
10 Acquisition Time	3.4079
11 Acquisition Date	2015-04-15T 20:38:00
12 Modification Date	2015-04-15T 20:38:45

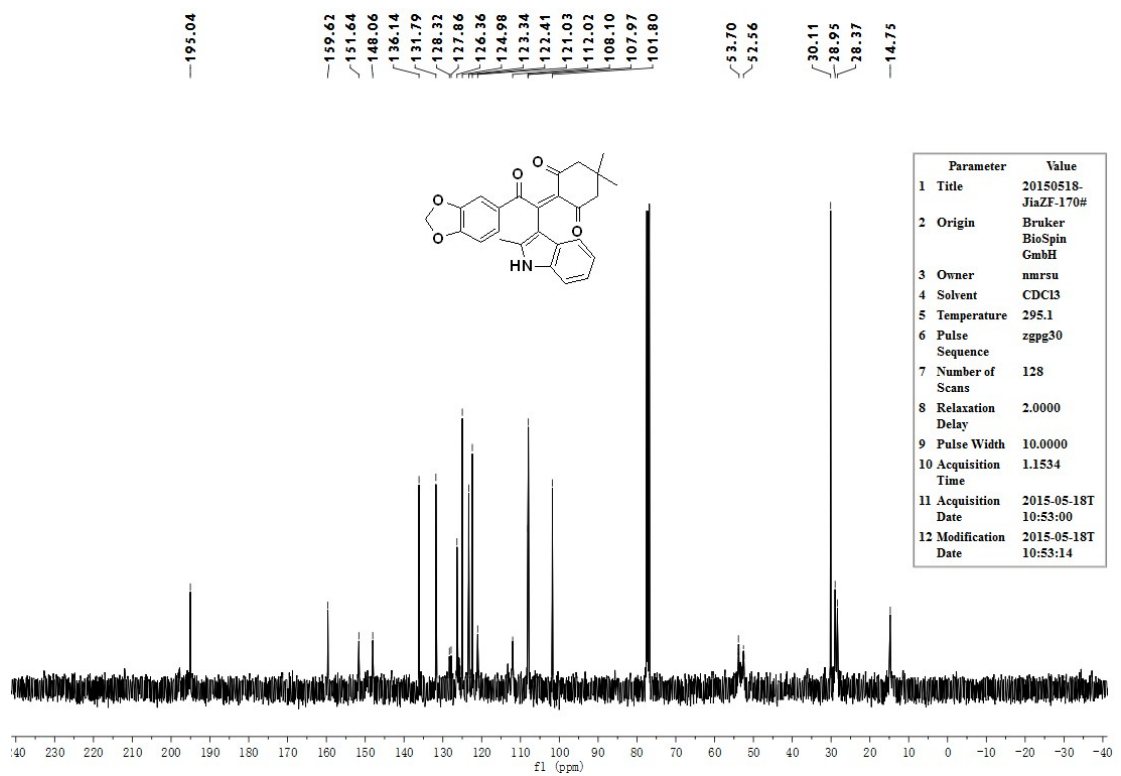


Parameter	Value
1 Title	20150415-JiaZF-136#
2 Origin	Bruker BioSpin GmbH
3 Owner	nrrsu
4 Solvent	DMSO
5 Temperature	297.9
6 Pulse Sequence	zgpg30
7 Number of Scans	256
8 Relaxation Delay	2.0000
9 Pulse Width	10.0000
10 Acquisition Time	1.1534
11 Acquisition Date	2015-04-15T 20:36:00
12 Modification Date	2015-04-15T 20:36:53

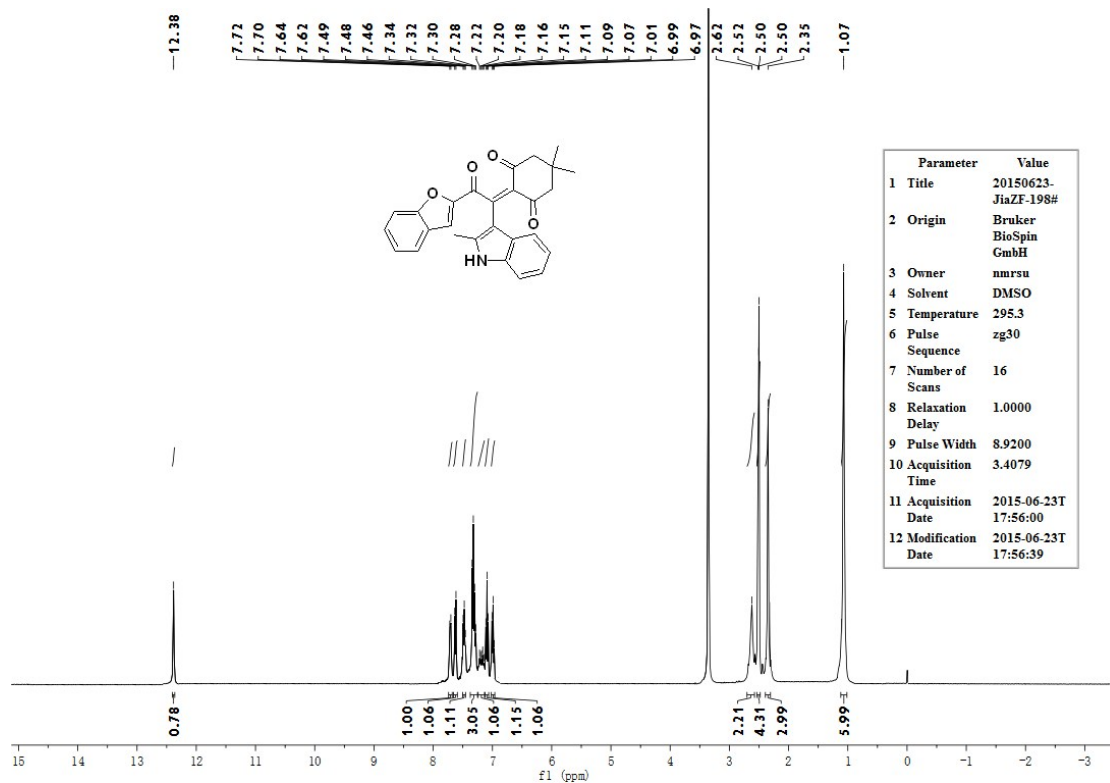




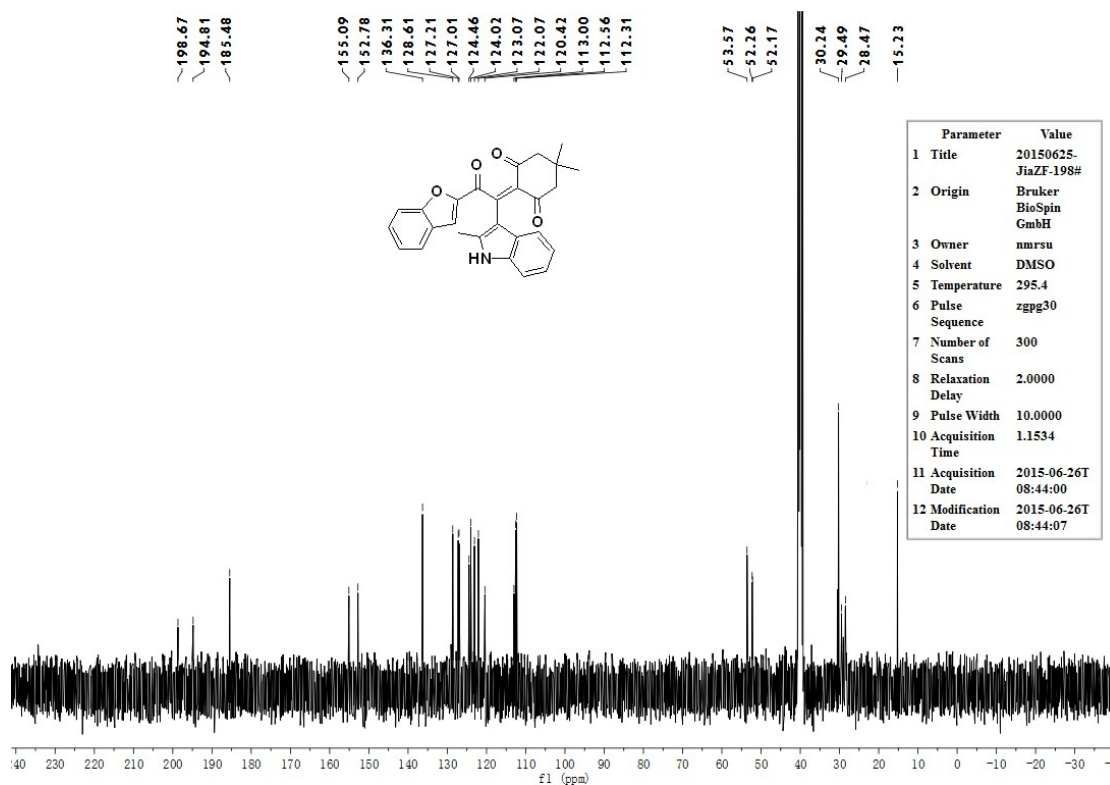
Parameter	Value
1 Title	20150623-JiaZF-170#
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Solvent	DMSO
5 Temperature	295.4
6 Pulse Sequence	zg30
7 Number of Scans	16
8 Relaxation Delay	1.0000
9 Pulse Width	8.9200
10 Acquisition Time	3.4079
11 Acquisition Date	2015-06-23T17:53:00
12 Modification Date	2015-06-23T17:53:22



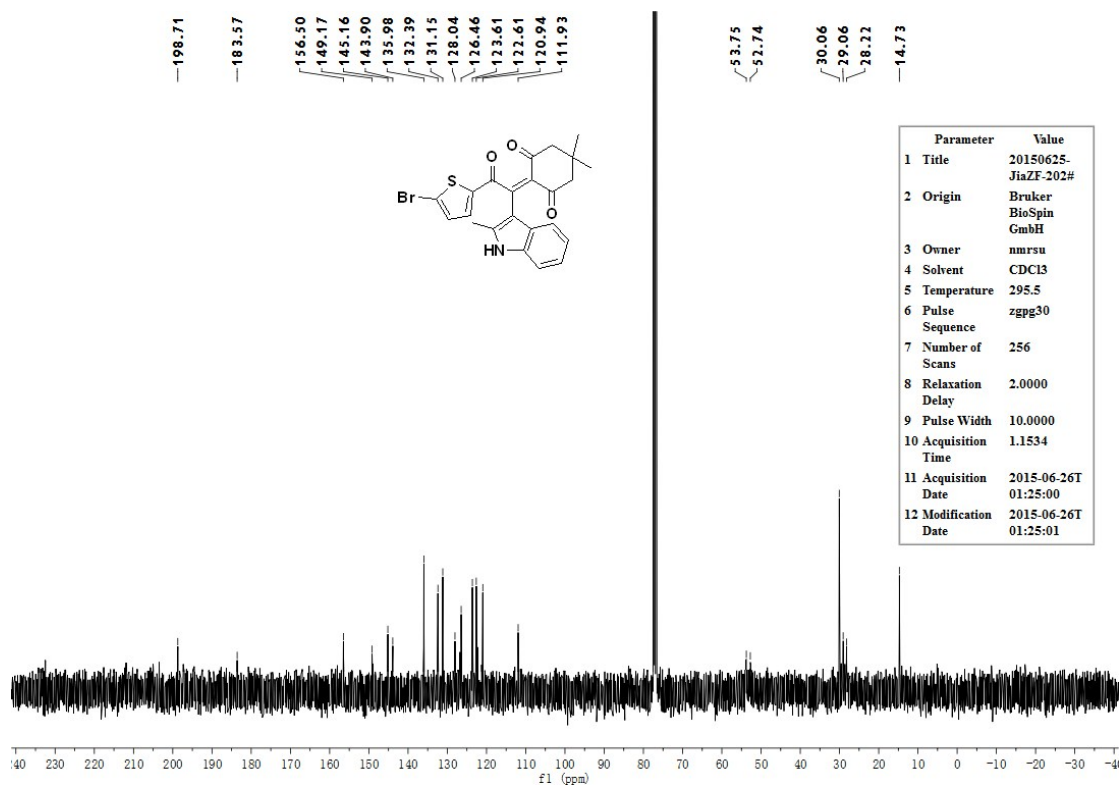
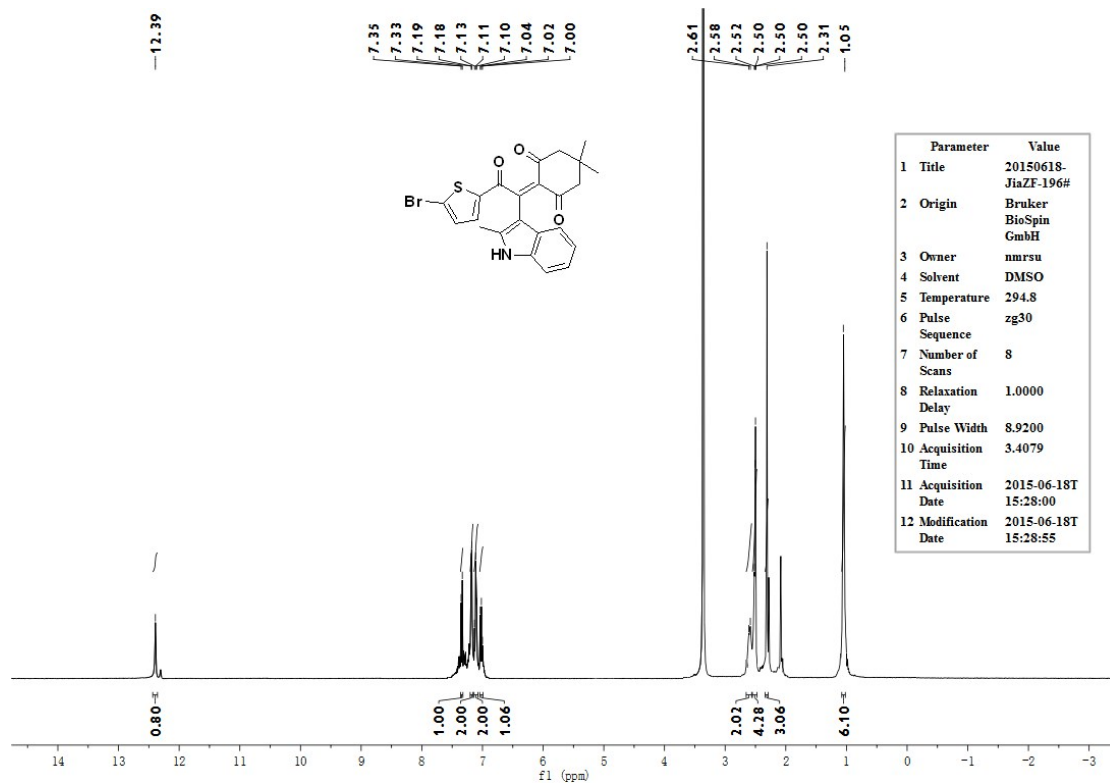
Parameter	Value
1 Title	20150518-JiaZF-170#
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Solvent	CDCl3
5 Temperature	295.1
6 Pulse Sequence	zgpg30
7 Number of Scans	128
8 Relaxation Delay	2.0000
9 Pulse Width	10.0000
10 Acquisition Time	1.1534
11 Acquisition Date	2015-05-18T10:53:00
12 Modification Date	2015-05-18T10:53:14

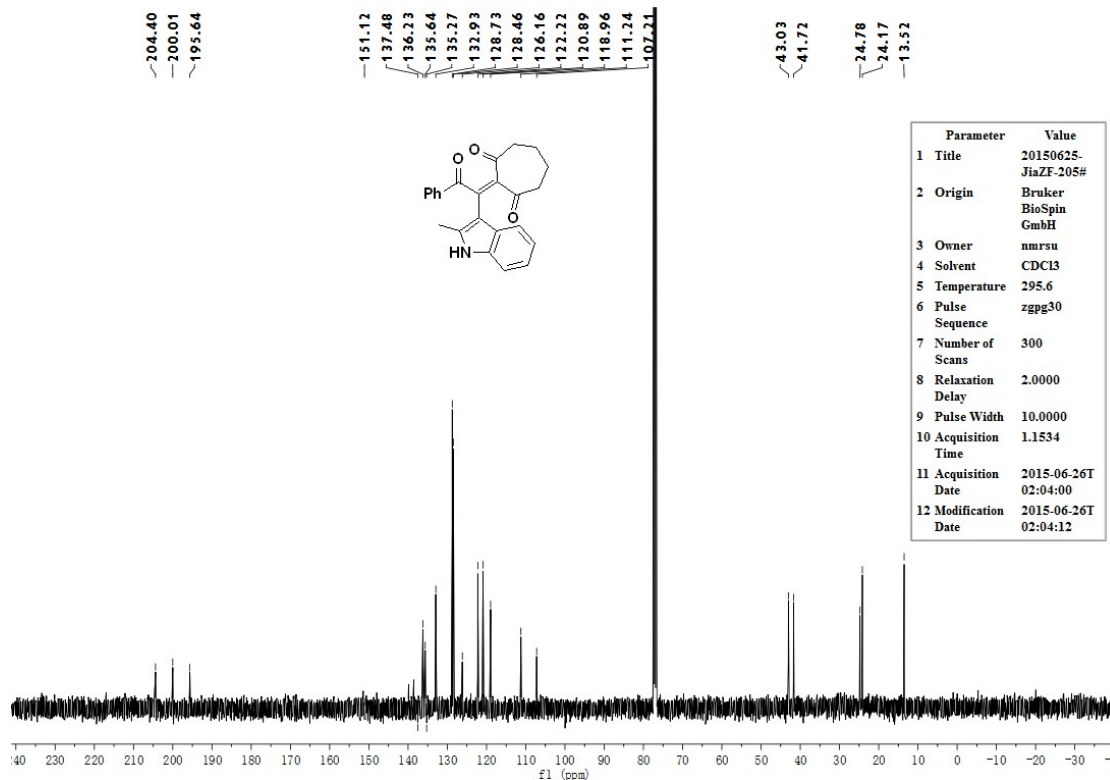
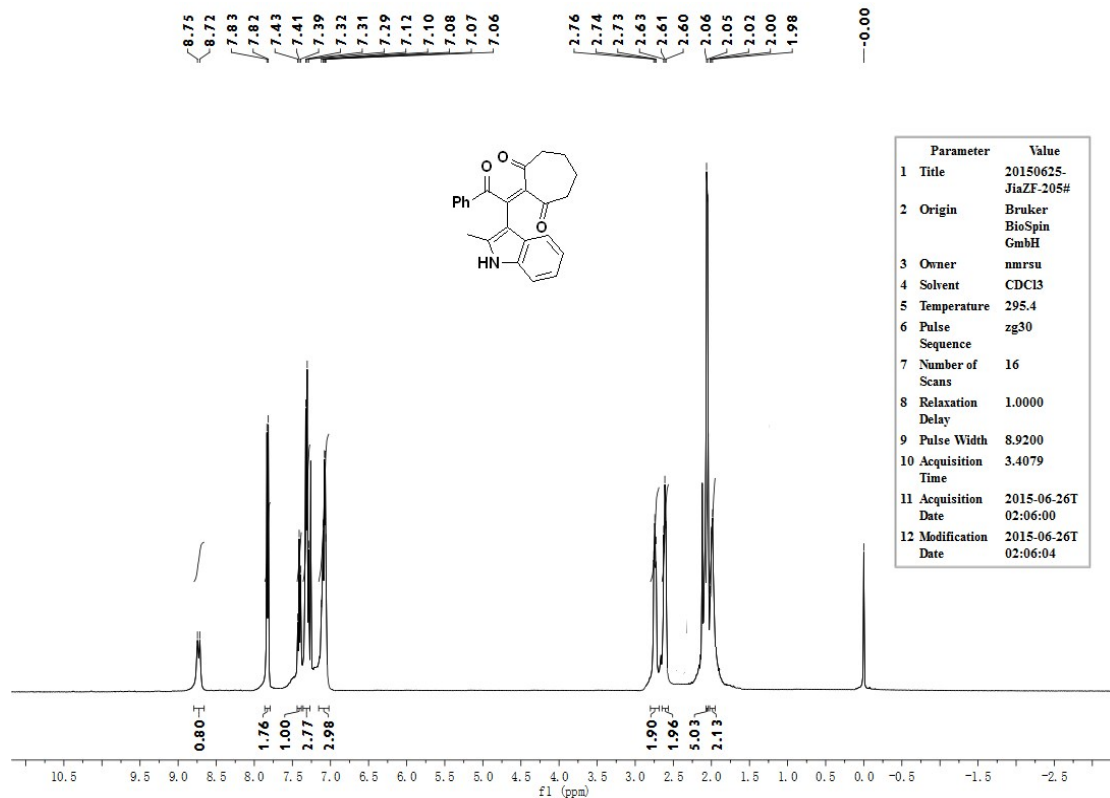


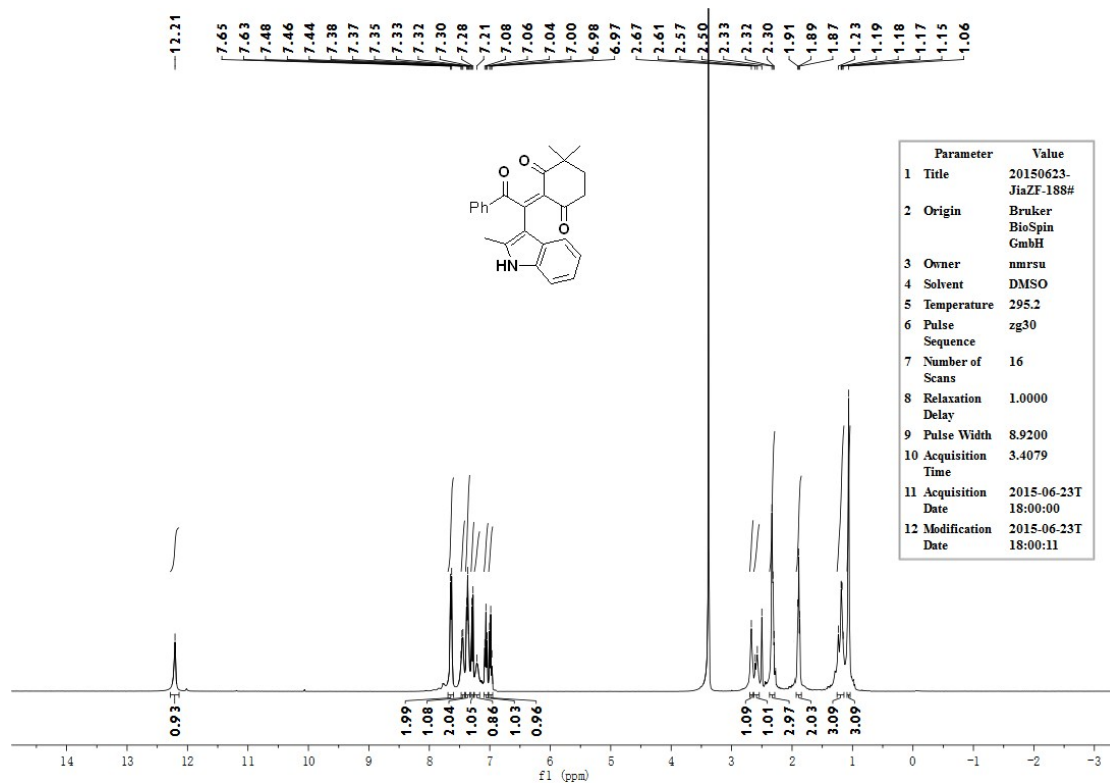
Parameter	Value
1 Title	20150623-JiaZF-198#
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Solvent	DMSO
5 Temperature	295.3
6 Pulse Sequence	zg30
7 Number of Scans	16
8 Relaxation Delay	1.0000
9 Pulse Width	8.9200
10 Acquisition Time	3.4079
11 Acquisition Date	2015-06-23T 17:56:00
12 Modification Date	2015-06-23T 17:56:39



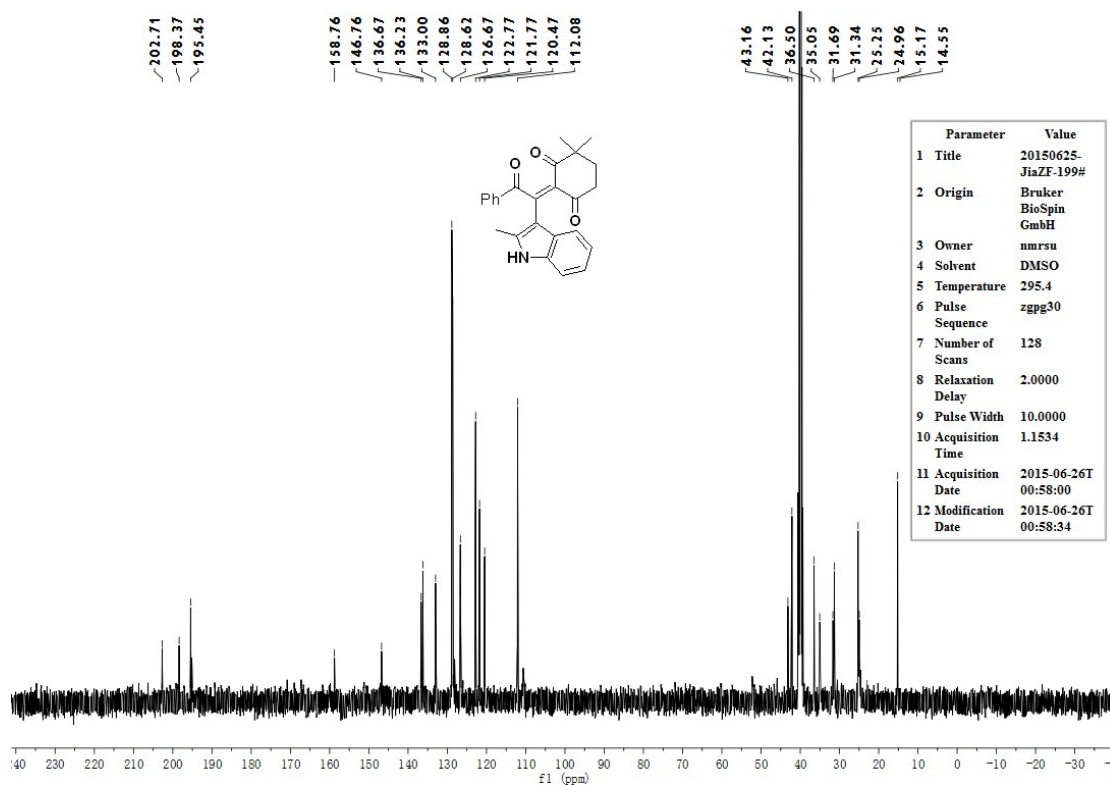
Parameter	Value
1 Title	20150625-JiaZF-198#
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Solvent	DMSO
5 Temperature	295.4
6 Pulse Sequence	zgpg30
7 Number of Scans	300
8 Relaxation Delay	2.0000
9 Pulse Width	10.0000
10 Acquisition Time	1.1534
11 Acquisition Date	2015-06-26T 08:44:00
12 Modification Date	2015-06-26T 08:44:07



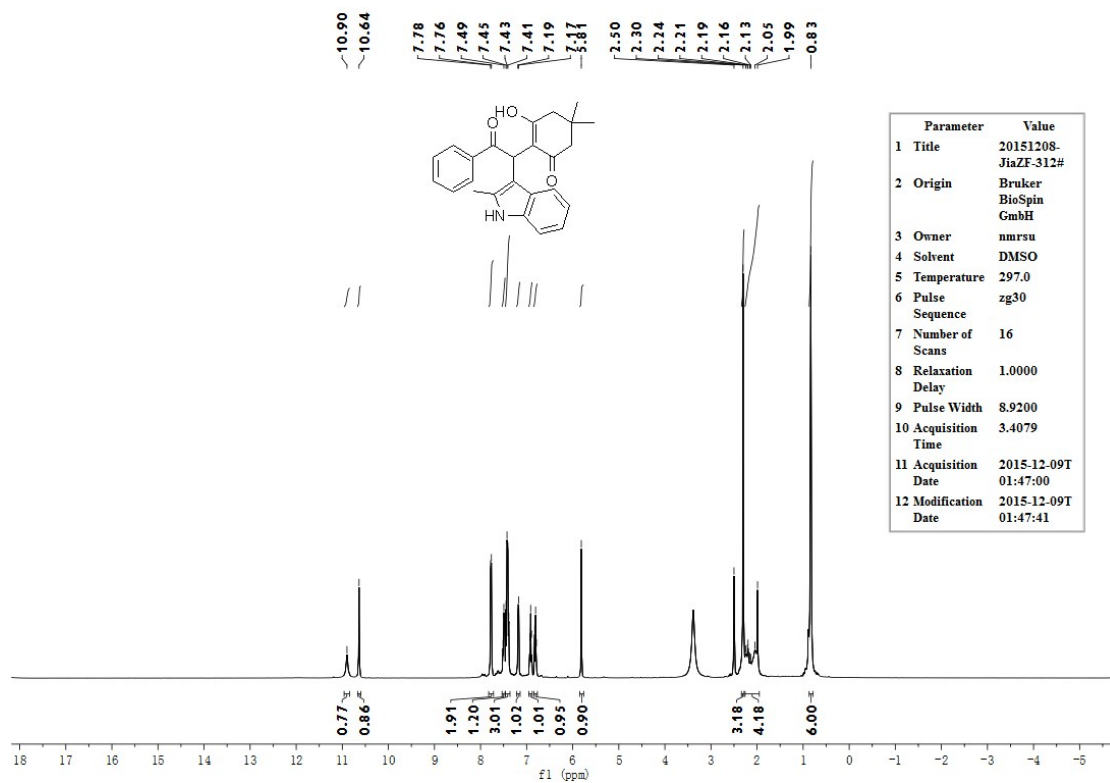




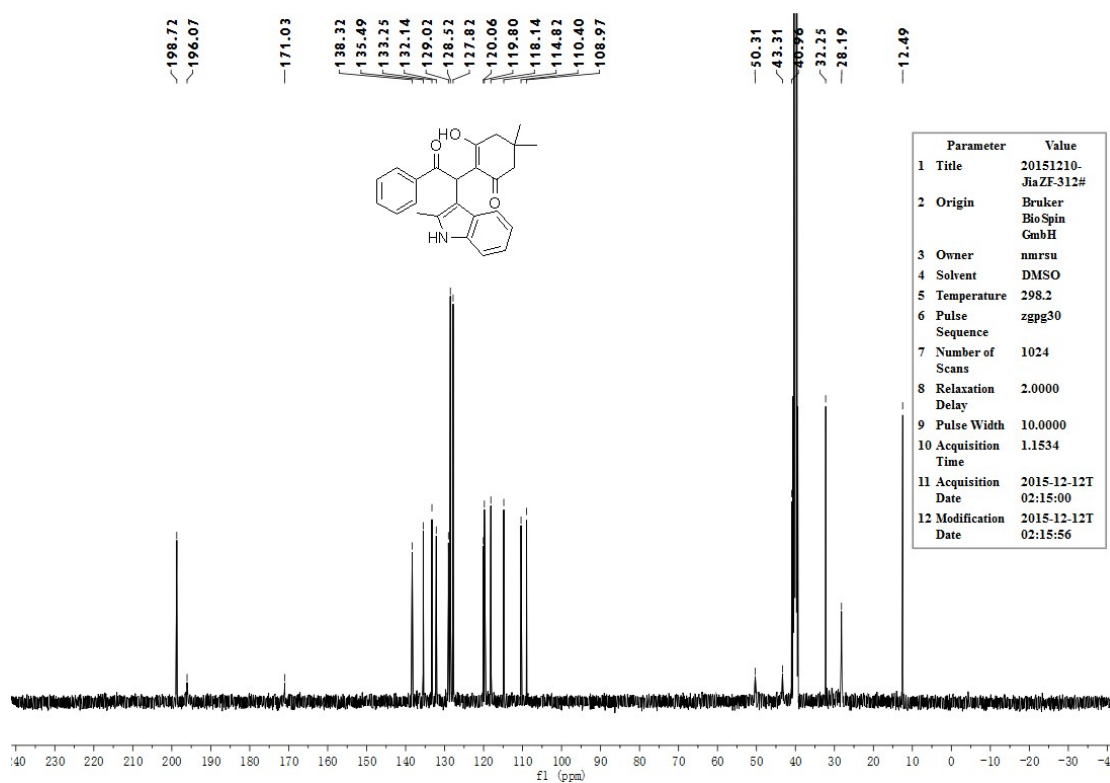
Parameter	Value
1 Title	20150623-JiaZF-188#
2 Origin	Bruker BioSpin GmbH
3 Owner	nrrsu
4 Solvent	DMSO
5 Temperature	295.2
6 Pulse Sequence	zg30
7 Number of Scans	16
8 Relaxation Delay	1.0000
9 Pulse Width	8.9200
10 Acquisition Time	3.4079
11 Acquisition Date	2015-06-23T18:00:00
12 Modification Date	2015-06-23T18:00:11



Parameter	Value
1 Title	20150625-JiaZF-199#
2 Origin	Bruker BioSpin GmbH
3 Owner	nrrsu
4 Solvent	DMSO
5 Temperature	295.4
6 Pulse Sequence	zgpg30
7 Number of Scans	128
8 Relaxation Delay	2.0000
9 Pulse Width	10.0000
10 Acquisition Time	1.1534
11 Acquisition Date	2015-06-26T00:58:00
12 Modification Date	2015-06-26T00:58:34

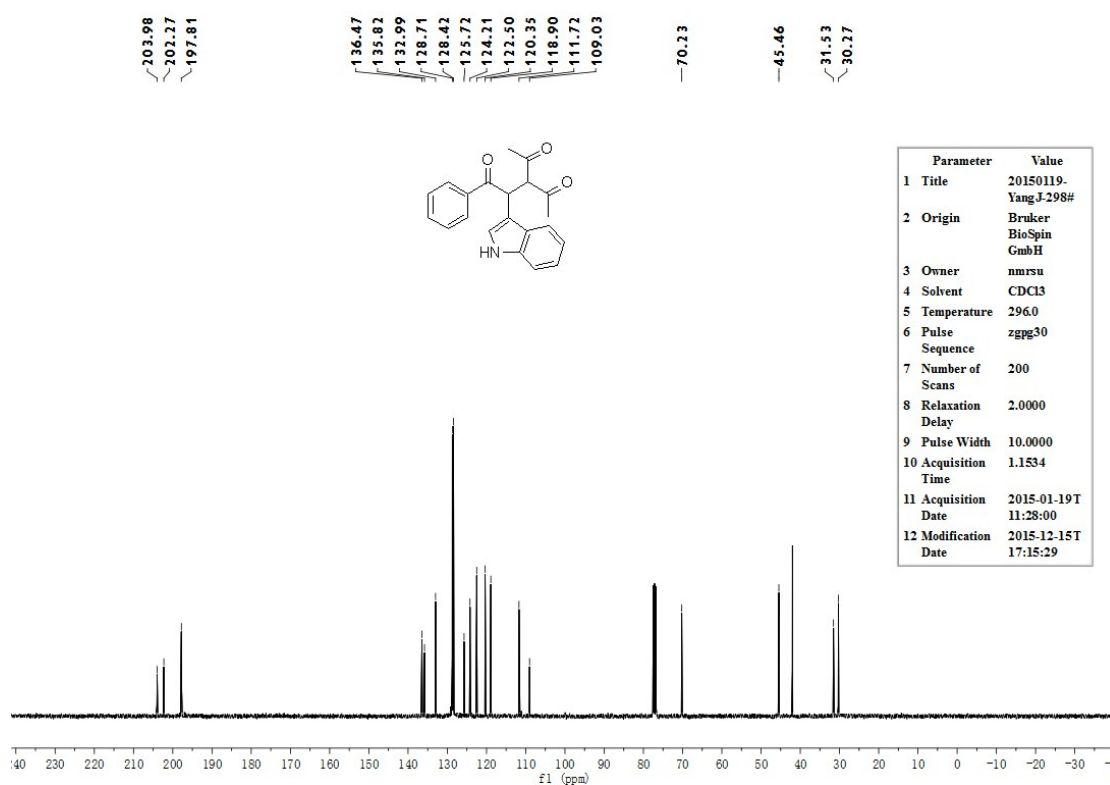
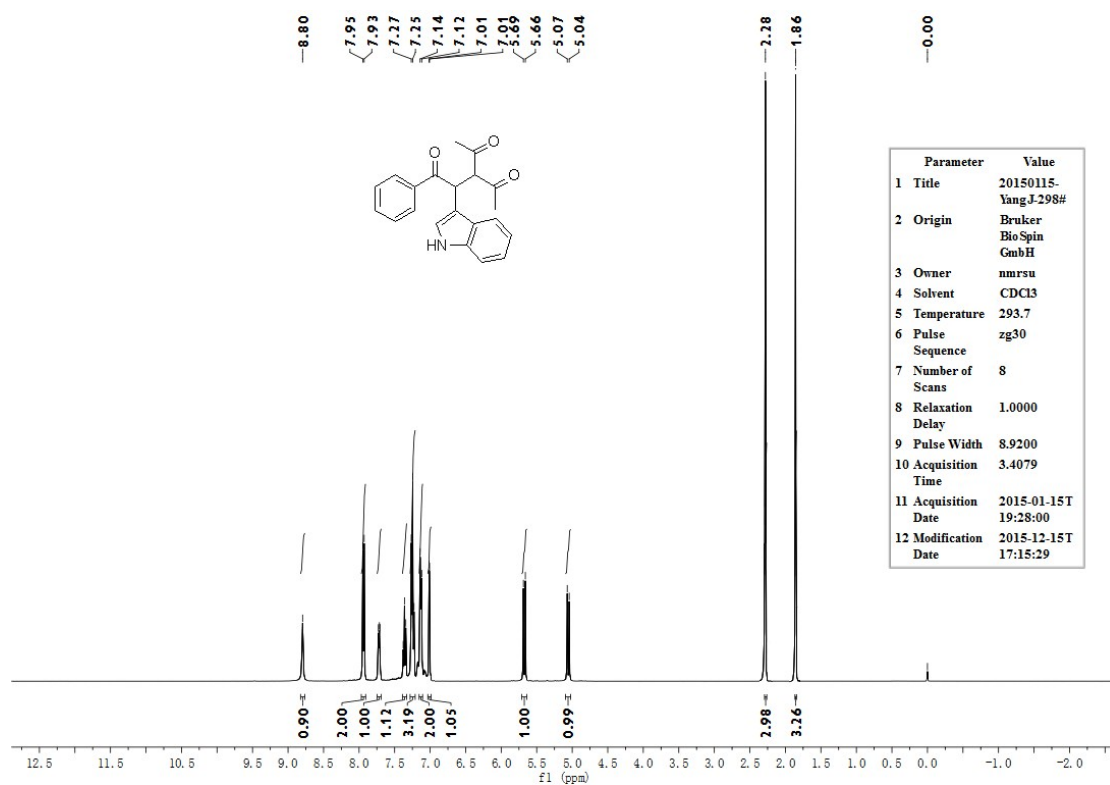


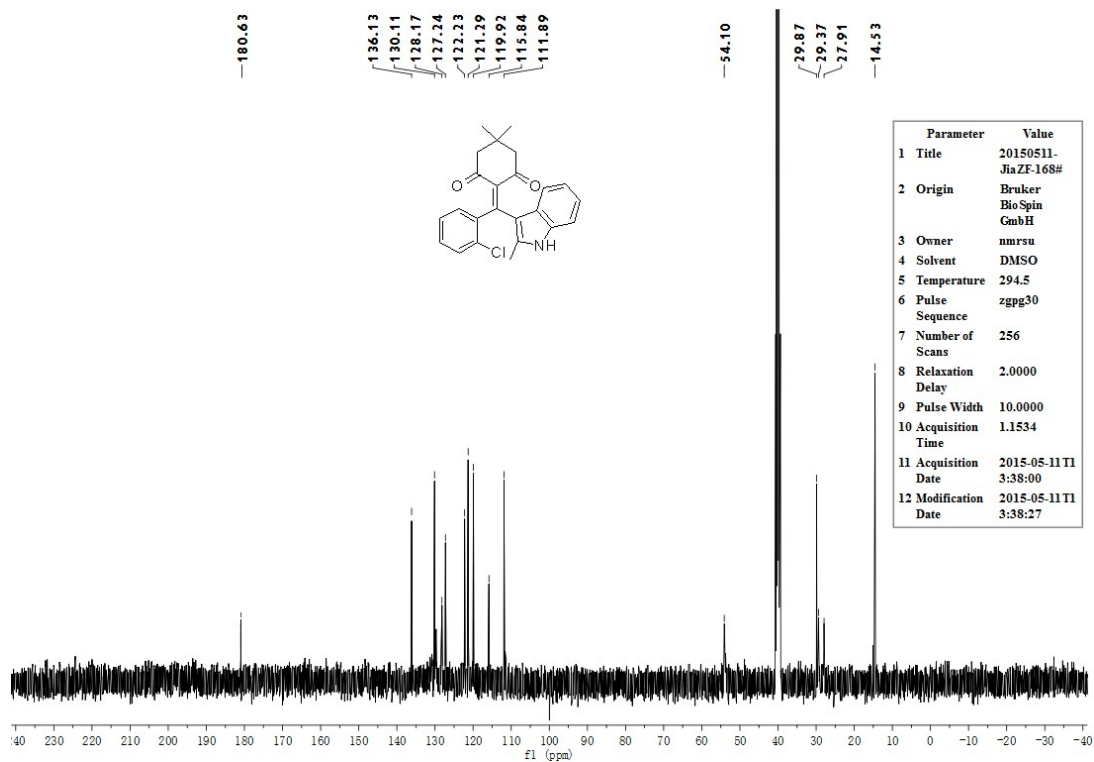
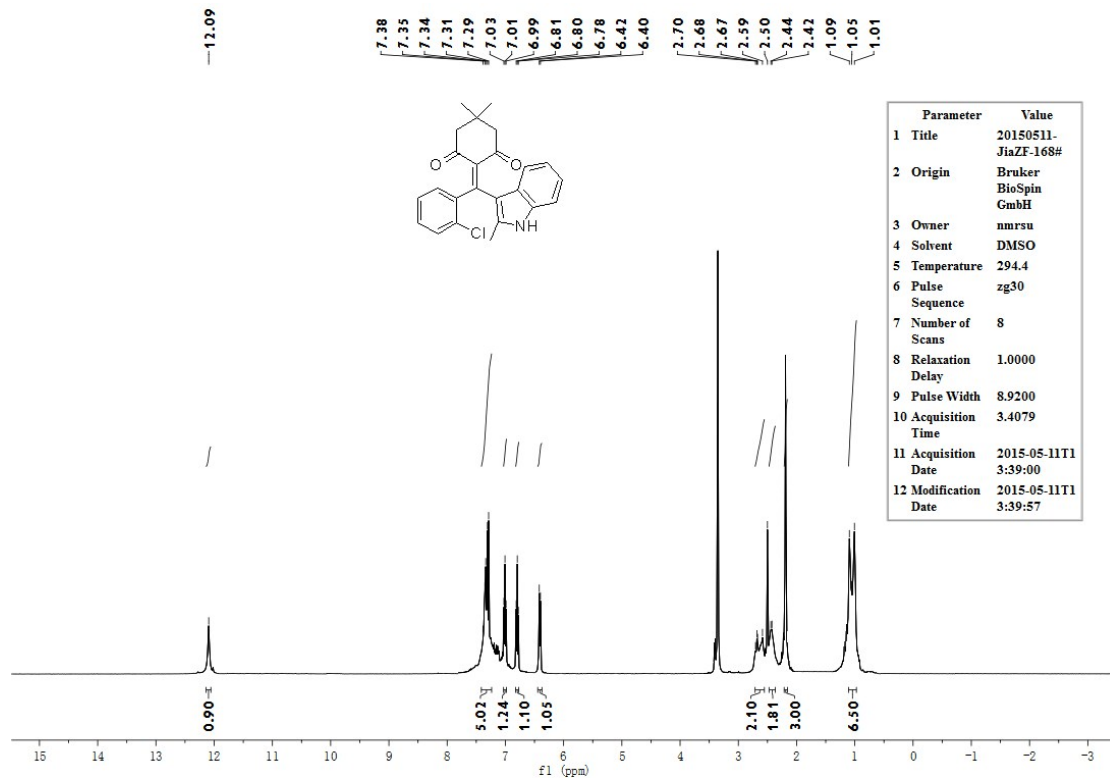
Parameter	Value
1 Title	20151208-JiaZF-312#
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Solvent	DMSO
5 Temperature	297.0
6 Pulse Sequence	zg30
7 Number of Scans	16
8 Relaxation Delay	1.0000
9 Pulse Width	8.9200
10 Acquisition Time	3.4079
11 Acquisition Date	2015-12-09T 01:47:00
12 Modification Date	2015-12-09T 01:47:41

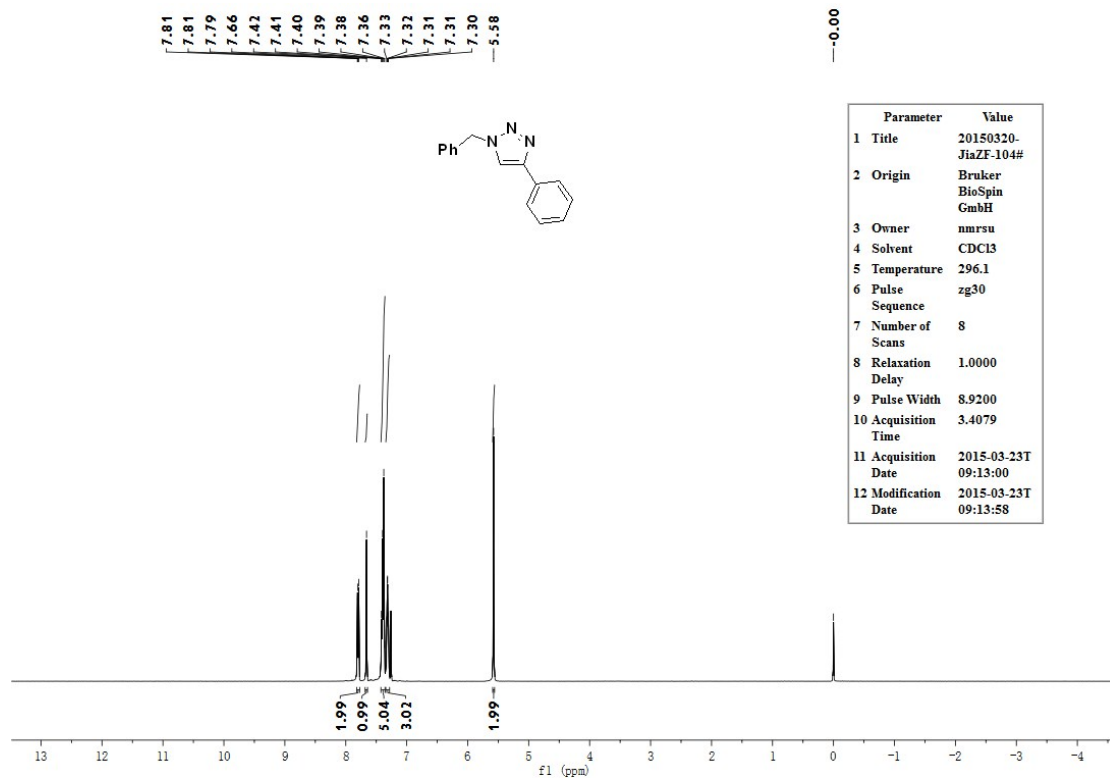


Parameter	Value
1 Title	20151210-JiaZF-312#
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Solvent	DMSO
5 Temperature	298.2
6 Pulse Sequence	zggg30
7 Number of Scans	1024
8 Relaxation Delay	2.0000
9 Pulse Width	10.0000
10 Acquisition Time	1.1534
11 Acquisition Date	2015-12-12T 02:15:00
12 Modification Date	2015-12-12T 02:15:56

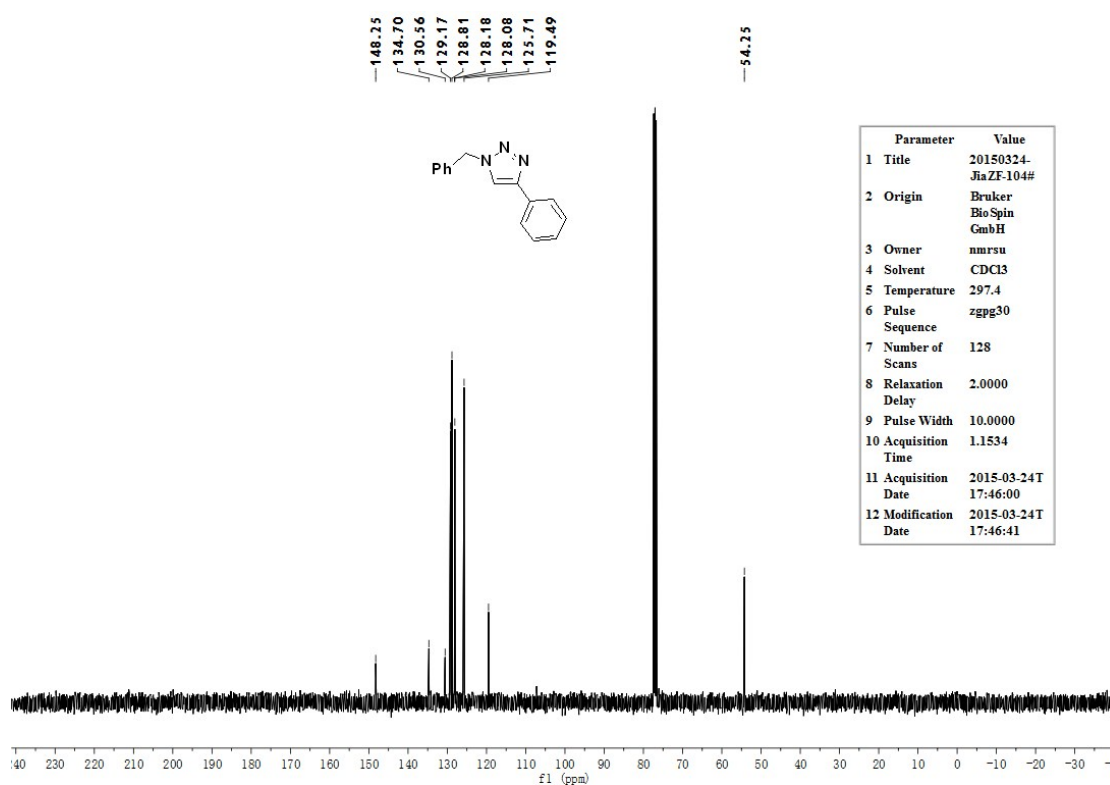




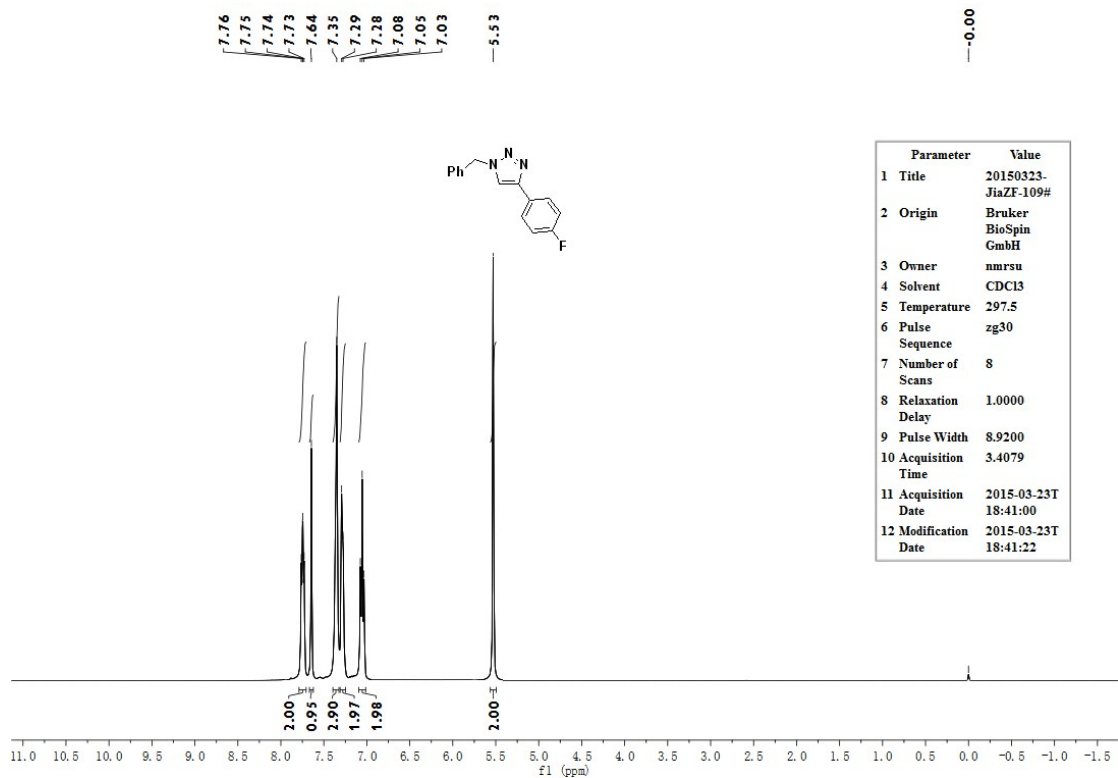




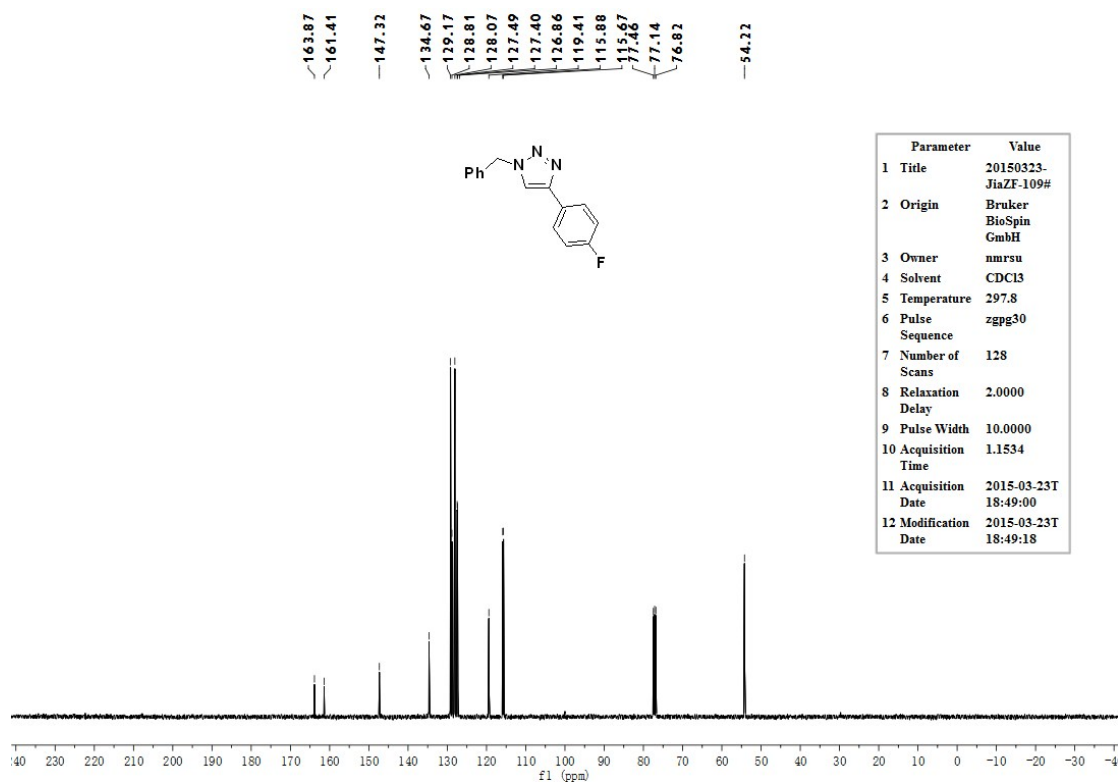
Parameter	Value
1 Title	20150320- JiaZF-104#
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsl
4 Solvent	CDCl3
5 Temperature	296.1
6 Pulse Sequence	zg30
7 Number of Scans	8
8 Relaxation Delay	1.0000
9 Pulse Width	8.9200
10 Acquisition Time	3.4079
11 Acquisition Date	2015-03-23T 09:13:00
12 Modification Date	2015-03-23T 09:13:58



Parameter	Value
1 Title	20150324- JiaZF-104#
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsl
4 Solvent	CDCl3
5 Temperature	297.4
6 Pulse Sequence	zgpg30
7 Number of Scans	128
8 Relaxation Delay	2.0000
9 Pulse Width	10.0000
10 Acquisition Time	1.1534
11 Acquisition Date	2015-03-24T 17:46:00
12 Modification Date	2015-03-24T 17:46:41

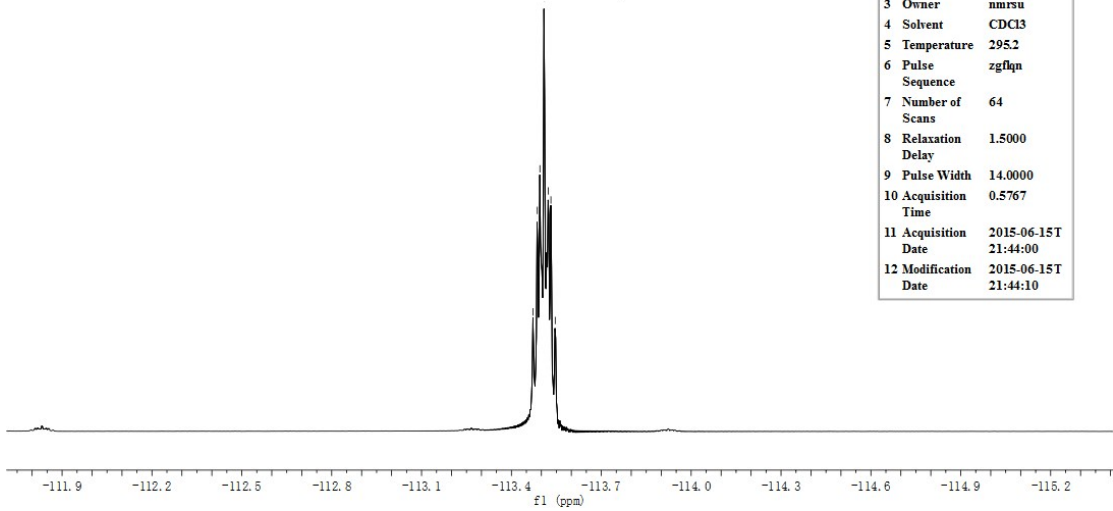
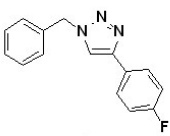


Parameter	Value
1 Title	20150323-JiaZF-109#
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Solvent	CDCl3
5 Temperature	297.5
6 Pulse Sequence	zg30
7 Number of Scans	8
8 Relaxation Delay	1.0000
9 Pulse Width	8.9200
10 Acquisition Time	3.4079
11 Acquisition Date	2015-03-23T 18:41:00
12 Modification Date	2015-03-23T 18:41:22

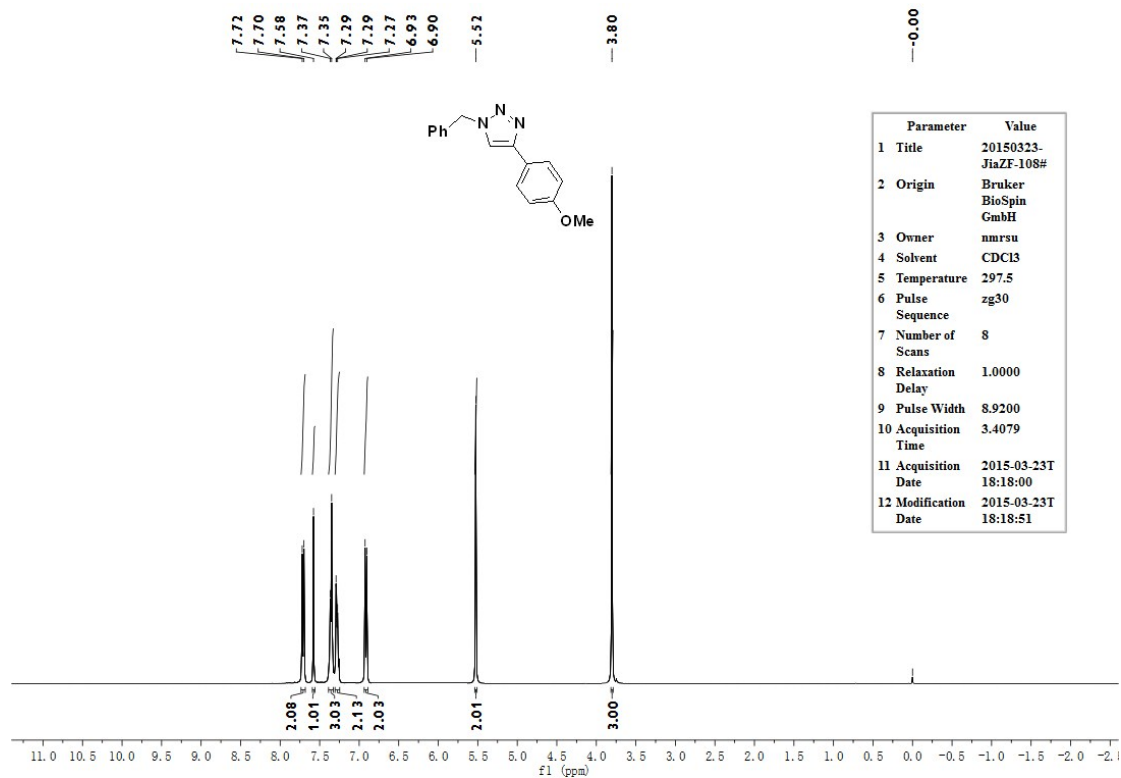


Parameter	Value
1 Title	20150323-JiaZF-109#
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Solvent	CDCl3
5 Temperature	297.8
6 Pulse Sequence	zgpg30
7 Number of Scans	128
8 Relaxation Delay	2.0000
9 Pulse Width	10.0000
10 Acquisition Time	1.1534
11 Acquisition Date	2015-03-23T 18:49:00
12 Modification Date	2015-03-23T 18:49:18

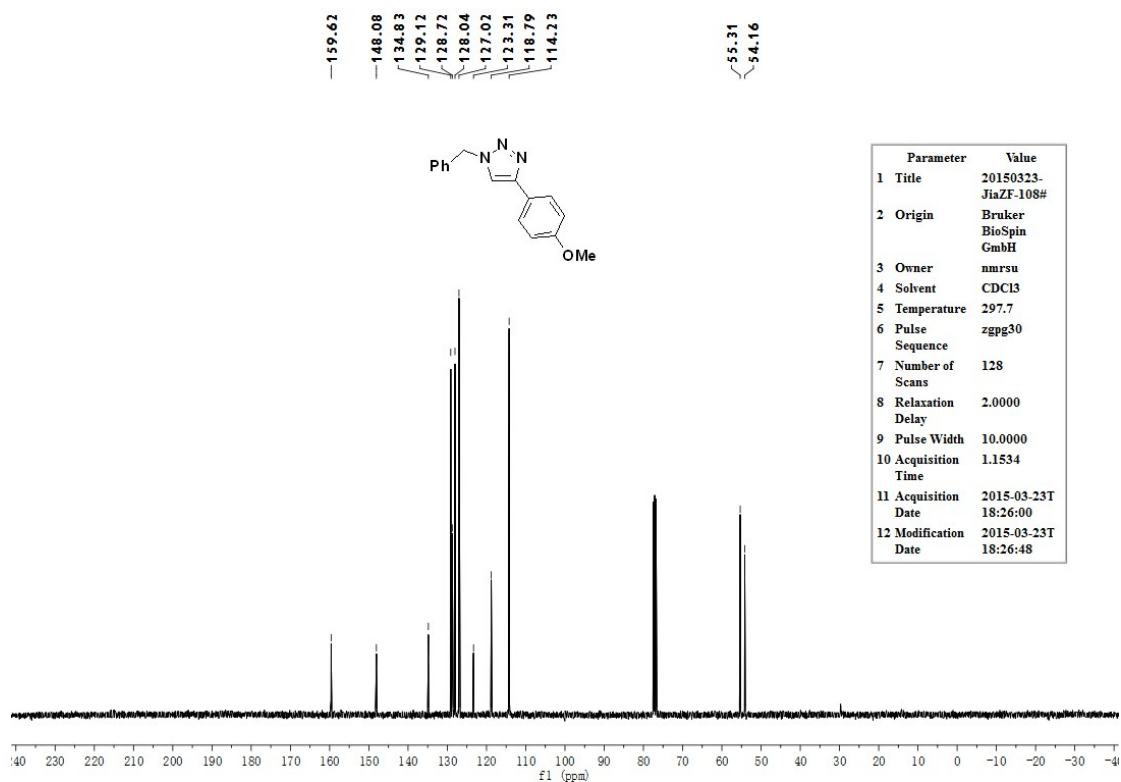
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-113.52  
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-113.55



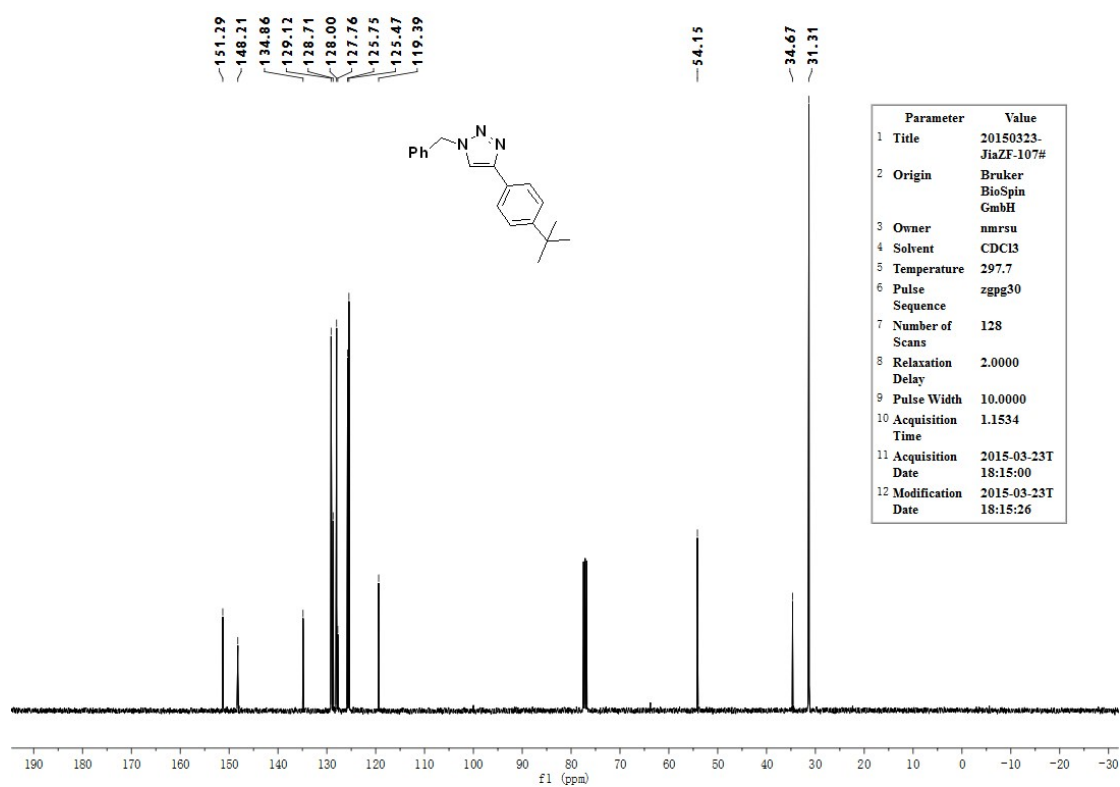
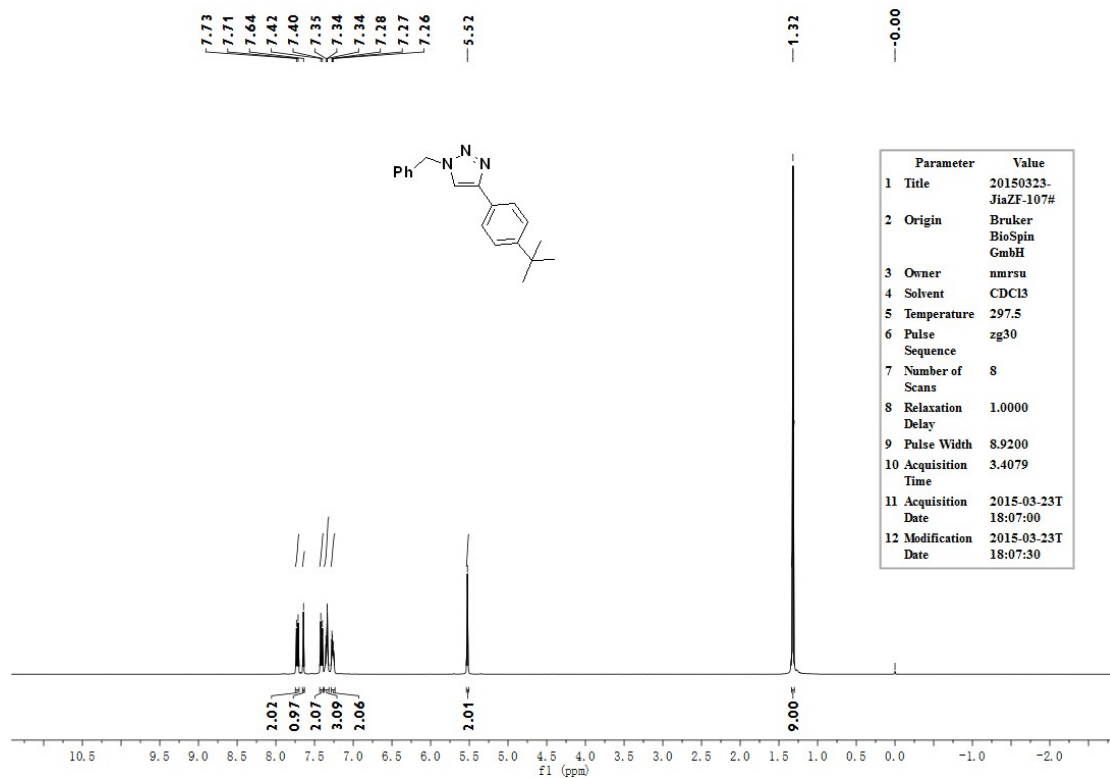
Parameter	Value
1 Title	20150615-JiaZE-109#
2 Origin	Bruker BioSpin GmbH
3 Owner	nmsu
4 Solvent	CDCl3
5 Temperature	295.2
6 Pulse Sequence	zgpgq
7 Number of Scans	64
8 Relaxation Delay	1.5000
9 Pulse Width	14.0000
10 Acquisition Time	0.5767
11 Acquisition Date	2015-06-15T 21:44:00
12 Modification Date	2015-06-15T 21:44:10

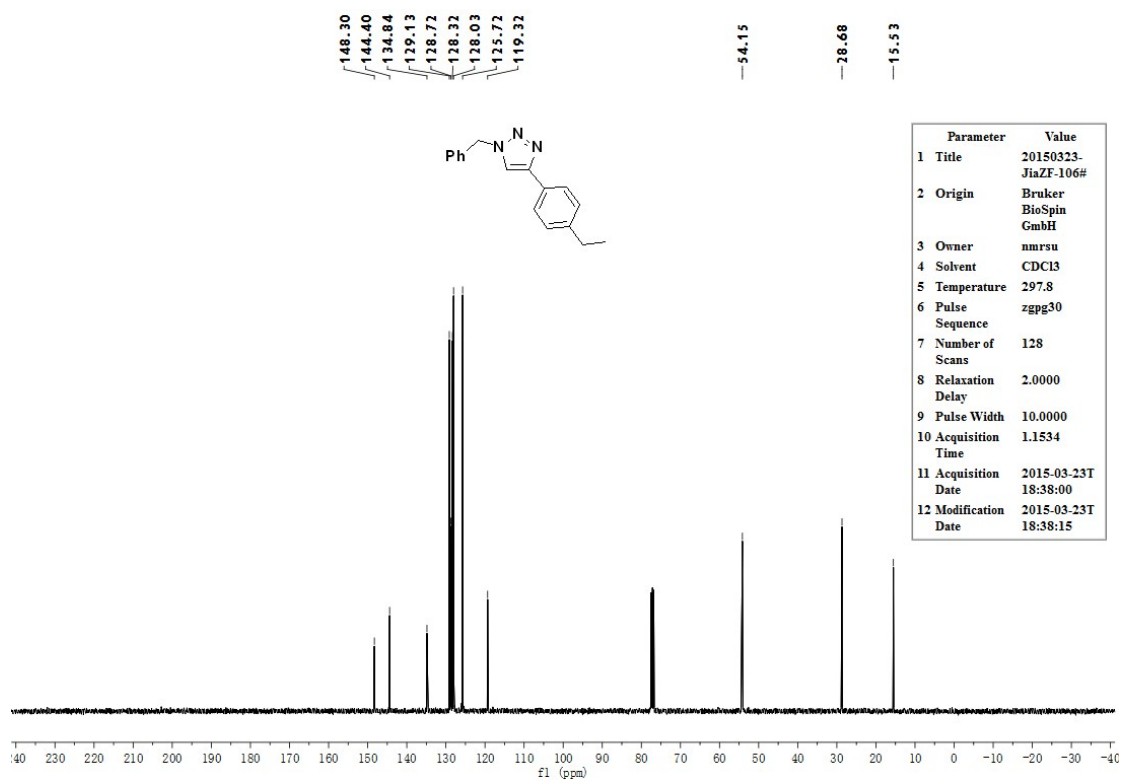
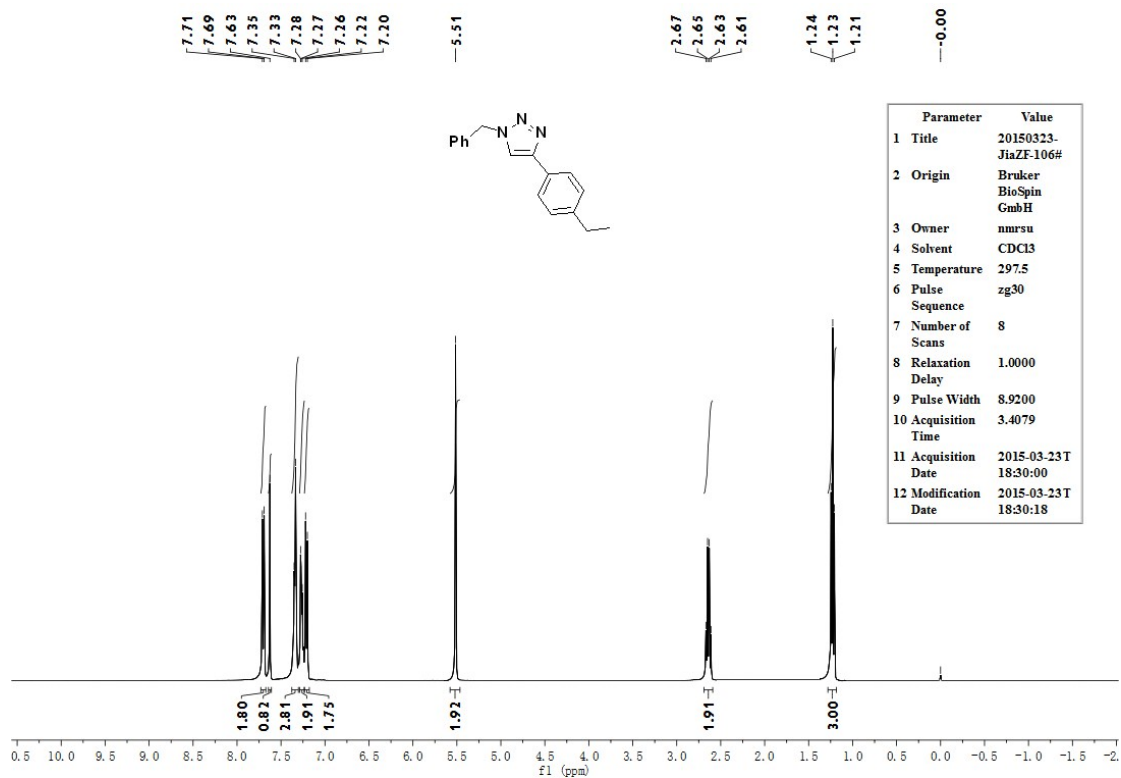


Parameter	Value
1 Title	20150323-JiaZF-108#
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Solvent	CDCl3
5 Temperature	297.5
6 Pulse	zg30
7 Number of Scans	8
8 Relaxation Delay	1.0000
9 Pulse Width	8.9200
10 Acquisition Time	3.4079
11 Acquisition Date	2015-03-23T 18:18:00
12 Modification Date	2015-03-23T 18:18:51

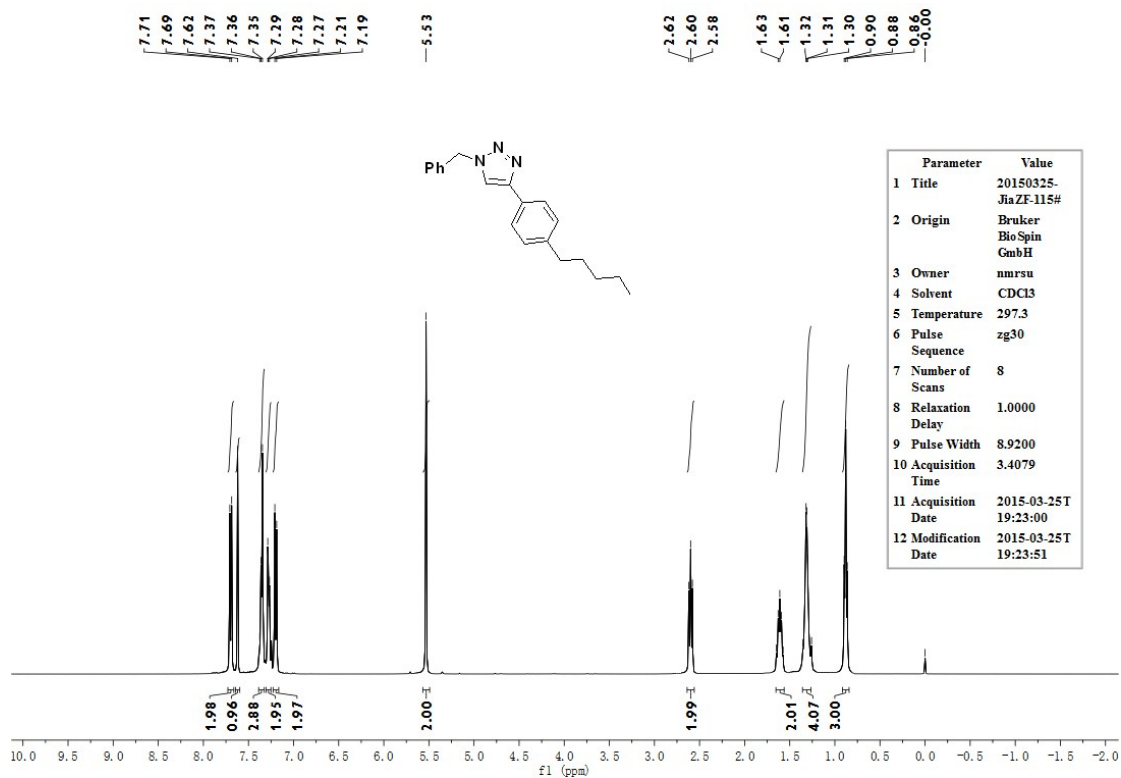


Parameter	Value
1 Title	20150323-JiaZF-108#
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Solvent	CDCl3
5 Temperature	297.7
6 Pulse	zpgg30
7 Number of Scans	128
8 Relaxation Delay	2.0000
9 Pulse Width	10.0000
10 Acquisition Time	1.1534
11 Acquisition Date	2015-03-23T 18:26:00
12 Modification Date	2015-03-23T 18:26:48

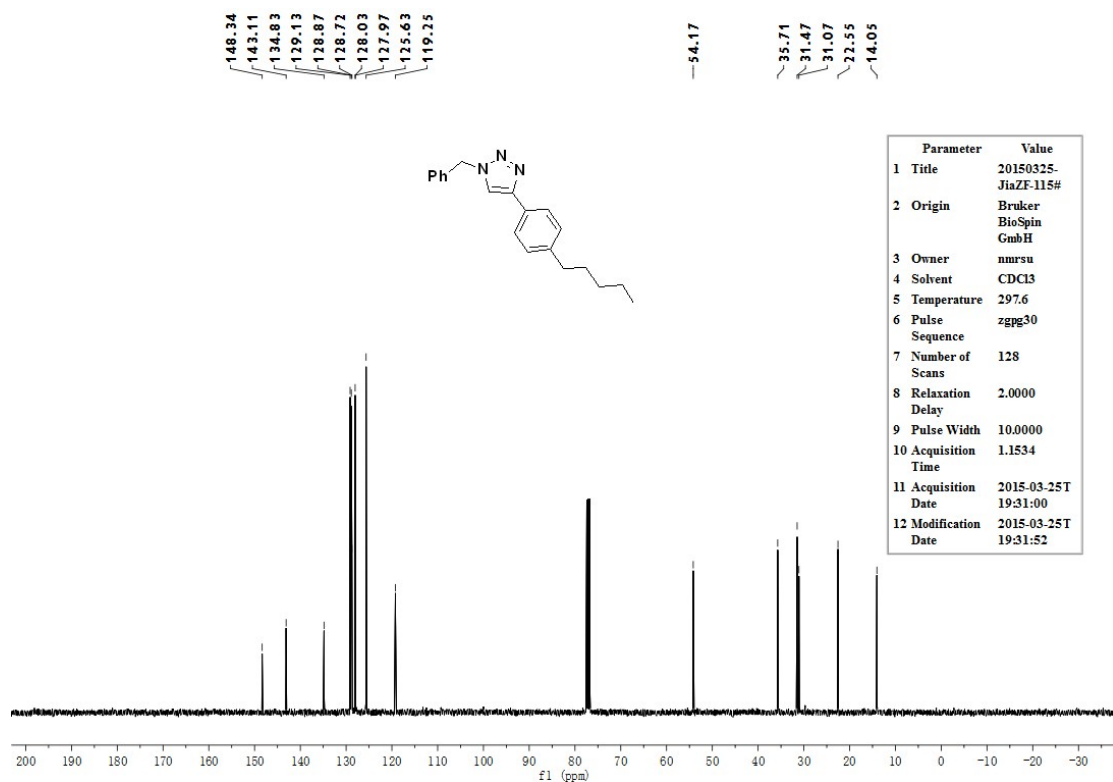




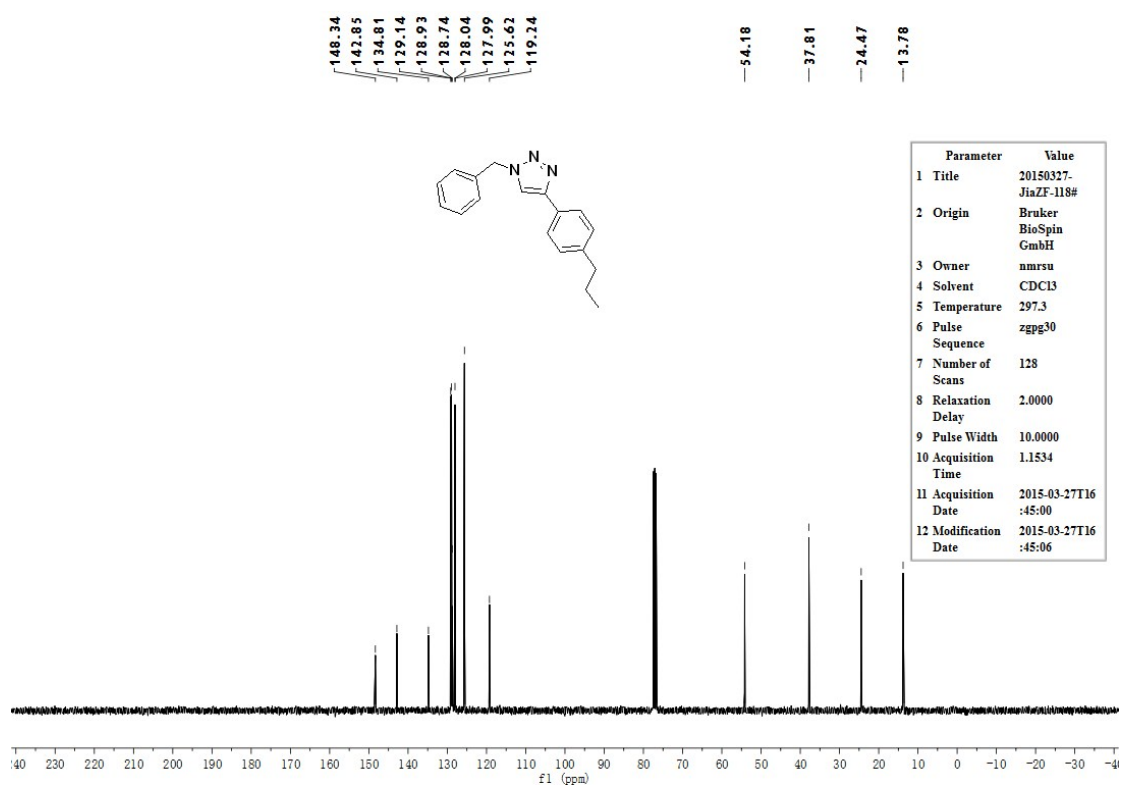
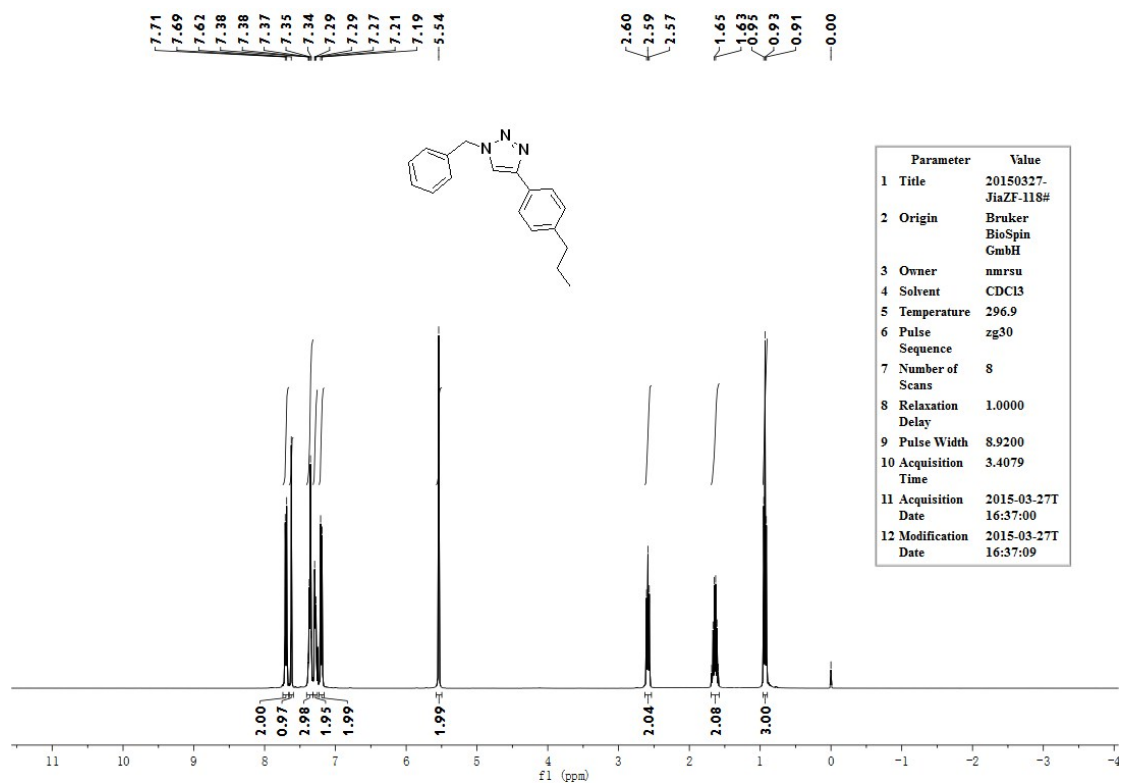


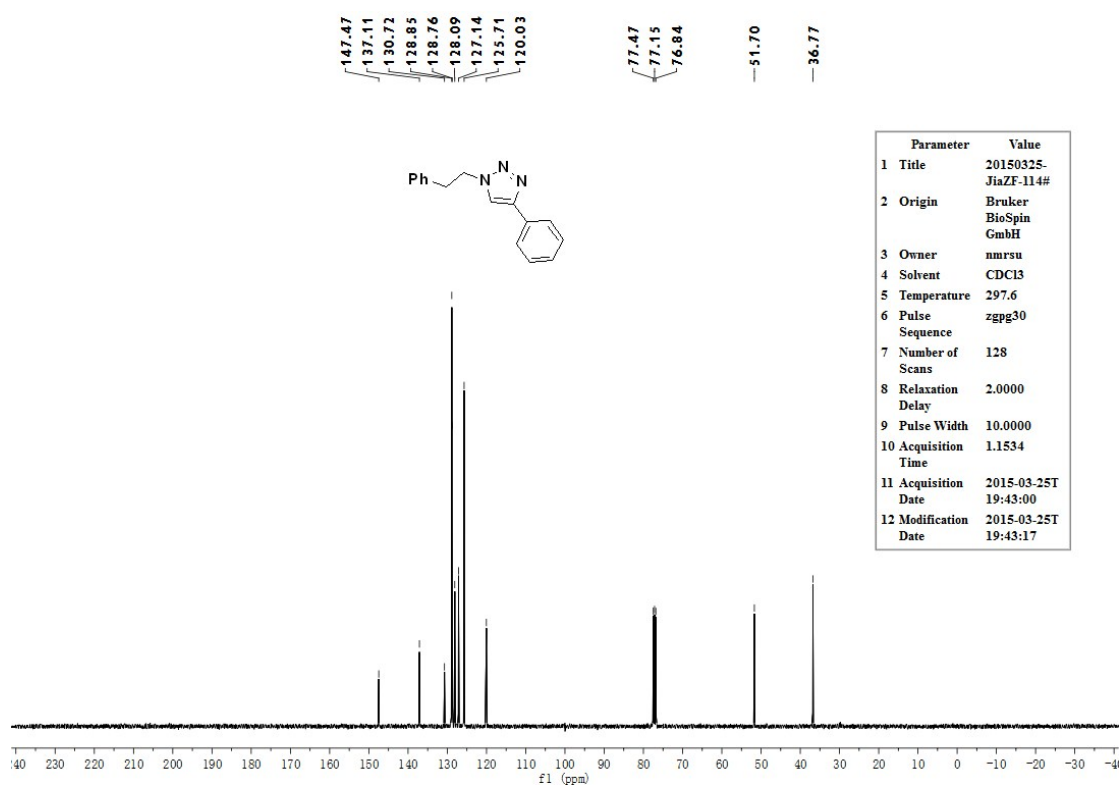
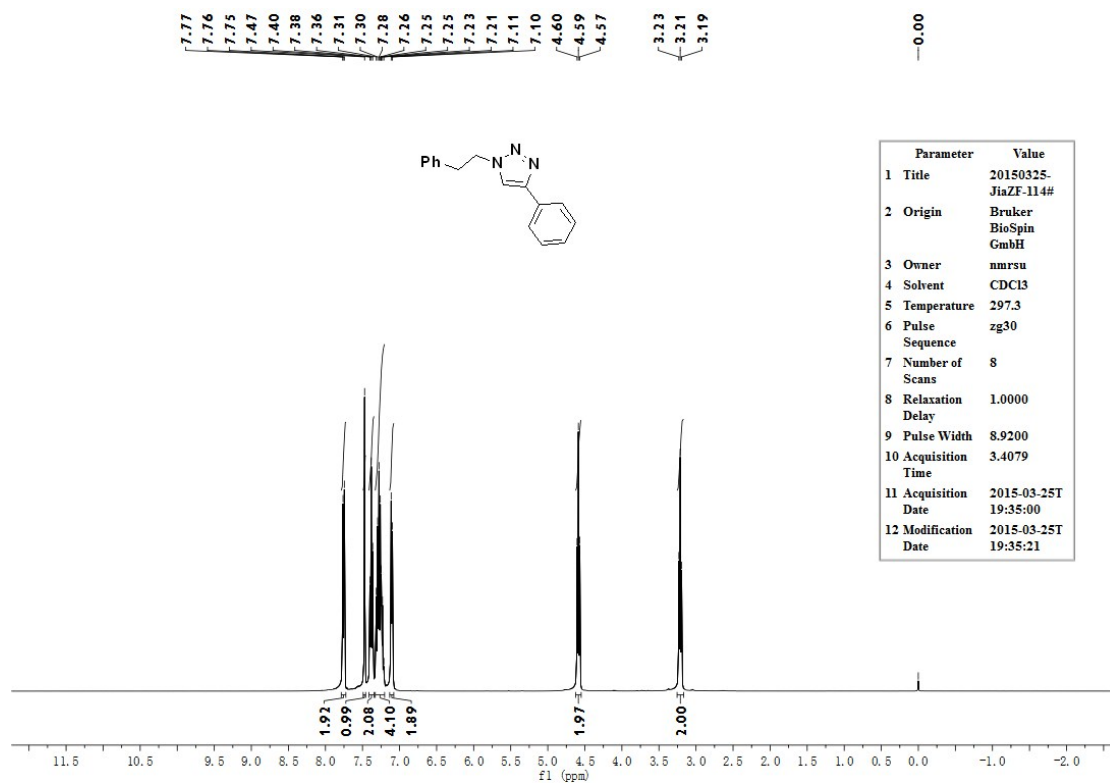


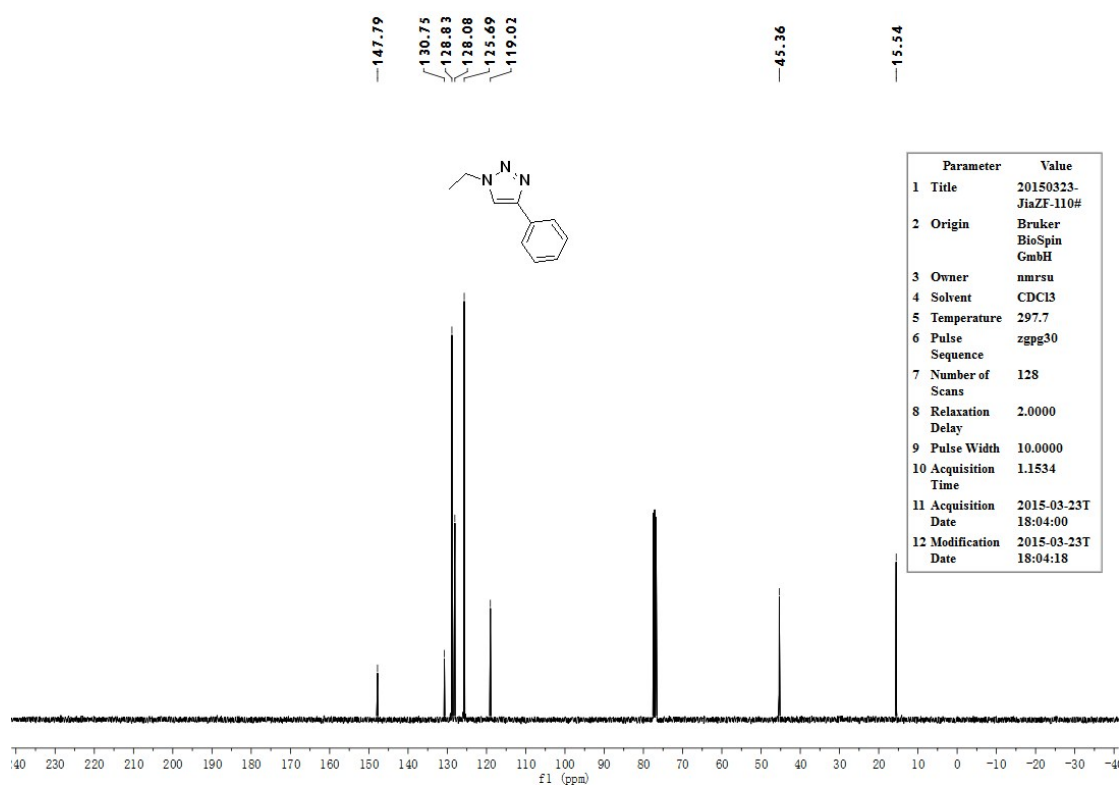
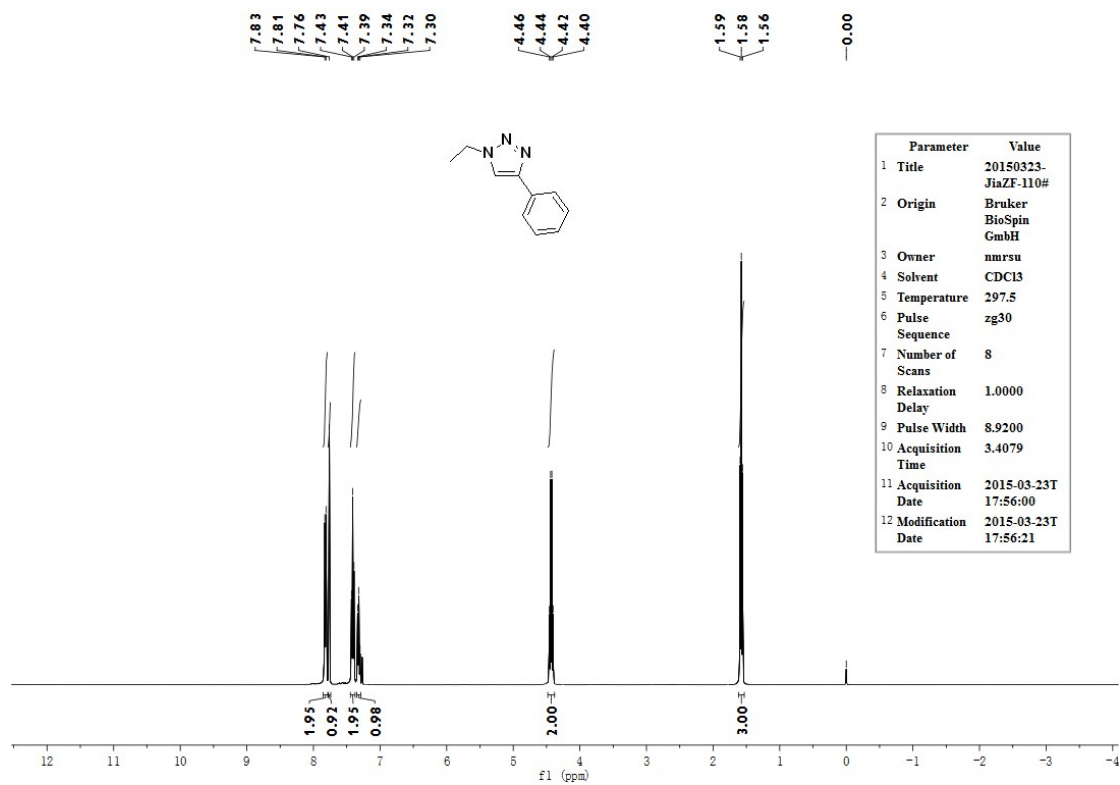
Parameter	Value
1 Title	20150325-JiaZF-115#
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Solvent	CDCl3
5 Temperature	297.3
6 Pulse Sequence	zg30
7 Number of Scans	8
8 Relaxation Delay	1.0000
9 Pulse Width	8.9200
10 Acquisition Time	3.4079
11 Acquisition Date	2015-03-25T 19:23:00
12 Modification Date	2015-03-25T 19:23:51

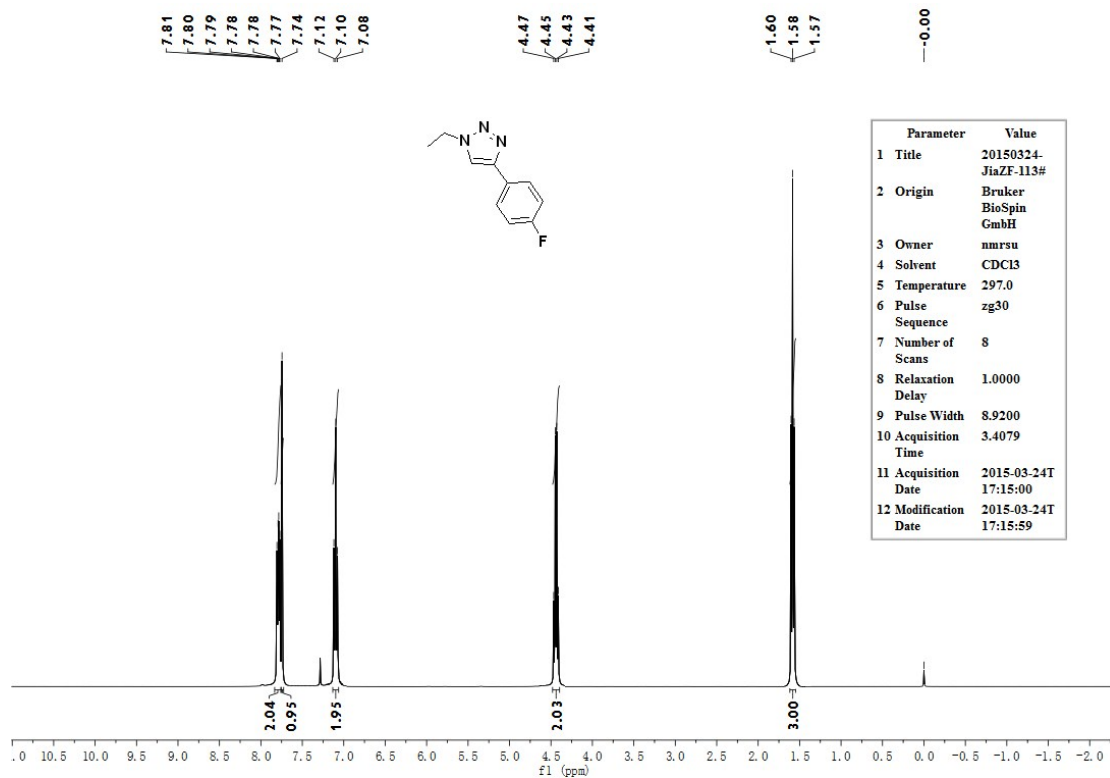


Parameter	Value
1 Title	20150325-JiaZF-115#
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Solvent	CDCl3
5 Temperature	297.6
6 Pulse Sequence	zgpg30
7 Number of Scans	128
8 Relaxation Delay	2.0000
9 Pulse Width	10.0000
10 Acquisition Time	1.1534
11 Acquisition Date	2015-03-25T 19:31:00
12 Modification Date	2015-03-25T 19:31:52

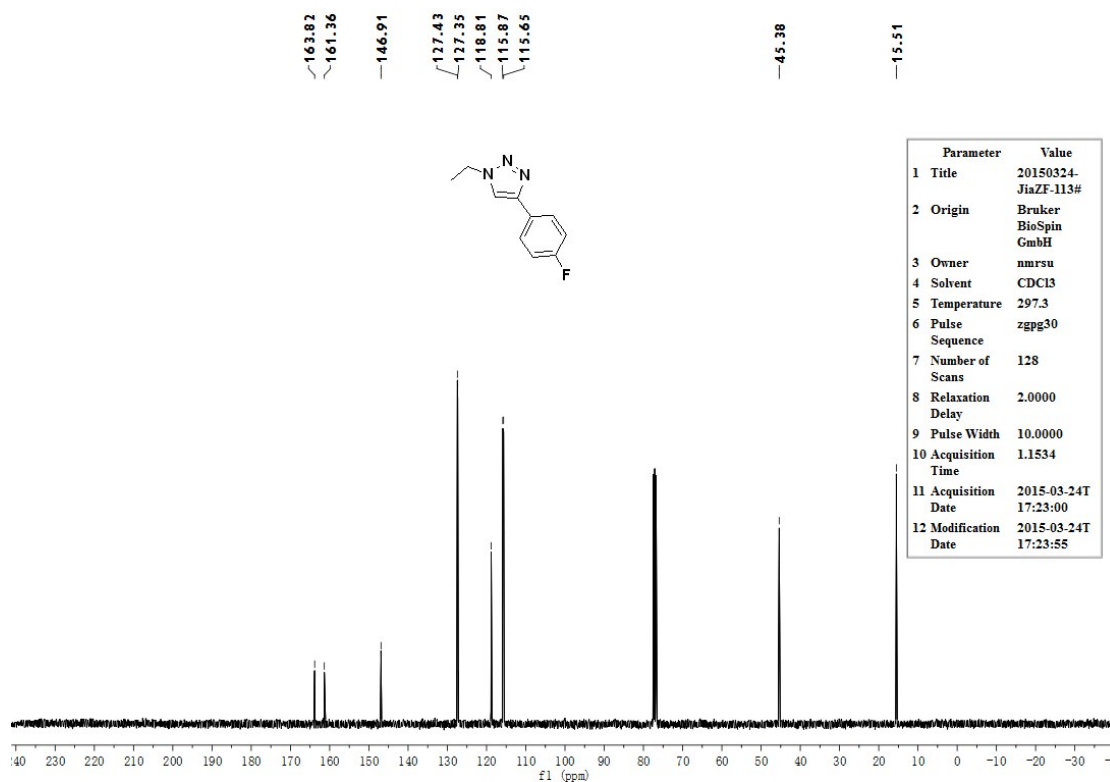




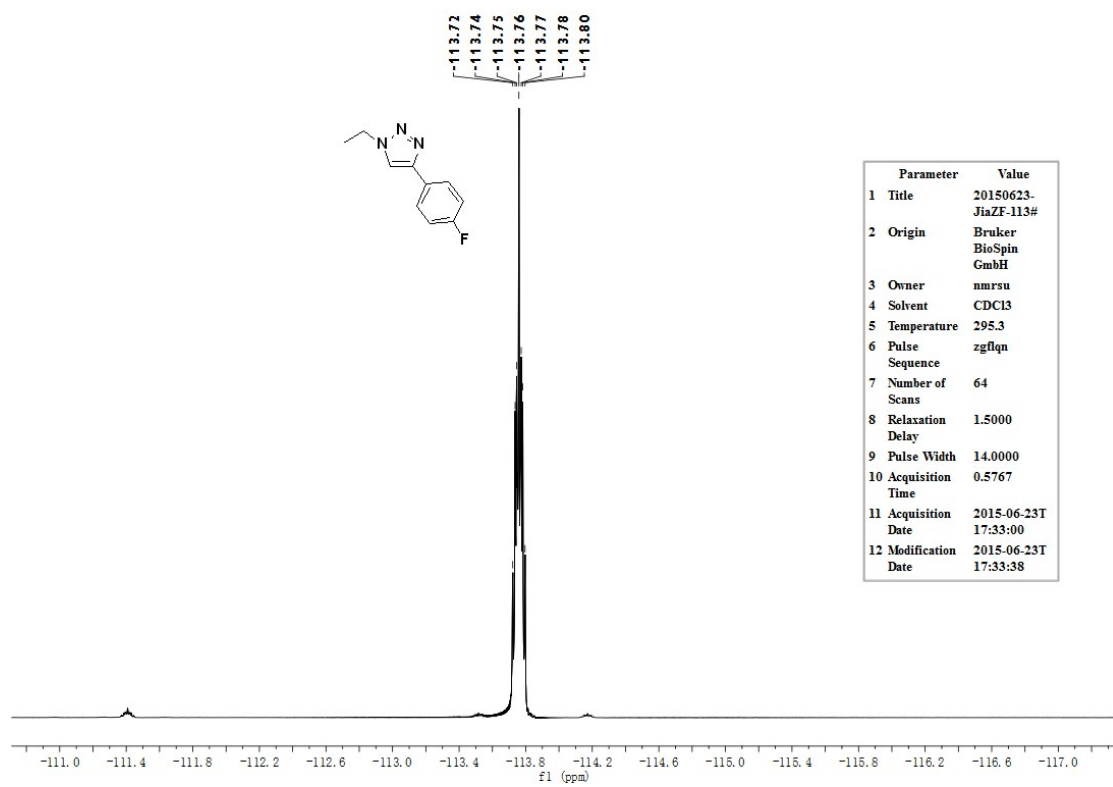




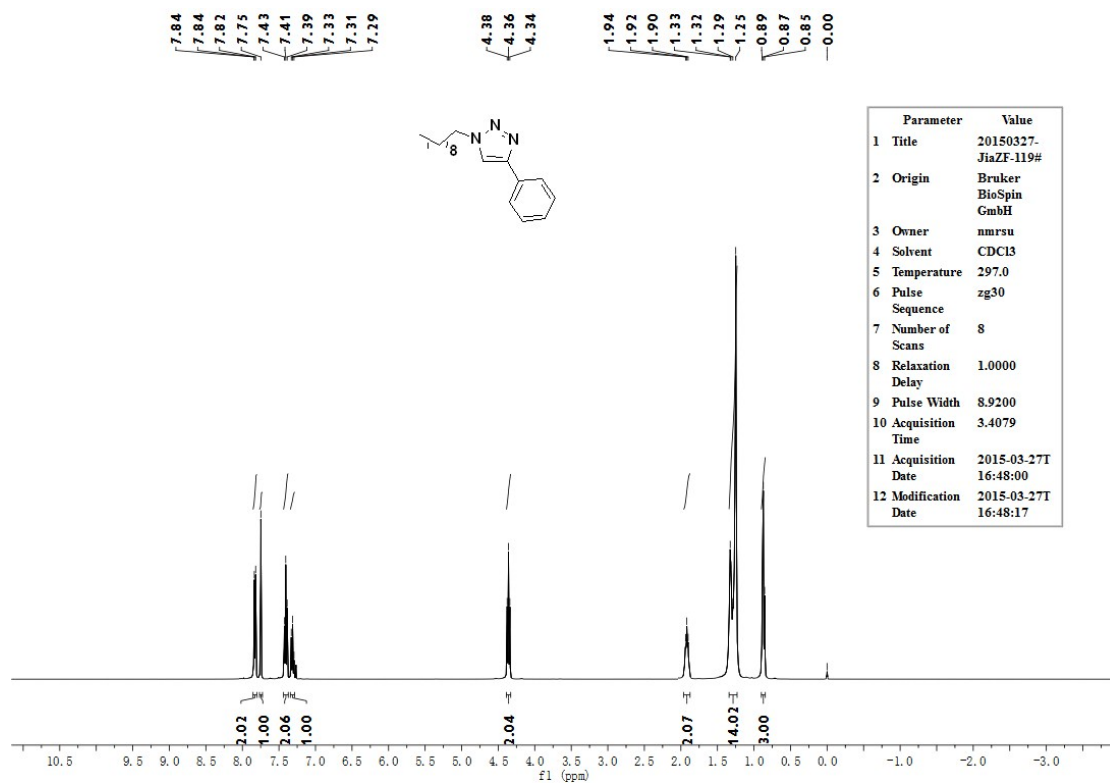
Parameter	Value
1 Title	20150324-JiaZF-113#
2 Origin	Bruker BioSpin GmbH
3 Owner	nmsru
4 Solvent	CDCl3
5 Temperature	297.0
6 Pulse Sequence	zg30
7 Number of Scans	8
8 Relaxation Delay	1.0000
9 Pulse Width	8.9200
10 Acquisition Time	3.4079
11 Acquisition Date	2015-03-24T17:15:00
12 Modification Date	2015-03-24T17:15:59



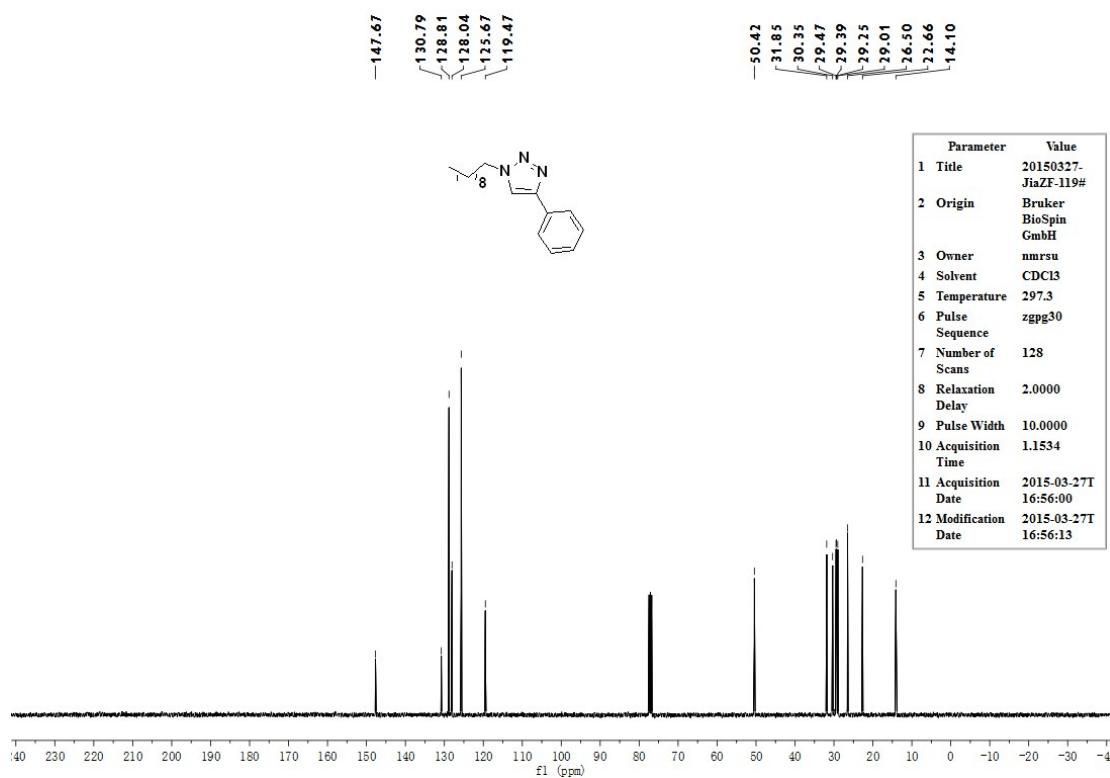
Parameter	Value
1 Title	20150324-JiaZF-113#
2 Origin	Bruker BioSpin GmbH
3 Owner	nmsru
4 Solvent	CDCl3
5 Temperature	297.3
6 Pulse Sequence	zgpg30
7 Number of Scans	128
8 Relaxation Delay	2.0000
9 Pulse Width	10.0000
10 Acquisition Time	1.1534
11 Acquisition Date	2015-03-24T17:23:00
12 Modification Date	2015-03-24T17:23:55



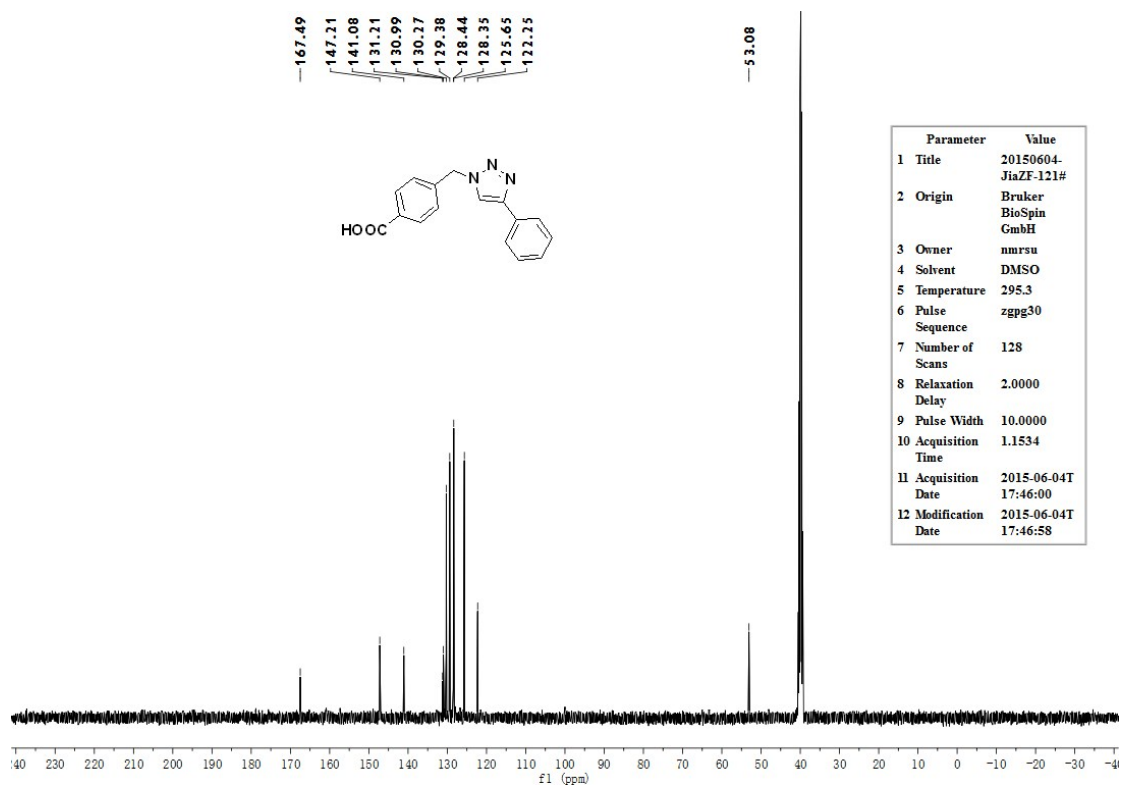
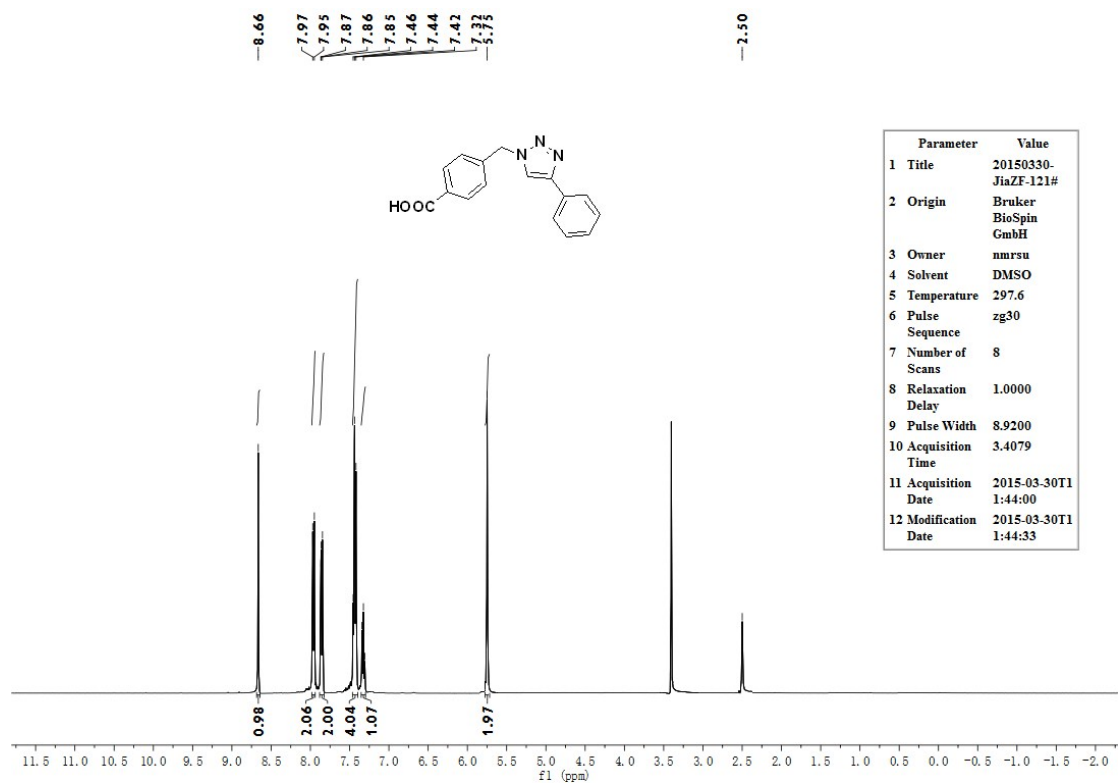
Parameter	Value
1 Title	20150623-JiaZF-113#
2 Origin	Bruker BioSpin GmbH
3 Owner	nmsru
4 Solvent	CDCl3
5 Temperature	295.3
6 Pulse Sequence	zgfgq
7 Number of Scans	64
8 Relaxation Delay	1.5000
9 Pulse Width	14.0000
10 Acquisition Time	0.5767
11 Acquisition Date	2015-06-23T17:33:00
12 Modification Date	2015-06-23T17:33:38



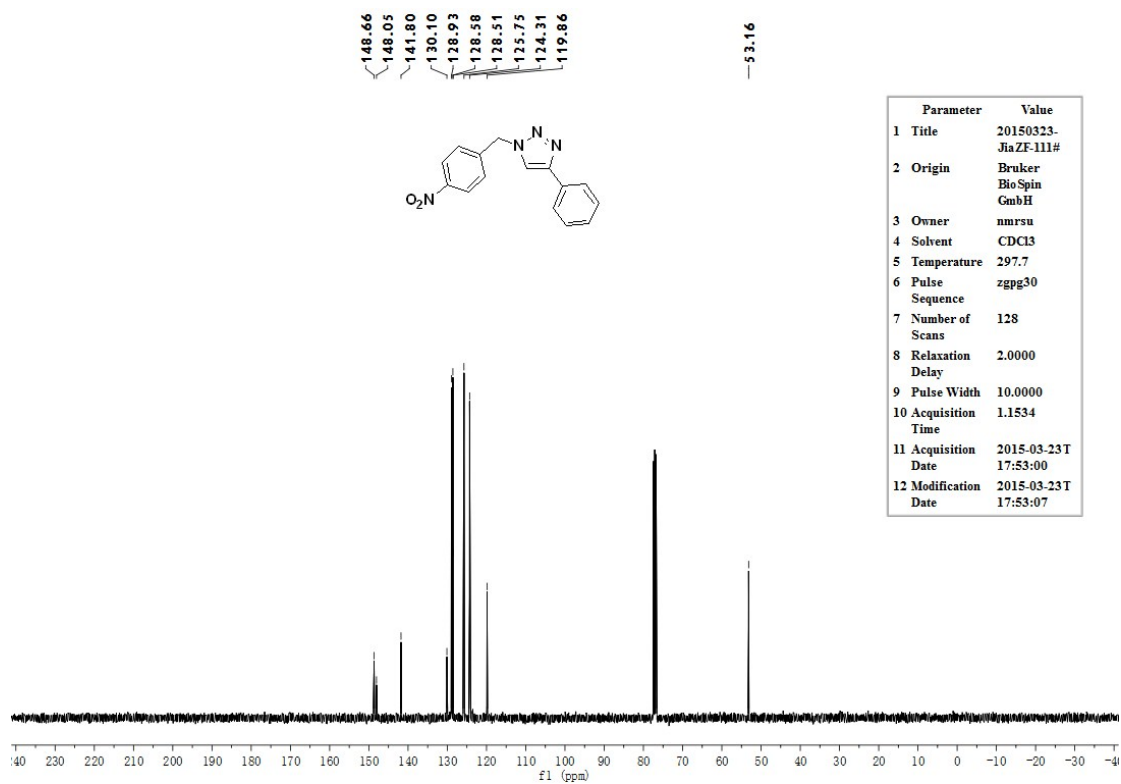
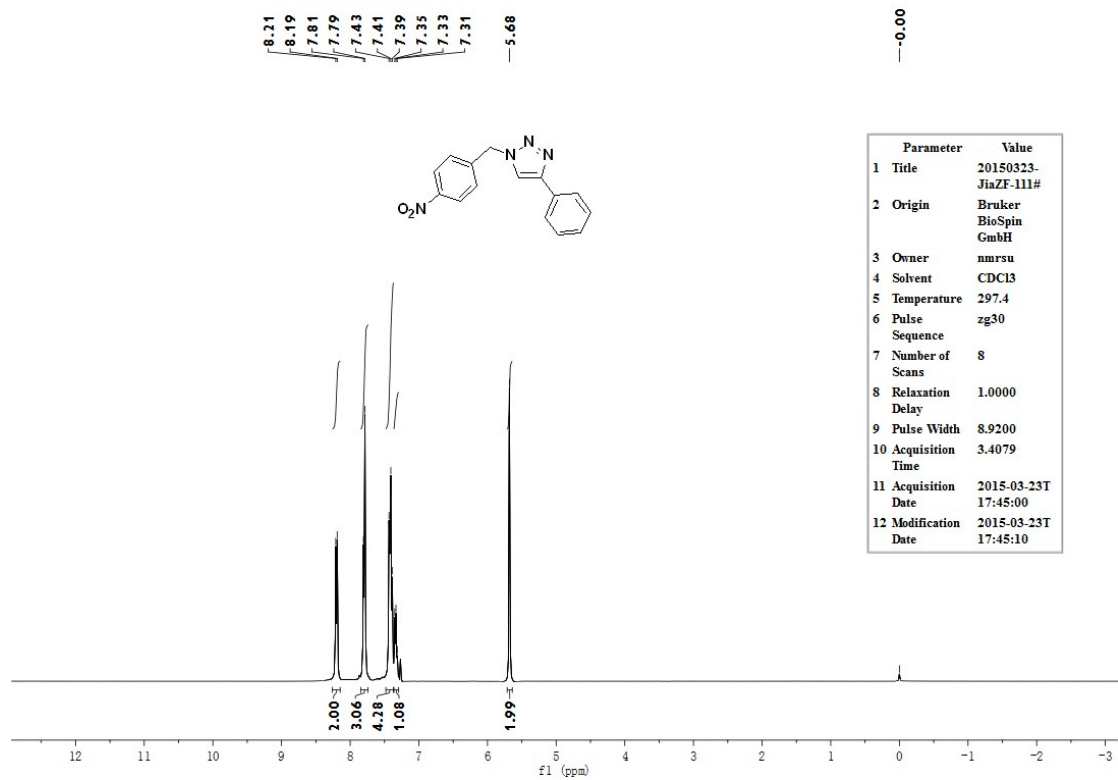
Parameter	Value
1 Title	20150327-JiaZF-119#
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Solvent	CDCl3
5 Temperature	297.0
6 Pulse Sequence	zg30
7 Number of Scans	8
8 Relaxation Delay	1.0000
9 Pulse Width	8.9200
10 Acquisition Time	3.4079
11 Acquisition Date	2015-03-27T16:48:00
12 Modification Date	2015-03-27T16:48:17

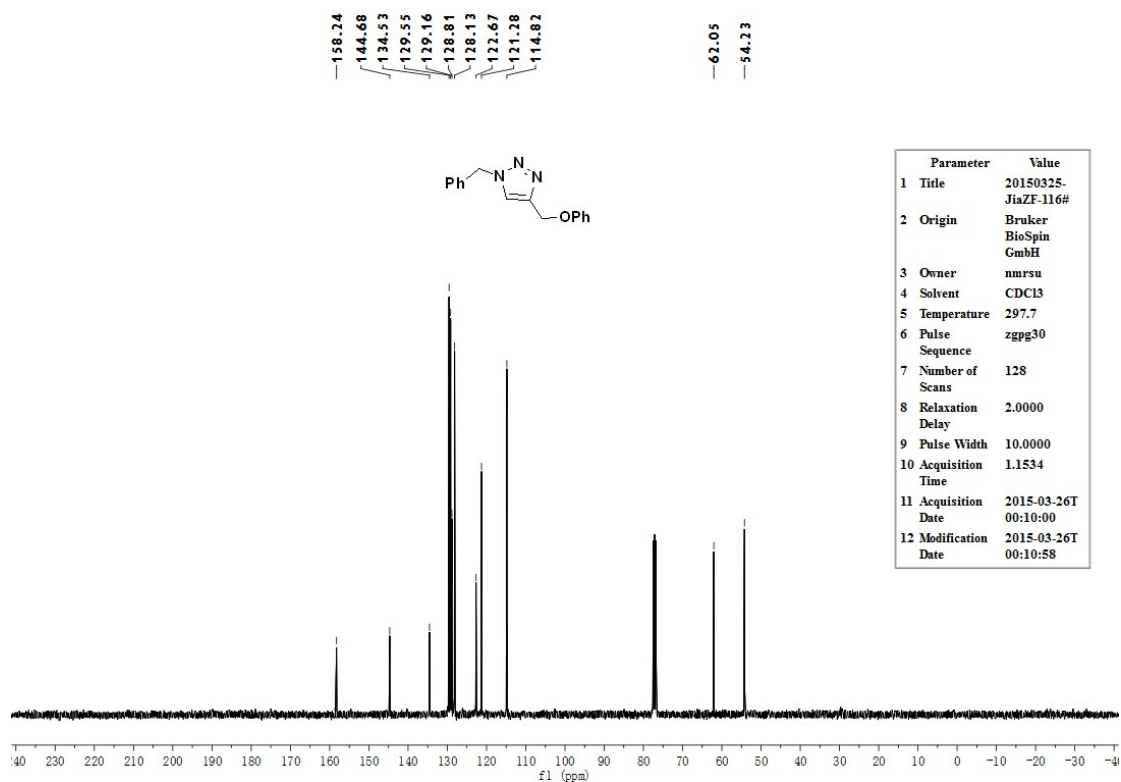
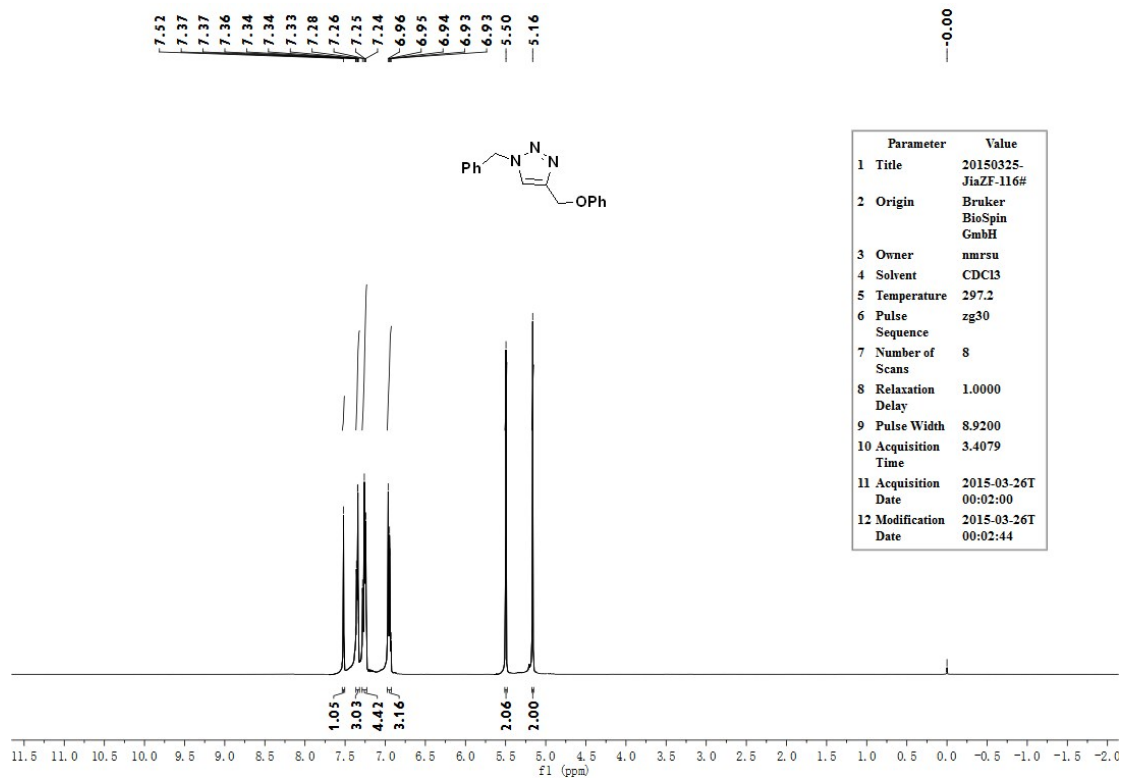


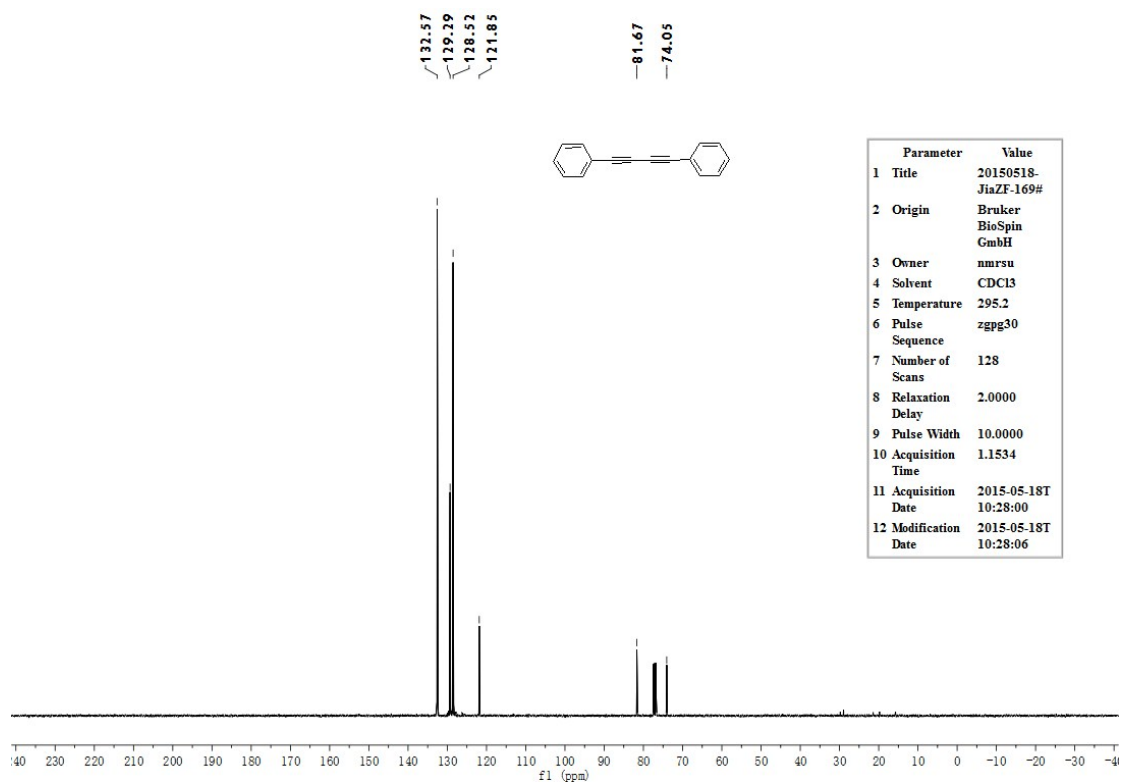
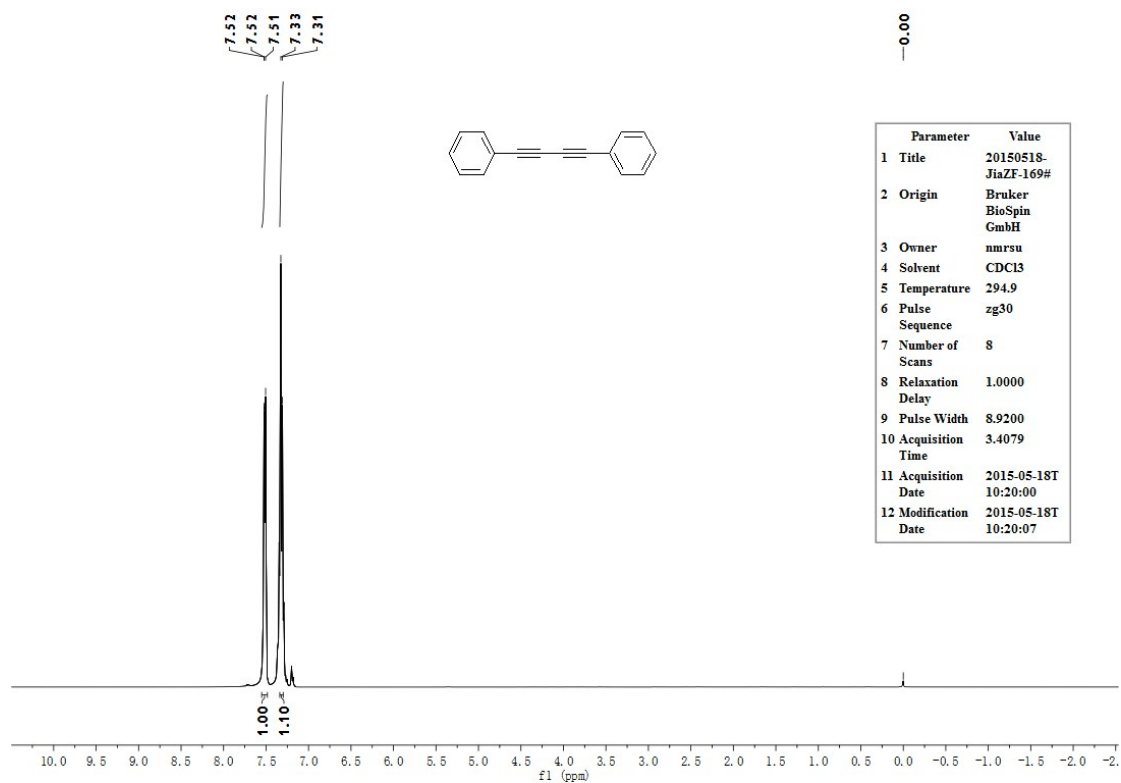
Parameter	Value
1 Title	20150327-JiaZF-119#
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Solvent	CDCl3
5 Temperature	297.3
6 Pulse Sequence	zgpg30
7 Number of Scans	128
8 Relaxation Delay	2.0000
9 Pulse Width	10.0000
10 Acquisition Time	1.1534
11 Acquisition Date	2015-03-27T16:56:00
12 Modification Date	2015-03-27T16:56:13

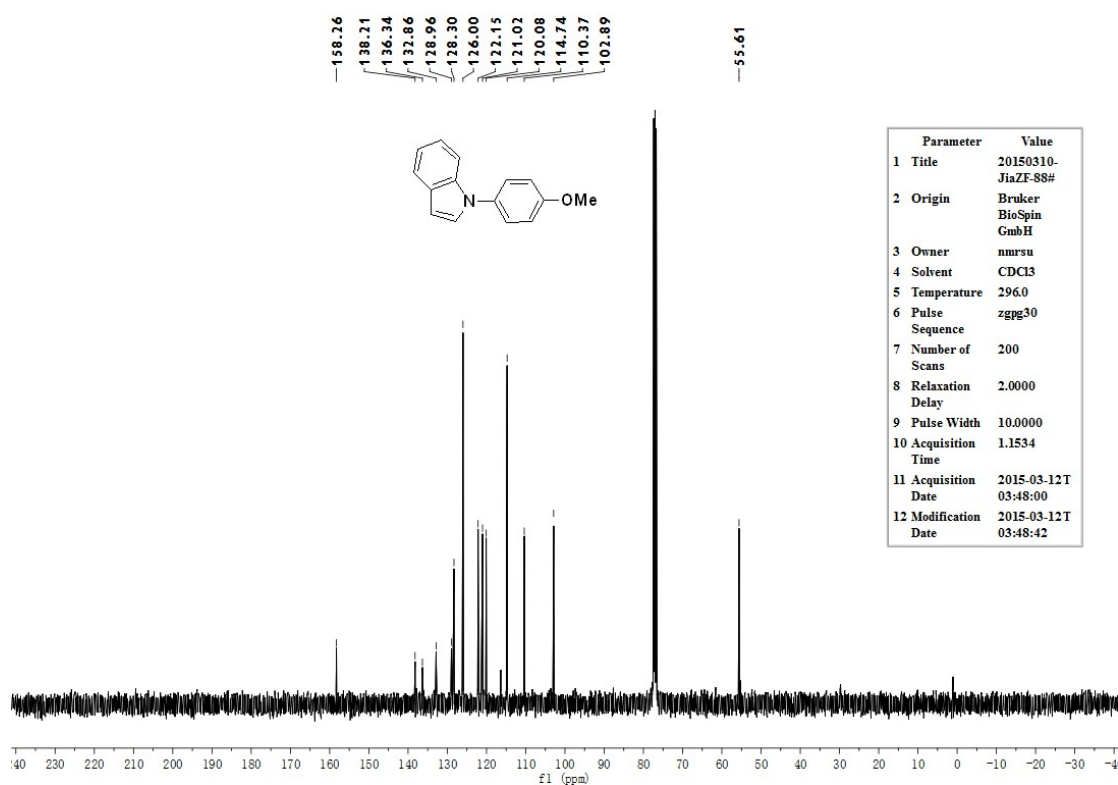
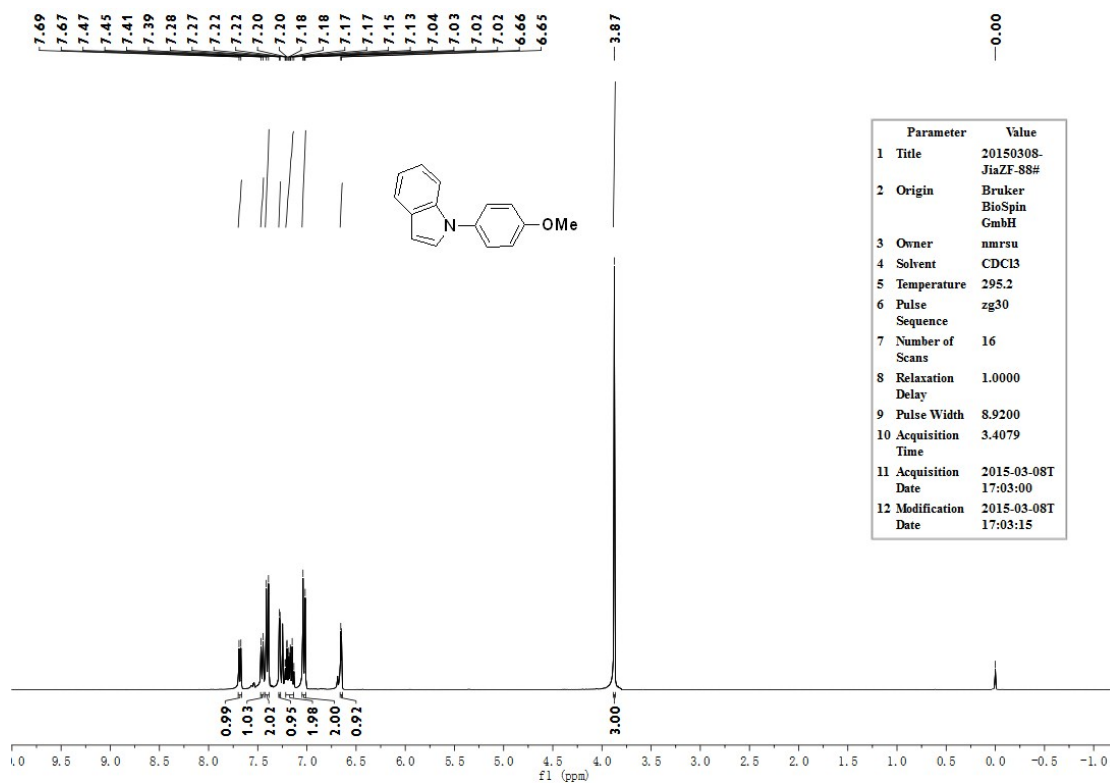












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