Replacing halogenated solvent by a butyl acetate solution of bisphenol S in the transformations of indoles

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General information

All reagents were purchased from available commercial suppliers and used without purification unless other noted. ^{1}H and ^{13}C NMR spectra were recorded on Bruker AV-400. Chemical shifts are expressed in ppm relative to Me_4Si in $CDCl_3$ or DMSO-d6. High-resolution mass spectra (HRMS) were obtained on Bruker Compass Data Analysis 4.0. A UV−vis spectrophotometer (UV2600, Shimadzu) is employed to measure the maximum absorption wavelength (λ_{max}).

Experimental Section

Typical procedure for the synthesis of 3a and 4a in butyl acetate assisted by BPS

To a V-type flask containing solution of **1a** (0.3 mmol) and **2a** (0.32 mmol) in 1 mL butyl acetate was added Amberlyst 15 (12 mg) and bisphenol S (BPS, 0.4 mmol). The tube reactor equipped with triangular magnetic stirrer was then sealed and heated at 80 °C for 5 hours and the reaction was monitored by TLC. After the completion of the reaction, reaction mixtures were allowed to cool to room temperature, and then subjected to an isolation with preparative TLC (20 cm × 20 cm) by using eluting solution (PE: EA = 5:1 (v: v)). Final compound **3a** and **4a** were obtained in 47% and yield 48% respectively after removing eluent by reduced pressure distillation.

Typical procedure for the synthesis of azepino[4,5-*b*]indole 6a in butyl acetate assisted by BPS

To a V-type flask containing the starting material **5a** (0.2 mmol) solution in butyl acetate (1 mL) was added Amberlyst 15 (12 mg) and bisphenol S (BPS, 0.4 mmol). The tube reactor equipped with triangular magnetic stirrer was then sealed and heated at 80 °C for 5 hours and reaction monitored by TLC. After the completion of the reaction, reaction mixture was allowed to cool to room temperature, and then subjected to an isolation with preparative TLC (20 cm × 20 cm) by using eluting solution (PE/EA = 5/1(v/v)). Final compound **6a** was obtained in 93% yield after removing eluent by reduced pressure distillation.

Typical procedure for the synthesis of 9a in butyl acetate assisted by BPS

To a V-type flask containing solution of **7a** (0.3 mmol) and **8a** (0.33 mmol) in 1 mL butyl acetate was added Amberlyst 15 (8 mg) and bisphenol S (BPS, 0.4 mmol). The tube equipped with triangular magnetic stirrer was then sealed and heated at 80 °C for 2 hours and the reaction was monitored by TLC. After the completion of the reaction, reaction mixtures were allowed to cool to room temperature, and then subjected to an isolation with preparative TLC (20 cm × 20 cm) by using eluting solution (PE/EA = 5/1 (v/v)). Final compound **9a** was obtained in 91% after removing eluent by reduced pressure distillation.

Specific procedure for recycle experiment of BPS and Amberlyst 15

To a round flask containing solution of **1a** (10 mmol) and **2a** (11 mmol) in 40 mL butyl acetate was added Amberlyst 15 (400 mg) and bisphenol S (BPS, 15 mmol). The round flask equipped with magnetic stirrer was then sealed and heated at 80 °C and the reaction was monitored by TLC. After the completion of reaction (~ 5 h), magnetic stirrer was taken out and butyl acetate was removed via reduced pressure evaporation and collected for recycle (~ 36 mL, 95%). Then 20 ml *p*-xylene was added to dissolve the precipitated products and unreacted starting materials. Insoluble solid (Amberlyst 15 and BPS) was separated by suction filtration and washed with 30 ml *p*-xylene for recycle. *p*-Xylene was removed and collected via reduced pressure evaporation as well. Thus, the liquid components, butyl acetate and p-xylene, BPS and Amberlyst-15, can all be recovered with high efficiency. Finally, crude products were purified by flash column chromatograph using PE/EA (10/1) as eluting solution.

Example for the E-factor Calculation (for the synthesis of 3a and 4a in a 10 mmol scale)

E-factor = {[1.311g $_{[1a]}$ + 1.277g $_{[2a]}$ + 35.28g $_{[BuOAc]}$ + 3.75g $_{[BPS]}$ + 0.4g $_{[Amberlyst]}$ + 43.05g $_{[p\text{-xylene}]}$] – [31.75g $_{[90\%\ recovered\ BuOAc]}$ + 43.05g $_{[recovered\ p\text{-xylene}]}$ + 0.4g $_{[recovered\ Amberlyst]}$ + 3.75g $_{[recovered\ BPS]}$ + 4.35g $_{[products]}$} / 4.35g $_{[products]}$ = 0.40

Example for the PMI Calculation (for the synthesis of 3a and 4a in a 10 mmol scale)

PMI = (total input mass – mass recovered materials)/ product mass

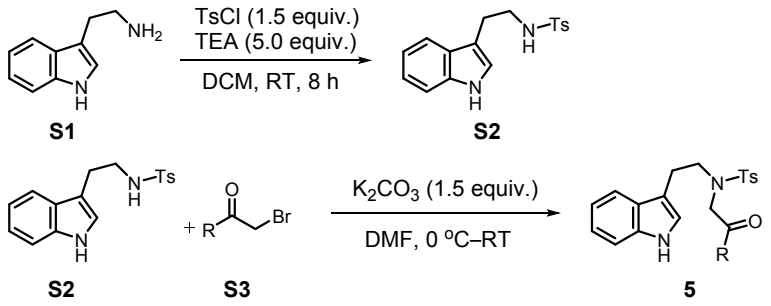
PMI = {[2.58g $_{[1a + 2a]}$ + 39.03g $_{[BuOAc + BPS]}$ + 0.4g $_{[Amberlyst]}$ + 43.05g $_{[p\text{-xylene}]}$] – 78.95g $_{[total\ mass\ of\ recovered\ materials]}$}/4.35g $_{[product]}$ = 1.40

***N*-substituted indoles (1b-1k) were prepared by following the reported procedure[1]**

To a solution of indole (10 mmol, 1 equiv.) in dry THF (15 mL) at 0 °C was added NaH (60% in mineraloil, 15 mmol, 1.5 equiv.) under N_2 atmosphere. After the mixture was stirred 30 min, alkylhalide (12 mmol, 1.2 equiv.) was added dropwise. The reaction mixture was warmed to room temperature and allowed to stir until the reaction was completed (monitored by TLC). Then 10 mL saturated NH_4Cl solution was added to quenched. The product was extracted with ethyl acetate (3 x 20 mL) and dried over anhydrous Na_2SO_4. The organic phase was concentrated in vacuum to obtain the crude mixture which was further purified by column chromatography (EA/PE) giving target products.

Typical procedure for synthesis of starting materials (5a-m)

Starting materials 1a -1n were synthesized strictly according to the reported methods.[2] Triethyl amine (5.0 equiv) was added into tryptamine (S1, 5 mmol) solution of DCM (50 mL) followed by tosyl chloride (1.5 equiv) at 0 ^oC. Then the reaction mixture was stirred at 25 ^oC for 8 h and reaction monitored by TLC. After reaction completed, reaction mass portioned between water and dichloromethane. The combined organic layer was washed with ammonium chloride solution and dried on sodium sulphate and evaporated under vacuum to obtain crude. The crude products were purified through flash column chromatography (100-200 silica gel; EA/Hexane). Then the obtained compound (S2; 2 mmol) in DMF (10 ml) was added to K_2CO_3 (1.5 equiv) at 0 ^oC and stirred at same temperature for half hour. Then the respective 2-bromoacetophenones (S3, 1.2 equiv) were added and slowly heated to RT and stirred till the completion of starting materials (0.5 to 2 h). After reaction completed (monitored by TLC), reaction mass quenched with ice-cold water and extracted into EA. The combined organic layer was washed with ice-cold water and sat. NH_4Cl. Then it was dried and evaporated to give crude residue. The obtained crude material passed through flash column chromatography to give pure starting products in high yields (**5a**-**5m**).



Scheme S1. Synthesis of starting materials **5a**-**m**.

Measurements of Kamlet-Taft solvatochromic parameters

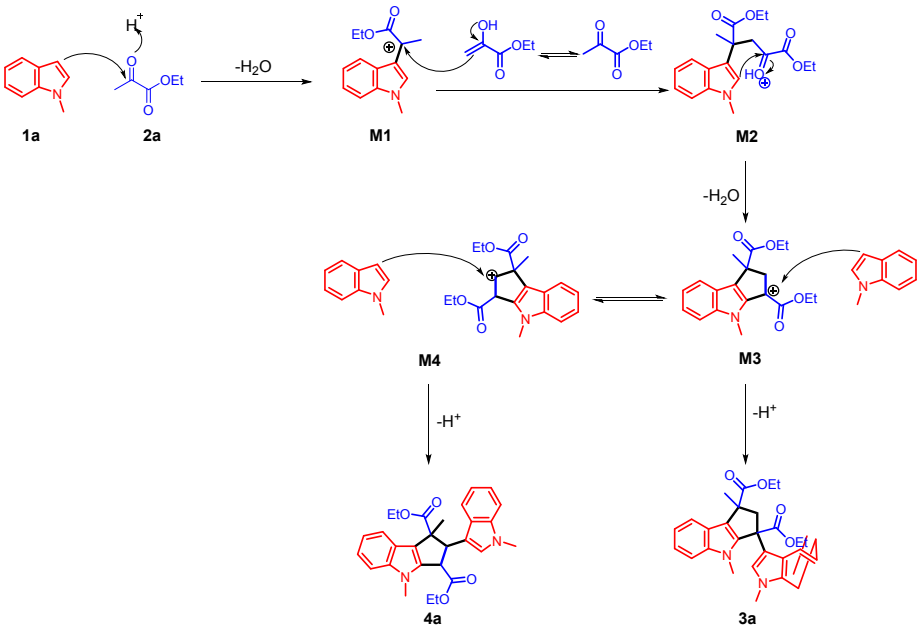
Solvent with different concentration of BPS in BuOAc were prepared firstly before measurement. Kamlet-Taft solvatochromic parameters of BPS solution were determined according to reported methods.[3] 4-Nitroanisole (4OMe), 4-nitroaniline (4NA), N,N-diethyl-4-nitroaniline (DMNA), N,N-diethyl-4-nitroaniline (DENA) and Rechardt's Dye and Rechardt's Dye were employed as indicators in this work. λ_{max} of BPS solvent in solvatochromic probes is measured at room temperature. Absorbance readings were collected by spectral scanning of BPS solvent in each indicator at 1 nm interval in triplicate. The concentration of each indicator in the mixed-solvent systems was was kept as low as 0.5×10^{-4} mol/L. K-T parameters of the solutions were calculated using equation bellow.[4-8]

$$\begin{aligned} &Indicator\,1:\ \pi^{*} = (28.10 - \nu_{\max 1})/3.51 \\ &Indicator\,2:\ \beta = 0.358\times(31.10 - \nu_{\max 2}) - 1.125\times\pi^{*} \\ &Indicator\,3:\ \alpha = (E_T(30) - 14.60\pi^{*} - 30.31)/16.50 \\ &E_T(30), kca\lg mol^{-1} = 28.591.5/\lambda_{\max 3} \\ &E_T^{N} = (E_T(30) - 30.7)/32.4 \end{aligned} \qquad \text{* MERGEFORMAT (1.1)}$$

The υ_{max} is the wavenumber in units of kiloKaiser (1kK=1000 cm^{-1}) obtained from the UV-Vis spectrophotometer.

To determine α, and E_T^N, the high-solubility coumarin 504 dye was used to replace Rechardt's Dye because it almost couldn't dissolve in BuOAc containing BPS. The correlation between the maximum wavelength in kK of Reichardt's dye and coumarin 504 was achieved by the following relationship:[9]

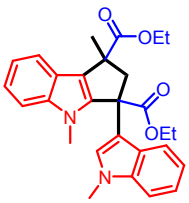
$$\nu_{\max 3} = -7.48\nu_{504} + 188.78,\ R^2 = 0.91 \qquad \text{* MERGEFORMAT (1.2)}$$



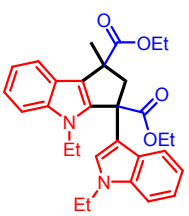
Scheme S2 Plausible mechanism of **3a** and **4a**. Based on the experiment results and corresponding reference, the plausible mechanism of **3a** and **4a** was proposed. The initial event should be the activation of the ketone carbonyl group of ethyl pyruvate **2a** with the acid catalyst, then *N*-methyl indole as nucleophile attacked the activated carbonyl group, followed by dehydration to form a carbocation intermediate **M1**. A nucleophilic attack of **2a** was then occurred, and **M1** was converted to a carbocation **M2**. Afterward, an intramolecular nucleophilic attack happened and a five-membered ring cationic intermediate **M3** was generated. Target product **3a** was formed finally after attacking of **1a** to **M3** and deprotonation. However, at the same time, **M4** might also be generated via a rearrangement of **M3**. It allowed concomitant formation of the target product **4a**.

Characterization data of the obtained compounds

Spectral Characterization Data for 3a–3m



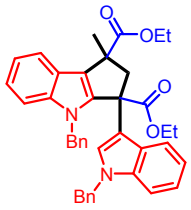
Diethyl 1,4-dimethyl-3-(1-methyl-1H-indol-3-yl)-1,2,3,4-tetrahydrocyclopenta[b]indole-1,3-dicarboxylate (**3a**): yield = 47%, yellow solid, mp: 130–132 °C, ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 7.72 (d, J = 7.8 Hz, 1H), 7.29 – 7.14 (m, 5H), 7.05 (d, J = 8.0 Hz, 1H), 6.93 – 6.82 (m, 2H), 4.32 (dq, J = 10.9, 7.1 Hz, 1H), 4.25 – 4.10 (m, 3H), 3.75 (s, 3H), 3.54 (d, J = 13.6 Hz, 1H), 3.43 (s, 3H), 3.38 (d, J = 14.8 Hz, 1H), 1.67 (s, 3H), 1.27 (t, J = 7.1 Hz, 3H), 1.19 (t, J = 7.1 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 176.4, 173.5, 142.4, 142.1, 137.7, 126.4, 125.9, 122.7, 122.4, 122.0, 121.3, 120.2, 119.8, 119.6, 119.6, 115.2, 110.0, 109.3, 61.9, 61.0, 55.4, 53.6, 48.5, 32.9, 30.8, 25.5, 14.4, 14.3 ppm. HRMS (TOF, ESI): m/z calcd for $C_{28}H_{30}N_2O_4Na$, $[M+Na]^+$= 481.2100, found 481.2103.



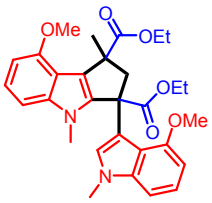
Diethyl 4-ethyl-3-(1-ethyl-1H-indol-3-yl)-1-methyl-1,2,3,4-tetrahydrocyclopenta[b]-indole-1,3-dicarboxylate (**3b**): yield = 46%, brown gum-like,^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 7.72 (d, J = 7.8 Hz, 1H), 7.31 (d, J = 8.2 Hz, 2H), 7.23 – 7.10 (m, 4H), 6.89 (dd, J = 13.7, 6.0 Hz, 2H), 4.36 (dq, J = 11.0, 7.1 Hz, 1H), 4.30 – 4.21 (m, 1H), 4.20 – 4.08 (m, 4H), 4.02 – 3.88 (m, 2H), 3.66 (d, J = 13.6 Hz, 1H), 3.39 (d, J = 13.6 Hz, 1H), 1.69 (s, 3H), 1.44 (t, J = 7.2 Hz, 3H), 1.30 (t, J = 7.1 Hz, 3H), 1.21 (t, J = 7.1 Hz, 3H), 0.92 (t, J = 7.1 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 176.5, 173.6, 142.3, 140.9, 136.7, 126.2, 124.7, 123.0, 122.1, 121.8, 121.1, 120.6, 119.8, 119.4, 119.4, 115.2, 110.7, 109.4, 61.8,

61.0, 55.4, 53.8, 48.5, 41.1, 39.3, 25.4, 15.6, 14.4 ppm. HRMS (TOF, ESI): m/z calcd for $C_{30}H_{34}N_2O_4Na$, $[M+Na]^+$= 509.2412, found 509.2416.

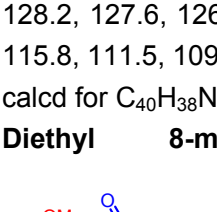
Diethyl 4-benzyl-3-(1-benzyl-1H-indol-3-yl)-1-methyl-1,2,3,4-tetrahydrocyclopenta-[b]indole-1,3-dicarboxylate (**3c**): yield = 78%, purple solid, mp: 63–65 °C,^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 7.75 (d, J = 7.8 Hz, 1H), 7.28 – 7.08 (m, 7H), 7.05 (t, J = 5.9 Hz, 4H), 6.99 – 6.85 (m, 5H), 6.73 (d, J = 5.9 Hz, 2H), 5.26 – 5.02 (m, 4H), 4.25 – 4.09 (m, 2H), 4.03 (dq, J = 14.1, 7.1 Hz, 1H), 3.89 – 3.78 (m, 1H), 3.74 (d, J = 13.7 Hz, 1H), 3.49 (d, J = 13.7 Hz, 1H), 1.76 (s, 3H), 1.22 (t, J = 7.1 Hz, 3H), 0.99 (t, J = 7.1 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 176.3, 173.3, 142.6, 141.9, 137.6, 137.4, 137.3, 128.8, 128.2, 127.6, 126.8, 126.6, 126.2, 126.1, 125.9, 123.1, 122.9, 122.2, 121.5, 120.5, 119.8, 119.8, 119.7, 115.8, 111.5, 109.9, 61.7, 61.0, 55.1, 53.8, 50.0, 48.6, 48.2, 25.7, 14.4, 14.0 ppm. HRMS (TOF, ESI): m/z calcd for $C_{40}H_{38}N_2O_4Na$, $[M+Na]^+$= 633.2733, found 633.2729.



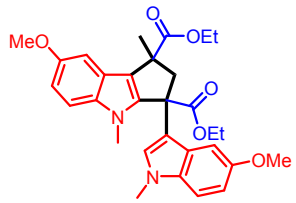
Diethyl 8-methoxy-3-(4-methoxy-1-methyl-1H-indol-3-yl)-1,4-dimethyl-1,2,3,4-tetrahydrocyclo-penta[b]indole-1,3-dicarboxylate (**3e**): yield = 45%, yellow solid, mp: 111–113 °C,^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 7.15 (q, J = 8.3 Hz, 2H), 6.95 (d, J = 8.2 Hz, 1H), 6.89 (d, J = 8.2 Hz, 1H), 6.55 (d, J = 7.8 Hz, 1H), 6.49 (d, J = 7.8 Hz, 1H), 6.45 (s, 1H), 4.25 – 4.09 (m, 2H), 3.93 (d, J = 7.1 Hz, 2H), 3.88 (s, 3H), 3.85 (s, 3H), 3.74 (s, 3H), 3.70 (s, 1H), 3.63 (s, 3H), 2.99 (d, J = 13.7 Hz, 1H), 1.83 (s, 3H), 1.19 (t, J = 7.1 Hz, 3H), 0.93 (t, J = 7.0 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 177.7, 173.9, 153.9, 153.7, 143.7, 141.5, 139.2, 125.5, 123.8, 122.8, 122.5, 118.3, 116.3, 114.0, 103.1, 102.8, 100.0, 99.2, 61.4, 60.3, 58.7, 55.2, 54.7, 54.5, 48.4, 33.0, 31.5, 26.1, 14.3, 14.0 ppm. HRMS (TOF, ESI): m/z calcd for $C_{30}H_{34}N_2O_6Na$, $[M+Na]^+$= 541.2310, found 541.2315.



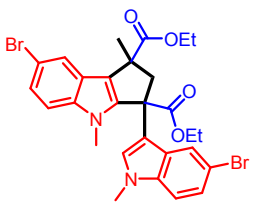
Diethyl 8-chloro-3-(4-chloro-1-methyl-1H-indol-3-yl)-1,4-dimethyl-1,2,3,4-tetrahydro-cyclopenta[b]-indole-1,3-dicarboxylate (**3f**): yield = 39%, yellow solid, mp: 181–183 °C,^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 7.20 – 7.10 (m, 3H), 7.06 (d, J = 8.2 Hz, 1H), 6.81 (ddd, J = 18.8, 10.5, 7.8 Hz, 2H), 6.41 (s, 1H), 4.25 (qd, J = 7.1, 3.0 Hz, 2H), 3.96 – 3.82 (m, 2H), 3.71 (s, 3H), 3.67 (d, J = 13.6 Hz, 1H), 3.64 (s, 3H), 3.26 (dd, J = 13.5, 1.4 Hz, 1H), 1.82 (s, 3H), 1.24 (t, J = 7.1 Hz, 3H), 0.91 (t, J = 7.1 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 176.7, 173.4, 157.9, 157.5, 155.4, 155.0, 144.9, 144.8, 142.9, 140.6, 140.4, 126.8, 122.8, 122.7, 122.3, 122.2, 121.5, 115.9, 115.0, 114.7, 112.6, 112.4, 106.0, 106.0, 105.8, 105.7, 105.4, 105.2, 104.9, 104.7, 62.0, 60.6, 57.3, 53.9, 48.7, 33.1, 31.4, 25.9, 14.2, 13.8 ppm. HRMS (TOF, ESI): m/z calcd for $C_{28}H_{28}Cl_2N_2O_4Na$, $[M+Na]^+$= 549.1319, found 549.1324.



Diethyl 7-methoxy-3-(5-methoxy-1-methyl-1H-indol-3-yl)-1,4-dimethyl-1,2,3,4-tetrahydrocyclo-penta[b]indole-1,3-dicarboxylate (**3g**): yield = 47%, brown solid, mp: 109–111 °C,^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ=7.23 – 7.09 (m, 3H), 6.92 – 6.75 (m, 3H), 6.33 (s, 1H), 4.32 (dt, J = 14.2, 7.2 Hz, 1H), 4.27 – 4.20 (m, 1H), 4.18 – 4.06 (m, 2H), 3.88 (s, 3H), 3.72 (s, 3H), 3.52 (d, J = 13.6 Hz, 1H), 3.42 (d, J = 4.8 Hz, 7H), 1.69 (s, 3H), 1.28 (t, J = 7.1 Hz, 3H), 1.20 (t, J = 7.1 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 176.4, 173.5, 154.1, 153.9, 143.0, 137.4, 132.9, 126.7, 126.2, 122.8, 121.9, 114.7, 112.4, 111.3, 110.5, 110.1, 101.9, 101.6, 61.8, 60.9, 56.1, 55.5, 53.4, 48.5, 33.1, 30.9, 25.7, 14.4, 14.3 ppm. HRMS (TOF, ESI): m/z calcd for $C_{30}H_{34}N_2O_6Na$, $[M+Na]^+$= 541.2312, found 541.2315.

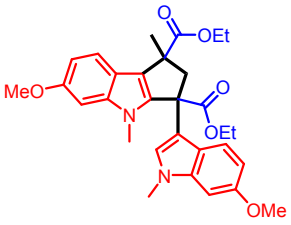


Diethyl 7-bromo-3-(5-bromo-1-methyl-1H-indol-3-yl)-1,4-dimethyl-1,2,3,4-tetrahydrocyclopenta[b]-indole-1,3-dicarboxylate (**3h**): yield = 76%, pale yellow solid, mp: 154–156 °C,^{1}H

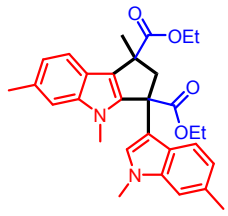


NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 7.84 (s, 1H), 7.32 – 7.27 (m, 1H), 7.25 (s, 1H), 7.22 (s, 1H), 7.15 (dd, J = 8.7, 3.2 Hz, 2H), 6.81 (s, 1H), 4.37 – 4.28 (m, 1H), 4.27 – 4.20 (m, 1H), 4.15 (dtd, J = 14.7, 7.1, 3.7 Hz, 2H), 3.71 (s, 3H), 3.50 (d, J = 13.7 Hz, 1H), 3.46 (s, 3H), 3.39 (d, J = 13.7 Hz, 1H), 1.66 (s, 3H), 1.27 (t, J = 7.1 Hz, 3H), 1.20 (t, J = 7.1 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 175.9, 173.0, 143.2, 140.9, 136.3, 127.6, 127.3, 125.1, 124.3, 124.1, 122.5, 122.4, 122.0, 114.7, 113.1, 111.5, 111.1, 62.1, 61.2, 55.2, 53.4, 48.5, 33.1, 31.1, 25.5, 14.3, 14.3 ppm. HRMS (TOF, ESI): m/z calcd for $C_{28}H_{28}Br_2N_2O_4Na$, $[M+Na]^+$= 637.0310, found 637.0314.

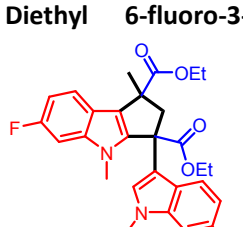
Diethyl 6-methoxy-3-(6-methoxy-1-methyl-1H-indol-3-yl)-1,4-dimethyl-1,2,3,4-tetrahydrocyclopenta[b]-indole-1,3-dicarboxylate (**3i**): yield = 48%, brown solid, mp: 75–77 °C, ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ=7.59 (d, J = 8.6 Hz, 1H), 6.91 (d, J = 8.8 Hz, 1H), 6.85 – 6.81 (m, 1H), 6.78 – 6.70 (m, 3H), 6.57 (dd, J = 8.6, 1.8 Hz, 1H), 4.32 (dd, J = 10.7, 7.1 Hz, 1H), 4.23 – 4.08 (m, 3H), 3.88 (s, 3H), 3.84 (s, 3H), 3.70 (s, 3H), 3.49 (d, J = 13.6 Hz, 1H), 3.39 (s, 3H), 3.35 (d, J = 11.1 Hz, 1H), 1.65 (s, 3H), 1.28 (t, J = 7.0 Hz, 3H), 1.21 (t, J = 7.0 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 176.4, 173.6, 156.5, 156.1, 142.8, 141.1, 138.4, 125.2, 122.3, 120.9, 120.3, 120.0, 117.1, 115.4, 109.4, 109.1, 94.1, 92.8, 61.8, 60.9, 55.9, 55.7, 55.4, 53.5, 48.5, 32.9, 30.8, 25.5, 14.4, 14.3 ppm. HRMS (TOF, ESI): m/z calcd for $C_{30}H_{34}N_2O_6Na$, $[M+Na]^+$= 541.2305, found 541.2315.



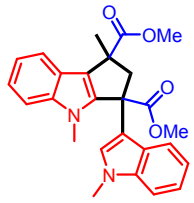
Diethyl 3-(1,6-dimethyl-1H-indol-3-yl)-1,4,6-trimethyl-1,2,3,4-tetrahydrocyclopenta[b]indole-1,3-dicarboxylate (**3j**): yield = 46%, brown gum-like,^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 7.60 (d, J = 8.0 Hz, 1H), 7.08 (d, J = 4.0 Hz, 2H), 7.00 (d, J = 8.0 Hz, 1H), 6.94 (d, J = 8.2 Hz, 1H), 6.79 (s, 1H), 6.73 (d, J = 8.2 Hz, 1H), 4.31 (dq, J = 10.9, 7.1 Hz, 1H), 4.25 – 4.09 (m, 3H), 3.72 (s, 3H), 3.45 (q, J = 21.8 Hz, 2H), 3.41 (s, 3H), 3.38 (s, 1H), 2.51 (s, 3H), 2.44 (s, 3H), 1.65 (s, 3H), 1.27 (t, J = 7.1 Hz, 3H), 1.22 (t, J = 7.1 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 176.5, 173.6, 142.5, 141.8, 138.1, 131.8, 131.1, 125.7, 123.8, 122.2, 121.3, 121.2, 120.4, 119.9, 119.3, 115.1, 110.1, 109.3, 61.8, 60.9, 55.3, 53.6, 48.5, 32.8, 30.7, 25.4, 22.1, 21.9, 14.4, 14.3 ppm. HRMS (TOF, ESI): m/z calcd for $C_{30}H_{34}N_2O_4Na$, $[M+Na]^+$= 509.2412, found 509.2416.



Diethyl 6-fluoro-3-(6-fluoro-1-methyl-1H-indol-3-yl)-1,4-dimethyl-1,2,3,4-tetrahydrocyclopenta-[b]indole-1,3-dicarboxylate (**3k**): yield = 47%, brown solid, mp: 150–152 °C, ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 7.62 (dd, J = 8.5, 5.5 Hz, 1H), 6.99 – 6.87 (m, 4H), 6.85 (s, 1H), 6.66 (td, J = 9.3, 2.0 Hz, 1H), 4.34 (dq, J = 10.8, 7.1 Hz, 1H), 4.28 – 4.20 (m, 1H), 4.19 – 4.11 (m, 2H), 3.71 (s, 3H), 3.44 (q, J = 16 Hz, 2H), 3.37 (s, 3H), 1.66 (s, 3H), 1.28 (t, J = 7.2 Hz, 3H), 1.20 (t, J = 7.1 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 176.2, 173.3, 161.1 (d, J = 29.3 Hz), 158.7 (d, J = 28.3 Hz), 142.4 (d, J = 3.4 Hz), 142.2 (d, J = 11.6 Hz), 137.8 (d, J = 11.8 Hz), 126.7 (d, J = 3.5 Hz), 122.5, 122.3, 121.0 (d, J = 10.0 Hz), 120.4 (d, J = 10.0 Hz), 119.1, 115.3, 108.4 (d, J = 19.1 Hz), 108.2 (d, J = 19.0 Hz), 96.6 (d, J = 26.1 Hz), 95.8 (d, J = 26.1 Hz), 62.0, 61.1, 55.3, 53.5, 48.5, 33.0, 30.9, 25.5, 14.3, 14.3 ppm. ^{19}F NMR (377 MHz, $CDCl_3$) δ = -120.30 (td, J = 9.6, 5.4 Hz), -120.79 (td, J = 9.7, 5.6 Hz) ppm. HRMS (TOF, ESI): m/z calcd for $C_{28}H_{28}F_2N_2O_4Na$, $[M+Na]^+$= 517.1904, found 517.1915.



Dimethyl 1,4-dimethyl-3-(1-methyl-1H-indol-3-yl)-1,2,3,4-tetra-hydrocyclopenta[b]indole-1,3-dicarboxylate (**3l**): yield = 43%, yellow solid, mp: 110–112 °C, ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 7.70 (d, J = 7.8 Hz, 1H), 7.32 – 7.26 (m, 2H), 7.25 – 7.21 (m, 1H), 7.17 (q, J = 7.4 Hz, 2H), 7.04 (d, J = 8.0 Hz, 1H), 6.92 (t, J = 7.5 Hz, 1H), 6.86 (s, 1H), 3.78 (s, 3H), 3.75 (s, 3H), 3.68 (s, 3H), 3.48 (q, J = 16 Hz, 2H), 3.44 (s, 3H), 1.67 (s, 3H)



ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 176.9, 174.1, 142.2, 142.1, 137.7, 126.4, 125.8, 122.6, 122.3, 122.1, 121.5, 120.0, 119.7, 119.7, 115.0, 110.0, 109.4, 55.5, 53.4, 52.9, 52.1, 48.5, 32.9, 30.7, 25.5 ppm. HRMS (TOF, ESI): m/z calcd for $C_{26}H_{26}N_2O_4Na$, $[M+Na]^+$= 453.1785, found 453.1790.

1,1'-(1,4-dimethyl-3-(1-methyl-1H-indol-3-yl)-1,2,3,4-tetrahydrocyclopenta[b]indole-1,3-diyl)bis-(ethan-1-one) (**3m**): yield = 28%, yellow solid, mp: 191–193 °C,^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 7.38 – 7.28 (m, 3H), 7.22 (dt, J = 15.0, 4.2 Hz, 2H), 6.99 (dt, J = 14.6, 7.4 Hz, 2H), 6.76 (s, 1H), 3.75 (s, 3H), 3.51 (s, 3H), 3.23 (q, J = 13.5 Hz, 2H), 2.33 (s, 3H), 2.10 (s, 3H), 1.54 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 211.9, 207.1, 144.1, 142.4, 137.9, 127.0, 126.0, 123.9, 122.9, 122.3, 121.9, 120.4, 119.9, 119.9, 119.1, 114.0, 110.4, 109.9, 60.6, 54.9, 54.6, 33.0, 31.3, 27.9, 26.3, 23.3 ppm. HRMS (TOF, ESI): m/z calcd for $C_{26}H_{26}N_2O_2Na$, $[M+Na]^+$= 421.1890, found 421.1892.

Spectral Characterization Data for 4a–4m

Diethyl 1,4-dimethyl-2-(1-methyl-1H-indol-3-yl)-1,2,3,4-tetrahydrocyclopenta[b]indole-1,3-dicarboxylate (**4a**): yield = 48%, brown solid, mp: 49–51 °C, ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 7.73 (d, J = 7.7 Hz, 1H), 7.27 (t, J = 9.2 Hz, 2H), 7.22 (t, J = 7.6 Hz, 1H), 7.17 (t, J = 7.3 Hz, 2H), 6.96 (s, 1H), 6.86 (t, J = 7.5 Hz, 1H), 6.76 (d, J = 8.0 Hz, 1H), 4.35 (dd, J = 10.8, 7.1 Hz, 1H), 4.19 (dd, J = 10.8, 7.1 Hz, 1H), 4.09 (td, J = 10.1, 4.8 Hz, 3H), 3.76 (s, 3H), 3.37 (s, 3H), 2.77 (d, J = 13.7 Hz, 1H), 1.74 (s, 3H), 1.59 (s, 1H), 1.28 (t, J = 7.1 Hz, 3H), 1.22 (t, J = 7.1 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 176.1, 173.0, 143.4, 142.0, 137.8, 126.6, 125.7, 122.9, 122.0, 121.6, 121.2, 119.7, 119.5, 119.4, 115.2, 110.1, 109.5, 61.6, 60.9, 56.9, 54.0, 48.5, 33.0, 30.6, 25.2, 14.3 ppm. HRMS (TOF, ESI): m/z calcd for $C_{28}H_{30}N_2O_4Na$, $[M+Na]^+$= 481.2100, found 481.2103.

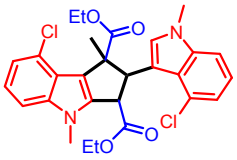
Diethyl 4-ethyl-2-(1-ethyl-1H-indol-3-yl)-1-methyl-1,2,3,4-tetrahydrocyclopenta[b]indole-1,3-dicarboxylate (**4b**): yield = 46%, brown solid, mp: 99–101 °C,^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 7.76 (d, J = 7.4 Hz, 1H), 7.31 (d, J = 8.2 Hz, 2H), 7.23 – 7.12 (m, 3H), 7.01 (s, 1H), 6.87 (d, J = 3.3 Hz, 2H), 4.36 (dd, J = 10.8, 7.1 Hz, 1H), 4.24 (dd, J = 10.8, 7.1 Hz, 1H), 4.19 – 4.06 (m, 5H), 3.86 (dt, J = 11.6, 7.2 Hz, 2H), 2.88 (d, J = 13.7 Hz, 1H), 1.76 (s, 3H), 1.45 (t, J = 7.3 Hz, 3H), 1.30 (t, J = 7.1 Hz, 3H), 1.24 (t, J = 7.1 Hz, 3H), 0.91 (t, J = 7.2 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 176.1, 173.1, 143.2, 140.9, 136.7, 126.1, 124.9, 123.3, 121.8, 121.2, 121.0, 120.1, 119.6, 119.5, 119.4, 115.2, 110.8, 109.6, 61.6, 60.9, 56.7, 54.1, 48.5, 41.1, 39.3, 25.2, 15.6, 14.4, 14.4, 14.2 ppm. HRMS (TOF, ESI): m/z calcd for $C_{30}H_{34}N_2O_4Na$, $[M+Na]^+$= 509.2412, found 509.2416.

Diethyl 4-benzyl-2-(1-benzyl-1H-indol-3-yl)-1-methyl-1,2,3,4-tetrahydrocyclopenta[b]indole-1,3-dicarboxylate (**4c**): yield = 18%, brown solid, mp: 56–58 °C,^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 7.77 (d, J = 7.8 Hz, 1H), 7.17 (ddd, J = 24.0, 11.2, 4.4 Hz, 6H), 7.09 – 6.99 (m, 5H), 6.99 – 6.88 (m, 5H), 6.74 (d, J = 6.6 Hz, 2H), 5.21 (q, J = 16.1 Hz, 2H), 5.04 (s, 2H), 4.19 – 4.09 (m, 3H), 4.04 (ddd, J = 14.3, 9.0, 5.4 Hz, 1H), 3.89 (dq, J = 10.7, 7.1 Hz, 1H), 2.97 (d, J = 13.8 Hz, 1H), 1.81 (s, 3H), 1.25 (t, J = 7.1 Hz, 3H), 1.00 (t, J = 7.1 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 1176.1, 172.9, 143.6, 141.8, 137.5, 137.4, 128.9, 128.2, 127.7, 126.8, 126.7, 126.4, 126.2, 126.1, 123.4, 122.2, 122.2, 121.4, 120.1, 119.9, 119.8, 119.6, 115.9, 111.7, 110.2, 61.5, 60.9, 56.3, 54.1, 50.1, 48.7, 48.3, 25.2, 14.4, 14.1 ppm. HRMS (TOF, ESI): m/z calcd for $C_{40}H_{38}N_2O_4Na$, $[M+Na]^+$= 633.2733, found 633.2729.

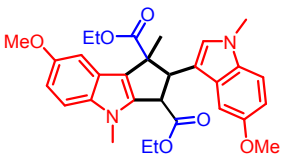
Diethyl 8-methoxy-2-(4-methoxy-1-methyl-1H-indol-3-yl)-1,4-dimethyl-1,2,3,4-tetrahydrocyclo-

penta[b]indole-1,3-dicarboxylate (**4e**): yield = 46%, yellow solid, mp: 62–64 °C, ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) *δ*= 7.15 (t, J = 7.9 Hz, 2H), 6.95 (d, J = 8.2 Hz, 1H), 6.89 (d, J = 8.2 Hz, 1H), 6.53 (d, J = 7.8 Hz, 1H), 6.48 (d, J = 7.7 Hz, 1H), 6.29 (s, 1H), 4.35 – 4.26 (m, 1H), 4.23 – 4.07 (m, 4H), 3.86 (s, 6H), 3.71 (s, 3H), 3.62 (s, 3H), 2.64 (d, J = 13.4 Hz, 1H), 1.45 (s, 3H), 1.20 (dt, J = 14.1, 7.1 Hz, 6H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) *δ* = 177.6, 173.6, 154.0, 153.7, 143.5, 141.4, 139.4, 125.2, 123.0, 122.5, 122.5, 116.3, 114.2, 113.9, 103.3, 102.8, 99.8, 99.4, 61.4, 60.6, 60.6, 58.1, 55.2, 54.8, 48.4, 33.0, 31.4, 26.8, 14.5, 14.3 ppm. HRMS (TOF, ESI): m/z calcd for $C_{30}H_{34}N_2O_6Na$, $[M+Na]^+$= 541.2310, found 541.2315.

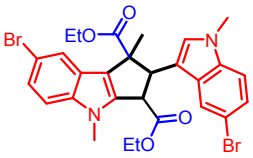
Diethyl 8-chloro-2-(4-chloro-1-methyl-1H-indol-3-yl)-1,4-dimethyl-1,2,3,4-tetrahydrocyclopenta[b]-indole-1,3-dicarboxylate (**4f**): yield = 33%, yellow solid, mp: 149–151 oC,1H NMR (400 MHz, CDCl3, TMS, 25 °C) δ= 7.21 – 7.03 (m, 4H), 6.82 (dd, J = 9.9, 7.9 Hz, 1H), 6.73 (dd, J = 10.8, 7.8 Hz, 1H), 6.59 (s, 1H), 4.30 – 4.04 (m, 5H), 3.71 (s, 3H), 3.62 (s, 3H), 2.71 (d, J = 13.6 Hz, 1H), 1.62 (s, 3H), 1.23 (td, J = 7.1, 2.2 Hz, 6H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 176.57, 173.0, 157.7, 157.5, 155.3, 155.0, 144.9, 144.8, 140.6, 140.5, 126.6, 122.97, 122.9, 122.1, 122.0, 114.7, 112.6, 112.4, 106.0, 105.8, 105.2, 105.1, 105.0, 104.9, 61.9, 60.9, 57.7, 54.0, 48.7, 33.3, 31.3, 26.6, 14.3, 14.2 ppm. HRMS (TOF, ESI): m/z calcd for $C_{28}H_{28}Cl_2N_2O_4Na$, $[M+Na]^+$= 549.1319, found 549.1324.



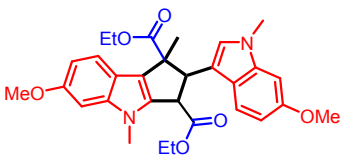
Diethyl 7-methoxy-2-(5-methoxy-1-methyl-1H-indol-3-yl)-1,4-dimethyl-1,2,3,4-tetrahydrocyclo-penta[b]indole-1,3-dicarboxylate (**4g**): yield = 43%, brown solid, mp: 122–124 °C,^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) *δ*= 7.15 (dd, J = 8.5, 2.2 Hz, 3H), 6.93 (s, 1H), 6.86 (dd, J = 9.0, 2.3 Hz, 1H), 6.79 (dd, J = 8.9, 2.2 Hz, 1H), 5.96 (s, 1H), 4.36 (dq, J = 10.7, 7.1 Hz, 1H), 4.23 (d, J = 7.1 Hz, 1H), 4.17 – 4.04 (m, 3H), 3.88 (s, 3H), 3.73 (s, 3H), 3.33 (s, 3H), 3.26 (s, 3H), 2.73 (d, J = 13.8 Hz, 1H), 1.73 (s, 3H), 1.30 (t, J = 7.1 Hz, 3H), 1.24 (t, J = 7.1 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) *δ* = 176.2, 173.0, 154.1, 153.9, 144.0, 137.3, 133.0, 126.8, 126.0, 122.9, 121.2, 114.9, 112.5, 111.2, 110.6, 110.2, 101.6, 100.7, 61.6, 60.9, 57.0, 56.1, 55.3, 53.7, 48.3, 33.1, 30.7, 24.95, 14.4 ppm. HRMS (TOF, ESI): m/z calcd for $C_{30}H_{34}N_2O_6Na$, $[M+Na]^+$= 541.2312, found 541.2315.



Diethyl 7-bromo-2-(5-bromo-1-methyl-1H-indol-3-yl)-1,4-dimethyl-1,2,3,4-tetrahydrocyclopenta-[b]indole-1,3-dicarboxylate (**4h**): yield = 13%, yellow solid, mp: 168–170 °C,^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) *δ*= 7.34 – 7.26 (m, 2H), 7.16 (d, J = 8.6 Hz, 2H), 7.04 (s, 1H), 6.88 (s, 1H), 4.32 (dq, J = 10.8, 7.1 Hz, 1H), 4.25 – 4.17 (m, 1H), 4.17 – 4.05 (m, 3H), 3.73 (s, 3H), 3.42 (s, 3H), 2.72 (d, J = 13.7 Hz, 1H), 1.68 (s, 3H), 1.28 (t, J = 5.5 Hz, 3H), 1.25 (t, J = 5.4 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) *δ* = 175.7, 172.5, 171.3, 143.9, 140.8, 136.5, 127.8, 127.2, 125.1, 124.3, 122.3, 122.2, 121.4, 114.9, 113.2, 113.1, 111.6, 111.2, 61.9, 61.2, 56.3, 53.7, 48.6, 33.2, 31.0, 25.5, 14.3, 14.3 ppm. HRMS (TOF, ESI): m/z calcd for $C_{28}H_{28}Br_2N_2O_4Na$, $[M+Na]^+$= 637.0310, found 637.0314.



Diethyl 6-methoxy-2-(6-methoxy-1-methyl-1H-indol-3-yl)-1,4-dimethyl-1,2,3,4-tetrahydrocyclo-penta[b]indole-1,3-dicarboxylate (**4i**): yield = 44%, yellow solid, mp: 111–113 °C,^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) *δ*= 7.58 (d, J = 8.6 Hz, 1H), 6.88 – 6.80 (m, 2H), 6.74 (dd, J = 12.0, 1.7 Hz, 2H), 6.64 (d, J = 8.8 Hz, 1H), 6.55 (dd, J = 8.8, 2.0 Hz, 1H), 4.34 (dq, J = 10.9, 7.1 Hz, 1H), 4.24 – 4.15 (m, 1H), 4.08 (dt, J = 21.3, 10.5 Hz, 3H), 3.88 (s, 3H), 3.83 (s, 3H), 3.70 (s, 3H), 3.33 (s, 3H), 2.71 (d, J = 13.7 Hz, 1H), 1.70 (s, 3H), 1.28 (t, J = 7.1 Hz, 3H), 1.22 (t, J = 7.1 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) *δ* = 176.2, 173.1, 156.5, 156.0, 142.7, 142.1, 138.6, 125.4, 121.5, 120.5, 120.1, 120.0,



117.3, 115.5, 109.4, 109.0, 94.2, 93.0, 61.5, 60.9, 56.9, 55.9, 55.7, 53.9, 48.5, 32.9, 30.7, 25.3, 14.3 ppm. HRMS (TOF, ESI): m/z calcd for $C_{30}H_{34}N_2O_6Na$, $[M+Na]^+$= 541.2305, found 541.2315.

Diethyl 2-(1,6-dimethyl-1H-indol-3-yl)-1,4,6-trimethyl-1,2,3,4-tetrahydrocyclopenta[b]indole-1,3-dicarboxylate (**4j**): yield = 41%, yellow solid, mp: 60–62 °C,^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 7.61 (d, J = 8.0 Hz, 1H), 7.09 (s, 2H), 7.01 (d, J = 8.0 Hz, 1H), 6.88 (s, 1H), 6.68 (dd, J = 19.4, 8.2 Hz, 2H), 4.34 (dq, J = 10.8, 7.1 Hz, 1H), 4.23 – 4.15 (m, 1H), 4.13 – 4.02 (m, 3H), 3.72 (s, 3H), 3.35 (s, 3H), 2.74 (d, J = 13.7 Hz, 1H), 2.51 (s, 3H), 2.43 (s, 3H), 1.72 (s, 3H), 1.28 (t, J = 7.1 Hz, 3H), 1.22 (t, J = 7.1 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 176.2, 173.1, 142.8, 142.4, 138.2, 131.9, 131.0, 126.0, 123.6, 121.4, 121.1, 120.7, 119.4, 119.0, 115.2, 110.2, 109.4, 61.5, 60.8, 56.9, 54.0, 48.4, 32.8, 30.6, 25.2, 22.1, 21.9, 14.3 ppm. HRMS (TOF, ESI): m/z calcd for $C_{30}H_{34}N_2O_4Na$, $[M+Na]^+$= 509.2412, found 509.2416.

Diethyl 6-fluoro-2-(6-fluoro-1-methyl-1H-indol-3-yl)-1,4-dimethyl-1,2,3,4-tetrahydrocyclopenta-[b]indole-1,3-dicarboxylate (**4k**): yield = 43%, yellow solid, mp: 146–148 °C,^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 7.61 (dd, J = 8.5, 5.5 Hz, 1H), 6.99 – 6.87 (m, 4H), 6.63 (dd, J = 6.3, 4.0 Hz, 2H), 4.35 (dq, J = 10.8, 7.1 Hz, 1H), 4.27 – 4.17 (m, 1H), 4.11 (dd, J = 13.8, 6.8 Hz, 3H), 3.72 (s, 3H), 3.31 (s, 3H), 2.71 (d, J = 13.7 Hz, 1H), 1.71 (s, 3H), 1.29 (t, J = 7.1 Hz, 3H), 1.21 (t, J = 7.1 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 175.7, 172.6, 160.9 (d, J = 31.2 Hz), 158.6 (d, J = 29.5 Hz), 143.2, 141.9 (d, J = 11.5 Hz), 137.8 (d, J = 11.8 Hz), 126.8 (d, J = 3.5 Hz), 122.1, 121.7, 120.3 (d, J = 10.0 Hz), 120.0 (d, J = 10.0 Hz), 119.2, 115.3, 108.4 (d, J = 24.4 Hz), 108.1 (d, J = 24.3 Hz), 96.6 (d, J = 26.2 Hz), 95.9 (d, J = 26.0 Hz), 61.6, 60.9, 56.7, 53.8, 48.4, 33.0, 30.7, 25.1, 14.2 ppm. ^{19}F NMR (377 MHz, $CDCl_3$) δ= -120.2 (dd, J = 15.6, 8.9 Hz), -120.9 (td, J = 9.8, 5.5 Hz) ppm. HRMS (TOF, ESI): m/z calcd for $C_{28}H_{28}F_2N_2O_4Na$, $[M+Na]^+$= 517.1904, found 517.1915.

Dimethyl 1,4-dimethyl-2-(1-methyl-1H-indol-3-yl)-1,2,3,4-tetrahydrocyclopenta[b]indole-1,3-dicarboxylate (**4l**): yield = 39%, yellow solid, mp: 181–183 °C, ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 7.70 (d, J = 7.7 Hz, 1H), 7.29 (d, J = 9.7 Hz, 2H), 7.24 – 7.13 (m, 3H), 6.96 (s, 1H), 6.87 (t, J = 7.5 Hz, 1H), 6.75 (d, J = 8.0 Hz, 1H), 4.00 (d, J = 13.7 Hz, 1H), 3.80 (s, 3H), 3.77 (s, 3H), 3.64 (s, 3H), 3.35 (s, 3H), 2.82 (d, J = 13.7 Hz, 1H), 1.75 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 176.7, 173.5, 143.4, 141.9, 137.8, 126.7, 125.7, 122.8, 122.1, 121.5, 121.3, 119.8, 119.6, 119.6, 119.3, 114.7, 110.2, 109.5, 57.3, 54.0, 52.7, 52.2, 48.3, 33.0, 30.5, 24.8 ppm. HRMS (TOF, ESI): m/z calcd for $C_{26}H_{26}N_2O_4Na$, $[M+Na]^+$= 453.1785, found 453.1790.

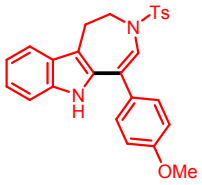
Diethyl 4-benzyl-2-(1-benzyl-1H-indol-3-yl)-1-methyl-1,2,3,4-tetrahydrocyclopenta[b]indole-1,3-dicarboxylate (**4m**): yield = 38%, brown gum-like, ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 7.66 (d, J = 7.1 Hz, 1H), 7.29 (t, J = 7.4 Hz, 2H), 7.20 (dt, J = 13.7, 7.2 Hz, 3H), 6.89 (t, J = 7.5 Hz, 1H), 6.86 – 6.78 (m, 2H), 3.90 (d, J = 13.5 Hz, 1H), 3.77 (s, 3H), 3.30 (s, 3H), 2.84 (d, J = 13.5 Hz, 1H), 2.45 (s, 3H), 2.31 (s, 3H), 1.72 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 210.9, 207.8, 145.0, 142.1, 137.7, 126.6, 126.0, 123.0, 122.2, 121.3, 121.0, 120.0, 119.8, 119.8, 118.8, 114.23, 110.5, 109.7, 60.1, 55.2, 54.9, 33.0, 30.6, 28.5, 26.8, 24.2 ppm. HRMS (TOF, ESI): m/z calcd for $C_{26}H_{26}N_2O_2Na$, $[M+Na]^+$= 421.1890, found 421.1892.

Spectral Characterization Data for 6a–6m

5-phenyl-3-tosyl-1,2,3,6-tetrahydroazepino[4,5-b]indole (**6a**)[2]: yield = 93%, yellow solid, mp: 190–192 °C,^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 7.77 (d, J = 8.2 Hz, 2H), 7.60 (s, 1H), 7.53

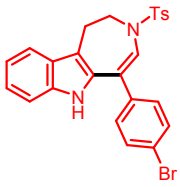
– 7.44 (m, 6H), 7.33 (d, J = 8.1 Hz, 2H), 7.20 – 7.06 (m, 3H), 6.92 (s, 1H), 3.95 – 3.88 (m, 2H), 4.02 – 3.76 (m, 2H), 3.11 – 3.04 (m, 2H), 3.26 – 2.90 (m, 2H), 2.43 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 144.2, 138.7, 136.3, 134.8, 130.8, 130.1, 129.9, 129.1, 128.5, 128.1, 127.1, 126.7, 122.5, 119.8, 118.3, 118.1, 113.8, 110.8, 46.5, 26.6, 21.7 ppm.

5-(4-methoxyphenyl)-3-tosyl-1,2,3,6-tetrahydroazepino[4,5-b] indole (**6b**)[2]: yield = 91%, yellow solid,



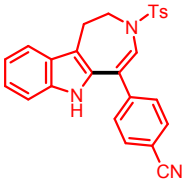
mp: 184–186 °C, ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 7.76 (d, J = 8.2 Hz, 2H), 7.63 (s, 1H), 7.47 (d, J = 7.6 Hz, 1H), 7.37 (d, J = 8.5 Hz, 2H), 7.32 (d, J = 8.1 Hz, 2H), 7.19 (d, J = 7.7 Hz, 1H), 7.16 – 7.06 (m, 2H), 7.01 (d, J = 8.5 Hz, 2H), 6.88 (s, 1H), 3.90 (d, J = 6.6 Hz, 5H), 3.11 – 3.02 (m, 2H), 2.42 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 159.5, 144.1, 136.3, 134.8, 131.1, 131.0, 130.9, 130.1, 128.6, 127.1, 126.4, 122.4, 119.7, 118.1, 118.0, 114.4, 113.6, 110.8, 55.5, 46.5, 26.6, 21.6 ppm. HRMS (TOF, ESI): m/z calcd for $C_{26}H_{24}N_2O_3SNa$, $[M+Na]^+$= 467.1402, found 467.1405.

5-(4-bromophenyl)-3-tosyl-1,2,3,6-tetrahydroazepino[4,5-b]indole (**6c**): yield = 82%, yellow solid, mp:



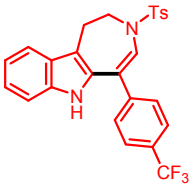
172–174 °C, ^{1}H NMR (400 MHz, CDCl3, TMS, 25 °C) δ= 7.73 (d, J = 8.2 Hz, 2H), 7.60 (d, J = 8.2 Hz, 2H), 7.49 (s, 1H), 7.44 (d, J = 7.8 Hz, 1H), 7.31 (d, J = 8.2 Hz, 4H), 7.18 (d, J = 7.8 Hz, 1H), 7.10 (dt, J = 20.5, 7.0 Hz, 2H), 6.86 (s, 1H), 3.90 – 3.83 (m, 2H), 3.07 – 3.00 (m, 2H), 2.41 (s, 3H ppm. 13C NMR (101 MHz, CDCl3, 25 oC) δ = 144.3, 137.7, 136.2, 134.9, 132.3, 131.6, 130.3, 130.2, 128.5, 127.1, 126.8, 122.8, 122.3, 120.0, 118.1, 116.9, 114.2, 110.8, 46.5, 26.6, 21.7 ppm. HRMS (TOF, ESI): m/z calcd for $C_{25}H_{21}BrN_2O_2SNa$, $[M+Na]^+$= 515.0400, found 515.0405.

4-(3-tosyl-1,2,3,6-tetrahydroazepino[4,5-b]indol-5-yl)benzonitrile (**6d**): yield = 86%, yellow solid, mp:



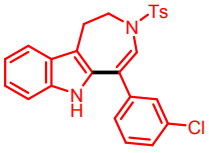
212–214 °C, ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 7.75 (dd, J = 12.5, 8.2 Hz, 4H), 7.57 (d, J = 8.2 Hz, 2H), 7.46 (s, 2H), 7.33 (d, J = 8.1 Hz, 2H), 7.20 (d, J = 7.9 Hz, 1H), 7.17 – 7.07 (m, 2H), 6.93 (s, 1H), 3.91 – 3.85 (m, 2H), 3.07 – 3.01 (m, 2H), 2.42 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 144.9, 144.2, 136.2, 135.4, 133.3, 130.8, 130.6, 129.9, 128.7, 128.0, 127.5, 123.3, 120.5, 119.0,118.5, 116.5, 115.2, 112.3, 111.2, 47.0, 26.8, 22.1 ppm. HRMS (TOF, ESI): m/z calcd for $C_{26}H_{22}N_3O_2S$, $[M+H]^+$= 440.1430, found 440.1432.

3-tosyl-5-(4-(trifluoromethyl)phenyl) -1,2,3,6 -tetrahy-droazepino-[4,5-b]indole (6e):



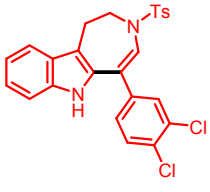
yield = 76%, yellow solid, mp: 184–186 °C, ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 7.75 (d, J = 8.2 Hz, 4H), 7.58 (d, J = 8.0 Hz, 2H), 7.46 (d, J = 7.2 Hz, 2H), 7.33 (d, J = 8.1 Hz, 2H), 7.20 (d, J = 7.8 Hz, 1H), 7.16 – 7.07 (m, 2H), 6.92 (s, 1H), 3.93 – 3.85 (m, 2H), 3.09 – 3.02 (m, 2H), 2.42 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 144.4, 142.6, 136.0, 135.0, 130.5, 130.2, 130.0, 128.5, 127.3, 127.2, 126.17 (q, J = 3.6 Hz), 125.6, 122.9, 120.0, 118.1, 116.7, 114.5, 110.9, 46.6, 26.5, 21.7 ppm. ^{19}F NMR (377 MHz, $CDCl_3$) δ= -62.5 ppm. HRMS (TOF, ESI): m/z calcd for $C_{26}H_{21}F_3N_2O_2SNa$, $[M+Na]^+$= 505.1165, found 505.1174.

5- (3-chlorophenyl) -3-tosyl-1,2,3,6-tetrahydroazepino [4,5-b] indole (**6f**): yield =



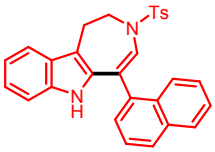
95%, yellow solid, mp: 176–178 °C,^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 7.75 (d, J = 8.3 Hz, 2H), 7.53 (s, 1H), 7.47 – 7.39 (m, 4H), 7.33 (d, J = 8.3 Hz, 3H), 7.20 (d, J = 7.9 Hz, 1H), 7.11 (ddd, J = 14.8, 13.9, 6.9 Hz, 2H), 6.90 (s, 1H), 3.91 – 3.84 (m, 2H), 3.08 – 3.01 (m, 2H), 2.42 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 144.3, 140.6, 136.1, 134.9, 130.4, 130.2, 130.0, 128.5, 128.4, 128.1, 127.1, 127.1, 122.7, 119.9, 118.1, 116.8, 114.2, 110.9, 46.5, 26.5, 21.7 ppm. HRMS (TOF, ESI): m/z calcd for $C_{25}H_{22}ClN_2O_2S$, $[M+H]^+$= 449.1088, found 449.1090.

5-(3,4-dichlorophenyl)-3-tosyl-1,2,3,6-tetrahydroazepino[4,5-b]indole (**6g**)[2]: yield = 87%, yellow solid,

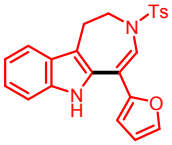


mp: 210–212 °C,^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 7.75 (d, J = 8.2 Hz, 2H), 7.58 – 7.51 (m, 3H), 7.46 (d, J = 7.8 Hz, 1H), 7.34 (d, J = 8.1 Hz, 2H), 7.29 (dd, J = 8.2, 2.0 Hz, 1H), 7.22 (d, J = 7.9 Hz, 1H), 7.17 – 7.07 (m, 2H), 6.90 (s, 1H), 3.90 – 3.83 (m, 2H), 3.07 – 3.00 (m, 2H), 2.43 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 144.4, 138.7, 135.9, 134.9, 133.1, 132.4, 131.6, 131.0, 130.1, 129.8, 129.2, 128.4, 127.1, 122.8, 119.9, 118.0, 115.6, 114.4, 110.8, 46.5, 26.4, 21.6 ppm. HRMS (TOF, ESI): m/z calcd for $C_{25}H_{21}Cl_2N_2O_2S$, $[M+H]^+$= 483.0698, found 483.0701.

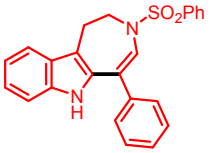
5-(naphthalen-1-yl)-3-tosyl-1,2,3,6-tetrahydroazepino[4,5-b]indole (**6h**)[2]: yield = 78%, yellow solid, mp: 203–205 °C,^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 7.93 (dt, J = 9.3, 7.1 Hz, 4H), 7.77 (d, J = 8.2 Hz, 2H), 7.61 – 7.52 (m, 4H), 7.48 (d, J = 7.3 Hz, 1H), 7.32 (d, J = 8.1 Hz, 2H), 7.16 – 7.06 (m, 3H), 7.01 (s, 1H), 3.93 (d, J = 4.7 Hz, 2H), 3.13 – 3.06 (m, 2H), 2.42 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 144.2, 136.3, 136.1, 134.9, 133.7, 133.0, 130.9, 130.2, 128.8, 128.7, 128.6, 128.2, 127.9, 127.8, 127.2, 127.0, 126.8, 126.6, 122.6, 119.8, 118.3, 118.1, 114.0, 110.8, 46.6, 26.7, 21.7 ppm. HRMS (TOF, ESI): m/z calcd for $C_{29}H_{25}N_2O_2S$, $[M+H]^+$= 465.1634, found 465.1636.



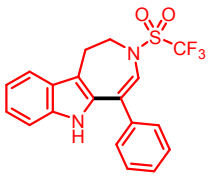
5-(furan-2-yl)-3-tosyl-1,2,3,6-tetrahydroazepino[4,5-b]indole (**6i**): yield = 86%, black solid, mp: 66–68 °C,^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 8.53 (s, 1H), 7.75 (d, J = 8.3 Hz, 2H), 7.57 (d, J = 0.6 Hz, 1H), 7.43 (d, J = 7.9 Hz, 1H), 7.34 – 7.28 (m, 4H), 7.16 (t, J = 7.1 Hz, 1H), 7.08 (t, J = 7.2 Hz, 1H), 6.55 – 6.48 (m, 2H), 3.90 – 3.84 (m, 2H), 3.02 – 2.95 (m, 2H), 2.41 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 153.0, 144.4, 142.4, 136.0, 135.0, 130.2, 129.3, 128.2, 127.4, 127.2, 122.6, 119.8, 118.0, 114.0, 111.5, 110.9, 108.3, 107.3, 46.6, 26.3, 21.7 ppm. HRMS (TOF, ESI): m/z calcd for $C_{23}H_{19}N_2O_3S$, $[M-H]^-$= 403.1122, found 403.1117.



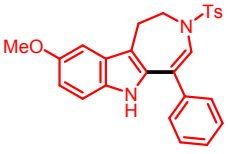
5-phenyl-3-(phenylsulfonyl)-1,2,3,6-tetrahydroazepino[4,5-b]indole (**6j**)[2]: yield = 85%, yellow solid, mp: 205–207 °C, ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 7.85 (d, J = 7.3 Hz, 2H), 7.55 (d, J = 7.3 Hz, 2H), 7.52 – 7.40 (m, 8H), 7.15 – 7.02 (m, 3H), 6.87 (s, 1H), 3.92 – 3.84 (m, 2H), 3.09 – 3.00 (m, 2H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 139.2, 138.6, 134.8, 133.2, 130.6, 129.8, 129.5, 129.1, 128.5, 128.2, 127.0, 126.5, 122.6, 119.8, 118.6, 118.1, 113.8, 110.8, 46.6, 26.6 ppm. HRMS (TOF, ESI): m/z calcd for $C_{24}H_{21}N_2O_2S$, $[M+H]^+$= 401.1322, found 401.1323.

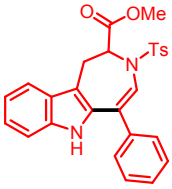


5-phenyl-3-((trifluoromethyl)sulfonyl)-1,2,3,6-tetrahydroaze-pino[4,5-b]indole (**6k**): yield = 71%, yellow solid, mp: 180–182 °C,^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 7.62 – 7.53 (m, 2H), 7.52 – 7.47 (m, 3H), 7.44 (dd, J = 7.1, 2.2 Hz, 2H), 7.23 – 7.16 (m, 2H), 7.16 – 7.10 (m, 1H), 6.54 (s, 1H), 4.15 – 4.08 (m, 2H), 3.41 – 3.34 (m, 2H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 136.19 (d, J = 224.8 Hz), 129.7, 129.4, 128.9, 128.6, 124.3, 124.2, 123.6, 120.2, 118.7, 114.7, 111.1, 48.4, 27.6 ppm. ^{19}F NMR (377 MHz, $CDCl_3$) δ =-75.1 ppm. HRMS (TOF, ESI): m/z calcd for $C_{19}H_{14}F_3N_2O_2S$, $[M-H]^-$= 391.0735, found 391.0728.



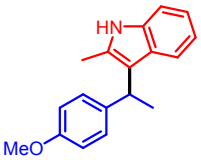
9-methoxy-5-phenyl-3-tosyl-1,2,3,6-tetrahydroazepino[4,5-b]indole (**6l**): yield = 92%, yellow solid, mp: 170–172 °C, ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 7.77 (d, J = 7.5 Hz, 2H), 7.54 – 7.42 (m, 6H), 7.33 (d, J = 8.0 Hz, 2H), 7.08 (d, J = 8.7 Hz, 1H), 6.90 (s, 2H), 6.80 (dd, J = 8.7, 1.0 Hz, 1H), 3.91 (d, J = 3.8 Hz, 2H), 3.85 (s, 3H), 3.05 (s, 2H), 2.43 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 154.2, 144.1, 138.7, 136.2, 131.5, 130.1, 130.0, 129.8, 129.1, 128.8, 128.1, 127.0, 126.4, 118.4, 113.5, 112.8, 111.6, 99.6, 55.9, 46.5, 26.7, 21.6 ppm. HRMS (TOF, ESI): m/z calcd for $C_{26}H_{23}N_2O_3S$, $[M-H]^-$= 443.1436, found 443.1430.



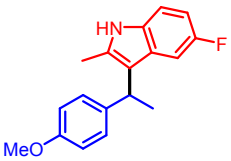


5-Phenyl-3-tosyl-1,2,3,6-tetrahydroazepino[4,5-b]indole-2-carboxylate (**6m**)[2]: yield = 76%, yellow solid, mp: 88–90 °C, ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 7.77 (d, J = 8.3 Hz, 2H), 7.59 (s, 1H), 7.51 – 7.42 (m, 6H), 7.33 (d, J = 8.1 Hz, 2H), 7.11 (ddt, J = 12.1, 6.7, 6.1 Hz, 3H), 7.01 (s, 1H), 5.60 (t, J = 3.5 Hz, 1H), 3.95 (dd, J = 15.9, 4.9 Hz, 1H), 3.29 (s, 3H), 2.81 (dd, J = 15.9, 3.0 Hz, 1H), 2.43 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 168.1, 144.5, 138.8, 135.6, 135.2, 131.3, 130.0, 129.8, 129.0, 128.5, 128.1, 127.4, 124.5, 122.4, 119.8, 117.8, 116.6, 110.8, 110.7, 57.7, 52.2, 28.3, 21.7 ppm. HRMS (TOF, ESI): m/z calcd for $C_{27}H_{23}N_2O_4S$, $[M-H]^-$= 471.1385, found 471.1379.

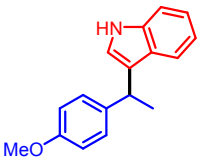
Spectral Characterization Data for 9a–9g



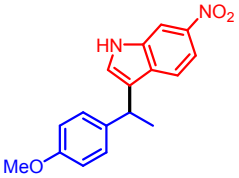
3-(1-(4-Methoxyphenyl)ethyl)-2-methyl-1H-indole (**9a**)[10]: yield = 91%, yellow solid, mp: 27–29 °C, ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 7.71 (s, 1H), 7.38 (d, J = 7.9 Hz, 1H), 7.27 – 7.21 (m, 3H), 7.06 (t, J = 7.5 Hz, 1H), 6.96 (t, J = 7.5 Hz, 1H), 6.80 (d, J = 8.3 Hz, 2H), 4.37 (q, J = 7.2 Hz, 1H), 3.76 (s, 3H), 2.32 (s, 3H), 1.74 (d, J = 7.3 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 157.5, 138.4, 135.3, 130.5, 128.3, 127.8, 120.7, 119.4, 119.0, 116.3, 113.5, 110.2, 55.4, 34.6, 20.8, 12.3 ppm.



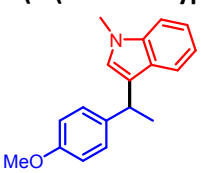
5-Fluoro-3-(1-(4-methoxyphenyl)ethyl)-2-methyl-1H-indole (**9b**): yield = 87%, yellow solid, mp: 26–28 °C, ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 7.70 (s, 1H), 7.22 (d, J = 8.7 Hz, 2H), 7.10 (dd, J = 8.7, 4.5 Hz, 1H), 6.99 (dd, J = 10.3, 1.9 Hz, 1H), 6.79 (dd, J = 8.1, 5.5 Hz, 3H), 4.30 (q, J = 7.3 Hz, 1H), 3.76 (s, 3H), 2.31 (s, 3H), 1.70 (d, J = 7.3 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 158.6, 157.6, 156.3, 137.9, 132.2 (d, J = 72.9 Hz), 128.2, 128.1 (d, J = 9.7 Hz), 116.7 (d, J = 4.5 Hz), 113.6, 110.6 (d, J = 9.8 Hz), 108.7 (d, J = 26.1 Hz), 104.4 (d, J = 23.8 Hz), 55.3, 34.6, 20.6, 12.3 ppm. ^{19}F NMR (377 MHz, $CDCl_3$) δ = -125.1 (td, J = 9.8, 4.5 Hz) ppm. HRMS (TOF, ESI): m/z calcd for $C_{18}H_{17}FNO$, $[M-H]^-$= 282.1299, found 282.1294.



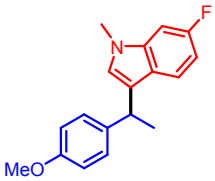
3-(1-(4-Methoxyphenyl)ethyl)-1H-indole (**9c**)[10]: yield = 88%, yellow solid, mp: 136–138 °C, ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 7.95 (s, 1H), 7.40 (d, J = 7.9 Hz, 1H), 7.34 (d, J = 8.1 Hz, 1H), 7.23 (d, J = 8.6 Hz, 2H), 7.17 (t, J = 7.6 Hz, 1H), 7.03 (t, J = 7.5 Hz, 1H), 7.00 (d, J = 1.4 Hz, 1H), 6.84 (d, J = 8.5 Hz, 2H), 4.36 (q, J = 7.1 Hz, 1H), 3.79 (s, 3H), 1.70 (d, J = 7.1 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 157.8, 139.2, 136.8, 128.4, 127.0, 122.0, 121.9, 121.1, 119.9, 119.3, 113.8, 111.1, 55.3, 36.2, 22.7 ppm.



3-(1-(4-Methoxyphenyl)ethyl)-6-nitro-1H-indole (**9d**): yield = 95%, yellow solid, mp: 98–100 °C, ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 8.87 (s, 1H), 8.32 (d, J = 1.9 Hz, 1H), 7.87 (dd, J = 8.8, 1.9 Hz, 1H), 7.34 (dd, J = 5.3, 3.3 Hz, 2H), 7.18 (d, J = 8.6 Hz, 2H), 6.85 (d, J = 8.6 Hz, 2H), 4.33 (q, J = 7.1 Hz, 1H), 3.79 (s, 3H), 1.69 (d, J = 7.1 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 158.0, 143.1, 138.3, 135.2, 131.7, 128.3, 127.3, 122.7, 119.6, 114.7, 114.0, 108.3, 55.3, 36.0, 22.5 ppm. HRMS (TOF, ESI): m/z calcd for $C_{17}H_{15}N_2O_3$, $[M-H]^-$= 295.1087, found 295.1083.



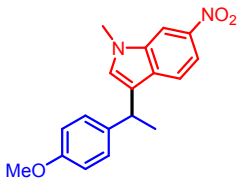
3-(1-(4-Methoxyphenyl)ethyl)-1-methyl-1H-indole (**9e**)[10]: yield = 89%, yellow gum-like, ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 7.36 (d, J = 7.9 Hz, 1H), 7.25 – 7.12 (m, 4H), 6.98 (t, J = 7.4 Hz, 1H), 6.83 – 6.77 (m, 3H), 4.31 (q, J = 7.1 Hz, 1H), 3.75 (s, 3H), 3.72 (s, 3H), 1.65 (d, J = 7.1 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 157.8, 139.3, 137.5, 128.4, 127.3, 126.0, 121.6, 120.5, 119.9, 118.7, 113.8, 109.2, 55.3, 36.2, 32.8, 22.8 ppm.



6-Fluoro-3-(1-(4-methoxyphenyl)ethyl)-1-methyl-1H-indole (**9f**): yield = 83%, brown gum-like, ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 7.19 (ddd, J = 9.7, 7.1, 1.5 Hz, 3H), 6.90 (d, J = 9.9 Hz,

1H), 6.79 (dd, J = 6.0, 4.2 Hz, 3H), 6.73 (t, J = 9.2 Hz, 1H), 4.26 (q, J = 6.9 Hz, 1H), 3.74 (s, 3H), 3.64 (s, 3H), 1.63 (dd, J = 7.1, 1.5 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 161.1, 158.8, 157.9, 139.0, 137.5 (d, J = 12.0 Hz), 128.4, 126.2 (d, J = 3.6 Hz), 123.9, 120.7 (d, J = 10.1 Hz), 120.6, 113.6, 107.4 (d, J = 24.4 Hz), 95.5 (d, J = 26.0 Hz), 55.3, 36.1, 32.8, 22.7 ppm. ^{19}F NMR (377 MHz, $CDCl_3$) δ = -121.1 – -121.2 (m) ppm. HRMS (TOF, ESI): m/z calcd for $C_{18}H_{19}FNO$, $[M+H]^+$= = 284.1448, found 284.1450.

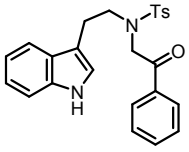
3-(1-(4-Methoxyphenyl)ethyl)-1-methyl-6-nitro-1H-indole (**9g**): yield = 96%, yellow solid, mp: 137–139 °C, ^{1}H



NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 8.23 (s, 1H), 7.85 (dd, J = 8.8, 1.5 Hz, 1H), 7.34 (d, J = 8.8 Hz, 1H), 7.19 (s, 1H), 7.17 (d, J = 5.7 Hz, 2H), 6.84 (d, J = 8.6 Hz, 2H), 4.32 (q, J = 7.0 Hz, 1H), 3.83 (s, 3H), 3.78 (s, 3H), 1.68 (d, J = 7.1 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 158.0, 142.8, 138.2, 135.9, 131.8, 131.8, 128.2, 121.6, 119.7, 114.1, 113.9, 106.3, 55.3, 35.9, 33.1, 22.5 ppm. HRMS (TOF, ESI): m/z calcd for $C_{18}H_{19}N_2O_3$, $[M+H]^+$= 311.1392, found 311.1393.

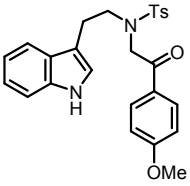
Spectral Characterization Data for 5a–5m

N-(2-(1H-indol-3-yl)ethyl)-4-methyl-N-(2-oxo-2-phenylethyl)ben-zenesulfonamide (**5a**)[2]: yield = 89%,



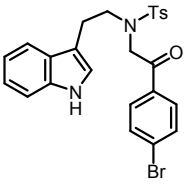
white solid, mp: 138–140 °C,^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ = 7.99 (s, 1H), 7.81 (d, J = 7.5 Hz, 2H), 7.75 (d, J = 8.2 Hz, 2H), 7.57 (t, J = 7.4 Hz, 1H), 7.49 (d, J = 7.9 Hz, 1H), 7.42 (t, J = 7.7 Hz, 2H), 7.32 – 7.25 (m, 3H), 7.15 (t, J = 7.5 Hz, 1H), 7.06 (t, J = 7.4 Hz, 1H), 6.96 (d, J = 1.6 Hz, 1H), 4.71 (s, 2H), 3.61 – 3.51 (m, 2H), 3.05 – 2.95 (m, 2H), 2.41 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 194.4, 143.5, 136.9, 136.3, 135.0, 133.8, 129.7, 128.9, 128.1, 127.7, 127.3, 122.3, 122.2, 119.6, 118.8, 112.6, 111.3, 53.7, 48.9, 24.9, 21.7 ppm.

N-(2-(1H-indol-3-yl)ethyl)-N-(2-(4-methoxyphenyl)-2-oxoethyl)-4-methylbenzenesulfonamide (**5b**)[2]:



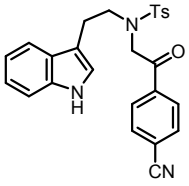
yield = 91%, yellow solid, mp: 175–177 °C,^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 7.96 (s, 1H), 7.85 (d, J = 8.8 Hz, 2H), 7.75 (d, J = 8.1 Hz, 2H), 7.51 (d, J = 7.9 Hz, 1H), 7.29 (dd, J = 18.5, 8.6 Hz, 4H), 7.16 (t, J = 7.4 Hz, 1H), 7.07 (t, J = 7.4 Hz, 1H), 6.98 (s, 1H), 6.90 (d, J = 8.8 Hz, 2H), 4.65 (s, 2H), 3.87 (s, 3H), 3.60 – 3.50 (m, 2H), 3.04 – 2.95 (m, 2H), 2.41 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 192.8, 164.4, 143.7, 136.8, 136.3, 130.6, 129.7, 128.1, 127.7, 127.3, 122.2, 119.6, 118.8, 114.1, 112.7, 111.2, 55.7, 53.5, 49.0, 24.9, 21.7 ppm.

N-(2-(1H-indol-3-yl)ethyl)-N-(2-(4-bromophenyl)-2-oxoethyl)-4-methylbenzenesulfonamide (**5c**):



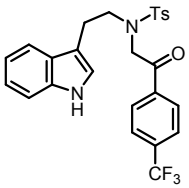
white solid, mp: 205–207 °C, The crude was taken into next without any purification and the product was confirmed by HRMS. HRMS (TOF, ESI): m/z calcd for $C_{25}H_{24}BrN_2O_3S$, $[M+H]^+$= 511.0687, found 511.0691.

N-(2-(1H-indol-3-yl)ethyl)-N-(2-(4-cyanophenyl)-2-oxoethyl)-4-methylbenzenesulfonamide (**5d**): The



crude was taken into next without any purification and the product was confirmed by HRMS. HRMS (TOF, ESI): m/z calcd for $C_{26}H_{24}N_3O_3S$, $[M+H]^+$= 458.1536, found 458.1538.

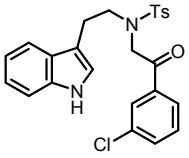
***N*-(2-(1H-indol-3-yl)ethyl)-4-methyl-*N*-(2-oxo-2-(4-(trifluoromethyl) phenyl)ethyl)benzenesulfon-amide** (**5e**): yield = 76%, white solid, mp: 217–219 °C,^{1}H NMR (400 MHz, DMSO-d_6,



25 °C) δ= 10.84 (s, 1H), 8.17 (d, J = 8.1 Hz, 2H), 7.92 (d, J = 8.2 Hz, 2H), 7.76 (d, J =

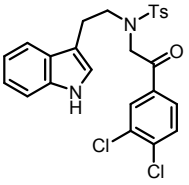
8.2 Hz, 2H), 7.40 (t, J = 6.7 Hz, 3H), 7.30 (d, J = 8.1 Hz, 1H), 7.08 (d, J = 1.8 Hz, 1H), 7.04 (t, J = 7.3 Hz, 1H), 6.94 (t, J = 7.3 Hz, 1H), 5.01 (s, 2H), 3.41 (dd, J = 9.5, 6.6 Hz, 2H), 3.35 (s, 3H), 2.90 (d, J = 8.4 Hz, 2H) ppm. ^{13}C NMR (101 MHz, DMSO-d_6) δ 194.3, 161.3, 143.1, 136.9, 136.2, 129.7, 128.9, 127.0, 126.9, 125.7, 122.9, 121.0, 118.3, 118.0, 111.4, 110.6, 54.2, 49.3, 24.2, 21.0 ppm. ^{19}F NMR (377 MHz, DMSO) δ =-61.6 ppm. HRMS (TOF, ESI): m/z calcd for $C_{26}H_{23}F_3N_2O_3S$ Na, $[M+Na]^+$= 523.1273, found 523.1279.

***N*-(2-(1H-indol-3-yl)ethyl)-*N*-(2-(3-chlorophenyl)-2-oxoethyl)-4-methylbenzenesulfonamide** (**5f**):



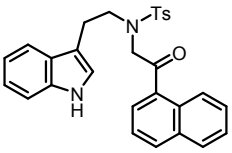
yield = 95%, white solid, mp: 177–179 °C,^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) *δ*= 1H NMR (400 MHz, CDCl3) δ 7.94 (s, 1H), 7.75 (d, J = 8.4 Hz, 3H), 7.66 (d, J = 7.8 Hz, 1H), 7.53 (d, J = 7.9 Hz, 1H), 7.48 (d, J = 7.9 Hz, 1H), 7.38 – 7.27 (m, 4H), 7.16 (t, J = 7.5 Hz, 1H), 7.06 (t, J = 7.4 Hz, 1H), 6.98 (d, J = 1.7 Hz, 1H), 4.62 (s, 2H), 3.61 – 3.53 (m, 2H), 3.01 (t, J = 7.5 Hz, 2H), 2.43 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) *δ* = 193.3, 143.7, 136.7, 136.4, 136.3, 135.2, 133.7, 130.2, 129.7, 128.2, 127.7, 127.2, 126.2, 122.4, 122.3, 119.7, 118.7, 112.6, 111.3, 53.8, 48.8, 25.0, 21.7 ppm. HRMS (TOF, ESI): m/z calcd for $C_{25}H_{23}ClN_2O_3S$ Na, $[M+Na]^+$= 489.1013, found 489.1016.

***N*-(2-(1H-indol-3-yl)ethyl)-*N*-(2-(3,4-dichlorophenyl)-2-oxoethyl)-4-methylbenzenesulfonamide** (**5g**)[2]:



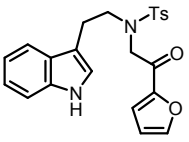
yield = 87%, yellow solid, mp: 202–204 °C,^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) *δ*= 7.93 (s, 1H), 7.81 (d, J = 1.8 Hz, 1H), 7.74 (d, J = 8.2 Hz, 2H), 7.58 (dd, J = 8.4, 1.9 Hz, 1H), 7.46 (t, J = 6.9 Hz, 2H), 7.34 – 7.27 (m, 3H), 7.16 (t, J = 7.5 Hz, 1H), 7.06 (t, J = 7.4 Hz, 1H), 6.98 (d, J = 1.8 Hz, 1H), 4.53 (s, 2H), 3.55 (t, J = 7.4 Hz, 2H), 3.00 (t, J = 7.4 Hz, 2H), 2.43 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) *δ* = 192.58, 143.79, 138.39, 136.40, 136.27, 133.54, 130.88, 130.09, 129.80, 127.67, 127.23, 127.13, 126.04, 122.87, 122.40, 119.77, 118.70, 112.49, 111.30,54.0, 48.9, 25.0, 21.7 ppm.

***N*-(2-(1H-indol-3-yl)ethyl)-4-methyl-*N*-(2-(naphthalen-1-yl)-2-oxoethyl)benzenesulfonamide** (**5h**)[2]:



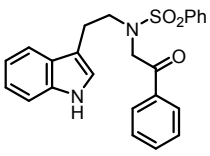
The crude was taken into next without any purification and the product was confirmed by HRMS. HRMS-ESI (m/z): calcd for $C_{29}H_{28}N_2O_3S$, $[M+H]^+$ = 483.1740, found 483.1742.

***N*-(2-(1H-indol-3-yl)ethyl)-*N*-(2-(furan-2-yl)-2-oxoethyl)-4-methyl-benzenesulfonamide** (**5i**): yield =



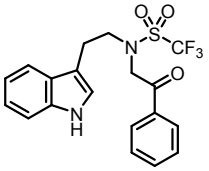
86%, white solid, mp: 106–108 °C, ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) *δ*= 8.02 (s, 1H), 7.75 (d, J = 8.2 Hz, 2H), 7.56 (s, 1H), 7.50 (d, J = 7.9 Hz, 1H), 7.32 (d, J = 8.1 Hz, 1H), 7.27 (d, J = 6.4 Hz, 3H), 7.21 (d, J = 3.6 Hz, 1H), 7.16 (t, J = 7.5 Hz, 1H), 7.07 (t, J = 7.4 Hz, 1H), 6.99 (d, J = 1.8 Hz, 1H), 6.52 (dd, J = 3.6, 1.6 Hz, 1H), 4.57 (s, 2H), 3.59 – 3.52 (m, 2H), 3.06 – 2.99 (m, 2H), 2.40 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) *δ* =183.6, 151.0, 147.0, 143.5, 136.8, 136.3, 129.7, 127.6, 127.3, 122.3, 122.2, 119.6, 118.8 118.4, 112.7, 112.6, 112.5, 111.3, 53.1, 49.2, 24.9, 21.7 ppm. HRMS (TOF, ESI): m/z calcd for $C_{23}H_{23}N_2O_4S$, $[M+H]^+$= 423.1375, found 423.1378.

***N*-(2-(1H-indol-3-yl)ethyl)-*N*-(2-oxo-2-phenylethyl)benzene-sulfonamide** (**5j**)[2]: yield = 85%, yellow



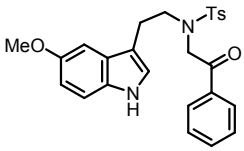
solid, mp: 142–144 °C, ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) *δ*= 8.02 (s, 1H), 7.87 (d, J = 7.5 Hz, 2H), 7.79 (d, J = 7.4 Hz, 2H), 7.56 (dd, J = 8.1, 6.4 Hz, 2H), 7.48 (dd, J = 12.7, 4.9 Hz, 3H), 7.42 (t, J = 7.7 Hz, 2H), 7.31 (d, J = 8.1 Hz, 1H), 7.15 (t, J = 7.5 Hz, 1H), 7.06 (t, J = 7.4 Hz, 1H), 6.95 (d, J = 1.5 Hz, 1H), 4.72 (s, 2H), 3.64 – 3.53 (m, 2H), 3.06 – 2.95 (m, 2H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) *δ* = 194.2, 139.9, 136.3, 134.9, 133.9, 132.8, 129.1, 128.9, 128.1, 127.5, 127.2, 122.3, 122.2, 119.6, 118.7, 112.4, 111.3, 53.6, 48.9, 24.9 ppm.

***N*-(2-(1*H*-indol-3-yl)ethyl)-1,1,1-trifluoro-*N*-(2-oxo-2-phenyl-ethyl)methanesulfonamide** (**5k**): yield =



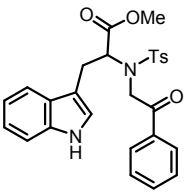
71%, yellow solid, mp: 117–119 °C,^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 8.03 (s, 1H), 7.70 (d, J = 7.4 Hz, 2H), 7.59 (t, J = 7.4 Hz, 1H), 7.53 (d, J = 7.9 Hz, 1H), 7.43 (t, J = 7.7 Hz, 2H), 7.35 (d, J = 8.1 Hz, 1H), 7.18 (t, J = 7.5 Hz, 1H), 7.07 (t, J = 7.4 Hz, 1H), 7.03 (d, J = 1.6 Hz, 1H), 4.69 (s, 2H), 3.86 (d, J = 15.8 Hz, 2H), 3.12 (t, J = 7.5 Hz, 2H)ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 192.0, 134.3, 131.7 (d, J = 939 Hz)，129.1, 127.9, 122.6, 122.4, 112.0, 118.5, 111.6, 111.5, 53.9, 50.1, 25.2 ppm. ^{19}F NMR (377 MHz, $CDCl_3$) δ = -75.84 ppm. HRMS (TOF, ESI): m/z calcd for $C_{19}H_{17}F_3N_2O_3SNa$, $[M+Na]^+$= 433.0808, found 433.0808.

***N*-(2-(5-methoxy-1*H*-indol-3-yl)ethyl)-4-methyl-*N*-(2-oxo-2-phenylethyl)benzenesulfonamide** (**5l**):



yield = 92%, yellow solid, mp: 127–129 °C, ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 7.92 (s, 1H), 7.81 (d, J = 7.5 Hz, 2H), 7.75 (d, J = 8.1 Hz, 2H), 7.57 (t, J = 7.3 Hz, 1H), 7.42 (t, J = 7.6 Hz, 2H), 7.26 (d, J = 8.3 Hz, 2H), 7.19 (d, J = 8.8 Hz, 1H), 6.99 (d, J = 1.4 Hz, 1H), 6.93 (s, 1H), 6.81 (dd, J = 8.7, 2.0 Hz, 1H), 4.70 (s, 2H), 3.81 (s, 3H), 3.59 – 3.51 (m, 2H), 3.04 – 2.92 (m, 2H), 2.40 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 194.4, 154.2, 143.5, 136.8, 135.0, 133.9, 131.4, 129.7, 128.9, 128.1, 127.6, 127.6, 123.0, 112.6, 112.3, 112.1, 100.4, 55.9, 53.7, 48.8, 25.1, 21.7 ppm. HRMS (TOF, ESI): m/z calcd for $C_{26}H_{26}N_2O_4SNa$, $[M+Na]^+$= 485.1509, found 485.1511.

Methyl *N*$^{\alpha}$-(2-oxo-2-phenylethyl)-*N*$^{\alpha}$-tosyltryptophanate (**5m**): yield = 76%, brown solid, mp: 64–66



°C,^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ= 8.12 (s, 1H), 7.96 (d, J = 7.3 Hz, 2H), 7.83 (d, J = 8.2 Hz, 2H), 7.59 (t, J = 7.4 Hz, 1H), 7.47 (t, J = 7.6 Hz, 2H), 7.39 (d, J = 7.8 Hz, 1H), 7.28 (d, J = 8.1 Hz, 1H), 7.22 (d, J = 8.1 Hz, 2H), 7.14 (t, J = 7.3 Hz, 1H), 7.05 (t, J = 7.2 Hz, 1H), 6.92 (d, J = 1.9 Hz, 1H), 5.10 (d, J = 1.2 Hz, 2H), 4.65 (dd, J = 9.6, 5.3 Hz, 1H), 3.39 (s, 3H), 3.18 (dt, J = 14.0, 6.6 Hz, 2H), 2.39 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C) δ = 194.4, 171.4, 143.7, 136.6, 136.2, 135.2, 133.7, 129.6, 129.4, 128.9, 128.2, 128.1, 127.1, 123.4, 122.1, 119.6, 118.5, 111.3, 109.7, 59.3, 52.1, 50.1, 26.9, 21.7 ppm. HRMS (TOF, ESI): m/z calcd for $C_{27}H_{26}N_2O_5SNa$, $[M+Na]^+$= 513.1456, found 513.1460.

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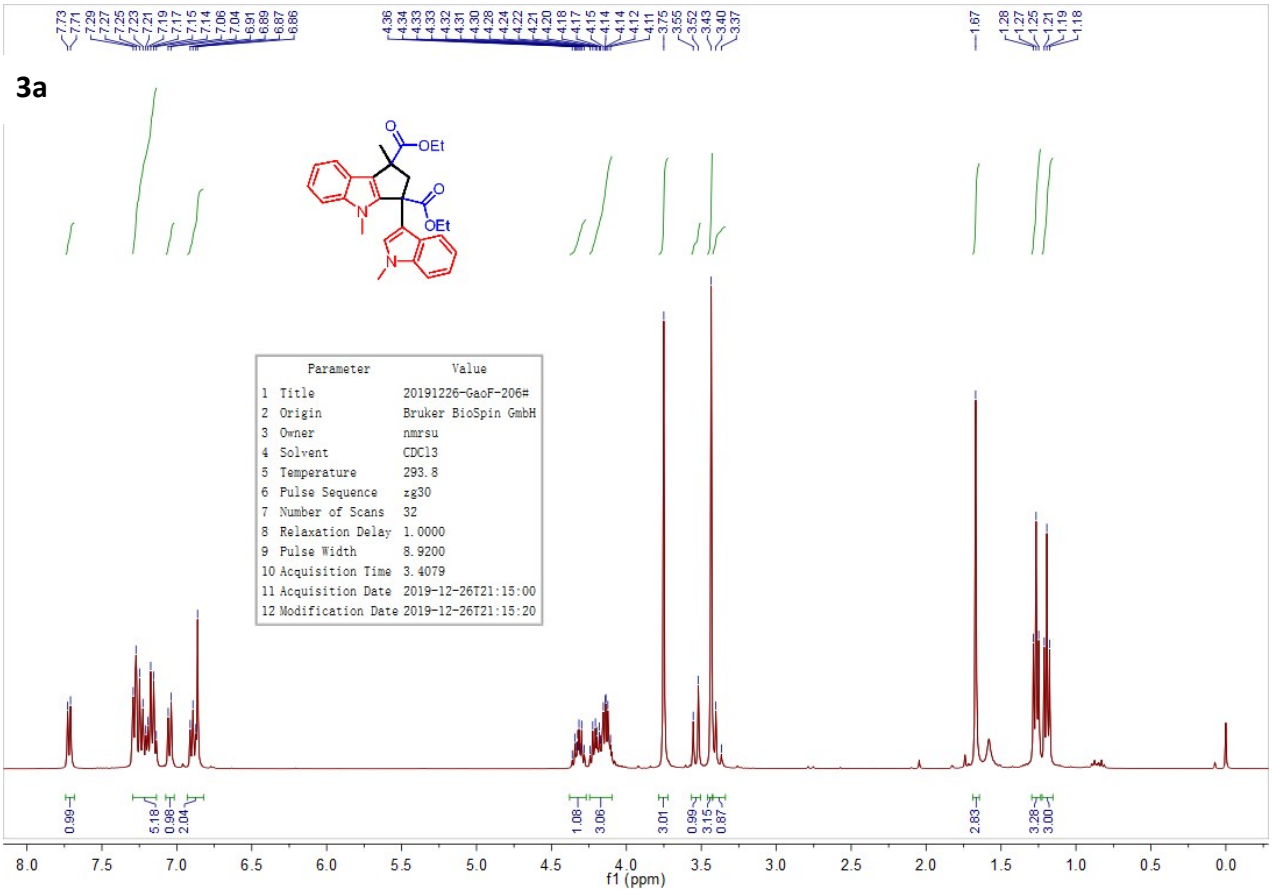
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7.71
7.29
7.27
7.25
7.23
7.21
7.19
7.17
7.15
7.14
7.06
7.04
6.91
6.89
6.87
6.86
4.36
4.34
4.33
4.32
4.31
4.30
4.28
4.24
4.22
4.21
4.20
4.18
4.17
4.15
4.14
4.12
4.11
3.75
3.55
3.52
3.43
3.40
3.37
1.67
1.28
1.27
1.25
1.21
1.19
1.18
OEt
OEt
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9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2019-12-26T21:15:00
12 Modification Date 2019-12-26T21:15:20
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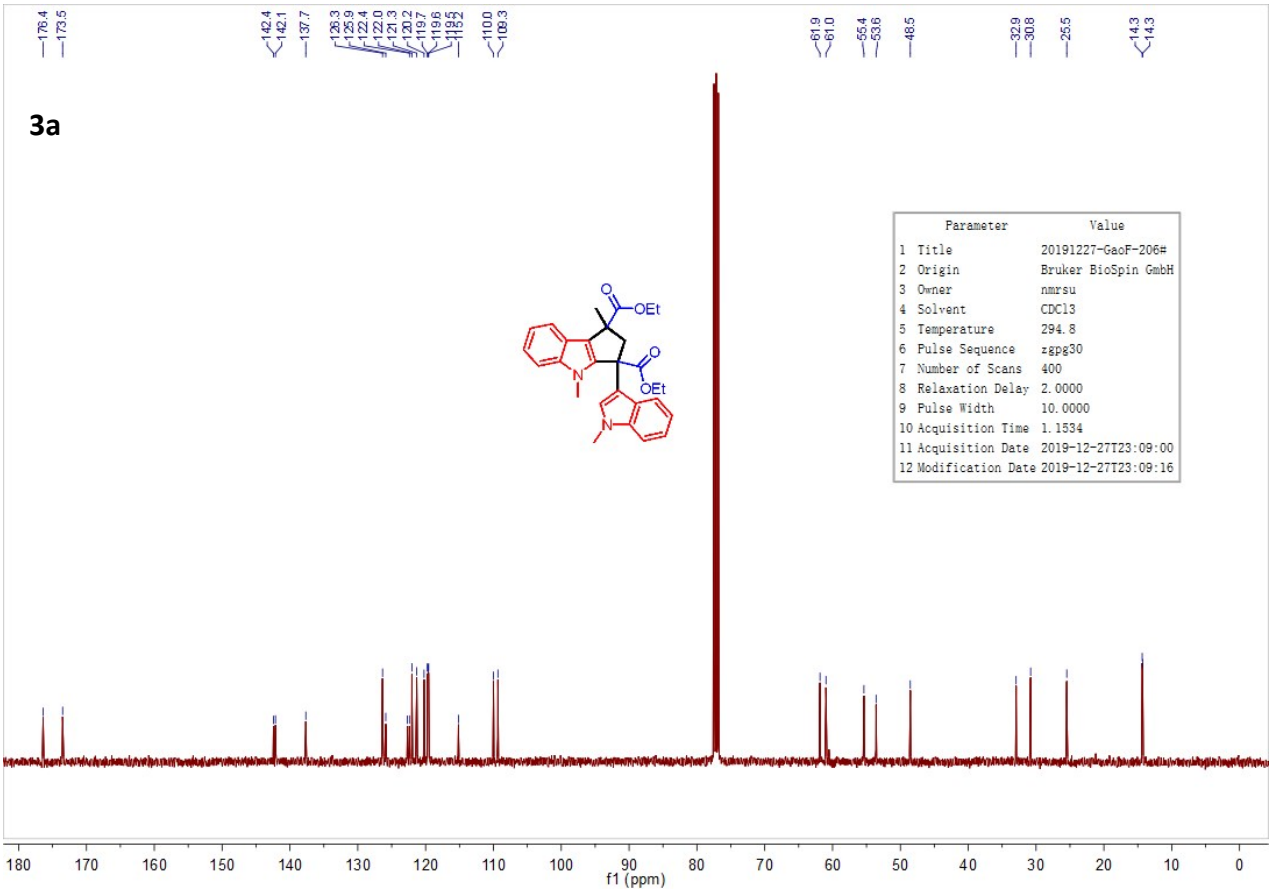
0.98
2.04
1.08
3.06
3.01
0.99
3.15
0.87
2.83
3.28
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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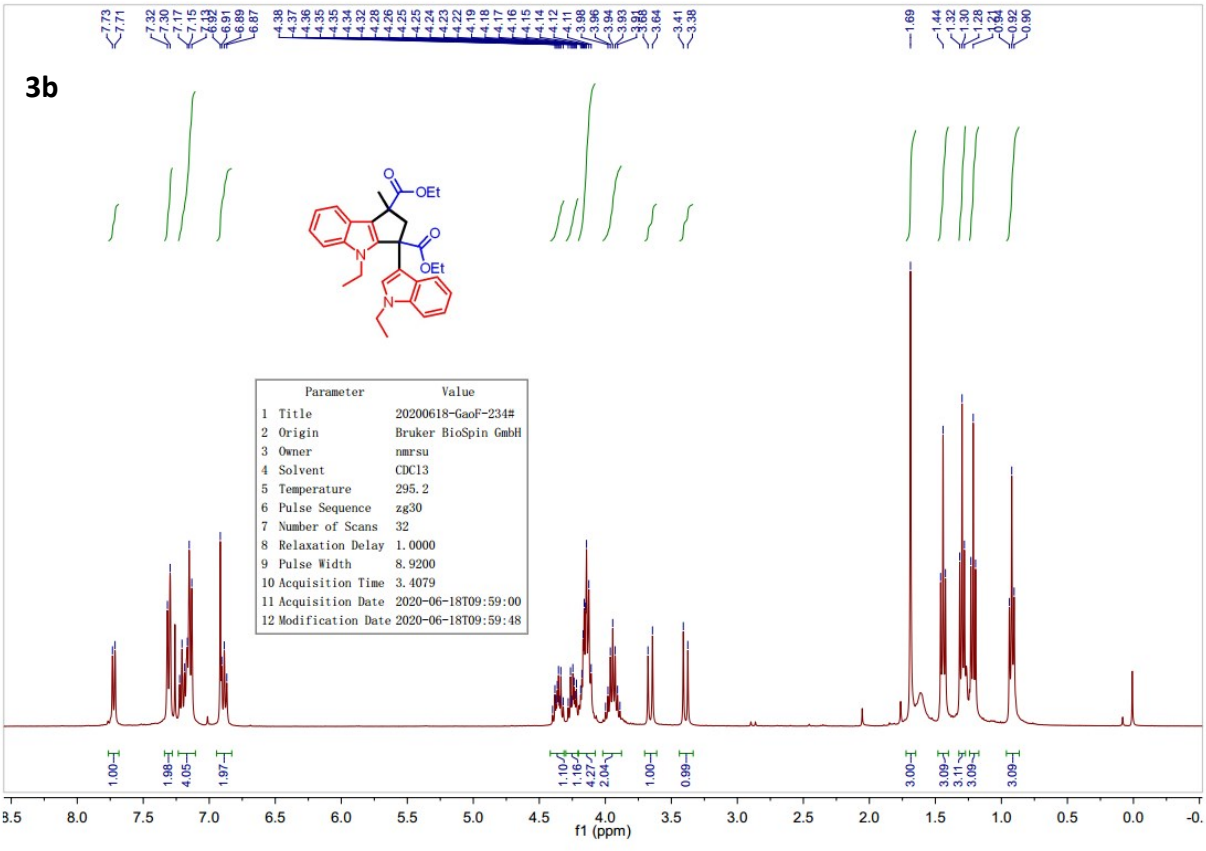
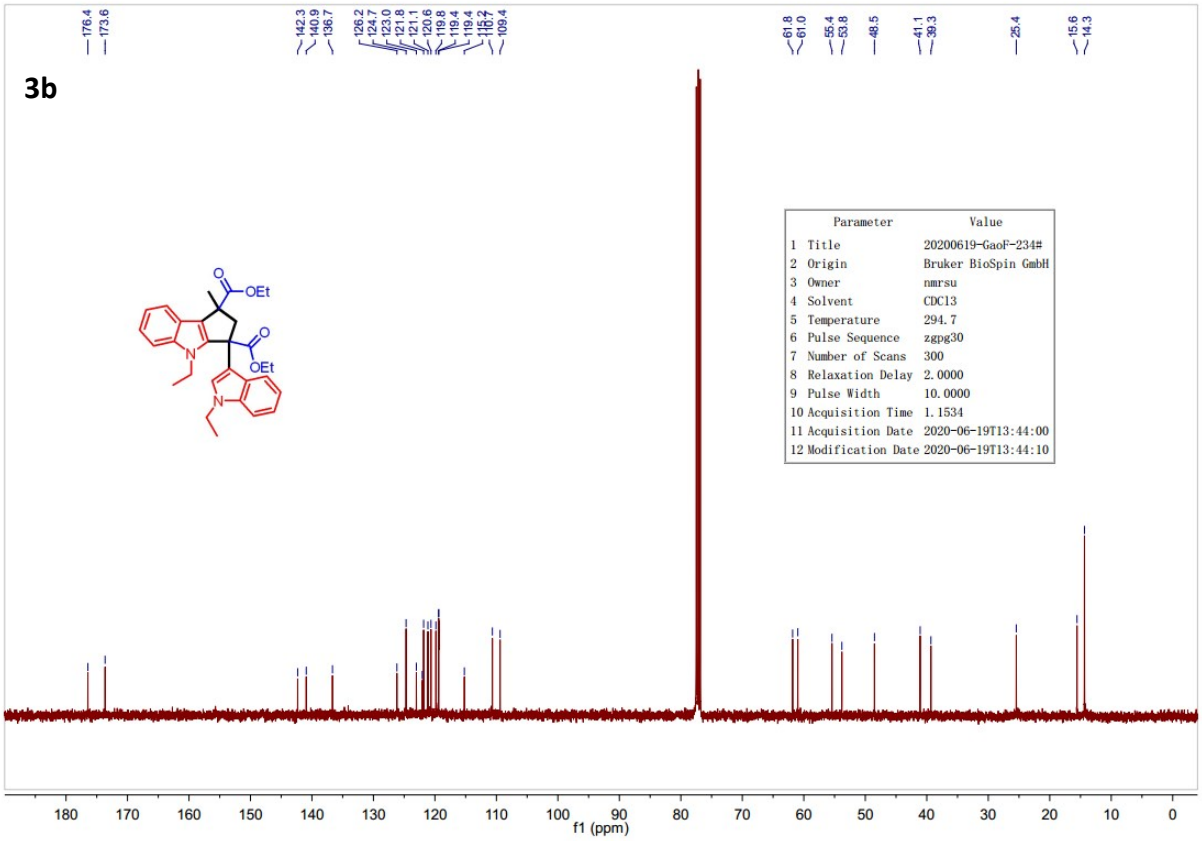
12 Modification Date 2019-12-27T23:09:16
f1 (ppm)


3b
Parameter Value
1 Title 20200618-GaoF-234#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 295.2
6 Pulse Sequence zg30
7 Number of Scans 32
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2020-06-18T09:59:00
12 Modification Date 2020-06-18T09:59:48
f1 (ppm)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142.3
140.9
136.7
126.2
124.7
123.0
121.8
121.1
120.6
119.8
119.4
119.4
109.4
61.8
61.0
55.4
53.8
48.5
41.1
39.3
25.4
15.6
14.3
OEt
OEt
Parameter Value
1 Title 20200619-GaoF-234#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 294.7
6 Pulse Sequence zgpg30
7 Number of Scans 300
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2020-06-19T13:44:00
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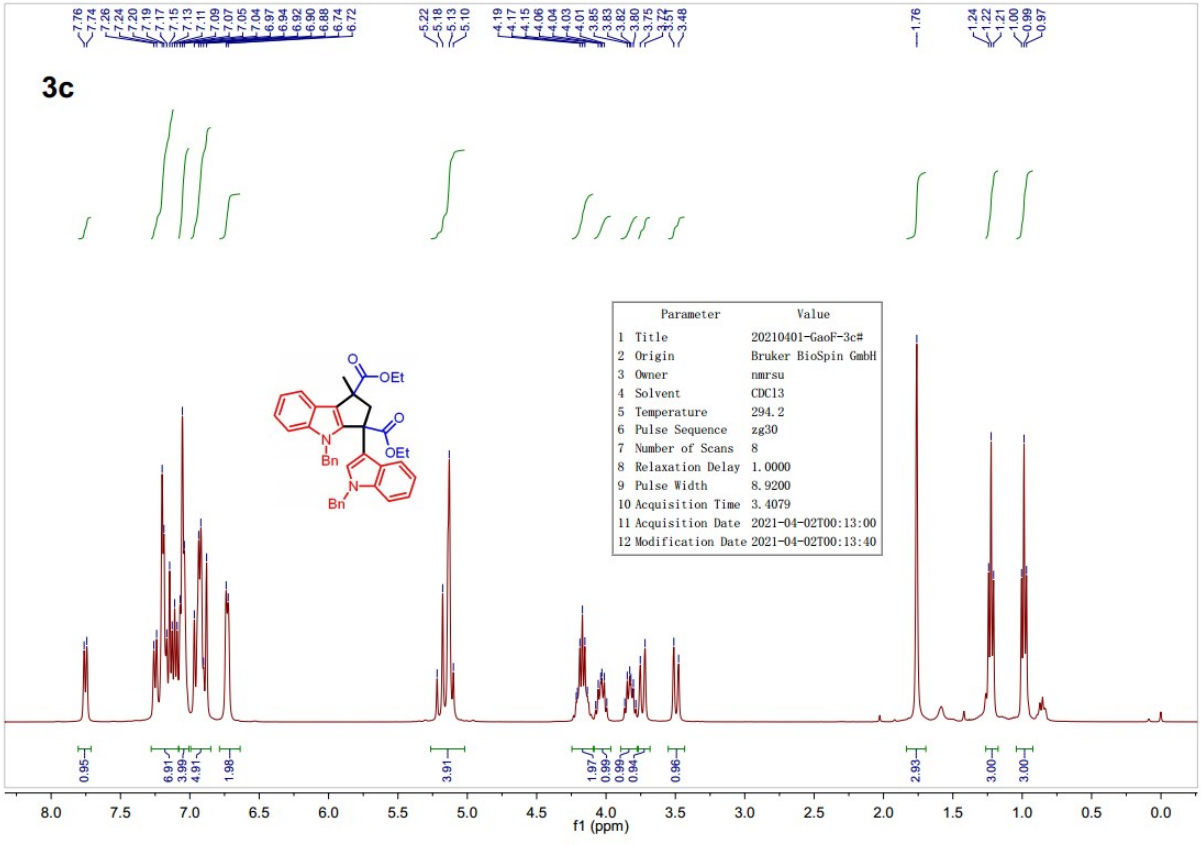
f1 (ppm)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7.20
7.19
7.17
7.15
7.13
7.11
7.09
7.07
7.05
7.04
6.97
6.94
6.92
6.90
6.88
6.74
6.72
5.22
5.18
5.13
5.10
4.19
4.17
4.15
4.06
4.04
4.03
4.01
3.85
3.83
3.82
3.80
3.75
3.57
3.48
1.76
1.24
1.22
1.21
1.00
0.99
0.97
OEt
OEt
Bn
Bn
Parameter Value
1 Title 20210401-GaoF-3c#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 294.2
6 Pulse Sequence zg30
7 Number of Scans 8
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2021-04-02T00:13:00
12 Modification Date 2021-04-02T00:13:40
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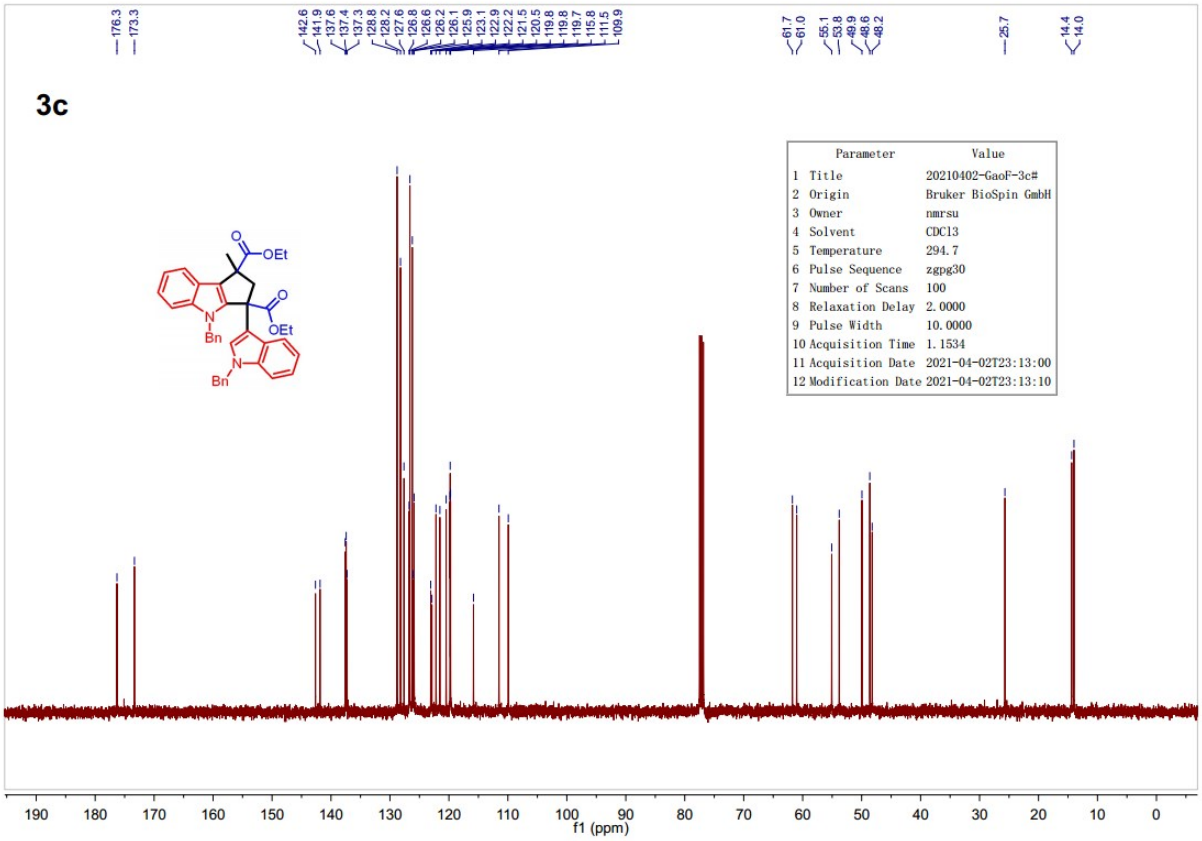
3.99
4.91
1.98
3.91
1.97
0.99
0.99
0.94
0.96
2.93
3.00
3.00
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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3 Owner nmrsu
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6 Pulse Sequence zgpg30
7 Number of Scans 100
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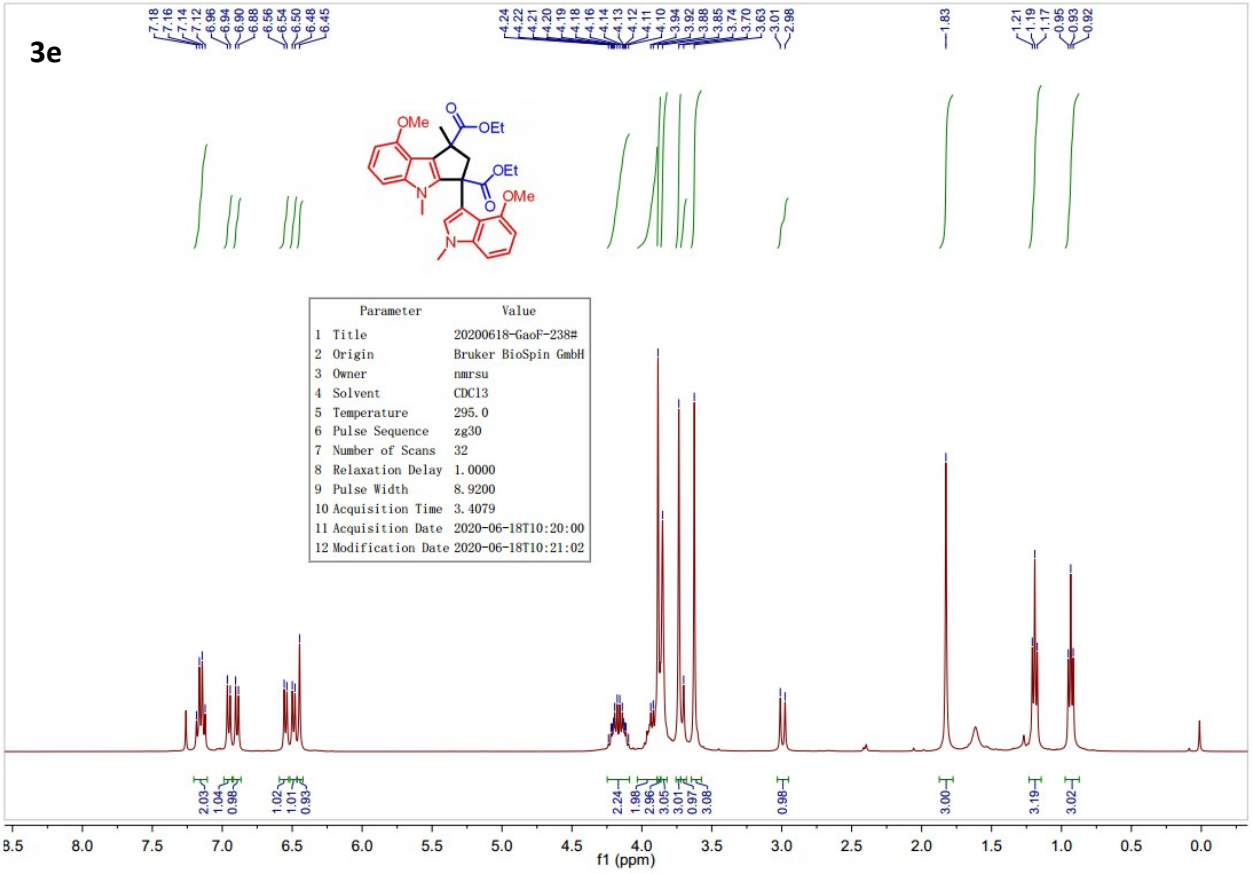
12 Modification Date 2021-04-02T23:13:10
f1 (ppm)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2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 295.0
6 Pulse Sequence zg30
7 Number of Scans 32
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
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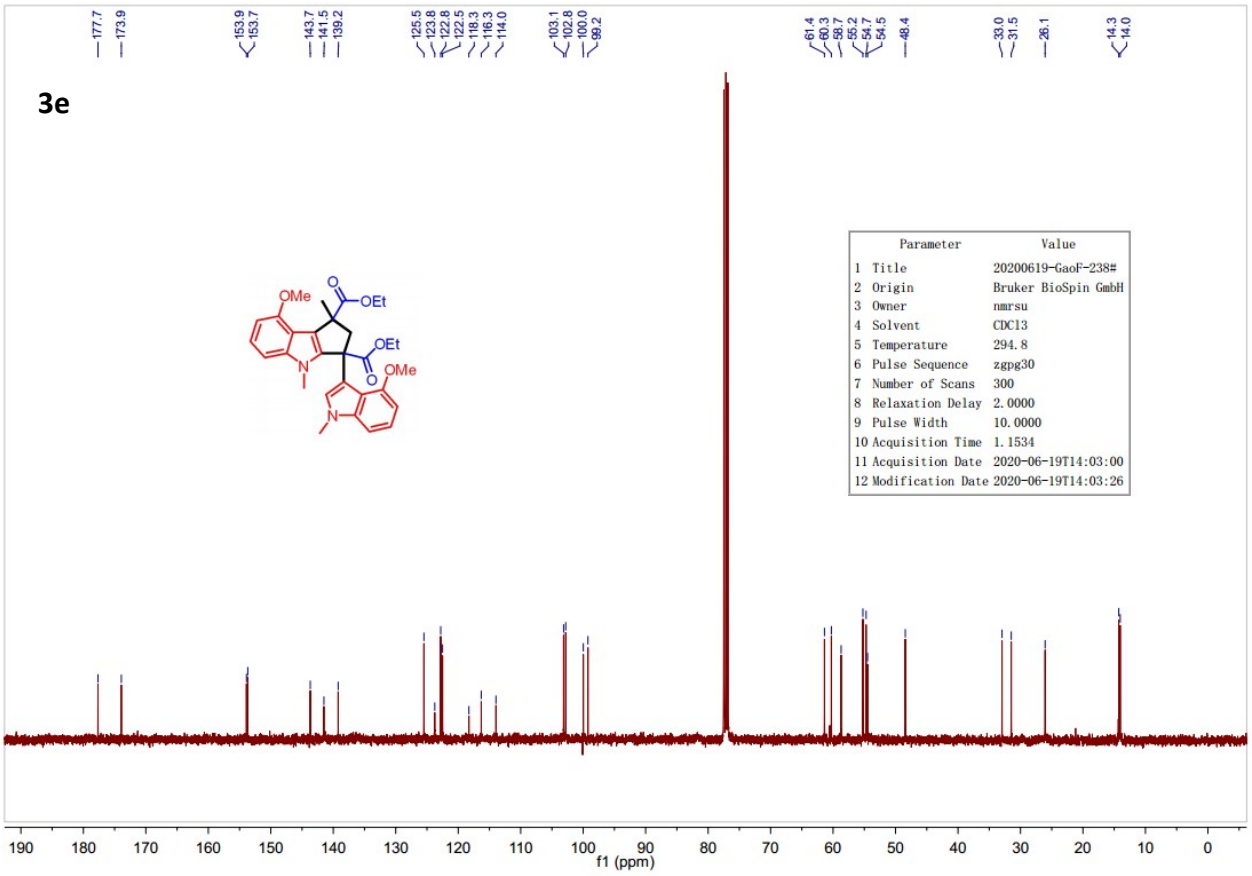
12 Modification Date 2020-06-18T10:21:02
f1 (ppm)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143.7
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123.8
122.8
122.5
118.3
116.3
114.0
103.1
102.8
100.0
99.2
61.4
60.3
58.7
55.2
54.7
54.5
48.4
33.0
31.5
26.1
14.3
14.0
OMe
OEt
OEt
OMe
Parameter Value
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3 Owner nmrsu
4 Solvent CDCl3
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6 Pulse Sequence zgpg30
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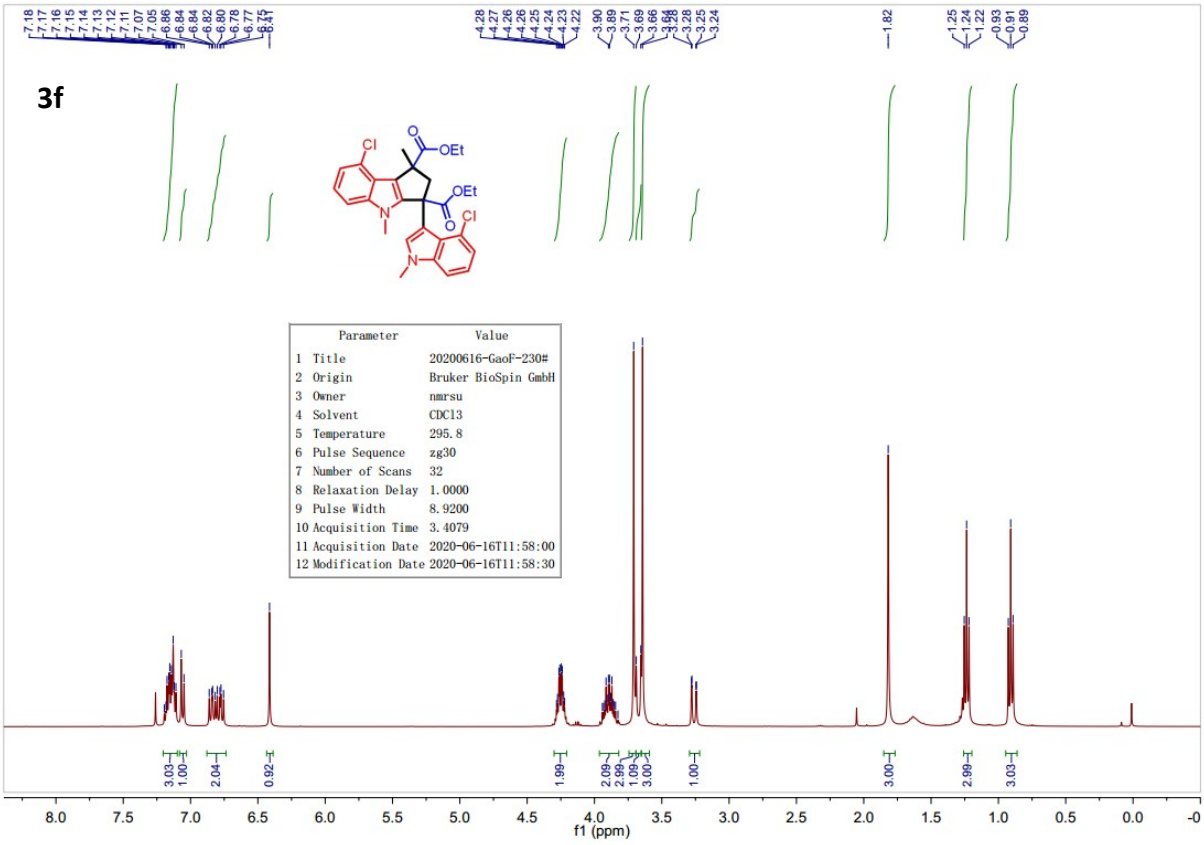
f1 (ppm)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6.82
6.80
6.78
6.77
6.75
6.41
4.28
4.27
4.26
4.25
4.24
4.23
4.22
3.90
3.89
3.71
3.69
3.66
3.28
3.25
3.24
1.82
1.25
1.24
1.22
0.93
0.91
0.89
Cl
OEt
OEt
Cl
Parameter Value
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2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
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5 Temperature 295.8
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10 Acquisition Time 3.4079
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1.09
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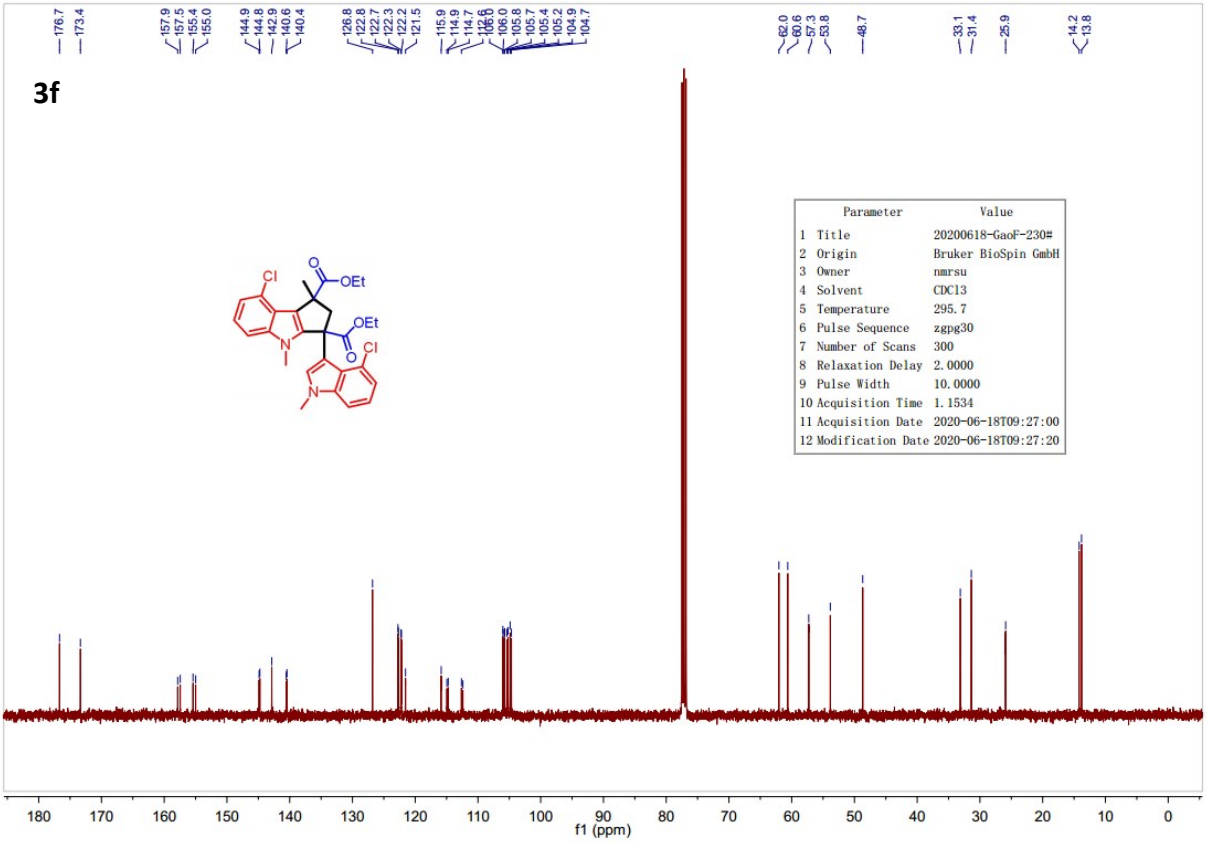
1.00
3.00
2.99
3.03
f1 (ppm)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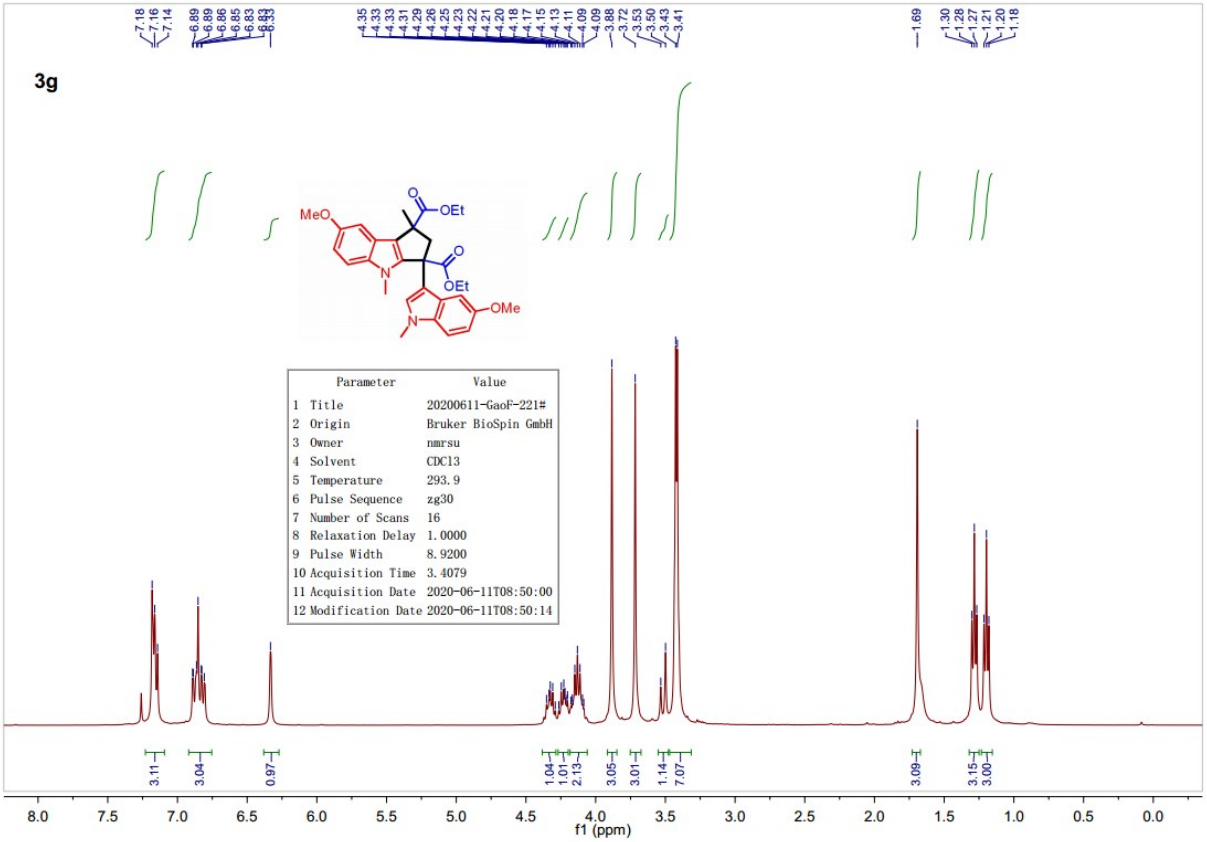
f1 (ppm)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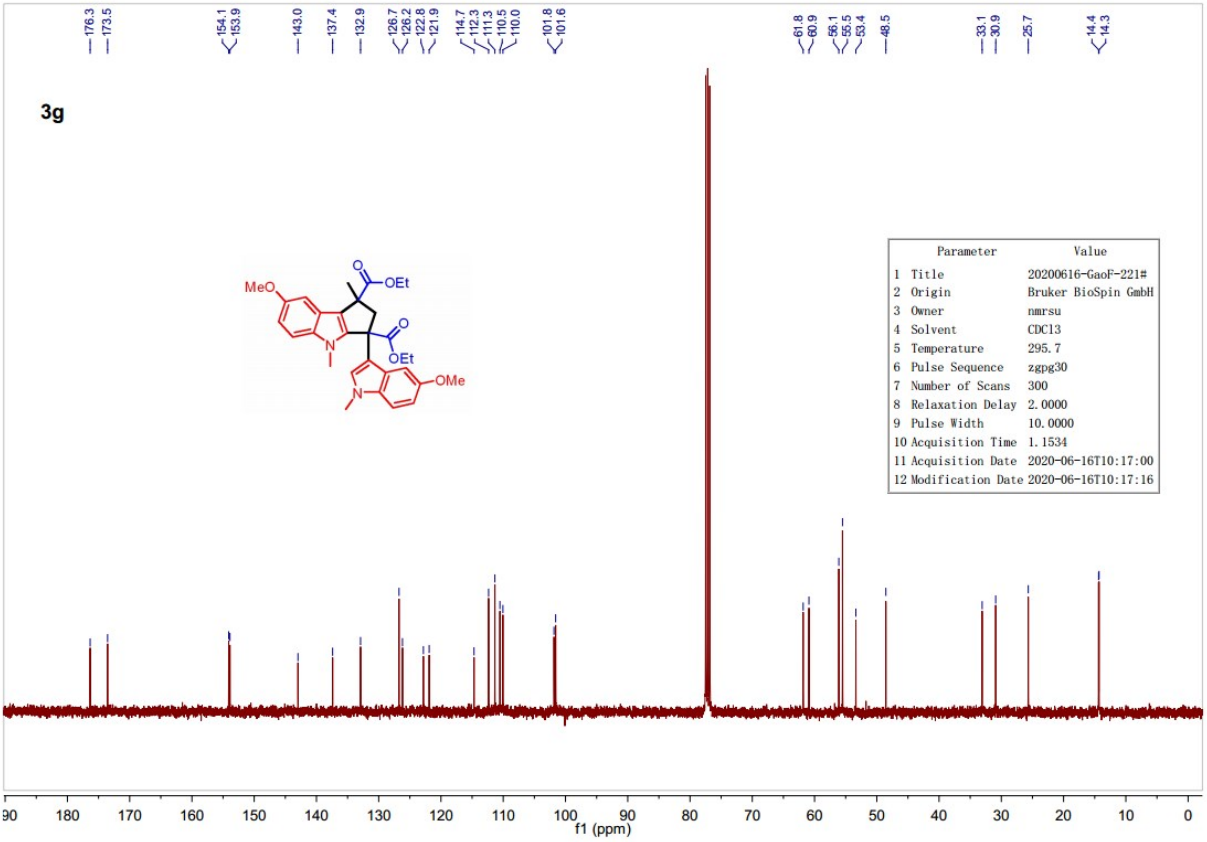
12 Modification Date 2020-06-11T08:50:14
f1 (ppm)


3g
MeO
OEt
OEt
OEt
OMe
Parameter Value
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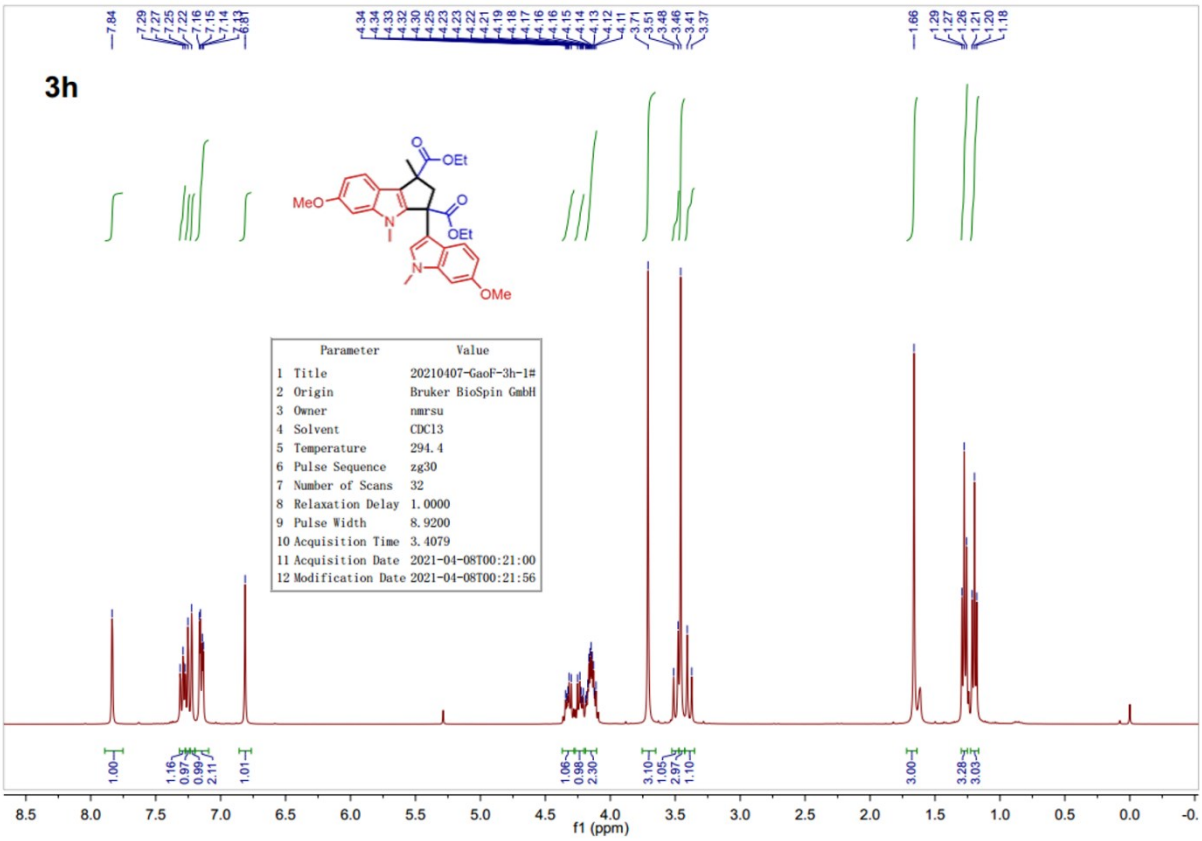
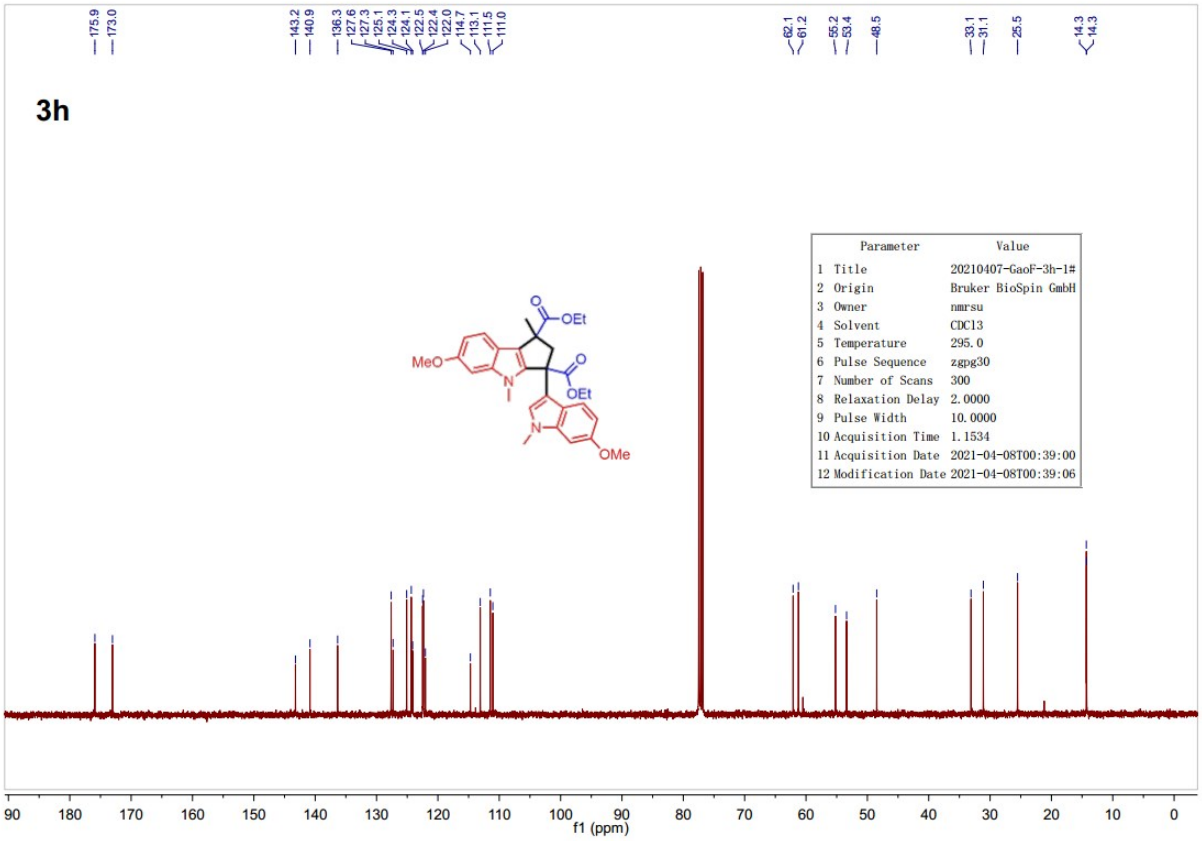
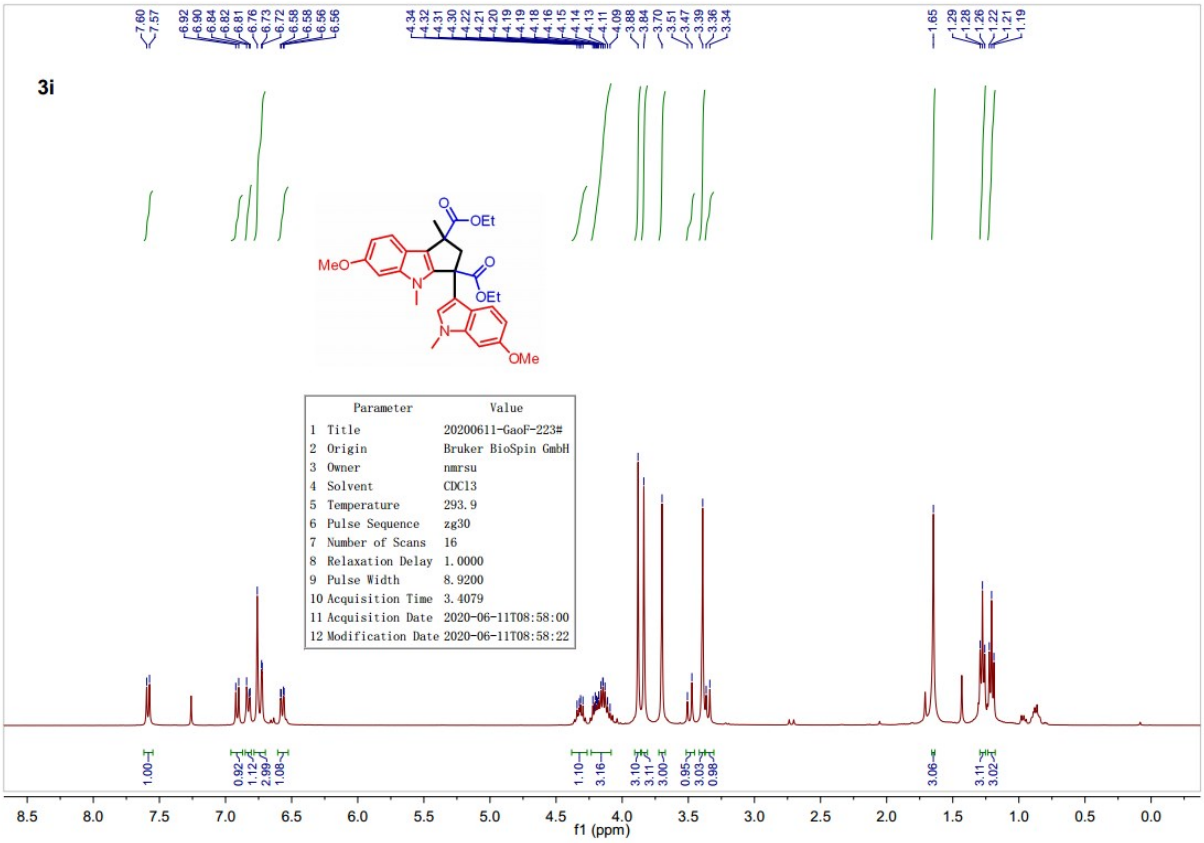
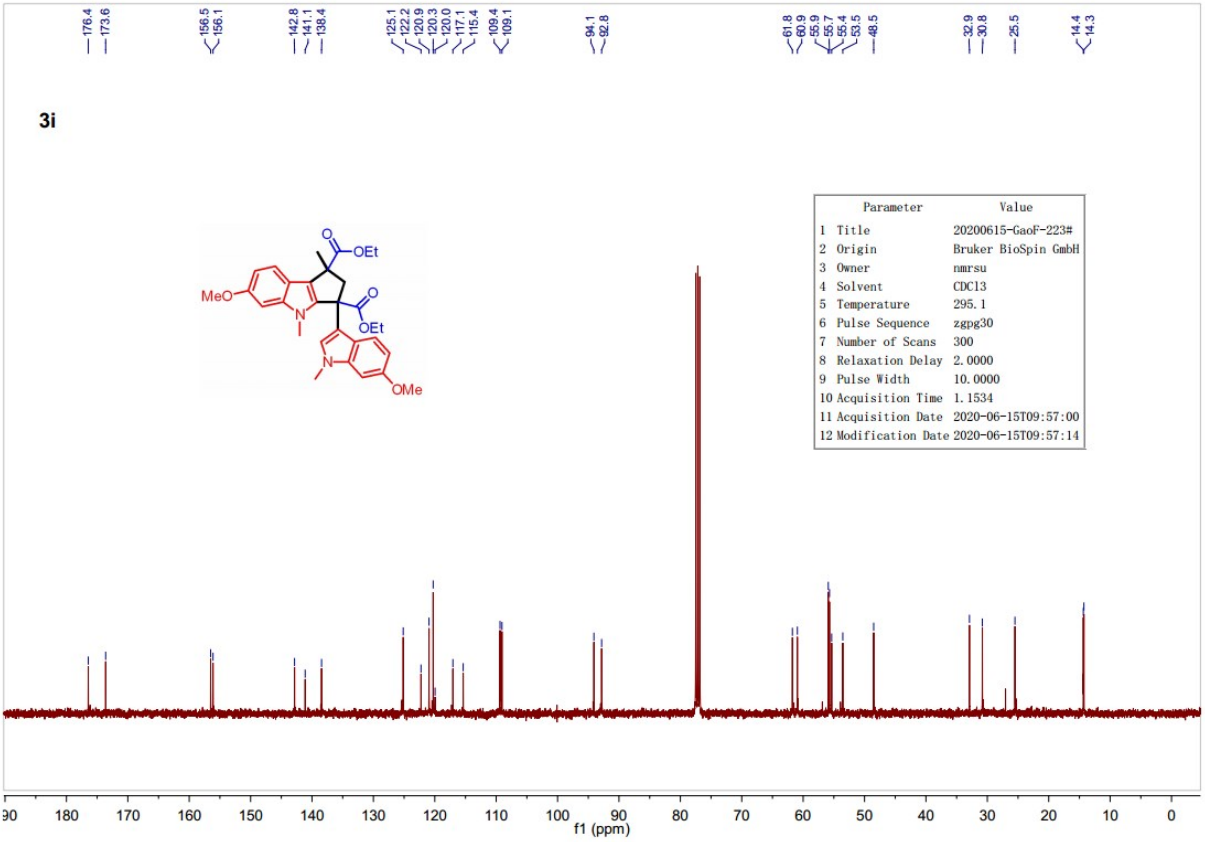
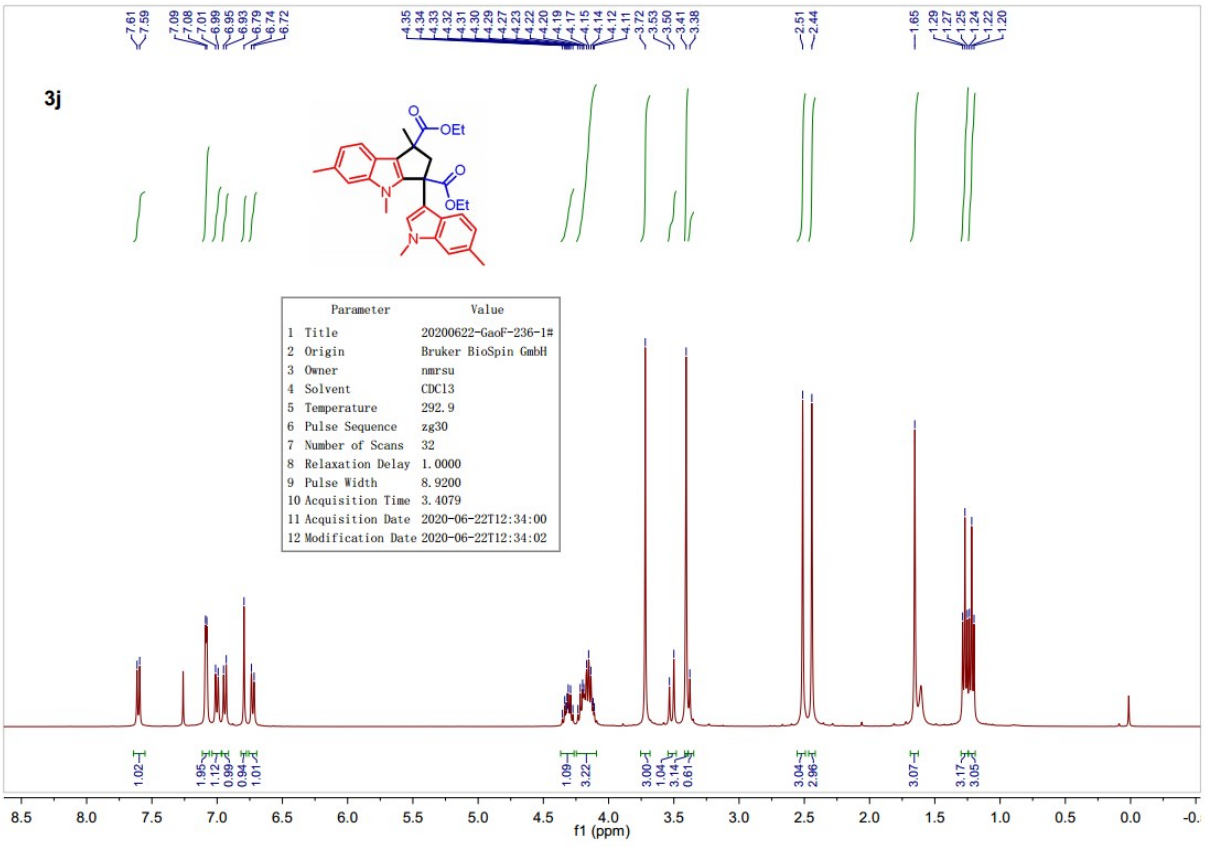
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2020-06-16T10:17:00
12 Modification Date 2020-06-16T10:17:16
f1 (ppm)

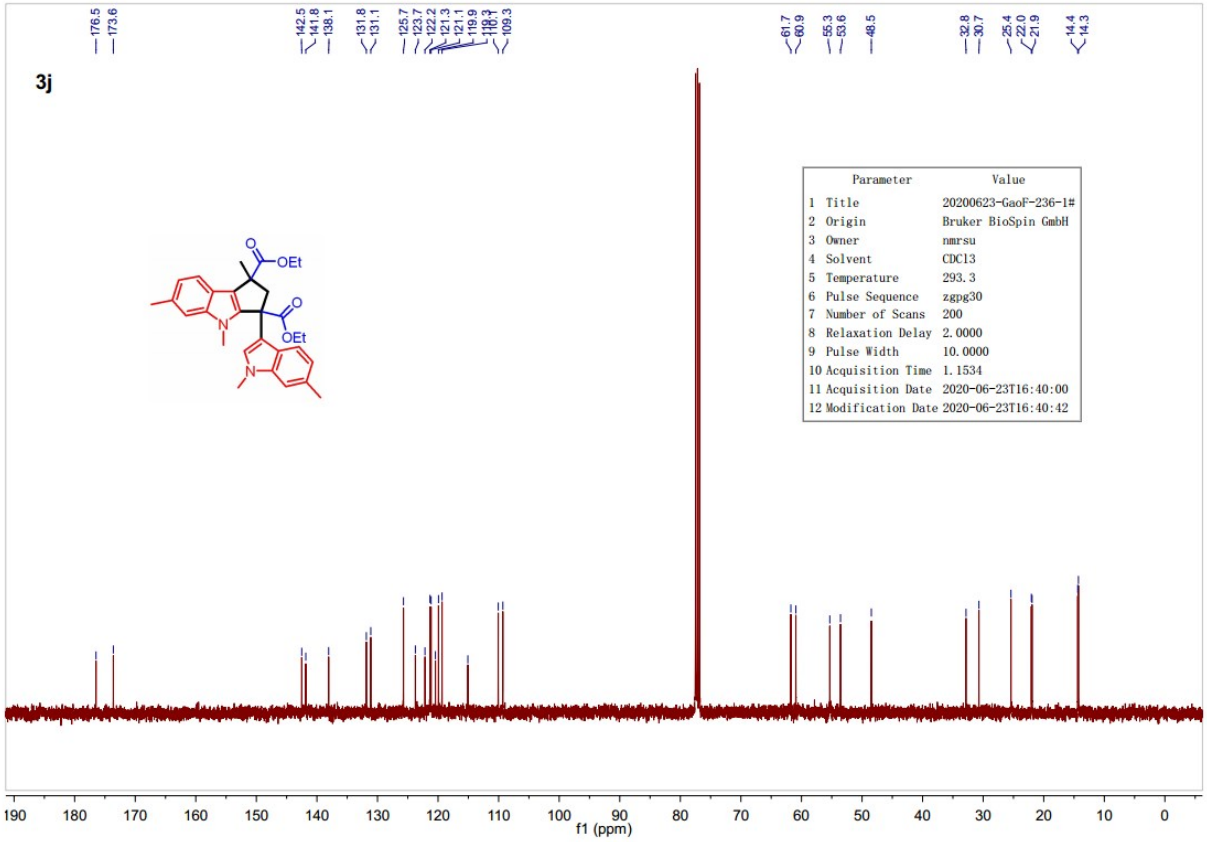

3h
MeO
OEt
OEt
OEt
OMe
Parameter Value
1 Title 20210407-GaoF-3h-1#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 294.4
6 Pulse Sequence zg30
7 Number of Scans 32
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2021-04-08T00:21:00
12 Modification Date 2021-04-08T00:21:56
f1 (ppm)

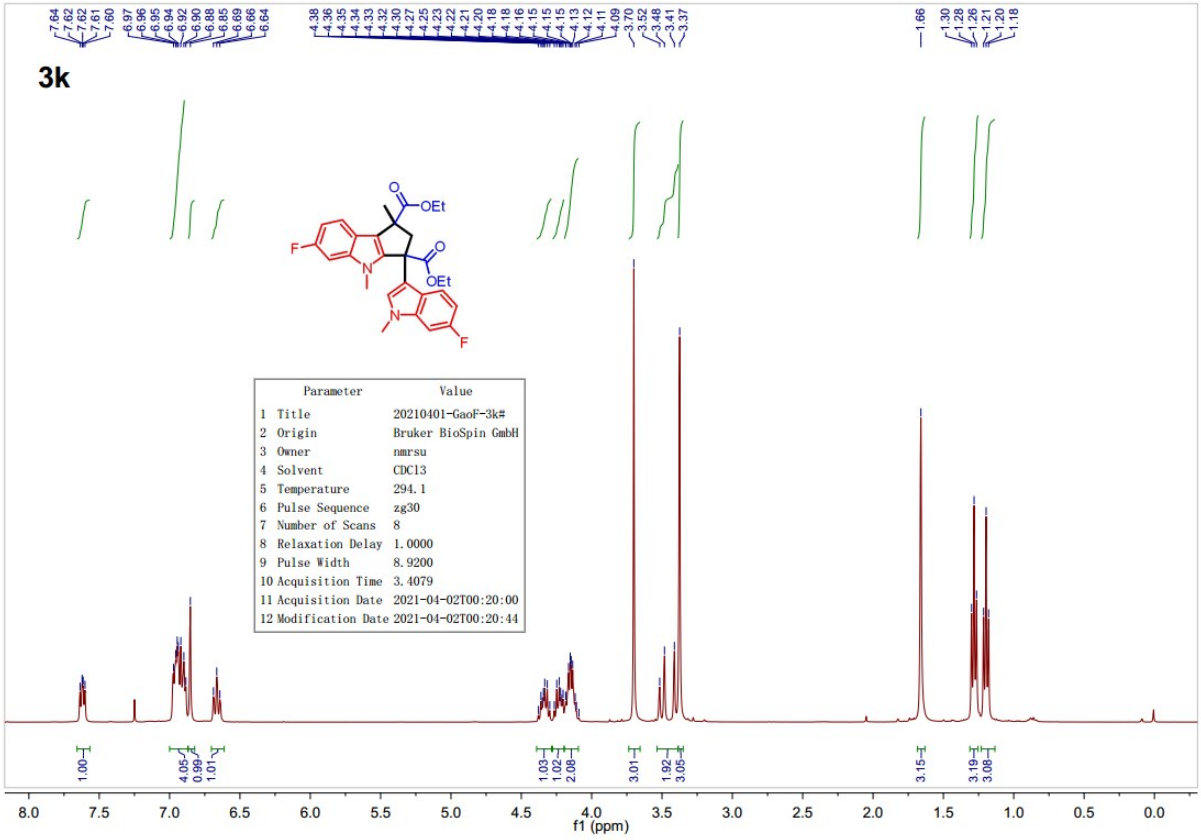

3h
175.9
173.0
143.2
140.9
136.3
127.6
127.3
125.1
124.3
124.1
122.5
122.4
122.0
114.7
113.1
111.5
111.0
62.1
61.2
55.2
53.4
48.5
33.1
31.1
25.5
14.3
14.3
Parameter Value
1 Title 20210407-GaoF-3h-1#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 295.0
6 Pulse Sequence zgpg30
7 Number of Scans 300
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2021-04-08T00:39:00
12 Modification Date 2021-04-08T00:39:06
MeO
OEt
OEt
OEt
OMe
f1 (ppm)

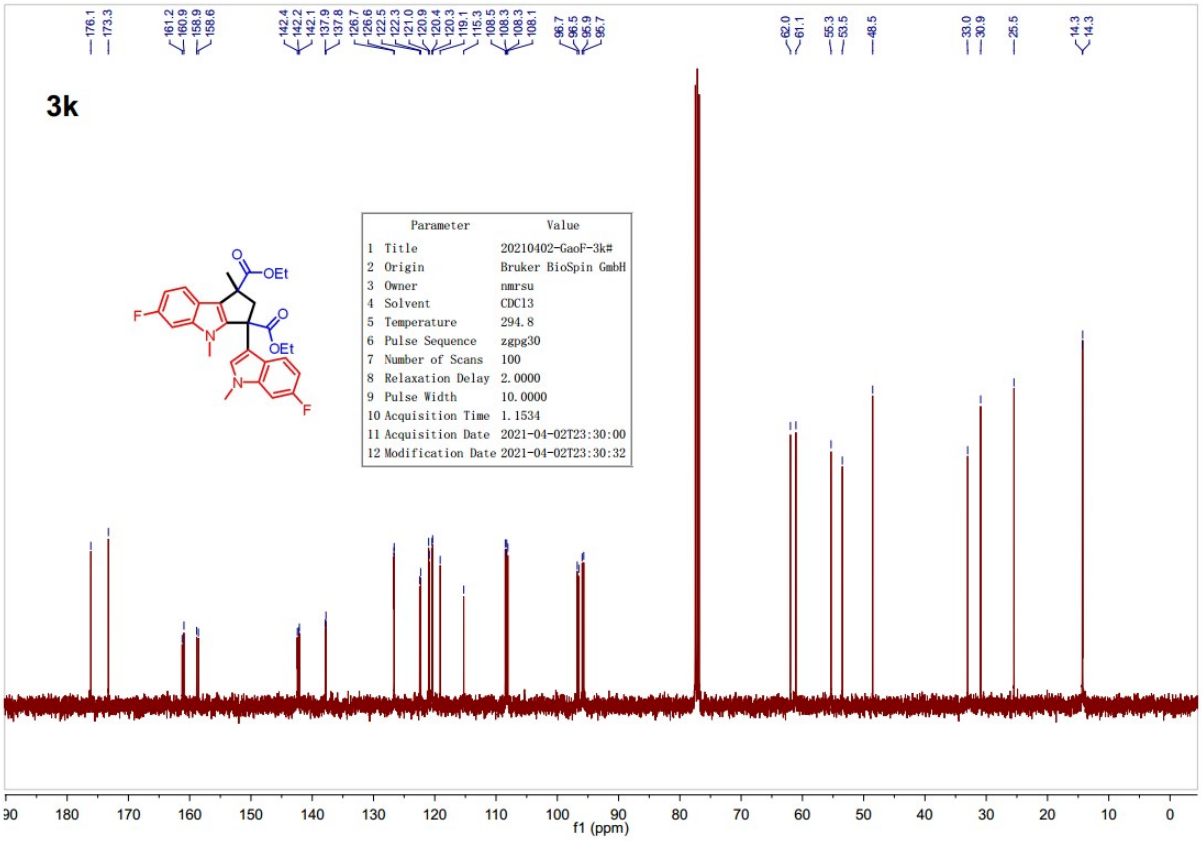

3i
7.60
7.57
6.92
6.90
6.84
6.82
6.81
6.76
6.73
6.72
6.58
6.58
6.56
6.56
4.34
4.32
4.31
4.30
4.22
4.21
4.20
4.19
4.19
4.18
4.16
4.15
4.14
4.13
4.11
4.09
3.88
3.84
3.70
3.51
3.47
3.39
3.36
3.34
1.65
1.29
1.28
1.26
1.22
1.21
1.19
Parameter Value
1 Title 20200611-GaoF-223#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 293.9
6 Pulse Sequence zg30
7 Number of Scans 16
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2020-06-11T08:58:00
12 Modification Date 2020-06-11T08:58:22
MeO
OEt
OEt
OEt
OMe
1.00
0.92
1.12
2.99
1.08
1.10
3.16
3.10
3.11
3.00
0.95
3.03
0.98
3.06
3.11
3.02
f1 (ppm)

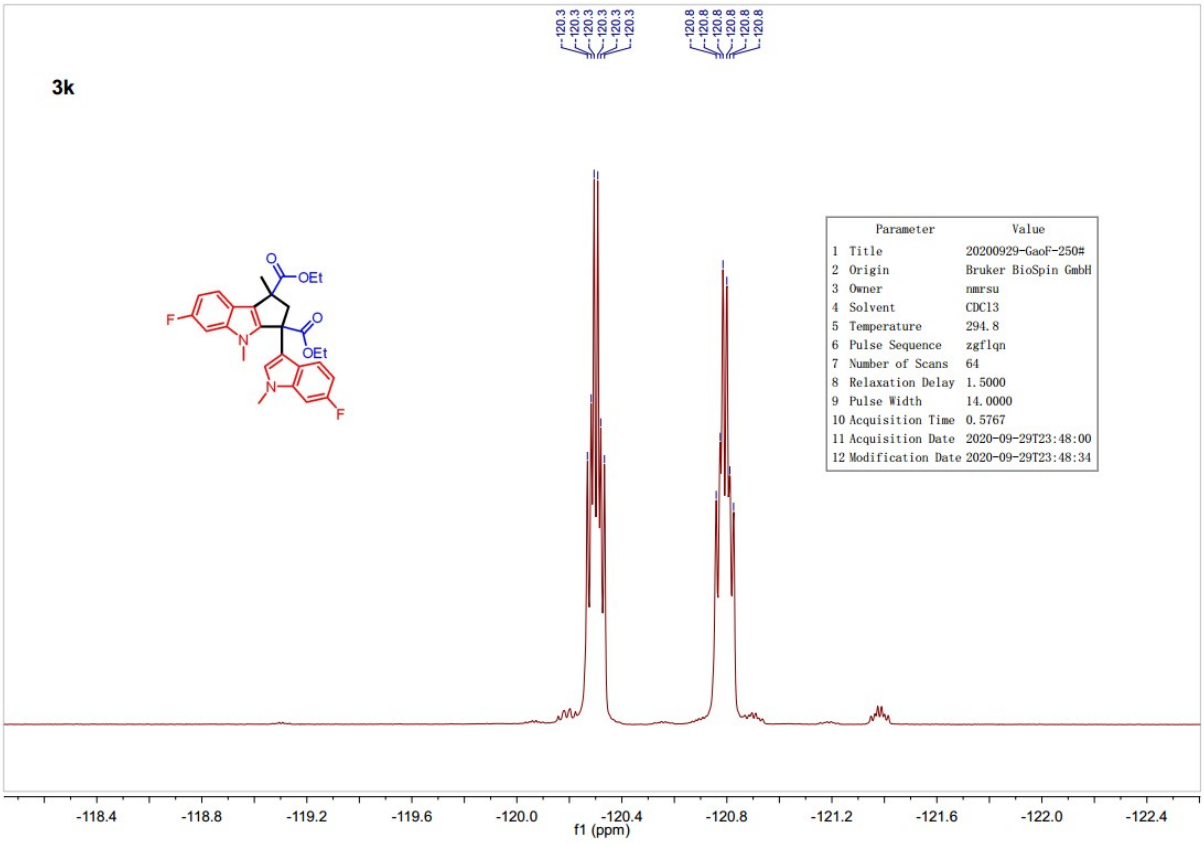

3i
176.4
173.6
156.5
156.1
142.8
141.1
138.4
125.1
122.2
120.9
120.3
120.0
117.1
115.4
109.4
109.1
94.1
92.8
61.8
60.9
55.9
55.7
55.4
53.5
48.5
32.9
30.8
25.5
14.4
14.3
OEt
MeO
OEt
OMe
Parameter Value
1 Title 20200615-GaoF-223#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 295.1
6 Pulse Sequence zgpg30
7 Number of Scans 300
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2020-06-15T09:57:00
12 Modification Date 2020-06-15T09:57:14
f1 (ppm)

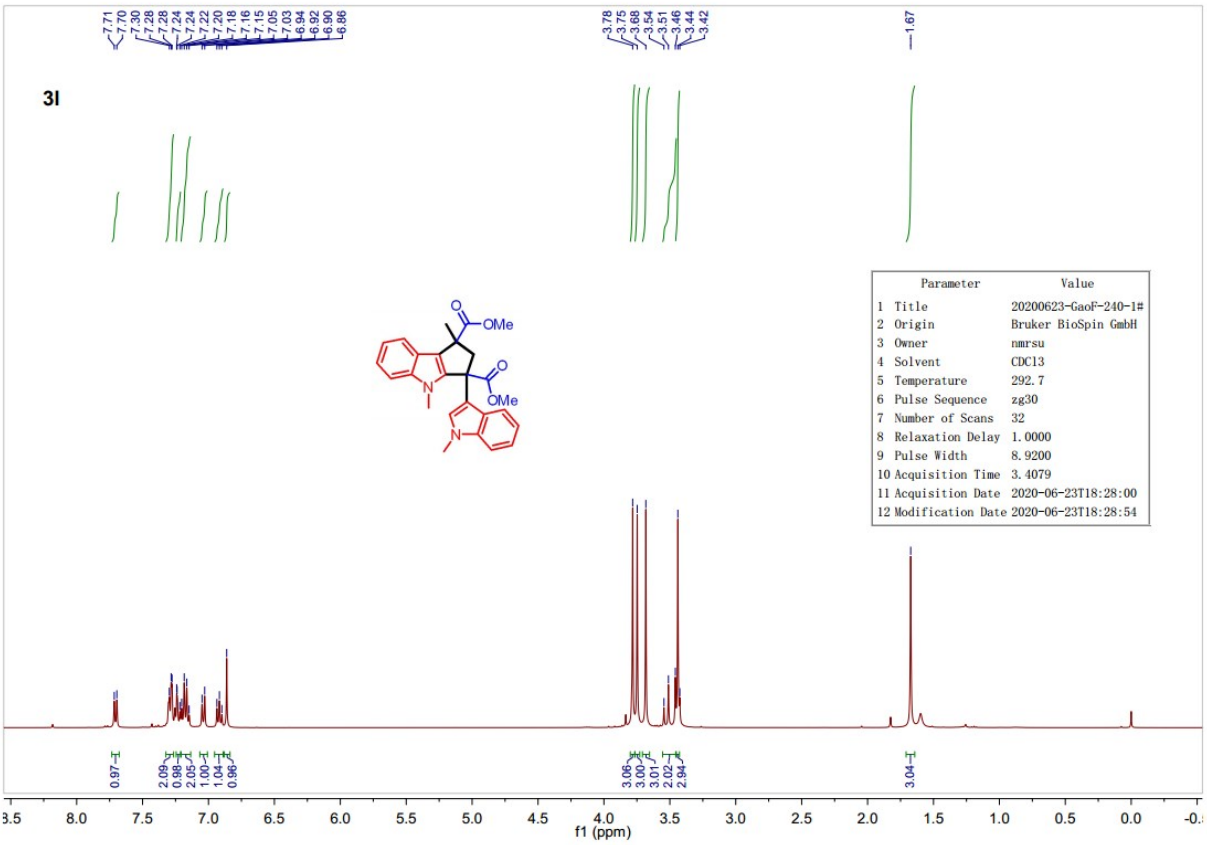

3j
7.61
7.59
7.09
7.08
7.01
6.99
6.95
6.93
6.79
6.74
6.72
4.35
4.34
4.33
4.32
4.31
4.30
4.29
4.27
4.23
4.22
4.20
4.19
4.17
4.15
4.14
4.12
4.11
3.72
3.53
3.50
3.41
3.38
2.51
2.44
1.65
1.29
1.27
1.25
1.24
1.22
1.20
OEt
OEt
Parameter Value
1 Title 20200622-GaoF-236-1#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 292.9
6 Pulse Sequence zg30
7 Number of Scans 32
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2020-06-22T12:34:00
12 Modification Date 2020-06-22T12:34:02
1.02
1.95
1.12
0.99
0.94
1.01
1.09
3.22
3.00
1.04
3.14
0.61
3.04
2.96
3.07
3.17
3.05
f1 (ppm)

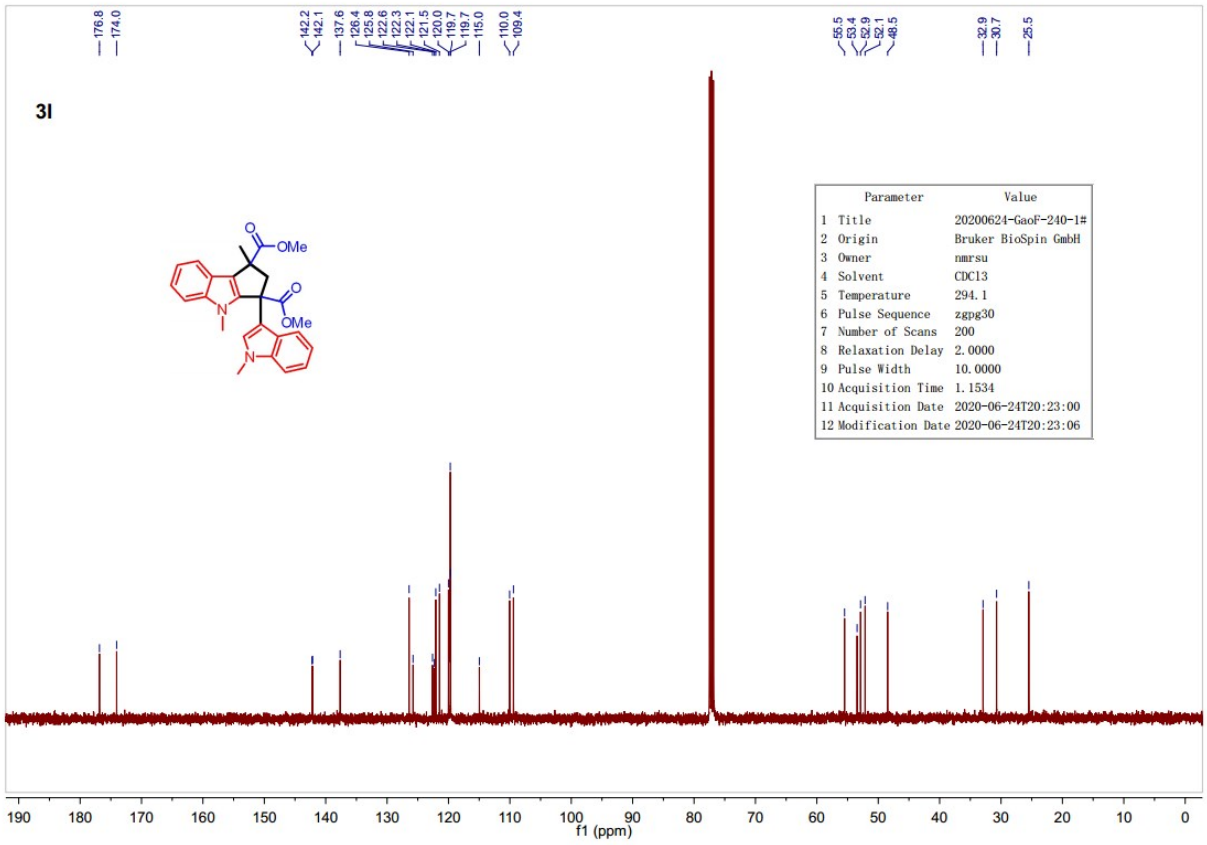

3j
176.5
173.6
142.5
141.8
138.1
131.8
131.1
125.7
123.7
122.2
121.3
121.1
119.9
118.3
118.2
109.3
61.7
60.9
55.3
53.6
48.5
32.8
30.7
25.4
22.0
21.9
14.4
14.3
OEt
OEt
Parameter Value
1 Title 20200623-GaoF-236-1#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 293.3
6 Pulse Sequence zgpg30
7 Number of Scans 200
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2020-06-23T16:40:00
12 Modification Date 2020-06-23T16:40:42
f1 (ppm)

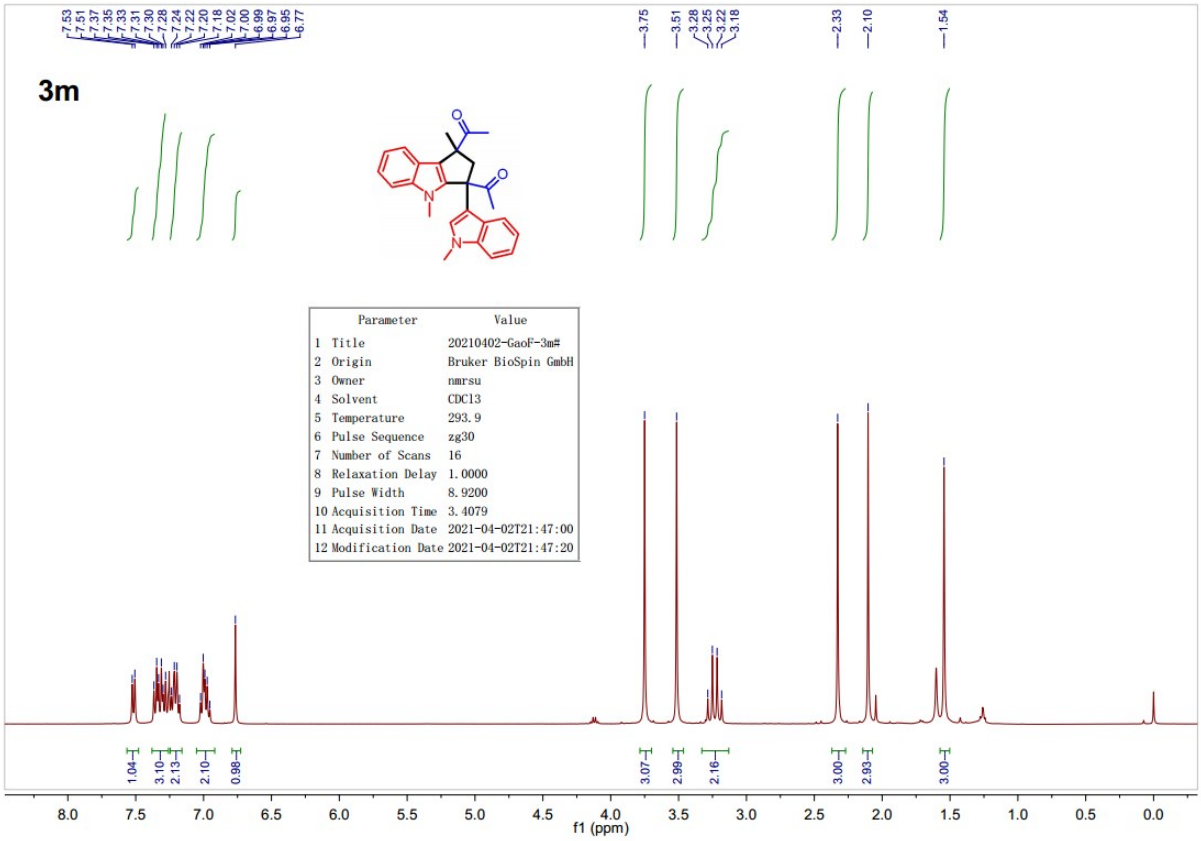

3k
7.64
7.62
7.62
7.61
7.60
6.97
6.96
6.95
6.94
6.92
6.90
6.88
6.85
6.69
6.66
6.64
4.38
4.36
4.35
4.34
4.33
4.32
4.30
4.27
4.25
4.23
4.22
4.21
4.20
4.18
4.18
4.16
4.15
4.15
4.13
4.12
4.11
4.09
3.70
3.52
3.48
3.41
3.37
1.66
1.30
1.28
1.26
1.21
1.20
1.18
OEt
OEt
F
F
Parameter Value
1 Title 20210401-GaoF-3k#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 294.1
6 Pulse Sequence zg30
7 Number of Scans 8
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2021-04-02T00:20:00
12 Modification Date 2021-04-02T00:20:44
1.00
4.05
0.99
1.01
1.03
1.02
2.08
3.01
1.92
3.05
3.15
3.19
3.08
f1 (ppm)

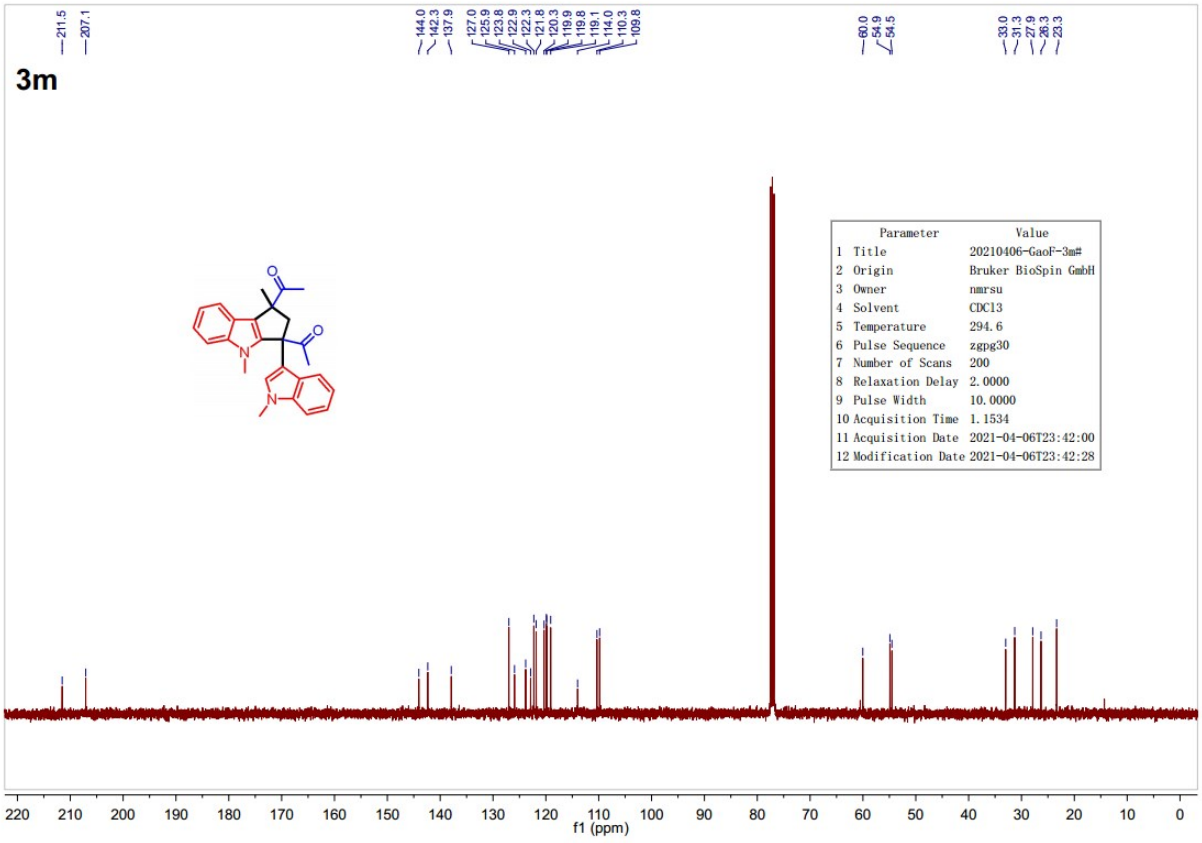

3k
176.1
173.3
161.2
160.9
158.9
158.6
142.4
142.2
142.1
137.9
137.8
126.7
126.6
122.5
122.3
121.0
120.9
120.4
120.3
119.1
115.3
108.5
108.3
108.3
108.1
96.7
96.5
95.9
95.7
62.0
61.1
55.3
53.5
48.5
33.0
30.9
25.5
14.3
14.3
Parameter Value
1 Title 20210402-GaoF-3k#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 294.8
6 Pulse Sequence zgpg30
7 Number of Scans 100
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2021-04-02T23:30:00
12 Modification Date 2021-04-02T23:30:32
OEt
OEt
F
F
N
O
O
f1 (ppm)

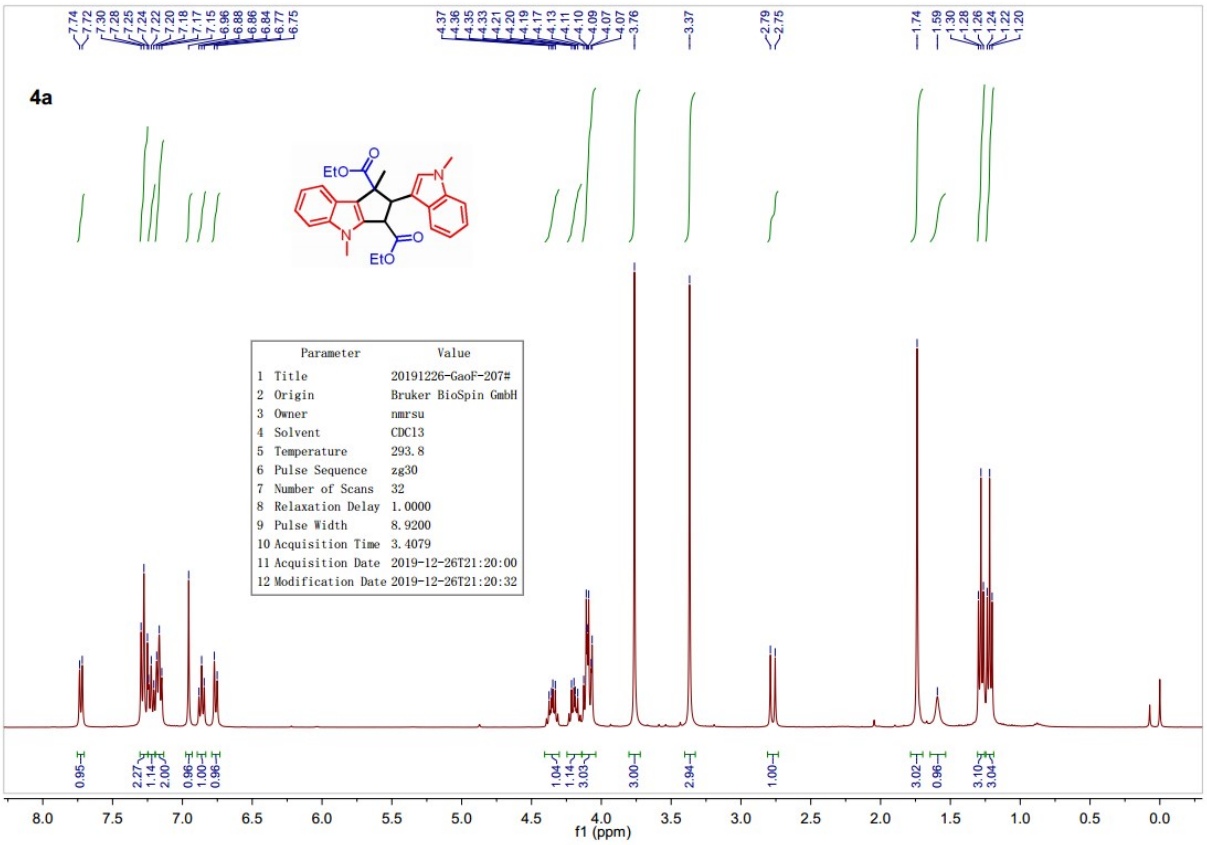

3k
120.3
120.3
120.3
120.3
120.3
120.3
120.8
120.8
120.8
120.8
120.8
120.8
Parameter Value
1 Title 20200929-GaoF-250#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 294.8
6 Pulse Sequence zgflqn
7 Number of Scans 64
8 Relaxation Delay 1.5000
9 Pulse Width 14.0000
10 Acquisition Time 0.5767
11 Acquisition Date 2020-09-29T23:48:00
12 Modification Date 2020-09-29T23:48:34
OEt
OEt
F
F
N
O
O
f1 (ppm)

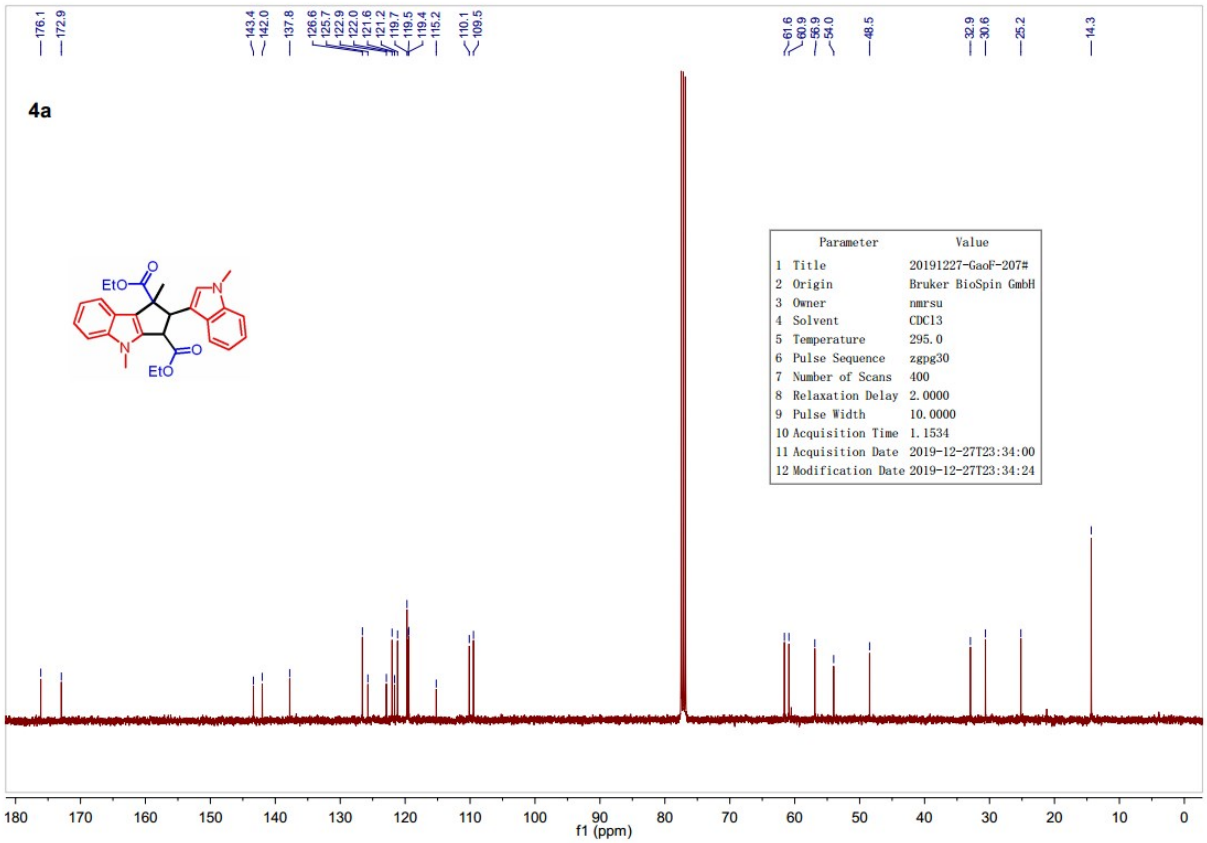

3l
7.71
7.70
7.30
7.28
7.28
7.24
7.24
7.22
7.20
7.18
7.16
7.15
7.05
7.03
6.94
6.92
6.90
6.86
3.78
3.75
3.68
3.54
3.51
3.46
3.44
3.42
1.67
OMe
OMe
Parameter Value
1 Title 20200623-GaoF-240-1#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 292.7
6 Pulse Sequence zg30
7 Number of Scans 32
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2020-06-23T18:28:00
12 Modification Date 2020-06-23T18:28:54
0.97
2.09
0.98
2.05
1.00
1.04
0.96
3.06
3.00
3.01
2.02
2.94
3.04
f1 (ppm)

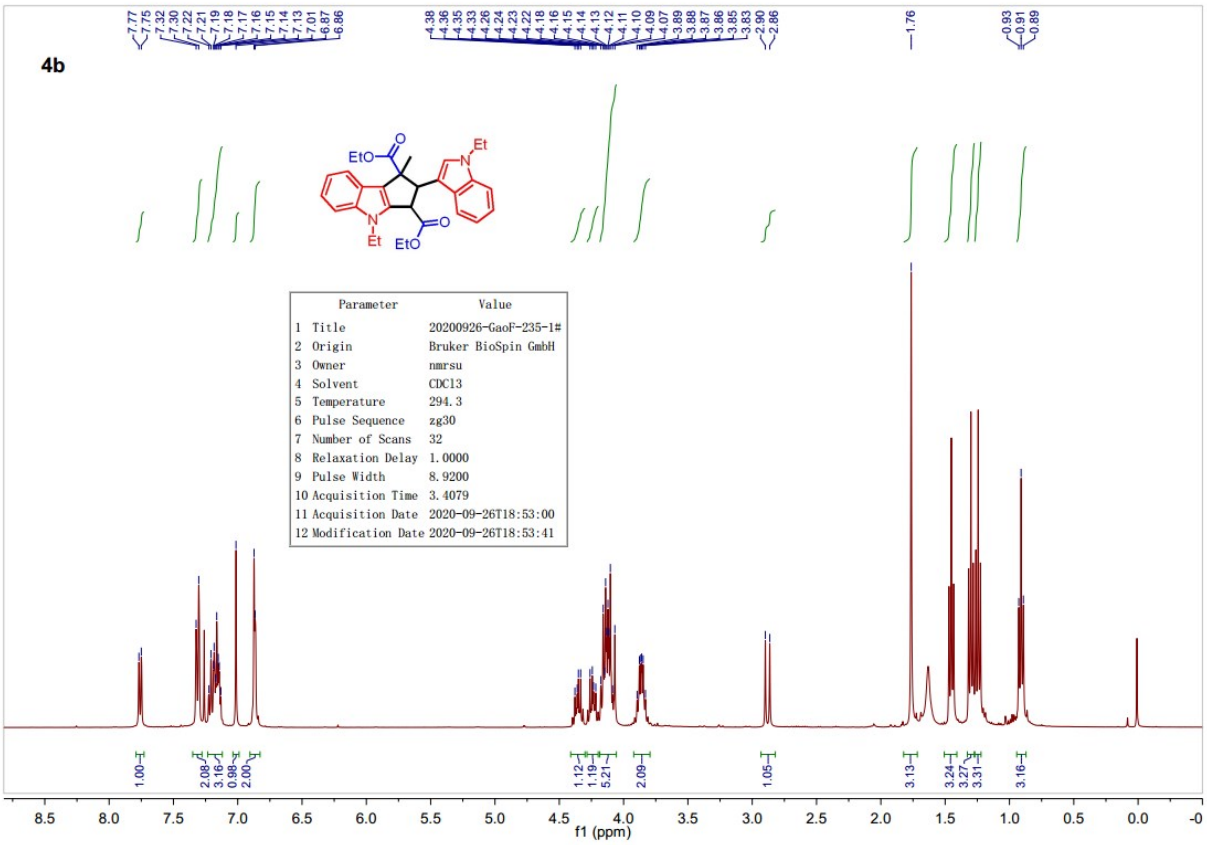

3l
176.8
174.0
142.2
142.1
137.6
126.4
125.8
122.6
122.3
122.1
121.5
120.0
119.7
119.7
115.0
110.0
109.4
55.5
53.4
52.9
52.1
48.5
32.9
30.7
25.5
OMe
OMe
Parameter Value
1 Title 20200624-GaoF-240-1#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 294.1
6 Pulse Sequence zgpg30
7 Number of Scans 200
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2020-06-24T20:23:00
12 Modification Date 2020-06-24T20:23:06
f1 (ppm)

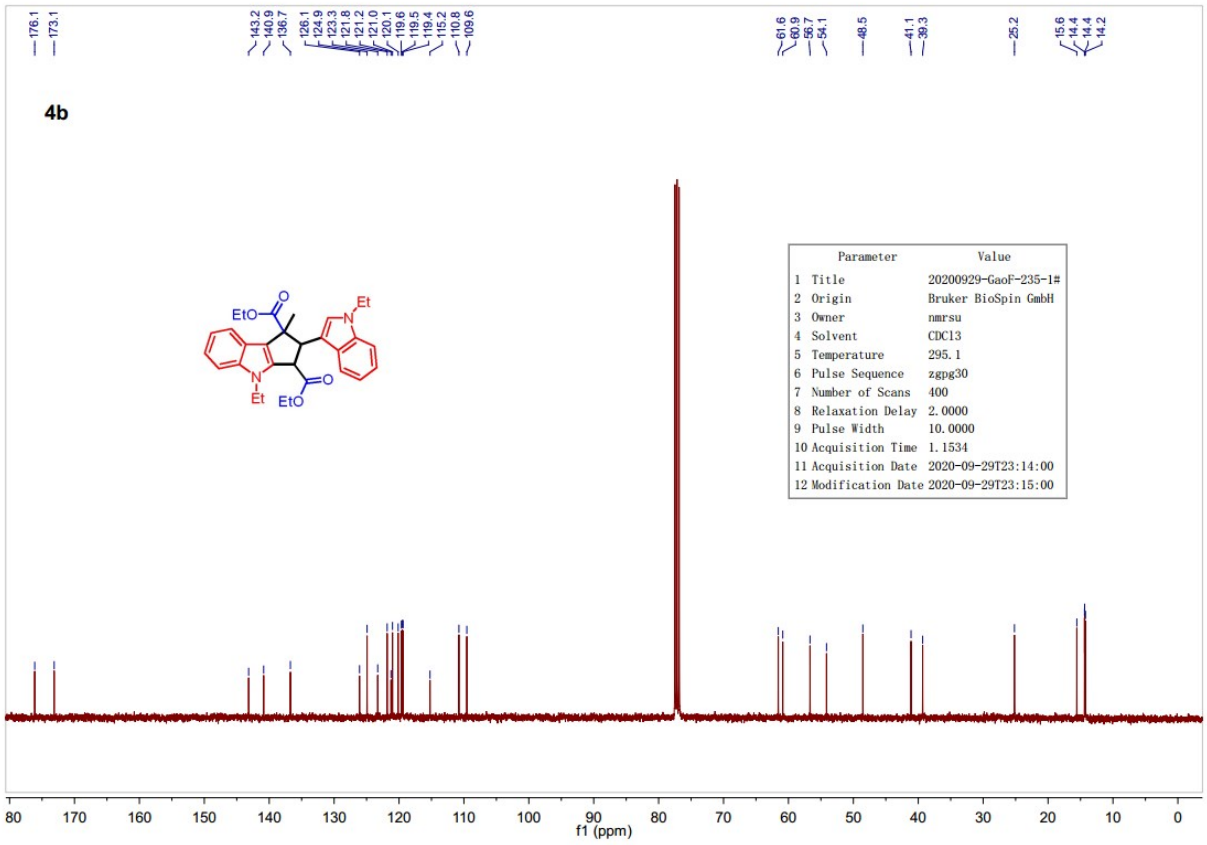

3m
7.53
7.51
7.37
7.35
7.33
7.31
7.30
7.28
7.24
7.22
7.20
7.18
7.02
7.00
6.99
6.97
6.95
6.77
3.75
3.51
3.28
3.25
3.22
3.18
2.33
2.10
1.54
Parameter Value
1 Title 20210402-GaoF-3m#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 293.9
6 Pulse Sequence zg30
7 Number of Scans 16
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2021-04-02T21:47:00
12 Modification Date 2021-04-02T21:47:20
1.04
3.10
2.13
2.10
0.98
3.07
2.99
2.16
3.00
2.93
3.00
f1 (ppm)

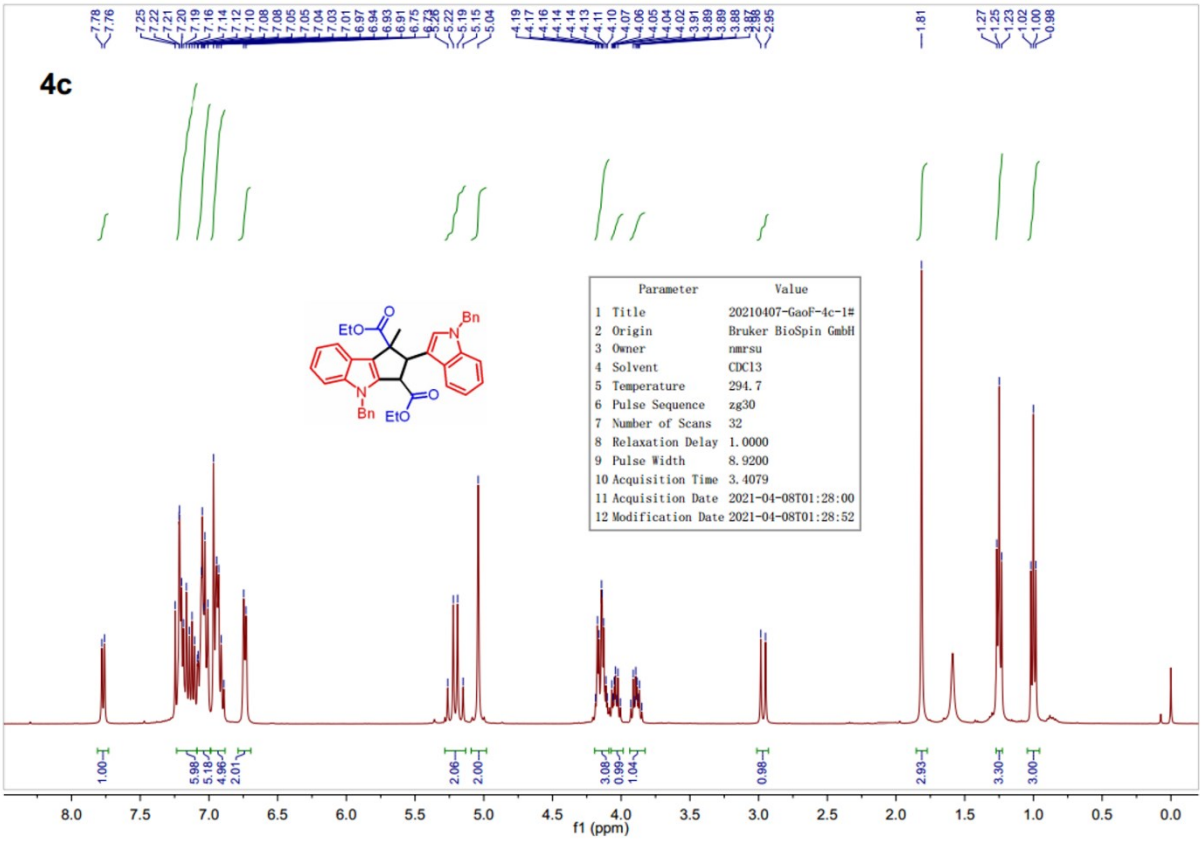

3m
211.5
207.1
144.0
142.3
137.9
127.0
125.9
123.8
122.9
122.3
121.8
120.3
119.9
119.8
119.1
114.0
110.3
109.8
60.0
54.9
54.5
33.0
31.3
27.9
26.3
23.3
Parameter Value
1 Title 20210406-GaoF-3m#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 294.6
6 Pulse Sequence zgpg30
7 Number of Scans 200
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2021-04-06T23:42:00
12 Modification Date 2021-04-06T23:42:28
f1 (ppm)

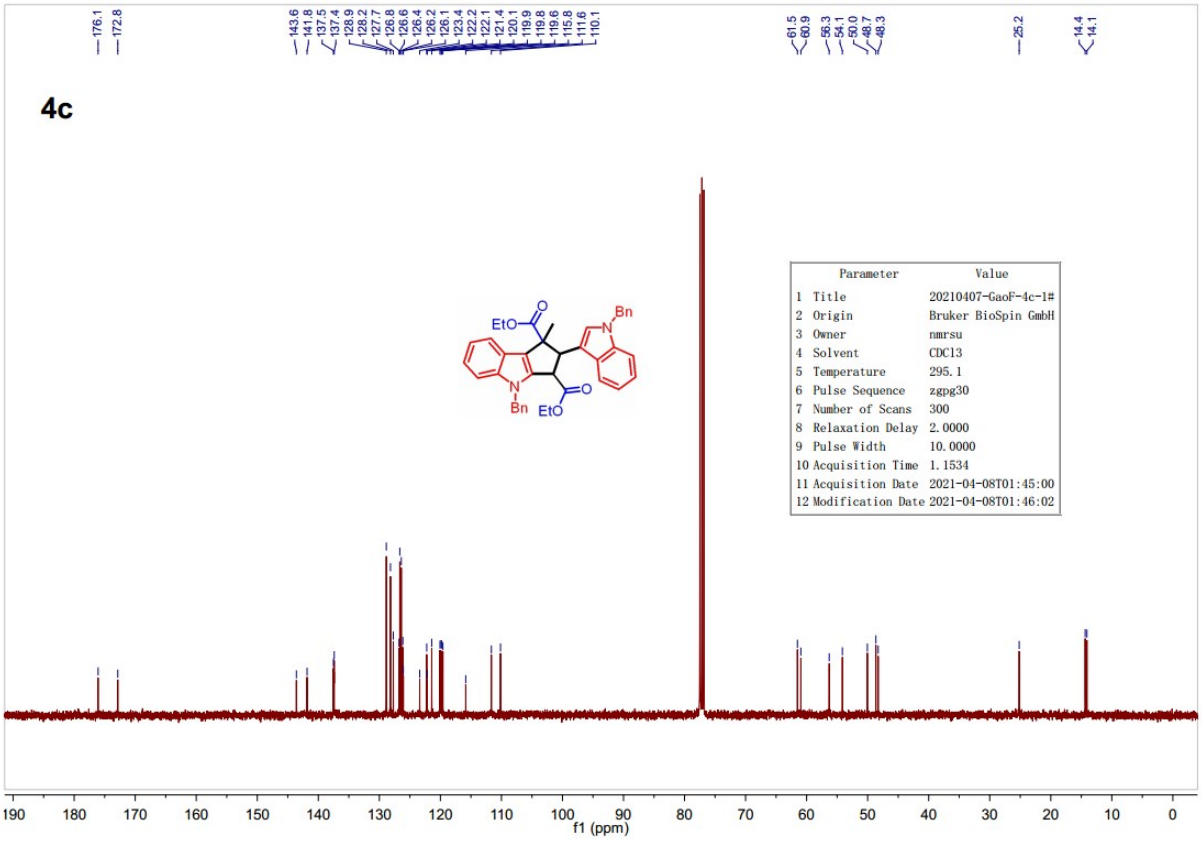

4a
7.74
7.72
7.30
7.28
7.25
7.24
7.22
7.20
7.18
7.17
7.15
6.96
6.88
6.86
6.84
6.77
6.75
4.37
4.36
4.35
4.33
4.21
4.20
4.19
4.17
4.13
4.11
4.10
4.09
4.07
4.07
3.76
3.37
2.79
2.75
1.74
1.59
1.30
1.28
1.26
1.24
1.22
1.20
EtO
O
N
O
EtO
Parameter Value
1 Title 20191226-GaoF-207#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 293.8
6 Pulse Sequence zg30
7 Number of Scans 32
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2019-12-26T21:20:00
12 Modification Date 2019-12-26T21:20:32
0.95
2.27
1.14
2.00
0.96
1.08
0.90
1.04
1.14
3.03
3.00
2.94
1.00
3.02
0.96
3.10
3.04
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)

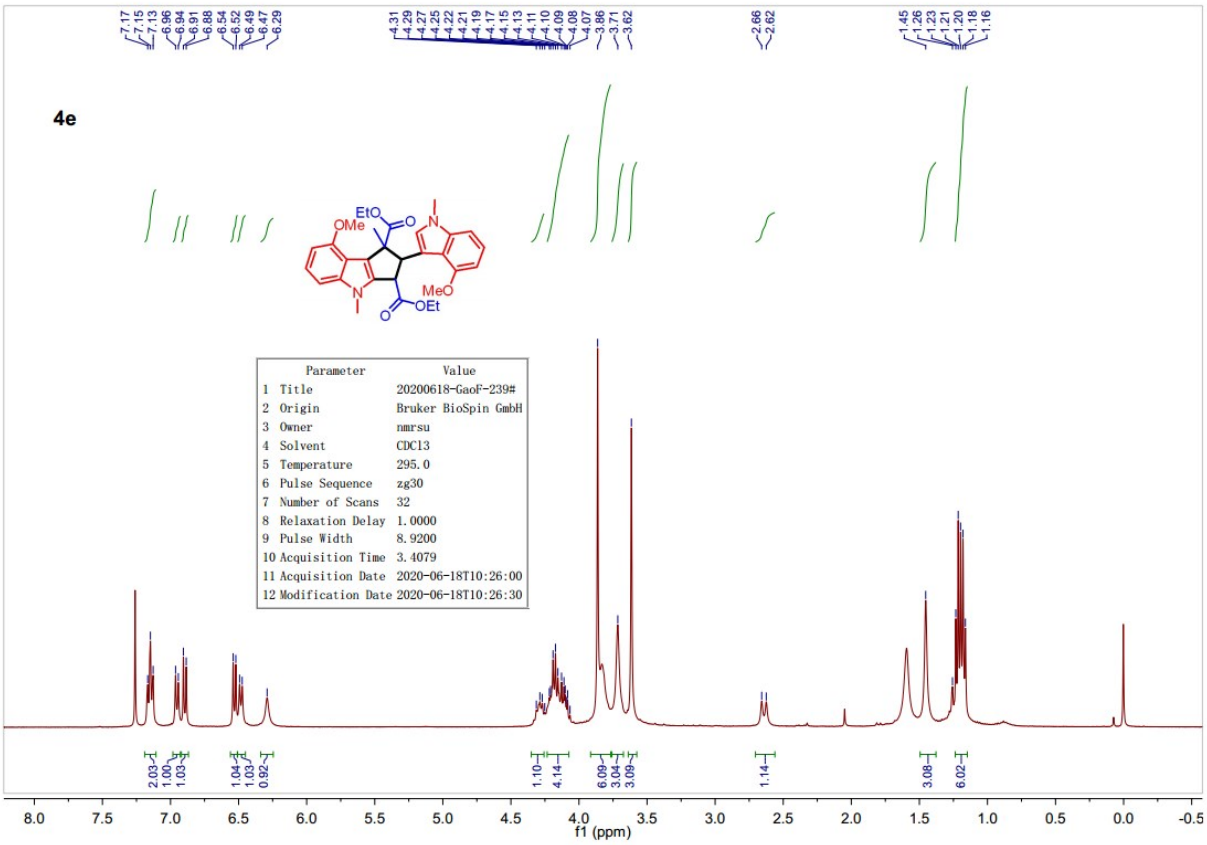

4a
176.1
172.9
143.4
142.0
137.8
126.6
125.7
122.9
122.0
121.6
121.2
119.7
119.5
119.4
115.2
110.1
109.5
61.6
60.9
56.9
54.0
48.5
32.9
30.6
25.2
14.3
EtO
O
N
O
EtO
Parameter Value
1 Title 20191227-GaoF-207#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 295.0
6 Pulse Sequence zgpg30
7 Number of Scans 400
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2019-12-27T23:34:00
12 Modification Date 2019-12-27T23:34:24
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

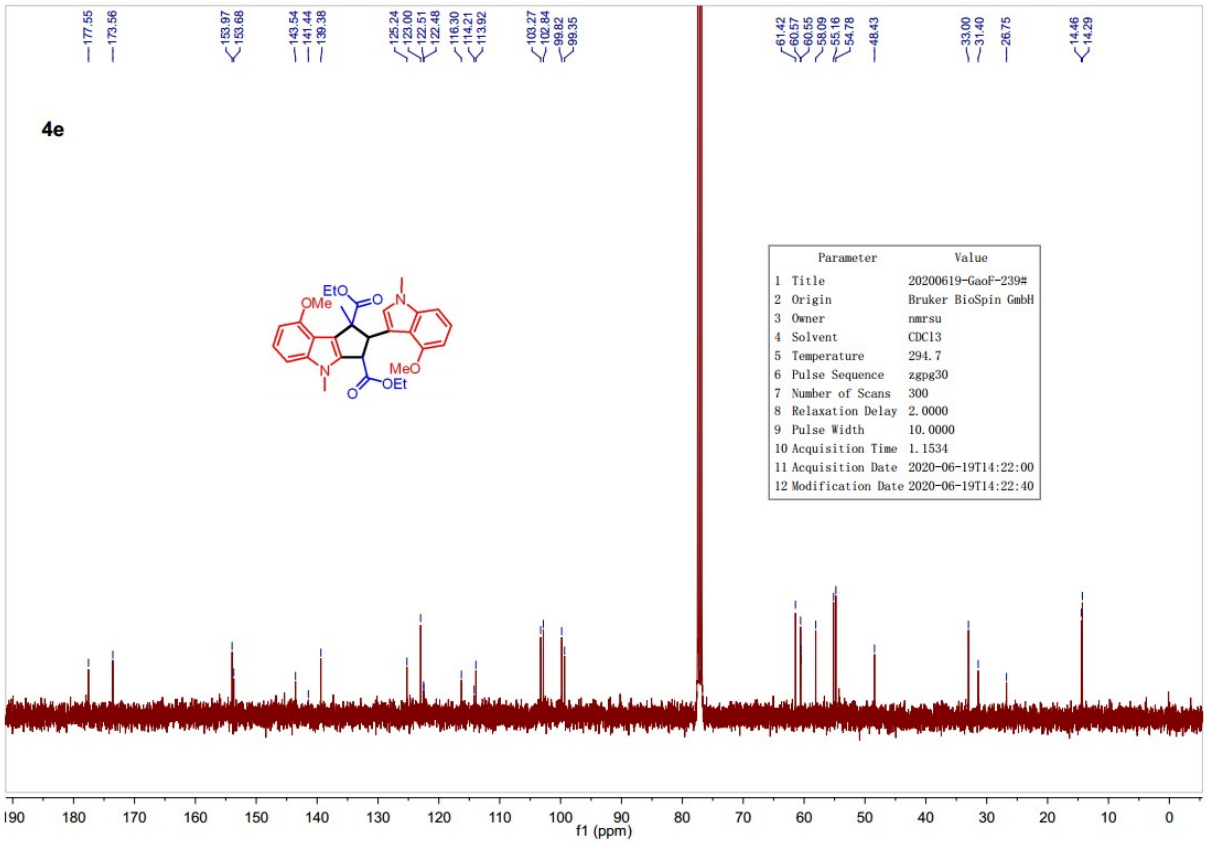

4b
7.77 7.75 7.32 7.30 7.22 7.21 7.19 7.18 7.17 7.16 7.15 7.14 7.13 7.01 6.87 6.86
4.38 4.36 4.35 4.33 4.26 4.24 4.23 4.22 4.18 4.16 4.15 4.14 4.13 4.12 4.11 4.10 4.09 4.07 3.89 3.88 3.87 3.86 3.85 3.83 2.90 2.86
1.76
0.93 0.91 0.89
EtO
O
N
Et
Et
N
O
EtO
Parameter Value
1 Title 20200926-GaoF-235-1#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 294.3
6 Pulse Sequence zg30
7 Number of Scans 32
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2020-09-26T18:53:00
12 Modification Date 2020-09-26T18:53:41
1.00 2.08 3.16 0.98 2.00 1.12 1.19 5.21 2.09 1.05 3.13 3.24 3.27 3.31 3.16
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 -0
f1 (ppm)

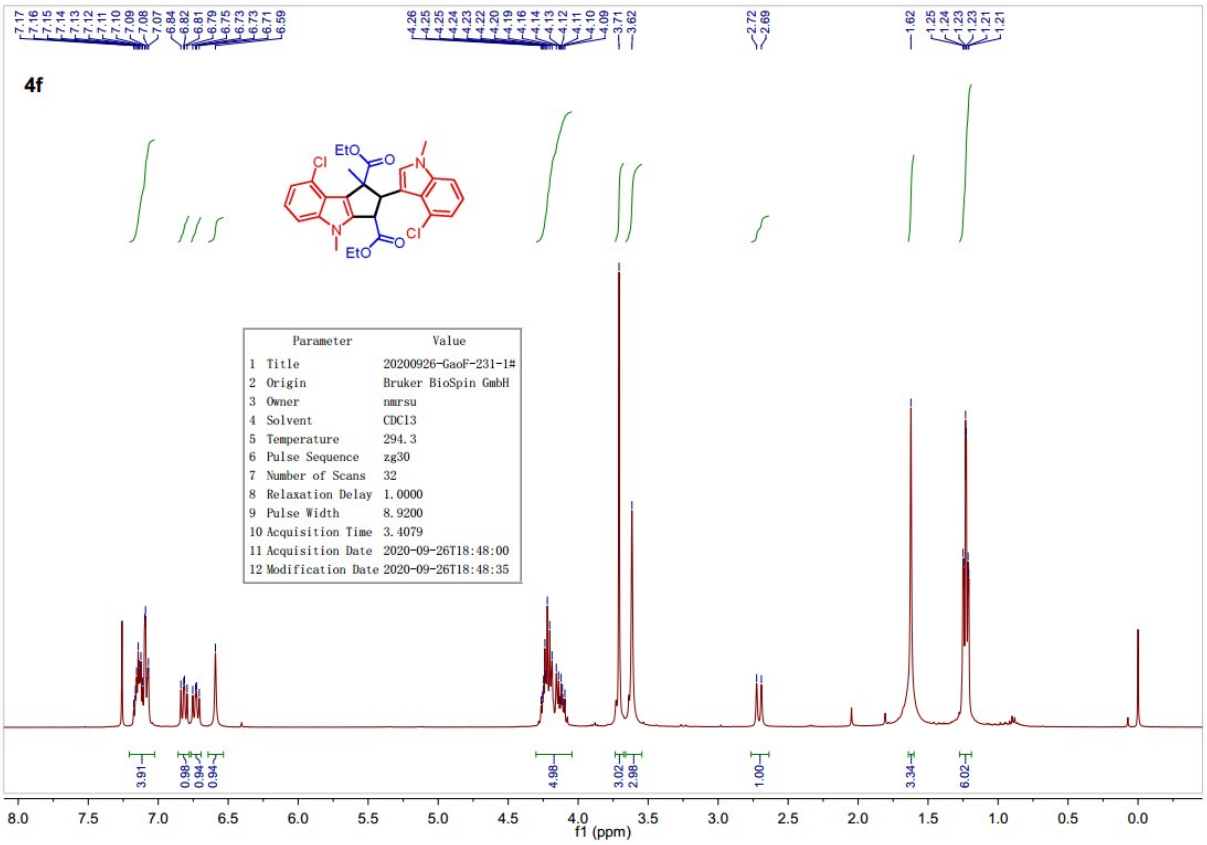

176.1 173.1
143.2 140.9 136.7 126.1 124.9 123.3 121.8 121.2 121.0 120.1 119.6 119.5 119.4 115.2 110.8 109.6
61.6 60.9 56.7 54.1 48.5 41.1 39.3 25.2 15.6 14.4 14.4 14.2
4b
EtO
O
N
Et
Et
N
O
EtO
Parameter Value
1 Title 20200929-GaoF-235-1#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 295.1
6 Pulse Sequence zgpg30
7 Number of Scans 400
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2020-09-29T23:14:00
12 Modification Date 2020-09-29T23:15:00
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

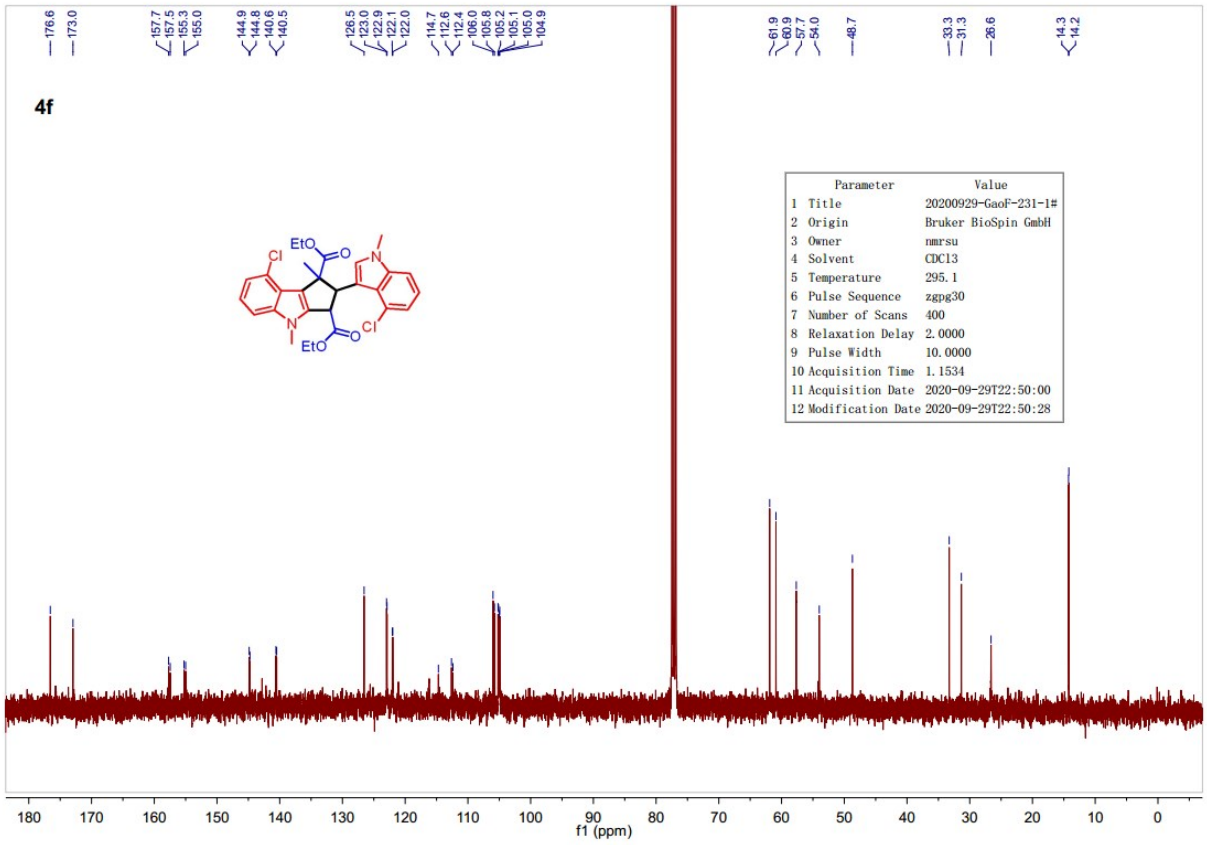

4c
Parameter Value
1 Title 20210407-GaoF-4c-1#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 294.7
6 Pulse Sequence zg30
7 Number of Scans 32
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2021-04-08T01:28:00
12 Modification Date 2021-04-08T01:28:52
f1 (ppm)

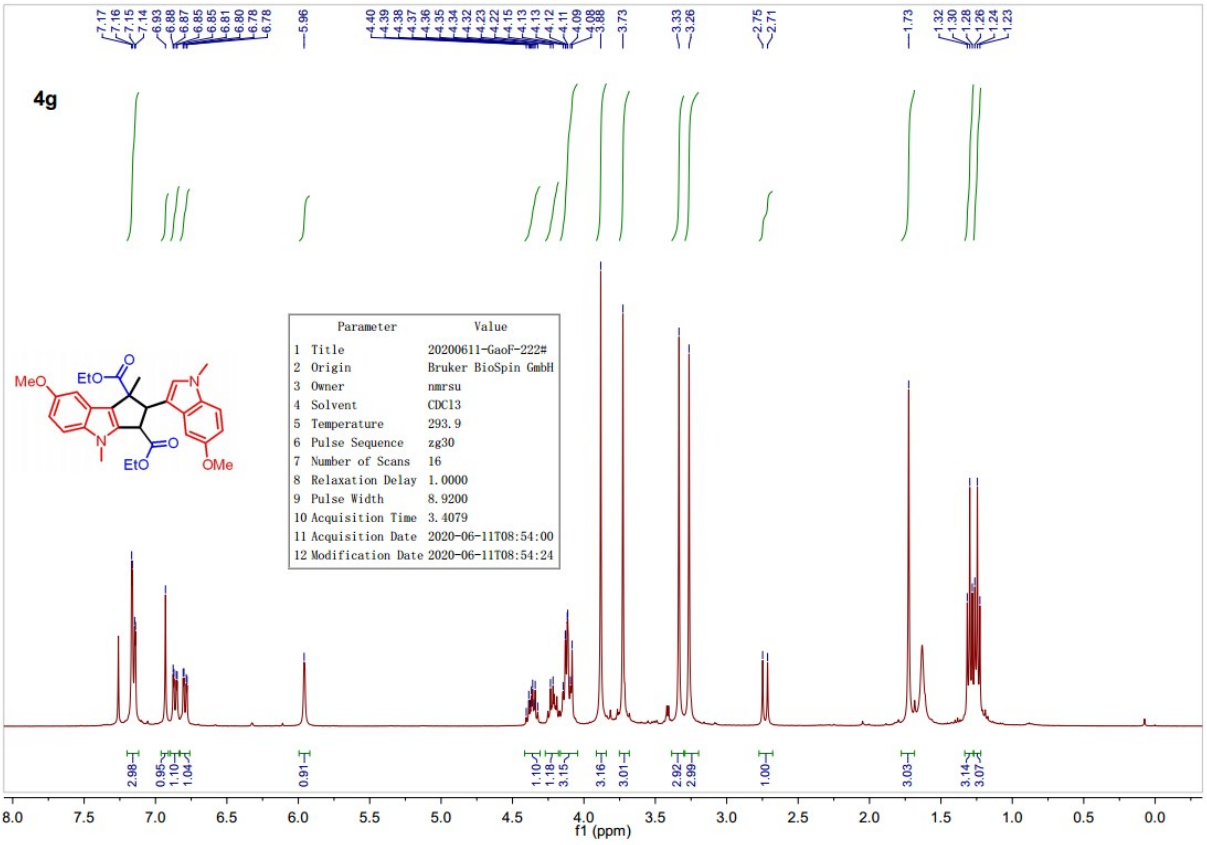

4c
Parameter Value
1 Title 20210407-GaoF-4c-1#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 295.1
6 Pulse Sequence zgpg30
7 Number of Scans 300
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2021-04-08T01:45:00
12 Modification Date 2021-04-08T01:46:02
f1 (ppm)

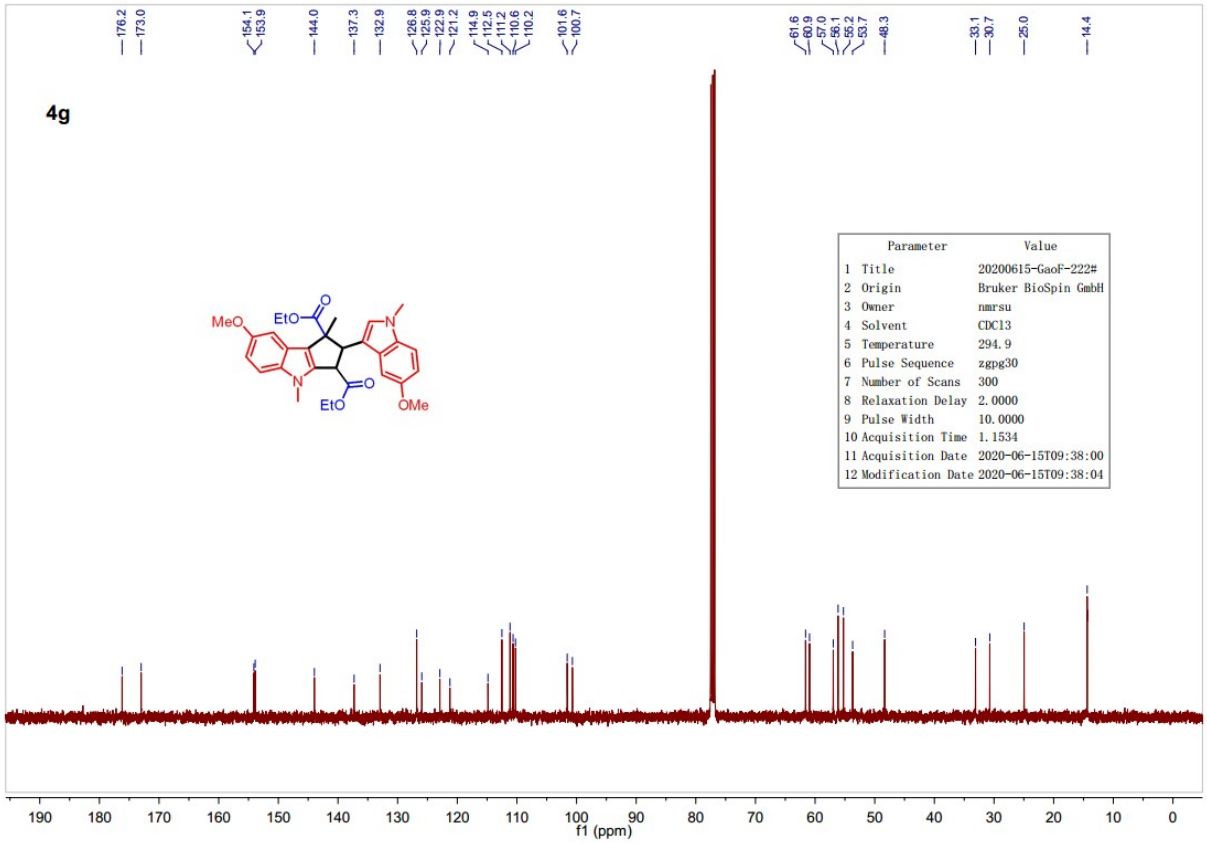

4e
7.17
7.15
7.13
6.96
6.94
6.91
6.88
6.54
6.52
6.49
6.47
6.29
4.31
4.29
4.27
4.25
4.22
4.21
4.19
4.17
4.15
4.13
4.11
4.10
4.09
4.08
4.07
3.86
3.71
3.62
2.66
2.62
1.45
1.26
1.23
1.21
1.20
1.18
1.16
EtO
OMe
MeO
OEt
Parameter Value
1 Title 20200618-GaoF-239#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 295.0
6 Pulse Sequence zg30
7 Number of Scans 32
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2020-06-18T10:26:00
12 Modification Date 2020-06-18T10:26:30
2.03
1.00
1.03
1.04
1.03
0.92
1.10
4.14
6.09
3.04
3.09
1.14
3.08
6.02
f1 (ppm)

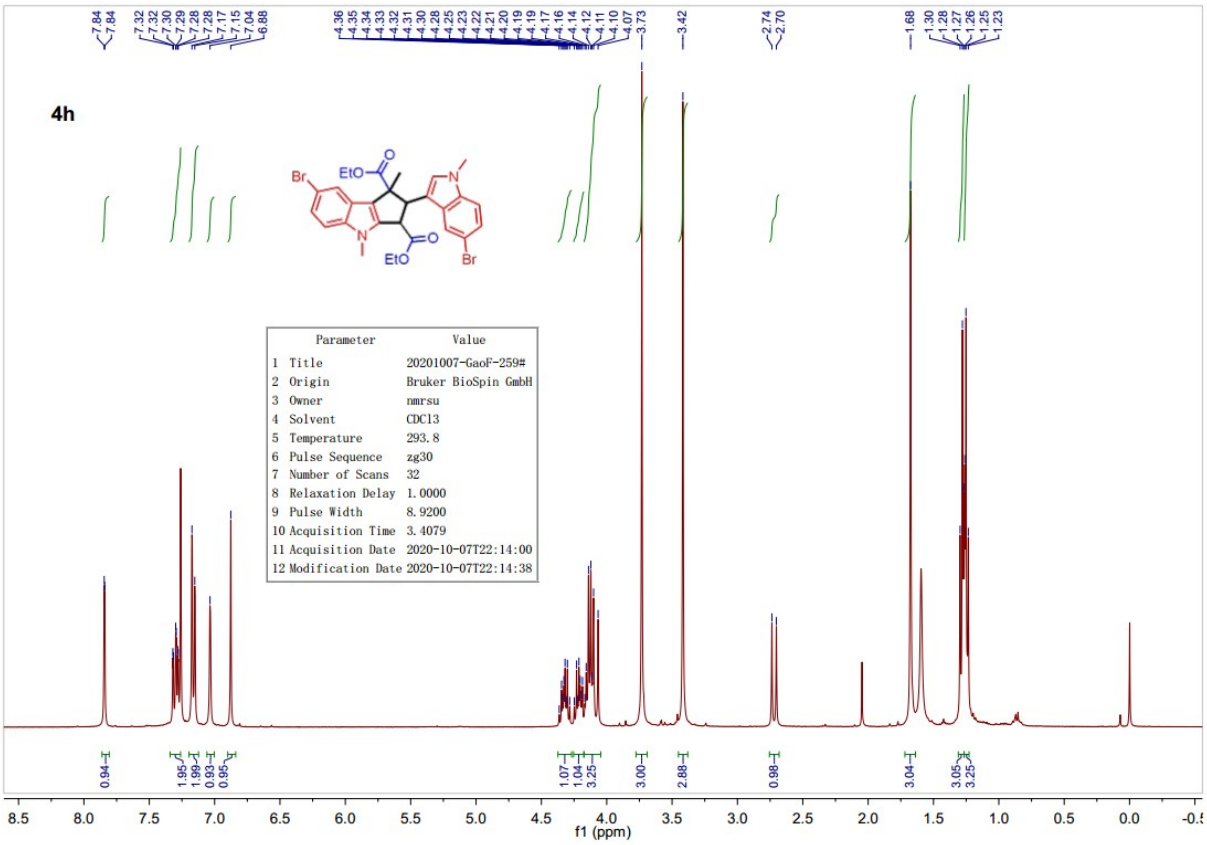

4e
177.55
173.56
153.97
153.68
143.54
141.44
139.38
125.24
123.00
122.51
122.48
116.30
114.21
113.92
103.27
102.84
99.82
99.35
61.42
60.57
60.55
58.09
55.16
54.78
48.43
33.00
31.40
26.75
14.46
14.29
EtO
OMe
MeO
OEt
Parameter Value
1 Title 20200619-GaoF-239#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 294.7
6 Pulse Sequence zgpg30
7 Number of Scans 300
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2020-06-19T14:22:00
12 Modification Date 2020-06-19T14:22:40
f1 (ppm)

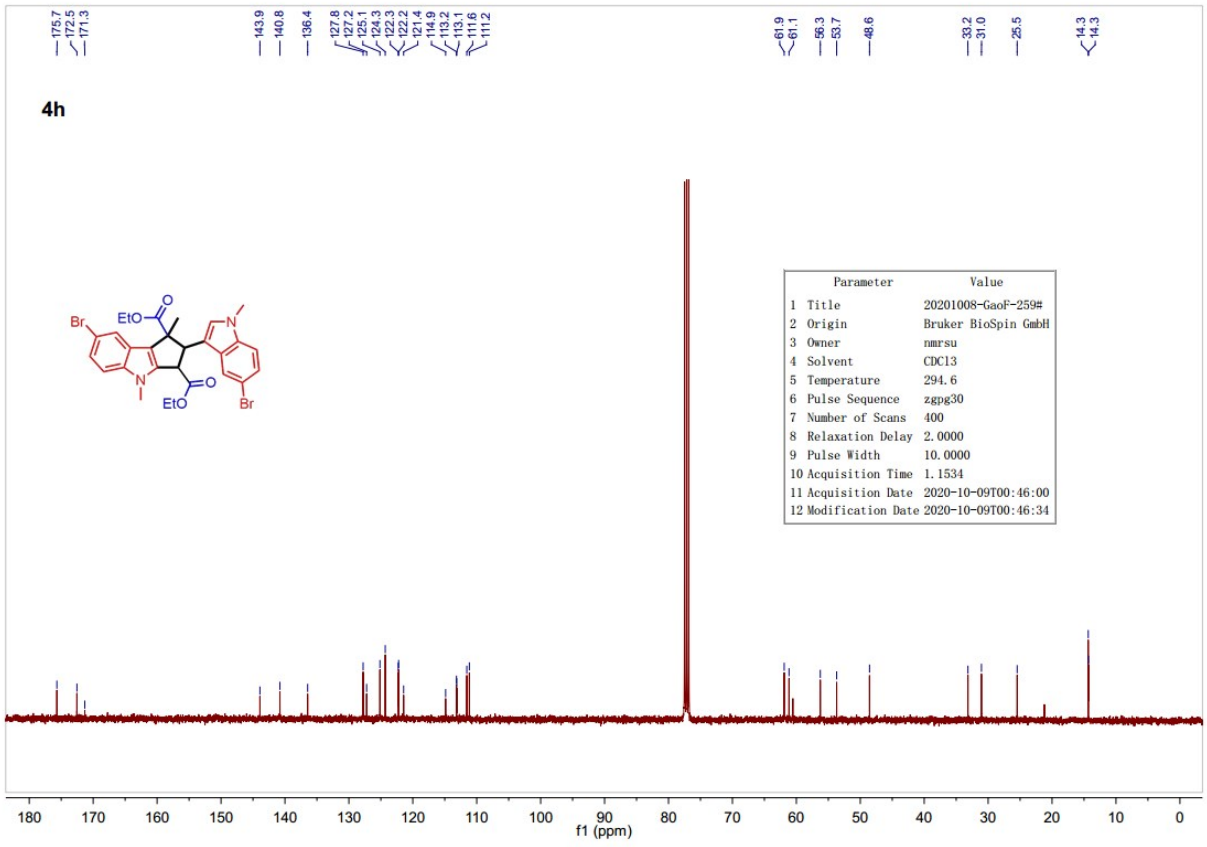

4f
7.17 7.16 7.15 7.14 7.13 7.12 7.11 7.10 7.09 7.08 7.07 6.84 6.82 6.81 6.79 6.75 6.73 6.73 6.71 6.59
4.26 4.25 4.24 4.23 4.22 4.20 4.19 4.16 4.14 4.13 4.12 4.11 4.10 4.09 3.71 3.62
2.72 2.69
1.62 1.25 1.24 1.23 1.23 1.21 1.21
EtO
O
Cl
N
Cl
N
EtO
O
Parameter Value
1 Title 20200926-GaoF-231-1#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 294.3
6 Pulse Sequence zg30
7 Number of Scans 32
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2020-09-26T18:48:00
12 Modification Date 2020-09-26T18:48:35
3.91 0.98 0.94 0.94 4.98 3.02 2.98 1.00 3.34 6.02
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)

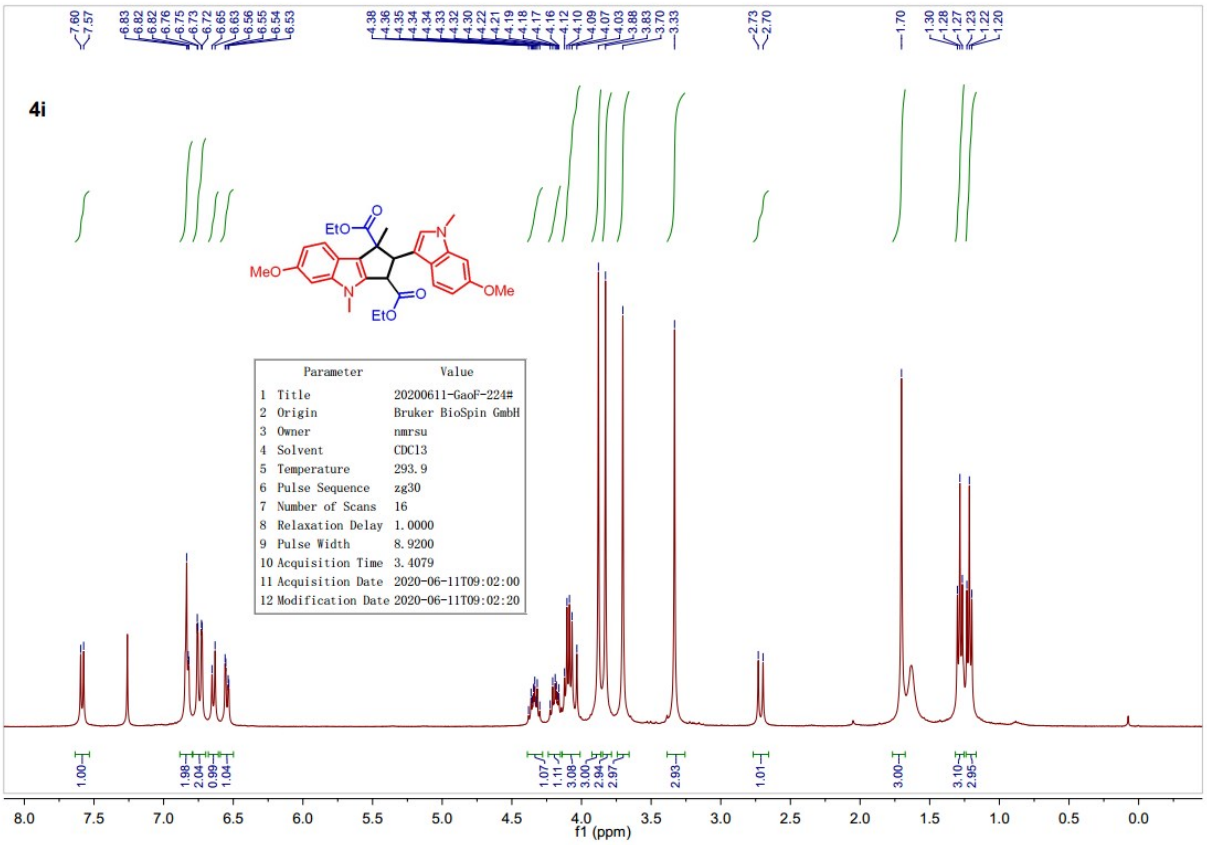

176.6 173.0
157.7 157.5 155.3 155.0 144.9 144.8 140.6 140.5 126.5 123.0 122.9 122.1 122.0 114.7 112.6 112.4 106.0 105.8 105.2 105.1 105.0 104.9
61.9 60.9 57.7 54.0 48.7 33.3 31.3 26.6 14.3 14.2
4f
EtO
O
Cl
N
Cl
N
EtO
O
Parameter Value
1 Title 20200929-GaoF-231-1#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 295.1
6 Pulse Sequence zgpg30
7 Number of Scans 400
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2020-09-29T22:50:00
12 Modification Date 2020-09-29T22:50:28
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

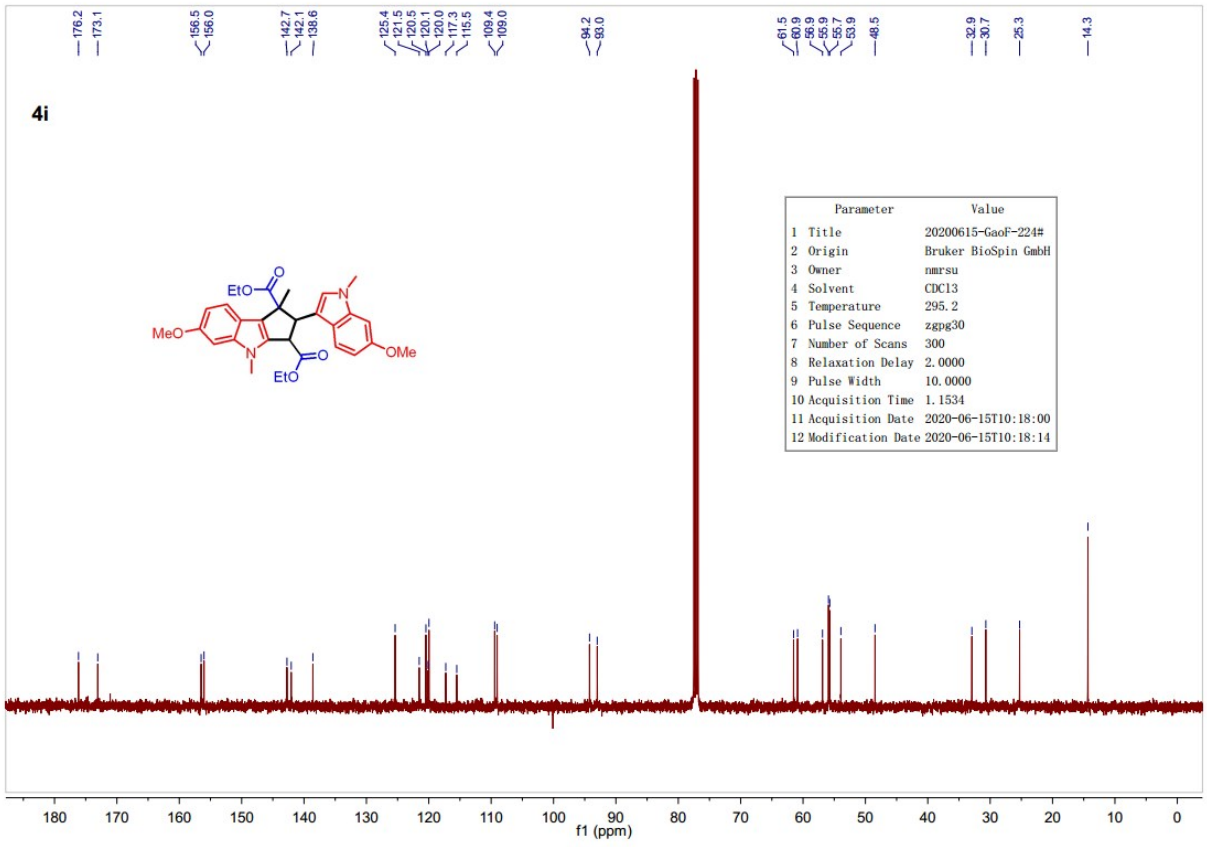

4g
7.17
7.16
7.15
7.14
6.93
6.88
6.87
6.85
6.85
6.81
6.80
6.78
6.78
5.96
4.40
4.39
4.38
4.37
4.36
4.35
4.34
4.32
4.23
4.22
4.15
4.13
4.12
4.11
4.09
4.08
3.88
3.73
3.33
3.26
2.75
2.71
1.73
1.32
1.30
1.28
1.26
1.24
1.23
MeO
EtO
EtO
OMe
Parameter Value
1 Title 20200611-GaoF-222#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 293.9
6 Pulse Sequence zg30
7 Number of Scans 16
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2020-06-11T08:54:00
12 Modification Date 2020-06-11T08:54:24
2.98
0.95
1.10
1.04
0.91
1.10
1.18
3.15
3.16
3.01
2.92
2.99
1.00
3.03
3.14
3.07
f1 (ppm)

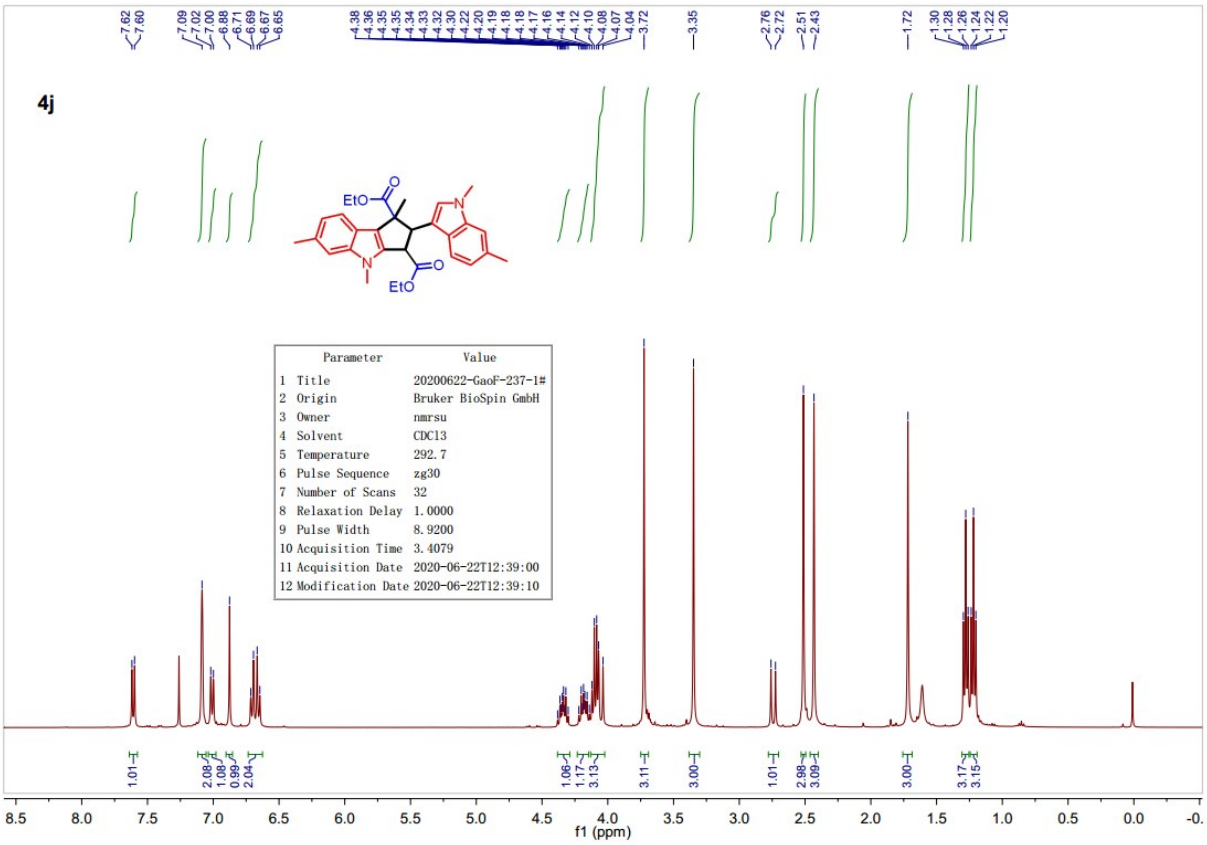

4g
176.2
173.0
154.1
153.9
144.0
137.3
132.9
126.8
125.9
122.9
121.2
114.9
112.5
111.2
110.6
110.2
101.6
100.7
61.6
60.9
57.0
56.1
55.2
53.7
48.3
33.1
30.7
25.0
14.4
MeO
EtO
EtO
OMe
Parameter Value
1 Title 20200615-GaoF-222#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 294.9
6 Pulse Sequence zgpg30
7 Number of Scans 300
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2020-06-15T09:38:00
12 Modification Date 2020-06-15T09:38:04
f1 (ppm)

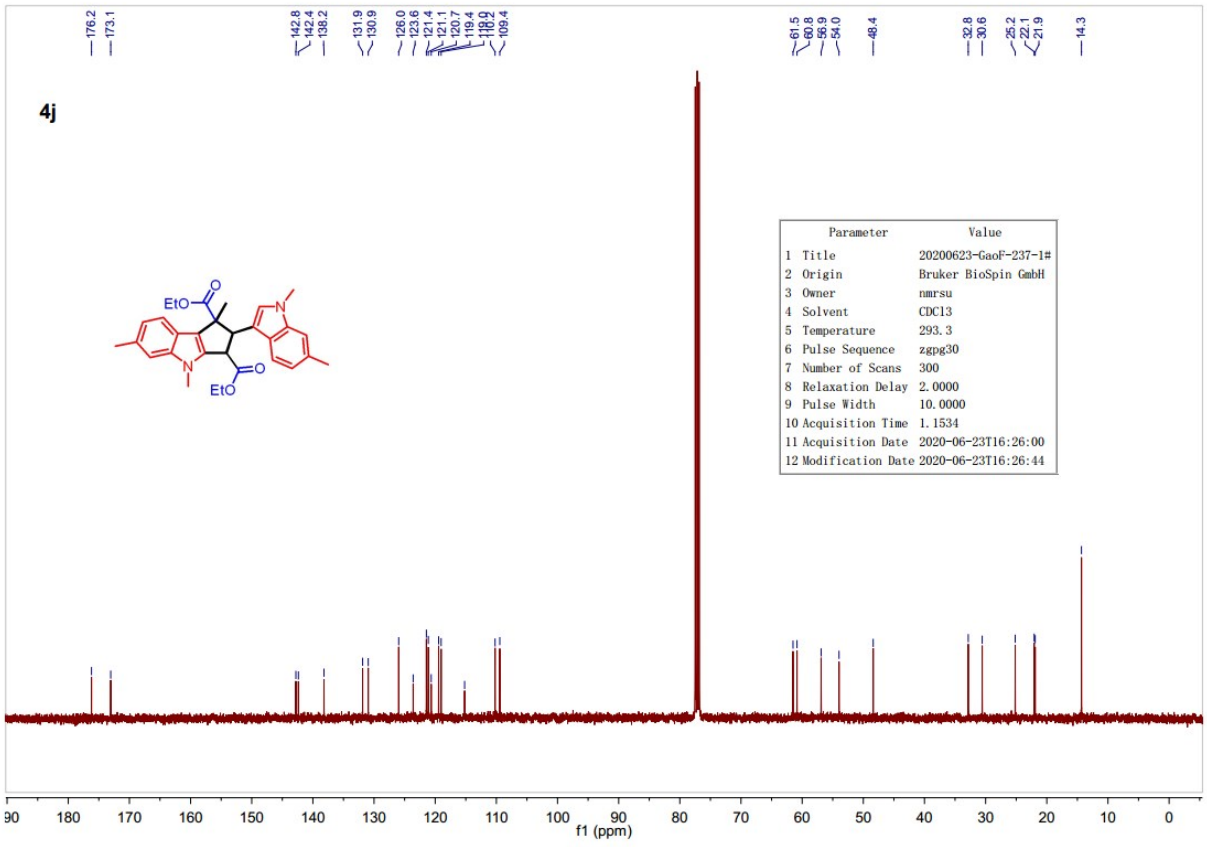

4h
Br
EtO
O
N
EtO
O
Br
Parameter Value
1 Title 20201007-GaoF-259#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 293.8
6 Pulse Sequence zg30
7 Number of Scans 32
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2020-10-07T22:14:00
12 Modification Date 2020-10-07T22:14:38
f1 (ppm)

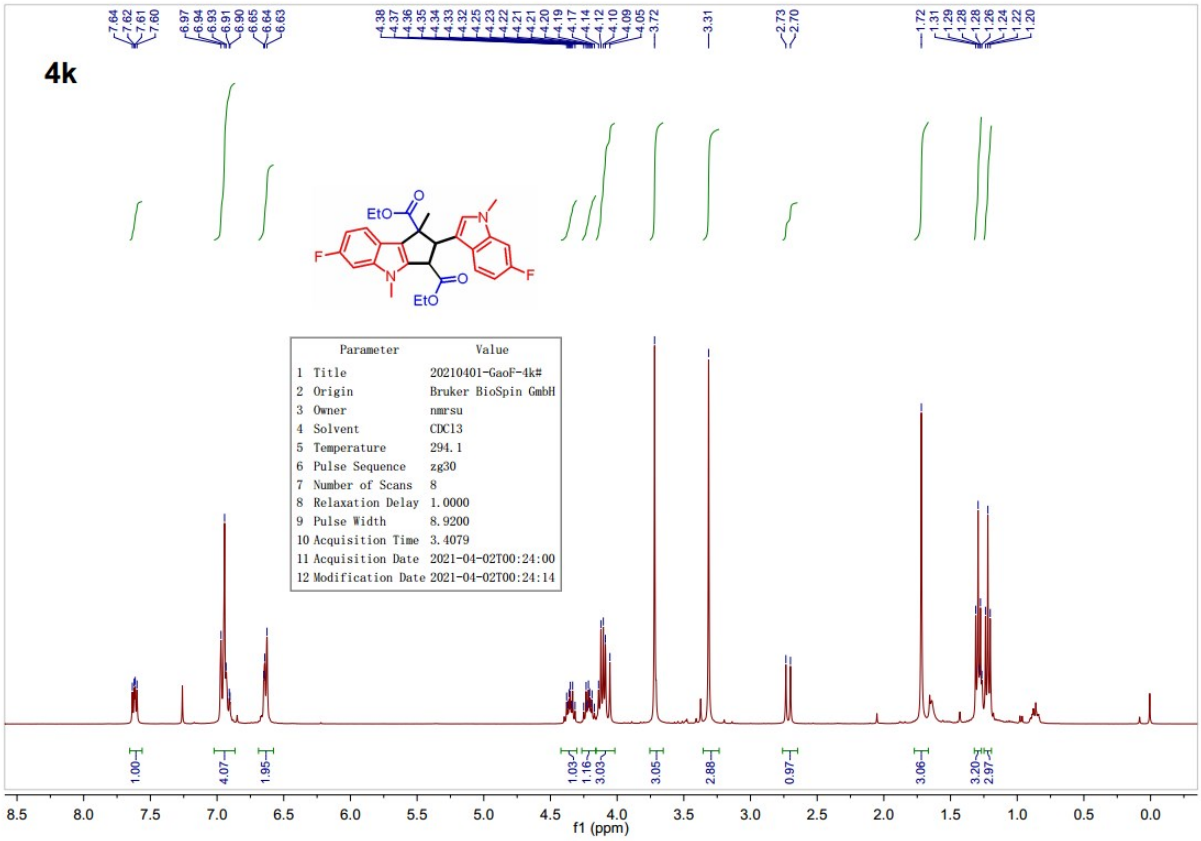

4h
Br
EtO
O
N
EtO
O
Br
Parameter Value
1 Title 20201008-GaoF-259#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 294.6
6 Pulse Sequence zgpg30
7 Number of Scans 400
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2020-10-09T00:46:00
12 Modification Date 2020-10-09T00:46:34
f1 (ppm)

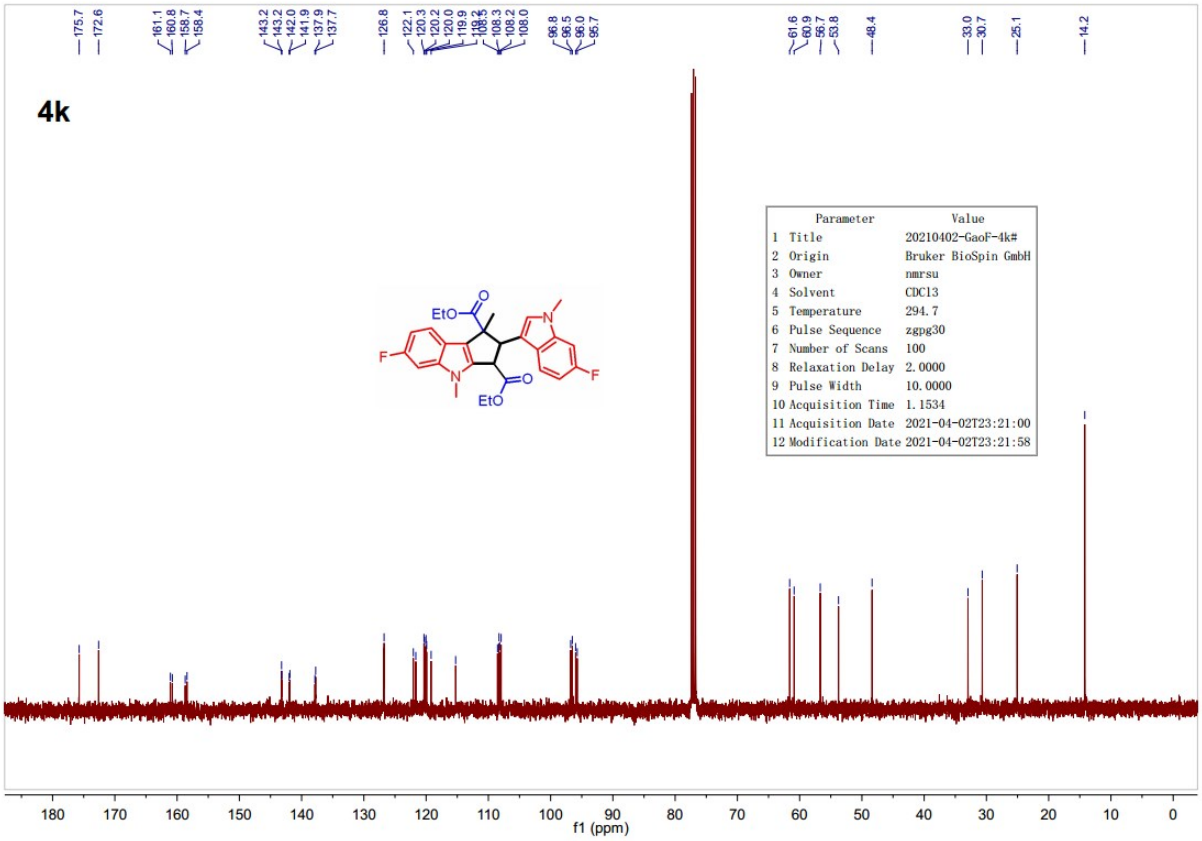

4i
EtO
MeO
OMe
EtO
Parameter Value
1 Title 20200611-GaoF-224#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 293.9
6 Pulse Sequence zg30
7 Number of Scans 16
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2020-06-11T09:02:00
12 Modification Date 2020-06-11T09:02:20
f1 (ppm)

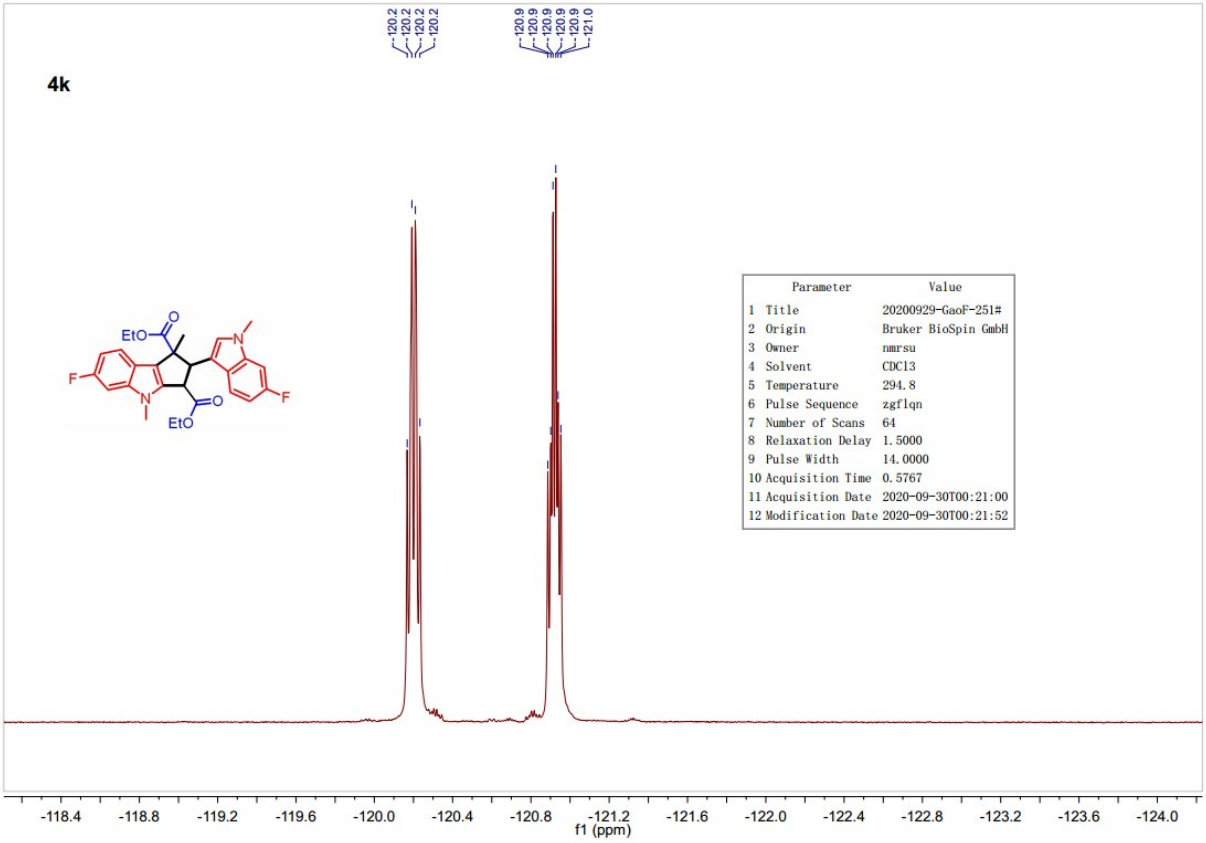

4i
EtO
MeO
OMe
EtO
Parameter Value
1 Title 20200615-GaoF-224#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 295.2
6 Pulse Sequence zgpg30
7 Number of Scans 300
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2020-06-15T10:18:00
12 Modification Date 2020-06-15T10:18:14
f1 (ppm)

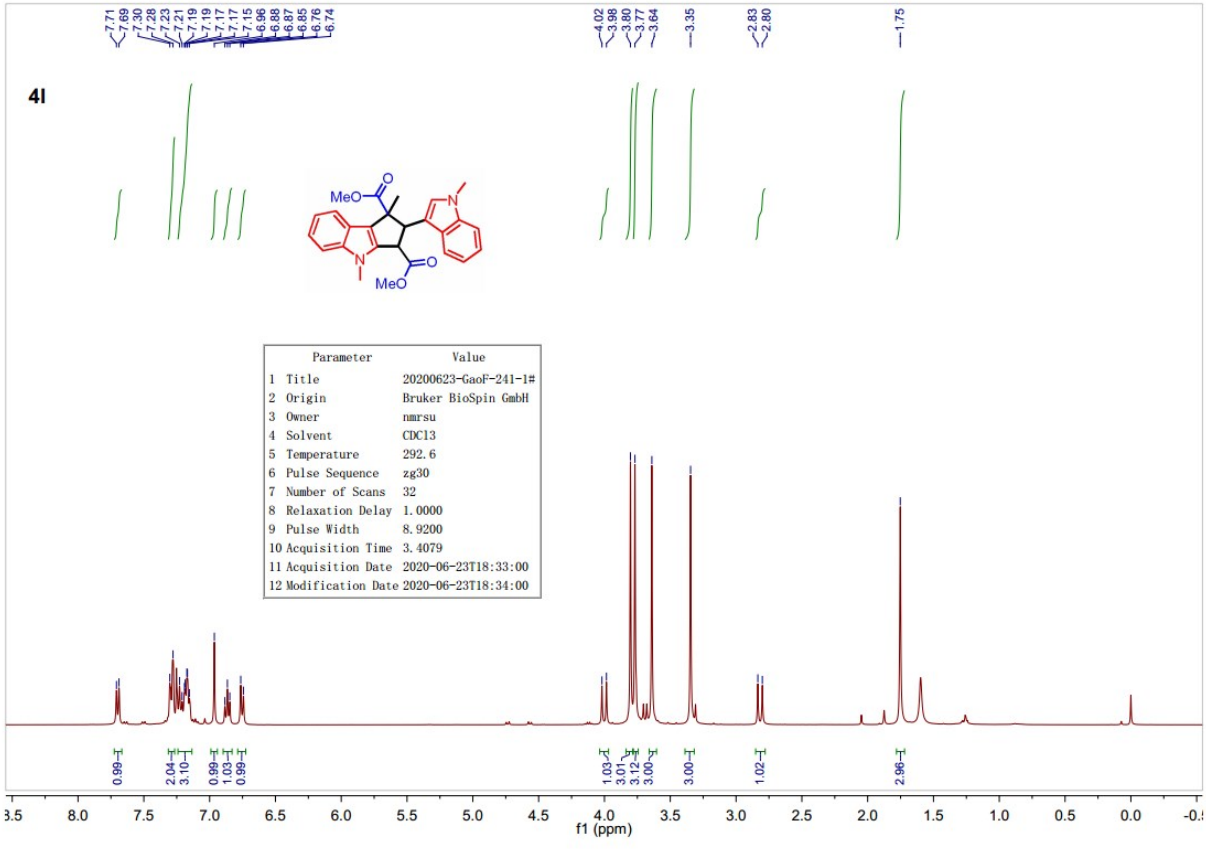

4j
7.62
7.60
7.09
7.02
7.00
6.88
6.71
6.69
6.67
6.65
4.38
4.36
4.35
4.35
4.34
4.33
4.32
4.30
4.22
4.20
4.19
4.18
4.18
4.17
4.16
4.14
4.12
4.10
4.08
4.07
4.04
3.72
3.35
2.76
2.72
2.51
2.43
1.72
1.30
1.28
1.26
1.24
1.22
1.20
EtO
EtO
Parameter Value
1 Title 20200622-GaoF-237-1#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 292.7
6 Pulse Sequence zg30
7 Number of Scans 32
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2020-06-22T12:39:00
12 Modification Date 2020-06-22T12:39:10
1.01
2.08
1.08
0.99
2.04
1.06
1.17
3.13
3.11
3.00
1.01
2.98
3.09
3.00
3.17
3.15
f1 (ppm)

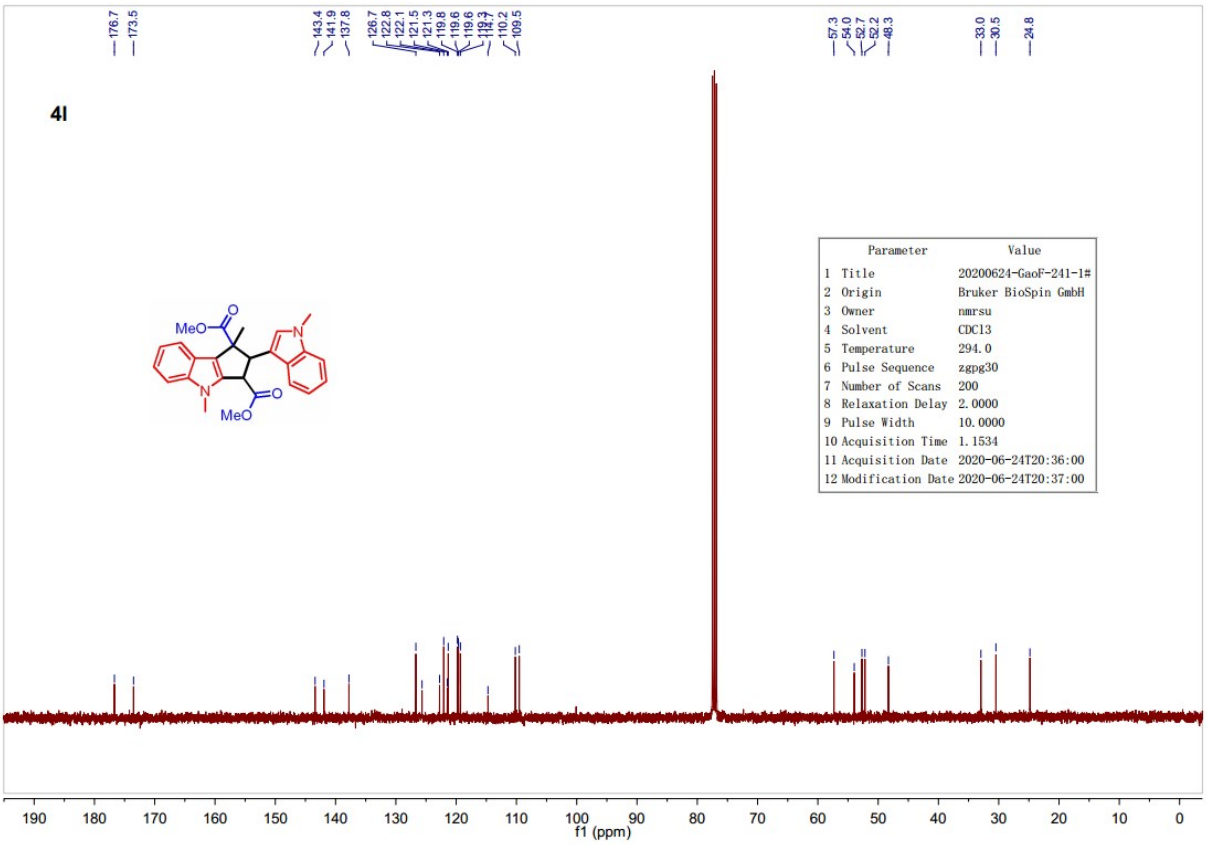

4j
176.2
173.1
142.8
142.4
138.2
131.9
130.9
126.0
123.6
121.4
121.1
120.7
119.4
118.2
118.0
109.4
61.5
60.8
56.9
54.0
48.4
32.8
30.6
25.2
22.1
21.9
14.3
EtO
EtO
Parameter Value
1 Title 20200623-GaoF-237-1#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 293.3
6 Pulse Sequence zgpg30
7 Number of Scans 300
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2020-06-23T16:26:00
12 Modification Date 2020-06-23T16:26:44
f1 (ppm)

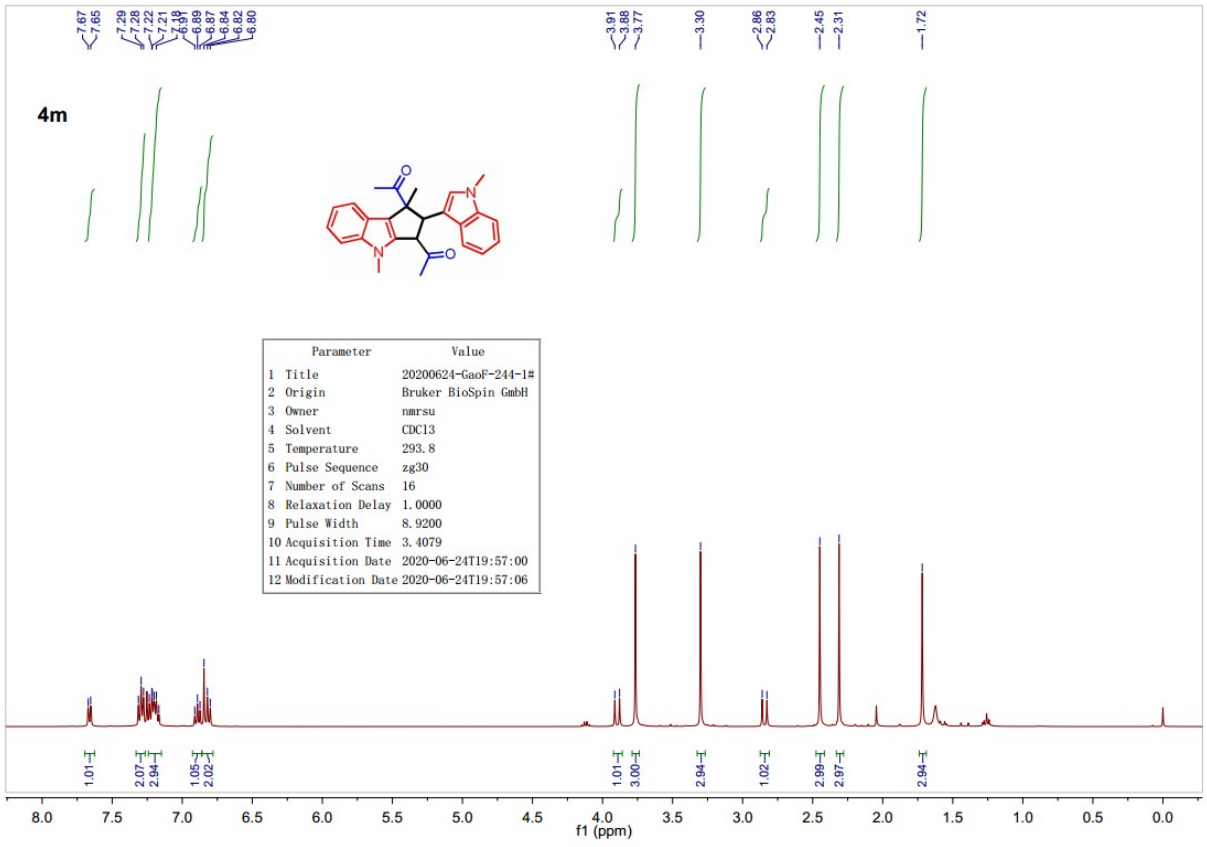

4k
EtO
O
N
F
F
N
O
EtO
Parameter Value
1 Title 20210401-GaoF-4k#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 294.1
6 Pulse Sequence zg30
7 Number of Scans 8
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2021-04-02T00:24:00
12 Modification Date 2021-04-02T00:24:14
f1 (ppm)

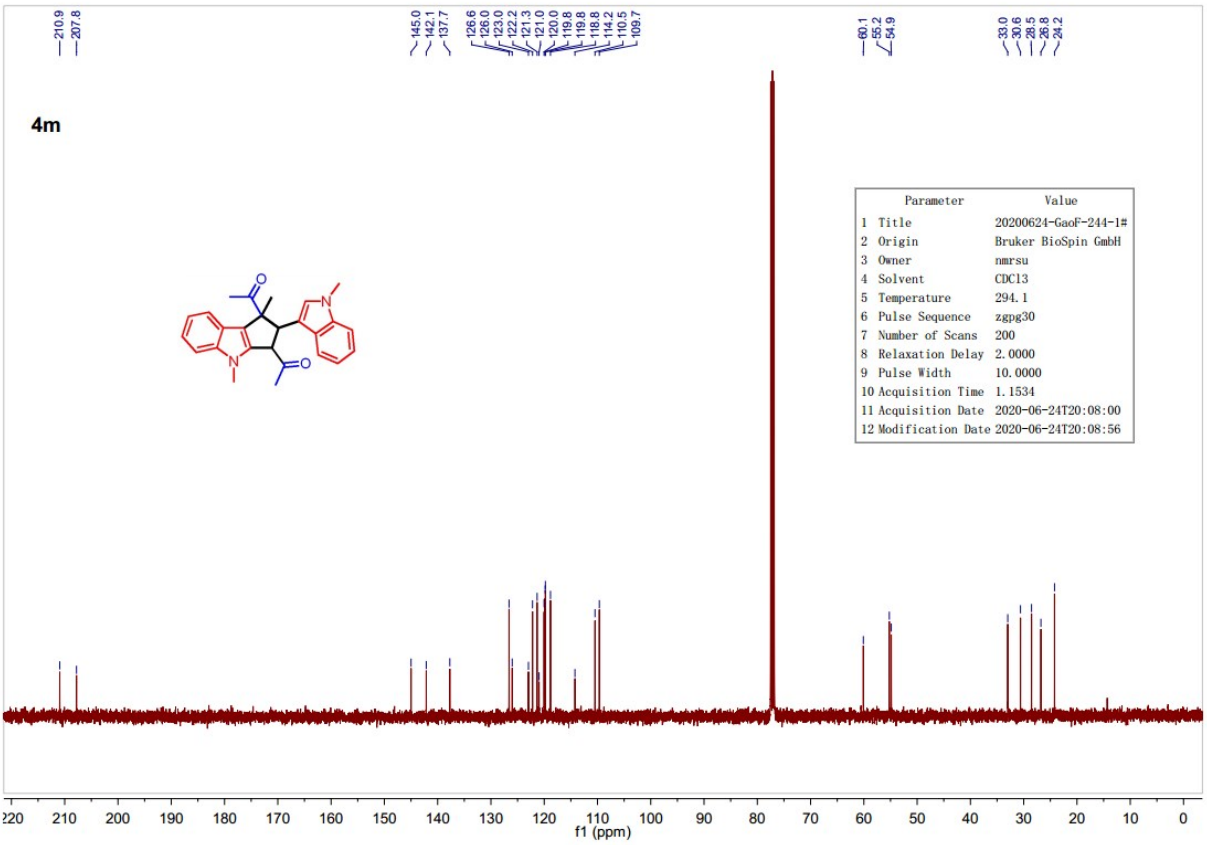

4k
EtO
O
N
F
F
N
O
EtO
Parameter Value
1 Title 20210402-GaoF-4k#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 294.7
6 Pulse Sequence zgpg30
7 Number of Scans 100
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2021-04-02T23:21:00
12 Modification Date 2021-04-02T23:21:58
f1 (ppm)

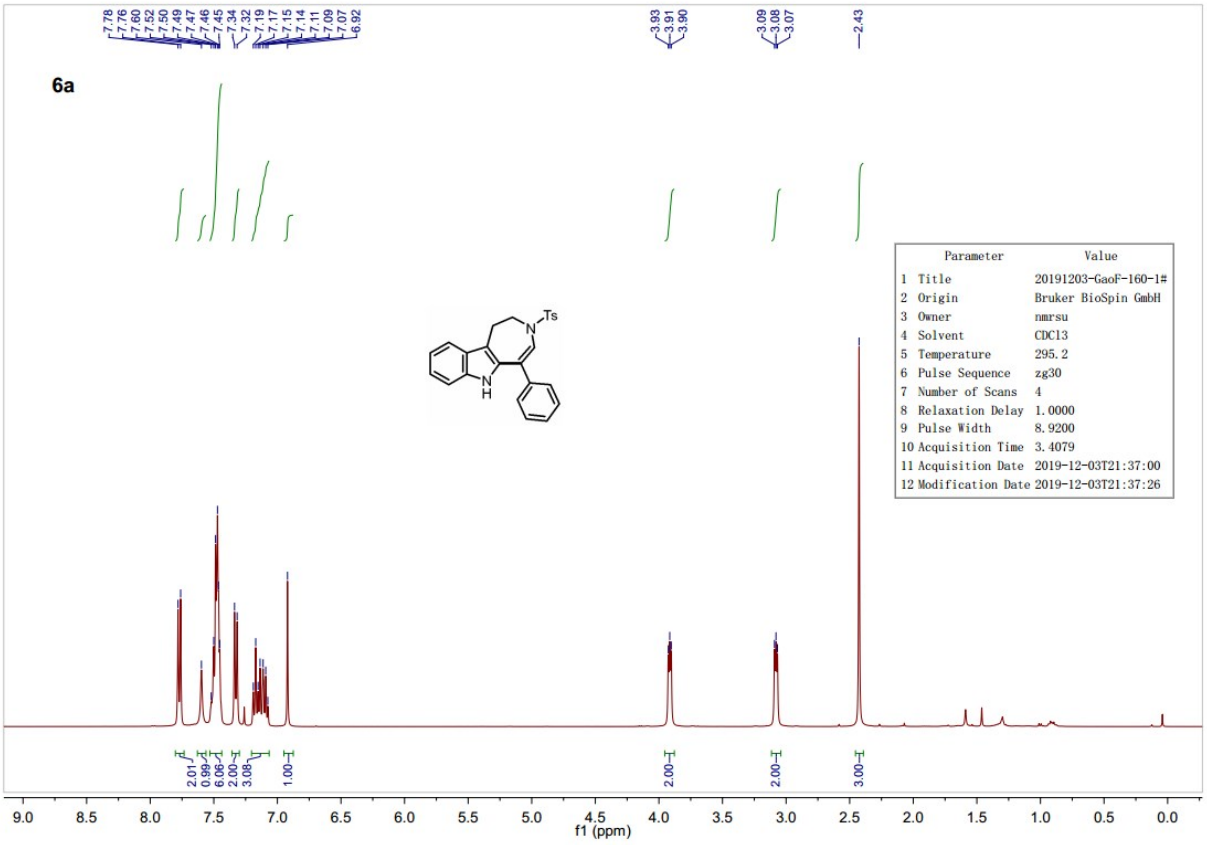

4k
120.2
120.2
120.2
120.2
120.9
120.9
120.9
120.9
120.9
121.0
EtO
O
N
F
F
N
O
EtO
Parameter Value
1 Title 20200929-GaoF-251#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 294.8
6 Pulse Sequence zgflqn
7 Number of Scans 64
8 Relaxation Delay 1.5000
9 Pulse Width 14.0000
10 Acquisition Time 0.5767
11 Acquisition Date 2020-09-30T00:21:00
12 Modification Date 2020-09-30T00:21:52
-118.4
-118.8
-119.2
-119.6
-120.0
-120.4
-120.8
-121.2
-121.6
-122.0
-122.4
-122.8
-123.2
-123.6
-124.0
f1 (ppm)

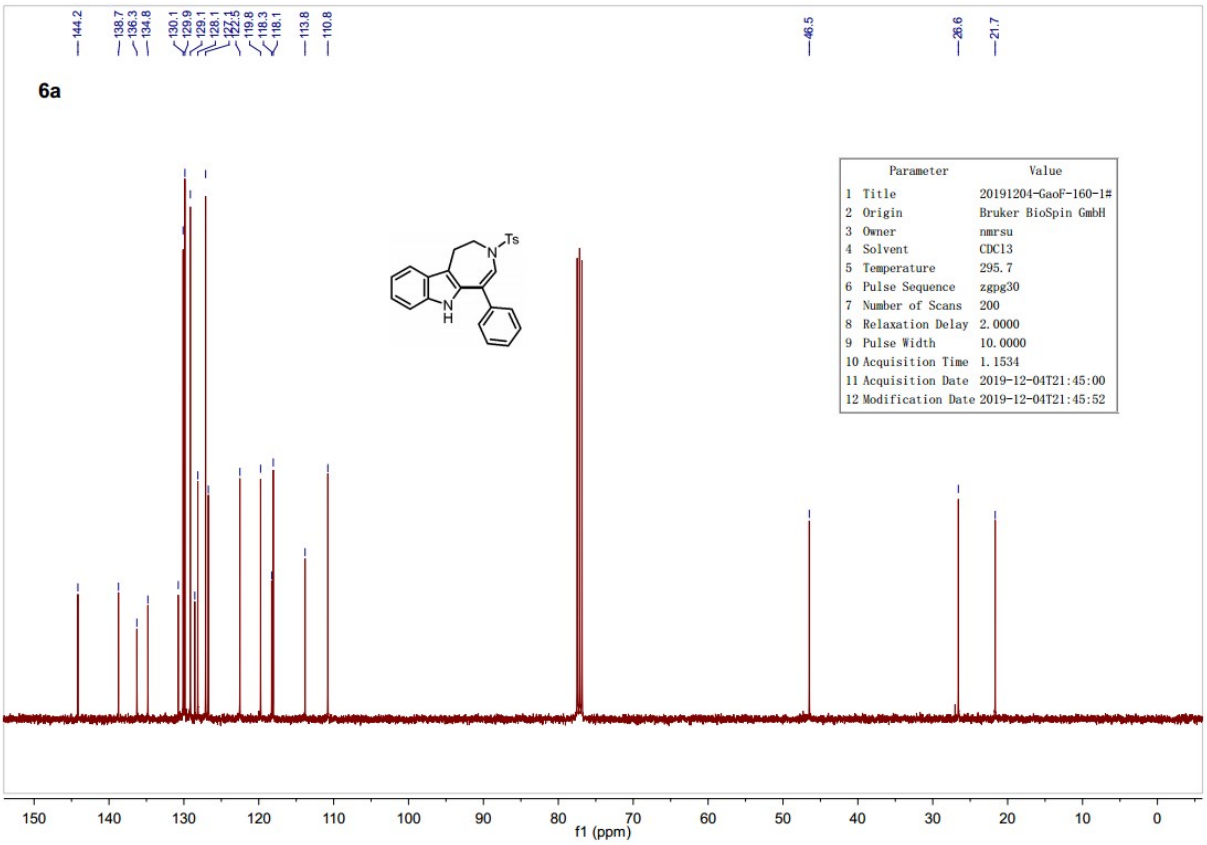

4l
7.71
7.69
7.30
7.28
7.23
7.21
7.19
7.19
7.17
7.17
7.15
6.96
6.88
6.87
6.85
6.76
6.74
4.02
3.98
3.80
3.77
3.64
3.35
2.83
2.80
1.75
MeO
O
N
N
O
MeO
Parameter Value
1 Title 20200623-GaoF-241-1#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 292.6
6 Pulse Sequence zg30
7 Number of Scans 32
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2020-06-23T18:33:00
12 Modification Date 2020-06-23T18:34:00
0.99
2.04
3.10
0.99
1.03
0.99
1.03
3.01
3.12
3.00
3.00
1.02
2.96
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)

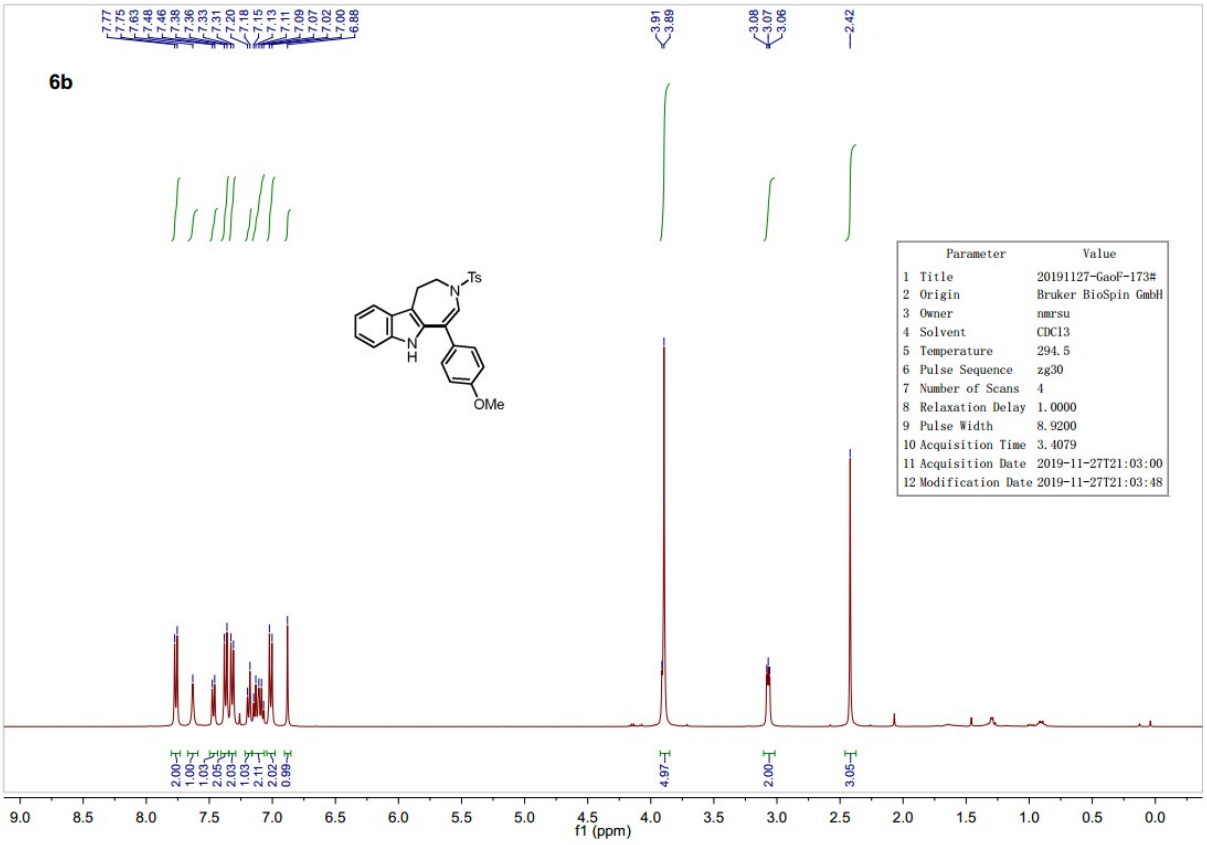

4l
MeO
MeO
Parameter Value
1 Title 20200624-GaoF-241-1#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 294.0
6 Pulse Sequence zgpg30
7 Number of Scans 200
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2020-06-24T20:36:00
12 Modification Date 2020-06-24T20:37:00
f1 (ppm)

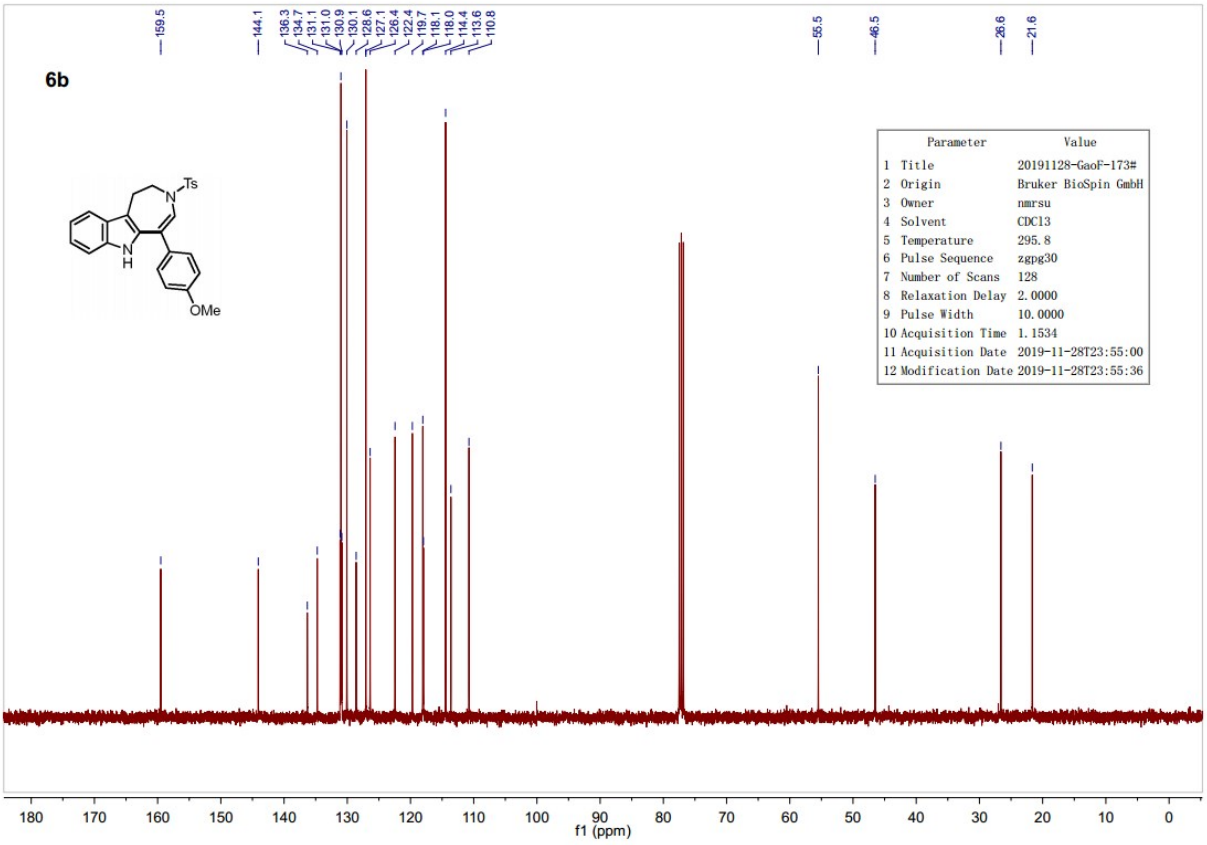

4m
Parameter Value
1 Title 20200624-GaoF-244-1#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 293.8
6 Pulse Sequence zg30
7 Number of Scans 16
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2020-06-24T19:57:00
12 Modification Date 2020-06-24T19:57:06
f1 (ppm)

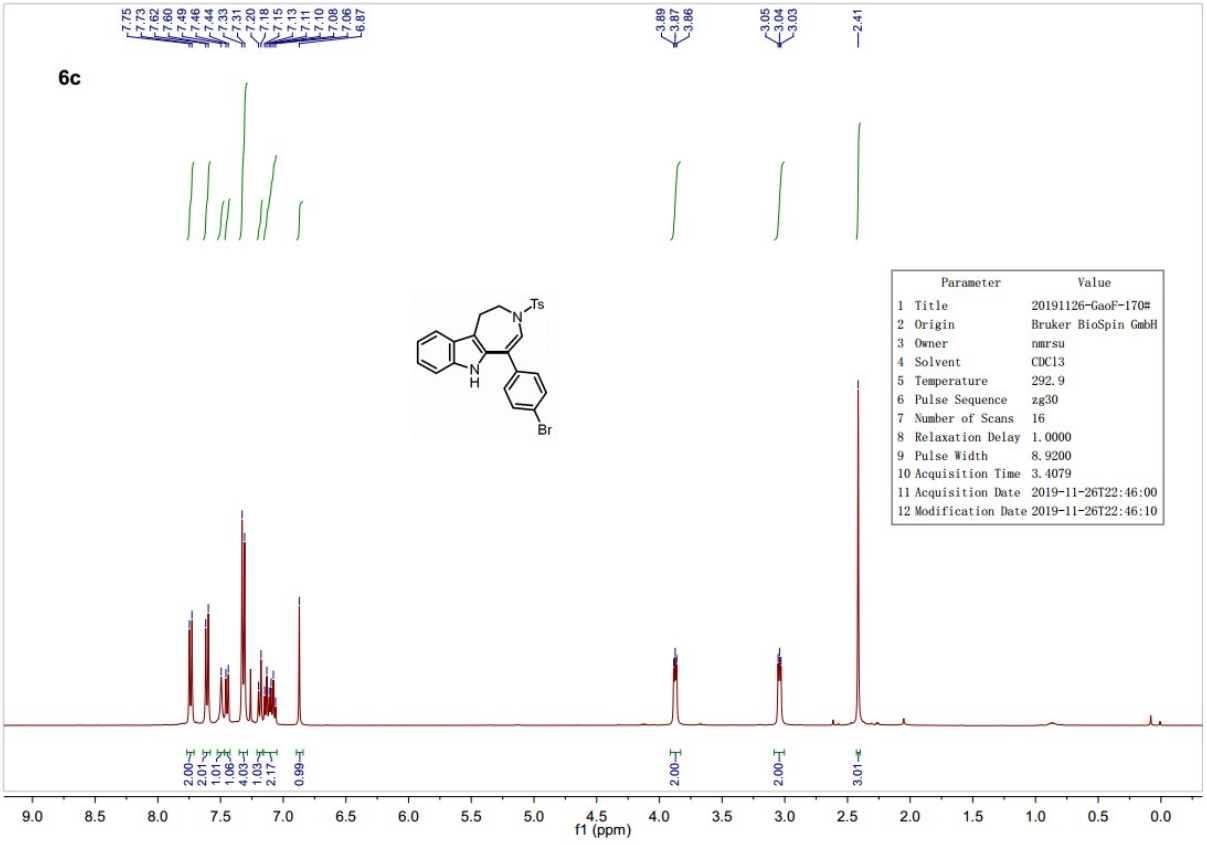

4m
210.9
207.8
145.0
142.1
137.7
126.6
126.0
123.0
122.2
121.3
121.0
120.0
119.8
119.6
118.8
114.2
110.5
109.7
60.1
55.2
54.9
33.0
30.6
28.5
26.8
24.2
Parameter Value
1 Title 20200624-GaoF-244-1#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 294.1
6 Pulse Sequence zgpg30
7 Number of Scans 200
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2020-06-24T20:08:00
12 Modification Date 2020-06-24T20:08:56
f1 (ppm)

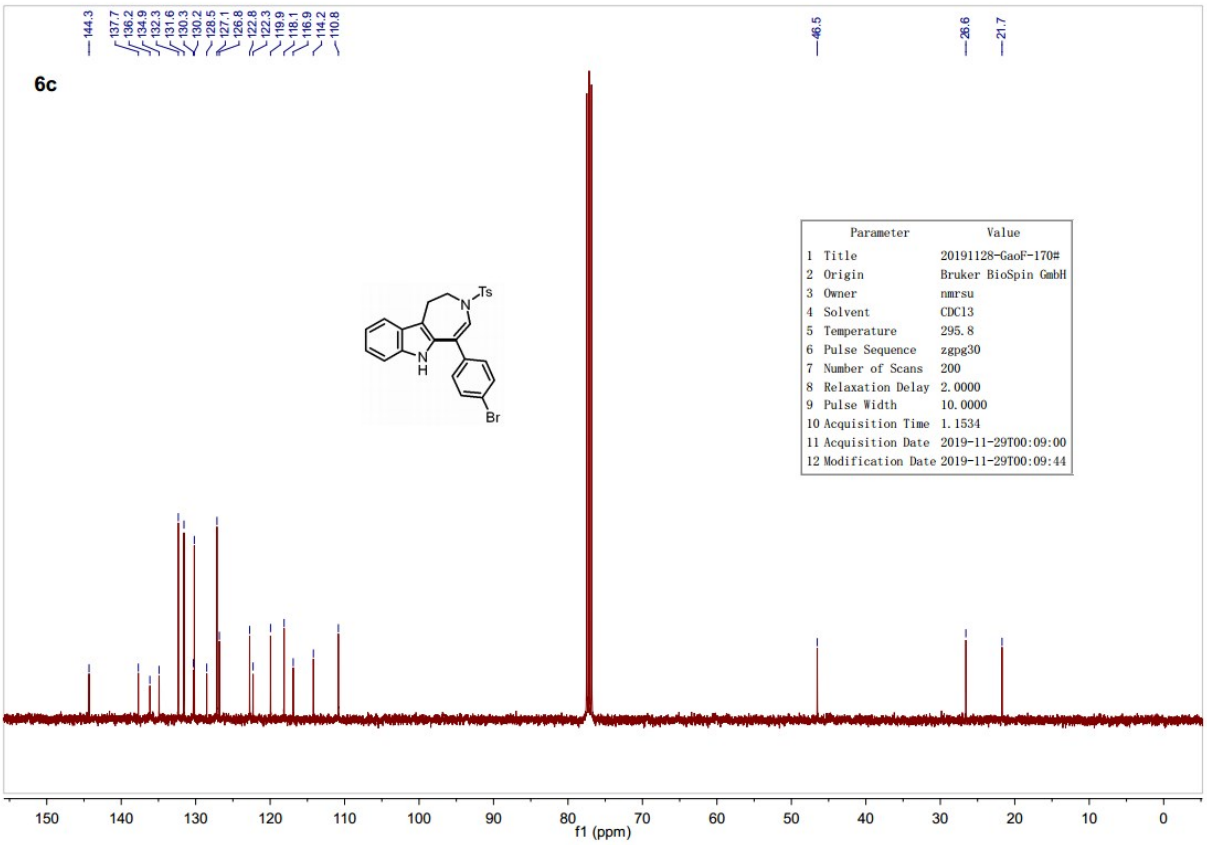

6a
7.78
7.76
7.60
7.52
7.50
7.49
7.47
7.46
7.45
7.34
7.32
7.19
7.17
7.15
7.14
7.11
7.09
7.07
6.92
3.93
3.91
3.90
3.09
3.08
3.07
2.43
Ts
N
H
Parameter Value
1 Title 20191203-GaoF-160-1#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 295.2
6 Pulse Sequence zg30
7 Number of Scans 4
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2019-12-03T21:37:00
12 Modification Date 2019-12-03T21:37:26
2.01
0.99
6.06
2.00
3.08
1.00
2.00
2.00
3.00
f1 (ppm)

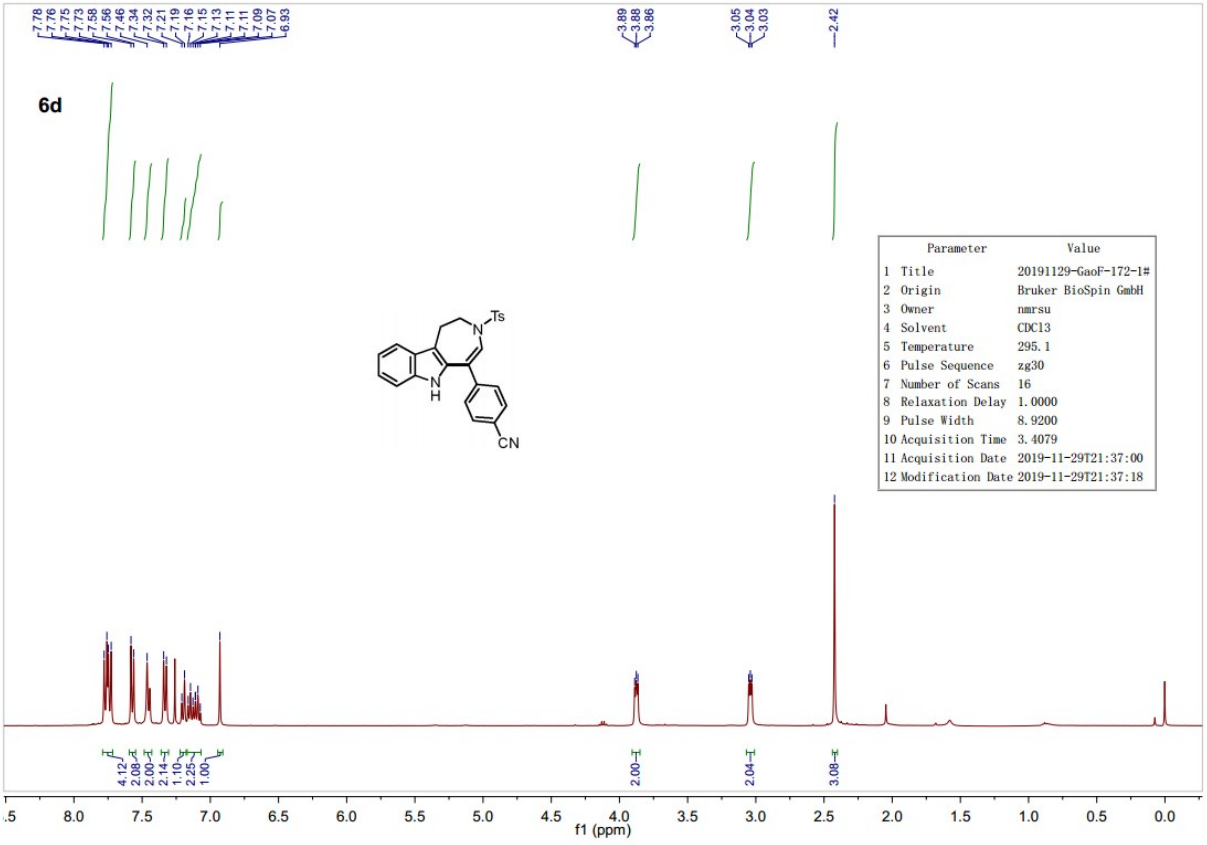

6a
144.2
138.7
136.3
134.8
130.1
129.9
129.1
128.1
127.1
122.5
119.8
118.3
118.1
113.8
110.8
46.5
26.6
21.7
Ts
N
H
Parameter Value
1 Title 20191204-GaoF-160-1#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 295.7
6 Pulse Sequence zgpg30
7 Number of Scans 200
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2019-12-04T21:45:00
12 Modification Date 2019-12-04T21:45:52
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

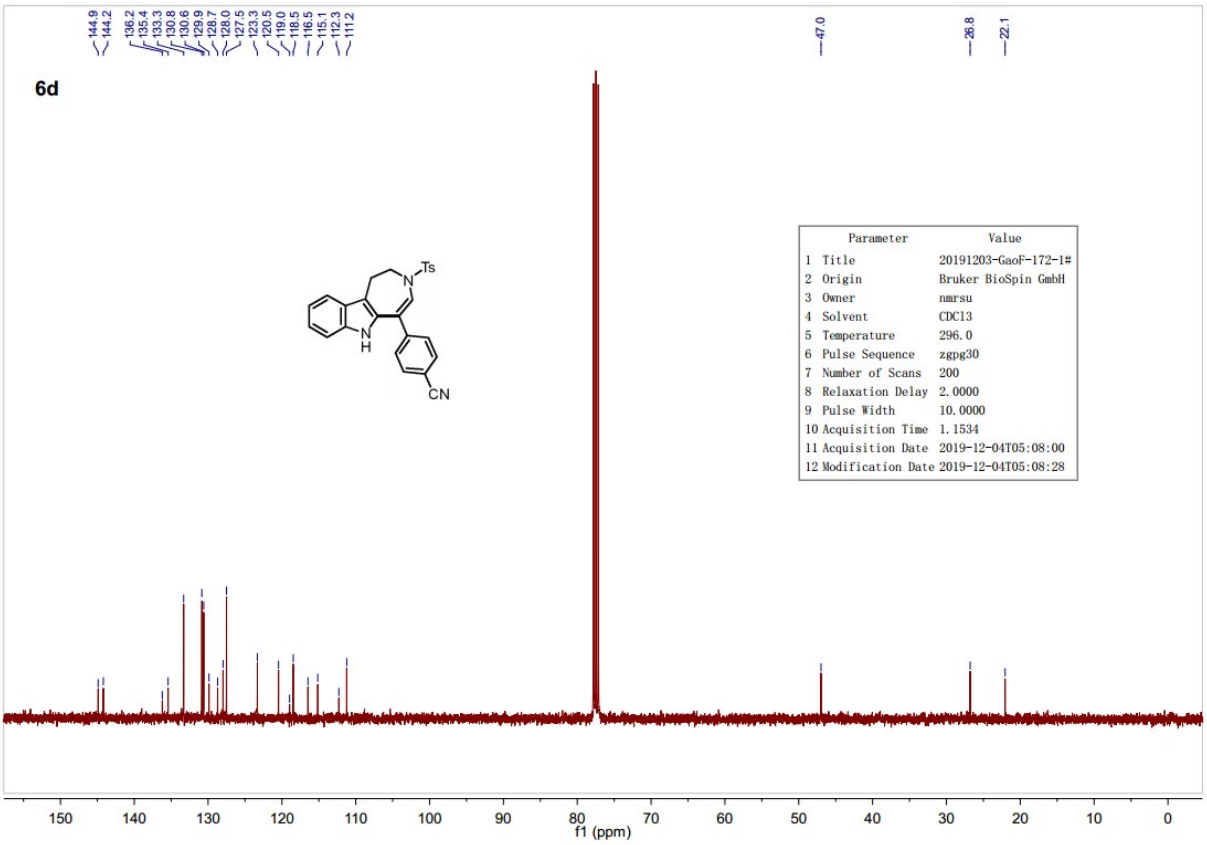

6b
7.77
7.75
7.63
7.48
7.46
7.38
7.36
7.33
7.31
7.20
7.18
7.15
7.13
7.11
7.09
7.07
7.02
7.00
6.88
3.91
3.89
3.08
3.07
3.06
2.42
Ts
N
H
OMe
Parameter Value
1 Title 20191127-GaoF-173#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 294.5
6 Pulse Sequence zg30
7 Number of Scans 4
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2019-11-27T21:03:00
12 Modification Date 2019-11-27T21:03:48
2.00
1.00
1.03
2.05
2.03
1.03
2.11
2.02
0.99
4.97
2.00
3.05
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)

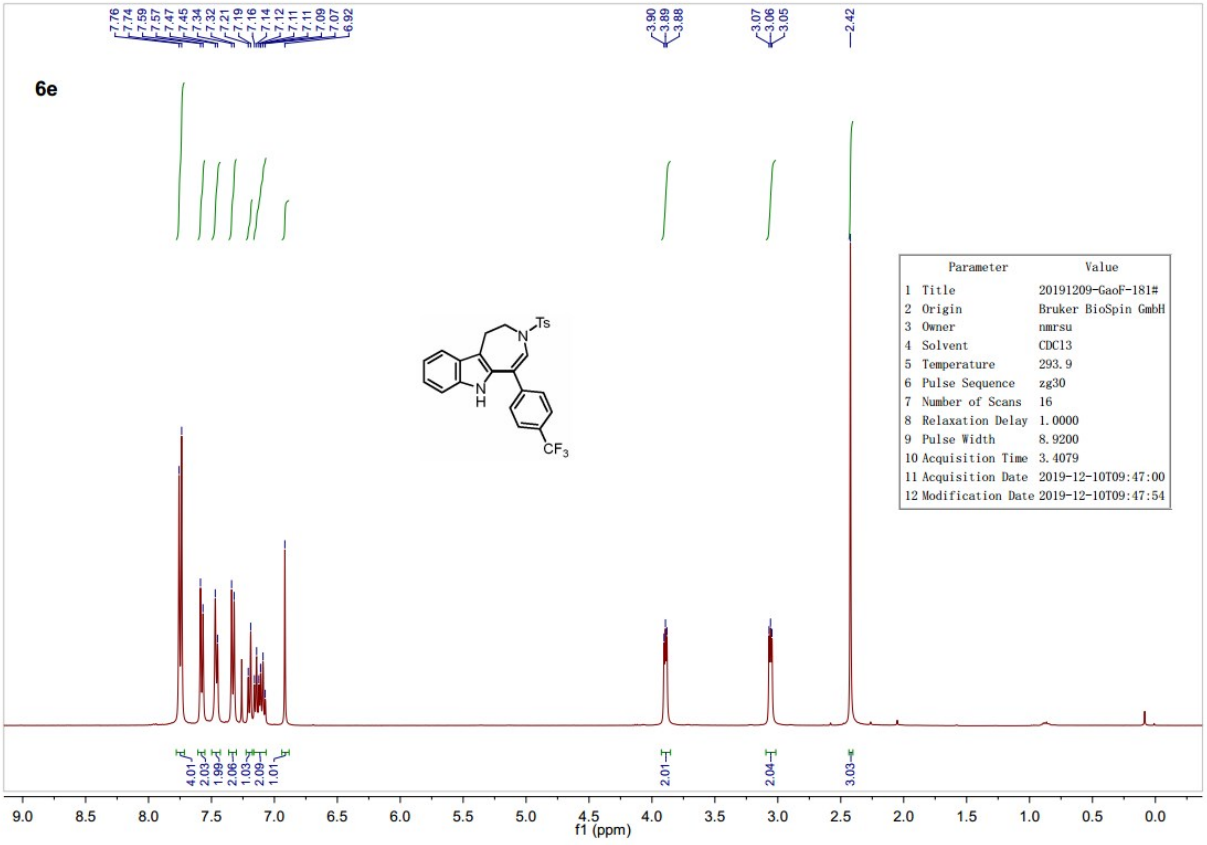

6b
159.5
144.1
136.3
134.7
131.1
131.0
130.9
130.1
128.6
127.1
126.4
122.4
119.7
118.1
118.0
114.4
113.6
110.8
55.5
46.5
26.6
21.6
Ts
N
H
OMe
Parameter Value
1 Title 20191128-GaoF-173#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 295.8
6 Pulse Sequence zgpg30
7 Number of Scans 128
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2019-11-28T23:55:00
12 Modification Date 2019-11-28T23:55:36
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

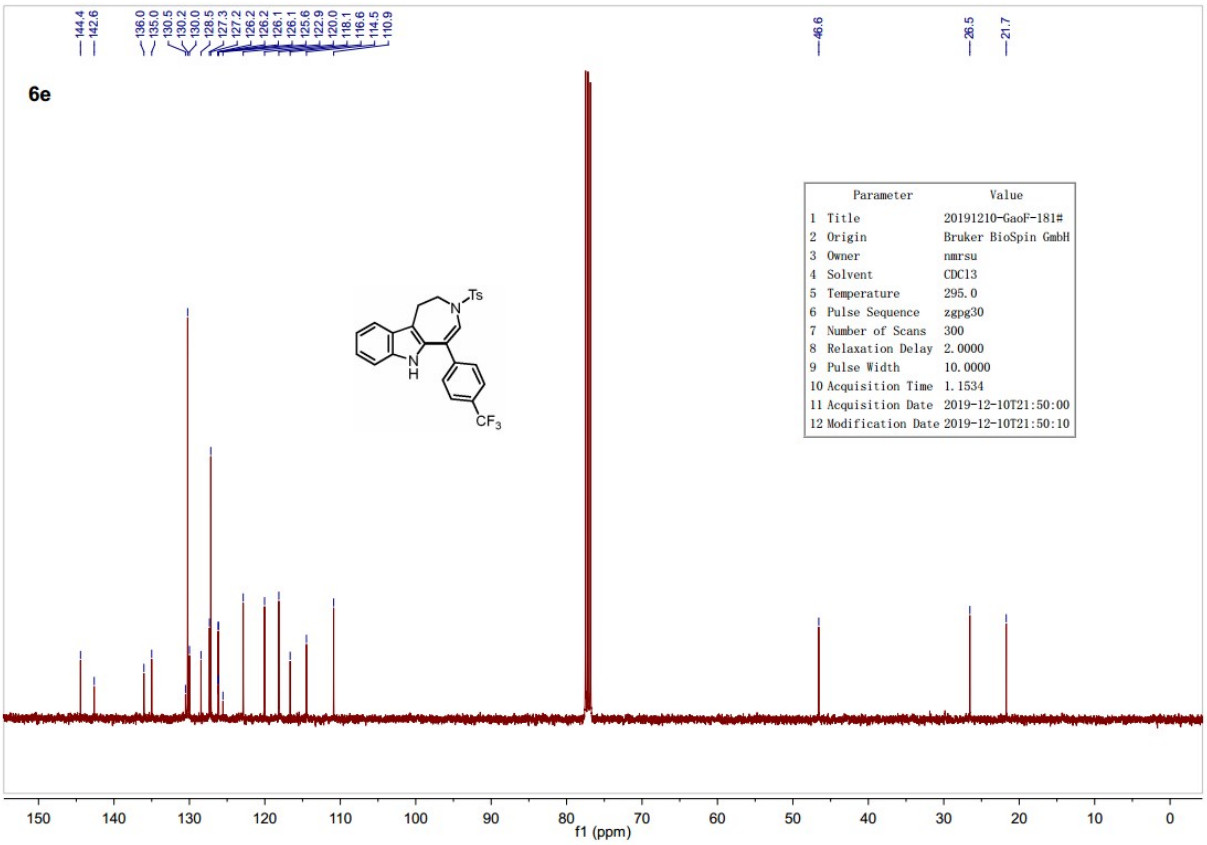

6c
7.75
7.73
7.62
7.60
7.49
7.46
7.44
7.33
7.31
7.20
7.18
7.15
7.13
7.11
7.10
7.08
7.06
6.87
3.89
3.87
3.86
3.05
3.04
3.03
2.41
Ts
N
H
Br
Parameter Value
1 Title 20191126-GaoF-170#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 292.9
6 Pulse Sequence zg30
7 Number of Scans 16
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2019-11-26T22:46:00
12 Modification Date 2019-11-26T22:46:10
2.00
2.01
1.01
1.08
4.03
1.03
2.17
0.99
2.00
2.00
3.01
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)

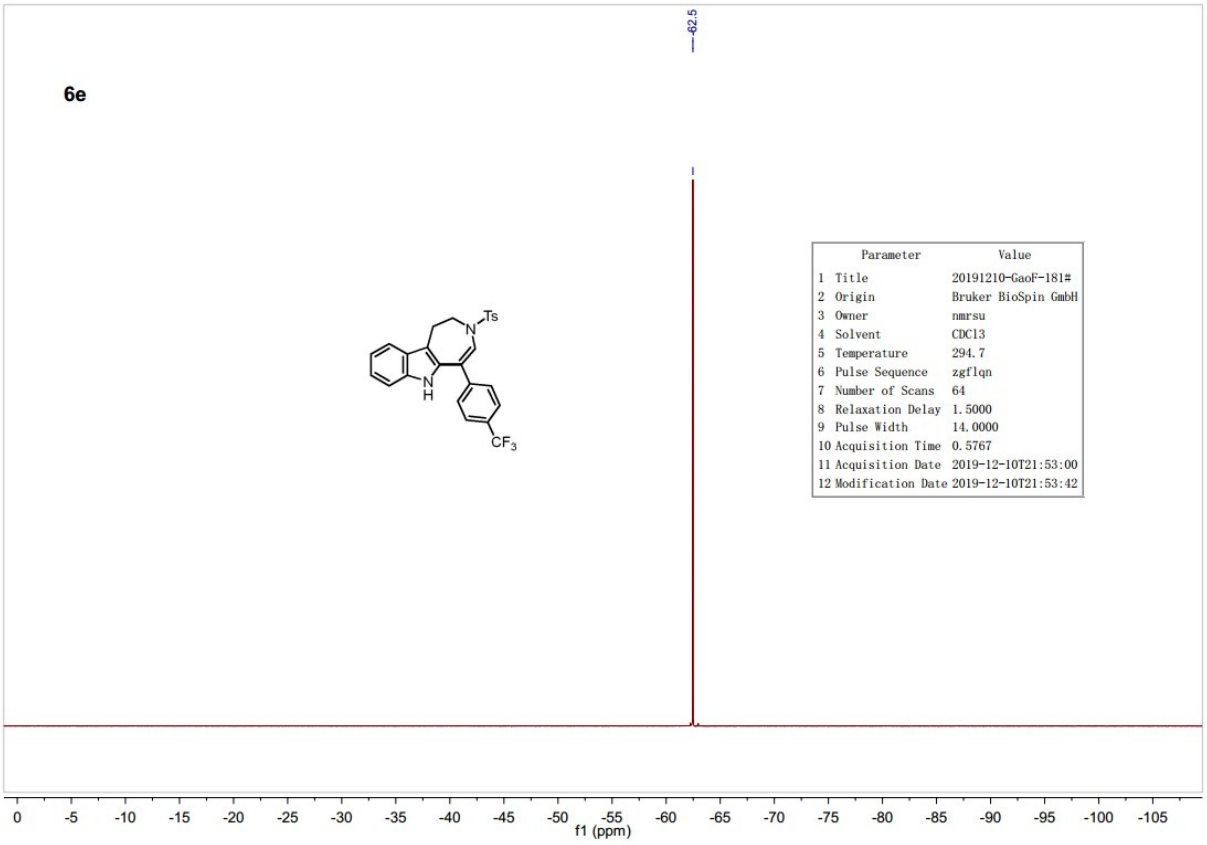

6c
144.3
137.7
136.2
134.9
132.3
131.6
130.3
130.2
128.5
127.1
126.8
122.8
122.3
119.9
118.1
116.9
114.2
110.8
46.5
26.6
21.7
Ts
N
H
Br
Parameter Value
1 Title 20191128-GaoF-170#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 295.8
6 Pulse Sequence zgpg30
7 Number of Scans 200
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2019-11-29T00:09:00
12 Modification Date 2019-11-29T00:09:44
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

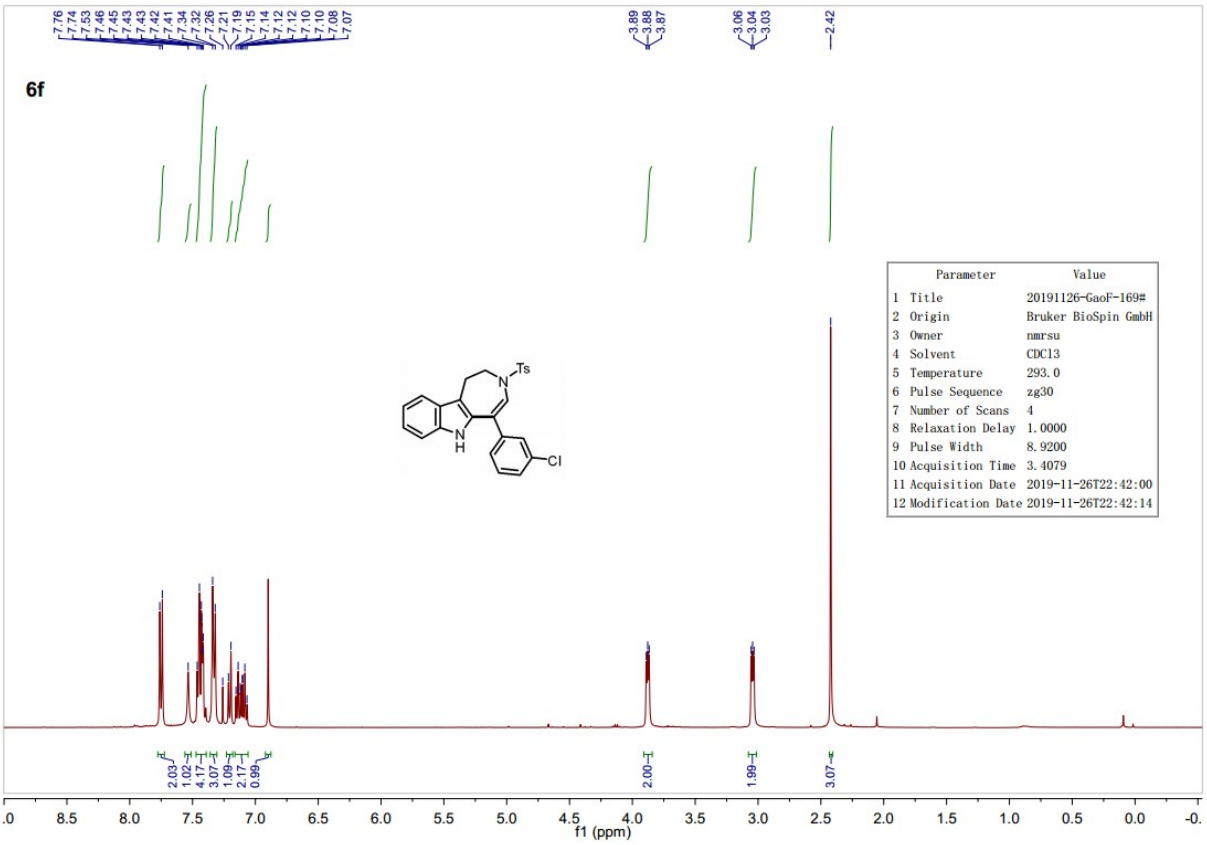

6d
7.78
7.76
7.75
7.73
7.58
7.56
7.46
7.34
7.32
7.21
7.19
7.16
7.15
7.13
7.11
7.11
7.09
7.07
6.93
3.89
3.88
3.86
3.05
3.04
3.03
2.42
Ts
N
H
CN
Parameter Value
1 Title 20191129-GaoF-172-1#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 295.1
6 Pulse Sequence zg30
7 Number of Scans 16
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2019-11-29T21:37:00
12 Modification Date 2019-11-29T21:37:18
4.12
2.08
2.00
2.14
1.10
2.25
1.00
2.00
2.04
3.08
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)

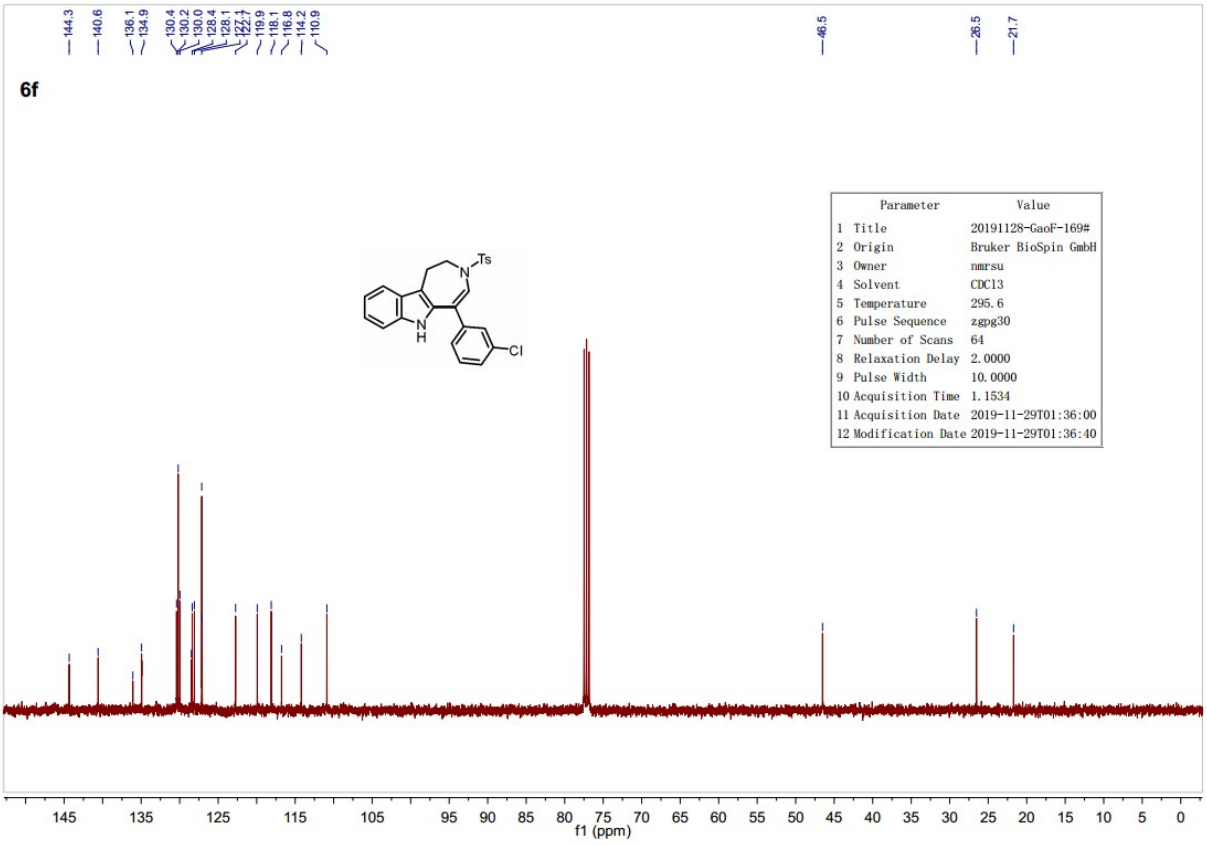

6d
144.9
144.2
136.2
135.4
133.3
130.8
130.6
129.9
128.7
128.0
127.5
123.3
120.5
119.0
118.5
116.5
115.1
112.3
111.2
47.0
26.8
22.1
Ts
N
H
CN
Parameter Value
1 Title 20191203-GaoF-172-1#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 296.0
6 Pulse Sequence zgpg30
7 Number of Scans 200
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2019-12-04T05:08:00
12 Modification Date 2019-12-04T05:08:28
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

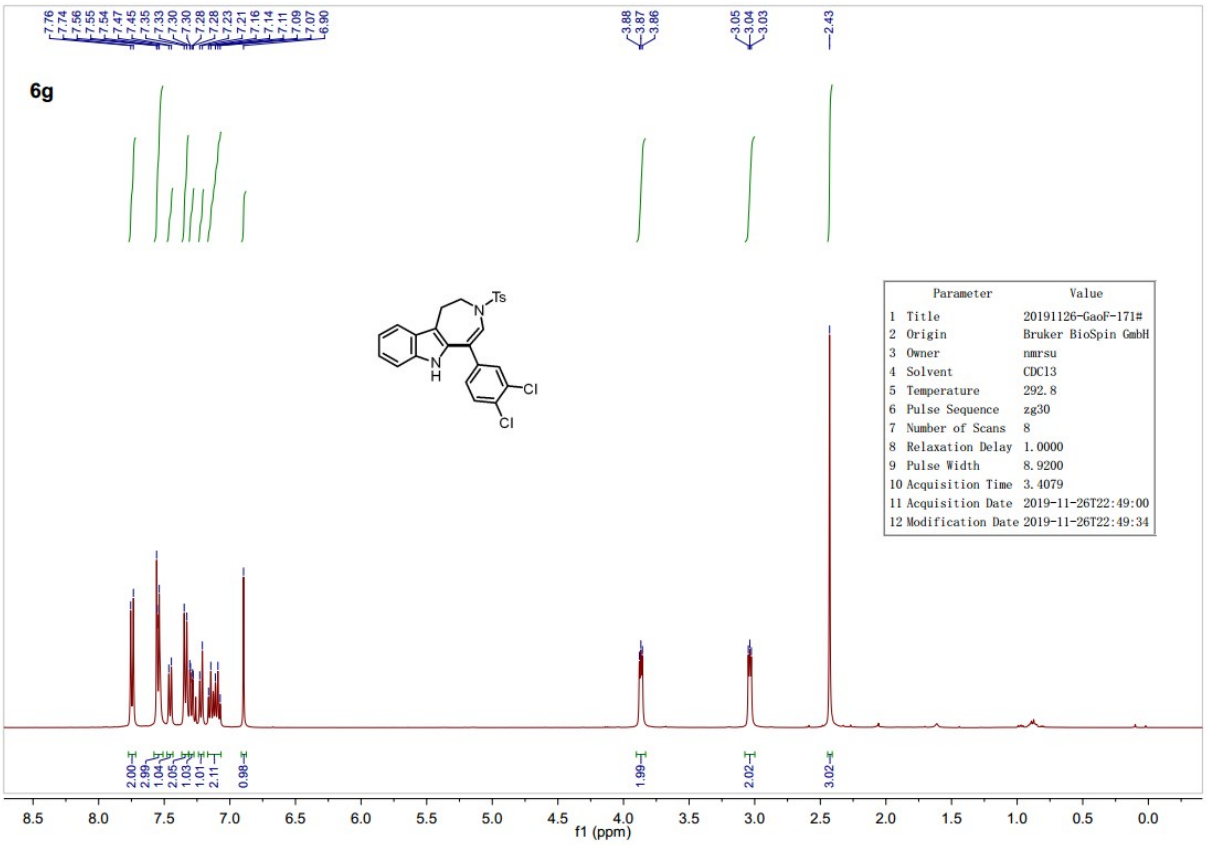

6e
7.76
7.74
7.59
7.57
7.47
7.45
7.34
7.32
7.21
7.19
7.16
7.14
7.12
7.11
7.11
7.09
7.07
6.92
3.90
3.89
3.88
3.07
3.06
3.05
2.42
Ts
N
H
CF3
Parameter Value
1 Title 20191209-GaoF-181#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 293.9
6 Pulse Sequence zg30
7 Number of Scans 16
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2019-12-10T09:47:00
12 Modification Date 2019-12-10T09:47:54
4.01
2.03
1.99
2.06
1.03
2.09
1.01
2.01
2.04
3.03
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)

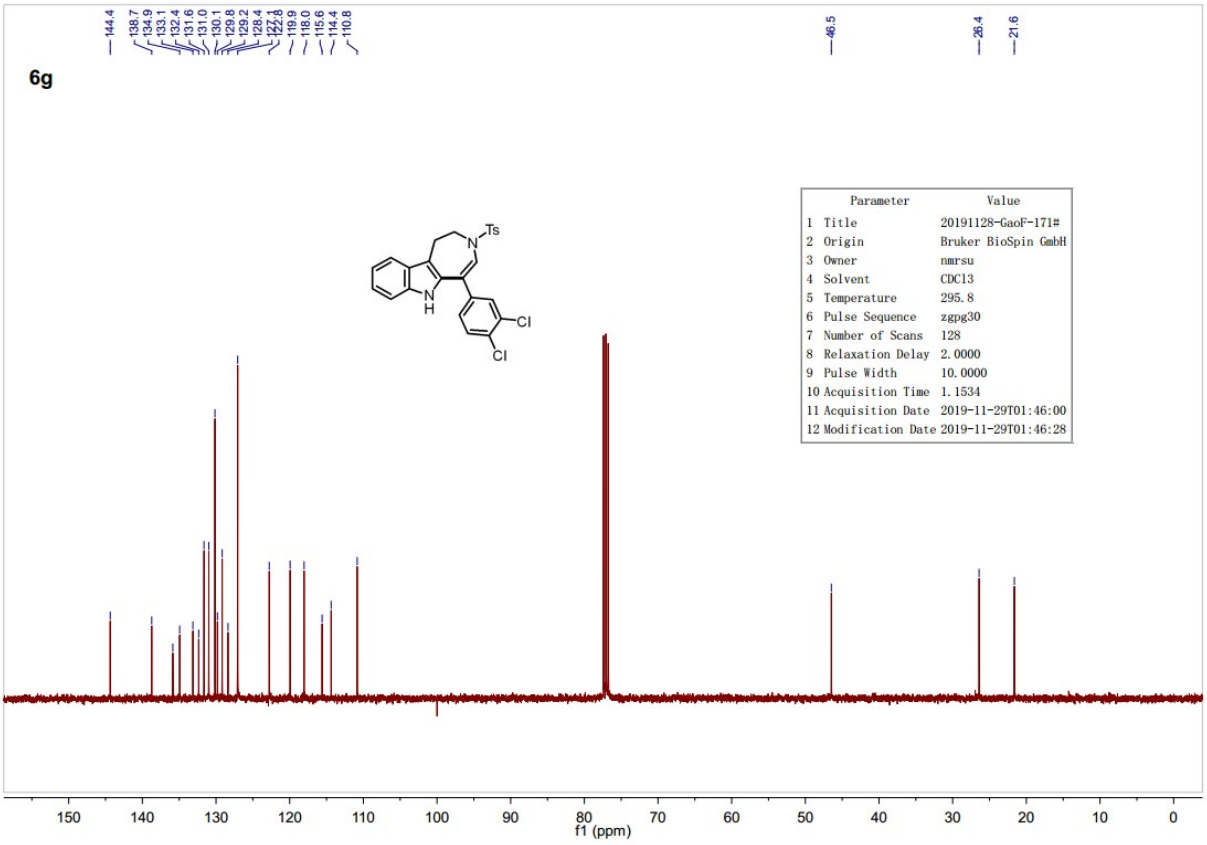

144.4
142.6
136.0
135.0
130.5
130.2
130.0
128.5
127.3
127.2
126.2
126.1
126.1
125.6
122.9
120.0
118.1
116.6
114.5
110.9
46.6
26.5
21.7
6e
Ts
N
H
CF3
Parameter Value
1 Title 20191210-GaoF-181#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 295.0
6 Pulse Sequence zgpg30
7 Number of Scans 300
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2019-12-10T21:50:00
12 Modification Date 2019-12-10T21:50:10
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

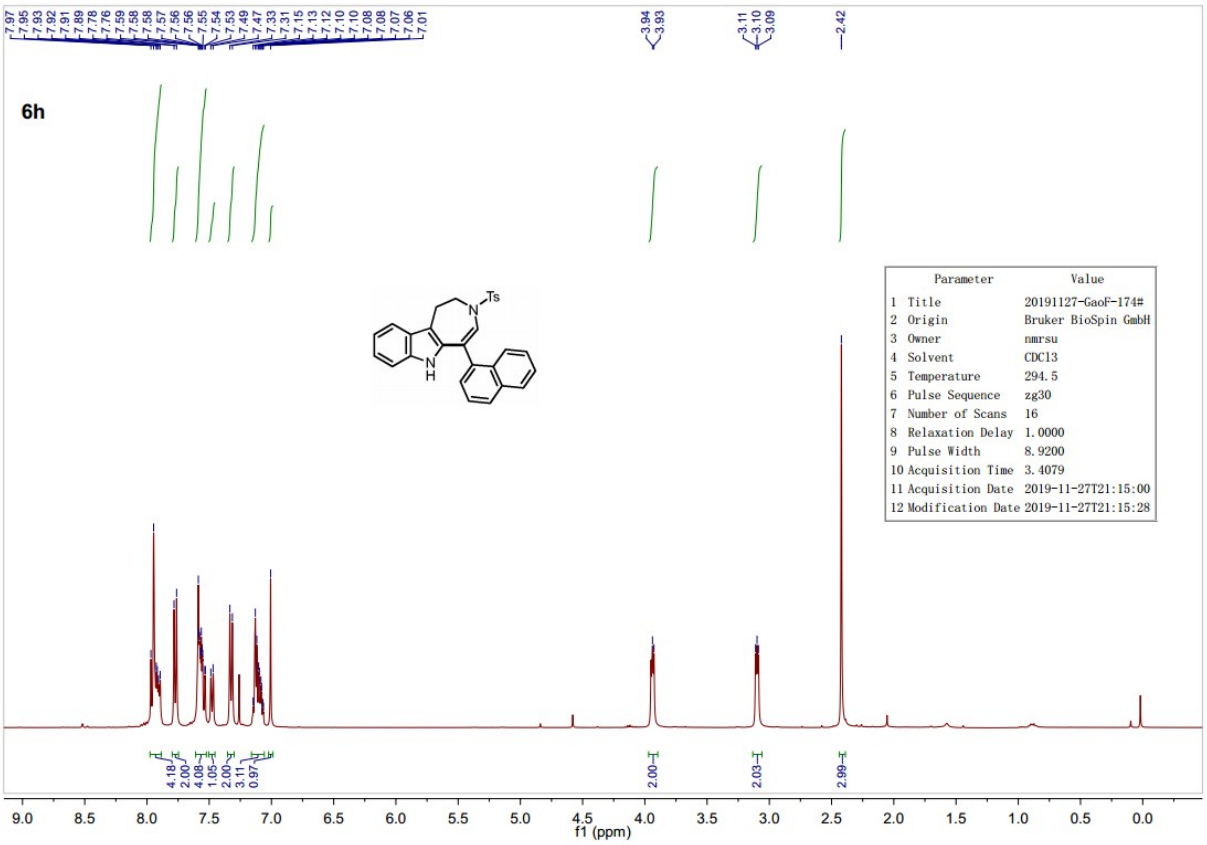

62.5
6e
Ts
N
H
CF3
Parameter Value
1 Title 20191210-GaoF-181#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 294.7
6 Pulse Sequence zgflqn
7 Number of Scans 64
8 Relaxation Delay 1.5000
9 Pulse Width 14.0000
10 Acquisition Time 0.5767
11 Acquisition Date 2019-12-10T21:53:00
12 Modification Date 2019-12-10T21:53:42
0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105
f1 (ppm)

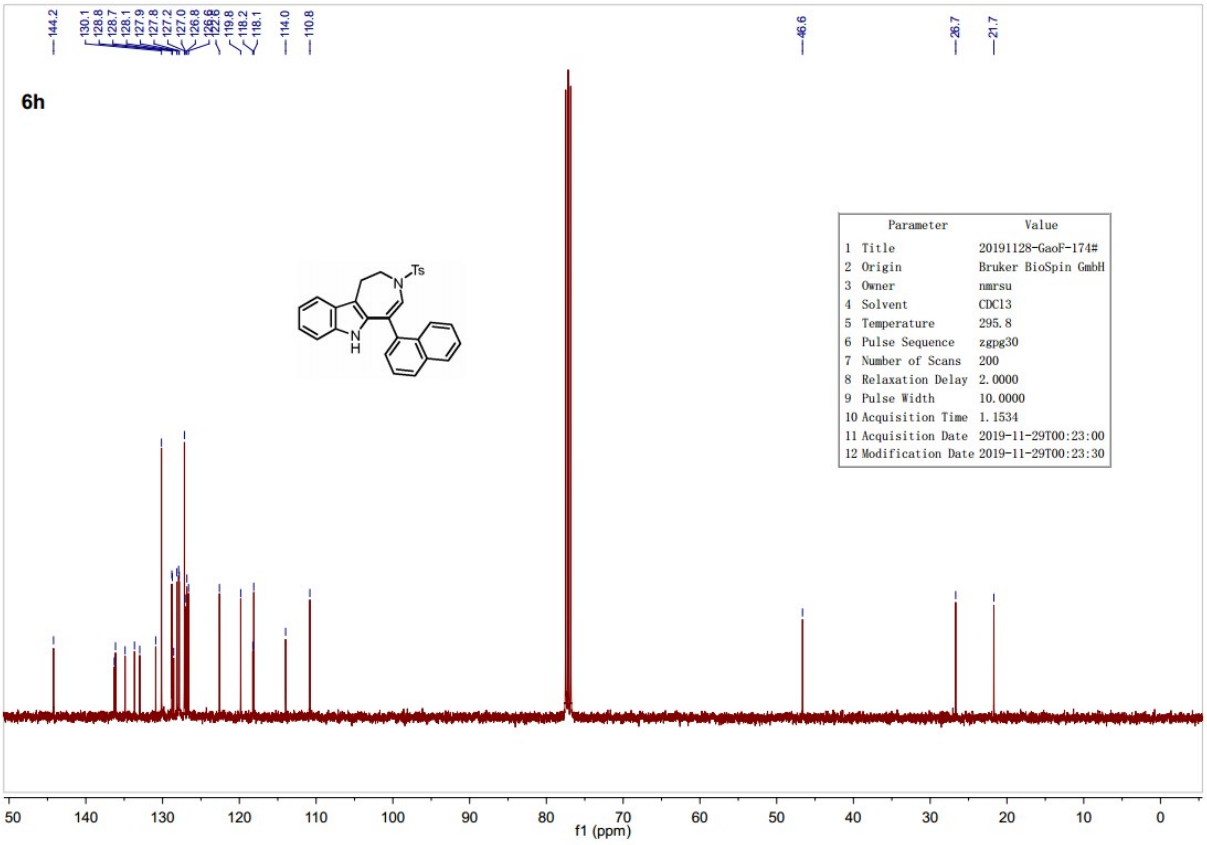

6f
7.76
7.74
7.53
7.46
7.45
7.43
7.43
7.42
7.41
7.34
7.32
7.26
7.21
7.19
7.15
7.14
7.12
7.12
7.10
7.10
7.08
7.07
3.89
3.88
3.87
3.06
3.04
3.03
2.42
Parameter Value
1 Title 20191126-GaoF-169#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 293.0
6 Pulse Sequence zg30
7 Number of Scans 4
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2019-11-26T22:42:00
12 Modification Date 2019-11-26T22:42:14
Ts
N
H
Cl
2.03
1.02
4.17
3.07
1.09
2.17
0.99
2.00
1.99
3.07
f1 (ppm)

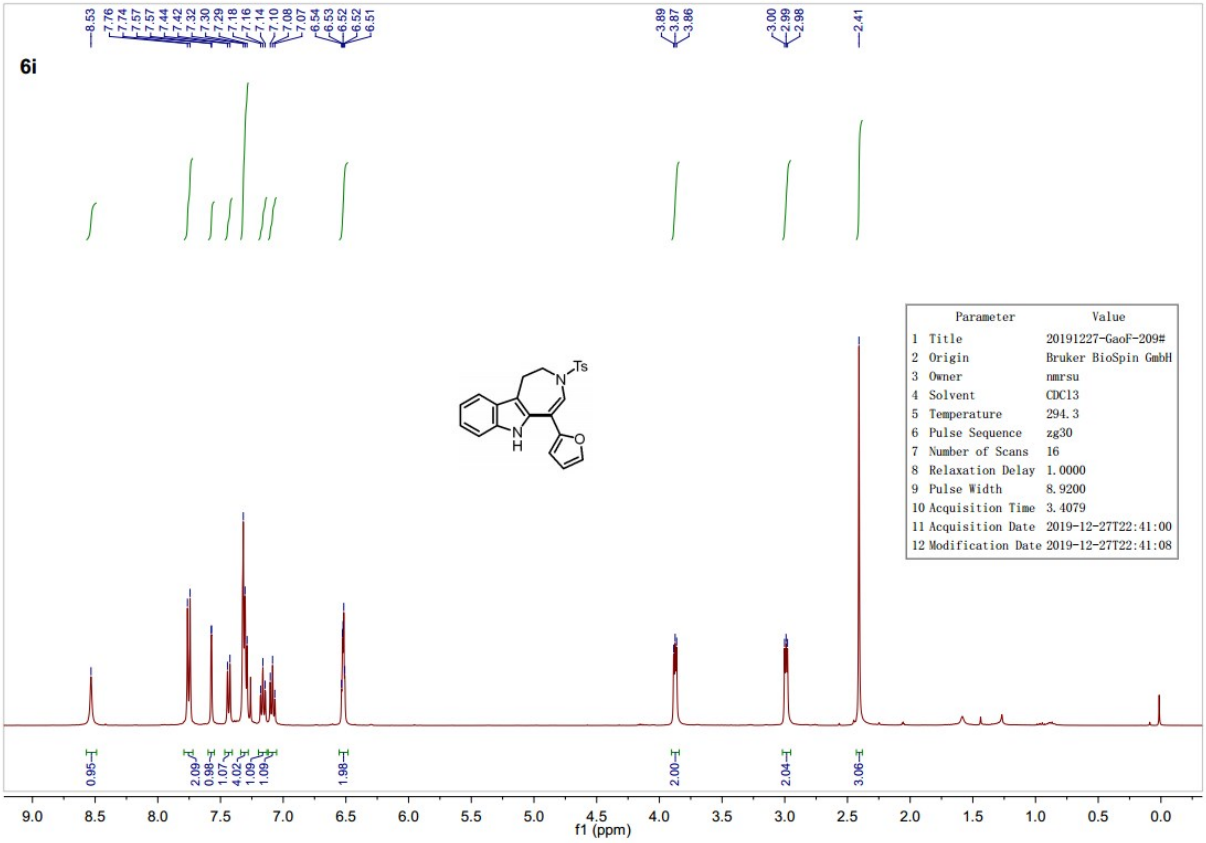

6f
144.3
140.6
136.1
134.9
130.4
130.2
130.0
128.4
128.1
127.1
122.7
119.9
118.1
116.8
114.2
110.9
46.5
26.5
21.7
Parameter Value
1 Title 20191128-GaoF-169#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 295.6
6 Pulse Sequence zgpg30
7 Number of Scans 64
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2019-11-29T01:36:00
12 Modification Date 2019-11-29T01:36:40
Ts
N
H
Cl
f1 (ppm)

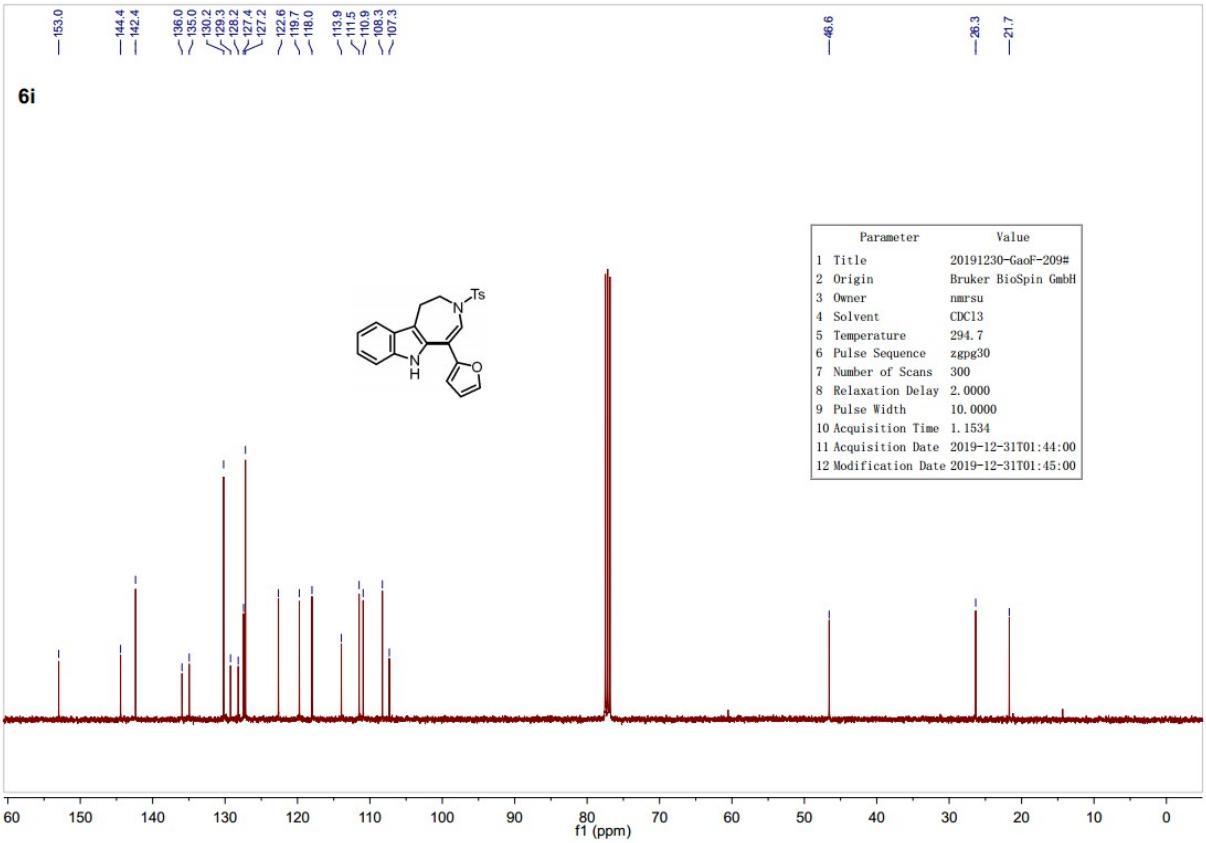

6g
7.76
7.74
7.56
7.55
7.54
7.47
7.45
7.35
7.33
7.30
7.28
7.23
7.21
7.16
7.14
7.11
7.09
7.07
6.90
3.88
3.87
3.86
3.05
3.04
3.03
2.43
Ts
N
H
Cl
Cl
Parameter Value
1 Title 20191126-GaoF-171#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 292.8
6 Pulse Sequence zg30
7 Number of Scans 8
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2019-11-26T22:49:00
12 Modification Date 2019-11-26T22:49:34
2.00
2.99
1.04
2.05
1.03
1.01
2.11
0.98
1.99
2.02
3.02
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)

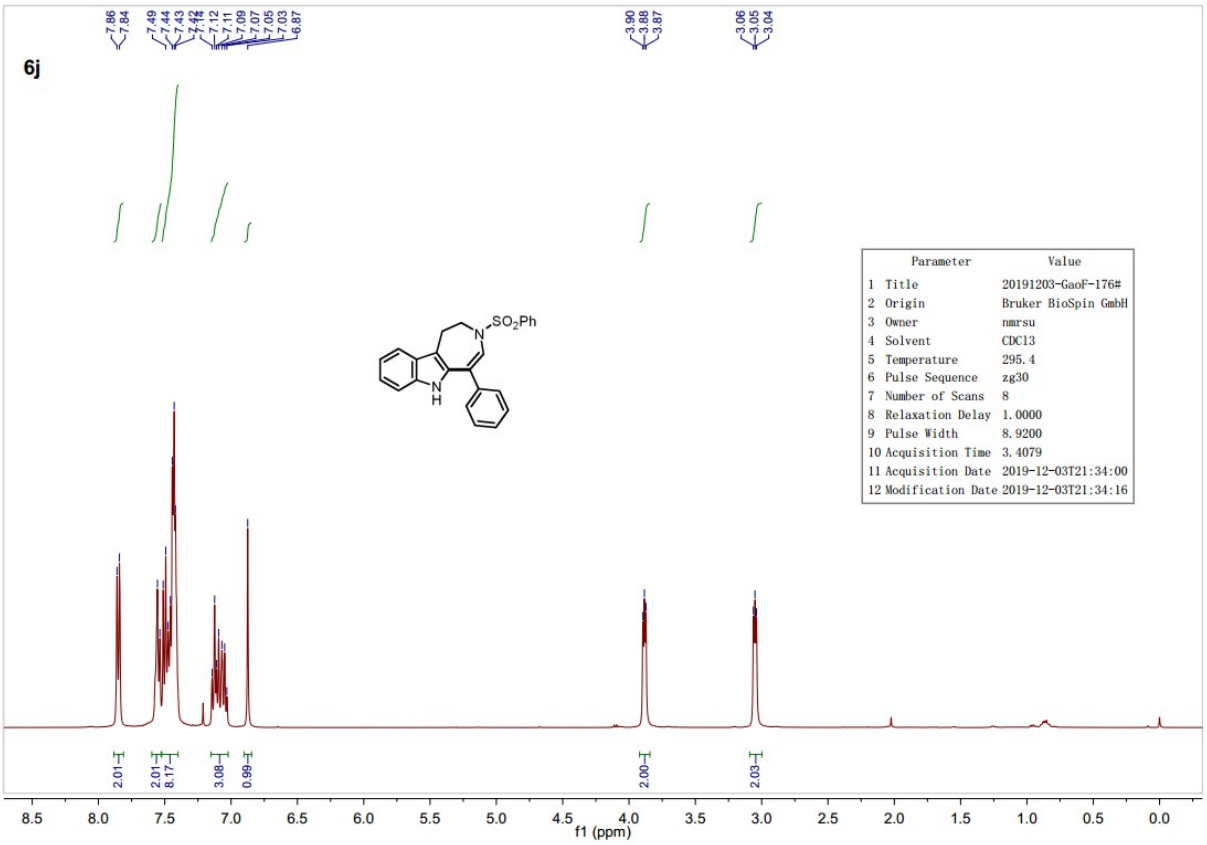

6g
144.4
138.7
134.9
133.1
132.4
131.6
131.0
130.1
129.8
129.2
128.4
122.8
119.9
118.0
115.6
114.4
110.8
46.5
26.4
21.6
Ts
N
H
Cl
Cl
Parameter Value
1 Title 20191128-GaoF-171#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 295.8
6 Pulse Sequence zgpg30
7 Number of Scans 128
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2019-11-29T01:46:00
12 Modification Date 2019-11-29T01:46:28
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

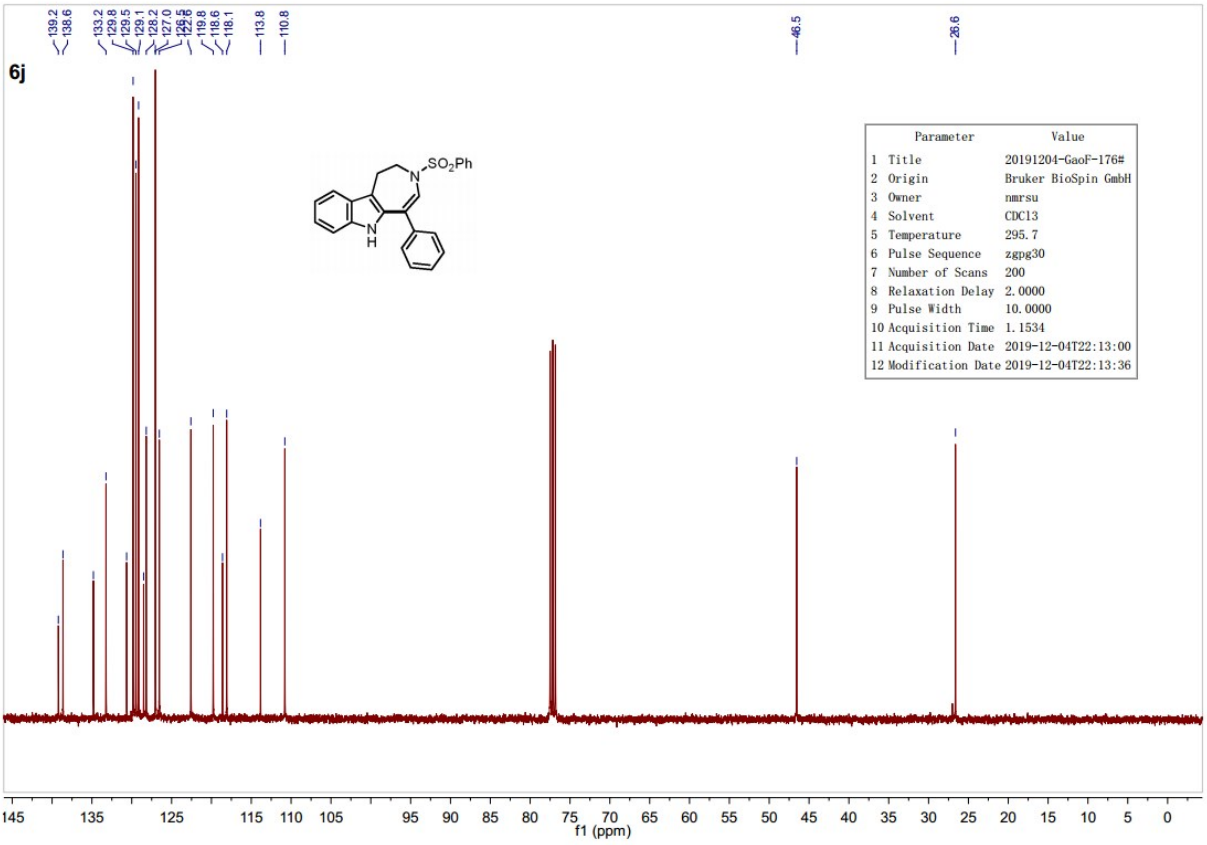

6h
7.97
7.95
7.93
7.92
7.91
7.89
7.78
7.76
7.59
7.58
7.57
7.56
7.56
7.55
7.54
7.53
7.49
7.47
7.33
7.31
7.15
7.13
7.12
7.10
7.10
7.08
7.08
7.07
7.06
7.01
3.94
3.93
3.11
3.10
3.09
2.42
Ts
N
H
Parameter Value
1 Title 20191127-GaoF-174#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 294.5
6 Pulse Sequence zg30
7 Number of Scans 16
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2019-11-27T21:15:00
12 Modification Date 2019-11-27T21:15:28
4.18
2.00
4.08
1.05
2.00
3.11
0.97
2.00
2.03
2.99
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)

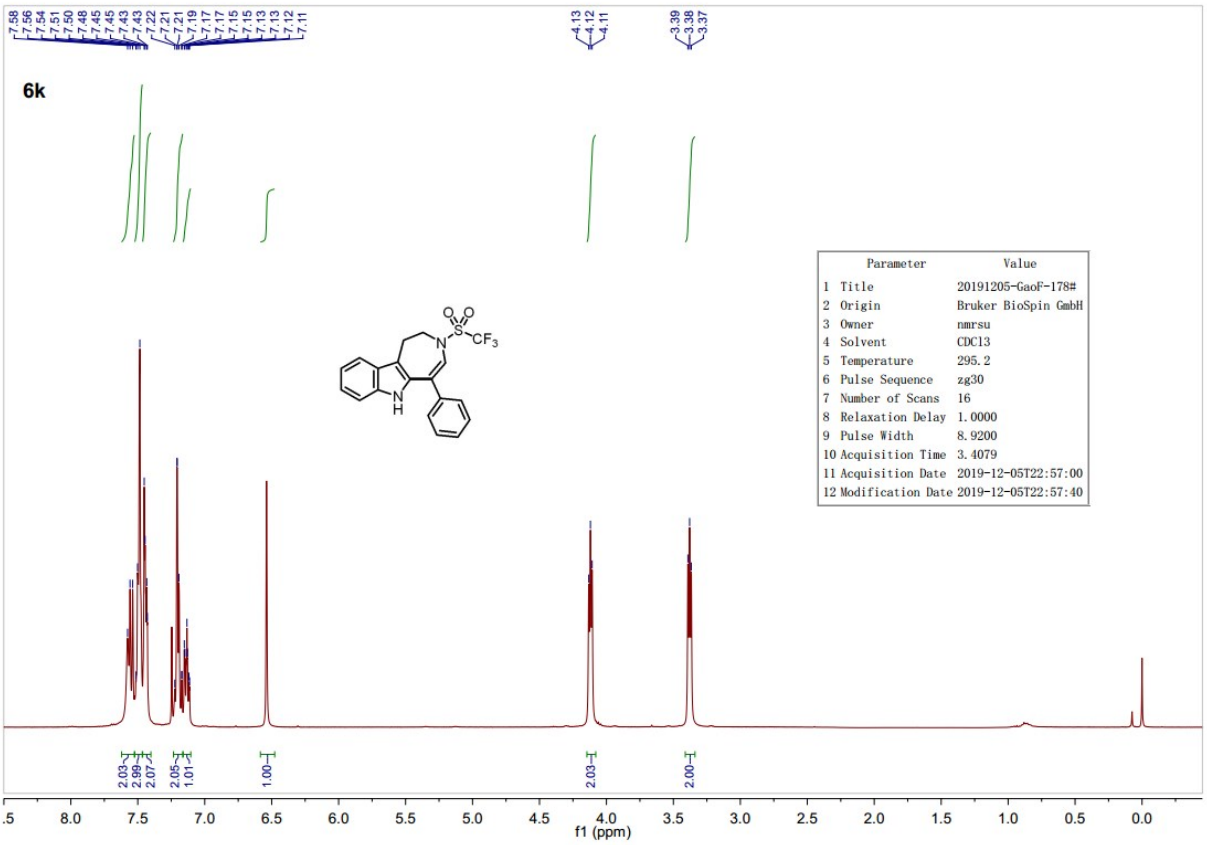

6h
144.2
130.1
128.8
128.7
128.1
127.9
127.8
127.2
127.0
126.8
119.8
118.2
118.1
114.0
110.8
46.6
26.7
21.7
Ts
N
H
Parameter Value
1 Title 20191128-GaoF-174#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 295.8
6 Pulse Sequence zgpg30
7 Number of Scans 200
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2019-11-29T00:23:00
12 Modification Date 2019-11-29T00:23:30
50 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

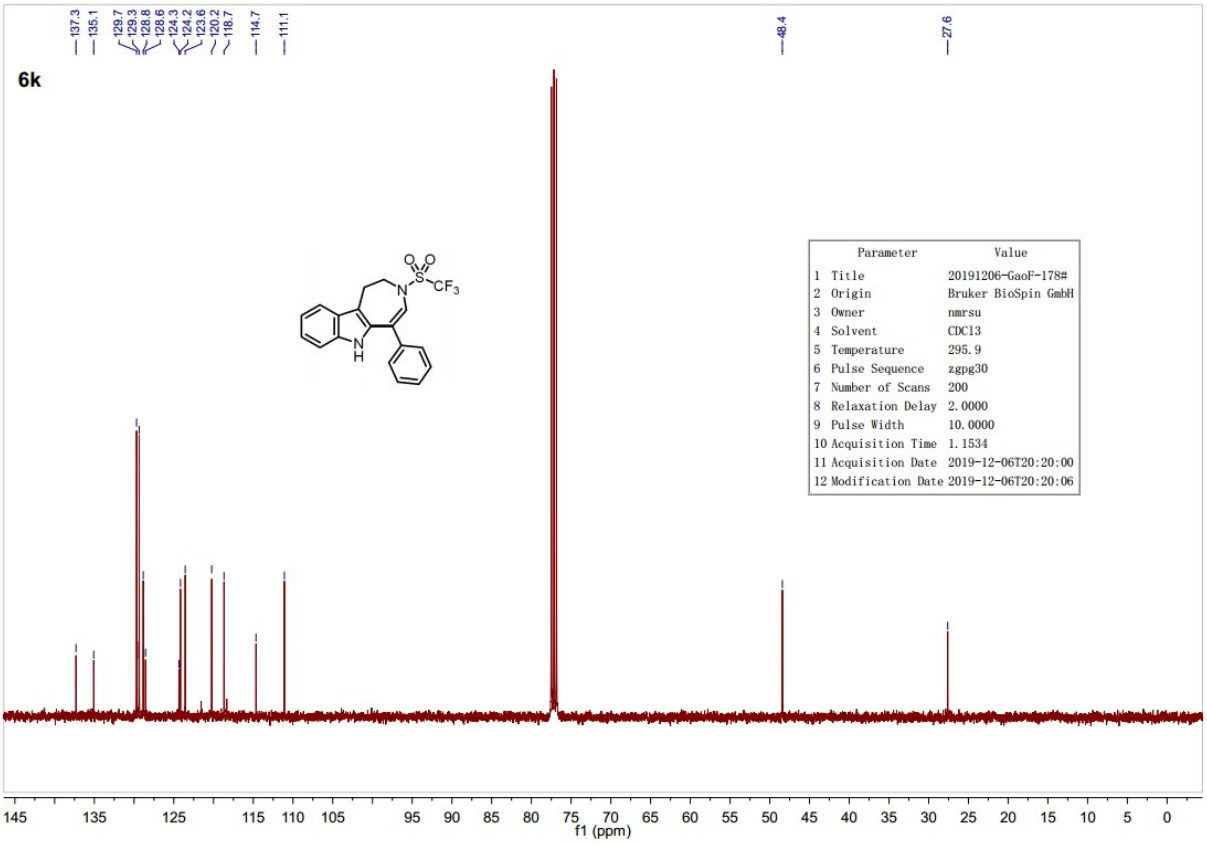

6i
8.53
7.76
7.74
7.57
7.57
7.44
7.42
7.32
7.30
7.29
7.18
7.16
7.14
7.10
7.08
7.07
6.54
6.53
6.52
6.52
6.51
3.89
3.87
3.86
3.00
2.99
2.98
2.41
Ts
N
H
O
Parameter Value
1 Title 20191227-GaoF-209#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 294.3
6 Pulse Sequence zg30
7 Number of Scans 16
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2019-12-27T22:41:00
12 Modification Date 2019-12-27T22:41:08
0.95
2.09
0.98
1.07
4.02
1.09
1.09
1.98
2.00
2.04
3.06
f1 (ppm)

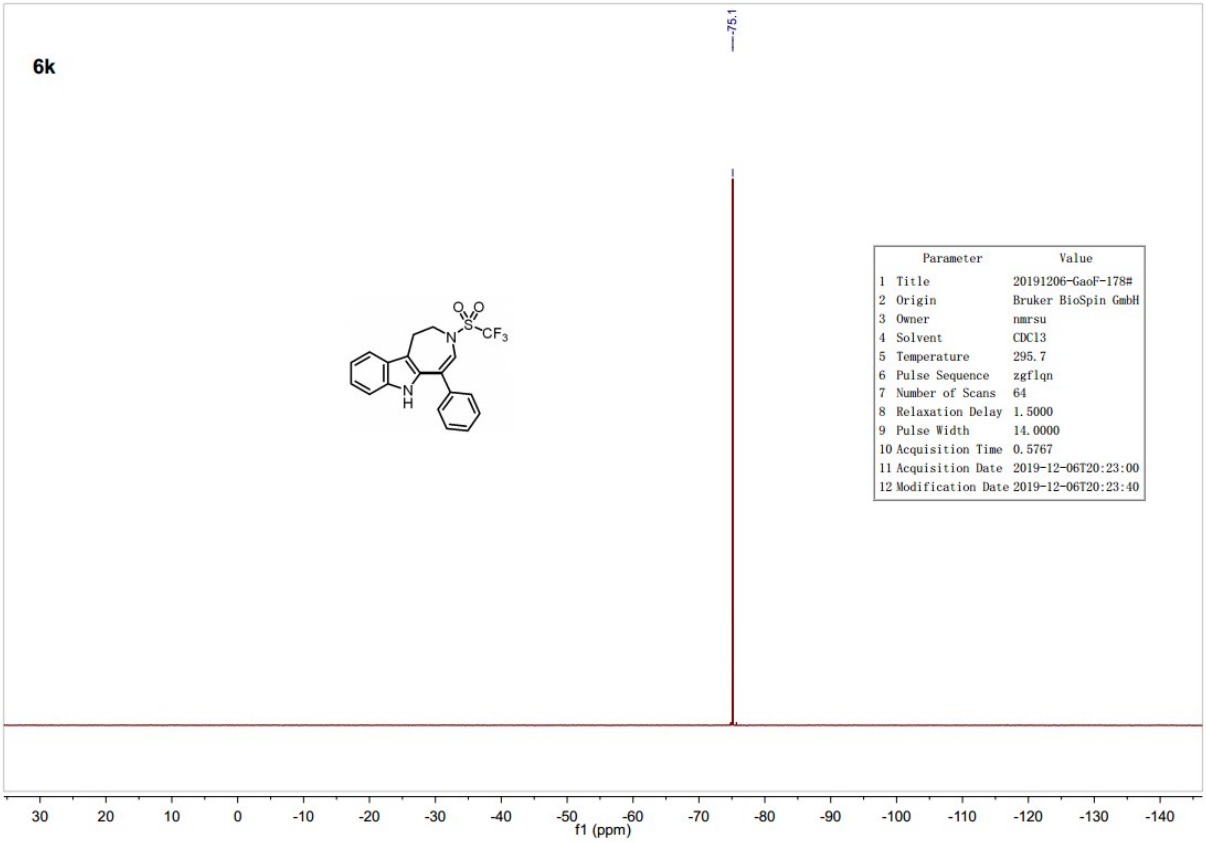

6i
153.0
144.4
142.4
136.0
135.0
130.2
129.3
128.2
127.4
127.2
122.6
119.7
118.0
113.9
111.5
110.9
108.3
107.3
46.6
26.3
21.7
Ts
N
H
O
Parameter Value
1 Title 20191230-GaoF-209#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 294.7
6 Pulse Sequence zgpg30
7 Number of Scans 300
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2019-12-31T01:44:00
12 Modification Date 2019-12-31T01:45:00
f1 (ppm)

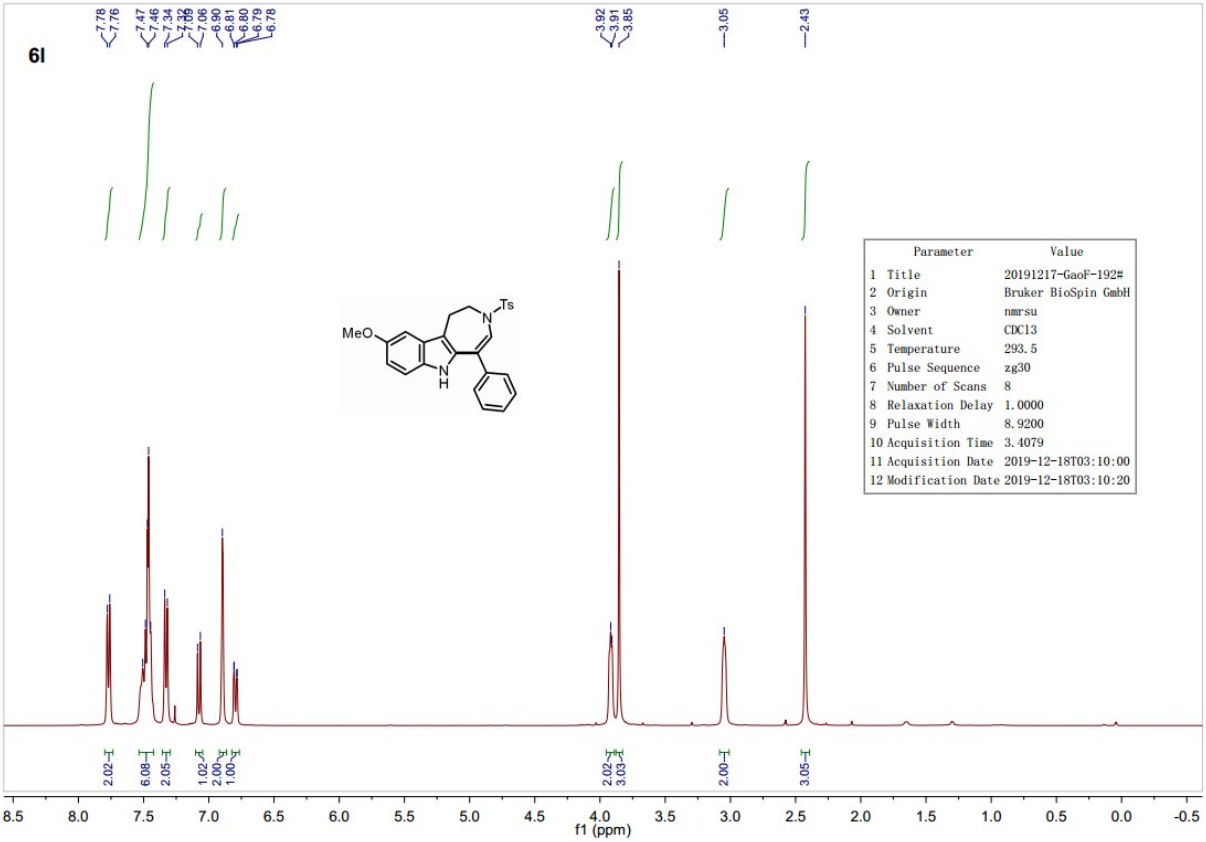

6j
7.86
7.84
7.49
7.44
7.43
7.12
7.11
7.09
7.07
7.05
7.03
6.87
3.90
3.88
3.87
3.06
3.05
3.04
SO2Ph
N
H
Parameter Value
1 Title 20191203-GaoF-176#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 295.4
6 Pulse Sequence zg30
7 Number of Scans 8
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2019-12-03T21:34:00
12 Modification Date 2019-12-03T21:34:16
2.01
2.01
8.17
3.08
0.99
2.00
2.03
f1 (ppm)

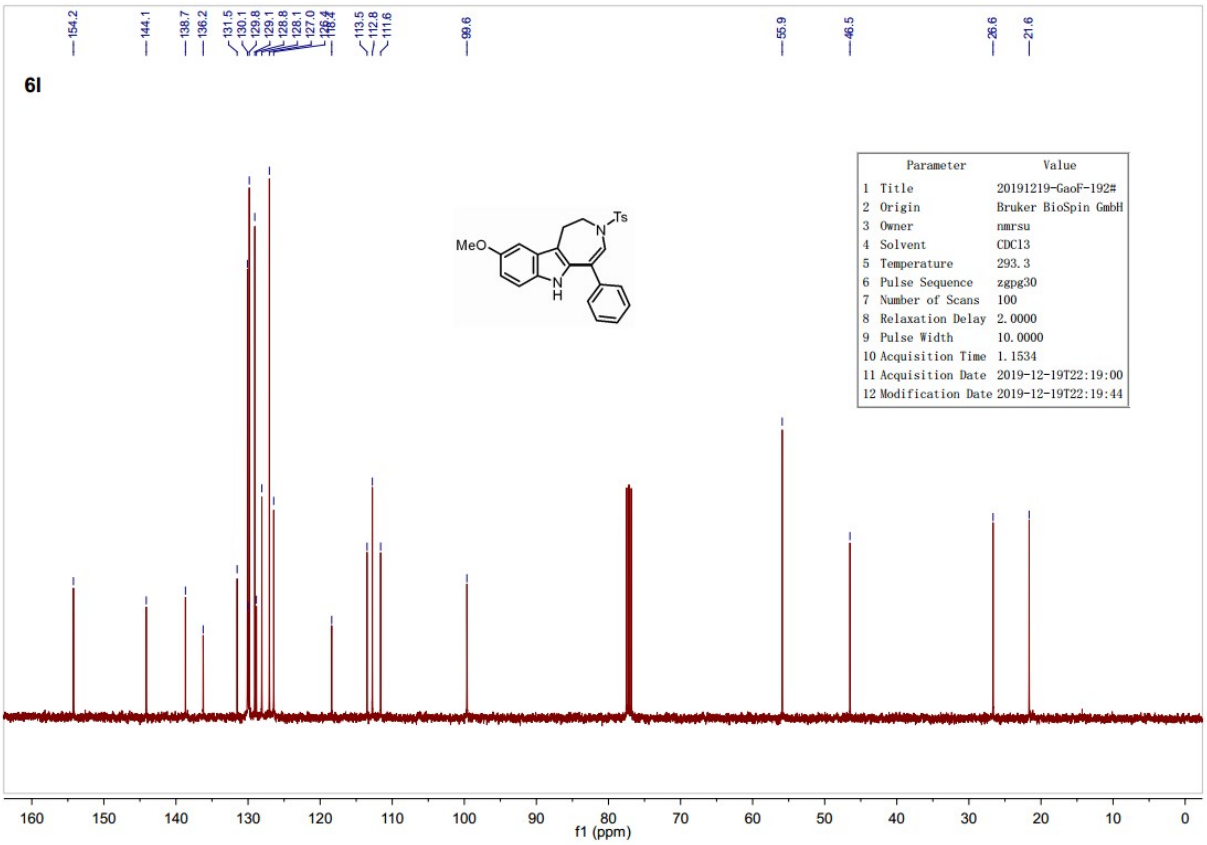

6j
139.2
138.6
133.2
129.8
129.5
129.1
128.2
127.0
119.8
118.6
118.1
113.8
110.8
46.5
26.6
SO2Ph
N
H
Parameter Value
1 Title 20191204-GaoF-176#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 295.7
6 Pulse Sequence zgpg30
7 Number of Scans 200
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2019-12-04T22:13:00
12 Modification Date 2019-12-04T22:13:36
f1 (ppm)

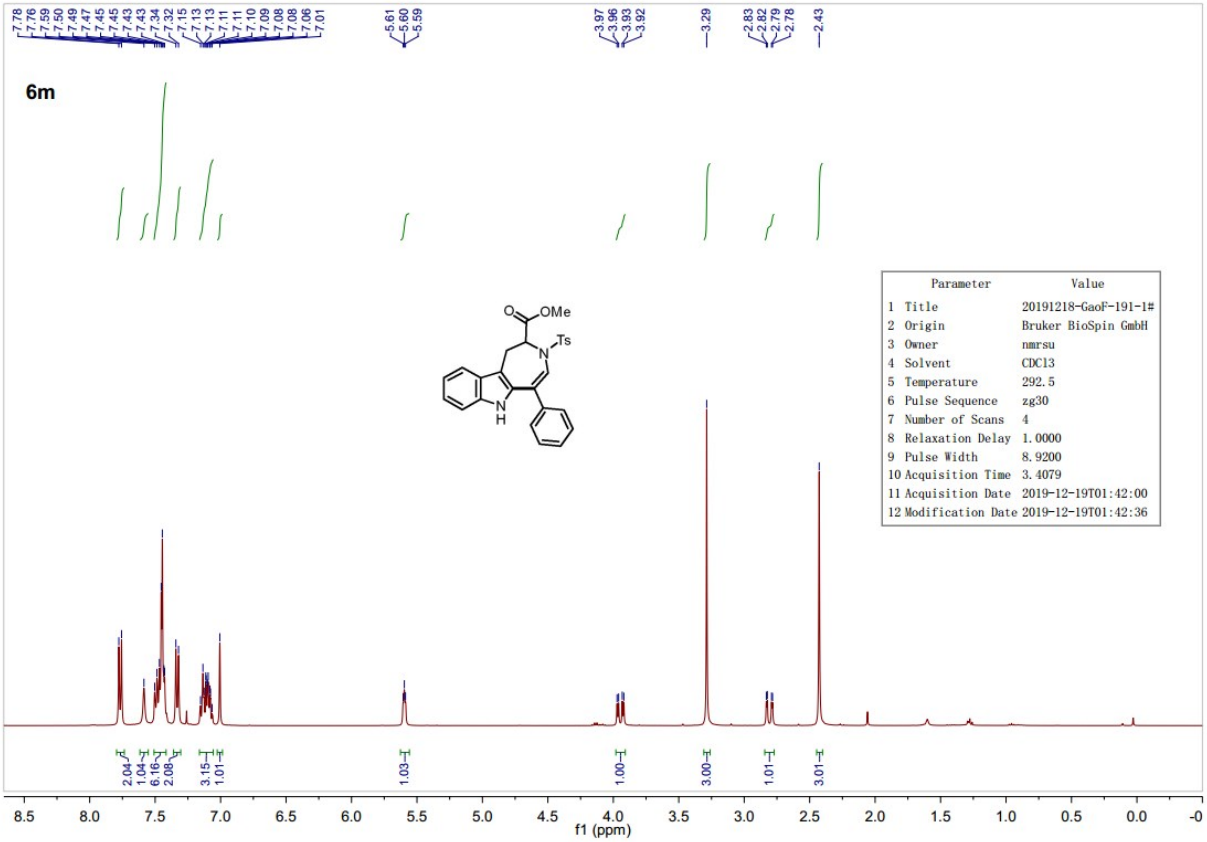

6k
7.58 7.56 7.54 7.51 7.50 7.48 7.45 7.45 7.43 7.43 7.22 7.21 7.21 7.19 7.17 7.17 7.15 7.15 7.13 7.13 7.12 7.11
4.13 4.12 4.11
3.39 3.38 3.37
Parameter Value
1 Title 20191205-GaoF-178#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 295.2
6 Pulse Sequence zg30
7 Number of Scans 16
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2019-12-05T22:57:00
12 Modification Date 2019-12-05T22:57:40
2.03 2.99 2.07 2.05 1.01 1.00 2.03 2.00
f1 (ppm)

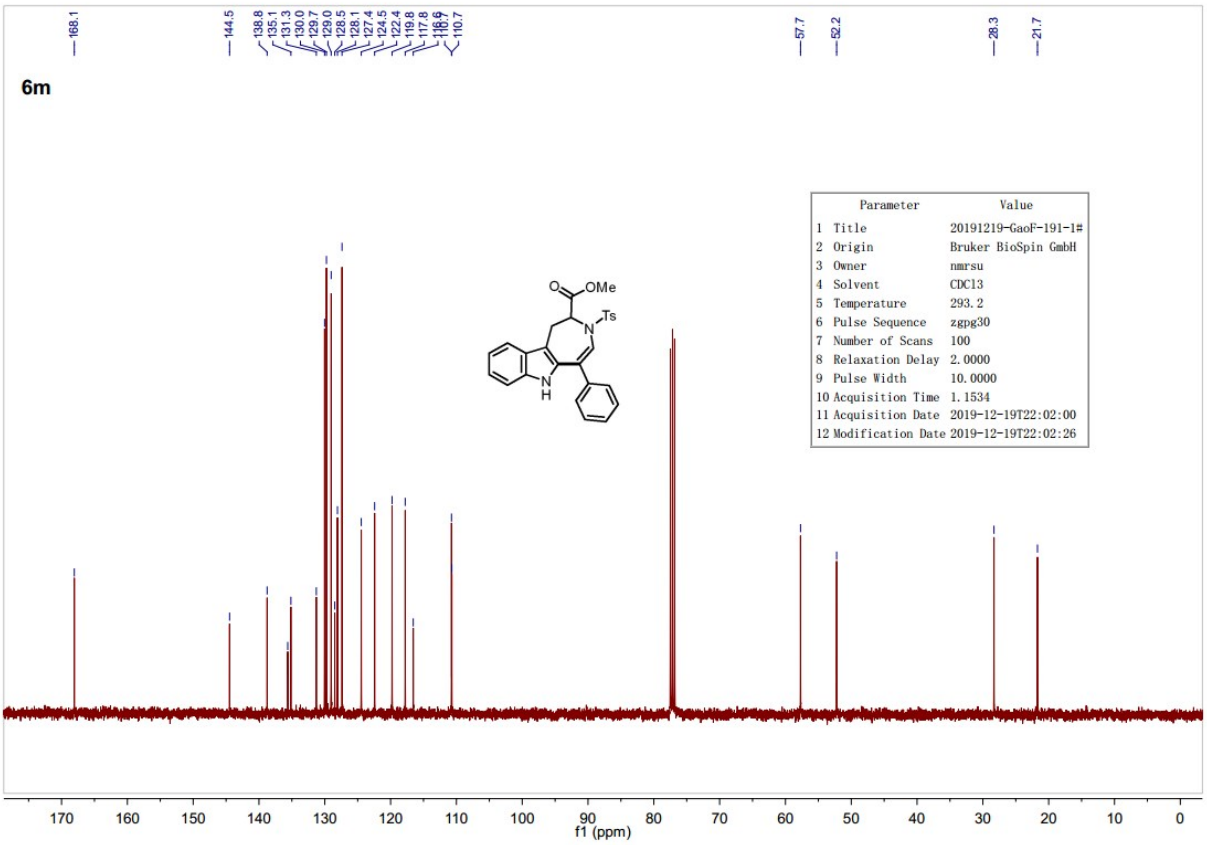

6k
137.3 135.1 129.7 129.3 128.8 128.6 124.3 124.2 123.6 120.2 118.7 114.7 111.1
48.4
27.6
Parameter Value
1 Title 20191206-GaoF-178#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 295.9
6 Pulse Sequence zgpg30
7 Number of Scans 200
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2019-12-06T20:20:00
12 Modification Date 2019-12-06T20:20:06
f1 (ppm)

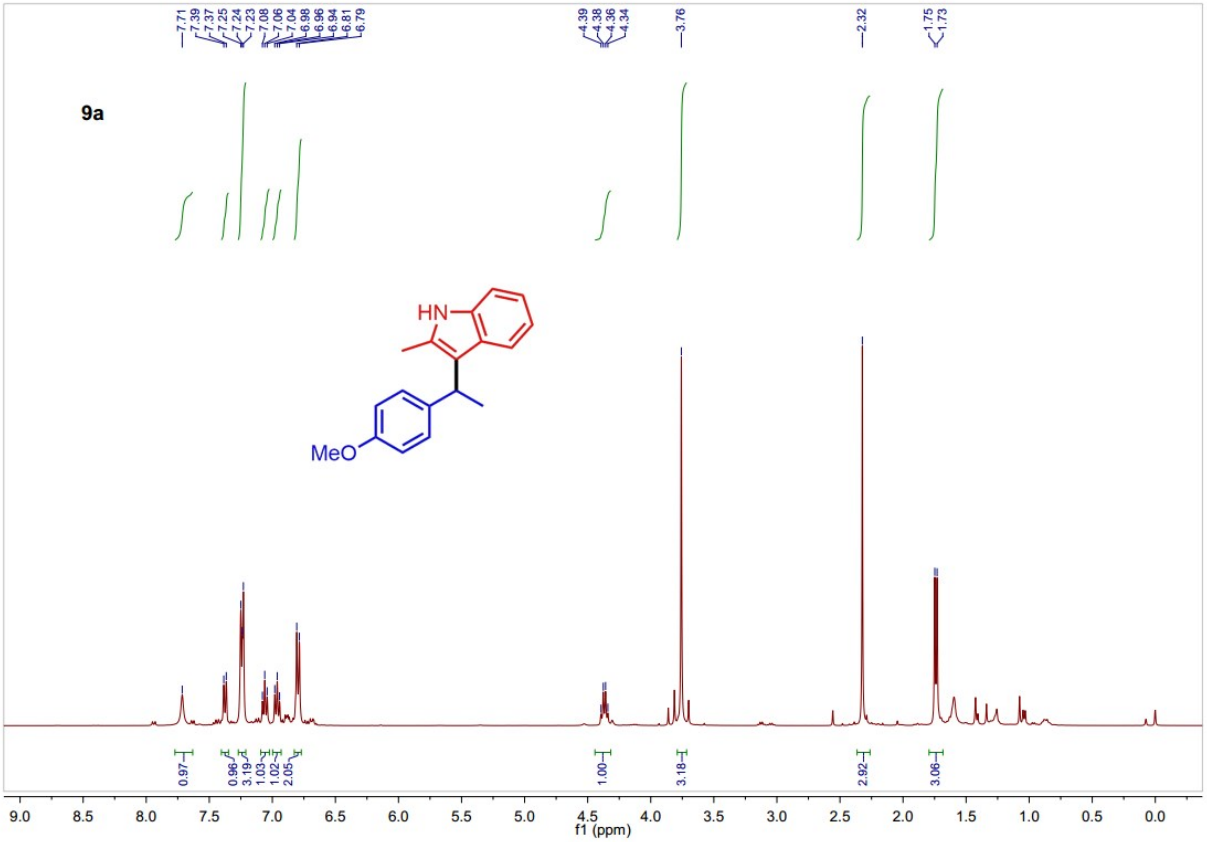

6k
-75.1
O
O
S
N
CF3
H
Parameter Value
1 Title 20191206-GaoF-178#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 295.7
6 Pulse Sequence zgflqn
7 Number of Scans 64
8 Relaxation Delay 1.5000
9 Pulse Width 14.0000
10 Acquisition Time 0.5767
11 Acquisition Date 2019-12-06T20:23:00
12 Modification Date 2019-12-06T20:23:40
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140
f1 (ppm)

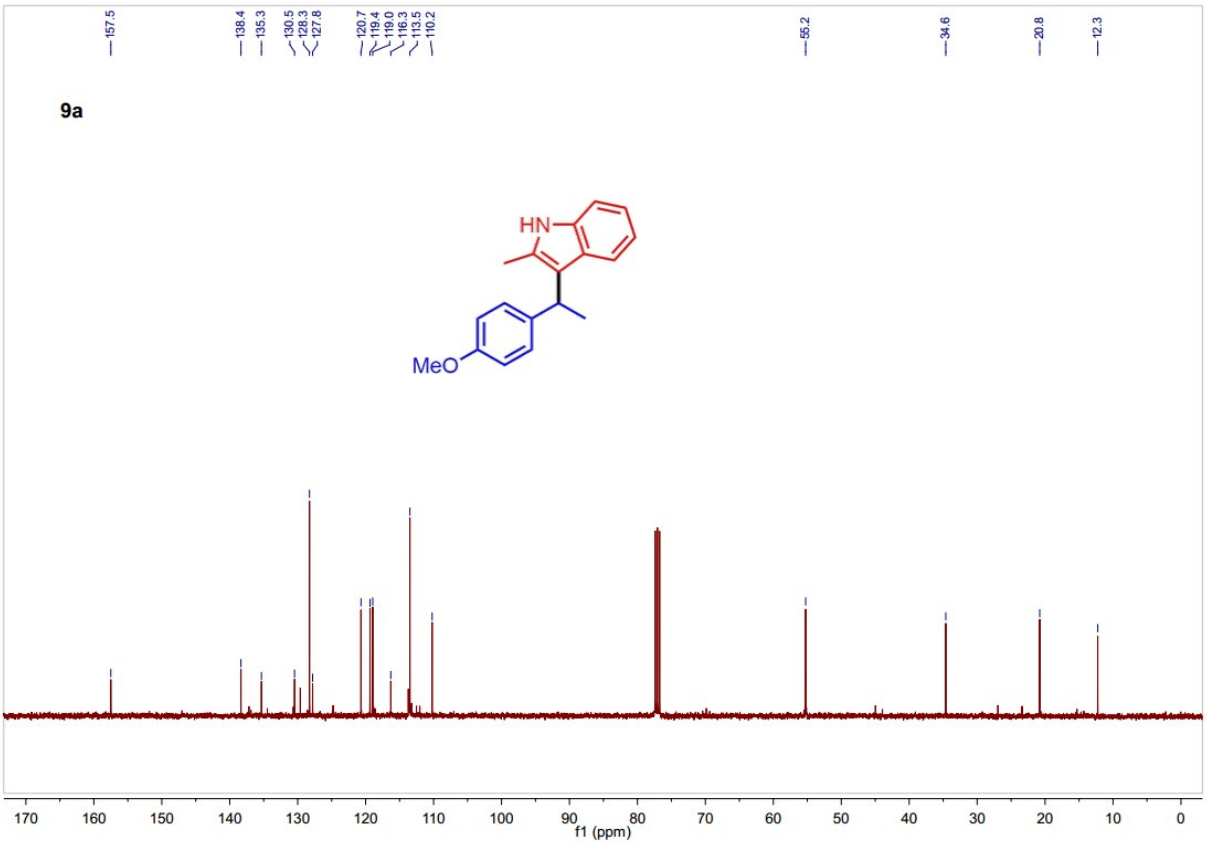

6l
7.78
7.76
7.47
7.46
7.34
7.32
7.09
7.06
6.80
6.61
6.60
6.79
6.78
3.92
3.91
3.85
3.05
2.43
Ts
N
MeO
H
Parameter Value
1 Title 20191217-GaoF-192#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 293.5
6 Pulse Sequence zg30
7 Number of Scans 8
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2019-12-18T03:10:00
12 Modification Date 2019-12-18T03:10:20
2.02
6.08
2.05
1.02
2.00
1.00
2.02
3.03
2.00
3.05
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 -0.5
f1 (ppm)

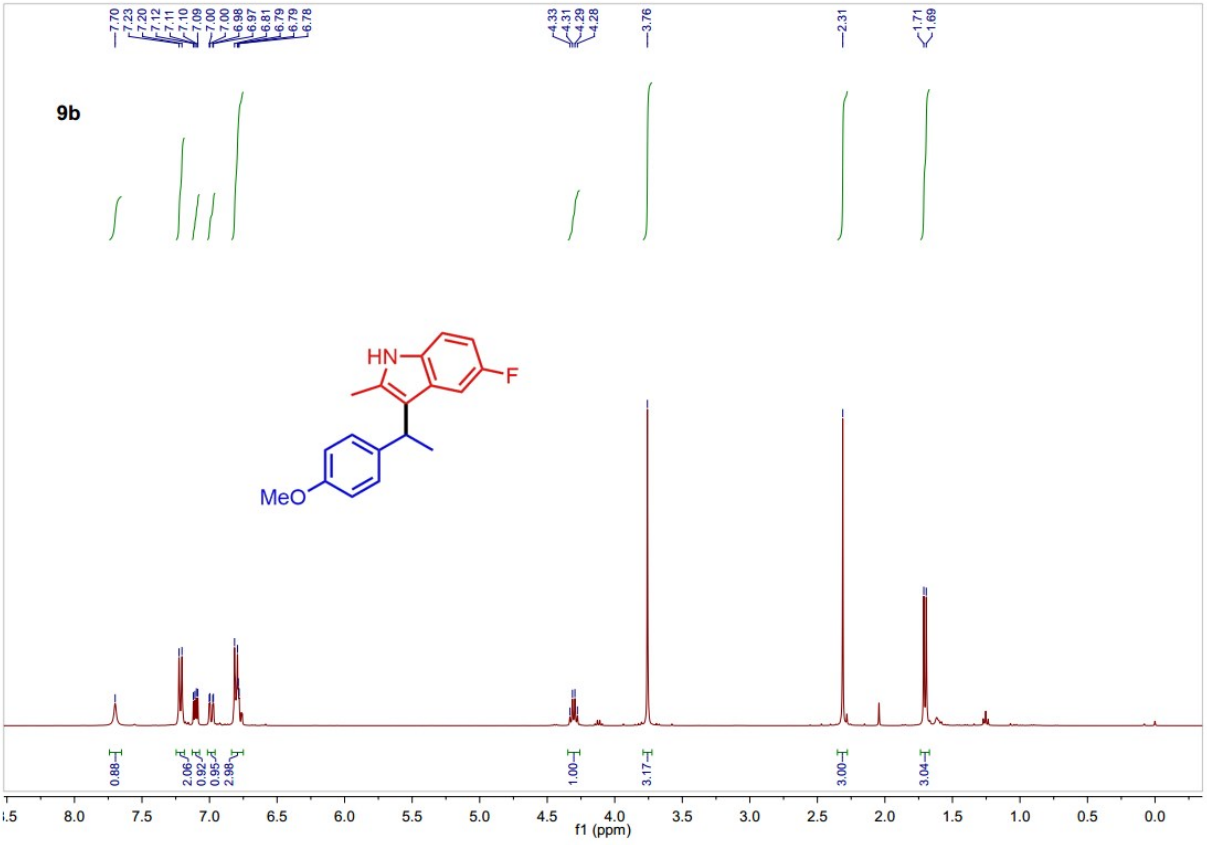

6l
154.2
144.1
138.7
136.2
131.5
130.1
129.8
129.1
128.8
128.1
127.0
126.4
118.4
113.5
112.8
111.6
99.6
55.9
46.5
26.6
21.6
MeO
Ts
N
H
Parameter Value
1 Title 20191219-GaoF-192#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 293.3
6 Pulse Sequence zgpg30
7 Number of Scans 100
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2019-12-19T22:19:00
12 Modification Date 2019-12-19T22:19:44
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

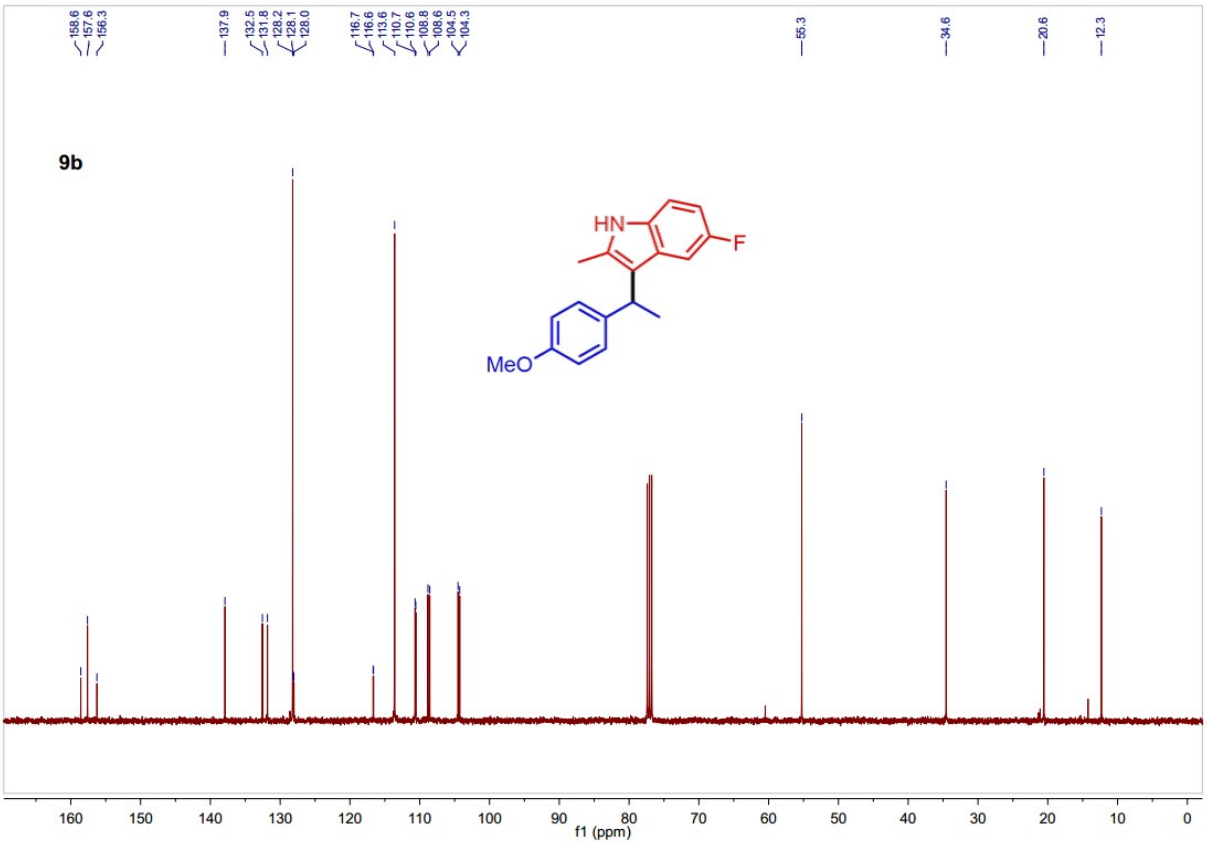

7.78
7.76
7.59
7.50
7.49
7.47
7.45
7.45
7.43
7.43
7.34
7.32
7.15
7.13
7.13
7.11
7.11
7.10
7.09
7.08
7.08
7.06
7.01
5.61
5.60
5.59
3.97
3.96
3.93
3.92
3.29
2.83
2.82
2.79
2.78
2.43
6m
OMe
O
Ts
N
H
Parameter Value
1 Title 20191218-GaoF-191-1#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 292.5
6 Pulse Sequence zg30
7 Number of Scans 4
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2019-12-19T01:42:00
12 Modification Date 2019-12-19T01:42:36
2.04
1.04
6.16
2.08
3.15
1.01
1.03
1.00
3.00
1.01
3.01
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 -0
f1 (ppm)

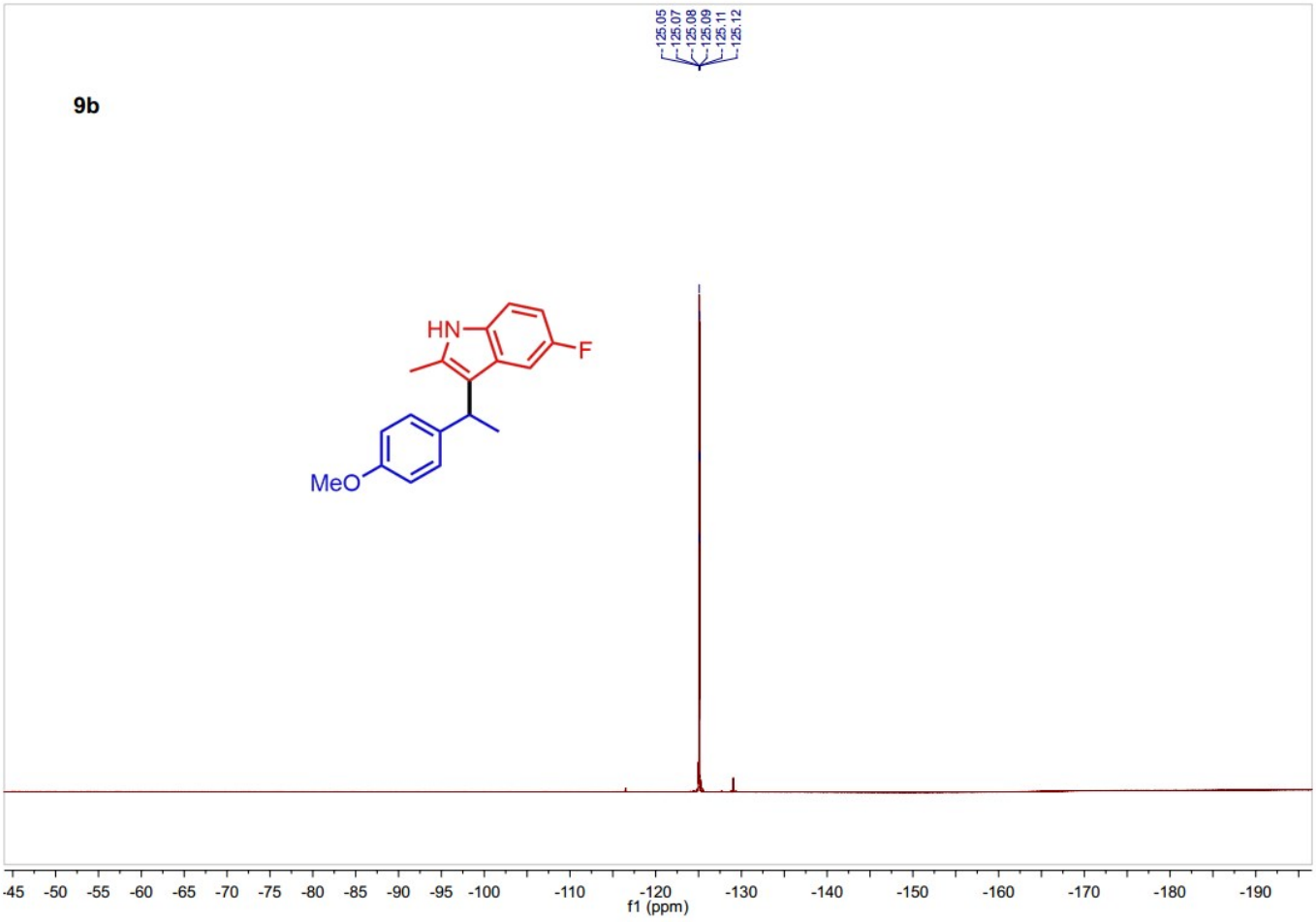

6m
168.1
144.5
138.8
135.1
131.3
130.0
129.7
129.0
128.5
128.1
127.4
124.5
122.4
119.8
117.8
116.6
116.4
110.7
57.7
52.2
28.3
21.7
Parameter Value
1 Title 20191219-GaoF-191-1#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 293.2
6 Pulse Sequence zgpg30
7 Number of Scans 100
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2019-12-19T22:02:00
12 Modification Date 2019-12-19T22:02:26
OMe
Ts
N
H
f1 (ppm)

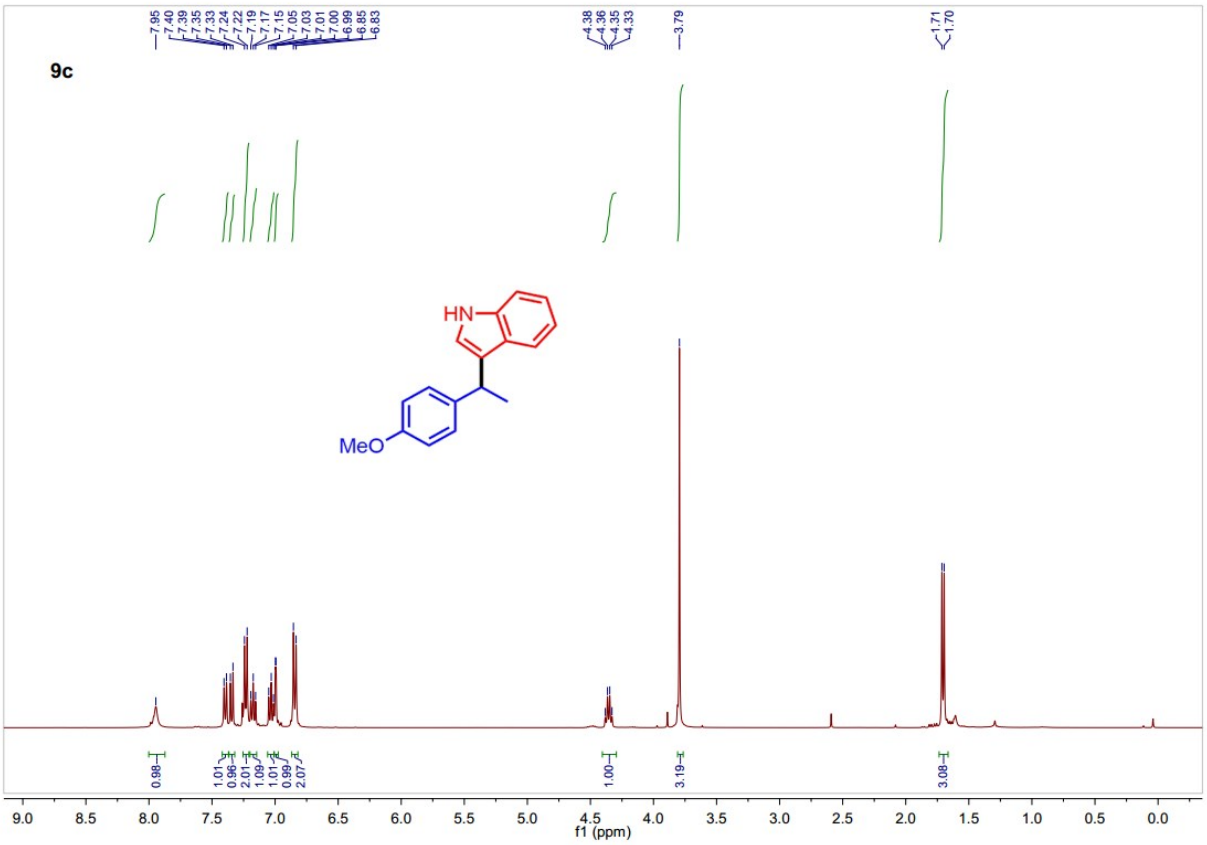

9a
7.71
7.39
7.37
7.25
7.24
7.23
7.08
7.06
7.04
6.98
6.96
6.94
6.81
6.79
4.39
4.38
4.36
4.34
3.76
2.32
1.75
1.73
HN
MeO
0.97
0.96
3.19
1.03
1.02
2.05
1.00
3.18
2.92
3.06
f1 (ppm)

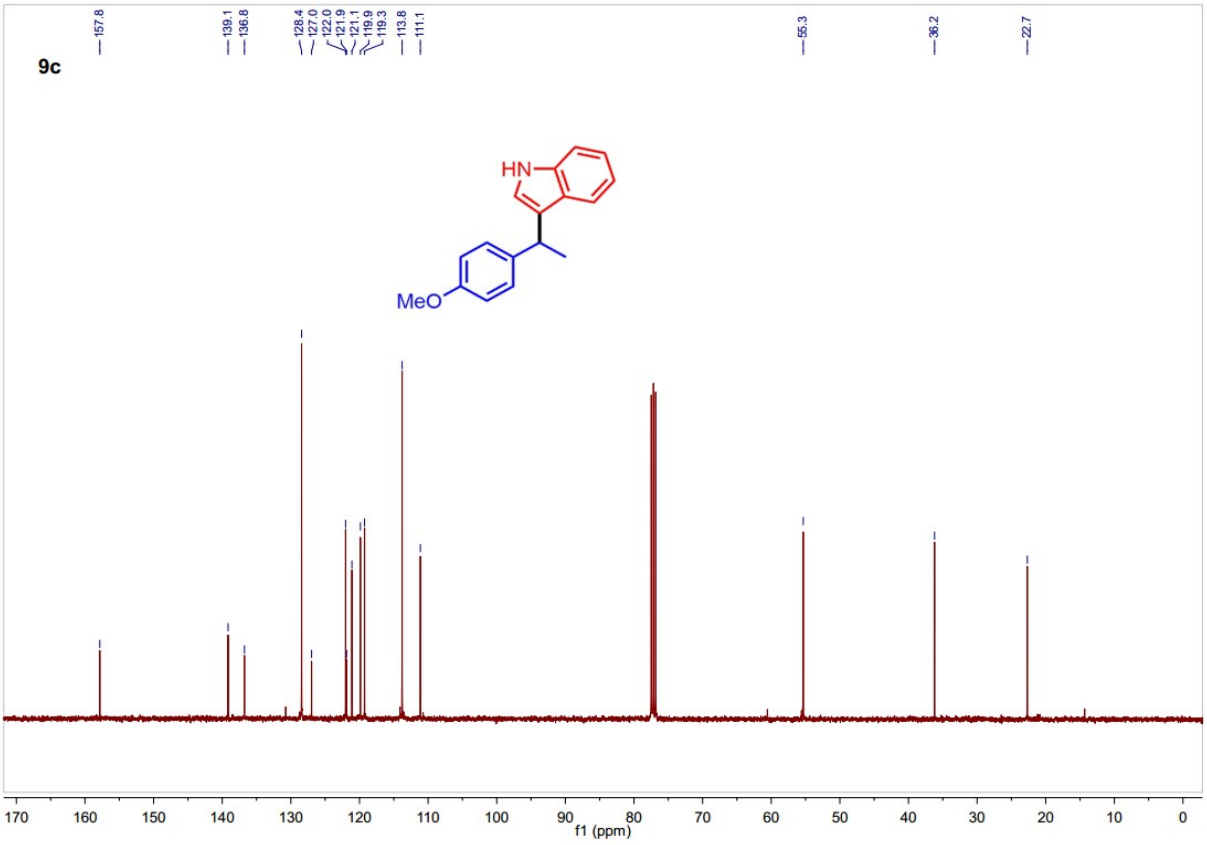

9a
157.5
138.4
135.3
130.5
128.3
127.8
120.7
119.4
119.0
116.3
113.5
110.2
55.2
34.6
20.8
12.3
HN
MeO
f1 (ppm)

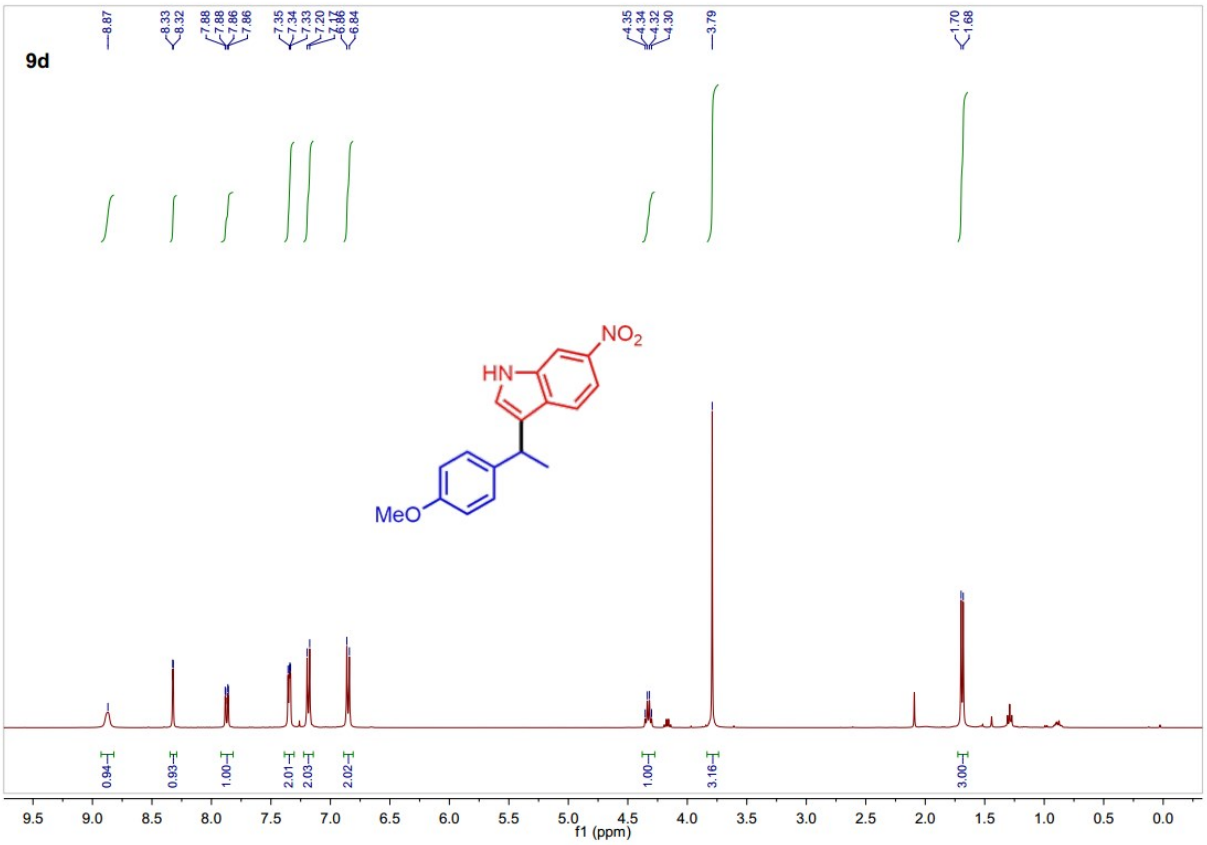

9b
7.70
7.23
7.20
7.12
7.11
7.10
7.09
7.00
7.00
6.98
6.97
6.81
6.79
6.79
6.78
4.33
4.31
4.29
4.28
3.76
2.31
1.71
1.69
HN
F
MeO
0.88
2.06
0.92
0.95
2.98
1.00
3.17
3.00
3.04
f1 (ppm)

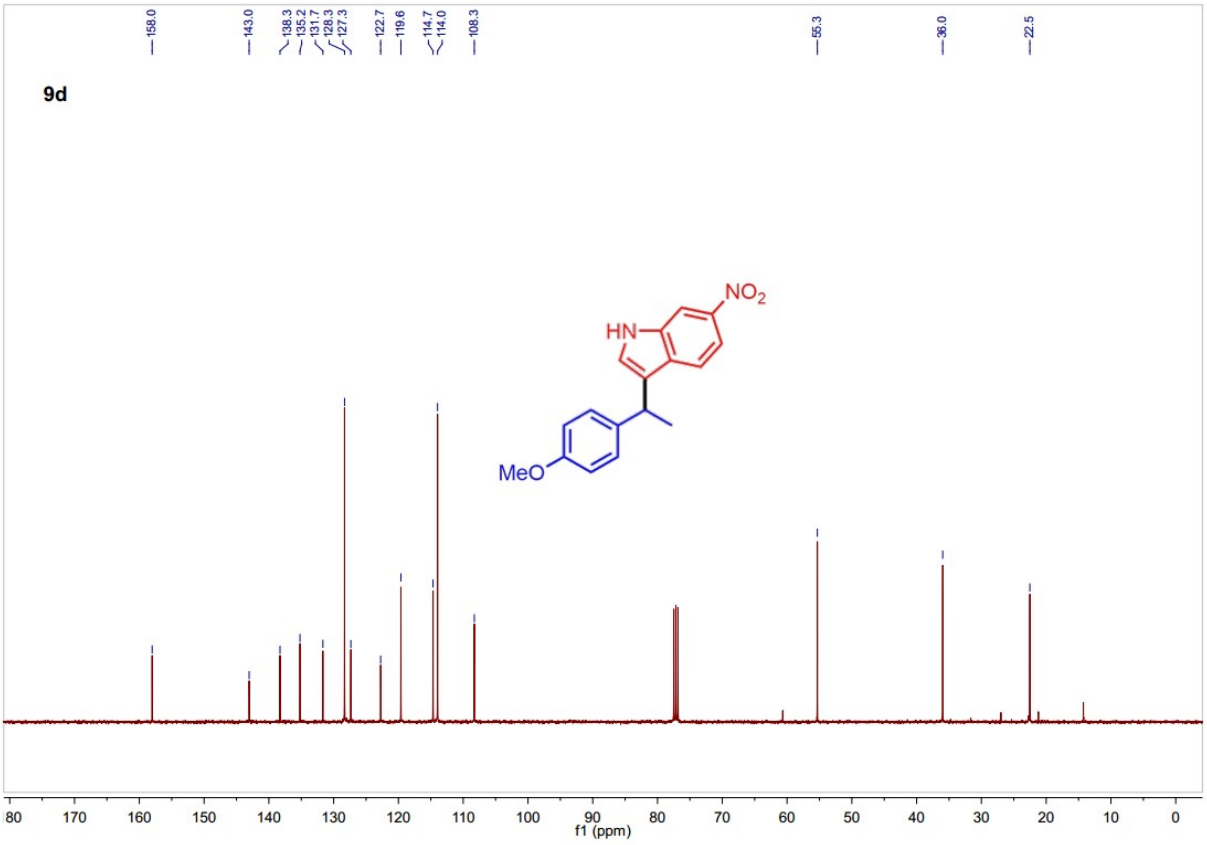

158.6
157.6
156.3
137.9
132.5
131.8
128.2
128.1
128.0
116.7
116.6
113.6
110.7
110.6
108.8
108.6
104.5
104.3
55.3
34.6
20.6
12.3
9b
HN
F
MeO
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

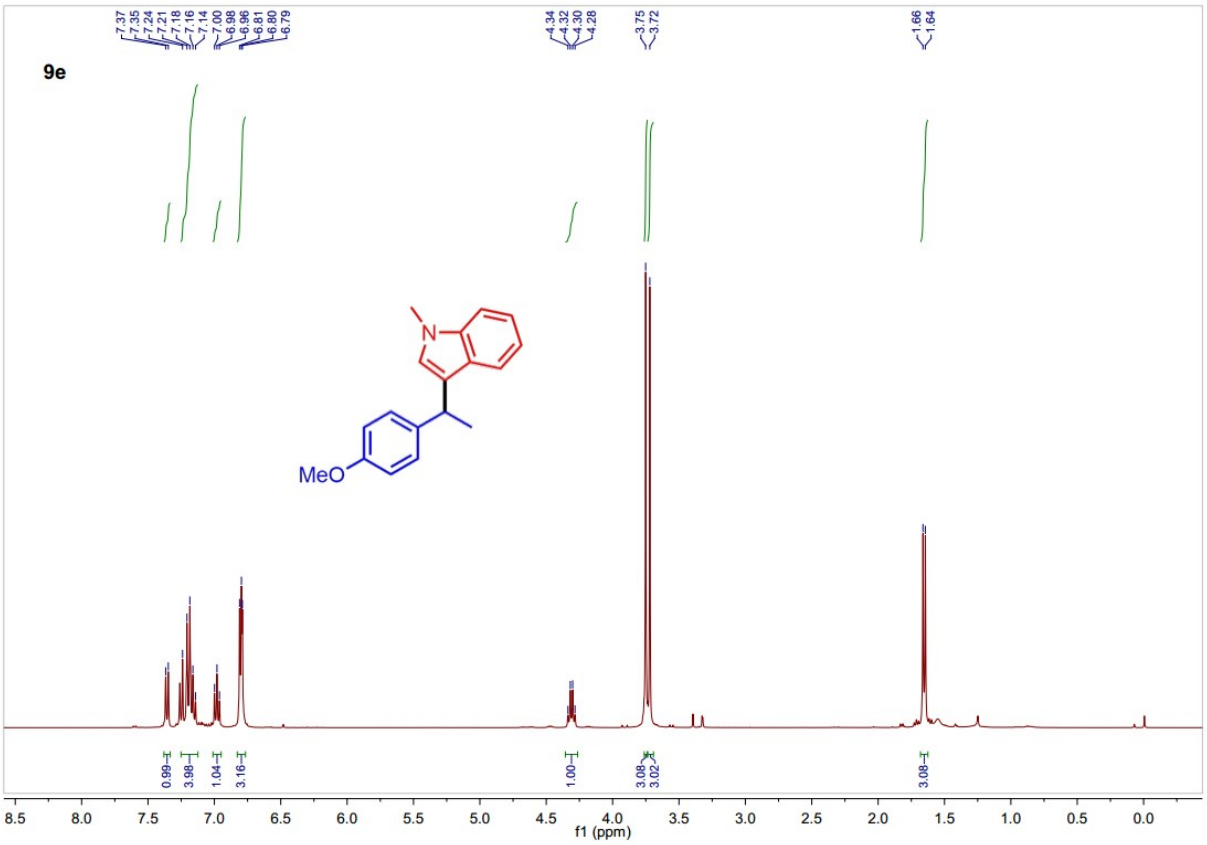

9b
-125.05
-125.07
-125.08
-125.09
-125.11
-125.12
HN
F
MeO
-45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190
f1 (ppm)

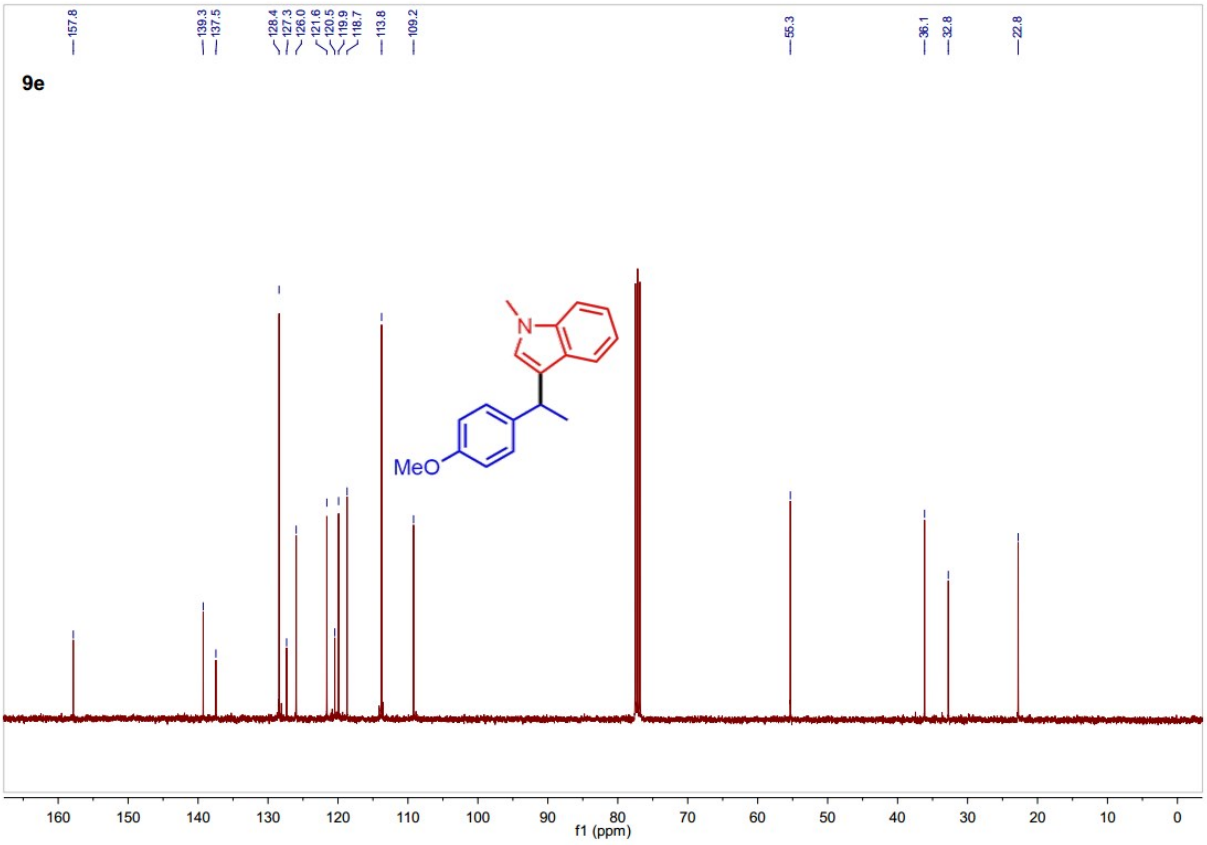

9c
7.95
7.40
7.39
7.35
7.33
7.24
7.22
7.19
7.17
7.15
7.05
7.03
7.01
7.00
6.99
6.85
6.83
4.38
4.36
4.35
4.33
3.79
1.71
1.70
HN
MeO
0.98
1.01
0.96
2.01
1.09
1.01
0.99
2.07
1.00
3.19
3.08
f1 (ppm)

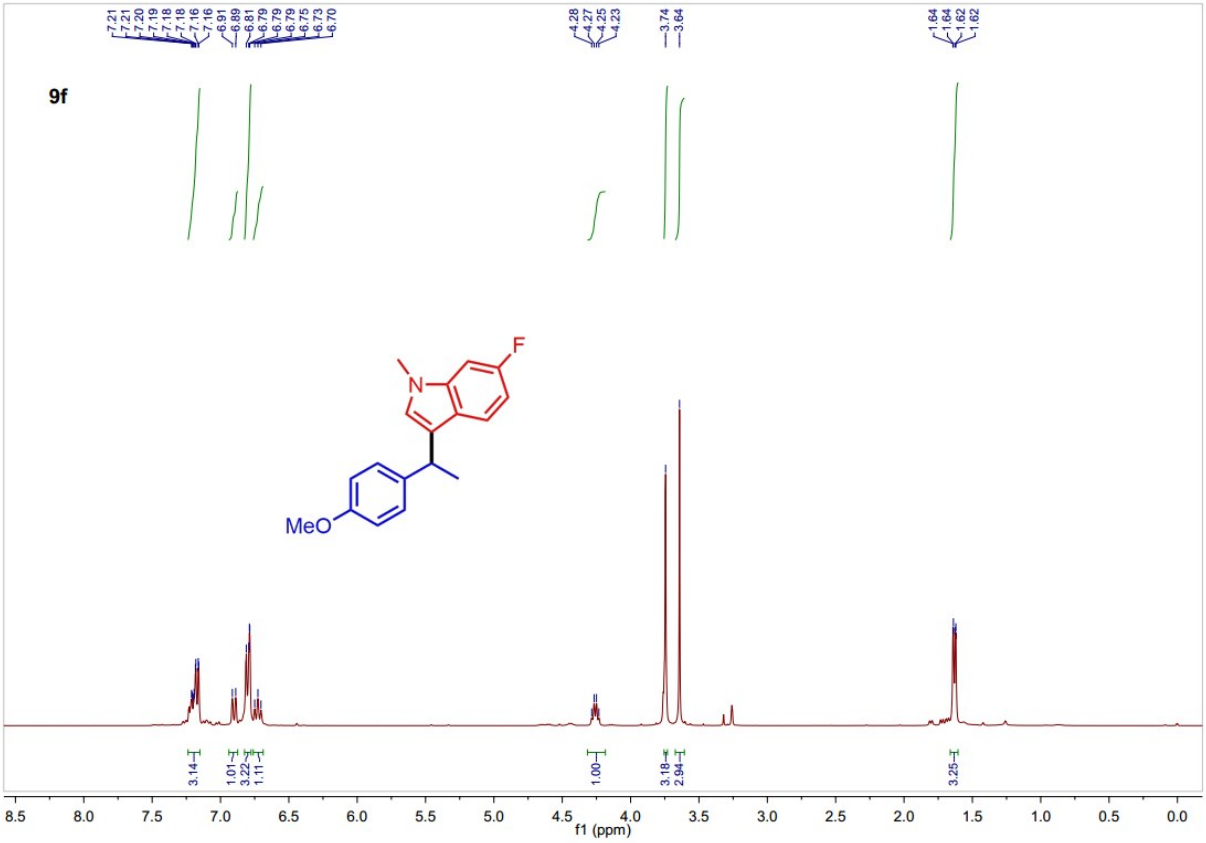

9c
157.8
139.1
136.8
128.4
127.0
122.0
121.9
121.1
119.9
119.3
113.8
111.1
55.3
36.2
22.7
HN
MeO
f1 (ppm)

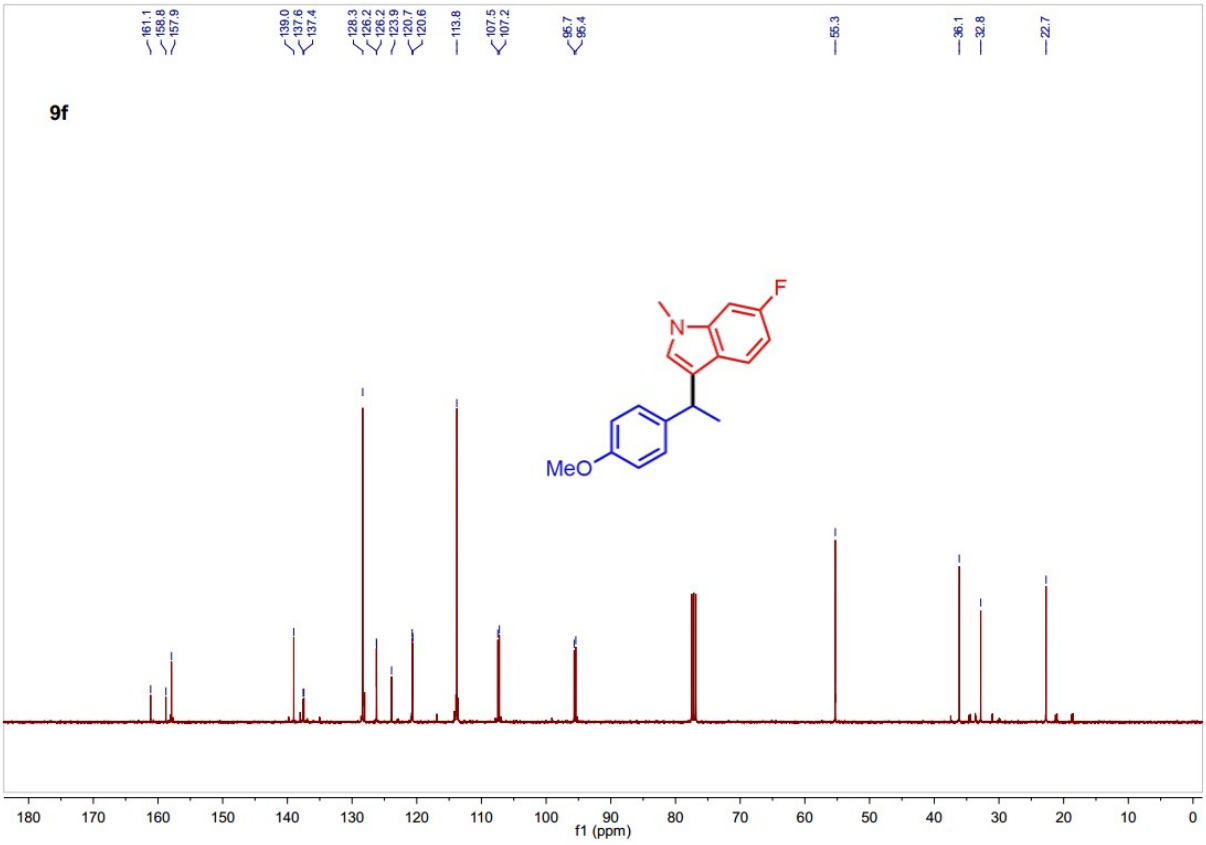

9d
8.87
8.33
8.32
7.88
7.88
7.86
7.86
7.35
7.34
7.33
7.20
6.86
6.84
4.35
4.34
4.32
4.30
3.79
1.70
1.68
NO2
HN
MeO
0.94
0.93
1.00
2.01
2.03
2.02
1.00
3.16
3.00
f1 (ppm)

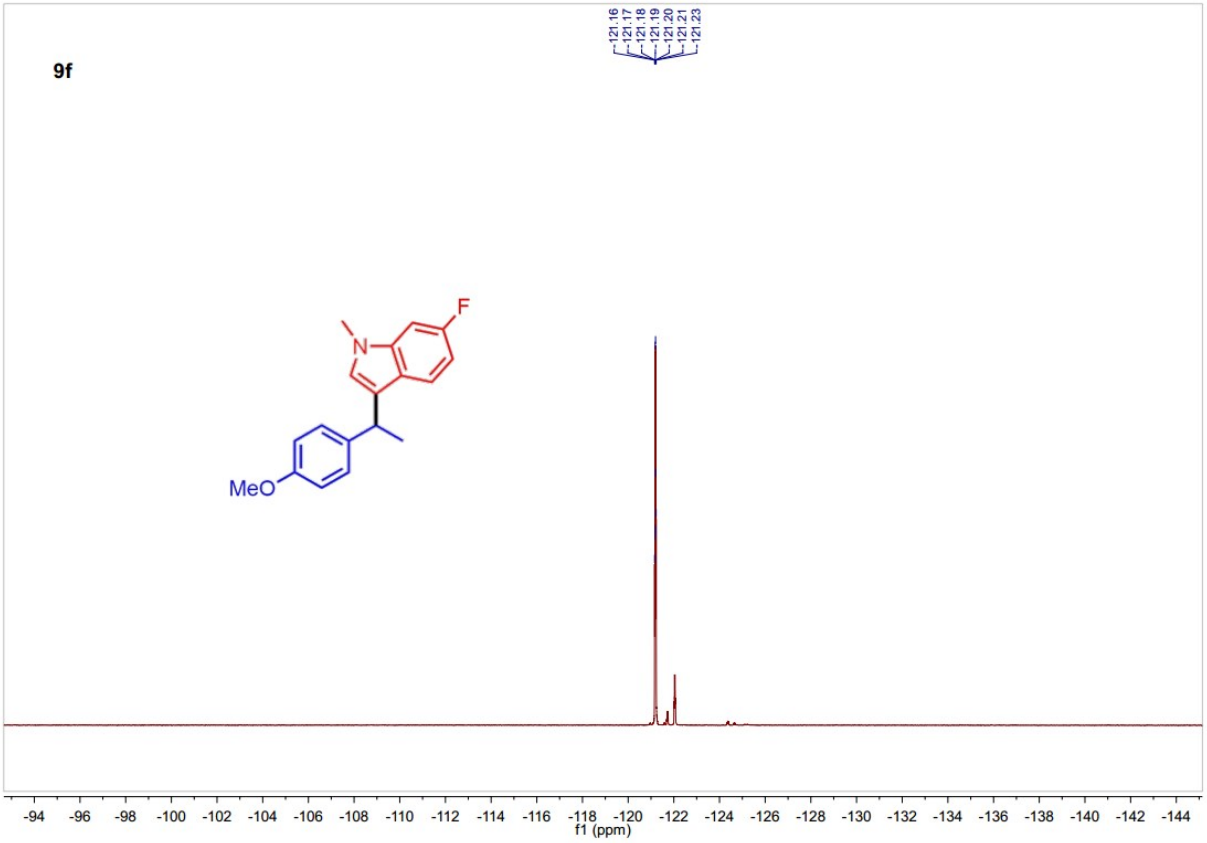

9d
158.0
143.0
138.3
135.2
131.7
128.3
127.3
122.7
119.6
114.7
114.0
108.3
55.3
36.0
22.5
NO2
HN
MeO
f1 (ppm)

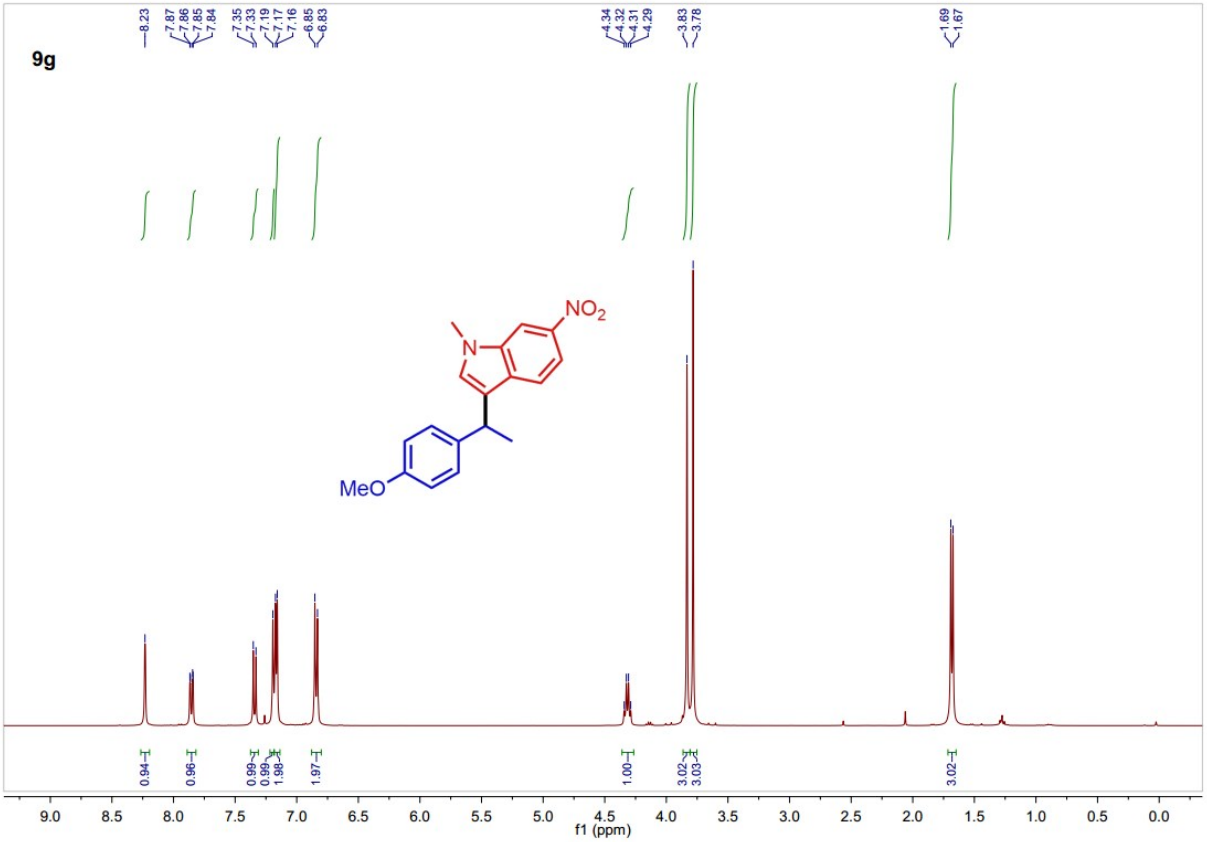

9e
7.37
7.35
7.24
7.21
7.18
7.16
7.14
7.00
6.98
6.96
6.81
6.80
6.79
4.34
4.32
4.30
4.28
3.75
3.72
1.66
1.64
MeO
0.99
3.98
1.04
3.16
1.00
3.08
3.02
3.08
f1 (ppm)

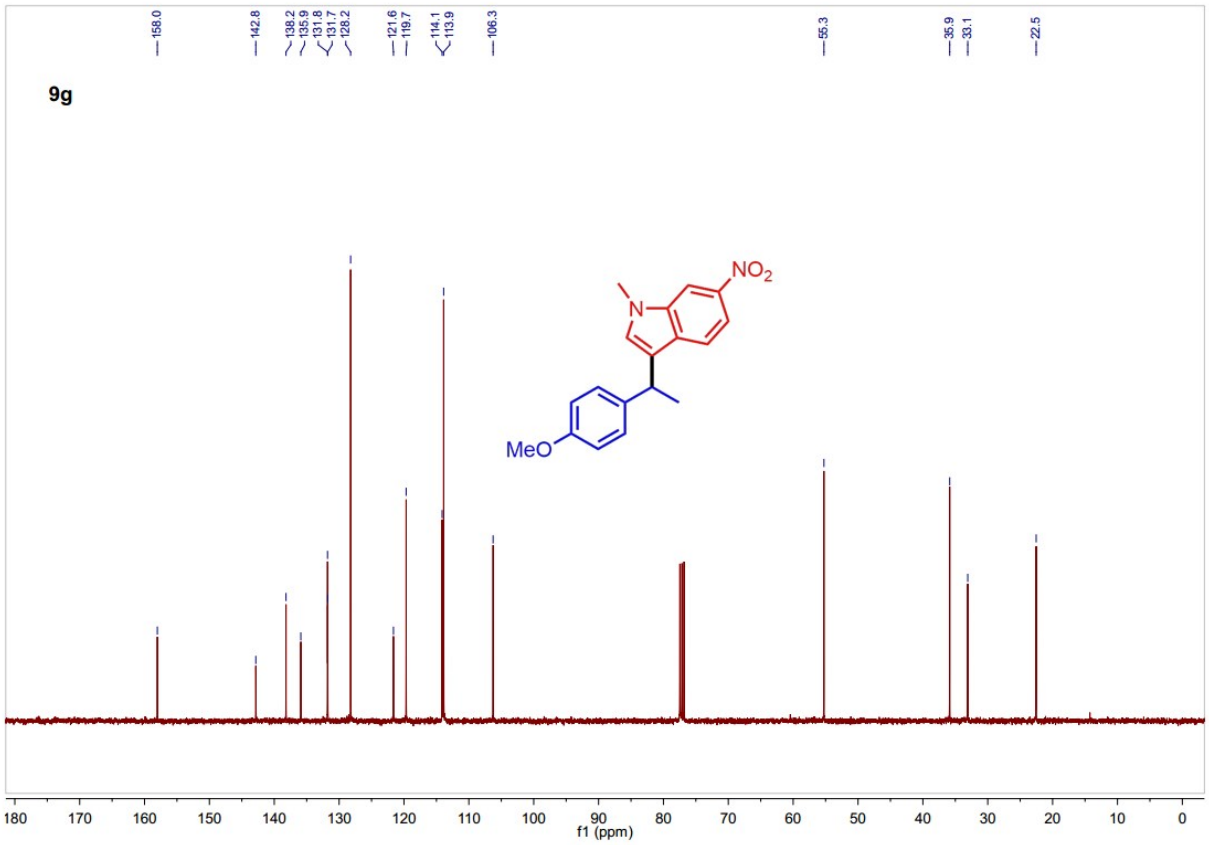

9e
157.8
139.3
137.5
128.4
127.3
126.0
121.6
120.5
119.9
118.7
113.8
109.2
55.3
36.1
32.8
22.8
MeO
f1 (ppm)

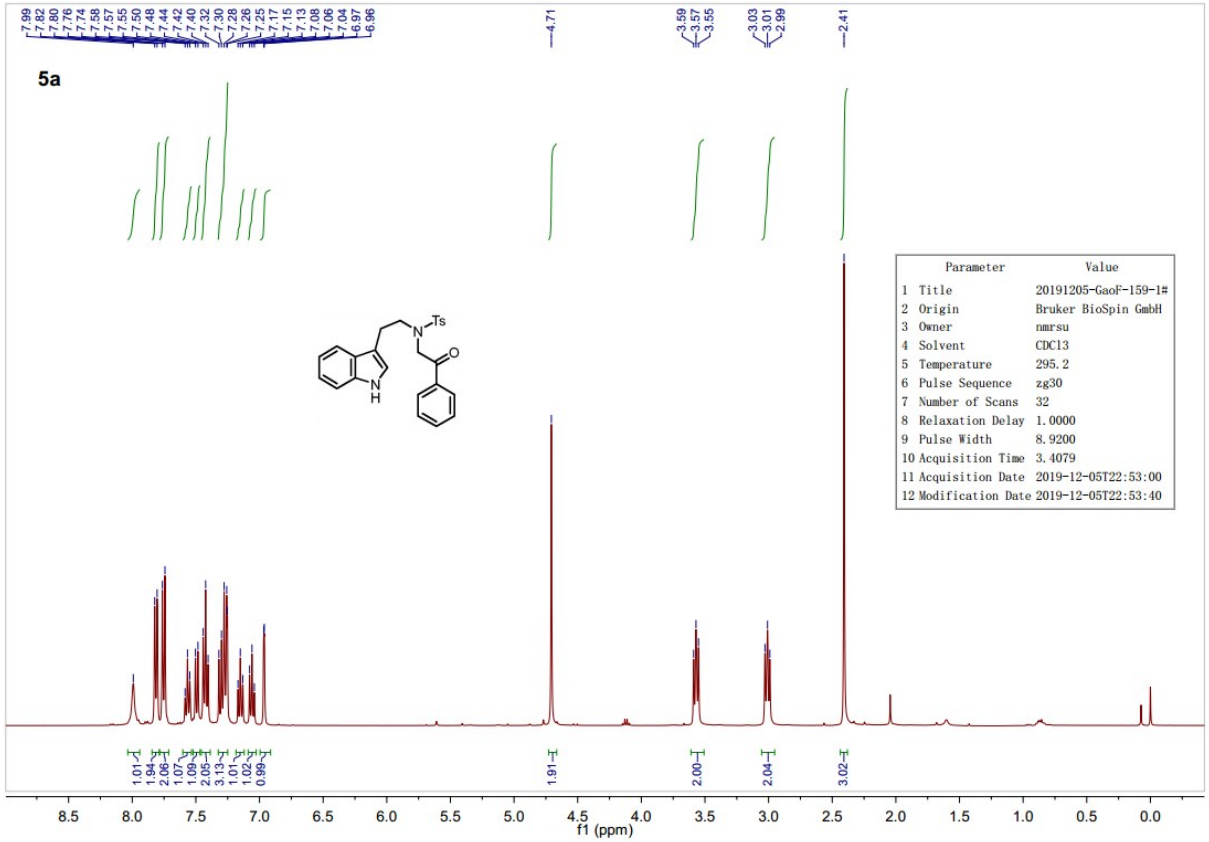

9f
7.21
7.21
7.20
7.19
7.18
7.18
7.16
7.16
6.91
6.89
6.81
6.79
6.79
6.79
6.75
6.73
6.70
4.28
4.27
4.25
4.23
3.74
3.64
1.64
1.64
1.62
1.62
F
N
MeO
3.14
1.01
3.22
1.11
1.00
3.18
2.94
3.25
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

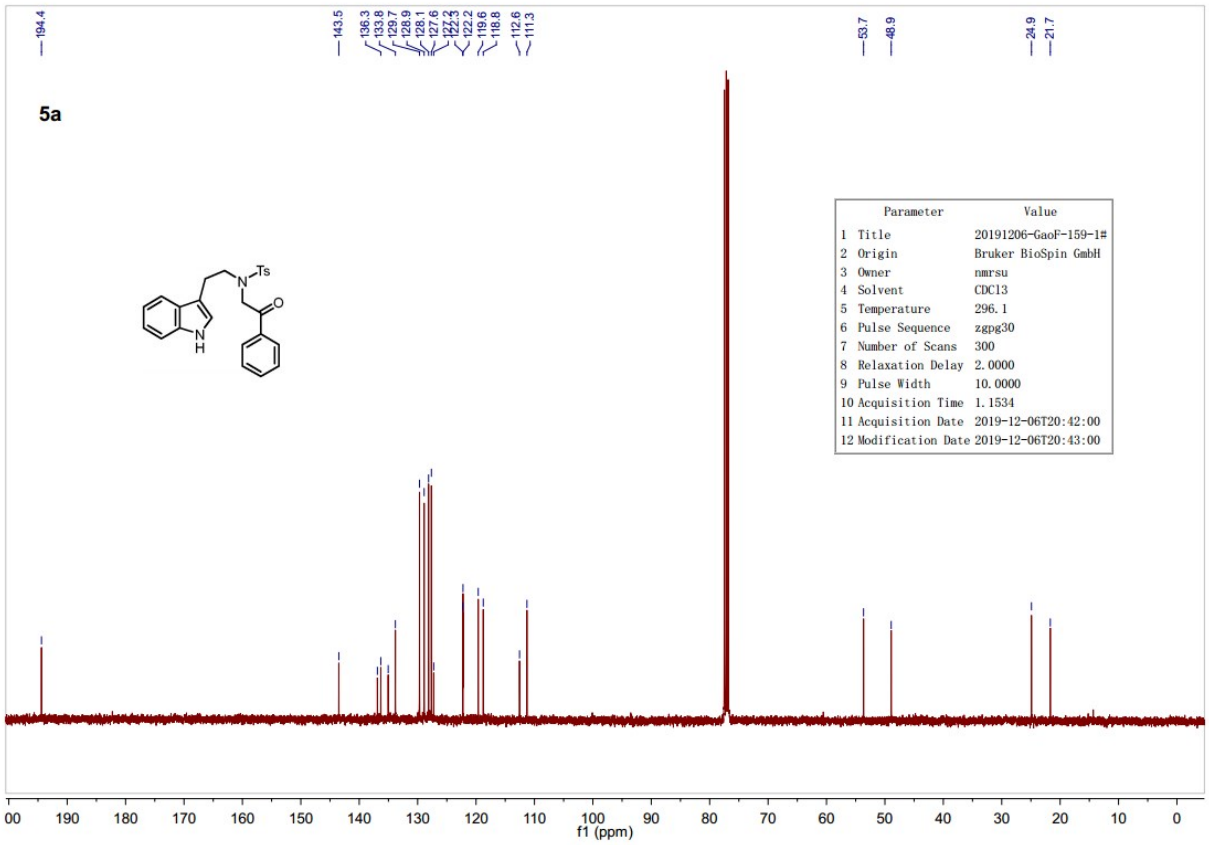

9f
161.1
158.8
157.9
139.0
137.6
137.4
128.3
126.2
126.2
123.9
120.7
120.6
113.8
107.5
107.2
95.7
95.4
55.3
36.1
32.8
22.7
F
N
MeO
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

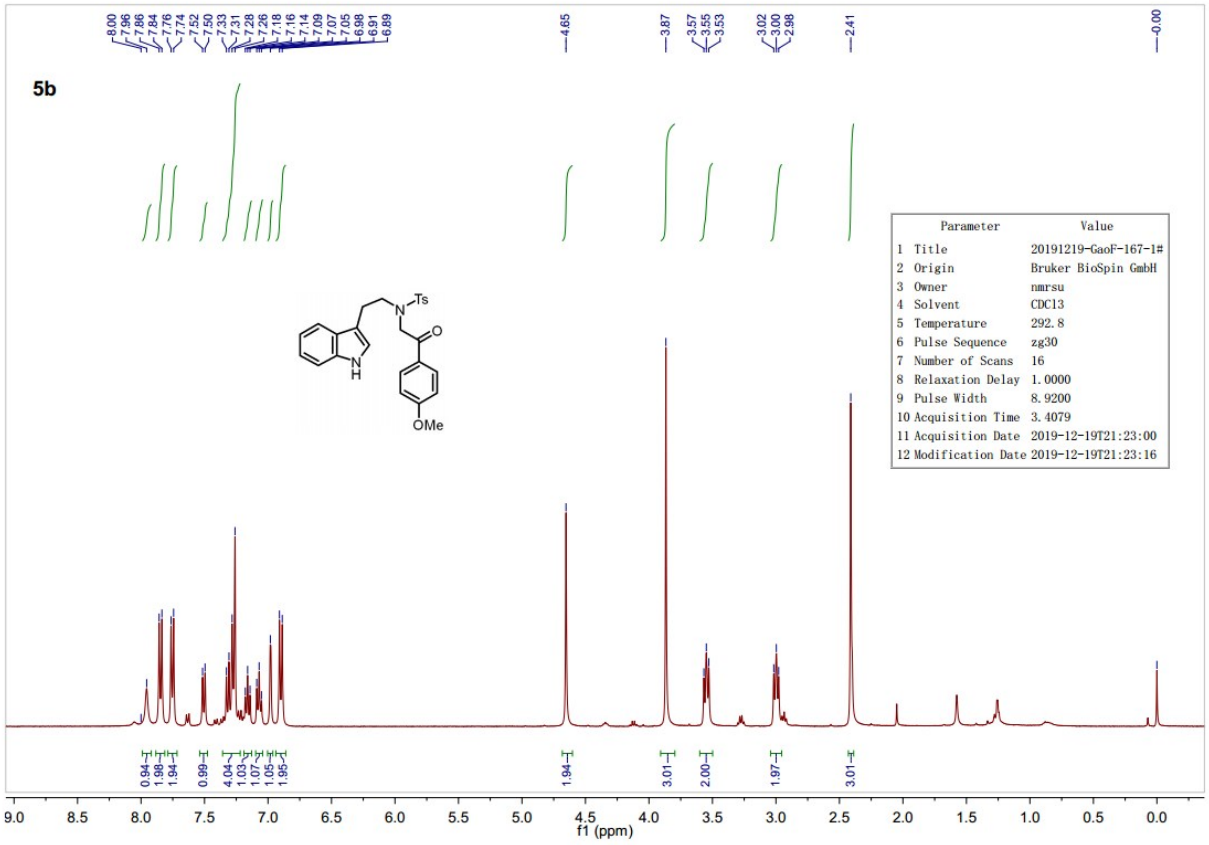

9f
-121.16
-121.17
-121.18
-121.19
-121.20
-121.21
-121.23
F
N
MeO
-94 -96 -98 -100 -102 -104 -106 -108 -110 -112 -114 -116 -118 -120 -122 -124 -126 -128 -130 -132 -134 -136 -138 -140 -142 -144
f1 (ppm)

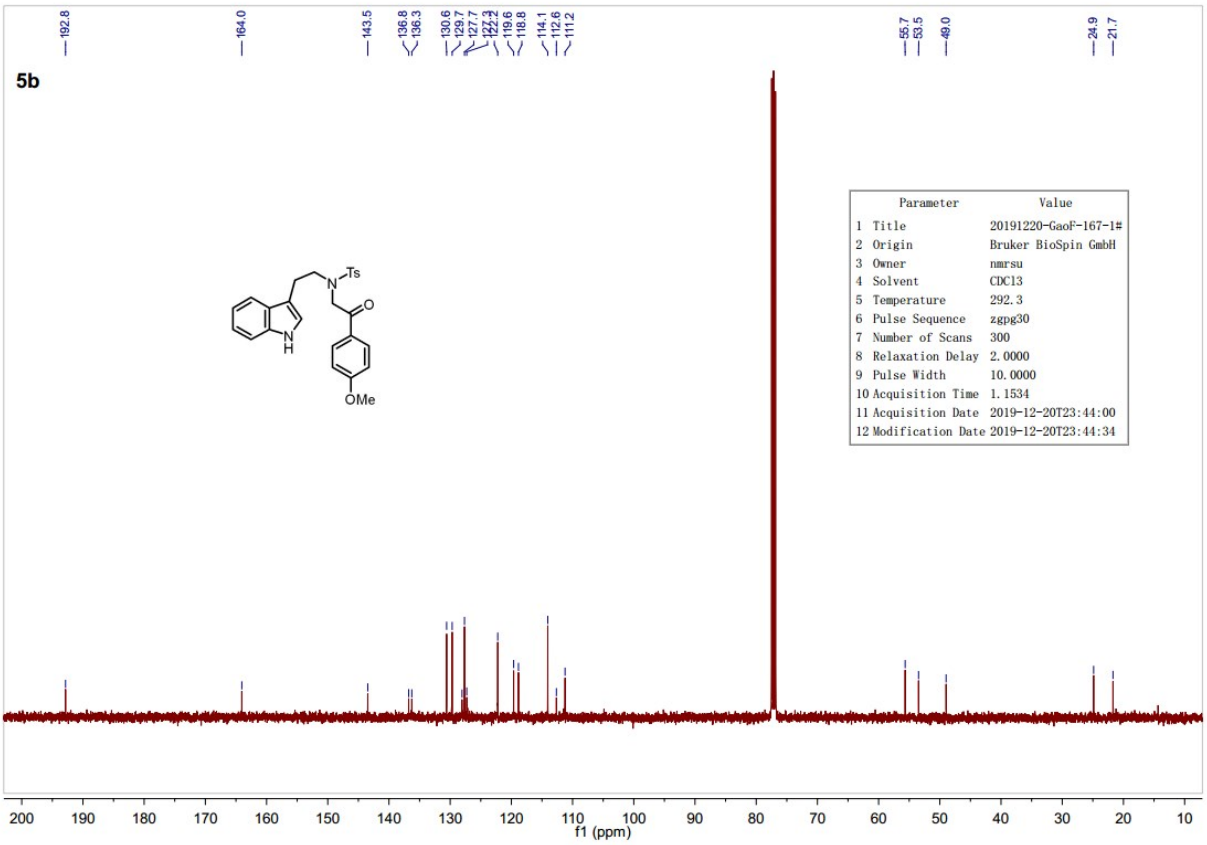

9g
8.23
7.87
7.86
7.85
7.84
7.35
7.33
7.19
7.17
7.16
6.85
6.83
4.34
4.32
4.31
4.29
3.83
3.78
1.69
1.67
NO2
N
MeO
0.94
0.96
0.99
0.99
1.98
1.97
1.00
3.02
3.03
3.02
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

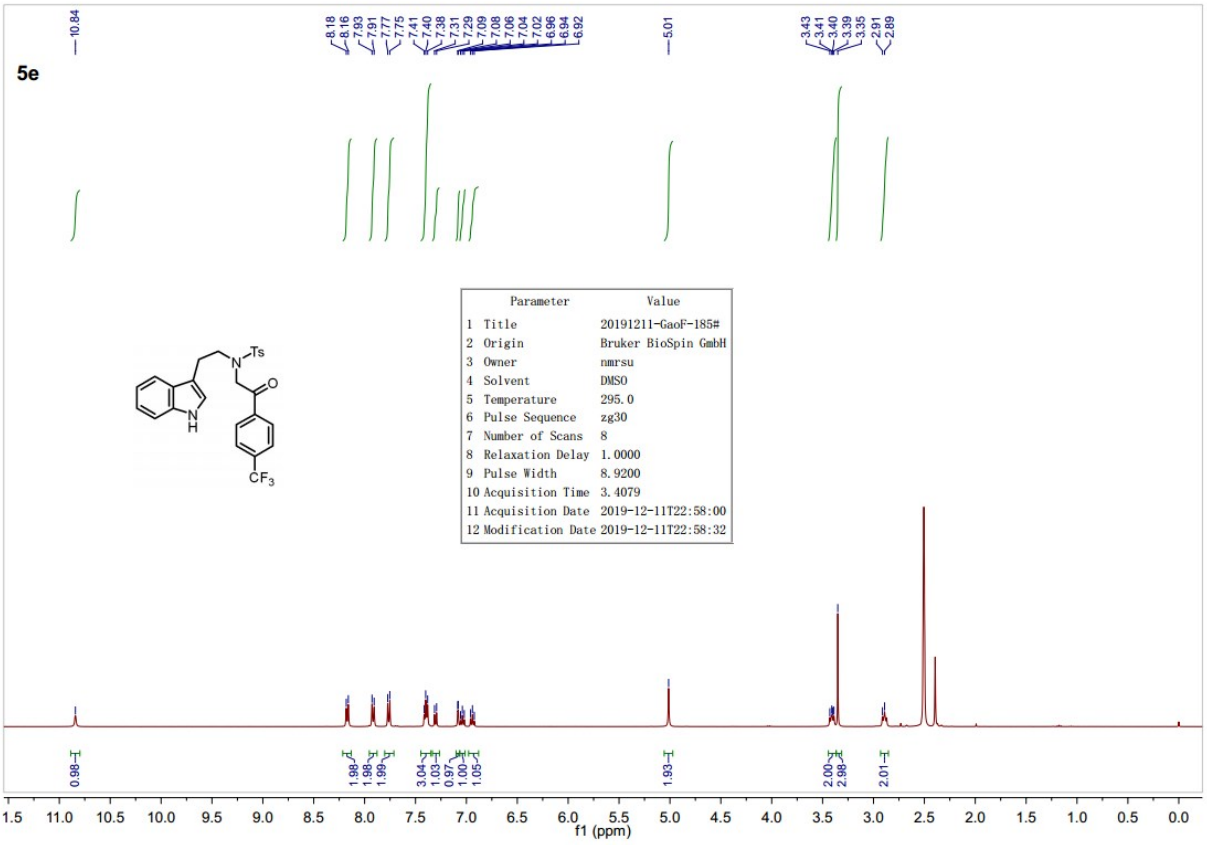

9g
158.0
142.8
138.2
135.9
131.8
131.7
128.2
121.6
119.7
114.1
113.9
106.3
55.3
35.9
33.1
22.5
NO2
N
MeO
f1 (ppm)

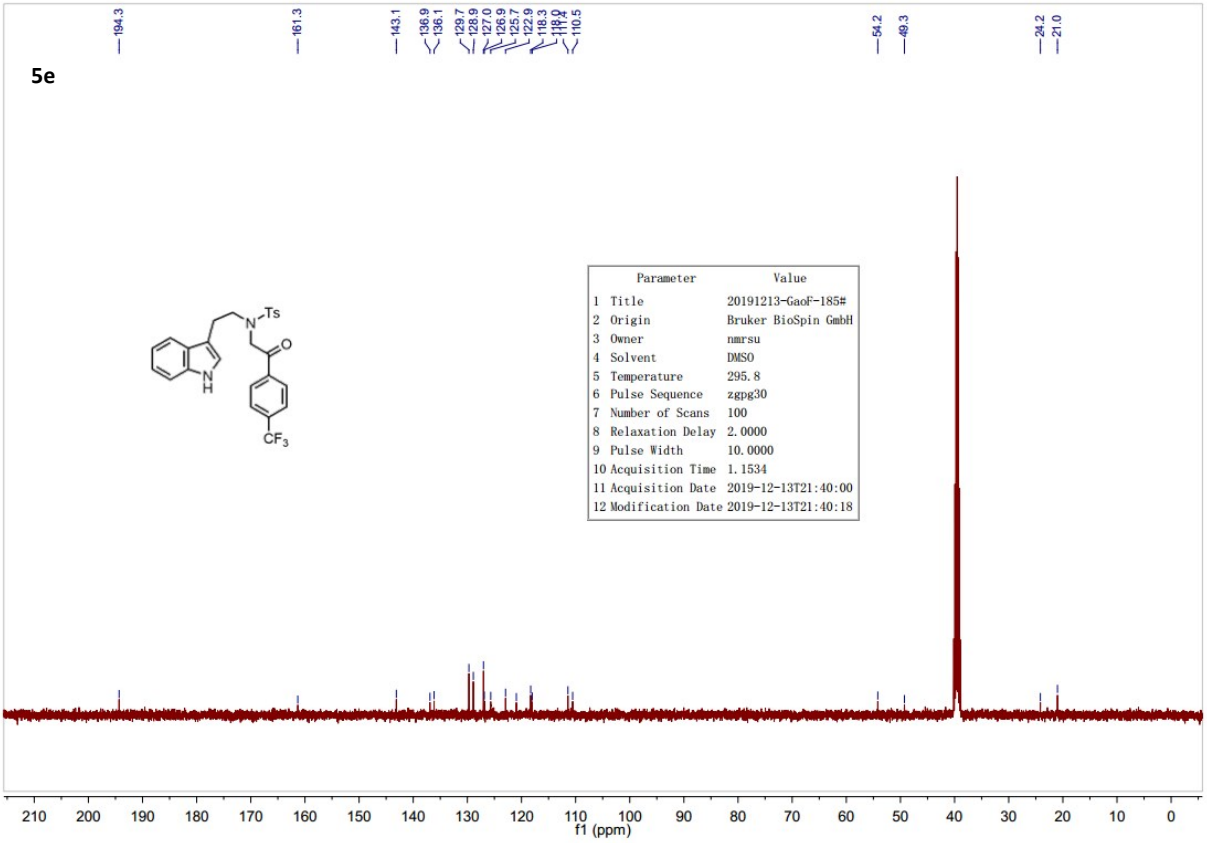

5a
7.99
7.82
7.80
7.76
7.74
7.58
7.57
7.55
7.50
7.48
7.44
7.42
7.40
7.32
7.30
7.28
7.26
7.25
7.17
7.15
7.13
7.08
7.06
7.04
6.97
6.96
4.71
3.59
3.57
3.55
3.03
3.01
2.99
2.41
Ts
N
H
O
Parameter Value
1 Title 20191205-GaoF-159-1#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 295.2
6 Pulse Sequence zg30
7 Number of Scans 32
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2019-12-05T22:53:00
12 Modification Date 2019-12-05T22:53:40
1.01
1.94
2.06
1.07
1.09
2.05
3.13
1.01
1.02
0.99
1.91
2.00
2.04
3.02
f1 (ppm)

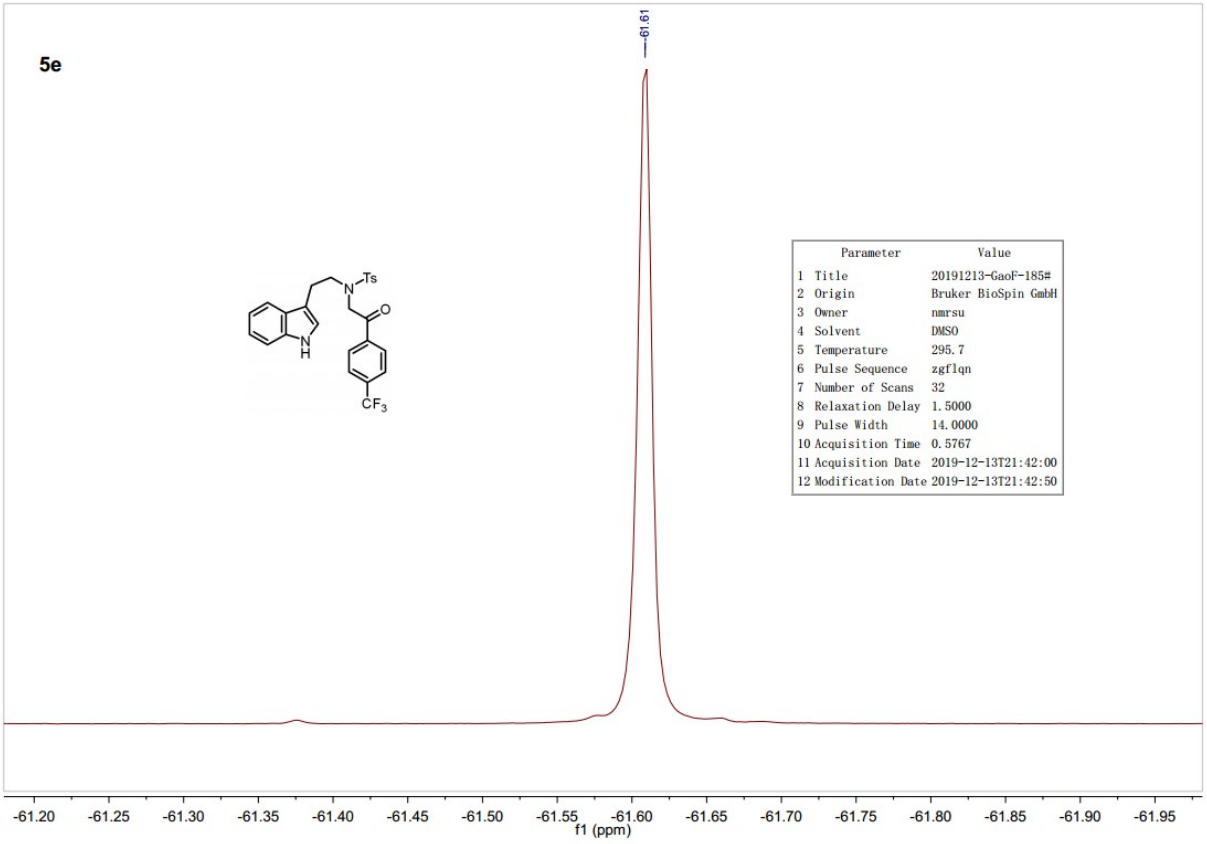

5a
194.4
143.5
136.3
133.8
129.7
128.9
128.1
127.6
122.2
119.6
118.8
112.6
111.3
53.7
48.9
24.9
21.7
Ts
N
O
H
Parameter Value
1 Title 20191206-GaoF-159-1#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 296.1
6 Pulse Sequence zgpg30
7 Number of Scans 300
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2019-12-06T20:42:00
12 Modification Date 2019-12-06T20:43:00
f1 (ppm)

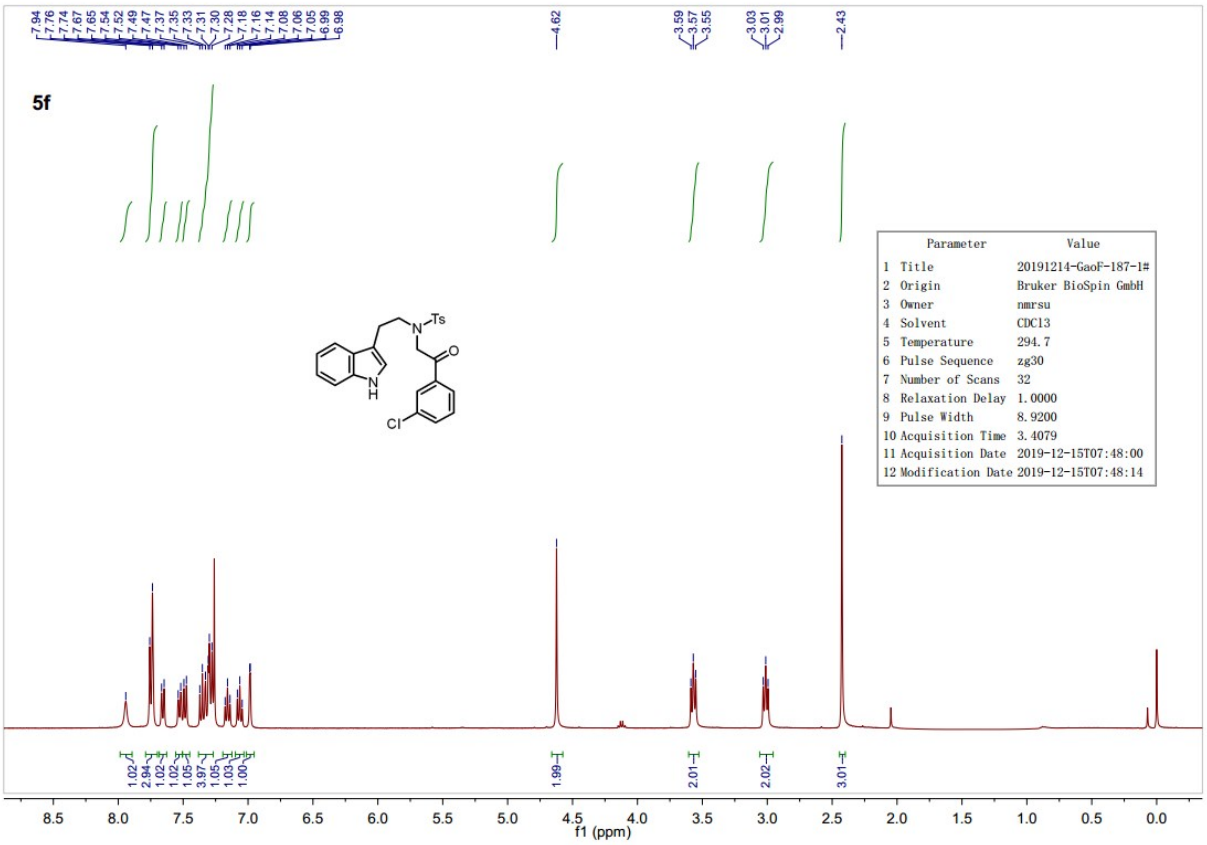

5b
8.00
7.96
7.86
7.84
7.76
7.74
7.52
7.50
7.33
7.31
7.28
7.26
7.18
7.16
7.14
7.09
7.07
7.05
6.98
6.91
6.89
4.65
3.87
3.57
3.55
3.53
3.02
3.00
2.98
2.41
0.00
0.94
1.98
1.94
0.99
4.04
1.03
1.07
1.05
1.95
1.94
3.01
2.00
1.97
3.01
Ts
N
O
H
OMe
Parameter Value
1 Title 20191219-GaoF-167-1#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 292.8
6 Pulse Sequence zg30
7 Number of Scans 16
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2019-12-19T21:23:00
12 Modification Date 2019-12-19T21:23:16
f1 (ppm)

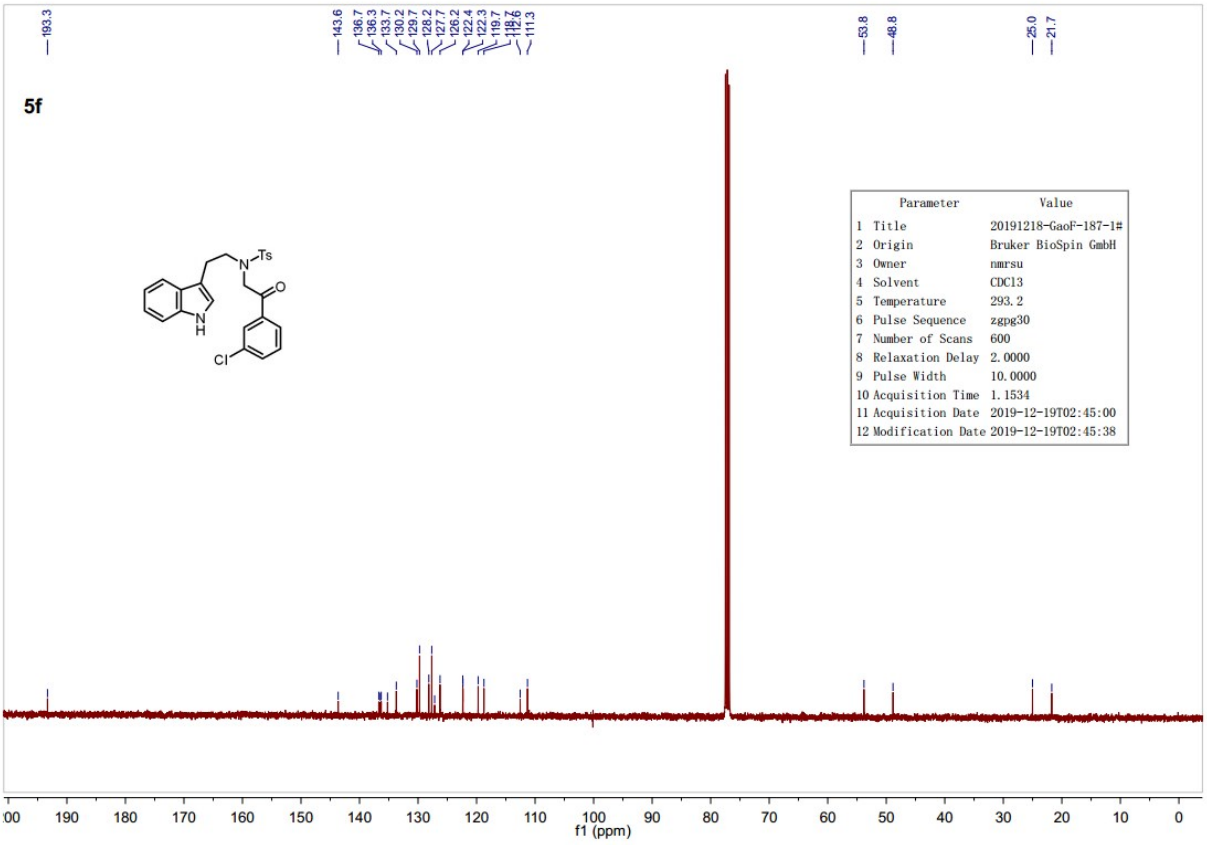

5b
192.8
164.0
143.5
136.8
136.3
130.6
129.7
127.7
122.3
122.2
119.6
118.8
114.1
112.6
111.2
55.7
53.5
49.0
24.9
21.7
Ts
N
O
N
H
OMe
Parameter Value
1 Title 20191220-GaoF-167-1#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 292.3
6 Pulse Sequence zgpg30
7 Number of Scans 300
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2019-12-20T23:44:00
12 Modification Date 2019-12-20T23:44:34
f1 (ppm)

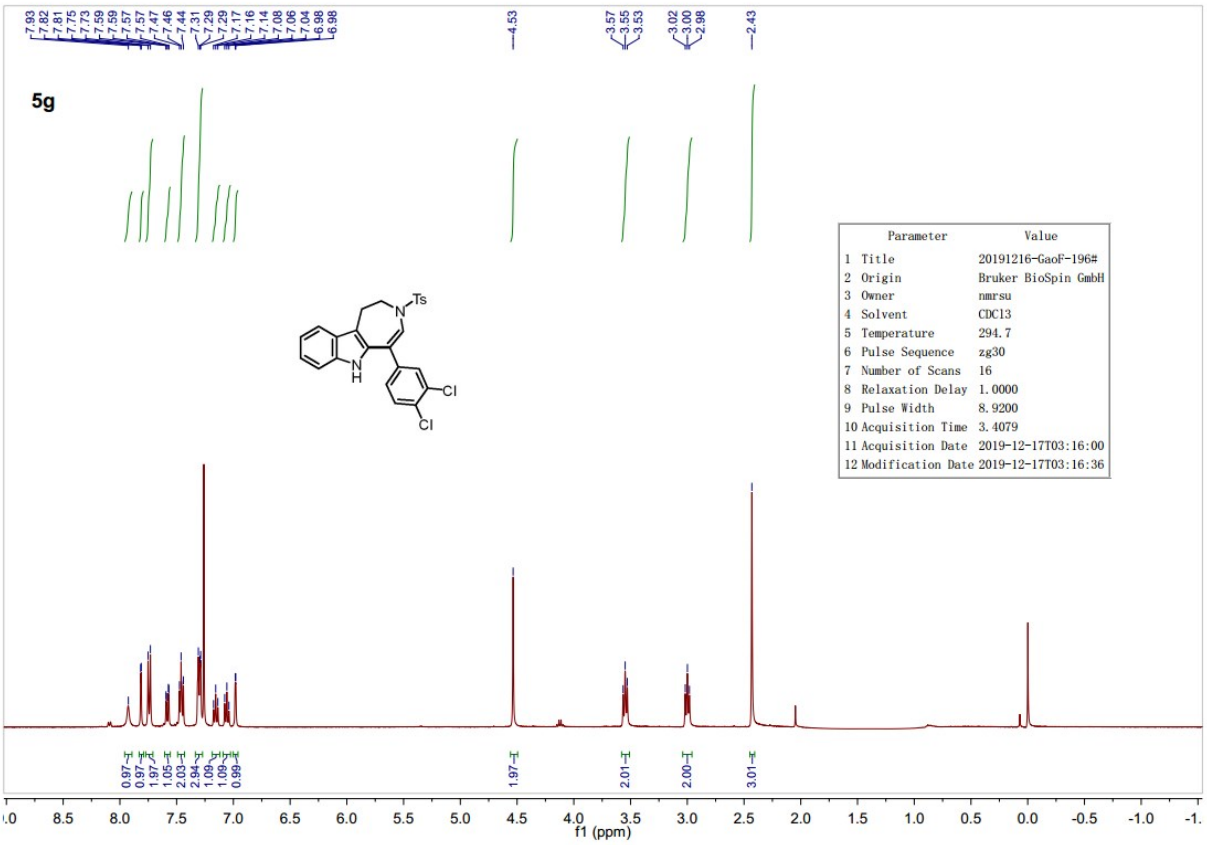

5e
10.84
8.18
8.16
7.93
7.91
7.77
7.75
7.41
7.40
7.38
7.31
7.29
7.09
7.08
7.06
7.04
7.02
6.96
6.94
6.92
5.01
3.43
3.41
3.40
3.39
3.35
2.91
2.89
Ts
N
O
N
H
CF3
Parameter Value
1 Title 20191211-GaoF-185#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent DMSO
5 Temperature 295.0
6 Pulse Sequence zg30
7 Number of Scans 8
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2019-12-11T22:58:00
12 Modification Date 2019-12-11T22:58:32
0.98
1.98
1.98
1.99
3.04
1.03
0.97
1.00
1.05
1.93
2.00
2.98
2.01
f1 (ppm)

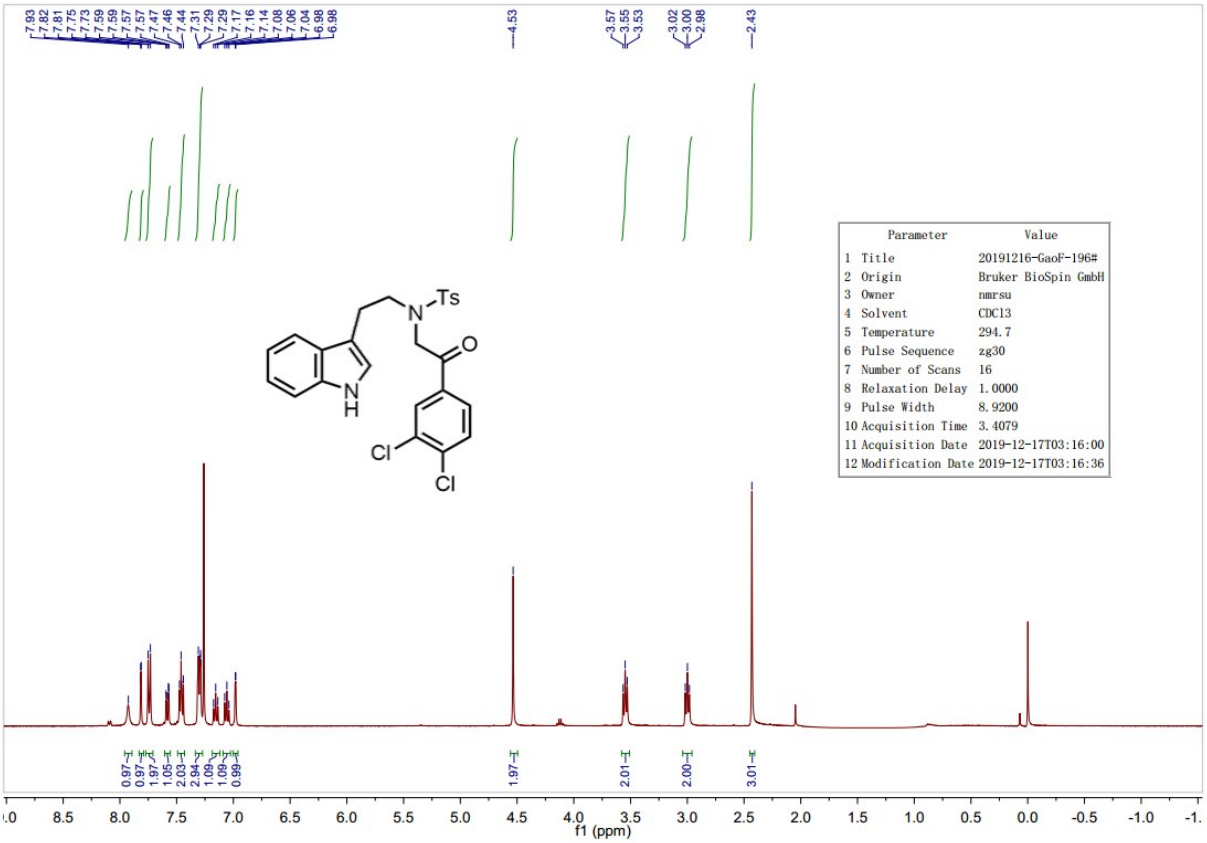

5e
194.3
161.3
143.1
136.9
136.1
129.7
128.9
127.0
126.9
125.7
122.9
118.3
110.5
54.2
49.3
24.2
21.0
Ts
N
O
H
CF3
Parameter Value
1 Title 20191213-GaoF-185#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent DMSO
5 Temperature 295.8
6 Pulse Sequence zgpg30
7 Number of Scans 100
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2019-12-13T21:40:00
12 Modification Date 2019-12-13T21:40:18
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

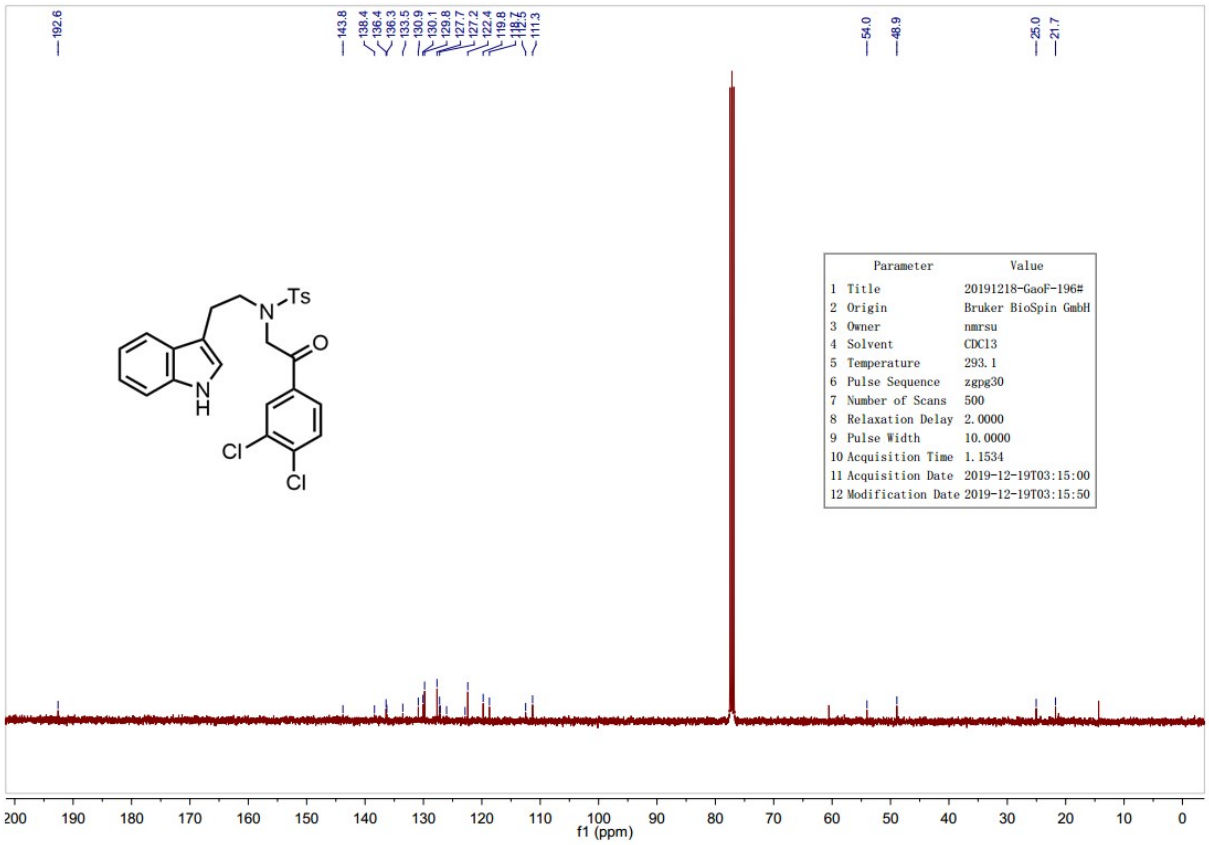

5e
61.61
Ts
N
O
H
CF3
Parameter Value
1 Title 20191213-GaoF-185#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent DMSO
5 Temperature 295.7
6 Pulse Sequence zgflqn
7 Number of Scans 32
8 Relaxation Delay 1.5000
9 Pulse Width 14.0000
10 Acquisition Time 0.5767
11 Acquisition Date 2019-12-13T21:42:00
12 Modification Date 2019-12-13T21:42:50
-61.20 -61.25 -61.30 -61.35 -61.40 -61.45 -61.50 -61.55 -61.60 -61.65 -61.70 -61.75 -61.80 -61.85 -61.90 -61.95
f1 (ppm)

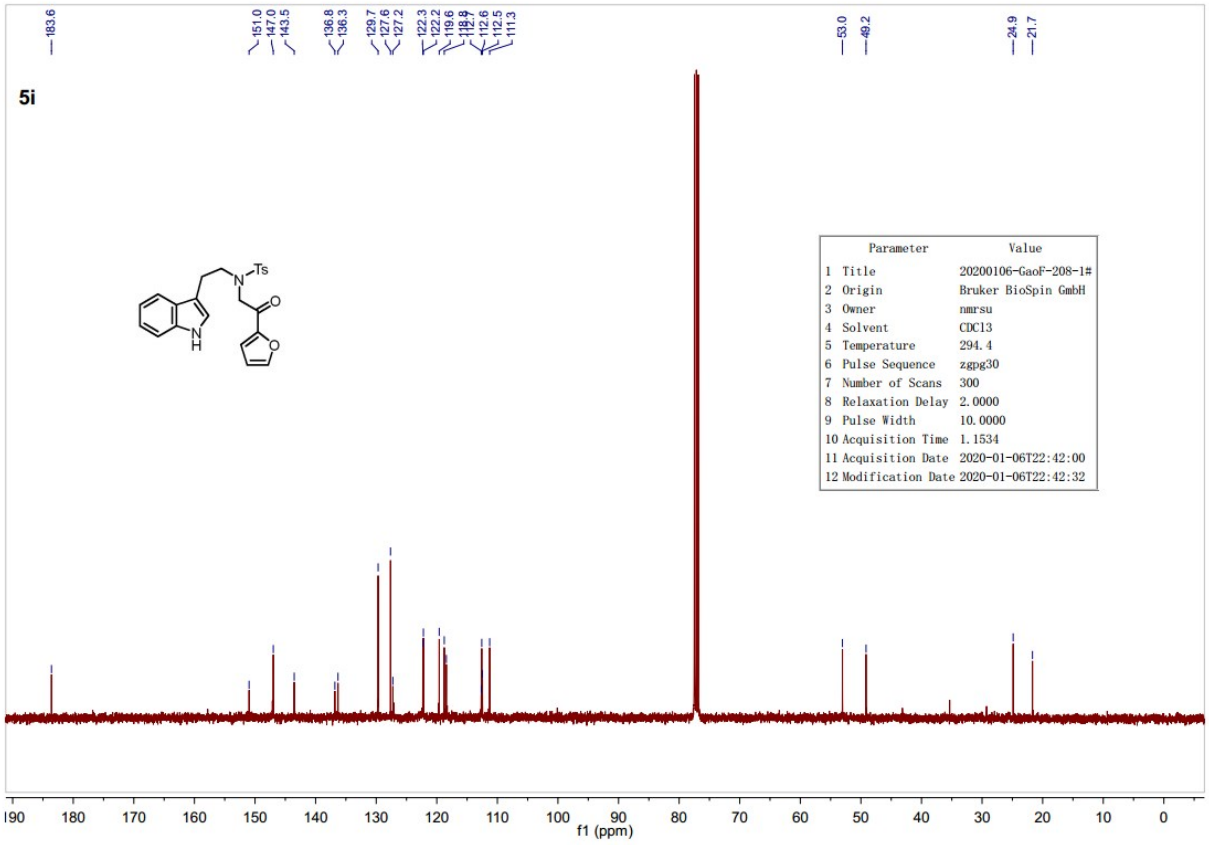

5f
7.94
7.76
7.74
7.67
7.65
7.54
7.52
7.49
7.47
7.37
7.35
7.33
7.31
7.30
7.28
7.18
7.16
7.14
7.08
7.06
7.05
6.99
6.98
4.62
3.59
3.57
3.55
3.03
3.01
2.99
2.43
Ts
N
O
H
Cl
Parameter Value
1 Title 20191214-GaoF-187-1#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 294.7
6 Pulse Sequence zg30
7 Number of Scans 32
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2019-12-15T07:48:00
12 Modification Date 2019-12-15T07:48:14
1.02
2.84
1.02
1.02
1.05
3.97
1.05
1.03
1.00
1.99
2.01
2.02
3.01
f1 (ppm)

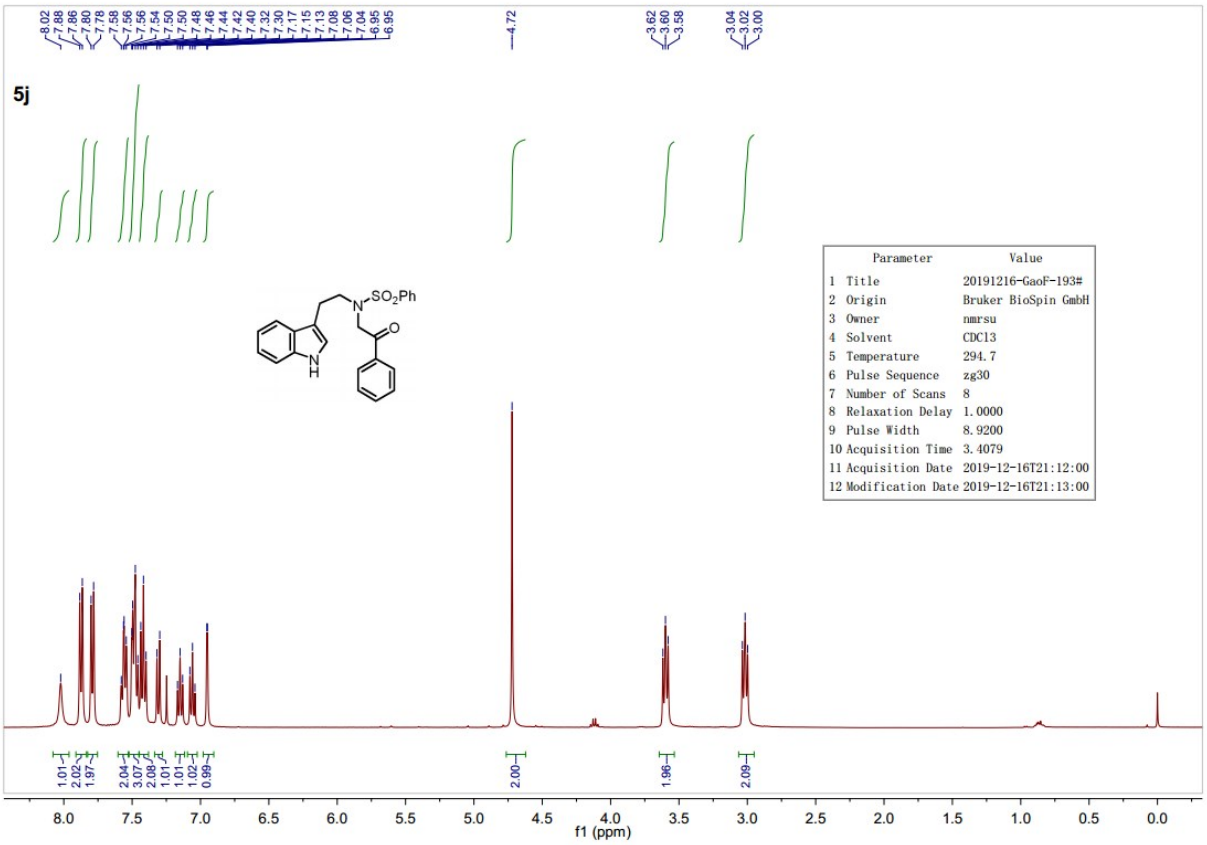

5f
193.3
143.6
136.7
136.3
133.7
130.2
129.7
128.2
127.7
126.2
122.4
122.3
119.7
112.6
111.3
53.8
48.8
25.0
21.7
Ts
N
O
H
Cl
Parameter Value
1 Title 20191218-GaoF-187-1#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 293.2
6 Pulse Sequence zgpg30
7 Number of Scans 600
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2019-12-19T02:45:00
12 Modification Date 2019-12-19T02:45:38
f1 (ppm)

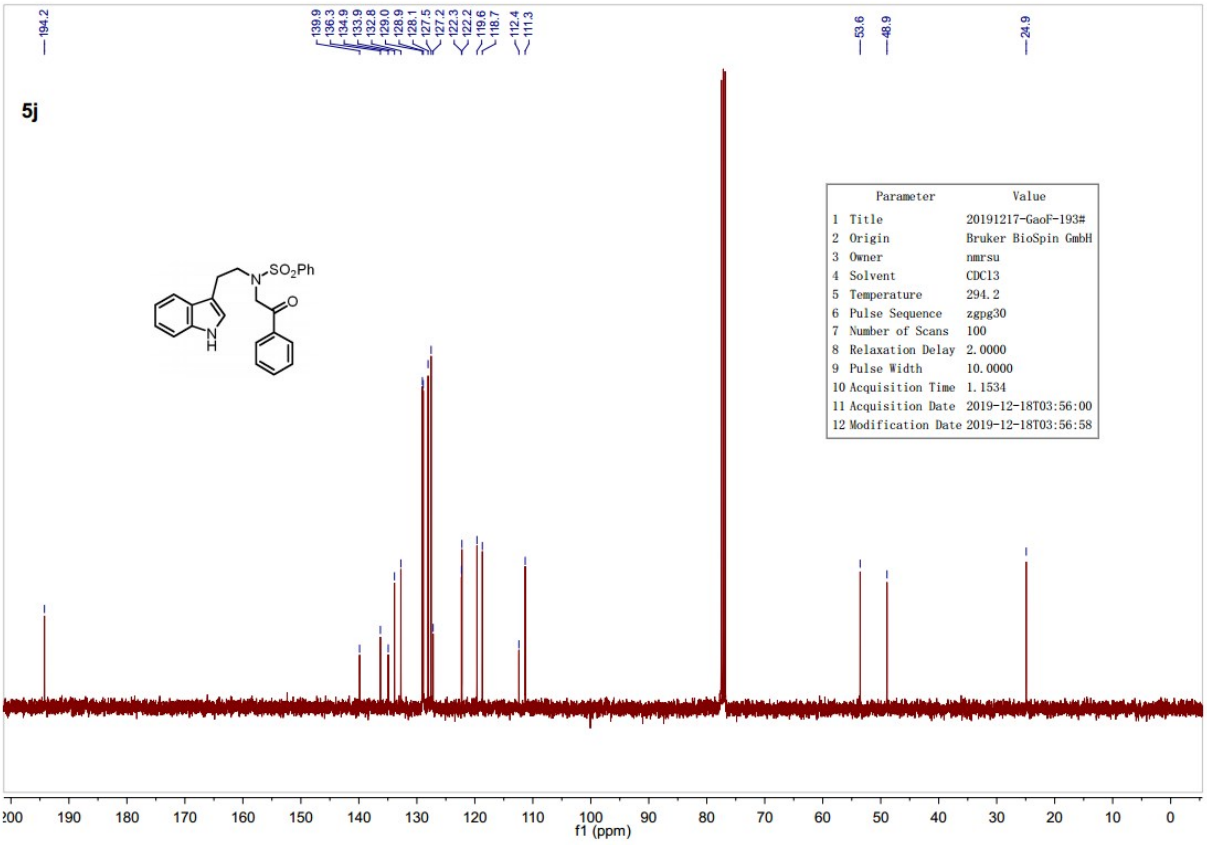

5g
7.93
7.82
7.81
7.75
7.73
7.59
7.59
7.57
7.57
7.47
7.46
7.44
7.31
7.29
7.29
7.17
7.16
7.14
7.08
7.06
7.04
6.98
6.98
4.53
3.57
3.55
3.53
3.02
3.00
2.98
2.43
Ts
N
H
Cl
Cl
Parameter Value
1 Title 20191216-GaoF-196#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 294.7
6 Pulse Sequence zg30
7 Number of Scans 16
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2019-12-17T03:16:00
12 Modification Date 2019-12-17T03:16:36
0.97
0.97
1.97
1.05
2.03
2.94
1.09
1.09
0.99
1.97
2.01
2.00
3.01
f1 (ppm)

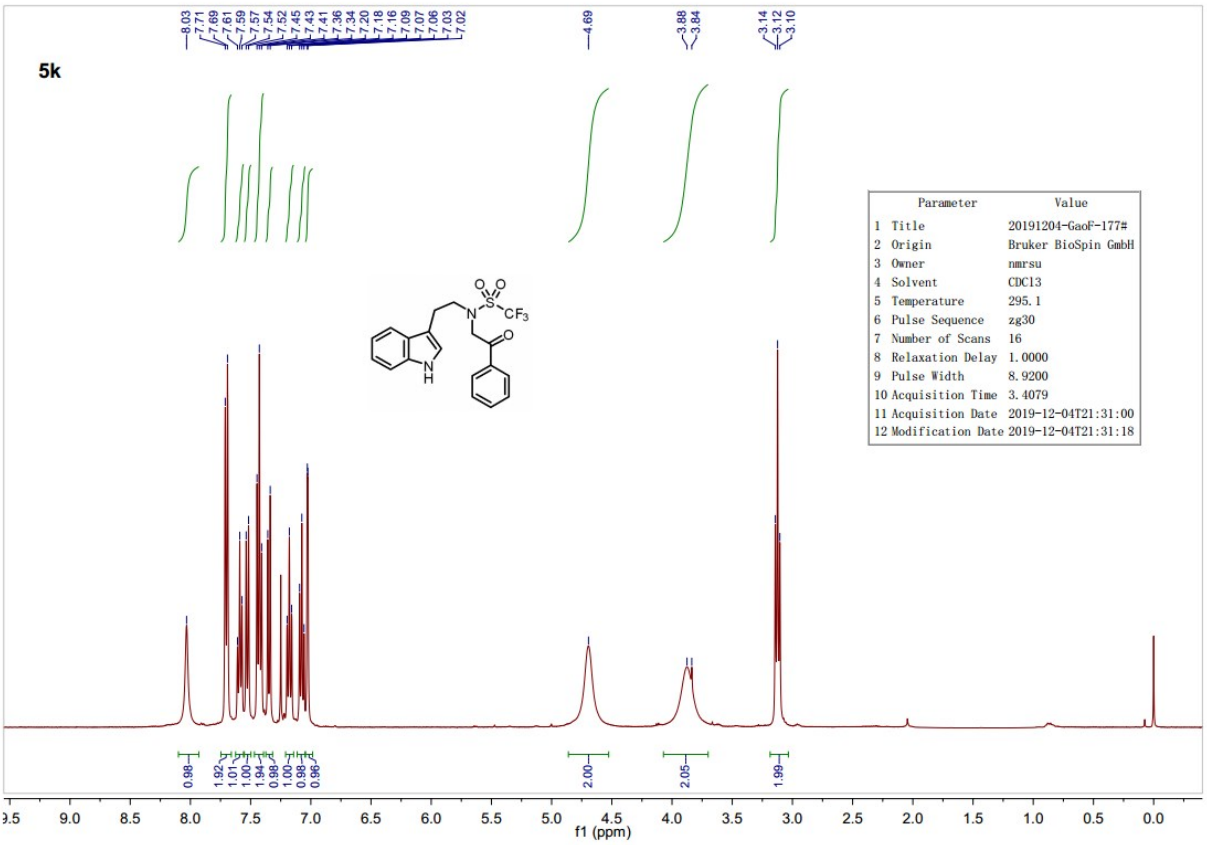

7.93
7.82
7.81
7.75
7.73
7.59
7.59
7.57
7.57
7.47
7.46
7.44
7.31
7.29
7.29
7.17
7.16
7.14
7.08
7.06
7.04
6.98
6.98
4.53
3.57
3.55
3.53
3.02
3.00
2.98
2.43
Ts
N
O
H
Cl
Cl
Parameter Value
1 Title 20191216-GaoF-196#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 294.7
6 Pulse Sequence zg30
7 Number of Scans 16
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2019-12-17T03:16:00
12 Modification Date 2019-12-17T03:16:36
0.97
0.97
1.97
1.05
2.03
2.94
1.09
1.09
0.99
1.97
2.01
2.00
3.01
f1 (ppm)

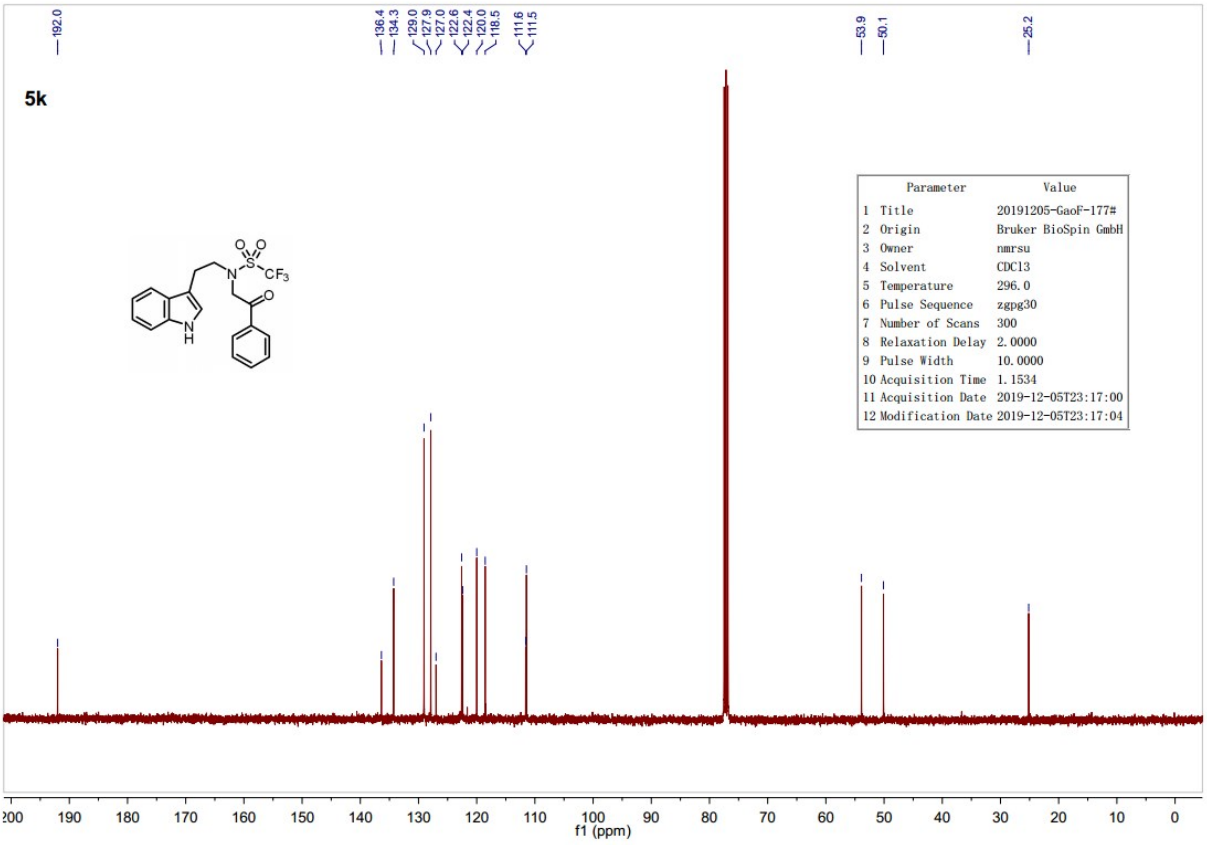

192.6
143.8
138.4
136.4
136.3
133.5
130.9
130.1
129.8
127.7
127.2
122.4
119.8
112.7
111.5
111.3
54.0
48.9
25.0
21.7
Ts
N
O
H
Cl
Cl
Parameter Value
1 Title 20191218-GaoF-196#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 293.1
6 Pulse Sequence zgpg30
7 Number of Scans 500
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2019-12-19T03:15:00
12 Modification Date 2019-12-19T03:15:50
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

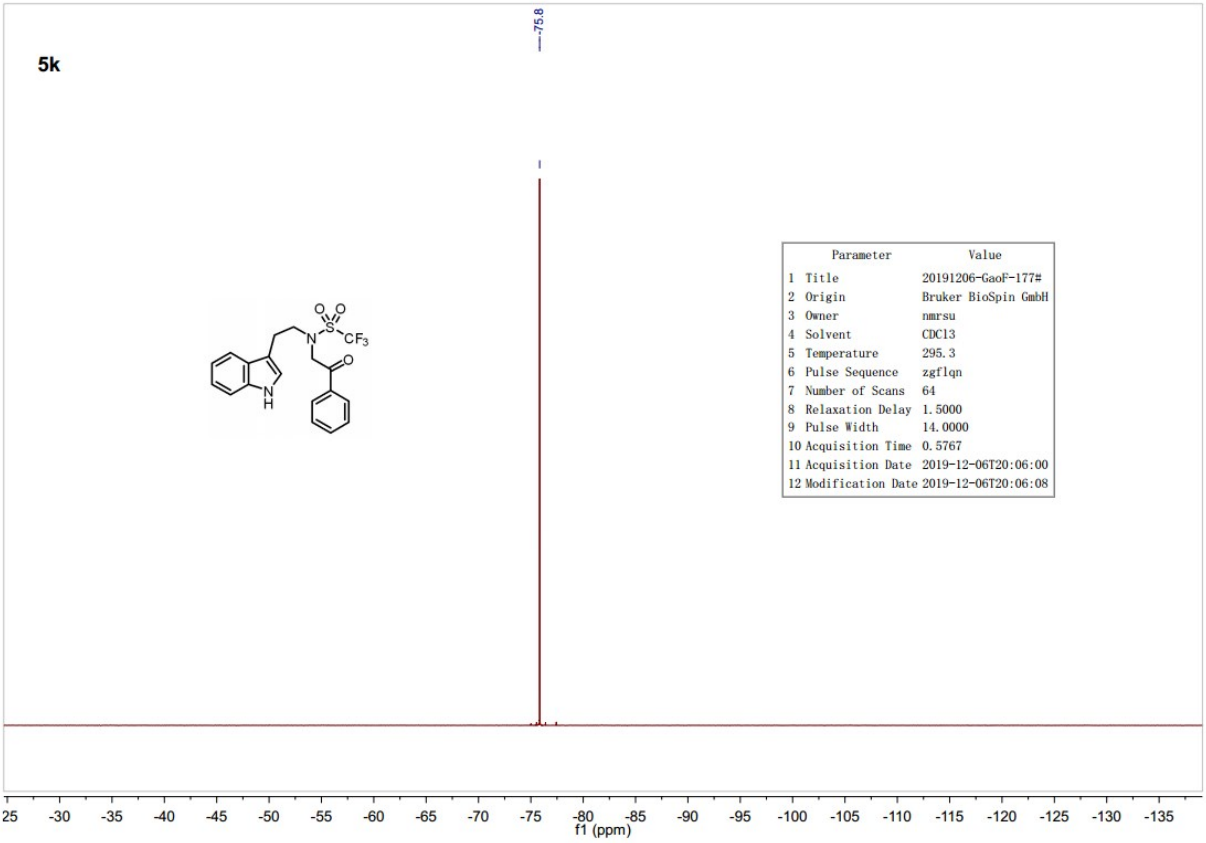

5i
183.6
151.0
147.0
143.5
136.8
136.3
129.7
127.6
127.2
122.3
122.2
119.6
112.6
112.5
111.3
53.0
49.2
24.9
21.7
Ts
N
O
H
O
Parameter Value
1 Title 20200106-GaoF-208-1#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 294.4
6 Pulse Sequence zgpg30
7 Number of Scans 300
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2020-01-06T22:42:00
12 Modification Date 2020-01-06T22:42:32
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

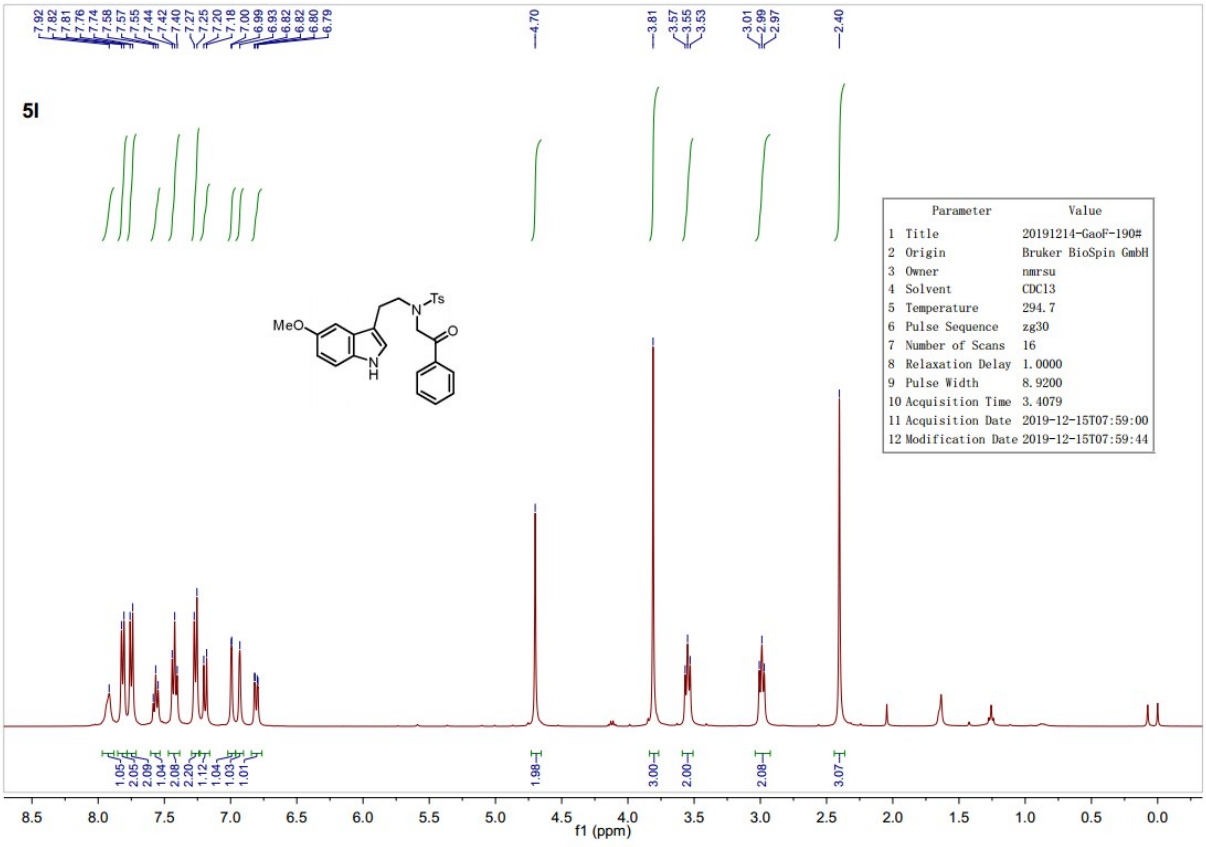

5j
8.02
7.88
7.86
7.80
7.78
7.58
7.56
7.56
7.54
7.50
7.50
7.48
7.46
7.44
7.42
7.40
7.32
7.30
7.17
7.15
7.13
7.08
7.06
7.04
6.95
6.95
4.72
3.62
3.60
3.58
3.04
3.02
3.00
SO2Ph
N
O
H
Parameter Value
1 Title 20191216-GaoF-193#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 294.7
6 Pulse Sequence zg30
7 Number of Scans 8
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2019-12-16T21:12:00
12 Modification Date 2019-12-16T21:13:00
1.01
2.02
1.97
2.04
3.07
2.08
1.01
1.01
1.02
0.99
2.00
1.96
2.09
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)

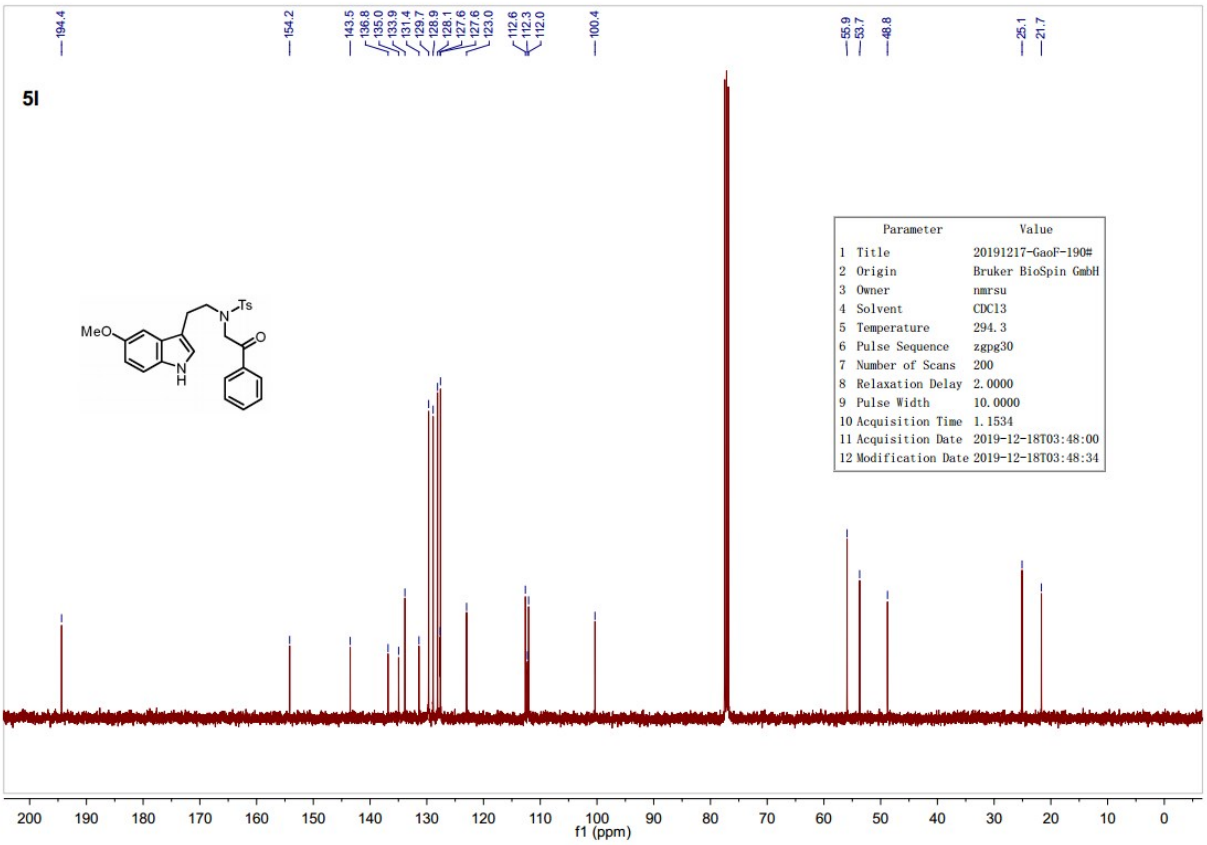

5j
194.2
139.9
136.3
134.9
133.9
132.8
129.0
128.9
128.1
127.5
127.2
122.3
122.2
119.6
118.7
112.4
111.3
53.6
48.9
24.9
SO2Ph
N
O
H
Parameter Value
1 Title 20191217-GaoF-193#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 294.2
6 Pulse Sequence zgpg30
7 Number of Scans 100
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2019-12-18T03:56:00
12 Modification Date 2019-12-18T03:56:58
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

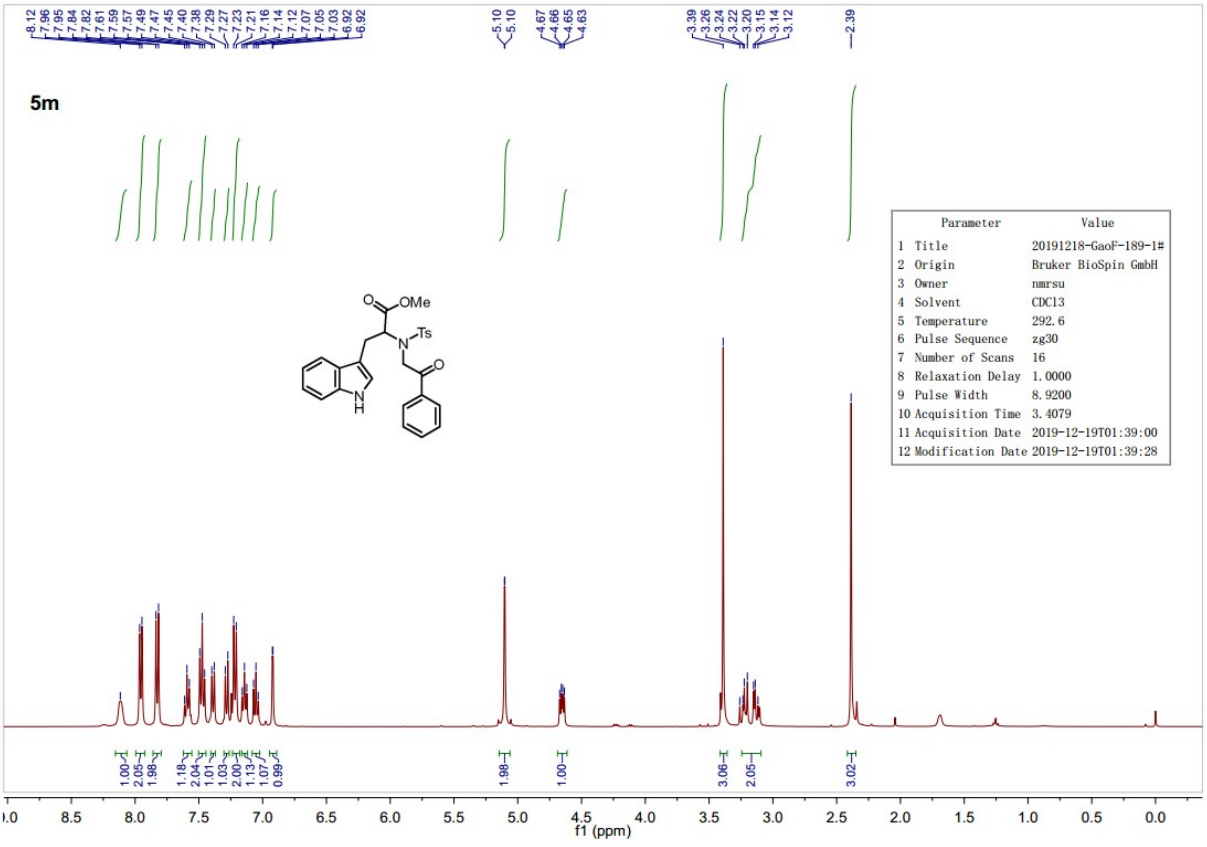

5k
8.03
7.71
7.69
7.61
7.59
7.57
7.54
7.52
7.45
7.43
7.41
7.36
7.34
7.20
7.18
7.16
7.09
7.07
7.06
7.03
7.02
4.69
3.88
3.84
3.14
3.12
3.10
Parameter Value
1 Title 20191204-GaoF-177#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 295.1
6 Pulse Sequence zg30
7 Number of Scans 16
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2019-12-04T21:31:00
12 Modification Date 2019-12-04T21:31:18
0.98
1.92
1.01
1.00
1.94
0.98
1.00
0.98
0.90
2.00
2.05
1.99
f1 (ppm)

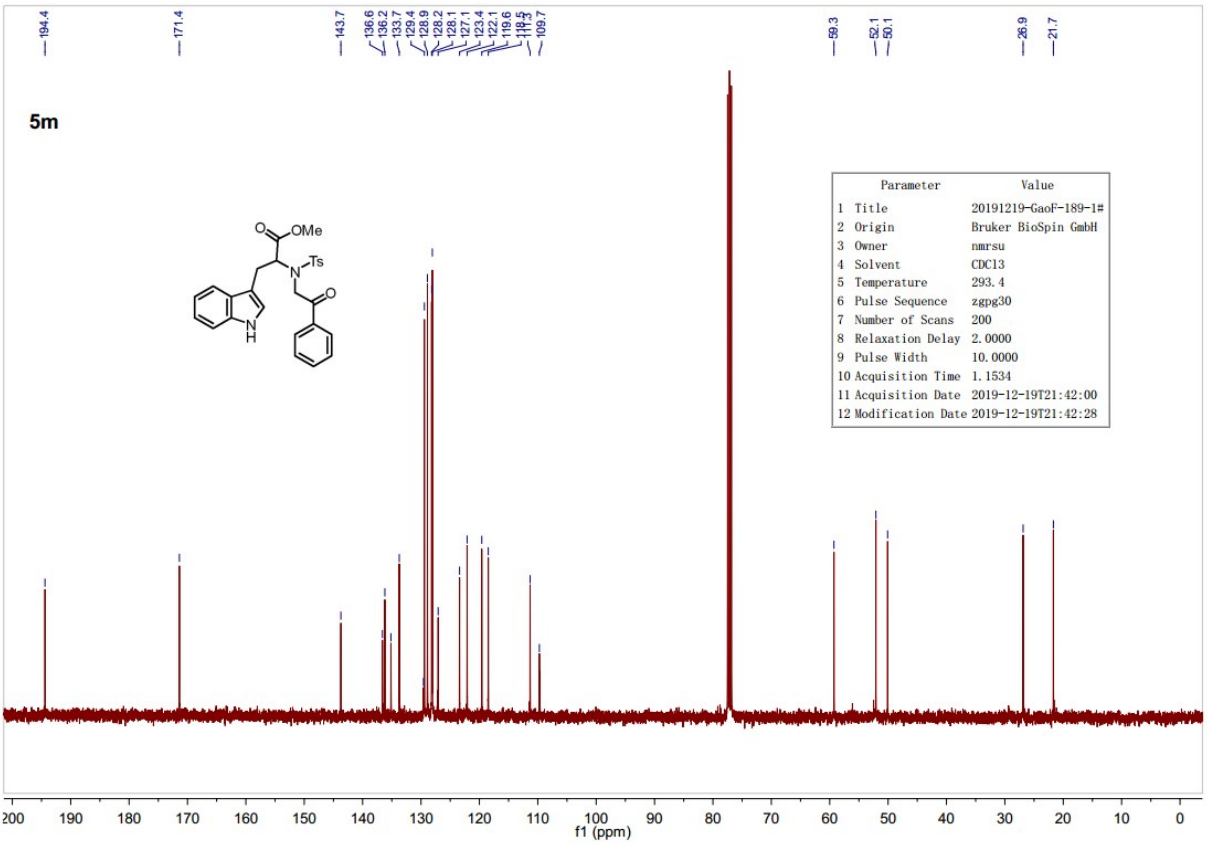

5k
192.0
136.4
134.3
129.0
127.9
127.0
122.6
122.4
120.0
118.5
111.6
111.5
53.9
50.1
25.2
Parameter Value
1 Title 20191205-GaoF-177#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 296.0
6 Pulse Sequence zgpg30
7 Number of Scans 300
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2019-12-05T23:17:00
12 Modification Date 2019-12-05T23:17:04
f1 (ppm)


5k
-75.8
Parameter Value
1 Title 20191206-GaoF-177#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 295.3
6 Pulse Sequence zgflqn
7 Number of Scans 64
8 Relaxation Delay 1.5000
9 Pulse Width 14.0000
10 Acquisition Time 0.5767
11 Acquisition Date 2019-12-06T20:06:00
12 Modification Date 2019-12-06T20:06:08
f1 (ppm)


5l
7.92
7.82
7.81
7.76
7.74
7.58
7.57
7.55
7.44
7.42
7.40
7.27
7.25
7.20
7.18
7.00
6.99
6.83
6.82
6.82
6.80
6.79
4.70
3.81
3.57
3.55
3.53
3.01
2.99
2.97
2.40
Parameter Value
1 Title 20191214-GaoF-190#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 294.7
6 Pulse Sequence zg30
7 Number of Scans 16
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2019-12-15T07:59:00
12 Modification Date 2019-12-15T07:59:44
1.05
2.05
2.09
1.04
2.08
2.20
1.12
1.04
1.03
1.01
1.98
3.00
2.00
2.08
3.07
f1 (ppm)


5l
194.4
154.2
143.5
136.8
135.0
133.9
131.4
129.7
128.9
128.1
127.6
127.6
123.0
112.6
112.3
112.0
100.4
55.9
53.7
48.8
25.1
21.7
MeO
Ts
N
O
H
Parameter Value
1 Title 20191217-GaoF-190#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 294.3
6 Pulse Sequence zgpg30
7 Number of Scans 200
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2019-12-18T03:48:00
12 Modification Date 2019-12-18T03:48:34
f1 (ppm)


8.12
7.96
7.95
7.84
7.82
7.61
7.59
7.57
7.49
7.47
7.45
7.40
7.38
7.29
7.27
7.23
7.21
7.16
7.14
7.12
7.07
7.05
7.03
6.92
6.92
5.10
5.10
4.67
4.66
4.65
4.63
3.39
3.26
3.24
3.22
3.20
3.15
3.14
3.12
2.39
5m
OMe
Ts
N
O
H
Parameter Value
1 Title 20191218-GaoF-189-1#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 292.6
6 Pulse Sequence zg30
7 Number of Scans 16
8 Relaxation Delay 1.0000
9 Pulse Width 8.9200
10 Acquisition Time 3.4079
11 Acquisition Date 2019-12-19T01:39:00
12 Modification Date 2019-12-19T01:39:28
1.00
2.05
1.98
1.18
2.04
1.01
1.03
2.00
1.13
1.07
0.99
1.98
1.00
3.06
2.05
3.02
f1 (ppm)


194.4
171.4
143.7
136.6
136.2
133.7
129.4
128.9
128.2
128.1
127.1
123.4
122.1
119.6
118.5
111.3
109.7
59.3
52.1
50.1
26.9
21.7
5m
OMe
Ts
N
H
O
Parameter Value
1 Title 20191219-GaoF-189-1#
2 Origin Bruker BioSpin GmbH
3 Owner nmrsu
4 Solvent CDCl3
5 Temperature 293.4
6 Pulse Sequence zgpg30
7 Number of Scans 200
8 Relaxation Delay 2.0000
9 Pulse Width 10.0000
10 Acquisition Time 1.1534
11 Acquisition Date 2019-12-19T21:42:00
12 Modification Date 2019-12-19T21:42:28
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)