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Mild cuprous halide mediated direct C^3 monohalogenation of indoles

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1. General

Information

All reactions were carried out under air. NMR spectra were recorded on a Bruker Avance spectrometer operating at 400 MHz (^{1}H NMR) or 101 MHz (^{13}C NMR) in DMSO-d_6 or $CDCl_3$. All ^{1}H NMR chemical shifts were reported in ppm and were referenced to the residual peaks of $CDCl_3$ at 7.26, coupling constants *J* were given in Hz. The following abbreviations are used to describe peak patterns where appropriate: singlet (s), doubet (d), doublet of doublets (dd), triplet (t), multiplet (m), and broad resonances (br). Mass spectra (MS) were obtained on a 6200 series TOF/6500 apparatus or a waters Q-TOF micro TM apparatus. The thin layer chromatography (TLC) was performed on pre-coated, glass-backed silica gel plates. Visualization of the developed chromatogram was performed by UV absorbance (254 nm).

Chemicals

Unless noted otherwise, the materials obtained from commercial suppliers were used without further purification. All solvents were analytical purity.

2. Experimental procedure

General Procedure for the Halogenation of indoles

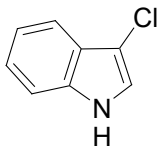
To a 25 mL flask equipped with a magnetic stirring bar and condenser tube were added indole derivatives (**1a~1i**) (1.0 mmol), cuprous halide (1.1 mmol), *N*-fluorobenzenesulfonimide (1.1 mmol), and acetonitrile (5 mL) under atmosphere. The reaction mixture was stirred at room temperature for 1-5 h, and then the mixture was filtered through a plug of celite, the filtrate was concentrated in a vacuum and purified to give **2** by chromatography (PE/EtOAc) as an eluent.

Radical Inhibition Experiments for Monohalogenation of indole at C^3 Position.

To a 25 mL flask equipped with a magnetic stirring bar and condenser tube was added indole **1a** (1.0 mmol), cuprous chloride (1.1 mmol), TEMPO (5.0 mmol), *N*-fluorobenzenesulfonimide (1.1 mmol), and acetonitrile (5 mL) under atmosphere. The reaction mixture was stirred at ambient temperature for 1 h. TLC indicated that C^3 mono-halogenated product **2a** with normal yield, and then the mixture was filtered through a plug of celite, the filtrate was concentrated in a vacuum and purified to give **2a** by chromatography (PE/EtOAc = 20:1~5:1) as an eluent.

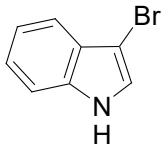
3. Characterization of all Products

3-Chloro-1H-indole **(2a)**



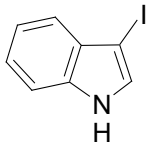
Obtained as an off-white solid (145 mg, 96%).
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 11.37 (s, 1H), 7.55 – 7.47 (m, 2H), 7.44 (dt, J = 8.1, 0.9 Hz, 1H), 7.19 (ddd, J = 8.2, 7.0, 1.3 Hz, 1H), 7.12 (ddd, J = 8.0, 6.9, 1.0 Hz, 1H)..
^{13}C NMR (101 MHz, DMSO) δ(ppm): 135.42, 125.02, 122.85, 122.68, 120.18, 117.52, 112.65, 103.62.
HRMS (ESI): $[M-H]^-$ calcd. for C_8H_6ClN,150.0116; found, 150.01149.

3-Bromo-1H-indole **(2′a)**



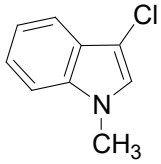
Obtained as off-white solid (160 mg, 82%).
^{1}H NMR (400 MHz, DMSO) δ (ppm): 11.47 (s, 1H), 7.55 (s, 1H), 7.43 (t, J = 8.2 Hz, 2H), 7.18 (ddd, J = 8.2, 7.0, 1.4 Hz, 1H), 7.14 – 7.09 (m, 1H).
^{13}C NMR (101 MHz, DMSO) δ (ppm): 135.83, 126.56, 125.24, 122.68, 120.33, 118.36, 112.55, 89.15.
HRMS (ESI): $[M-H]^-$ calcd. for C_8H_6BrN, 193.96109; found, 193.96094.

3-Iodo-1H-indole **(2″a)**



Obtained as white solid (199 mg, 82%).
^{1}H NMR (400 MHz, DMSO) δ(ppm): 11.53 (s, 1H), 7.55 (s, 1H), 7.46 – 7.41 (m, 1H), 7.32 – 7.27 (m, 1H), 7.17 (ddd, J = 8.1, 6.9, 1.4 Hz, 1H), 7.11 (ddd, J = 8.0, 6.9, 1.1 Hz, 1H).
^{13}C NMR (101 MHz, DMSO) δ (ppm): 136.38, 130.10, 129.79, 122.67, 120.42, 120.26, 112.39, 56.37.
HRMS (ESI): $[M-H]^-$ calcd. for C_8H_6IN, 241.94722; found, 241.94638.

3-Chloro-1-methyl-1H-indole **(2b)**



Obtained as colorless liquid (158 mg, 96%).

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm):7.66 (dt, J = 7.9, 1.0 Hz, 1H), 7.37-7.29 (m, 2H), 7.22 (ddd, J = 7.9, 6.6, 1.4 Hz, 1H), 7.05 (s, 1H), 3.79 (s, 3H).

^{13}C NMR (101 MHz, DMSO) δ (ppm): 147.56, 135.98, 126.76, 125.33, 122.76, 120.28, 117.78, 110.81, 102.58, 33.11.

HRMS (ESI): $[M-H]^-$ calcd. for C_9H_7ClN, 164.02725; found, 164.02745.

3-Bromo-1-methyl-1H-indole **(2′b)**

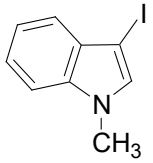
Obtained as slight yellow liquid (202 mg, 96%).

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.63-7.57 (m, 1H), 7.36-7.29 (m, 2H), 7.23 (ddd, J = 8.1, 6.6, 1.4 Hz, 1H), 7.10 (s, 1H), 3.81 (s, 3H).

^{13}C NMR (151 MHz, DMSO) δ(ppm): 136.45, 129.11, 126.91, 122.75, 120.44, 118.66, 110.80, 87.91, 33.21.

HRMS (ESI): $[M-H]^-$ calcd. for C_9H_7BrN, 207.97674; found, 207.97647.

3-Iodo-1-methyl-1H-indole **(2″b)**



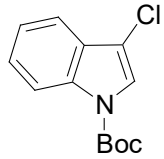
Obtained as colorless liquid (242 mg, 94%).

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.49 (dt, J = 8.0, 1.0 Hz, 1H), 7.36-7.30 (m, 2H), 7.25 (ddd, J = 8.0, 5.6, 2.6 Hz, 1H), 7.16 (s, 1H), 3.83 (s, 3H).

^{13}C NMR (101 MHz, DMSO) δ(ppm): 137.08, 133.94, 130.26, 122.67, 120.58, 120.47, 110.66, 54.96, 33.23.

HRMS (ESI): $[M-H]^-$ calcd. for C_9H_7IN, 255.96287; found, 255.96358.

***tert-Butyl 3-chloro-1H-indole-1-carboxylate* (2c)**



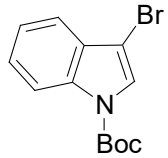
Obtained as white solid (220 mg, 88%).

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.18 (d, J = 8.3 Hz, 1H), 7.61 (d, J = 8.7 Hz, 2H), 7.43-7.32 (m, 2H), 1.69 (s, 9H).

^{13}C NMR (101 MHz, DMSO) δ(ppm): 148.79, 134.12, 127.66, 126.14, 123.88, 123.19, 118.55, 115.46, 111.02, 84.96, 28.05.

MS (ESI): $[M+Na]^+$ calcd. for $C_{13}H_{14}ClNNaO_2$, 274. 1; found,274.3.

***tert-Butyl 3-bromo-1H-indole-1-carboxylate* (2′c)**



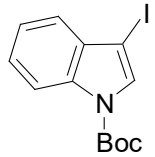
Obtained as slight yellow liquid (263 mg, 89%).

^{1}H NMR (400 MHz, DMSO-*d6*) δ (ppm): 8.09 (dt, J = 8.4, 0.9 Hz, 1H), 7.87 (s, 1H), 7.49 (ddd, J = 7.8, 1.4, 0.8 Hz, 1H), 7.43 (ddd, J = 8.4, 7.2, 1.4 Hz, 1H), 7.35 (td, J = 7.5, 1.1 Hz, 1H), 1.62 (s, 9H).

^{13}C NMR (101 MHz, DMSO) δ(ppm): 148.71, 134.43, 129.13, 126.08, 125.65, 123.96, 119.56, 115.36, 97.46, 84.99, 28.06.

MS (ESI): $[M+Na]^+$ calcd. for $C_{13}H_{14}BrNNaO_2$,318.0; found, 318.2.

***tert-Butyl 3-iodo-1H-indole-1-carboxylate* (2″c)**



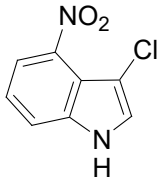
Obtained as slight yellow liquid (308 mg, 90%).

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.16 (d, J = 8.2 Hz, 1H), 7.76 (s, 1H), 7.45-7.32 (m, 3H), 1.70 (s, 9H).

^{13}C NMR (101 MHz, DMSO) δ(ppm): 148.60, 134.75, 132.24, 130.58, 125.90, 123.93, 121.66, 115.18, 84.86, 67.05, 28.09.

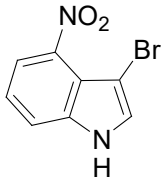
MS (ESI): $[M+CH_3CN+H]^+$ calcd. for $C_{15}H_{18}IN_2O_2$, 385.0; found, 385.2.

3-Chloro-4-nitro-1H-indole **(2d)**



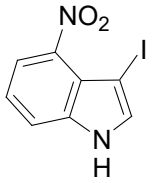
Obtained as yellow solid (171 mg, 87%).
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.60 (s, 1H), 7.82 (dd, J = 7.8, 0.9 Hz, 1H), 7.66 (dd, J = 8.2, 0.9 Hz, 1H), 7.45 (d, J = 2.8 Hz, 1H), 7.32 (t, J = 8.0 Hz, 1H).
^{13}C NMR (101 MHz, DMSO) δ(ppm): 141.70, 137.83, 128.58, 121.65, 118.76, 117.54, 115.69, 102.17.
HRMS (ESI): $[M-H]^-$ calcd. for $C_8H_4ClN_2O_2$, 194.99668; found 194.99629.

3-Bromo-4-nitro-1H-indole **(2′d)**



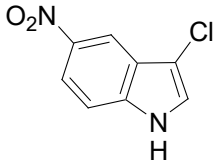
Obtained as yellow solid (205 mg, 85%).
^{1}H NMR (400 MHz, DMSO) δ(ppm): 12.35 (s, 1H), 7.90 (d, J = 2.8 Hz, 1H), 7.86 – 7.81 (m, 1H), 7.78 – 7.71 (m, 1H), 7.32 (t, J = 8.0 Hz, 1H).
^{13}C NMR (101 MHz, DMSO) δ(ppm): 142.01, 138.25, 131.12, 121.60, 118.37, 117.31, 116.81, 86.31.
HRMS (ESI): $[M-H]^-$ calcd. for $C_8H_4BrN_2O_2$, 238.94616; found,238.94586.

3-Iodo-4-nitro-1H-indole **(2″d)**



Obtained as yellow solid (274 mg, 95%).
^{1}H NMR (400 MHz, DMSO) δ (ppm): 11.98 (s, 1H), 8.07 (dd, J = 8.0, 0.8 Hz, 1H), 7.91 (dd, J = 7.9, 0.9 Hz, 1H), 7.78 (d, J = 3.0 Hz, 1H), 7.31 (t, J = 8.0 Hz, 1H), 7.05 (d, J = 3.0 Hz, 1H).
^{13}C NMR (101 MHz, DMSO) δ(ppm): 139.69, 138.75, 131.35, 121.83, 120.72, 119.78, 117.42, 101.66.
HRMS (ESI): $[M-H]^-$ calcd. for $C_8H_4IN_2O_2$, 286.93229; found,286.93183.

3-Chloro-5-nitro-1H-indole **(2e)**



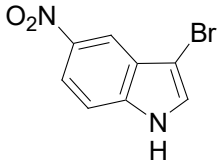
Obtained as yellow solid (195 mg, 99%).

^{1}H NMR (400 MHz, DMSO) δ(ppm): 12.10 (s, 1H), 8.36 (d, *J* = 2.3 Hz, 1H), 8.05 (dd, *J* = 9.0, 2.3 Hz, 1H), 7.82 (d, *J* = 2.7 Hz, 1H), 7.60 (d, *J* = 9.0 Hz, 1H).

^{13}C NMR (101 MHz, DMSO) δ(ppm): 141.68, 138.40, 127.03, 124.41, 117.91, 114.57, 113.45, 106.12.

HRMS (ESI): $[M-H]^-$ calcd. for $C_8H_4ClN_2O_2$, 194.99668; found 194.99623.

3-Bromo-5-nitro-1H-indole **(2′e)**



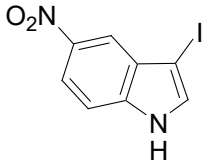
Obtained as yellow solid (211 mg, 88%).

H NMR (400 MHz, DMSO) δ(ppm): 12.21 (s, 1H), 8.32 (d, *J* = 2.3 Hz, 1H), 8.07 (dd, *J* = 9.0, 2.3 Hz, 1H), 7.88 (s, 1H), 7.64 (d, *J* = 9.0 Hz, 1H).

^{13}C NMR (101 MHz, DMSO) δ(ppm): 141.83, 139.03, 129.53, 126.11, 117.96, 115.40, 113.44, 91.50.

HRMS (ESI): $[M-H]^-$ calcd. for $C_8H_4BrN_2O_2$, 238.94616; found,238.94541.

3-Iodo-5-nitro-1H-indole **(2″e)**



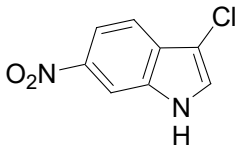
Obtained as yellow solid (250 mg, 87%).

^{1}H NMR (400 MHz, $CDCl_3$) *δ* (ppm): 8.72 (s, 1H), 8.48 (d, *J* = 2.2 Hz, 1H), 8.19 (dd, *J* = 9.0, 2.2 Hz, 1H), 7.50-7.45 (m, 2H).

^{13}C NMR (101 MHz, DMSO) δ(ppm): 141.83, 139.81, 134.31, 129.51, 117.88, 117.19, 113.15, 59.16.

HRMS (ESI): $[M-H]^-$ calcd. for $C_8H_4IN_2O_2$, 286.93229; found,286.93120.

3-Chloro-6-nitro-1H-indole **(2f)**



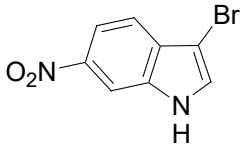
Obtained as yellow solid (169 mg, 86%).

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.70 (s, 1H), 8.40 (d, J = 2.0 Hz, 1H), 8.13 (dd, J = 8.9, 2.0 Hz, 1H), 7.74 (d, J = 8.9 Hz, 1H), 7.51 (d, J = 2.7 Hz, 1H).

^{13}C NMR (101 MHz, DMSO) δ(ppm): 143.29, 133.75, 129.81, 129.37, 118.13, 115.32, 109.58, 104.71.

HRMS (ESI): $[M-H]^-$ calcd. for $C_8H_4ClN_2O_2$, 194.99668; found 194.99629.

3-Bromo-6-nitro-1H-indole **(2′f)**



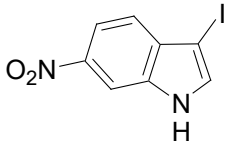
Obtained as yellow solid (204 mg, 85%).

^{1}H NMR (400 MHz, DMSO) δ(ppm): 12.28 – 12.17 (m, 1H), 8.38 (d, J = 2.1 Hz, 1H), 8.01 (s, 1H), 7.99 (dd, J = 8.8, 2.1 Hz, 1H), 7.61 (d, J = 8.8 Hz, 1H).

^{13}C NMR (101 MHz, DMSO) δ(ppm): 143.25, 134.21, 132.09, 131.09, 118.90, 115.39, 109.38, 90.08.

HRMS (ESI): $[M-H]^-$ calcd. for $C_8H_4BrN_2O_2$, 238.94616; found,238.94547.

3-Iodo-6-nitro-1H-indole **(2″f)**



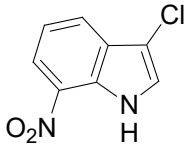
Obtained as yellow solid (267 mg, 93%).

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.87 (s, 1H), 8.41 (d, J = 2.1 Hz, 1H), 8.13 (dd, J = 8.8, 2.0 Hz, 1H), 7.64-7.53 (m, 2H).

^{13}C NMR (101 MHz, DMSO) δ(ppm): 143.24, 136.92, 134.79, 134.68, 120.79, 115.45, 109.06, 57.59.

HRMS (ESI): $[M-H]^-$ calcd. for $C_8H_4IN_2O_2$, 286.93229; found,286.93123.

3-Chloro-7-nitro-1H-indole **(2g)**



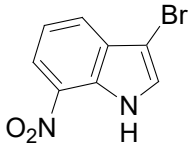
Obtained as yellow solid (188 mg, 96%).

^{1}H NMR (400 MHz, DMSO) δ(ppm): 12.14 (s, 1H), 8.20 (dd, *J* = 8.1, 1.0 Hz, 1H), 8.01 (dd, *J* = 7.8, 1.0 Hz, 1H), 7.72 (d, *J* = 2.5 Hz, 1H), 7.35 (t, *J* = 7.9 Hz, 1H).

^{13}C NMR (101 MHz, DMSO) δ(ppm): 133.46, 129.14, 127.58, 126.34, 126.24, 120.36, 120.08, 105.96.

HRMS (ESI): $[M-H]^-$ calcd. for $C_8H_4ClN_2O_2$, 194.99668; found 194.99635.

3-Bromo-7-nitro-1H-indole **(2′g)**



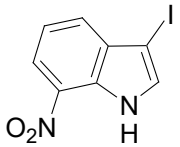
Obtained as yellow solid (210 mg, 87%).

^{1}H NMR (400 MHz, DMSO) δ(ppm): 12.24 (s, 1H), 8.21 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.94 (dd, *J* = 7.8, 1.0 Hz, 1H), 7.75 (s, 1H), 7.36 (t, *J* = 7.9 Hz, 1H).

^{13}C NMR (101 MHz, DMSO) δ(ppm): 133.35, 130.66, 128.63, 128.11, 127.14, 120.21, 120.06, 91.43.

HRMS (ESI): $[M-H]^-$ calcd. for $C_8H_4BrN_2O_2$, 238.94616; found,238.94555.

3-Iodo-7-nitro-1H-indole **(2″g)**



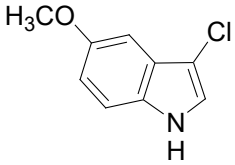
Obtained as yellow solid (247 mg, 86%).

^{1}H NMR (400 MHz, $CDCl_3$) *δ* (ppm): 10.10 (s, 1H), 8.26 (d, *J* = 8.1 Hz, 1H), 7.85 (d, *J* = 7.8 Hz, 1H), 7.52 (d, *J* = 2.4 Hz, 1H), 7.34 (t, *J* = 7.9 Hz, 1H).

^{13}C NMR (101 MHz, DMSO) δ(ppm): 133.92, 133.55, 133.21, 129.05, 128.78, 120.00, 119.95, 59.11.

HRMS (ESI): $[M-H]^-$ calcd. for $C_8H_4IN_2O_2$, 286.93229; found,286.93125.

3-Chloro-5-methoxy-1H-indole **(2h)**



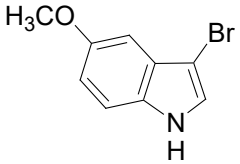
Obtained as off-white solid (143 mg, 79%).

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.99 (s, 1H), 7.26 (s, 1H), 7.17 (d, J = 2.7 Hz, 1H), 7.07 (d, J = 2.5 Hz, 1H), 6.93 (dd, J = 8.9, 2.5 Hz, 1H), 3.91 (s, 3H).

^{13}C NMR (101 MHz, DMSO) δ(ppm): 154.44, 130.43, 125.32, 123.26, 113.60, 113.32, 103.23, 98.62, 55.76.

HRMS (ESI): $[M-H]^-$ calcd. for C_9H_7ClNO, 180.02217; found, 180.02243.

3-Bromo-5-methoxy-1H-indole **(2′h)**



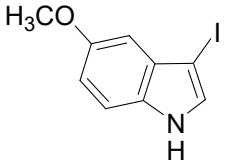
Obtained as off-white solid (183 mg, 81%).

^{1}H NMR (400 MHz, DMSO) δ (ppm): 11.32 (s, 1H), 7.49 (d, J = 2.7 Hz, 1H), 7.33 (dd, J = 8.6, 0.7 Hz, 1H), 6.85-6.80 (m, 2H), 3.79 (s, 3H).

^{13}C NMR (101 MHz, DMSO) δ (ppm): 154.57, 130.81, 126.89, 125.64, 113.50, 113.26, 99.49, 88.73, 55.78.

HRMS (ESI): $[M-H]^-$ calcd. for C_9H_7BrNO, 223.97166; found.223.97870.

3-Iodo-5-methoxy-1H-indole **(2″h)**



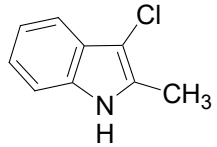
Obtained as off-white solid (206 mg, 76%).

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.28 (s, 1H), 7.28 (td, J = 3.4, 1.4 Hz, 2H), 6.93 (d, J = 8.0 Hz, 2H), 3.93 (s, 3H).

^{13}C NMR (101 MHz, DMSO) δ (ppm): 154.68, 131.34, 130.53, 130.22, 113.28, 113.08, 101.55, 55.91, 55.80.

HRMS (ESI): $[M-H]^-$ calcd. for C_9H_7INO, 271.95778; found, 271.95732.

3-Chloro-2-methyl-1H-indole **(2i)**



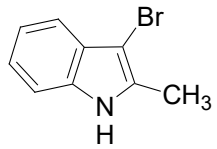
Obtained as slight yellow solid (126 mg, 76%).

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.87 (s, 1H), 7.61-7.48 (m, 1H), 7.29 (s, 1H), 7.19 (dd, J = 7.0, 3.5 Hz, 2H), 2.46 (s, 3H).

^{13}C NMR (101 MHz, DMSO) δ (ppm): 134.42, 131.77, 125.70, 121.82, 119.94, 116.72, 111.72, 101.03, 11.29.

HRMS (ESI): $[M-H]^-$ calcd. for C_9H_7ClN, 164.02725; found, 164.02733.

3-Bromo-2-methyl-1H-indole **(2′i)**



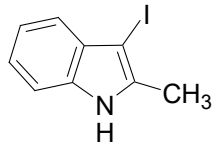
Obtained as slight yellow solid (161 mg, 77%).

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.00 (s, 1H), 7.54-7.47 (m, 1H), 7.29 (d, J = 6.8 Hz, 1H), 7.22-7.15 (m, 2H), 2.47 (s, 3H).

^{13}C NMR (101 MHz, DMSO) δ (ppm): 135.25, 133.70, 127.35, 121.88, 120.08, 117.62, 111.68, 88.24, 12.38.

HRMS (ESI): $[M-H]^-$ calcd. for C_9H_7BrN, 207.97674; found, 207.97640.

3-Iodo-2-methyl-1H-indole **(2″i)**



Obtained as slight yellow solid (224 mg, 87%).

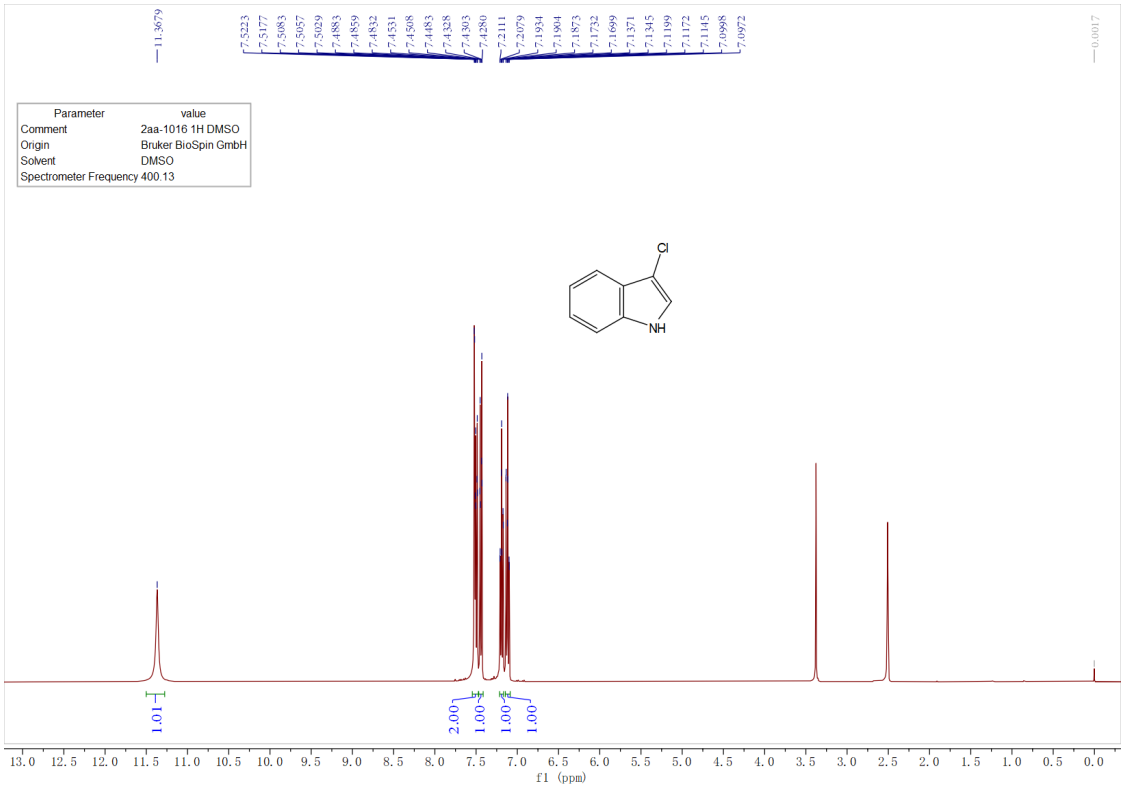
^{1}H NMR (400 MHz, DMSO) δ (ppm): 11.50 (s, 1H), 7.30 (dt, J = 8.1, 0.8 Hz, 1H), 7.20-7.15 (m, 1H), 7.12-7.02 (m, 2H), 2.41 (s, 3H).

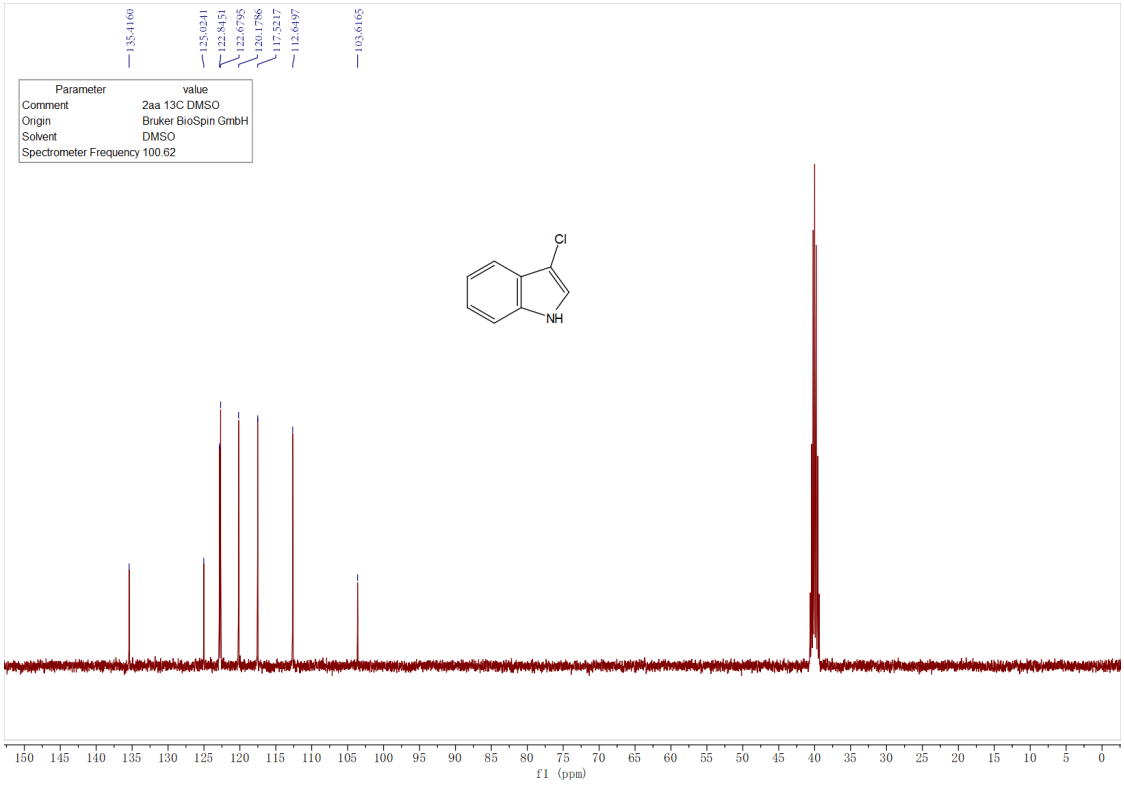
^{13}C NMR (101 MHz, DMSO) δ (ppm): 137.56, 136.56, 130.67, 121.93, 120.13, 119.53, 111.58, 58.05, 14.36.

HRMS (ESI): $[M-H]^-$ calcd. for C_9H_7IN, 255.96287; found, 255.96236.

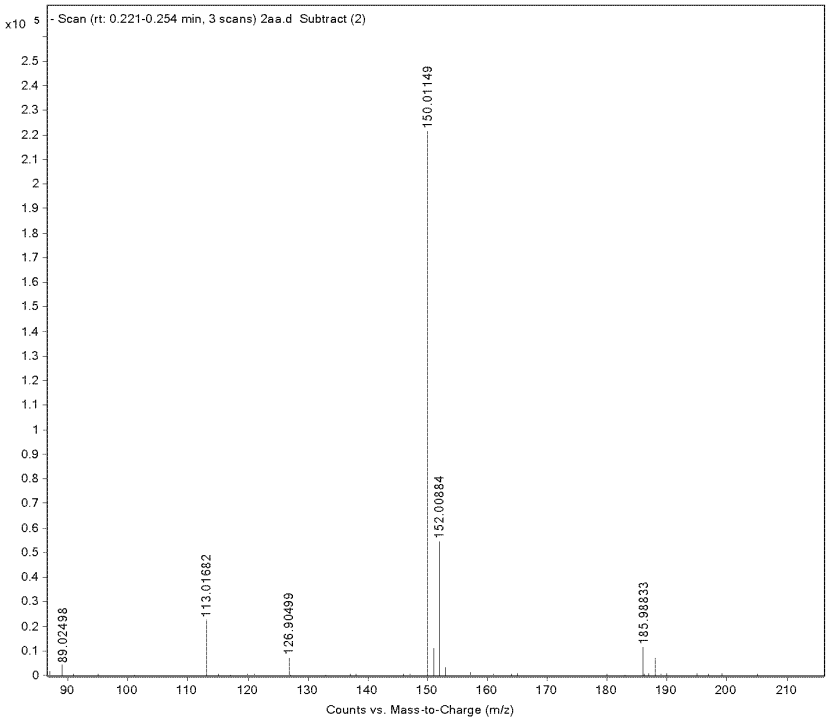
4. ^{1}H NMR and MS spectra of all products

2a

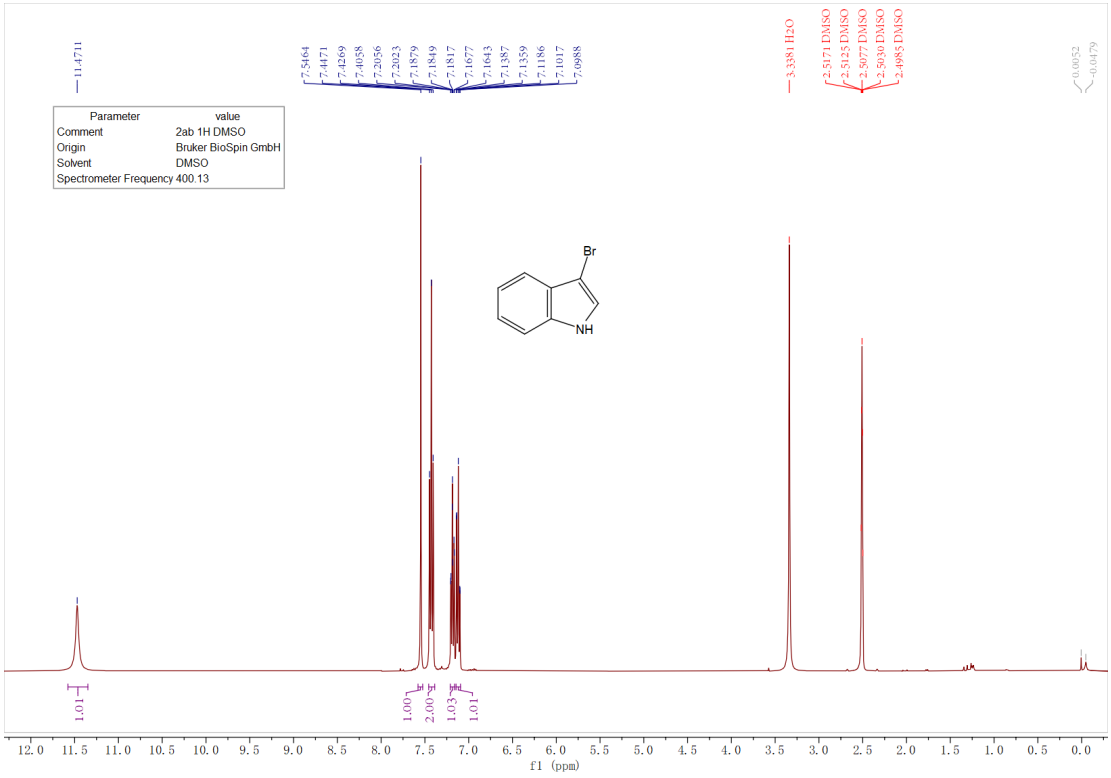


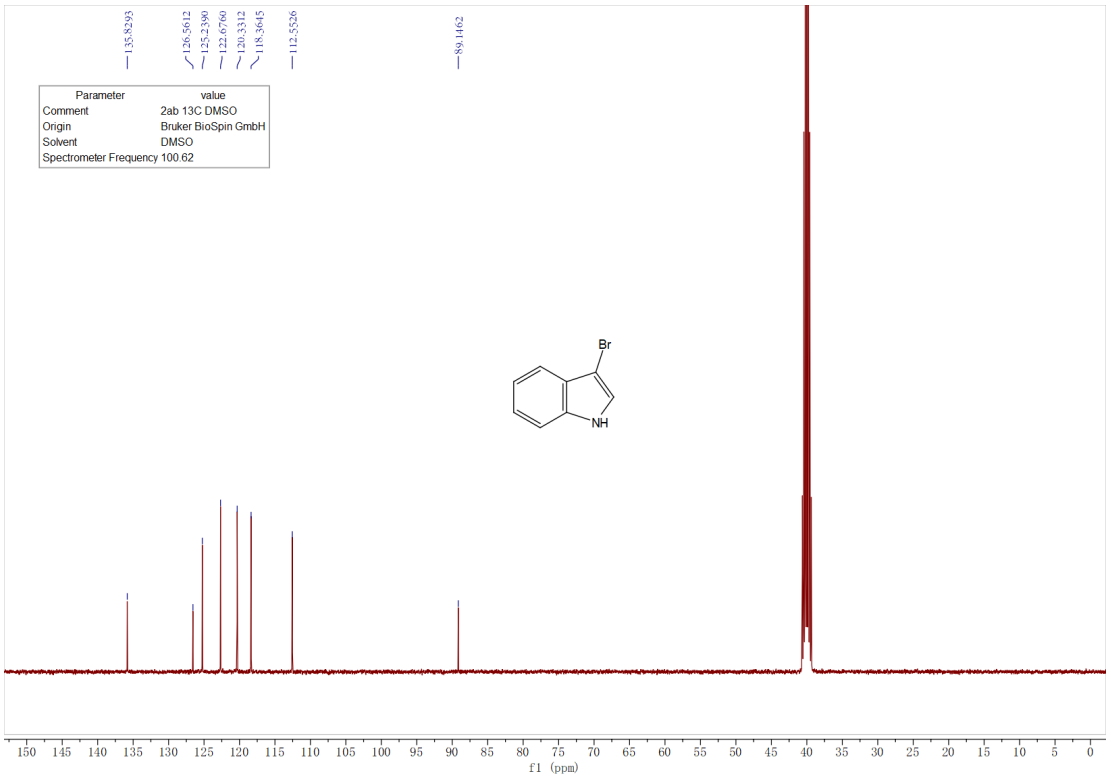


Sample Name	2aa	**Position**	Vial 1	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	6	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	2aa.d
ACQ Method	E-R.m	**Comment**		**Acquired Time**	29/04/2024 20:16:13 (UTC+08:00)

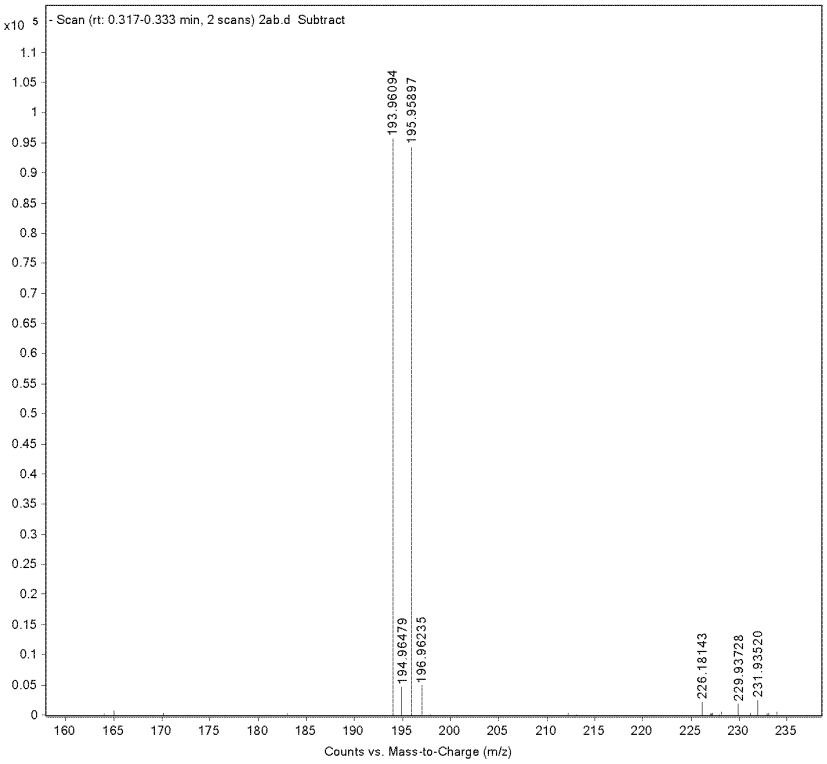


2'a

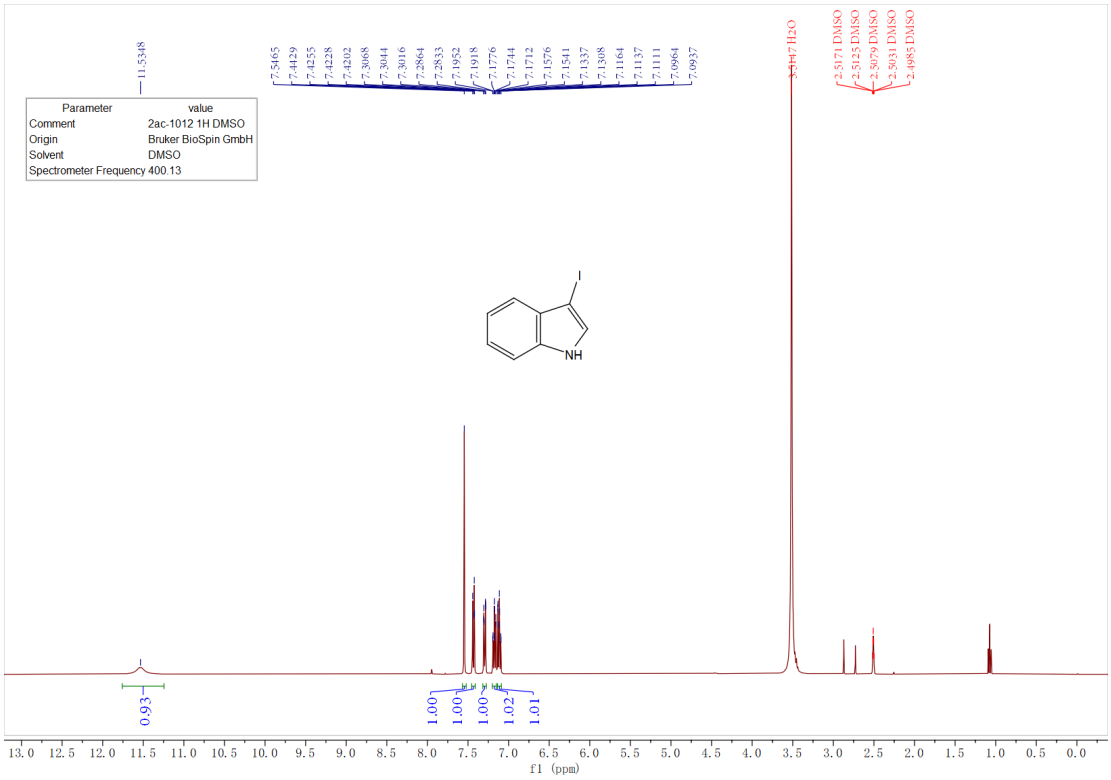

11.4711
7.5464
7.4471
7.4269
7.4058
7.2056
7.2023
7.1879
7.1849
7.1817
7.1677
7.1643
7.1387
7.1359
7.1186
7.1017
7.0988
3.3381 H2O
2.5171 DMSO
2.5125 DMSO
2.5077 DMSO
2.5030 DMSO
2.4985 DMSO
0.0052
-0.0479
Parameter value
Comment 2ab 1H DMSO
Origin Bruker BioSpin GmbH
Solvent DMSO
Spectrometer Frequency 400.13
Br
NH
1.01
1.00
2.00
1.03
1.01
f1 (ppm)

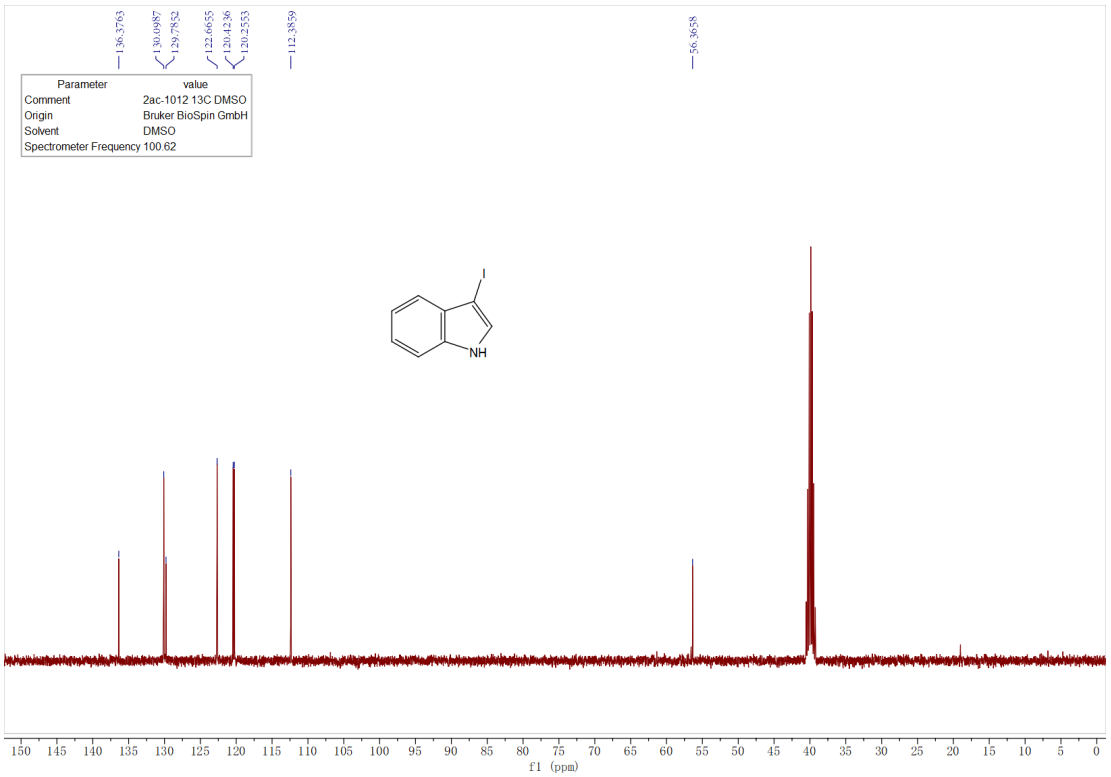

135.8293
126.5612
125.2390
122.6760
120.3312
118.3645
112.5526
89.1462
Parameter value
Comment 2ab 13C DMSO
Origin Bruker BioSpin GmbH
Solvent DMSO
Spectrometer Frequency 100.62
Br
NH
f1 (ppm)

Sample Name	2ab	**Position**	Vial 2	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	2ab.d
ACQ Method	E-R.m	**Comment**		**Acquired Time**	29/04/2024 20:25:02 (UTC+08:00)

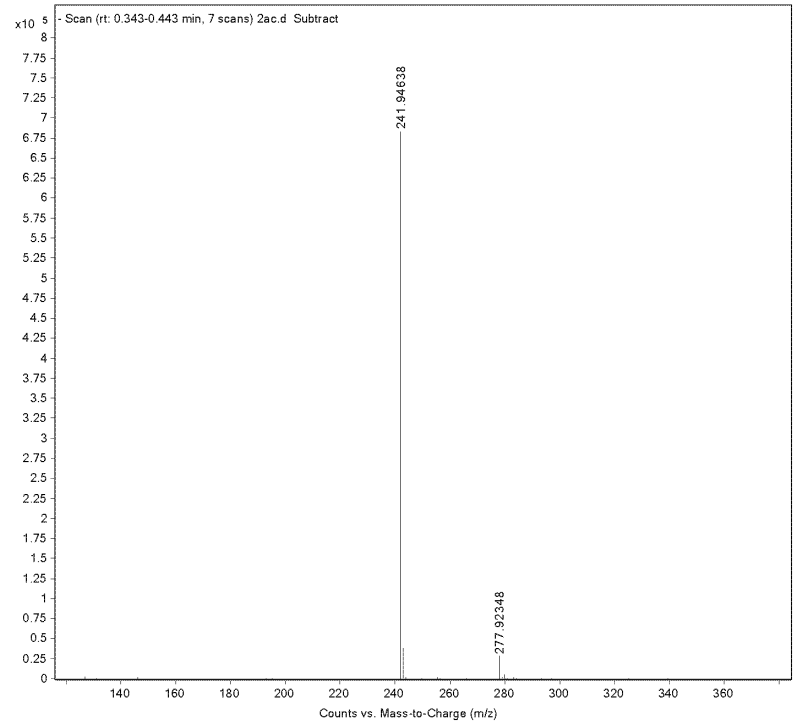


2"a

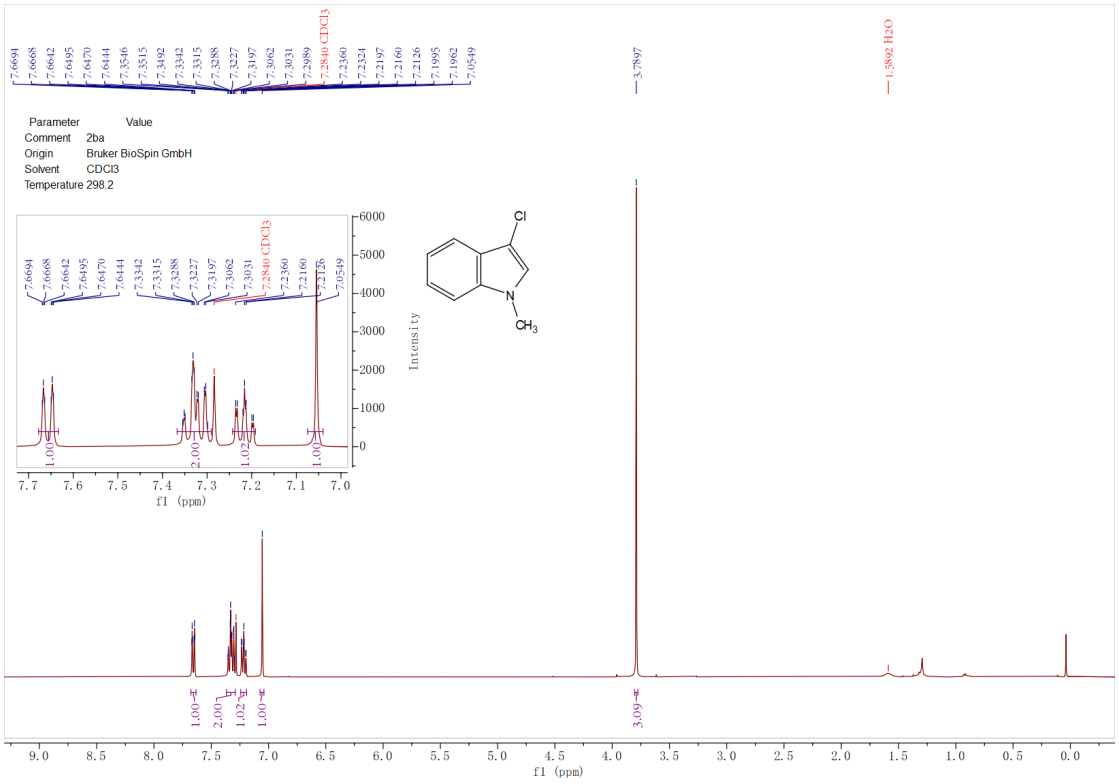

11.5348
7.5465
7.4429
7.4255
7.4228
7.4202
7.3068
7.3044
7.3016
7.2864
7.2833
7.1952
7.1918
7.1776
7.1744
7.1712
7.1576
7.1541
7.1337
7.1308
7.1164
7.1137
7.1111
7.0964
7.0937
3.3347 H2O
2.5171 DMSO
2.5125 DMSO
2.5079 DMSO
2.5031 DMSO
2.4985 DMSO
Parameter value
Comment 2ac-1012 1H DMSO
Origin Bruker BioSpin GmbH
Solvent DMSO
Spectrometer Frequency 400.13
I
NH
0.93
1.00
1.00
1.00
1.02
1.01
f1 (ppm)

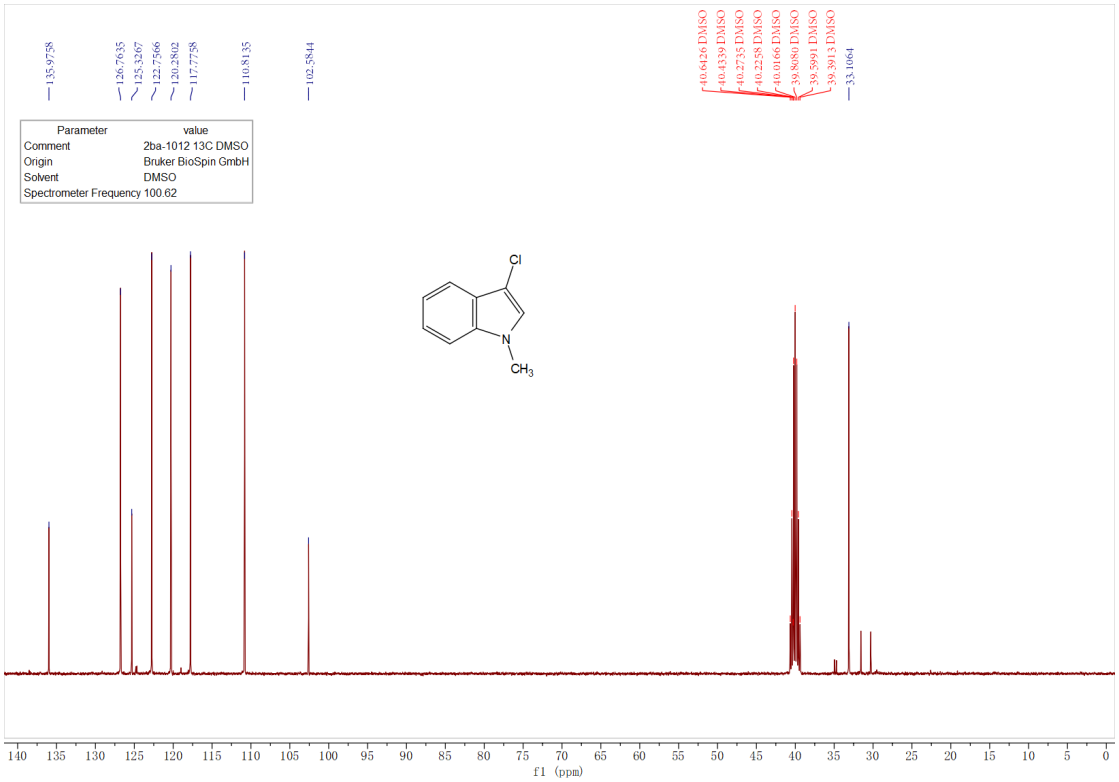

136.3763
130.0987
129.7852
122.6655
120.4236
120.2553
112.3859
56.3658
Parameter value
Comment 2ac-1012 13C DMSO
Origin Bruker BioSpin GmbH
Solvent DMSO
Spectrometer Frequency 100.62
I
NH
f1 (ppm)

Sample Name	2ac	**Position**	Vial 3	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	2ac.d
ACQ Method	E-R.m	**Comment**		**Acquired Time**	29/04/2024 20:28:32 (UTC+08:00)

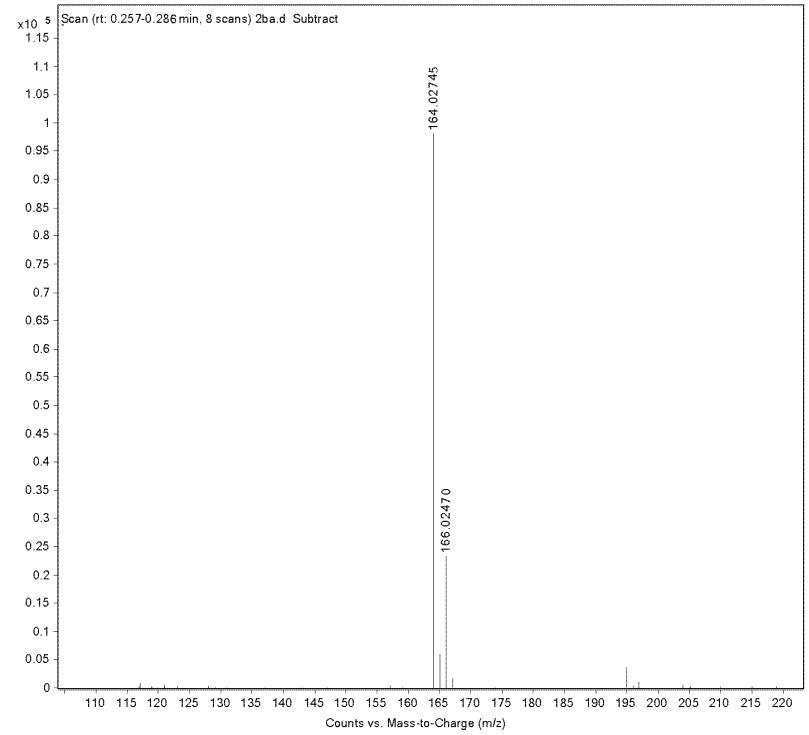


2b

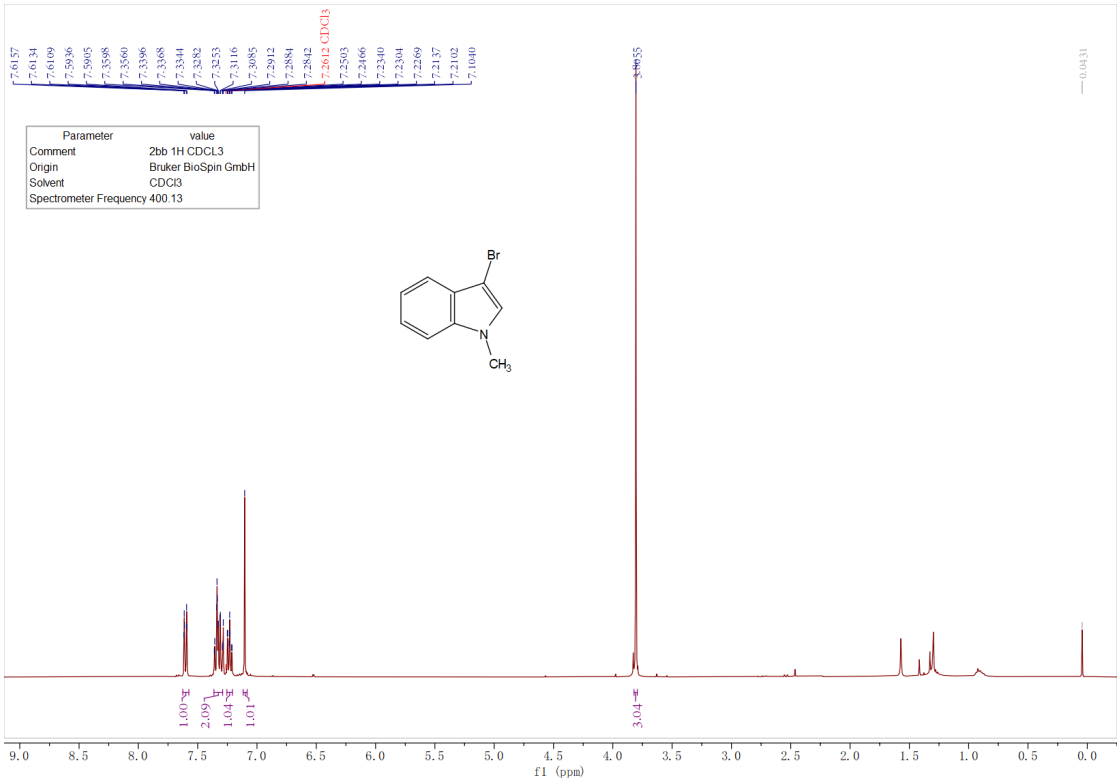

Parameter Value
Comment 2ba
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Intensity
f1 (ppm)

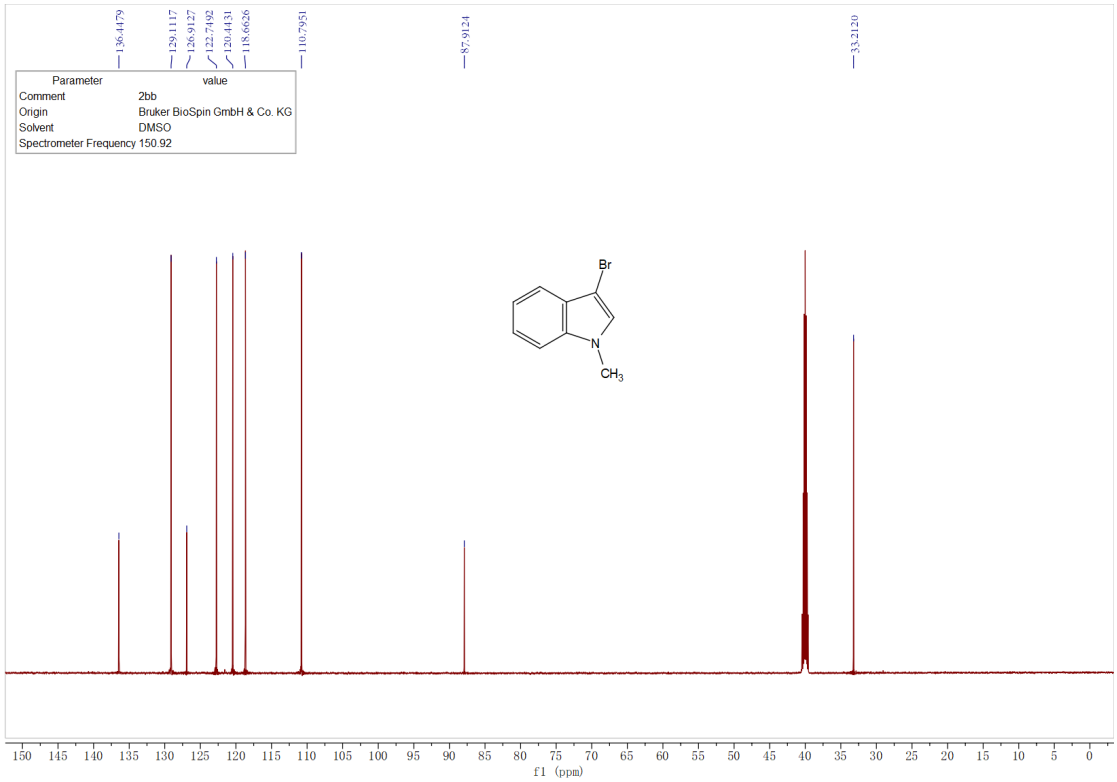

Parameter value
Comment 2ba-1012 13C DMSO
Origin Bruker BioSpin GmbH
Solvent DMSO
Spectrometer Frequency 100.62
f1 (ppm)

Sample Name	2ba	**Position**	Vial 28	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	2ba.d
ACQ Method	E-R.m	**Comment**		**Acquired Time**	29/04/2024 21:51:34 (UTC+08:00)

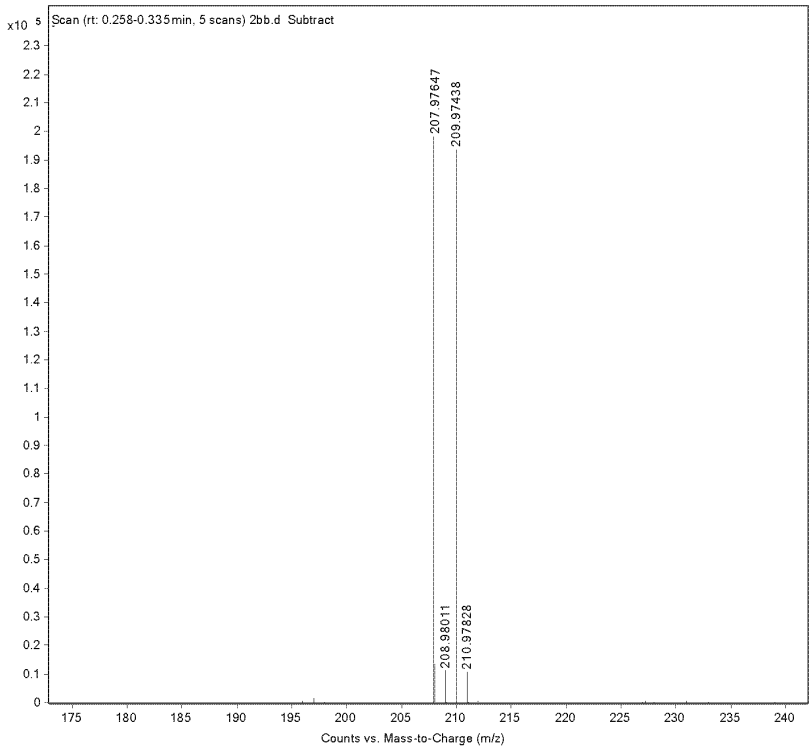


2'b

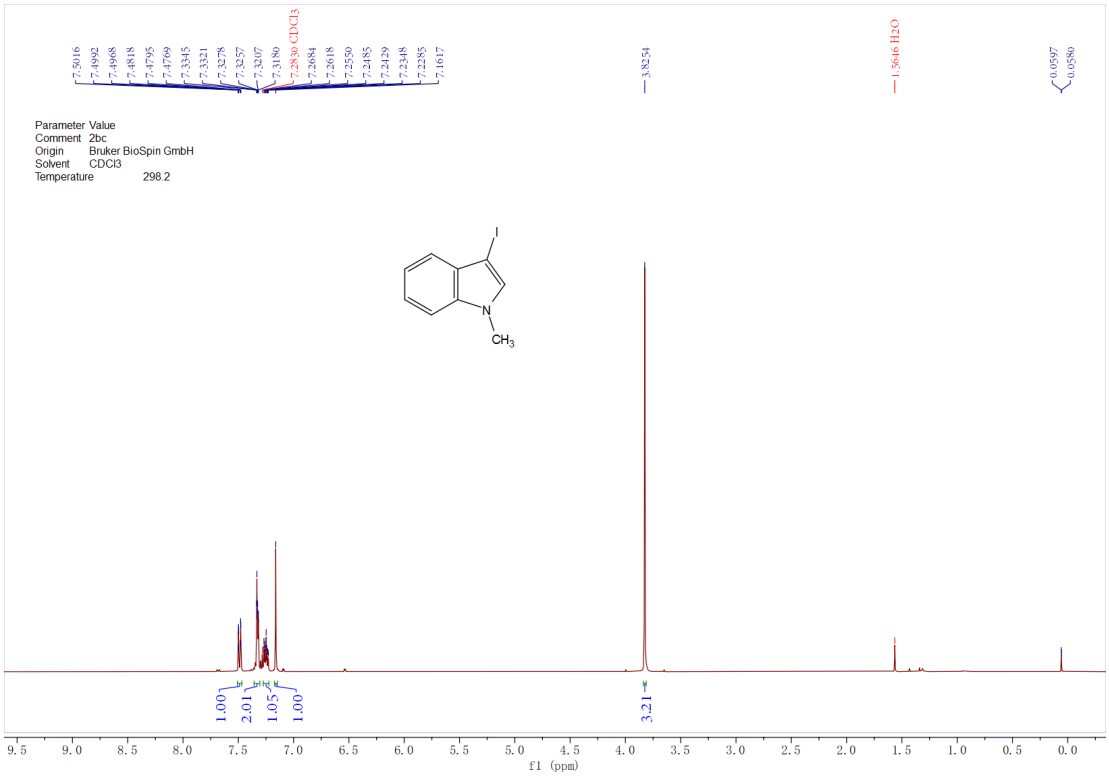

Parameter value
Comment 2bb 1H CDCL3
Origin Bruker BioSpin GmbH
Solvent CDCl3
Spectrometer Frequency 400.13
Br
N
CH3
f1 (ppm)

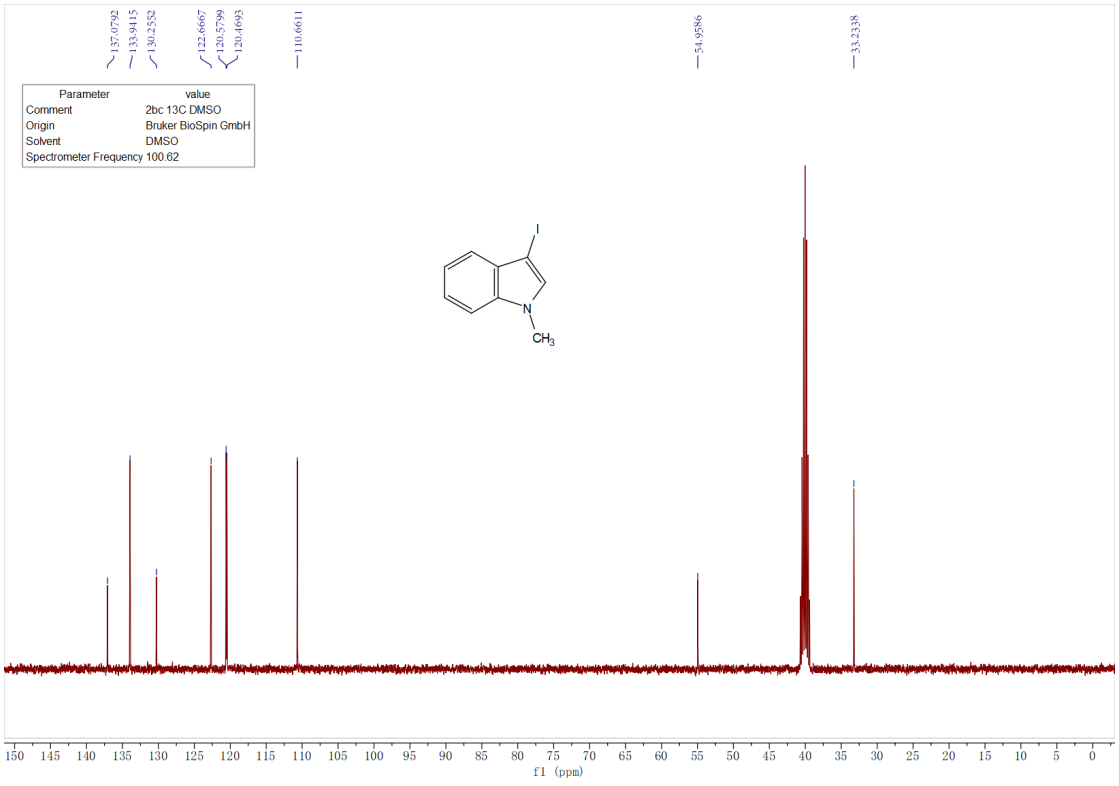

Parameter value
Comment 2bb
Origin Bruker BioSpin GmbH & Co. KG
Solvent DMSO
Spectrometer Frequency 150.92
Br
N
CH3
f1 (ppm)

Sample Name	2bb	**Position**	Vial 29	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	2bb.d
ACQ Method	E-R.m	**Comment**		**Acquired Time**	29/04/2024 21:52:04 (UTC+08:00)

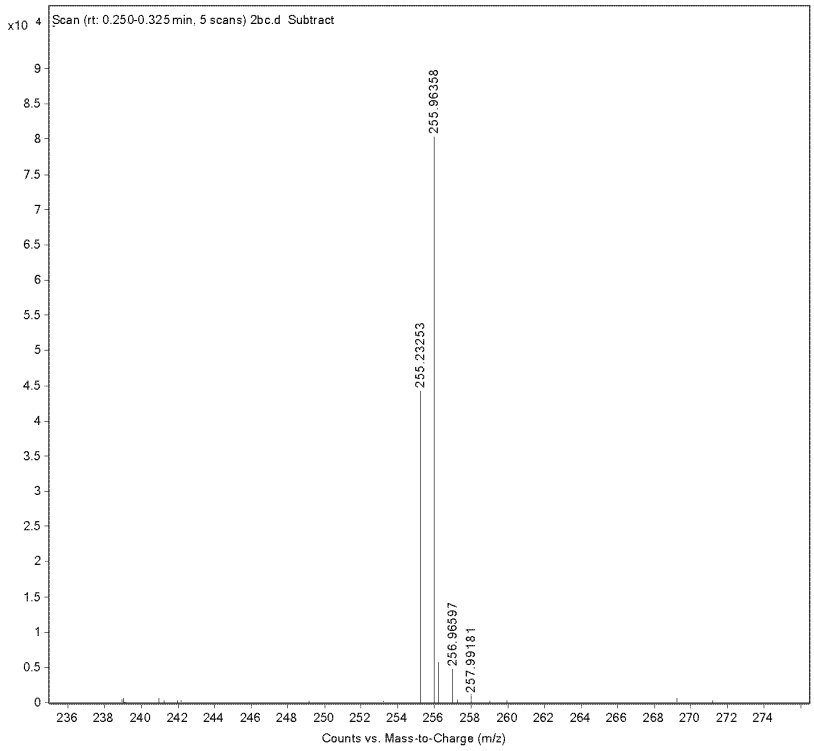


2"b

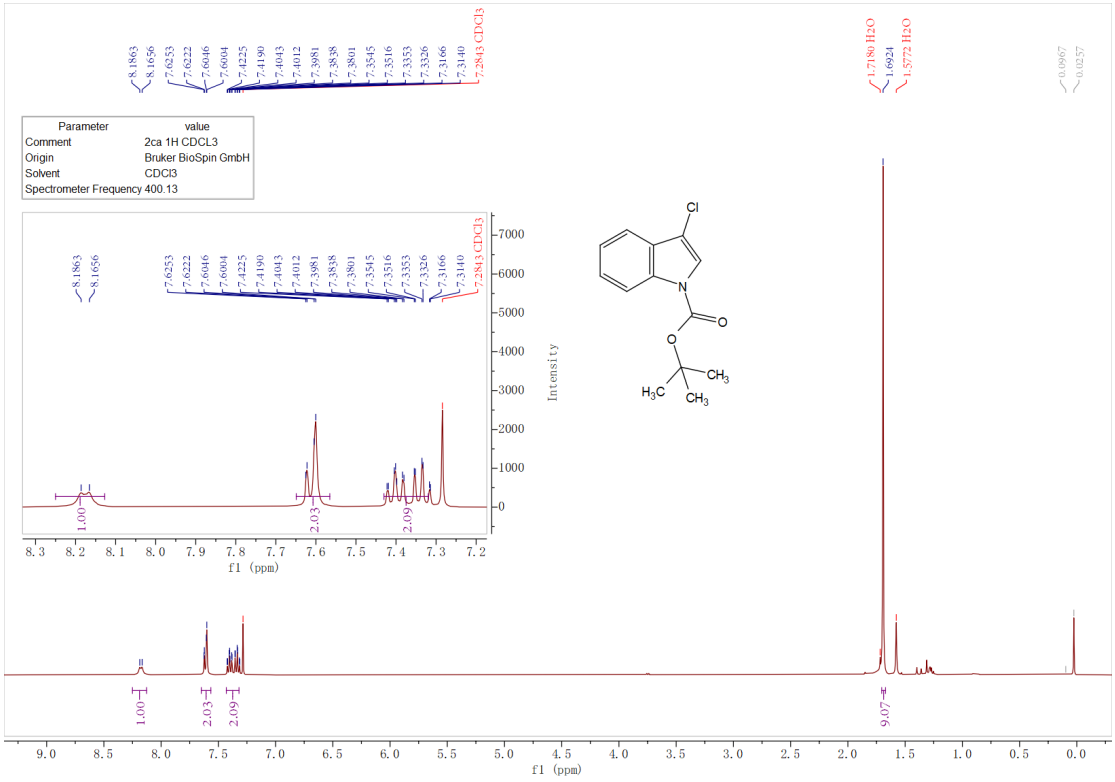

7.5016
7.4992
7.4968
7.4818
7.4795
7.4769
7.3345
7.3321
7.3278
7.3257
7.3207
7.3180
7.2830 CDCl3
7.2684
7.2618
7.2550
7.2485
7.2429
7.2348
7.2285
7.1617
3.8254
1.5646 H2O
0.0597
0.0580
Parameter Value
Comment 2bc
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
I
N
CH3
1.00
2.01
1.05
1.00
3.21
f1 (ppm)

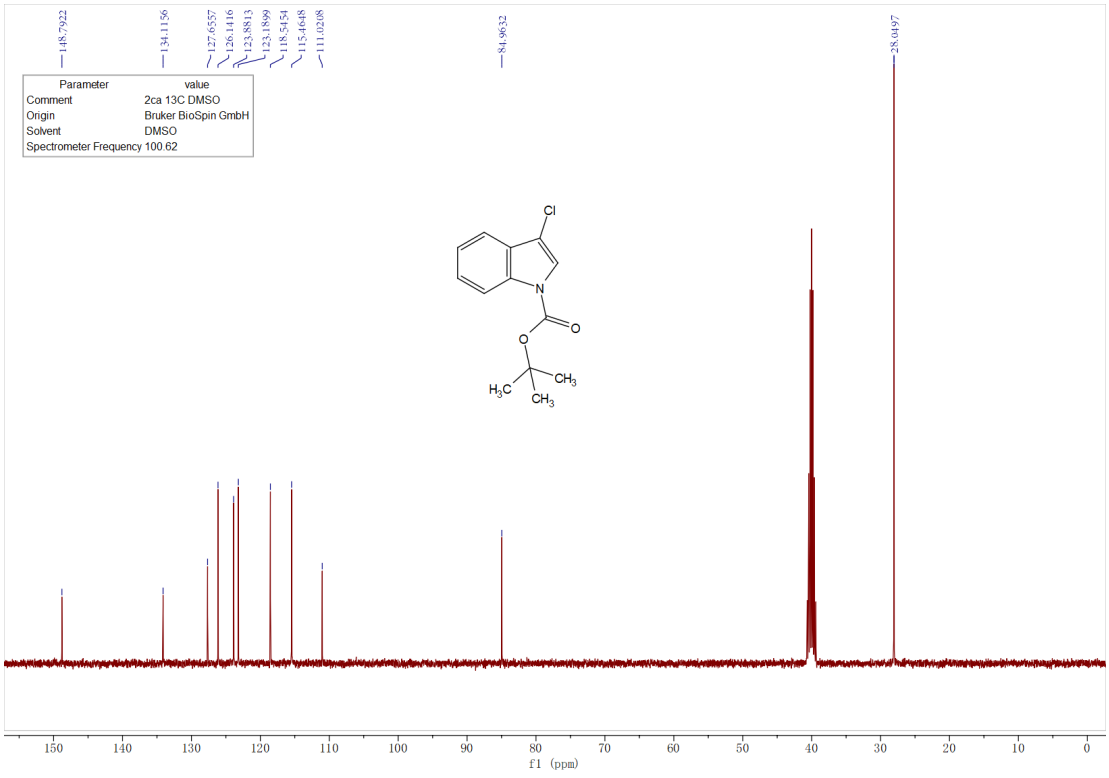

137.0792
133.9415
130.2552
122.6667
120.5799
120.4693
110.6611
54.9586
33.2338
Parameter value
Comment 2bc 13C DMSO
Origin Bruker BioSpin GmbH
Solvent DMSO
Spectrometer Frequency 100.62
I
N
CH3
f1 (ppm)

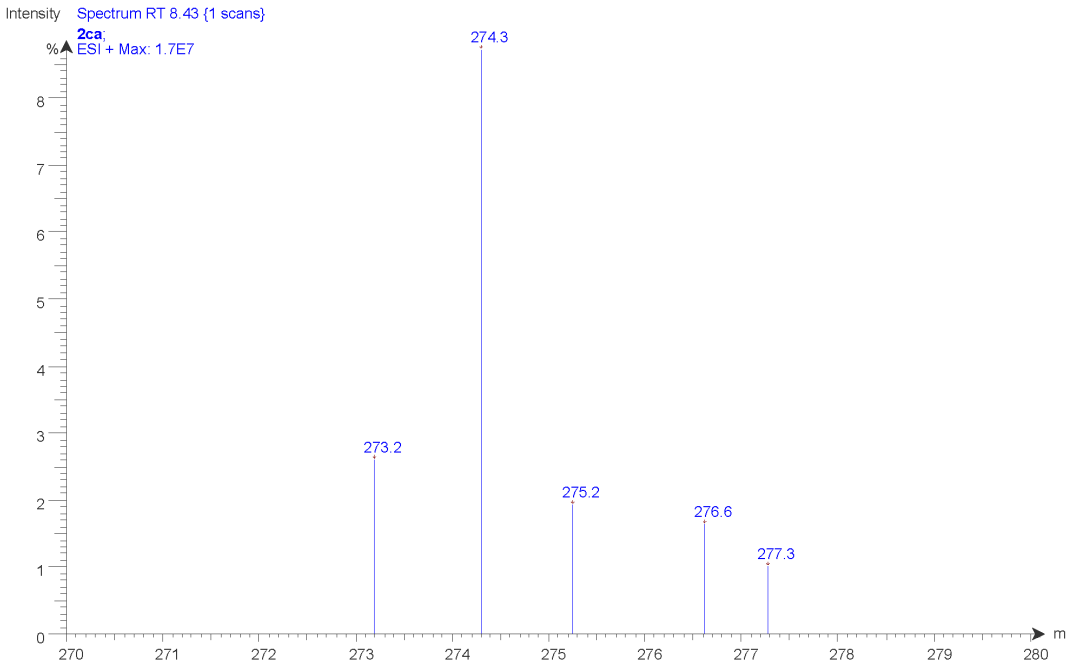
Sample Name	2bc	**Position**	Vial 30	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	2bc.d
ACQ Method	E-R.m	**Comment**		**Acquired Time**	29/04/2024 21:52:21 (UTC+08:00)



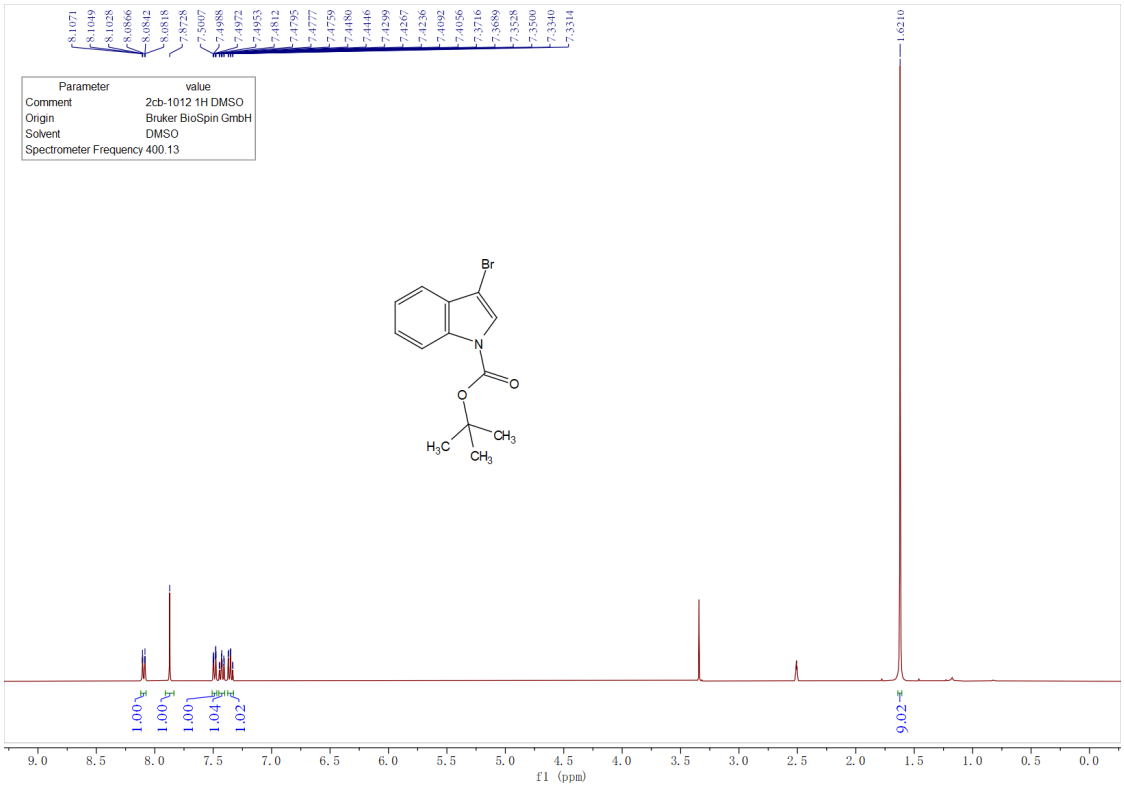
2c

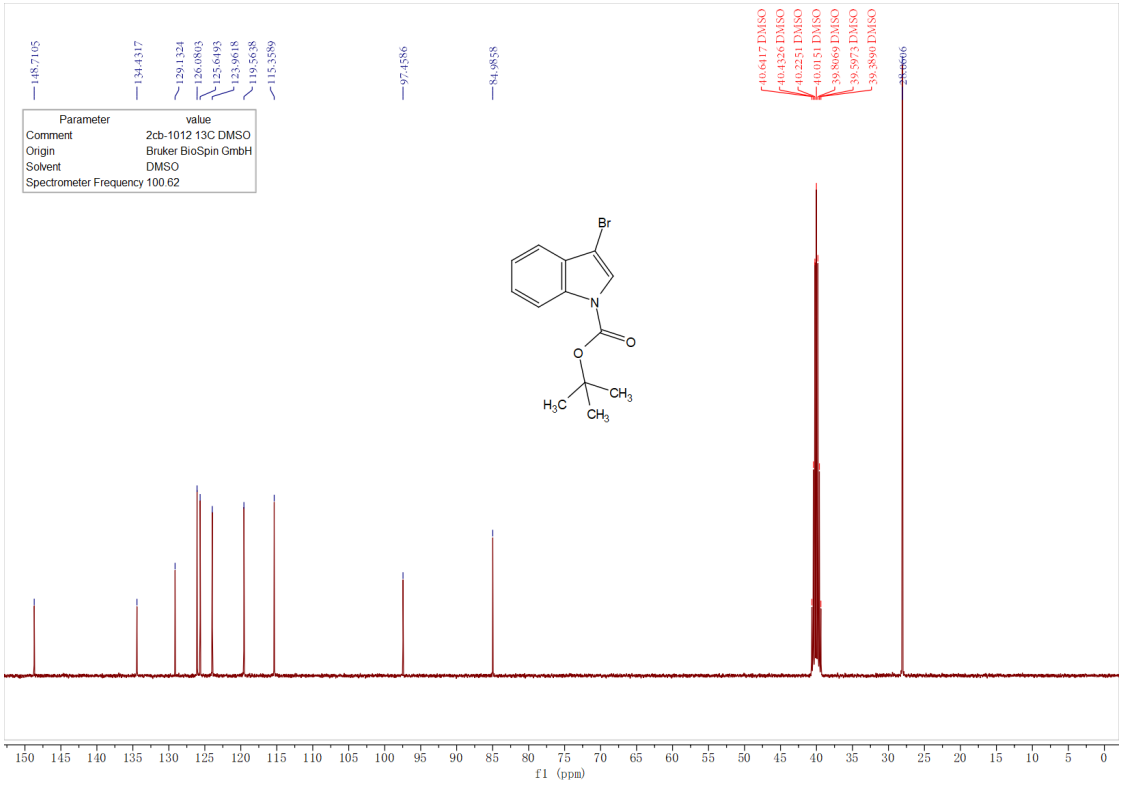

Parameter value
Comment 2ca 1H CDCL3
Origin Bruker BioSpin GmbH
Solvent CDCl3
Spectrometer Frequency 400.13
f1 (ppm)
Intensity


Parameter value
Comment 2ca 13C DMSO
Origin Bruker BioSpin GmbH
Solvent DMSO
Spectrometer Frequency 100.62
f1 (ppm)


Intensity
Spectrum RT 8.43 {1 scans}
2ca;
ESI + Max: 1.7E7
%
8
7
6
5
4
3
2
1
0
274.3
273.2
275.2
276.6
277.3
270
271
272
273
274
275
276
277
278
279
280
m

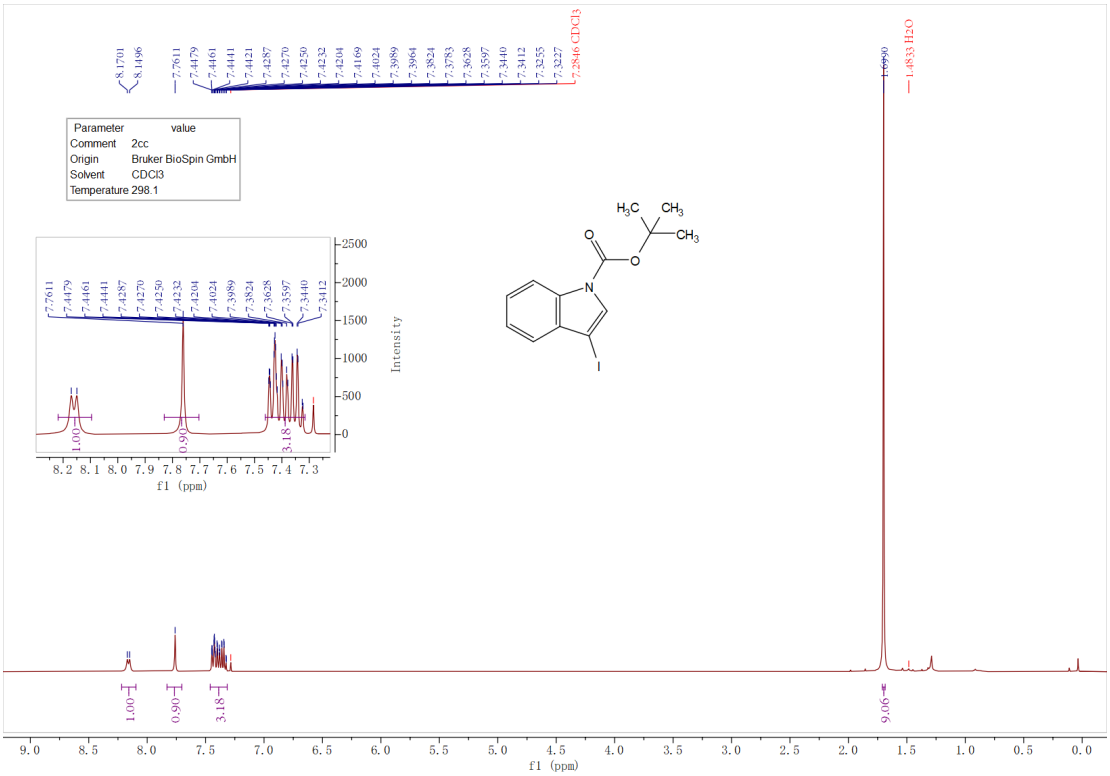
2'c

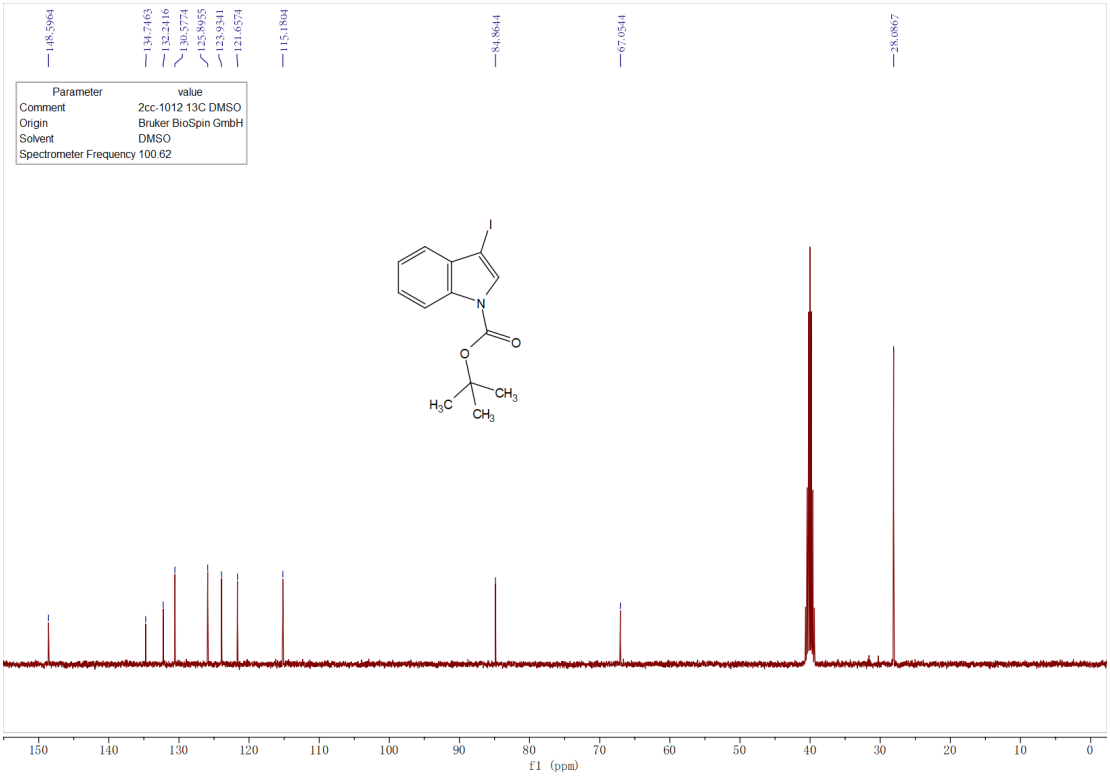

8.1071
8.1049
8.1028
8.0866
8.0842
8.0818
7.8728
7.5007
7.4988
7.4972
7.4953
7.4812
7.4795
7.4777
7.4759
7.4480
7.4446
7.4299
7.4267
7.4236
7.4092
7.4056
7.3716
7.3689
7.3528
7.3500
7.3340
7.3314
1.6210
Parameter value
Comment 2cb-1012 1H DMSO
Origin Bruker BioSpin GmbH
Solvent DMSO
Spectrometer Frequency 400.13
Br
N
O
O
H3C
CH3
CH3
1.00
1.00
1.00
1.04
1.02
9.02
f1 (ppm)

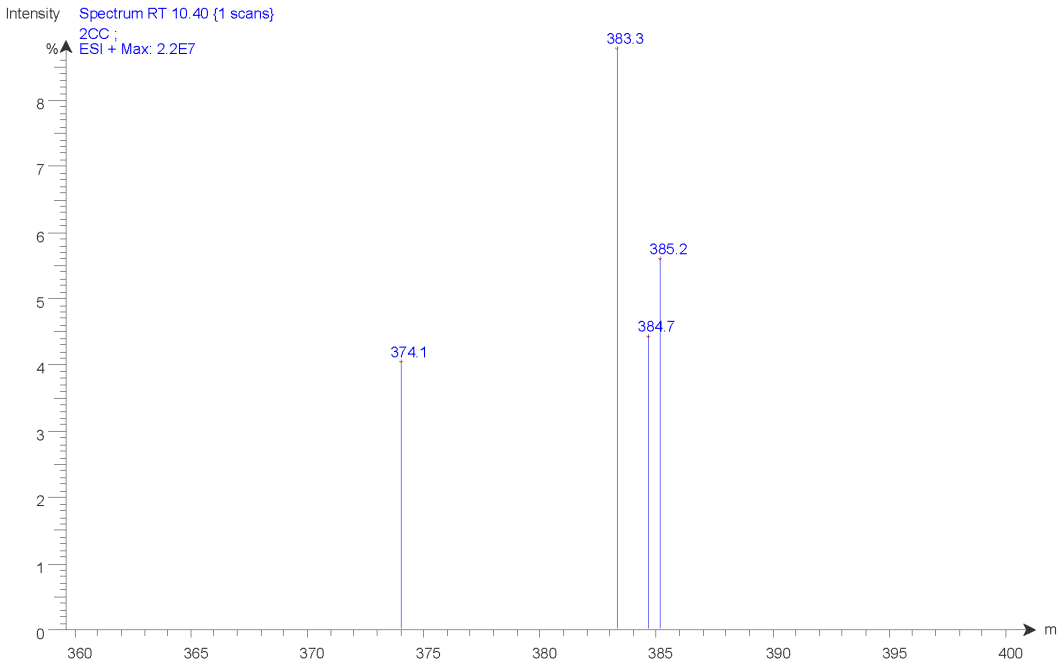

148.7105
134.4317
129.1324
126.0803
125.6493
123.9618
119.5638
115.3589
97.4586
84.9858
40.6417 DMSO
40.4326 DMSO
40.2251 DMSO
40.0151 DMSO
39.8069 DMSO
39.5973 DMSO
39.3890 DMSO
28.0606
Parameter value
Comment 2cb-1012 13C DMSO
Origin Bruker BioSpin GmbH
Solvent DMSO
Spectrometer Frequency 100.62
Br
N
O
O
H3C
CH3
CH3
f1 (ppm)


Intensity
Spectrum RT 12.99 {1 scans}
2cb;
ESI + Max: 1.5E7
318.2
%
6
5
4
3
2
1
0
300
302
304
306
308
310
312
314
316
318
320
m

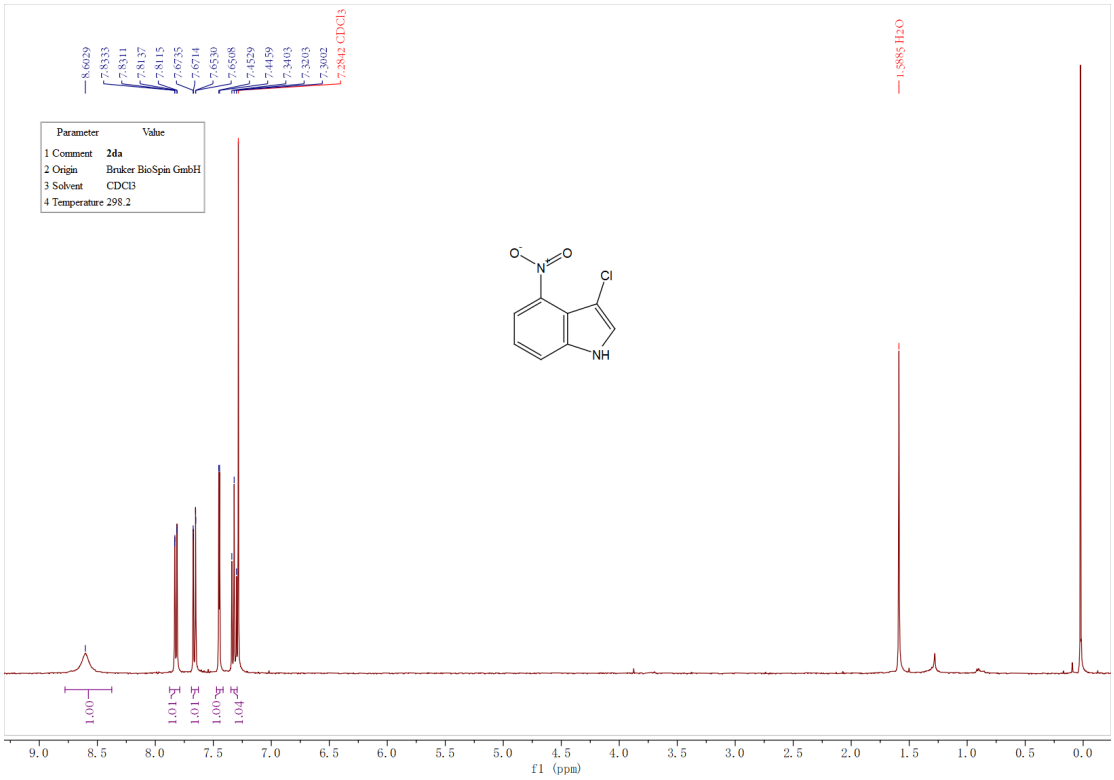
2"c

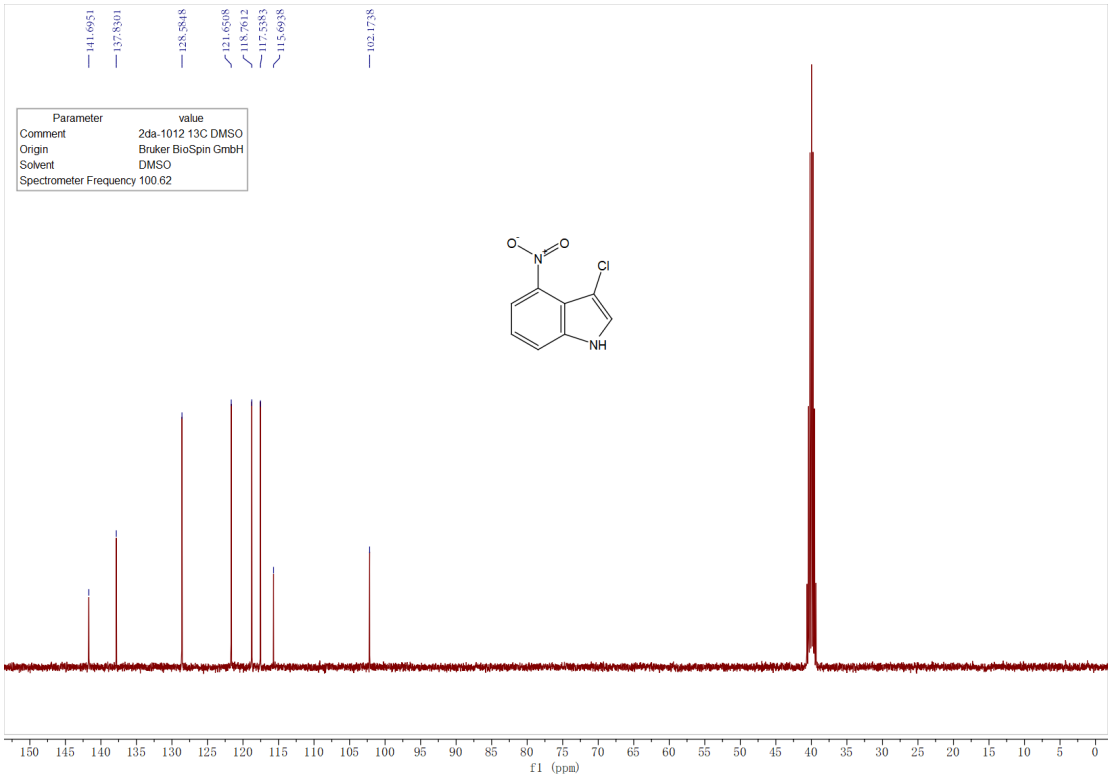

Parameter value
Comment 2cc
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Intensity
f1 (ppm)
1.00
0.90
3.18
9.06


Parameter value
Comment 2cc-1012 13C DMSO
Origin Bruker BioSpin GmbH
Solvent DMSO
Spectrometer Frequency 100.62
f1 (ppm)

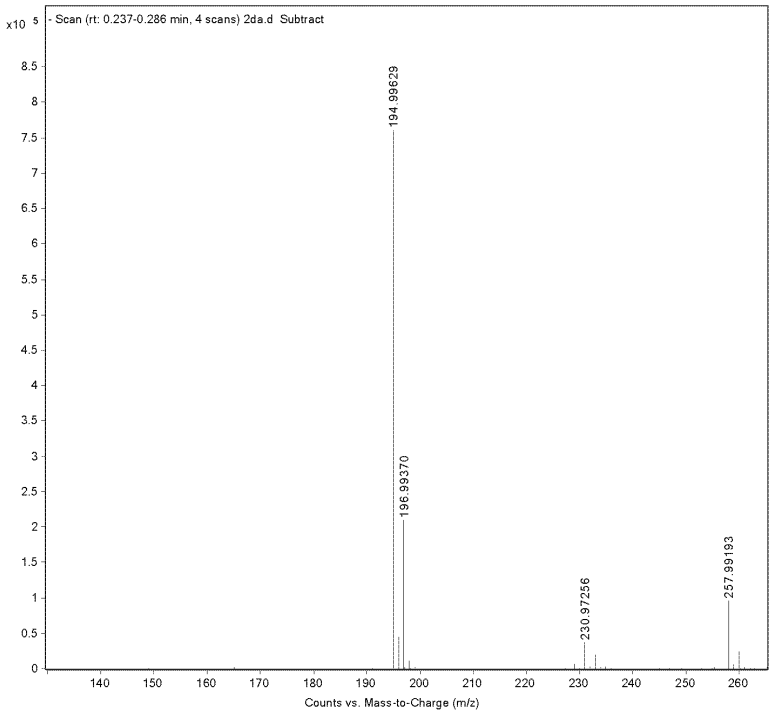

Intensity
Spectrum RT 10.40 {1 scans}
2CC ;
ESI + Max: 2.2E7
%
8
7
6
5
4
3
2
1
0
383.3
385.2
384.7
374.1
360
365
370
375
380
385
390
395
400
m

2d

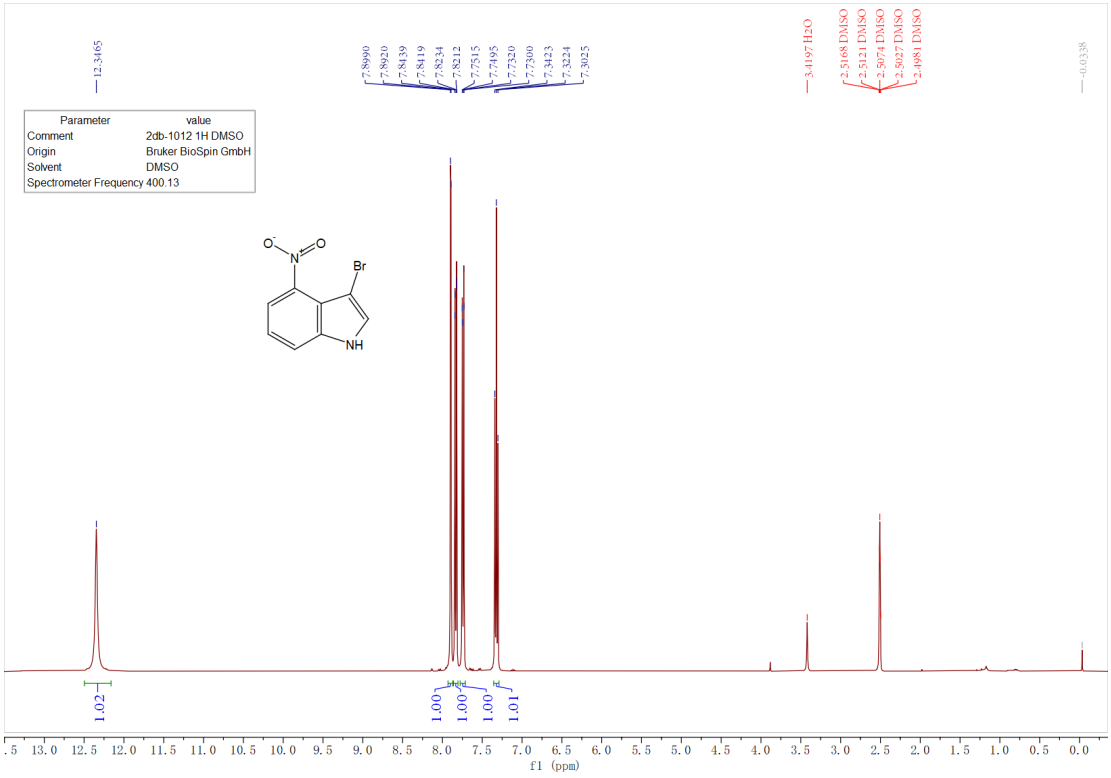

8.6029
7.8333
7.8311
7.8137
7.8115
7.6735
7.6714
7.6530
7.6508
7.4529
7.4459
7.3403
7.3203
7.3002
7.2842 CDCl3
1.5885 H2O
Parameter Value
1 Comment 2da
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.2
O
N
O
Cl
NH
1.00
1.01
1.01
1.00
1.04
f1 (ppm)

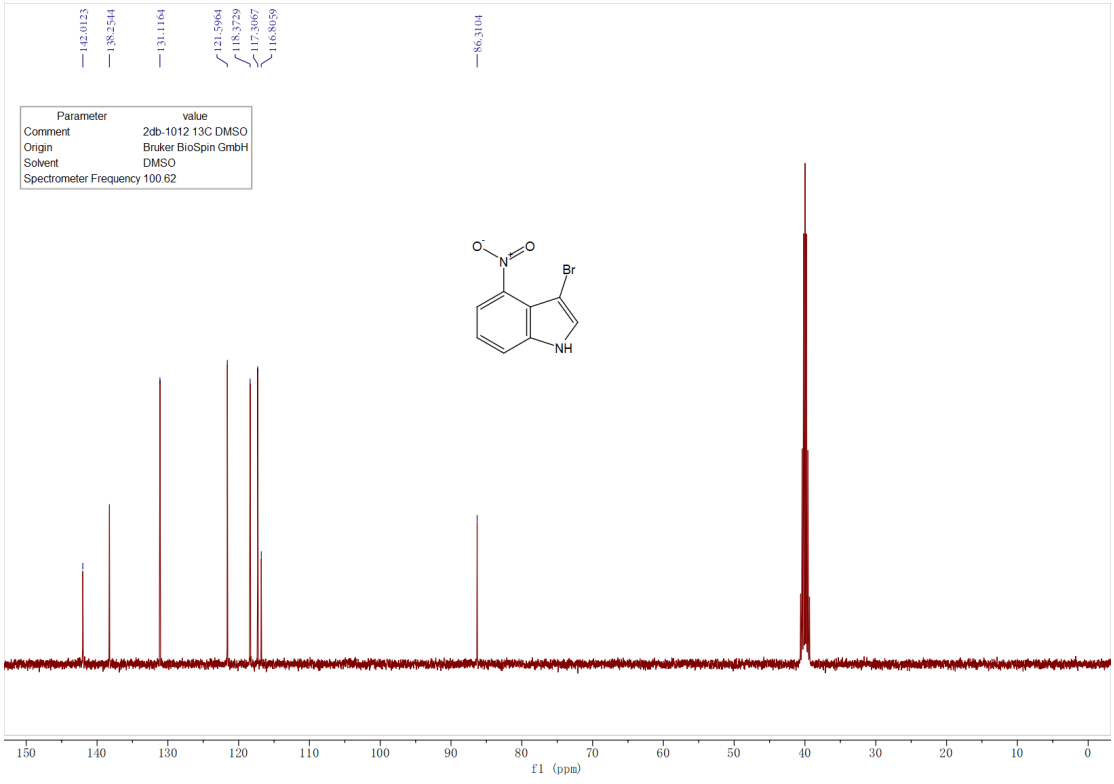

141.6951
137.8301
128.5848
121.6508
118.7612
117.5383
115.6938
102.1738
Parameter value
Comment 2da-1012 13C DMSO
Origin Bruker BioSpin GmbH
Solvent DMSO
Spectrometer Frequency 100.62
O
N
O
Cl
NH
f1 (ppm)

Sample Name	2da	**Position**	Vial 10	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	2da.d
ACQ Method	E-R.m	**Comment**		**Acquired Time**	29/04/2024 20:52:29 (UTC+08:00)

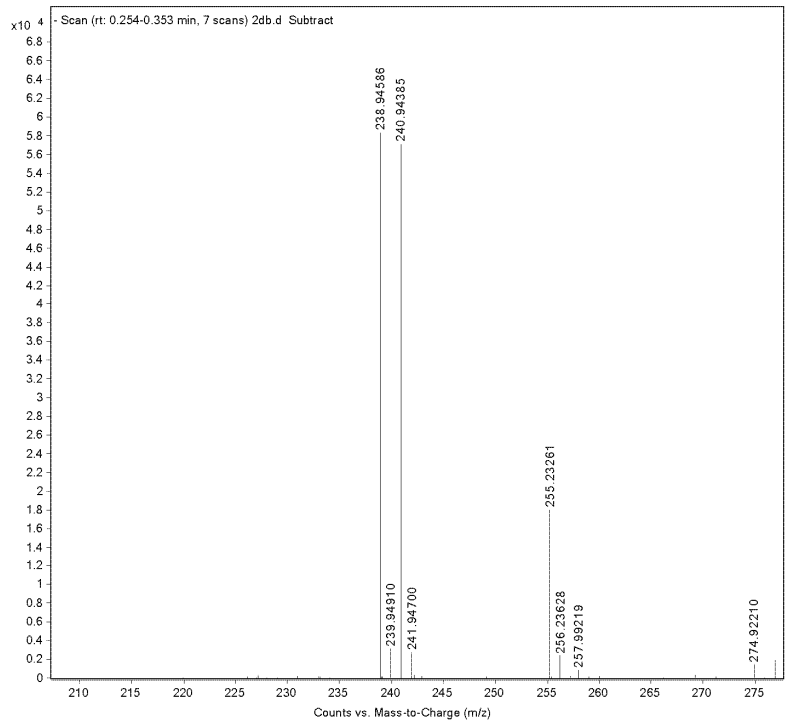


2'd

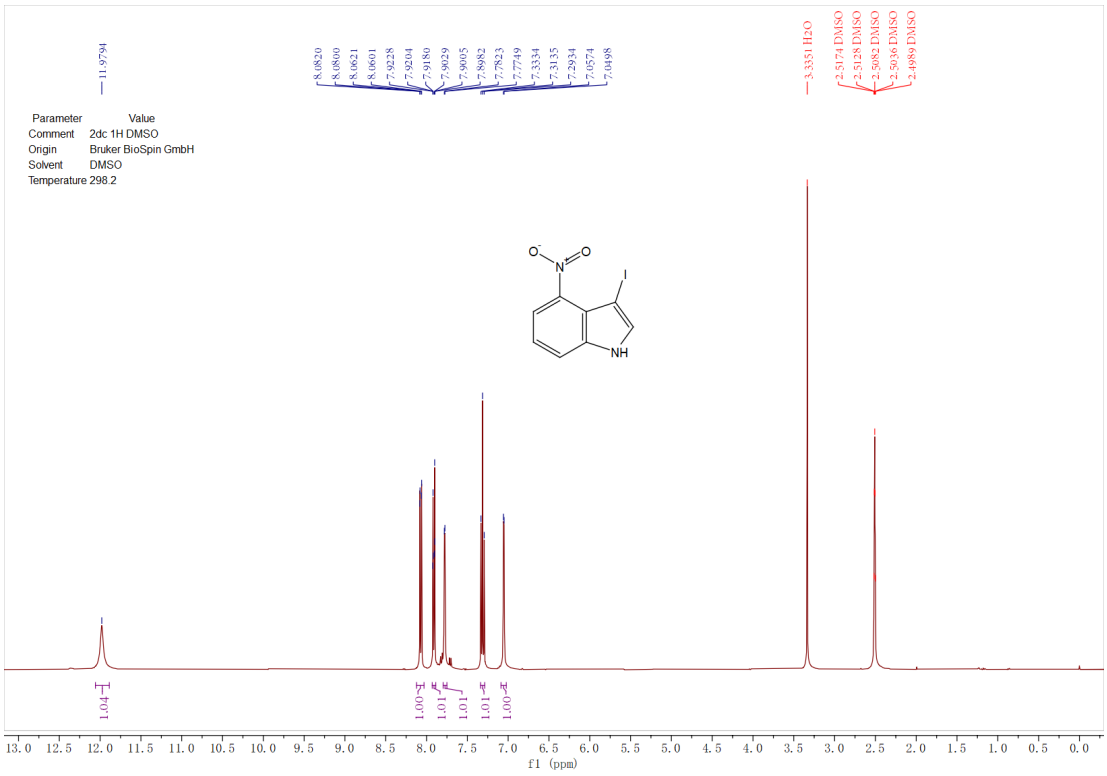

12.3465
7.8990
7.8920
7.8439
7.8419
7.8234
7.8212
7.7515
7.7495
7.7320
7.7300
7.3423
7.3224
7.3025
3.4197 H2O
2.5168 DMSO
2.5121 DMSO
2.5074 DMSO
2.5027 DMSO
2.4981 DMSO
-0.0338
Parameter value
Comment 2db-1012 1H DMSO
Origin Bruker BioSpin GmbH
Solvent DMSO
Spectrometer Frequency 400.13
Br
NH
1.02
1.00
1.00
1.00
1.01
f1 (ppm)

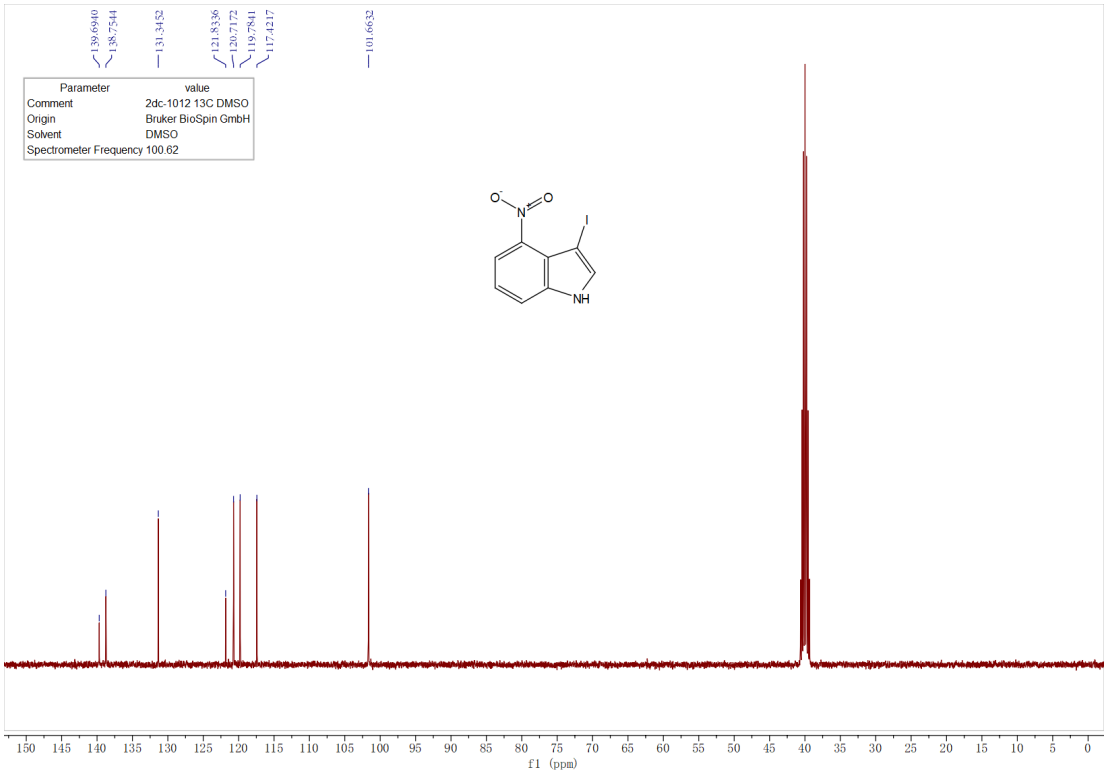

142.0123
138.2544
131.1164
121.5964
118.3729
117.3067
116.8059
86.3104
Parameter value
Comment 2db-1012 13C DMSO
Origin Bruker BioSpin GmbH
Solvent DMSO
Spectrometer Frequency 100.62
Br
NH
f1 (ppm)

Sample Name	2db	**Position**	Vial 11	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	2db.d
ACQ Method	E-R.m	**Comment**		**Acquired Time**	29/04/2024 20:56:00 (UTC+08:00)

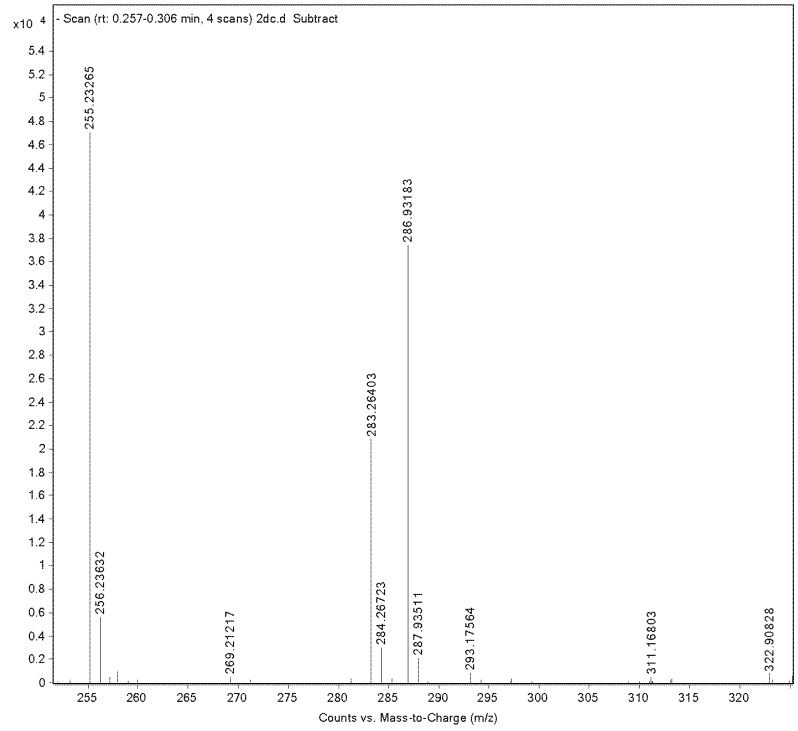


2"d

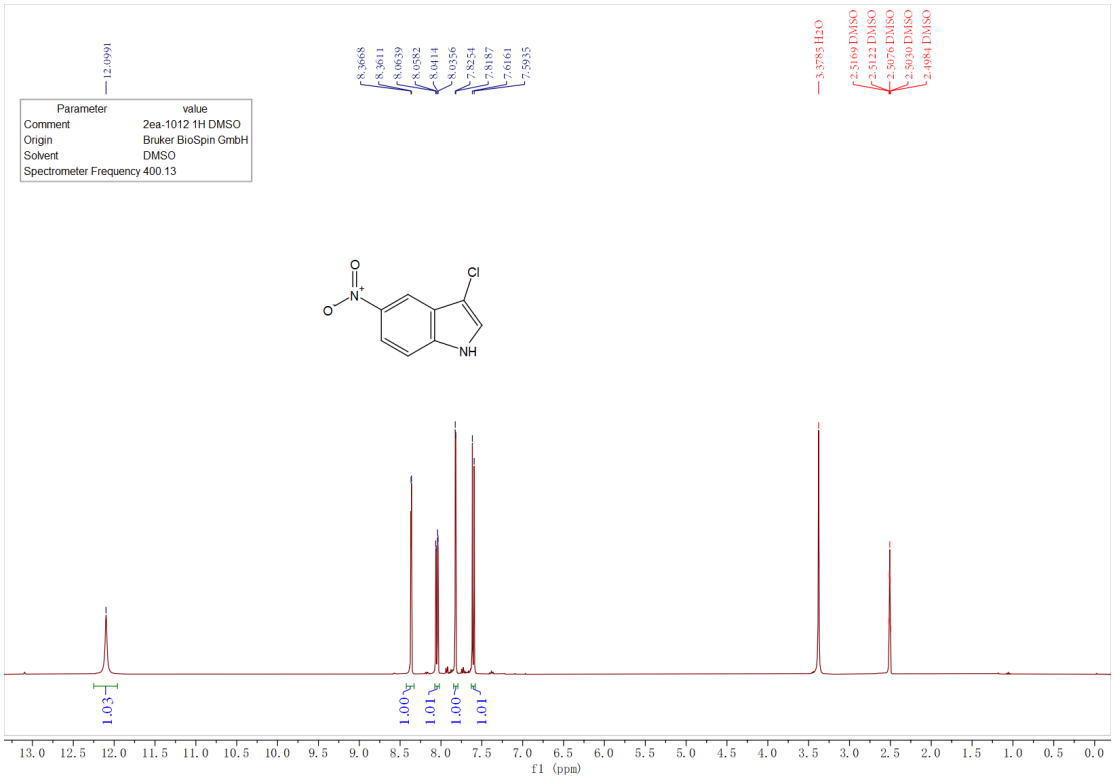

11.9794
8.0820
8.0800
8.0621
8.0601
7.9228
7.9204
7.9180
7.9029
7.9005
7.8982
7.7823
7.7749
7.3334
7.3135
7.2934
7.0574
7.0498
3.3351 H2O
2.5174 DMSO
2.5128 DMSO
2.5082 DMSO
2.5036 DMSO
2.4989 DMSO
Parameter Value
Comment 2dc 1H DMSO
Origin Bruker BioSpin GmbH
Solvent DMSO
Temperature 298.2
1.04
1.00
1.01
1.01
1.01
1.00
f1 (ppm)

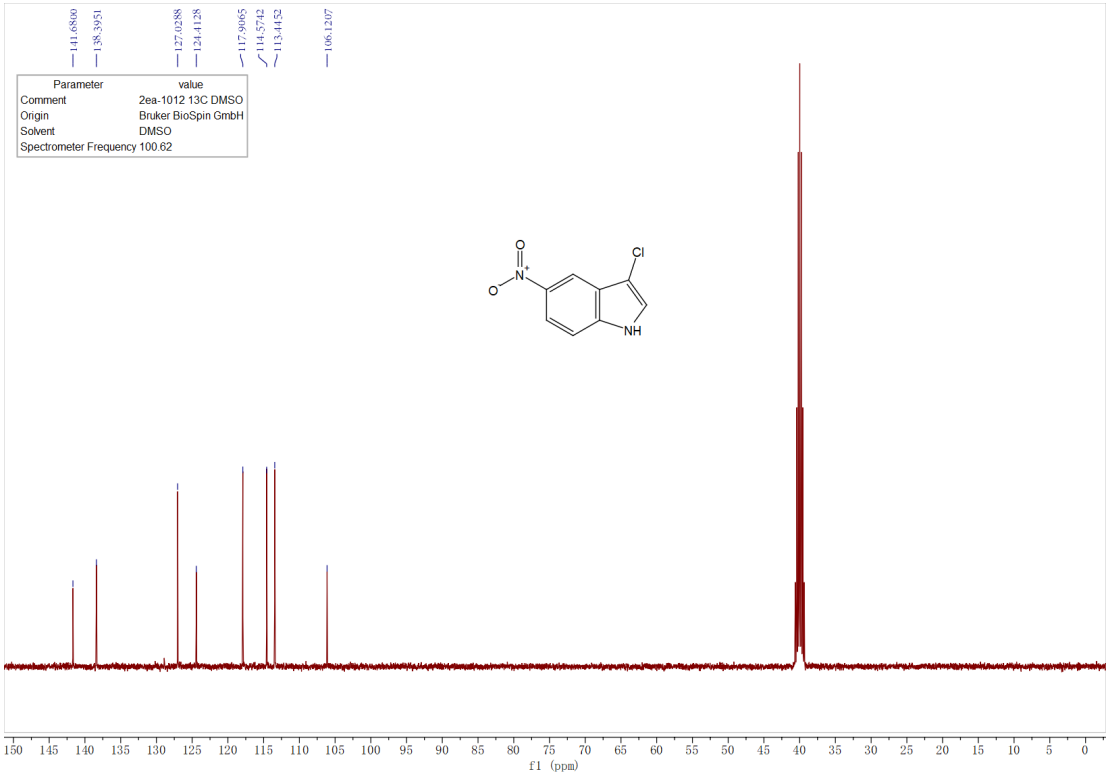

139.6940
138.7544
131.3452
121.8336
120.7172
119.7841
117.4217
101.6632
Parameter value
Comment 2dc-1012 13C DMSO
Origin Bruker BioSpin GmbH
Solvent DMSO
Spectrometer Frequency 100.62
f1 (ppm)

Sample Name	2dc	**Position**	Vial 12	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	2dc.d
ACQ Method	E-R.m	**Comment**		**Acquired Time**	29/04/2024 20:59:26 (UTC+08:00)

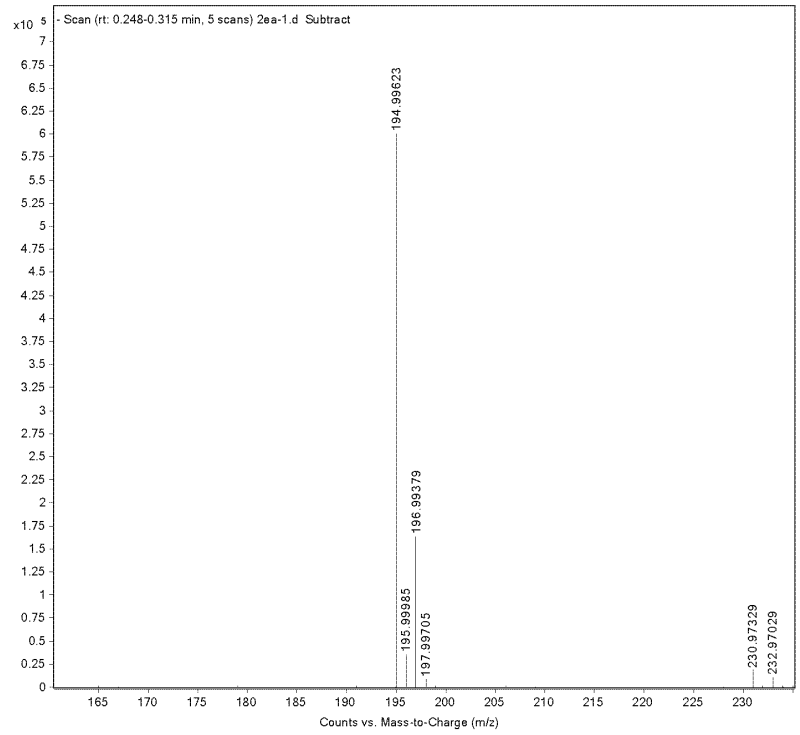


2e

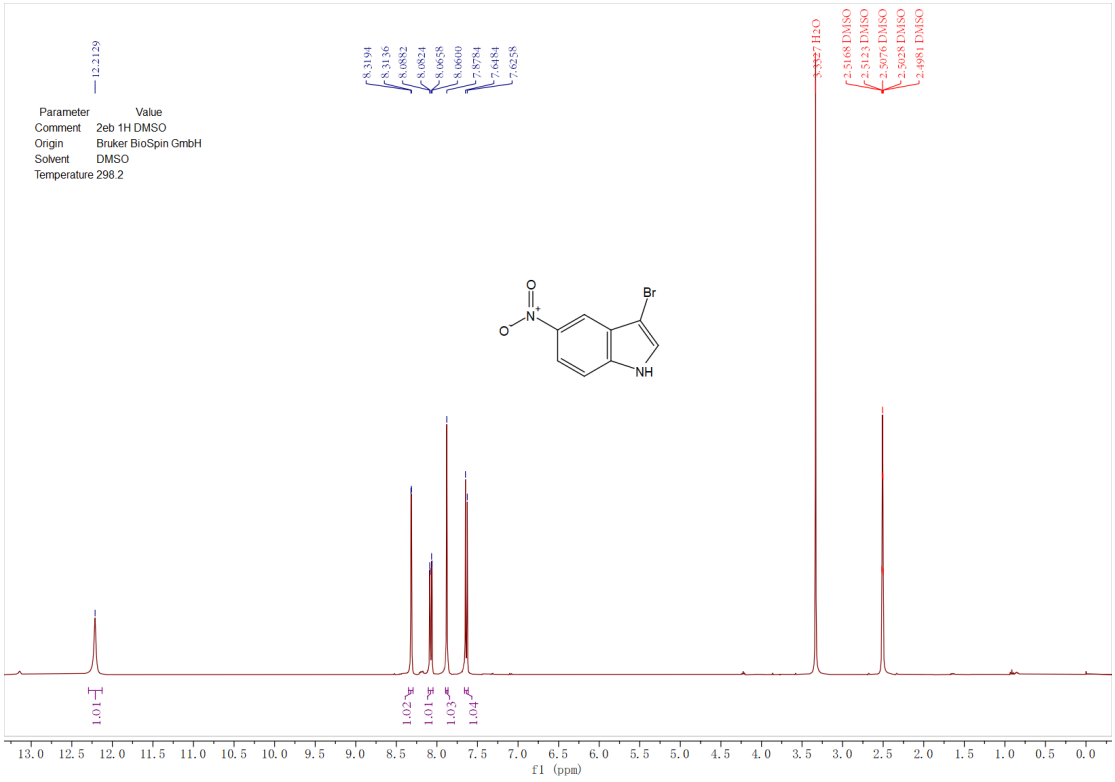

12.0991
8.3668
8.3611
8.0639
8.0582
8.0414
8.0356
7.8254
7.8187
7.6161
7.5935
3.3785 H2O
2.5169 DMSO
2.5122 DMSO
2.5076 DMSO
2.5030 DMSO
2.4984 DMSO
Parameter value
Comment 2ea-1012 1H DMSO
Origin Bruker BioSpin GmbH
Solvent DMSO
Spectrometer Frequency 400.13
Cl
NH
1.03
1.00
1.01
1.00
1.01
f1 (ppm)

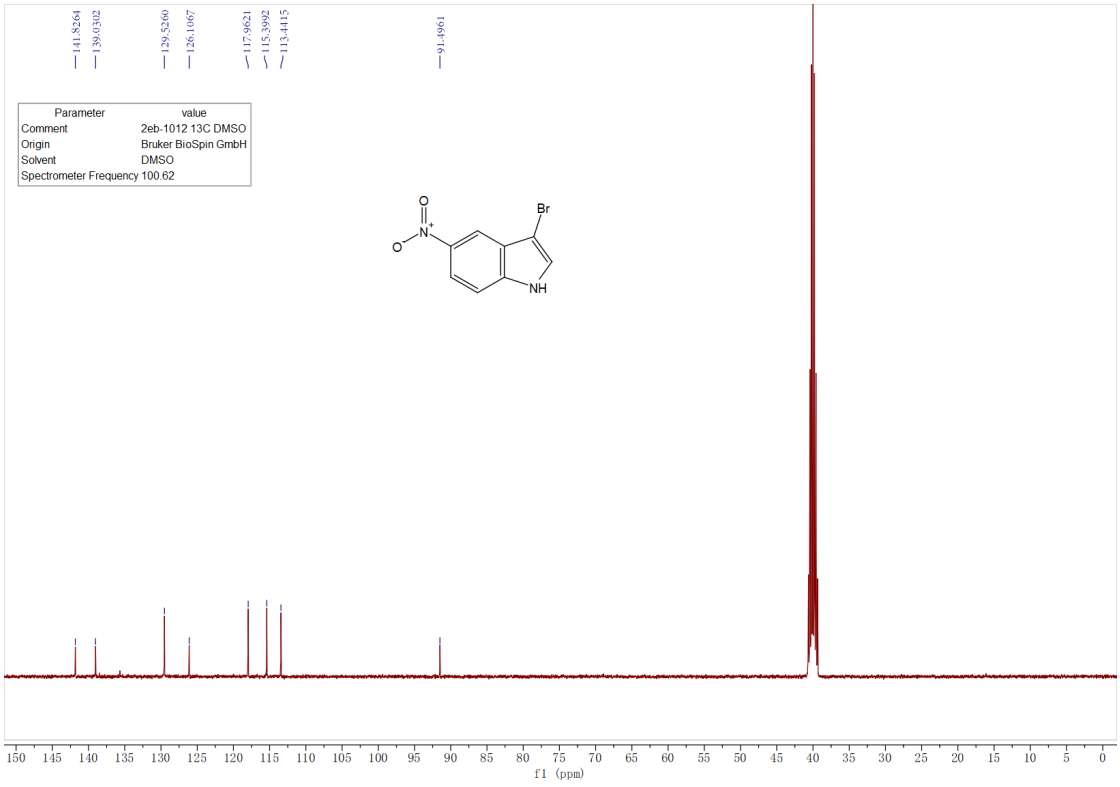

141.6800
138.3951
127.0288
124.4128
117.9065
114.5742
113.4452
106.1207
Parameter value
Comment 2ea-1012 13C DMSO
Origin Bruker BioSpin GmbH
Solvent DMSO
Spectrometer Frequency 100.62
Cl
NH
f1 (ppm)

Sample Name	2ea	**Position**	Vial 5	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	2ea-1.d
ACQ Method	E-R.m	**Comment**		**Acquired Time**	29/04/2024 20:35:24 (UTC+08:00)

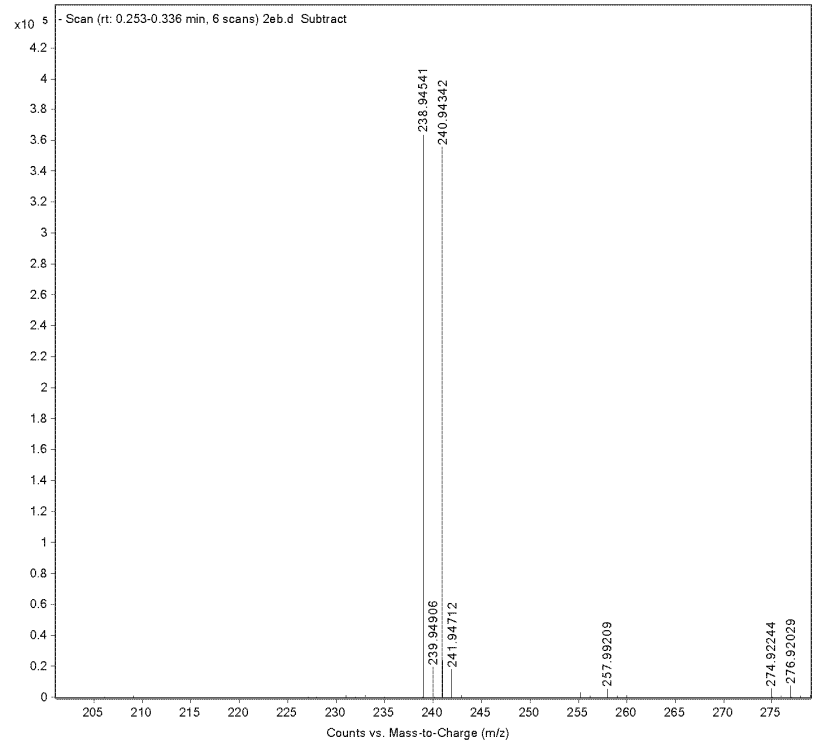


2'e

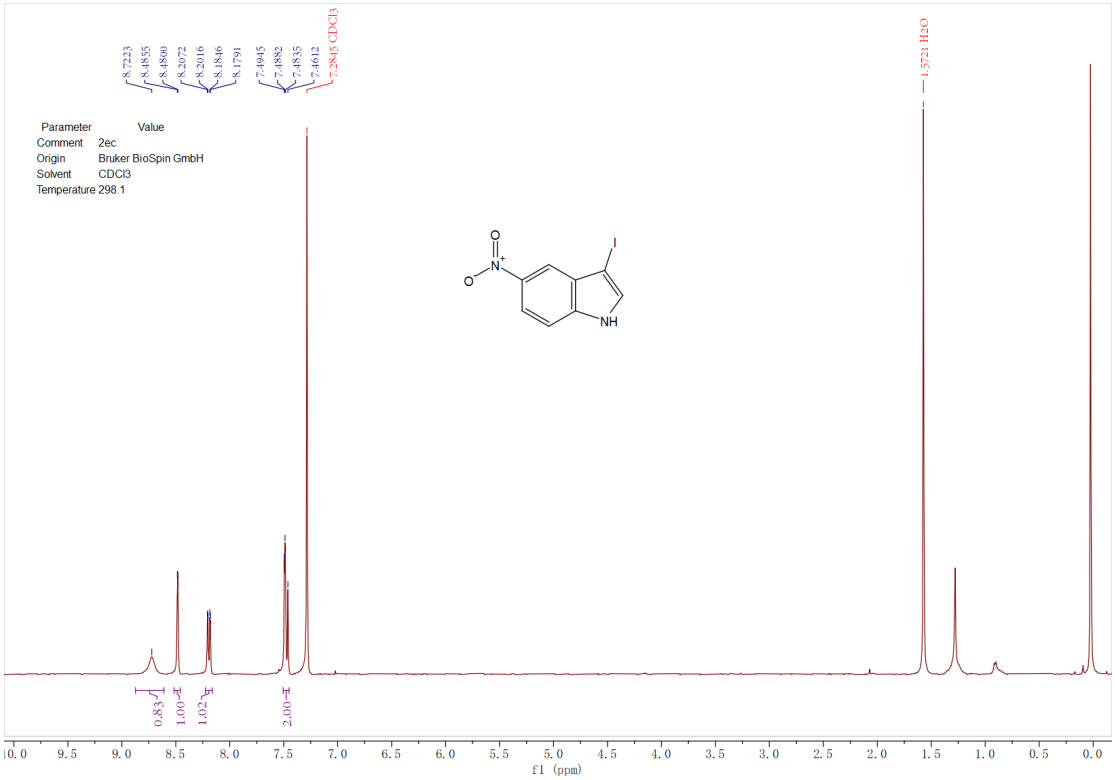

12.2129
8.3194
8.3136
8.0882
8.0824
8.0658
8.0600
7.8784
7.6484
7.6258
3.3327 H2O
2.5168 DMSO
2.5123 DMSO
2.5076 DMSO
2.5028 DMSO
2.4981 DMSO
Parameter Value
Comment 2eb 1H DMSO
Origin Bruker BioSpin GmbH
Solvent DMSO
Temperature 298.2
Br
NH
1.01
1.02
1.01
1.03
1.04
f1 (ppm)

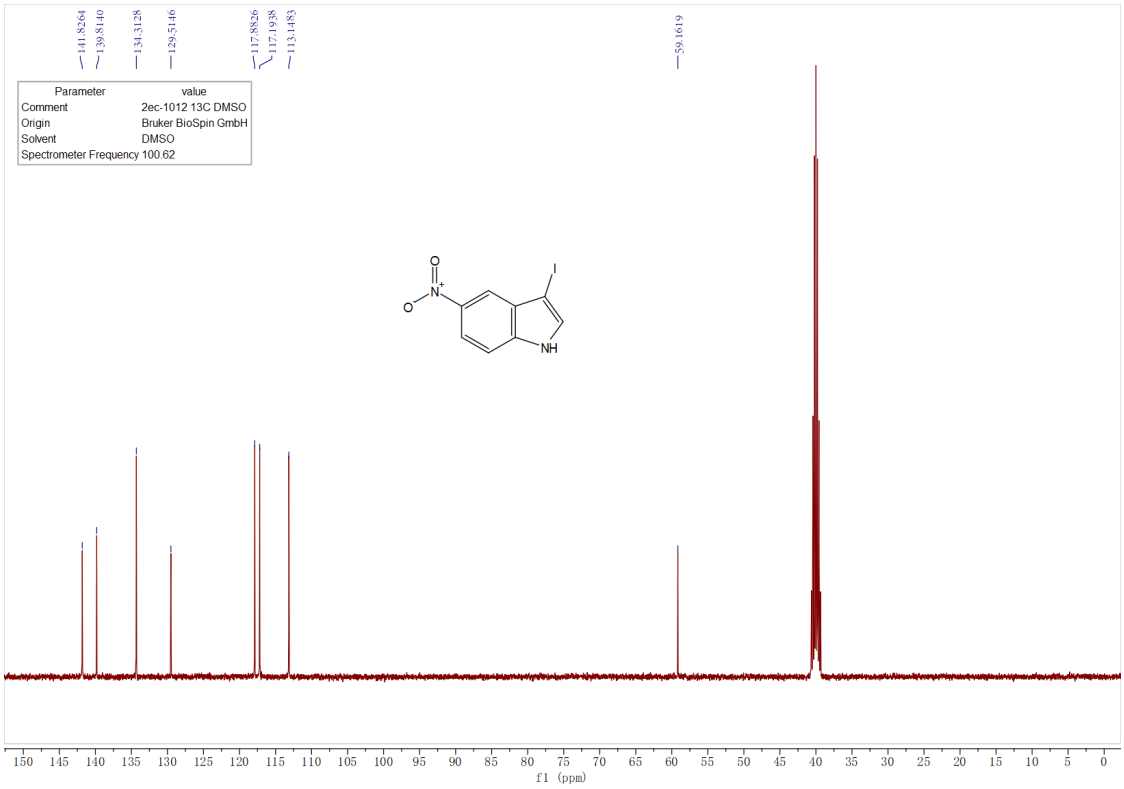

141.8264
139.0302
129.5260
126.1067
117.9621
115.3992
113.4415
91.4961
Parameter value
Comment 2eb-1012 13C DMSO
Origin Bruker BioSpin GmbH
Solvent DMSO
Spectrometer Frequency 100.62
Br
NH
f1 (ppm)

Sample Name	2eb	**Position**	Vial 14	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	2eb.d
ACQ Method	E-R.m	**Comment**		**Acquired Time**	29/04/2024 21:06:19 (UTC+08:00)

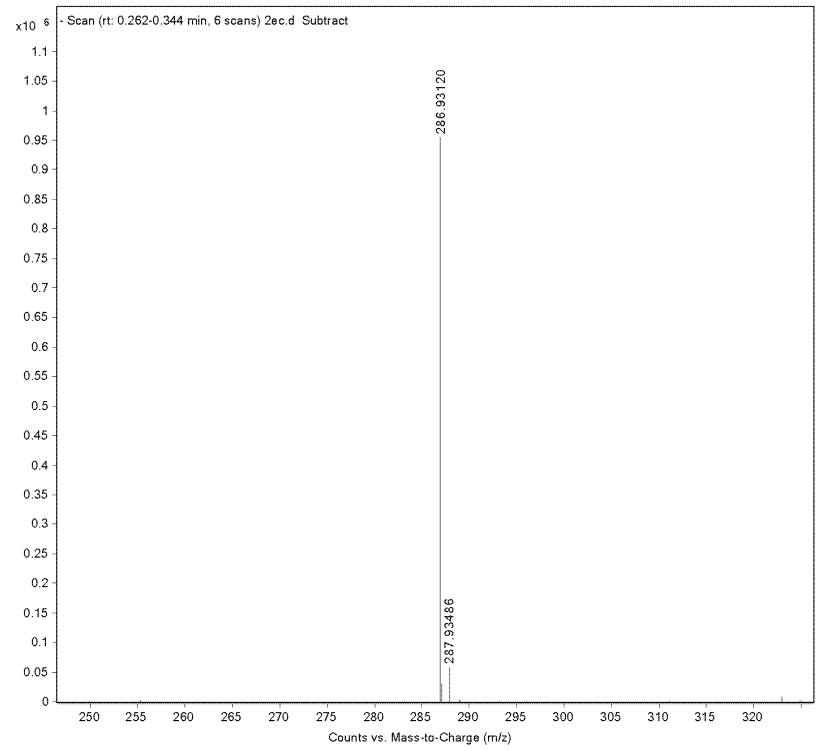


2"e

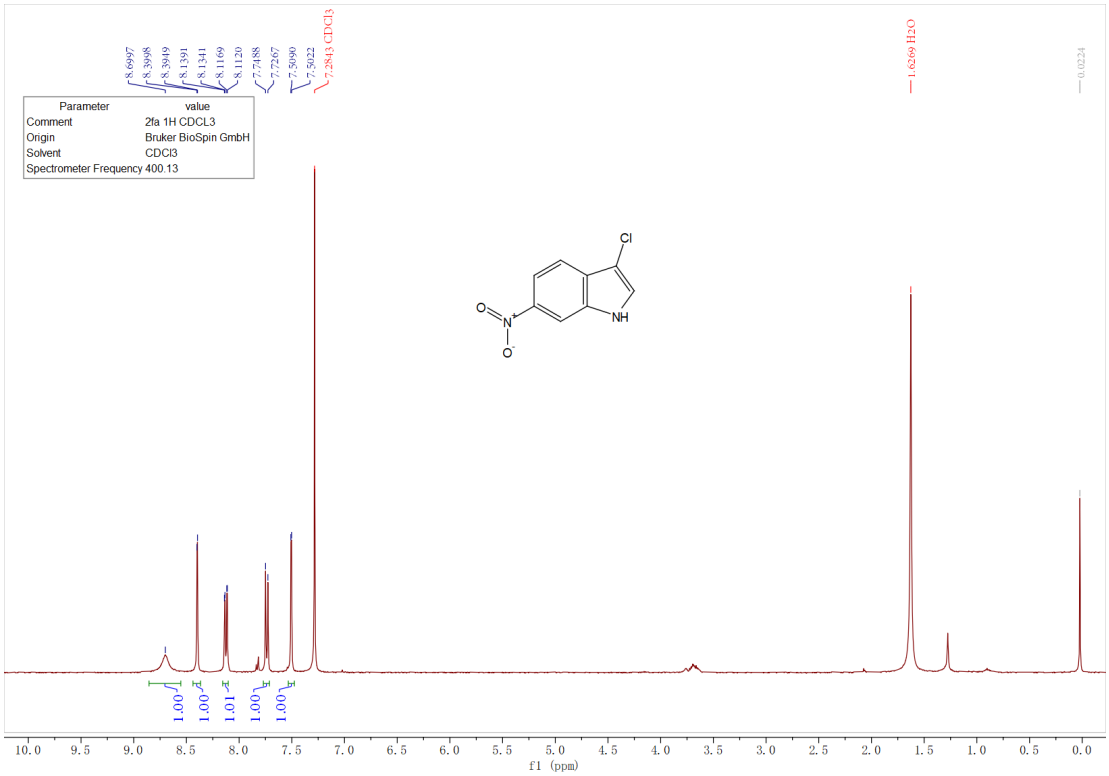

8.7223
8.4855
8.4800
8.2072
8.2016
8.1846
8.1791
7.4945
7.4882
7.4835
7.4612
7.2845 CDCl3
1.5721 H2O
Parameter Value
Comment 2ec
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
0.83
1.00
1.02
2.00
f1 (ppm)

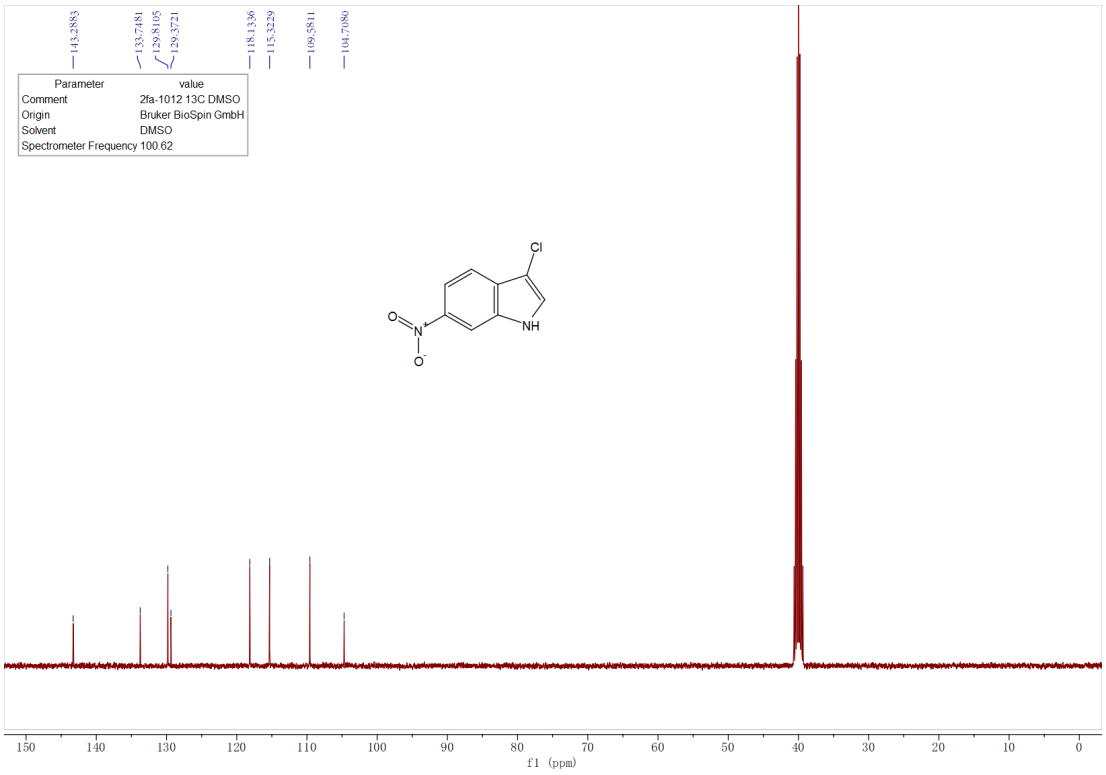

141.8264
139.8140
134.3128
129.5146
117.8826
117.1938
113.1483
59.1619
Parameter value
Comment 2ec-1012 13C DMSO
Origin Bruker BioSpin GmbH
Solvent DMSO
Spectrometer Frequency 100.62
f1 (ppm)

Sample Name	2ec	**Position**	Vial 15	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	2ec.d
ACQ Method	E-R.m	**Comment**		**Acquired Time**	29/04/2024 21:09:46 (UTC+08:00)

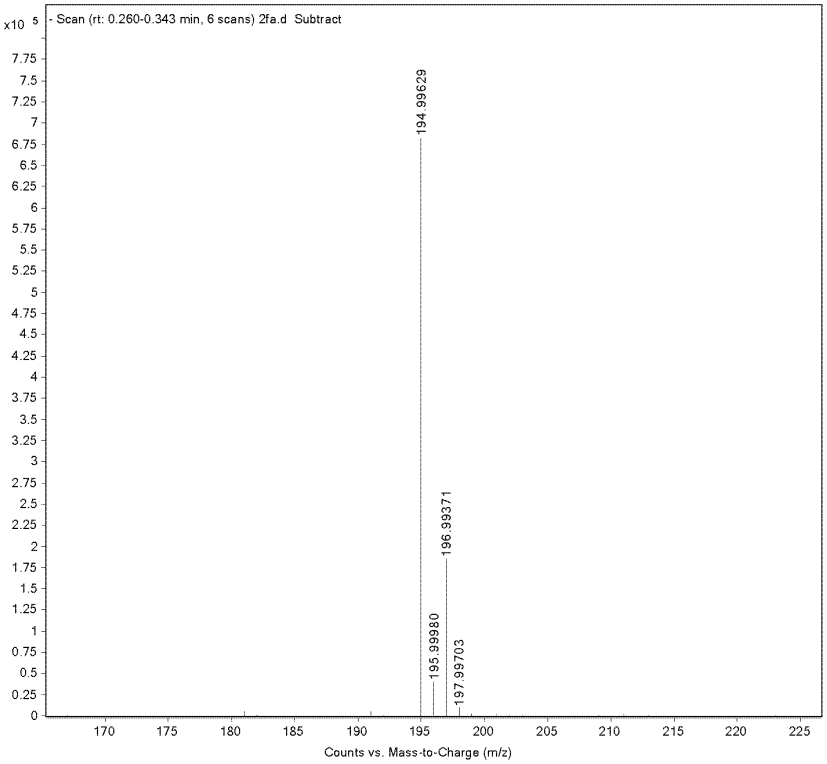


2f

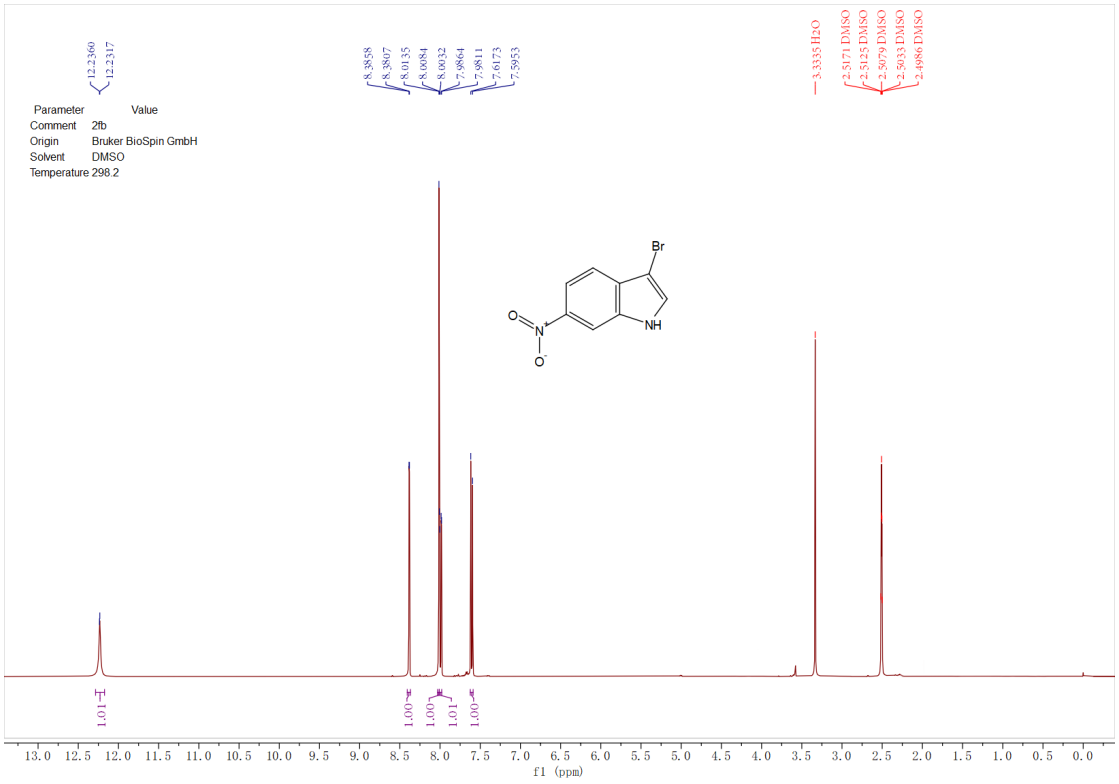

8.6997
8.3998
8.3949
8.1391
8.1341
8.1169
8.1120
7.7488
7.7267
7.5090
7.5022
7.2843 CDCl3
1.6269 H2O
0.0224
Parameter value
Comment 2fa 1H CDCL3
Origin Bruker BioSpin GmbH
Solvent CDCl3
Spectrometer Frequency 400.13
Cl
NH
1.00
1.00
1.01
1.00
1.00
f1 (ppm)

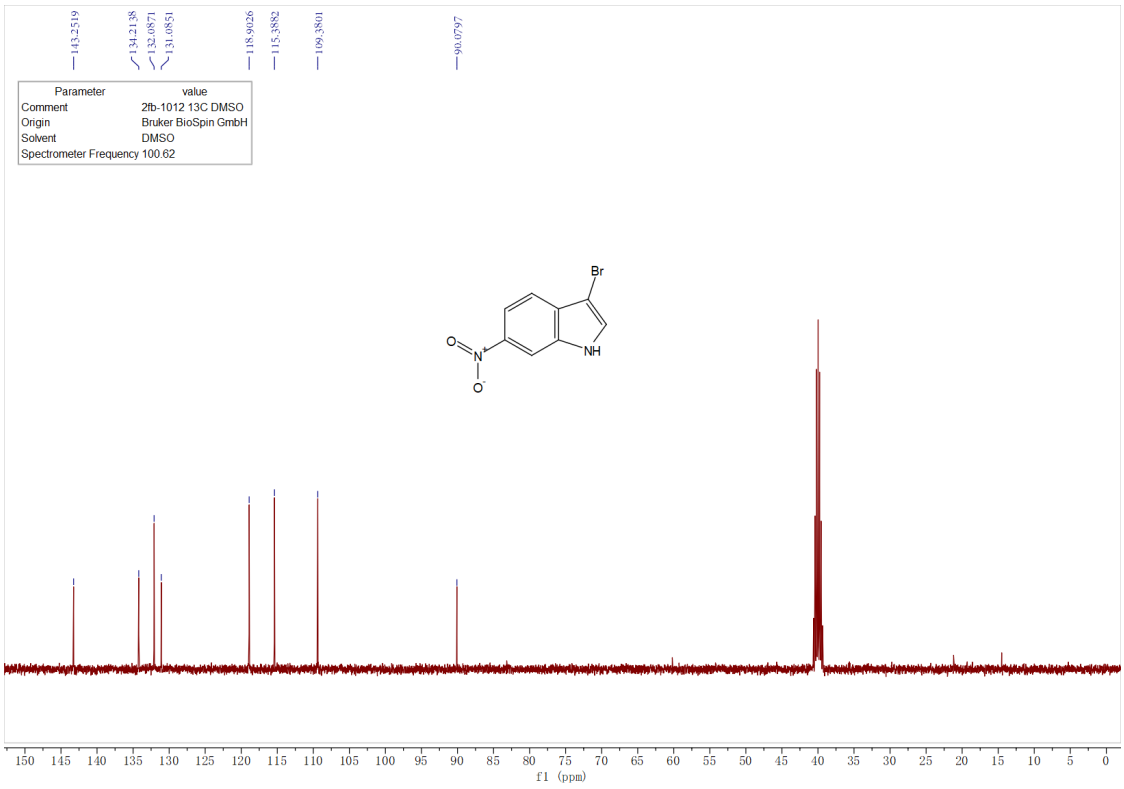

143.2883
133.7481
129.8105
129.3721
118.1336
115.3229
109.5811
104.7080
Parameter value
Comment 2fa-1012 13C DMSO
Origin Bruker BioSpin GmbH
Solvent DMSO
Spectrometer Frequency 100.62
Cl
NH
f1 (ppm)

Sample Name	2fa	**Position**	Vial 16	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	2fa.d
ACQ Method	E-R.m	**Comment**		**Acquired Time**	29/04/2024 21:13:09 (UTC+08:00)

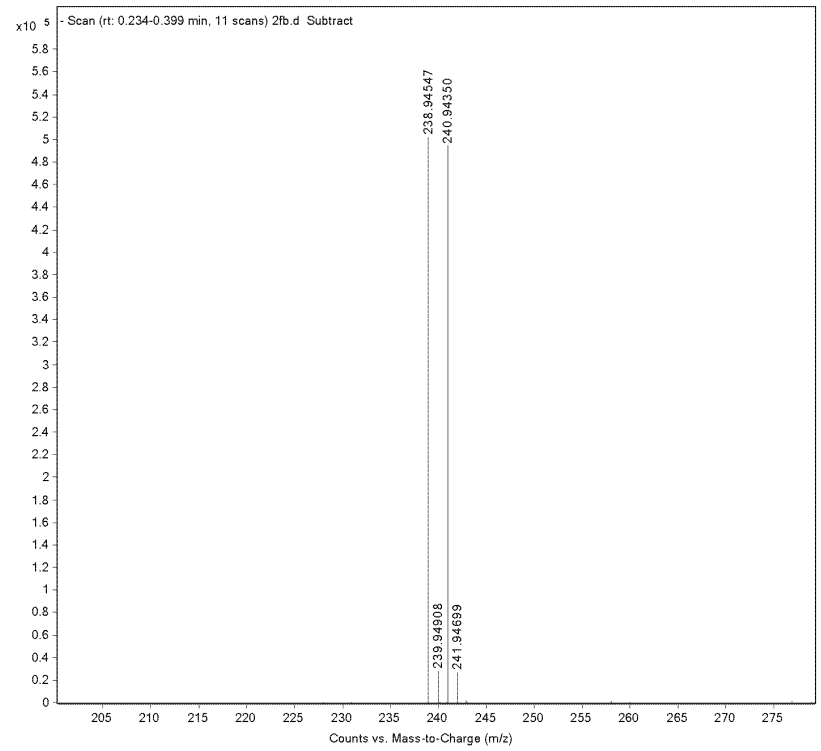


2'f

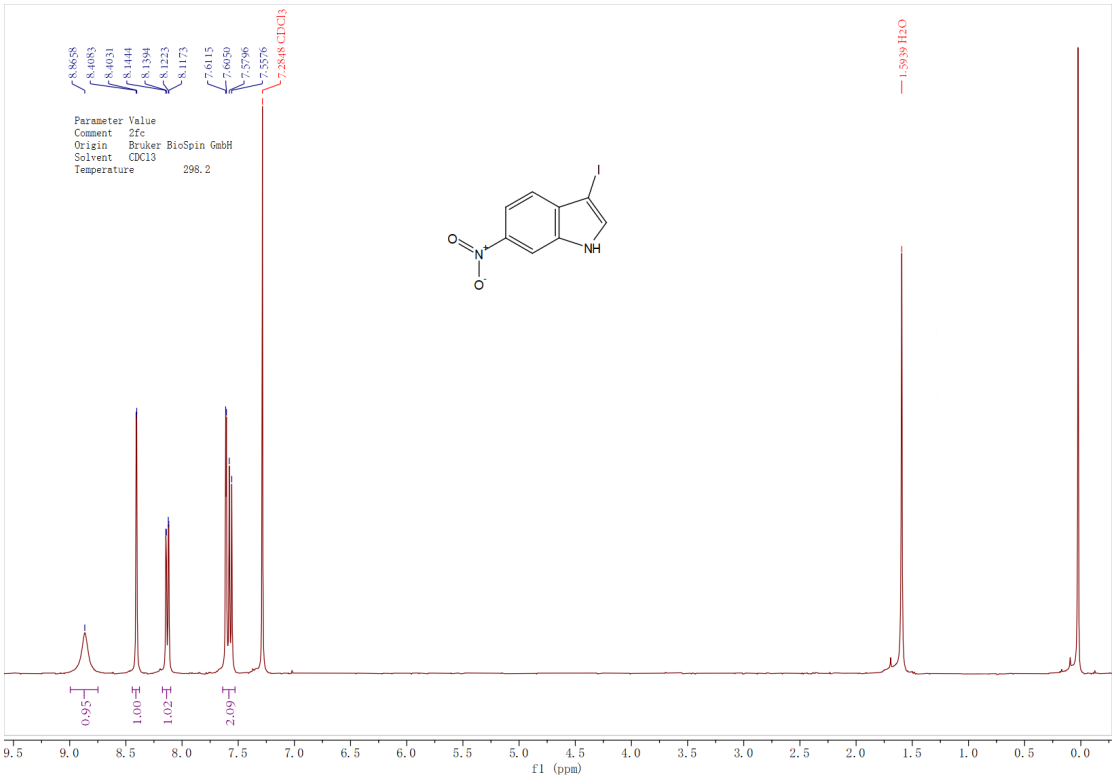

12.2366
12.2317
8.3858
8.3807
8.0135
8.0084
8.0032
7.9864
7.9811
7.6173
7.5953
3.3335 H2O
2.5171 DMSO
2.5125 DMSO
2.5079 DMSO
2.5033 DMSO
2.4986 DMSO
Parameter Value
Comment 2fb
Origin Bruker BioSpin GmbH
Solvent DMSO
Temperature 298.2
Br
NH
1.01
1.00
1.00
1.01
1.00
f1 (ppm)

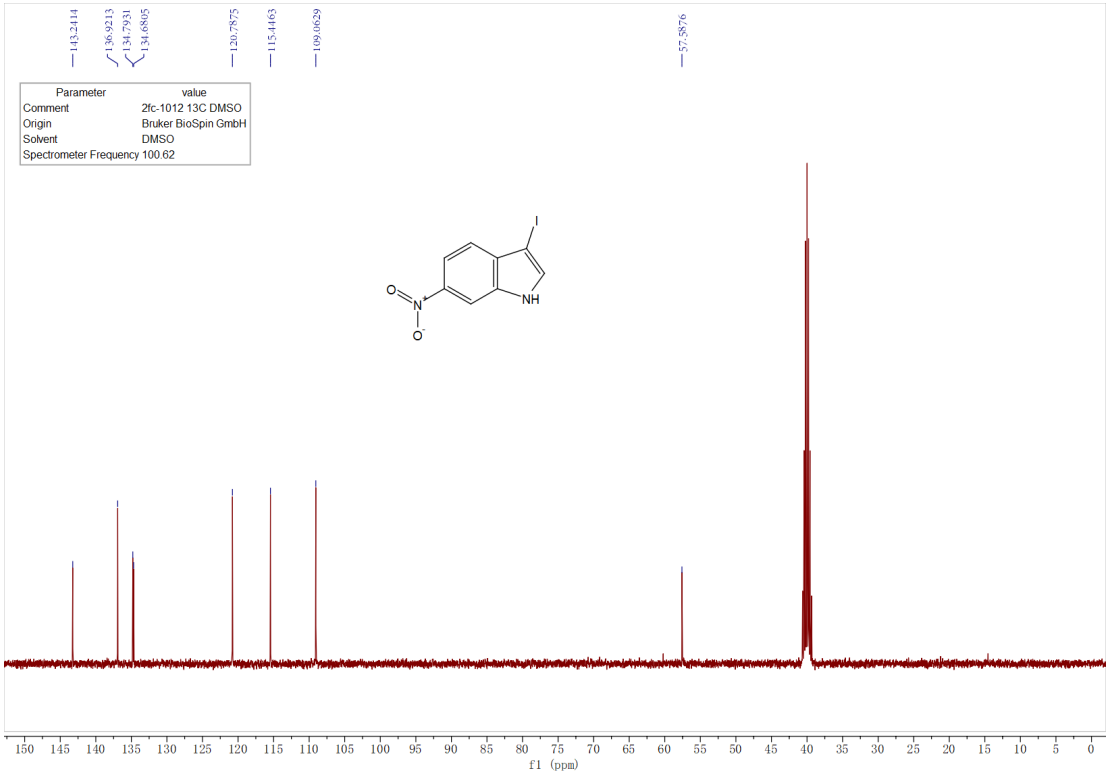

143.2519
134.2138
132.0871
131.0851
118.9026
115.3882
109.3801
90.0797
Parameter value
Comment 2fb-1012 13C DMSO
Origin Bruker BioSpin GmbH
Solvent DMSO
Spectrometer Frequency 100.62
Br
NH
f1 (ppm)

Sample Name	2fb	**Position**	Vial 17	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	2fb.d
ACQ Method	E-R.m	**Comment**		**Acquired Time**	29/04/2024 21:16:35 (UTC+08:00)

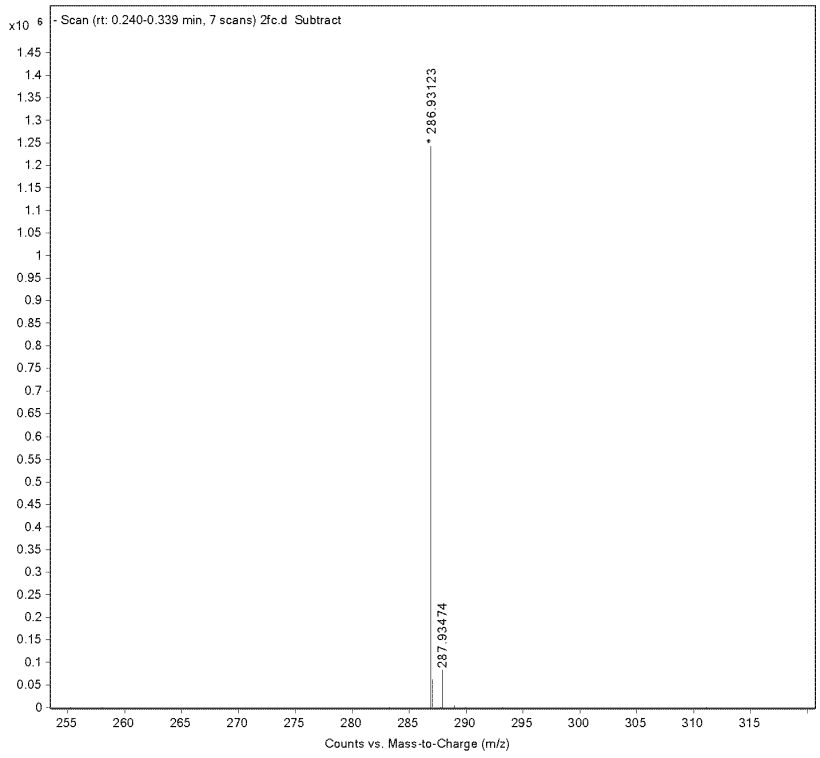


2"f

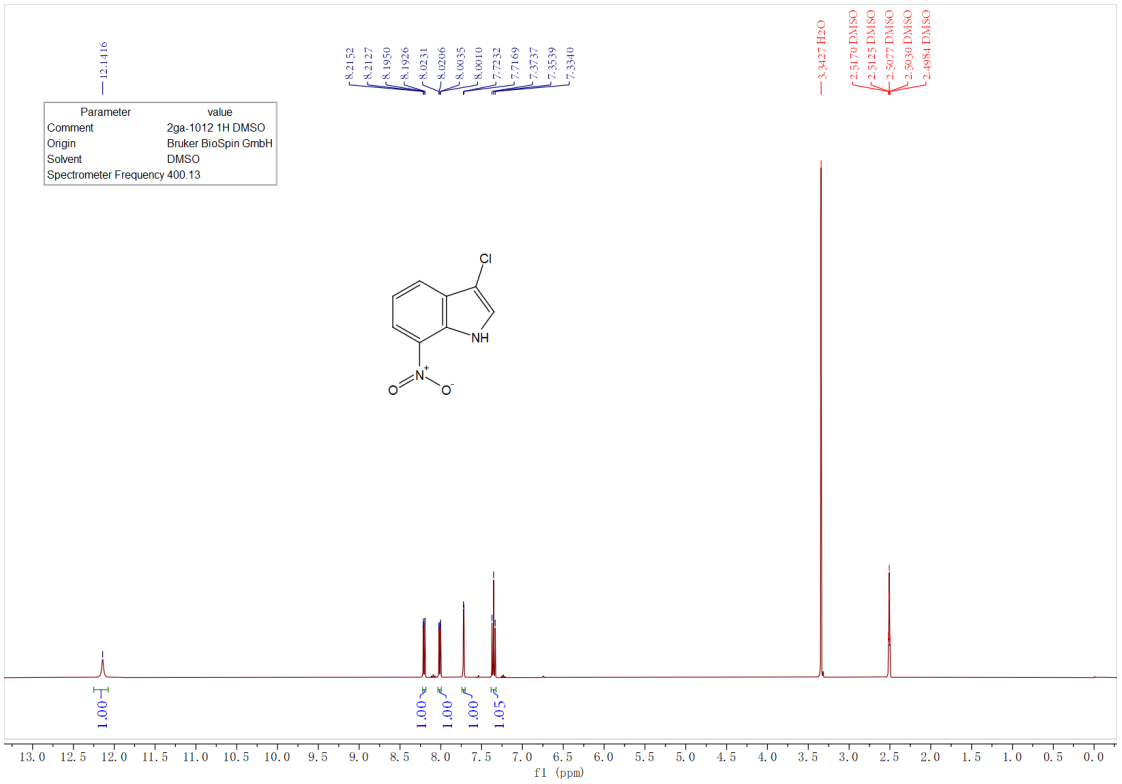

8.8658
8.4083
8.4031
8.1444
8.1394
8.1223
8.1173
7.6115
7.6050
7.5796
7.5576
7.2848 CDCl3
1.5939 H2O
Parameter Value
Comment 2fc
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
I
O
N+
O-
NH
0.95
1.00
1.02
2.09
f1 (ppm)

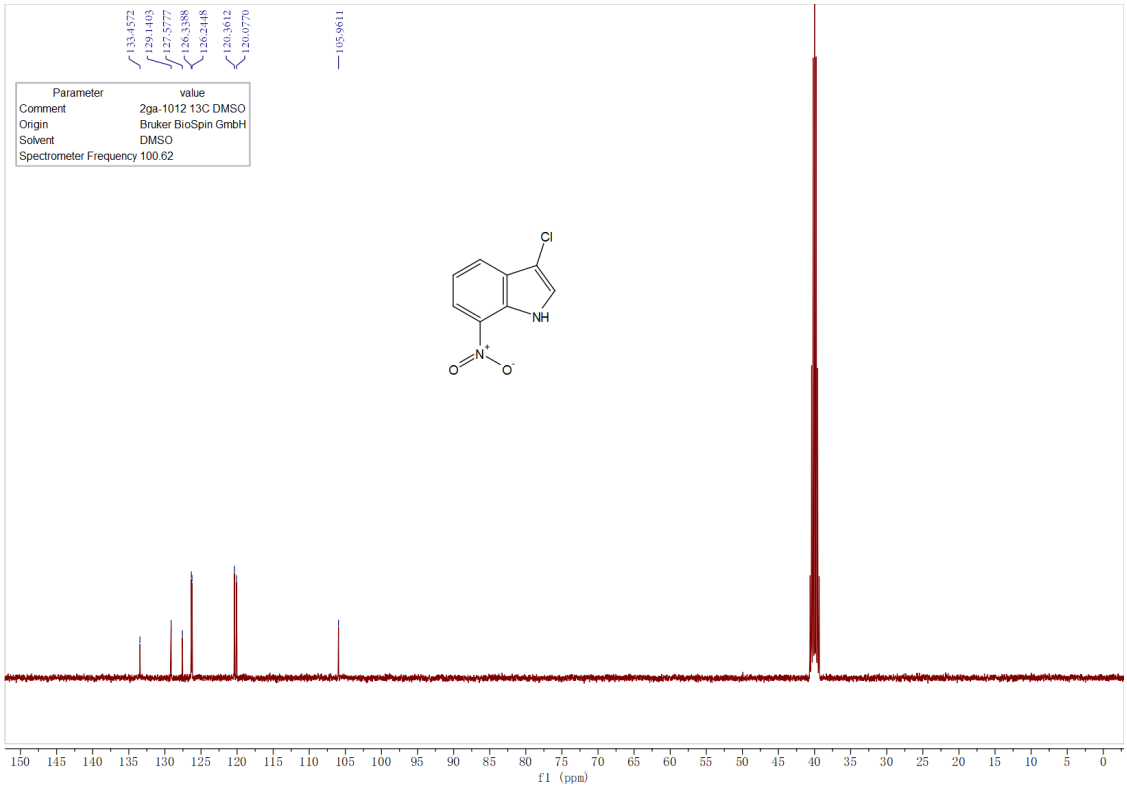

143.2414
136.9213
134.7931
134.6805
120.7875
115.4463
109.0629
57.5876
Parameter value
Comment 2fc-1012 13C DMSO
Origin Bruker BioSpin GmbH
Solvent DMSO
Spectrometer Frequency 100.62
I
O
N+
O-
NH
f1 (ppm)

Sample Name	2fc	**Position**	Vial 18	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	2fc.d
ACQ Method	E-R.m	**Comment**		**Acquired Time**	29/04/2024 21:19:58 (UTC+08:00)

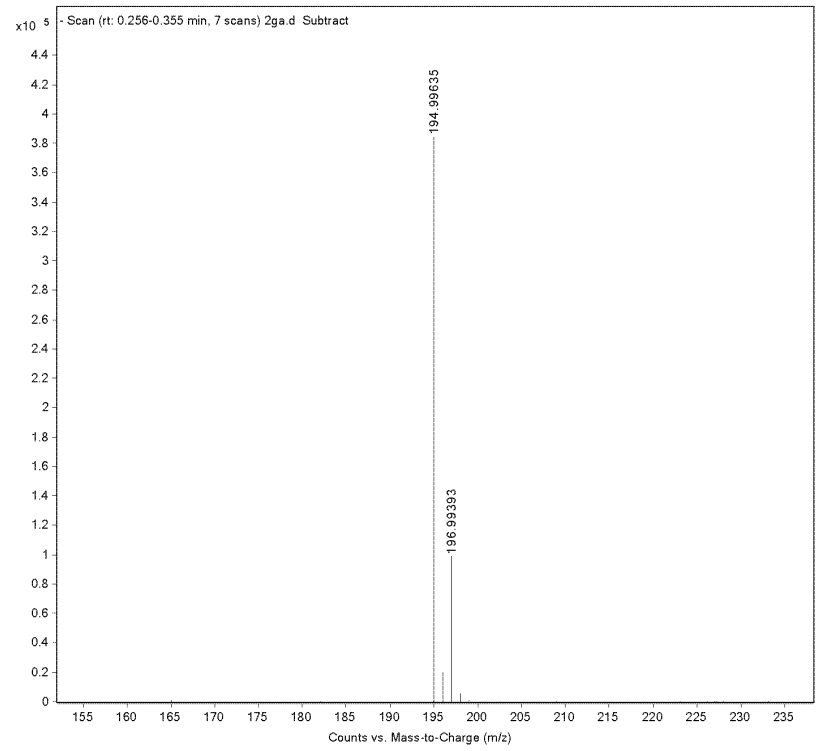


2g

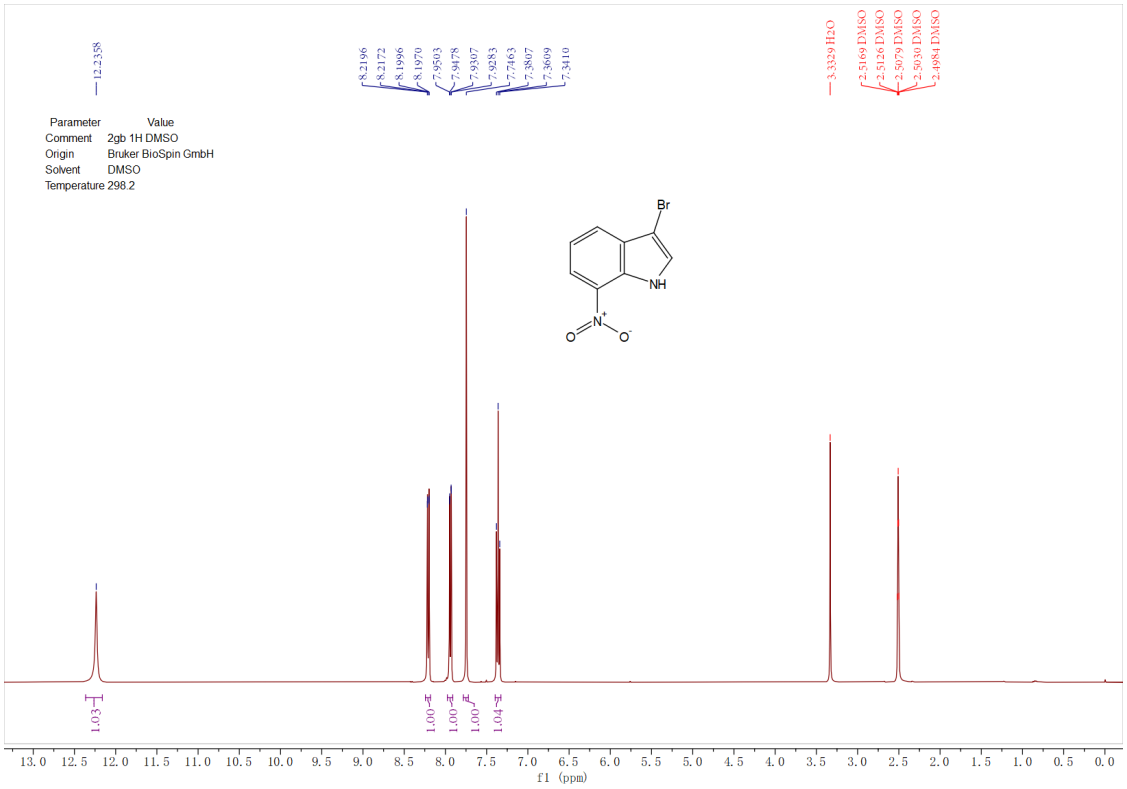

12.1416
8.2152
8.2127
8.1950
8.1926
8.0231
8.0206
8.0035
8.0010
7.7232
7.7169
7.3737
7.3539
7.3340
3.3427 H2O
2.5170 DMSO
2.5125 DMSO
2.5077 DMSO
2.5030 DMSO
2.4984 DMSO
Parameter value
Comment 2ga-1012 1H DMSO
Origin Bruker BioSpin GmbH
Solvent DMSO
Spectrometer Frequency 400.13
Cl
NH
O
N+
O-
1.00
1.00
1.00
1.00
1.05
f1 (ppm)

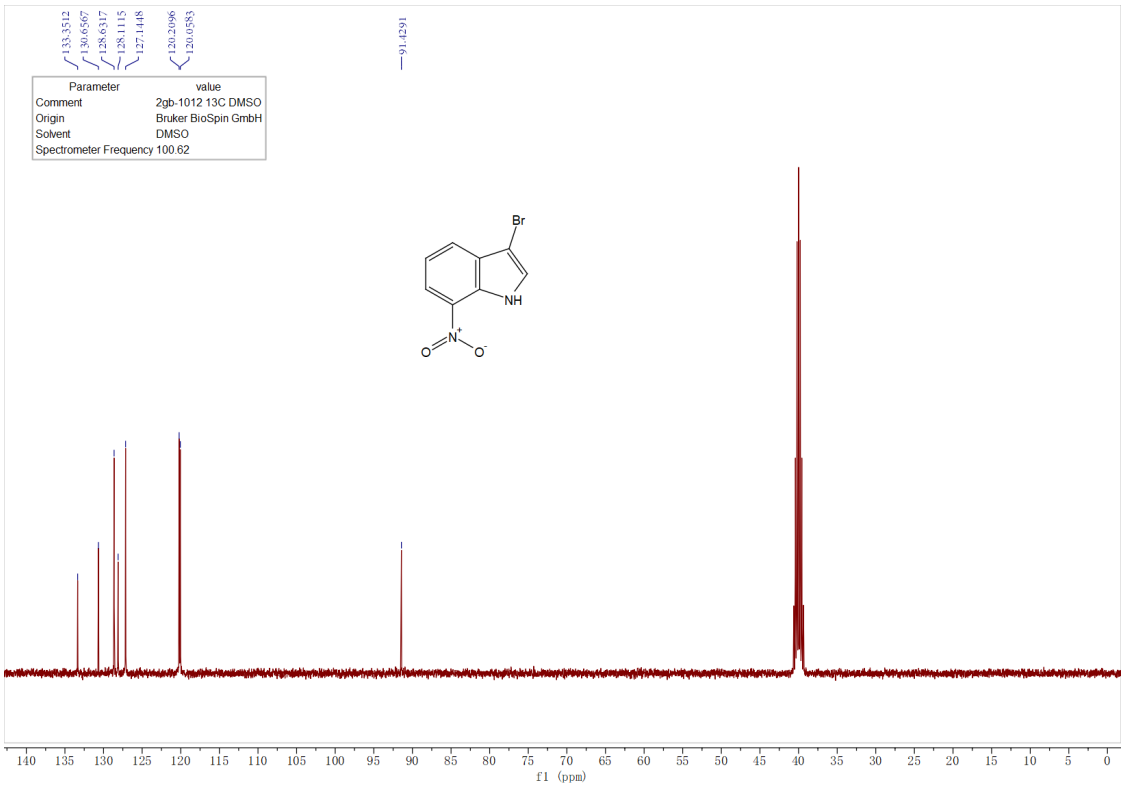

133.4572
129.1403
127.5777
126.3388
126.2448
120.3612
120.0770
105.9611
Parameter value
Comment 2ga-1012 13C DMSO
Origin Bruker BioSpin GmbH
Solvent DMSO
Spectrometer Frequency 100.62
Cl
NH
O
N+
O-
f1 (ppm)

Sample Name	2ga	**Position**	Vial 19	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	2ga.d
ACQ Method	E-R.m	**Comment**		**Acquired Time**	29/04/2024 21:23:22 (UTC+08:00)

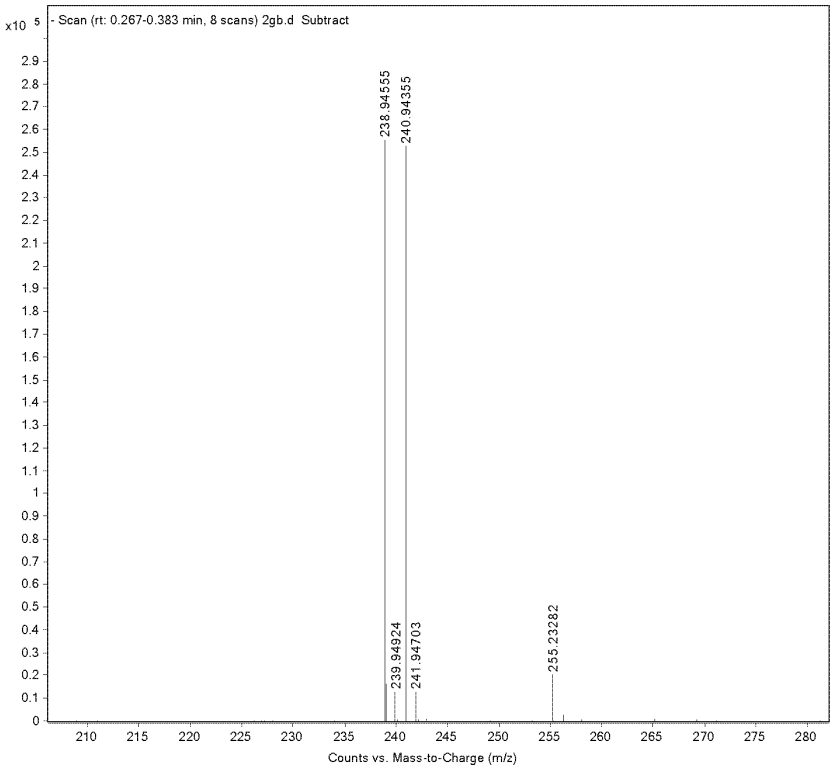


2'g

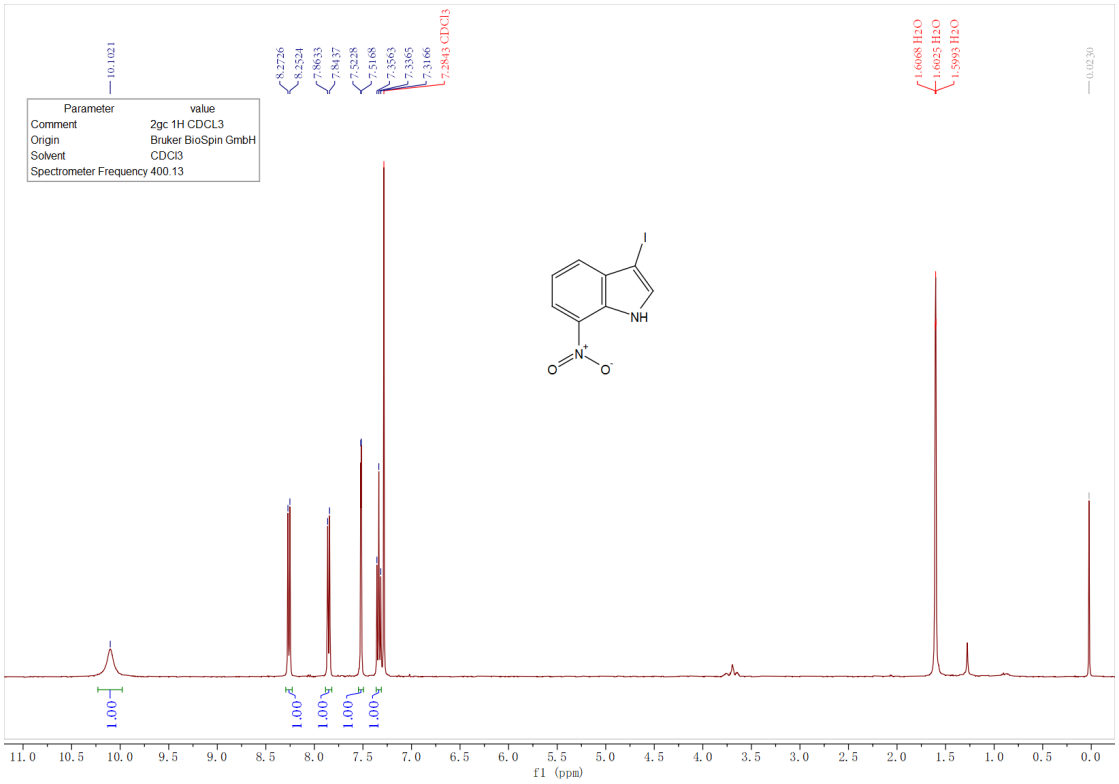

12.2358
8.2196
8.2172
8.1996
8.1970
7.9503
7.9478
7.9307
7.9283
7.7463
7.3807
7.3669
7.3410
3.3329 H2O
2.5169 DMSO
2.5126 DMSO
2.5079 DMSO
2.5030 DMSO
2.4984 DMSO
Parameter Value
Comment 2gb 1H DMSO
Origin Bruker BioSpin GmbH
Solvent DMSO
Temperature 298.2
Br
NH
1.03
1.00
1.00
1.00
1.04
f1 (ppm)

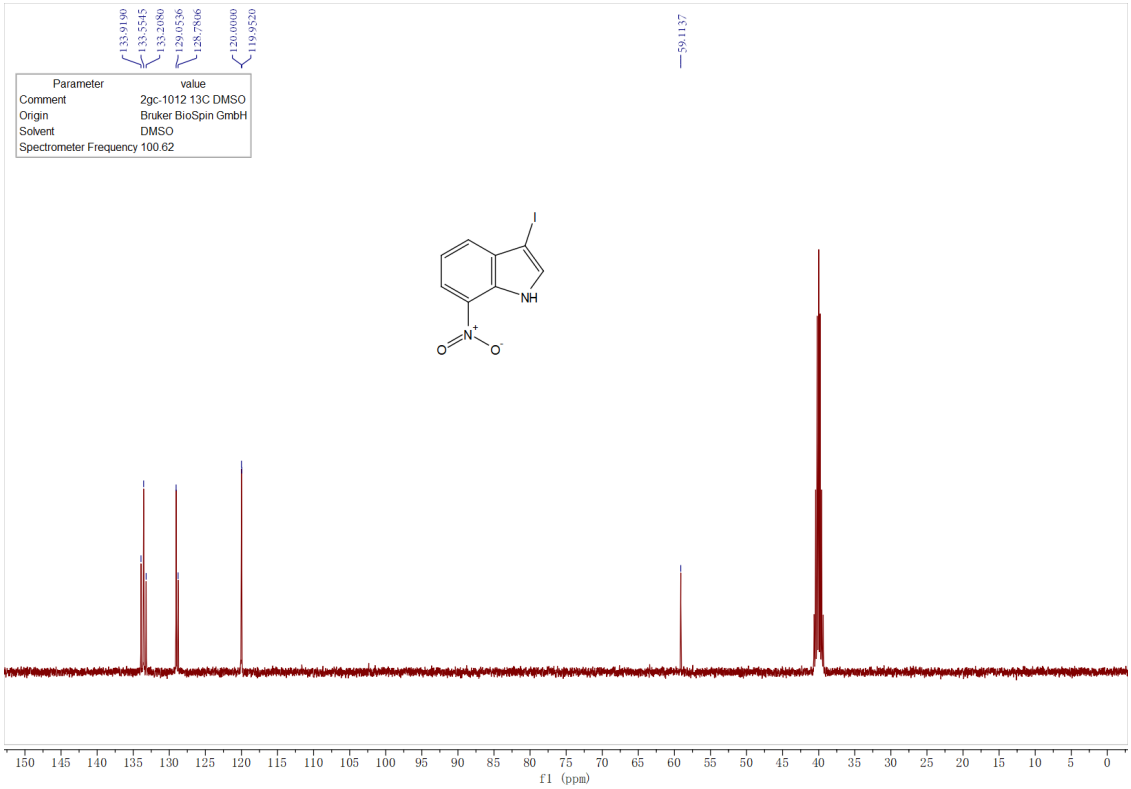

133.3512
130.6567
128.6317
128.1115
127.1448
120.2096
120.0583
91.4291
Parameter value
Comment 2gb-1012 13C DMSO
Origin Bruker BioSpin GmbH
Solvent DMSO
Spectrometer Frequency 100.62
Br
NH
f1 (ppm)

Sample Name	2gb	**Position**	Vial 20	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	2gb.d
ACQ Method	E-R.m	**Comment**		**Acquired Time**	29/04/2024 21:26:51 (UTC+08:00)

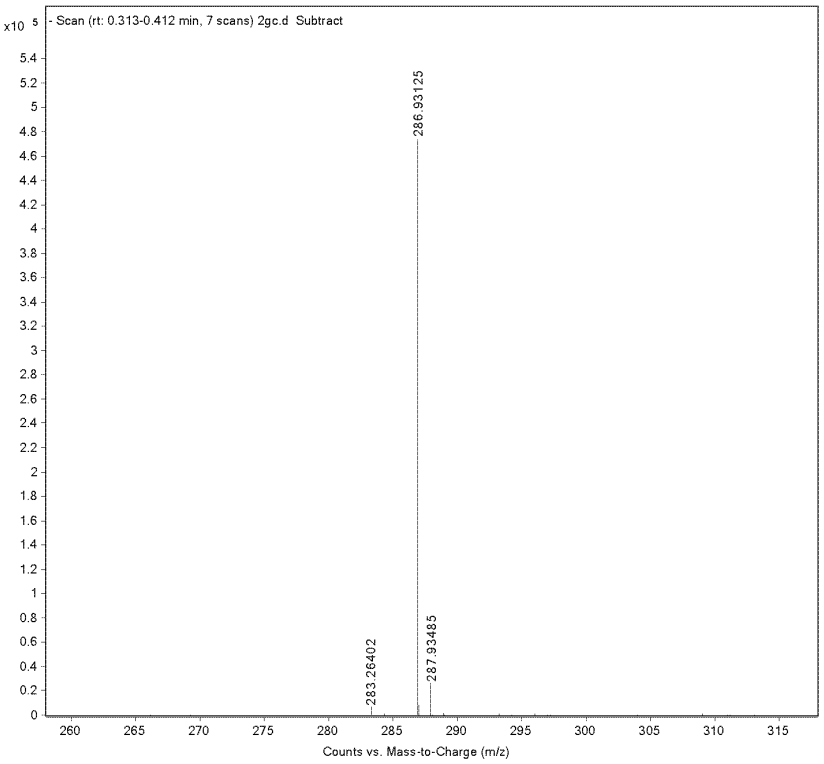


2"g

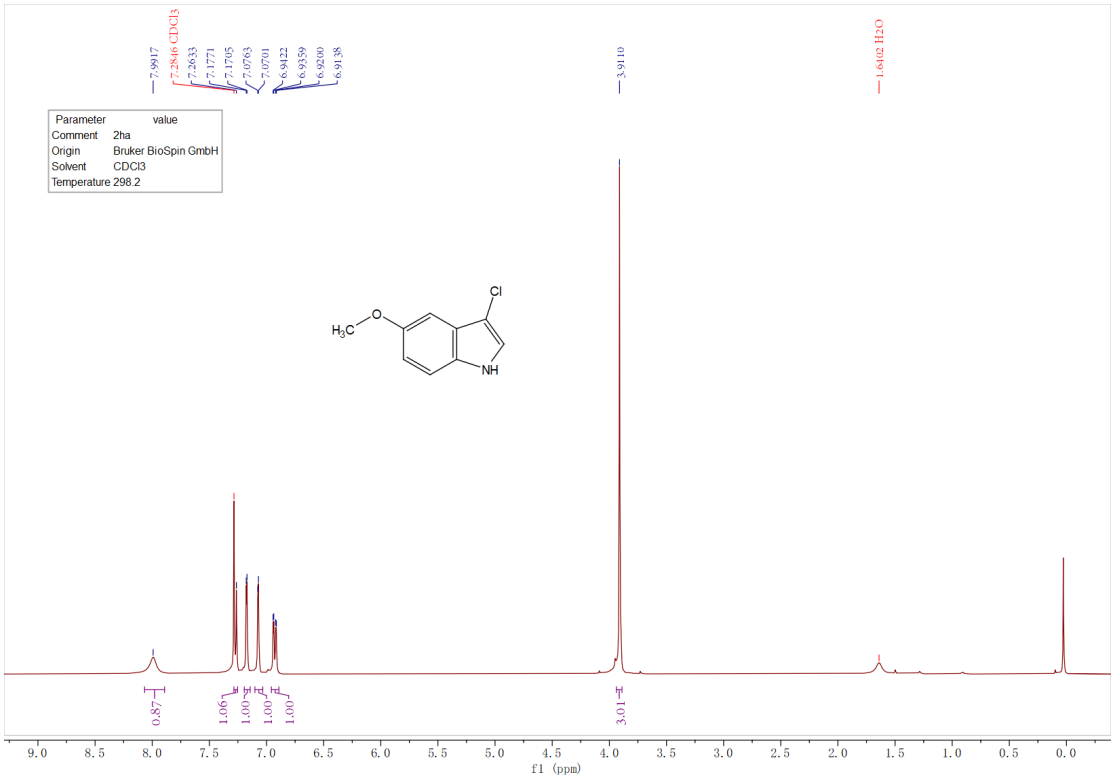

10.1021
8.2726
8.2524
7.8633
7.8437
7.5228
7.5168
7.3563
7.3365
7.3166
7.2843 CDCl3
1.6068 H2O
1.6025 H2O
1.5993 H2O
0.0230
Parameter value
Comment 2gc 1H CDCL3
Origin Bruker BioSpin GmbH
Solvent CDCl3
Spectrometer Frequency 400.13
I
NH
N+
O
O-
1.00
1.00
1.00
1.00
1.00
f1 (ppm)

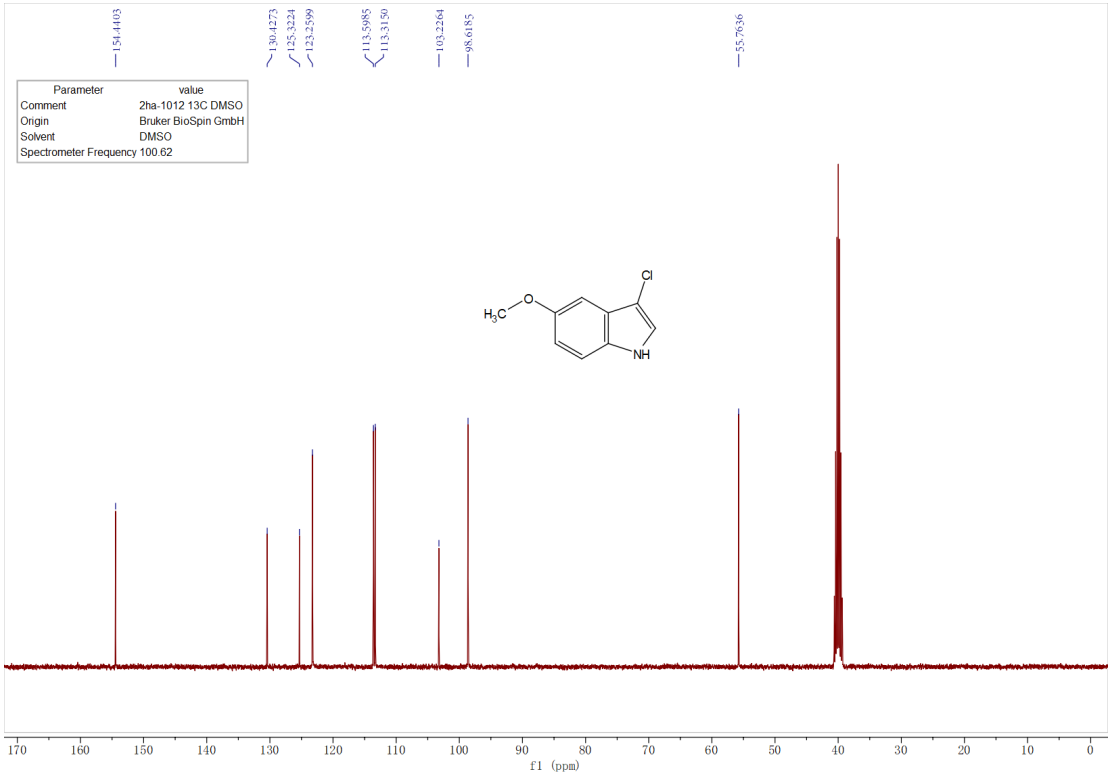

133.9190
133.5545
133.2080
129.0536
128.7866
120.0000
119.9520
59.1137
Parameter value
Comment 2gc-1012 13C DMSO
Origin Bruker BioSpin GmbH
Solvent DMSO
Spectrometer Frequency 100.62
I
NH
N+
O
O-
f1 (ppm)

Sample Name	2gc	**Position**	Vial 21	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	2gc.d
ACQ Method	E-R.m	**Comment**		**Acquired Time**	29/04/2024 21:30:18 (UTC+08:00)

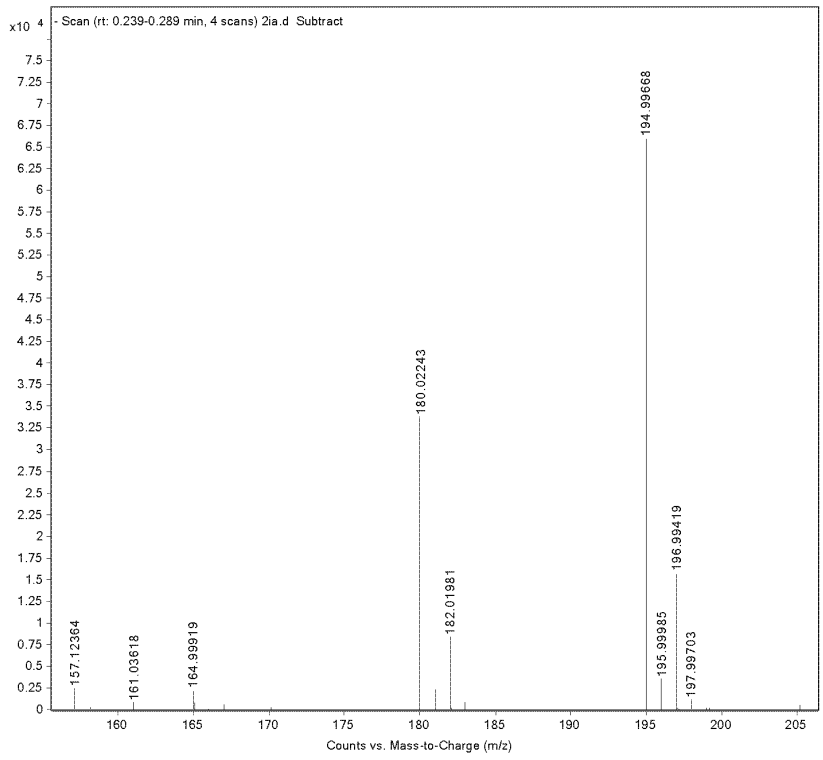


2h

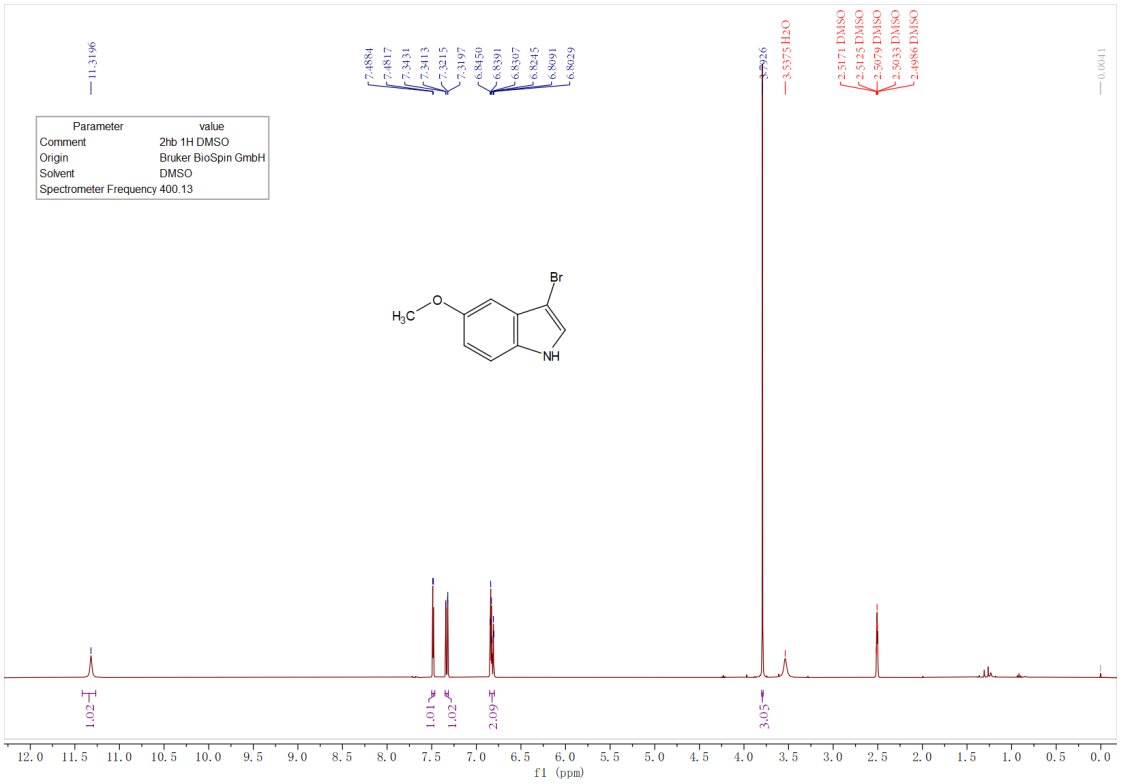

7.9917
7.2846 CDCl3
7.2633
7.1771
7.1705
7.0763
7.0701
6.9422
6.9359
6.9200
6.9138
3.9110
1.6402 H2O
Parameter value
Comment 2ha
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Cl
O
H3C
NH
0.87
1.06
1.00
1.00
1.00
3.01
f1 (ppm)

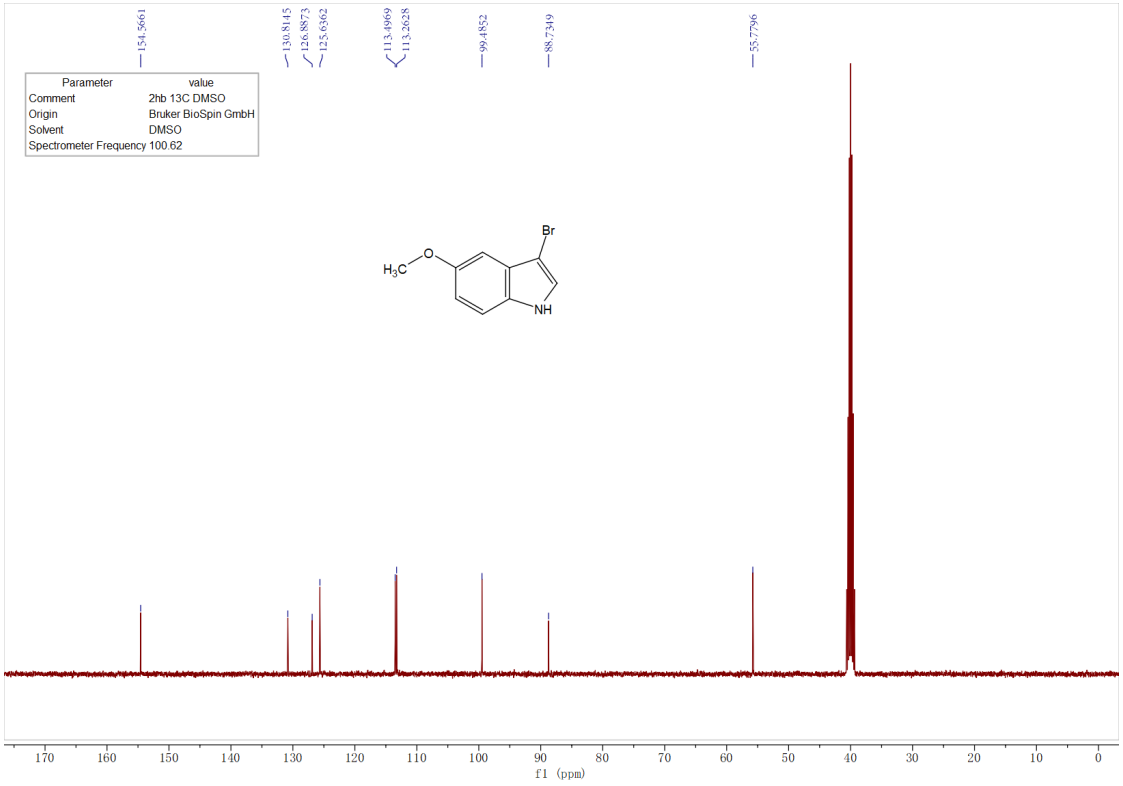

154.4403
130.4273
125.3224
123.2599
113.5985
113.3150
103.2264
98.6185
55.7636
Parameter value
Comment 2ha-1012 13C DMSO
Origin Bruker BioSpin GmbH
Solvent DMSO
Spectrometer Frequency 100.62
Cl
O
H3C
NH
f1 (ppm)

Sample Name	2ia	**Position**	Vial 22	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	2ia.d
ACQ Method	E-R.m	**Comment**		**Acquired Time**	29/04/2024 21:33:43 (UTC+08:00)

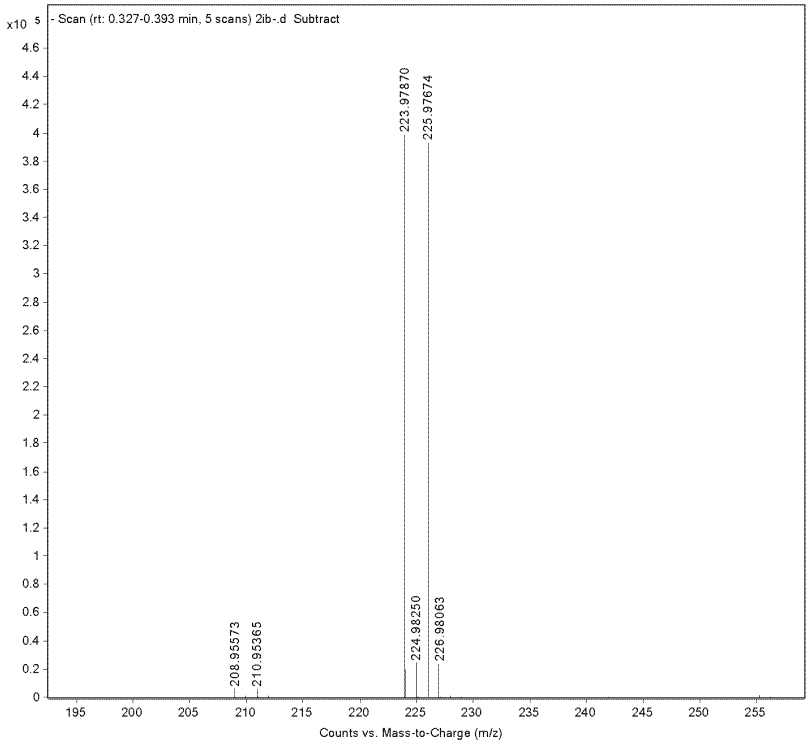


2'h

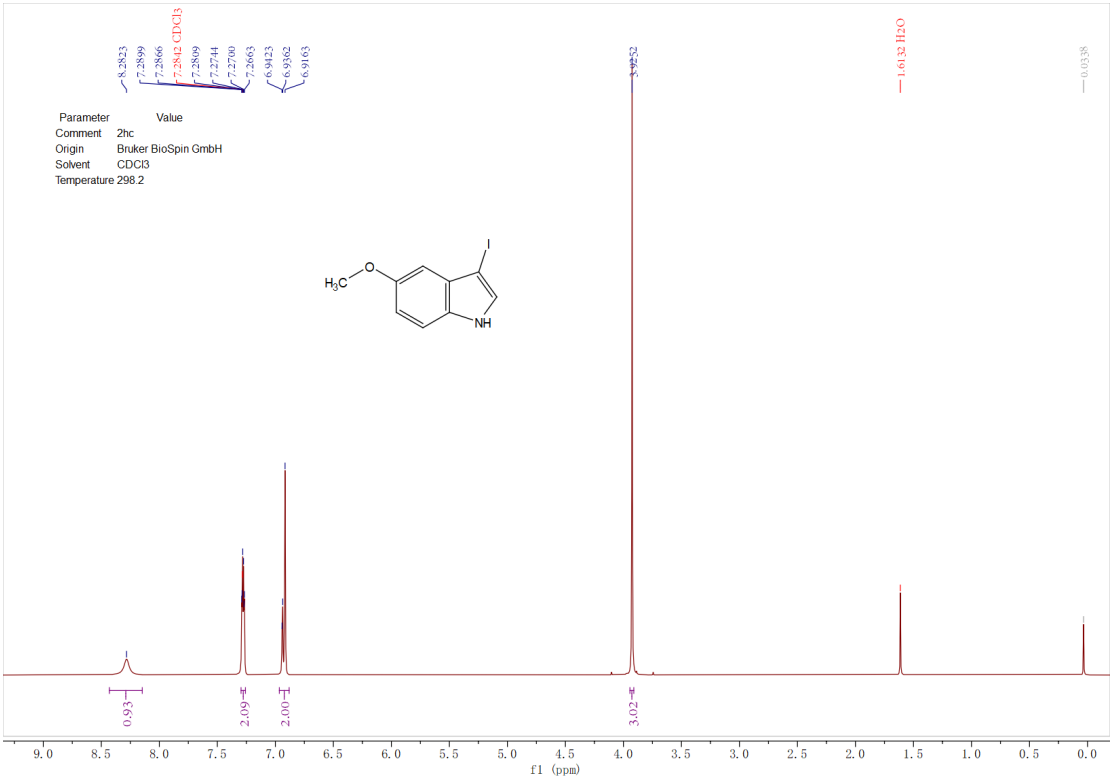

11.3196
7.4884
7.4817
7.3431
7.3413
7.3215
7.3197
6.8450
6.8391
6.8307
6.8245
6.8091
6.8029
3.5926
3.5375 H2O
2.5171 DMSO
2.5125 DMSO
2.5079 DMSO
2.5033 DMSO
2.4986 DMSO
0.0041
Parameter value
Comment 2hb 1H DMSO
Origin Bruker BioSpin GmbH
Solvent DMSO
Spectrometer Frequency 400.13
Br
H3C
O
NH
1.02
1.01
1.02
2.09
3.05
f1 (ppm)

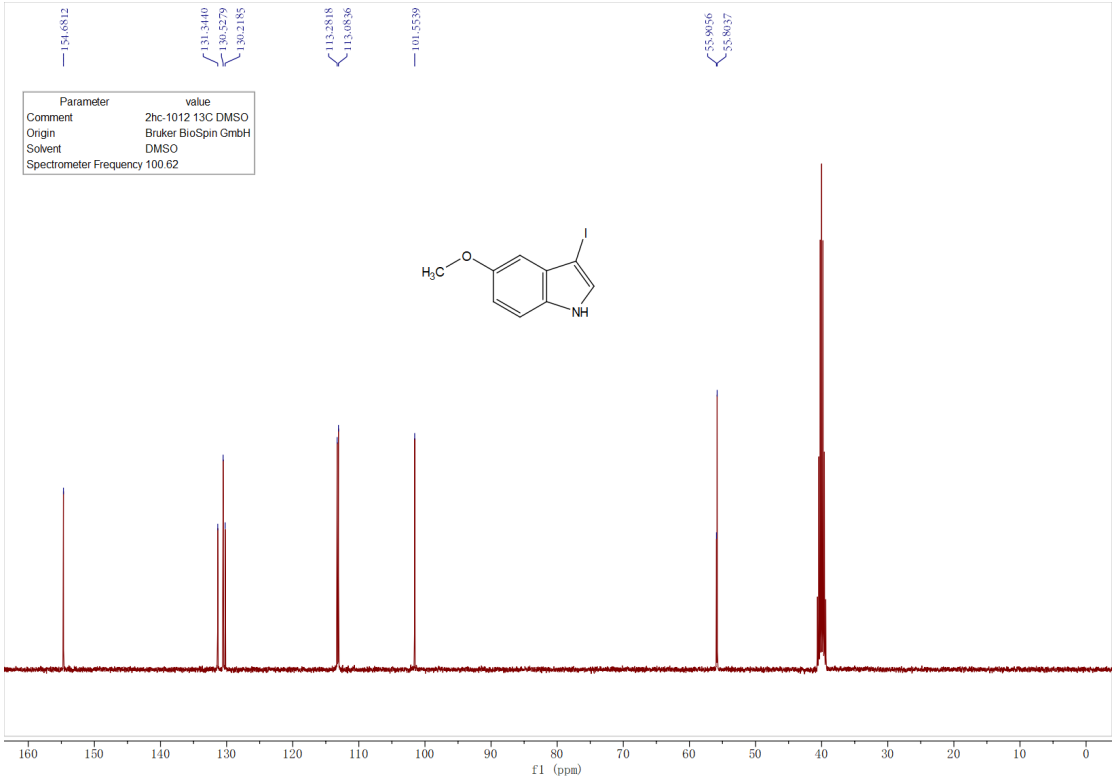

154.5661
130.8145
126.8873
125.6362
113.4969
113.2628
99.4852
88.7349
55.7796
Parameter value
Comment 2hb 13C DMSO
Origin Bruker BioSpin GmbH
Solvent DMSO
Spectrometer Frequency 100.62
Br
H3C
O
NH
f1 (ppm)

Sample Name	2ib	**Position**	Vial 1	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	2ib-.d
ACQ Method	ESI-.m	**Comment**		**Acquired Time**	07/05/2024 09:56:41 (UTC+08:00)

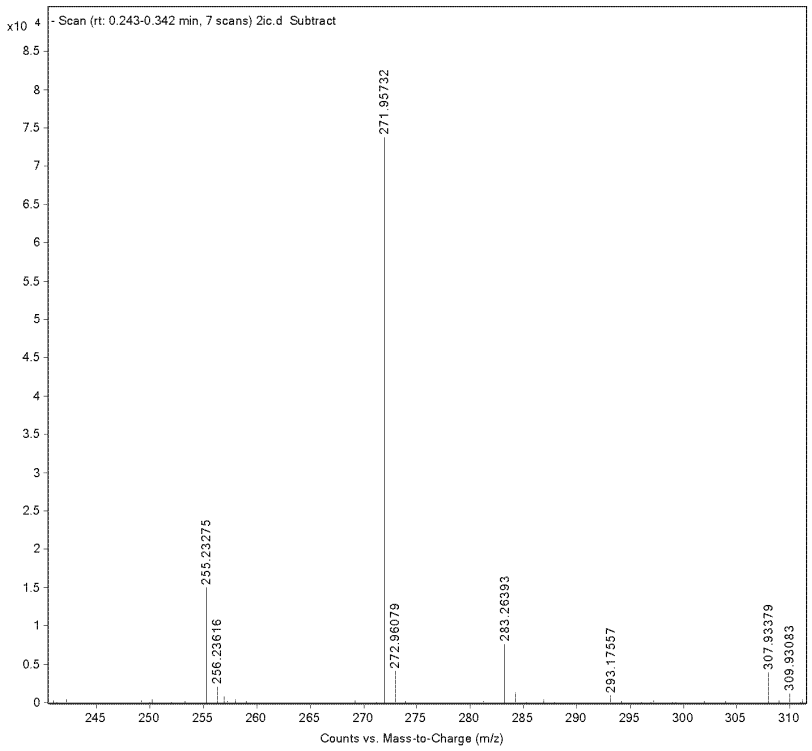


2"h

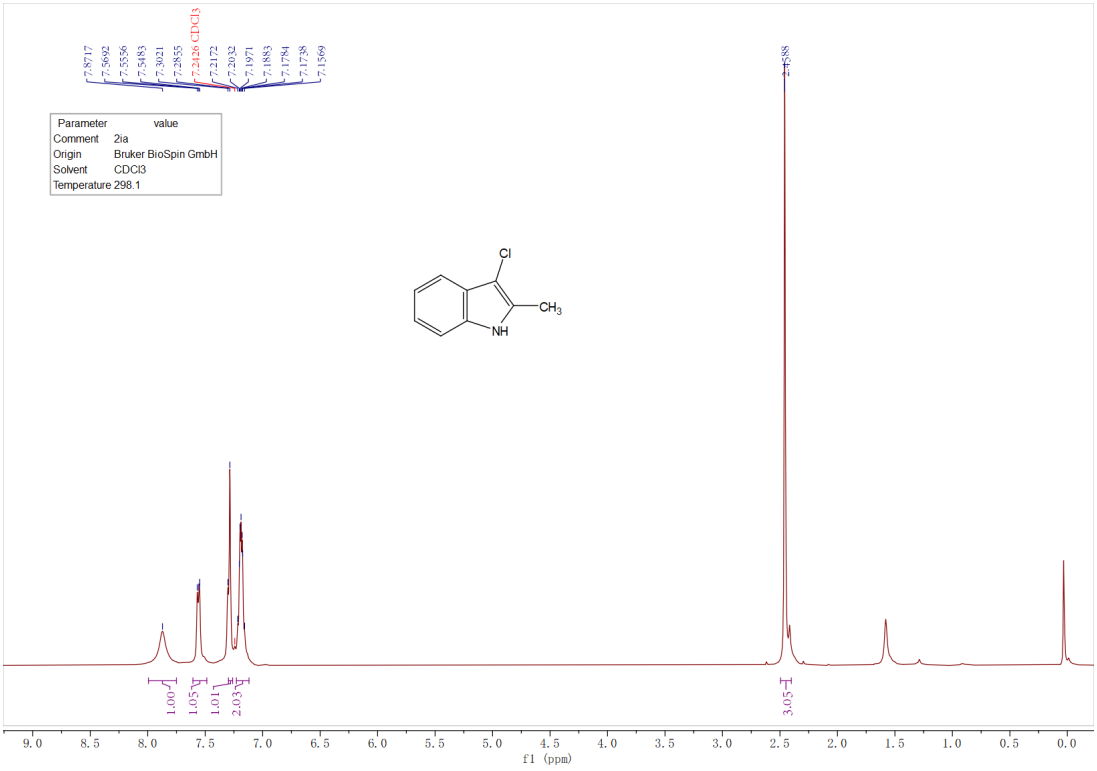

8.2823
7.2899
7.2866
7.2842 CDCl3
7.2809
7.2744
7.2700
7.2663
6.9423
6.9362
6.9163
3.9252
1.6132 H2O
0.0338
Parameter Value
Comment 2hc
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
H3C
O
I
NH
0.93
2.09
2.00
3.02
f1 (ppm)

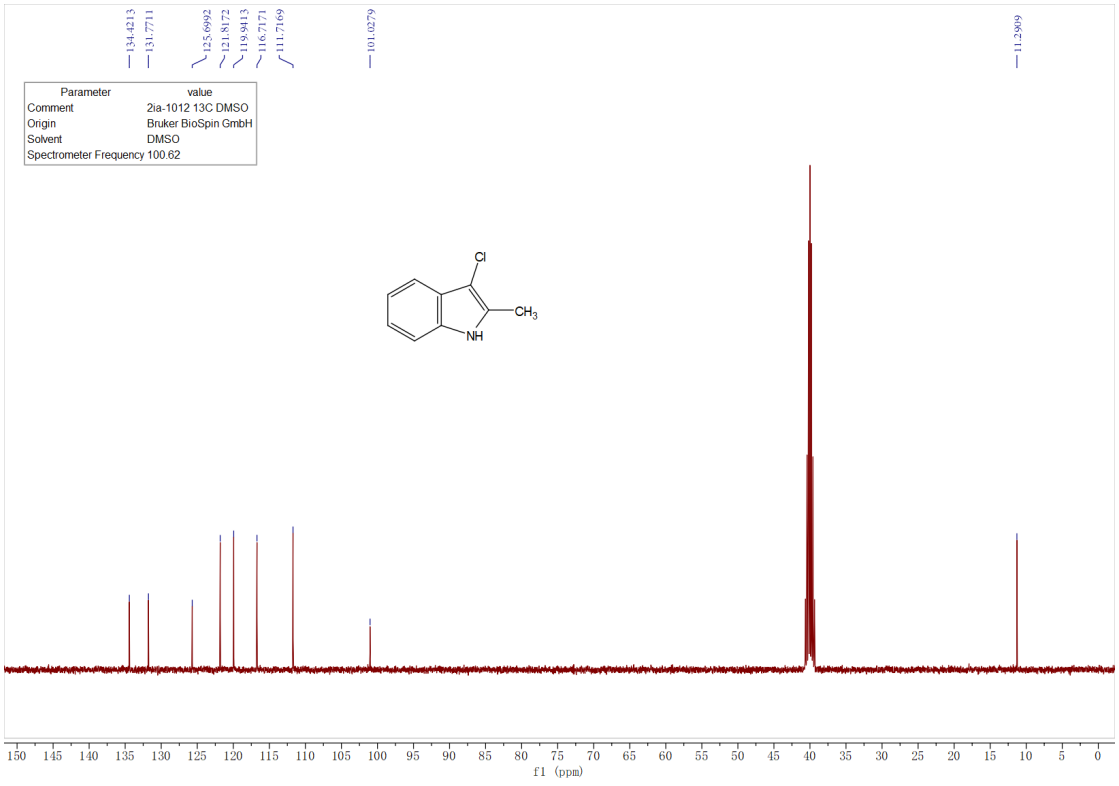

154.6812
131.3440
130.5279
130.2185
113.2818
113.0836
101.5539
55.9056
55.8637
Parameter value
Comment 2hc-1012 13C DMSO
Origin Bruker BioSpin GmbH
Solvent DMSO
Spectrometer Frequency 100.62
H3C
O
I
NH
f1 (ppm)

Sample Name	2ic	**Position**	Vial 24	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	2ic.d
ACQ Method	E-R.m	**Comment**		**Acquired Time**	29/04/2024 21:40:42 (UTC+08:00)

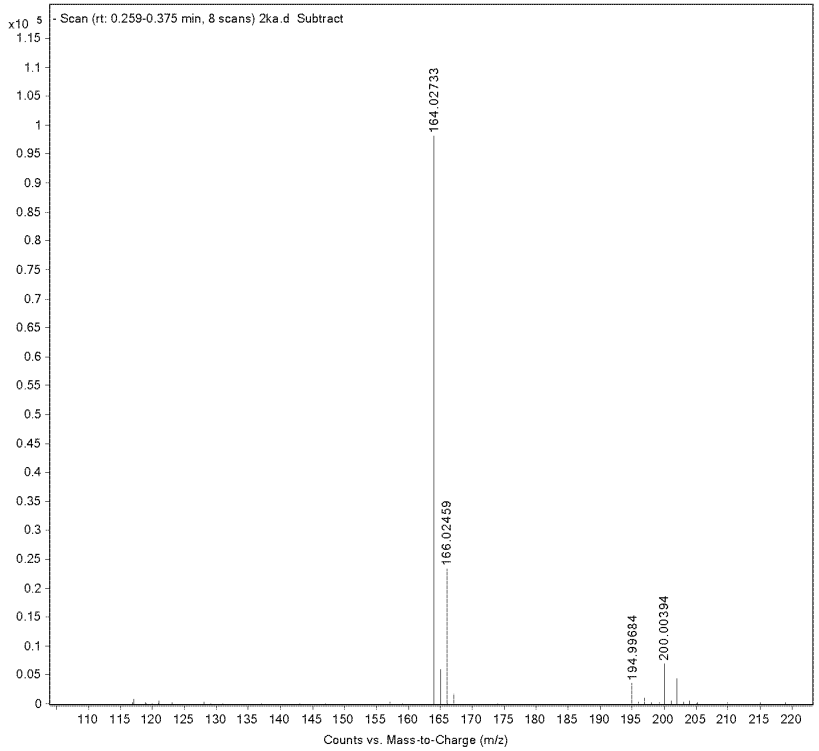


2i

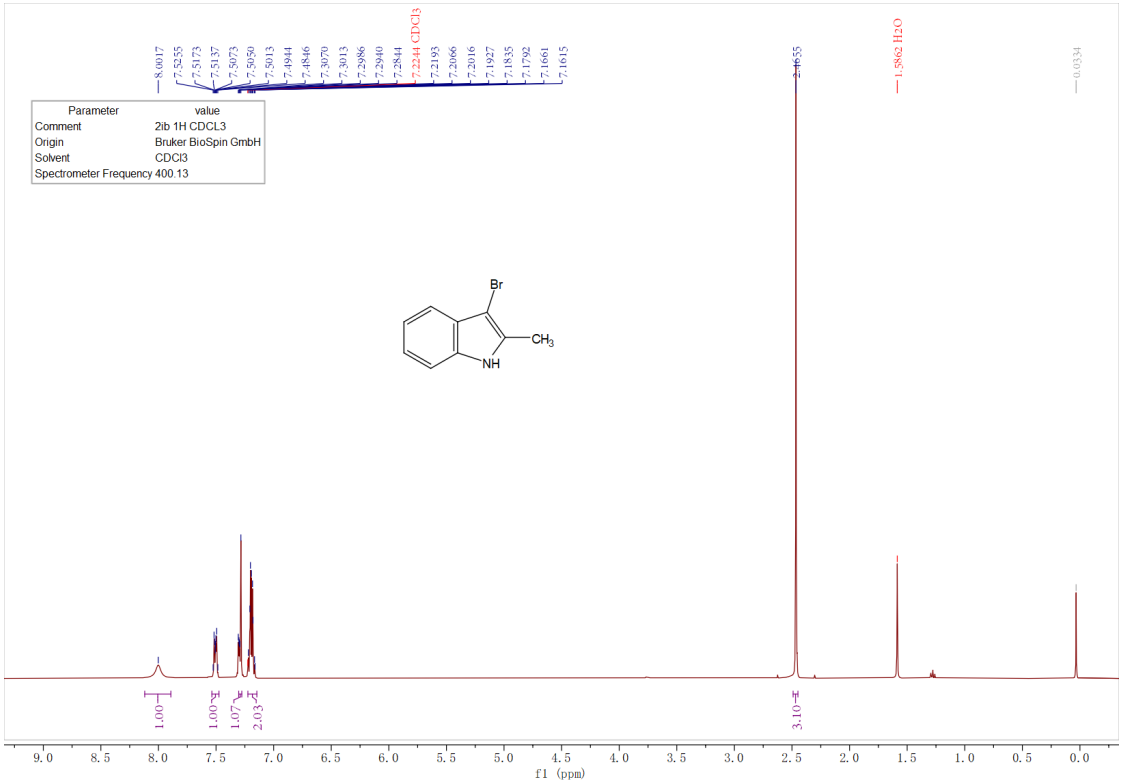

7.8717
7.5692
7.5536
7.5483
7.3021
7.2855
7.2126 CDCl3
7.2172
7.2032
7.1971
7.1885
7.1784
7.1738
7.1569
2.4888
Parameter value
Comment 2ia
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Cl
CH3
NH
1.00
1.05
1.01
2.03
3.05
f1 (ppm)

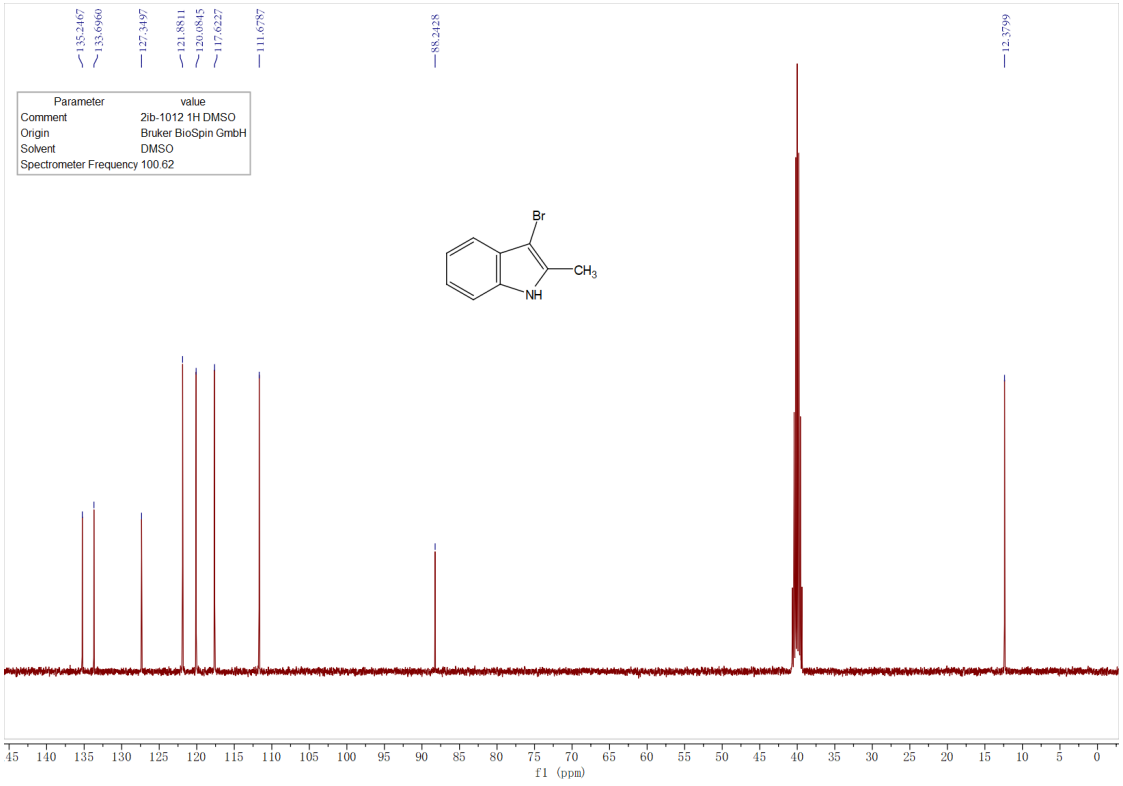

134.4213
131.7711
125.6992
121.8172
119.9413
116.7171
111.7169
101.0279
11.2989
Parameter value
Comment 2ia-1012 13C DMSO
Origin Bruker BioSpin GmbH
Solvent DMSO
Spectrometer Frequency 100.62
Cl
CH3
NH
f1 (ppm)

Sample Name	2ka	**Position**	Vial 25	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	2ka.d
ACQ Method	E-R.m	**Comment**		**Acquired Time**	29/04/2024 21:44:06 (UTC+08:00)

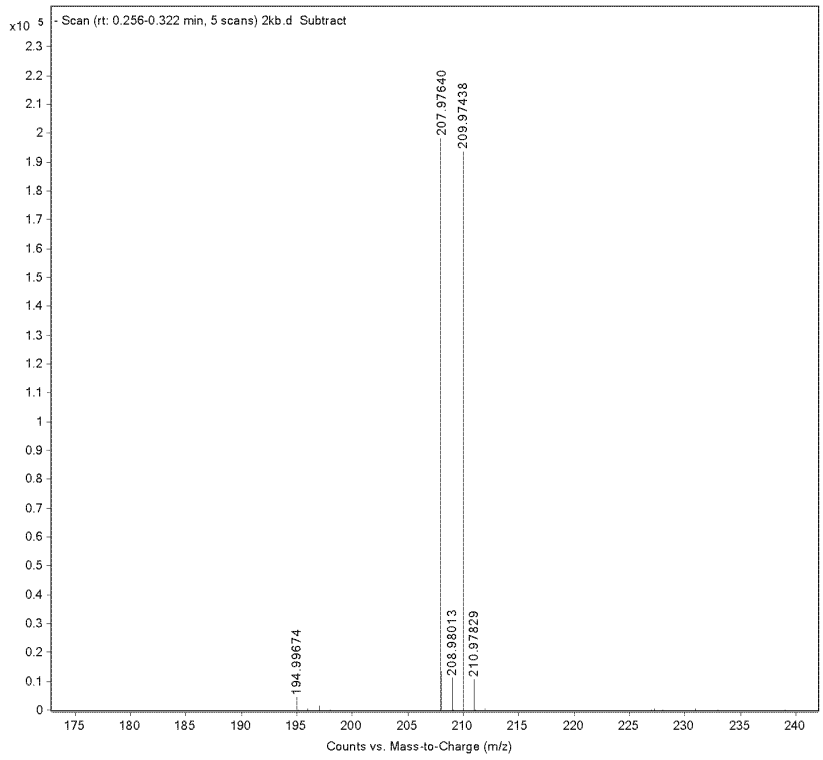


2'i

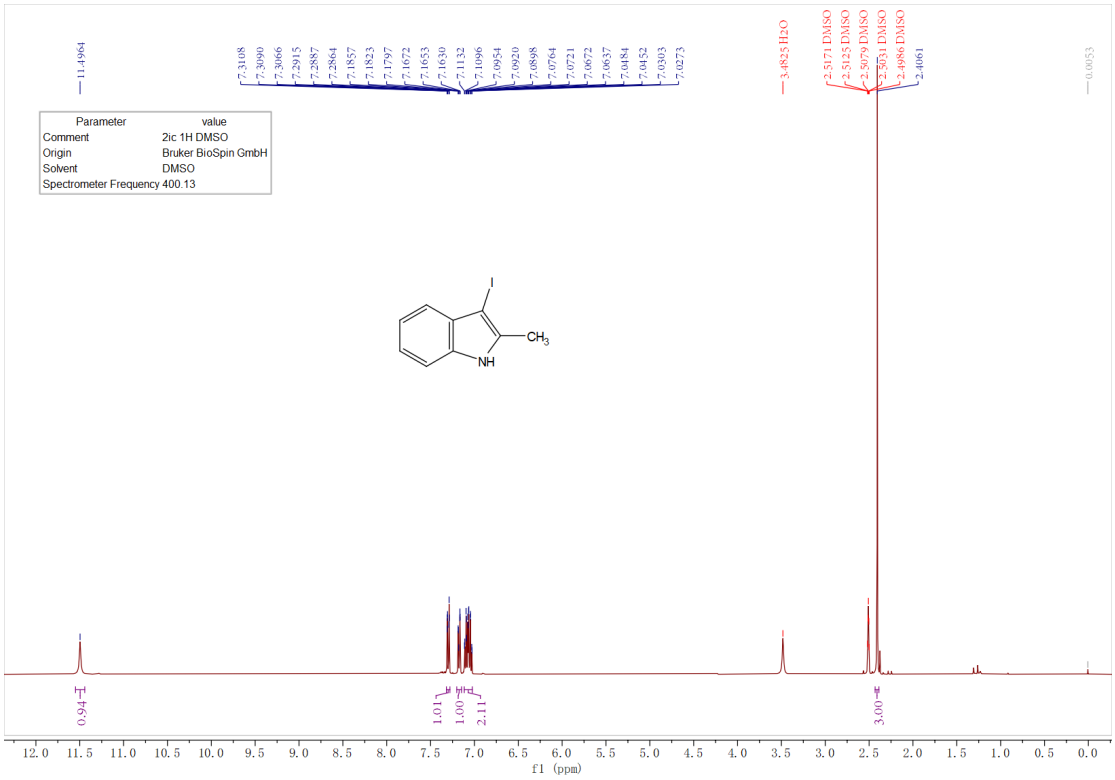

8.0017
7.5255
7.5173
7.5137
7.5073
7.5050
7.5013
7.4944
7.4846
7.3070
7.3013
7.2986
7.2940
7.2844
7.2244 CDCl3
7.2193
7.2066
7.2016
7.1927
7.1835
7.1792
7.1661
7.1615
2.4655
1.5862 H2O
0.0334
Parameter value
Comment 2ib 1H CDCL3
Origin Bruker BioSpin GmbH
Solvent CDCl3
Spectrometer Frequency 400.13
Br
CH3
NH
1.00
1.00
1.07
2.03
3.10
f1 (ppm)

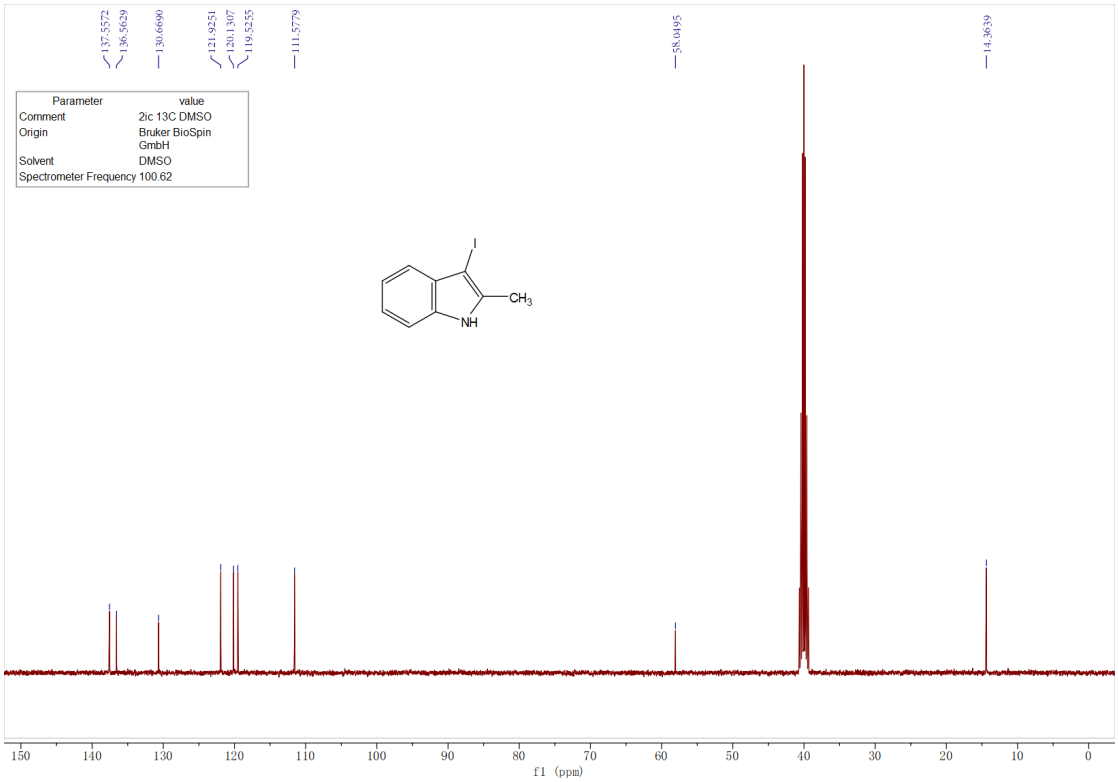

135.2467
133.6960
127.3497
121.8811
120.0845
117.6227
111.6787
68.2428
12.3799
Parameter value
Comment 2ib-1012 1H DMSO
Origin Bruker BioSpin GmbH
Solvent DMSO
Spectrometer Frequency 100.62
Br
CH3
NH
f1 (ppm)

Sample Name	2kb	**Position**	Vial 26	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	2kb.d
ACQ Method	E-R.m	**Comment**		**Acquired Time**	29/04/2024 21:47:34 (UTC+08:00)



2"i


11.4964
7.3108
7.3090
7.3066
7.2915
7.2887
7.2864
7.1857
7.1823
7.1797
7.1672
7.1653
7.1630
7.1132
7.1096
7.0954
7.0920
7.0898
7.0764
7.0721
7.0672
7.0637
7.0484
7.0452
7.0303
7.0273
3.4825 H2O
2.5171 DMSO
2.5125 DMSO
2.5079 DMSO
2.5031 DMSO
2.4986 DMSO
2.4061
0.0053
Parameter value
Comment 2ic 1H DMSO
Origin Bruker BioSpin GmbH
Solvent DMSO
Spectrometer Frequency 400.13
I
CH3
NH
0.94
1.01
1.00
2.11
3.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


137.5572
136.5629
130.6690
121.9251
120.1307
119.5255
111.5779
58.0495
14.3639
Parameter value
Comment 2ic 13C DMSO
Origin Bruker BioSpin GmbH
Solvent DMSO
Spectrometer Frequency 100.62
I
CH3
NH
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

Sample Name	2kc	**Position**	Vial 27	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	2kc.d
ACQ Method	E-R.m	**Comment**		**Acquired Time**	29/04/2024 21:51:01 (UTC+08:00)