Direct Intramolecular Amination of Tryptophan Esters to Prepare Pyrrolo[2,3-b]indoles

Zhao-Ying Yang,† Tian Tian,† Ya-Fei Du,† Shi-Yi Li,† Cen-Cen Chu,† Lu-Ying Chen,† Dan Li,† Jia-Yi Liu,‡ and Bin Wang*,†

*E-mail: wangbin@nankai.edu.cn

†State Key Laboratory of Medicinal Chemical Biology, College of Pharmacy and Tianjin Key Laboratory of Molecular Drug Research, Nankai University, Haihe Education Park, 38 Tongyan Road, Tianjin 300353, People's Republic of China

‡IUT of Limousin 12, road André Maurois 87065 Limoges, France

Supporting Information

Table of Contents Page

1. Experimental Section

(i) General Remarks

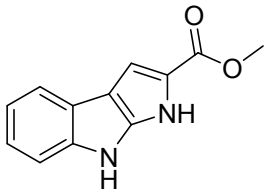
^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker AVANCE AV400 (400MHz for H and 101MHz for C). Signal positions were recorded in ppm with the abbreviations s, d, t, q, and m denoting singlet, doublet, triplet, quartet, and multiplet respectively. All NMR chemical shifts were referenced to residual solvent peaks or to $Si(CH_3)_4$ as an internal standard. NMR Spectra recorded in $CDCl_3$ were referenced to residual $CHCl_3$ at 7.26 ppm for ^{1}H or 77.0 ppm for ^{13}C. NMR spectra recorded in DMSO-d_6 were referenced to residual DMSO at 2.49 ppm and 3.33 ppm for ^{1}H or 39.6 ppm for ^{13}C. All coupling constants *J* were quoted in Hz. Data were reported as follows: chemical shift, multiplicity, coupling constant and integration. HRMS were measured using Q-TOF LC−MS and the ESI-FTICR technique. Reactions were monitored by thin-layer chromatography (TLC) on 0.25mm silica gel glass plates coated with 60 F254. Column chromatography was performed on silica gel (200-300 mesh) using a mixture of petroleum ether (60-90°C) and acetone as eluant. Commercially available reagents were used as received without further purification. Raw materials **1d-m**[1], **1s**[1], **1n-1p**[2], **1q-r**[3], **1t-w**[3] were prepared by the known methods.[1-3]

(ii) General Procedure for the Preparation of Product **2a-w**

Methyl 2-amino-3-(1H-indol-3-yl) propanoate hydrochloride **1a** (0.5 mmol, 130.0 mg, 1 equiv) was added to a mixture of I_2 (0.15 mmol, 38.1 mg, 0.3 equiv) and $Na_2HPO_4 \cdot 12H_2O$ (1.75 mmol, 626.8 mg, 3.5 equiv) under air, and then *tert*-butyl hydroperoxide (0.5 mmol, 68.6 μL, 1 equiv) and 1,4-dioxane (2 mL) were added. After the mixture was stirred at 80°C for 1.5h, the residue was mixed with silica gel and concentrated. The resulting mixture was purified by silica gel column chromatography on silica gel with petroleum ether: acetone (5:1) as eluent to give the desired product methyl 1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate **2a** (94.3mg, 88%).

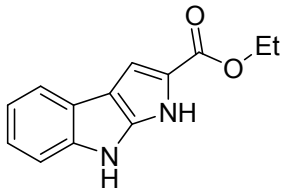
2. The Characterization of Products

methyl 1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2a)



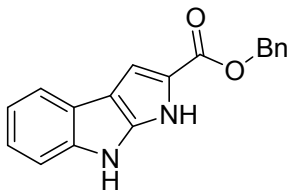
White solid (94.3 mg, 88%). Mp: 248−249 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 11.90 (s, 1H), 11.11 (s, 1H), 7.63 (d, J = 7.6 Hz, 1H), 7.33 (d, J = 7.9 Hz, 1H), 7.14 – 7.08 (m, 2H), 7.02 (t, J = 7.4 Hz, 1H), 3.79 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 162.0, 142.9, 141.8, 121.9, 121.2, 120.1, 119.5, 119.2, 112.2, 109.7, 107.4, 51.3. HRMS (ESI): m/z calcd for $C_{12}H_{11}N_2O_2^+$[M + H]$^+$: 215.0815, found 215.0811.

ethyl 1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2b)



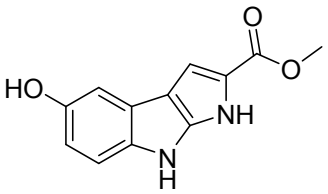
White solid (106.5 mg, 93%). Mp: 181−182 °C. ^{1}H NMR (400 MHz, DMSO-d_6): 11.86 (s, 1H), 11.10 (s, 1H), 7.63 (d, J = 7.6 Hz, 1H), 7.34 (d, J = 7.9 Hz, 1H), 7.13–7.08 (m, 2H), 7.02 (t, J = 7.5 Hz, 1H), 4.26 (q, J = 6.8 Hz, 2H), 1.31 (t, J = 6.9 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 161.6, 142.9, 141.8, 121.8, 121.2, 120.4, 119.4, 119.2, 112.2, 109.6, 107.2, 59.7, 15.0. HRMS (ESI): m/z calcd for $C_{13}H_{13}N_2O_2^+$[M + H]$^+$: 229.0972, found 229.0970.

benzyl 1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2c)



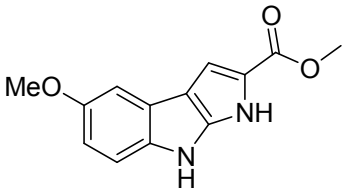
White solid (140.5 mg, 97%). Mp: 163−164 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 11.93 (s, 1H), 11.12 (s, 1H), 7.63 (d, J = 7.7 Hz, 1H), 7.48 (d, J = 7.5 Hz, 2H), 7.41 (t, J = 7.5 Hz, 2H), 7.36–7.33 (m, 2H), 7.20 (s, 1H), 7.10 (t, J = 7.6 Hz, 1H), 7.02 (t, J = 7.4 Hz, 1H), 5.31 (s, 2H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 161.3, 143.1, 141.9, 137.5, 128.9, 128.3, 128.2, 121.9, 121.2, 120.0, 119.5, 119.3, 112.2, 109.8, 107.8, 65.1. HRMS (ESI): m/z calcd for $C_{18}H_{15}N_2O_2^+$[M + H]$^+$: 291.1128, found 291.1131.

methyl 5-hydroxy-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2d)



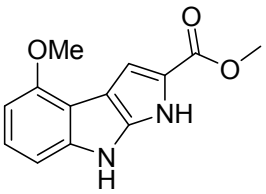
Yellow solid (42.0 mg, 37%). Mp: 243−244 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 11.74 (s, 1H), 10.69 (s, 1H), 8.75 (s, 1H), 7.11–7.07 (m, 2H), 7.00 (s, 1H), 6.59 (d, J = 7.4 Hz, 1H), 3.77 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 162.0, 151.2, 143.8, 135.7, 122.0, 119.7, 112.4, 110.5, 109.8, 107.5, 105.1, 51.2. HRMS (ESI): m/z calcd for $C_{12}H_{11}N_2O_3^+$[M + H]$^+$: 231.0764, found 231.0764.

methyl 5-methoxy-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2e)



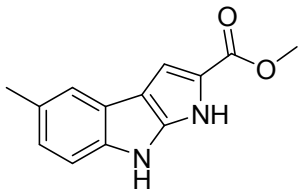
Yellowish solid (50.1 mg, 41%). Mp: 216−217 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 11.80 (s, 1H), 10.84 (s, 1H), 7.21–7.19 (m, 2H), 7.09 (s, 1H), 6.72 (dd, J = 8.8, 2.5 Hz, 1H), 3.78 (s, 3H), 3.77 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 162.0, 153.8, 143.7, 136.5, 129.8, 121.7, 120.0, 112.6, 109.9, 107.4, 103.3, 55.9, 51.3. HRMS (ESI): m/z calcd for $C_{13}H_{13}N_2O_3^+$[M + H]$^+$: 245.0921, found 245.0923.

methyl 4-methoxy-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2f)



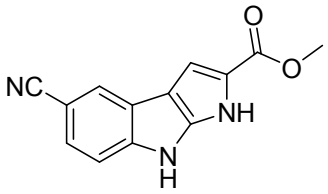
Yellowish solid (71.0 mg, 63%). Mp: 212−213 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 11.90 (s, 1H), 11.14 (s, 1H), 7.06–7.01 (m, 2H), 6.96 (d, J = 8.0 Hz, 1H), 6.61 (d, J = 7.9 Hz, 1H), 3.91 (s, 3H), 3.78 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 162.0, 153.1, 142.8, 141.8, 123.0, 120.0, 110.7, 108.3, 107.7, 105.7, 101.3, 55.7, 51.3. HRMS (ESI): m/z calcd for $C_{13}H_{13}N_2O_3^+$[M + H]$^+$: 245.0921, found 245.0922.

methyl 5-methyl-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2g)



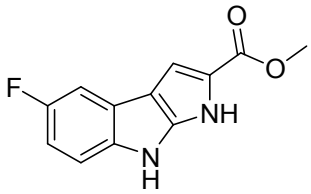
Yellowish solid (85.5 mg, 75%). Mp: 236−237 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 11.85 (s, 1H), 10.96 (s, 1H), 7.42 (s, 1H), 7.21 (d, J = 8.2 Hz, 1H), 7.10 (s, 1H), 6.92 (d, J = 8.2 Hz, 1H), 3.78 (s, 3H), 2.38 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 162.0, 143.3, 140.0, 128.0, 123.0, 121.3, 119.9, 119.4, 111.9, 109.6, 107.3, 51.3, 21.6. HRMS (ESI): m/z calcd for $C_{13}H_{13}N_2O_2^+$[M + H]$^+$: 229.0972, found 229.0975.

methyl 5-cyano-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2h)



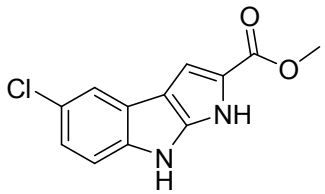
Yellowish solid (55.5 mg, 46%). Mp: 260−261 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 12.21 (s, 1H), 11.85 (s, 1H), 8.14 (s, 1H), 7.49 (s, 2H), 7.21 (s, 1H), 3.81 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 161.9, 143.8, 143.3, 125.2, 123.7, 121.6, 121.2, 113.1, 108.9, 107.5, 101.1, 51.5. HRMS (ESI): m/z calcd for $C_{13}H_{10}N_3O_2^+$[M + H]$^+$: 240.0768, found 240.0768.

methyl 5-fluoro-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2i)



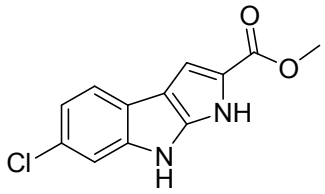
Yellowish solid (70.5 mg, 61%). Mp: 247−248 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 11.95 (s, 1H), 11.18 (s, 1H), 7.43 (dd, J = 9.8, 2.6 Hz, 1H), 7.31–7.27 (m, 1H), 7.13 (s, 1H), 6.92 (td, J = 9.2, 2.7 Hz, 1H), 3.79 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 162.0, 158.4, 156.1, 144.0, 138.2, 121.7, 121.6, 120.6, 112.7, 112.6, 109.6, 109.6, 108.9, 108.7, 107.5, 105.2, 104.9, 51.4. HRMS (ESI): m/z calcd for $C_{12}H_{10}FN_2O_2^+$[M + H]$^+$: 233.0721, found 233.0722.

methyl 5-chloro-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2j)



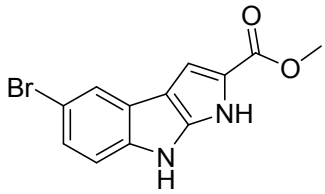
Yellowish solid (90.1 mg, 72%). Mp: 288−289 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 12.01 (s, 1H), 11.33 (s, 1H), 7.70 (s, 1H), 7.34 (d, J = 8.5 Hz, 1H), 7.16 (s, 1H), 7.12 (d, J = 8.4 Hz, 1H), 3.81 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 162.0, 143.5, 140.2, 123.8, 122.4, 121.4, 120.9, 118.7, 113.4, 109.0, 107.5, 51.4. HRMS (ESI): m/z calcd for $C_{12}H_{10}ClN_2O_2^+$[M + H]$^+$: 249.0425, found 249.0420.

methyl 6-chloro-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2k)



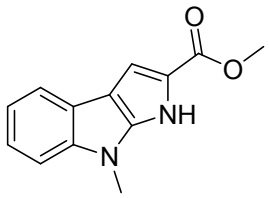
Yellowish solid (79.8 mg, 64%). Mp: 292−293 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 12.05 (s, 1H), 11.37 (s, 1H), 7.66 (d, J = 8.3 Hz, 1H), 7.38 (s, 1H), 7.18 (s, 1H), 7.09 (d, J = 8.4 Hz, 1H), 3.83 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 162.0, 143.1, 142.3, 126.0, 120.7, 120.3, 120.0, 119.4, 111.9, 109.1, 107.3, 51.4. HRMS (ESI): m/z calcd for $C_{12}H_{10}ClN_2O_2^+$[M + H]$^+$: 249.0425, found 249.0427.

methyl 5-bromo-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2l)



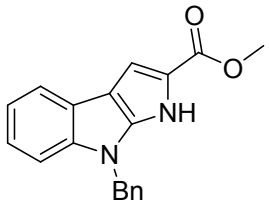
Yellowish solid (130.1 mg, 89%). Mp: 277−278 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 12.03 (s, 1H), 11.37 (s, 1H), 7.83 (s, 1H), 7.29 (d, J = 8.5 Hz, 1H), 7.22 (d, J = 8.6 Hz, 1H), 7.15 (s, 1H), 3.79 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 161.9, 143.3, 140.4, 124.0, 123.0, 121.6, 120.9, 114.0, 111.6, 108.9, 107.5, 51.4. HRMS (ESI): m/z calcd for $C_{12}H_{10}BrN_2O_2^+$[M + H]$^+$: 292.9926, 293,9959, 294.9905, 295.9939, found 292.9920, 293,9953, 294.9901. 295.9937.

methyl 8-methyl-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2m)



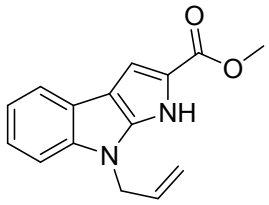
White solid (95.0 mg, 83%). Mp: 256−257 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 12.11 (s, 1H), 7.66 (d, J = 7.4 Hz, 1H), 7.38 (d, J = 8.0 Hz, 1H), 7.20–7.17 (m, 2H), 7.10–7.06 (m, 1H), 3.81 (s, 3H), 3.80 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 162.0, 144.3, 142.2, 121.9, 120.9, 120.3, 119.7, 119.5, 110.1, 108.4, 107.8, 51.4, 30.3. HRMS (ESI): m/z calcd for $C_{13}H_{13}N_2O_2^+$[M + H]$^+$: 229.0972, found 229.0976.

methyl 8-benzyl-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2n)



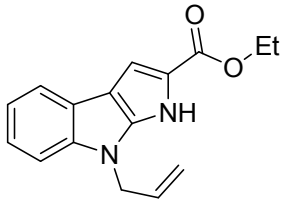
White solid (118.0 mg, 78%). Mp: 244−245 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 12.25 (s, 1H), 7.68 (d, J = 7.5 Hz, 1H), 7.39 (d, J = 8.0 Hz, 1H), 7.30–7.26 (m, 2H), 7.23–7.20 (m, 4H), 7.14–7.05 (m, 2H), 5.55 (s, 2H), 3.80 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 162.0, 143.8, 141.3, 138.0, 129.0, 127.8, 127.4, 122.0, 121.2, 120.6, 119.9, 119.6, 110.8, 108.8, 107.8, 51.4, 46.8. HRMS (ESI): m/z calcd for $C_{19}H_{17}N_2O_2^+$[M + H]$^+$: 305.1285, found 305.1286.

methyl 8-allyl-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2o)



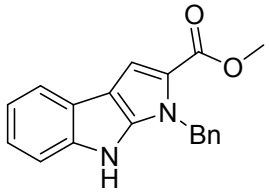
White solid (100.0 mg, 79%). Mp: 224−225 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 12.09 (s, 1H), 7.67 (d, J = 7.6 Hz, 1H), 7.37 (d, J = 8.0 Hz, 1H), 7.18–7.14 (m, 2H), 7.08 (t, J = 7.6 Hz, 1H), 5.99–5.92 (m, 1H), 5.12 (d, J = 10.3 Hz, 1H), 5.02 (d, J = 17.1 Hz, 1H), 4.94 (s, 2H), 3.80 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 162.0, 143.6, 141.4, 133.6, 122.0, 121.1, 120.4, 119.8, 119.6, 117.2, 110.6, 108.6, 107.7, 51.4, 45.8. HRMS (ESI): m/z calcd for $C_{15}H_{15}N_2O_2^+$[M + H]$^+$: 255.1128, found 255.1132.

ethyl 8-allyl-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2p)



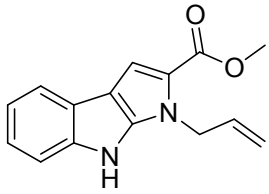
White solid (120.2 mg, 94%). Mp: 176−177 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 12.04 (s, 1H), 7.67 (d, J = 7.6 Hz, 1H), 7.37 (d, J = 8.1 Hz, 1H), 7.17–7.14 (m, 2H), 7.07 (t, J = 7.4 Hz, 1H), 5.99–5.92 (m, 1H), 5.12 (d, J = 10.2 Hz, 1H), 5.00 (d, J = 17.1 Hz, 1H), 4.94 (d, J = 5.2 Hz, 2H), 4.27 (q, J = 7.1 Hz, 2H), 1.32 (t, J = 7.0 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 161.6, 143.5, 141.3, 133.7, 121.9, 121.1, 120.7, 119.8, 119.5, 117.1, 110.6, 108.6, 107.6, 59.8, 45.8, 15.1. HRMS (ESI): m/z calcd for $C_{16}H_{17}N_2O_2^+$[M + H]$^+$: 269.1285, found 269.1285.

methyl 1-benzyl-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2q)



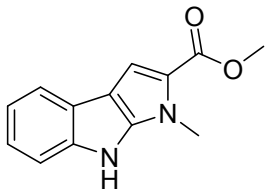
Yellowish solid (60.5 mg, 40%). Mp: 156−157 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 11.53 (s, 1H), 7.71 (d, J = 7.6 Hz, 1H), 7.40 (d, J = 7.9 Hz, 1H), 7.36 (s, 1H), 7.32 (t, J = 7.3 Hz, 2H), 7.26–7.23 (m, 1H), 7.20–7.08 (m, 4H), 5.77 (s, 2H), 3.75 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 162.5, 144.2, 140.8, 136.9, 129.0, 127.8, 126.9, 122.3, 121.8, 120.6, 120.3, 119.6, 111.7, 110.0, 108.9, 51.1, 49.3. HRMS (ESI): m/z calcd for $C_{19}H_{17}N_2O_2^+$[M + H]$^+$: 305.1285, found 305.1289.

methyl 1-allyl-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2r)



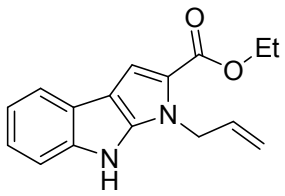
Yellowish solid (30.0 mg, 24%). Mp: 133−134 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.92 (s, 1H), 7.71–7.69 (m, 1H), 7.34 (s, 1H), 7.30–7.28 (m, 1H), 7.20–7.16 (m, 2H), 6.07–6.00 (m, 1H), 5.20 (d, J = 10.3 Hz, 1H), 5.14 (d, J = 5.2 Hz, 2H), 5.06 (d, J = 17.1 Hz, 1H), 3.84 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 162.5, 144.2, 140.9, 133.5, 122.3, 121.9, 120.6, 120.0, 119.6, 117.1, 111.7, 109.7, 108.8, 51.1, 48.2. HRMS (ESI): m/z calcd for $C_{15}H_{15}N_2O_2^+$[M + H]$^+$: 255.1128, found 255.1132.

methyl 1-methyl-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2s)



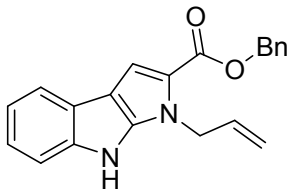
White solid (20.0 mg, 18%). Mp: 195−196 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 11.42 (s, 1H), 7.65 (d, J = 7.6 Hz, 1H), 7.38 (d, J = 7.9 Hz, 1H), 7.23 (s, 1H), 7.14 (t, J = 7.6 Hz, 1H), 7.06 (t, J = 7.5 Hz, 1H), 3.98 (s, 3H), 3.76 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 162.0, 145.5, 141.4, 122.2, 121.4, 120.0, 119.8, 119.5, 112.2, 109.0, 107.4, 51.1, 33.5. HRMS (ESI): m/z calcd for $C_{13}H_{13}N_2O_2^+$[M + H]$^+$: 229.0972, found 229.0970.

ethyl 1-allyl-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2t)



Yellowish solid (39.0 mg, 29%). Mp: 97−98 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.95 (s, 1H), 7.70–7.68 (m, 1H), 7.37 (s, 1H), 7.30–7.28 (m, 1H), 7.19–7.14 (m, 2H), 6.08 –5.98 (m, 1H), 5.19 (d, J = 10.3 Hz, 1H), 5.13 (d, J = 5.1 Hz, 2H), 5.05 (d, J = 17.1 Hz, 1H), 4.30 (q, J = 7.1 Hz, 2H), 1.37 (t, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 162.2, 144.1, 140.9, 133.5, 122.2, 121.9, 120.6, 120.3, 119.5, 117.0, 111.7, 109.7, 108.7, 59.8, 48.2, 14.6. HRMS (ESI): m/z calcd for $C_{16}H_{17}N_2O_2^+$[M + H]$^+$: 269.1285, found 269.1287.

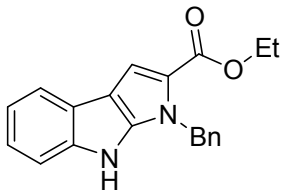
benzyl 1-allyl-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2u)



Yellowish solid (44.9 mg, 27%). Mp: 111−112 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.86 (s, 1H), 7.69–7.66 (m, 1H), 7.44–7.41 (m, 3H), 7.37 (t, J = 7.2 Hz, 2H), 7.32 (d, J = 7.2 Hz, 1H), 7.29–7.26 (m, 1H), 7.19–7.13 (m, 2H), 6.05–5.98 (m, 1H), 5.30 (s, 2H), 5.19 (d, J = 10.3 Hz, 1H), 5.11 (d, J = 4.9 Hz, 2H), 5.04 (d, J = 17.1 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 161.8, 144.3, 140.9, 136.8, 133.4, 128.6, 128.1, 128.0,

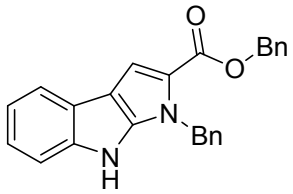
122.4, 121.8, 120.7, 119.9, 119.6, 117.2, 111.8, 110.1, 108.9, 65.5, 48.2. HRMS (ESI): m/z calcd for $C_{21}H_{19}N_2O_2^+[M + H]^+$: 331.1441, found 331.1441.

ethyl 1-benzyl-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2v)



Yellowish solid (61.9 mg, 39%). Mp: 167−168 °C. ^{1}H NMR (400 MHz, DMSO-*d6*): δ 11.51 (s, 1H), 7.70 (d, J = 7.6 Hz, 1H), 7.39 (d, J = 7.9 Hz, 1H), 7.35 (s, 1H), 7.30 (t, J = 7.4 Hz, 2H), 7.25–7.21 (m, 1H), 7.18–7.07 (m, 4H), 5.76 (s, 2H), 4.20 (q, J = 7.1 Hz, 2H), 1.26 (t, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 162.2, 144.2, 140.8, 137.1, 128.9, 127.8, 126.9, 122.2, 121.8, 120.6, 120.5, 119.5, 111.7, 109.9, 108.8, 59.8, 49.3, 14.5. HRMS (ESI): m/z calcd for $C_{20}H_{19}N_2O_2^+[M + H]^+$: 319.1441, found 319.1442.

benzyl 1-benzyl-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2w)



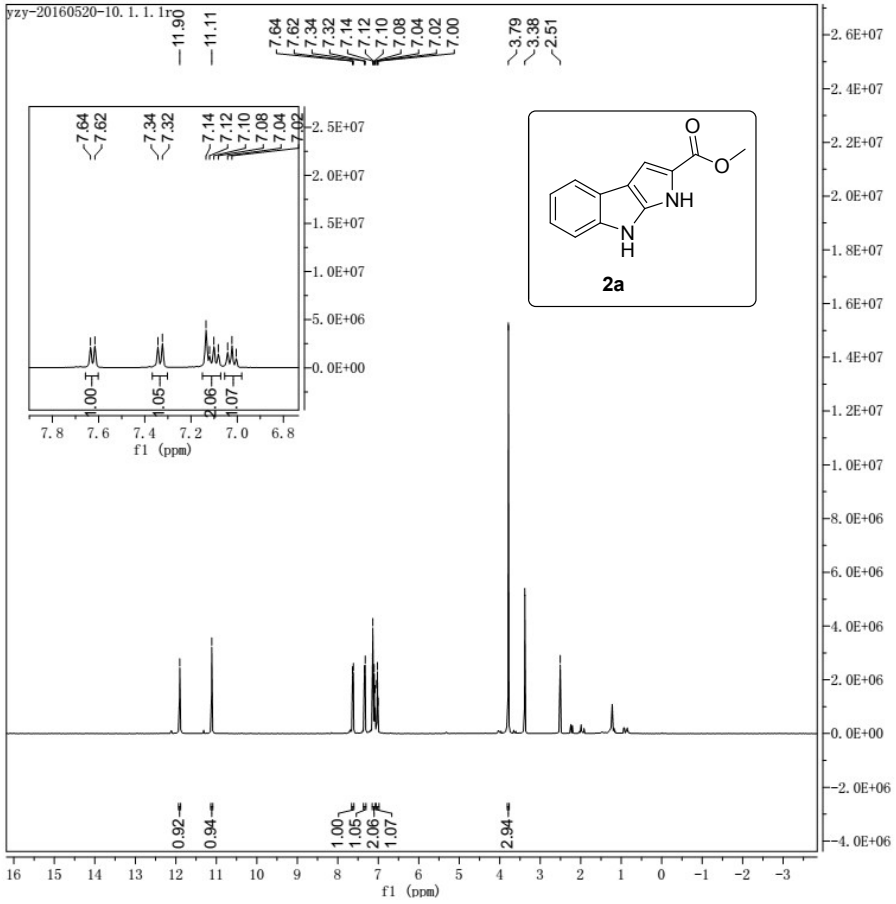
Yellowish solid (67.5 mg, 36%). Mp: 153−154 °C.^{1}H NMR (400 MHz, DMSO-d_6): δ 11.56 (s, 1H), 7.72 (d, *J* = 7.6 Hz, 1H), 7.44–7.35 (m, 7H), 7.33–7.30 (m, 2H), 7.27–7.24 (m, 1H), 7.15–7.08 (m, 4H), 5.78 (s, 2H), 5.27 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 161.8, 144.3, 140.9, 136.9, 136.7, 129.0, 128.6, 128.0, 128.0, 127.9, 127.0, 122.3, 121.8, 120.6, 120.3, 119.6, 111.7, 110.3, 109.0, 65.5, 49.4. HRMS (ESI): m/z calcd for $C_{25}H_{21}N_2O_2^+[M + H]^+$: 381.1598, found 381.1597.

3. References

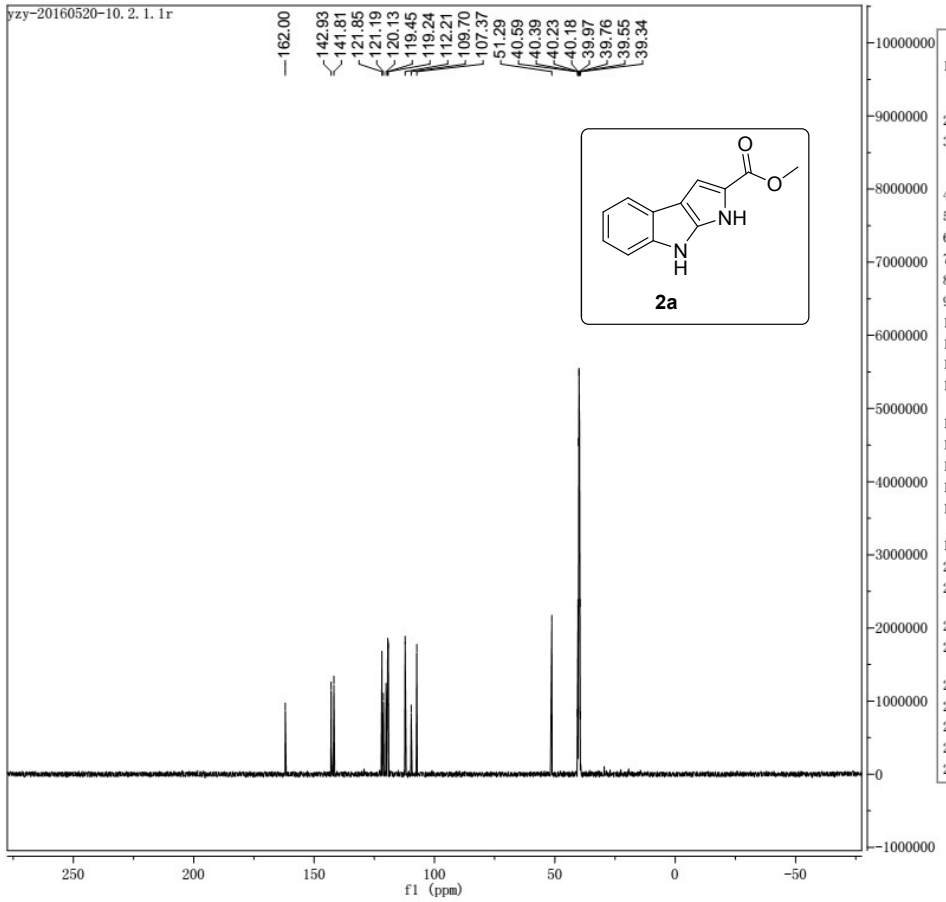
1. Chiotellis, A.; Muller, A.; Mu, L.; Keller, C.; Schibli, R.; Krämer, S. D.; Ametamey, S. M. *Mol. Pharmaceutics* **2014,** *11*, 3839.
2. Benson, S. C.; Lee, L.; Yang, L.; Snyder, J. K. *Tetrahedron* **2000,** *56*, 1165.
3. Kumaraswamy, G.; Pitchaiah, A.; Ramakrishna, G.; Ramakrishna, D. S.; Sadaiah, K. *Tetrahedron Lett.* **2006,** *47*, 2013.

4. NMR and HRMS Spectra

^{1}H，^{13}C NMR and MS spectra for products 2.
methyl 1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2a)

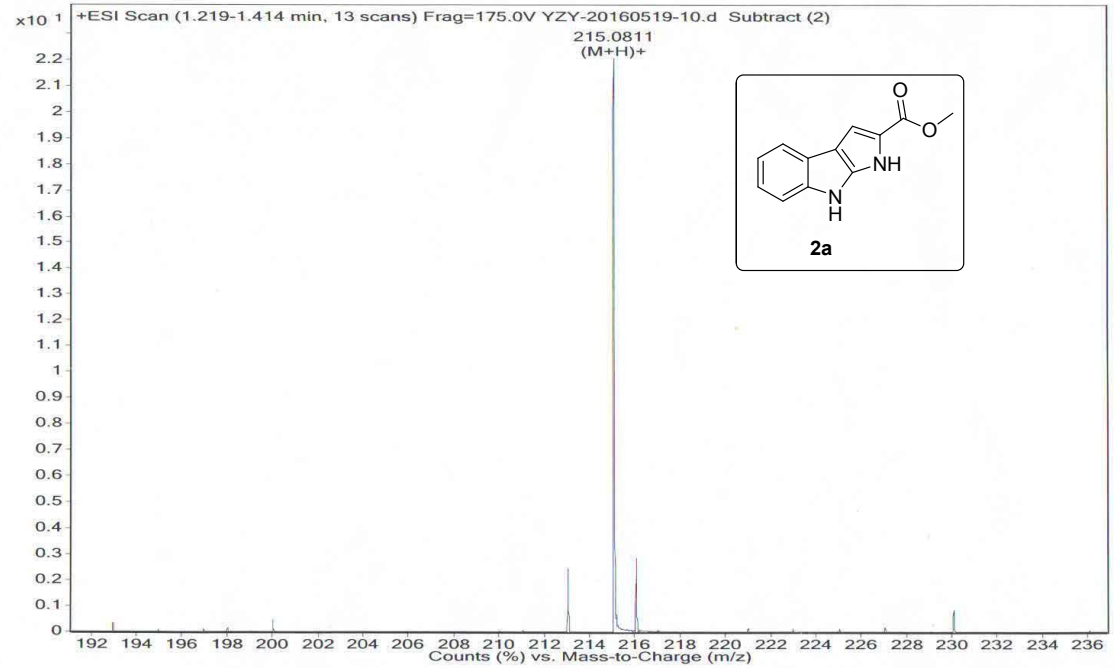


	Parameter	Value
1	Data File Name	E:/ 杨钊英 核磁数据/ 我的课题C-N键偶联/ 主产物谱图/ 1/ pdata/ 1/ 1r
2	Title	yzy-20160520-10.1.1.1r
3	Comment	PROTON DMSO {D:\ NMR_DATA\ Wangbin} Wangbin 1
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	294.5
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	16
15	Receiver Gain	113
16	Relaxation Delay	1.0000
17	Pulse Width	14.4000
18	Presaturation Frequency	
19	Acquisition Time	4.0894
20	Acquisition Date	2016-05-22T13:02:00
21	Modification Date	2016-05-22T13:02:02
22	Class	
23	Spectrometer Frequency	400.13
24	Spectral Width	8012.8
25	Lowest Frequency	-1537.1
26	Nucleus	1H
27	Acquired Size	32768
28	Spectral Size	65536

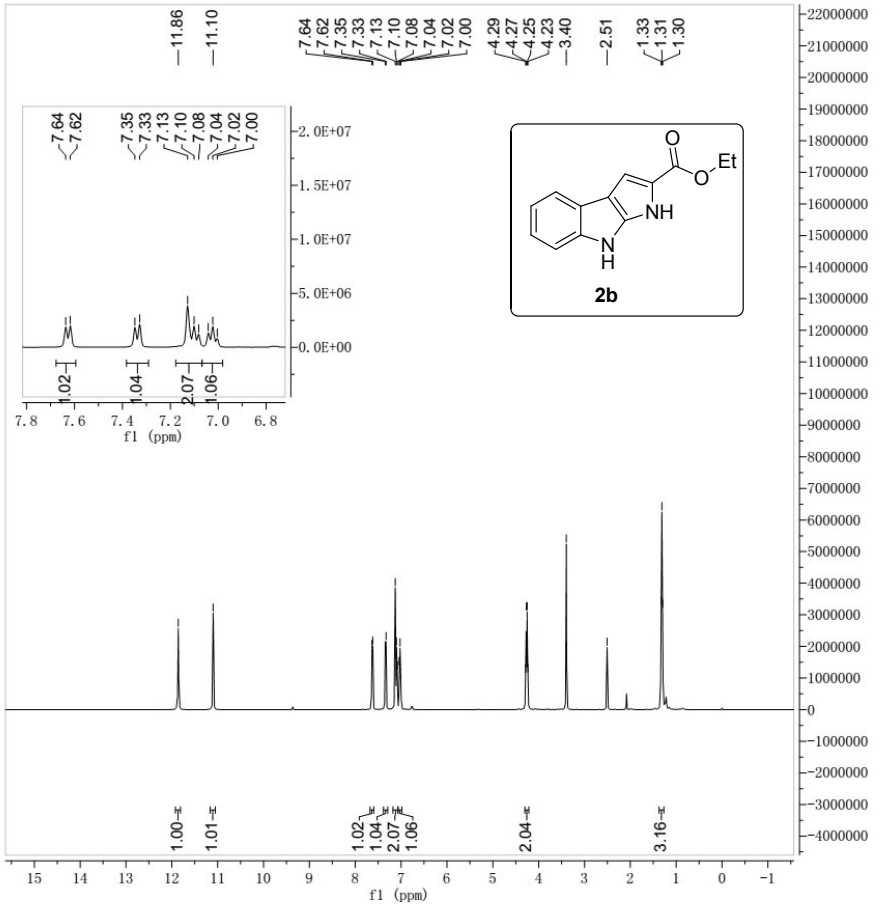


	Parameter	Value
1	Data File Name	E:/ 杨钊英 核磁数据/ 我的课题C-N键偶联/ 主产物谱图/ 2/ pdata/ 1/ 1r
2	Title	yzy-20160520-10.2.1.1r
3	Comment	C13CPD DMSO {D:\ NMR_DATA\ Wangbin} Wangbin 1
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	295.7
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	1024
15	Receiver Gain	113
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	0.4999
20	Acquisition Date	2016-05-22T13:30:00
21	Modification Date	2016-05-22T13:29:42
22	Class	
23	Spectrometer Frequency	100.61
24	Spectral Width	35714.3
25	Lowest Frequency	-7796.8
26	Nucleus	13C
27	Acquired Size	17855
28	Spectral Size	32768

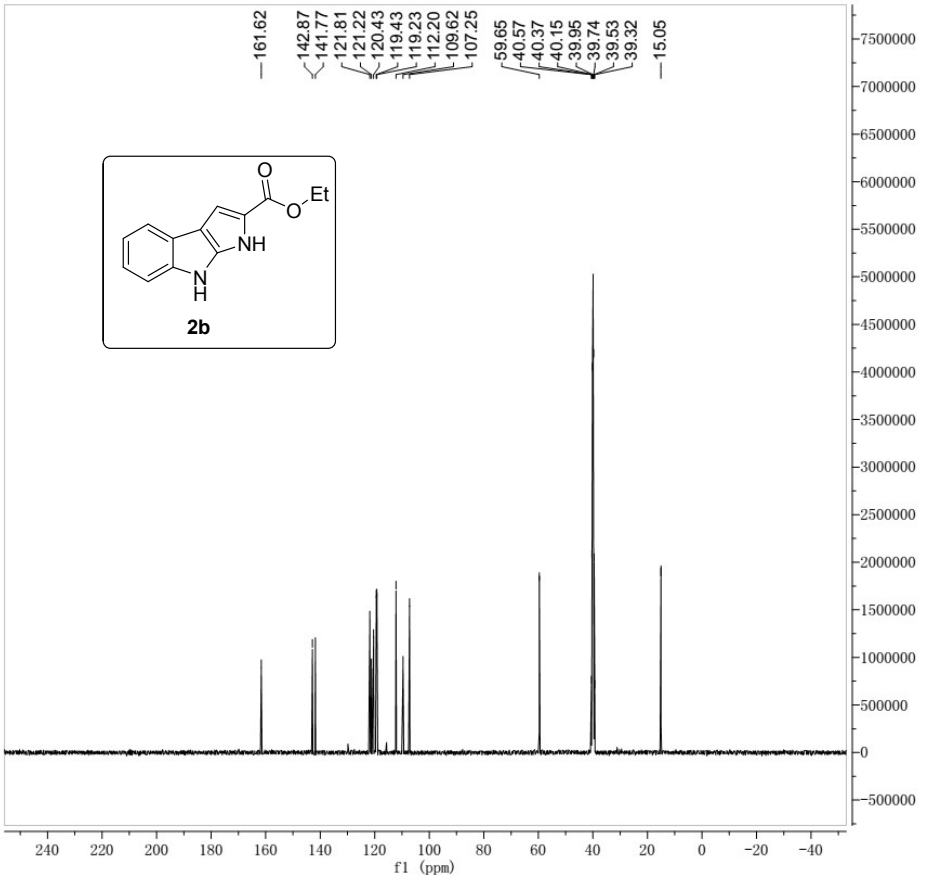
Sample Name	Sample9	**Position**	P1-A9	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YZY-20160519-10.d	**ACQ Method**	chen-ms.m	**Comment**		**Acquired Time**	6/14/2016 10:35:44 AM



ethyl 1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2b)

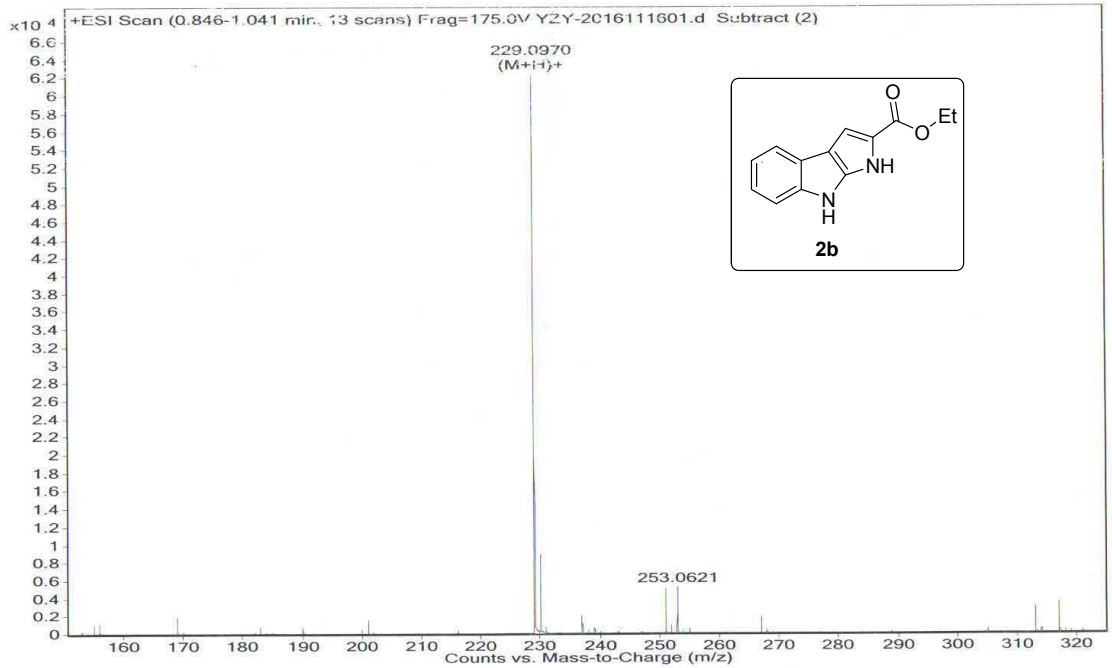


Parameter	Value
1 Data File Name	E:/ 杨钊英 核磁数据/ 色氨酸乙酯盐酸盐产物/ 1/ pdata/ 1/ 1r
2 Title	yzy-20161020-3.1.1.1r
3 Comment	PROTON DMSO {D:\ NMR_DATA\ Wangbin} Wangbin 12
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	292.4
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	88
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2016-10-20T10:10:00
21 Modification Date	2016-10-20T10:07:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1536.7
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

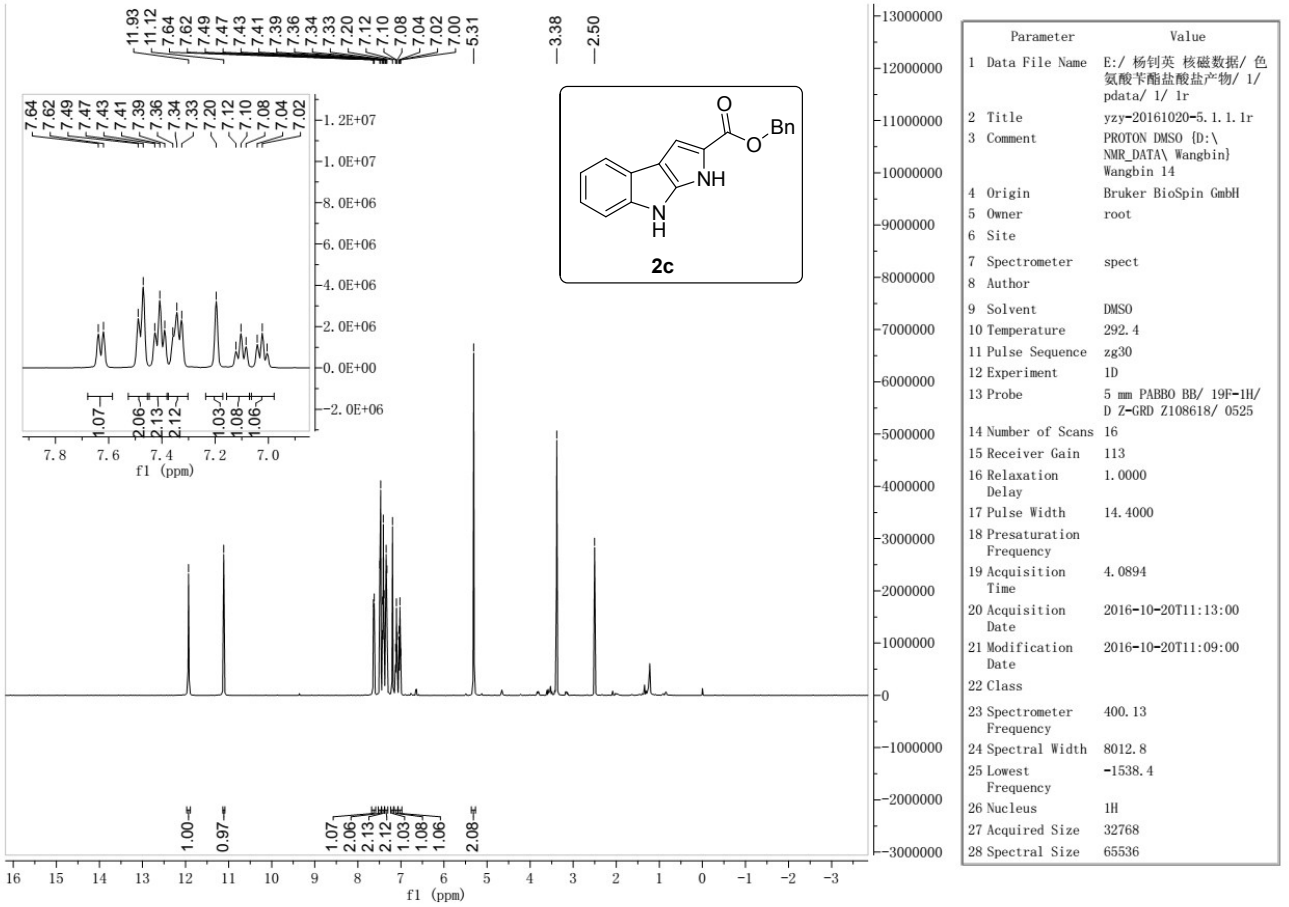


	Parameter	Value
1	Data File Name	E:/ 杨钊英 核磁数据/ 色氨酸乙酯盐酸盐产物/ 2/ pdata/ 1/ 1r
2	Title	yzy-20161020-3.2.1.1r
3	Comment	C13CPD DMSO {D:\ NMR_DATA\ Wangbin} Wangbin 12
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	293.3
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	1024
15	Receiver Gain	78
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	0.4999
20	Acquisition Date	2016-10-20T10:38:00
21	Modification Date	2016-10-20T10:34:00
22	Class	
23	Spectrometer Frequency	100.61
24	Spectral Width	35714.3
25	Lowest Frequency	-7796.8
26	Nucleus	13C
27	Acquired Size	17855
28	Spectral Size	32768

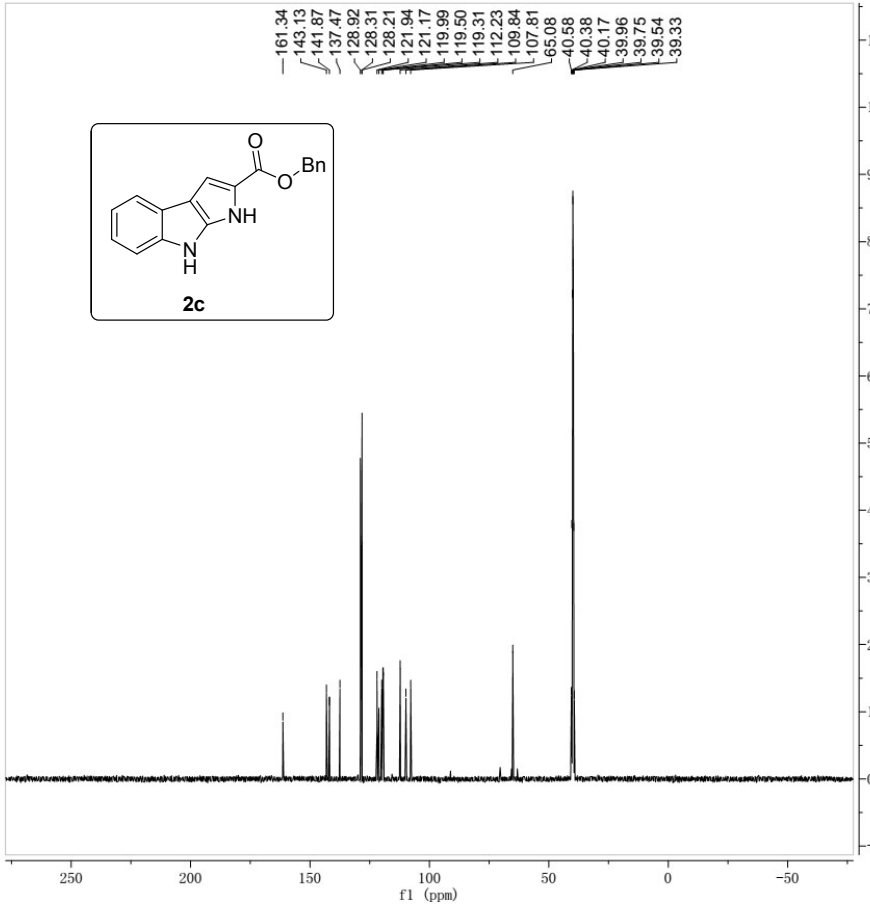
Sample Name	Sample1	**Position**	P1-A1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YZY-2016111601.d	**ACQ Method**	chen-ms.m	**Comment**		**Acquired Time**	11/16/2016 4:46:16 PM



benzyl 1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2c)

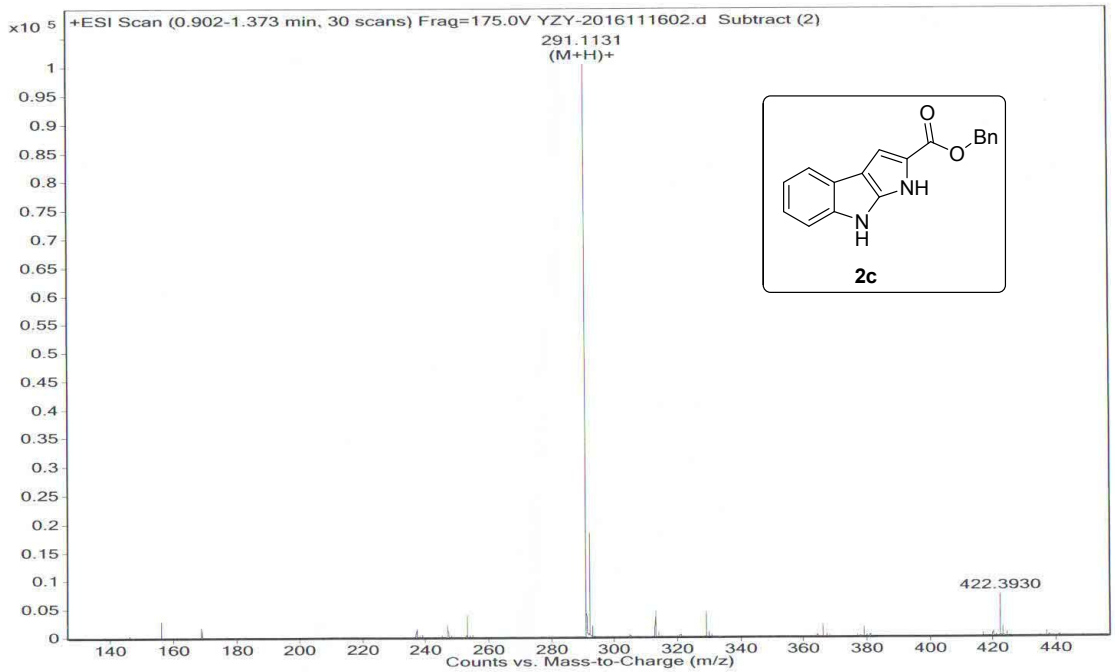


	Parameter	Value
1	Data File Name	E:/ 杨钊英 核磁数据/ 色氨酸苄酯盐酸盐产物/ 1/ pdata/ 1/ 1r
2	Title	yzy-20161020-5.1.1.1r
3	Comment	PROTON DMSO {D:\ NMR_DATA\ Wangbin} Wangbin 14
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	292.4
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	16
15	Receiver Gain	113
16	Relaxation Delay	1.0000
17	Pulse Width	14.4000
18	Presaturation Frequency	
19	Acquisition Time	4.0894
20	Acquisition Date	2016-10-20T11:13:00
21	Modification Date	2016-10-20T11:09:00
22	Class	
23	Spectrometer Frequency	400.13
24	Spectral Width	8012.8
25	Lowest Frequency	-1538.4
26	Nucleus	1H
27	Acquired Size	32768
28	Spectral Size	65536

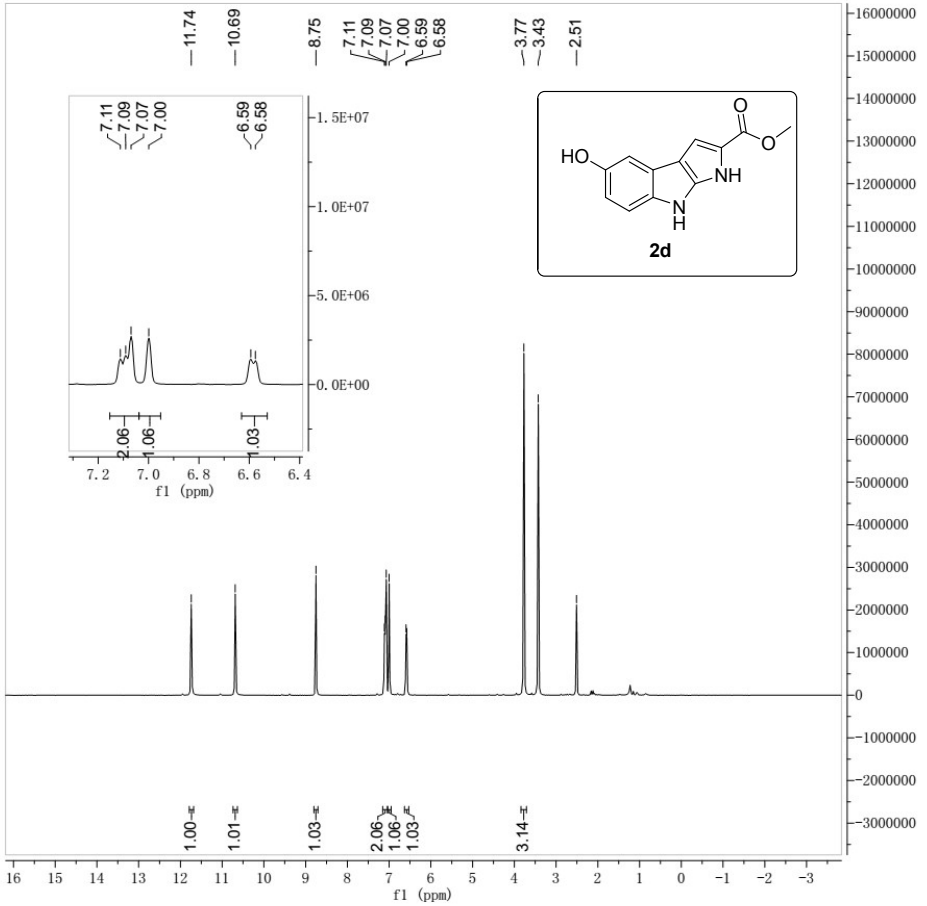


	Parameter	Value
1	Data File Name	E:/ 杨钊英 核磁数据/ 色氨酸苄酯盐酸盐产物/ 2/ pdata/ 1/ 1r
2	Title	yzy-20161020-5.2.1.1r
3	Comment	C13CPD DMSO {D:\ NMR_DATA\ Wangbin} Wangbin 14
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	293.3
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	1024
15	Receiver Gain	133
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	0.4999
20	Acquisition Date	2016-10-20T11:40:00
21	Modification Date	2016-10-20T11:37:00
22	Class	
23	Spectrometer Frequency	100.61
24	Spectral Width	35714.3
25	Lowest Frequency	-7796.8
26	Nucleus	13C
27	Acquired Size	17855
28	Spectral Size	32768

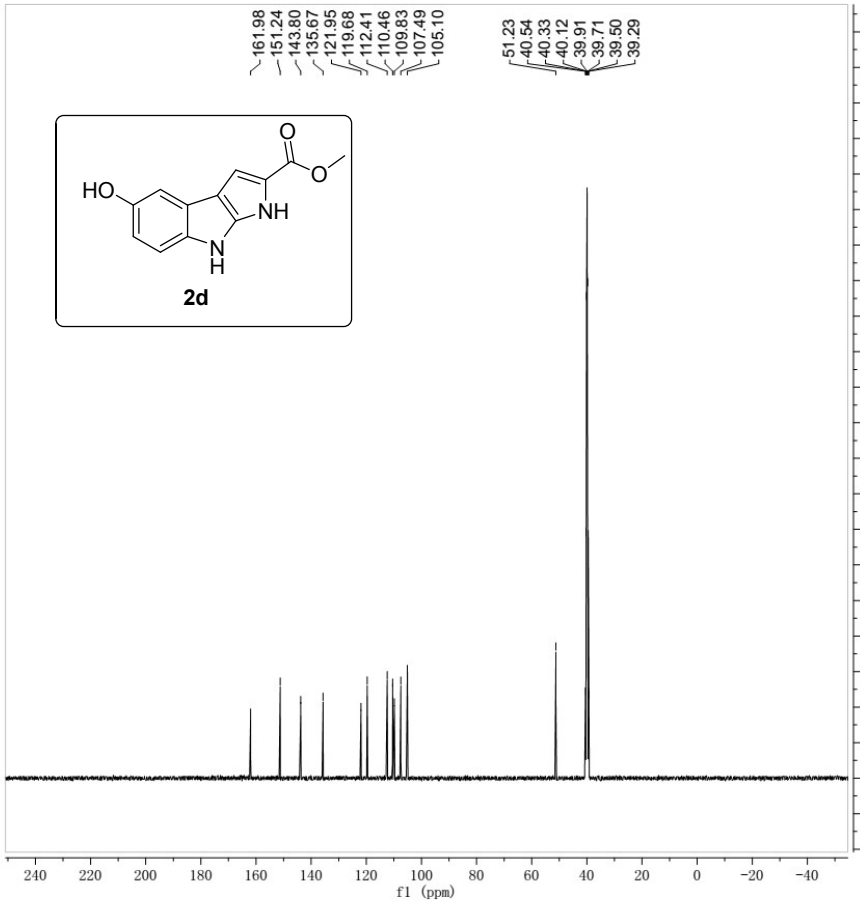
Sample Name	Sample2	**Position**	P1-A2	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YZY-2016111602.d	**ACQ Method**	chen-ms.m	**Comment**		**Acquired Time**	11/16/2016 4:51:56 PM



methyl 5-hydroxy-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2d)

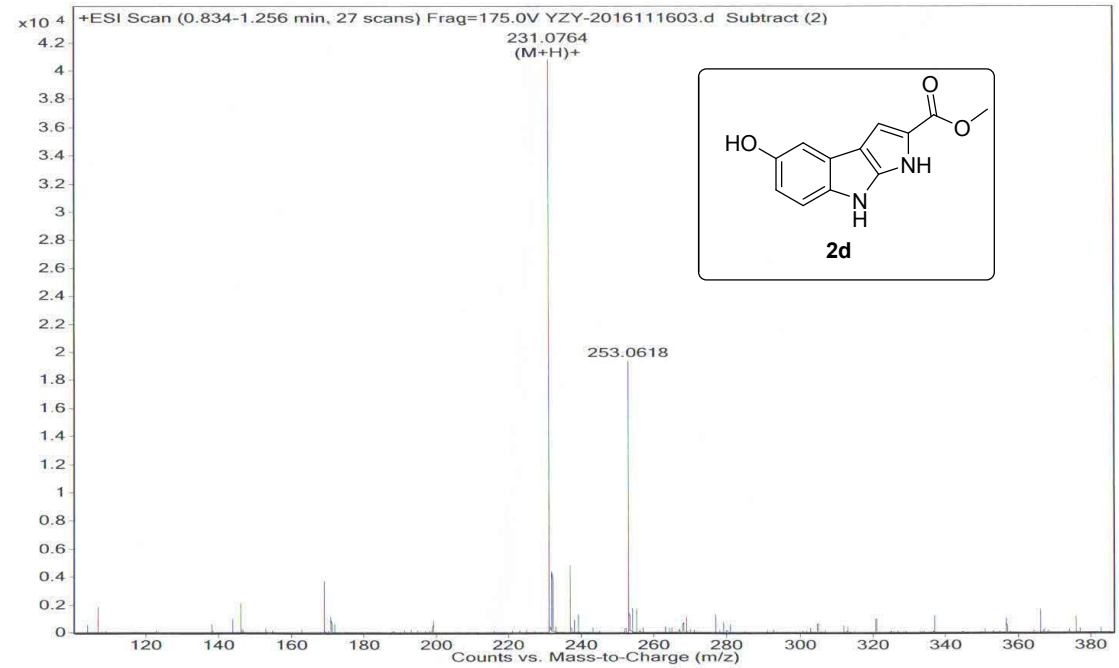


	Parameter	Value
1	Data File Name	E:/ 杨钊英 核磁数据/ yzy-20161026-1/ 1/ pdata/ 1/ 1r
2	Title	yzy-20161026-1.1.1.1r
3	Comment	PROTON DMSO {D:\ NMR_DATA\ Wangbin} Wangbin 19
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	291.2
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	16
15	Receiver Gain	100
16	Relaxation Delay	1.0000
17	Pulse Width	14.4000
18	Presaturation Frequency	
19	Acquisition Time	4.0894
20	Acquisition Date	2016-10-26T21:38:00
21	Modification Date	2016-10-26T21:34:00
22	Class	
23	Spectrometer Frequency	400.13
24	Spectral Width	8012.8
25	Lowest Frequency	-1535.4
26	Nucleus	1H
27	Acquired Size	32768
28	Spectral Size	65536

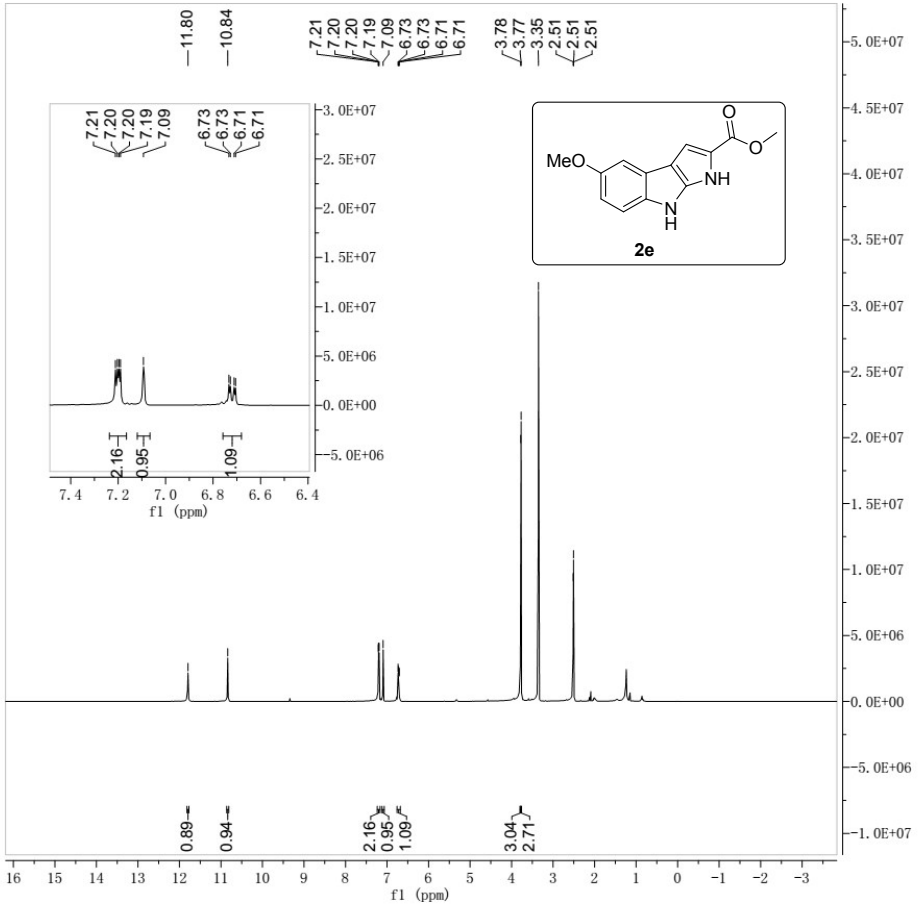


	Parameter	Value
1	Data File Name	E:/ 杨钊英 核磁数据/ yzy-20161026-1/ 2/ pdata/ 1/ 1r
2	Title	yzy-20161026-1.2.1.1r
3	Comment	C13CPD DMSO {D:\ NMR_DATA\ Wangbin} Wangbin 19
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	291.7
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	1024
15	Receiver Gain	200
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	0.4999
20	Acquisition Date	2016-10-26T22:06:00
21	Modification Date	2016-10-26T22:02:00
22	Class	
23	Spectrometer Frequency	100.61
24	Spectral Width	35714.3
25	Lowest Frequency	-7796.8
26	Nucleus	13C
27	Acquired Size	17855
28	Spectral Size	32768

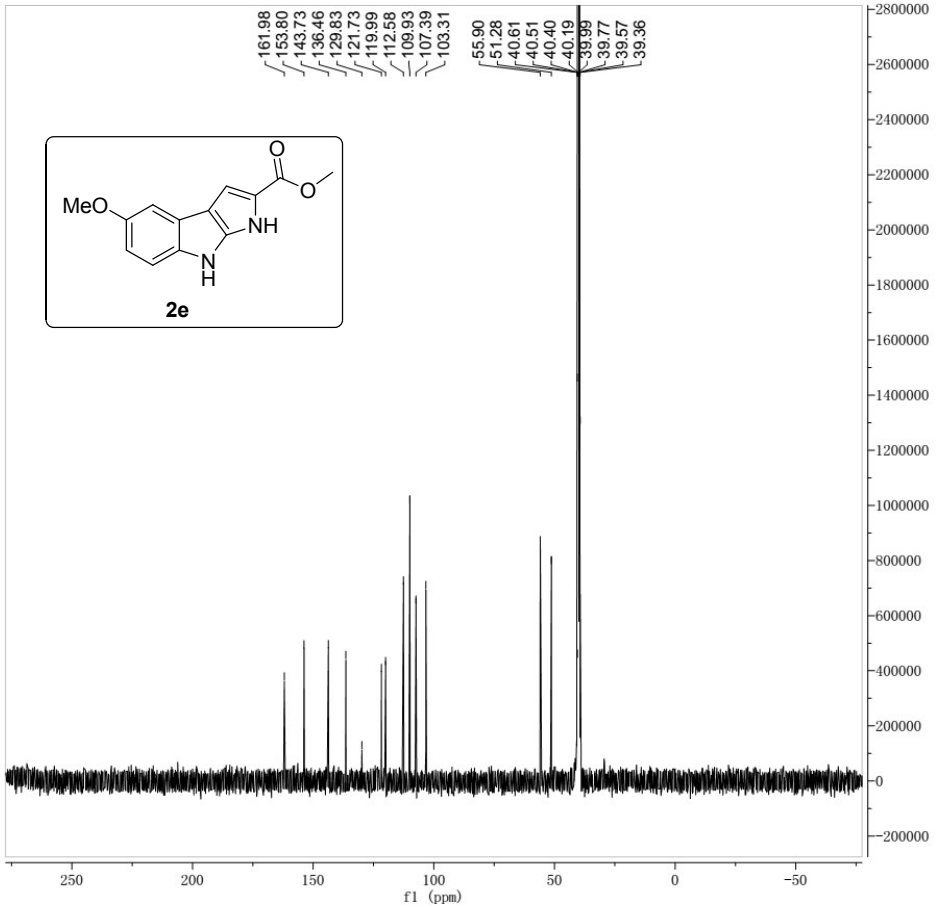
Sample Name	Sample3	**Position**	P1-A3	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YZY-2016111603.d	**ACQ Method**	chen-ms.m	**Comment**		**Acquired Time**	11/16/2016 4:57:37 PM



methyl 5-methoxy-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2e)

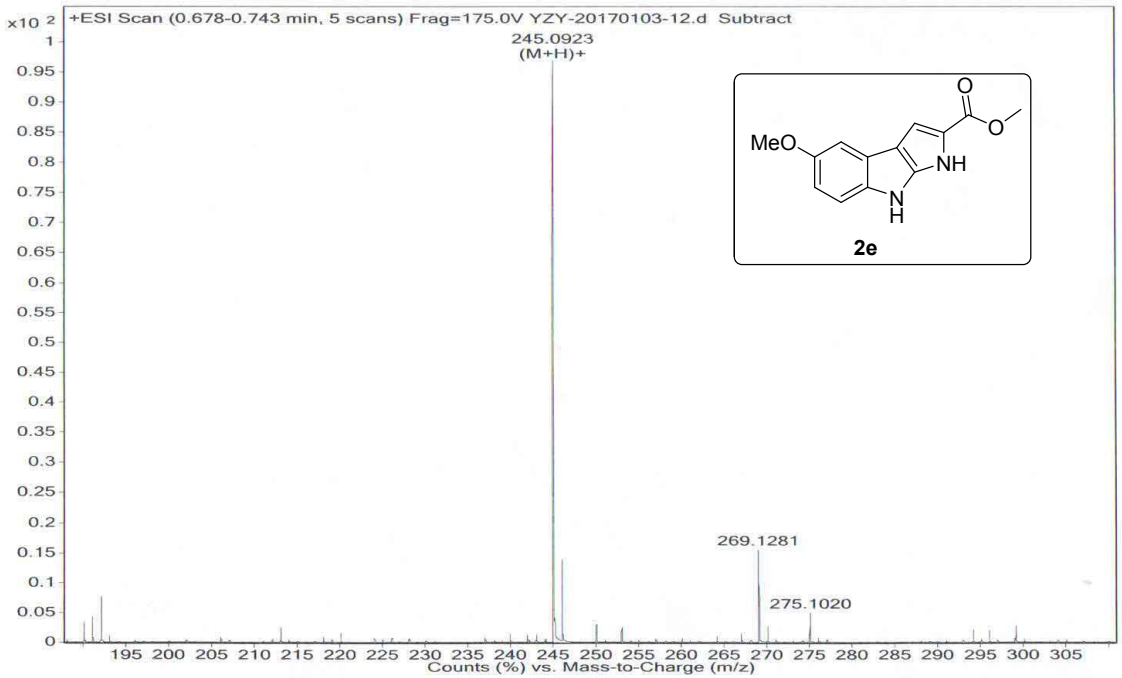


	Parameter	Value
1	Data File Name	E:/ yzy-20170112-3/ 1/ pdata/ 1/ 1r
2	Title	yzy-20170112-3.1.1.1r
3	Comment	PROTON DMSO {D:\ NMR_DATA\ Wangbin} Wangbin 3
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	294.8
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	48
15	Receiver Gain	159
16	Relaxation Delay	1.0000
17	Pulse Width	14.4000
18	Presaturation Frequency	
19	Acquisition Time	4.0894
20	Acquisition Date	2017-01-12T16:54:00
21	Modification Date	2017-01-12T16:50:00
22	Class	
23	Spectrometer Frequency	400.13
24	Spectral Width	8012.8
25	Lowest Frequency	-1535.4
26	Nucleus	1H
27	Acquired Size	32768
28	Spectral Size	65536

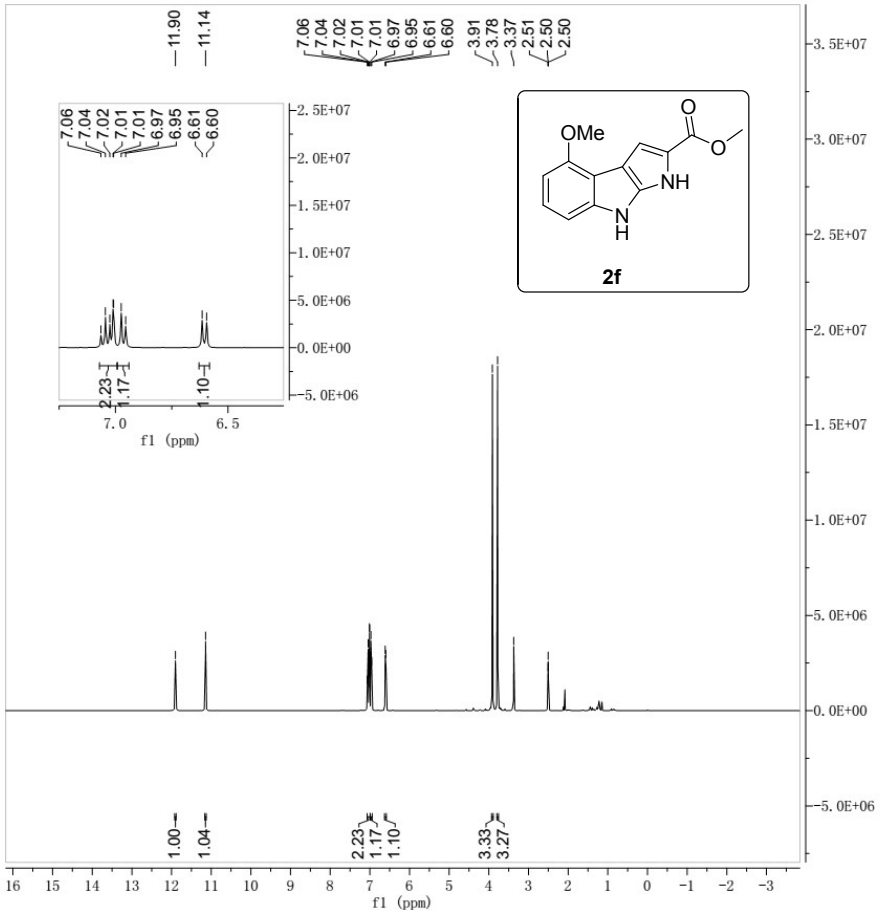


	Parameter	Value
1	Data File Name	E:/ yzy-20170112-3/ 2/ pdata/ 1/ 1r
2	Title	yzy-20170113-1.1.1.1r
3	Comment	C13CPD DMSO {D:\ NMR_DATA\ Wangbin} Wangbin 21
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	296.1
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	1800
15	Receiver Gain	113
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	0.4999
20	Acquisition Date	2017-01-13T10:23:00
21	Modification Date	2017-01-13T10:19:00
22	Class	
23	Spectrometer Frequency	100.61
24	Spectral Width	35714.3
25	Lowest Frequency	-7796.8
26	Nucleus	13C
27	Acquired Size	17855
28	Spectral Size	32768

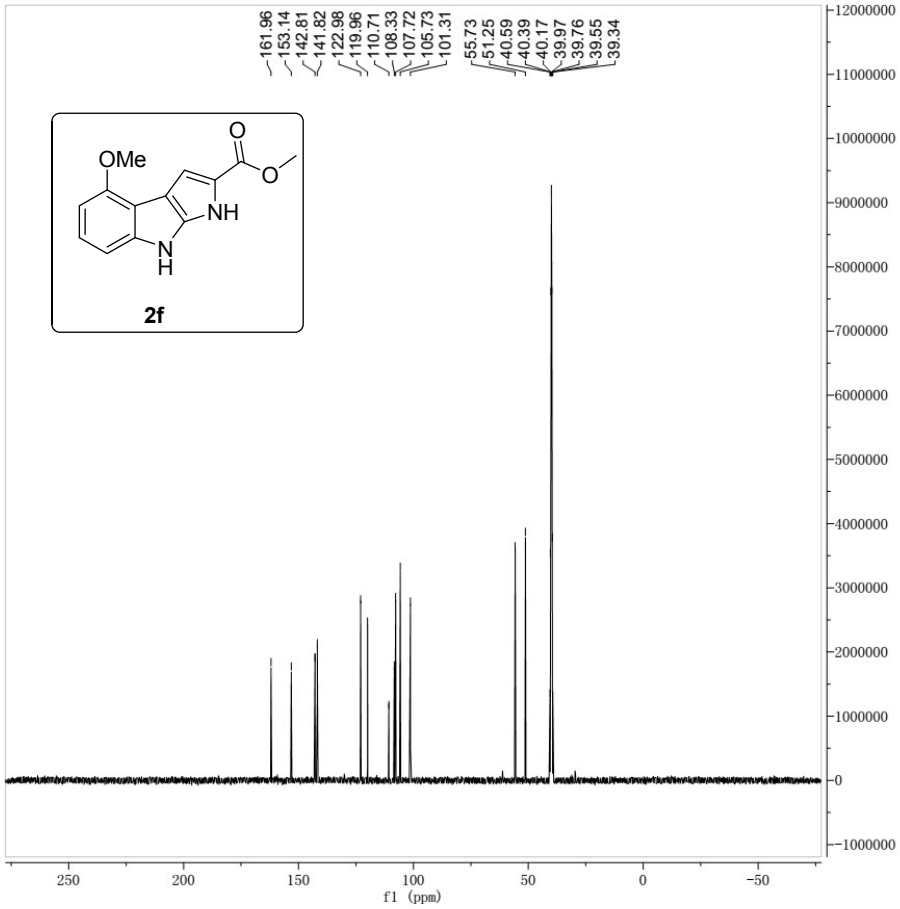
Sample Name	Sample3	**Position**	P1-A3	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YZY-20170103-12.d	**ACQ Method**	chen-ms.m	**Comment**		**Acquired Time**	1/3/2017 4:47:57 PM



methyl 4-methoxy-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2f)

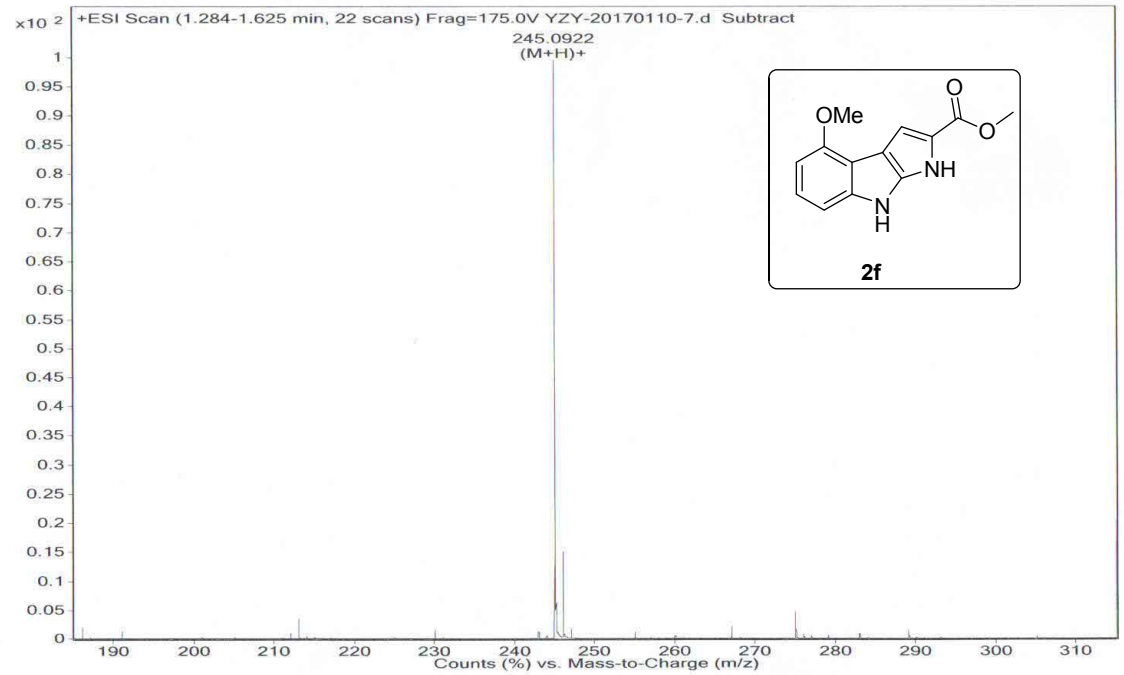


Parameter	Value
1 Data File Name	E:/ yzy-20170111-2/ 1/ pdata/ 1/ 1r
2 Title	yzy-20170111-2.1.1.1r
3 Comment	PROTON DMSO {D:\ NMR_DATA\ Wangbin} Wangbin 23
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	294.9
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	88
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2017-01-11T09:24:00
21 Modification Date	2017-01-11T09:20:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1538.0
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

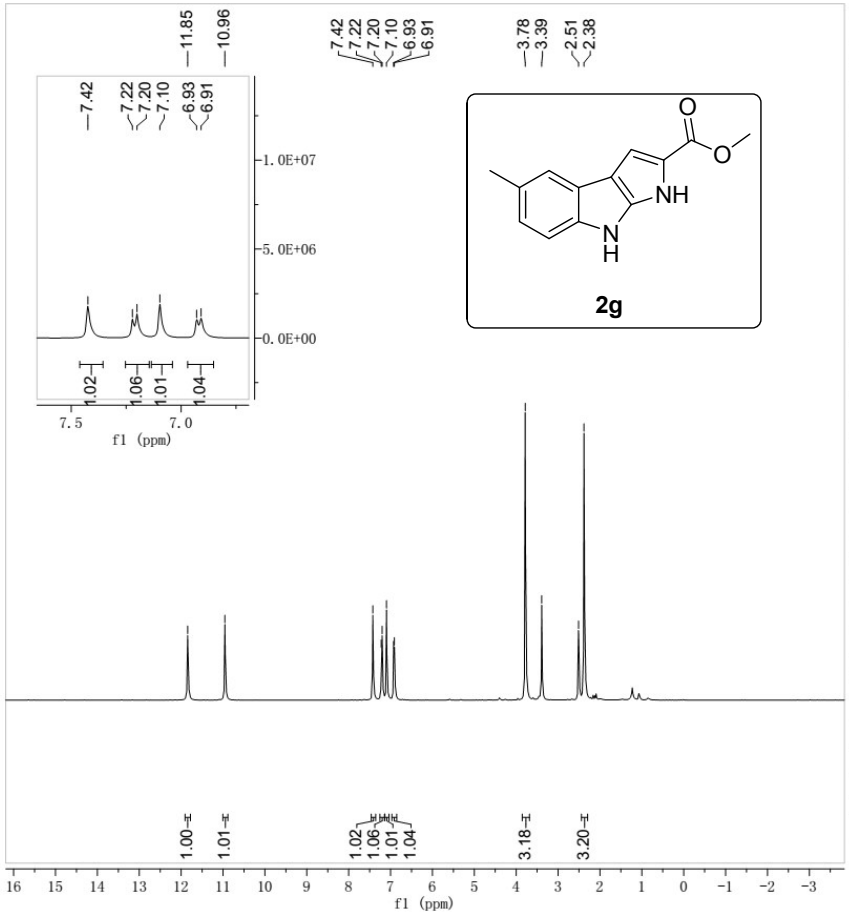


Parameter	Value
1 Data File Name	E:/ yzy-20170111-2/ 2/ pdata/ 1/ 1r
2 Title	yzy-20170111-2.2.1.1r
3 Comment	C13CPD DMSO {D:\ NMR_DATA\ Wangbin} Wangbin 23
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	295.0
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	800
15 Receiver Gain	200
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.4999
20 Acquisition Date	2017-01-11T09:46:00
21 Modification Date	2017-01-11T09:42:00
22 Class	
23 Spectrometer Frequency	100.61
24 Spectral Width	35714.3
25 Lowest Frequency	-7796.8
26 Nucleus	13C
27 Acquired Size	17855
28 Spectral Size	32768

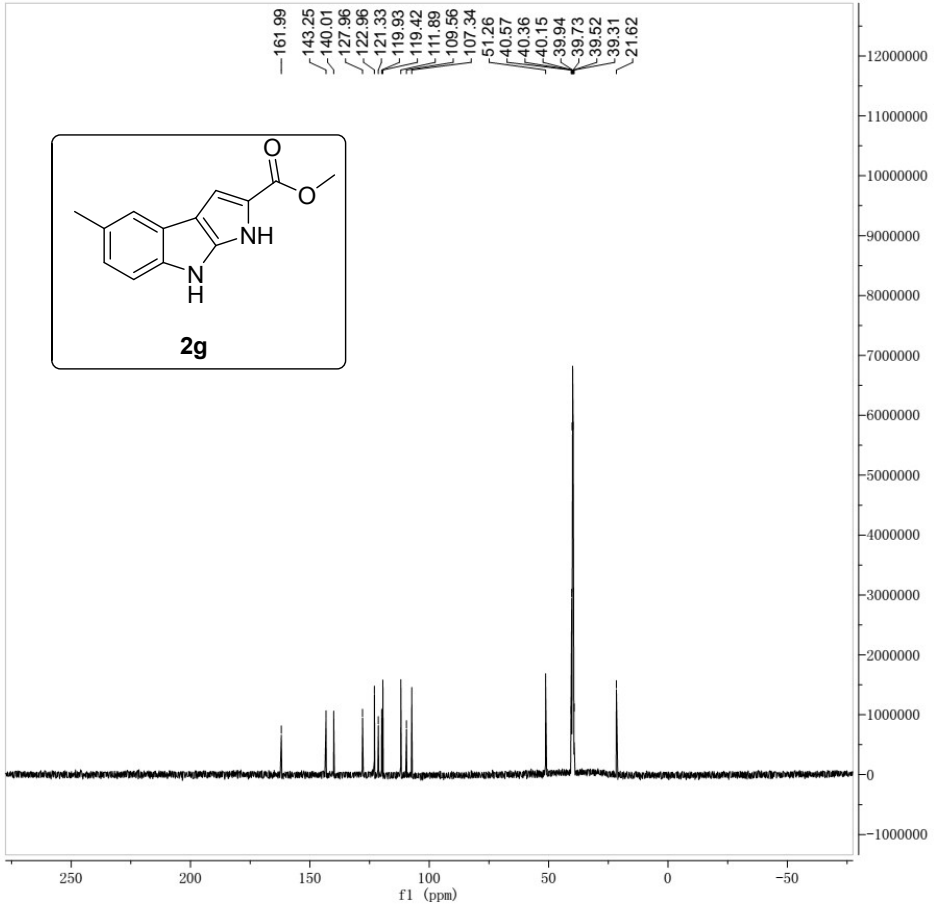
Sample Name	Sample47	**Position**	P1-F2	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YZY-20170110-7.d	**ACQ Method**	chen-ms.m	**Comment**		**Acquired Time**	2/21/2017 8:59:37 PM



methyl-5-methyl-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2g)

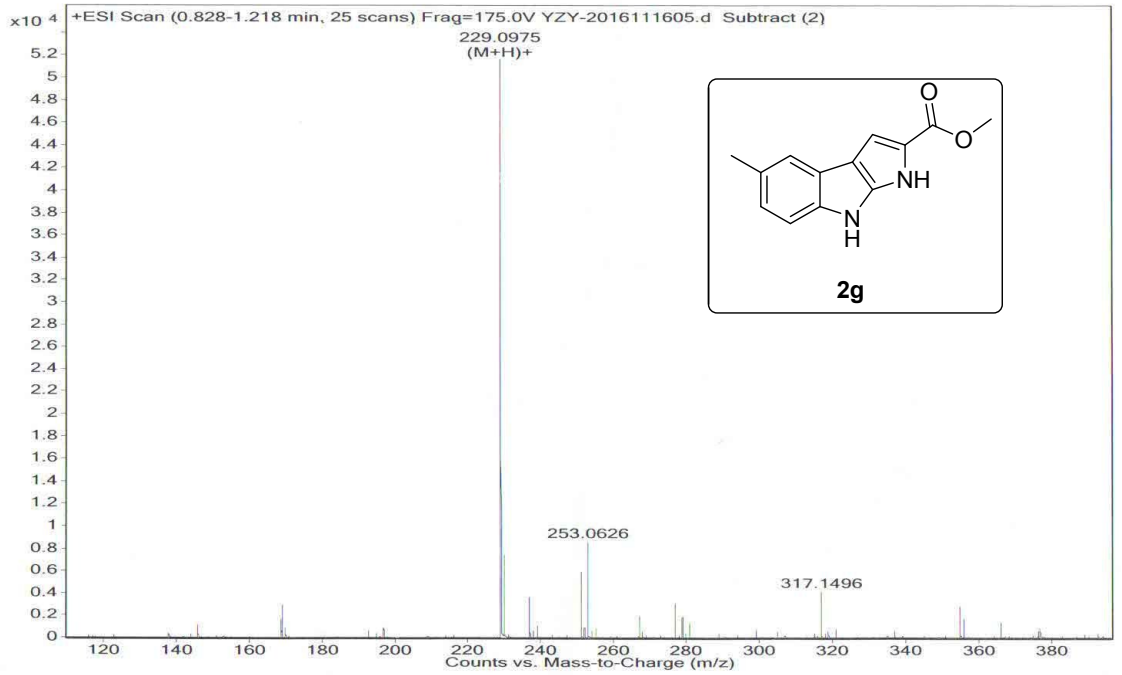


	Parameter	Value
1	Data File Name	E:/ yzy-20161113-2/ 1/ pdata/ 1/ 1r
2	Title	yzy-20161113-2.1.1.1r
3	Comment	PROTON DMSO {D:\ NMR_DATA\ Wangbin} Wangbin 13
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	291.0
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	16
15	Receiver Gain	100
16	Relaxation Delay	1.0000
17	Pulse Width	14.4000
18	Presaturation Frequency	
19	Acquisition Time	4.0894
20	Acquisition Date	2016-11-13T20:46:00
21	Modification Date	2016-11-13T20:43:00
22	Class	
23	Spectrometer Frequency	400.13
24	Spectral Width	8012.8
25	Lowest Frequency	-1535.4
26	Nucleus	1H
27	Acquired Size	32768
28	Spectral Size	65536

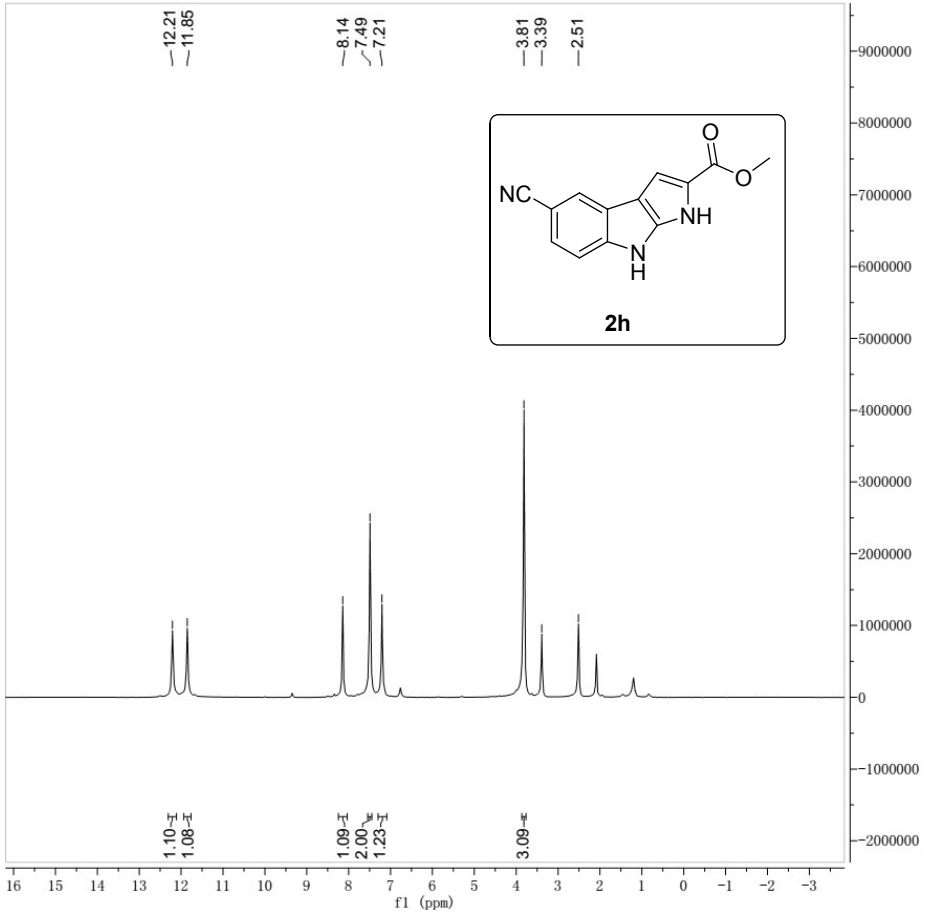


	Parameter	Value
1	Data File Name	E:/ yzy-20161113-2/ 2/ pdata/ 1/ 1r
2	Title	yzy-20161113-2.2.1.1r
3	Comment	C13CPD DMSO {D:\ NMR_DATA\ Wangbin} Wangbin 13
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	291.8
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	950
15	Receiver Gain	200
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	0.4999
20	Acquisition Date	2016-11-13T21:13:00
21	Modification Date	2016-11-13T21:10:00
22	Class	
23	Spectrometer Frequency	100.61
24	Spectral Width	35714.3
25	Lowest Frequency	-7796.8
26	Nucleus	13C
27	Acquired Size	17855
28	Spectral Size	32768

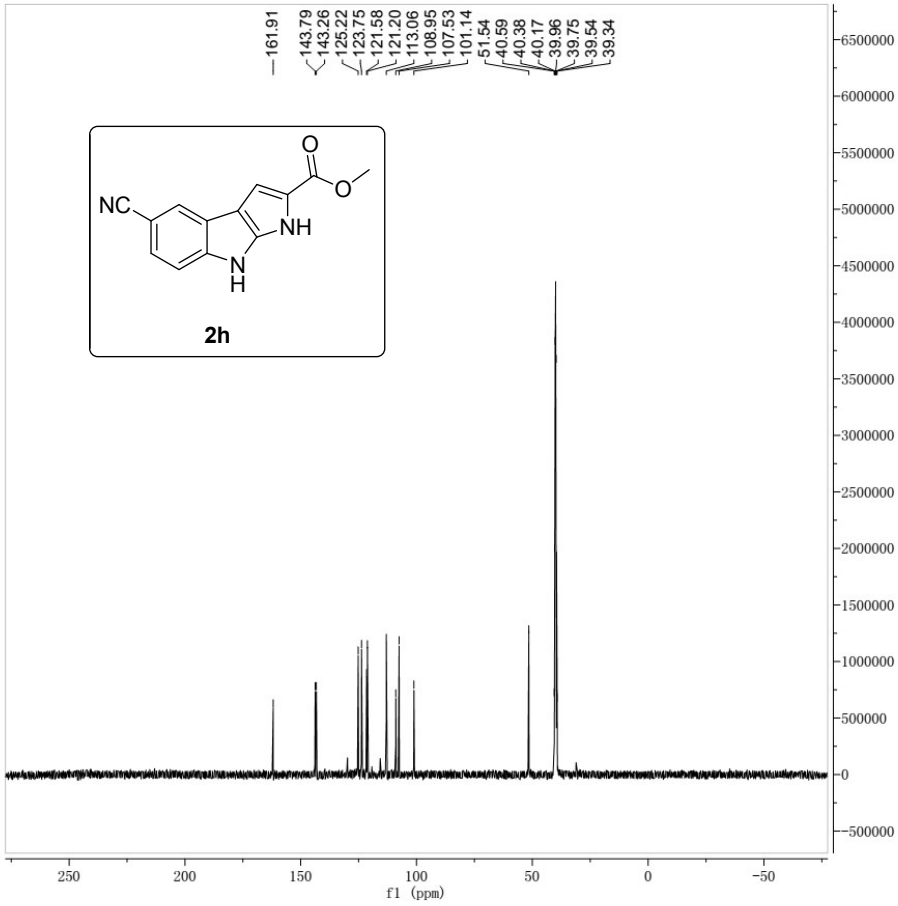
Sample Name	Sample5	**Position**	P1-A5	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YZY-2016111605.d	**ACQ Method**	chen-ms.m	**Comment**		**Acquired Time**	11/16/2016 5:09:00 PM



methyl 5-cyano-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2h)

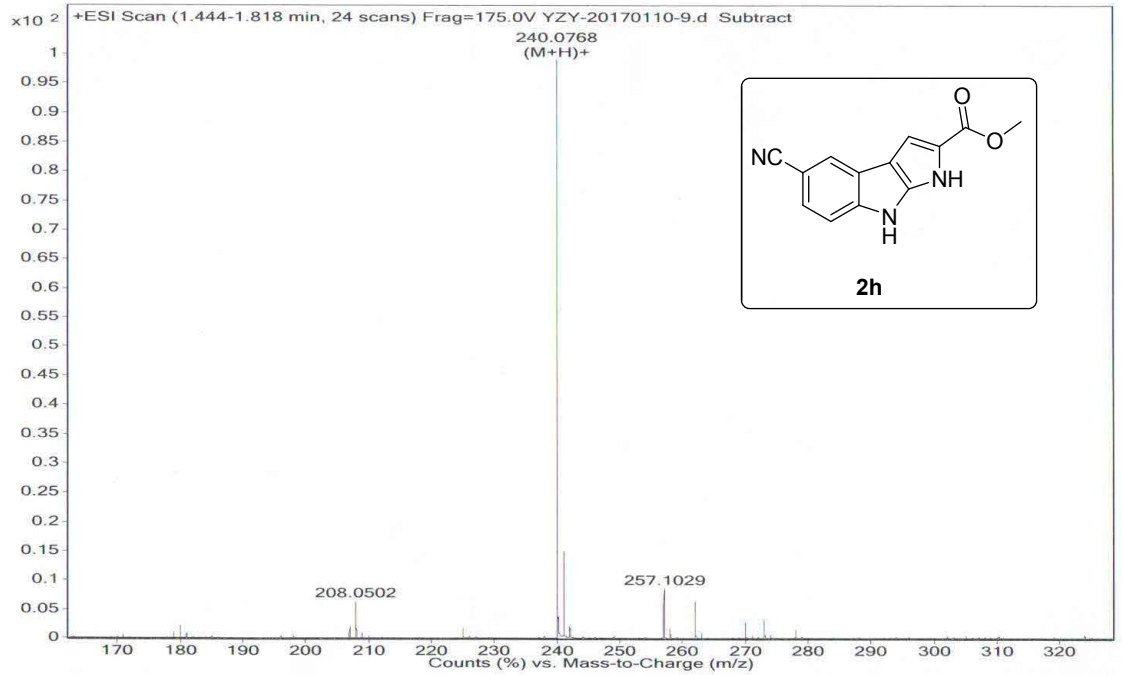


	Parameter	Value
1	Data File Name	E:/ yzy-20170112-2/ 1/ pdata/ 1/ 1r
2	Title	yzy-20170112-2.1.1.1r
3	Comment	PROTON DMSO {D:\ NMR_DATA\ Wangbin} Wangbin 1
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	294.8
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	16
15	Receiver Gain	100
16	Relaxation Delay	1.0000
17	Pulse Width	14.4000
18	Presaturation Frequency	
19	Acquisition Time	4.0894
20	Acquisition Date	2017-01-12T11:17:00
21	Modification Date	2017-01-12T11:13:00
22	Class	
23	Spectrometer Frequency	400.13
24	Spectral Width	8012.8
25	Lowest Frequency	-1535.4
26	Nucleus	1H
27	Acquired Size	32768
28	Spectral Size	65536

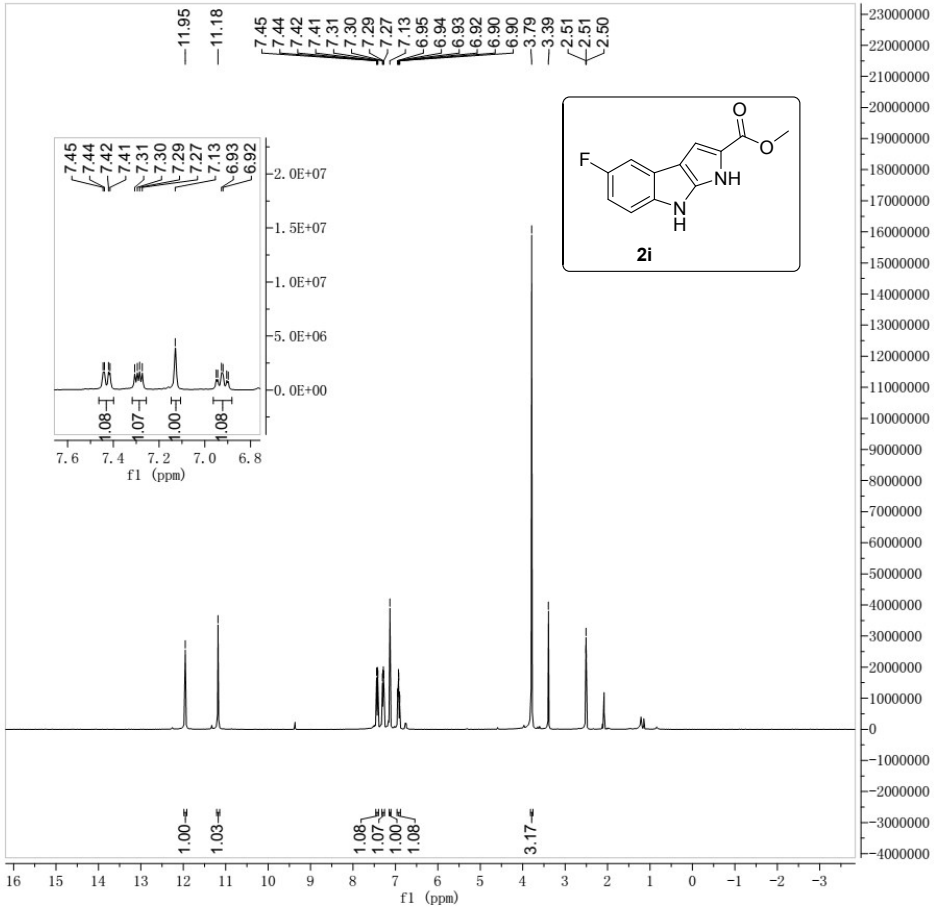


	Parameter	Value
1	Data File Name	E:/ yzy-20170112-2/ 2/ pdata/ 1/ 1r
2	Title	yzy-20170112-2.2.1.1r
3	Comment	C13CPD DMSO {D:\ NMR_DATA\ Wangbin} Wangbin 1
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	295.8
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	900
15	Receiver Gain	133
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	0.4999
20	Acquisition Date	2017-01-12T11:41:00
21	Modification Date	2017-01-12T11:37:00
22	Class	
23	Spectrometer Frequency	100.61
24	Spectral Width	35714.3
25	Lowest Frequency	-7796.8
26	Nucleus	13C
27	Acquired Size	17855
28	Spectral Size	32768

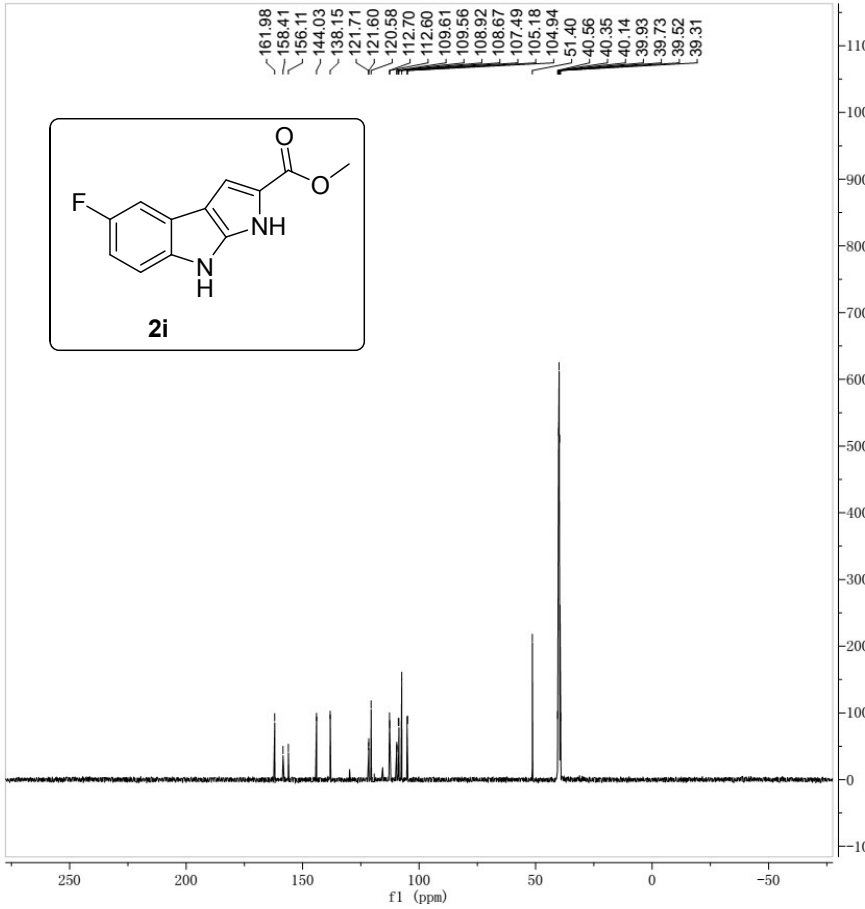
Sample Name	Sample49	**Position**	P1-F4	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YZY-20170110-9.d	**ACQ Method**	chen-ms.m	**Comment**		**Acquired Time**	2/21/2017 9:10:58 PM



methyl 5-fluoro-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2i)

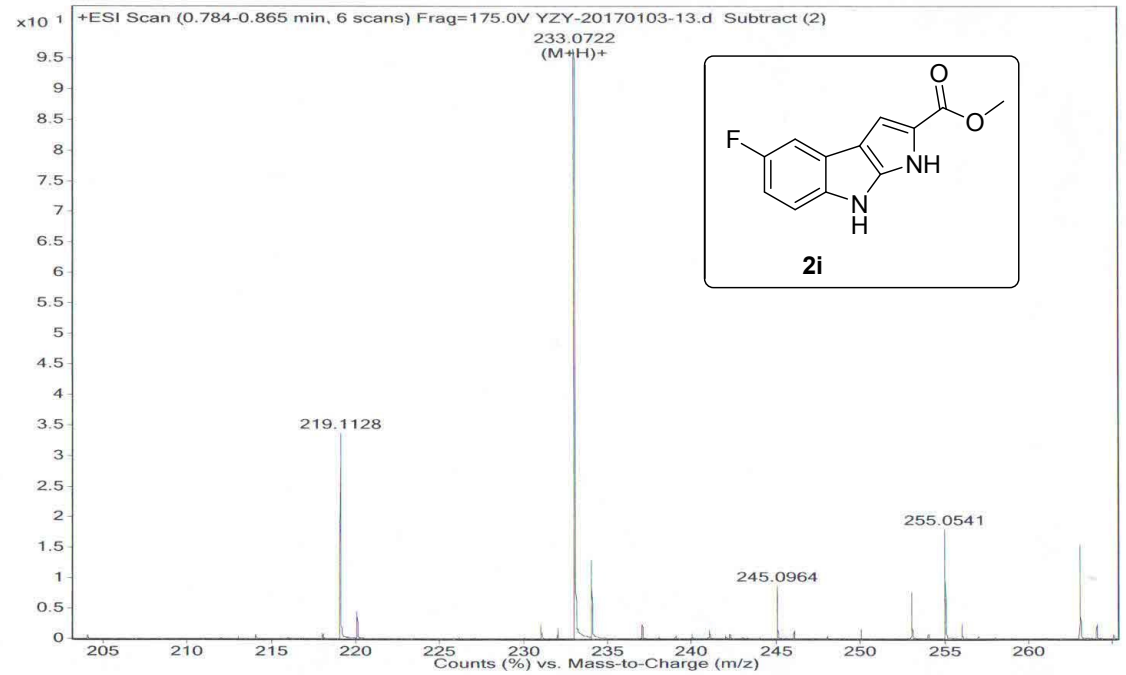


Parameter	Value
1 Data File Name	E:/ yzy-20161225-1/ 1/ pdata/ 1/ 1r
2 Title	yzy-20161225-1.1.1.1r
3 Comment	PROTON DMSO {D:\ NMR_DATA\ Wangbin} Wangbin 20
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	290.9
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	113
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2016-12-25T16:37:00
21 Modification Date	2016-12-25T16:33:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1535.4
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

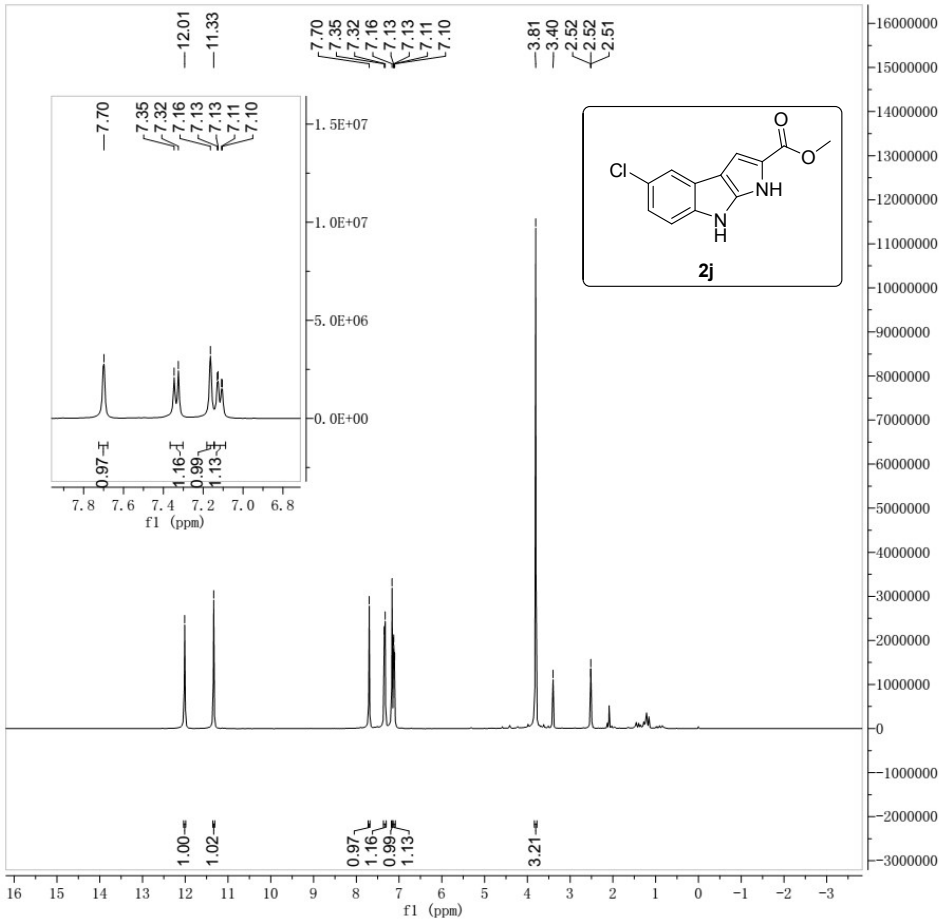


	Parameter	Value
1	Data File Name	E:/ yzy-20161225-1/ 2/ pdata/ 1/ 1r
2	Title	yzy-20161225-1.2.1.1r
3	Comment	C13CPD DMSO {D:\ NMR_DATA\ Wangbin} Wangbin 20
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	292.2
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	950
15	Receiver Gain	119
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	0.4999
20	Acquisition Date	2016-12-25T17:04:00
21	Modification Date	2016-12-25T17:00:00
22	Class	
23	Spectrometer Frequency	100.61
24	Spectral Width	35714.3
25	Lowest Frequency	-7796.8
26	Nucleus	13C
27	Acquired Size	17855
28	Spectral Size	32768

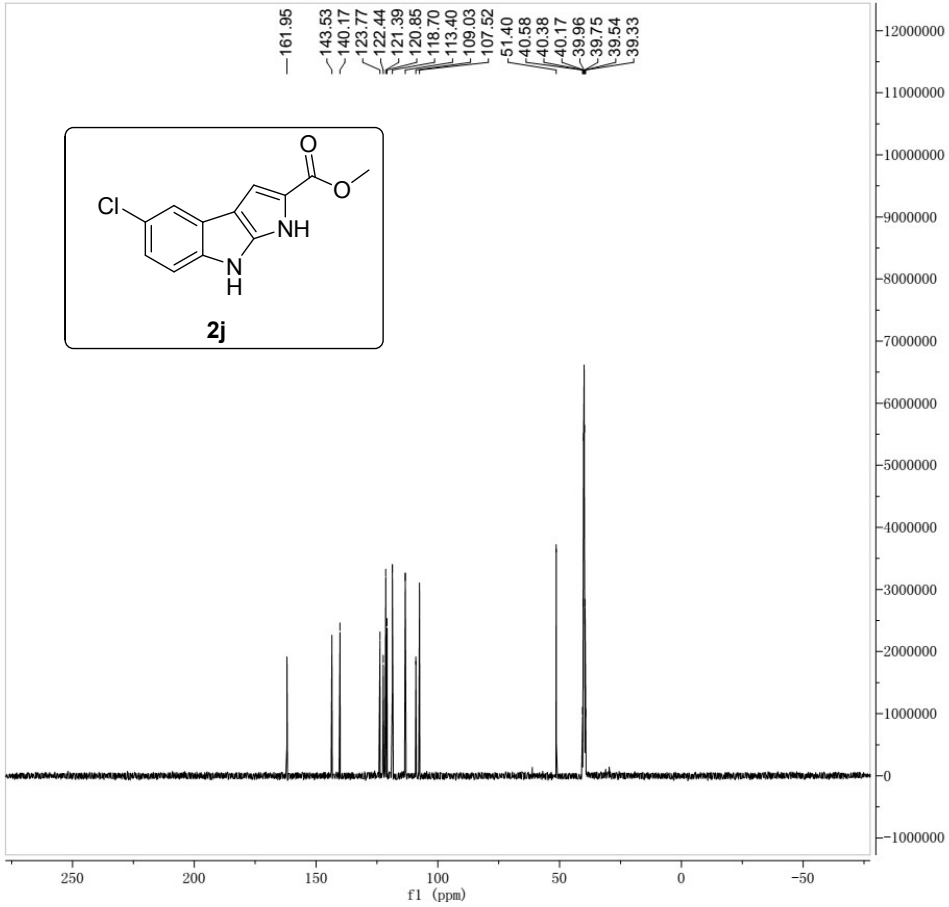
Sample Name	Sample	**Position**	P1-A4	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YZY-20170103-13.d	**ACQ Method**	chen-ms.m	**Comment**		**Acquired Time**	1/3/2017 4:53:38 PM



methyl 5-chloro-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2j)

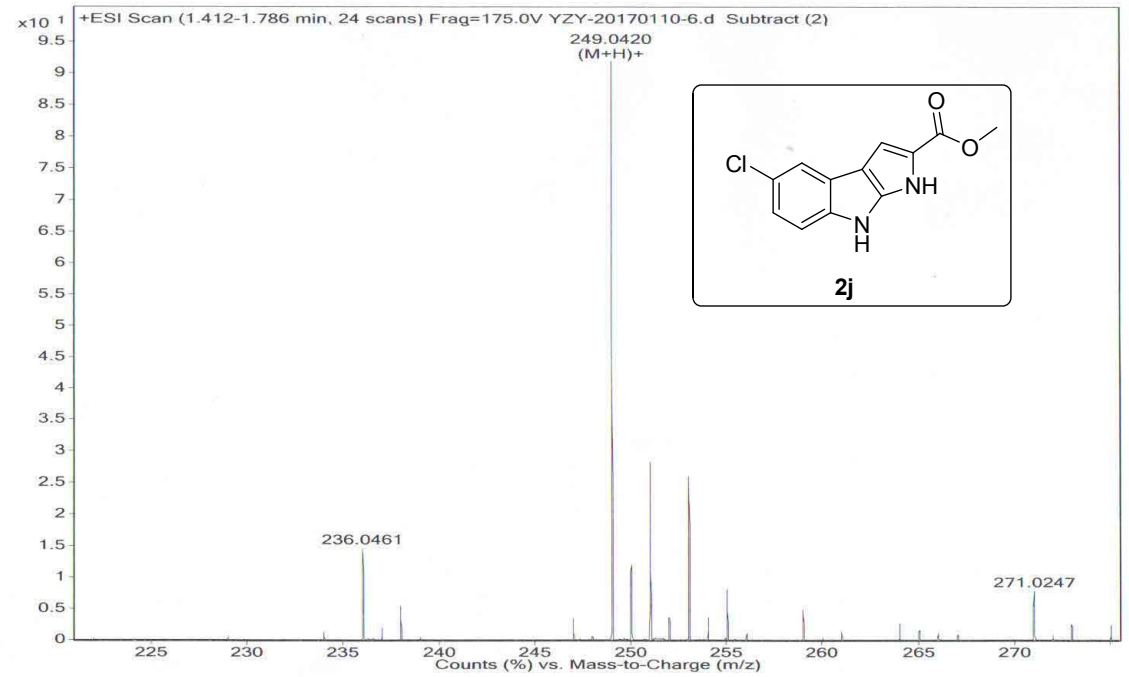


	Parameter	Value
1	Data File Name	E:/ yzy-20170111-3/ 1/ pdata/ 1/ 1r
2	Title	yzy-20170111-3.1.1.1r
3	Comment	PROTON DMSO {D:\ NMR_DATA\ Wangbin} Wangbin 24
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	294.0
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	16
15	Receiver Gain	88
16	Relaxation Delay	1.0000
17	Pulse Width	14.4000
18	Presaturation Frequency	
19	Acquisition Time	4.0894
20	Acquisition Date	2017-01-11T09:53:00
21	Modification Date	2017-01-11T09:49:00
22	Class	
23	Spectrometer Frequency	400.13
24	Spectral Width	8012.8
25	Lowest Frequency	-1533.1
26	Nucleus	1H
27	Acquired Size	32768
28	Spectral Size	65536

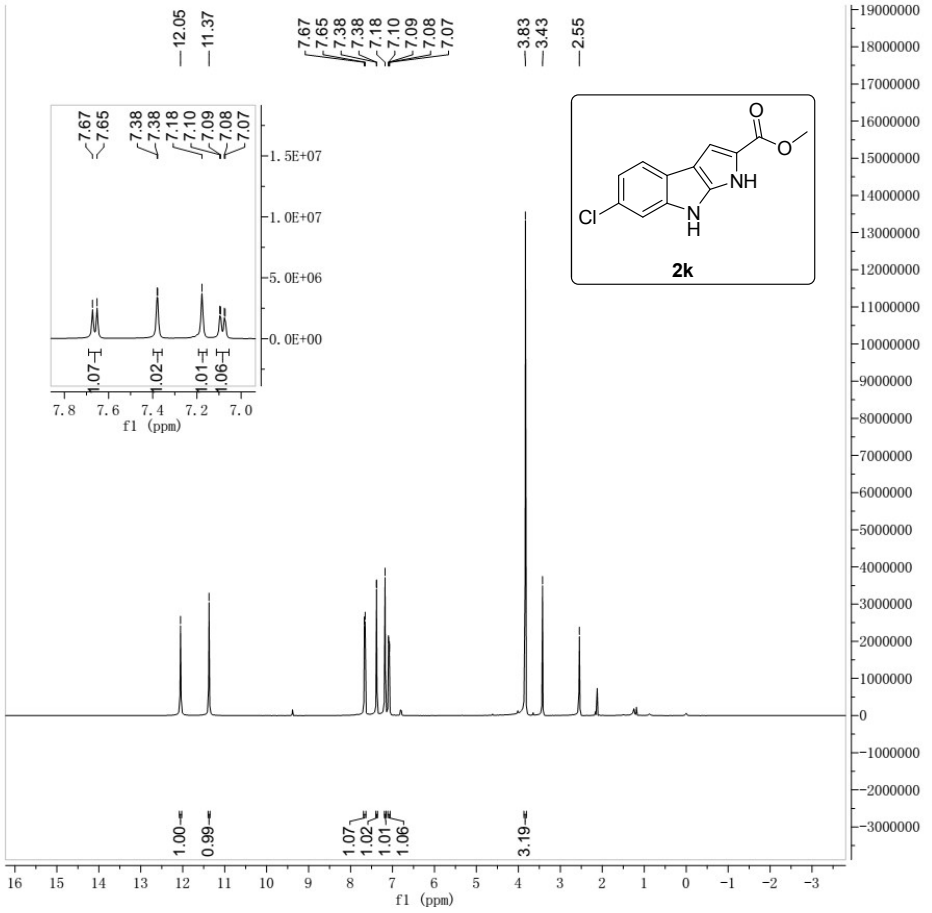


	Parameter	Value
1	Data File Name	E:/ yzy-20170111-3/ 2/ pdata/ 1/ 1r
2	Title	yzy-20170111-3.2.1.1r
3	Comment	C13CPD DMSO {D:\ NMR_DATA\ Wangbin} Wangbin 24
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	295.4
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	800
15	Receiver Gain	200
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	0.4999
20	Acquisition Date	2017-01-11T10:14:00
21	Modification Date	2017-01-11T10:11:00
22	Class	
23	Spectrometer Frequency	100.61
24	Spectral Width	35714.3
25	Lowest Frequency	-7796.8
26	Nucleus	13C
27	Acquired Size	17855
28	Spectral Size	32768

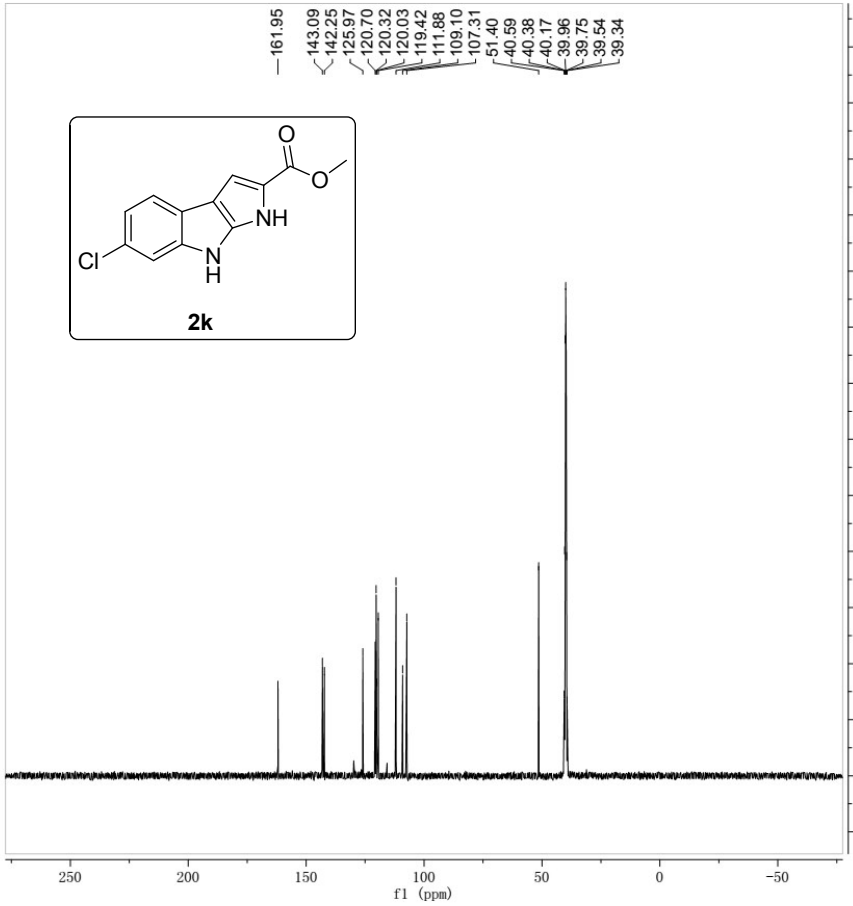
Sample Name	Sample46	**Position**	P1-F1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YZY-20170110-6.d	**ACQ Method**	chen-ms.m	**Comment**		**Acquired Time**	2/21/2017 8:53:55 PM



methyl 6-chloro-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2k)

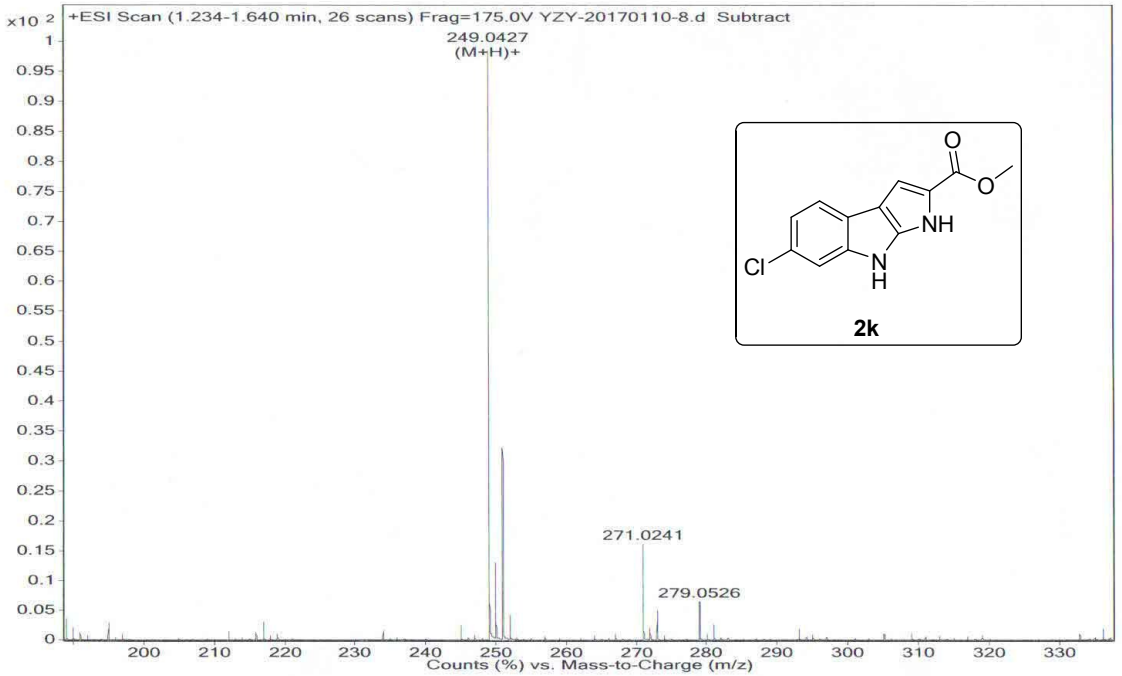


	Parameter	Value
1	Data File Name	E:/ yzy-20170112-1/ 1/ pdata/ 1/ 1r
2	Title	yzy-20170112-1.1.1.1r
3	Comment	PROTON DMSO {D:\ NMR_DATA\ Wangbin} Wangbin 24
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	294.4
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	16
15	Receiver Gain	100
16	Relaxation Delay	1.0000
17	Pulse Width	14.4000
18	Presaturation Frequency	
19	Acquisition Time	4.0894
20	Acquisition Date	2017-01-12T10:51:00
21	Modification Date	2017-01-12T10:47:00
22	Class	
23	Spectrometer Frequency	400.13
24	Spectral Width	8012.8
25	Lowest Frequency	-1521.1
26	Nucleus	1H
27	Acquired Size	32768
28	Spectral Size	65536

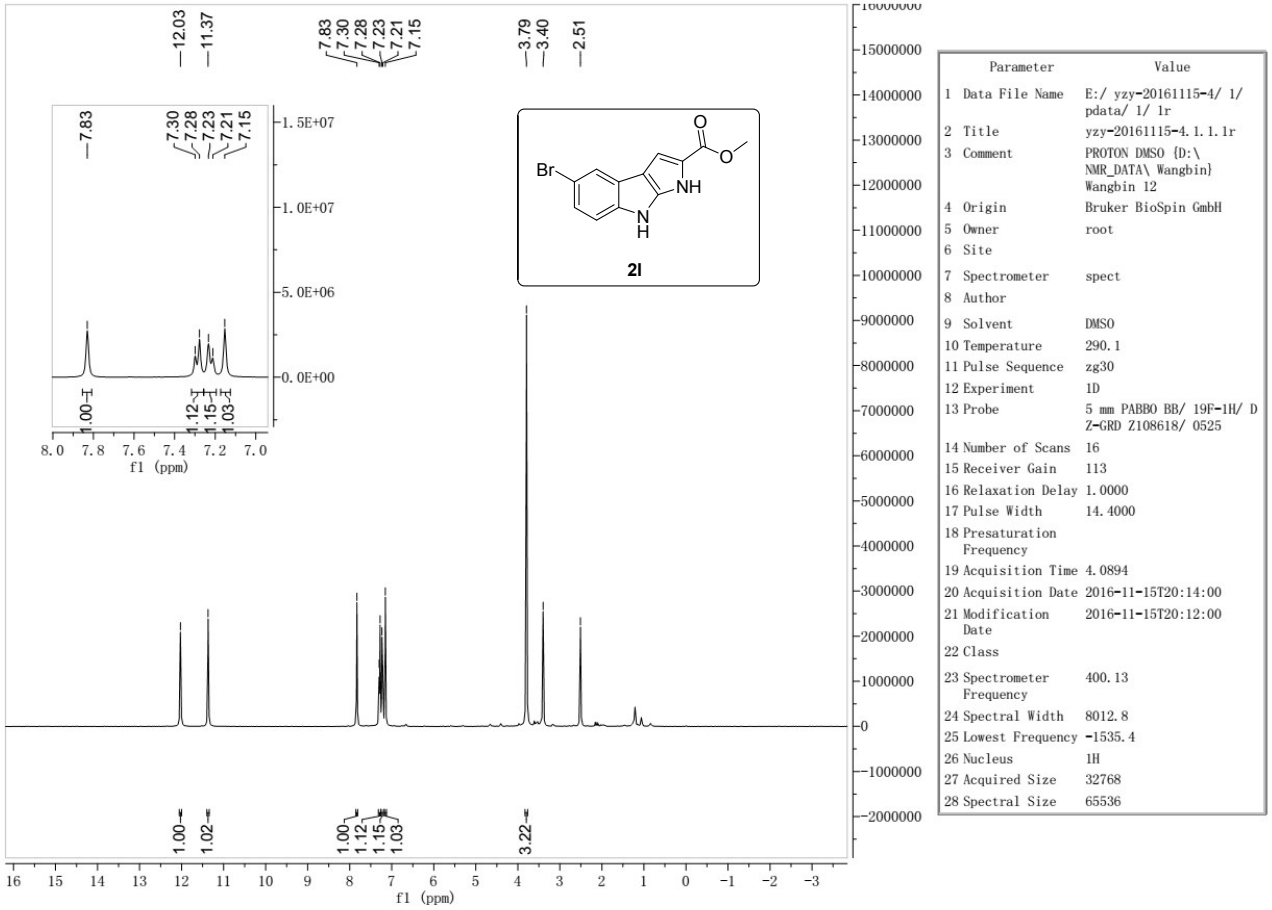


Parameter	Value
1 Data File Name	E:/ yzy-20170112-1/ 2/ pdata/ 1/ 1r
2 Title	yzy-20170112-1.2.1.1r
3 Comment	C13CPD DMSO {D:\ NMR_DATA\ Wangbin} Wangbin 24
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	295.7
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	800
15 Receiver Gain	119
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.4999
20 Acquisition Date	2017-01-12T11:13:00
21 Modification Date	2017-01-12T11:09:00
22 Class	
23 Spectrometer Frequency	100.61
24 Spectral Width	35714.3
25 Lowest Frequency	-7796.8
26 Nucleus	13C
27 Acquired Size	17855
28 Spectral Size	32768

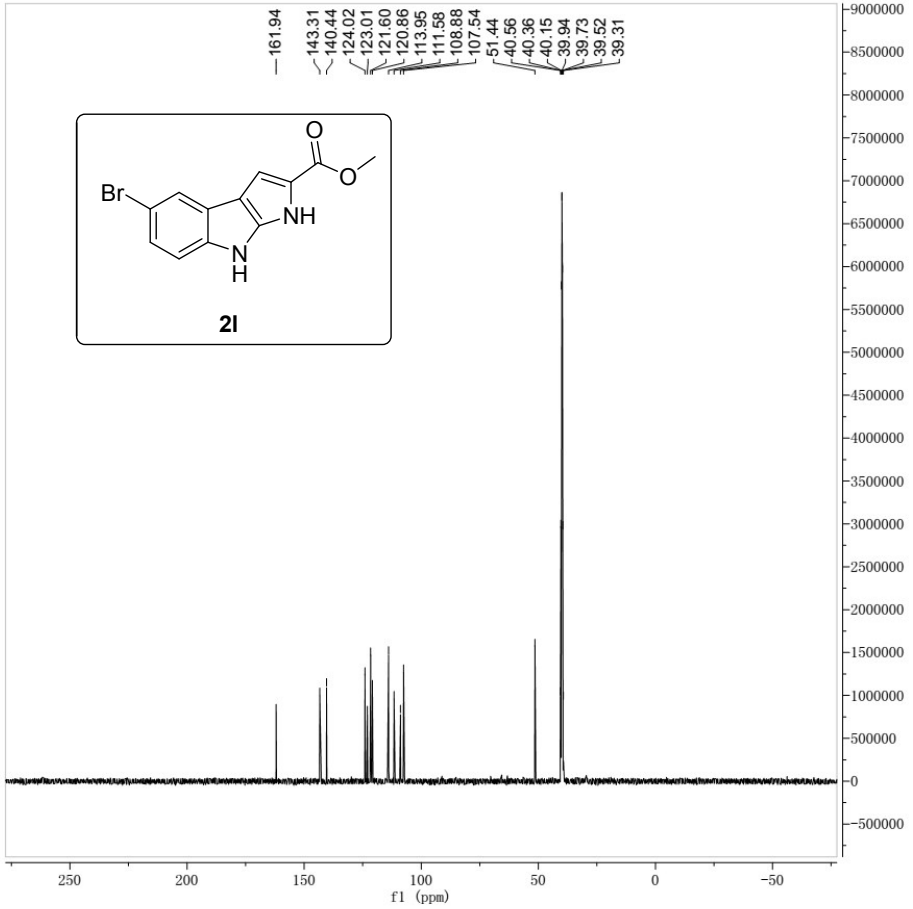
Sample Name	Sample48	**Position**	P1-F3	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YZY-20170110-8.d	**ACQ Method**	chen-ms.m	**Comment**		**Acquired Time**	2/21/2017 9:05:16 PM



methyl 5-bromo-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2l)

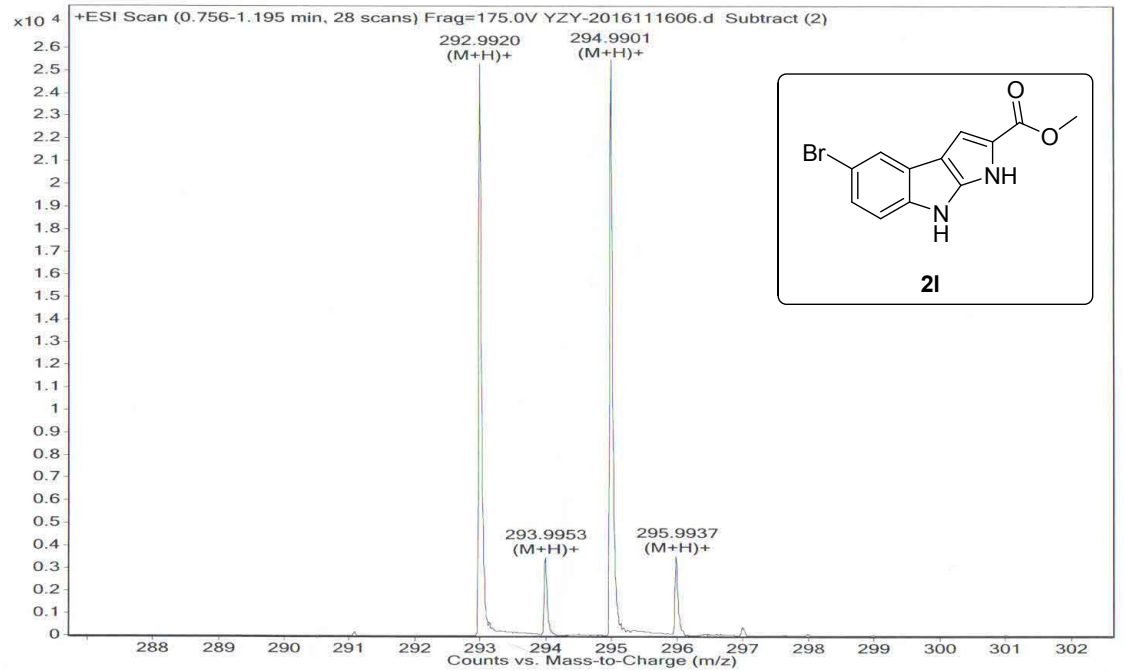


	Parameter	Value
1	Data File Name	E:/ yzy-20161115-4/ 1/ pdata/ 1/ 1r
2	Title	yzy-20161115-4.1.1.1r
3	Comment	PROTON DMSO {D:\ NMR_DATA\ Wangbin} Wangbin 12
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	290.1
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	16
15	Receiver Gain	113
16	Relaxation Delay	1.0000
17	Pulse Width	14.4000
18	Presaturation Frequency	
19	Acquisition Time	4.0894
20	Acquisition Date	2016-11-15T20:14:00
21	Modification Date	2016-11-15T20:12:00
22	Class	
23	Spectrometer Frequency	400.13
24	Spectral Width	8012.8
25	Lowest Frequency	-1535.4
26	Nucleus	1H
27	Acquired Size	32768
28	Spectral Size	65536

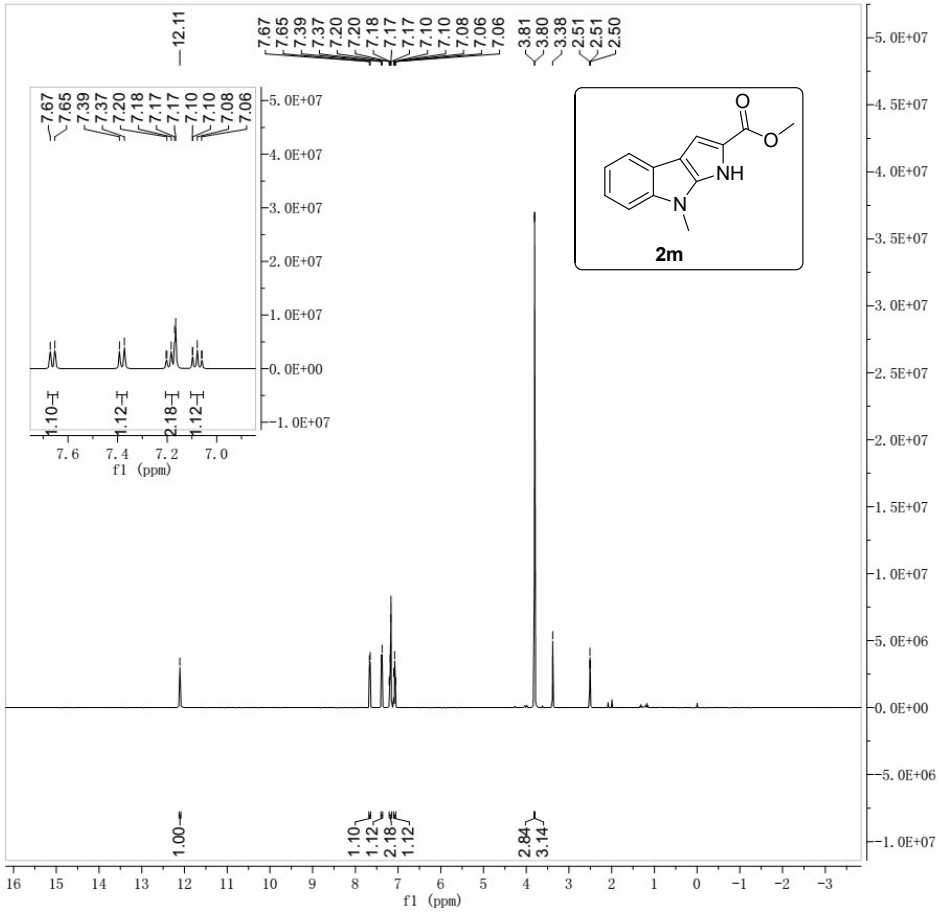


	Parameter	Value
1	Data File Name	E:/ yzy-20161115-4/ 2/ pdata/ 1/ 1r
2	Title	yzy-20161115-4.2.1.1r
3	Comment	C13CPD DMSO {D:\ NMR_DATA\ Wangbin} Wangbin 12
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	291.3
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	1024
15	Receiver Gain	113
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	0.4999
20	Acquisition Date	2016-11-15T20:42:00
21	Modification Date	2016-11-15T20:39:00
22	Class	
23	Spectrometer Frequency	100.61
24	Spectral Width	35714.3
25	Lowest Frequency	-7796.8
26	Nucleus	13C
27	Acquired Size	17855
28	Spectral Size	32768

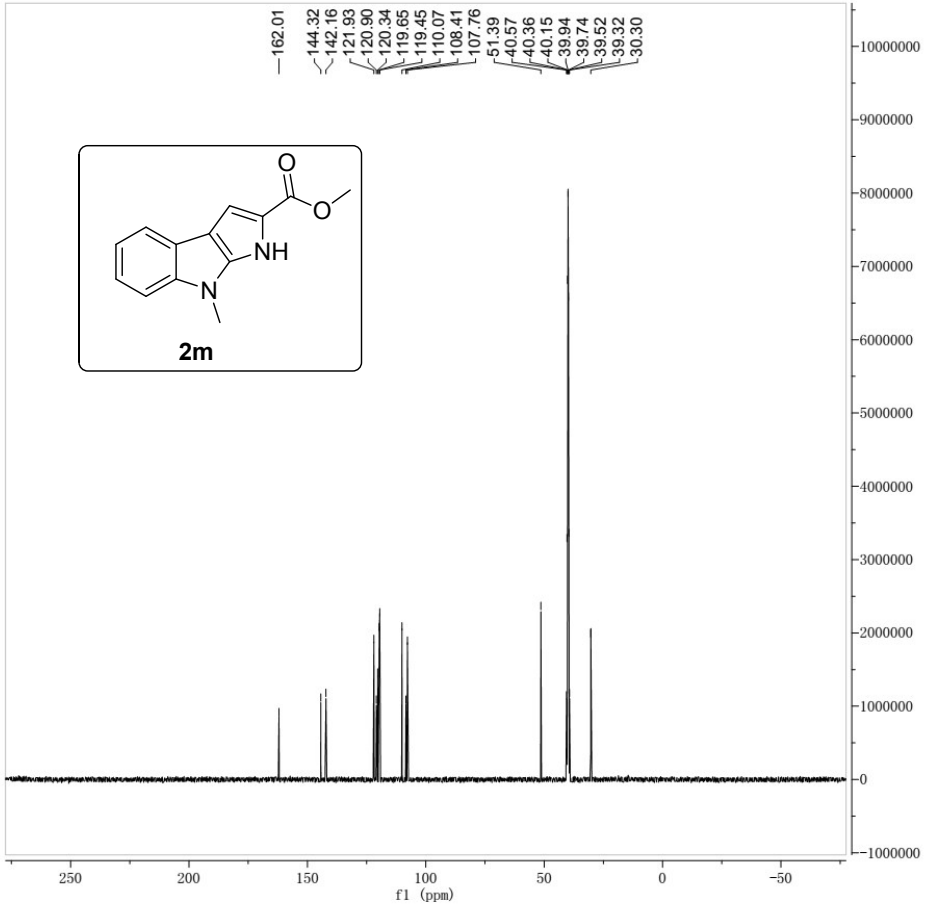
Sample Name	Sample6	**Position**	P1-A6	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YZY-2016111606.d	**ACQ Method**	chen-ms.m	**Comment**		**Acquired Time**	11/16/2016 5:14:42 PM



methyl 8-methyl-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2m)

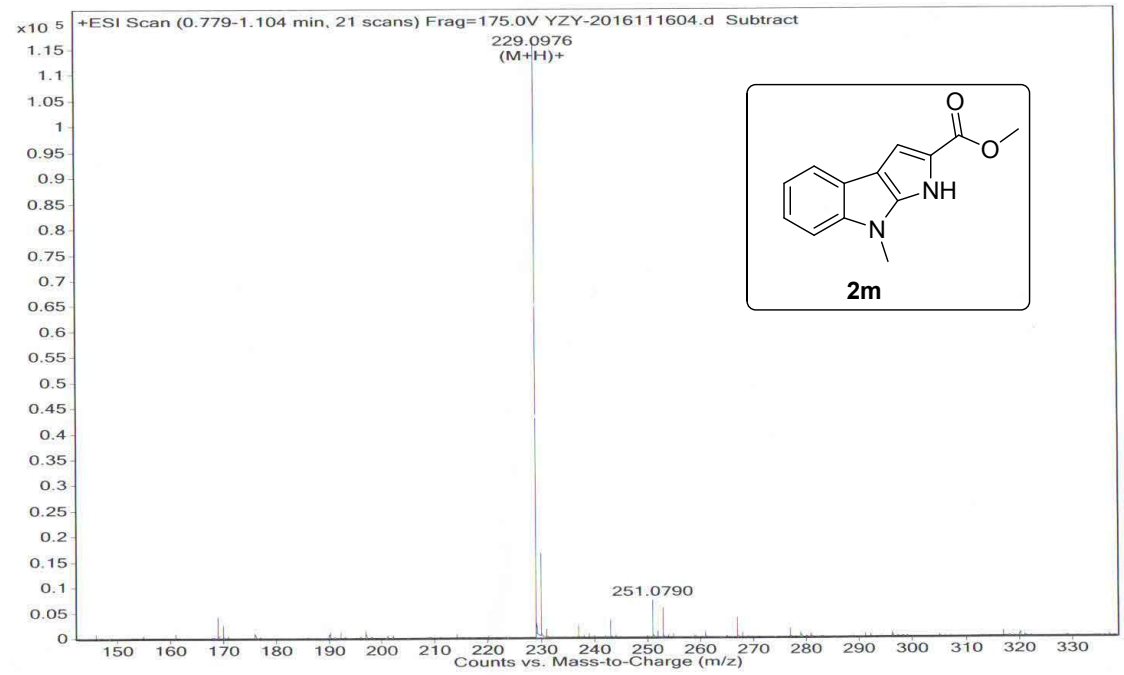


Parameter	Value
1 Data File Name	E:/ 杨钊英 核磁数据/ yzy-20161026-1/ 3/ pdata/ 1/ 1r
2 Title	yzy-20161026-1.3.1.1r
3 Comment	PROTON DMSO {D:\ NMR_DATA\ Wangbin} Wangbin 21
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	290.4
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	113
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2016-10-27T21:38:00
21 Modification Date	2016-10-27T21:35:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1536.5
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

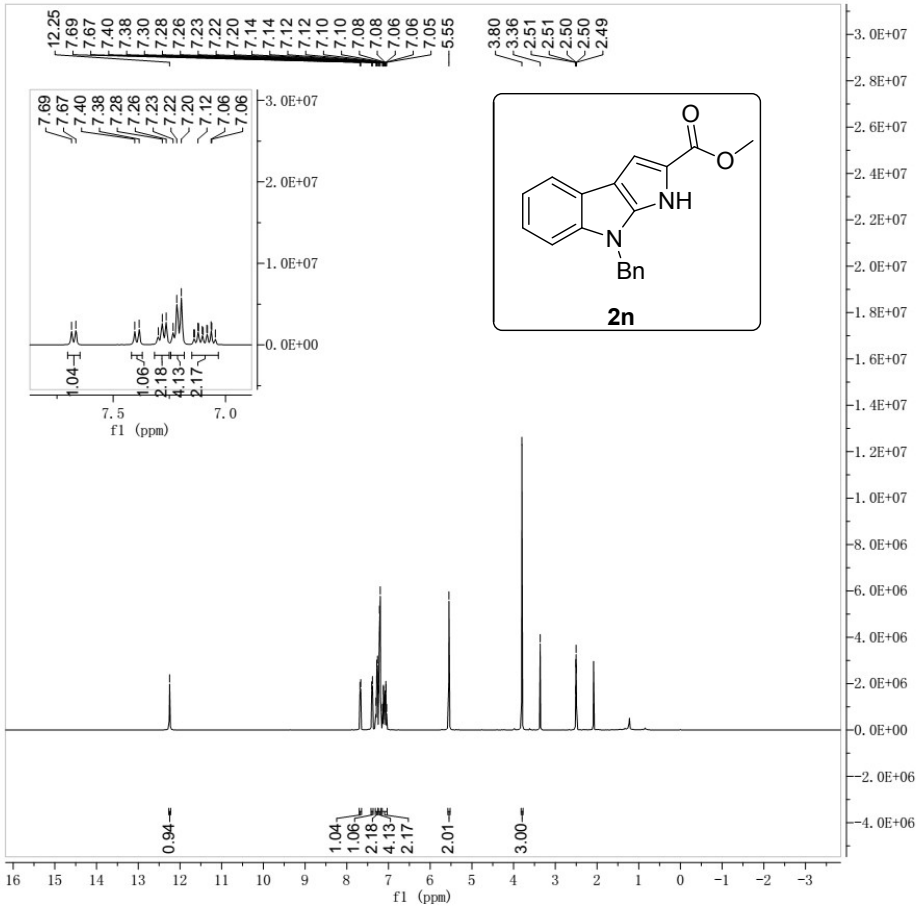


Parameter	Value
1 Data File Name	E:/ 杨钊英 核磁数据/ yzy-20161026-1/ 4/ pdata/ 1/ 1r
2 Title	yzy-20161026-1.4.1.1r
3 Comment	C13CPD DMSO {D:\ NMR_DATA\ Wangbin} Wangbin 21
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	291.4
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	1024
15 Receiver Gain	113
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.4999
20 Acquisition Date	2016-10-27T22:06:00
21 Modification Date	2016-10-27T22:03:00
22 Class	
23 Spectrometer Frequency	100.61
24 Spectral Width	35714.3
25 Lowest Frequency	-7796.8
26 Nucleus	13C
27 Acquired Size	17855
28 Spectral Size	32768

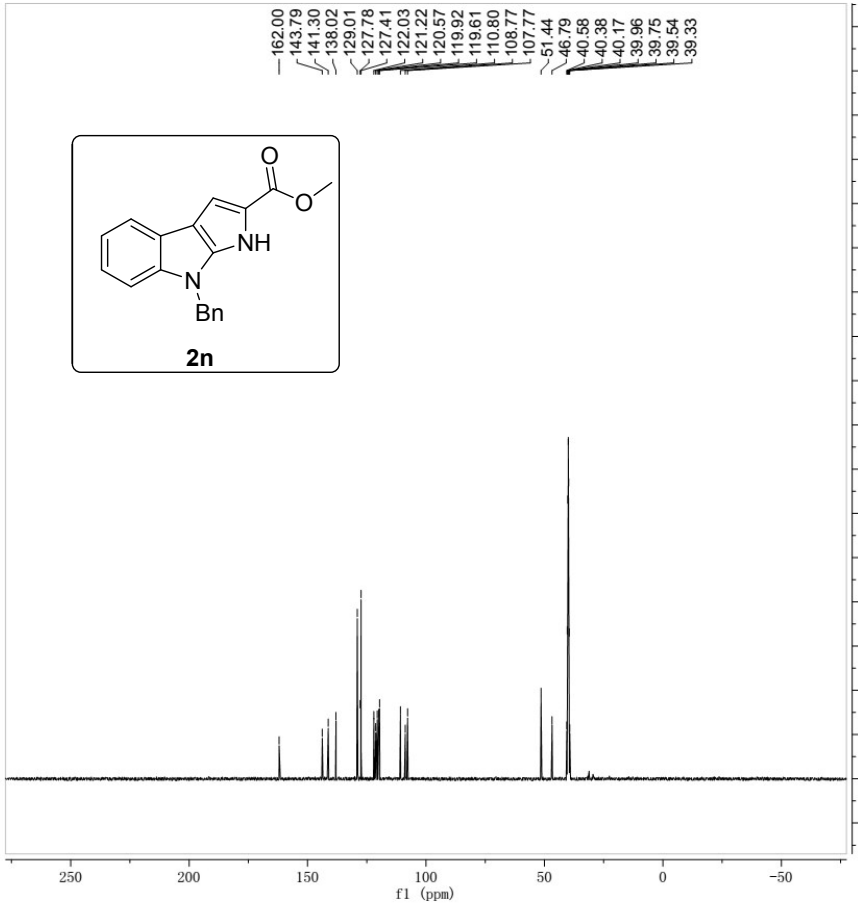
Sample Name	Sample4	**Position**	P1-A4	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YZY-2016111604.d	**ACQ Method**	chen-ms.m	**Comment**		**Acquired Time**	11/16/2016 5:03:18 PM



methyl 8-benzyl-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2n)

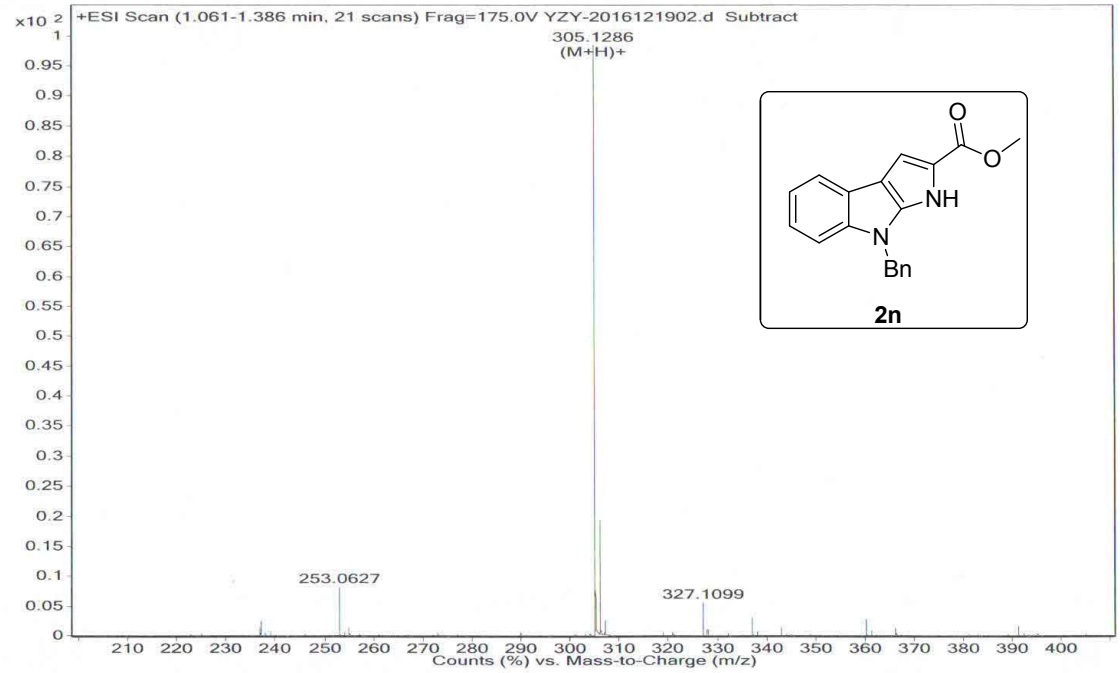


	Parameter	Value
1	Data File Name	E:/ yzy-20161217-1/ 1/ pdata/ 1/ 1r
2	Title	yzy-20161217-1.1.1.1r
3	Comment	PROTON DMSO {D:\ NMR_DATA\ Wangbin} Wangbin 21
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	293.1
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	16
15	Receiver Gain	100
16	Relaxation Delay	1.0000
17	Pulse Width	14.4000
18	Presaturation Frequency	
19	Acquisition Time	4.0894
20	Acquisition Date	2016-12-17T10:34:00
21	Modification Date	2016-12-17T10:30:00
22	Class	
23	Spectrometer Frequency	400.13
24	Spectral Width	8012.8
25	Lowest Frequency	-1537.9
26	Nucleus	1H
27	Acquired Size	32768
28	Spectral Size	65536

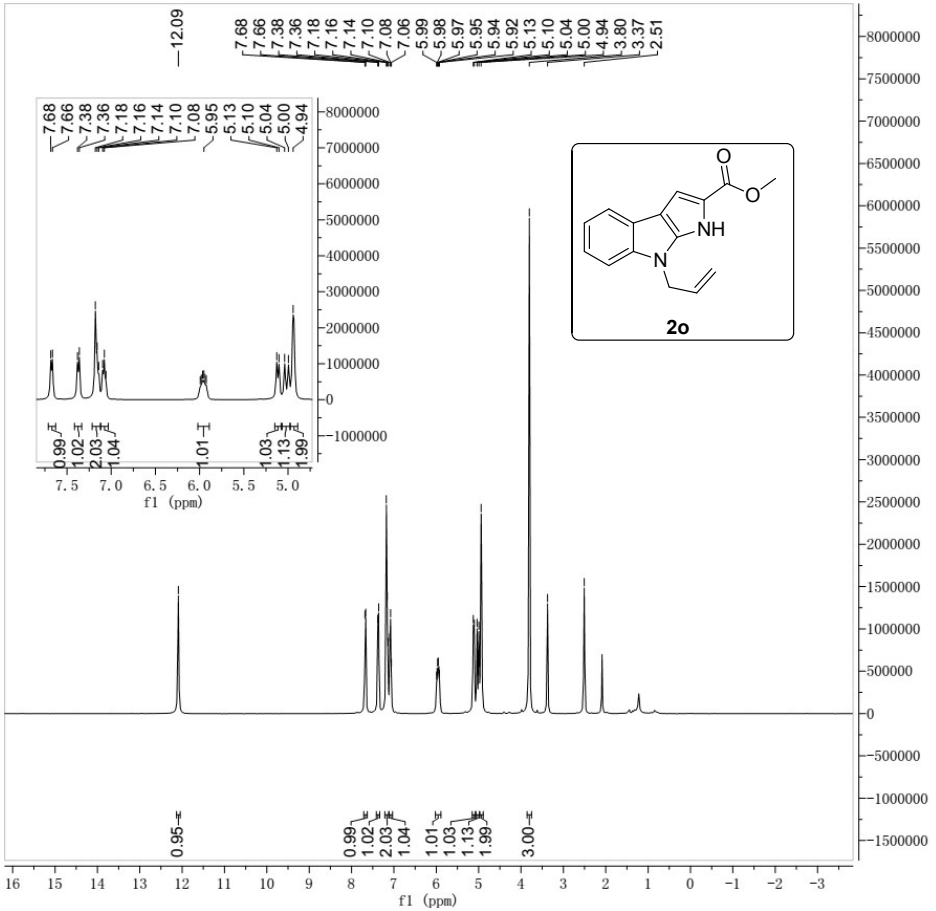


	Parameter	Value
1	Data File Name	E:/ yzy-20161208-3/ 2/ pdata/ 1/ 1r
2	Title	yzy-20161208-3.2.1.1r
3	Comment	C13CPD DMSO {D:\ NMR_DATA\ Wangbin} Wangbin 1
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	293.2
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	1024
15	Receiver Gain	113
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	0.4999
20	Acquisition Date	2016-12-08T20:02:00
21	Modification Date	2016-12-08T19:58:00
22	Class	
23	Spectrometer Frequency	100.61
24	Spectral Width	35714.3
25	Lowest Frequency	-7796.8
26	Nucleus	13C
27	Acquired Size	17855
28	Spectral Size	32768

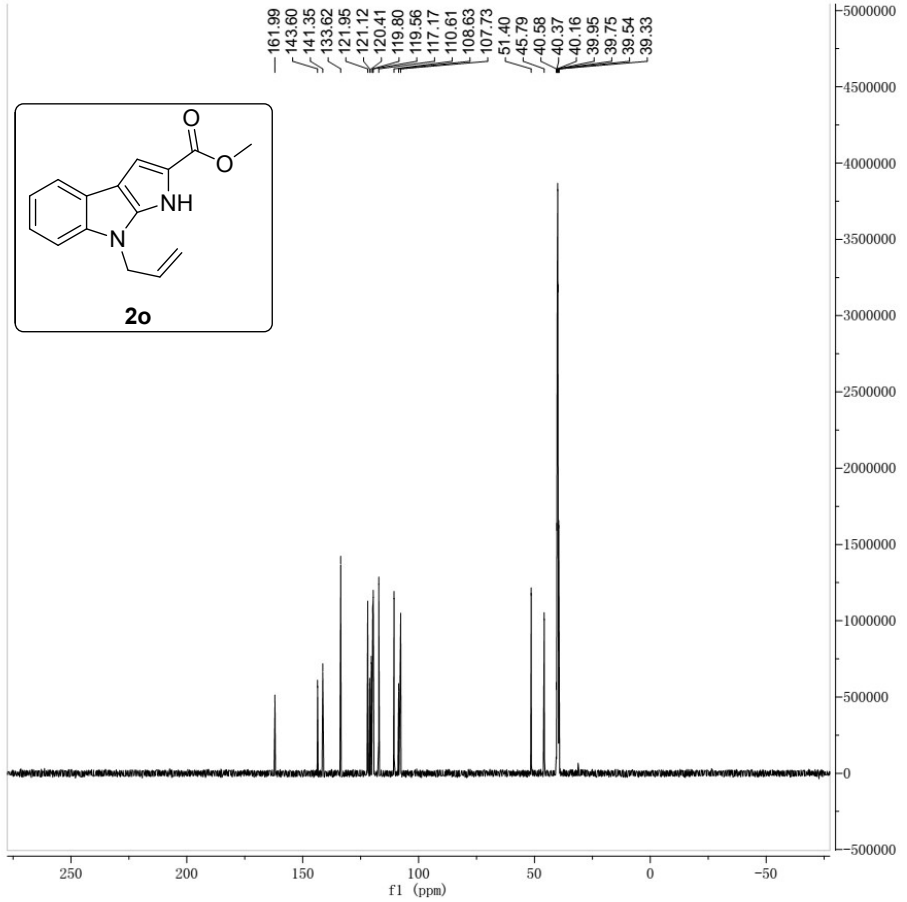
Sample Name	Sample10	**Position**	P1-B1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YZY-2016121902.d	**ACQ Method**	chen-ms.m	**Comment**		**Acquired Time**	12/22/2016 4:58:13 PM



methyl 8-allyl-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2o)

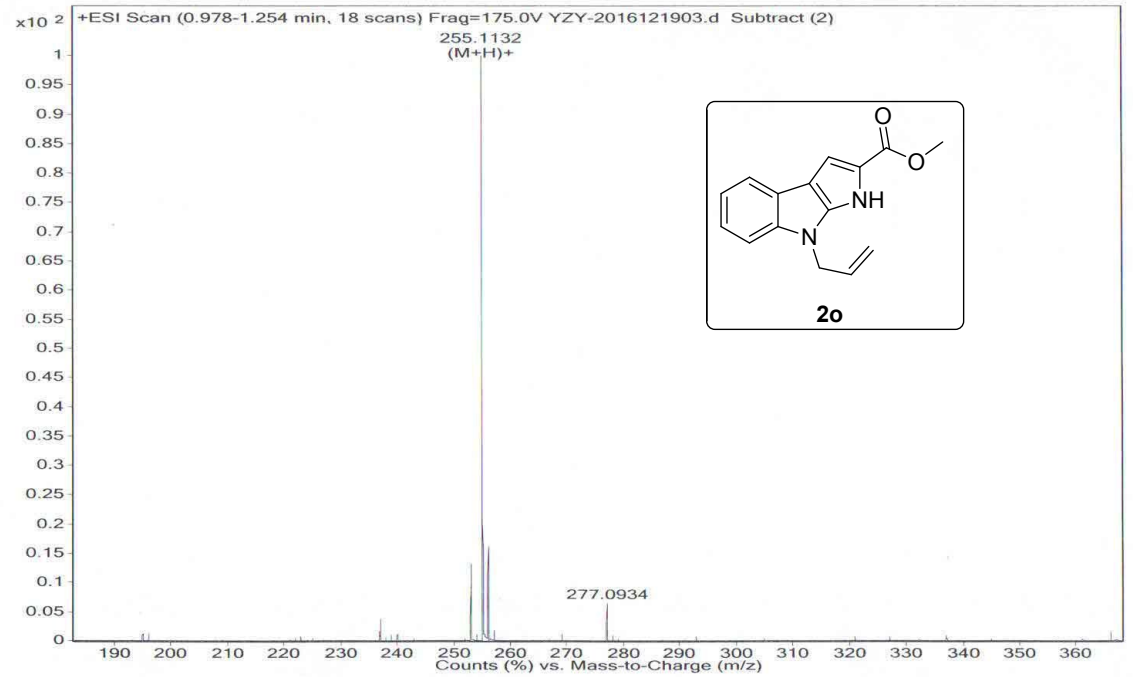


Parameter	Value
1 Data File Name	E:/ yzy-20161217-2/ 1/ pdata/ 1/ 1r
2 Title	yzy-20161217-2.1.1.1r
3 Comment	PROTON DMSO {D:\ NMR_DATA\ Wangbin} Wangbin 22
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	293.2
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	78
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2016-12-17T10:38:00
21 Modification Date	2016-12-17T10:34:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1535.4
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

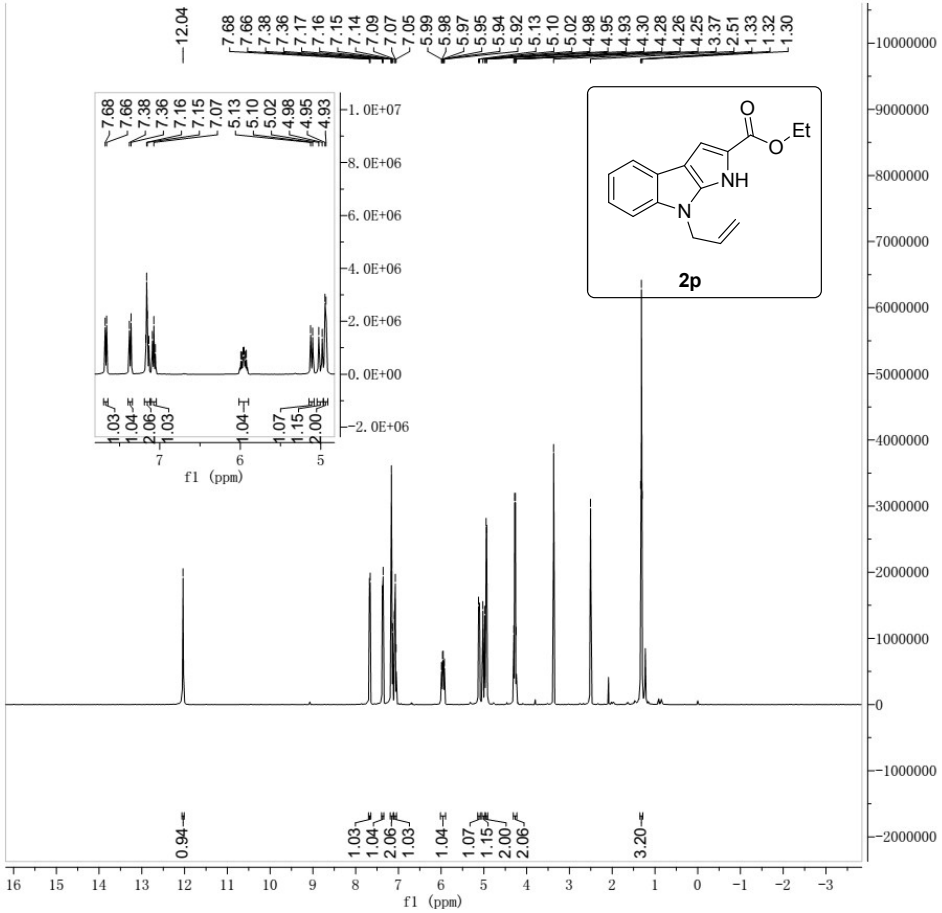


	Parameter	Value
1	Data File Name	E:/ yzy-20161217-2/ 2/ pdata/ 1/ 1r
2	Title	yzy-20161217-2.2.1.1r
3	Comment	C13CPD DMSO {D:\ NMR_DATA\ Wangbin} Wangbin 22
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	293.2
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	950
15	Receiver Gain	78
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	0.4999
20	Acquisition Date	2016-12-17T11:04:00
21	Modification Date	2016-12-17T11:00:00
22	Class	
23	Spectrometer Frequency	100.61
24	Spectral Width	35714.3
25	Lowest Frequency	-7796.8
26	Nucleus	13C
27	Acquired Size	17855
28	Spectral Size	32768

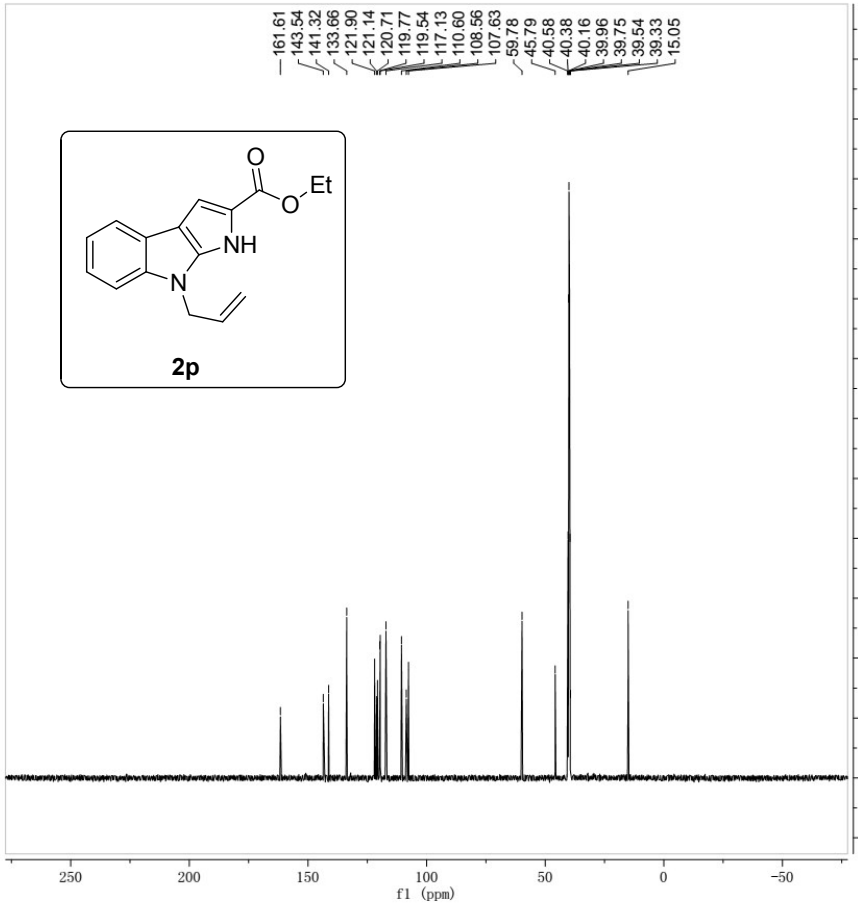
Sample Name	Sample11	**Position**	P1-B2	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YZY-2016121903.d	**ACQ Method**	chen-ms.m	**Comment**		**Acquired Time**	12/22/2016 5:03:53 PM



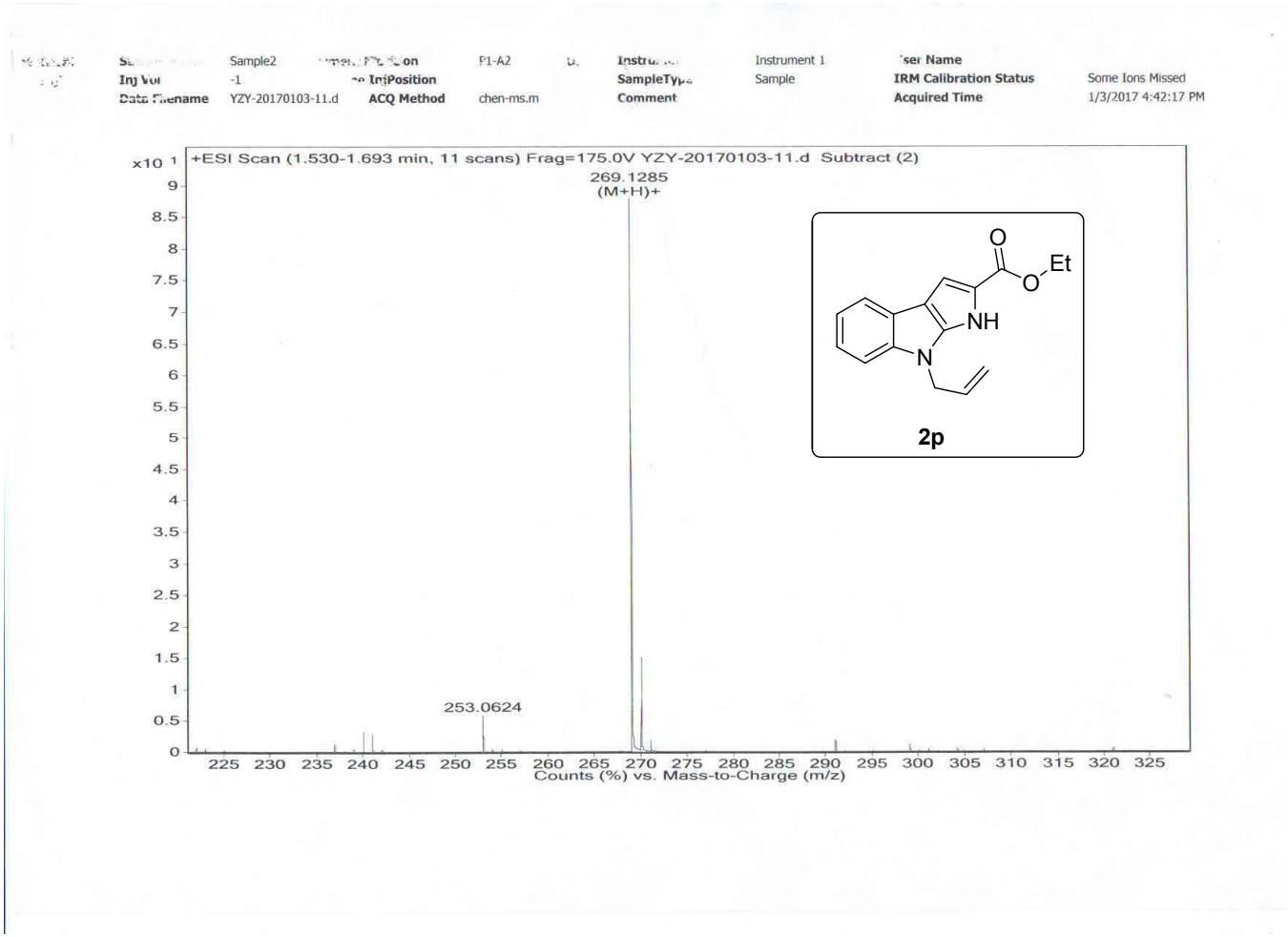
ethyl 8-allyl-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2p)



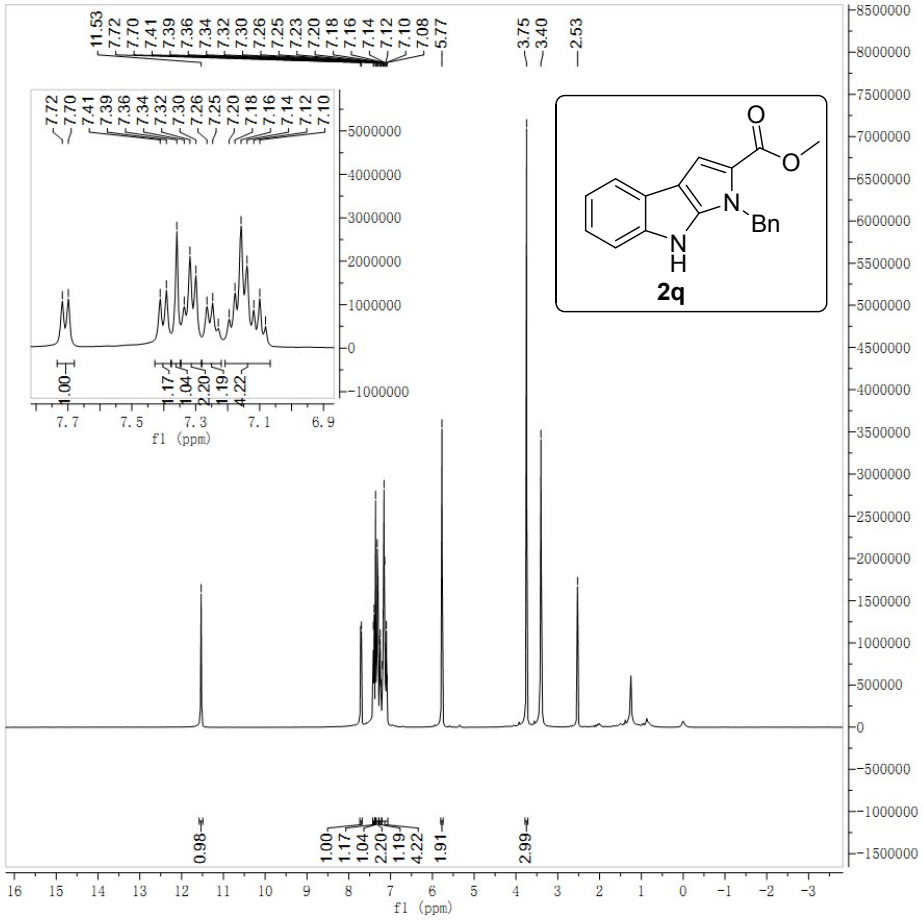
Parameter	Value
1 Data File Name	E:/ yzy-20161225-2/ 1/ pdata/ 1/ 1r
2 Title	yzy-20161225-2.1.1.1r
3 Comment	PROTON DMSO {D:\ NMR_DATA\ Wangbin} Wangbin 21
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	291.3
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	100
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2016-12-25T17:08:00
21 Modification Date	2016-12-25T17:04:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1536.8
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



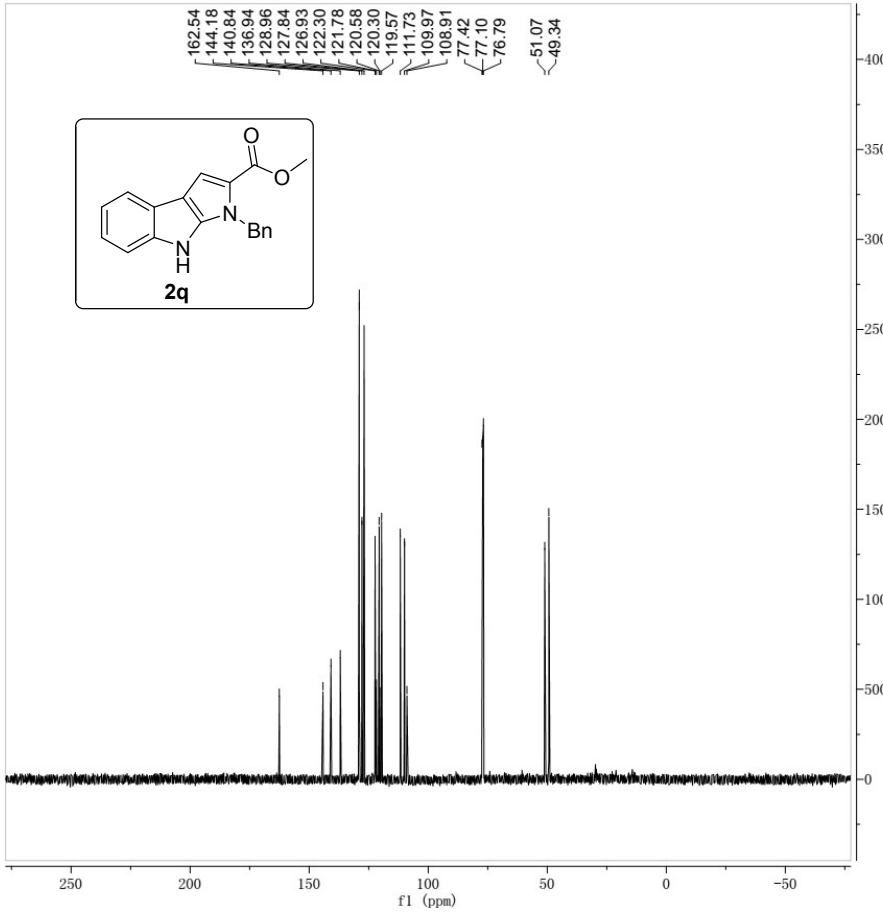
	Parameter	Value
1	Data File Name	E:/ yzy-20161225-2/ 2/ pdata/ 1/ 1r
2	Title	yzy-20161225-2.2.1.1r
3	Comment	C13CPD DMSO {D:\ NMR_DATA\ Wangbin} Wangbin 21
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	292.4
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	1024
15	Receiver Gain	159
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	0.4999
20	Acquisition Date	2016-12-25T17:36:00
21	Modification Date	2016-12-25T17:32:00
22	Class	
23	Spectrometer Frequency	100.61
24	Spectral Width	35714.3
25	Lowest Frequency	-7796.8
26	Nucleus	13C
27	Acquired Size	17855
28	Spectral Size	32768


Sample2
P1-A2
Instrument 1
User Name
Inj Vol
-1
Position
SampleType
Sample
IRM Calibration Status
Some Ions Missed
Data Filename
YZY-20170103-11.d
ACQ Method
chen-ms.m
Comment
Acquired Time
1/3/2017 4:42:17 PM
+ESI Scan (1.530-1.693 min, 11 scans) Frag=175.0V YZY-20170103-11.d Subtract (2)
x10 1
269.1285
(M+H)+
253.0624
Counts (%) vs. Mass-to-Charge (m/z)
O
O
Et
NH
N
2p

methyl 1-benzyl-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2q)

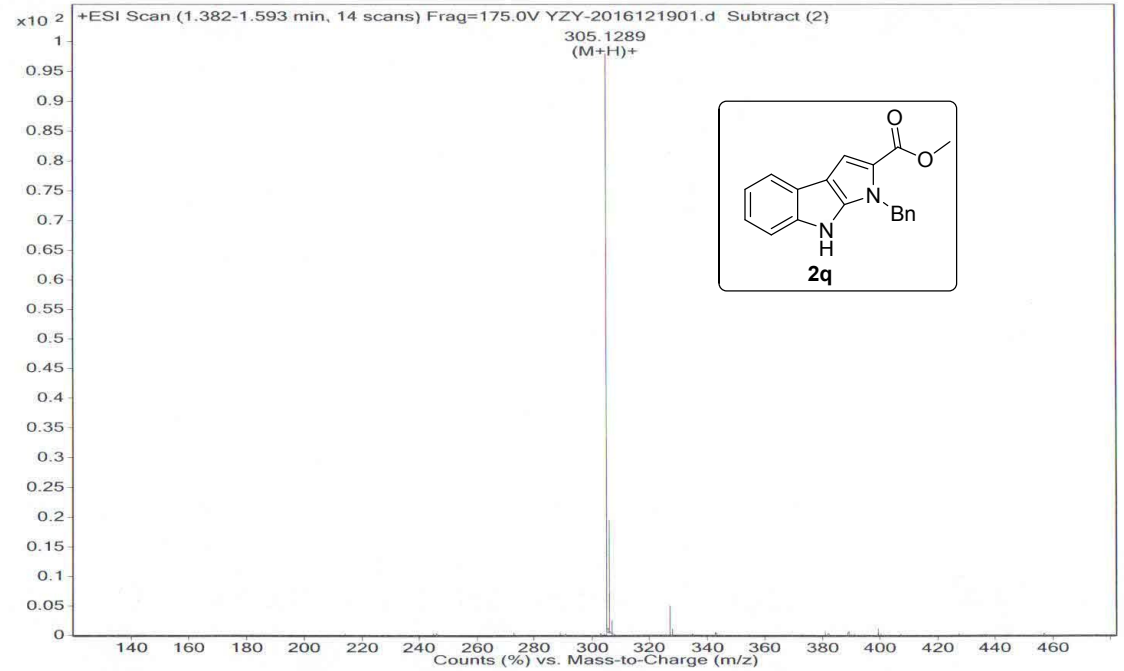


Parameter	Value
1 Data File Name	E:/ 杨钊英 核磁数据/ 吲哚并吡咯产物谱图/ N-苄基色氨酸甲酯产物/ d-DMSO 2q氢谱/ pdata/ 1/ 1r
2 Title	yzy-20170613-2q.1.1.1r
3 Comment	PROTON DMSO {D:\ NMR_DATA\ Wangbin} Wangbin 1
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	78
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2017-06-15T12:41:00
21 Modification Date	2017-06-15T12:42:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1528.8
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

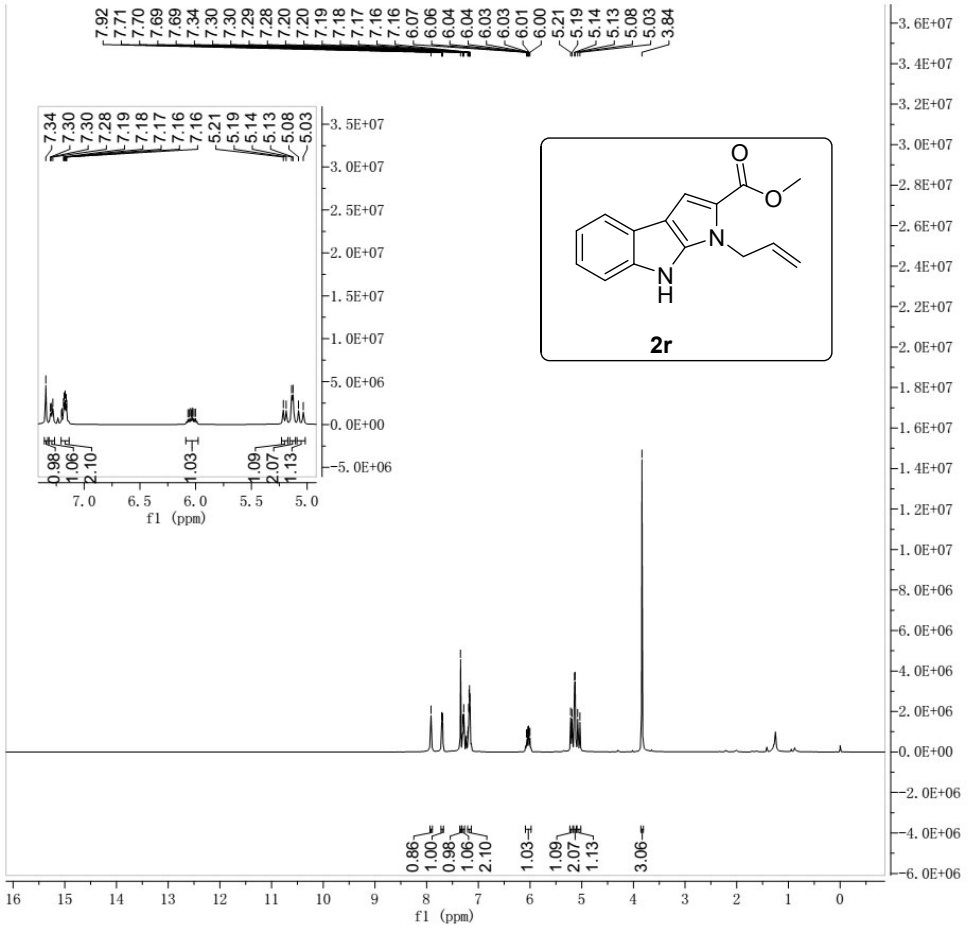


	Parameter	Value
1	Data File Name	E:/ yzy-20161126-2/ 2/ pdata/ 1/ 1r
2	Title	yzy-20161126-2.2.1.1r
3	Comment	C13CPD CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 13
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	293.7
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	900
15	Receiver Gain	100
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	0.4999
20	Acquisition Date	2016-11-26T16:04:00
21	Modification Date	2016-11-26T16:01:00
22	Class	
23	Spectrometer Frequency	100.61
24	Spectral Width	35714.3
25	Lowest Frequency	-7796.8
26	Nucleus	13C
27	Acquired Size	17855
28	Spectral Size	32768

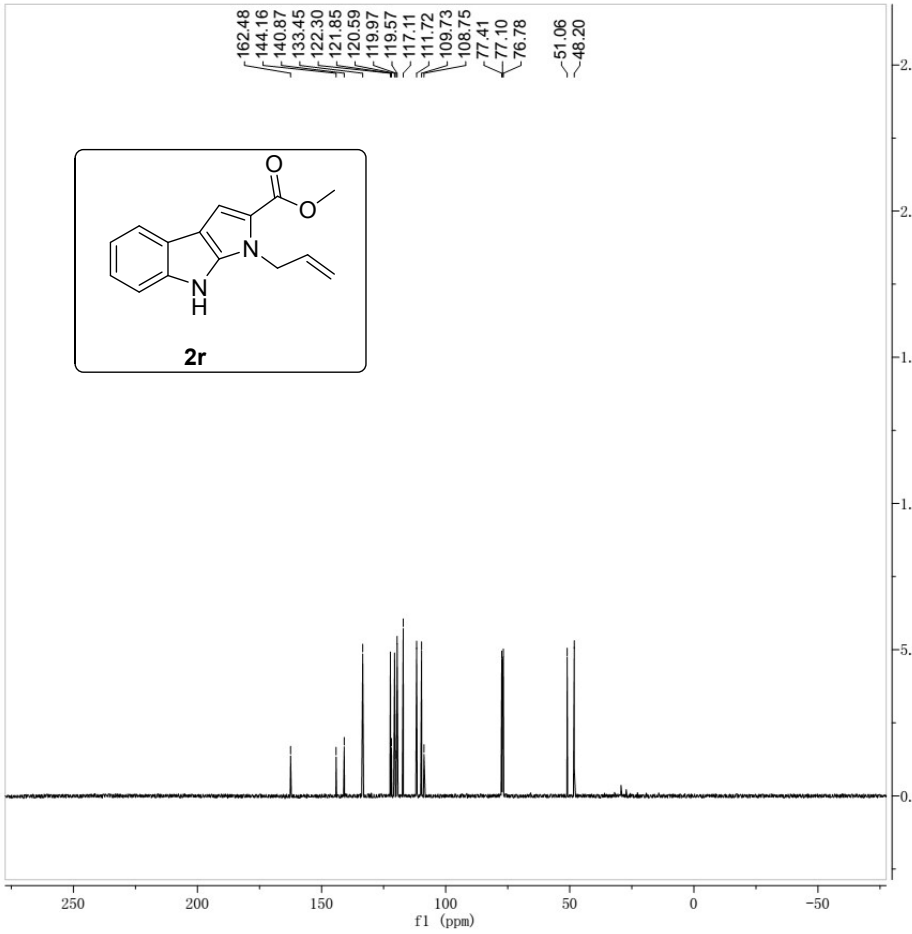
Sample Name	Sample9	**Position**	P1-A9	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YZY-2016121901.d	**ACQ Method**	chen-ms.m	**Comment**		**Acquired Time**	12/22/2016 4:52:31 PM



methyl 1-allyl-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2r)

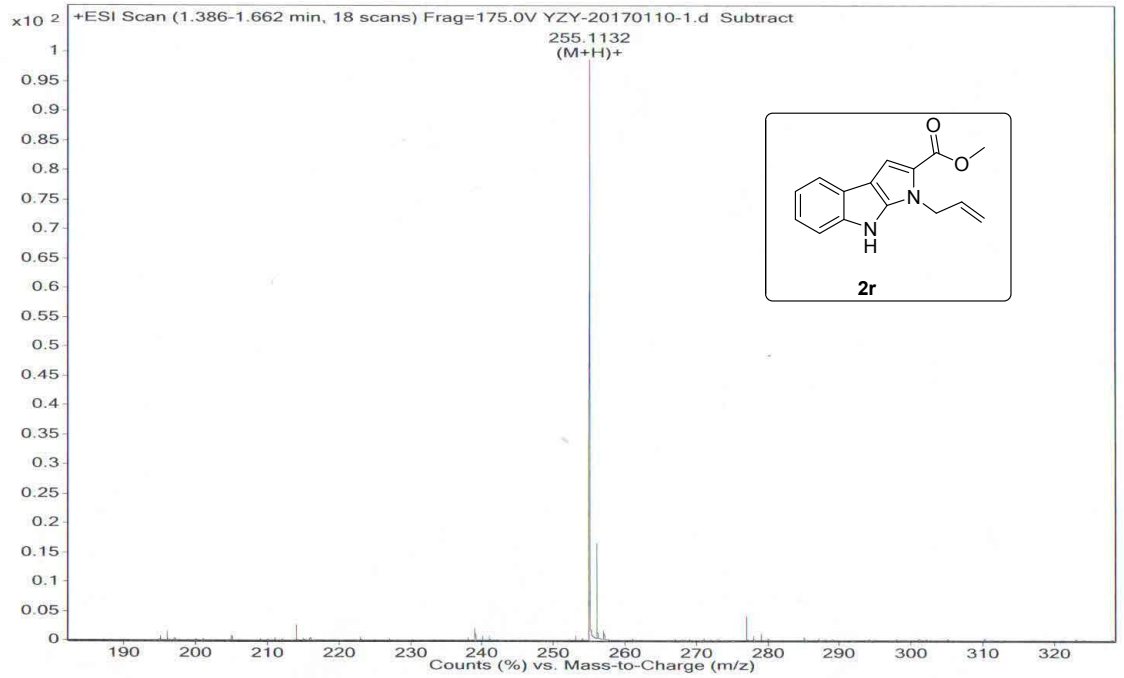


Parameter	Value
1 Data File Name	E:/ yzy-20170104-1/ 1/ pdata/ 1/ 1r
2 Title	yzy-20170104-1.1.1.1r
3 Comment	PROTON CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 8
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	293.2
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	78
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2017-01-04T11:37:00
21 Modification Date	2017-01-04T11:33:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1555.2
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

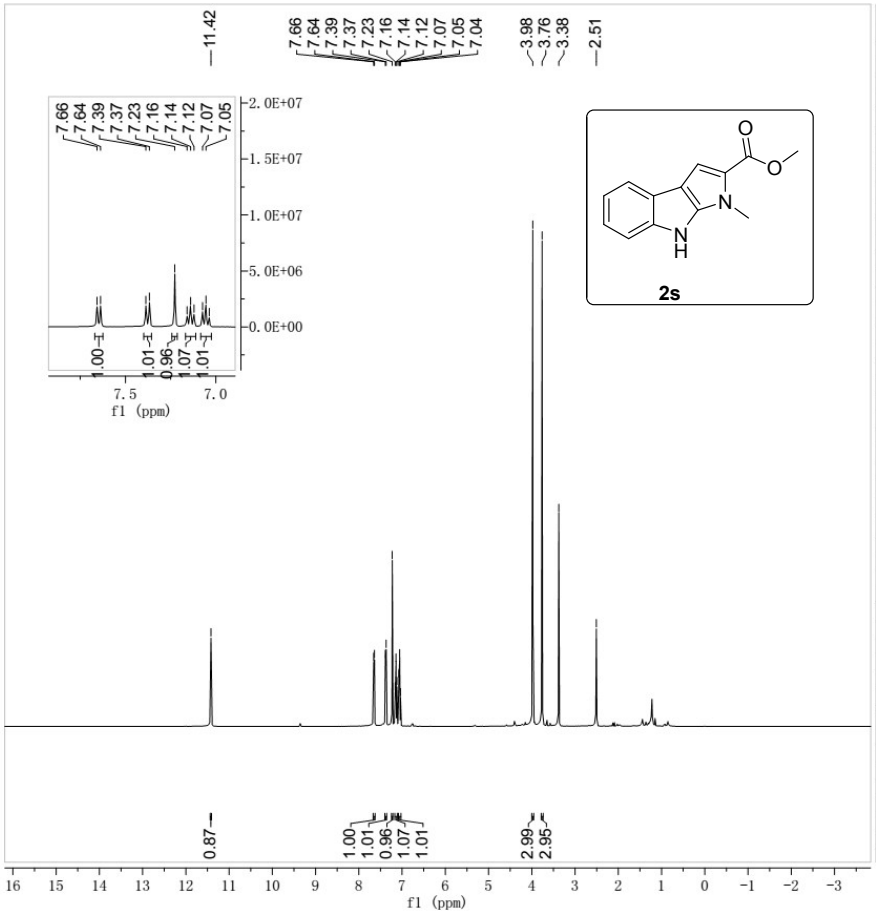


	Parameter	Value
1	Data File Name	E:/ yzy-20170104-1/ 2/ pdata/ 1/ 1r
2	Title	yzy-20170104-1.2.1.1r
3	Comment	C13CPD CDC13 {D:\ NMR_DATA\ Wangbin} Wangbin 8
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDC13
10	Temperature	294.2
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	1024
15	Receiver Gain	200
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	0.4999
20	Acquisition Date	2017-01-04T11:45:00
21	Modification Date	2017-01-04T12:01:00
22	Class	
23	Spectrometer Frequency	100.61
24	Spectral Width	35714.3
25	Lowest Frequency	-7796.8
26	Nucleus	13C
27	Acquired Size	17855
28	Spectral Size	32768

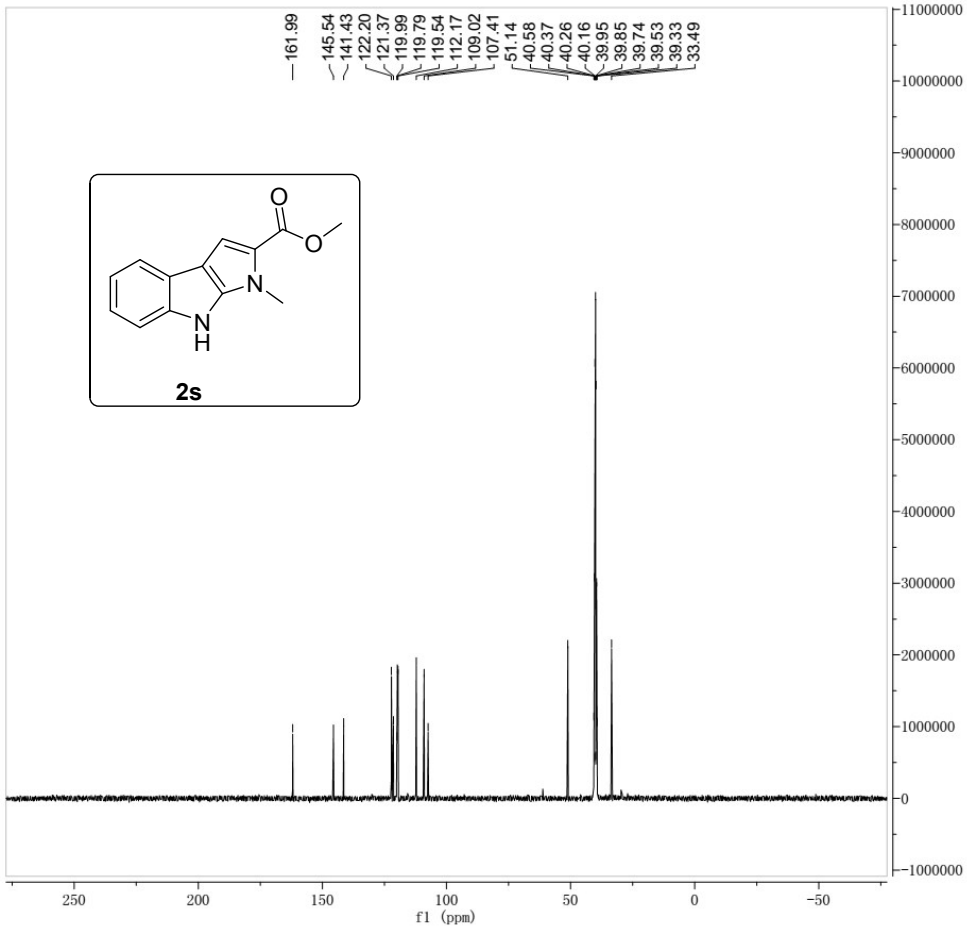
Sample Name	Sample41	**Position**	P1-E5	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YZY-20170110-1.d	**ACQ Method**	chen-ms.m	**Comment**		**Acquired Time**	2/21/2017 8:25:31 PM



methyl 1-methyl-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2s)

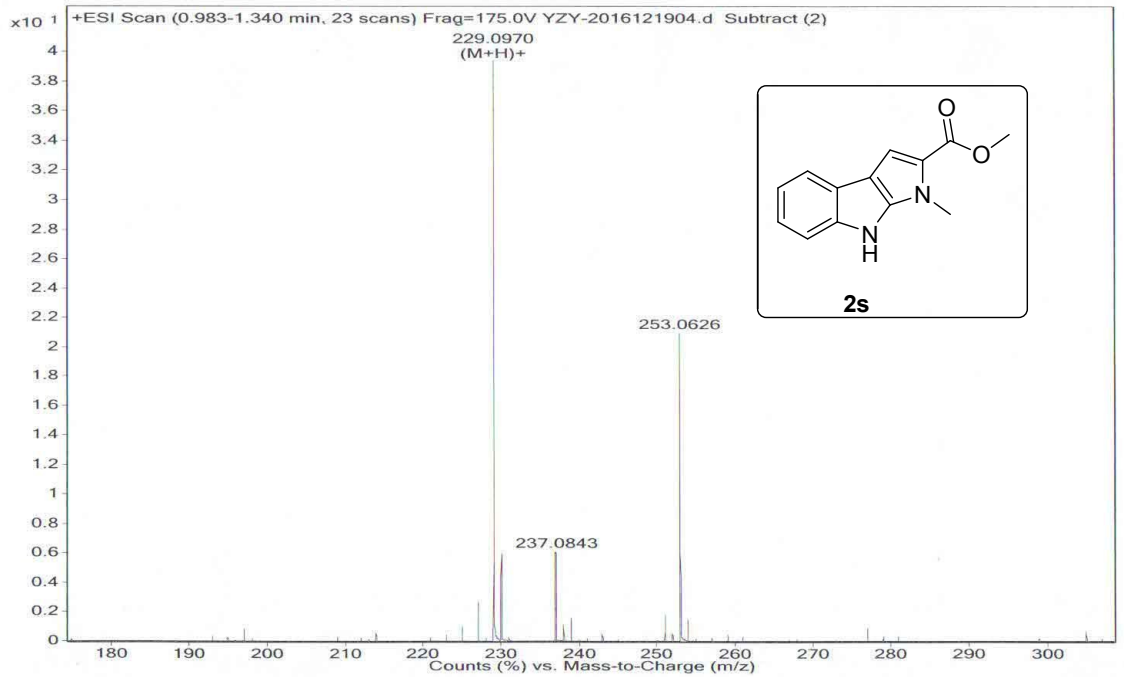


Parameter		Value
1	Data File Name	E:/ yzy-201612-8-4/ 1/ pdata/ 1/ 1r
2	Title	yzy-201612-8-4.1.1.1r
3	Comment	PROTON DMSO {D:\ NMR_DATA\ Wangbin} Wangbin 3
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	293.2
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	16
15	Receiver Gain	100
16	Relaxation Delay	1.0000
17	Pulse Width	14.4000
18	Presaturation Frequency	
19	Acquisition Time	4.0894
20	Acquisition Date	2016-12-08T20:13:00
21	Modification Date	2016-12-08T20:09:00
22	Class	
23	Spectrometer Frequency	400.13
24	Spectral Width	8012.8
25	Lowest Frequency	-1535.4
26	Nucleus	1H
27	Acquired Size	32768
28	Spectral Size	65536

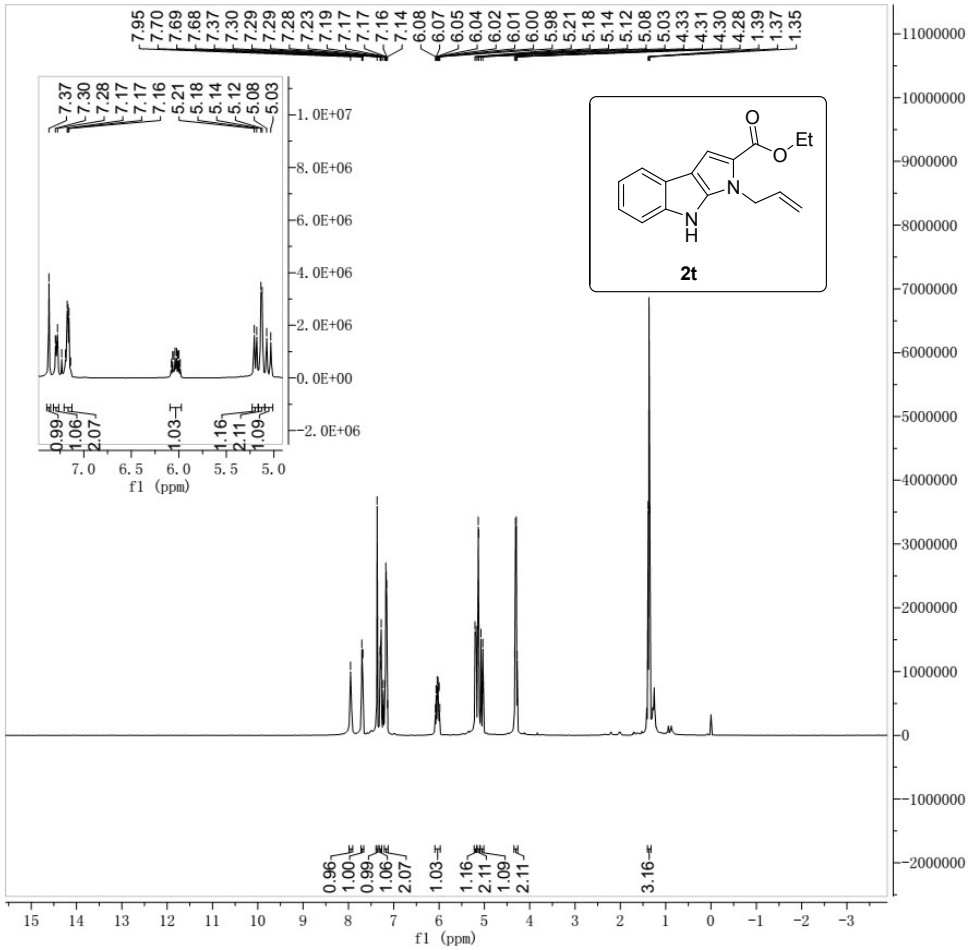


	Parameter	Value
1	Data File Name	E:/ yzy-201612-8-4/ 2/ pdata/ 1/ 1r
2	Title	yzy-201612-8-4.2.1.1r
3	Comment	C13CPD DMSO {D:\ NMR_DATA\ Wangbin} Wangbin 3
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	293.1
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	1150
15	Receiver Gain	113
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	0.4999
20	Acquisition Date	2016-12-08T20:44:00
21	Modification Date	2016-12-08T20:40:00
22	Class	
23	Spectrometer Frequency	100.61
24	Spectral Width	35714.3
25	Lowest Frequency	-7796.8
26	Nucleus	13C
27	Acquired Size	17855
28	Spectral Size	32768

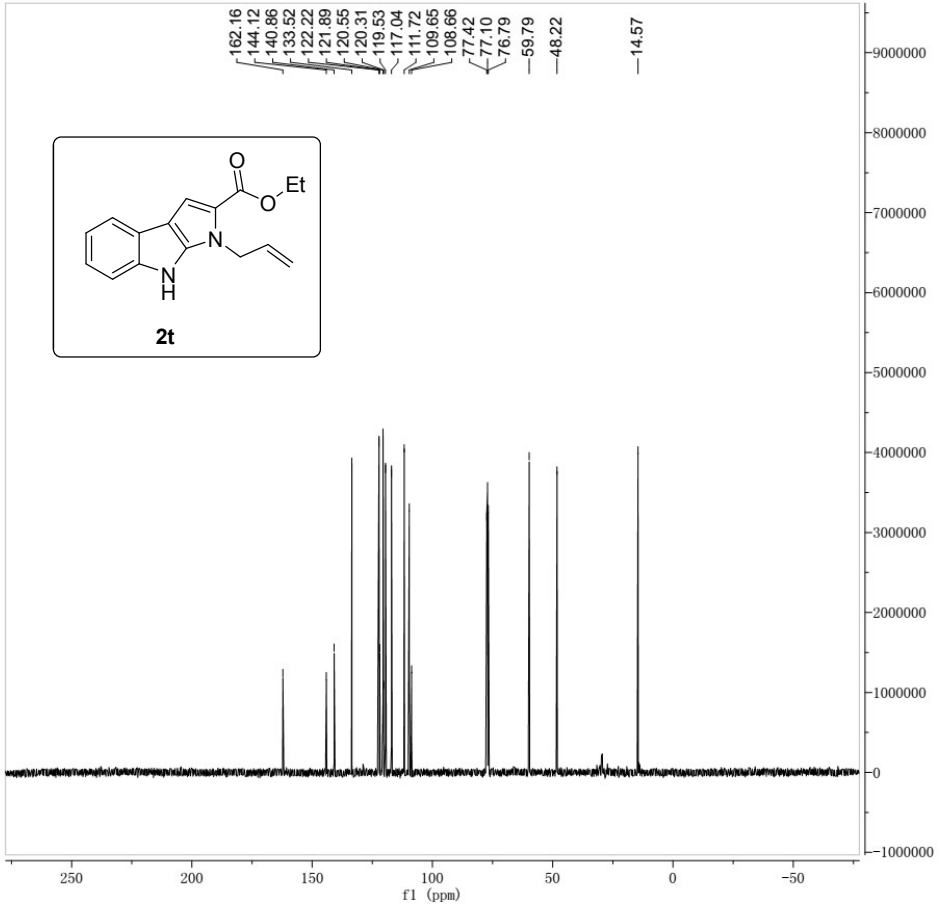
Sample Name	Sample12	**Position**	P1-B3	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YZY-2016121904.d	**ACQ Method**	chen-ms.m	**Comment**		**Acquired Time**	12/22/2016 5:09:33 PM



ethyl 1-allyl-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2t)

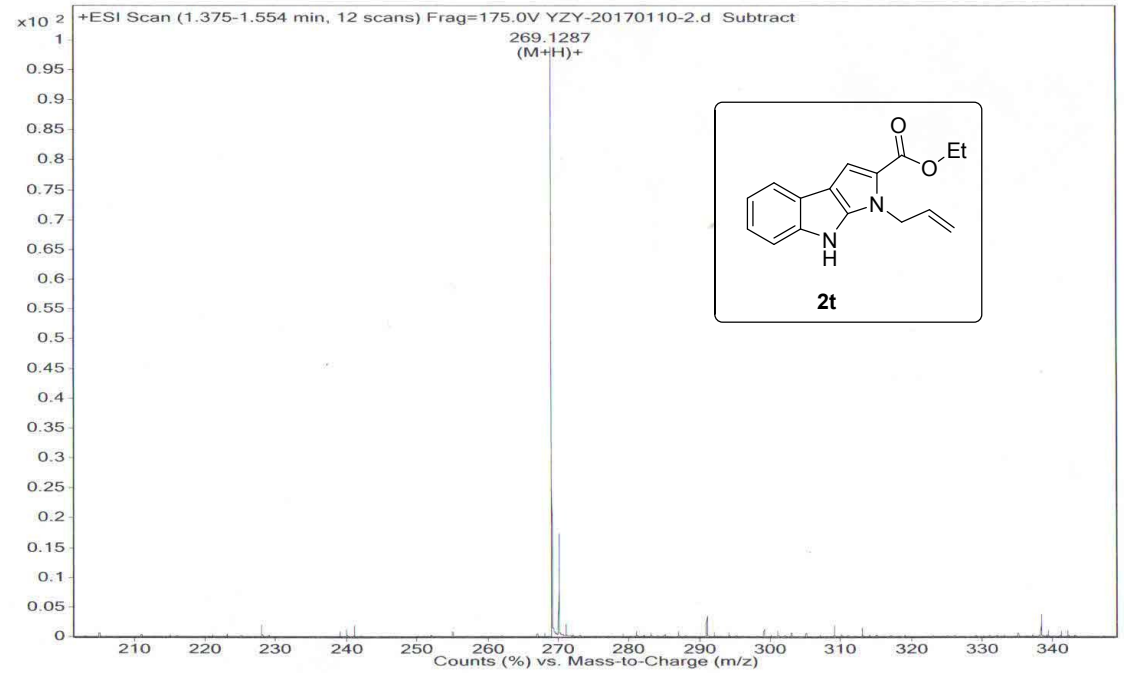


	Parameter	Value
1	Data File Name	E:/ yzy-20170104-2/ 1/ pdata/ 1/ 1r
2	Title	yzy-20170104-2.1.1.1r
3	Comment	PROTON CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 5
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	293.2
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	16
15	Receiver Gain	61
16	Relaxation Delay	1.0000
17	Pulse Width	14.4000
18	Presaturation Frequency	
19	Acquisition Time	4.0894
20	Acquisition Date	2017-01-04T20:59:00
21	Modification Date	2017-01-04T20:55:00
22	Class	
23	Spectrometer Frequency	400.13
24	Spectral Width	8012.8
25	Lowest Frequency	-1556.2
26	Nucleus	1H
27	Acquired Size	32768
28	Spectral Size	65536



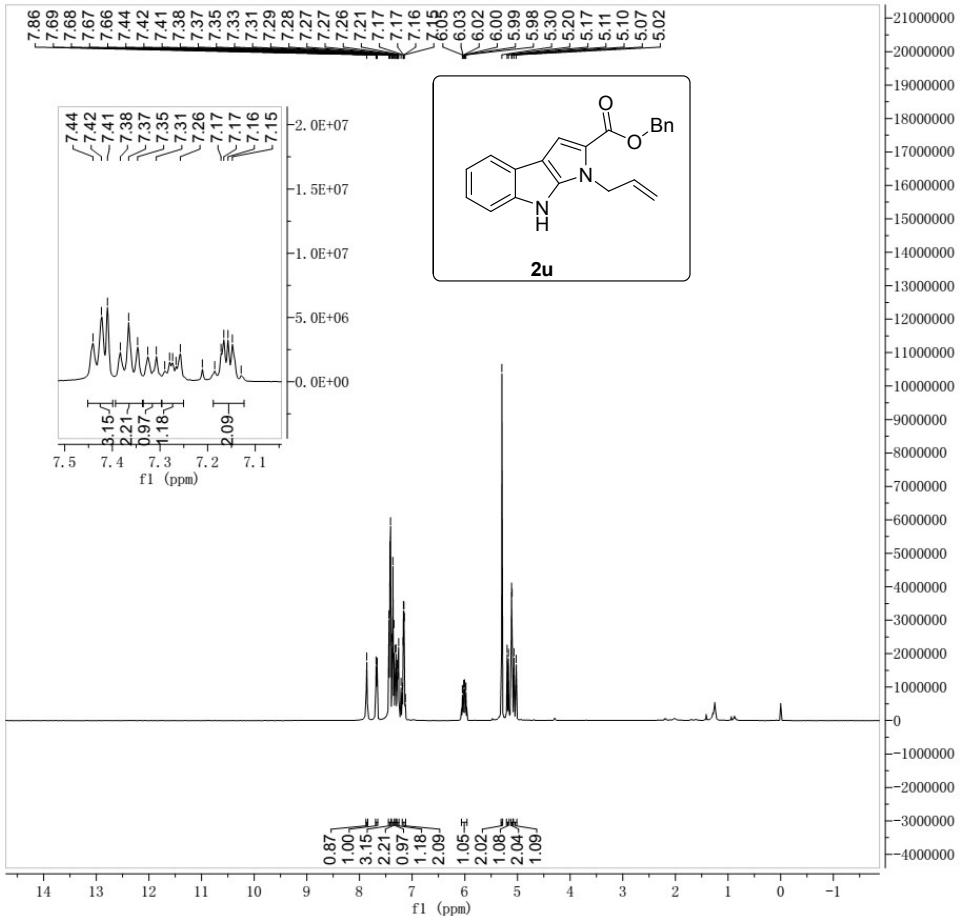
	Parameter	Value
1	Data File Name	E:/ yzy-20170104-2/ 2/ pdata/ 1/ 1r
2	Title	yzy-20170104-2.2.1.1r
3	Comment	C13CPD CDC13 {D:\ NMR_DATA\ Wangbin} Wangbin 5
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	294.4
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	850
15	Receiver Gain	176
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	0.4999
20	Acquisition Date	2017-01-04T21:23:00
21	Modification Date	2017-01-04T21:19:00
22	Class	
23	Spectrometer Frequency	100.61
24	Spectral Width	35714.3
25	Lowest Frequency	-7796.8
26	Nucleus	13C
27	Acquired Size	17855
28	Spectral Size	32768

Sample Name	Sample42	**Position**	P1-E6	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YZY-20170110-2.d	**ACQ Method**	chen-ms.m	**Comment**		**Acquired Time**	2/21/2017 8:31:12 PM

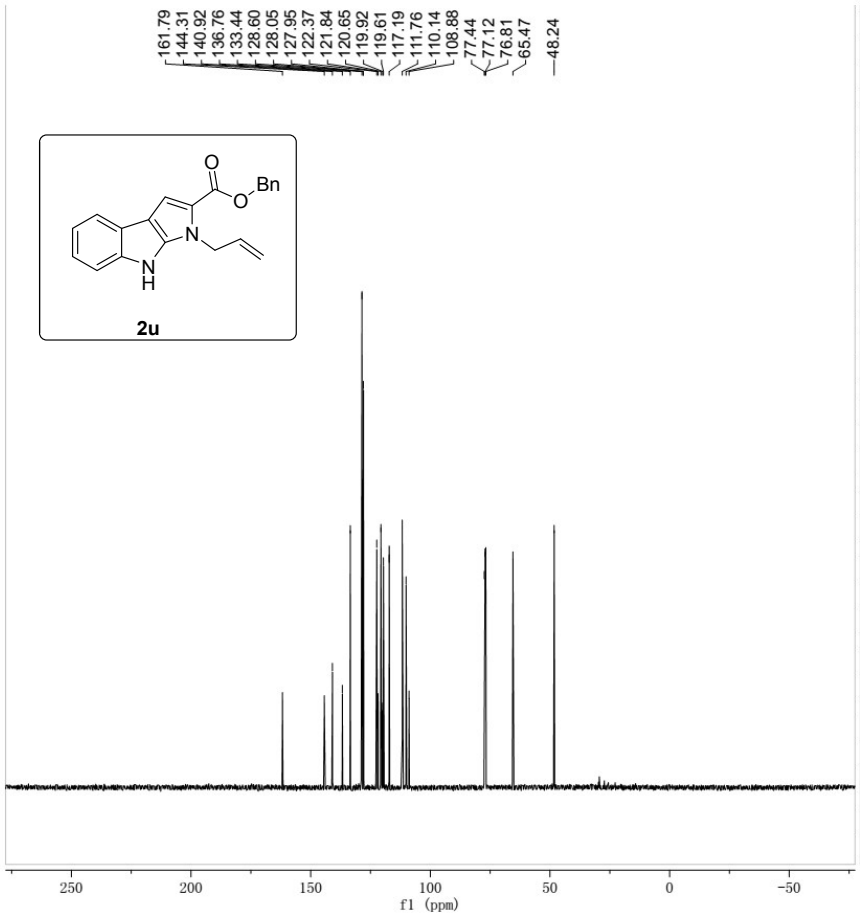


2t

benzyl 1-allyl-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2u)

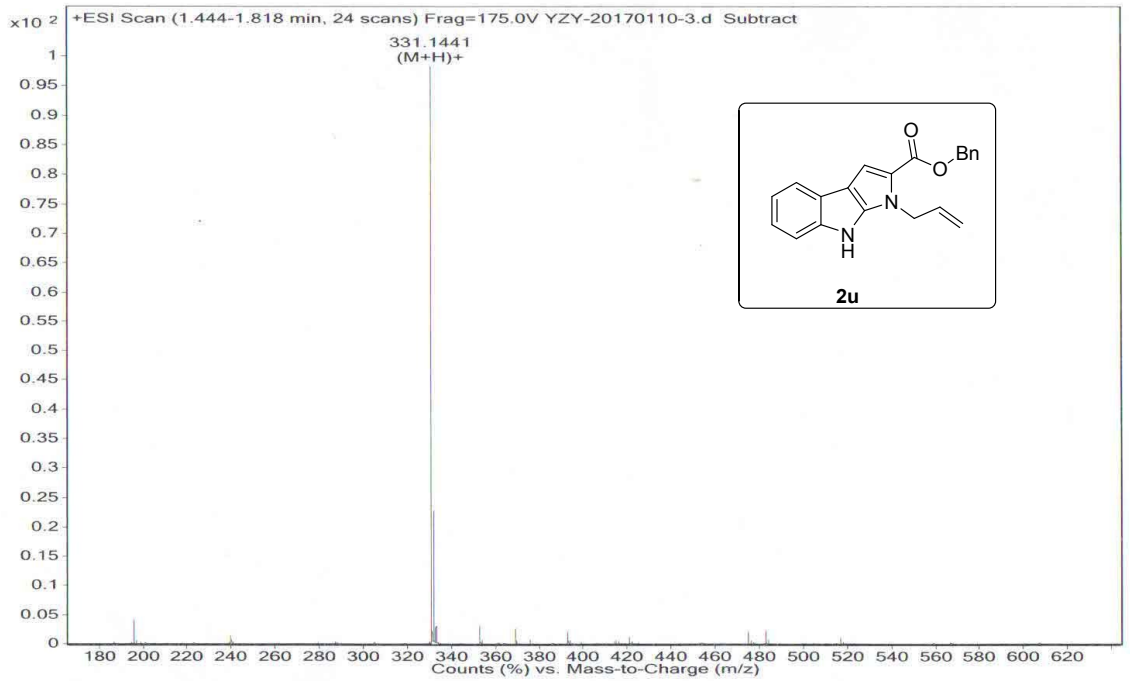


	Parameter	Value
1	Data File Name	E:/ yzy-20170104-3/ 1/ pdata/ 1/ 1r
2	Title	yzy-20170104-3.1.1.1r
3	Comment	PROTON CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 6
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	293.4
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	16
15	Receiver Gain	61
16	Relaxation Delay	1.0000
17	Pulse Width	14.4000
18	Presaturation Frequency	
19	Acquisition Time	4.0894
20	Acquisition Date	2017-01-04T21:28:00
21	Modification Date	2017-01-04T21:25:00
22	Class	
23	Spectrometer Frequency	400.13
24	Spectral Width	8012.8
25	Lowest Frequency	-1565.1
26	Nucleus	1H
27	Acquired Size	32768
28	Spectral Size	65536

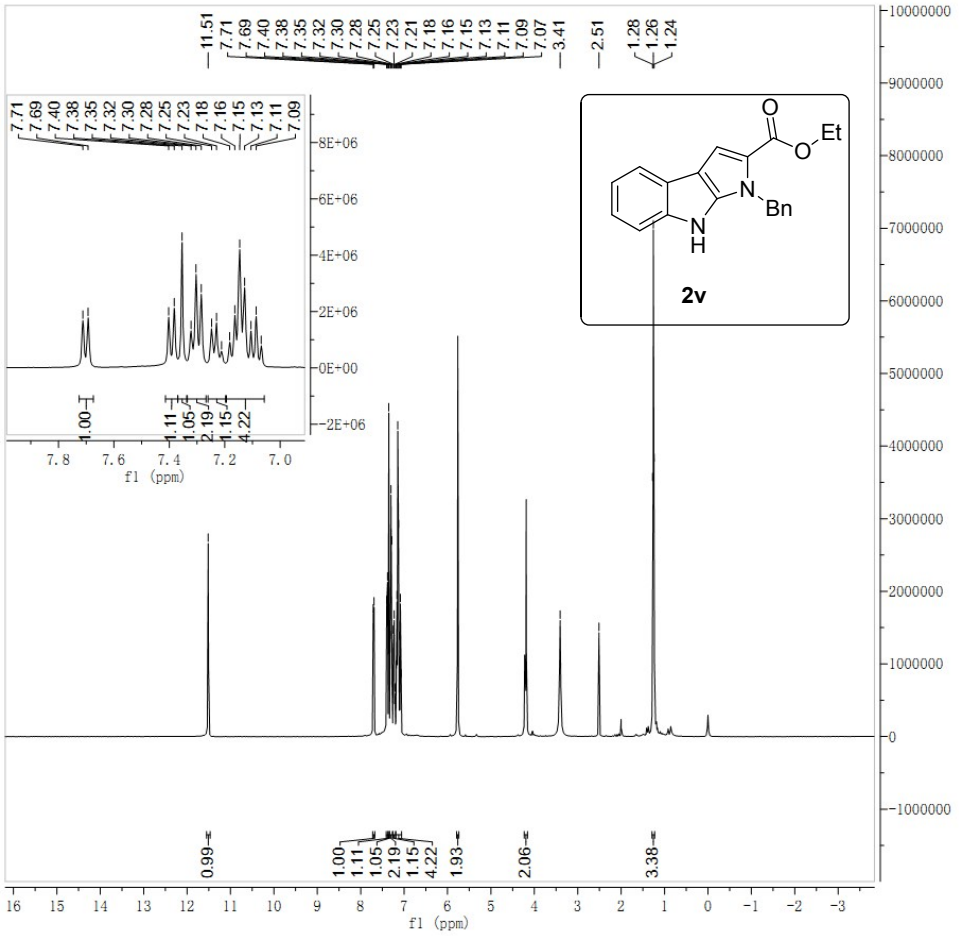


Parameter	Value
1 Data File Name	E:/ yzy-20170104-3/ 2/ pdata/ 1/ 1r
2 Title	yzy-20170104-3.2.1.1r
3 Comment	C13CPD CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 6
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	294.4
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	850
15 Receiver Gain	200
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.4999
20 Acquisition Date	2017-01-04T21:51:00
21 Modification Date	2017-01-04T21:47:00
22 Class	
23 Spectrometer Frequency	100.61
24 Spectral Width	35714.3
25 Lowest Frequency	-7796.8
26 Nucleus	13C
27 Acquired Size	17855
28 Spectral Size	32768

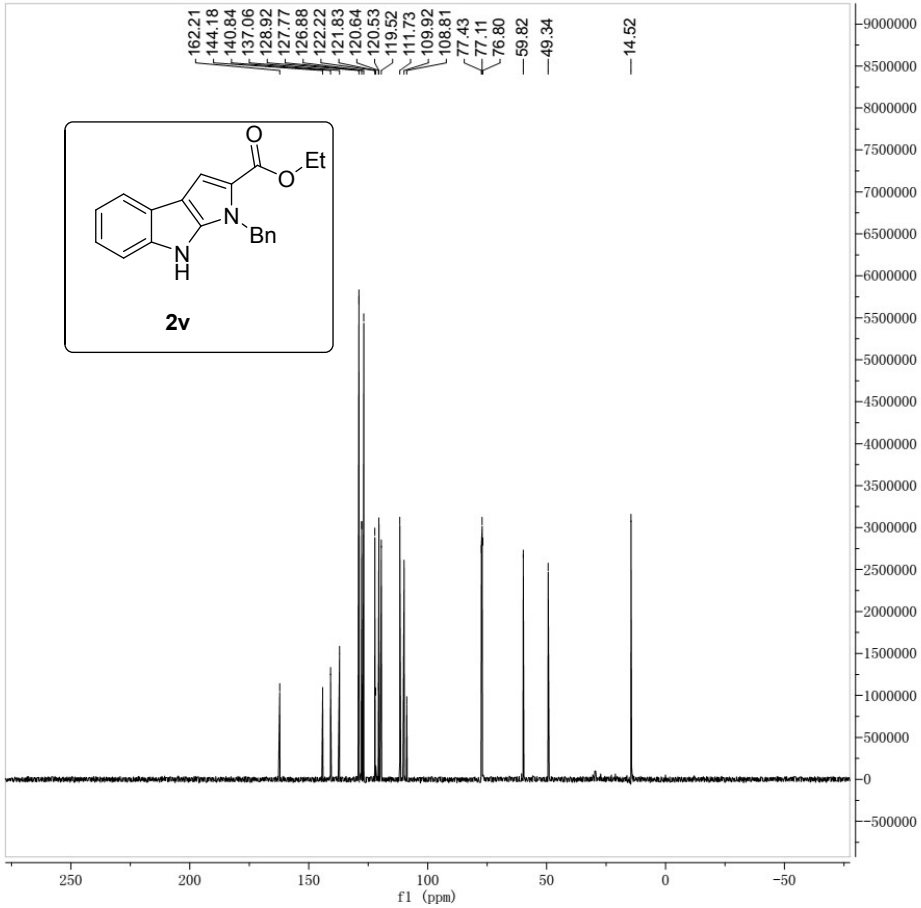
Sample Name	Sample43	**Position**	P1-E7	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YZY-20170110-3.d	**ACQ Method**	chen-ms.m	**Comment**		**Acquired Time**	2/21/2017 8:36:52 PM



ethyl 1-benzyl-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2v)

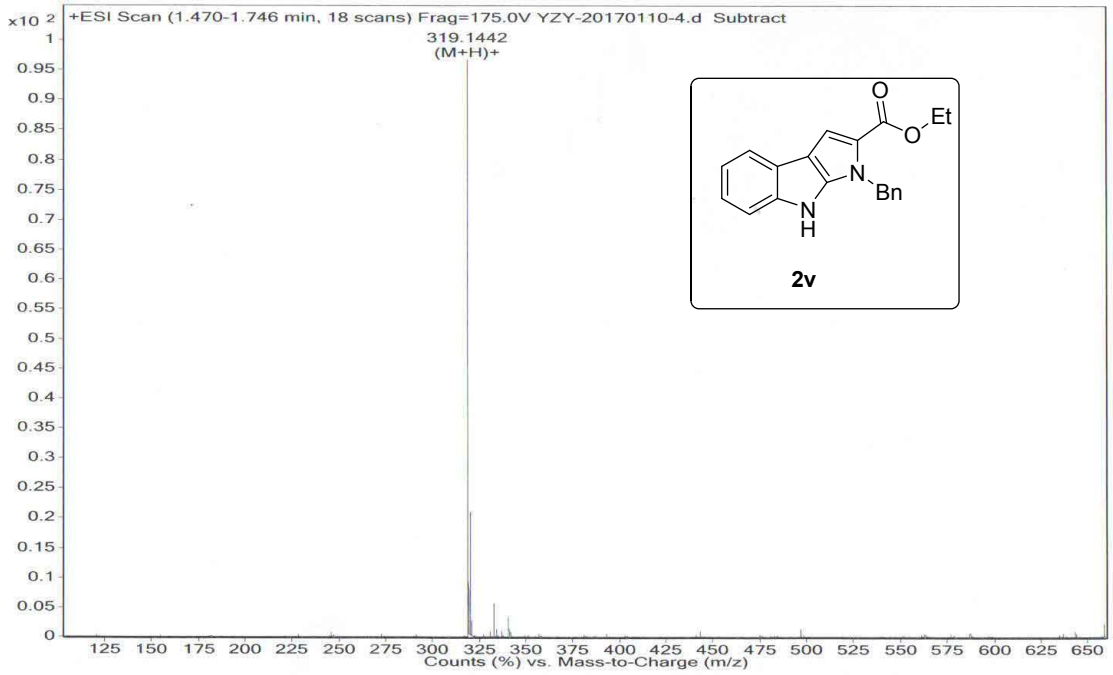


	Parameter	Value
1	Data File Name	E:/ 杨钊英 核磁数据/ 吲哚并吡咯产物谱图/ N-苄基色氨酸乙酯产物/ d-DMSO 2V氢谱/ pdata/ 1/ 1r
2	Title	yzy-20170613-2v.1.1.1r
3	Comment	PROTON DMSO {D:\ NMR_DATA\ Wangbin} Wangbin 2
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	298.0
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	16
15	Receiver Gain	56
16	Relaxation Delay	1.0000
17	Pulse Width	14.4000
18	Presaturation Frequency	
19	Acquisition Time	4.0894
20	Acquisition Date	2017-06-15T12:45:00
21	Modification Date	2017-06-15T12:46:00
22	Class	
23	Spectrometer Frequency	400.13
24	Spectral Width	8012.8
25	Lowest Frequency	-1535.0
26	Nucleus	1H
27	Acquired Size	32768
28	Spectral Size	65536

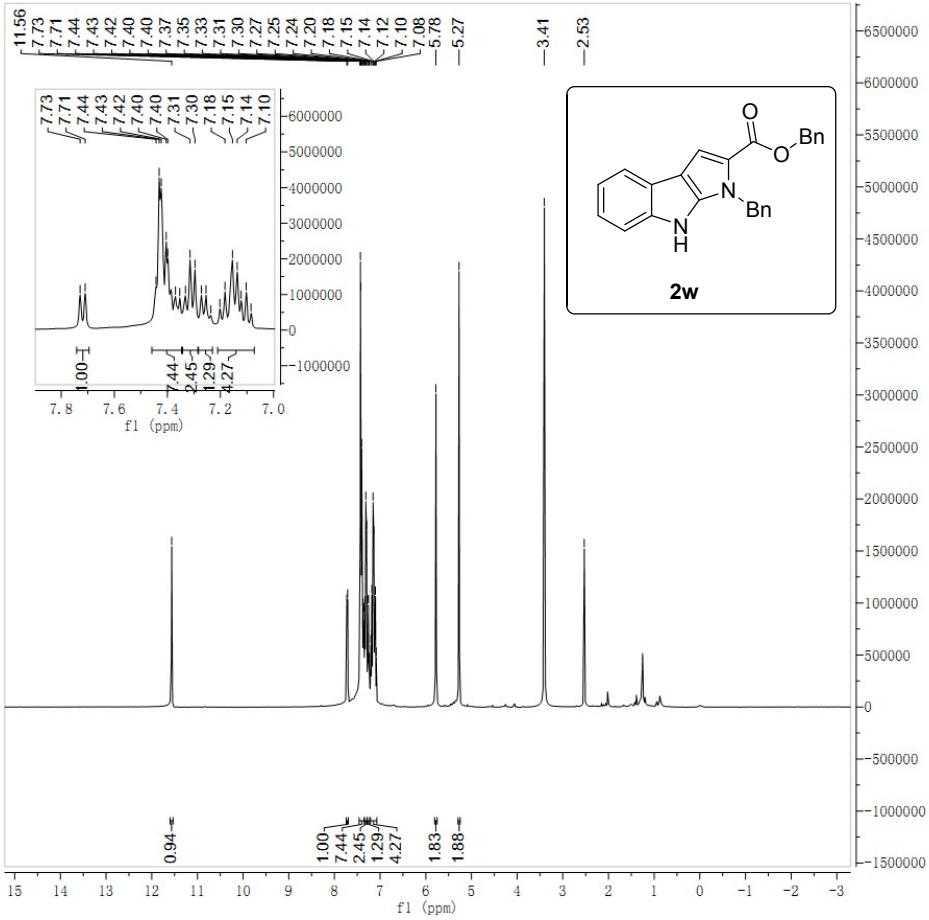


	Parameter	Value
1	Data File Name	E:/ yzy-20170106-1/ 2/ pdata/ 1/ 1r
2	Title	yzy-20170106-1.2.1.1r
3	Comment	C13CPD CDC13 {D:\ NMR_DATA\ Wangbin} Wangbin 16
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	295.0
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	850
15	Receiver Gain	113
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	0.4999
20	Acquisition Date	2017-01-06T10:33:00
21	Modification Date	2017-01-06T10:29:00
22	Class	
23	Spectrometer Frequency	100.61
24	Spectral Width	35714.3
25	Lowest Frequency	-7796.8
26	Nucleus	13C
27	Acquired Size	17855
28	Spectral Size	32768

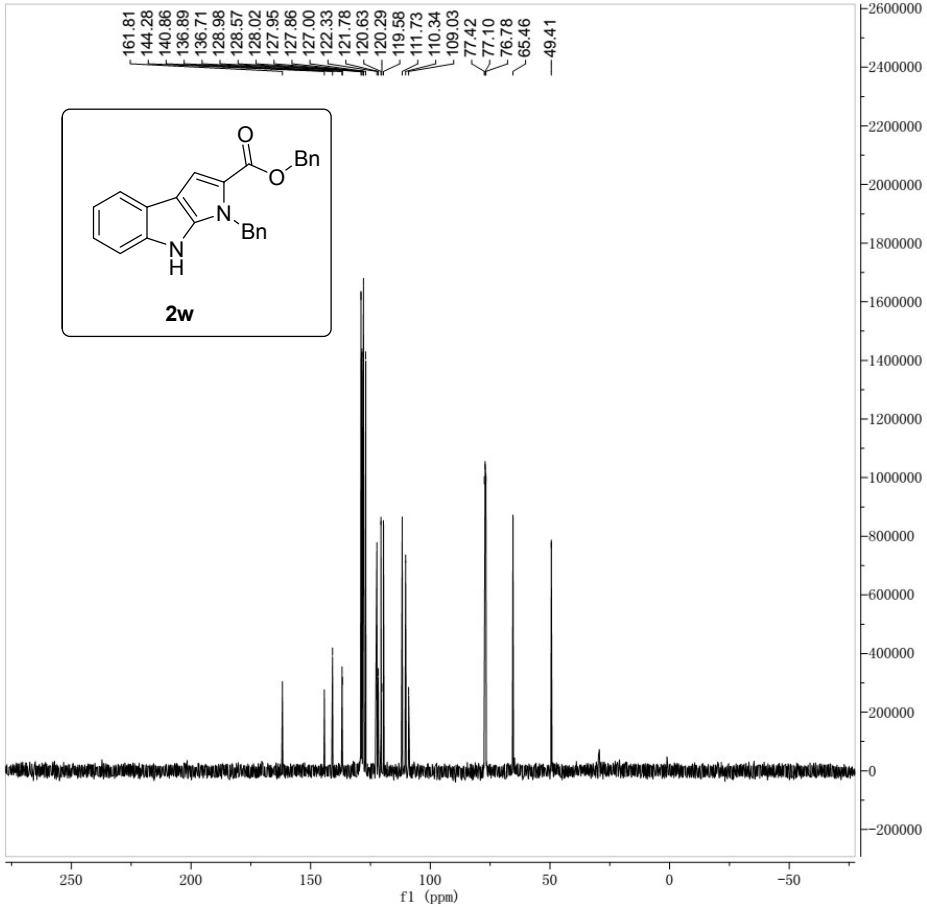
Sample Name	Sample44	**Position**	P1-E8	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YZY-20170110-4.d	**ACQ Method**	chen-ms.m	**Comment**		**Acquired Time**	2/21/2017 8:42:34 PM



benzyl 1-benzyl-1,8-dihydropyrrolo[2,3-b]indole-2-carboxylate (2w)



Parameter	Value
1 Data File Name	E:/ 杨钊英 核磁数据/ 吲哚并吡咯产物谱图/ N-苄基色氨酸苄酯产物/ d-DMSO 2W氢谱/ pdata/ 1/ 1r
2 Title	yzy-20170613-2w.1.1.1r
3 Comment	PROTON DMSO {D:\ NMR_DATA\ Wangbin} Wangbin 3
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	71
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2017-06-15T12:50:00
21 Modification Date	2017-06-15T12:51:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1527.3
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



	Parameter	Value
1	Data File Name	E:/ yzy-20170111-1/ 2/ pdata/ 1/ 1r
2	Title	yzy-20170111-1.2.1.1r
3	Comment	C13CPD CDC13 {D:\ NMR_DATA\ Wangbin} Wangbin 22
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	295.7
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	543
15	Receiver Gain	113
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	0.4999
20	Acquisition Date	2017-01-11T09:18:00
21	Modification Date	2017-01-11T09:16:00
22	Class	
23	Spectrometer Frequency	100.61
24	Spectral Width	35714.3
25	Lowest Frequency	-7796.8
26	Nucleus	13C
27	Acquired Size	17855
28	Spectral Size	32768

Sample Name	Sample45	**Position**	P1-E9	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YZY-20170110-5.d	**ACQ Method**	chen-ms.m	**Comment**		**Acquired Time**	2/21/2017 8:48:15 PM