SUPPORTING INFORMATION

Pd-catalyzed intramolecular C-H activation for the synthesis of fused-1,2,3-triazole quinolines and dihydroquinolines

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Contents

1. GENERAL INFORMATION

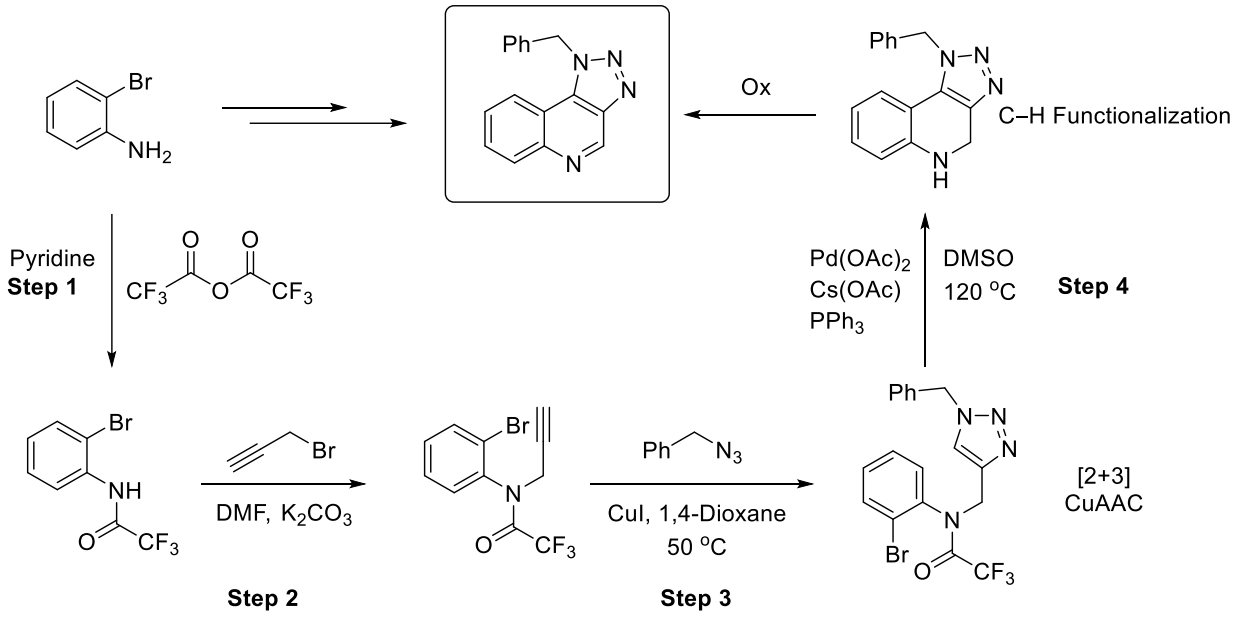
1.1. Reagents and methods

All the commercially available reagents, catalysts, bases, and solvents were used as purchased, without further purification. Starting materials and reaction products were purified by flash chromatography using SiO_2 as stationary phase, eluting with *n*-hexane/ethyl acetate. ^{1}H NMR (400.13 MHz), ^{13}C NMR (100.6 MHz), and ^{19}F spectra (376.5 MHz) were recorded with a Bruker Avance 400 spectrometer equipped with a Nanobay console and Cryoprobe Prodigy probe. Splitting patterns are designed as s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), or bs (broad singlet). IR spectra were recorded with a Jasco FT/IR-430 spectrometer. Mass spectra were determined with a Shimadzu QP2010-Plus Gas Chromatograph Mass spectrometer (EI ion source). HRMS were recorded with an Orbitrap Exactive Mass spectrometer with ESI source. Melting points were determined with a Büchi B-545 apparatus and are uncorrected. All the azides are commercially available except for 5-azido-1,2,3-trimethoxybenzene that was synthesized according to the reported procedure.

2. SYNTHETIC PROCEDURES

2.1. Typical procedure for the preparation of [1,2,3]triazolo[4,5-*c*]quinoline 5a-5q

1-benzyl-1*H*-[1,2,3]triazolo[4,5-*c*]quinoline **5a-5m** were prepared according to the sequence outlined in Scheme 1.

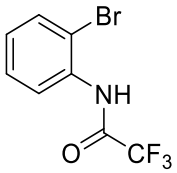


Scheme 1

STEP 1*: *synthesis of N-(2-bromophenyl)-2,2,2-trifluoroacetamide [S1]

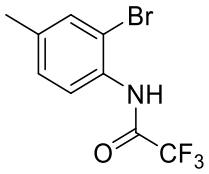
Following a slight modification of the literature procedure.[S1]

To a stirred solution of 2-bromoaniline (1.72 g, 10.0 mmol, 1.0 equiv.) in pyridine (15 mL), 2,2,2-trifluoroacetic anhydride (1.66 mL, 12.0 mmol, 1.2 equiv.) was added dropwise at 0°C. The reaction mixture was then allowed to warm to room temperature and stirred for 1 hour. The progress of the reaction was monitored by TLC (*n*-hexane/AcOEt, 80:20). After completion, the reaction was diluted with Et_2O and sequentially washed with 2N HCl, saturated $NaHCO_3$ solution, and brine. The organic layer was dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The reaction yielded *N*-(2-bromophenyl)-2,2,2-trifluoroacetamide in 97% yield (2.60 g, 9.7 mmol).

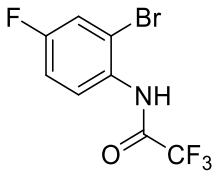


***N*-(2-bromophenyl)-2,2,2-trifluoroacetamide:** 97% yield, 2.60 g, 9.70 mmol; white solid; lit. mp [S1]: 57 – 59 °C; mp: 60 - 62 °C; R_f = 0.19 (*n*-hexane-EtOAc, 80:20); IR (neat): 3244, 1710, 1411, 1242,

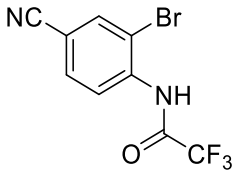
761 cm^{-1}; ^{1}H NMR (400.13 MHz, $CDCl_3$) δ 8.47 (bs, NH), 8.37 – 8.27 (m, 1H), 7.67 – 7.57 (m, 1H), 7.41 (t, *J* = 7.6 Hz, 1H), 7.18 – 7.10 (m, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 154.6 (q, J_{C-F} = 37.0 Hz) (C), 133.2 (C), 132.6 (CH), 128.7 (CH), 127.2 (CH), 122.0 (CH), 117.0 (q, J_{C-F} = 289.4 Hz) (C), 114.0 (C); HRMS: *m/z* $[M + H]^+$ calcd for $C_8H_6BrF_3NO$: 267.9579; found: 267.9554.



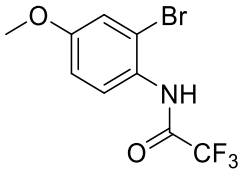
***N*-(2-bromo-4-methylphenyl)-2,2,2-trifluoroacetamide:** 95% yield, 2.66 g, 9.50 mmol; white solid; lit. mp [S1]: 67 – 69 °C; mp: 70 - 72 °C; R_f = 0.23 (*n*-hexane-EtOAc, 80:20); IR (neat): 3451, 1718, 1521, 1177, 822 cm^{-1}; $^{1}HNMR$ (400.13 MHz, $CDCl_3$) δ 8.34 (bs, NH), 8.12 (d, *J* = 8.3 Hz, 1H), 7.42 – 7.38 (m, 1H), 7.18 – 7.11 (m, 1H), 7.19 – 7.05 (m, 1H), 2.31 (s, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 154.6 (q, J_{C-F} = 37.0 Hz) (C), 137.6 (C), 132.9 (CH), 130.6 (C), 129.3 (CH), 121.9 (CH), 117.1 (q, J_{C-F} = 289.3 Hz) (C), 114.0 (C), 20.6 (CH_3); HRMS: *m/z* $[M + H]^+$ calcd for $C_9H_8BrF_3NO$: 281.9736; found: 281.9725.



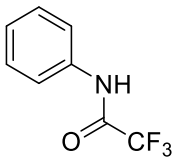
***N*-(2-bromo-4-fluorophenyl)-2,2,2-trifluoroacetamide:** 96% yield, 2.61 g, 9.12 mmol; pale yellow solid; mp: 80 - 82 °C; R_f = 0.21 (*n*-hexane-EtOAc, 90:10); IR (neat): 3252, 2158, 2029, 1715, 1547, 1151 cm^{-1}; $^{1}HNMR$ (400.13 MHz, $CDCl_3$) δ 8.36 (bs, NH), 8.30 – 8.22 (m, 1H), 7.38 (dd, J_1 = 7.7 Hz, J_2 = 2.8 Hz, 1H), 7.18 – 7.10 (m, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 159.7 (d, J_{C-F} = 251.9 Hz) (C), 154.8 (q, J_{C-F} = 38.1 Hz) (C), 129.6 (d, J_{C-F} = 3.3 Hz) (C), 123.5 (d, J_{C-F} = 8.5 Hz) (CH), 119.9 (d, J_{C-F} = 25.5 Hz) (CH), 115.7 (d, J_{C-F} = 22.3 Hz) (CH), 115.6 (q, J_{C-F} = 288.0 Hz) (C), 114.8 (d, J_{C-F} = 9.6 Hz) (C); HRMS: *m/z* $[M + H]^+$ calcd for $C_8H_5BrF_4NO$: 285.9485; found 285.9491.



***N*-(2-bromo-4-cyanophenyl)-2,2,2-trifluoroacetamide:** 97% yield, 2.68 g, 9.14 mmol; white solid; mp: 100 - 102 °C; R_f = 0.22 (*n*-hexane-EtOAc, 80:20); IR (neat): 3335, 3072, 1714, 1525, 1159, 834 cm^{-1}; ^{1}HNMR (400.13 MHz, $CDCl_3$) δ 8.63 (bs, NH), 8.55 (d, *J* = 8.6 Hz, 1H), 7.94 (d, *J* = 1.7 Hz, 1H), 7.72 (dd, J_1 = 8.6 Hz, J_2 = 1.7 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 154.9 (q, $J_{C\text{-}F}$ = 38.5 Hz) (C), 137.2 (C), 136.0 (CH), 132.8 (CH), 121.6 (CH), 116.7 (C) 115.2 (q, $J_{C\text{-}F}$ = 289.5 Hz) (C), 113.9 (C), 110.7 (C) 20.6 (CH_3); HRMS: *m/z* $[M + H]^+$ calcd for $C_9H_5BrF_3N_2O$: 292.9532; found 292.9548.



***N*-(2-bromo-4-methoxyphenyl)-2,2,2-trifluoroacetamide:** 98% yield, 2.79 g, 9.36 mmol; white solid; mp: 116-118 °C; R_f = 0.23 (*n*-hexane-EtOAc, 85:15); IR (neat): 3289, 1701, 1542, 1160, 818 cm^{-1}; ^{1}HNMR (400.13 MHz, $CDCl_3$) δ 8.17 (bs, NH), 7.99 (d, *J* = 9.1 Hz, 1H), 7.04 (d, *J* = 2.8 Hz, 1H), 6.81 (dd, J_1 = 9.1 Hz, J_2 = 2.8 Hz, 1H), 3.72 (s, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 157.9 (C) 154.6 (q, $J_{C\text{-}F}$ = 37.4 Hz) (C), 126.2 (C), 123.5 (CH), 117.9 (CH), 115.4 (C), 114.0 (CH), 116.1 (q, $J_{C\text{-}F}$ = 289.3 Hz) (C), 55.7 (CH_3); HRMS: *m/z* $[M + H]^+$ calcd for $C_9H_8BrF_3NO_2$: 297.9685; found 297.9664.



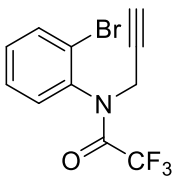
2,2,2-trifluoro-*N*-phenylacetamide: 99% yield, 1.88 g, 9.90 mmol; white solid; lit. mp [S2]: 90 - 92 °C; mp: 88 - 90 °C; R_f = 0.20 (*n*-hexane-EtOAc, 85:15); IR (neat): 3311, 1709, 1554, 1242, 760 cm^{-1}; ^{1}HNMR (400.13 MHz, $CDCl_3$) δ 7.91 (bs, NH), 7.49 (d, *J* = 7.8 Hz, 2H), 7.31 (t *J* = 7.8 Hz, 2H), 7.20 – 7.14 (m, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 154.8 (q, $J_{C\text{-}F}$ = 37.2 Hz), 135.0 (C), 129.3 (CH), 126.4

(C), 120.5 (CH), 115.6 (q, $J_{C\text{-}F}$ = 289.4 Hz) (C); HRMS: *m/z* $[M + H]^+$ calcd for $C_8H_7F_3NO$: 190.0474; found: 190.0492.

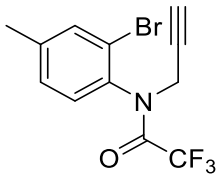
STEP 2*: *synthesis of N-(2-bromophenyl)-2,2,2-trifluoro-N-(prop-2-yn-1-yl)acetamide

Following a slight modification of the literature procedure.[S1]

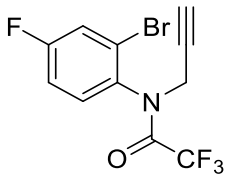
To a solution of *N*-(2-bromophenyl)-2,2,2-trifluoroacetamide (2.6 g, 9.70 mmol, 1.0 equiv.) in 15 mL of DMF, K_2CO_3 (2.67 g, 19.40 mmol, 2.0 equiv.) and propargyl bromide (0.808 mL, 10.67 mmol, 1.1 equiv.) were added. The reaction mixture was stirred at room temperature for 6 hours. Upon completion, the mixture was diluted with diethyl ether, extracted with brine and dried over anhydrous Na_2SO_4. Then was concentrated under reduced pressure, and purified by flash column chromatography, affording *N*-(2-bromophenyl)-2,2,2-trifluoro-*N*-(prop-2-yn-1-yl)acetamide in 90% yield (2.67 g, 8.73 mmol).



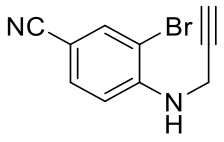
***N*-(2-bromophenyl)-2,2,2-trifluoro-*N*-(prop-2-yn-1-yl)acetamide:** 90% yield, 2.66 g, 8.73 mmol; brown solid; mp: 52 - 54 °C; R_f = 0.22 (*n*-hexane-EtOAc, 90:10); IR (neat): 3311, 2994, 1721, 1481, 1114 cm^{-1}; ^1H NMR (400.13 MHz, $CDCl_3$) δ 7.76 – 7.68 (m, 1H), 7.51 – 7.32 (m, 3H), 5.13 (dd, J_1 = 17.4 Hz, J_2 = 2.4 Hz, 1H), 3.96 (dd, J_1 = 17.4 Hz, J_2 = 2.4 Hz, 1H), 2.29 (t, *J* = 2.4 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 156.49 (q, $J_{C\text{-}F}$ = 37.6 Hz) (C), 136.5 (C), 133.6 (CH), 131.8 (CH), 131.2 (CH), 128.1 (CH), 123.4 (C), 115.9 (q, $J_{C\text{-}F}$ = 287.1 Hz) (C), 76.4 (C), 74.1 (CH) 39.1 (CH_2); HRMS: *m/z* $[M + H]^+$ calcd for $C_{11}H_8BrF_3NO$: 305.9736; found: 305.9717.



***N*-(2-bromo-4-methylphenyl)-2,2,2-trifluoro-*N*-(prop-2-yn-1-yl)acetamide:** 92% yield, 2.85 g, 8.92 mmol; brown solid; mp: 66 - 68 °C; R_f = 0.24 (*n*-hexane-EtOAc, 90:10); IR (neat): 3414, 2899, 1714, 1389, 758 cm^{-1}; ^1H NMR (400.13 MHz, $CDCl_3$) δ 7.57 – 7.49 (m, 1H), 7.33 (d, *J* = 7.6 Hz 3H), 7.24 – 7.17 (m, 1H), 5.10 (dd, J_1 = 17.4 Hz, J_2 = 2.4 Hz, 1H), 3.93 (dd, J_1 = 17.4 Hz, J_2 = 2.4 Hz, 1H), 2.41 (s, 3H), 2.28 (t, *J* = 2.4 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 156.6 (q, $J_{C\text{-}F}$ = 37.6 Hz) (C), 141.9 (C), 133.9 (CH), 133.8 (C), 128.8 (CH), 122.9 (CH), 123.4 (C), 115.6 (q, $J_{C\text{-}F}$ = 287.1 Hz) (C), 76.5 (C), 73.9 (CH), 39.2 (CH_2), 20.9 (CH_3); HRMS: *m/z* $[M + H]^+$ calcd for $C_{12}H_{10}BrF_3NO$: 319.9892; found: 319.9870.

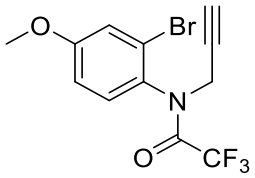


***N*-(2-bromo-4-fluorophenyl)-2,2,2-trifluoro-*N*-(prop-2-yn-1-yl)acetamide:** 70% yield, 0.57 g, 1.75 mmol; pale yellow wax; R_f = 0.27 (*n*-hexane-EtOAc, 90:10); IR (neat): 3393, 2960, 1764, 1453, 1045, cm^{-1}; ^1H NMR (400.13 MHz, $CDCl_3$) δ 7.51 – 7.42 (m, 2H), 7.19 – 7.12 (m, 1H), 5.13 (dd, J_1 = 17.3 Hz, J_2 = 2.5 Hz, 1H), 3.95 (dd, J_1 = 17.3 Hz, J_2 = 2.5 Hz, 1H), 2.30 (t, *J* = 2.5 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 162.6 (d, $J_{C\text{-}F}$ = 254.5 Hz) (C), 156.5 (q, $J_{C\text{-}F}$ = 36.4 Hz) (C), 133.0 (d, $J_{C\text{-}F}$ = 8.8 Hz) (CH),132.8 (d, $J_{C\text{-}F}$ = 4.1 Hz) (C), 124.4 (d, $J_{C\text{-}F}$ = 10.2 Hz) (C), 121.0 (d, $J_{C\text{-}F}$ = 25.8 Hz) (CH), 115.8 (q, $J_{C\text{-}F}$ = 289.0 Hz) (C), 115.3 (d, $J_{C\text{-}F}$ = 22.4 Hz) (CH); 76.2 (C), 74.4 (CH), 39.1 (CH_2), HRMS: *m/z* $[M + H]^+$ calcd for $C_{11}H_7BrF_4NO$: 323.9442; found: 323.9433.

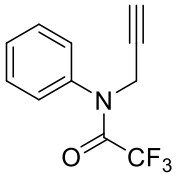


***3*-bromo-4-(prop-2-yn-1-ylamino)benzonitrile:** 50% yield, 0.29 g, 1.25 mmol; brown oil; R_f = 0.21 (*n*-hexane-EtOAc, 60:40); IR (neat): 3392, 3276, 2159, 1518, 814 cm^{-1}; ^1H NMR (400.13 MHz, $CDCl_3$) δ 7.64 (d, *J* = 1.8 Hz, 1H), 7.43 (dd, J_1 = 8.4 Hz, J_2 = 1.8 Hz, 1H), 6.67 (d, *J* = 8.5 Hz, 1H), 5.04

(bs, 1H), 3.99 (s, 2H), 2.22 (t, *J* = 2.4 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 147.1 (C), 135.9 (CH), 132.9 (CH), 118.7 (C), 111.1 (CH), 109.1 (C), 101.1 (C), 78.6 (C), 72.6 (CH), 33.1 (CH_2); HRMS: *m/z* $[M + H]^+$ calcd for $C_{10}H_8BrN_2$: 234.9865; found: 234.9874.



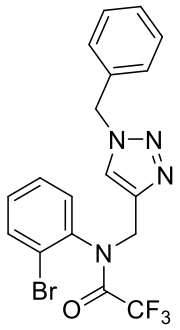
***N*-(2-bromo-4-methoxyphenyl)-2,2,2-trifluoro-*N*-(prop-2-yn-1-yl)acetamide:** 90% yield, 0.76 g, 2.25 mmol; yellow oil; R_f = 0.24 (*n*-hexane-EtOAc, 90:10); IR (neat): 3711, 3293, 2158, 1702, 1206, 842 cm^{-1}; ^{1}H NMR (400.13 MHz, $CDCl_3$) δ 7.36 (d, *J* = 8.8 Hz, 1H), 7.22 (d, *J* = 2.8 Hz, 1H), 6.92 (dd, J_1 = 8.8 Hz, J_2 = 2.8 Hz, 1H), 5.10 (dd, J_1 = 17.3 Hz, J_2 = 2.5 Hz, 1H), 3.93 (dd, J_1 = 17.3 Hz, J_2 = 2.5 Hz, 1H), 3.86 (s, 3H), 2.28 (t, *J* = 2.5 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 160.8 (C), 158.3 (q, J_{C-F} = 37.1 Hz) (C), 132.3 (CH), 129.1 (C), 124.0 (C), 118.6 (CH), 115.9 (q, J_{C-F} = 288.0 Hz) (C), 113.5 (CH), 76.6 (C), 74.0 (CH), 55.8 (CH_3), 39.4 (CH_2); HRMS: *m/z* $[M + H]^+$ calcd for $C_{12}H_{10}BrF_3NO_2$: 335.9841; found: 335.9828.



2,2,2-trifluoro-*N*-phenyl-*N*-(prop-2-yn-1-yl)acetamide: 91% yield, 2.01 g, 8.83 mmol; yellow solid; mp: 58 - 60 °C; R_f = 0.20 (*n*-hexane-EtOAc, 90:10); IR (neat): 3398, 2915, 1722, 1415, 765 cm^{-1}; ^{1}H NMR (400.13 MHz, $CDCl_3$) δ 7.44 – 7.32 (m, 3H), 7.31 – 7.21 (m, 2H), 4.29 (d, *J* = 2.3 Hz, 2H), 2.22 (t, *J* = 2.4 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 156.4 (q, J_{C-F} = 37.6 Hz) (C), 138.3 (C), 129.6 (CH), 129.4 (CH), 128.4 (CH), 116.2 (q, J_{C-F} = 287.1 Hz) (C), 76.9 (C), 73.7 (CH) 41.0 (CH_2); HRMS: *m/z* $[M + H]^+$ calcd for $C_{11}H_9F_3NO$: 228.0631; found: 228.0647.

STEP 3: synthesis of N-((1-benzyl-1H-1,2,3-triazol-4-yl)methyl)-N-(2-bromophenyl)-2,2,2-trifluoroacetamide (2a)

To a vial containing *N*-(2-bromophenyl)-2,2,2-trifluoro-*N*-(prop-2-yn-1-yl)acetamide (306.2 mg, 1.00 mmol, 1.00 equiv.) in 2 mL of dioxane, CuI (38.1 mg, 0.20 mmol, 0.20 equiv.) and benzyl azide (146.3 mg, 1.10 mmol, 1.10 equiv.) were added. The vial was sealed, and the reaction mixture was stirred at 50°C overnight. Upon completion, the mixture was concentrated under reduced pressure and purified by flash column chromatography (70:30 *n*-hexane/EtOAc, R_f = 0.22) to afford the pure product as a yellow solid (413.0 mg, 0.94 mmol, 94% yield).

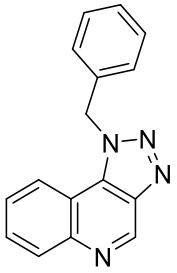


***N*-((1-benzyl-1*H*-1,2,3-triazol-4-yl)methyl)-*N*-(2-bromophenyl)-2,2,2-trifluoroacetamide, 2a:** 90% yield, 413.0 mg, 0.94 mmol; yellow solid; mp: 120-122 °C; R_f = 0.23 (*n*-hexane-EtOAc, 70:30); IR (neat): 3121, 3073, 1694, 1478, 1149, 719 cm^{-1}; ^1H NMR (400.13 MHz, $CDCl_3$) δ 7.59 – 7.56 (m, 1H), 7.50 (s, 1H), 7.31 - 7.28 (m, 3H), 7.20 – 7.14 (m, 4H), 7.00 - 6.96 (m, 1H), 5.49 (d, *J* = 14.6 Hz, 1H), 5.39 – 5.28 (m, 2H), 4.36 (d, *J* = 14.6 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 156.9 (q, J_{C-F} = 36.7 Hz) (C), 142.0 (C), 137.6 (C), 134.4 (C), 133.5 (CH), 131.6 (CH), 130.9 (CH), 129.2 (CH), 128.9 (CH), 128.2 (CH), 128.0 (CH), 124.0 (CH), 123.4 (C), 116.1 (q, J_{C-F} = 288.9 Hz) (C), 54.2 (CH_2), 45.7 (CH_2); ^{19}F NMR (376.5 MHz, $CDCl_3$) δ -68.9. HRMS: *m/z* $[M + H]^+$ calcd for $C_{18}H_{15}BrF_3N_4O$: 439.0354; found: 439.0377.

STEP 4: synthesis of 1-benzyl-1H-[1,2,3]triazolo[4,5-c]quinoline (5a)

To a vial containing $Pd(OAc)_2$ (2.8 mg, 0.013 mmol, 0.05 equiv.), PPh_3 (13.1 mg, 0.050 mmol, 0.20 equiv.) in DMSO (2 mL) was added *N*-((1-benzyl-1*H*-1,2,3-triazol-4-yl)methyl)-*N*-(2-

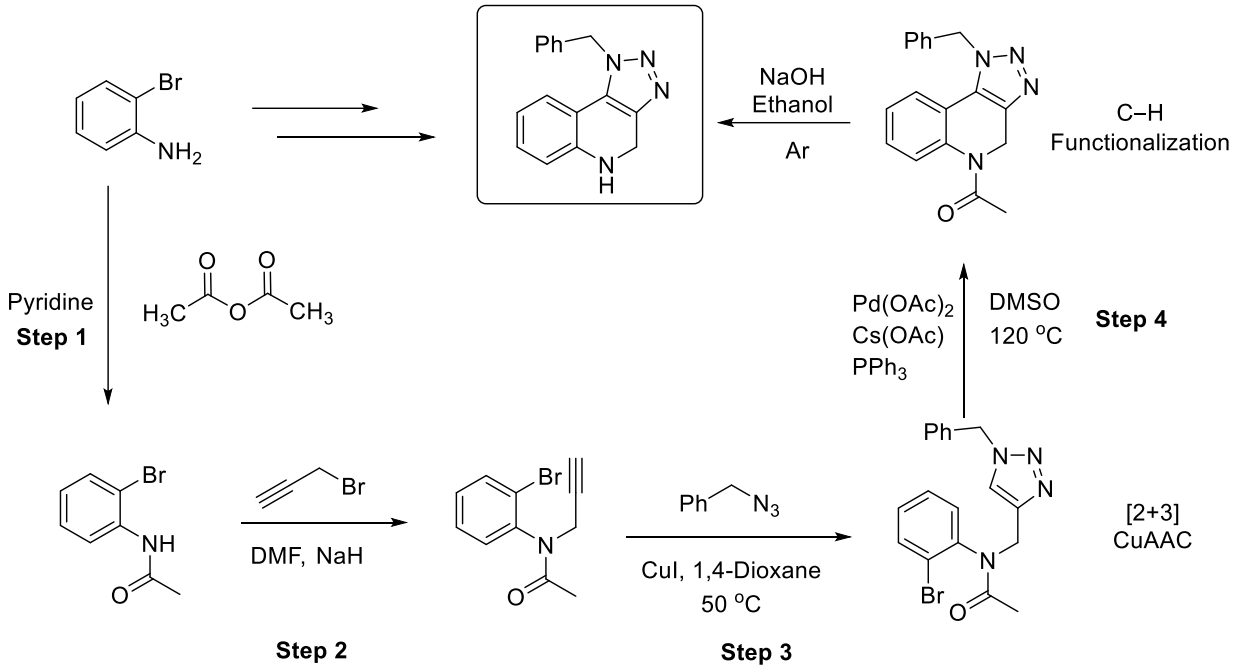
bromophenyl)-2,2,2-trifluoroacetamide (110.0 mg, 0.250 mmol, 1.00 equiv.), and Cs(OAc) (96.0 mg, 0.500 mmol, 2.00 equiv.). The mixture was stirred at 120 ^{o}C for 0.5 hours. Upon completion of reaction (monitored by TLC), an oxygen balloon was then applied. The reaction was monitored by TLC upon completion, the mixture was then diluted with diethyl ether, extracted with brine and dried over anhydrous Na_2SO_4. The residue was purified by flash column chromatography 50/50 *n*-hexane and EtOAc (R_f = 0.19) to give the pure product (61.2 mg, 0.24 mmol, 95%) as yellow solid.



1-benzyl-1*H*-[1,2,3]triazolo[4,5-*c*]quinoline, 5a: 95% yield, 61.2 mg, 0.24 mmol; yellow solid; mp: 140-142 °C; R_f = 0.22 (*n*-hexane-EtOAc, 50:50); IR (neat): 3386, 2961, 1688, 1453, 722 cm^{-1}; ^{1}H NMR (400.13 MHz, $CDCl_3$) δ 9.61 (s, 1H), 8.38 (d, *J* = 8.3 Hz, 1H), 8.11 (d, *J* = 8.3 Hz, 1H), 7.88 – 7.76 (m, 1H), 7.71 – 7.60 (m, 1H), 7.43 – 7.29 (m, 3H), 7.20 (d, *J* = 7.5 Hz, 2H), 6.29 (s, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 145.6 (C), 145.0 (CH), 141.2 (C), 134.2 (C), 133.2 (C), 130.8 (CH), 129.6 (CH), 129.3 (CH), 128.6 (CH), 127.7 (CH), 126.4 (CH), 122.1 (CH), 115.2 (C), 53.9 (CH_2); MS (EI, 70 eV): *m/z* (%)= 231 (100), 260 (M^+, 100), 91 (100), 128 (90); HRMS: *m/z* $[M + H]^+$ calcd for $C_{16}H_{13}N_4$: 261.1135; found: 261.1115.

2.2. Typical procedure for the preparation of 4,5-dihydro-1*H*-[1,2,3]triazolo[4,5-*c*]quinoline 4a-4h

1-benzyl-1*H*-[1,2,3]triazolo[4,5-*c*]quinoline **4a-4h** were prepared following the procedures outlined in Scheme 2.

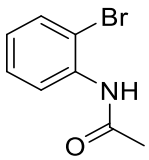


Scheme 2

STEP 1: Synthesis of N-(2-bromophenyl)acetamide

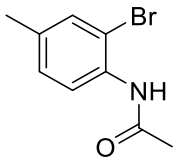
Following a slight modification of the literature procedure.[S3]

To a stirred solution of 2-bromoaniline (1.72 g, 10.0 mmol, 1.0 equiv.) in pyridine (15 mL), acetic anhydride (1.66 mL, 12.0 mmol, 1.2 equiv.) was added drop wise at room temperature. The reaction mixture was stirred for 3 hours, with progress monitored by TLC (*n*-hexane/AcOEt, 80:20). Upon completion, the reaction was diluted with diethyl ether and the organic phase was sequentially washed with 2N HCl, saturated $NaHCO_3$ solution, and brine. The organic layer was dried over Na_2SO_4, filtered, and concentrated under reduced pressure to yield *N*-(2-bromophenyl)-2,2,2-trifluoroacetamide as a residue in 95% yield (2.03 g, 9.5 mmol)



***N*-(2-bromophenyl)acetamide :** 95% yield, 2.03 g, 9.5 mmol; white solid; lit. mp [S3]: 96 - 98 °C; mp: 92 - 94 °C; R_f = 0.19 (*n*-hexane-EtOAc, 80:20); IR (neat): 3361, 1664, 1541, 1285, 759 cm^{-1}; ^1H

NMR (400.13 MHz, $CDCl_3$) δ 8.25 (d, *J* = 8.0 Hz, 1H), 7.53 (bs, 1H), 7.45 (d, *J* = 8.0 Hz, 1H), 7.23 (t, *J* = 7.5 Hz, 1H), 6.90 (t, *J* = 7.5 Hz, 1H), 2.17 (s, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 168.2 (C), 135.7 (C), 132.2 (CH), 128.4 (CH), 125.1 (CH), 121.9 (CH), 113.2 (C), 24.8 (CH_3); HRMS: *m/z* $[M + H]^+$ calcd for C_8H_9BrNO: 213.9862; found: 213.9855.

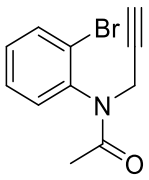


***N*-(2-bromo-4-methylphenyl)acetamide :** 94% yield, 2.15 g, 9.45 mmol; white solid; lit. mp [S3]: 86 - 88 °C; mp: 83 - 85 °C; R_f = 0.20 (*n*-hexane-EtOAc, 85:15); IR (neat): 3245, 1685, 1512, 1287, 754 cm^{-1}; ^1H NMR (400.13 MHz, $CDCl_3$) δ 8.05 (d, *J* = 8.4 Hz, 1H), 7.46 (bs, 1H), 7.26 (s, 1H), 7.01 (d, *J* = 8.3 Hz, 1H), 2.21 (s, 3H), 2.13 (s, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 168.2 (C), 135.3 (C), 133.1 (C), 132.4 (CH), 128.9 (CH), 122.0 (CH), 113.3 (C), 24.7 (CH_3), 24.5 (CH_3); HRMS: *m/z* $[M + H]^+$ calcd for $C_9H_{11}BrNO$: 228.0018; found: 228.0033.

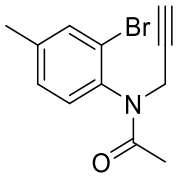
STEP 2: synthesis of N-(2-bromophenyl)-N-(prop-2-yn-1-yl)acetamide.

Following a slight modification of the literature procedure.[S4]

Sodium hydride (60% in paraffin oil, 0.48 g, 12.0 mmol, 1.2 equiv.) was added to *n*-hexane to remove the mineral oil. After 10 minutes, the *n*-hexane was removed, and a solution of *N*-(2-bromophenyl)acetamide (2.14 g, 10.0 mmol, 1.0 equiv.) in DMF was added, followed by propargyl bromide (11.0 mmol, 0.83 mL, 1.1 equiv.) at 0°C. The reaction was then warmed to room temperature and stirred for 6 hours. After completion, the mixture was then diluted with diethyl ether, extracted with brine and dried over anhydrous Na_2SO_4, concentrated under vacuum, and purified by flash column chromatography to give *N*-(2-bromophenyl)-*N*-(prop-2-yn-1-yl)acetamide in 90% yield (2.27 g, 9.0 mmol).



***N*-(2-bromophenyl)-*N*-(prop-2-yn-1-yl)acetamide:** 90% yield, 2.27 g, 9.0 mmol; white solid; lit. mp[S5]: 45 - 47 °C; mp: 52 - 54 °C; R_f = 0.19 (*n*-hexane-EtOAc, 95:5); IR (neat): 3389, 2918, 1731, 1364, 1245 cm^{-1}; ^{1}HNMR (400.13 MHz, $CDCl_3$) δ 7.67 – 7.58 (m, 1H), 7.40 – 7.30 (m, 2H), 7.25 – 7.18 (m, 1H), 5.00 (dd, J_1 = 17.3 Hz, J_2 = 2.5 Hz, 1H), 3.77 (dd, J_1 = 17.3 Hz, J_2 = 2.5 Hz 1H), 2.12 (t, *J* = 2.5 Hz, 1H), 1.74 (s, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 169.8 (C), 140.3 (C), 133.7 (CH), 131.3 (CH), 130.3 (CH), 128.7 (CH), 123.6 (C), 78.6 (C), 72.5 (CH), 36.6 (CH_2), 22.1 (CH_3); HRMS: *m/z* [M + H]$^+$ calcd for $C_{11}H_{11}BrNO$: 252.0018; found: 252.0031.

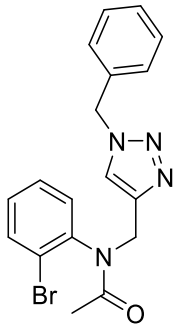


***N*-(2-bromo-4-methylphenyl)-*N*-(prop-2-yn-1-yl)acetamide:** 91% yield, 2.41 g, 9.1 mmol; white solid; mp: 46 - 48 °C; R_f = 0.22 (*n*-hexane-EtOAc, 95:5); IR (neat): 3258, 2901, 1738, 1352, 1277 cm^{-1}; ^{1}HNMR (400.13 MHz, $CDCl_3$) δ 7.50 (s, 1H), 7.33 – 7.25 (m, 1H), 7.23 – 7.13 (m, 1H), 5.04 (d, *J* = 17.5 Hz, 1H), 3.80 (d, *J* = 17.5 Hz, 1H), 2.37 (s, 3H), 2.19 – 2.13 (m, 1H), 1.80 (s, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 170.0 (C), 140.8 (C), 137.7 (C), 134.1 (CH), 133.7 (C), 130.7 (CH), 129.4 (CH), 123.2 (C), 78.7 (C), 72.4 (CH), 36.7 (CH_2), 22.1 (CH_3), 20.9 (CH_3); HRMS: *m/z* [M + H]$^+$ calcd for $C_{12}H_{13}BrNO$: 266.0118; found: 266.0131.

STEP 3: synthesis of N-((1-benzyl-1H-1,2,3-triazol-4-yl)methyl)-N-(2-bromophenyl)acetamide (3a).

To a vial containing *N*-(2-bromophenyl)-*N*-(prop-2-yn-1-yl)acetamide (252.0 mg, 1.00 mmol, 1.00 equiv.) in 2 mL of dioxane, CuI (38.1 mg, 0.20 mmol, 0.20 equiv.) and benzyl azide (146.3 mg, 1.10 mmol, 1.10 equiv.) were added. The vial was sealed, and the reaction mixture was stirred at 50°C overnight. After completion, the mixture was concentrated under reduced pressure and purified

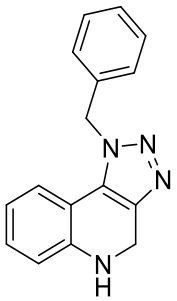
by flash column chromatography (70:30 *n*-hexane/EtOAc, R_f = 0.20) to afford the pure product as a yellow solid (366.2 mg, 0.95 mmol,95% yield).



***N*-((1-benzyl-1*H*-1,2,3-triazol-4-yl)methyl)-*N*-(2-bromophenyl)acetamide, 3a**: 95% yield, 365.7 mg, 0.95 mmol; pale yellow solid; mp: 112-114 °C; R_f = 0.20 (n-hexane-EtOAc, 60:40); IR (neat): 3139, 2955, 1655, 1369, 1044, 709 cm^{-1}; ^1H NMR (400.13 MHz, $CDCl_3$) δ 7.65 (dd, J_1 = 8.0 Hz, J_2 = 1.3 Hz, 1H), 7.60 (s, 1H), 7.41 – 7.35 (m, 3H), 7.32 – 7.19 (m, 4H), 7.11 (dd, J_1 = 8.0 Hz, J_2 = 1.3 Hz, 1H), 5.56 (d, *J* = 14.8 Hz, 1H), 5.44 (d, *J* = 14.8 Hz, 1H), 5.26 (d, *J* = 14.8 Hz, 1H), 4.45 (d, *J* = 14.8 Hz, 1H), 1.80 (s, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 170.4 (C), 144.1 (C), 141.5 (C), 134.7 (C), 133.8 (CH), 131.0 (CH), 130.0 (CH), 129.1 (CH), 128.8 (CH), 128.7 (CH), 128.0 (CH), 123.7 (CH), 123.7 (C), 54.1 (CH_2), 43.6 (CH_2), 22.3 (CH_3); HRMS: *m/z* $[M + H]^+$ calcd for $C_{18}H_{18}BrN_4O$:385.0658; found: 385.0634.

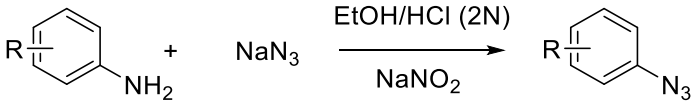
STEP 4: 1-benzyl-4,5-dihydro-1H-[1,2,3]triazolo[4,5-c]quinoline (4a)

To a vial containing $Pd(OAc)_2$ (2.8 mg, 0.013 mmol, 0.05 equiv.), PPh_3 (13.1 mg, 0.050 mmol, 0.20 equiv.) in DMSO (2 mL), was added *N*-((1-benzyl-1*H*-1,2,3-triazol-4-yl)methyl)-*N*-(2-bromophenyl)acetamide (96.8 mg, 0.250 mmol, 1.00 equiv.) and Cs(OAc) (96.2 mg, 0.500 mmol, 2.00 equiv.). The mixture was stirred at 120 °C for 0.5 hours. Upon completion of the reaction (monitored by TLC), NaOH (2N, 1 mL) and EtOH (1 mL) were added to hydrolyze the acetamide protecting group. The mixture was then diluted with diethyl ether, extracted with brine and dried over anhydrous Na_2SO_4. The residue was purified by flash column chromatography 50/50 *n*-hexane and EtOAc (R_f = 0.21) to give the pure product (61 mg, 0.193 mmol, 77%) as a pale yellow solid.



1-benzyl-4,5-dihydro-1*H*-[1,2,3]triazolo[4,5-*c*]quinoline, 4a: 77% yield, 61 mg, 0.193 mmol; pale yellow solid; mp: 182-184 °C; R_f = 0.21 (*n*-hexane-EtOAc, 50:50); IR (neat): 3367, 3063, 1622, 1122, 713 cm^{-1}; ^1H NMR (400.13 MHz, $CDCl_3$) δ 7.29 – 7.15 (m, 3H), 7.07 (d, *J* = 7.7 Hz, 2H), 7.01 (d, *J* = 7.7 Hz, 1H), 6.95 – 6.88 (m, 1H), 6.55 – 6.40 (m, 2H), 5.69 (s, 2H), 4.72 (s, 2H), 4.09 (bs, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 144.8 (C), 140.0 (C), 135.0 (C), 130.0 (CH), 129.4 (C), 129.1 (CH), 128.2 (CH), 126.4 (CH), 122.9 (CH), 118.0 (CH), 114.6 (CH), 110.5 (C), 53.0 (CH_2), 41.3 (CH_2); MS (EI, 70 eV): *m/z* (%)= 207 (100), 73 (76), 281 (47), 260 (30), 262 (M^+, 6); HRMS: *m/z* $[M + H]^+$ calcd for $C_{16}H_{15}N_4$: 263.1291; found: 263.1276.

2.3. Typical procedure for the preparation of azides

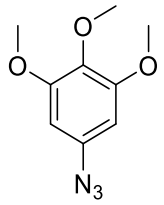


Scheme 3

Procedure for 5-azido-1,2,3-trimethoxybenzene

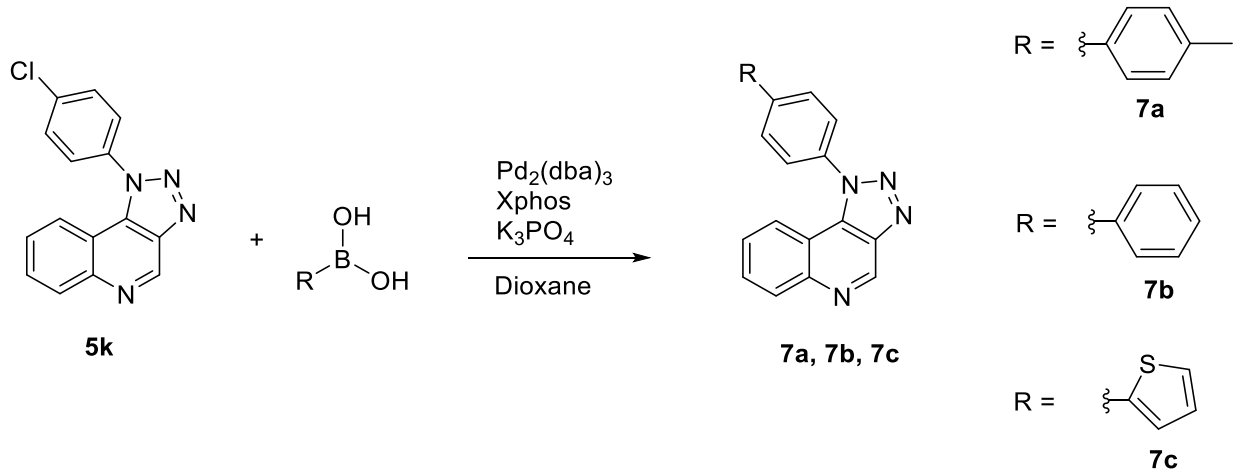
Following the same procedure reported in literature [S6], the 3,4,5-trimethoxyaniline (1.832 g, 10.0 mmol, 1.0 equiv.) was suspended in 17% hydrochloric acid at room temperature, and ethanol was added until a clear solution was obtained. The solution was then cooled to 0°C, and $NaNO_2$ (1.035 g, 15.0 mmol, 1.5 equiv.) was added in small portions. After stirring at 0°C for 15-30 minutes, NaN_3 (0.975 g, 15.0 mmol, 1.5 equiv.) was added slowly, and the mixture was stirred for an additional 2 hours at room temperature. The reaction mixture was extracted with diethyl ether, and the combined organic fractions were washed with saturated $NaHCO_3$ solution and

brine, dried over Na_2SO_2, and concentrated under reduced pressure. The desired azide was obtained in quantitative yield without further purification.



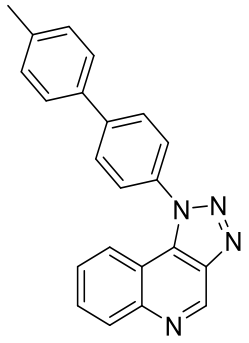
5-azido-1,2,3-trimethoxybenzene: 99% yield, 2.08 g, 9.9 mmol; brown solid; lit. mp [S7]: 42 – 43; mp: 45 - 47 °C; R_f = 0.20 (*n*-hexane-EtOAc, 75:25); IR (neat): 2910, 2485, 1461, 1135, 993 cm^{-1}; ^1H NMR (400.13 MHz, $CDCl_3$) δ 6.18 (s, 2H), 3.78 (s, 6H), 3.74 (s, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 154.1 (C), 135.7 (C), 135.4 (C), 96.4 (CH), 61.0 (CH_3), 56.2 (CH_3). HRMS: m/z $[M + H]^+$ calcd for $C_9H_{12}N_3O_3$:210.0873; found: 210.0888.

2.4. Procedure for the synthesis of compounds (7a, 7b, 7c)

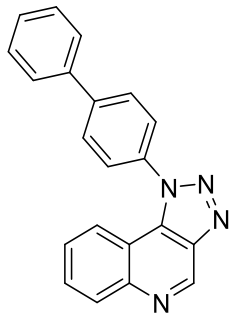


To a mixture of $Pd_2(dba)_3$ (4.6 mg, 0.005 mmol, 0.02 equiv.) and Xphos ligand (4.7 mg, 0.010 mmol, 0.04 equiv.) in dry dioxane (2 mL), compound **5k** (70.0 mg, 0.250 mmol, 1.00 equiv.), *p*-tolyl boronic acid (51.0 mg, 0.375 mmol, 1.50 equiv.), and K_3PO_4 (0.159 g, 0.750 mmol, 3.00 equiv.) were added. The reaction mixture was then stirred under argon at 100°C and monitored by TLC. After completion, the mixture was concentrated under reduced pressure and purified by

flash column chromatography (90:10 *n*-hexane/EtOAc) to afford the pure product **7a** (86% yield, 72.5 mg, 0.215 mmol).

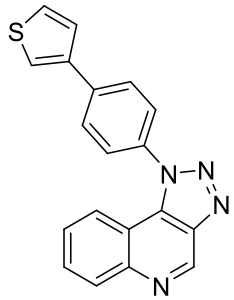


1-(4'-methyl-[1,1'-biphenyl]-4-yl)-1*H*-[1,2,3]triazolo[4,5-*c*]quinoline, 7a: 86% yield, 72.3 mg, 0.22 mmol; pale yellow solid; mp: 197-199 °C; R_f = 0.24 (*n*-hexane-EtOAc, 75:25); IR (neat): 3055, 1504, 992, 801, 767 cm^{-1}; ^1H NMR (400.13 MHz, $CDCl_3$) δ 9.51 (s, 1H), 8.22 (d, *J* = 8.3 Hz, 1H), 7.83 – 7.73 (m, 3H), 7.72 – 7.66 (m, 1H), 7.65 – 7.61 (m, 2H), 7.53 (d, *J* = 8.3 Hz, 2H), 7.42 (m, 1H), 7.24 (d, *J* = 8.3 Hz, 2H), 2.35 (s, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 145.9 (C), 144.9 (CH), 143.7 (C), 140.5 (C), 138.4 (C), 136.4 (C), 135.7 (C), 133.7 (C), 130.8 (CH), 129.95 (CH), 129.86 (CH), 128.3 (CH), 127.4 (CH), 127.1 (CH), 126.7 (CH), 121.9 (CH), 115.3 (C), 21.2 (CH_3); MS (EI, 70 eV): *m/z* (%)= 207 (100), 73 (82), 281 (49), 336 (M^+, 4); HRMS: *m/z* $[M + H]^+$ calcd for $C_{22}H_{17}N_4$: 337.1448; found: 337.1463.



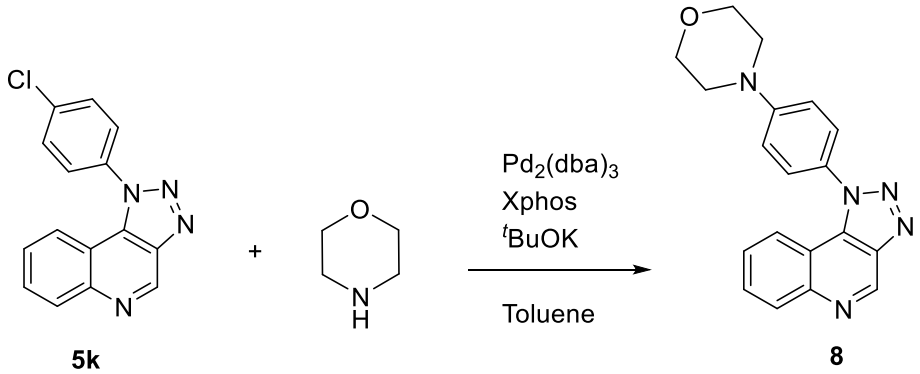
1-([1,1'-biphenyl]-4-yl)-1*H*-[1,2,3]triazolo[4,5-*c*]quinoline, 7b: 95% yield, 76.5 mg, 0.24 mmol; grey solid; mp: 178-180 °C; R_f = 0.22 (*n*-hexane-EtOAc, 75:25); IR (neat): 3063, 1527, 1087, 984, 758 cm^{-1}; ^1H NMR (400.13 MHz, $CDCl_3$) δ 9.49 (s, 1H), 8.21 (d, *J* = 8.2, 1H), 7.85 – 7.81 (m, 3H), 7.80 – 7.70 (m, 5H), 7.57 – 7.48 (m, 3H), 7.47 – 7.39 (m, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 145.9 (C), 144.9 (CH), 143.8 (C), 140.5 (C), 139.3 (C), 136.0 (C), 133.7 (C), 130.8 (CH), 130.0 (CH), 129.1

(CH), 128.6 (CH), 128.4 (CH), 127.4 (CH), 127.3 (CH), 126.8 (CH), 121.8 (CH), 115.2 (C); MS (EI, 70 eV): *m/z* (%)= 207 (100), 73 (73), 281 (55), 322 (M^+, 1); HRMS: *m/z* $[M + H]^+$ calcd for $C_{21}H_{15}N_4$: 323.1291; found: 323.1276.



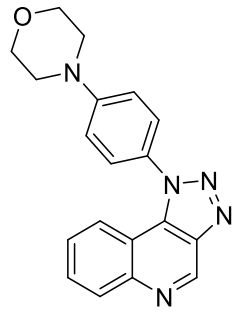
1-(4-(thiophen-3-yl)phenyl)-1*H*-[1,2,3]triazolo[4,5-*c*]quinoline, 7c: 85% yield, 69.7 mg, 0.22 mmol; pale yellow solid; mp: 230-232 °C; R_f = 0.18 (*n*-hexane-EtOAc, 70:30); IR (neat): 2967, 1535, 1267, 762, 567 cm^{-1}; ^1H NMR (400.13 MHz, $CDCl_3$) δ 9.60 (s, 1H), 8.41 – 8.38 (m, 1H), 7.91 – 7.85 (m, 2H), 7.85 – 7.72 (m, 2H), 7.71 – 7.57 (m, 3H), 7.55 – 7.40 (m, 2H), 7.19 (s, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 145.9 (C), 144.9 (CH), 140.50 (C), 140.47 (C), 138.3 (C), 135.6 (C), 133.7 (C), 130.8 (CH), 129.9 (CH), 127.7 (CH), 127.4 (CH), 127.1 (CH), 126.9 (CH), 126.1 (CH), 122.0 (CH), 121.8 (CH), 115.2 (C); MS (EI, 70 eV): *m/z* (%)= 207 (100), 73 (83), 281 (34), 328 (M^+, 2); HRMS: *m/z* $[M + H]^+$ calcd for $C_{19}H_{13}N_4S$: 329.0855; found: 329.0874.

2.5. Procedure for the synthesis of compound 8



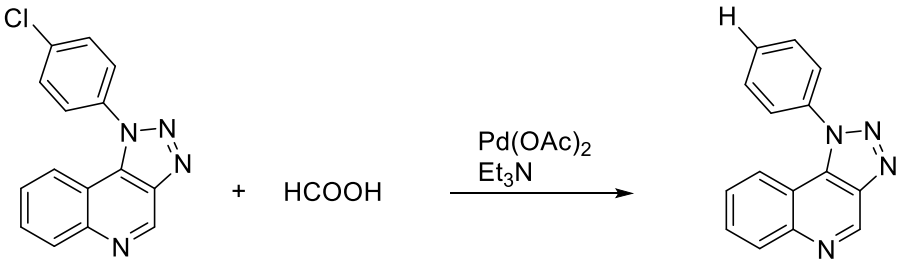
5k **8**

To a mixture of $Pd(OAc)_2$ (5.7 mg, 0.0063 mmol, 0.025 equiv.) and Xphos ligand (5.9 mg, 0.0125 mmol, 0.050 equiv.) in dry toluene (2.0 mL), compound **5k** (70.1 mg, 0.25 mmol, 1.0 equiv.), morpholine (32.7 mg, 0.37 mmol, 1.5 equiv.), and ^{t}BuOK (56.1 mg, 0.5 mmol, 2.0 equiv.) were added. The reaction mixture was then stirred under argon at 100°C and monitored by TLC. After completion, the mixture was concentrated under reduced pressure and purified by flash column chromatography (50:50 *n*-hexane/EtOAc) to afford the pure product **8** (52% Yield, 43.2 mg, 0.13 mmol).



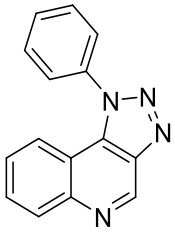
4-(4-(1*H*-[1,2,3]triazolo[4,5-*c*]quinolin-1-yl)phenyl)morpholine, 8: 52% yield, 43.2 mg, 0.13 mmol; grey solid; mp: 245-247 °C; R_f = 0.21 (*n*-hexane-EtOAc, 50:50); IR (neat): 2841, 1527, 1110, 754, 560 cm^{-1}; ^{1}H NMR (400.13 MHz, $CDCl_3$) δ 9.51 (s, 1H), 8.22 (d, *J* = 8.2 Hz, 1H), 7.75 – 7.66 (m, 2H), 7.49 – 7.38 (m, 3H), 7.09 – 7.02 (m, 2H), 3.86 (t, *J* = 4.8 Hz, 4H), 3.28 (t, *J* = 4.8 Hz, 4H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 152.6 (C), 145.9 (C), 145.0 (CH), 140.3 (C), 133.9 (C), 130.7 (CH), 129.7 (CH), 128.1 (C), 127.4 (CH), 127.3 (CH), 121.8 (CH), 115.5 (CH), 66.7 (CH_2), 48.4 (CH_2); MS (EI, 70 eV): *m/z* (%)= 300 (100), 115 (55), 207 (36), 331 (M^+, 4); HRMS: *m/z* $[M + H]^+$ calcd for $C_{19}H_{18}N_5O$: 332.1506; found: 332.1528.

2.6. Procedure for the synthesis of compound 9



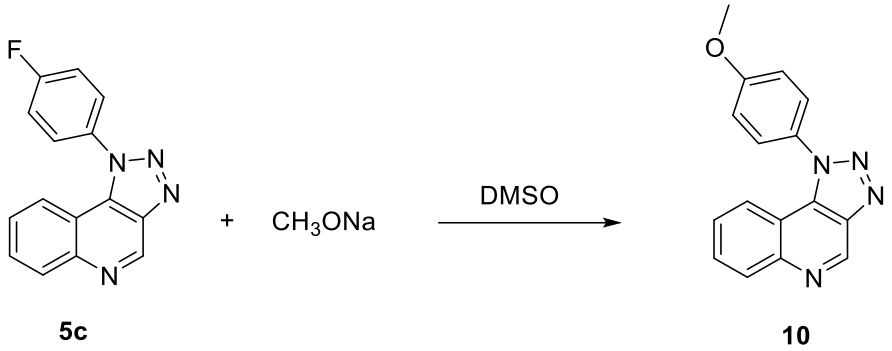
5k **9**

To a mixture of $Pd(OAc)_2$ (1.4 mg, 0.0062 mmol, 0.025 equiv.) and Et_3N (75.9 mg, 0.75 mmol, 3.0 equiv.) in dry DMSO (2.0 mL), compound **5k** (70 mg, 0.25 mmol, 1.0 equiv.) and formic acid (0.023 g, 0.50 mmol, 2.000 equiv.) were added. The reaction mixture was then stirred under argon at 120°C and monitored by TLC. After completion, the mixture was diluted with diethyl ether, extracted with brine, dried over anhydrous Na_2SO_4, and concentrated under reduced pressure. The residue was purified by flash column chromatography (60:40 *n*-hexane/EtOAc) to afford the pure product **9** (71% Yield, 43.8 mg, 0.1775 mmol).



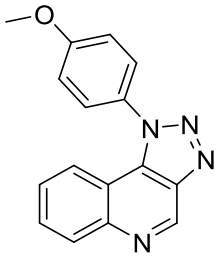
1-phenyl-1*H*-[1,2,3]triazolo[4,5-*c*]quinoline, 9: 71% yield, 43.8 mg, 0.1775 mmol; pale yellow solid; mp: 153-155 °C; R_f = 0.16 (*n*-hexane-EtOAc, 60:40); IR (neat): 3073, 1504, 992, 767, 696 cm^{-1}; ^1H NMR (400.13 MHz, $CDCl_3$) δ 9.52 (s, 1H), 8.23 (d, *J* = 8.1 Hz, 1H), 7.79 – 7.66 (m, 7H), 7.44 – 7.39 (m, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 145.9 (C), 144.9 (CH), 140.4 (C), 137.1 (C), 130.82 (CH), 130.80 (C), 130.1 (CH), 129.94 (CH), 129.90 (C), 127.4 (CH), 126.5 (CH), 121.7 (CH), 115.2 (C); MS (EI, 70 eV): *m/z* (%)= 218 (100), 190 (37), 77 (40), 246 (M^+, 15); HRMS: *m/z* $[M + H]^+$ calcd for $C_{15}H_{11}N_4$: 247.0978; found: 247.0999.

2.7. Procedure for the synthesis compound 10



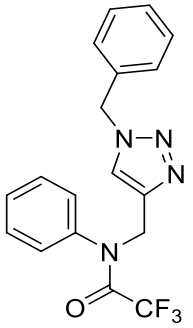
5c **10**

Compound **5c** (66 mg, 0.250 mmol, 1.000 equiv.) and sodium methoxide (20.2 mg, 0.375 mmol, 1.5 equiv.) were added to DMSO (2 mL). The reaction mixture was stirred at 140°C for 10 hours and monitored by TLC. Upon completion, the mixture was diluted with diethyl ether, extracted with brine, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash column chromatography (70:30 *n*-hexane/EtOAc) to afford the pure product **10** (78% Yield, 54.0 mg, 0.195 mmol).

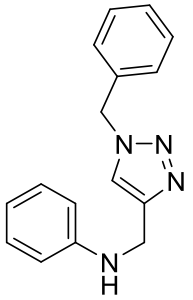


1-(4-methoxyphenyl)-1*H*-[1,2,3]triazolo[4,5-*c*]quinoline, 10: 78% yield, 54.0 mg, 0.195 mmol; brown solid; mp: 174-176 °C; R_f = 0.22 (*n*-hexane-EtOAc, 70:30); IR (neat): 2922, 1522, 1253, 843, 760 cm^{-1}; ^1H NMR (400.13 MHz, $CDCl_3$) δ 9.52 (s, 1H), 8.22 (d, *J* = 8.8 Hz, 1H), 7.73 – 7.63 (m, 2H), 7.53 – 7.46 (m, 2H), 7.44 – 7.38 (m, 1H), 7.14 – 7.07 (m, 2H), 3.89 (*s*, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 161.3 (C), 145.9 (C), 144.9 (CH), 140.3 (C), 133.9 (C), 130.7 (CH), 129.83 (CH), 129.67 (C), 127.9 (CH), 127.4 (CH), 121.7 (CH), 115.3 (C), 115.1 (CH), 55.8 (CH_3); MS (EI, 70 eV): *m/z* (%)= 205 (100), 233 (75), 151 (16), 276 (M^+, 10); HRMS: *m/z* $[M + H]^+$ calcd for $C_{16}H_{13}N_4O$: 277.1084; found: 277.1069.

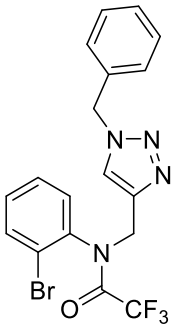
CHARACTERIZATION DATA OF COMPOUNDS 1a, 1a', 2a-q, 3a-h



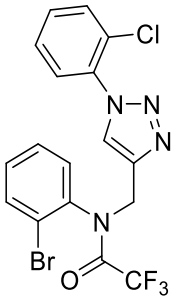
***N*-((1-benzyl-1*H*-1,2,3-triazol-4-yl)methyl)-2,2,2-trifluoro-*N*-phenylacetamide, 1a:** 91% yield, 327.6 mg, 0.91 mmol; white solid; mp: 100-102 °C; R_f = 0.21 (*n*-hexane-EtOAc, 80:20); IR (neat): 3118, 2359, 1685, 1455, 1074, 747 cm^{-1}; ^1H NMR (400.13 MHz, $CDCl_3$) δ 7.58 (s, 1H), 7.42 – 7.32 (s, 6H), 7.27 – 7.21 (m, 2H), 7.19 – 7.11 (m, 2H), 5.52 (s, 2H), 4.94 (s, 2H), 4.36; ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 156.9 (q, J_{C-F} = 36.2 Hz) (C), 142.4 (C), 139.0 (C), 134.5 (C), 129.4 (CH), 129.3 (CH), 129.1 (CH), 128.8 (CH), 128.2 (CH) 128.0 (CH), 123.9 (CH), 116.2 (q, J_{C-F} = 287.2 Hz) (C), 54.2 (CH_2), 47.3 (CH_2); HRMS: *m/z* $[M + H]^+$ calcd for $C_{18}H_{16}F_3N_4O$: 361.1249; found: 361.1255.



***N*-((1-benzyl-1*H*-1,2,3-triazol-4-yl)methyl)aniline, 1a':** 89% yield, 214.6 mg, 0.81 mmol; pale yellow liquid; R_f = 0.20 (*n*-hexane-EtOAc, 75:25); IR (neat): 3680, 2965, 1594, 1320, 1119, 747 cm^{-1}; ^1H NMR (400.13 MHz, $CDCl_3$) δ 7.21 – 7.09 (m, 4H), 7.04 – 6.91 (m, 4H), 6.52 (t, *J* = 7.4 Hz, 1H), 6.43 (d, *J* = 7.6 Hz, 2H), 5.24 (s, 2H), 4.20 (s, 2H), 3.78 (bs, NH, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 147.6 (C), 146.6 (C), 134.7 (C), 129.2 (CH), 129.1 (CH), 128.7 (CH), 128.0 (CH), 121.6 (CH), 118.0 (CH), 113.2 (CH), 54.1 (CH_2), 39.9 (CH_2); HRMS: *m/z* $[M + H]^+$ calcd for $C_{16}H_{17}N_4$: 265.1448; found: 265.1431.

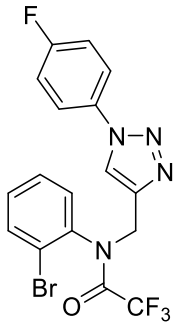


***N*-((1-benzyl-1*H*-1,2,3-triazol-4-yl)methyl)-*N*-(2-bromophenyl)-2,2,2-trifluoroacetamide, 2a:** 90% yield, 413.0 mg, 0.94 mmol; white solid; mp: 120-122 °C; R_f = 0.23 (*n*-hexane-EtOAc, 70:30); IR (neat): 3121, 3073, 1694, 1478, 1149, 719 cm^{-1}; ^1H NMR (400.13 MHz, $CDCl_3$) δ 7.59 – 7.56 (m, 1H), 7.50 (s, 1H), 7.31 - 7.28 (m, 3H), 7.20 – 7.14 (m, 4H), 7.00 - 6.96 (m, 1H), 5.49 (q, *J* = 14.6 Hz, 1H), 5.39 – 5.28 (m, 2H), 4.36 (d, *J* = 14.6 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 156.9 (q, J_{C-F} = 36.7 Hz) (C), 142.0 (C), 137.6 (C), 134.4 (C), 133.5 (CH), 131.6 (CH), 130.9 (CH), 129.2 (CH), 128.9 (CH), 128.2 (CH), 128.0 (CH), 124.0 (CH), 123.4 (C), 116.1 (d, J_{C-F} = 288.9 Hz) (C), 54.2 (CH_2), 45.7 (CH_2); ^{19}F NMR (376.5 MHz, $CDCl_3$) δ -68.9 (s); HRMS: *m/z* $[M + H]^+$ calcd for $C_{18}H_{15}BrF_3N_4O$: 439.0376; found: 439.0354.

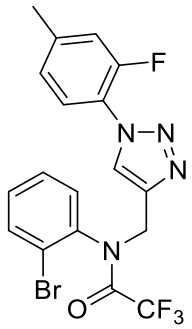


***N*-(2-bromophenyl)-*N*-((1-(2-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-2,2,2-trifluoroacetamide, 2b:** 93% yield, 425.0 mg, 0.93 mmol; white solid; mp: 121-123 °C; R_f = 0.19 (*n*-hexane-EtOAc, 70:30); IR (neat): 3144, 1698, 1481, 1153, 762 cm^{-1}; ^1H NMR (400.13 MHz, $CDCl_3$) δ 8.09 (s, 1H), 7.74 – 7.67 (m, 1H), 7.65 – 7.53 (m, 2H), 7.52 – 7.42 (m, 2H), 7.35 – 7.26 (m, 2H), 7.15 (dd, J_1 = 6.8 Hz, J_2 = 2.5 Hz, 1H), 5.57 (d, *J* = 14.8 Hz, 1H), 4.59 (d, *J* = 14.8 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 157.0 (q, J_{C-F} = 36.8 Hz) (C), 141.3 (C), 137.5 (C), 134.6 (C), 133.6 (CH), 131.6 (CH), 131.1 (CH), 131.0 (CH), 130.80 (CH), 130.78 (C), 128.7 (C), 128.3 (CH), 128.0 (CH),

127.7 (CH), 126.3 (CH), 123.5 (C), 116.0 (q, $J_{C\text{-}F}$ = 288.1 Hz) (C), 45.5 (CH_2); ^{19}F NMR (376.5 MHz, $CDCl_3$) δ -68.9 (s); HRMS: *m/z* $[M + H]^+$ calcd for $C_{17}H_{12}BrClF_3N_4O$: 458.9830; found: 458.9848.

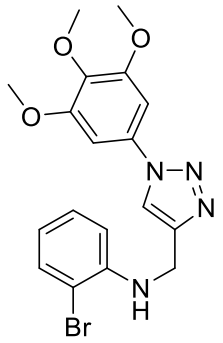


***N*-(2-bromophenyl)-2,2,2-trifluoro-*N*-((1-(4-fluorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)acetamide, 2c:** 85% yield, 376.5 mg, 0.85 mmol; brown solid; mp: 115-117 °C; R_f = 0.25 (*n*-hexane-EtOAc, 70:30); IR (neat): 3145, 3100, 1685, 1519, 1149, 833 cm^{-1}; ^1H NMR (400.13 MHz, $CDCl_3$) δ 8.05 (s, 1H), 7.68 – 7.61 (m, 3H), 7.27 – 7.19 (m, 2H), 7.18 –7.07 (m, 3H), 5.41 (d, *J* = 14.8 Hz, 1H), 4.40 (d, *J* = 14.8 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 162.5 (d, $J_{C\text{-}F}$ = 248.7 Hz) (C), 157.0 (q, $J_{C\text{-}F}$ = 36.7 Hz) (C), 142.5 (C), 137.8 (C), 133.6 (CH), 133.1 (d, $J_{C\text{-}F}$ = 2.9 Hz) (C), 131.5 (CH), 131.1 (CH), 128.3 (CH), 123.3 (C), 122.5 (d, $J_{C\text{-}F}$ = 8.5 Hz) (CH), 116.9 (CH), 116.7 (CH), 115.8 (q, $J_{C\text{-}F}$ = 288.4 Hz) (C), 46.9 (CH_2); ^{19}F NMR (376.5 MHz, $CDCl_3$) δ -68.9 (s), -111.8 (m); HRMS: *m/z* $[M + H]^+$ calcd for $C_{17}H_{12}BrF_4N_4O$: 443.0125; found: 443.0145.

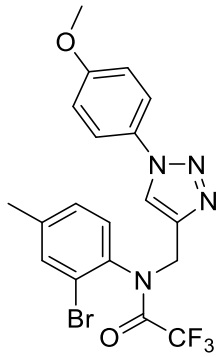


***N*-(2-bromophenyl)-2,2,2-trifluoro-*N*-((1-(2-fluoro-4-methylphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)acetamide, 2d:** 86% yield, 392.1 mg, 0.86 mmol; pale pink solid; mp: 83-85 °C; R_f = 0.17 (*n*-hexane-EtOAc, 70:30); IR (neat): 3178, 3076, 1694, 1477, 1143 cm^{-1}; ^1H NMR (400.13 MHz, $CDCl_3$) δ 8.14 (s, 1H), 7.83 – 7.61 (m, 2H), 7.37 – 7.24 (m, 2H), 7.22 – 6.98 (m, 3H), 5.54 (d, *J* = 14.8 Hz, 1H), 4.53 (d, *J* = 14.8 Hz, 1H), 2.43 (s, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 156.9 (q, $J_{C\text{-}F}$ = 36.6

Hz), 153.2 (d, $J_{C\text{-}F}$ = 248.8 Hz) (C), 141.8 (C), 141.5 (d, $J_{C\text{-}F}$ = 7.8 Hz) (C), 137.6 (C), 133.6 (CH), 131.6 (CH), 131.0 (CH), 128.3 (CH), 125.8 (d, $J_{C\text{-}F}$ = 3.1 Hz) (CH), 125.2 (d, $J_{C\text{-}F}$ = 7.6 Hz) (CH), 124.5 (CH), 123.4 (C), 122.5 (d, $J_{C\text{-}F}$ = 10.4 Hz) (C), 117.3 (d, $J_{C\text{-}F}$ = 19.6 Hz) (CH), 116.1 (q, $J_{C\text{-}F}$ = 288.5 Hz) (C), 45.6 (CH_2), 21.2 (CH_3); ^{19}F NMR (376.5 MHz, $CDCl_3$) δ -68.9 (s), -124.4 (t, *J* = 9.5 Hz); HRMS: *m/z* $[M + H]^+$ calcd for $C_{18}H_{14}BrF_4N_4O$: 457.0282; found: 457.0296.

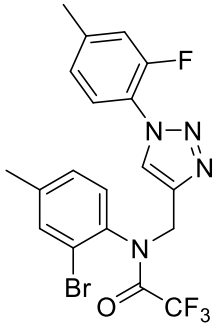


2-bromo-*N*-((1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)aniline, 2e: 81% yield, 337.8 mg, 0.81 mmol; pale yellow solid; mp: 138-140 °C; R_f = 0.20 (*n*-hexane-EtOAc, 70:30); IR (neat): 3346, 2938, 1595, 1508, 1126 cm^{-1}; ^1H NMR (400.13 MHz, $CDCl_3$) δ 7.90 (s, 1H), 7.48 (d, *J* = 7.8 Hz, 1H), 7.20 (t, *J* = 7.7 Hz, 1H), 6.94 (s, 2H), 6.79 (d, *J* = 8.1 Hz, 1H), 6.66 (t, *J* = 7.5 Hz, 1H), 4.65 (s, 2H), 4.24 (bs, 1H), 3.94 (s, 6H), 3.90 (s, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 153.9 (C), 146.7 (C), 144.1 (C), 138.3 (C), 132.9 (C), 132.6 (CH), 128.6 (CH), 120.2 (CH), 118.8 (CH), 111.9 (CH), 110.1 (C), 98.5 (CH), 61.1 (CH_3), 56.5 (CH_2), 40.1 (CH_3); HRMS: *m/z* $[M + H]^+$ calcd for $C_{18}H_{20}BrN_4O_3$: 419.0713; found: 419.0708.

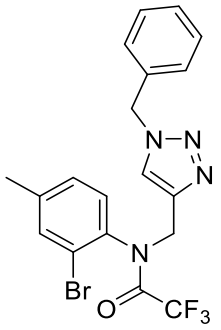


***N*-(2-bromo-4-methylphenyl)-2,2,2-trifluoro-*N*-((1-(4-methoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)acetamide, 2f:** 98% yield, 458.6 mg, 0.98 mmol; pale yellow solid; mp: 124-126 °C; R_f

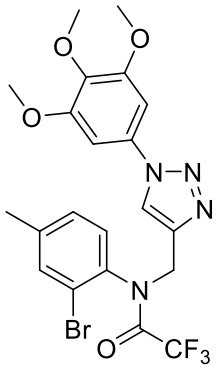
= 0.24 (*n*-hexane-EtOAc, 60:40); IR (neat): 3153, 2962, 1677, 1151, 600 cm-1; ^{1}H NMR (400.13 MHz, $CDCl_3$) δ 8.06 (s, 1H), 7.65 – 7.60 (m, 2H), 7.50 (d, J = 1.5 Hz, 1H), 7.07 (dd, J_1 = 8.1 Hz, J_2 = 1.2 Hz, 1H), 7.05 – 6.94 (m, 3H), 5.47 (d, J = 14.7 Hz, 1H), 4.45 (d, J = 14.7 Hz, 1H), 3.85 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 159.9 (C), 157, (q, $J_{C\text{-}F}$ = 36.5 Hz) (C), 142.2 (C), 141.7 (C), 135.0 (C), 133.9 (CH), 131.1 (CH), 130.3 (C), 128.9 (CH), 122.8 (C), 122.2 (CH), 122.0 (CH), 115.7 (q, $J_{C\text{-}F}$ = 285.2 Hz) (C), 114.8 (CH), 55.6 (CH_3), 46.0 (CH_2), 20.9 (CH_3); ^{19}F NMR (376.5 MHz, $CDCl_3$) δ -68.9 (s); HRMS: *m/z* $[M + H]^+$ calcd for $C_{19}H_{17}BrF_3N_4O_2$: 469.0481; found: 469.0497.



***N*-(2-bromo-4-methylphenyl)-2,2,2-trifluoro-*N*-((1-(2-fluoro-4-methylphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)acetamide, 2g:** 91% yield, 427.7 mg, 0.91 mmol; yellow solid; mp: 82-84 °C; R_f = 0.23 (*n*-hexane-EtOAc, 70:30); IR (neat): 3155, 1695, 1497, 1148, 823 cm^{-1}; ^{1}H NMR (400.13 MHz, $CDCl_3$) δ 8.14 (d, J = 2.5 Hz, 1H), 7.79 – 7.76 (m, 1H), 7.53 (s, 1H), 7.12 – 7.11 (m, 3H), 7.09 – 6.98 (m, 1H), 5.53 (d, J = 14.7 Hz, 1H), 4.50 (d, J = 14.7 Hz, 1H), 2.44 (s, 3H), 2.38 (s, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 157.1 (q, $J_{C\text{-}F}$ = 36.6 Hz) (C), 153.0 (d, $J_{C\text{-}F}$ = 250.5 Hz) (C), 141.9 (C), 141.7 (C), 141.4 (d, $J_{C\text{-}F}$ = 7.6 Hz) (C), 134.9 (C), 133.9 (CH), 131.1 (CH), 128.9 (CH), 125.8 (d, $J_{C\text{-}F}$ = 3.3 Hz) (CH), 125.2 (d, $J_{C\text{-}F}$ = 7.6 Hz) (CH), 124.5 (CH), 122.9 (C), 122.5 (d, $J_{C\text{-}F}$ = 7.6 Hz) (C), 117.3 (d, $J_{C\text{-}F}$ = 19.4 Hz) (CH), 115.9 (q, $J_{C\text{-}F}$ = 285.2 Hz), 45.7 (CH_2), 21.8 (CH_3), 20.9 (CH_3); ^{19}F NMR (376.5 MHz, $CDCl_3$) δ -68.9 (s), -124.4 (t, J = 9.5 Hz); HRMS: *m/z* $[M + H]^+$ calcd for $C_{19}H_{16}BrF_4N_4O$: 471.0438; found: 471.0422.

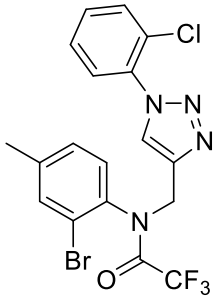


***N*-((1-benzyl-1*H*-1,2,3-triazol-4-yl)methyl)-*N*-(2-bromo-4-methylphenyl)-2,2,2-trifluoroacetamide, 2h:** 97% yield, 438.5 mg, 0.97 mmol; white solid; mp: 112-114 °C; R_f = 0.26 (*n*-hexane-EtOAc, 70:30); IR (neat): 3061, 1692, 1496, 1151, 727 cm^{-1}; ^1H NMR (400.13 MHz, $CDCl_3$) δ 7.58 (s, 1H), 7.47 (d, J_1 = 1.2 Hz, 1H), 7.43 – 7.36 (m, 3H), 7.29 – 7.24 (m, 2H), 7.09 - 7.04 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 6.91 (d, J = 8.0 Hz, 1H), 5.58 (d, J = 14.8 Hz, 1H), 5.43 (d, J = 14.8 Hz, 1H), 5.37 (d, J = 14.6 Hz, 1H), 4.39 (d, J = 14.6 Hz, 1H), 2.36 (s, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 157.1 (q, $J_{C\text{-}F}$ = 36.6 Hz) (C), 142.1 (C), 141.6 (C), 134.8 (C), 134.4 (C), 133.9 (CH), 131.0 (CH), 131.0 (CH), 129.1 (CH), 128.9 (CH), 128.0 (CH), 123.9 (CH), 122.9 (C), 115.8 (q, $J_{C\text{-}F}$ = 288.2 Hz) (C), 54.2 (CH_2), 45.8 (CH_2), 20.9 (CH_3); ^{19}F NMR (376.5 MHz, $CDCl_3$) δ -68.9 (s); HRMS: *m/z* $[M + H]^+$ calcd for $C_{19}H_{17}BrF_3N_4O$: 453.0532; found: 453.0519.

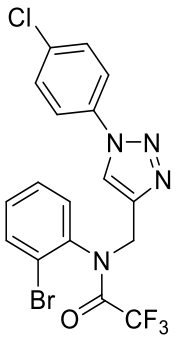


***N*-(2-bromo-4-methylphenyl)-2,2,2-trifluoro-*N*-((1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)acetamide, 2i:** 92% yield, 485.8 mg, 0.92 mmol; white solid; mp: 108-110 °C; R_f = 0.22 (*n*-hexane-EtOAc, 70:30); IR (neat): 3008, 1695, 1508, 1151, 774 cm^{-1}; ^1H NMR (400.13 MHz, $CDCl_3$) δ 8.08 (b*s*, 1H), 7.45 (s, 1H), 7.03 (d, J = 7.3 Hz, 1H), 6.97 – 6.82 (m, 3H), 5.39 (d, J = 12.9 Hz, 1H), 4.37 (d, J = 12.9 Hz, 1H), 3.86 (s, 6H), 3.81 (s, 3H), 2.29 (s, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 157.2 (q, $J_{C\text{-}F}$ = 36.7 Hz) (C), 153.9 (C), 142.4 (C), 141.7 (C), 138.4 (C), 135.1 (C), 134.0 (CH),

132.7 (C), 130.9 (CH), 128.9 (CH), 122.8 (C), 122.3 (C), 115.8 (q, $J_{C\text{-}F}$ = 287.5 Hz) (C), 98.2 (CH), 61.1 (CH_3), 56.4 (CH_3), 46.1 (CH_2), 20.9 (CH_3); ^{19}F NMR (376.5 MHz, $CDCl_3$) δ -68.9 (s); HRMS: *m/z* [M + H]$^+$ calcd for $C_{21}H_{21}BrF_3N_4O_4$: 529.0693; found: 529.0675.

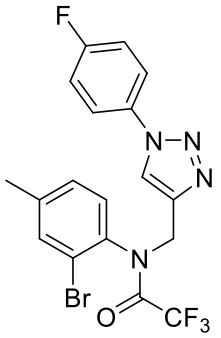


***N*-(2-bromophenyl)-*N*-((1-(2-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-2,2,2-trifluoroacetamide, 2j:** 89% yield, 419.3 mg, 0.89 mmol; pale brown solid; mp: 125-127 °C; R_f = 0.24 (*n*-hexane-EtOAc, 70:30); IR (neat): 3142, 1694, 1518, 1148, 840 cm^{-1}; ^{1}H NMR (400.13 MHz, $CDCl_3$) δ 8.09 (s, 1H), 7.67 – 7.56 (m, 2H), 7.53 (d, *J* = 1.2 Hz, 1H), 7.50 – 7.45 (m, 2H), 7.11 (dd, J_1 = 8.1 Hz, J_2 = 1.2 Hz, 1H), 7.01 (d, *J* = 8.1 Hz, 1H), 5.55 (d, *J* = 14.7 Hz, 1H), 4.55 (d, *J* = 14.7 Hz, 1H), 2.38 (s, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 157.1 (q, $J_{C\text{-}F}$ = 35.2 Hz) (C), 141.7 (C), 141.4 (C), 134.8 (C), 134.7 (C), 134.0 (CH), 131.1 (CH), 130.9 (CH), 130.7 (CH), 128.9 (CH), 128.6 (C), 127.9 (CH), 127.7 (CH), 126.1 (CH), 123.0 (C), 116.1 (q, $J_{C\text{-}F}$ = 288.0 Hz) (C), 45.6 (CH_2), 20.9 (CH_3); ^{19}F NMR (376.5 MHz, $CDCl_3$) δ -68.9 (s); HRMS: *m/z* [M + H]$^+$ calcd for $C_{18}H_{14}BrClF_3N_4O$: 472.9986; found: 472.9966.

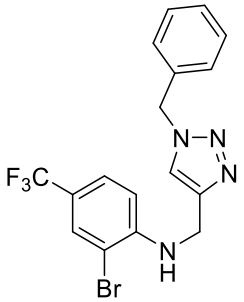


***N*-(2-bromophenyl)-*N*-((1-(4-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-2,2,2-trifluoroacetamide, 2k:** 93% yield, 426.5 mg, 0.93 mmol; pale yellow solid; mp: 127-129 °C; R_f = 0.21 (*n*-hexane-EtOAc, 70:30); IR (neat): 3146, 1698, 1473, 1155, 727 cm^{-1}; ^{1}H NMR (400.13 MHz,

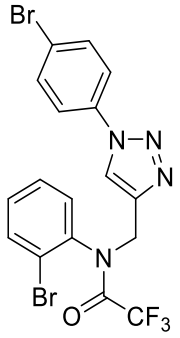
$CDCl_3$) δ 8.16 (s, 1H), 7.76 – 7.68 (m, 3H), 7.55 – 7.50 (m, 2H), 7.38 – 7.30 (m, 2H), 7.23 – 7.14 (m, 1H), 5.51 (d, *J* = 14.7 Hz, 1H), 4.50 (d, *J* = 14.7 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 157 (q, $J_{C\text{-}F}$ = 36.7 Hz) (C), 142.6 (C), 137.8 (C), 135.3 (C), 134.8 (C), 133.7 (CH), 131.5 (CH), 131.1 (CH), 130.0 (CH), 128.4 (CH), 123.3 (C), 122.2 (CH), 121.6 (CH), 115.9 (q, $J_{C\text{-}F}$ = 285.8 Hz) (C), 46.0 (CH_2); ^{19}F NMR (376.5 MHz, $CDCl_3$) δ -68.9 (s); HRMS: *m/z* $[M + H]^+$ calcd for $C_{17}H_{12}BrClF_3N_4O$: 458.9830; found: 458.9848.



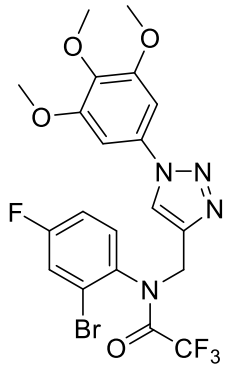
***N*-(2-bromo-4-methylphenyl)-2,2,2-trifluoro-*N*-((1-(4-fluorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)acetamide, 2l:** 94% yield, 428.6 mg, 0.94 mmol; yellow solid; mp: 128-130 °C; R_f = 0.19 (*n*-hexane-EtOAc, 70:30); IR (neat): 3138, 1695, 1518, 1144, 840 cm^{-1}; ^{1}H NMR (400.13 MHz, $CDCl_3$) δ 8.13 (s, 1H), 7.78 – 7.71 (m, 2H), 7.54 (d, *J* =1.2 Hz, 1H), 7.29 – 7.21 (m, 2H), 7.13 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.03 (d, J_1 = 8.0 Hz, 1H), 5.49 (d, *J* = 14.6 Hz, 1H), 4.48 (d, *J* = 14.6 Hz, 1H), 2.39 (s, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 162.5 (d, $J_{C\text{-}F}$ = 248.5 Hz) (C), 157.2 (q, $J_{C\text{-}F}$ = 37.2 Hz) (C), 142.6 (C), 141.8 (C), 135.1 (C), 134.0 (CH), 133.2 (C), 131.0 (CH), 129.0 (CH), 122.8 (C), 122.5 (CH), 122.4 (d, $J_{C\text{-}F}$ = 3.7 Hz) (CH), 116.8 (d, $J_{C\text{-}F}$ = 23.1 Hz) (CH), 115.8 (q, $J_{C\text{-}F}$ = 288.2 Hz) (C), 46.1 (CH_2), 20.9 (CH_3); ^{19}F NMR (376.5 MHz, $CDCl_3$) δ -68.9 (s), -111.8 (m); HRMS: *m/z* $[M + H]^+$ calcd for $C_{18}H_{14}BrF_4N_4O$: 457.0282; found: 457.0275.



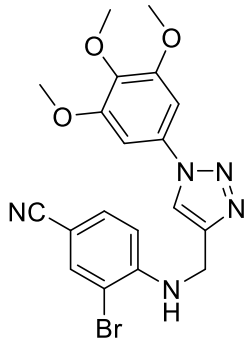
***N*-((1-benzyl-1H-1,2,3-triazol-4-yl)methyl)-2-bromo-4-(trifluoromethyl)aniline, 2m:** 70% yield, 287.7 mg, 0.70 mmol; yellow solid; mp: 118-120 °C; R_f = 0.16 (*n*-hexane-EtOAc, 75:25); IR (neat): 3378, 3068, 1324, 1109, 745 cm^{-1}; ^1H NMR (400.13 MHz, $CDCl_3$) δ 7.67 (d, *J* = 1.2 Hz, 1H), 7.45 – 7.32 (m, 5H), 7.31 – 7.21 (m, 2H), 6.70 (d, *J* = 8.6 Hz, 1H), 5.51 (s, 2H), 5.22 (bs, 1H), 4.54 (d, *J* = 5.7 Hz, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 146.8 (C), 145.3 (C), 134.5 (C), 129.6 (q, J_{C-F} = 3.7 Hz) (CH), 129.2 (CH), 128.8 (CH), 128.0 (CH), 125.8 (q, J_{C-F} = 3.7 Hz) (CH), 123.8 (q, J_{C-F} = 271.8 Hz) (C), 121.6 (CH), 119.9 (q, J_{C-F} = 33.3 Hz) (C), 110.6 (CH), 108.9 (C), 54.3 (CH_2), 39.6 (CH_2); ^{19}F NMR (376.5 MHz, $CDCl_3$) δ -60.9 (s); HRMS: *m/z* $[M + H]^+$ calcd for $C_{17}H_{15}BrF_3N_4$: 411.0354; found: 411.0337.



***N*-(2-bromophenyl)-*N*-((1-(4-bromophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-2,2,2-trifluoroacetamide, 2n:** 81% yield, 408.3 mg, 0.81 mmol; pale yellow solid; mp: 135-137 °C; R_f = 0.22 (*n*-hexane-EtOAc, 85:15); IR (neat): 3149, 1698, 1483, 1159, 731 cm^{-1}; ^1H NMR (400.13 MHz, $CDCl_3$) δ 8.16 (s, 1H), 7.75 – 7.71 (m, 1H), 7.71 – 7.63 (m, 4H), 7.38 – 7.29 (m, 2H), 7.21 – 7.14 (m, 1H), 5.50 (d, *J* = 14.7 Hz, 1H), 4.50 (d, *J* = 14.7 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 156.9 (q, J_{C-F} = 36.2 Hz), 142.7 (C), 137.8 (C), 135.8 (C), 133.7 (CH), 133.0 (CH), 131.5 (CH), 131.1 (CH), 128.4 (CH), 123.3 (C), 122.6 (C), 122.1 (CH), 121.9 (CH), 115.7 (q, J_{C-F} = 285.1 Hz), 46.0 (CH_2); ^{19}F NMR (376.5 MHz, $CDCl_3$) δ -68.9 (s); HRMS: *m/z* $[M + H]^+$ calcd for $C_{17}H_{12}Br_2F_3N_4O$: 504.9304; found: 504.9327.

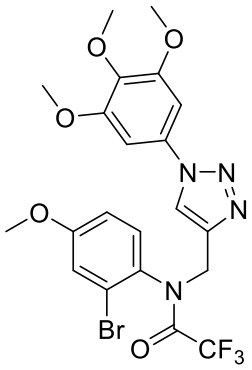


***N*-(2-bromo-4-fluorophenyl)-2,2,2-trifluoro-*N*-((1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)acetamide, 2o:** 73% yield, 389.3 mg, 0.73 mmol; white solid; mp: 118-120 °C; R_f = 0.22 (*n*-hexane-EtOAc, 60:40); IR (neat): 3723, 1705, 1504, 1151, 773 cm^{-1}; ^1H NMR (400.13 MHz, $CDCl_3$) δ 8.13 (*s*, 1H), 7.46 (dd, J_1 = 7.8 Hz, J_2 = 2.7 Hz, 1H), 7.23 – 7.14 (m, 1H), 7.10 – 7.02 (m, 1H), 6.96 (s, 2H), 5.48 (d, *J* = 14.8 Hz, 1H), 4.43 (d, *J* = 14.8 Hz, 1H), 3.94 (s, 6H), 3.89 (s, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 162.4 (d, J_{C-F} = 255.5 Hz) (C), 157.1 (q, J_{C-F} = 36.7 Hz) (C), 153.9 (C), 142.1 (C), 138.4 (C), 134.8 (d, J_{C-F} = 3.4 Hz) (C), 133.7 (d, J_{C-F} = 9.0 Hz) (CH), 132.6.0 (C), 124.2 (d, J_{C-F} = 10.2 Hz) (C), 122.3 (CH), 121.0 (d, J_{C-F} = 25.6 Hz) (CH), 115.8 (q, J_{C-F} = 288.0 Hz) (C), 115.5 (d, J_{C-F} = 22.3 Hz) (CH), 98.2 (CH), 61.0 (CH_3), 56.4 (CH_3), 46.0 (CH_2); ^{19}F NMR (376.5 MHz, $CDCl_3$) δ -68.9 (s), -68.9 (s), -111.8 (m); HRMS: *m/z* $[M + H]^+$ calcd $C_{20}H_{18}BrF_4N_4O_4$: 535.0442; found: 535.0463.

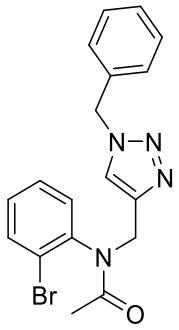


3-bromo-4-(((1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)amino)benzonitrile, 2p: 90% yield, 400,0 mg, 0.9 mmol; white solid; mp: 121-123 °C; R_f = 0.22 (*n*-hexane-EtOAc, 50:50); IR (neat): 3753, 3712, 3252, 2158, 2029, 1510, 1127, 826 cm^{-1}; ^1H NMR (400.13 MHz, $CDCl_3$) δ 7.81 (*s*, 1H), 7.63 (s, 1H), 7.38 (d, *J* = 8.4 Hz, 1H), 6.84 (s, 2H), 6.69 (d, *J* = 8.4 Hz, 1H), 5.42 (bs, 1H),

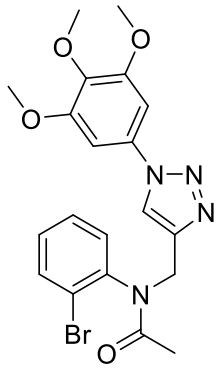
4.58 (s, 2H), 3.85 (s, 6H), 3.81 (s, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 153.9 (C), 147.6 (C), 144.9 (C), 138.6 (C), 135.9 (CH), 133.0 (CH), 132.7 (C), 120.2 (CH), 118.7(C), 110.8 (CH), 109.0 (C), 100.6 (C), 98.6 (CH), 61.1 (CH_3), 56.5 (CH_3), 39.4 (CH_2); HRMS: *m/z* $[M + H]^+$ calcd for $C_{19}H_{19}BrN_5O_3$: 444.0666; found: 444.0689.



***N*-(2-bromo-4-methoxyphenyl)-2,2,2-trifluoro-*N*-((1-(3,4,5-trimethoxyphenyl)-1H-1,2,3-triazol-4-yl)methyl)acetamide 2q:** 85% yield, 463.5 mg, 0.85 mmol; white solid; mp: 119-121 °C; R_f = 0.23 (*n*-hexane-EtOAc, 60:40); IR (neat): 3711, 2158, 1702, 1500, 1156, 775 cm^{-1}; ^{1}H NMR (400.13 MHz, $CDCl_3$) δ 8.13 (s, 1H), 7.24 (d, *J* = 2.7 Hz, 1H), 7.064 (d, *J* = 8.9 Hz, 1H), 6.97 (s, 2H), 6.93 (dd, J_1 = 8.9 Hz, J_2 = 2.7 Hz, 1H), 5.47 (d, *J* = 14.4 Hz, 1H), 4.46 (d, *J* = 14.4 Hz, 1H), 3.89 (s, 6H), 3.90 (s, 3H), 3.84 (s, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 160.6 (C), 157.4 (q, $J_{C\text{-}F}$ = 36.2 Hz) (C), 154.0 (C), 142.5 (C), 138.4 (C), 132.7 (C), 131.9 (CH), 130.3 (C), 123.9 (C), 122.3 (CH), 118.8 (CH), 115.9 (q, $J_{C\text{-}F}$ = 287.5 Hz) (C), 113.6 (CH), 98.2 (CH), 61.1 (CH_3), 56.5 (CH_3), 55.8 (CH_3), 46.2 (CH_2); ^{19}F NMR (376.5 MHz, $CDCl_3$) δ -68.9 (s); HRMS: *m/z* $[M + H]^+$ calcd for $C_{21}H_{21}BrF_3N_4O_5$: 545.0642; found: 545.0623.

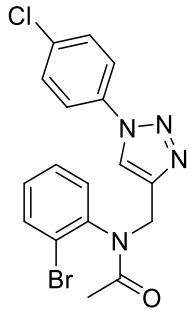


***N*-((1-benzyl-1*H*-1,2,3-triazol-4-yl)methyl)-N-(2-bromophenyl)acetamide, 3a:** 92% yield, 365.7 mg, 0.95 mmol; pale yellow solid; mp: 112-114 °C; R_f = 0.20 (*n*-hexane-EtOAc, 60:40); IR (neat): 3139, 2955, 1655, 1369, 1044, 709 cm^{-1}; ^1H NMR (400.13 MHz, $CDCl_3$) δ 7.65 (dd, J_1 = 8.0 Hz, J_2 = 1.3 Hz, 1H), 7.60 (s, 1H), 7.41 – 7.35 (m, 3H), 7.32 – 7.19 (m, 4H), 7.11 (dd, J_1 = 8.0 Hz, J_2 = 1.3 Hz, 1H), 5.56 (d, *J* = 14.8 Hz, 1H), 5.44 (d, *J* = 14.8 Hz, 1H), 5.26 (d, *J* = 14.8 Hz, 1H), 4.45 (d, *J* = 14.8 Hz, 1H), 1.80 (s, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 170.4 (C), 144.1 (C), 141.5 (C), 134.7 (C), 133.8 (CH), 131.0 (CH), 130.0 (CH), 129.1 (CH), 128.8 (CH), 128.7 (CH), 128.0 (CH), 123.7 (CH), 123.6 (C), 54.1 (CH_2), 43.6 (CH_2), 22.3 (CH_3); HRMS: *m/z* $[M + H]^+$ calcd for $C_{18}H_{18}BrN_4O$: 385.0858; found: 385.0839.

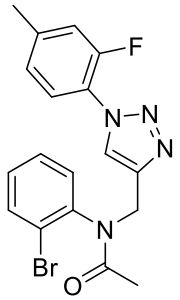


***N*-(2-bromophenyl)-*N*-((1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)acetamide, 3b:** 96% yield, 442.6 mg, 0.96 mmol; pale yellow solid; mp: 156-158 °C; R_f = 0.24 (*n*-hexane-EtOAc, 60:40); IR (neat): 3117, 2983, 1663, 1473, 763 cm^{-1}; ^1H NMR (400.13 MHz, $CDCl_3$) δ 8.13 (s, 1H), 7.67 (dd, J_1 = 8.0 Hz, J_2 = 1.0 Hz, 1H), 7.30 – 7.21 (m, 1H), 7.20 – 7.08 (m, 2H), 6.89 (s, 2H), 5.28 (d, *J* = 14.8 Hz, 1H), 4.36 (d, *J* = 14.8 Hz, 1H), 3.85 (s, 6H), 3.80 (s, 3H), 1.75 (s, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 170.6 (C), 153.9 (C), 144.4 (C), 141.6 (C), 138.2 (C), 133.8 (CH), 132.9 (C), 130.9

(CH), 130.1 (CH), 128.9 (CH), 123.5 (C), 122.1 (CH), 98.1 (CH), 61.0 (CH_3), 56.4 (CH_3), 43.8 (CH_2), 22.3 (CH_3); HRMS: *m/z* $[M + H]^+$ calcd for $C_{20}H_{22}BrN_4O_4$: 461.0819; found: 461.0833.

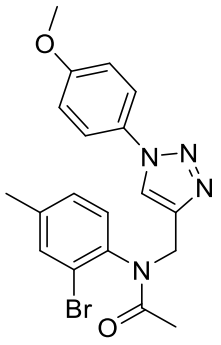


***N*-(2-bromophenyl)-*N*-((1-(2-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)acetamide, 3c:** 85% yield, 344.2 mg, 0.85 mmol; yellow liquid; R_f = 0.18 (*n*-hexane-EtOAc, 60:40); IR (neat): 3068, 1665, 1476, 1038, 759 cm^{-1}; ^1H NMR (400.13 MHz, $CDCl_3$) δ 7.61 (s, 1H), 7.59 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.58 – 7.56 (m, 2H), 7.48 – 7.44 (m, 2H), 7.35 (td, J_1 = 7.6 Hz, J_2 = 1.2 Hz, 1H), 7.29 – 7.16 (m, 2H), 5.41 (d, *J* = 14.8 Hz, 1H), 4.57 (d, *J* = 14.8 Hz, 1H), 1.86 (s, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 170.5 (C), 143.5 (C), 141.5 (C), 134.9 (C), 133.8 (CH), 131.1 (CH), 130.7 (CH), 130.1 (CH), 128.9 (CH), 128.7 (C), 127.9 (CH), 127.8 (CH), 125.9 (CH), 123.7 (C), 43.5 (CH_2), 22.3 (CH_3); HRMS: *m/z* $[M + H]^+$ calcd for $C_{17}H_{15}BrClN_4O$: 405.0112; found: 405.0127.

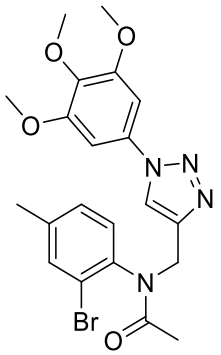


***N*-(2-bromophenyl)-*N*-((1-(2-fluoro-4-methylphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)acetamide, 3d:** 85% yield, 341.7 mg, 0.85 mmol; white oil; R_f = 0.25 (*n*-hexane-EtOAc, 50:50); IR (neat): 3178, 1657, 1046, 766, 562 cm^{-1}; ^1H NMR (400.13 MHz, $CDCl_3$) δ 8.16 (s, 1H), 7.78 (t, *J* = 7.9 Hz, 1H), 7.70 (d, *J* = 7.7 Hz, 1H), 7.36 (t, *J* = 7.1 Hz, 1H), 7.31 – 7.18 (m, 2H), 7.17 – 7.06 (m, 2H), 5.42 (d, *J* = 14.8 Hz, 1H), 4.53 (d, *J* = 14.8 Hz, 1H), 2.49 (s, 3H), 1.86 (s, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 170.5 (C), 153.2 (d, J_{C-F} = 250.9 Hz) (C), 143.7 (C), 141.5 (C), 141.2 (d, J_{C-F} = 7.9 Hz) (C),133.8 (CH), 131.1 (CH), 130.1 (CH), 128.9 (CH), 125.7 (d, J_{C-F} = 3.1 Hz) (CH), 125.1 (d, J_{C-F} = 7.3 Hz) (C), 124.5

(CH), 123.7 (C), 122.7 (d, $J_{C\text{-}F}$ = 10.1 Hz) (C), 117.3 (d, $J_{C\text{-}F}$ = 19.7 Hz) (CH), 43.5 (CH_2), 22.3 (CH_3), 21.2 (CH_3); ^{19}F NMR (376.5 MHz, $CDCl_3$) δ -124.30 (t, *J* = 9.5 Hz); HRMS: *m/z* $[M + H]^+$ calcd for $C_{18}H_{17}BrFN_4O$: 403.0564; found: 403.0539.

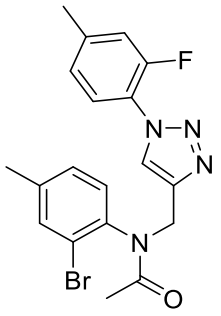


***N*-(2-bromo-4-methylphenyl)-*N*-((1-(4-methoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)acetamide, 3e:** 98% yield, 405.7 mg, 0.98 mmol; white solid; mp: 120-122 °C; R_f = 0.24 (*n*-hexane-EtOAc, 60:40); IR (neat): 3144, 1649, 1431, 1042, 567 cm^{-1}; ^1H NMR (400.13 MHz, $CDCl_3$) δ 8.20 (bs, 1H), 7.66 (d, *J* = 7.3 Hz, 2H), 7.51 (s, 1H), 7.20 – 6.92 (m, 4H), 5.35 (bs, 1H), 4.46 (bs, 1H), 3.88 (s, 3H), 2.37 (s, 3H), 1.85 (s, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 170.7 (C), 159.7 (C), 144.3 (CH), 141.3 (C), 140.5 (C), 138.9 (C), 134.1 (CH), 130.5 (C), 130.4 (CH), 129.6 (CH), 123.1 (C), 122.0 (CH), 114.7 (CH), 55.6 (CH_3), 43.8 (CH_2), 22.3 (CH_3), 20.8 (CH_3); HRMS: *m/z* $[M + H]^+$ calcd for $C_{19}H_{20}BrN_4O_2$: 415.0764; found: 415.0776.

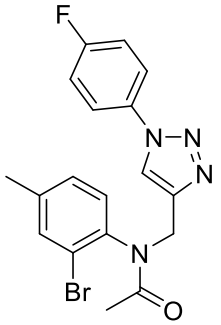


***N*-(2-bromo-4-methylphenyl)-*N*-((1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)acetamide, 3f:** 83% yield, 394.2 mg, 0.83 mmol; white oil; mp: 138-140 °C; R_f = 0.22 (*n*-hexane-EtOAc, 60:40); IR (neat): 3415, 2967, 1656, 1127, 572 cm^{-1}; ^1H NMR (400.13 MHz, $CDCl_3$) δ 8.14 (s, 1H), 7.51 (s, 1H), 7.13 (d, *J* = 7.8 Hz, 1H), 7.04 (d, *J* = 7.8 Hz, 1H), 6.97 (s, 2H), 5.33

(d, *J* = 14.8 Hz, 1H), 4.44 (d, *J* = 14.8 Hz, 1H), 3.94 (s, 6H), 3.89 (s, 3H), 2.36 (s, 3H), 1.84 (s, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 170.8 (C), 153.9 (C), 144.4 (C), 140.6 (C), 138.9 (C), 138.2 (C), 134.2 (CH), 132.9 (C), 130.4 (CH), 129.6 (CH), 123.0 (C), 122.1 (CH), 98.1 (CH), 61.1 (CH_3), 56.5 (CH_3), 43.8 (CH_2), 22.3 (CH_3), 20.8 (CH_3); HRMS: *m/z* $[M + H]^+$ calcd for $C_{21}H_{24}BrN_4O_4$: 475.0975; found: 475.0954.



***N*-(2-bromo-4-methylphenyl)-*N*-((1-(2-fluoro-4-methylphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)acetamide, 3g:** 99% yield, 411.8 mg, 0.99 mmol; yellow solid; mp: 119-121 °C; R_f = 0.21 (*n*-hexane-EtOAc, 50:50); IR (neat): 3074, 2922, 1665, 1042, 824 cm^{-1}; ^{1}H NMR (400.13 MHz, $CDCl_3$) δ 8.15 (s, 1H), 7.77 (t, *J* = 7.8 Hz, 1H), 7.51 (s, 1H), 7.19 – 6.93 (m, 4H), 5.39 (d, *J* = 14.8 Hz, 1H), 4.48 (d, *J* = 14.8 Hz, 1H), 2.44 (s, 3H), 2.37 (s, 3H), 1.85 (s, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 170.7 (C), 154.2 (d, J_{C-F} = 60.3 Hz) (C), 152.0 (C), 143.9 (C), 141.2 (d, J_{C-F} = 7.3 Hz) (C), 140.5 (C), 138.8 (C), 134.1 (CH), 130.5 (CH), 129.6 (CH), 125.7 (d, J_{C-F} = 3.1 Hz) (CH), 124.9 (d, J_{C-F} = 7.5 Hz) (C), 124.5 (CH), 123.2 (C), 117.30 (d, J_{C-F} = 19.5 Hz) (CH), 43.8 (CH_2), 22.3 (CH_3), 21.2 (CH_3), 20.8 (CH_3); ^{19}F NMR (376.5 MHz, $CDCl_3$) δ -124.3 (m); HRMS: *m/z* $[M + H]^+$ calcd for $C_{19}H_{19}BrFN_4O$: 417.0721; found: 417.0740.



***N*-(2-bromo-4-methylphenyl)-*N*-((1-(4-fluorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)acetamide, 3h:** 93% yield, 374.8 mg, 0.93 mmol; white solid; mp: 155-157 °C; R_f = 0.23 (*n*-hexane-EtOAc, 60:40); IR (neat): 3140, 1653, 1515, 1042, 839 cm^{-1}; ^1H NMR (400.13 MHz, $CDCl_3$) δ 8.12 (s, 1H), 7.76 – 7.67 (m, 2H), 7.50 (d, *J* = 1.5 Hz, 1H), 7.25 – 7.14 (m, 2H), 7.13 – 7.05 (m, 2H), 5.33 (d, *J* = 14.8 Hz, 1H), 4.45 (d, *J* = 14.8 Hz, 1H), 2.36 (s, 3H), 1.84 (s, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 170.8 (C), 162.3 (d, J_{C-F} = 250.1 Hz) (C), 144.7 (C), 140.6 (C), 139.0 (C), 134.2 (CH), 133.3 (d, J_{C-F} = 3.0 Hz) (C), 130.4 (CH), 129.7 (CH), 123.1 (C), 122.4 (d, J_{C-F} = 8.7 Hz) (CH), 122.1 (CH), 116.6 (d, J_{C-F} = 23.2 Hz) (CH), 43.8 (CH_2), 22.3 (CH_3), 20.8 (CH_3); ^{19}F NMR (376.5 MHz, $CDCl_3$) δ -111.8 (m); HRMS: *m/z* $[M + H]^+$ calcd for $C_{18}H_{17}BrFN_4O$: 403.0564; found: 403.0580.

References

S1. Leggy, Arnold A.; Wenchen, Luo; and Kiplin, Guy R.; **Org. Lett.,** *2004*, 6, 17, 3005 – 3007.

S2. Losa, Romain; Lorton, Charlotte; Retailleau, Pascal; Bignon, Jérôme; and Voituriez, Arnaud; **Org. Lett.,** *2023*, 25, 27, 5140 – 5144.

S3. Benedí, Carolina; Bravo, Fernando; Uriz, Pedro; Fernández, Elena; Claver, Carmen; and Castillón, Sergio; **Tetrahedron Lett**., *2003*, 44, 6073 – 6077.

S4. Alcaide Benito, Almendros Pedro, Cembellín Sara, Martínez Teresa del Campo, Alejandro Muñoza; **Chem. Commun.,** *2016*, 52, 6813 - 6816.

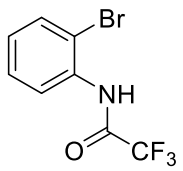
S5. Tietze, Lutz F.; Hungerland, Tim; Ammermann, Jonas; Eichhorst, Christoph; Reichmann, Sven O.; Stalke, Dietmar; **J. Indian. Chem. Soc.,** *2013*, 90, 10, 1537 – 1555.

S6. Wilkening, Ina; del Signore, Giuseppe; and Hackenberger, Christian P. R.; **Chem. Commun.**, *2011*, 47, 349 - 351.

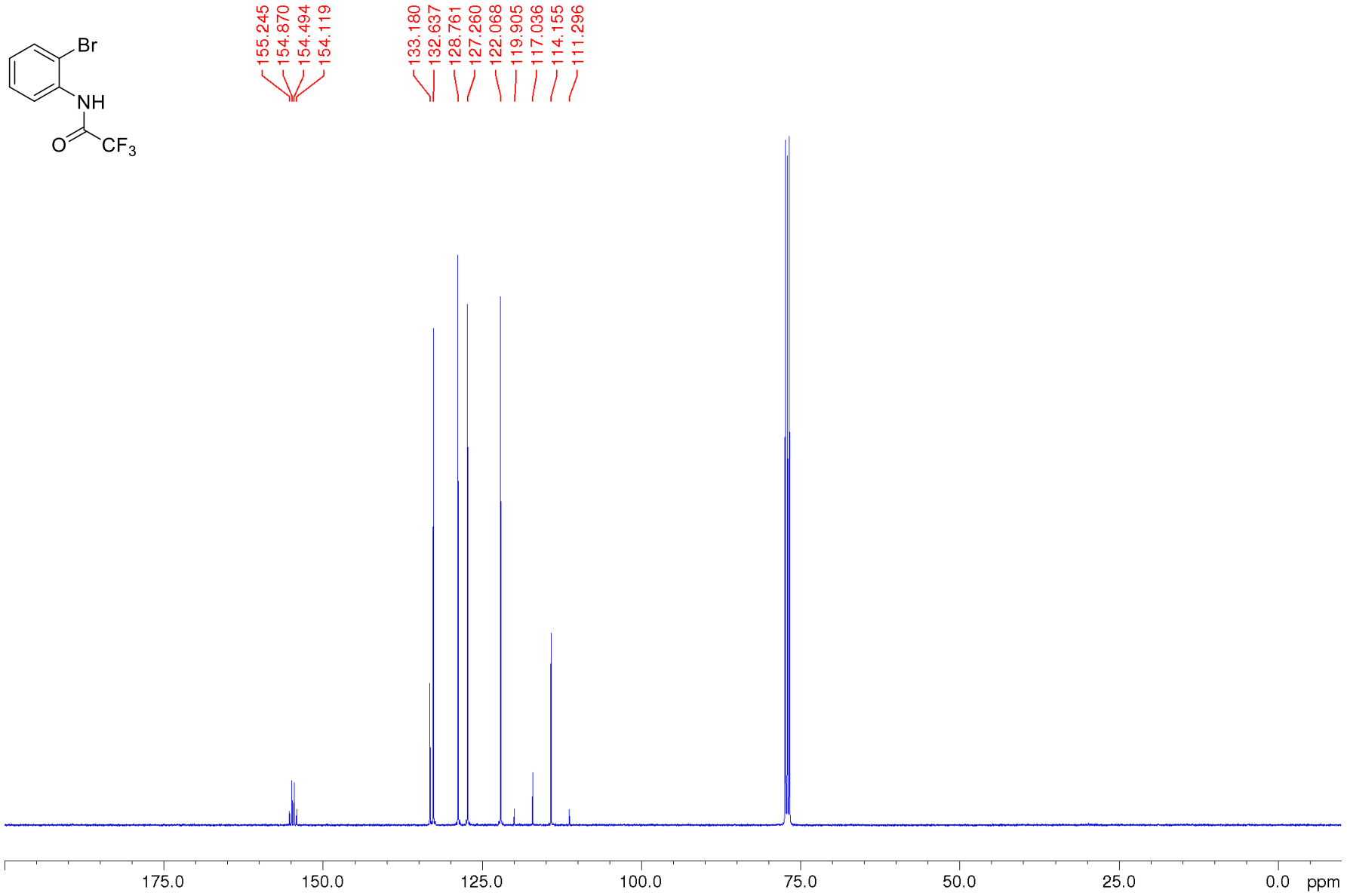
S7. Wang, Fu-Cheng; Peng, Bin; Ren, Ting-Ting; Liu, Shao-Peng; Du, Jing-Rui; Chen, Zi-Hao; Zhang, Ting-Ting; Cao, Sheng-Li; Xu, Xingzhi; **J. Med. Chem.,** *2022*, 65, 22, 15028 – 15047.

^{1}H, ^{13}C, ^{13}C DEPT, ^{19}F NMR Spectra

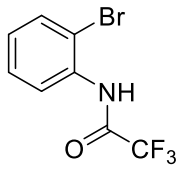
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



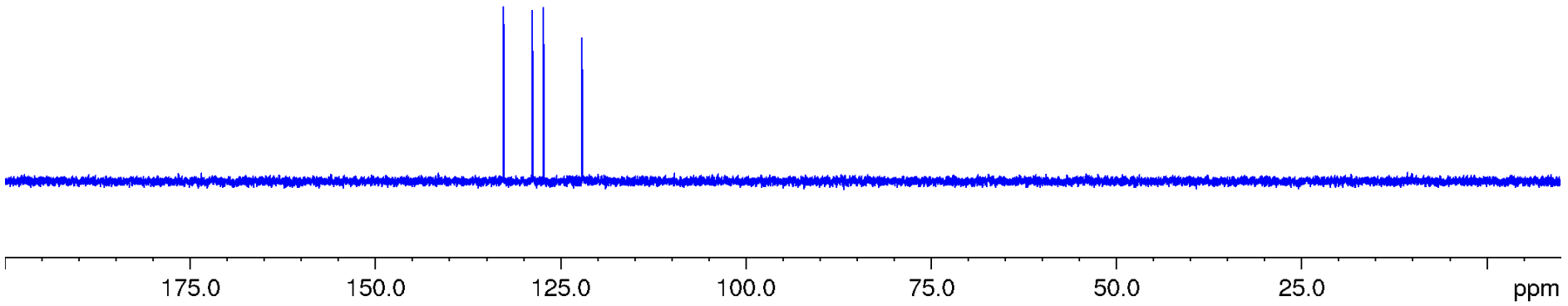
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



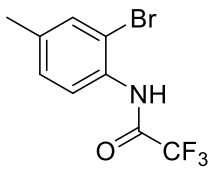
DEPT 135 NMR-spectrum ($CDCl_3$)



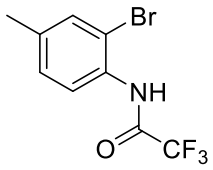
132.639
128.769
127.257
122.062



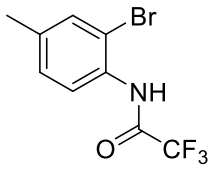
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



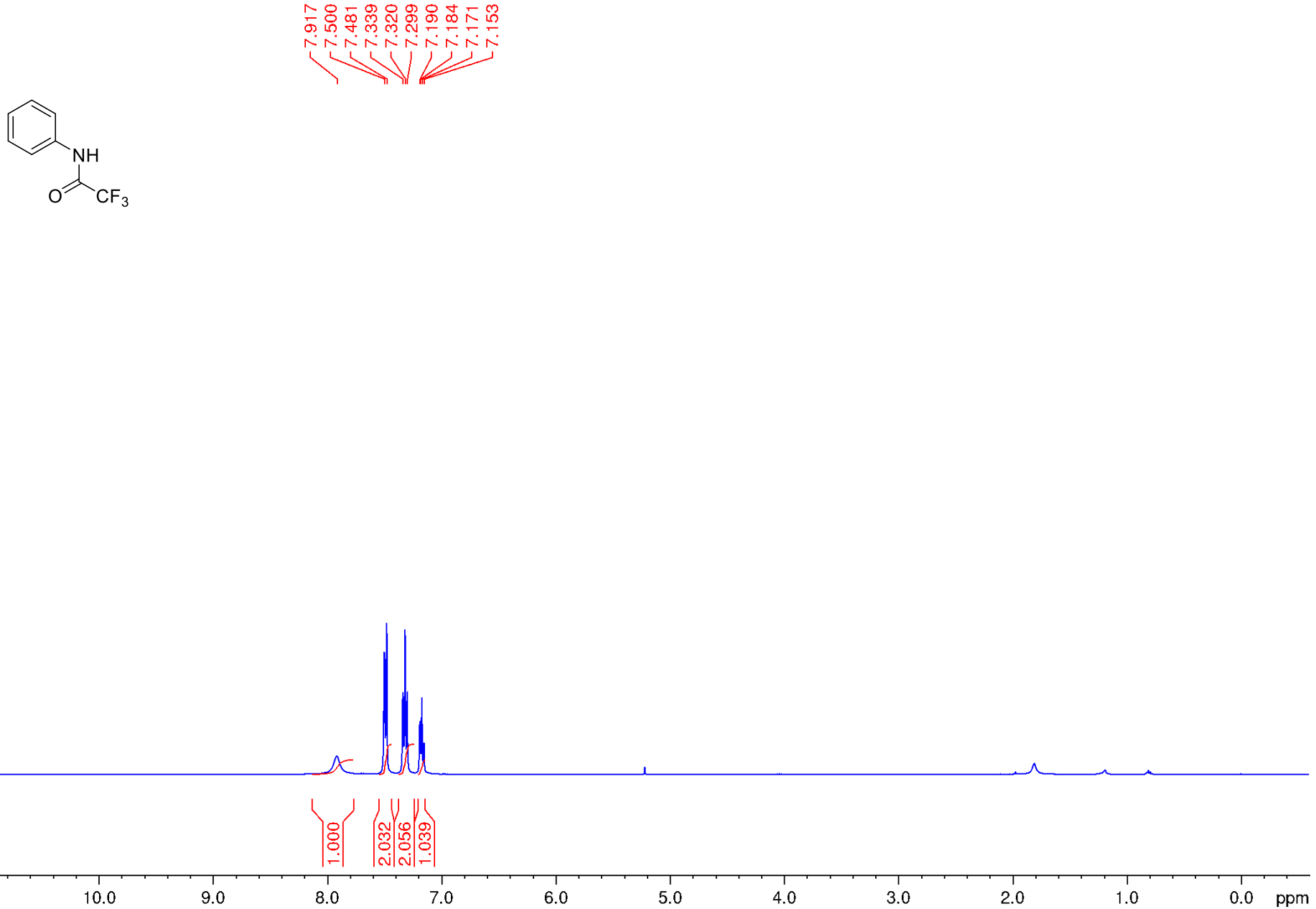
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



DEPT 135 NMR-spectrum ($CDCl_3$)



^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



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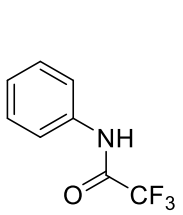
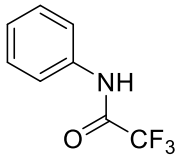
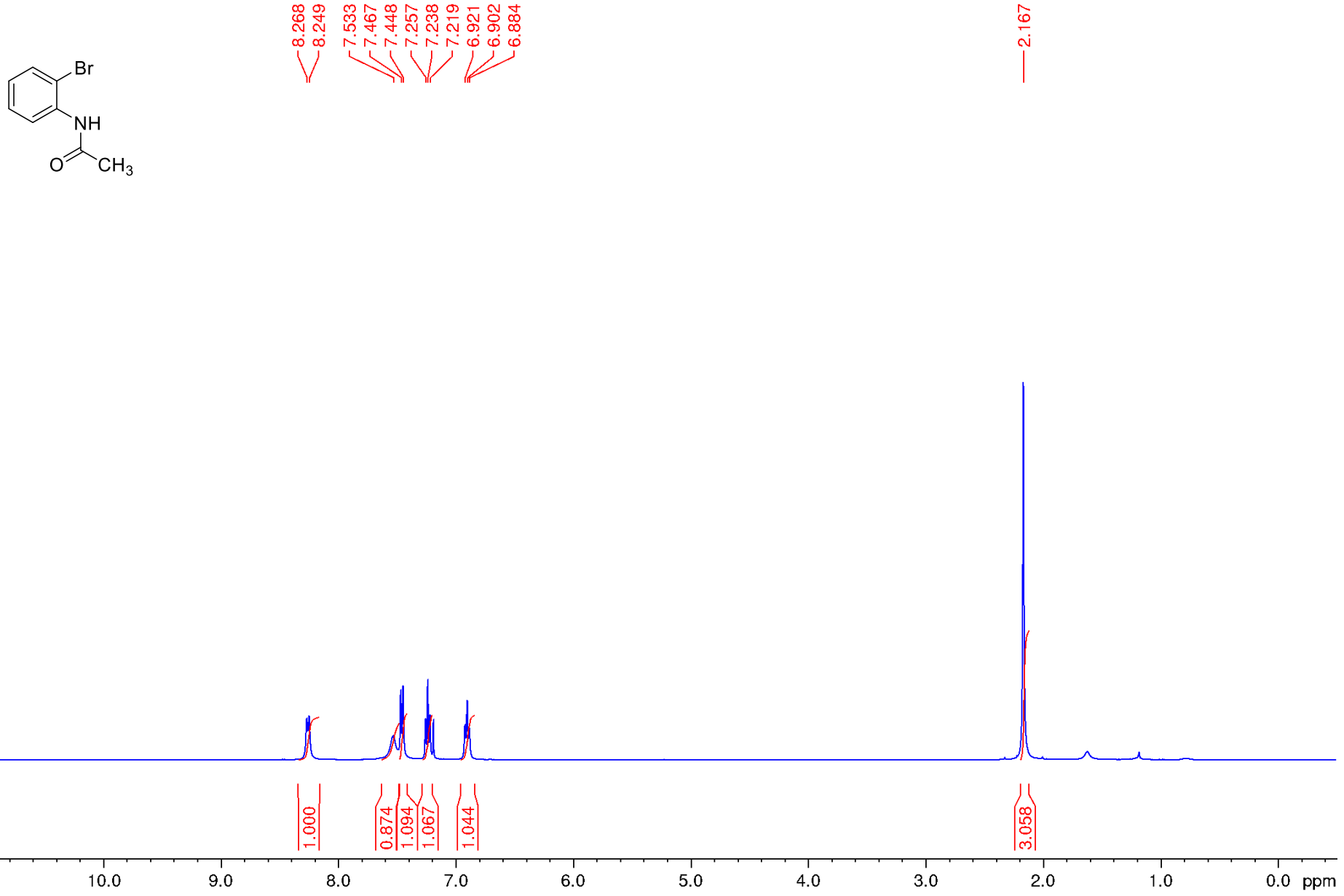


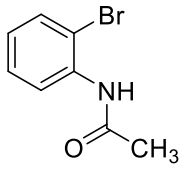
DEPT 135 NMR-spectrum ($CDCl_3$)



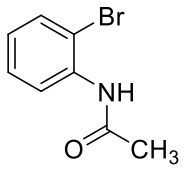
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



DEPT 135 NMR-spectrum ($CDCl_3$)



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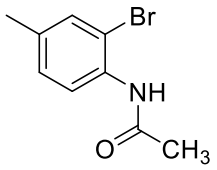
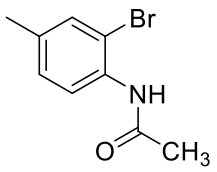
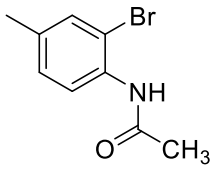


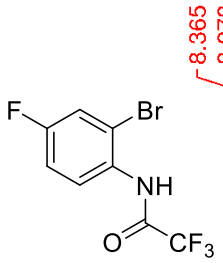
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)

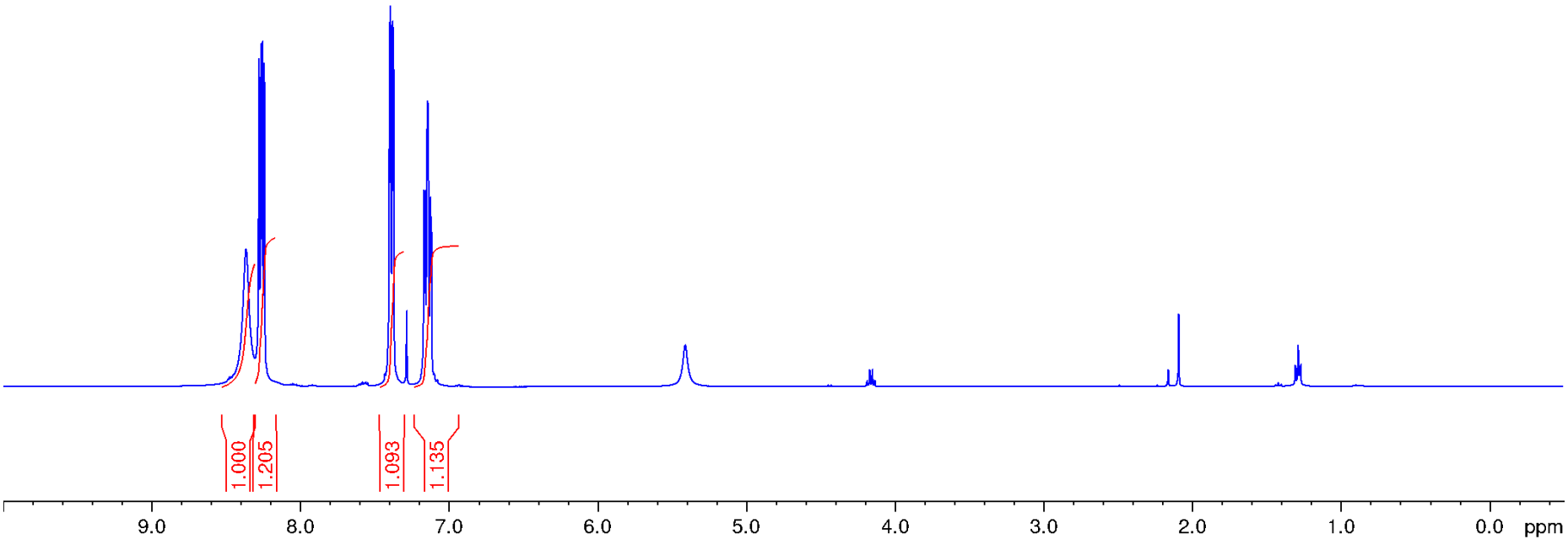


DEPT 135 NMR-spectrum ($CDCl_3$)

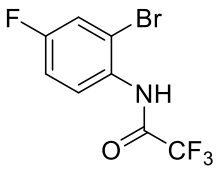


^{1}H NMR-spectrum (400 MHz, $CDCl_3$)

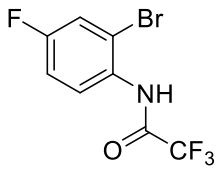




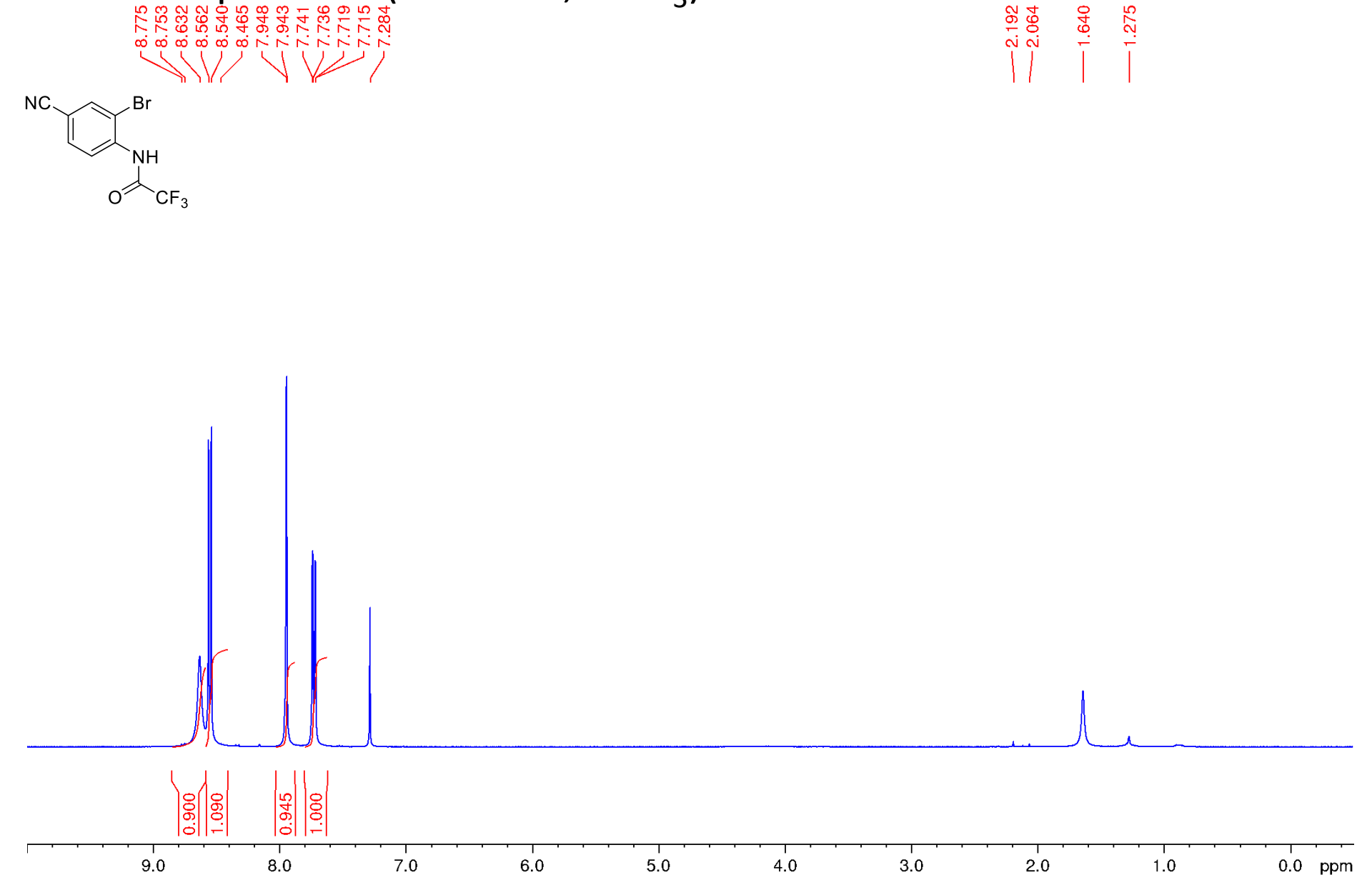
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



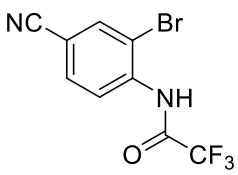
DEPT 135 NMR-spectrum ($CDCl_3$)



^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



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155.119
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154.367
137.257
135.967
132.810
121.636
119.555
116.677
113.876
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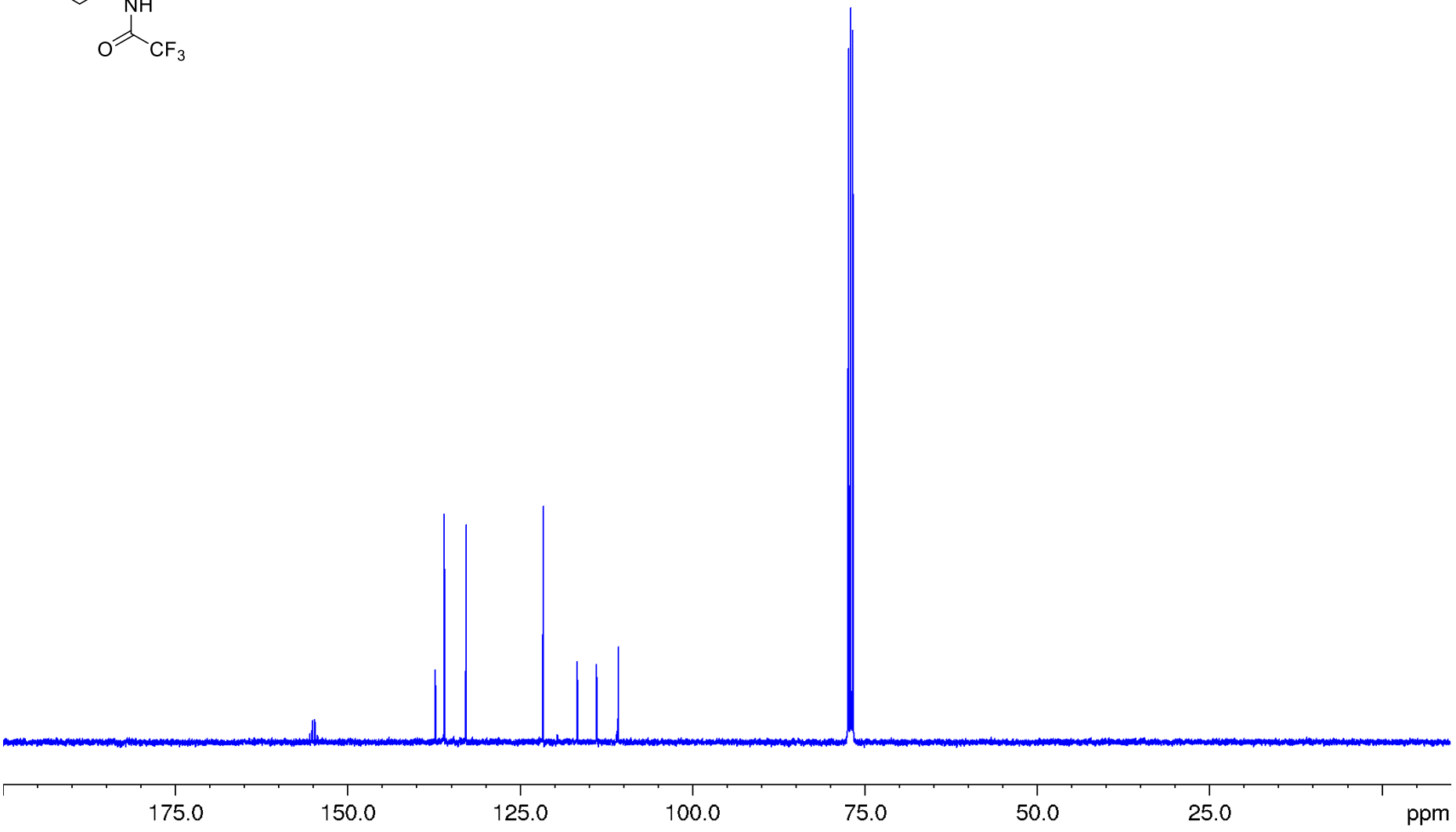
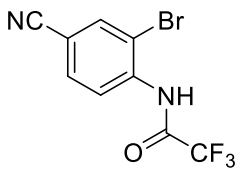
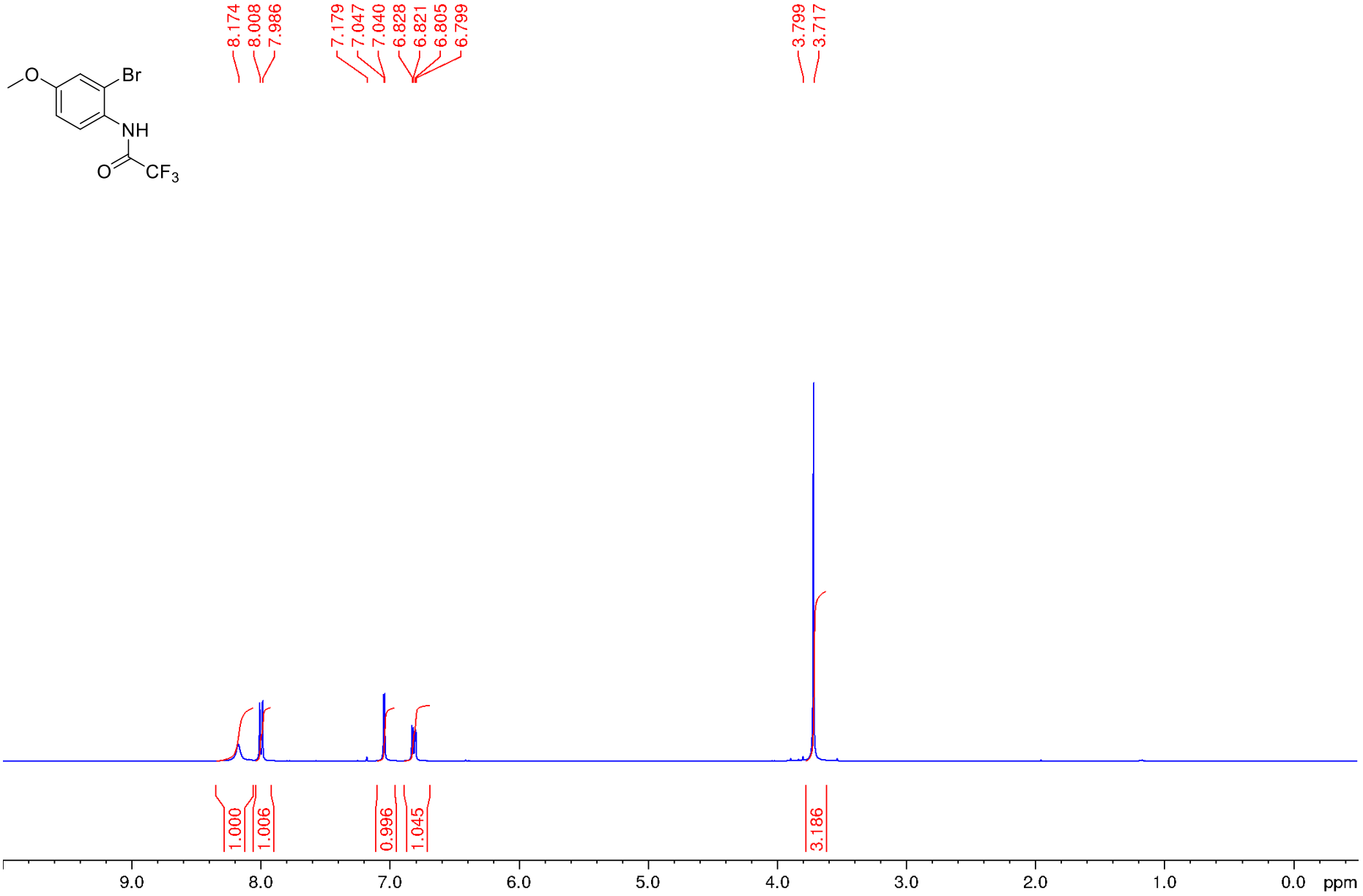
110.948
110.692



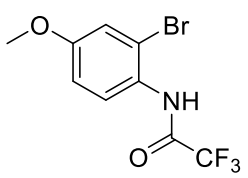
DEPT 135 NMR-spectrum ($CDCl_3$)



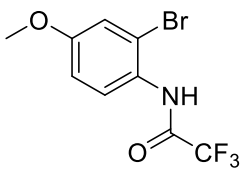
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



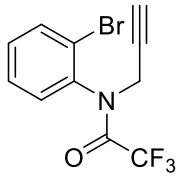
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



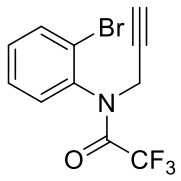
DEPT 135 NMR-spectrum ($CDCl_3$)



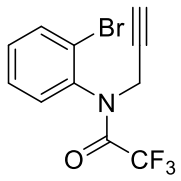
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



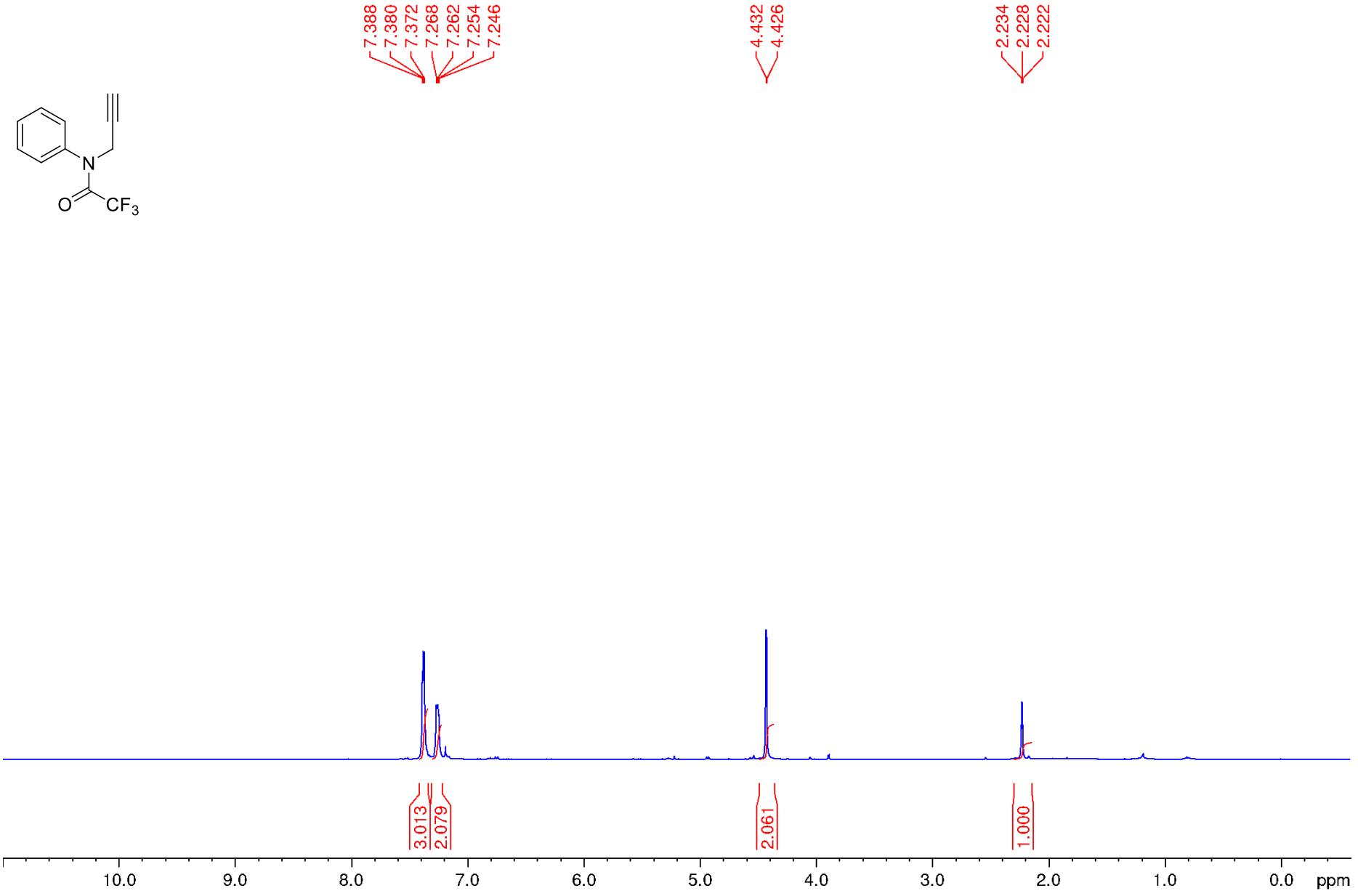
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



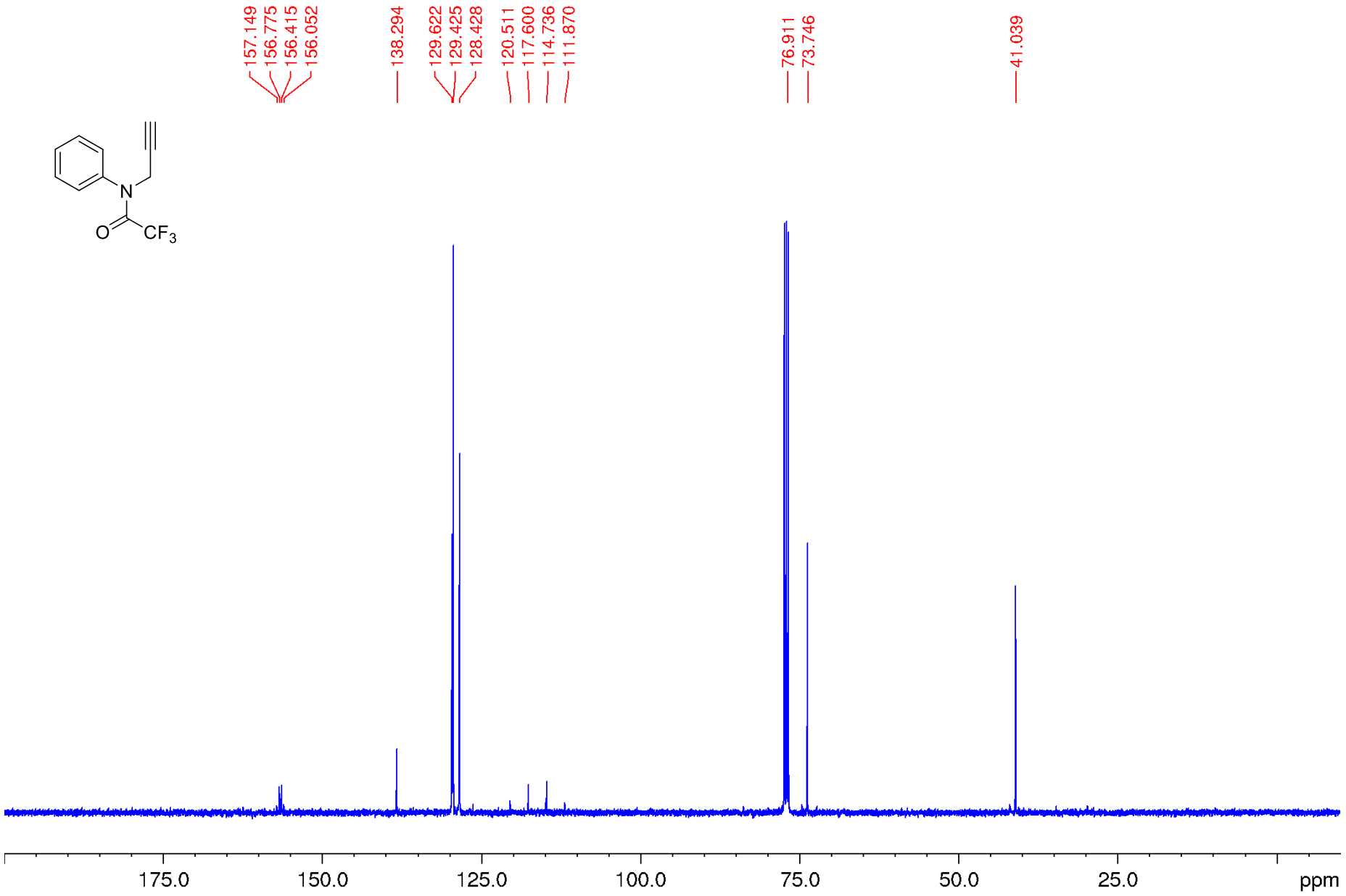
DEPT 135 NMR-spectrum ($CDCl_3$)



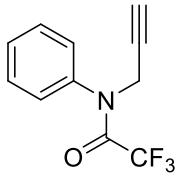
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



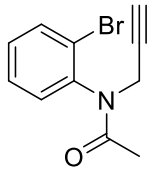
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



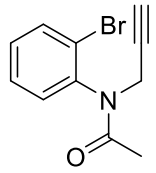
DEPT 135 NMR-spectrum ($CDCl_3$)



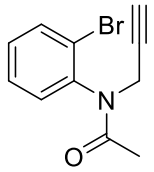
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



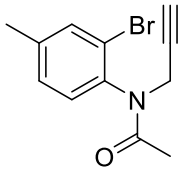
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



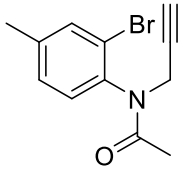
DEPT 135 NMR-spectrum ($CDCl_3$)



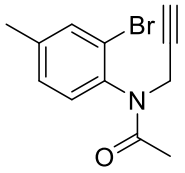
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



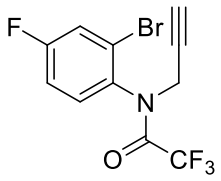
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



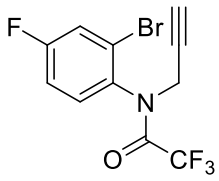
DEPT 135 NMR-spectrum ($CDCl_3$)



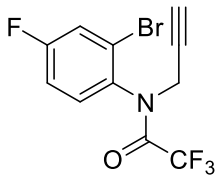
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



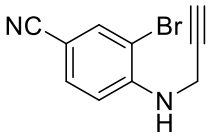
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



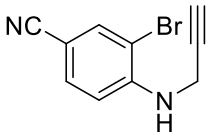
DEPT 135 NMR-spectrum ($CDCl_3$)



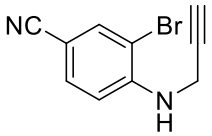
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



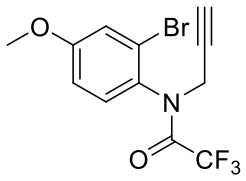
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



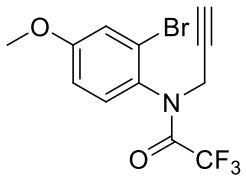
DEPT 135 NMR-spectrum ($CDCl_3$)



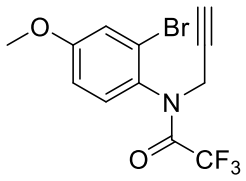
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



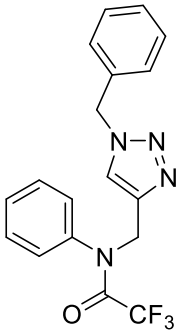
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



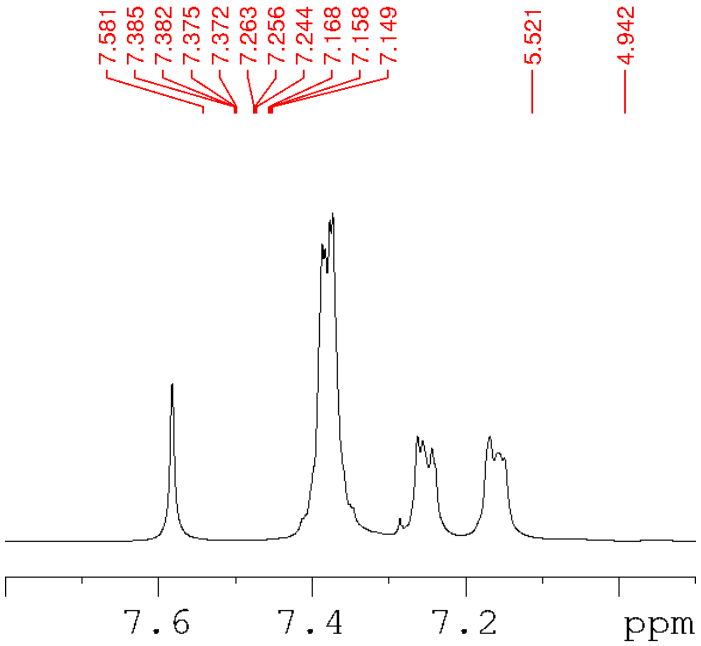
DEPT 135 NMR-spectrum ($CDCl_3$)

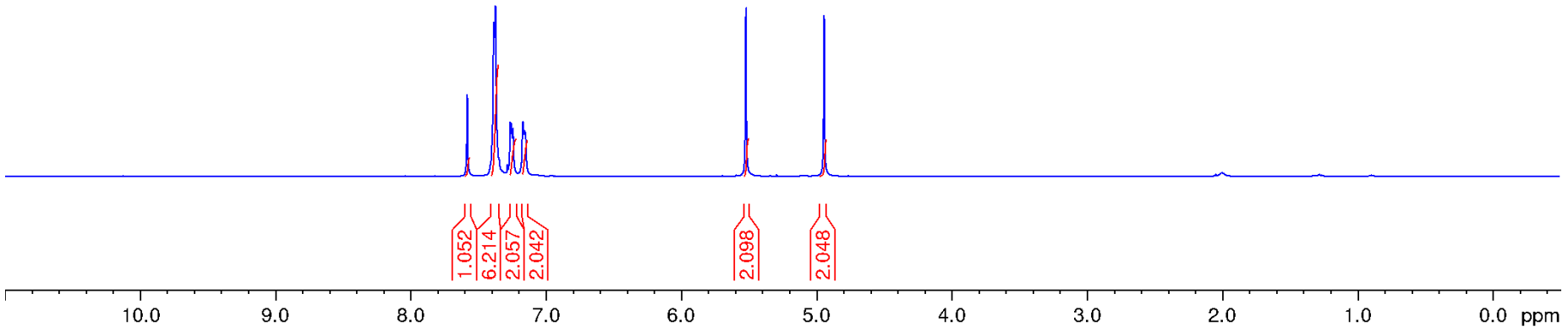


^{1}H NMR-spectrum (400 MHz, $CDCl_3$)

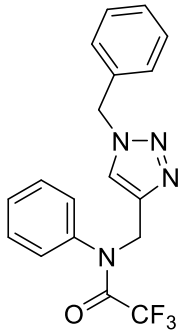


1a



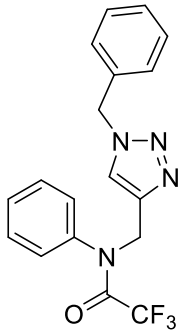


^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



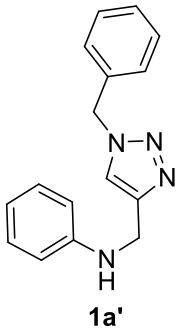
1a

DEPT 135 NMR-spectrum ($CDCl_3$)

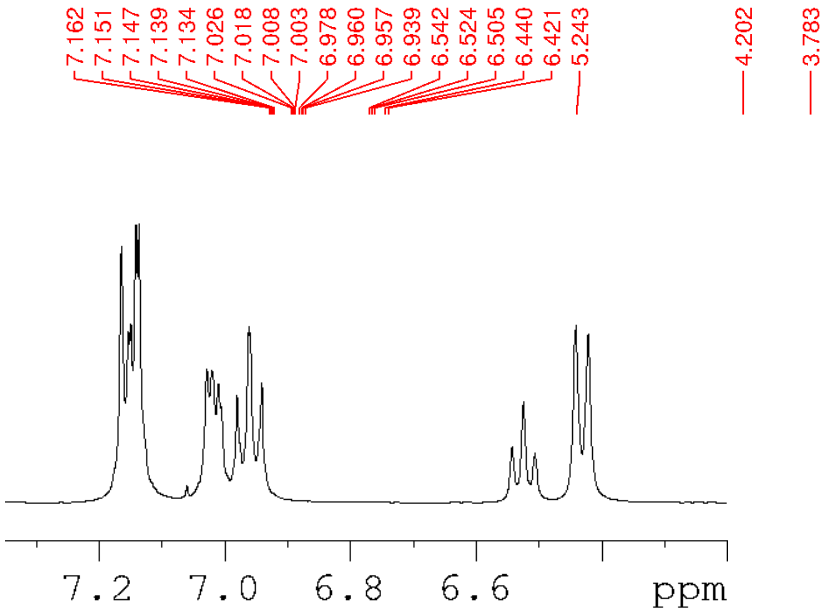


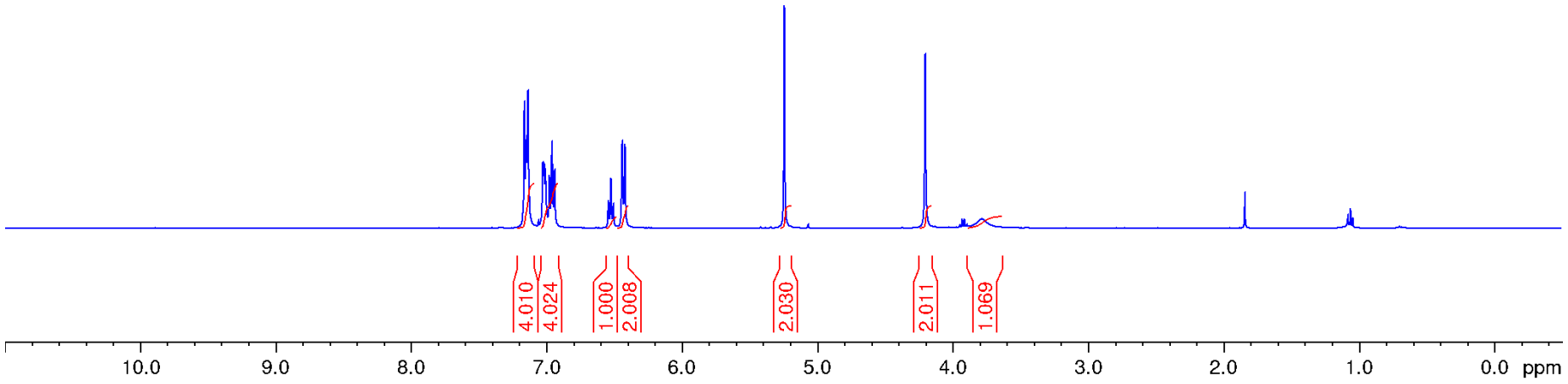
1a

^{1}H NMR-spectrum (400 MHz, $CDCl_3$)

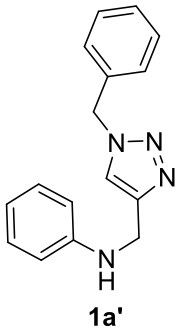


1a'





^{13}C NMR-spectrum (100 MHz, $CDCl_3$)

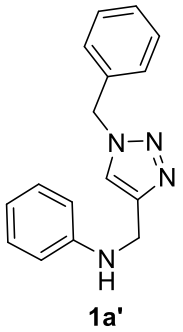


1a'

147.610
146.667
134.738
129.300
129.118
128.736
128.010
121.659
118.012
113.219
54.114
39.950

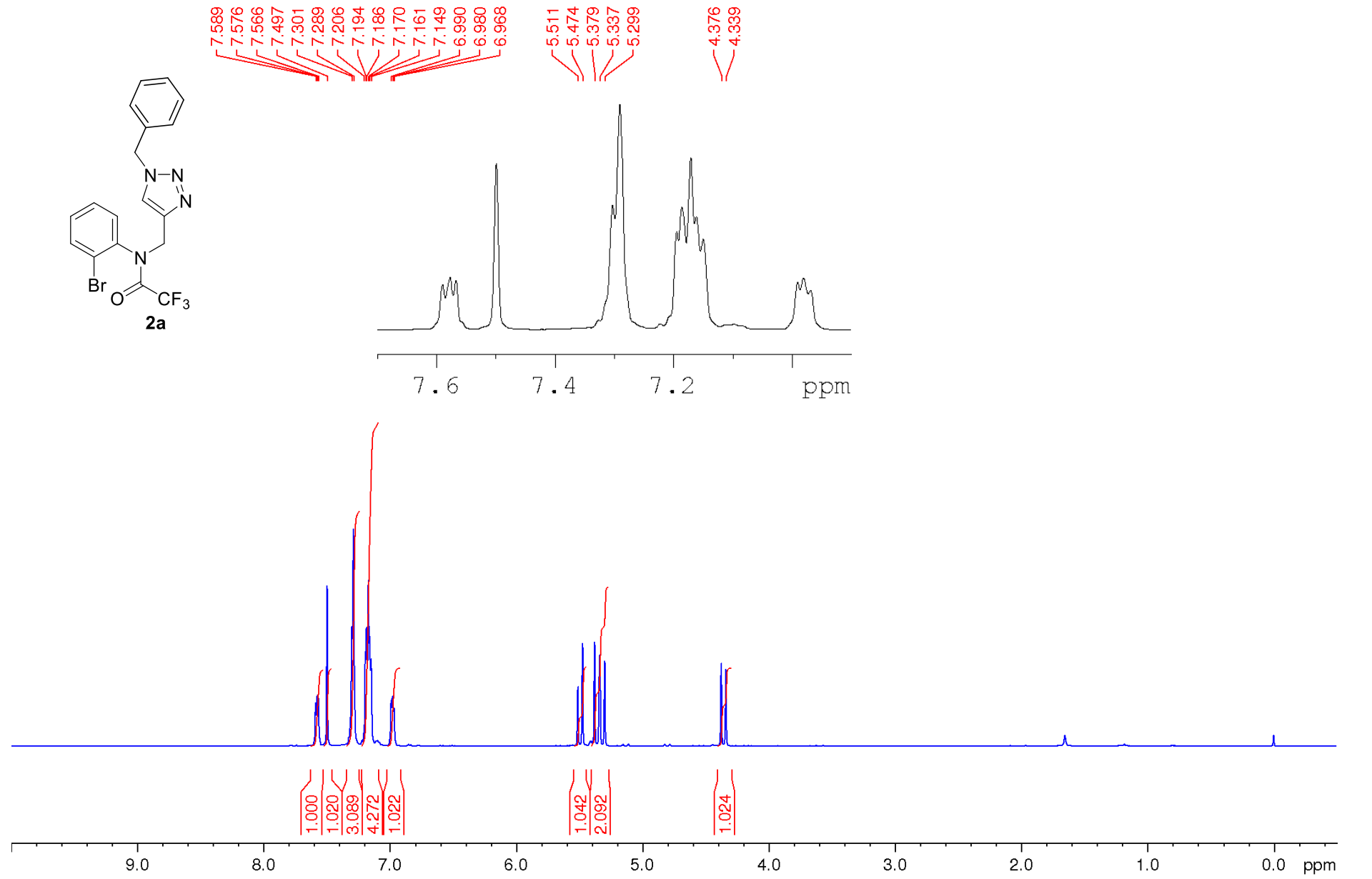
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm

DEPT 135 NMR-spectrum ($CDCl_3$)

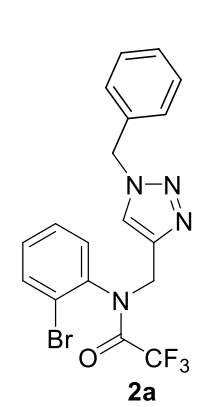


1a'

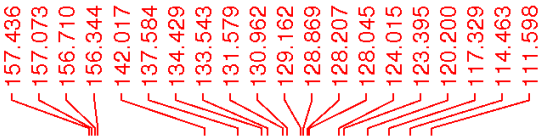
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)

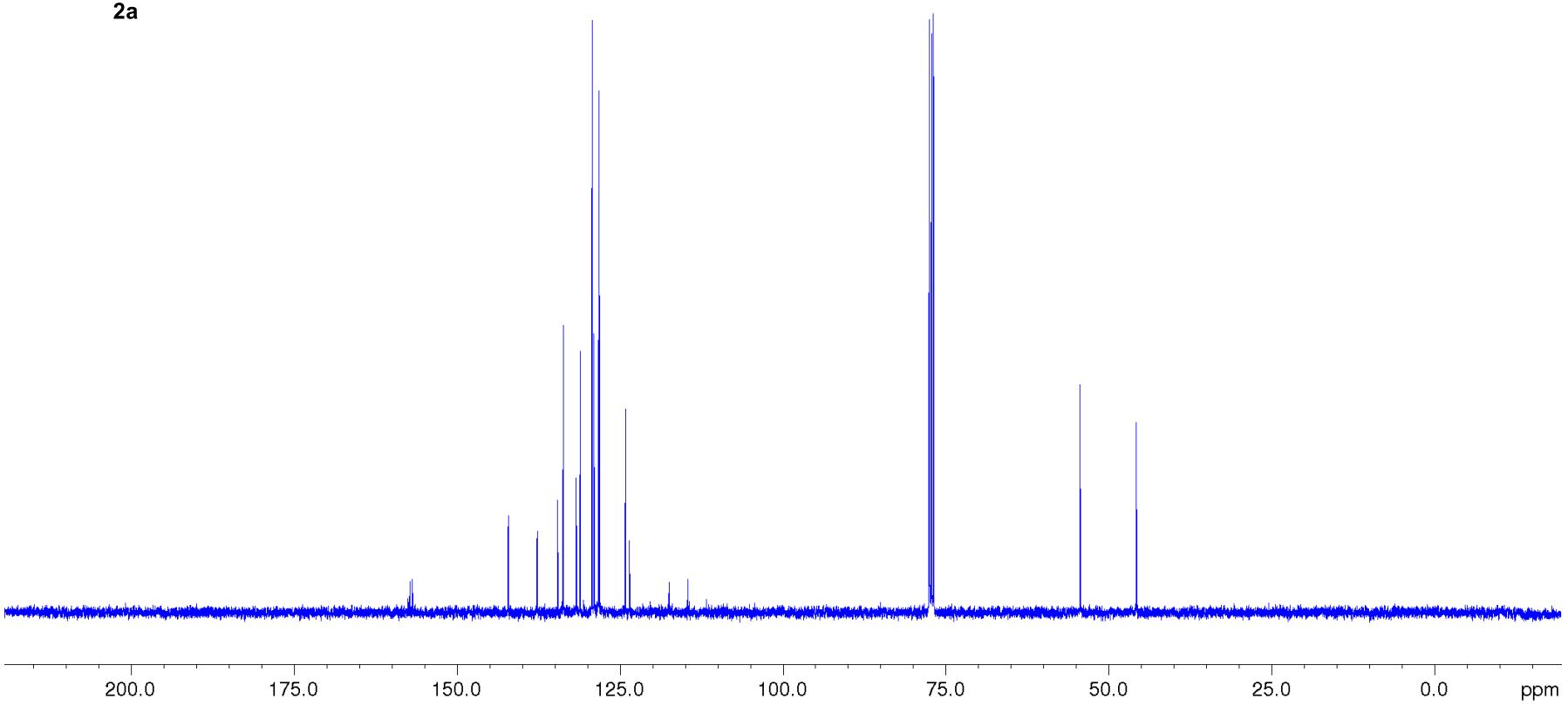


^{13}C NMR-spectrum (100 MHz, $CDCl_3$)

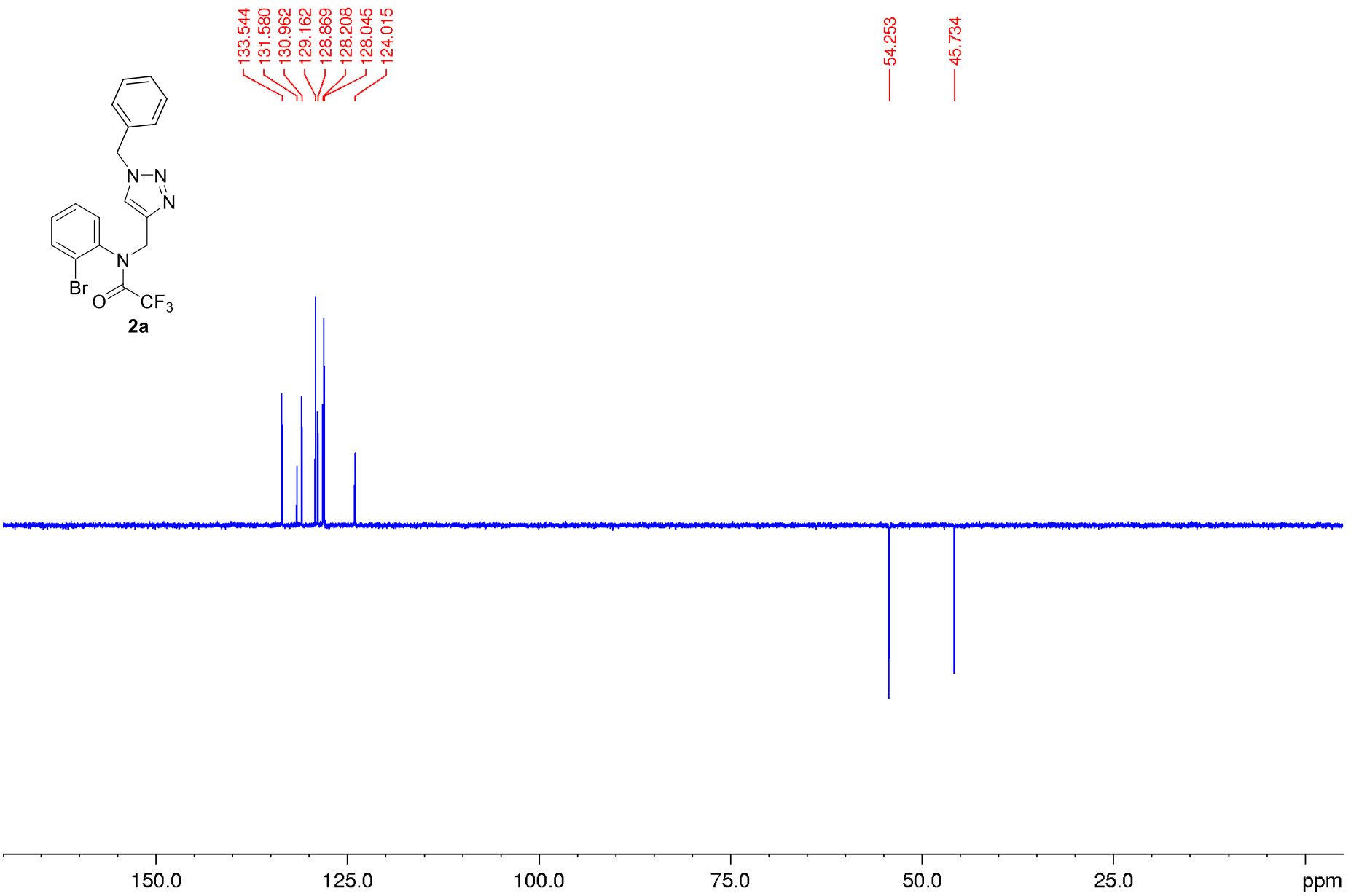


2a

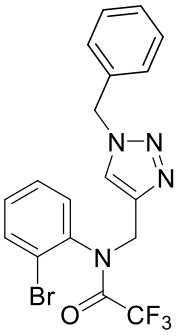




DEPT 135 NMR-spectrum ($CDCl_3$)

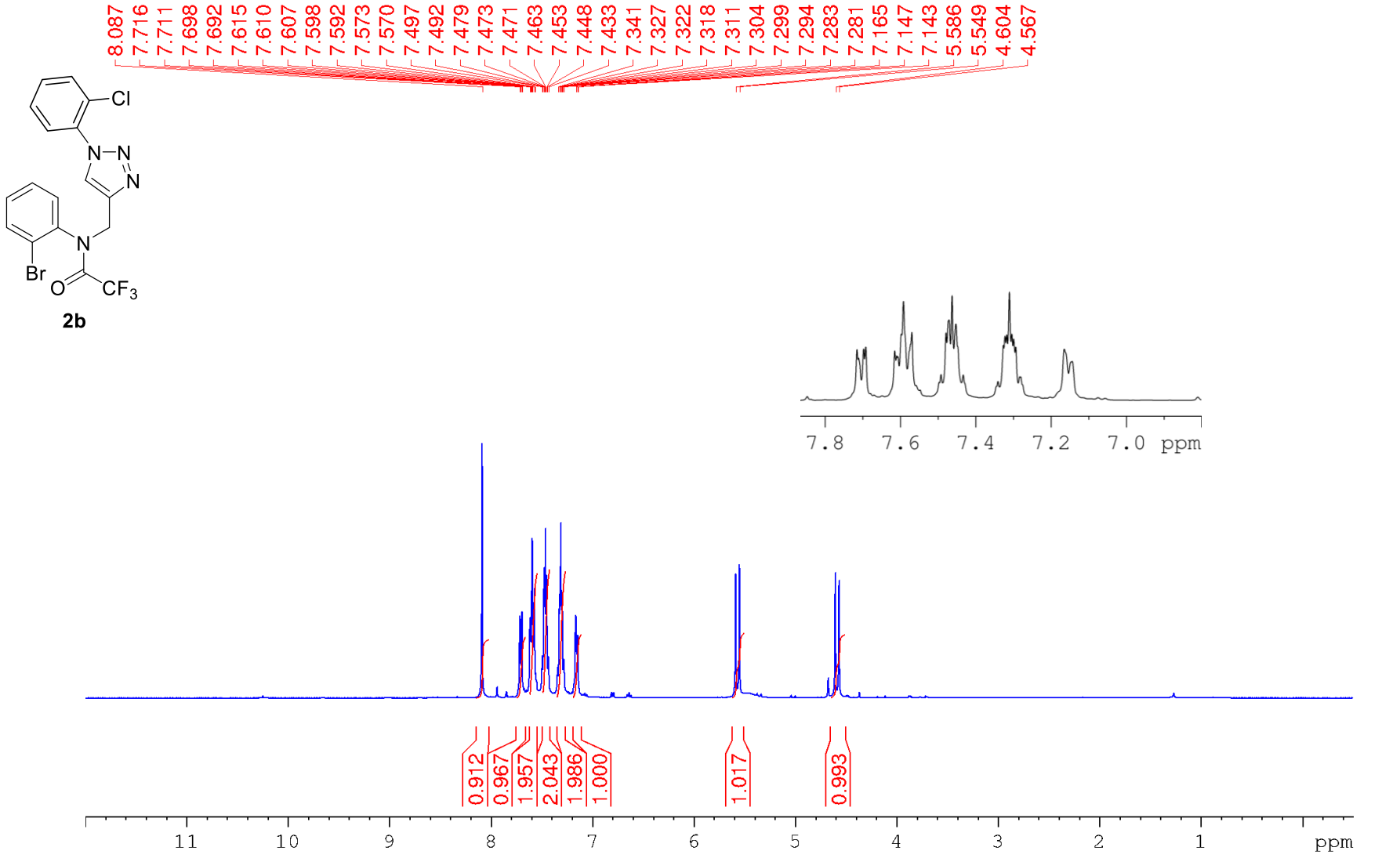


^{19}F NMR-spectrum (376.5 Hz, $CDCl_3$)

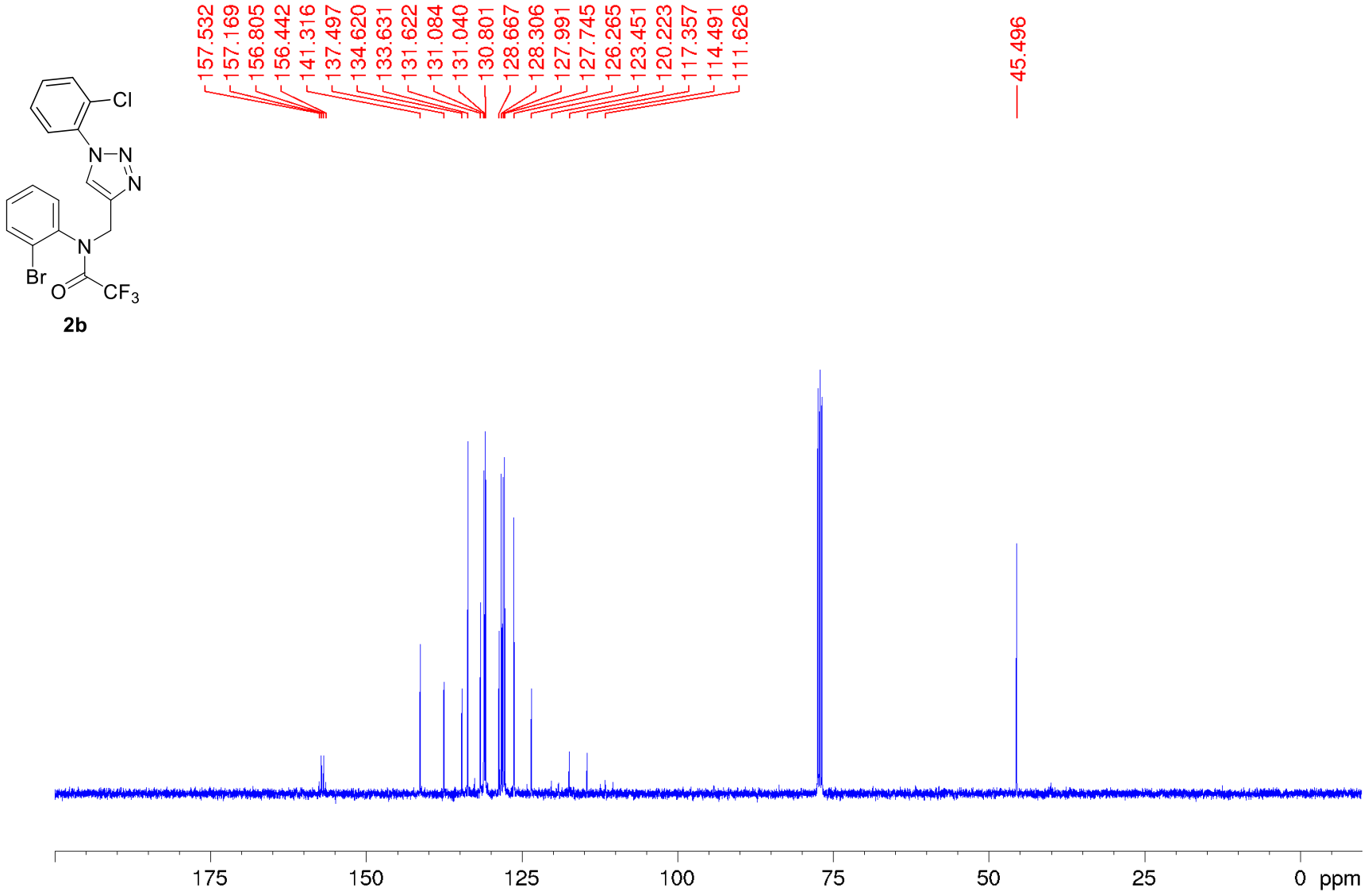


2a

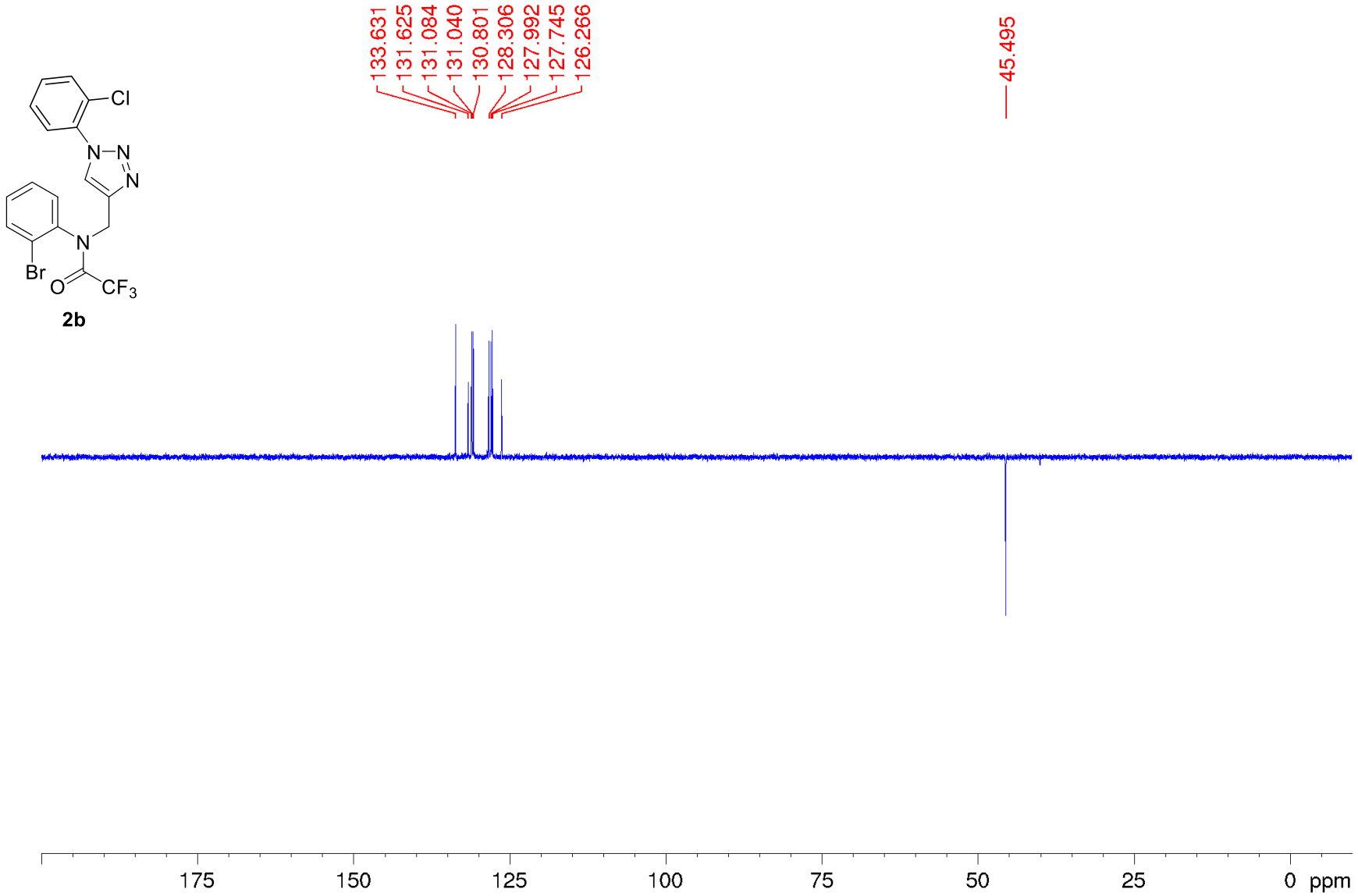
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



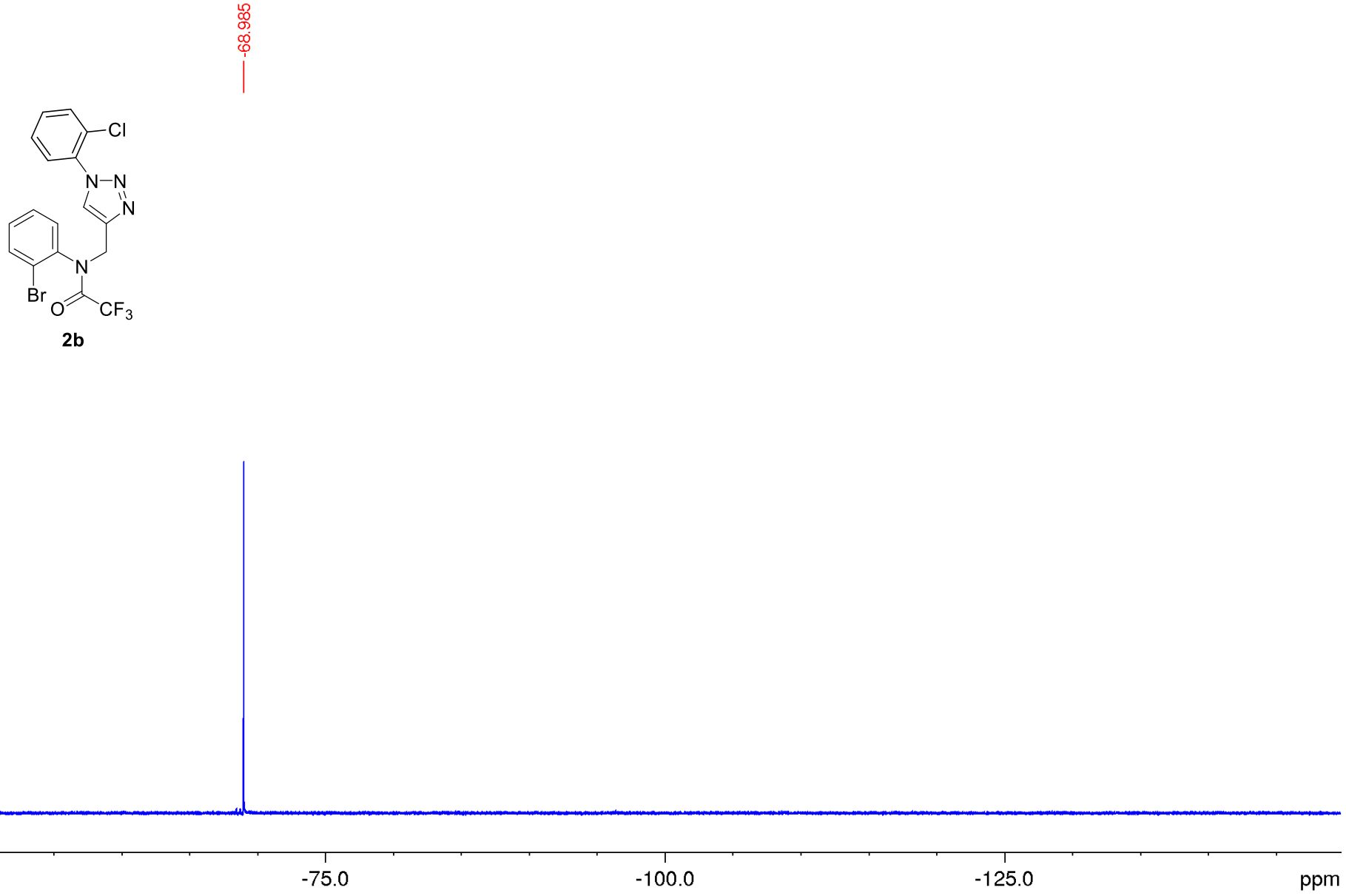
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



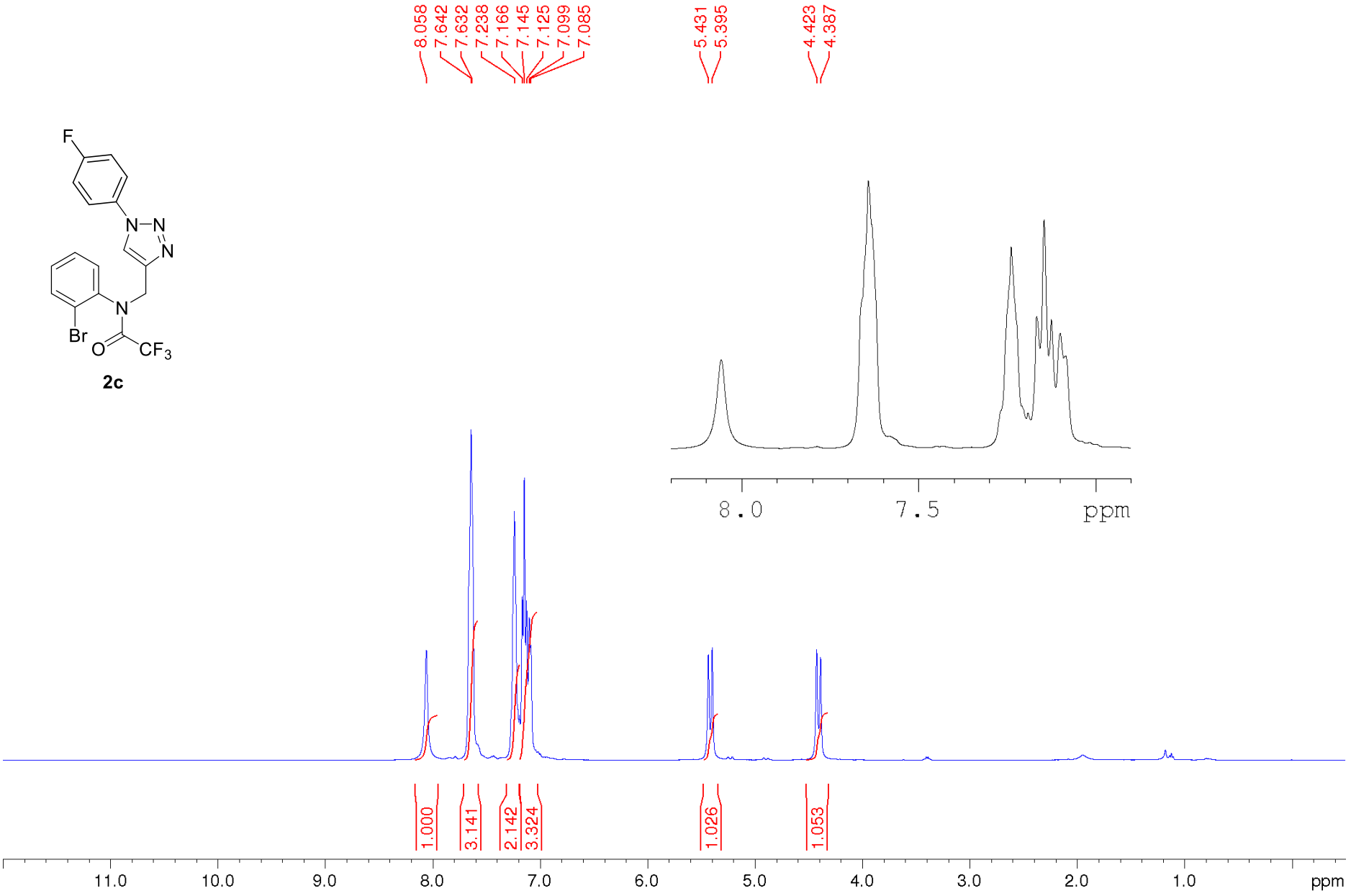
DEPT 135 NMR-spectrum ($CDCl_3$)



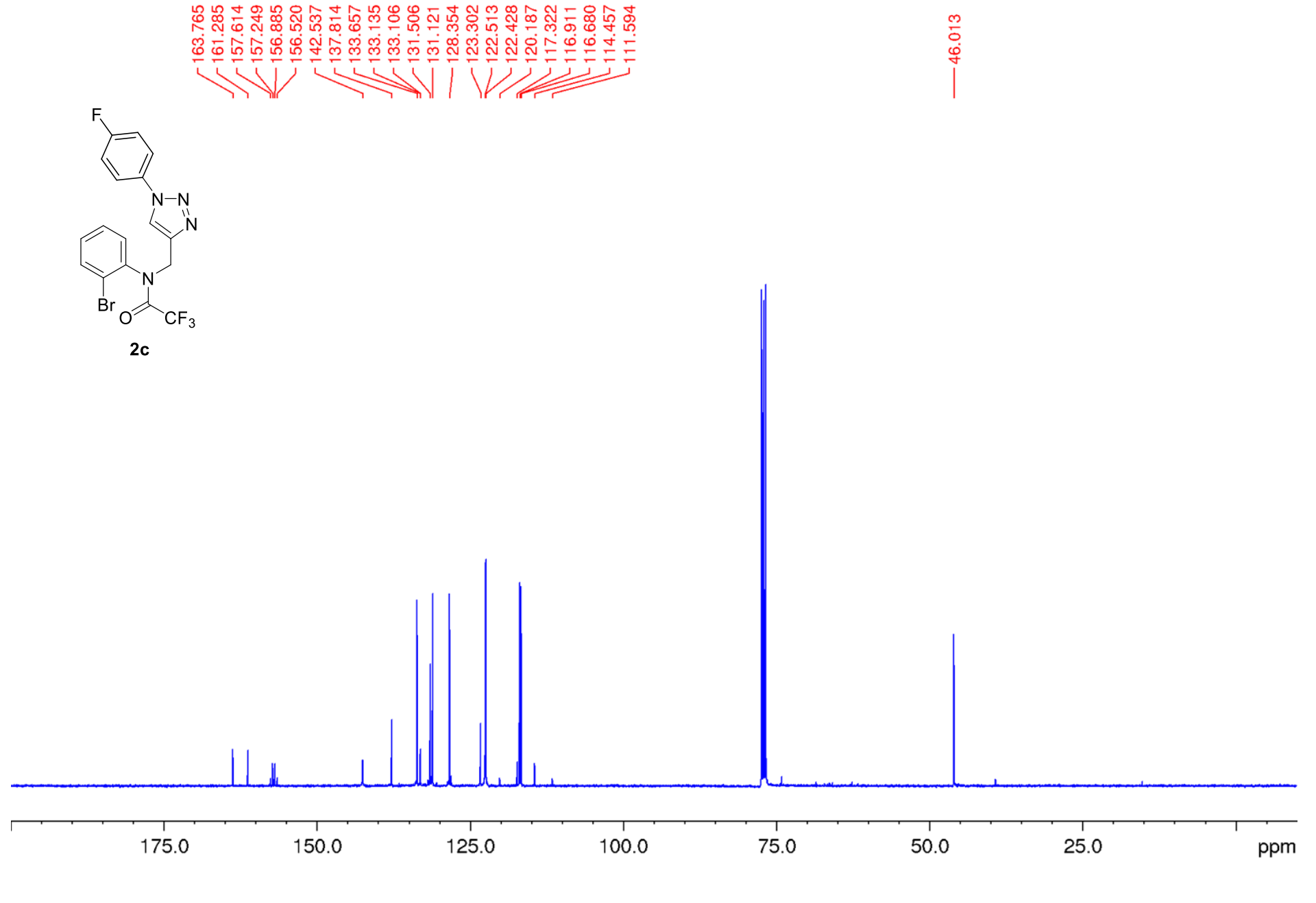
^{19}F NMR-spectrum (376.5 Hz, $CDCl_3$)



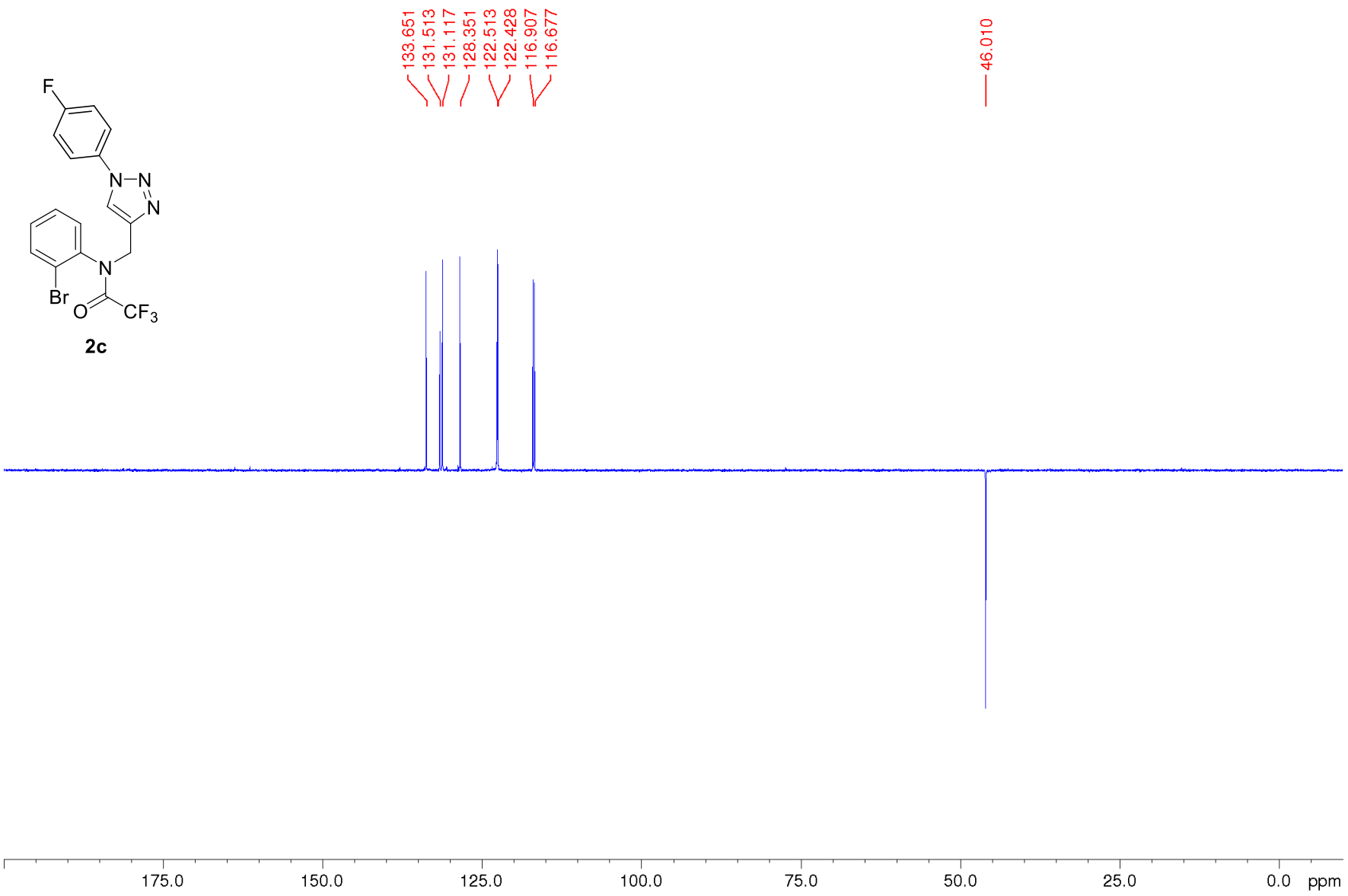
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



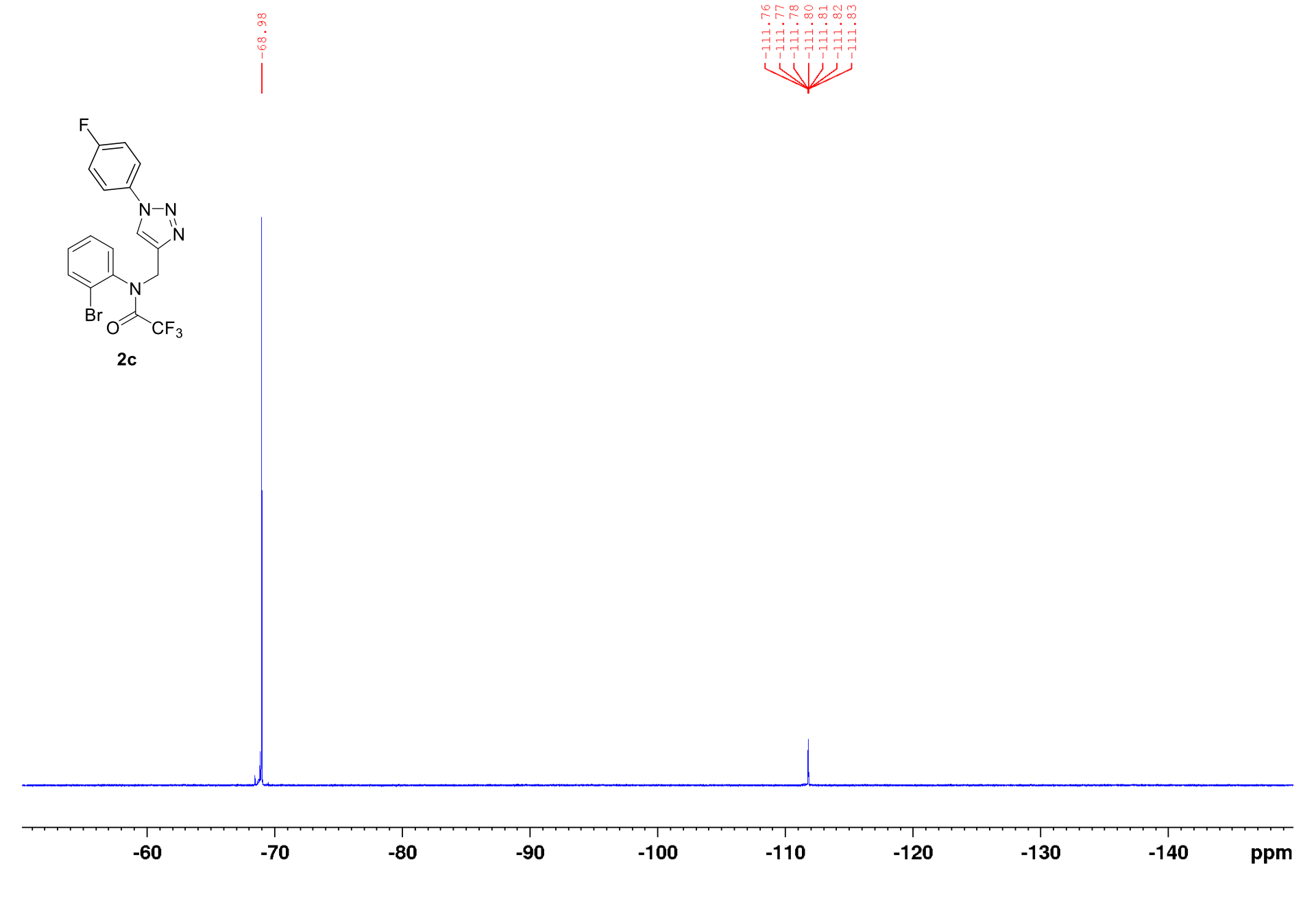
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



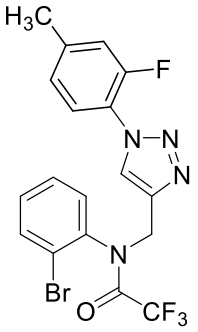
DEPT 135 NMR-spectrum ($CDCl_3$)



^{19}F NMR-spectrum (376.5 Hz, $CDCl_3$)

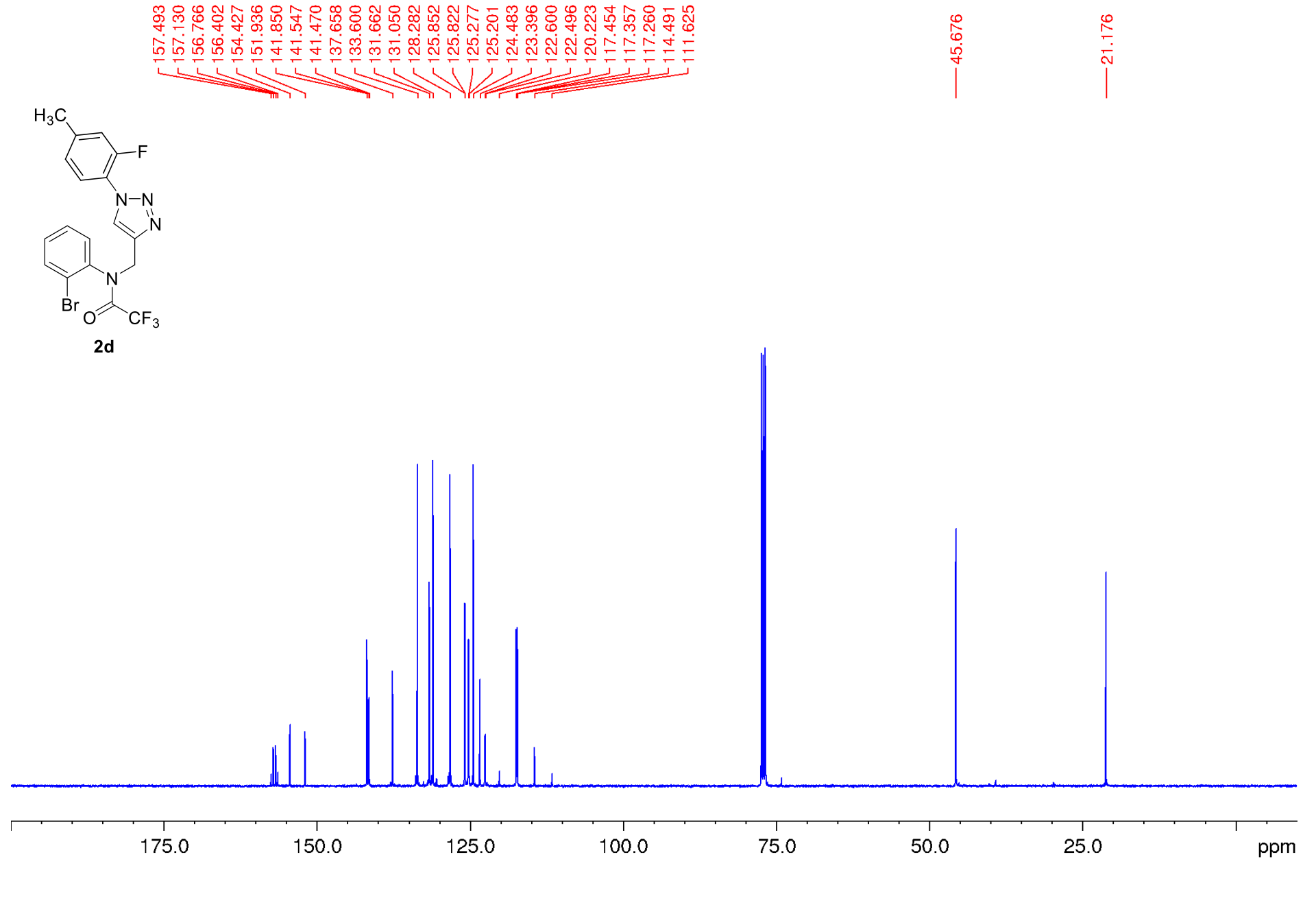


^{1}H NMR-spectrum (400 MHz, $CDCl_3$)

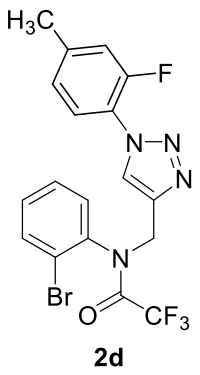


2d

^{13}C NMR-spectrum (100 MHz, $CDCl_3$)

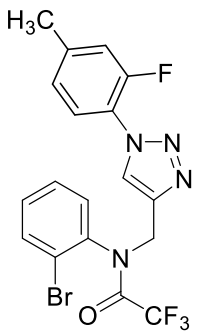


DEPT 135 NMR-spectrum ($CDCl_3$)



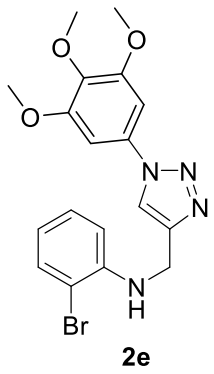
2d

^{19}F NMR-spectrum (376.5 Hz, $CDCl_3$)



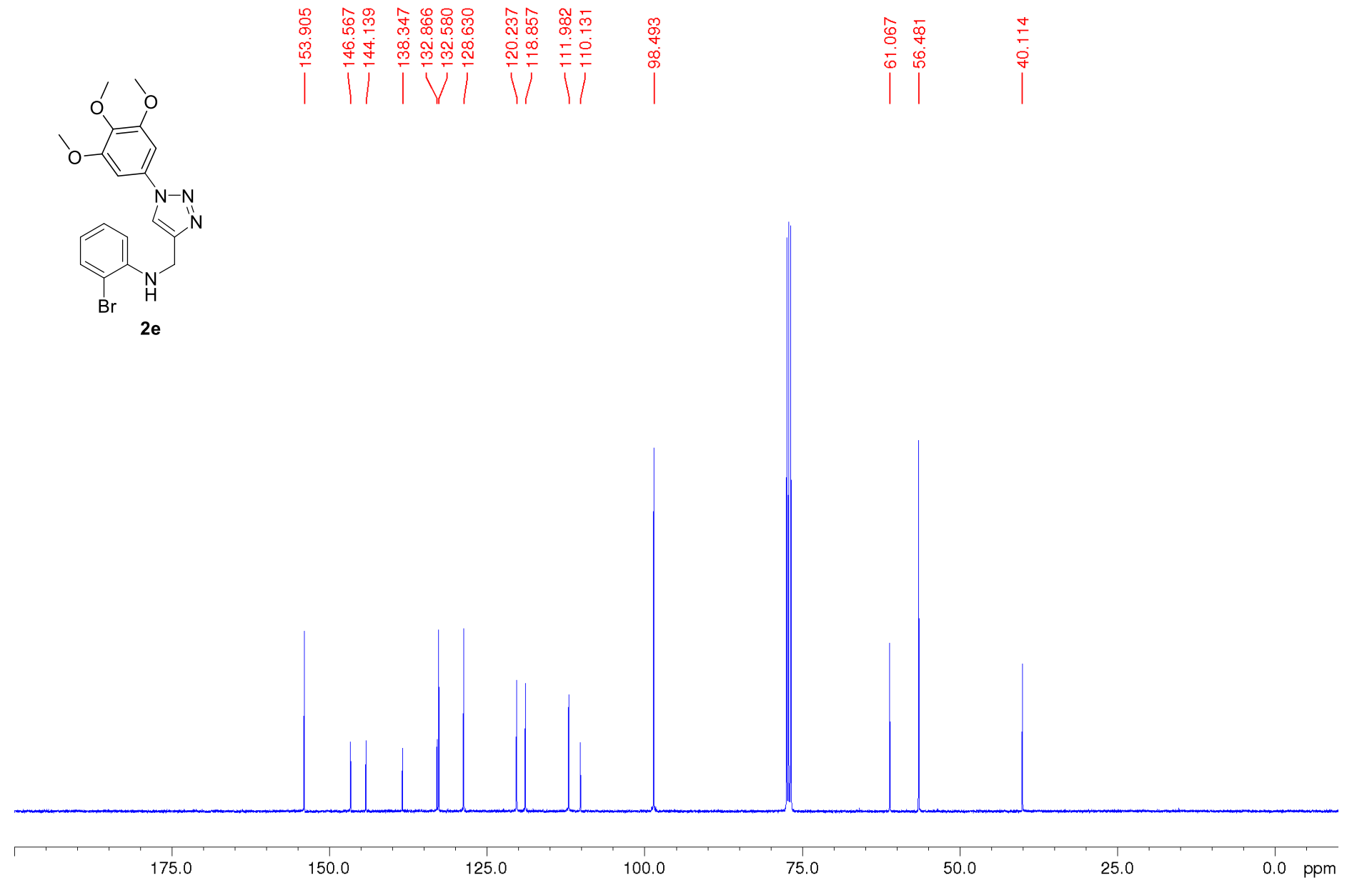
2d

^{1}H NMR-spectrum (400 MHz, $CDCl_3$)

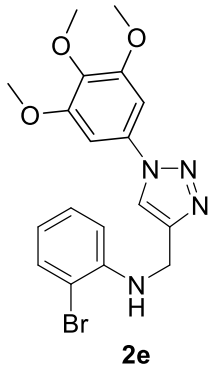


2e

^{13}C NMR-spectrum (100 MHz, $CDCl_3$)

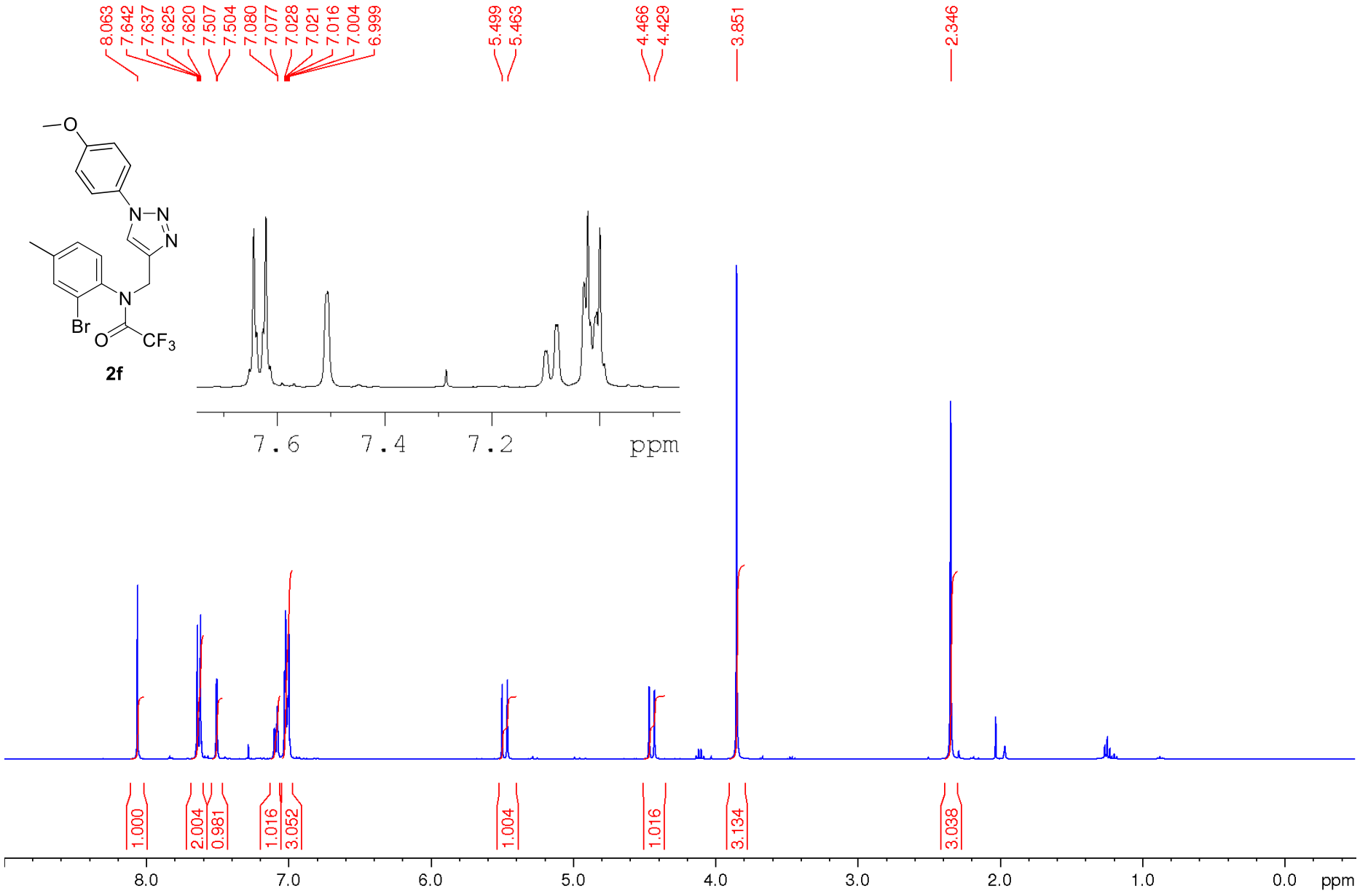


DEPT 135 NMR-spectrum ($CDCl_3$)

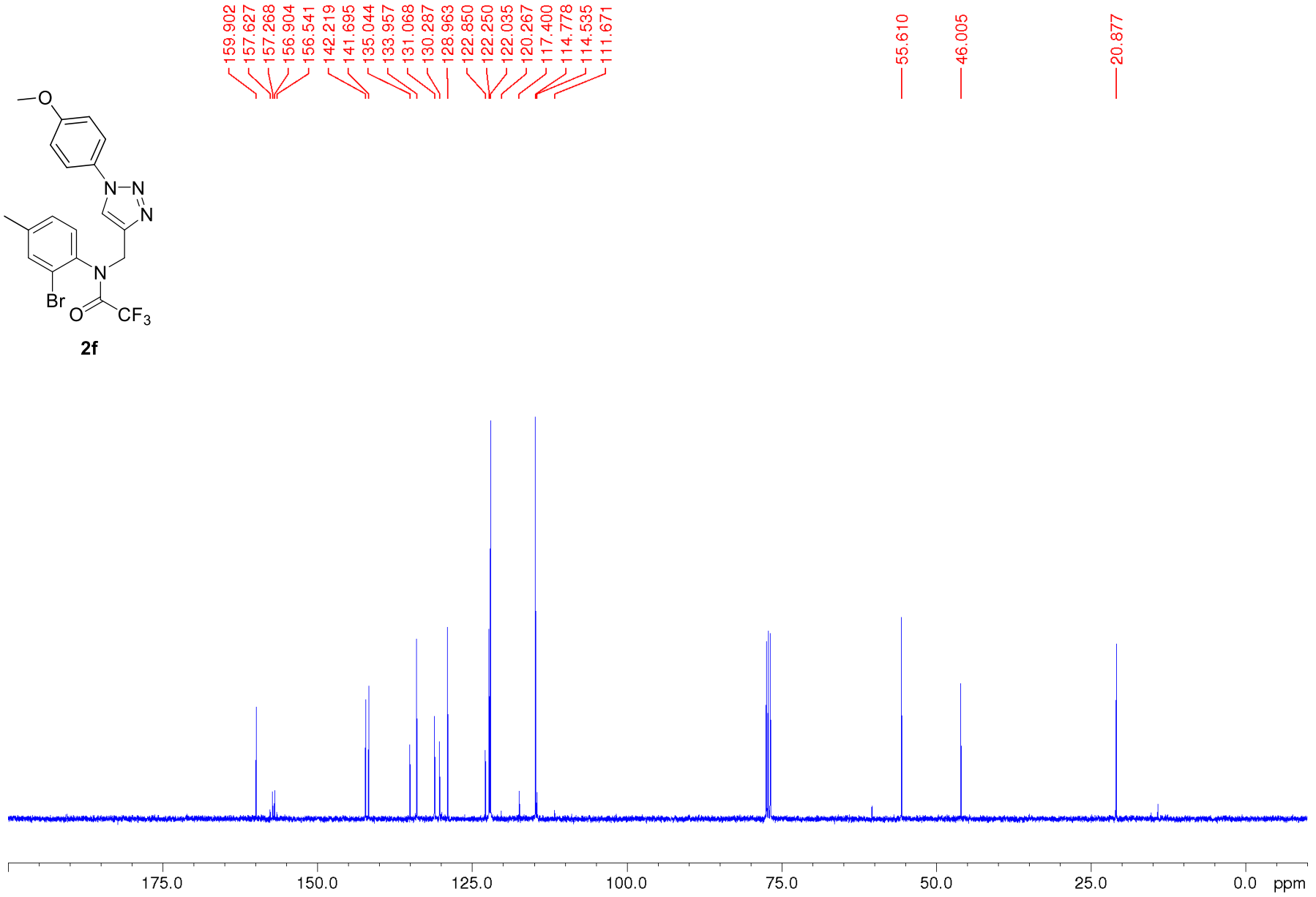


2e

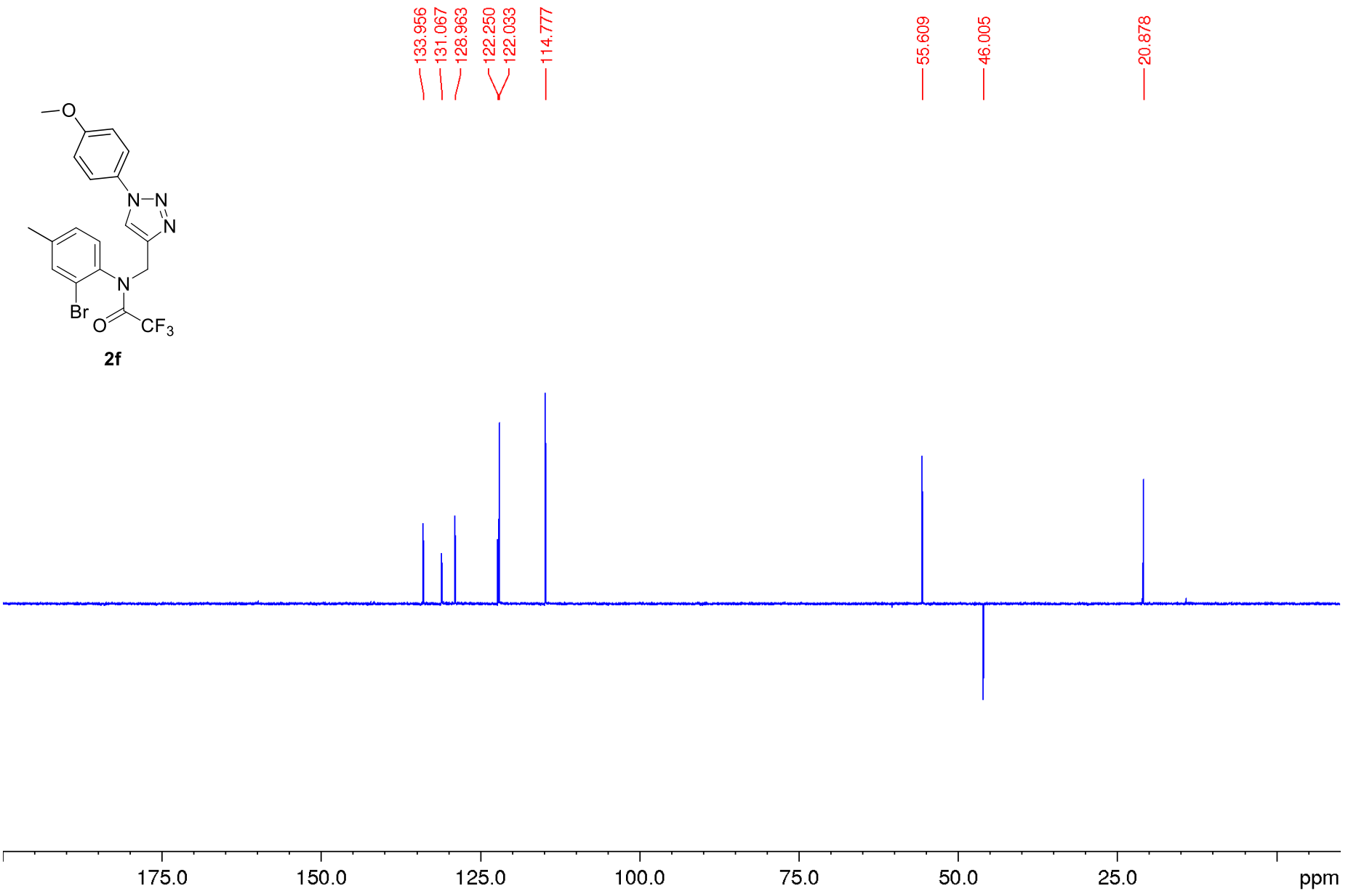
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



^{13}C NMR-spectrum (100 MHz, $CDCl_3$)

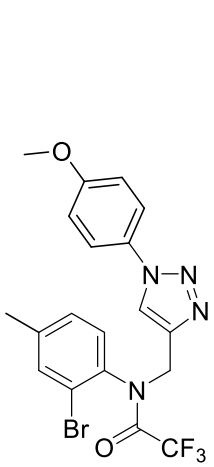


DEPT 135 NMR-spectrum ($CDCl_3$)



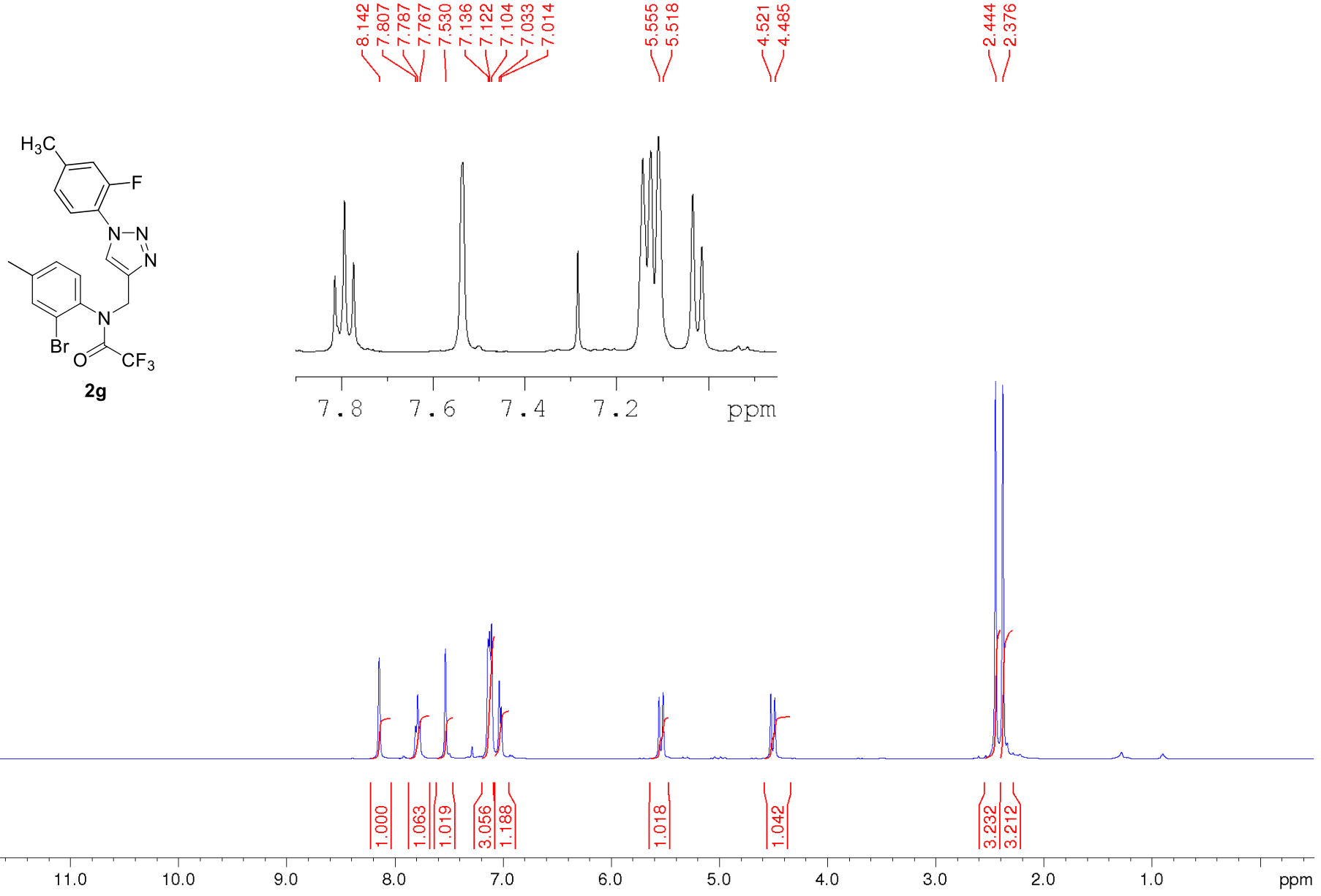
2f

^{19}F NMR-spectrum (376.5 Hz, $CDCl_3$)

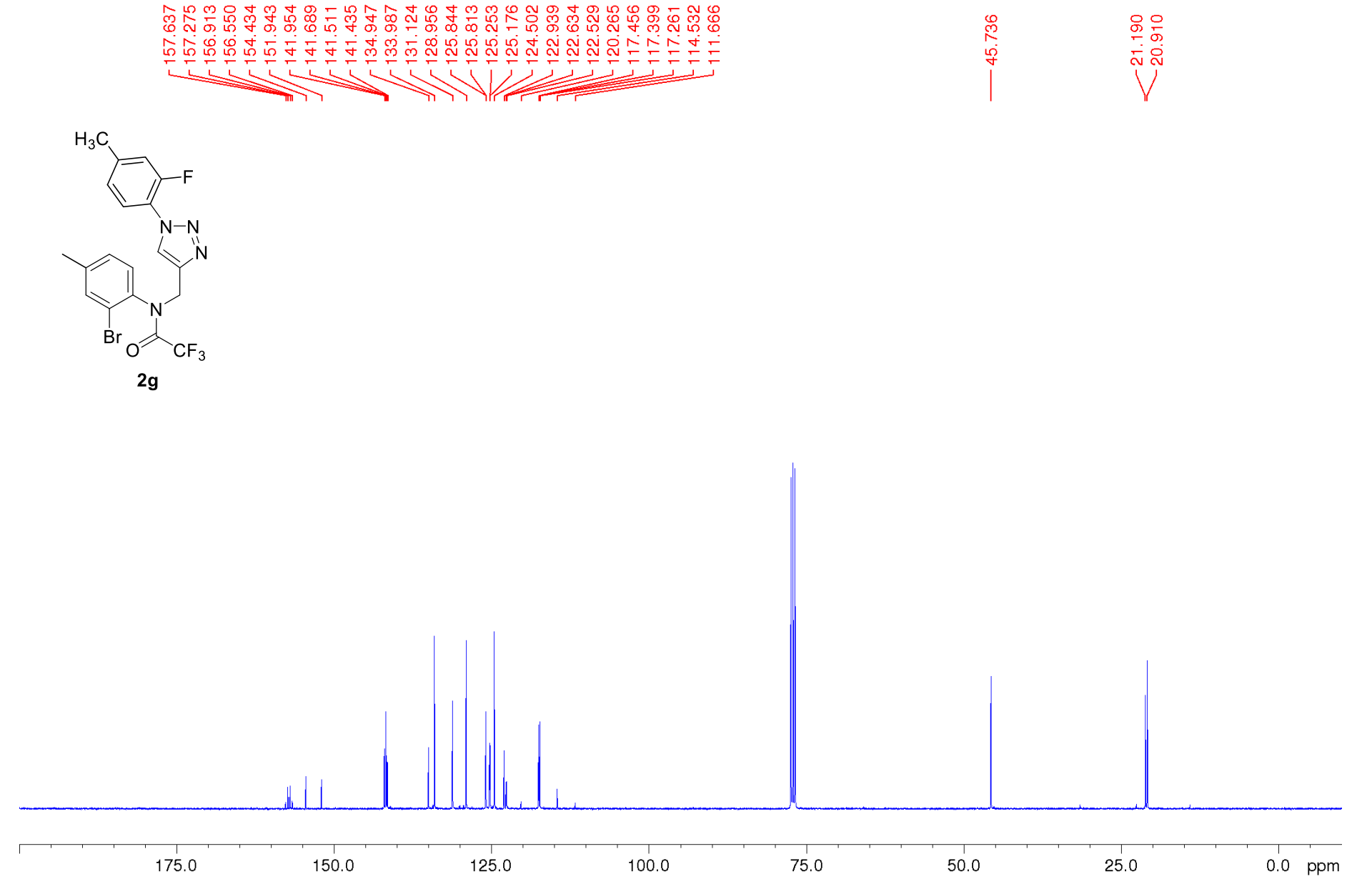


2f

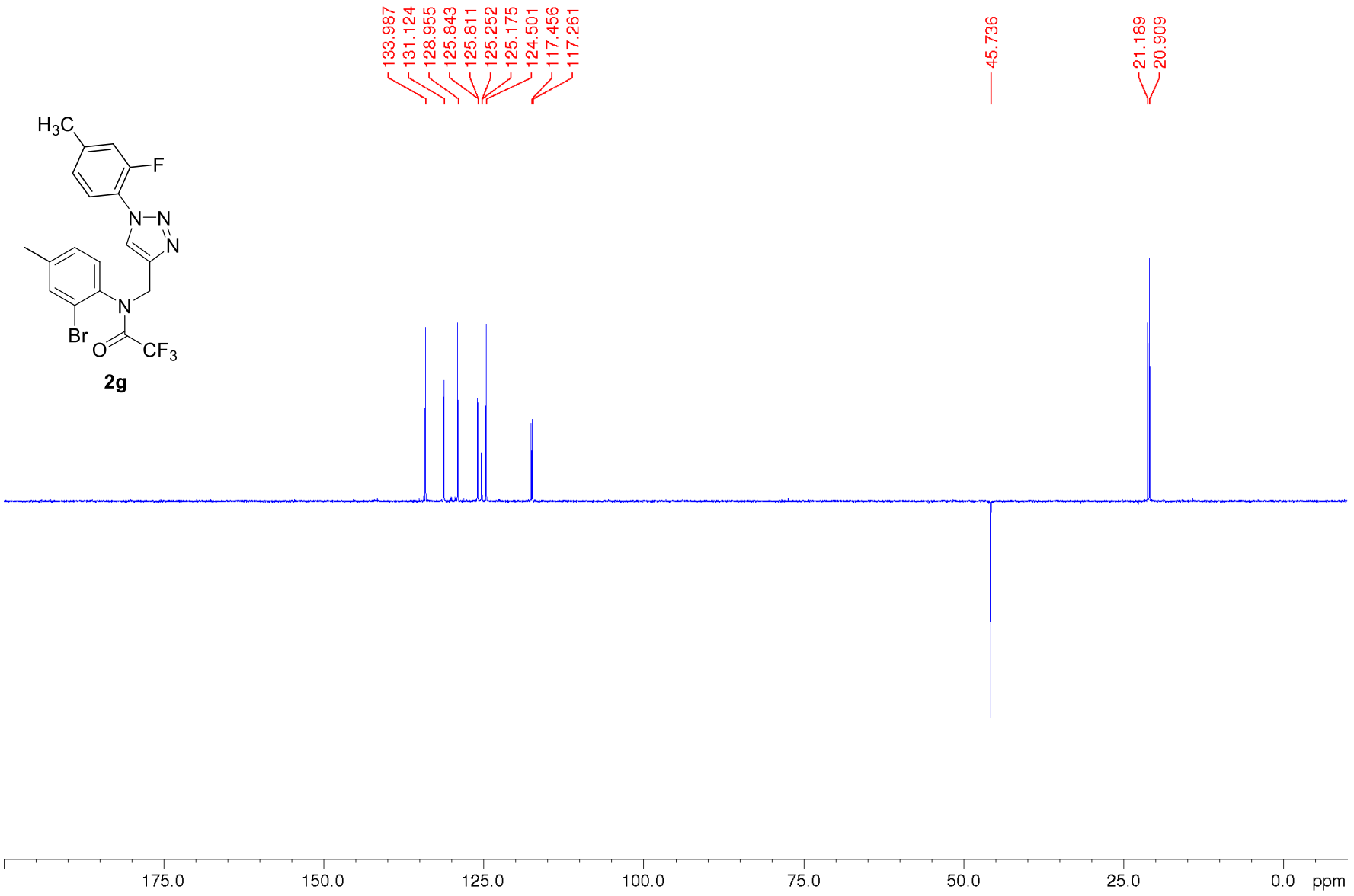
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



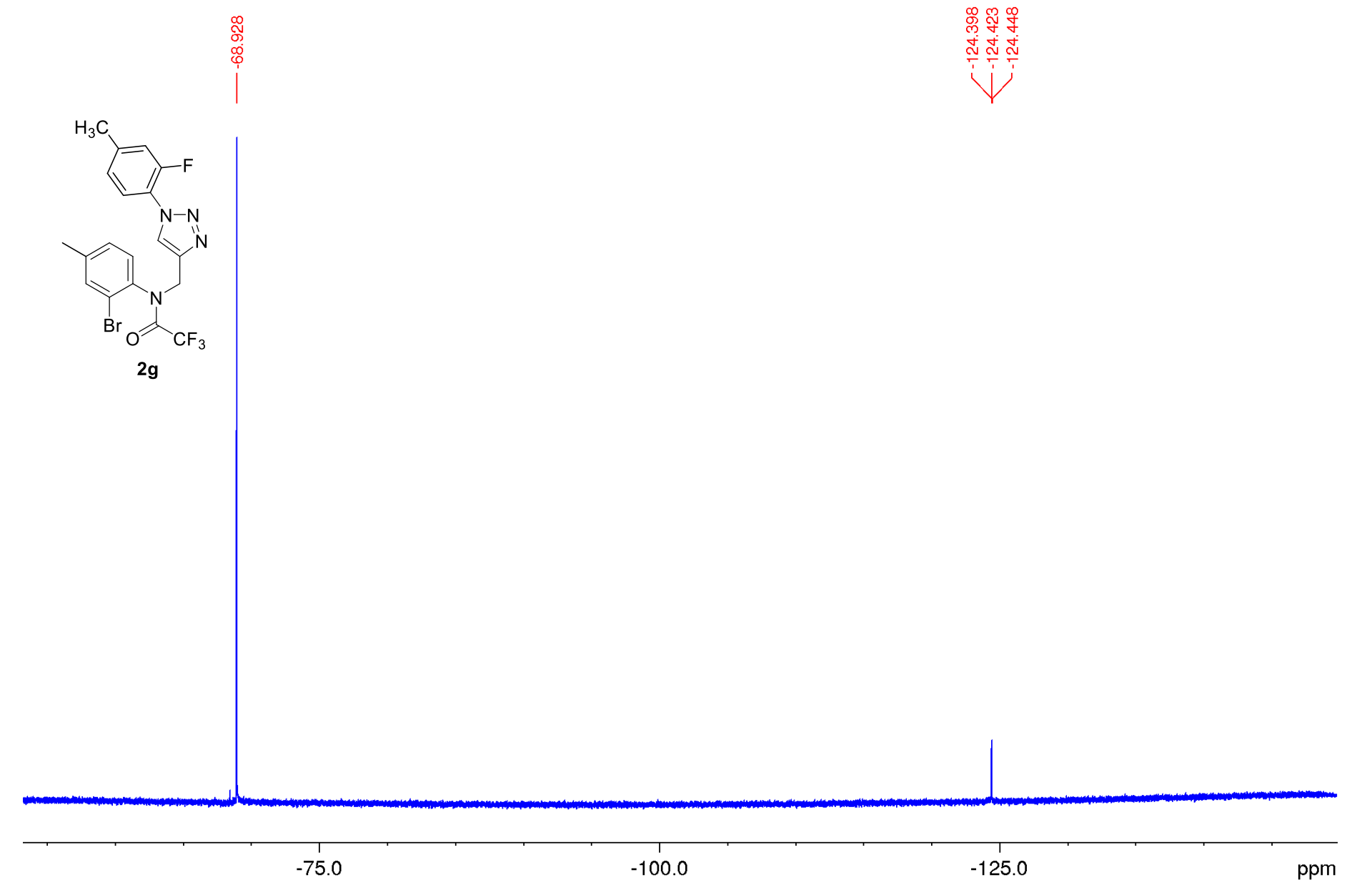
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



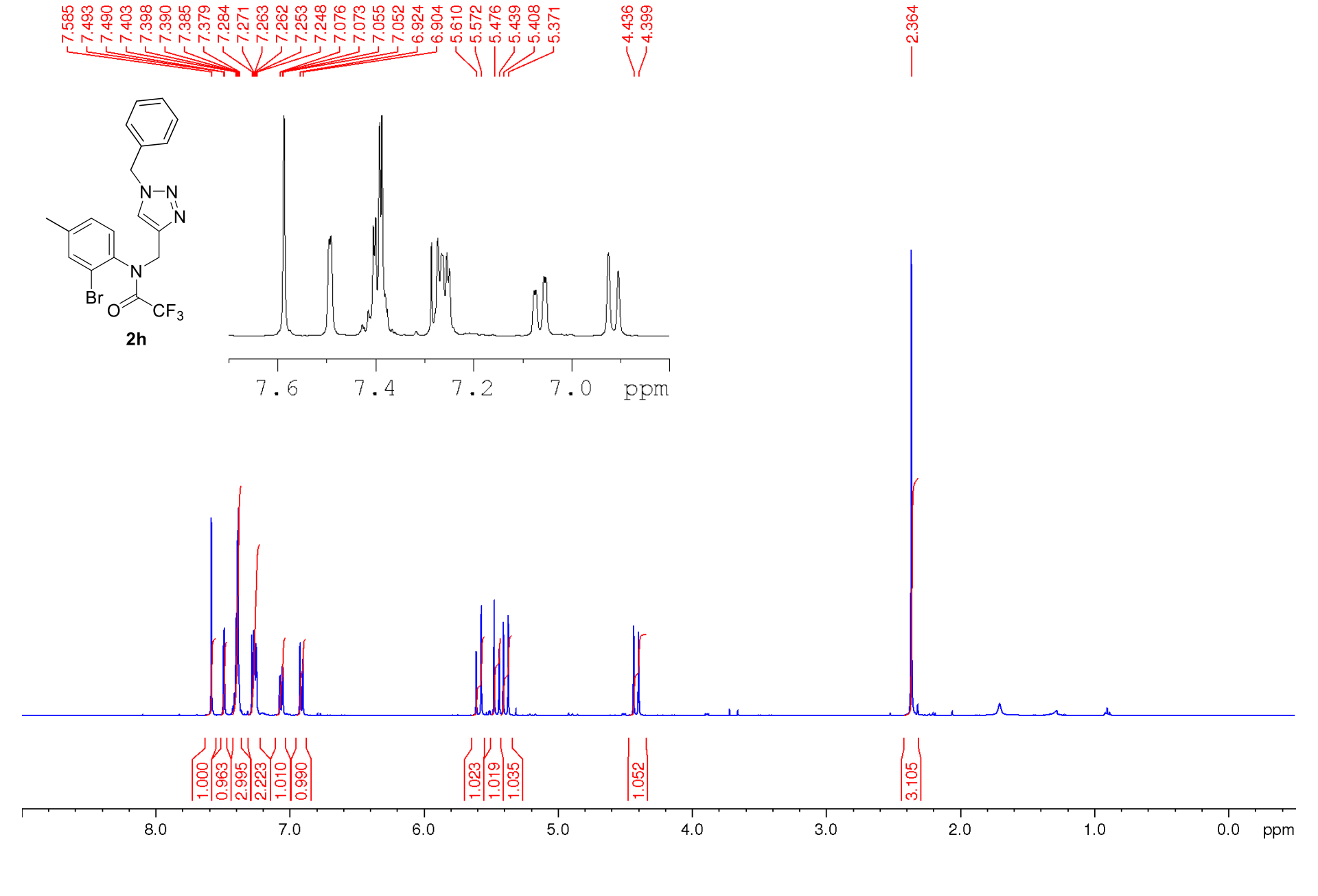
DEPT 135 NMR-spectrum ($CDCl_3$)



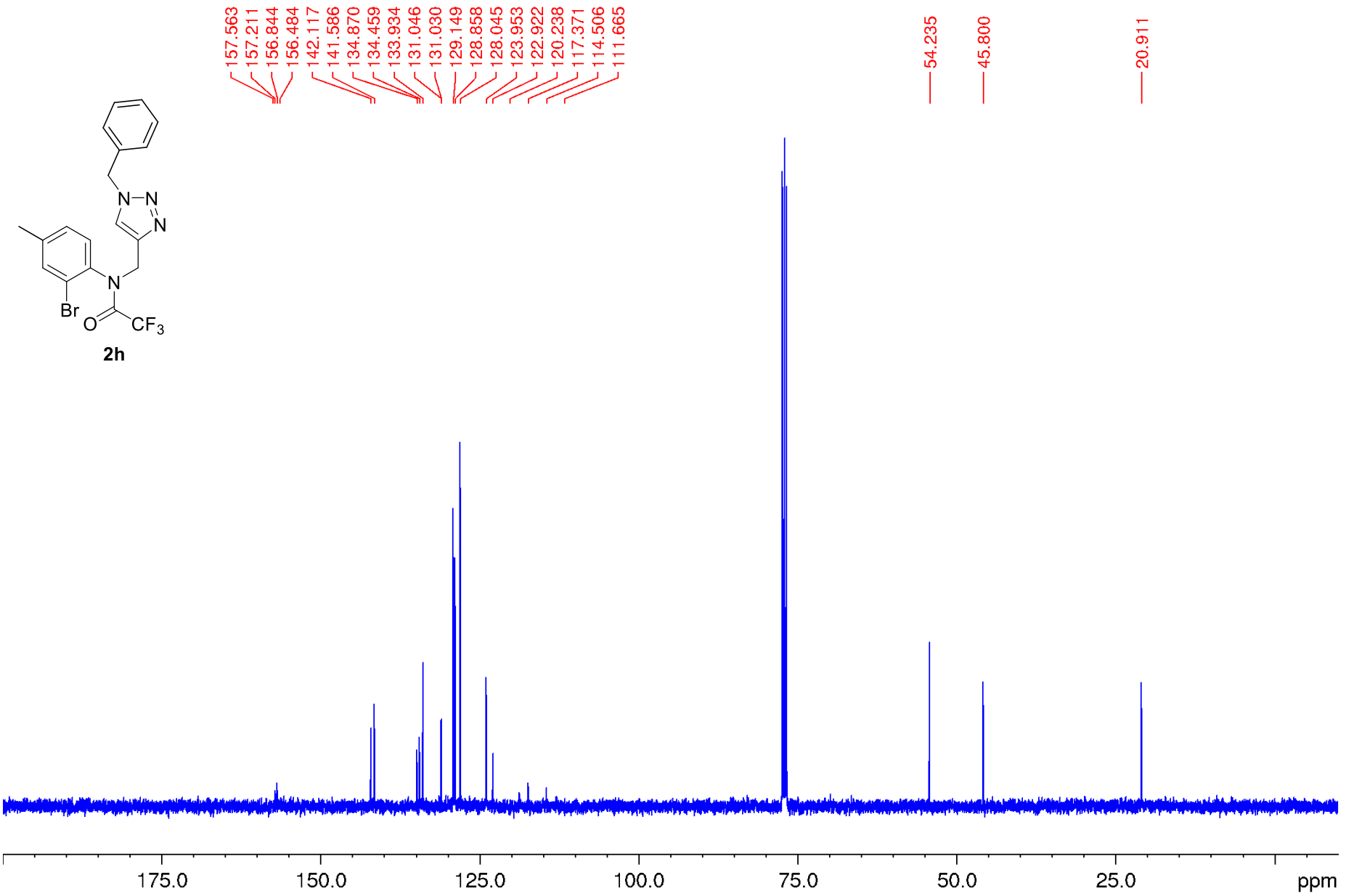
^{19}F NMR-spectrum (376.5 Hz, $CDCl_3$)



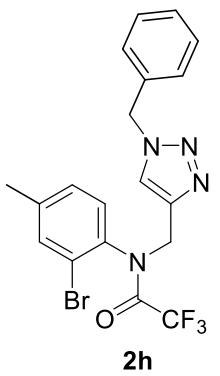
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



^{13}C NMR-spectrum (100 MHz, $CDCl_3$)

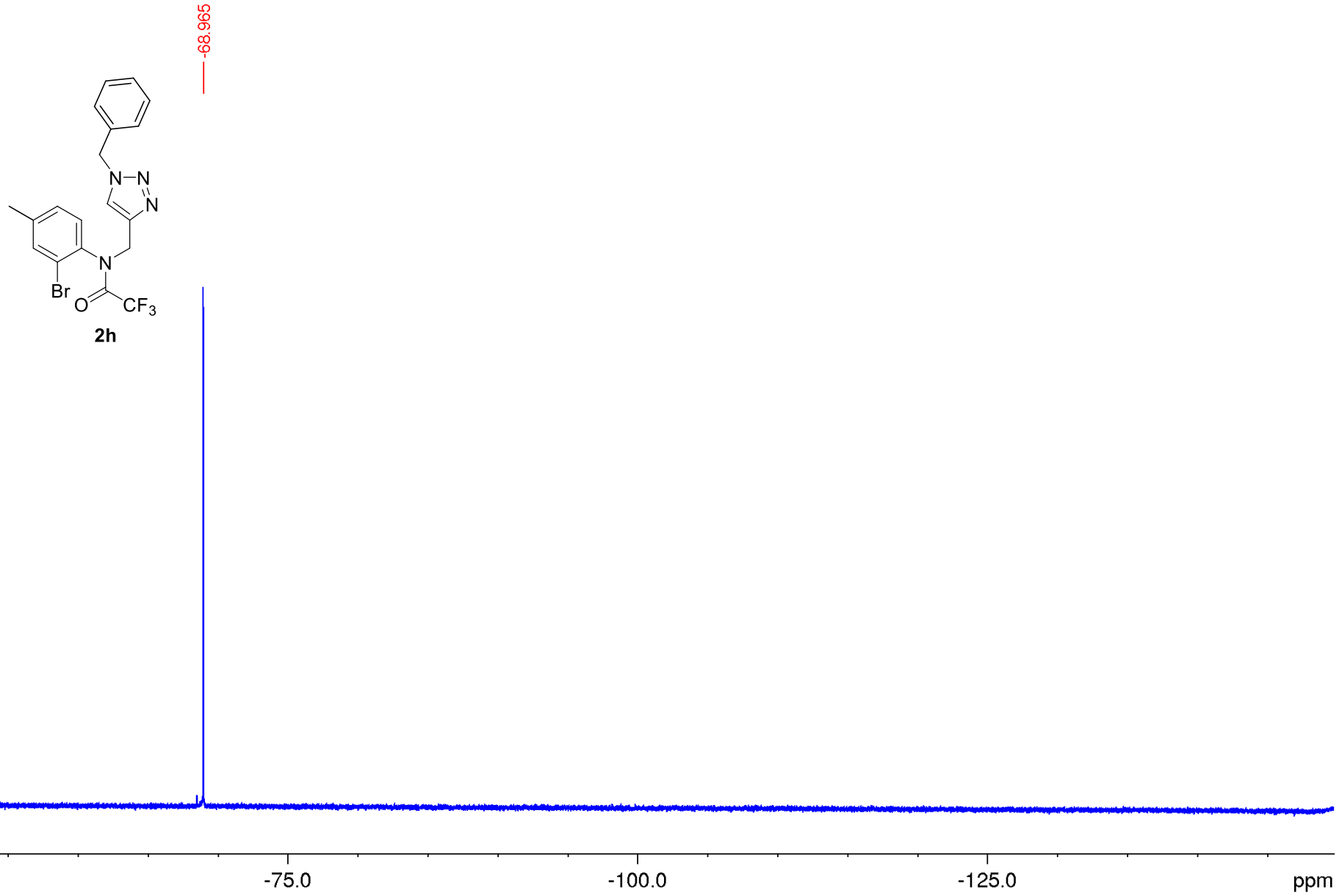


DEPT 135 NMR-spectrum ($CDCl_3$)

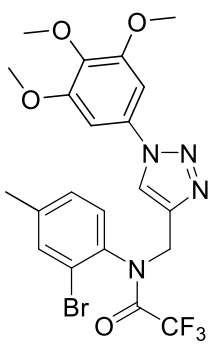


2h

^{19}F NMR-spectrum (376.5 Hz, $CDCl_3$)

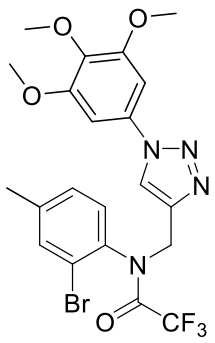


^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



2i

^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



2i

157.758
157.387
157.024
156.668
153.957
142.442
141.768
138.405
135.074
134.026
132.692
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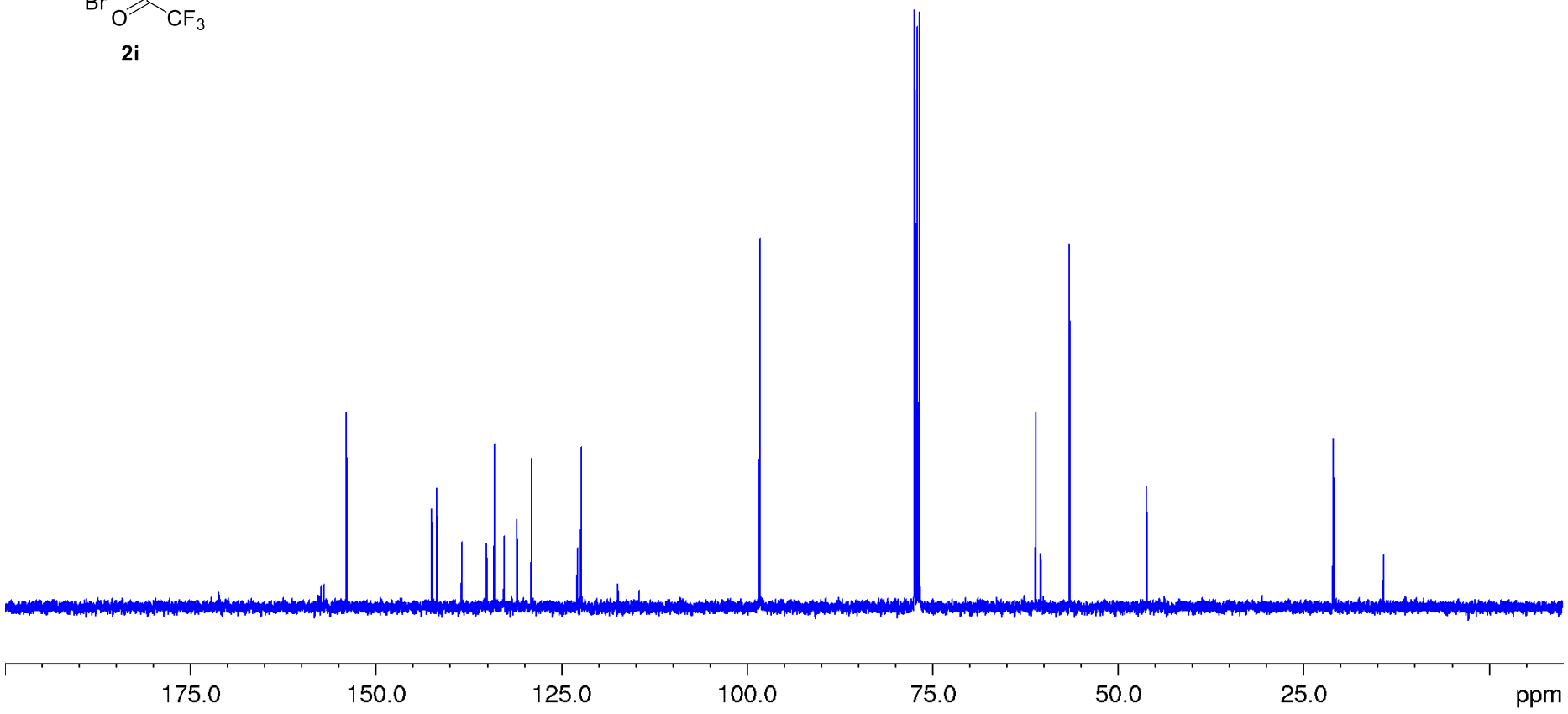
98.246
61.061
56.495
46.114
20.921



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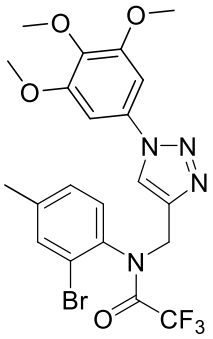
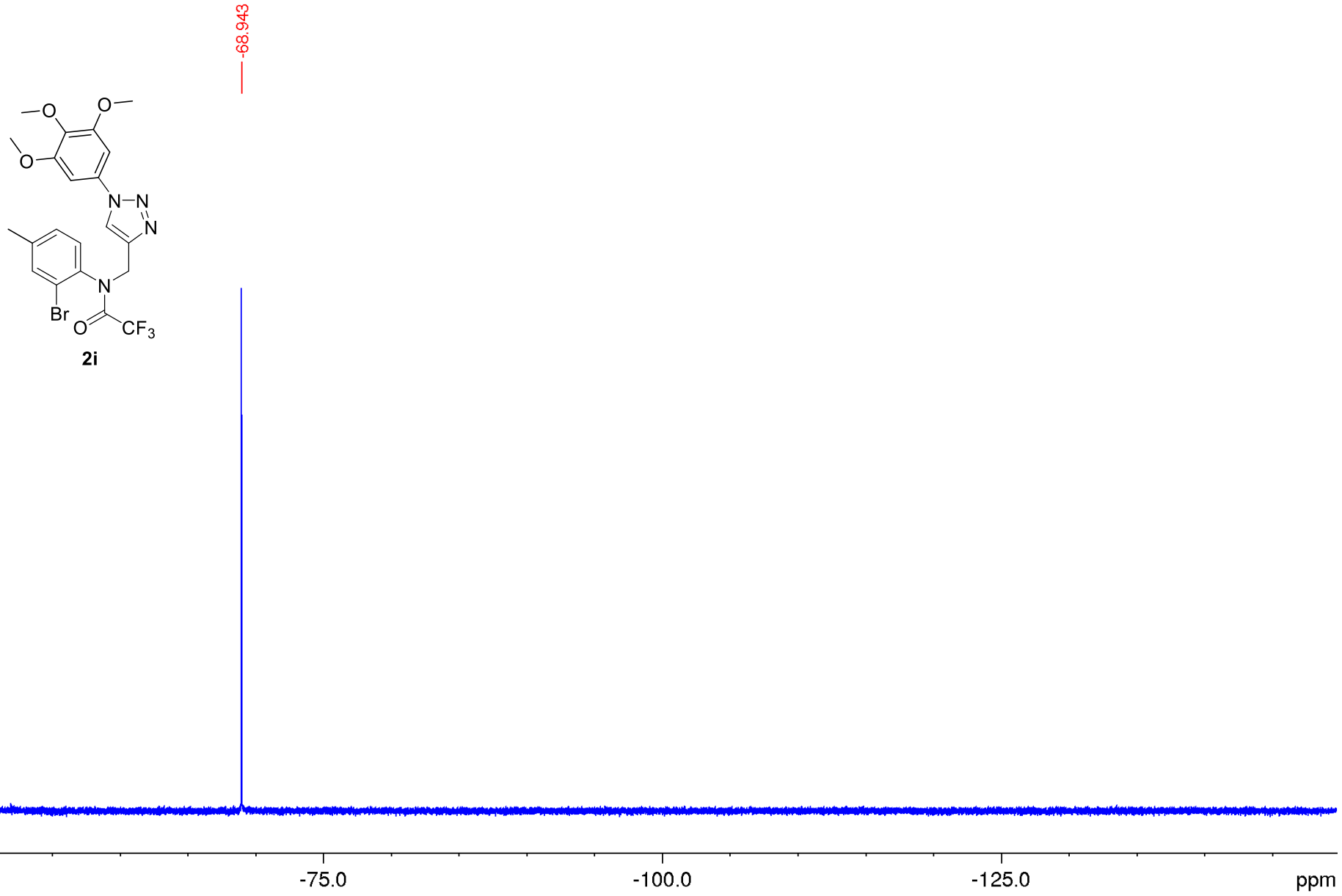
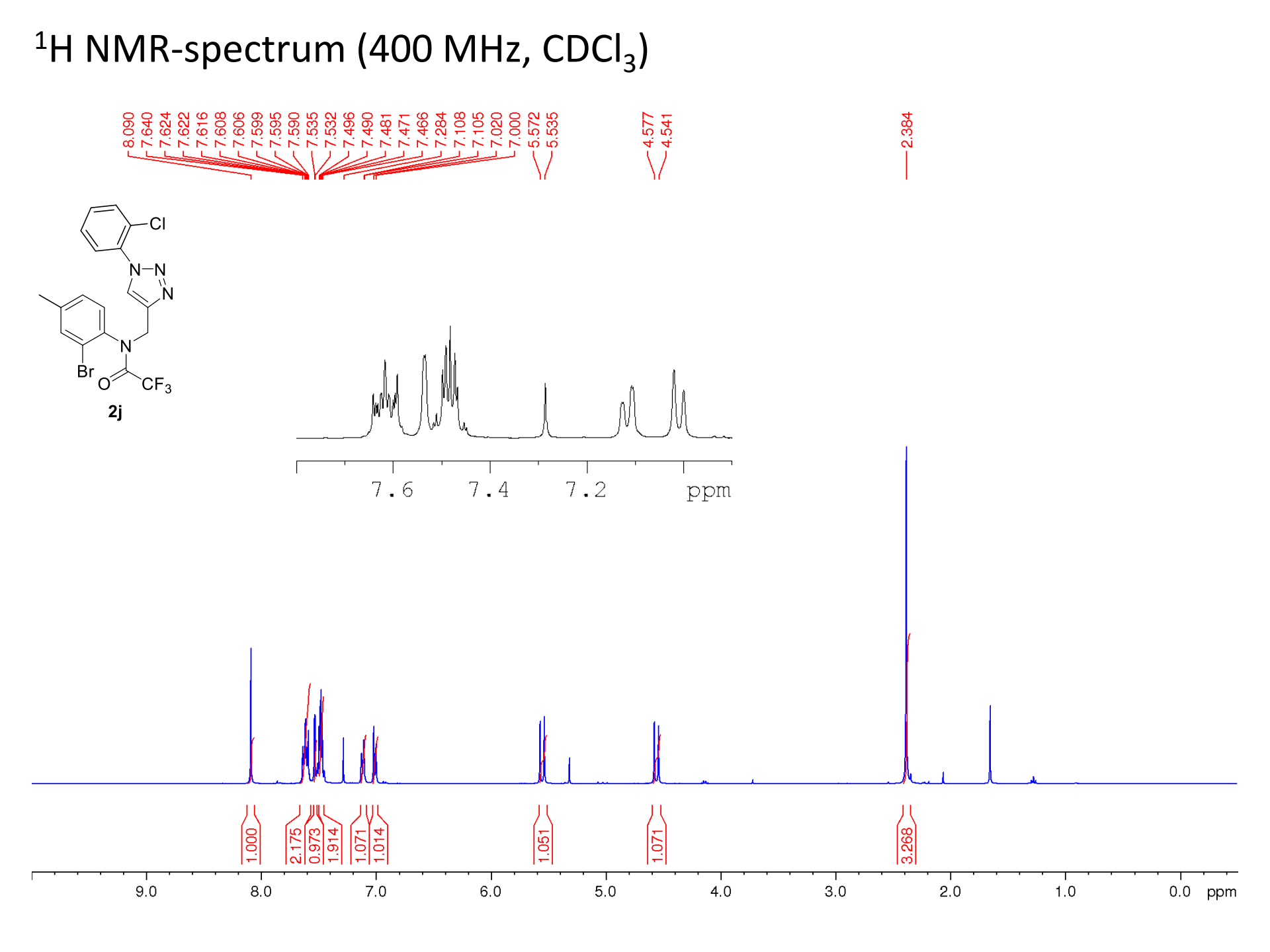


2i

^{19}F NMR-spectrum (376.5 Hz, $CDCl_3$)



^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



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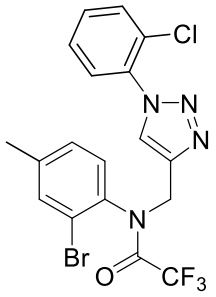
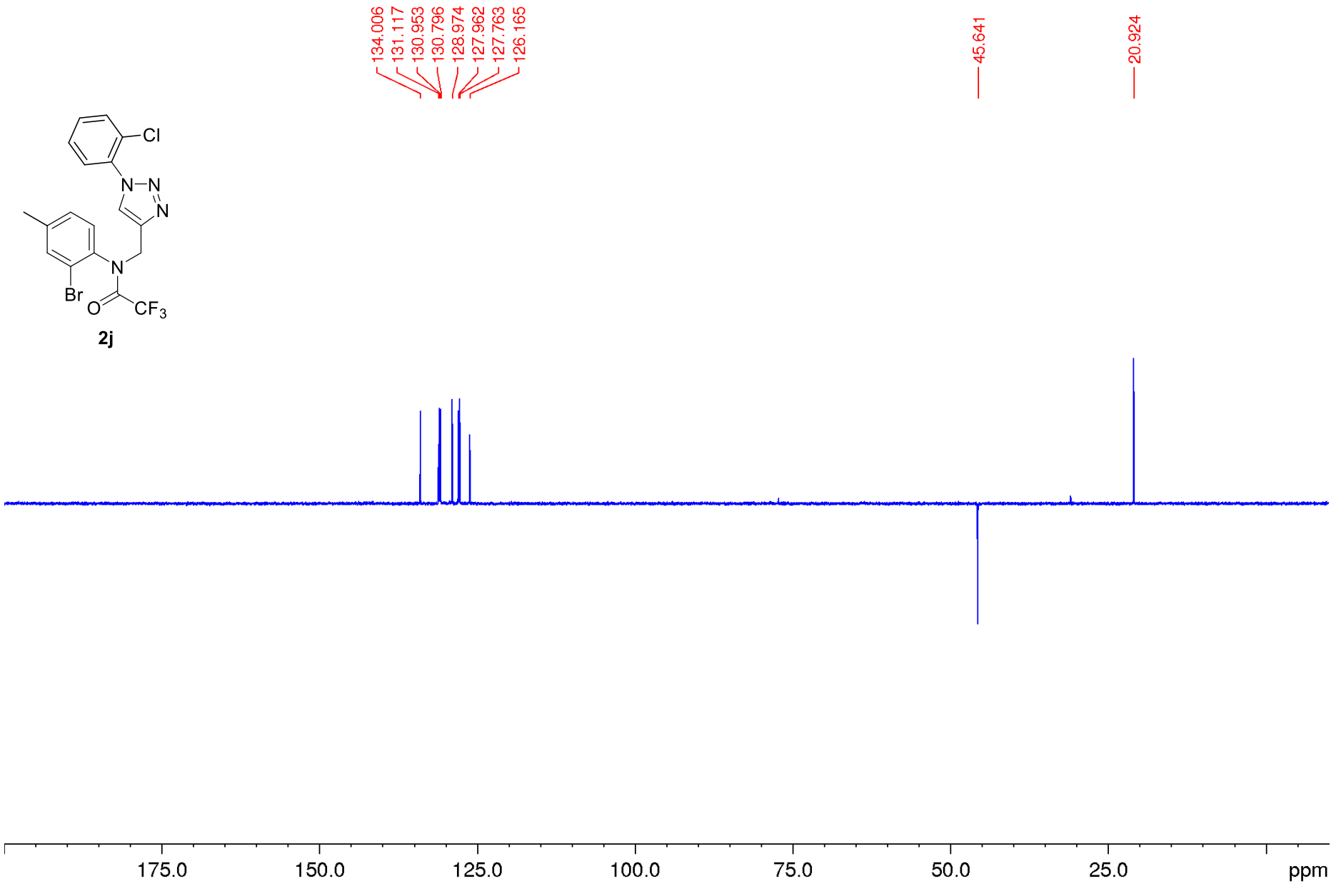
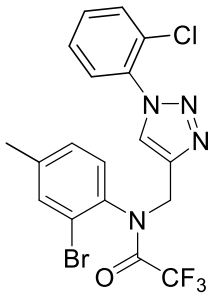


2j

DEPT 135 NMR-spectrum ($CDCl_3$)

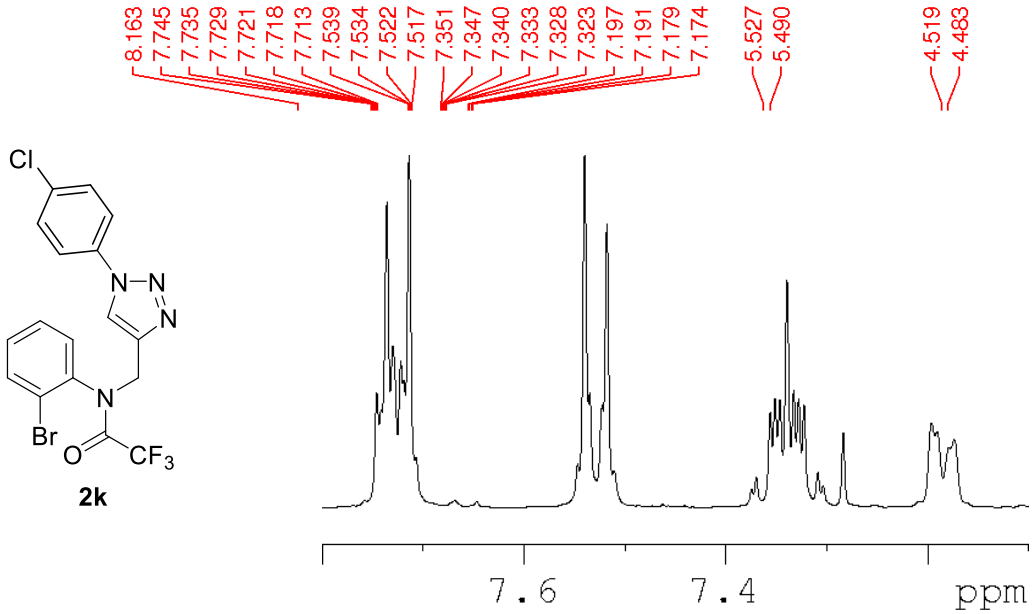


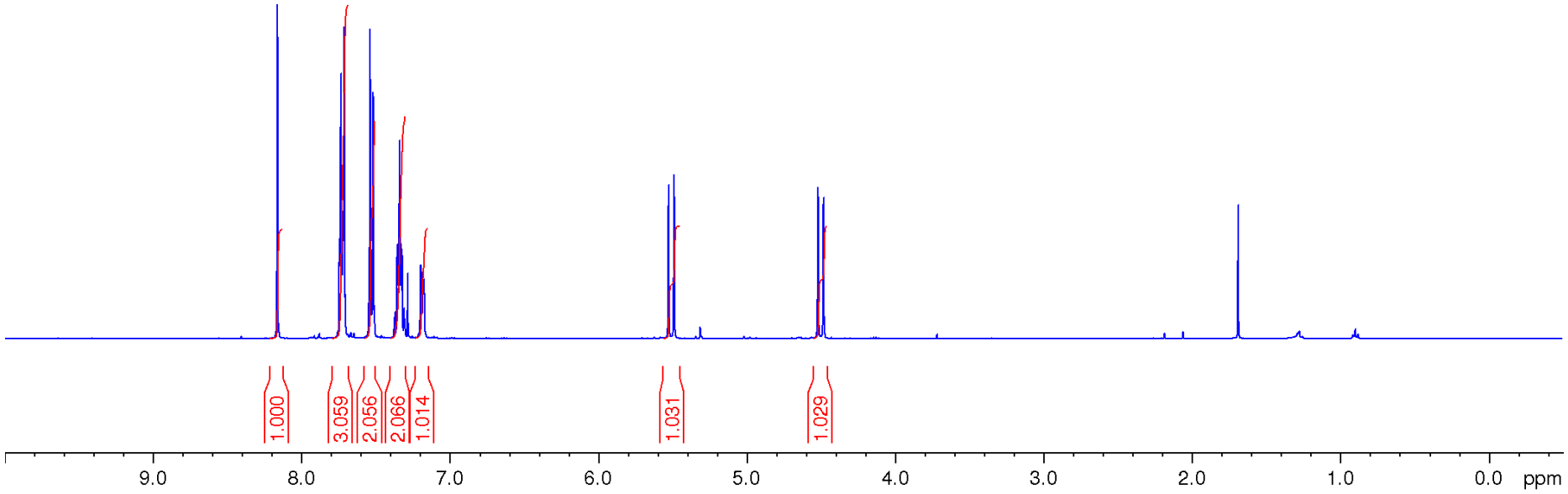
^{19}F NMR-spectrum (376.5 Hz, $CDCl_3$)



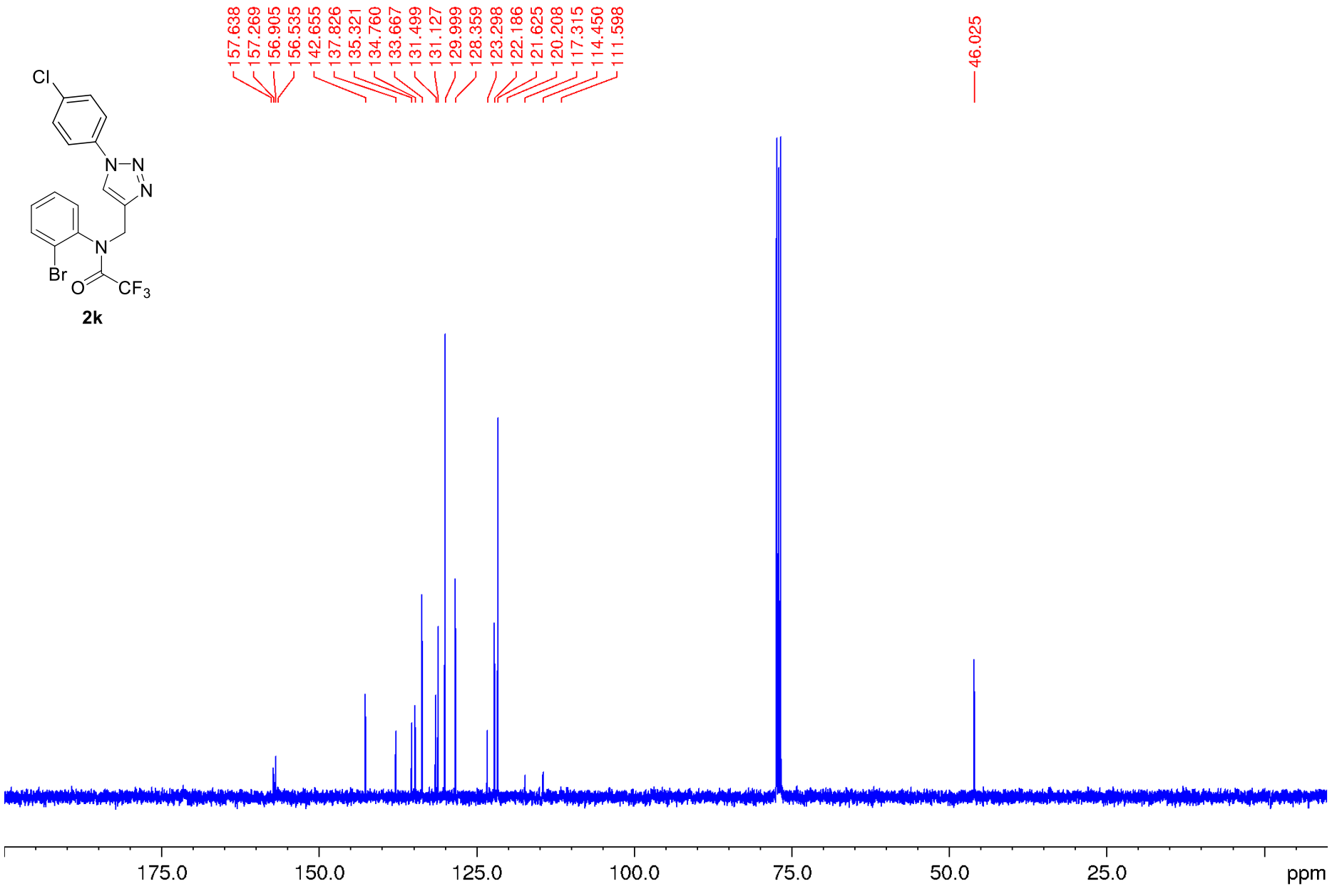
2j

^{1}H NMR-spectrum (400 MHz, $CDCl_3$)

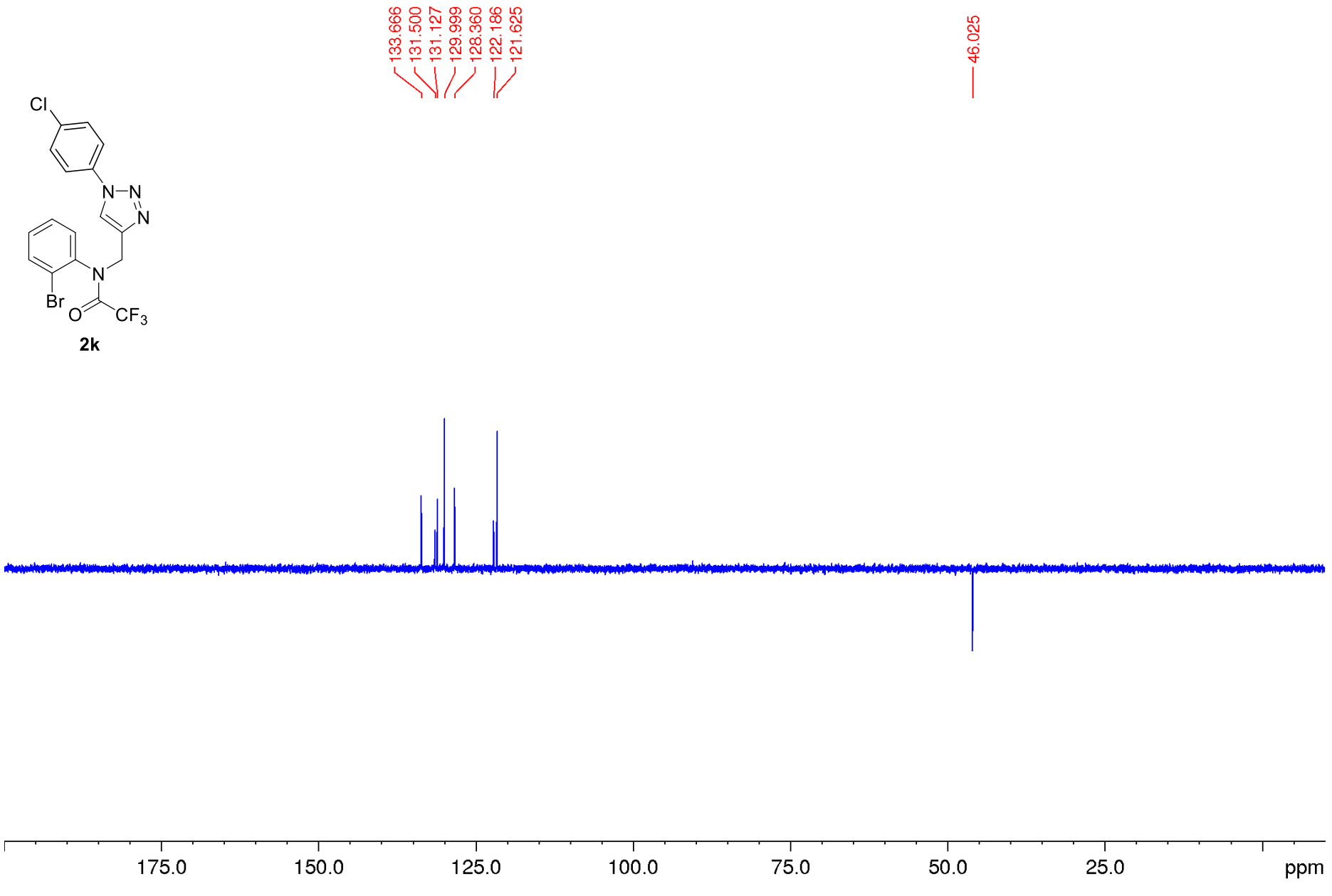




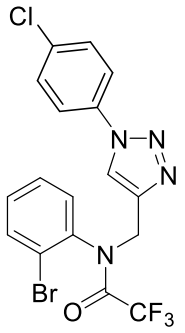
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



DEPT 135 NMR-spectrum ($CDCl_3$)

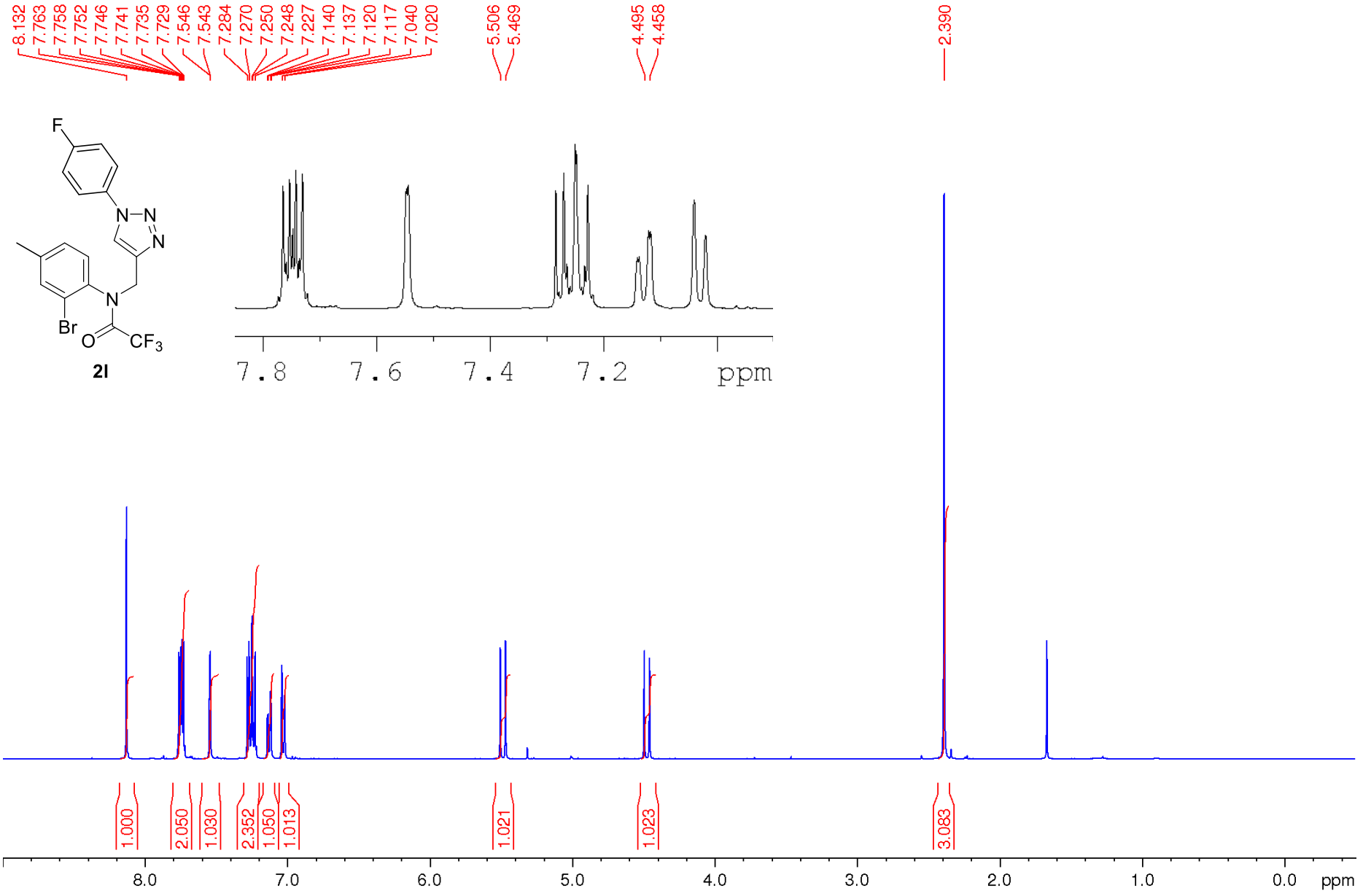


^{19}F NMR-spectrum (376.5 Hz, $CDCl_3$)

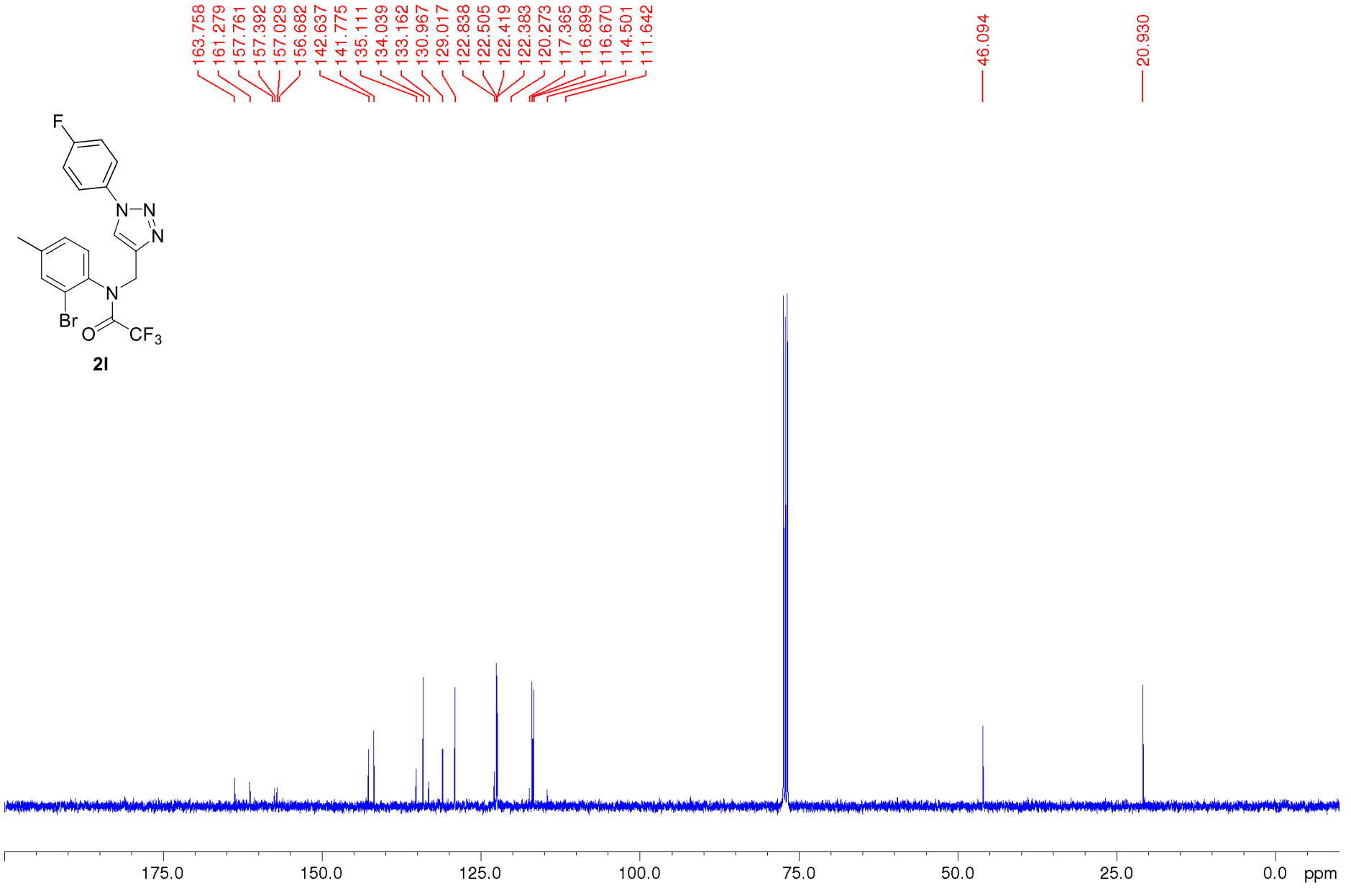


2k

^{1}H NMR-spectrum (400 MHz, $CDCl_3$)

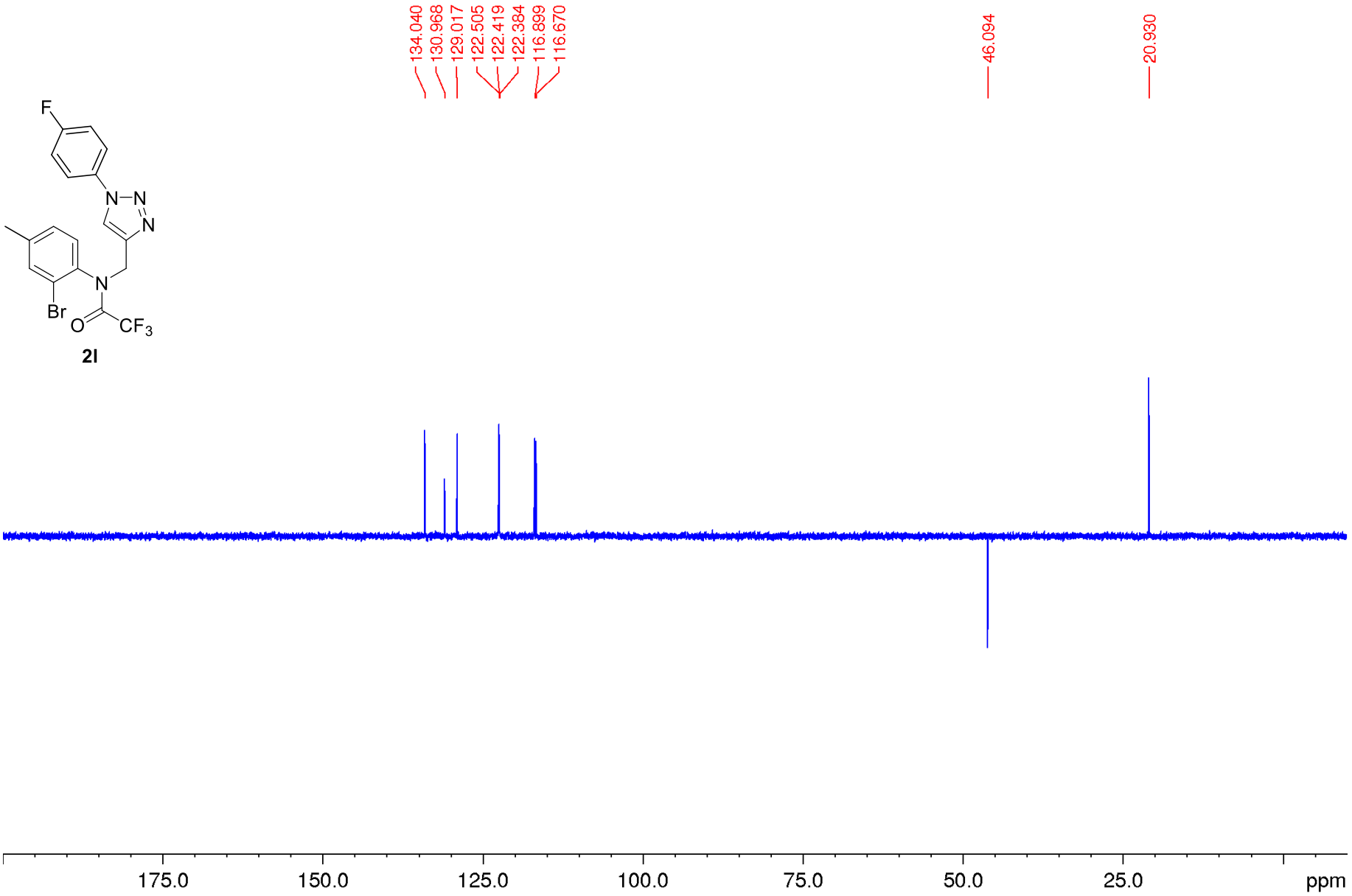


^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



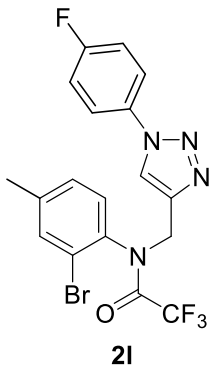
2l

DEPT 135 NMR-spectrum ($CDCl_3$)



2l

^{19}F NMR-spectrum (376.5 Hz, $CDCl_3$)



2l

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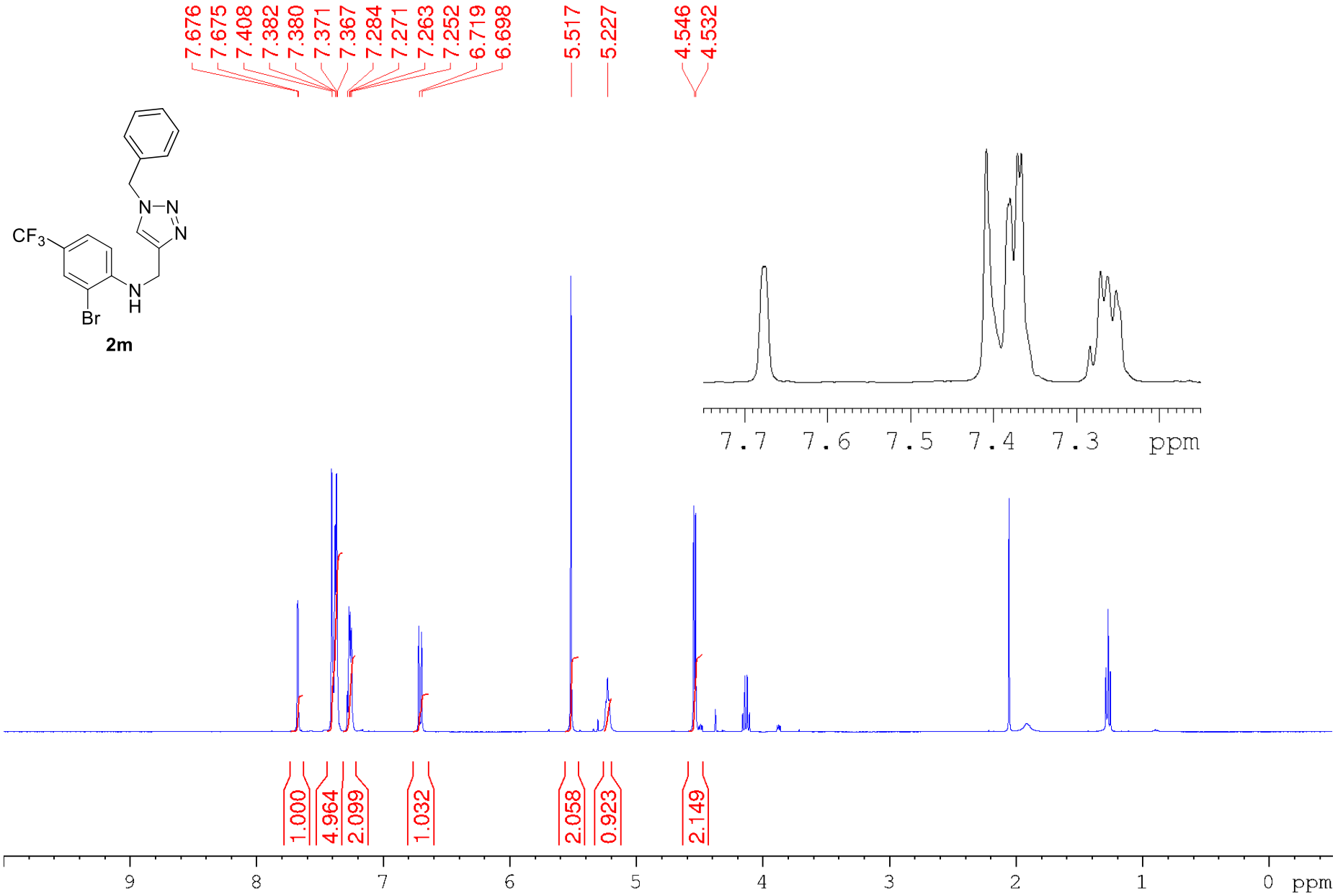
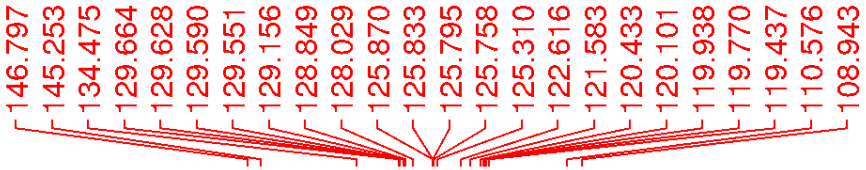
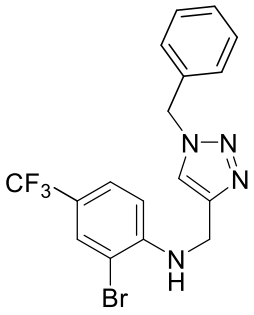
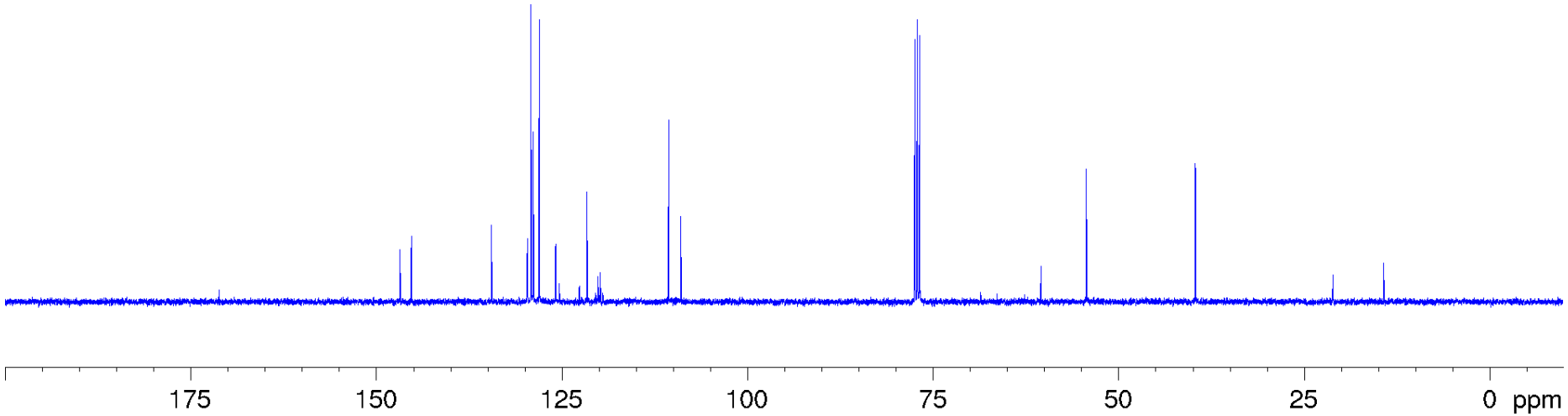


^{13}C NMR-spectrum (100 MHz, $CDCl_3$)

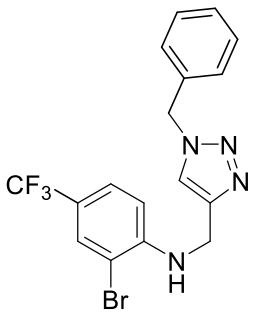




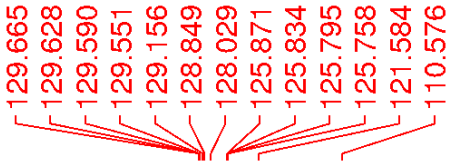
2m

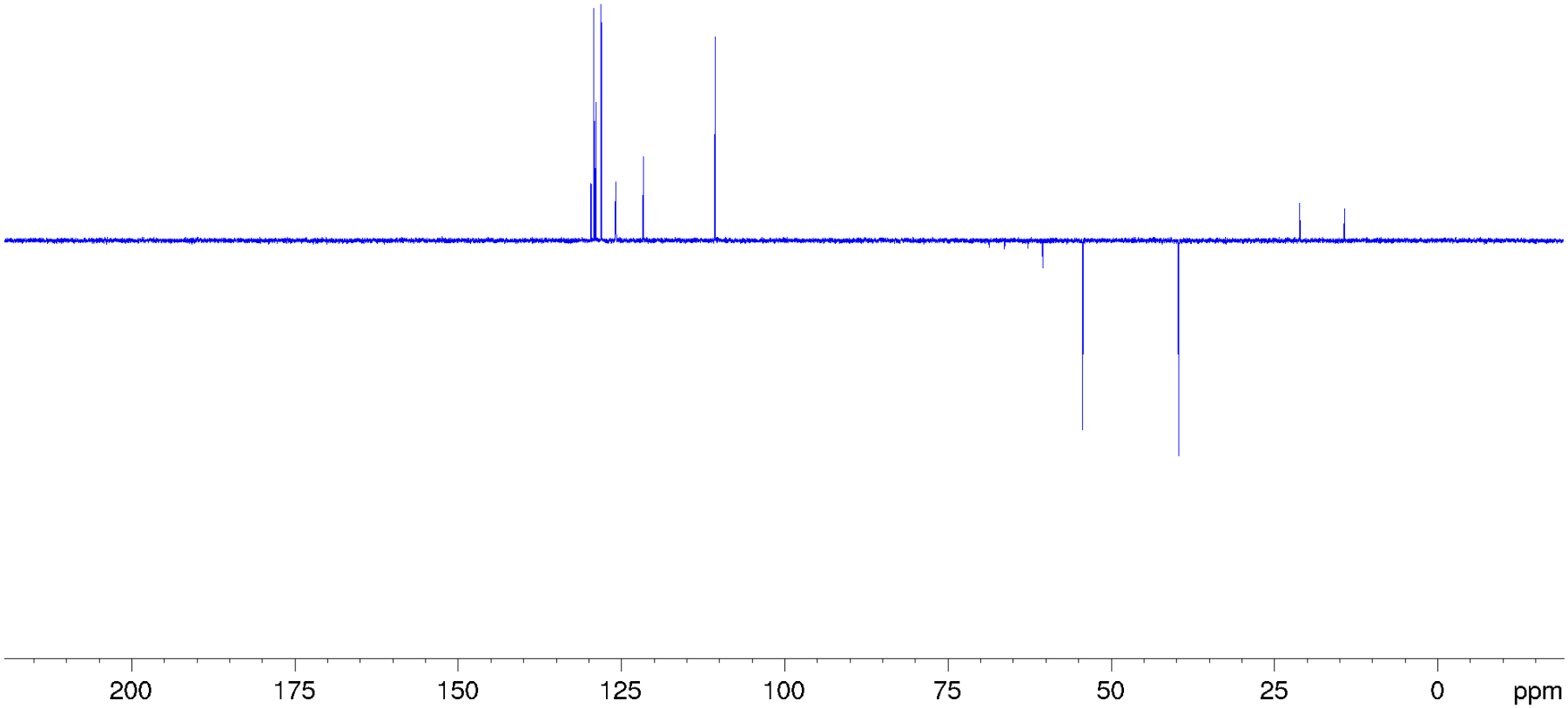


DEPT 135 NMR-spectrum ($CDCl_3$)

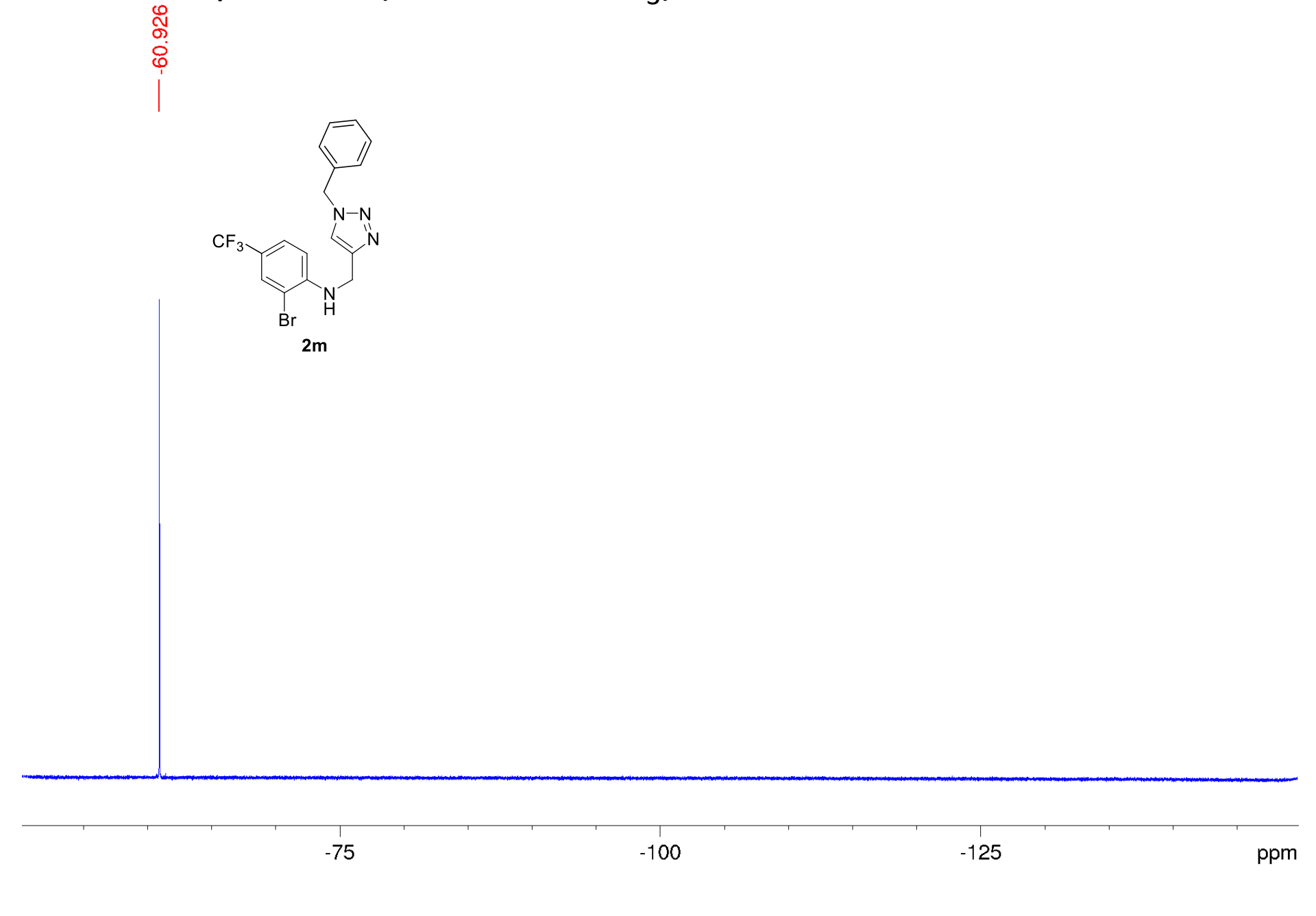


2m

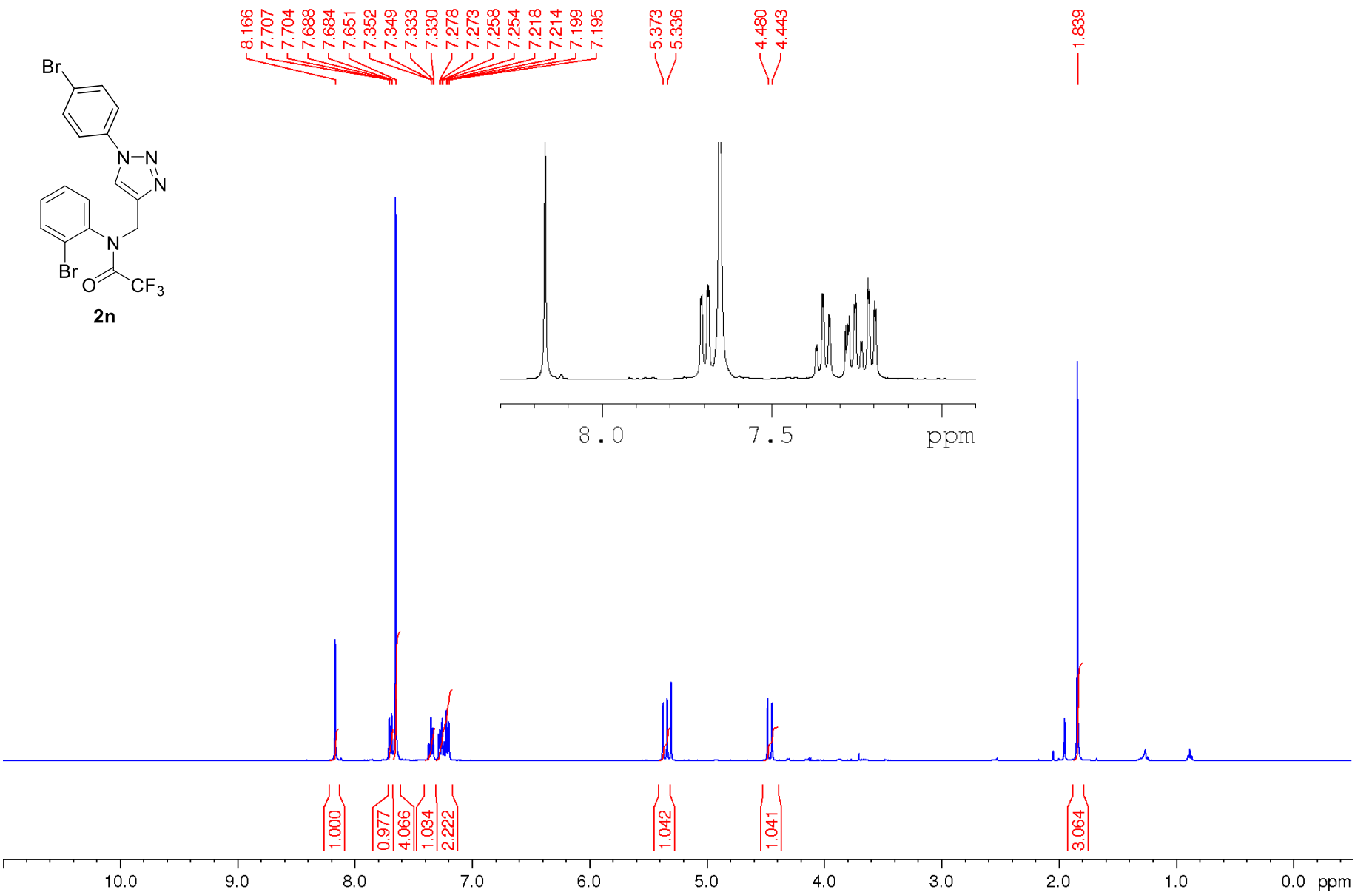




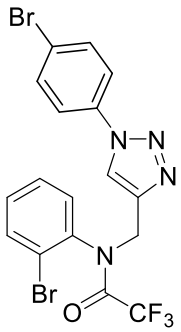
^{19}F NMR-spectrum (376.5 Hz, $CDCl_3$)



^{1}H NMR-spectrum (400 MHz, $CDCl_3$)

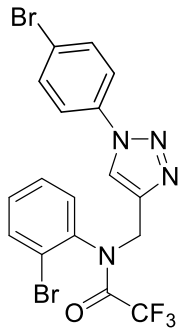


^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



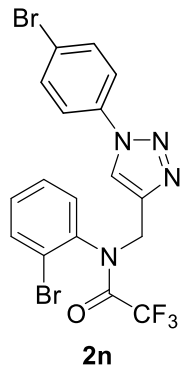
2n

DEPT 135 NMR-spectrum ($CDCl_3$)



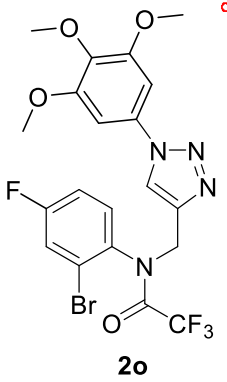
2n

^{19}F NMR-spectrum (376.5 Hz, $CDCl_3$)

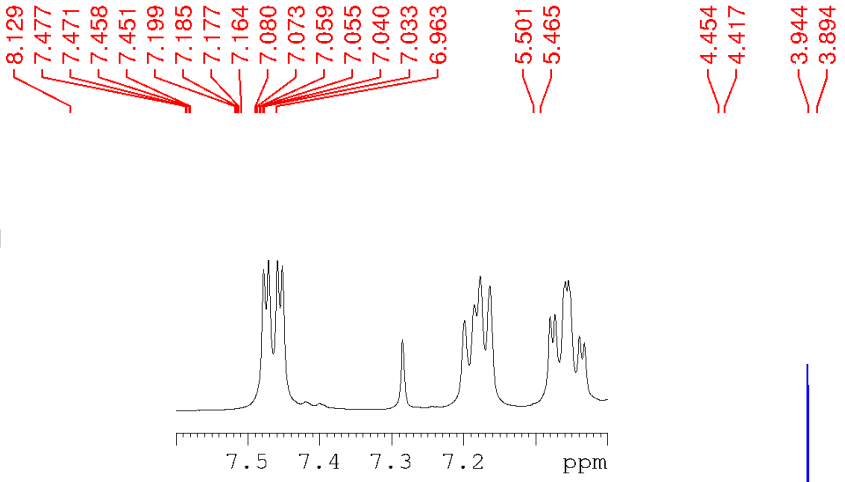


2n

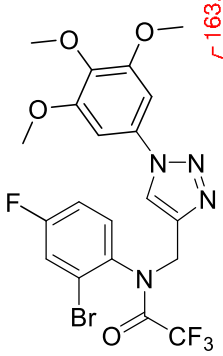
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



2o

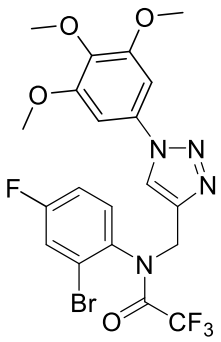


^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



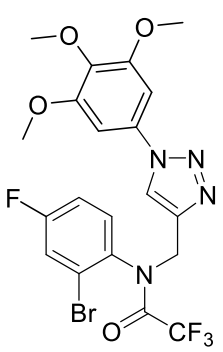
2o

DEPT 135 NMR-spectrum ($CDCl_3$)



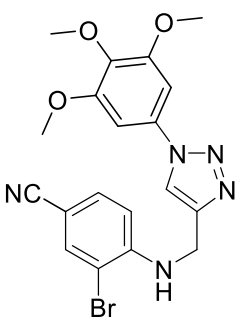
2o

^{19}F NMR-spectrum (376.5 Hz, $CDCl_3$)

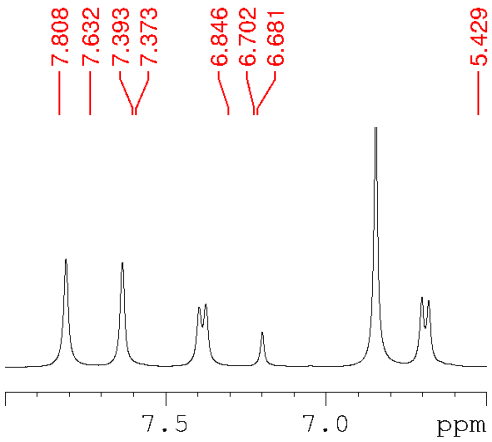


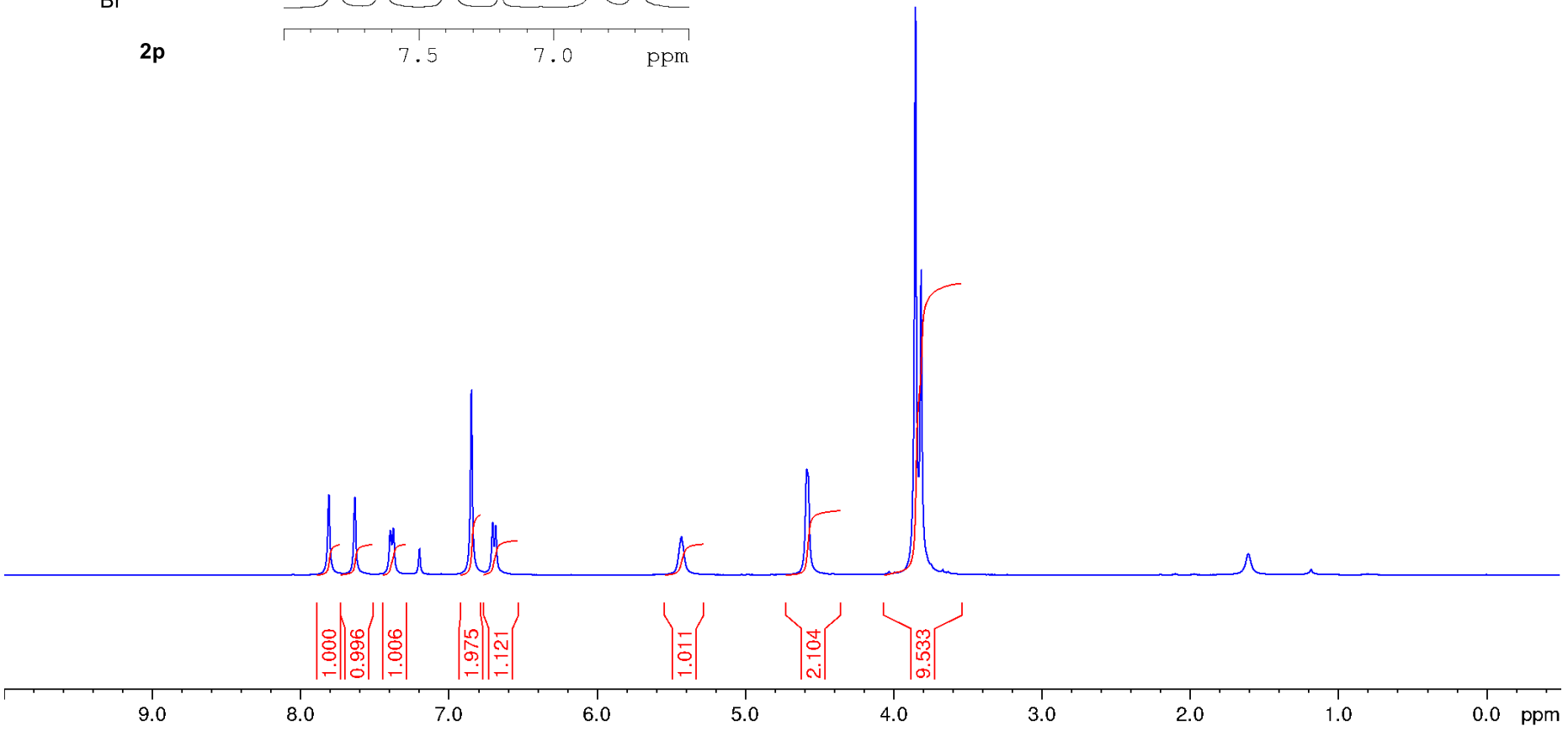
2o

^{1}H NMR-spectrum (400 MHz, $CDCl_3$)

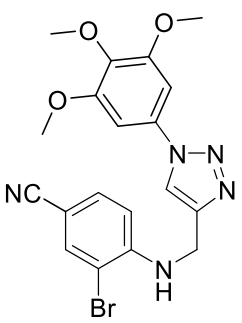


2p





^{13}C NMR-spectrum (100 MHz, $CDCl_3$)

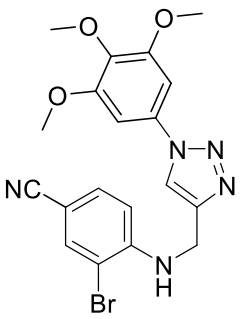


2p

153.972
147.602
144.941
138.564
135.892
133.040
132.675
120.203
118.689
110.804
108.982
100.600
98.575
61.084
56.503
39.388

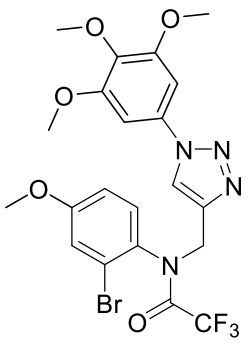
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm

DEPT 135 NMR-spectrum ($CDCl_3$)



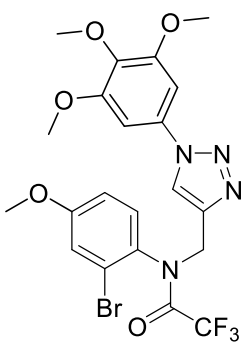
2p

^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



2q

^{13}C NMR-spectrum (100 MHz, $CDCl_3$)

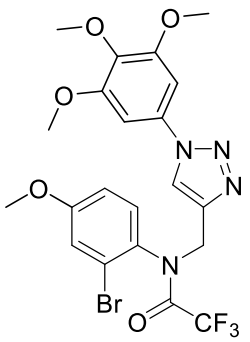


2q

160.645
157.976
157.583
157.224
156.861
153.966
142.470
138.410
132.689
131.886
130.339
123.884
122.336
118.809
117.400
114.535
113.597
98.240
77.364
77.045
76.728
61.082
56.504
55.810
46.256

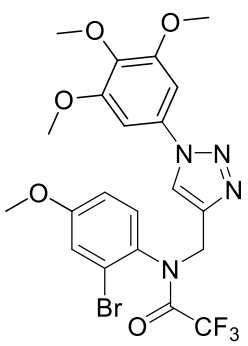
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm

DEPT 135 NMR-spectrum ($CDCl_3$)



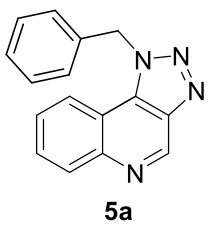
2q

^{19}F NMR-spectrum (376.5 Hz, $CDCl_3$)

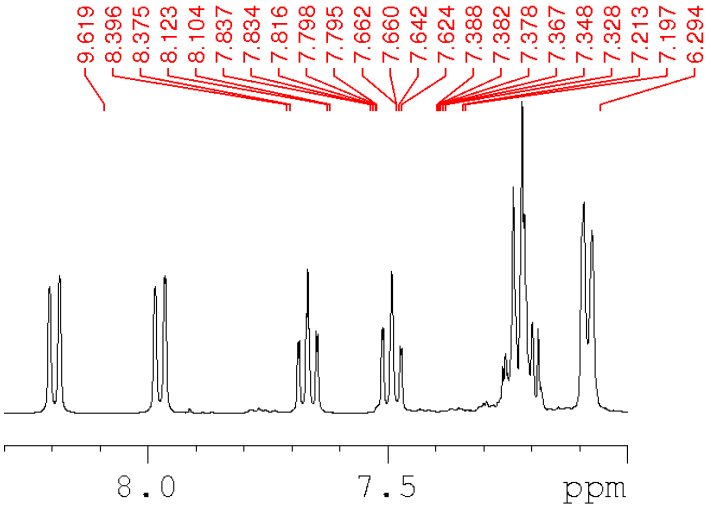


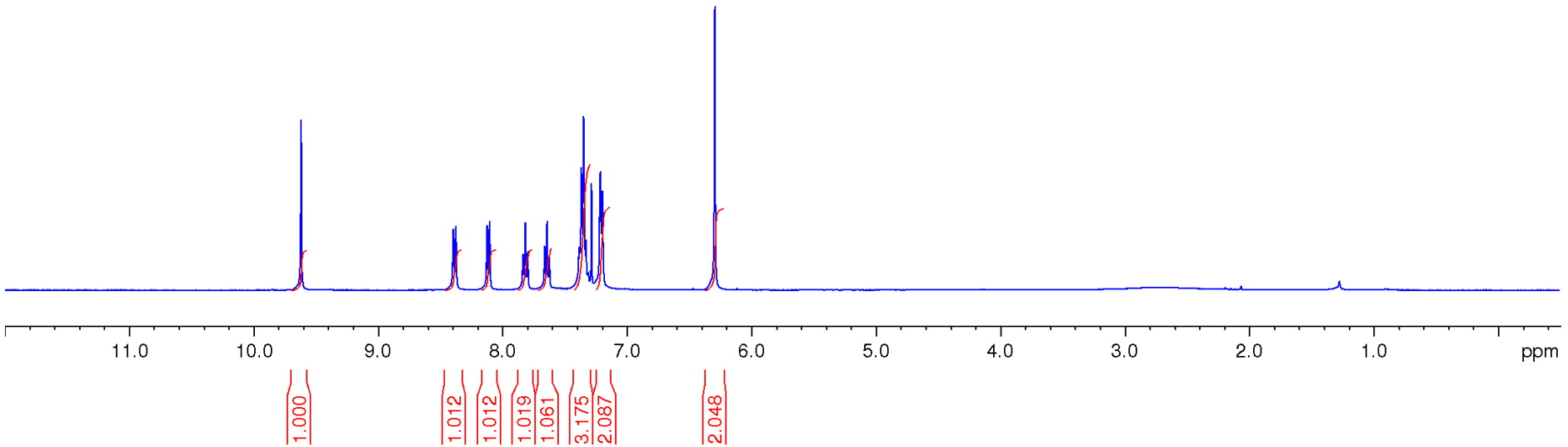
2q

^{1}H NMR-spectrum (400 MHz, $CDCl_3$)

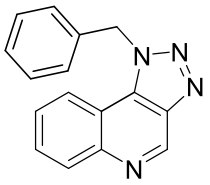


5a



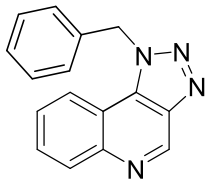


^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



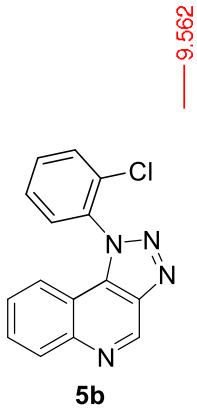
5a

DEPT 135 NMR-spectrum ($CDCl_3$)

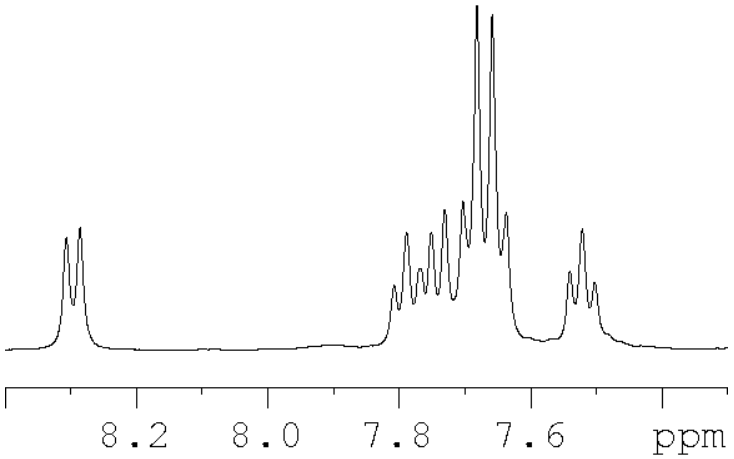


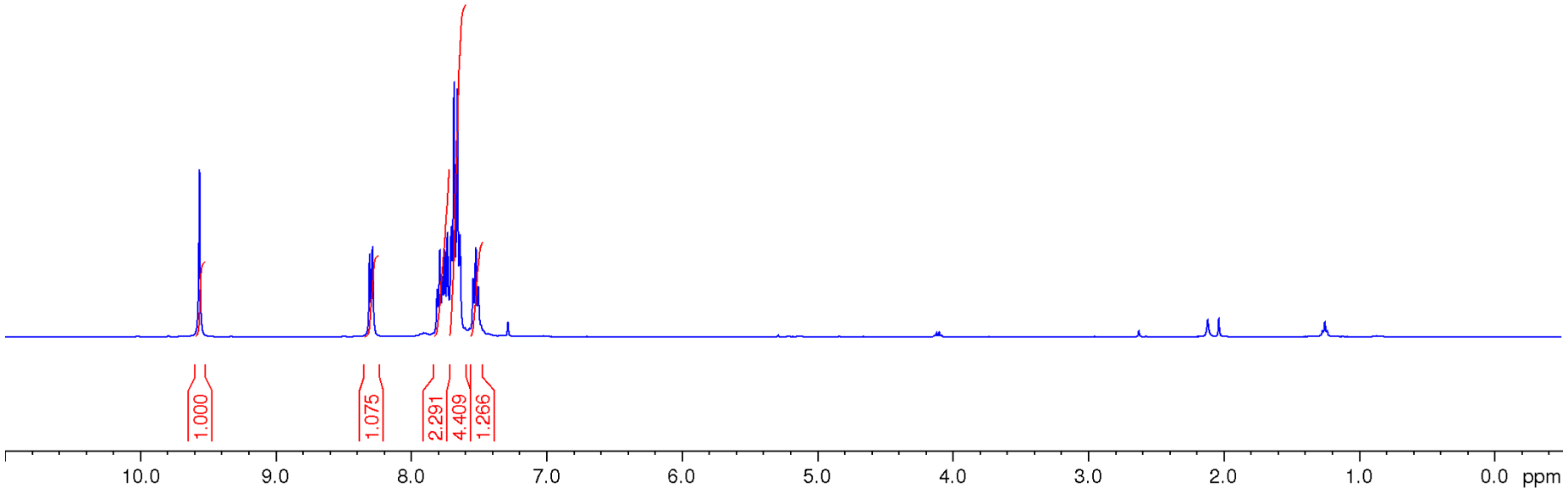
5a

^{1}H NMR-spectrum (400 MHz, $CDCl_3$)

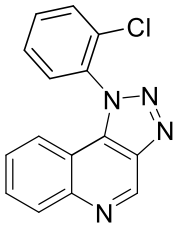


5b



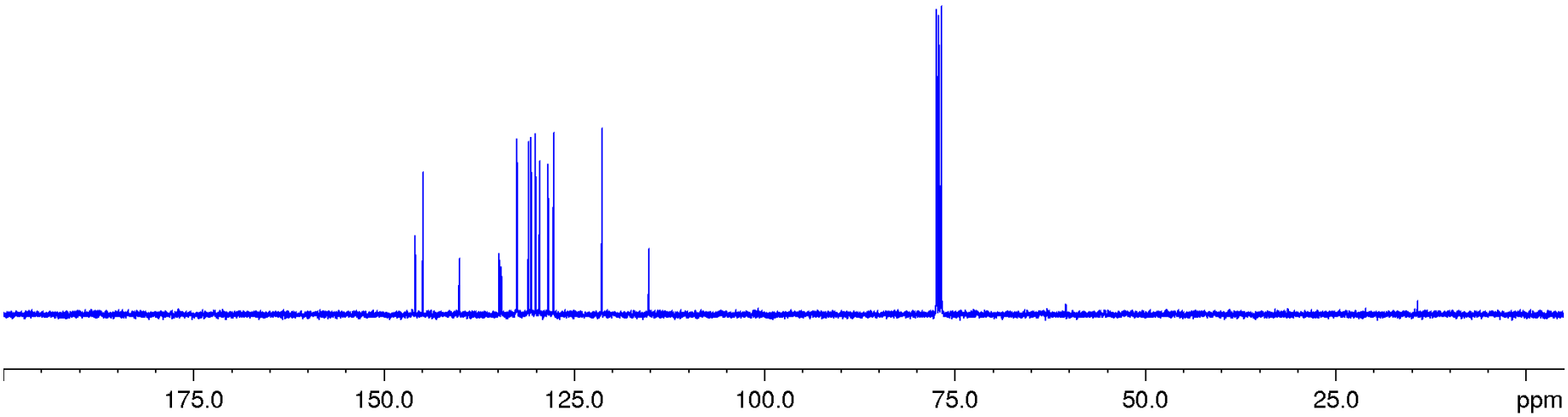


^{13}C NMR-spectrum (100 MHz, $CDCl_3$)

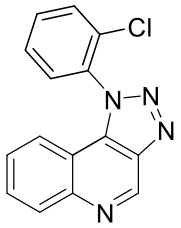


5b

145.902
144.862
140.096
134.834
134.550
132.509
132.471
131.005
130.648
130.080
129.553
128.413
127.703
121.352
115.178

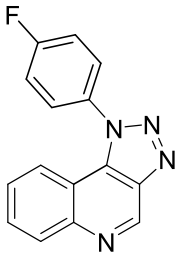


DEPT 135 NMR-spectrum ($CDCl_3$)

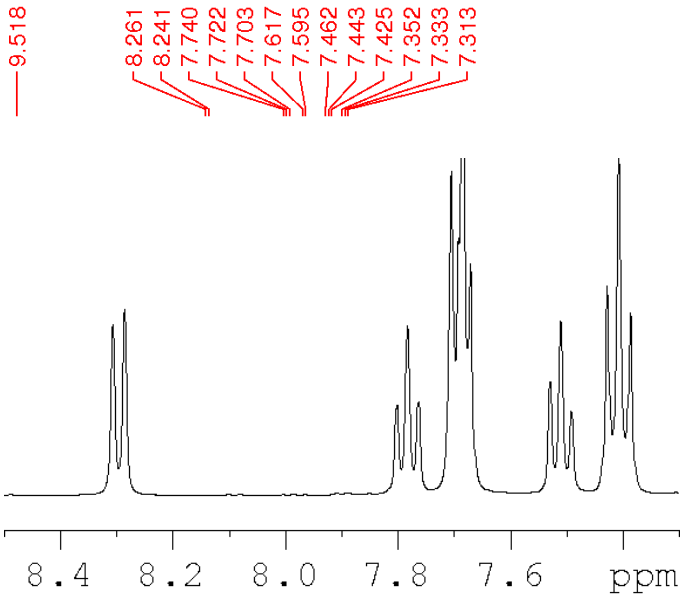


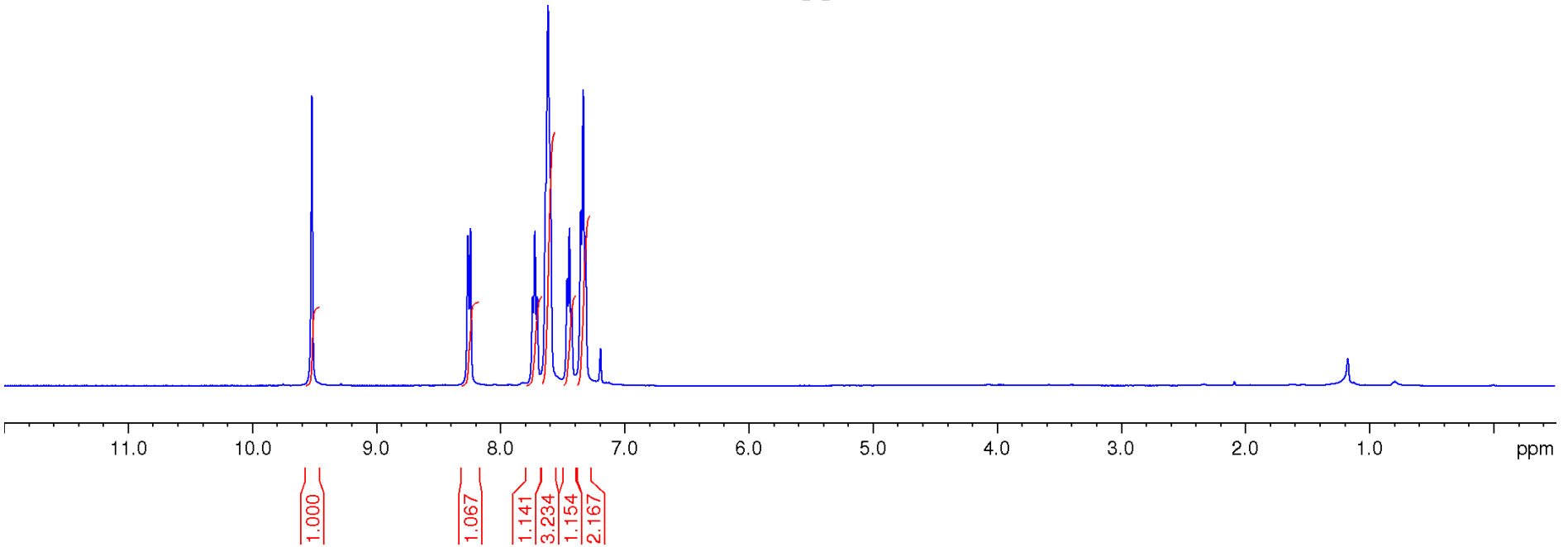
5b

^{1}H NMR-spectrum (400 MHz, $CDCl_3$)

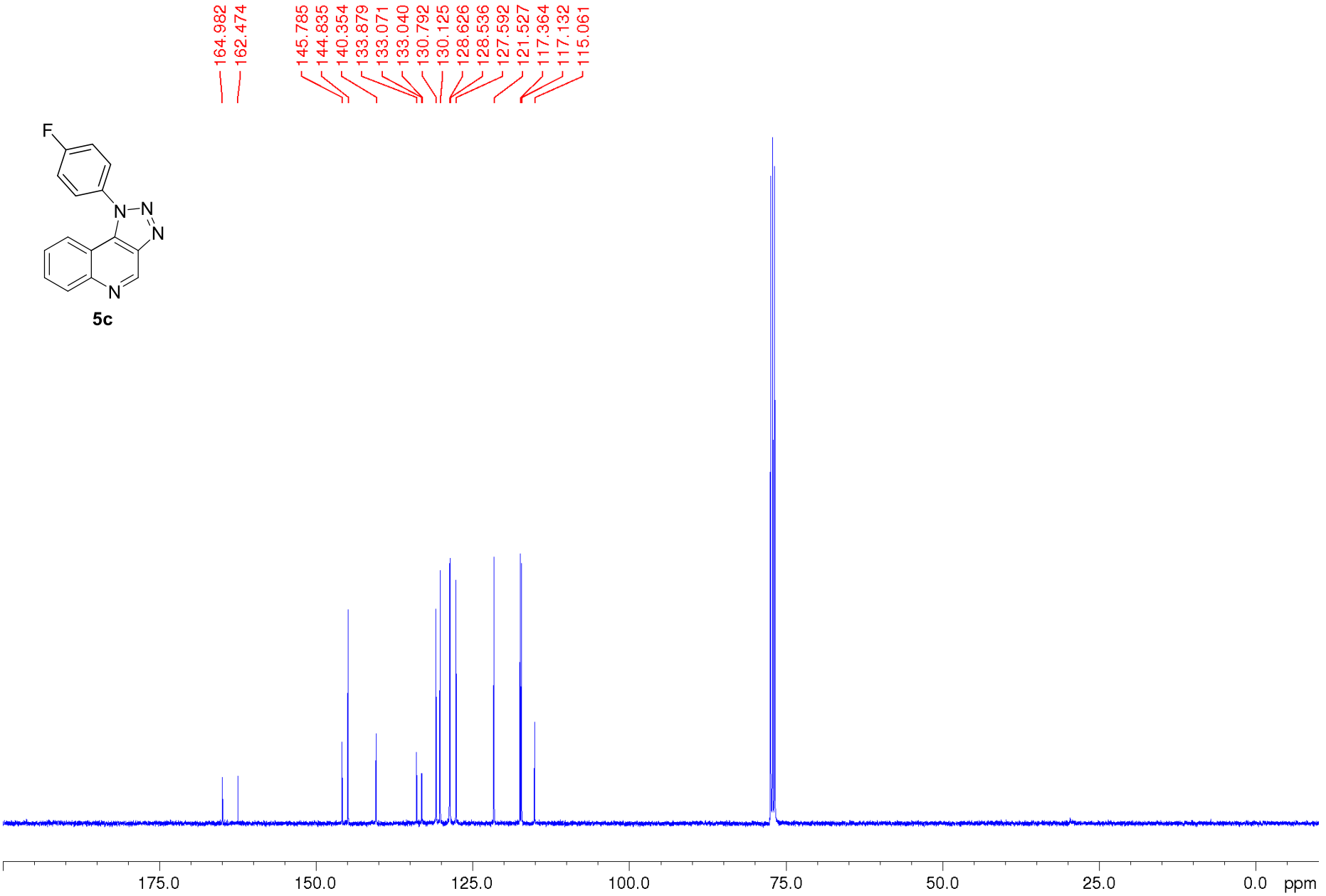


5c

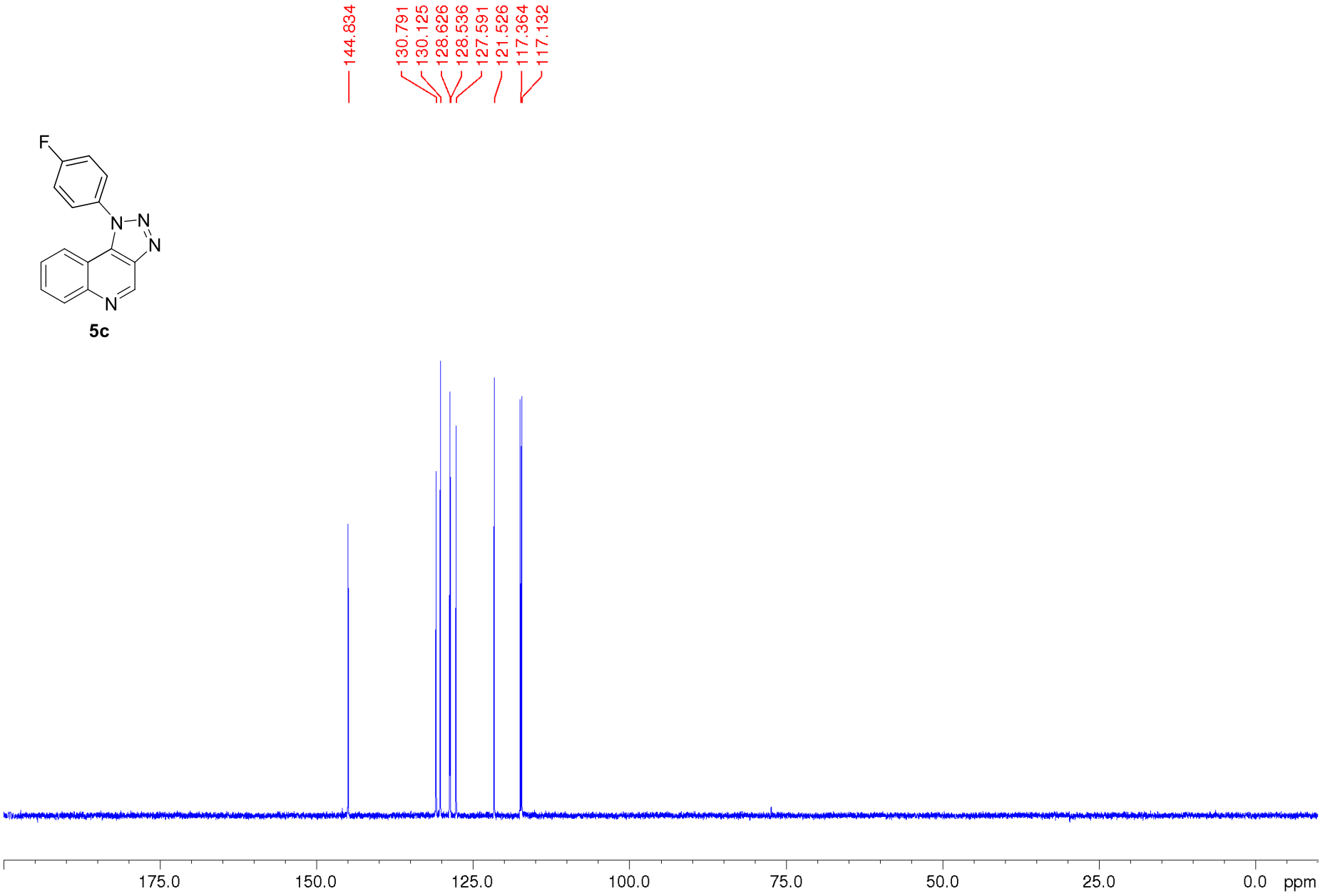




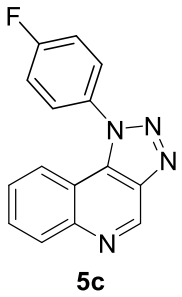
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



DEPT 135 NMR-spectrum ($CDCl_3$)

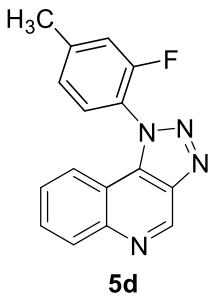


^{19}F NMR-spectrum (376.5 Hz, $CDCl_3$)

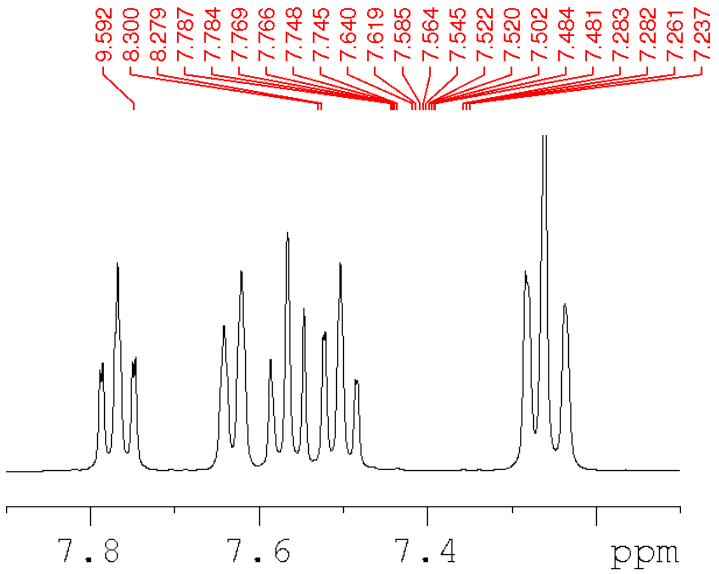


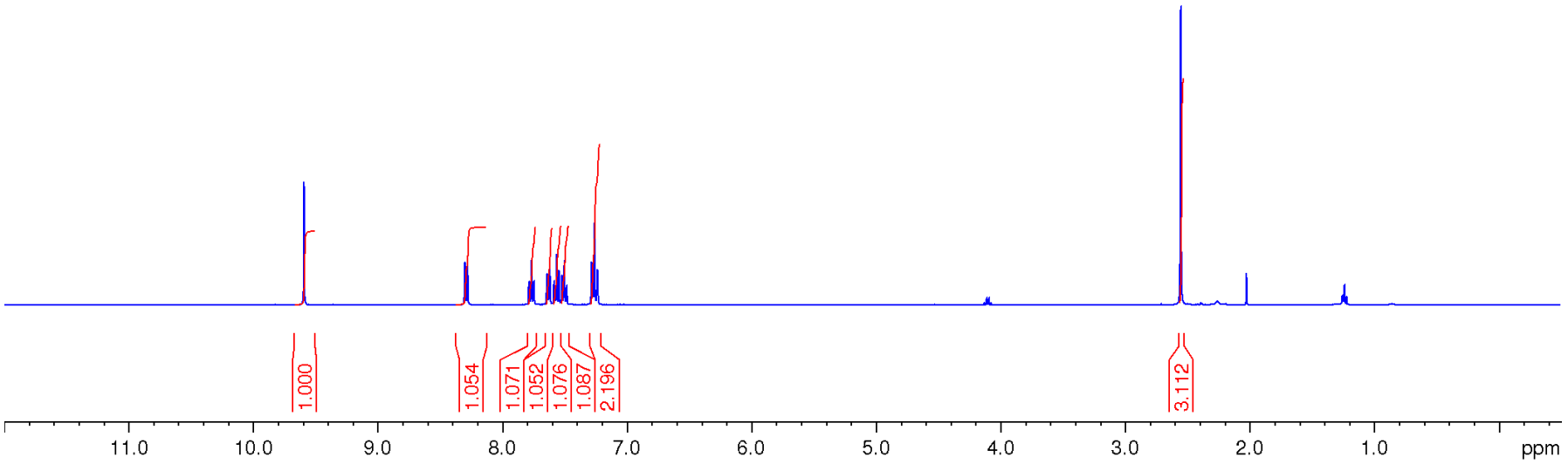
5c

^{1}H NMR-spectrum (400 MHz, $CDCl_3$)

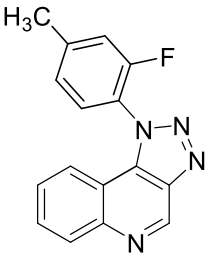


5d





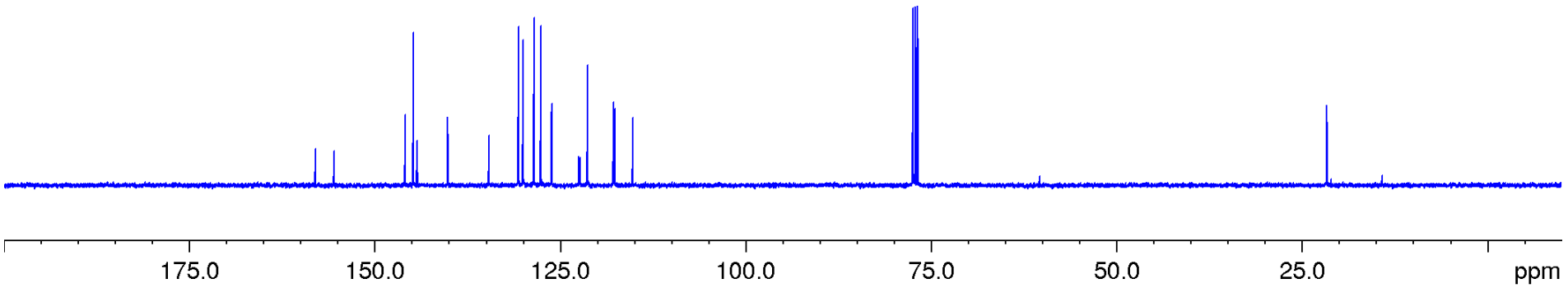
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



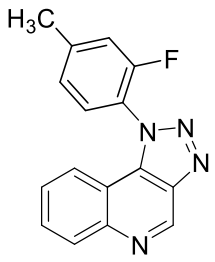
5d

158.013
155.484
145.903
144.787
144.319
144.245
140.177
134.594
130.627
129.995
128.541
127.594
126.146
126.113
122.445
122.316
121.298
117.816
117.632
115.200

21.627

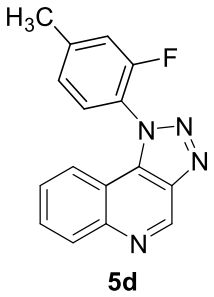


DEPT 135 NMR-spectrum ($CDCl_3$)



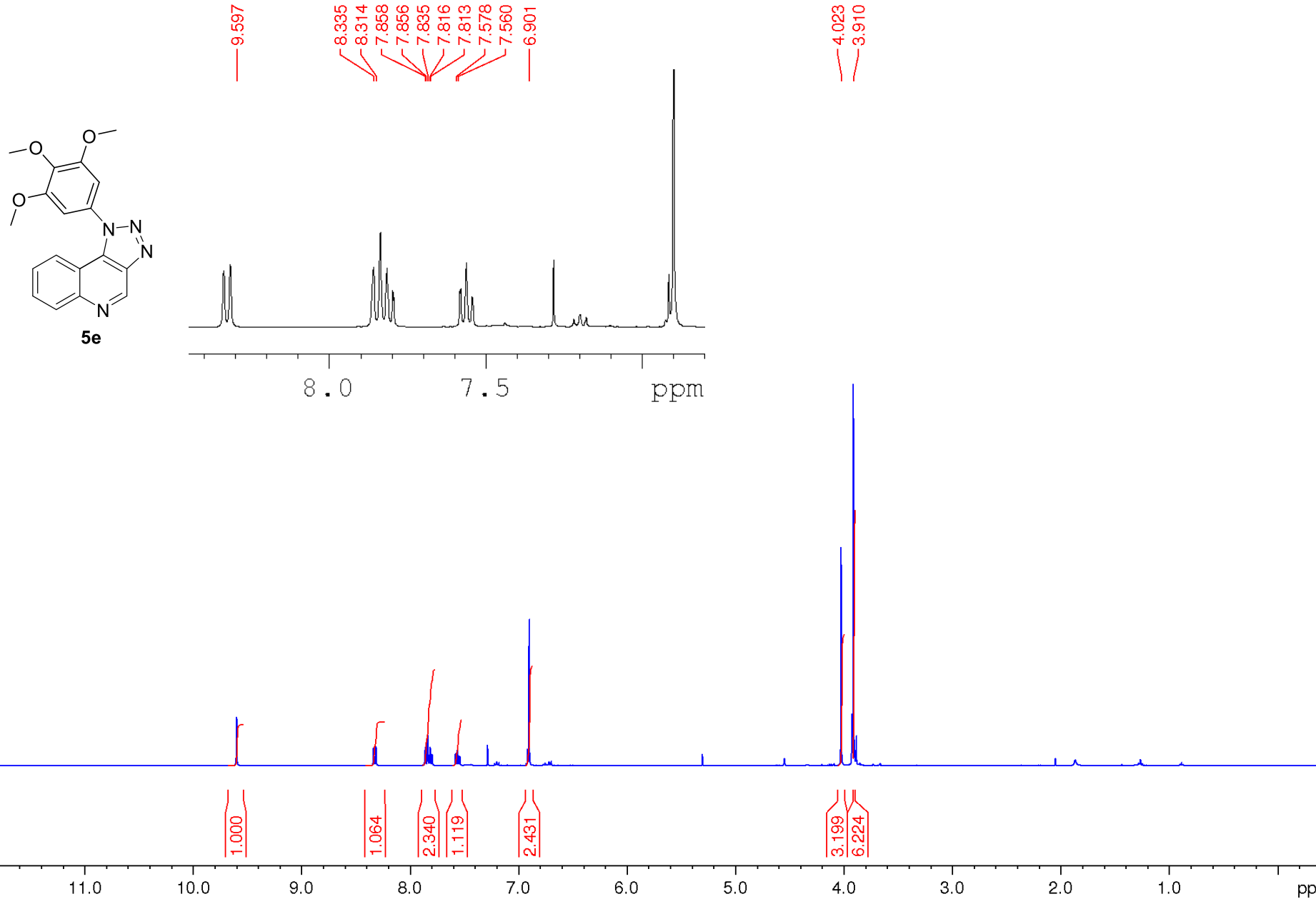
5d

^{19}F NMR-spectrum (376.5 Hz, $CDCl_3$)



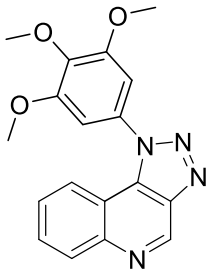
5d

^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



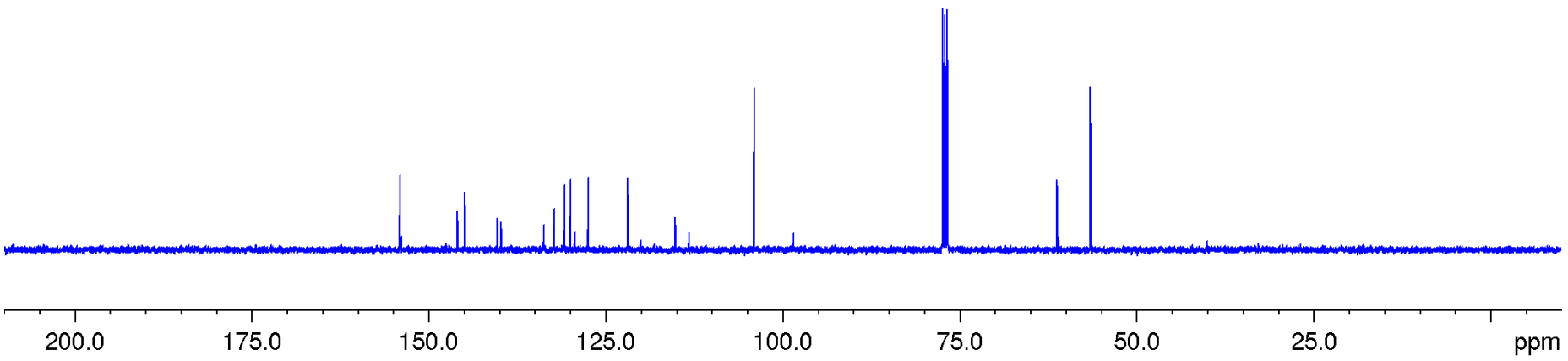
5e

^{13}C NMR-spectrum (100 MHz, $CDCl_3$)

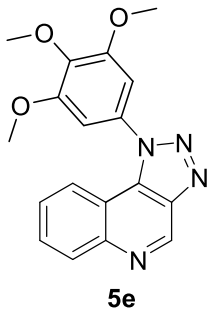


5e

154.080
145.961
144.916
140.272
139.763
133.749
132.303
130.817
129.995
127.464
121.878
115.174
104.035
61.213
56.518



DEPT 135 NMR-spectrum ($CDCl_3$)

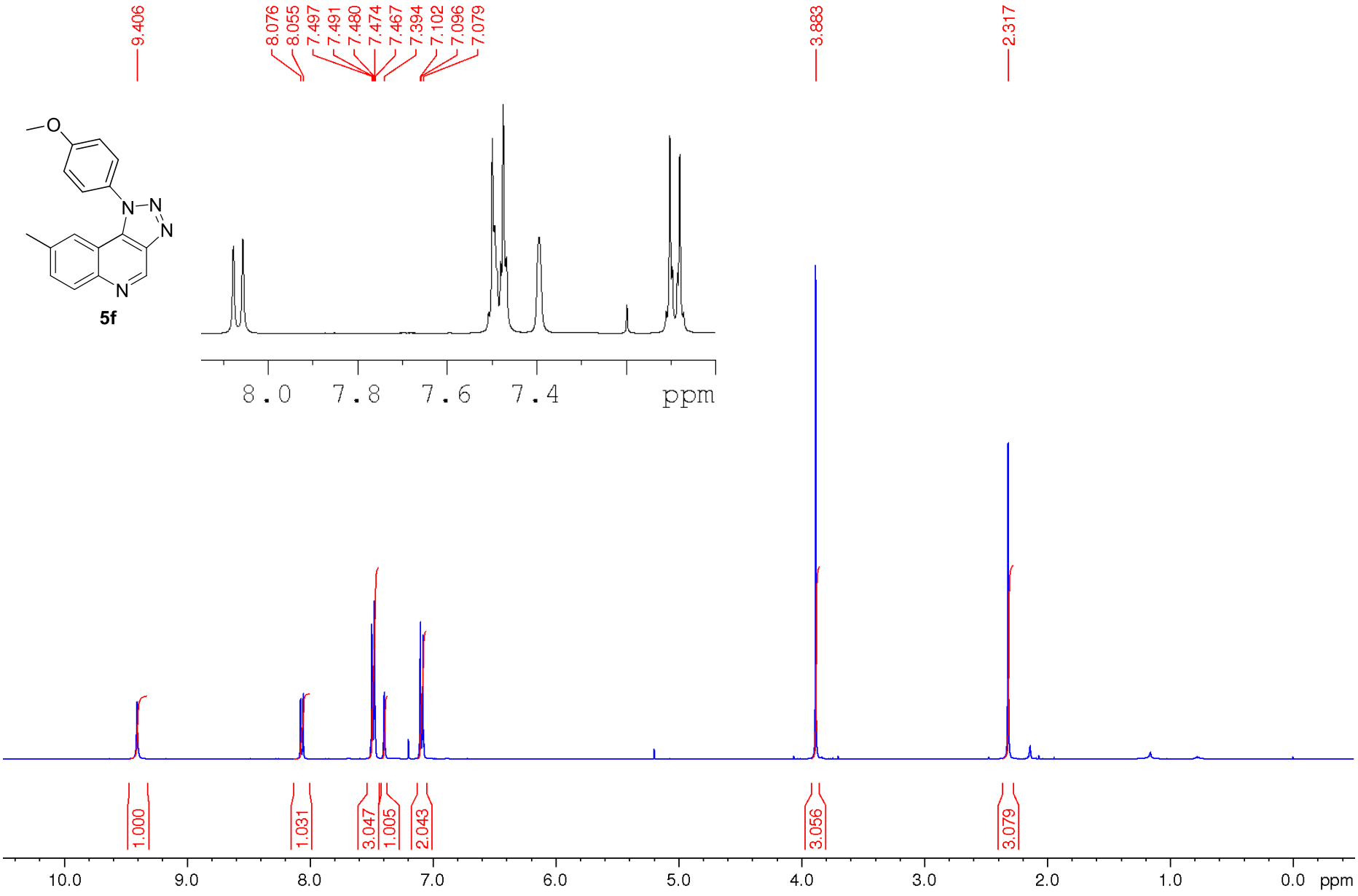


5e

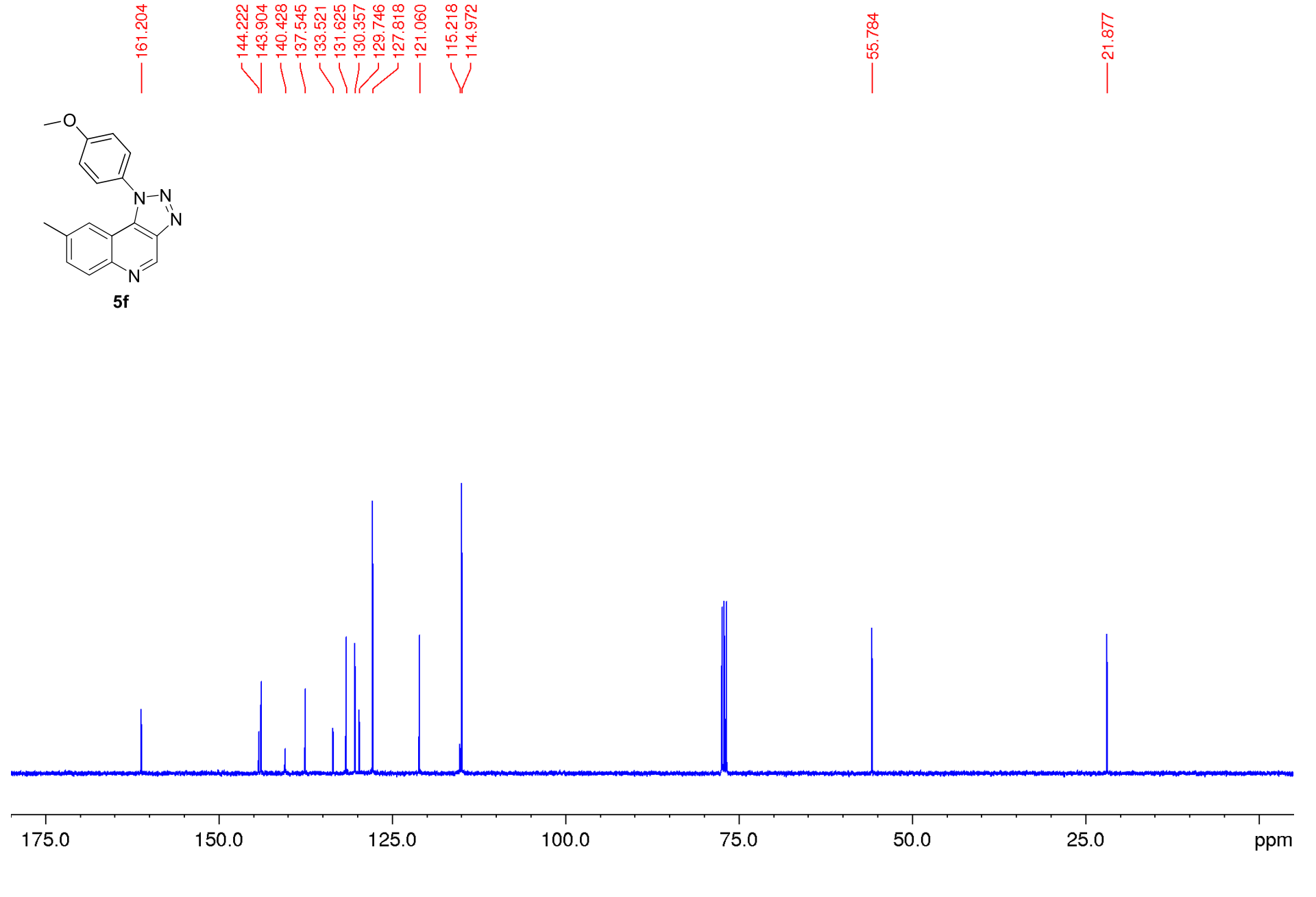
144.917
130.817
129.997
127.464
121.879
104.035
61.213
56.518

175.0 150.0 125.0 100.0 75.0 50.0 25.0 ppm

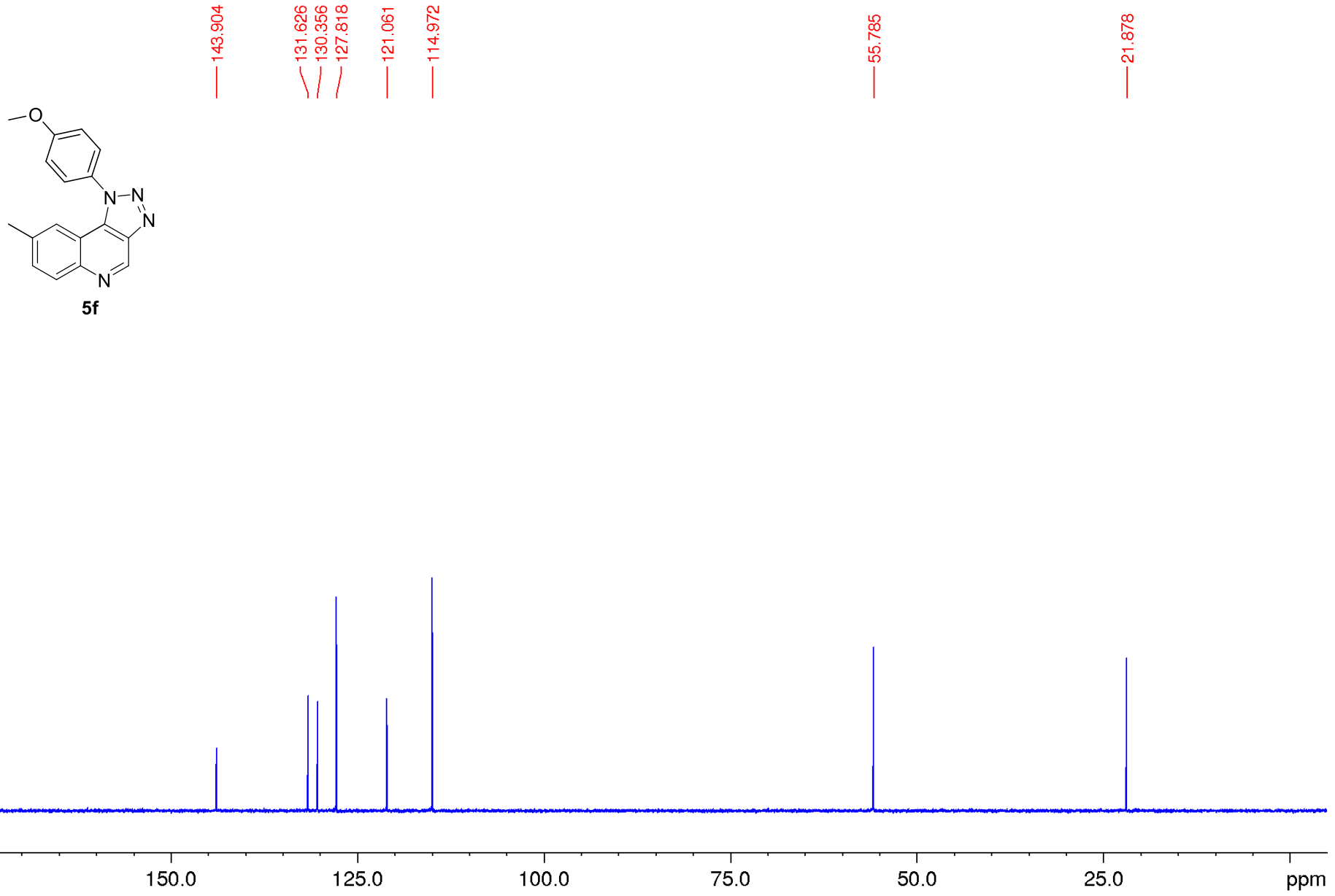
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



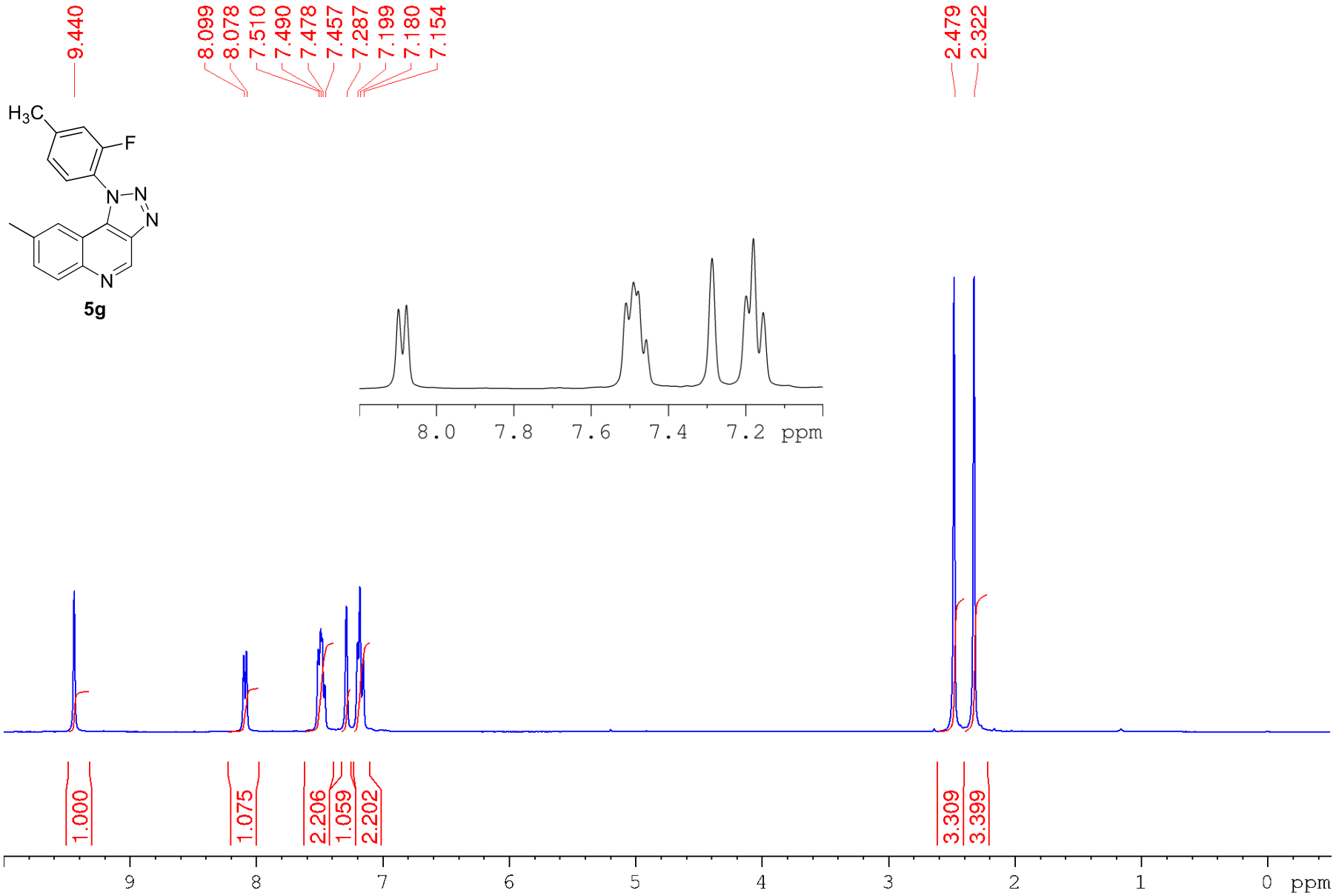
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



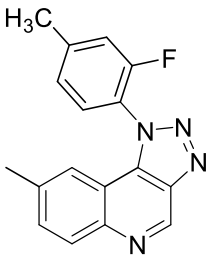
DEPT 135 NMR-spectrum ($CDCl_3$)



^{1}H NMR-spectrum (400 MHz, $CDCl_3$)

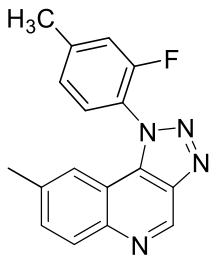


^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



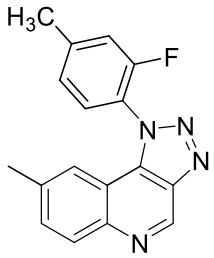
5g

DEPT 135 NMR-spectrum ($CDCl_3$)



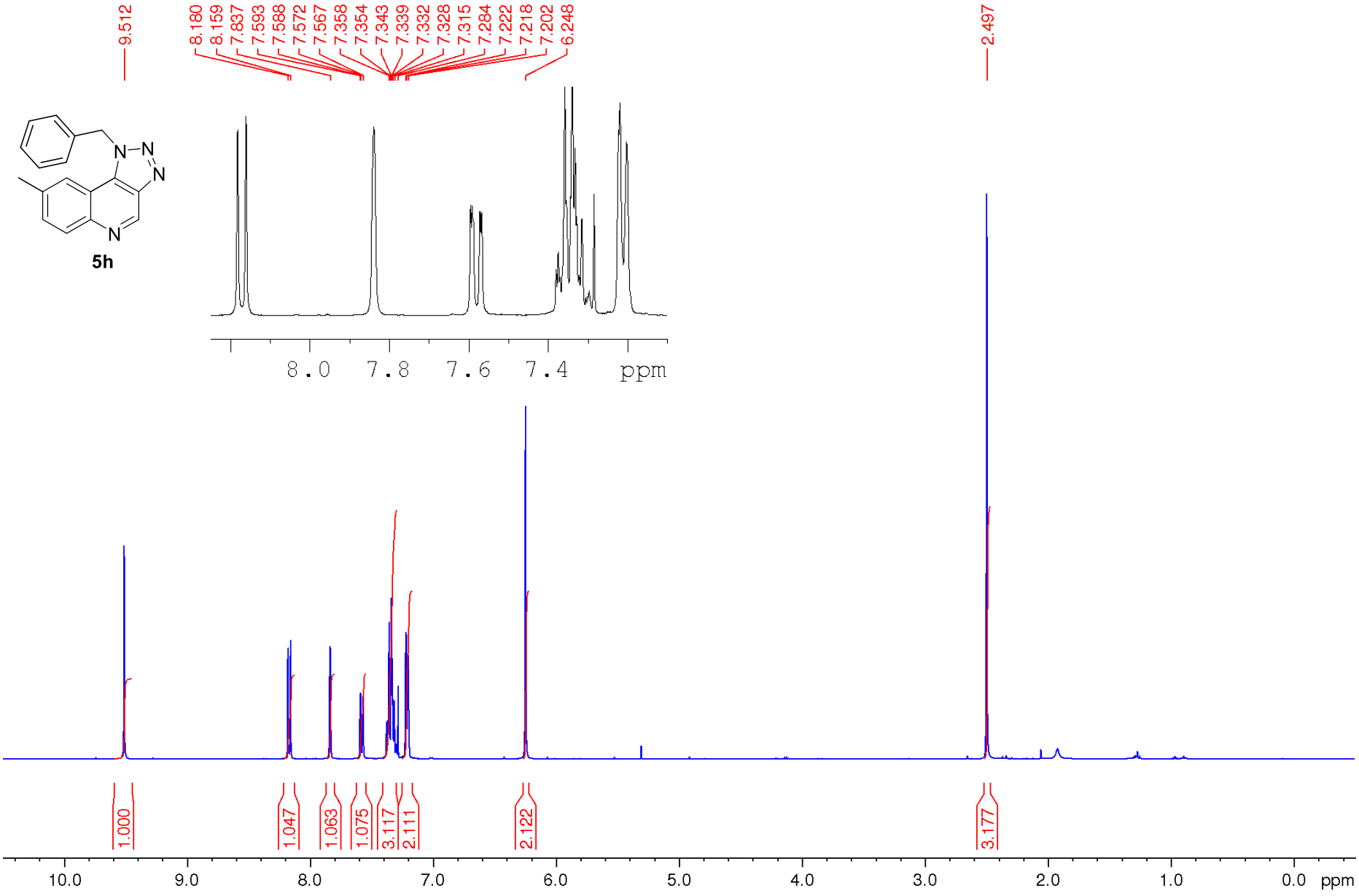
5g

^{19}F NMR-spectrum (376.5 Hz, $CDCl_3$)

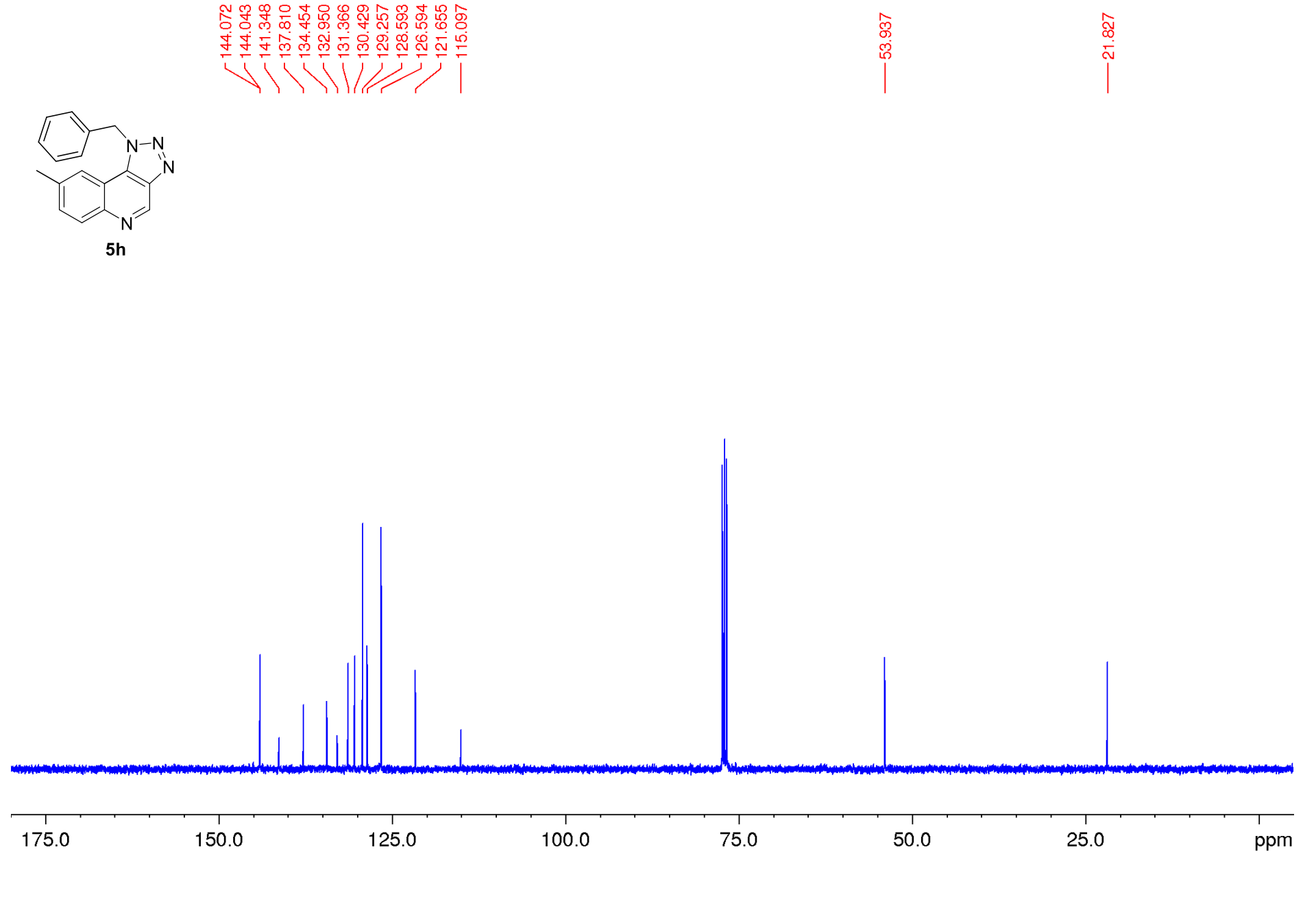


5g

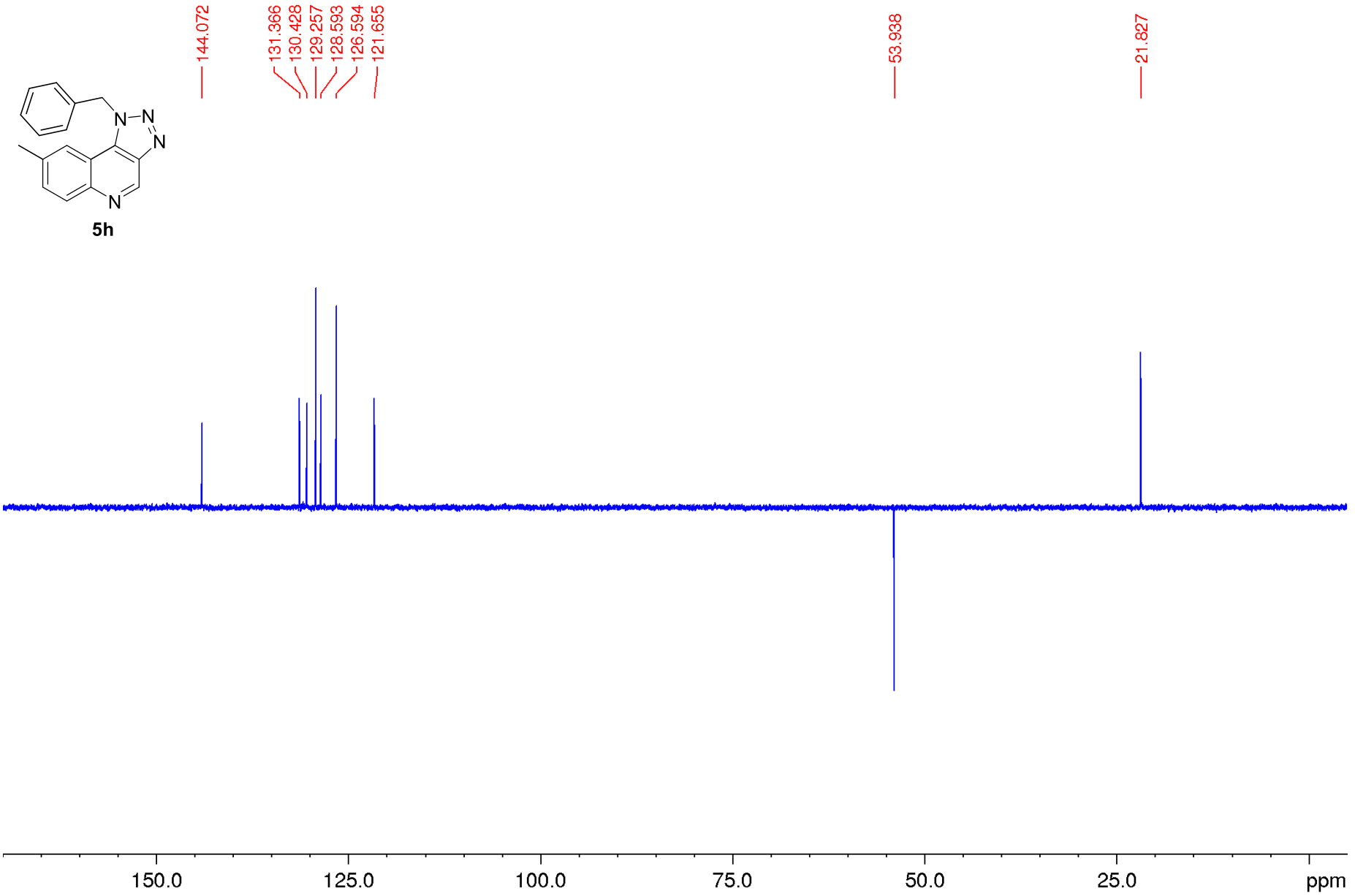
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



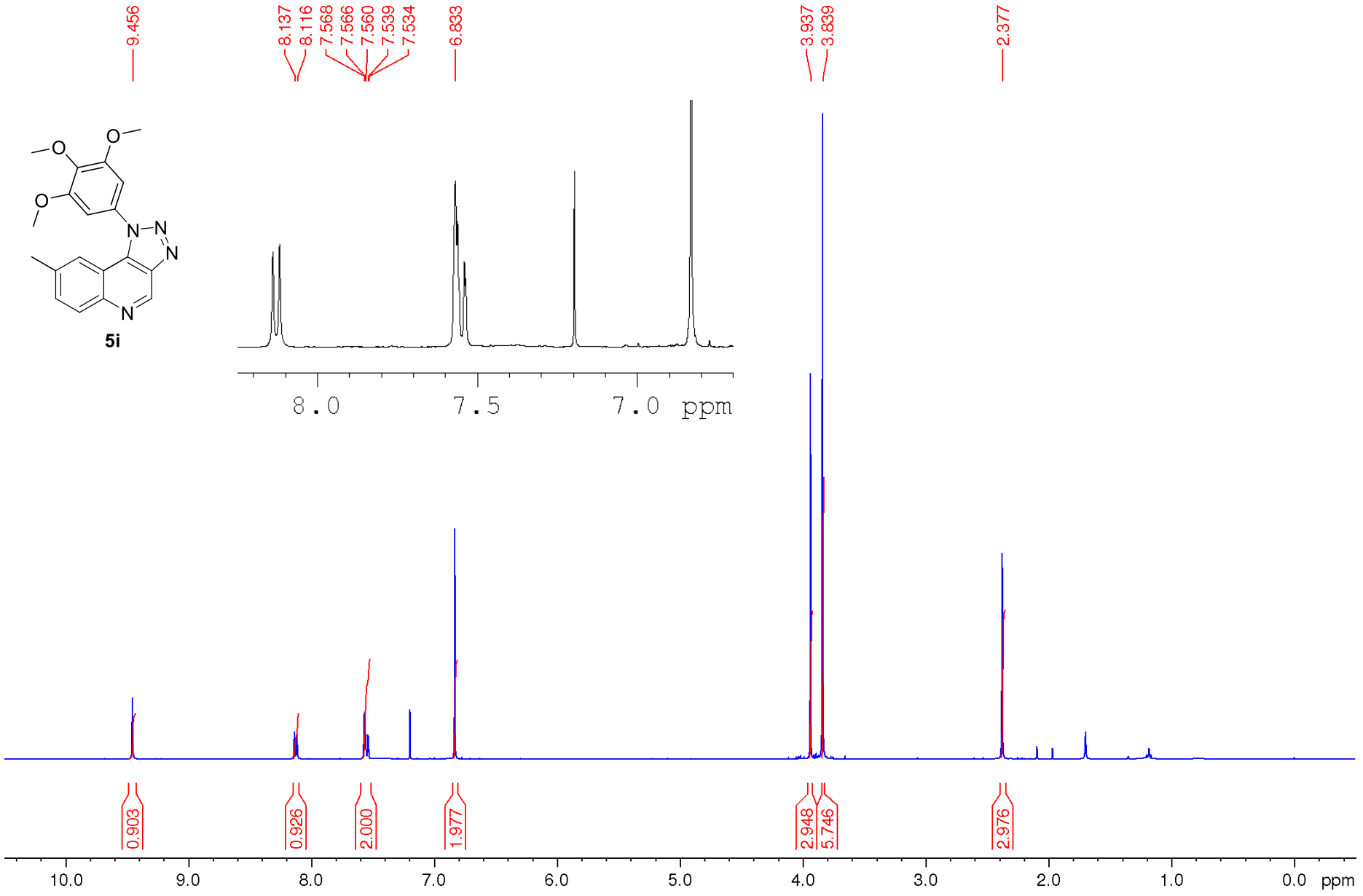
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



DEPT 135 NMR-spectrum ($CDCl_3$)

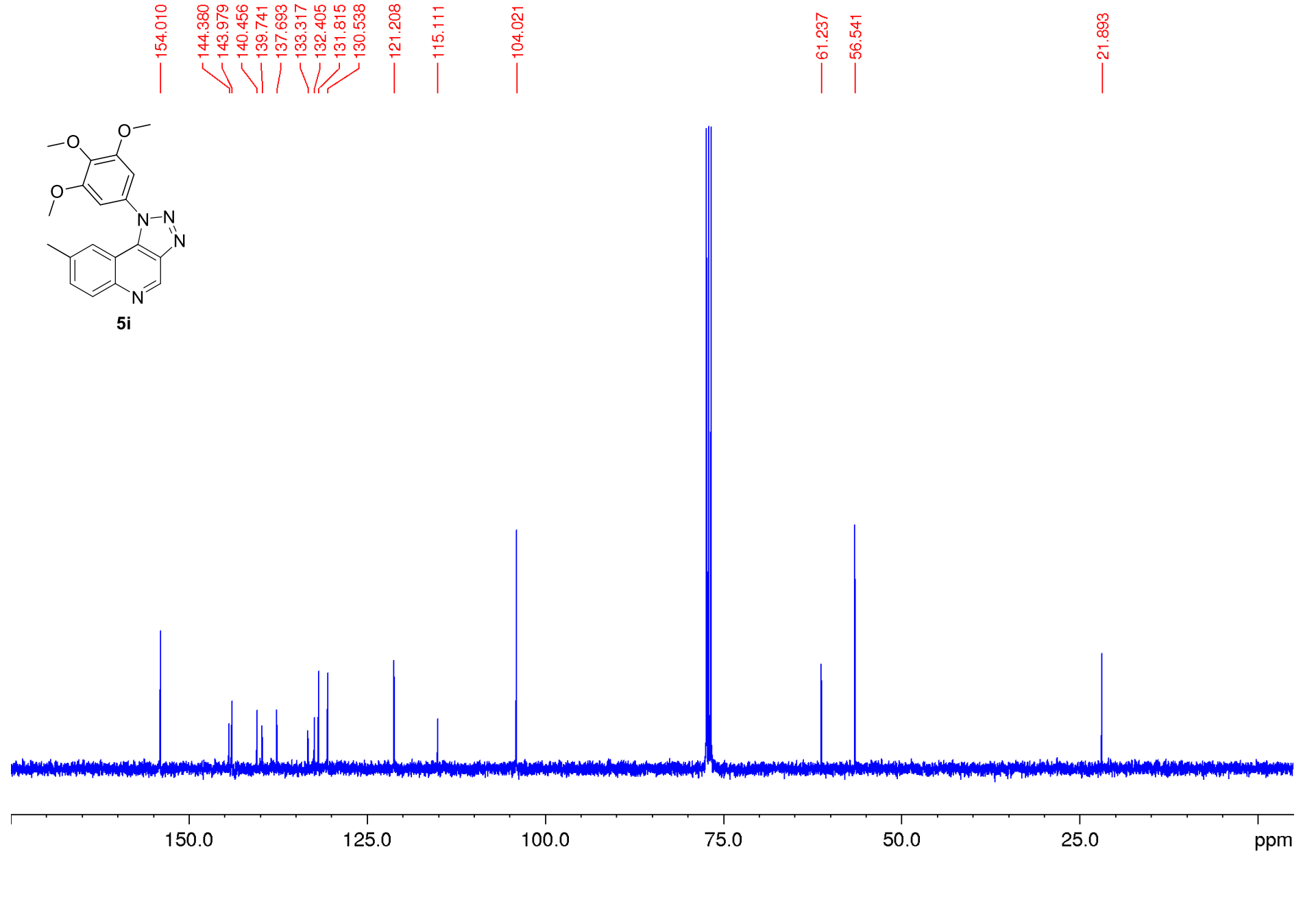


^{1}H NMR-spectrum (400 MHz, $CDCl_3$)

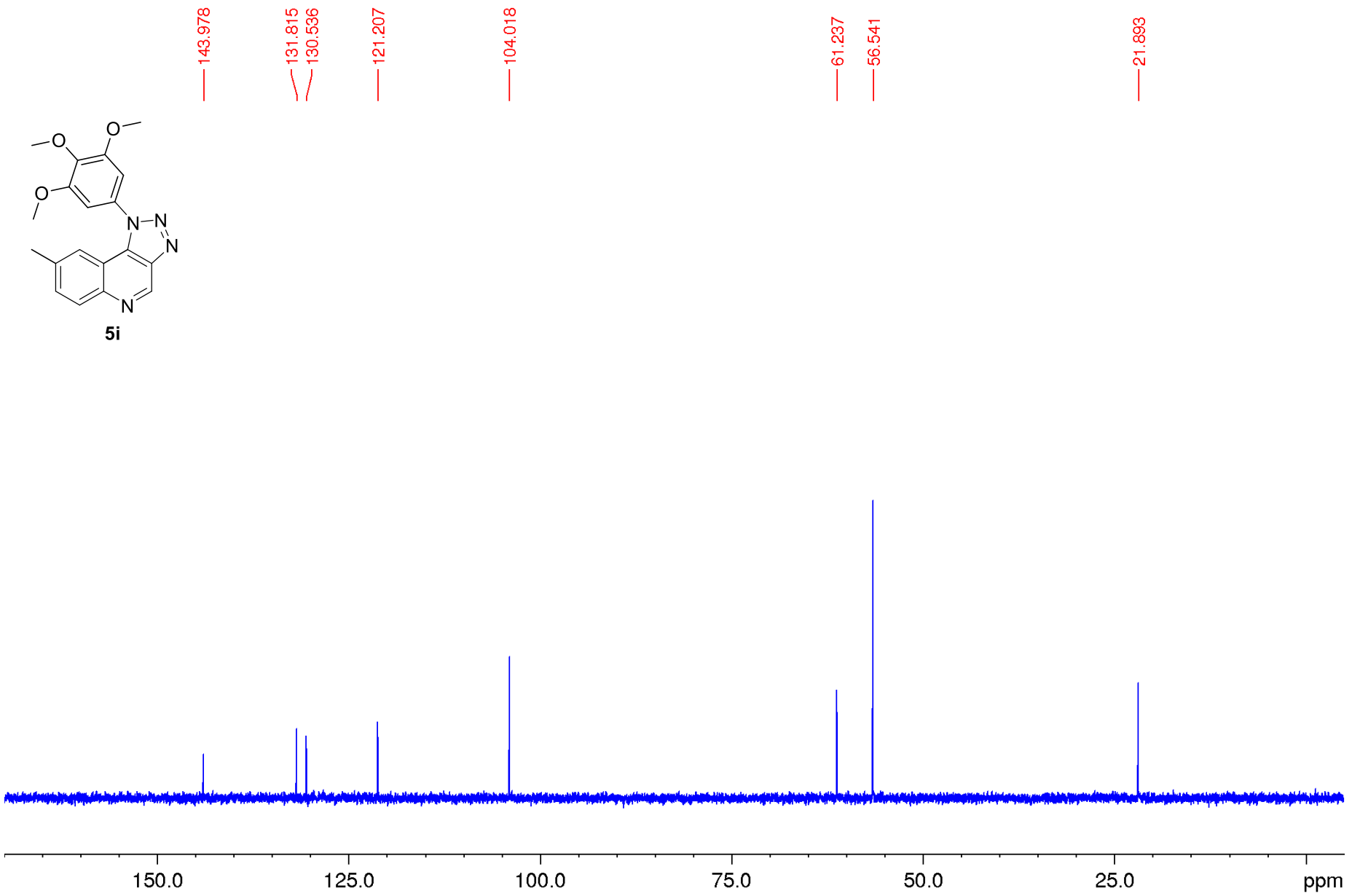


5i

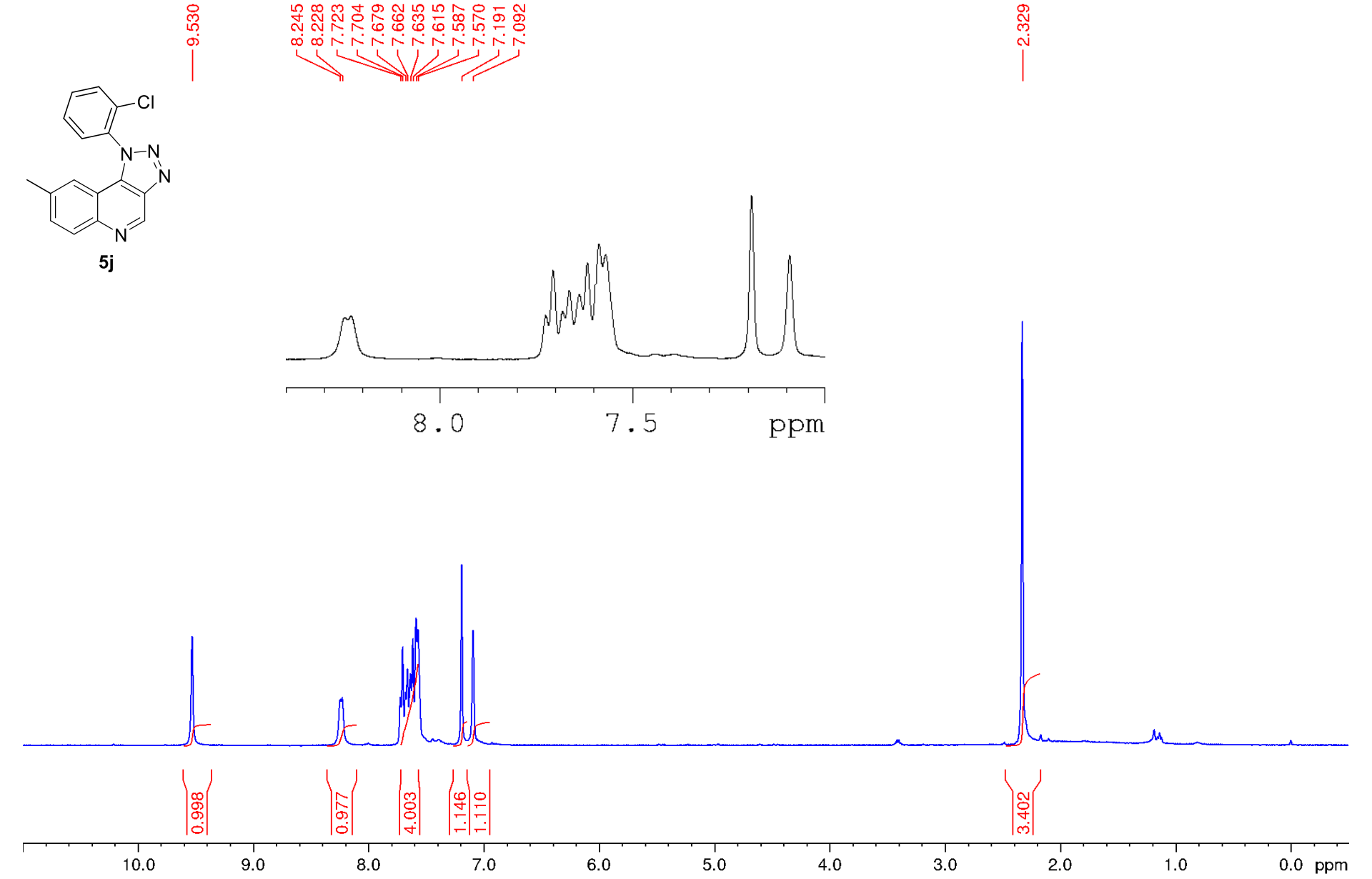
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



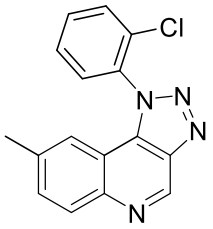
DEPT 135 NMR-spectrum ($CDCl_3$)



^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



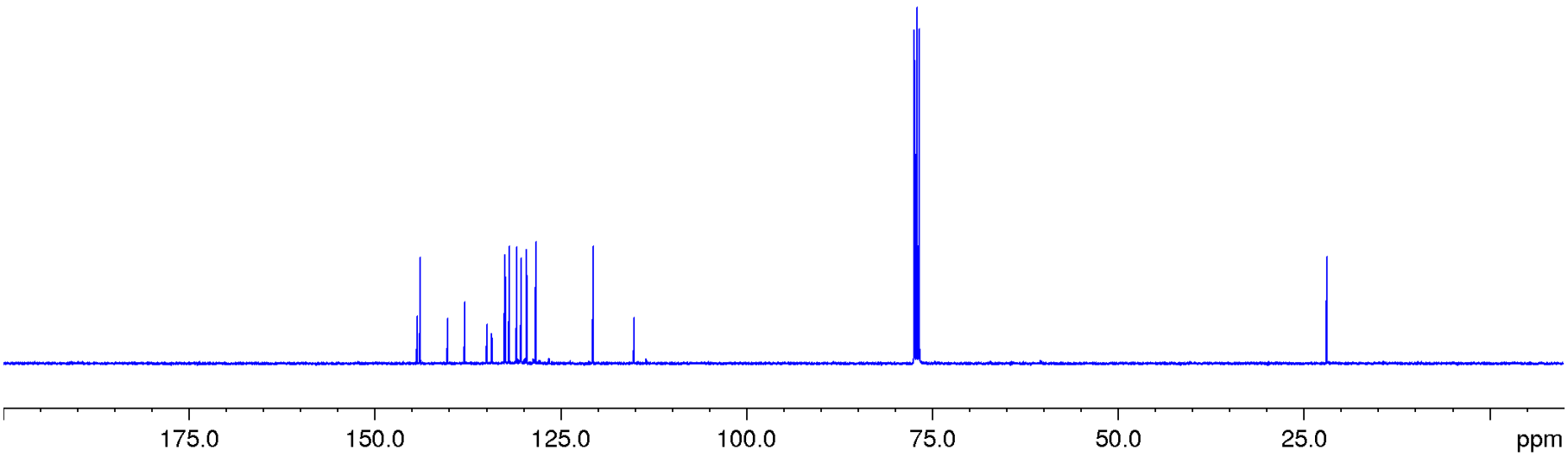
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



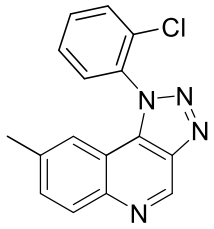
5j

144.307
143.889
140.215
137.891
134.927
134.246
132.544
132.452
131.925
130.913
130.319
129.568
128.337
120.632
115.111

21.892

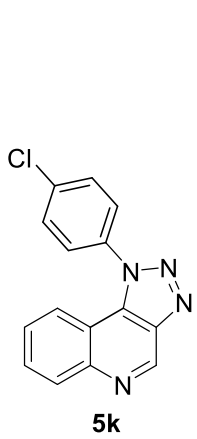


DEPT 135 NMR-spectrum ($CDCl_3$)

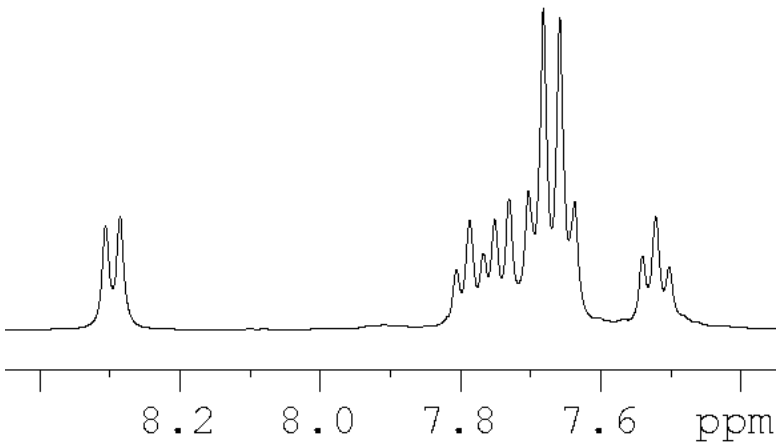


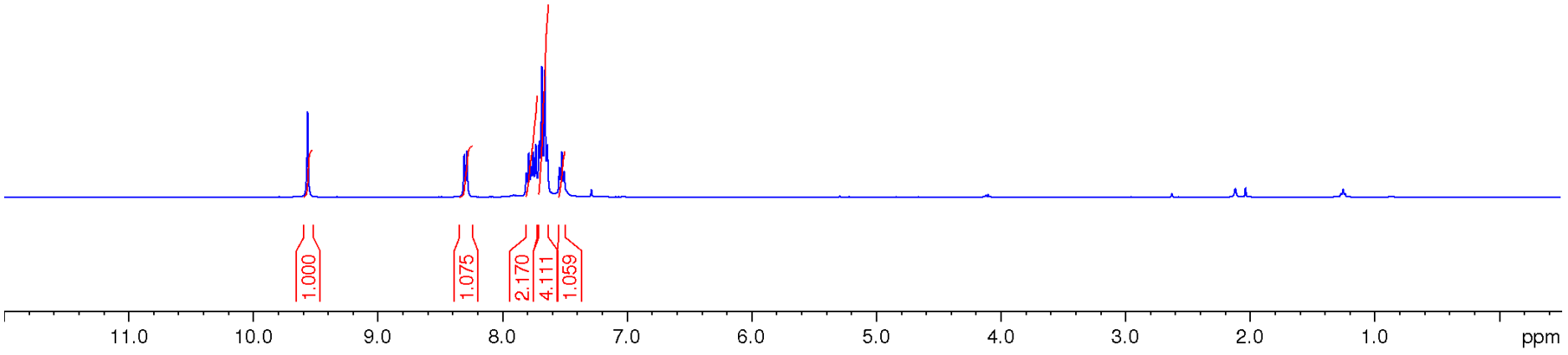
5j

^{1}H NMR-spectrum (400 MHz, $CDCl_3$)

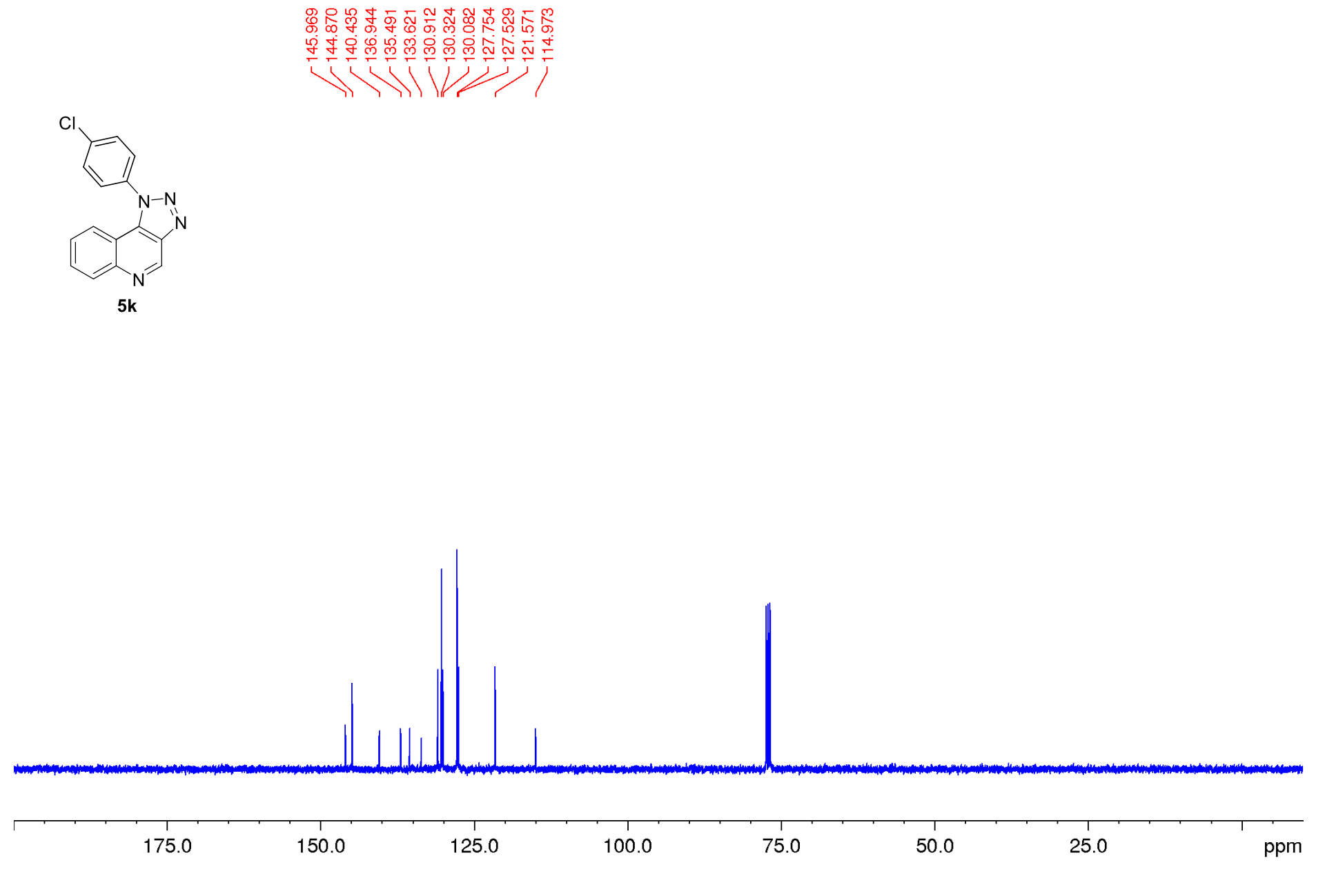


5k

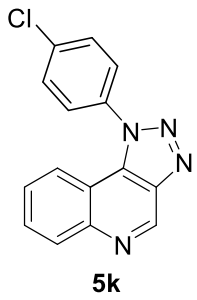




^{13}C NMR-spectrum (100 MHz, $CDCl_3$)

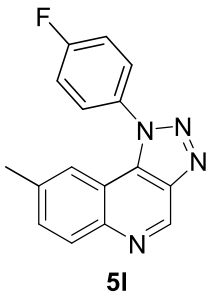


DEPT 135 NMR-spectrum ($CDCl_3$)



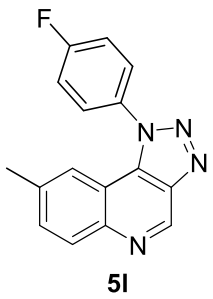
5k

^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



5l

^{13}C NMR-spectrum (100 MHz, $CDCl_3$)

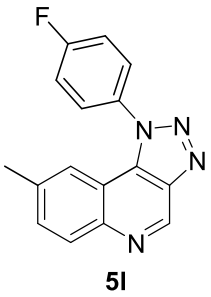


5l

164.955
162.451
144.124
143.804
140.471
137.890
133.535
133.155
133.122
131.969
130.424
128.615
128.527
120.890
117.235
117.005
114.980
21.900

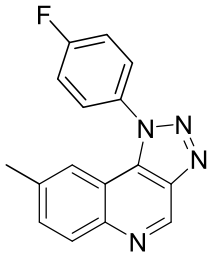
175.0
150.0
125.0
100.0
75.0
50.0
25.0
0.0
ppm

DEPT 135 NMR-spectrum ($CDCl_3$)

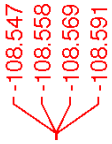


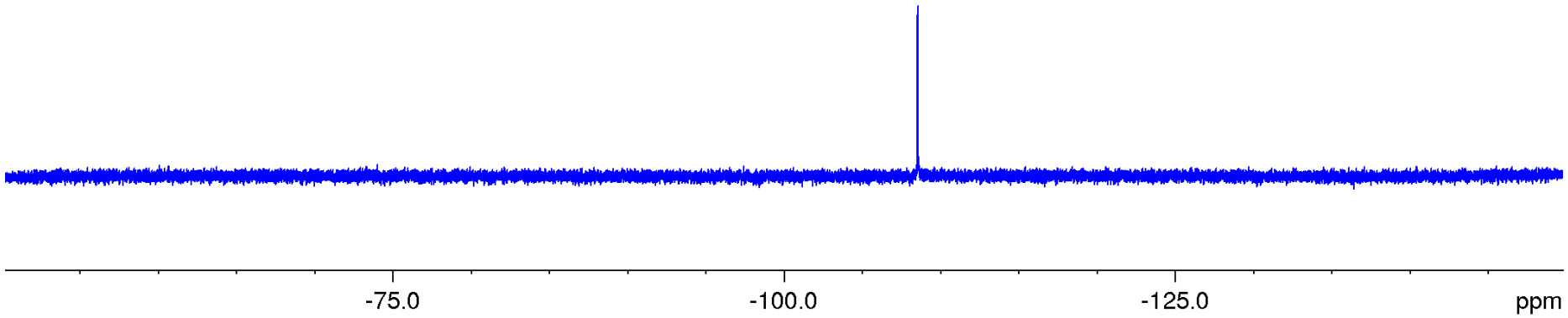
5l

^{19}F NMR-spectrum (376.5 Hz, $CDCl_3$)

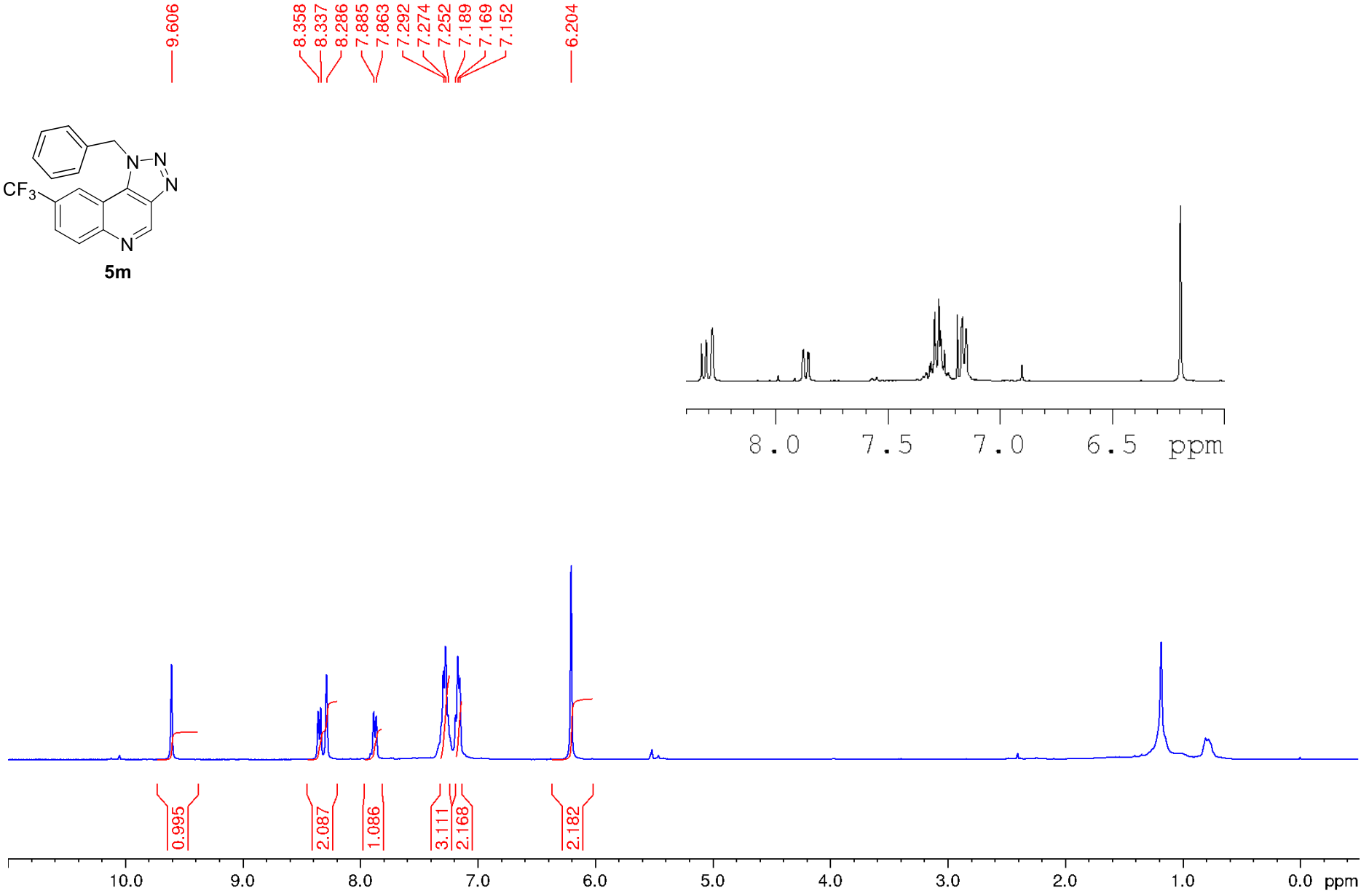


5l

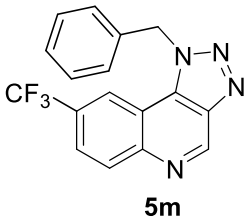




^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



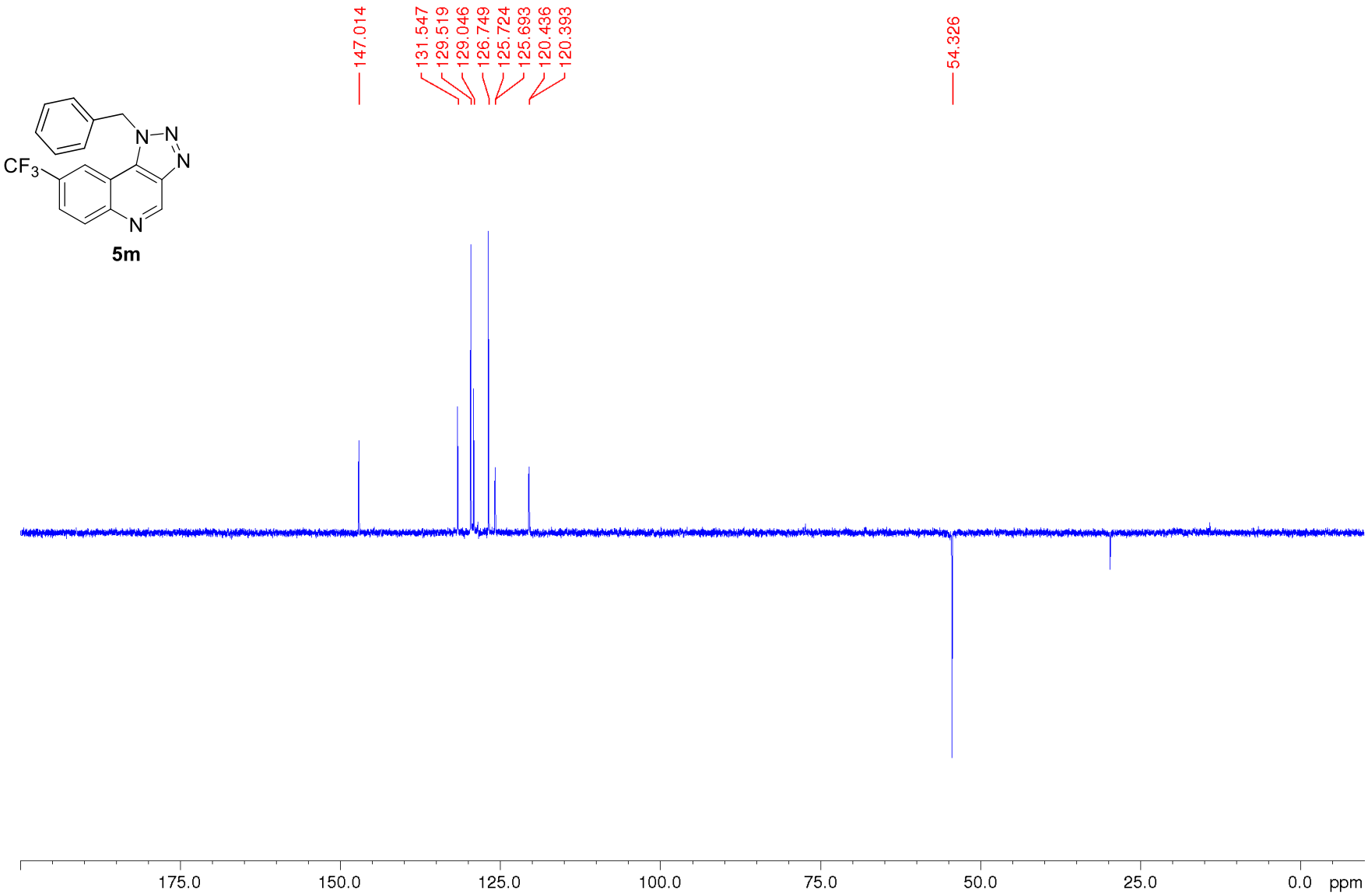
5m

147.050
146.640
141.638
133.465
133.286
131.590
129.517
129.162
129.041
126.750
125.737
125.701
125.671
125.641
124.992
122.307
120.475
120.430
120.389
120.348
114.690

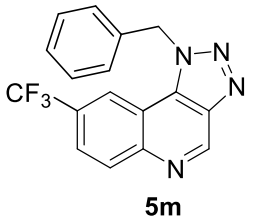
54.320

175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm

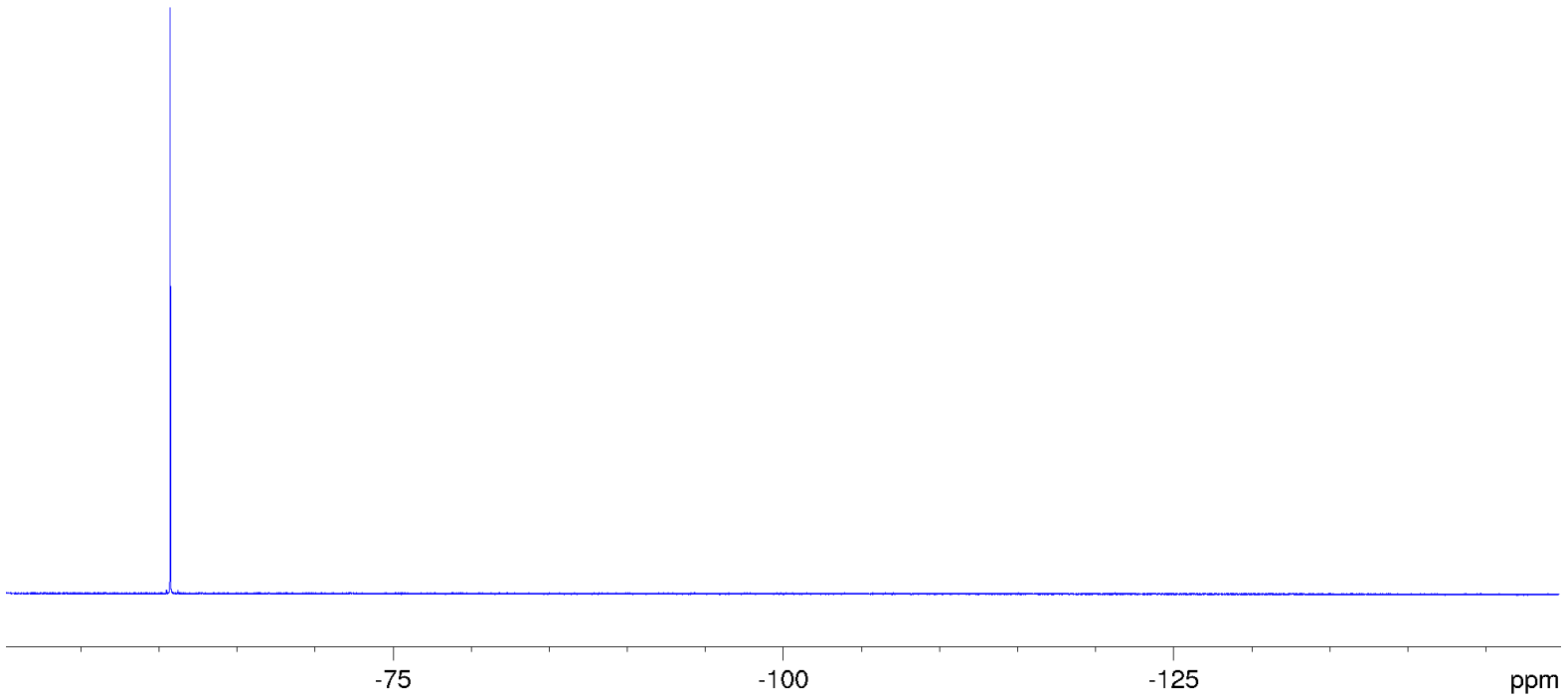
DEPT 135 NMR-spectrum ($CDCl_3$)



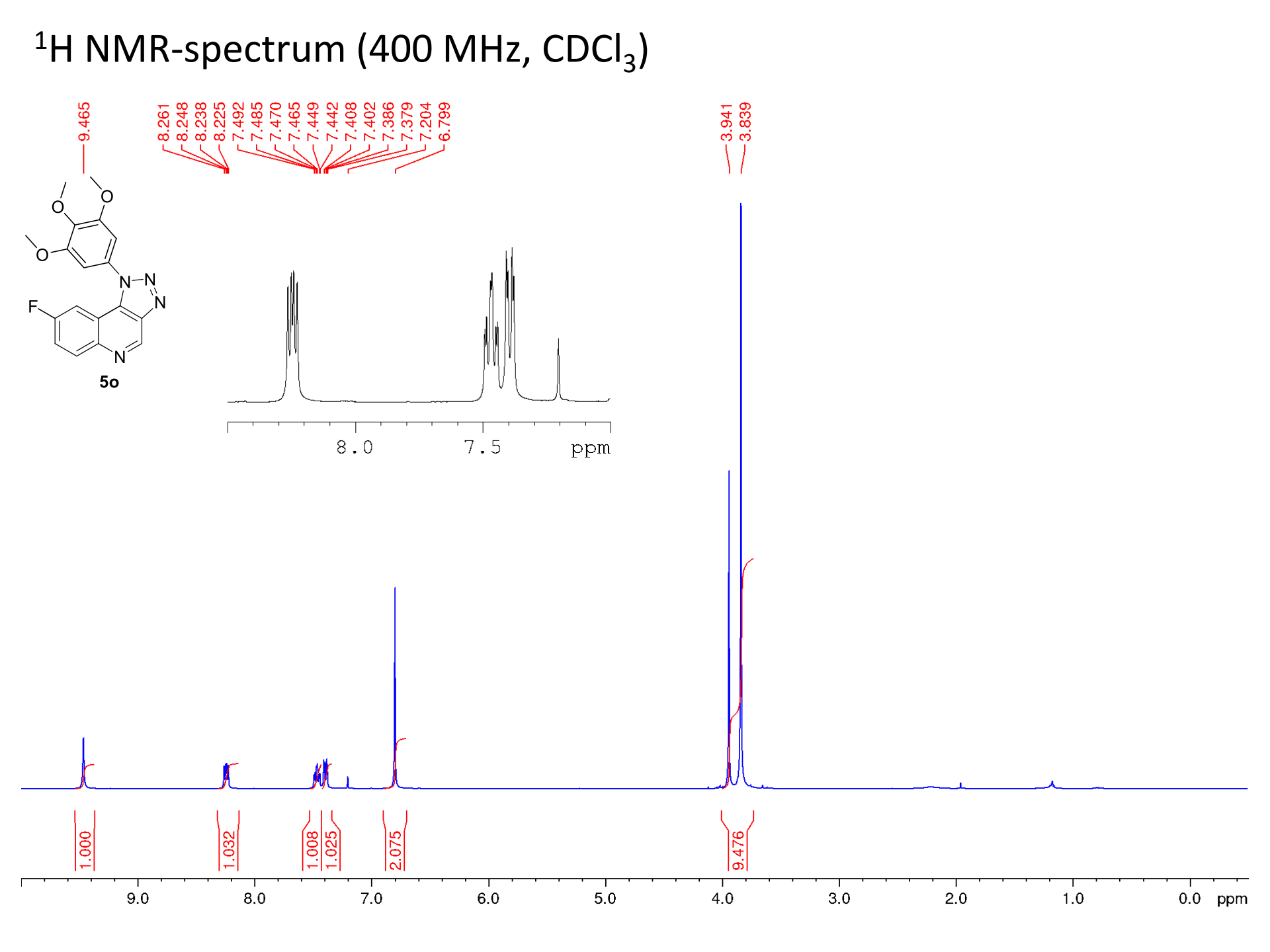
^{19}F NMR-spectrum (376.5 Hz, $CDCl_3$)



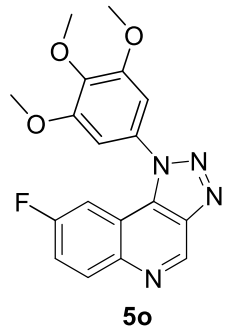
5m



^{1}H NMR-spectrum (400 MHz, $CDCl_3$)

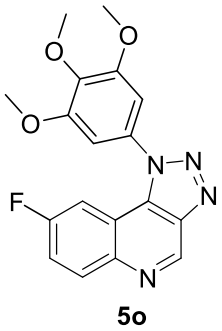


^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



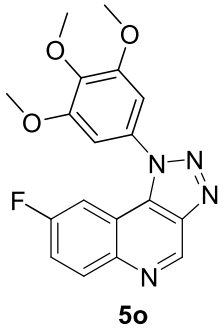
5o

DEPT 135 NMR-spectrum ($CDCl_3$)



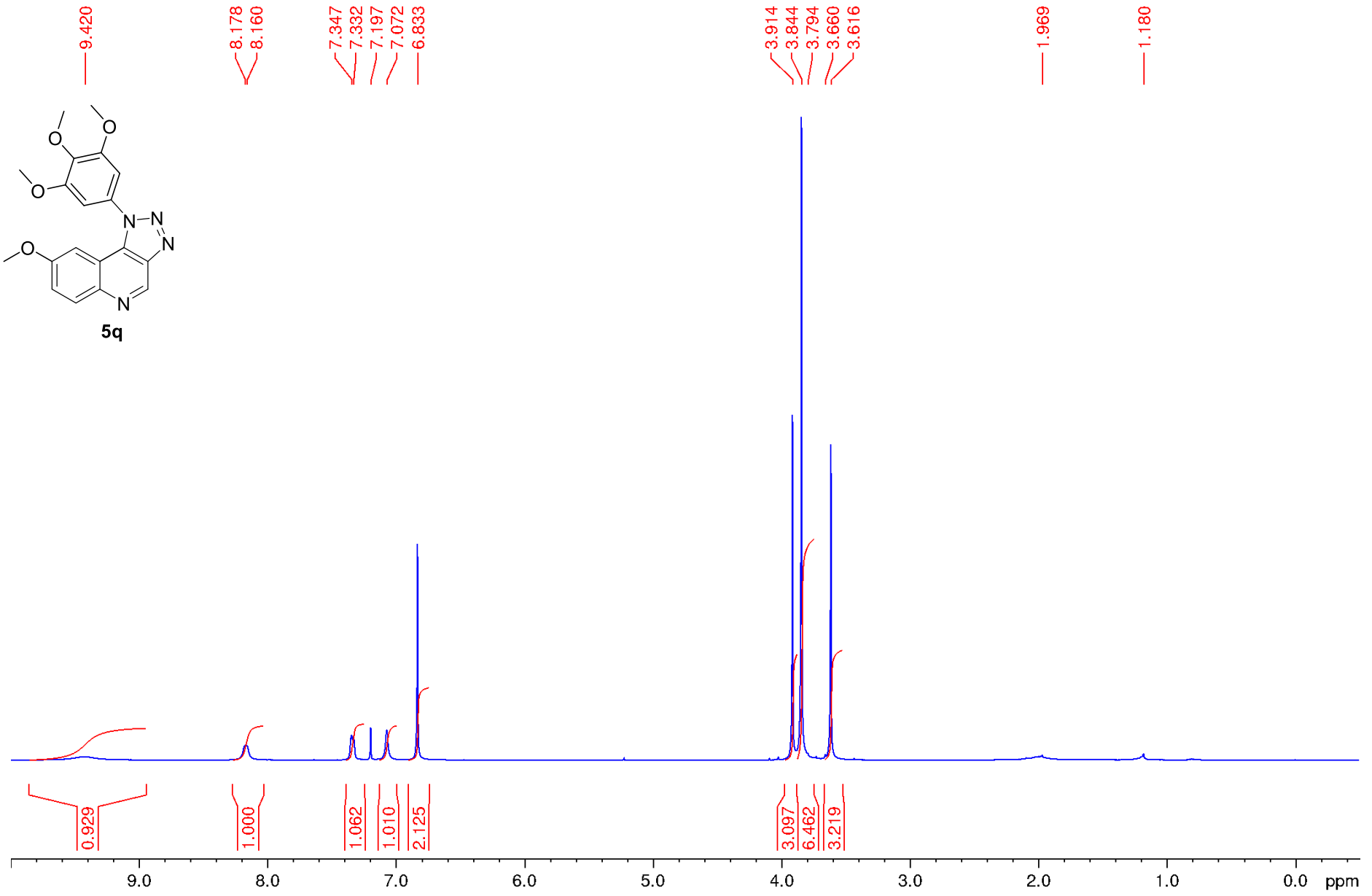
5o

^{19}F NMR-spectrum (376.5 Hz, $CDCl_3$)



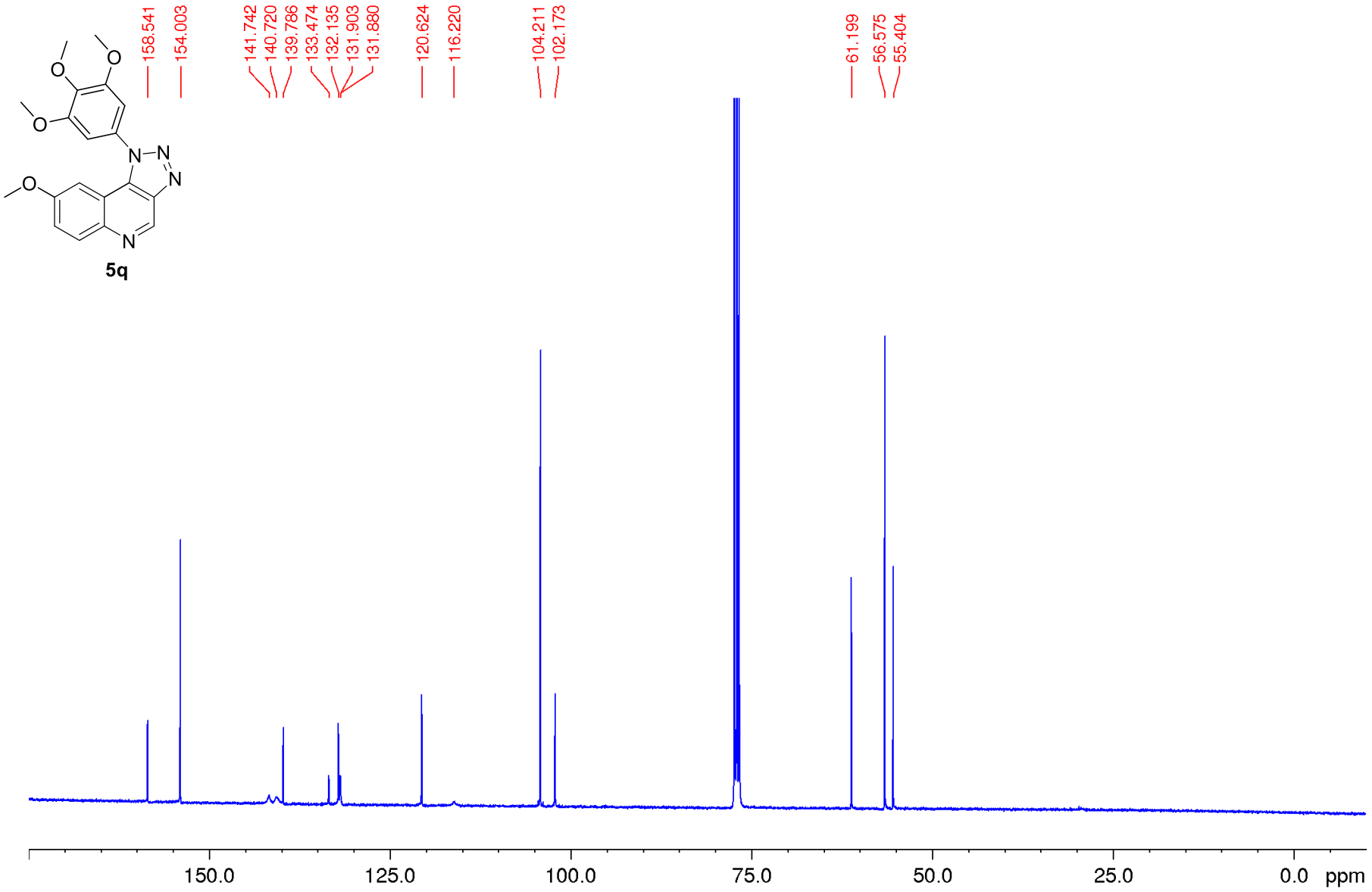
5o

^{1}H NMR-spectrum (400 MHz, $CDCl_3$)

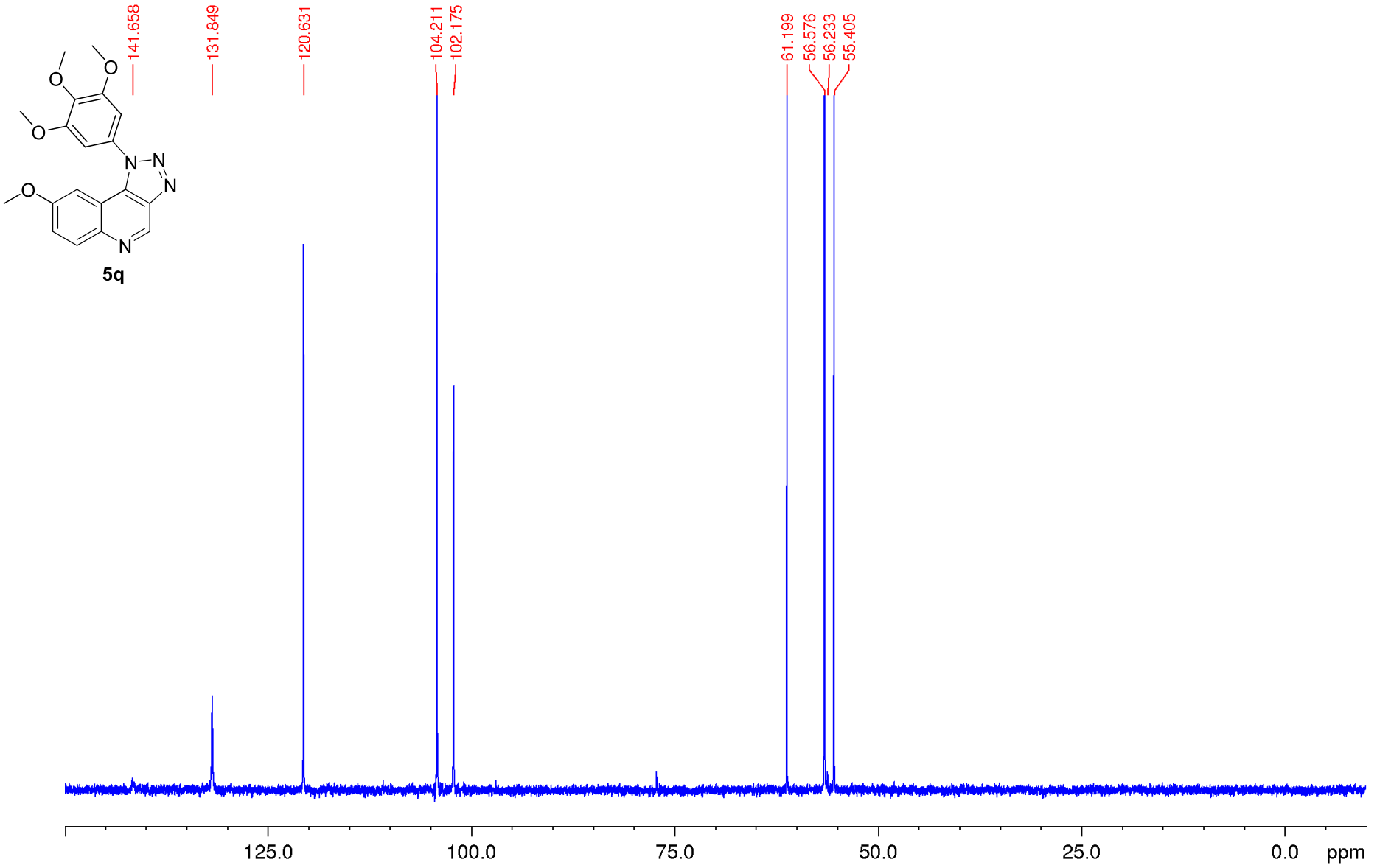


5q

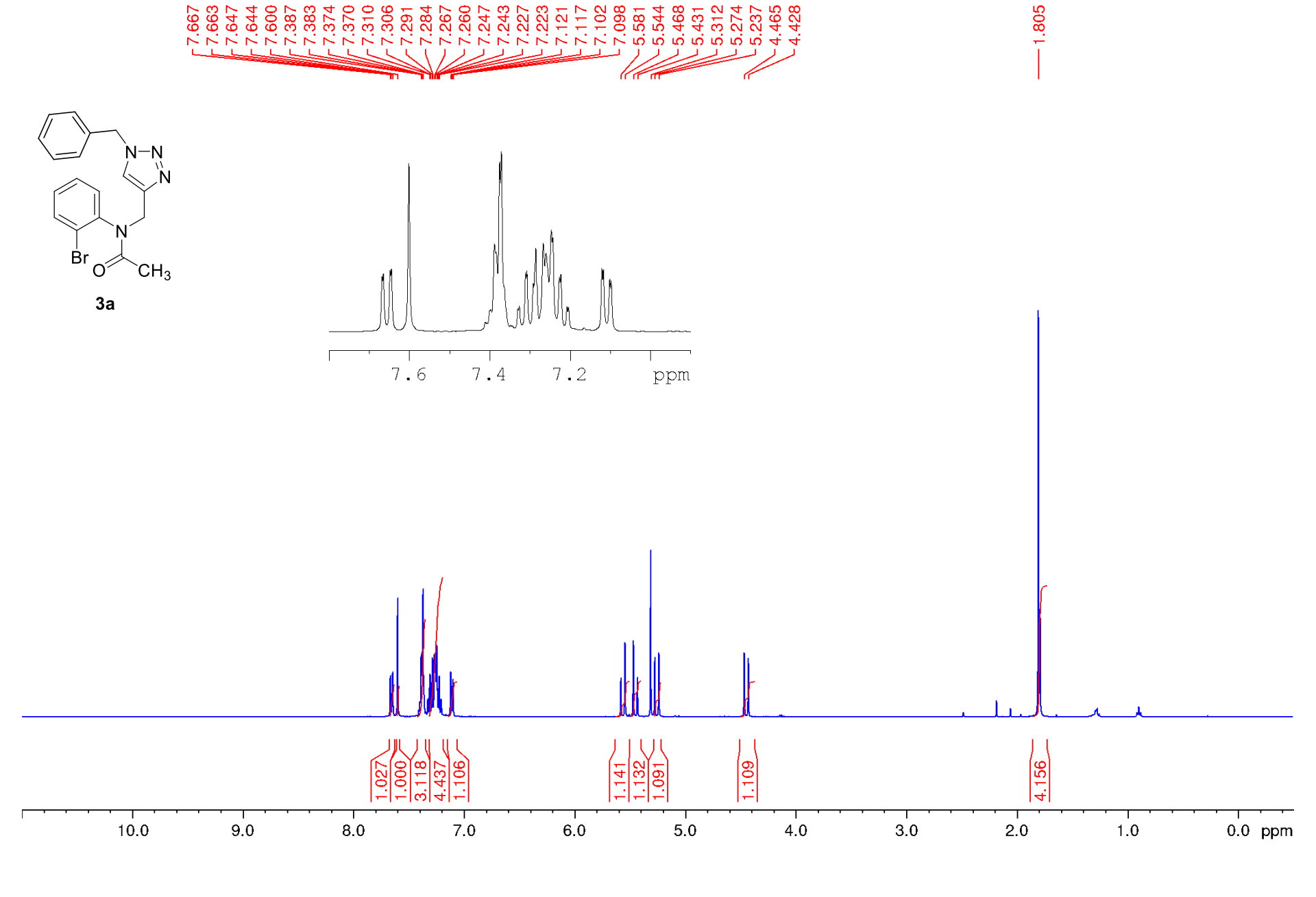
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



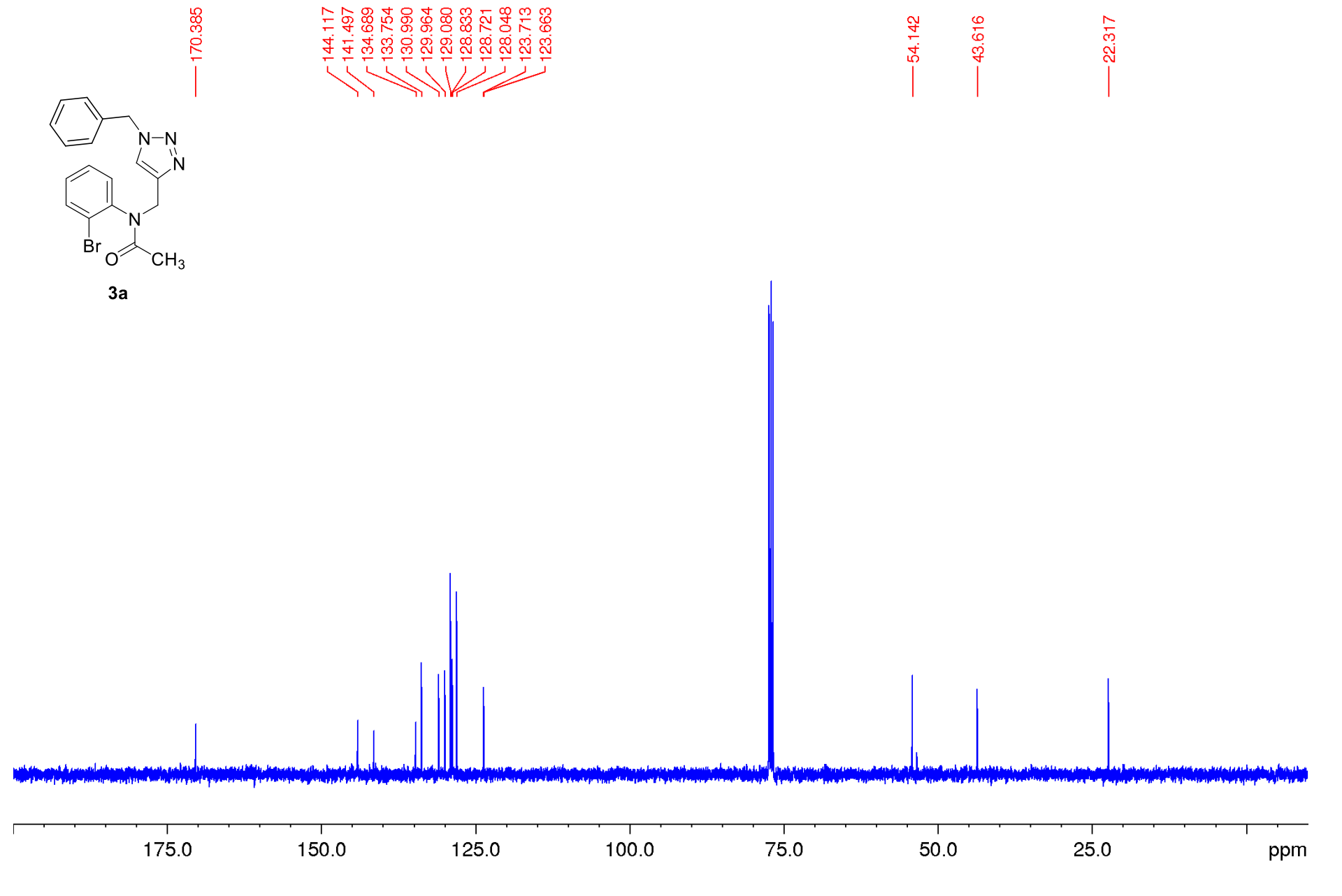
DEPT 135 NMR-spectrum ($CDCl_3$)



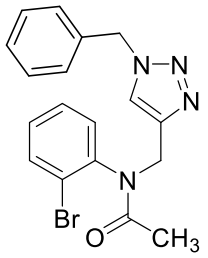
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



^{13}C NMR-spectrum (100 MHz, $CDCl_3$)

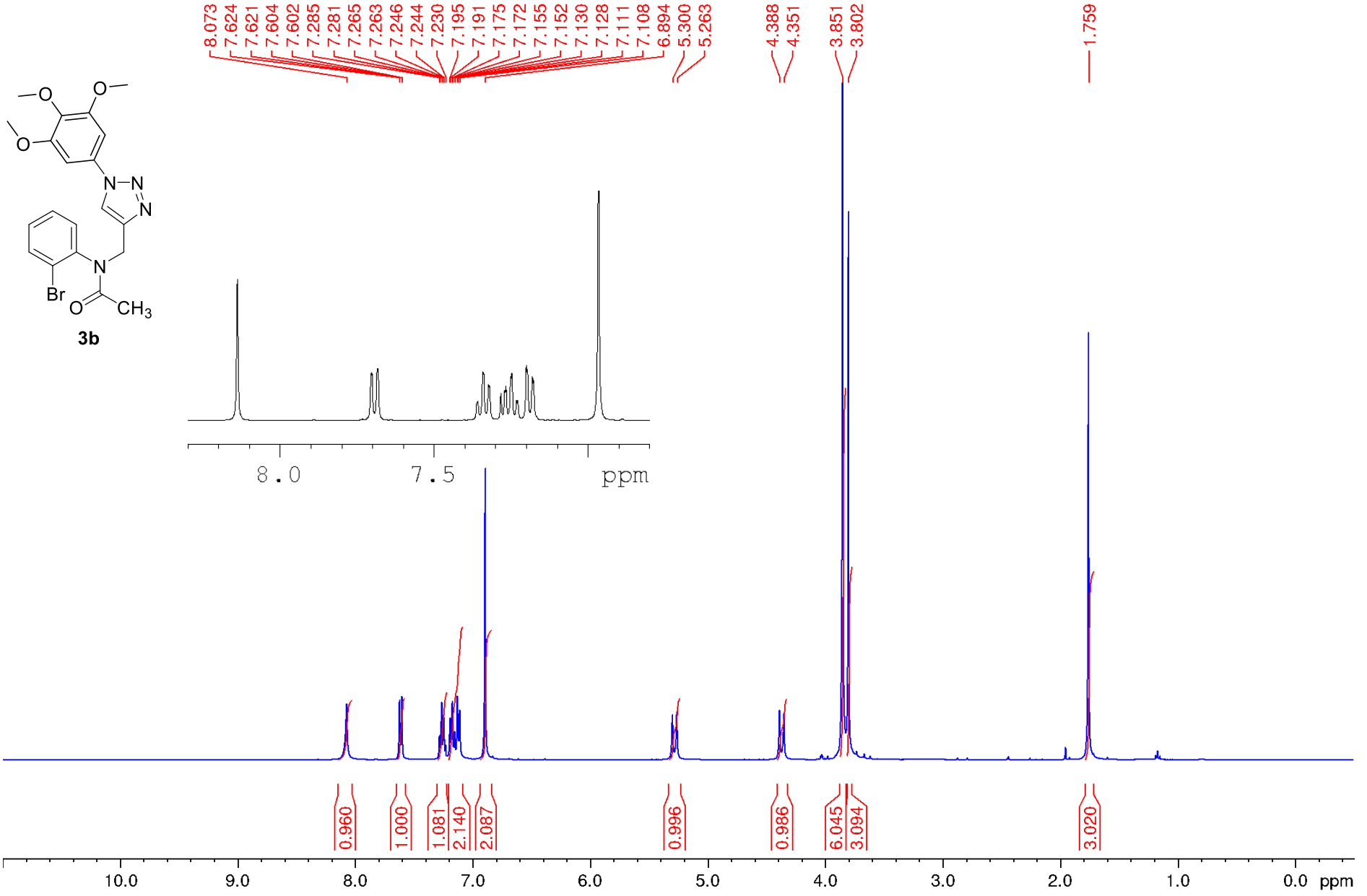


DEPT 135 NMR-spectrum ($CDCl_3$)



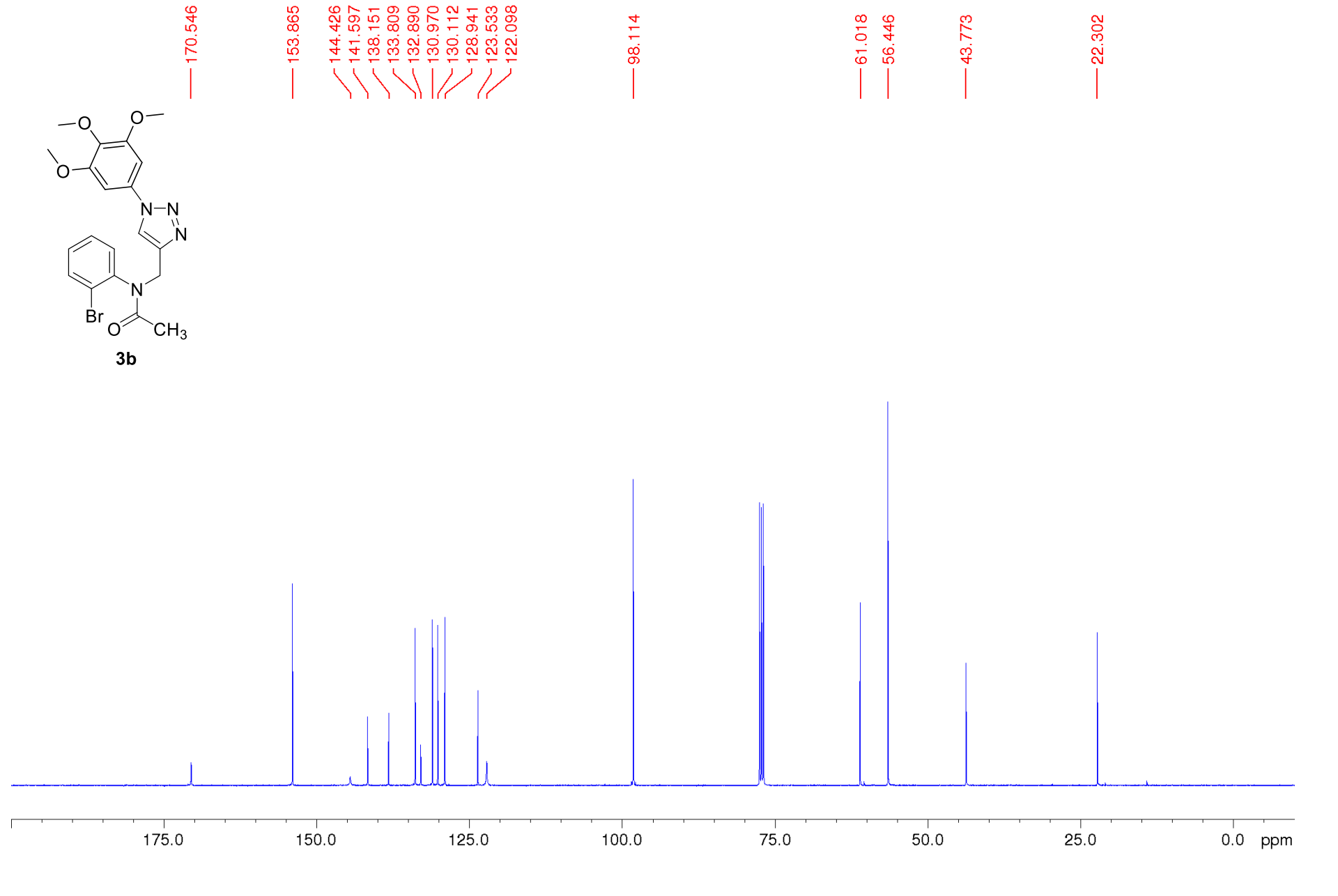
3a

^{1}H NMR-spectrum (400 MHz, $CDCl_3$)

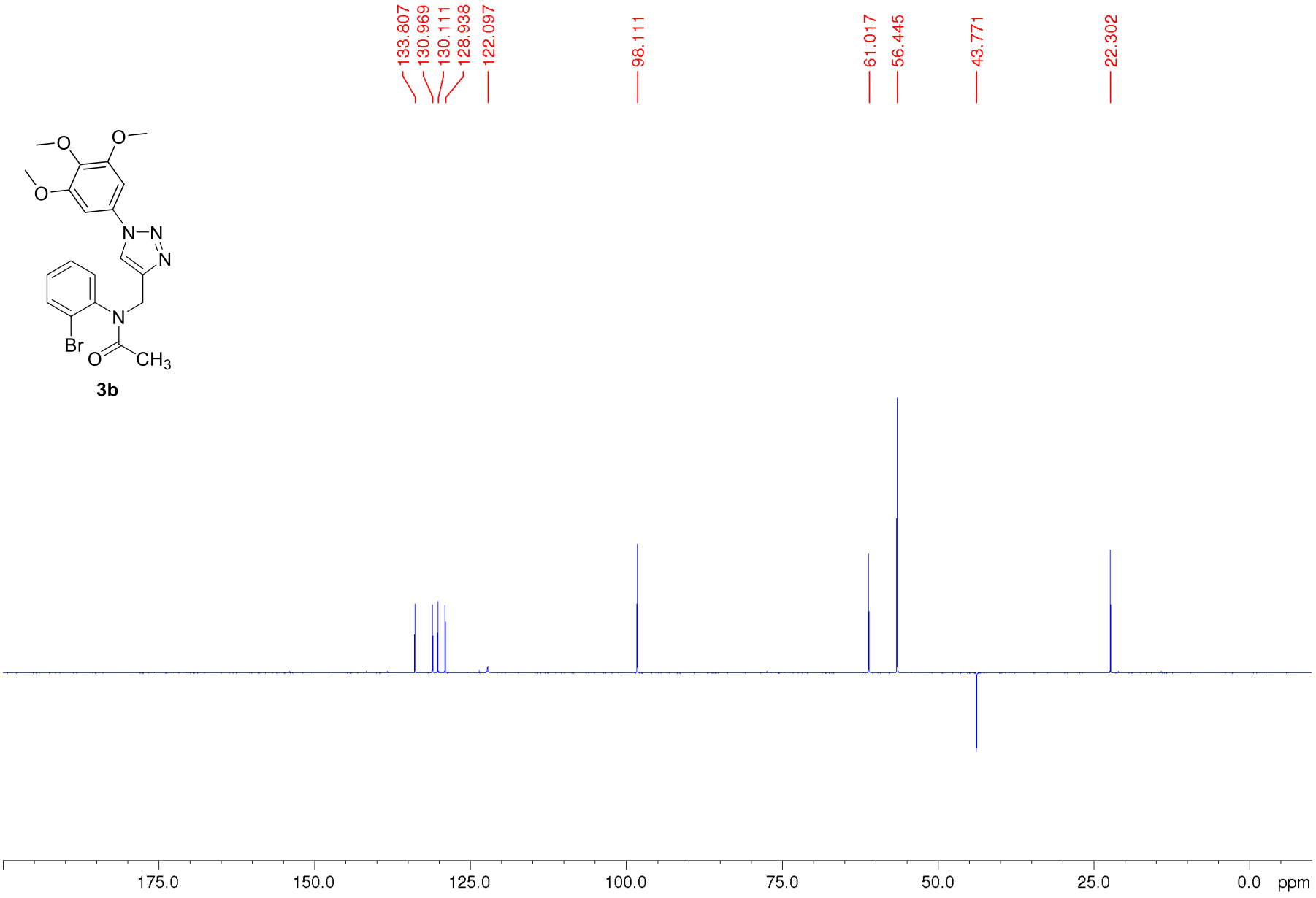


3b

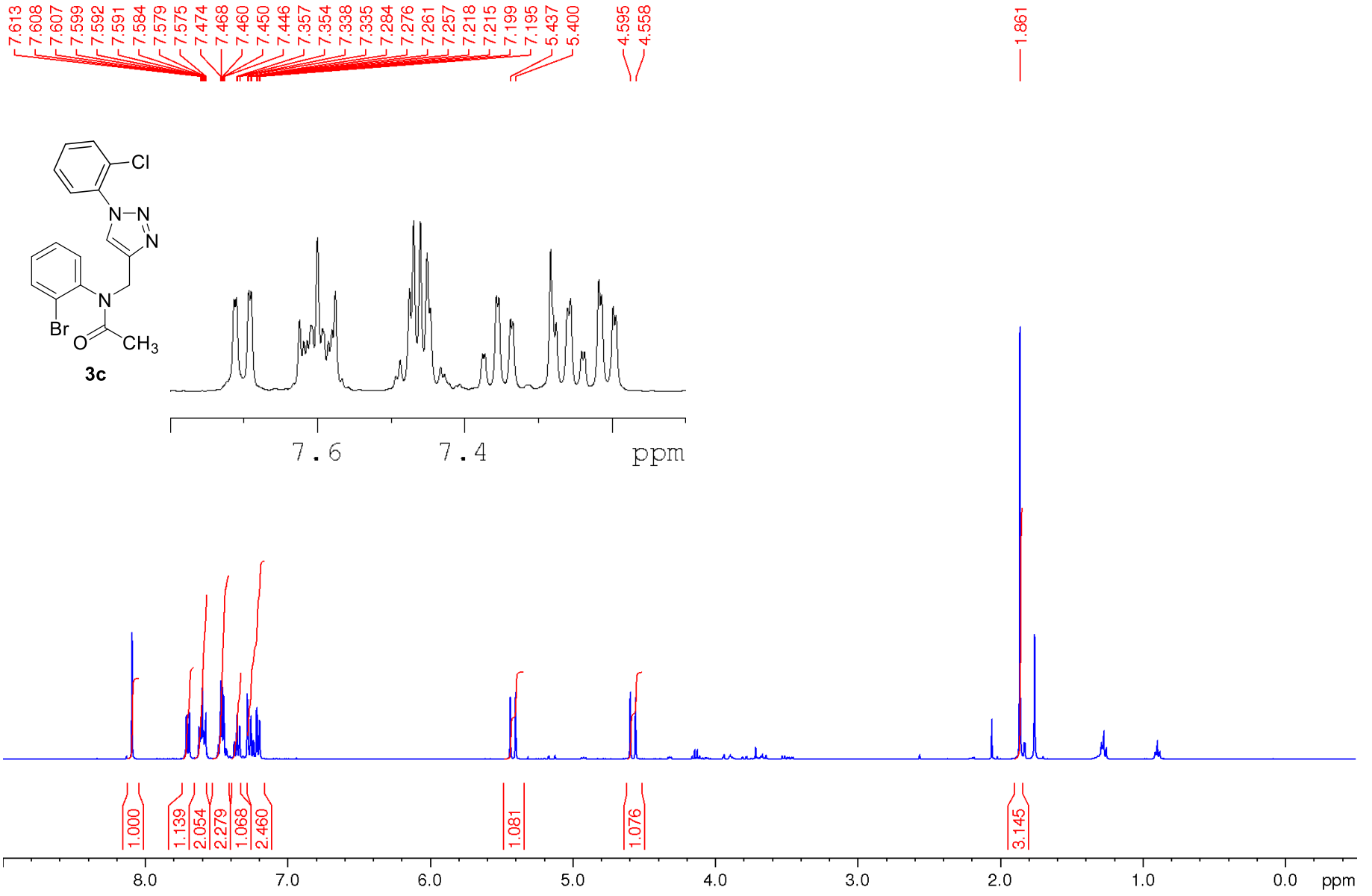
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



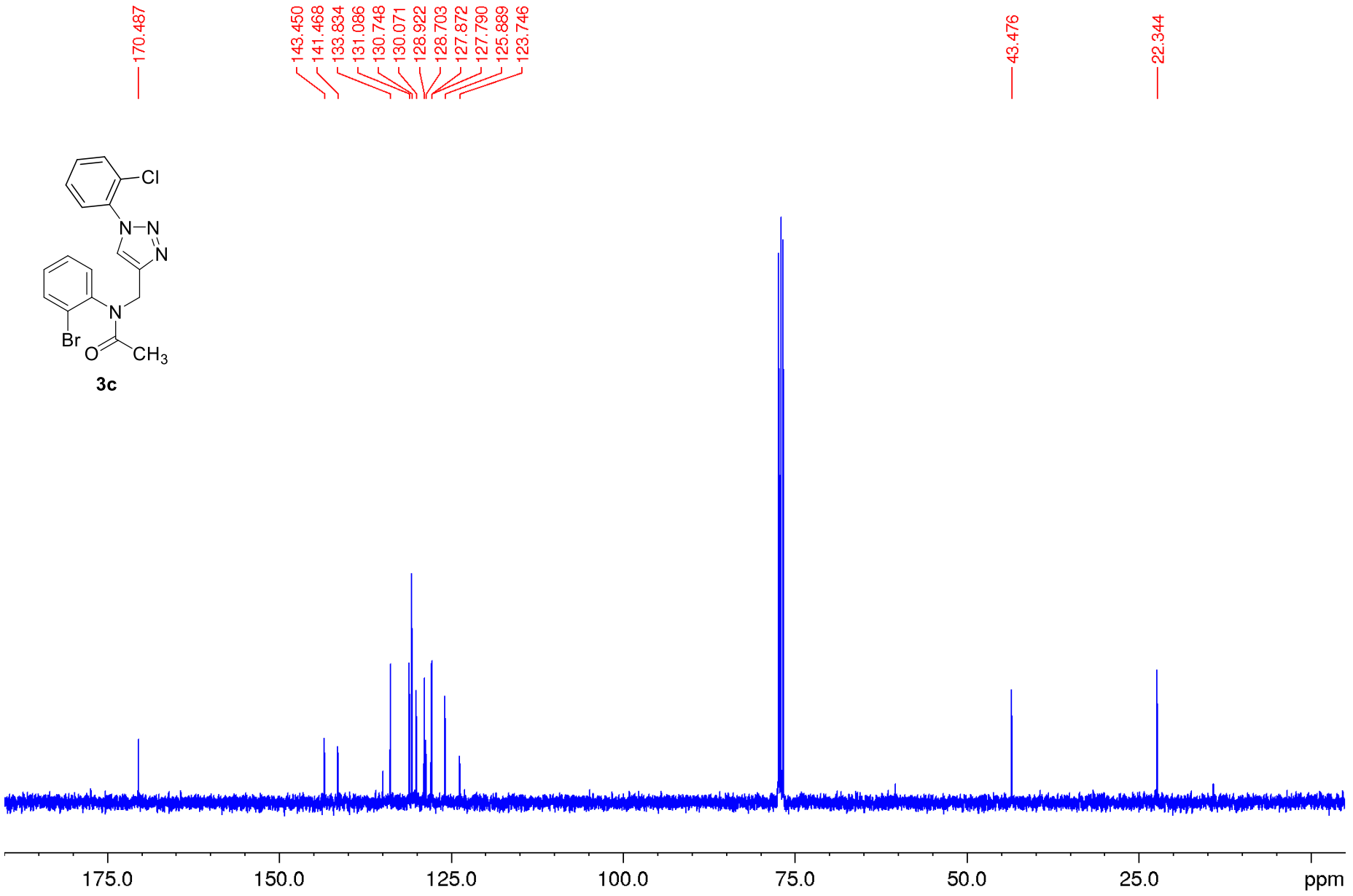
DEPT 135 NMR-spectrum ($CDCl_3$)



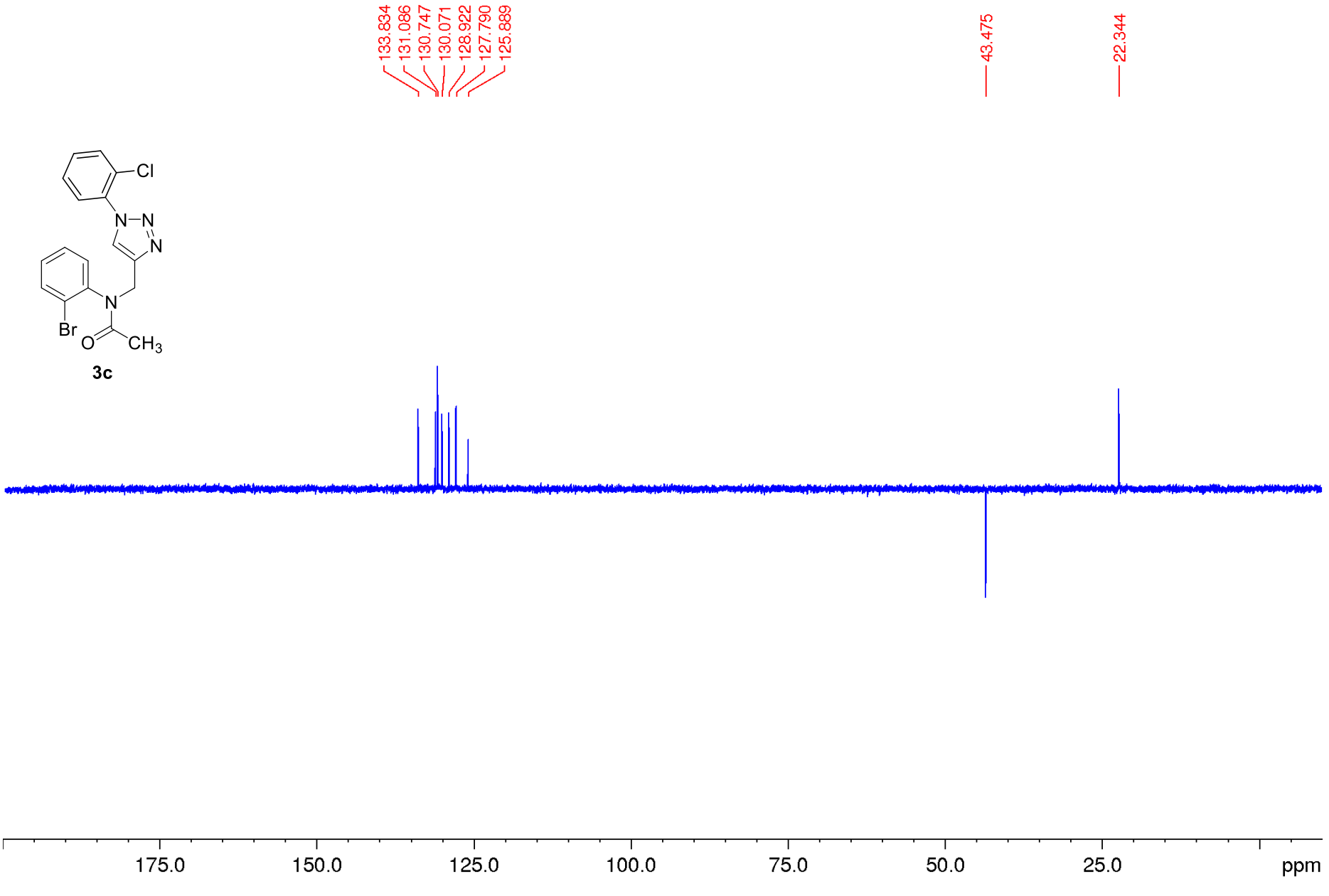
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



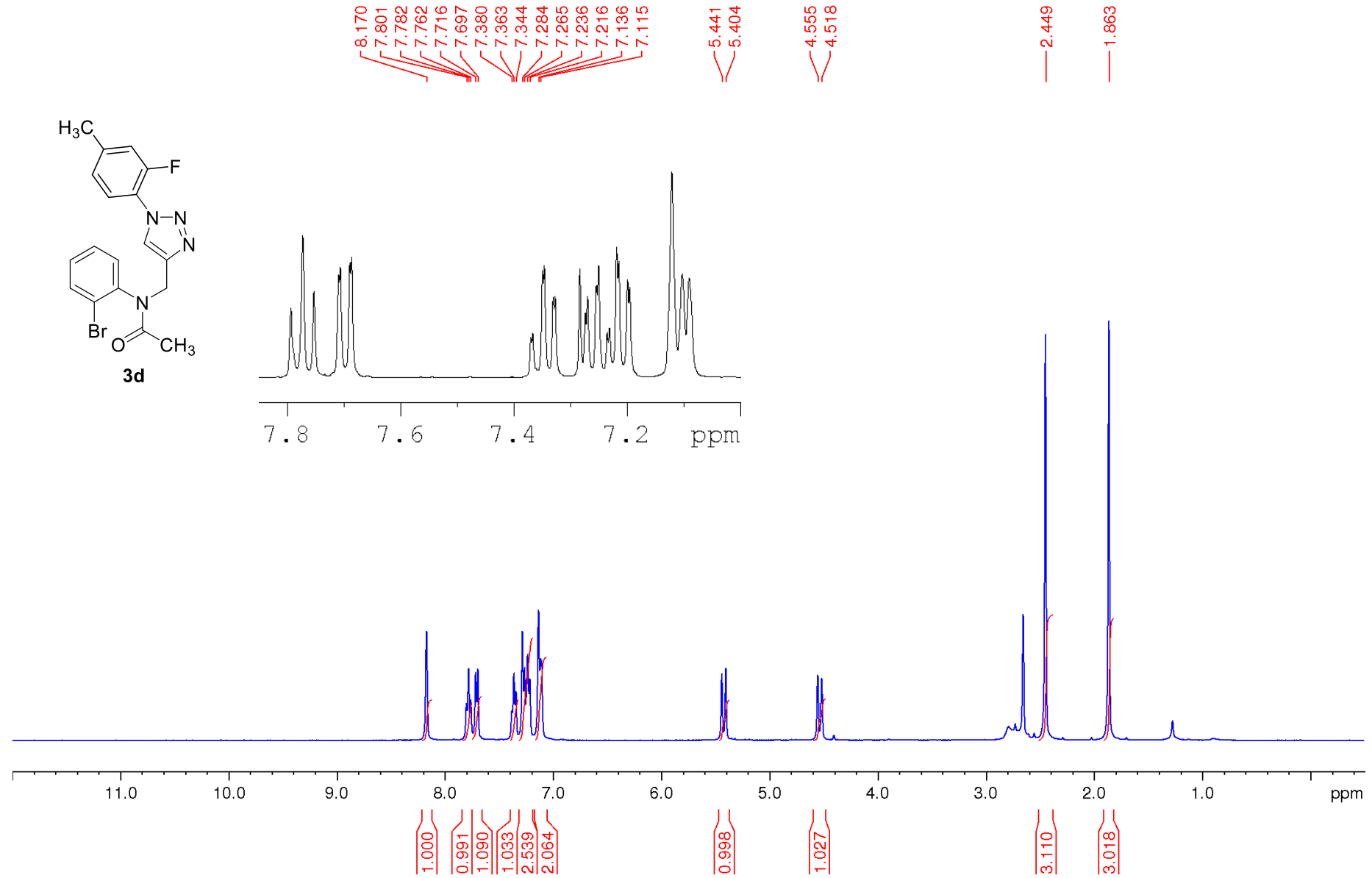
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



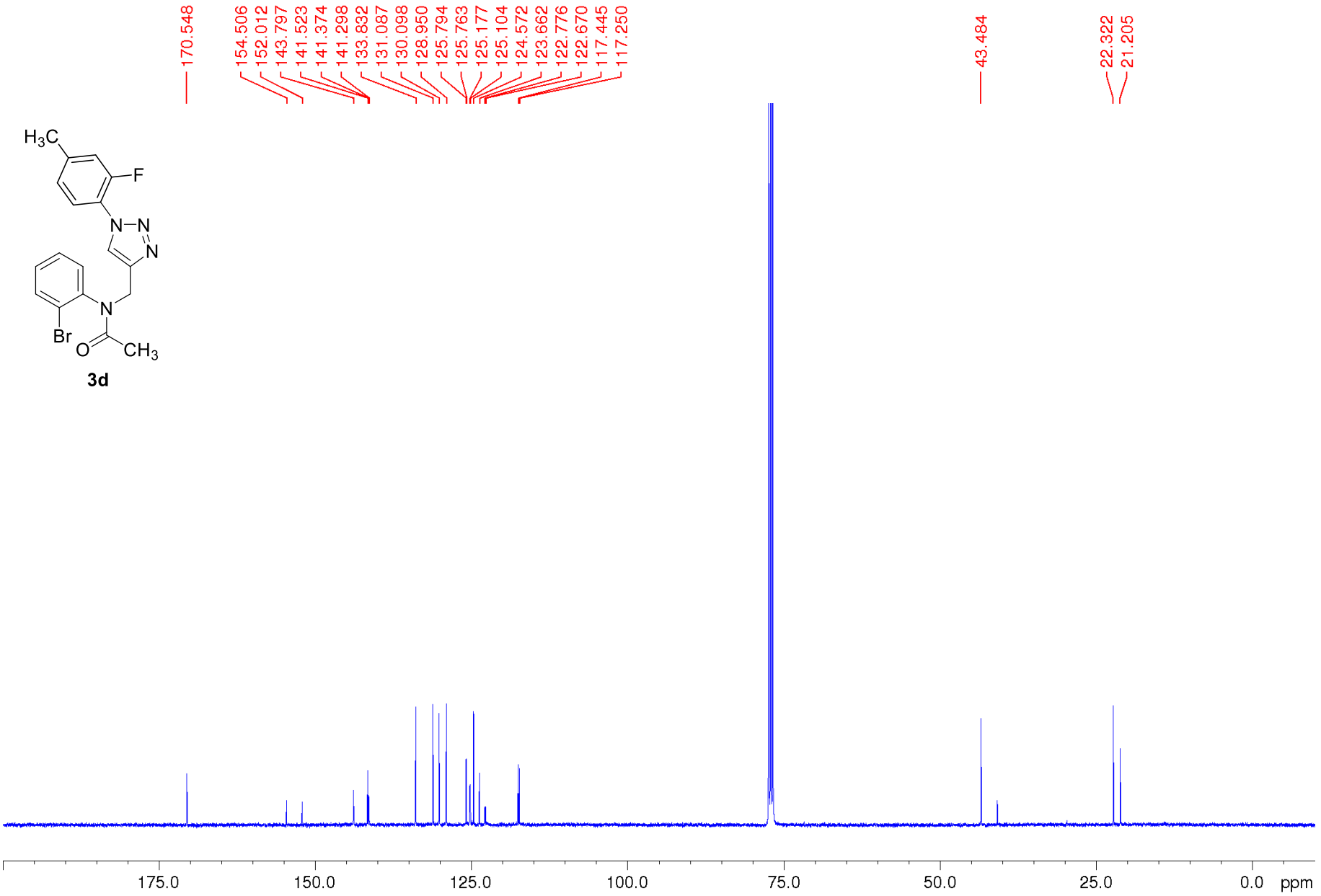
DEPT 135 NMR-spectrum ($CDCl_3$)



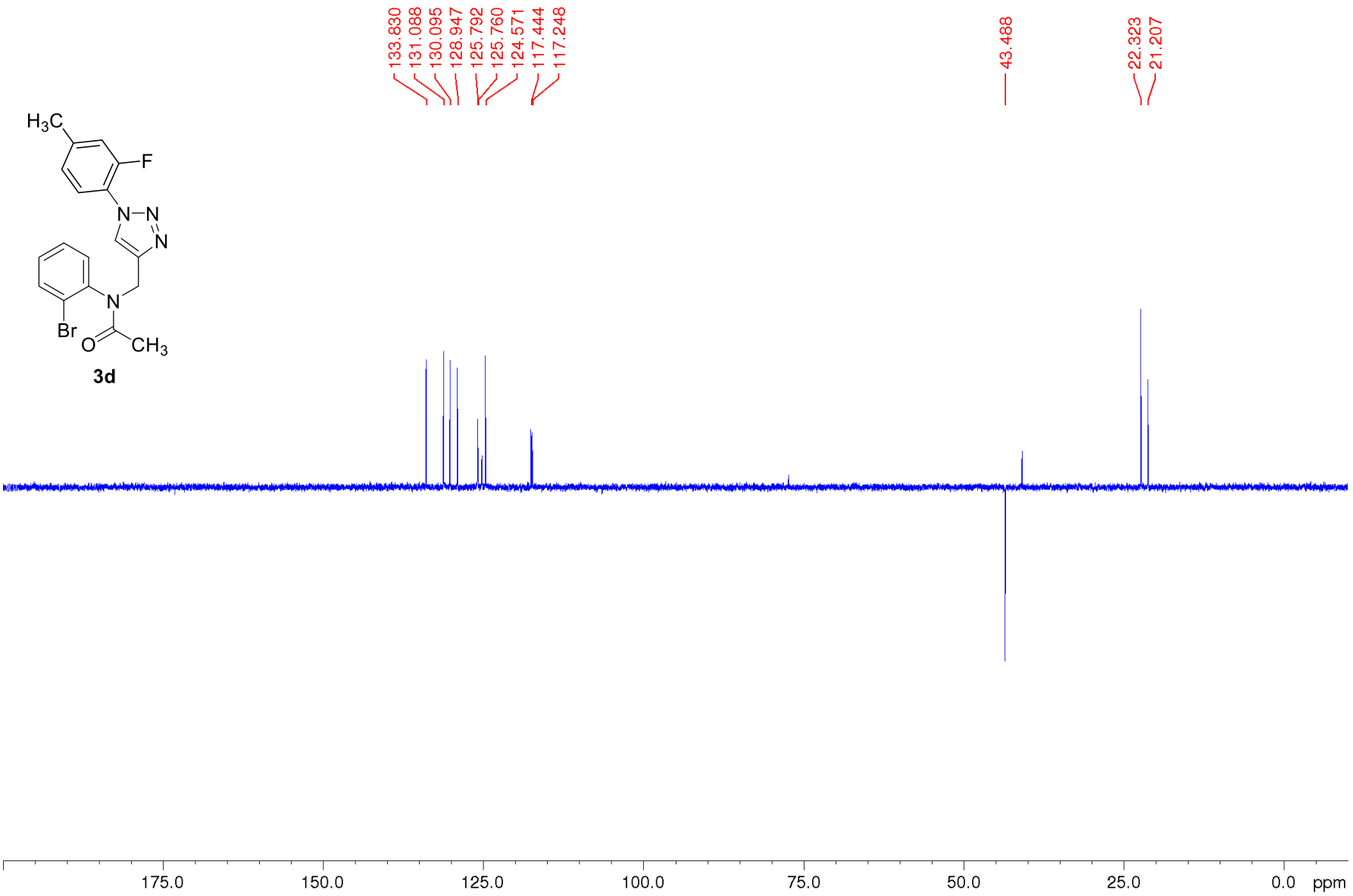
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



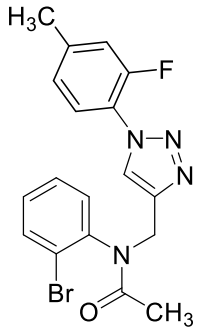
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



DEPT 135 NMR-spectrum ($CDCl_3$)

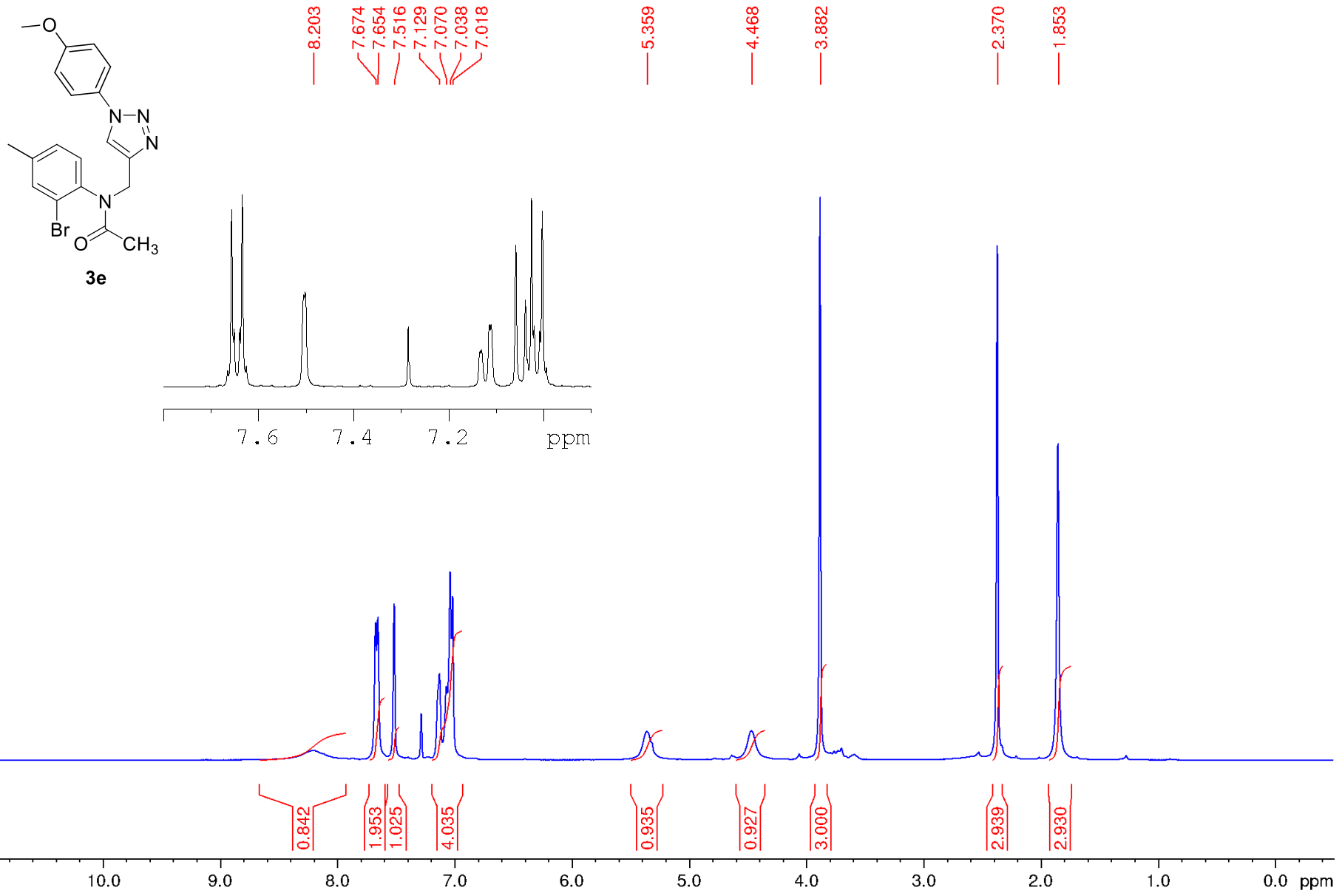


^{19}F NMR-spectrum (376.5 Hz, $CDCl_3$)

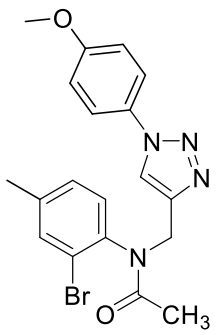


3d

^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



3e

170.750
159.747
144.318
141.307
140.529
138.961
134.124
130.560
130.467
129.631
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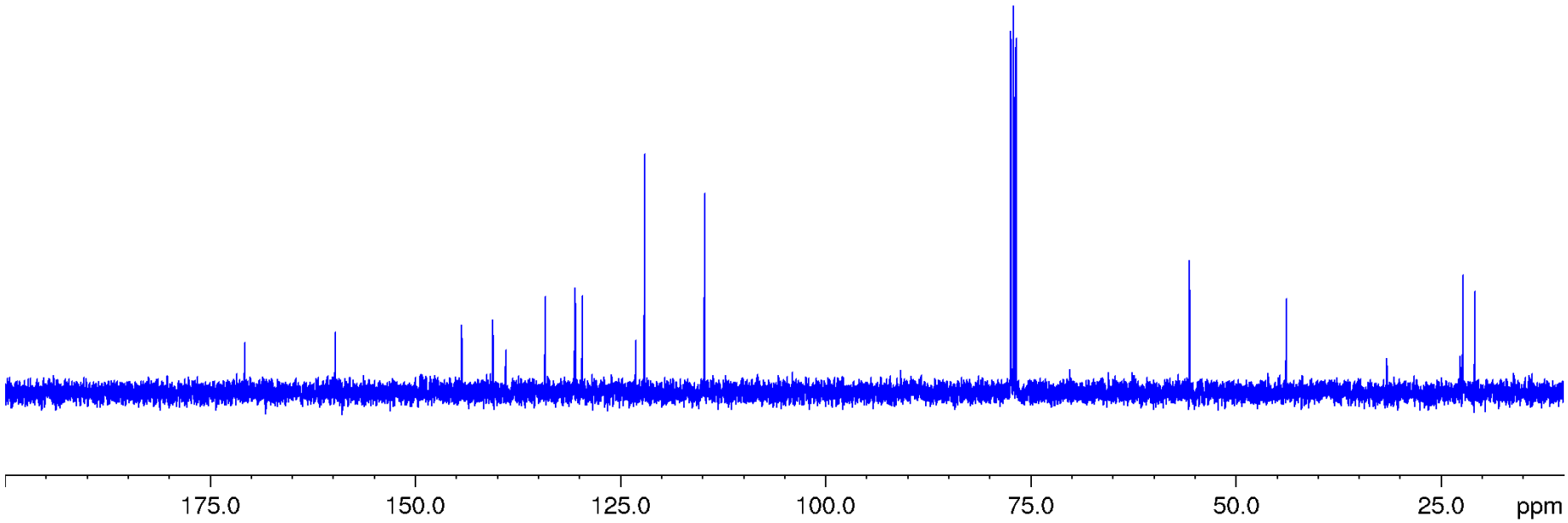
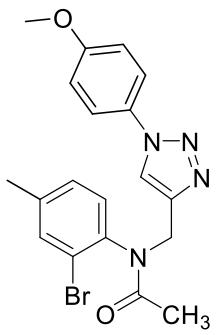
122.018
114.720
55.622
43.804
22.284
20.813

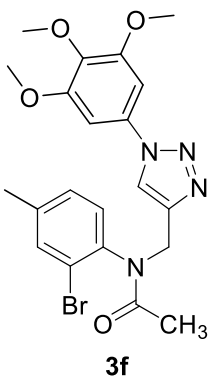


DEPT 135 NMR-spectrum ($CDCl_3$)



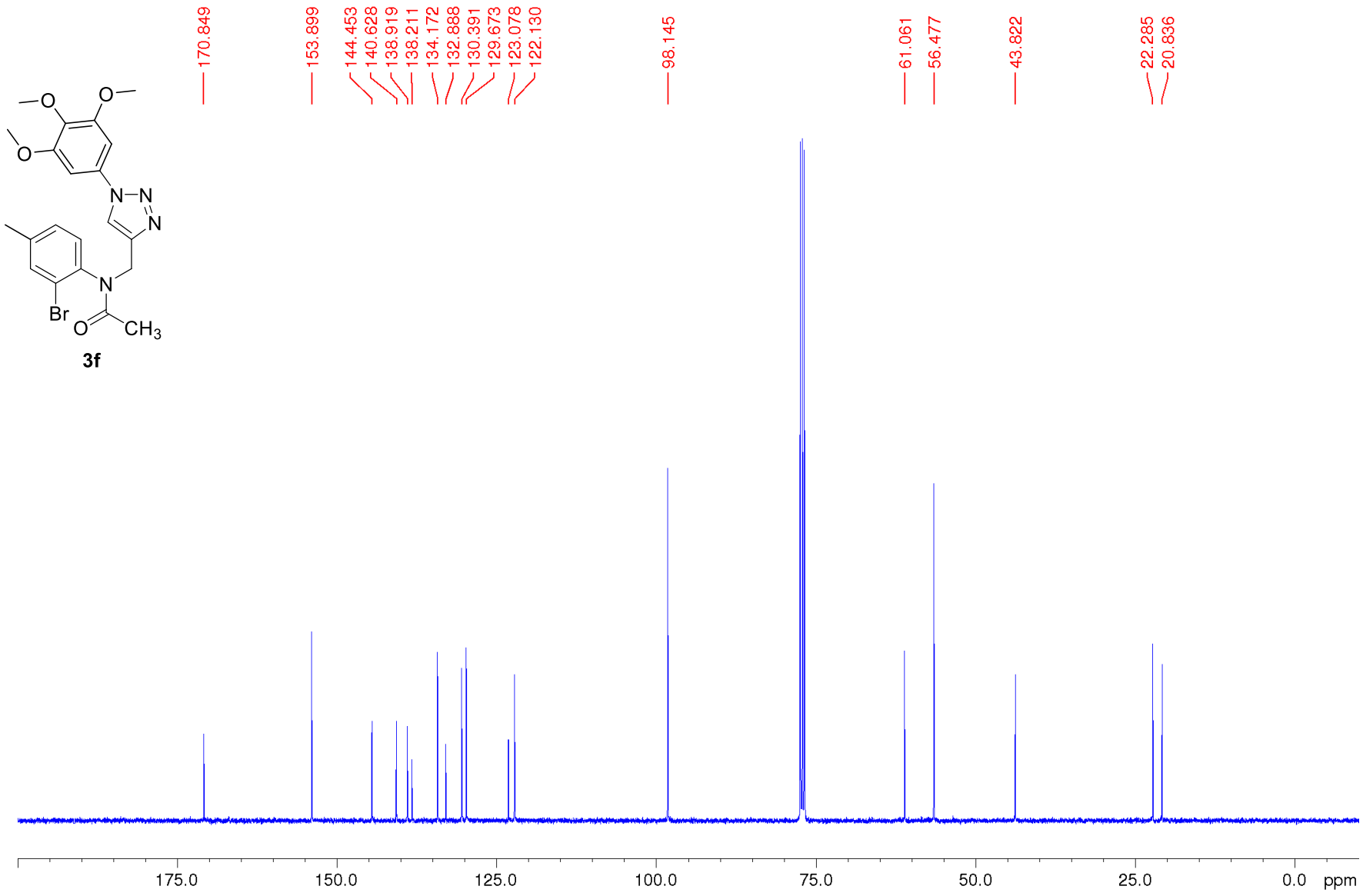
3e

^{1}H NMR-spectrum (400 MHz, $CDCl_3$)

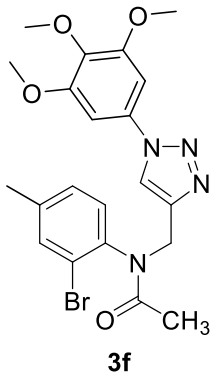


3f

^{13}C NMR-spectrum (100 MHz, $CDCl_3$)

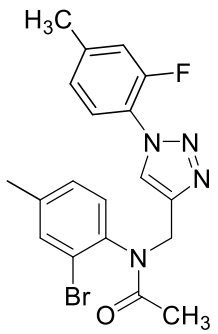


DEPT 135 NMR-spectrum ($CDCl_3$)



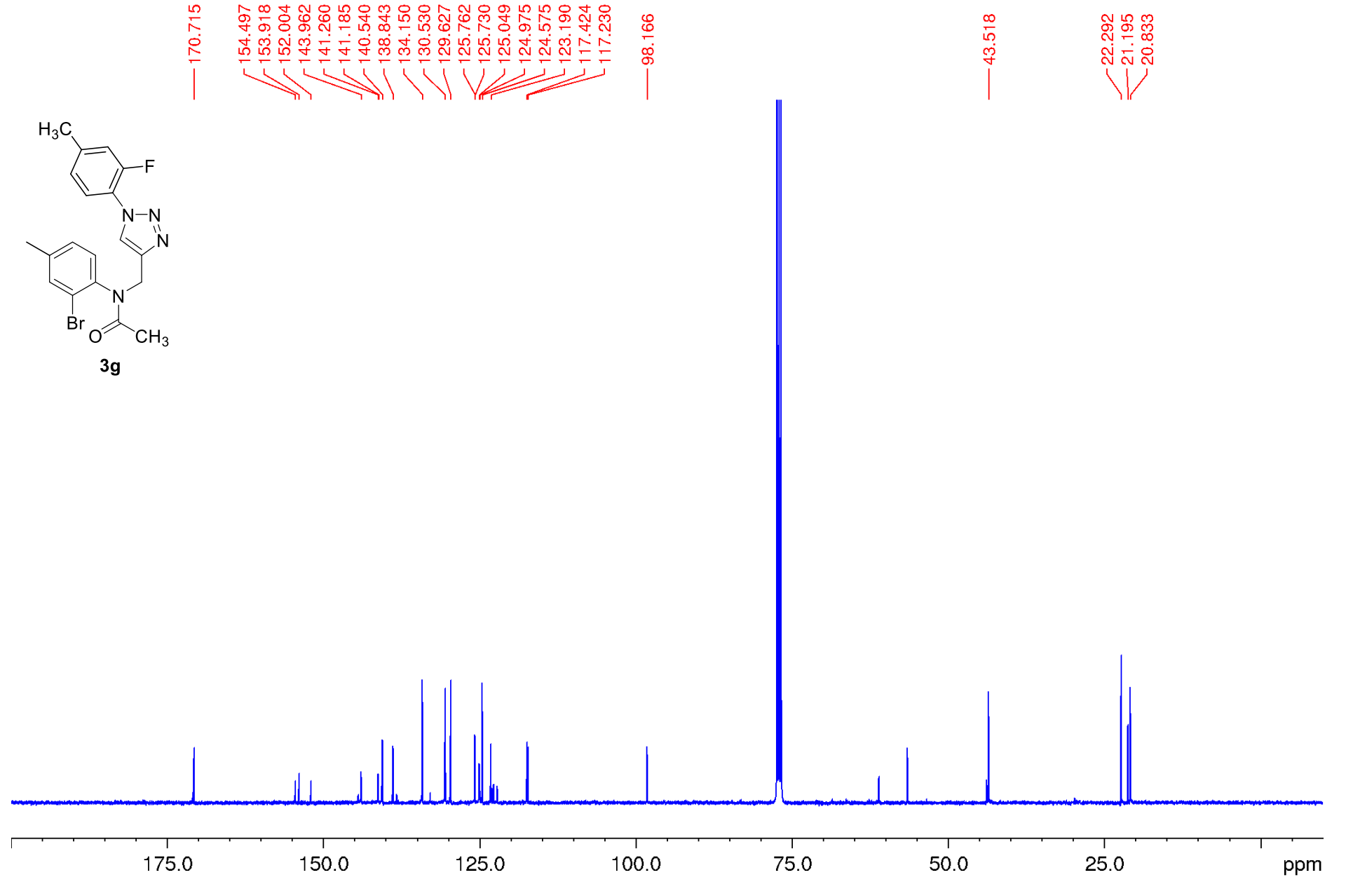
3f

^{1}H NMR-spectrum (400 MHz, $CDCl_3$)

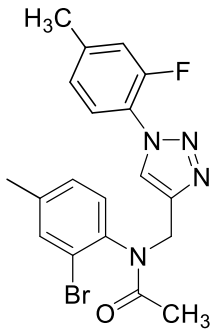


3g

^{13}C NMR-spectrum (100 MHz, $CDCl_3$)

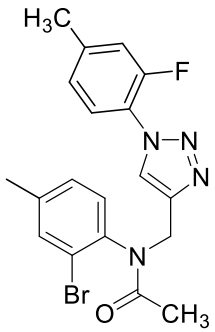


DEPT 135 NMR-spectrum ($CDCl_3$)



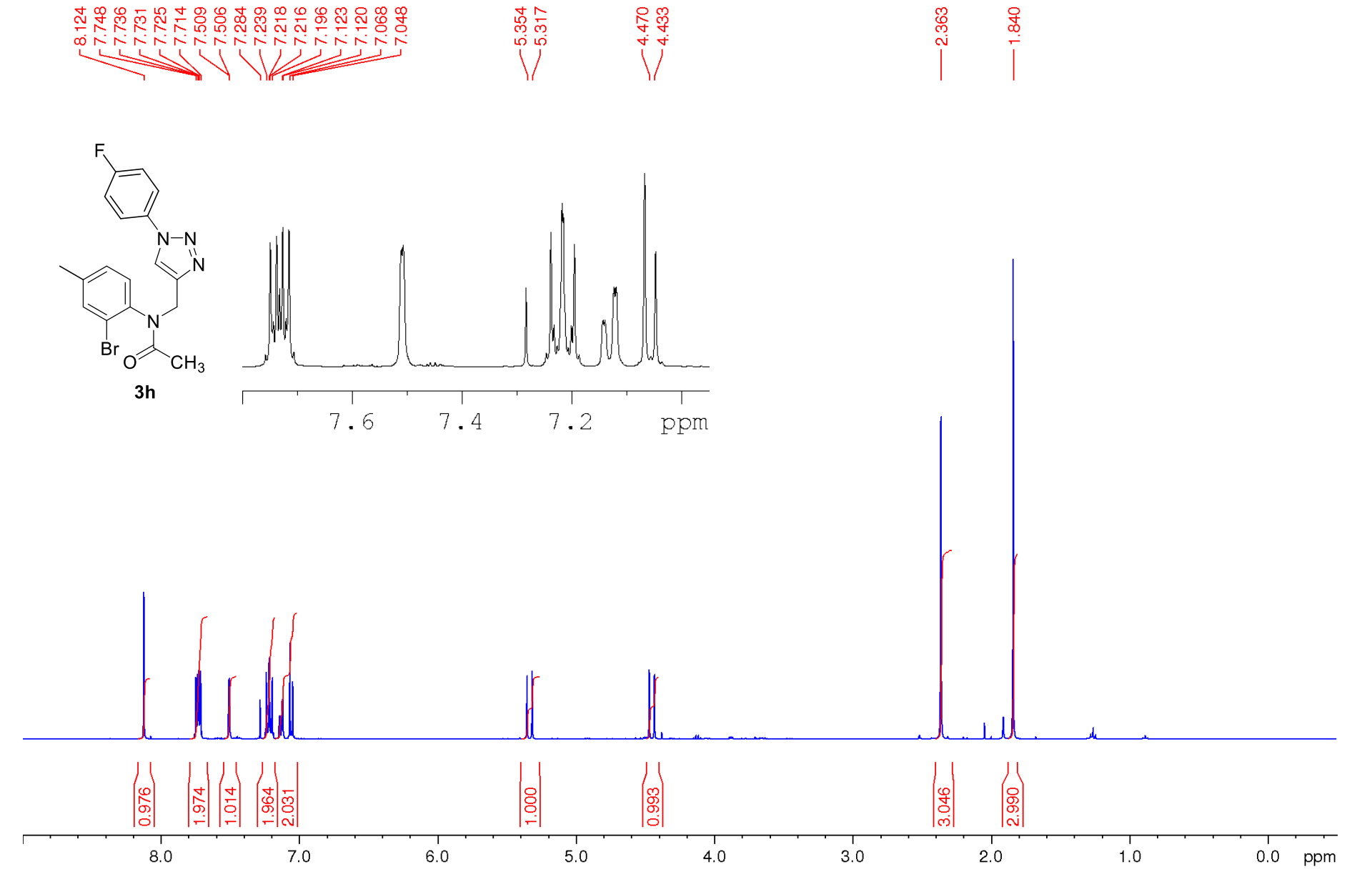
3g

^{19}F NMR-spectrum (376.5 Hz, $CDCl_3$)

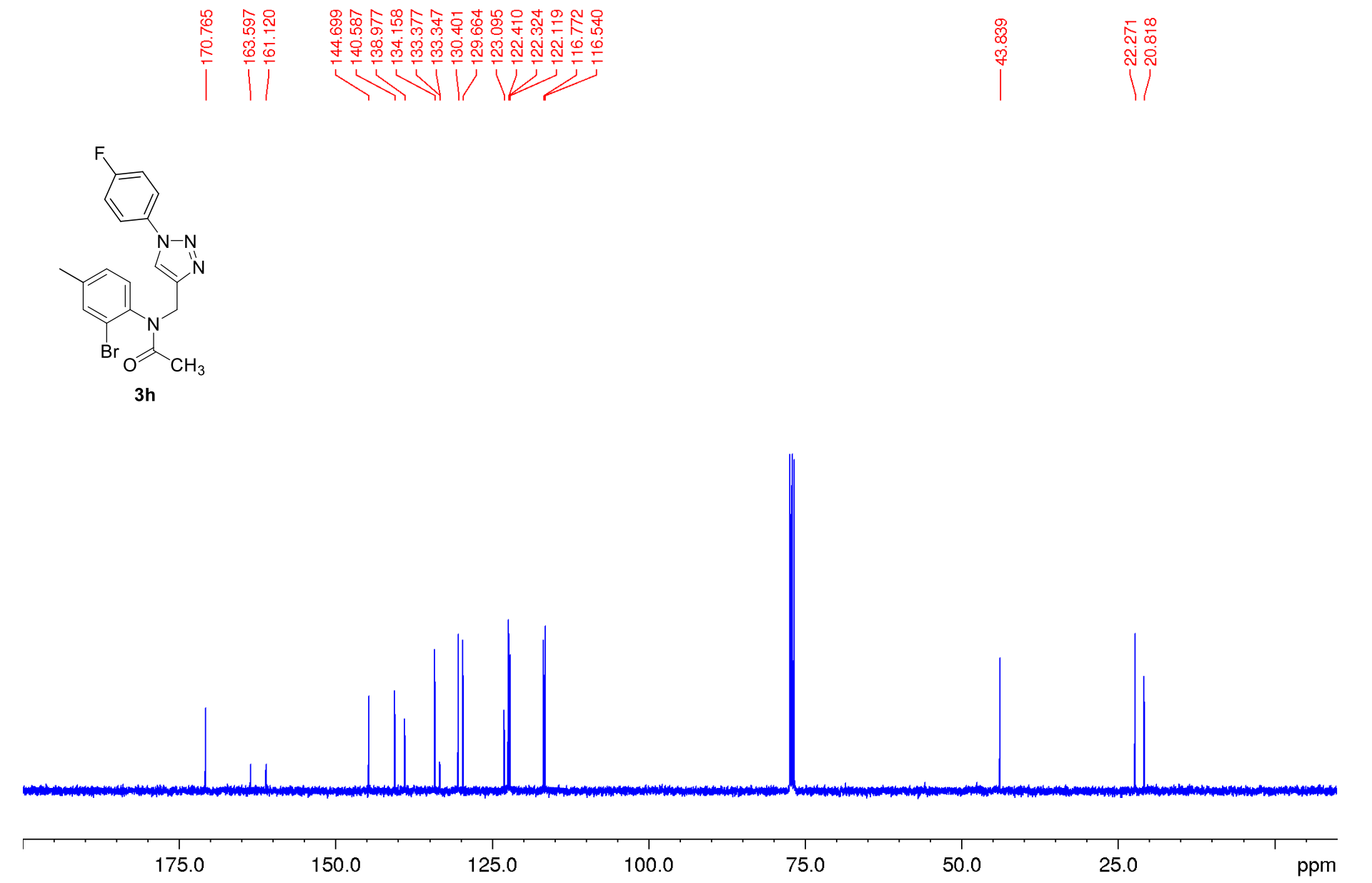


3g

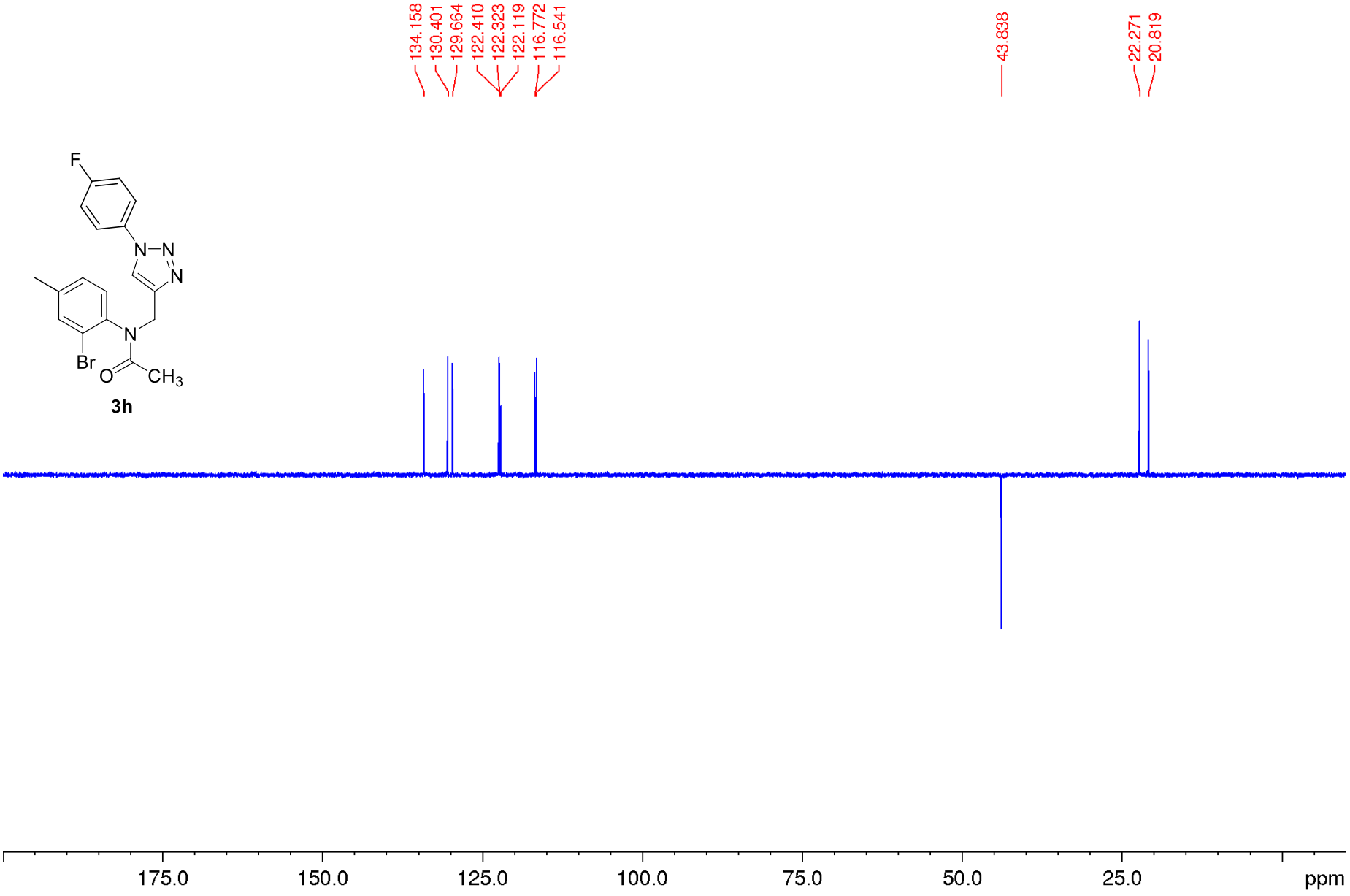
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



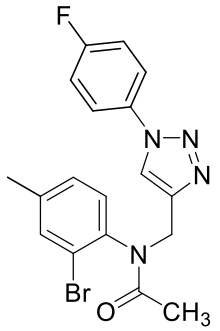
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



DEPT 135 NMR-spectrum ($CDCl_3$)

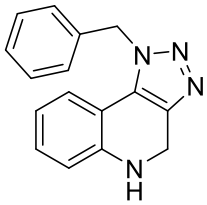


^{19}F NMR-spectrum (376.5 Hz, $CDCl_3$)

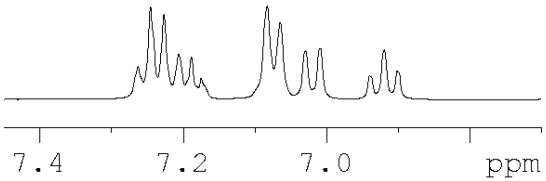


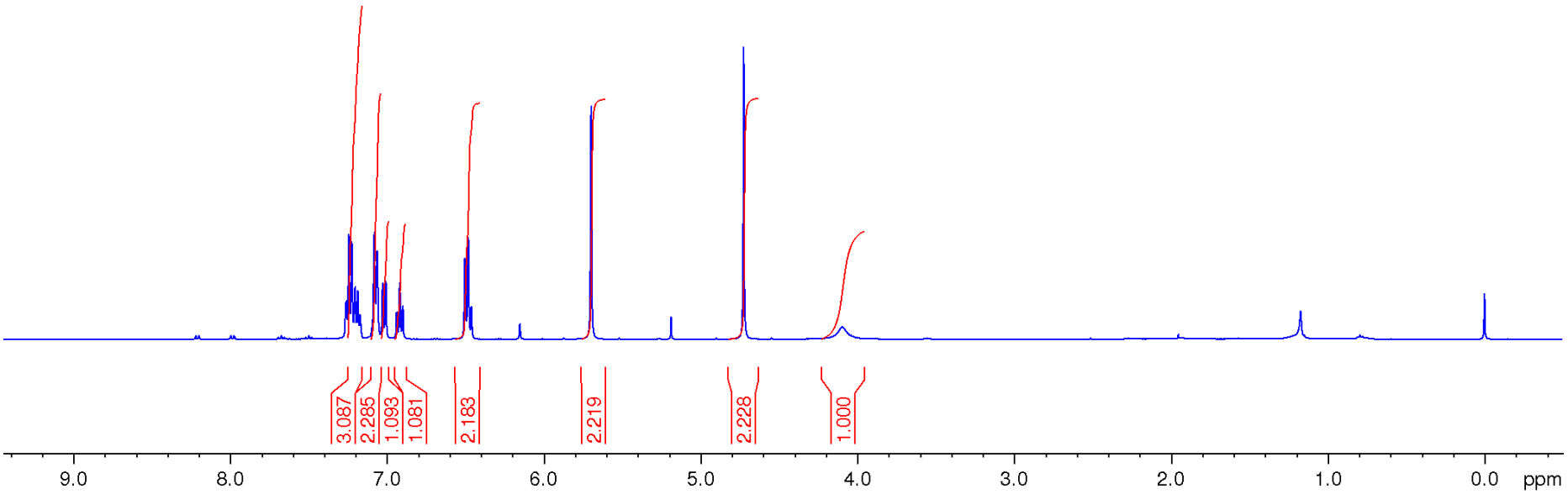
3h

^{1}H NMR-spectrum (400 MHz, $CDCl_3$)

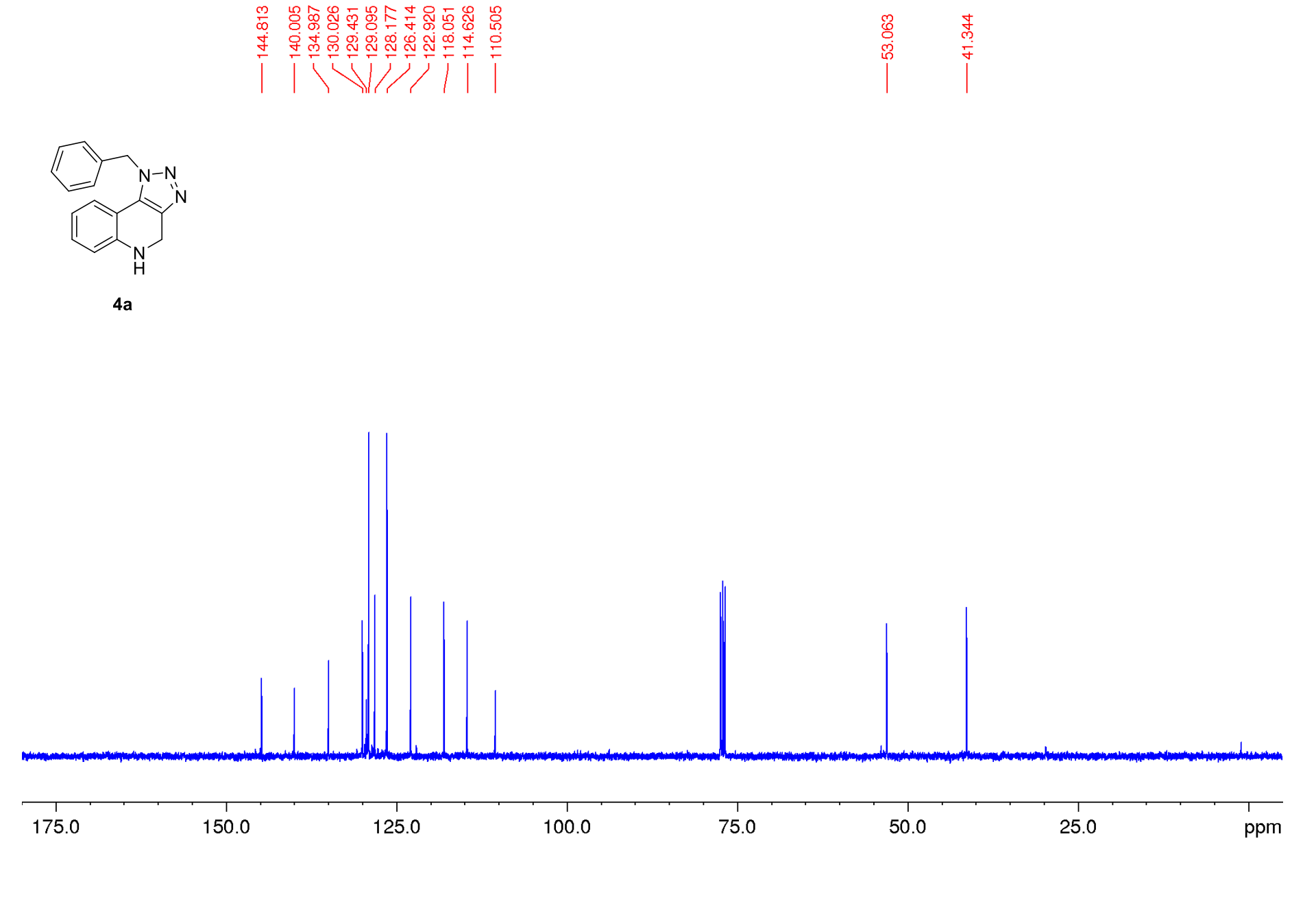


4a

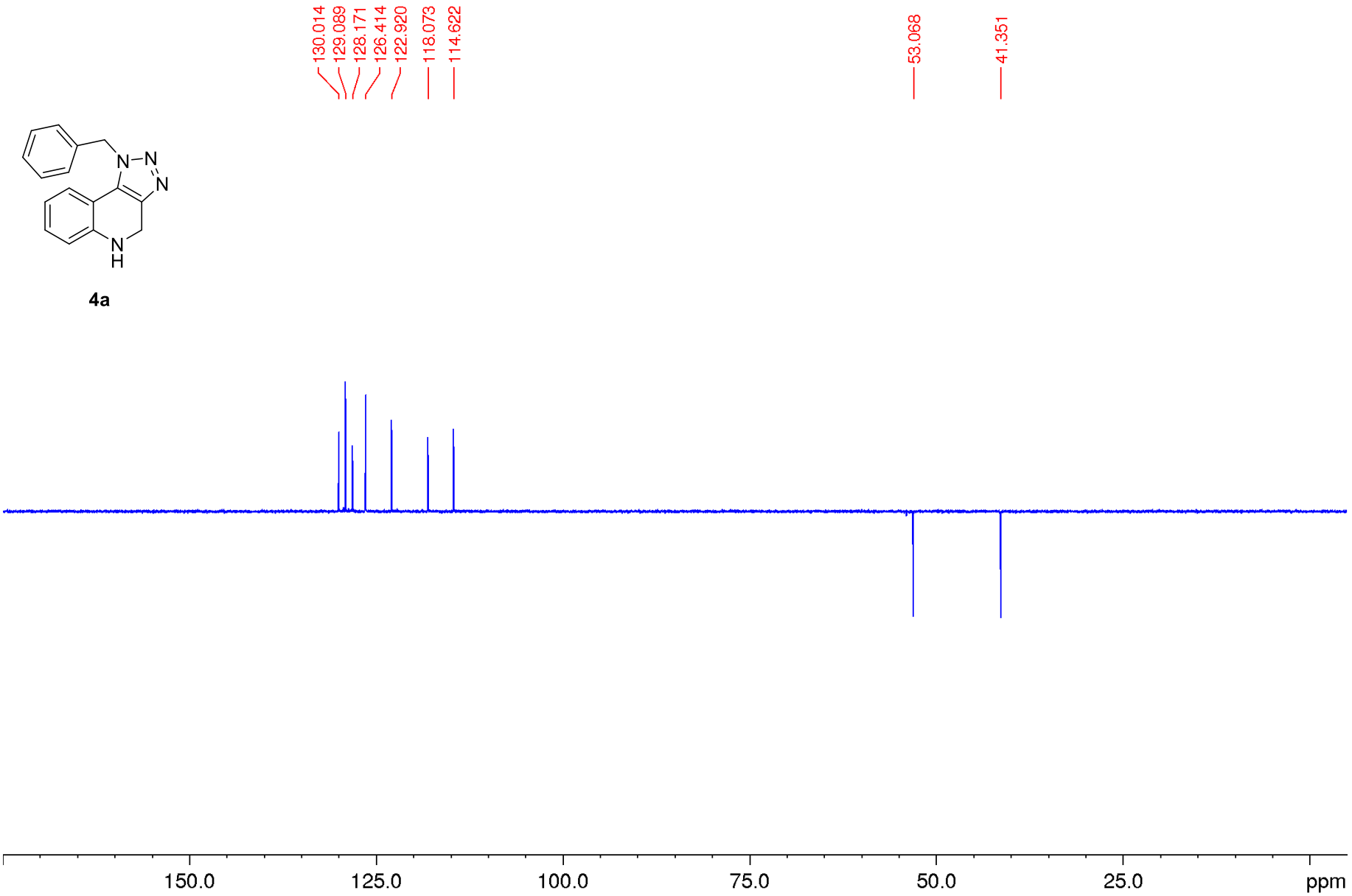




^{13}C NMR-spectrum (100 MHz, $CDCl_3$)

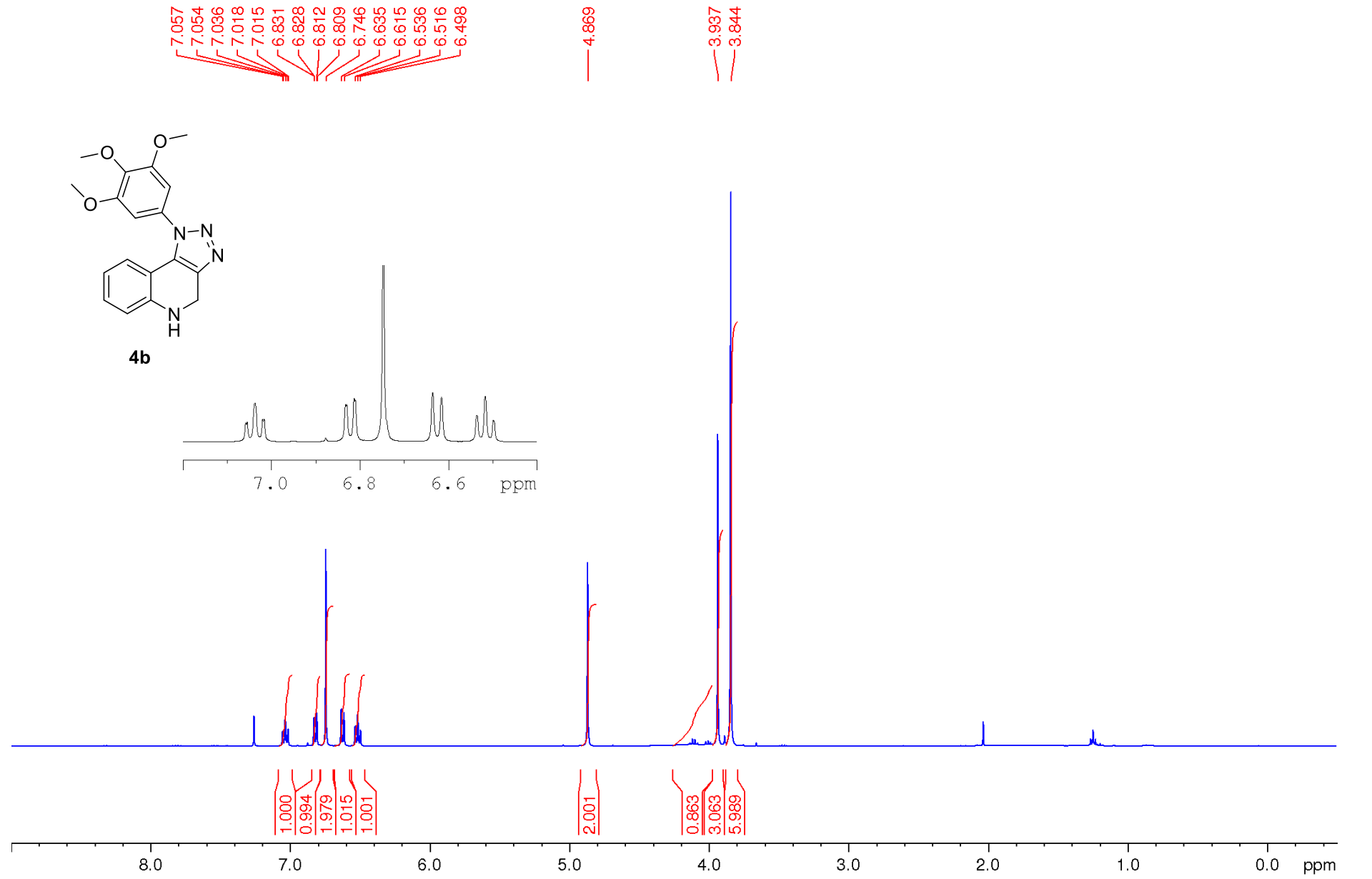


DEPT 135 NMR-spectrum ($CDCl_3$)

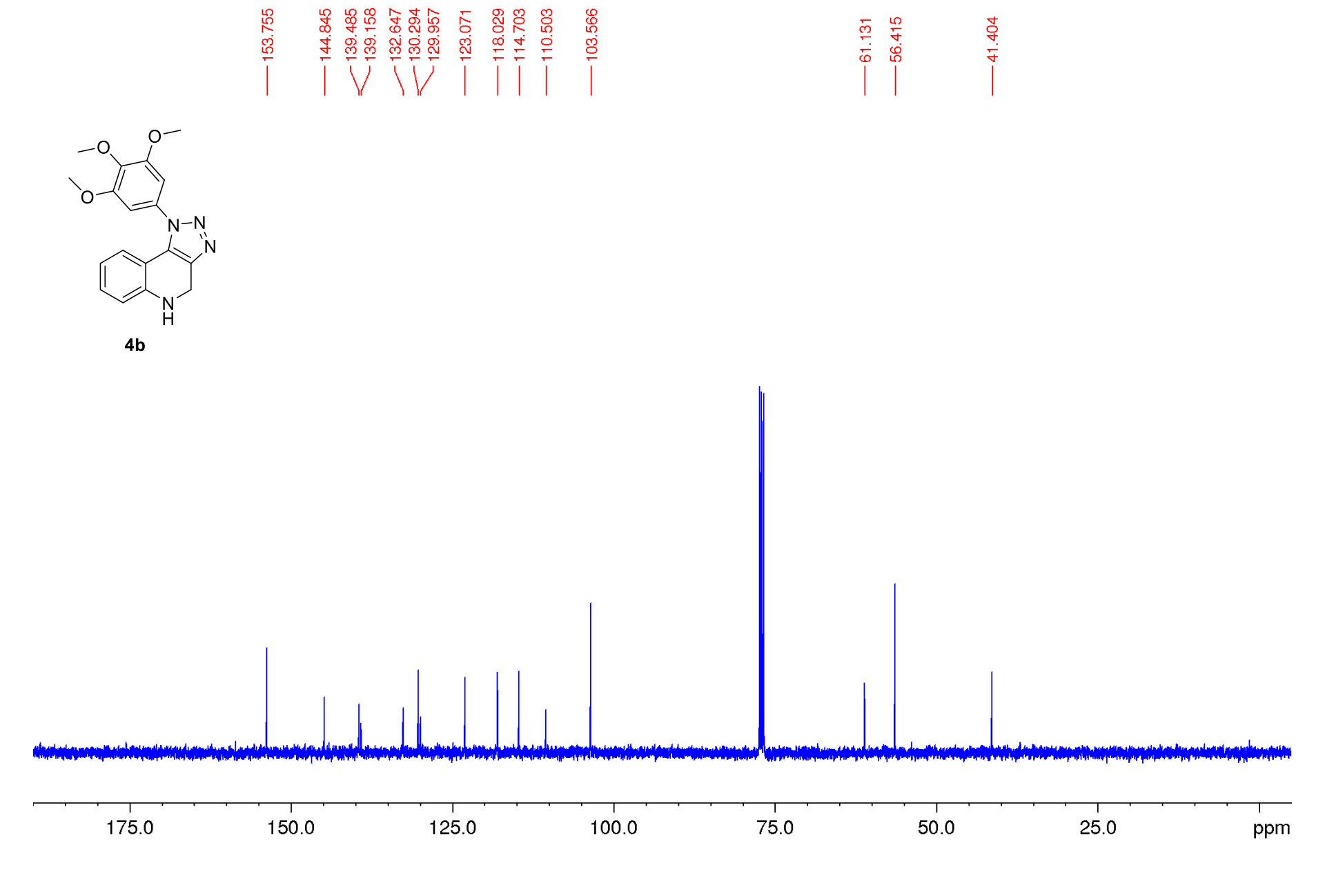


4a

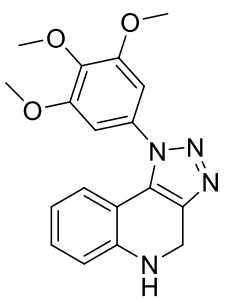
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



^{13}C NMR-spectrum (100 MHz, $CDCl_3$)

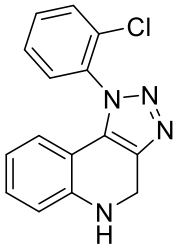


DEPT 135 NMR-spectrum ($CDCl_3$)

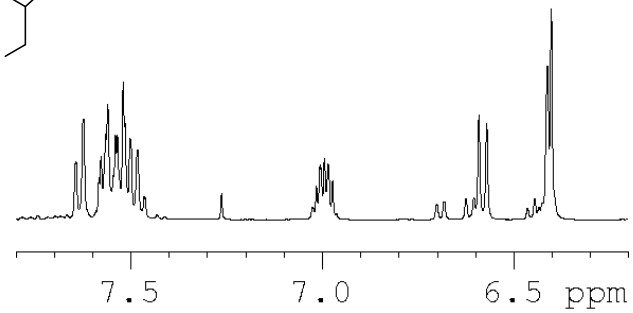


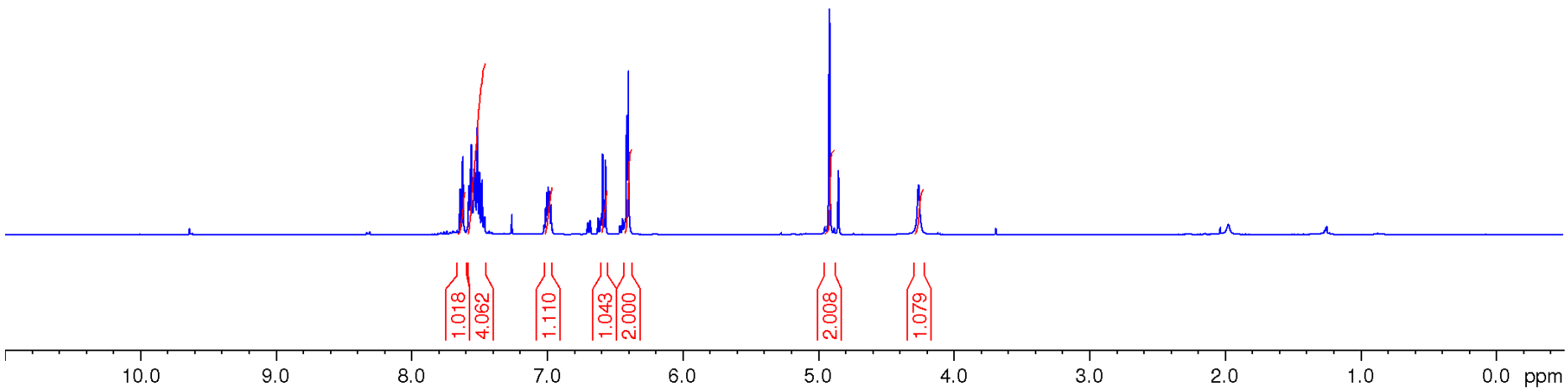
4b

^{1}H NMR-spectrum (400 MHz, $CDCl_3$)

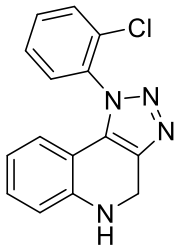


4c



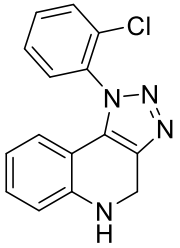


^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



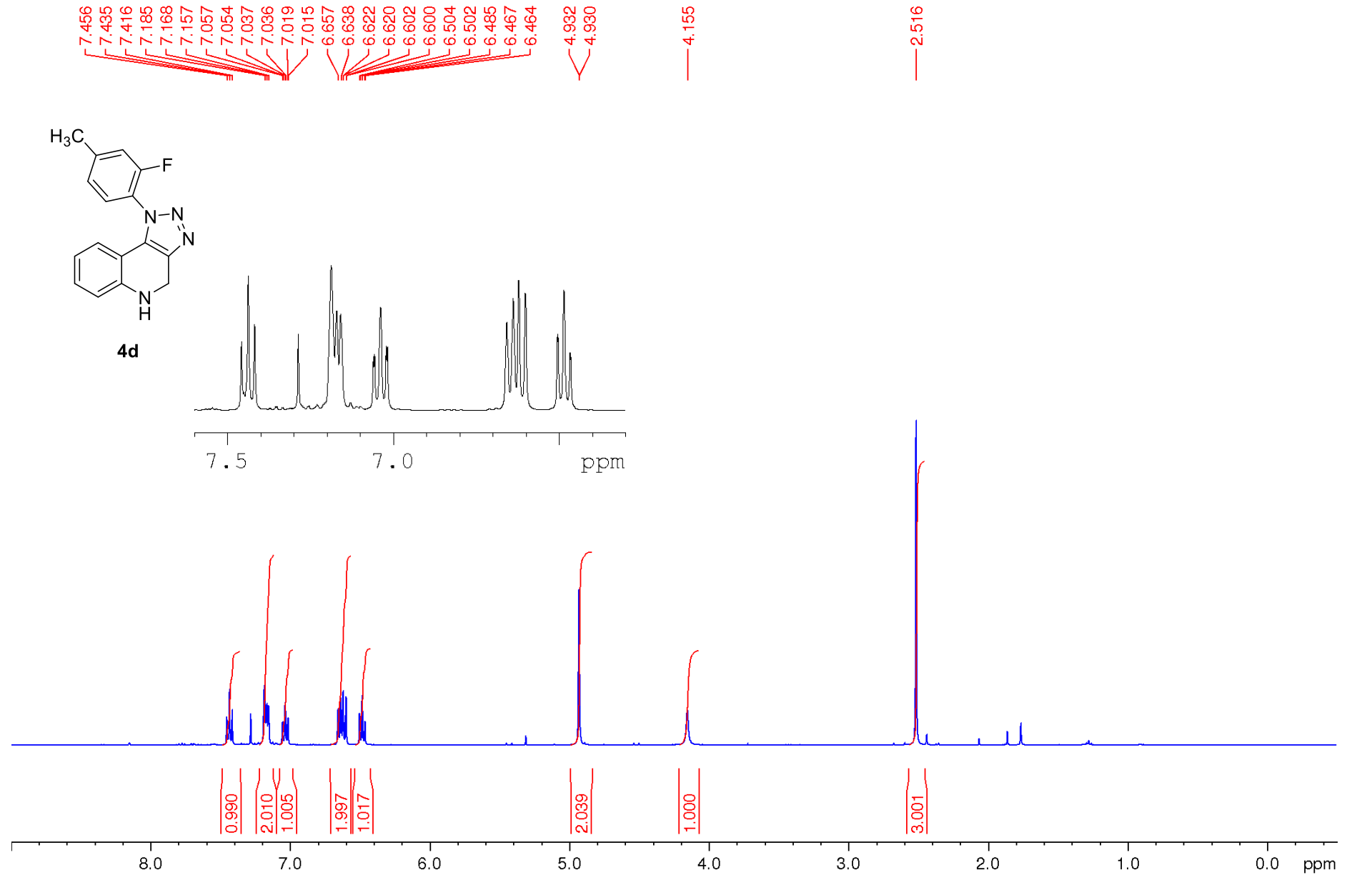
4c

DEPT 135 NMR-spectrum ($CDCl_3$)

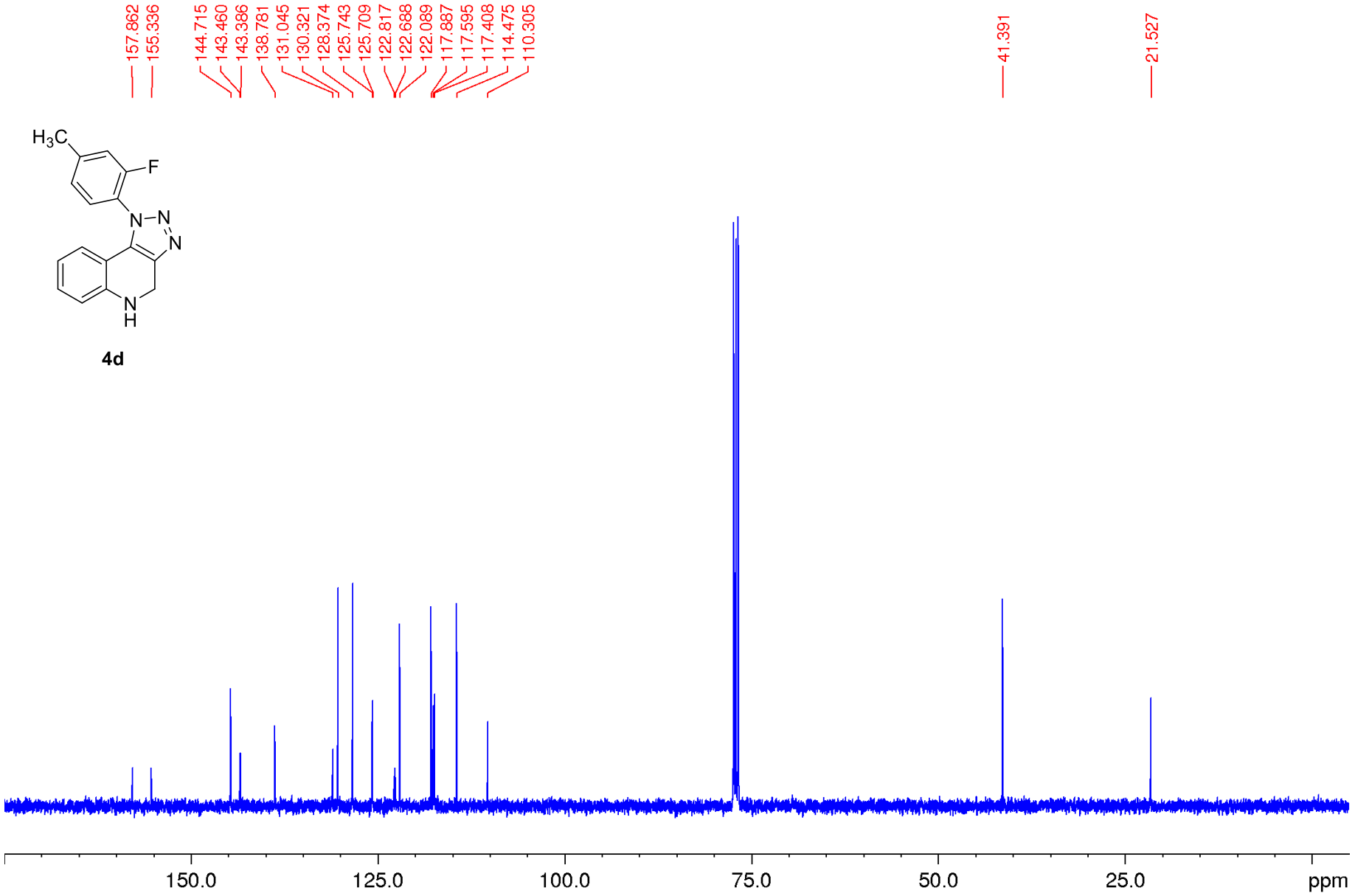


4c

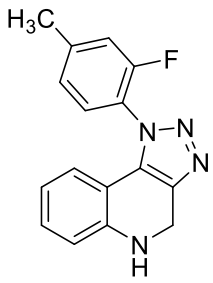
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



^{13}C NMR-spectrum (100 MHz, $CDCl_3$)

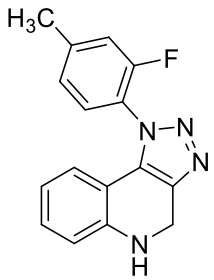


DEPT 135 NMR-spectrum ($CDCl_3$)



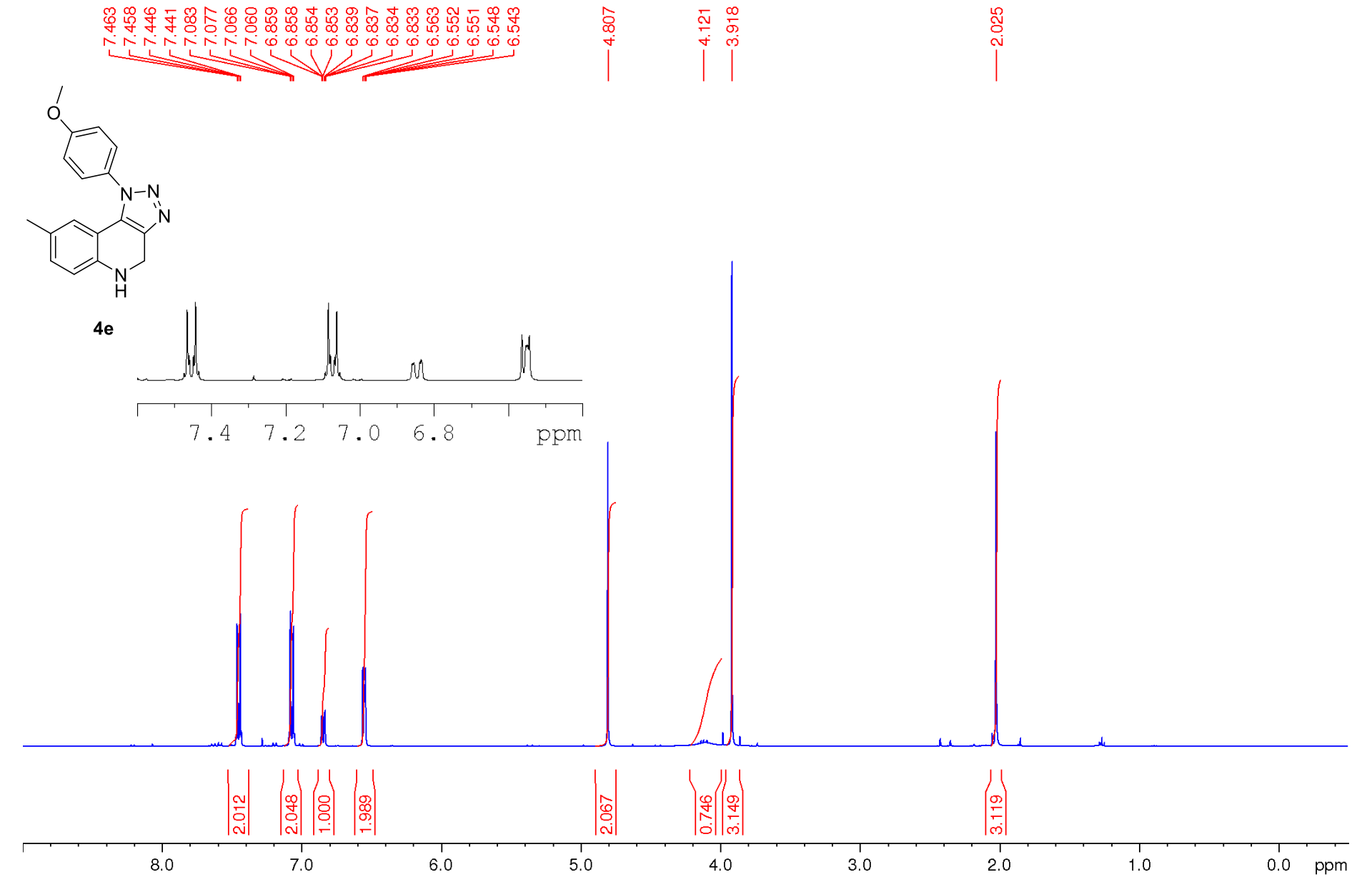
4d

^{19}F NMR-spectrum (376.5 Hz, $CDCl_3$)

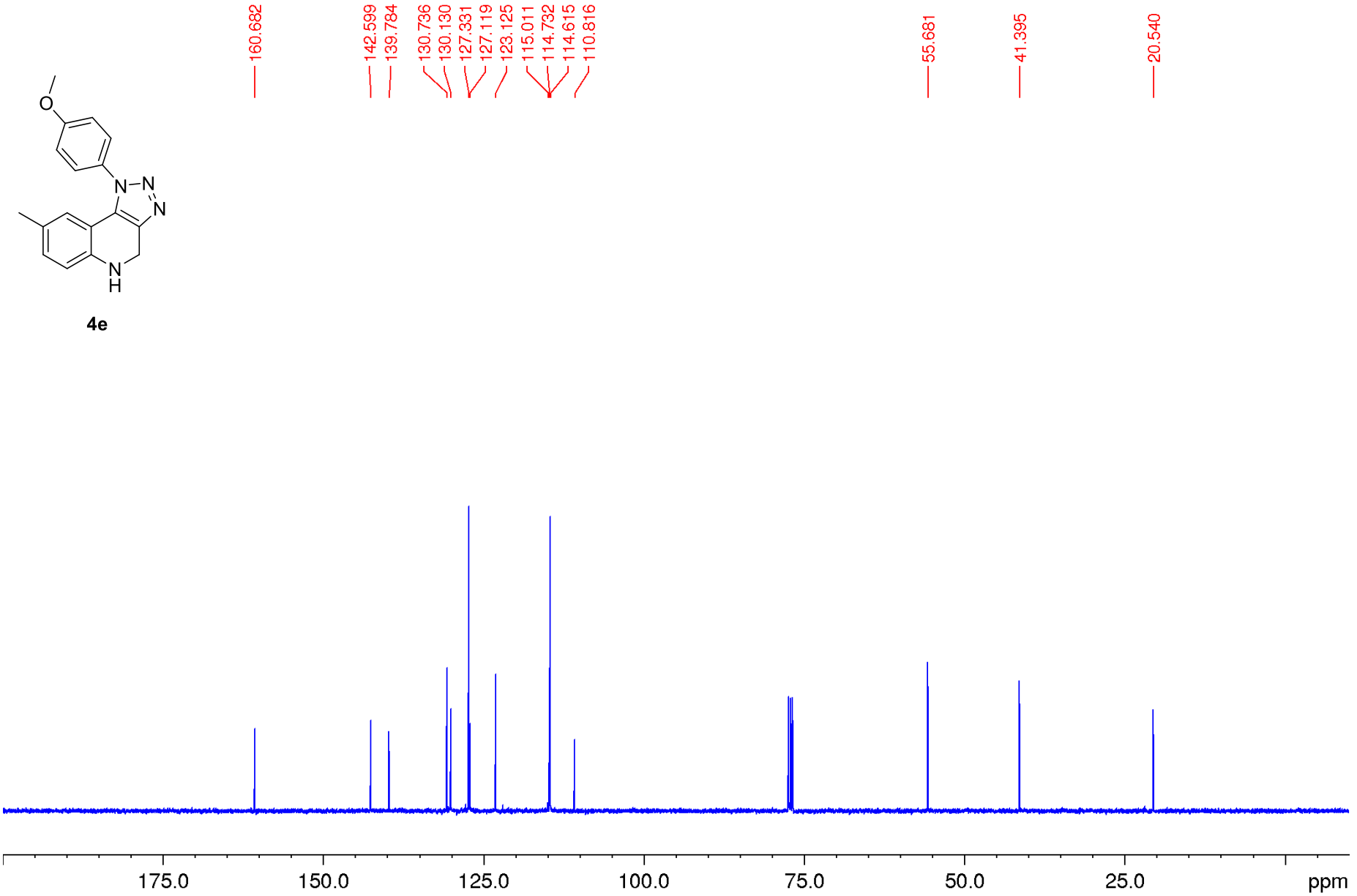


4d

^{1}H NMR-spectrum (400 MHz, $CDCl_3$)

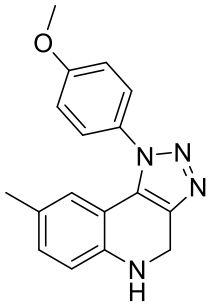


^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



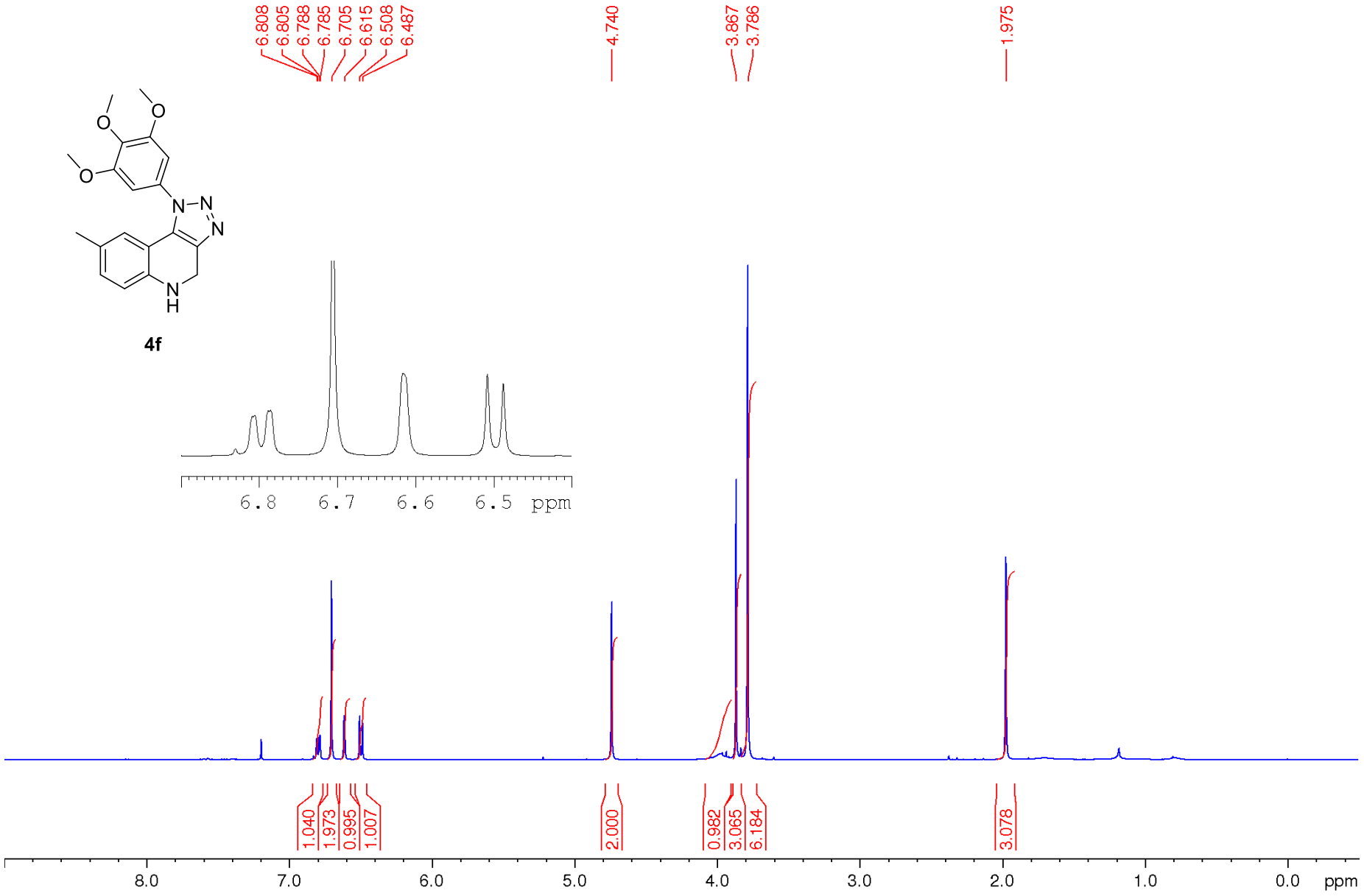
4e

DEPT 135 NMR-spectrum ($CDCl_3$)

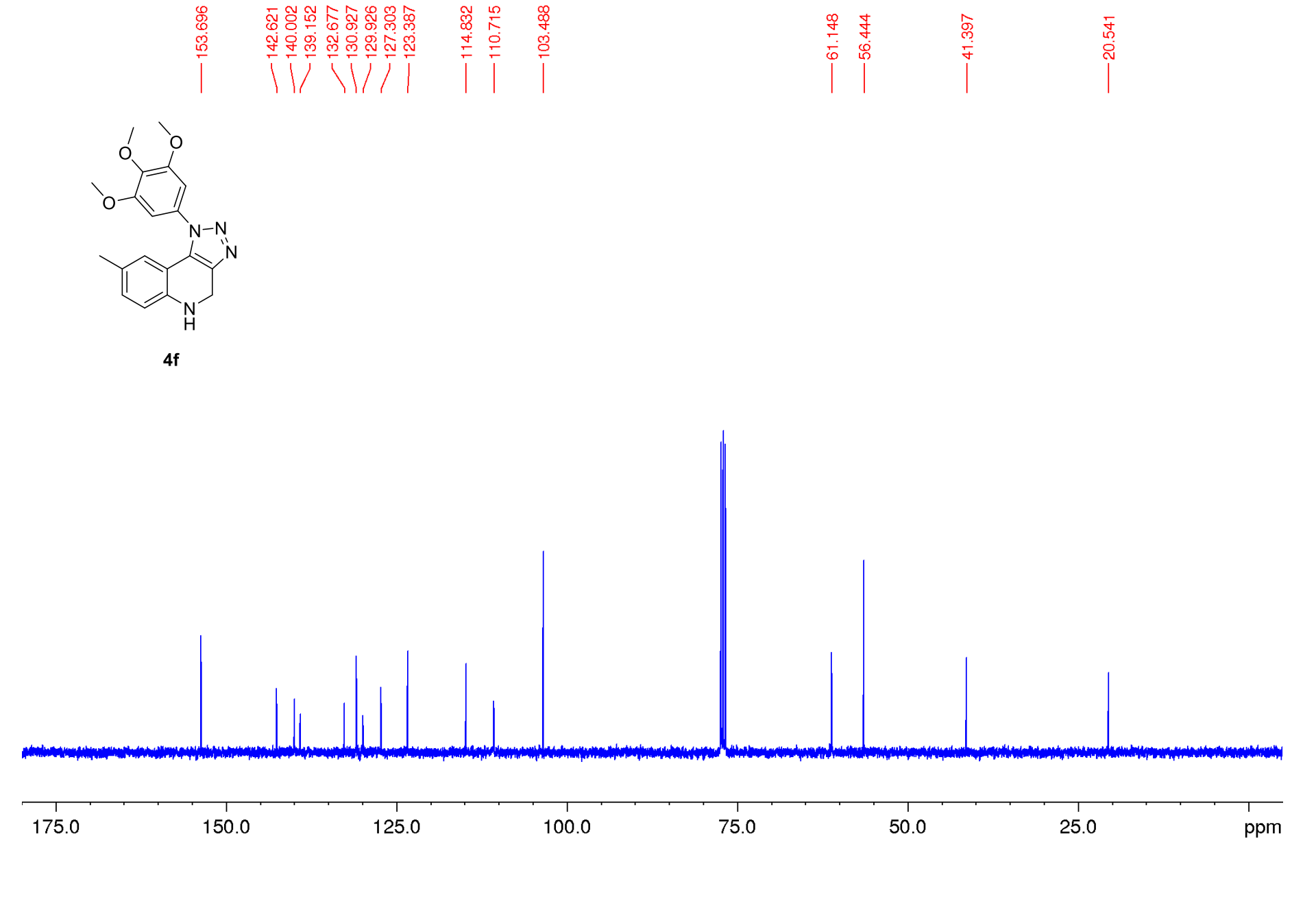


4e

^{1}H NMR-spectrum (400 MHz, $CDCl_3$)

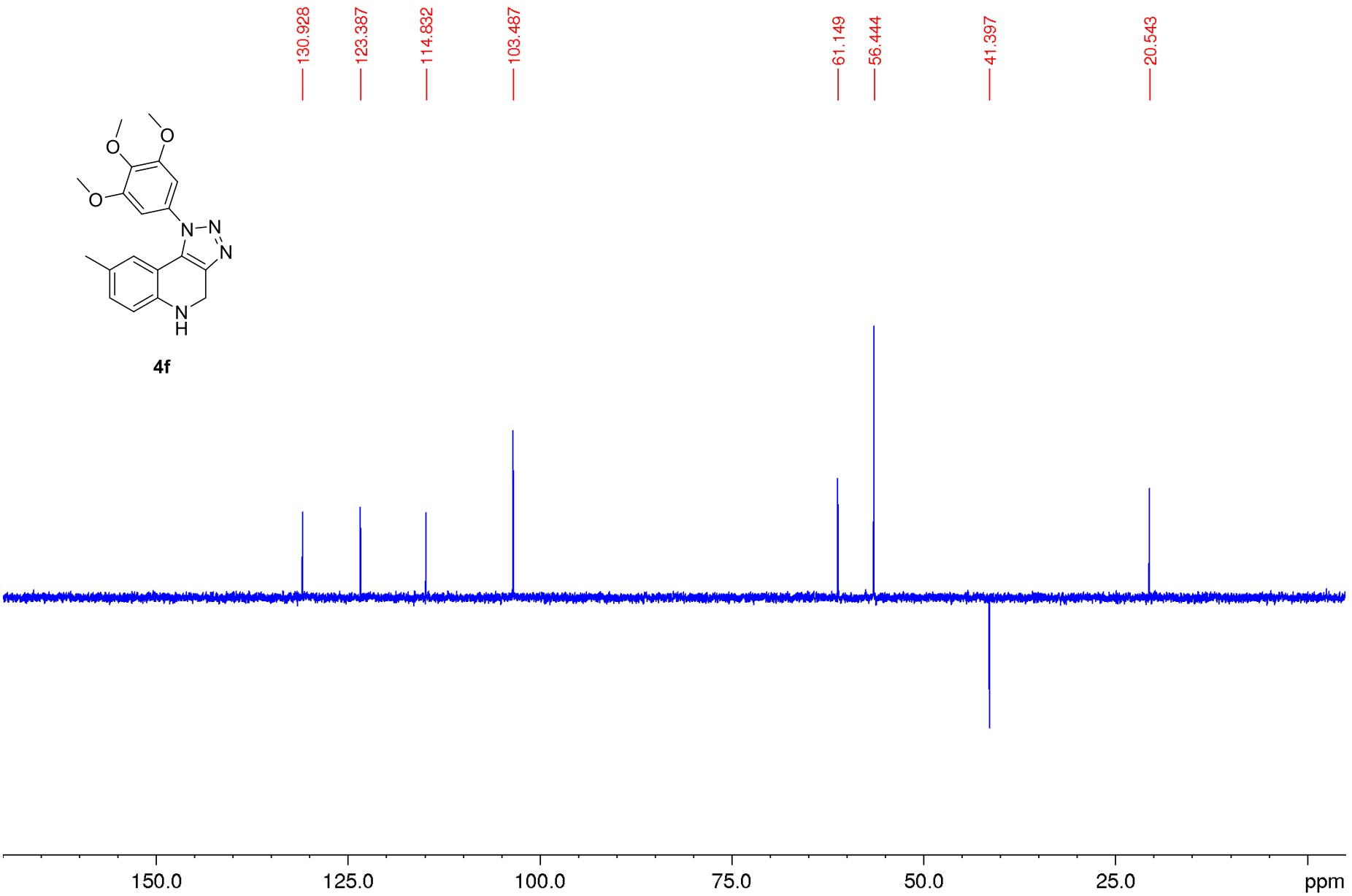


^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



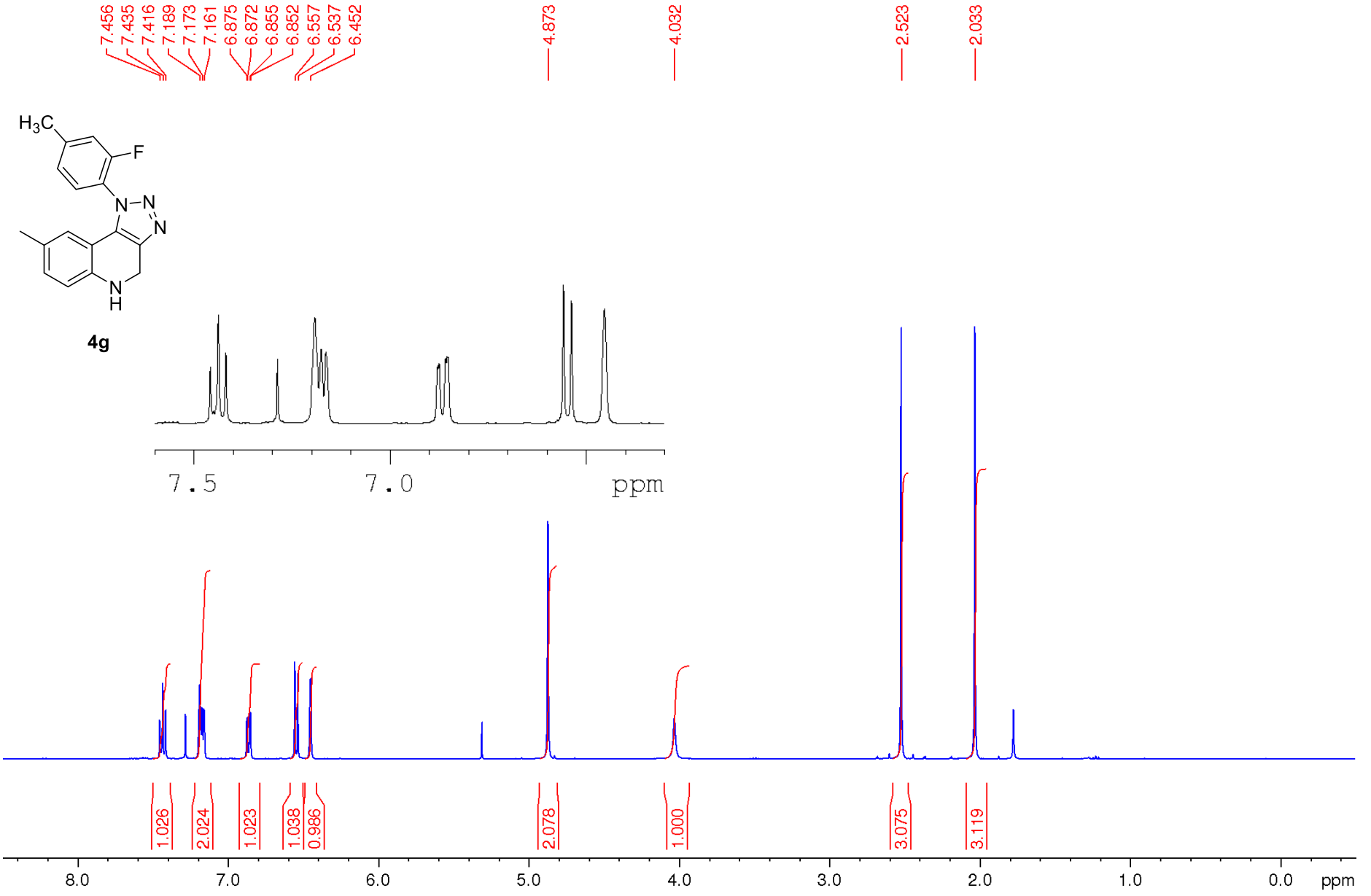
4f

DEPT 135 NMR-spectrum ($CDCl_3$)

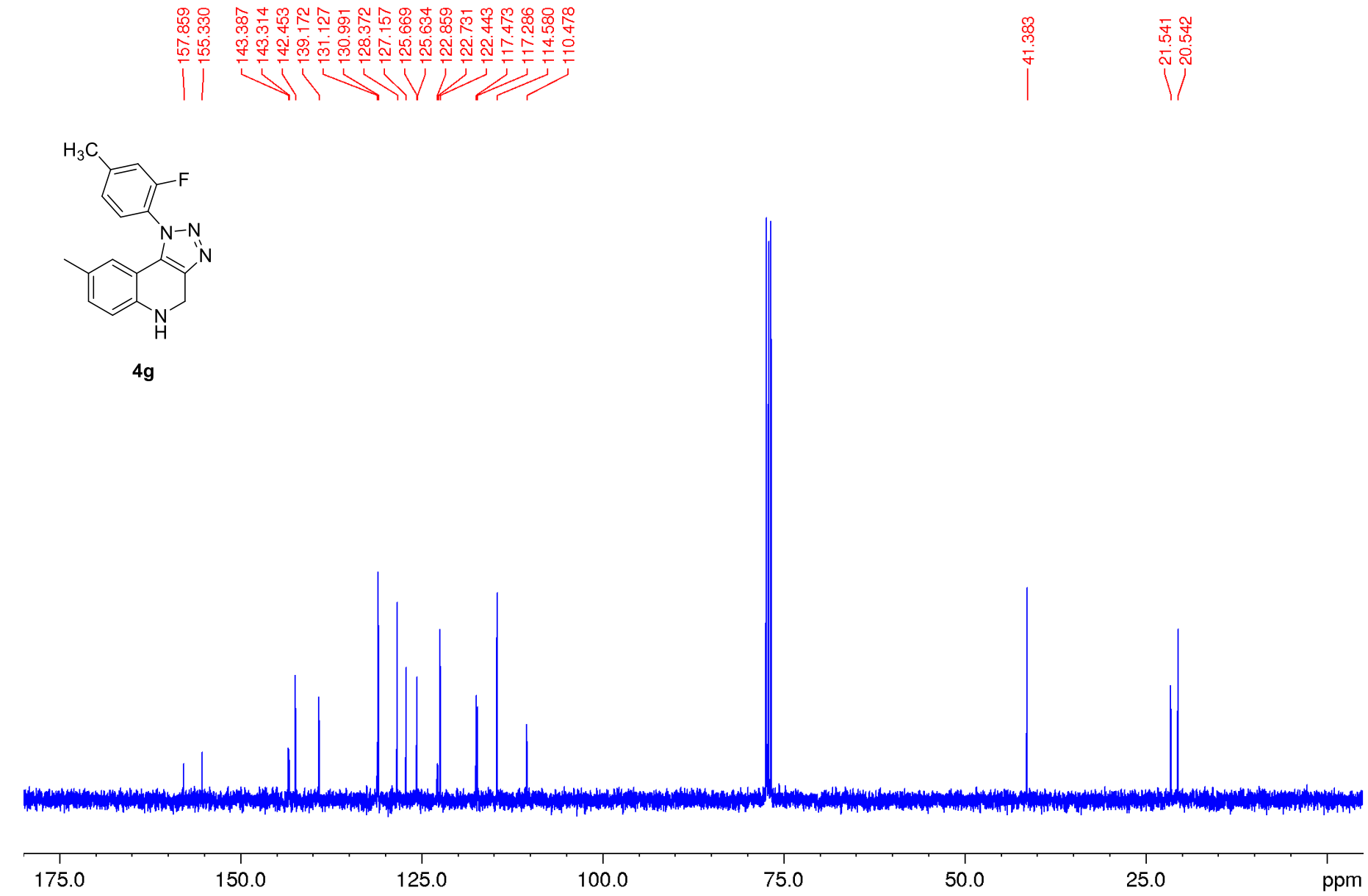


4f

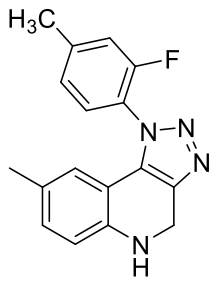
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



^{13}C NMR-spectrum (100 MHz, $CDCl_3$)

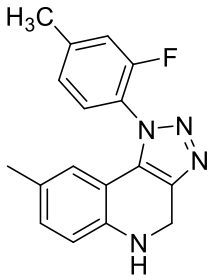


DEPT 135 NMR-spectrum ($CDCl_3$)



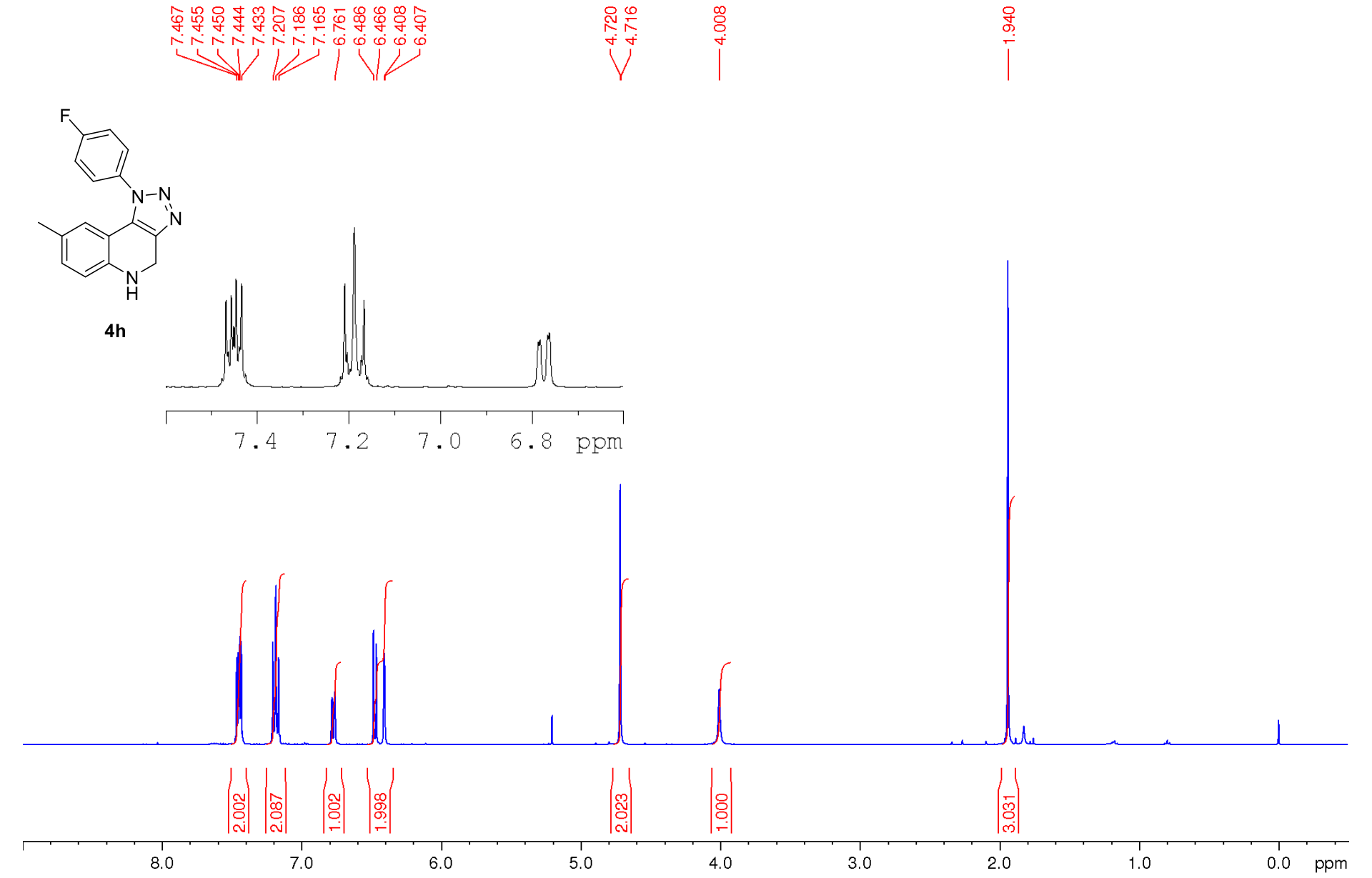
4g

^{19}F NMR-spectrum (376.5 Hz, $CDCl_3$)

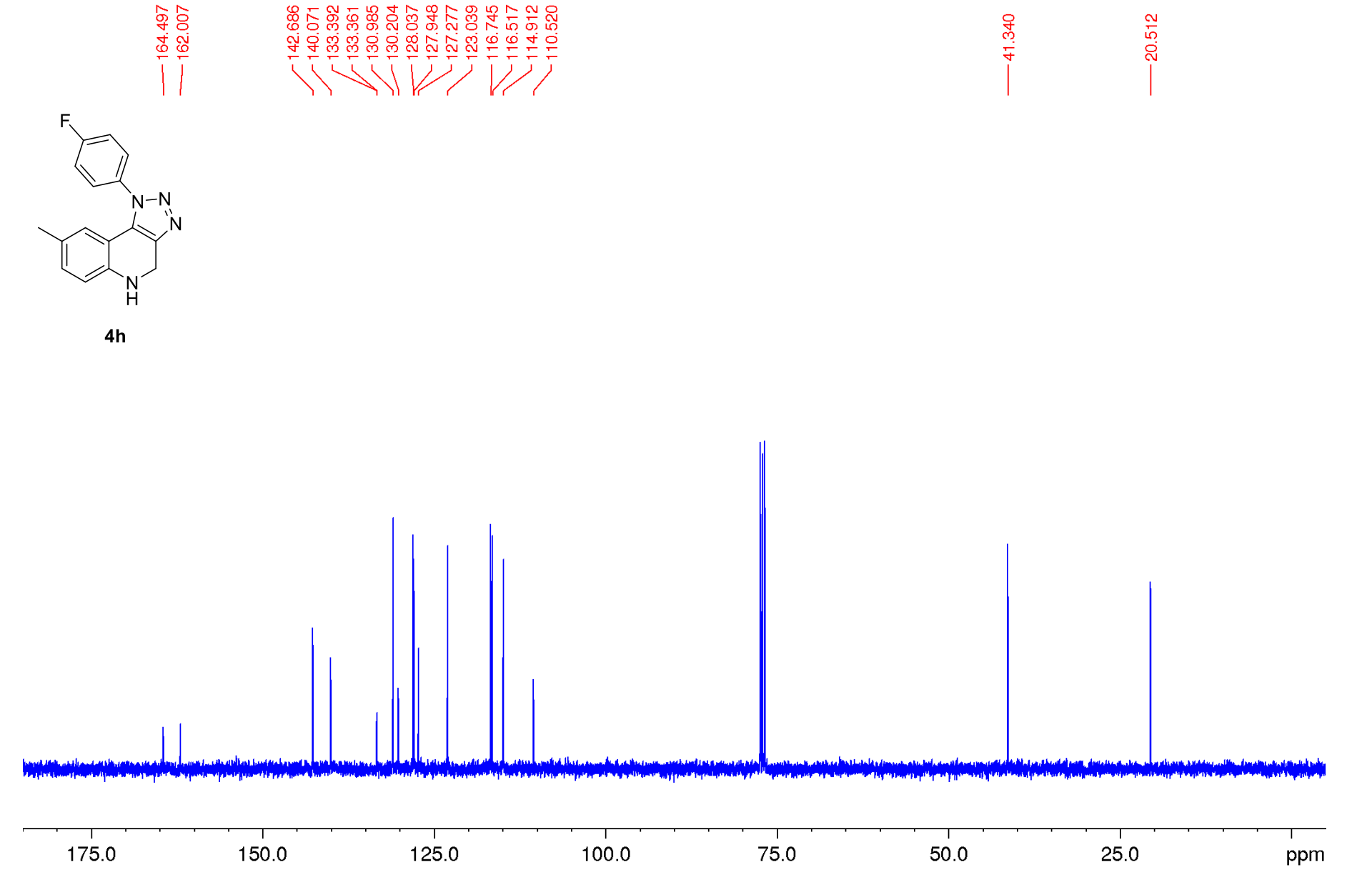


4g

^{1}H NMR-spectrum (400 MHz, $CDCl_3$)

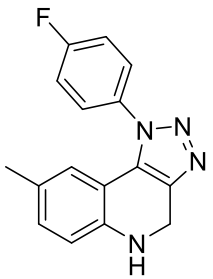


^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



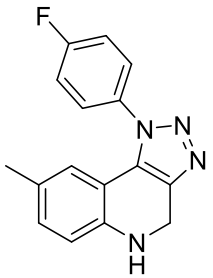
4h

DEPT 135 NMR-spectrum ($CDCl_3$)

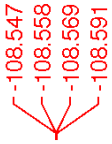


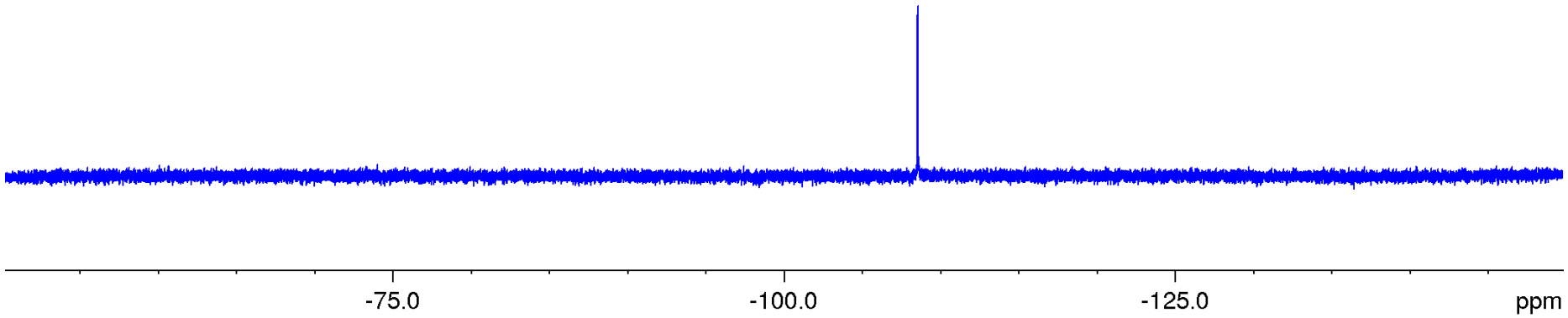
4h

^{19}F NMR-spectrum (376.5 Hz, $CDCl_3$)

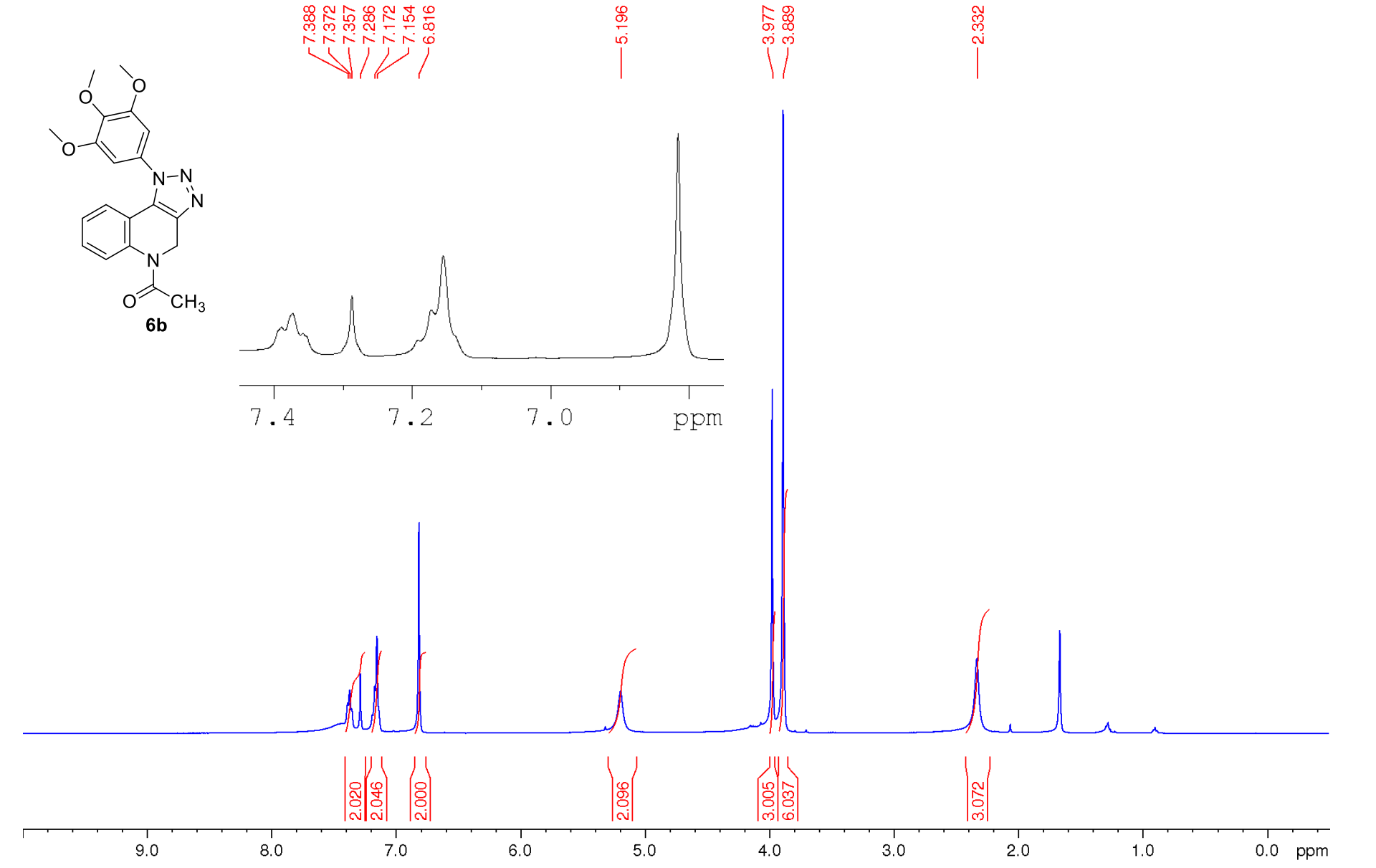


4h

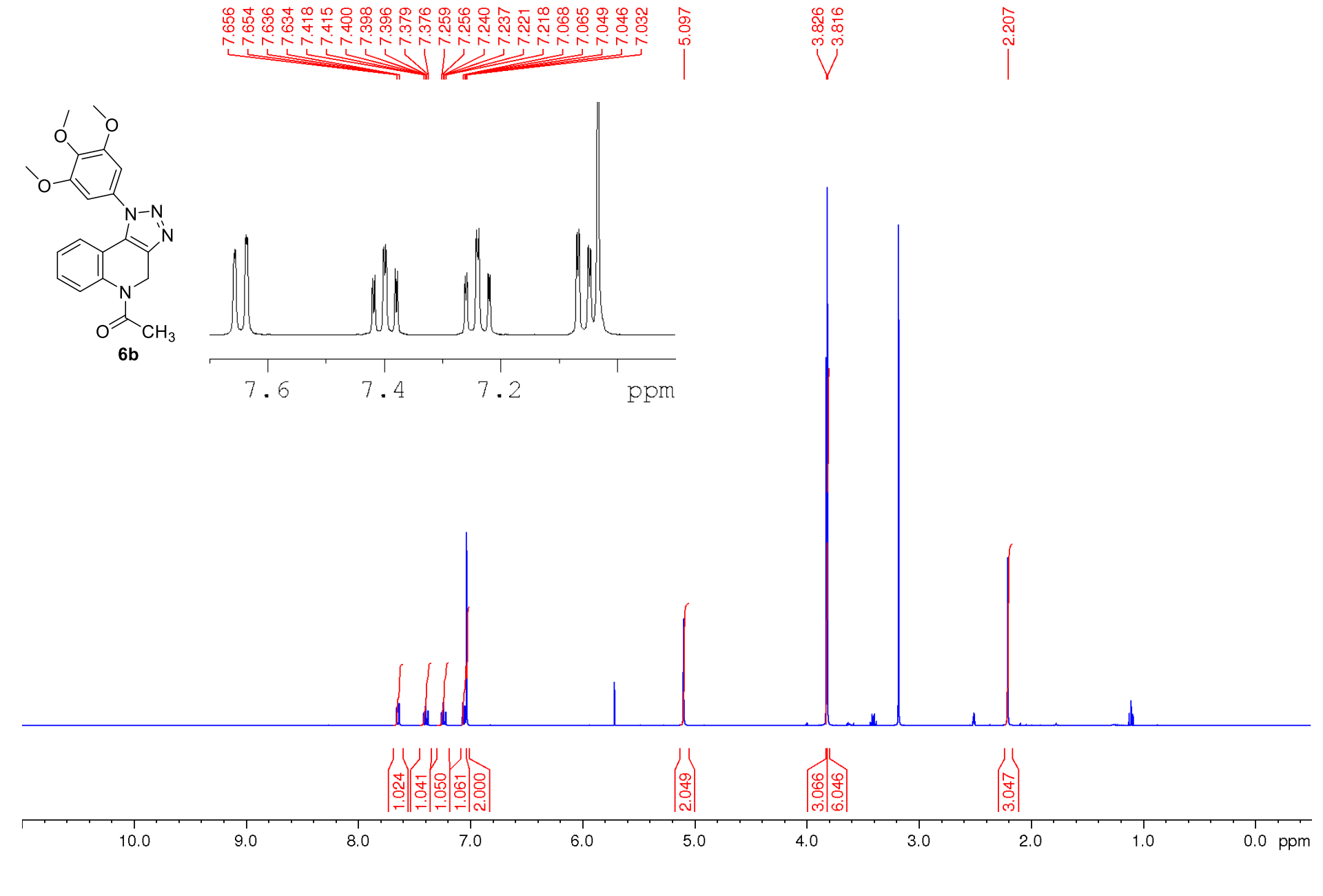




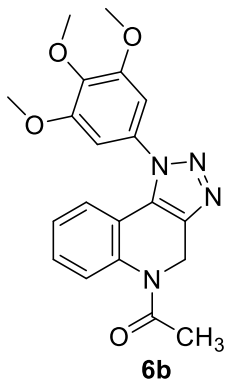
^{1}H NMR-spectrum at 25 ^{o}C(400 MHz, $CDCl_3$)



^{1}H NMR-spectrum at 60 ^{o}C(400 MHz, DMSO)



^{13}C NMR-spectrum, 10 thousands scanes (100 MHz, $CDCl_3$)

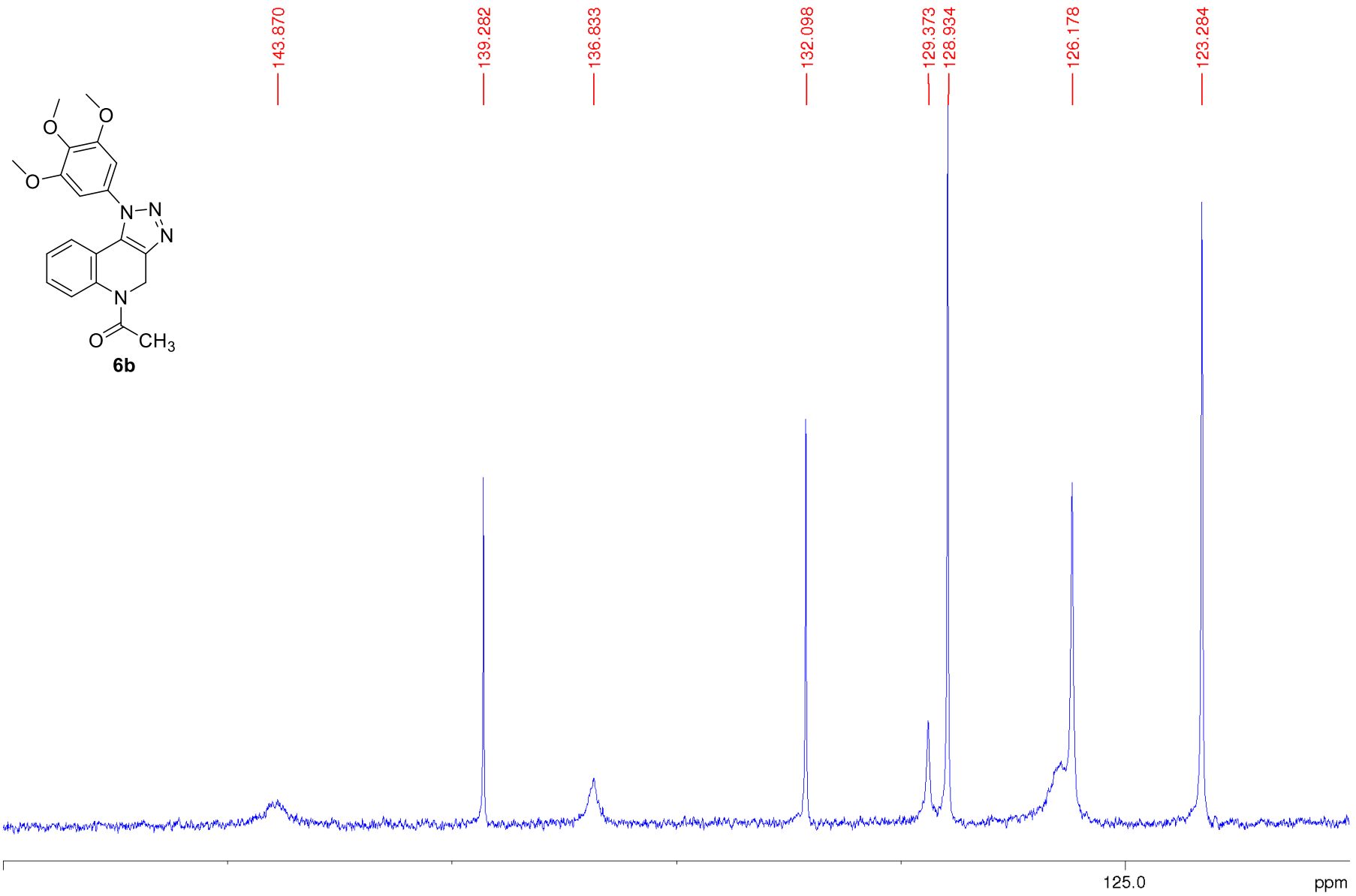


6b

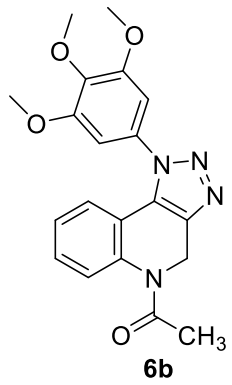
169.820
153.923
143.870
139.282
136.833
132.098
129.373
128.934
126.178
123.284
119.614
102.822
61.160
56.508
40.093
22.782

175.0 150.0 125.0 100.0 75.0 50.0 25.0 0.0 ppm

^{13}C NMR-spectrum, 10 thousand scanes (100 MHz, $CDCl_3$)

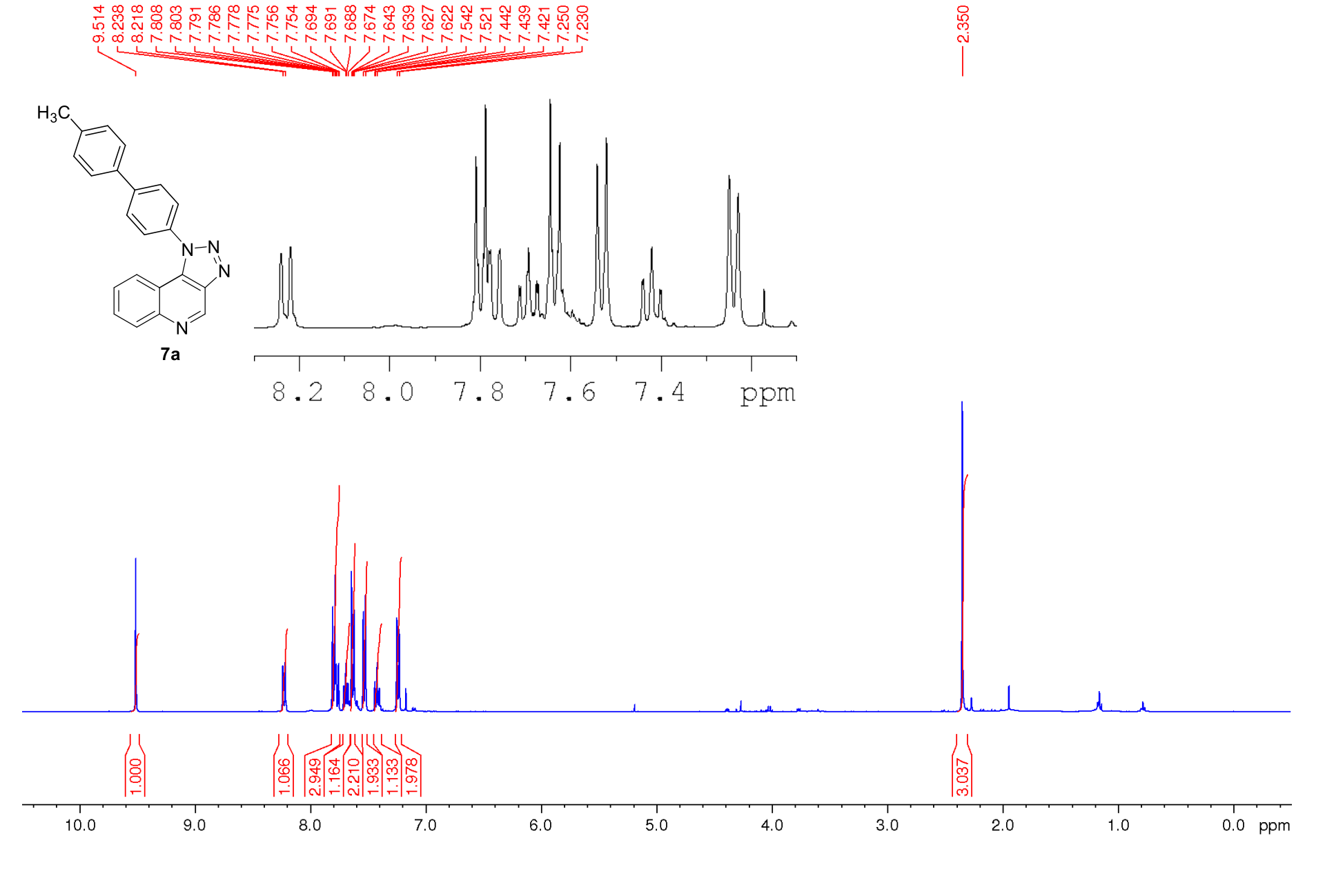


DEPT 135 NMR-spectrum ($CDCl_3$)

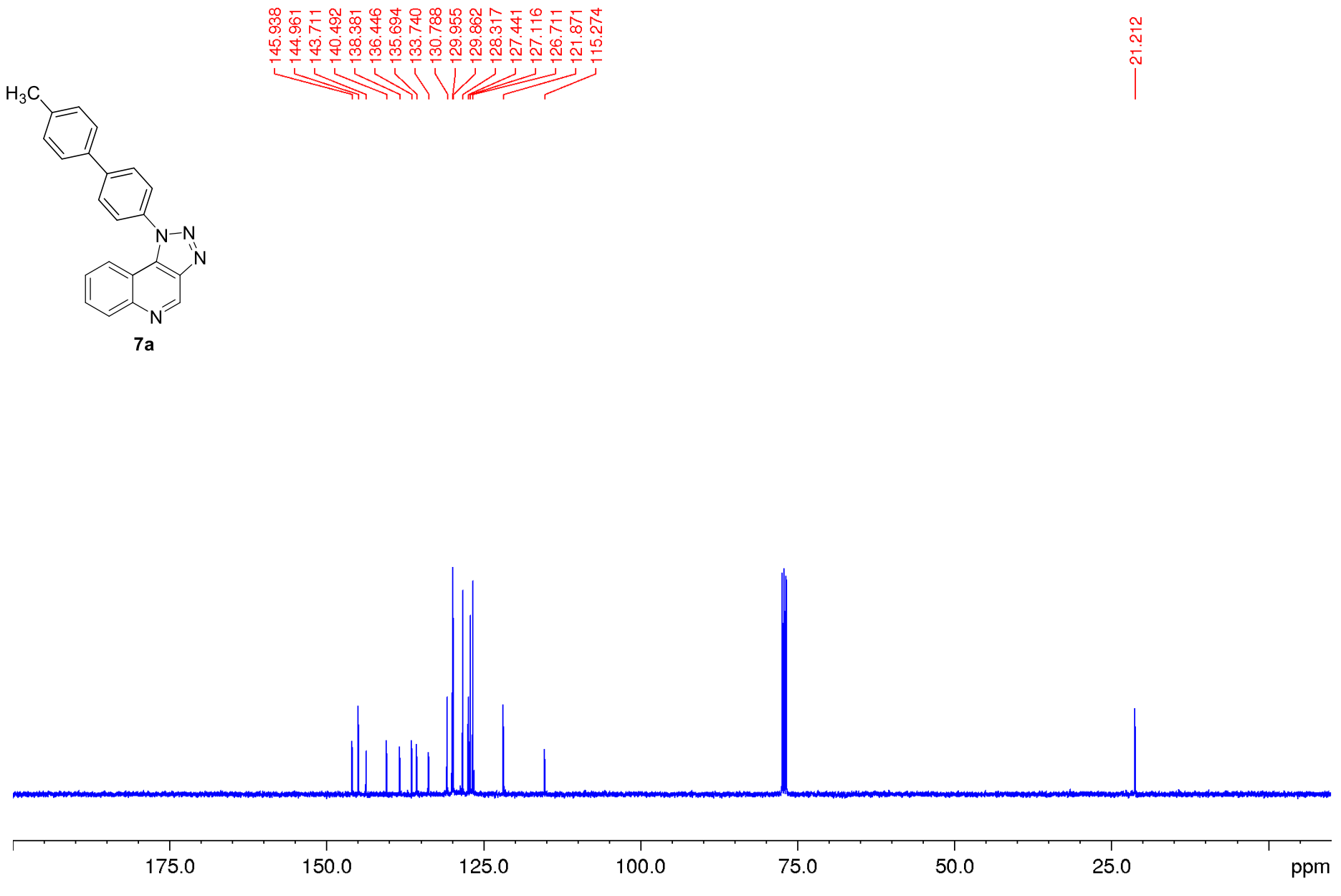


6b

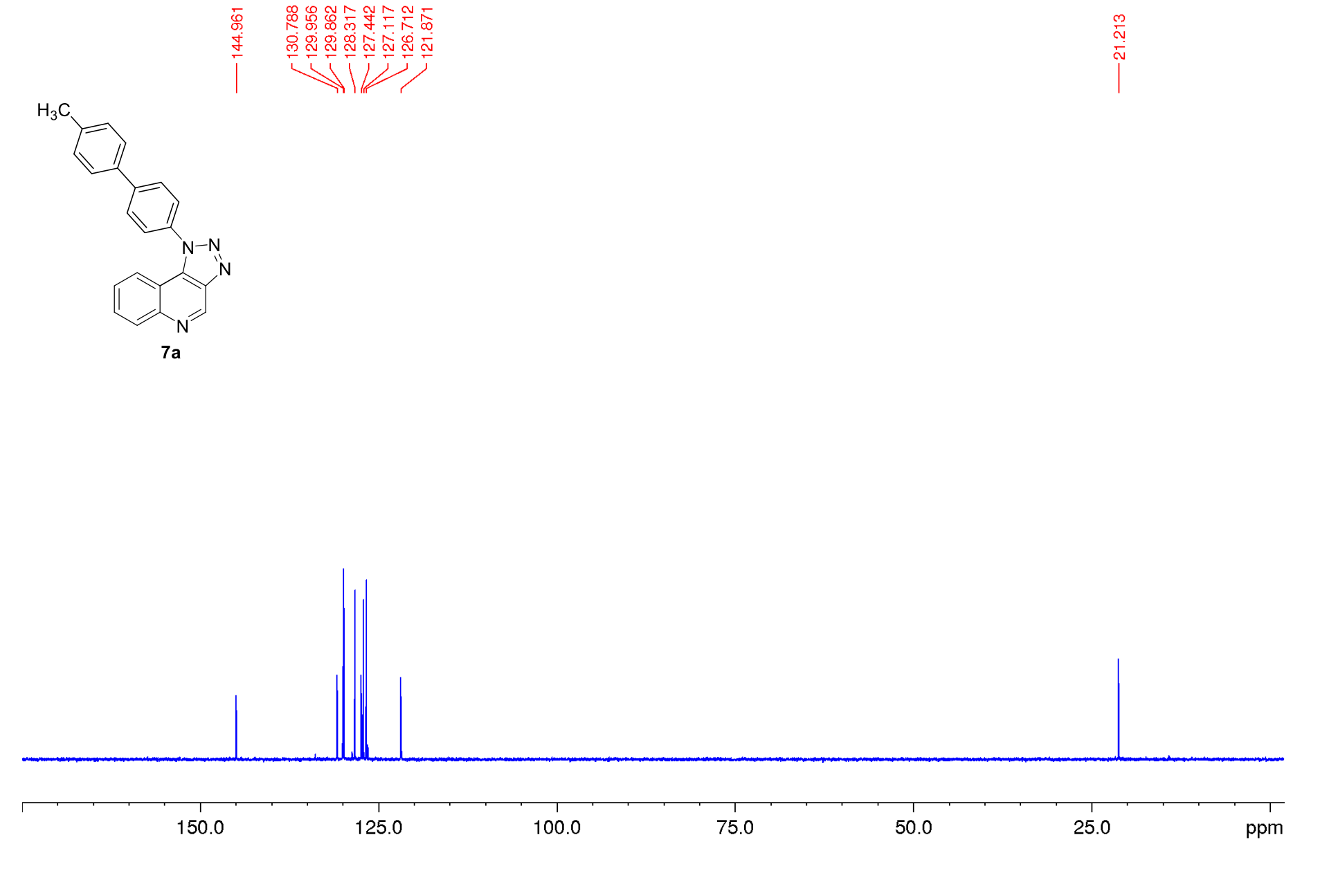
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



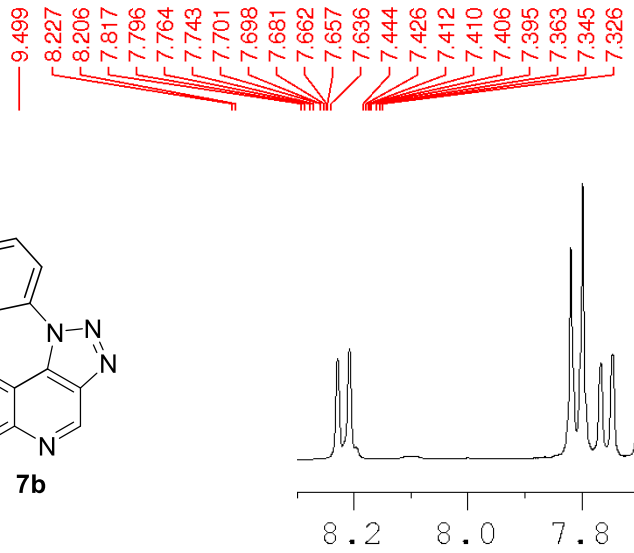
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)

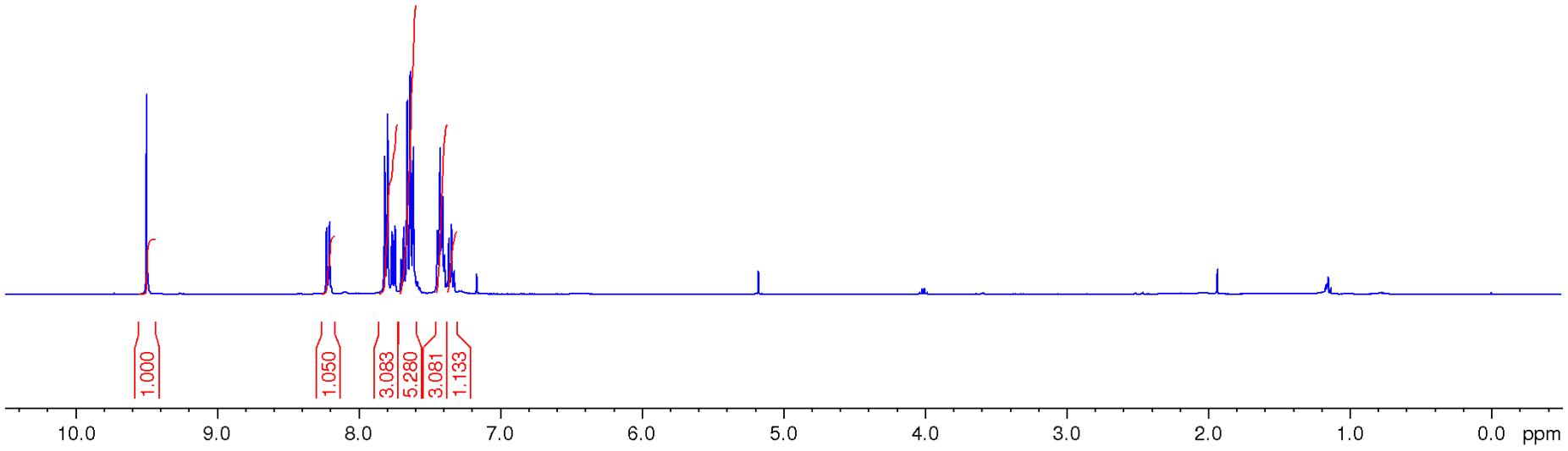


DEPT 135 NMR-spectrum ($CDCl_3$)

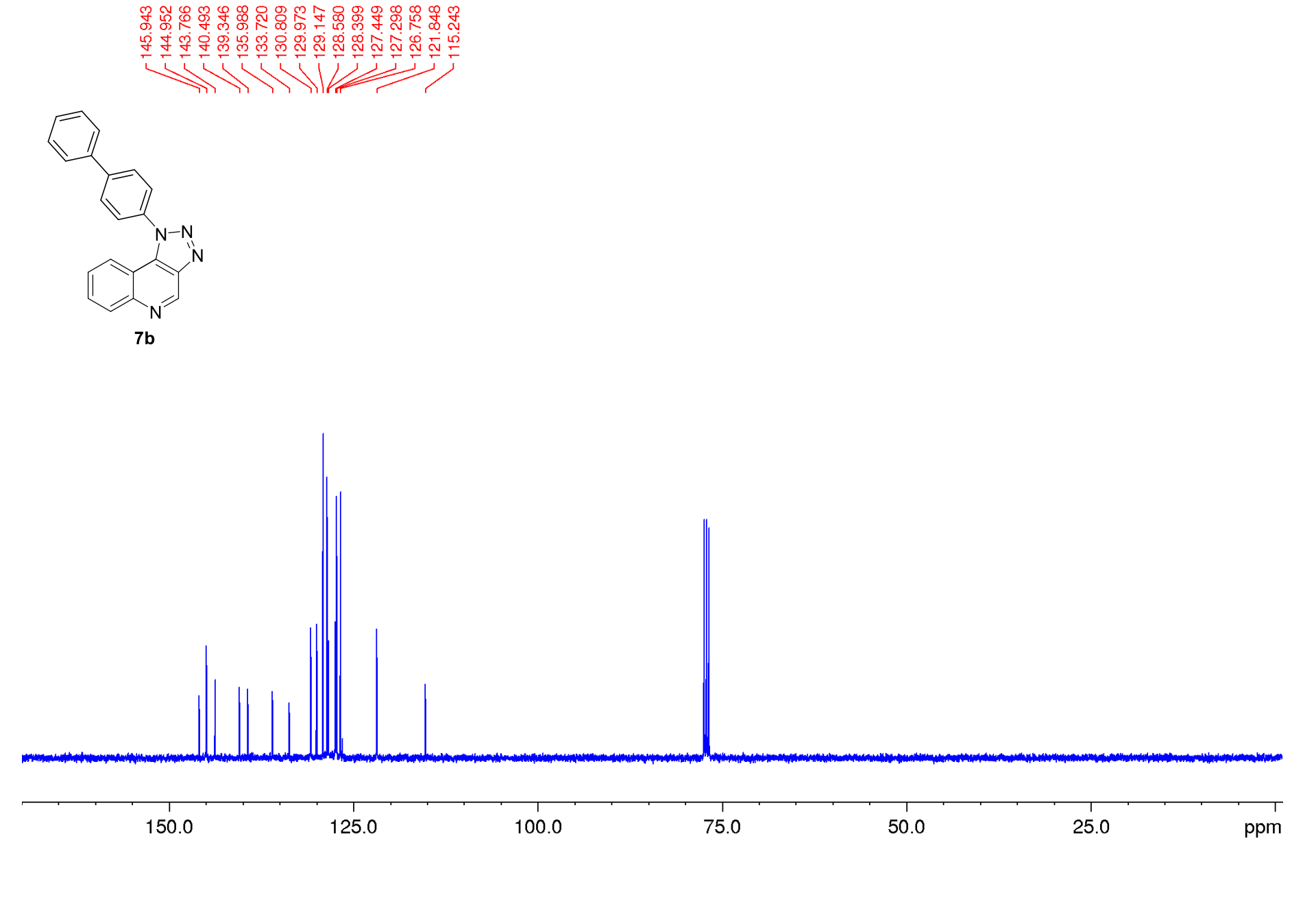


^{1}H NMR-spectrum (400 MHz, $CDCl_3$)

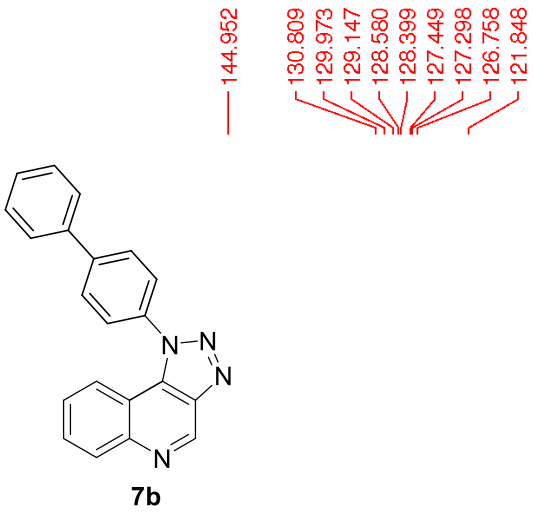




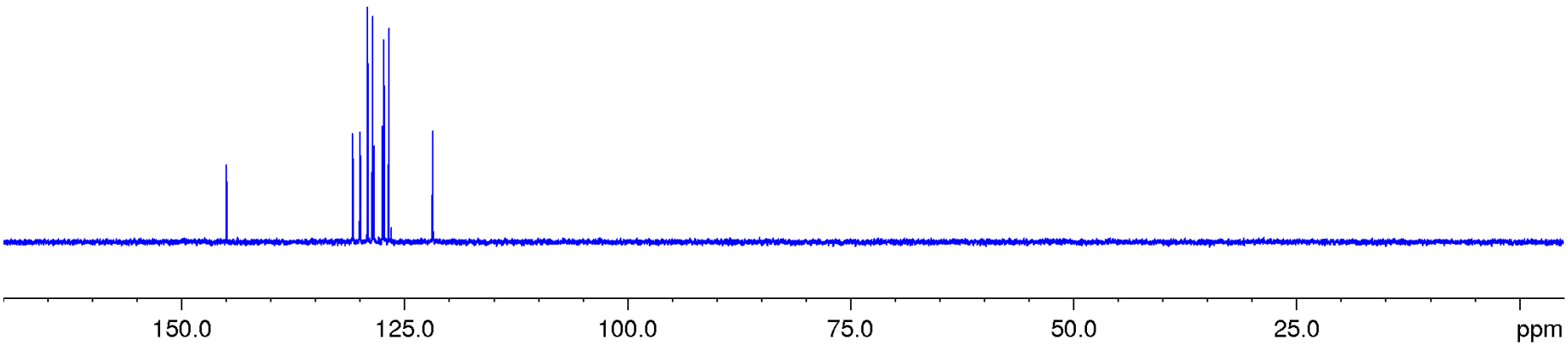
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



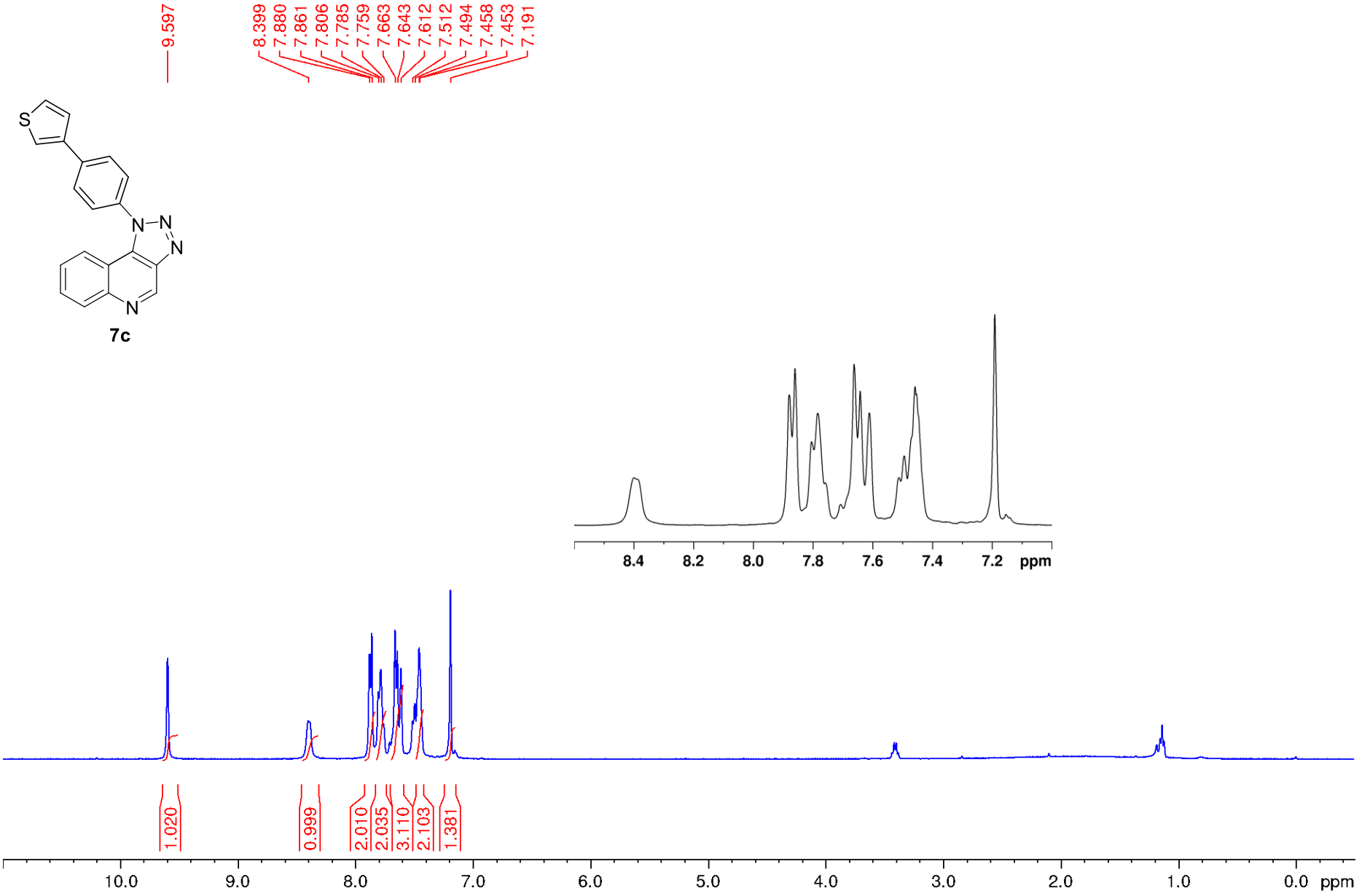
DEPT 135 NMR-spectrum ($CDCl_3$)



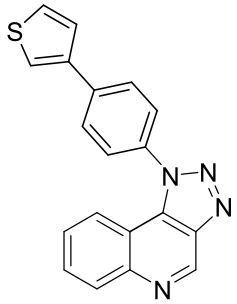
7b



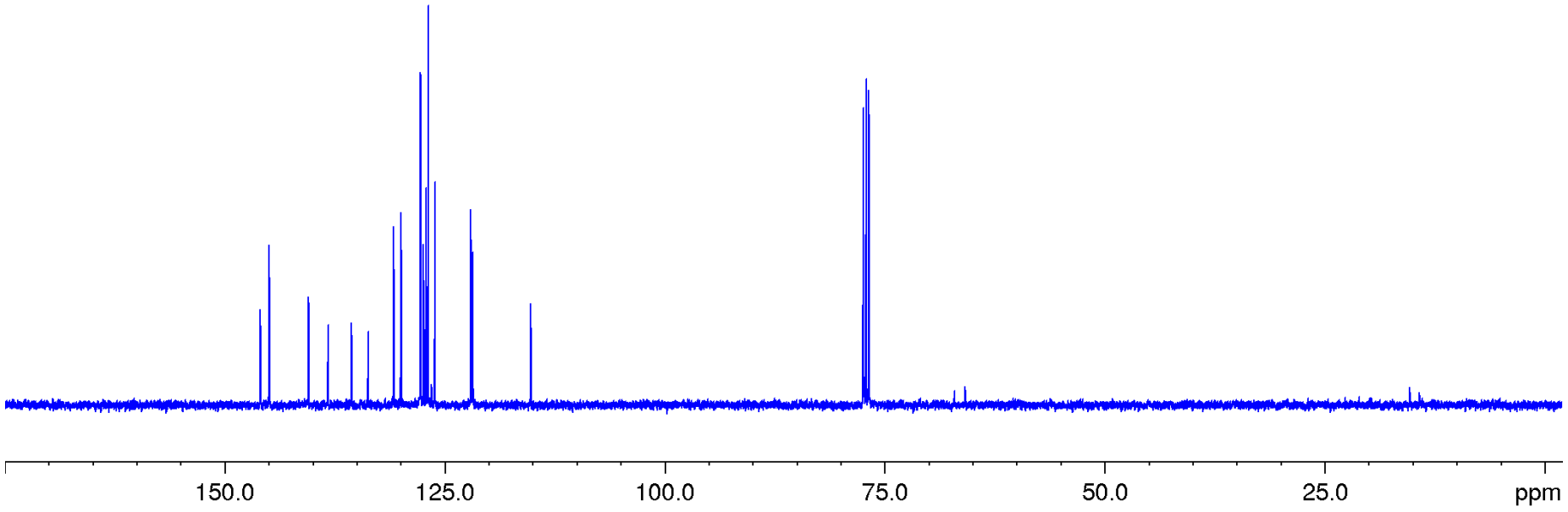
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



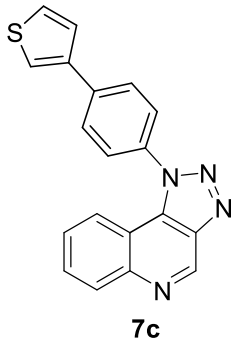
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



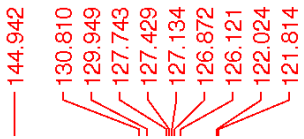
7c

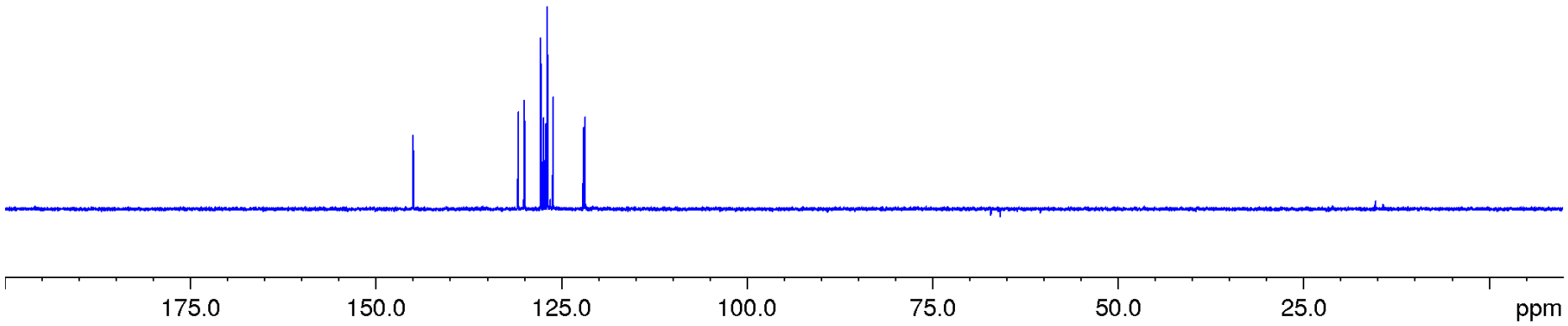


DEPT 135 NMR-spectrum ($CDCl_3$)

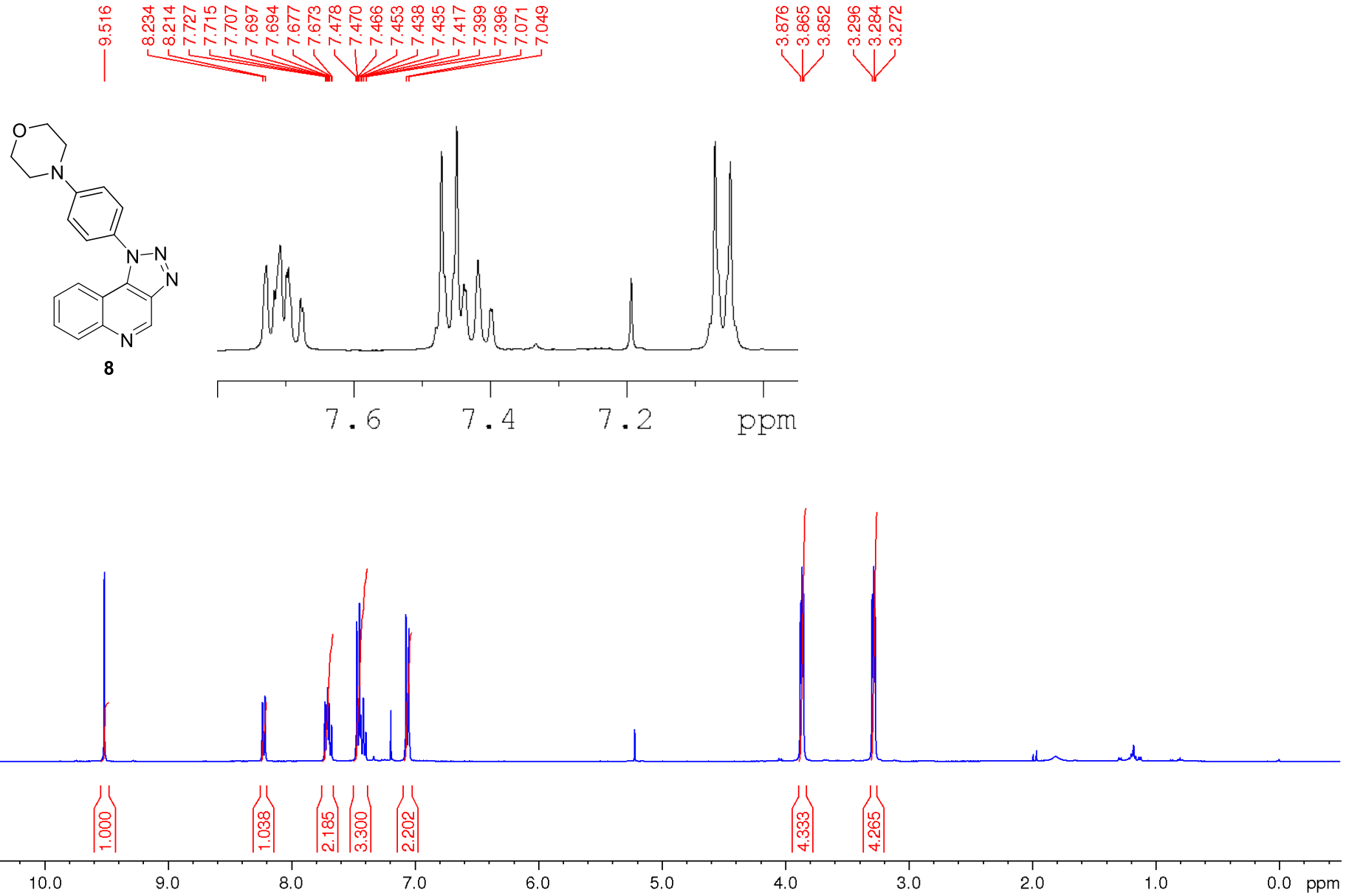


7c

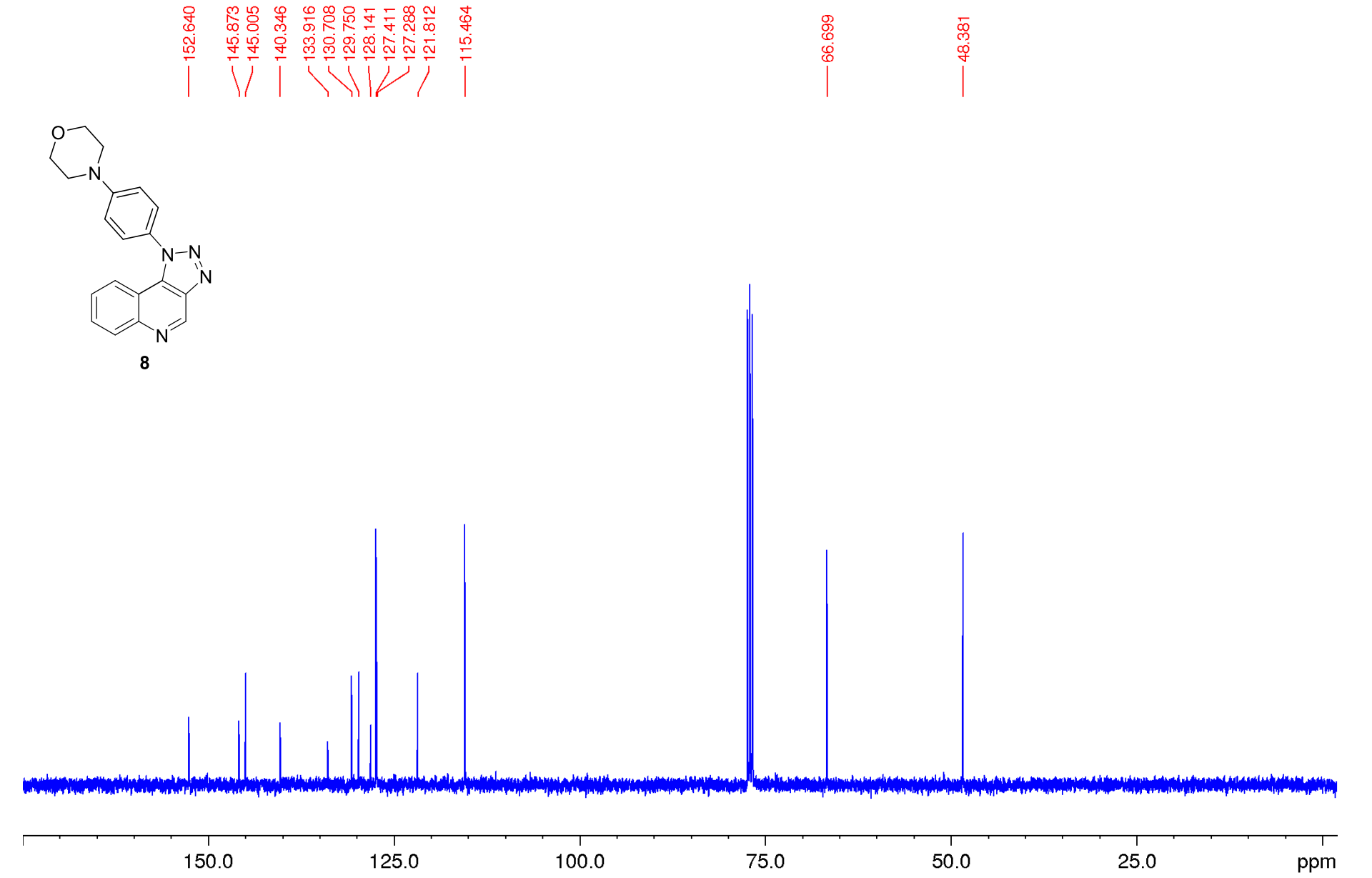




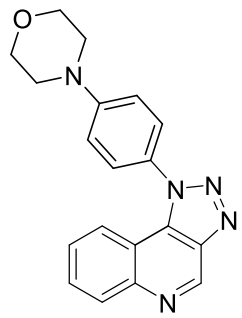
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



^{13}C NMR-spectrum (100 MHz, $CDCl_3$)

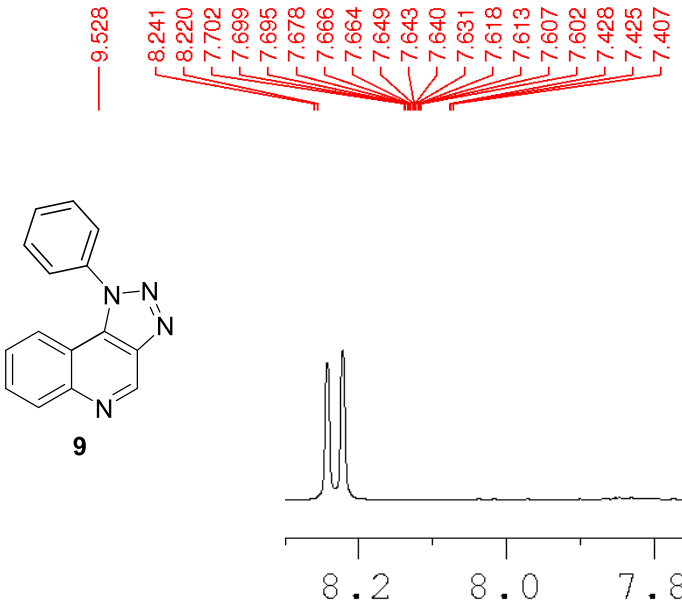


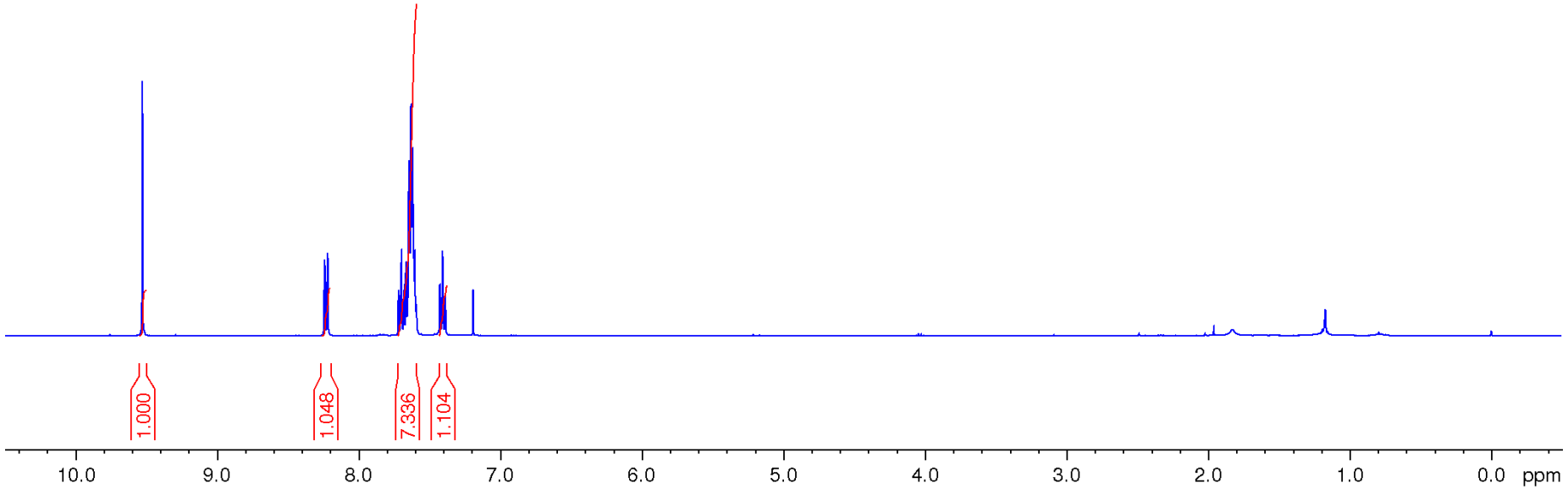
DEPT 135 NMR-spectrum ($CDCl_3$)



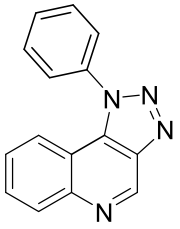
8

^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



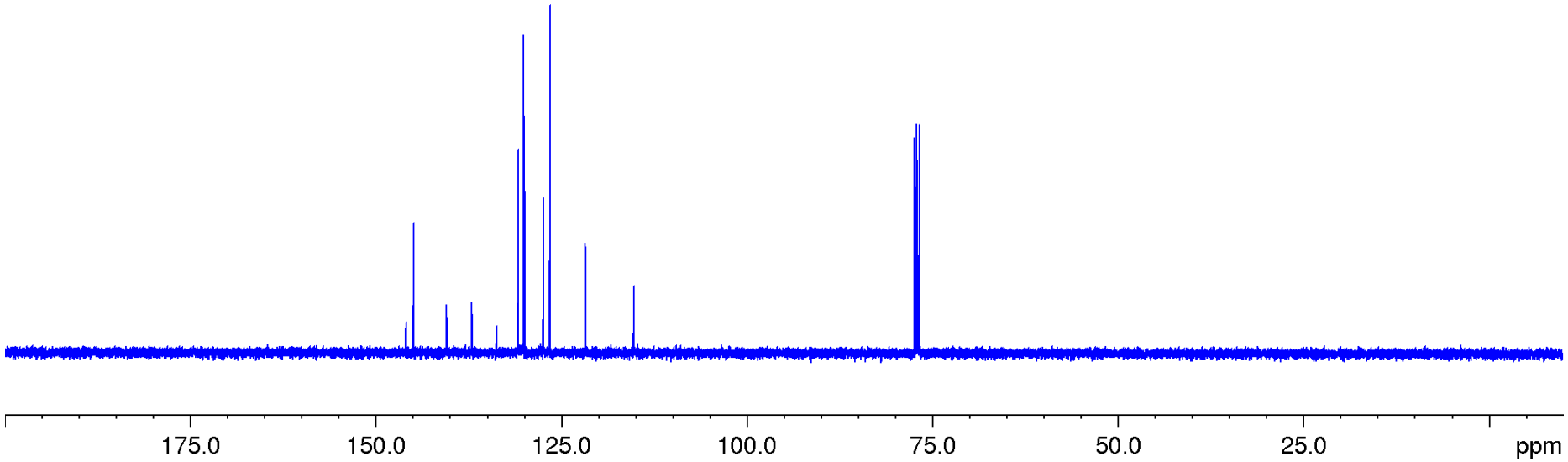


^{13}C NMR-spectrum (100 MHz, $CDCl_3$)

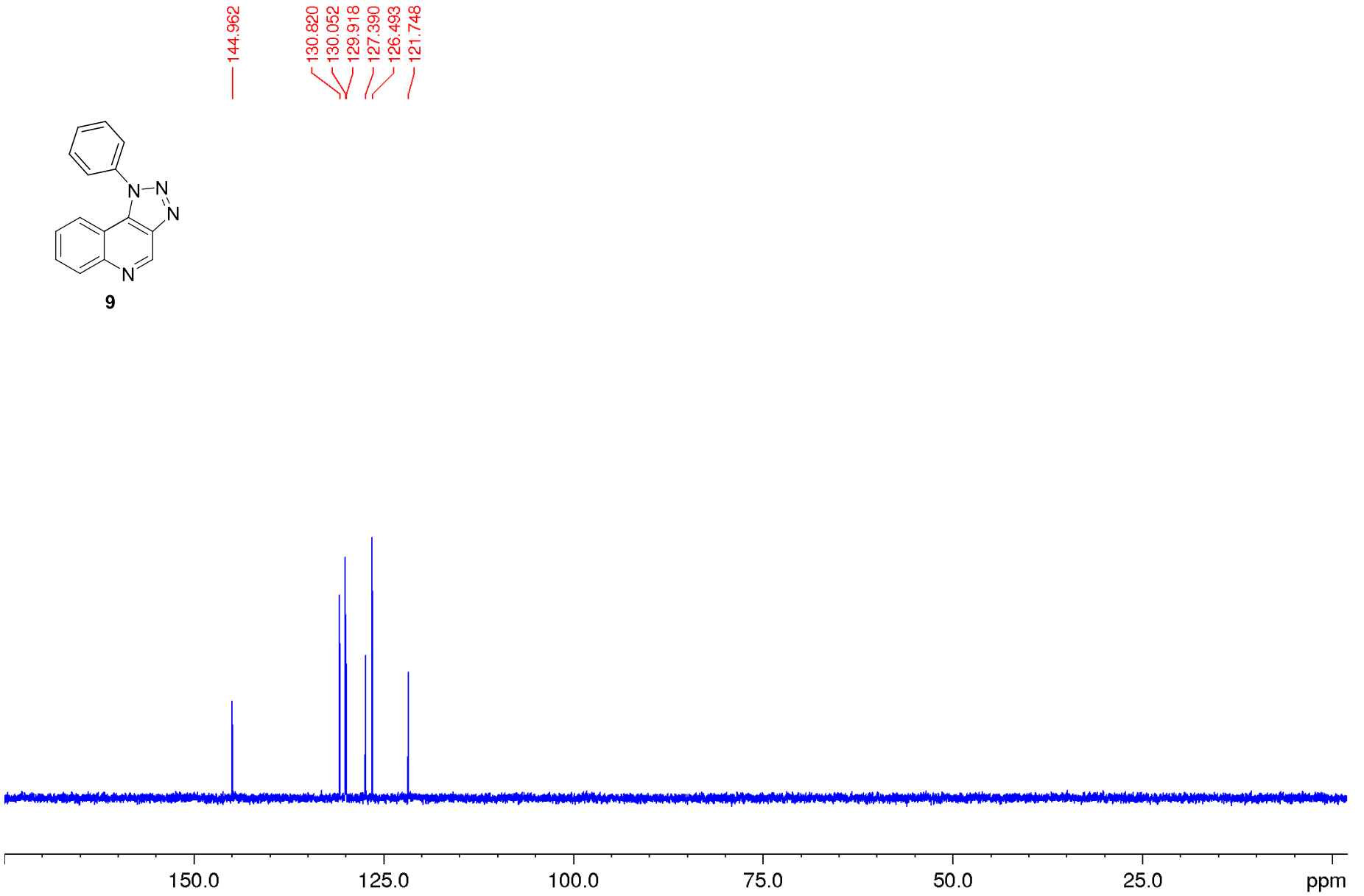


9

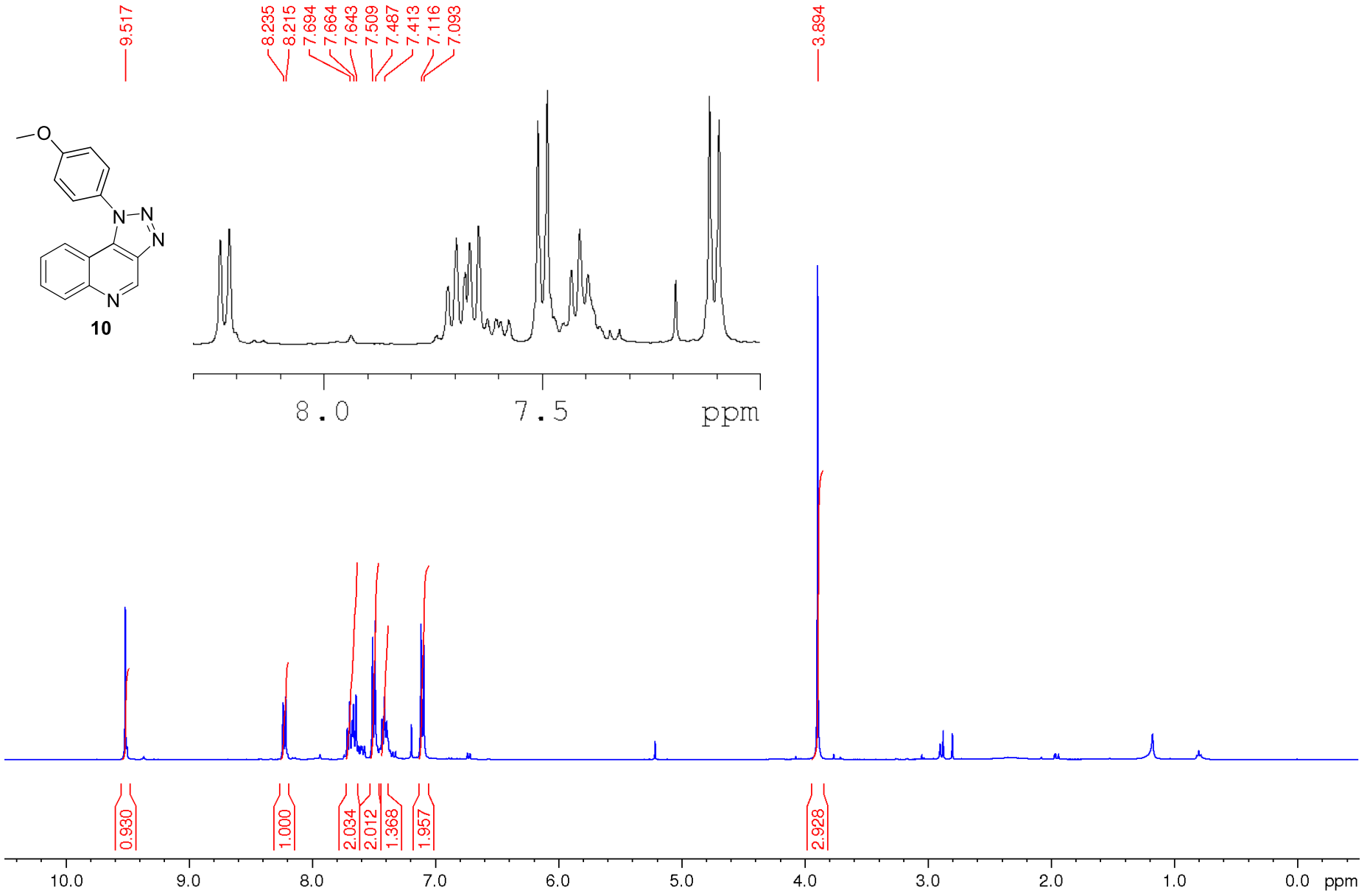
145.934
144.933
140.448
137.053
130.818
130.796
130.050
129.942
129.909
127.384
126.484
121.743
115.208



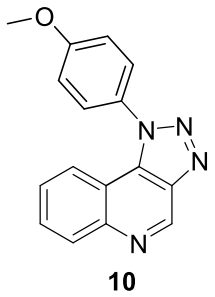
DEPT 135 NMR-spectrum ($CDCl_3$)



^{1}H NMR-spectrum (400 MHz, $CDCl_3$)

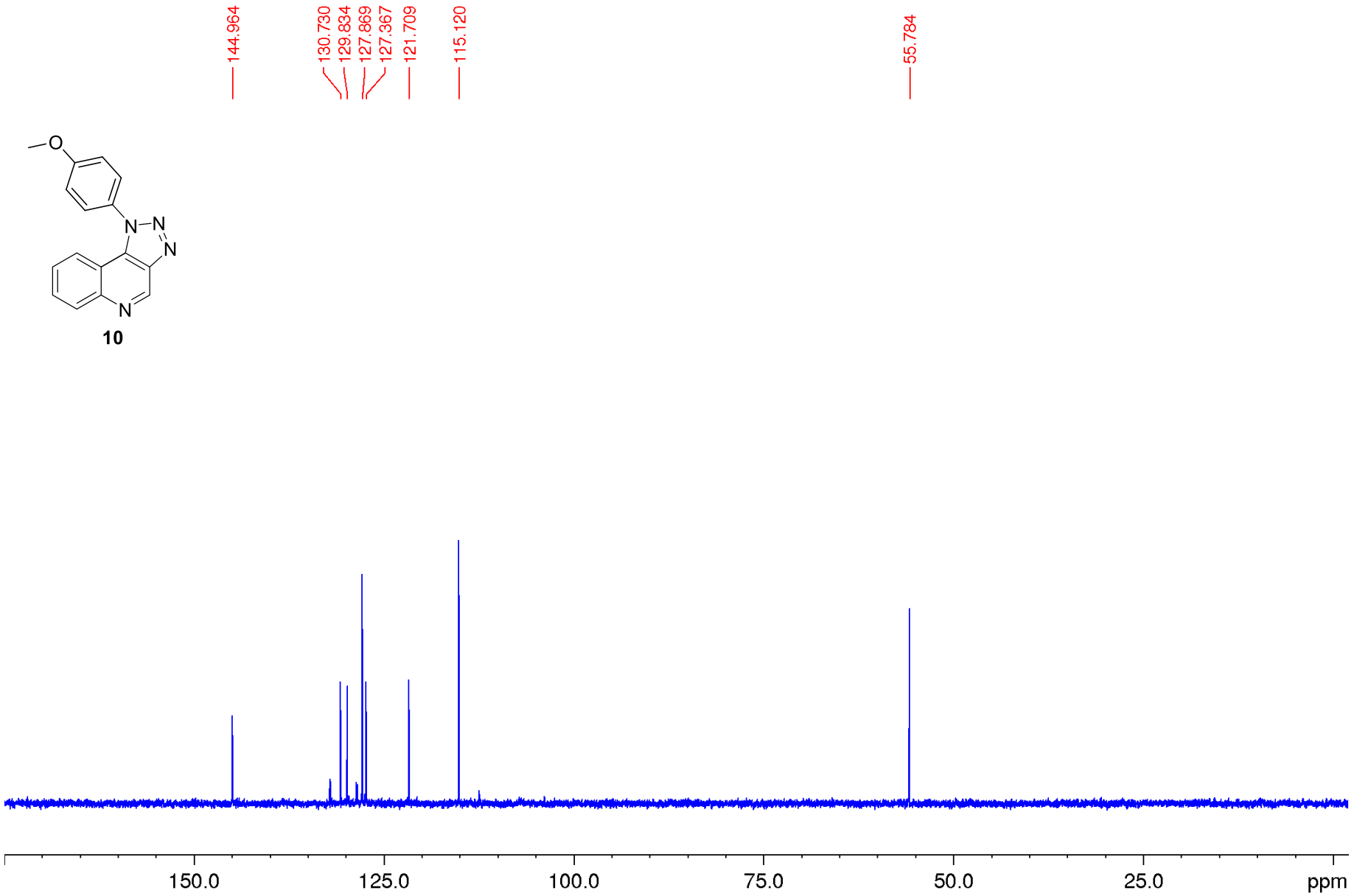


^{13}C NMR-spectrum (100 MHz, $CDCl_3$)

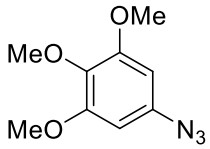


10

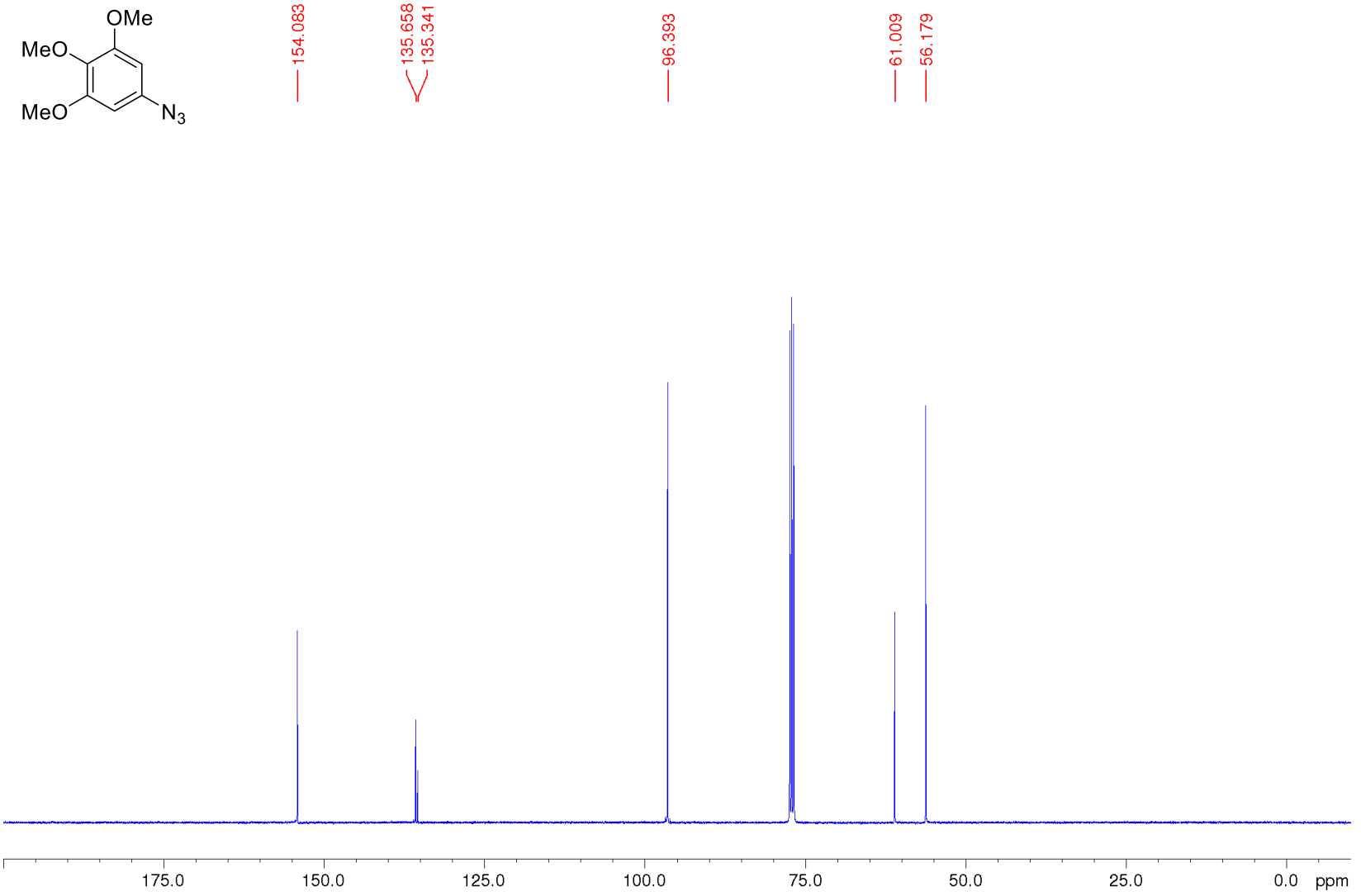
DEPT 135 NMR-spectrum ($CDCl_3$)



^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



DEPT 135 NMR-spectrum ($CDCl_3$)