Supporting Information

Photocatalytic Intermolecular Carboarylation of Alkenes by Selective C−O Bond Cleavage of Diarylethers

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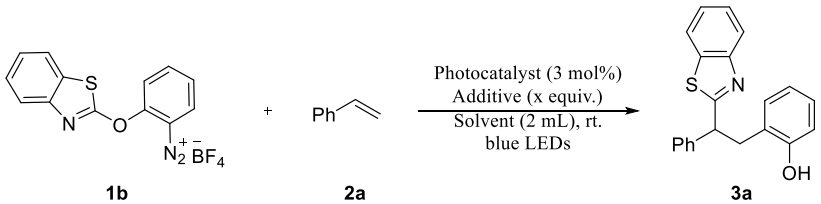
1. General experimental details

All reactions were maintained under a nitrogen atmosphere unless otherwise stated. Commercially available reagents and solvents were purchased from Macklin, Energy, Sigma-Aldrich or TCI and were used without further purification. Infrared (FT-IR) spectra were recorded on a BRUKER VERTEX 70, ν_{max} in cm^{-1}. ^{1}H-NMR spectra were recorded on a BRUKER AVANCE III HD (400 MHz) spectrometer. Chemical shifts were reported in ppm from tetramethylsilane with the solvent resonance as internal standard ($CDCl_3$: δ 7.26, DMSO-d^6: δ 2.50). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quadruplet, br = broad, m = multiplet), coupling constants (Hz) and integration. ^{13}C-NMR spectra were recorded on a BRUKER AVANCE III HD (100 MHz) spectrometer with complete proton decoupling. Chemical shifts were reported in ppm from tetramethylsilane with the solvent resonance as the internal standard ($CDCl_3$: δ 77.00, DMSO-d^6: δ 39.52). ^{19}F-NMR spectra were recorded on a BRUKER AVANCE III HD (376 MHz) spectrometer. ^{11}B-NMR spectra were recorded on a BRUKER AVANCE III HD (128 MHz) spectrometer. High resolution mass spectrometry (HRMS) were measured with a GCT PremierTM and BRUKER micrOTF-Q III. Melting points were measured using INESA WRR and values were uncorrected. Single-crystal X-ray diffraction measurements were performed on Bruker Photon II CPAD diffractometer with nitrogen-flow temperature controlled using graphite-monchromated Mo-Kα (λ =0.71073 Å) radiation at 120 K. The structure was solved by direct method using SHELXL2014 and the refinement against all reflections of the compound was performed using SHELXL2014. Powder X-ray diffraction (PXRD) data were collected on a desktop diffractometer (D2 PHASER, Bruker, Germany) using Cu-Kα (λ=1.54056 Å) radiation operated at 30 kV and 10 mA.

2. Reaction condition survey[a]



1b **2a** **3a**

Entry	Photocatalyst	Additive (x equiv.)	Solvent	Yield (%)[b]
1	$[Ir(ppy)_2(dtbbpy)]PF_6$	PhSH (1.5)	MeCN	31
2	$Ir(ppy)_3$	PhSH (1.5)	MeCN	<10
3	Eosin Y	PhSH (1.5)	MeCN	39
4	$Ru(bpy)_3Cl_2·6H_2O$	PhSH (1.5)	MeCN	37
5	$[Ir(dF(CF_3)ppy)_2(dtbbpy)]PF_6$	PhSH (1.5)	MeCN	48
6	9-mesityl-10-methylacridinium perchlorate	PhSH (1.5)	MeCN	46
7	2,4,6-triphenylpyrylium tetrafluoroborate	PhSH (1.5)	MeCN	38
8	4CzIPN	PhSH (1.5)	MeCN	55
9	Fluorescein	PhSH (1.5)	MeCN	37
10	4CzIPN	PhSH (1.5)	DCM	38
11	4CzIPN	PhSH (1.5)	DMSO	n.d.
12	4CzIPN	PhSH (1.5)	DMF	n.d.
13	4CzIPN	PhSH (1.5)	DME	<10
14	4CzIPN	PhSH (1.5)	$PhCF_3$	<10
15	4CzIPN	PhSH (1.5)	PhCl	<10
16	4CzIPN	PhSH (1.5)	Acetone	65
17	4CzIPN	PhSH (1.5)	EtOAc	45
18	4CzIPN	PhSH (1.5)	THF	21
19	4CzIPN	L(+)-Ascorbic acid (1.5)	Acetone	37

20	4CzIPN	$NaBH_4$ (1.5)	Acetone	trace
21	4CzIPN	Sodium ascorbate (1.5)	Acetone	trace
22	4CzIPN	Cyclohexa-1,4-diene (1.5)	Acetone	<10
23	$[Ir(ppy)_2(dtbbpy)]PF_6$	TTMSS (1.5)	MeCN	19
24	$[Ir(ppy)_2(dtbbpy)]PF_6$	$^iPr_2NH$ (1.5)	MeCN	n.d.
25[c]	$[Ir(ppy)_2(dtbbpy)]PF_6$	HEH (2.0)	MeCN	n.d.
26	4CzIPN	L(+)-Ascorbic acid (1.5)	MeCN	66
27	4CzIPN	L(+)-Ascorbic acid (1.5)	DCM	24
28	4CzIPN	L(+)-Ascorbic acid (1.5)	EtOAc	63
29	4CzIPN	L(+)-Ascorbic acid (2.0)	MeCN	71
30[c]	**4CzIPN**	**L(+)-Ascorbic acid (2.0)**	**MeCN**	**71**
31[c]	4CzIPN	L(+)-Ascorbic acid (2.5)	MeCN	70
32[c,d]	4CzIPN	L(+)-Ascorbic acid (2.0)	MeCN	trace
33[c,d]	-	L(+)-Ascorbic acid (2.0)	MeCN	trace
34[c]	4CzIPN	-	MeCN	22
35[c]	-	L(+)-Ascorbic acid (2.0)	MeCN	22

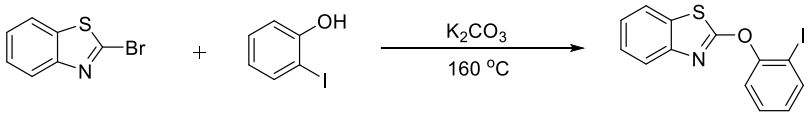
[a]Reaction condition: **1b** (0.2 mmol), **2a** (0.4 mmol), photocatalyst (3 mol %), and additive in solvent (2.0 mL) were irradiated with 30 W×2 blue LEDs at rt under N_2. [b]Yields of isolated products. [c]**1b** (0.3 mmol), **2a** (0.2 mmol). [d]In dark. The "n.d." means no product was detected.

3. General procedure for the carboarylation of alkenes

Alkene **2** (0.2 mmol, 1.0 equiv.), benzenediazonium tetrafluoroborate **1b-1o** (0.3 mmol, 1.5 equiv.), 4CzIPN (0.006 mmol, 3 mol %), and L(+)-ascorbic acid (0.4 mmol, 2.0 equiv.) were loaded in a reaction vial which was subjected to evacuation/ flushing with N_2 three times. MeCN (2.0 mL) was added to the mixture via syringe and the reaction was irradiated with 30 W×2 blue LEDs. After reaction completion monitored by TLC, the reaction mixture was extracted with ethyl acetate (3 x 15 mL). The combined organic extract was washed by brine, dried over Na_2SO_4, filtered, concentrated, and purified by flash column chromatography on silica gel (eluent: ethyl acetate/ petroleum ether) to give the desired product **3** or **4**.

4. Synthesis of dual-function reagents 1 and 4CzIPN

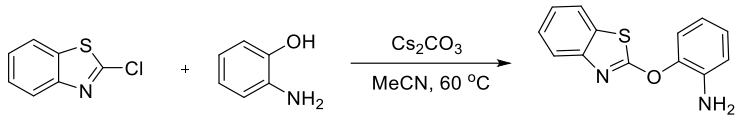
4.1 Synthesis of **1a**



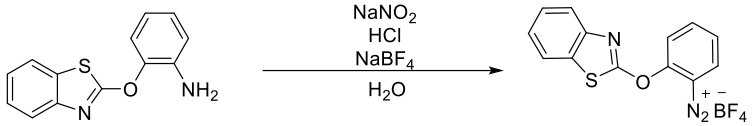
2-Bromobenzothiazole (10 mmol 1.0 equiv.), 2-iodophenol (15 mmol 1.5 equiv.), and K_2CO_3 (20 mmol, 2.0 equiv.) were loaded in a 100 mL flame-dried Schlenk tube which was subjected to evacuation/ flushing with N_2 three times. The reaction was heated to 160°C for 24 h in oil bath. After reaction completion monitored by TLC, the reaction mixture was cooled to room temperature and extracted with ethyl acetate (3 x 25 mL). The combined organic extract was washed by brine,

dried over Na_2SO_4, filtered, concentrated, and purified by flash column chromatography on silica gel (eluent: ethyl acetate/ petroleum ether = 1:200) to give product as white solid (1.9 g) in 54% yield.

4.2 Representative procedures for synthesis of **1b-1o**

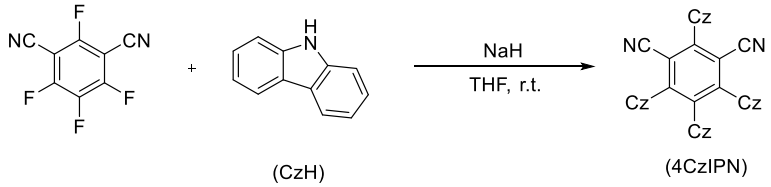


First step: 2-Aminophenol (10 mmol, 1.0 equiv.) and Cs_2CO_3 (21 mmol, 2.1 equiv.) were loaded in a 100 mL round-bottom flask which was subjected to evacuation/ flushing with N_2 three times. MeCN (25 mL) and 2-chlorobenzothiazole (20 mmol, 2.0 equiv.) were added in sequence to the mixture via syringe and the reaction was heated to 60°C for 12 h in oil bath. After reaction completion monitored by TLC, the reaction mixture was cooled to room temperature and extracted with ethyl acetate (3 x 20 mL).The combined organic extract was washed by brine, dried over Na_2SO_4, filtered, concentrated, and purified by flash column chromatography on silica gel (eluent: ethyl acetate/ petroleum ether = 1:10) to give product as pink solid (2.1g) in 87% yield.



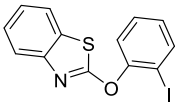
Second step: 2-Benzothiazolyloxy aniline (1 mmol, 1 equiv.) was milled into powder and poured into a 100 mL round-bottom flask containing a stirrer. Concentrated hydrochloric acid (2 mL) was added portion wise to the mixture in a state of agitation. After 1 h, the mixture become homogenous white viscous liquid and was placed in an ice bath. Sodium nitrite (1.1 mmol, 1.1 equiv.) in 1.0 mL of distilled water was added drop wise. After 15 minutes, a yellow clear solution was obtained. Sodium tetrafluoroborate (10 mmol, 10 equiv.) was added to this solution, and then a lot of precipitate can be observed. After filtration, the cake was washed by distilled water (5 mL×3) (0 °C) and ether (5 mL×4) and evaporated to dryness under reduced pressure, giving 2-benzothiazolyloxy benzenediazonium tetrafluoroborate (306.5 mg) in 90% yield.

4.3 Synthesis of 4CzIPN



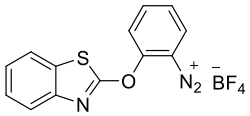
NaH (60% in oil, 0.60 g, 15 mmol) was added slowly to a stirred solution of carbazole (1.67 g, 10.0 mmol) in dry THF (40 mL) under a nitrogen atmosphere at room temperature. After 30 min, tetrafluoroisophthalonitrile (0.40 g, 2 mmol) was added. After stirred at room temperature for 12 h, 2 mL water was added to the reaction mixture to quench the excess NaH. The resulting mixture was then concentrated under reduced pressure and washed by water and EtOH to yield the crude product, which was purified by recrystalization from hexane/DCM to give the product (1.5 g) in 95 % yield.

5. Characterization of starting materials

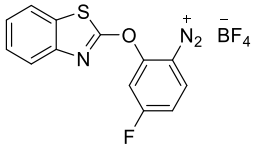


1a: 1.9 g, 54%, yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93-7.88 (m, 1H), 7.78-7.73 (m, 1H), 7.72-7.67 (m, 1H), 7.48-7.36 (m, 3H), 7.32-7.26 (m, 1H), 7.09-7.02 (m, 1H); ^{13}C NMR (100 MHz,

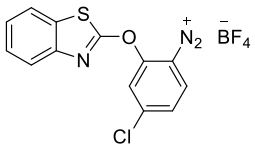
$CDCl_3$) δ 167.8, 154.2, 147.6, 143.6, 133.8, 133.1, 127.9, 127.5, 126.1, 123.3, 122.6, 122.5, 107.9. FT-IR: ν (cm^{-1}) 3068, 2925, 2744, 1595, 1518, 1463. HRMS [ESI] calcd for $C_{13}H_9INOS^+$ $[M+H]^+$ 353.9444, found 353.9443.



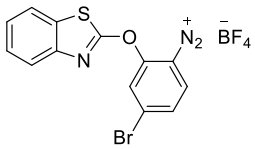
1b: 306.5 mg, 90%, yellow solid, m.p. 123 ºC (decomp.). ^{1}H NMR (400 MHz, DMSO-d^6) δ 8.85-8.78 (m, 1H), 8.43-8.34 (m, 2H), 8.14 (dd, *J* = 8.0, 0.8 Hz, 1H), 7.90-7.80 (m, 2H), 7.59-7.53 (m, 1H), 7.52-7.46 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d^6) δ 167.8, 154.2, 147.6, 143.6, 133.8, 133.1, 127.9, 127.5, 126.1, 123.3, 122.6, 122.5, 107.9. FT-IR: ν (cm^{-1}) 2988, 2902, 2260, 1599, 1573, 1257. HRMS [ESI] calcd for $C_{13}H_8N_3OS^+$ 254.0383, found 254.0394.



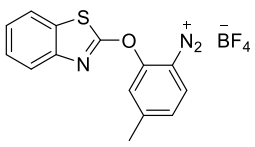
1c: 298.3 mg, 83%, yellow solid, m.p. 196 ºC (decomp.). ^{1}H NMR (400 MHz, DMSO-d^6) δ 8.94 (dd, *J* = 9.6, 5.2 Hz, 1H), 8.49 (dd, *J* = 10.0, 2.4 Hz, 1H), 8.15 (d, *J* = 8.0 Hz, 1H), 7.92 (d, *J* = 8.0 Hz, 1H), 7.82-7.75 (m, 1H), 7.60-7.54 (m, 1H), 7.54-7.47 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d^6) δ 169.9 (d, $J_{C\text{-}F}$ = 267.3 Hz), 167.3, 156.8 (d, $J_{C\text{-}F}$ = 14.8 Hz), 147.6, 137.0 (d, $J_{C\text{-}F}$ = 13.3 Hz), 133.2, 127.5, 126.2, 123.3, 122.8, 116.5 (d, $J_{C\text{-}F}$ = 25.3 Hz), 111.2 (d, $J_{C\text{-}F}$ = 29.6 Hz), 104.2 (d, *J* = 2.7 Hz); ^{19}F NMR (376 MHz, DMSO-d^6) δ -81.8 (s), -148.2 (s), -148.3 (s). FT-IR: ν (cm^{-1}) 3440, 3333, 3057, 2366, 1634, 1597, 1513. HRMS [ESI] calcd for $C_{13}H_7FN_3OS^+$ 272.0288, found 272.0284.



1d: 240.6 mg, 64%, yellow solid, m.p. 182 ºC (decomp.). ^{1}H NMR (400 MHz, DMSO-d^6) δ 8.83 (d, *J* = 9.2 Hz, 1H), 8.67 (d, *J* = 1.6 Hz, 1H), 8.14 (d, *J* = 7.6 Hz, 1H), 7.98 (dd, *J* = 9.2, 2.0 Hz, 1H), 7.92 (d, *J* = 8.0 Hz, 1H), 7.60-7.54 (m, 1H), 7.53-7.47 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d^6) δ 167.5, 154.6, 148.7, 147.6, 134.8, 133.2, 128.5, 127.5, 126.2, 123.3, 123.0, 122.8, 106.9. FT-IR: ν (cm^{-1}) 3114, 3091, 2286, 1598, 1582, 1313. HRMS [ESI] calcd for $C_{13}H_7ClN_3OS^+$ 287.9993, found 287.9986.

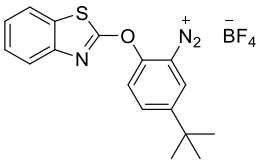


1e: 322.3 mg, 77%, yellow solid, m.p. 180 ºC (decomp.). ^{1}H NMR (400 MHz, DMSO-d^6) δ 8.90-8.76 (m, 1H), 8.75-8.65 (m, 1H), 8.22-8.06 (m, 2H), 7.92 (d, *J* = 8.0 Hz, 1H), 7.60-7.53 (m, 1H), 7.53-7.46 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d^6) δ 167.6, 154.0, 147.6, 138.6, 134.4, 133.3, 131.4, 127.5, 126.1, 125.8, 123.3, 122.8, 107.2. FT-IR: ν (cm^{-1}) 3109, 2988, 2901, 2280, 1598, 1579, 1288. HRMS [ESI] calcd for $C_{13}H_7BrN_3OS^+$ 331.9488, found 331.9485.

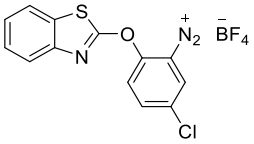


1f: 312.2 mg, 88%, yellow solid, m.p. 169 ºC (decomp.). ^{1}H NMR (400 MHz, DMSO-d^6) δ 8.67 (d, *J* = 8.4 Hz, 1H), 8.24-8.16 (m, 1H), 8.13 (d, *J* = 8.0 Hz, 1H), 7.89 (d, *J* = 7.6 Hz, 1H), 7.66 (d, *J* =

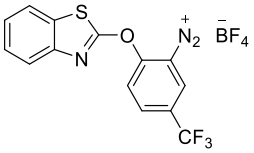
8.4 Hz, 1H), 7.60-7.52 (m, 1H), 7.52-7.46 (m, 1H), 2.61 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d^6) δ 167.7, 157.8, 154.6, 147.7, 133.4, 133.3, 128.8, 127.5, 126.1, 123.3, 122.7, 122.3, 103.9, 23.4. FT-IR: ν (cm^{-1}) 3100, 2987, 2901, 2257, 1599, 1580, 1311. HRMS [ESI] calcd for $C_{14}H_{10}N_3OS^+$ 268.0539, found 268.0545.



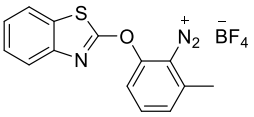
1g: 280.5 mg, 71%, yellow solid, m.p. 152 ºC (decomp.). ^{1}H NMR (400 MHz, DMSO-d^6) δ 8.86 (d, *J* = 2.4 Hz, 1H), 8.52-8.44 (m, 1H), 8.36-8.30 (m, 1H), 8.16-8.10 (m, 1H), 7.88-7.82 (m, 1H), 7.60-7.52 (m, 1H), 7.51-7.46 (m, 1H), 1.38 (s, 9H); ^{13}C NMR (100 MHz, DMSO-d^6) δ 168.2, 152.2, 151.0, 147.7, 141.3, 133.0, 130.0, 127.5, 126.0, 123.3, 122.7, 122.5, 107.5, 35.9, 30.8. FT-IR: ν (cm^{-1}) 3085, 2974, 2265, 1605, 1562, 1498, 1401, 1258. HRMS [ESI] calcd for $C_{17}H_{16}N_3OS^+$ 310.1009, found 310.1013.



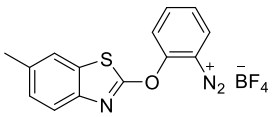
1h: 259.6 mg, 69%, yellow solid, m.p. 193 ºC (decomp.). ^{1}H NMR (400 MHz, DMSO-d^6) δ 9.04-8.92 (m, 1H), 8.54-8.42 (m, 2H), 8.14 (d, *J* = 8.0 Hz, 1H), 7.87 (d, *J* = 8.0 Hz, 1H), 7.60-7.53 (m, 1H), 7.53-7.46 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d^6) δ 167.7, 153.3, 147.5, 143.6, 133.1, 132.1, 130.5, 127.6, 126.2, 124.2, 123.3, 122.6, 109.3. FT-IR: ν (cm^{-1}) 3303, 3091, 3010, 1684, 1616, 1587, 1490, 1311. HRMS [ESI] calcd for $C_{13}H_7ClN_3OS^+$ 287.9993, found 287.9989.



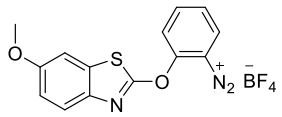
1i: 266.1 mg, 65%, yellow solid, m.p. 161 ºC (decomp.). ^{1}H NMR (400 MHz, DMSO-d^6) δ 9.36 (d, *J* = 2.0 Hz, 1H), 8.82-8.76 (m, 1H), 8.70-8.62 (m, 1H), 8.20-8.14 (m, 1H), 7.93-7.88 (m, 1H), 7.62-7.56 (m, 1H), 7.55-7.50 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d^6) δ 167.2, 156.5, 147.4, 140.3 (q, $J_{C\text{-}F}$ = 2.7 Hz), 133.3, 131.8 (q, $J_{C\text{-}F}$ = 4.2 Hz), 127.7, 126.9 (q, $J_{C\text{-}F}$ = 35.0 Hz), 126.3, 123.5, 123.4, 122.8, 122.4 (q, $J_{C\text{-}F}$ = 271.6 Hz), 109.4; ^{19}F NMR (376 MHz, DMSO-d^6) δ -61.5 (s), -148.2 (s), -148.3 (s). FT-IR: ν (cm^{-1}) 3097, 3074, 2280, 1616, 1575, 1281. HRMS [ESI] calcd for $C_{14}H_7F_3N_3OS^+$ 322.0256, found 322.0249.



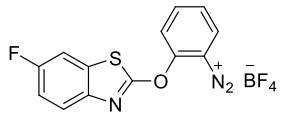
1j: 306.8 mg, 86%, yellow solid, m.p. 158 ºC (decomp.). ^{1}H NMR (400 MHz, DMSO-d^6) δ 8.30-8.24 (m, 1H), 8.22-8.17 (m, 1H), 8.16-8.11 (m, 1H), 7.89-7.84 (m, 1H), 7.76-7.70 (m, 1H), 7.59-7.53 (m, 1H), 7.52-7.46 (m, 1H), 2.83 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d^6) δ 168.0, 154.4, 147.7, 145.8, 143.0, 133.2, 129.1, 127.5, 126.1, 123.3, 122.6, 119.8, 108.2, 18.8. FT-IR: ν (cm^{-1}) 2988, 2923, 2263, 1596, 1574, 1288, 1276. HRMS [ESI] calcd for $C_{14}H_{10}N_3OS^+$ 268.0539, found 268.0540.



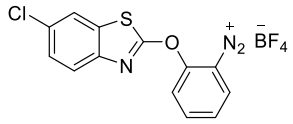
1k: 311.1 mg, 88%, yellow solid, m.p. 165 ºC (decomp.). ^{1}H NMR (400 MHz, DMSO-d^{6}) δ 8.79 (d, *J* = 8.4 Hz, 1H), 8.46-8.30 (m, 2H), 7.98-7.90 (m, 1H), 7.88-7.80 (m, 1H), 7.79-7.71 (m, 1H), 7.43-7.32 (m, 1H), 2.45 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d^{6}) δ 166.9, 154.4, 145.5, 143.7, 135.9, 133.8, 133.1, 128.8, 127.8, 122.8, 122.3, 122.2, 107.7, 21.6. FT-IR: ν (cm^{-1}) 3112, 2988, 2902, 2288, 1596, 1523, 1307. HRMS [ESI] calcd for $C_{14}H_{10}N_3OS^+$ 268.0539, found 268.0541.



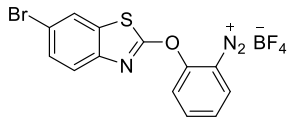
1l: 258.8 mg, 70%, yellow solid, m.p. 167 ºC (decomp.). ^{1}H NMR (400 MHz, DMSO-d^{6}) δ 8.84-8.74 (m, 1H), 8.40-8.30 (m, 2H), 7.85-7.71 (m, 3H), 7.14 (dd, *J* = 8.8, 2.8 Hz, 1H), 3.84 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d^{6}) δ 165.2, 157.8, 154.6, 143.7, 141.5, 134.5, 133.8, 127.7, 123.3, 121.9, 116.2, 107.5, 106.4, 56.2. FT-IR: ν (cm^{-1}) 3111, 2988, 2902, 2283, 1597, 1576, 1473, 1259. HRMS [ESI] calcd for $C_{14}H_{10}N_3O_2S^+$ 284.0488, found 284.0490.



1m: 291.2 mg, 81%, yellow solid, m.p. 162 ºC (decomp.). ^{1}H NMR (400 MHz, DMSO-d^{6}) δ 8.81 (d, *J* = 8.0 Hz, 1H), 8.38 (d, *J* = 3.6 Hz, 1H), 8.06 (dd, *J* = 8.4, 2.4 Hz, 1H), 7.90 (dd, *J* = 8.8, 4.8 Hz, 1H), 7.87-7.81 (m, 1H), 7.46-7.39 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d^{6}) δ 167.5, 160.0 (d, $J_{C\text{-}F}$ = 241.3 Hz), 154.1, 144.4 (d, $J_{C\text{-}F}$ = 1.8 Hz), 143.7, 134.3 (d, $J_{C\text{-}F}$ = 11.7 Hz), 133.9, 128.0, 124.0 (d, $J_{C\text{-}F}$ = 9.4 Hz), 122.4, 115.8 (d, $J_{C\text{-}F}$ = 24.5 Hz), 110.0 (d, $J_{C\text{-}F}$ = 27.9 Hz), 107.9; ^{19}F NMR (376 MHz, DMSO-d^{6}) δ -115.1 (s), -148.2 (s), -148.2 (s). FT-IR: ν (cm^{-1}) 3125, 2974, 2901, 2271, 1608, 1475, 1414, 1251. HRMS [ESI] calcd for $C_{13}H_7FN_3OS^+$ 272.0288, found 272.0289.

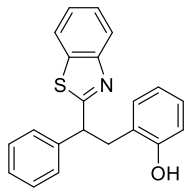


1n: 251.6 mg, 67%, yellow solid, m.p. 171 ºC (decomp.). ^{1}H NMR (400 MHz, DMSO-d^{6}) δ 8.82 (d, *J* = 8.4 Hz, 1H), 8.44-8.34 (m, 2H), 8.31-8.26 (m, 1H), 7.92-7.82 (m, 2H), 7.58 (dd, *J* = 8.4, 1.6Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d^{6}) δ 168.6, 154.0, 146.5, 143.6, 134.6, 133.9, 130.2, 128.1, 127.9, 123.9, 123.0, 122.6, 107.9. FT-IR: ν (cm^{-1}) 3111, 3093, 2292, 1593, 1522, 1304. HRMS [ESI] calcd for $C_{13}H_7ClN_3OS^+$ 287.9993, found 287.9992.

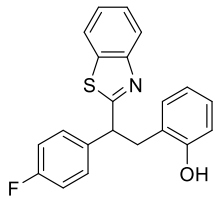


1o: 263.2 mg, 63%, yellow solid, m.p. 200 ºC (decomp.). ^{1}H NMR (400 MHz, DMSO-d^{6}) δ 8.86-8.78 (m, 1H), 8.47-8.32 (m, 3H), 7.90-7.78 (m, 2H), 7.71 (dd, *J* = 8.8, 2.0 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d^{6}) δ 168.6, 153.9, 146.8, 143.6, 135.0, 133.9, 130.6, 128.1, 125.8, 124.2, 122.7, 118.1, 108.0. FT-IR: ν (cm^{-1}) 3110, 3091, 2292, 1592, 1521, 1304, 1257. HRMS [ESI] calcd for $C_{13}H_7BrN_3OS^+$ 331.9488, found 331.9491.

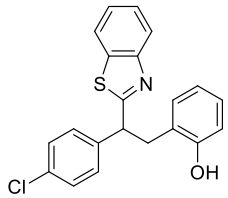
6. Characterization of products



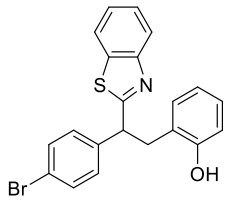
3a: 46.8 mg, 71%, white solid, m.p. 148-149 °C. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.09 (br, 1H), 8.16-8.10 (m, 1H), 7.76-7.70 (m, 1H), 7.54-7.47 (m, 1H), 7.42-7.28 (m, 6H), 7.17-7.10 (m, 2H), 6.99-6.93 (m, 1H), 6.89-6.83(m, 1H), 4.75 (dd, *J* = 10.4, 2.8 Hz, 1H), 3.94 (dd, *J* = 14.0, 10.8 Hz, 1H), 3.21 (dd, *J* = 14.0, 2.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.7, 155.0, 150.8, 142.9, 135.5, 131.2, 129.1, 128.2, 127.7, 127.7, 126.9, 126.4, 125.5, 122.6, 121.6, 120.5, 118.8, 53.7, 35.9. FT-IR: ν (cm^{-1}) 3059, 3027, 2904, 1600, 1512, 1387, 1235. HRMS [ESI] calcd for $C_{21}H_{18}NOS$ $[M+H]^+$ 332.1104, found 332.1109.



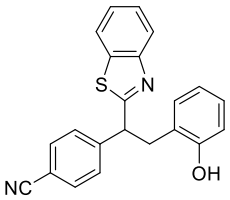
3b: 51.1 mg, 73%, yellow solid, m.p. 131-132 °C. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.91 (br, 1H), 8.14-8.08 (m, 1H), 7.78-7.70 (m, 1H), 7.54-7.48 (m, 1H), 7.40-7.34 (m, 1H), 7.32-7.24 (m, 2H), 7.16-7.00 (m, 4H), 6.93 (dd, *J* = 8.0, 1.2 Hz, 1H), 6.86-6.81 (m, 1H), 4.74 (dd, *J* = 10.4, 3.2 Hz, 1H), 3.86 (dd, *J* = 14.0, 10.4 Hz, 1H), 3.19 (dd, *J* = 14.0, 3.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.4, 162.2 (d, $J_{C\text{-}F}$ = 245.2 Hz), 155.0, 150.9, 138.5 (d, $J_{C\text{-}F}$ = 3.3 Hz), 135.4, 131.3, 129.4 (d, $J_{C\text{-}F}$ = 8.1 Hz), 128.3, 126.5, 126.4, 125.6, 122.6, 121.7, 120.5, 118.7, 116.0 (d, $J_{C\text{-}F}$ = 21.4 Hz), 52.6, 36.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ -114.4 (s). FT-IR: ν (cm^{-1}) 3069, 3088, 2918, 2855, 1679, 1509, 1440. HRMS [ESI] calcd for $C_{21}H_{16}FNOSNa$ $[M+Na]^+$ 372.0829, found 372.0824.



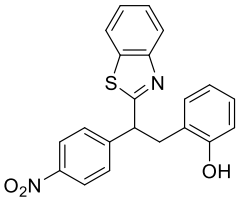
3c: 54.7 mg, 75%, yellow solid, m.p. 113-114 °C. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.87 (br, 1H), 8.11 (d, *J* = 8.4 Hz, 1H), 7.74 (d, *J* = 8.0 Hz, 1H), 7.54-7.46 (m, 1H), 7.40-7.30 (m, 3H), 7.28-7.22 (m, 2H), 7.14-7.05 (m, 2H), 6.96-6.90 (m, 1H), 6.87-6.80 (m, 1H), 4.76 (dd, *J* = 10.0, 3.2 Hz, 1H), 3.86 (dd, *J* = 14.0, 10.4 Hz, 1H), 3.20 (dd, *J* = 14.0, 3.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.1, 155.0, 151.0, 141.1, 135.4, 133.6, 131.3, 129.2, 128.4, 126.5, 126.3, 125.7, 122.6, 121.7, 120.5, 118.5, 52.6, 36.0. FT-IR: ν (cm^{-1}) 3675, 2970, 2862, 1581, 1511, 1338. HRMS [ESI] calcd for $C_{21}H_{17}ClNOS$ $[M+H]^+$ 366.0714, found 366.0708.



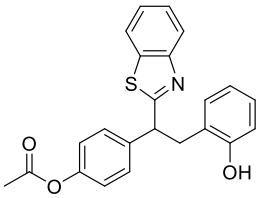
3d: 45.7 mg, 56%, yellow solid, m.p. 142-143 °C. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.84 (br, 1H), 8.11 (d, *J* = 8.4 Hz, 1H), 7.74 (d, *J* = 8.0 Hz, 1H), 7.54-7.46 (m, 3H), 7.41-7.34 (m, 1H), 7.22-7.16 (m, 2H), 7.14-7.05 (m, 2H), 6.95 (d, *J* = 8.0 Hz, 1H), 6.87-6.80 (m, 1H), 4.75 (dd, *J* = 10.4, 3.2 Hz, 1H), 3.86 (dd, *J* = 14.0, 10.4 Hz, 1H), 3.19 (dd, *J* = 14.0, 3.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.9, 155.0, 150.9, 141.6, 135.4, 132.2, 131.2, 129.6, 128.4, 126.5, 126.3, 125.7, 122.7, 121.7, 121.7, 120.6, 118.6, 52.8, 35.9. FT-IR: ν (cm^{-1}) 3067, 2922, 2731, 1596, 1514, 1455, 1376. HRMS [ESI] calcd for $C_{21}H_{17}BrNOS$ $[M+H]^+$ 410.0209, found 410.0212.



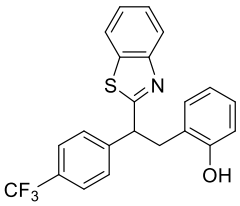
3e: 65.2 mg, 92%, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.50 (br, 1H), 8.11 (d, *J* = 8.4 Hz, 1H), 7.77 (d, *J* = 7.6 Hz, 1H), 7.66-7.60 (m, 2H), 7.55-7.49 (m, 1H), 7.45-7.37 (m, 3H), 7.14-7.08 (m, 1H), 7.06-7.02 (m, 1H), 6.90 (dd, *J* = 8.0, 1.2 Hz, 1H), 6.84-6.79 (m, 1H), 4.86 (dd, *J* = 10.0, 4.0 Hz, 1H), 3.86 (dd, *J* = 14.4, 10.4 Hz, 1H), 3.23 (dd, *J* = 14.0, 3.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.6, 154.9, 151.0, 147.4, 135.3, 132.9, 131.2, 128.8, 128.5, 126.7, 125.9, 125.6, 122.8, 121.7, 120.6, 118.5, 118.4, 111.6, 52.7, 35.9. FT-IR: ν (cm^{-1}) 3065, 2925, 2852, 2228, 1606, 1503, 1456. HRMS [ESI] calcd for $C_{22}H_{16}N_2OSNa$ $[M+Na]^+$ 379.0876, found 379.0878.



3f: 23.2 mg, 31%, yellow solid, m.p. 144-145 °C. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/10). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.39 (br, 1H), 8.24-8.18 (m, 2H), 8.13 (d, *J* = 8.4 Hz, 1H), 7.77 (d, *J* = 8.0 Hz, 1H), 7.57-7.51 (m, 1H), 7.51-7.45 (m, 2H), 7.43-7.37 (m, 1H), 7.14-7.08 (m, 1H), 7.06-7.02 (m, 1H), 6.94-6.88 (m, 1H), 6.85-6.79 (m, 1H), 4.88 (dd, *J* = 10.4, 3.6 Hz, 1H), 3.89 (dd, *J* = 14.0, 10.4 Hz, 1H), 3.22 (dd, *J* = 14.0, 3.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.2, 154.9, 151.1, 149.3, 147.4, 135.3, 131.2, 128.9, 128.6, 126.7, 125.9, 125.5, 124.3, 122.8, 121.7, 120.7, 118.6, 52.7, 35.8. FT-IR: ν (cm^{-1}) 3312, 2923, 2853, 1703, 1622, 1595, 1375. HRMS [ESI] calcd for $C_{21}H_{16}N_2O_3SNa$ $[M+Na]^+$ 399.0774, found 399.0776.

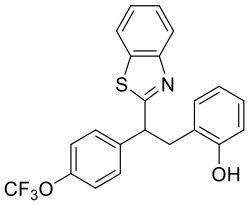


3g: 69.3 mg, 89%, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.93 (br, 1H), 8.13-8.08 (m, 1H), 7.76-7.70 (m, 1H), 7.52-7.46 (m, 1H), 7.39-7.31 (m, 3H), 7.14-7.06 (m, 4H), 6.95-6.90 (m, 1H), 6.87-6.81 (m, 1H), 4.76 (dd, *J* = 10.4, 3.2 Hz, 1H), 3.89 (dd, *J* = 14.0, 10.4 Hz, 1H), 3.20 (dd, *J* = 14.0, 3.2 Hz, 1H), 2.31 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.4, 169.4, 155.0, 150.9, 150.1, 140.2, 135.5, 131.2, 128.9, 128.3, 126.6, 126.5, 125.6, 122.6, 122.2, 121.7, 120.6, 118.6, 52.8, 36.0, 21.2. FT-IR: ν (cm^{-1}) 3065, 2932, 1756, 1594, 1504, 1439, 1314. HRMS [ESI] calcd for $C_{23}H_{19}NO_3SNa$ $[M+Na]^+$ 412.0978, found 412.0972.

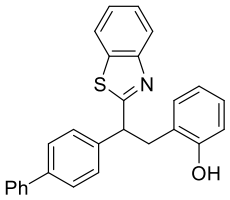


3h: 45.3 mg, 57%, yellow solid, m.p. 85-86 °C. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.75 (br, 1H),

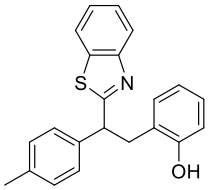
8.15-8.10 (m, 1H), 7.78-7.72 (m, 1H), 7.66-7.58 (m, 2H), 7.55-7.49 (m, 1H), 7.48-7.42 (m, 2H), 7.41-7.35 (m, 1H), 7.14-7.06 (m, 2H), 6.95 (dd, *J* = 8.0, 1.2 Hz, 1H), 6.87-6.81 (m, 1H), 4.85 (dd, *J* = 10.4, 3.2 Hz, 1H), 3.91 (dd, *J* = 14.4, 10.8 Hz, 1H), 3.20 (dd, *J* = 14.4, 3.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.3, 155.0, 151.0, 146.4 (q, J_{C-F} = 0.9 Hz), 135.4, 131.2, 130.0 (q, J_{C-F} = 32.5 Hz), 128.4, 128.2, 126.6, 126.1 (q, J_{C-F} = 3.6 Hz), 125.8, 124.0 (q, J_{C-F} = 270.3 Hz), 122.7, 121.7, 120.6, 118.6, 53.0, 35.9; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.5 (s). FT-IR: ν (cm^{-1}) 3062, 2927, 2849, 2734, 1617, 1414, 1385. HRMS [ESI] calcd for $C_{22}H_{17}F_3NOS$ $[M+H]^+$ 400.0977, found 400.0976.



3i: 44.1 mg, 53%, yellow solid, m.p. 88-89 ºC. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.78 (br, 1H), 8.12 (d, *J* = 8.4 Hz, 1H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.55-7.48 (m, 1H), 7.41-7.32 (m, 3H), 7.24-7.18 (m, 2H), 7.14-7.06 (m, 2H), 6.92 (dd, *J* = 8.0, 1.2 Hz, 1H), 6.87-6.80 (m, 1H), 4.78 (dd, *J* = 10.4, 3.2 Hz, 1H), 3.88 (dd, *J* = 14.0, 10.4 Hz, 1H), 3.20 (dd, *J* = 14.0, 3.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.8, 155.0, 151.0, 148.6 (q, J_{C-F} = 1.4 Hz), 141.3, 135.4, 131.2, 129.3, 128.4, 126.5, 126.2, 125.7, 122.7, 121.7, 121.5, 120.6, 120.5 (q, J_{C-F} = 255.7 Hz), 118.6, 52.6, 36.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.8 (s). FT-IR: ν (cm^{-1}) 3312, 2921, 2851, 1561, 1508, 1457, 1254. HRMS [ESI] calcd for $C_{22}H_{17}F_3NO_2S$ $[M+H]^+$ 416.0927, found 416.0930.

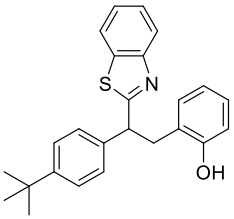


3j: 29.2 mg, 36%, yellow solid, m.p. 98-99 ºC. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.03 (br, 1H), 8.15-8.10 (m, 1H), 7.76-7.72 (m, 1H), 7.63-7.56 (m, 4H), 7.54-7.48 (m, 1H), 7.48-7.42 (m, 2H), 7.41-7.33 (m, 4H), 7.18-7.08 (m, 2H), 6.95 (dd, *J* = 8.0, 0.8 Hz, 1H), 6.89-6.83 (m, 1H), 4.76 (dd, *J* = 10.8, 2.8 Hz, 1H), 3.96 (dd, *J* = 14.4, 10.8 Hz, 1H), 3.21 (dd, *J* = 14.0, 2.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.6, 155.0, 150.9, 141.9, 140.7, 140.5, 135.6, 131.3, 128.8, 128.3, 128.2, 127.8, 127.5, 127.1, 126.8, 126.4, 125.6, 122.6, 121.6, 120.6, 118.8, 53.4, 35.9. FT-IR: ν (cm^{-1}) 3074, 2923, 2839, 1606, 1581, 1515, 1485. HRMS [ESI] calcd for $C_{27}H_{21}NOSNa$ $[M+Na]^+$ 430.1236, found 430.1237.

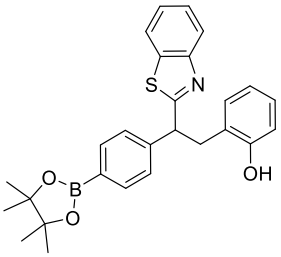


3k: 35.8 mg, 52%, yellow solid, m.p. 141-142 ºC. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.08 (br, 1H), 8.10 (d, *J* = 8.0 Hz, 1H), 7.72 (d, *J* = 7.6 Hz, 1H), 7.54-7.46 (m, 1H), 7.40-7.34 (m, 1H), 7.24-7.16 (m, 4H), 7.16-7.08 (m, 2H), 6.94 (d, *J* = 7.6 Hz, 1H), 6.88-6.82 (m, 1H), 4.68 (dd, *J* = 10.4, 2.8 Hz, 1H), 3.92 (dd, *J* = 14.4, 10.8 Hz, 1H), 3.15 (dd, *J* = 14.4, 2.8 Hz, 1H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.1, 155.1, 150.9, 140.1, 137.5, 135.6, 131.2, 129.8, 128.2, 127.6, 127.0, 126.4,

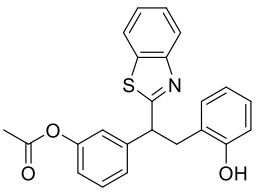
125.5, 122.5, 121.6, 120.5, 118.8, 53.4, 35.9, 21.1. FT-IR: ν (cm^{-1}) 3567, 2922, 2849, 1695, 1578, 1440, 1260. HRMS [ESI] calcd for $C_{22}H_{19}NOSNa$ $[M+Na]^+$ 368.1080, found 368.1086.



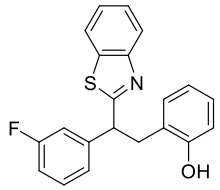
3l: 47.9 mg, 62%, yellow solid, m.p. 98-99 ºC. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^{1}H NMR (400 MHz, $CDCl_3$) 10.08 (br, 1H), 8.14-8.08 (m, 1H), 7.75-7.69 (m, 1H), 7.53-7.46 (m, 1H), 7.42-7.32 (m, 3H), 7.29-7.24 (m, 2H), 7.16 (dd, *J* = 7.6, 1.6Hz, 1H), 7.14-7.08 (m, 1H), 6.94 (dd, *J* = 8.0, 1.2 Hz, 1H), 6.88-6.83(m, 1H), 4.69 (dd, *J* = 10.8, 2.8 Hz, 1H), 3.95 (dd, *J* = 14.0, 10.8 Hz, 1H), 3.15 (dd, *J* = 14.0, 2.8 Hz, 1H), 1.33 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.0, 155.0, 150.9, 150.7, 139.9, 135.5, 131.2, 128.2, 127.3, 127.1, 126.4, 126.0, 125.5, 122.5, 121.6, 120.5, 118.8, 53.3, 35.9, 34.6, 31.3. FT-IR: ν (cm^{-1}) 3629, 3055, 2962, 2865, 1669, 1580, 1439. HRMS [ESI] calcd for $C_{25}H_{25}NOSNa$ $[M+Na]^+$ 410.1549, found 410.1545.



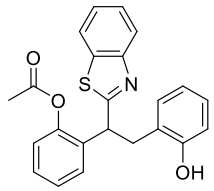
3m: 28.5 mg, 31%, yellow solid, m.p. 202-203 ºC. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^{1}H NMR (400 MHz, $CDCl_3$) 10.04 (br, 1H), 8.14-8.08 (m, 1H), 7.85-7.79 (m, 2H), 7.75-7.69 (m, 1H), 7.54-7.46 (m, 1H), 7.39-7.30 (m, 3H), 7.16-7.08 (m, 2H), 6.96-6.91 (m, 1H), 6.88-6.81 (m, 1H), 4.72 (dd, *J* = 10.4, 2.8 Hz, 1H), 3.95 (dd, *J* = 14.0, 10.4 Hz, 1H), 3.15 (dd, *J* = 14.0, 2.8 Hz, 1H), 1.35 (s, 12H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.4, 155.0, 150.8, 145.8, 135.6, 135.6, 131.2, 128.2, 127.2, 126.8, 126.4, 125.5, 122.6, 121.6, 120.6, 118.8, 83.9, 53.9, 35.7, 24.9, 24.8; ^{11}B NMR (128 MHz, $CDCl_3$) δ -13.2 (br). FT-IR: ν (cm^{-1}) 3066, 2957, 2853, 1684, 1608, 1507, 1487, 1440. HRMS [ESI] calcd for $C_{27}H_{28}BNO_3SNa$ $[M+Na]^+$ 480.1775, found 480.1790.



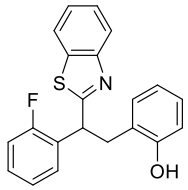
3n: 46.7 mg, 60%, yellow solid, m.p. 161-162 ºC. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/7). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.87 (br, 1H), 8.14-8.08 (m, 1H), 7.78-7.70 (m, 1H), 7.54-7.46 (m, 1H), 7.42-7.32 (m, 2H), 7.23-7.17 (m, 1H), 7.15-7.03 (m, 4H), 6.95-6.90 (m, 1H), 6.88-6.80 (m, 1H), 4.76 (dd, *J* = 10.4, 2.8 Hz, 1H), 3.90 (dd, *J* = 14.0, 10.4 Hz, 1H), 3.22 (dd, *J* = 14.4, 3.2 Hz, 1H), 2.29 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.0, 169.3, 155.0, 151.1, 151.0, 144.2, 135.5, 131.2, 130.0, 128.3, 126.5, 125.6, 125.3, 122.6, 121.7, 121.0, 120.6, 118.6, 53.1, 35.9, 21.2. FT-IR: ν (cm^{-1}) 3629, 3066, 2922, 2854, 1698, 1606, 1418, 1343. HRMS [ESI] calcd for $C_{23}H_{19}NO_3SNa$ $[M+Na]^+$ 412.0978, found 412.0972.



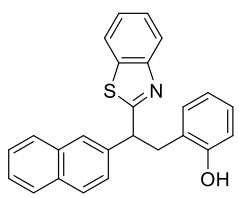
3o: 36.7 mg, 53%, yellow solid, m.p. 146-147 ºC. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15).^{1}H NMR (400 MHz, $CDCl_3$) δ 9.82 (br, 1H), 8.14-8.09 (m, 1H), 7.78-7.72 (m, 1H), 7.55-7.48 (m, 1H), 7.41-7.35 (m, 1H), 7.35-7.29 (m, 1H), 7.15-7.06 (m, 3H), 7.06-6.96 (m, 2H), 6.95-6.90 (m, 1H), 6.88-6.81 (m, 1H), 4.74 (dd, *J* = 10.8, 2.8 Hz, 1H), 3.90 (dd, *J* = 14.0, 10.8 Hz, 1H), 3.18 (dd, *J* = 14.0, 2.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.7, 163.1 (d, J_{C-F} = 246.1 Hz), 155.0, 150.9, 145.0 (d, J_{C-F} = 7.1 Hz), 135.4, 131.2, 130.6 (d, J_{C-F} = 8.2 Hz), 128.4, 126.5, 126.4, 125.7, 123.5 (d, J_{C-F} = 2.8 Hz), 122.7, 121.7, 120.6, 118.7, 114.9 (d, J_{C-F} = 12.9 Hz), 114.7 (d, J_{C-F} = 12.3 Hz), 53.1, 35.8; ^{19}F NMR (376 MHz, $CDCl_3$) δ -111.7 (s). FT-IR: ν (cm^{-1}) 3567, 3062, 2958, 2923, 1734, 1579, 1438. HRMS [ESI] calcd for $C_{21}H_{16}FNOSNa$ $[M+Na]^+$ 372.0829, found 372.0833.



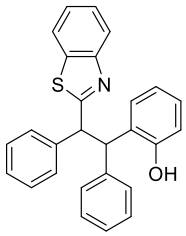
3p: 57.6 mg, 74%, yellow solid, m.p. 135-136 ºC. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/7). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.16 (br, 1H), 8.14-8.08 (m, 1H), 7.76-7.70 (m, 1H), 7.54-7.47 (m, 1H), 7.40-7.32 (m, 2H), 7.24-7.15 (m, 3H), 7.15-7.06 (m, 2H), 6.98-6.92 (m, 1H), 6.89-6.82 (m, 1H), 4.84 (dd, *J* = 10.4, 2.4 Hz, 1H), 3.91 (dd, *J* = 14.0, 10.4 Hz, 1H), 3.11 (dd, *J* = 14.4, 2.4 Hz, 1H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.0, 169.3, 155.1, 150.6, 147.7, 135.6, 134.7, 131.1, 129.4, 128.9, 128.4, 126.8, 126.8, 126.5, 125.7, 123.1, 122.4, 121.7, 120.6, 118.8, 47.6, 34.6, 21.0. FT-IR: ν (cm^{-1}) 3629, 3063, 2933, 2847, 1760, 1653, 1560, 1455. HRMS [ESI] calcd for $C_{23}H_{19}NO_3SNa$ $[M+Na]^+$ 412.0978, found 412.0984.



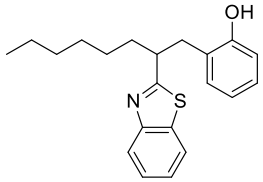
3q: 46.9 mg, 67%, yellow solid, m.p. 124-125 ºC. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.02 (br, 1H), 8.16-8.11 (m, 1H), 7.78-7.72 (m, 1H), 7.55-7.48 (m, 1H), 7.41-7.34 (m, 1H), 7.34-7.27 (m, 1H), 7.22-7.06 (m, 5H), 6.96 (dd, *J* = 8.0, 0.8 Hz, 1H), 6.90-6.83 (m, 1H), 5.14 (dd, *J* = 10.8, 3.2 Hz, 1H), 3.93 (dd, *J* = 14.0, 10.4 Hz, 1H), 3.19 (dd, *J* = 14.4, 2.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.5, 159.8 (d, J_{C-F} = 245.1 Hz), 155.0, 150.8, 135.5, 131.3, 129.7 (d, J_{C-F} = 14.4 Hz), 129.4 (d, J_{C-F} = 3.7 Hz), 129.4, 128.3, 126.6, 126.5, 125.7, 124.7 (d, J_{C-F} = 3.6 Hz), 122.6, 121.7, 120.6, 118.7, 115.9 (d, J_{C-F} = 21.8 Hz), 45.8 (d, J_{C-F} = 2.6 Hz), 34.6; ^{19}F NMR (376 MHz, $CDCl_3$) δ -118.4 (s). FT-IR: ν (cm^{-1}) 3065, 2921, 2852, 1647, 1609, 1486, 1391. HRMS [ESI] calcd for $C_{21}H_{16}FNOSNa$ $[M+Na]^+$ 372.0829, found 372.0830.



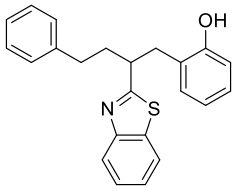
3r: 30.3 mg, 40%, yellow solid, m.p. 72-73 ºC. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.12 (br, 1H), 8.18-8.12 (m, 1H), 7.88-7.78 (m, 4H), 7.76-7.68 (m, 1H), 7.56-7.46 (m, 3H), 7.44-7.32 (m, 2H), 7.20-7.08 (m, 2H), 6.96 (dd, *J* = 8.0, 1.2 Hz, 1H), 6.88-6.83(m, 1H), 4.88 (dd, *J* = 10.8, 2.8 Hz, 1H), 4.03 (dd, *J* = 14.0, 10.4 Hz, 1H), 3.24 (dd, *J* = 14.0, 2.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.7, 155.1, 151.0, 140.3, 135.6, 133.6, 132.8, 131.3, 129.0, 128.3, 127.9, 127.8, 126.8, 126.6, 126.5, 126.4, 126.3, 125.6, 125.6, 122.6, 121.6, 120.6, 118.8, 53.9, 35.9. FT-IR: ν (cm^{-1}) 3056, 2923, 2850, 1559, 1507, 1438, 1315. HRMS [ESI] calcd for $C_{25}H_{20}NOS$ $[M+H]^+$ 382.1260, found 382.1252.



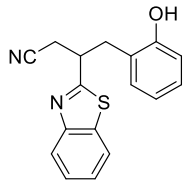
3s (*d.r.*> 19:1): 56.7 mg, 70%, yellow solid, m.p. 177-178ºC. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/10). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.72 (br, 1H), 8.06-8.00 (m, 1H), 7.70-7.64 (m, 1H), 7.49-7.40 (m, 3H), 7.35-7.27 (m, 4H), 7.22-7.10 (m, 4H), 7.10-7.06 (m, 1H), 7.06-6.99 (m, 1H), 6.98-6.90 (m, 1H), 6.84 (dd, *J* = 8.0, 1.2 Hz, 1H), 6.81-6.74 (m, 1H), 5.76 (d, *J* = 12.4 Hz, 1H), 5.30 (d, *J* = 12.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.8, 153.4, 151.6, 141.7, 140.5, 134.9, 131.5, 128.9, 128.7, 128.7, 128.4, 128.2, 127.6, 127.2, 126.3, 126.2, 125.2, 122.6, 121.5, 121.4, 119.1, 55.6, 46.5. FT-IR: ν (cm^{-1}) 3681, 3062, 2981, 2934, 1666, 1594, 1525. HRMS [ESI] calcd for $C_{27}H_{22}NOS$ $[M+H]^+$ 408.1417, found 408.1415.



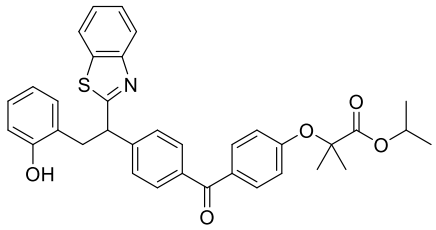
3t: 21.7 mg, 32%, yellow solid, m.p. 104-105 ºC. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/20). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.54 (br, 1H), 8.05-7.99 (m, 1H), 7.83-7.78 (m, 1H), 7.50-7.44 (m, 1H), 7.39-7.33 (m, 1H), 7.13-7.09 (m, 1H), 7.07-7.01 (m, 1H), 6.85-6.77 (m, 2H), 3.62-3.52 (m, 1H), 3.52-3.42 (m, 1H), 2.96 (dd, *J* = 13.6, 3.2 Hz, 1H), 2.00-1.85 (m, 2H), 1.55-1.24 (m, 8H), 0.88 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 177.6, 155.0, 151.3, 134.7, 130.8, 127.9, 127.2, 126.2, 125.2, 122.3, 121.6, 120.3, 118.0, 47.0, 38.0, 33.5, 31.6, 29.3, 26.7, 22.6, 14.0. FT-IR: ν (cm^{-1}) 3069, 2920, 2853, 1606, 1562, 1456, 1440. HRMS [ESI] calcd for $C_{21}H_{26}NOS$ $[M+H]^+$ 340.1730, found 340.1731.



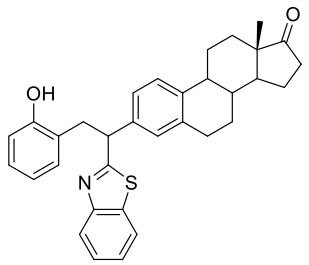
3u: 18.7 mg, 26%, yellow solid, m.p. 142-143 ºC. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.20 (br, 1H), 8.08-8.01 (m, 1H), 7.86-7.78 (m, 1H), 7.54-7.44 (m, 1H), 7.42-7.34 (m, 1H), 7.34-7.26 (m, 2H), 7.25-7.16 (m, 3H), 7.14-7.02 (m, 2H), 6.90-6.72 (m, 2H), 3.66-3.50 (m, 2H), 3.04 (dd, *J* = 12.8, 2.4 Hz, 1H), 2.88-2.70 (m, 2H), 2.36-2.18 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 177.0, 154.9, 151.3, 141.1, 134.7, 130.9, 128.6, 128.4, 128.0, 126.9, 126.4, 126.2, 125.3, 122.4, 121.6, 120.4, 118.1, 46.3, 39.5, 33.3, 32.8. FT-IR: ν (cm^{-1}) 3067, 2922, 2852, 1698, 1670, 1636, 1559. HRMS [ESI] calcd for $C_{23}H_{21}NOSNa$ $[M+Na]^+$ 382.1236, found 382.1243.



3v: 11.8 mg, 20%, yellow solid, m.p. 133-134 °C. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08-8.03 (m, 1H), 7.88-7.82 (m, 1H), 7.55-7.49 (m, 1H), 7.45-7.39 (m, 1H), 7.20-7.08 (m, 2H), 6.90-6.80 (m, 2H), 4.00-3.90 (m, 1H), 3.54 (dd, *J* = 14.0, 8.8 Hz, 1H), 3.21 (dd, *J* = 14.0, 5.6 Hz, 1H), 3.00-2.86 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.6, 154.5, 151.7, 134.7, 131.3, 128.8, 126.7, 125.8, 124.2, 122.9, 121.8, 120.9, 117.5, 117.4, 42.1, 34.1, 24.1. FT-IR: ν (cm^{-1}) 3643, 2922, 2850, 1684, 1616, 1587, 1490. HRMS [ESI] calcd for $C_{17}H_{14}N_2OSNa$ $[M+Na]^+$ 317.0719, found 317.0707.

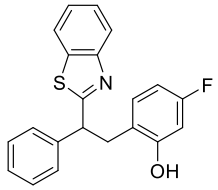


3w: 69.7 mg, 60%, yellow solid, m.p. 56-57 °C. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.80 (br, 1H), 8.12 (d, *J* = 8.0 Hz, 1H), 7.80-7.70 (m, 5H), 7.55-7.48 (m, 1H), 7.46-7.35 (m, 3H), 7.14-7.06 (m, 2H), 6.96-6.90 (m, 1H), 6.90-6.80 (m, 3H), 5.14-5.02 (m, 1H), 4.85 (dd, *J* = 10.4, 3.2 Hz, 1H), 3.93 (dd, *J* = 14.0, 10.8 Hz, 1H), 3.22 (dd, *J* = 14.0, 3.2 Hz, 1H), 1.67 (s, 6H), 1.20 (d, *J* = 6.0 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.9, 174.5, 173.2, 159.7, 155.0, 151.0, 146.5, 137.5, 135.4, 132.1, 131.2, 130.6, 130.4, 128.4, 127.7, 126.5, 126.3, 125.7, 122.7, 121.7, 120.6, 118.6, 117.2, 79.4, 69.4, 53.2, 35.8, 25.4, 25.4, 21.5. FT-IR: ν (cm^{-1}) 3063, 2982, 2936, 1772, 1648, 1541, 1466. HRMS [ESI] calcd for $C_{35}H_{33}NO_5SNa$ $[M+Na]^+$ 602.1972, found 602.1963.

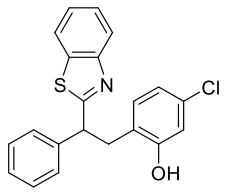


3x (*d.r.* = 1:1): 30.1 mg, 30%, yellow solid, m.p. 109-110 °C. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/7).^{1}H NMR (400 MHz, $CDCl_3$) δ 10.07 (br, 1H, two isomers), 8.14-8.08 (m, 1H, two isomers), 7.76-7.69 (m, 1H, two isomers), 7.54-7.46 (m, 1H, two isomers), 7.40-7.32 (m, 1H, two isomers), 7.31-7.26 (m, 1H, two isomers), 7.20-7.14 (m, 1H, two isomers), 7.14-7.07 (m, 2H, two isomers), 7.07-7.02 (m, 1H, two isomers), 6.96-6.90 (m, 1H, two isomers), 6.89-6.82(m, 1H, two isomers), 4.68-4.60 (m, 1H, two isomers), 3.98-3.87 (m, 1H, two isomers), 3.18-3.06 (m, 1H, two isomers), 2.98-2.82 (m, 2H, two isomers), 2.58-2.46 (m, 1H, two isomers), 2.46-2.38 (m, 1H, two isomers), 2.36-2.26 (m, 1H, two isomers), 2.25-1.94 (m, 4H, two isomers), 1.74-1.36 (m, 6H, two isomers), 0.92 (s, 3H, two isomers); ^{13}C NMR (100 MHz, $CDCl_3$) δ 220.8 (overlap, two isomers), 175.9 & 175.9 (two isomers), 155.0 (overlap, two isomers), 150.9 (overlap, two isomers), 140.5 & 140.5 (two isomers), 139.3 (overlap, two isomers), 137.4 & 137.4 (two isomers), 135.5 (overlap, two isomers), 131.1 (overlap, two isomers), 128.2 (overlap, two isomers), 128.2 & 128.1 (two isomers), 127.2 & 127.1 (two isomers), 126.4 (overlap, two isomers), 126.1 & 126.1 (two isomers), 125.5 (overlap, two isomers), 125.0 & 125.0 (two isomers), 122.5 (overlap, two isomers), 121.6 (overlap, two isomers), 120.6 (overlap, two

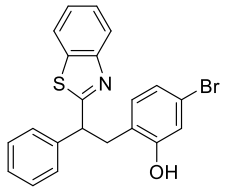
isomers), 118.8 (overlap, two isomers), 53.4 & 53.4 (two isomers), 50.5 (overlap, two isomers), 48.0 (overlap, two isomers), 44.3 (overlap, two isomers), 38.0 (overlap, two isomers), 35.9 (overlap, two isomers), 31.6 (overlap, two isomers), 29.4 & 29.4 (two isomers), 26.4 (overlap, two isomers), 25.7 (overlap, two isomers), 21.6 (overlap, two isomers), 13.9 (overlap, two isomers). FT-IR: ν (cm^{-1}) 3085, 2927, 2856, 1734, 1637, 1541. HRMS [ESI] calcd for $C_{33}H_{34}NO_2S$ $[M+H]^+$ 508.2305, found 508.2314.



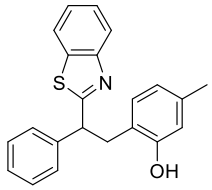
4a: 42.8 mg, 61%, yellow solid, m.p. 59-60 °C. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.52 (br, 1H), 8.14-8.08 (m, 1H), 7.78-7.72 (m, 1H), 7.55-7.48 (m, 1H), 7.42-7.34 (m, 3H), 7.34-7.27 (m, 3H), 7.00 (dd, *J* = 8.4, 6.8 Hz, 1H), 6.64 (dd, *J* = 10.4, 2.8 Hz, 1H), 6.57-6.51 (m, 1H), 4.75-4.68 (m, 1H), 3.81 (dd, *J* = 14.0, 10.4 Hz, 1H), 3.20 (dd, *J* = 14.4, 2.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.9, 162.6 (d, J_{C-F} = 242.6 Hz), 156.5, 156.4, 150.7, 142.5, 135.5, 132.0 (d, J_{C-F} = 39.2 Hz), 129.1, 127.9, 127.8, 126.5, 125.7, 122.4, 121.7, 107.3 (d, J_{C-F} = 21.3 Hz), 105.8 (d, J_{C-F} = 22.8 Hz), 53.4, 35.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ -114.4 (s). FT-IR: ν (cm^{-1}) 3671, 2979, 2933, 1609, 1515, 1498, 1456. HRMS [ESI] calcd for $C_{21}H_{17}FNOS$ $[M+H]^+$ 350.1009, found 350.1007.



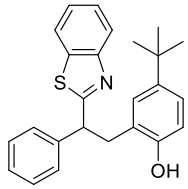
4b: 46.6 mg, 64%, yellow solid, m.p. 171-172 °C. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12-8.06 (m, 1H), 7.76-7.71 (m, 1H), 7.56-7.48 (m, 1H), 7.42-7.30 (m, 4H), 7.30-7.26 (m, 2H), 7.00-6.96 (m, 1H), 6.94 (d, *J* = 2.0 Hz, 1H), 6.80 (dd, *J* = 8.0, 2.0 Hz, 1H), 4.68 (dd, *J* = 10.8, 2.8 Hz, 1H), 3.82 (dd, *J* = 14.0, 10.4 Hz, 1H), 3.17 (dd, *J* = 14.4, 2.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.8, 156.0, 150.7, 142.4, 135.5, 133.2, 132.1, 129.2, 127.9, 127.9, 126.6, 125.7, 125.3, 122.5, 121.7, 120.6, 119.0, 53.3, 35.5. FT-IR: ν (cm^{-1}) 3060, 2923, 2850, 2590, 1688, 1496, 1437. HRMS [ESI] calcd for $C_{21}H_{17}ClNOS$ $[M+H]^+$ 366.0714, found 366.0706.



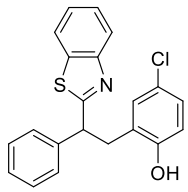
4c: 51.7 mg, 63%, yellow solid, m.p. 144-145 °C. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12-8.06 (m, 1H), 7.78-7.70 (m, 1H), 7.55-7.48 (m, 1H), 7.42-7.31 (m, 4H), 7.31-7.25 (m, 2H), 7.10 (d, *J* = 1.6 Hz, 1H), 6.98-6.89 (m, 2H), 4.68 (dd, *J* = 10.4, 2.8 Hz, 1H), 3.81 (dd, *J* = 14.4, 10.4 Hz, 1H), 3.15 (dd, *J* = 14.4, 2.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.7, 156.2, 150.6, 142.4, 135.5, 132.4, 129.2, 127.9, 127.8, 126.6, 125.8, 125.7, 123.5, 122.5, 122.0, 121.7, 121.1, 53.3, 35.5. FT-IR: ν (cm^{-1}) 3062, 2927, 2857, 2605, 1589, 1497, 1436, 1416. HRMS [ESI] calcd for $C_{21}H_{17}BrNOS$ $[M+H]^+$ 410.0209, found 410.0199.



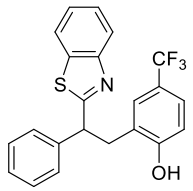
4d: 49.6 mg, 72%, yellow solid, m.p. 131-132 ºC. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.86 (br, 1H), 8.04-7.98 (m, 1H), 7.66-7.58 (m, 1H), 7.44-7.36 (m, 1H), 7.32-7.18 (m, 6H), 6.96-6.90 (m, 1H), 6.70-6.66 (m, 1H), 6.61-6.55 (m, 1H), 4.60 (dd, *J* = 10.8, 3.2 Hz, 1H), 3.79 (dd, *J* = 14.0, 10.8 Hz, 1H), 3.04 (dd, *J* = 14.0, 2.8 Hz, 1H), 2.15 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.8, 154.8, 150.9, 143.0, 138.2, 135.6, 131.0, 129.1, 127.8, 127.8, 126.4, 125.5, 123.8, 122.6, 121.6, 121.4, 119.3, 53.8, 35.6, 21.1. FT-IR: ν (cm^{-1}) 3075, 3027, 2915, 1581, 1561, 1486, 1421. HRMS [ESI] calcd for $C_{22}H_{19}NOSNa$ $[M+Na]^+$ 368.1080, found 368.1077.



4e: 55.7 mg, 72%, yellow solid, m.p. 68-69 ºC. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^{1}H NMR (400 MHz, $CDCl_3$) 8.15-8.09 (m, 1H), 7.76-7.70 (m, 1H), 7.53-7.46 (m, 1H), 7.42-7.28 (m, 6H), 7.15 (dd, *J* = 8.4, 2.4 Hz, 1H), 7.04-6.98 (m, 1H), 6.93-6.87 (m, 1H), 4.79 (dd, *J* = 10.0, 3.2 Hz, 1H), 3.85 (dd, *J* = 14.0, 10.0 Hz, 1H), 3.30 (dd, *J* = 14.0, 3.2 Hz, 1H), 1.25 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.9, 152.7, 150.9, 143.0, 142.7, 135.5, 129.0, 128.2, 128.1, 127.7, 126.4, 125.6, 125.5, 125.2, 122.6, 121.6, 118.0, 53.4, 36.1, 34.0, 31.6. FT-IR: ν (cm^{-1}) 3613, 2964, 2902, 1601, 1502, 1454, 1439. HRMS [ESI] calcd for $C_{25}H_{25}NOSNa$ $[M+Na]^+$ 410.1549, found 410.1542.

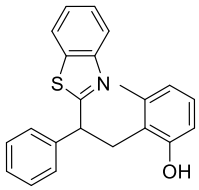


4f: 37.7 mg, 52 %, yellow solid, m.p. 141-142 ºC. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14-8.08 (m, 1H), 7.78-7.70 (m, 1H), 7.55-7.48 (m, 1H), 7.42-7.28 (m, 6H), 7.12-7.08 (m, 1H), 7.06 (dd, *J* = 8.4, 2.4 Hz, 1H), 6.90-6.84 (m, 1H), 4.71 (dd, *J* = 10.8, 2.8 Hz, 1H), 3.87 (dd, *J* = 14.4, 10.8 Hz, 1H), 3.14 (dd, *J* = 14.4, 2.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.6, 153.8, 150.7, 142.5, 135.5, 130.7, 129.2, 128.5, 128.1, 127.9, 127.7, 126.5, 125.7, 125.0, 122.5, 121.7, 120.2, 53.4, 35.7. FT-IR: ν (cm^{-1}) 3061, 2730, 2657, 1514, 1461, 1440, 1240. HRMS [ESI] calcd for $C_{21}H_{16}ClNOSNa$ $[M+Na]^+$ 388.0533, found 388.0524.

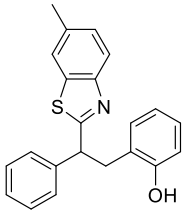


4g: 44.1 mg, 55%, yellow solid, m.p. 58-59 ºC. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14-8.08 (m, 1H), 7.78-7.72 (m, 1H), 7.56-7.48 (m, 1H), 7.42-7.32 (m, 5H), 7.32-7.27 (m, 3H), 7.02-6.96 (m, 1H), 4.77 (dd, *J* = 10.4, 2.8 Hz, 1H), 3.87 (dd, *J* = 14.4, 10.4 Hz, 1H), 3.28 (dd, *J* = 14.4, 2.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.8, 158.3, 150.5, 142.2, 135.5, 129.2, 128.6 (q, J_{C-F} = 3.6 Hz), 128.0,

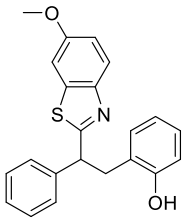
127.8, 126.8, 126.6, 125.8, 125.5 (q, J_{C-F} = 3.6 Hz), 124.5 (q, J_{C-F} = 269.5 Hz), 122.4, 122.4 (q, J_{C-F} = 32.1 Hz), 121.7, 119.0, 53.1, 35.8; ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.3 (s). FT-IR: ν (cm^{-1}) 3063, 2927, 2849, 2621, 1871, 1616, 1438, 1386. HRMS [ESI] calcd for $C_{22}H_{16}F_3NOSNa$ $[M+Na]^+$ 422.0797, found 422.0791.



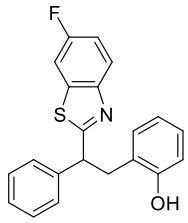
4h: 46.1 mg, 67%, yellow solid, m.p. 189-190 ºC. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/20). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.34 (br, 1H), 8.18-8.11 (m, 1H), 7.75-7.68 (m, 1H), 7.54-7.48 (m, 1H), 7.44-7.30 (m, 6H), 7.09-7.02 (m, 1H), 6.90-6.84 (m, 1H), 6.82-6.76 (m, 1H), 4.69 (dd, *J* = 10.8, 2.4 Hz, 1H), 4.09 (dd, *J* = 14.8, 11.2 Hz, 1H), 3.13 (dd, *J* = 14.4, 2.4 Hz, 1H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.2, 155.4, 150.8, 143.5, 138.0, 135.6, 129.3, 127.8, 127.8, 127.5, 126.4, 126.0, 125.6, 122.7, 122.6, 121.6, 116.7, 51.5, 33.1, 20.0; FT-IR: ν (cm^{-1}) 3061, 2955, 2851, 1574, 1514, 1493, 1459. HRMS [ESI] calcd for $C_{22}H_{19}NOSNa$ $[M+Na]^+$ 368.1080, found 368.1082.



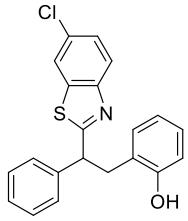
4i: 56.5 mg, 82%, yellow solid, m.p. 69-70 ºC. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02-7.97 (m, 1H), 7.54-7.48 (m, 1H), 7.41-7.28 (m, 6H), 7.16-7.08 (m, 2H), 6.98-6.92 (m, 1H), 6.88-6.82 (m, 1H), 4.71 (dd, *J* = 10.8, 3.2 Hz, 1H), 3.91 (dd, *J* = 14.0, 10.8 Hz, 1H), 3.18 (dd, *J* = 14.0, 2.8 Hz, 1H), 2.45 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.6, 155.1, 148.9, 143.0, 135.8, 135.7, 131.3, 129.1, 128.2, 127.9, 127.8, 127.7, 126.9, 122.0, 121.3, 120.5, 118.8, 53.6, 36.0, 21.5. FT-IR: ν (cm^{-1}) 3060, 3029, 2922, 2847, 1596, 1489, 1241. HRMS [ESI] calcd for $C_{22}H_{19}NOSNa$ $[M+Na]^+$ 368.1080, found 368.1086.



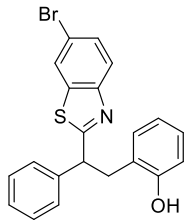
4j: 28.8 mg, 40%, yellow solid, m.p. 95-96 ºC. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.8 Hz, 1H), 7.41-7.27 (m, 5H), 7.19-7.15 (m, 1H), 7.15-7.06 (m, 3H), 6.97-6.91 (m, 1H), 6.87-6.81(m, 1H), 4.67 (dd, *J* = 10.4, 2.4 Hz, 1H), 3.89 (dd, *J* = 14.4, 10.8 Hz, 1H), 3.83 (s, 3H), 3.16 (dd, *J* = 14.0, 2.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.1, 157.9, 155.1, 145.3, 143.0, 136.9, 131.3, 129.1, 128.2, 127.8, 127.7, 127.0, 123.0, 120.5, 118.8, 115.6, 104.3, 55.8, 53.6, 36.0. FT-IR: ν (cm^{-1}) 3661, 3062, 2933, 2633, 1602, 1564, 1474. HRMS [ESI] calcd for $C_{22}H_{20}NO_2S$ $[M+H]^+$ 362.1209, found 362.1215.



4k: 46.8 mg, 67%, yellow solid, m.p. 119-120 ºC. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (dd, *J* = 9.2, 4.8 Hz, 1H), 7.44-7.35 (m, 3H), 7.35-7.28 (m, 3H), 7.26-7.20 (m, 1H), 7.16-7.08 (m, 2H), 6.94 (dd, *J* = 8.4, 1.2 Hz, 1H), 6.88-6.82 (m, 1H), 4.72 (dd, *J* = 10.4, 2.8 Hz, 1H), 3.90 (dd, *J* = 14.0, 10.4 Hz, 1H), 3.20 (dd, *J* = 10.4, 3.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.6, 160.6 (d, J_{C-F} = 244.9 Hz), 154.9, 147.6, 142.6, 136.6 (d, J_{C-F} = 11.2 Hz), 131.3, 129.2, 128.3, 127.8, 127.8, 126.6, 123.5 (d, J_{C-F} = 9.4 Hz), 120.6, 118.6, 115.1 (d, J_{C-F} = 24.7 Hz), 107.9 (d, J_{C-F} = 26.7 Hz), 53.5, 35.9; ^{19}F NMR (376 MHz, $CDCl_3$) δ -115.1 (s). FT-IR: ν (cm^{-1}) 3085, 3028, 2848, 2710, 1603, 1583, 1483. HRMS [ESI] calcd for $C_{21}H_{17}FNOS$ $[M+H]^+$ 350.1009, found 350.1006.



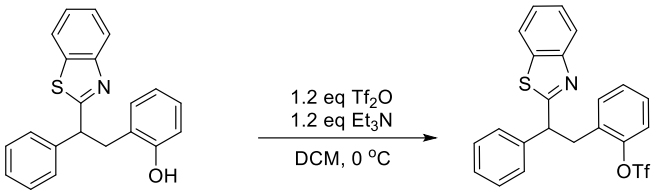
4l: 43.7 mg, 60%, yellow solid, m.p. 58-59 ºC. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 8.8 Hz, 1H), 7.69 (d, *J* = 2.0 Hz, 1H), 7.45 (dd, *J* = 8.8, 2.0 Hz, 1H), 7.42-7.35 (m, 2H), 7.35-7.29 (m, 3H), 7.16-7.08 (m, 2H), 6.96-6.91 (m, 1H), 6.88-6.82 (m, 1H), 4.73 (dd, *J* = 10.4, 3.2 Hz, 1H), 3.90 (dd, *J* = 14.4, 10.8 Hz, 1H), 3.21 (dd, *J* = 14.4, 3.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.4, 154.9, 149.5, 142.5, 136.7, 131.6, 131.3, 129.2, 128.3, 127.9, 127.8, 127.2, 126.6, 123.3, 121.3, 120.6, 118.6, 53.5, 35.9. FT-IR: ν (cm^{-1}) 3062, 2923, 2852, 1594, 1489, 1455, 1240. HRMS [ESI] calcd for $C_{21}H_{17}ClNOS$ $[M+H]^+$ 366.0714, found 366.0709.



4m: 59.9 mg, 73%, yellow solid, m.p. 121-122 ºC. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15).^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 8.8 Hz, 1H), 7.85 (d, *J* = 2.0 Hz, 1H), 7.59 (dd, *J* = 8.8, 2.0 Hz, 1H), 7.41-7.34 (m, 2H), 7.34-7.28 (m, 3H), 7.16-7.08 (m, 2H), 6.93 (dd, *J* = 8.4, 1.2 Hz, 1H), 6.88-6.82 (m, 1H), 4.72 (dd, *J* = 10.4, 3.2 Hz, 1H), 3.89 (dd, *J* = 14.4, 10.8 Hz, 1H), 3.20 (dd, *J* = 14.0, 3.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.4, 154.9, 149.9, 142.5, 137.2, 131.3, 129.9, 129.2, 128.3, 127.9, 127.8, 126.5, 124.2, 123.7, 120.6, 119.2, 118.5, 53.5, 35.9. FT-IR: ν (cm^{-1}) 3062, 3028, 2849, 1581, 1515, 1452, 1396. HRMS [ESI] calcd for $C_{21}H_{17}BrNOS$ $[M+H]^+$ 410.0209, found 410.0202.

7. Transformation of compound 3a

7.1. Synthesis of **5**

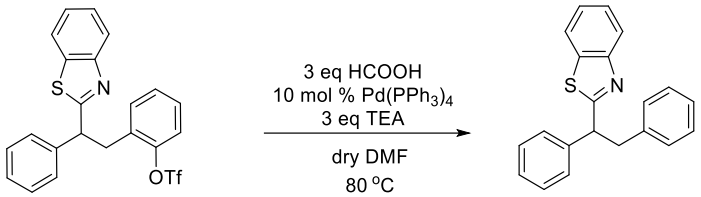


3a **5**

3a (1 mmol, 1.0 equiv.) was dissolved in DCM (10 mL) and cooled to 0 °C. Et_3N (1.2 mmol, 1.2 equiv) was added dropwise to the solution, which was followed by the addition of triflic anhydride (1.2 mmol, 1.2 equiv). After 5 min, the ice bath was removed, and the reaction was monitored by TLC. Once the **3a** was completely consumed, the reaction was stopped. The solvent was evaporated under vacuum and the residue was purified by flash column chromatography on silica gel (EtOAc/petroleum ether =1:20) to afford the desired product **5** (421.7 mg, 91% yield, 15 min).

5: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12-8.05 (m, 1H), 7.82-7.76 (m, 1H), 7.52-7.44 (m, 1H), 7.42-7.34 (m, 3H), 7.34-7.29 (m, 2H), 7.29-7.22 (m, 3H), 7.22-7.17 (m, 1H), 7.16-7.10 (m, 1H), 4.84-4.74 (m, 1H), 4.02-3.90 (m, 1H), 3.66-3.54 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.8, 153.2, 148.2, 140.6, 135.3, 132.4, 131.9, 128.8, 128.5, 128.2, 128.1, 127.7, 126.0, 125.0, 123.1, 121.6, 121.3, 118.6 (q, J_{C-F} = 318.2 Hz), 50.7, 36.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ -73.7 (s). FT-IR: ν (cm^{-1}) 3031, 2968, 2944, 1558, 1487, 1456, 1285. HRMS [ESI] calcd for $C_{22}H_{16}F_3NO_3S_2Na$ $[M+Na]^+$ 486.0416, found 486.0425.

7.2. Synthesis of **6**

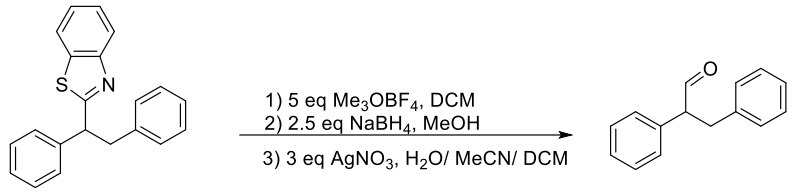


5 **6**

5 (0.2 mmol, 1.0 equiv.), formic acid (0.6 mmol, 3.0 equiv.), $Pd(PPh_3)_4$ (0.02 mmol, 10 mol %), TEA (0.6 mmol, 3.0 equiv.), and dry DMF (2.0 mL) were added to an oven-dried 5-mL flask. The flask was capped and then backfilled with nitrogen for three times. The reaction mixture was heated to 80 °C until **5** had been completely consumed as determined by TLC. Then, the reaction mixture was cooled down to room temperature and diluted with ethyl acetate (50 mL). The organic phase was washed with brine (3*15 mL) and dried with $MgSO_4$. The solvent was removed under reduced pressure to get the crude product, which was purified by flash column chromatography on silica gel (EtOAc/petroleum ether =1:40) to afford the pure product as a yellow solid (58.6 mg, 93% yield, 8.5 h).

6: yellow solid, m.p. 50-51 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98-7.92 (m, 1H), 7.74-7.66 (m, 1H), 7.40-7.34 (m, 1H), 7.31-7.23 (m, 3H), 7.23-7.18 (m, 2H), 7.18-7.05 (m, 4H), 7.05-7.00 (m, 2H), 4.60 (dd, *J* = 8.0, 8.0 Hz, 1H), 3.75 (dd, *J* = 14.0, 7.2 Hz, 1H), 3.37 (dd, *J* = 14.0, 8.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.2, 153.2, 141.2, 139.1, 135.3, 129.1, 128.7, 128.3, 128.3, 127.4, 126.3, 125.9, 124.8, 123.0, 121.5, 52.7, 41.9. FT-IR: ν (cm^{-1}) 3025, 2926, 2894, 1654, 1601, 1511, 1436. HRMS [ESI] calcd for $C_{21}H_{18}NS$ $[M+H]^+$ 316.1154, found 316.1156.

7.3. Synthesis of **7**

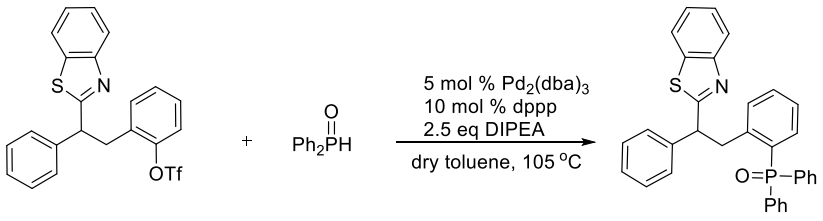


6 7

6 (0.15 mmol, 1.0 equiv.), activated 4 Å powdered molecular sieves (300 mg), and anhydrous CH_2Cl_2 (2 mL) was stirred at r.t. for 10 min, and then Me_3OBF_4 (1.0 mmol, 5 equiv.) was added in twice. The suspension was stirred at r.t. for 4 h and then concentrated to dryness without filtering off the molecular sieves. To a cooled (0 °C), stirred suspension of the crude *N*-methylbenzothiazolium salt in CH_3OH (2 mL) was added $NaBH_4$ (0.5 mmol, 2.5 equiv.). The mixture was stirred at rt. for an additional 30 min, diluted with acetone, filtered through a pad of Celite, and concentrated. To a vigorously stirred solution of the crude benzothiazoline in CH_2Cl_2 (0.6 mL) and CH_3CN (3.0 mL) were added H_2O (0.36 mL) and then $AgNO_3$ (0.45 mmol, 3 equiv.). The mixture was stirred at r.t. until the benzothiazoline were completely consumed as determined by TLC, and then diluted with 1 M phosphate buffer at pH 7 (0.1 mL). Stirring was continued for an additional 15 min, and then the reaction mixture was diluted with 1 M phosphate buffer at pH 7 (5 mL) and the suspension was extracted with EtOAc (2 × 10 mL), and the combined organic layers were dried over Na_2SO_4, filtered through a pad of Celite, and concentrated. The residue was eluted from a short column of silica gel (EtOAc/petroleum ether =1:40) to afford **7** (27.4 mg, 87% for 3 steps)

7: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.66 (d, *J* = 1.6 Hz, 1H), 7.30-7.17 (m, 3H), 7.17-7.10 (m, 2H), 7.10-7.02 (m, 3H), 7.01-6.94 (m, 2H), 3.80-3.72 (m, 1H), 3.39 (dd, *J* = 14.0, 6.8 Hz, 1H), 2.89 (dd, *J* = 14.0, 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.9, 138.8, 135.7, 129.1, 128.4, 127.7, 126.3, 61.0, 36.2. FT-IR: ν (cm^{-1}) 3062, 3029, 2923, 1703, 1601, 1495, 1453. HRMS [ESI] calcd for $C_{15}H_{14}ONa$ $[M+Na]^+$ 233.0937, found 233.0939.

7.4. Synthesis of **8**

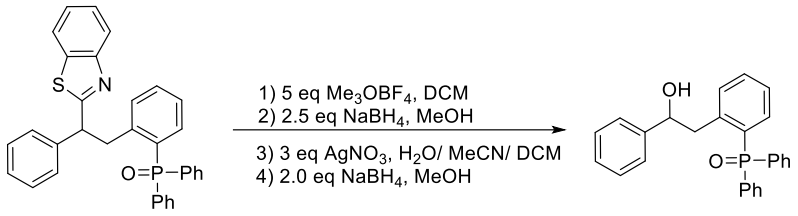


5 8

Under N_2, a 5 mL vial was charged with trifluoromethanesulfonate **5** (0.2 mmol, 1.0 equiv.), diphenylphosphine oxide (0.4 mmol, 2.0 equiv.), *N*, *N*-diisopropylethylamine (0.5 mmol, 2.5 equiv.), 1, 3-bis-(diphenylphosphino)propane (0.02 mmol, 10 mol%), $Pd_2(dba)_3$ (0.01 mmol, 5 mol%), and degassed toluene (1 mL). The vial was sealed and stirred at 105 °C for 48 h. Upon completion, the mixture was cooled to room temperature, and directly subject to flash column chromatography on silica gel (EtOAc/petroleum ether = 1 : 1) to afford **8** as a yellow solid (99 mg, 96% yield, 46.5 h).

8: yellow solid, m.p. 83-84 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06-7.98 (m, 1H), 7.77-7.72 (m, 1H), 7.72-7.63 (m, 4H), 7.59-7.50 (m, 2H), 7.50-7.39 (m, 5H), 7.36-7.26 (m, 3H), 7.25-7.12 (m, 4H), 7.11-6.99 (m, 3H), 5.01 (dd, *J* = 7.6, 7.6 Hz, 1H), 4.03 (dd, *J* = 14.0, 7.6 Hz, 1H), 3.75 (dd, *J* = 14.0, 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.9, 153.2, 144.5 (d, $J_{C\text{-}P}$ = 7.8 Hz), 141.4, 135.4, 133.7 (d, $J_{C\text{-}P}$ = 13.0 Hz), 133.7 (d, $J_{C\text{-}P}$ = 4.0 Hz), 132.7 (d, $J_{C\text{-}P}$ = 3.1 Hz), 132.5 (d, $J_{C\text{-}P}$ = 10.2 Hz), 132.1, 132.0, 131.9, 131.5 (d, $J_{C\text{-}P}$ = 2.1 Hz), 131.1 (d, $J_{C\text{-}P}$ = 90.9 Hz), 128.7, 128.6, 128.5, 128.5, 128.4, 126.9, 125.7 (d, $J_{C\text{-}P}$ = 13.1 Hz), 125.6, 124.6, 122.9, 121.5, 51.0, 40.8 (d, $J_{C\text{-}P}$ = 4.5 Hz); ^{31}P NMR (162 MHz, $CDCl_3$) δ 31.6 (s). FT-IR: ν (cm^{-1}) 3057, 2927, 2893, 1726, 1513, 1493, 1238. HRMS [ESI] calcd for $C_{33}H_{27}NOPS$ $[M+H]^+$ 516.1545, found 516.1545.

7.5. Synthesis of **9**

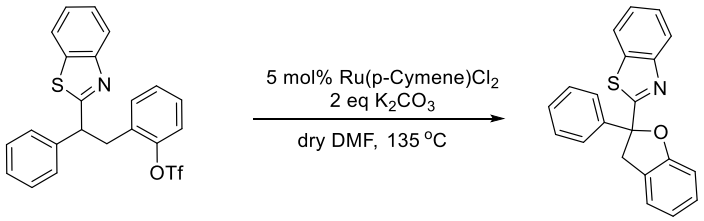


8 **9**

8 (0.1 mmol, 1.0 equiv.), activated 4 Å powdered molecular sieves (150 mg), anhydrous CH_2Cl_2 (1 mL) and MeCN (1 mL) was stirred at r.t. for 10 min, and then MeOTf (0.5 mmol, 5 equiv.) was added in twice. The suspension was stirred at r.t. for 4 h and then concentrated to dryness without filtering off the molecular sieves. To a cooled (0 °C), stirred suspension of the crude *N*-methylbenzothiazolium salt in CH_3OH (2 mL) was added $NaBH_4$ (0.25 mmol, 2.5 equiv.). The mixture was stirred at r.t. for an additional 30 min, diluted with acetone, filtered through a pad of Celite, and concentrated. To avigorously stirred solution of the crude benzothiazolines in CH_2Cl_2 (0.3 mL) and CH_3CN (1.5 mL) were added H_2O (0.18 mL) and then $AgNO_3$ (0.3 mmol, 3 equiv.). The mixture was stirred at rt. until the benzothiazolines were completely consumed as determined by TLC, and then diluted with 1 M phosphate buffer at pH 7 (0.1 mL). Stirring was continued for an additional 15 min, and then the reaction mixture was diluted with 1 M phosphate buffer at pH 7 (5 mL) and the suspension was extracted with EtOAc (3 × 15 mL), and the combined organic layers were dried over Na_2SO_4, filtered through a pad of Celite, and concentrated. The mixture was diluted in CH_3OH (2 mL) and added $NaBH_4$ (0.2 mmol, 2.0 equiv.) in 0 °C. After stired at r.t. for 30 min (TLC), the residue was eluted from a short column of silica gel (EtOAc/petroleum ether = 1:3) to afford **9** (21.6 mg, 54% for 4 steps).

9: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68-7.54 (m, 5H), 7.54-7.40 (m, 7H), 7.37-7.28 (m, 3H), 7.25-7.16 (m, 2H), 7.05-6.93 (m, 1H), 6.71 (d, J = 7.6 Hz, 1H), 4.96-4.84 (m, 1H), 3.36 (dd, J = 13.2, 9.6 Hz, 1H), 3.06 (dd, J = 14.0, 3.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.0, 144.5 (d, $J_{C\text{-}P}$ = 7.8 Hz), 133.3 (d, $J_{C\text{-}P}$ = 13.3 Hz), 132.9, 132.5 (d, $J_{C\text{-}P}$ = 2.7 Hz), 132.3 (d, $J_{C\text{-}P}$ = 18.3 Hz), 132.3, 132.2, 132.1 (d, $J_{C\text{-}P}$ = 6.7 Hz), 131.9, 131.8 (d, $J_{C\text{-}P}$ = 10.0 Hz), 131.0 (d, $J_{C\text{-}P}$ = 47.6 Hz), 128.8 (d, $J_{C\text{-}P}$ = 7.8 Hz), 128.8 (d, $J_{C\text{-}P}$ = 7.8 Hz), 128.2, 126.8, 126.0, 125.9, 75.5, 44.6 (d, $J_{C\text{-}P}$ = 4.9 Hz); ^{31}P NMR (162 MHz, $CDCl_3$) δ 35.8 (s). FT-IR: ν (cm^{-1}) 3057, 2964, 2923, 1825, 1773, 1559, 1477. HRMS [ESI] calcd for $C_{26}H_{23}O_2PNa$ $[M+Na]^+$ 421.1328, found 421.1308.

7.6. Synthesis of **10**

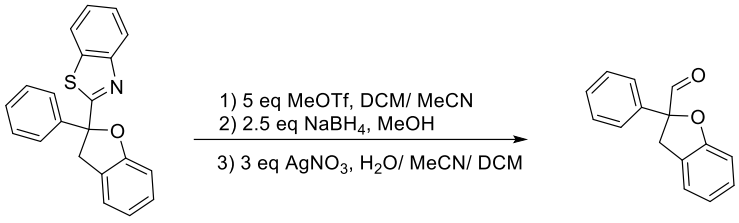


5 **10**

5 (0.2 mmol, 1.0 equiv.), potassium carbonate (0.4 mmol, 2.0 equiv.), Ru(p-cymene)Cl_2 (0.01 mmol, 5 mol %), and dry DMF (2.0 mL) were added to an oven-dried 5mL flask. The flask was capped and then backfilled with nitrogen for three times. The reaction mixture was heated to 135 °C until **5** had been completely consumed as determined by TLC. Then, the reaction mixture was cooled down to room temperature and solvent was removed under reduced pressure to get the crude product, which was purified by flash column chromatography on silica gel (EtOAc/petroleum ether = 1:30) to afford product **10** as a white solid (62.2 mg, 94% yield, 11 h).

10: white solid, m.p. 130-131°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06-8.01 (m, 1H), 7.84-7.79 (m, 1H), 7.77-7.70 (m, 2H), 7.49-7.42 (m, 1H), 7.42-7.36 (m, 2H), 7.36-7.27 (m, 2H), 7.24-7.21 (m, 2H), 7.11-7.06 (m, 1H), 6.96-6.90 (m, 1H), 4.64 (d, *J* = 15.6 Hz, 1H), 3.84 (d, *J* = 15.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.6, 158.1, 153.2, 142.6, 135.7, 128.6, 128.4, 128.1, 126.0, 125.9, 125.4, 125.1, 125.0, 123.3, 121.7, 121.7, 110.1, 91.9, 44.3. FT-IR: ν (cm^{-1}) 3054, 2922, 2852, 1685, 1613, 1433, 1327. HRMS [ESI] calcd for $C_{21}H_{16}NOS$ $[M+H]^+$ 330.0947, found 330.0944.

7.7. Synthesis of **11**

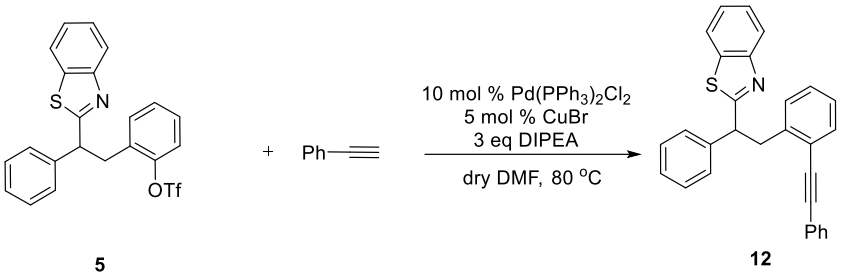


10 **11**

10 (0. 1 mmol, 1.0 equiv.), activated 4 Å powdered molecular sieves (150 mg), anhydrous CH_2Cl_2 (1 mL) and MeCN (1 mL) was stirred at r.t. for 10 min, and then MeOTf (0.5 mmol, 5 equiv.) was added in twice. The suspension was stirred at r.t. for 4 h and then concentrated to dryness without filtering off the molecular sieves. To a cooled (0 °C), stirred suspension of the crude *N*-methylbenzothiazolium salt in CH_3OH (2 mL) was added $NaBH_4$ (0.25 mmol, 2.5 equiv.). The mixture was stirred at r.t. for an additional 30 min, diluted with acetone, filtered through a pad of Celite, and concentrated. To avigorously stirred solution of the crude benzothiazolines in CH_2Cl_2 (0.3 mL) and CH_3CN (1.5 mL) were added H_2O (0.18 mL) and then $AgNO_3$ (0.3 mmol, 3 equiv.). The mixture was stirred at r.t. until the benzothiazolines were completely consumed as determined by TLC, and then diluted with 1 M phosphate buffer at pH 7 (0.1 mL). Stirring was continued for an additional 15 min, and then the reaction mixture was diluted with 1 M phosphate buffer at pH 7 (5 mL) and the suspension was extracted with EtOAc (3 × 15 mL), and the combined organic layers were dried over Na_2SO_4, filtered through a pad of Celite, and concentrated. The crude product was purified by flash column chromatography on silica gel (EtOAc/petroleum ether = 1:7) to afford product **11** as a yellow oil (12.3 mg, 55% yield for 3 steps).

11: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14-8.07 (m, 2H), 7.69 (s, 1H), 7.66-7.59 (m, 1H), 7.55-7.48 (m, 2H), 7.22-7.15 (m, 2H), 6.99-6.94 (m, 1H), 6.91-6.85 (m, 1H), 4.29 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.2, 155.7, 135.8, 134.1, 131.0, 129.1, 128.9, 125.6, 121.0, 120.9, 117.8, 41.1. FT-IR: ν (cm^{-1}) 3408, 3062, 2917, 2851, 1673, 1608, 1594, 1341. HRMS [ESI] calcd for $C_{15}H_{13}O_2$ $[M+H]^+$ 225.0910, found 225.0919.

7.8. Synthesis of **12**



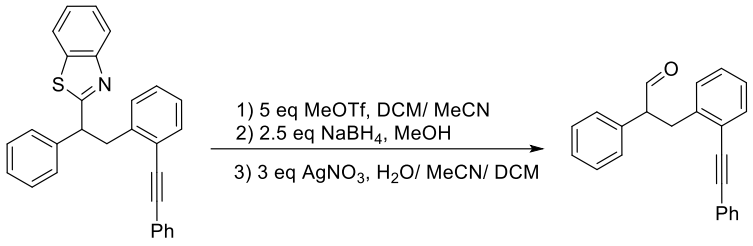
5 **12**

5 (0.2 mmol, 1.0 equiv.), phenylacetylene (0.6 mmol, 3.0 equiv.), $Pd(PPh_3)_2Cl_2$ (0.02 mmol, 10 mol %), CuBr (0.01 mmol, 5 mol %), DIPEA (0.6 mmol, 3.0 equiv.), and dry DMF (2.0 mL) were added to an oven-dried 5 mL flask. The flask was capped and then backfilled with nitrogen for three times. The reaction mixture was heated to 80 °C until **5** had been completely consumed as

determined by TLC. Then, the reaction mixture was cooled down to room temperature and then diluted with ethyl acetate (50 mL). The organic phase was washed with brine (4×10 mL) and dried with $MgSO_4$. The solvent was removed under reduced pressure to get the crude product, which was purified by flash column chromatography on silica gel (EtOAc/petroleum ether = 1:40) to afford product **12** as a yellow solid (74.4 mg, 90% yield, 10 h).

12: yellow solid, m.p. 82-83°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 -7.98 (m, 1H), 7.76-7.70 (m, 1H), 7.50-7.38 (m, 4H), 7.36-7.30 (m, 2H), 7.30-7.16 (m, 7H), 7.12-7.06 (m, 1H), 7.05-6.99 (m, 1H), 6.99-6.94 (m, 1H), 4.90 (dd, *J* = 7.6, 7.6 Hz, 1H), 4.05 (dd, *J* = 13.2, 7.2 Hz, 1H), 3.62 (dd, *J* = 13.2, 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.9, 153.3, 141.4, 141.2, 135.4, 132.3, 131.7, 130.1, 128.6, 128.4, 128.3, 128.3, 128.1, 127.3, 126.4, 125.8, 124.8, 123.3, 123.0, 121.5, 93.9, 88.1, 51.4, 41.1. FT-IR: ν (cm^{-1}) 3059, 3028, 2958, 1637, 1493, 1436, 1328. HRMS [ESI] calcd for $C_{29}H_{22}NS$ $[M+H]^+$ 416.1467, found 416.1456.

7.9. Synthesis of **13**

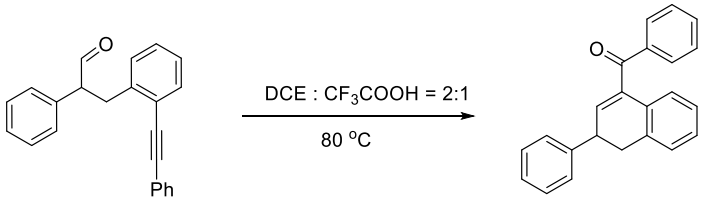


12 **13**

13 was prepared from **12** (0.2 mmol) according to the same procedures as the synthesis of **11**, the crude product was purified by flash column chromatography on silica gel (EtOAc/petroleum ether = 1:7) to afford product **13** as a yellow oil (50.8 mg, 82% yield for 3 steps).

13: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.83 (d, *J* = 1.2 Hz, 1H), 7.62-7.50 (m, 3H), 7.44-7.30 (m, 6H), 7.25-7.16 (m, 4H), 7.12-7.08 (m, 1H), 4.16 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 3.84 (dd, *J* = 13.6, 6.8 Hz, 1H), 3.21 (dd, *J* = 13.6, 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.9, 141.1, 136.0, 132.4, 131.6, 130.2, 129.2, 129.0, 128.5, 128.5, 128.4, 127.7, 126.5, 123.2, 122.9, 94.0, 88.0, 59.9, 35.4. FT-IR: ν (cm^{-1}) 3028, 2814, 2214, 1720, 1599, 1493, 1444, 1387. HRMS [ESI] calcd for $C_{23}H_{18}ONa$ $[M+Na]^+$ 333.1250, found 333.1258.

7.10. Synthesis of **14**

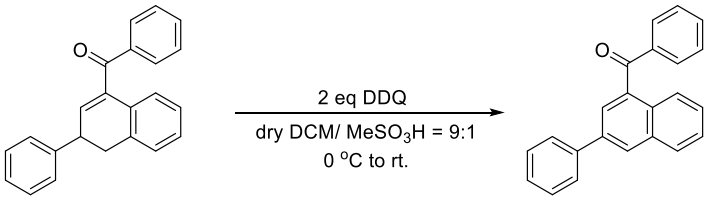


13 **14**

To a solution of **13** (32 mg, 0.1 mmol) in DCE (2.0 mL) was added TFA (1.0 mL) and the resulting solution was stirred at 80 °C for 1 h. Then the mixture was cooled down to r.t. and concentrated in vacuo to yield the crude product. Purification by flash column chromatography on silica gel (EtOAc/petroleum ether = 1:40) afforded product **14** as a yellow oil (24.0 mg, 77%).

14: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86-7.79 (m, 2H), 7.47-7.40 (m, 1H), 7.36-7.29 (m, 2H), 7.25-7.12 (m, 6H), 7.11-7.04 (m, 3H), 6.37 (d, *J* = 3.2 Hz, 1H), 3.88-3.79 (m, 1H), 3.08-2.94 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.9, 143.5, 139.3, 138.8, 137.8, 134.9, 133.1, 131.6, 130.0, 128.8, 128.5, 128.3, 128.0, 127.6, 127.0, 127.0, 125.9, 41.4, 37.0. FT-IR: ν (cm^{-1}) 3059, 2923, 2853, 1723, 1596, 1448, 1253. HRMS [ESI] calcd for $C_{23}H_{18}ONa$ $[M+Na]^+$ 333.1250, found 333.1259.

7.11. Synthesis of **15**

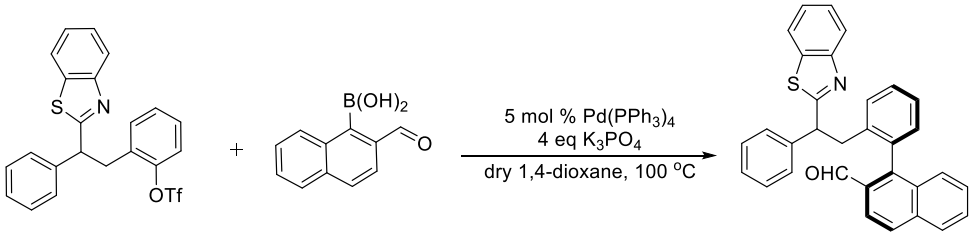


14 **15**

Compound **15** (0.1 mmol) was dissolved in dry CH_2Cl_2 (9 mL) and methanesulfonic acid (1 mL) at 0 °C. The solution was treated with DDQ (0.2 mmol), stirred at 0 °C for 30 min and then rt for 6 h. The mixture was extracted with CH_2Cl_2 (3×10 mL), and the combined organic layers were washed with water and brine, dried over Na_2SO_4, filtered, and purified through a short pad of silica gel (EtOAc/ petroleum ether = 1:40) to afford product **15** as a yellow oil (24.3 mg, 79%).

15: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24-8.19 (m, 1H), 8.12-8.06 (m, 1H), 8.02-7.97 (m, 1H), 7.96-7.91 (m, 2H), 7.88-7.84 (m, 1H), 7.74-7.67 (m, 2H), 7.65-7.59 (m, 1H), 7.59-7.54 (m, 1H), 7.54-7.45 (m, 5H), 7.43-7.36 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.9, 140.1, 138.2, 137.2, 137.1, 134.1, 133.4, 130.5, 130.2, 129.0, 128.8, 128.7, 128.6, 127.8, 127.4, 127.3, 127.2, 126.9, 125.6. FT-IR: ν (cm^{-1}) 3080, 2956, 2924, 1652, 1577, 1495, 1321.$C_{23}H_{16}ONa$ $[M+Na]^+$ 331.1093, found 331.1095.

7.12. Synthesis of **16**



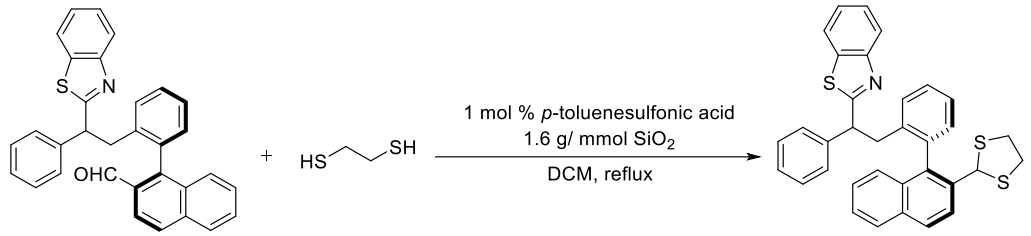
5 **16**

5 (0.2 mmol, 1.0 equiv.), (2-formylnaphthalen-1-yl)boronic acid (0.8 mmol, 4.0 equiv.), $Pd(PPh_3)_4$ (0.01 mmol, 5 mol %), K_3PO_4 (0.8 mmol, 4.0 equiv.), and dry 1, 4-dioxane (2.0 mL) were added to an oven-dried 5 mL flask. The flask was capped and then backfilled with nitrogen for three times. The reaction mixture was heated to 100°C until **5** had been completely consumed as determined by TLC. Then, the reaction mixture was cooled down to room temperature and solvent was removed under reduced pressure to get the crude product, which was purified by flash column chromatography on silica gel (EtOAc/petroleum ether = 1:30) to afford product **16** as a yellow oil (44.5 mg, 47% yield, 24 h).

16 (*d.r.* = 5:1): yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.81 (d, *J* = 0.4 Hz, 1H, major), 9.44 (d, *J* = 0.8 Hz, 1H, minor), 8.13-8.08 (m, 1H, major), 8.08-8.04 (m, 1H, minor), 8.02-7.95 (m, 3H, major), 7.95-7.87 (m, 3H, minor),7.73-7.68 (m, 1H, major), 7.68-7.72 (m, 1H, major & 1H, minor, overlap), 7.62-7.56 (m, 1H, major), 7.52-7.38 (m, 4H, major & 4H, minor, overlap), 7.39-7.26 (m, 3H, major & 3H, minor, overlap), 7.25-7.20 (m, 1H, major & 1H, minor, overlap), 7.19-7.12 (m, 1H, major), 7.13-7.10 (m, 1H, minor), 7.10-7.06 (m, 2H, major & 2H, minor, overlap), 6.98-6.94 (m, 2H, minor), 6.91-6.84 (m, 2H, major), 4.47 (dd, *J* = 8.4, 6.8 Hz, 1H, minor), 4.40 (dd, *J* = 8.8, 6.4 Hz, 1H, major), 3.61 (dd, *J* = 14.4, 6.8 Hz, 1H, minor), 3.54 (dd, *J* = 14.4, 8.8 Hz, 1H, major), 3.13-3.03 (m, 1H, major & 1H, minor, overlap); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major) 192.6, 172.6, 153.1, 145.4, 141.0, 138.5, 136.2, 135.1, 135.0, 132.5, 131.4, 131.3, 129.8, 129.0, 128.7, 128.6, 128.6, 128.4, 128.0, 127.7, 127.5, 127.2, 126.3, 125.8, 124.8, 123.0, 122.2, 121.4, 50.5, 39.6; (minor) 192.4, 173.5, 153.0, 145.1, 140.5, 138.5, 136.0, 135.1, 134.9, 131.8, 131.6, 131.1, 130.0, 128.9, 128.7,

128.6, 128.6, 128.4, 128.0, 127.6, 127.3, 127.2, 126.3, 125.9, 124.7, 122.9, 122.1, 121.4, 51.5, 39.3. FT-IR: ν (cm^{-1}) 2960, 2917, 1618, 1592, 1482, 1430, 1309. HRMS [ESI] calcd for $C_{32}H_{24}NOS$ $[M+H]^+$ 470.1573, found 470.1578.

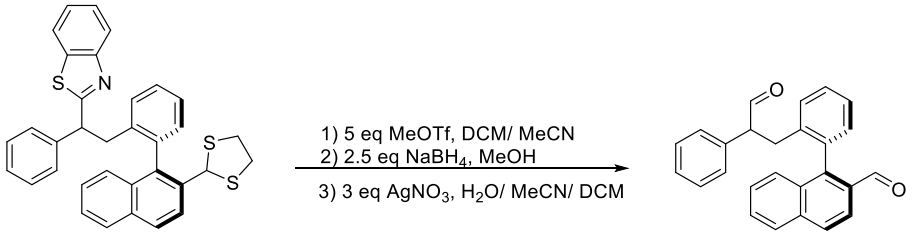
7.13. Protection of aldehyde



16

A 50 mL round-bottom flask fitted with a condenser was charged with silica gel (145 mg), CH_2Cl_2 (5 mL), **16** (0.09 mmol), 1, 2-ethanedithiol (0.1 mmol, 1.1 equiv.), and *p*-toluenesulfonic acid (1.5 mg, 1 mol %). The heterogeneous mixture was refluxed under stirring with a magnetic stirrer. Progress of the reaction was monitored by TLC. After complete disappearance of **16**, the reaction mixture was filtered through a sintered glass funnel. The solid residue was washed with CH_2Cl_2 (10mL). The solvent was evaporated under vacuum to get the crude product as a white solid, which was pure enough to be directly used in the next step.

7.14. Synthesis of **17**



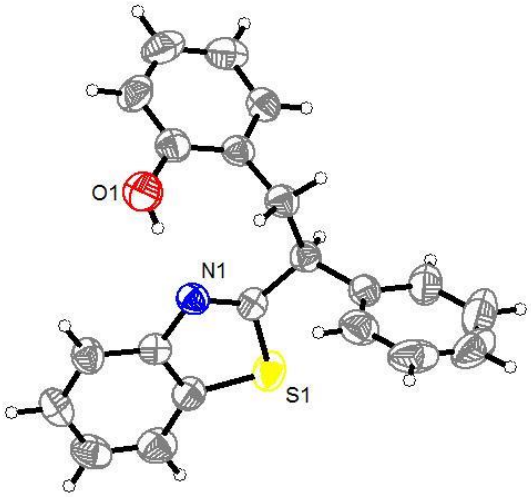
17

The disulfide (0.07 mmol, 1.0 equiv.), activated 4 Å powdered molecular sieves (140 mg), anhydrous CH_2Cl_2 (1 mL), and MeCN (1 mL) was stirred at r.t. for 10 min, and then MeOTf (0.35 mmol, 5 equiv.) was added in twice. The suspension was stirred at r.t. for 4 h and then concentrated to dryness without filtering off the molecular sieves. To a cooled (0 °C), stirred suspension of the crude *N*-methylbenzothiazolium salt in CH_3OH (2 mL) was added $NaBH_4$ (0.175 mmol, 2.5 equiv.). The mixture was stirred at r.t. for an additional 30 min, diluted with acetone, filtered through a pad of Celite, and concentrated. To avigorously stirred solution of the crude benzothiazolines in CH_2Cl_2 (0.2 mL) and CH_3CN (1.0 mL) were added H_2O (0.13 mL) and then $AgNO_3$ (0.21 mmol, 3 equiv.). The mixture was stirred at r.t. until the benzothiazolines were completely consumed as determined by TLC, and then diluted with 1 M phosphate buffer at pH 7 (0.1 mL). Stirring was continued for an additional 15 min, and then the reaction mixture was diluted with 1 M phosphate buffer at pH 7 (5 mL) and the suspension was extracted with EtOAc (2 × 10 mL), and the combined organic layers were dried over Na_2SO_4, filtered through a pad of Celite, and concentrated. The residue was eluted from a short column of silica gel (EtOAc/petroleum ether = 1:15) to afford product **17** (8.0 mg, 31% for 3 steps).

17 (*d.r.* = 4.1:1): yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.95 (s, 1H, minor), 9.83 (m, 1H, major), 9.43 (d, *J* = 1.2 Hz, 1H, major), 9.25 (s, 1H, minor), 8.10-8.05 (m, 1H, major), 8.00-7.91 (m, 2H, major & 3H, minor, overlap), 7.67-7.60 (m, 1H, minor & 1H, major, overlap), 7.50-7.26 (m, 6H, major & 6H, minor, overlap), 7.20-7.11 (m, 3H, major & 3H, minor, overlap), 6.75-6.70 (m, 2H, minor), 6.70-6.60 (m, 2H, major), 3.63-3.58 (m, 1H, minor), 3.53-3.47 (m, 1H, major), 3.26-3.18 (m, 1H, minor), 3.11 (dd, *J* = 14.4, 6.8 Hz, 1H, major), 2.66 (dd, *J* = 14.4, 7.6 Hz, 1H, major), 2.56 (dd, *J* = 14.4, 9.2Hz, 1H, minor); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major) 199.0, 192.5, 145.3, 138.2,

136.2, 135.0, 134.9, 132.4, 131.8, 131.4, 130.1, 129.1, 129.0, 128.7, 128.7, 128.6, 128.4, 127.7, 127.3, 127.2, 126.4, 122.2, 59.3, 33.6; (minor) 199.3, 192.0, 144.9, 138.2, 135.9, 134.9, 134.8, 132.2, 131.5, 131.2, 129.7, 129.2, 128.9, 128.8, 128.6, 128.5, 128.4, 127.7, 127.3, 127.0, 126.4, 122.1, 60.0, 33.2. FT-IR: ν (cm^{-1}) 3060, 2925, 2850, 2730, 1721, 1687, 1616, 1490, 1380. HRMS [ESI] calcd for $C_{26}H_{20}O_2Na$ $[M+Na]^+$ 387.1356, found 387.1348.

8. Single-crystal X-ray diffraction data for 3a



Bond precision:	C-C = 0.0047 A	Wavelength=0.71073	
Cell:	a=12.840(3)	b=14.882(3)	c=17.928(4)
	alpha=90	beta=99.99(3)	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	3373.8(13)	3373.8(12)	
Space group	P 21/n	P 1 21/n 1	
Hall group	-P 2yn	-P 2yn	
Moiety formula	C21 H17 N O S	C21 H17 N O S	
Sum formula	C21 H17 N O S	C21 H17 N O S	
Mr	331.42	331.42	
Dx, g cm^{-3}	1.305	1.305	
Z	8	8	
Mu (mm^{-1})	0.198	0.198	
F000	1392.0	1392.0	
F000’	1393.49		
h, k, lmax	15, 17, 21	15, 17, 21	
Nref	5950	5889	
Tmin, Tmax	0.977, 0.980	0.961, 0.980	
Tmin’	0.961		
Correction method = # Reported T Limits: Tmin=0.961 Tmax=0.980			
AbsCorr = MULTI-SCAN			
Data completeness = 0.990		Theta (max) = 25.000	
R(reflections)= 0.0673 (4639)		wR2(reflections)= 0.1679 (5889)	
S = 1.157		Npar= 435	

9. Emission quenching experiments (Stern–Volmer Studies):

Emission intensities were recorded using a FLS980 (Edinburgh Instrument, UK) luminescence spectrophotometer. All 4CzIPN solutions were excited at 460 nm and the emission intensity was collected at 558 nm. In a typical experiment, to a $3 \cdot 10^{-6}$ M solution of 4CzIPN in MeCN was added the appropriate amount of a quencher diazonium salt **1b** in a screw-top quartz cuvette. After degassing the sample with a stream of N_2 for 10 minutes, the emission of the sample was collected. Then, another quencher ascorbic acid ($AscH_2$) was test in the same way.

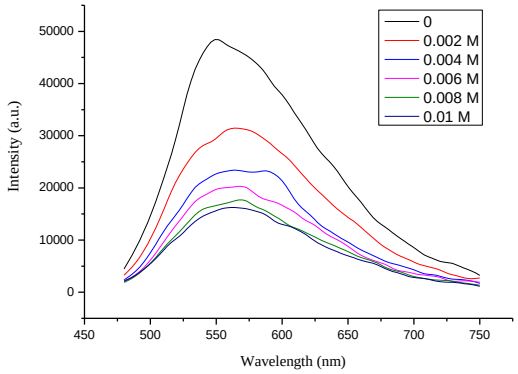


Fig. S1 Quenching of 4CzIPN emission in the presence of increasing amounts of the diazonium salt **1b**.

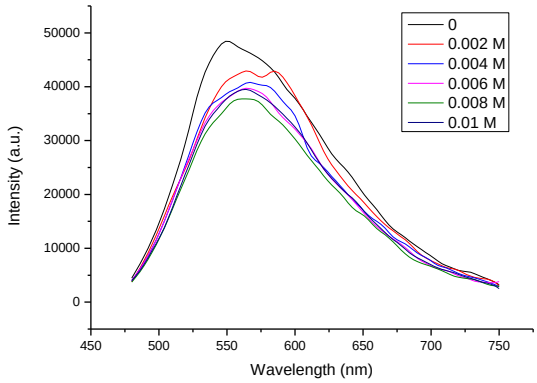


Fig. S2 Quenching of 4CzIPN emission in the presence of increasing amounts of ascorbic acid.

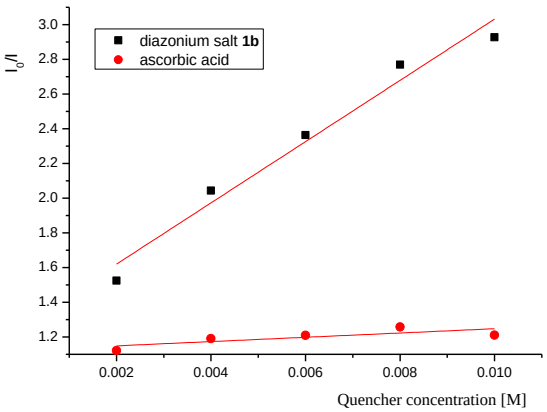


Fig. S3 Stern-Volmer quenching plot.

10. Absorption experiments:

Solutions of different complexes were introduced to a 1 cm path length quartz cuvette equipped with a Teflon® septum and analyzed using an ultraviolet spectrometer (Agilent Technologies Cary 5000 UV-vis-NIR). For diazonium salt **1b**, ascorbic acid ($AscH_2$), the mixtures (**1b** (0.01 mmol) and **2a** (0.02 mmol)) and the mixtures (**1b** (0.01 mmol) and ascorbic acid (0.02 mmol)) were dissolved in MeCN (4 mL) respectively. The mixtures were stirred for 5 min, then transformed to 1 cm path length quartz cuvettes, sealed with Teflon® septa and degassed with a stream of argon for 10 minutes.

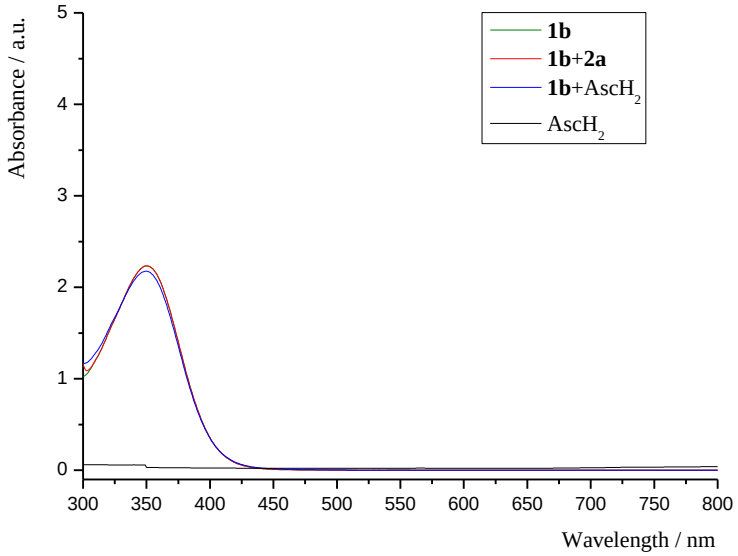


Fig. S4 Absorption spectra of **1b**, $AscH_2$, the mixture of **1b** and **2a** and the mixture of **1b** and $AscH_2$.

11. Determination of quantum yield:

The quantum yield (Φ) was determined by the known ferrioxalate actinometry method. A ferrioxalate actinometry solution was prepared by following the Hammond variation of the Hatchard and Parker procedure outlined in Handbook of Photochemistry. The actinometry solutions (1mL) were irradiated with 15 W blue LEDs (400±5 nm) for specified time intervals (0 sec, 20 sec, 40sec, 60 sec, 80 sec, 100 sec). The UV-Vis spectra is shown in **Fig. S5**. Based on the data, we got the graph (**Fig. S6**) between the number of moles of products (y axis) and time (x axis). Then, the irradiated light intensity was estimated to 3.78 x 10^{-8} einstein S^{-1} by using $K_3[Fe(C_2O_4)_3]$ as an actinometer. For four clean tubes, according to the general procedure, the 0.1 mmol scale model reaction solution was irradiated with 15 W blue LEDs (400±5 nm) for specified time intervals (0 min, 3 min, 5 min, 15 min, 20 min). The moles of products formed were determined by H-NMR yield with Toluene as reference standard. The number of moles of products (y axis) per unit time is related to the number of photons (x axis, calculated from the light intensity) (**Fig. S7**). The slope gives the quantum yield (Φ) of the photoreaction, 1.04 (104%).

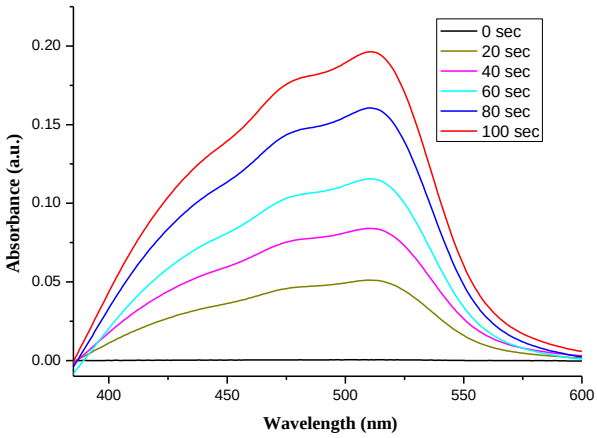


Fig. S5

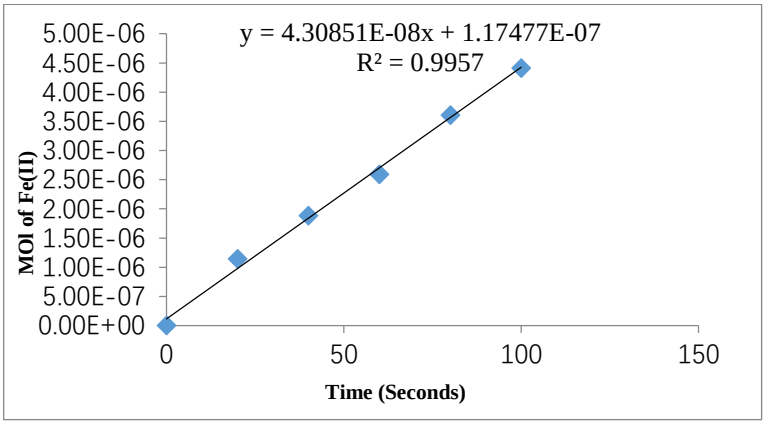


Fig. S6

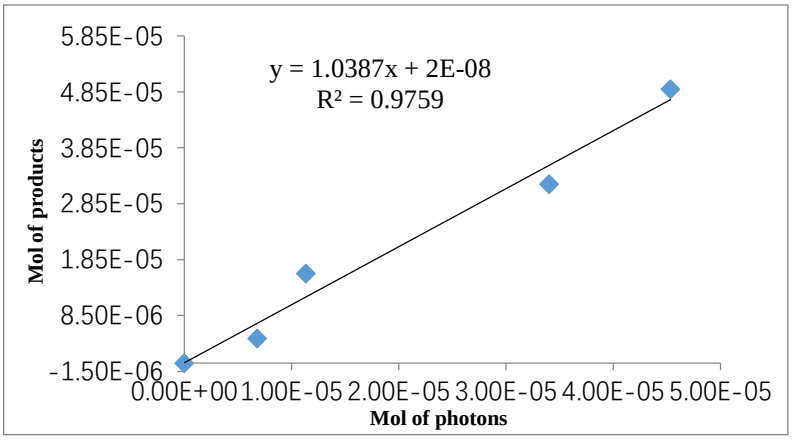


Fig. S7

12. Cyclic voltammograms:

All voltammograms were taken at room temperature using a meshplatinum (Pt) counter electrode, a glassy carbon working electrode (3 mm diameter), and a saturated KCl Ag/AgCl reference electrode. The conditions of the experiments were the following: an acetonitrile solution of 0.1 M tetrabutylammonium tetrafluoroborate (Bu_4NBF_4) and 0.01 M diazonium salt **1b**, dehydroascorbate **A** or **3a**, a scan rate of 0.1 V/s, and a negative initial scan direction. The reported potentials were averages over segments, and were taken at half-height of the cathodic peaks ($E_{p/2}$) of **1b**, **A** or **3a**, since all reductions were nonreversible. To convert the potentials from SCE to Fc/Fc^+ reference, 380 mV were subtracted from the measured values. The positive peaks on the return sweep of most

substrates were thought to signify an ECE-type mechanism.

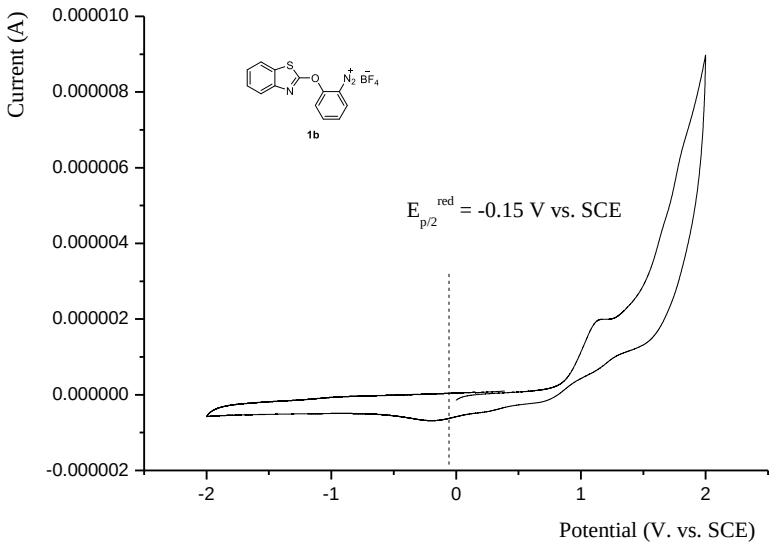


Fig. S8 Cyclic voltammogram of diazonium salt **1b** in MeCN.

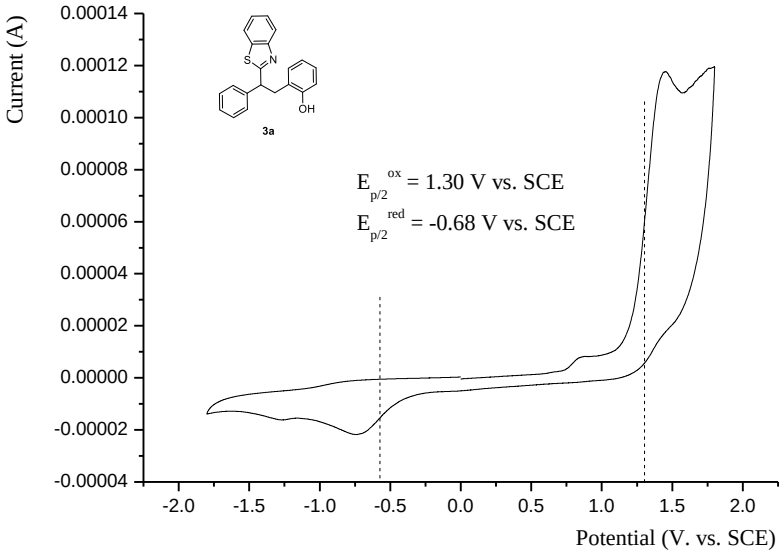


Fig. S9 Cyclic voltammogram of **3a** in MeCN.

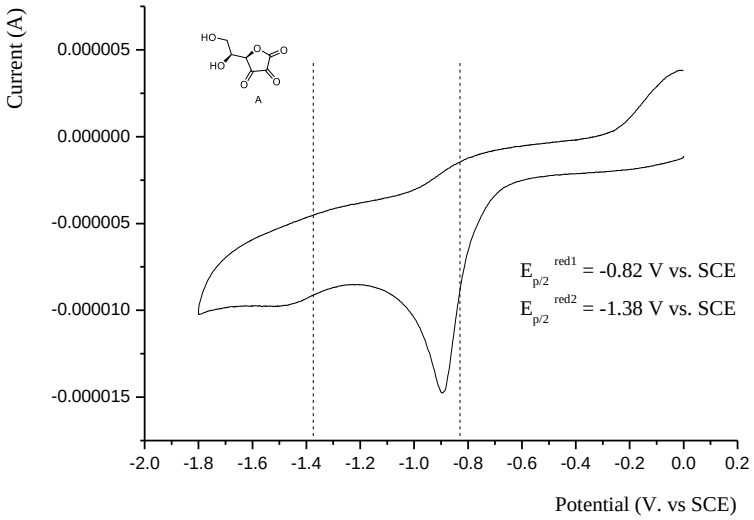


Fig. S10 Cyclic voltammogram of dehydroascorbate **A** in MeCN.

13. Light on-and-off experiments:

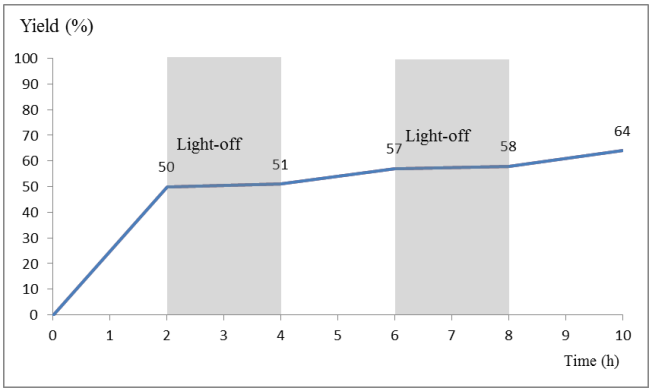


Fig. S11

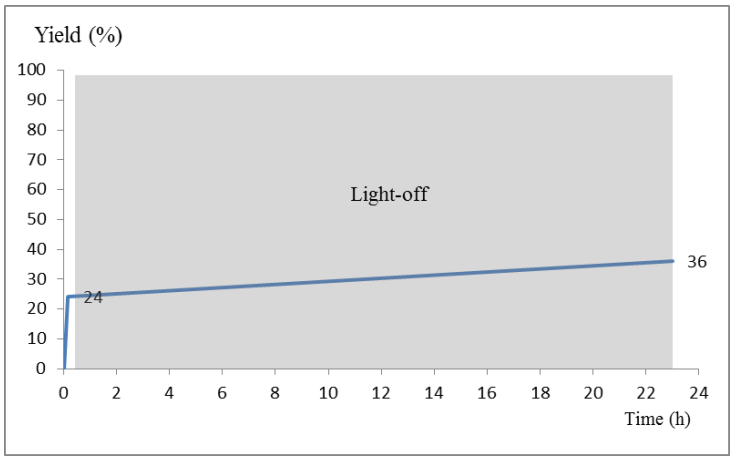
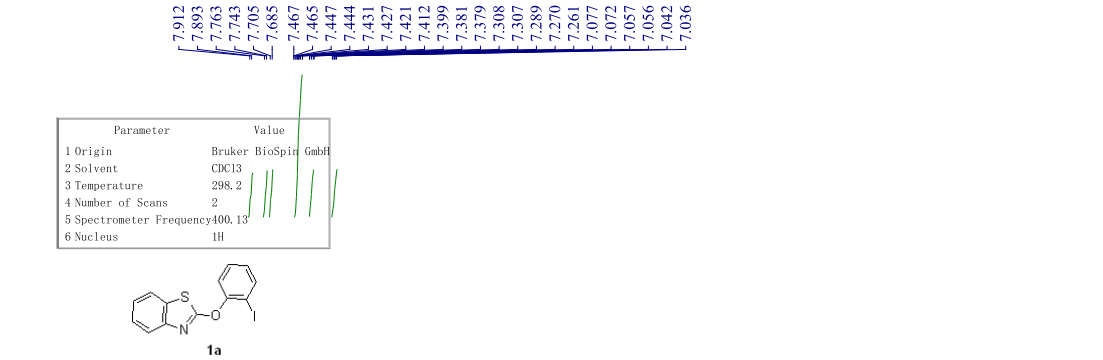
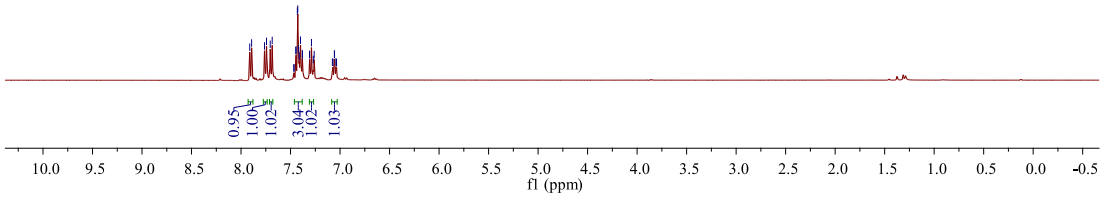
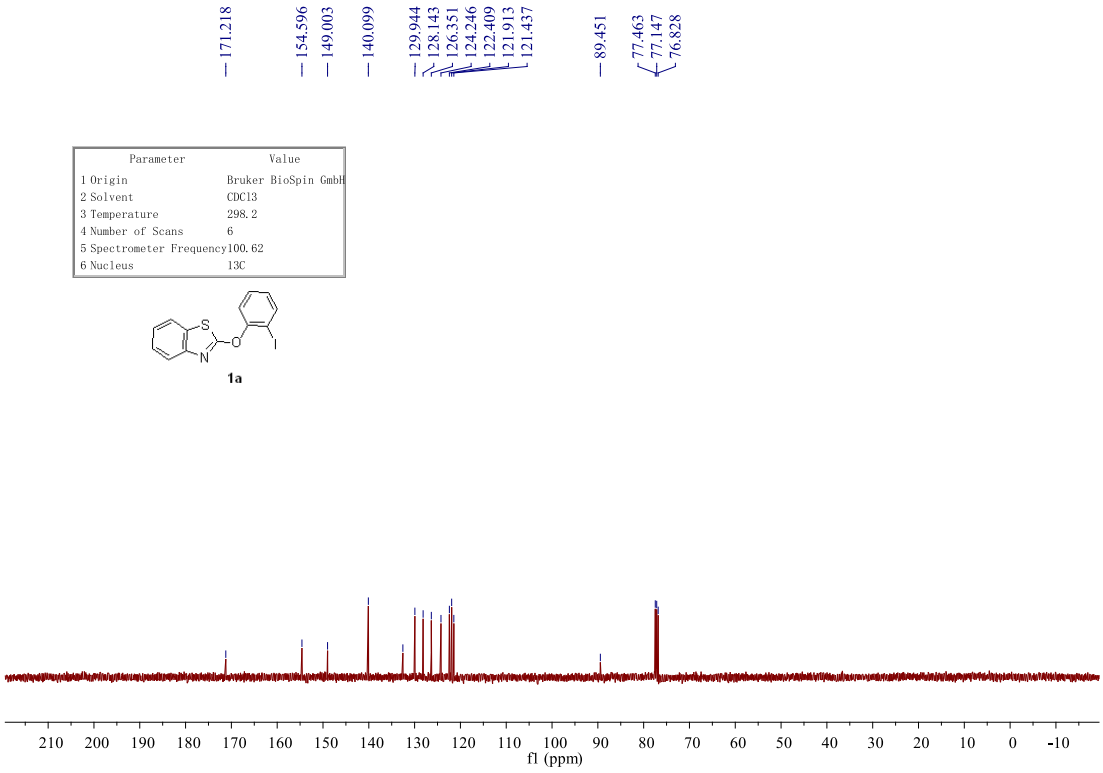


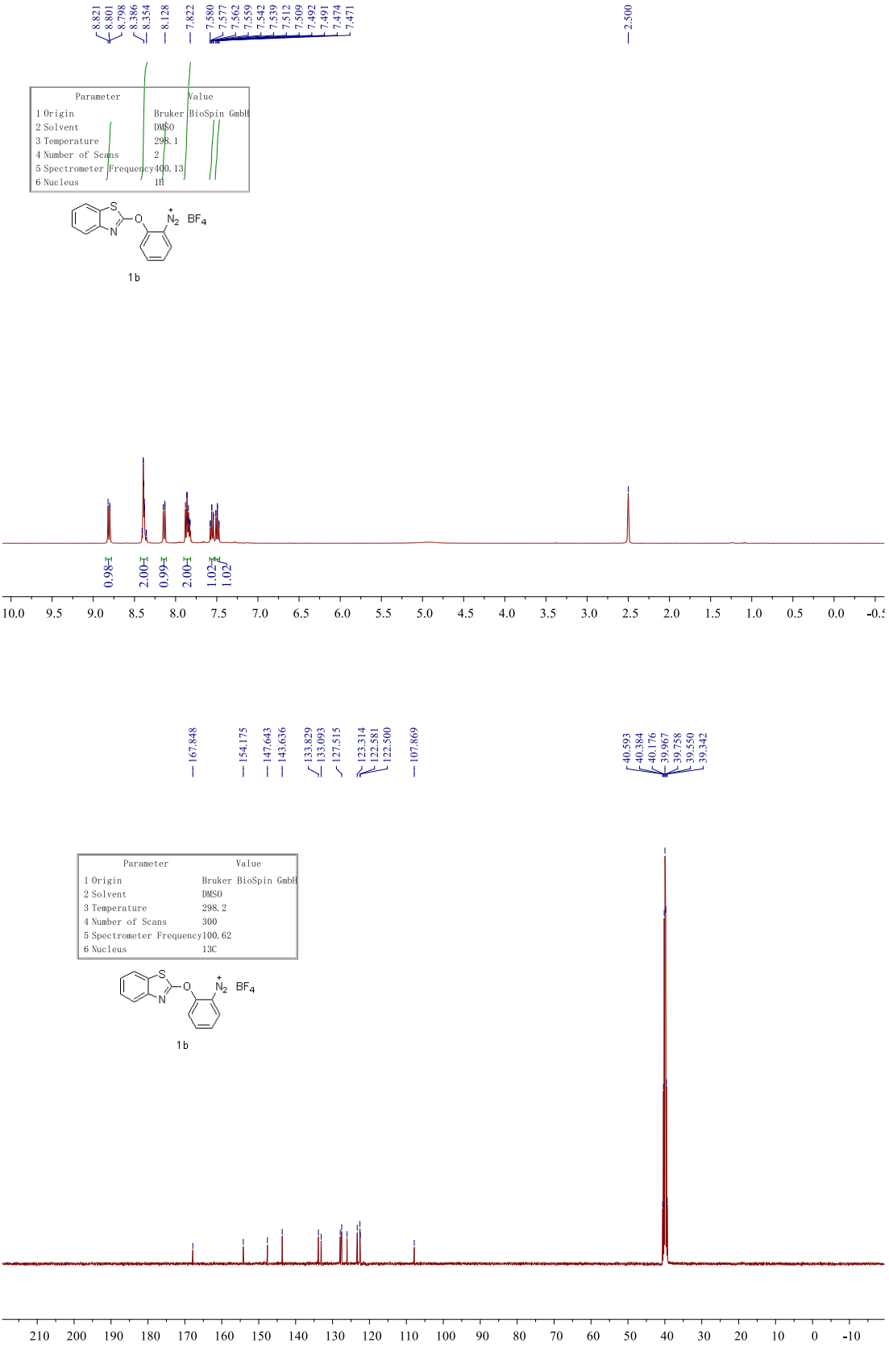
Fig. S12

14. ^{1}H, ^{13}C, and ^{19}F NMR Spectra





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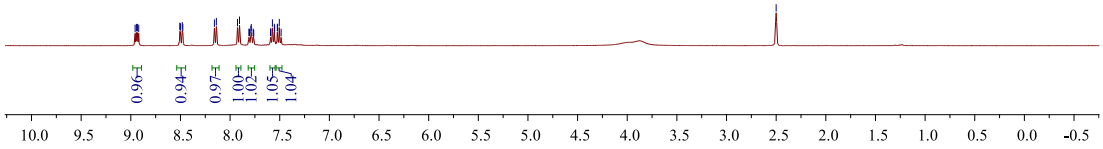
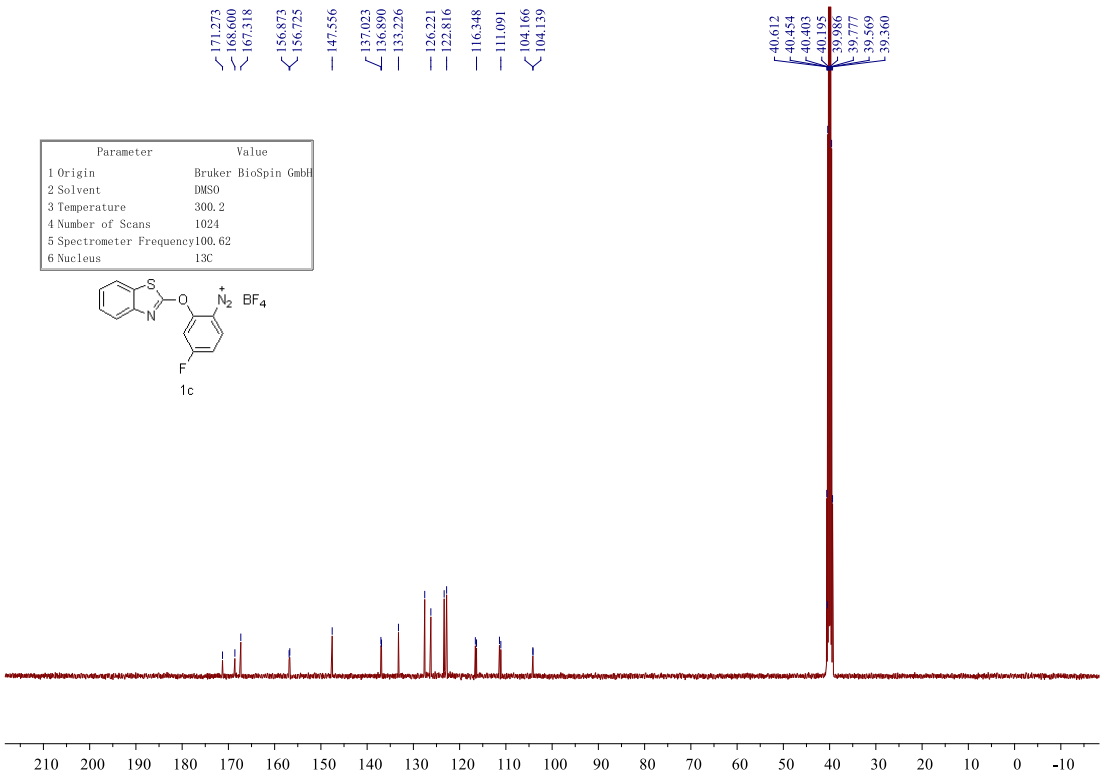
8.801
8.798
8.386
8.354
8.128
7.822
7.580
7.577
7.562
7.559
7.542
7.539
7.512
7.509
7.492
7.491
7.474
7.471
2.500
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
BF4
1b
0.98
2.00
0.99
2.00
1.02
1.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
167.848
154.175
147.643
143.636
133.829
133.093
127.515
123.314
122.581
122.500
107.869
40.593
40.384
40.176
39.967
39.758
39.550
39.342
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 298.2
4 Number of Scans 300
5 Spectrometer Frequency 100.62
6 Nucleus 13C
BF4
1b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10


8.957
8.944
8.933
8.920
8.501
8.476
8.158
8.138
7.805
7.762
7.593
7.590
7.574
7.554
7.551
7.524
7.522
7.504
7.486
2.500
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 300.2
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
S
O
N
N2 BF4
F
1c


0.96
0.94
0.97
1.00
1.02
1.05
1.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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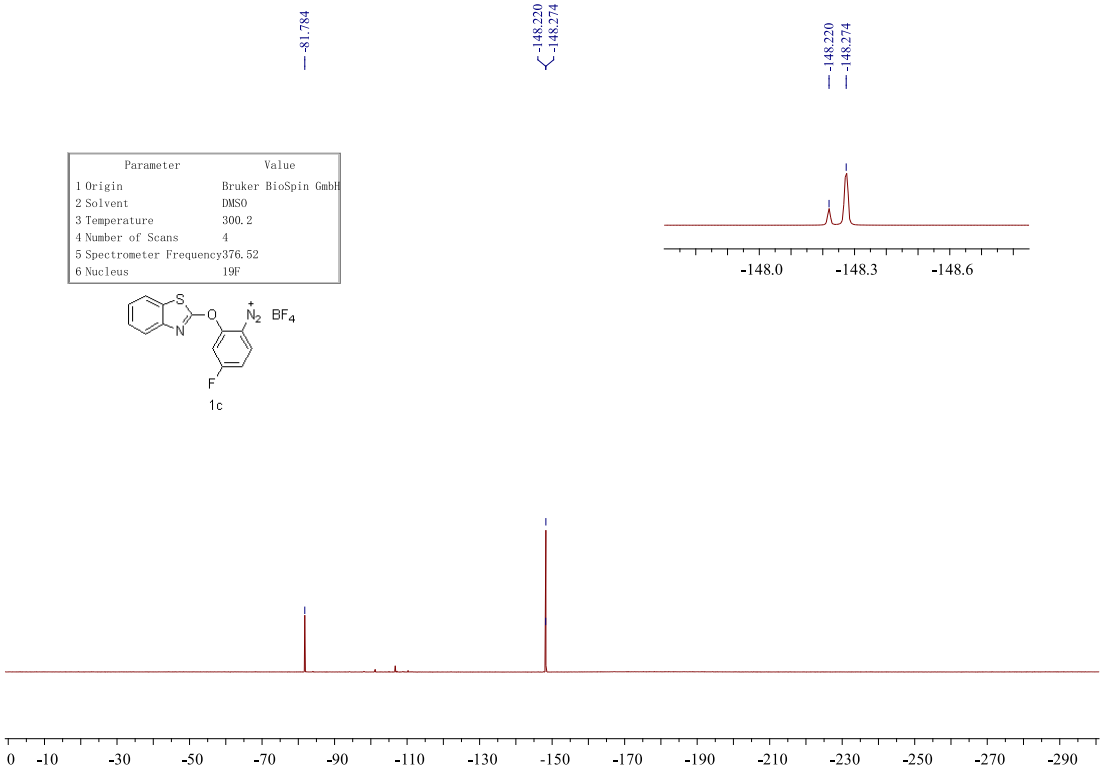
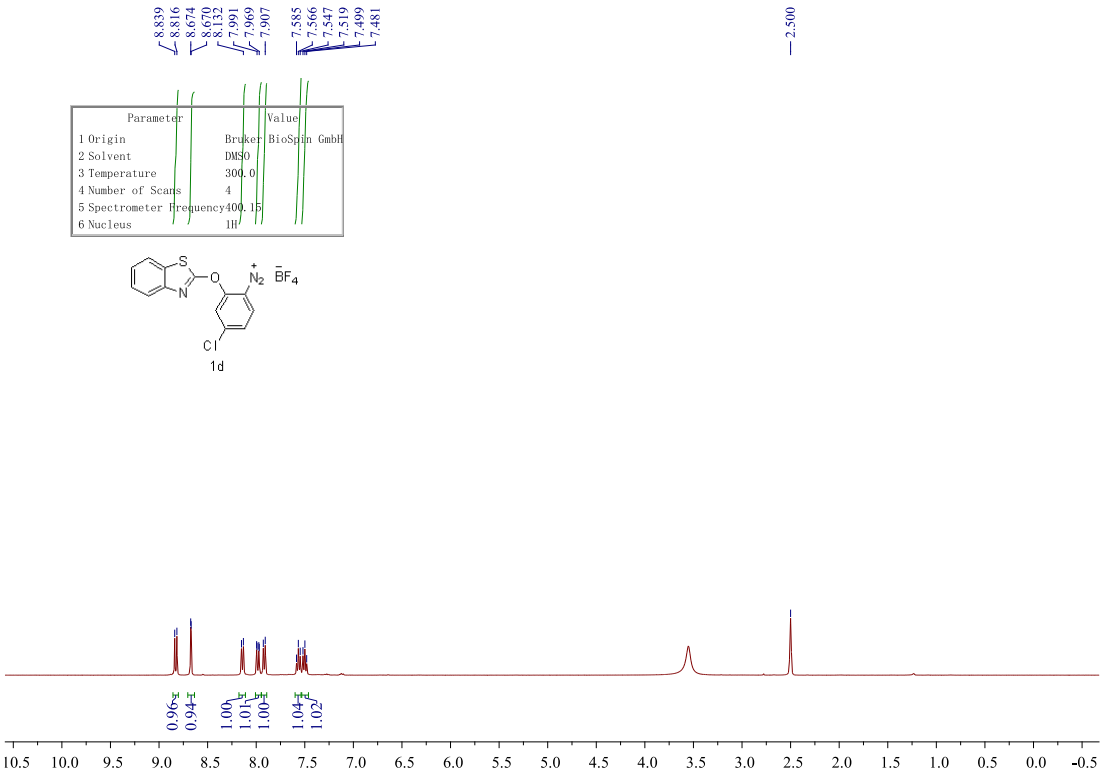
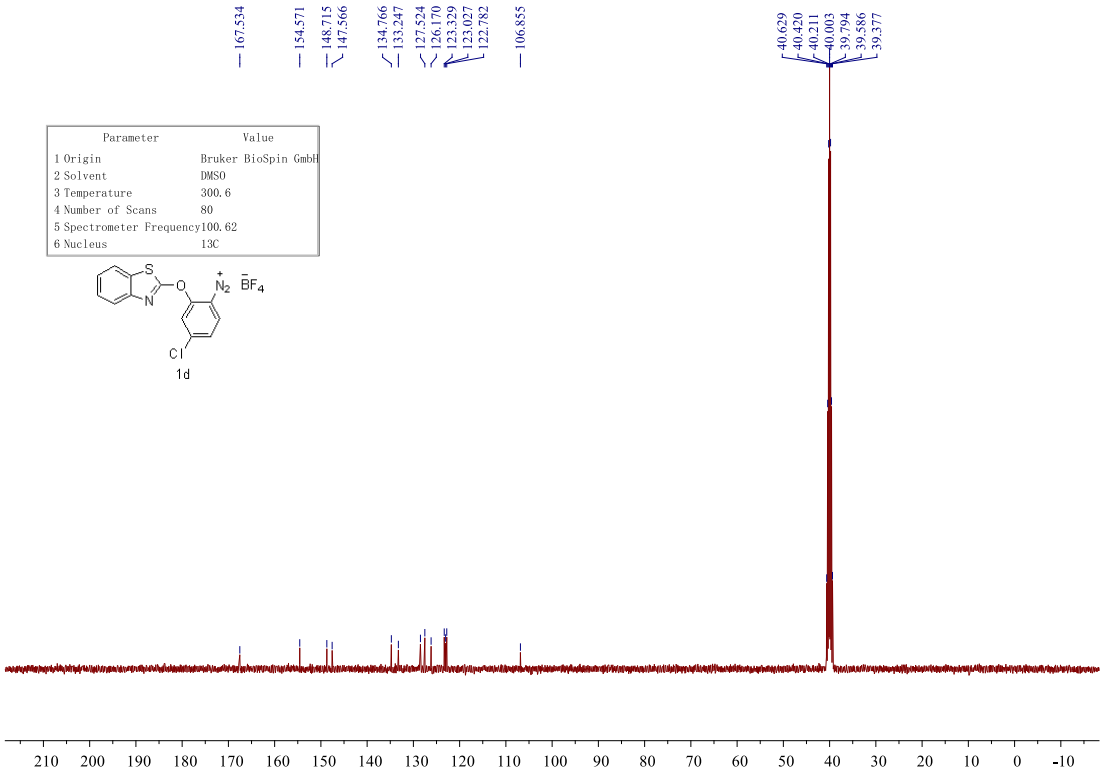
168.600
167.318
156.873
156.725
147.556
137.023
136.890
133.226
126.221
122.816
116.348
111.091
104.166
104.139
40.612
40.454
40.403
40.195
39.986
39.777
39.569
39.360
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 300.2
4 Number of Scans 1024
5 Spectrometer Frequency 100.62
6 Nucleus 13C
S
O
N
N2 BF4
F
1c
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10


-81.784
-148.220
-148.274
-148.220
-148.274
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 300.2
4 Number of Scans 4
5 Spectrometer Frequency 376.52
6 Nucleus 19F
-148.0
-148.3
-148.6
0 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290

1c


8.839
8.816
8.674
8.670
8.132
7.991
7.969
7.907
7.585
7.566
7.547
7.519
7.499
7.481
2.500
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 300.0
4 Number of Scans 4
5 Spectrometer Frequency 400.15
6 Nucleus 1H
0.96
0.94
1.00
1.01
1.00
1.04
1.02
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

1d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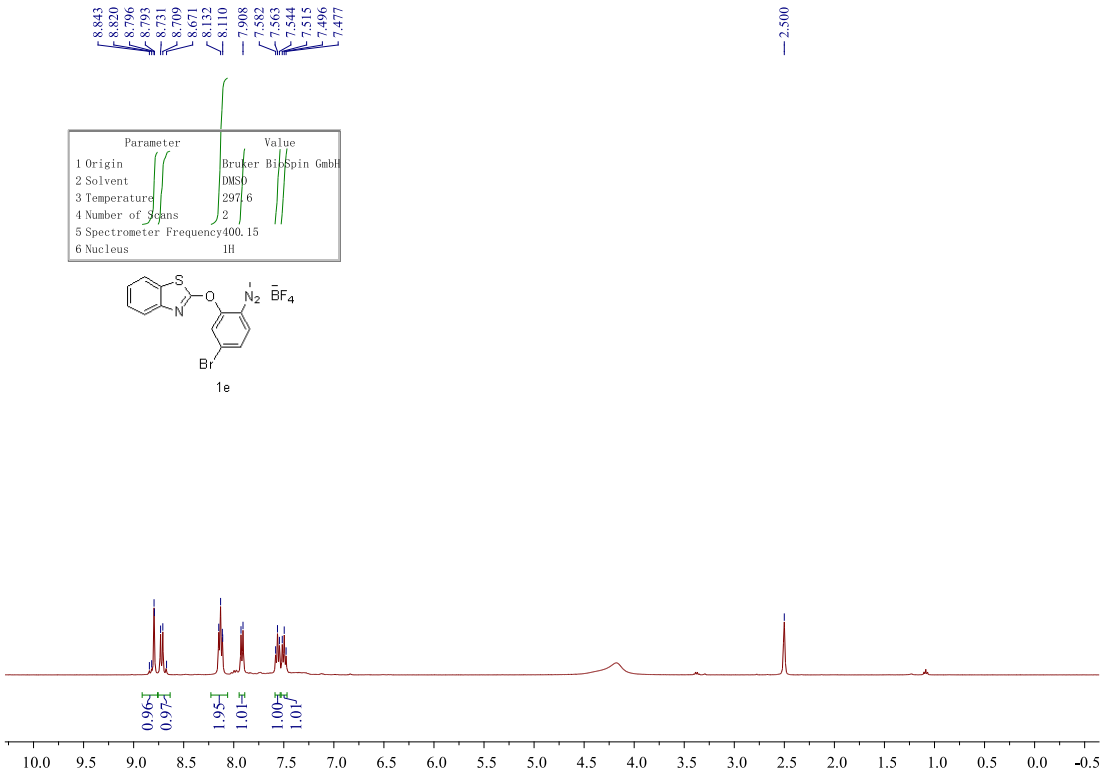
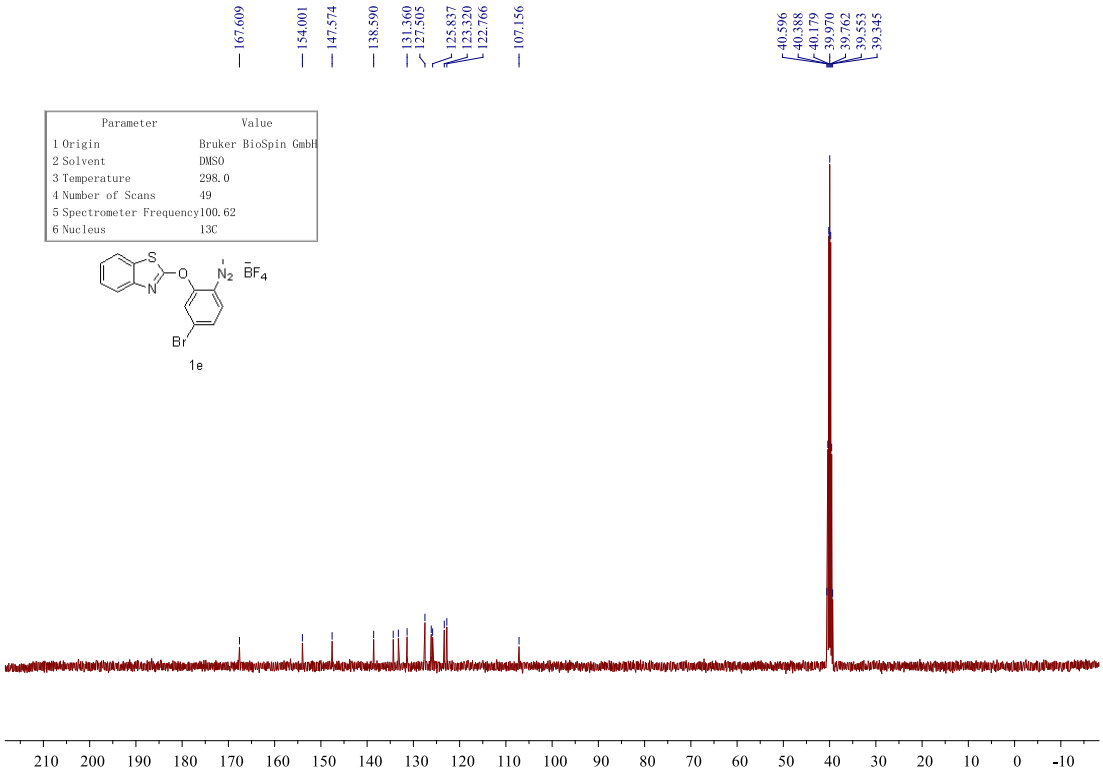
154.571
148.715
147.566
134.766
133.247
127.524
126.170
123.329
123.027
122.782
106.855
40.629
40.420
40.211
40.003
39.794
39.586
39.377
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 300.6
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
1d


8.843
8.820
8.796
8.793
8.731
8.709
8.671
8.132
8.110
7.908
7.582
7.563
7.544
7.515
7.496
7.477
2.500
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 297.6
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
1e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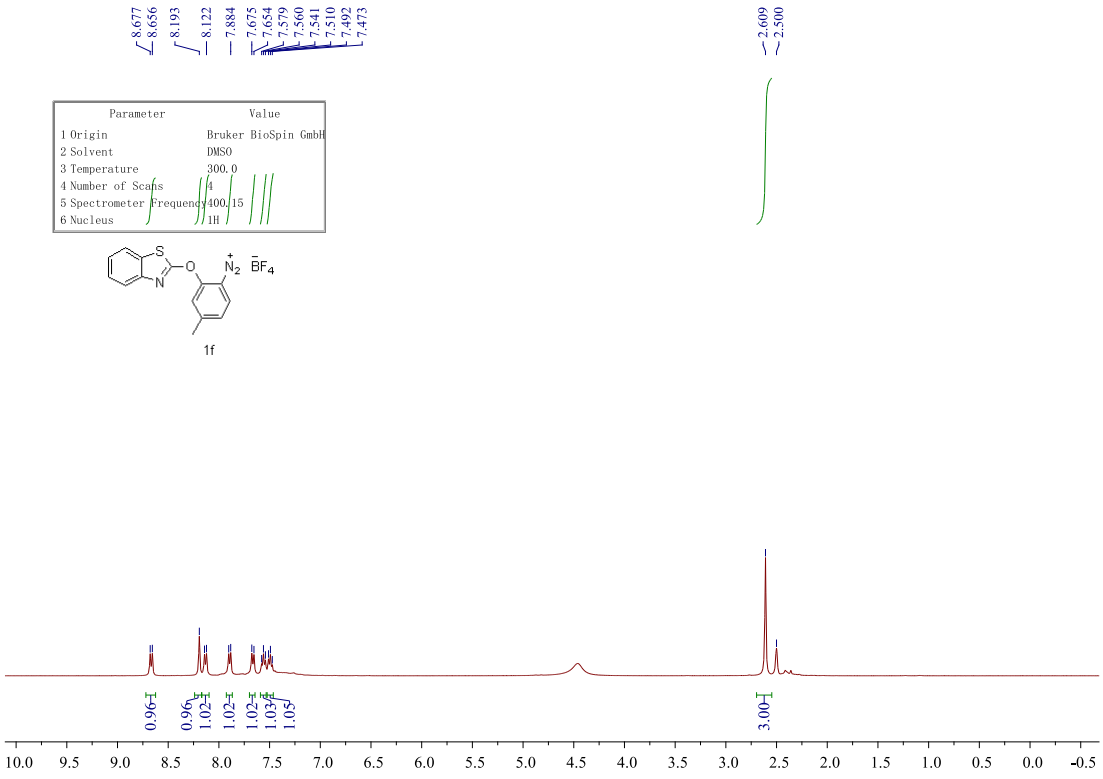
154.001
147.574
138.590
131.360
127.505
125.837
123.320
122.766
107.156
40.596
40.388
40.179
39.970
39.762
39.553
39.345
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 298.0
4 Number of Scans 49
5 Spectrometer Frequency 100.62
6 Nucleus 13C
1e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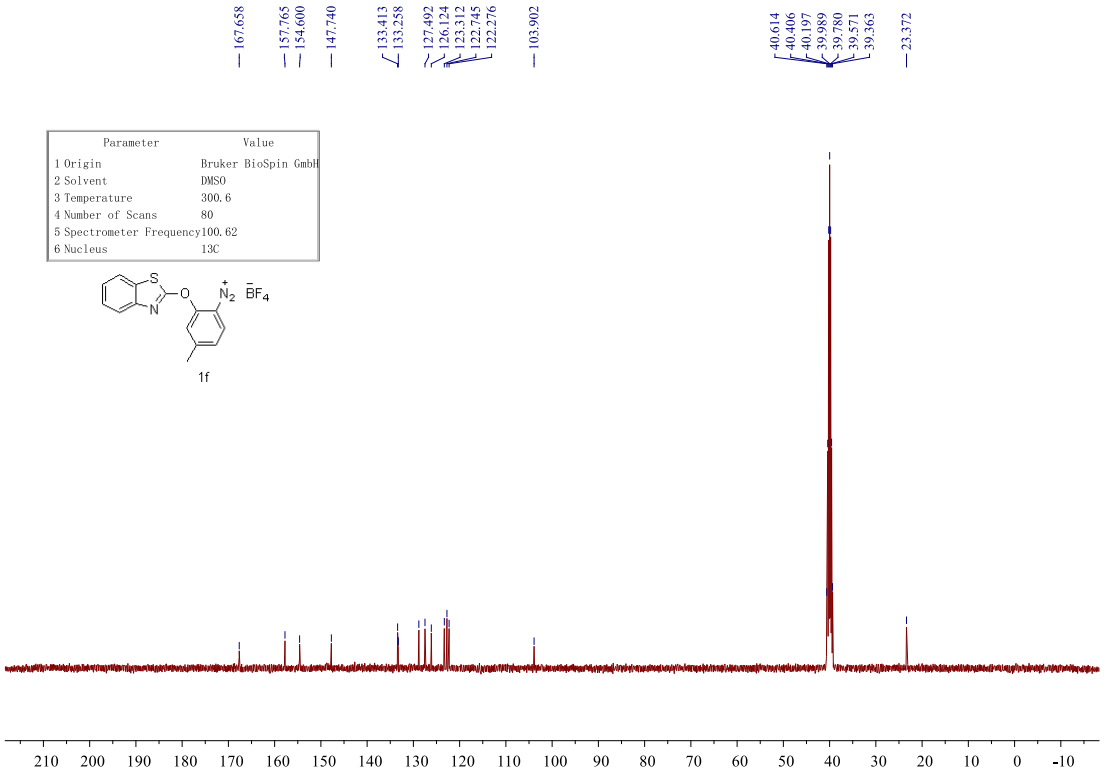
8.656
8.193
8.122
7.884
7.675
7.654
7.579
7.560
7.541
7.510
7.492
7.473
2.609
2.500
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 300.0
4 Number of Scans 4
5 Spectrometer Frequency 400.15
6 Nucleus 1H
1f
0.96
0.96
1.02
1.02
1.02
1.03
1.05
3.00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147.740
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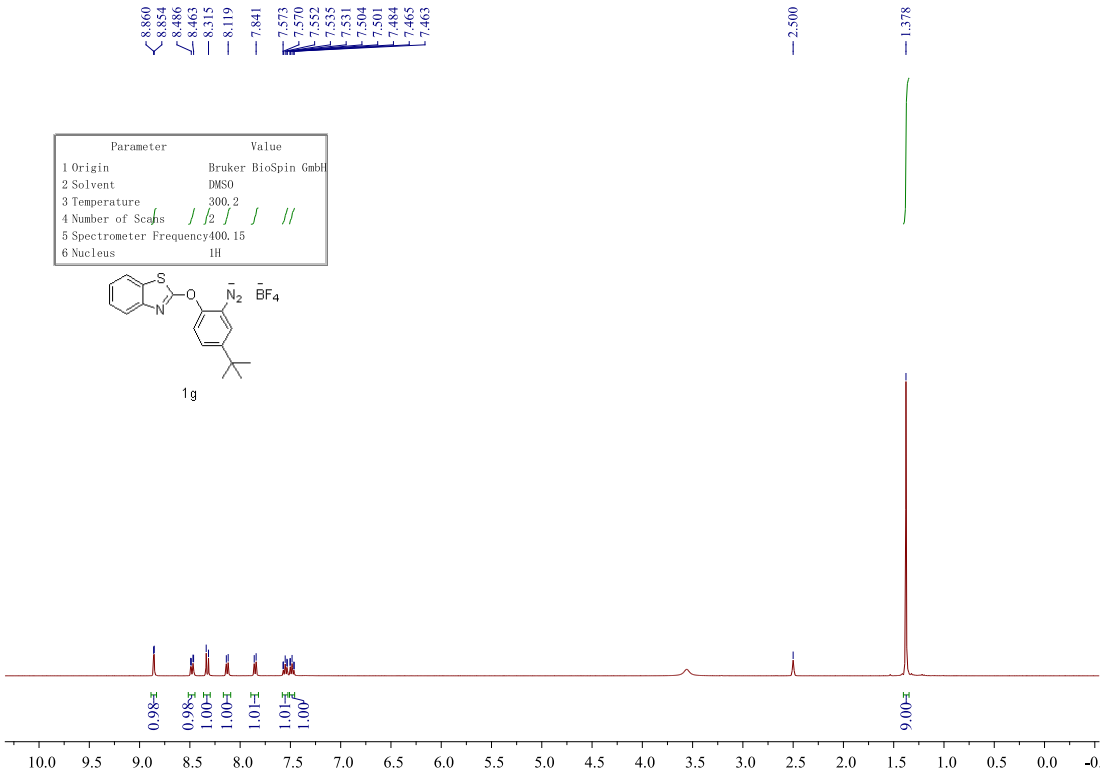
133.258
127.492
126.124
123.312
122.745
122.276
103.902
40.614
40.406
40.197
39.989
39.780
39.571
39.363
23.372
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 300.6
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
1f
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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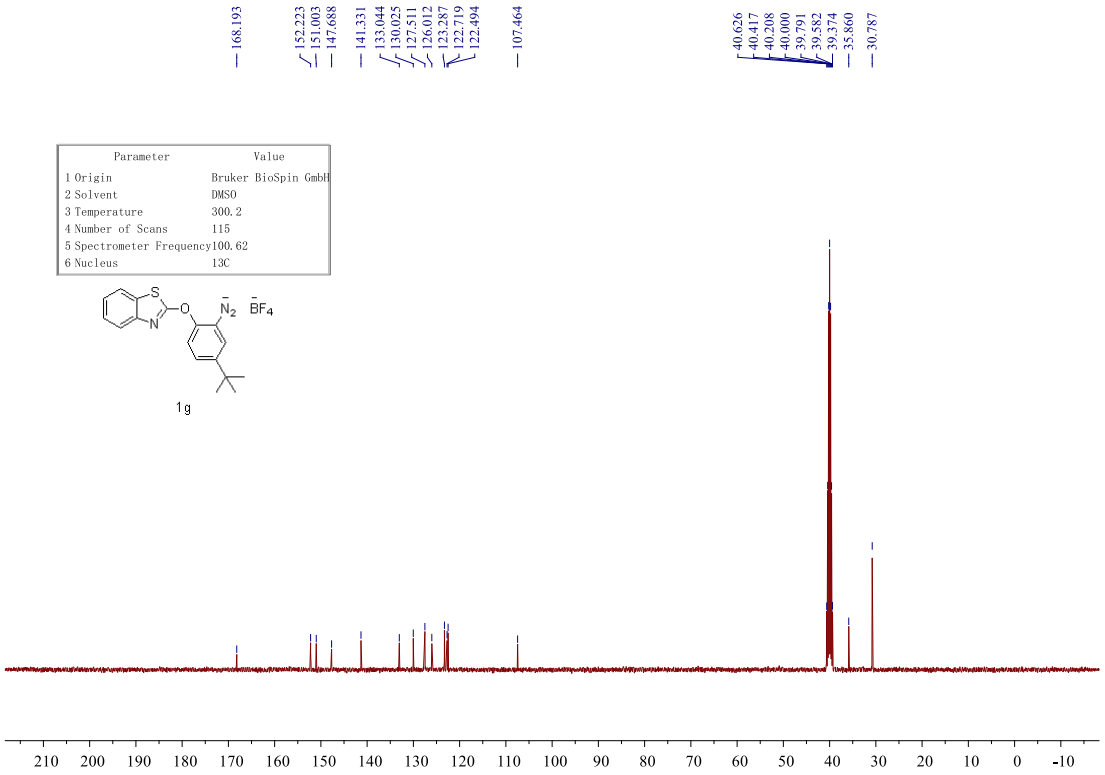
8.854
8.486
8.463
8.315
8.119
7.841
7.573
7.570
7.552
7.535
7.531
7.504
7.501
7.484
7.465
7.463
2.500
1.378
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 300.2
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
1g
0.98
0.98
1.00
1.00
1.01
1.01
1.00
9.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0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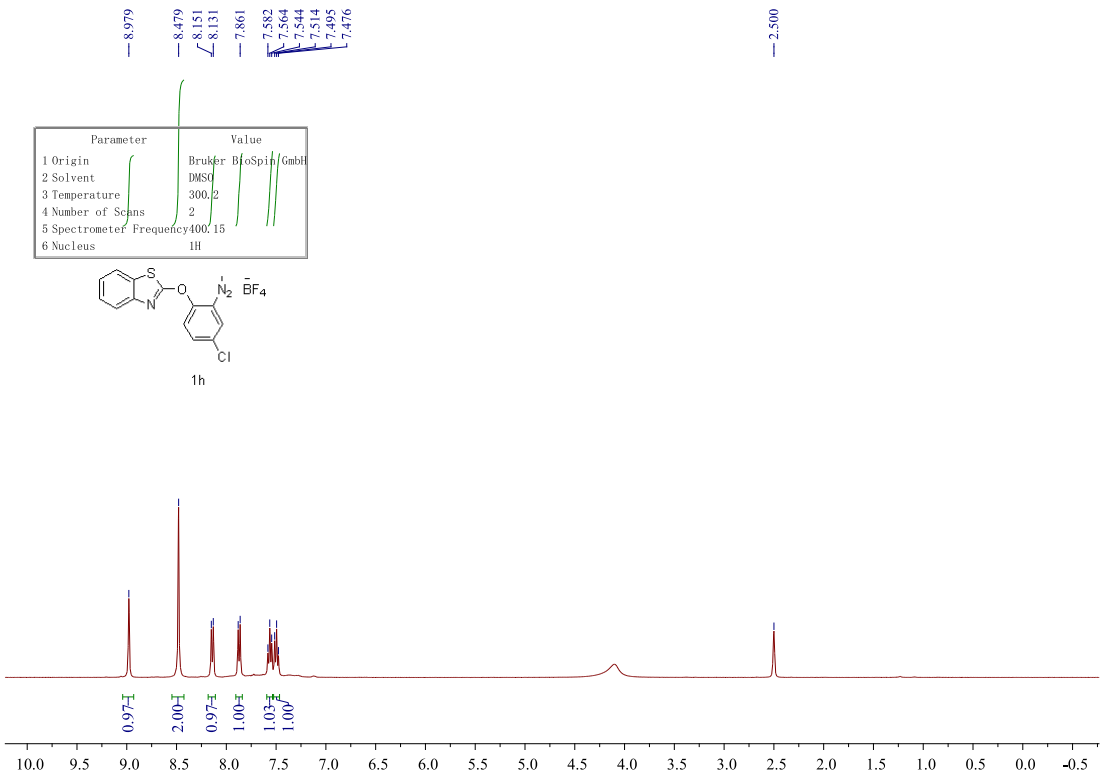
152.223
151.003
147.688
141.331
133.044
130.025
127.511
126.012
123.287
122.719
122.494
107.464
40.626
40.417
40.208
40.000
39.791
39.582
39.374
35.860
30.787
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 300.2
4 Number of Scans 115
5 Spectrometer Frequency 100.62
6 Nucleus 13C
1g
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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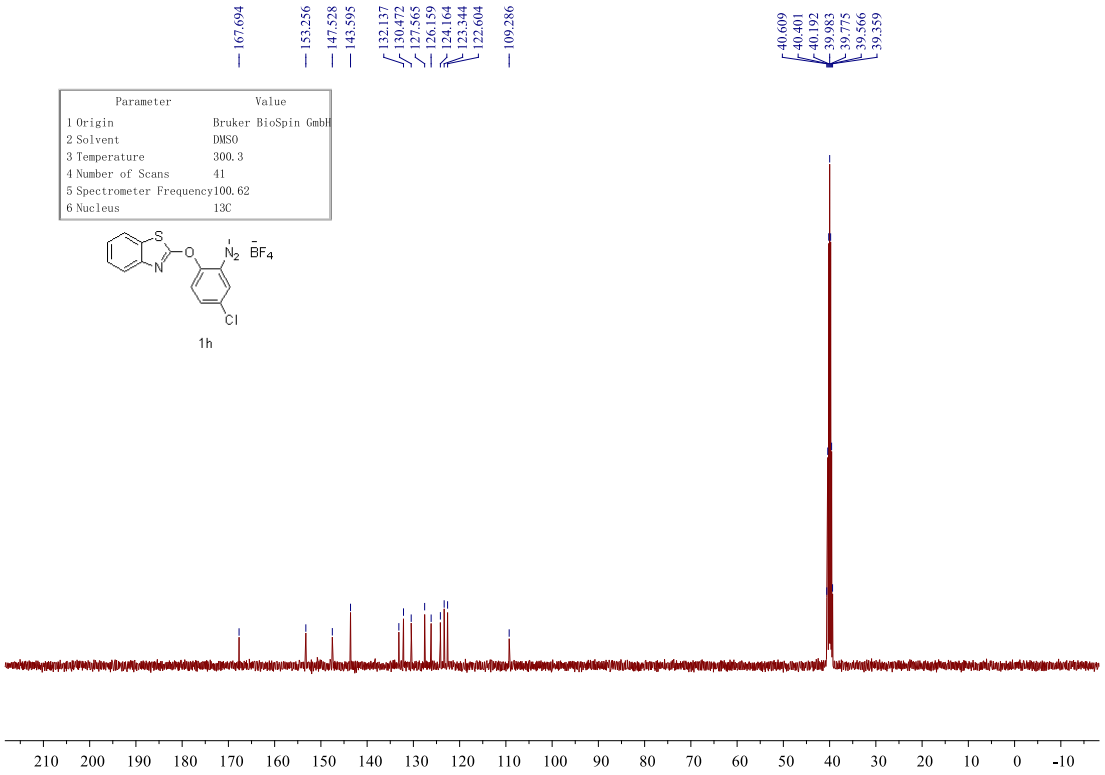
8.151
8.131
7.861
7.582
7.564
7.544
7.514
7.495
7.476
2.500
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 300.2
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
1h
0.97
2.00
0.97
1.00
1.03
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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143.595
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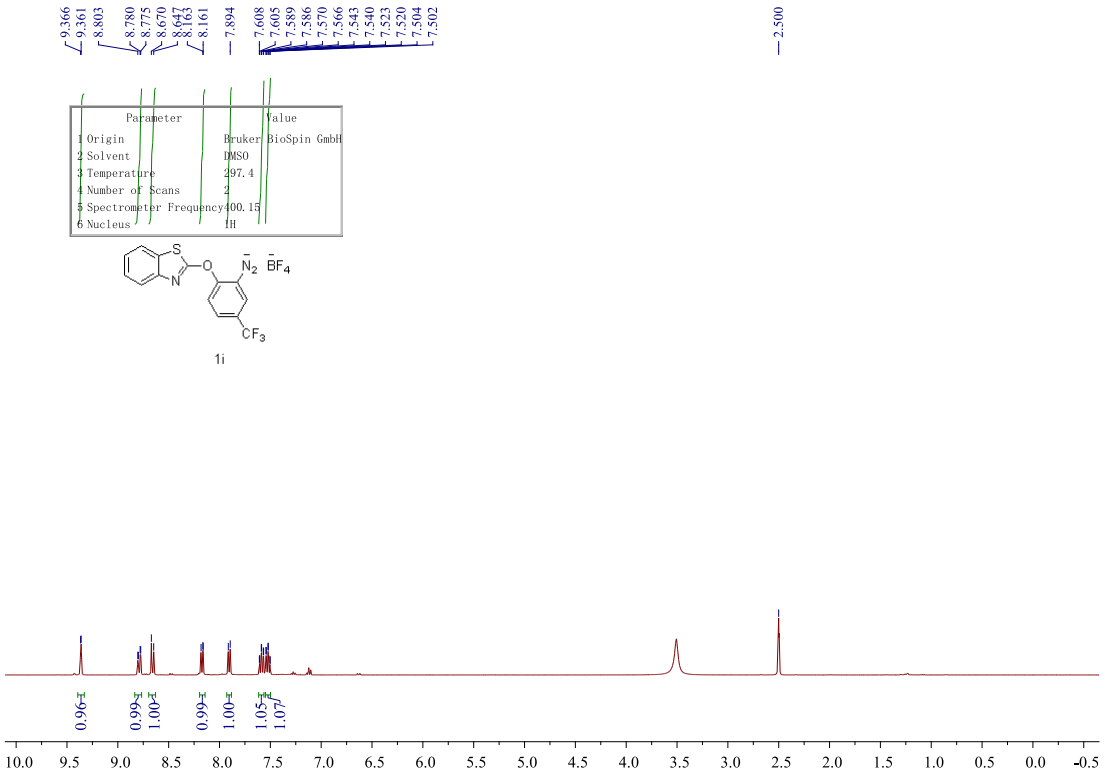
130.472
127.565
126.159
124.164
123.344
122.604
109.286
40.609
40.401
40.192
39.983
39.775
39.566
39.359
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 300.3
4 Number of Scans 41
5 Spectrometer Frequency 100.62
6 Nucleus 13C
S
O
N
N2
BF4
Cl
1h
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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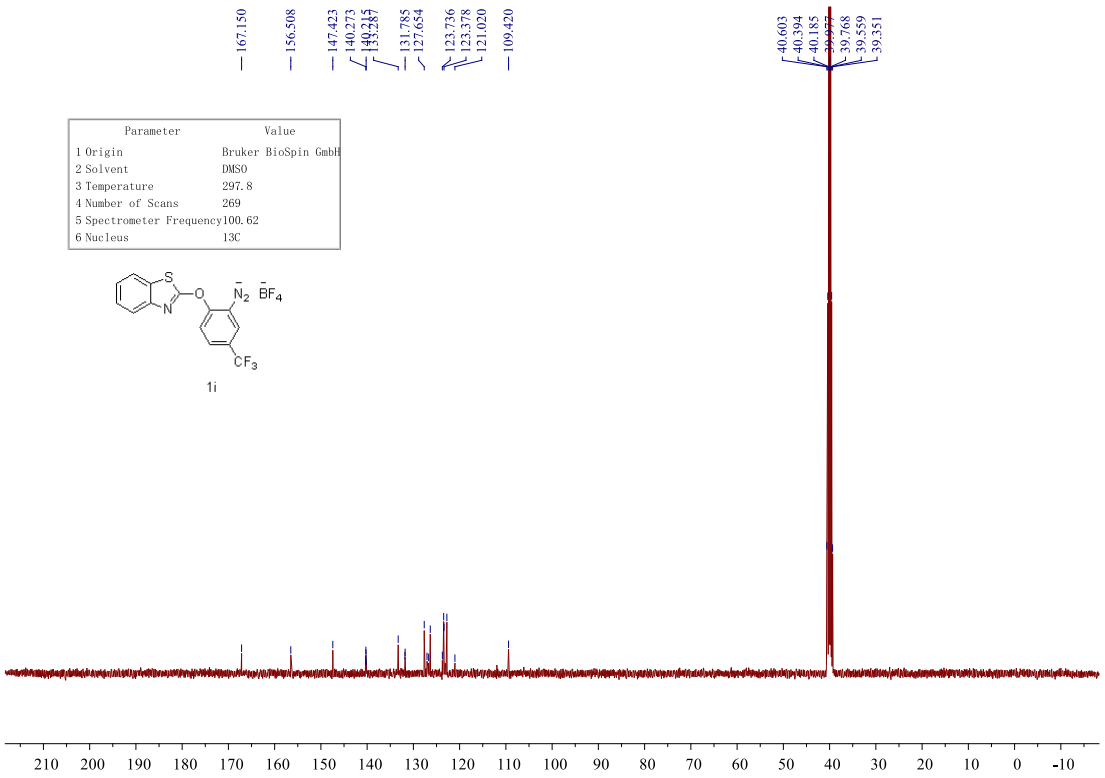
8.780
8.775
8.670
8.647
8.163
8.161
7.894
7.608
7.605
7.589
7.586
7.570
7.566
7.543
7.540
7.523
7.520
7.504
7.502
2.500
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 297.4
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
S
O
N
N2
BF4
CF3
1i
0.96
0.99
1.00
0.99
1.00
1.05
1.07
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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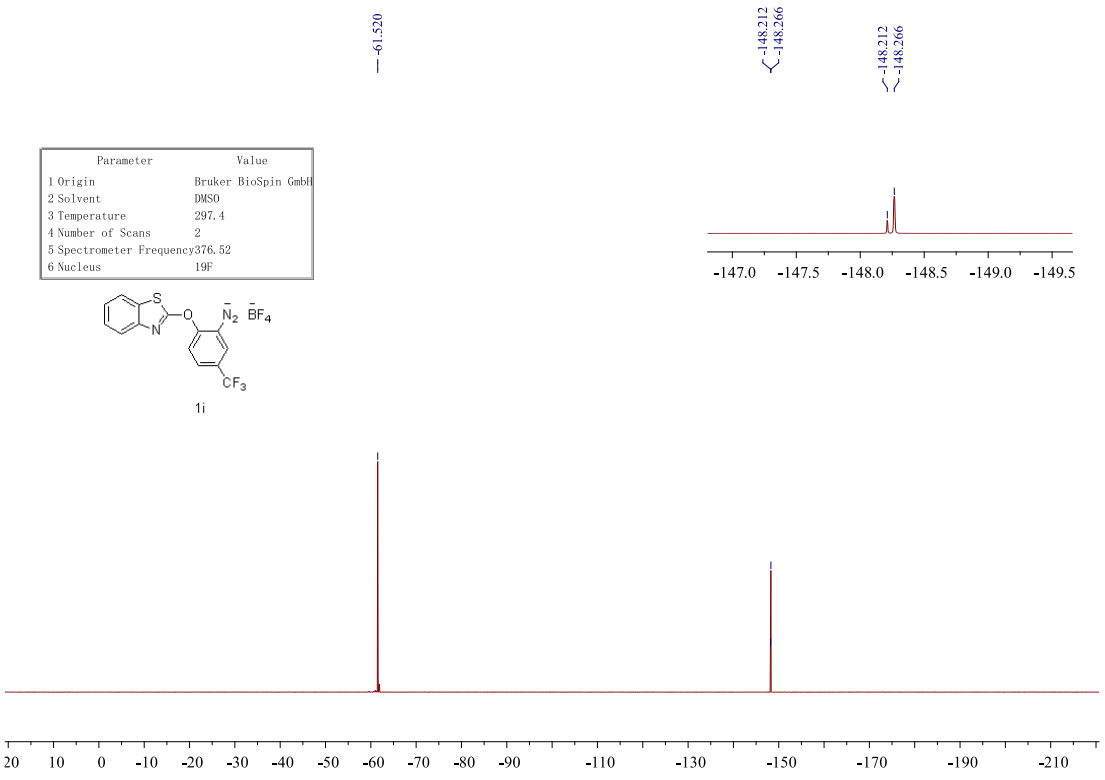
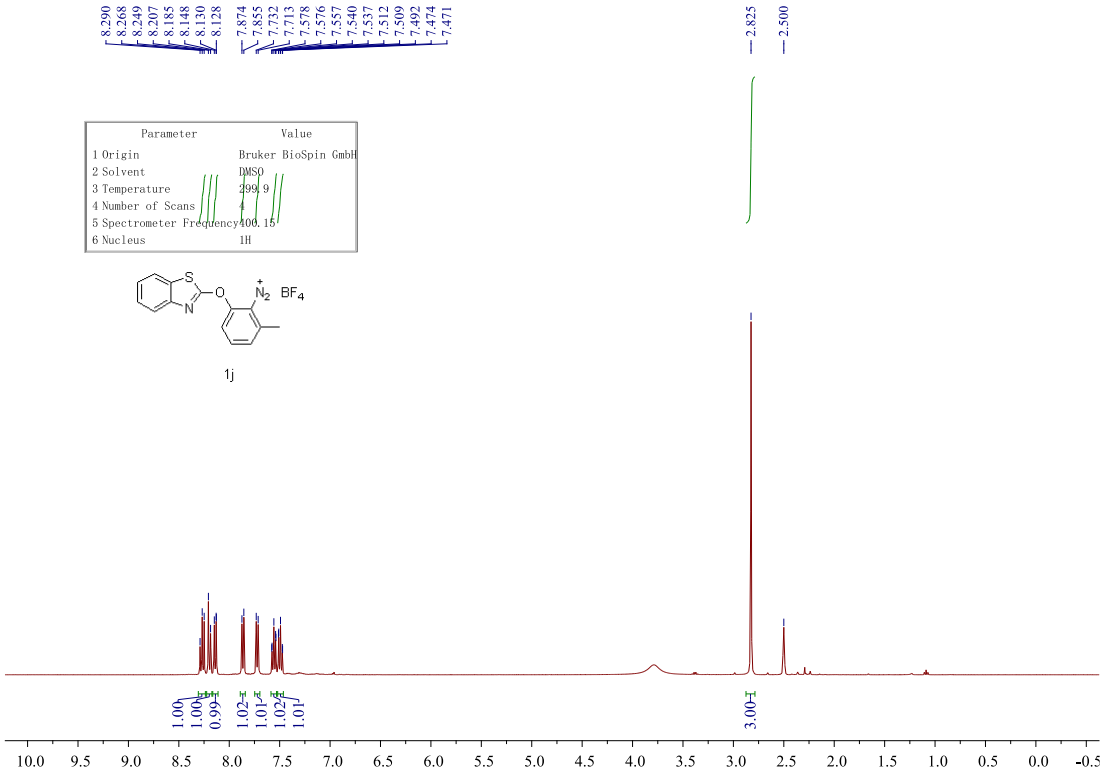
147.423
140.273
140.215
139.287
131.785
127.654
123.736
123.378
121.020
109.420
40.603
40.394
40.185
39.977
39.768
39.559
39.351
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 297.8
4 Number of Scans 269
5 Spectrometer Frequency 100.62
6 Nucleus 13C
1i


-61.520
-148.212
-148.266
-148.212
-148.266
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 297.4
4 Number of Scans 2
5 Spectrometer Frequency 376.52
6 Nucleus 19F
1i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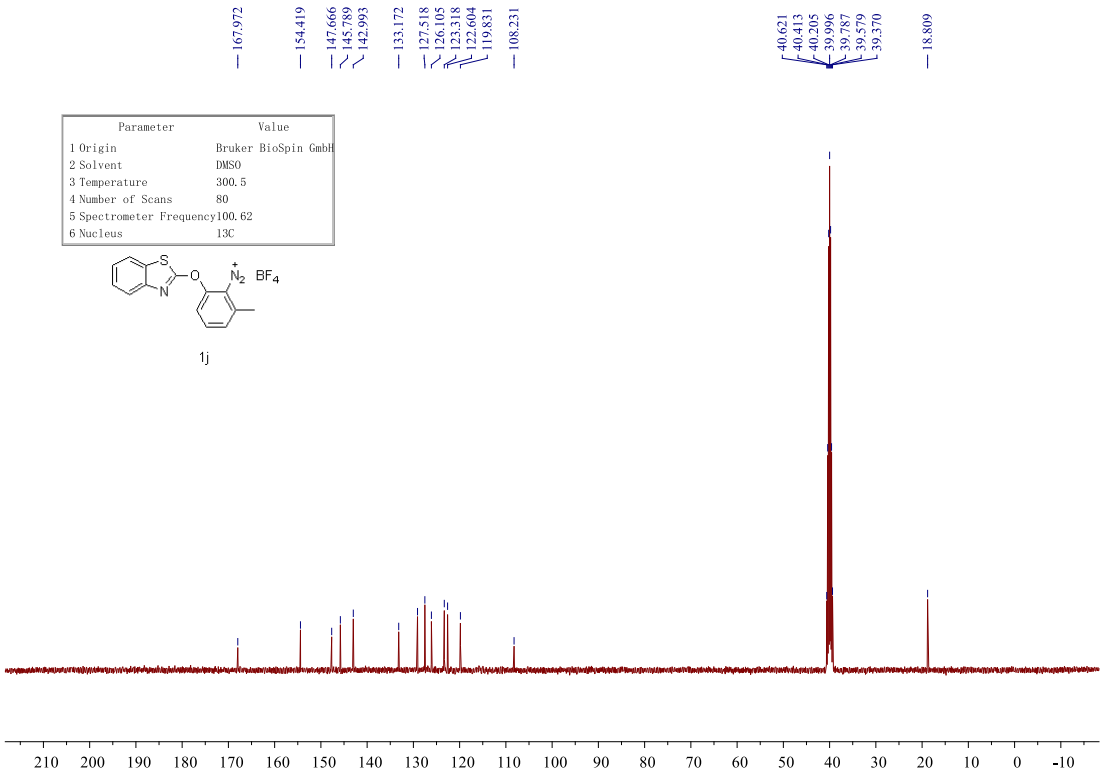
8.148
8.130
8.128
7.874
7.855
7.732
7.713
7.578
7.576
7.557
7.540
7.537
7.512
7.509
7.492
7.474
7.471
2.825
2.500
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 299.9
4 Number of Scans 4
5 Spectrometer Frequency 400.15
6 Nucleus 1H
1j
1.00
1.00
0.99
1.02
1.01
1.02
1.01
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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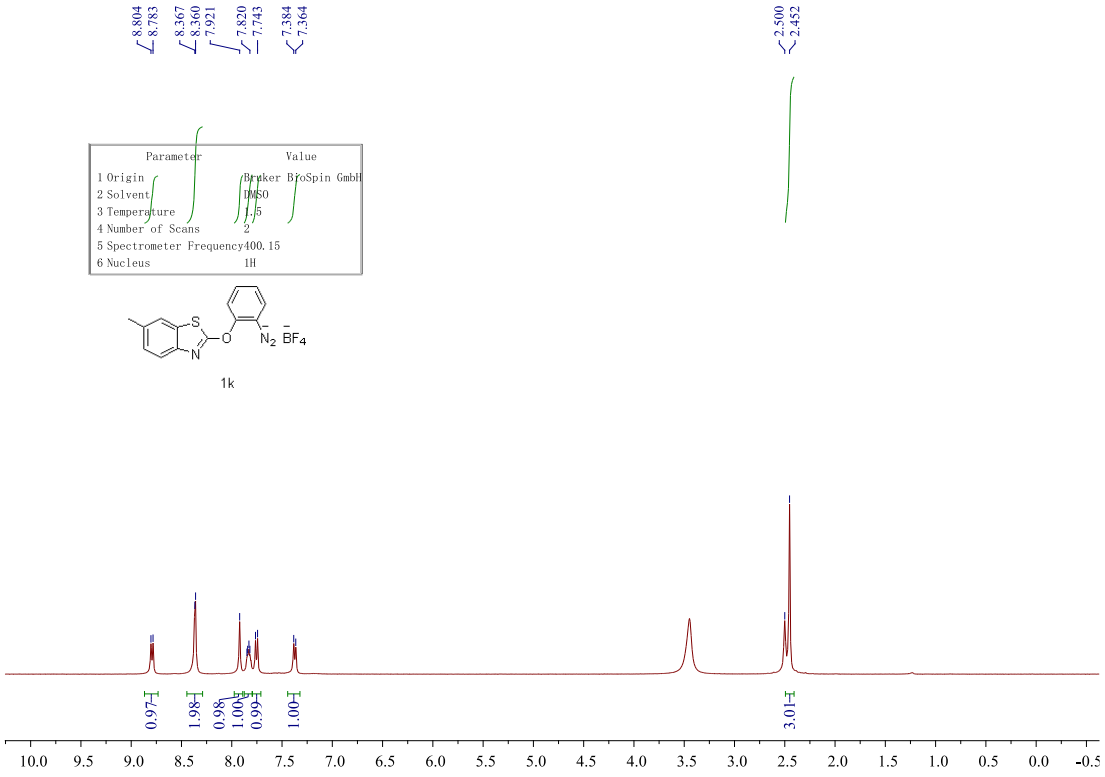
133.172
127.518
126.105
123.318
122.604
119.831
108.231
40.621
40.413
40.205
39.996
39.787
39.579
39.370
18.809
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 300.5
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
1j
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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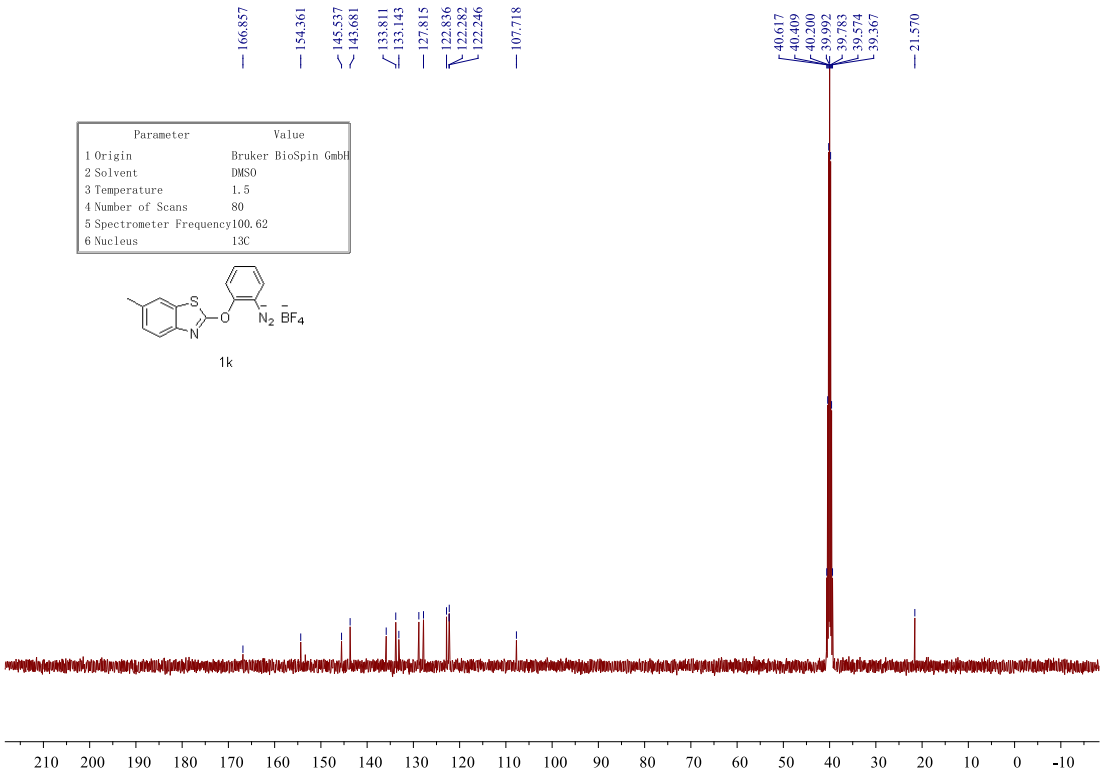
8.783
8.367
8.360
7.921
7.820
7.743
7.384
7.364
2.500
2.452
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 1.5
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
1k
0.97
1.98
0.98
1.00
0.99
1.00
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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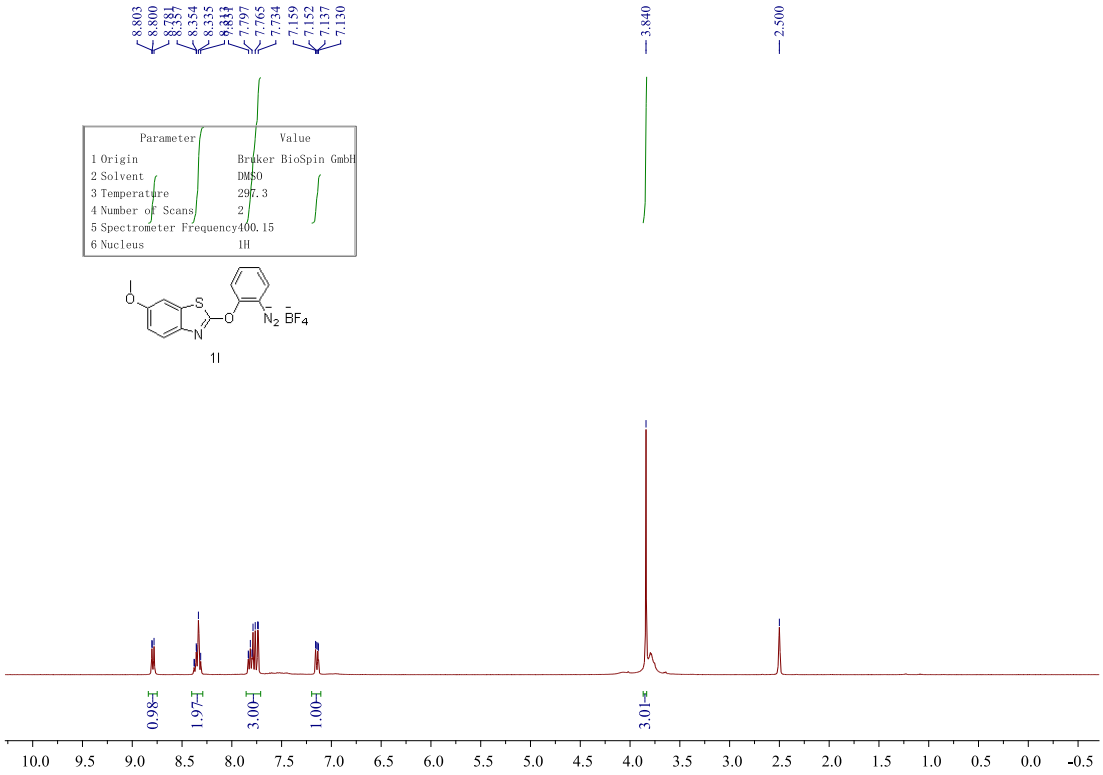
145.537
143.681
133.811
133.143
127.815
122.836
122.282
122.246
107.718
40.617
40.409
40.200
39.992
39.783
39.574
39.367
21.570
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 1.5
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
1k
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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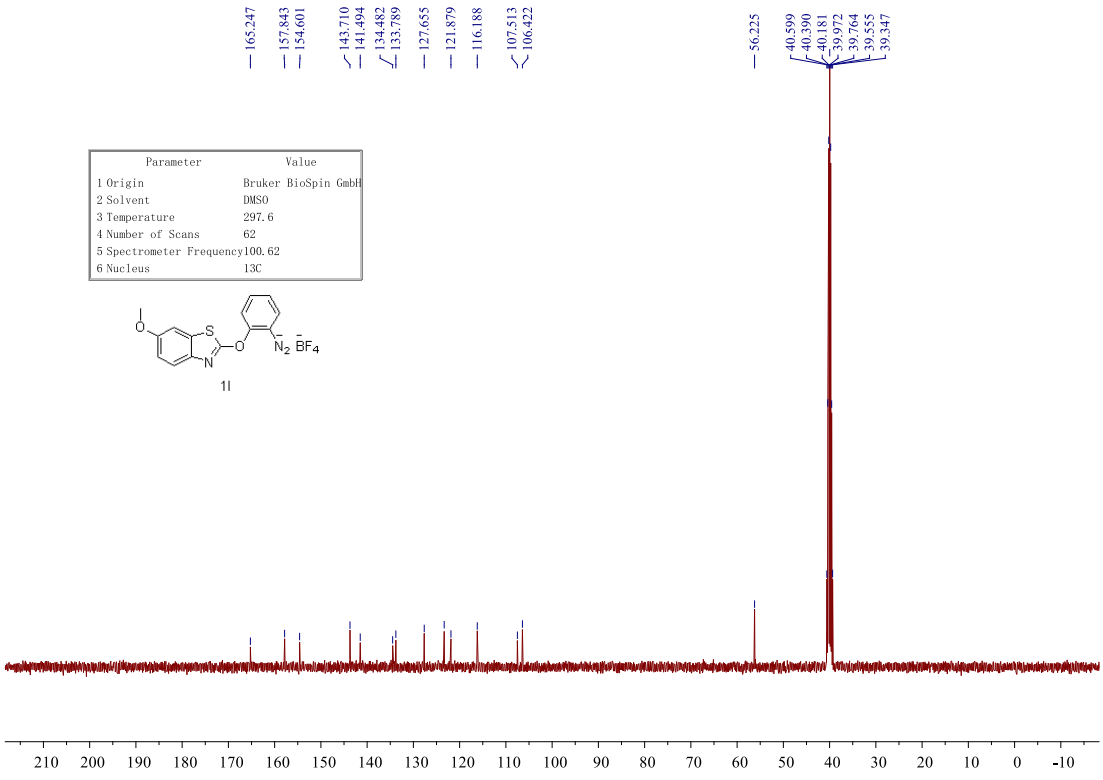
8.800
8.781
8.357
8.354
8.335
7.797
7.765
7.734
7.159
7.152
7.137
7.130
3.840
2.500
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 297.3
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
1l
0.98
1.97
3.00
1.00
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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154.601
143.710
141.494
134.482
133.789
127.655
121.879
116.188
107.513
106.422
56.225
40.599
40.390
40.181
39.972
39.764
39.555
39.347
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 297.6
4 Number of Scans 62
5 Spectrometer Frequency 100.62
6 Nucleus 13C
1l
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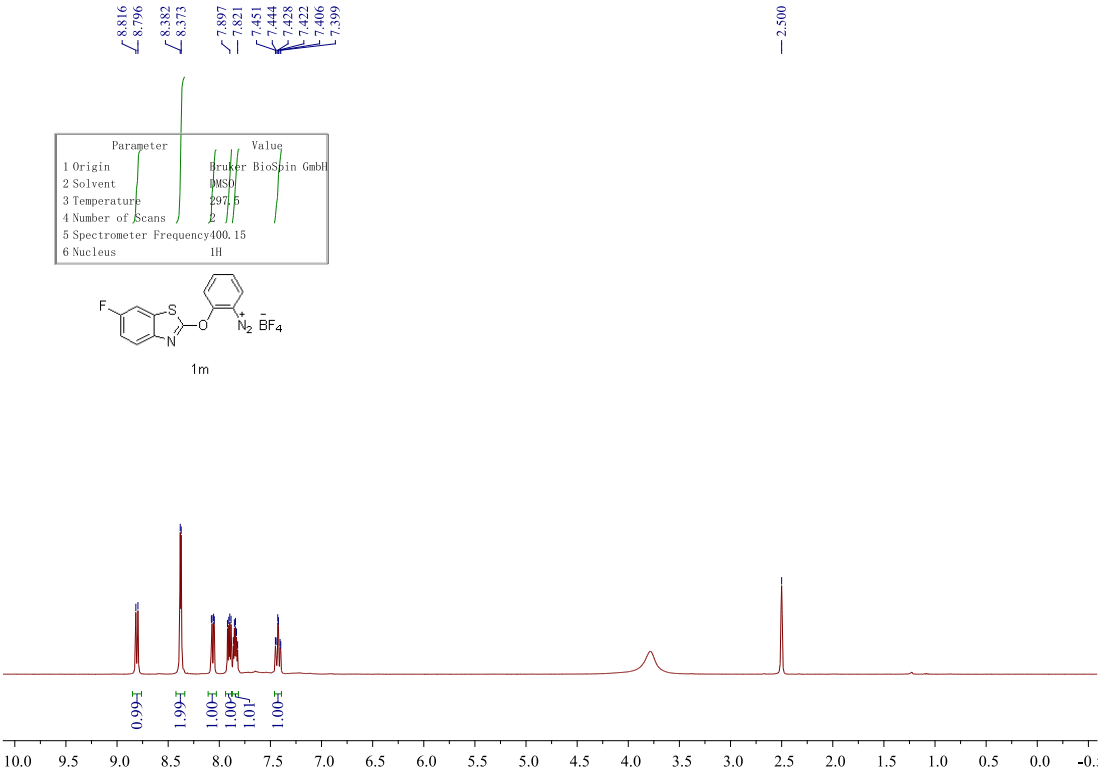
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7.444
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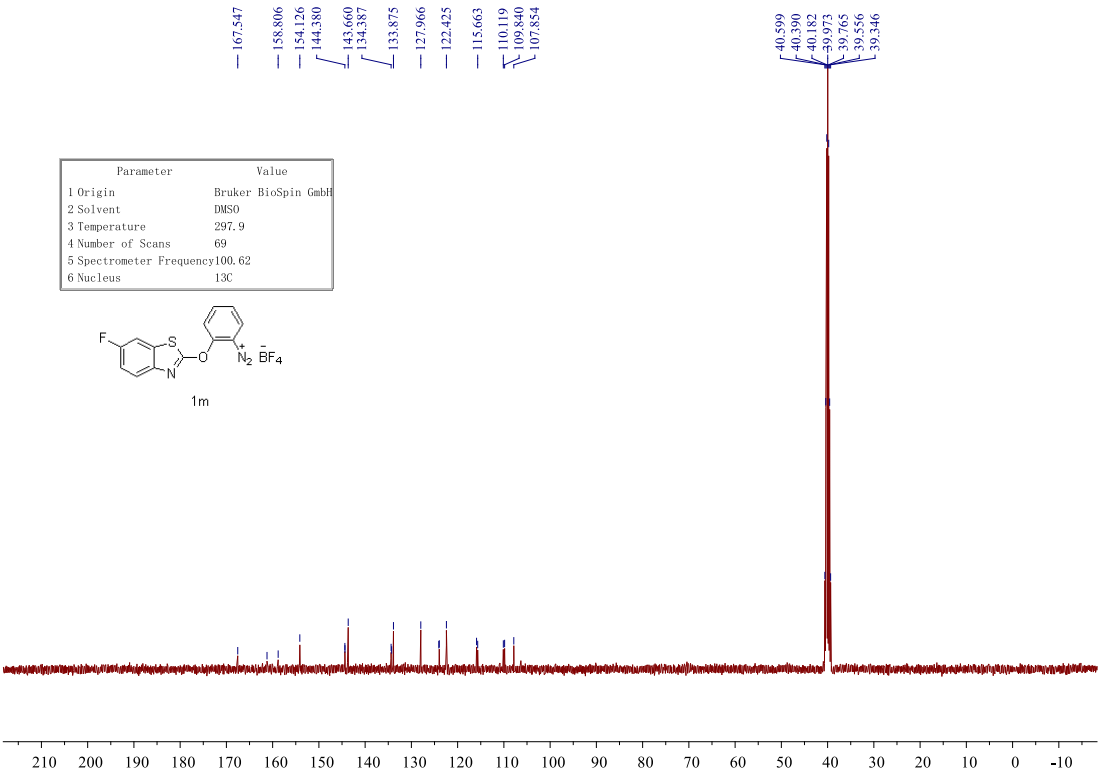
7.422
7.406
7.399
2.500
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 297.5
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
F
S
N
O
N2
BF4
1m
0.99
1.99
1.00
1.00
1.01
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0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115.663
110.119
109.840
107.854
40.599
40.390
40.182
39.973
39.765
39.556
39.346
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 297.9
4 Number of Scans 69
5 Spectrometer Frequency 100.62
6 Nucleus 13C
F
S
N
O
N2
BF4
1m
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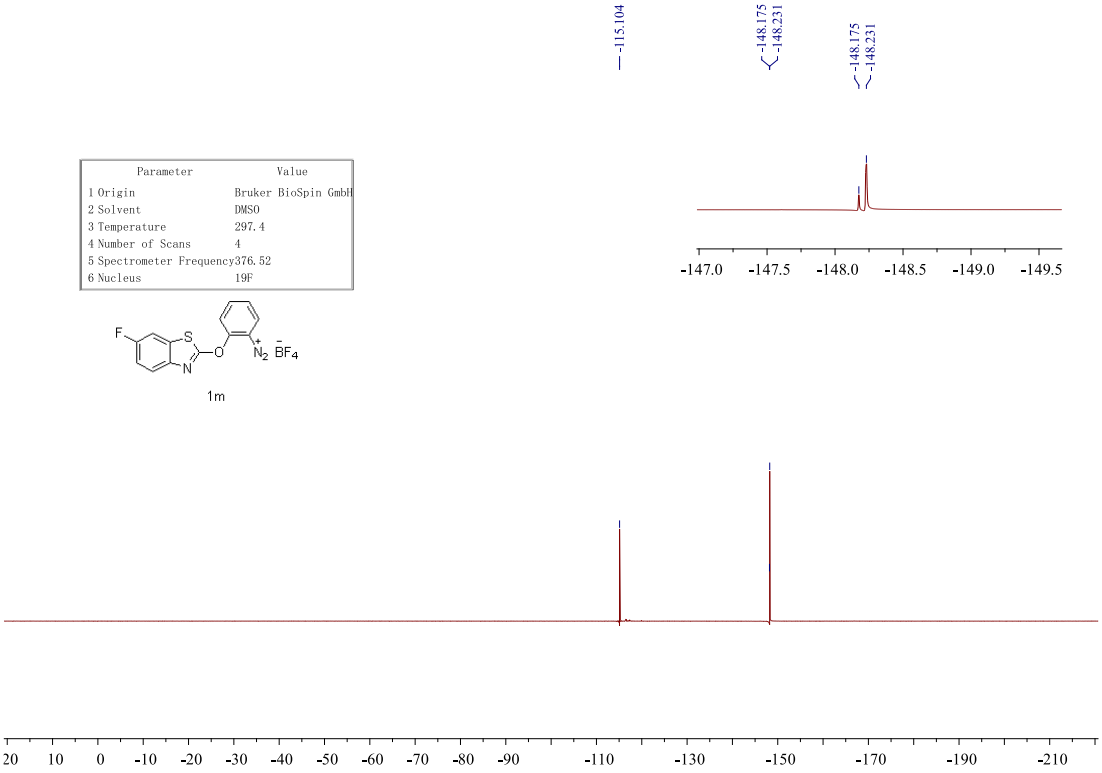
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-148.175
-148.231
-148.175
-148.231
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 297.4
4 Number of Scans 4
5 Spectrometer Frequency 376.52
6 Nucleus 19F
F
S
O
N
N2 BF4
1m
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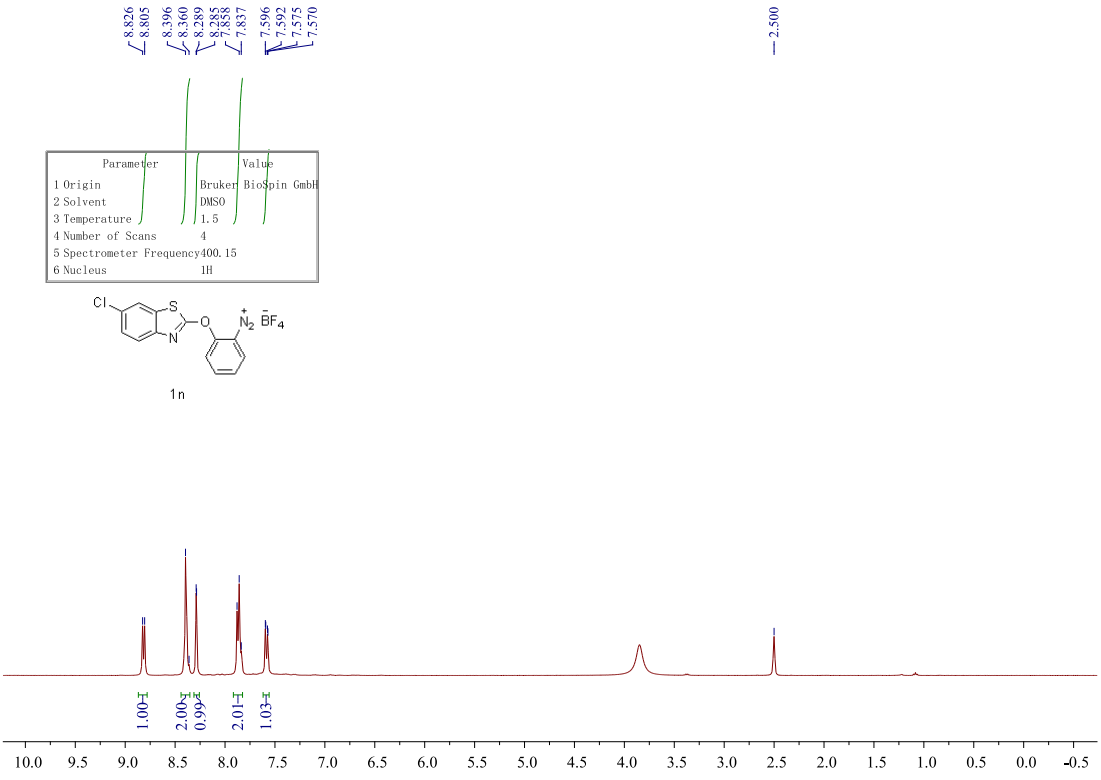
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210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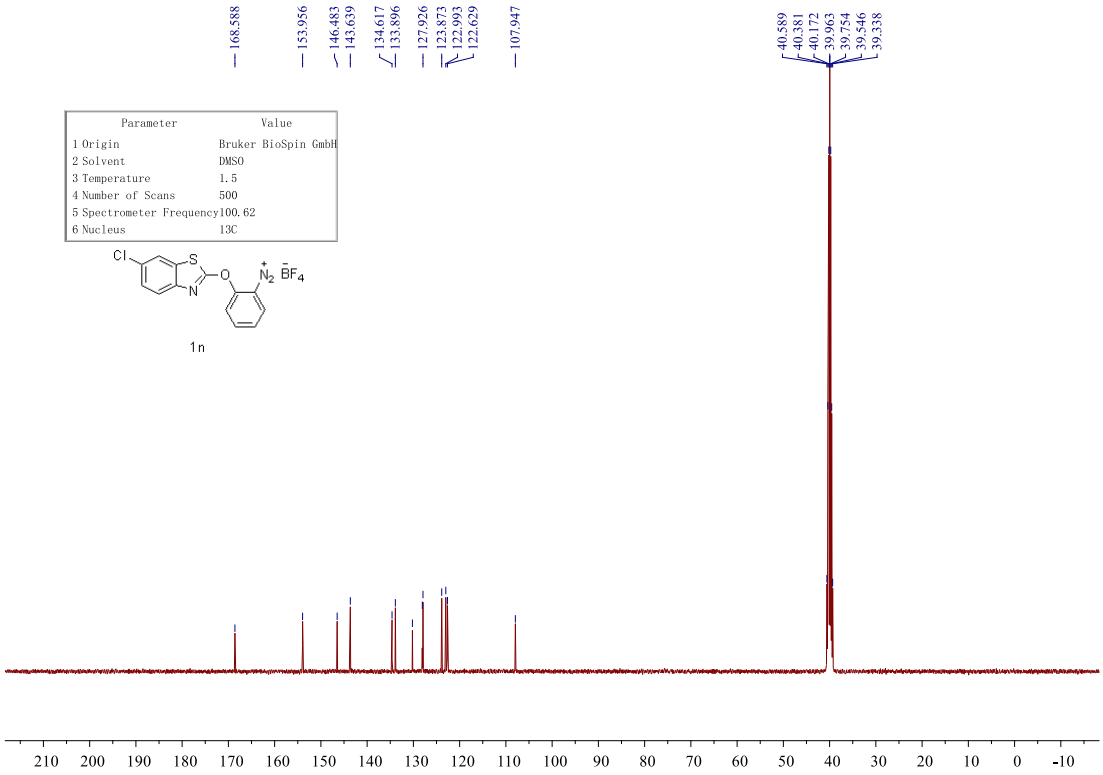
8.289
8.285
7.858
7.837
7.596
7.592
7.575
7.570
2.500
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 1.5
4 Number of Scans 4
5 Spectrometer Frequency 400.15
6 Nucleus 1H
Cl
S
O
N
N2 BF4
1n
1.00
2.00
0.99
2.01
1.03
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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146.483
143.639
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133.896
127.926
123.873
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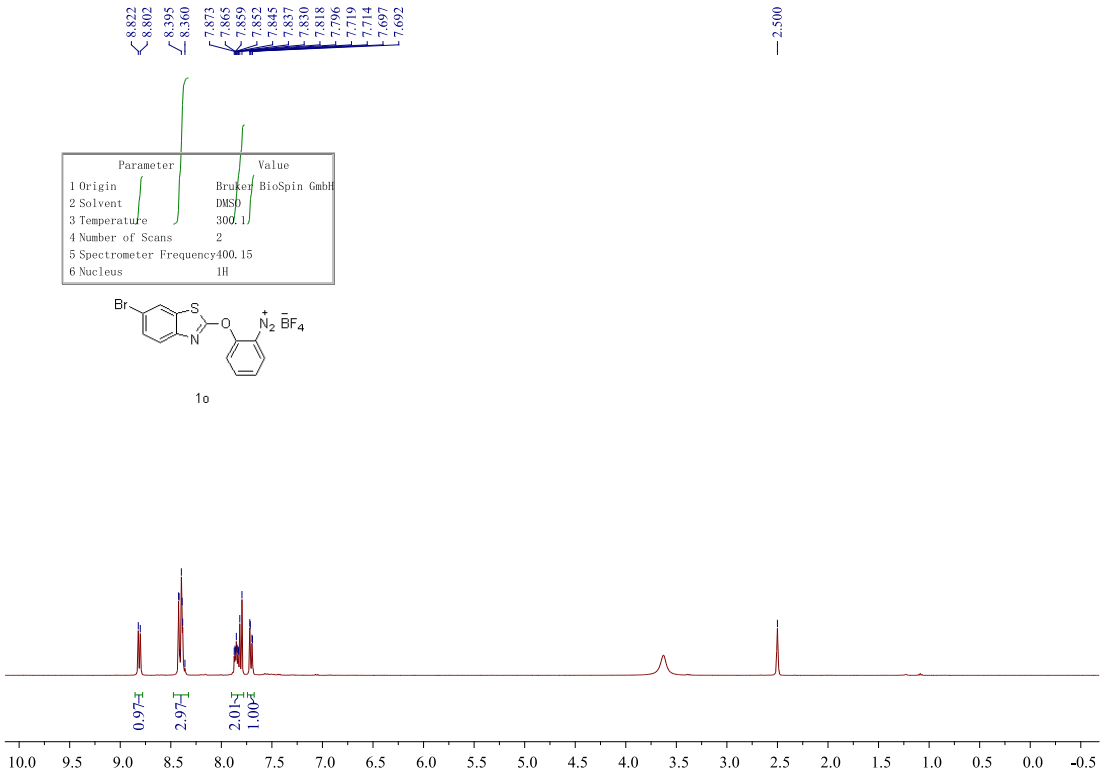
122.629
107.947
40.589
40.381
40.172
39.963
39.754
39.546
39.338
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 1.5
4 Number of Scans 500
5 Spectrometer Frequency 100.62
6 Nucleus 13C
Cl
S
N
O
N2 BF4
1n
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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8.395
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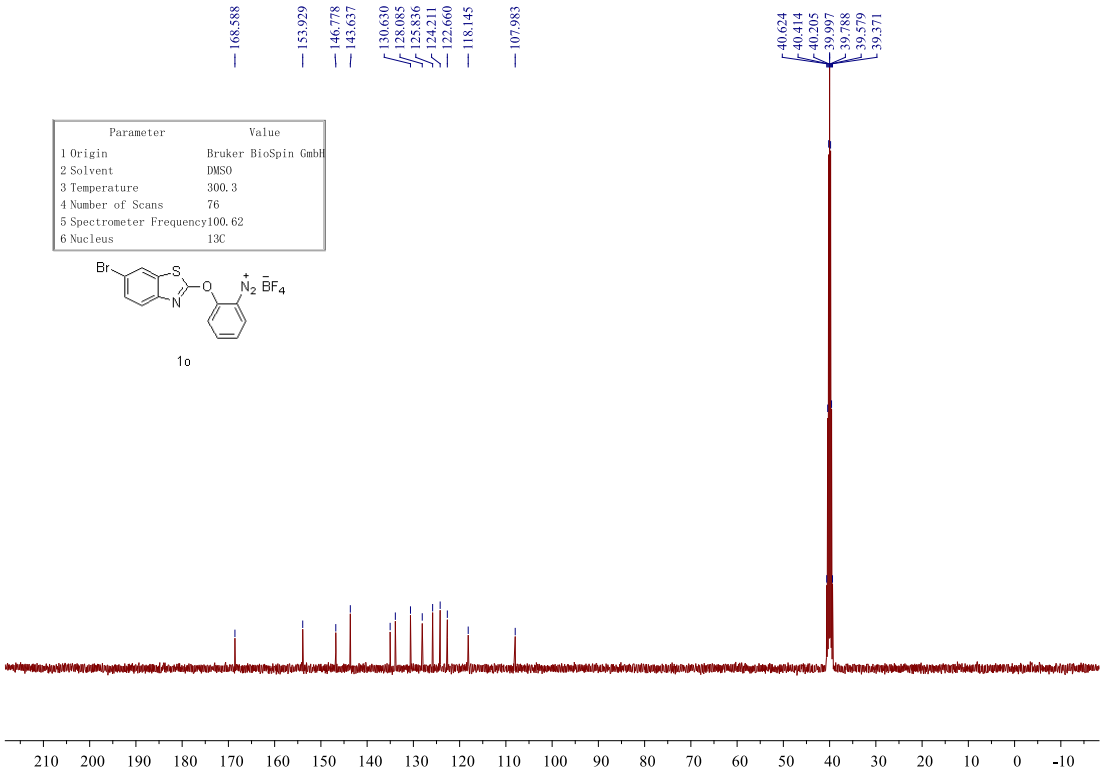
7.859
7.852
7.845
7.837
7.830
7.818
7.796
7.719
7.714
7.697
7.692
2.500
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 300.1
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
Br
S
N
O
N2 BF4
1o
0.97
2.97
2.01
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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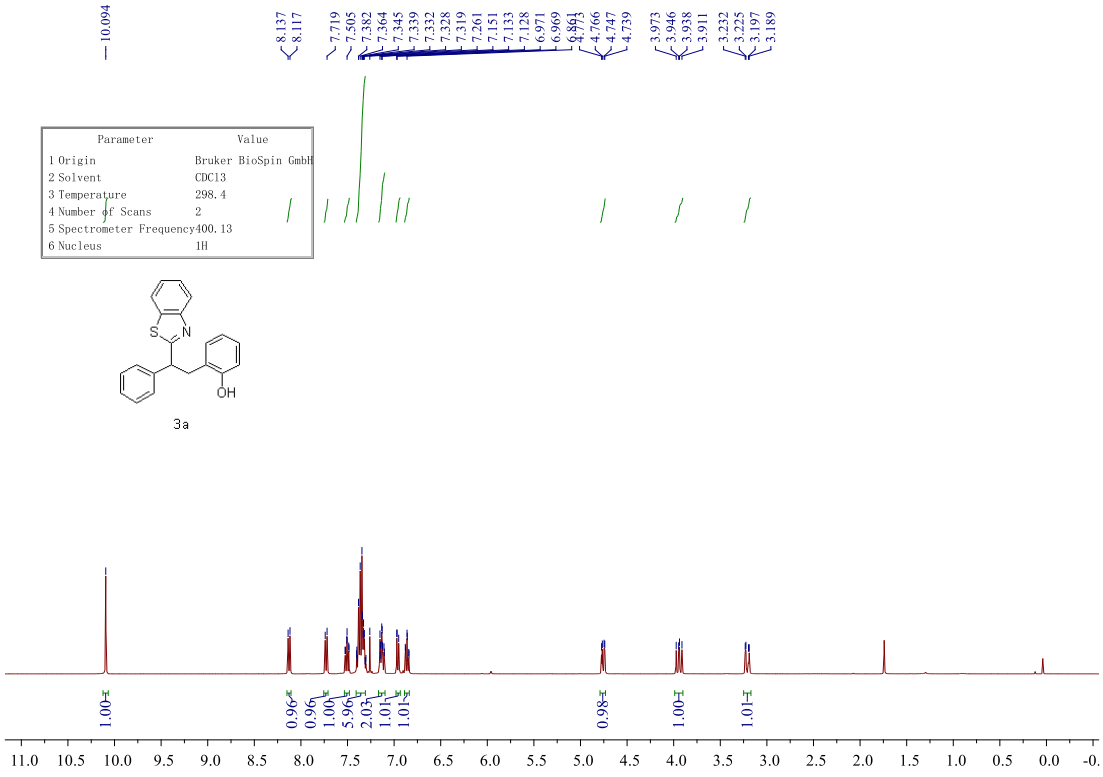
128.085
125.836
124.211
122.660
118.145
107.983
40.624
40.414
40.205
39.997
39.788
39.579
39.371
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 300.3
4 Number of Scans 76
5 Spectrometer Frequency 100.62
6 Nucleus 13C
Br
S
N
O
N2
BF4
1o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8.117
7.719
7.505
7.382
7.364
7.345
7.339
7.332
7.328
7.319
7.261
7.151
7.133
7.128
6.971
6.969
4.766
4.747
4.739
3.973
3.946
3.938
3.911
3.232
3.225
3.197
3.189
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.4
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
S
N
OH
3a
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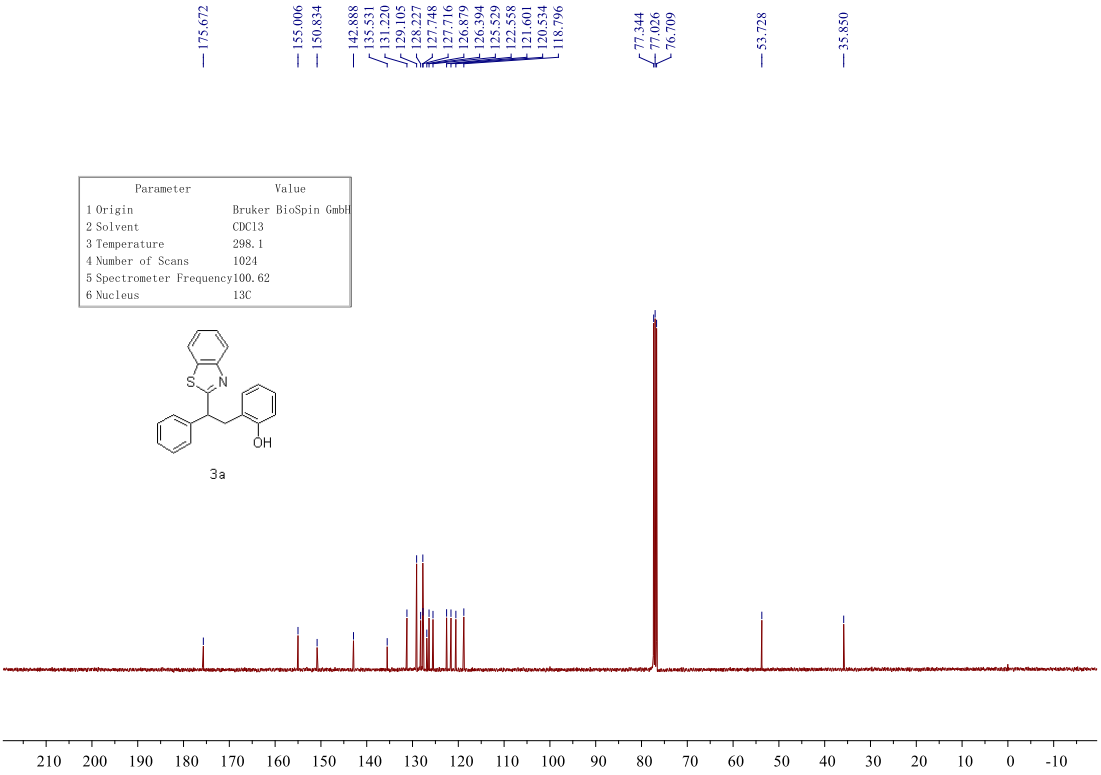
0.96
0.96
1.00
5.96
2.03
1.01
1.01
0.98
1.00
1.01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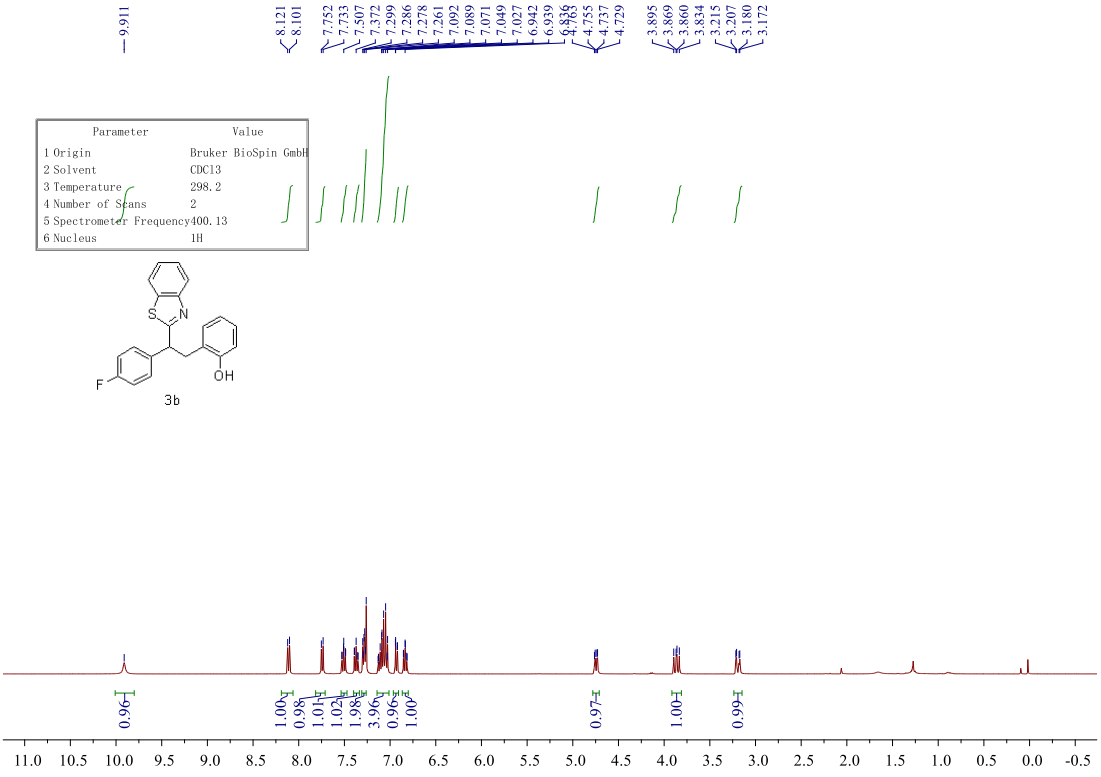
126.394
125.529
122.558
121.601
120.534
118.796
77.344
77.026
76.709
53.728
35.850
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 1024
5 Spectrometer Frequency 100.62
6 Nucleus 13C
S
N
OH
3a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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7.299
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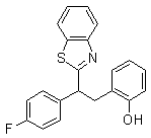
7.278
7.261
7.092
7.089
7.071
7.049
7.027
6.942
6.939
6.836
6.763
4.755
4.737
4.729
3.895
3.869
3.860
3.834
3.215
3.207
3.180
3.172
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
S
N
OH
F
3b
0.96
1.00
0.98
1.01
1.02
1.98
3.96
0.96
1.00
0.97
1.00
0.99
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Spectrometer	spect
3 Solvent	CDCl3
4 Temperature	298.1
5 Number of Scans	40
6 Spectrometer Frequency	100.61
7 Nucleus	13C



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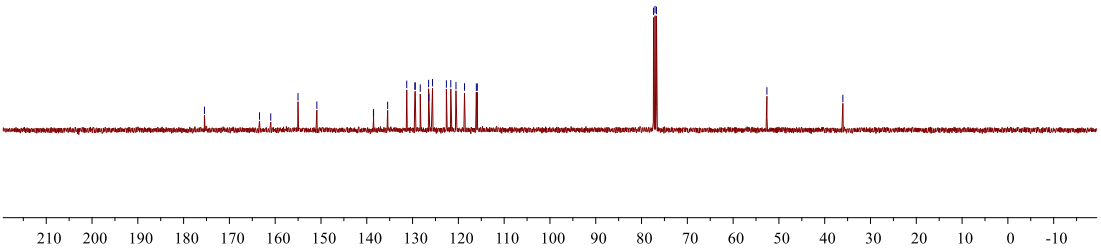
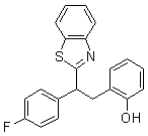


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Spectrometer	spect
3 Solvent	CDCl3
4 Temperature	298.2
5 Number of Scans	2
6 Spectrometer Frequency	376.46
7 Nucleus	19F



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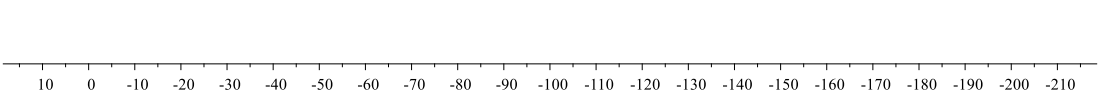

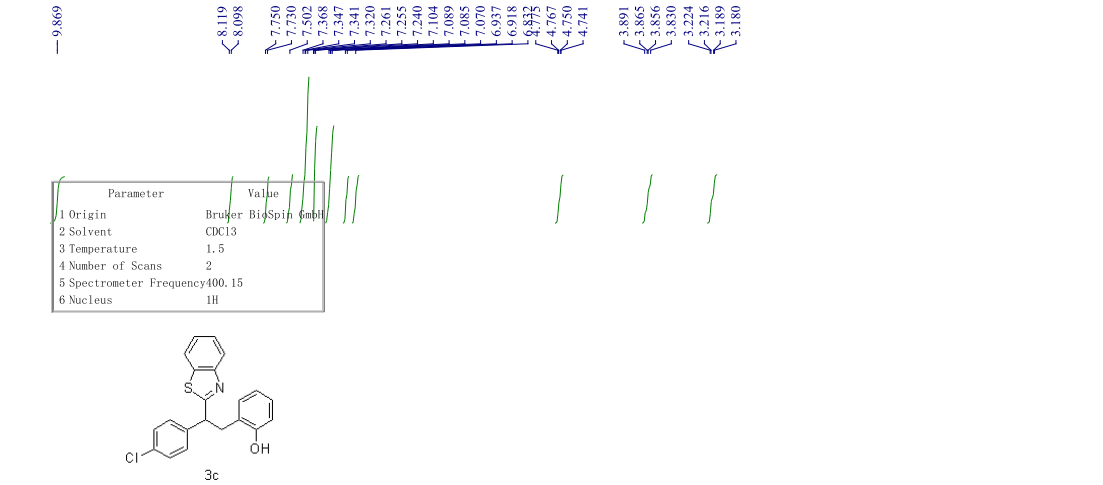
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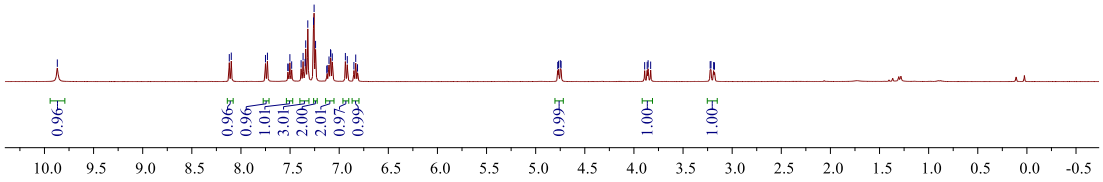
7.320
7.261
7.255
7.240
7.104
7.089
7.085
7.070
6.937
6.918
4.767
4.750
4.741
3.891
3.865
3.856
3.830
3.224
3.216
3.189
3.180
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 1.5
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
S
N
Cl
OH
3c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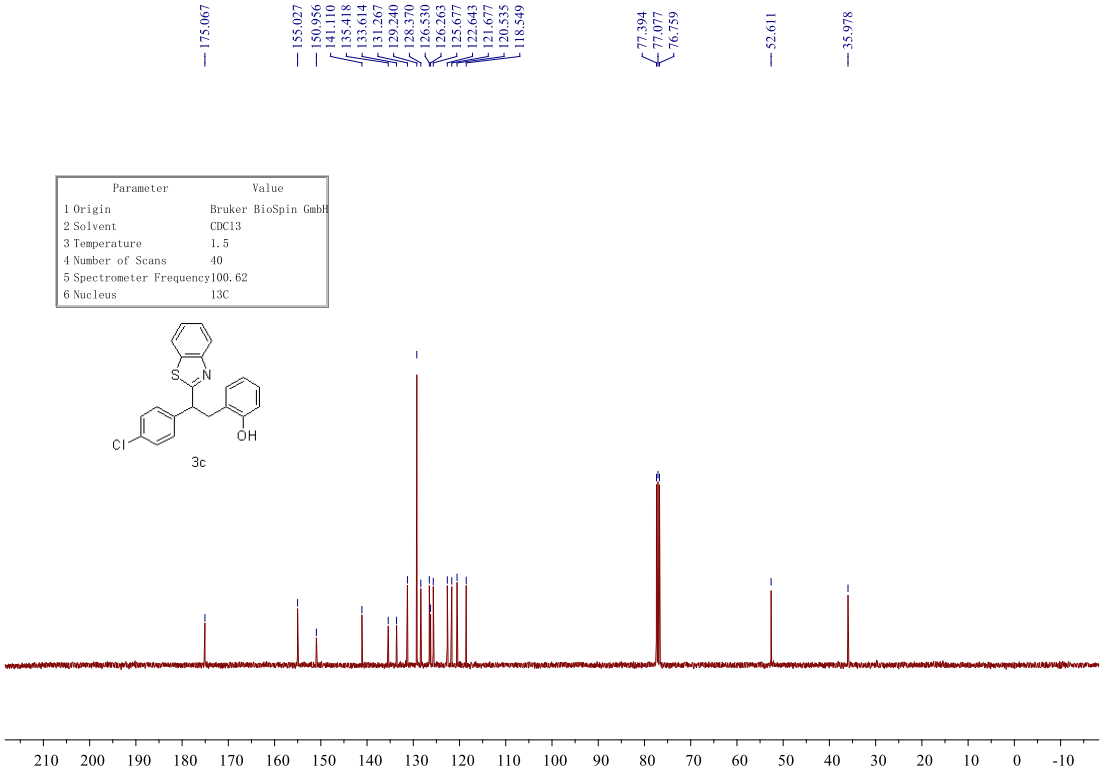
0.96
0.96
1.01
3.01
2.00
2.01
0.97
0.99
0.99
1.00
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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133.614
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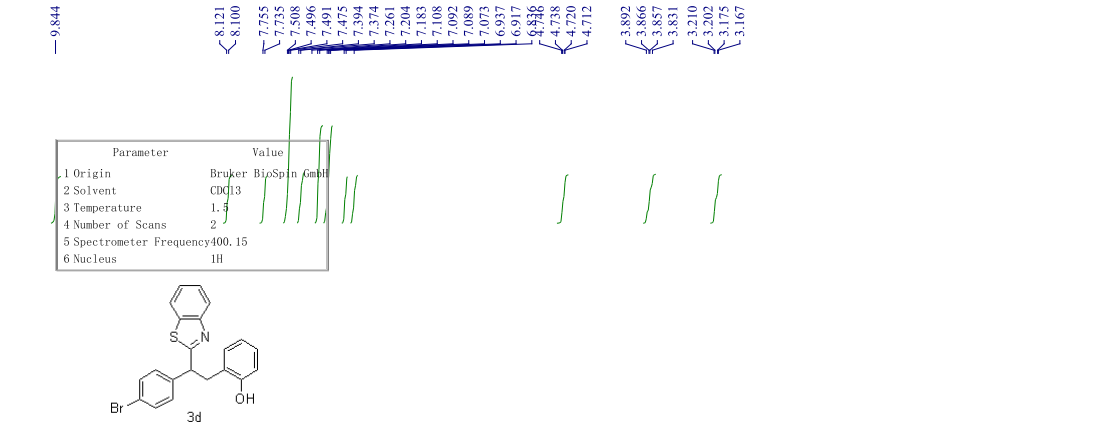
129.240
128.370
126.530
126.263
125.677
122.643
121.677
120.535
118.549
77.394
77.077
76.759
52.611
35.978
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 1.5
4 Number of Scans 40
5 Spectrometer Frequency 100.62
6 Nucleus 13C
S
N
Cl
OH
3c
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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7.755
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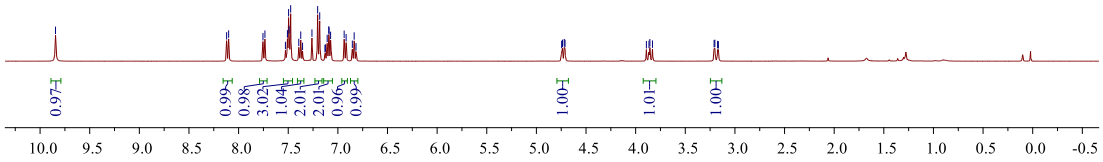
7.508
7.496
7.491
7.475
7.394
7.374
7.261
7.204
7.183
7.108
7.092
7.089
7.073
6.937
6.917
4.738
4.720
4.712
3.892
3.866
3.857
3.831
3.210
3.202
3.175
3.167
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 1.5
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
S
N
Br
OH
3d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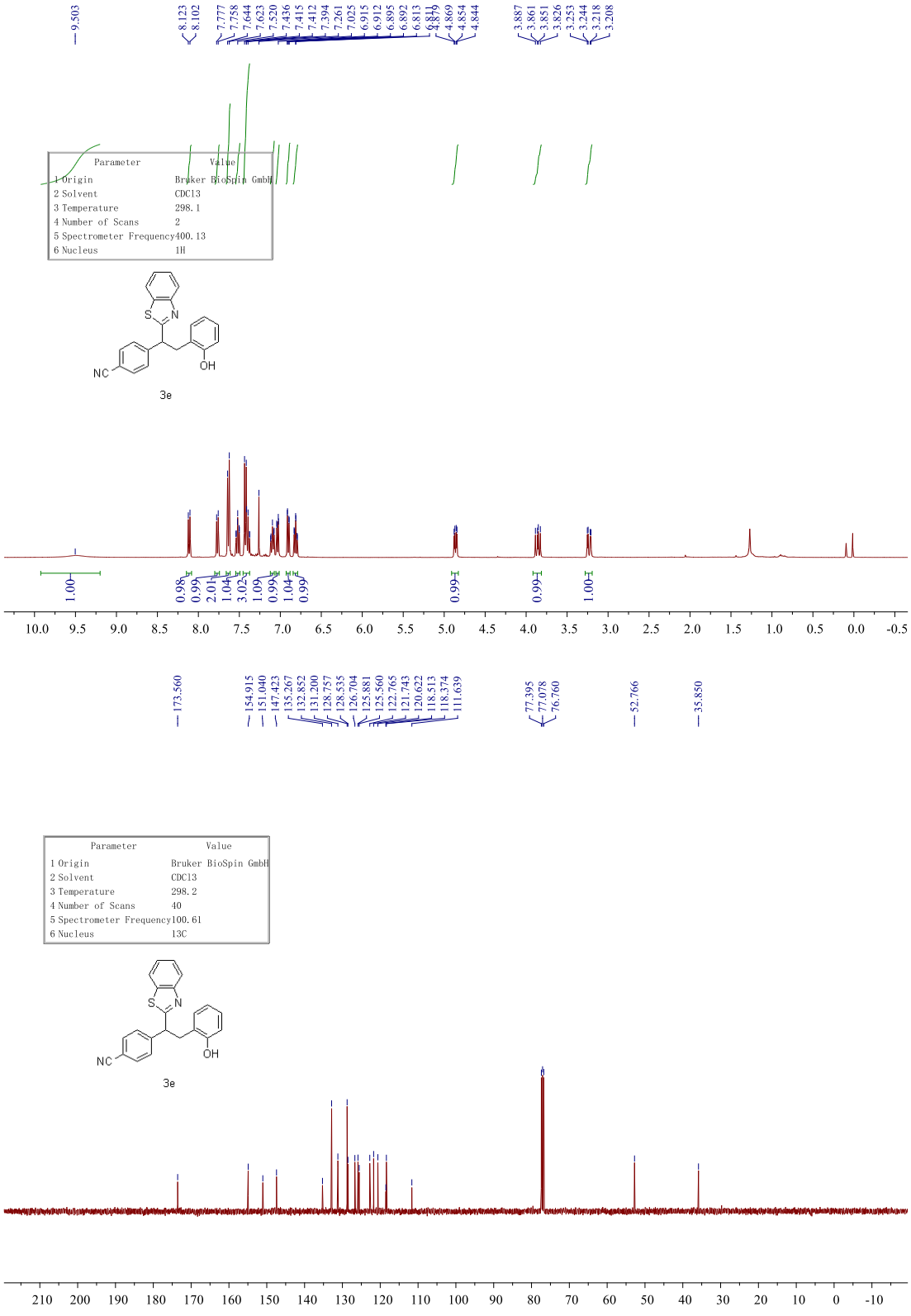
0.99
0.98
3.02
1.04
2.01
2.01
0.96
0.99
1.00
1.01
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5


174.893
155.004
150.934
141.636
135.422
132.206
131.249
129.562
128.371
126.533
126.260
125.688
122.650
121.718
121.669
120.556
118.614
77.375
77.057
76.740
52.755
35.868
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 1.5
4 Number of Scans 50
5 Spectrometer Frequency 100.62
6 Nucleus 13C
S
N
Br
OH
3d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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7.520
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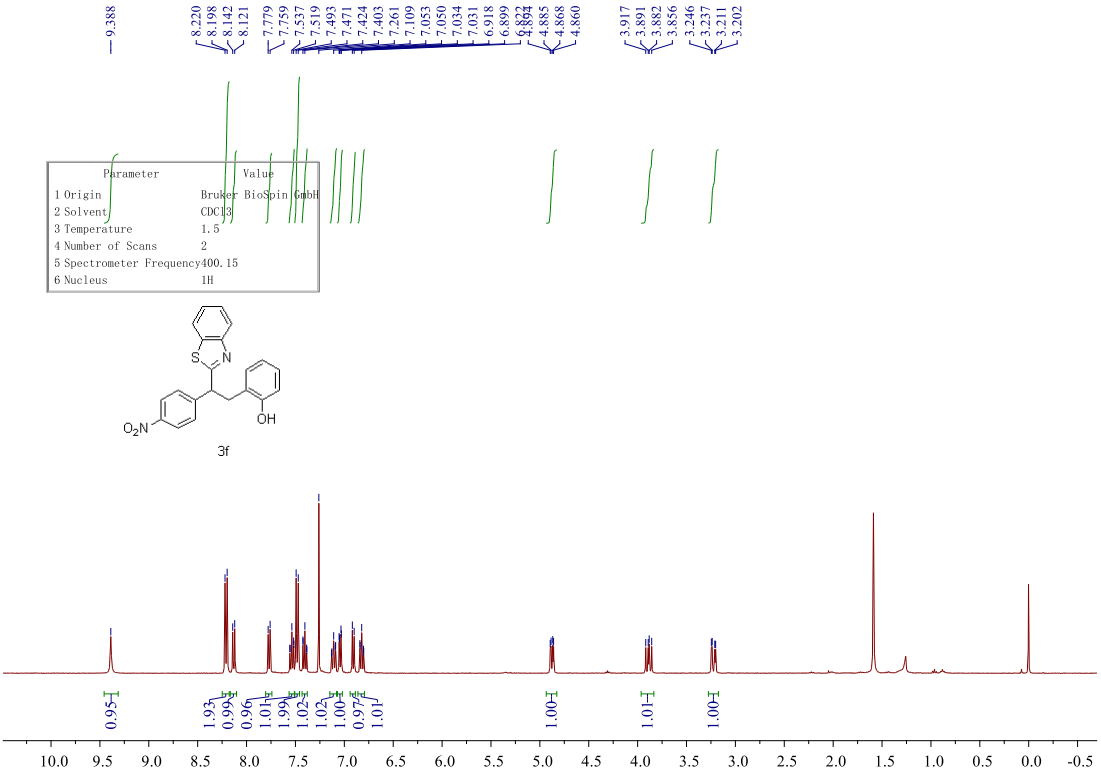
7.415
7.412
7.394
7.261
7.025
6.915
6.912
6.895
6.892
6.813
6.811
4.879
4.869
4.854
4.844
3.887
3.861
3.851
3.826
3.253
3.244
3.218
3.208
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
S
N
NC
OH
3e
1.00
0.98
0.99
2.01
1.04
3.02
1.09
0.99
1.04
0.99
0.99
0.99
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
173.560
154.915
151.040
147.423
135.267
132.852
131.200
128.757
128.535
126.704
125.881
125.560
122.765
121.743
120.622
118.513
118.374
111.639
77.395
77.078
76.760
52.766
35.850
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 40
5 Spectrometer Frequency 100.61
6 Nucleus 13C
S
N
NC
OH
3e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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7.403
7.261
7.109
7.053
7.050
7.034
7.031
6.918
6.899
4.885
4.868
4.860
3.917
3.891
3.882
3.856
3.246
3.237
3.211
3.202
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 1.5
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
S
N
O2N
OH
3f
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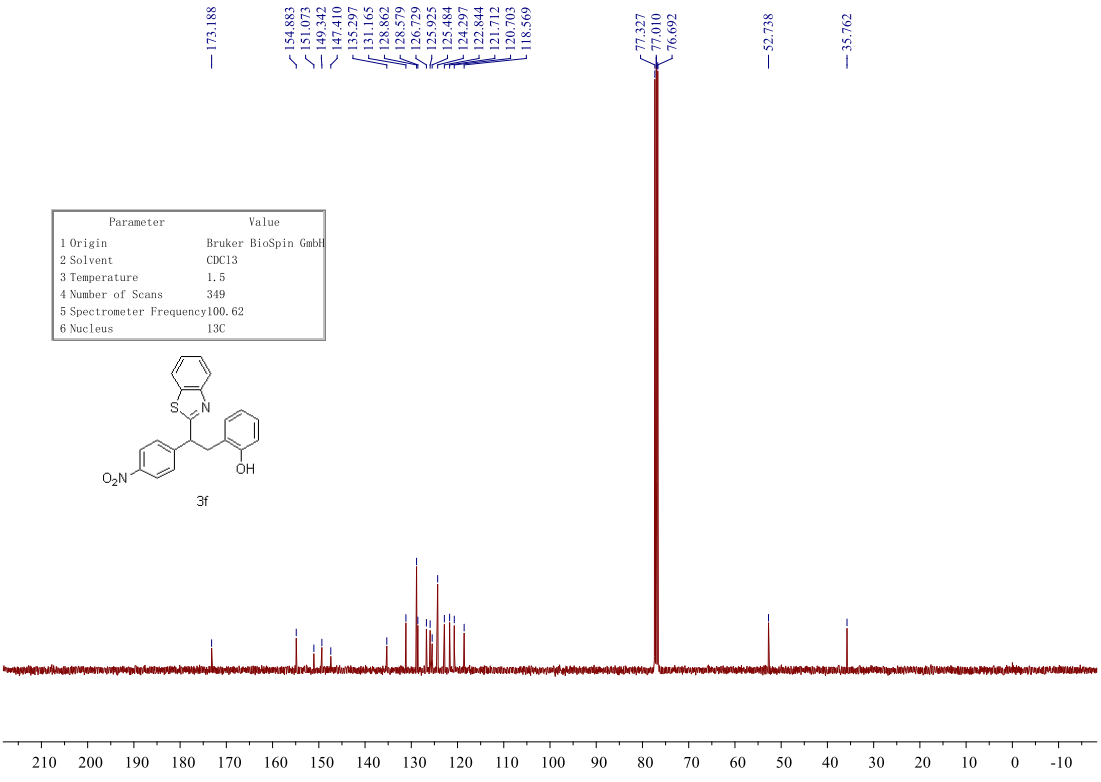
1.93
0.99
0.96
1.01
1.99
1.02
1.02
1.00
0.97
1.01
1.00
1.01
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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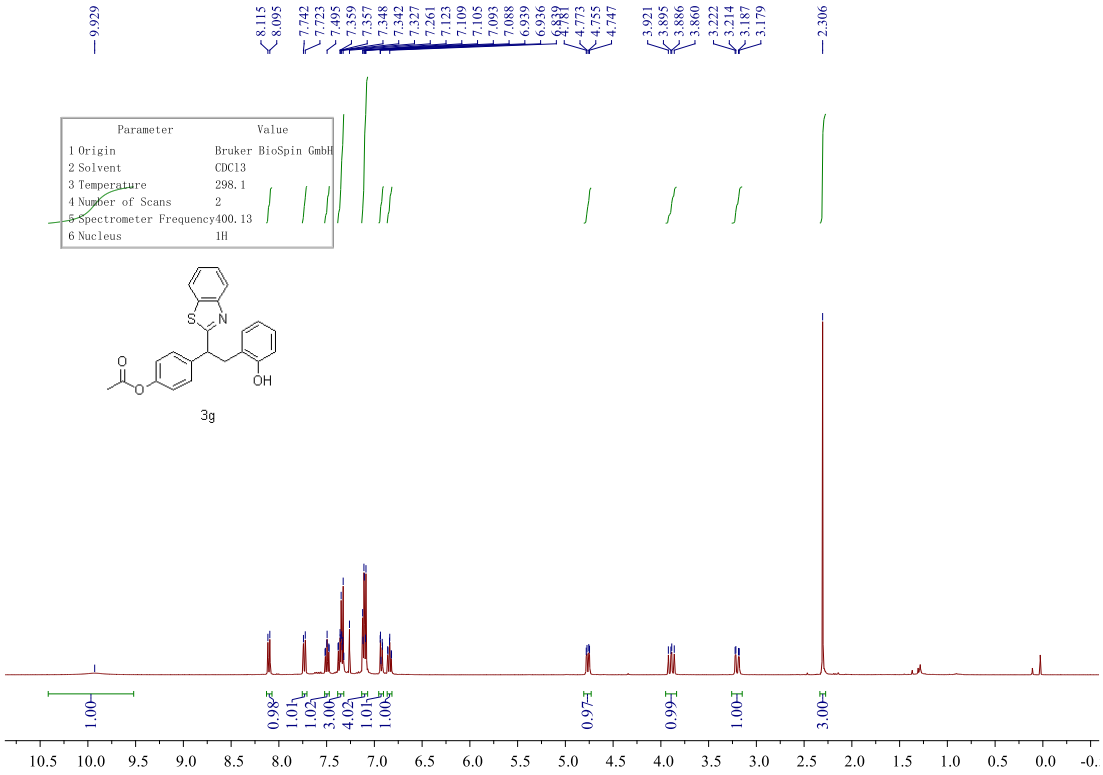
124.297
122.844
121.712
120.703
118.569
77.327
77.010
76.692
52.738
35.762
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 1.5
4 Number of Scans 349
5 Spectrometer Frequency 100.62
6 Nucleus 13C
S
N
O2N
OH
3f
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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7.342
7.327
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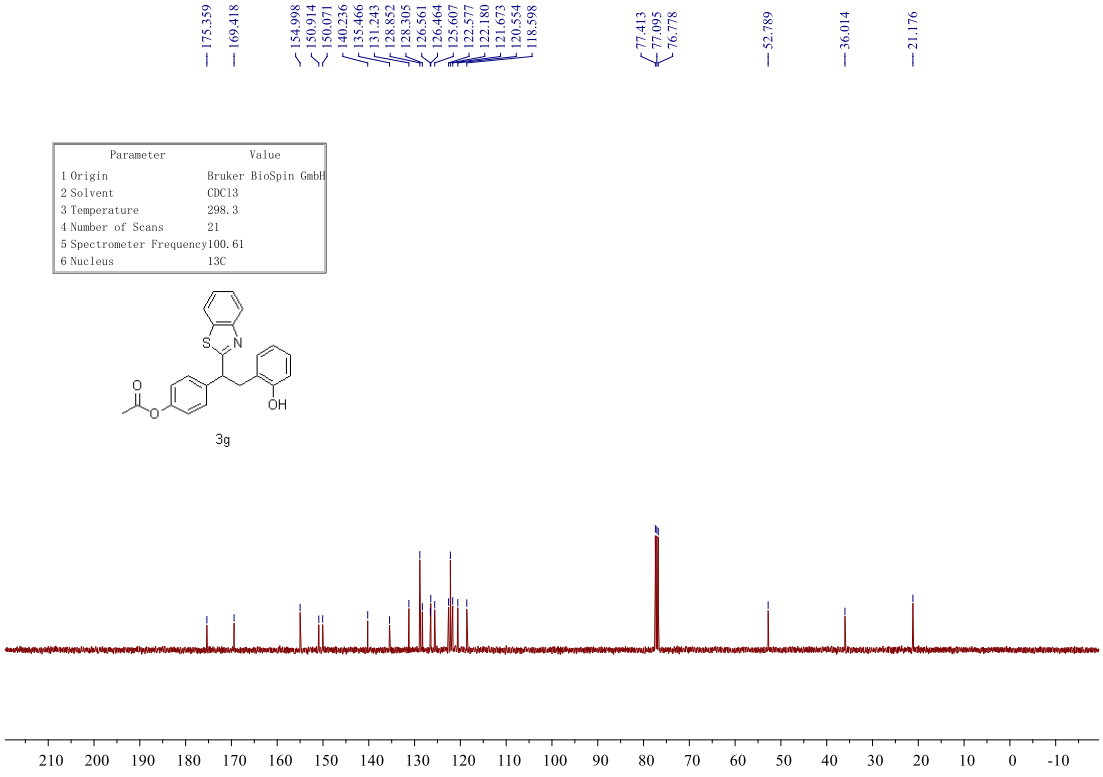
7.123
7.109
7.105
7.093
7.088
6.939
6.936
6.839
6.837
4.773
4.755
4.747
3.921
3.895
3.886
3.860
3.222
3.214
3.187
3.179
2.306
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
3g
1.00
0.98
1.01
1.02
3.00
4.02
1.01
1.00
0.97
0.99
1.00
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.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125.607
122.577
122.180
121.673
120.554
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77.413
77.095
76.778
52.789
36.014
21.176
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.3
4 Number of Scans 21
5 Spectrometer Frequency 100.61
6 Nucleus 13C
3g
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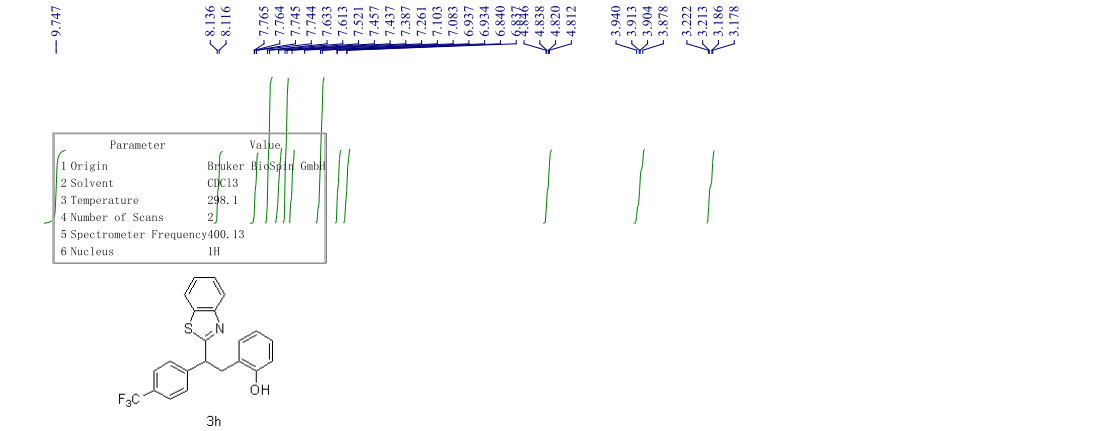
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7.744
7.633
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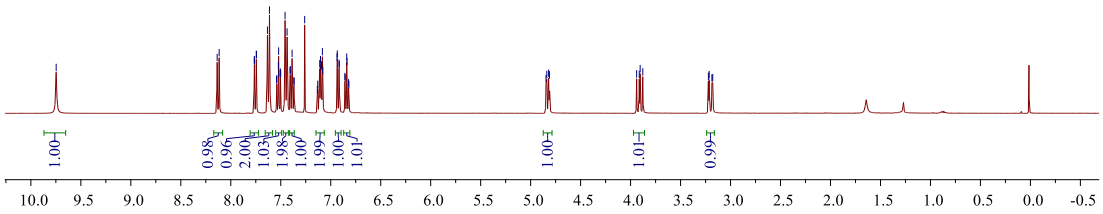
7.457
7.437
7.387
7.261
7.103
7.083
6.937
6.934
6.840
4.838
4.820
4.812
3.940
3.913
3.904
3.878
3.222
3.213
3.186
3.178
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
S
N
F3C
OH
3h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1.99
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1.01
1.00
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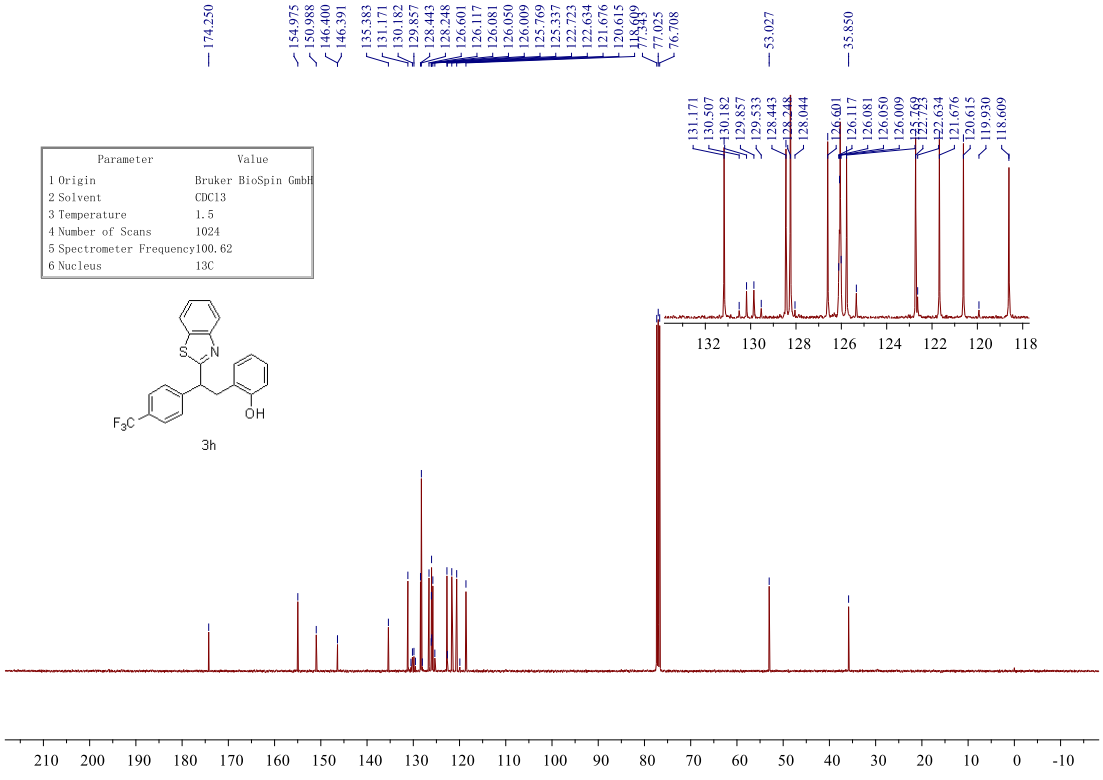
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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126.601
126.117
126.081
126.050
126.009
125.769
125.337
122.723
122.634
121.676
120.615
118.609
77.343
77.025
76.708
53.027
35.850
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 1.5
4 Number of Scans 1024
5 Spectrometer Frequency 100.62
6 Nucleus 13C
S
N
F3C
OH
3h
132 130 128 126 124 122 120 118
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10


-62.522
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 376.46
6 Nucleus 19F
S
N
F3C
OH
3h
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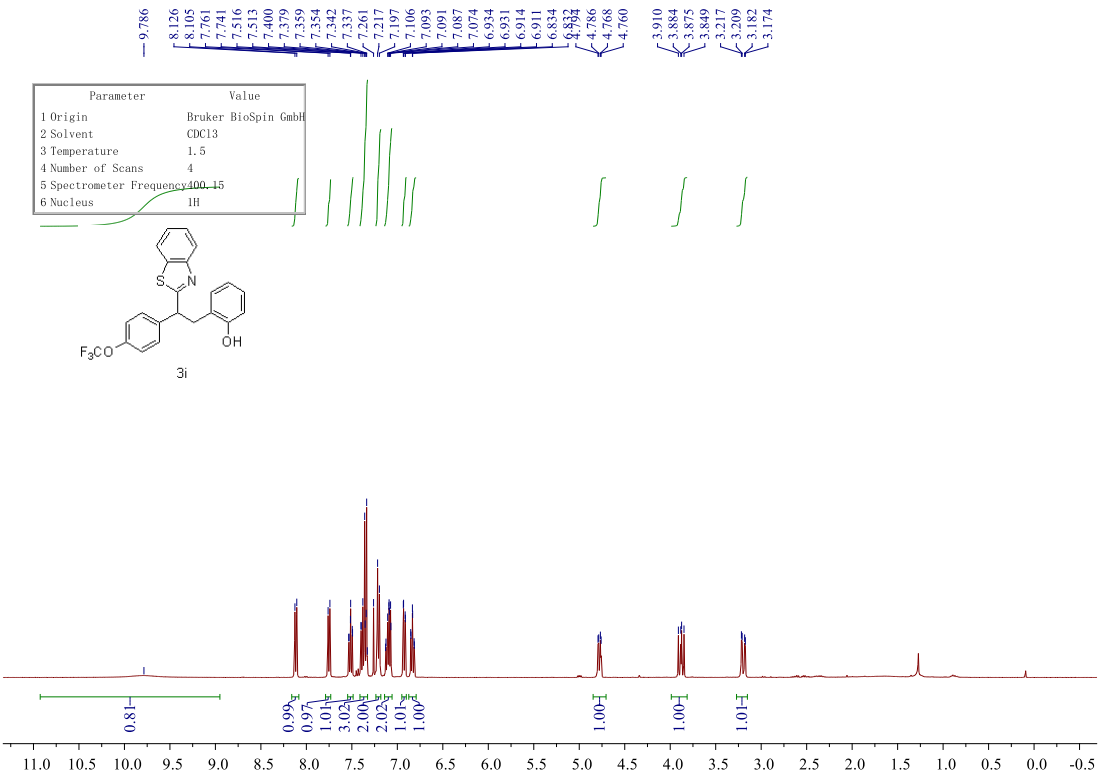
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7.091
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7.074
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6.931
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6.911
6.834
6.833
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4.768
4.760
3.910
3.884
3.875
3.849
3.217
3.209
3.182
3.174
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 1.5
4 Number of Scans 4
5 Spectrometer Frequency 400.15
6 Nucleus 1H
S
N
F3CO
OH
3i
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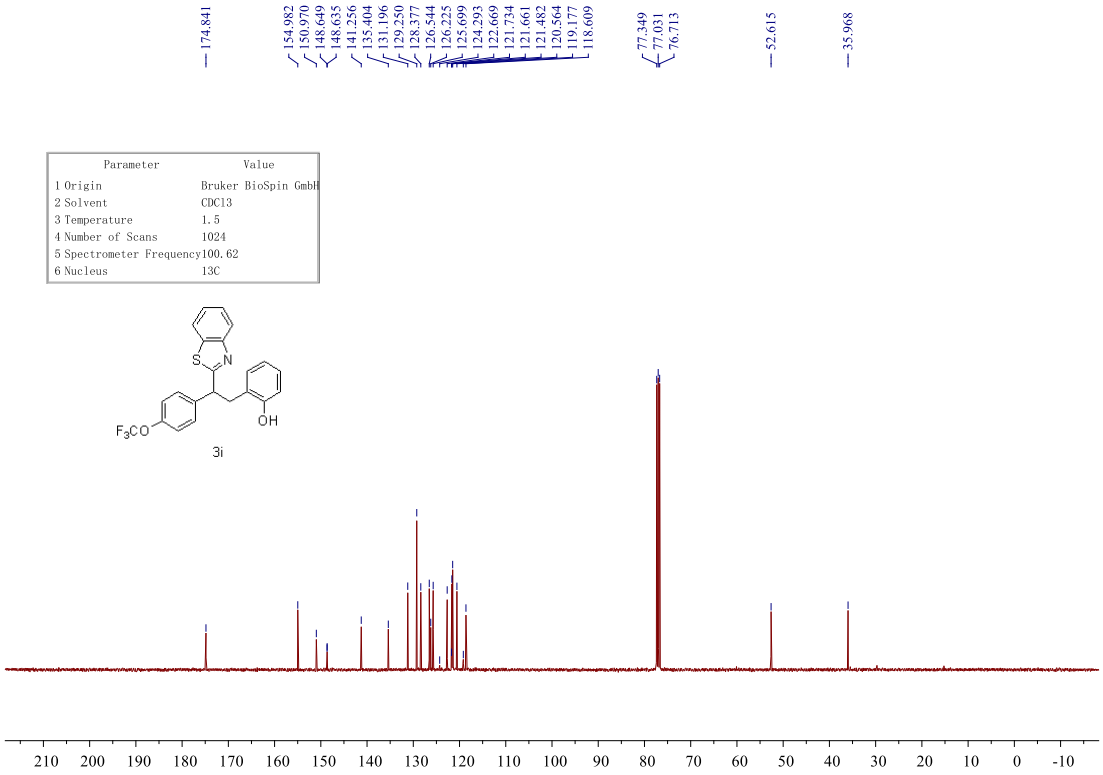
0.99
0.97
1.01
3.02
2.00
2.02
1.01
1.00
1.00
1.00
1.01
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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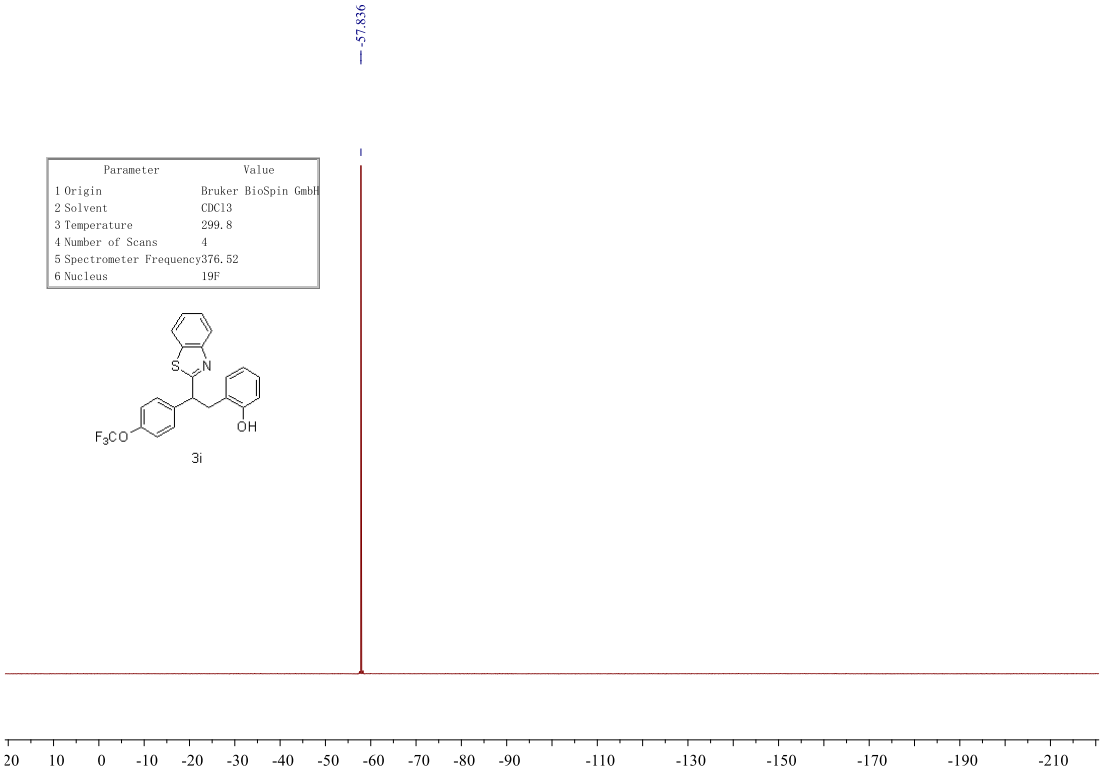
125.699
124.293
122.669
121.734
121.661
121.482
120.564
119.177
118.609
77.349
77.031
76.713
52.615
35.968
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 1.5
4 Number of Scans 1024
5 Spectrometer Frequency 100.62
6 Nucleus 13C
S
N
F3CO
OH
3i
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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2 Solvent CDCl3
3 Temperature 299.8
4 Number of Scans 4
5 Spectrometer Frequency 376.52
6 Nucleus 19F
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N
F3CO
OH
3i
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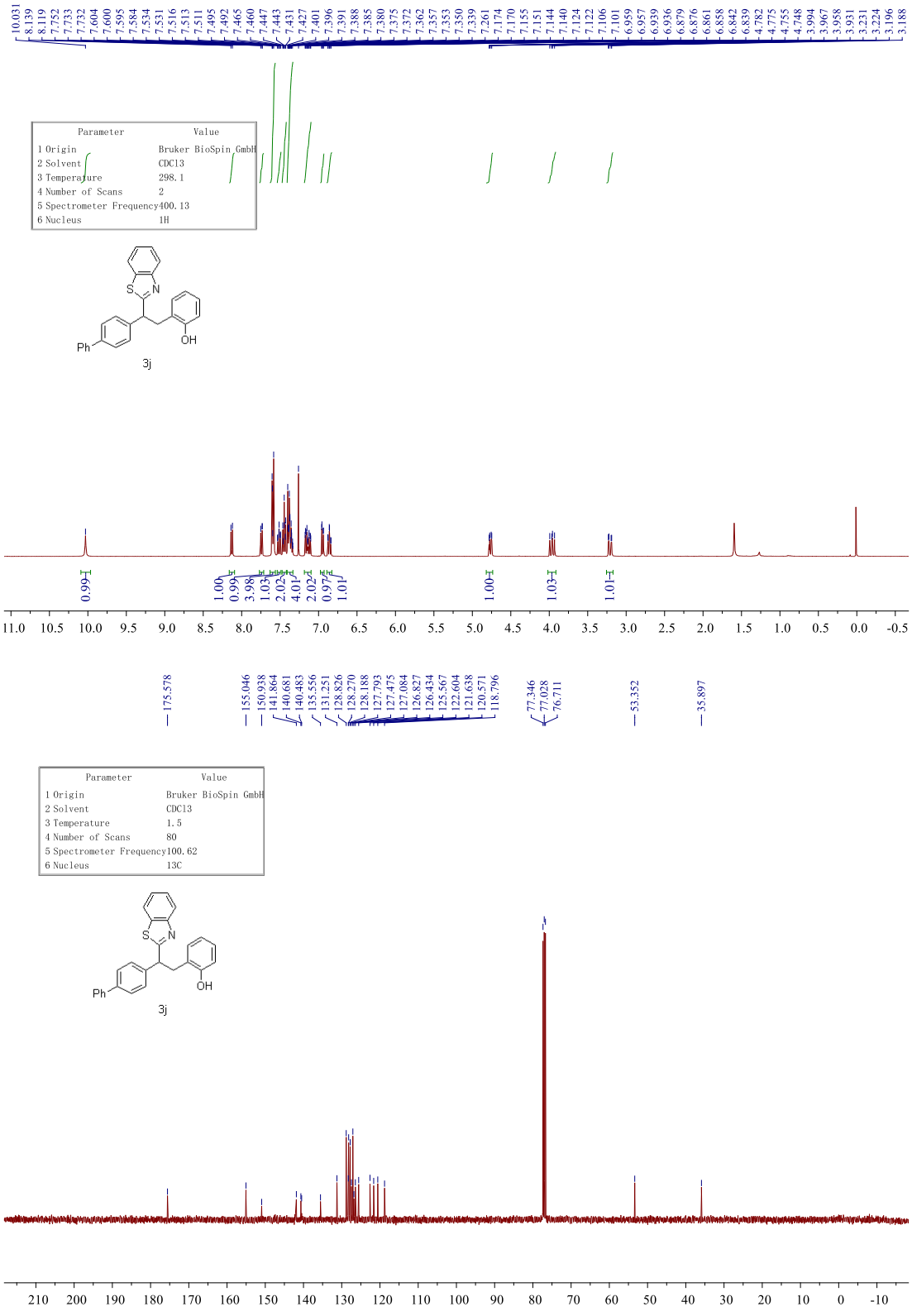
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7.513
7.511
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7.492
7.465
7.460
7.447
7.443
7.431
7.427
7.401
7.396
7.391
7.388
7.385
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7.362
7.357
7.353
7.350
7.339
7.261
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7.170
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7.151
7.144
7.140
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7.106
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6.957
6.939
6.936
6.879
6.876
6.861
6.858
6.842
6.839
4.782
4.775
4.755
4.748
3.994
3.967
3.958
3.931
3.231
3.224
3.196
3.188
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
S
N
Ph
OH
3j
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0.99
3.98
1.03
2.02
4.01
2.02
0.97
1.01
1.00
1.03
1.01
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
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140.483
135.556
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128.826
128.270
128.188
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127.475
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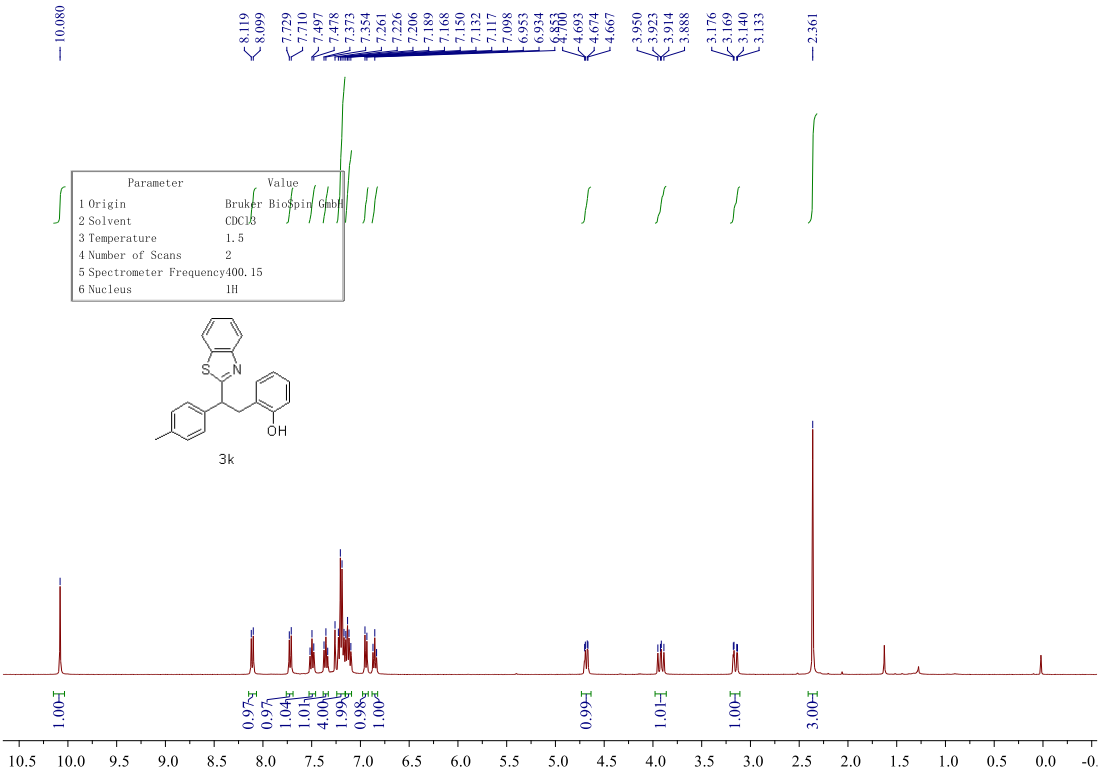
126.827
126.434
125.567
122.604
121.638
120.571
118.796
77.346
77.028
76.711
53.352
35.897
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 1.5
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
S
N
Ph
OH
3j
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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7.206
7.189
7.168
7.150
7.132
7.117
7.098
6.953
6.934
4.693
4.674
4.667
3.950
3.923
3.914
3.888
3.176
3.169
3.140
3.133
2.361
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 1.5
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
S
N
OH
3k
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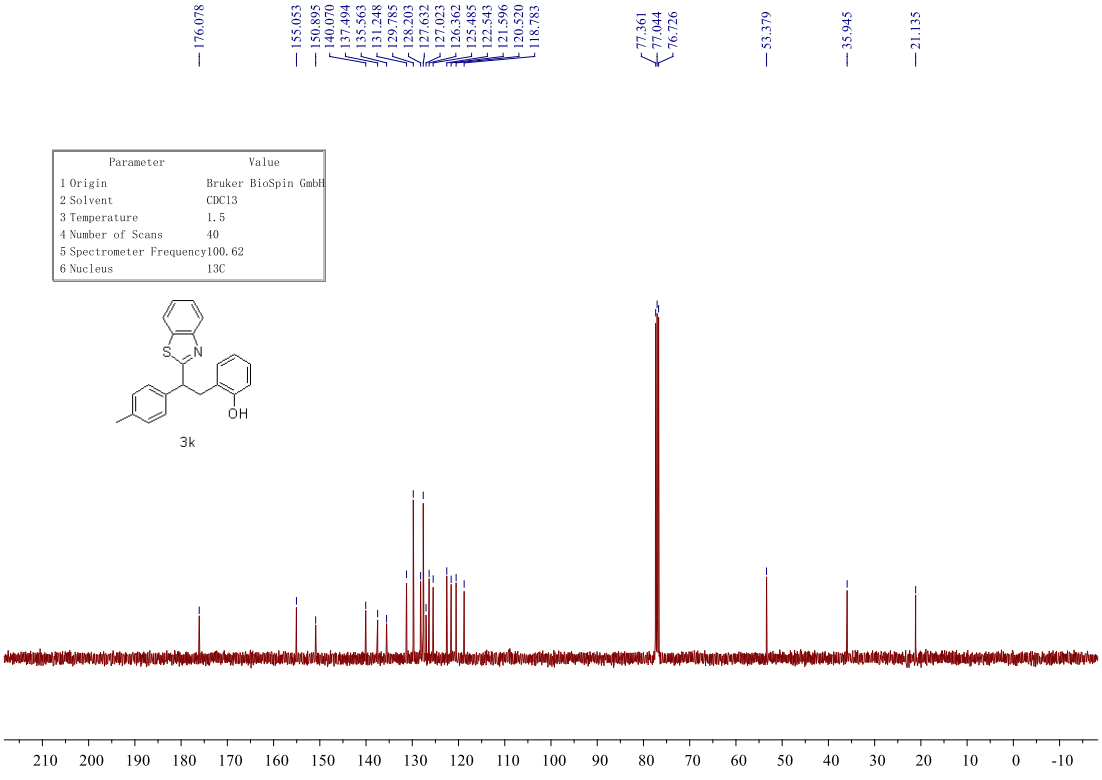
0.97
0.97
1.04
1.01
4.00
1.99
0.98
1.00
0.99
1.01
1.00
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.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127.023
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125.485
122.543
121.596
120.520
118.783
77.361
77.044
76.726
53.379
35.945
21.135
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 1.5
4 Number of Scans 40
5 Spectrometer Frequency 100.62
6 Nucleus 13C
S
N
OH
3k
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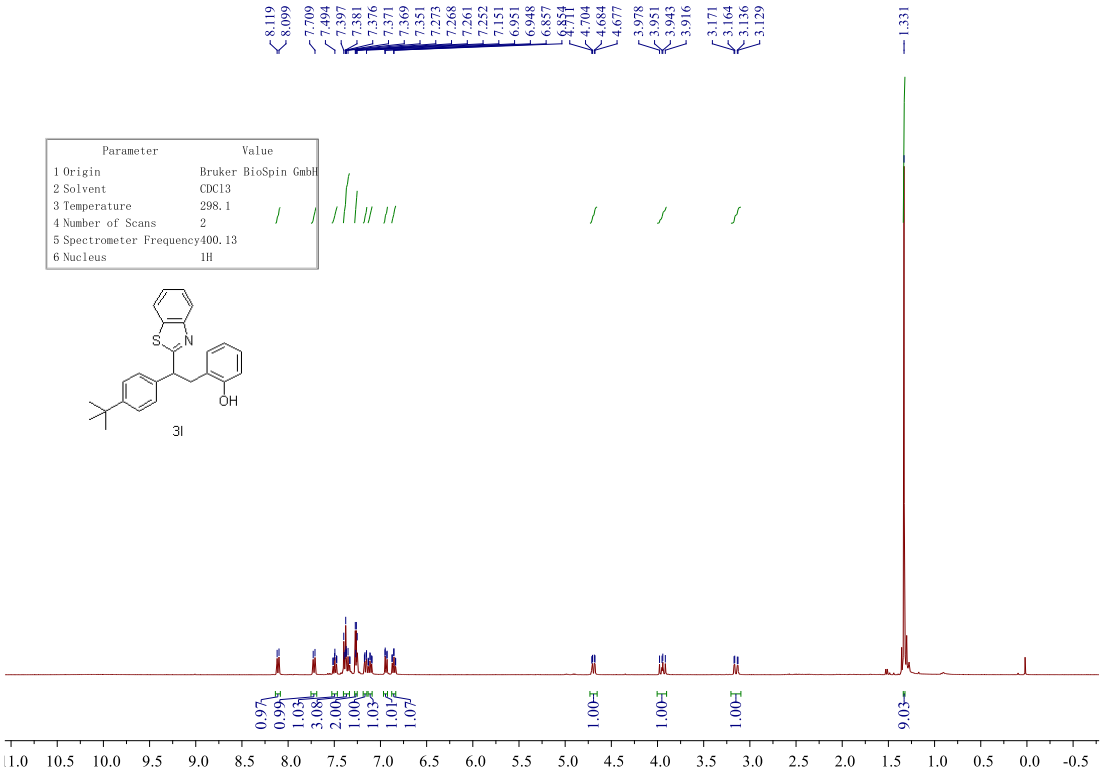
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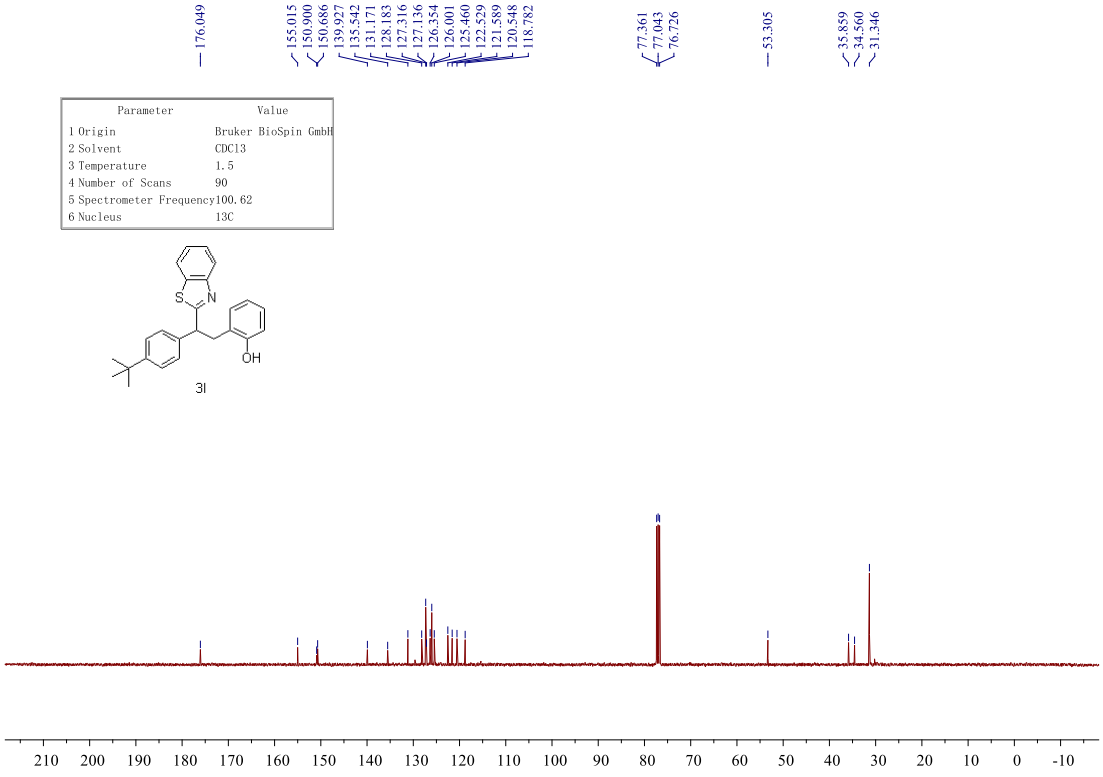
7.273
7.268
7.261
7.252
7.151
6.951
6.948
6.857
4.711
4.704
4.684
4.677
3.978
3.951
3.943
3.916
3.171
3.164
3.136
3.129
1.331
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
S
N
OH
3l
0.97
0.99
1.03
3.08
2.00
1.00
1.03
1.01
1.07
1.00
1.00
1.00
9.03
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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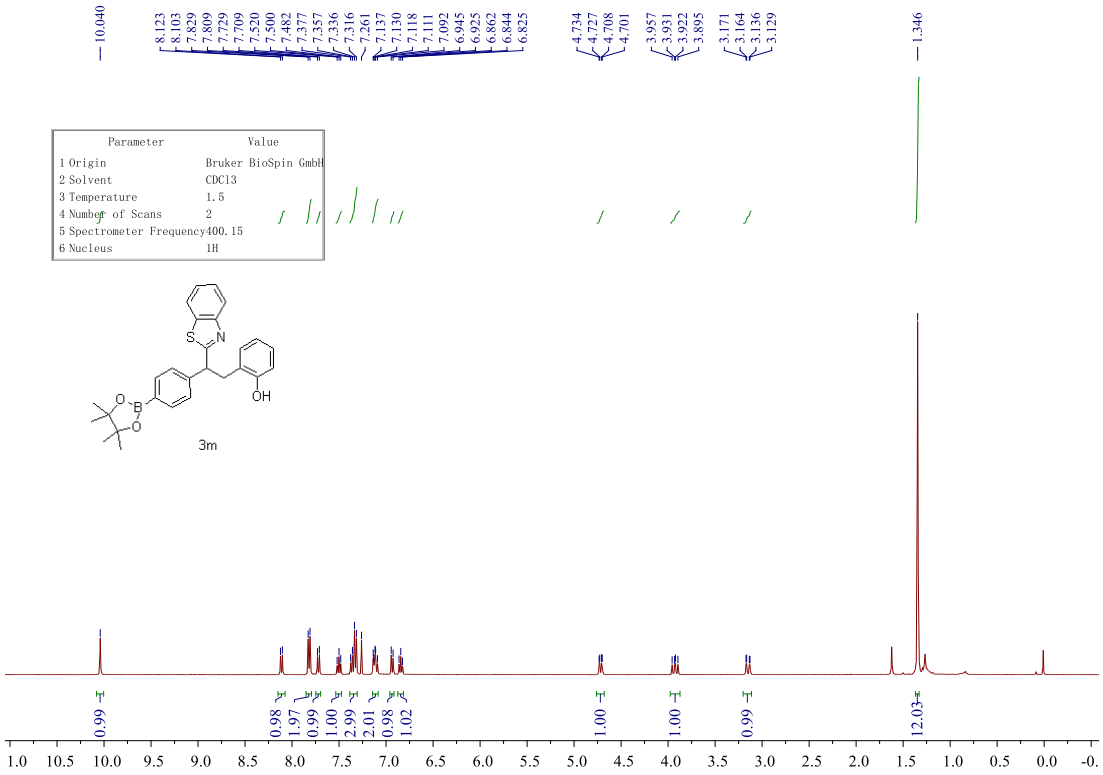
122.529
121.589
120.548
118.782
77.361
77.043
76.726
53.305
35.859
34.560
31.346
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 1.5
4 Number of Scans 90
5 Spectrometer Frequency 100.62
6 Nucleus 13C
S
N
OH
3l
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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7.336
7.316
7.261
7.137
7.130
7.118
7.111
7.092
6.945
6.925
6.862
6.844
6.825
4.734
4.727
4.708
4.701
3.957
3.931
3.922
3.895
3.171
3.164
3.136
3.129
1.346
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 1.5
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
3m
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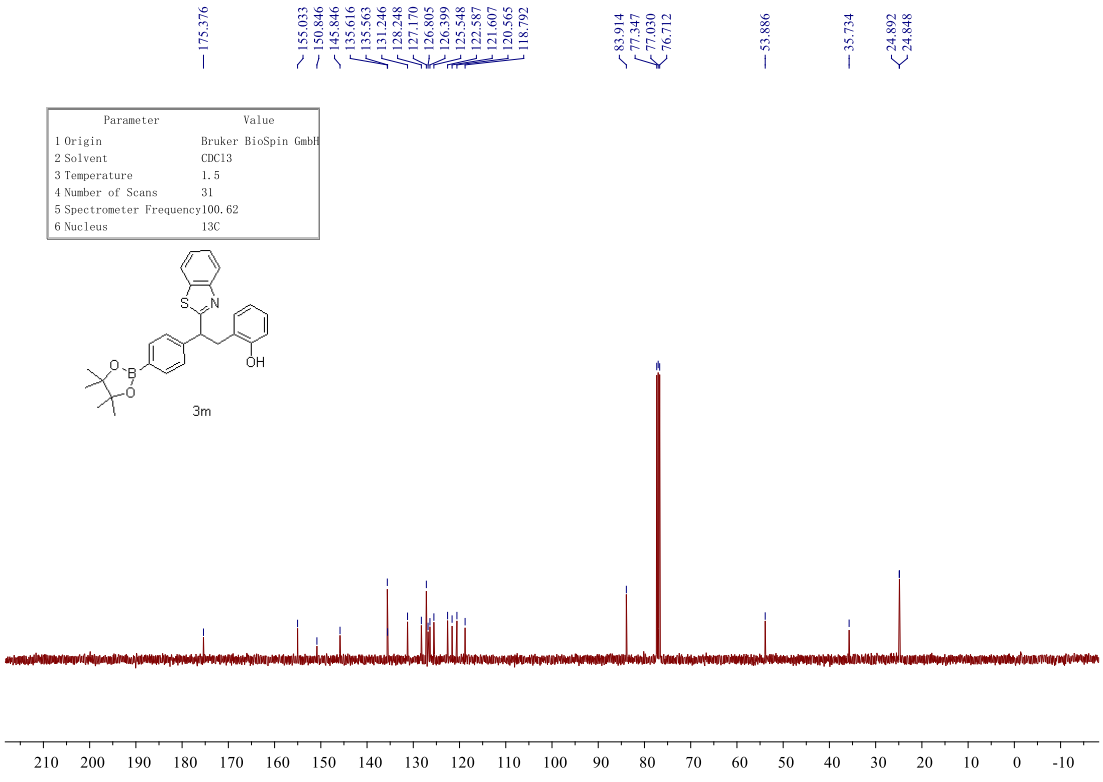
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125.548
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121.607
120.565
118.792
83.914
77.347
77.030
76.712
53.886
35.734
24.892
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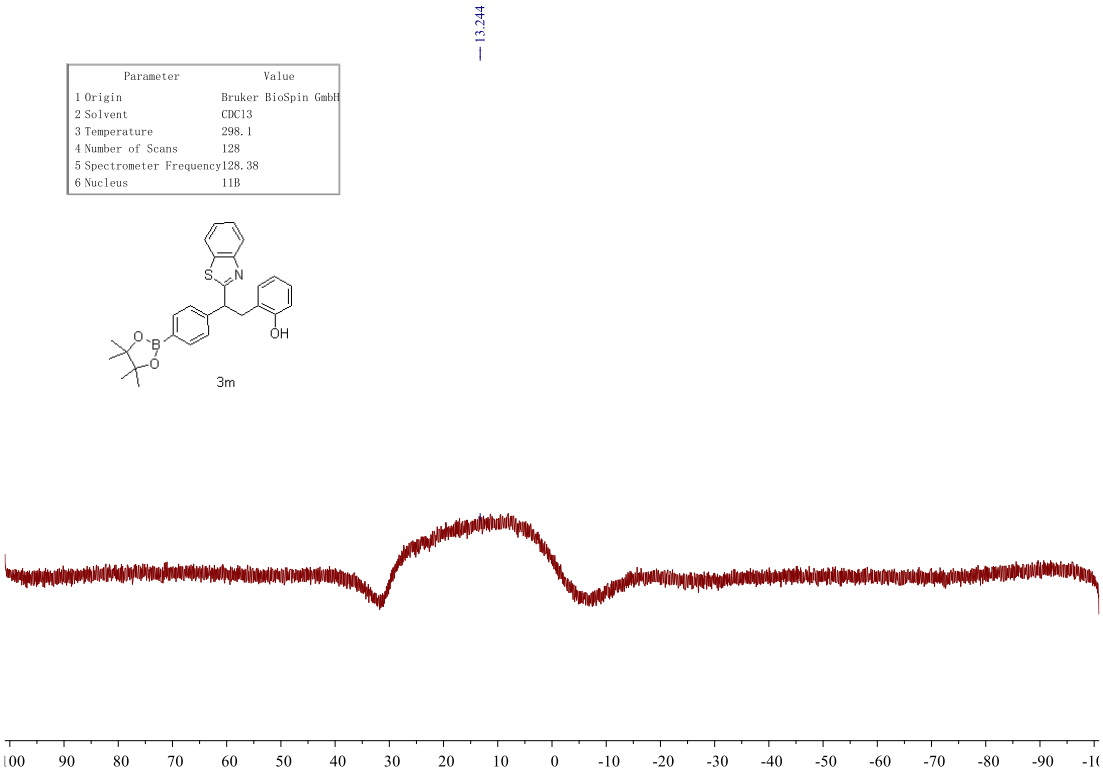
2 Solvent CDCl3
3 Temperature 1.5
4 Number of Scans 31
5 Spectrometer Frequency 100.62
6 Nucleus 13C
3m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2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 128
5 Spectrometer Frequency 128.38
6 Nucleus 11B
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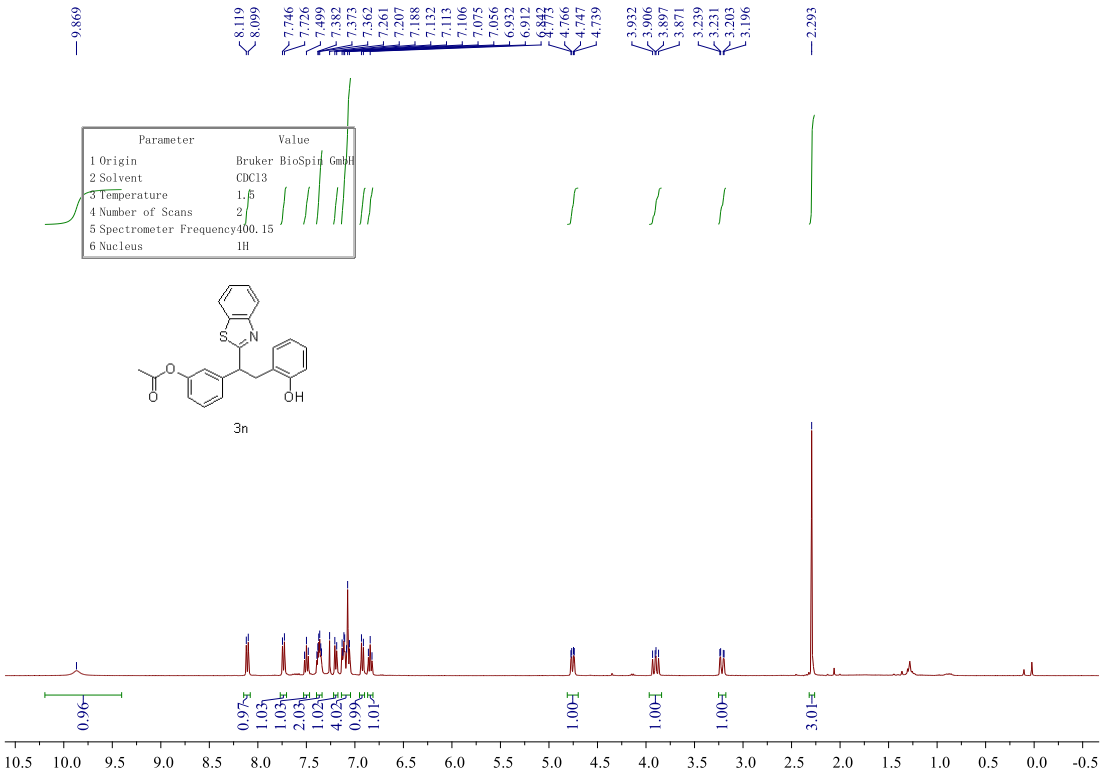
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7.113
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7.075
7.056
6.932
6.912
6.842
4.773
4.766
4.747
4.739
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3.906
3.897
3.871
3.239
3.231
3.203
3.196
2.293
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 1.5
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
3n
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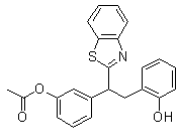
0.97
1.03
1.03
2.03
1.02
4.02
0.99
1.01
1.00
1.00
1.00
3.01

Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	1.5
4 Number of Scans	30
5 Spectrometer Frequency	100.62
6 Nucleus	13C



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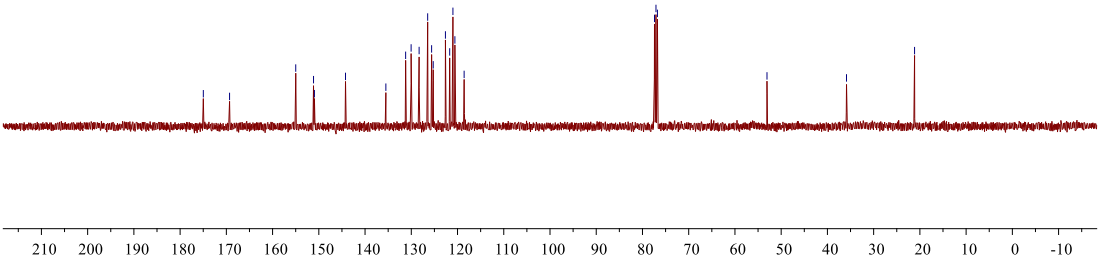
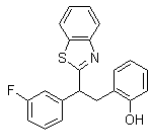


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	1.5
4 Number of Scans	2
5 Spectrometer Frequency	400.15
6 Nucleus	1H



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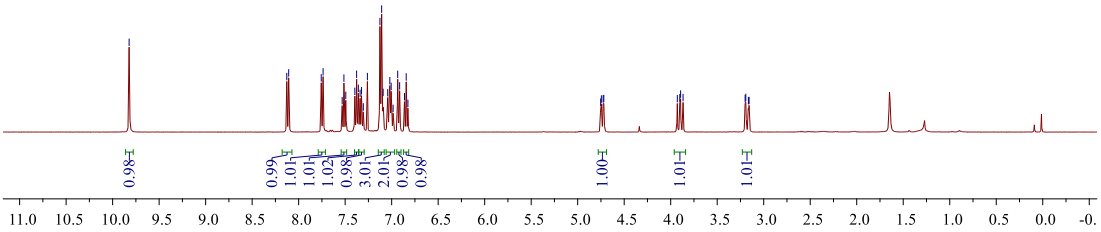

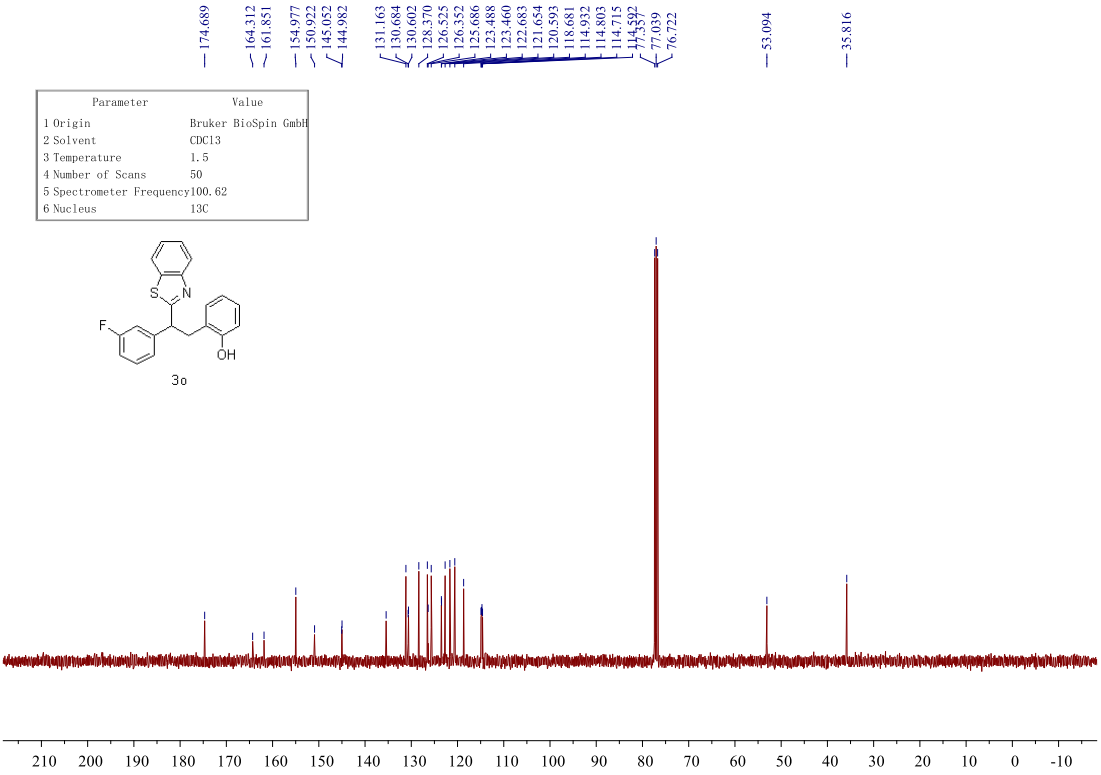
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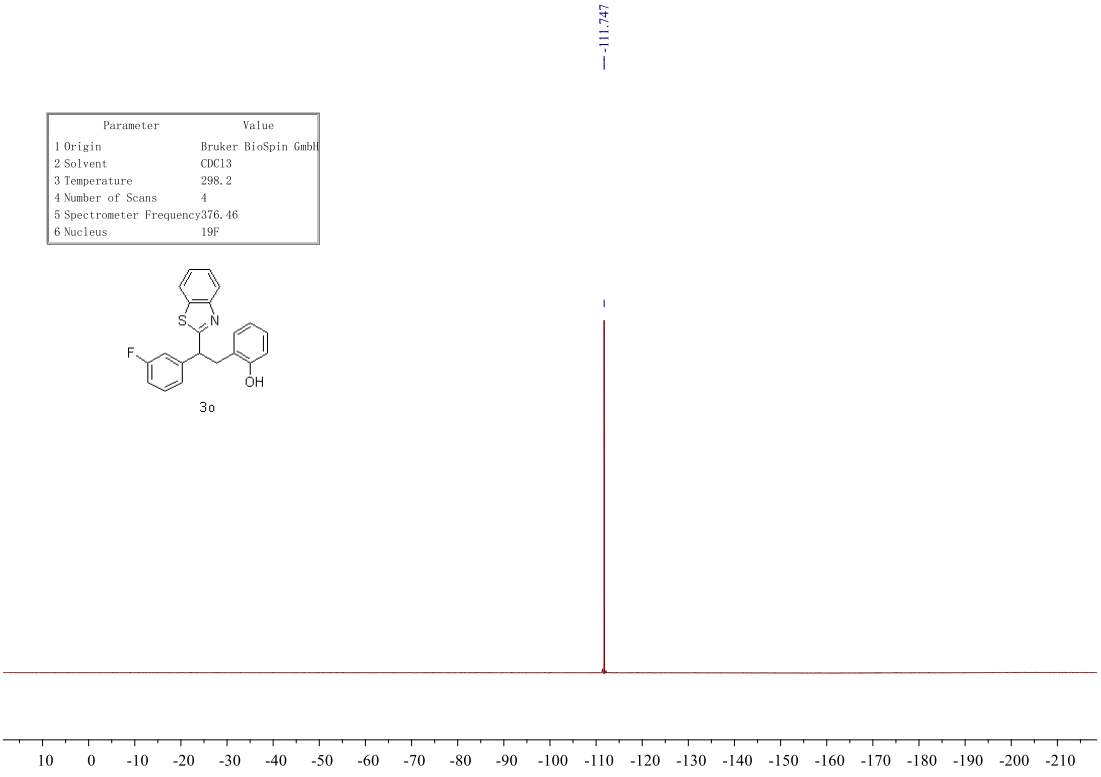
121.654
120.593
118.681
114.932
114.803
114.715
114.592
77.357
77.039
76.722
53.094
35.816
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 1.5
4 Number of Scans 50
5 Spectrometer Frequency 100.62
6 Nucleus 13C
S
N
F
OH
3o
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 376.46
6 Nucleus 19F
S
N
F
OH
3o
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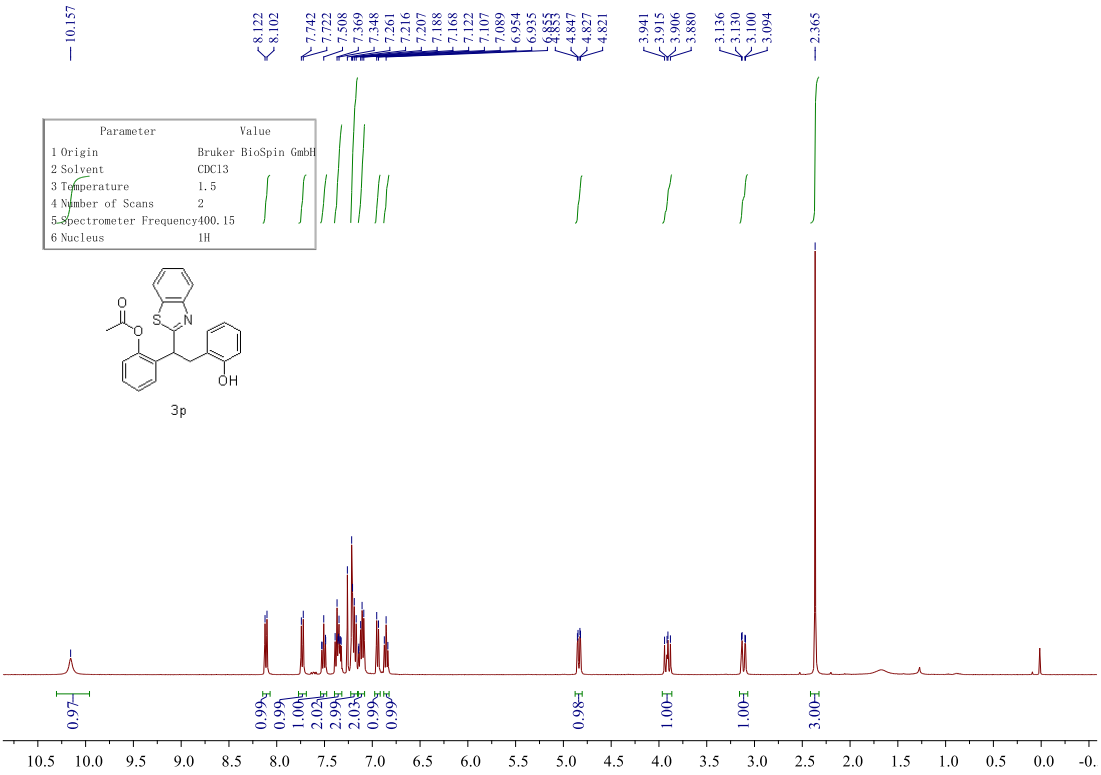
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6.935
6.855
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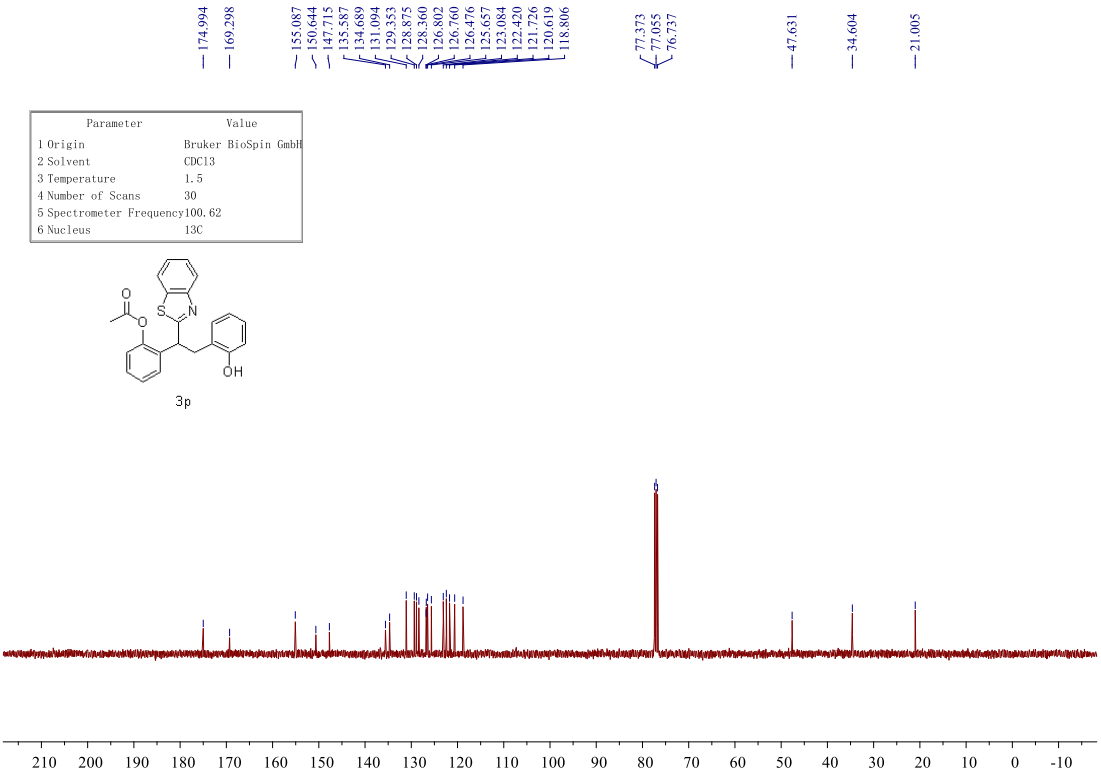
4.827
4.821
3.941
3.915
3.906
3.880
3.136
3.130
3.100
3.094
2.365
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 1.5
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
3p
0.97
0.99
0.99
1.00
2.02
2.99
2.03
0.98
0.99
0.98
1.00
1.00
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.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131.094
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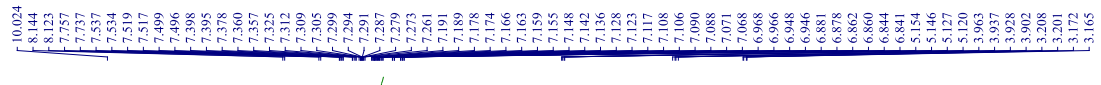
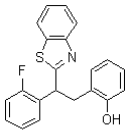
128.875
128.360
126.802
126.760
126.476
125.657
123.084
122.420
121.726
120.619
118.806
77.373
77.055
76.737
47.631
34.604
21.005
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 1.5
4 Number of Scans 30
5 Spectrometer Frequency 100.62
6 Nucleus 13C
3p
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10



Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	298.1
4 Number of Scans	2
5 Spectrometer Frequency	400.13
6 Nucleus	1H



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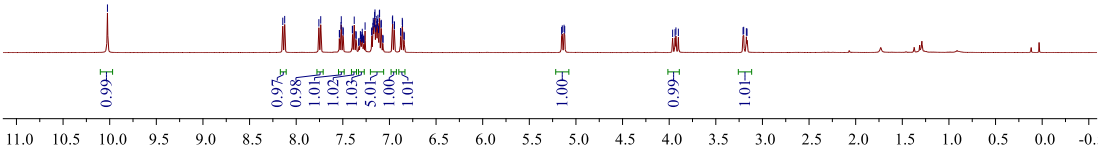
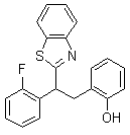


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	1.5
4 Number of Scans	40
5 Spectrometer Frequency	100.62
6 Nucleus	13C



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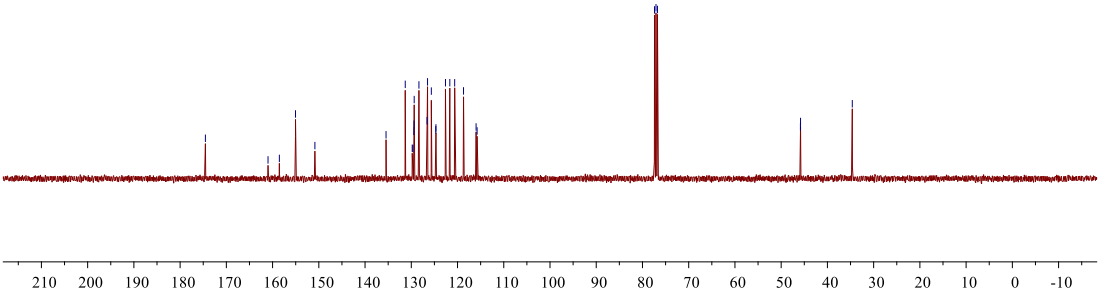
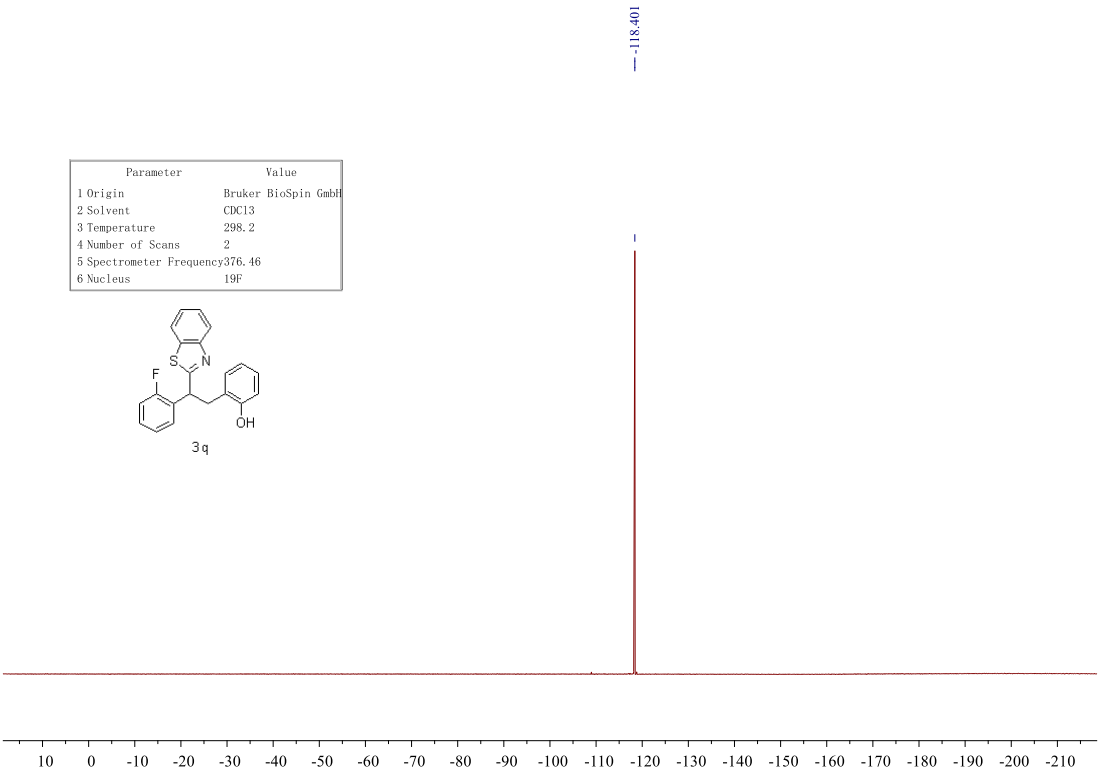
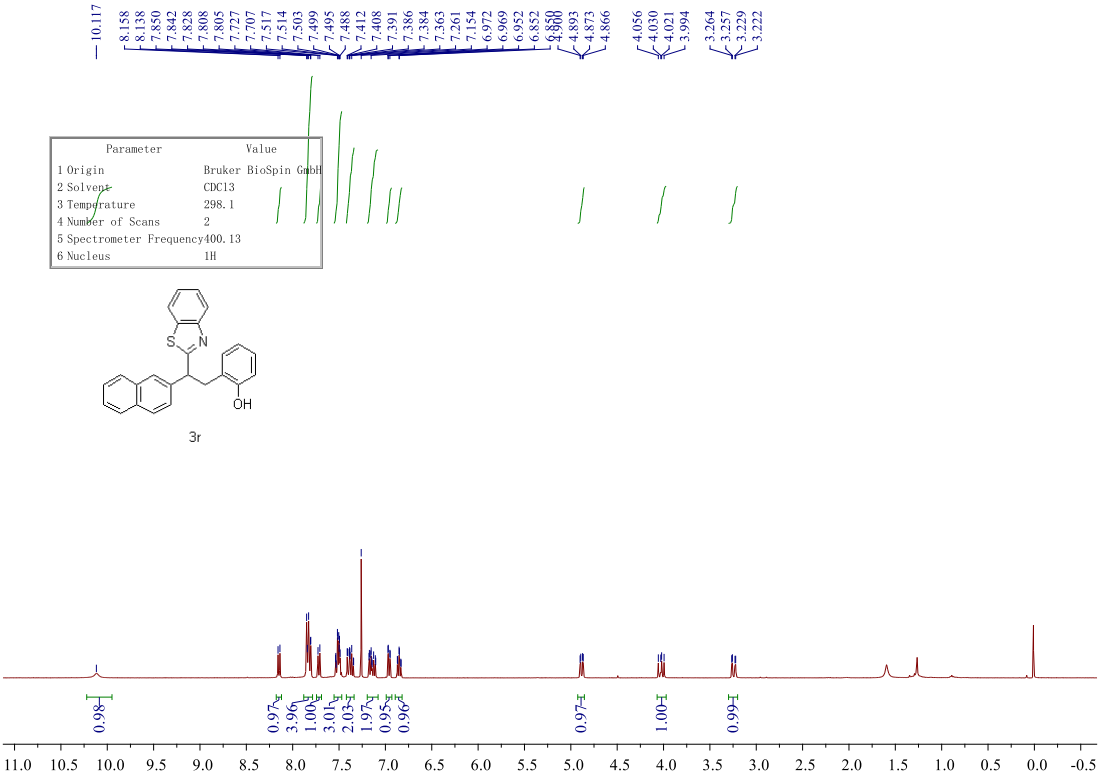



-118.401
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 376.46
6 Nucleus 19F
F
S
N
OH
3q
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210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7.805
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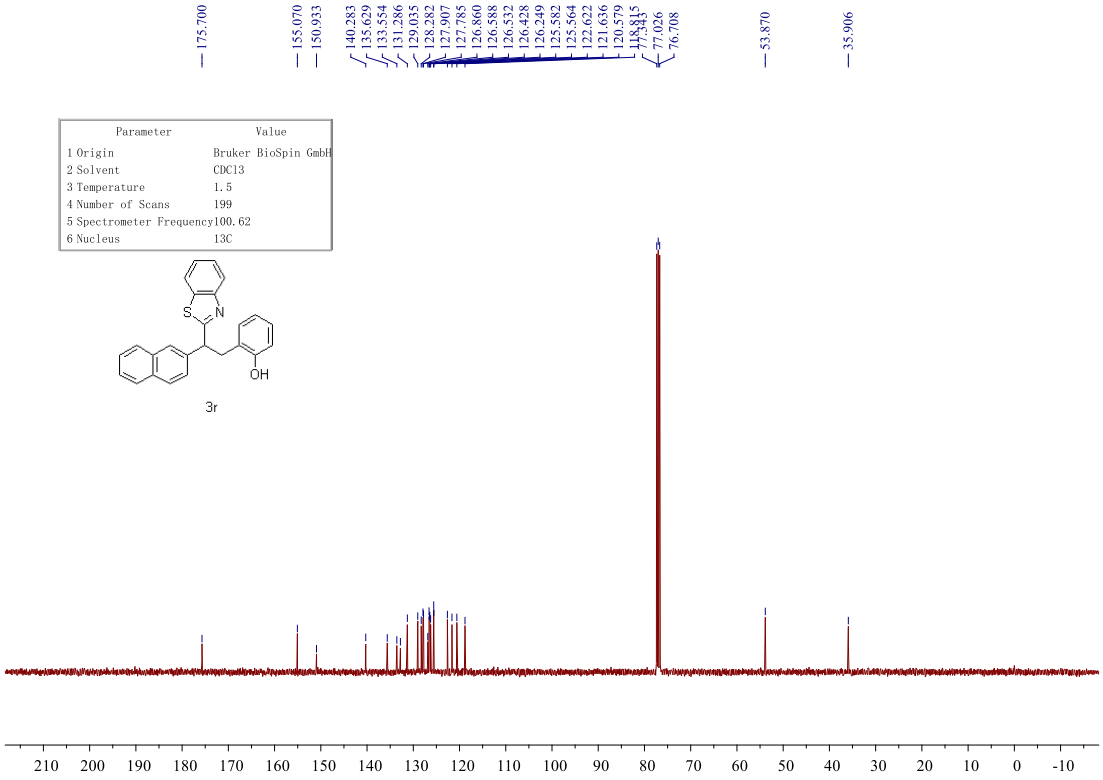
7.707
7.517
7.514
7.503
7.499
7.495
7.488
7.412
7.408
7.391
7.386
7.384
7.363
7.261
7.154
6.972
6.969
6.952
6.852
6.850
4.900
4.893
4.873
4.866
4.056
4.030
4.021
3.994
3.264
3.257
3.229
3.222
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
S
N
OH
3r
0.98
0.97
3.96
1.00
3.01
2.03
1.97
0.95
0.96
0.97
1.00
0.99
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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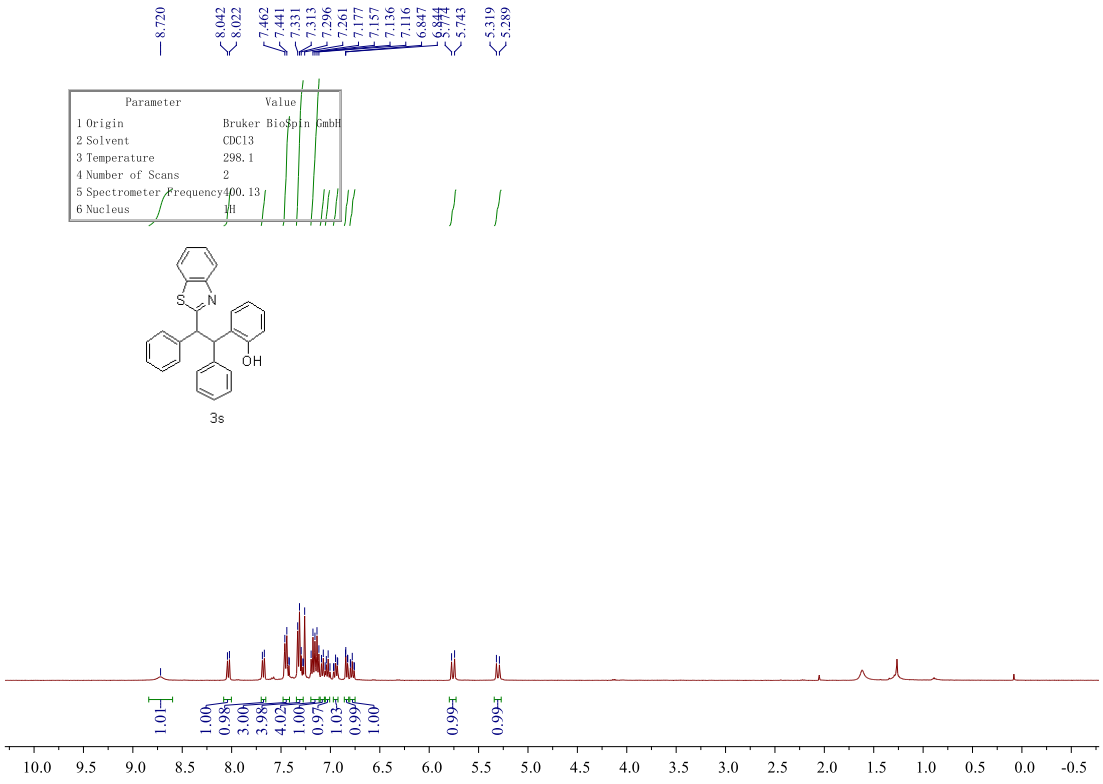
127.907
127.785
126.860
126.588
126.532
126.428
126.249
125.582
125.564
122.622
121.636
120.579
118.815
77.343
77.026
76.708
53.870
35.906
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 1.5
4 Number of Scans 199
5 Spectrometer Frequency 100.62
6 Nucleus 13C
S
N
OH
3r
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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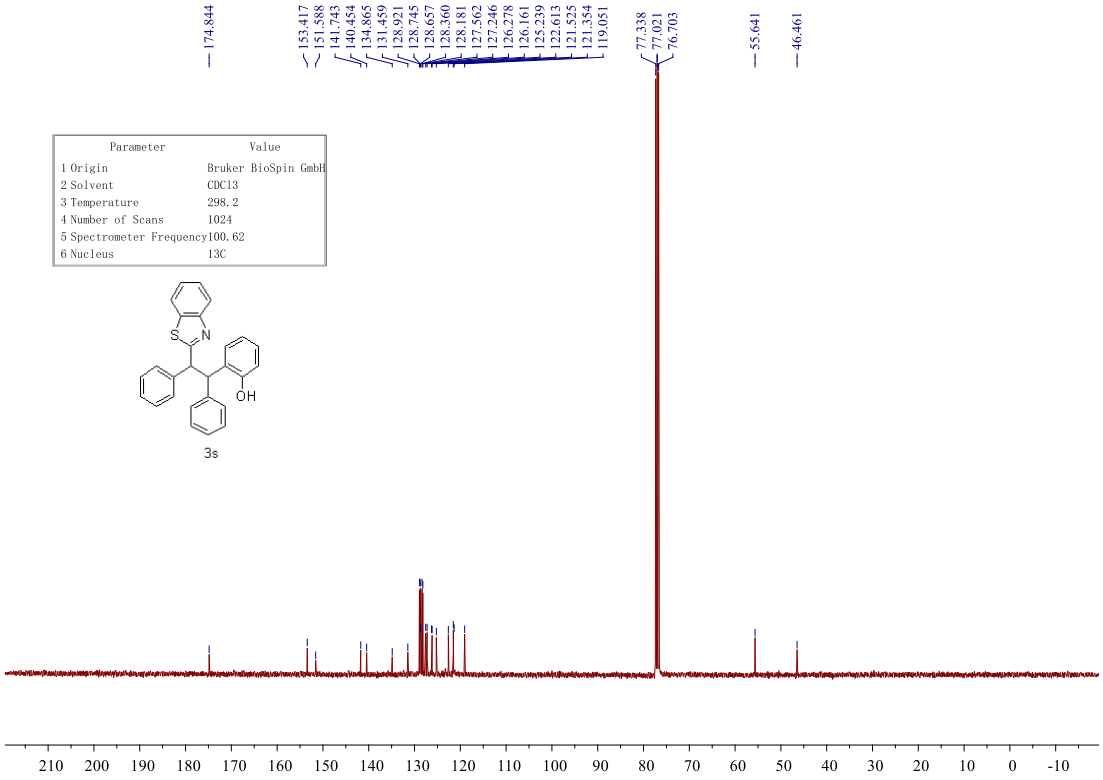
8.022
7.462
7.441
7.331
7.313
7.296
7.261
7.177
7.157
7.136
7.116
6.847
6.844
5.774
5.743
5.319
5.289
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
S
N
OH
3s
1.01
1.00
0.98
3.00
3.98
4.02
1.00
0.97
1.03
0.99
1.00
0.99
0.99
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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128.745
128.657
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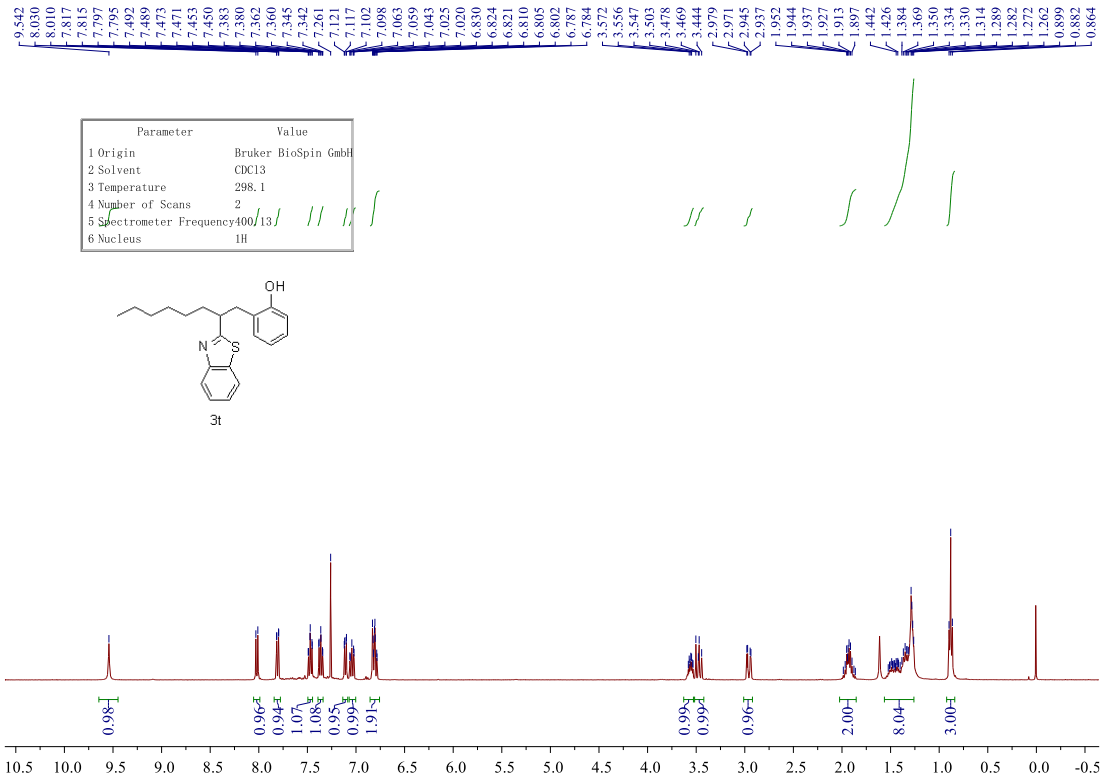
127.562
127.246
126.278
126.161
125.239
122.613
121.525
121.354
119.051
77.338
77.021
76.703
55.641
46.461
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 1024
5 Spectrometer Frequency 100.62
6 Nucleus 13C
S
N
OH
3s
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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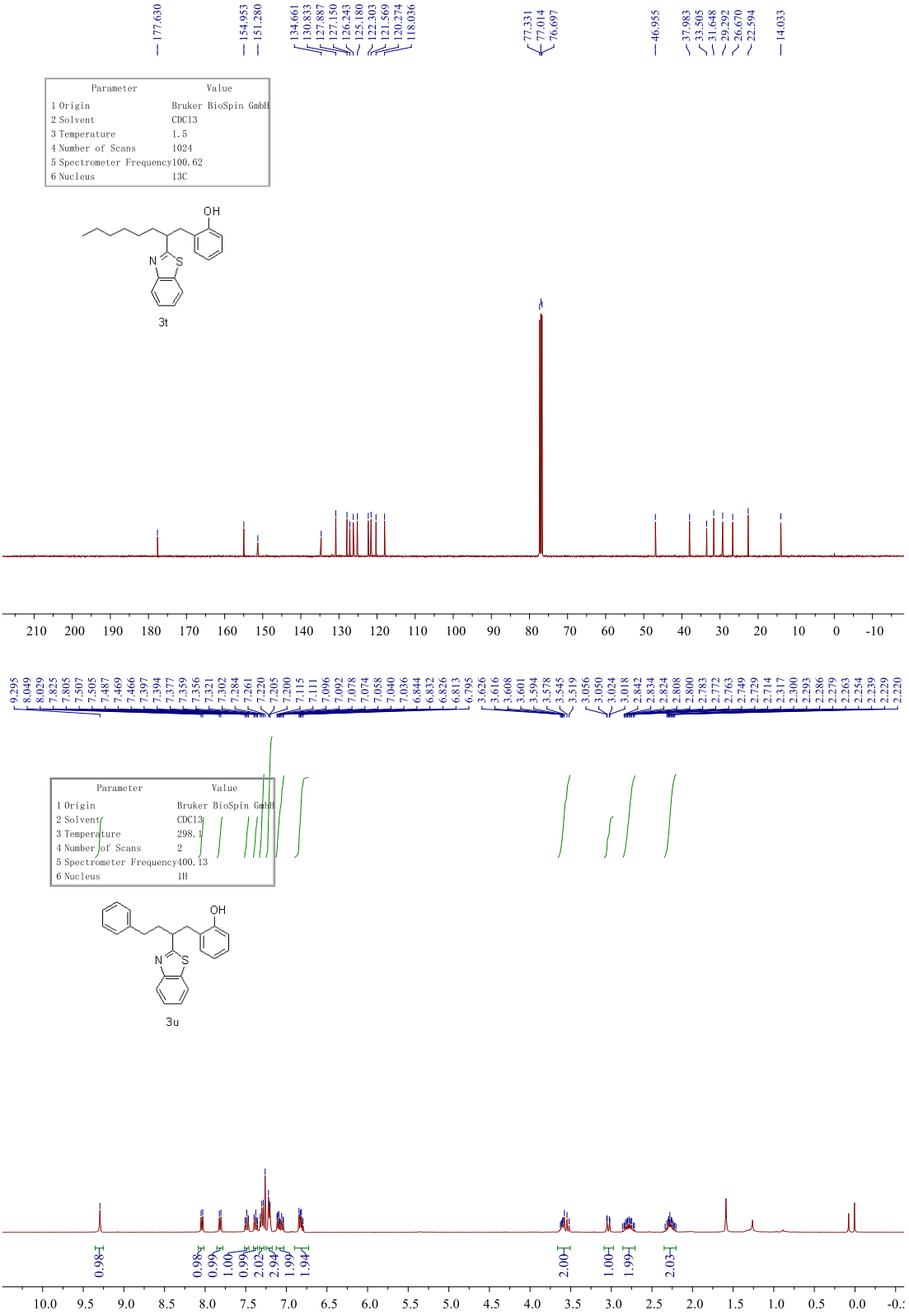
7.797
7.795
7.492
7.489
7.473
7.471
7.453
7.450
7.383
7.380
7.362
7.360
7.345
7.342
7.261
7.121
7.117
7.102
7.098
7.063
7.059
7.043
7.025
7.020
6.830
6.824
6.821
6.810
6.805
6.802
6.787
6.784
3.572
3.556
3.547
3.503
3.478
3.469
3.444
2.979
2.971
2.945
2.937
1.952
1.944
1.937
1.927
1.913
1.897
1.442
1.426
1.384
1.369
1.350
1.334
1.330
1.314
1.289
1.282
1.272
1.262
0.899
0.882
0.864
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
OH
N
S
3t
0.98
0.96
0.94
1.07
1.08
0.95
0.99
1.91
0.99
0.99
0.96
2.00
8.04
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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121.569
120.274
118.036
77.331
77.014
76.697
46.955
37.983
33.505
31.648
29.292
26.670
22.594
14.033
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 1.5
4 Number of Scans 1024
5 Spectrometer Frequency 100.62
6 Nucleus 13C
OH
N
S
3t
9.295
8.049
8.029
7.825
7.805
7.507
7.505
7.487
7.469
7.466
7.397
7.394
7.377
7.359
7.356
7.321
7.302
7.284
7.261
7.220
7.205
7.200
7.115
7.111
7.096
7.092
7.078
7.074
7.058
7.040
7.036
6.844
6.832
6.826
6.813
6.795
3.626
3.616
3.608
3.601
3.594
3.578
3.545
3.519
3.056
3.050
3.024
3.018
2.842
2.834
2.824
2.808
2.800
2.783
2.772
2.763
2.749
2.729
2.714
2.317
2.300
2.293
2.286
2.279
2.263
2.254
2.239
2.229
2.220
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
OH
N
S
3u
0.98
0.98
0.99
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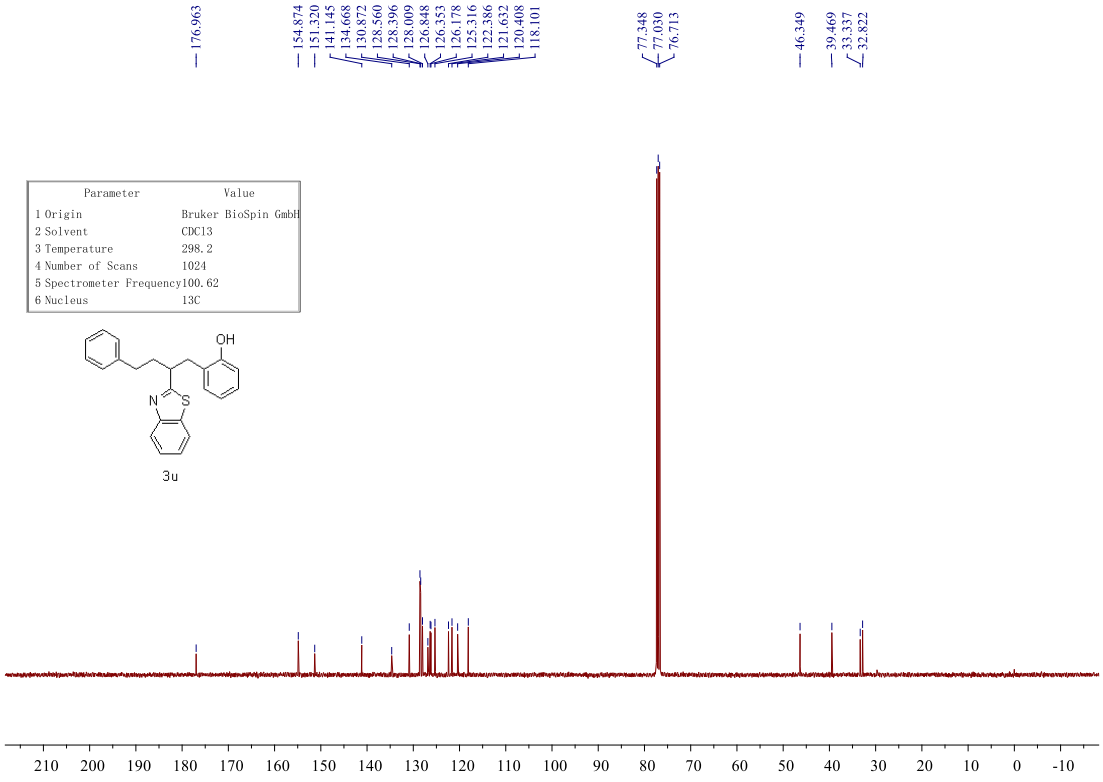
0.99
2.02
2.94
1.99
1.94
2.00
1.00
1.99
2.03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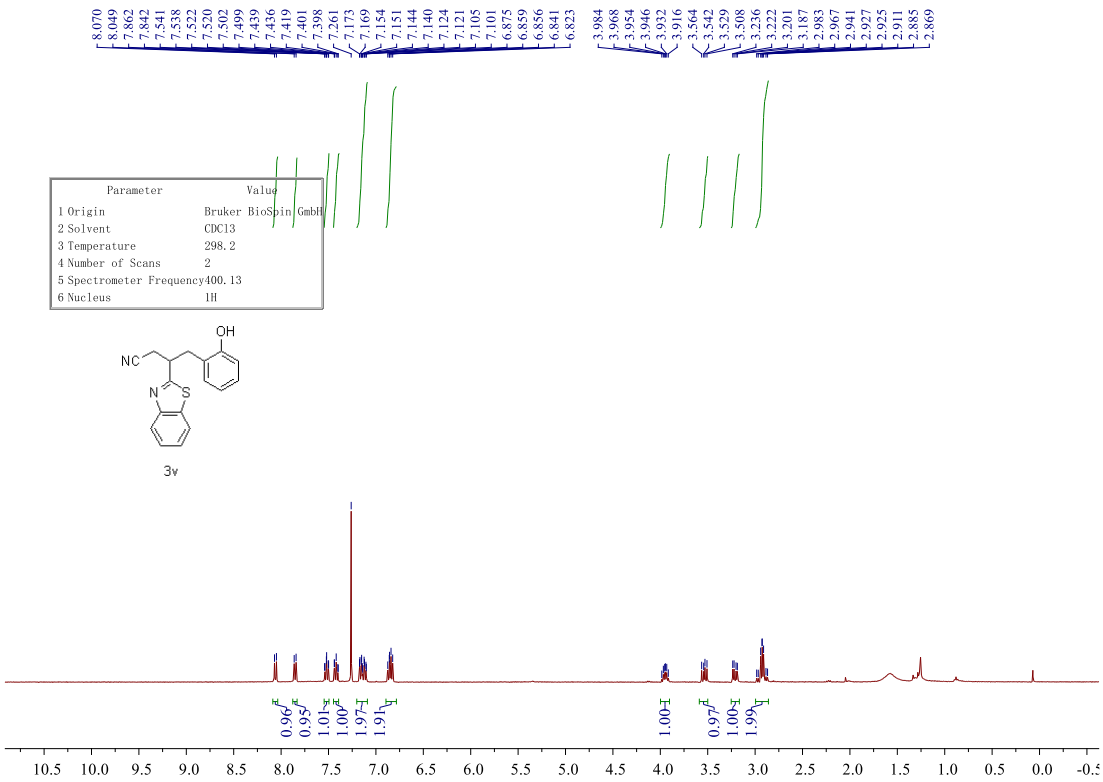
125.316
122.386
121.632
120.408
118.101
77.348
77.030
76.713
46.349
39.469
33.337
32.822
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 1024
5 Spectrometer Frequency 100.62
6 Nucleus 13C
OH
N
S
3u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7.520
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7.499
7.439
7.436
7.419
7.401
7.398
7.261
7.173
7.169
7.154
7.151
7.144
7.140
7.124
7.121
7.105
7.101
6.875
6.859
6.856
6.841
6.823
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3.968
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3.946
3.932
3.916
3.564
3.542
3.529
3.508
3.236
3.222
3.201
3.187
2.983
2.967
2.941
2.927
2.925
2.911
2.885
2.869
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
OH
NC
N
S
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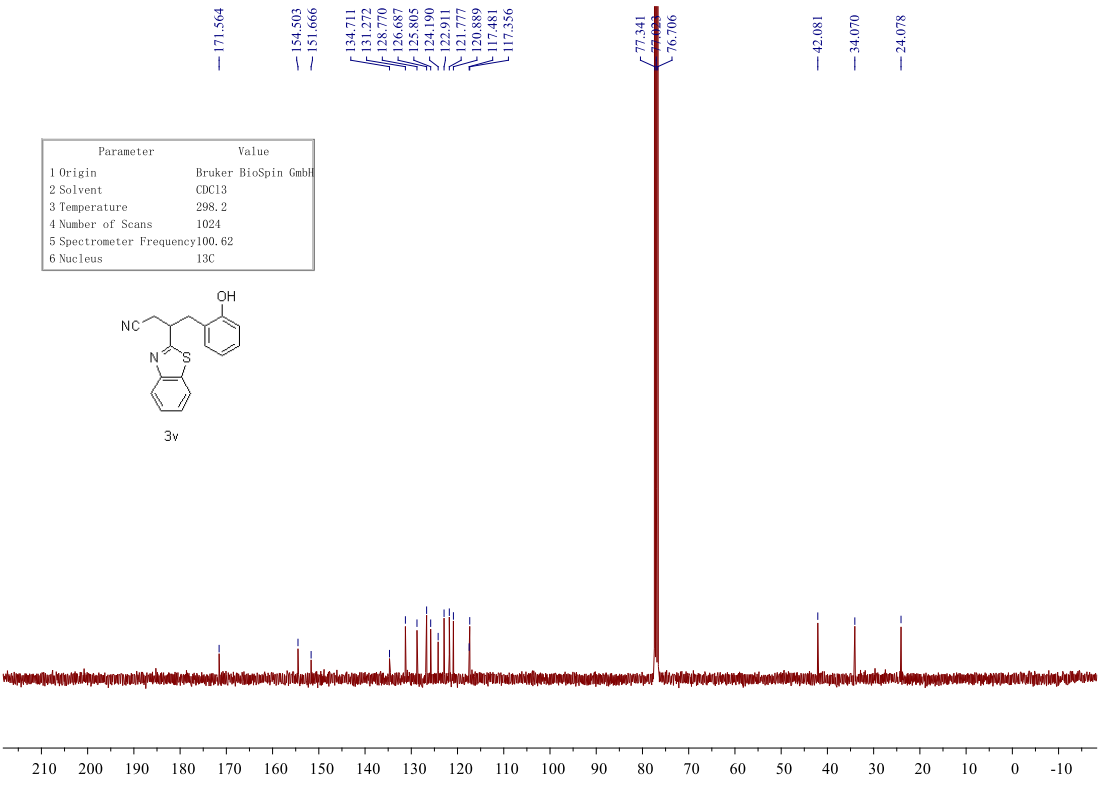
1.91
1.00
0.97
1.00
1.99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134.711
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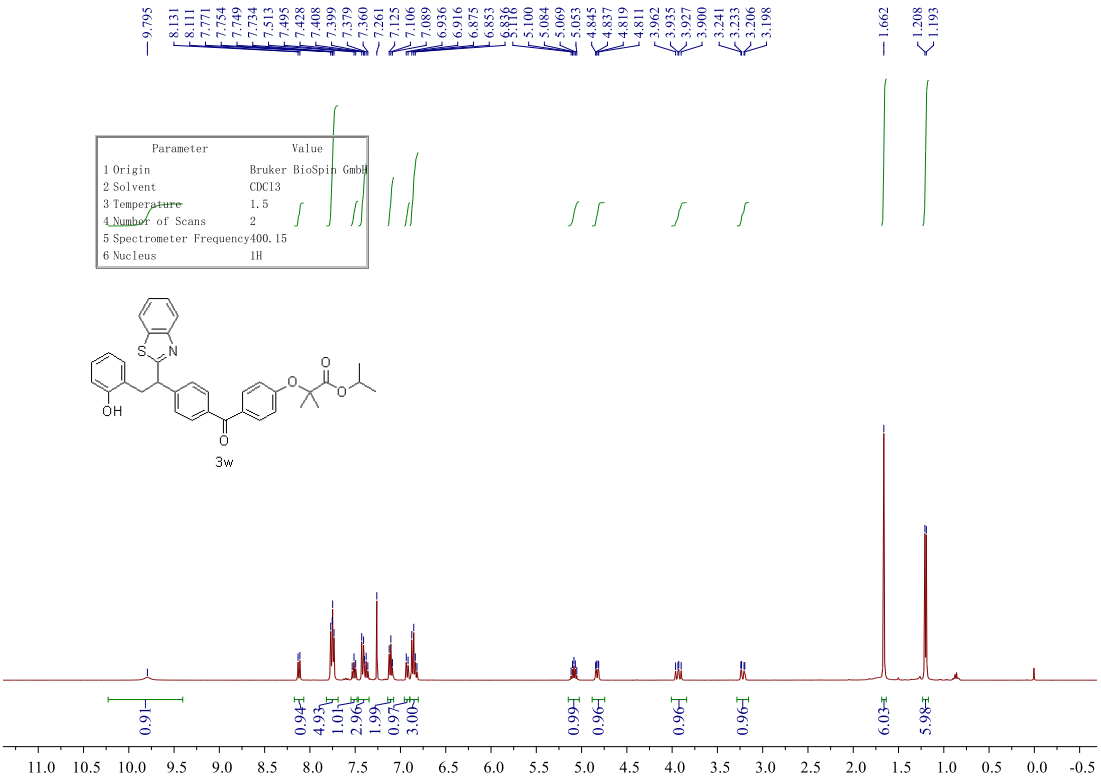
121.777
120.889
117.481
117.356
77.341
77.023
76.706
42.081
34.070
24.078
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 1024
5 Spectrometer Frequency 100.62
6 Nucleus 13C
OH
NC
N
S
3v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7.408
7.399
7.379
7.360
7.261
7.125
7.106
7.089
6.936
6.916
6.875
6.853
5.118
5.100
5.084
5.069
5.053
4.845
4.837
4.819
4.811
3.962
3.935
3.927
3.900
3.241
3.233
3.206
3.198
1.662
1.208
1.193
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 1.5
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
S
N
OH
O
O
O
O
3w
0.91
0.94
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0.96
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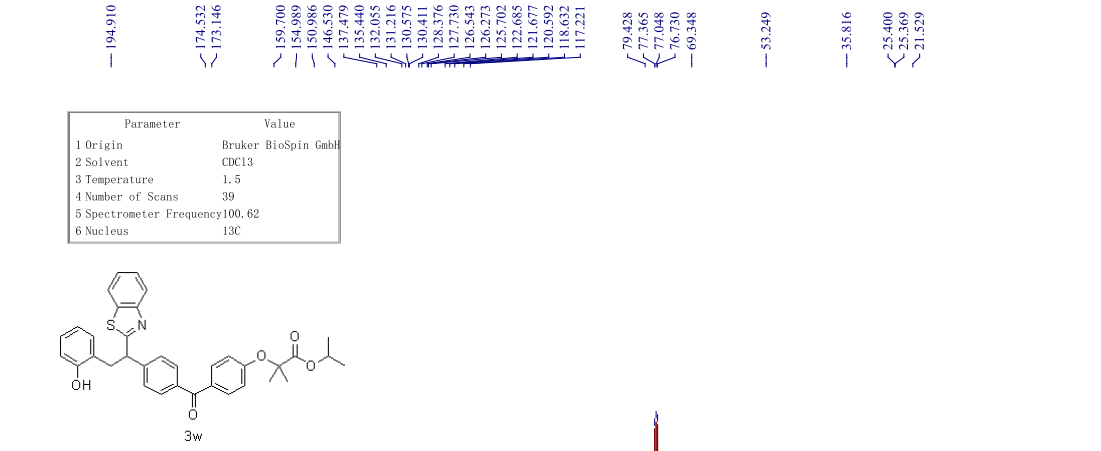
5.98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130.411
128.376
127.730
126.543
126.273
125.702
122.685
121.677
120.592
118.632
117.221
79.428
77.365
77.048
76.730
69.348
53.249
35.816
25.400
25.369
21.529
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 1.5
4 Number of Scans 39
5 Spectrometer Frequency 100.62
6 Nucleus 13C
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S
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O
O
O
O
3w
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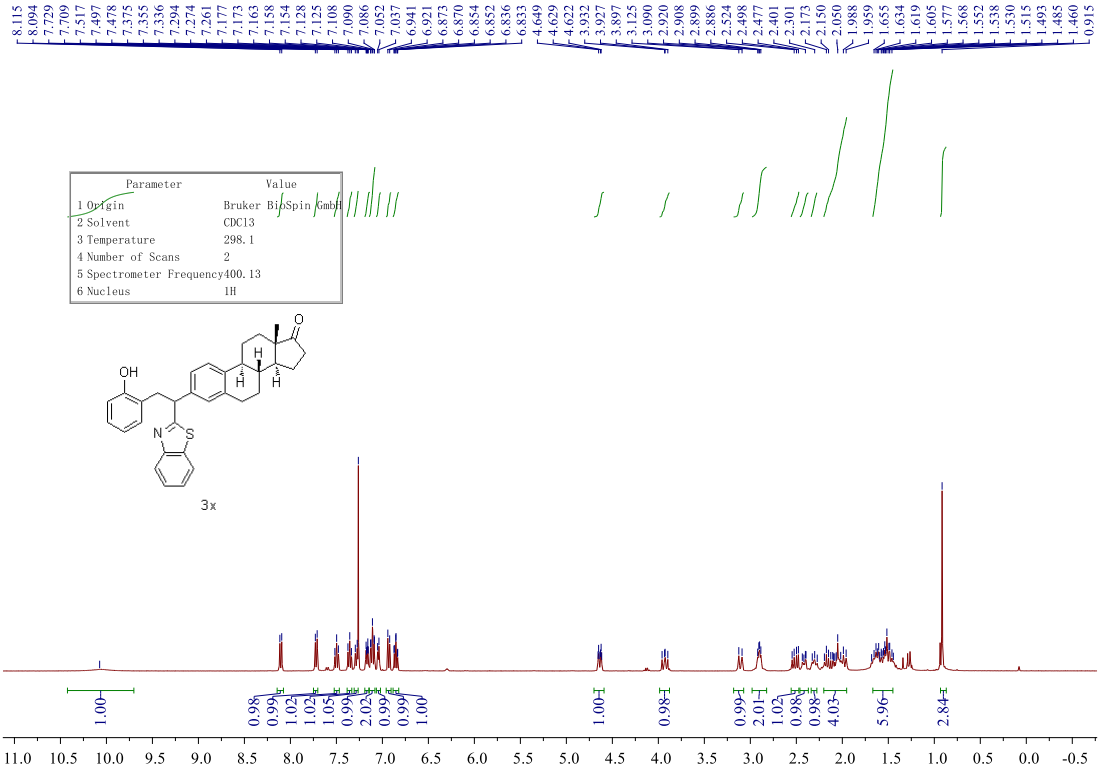
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7.294
7.274
7.261
7.177
7.173
7.163
7.158
7.154
7.128
7.125
7.108
7.090
7.086
7.052
7.037
6.941
6.921
6.873
6.870
6.854
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6.836
6.833
4.649
4.629
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3.932
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3.897
3.125
3.090
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2.899
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2.524
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2.173
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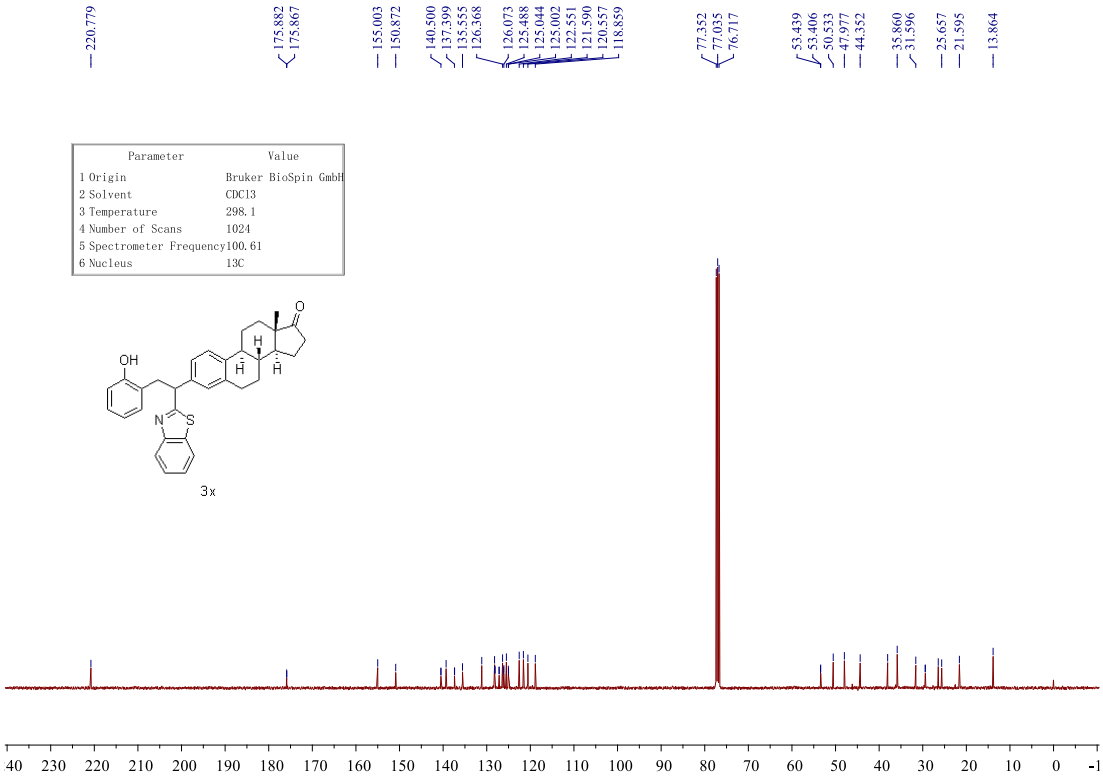
2.050
1.988
1.959
1.655
1.634
1.619
1.605
1.577
1.568
1.552
1.538
1.530
1.515
1.493
1.485
1.460
0.915
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
OH
N
S
O
H
H
H
3x
1.00
0.98
0.99
1.02
1.02
1.05
0.99
2.02
0.99
0.99
1.00
1.00
0.98
0.99
2.01
1.02
0.98
0.98
4.03
5.96
2.84
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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122.551
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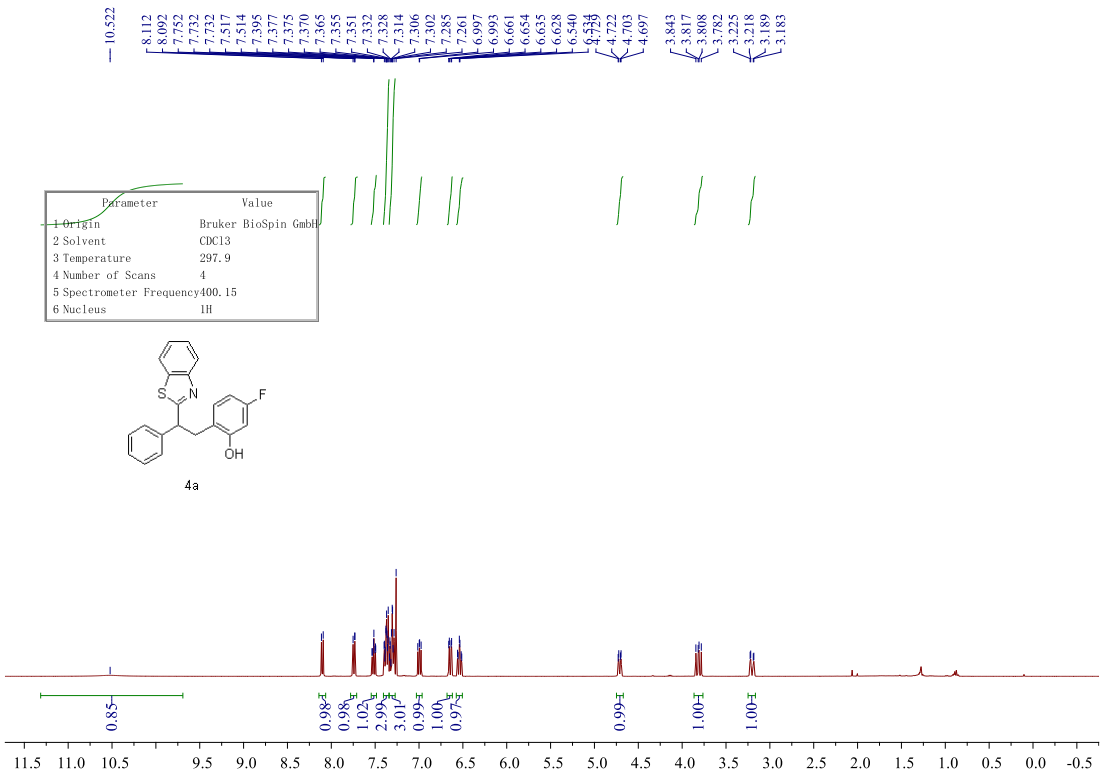
77.352
77.035
76.717
53.439
53.406
50.533
47.977
44.352
35.860
31.596
25.657
21.595
13.864
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
OH
O
H
N
S
3x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7.377
7.375
7.370
7.365
7.355
7.351
7.332
7.328
7.314
7.306
7.302
7.285
7.261
6.997
6.993
6.661
6.654
6.635
6.628
6.540
4.722
4.703
4.697
3.843
3.817
3.808
3.782
3.225
3.218
3.189
3.183
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 297.9
4 Number of Scans 4
5 Spectrometer Frequency 400.15
6 Nucleus 1H
S
N
F
OH
4a
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3.01
0.99
1.00
0.97
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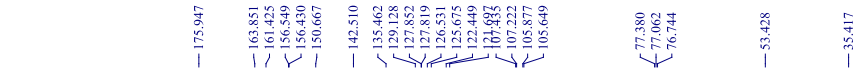
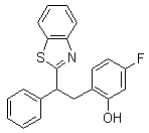
1.00
1.00



Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	300.4
4 Number of Scans	71
5 Spectrometer Frequency	100.62
6 Nucleus	13C



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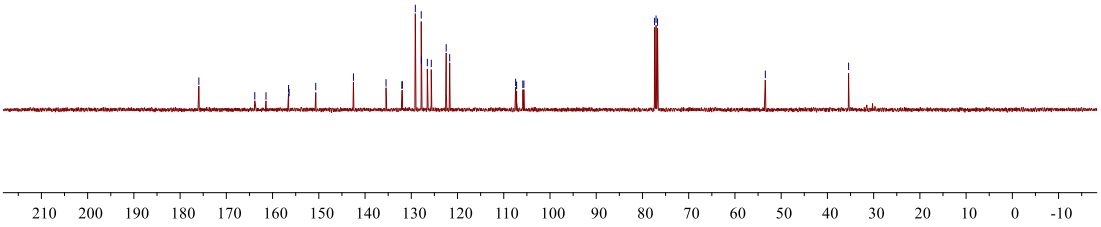
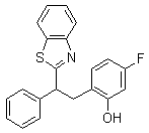
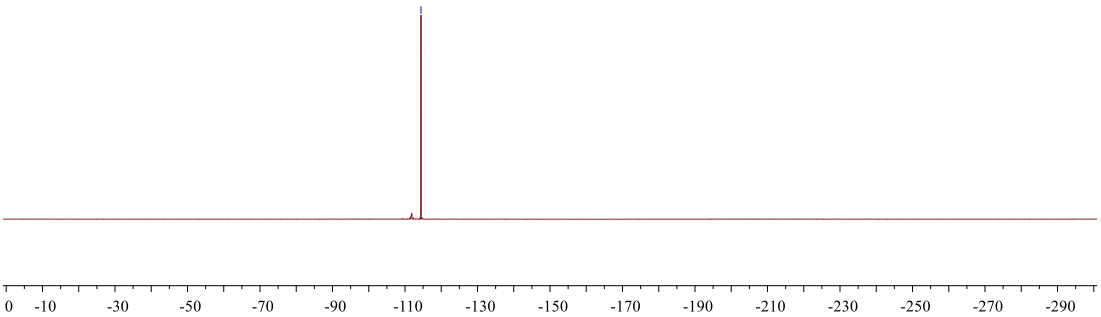
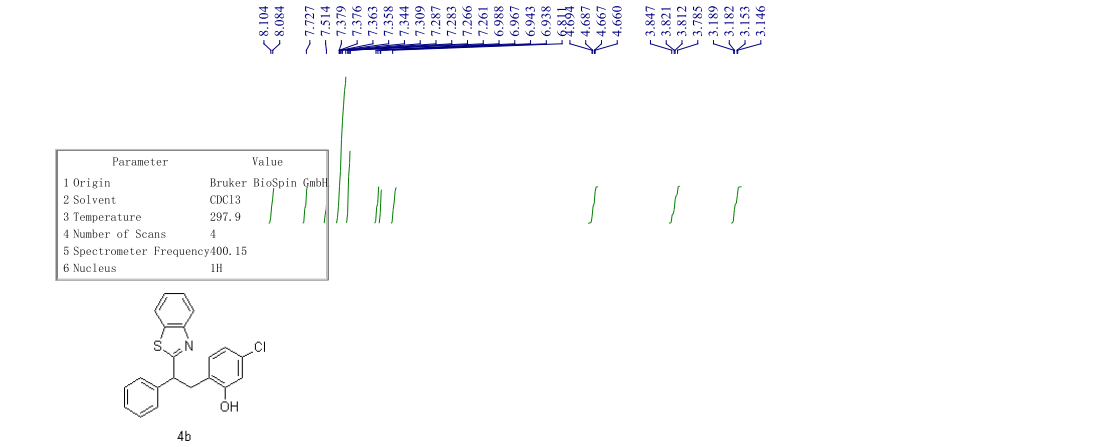


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	300.2
4 Number of Scans	4
5 Spectrometer Frequency	376.52
6 Nucleus	19F



4a

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7.727
7.514
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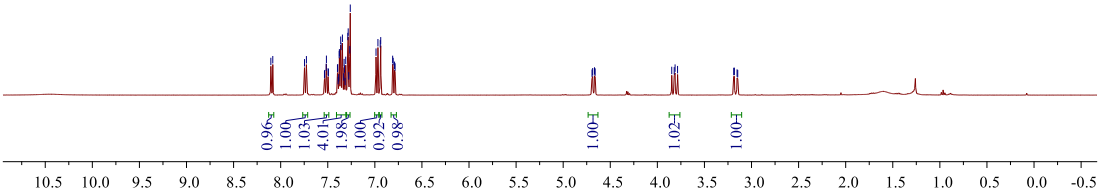
7.376
7.365
7.358
7.344
7.309
7.287
7.283
7.266
7.261
6.988
6.967
6.943
6.938
6.881
4.694
4.687
4.667
4.660
3.847
3.821
3.812
3.785
3.189
3.182
3.153
3.146
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 297.9
4 Number of Scans 4
5 Spectrometer Frequency 400.15
6 Nucleus 1H
S
N
Cl
OH

4b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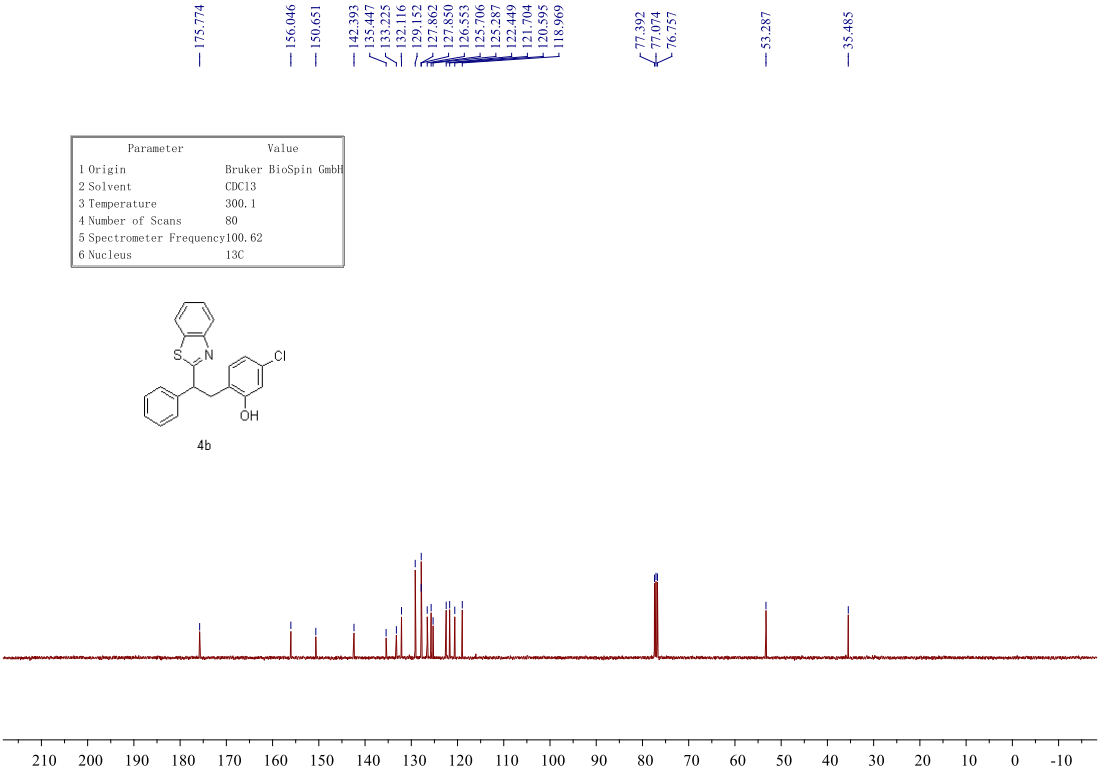
1.00
1.03
4.01
1.98
1.00
0.92
0.98
1.00
1.02
1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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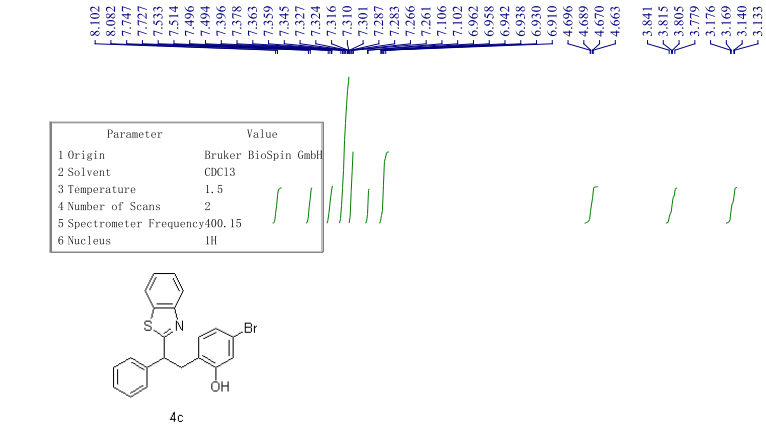
150.651
142.393
135.447
133.225
132.116
129.152
127.862
127.850
126.553
125.706
125.287
122.449
121.704
120.595
118.969
77.392
77.074
76.757
53.287
35.485
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 300.1
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
S
N
Cl
OH
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

4b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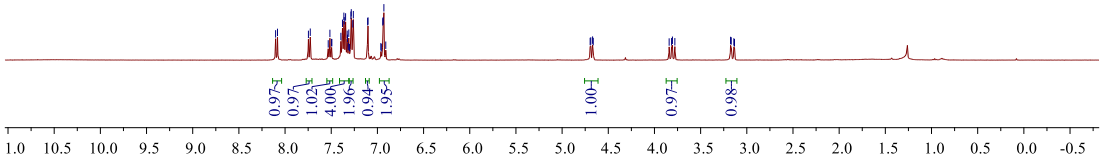
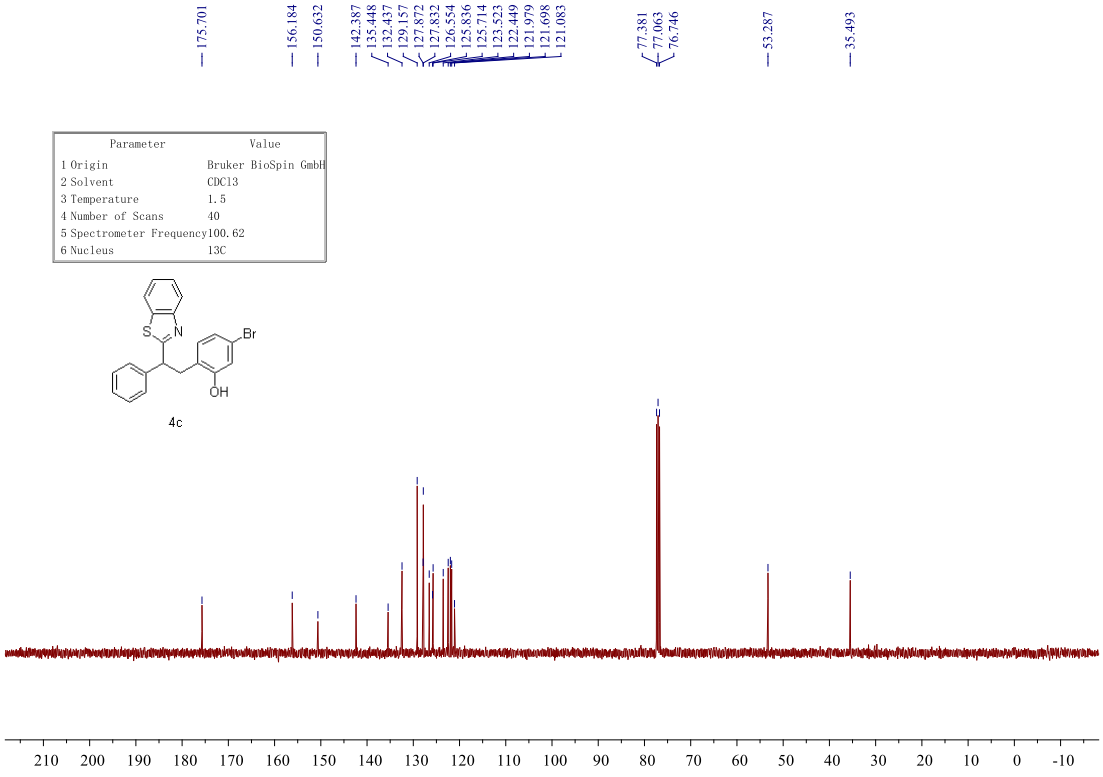
7.747
7.727
7.533
7.514
7.496
7.494
7.396
7.378
7.363
7.359
7.345
7.327
7.324
7.316
7.310
7.301
7.287
7.283
7.266
7.261
7.106
7.102
6.962
6.958
6.942
6.938
6.930
6.910
4.696
4.689
4.670
4.663
3.841
3.815
3.805
3.779
3.176
3.169
3.140
3.133
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 1.5
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
S
N
Br
OH

4c


0.97
0.97
1.02
4.00
1.96
0.94
1.95
1.00
0.97
0.98
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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132.437
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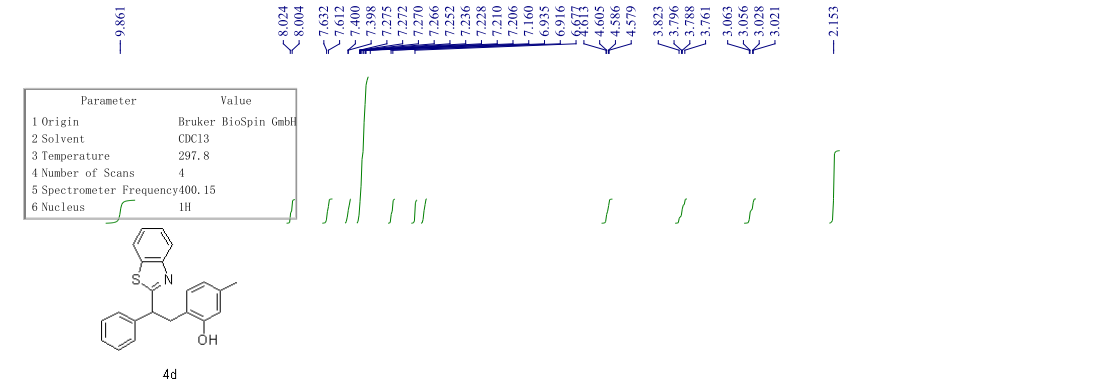
126.554
125.836
125.714
123.523
122.449
121.979
121.698
121.083
77.381
77.063
76.746
53.287
35.493
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 1.5
4 Number of Scans 40
5 Spectrometer Frequency 100.62
6 Nucleus 13C
S
N
Br
OH
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

4c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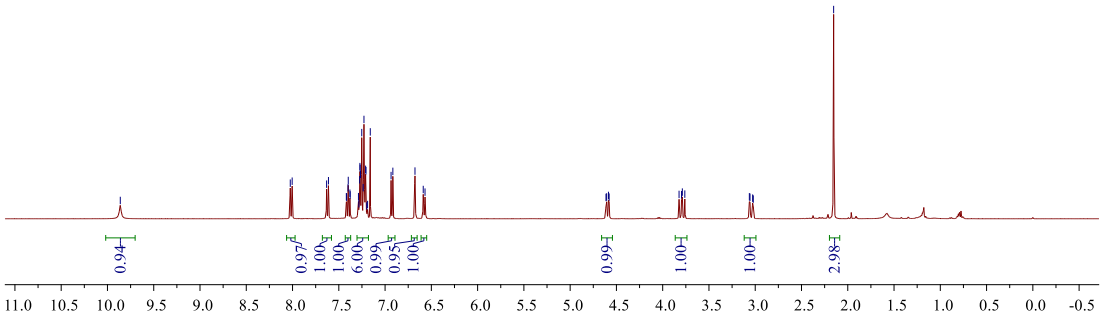
7.400
7.398
7.275
7.272
7.270
7.266
7.252
7.236
7.228
7.210
7.206
7.160
6.935
6.916
4.605
4.586
4.579
3.823
3.796
3.788
3.761
3.063
3.056
3.028
3.021
2.153
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 297.8
4 Number of Scans 4
5 Spectrometer Frequency 400.15
6 Nucleus 1H
S
N
OH

4d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0.97
1.00
1.00
6.00
0.99
0.95
1.00
0.99
1.00
1.00
2.98
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5


175.756
154.802
150.919
142.974
138.231
135.554
131.028
129.100
127.778
127.684
126.380
125.503
123.779
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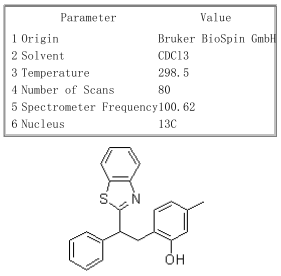
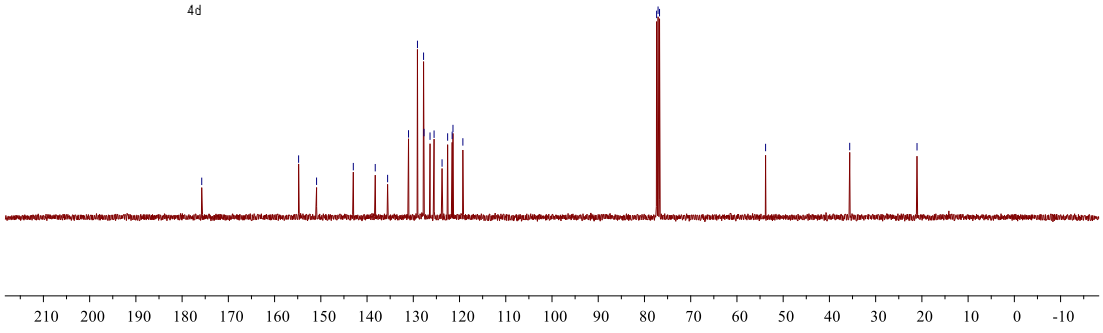
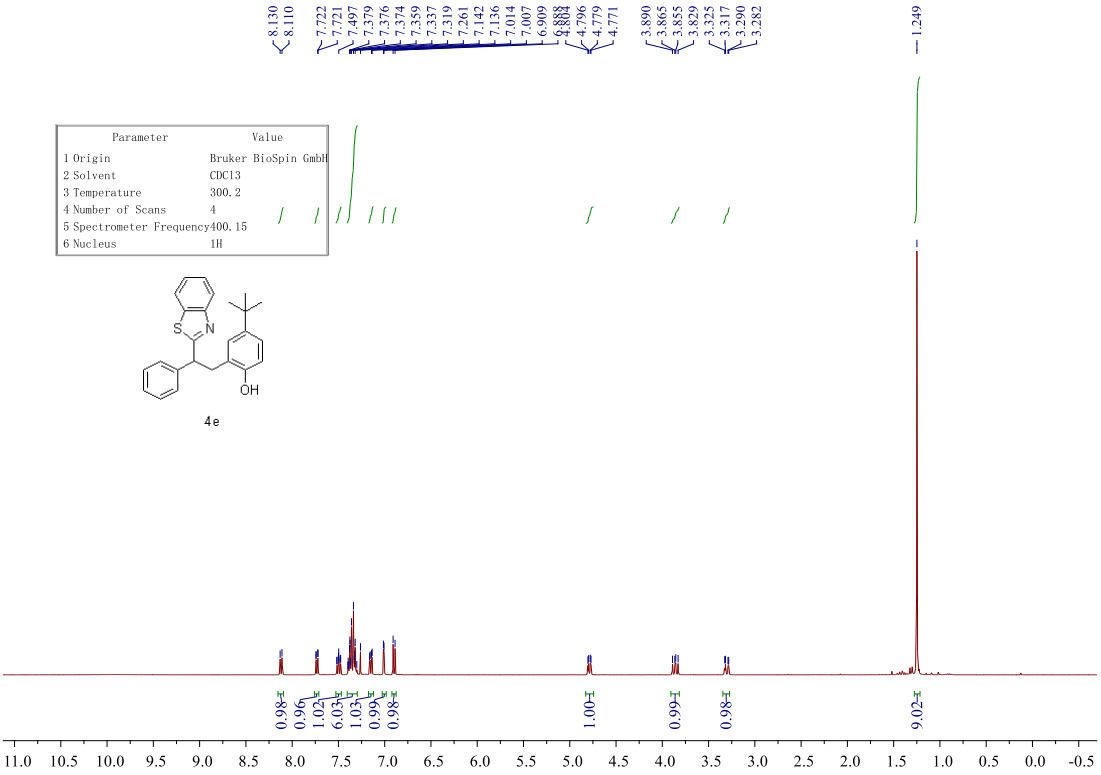
121.598
121.416
119.275
77.376
77.059
76.741
53.804
35.609
21.053


Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.5
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
S
N
OH

4d


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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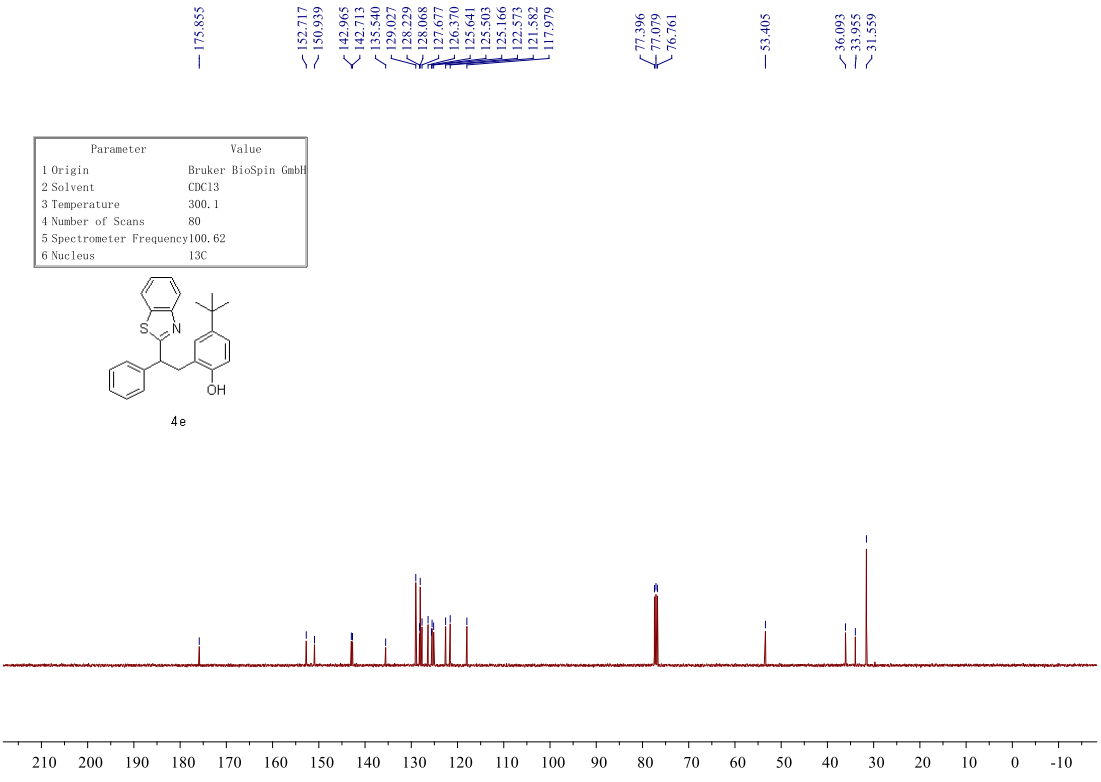
7.721
7.497
7.379
7.376
7.374
7.359
7.337
7.319
7.261
7.142
7.136
7.014
7.007
6.909
4.796
4.779
4.771
3.890
3.865
3.855
3.829
3.325
3.317
3.290
3.282
1.249
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 300.2
4 Number of Scans 4
5 Spectrometer Frequency 400.15
6 Nucleus 1H
S
N
OH
4e
0.98
0.96
1.02
6.03
1.03
0.99
0.98
1.00
0.99
0.98
9.02
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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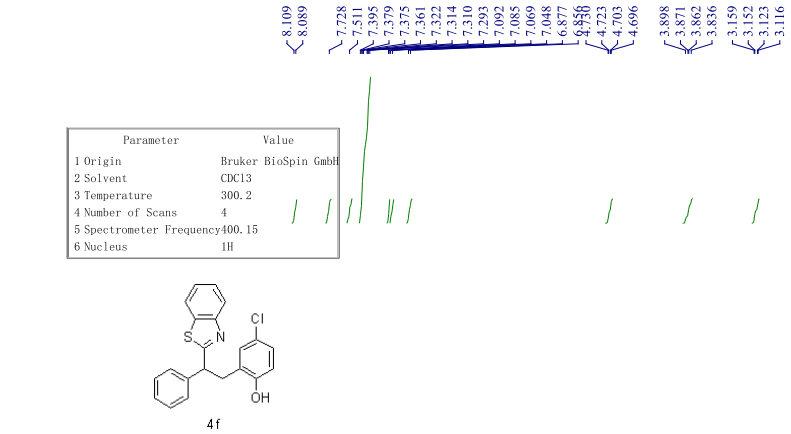
126.370
125.641
125.503
125.166
122.573
121.582
117.979
77.396
77.079
76.761
53.405
36.093
33.955
31.559
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 300.1
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
S
N
OH
4e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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7.379
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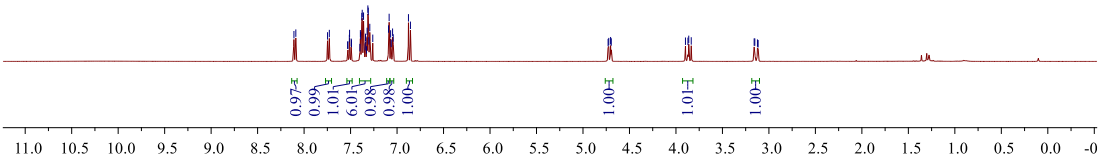
7.361
7.322
7.314
7.310
7.293
7.092
7.085
7.069
7.048
6.877
6.856
4.730
4.723
4.703
4.696
3.898
3.871
3.862
3.836
3.159
3.152
3.123
3.116
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 300.2
4 Number of Scans 4
5 Spectrometer Frequency 400.15
6 Nucleus 1H
Cl
S
N
OH

4f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0.99
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0.98
0.98
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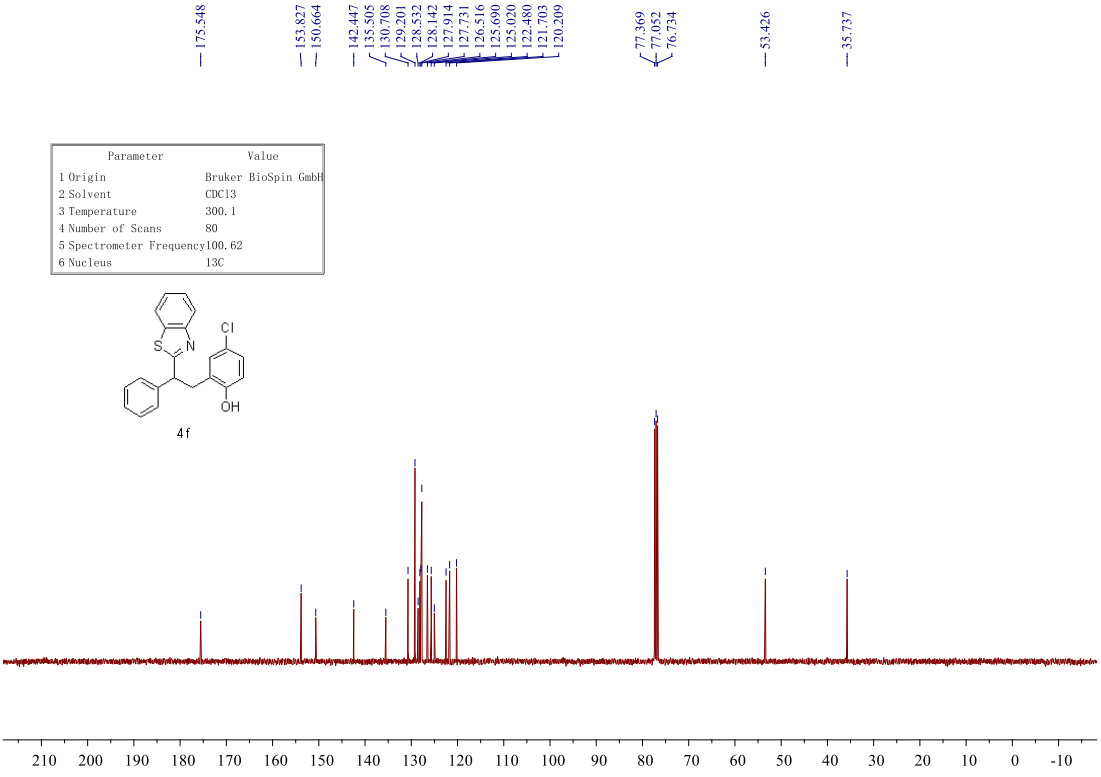
1.00
1.01
1.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0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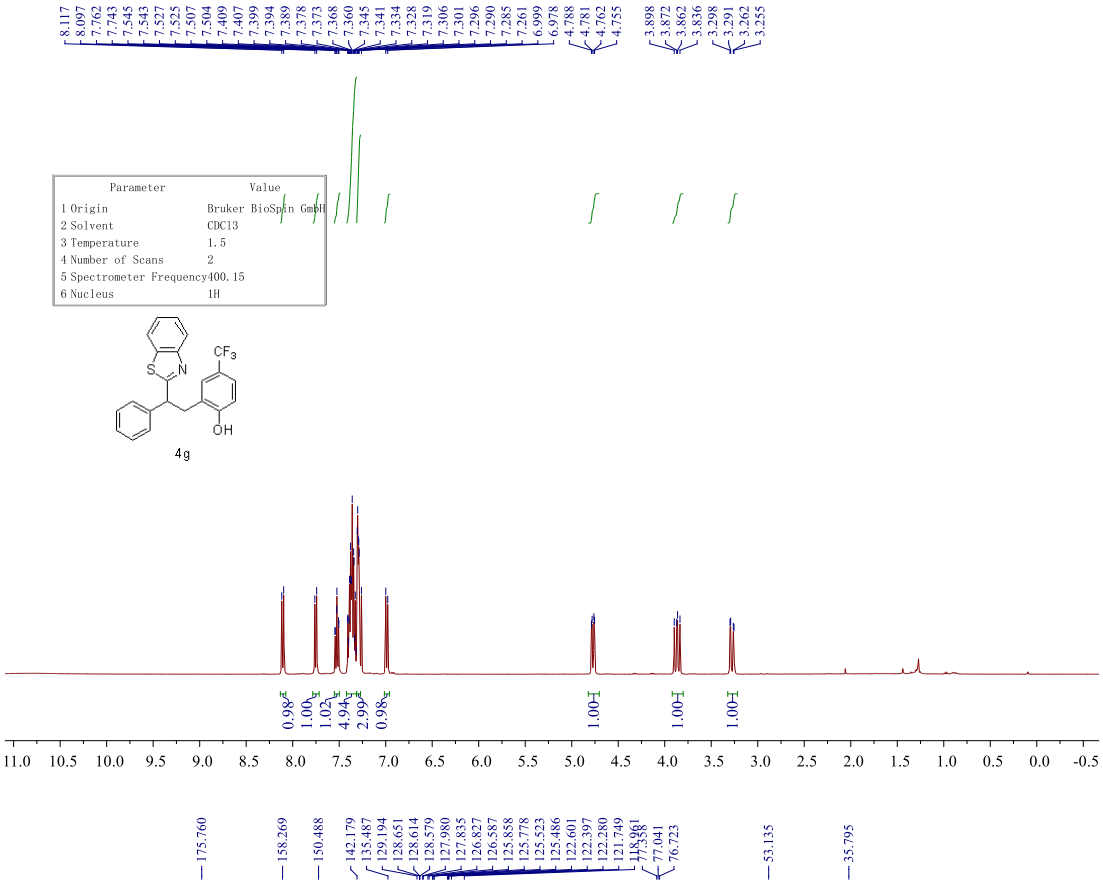
128.142
127.914
127.731
126.516
125.690
125.020
122.480
121.703
120.209
77.369
77.052
76.734
53.426
35.737
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 300.1
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
Cl
S
N
OH
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

4f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7.525
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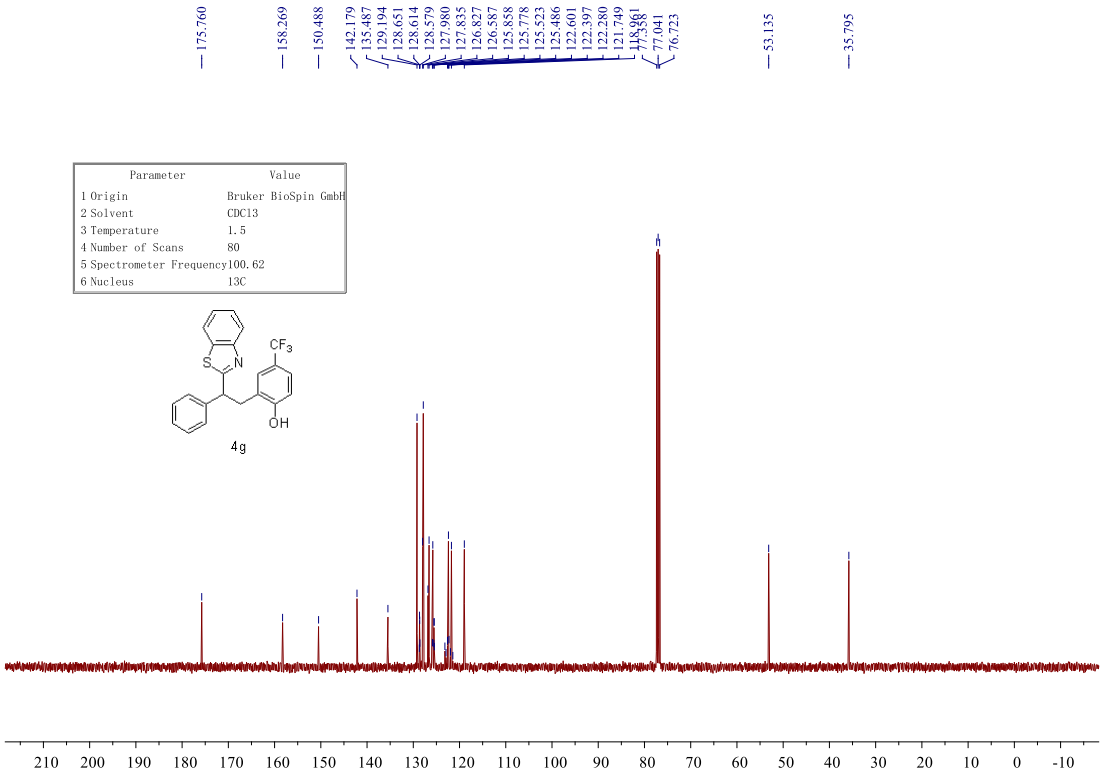
7.407
7.399
7.394
7.389
7.378
7.373
7.368
7.360
7.345
7.341
7.334
7.328
7.319
7.306
7.301
7.296
7.290
7.285
7.261
6.999
6.978
4.788
4.781
4.762
4.755
3.898
3.872
3.862
3.836
3.298
3.291
3.262
3.255
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 1.5
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
CF3
S
N
OH
4g
0.98
1.00
1.02
4.94
2.99
0.98
1.00
1.00
1.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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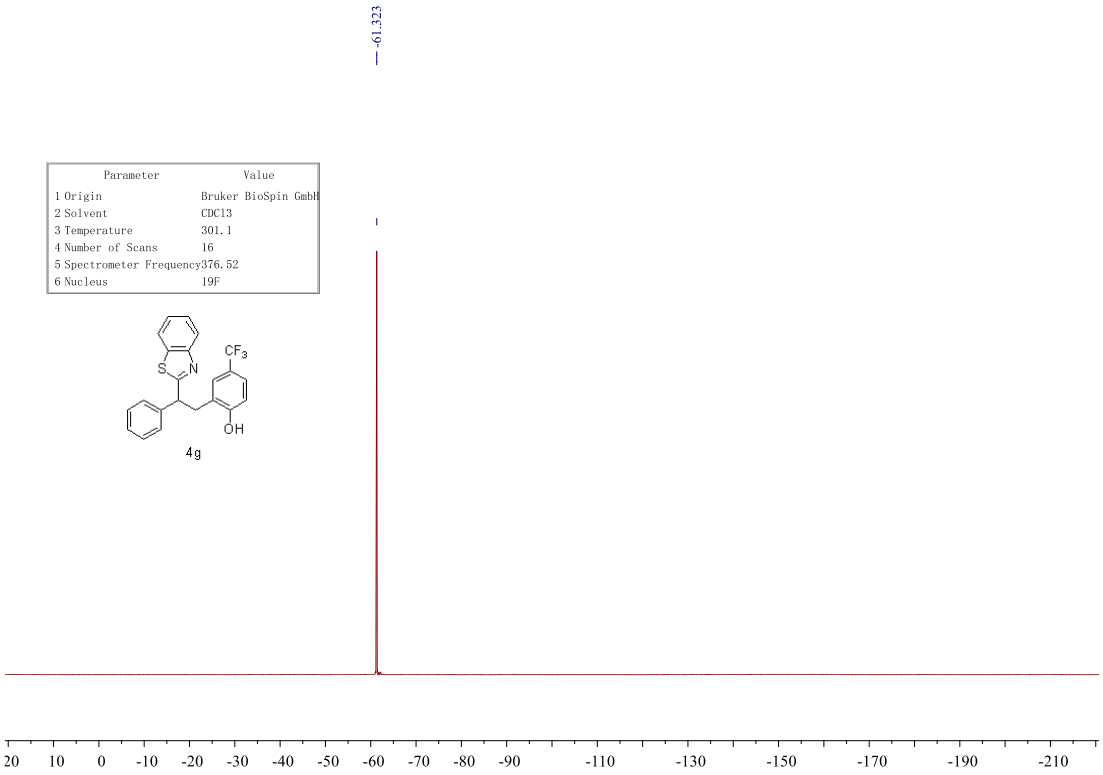
127.835
126.827
126.587
125.858
125.778
125.523
125.486
122.601
122.397
122.280
121.749
118.961
77.358
77.041
76.723
53.135
35.795
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 1.5
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
CF3
S
N
OH
4g
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 301.1
4 Number of Scans 16
5 Spectrometer Frequency 376.52
6 Nucleus 19F
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S
N
OH
4g
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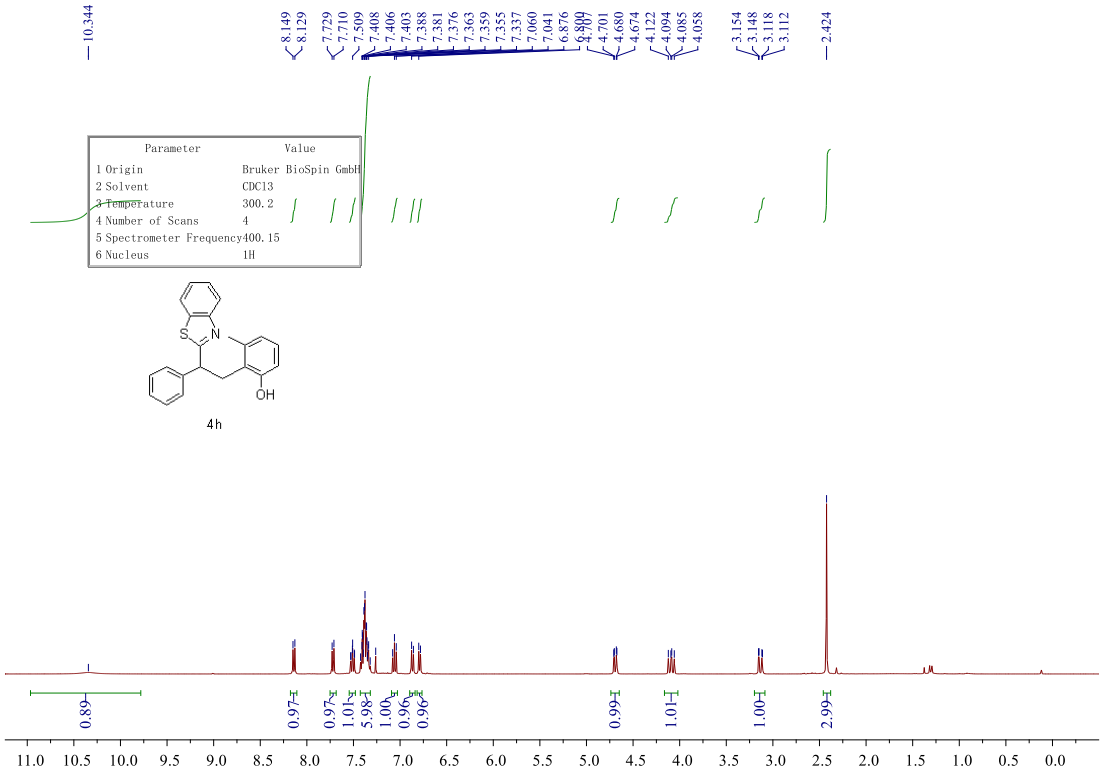
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7.388
7.381
7.376
7.363
7.359
7.355
7.337
7.060
7.041
6.876
6.800
6.797
4.701
4.680
4.674
4.122
4.094
4.085
4.058
3.154
3.148
3.118
3.112
2.424
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 300.2
4 Number of Scans 4
5 Spectrometer Frequency 400.15
6 Nucleus 1H
S
N
OH
4h
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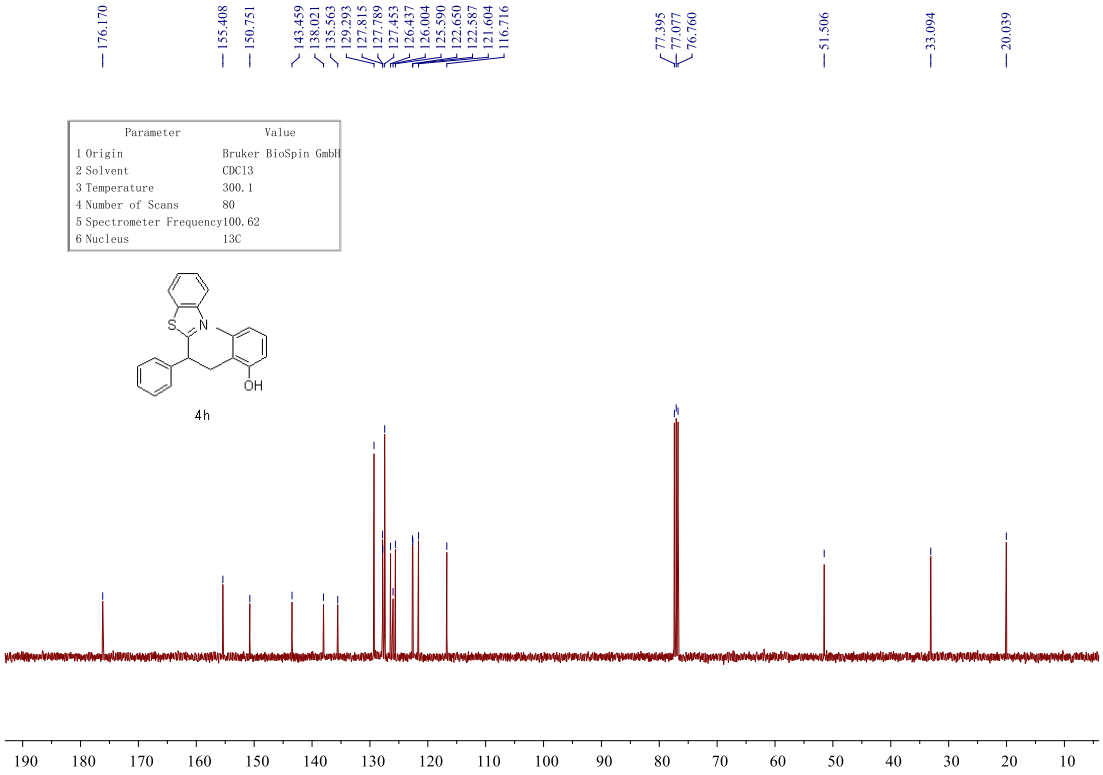
0.97
1.01
5.98
1.00
0.96
0.96
0.99
1.01
1.00
2.99
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0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126.437
126.004
125.590
122.650
122.587
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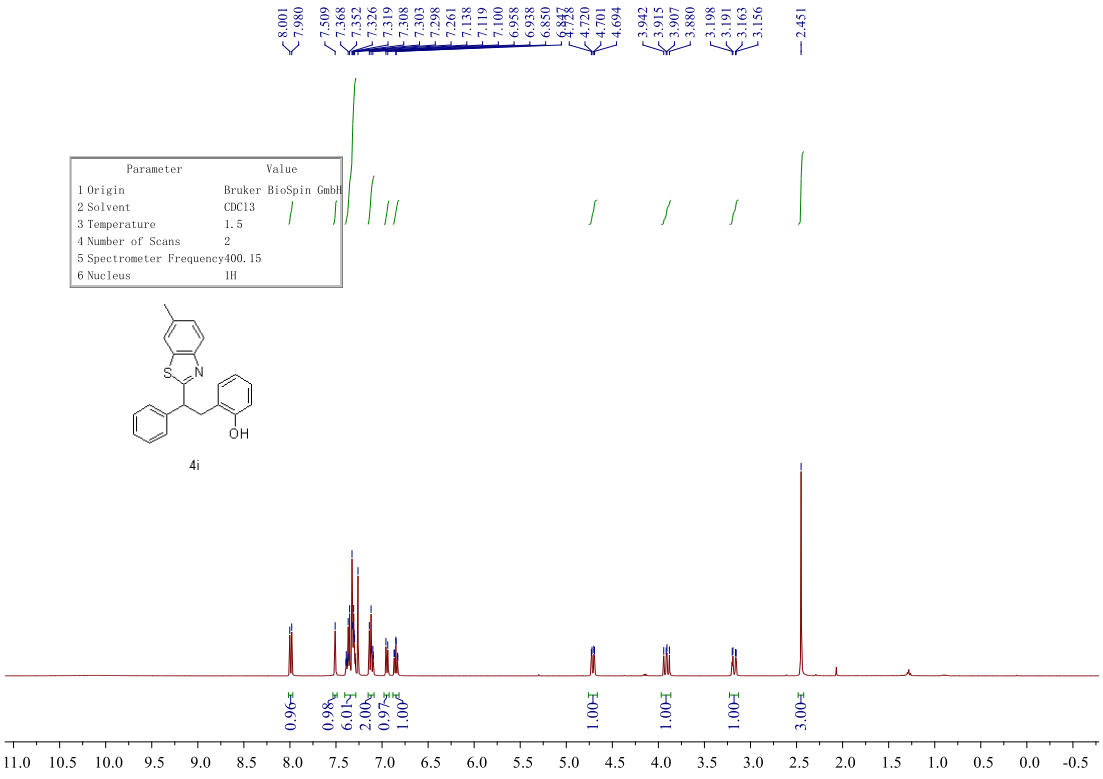
116.716
77.395
77.077
76.760
51.506
33.094
20.039
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 300.1
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
S
N
OH
4h
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10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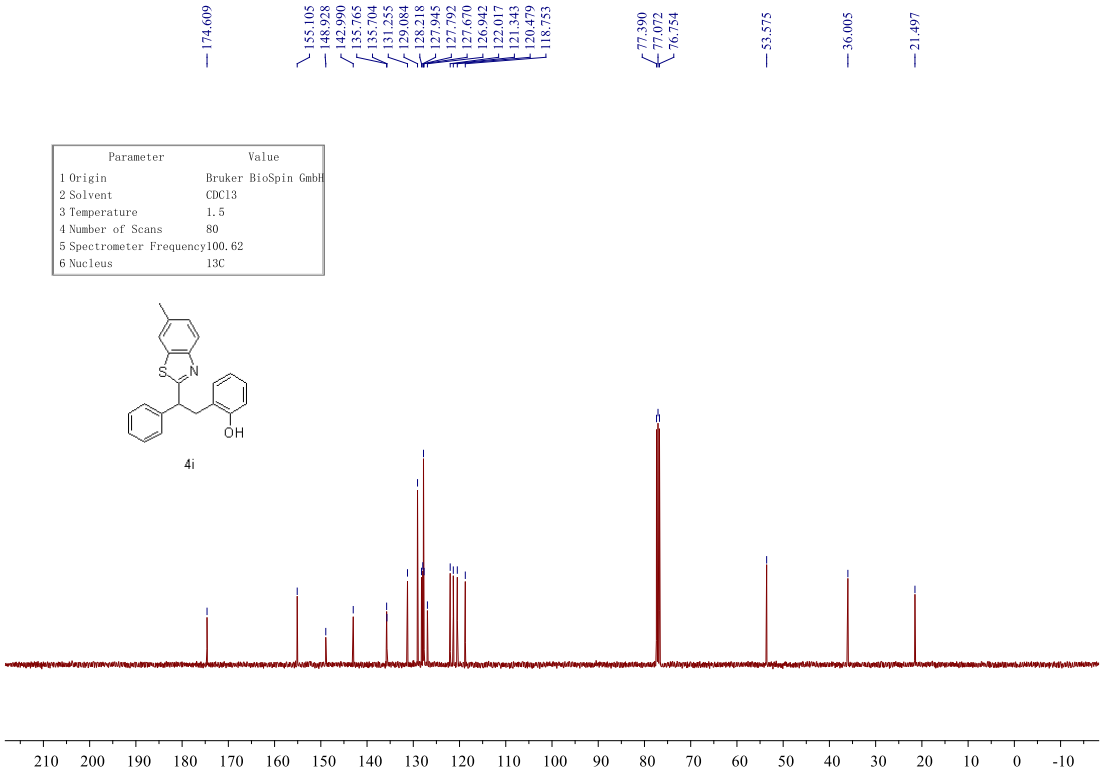
7.100
6.958
6.938
6.850
4.728
4.720
4.701
4.694
3.942
3.915
3.907
3.880
3.198
3.191
3.163
3.156
2.451
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 1.5
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
S
N
OH
4i
0.96
0.98
6.01
2.00
0.97
1.00
1.00
1.00
1.00
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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155.105
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129.084
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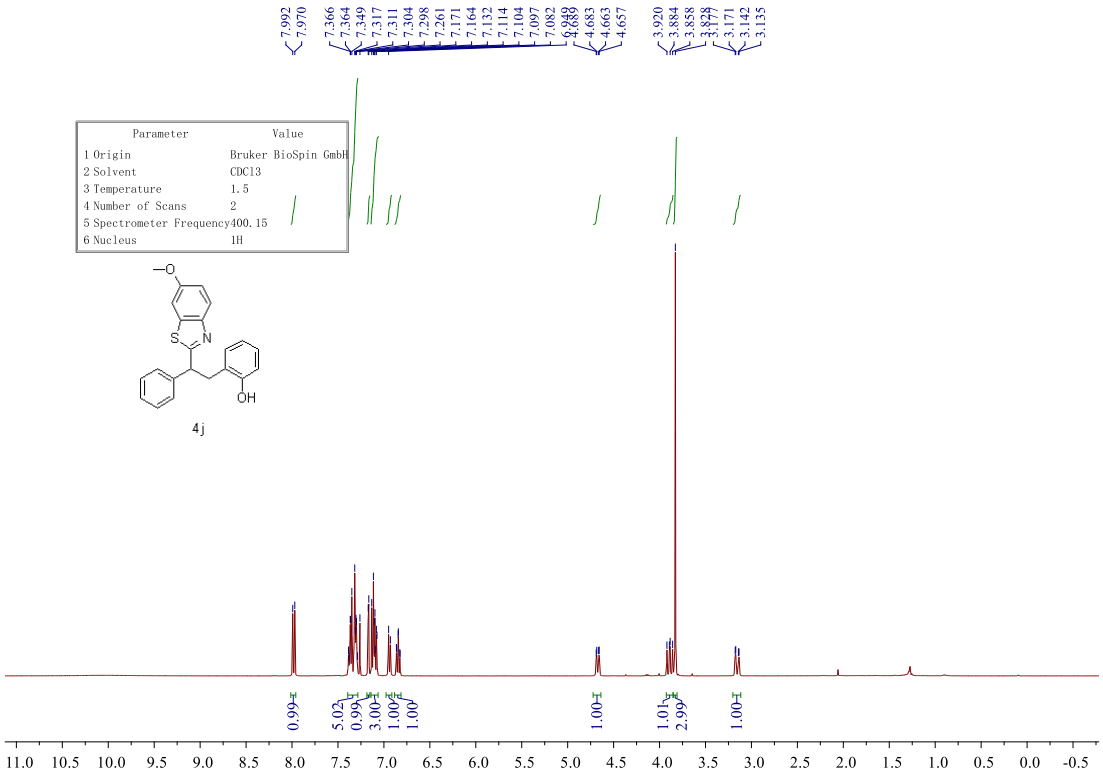
127.945
127.792
127.670
126.942
122.017
121.343
120.479
118.753
77.390
77.072
76.754
53.575
36.005
21.497
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 1.5
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
S
N
OH
4i
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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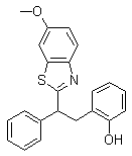
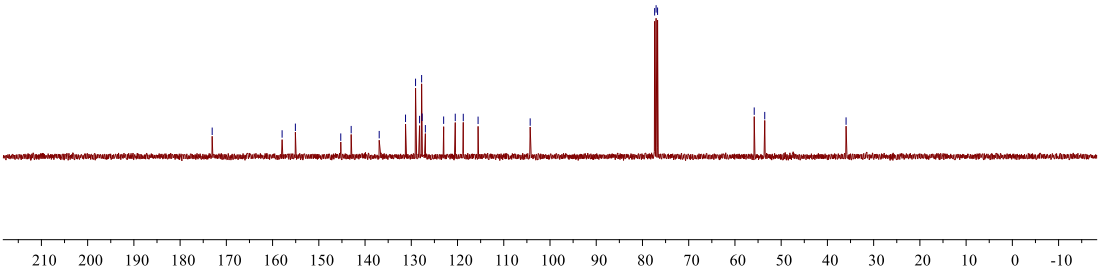
7.364
7.349
7.317
7.311
7.304
7.298
7.261
7.171
7.164
7.132
7.114
7.104
7.097
7.082
6.949
6.689
4.683
4.663
4.657
3.920
3.884
3.858
3.828
3.177
3.171
3.142
3.135
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 1.5
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
O
S
N
OH
4j
0.99
5.02
0.99
3.00
1.00
1.00
1.00
1.01
2.99
1.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

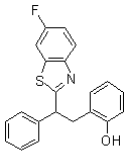
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	1.5
4 Number of Scans	40
5 Spectrometer Frequency	100.62
6 Nucleus	13C



4j



Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	298.1
4 Number of Scans	2
5 Spectrometer Frequency	400.13
6 Nucleus	1H



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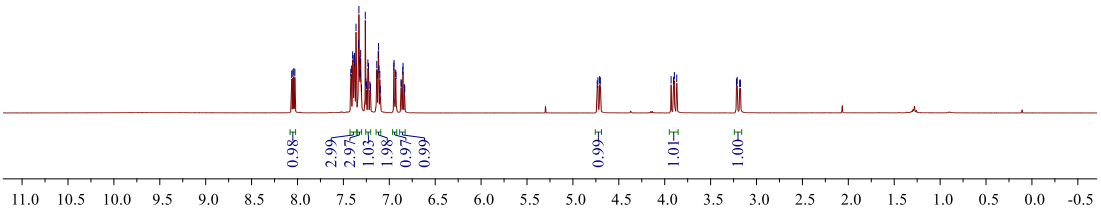
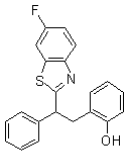
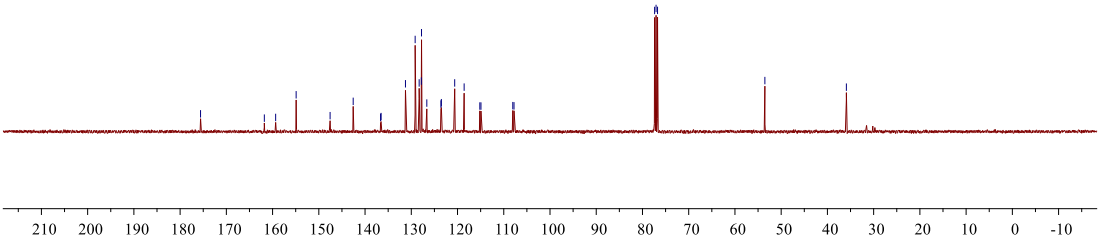


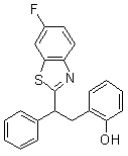
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	1.5
4 Number of Scans	80
5 Spectrometer Frequency	100.62
6 Nucleus	13C



4k

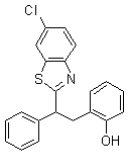


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	301.2
4 Number of Scans	16
5 Spectrometer Frequency	376.52
6 Nucleus	19F

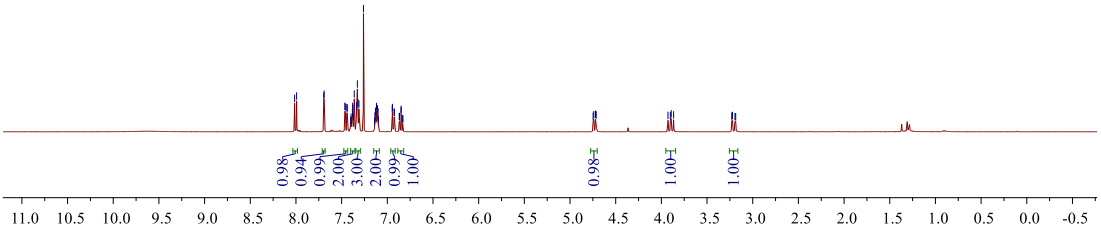


4k

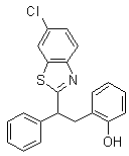
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	298.2
4 Number of Scans	2
5 Spectrometer Frequency	400.13
6 Nucleus	1H



4l



Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	298.5
4 Number of Scans	80
5 Spectrometer Frequency	100.62
6 Nucleus	13C



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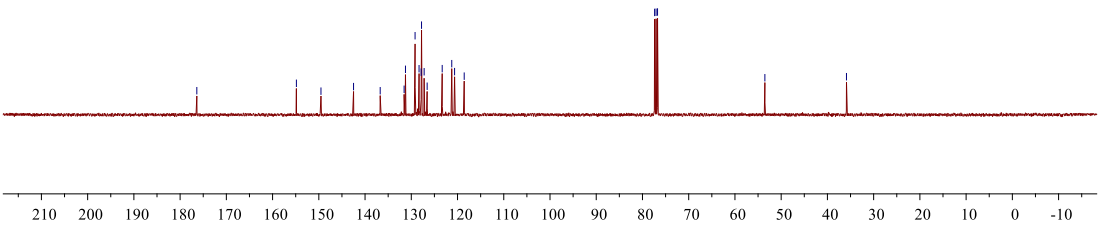

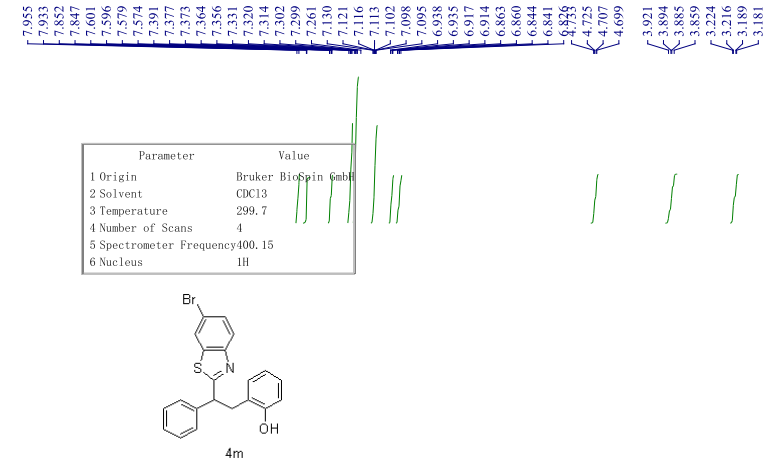
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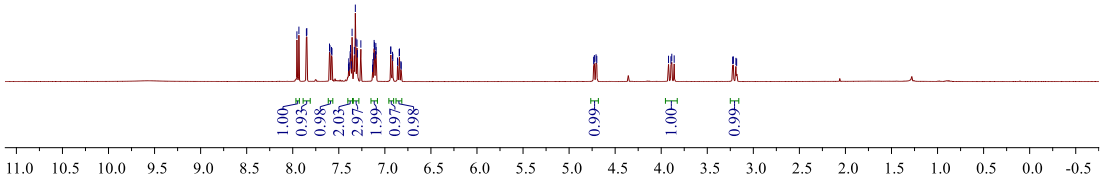
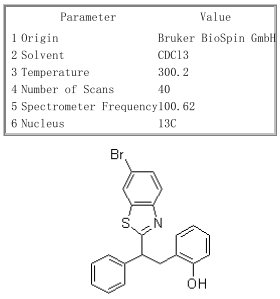
7.847
7.601
7.596
7.579
7.574
7.391
7.377
7.373
7.364
7.356
7.331
7.320
7.314
7.302
7.299
7.261
7.130
7.121
7.116
7.113
7.102
7.098
7.095
6.938
6.935
6.917
6.914
6.863
6.860
6.844
6.841
6.826
4.733
4.725
4.707
4.699
3.921
3.894
3.885
3.859
3.224
3.216
3.189
3.181
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 299.7
4 Number of Scans 4
5 Spectrometer Frequency 400.15
6 Nucleus 1H
Br
S
N
OH

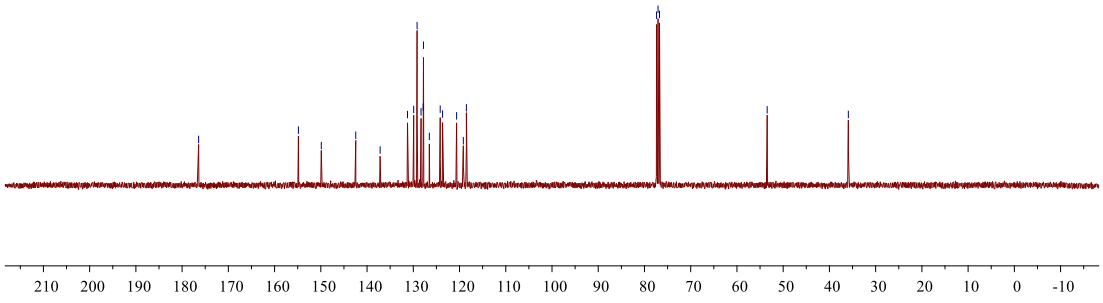
4m

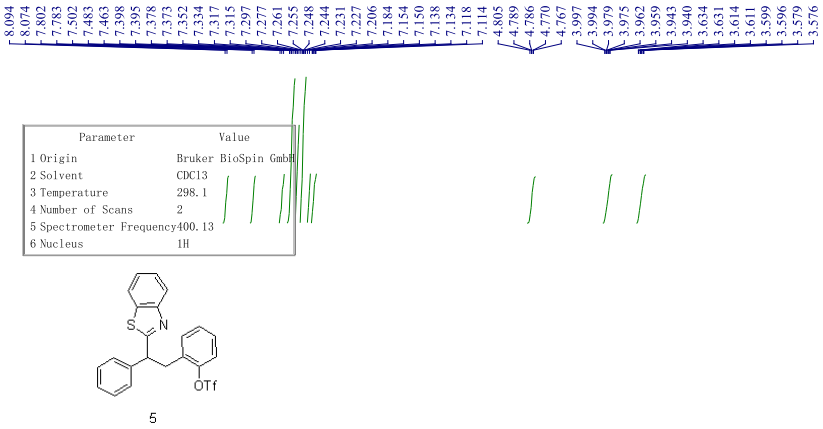

1.00
0.93
0.98
2.03
2.97
1.99
0.97
0.98
0.99
1.00
0.99
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5


176.431
154.847
149.898
142.446
137.171
131.255
129.915
129.179
128.322
127.864
127.797
126.532
124.177
123.666
120.634
119.177
118.513
77.383
77.065
76.747
53.461
35.905


Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 300.2
4 Number of Scans 40
5 Spectrometer Frequency 100.62
6 Nucleus 13C
Br
S
N
OH

4m


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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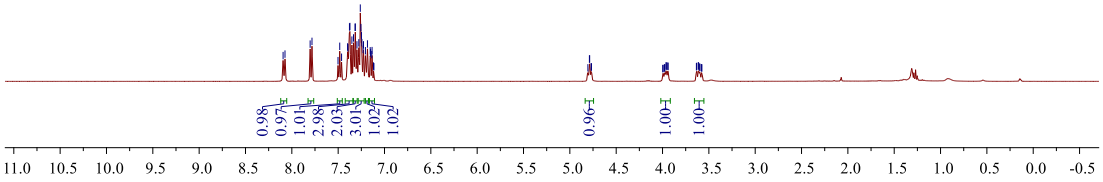
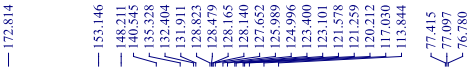
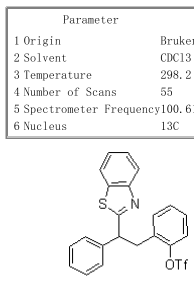
8.074
7.802
7.783
7.502
7.483
7.463
7.398
7.395
7.378
7.373
7.352
7.334
7.317
7.315
7.297
7.277
7.261
7.255
7.248
7.244
7.231
7.227
7.206
7.184
7.154
7.150
7.138
7.134
7.118
7.114
4.805
4.789
4.786
4.770
4.767
3.997
3.994
3.979
3.975
3.962
3.959
3.943
3.940
3.634
3.631
3.614
3.611
3.599
3.596
3.579
3.576
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
S
N
OTf

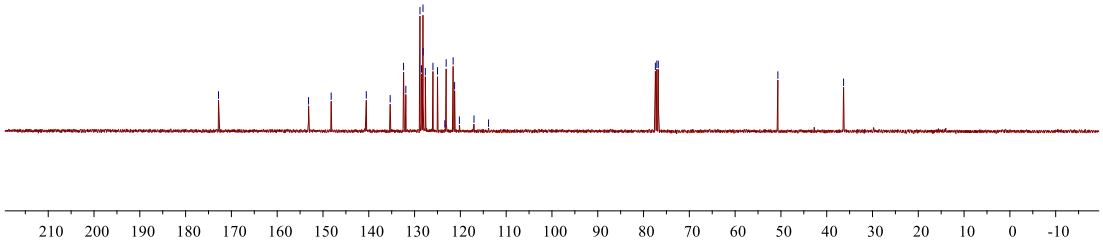
5


0.98
0.97
1.01
2.98
2.03
3.01
1.02
1.02
0.96
1.00
1.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5


172.814
153.146
148.211
140.545
135.328
132.404
131.911
128.823
128.479
128.165
128.140
127.652
125.989
124.996
123.400
123.101
121.578
121.259
120.212
117.030
113.844
77.415
77.097
76.780
50.667
36.316


Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 55
5 Spectrometer Frequency 100.61
6 Nucleus 13C
S
N
OTf

5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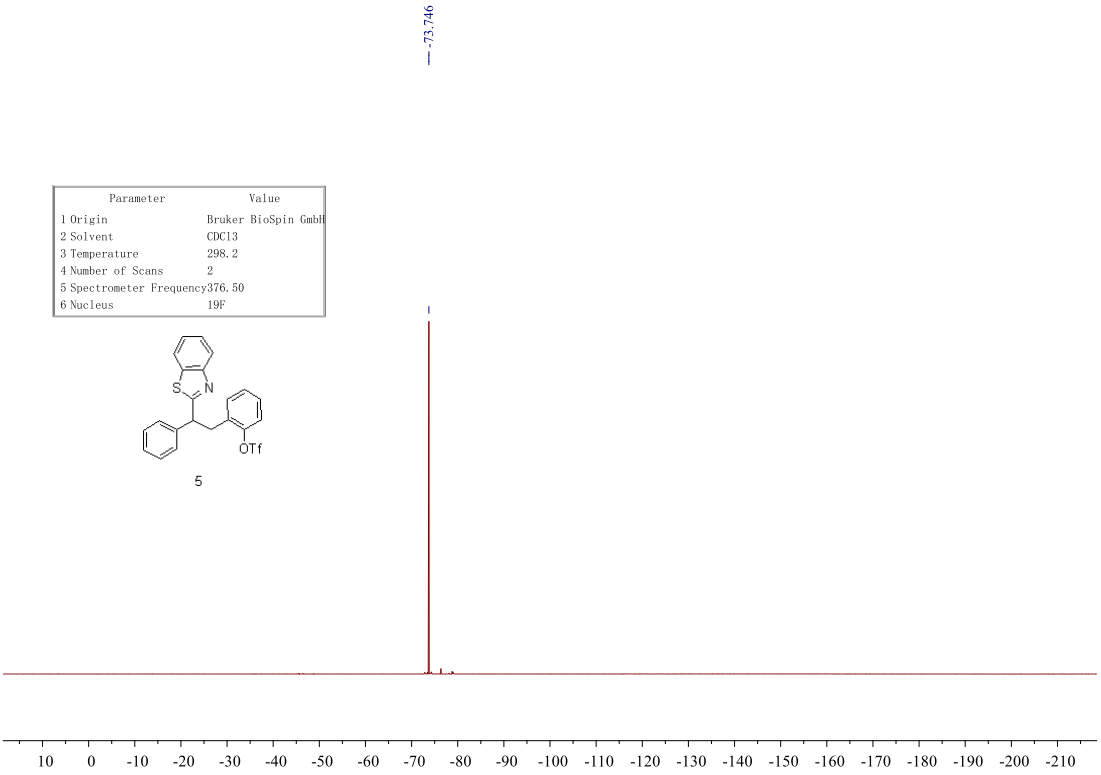
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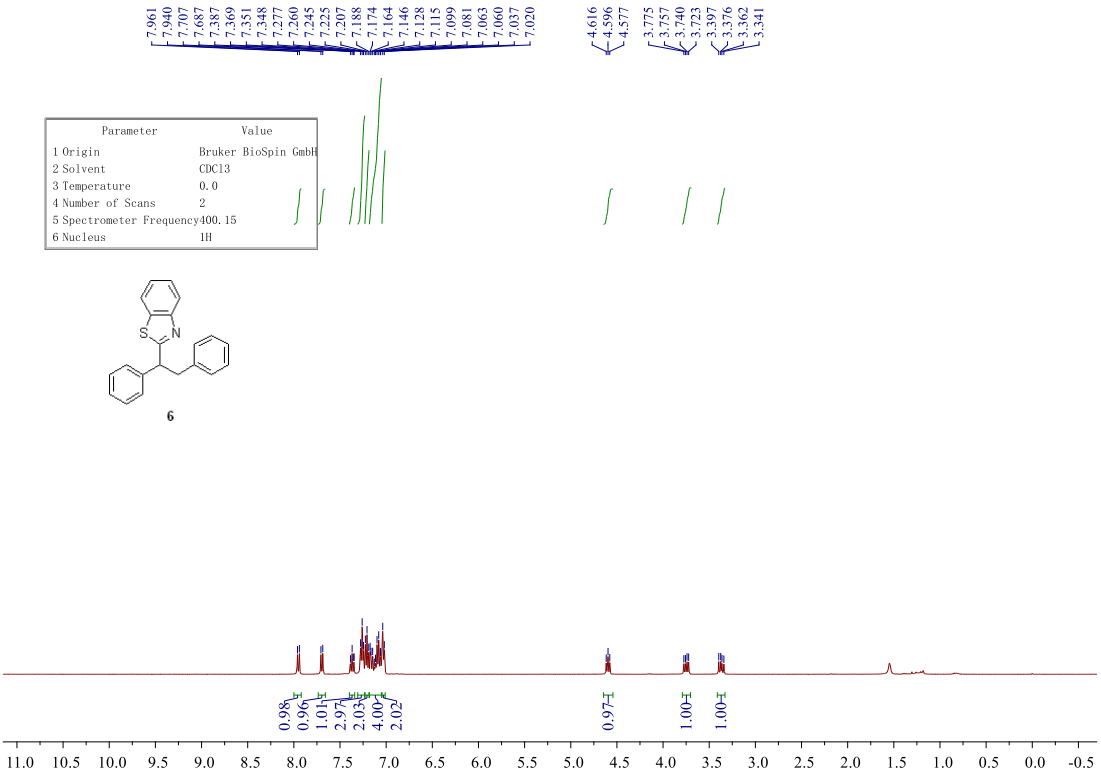
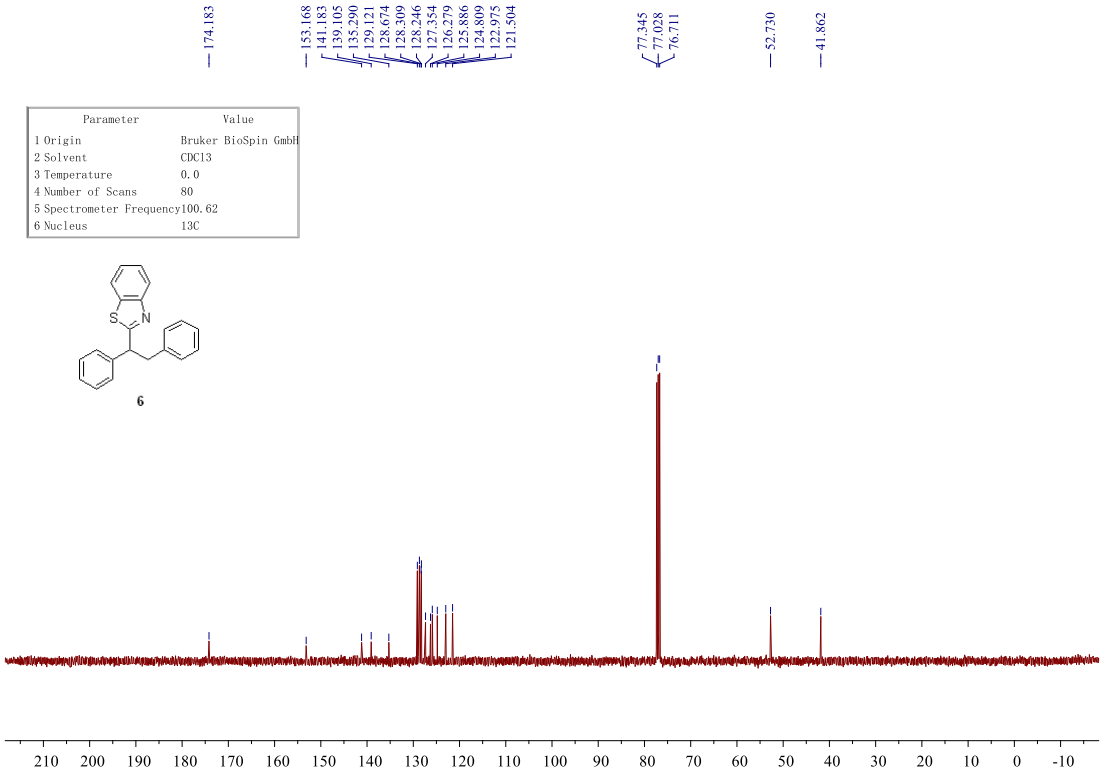
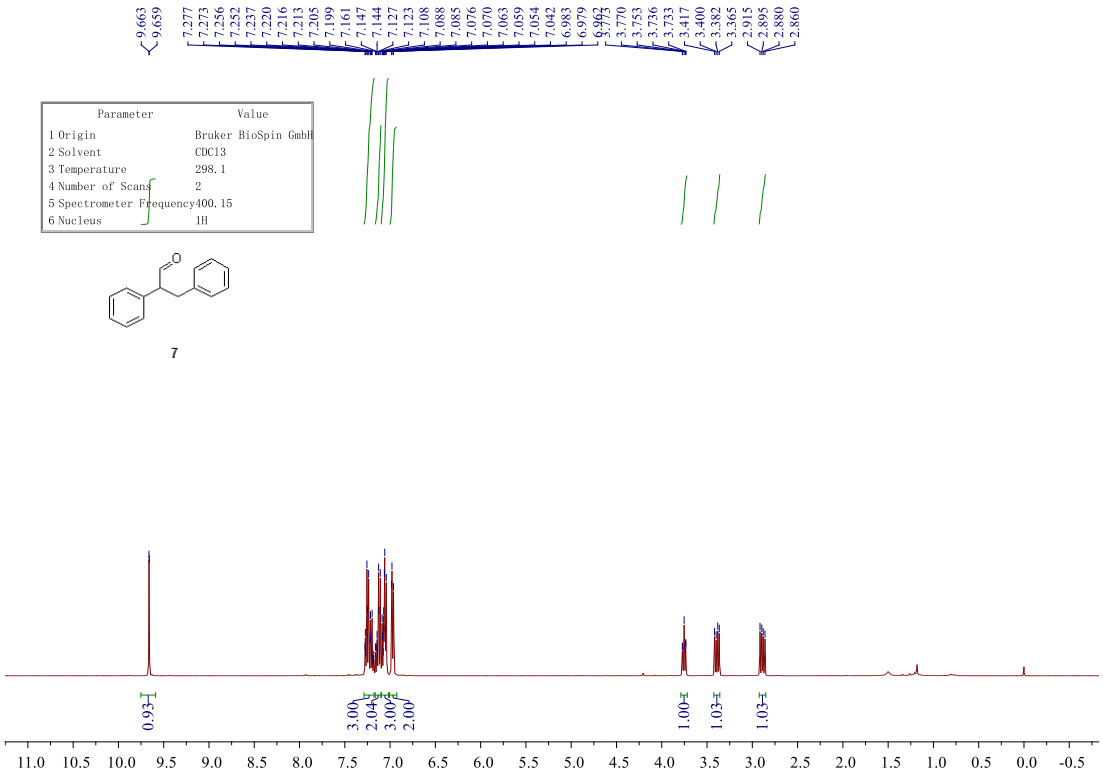
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency376.50
6 Nucleus 19F
S
N
OTf
5
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210


7.961 7.940 7.707 7.687 7.387 7.369 7.351 7.348 7.277 7.260 7.245 7.225 7.207 7.188 7.174 7.164 7.146 7.128 7.115 7.099 7.081 7.063 7.060 7.037 7.020
4.616 4.596 4.577
3.775 3.757 3.740 3.723
3.397 3.376 3.362 3.341
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 0.0
4 Number of Scans 2
5 Spectrometer Frequency400.15
6 Nucleus 1H
S
N
6
0.98 0.96 1.01 2.97 2.03 4.00 2.02
0.97 1.00 1.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5


174.183
153.168
141.183
139.105
135.290
129.121
128.674
128.309
128.246
127.354
126.279
125.886
124.809
122.975
121.504
77.345
77.028
76.711
52.730
41.862
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 0.0
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
S
N
6
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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9.659
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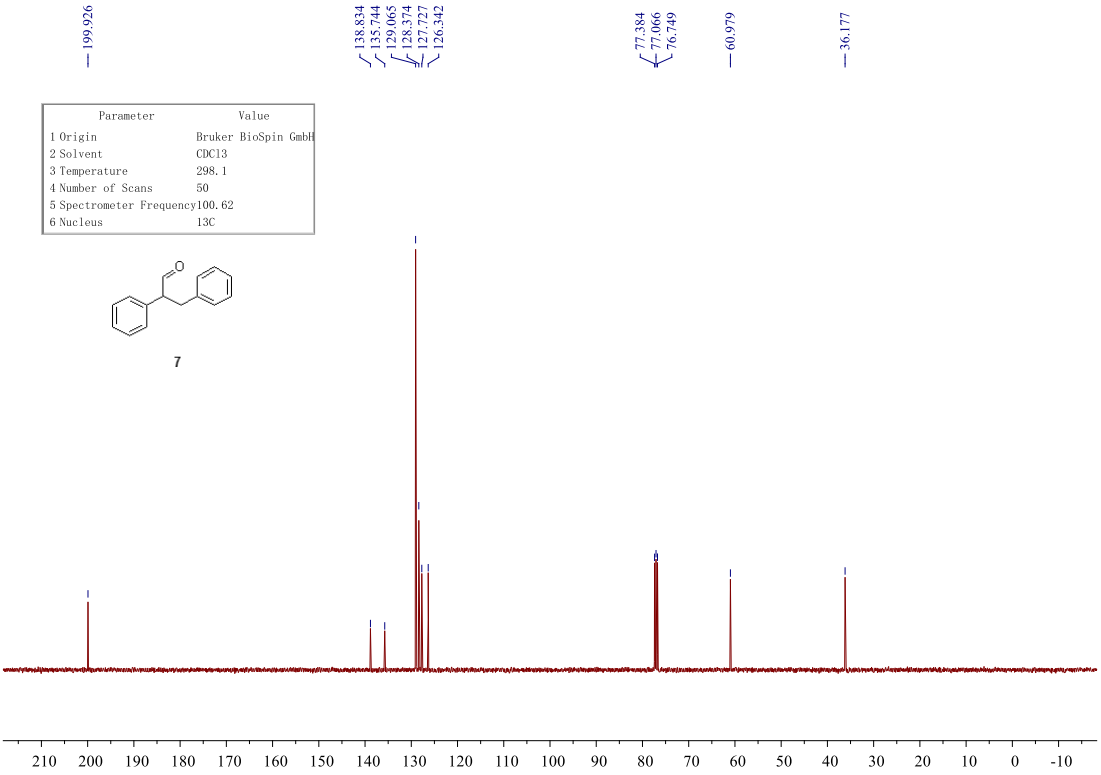
7.273
7.256
7.252
7.237
7.220
7.216
7.213
7.205
7.199
7.161
7.147
7.144
7.127
7.123
7.108
7.088
7.085
7.076
7.070
7.063
7.059
7.054
7.042
6.983
6.979
6.962
3.770
3.753
3.736
3.733
3.417
3.400
3.382
3.365
2.915
2.895
2.880
2.860
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
O
7
0.93
3.00
2.04
3.00
2.00
1.00
1.03
1.03
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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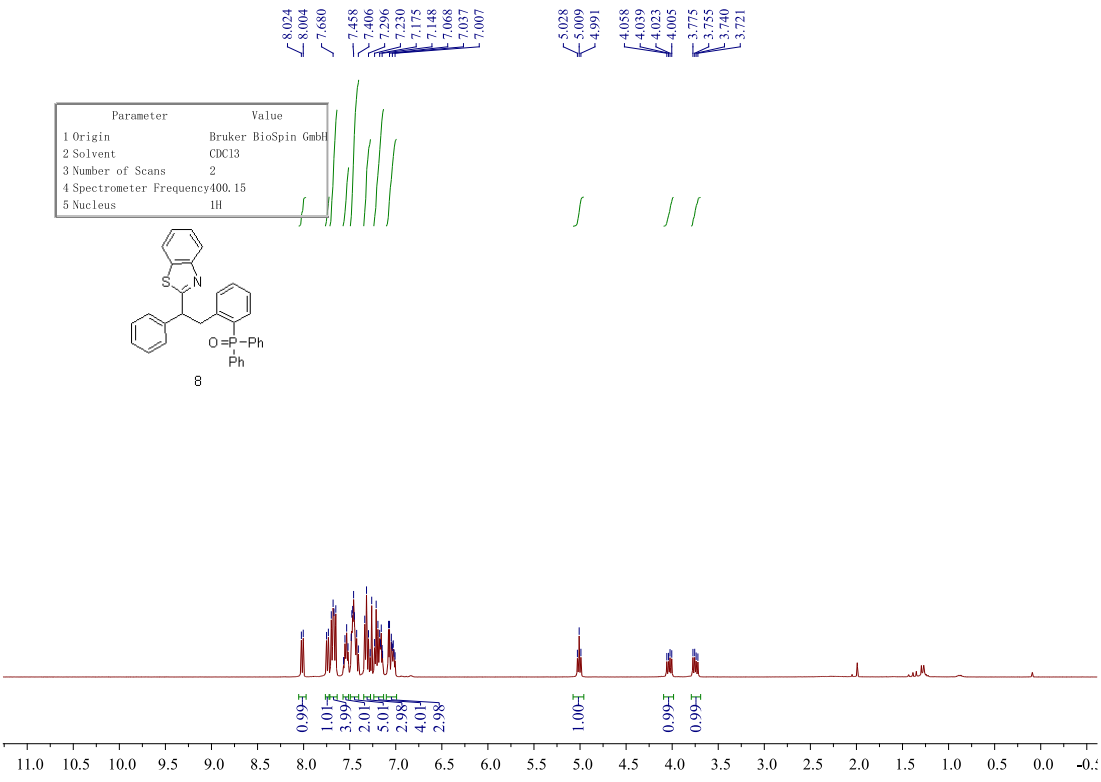
135.744
129.065
128.374
127.727
126.342
77.384
77.066
76.749
60.979
36.177
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 50
5 Spectrometer Frequency 100.62
6 Nucleus 13C
O
7
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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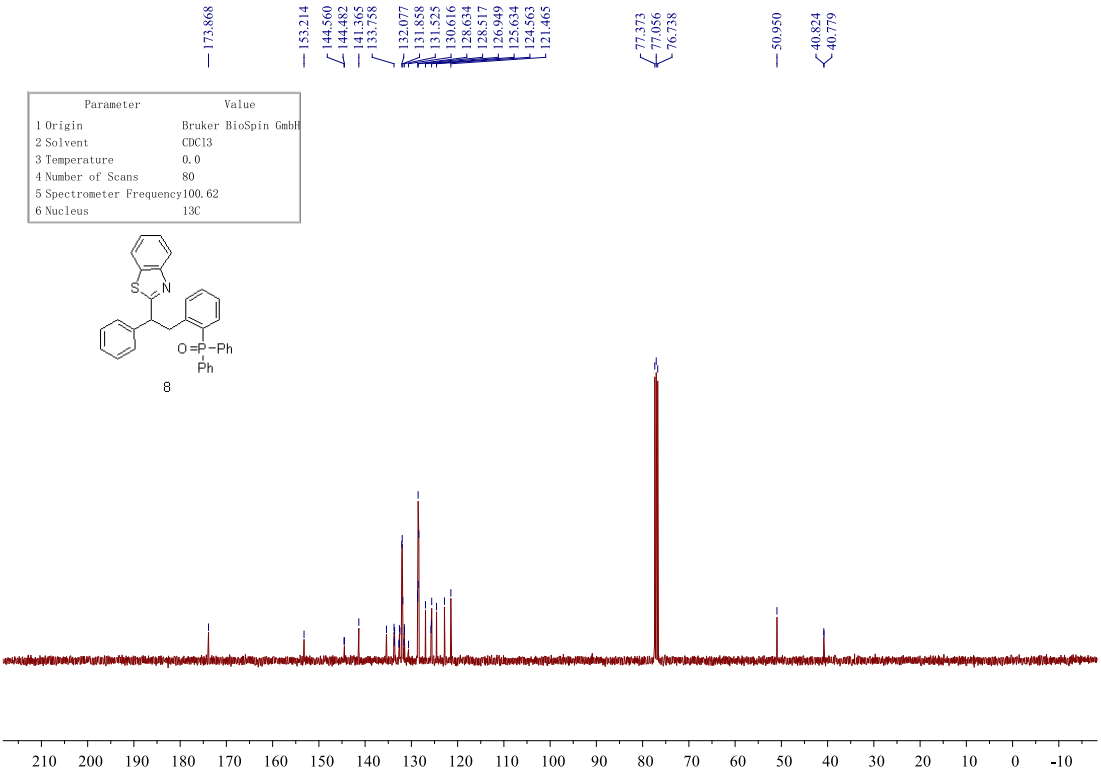
7.458
7.406
7.296
7.230
7.175
7.148
7.068
7.037
7.007
5.028
5.009
4.991
4.058
4.039
4.023
4.005
3.775
3.755
3.740
3.721
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Number of Scans 2
4 Spectrometer Frequency 400.15
5 Nucleus 1H
S
N
O=P–Ph
Ph
8
0.99
1.01
3.99
2.01
5.01
2.98
4.01
2.98
1.00
0.99
0.99
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0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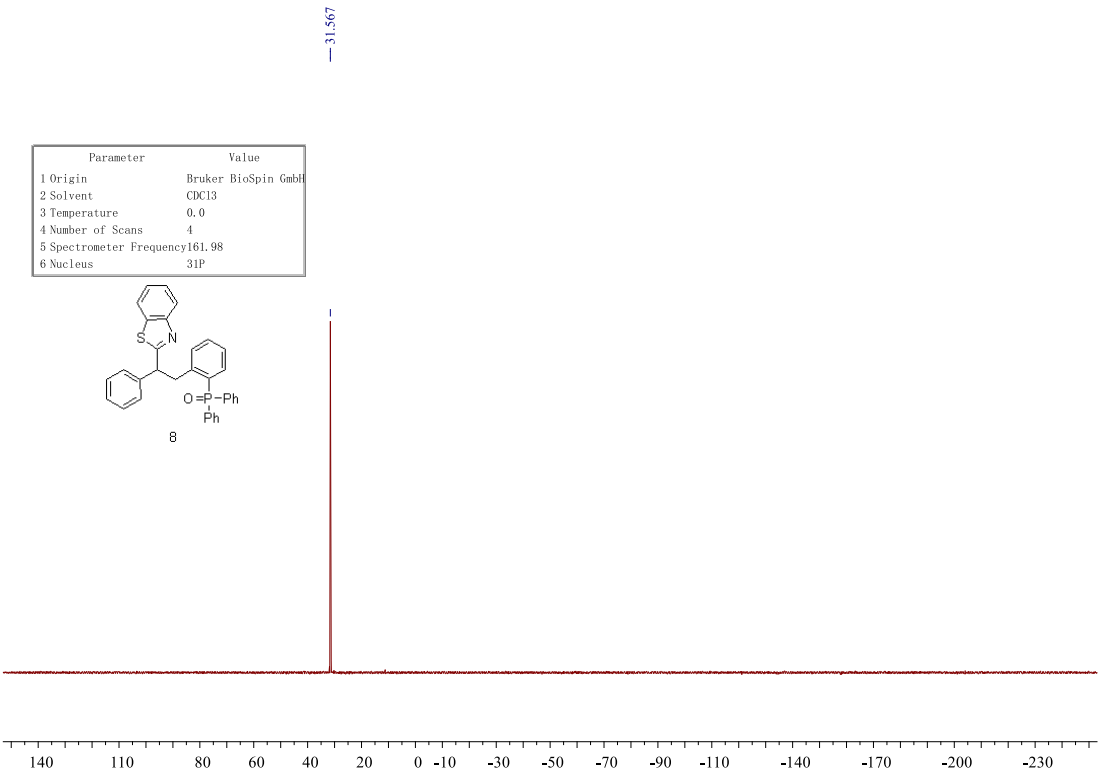
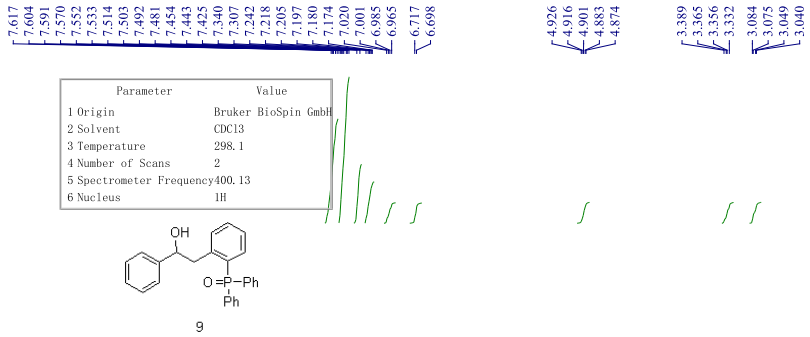
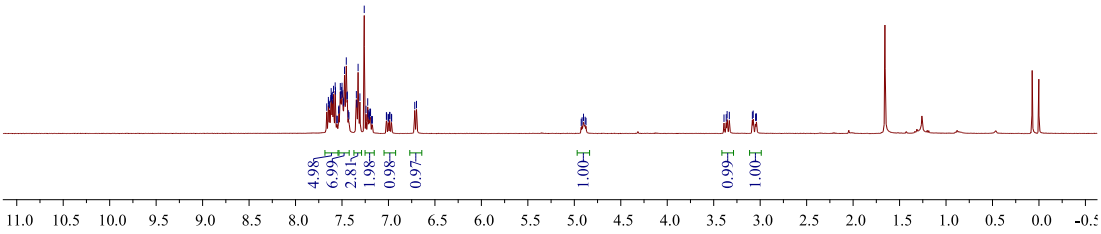
144.560
144.482
141.365
133.758
132.077
131.858
131.525
130.616
128.634
128.517
126.949
125.634
124.563
121.465
77.373
77.056
76.738
50.950
40.824
40.779
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 0.0
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
S
N
O=P-Ph
Ph
8
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10


31.567
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 0.0
4 Number of Scans 4
5 Spectrometer Frequency 161.98
6 Nucleus 31P
S
N
O=P-Ph
Ph
8
140 110 80 60 40 20 0 -10 -30 -50 -70 -90 -110 -140 -170 -200 -230



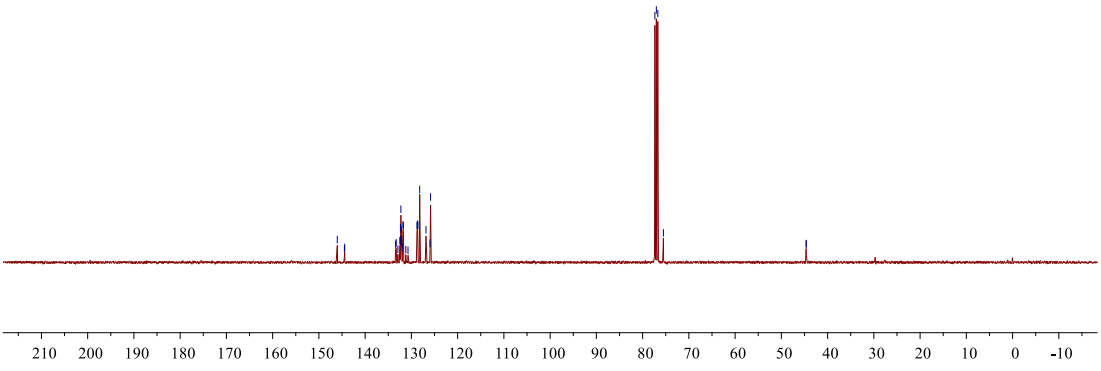
9

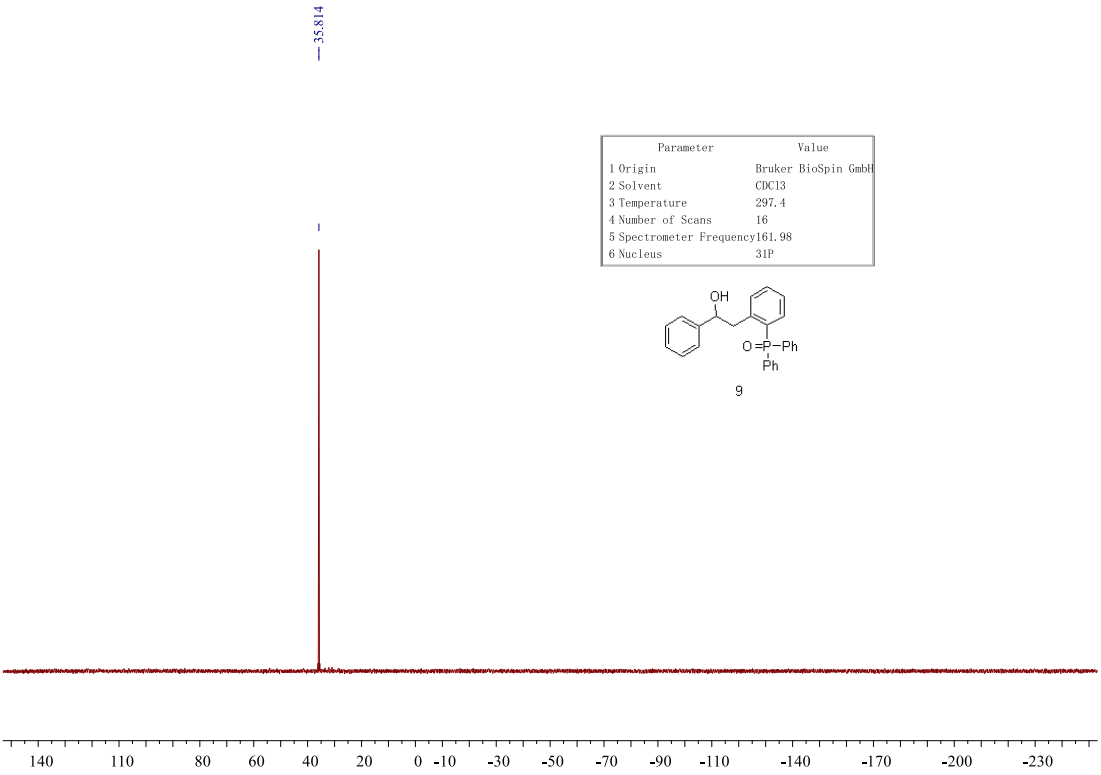


Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 297.9
4 Number of Scans 1024
5 Spectrometer Frequency 100.62
6 Nucleus 13C

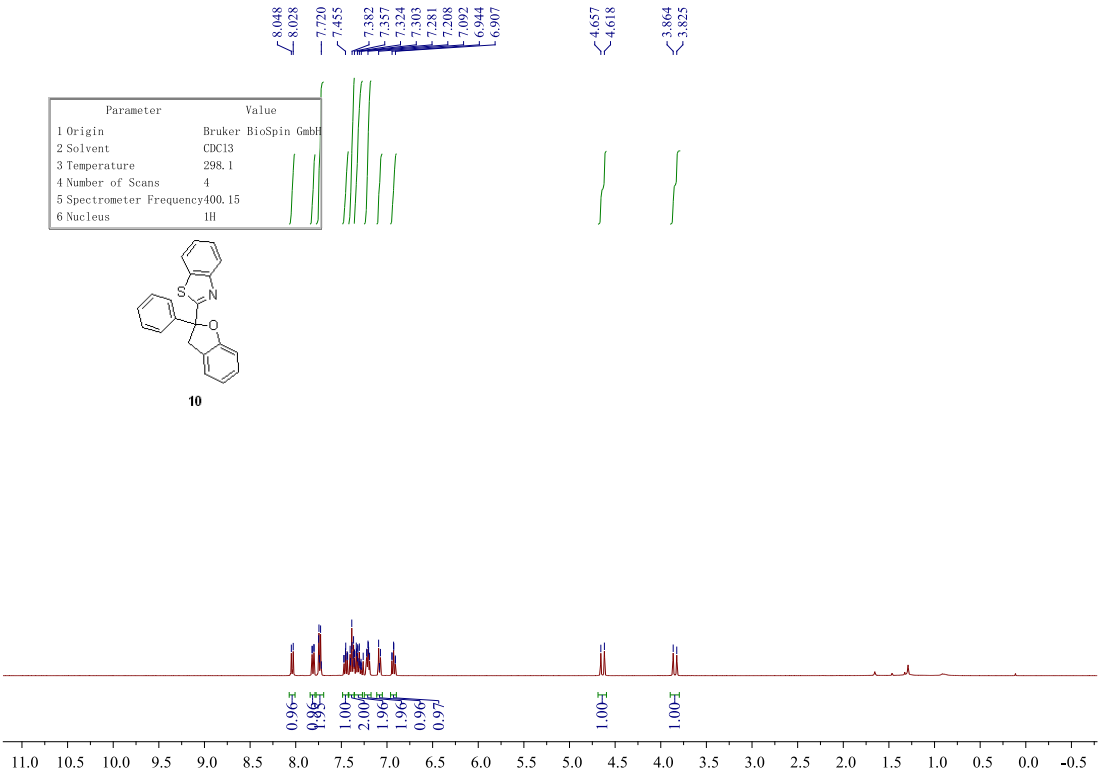
OH
O=P–Ph
Ph

9

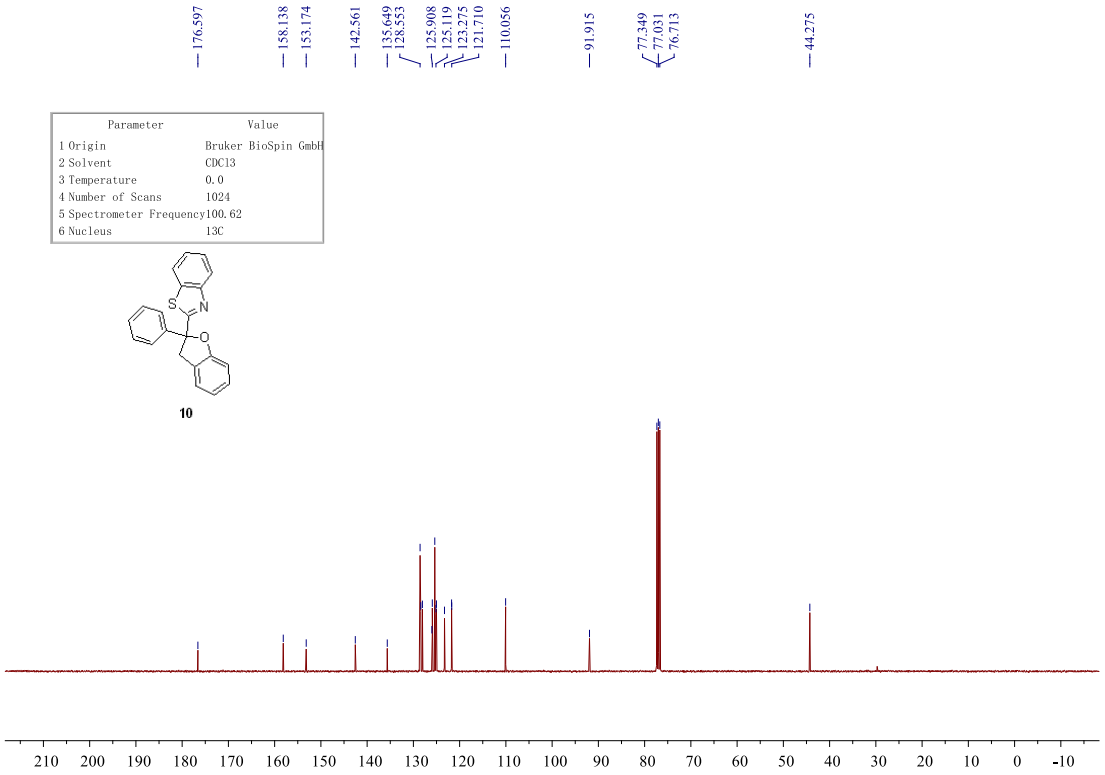


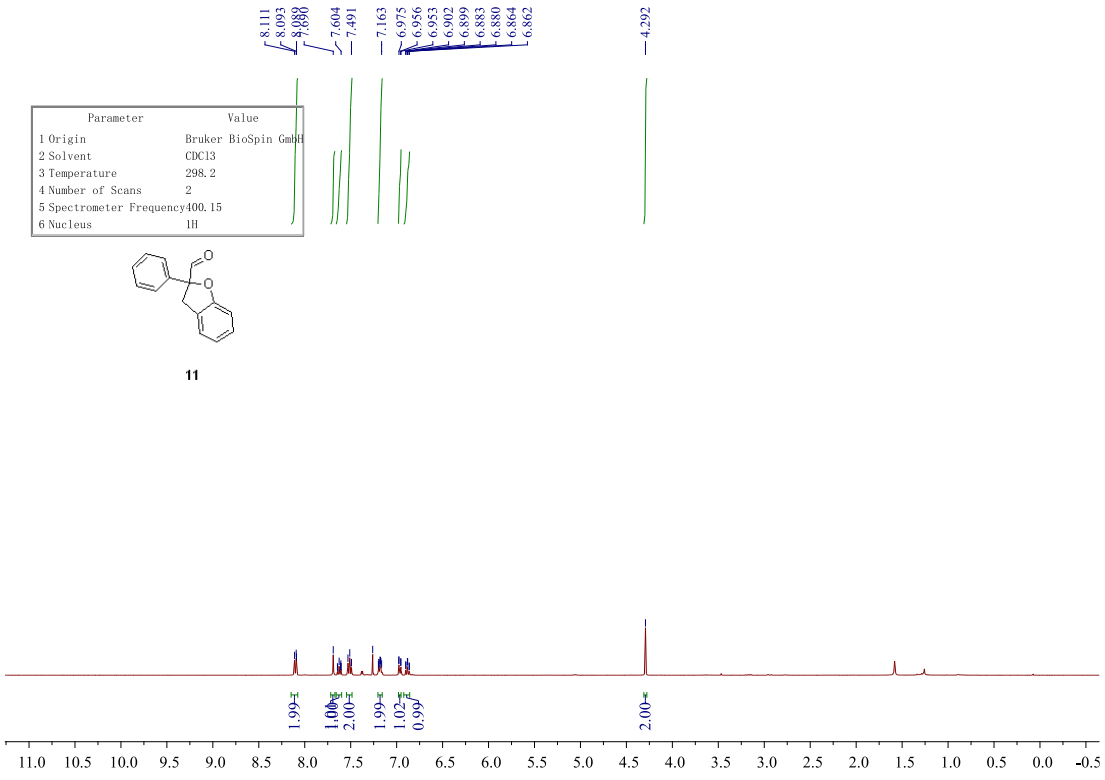

35.814
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 297.4
4 Number of Scans 16
5 Spectrometer Frequency 161.98
6 Nucleus 31P
OH
O=P-Ph
Ph
140 110 80 60 40 20 0 -10 -30 -50 -70 -90 -110 -140 -170 -200 -230

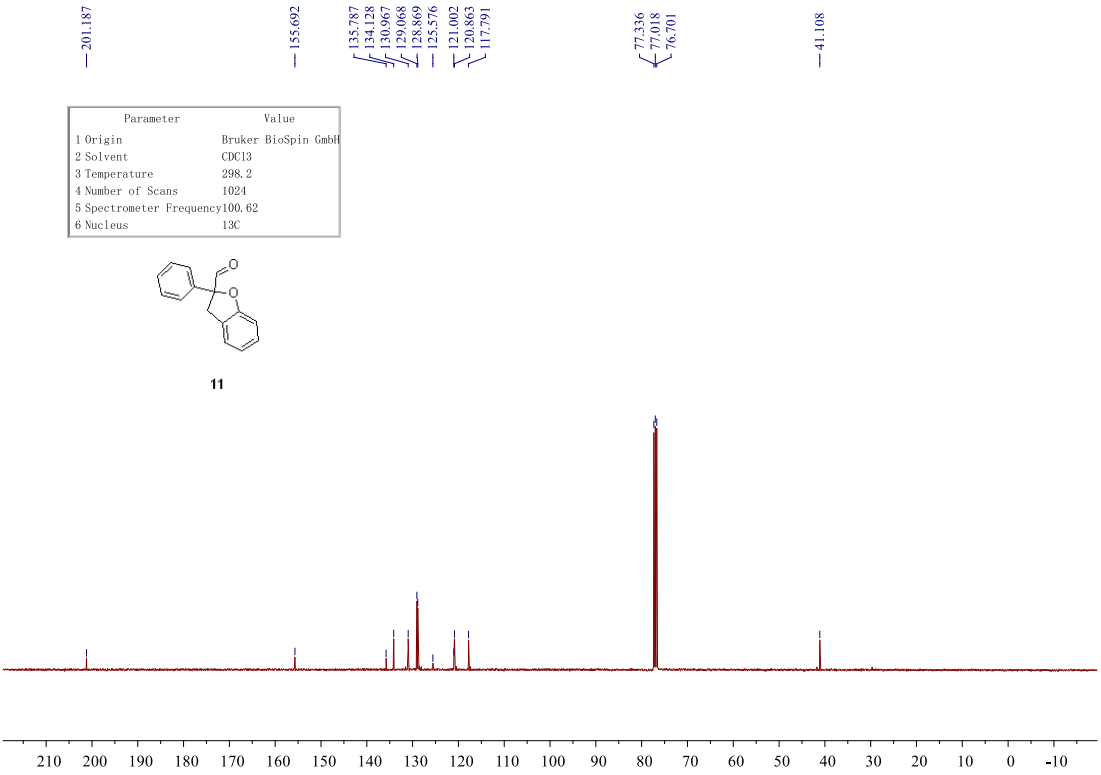
9

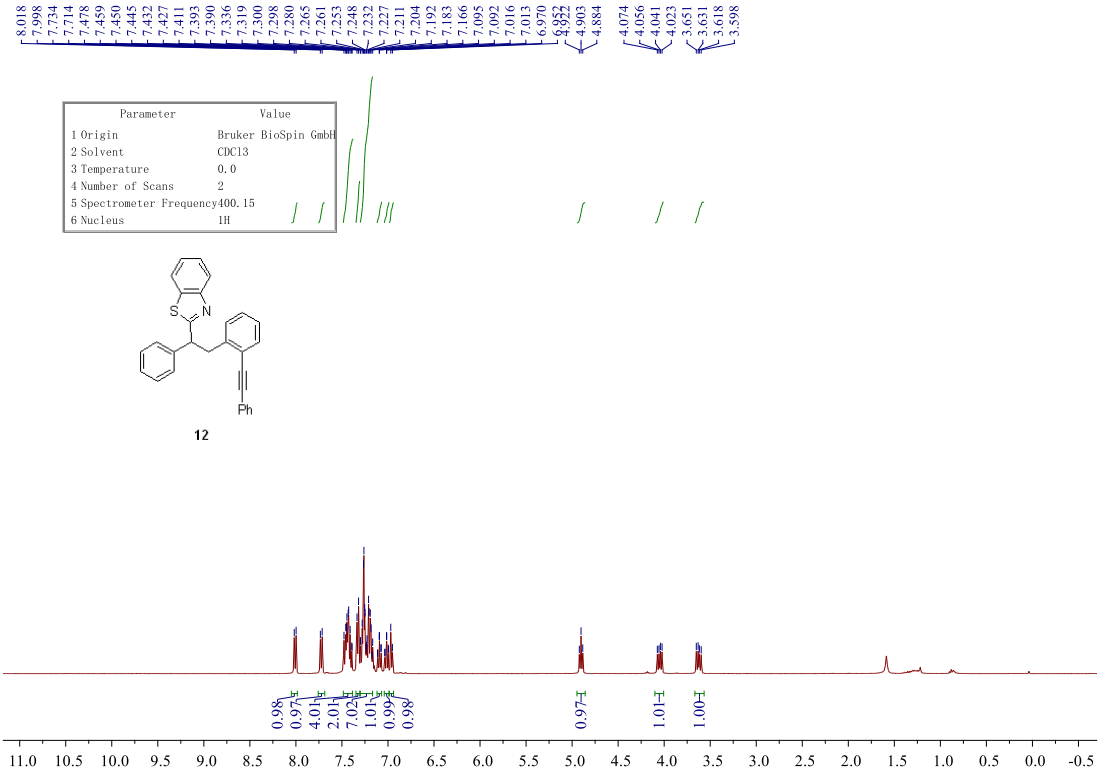

8.048 8.028 7.720 7.455 7.382 7.357 7.324 7.303 7.281 7.208 7.092 6.944 6.907
4.657 4.618
3.864 3.825
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 4
5 Spectrometer Frequency 400.15
6 Nucleus 1H
S
N
O
0.96 0.96 1.00 2.00 1.96 1.96 0.96 0.97 1.00 1.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

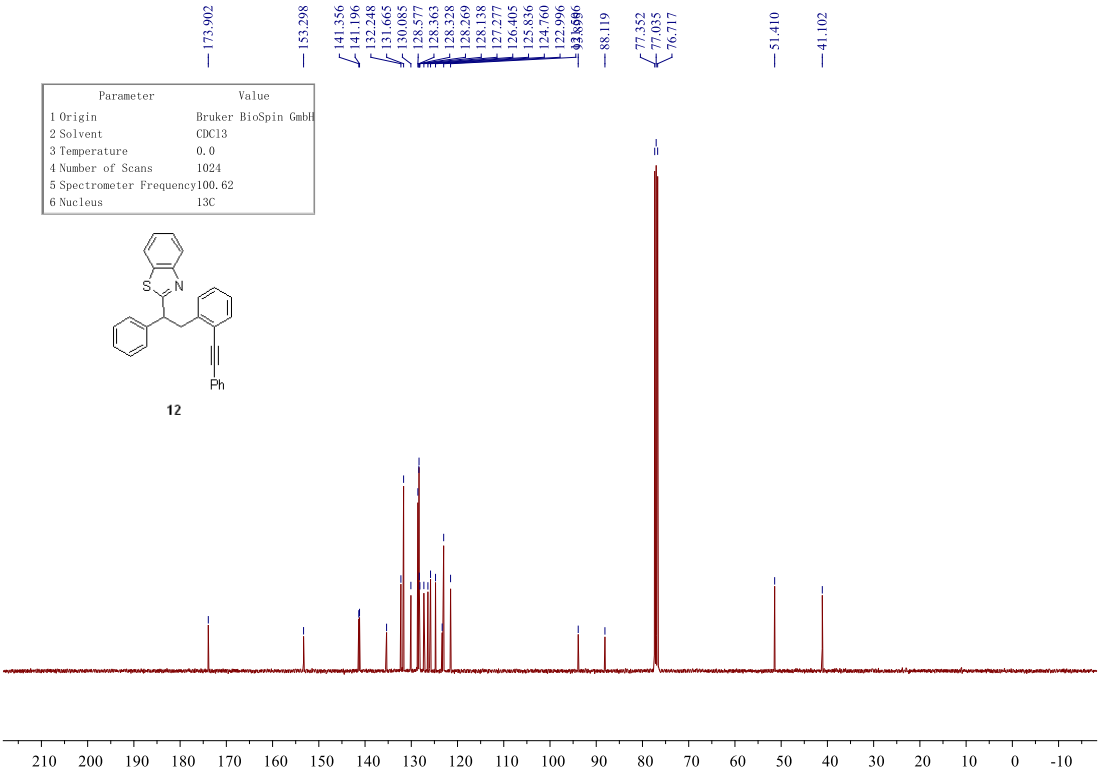
10


176.597
158.138
153.174
142.561
135.649
128.553
125.908
125.119
123.275
121.710
110.056
91.915
77.349
77.031
76.713
44.275
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 0.0
4 Number of Scans 1024
5 Spectrometer Frequency 100.62
6 Nucleus 13C
S
N
O
10
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

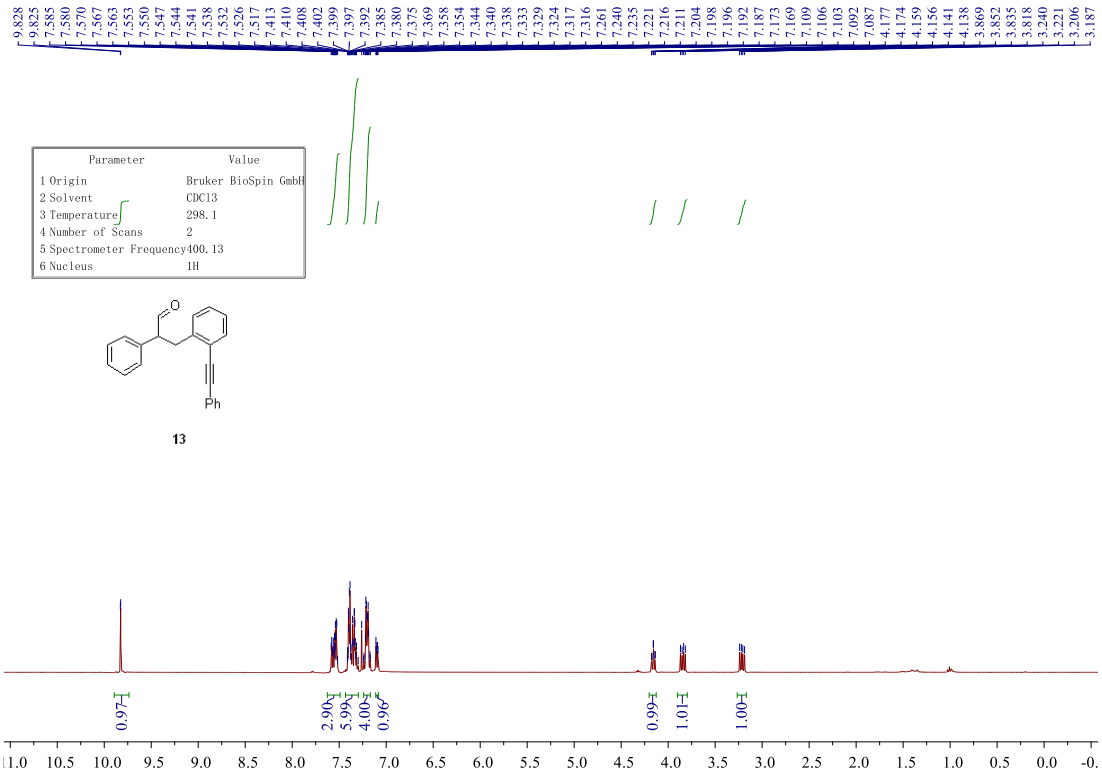

8.111
8.093
8.088
8.080
7.690
7.604
7.491
7.163
6.975
6.956
6.953
6.902
6.899
6.883
6.880
6.864
6.862
4.292
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
O
O
11
1.99
1.00
2.00
1.99
1.02
0.99
2.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5


201.187
155.692
135.787
134.128
130.967
129.068
128.869
125.576
121.002
120.863
117.791
77.336
77.018
76.701
41.108
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 1024
5 Spectrometer Frequency 100.62
6 Nucleus 13C
O
O
11
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

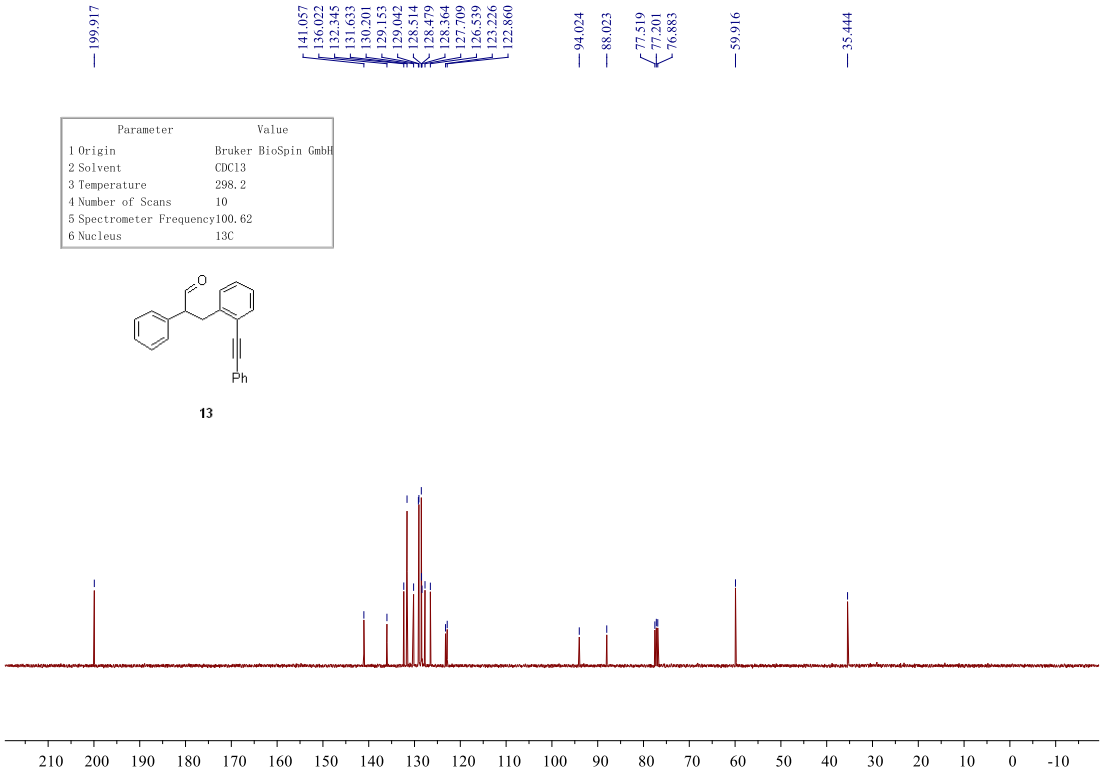

8.018
7.998
7.734
7.714
7.478
7.459
7.450
7.445
7.432
7.427
7.411
7.393
7.390
7.336
7.319
7.300
7.298
7.280
7.265
7.261
7.253
7.248
7.232
7.227
7.211
7.204
7.192
7.183
7.166
7.095
7.092
7.016
7.013
6.970
4.903
4.884
4.074
4.056
4.041
4.023
3.651
3.631
3.618
3.598
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 0.0
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
S
N
Ph
12
0.98
0.97
4.01
2.01
7.02
1.01
0.99
0.98
0.97
1.01
1.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5


173.902
153.298
141.356
141.196
132.248
131.665
130.085
128.577
128.363
128.328
128.269
128.138
127.277
126.405
125.836
124.760
122.996
88.119
77.352
77.035
76.717
51.410
41.102
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 0.0
4 Number of Scans 1024
5 Spectrometer Frequency 100.62
6 Nucleus 13C
S
N
Ph
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

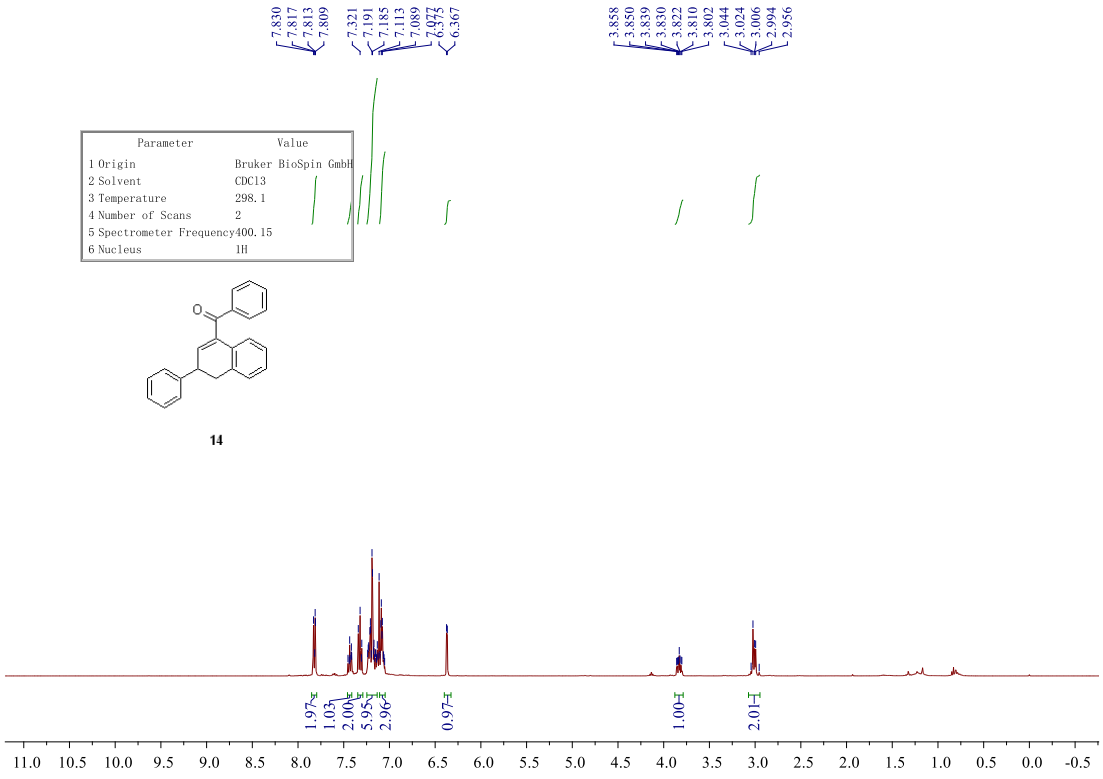
12


9.828
9.825
7.585
7.580
7.570
7.567
7.563
7.553
7.550
7.547
7.544
7.541
7.538
7.532
7.526
7.517
7.413
7.410
7.408
7.402
7.399
7.397
7.392
7.385
7.380
7.375
7.369
7.358
7.354
7.344
7.340
7.338
7.333
7.329
7.324
7.317
7.316
7.261
7.240
7.235
7.221
7.216
7.211
7.204
7.198
7.196
7.192
7.187
7.173
7.169
7.109
7.106
7.103
7.092
7.087
4.177
4.174
4.159
4.156
4.141
4.138
3.869
3.852
3.835
3.818
3.240
3.221
3.206
3.187
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
Ph
0.97
2.90
5.99
4.00
0.96
0.99
1.01
1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

13


199.917
141.057
136.022
132.345
131.633
130.201
129.153
129.042
128.514
128.479
128.364
127.709
126.539
123.226
122.860
94.024
88.023
77.519
77.201
76.883
59.916
35.444
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 10
5 Spectrometer Frequency 100.62
6 Nucleus 13C
O
Ph
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

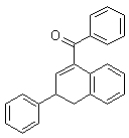
13


7.830
7.817
7.813
7.809
7.321
7.191
7.185
7.113
7.089
7.077
6.975
6.367
3.858
3.850
3.839
3.830
3.822
3.810
3.802
3.044
3.024
3.006
2.994
2.956
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
O
1.97
1.03
2.00
5.95
2.96
0.97
1.00
2.01
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

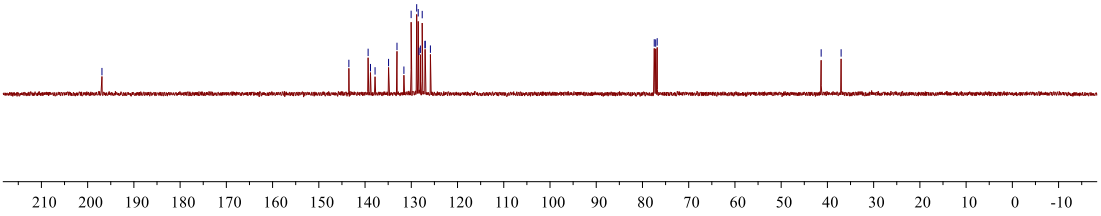
14

196.904
143.500
139.339
138.827
137.835
134.913
133.093
131.598
130.034
128.831
128.503
128.322
128.032
127.638
127.028
126.999
125.866
77.452
77.135
76.817
41.353
37.035

Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	298.2
4 Number of Scans	8
5 Spectrometer Frequency	100.62
6 Nucleus	13C

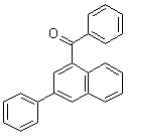


14



8.214
8.097
8.076
8.001
7.981
7.944
7.926
7.923
7.857
7.853
7.718
7.714
7.696
7.641
7.638
7.635
7.619
7.604
7.601
7.598
7.590
7.587
7.573
7.570
7.553
7.550
7.530
7.526
7.508
7.503
7.485
7.465
7.415
7.412
7.410
7.394
7.389
7.378
7.376
7.261

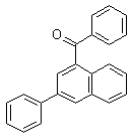
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Number of Scans	2
4 Spectrometer Frequency	400.15
5 Nucleus	1H



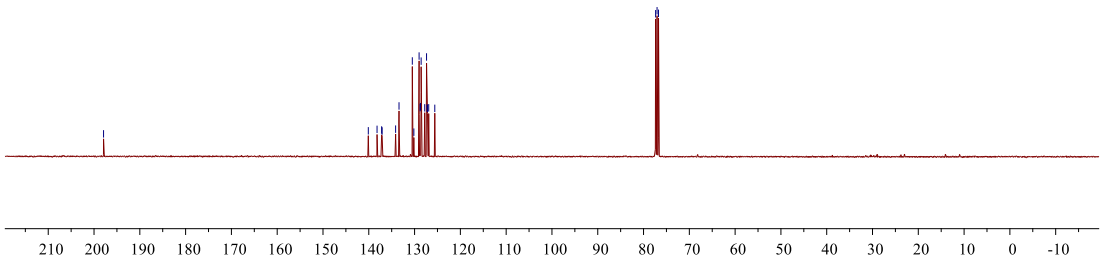
15

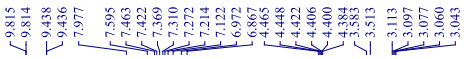
0.99
0.98
0.99
1.97
0.98
2.01
0.97
1.01
4.99
1.00

Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	298.2
4 Number of Scans	1024
5 Spectrometer Frequency	100.61
6 Nucleus	13C

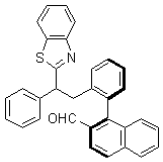


15

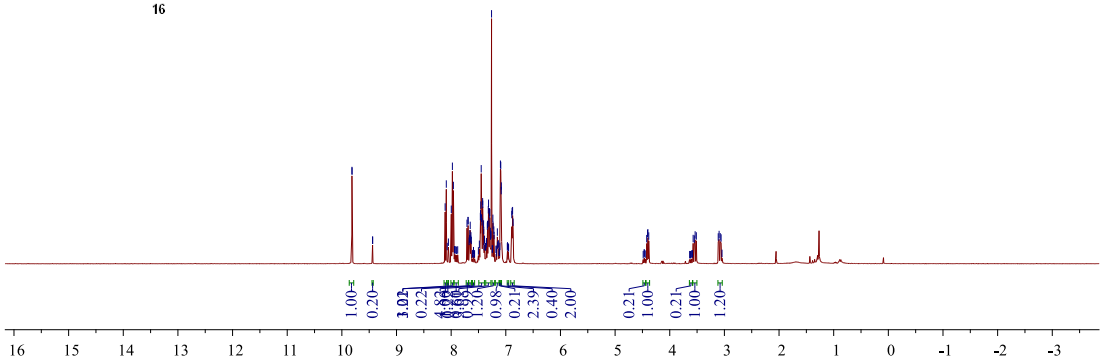


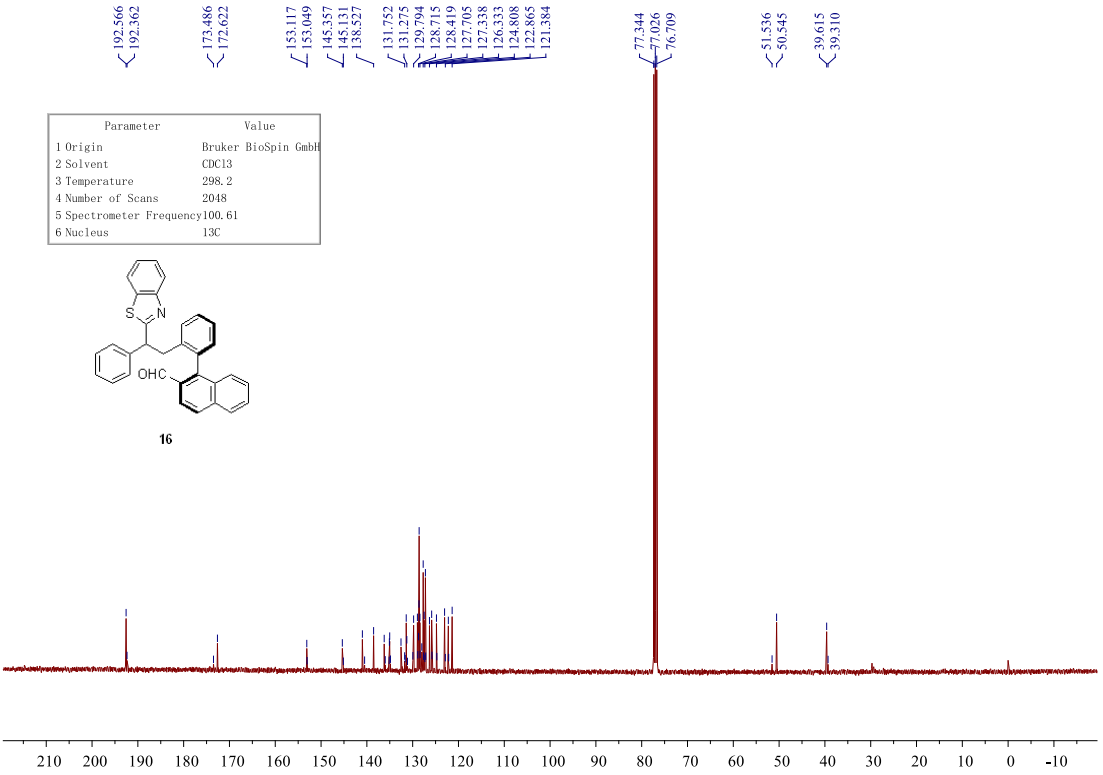


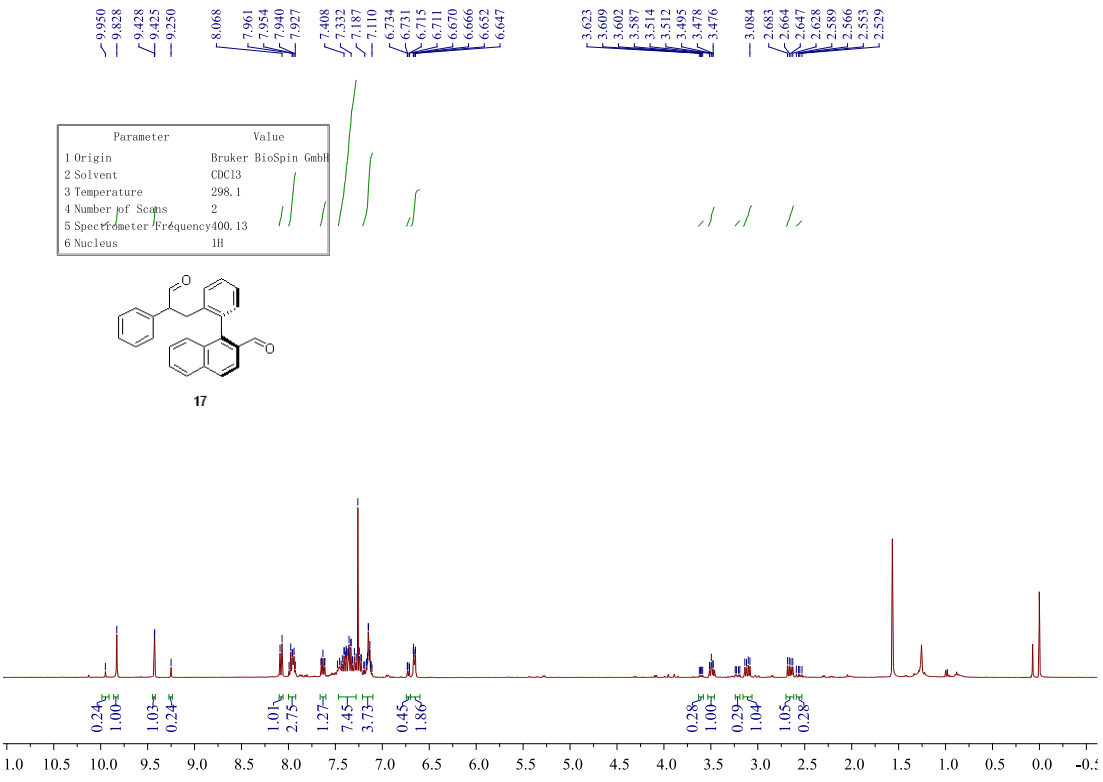
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	298.2
4 Number of Scans	2
5 Spectrometer Frequency	400.13
6 Nucleus	1H



16




192.566
192.362
173.486
172.622
153.117
153.049
145.357
145.131
138.527
131.752
131.275
129.794
128.715
128.419
127.705
127.338
126.333
124.808
122.865
121.384
77.344
77.026
76.709
51.536
50.545
39.615
39.310
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2048
5 Spectrometer Frequency 100.61
6 Nucleus 13C
S
N
OHC
16
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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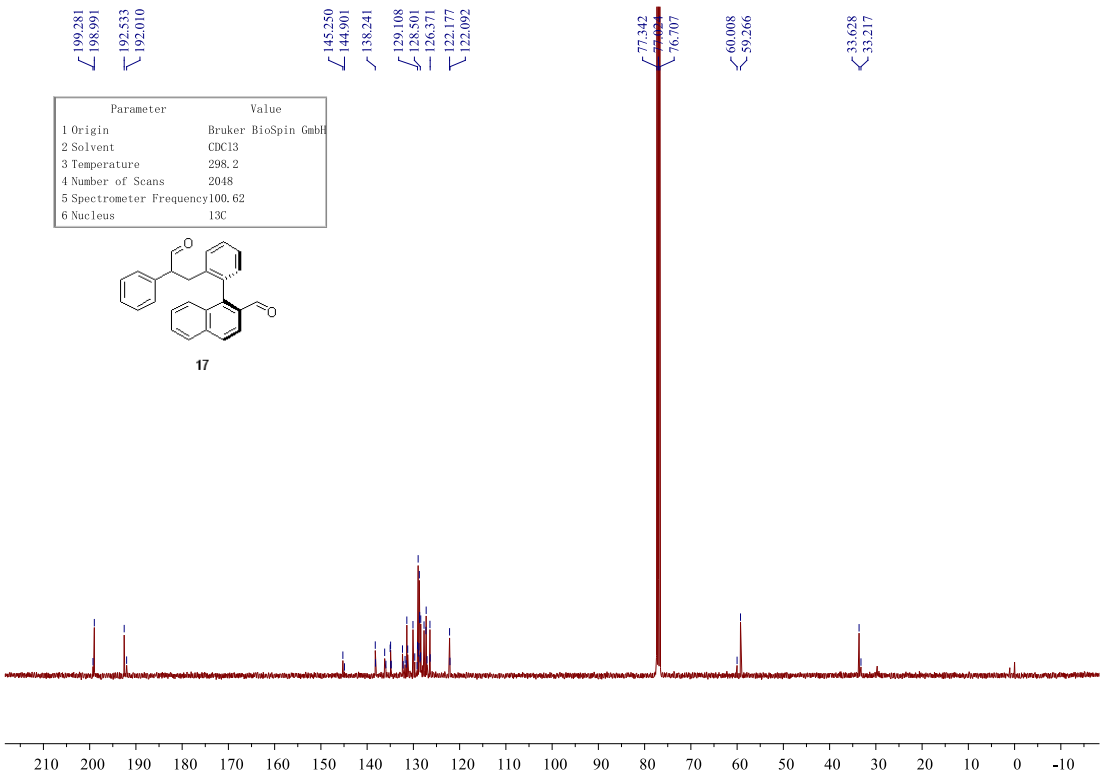
9.828
9.428
9.425
9.250
8.068
7.961
7.954
7.940
7.927
7.408
7.332
7.187
7.110
6.734
6.731
6.715
6.711
6.670
6.666
6.652
6.647
3.623
3.609
3.602
3.587
3.514
3.512
3.495
3.478
3.476
3.084
2.683
2.664
2.647
2.628
2.589
2.566
2.553
2.529
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
O
17
0.24
1.00
1.03
0.24
1.01
2.75
1.27
7.45
3.73
0.45
1.86
0.28
1.00
0.29
1.04
1.05
0.28
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0


199.281
198.991
192.533
192.010
145.250
144.901
138.241
129.108
128.501
126.371
122.177
122.092
77.342
77.024
76.707
60.008
59.266
33.628
33.217
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2048
5 Spectrometer Frequency 100.62
6 Nucleus 13C
O
O
17
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10