Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Organocatalytic enantioselective Mukaiyama-Mannich reaction of fluorinated enol silyl ethers and cyclic *N*-sulfonyl ketimines

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Contents **Page**

General: Reactions were monitored by thin layer chromatography using UV light to visualize the course of reaction. Purification of reaction products was carried out by flash chromatography on silica gel. Chemical yields referred to pure isolated substances. Infrared (IR) spectra were obtained using Nicolet Fourier Transform Infrared (FT-IR) Spectrometer. The $[\alpha]_D$ was recorded using PolAAr 3005 High Accuracy Polarimeter. ^1H, ^{19}F, ^{13}C NMR spectra were obtained using a Bruker DPX-400 and 300 MHz spectrometer. Chemical shifts are reported in ppm from $CDCl_3$, acetone-d_6 with the solvent resonance or $(CH_3)_4Si$ as the internal standard. The following abbreviations were used to designate chemical shift multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, h = heptet, m = multiplet, br = broad. Coupling constants (*J*) are reported in Hertz.

Anhydrous toluene and THF was prepared by distillation over sodium-benzophenone ketyl prior to use. Anhydrous CH_2Cl_2 and CH_3CN were prepared by first distillation over P_2O_5 and then from CaH_2. Anhydrous EtOAc were prepared by first distillation over activated $CaSO_4$ and MS 5Å prior to use. The cyclic *N*-sulfonyl ketimines **7**[1] were prepared according to the corresponding literature report. The difluoroenoxysilanes **1**, monofluorinated enol silyl ethers **4** and nonfluorinated analogue **8** were prepared according to literature reports.[2]

List of abbreviation:

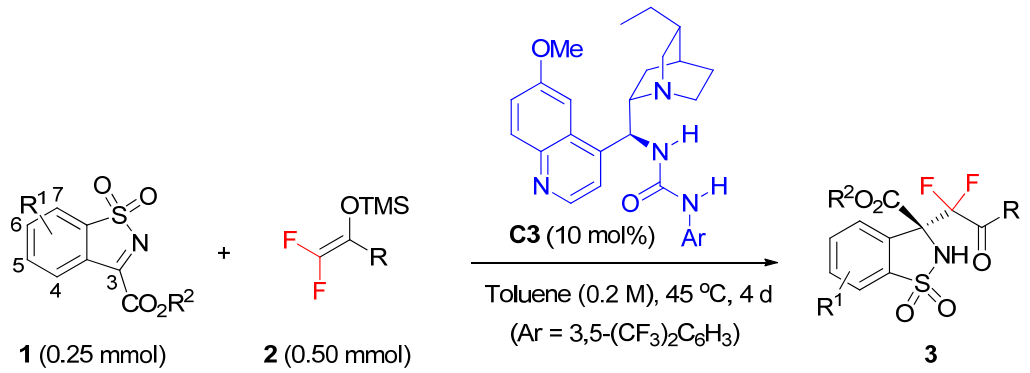
Entry	Chemical name	Abbreviation
1	Petroleum ether	PE
2	Hexafluoroisopropyl alcohol	HFIP

[1] (*a*) H. Wang, T. Jiang and M.-H. Xu, *J. Am. Chem. Soc.,* 2013, **135**, 971; (*b*) S. Zhang, L. Li, Y. Hu, Z. Zha, Z. Wang and T.-P. Loh, *Org. Lett.*, 2015, **17**, 1050.

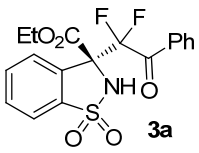
[2] (*a*) H. Amii, T. Kobayashi, Y. Hatamoto and K. Uneyama, *Chem. Commun.* 1999, 1323; (*b*) G. K. S. Prakash, J. Hu and G. A. Olah, *J. Fluorine Chem.* 2001, **112**, 357; (*c*) É. Bélanger, K. Cantin, O. Messe, M. Tremblay and J.-F. Paquin, *J. Am. Chem. Soc.*, 2007, **129**, 1034; (*d*) J. Eames, G. S. Coumbarides, M. J. Suggate and N. Weerasooriya, *Eur. J. Org. Chem.* 2003, 634.

Part I. General procedure for the asymmetric Mukaiyama-Mannich reaction.

The Mukaiyama-Mannich reaction of difluoroenoxysilanes.

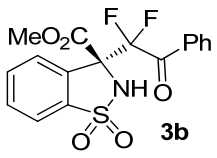


To a 5.0 mL vial were added hydroquinine derived bifunctional urea catalyst **C3** (14.5 mg, 0.025 mmol) and cyclic *N*-sulfonyl ketimine **1** (0.25 mmol), followed by 1.25 mL of anhydrous toluene. The resulting mixture was stirred at 45 °C for about 10 min and then difluoroenoxysilanes **2** (0.50 mmol) was added. The resulting mixture was stirred at 45 °C for 4 days when **1** was almost full consumed by TLC analysis. Then the reaction mixture was directly subjected to flash column chromatography to afford the corresponding product **3**, using indicated eluent.



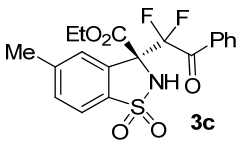
Column chromatography (PE/EtOAc = 5:1 to 3:1) afforded product **3a** in 90% yield as white colloidal solid.[3] HPLC analysis (Chiralpak AD-H, ^{i}PrOH/hexane = 40/60, 1.0 mL/min, 230 nm, 30 °C; t_r (minor) = 27.706 min, t_r (major) = 15.889 min) gave the isomeric composition of the product: 93% ee, $[\alpha]^{28}_{D}$ = -97.8 (c = 0.99, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.09-8.07 (m, 2H), 7.96-7.94 (m, 1H), 7.86-7.84 (m, 1H), 7.77-7.71 (m, 2H), 7.70-7.64 (m, 1H), 7.51-7.47 (m, 2H), 6.03 (s, 1H), 4.42-4.37 (m, 2H), 1.34 (t, *J* = 7.2 Hz, 3H); ^{19}F NMR (376 MHz, $CDCl_3$): δ -99.70 (d, *J* = 297 Hz, 1F), -105.70 (d, *J* = 297 Hz, 1F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 187.73 (dd, *J* = 32 Hz, *J* = 29 Hz), 165.56 (dd, *J* = 7.3 Hz, *J* = 2.0 Hz), 136.53, 135.19, 133.57, 131.77, 131.10, 130.34 (dd, *J* = 3.7 Hz, *J* = 2.1 Hz), 130.26 (d, *J* = 1.4 Hz), 128.79, 126.98 (d, *J* = 5.6 Hz), 121.87, 115.37 (t, *J* = 268 Hz), 68.51 (dd, *J* = 26 Hz, *J* = 24 Hz), 64.36, 13.78.

[3] J.-S.Yu and J. Zhou, *Org. Biomol. Chem.*, 2015, **13**, 10968.



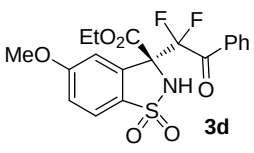
3b

Column chromatography (PE/EtOAc = 4:1) afforded product **3b** in 93% yield as white colloidal solid; HPLC analysis (Chiralpak AS-H, ^{i}PrOH/hexane = 40/60, 1.0 mL/min, 230 nm, 30 ^{o}C; t_r (minor) = 24.952 min, t_r (major) = 15.804 min) gave the isomeric composition of the product: 94% ee, $[\alpha]^{28}_{D}$ = -110.9 (c = 0.77, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.09-8.07 (m, 2H), 7.96-7.93 (m, 1H), 7.87-7.85 (m, 1H), 7.76-7.64 (m, 3H), 7.51-7.47 (m, 2H), 6.05 (s, 1H), 3.93 (s, 3H); ^{19}F NMR (376 MHz, $CDCl_3$): δ -99.71 (d, *J* = 298 Hz, 1F), -106.06 (d, *J* = 298 Hz, 1F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 187.73 (dd, *J* = 32 Hz, *J* = 29 Hz), 166.16 (dd, *J* = 7.4 Hz, *J* = 2.0 Hz), 136.41, 135.27, 133.63, 131.82, 130.95 (t, *J* = 3.6 Hz), 130.36 (dd, *J* = 3.7 Hz, *J* = 2.1 Hz), 129.98 (d, *J* = 1.7 Hz), 128.80, 127.03 (d, *J* = 5.7 Hz), 121.86, 115.34 (t, *J* = 268 Hz), 68.40 (dd, *J* = 26 Hz, *J* = 24 Hz), 54.67. IR (KBr): 3279, 1958, 1753, 1698, 1598, 1451, 1321, 1259, 1180, 1097, 1032, 864, 763, 713, 576 cm^{-1}. MS (EI): 381 (M^+, 0.2), 322 (12), 274 (1), 226 (34), 166 (8), 105 (100), 77 (35), 51 (7). HRMS (EI): Exact mass calcd for $C_{17}H_{13}NO_5F_2S$ $[M]^+$: 381.0483, Found: 381.0485.



3c

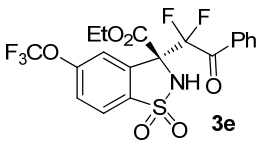
Column chromatography (PE/EtOAc = 4:1 to 2:1) afforded product **3c** in 89% yield as white colloidal solid;[3] HPLC analysis (Chiralpak AD-H, ^{i}PrOH/hexane = 40/60, 1.0 mL/min, 230 nm, 30 ^{o}C; t_r (minor) = 24.750 min, t_r (major) = 17.218 min) gave the isomeric composition of the product: 92% ee, $[\alpha]^{28}_{D}$ = -124.4 (c = 1.05, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.09-8.07 (m, 2H), 7.73-7.72 (m, 2H), 7.67-7.64 (m, 1H), 7.52-7.47 (m, 3H), 6.01 (s, 1H), 4.43-4.36 (m, 2H), 2.52 (s, 3H), 1.34 (t, *J* = 7.2 Hz, 3H); ^{19}F NMR (376 MHz, $CDCl_3$): δ -99.67 (d, *J* = 298 Hz, 1F), -105.87 (d, *J* = 298 Hz, 1F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 187.72 (dd, *J* = 32 Hz, *J* = 29 Hz), 165.59 (dd, *J* = 7.4 Hz, *J* = 2.1 Hz), 144.83, 135.14, 133.83, 132.67, 131.07 (t, *J* = 3.4 Hz), 130.52 (d, *J* = 1.7 Hz), 130.30 (dd, *J* = 3.7 Hz, *J* = 2.1 Hz), 128.75, 127.03 (d, *J* = 5.5 Hz), 121.52, 115.36 (t, *J* = 268 Hz), 68.27 (dd, *J* = 25 Hz, *J* = 24 Hz), 64.23, 21.81, 13.76.



3d

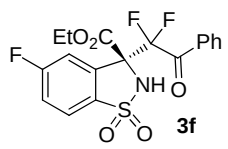
Column chromatography (PE/EtOAc = 4:1 to 2:1) afforded product **3d** in 87% yield as pale yellow colloidal solid;[3] HPLC analysis (Chiralpak AD-H, ^{i}PrOH/hexane = 40/60, 1.0 mL/min, 230 nm, 30 ^{o}C; t_r (minor) = 35.989 min, t_r

(major) = 19.864 min) gave the isomeric composition of the product: 94% ee, $[\alpha]^{28}_D$ = -115.0 (c = 0.52, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.09-8.07 (m, 2H), 7.75 (d, *J* = 8.8 Hz, 1H), 7.68-7.64 (m, 1H), 7.49 (t, *J* = 8.0 Hz, 2H), 7.37-7.36 (m, 1H), 7.22-7.19 (m, 1H), 6.01 (s, 1H), 4.45-4.35 (m, 2H), 3.92 (s, 3H), 1.35 (t, *J* = 7.2 Hz, 3H); ^{19}F NMR (376 MHz, $CDCl_3$): δ -99.81 (d, *J* = 297 Hz, 1F), -106.05 (d, *J* = 297 Hz, 1F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 187.80 (dd, *J* = 32 Hz, *J* = 29 Hz), 165.58 (dd, *J* = 7.4 Hz, *J* = 2.1 Hz), 163.81, 135.26, 132.81 (d, *J* =1.7 Hz), 131.18 (t, *J* = 3.5 Hz), 130.41 (dd, *J* = 3.7 Hz, *J* = 2.0 Hz), 128.87, 128.53, 123.22, 118.30, 115.44 (t, *J* = 269 Hz), 111.41 (d, *J* = 5.8 Hz), 68.18 (dd, *J* = 25 Hz, *J* = 24 Hz), 64.39, 56.10, 13.90.



3e

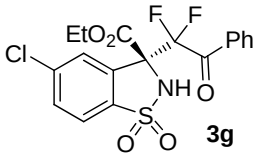
Column chromatography (PE/EtOAc = 4:1) gave **3e** in 95% yield as pale yellow colloidal solid; HPLC analysis (Chiralpak AD-H, ^{i}PrOH/hexane = 25/75, 1.0 mL/min, 230 nm, 30 ^{o}C; t_r (minor) = 13.312 min, t_r (major) = 15.575 min) gave the isomeric composition of the product: 87% ee, $[\alpha]^{28}_D$ = -82.4 (c = 0.46, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.09-8.07 (m, 2H), 7.91 (d, *J* = 8.4 Hz, 1H), 7.78 (s, 1H), 7.70-7.66 (m, 1H), 7.58-7.56 (m, 1H), 7.53-7.49 (m, 2H), 6.15 (s, 1H), 4.50-4.35 (m, 2H), 1.35 (t, *J* = 7.2 Hz, 3H); ^{19}F NMR (376 MHz, $CDCl_3$): δ -57.88 (s, 3F, *CF*$_3$), -99.70 (d, *J* = 297 Hz, 1F), -105.31 (d, *J* = 297 Hz, 1F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 187.42 (dd, *J* = 32 Hz, *J* = 29 Hz), 164.97 (d, *J* = 7.1 Hz), 152.69, 135.39, 134.82, 132.97 (d, *J* =1.5 Hz), 130.94 (t, *J* = 3.6 Hz), 130.39 (dd, *J* = 3.6 Hz, *J* = 2.0 Hz), 128.88, 124.32, 123.77, 120.14 (q, *J* = 259 Hz), 119.17, 119.12, 115.26 (t, *J* = 269 Hz), 68.13 (dd, *J* = 26 Hz, *J* = 24 Hz), 64.78, 13.73. IR (KBr): 3275, 1752, 1701, 1598, 1475, 1259, 1185, 1099, 855, 711, 594 cm^{-1}. MS (EI): 479 (M^+, 0.7), 406 (6), 324 (10), 296 (5), 156 (7), 105 (100), 77 (29), 51 (4). HRMS (EI): Exact mass calcd for $C_{19}H_{14}F_5NO_6S$ $[M]^+$: 479.0462, Found: 479.0455.



3f

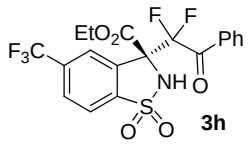
Column chromatography (PE/EtOAc = 4:1 to 3:1) afforded product **3f** in 79% yield as pale white colloidal solid; HPLC analysis (Chiralpak AD-H, ^{i}PrOH/hexane = 25/75, 1.0 mL/min, 230 nm, 30 ^{o}C; t_r (minor) = 22.250 min, t_r (major) = 26.887 min) gave the isomeric composition of the product: 92% ee, $[\alpha]^{28}_D$ = -98.6 (c = 0.65, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.09-8.07 (m, 2H), 7.88-7.84 (m, 1H), 7.69-7.61 (m, 2H), 7.53-7.49 (m, 2H), 7.45-7.40 (m, 1H), 6.10 (s, 1H), 4.42 (q, *J* = 6.8 Hz, 2H), 1.36 (t, *J* = 6.8

Hz, 3H); ^{19}F NMR (376 MHz, $CDCl_3$): δ -99.73 (d, *J* = 297 Hz, 1F), -102.62 (s, 1F), -105.53 (d, *J* = 297 Hz, 1F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 187.48 (dd, *J* = 32 Hz, *J* = 29 Hz), 165.40 (d, *J* = 255 Hz), 165.06 (d, *J* = 7.2 Hz), 135.33, 133.35 (dd, *J* = 9.9 Hz, *J* = 1.8 Hz), 132.66 (d, *J* = 2.9 Hz), 130.97 (t, *J* = 2.8 Hz), 130.36 (dd, *J* = 3.7 Hz, *J* = 2.1 Hz), 128.85, 124.07 (d, *J* = 9.9 Hz), 119.83 (d, *J* = 24 Hz), 115.27 (t, *J* = 269 Hz), 114.415 (dd, *J* = 26 Hz, *J* = 5.7 Hz), 68.04 (t, *J* = 26 Hz), 64.69, 13.79. IR (KBr): 3276, 1751, 1700, 1596, 1481, 1326, 1258, 1183, 1098, 820, 725 cm^{-1}. MS (EI): 340 (7), 258 (11), 249 (4), 195 (27), 156 (6), 105 (95), 103 (100), 77 (33). HRMS (EI): Exact mass calcd for $C_{18}H_{14}NO_5F_3S$ $[M]^+$: 413.0545, Found: 413.0554.



3g

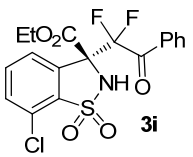
Column chromatography (PE/EtOAc = 4:1) gave **3g** in 74% yield as pale white colloidal solid;[3] HPLC analysis (Chiralpak AS-H, ^{i}PrOH/hexane = 40/60, 1.0 mL/min, 230 nm, 30 ^{o}C; t_r (minor) = 23.453 min, t_r (major) = 12.626 min) gave the isomeric composition of the product: 92% ee, $[\alpha]^{28}_D$ = -108.8 (c = 0.60, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.09-8.07 (m, 2H), 7.92-7.91 (m, 1H), 7.81-7.79 (m, 1H), 7.71-7.66 (m, 2H), 7.53-7.49 (m, 2H), 6.08 (s, 1H), 4.42 (q, *J* = 7.2 Hz, 2H), 1.36 (t, *J* = 7.2 Hz, 3H); ^{19}F NMR (376 MHz, $CDCl_3$): δ -99.52 (d, *J* = 298 Hz, 1F), -105.41 (d, *J* = 298 Hz, 1F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 187.45 (dd, *J* = 32 Hz, *J* = 29 Hz), 165.02 (dd, *J* = 7.2 Hz, *J* = 2.0 Hz), 140.15, 135.33, 135.11, 132.30, 132.25 (d, *J* = 1.8 Hz), 130.95 (t, *J* = 3.6 Hz), 130.37 (dd, *J* = 3.6 Hz, *J* = 2.1 Hz), 128.86, 127.16 (d, *J* = 5.9 Hz), 123.02, 115.27 (t, *J* = 269 Hz), 68.11 (dd, *J* = 26 Hz, *J* = 24 Hz), 64.69, 13.80.



3h

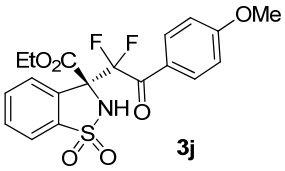
Column chromatography (PE/EtOAc = 4:1) gave **3h** in 94% yield as pale white colloidal solid; HPLC analysis (Chiralpak AD-H, ^{i}PrOH/hexane = 40/60, 1.0 mL/min, 230 nm, 30 ^{o}C; t_r (minor) = 7.52 min, t_r (major) = 11.35 min) gave the isomeric composition of **3h**: 84% ee, $[\alpha]^{28}_D$ = -66.2 (c = 0.90, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.21-8.20 (m, 1H), 8.09-8.07 (m, 2H), 8.01 (s, 2H), 7.70-7.66 (m, 1H), 7.53-7.49 (m, 2H), 6.20 (s, 1H), 4.51-4.36 (m, 2H), 1.35 (t, *J* = 7.2 Hz, 3H); ^{19}F NMR (376 MHz, $CDCl_3$): δ -62.82 (s, 3F, *CF*$_3$), -99.41 (d, *J* = 299 Hz, 1F), -105.09 (d, *J* = 299 Hz, 1F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 187.37 (dd, *J* = 31 Hz, *J* = 29 Hz), 164.90 (dd, *J* = 7.2 Hz, *J* = 1.9 Hz), 139.85, 135.70 (q, *J* = 33 Hz), 135.42, 131.45 (d, *J* = 1.7 Hz), 130.89 (t, *J* = 3.6 Hz), 130.39 (dd, *J* = 3.6 Hz, *J* = 2.3 Hz), 129.13 (q, *J* = 3.5

Hz), 128.90, 124.41 (q, J = 3.9 Hz), 122.89, 122.79 (q, J = 272 Hz), 115.28 (t, J = 269 Hz), 68.41 (dd, J = 26 Hz, J = 24 Hz), 64.81, 13.75. IR (KBr): 3277, 1752, 1702, 1371, 1329, 1178, 1031, 850, 715 cm^{-1}. MS (EI): 463 (M^+, 0.6), 390 (5), 308 (7), 234 (4), 156 (11), 105 (100), 77 (29), 43 (13). HRMS (EI): Exact mass calcd for $C_{19}H_{14}NO_5F_5S$ $[M]^+$: 463.0513, Found: 463.0511.



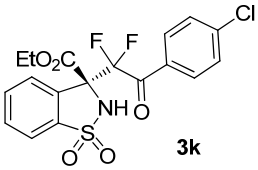
3i

Column chromatography (PE/EtOAc = 4:1 to 3:1) afforded product **3i** in 98% yield as pale white colloidal solid; HPLC analysis (Chiralpak AD-H, ^{i}PrOH/hexane = 40/60, 1.0 mL/min, 230 nm, 30 ^{o}C; t_r (minor) = 13.557 min, t_r (major) = 16.901 min) gave the isomeric composition of the product: 90% ee, $[\alpha]^{28}_D$ = -89.8 (c = 0.86, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.09-8.07 (m, 2H), 7.86-7.84 (m, 1H), 7.70-7.64 (m, 3H), 7.52-7.49 (m, 2H), 6.11 (s, 1H), 4.43-4.38 (m, 2H), 1.35 (t, J = 7.2 Hz, 3H); ^{19}F NMR (282 MHz, $CDCl_3$): δ -99.30 (d, J = 298 Hz, 1F,), -105.44 (d, J = 298 Hz, 1F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 187.54 (dd, J = 30 Hz, J = 29 Hz), 165.17 (dd, J = 7.4 Hz, J = 2.1 Hz), 135.31, 134.64, 134.58. 132.91 (d, J = 1.7 Hz), 132.60, 131.03 (t, J = 3.6 Hz), 130.37 (dd, J = 3.8 Hz, J = 2.1 Hz), 129.61, 128.86, 125.28 (d, J = 5.8 Hz), 115.31 (t, J = 269 Hz), 67.54 (dd, J = 26 Hz, J = 24 Hz), 64.63, 13.81. IR (KBr): 3305, 1739, 1698, 1455, 1262, 1182, 1095, 843, 778, 589 cm^{-1}. MS (EI): 429 (M^+, 0.3), 356 (9), 274 (16), 246 (6), 156 (4), 105 (100), 77 (30), 51 (5). HRMS (EI): Exact mass calcd for $C_{18}H_{14}NO_5F_2S^{35}Cl$ $[M]^+$: 429.0249, Found: 429.0251.



3j

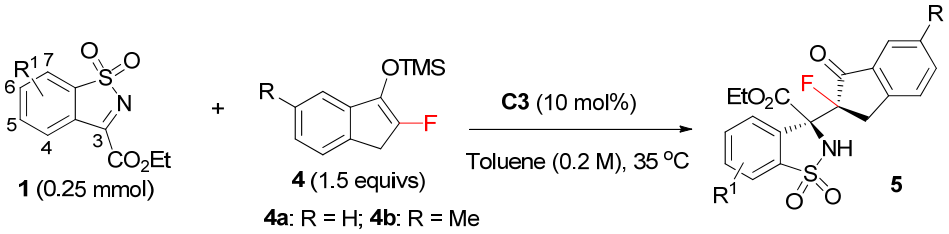
Column chromatography (PE/EtOAc = 5:1 to 3:1) afforded product **3j** in 75% yield as pale white foamy solid;[3] HPLC analysis (Chiralpak AD-H, ^{i}PrOH/hexane = 40/60, 1.0 mL/min, 230 nm, 30 ^{o}C; t_r (minor) = 39.292 min, t_r (major) = 20.875 min) gave the isomeric composition of the product: 92% ee, $[\alpha]^{28}_D$ = -101.5 (c = 1.00, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.09-8.07 (m, 2H), 7.96-7.93 (m, 1H), 7.87-7.85 (m, 1H), 7.75-7.72 (m, 2H), 6.98-6.94 (m, 2H), 6.00 (s, 1H), 4.41-4.34 (m, 2H), 3.89 (s, 3H), 1.34 (t, J = 7.2 Hz, 3H); ^{19}F NMR (376 MHz, $CDCl_3$): δ -99.29 (d, J = 296 Hz, 1F), -105.08 (dd, J = 296 Hz, 1F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 185.86 (dd, J = 31 Hz, J = 29 Hz), 165.68 (dd, J = 7.4 Hz, J = 2.0 Hz), 165.23, 136.57, 133.51, 133.07 (dd, J = 3.9 Hz, J = 1.9 Hz), 131.70, 130.44 (d, J = 1.8 Hz), 127.03 (d, J = 5.7 Hz), 123.95 (dd, J = 3.8 Hz, J = 2.8 Hz), 121.87, 115.74 (t, J = 268 Hz), 114.19, 68.54 (dd, J = 26 Hz, J = 24 Hz), 64.24, 55.63, 13.81.



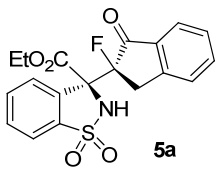
3k

Column chromatography (PE/EtOAc = 4:1 to 3:1) gave **3k** in 74% yield as pale white colloidal solid;[3] HPLC analysis (Chiralpak AD-H, ^{i}PrOH/hexane = 40/60, 1.0 mL/min, 230 nm, 30 ^{o}C; t_r (minor) = 24.700 min, t_r (major) = 15.211 min) gave the isomeric composition of the product: 93% ee, $[\alpha]^{28}_{D}$ = -100.8 (c = 1.08, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.04-8.01 (m, 2H), 7.96-7.93 (m, 1H), 7.87-7.85 (m, 1H), 7.78-7.73 (m, 2H), 7.49-7.46 (m, 2H), 6.04 (s, 1H), 4.43-4.37 (m, 2H), 1.34 (t, *J* = 7.2 Hz, 3H); ^{19}F NMR (376 MHz, $CDCl_3$): δ -99.87 (d, *J* = 297 Hz, 1F), -105.86 (d, *J* = 297 Hz, 1F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 186.73 (dd, *J* = 32 Hz, *J* = 29 Hz), 165.40 (dd, *J* = 7.3 Hz, *J* = 2.0 Hz), 142.01, 136.51, 133.61, 131.84, 131.72 (dd, *J* = 3.9 Hz, *J* = 2.1 Hz), 130.08 (d, *J* = 1.7 Hz), 129.47 (t, *J* = 3.0 Hz), 129.23, 126.95 (d, *J* = 5.4 Hz), 121.90, 115.25 (t, *J* = 267 Hz), 68.42 (dd, *J* = 26 Hz, *J* = 24 Hz), 64.46, 13.78.

The Mukaiyama-Mannich reaction of monofluorinated enol silyl ethers



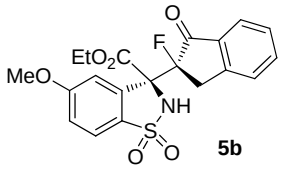
To a 5.0 mL vial were added hydroquinine derived bifunctional urea catalyst **C3** (14.5 mg, 0.025 mmol) and cyclic *N*-sulfonyl ketimine **1** (0.25 mmol), followed by 1.25 mL of anhydrous toluene. The resulting mixture was stirred at 35 ^{o}C for about 10 min and then mono-fluorinated enol silyl ether **4** (0.375 mmol) was added. The resulting mixture was stirred at 35 ^{o}C till full conversion of **1** by TLC analysis. The reaction mixturing was directly subjected to flash column chromatography to afford the corresponding product **5**, using indicated eluent.



5a

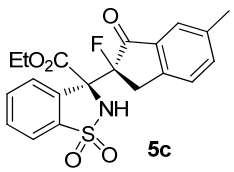
Column chromatography (PE/EtOAc = 5:1 to 3:1) gave **5a** in 99% yield as white solid (m.p. = 146-148 ^{o}C), dr value was determined by ^{1}H NMR or ^{19}F NMR of crude mixture. HPLC analysis (Chiralpak AD-H, ^{i}PrOH/hexane = 40/60, 1.0 mL/min, 230 nm, 30 ^{o}C; t_r (minor) = 18.152 min, t_r (major) = 9.277 min) gave the isomeric composition of the product: 90% ee, $[\alpha]^{28}_{D}$ = +19.4 (c = 0.72, $CHCl_3$); ^{1}H NMR (400 MHz,

$CDCl_3$): δ 7.92-7.89 (m, 1H), 7.78-7.77 (m, 2H), 7.69-7.63 (m, 3H), 7.44-7.40 (m, 2H), 6.21 (s, 1H), 4.42-4.28 (m, 2H), 3.63 (dd, *J* = 18 Hz, *J* = 15.6 Hz, 1H), 3.37 (dd, *J* = 24.4 Hz, *J* = 16.4 Hz, 1H), 1.31 (t, *J* = 7.2 Hz, 3H); ^{19}F NMR (282 MHz, $CDCl_3$): δ -158.71 (s, 1F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 196.18 (d, *J* = 18 Hz), 167.63, 149.59 (d, *J* = 2 Hz), 136.55, 135.72, 134.45, 133.12, 131.74, 131.12, 128.59, 127.33 (d, *J* = 5 Hz), 126.14, 125.31, 121.44, 95.74 (d, *J* = 201 Hz), 69.72 (d, *J* = 27 Hz), 64.22, 36.84 (d, *J* = 24 Hz), 13.83. IR (KBr): 3289, 3001, 1724, 1605, 1467, 1360, 1314, 1174, 1024, 888, 739, 577 cm^{-1}. MS (EI): 389 (M^+, 0.5), 316 (100), 296 (6), 150 (80), 130 (14), 103 (52). HRMS (EI): Exact mass calcd for $C_{19}H_{16}NO_5FS$ $[M]^+$: 389.0733, Found: 389.0735.



5b

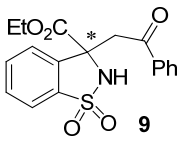
Column chromatography (PE/EtOAc = 5:1 to 3:1) afforded product **5b** in 78% yield as white solid (m.p. = 68-70 °C), dr value was determined by ^{1}H NMR or ^{19}F NMR of crude reaction mixture. HPLC analysis (Chiralpak AD-H, ^{i}PrOH/hexane = 40/60, 1.0 mL/min, 230 nm, 30 °C; t_r (minor) = 19.698 min, t_r (major) = 10.810 min) gave the isomeric composition of the product: 92% ee, $[\alpha]^{28}_D$ = +14.7 (c = 0.49, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.79-7.77 (m, 1H), 7.69-7.63 (m, 2H), 7.44-7.40 (m, 2H), 7.30-7.29 (m, 1H), 7.16-7.13 (m, 1H), 6.11 (s, 1H), 4.41-4.33 (m, 2H), 3.86 (s, 3H), 3.58 (t, *J* = 17.6 Hz, 1H), 3.36 (dd, *J* = 24.8 Hz, *J* = 18 Hz, 1H), 1.34 (t, *J* = 7.2 Hz, 3H); ^{19}F NMR (282 MHz, $CDCl_3$): δ -158.71 (s, 1F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 196.01 (d, *J* = 18 Hz), 167.53, 163.34, 149.60 (d, *J* = 3 Hz), 136.50, 134.57, 134.16, 128.57, 127.87, 126.15, 125.23, 122.69, 117.75, 111.80 (d, *J* = 5 Hz), 95.97 (d, *J* = 201 Hz), 69.31 (d, *J* = 26 Hz), 64.19, 55.87, 36.87 (d, *J* = 24 Hz), 13.88. IR (KBr): 3415, 1729, 1602, 1485, 1306, 1259, 1169, 1021 cm^{-1}. MS (EI): 346 (54), 309 (5), 195 (24), 150 (36), 133 (41), 103 (100). HRMS (EI): Exact mass calcd for $C_{20}H_{18}NO_6FS$ $[M]^+$: 419.0839, Found: 419.0836.



5c

Column chromatography (PE/EtOAc = 5:1 to 3:1) afforded product **5c** in 88% yield as white solid (m.p. = 76-78 °C), dr value was determined by ^{1}H NMR or ^{19}F NMR of crude reaction mixture. HPLC analysis (Chiralpak AD-H, ^{i}PrOH/hexane = 40/60, 1.0 mL/min, 230 nm, 30 °C; t_r (minor) = 19.178 min, t_r (major) = 9.397 min) gave the isomeric composition of the product: 90% ee, $[\alpha]^{28}_D$ = +18.5 (c = 0.61, $CHCl_3$); ^{1}H NMR

(400 MHz, $CDCl_3$): δ 7.91-7.89 (m, 1H), 7.80-7.78 (m, 1H), 7.71-7.66 (m, 2H), 7.57 (s, 1H), 7.48-7.45 (m, 1H), 7.31-7.29 (m, 1H), 6.24 (s, 1H), 4.41-4.27 (m, 2H), 3.58 (t, *J* = 17.6 Hz, 1H), 3.32 (dd, *J* = 24.8 Hz, *J* = 18 Hz, 1H), 2.39 (s, 3H), 1.30 (t, *J* = 7.2 Hz, 3H); ^{19}F NMR (282 MHz, $CDCl_3$): δ -158.51 (s, 1F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 196.23 (d, *J* = 18 Hz), 167.66, 147.02 (d, *J* = 3 Hz), 138.74, 137.85, 135.71, 134.55, 133.08, 131.83, 131.06, 127.30 (d, *J* = 5 Hz), 125.82, 125.12, 121.40, 95.98 (d, *J* = 200 Hz), 69.80 (d, *J* = 27 Hz), 64.14, 36.53 (d, *J* = 24 Hz), 21.03, 13.81. IR (KBr): 3264, 2932, 1728, 1369, 1312, 1253, 1176, 1067, 758, 578 cm^{-1}. MS (EI): 330 (9), 310 (3), 195 (24), 164 (11), 103 (100), 76 (16). HRMS (EI): Exact mass calcd for $C_{20}H_{18}NO_5FS$ $[M]^+$: 403.0890, Found: 403.0888.

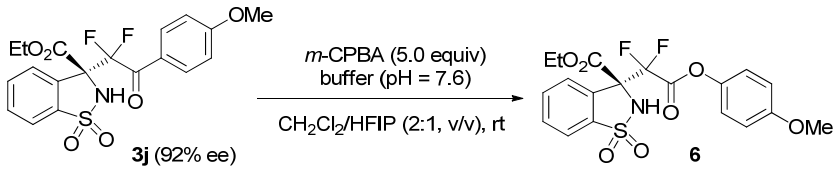


9

Column chromatography (PE/EtOAc = 2:1) afforded product **9** in 24% yield as white solid.[4] HPLC analysis (Chiralpak IC, ^{i}PrOH/hexane = 40/60, 1.0 mL/min, 230 nm, 30 ^{o}C; t_r (minor) = 30.409 min, t_r (major) = 20.532 min) gave the isomeric composition of the product: 32% ee; ^1H NMR (400 MHz, $CDCl_3$): δ 7.93-7.91 (m, 2H), 7.85-7.83 (m, 1H), 7.72-7.71 (m, 2H), 7.67-7.59 (m, 2H), 7.49-7.45 (m, 2H), 6.08 (s, 1H), 4.38-4.27 (m, 2H), 4.09 (d, *J* = 17.6 Hz, 1H), 3.73 (d, *J* = 17.6 Hz, 1H), 1.31 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 195.92, 169.58, 136.87, 135.52, 134.01, 133.64, 130.80, 128.78, 128.17, 124.20, 121.88, 65.43, 63.50, 49.13, 13.94.

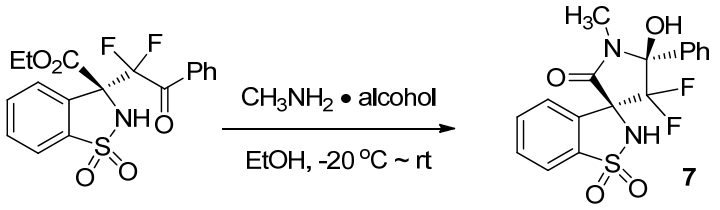
[4] S. Nakamura, M. Sano, A. Toda, D. Nakane and H. Masuda, *Chem. Eur. J.*, 2015, **21**, 3929.

Part II. Synthetic elaborations.



The product **3j** (107.0 mg, 0.25 mmol) was dissolved in CH_2Cl_2/HFIP (2:1, 3.0 mL), followed by the addition of *m*-chloroperoxybenzoic acid (*m*-CPBA) (276.0 mg, 1.25 mmol, 85% wt) and phosphate buffer (0.25 mL, pH = 7.6) at ambient temperature.[5] The mixture was stirred until full consumption of **3j** by TLC analysis (ca. 5 h), and then quenched by saturated $Na_2S_2O_3$ (aq), followed by extraction using CH_2Cl_2 (10.0 mL × 3). The combined organic layers were washed with saturated $NaHCO_3$ and brine (10.0 mL × 3), and then dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified by column chromatography (using PE/EtOAc = 2/1 as eluent) to afford **6** (107.0 mg, 97% yield) as pale yellow oil. HPLC analysis (Chiralpak AD-H, ^{i}PrOH/hexane = 40/60, 1.0 mL/min, 230 nm, 30 ^{o}C; t_r (minor) = 20.938 min, t_r (major) = 13.596 min) gave the isomeric composition of the product: 91% ee, $[\alpha]^{25}_{D}$ = -54.8 (c = 1.0, $CHCl_3$); IR (KBr): 3264, 2966, 1793, 1748, 1505, 1455, 1324, 1251, 1108, 1030, 861, 761, 573 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.03-8.01 (m, 1H), 7.84-7.82 (m, 1H), 7.78-7.71 (m, 2H), 7.08-7.04 (m, 2H), 6.90-6.85 (m, 2H), 6.09 (s, 1H), 4.49-4.36 (m, 2H), 3.78 (s, 3H), 1.37 (t, *J* = 7.2 Hz, 3H); ^{19}F NMR (282 MHz, $CDCl_3$): δ -107.88 (d, *J* = 266 Hz, 1F), -109.81 (d, *J* = 266 Hz, 1F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.91 (d, *J* = 3 Hz), 160.09 (t, *J* = 32 Hz), 158.04, 142.98, 135.90, 133.77, 131.95, 127.23 (t, *J* = 3 Hz), 121.80, 121.59, 114.63, 112.95 (t, *J* = 264 Hz), 69.12 (dd, *J* = 27 Hz, *J* = 26 Hz), 65.01, 55.58, 13.86. MS (EI): 441 (M^+, 5), 368 (3), 262 (2), 124 (53), 105 (55), 85 (72), 83 (100), 43 (22); HRMS (EI): Exact mass calcd for $C_{19}H_{17}NO_7SF_2$ $[M]^+$: 441.0694, Found: 441.0692.

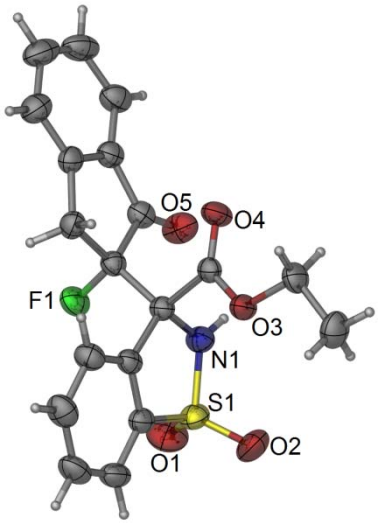
[5] S. Kobayashi, H. Tanaka, H. Amii and K. Uneyama, *Tetrahedron* 2003, **59**, 1547.



3a (92% ee) (63% yield, 92% ee)

To a 25.0 mL Schlenk tube was added product **3a** (100 mg, 0.253 mmol), followed by 3.0 mL anhydrous EtOH under N_2 atmosphere. The mixture was cooled to -20 °C, and then 0.6 mL CH_3NH_2 in ethanol (27-30% wt) was added dropwise at -20 °C. The mixture was stirred at room temperature until full consumption of **3a** by TLC analysis (about 5 h). Then the reaction mixture was concentrated under reduced pressure, and the residue was purified by column chromatography (PE/ethyl acetate = 1/1) to afford product **7** as a single isomer and white solid in 63% yield (60.7 mg). M. p. 240-242 ^{o}C. HPLC analysis (Chiralpak AD-H, ^{i}PrOH/hexane = 40/60, 0.8 mL/min, 230 nm, t_r (minor) = 10.973 min, t_r (major) = 8.275 min) gave the isomeric composition of the product: 92% ee, $[\alpha]^{25}_{D}$ = +8.4 (c = 0.55, acetone); ^{1}H NMR (400 MHz, acetone-d_6): δ 7.80-7.76 (m, 1H), 7.69-7.64 (m, 2H), 7.61-7.58 (m, 2H), 7.54-7.50 (m, 1H), 7.44-7.36 (m, 3H), 7.04 (s, br, 1H), 2.73 (s, 4H); ^{19}F NMR (282 MHz, acetone-d_6): δ -109.41 (d, J = 230 Hz, 1F), -128.38 (d, J = 230 Hz, 1F); ^{13}C NMR (100 MHz, acetone-d_6): δ 169.30 (d, J = 6 Hz), 138.69, 133.88, 133.75, 132.17, 132.04, 130.61, 129.40 (d, J = 2.5 Hz), 129.29, 128.74 (d, J = 7 Hz), 121.72, 118.51 (dd, J = 273 Hz, J = 253 Hz), 92.66 (dd, J = 29 Hz, J = 24 Hz), 67.60 (dd, J = 29 Hz, J = 19 Hz), 27.31; IR (KBr): 3375, 1737, 1452, 1419, 1364, 1302, 1243, 1158, 1113, 1063, 768, 754, 526 cm^{-1}; HRMS (ESI): Exact mass calcd for $C_{17}H_{18}F_2N_3O_4S$ $[M+NH_4]^+$: 398.0981, Found: 398.0981.

Part III. X-ray crystal data of 5a.[6]



Data intensity of $C_{19}H_{16}FNO_5S$ (**5a**) was collected using a Bruker SMART APEX II (Mo radiation) at 296 K in a nitrogen stream. Data collection and reduction were done by using the Bruker ApexII software package. The structures were solved by direct methods and refined by full-matrix least-squares on F^2 with anisotropic displacement parameters for non-H atoms using SHELX-97. Hydrogen atoms were added at their geometrically idea positions and refined isotropically. Crystal data for **5a**: $C_{19}H_{16}FNO_5S$, T = 296(2) K, Orthorhombic, P2(1)2(1)2(1) a = 10.342(2) Å, b = 12.672(3) Å, c = 13.549(3) Å, alpha = 90 deg, beta = 90 deg, gamma = 90 deg. V = 1775.6(7) Å^3. Z = 4, d_{calc} = 1.457 mg/m^3. Total number of reflections 20679 [R(int) = 0.0282], R_1 = 0.0294, wR_2 = 0.0739 (all data), GOF = 1.029, and 244 parameter.

Table 1. Crystal data and structure refinement for z.

Identification code	z
Empirical formula	$C_{19}H_{16}FNO_5S$
Formula weight	389.39
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 10.342(2) Å alpha = 90 deg.
	b = 12.672(3) Å beta = 90 deg.
	c = 13.549(3) Å gamma = 90 deg.

[6] Supplementary crystallographic data have been deposited at the Cambridge Crystallographic Data Center. (CCDC 1439365).

Volume	1775.6(7) $Å^3$
Z, Calculated density	4, 1.457 Mg/m^3
Absorption coefficient	0.224 mm^{-1}
F(000)	808
Crystal size	0.46 x 0.32 x 0.26 mm
Theta range for data collection	2.20 to 24.99 deg.
Limiting indices	-12<=h<=12, -15<=k<=15, -16<=l<=16
Reflections collected / unique	20679 / 3128 [R(int) = 0.0282]
Completeness to theta = 24.99	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9441 and 0.9040
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3128 / 0 / 244
Goodness-of-fit on F^2	1.029
Final R indices [I>2sigma(I)]	R_1 = 0.0273, wR_2 = 0.0720
R indices (all data)	R_1 = 0.0294, wR_2 = 0.0739
Absolute structure parameter	0.00(6)
Largest diff. peak and hole	0.254 and -0.220 $e.A^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for z. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
S(1)	9204(1)	9407(1)	763(1)	42(1)
O(1)	9824(2)	8747(1)	53(1)	66(1)
O(2)	9627(2)	9312(1)	1762(1)	65(1)
O(3)	7761(1)	11865(1)	1769(1)	39(1)
O(4)	8190(1)	12998(1)	537(1)	43(1)
O(5)	10200(1)	11982(1)	-1093(1)	51(1)
N(1)	9273(2)	10638(1)	390(1)	38(1)
F(1)	8059(1)	10538(1)	-1465(1)	46(1)
C(1)	7517(2)	9349(1)	707(1)	36(1)
C(2)	6766(2)	8474(2)	927(1)	46(1)
C(3)	5449(2)	8572(2)	856(2)	50(1)
C(4)	4902(2)	9527(2)	584(2)	50(1)
C(5)	5661(2)	10397(2)	370(1)	41(1)
C(6)	6994(2)	10304(1)	425(1)	33(1)
C(7)	8010(2)	11137(1)	181(1)	31(1)

C(8)	7932(2)	11467(1)	-916(1)	33(1)
C(9)	6708(2)	12050(2)	-1235(1)	38(1)
C(10)	7187(2)	12932(1)	-1889(1)	37(1)
C(11)	6457(2)	13641(2)	-2432(2)	49(1)
C(12)	7103(3)	14390(2)	-2993(2)	58(1)
C(13)	8438(3)	14440(2)	-3012(2)	56(1)
C(14)	9176(2)	13747(2)	-2466(1)	46(1)
C(15)	8524(2)	12994(1)	-1902(1)	37(1)
C(16)	9068(2)	12168(1)	-1280(1)	36(1)
C(17)	7970(2)	12124(1)	840(1)	31(1)
C(18)	7855(2)	12716(2)	2494(1)	45(1)
C(19)	7865(2)	12216(2)	3494(2)	56(1)

Table 3. Bond lengths [Å] and angles [deg] for z.

S(1)-O(1)	1.4275(17)
S(1)-O(2)	1.4282(16)
S(1)-N(1)	1.6408(16)
S(1)-C(1)	1.7484(19)
O(3)-C(17)	1.318(2)
O(3)-C(18)	1.462(2)
O(4)-C(17)	1.203(2)
O(5)-C(16)	1.220(2)
N(1)-C(7)	1.478(2)
N(1)-H(1A)	0.8600
F(1)-C(8)	1.399(2)
C(1)-C(6)	1.379(3)
C(1)-C(2)	1.386(3)
C(2)-C(3)	1.371(3)
C(2)-H(2A)	0.9300
C(3)-C(4)	1.386(3)
C(3)-H(3A)	0.9300
C(4)-C(5)	1.384(3)
C(4)-H(4A)	0.9300
C(5)-C(6)	1.386(3)
C(5)-H(5A)	0.9300
C(6)-C(7)	1.526(2)
C(7)-C(17)	1.537(2)
C(7)-C(8)	1.546(2)
C(8)-C(9)	1.528(3)
C(8)-C(16)	1.553(2)
C(9)-C(10)	1.510(3)
C(9)-H(9A)	0.9700

C(9)-H(9B)	0.9700
C(10)-C(15)	1.384(3)
C(10)-C(11)	1.384(3)
C(11)-C(12)	1.388(3)
C(11)-H(11A)	0.9300
C(12)-C(13)	1.383(4)
C(12)-H(12A)	0.9300
C(13)-C(14)	1.379(3)
C(13)-H(13A)	0.9300
C(14)-C(15)	1.396(3)
C(14)-H(14A)	0.9300
C(15)-C(16)	1.457(3)
C(18)-C(19)	1.495(3)
C(18)-H(18A)	0.9700
C(18)-H(18B)	0.9700
C(19)-H(19B)	0.9600
C(19)-H(19C)	0.9600
C(19)-H(19D)	0.9600

O(1)-S(1)-O(2)	116.87(11)
O(1)-S(1)-N(1)	109.30(10)
O(2)-S(1)-N(1)	111.03(10)
O(1)-S(1)-C(1)	113.23(10)
O(2)-S(1)-C(1)	110.08(10)
N(1)-S(1)-C(1)	94.02(9)
C(17)-O(3)-C(18)	116.61(14)
C(7)-N(1)-S(1)	115.31(12)
C(7)-N(1)-H(1A)	122.3
S(1)-N(1)-H(1A)	122.3
C(6)-C(1)-C(2)	122.82(18)
C(6)-C(1)-S(1)	111.46(14)
C(2)-C(1)-S(1)	125.71(15)
C(3)-C(2)-C(1)	118.00(18)
C(3)-C(2)-H(2A)	121.0
C(1)-C(2)-H(2A)	121.0
C(2)-C(3)-C(4)	120.16(19)
C(2)-C(3)-H(3A)	119.9
C(4)-C(3)-H(3A)	119.9
C(5)-C(4)-C(3)	121.3(2)
C(5)-C(4)-H(4A)	119.3
C(3)-C(4)-H(4A)	119.3
C(4)-C(5)-C(6)	119.04(19)
C(4)-C(5)-H(5A)	120.5

C(6)-C(5)-H(5A)	120.5
C(1)-C(6)-C(5)	118.63(16)
C(1)-C(6)-C(7)	113.42(16)
C(5)-C(6)-C(7)	127.93(17)
N(1)-C(7)-C(6)	105.69(13)
N(1)-C(7)-C(17)	105.12(13)
C(6)-C(7)-C(17)	114.73(14)
N(1)-C(7)-C(8)	110.29(14)
C(6)-C(7)-C(8)	111.05(14)
C(17)-C(7)-C(8)	109.67(14)
F(1)-C(8)-C(9)	109.53(14)
F(1)-C(8)-C(7)	106.14(13)
C(9)-C(8)-C(7)	116.54(14)
F(1)-C(8)-C(16)	103.98(13)
C(9)-C(8)-C(16)	105.11(14)
C(7)-C(8)-C(16)	114.82(15)
C(10)-C(9)-C(8)	104.58(15)
C(10)-C(9)-H(9A)	110.8
C(8)-C(9)-H(9A)	110.8
C(10)-C(9)-H(9B)	110.8
C(8)-C(9)-H(9B)	110.8
H(9A)-C(9)-H(9B)	108.9
C(15)-C(10)-C(11)	120.07(18)
C(15)-C(10)-C(9)	112.17(16)
C(11)-C(10)-C(9)	127.76(18)
C(10)-C(11)-C(12)	118.2(2)
C(10)-C(11)-H(11A)	120.9
C(12)-C(11)-H(11A)	120.9
C(13)-C(12)-C(11)	121.5(2)
C(13)-C(12)-H(12A)	119.3
C(11)-C(12)-H(12A)	119.3
C(14)-C(13)-C(12)	120.9(2)
C(14)-C(13)-H(13A)	119.6
C(12)-C(13)-H(13A)	119.6
C(13)-C(14)-C(15)	117.5(2)
C(13)-C(14)-H(14A)	121.2
C(15)-C(14)-H(14A)	121.2
C(10)-C(15)-C(14)	121.87(19)
C(10)-C(15)-C(16)	109.73(16)
C(14)-C(15)-C(16)	128.38(19)
O(5)-C(16)-C(15)	128.96(17)
O(5)-C(16)-C(8)	123.35(16)
C(15)-C(16)-C(8)	107.58(15)

O(4)-C(17)-O(3)	125.85(16)
O(4)-C(17)-C(7)	123.08(16)
O(3)-C(17)-C(7)	110.89(14)
O(3)-C(18)-C(19)	107.29(17)
O(3)-C(18)-H(18A)	110.3
C(19)-C(18)-H(18A)	110.3
O(3)-C(18)-H(18B)	110.3
C(19)-C(18)-H(18B)	110.3
H(18A)-C(18)-H(18B)	108.5
C(18)-C(19)-H(19B)	109.5
C(18)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(18)-C(19)-H(19D)	109.5
H(19B)-C(19)-H(19D)	109.5
H(19C)-C(19)-H(19D)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2$ x 10^3) for z. The anisotropic displacement factor exponent takes the form: $-2\ pi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
S(1)	46(1)	35(1)	44(1)	4(1)	-4(1)	8(1)
O(1)	68(1)	46(1)	84(1)	-9(1)	11(1)	18(1)
O(2)	68(1)	70(1)	57(1)	24(1)	-21(1)	-3(1)
O(3)	53(1)	33(1)	30(1)	-1(1)	0(1)	-3(1)
O(4)	56(1)	32(1)	41(1)	2(1)	5(1)	-8(1)
O(5)	33(1)	59(1)	61(1)	14(1)	7(1)	2(1)
N(1)	33(1)	36(1)	45(1)	4(1)	-1(1)	2(1)
F(1)	62(1)	37(1)	39(1)	-9(1)	3(1)	-3(1)
C(1)	48(1)	32(1)	28(1)	-1(1)	-1(1)	0(1)
C(2)	70(1)	32(1)	38(1)	4(1)	2(1)	-4(1)
C(3)	62(1)	41(1)	48(1)	0(1)	9(1)	-18(1)
C(4)	44(1)	53(1)	52(1)	-3(1)	7(1)	-12(1)
C(5)	40(1)	37(1)	46(1)	0(1)	6(1)	-2(1)
C(6)	41(1)	30(1)	28(1)	-2(1)	3(1)	-4(1)
C(7)	31(1)	30(1)	33(1)	1(1)	0(1)	0(1)
C(8)	37(1)	30(1)	32(1)	-2(1)	1(1)	0(1)
C(9)	36(1)	43(1)	35(1)	4(1)	-3(1)	-3(1)
C(10)	44(1)	37(1)	29(1)	-2(1)	-2(1)	0(1)
C(11)	54(1)	48(1)	45(1)	5(1)	-3(1)	6(1)
C(12)	84(2)	45(1)	46(1)	10(1)	0(1)	13(1)
C(13)	84(2)	40(1)	44(1)	8(1)	14(1)	-5(1)

C(14)	58(1)	41(1)	39(1)	0(1)	9(1)	-6(1)
C(15)	45(1)	35(1)	30(1)	-2(1)	4(1)	-2(1)
C(16)	37(1)	36(1)	34(1)	-3(1)	6(1)	-1(1)
C(17)	26(1)	33(1)	35(1)	0(1)	-2(1)	-1(1)
C(18)	56(1)	42(1)	37(1)	-9(1)	-3(1)	-3(1)
C(19)	61(1)	71(1)	35(1)	-4(1)	-2(1)	-3(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for z.

	x	y	z	U(eq)
H(1A)	9993	10969	322	45
H(2A)	7144	7840	1117	56
H(3A)	4921	7995	990	60
H(4A)	4007	9585	544	60
H(5A)	5282	11035	192	49
H(9A)	6134	11584	-1597	46
H(9B)	6250	12329	-668	46
H(11A)	5559	13615	-2420	59
H(12A)	6627	14869	-3365	70
H(13A)	8844	14948	-3399	67
H(14A)	10074	13780	-2473	55
H(18A)	7122	13190	2432	54
H(18B)	8642	13118	2392	54
H(19B)	7923	12755	3990	83
H(19C)	8595	11752	3548	83
H(19D)	7082	11820	3586	83

Table 6. Torsion angles [deg] for z.

O(1)-S(1)-N(1)-C(7)	116.24(14)
O(2)-S(1)-N(1)-C(7)	-113.40(14)
C(1)-S(1)-N(1)-C(7)	-0.09(13)
O(1)-S(1)-C(1)-C(6)	-114.89(15)
O(2)-S(1)-C(1)-C(6)	112.23(14)
N(1)-S(1)-C(1)-C(6)	-1.90(14)
O(1)-S(1)-C(1)-C(2)	66.09(19)
O(2)-S(1)-C(1)-C(2)	-66.79(19)
N(1)-S(1)-C(1)-C(2)	179.09(17)
C(6)-C(1)-C(2)-C(3)	0.2(3)
S(1)-C(1)-C(2)-C(3)	179.14(16)
C(1)-C(2)-C(3)-C(4)	-0.9(3)
C(2)-C(3)-C(4)-C(5)	0.6(3)

C(3)-C(4)-C(5)-C(6)	0.3(3)
C(2)-C(1)-C(6)-C(5)	0.7(3)
S(1)-C(1)-C(6)-C(5)	-178.36(14)
C(2)-C(1)-C(6)-C(7)	-177.67(16)
S(1)-C(1)-C(6)-C(7)	3.28(18)
C(4)-C(5)-C(6)-C(1)	-0.9(3)
C(4)-C(5)-C(6)-C(7)	177.14(17)
S(1)-N(1)-C(7)-C(6)	1.79(17)
S(1)-N(1)-C(7)-C(17)	123.53(13)
S(1)-N(1)-C(7)-C(8)	-118.32(13)
C(1)-C(6)-C(7)-N(1)	-3.20(19)
C(5)-C(6)-C(7)-N(1)	178.63(17)
C(1)-C(6)-C(7)-C(17)	-118.52(17)
C(5)-C(6)-C(7)-C(17)	63.3(2)
C(1)-C(6)-C(7)-C(8)	116.42(16)
C(5)-C(6)-C(7)-C(8)	-61.8(2)
N(1)-C(7)-C(8)-F(1)	60.91(17)
C(6)-C(7)-C(8)-F(1)	-55.92(17)
C(17)-C(7)-C(8)-F(1)	176.23(13)
N(1)-C(7)-C(8)-C(9)	-176.84(14)
C(6)-C(7)-C(8)-C(9)	66.32(19)
C(17)-C(7)-C(8)-C(9)	-61.53(19)
N(1)-C(7)-C(8)-C(16)	-53.34(19)
C(6)-C(7)-C(8)-C(16)	-170.17(14)
C(17)-C(7)-C(8)-C(16)	61.97(18)
F(1)-C(8)-C(9)-C(10)	-102.46(16)
C(7)-C(8)-C(9)-C(10)	137.09(15)
C(16)-C(8)-C(9)-C(10)	8.72(18)
C(8)-C(9)-C(10)-C(15)	-6.1(2)
C(8)-C(9)-C(10)-C(11)	174.37(18)
C(15)-C(10)-C(11)-C(12)	1.1(3)
C(9)-C(10)-C(11)-C(12)	-179.5(2)
C(10)-C(11)-C(12)-C(13)	-0.4(3)
C(11)-C(12)-C(13)-C(14)	-0.4(4)
C(12)-C(13)-C(14)-C(15)	0.4(3)
C(11)-C(10)-C(15)-C(14)	-1.1(3)
C(9)-C(10)-C(15)-C(14)	179.40(17)
C(11)-C(10)-C(15)-C(16)	-179.88(17)
C(9)-C(10)-C(15)-C(16)	0.6(2)
C(13)-C(14)-C(15)-C(10)	0.3(3)
C(13)-C(14)-C(15)-C(16)	178.88(19)
C(10)-C(15)-C(16)-O(5)	-178.55(19)
C(14)-C(15)-C(16)-O(5)	2.8(3)

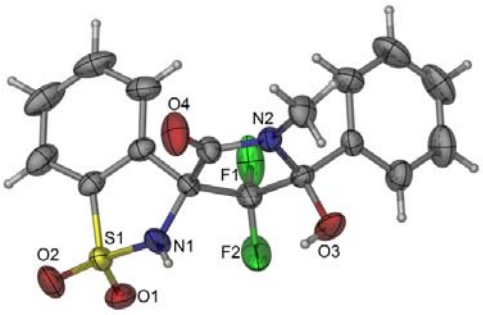
C(10)-C(15)-C(16)-C(8)	5.2(2)
C(14)-C(15)-C(16)-C(8)	-173.50(18)
F(1)-C(8)-C(16)-O(5)	-70.2(2)
C(9)-C(8)-C(16)-O(5)	174.75(18)
C(7)-C(8)-C(16)-O(5)	45.3(2)
F(1)-C(8)-C(16)-C(15)	106.35(15)
C(9)-C(8)-C(16)-C(15)	-8.74(18)
C(7)-C(8)-C(16)-C(15)	-138.14(15)
C(18)-O(3)-C(17)-O(4)	-2.4(3)
C(18)-O(3)-C(17)-C(7)	172.85(15)
N(1)-C(7)-C(17)-O(4)	100.68(19)
C(6)-C(7)-C(17)-O(4)	-143.66(17)
C(8)-C(7)-C(17)-O(4)	-17.9(2)
N(1)-C(7)-C(17)-O(3)	-74.72(16)
C(6)-C(7)-C(17)-O(3)	40.9(2)
C(8)-C(7)-C(17)-O(3)	166.72(14)
C(17)-O(3)-C(18)-C(19)	-168.24(17)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for z [Å and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)

Part IV. X-ray data of 7.[7]



Data intensity of $C_{17}H_{14}F_2N_2O_4S$ (**7**) was collected using a Bruker SMART APEX II (Mo radiation) at 296 K in a nitrogen stream. Data collection and reduction were done by using the Bruker ApexII software package. The structures were solved by direct methods and refined by full-matrix least-squares on F^2 with anisotropic displacement parameters for non-H atoms using SHELX-97. Hydrogen atoms were added at their geometrically idea positions and refined isotropically. Crystal data for **7**: $C_{17}H_{14}F_2N_2O_4S$, T = 296(2) K, Orthorhombic, P2(1)2(1)2(1). a = 7.1956(3) Å, b = 9.6833(3) Å, c = 23.2873(8) Å, alpha = 90 deg, beta = 90 deg, gamma = 90 deg. V = 1622.59(10) Å^3. Z = 4, d_{calc} = 1.557 mg/m^3. Total number of reflections 18989/[R(int) = 0.0297], R_1 = 0.0337, wR_2 = 0.0801 (all data), GOF = 1.052, and 235 parameter.

Table 1. Crystal data and structure refinement for z.

Identification code	z
Empirical formula	$C_{17}H_{14}F_2N_2O_4S$
Formula weight	380.36
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 7.1956(3) Å alpha = 90 deg.
	b = 9.6833(3) Å beta = 90 deg.
	c = 23.2873(8) Å gamma = 90 deg.
Volume	1622.59(10) Å^3
Z, Calculated density	4, 1.557 Mg/m^3
Absorption coefficient	0.249 mm^{-1}

[7] Supplementary crystallographic data have been deposited at the Cambridge Crystallographic Data Center. (CCDC 1439366).

F(000)	784
Crystal size	0.41 x 0.25 x 0.17 mm
Theta range for data collection	1.75 to 25.01 deg.
Limiting indices	-8<=h<=8, -10<=k<=11, -27<=l<=27
Reflections collected / unique	18989 / 2871 [R(int) = 0.0297]
Completeness to theta = 25.01	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9590 and 0.9049
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2871 / 0 / 235
Goodness-of-fit on F^2	1.052
Final R indices [I>2sigma(I)]	R_1 = 0.0314, wR_2 = 0.0781
R indices (all data)	R_1 = 0.0337, wR_2 = 0.0801
Absolute structure parameter	-0.03(8)
Largest diff. peak and hole	0.258 and -0.230 e. $Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for z. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
S(1)	1952(1)	5451(1)	304(1)	34(1)
F(1)	3297(2)	5852(2)	-1405(1)	71(1)
F(2)	3229(3)	7570(2)	-819(1)	94(1)
O(1)	3828(2)	5964(2)	353(1)	48(1)
O(2)	989(3)	5282(2)	831(1)	54(1)
O(3)	719(3)	8924(2)	-1391(1)	50(1)
O(4)	-2518(2)	5587(2)	-856(1)	64(1)
N(1)	738(3)	6368(2)	-143(1)	42(1)
N(2)	-828(3)	6802(2)	-1517(1)	33(1)
C(1)	1914(3)	3997(2)	-140(1)	34(1)
C(2)	2386(3)	2658(3)	12(1)	48(1)
C(3)	2251(4)	1669(3)	-411(2)	62(1)
C(4)	1703(4)	2017(3)	-958(2)	62(1)
C(5)	1233(4)	3354(3)	-1100(1)	50(1)
C(6)	1331(3)	4360(2)	-682(1)	34(1)
C(7)	815(3)	5879(2)	-733(1)	31(1)
C(8)	-1079(3)	6062(2)	-1030(1)	37(1)
C(9)	930(3)	7543(2)	-1556(1)	32(1)

C(10)	2142(3)	6717(3)	-1122(1)	40(1)
C(11)	1790(3)	7551(2)	-2149(1)	33(1)
C(12)	3041(4)	8583(3)	-2291(1)	47(1)
C(13)	3953(4)	8542(3)	-2816(1)	64(1)
C(14)	3626(5)	7477(4)	-3194(1)	68(1)
C(15)	2393(4)	6461(4)	-3052(1)	64(1)
C(16)	1481(4)	6480(3)	-2534(1)	48(1)
C(17)	-2431(4)	7242(3)	-1859(1)	47(1)

Table 3. Bond lengths [Å] and angles [deg] for z.

S(1)-O(2)	1.4176(18)
S(1)-O(1)	1.4431(18)
S(1)-N(1)	1.6247(19)
S(1)-C(1)	1.748(2)
F(1)-C(10)	1.352(3)
F(2)-C(10)	1.338(3)
O(3)-C(9)	1.399(3)
O(3)-H(3B)	0.8200
O(4)-C(8)	1.203(3)
N(1)-C(7)	1.453(3)
N(1)-H(1A)	0.8600
N(2)-C(8)	1.353(3)
N(2)-C(9)	1.457(3)
N(2)-C(17)	1.466(3)
C(1)-C(6)	1.374(3)
C(1)-C(2)	1.387(3)
C(2)-C(3)	1.377(4)
C(2)-H(2A)	0.9300
C(3)-C(4)	1.375(4)
C(3)-H(3A)	0.9300
C(4)-C(5)	1.378(4)
C(4)-H(4A)	0.9300
C(5)-C(6)	1.379(3)
C(5)-H(5A)	0.9300
C(6)-C(7)	1.522(3)
C(7)-C(8)	1.539(3)
C(7)-C(10)	1.546(3)
C(9)-C(11)	1.514(3)
C(9)-C(10)	1.556(3)
C(11)-C(12)	1.384(3)
C(11)-C(16)	1.388(3)

C(12)-C(13)	1.388(4)
C(12)-H(12A)	0.9300
C(13)-C(14)	1.377(5)
C(13)-H(13A)	0.9300
C(14)-C(15)	1.366(5)
C(14)-H(14A)	0.9300
C(15)-C(16)	1.374(4)
C(15)-H(15A)	0.9300
C(16)-H(16A)	0.9300
C(17)-H(17A)	0.9600
C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600

O(2)-S(1)-O(1)	115.41(11)
O(2)-S(1)-N(1)	110.81(11)
O(1)-S(1)-N(1)	111.41(11)
O(2)-S(1)-C(1)	114.34(11)
O(1)-S(1)-C(1)	109.79(10)
N(1)-S(1)-C(1)	92.93(10)
C(9)-O(3)-H(3B)	109.5
C(7)-N(1)-S(1)	114.06(15)
C(7)-N(1)-H(1A)	123.0
S(1)-N(1)-H(1A)	123.0
C(8)-N(2)-C(9)	115.40(18)
C(8)-N(2)-C(17)	120.30(19)
C(9)-N(2)-C(17)	120.42(17)
C(6)-C(1)-C(2)	123.2(2)
C(6)-C(1)-S(1)	110.05(16)
C(2)-C(1)-S(1)	126.71(19)
C(3)-C(2)-C(1)	116.7(3)
C(3)-C(2)-H(2A)	121.6
C(1)-C(2)-H(2A)	121.6
C(4)-C(3)-C(2)	120.8(2)
C(4)-C(3)-H(3A)	119.6
C(2)-C(3)-H(3A)	119.6
C(3)-C(4)-C(5)	121.5(2)
C(3)-C(4)-H(4A)	119.2
C(5)-C(4)-H(4A)	119.2
C(4)-C(5)-C(6)	118.8(3)
C(4)-C(5)-H(5A)	120.6
C(6)-C(5)-H(5A)	120.6
C(1)-C(6)-C(5)	118.9(2)
C(1)-C(6)-C(7)	113.14(18)

C(5)-C(6)-C(7)	128.0(2)
N(1)-C(7)-C(6)	104.53(17)
N(1)-C(7)-C(8)	110.69(18)
C(6)-C(7)-C(8)	111.29(18)
N(1)-C(7)-C(10)	113.94(18)
C(6)-C(7)-C(10)	113.72(18)
C(8)-C(7)-C(10)	102.87(17)
O(4)-C(8)-N(2)	126.8(2)
O(4)-C(8)-C(7)	124.56(19)
N(2)-C(8)-C(7)	108.65(19)
O(3)-C(9)-N(2)	111.05(18)
O(3)-C(9)-C(11)	106.82(17)
N(2)-C(9)-C(11)	114.49(17)
O(3)-C(9)-C(10)	111.98(19)
N(2)-C(9)-C(10)	101.10(16)
C(11)-C(9)-C(10)	111.49(18)
F(2)-C(10)-F(1)	106.3(2)
F(2)-C(10)-C(7)	112.11(18)
F(1)-C(10)-C(7)	109.93(19)
F(2)-C(10)-C(9)	110.6(2)
F(1)-C(10)-C(9)	110.21(17)
C(7)-C(10)-C(9)	107.72(18)
C(12)-C(11)-C(16)	119.3(2)
C(12)-C(11)-C(9)	119.1(2)
C(16)-C(11)-C(9)	121.3(2)
C(11)-C(12)-C(13)	119.8(3)
C(11)-C(12)-H(12A)	120.1
C(13)-C(12)-H(12A)	120.1
C(14)-C(13)-C(12)	120.3(3)
C(14)-C(13)-H(13A)	119.8
C(12)-C(13)-H(13A)	119.8
C(15)-C(14)-C(13)	119.7(3)
C(15)-C(14)-H(14A)	120.2
C(13)-C(14)-H(14A)	120.2
C(14)-C(15)-C(16)	120.9(3)
C(14)-C(15)-H(15A)	119.5
C(16)-C(15)-H(15A)	119.5
C(15)-C(16)-C(11)	120.0(3)
C(15)-C(16)-H(16A)	120.0
C(11)-C(16)-H(16A)	120.0
N(2)-C(17)-H(17A)	109.5
N(2)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5

N(2)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2$ x 10^3) for z. The anisotropic displacement factor exponent takes the form: $-2\ pi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
S(1)	43(1)	30(1)	30(1)	1(1)	-6(1)	2(1)
F(1)	40(1)	98(1)	77(1)	45(1)	25(1)	29(1)
F(2)	106(2)	112(2)	65(1)	36(1)	-48(1)	-79(1)
O(1)	51(1)	42(1)	52(1)	-4(1)	-14(1)	-9(1)
O(2)	69(1)	61(1)	32(1)	7(1)	-1(1)	5(1)
O(3)	63(1)	32(1)	57(1)	-12(1)	25(1)	-6(1)
O(4)	35(1)	89(2)	68(1)	33(1)	3(1)	-12(1)
N(1)	64(1)	33(1)	28(1)	-4(1)	-4(1)	17(1)
N(2)	32(1)	34(1)	34(1)	3(1)	-2(1)	-3(1)
C(1)	25(1)	29(1)	47(1)	-1(1)	-2(1)	-2(1)
C(2)	36(1)	33(1)	77(2)	4(1)	-10(1)	3(1)
C(3)	38(1)	29(1)	118(3)	-10(2)	-8(2)	4(1)
C(4)	52(2)	42(1)	91(2)	-31(2)	6(2)	-4(1)
C(5)	47(2)	50(1)	53(1)	-18(1)	4(1)	-9(1)
C(6)	28(1)	32(1)	42(1)	-5(1)	3(1)	-4(1)
C(7)	34(1)	33(1)	26(1)	0(1)	0(1)	-2(1)
C(8)	34(1)	41(1)	36(1)	4(1)	-1(1)	-3(1)
C(9)	36(1)	28(1)	31(1)	-3(1)	3(1)	-3(1)
C(10)	36(1)	48(1)	36(1)	4(1)	-5(1)	-14(1)
C(11)	35(1)	34(1)	31(1)	4(1)	1(1)	4(1)
C(12)	51(1)	43(1)	48(1)	5(1)	11(1)	-2(1)
C(13)	57(2)	74(2)	62(2)	22(2)	21(2)	0(2)
C(14)	64(2)	105(3)	35(1)	5(2)	14(1)	16(2)
C(15)	68(2)	87(2)	36(1)	-17(1)	8(1)	6(2)
C(16)	55(2)	49(1)	40(1)	-9(1)	2(1)	1(1)
C(17)	38(1)	52(2)	49(1)	10(1)	-8(1)	1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for z.

	x	y	z	U(eq)
H(3B)	164	8961	-1084	76
H(1A)	106	7080	-41	50
H(2A)	2774	2438	382	58
H(3A)	2534	755	-326	74
H(4A)	1649	1335	-1238	74
H(5A)	855	3573	-1470	60
H(12A)	3270	9301	-2035	57
H(13A)	4788	9237	-2912	77
H(14A)	4243	7450	-3545	81
H(15A)	2167	5747	-3310	77
H(16A)	657	5775	-2440	58
H(17A)	-3465	6642	-1783	70
H(17B)	-2122	7198	-2260	70
H(17C)	-2757	8173	-1759	70

Table 6. Torsion angles [deg] for z.

O(2)-S(1)-N(1)-C(7)	-139.92(17)
O(1)-S(1)-N(1)-C(7)	90.13(18)
C(1)-S(1)-N(1)-C(7)	-22.47(18)
O(2)-S(1)-C(1)-C(6)	128.45(17)
O(1)-S(1)-C(1)-C(6)	-99.99(17)
N(1)-S(1)-C(1)-C(6)	14.02(17)
O(2)-S(1)-C(1)-C(2)	-51.4(2)
O(1)-S(1)-C(1)-C(2)	80.1(2)
N(1)-S(1)-C(1)-C(2)	-165.9(2)
C(6)-C(1)-C(2)-C(3)	0.1(4)
S(1)-C(1)-C(2)-C(3)	180.00(19)
C(1)-C(2)-C(3)-C(4)	1.1(4)
C(2)-C(3)-C(4)-C(5)	-1.4(5)
C(3)-C(4)-C(5)-C(6)	0.5(4)
C(2)-C(1)-C(6)-C(5)	-1.0(3)
S(1)-C(1)-C(6)-C(5)	179.09(18)
C(2)-C(1)-C(6)-C(7)	177.4(2)
S(1)-C(1)-C(6)-C(7)	-2.4(2)
C(4)-C(5)-C(6)-C(1)	0.7(4)
C(4)-C(5)-C(6)-C(7)	-177.5(2)
S(1)-N(1)-C(7)-C(6)	23.3(2)

S(1)-N(1)-C(7)-C(8)	143.21(17)
S(1)-N(1)-C(7)-C(10)	-101.4(2)
C(1)-C(6)-C(7)-N(1)	-12.2(2)
C(5)-C(6)-C(7)-N(1)	166.1(2)
C(1)-C(6)-C(7)-C(8)	-131.67(19)
C(5)-C(6)-C(7)-C(8)	46.6(3)
C(1)-C(6)-C(7)-C(10)	112.7(2)
C(5)-C(6)-C(7)-C(10)	-69.0(3)
C(9)-N(2)-C(8)-O(4)	165.3(2)
C(17)-N(2)-C(8)-O(4)	7.4(4)
C(9)-N(2)-C(8)-C(7)	-16.4(3)
C(17)-N(2)-C(8)-C(7)	-174.4(2)
N(1)-C(7)-C(8)-O(4)	-56.5(3)
C(6)-C(7)-C(8)-O(4)	59.3(3)
C(10)-C(7)-C(8)-O(4)	-178.6(2)
N(1)-C(7)-C(8)-N(2)	125.20(19)
C(6)-C(7)-C(8)-N(2)	-119.0(2)
C(10)-C(7)-C(8)-N(2)	3.1(2)
C(8)-N(2)-C(9)-O(3)	-97.3(2)
C(17)-N(2)-C(9)-O(3)	60.5(3)
C(8)-N(2)-C(9)-C(11)	141.59(19)
C(17)-N(2)-C(9)-C(11)	-60.5(3)
C(8)-N(2)-C(9)-C(10)	21.6(2)
C(17)-N(2)-C(9)-C(10)	179.50(19)
N(1)-C(7)-C(10)-F(2)	11.7(3)
C(6)-C(7)-C(10)-F(2)	-108.0(2)
C(8)-C(7)-C(10)-F(2)	131.6(2)
N(1)-C(7)-C(10)-F(1)	129.66(19)
C(6)-C(7)-C(10)-F(1)	10.0(3)
C(8)-C(7)-C(10)-F(1)	-110.5(2)
N(1)-C(7)-C(10)-C(9)	-110.2(2)
C(6)-C(7)-C(10)-C(9)	130.11(19)
C(8)-C(7)-C(10)-C(9)	9.6(2)
O(3)-C(9)-C(10)-F(2)	-22.4(3)
N(2)-C(9)-C(10)-F(2)	-140.7(2)
C(11)-C(9)-C(10)-F(2)	97.2(2)
O(3)-C(9)-C(10)-F(1)	-139.62(19)
N(2)-C(9)-C(10)-F(1)	102.09(19)
C(11)-C(9)-C(10)-F(1)	-20.0(2)
O(3)-C(9)-C(10)-C(7)	100.4(2)
N(2)-C(9)-C(10)-C(7)	-17.8(2)
C(11)-C(9)-C(10)-C(7)	-139.93(18)
O(3)-C(9)-C(11)-C(12)	33.8(3)

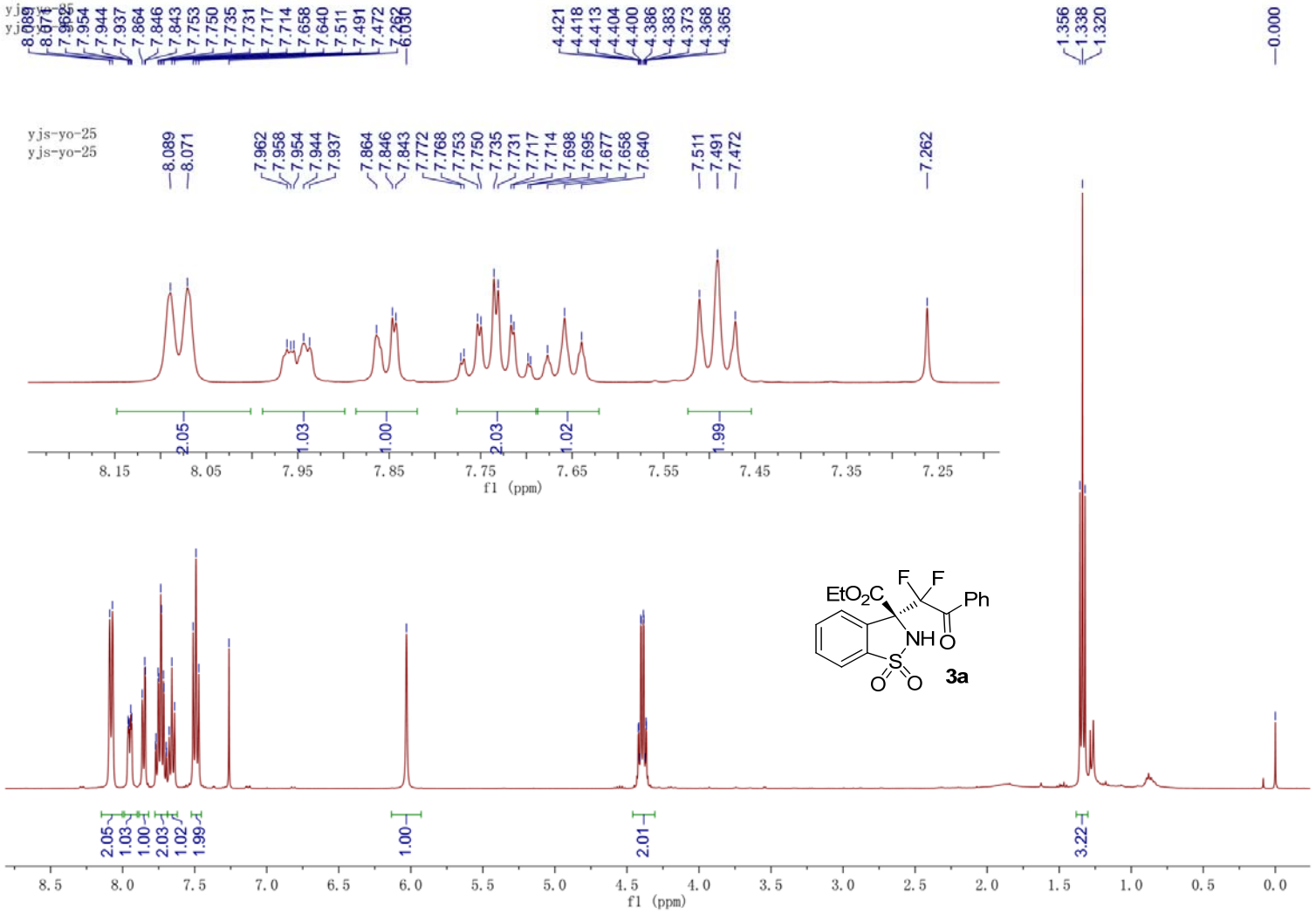
N(2)-C(9)-C(11)-C(12)	157.2(2)
C(10)-C(9)-C(11)-C(12)	-88.8(2)
O(3)-C(9)-C(11)-C(16)	-152.1(2)
N(2)-C(9)-C(11)-C(16)	-28.7(3)
C(10)-C(9)-C(11)-C(16)	85.3(3)
C(16)-C(11)-C(12)-C(13)	0.7(4)
C(9)-C(11)-C(12)-C(13)	174.9(2)
C(11)-C(12)-C(13)-C(14)	-0.4(4)
C(12)-C(13)-C(14)-C(15)	0.3(5)
C(13)-C(14)-C(15)-C(16)	-0.5(5)
C(14)-C(15)-C(16)-C(11)	0.8(4)
C(12)-C(11)-C(16)-C(15)	-0.9(4)
C(9)-C(11)-C(16)-C(15)	-175.0(2)

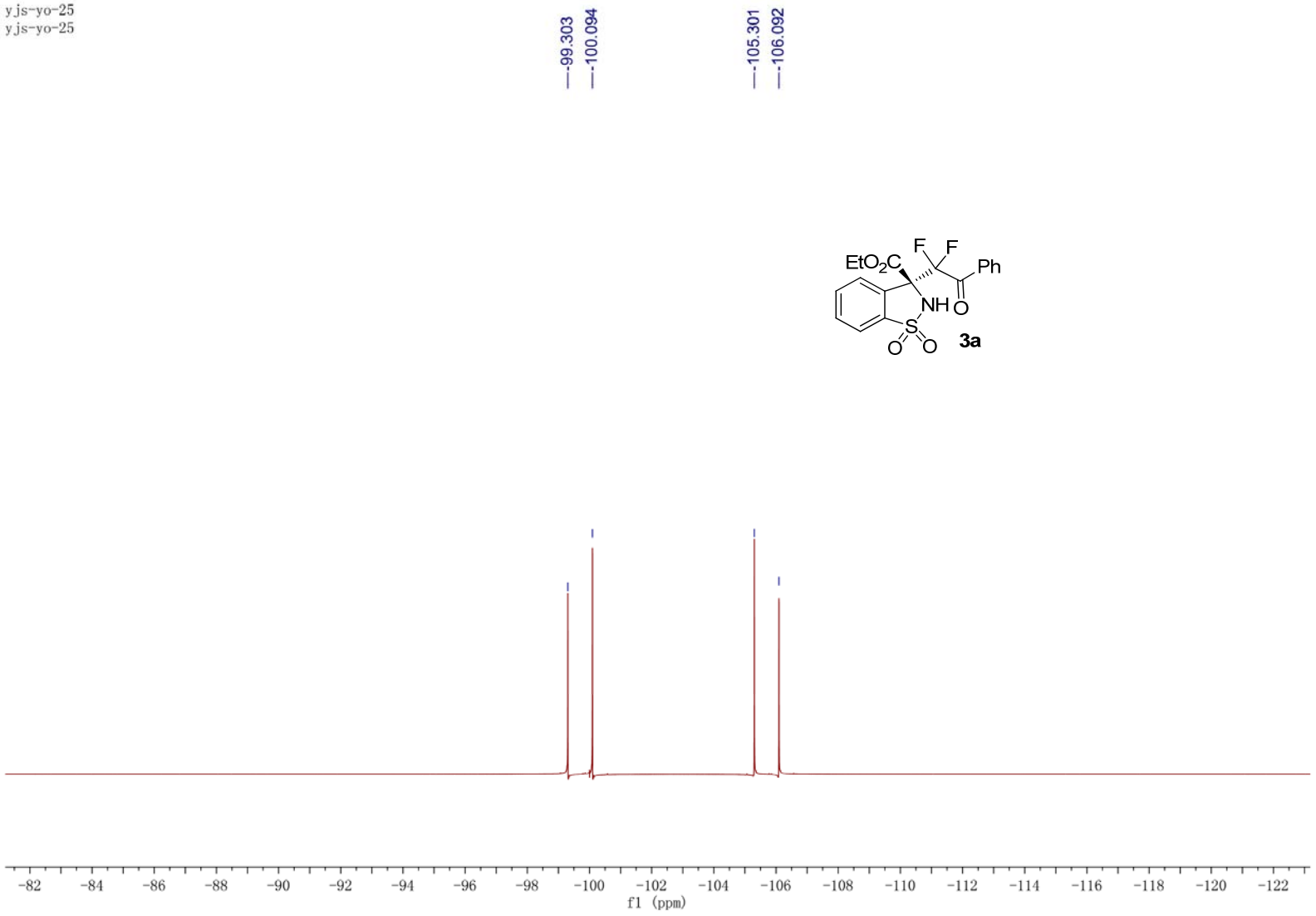
Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for z [Å and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)

Part IV. ^{1}H, ^{19}F, ^{13}C NMR spectra

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yjs-yo-25
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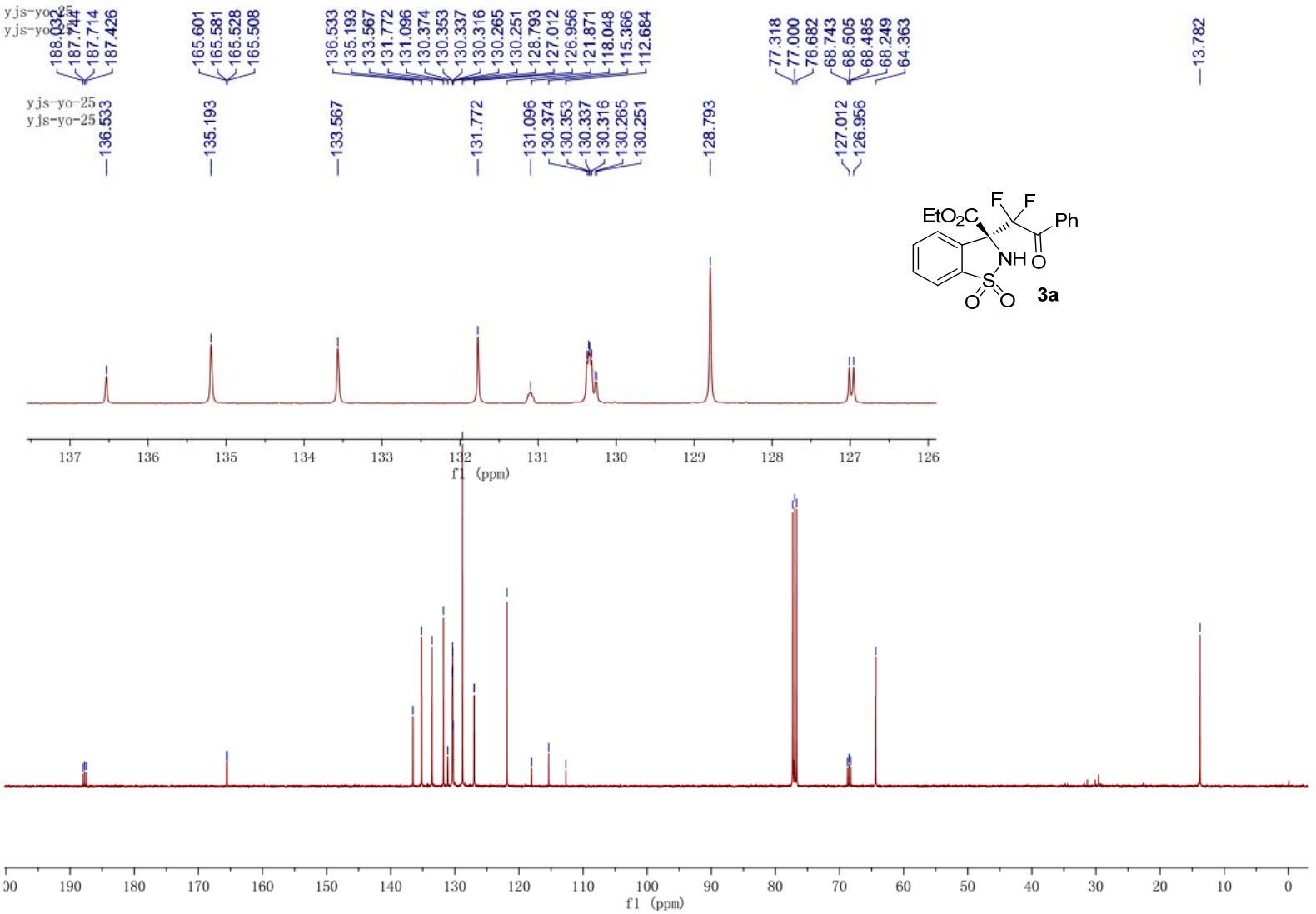
-100.094
-105.301
-106.092
EtO2C
F
F
Ph
NH
O
S
O
O
3a
-82
-84
-86
-88
-90
-92
-94
-96
-98
-100
-102
-104
-106
-108
-110
-112
-114
-116
-118
-120
-122
f1 (ppm)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133.567
131.772
131.096
130.374
130.353
130.337
130.316
130.265
130.251
128.793
127.012
126.956
121.871
118.048
115.366
112.684
77.318
77.000
76.682
68.743
68.505
68.485
68.249
64.363
13.782
yjs-yo-25
yjs-yo-25
136.533
135.193
133.567
131.772
131.096
130.374
130.353
130.337
130.316
130.265
130.251
128.793
127.012
126.956
EtO2C
F
F
Ph
NH
O
S
O
O
3a
137
136
135
134
133
132
131
130
129
128
127
126
f1 (ppm)
190
180
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70
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50
40
30
20
10
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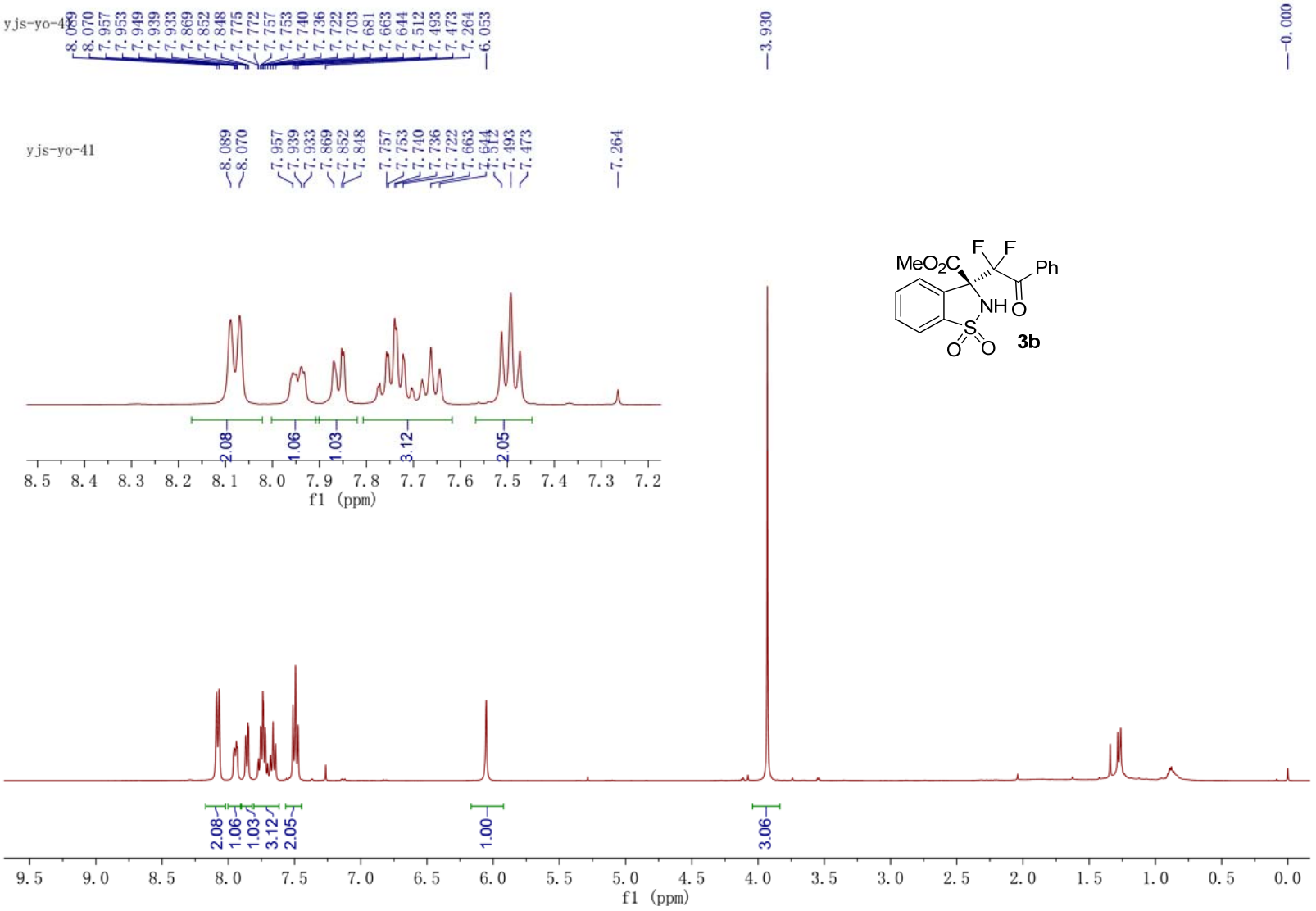
f1 (ppm)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7.848
7.775
7.772
7.757
7.753
7.740
7.736
7.722
7.703
7.681
7.663
7.644
7.512
7.493
7.473
7.264
6.053
3.930
0.000
MeO2C
F
F
Ph
NH
O
S
O
O
3b
2.08
1.06
1.03
3.12
2.05
1.00
3.06
f1 (ppm)

yjs-yo-41

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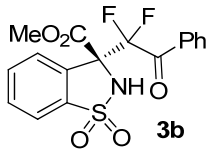
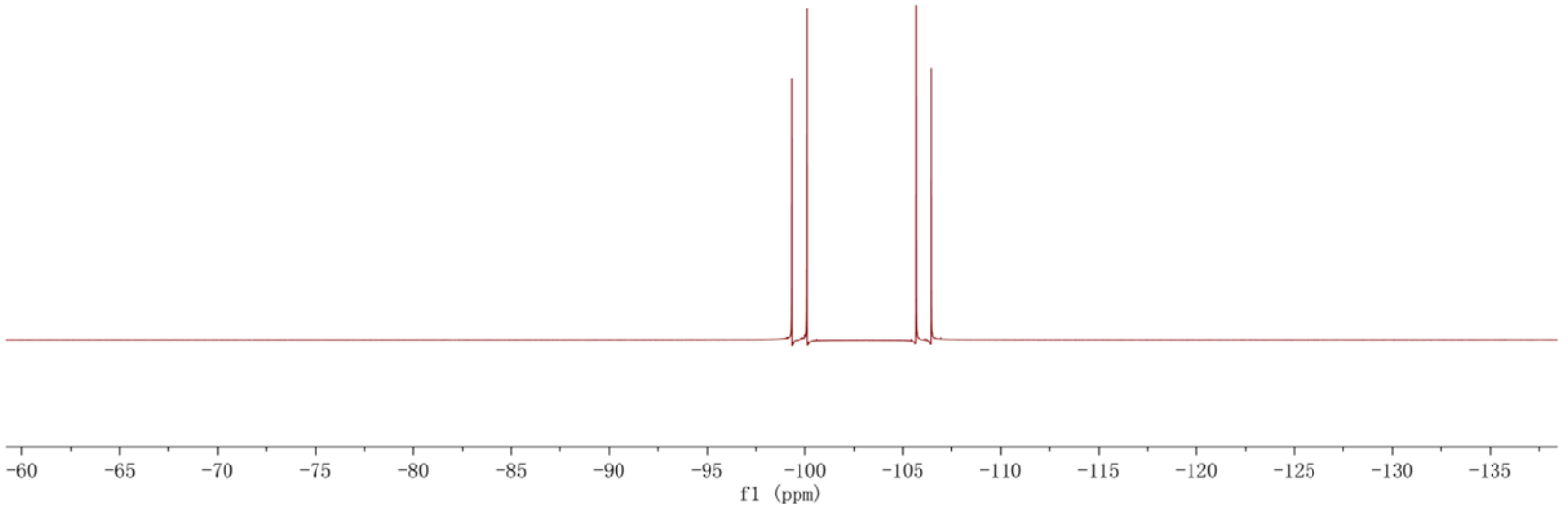
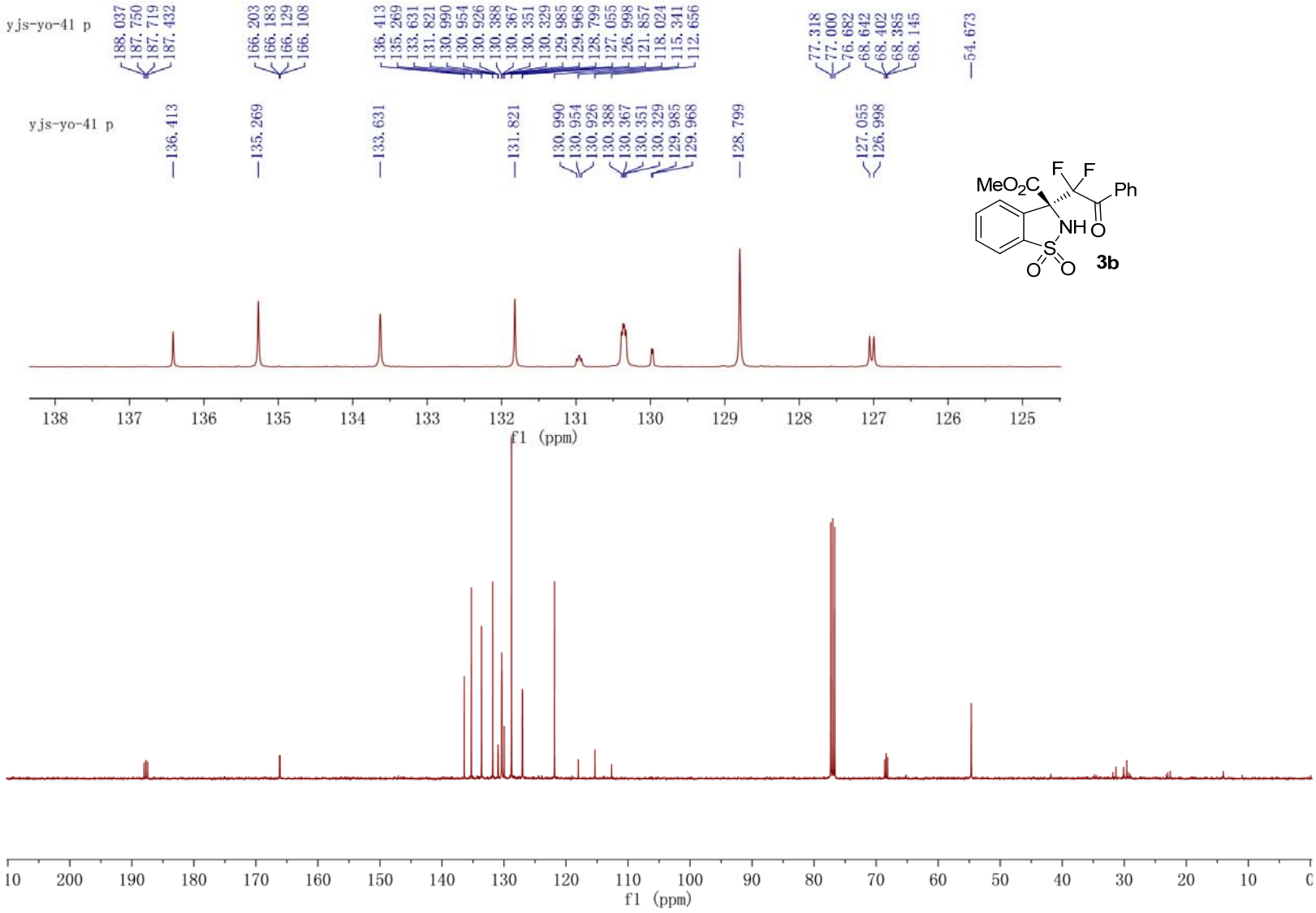
-105.659
-106.452



3b

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130.954
130.926
130.388
130.367
130.351
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129.968
128.799
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126.998
121.857
118.024
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68.402
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130.329
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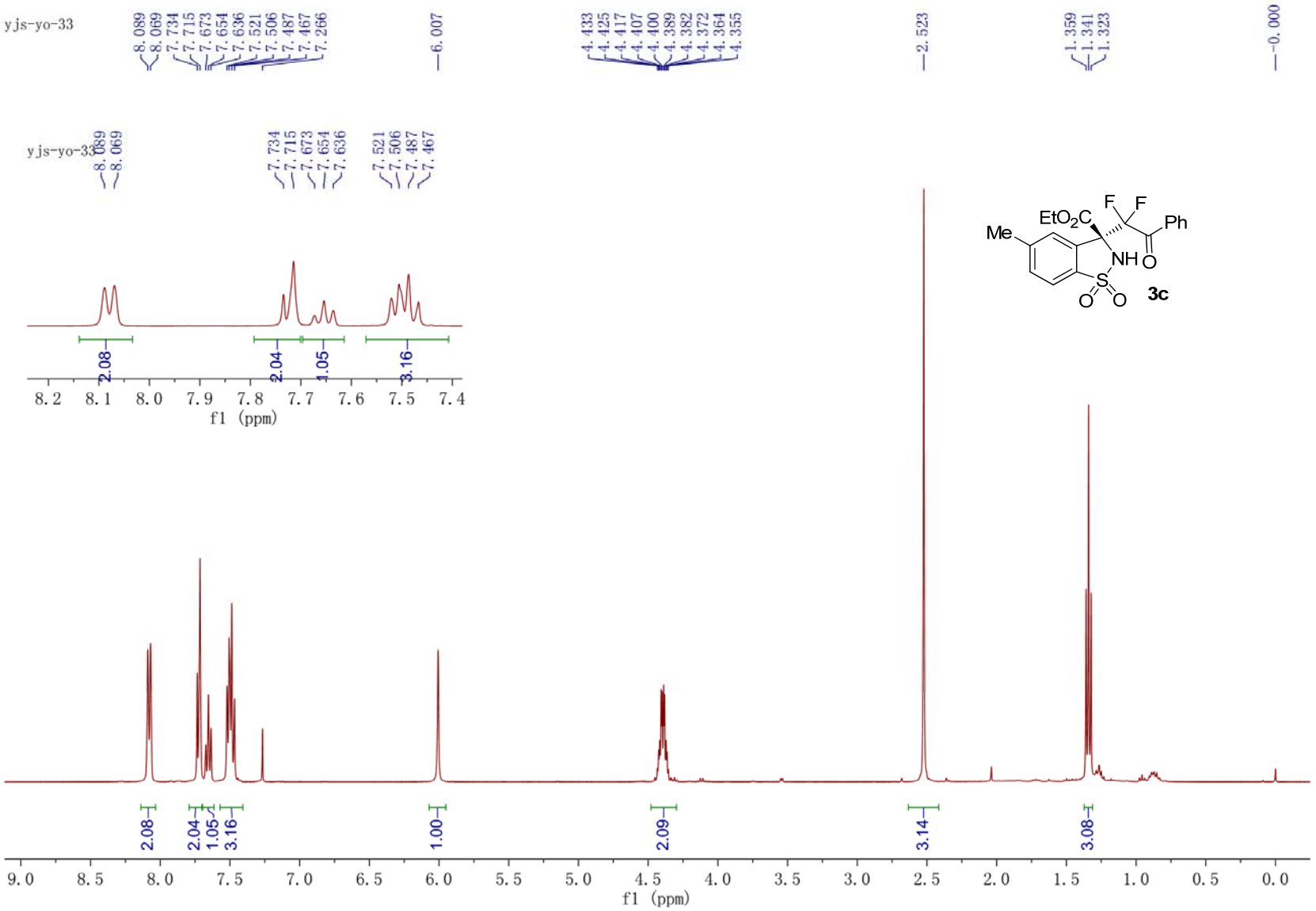
127.055
126.998
MeO2C
F
F
Ph
NH
O
S
O
O
3b
138
137
136
135
134
133
132
131
130
129
128
127
126
125
f1 (ppm)
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.673
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7.636
7.521
7.506
7.487
7.467
7.266
6.007
4.433
4.425
4.417
4.407
4.400
4.389
4.382
4.372
4.364
4.355
2.523
1.359
1.341
1.323
-0.000
yjs-yo-33
2.08
2.04
1.05
3.16
f1 (ppm)
EtO2C
F
F
Ph
Me
NH
O
S
O
O
3c
2.08
2.04
1.05
3.16
1.00
2.09
3.14
3.08
f1 (ppm)

yjs-yo-33

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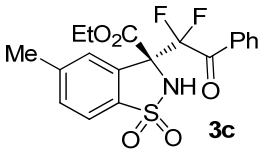
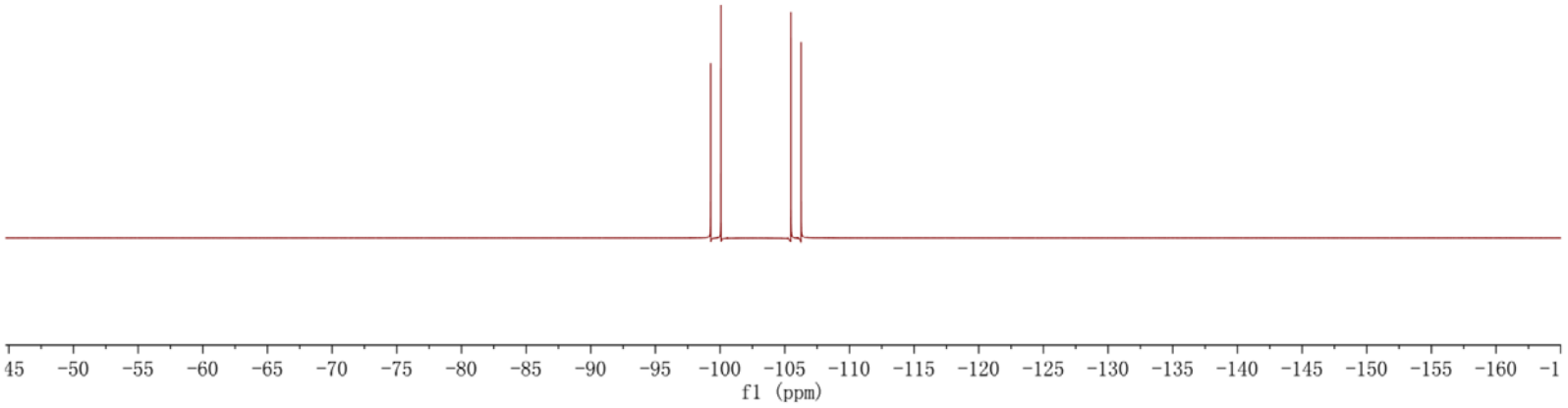
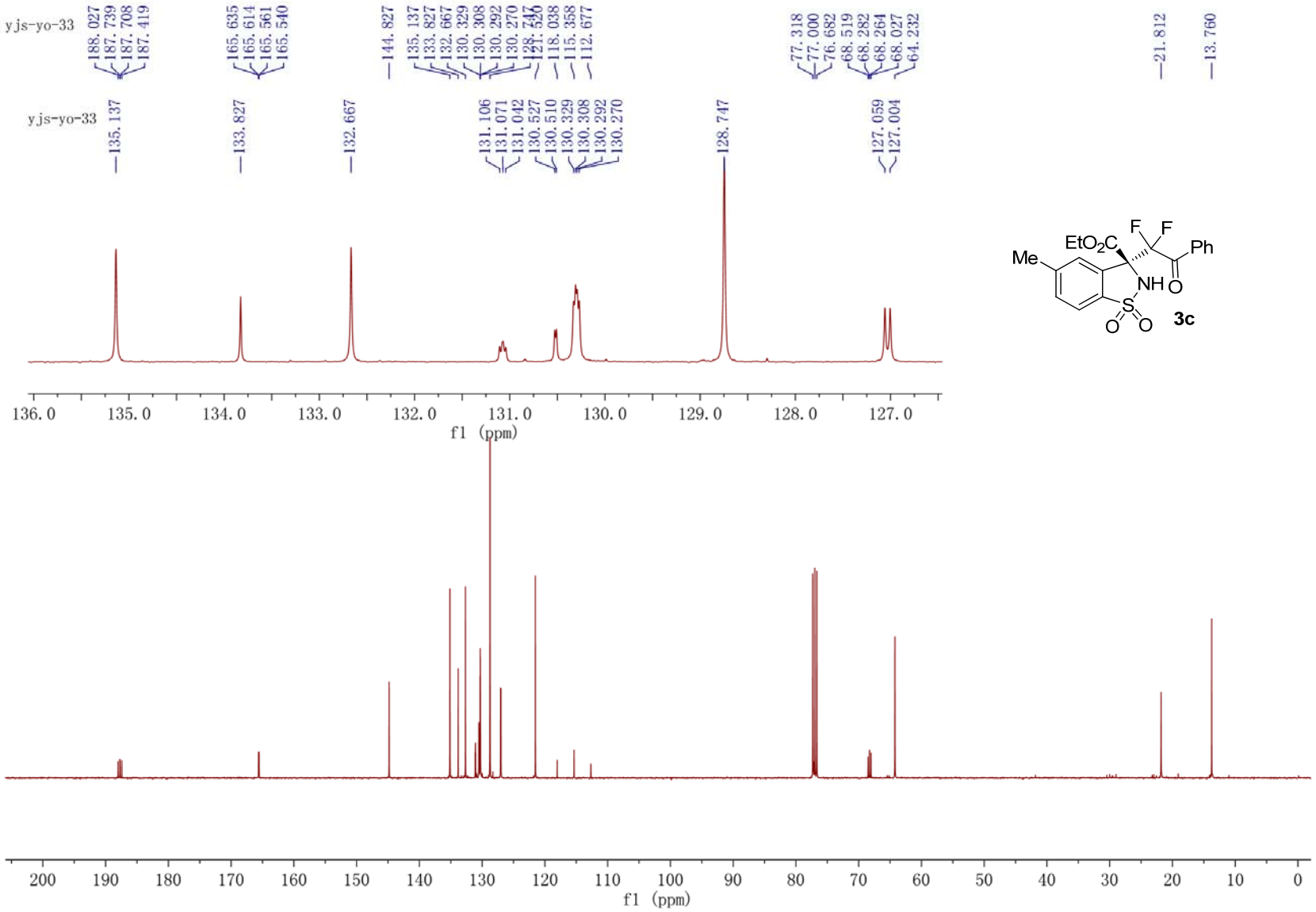
-105.471
-106.263



3c

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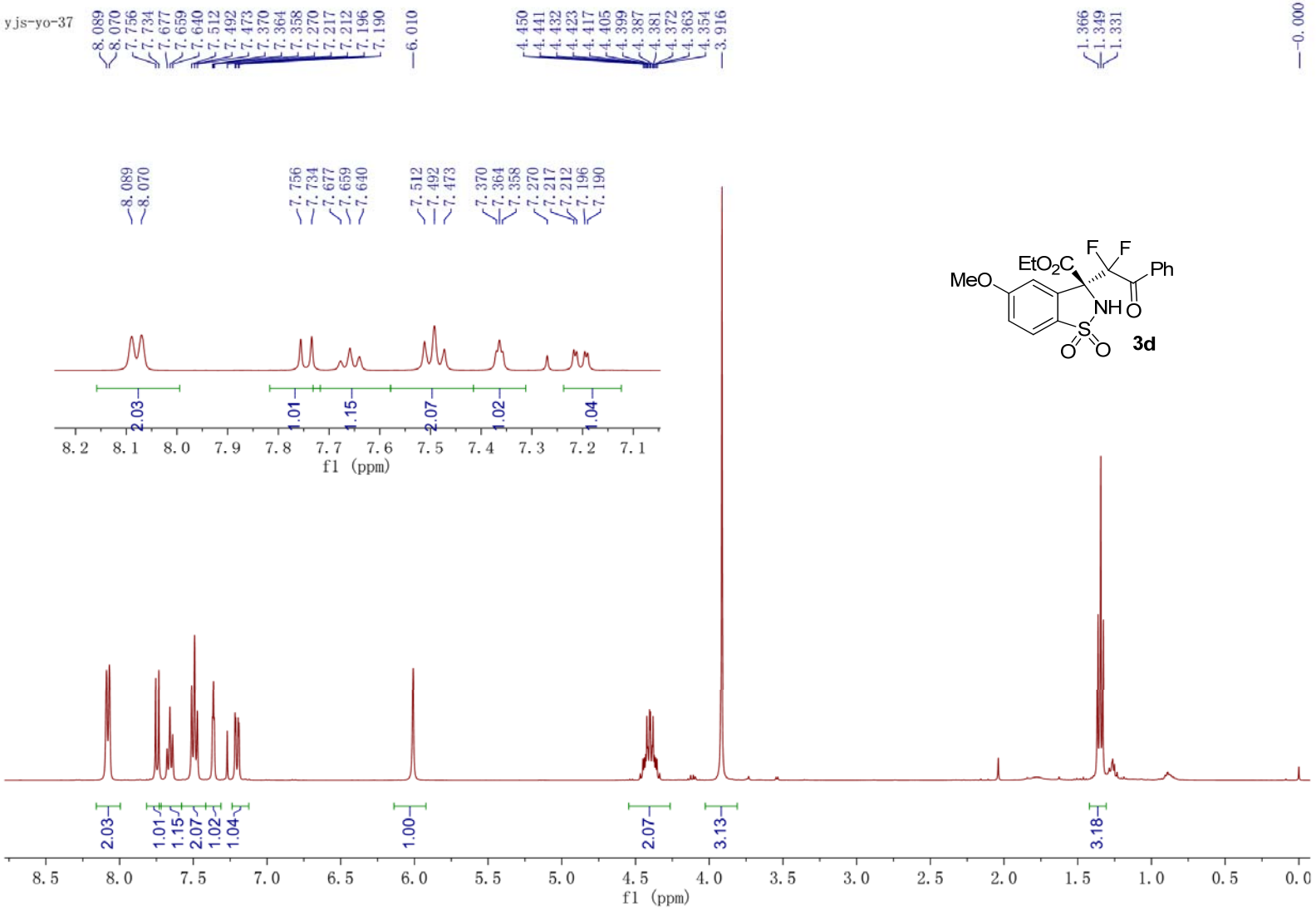
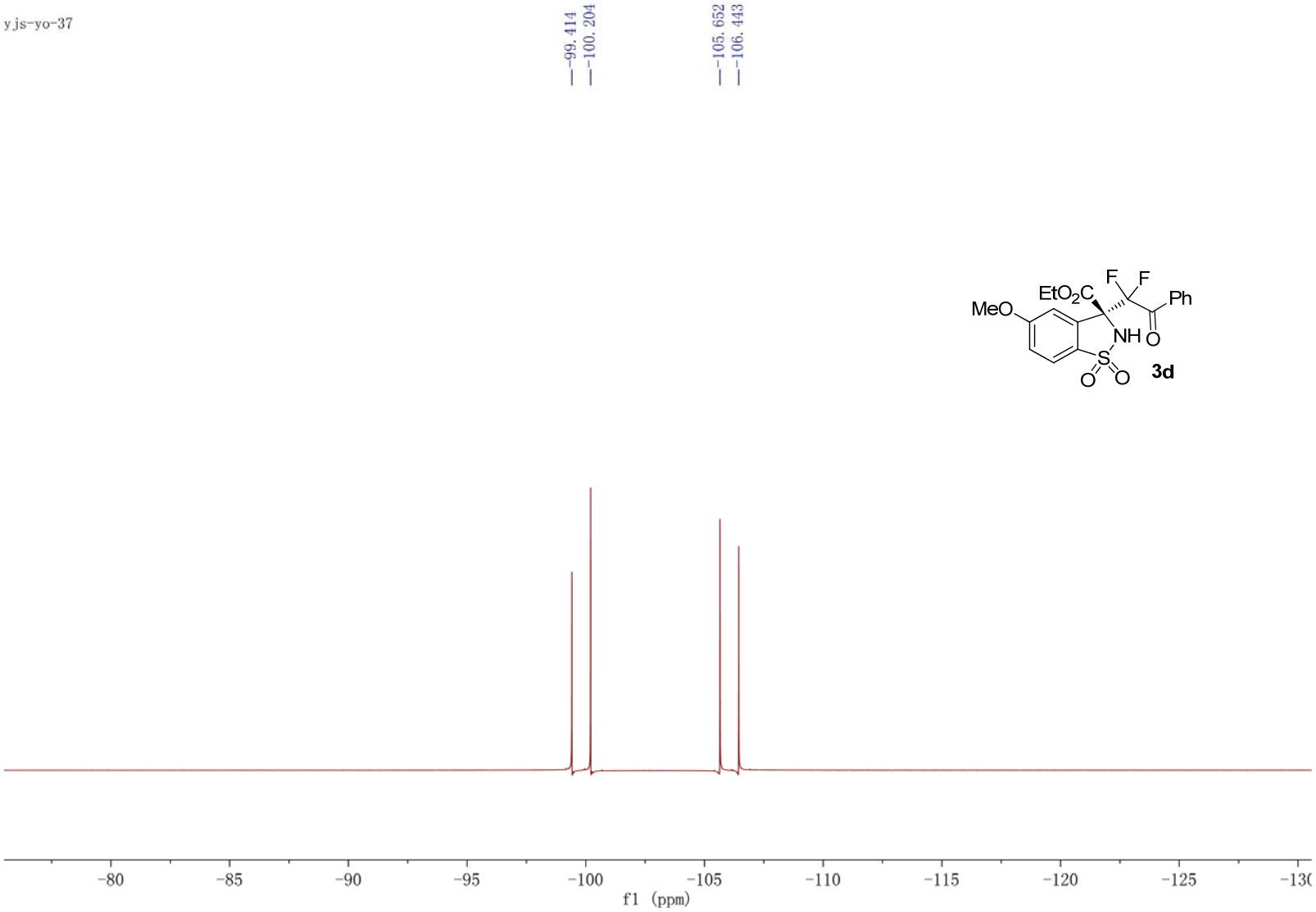
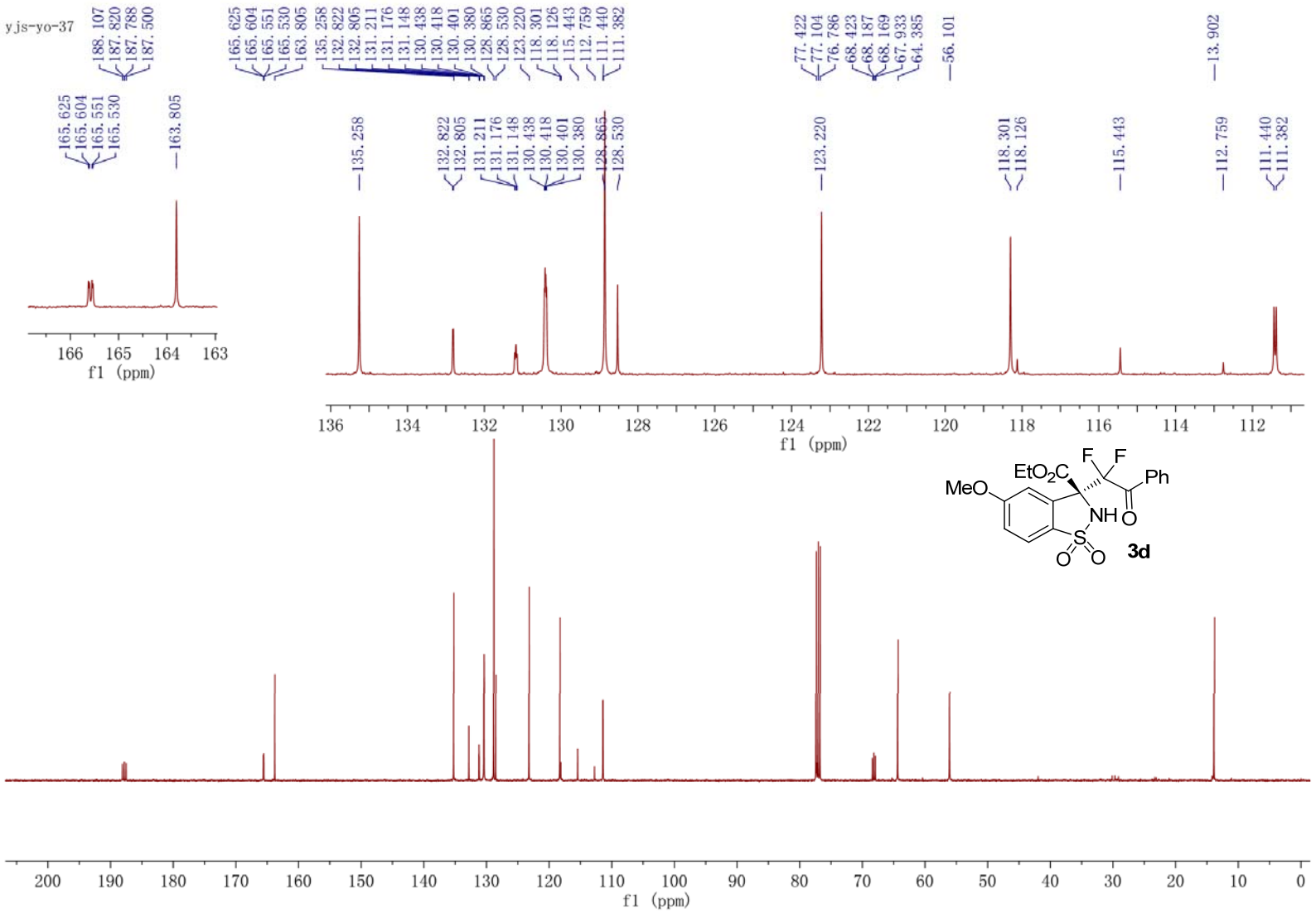
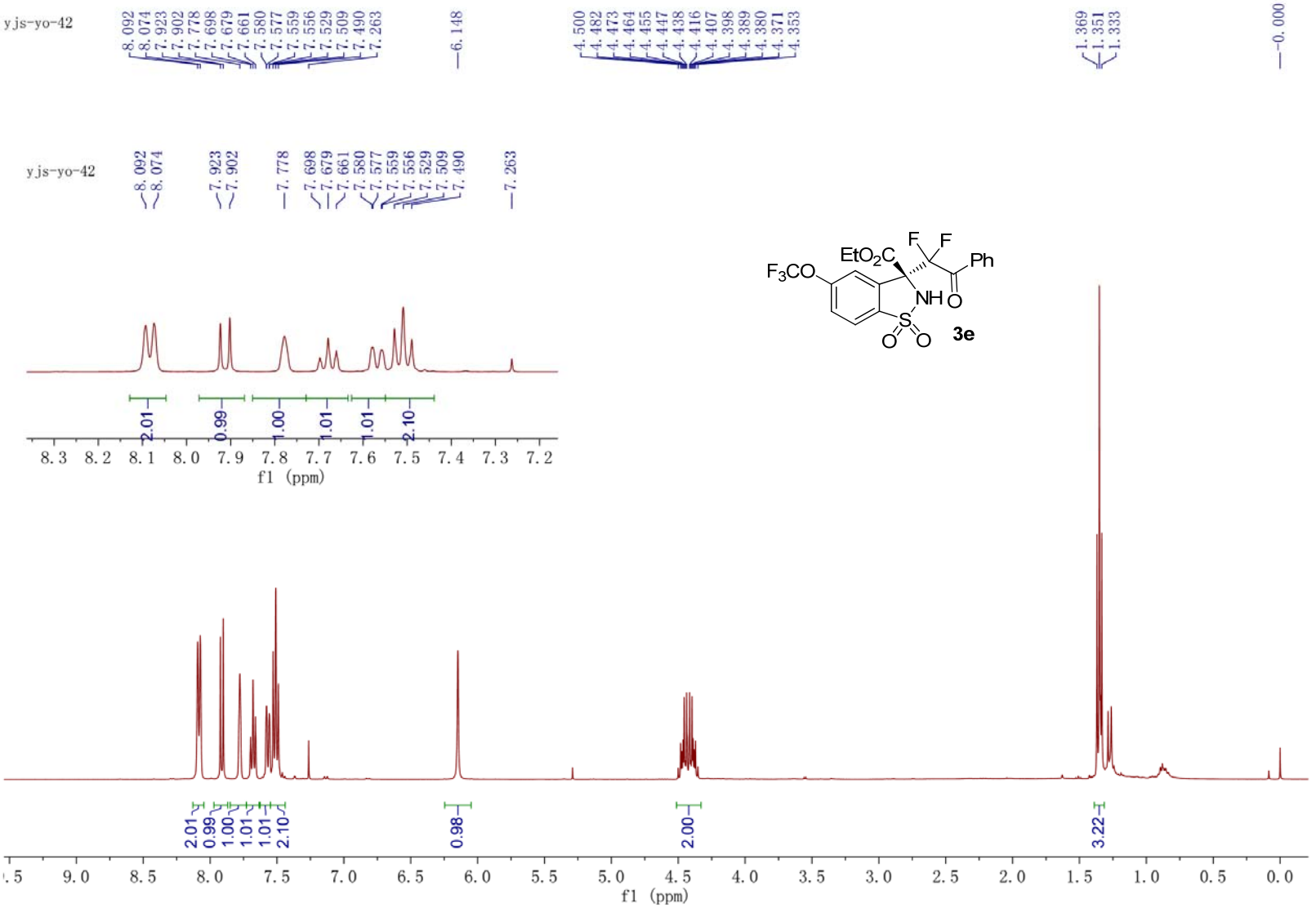
135.137
133.827
132.667
130.329
130.308
130.292
130.270
128.747
121.520
118.038
115.358
112.677
77.318
77.000
76.682
68.519
68.282
68.264
68.027
64.232
21.812
13.760
yjs-yo-33
135.137
133.827
132.667
131.106
131.071
131.042
130.527
130.510
130.329
130.308
130.292
130.270
128.747
127.059
127.004
136.0
135.0
134.0
133.0
132.0
131.0
130.0
129.0
128.0
127.0
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
Me
EtO2C
F
F
Ph
NH
O
S
O
O
3c

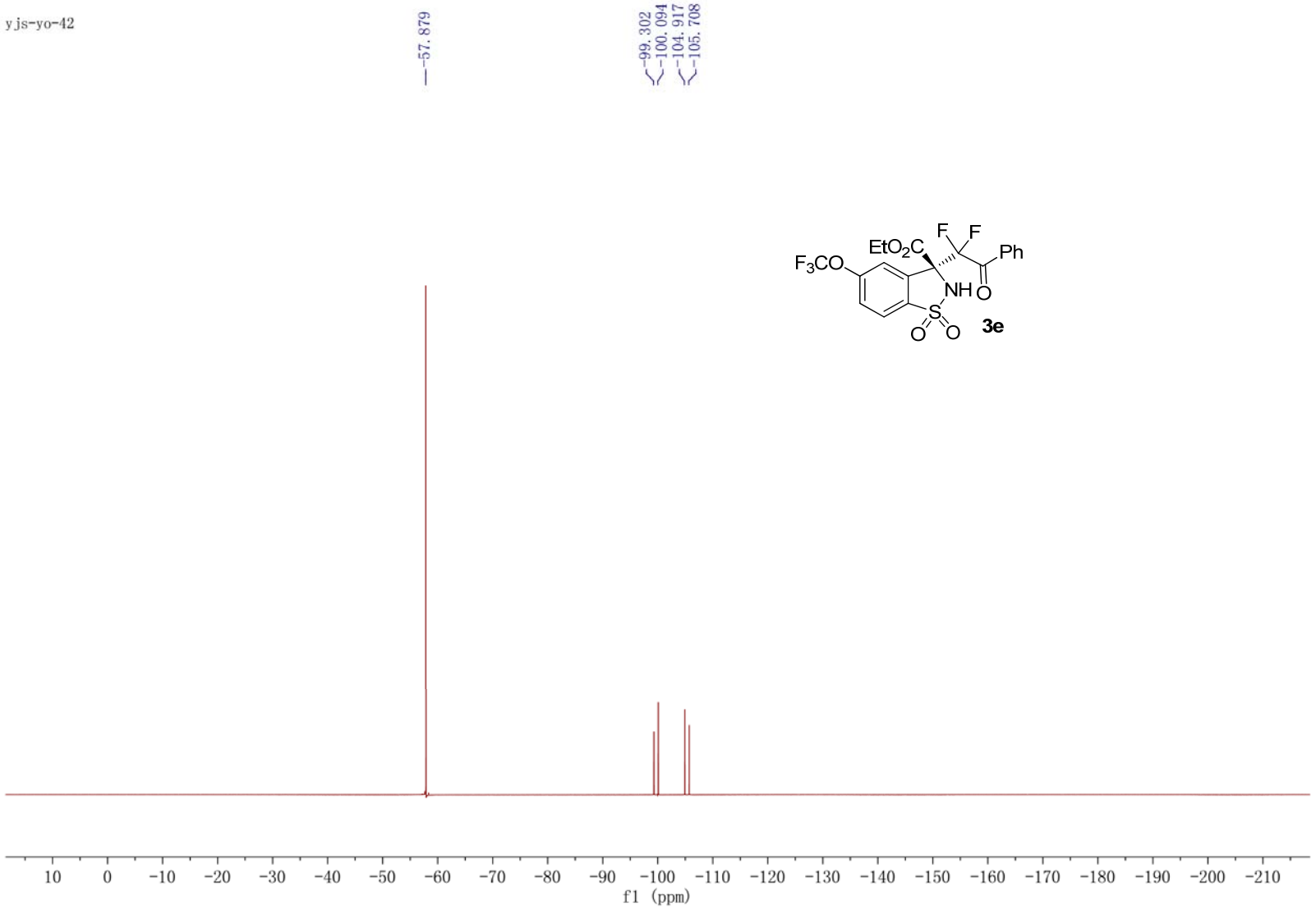

yjs-yo-37
8.089
8.070
7.756
7.734
7.677
7.659
7.640
7.512
7.492
7.473
7.370
7.364
7.358
7.270
7.217
7.212
7.196
7.190
6.010
4.450
4.441
4.432
4.423
4.417
4.405
4.399
4.387
4.381
4.372
4.363
4.354
3.916
1.366
1.349
1.331
0.000
2.03
1.01
1.15
2.07
1.02
1.04
f1 (ppm)
1.00
2.07
3.13
3.18
MeO
EtO2C
F
F
Ph
NH
O
S
O
O
3d

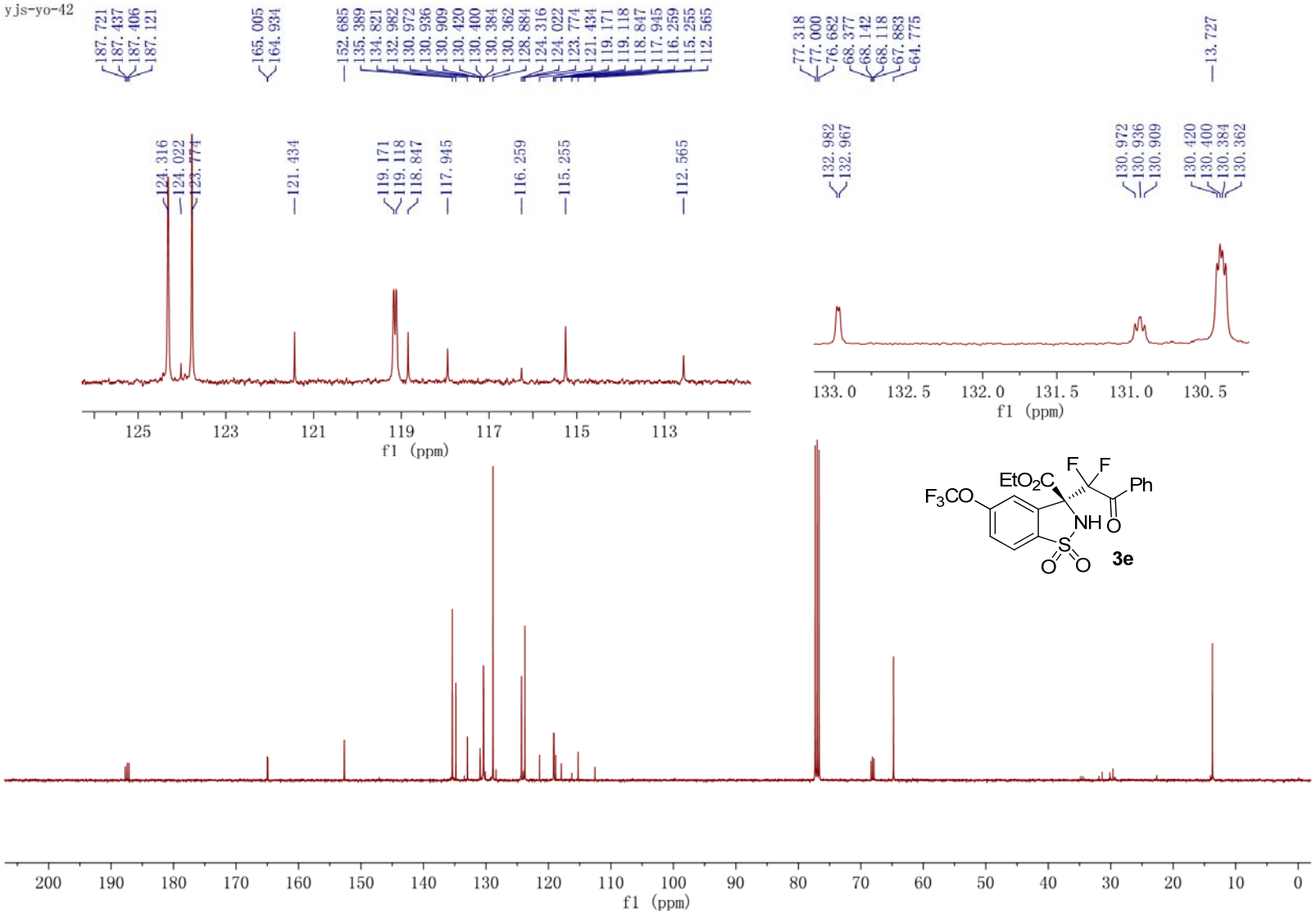
yjs-yo-37

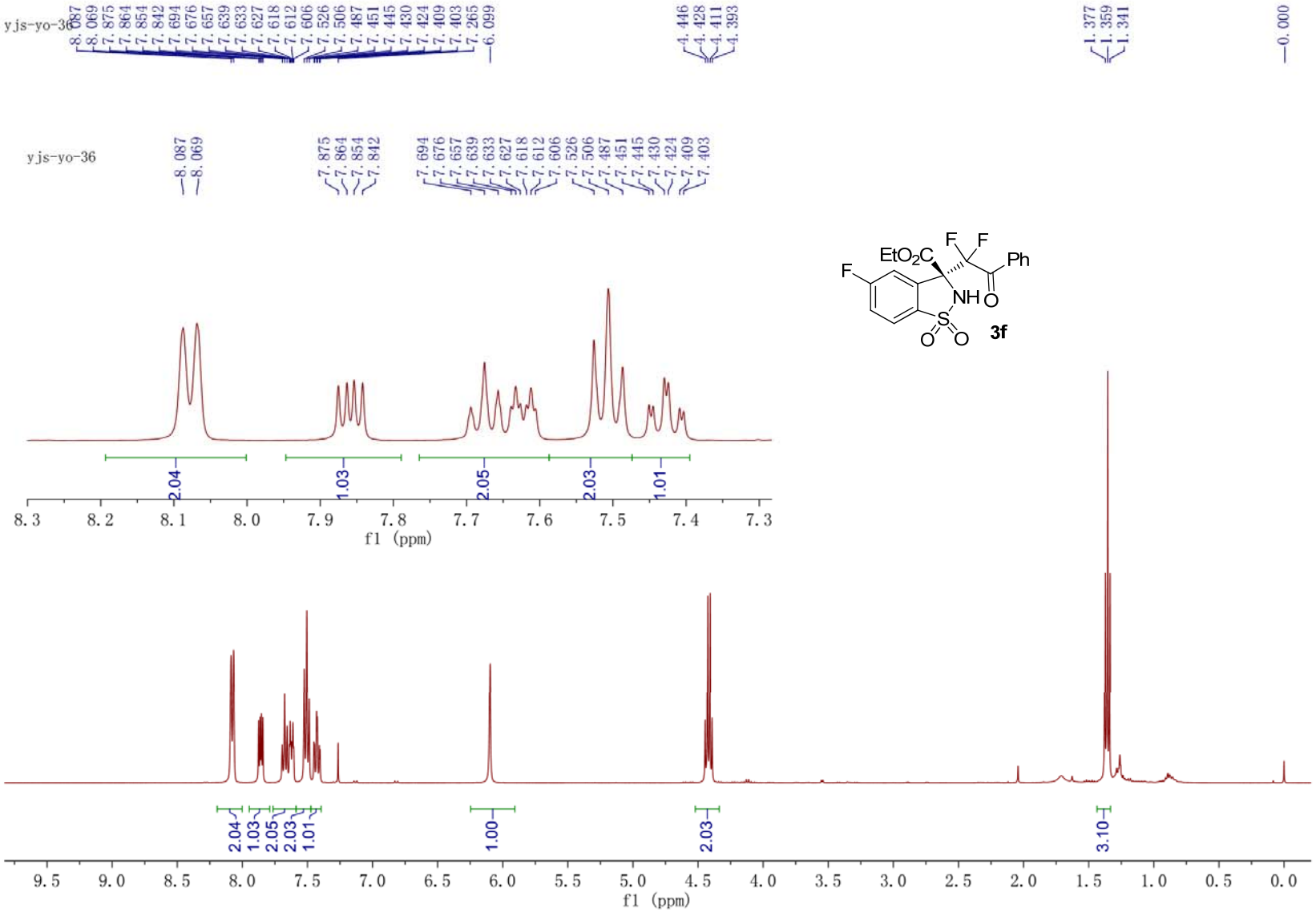

-99.414
-100.204
-105.652
-106.443
F
F
EtO2C
Ph
MeO
NH
O
S
O
O
3d
-80
-85
-90
-95
-100
-105
-110
-115
-120
-125
f1 (ppm)


yjs-yo-37
188.107
187.820
187.788
187.500
165.625
165.604
165.551
165.530
163.805
135.258
132.822
132.805
131.211
131.176
131.148
130.438
130.418
130.401
130.380
128.865
128.530
123.220
118.301
118.126
115.443
112.759
111.440
111.382
77.422
77.104
76.786
68.423
68.187
68.169
67.933
64.385
56.101
13.902
f1 (ppm)
MeO
EtO2C
F
F
Ph
NH
O
S
O
O
3d

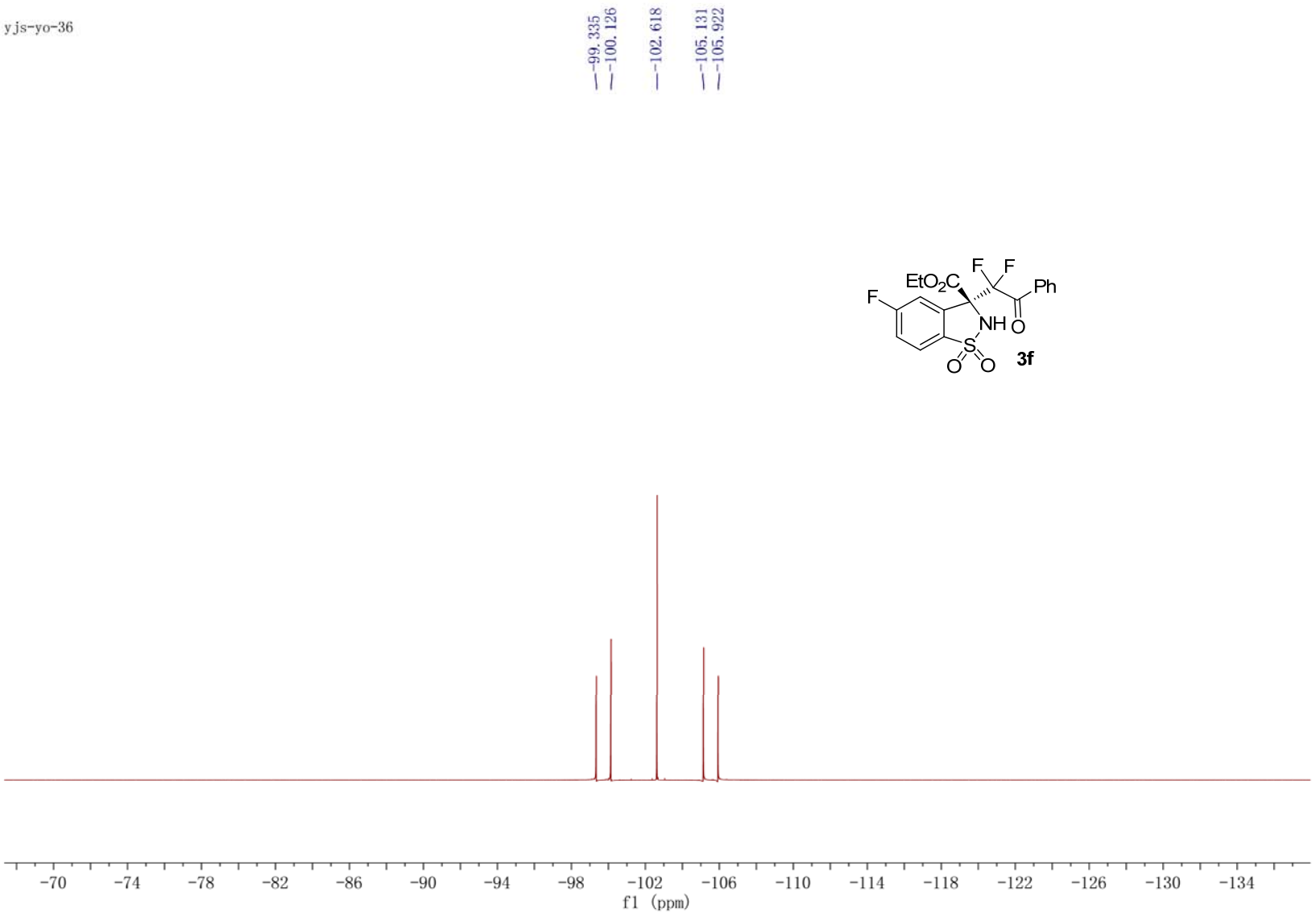

yjs-yo-42
8.092
8.074
7.923
7.902
7.778
7.698
7.679
7.661
7.580
7.577
7.559
7.556
7.529
7.509
7.490
7.263
6.148
4.500
4.482
4.473
4.464
4.455
4.447
4.438
4.416
4.407
4.398
4.389
4.380
4.371
4.353
1.369
1.351
1.333
0.000
yjs-yo-42
F
F
EtO2C
Ph
F3CO
NH
O
S
O
O
3e
2.01
0.99
1.00
1.01
1.01
2.10
f1 (ppm)
0.98
2.00
3.22

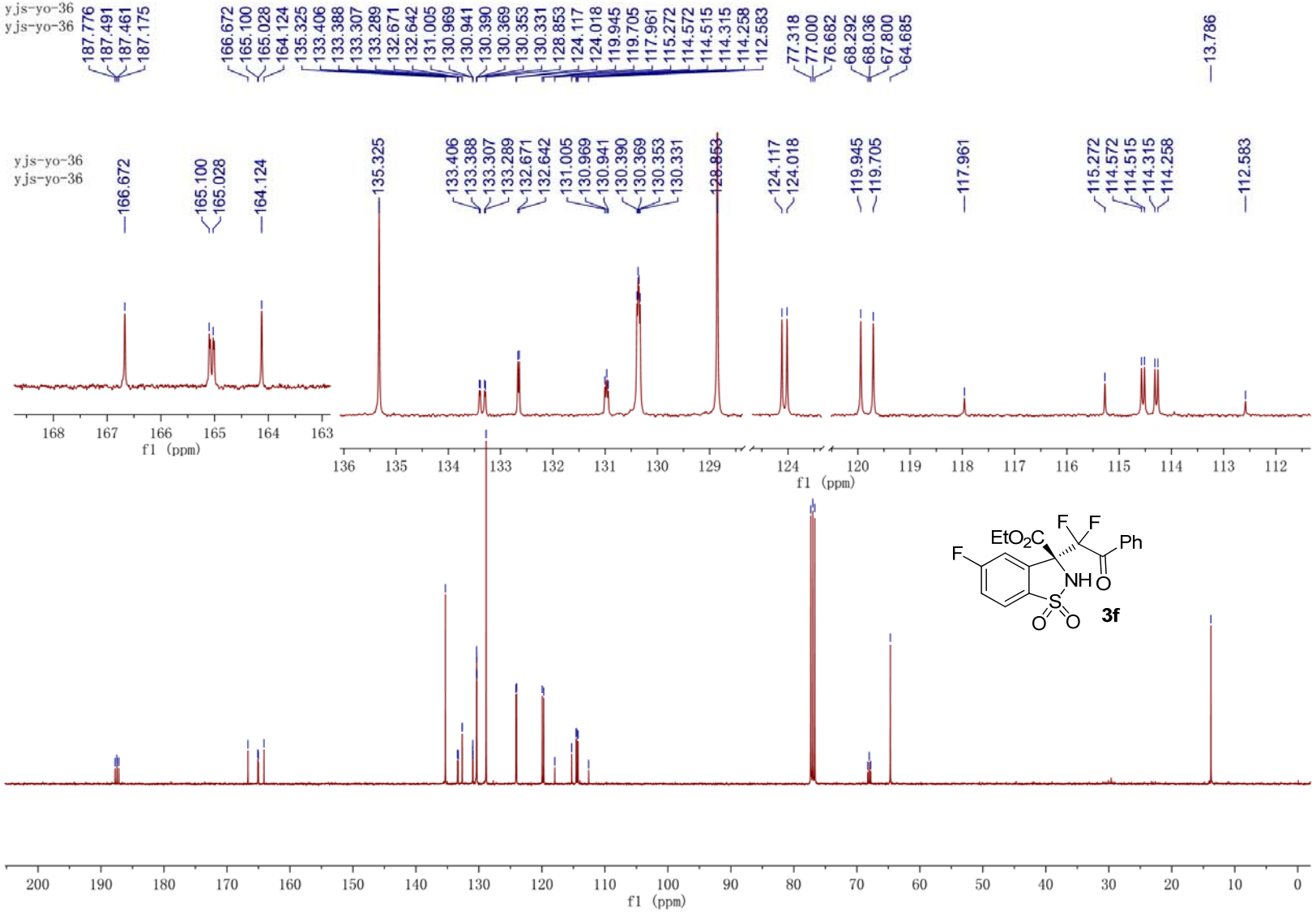

yjs-yo-42
-57.879
-99.302
-100.094
-104.917
-105.708
F
F
EtO2C
Ph
F3CO
NH
O
S
O
O
3e
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

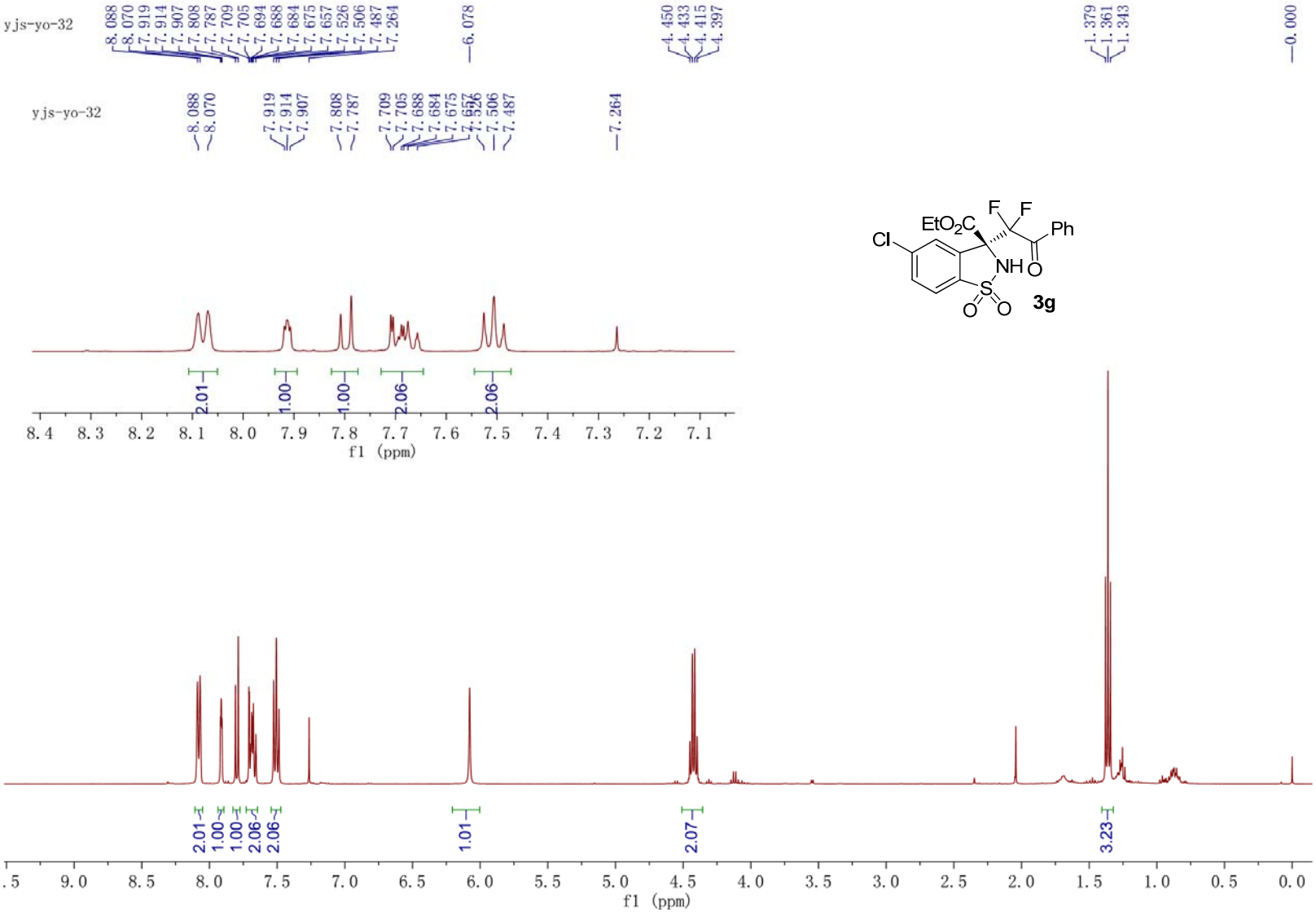

yjs-yo-42
187.721
187.437
187.406
187.121
165.005
164.934
152.685
135.389
134.821
132.982
130.972
130.936
130.909
130.420
130.400
130.384
130.362
128.884
124.316
124.022
123.774
121.434
119.171
119.118
118.847
117.945
116.259
115.255
112.565
77.318
77.000
76.682
68.377
68.142
68.118
67.883
64.775
13.727
f1 (ppm)
f1 (ppm)
f1 (ppm)
F3CO
EtO2C
F
F
Ph
NH
O
S
O
O
3e


yjs-yo-36
8.087
8.069
7.875
7.864
7.854
7.842
7.694
7.676
7.657
7.639
7.633
7.627
7.618
7.612
7.606
7.526
7.506
7.487
7.451
7.445
7.430
7.424
7.409
7.403
7.265
6.099
4.446
4.428
4.411
4.393
1.377
1.359
1.341
0.000
EtO2C
F
F
Ph
F
NH
O
S
O
O
3f
2.04
1.03
2.05
2.03
1.01
1.00
2.03
3.10
f1 (ppm)

yjs-yo-36

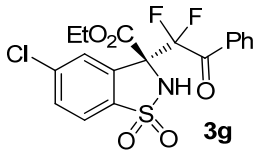

-99.335
-100.126
-102.618
-105.131
-105.922
EtO2C
F
F
Ph
F
NH
O
S
O
O
3f
-70
-74
-78
-82
-86
-90
-94
-98
-102
-106
-110
-114
-118
-122
-126
-130
-134
f1 (ppm)


yjs-yo-36
yjs-yo-36
187.776
187.491
187.461
187.175
166.672
165.100
165.028
164.124
135.325
133.406
133.388
133.307
133.289
132.671
132.642
131.005
130.969
130.941
130.390
130.369
130.353
130.331
128.853
124.117
124.018
119.945
119.705
117.961
115.272
114.572
114.515
114.315
114.258
112.583
77.318
77.000
76.682
68.292
68.036
67.800
64.685
13.786
f1 (ppm)
EtO2C
F
F
Ph
NH
O
S
O
O
3f

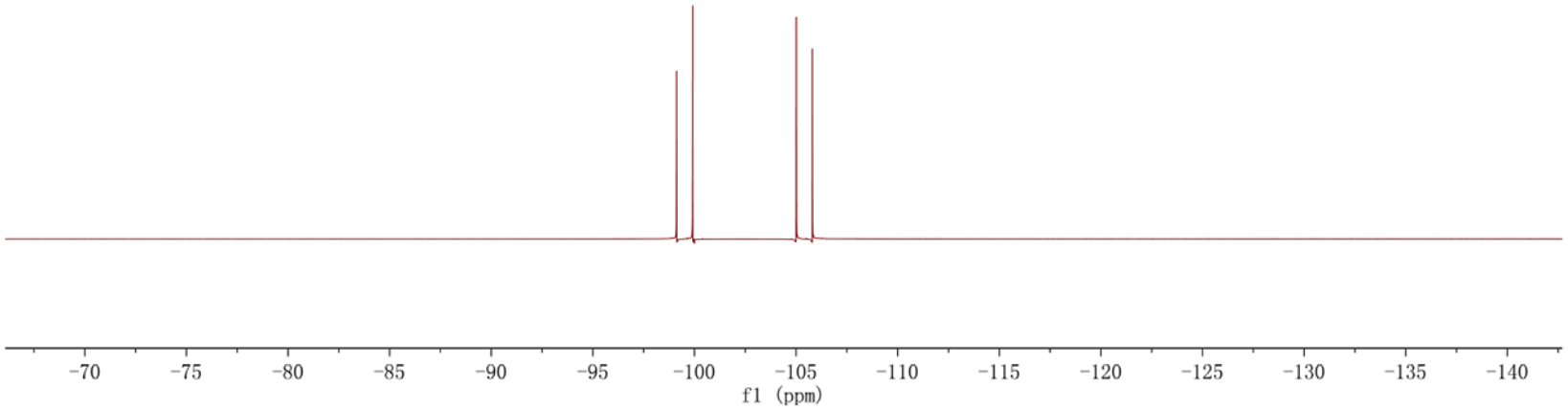

yjs-yo-32
8.088
8.070
7.919
7.914
7.907
7.808
7.787
7.709
7.705
7.694
7.688
7.684
7.675
7.657
7.526
7.506
7.487
7.264
6.078
4.450
4.433
4.415
4.397
1.379
1.361
1.343
0.000
yjs-yo-32
EtO2C
F
F
Ph
Cl
NH
O
S
O
O
3g
2.01
1.00
1.00
2.06
2.06
f1 (ppm)
2.01
1.00
1.00
2.06
2.06
1.01
2.07
3.23
f1 (ppm)

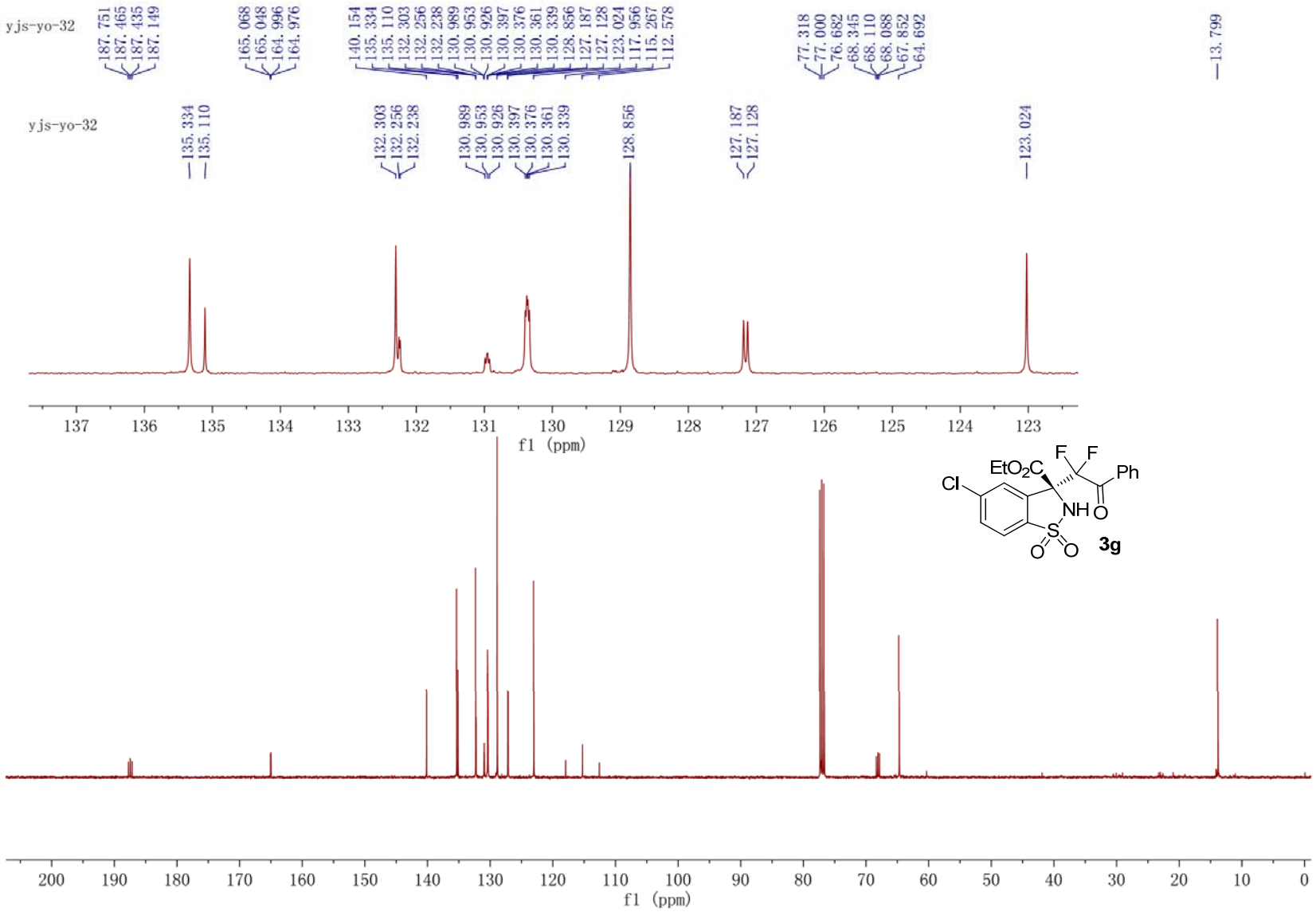
yjs-yo-32

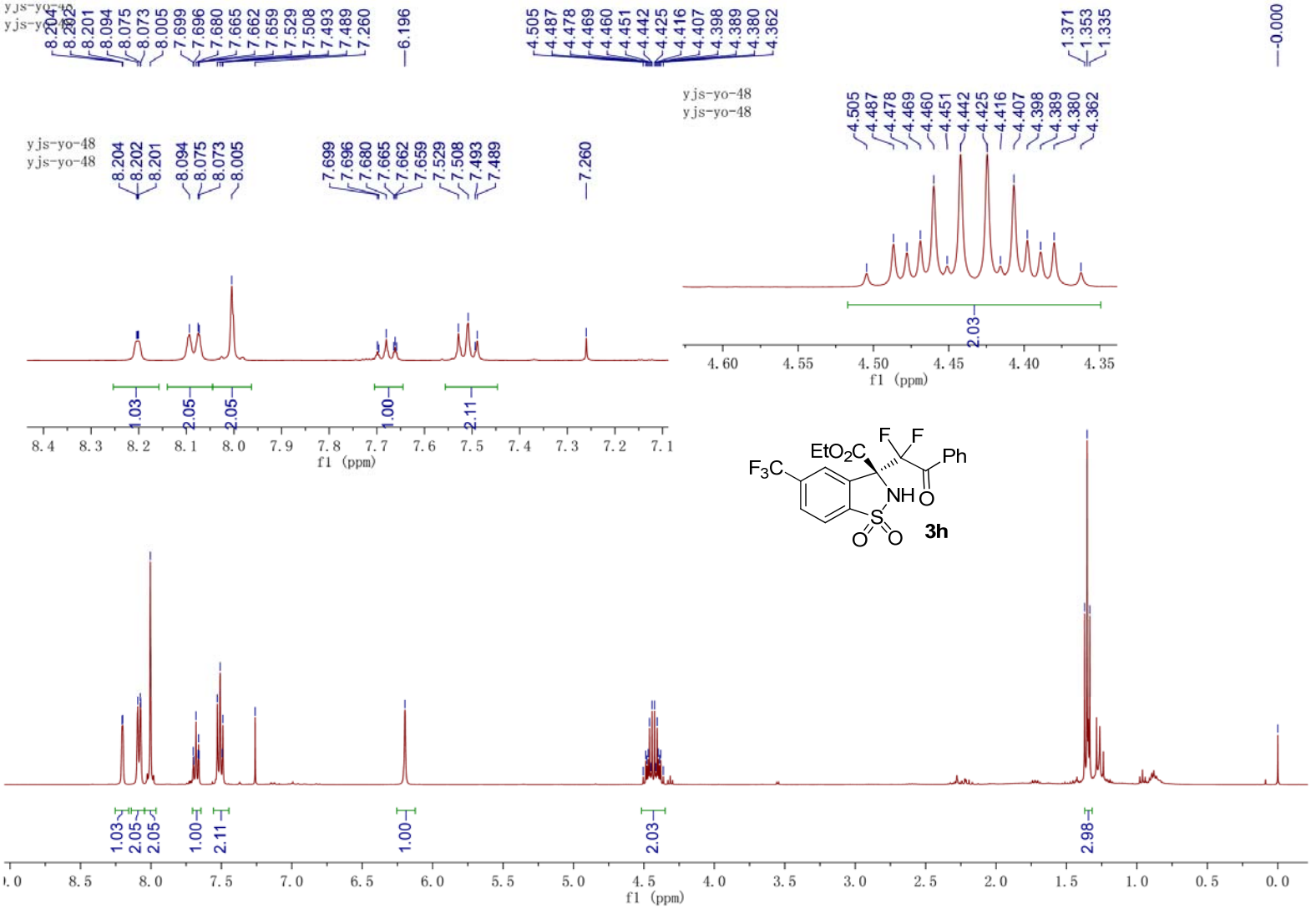
-99.120
-99.912
-105.010
-105.802

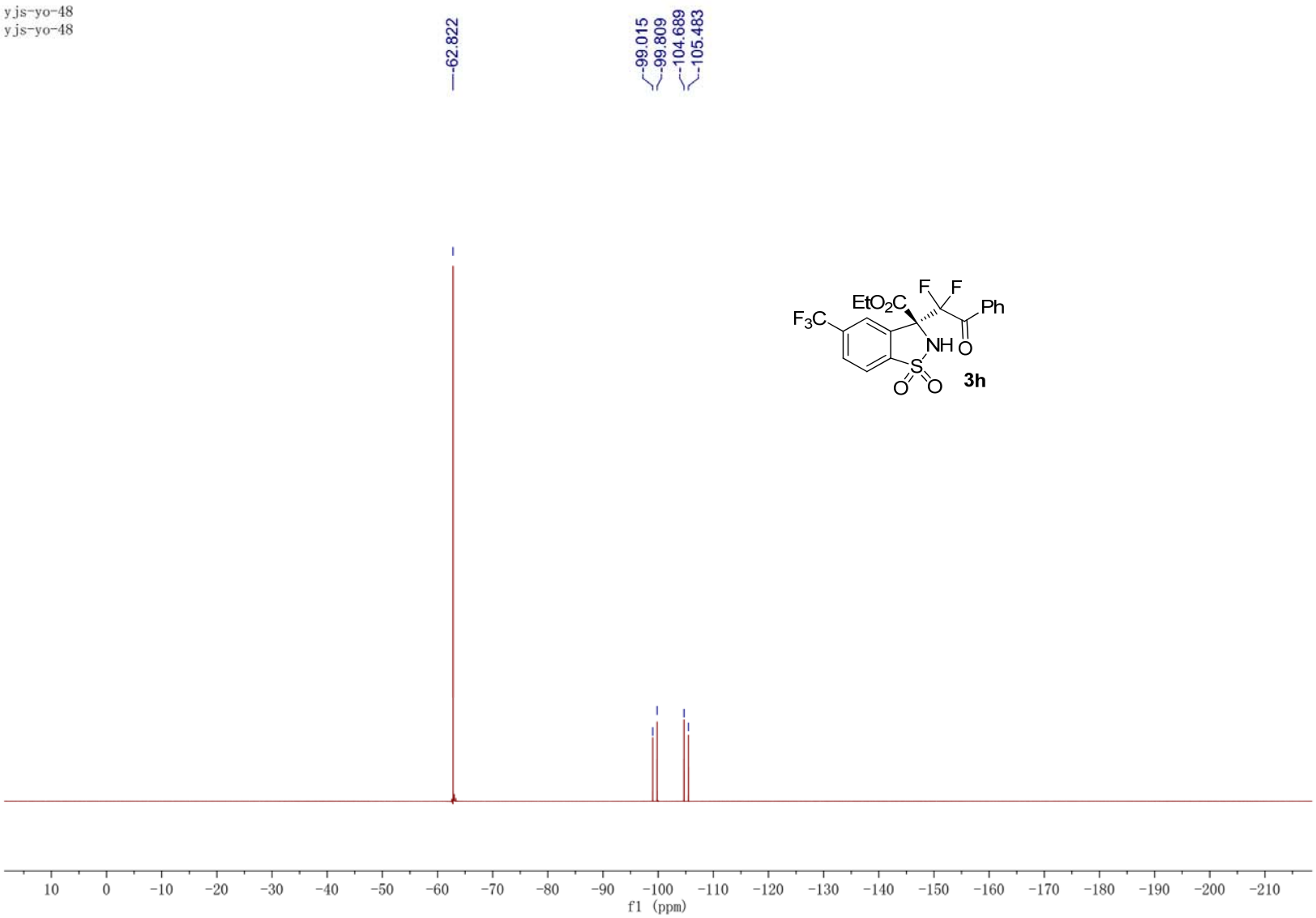


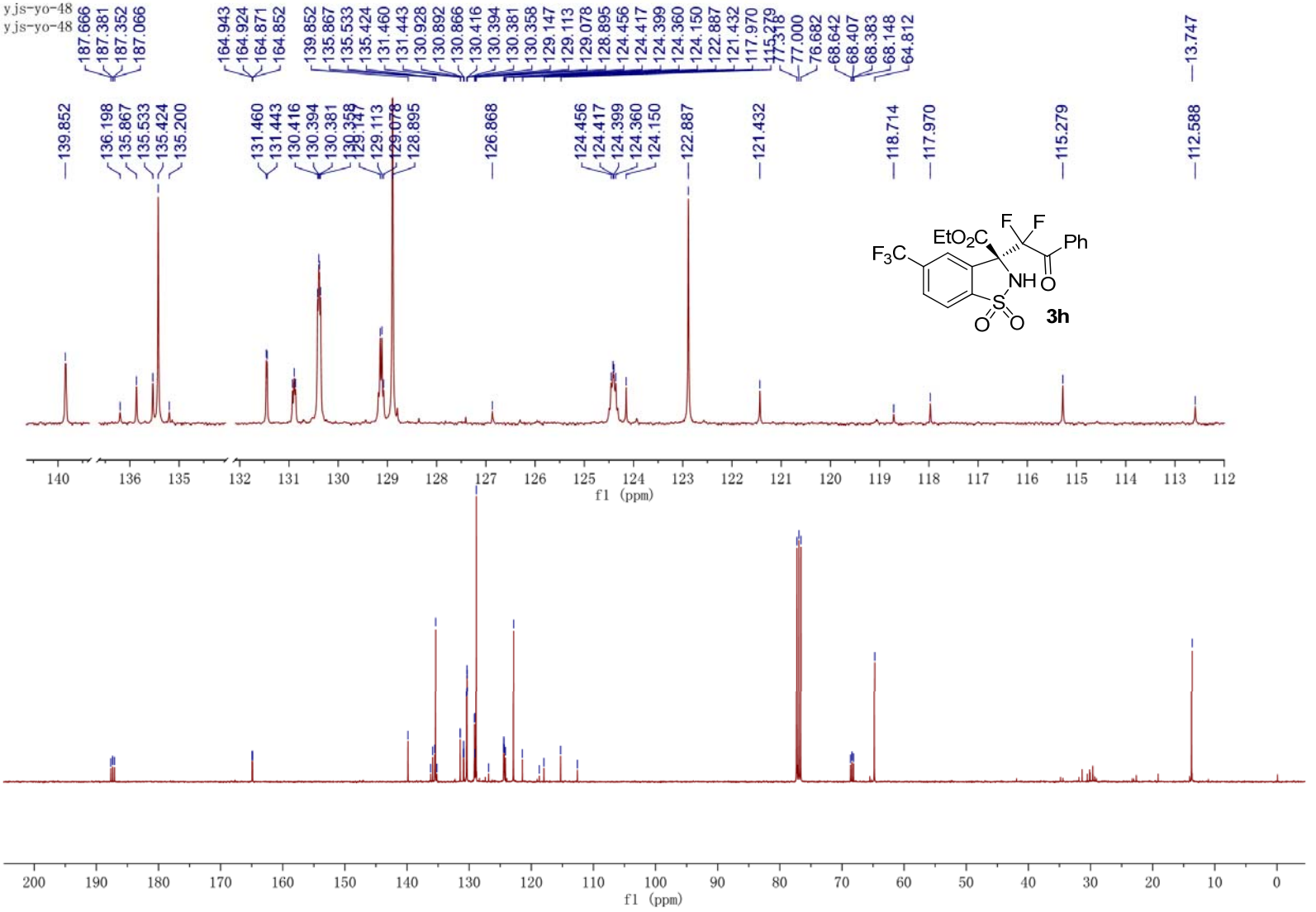
3g

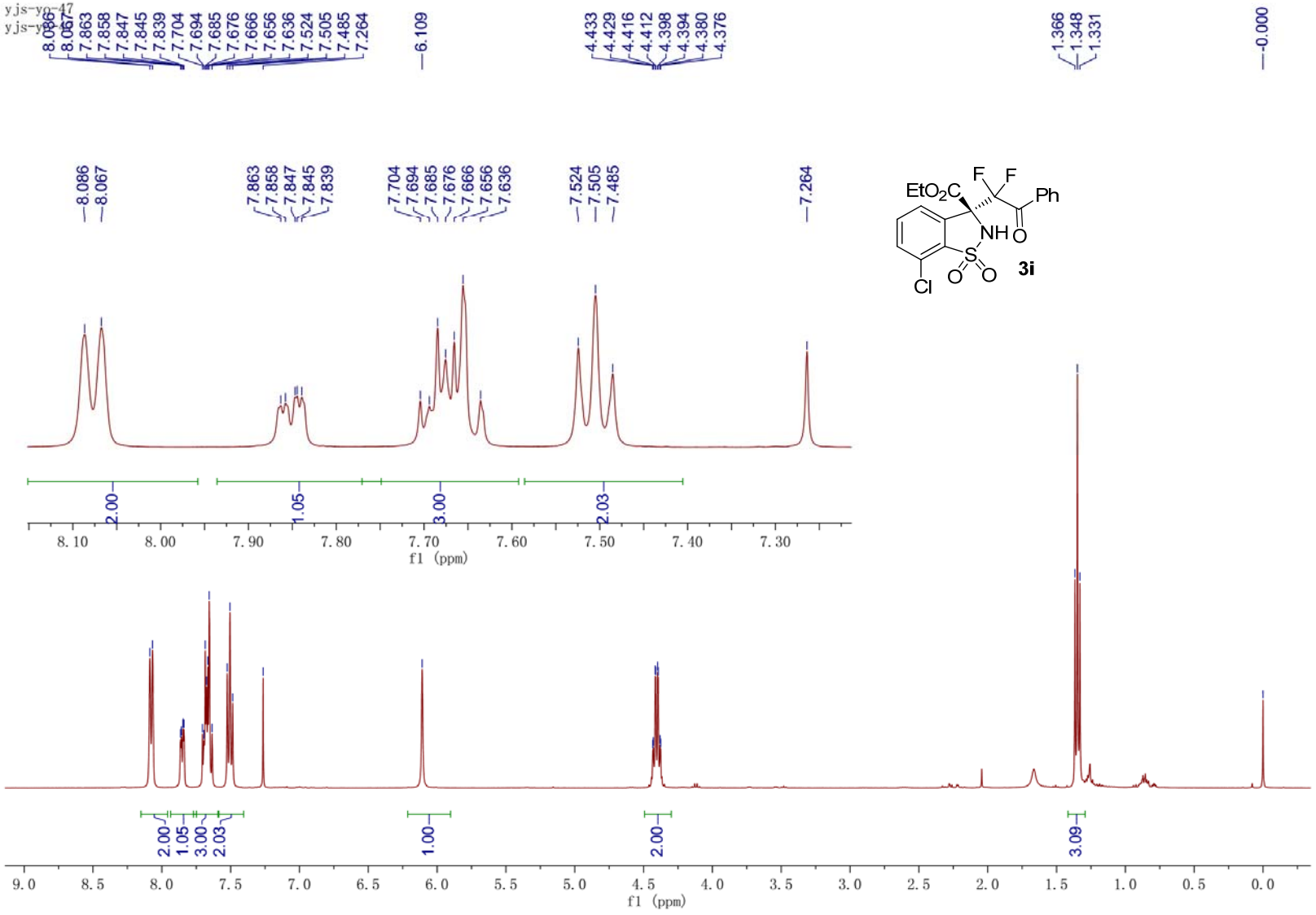



yjs-yo-32
187.751
187.465
187.435
187.149
165.068
165.048
164.996
164.976
140.154
135.334
135.110
132.303
132.256
132.238
130.989
130.953
130.926
130.397
130.376
130.361
130.339
128.856
127.187
127.128
123.024
117.956
115.267
112.578
77.318
77.000
76.682
68.345
68.110
68.088
67.852
64.692
13.799
yjs-yo-32
135.334
135.110
132.303
132.256
132.238
130.989
130.953
130.926
130.397
130.376
130.361
130.339
128.856
127.187
127.128
123.024
137
136
135
134
133
132
131
130
129
128
127
126
125
124
123
f1 (ppm)
EtO2C
F
F
Ph
Cl
NH
O
S
O
O
3g
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


yjs-yo-48
yjs-yo-48
8.204
8.202
8.201
8.094
8.075
8.073
8.005
7.699
7.696
7.680
7.665
7.662
7.659
7.529
7.508
7.493
7.489
7.260
6.196
4.505
4.487
4.478
4.469
4.460
4.451
4.442
4.425
4.416
4.407
4.398
4.389
4.380
4.362
1.371
1.353
1.335
-0.000
1.03
2.05
2.05
1.00
2.11
2.03
f1 (ppm)
F
F
EtO2C
Ph
F3C
NH
O
S
O
O
3h

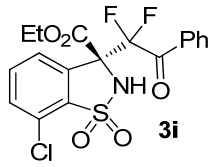

yjs-yo-48
yjs-yo-48
-62.822
-99.015
-99.809
-104.689
-105.483
F
F
EtO2C
Ph
F3C
NH
O
S
O
O
3h
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


yjs-yo-48
yjs-yo-48
187.666
187.381
187.352
187.066
164.943
164.924
164.871
164.852
139.852
135.867
135.533
135.424
131.460
131.443
130.928
130.892
130.866
130.416
130.394
130.381
130.358
129.147
129.113
129.078
128.895
124.456
124.417
124.399
124.360
124.150
122.887
121.432
117.970
115.279
77.318
77.000
76.682
68.642
68.407
68.383
68.148
64.812
13.747
139.852
136.198
135.867
135.533
135.424
135.200
131.460
131.443
130.416
130.394
130.381
129.147
129.113
129.078
128.895
126.868
124.456
124.417
124.399
124.360
124.150
122.887
121.432
118.714
117.970
115.279
112.588
F
F
EtO2C
Ph
F3C
NH
O
S
O
O
3h
f1 (ppm)
f1 (ppm)

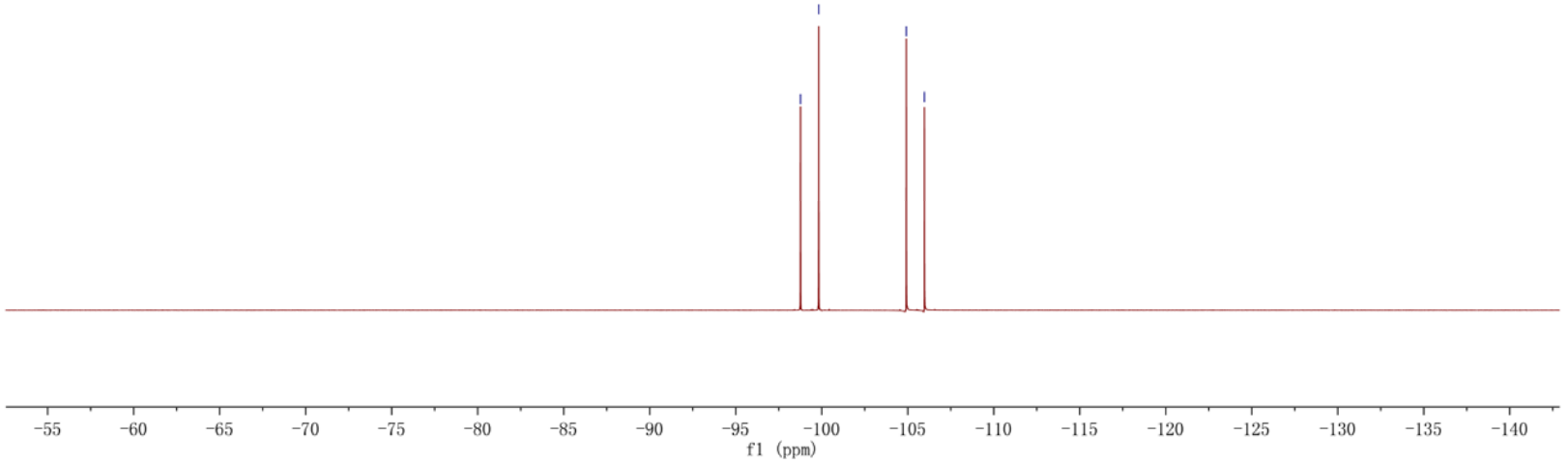

yjs-yq-47
yjs-yq
8.086
8.067
7.863
7.858
7.847
7.845
7.839
7.704
7.694
7.685
7.676
7.666
7.656
7.636
7.524
7.505
7.485
7.264
6.109
4.433
4.429
4.416
4.412
4.398
4.394
4.380
4.376
1.366
1.348
1.331
-0.000
F
F
EtO2C
Ph
NH
O
S
O
O
Cl
3i
2.00
1.05
3.00
2.03
1.00
2.00
3.09
f1 (ppm)

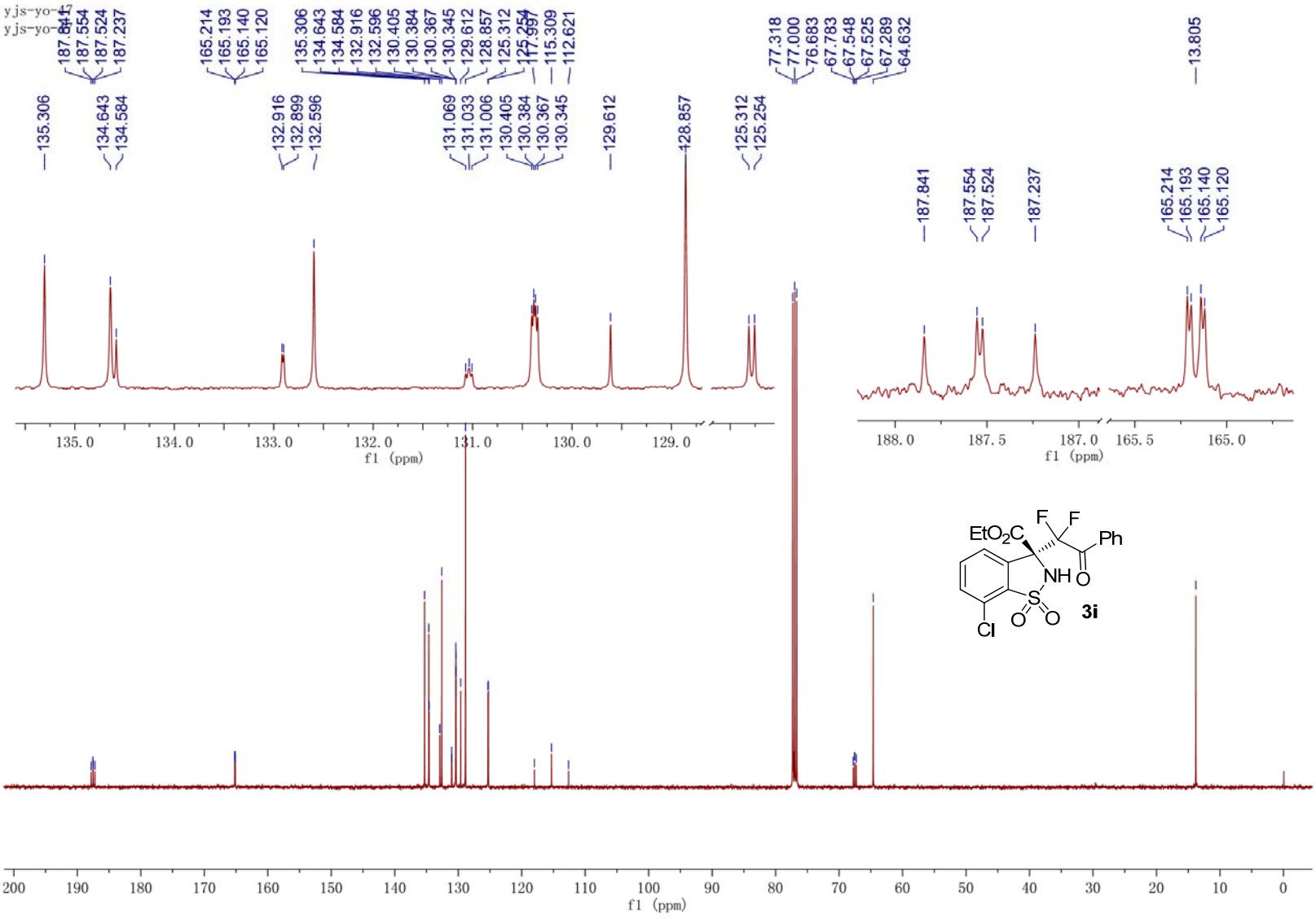
yjs-yo-47 300MHz
yjs-yo-47 300MHz

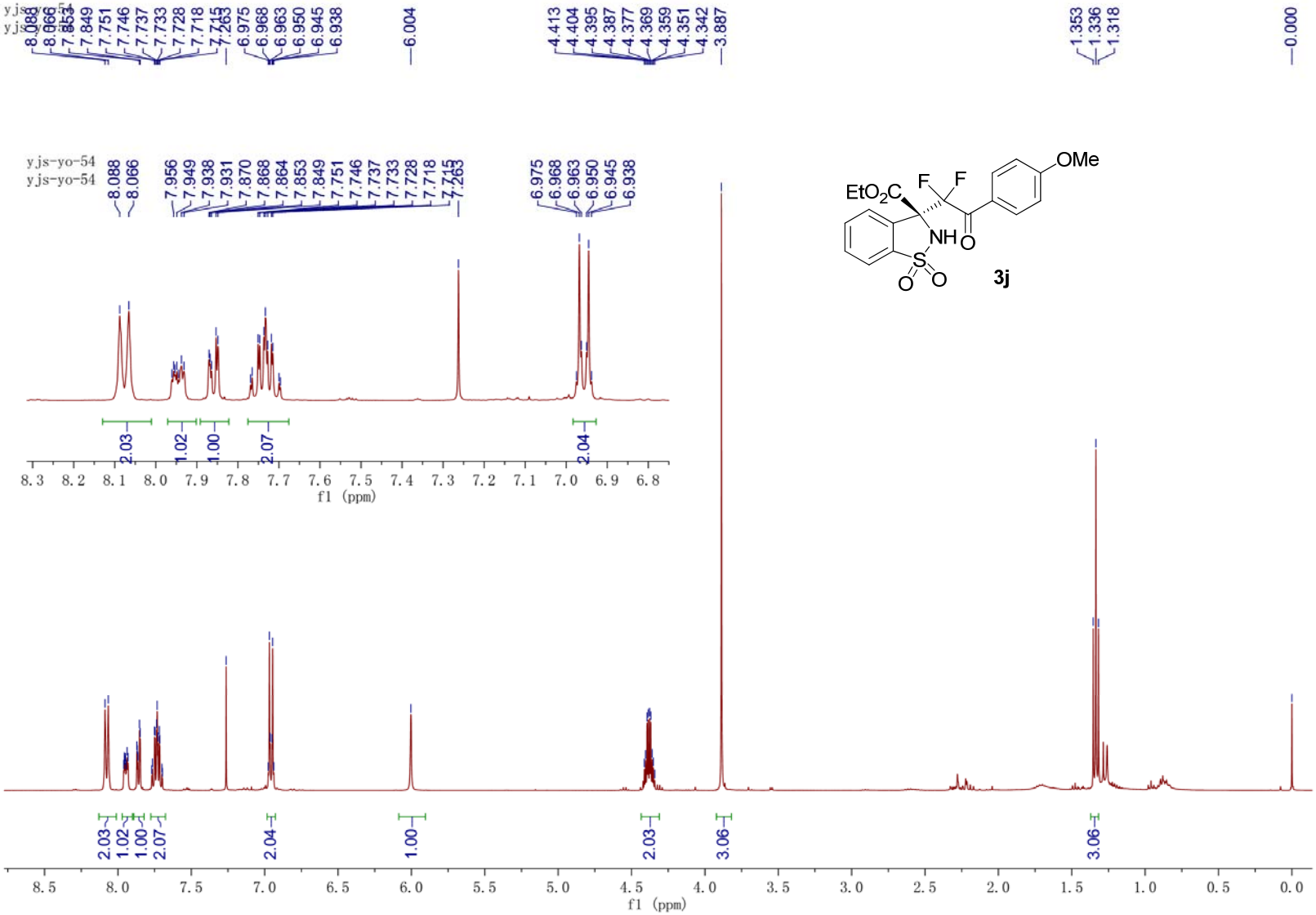
-98.768
-99.825
-104.915
-105.972



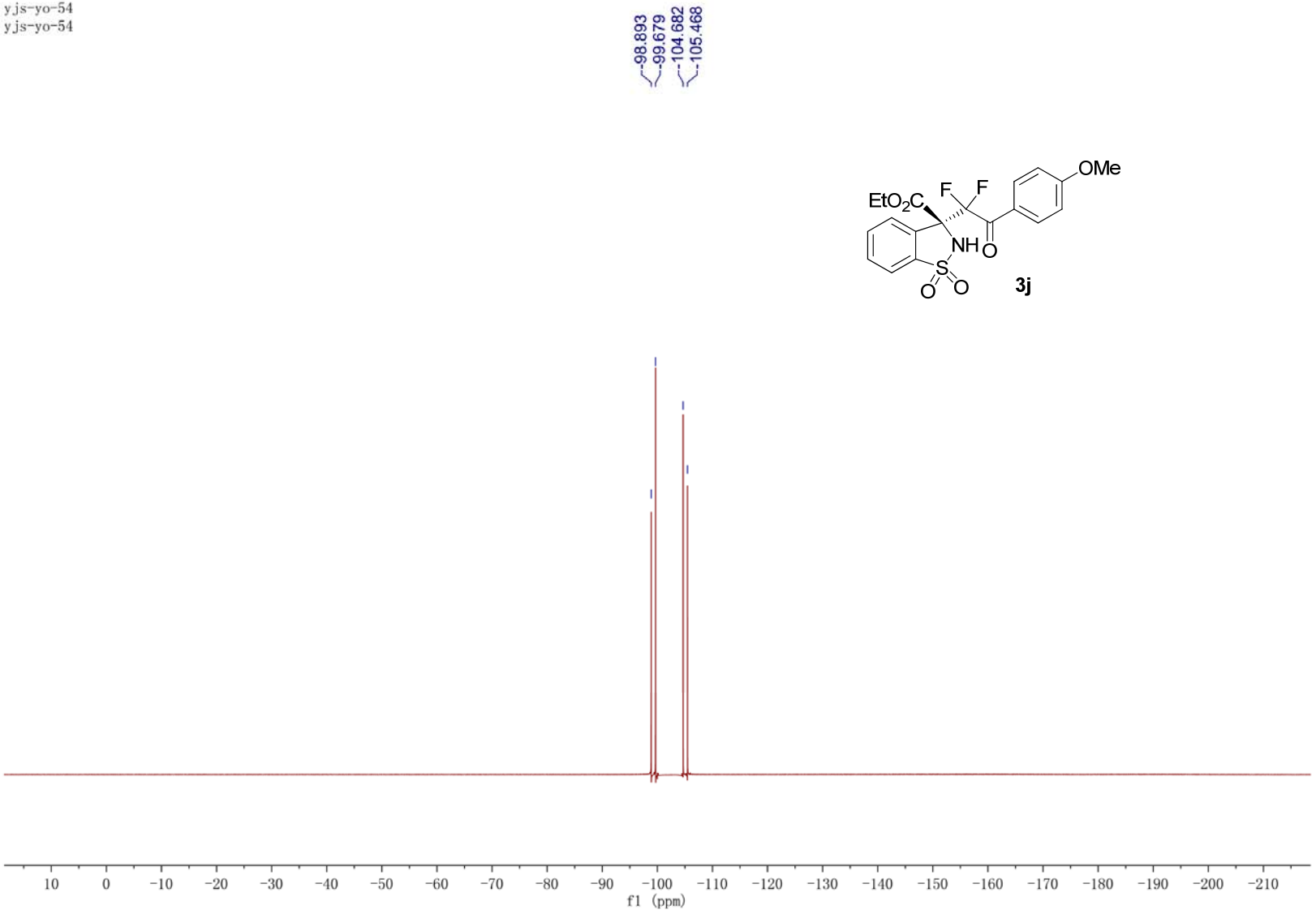
3i

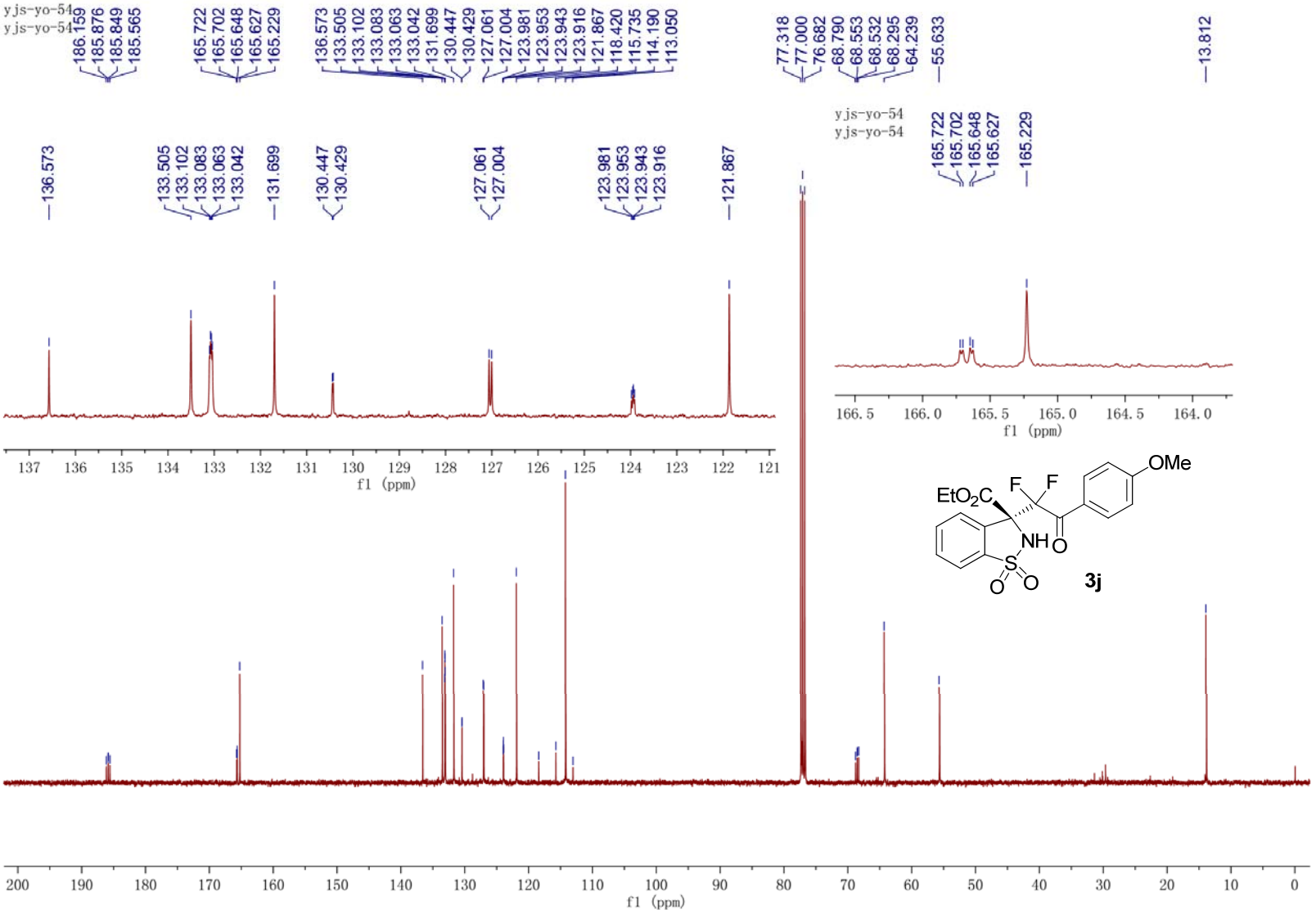


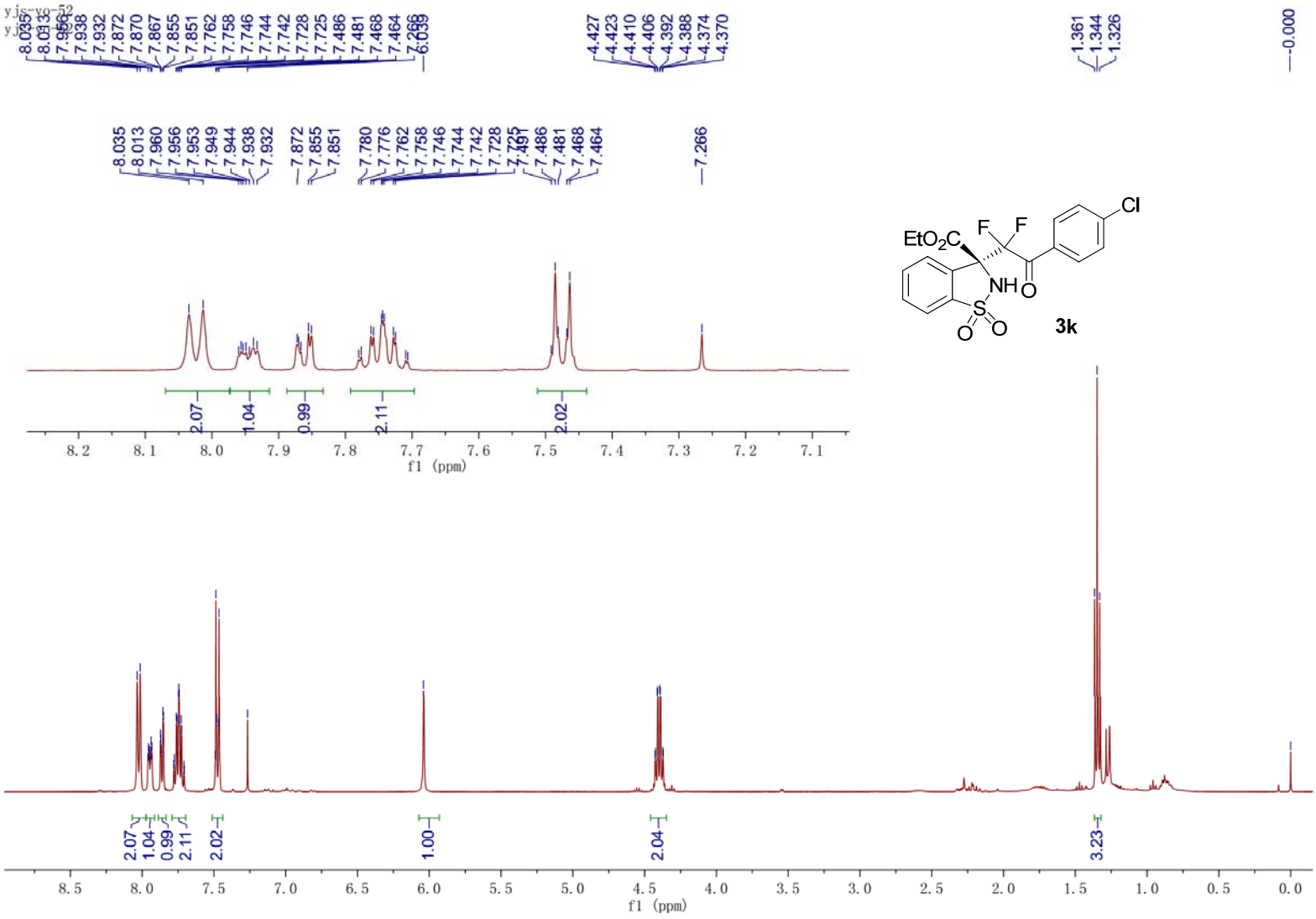

yjs-yo-47
yjs-yo-47
187.841
187.554
187.524
187.237
165.214
165.193
165.140
165.120
135.306
134.643
134.584
132.916
132.596
130.405
130.384
130.367
130.345
129.612
128.857
125.312
125.254
117.997
115.309
112.621
77.318
77.000
76.683
67.783
67.548
67.525
67.289
64.632
13.805
135.306
134.643
134.584
132.916
132.899
132.596
131.069
131.033
131.006
130.405
130.384
130.367
130.345
129.612
128.857
125.312
125.254
187.841
187.554
187.524
187.237
165.214
165.193
165.140
165.120
135.0
134.0
133.0
132.0
131.0
130.0
129.0
f1 (ppm)
188.0
187.5
187.0
165.5
165.0
f1 (ppm)
EtO2C
F
F
Ph
NH
O
S
O
O
Cl
3i
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


yjs-yo-54
yjs-yo-54
8.088
8.066
7.956
7.949
7.938
7.931
7.870
7.868
7.864
7.853
7.849
7.751
7.746
7.737
7.733
7.728
7.718
7.715
7.263
6.975
6.968
6.963
6.950
6.945
6.938
6.004
4.413
4.404
4.395
4.387
4.377
4.369
4.359
4.351
4.342
3.887
1.353
1.336
1.318
0.000
2.03
1.02
1.00
2.07
2.04
f1 (ppm)
EtO2C
F
F
OMe
NH
O
S
O
O
3j

yjs-yo-54
yjs-yo-54

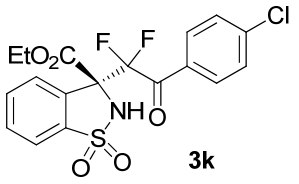



yjs-yo-54
yjs-yo-54
186.159
185.876
185.849
185.565
165.722
165.702
165.648
165.627
165.229
136.573
133.505
133.102
133.083
133.063
133.042
131.699
130.447
130.429
127.061
127.004
123.981
123.953
123.943
123.916
121.867
118.420
115.735
114.190
113.050
77.318
77.000
76.682
68.790
68.553
68.532
68.295
64.239
55.633
13.812
f1 (ppm)
OMe
EtO2C
F
F
NH
O
S
O
O
3j

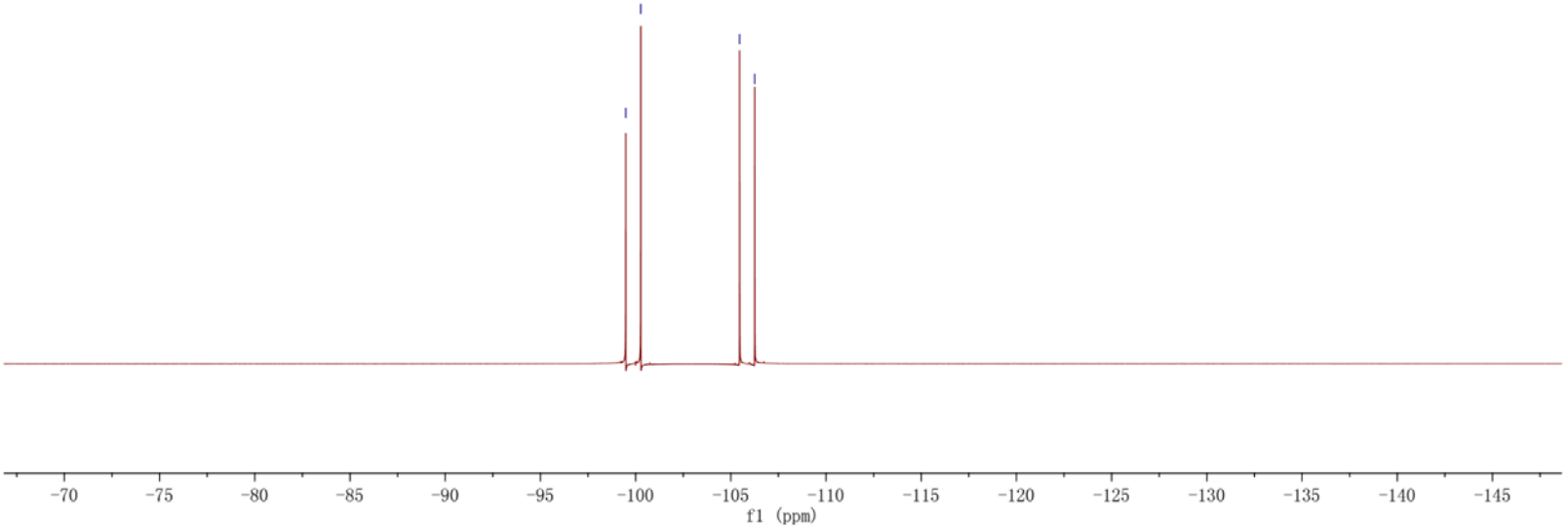

8.035
8.013
7.960
7.956
7.953
7.949
7.944
7.938
7.932
7.872
7.855
7.851
7.780
7.776
7.762
7.758
7.746
7.744
7.742
7.728
7.725
7.491
7.486
7.481
7.468
7.464
7.266
4.427
4.423
4.410
4.406
4.392
4.388
4.374
4.370
1.361
1.344
1.326
0.000
2.07
1.04
0.99
2.11
2.02
1.00
2.04
3.23
f1 (ppm)
EtO2C
F
F
Cl
NH
O
S
O
O
3k

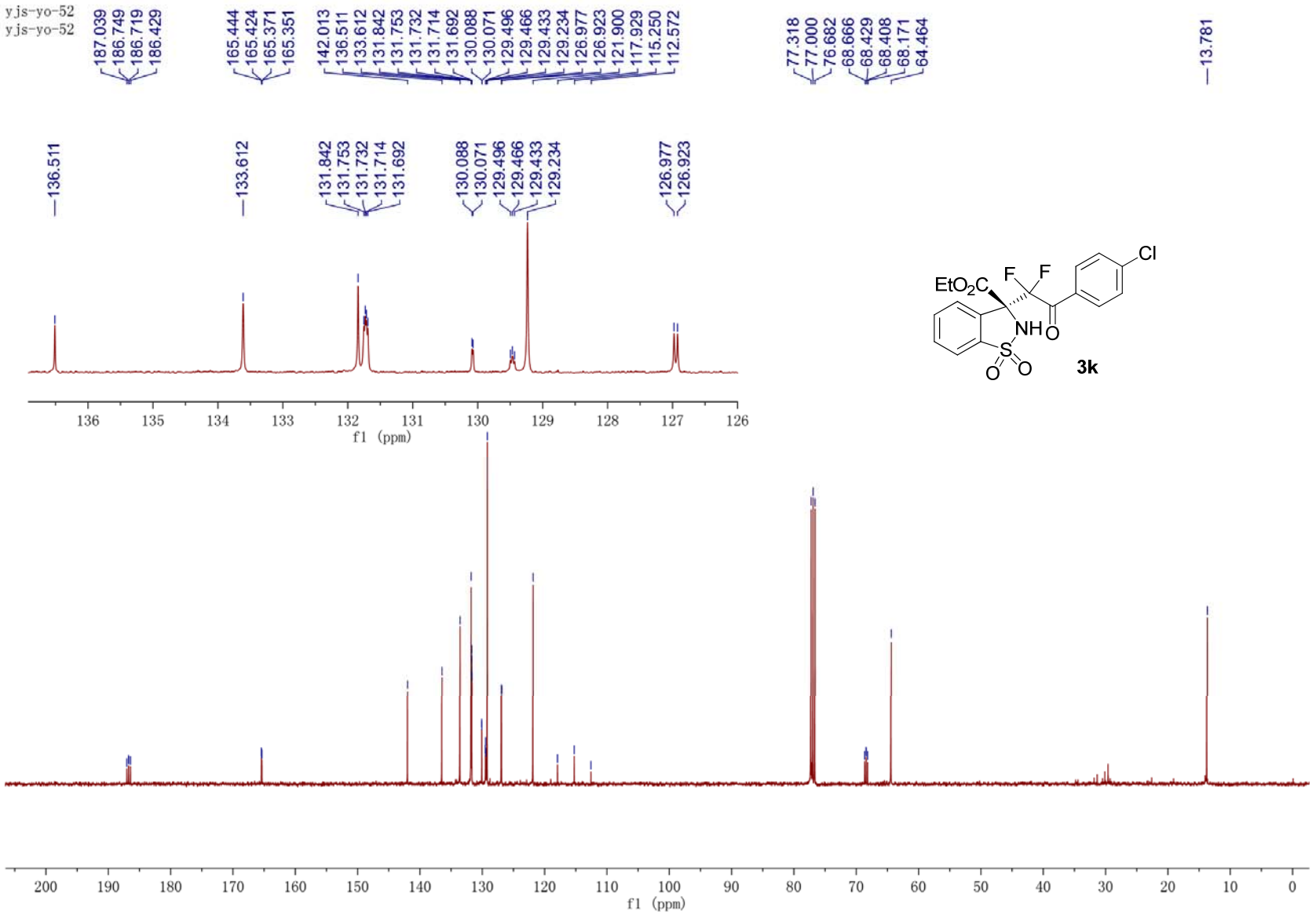
yjs-yo-52
yjs-yo-52

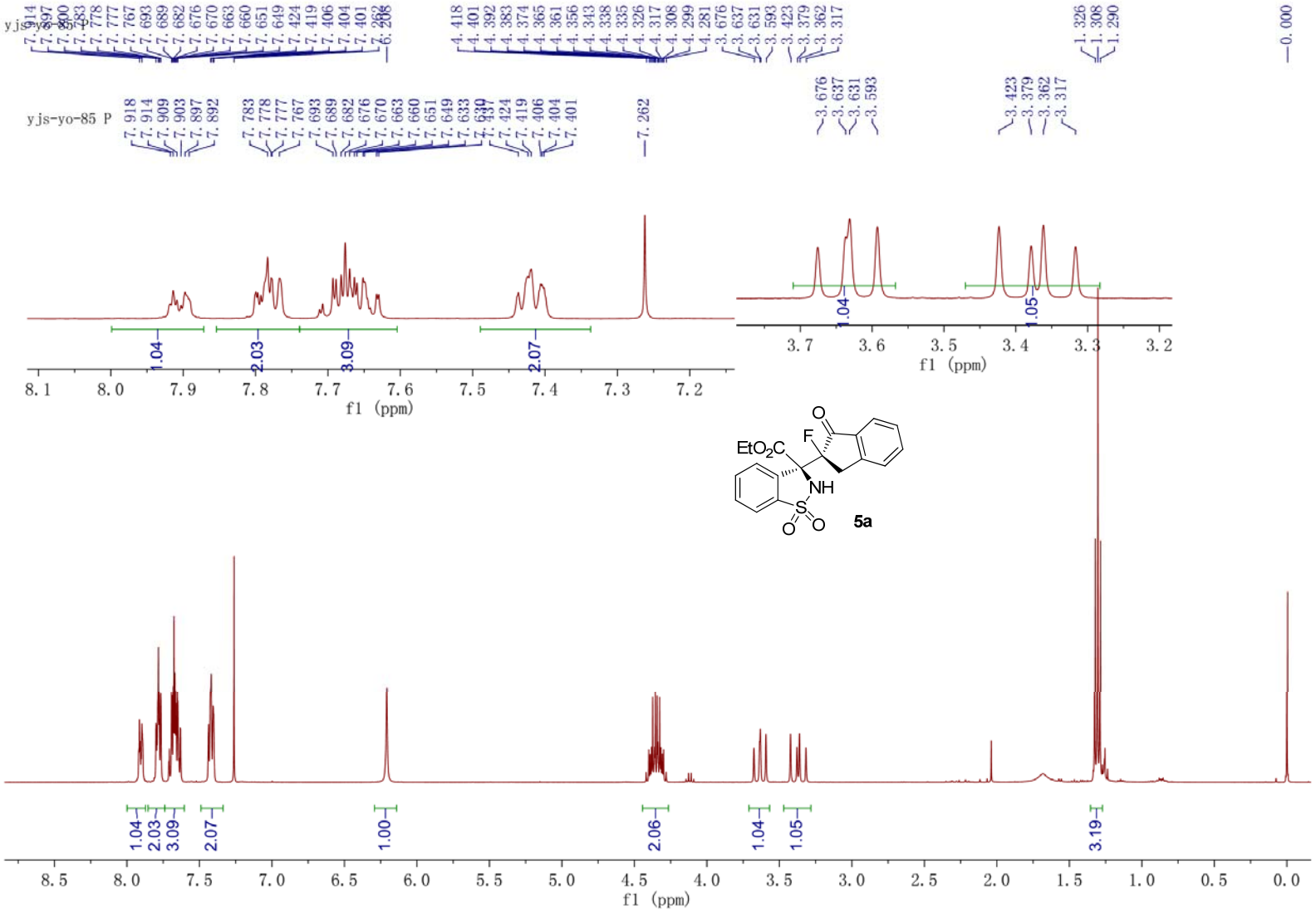
-99.479
-100.268
-105.465
-106.254



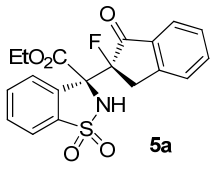
3k



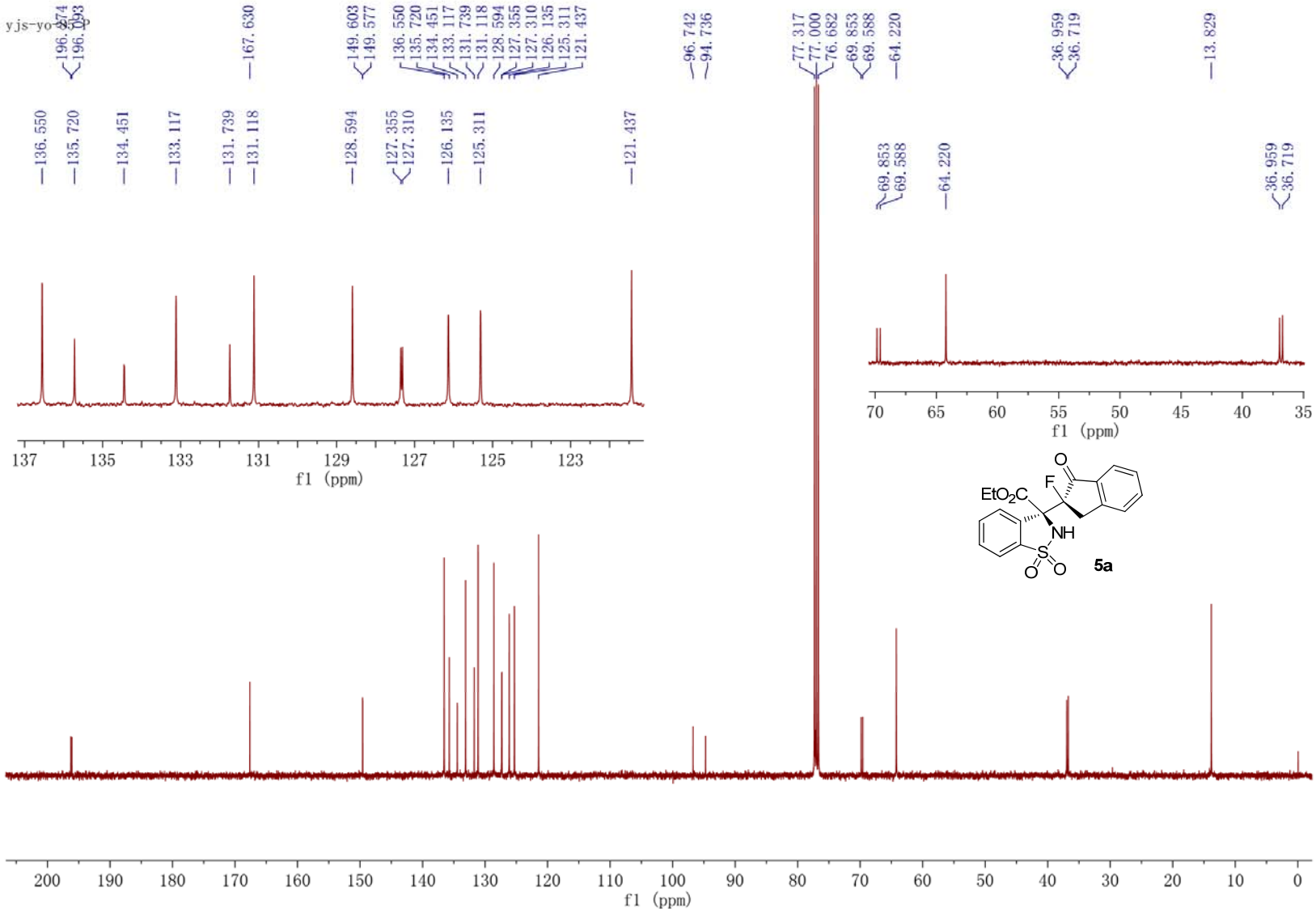

yjs-yo-52
yjs-yo-52
187.039
186.749
186.719
186.429
165.444
165.424
165.371
165.351
142.013
136.511
133.612
131.842
131.753
131.732
131.714
131.692
130.088
130.071
129.496
129.466
129.433
129.234
126.977
126.923
121.900
117.929
115.250
112.572
77.318
77.000
76.682
68.666
68.429
68.408
68.171
64.464
13.781
f1 (ppm)
EtO2C
F
F
Cl
NH
O
S
O
O
3k

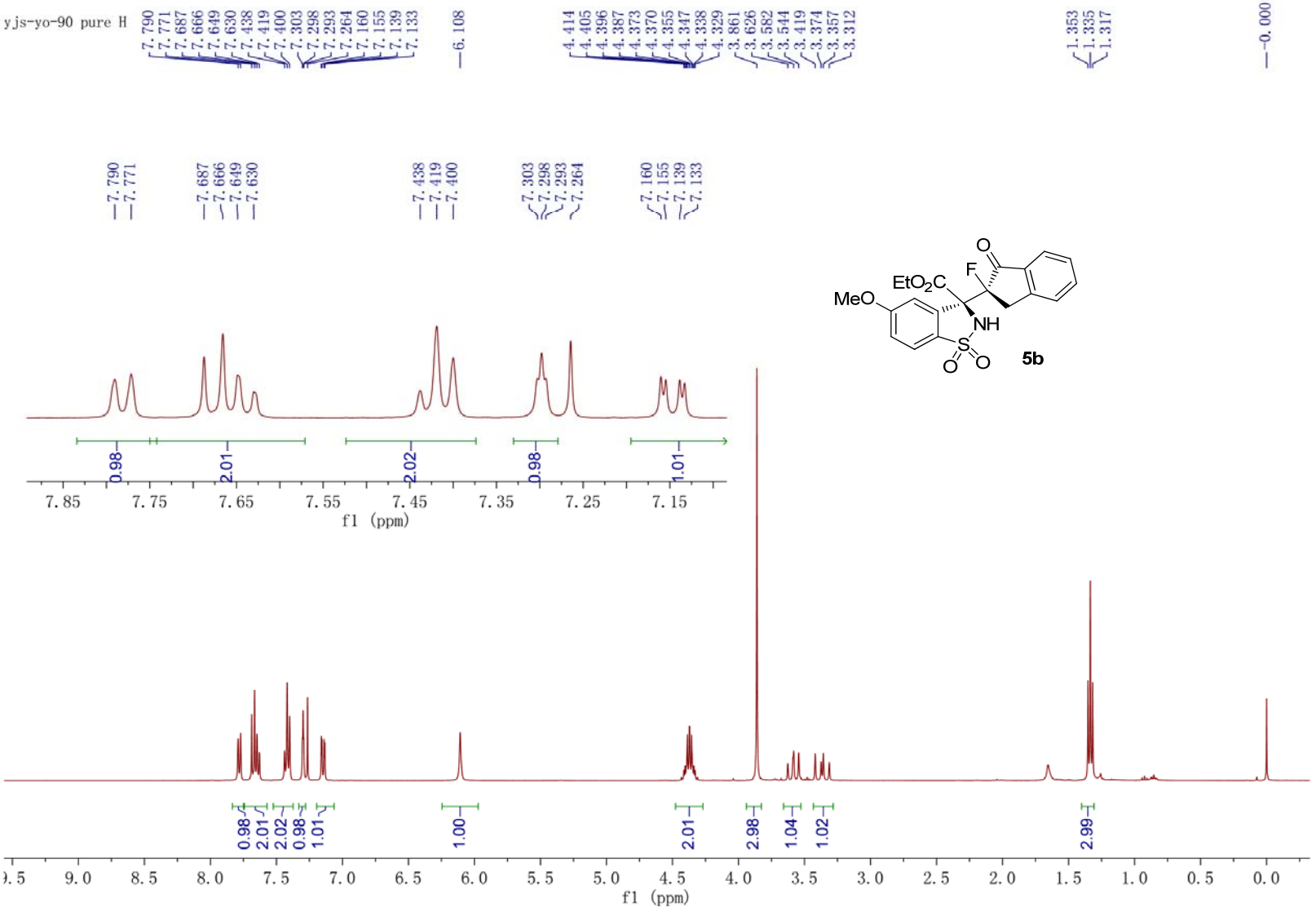

yjs-yo-85 P
f1 (ppm)
EtO2C
F
NH
S
O
5a

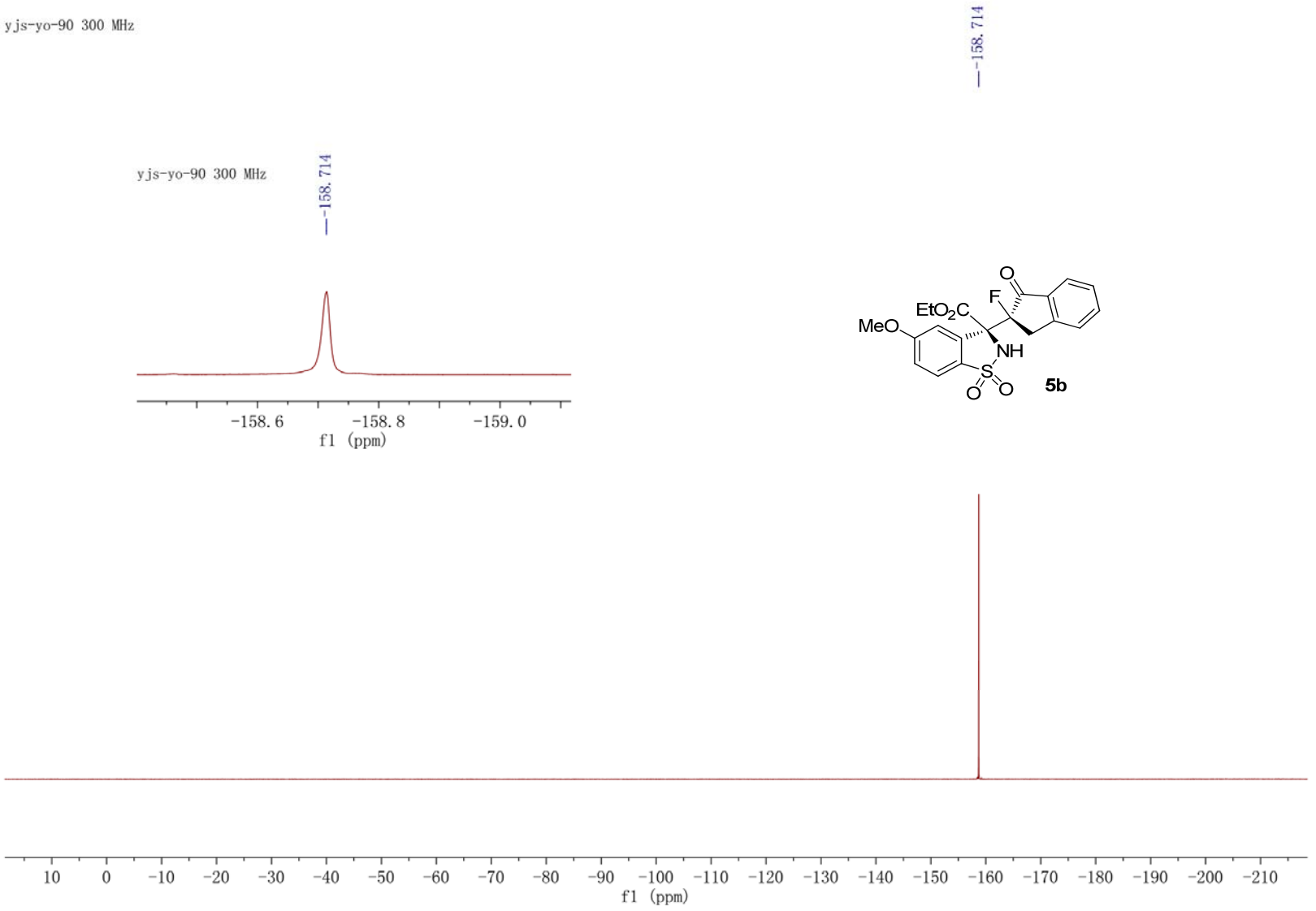
yjs-yo-85 P
yjs-yo-85 P

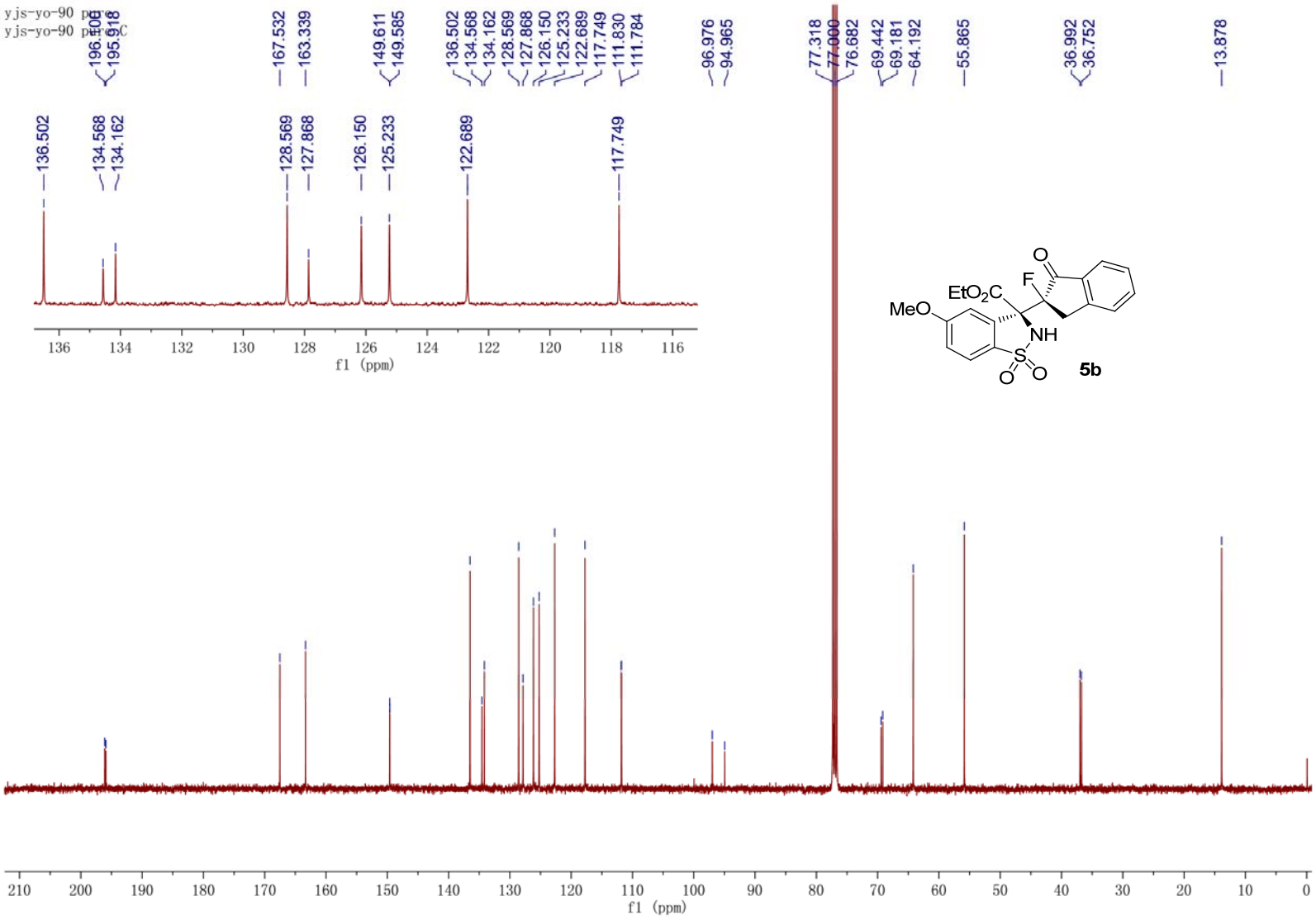


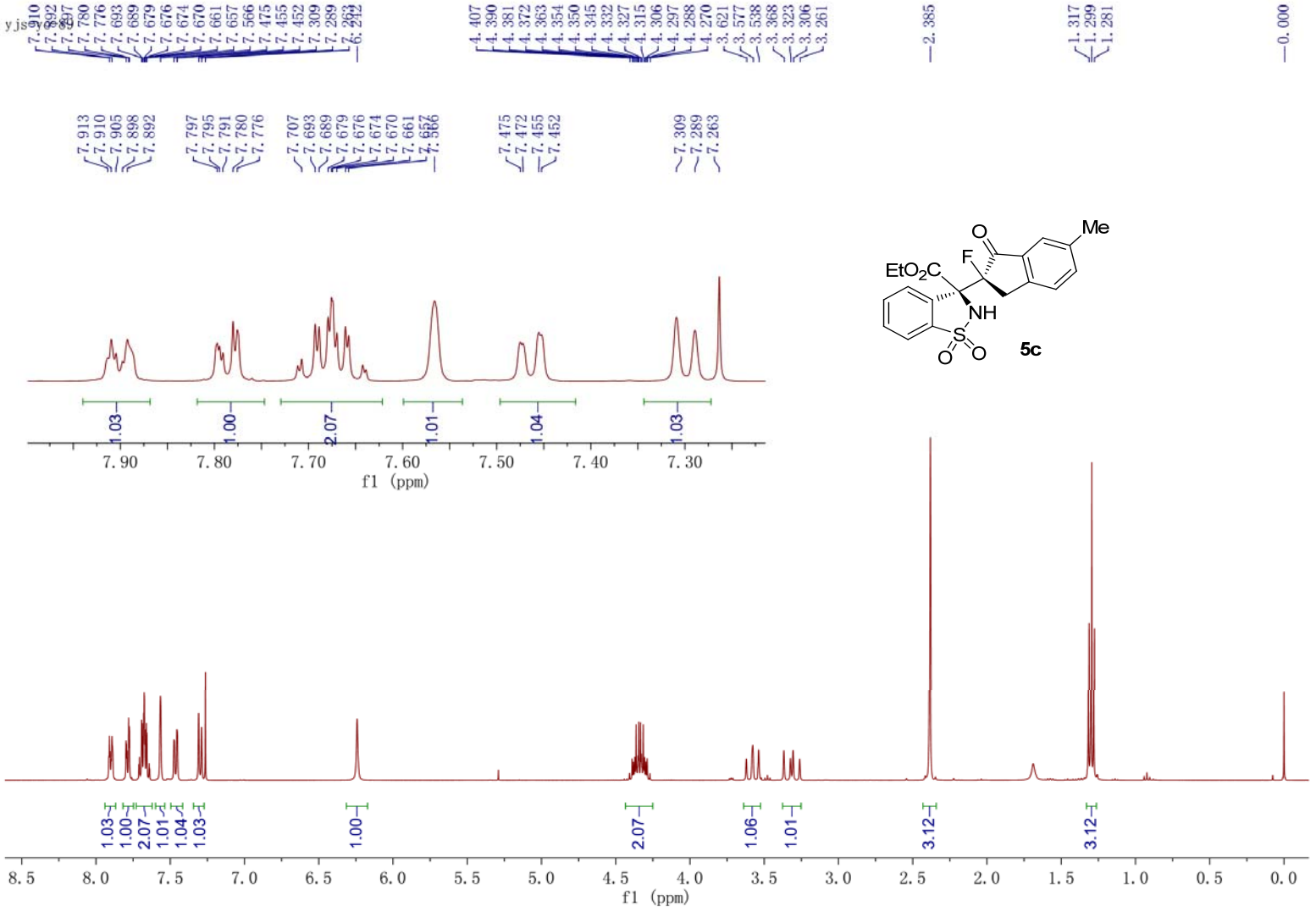
5a

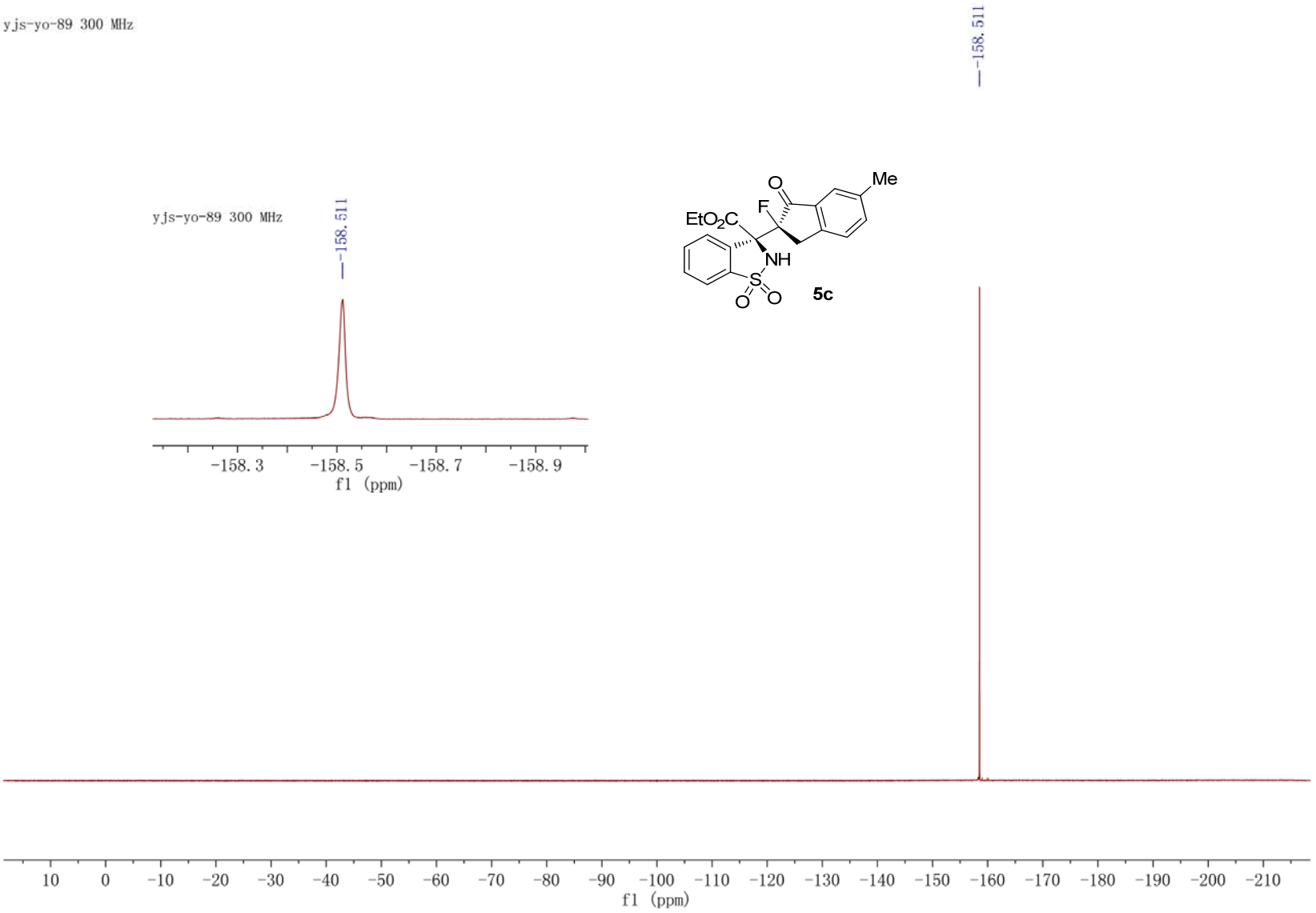

196.474
196.193
167.630
149.603
149.577
136.550
135.720
134.451
133.117
131.739
131.118
128.594
127.355
127.310
126.135
125.311
121.437
96.742
94.736
77.317
77.000
76.682
69.853
69.588
64.220
36.959
36.719
13.829
f1 (ppm)
EtO2C
F
O
NH
S
O
O
5a

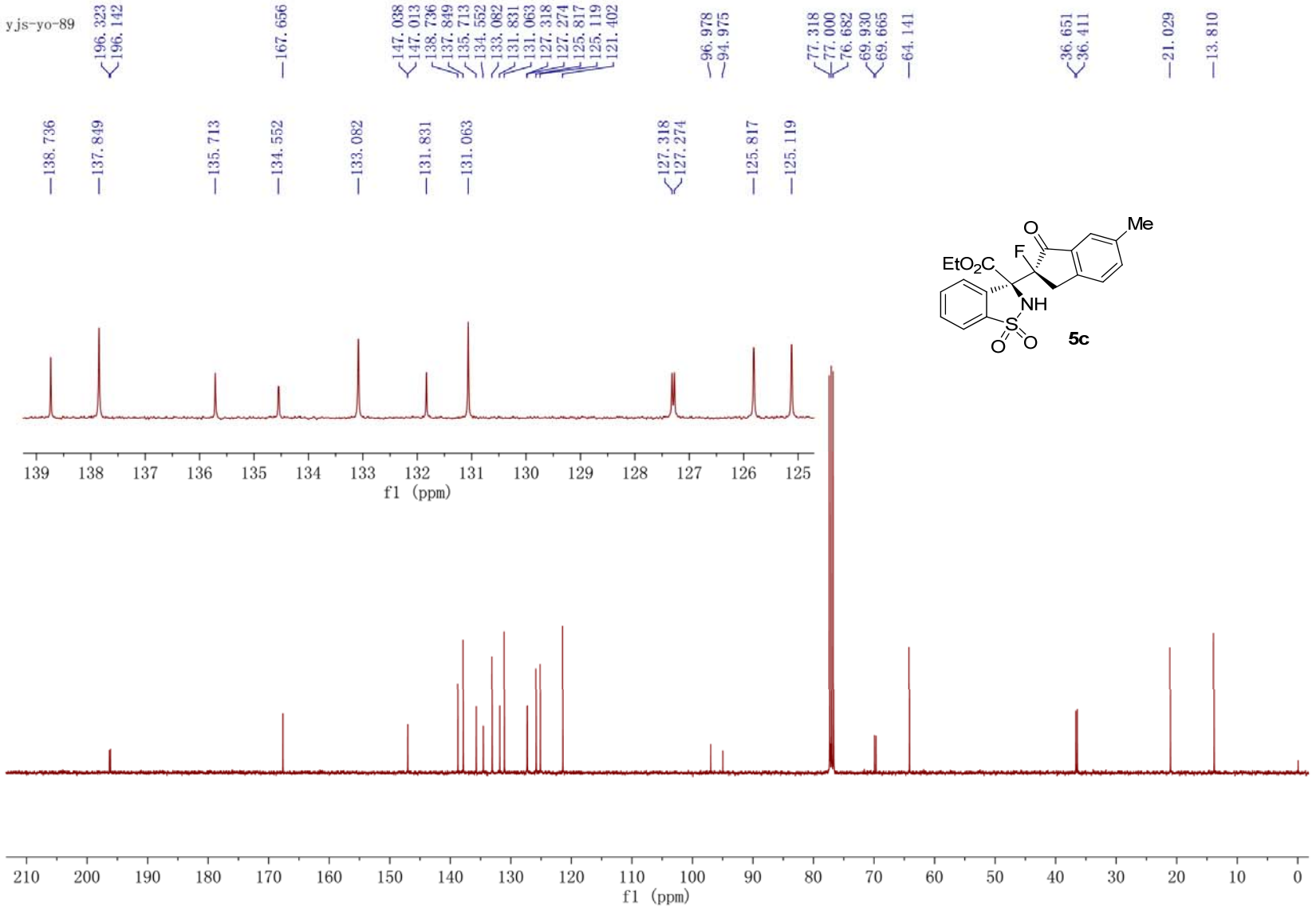

yjs-yo-90 pure H
7.790
7.771
7.687
7.666
7.649
7.630
7.438
7.419
7.400
7.303
7.298
7.293
7.264
7.160
7.155
7.139
7.133
6.108
4.414
4.405
4.396
4.387
4.373
4.370
4.355
4.347
4.338
4.329
3.861
3.626
3.582
3.544
3.419
3.374
3.357
3.312
1.353
1.335
1.317
0.000
0.98
2.01
2.02
0.98
1.01
7.85
7.75
7.65
7.55
7.45
7.35
7.25
7.15
f1 (ppm)
O
F
EtO2C
MeO
NH
S
O
O
5b
0.98
2.01
2.02
0.98
1.01
1.00
2.01
2.98
1.04
1.02
2.99
f1 (ppm)

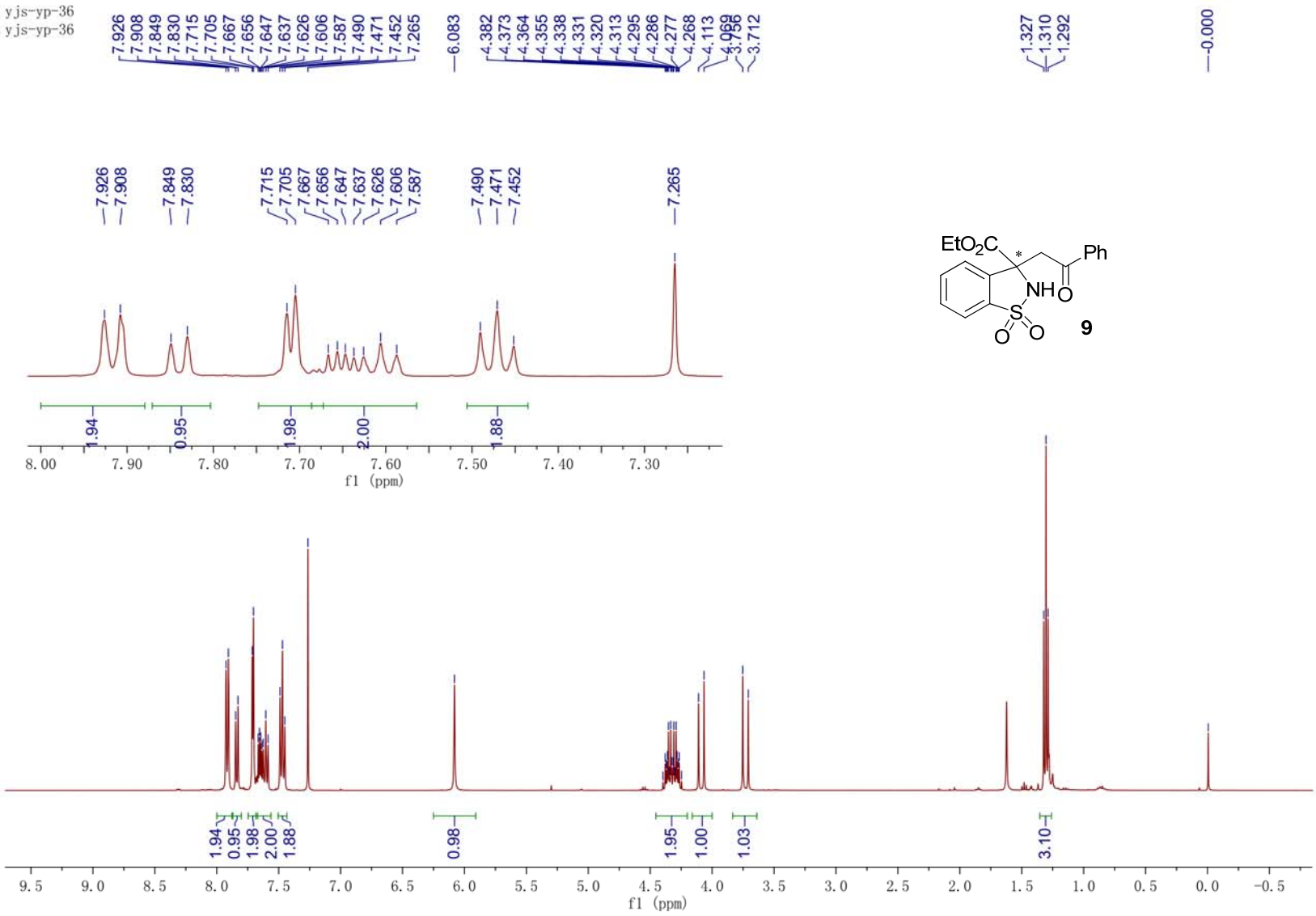

yjs-yo-90 300 MHz
-158.714
yjs-yo-90 300 MHz
-158.714
-158.6
-158.8
-159.0
f1 (ppm)
O
F
EtO2C
MeO
NH
S
O
O
5b
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

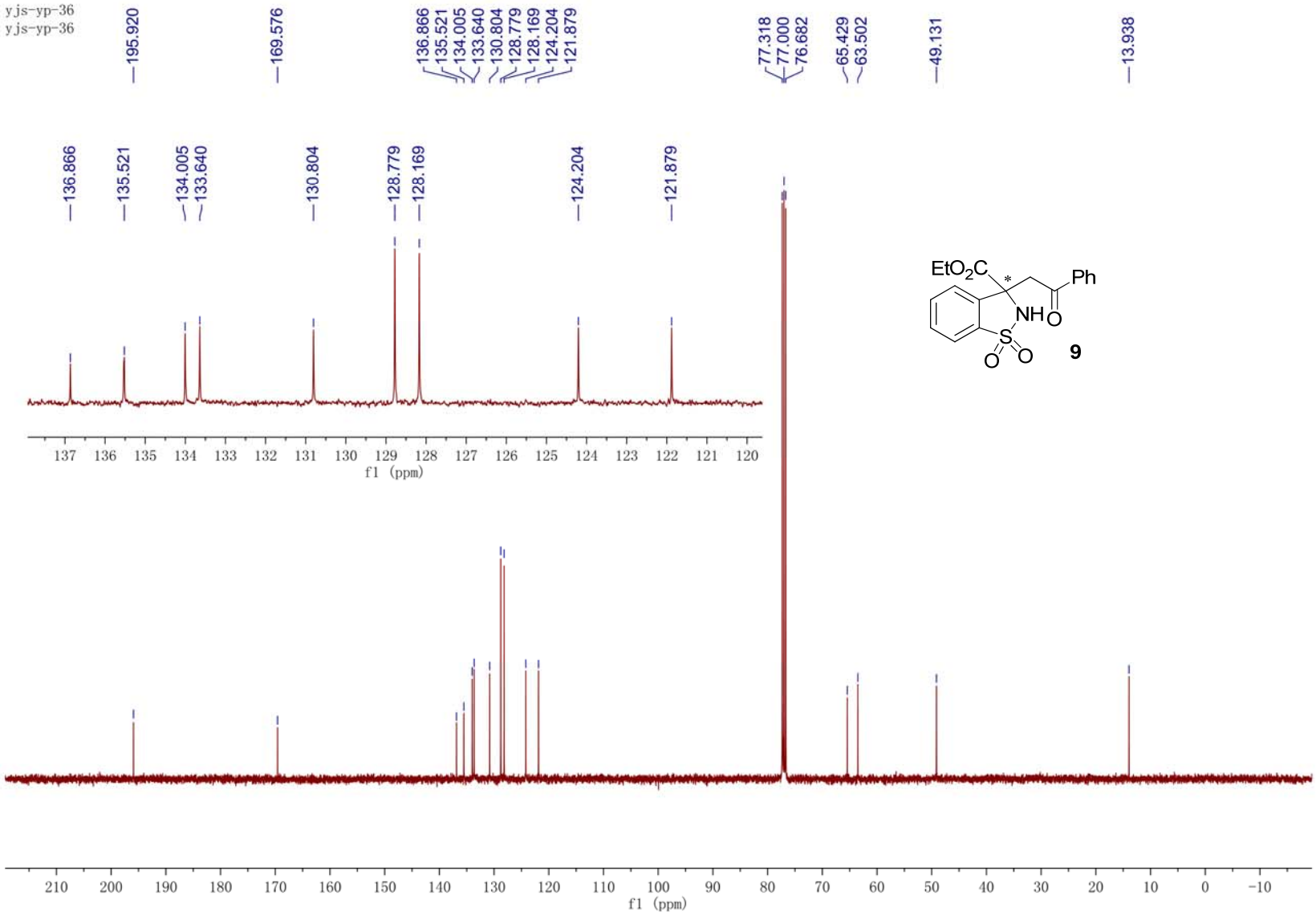

yjs-yo-90 pd
yjs-yo-90 pure 13C
196.608
195.918
167.532
163.339
149.611
149.585
136.502
134.568
134.162
128.569
127.868
126.150
125.233
122.689
117.749
111.830
111.784
96.976
94.965
77.318
77.000
76.682
69.442
69.181
64.192
55.865
36.992
36.752
13.878
f1 (ppm)
MeO
EtO2C
F
O
NH
S
O
O
5b

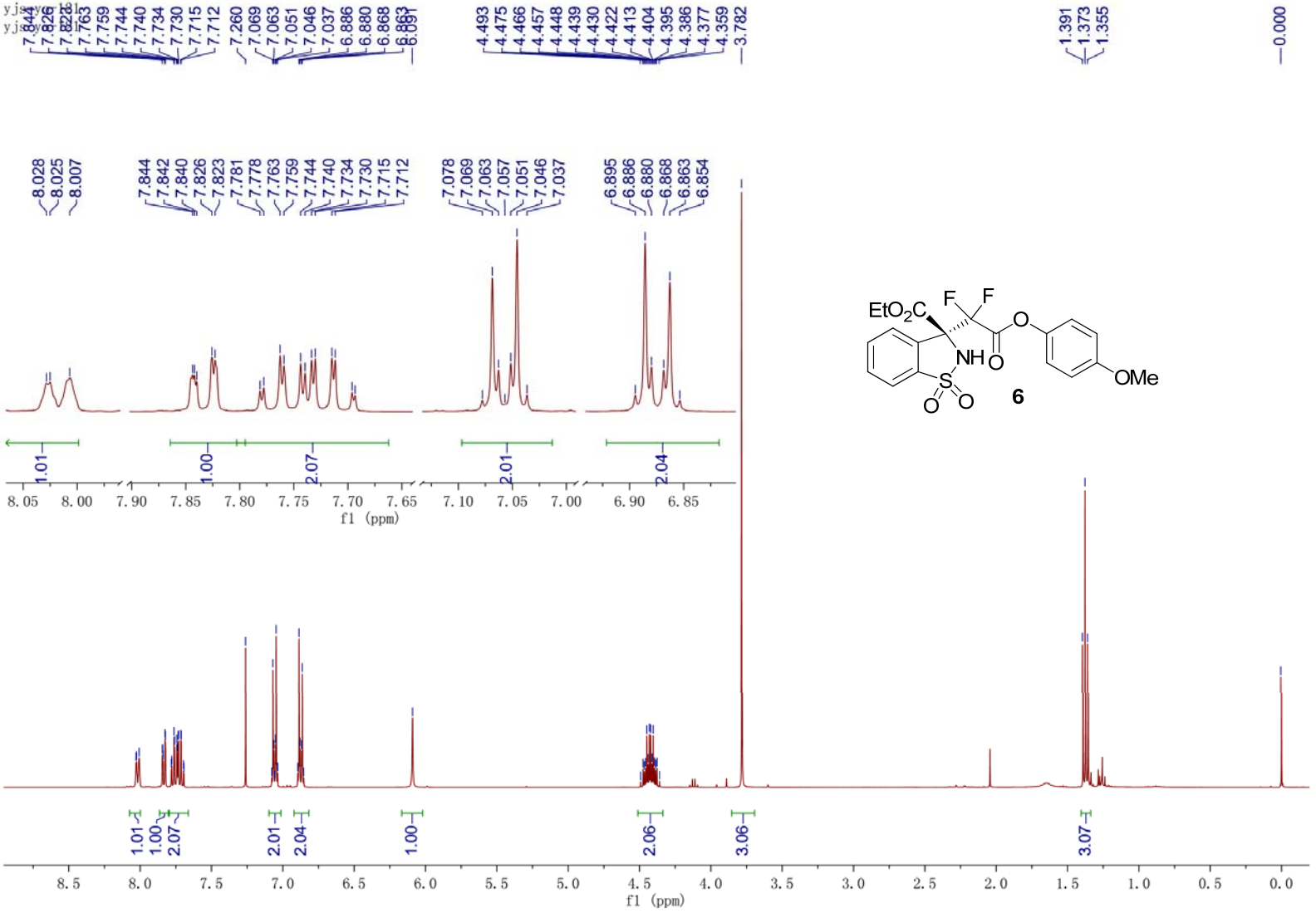

7.913
7.910
7.905
7.898
7.892
7.797
7.795
7.791
7.780
7.776
7.707
7.693
7.689
7.679
7.676
7.674
7.670
7.661
7.657
7.566
7.475
7.472
7.455
7.452
7.309
7.289
7.263
4.407
4.390
4.381
4.372
4.363
4.354
4.350
4.345
4.332
4.327
4.315
4.306
4.297
4.288
4.270
3.621
3.577
3.538
3.368
3.323
3.306
3.261
2.385
1.317
1.299
1.281
0.000
1.03
1.00
2.07
1.01
1.04
1.03
7.90
7.80
7.70
7.60
7.50
7.40
7.30
f1 (ppm)
Me
O
F
EtO2C
NH
S
O
O
5c
1.03
1.00
2.07
1.01
1.04
1.03
1.00
2.07
1.06
1.01
3.12
3.12
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


yjs-yo-89 300 MHz
-158.511
yjs-yo-89 300 MHz
-158.511
-158.3
-158.5
-158.7
-158.9
f1 (ppm)
EtO2C
F
O
Me
NH
S
O
O
5c
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


yjs-yo-89
196.323
196.142
167.656
147.038
147.013
138.736
137.849
135.713
134.552
133.082
131.831
131.063
127.318
127.274
125.817
125.119
121.402
96.978
94.975
77.318
77.000
76.682
69.930
69.665
64.141
36.651
36.411
21.029
13.810
O
F
Me
EtO2C
NH
S
O
O
5c
f1 (ppm)
f1 (ppm)

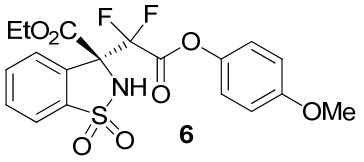

yjs-yp-36
yjs-yp-36
7.926
7.908
7.849
7.830
7.715
7.705
7.667
7.656
7.647
7.637
7.626
7.606
7.587
7.490
7.471
7.452
7.265
6.083
4.382
4.373
4.364
4.355
4.338
4.331
4.320
4.313
4.295
4.286
4.277
4.268
4.113
3.712
1.327
1.310
1.292
0.000
EtO2C
Ph
NH
O
S
O
O
9
1.94
0.95
1.98
2.00
1.88
0.98
1.95
1.00
1.03
3.10
f1 (ppm)


yjs-yp-36
yjs-yp-36
195.920
169.576
136.866
135.521
134.005
133.640
130.804
128.779
128.169
124.204
121.879
77.318
77.000
76.682
65.429
63.502
49.131
13.938
EtO2C
Ph
NH
O
S
O
O
9
f1 (ppm)
f1 (ppm)

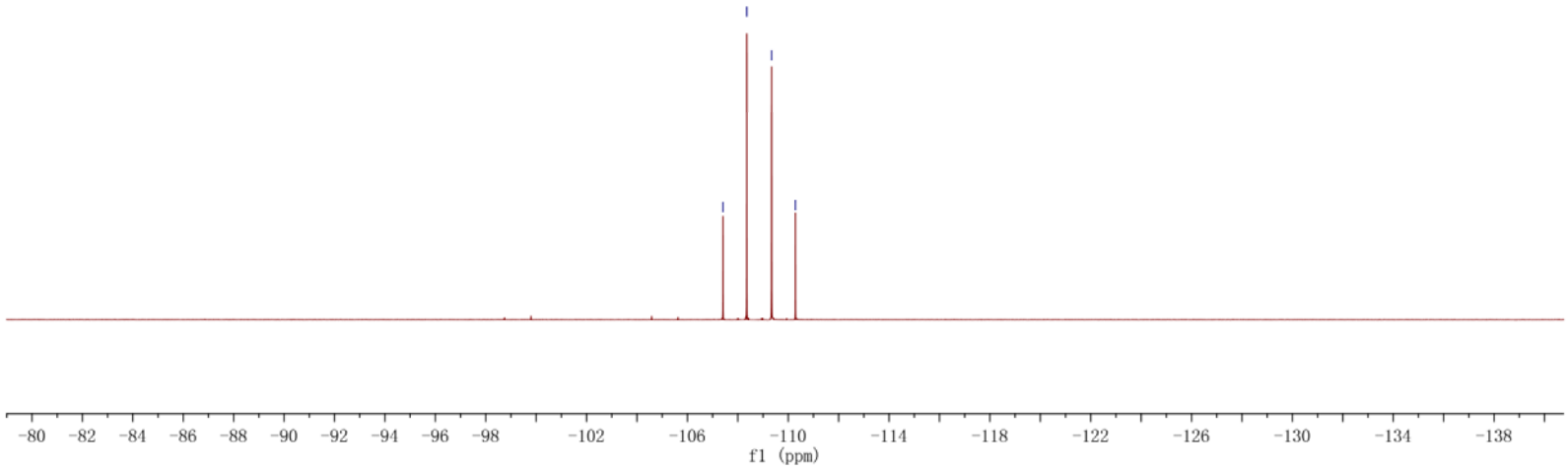

7.844
7.826
7.763
7.759
7.744
7.740
7.734
7.730
7.715
7.712
7.260
7.069
7.063
7.051
7.046
7.037
6.886
6.880
6.868
6.863
4.493
4.475
4.466
4.457
4.448
4.439
4.430
4.422
4.413
4.404
4.395
4.386
4.377
4.359
3.782
1.391
1.373
1.355
0.000
8.028
8.025
8.007
7.844
7.842
7.840
7.826
7.823
7.781
7.778
7.763
7.759
7.744
7.740
7.734
7.730
7.715
7.712
7.078
7.069
7.063
7.057
7.051
7.046
7.037
6.895
6.886
6.880
6.868
6.863
6.854
1.01
1.00
2.07
2.01
2.04
f1 (ppm)
1.01
1.00
2.07
2.01
2.04
1.00
2.06
3.06
3.07
f1 (ppm)
EtO2C
F
F
O
NH
O
S
O
O
OMe
6

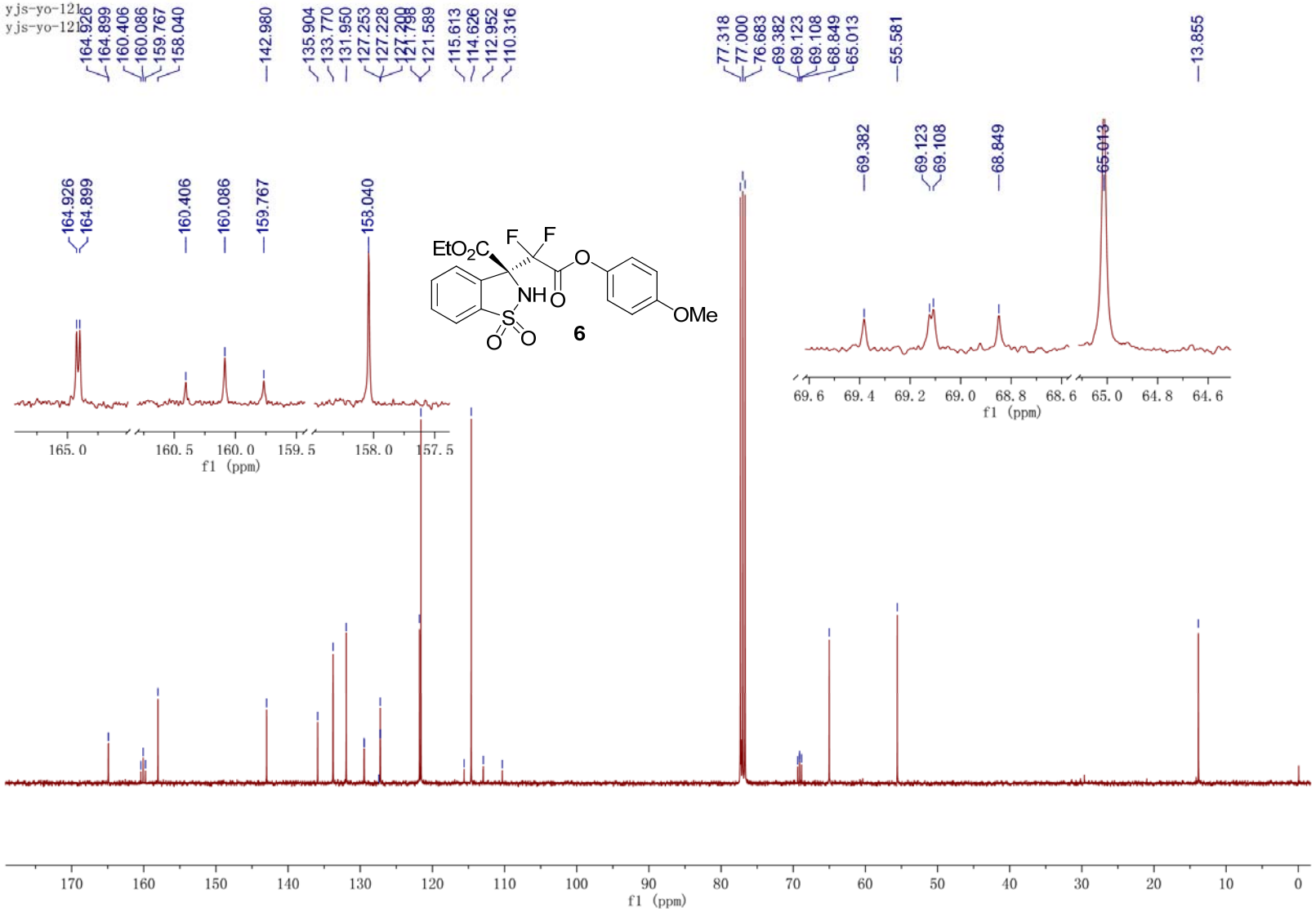
yjs-yo-121
yjs-yo-121

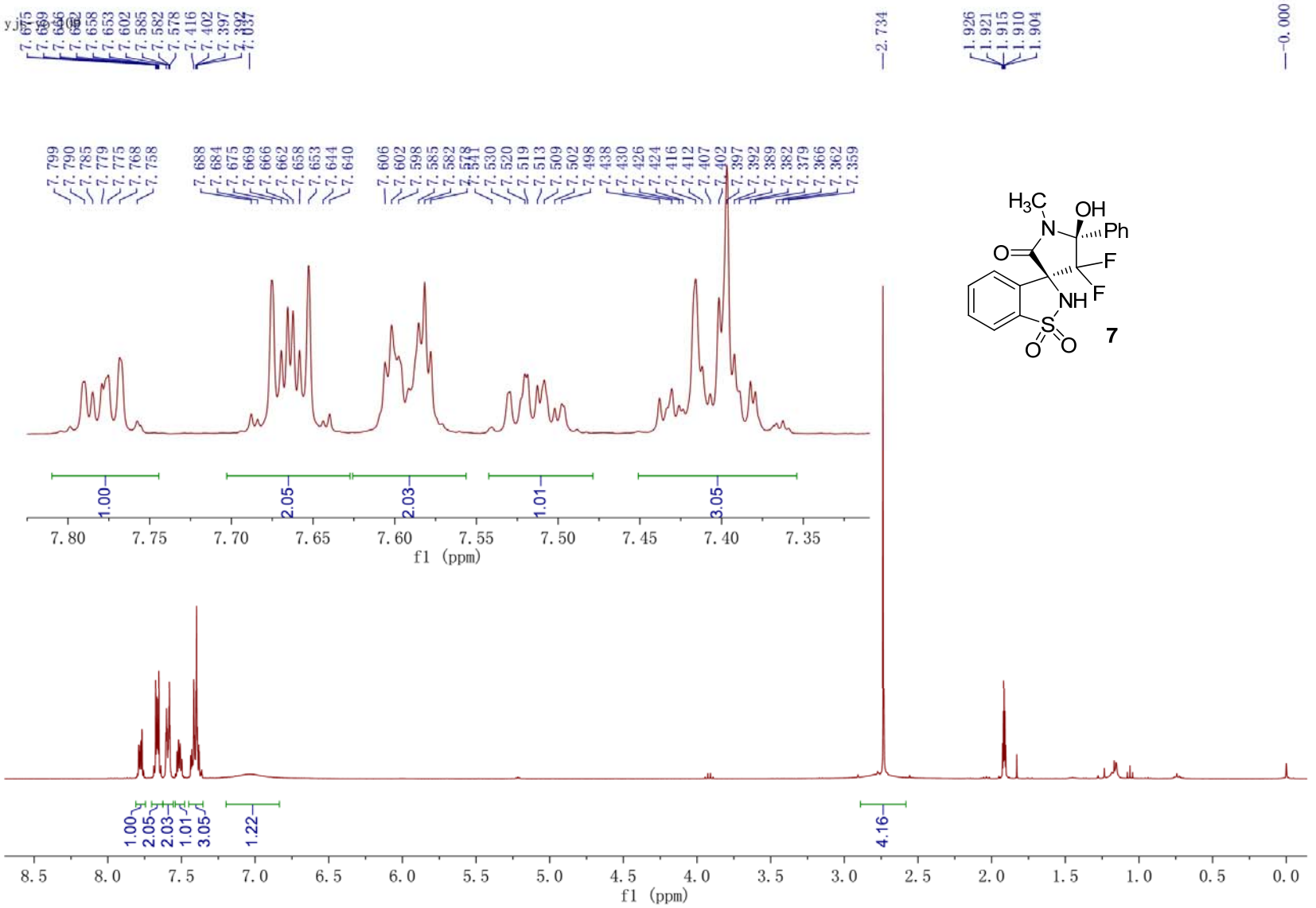
-107.411
-108.354
-109.340
-110.283

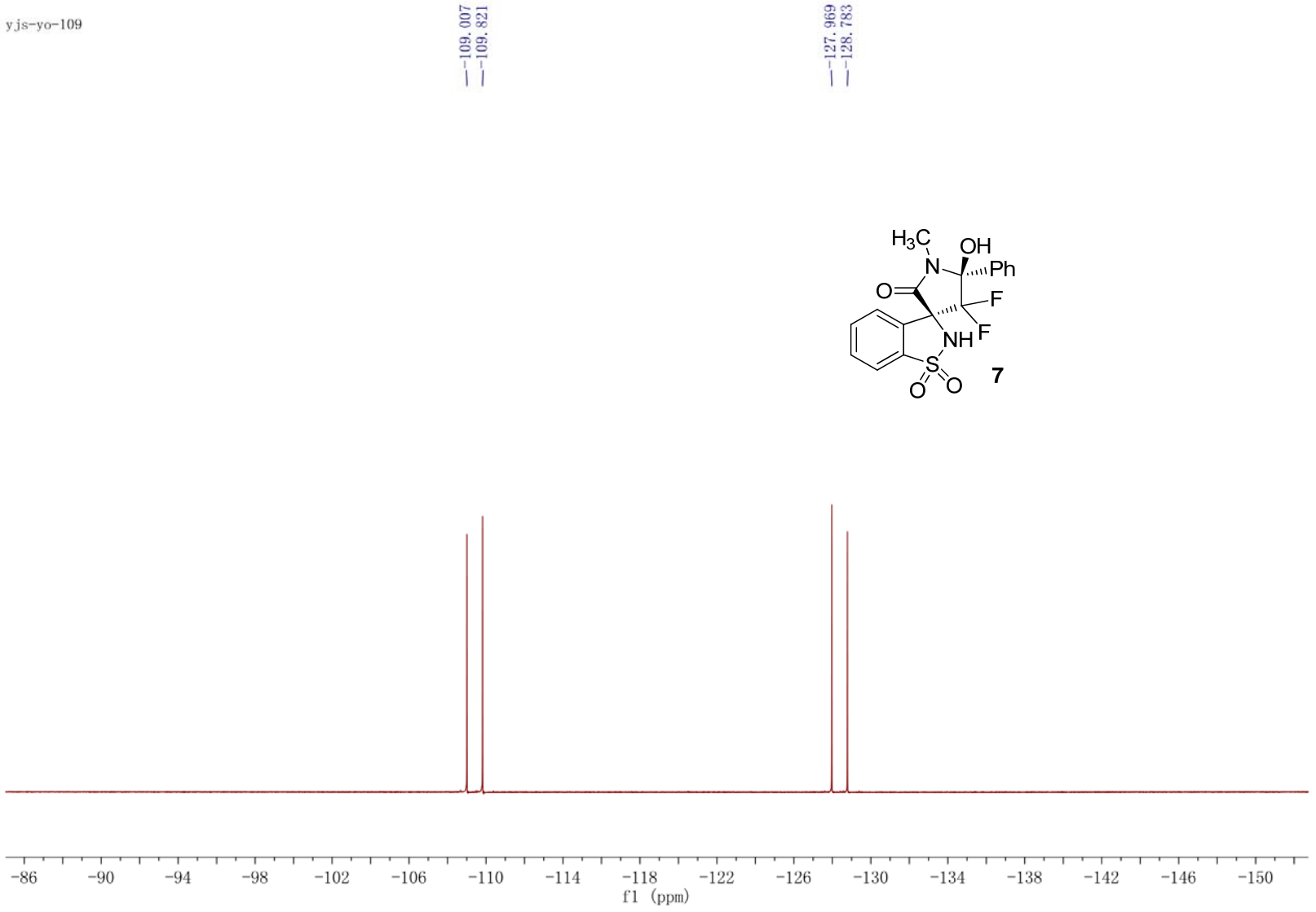


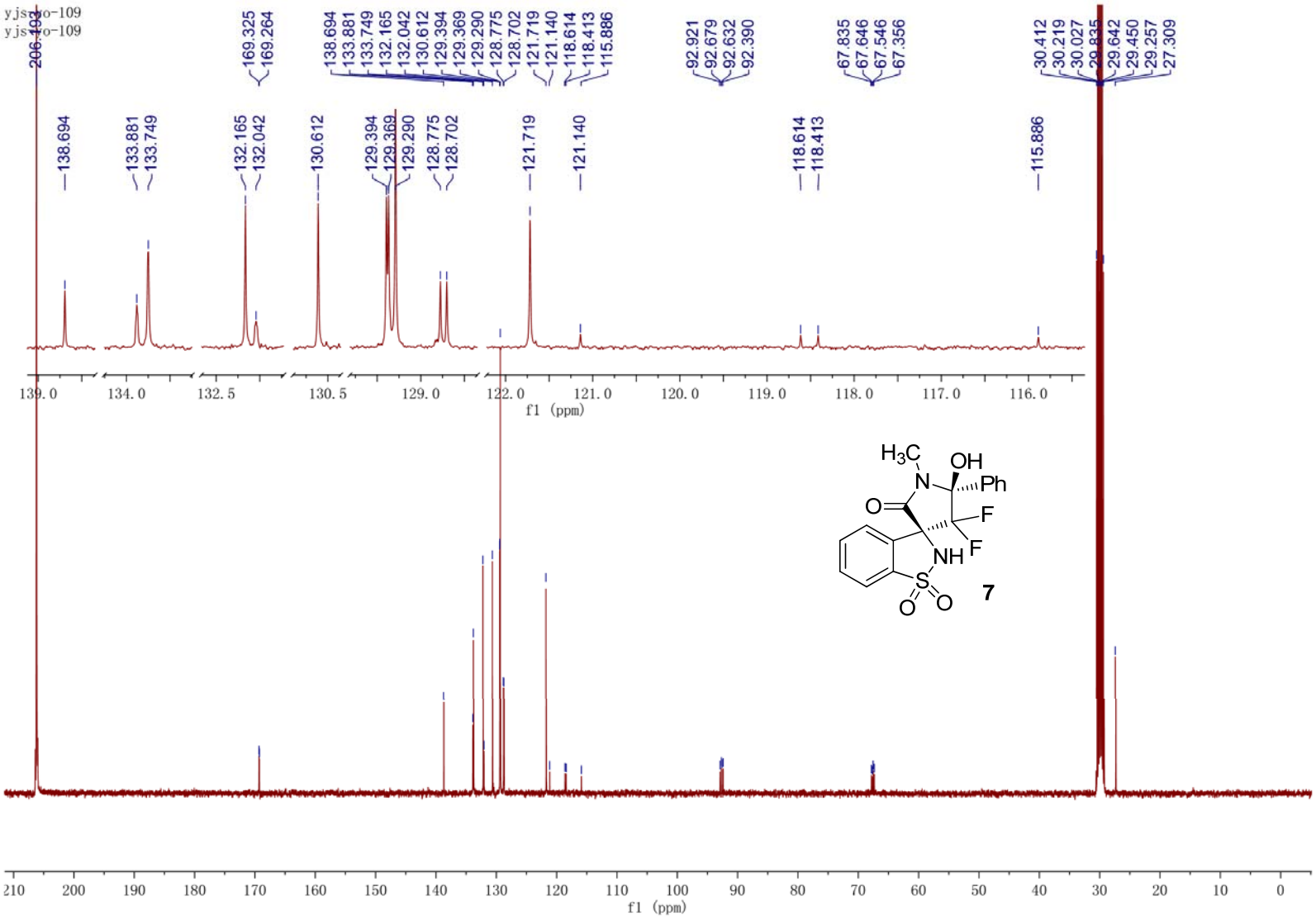
6




yjs-yo-121
yjs-yo-121
164.926
164.899
160.406
160.086
159.767
158.040
142.980
135.904
133.770
131.950
127.253
127.228
121.589
115.613
114.626
112.952
110.316
77.318
77.000
76.683
69.382
69.123
69.108
68.849
65.013
55.581
13.855
EtO2C
F
F
O
NH
O
S
O
O
OMe
6
f1 (ppm)


7.799
7.790
7.785
7.779
7.775
7.768
7.758
7.688
7.684
7.675
7.669
7.666
7.662
7.658
7.653
7.644
7.640
7.606
7.602
7.598
7.585
7.582
7.541
7.530
7.520
7.519
7.513
7.509
7.502
7.498
7.438
7.430
7.426
7.424
7.416
7.412
7.407
7.402
7.397
7.392
7.389
7.382
7.379
7.366
7.362
7.359
2.734
1.926
1.921
1.915
1.910
1.904
0.000
1.00
2.05
2.03
1.01
3.05
1.22
4.16
f1 (ppm)
H3C
N
OH
Ph
O
F
NH
F
S
O
O
7


yjs-yo-109
-109.007
-109.821
-127.969
-128.783
H3C
N
OH
Ph
O
F
F
NH
S
O
O
7
-86
-90
-94
-98
-102
-106
-110
-114
-118
-122
-126
-130
-134
-138
-142
-146
-150
f1 (ppm)


yjs-fo-109
yjs-fo-109
206.103
169.325
169.264
138.694
133.881
133.749
132.165
132.042
130.612
129.394
129.369
129.290
128.775
128.702
121.719
121.140
118.614
118.413
115.886
92.921
92.679
92.632
92.390
67.835
67.646
67.546
67.356
30.412
30.219
30.027
29.835
29.642
29.450
29.257
27.309
f1 (ppm)
f1 (ppm)
H3C
N
OH
Ph
O
F
F
NH
S
O
O
7

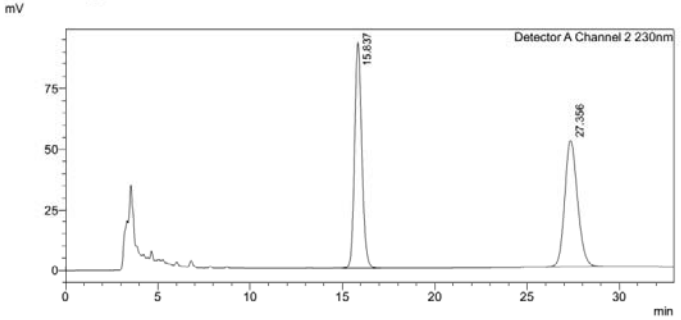
SHIMADZU LabSolutions

Analysis Report

<Sample Information>

Sample Name	: yjs-yn-30		
Sample ID	:		
Data Filename	: yjs-yo-25-rac-ADH-60-40-1.0-30oC.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/6/22 15:14:37	Acquired by	: System Administrator
Date Processed	: 2015/6/22 15:48:08	Processed by	: System Administrator

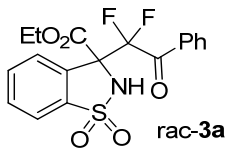
<Chromatogram>



<Peak Table>

Detector A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	15.837	2517679	92795	50.092
2	27.356	2508408	52185	49.908
Total		5026087	144980	



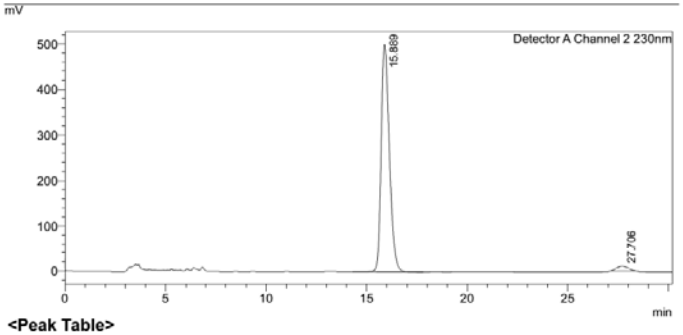
rac-**3a**

Analysis Report

<Sample Information>

Sample Name	: yjs-yo-25-asy		
Sample ID	:		
Data Filename	: yjs-yo-25-asy-ADH-60-40-1.0-30oC.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/6/22 14:12:51	Acquired by	: System Administrator
Date Processed	: 2015/6/22 14:43:03	Processed by	: System Administrator

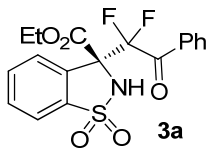
<Chromatogram>



<Peak Table>

Detector A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	15.889	14189785	501101	96.596
2	27.706	500114	11684	3.404
Total		14689899	512785	



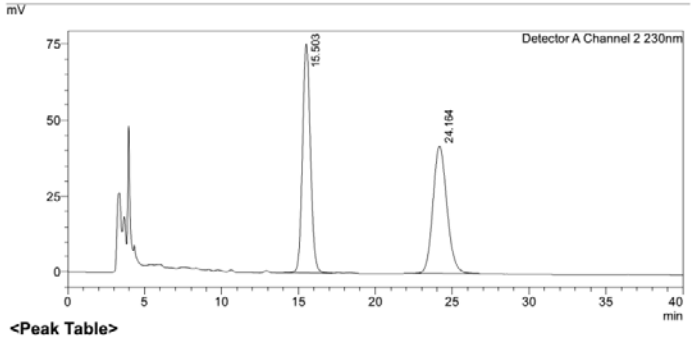
3a

Analysis Report

<Sample Information>

Sample Name	: yjs-yo-43-3		
Sample ID	:		
Data Filename	: yjs-yo-43-3-rac-ASH-60-40-1.0-70.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/6/25 11:30:16	Acquired by	: System Administrator
Date Processed	: 2015/6/26 21:43:00	Processed by	: System Administrator

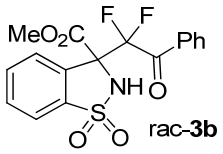
<Chromatogram>



<Peak Table>

Detector A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	15.503	2709441	75392	50.230
2	24.164	2684642	42183	49.770
Total		5394083	117575	



rac-**3b**

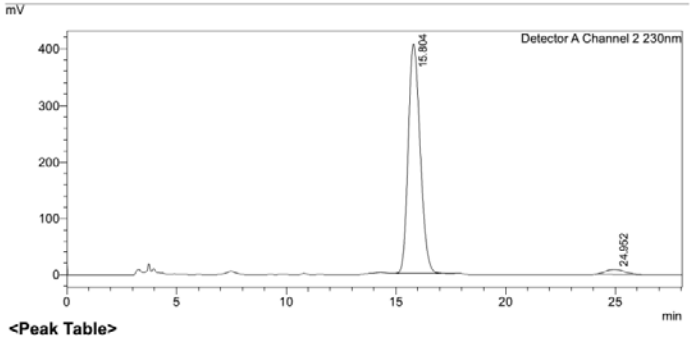
D:\Data\yujinsheng\yjs-yo-43-3-rac-ASH-60-40-1.0-70.lcd

Analysis Report

<Sample Information>

Sample Name	: yjs-yo-41		
Sample ID	:		
Data Filename	: yjs-yo-41-asy-ASH-60-40-1.0-30 oC.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/6/26 21:57:09	Acquired by	: System Administrator
Date Processed	: 2015/6/26 22:27:20	Processed by	: System Administrator

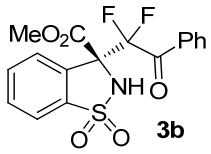
<Chromatogram>



<Peak Table>

Detector A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	15.804	15457782	406497	96.866
2	24.952	500079	8526	3.134
Total		15957861	415023	



3b

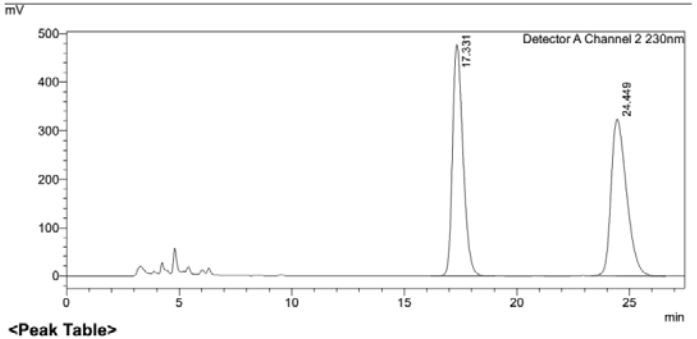
D:\Data\yujinsheng\yjs-yo-41-asy-ASH-60-40-1.0-30 oC.lcd

Analysis Report

<Sample Information>

Sample Name	: yjs-yn-40		
Sample ID	:		
Data Filename	: yjs-yo-33-rac-ADH--60-40-1.0-30oC.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/6/22 21:39:23	Acquired by	: System Administrator
Date Processed	: 2015/6/22 22:08:13	Processed by	: System Administrator

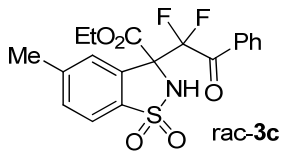
<Chromatogram>



<Peak Table>

Detector A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	17.331	15434406	477606	49.971
2	24.449	15452284	323224	50.029
Total		30886690	800831	



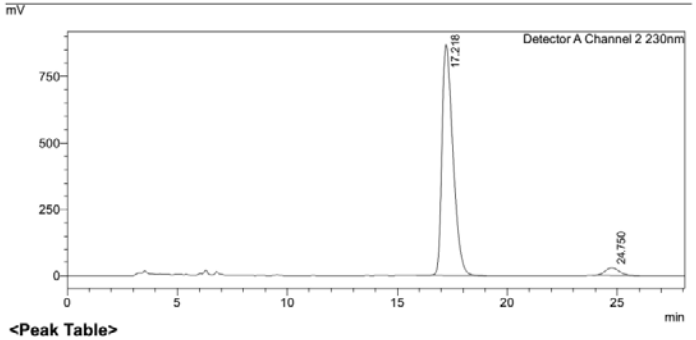
rac-**3c**

Analysis Report

<Sample Information>

Sample Name	: yjs-yo-33		
Sample ID	:		
Data Filename	: yjs-yo-33-asy-ADH-60-40-1.0-30oC.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/6/22 20:40:58	Acquired by	: System Administrator
Date Processed	: 2015/6/22 22:08:44	Processed by	: System Administrator

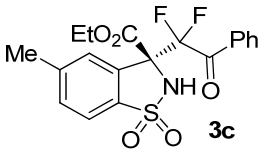
<Chromatogram>



<Peak Table>

Detector A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	17.218	30199480	869152	96.011
2	24.750	1254561	28816	3.989
Total		31454041	897968	



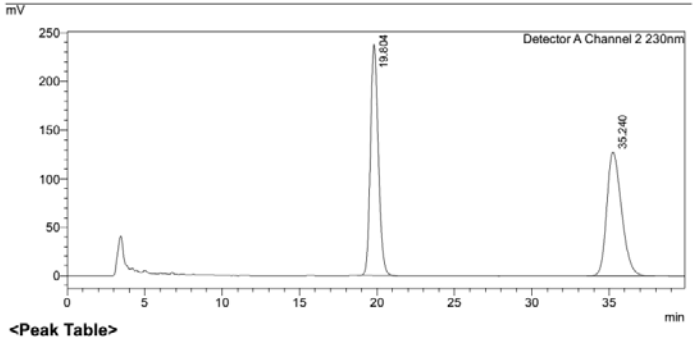
3c

Analysis Report

<Sample Information>

Sample Name	: yjs-yn-34		
Sample ID	:		
Data Filename	: yjs-yo-37--rac-ADH-60-40-1.0-30 oC.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/6/25 17:32:20	Acquired by	: System Administrator
Date Processed	: 2015/6/25 18:12:30	Processed by	: System Administrator

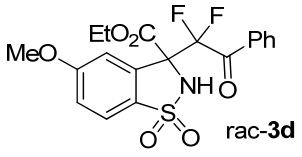
<Chromatogram>



<Peak Table>

Detector A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	19.804	8453927	237919	49.964
2	35.240	8466108	127806	50.036
Total		16920035	365725	



rac-**3d**

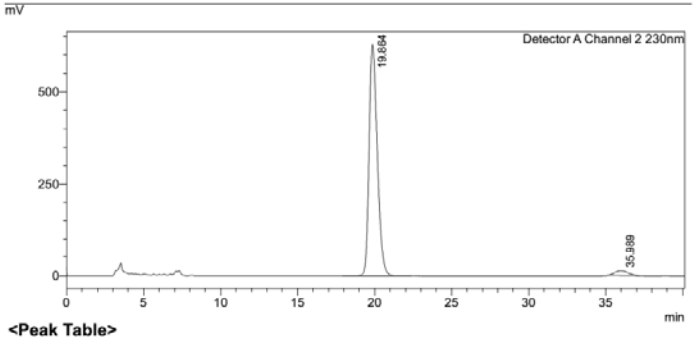
D:\Data\yujinsheng\yjs-yo-37--rac-ADH-60-40-1.0-30 oC.lcd

Analysis Report

<Sample Information>

Sample Name	: yjs-yo-37		
Sample ID	:		
Data Filename	: yjs-yo-37-asy-ADH-60-40-1.0-30 oC.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/6/25 16:11:57	Acquired by	: System Administrator
Date Processed	: 2015/6/25 18:13:33	Processed by	: System Administrator

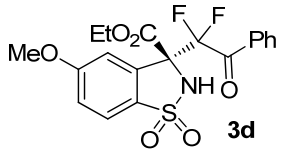
<Chromatogram>



<Peak Table>

Detector A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	19.864	23289963	627917	96.860
2	35.989	755040	12787	3.140
Total		24045003	640704	



3d

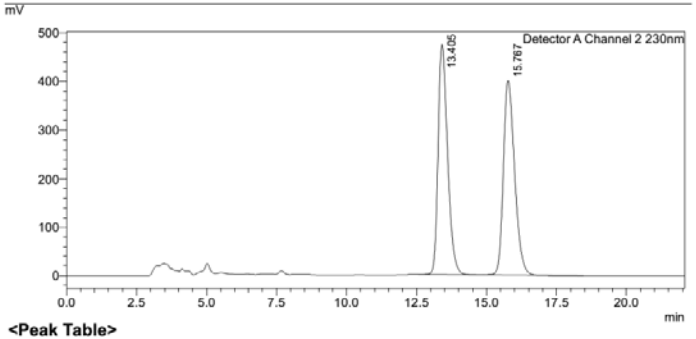
D:\Data\yujinsheng\yjs-yo-37-asy-ADH-60-40-1.0-30 oC.lcd

Analysis Report

<Sample Information>

Sample Name	: yjs-yo-43-2		
Sample ID	:		
Data Filename	: yjs-yo-43-2-rac-ADH-75-25-1.0.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/6/23 21:25:08	Acquired by	: System Administrator
Date Processed	: 2015/6/26 21:42:37	Processed by	: System Administrator

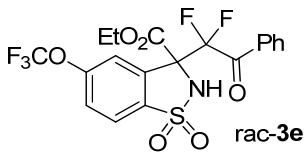
<Chromatogram>



<Peak Table>

Detector A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	13.405	11208005	474205	50.026
2	15.767	11196186	400511	49.974
Total		22404191	874716	



rac-**3e**

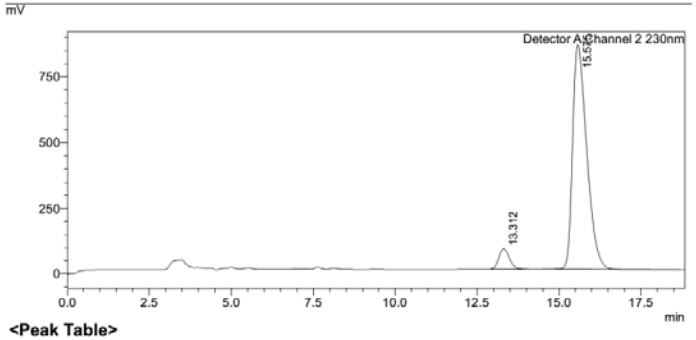
D:\Data\yujinsheng\yjs-yo-43-2-rac-ADH-75-25-1.0.lcd

Analysis Report

<Sample Information>

Sample Name	: yjs-yo-42		
Sample ID	:		
Data Filename	: yjs-yo-42-asy-ADH-75-25-1.0-30 oC.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/6/26 22:31:59	Acquired by	: System Administrator
Date Processed	: 2015/6/27 9:15:39	Processed by	: System Administrator

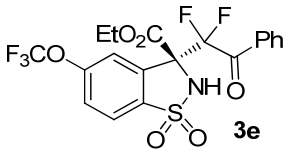
<Chromatogram>



<Peak Table>

Detector A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	13.312	1750365	80354	6.390
2	15.575	25642720	856595	93.610
Total		27393085	936949	



3e

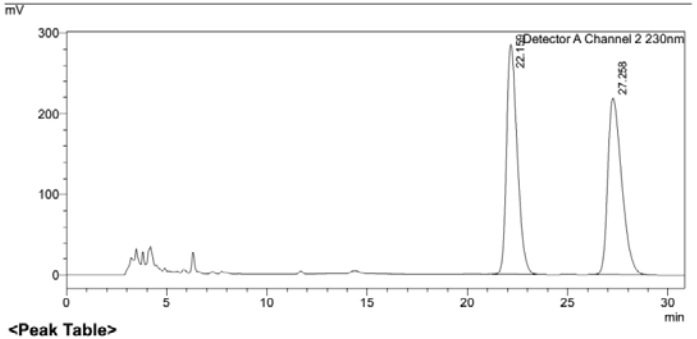
D:\Data\yujinsheng\yjs-yo-42-asy-ADH-75-25-1.0-30 oC.lcd

Analysis Report

<Sample Information>

Sample Name	: yjs-yo-43-1		
Sample ID	:		
Data Filename	: yjs-yo-36-rac-ADH-75-25-1.0-30 oC.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/6/25 20:09:06	Acquired by	: System Administrator
Date Processed	: 2015/6/25 20:40:31	Processed by	: System Administrator

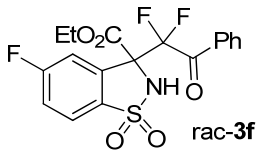
<Chromatogram>



<Peak Table>

Detector A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	22.159	10615291	285524	49.932
2	27.258	10644142	219800	50.068
Total		21259433	505324	



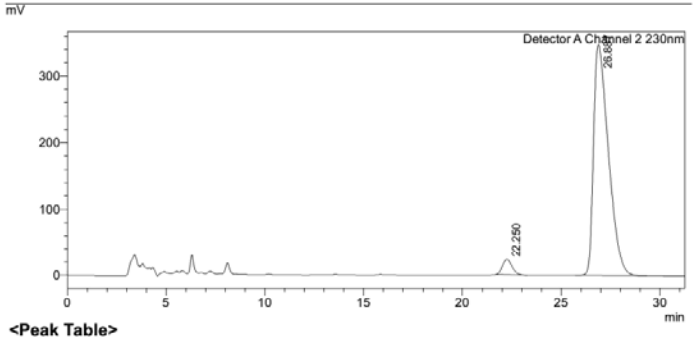
rac-**3f**

Analysis Report

<Sample Information>

Sample Name	: yjs-yo-36		
Sample ID	:		
Data Filename	: yjs-yo-36-asy-ADH-75-25-1.0-30 oC.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/6/25 19:36:24	Acquired by	: System Administrator
Date Processed	: 2015/6/25 20:39:51	Processed by	: System Administrator

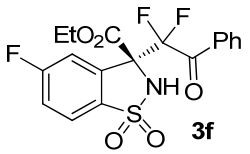
<Chromatogram>



<Peak Table>

Detector A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	22.250	797797	23337	4.193
2	26.887	18230562	348156	95.807
Total		19028359	371493	



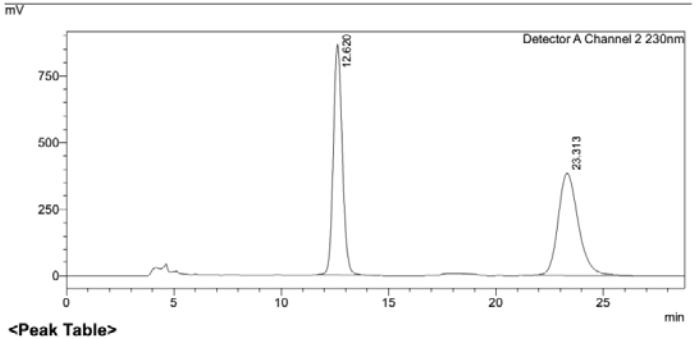
3f

Analysis Report

<Sample Information>

Sample Name	: yjs-yn-35		
Sample ID	:		
Data Filename	: yjs-yo-32--rac-ASH--60-40-0.8-30oC.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/6/23 9:41:28	Acquired by	: System Administrator
Date Processed	: 2015/6/23 10:10:16	Processed by	: System Administrator

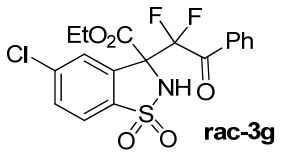
<Chromatogram>



<Peak Table>

Detector A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	12.620	25316656	866379	50.164
2	23.313	25151586	385830	49.836
Total		50468242	1252209	



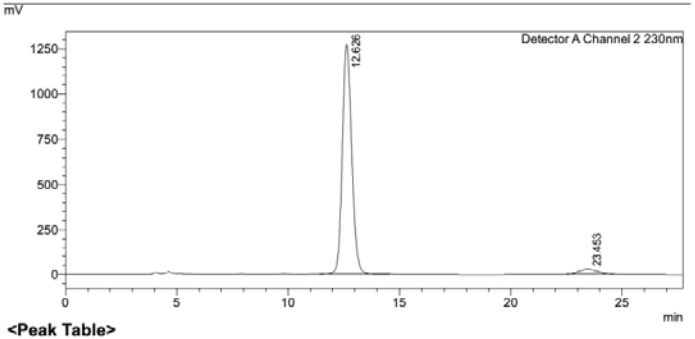
rac-3g

Analysis Report

<Sample Information>

Sample Name	: yjs-yo-32		
Sample ID	:		
Data Filename	: yjs-yo-32-asy-ASH--60-40-0.8-30oC.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/6/23 9:13:00	Acquired by	: System Administrator
Date Processed	: 2015/6/23 10:12:37	Processed by	: System Administrator

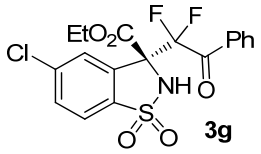
<Chromatogram>



<Peak Table>

Detector A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	12.626	37455266	1271889	95.879
2	23.453	1609983	27173	4.121
Total		39065249	1299062	



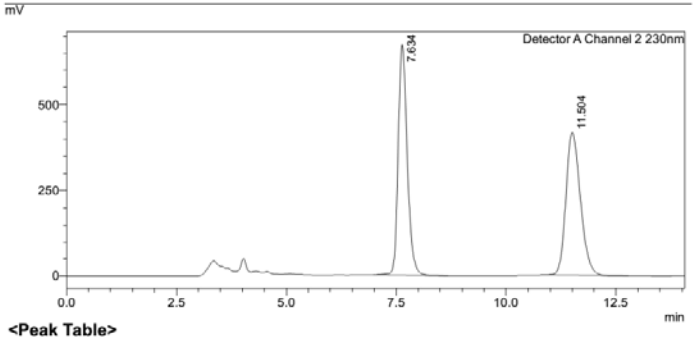
3g

Analysis Report

<Sample Information>

Sample Name	: yjs-yo-46-2		
Sample ID	:		
Data Filename	: yjs-yo-46-2-rac-ADH-60-40-1.0-60.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/6/25 11:06:31	Acquired by	: System Administrator
Date Processed	: 2015/6/25 11:20:36	Processed by	: System Administrator

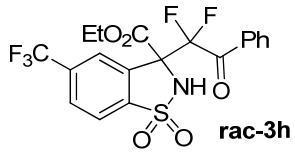
<Chromatogram>



<Peak Table>

Detector A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	7.634	9667010	673767	50.049
2	11.504	9648148	418082	49.951
Total		19315158	1091849	



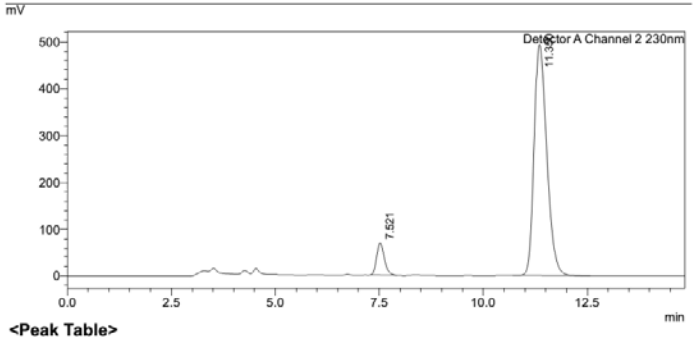
rac-3h

Analysis Report

<Sample Information>

Sample Name	: yjs-yo-48		
Sample ID	:		
Data Filename	: yjs-yo-48--asy-ADH-60-40-1.0.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/6/30 20:10:35	Acquired by	: System Administrator
Date Processed	: 2015/6/30 20:25:50	Processed by	: System Administrator

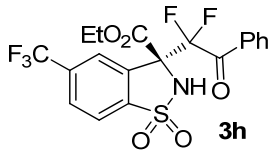
<Chromatogram>



<Peak Table>

Detector A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	7.521	901964	70145	7.934
2	11.350	10467027	493775	92.066
Total		11368991	563921	



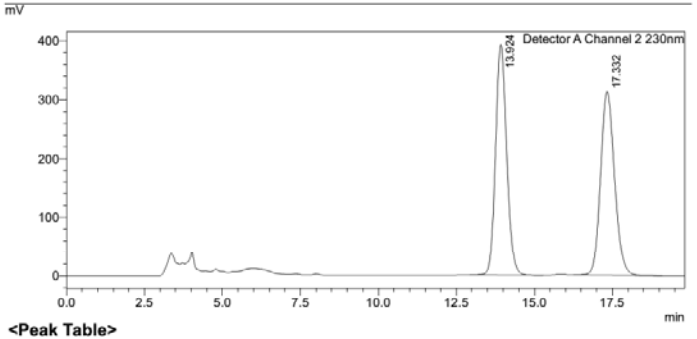
3h

Analysis Report

<Sample Information>

Sample Name	: yjs-yo-46-1		
Sample ID	:		
Data Filename	: yjs-yo-46-1-rac-ADH-60-40-1.0-60.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/6/25 10:45:55	Acquired by	: System Administrator
Date Processed	: 2015/6/30 17:26:55	Processed by	: System Administrator

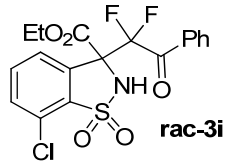
<Chromatogram>



<Peak Table>

Detector A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	13.924	9771498	393230	49.985
2	17.332	9777276	312655	50.015
Total		19548774	705885	



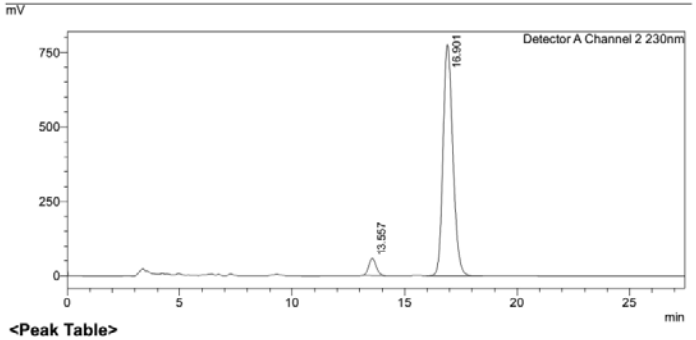
rac-3i

Analysis Report

<Sample Information>

Sample Name	: yjs-yo-47		
Sample ID	:		
Data Filename	: yjs-yo-47-asy-ADH-60-40-1.0.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/6/30 16:58:48	Acquired by	: System Administrator
Date Processed	: 2015/7/9 21:36:38	Processed by	: System Administrator

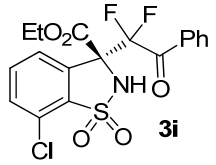
<Chromatogram>



<Peak Table>

Detector A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	13.557	1298862	57048	5.217
2	16.901	23599005	776097	94.783
Total		24897867	833145	



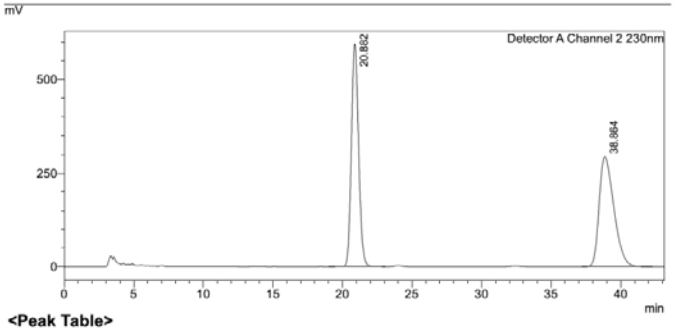
3i

Analysis Report

<Sample Information>

Sample Name	: yjs-yn-57		
Sample ID	:		
Data Filename	: yjs-yo-61-rac-ADH-60-40-1.0-30oC.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/7/9 21:12:20	Acquired by	: System Administrator
Date Processed	: 2015/7/9 21:55:29	Processed by	: System Administrator

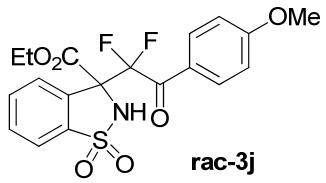
<Chromatogram>



<Peak Table>

Detector A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	20.882	21423891	594982	49.824
2	38.864	21575096	294442	50.176
Total		42998987	889424	



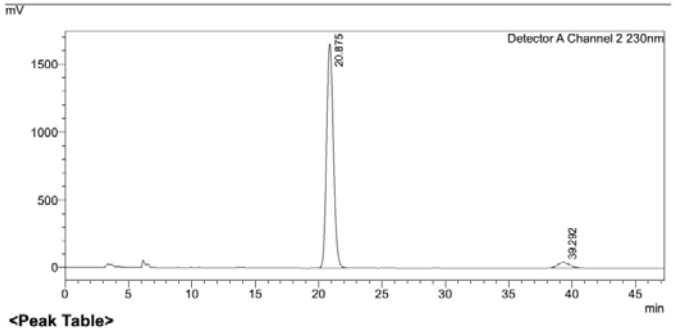
rac-3j

Analysis Report

<Sample Information>

Sample Name	: yjs-yo-61-asy		
Sample ID	:		
Data Filename	: yjs-yo-61-asy-ADH-60-40-1.0-30oC.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/7/9 20:23:51	Acquired by	: System Administrator
Date Processed	: 2015/7/9 21:37:26	Processed by	: System Administrator

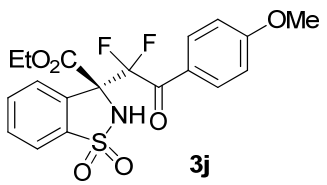
<Chromatogram>



<Peak Table>

Detector A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	20.875	61811330	1653485	95.966
2	39.292	2598302	39762	4.034
Total		64409633	1693247	



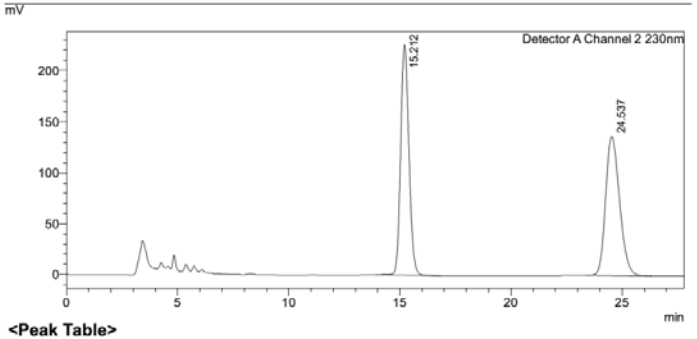
3j

Analysis Report

<Sample Information>

Sample Name	: yjs-yn-85		
Sample ID	:		
Data Filename	: yjs-yo-52-rac--60-40-1.0-30oC.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/7/4 18:05:26	Acquired by	: System Administrator
Date Processed	: 2015/7/4 18:33:16	Processed by	: System Administrator

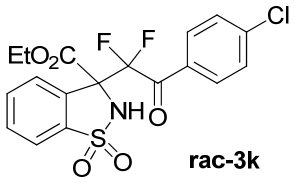
<Chromatogram>



<Peak Table>

Detector A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	15.212	5859055	226137	49.623
2	24.537	5948123	136741	50.377
Total		11807178	362878	



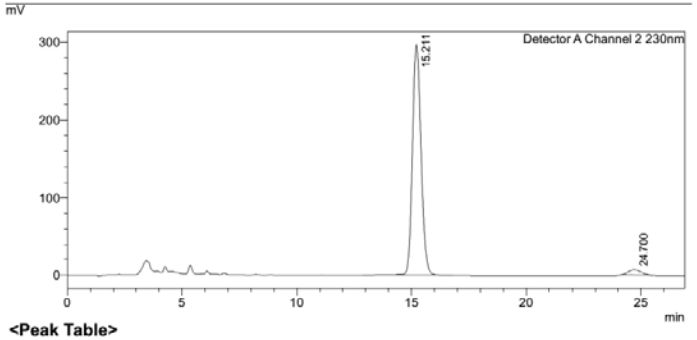
rac-3k

Analysis Report

<Sample Information>

Sample Name	: yjs-yo-52		
Sample ID	:		
Data Filename	: yjs-yo-52-asy-60-40-1.0-30oC.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/7/4 16:57:53	Acquired by	: System Administrator
Date Processed	: 2015/7/4 18:06:44	Processed by	: System Administrator

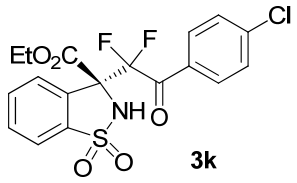
<Chromatogram>



<Peak Table>

Detector A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	15.211	7773930	297027	96.523
2	24.700	280048	7143	3.477
Total		8053979	304170	



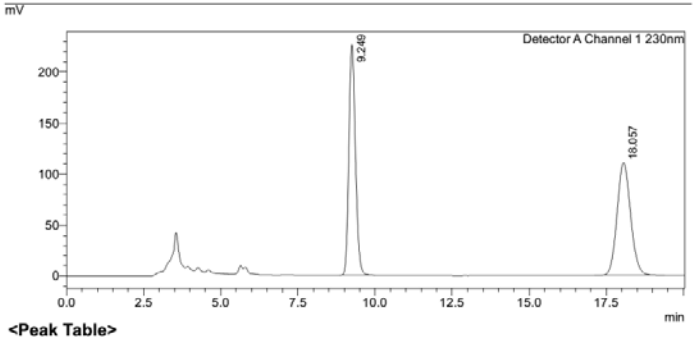
3k

Analysis Report

<Sample Information>

Sample Name	: yjs-yo-83-1		
Sample ID	:		
Data Filename	: yjs-yo-83-1-rac-ADH-60-40-1.0-30oC.lcd		
Method Filename	: 2.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/7/30 16:06:37	Acquired by	: System Administrator
Date Processed	: 2015/8/25 10:00:02	Processed by	: System Administrator

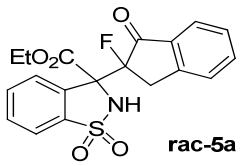
<Chromatogram>



<Peak Table>

Detector A Channel 1 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	9.249	3371490	226353	49.851
2	18.057	3391588	110938	50.149
Total		6763079	337290	



rac-5a

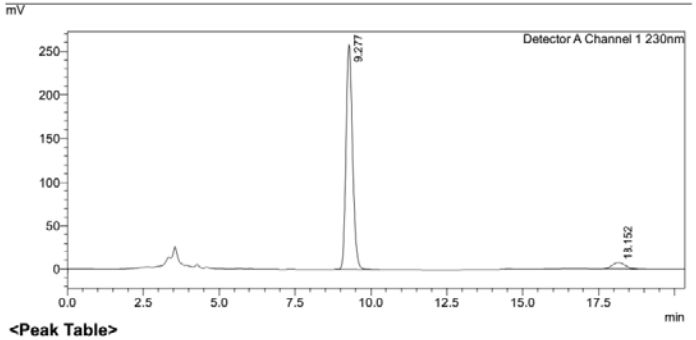
D:\Data\yujinsheng\yjs-yo-83-1-rac-ADH-60-40-1.0-30oC.lcd

Analysis Report

<Sample Information>

Sample Name	: yjs-yo-85		
Sample ID	:		
Data Filename	: yjs-yo-85-asy-ADH-60-40-1.0-30oC.lcd		
Method Filename	: 2.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/7/30 15:02:32	Acquired by	: System Administrator
Date Processed	: 2015/7/30 15:25:17	Processed by	: System Administrator

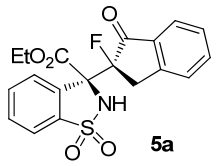
<Chromatogram>



<Peak Table>

Detector A Channel 1 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	9.277	3879831	258240	94.844
2	18.152	210935	7296	5.156
Total		4090766	265536	



5a

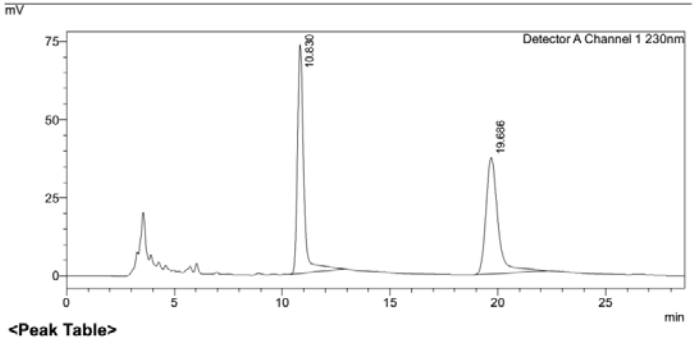
D:\Data\yujinsheng\yjs-yo-85-asy-ADH-60-40-1.0-30oC.lcd

Analysis Report

<Sample Information>

Sample Name	: yjs-yo-83-3		
Sample ID	:		
Data Filename	: yjs-yo-90-RAC-ADH-60-40-1.0-30oC.lcd		
Method Filename	: 2.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/8/6 10:48:00	Acquired by	: System Administrator
Date Processed	: 2015/8/25 9:59:10	Processed by	: System Administrator

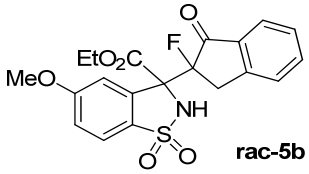
<Chromatogram>



<Peak Table>

Detector A Channel 1 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	10.830	1502076	73446	50.709
2	19.686	1460067	37446	49.291
Total		2962143	110892	



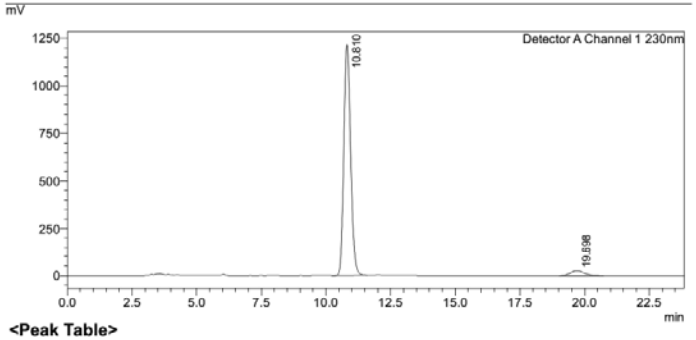
rac-5b

Analysis Report

<Sample Information>

Sample Name	: yjs-yo-90		
Sample ID	:		
Data Filename	: yjs-yo-90-asy-ADH-60-40-1.0-30oC.lcd		
Method Filename	: 2.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/8/6 10:22:41	Acquired by	: System Administrator
Date Processed	: 2015/8/25 9:59:13	Processed by	: System Administrator

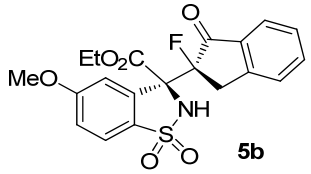
<Chromatogram>



<Peak Table>

Detector A Channel 1 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	10.810	22298635	1216664	96.209
2	19.698	878665	25067	3.791
Total		23177300	1241731	



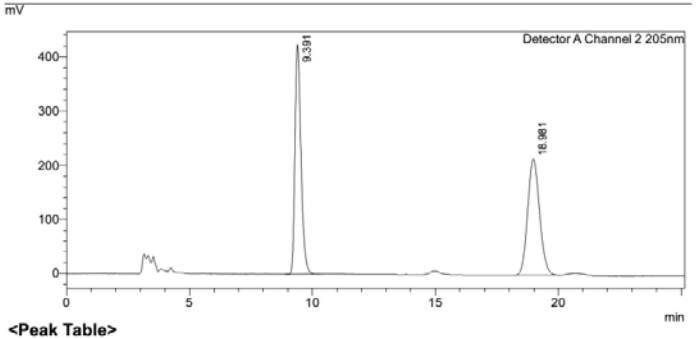
5b

Analysis Report

<Sample Information>

Sample Name	: yjs-yo-77 rac		
Sample ID	:		
Data Filename	: yjs-yo-73-2-rac-ADH-60-40-1.0-30 oC.lcd		
Method Filename	: 2.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/7/23 15:23:01	Acquired by	: System Administrator
Date Processed	: 2015/8/6 10:25:58	Processed by	: System Administrator

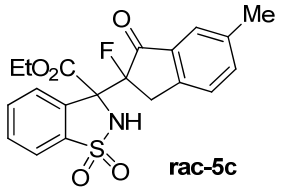
<Chromatogram>



<Peak Table>

Detector A Channel 2 205nm

Peak#	Ret. Time	Area	Height	Conc.
1	9.391	7230600	424102	49.913
2	18.981	7255720	215574	50.087
Total		14486319	639676	



rac-5c

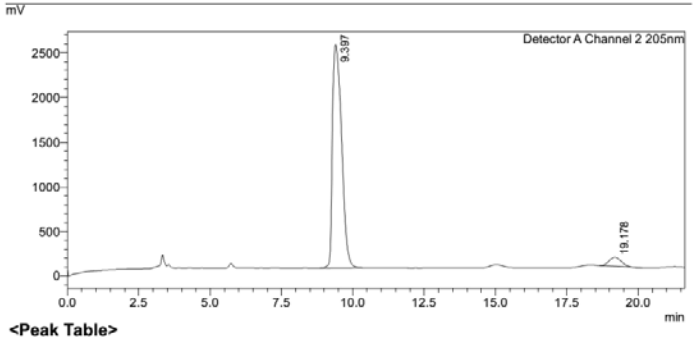
D:\Data\yujinsheng\yjs-yo-73-2-rac-ADH-60-40-1.0-30 oC.lcd

Analysis Report

<Sample Information>

Sample Name	: yjs-yo-89		
Sample ID	:		
Data Filename	: yjs-yo-89-asy-ADH-60-40-1.0-30oC.lcd		
Method Filename	: 2.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/8/6 9:59:31	Acquired by	: System Administrator
Date Processed	: 2015/8/25 9:59:36	Processed by	: System Administrator

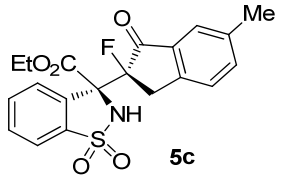
<Chromatogram>



<Peak Table>

Detector A Channel 2 205nm

Peak#	Ret. Time	Area	Height	Conc.
1	9.397	55903166	2503747	94.935
2	19.178	2982657	100253	5.065
Total		58885823	2604000	



5c

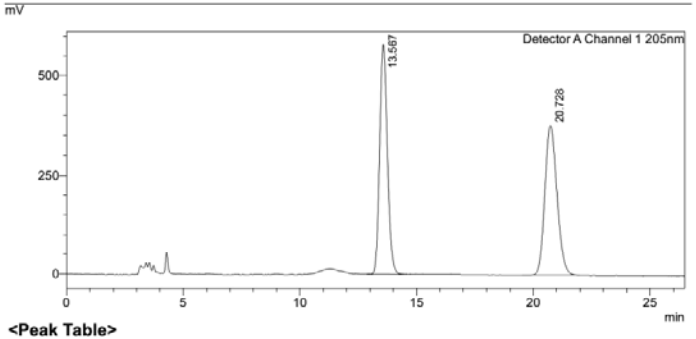
D:\Data\yujinsheng\yjs-yo-89-asy-ADH-60-40-1.0-30oC.lcd

Analysis Report

<Sample Information>

Sample Name	: yjs-yo-121-rac		
Sample ID	:		
Data Filename	: yjs-yo-125-rac-ADH-60-40-1.0-30oC.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/9/23 11:25:04	Acquired by	: System Administrator
Date Processed	: 2015/9/23 11:51:35	Processed by	: System Administrator

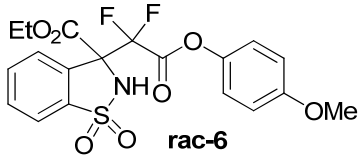
<Chromatogram>



<Peak Table>

Detector A Channel 1 205nm

Peak#	Ret. Time	Area	Height	Conc.
1	13.567	13431145	580226	49.409
2	20.728	13752328	378549	50.591
Total		27183472	958775	



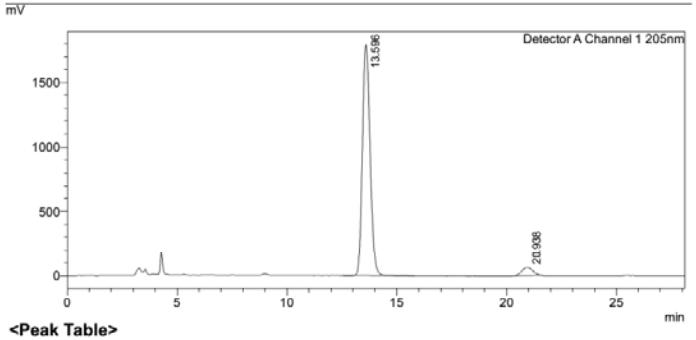
rac-6

Analysis Report

<Sample Information>

Sample Name	: yjs-yo-125-asy		
Sample ID	:		
Data Filename	: yjs-yo-125-asy-ADH-60-40-1.0-30oC.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/9/22 21:22:09	Acquired by	: System Administrator
Date Processed	: 2015/9/22 21:52:34	Processed by	: System Administrator

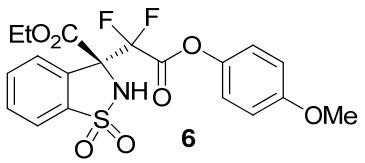
<Chromatogram>



<Peak Table>

Detector A Channel 1 205nm

Peak#	Ret. Time	Area	Height	Conc.
1	13.596	43672025	1794141	95.297
2	20.938	2155129	63613	4.703
Total		45827154	1857754	



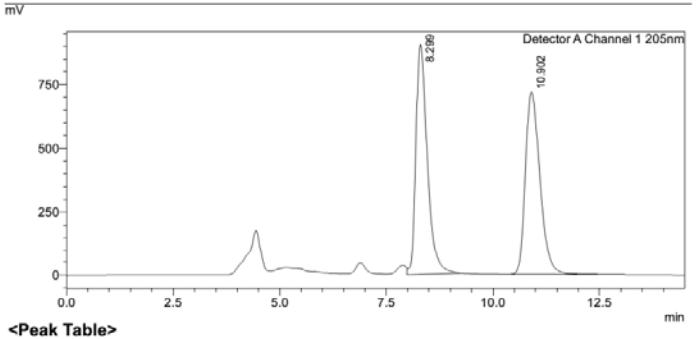
6

Analysis Report

<Sample Information>

Sample Name	: yjs-yo-109-rac-60-40-0.8		
Sample ID	:		
Data Filename	: yjs-yo-93--rac--ADH-60-40-0.8-230.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/9/10 15:51:13	Acquired by	: System Administrator
Date Processed	: 2015/9/10 16:06:33	Processed by	: System Administrator

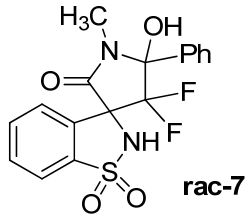
<Chromatogram>



<Peak Table>

Detector A Channel 1 205nm

Peak#	Ret. Time	Area	Height	Conc.
1	8.299	16951251	905067	49.700
2	10.902	17155762	717750	50.300
Total		34107013	1622817	



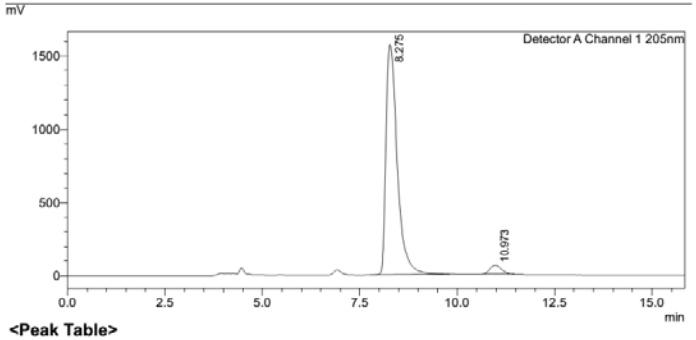
rac-7

Analysis Report

<Sample Information>

Sample Name	: yjs-yo-109-asy-60-40-0.8		
Sample ID	:		
Data Filename	: yjs-yo-109-asy--ADH-60-40-0.8-230.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/9/10 16:09:27	Acquired by	: System Administrator
Date Processed	: 2015/9/10 16:25:17	Processed by	: System Administrator

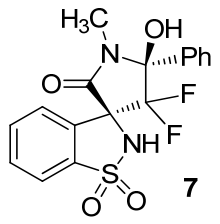
<Chromatogram>



<Peak Table>

Detector A Channel 1 205nm

Peak#	Ret. Time	Area	Height	Conc.
1	8.275	31826783	1573605	96.144
2	10.973	1276561	60770	3.856
Total		33103344	1634375	



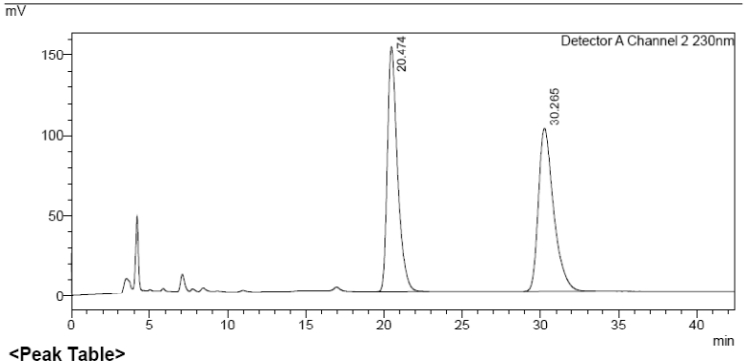
7

Analysis Report

<Sample Information>

Sample Name	: yjs-yo-36-rac		
Sample ID	:		
Data Filename	: yjs-yo-36-rac-IC-60-40-1.0-50 Pa-30 oC1.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 20 uL		
Date Acquired	: 2015/11/27 9:28:27	Acquired by	: System Administrator
Date Processed	: 2015/11/27 10:10:53	Processed by	: System Administrator

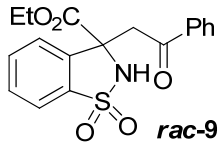
<Chromatogram>



<Peak Table>

Detector A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	20.474	6851387	152437	49.948
2	30.265	6865775	101629	50.052
Total		13717162	254066	



***rac*-9**

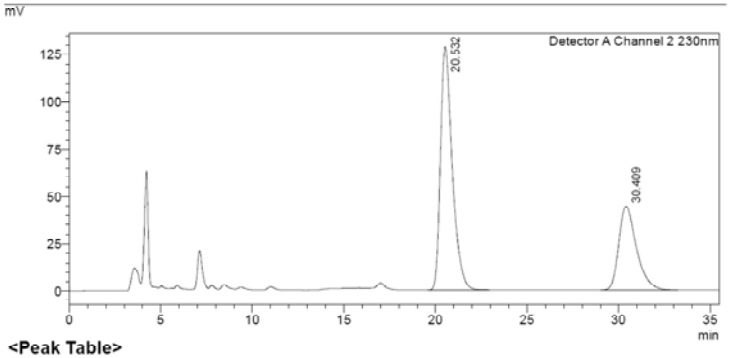
D:\Data\yujinsheng\yjs-yo-36-rac-IC-60-40-1.0-50 Pa-30 oC1.lcd

Analysis Report

<Sample Information>

Sample Name	: yjs-yo-36-asy		
Sample ID	:		
Data Filename	: yjs-yo-36-asy-IC-60-40-1.0-50 Pa-30 oC2.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 20 uL		
Date Acquired	: 2015/11/27 10:26:32	Acquired by	: System Administrator
Date Processed	: 2015/11/27 11:02:02	Processed by	: System Administrator

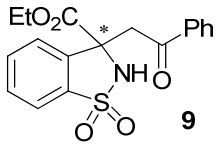
<Chromatogram>



<Peak Table>

Detector A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	20.532	5777663	128586	65.862
2	30.409	2994758	44394	34.138
Total		8772421	172980	



9

D:\Data\yujinsheng\yjs-yo-36-asy-IC-60-40-1.0-50 Pa-30 oC2.lcd