

SUPPORTING INFORMATION

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

Karim Ullah,^a Dario Allevi,^b Giancarlo Fabrizi,^a Antonella Goggiamani,^a Federico Marrone,^a
and Antonia Iazzetti.^{*b,c}

a. Dipartimento di Chimica e Tecnologie del Farmaco, Sapienza, Università di Roma, P.le A. Moro 5, 00185 Rome, Italy.

b. Dipartimento di Scienze Biotechnologiche di base, Cliniche Intensivologiche e Perioperatorie, Università Cattolica del Sacro Cuore, L.go Francesco Vito 1, 00168 Rome, Italy.

c. Policlinico Universitario 'A. Gemelli' Foundation-IRCCS, Rome, 00168, Italy.

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1. GENERAL INFORMATION

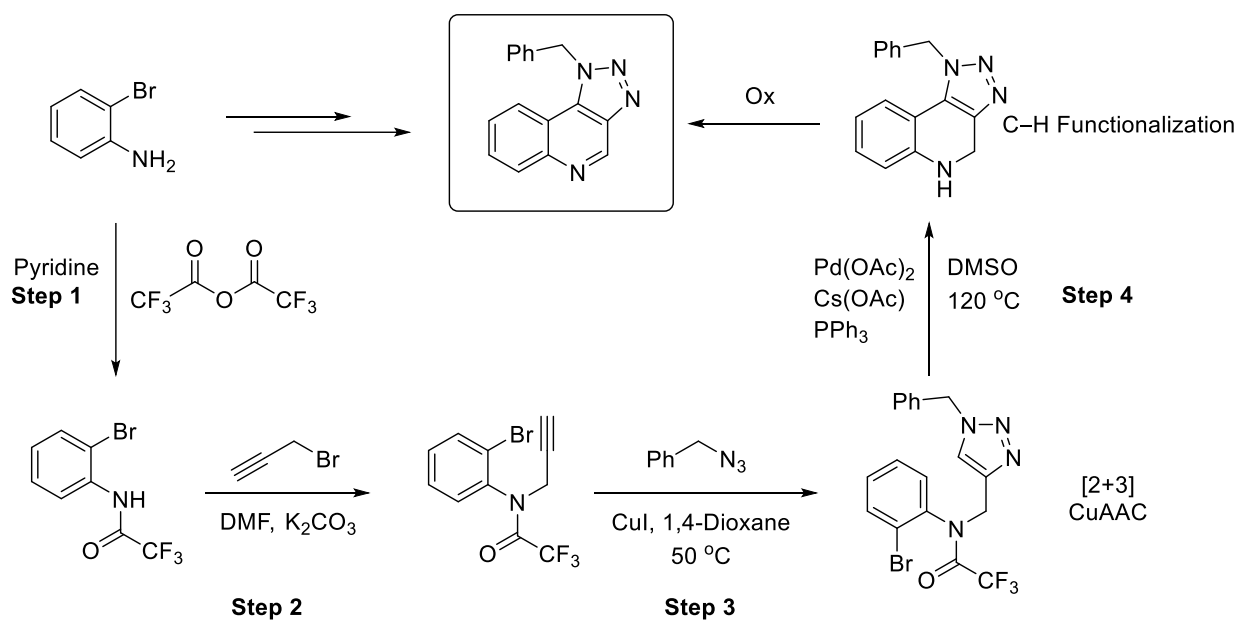
1.1. Reagents and methods

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 SiO₂ as stationary phase, eluting with *n*-hexane/ethyl acetate. ¹H NMR (400.13 MHz), ¹³C NMR (100.6 MHz), and ¹⁹F 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.

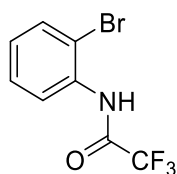


Scheme 1

STEP 1: synthesis of *N*-(2-bromophenyl)-2,2,2-trifluoroacetamide^{S1}

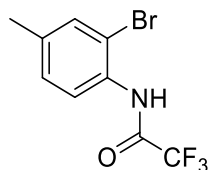
Following a slight modification of the literature procedure.^{S1}

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 Et₂O and sequentially washed with 2N HCl, saturated NaHCO₃ solution, and brine. The organic layer was dried over Na₂SO₄, 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).

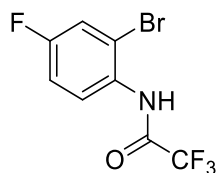


***N*-(2-bromophenyl)-2,2,2-trifluoroacetamide:** 97% yield, 2.60 g, 9.70 mmol; white solid; lit. mp ^{S1}: 57 – 59 °C; mp: 60 - 62 °C; *R*_f = 0.19 (*n*-hexane-EtOAc, 80:20); IR (neat): 3244, 1710, 1411, 1242,

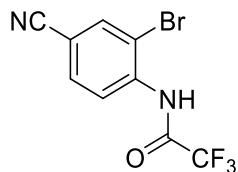
761 cm⁻¹; ¹H NMR (400.13 MHz, CDCl₃) δ 8.47 (bs, NH), 8.37 – 8.27 (m, 1H), 7.67 – 7.57 (m, 1H), 7.41 (t, *J* = 7.6 Hz, 1H), 7.18 – 7.10 (m, 1H); ¹³C NMR (100.6 MHz, CDCl₃) δ 154.6 (q, *J*_{C-F} = 37.0 Hz) (C), 133.2 (C), 132.6 (CH), 128.7 (CH), 127.2 (CH), 122.0 (CH), 117.0 (q, *J*_{C-F} = 289.4 Hz) (C), 114.0 (C); HRMS: *m/z* [M + H]⁺ calcd for C₈H₆BrF₃NO: 267.9579; found: 267.9554.



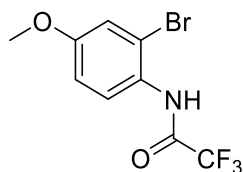
***N*-(2-bromo-4-methylphenyl)-2,2,2-trifluoroacetamide:** 95% yield, 2.66 g, 9.50 mmol; white solid; lit. mp ^{S1}: 67 – 69 °C; mp: 70 - 72 °C; *R*_f = 0.23 (*n*-hexane-EtOAc, 80:20); IR (neat): 3451, 1718, 1521, 1177, 822 cm⁻¹; ¹H NMR (400.13 MHz, CDCl₃) δ 8.34 (bs, NH), 8.12 (d, *J* = 8.3 Hz, 1H), 7.42 – 7.38 (m, 1H), 7.18 – 7.11 (m, 1H), 7.19 – 7.05 (m, 1H), 2.31 (s, 3H); ¹³C NMR (100.6 MHz, CDCl₃) 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 (CH₃); HRMS: *m/z* [M + H]⁺ calcd for C₉H₈BrF₃NO: 281.9736; found: 281.9725.



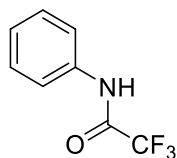
***N*-(2-bromo-4-fluorophenyl)-2,2,2-trifluoroacetamide:** 96% yield, 2.61 g, 9.12 mmol; pale yellow solid; mp: 80 - 82 °C; *R*_f = 0.21 (*n*-hexane-EtOAc, 90:10); IR (neat): 3252, 2158, 2029, 1715, 1547, 1151 cm⁻¹; ¹H NMR (400.13 MHz, CDCl₃) δ 8.36 (bs, NH), 8.30 – 8.22 (m, 1H), 7.38 (dd, *J*₁ = 7.7 Hz, *J*₂ = 2.8 Hz, 1H), 7.18 – 7.10 (m, 1H); ¹³C NMR (100.6 MHz, CDCl₃) 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 C₈H₅BrF₄NO: 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} ; ^1H NMR (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, $J_{\text{C-F}}$ = 38.5 Hz) (C), 137.2 (C), 136.0 (CH), 132.8 (CH), 121.6 (CH), 116.7 (C) 115.2 (q, $J_{\text{C-F}}$ = 289.5 Hz) (C), 113.9 (C), 110.7 (C) 20.6 (CH_3); HRMS: m/z $[\text{M} + \text{H}]^+$ calcd for $\text{C}_9\text{H}_5\text{BrF}_3\text{N}_2\text{O}$: 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} ; ^1H NMR (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, $J_{\text{C-F}}$ = 37.4 Hz) (C), 126.2 (C), 123.5 (CH), 117.9 (CH), 115.4 (C), 114.0 (CH), 116.1 (q, $J_{\text{C-F}}$ = 289.3 Hz) (C), 55.7 (CH_3); HRMS: m/z $[\text{M} + \text{H}]^+$ calcd for $\text{C}_9\text{H}_8\text{BrF}_3\text{NO}_2$: 297.9685; found 297.9664.



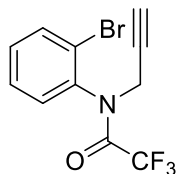
2,2,2-trifluoro-N-phenylacetamide: 99% yield, 1.88 g, 9.90 mmol; white solid; lit. mp ^{S2}: 90 - 92 °C; mp: 88 - 90 °C; R_f = 0.20 (*n*-hexane-EtOAc, 85:15); IR (neat): 3311, 1709, 1554, 1242, 760 cm^{-1} ; ^1H NMR (400.13 MHz, CDCl_3) δ 7.91 (bs, NH), 7.49 (d, J = 7.8 Hz, 2H), 7.31 (t J = 7.8 Hz, 2H),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

(C), 120.5 (CH), 115.6 (q, $J_{\text{C-F}} = 289.4$ Hz) (C); HRMS: m/z $[M + H]^+$ calcd for $\text{C}_8\text{H}_7\text{F}_3\text{NO}$: 190.0474; found: 190.0492.

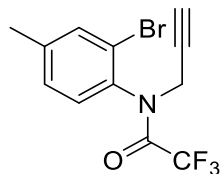
STEP 2: synthesis of *N*-(2-bromophenyl)-2,2,2-trifluoro-*N*-(prop-2-yn-1-yl)acetamide

Following a slight modification of the literature procedure.^{S1}

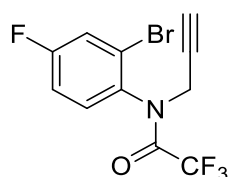
To a solution of *N*-(2-bromophenyl)-2,2,2-trifluoroacetamide (2.6 g, 9.70 mmol, 1.0 equiv.) in 15 mL of DMF, K_2CO_3 (2.67 g, 19.40 mmol, 2.0 equiv.) and propargyl bromide (0.808 mL, 10.67 mmol, 1.1 equiv.) were added. The reaction mixture was stirred at room temperature for 6 hours. Upon completion, 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).



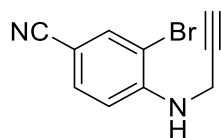
***N*-(2-bromophenyl)-2,2,2-trifluoro-*N*-(prop-2-yn-1-yl)acetamide:** 90% yield, 2.66 g, 8.73 mmol; brown solid; mp: 52 - 54 °C; $R_f = 0.22$ (*n*-hexane-EtOAc, 90:10); IR (neat): 3311, 2994, 1721, 1481, 1114 cm^{-1} ; ^1H NMR (400.13 MHz, CDCl_3) δ 7.76 – 7.68 (m, 1H), 7.51 – 7.32 (m, 3H), 5.13 (dd, $J_1 = 17.4$ 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, $J_{\text{C-F}} = 37.6$ Hz) (C), 136.5 (C), 133.6 (CH), 131.8 (CH), 131.2 (CH), 128.1 (CH), 123.4 (C), 115.9 (q, $J_{\text{C-F}} = 287.1$ Hz) (C), 76.4 (C), 74.1 (CH) 39.1 (CH_2); HRMS: m/z $[M + H]^+$ calcd for $\text{C}_{11}\text{H}_8\text{BrF}_3\text{NO}$: 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, $J_{\text{C-F}}$ = 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, $J_{\text{C-F}}$ = 287.1 Hz) (C), 76.5 (C), 73.9 (CH), 39.2 (CH_2), 20.9 (CH_3); HRMS: m/z $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{12}\text{H}_{10}\text{BrF}_3\text{NO}$: 319.9892; found: 319.9870.

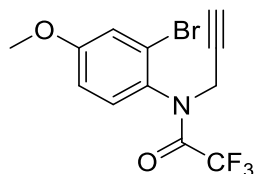


***N*-(2-bromo-4-fluorophenyl)-2,2,2-trifluoro-*N*-(prop-2-yn-1-yl)acetamide:** 70% yield, 0.57 g, 1.75 mmol; pale yellow wax; R_f = 0.27 (*n*-hexane-EtOAc, 90:10); IR (neat): 3393, 2960, 1764, 1453, 1045, cm^{-1} ; ^1H NMR (400.13 MHz, CDCl_3) δ 7.51 – 7.42 (m, 2H), 7.19 – 7.12 (m, 1H), 5.13 (dd, J_1 = 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, $J_{\text{C-F}}$ = 254.5 Hz) (C), 156.5 (q, $J_{\text{C-F}}$ = 36.4 Hz) (C), 133.0 (d, $J_{\text{C-F}}$ = 8.8 Hz) (CH), 132.8 (d, $J_{\text{C-F}}$ = 4.1 Hz) (C), 124.4 (d, $J_{\text{C-F}}$ = 10.2 Hz) (C), 121.0 (d, $J_{\text{C-F}}$ = 25.8 Hz) (CH), 115.8 (q, $J_{\text{C-F}}$ = 289.0 Hz) (C), 115.3 (d, $J_{\text{C-F}}$ = 22.4 Hz) (CH); 76.2 (C), 74.4 (CH), 39.1 (CH_2), HRMS: m/z $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{11}\text{H}_7\text{BrF}_4\text{NO}$: 323.9442; found: 323.9433.

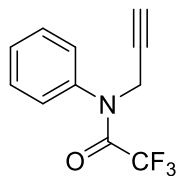


3-bromo-4-(prop-2-yn-1-ylamino)benzonitrile: 50% yield, 0.29 g, 1.25 mmol; brown oil; R_f = 0.21 (*n*-hexane-EtOAc, 60:40); IR (neat): 3392, 3276, 2159, 1518, 814 cm^{-1} ; ^1H NMR (400.13 MHz, CDCl_3) δ 7.64 (d, J = 1.8 Hz, 1H), 7.43 (dd, J_1 = 8.4 Hz, J_2 = 1.8 Hz, 1H), 6.67 (d, J = 8.5 Hz, 1H), 5.04

(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 $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{10}\text{H}_8\text{BrN}_2$: 234.9865; found: 234.9874.



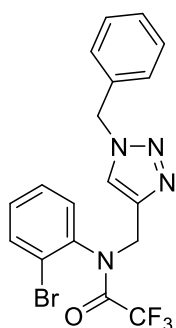
***N*-(2-bromo-4-methoxyphenyl)-2,2,2-trifluoro-*N*-(prop-2-yn-1-yl)acetamide**: 90% yield, 0.76 g, 2.25 mmol; yellow oil; $R_f = 0.24$ (*n*-hexane-EtOAc, 90:10); IR (neat): 3711, 3293, 2158, 1702, 1206, 842 cm^{-1} ; ^1H NMR (400.13 MHz, CDCl_3) δ 7.36 (d, $J = 8.8$ Hz, 1H), 7.22 (d, $J = 2.8$ Hz, 1H), 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, $J_{\text{C-F}} = 37.1$ Hz) (C), 132.3 (CH), 129.1 (C), 124.0 (C), 118.6 (CH), 115.9 (q, $J_{\text{C-F}} = 288.0$ Hz) (C), 113.5 (CH), 76.6 (C), 74.0 (CH), 55.8 (CH_3), 39.4 (CH_2); HRMS: m/z $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{12}\text{H}_{10}\text{BrF}_3\text{NO}_2$: 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 $^{\circ}\text{C}$; $R_f = 0.20$ (*n*-hexane-EtOAc, 90:10); IR (neat): 3398, 2915, 1722, 1415, 765 cm^{-1} ; ^1H 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, $J_{\text{C-F}} = 37.6$ Hz) (C), 138.3 (C), 129.6 (CH), 129.4 (CH), 128.4 (CH), 116.2 (q, $J_{\text{C-F}} = 287.1$ Hz) (C), 76.9 (C), 73.7 (CH), 41.0 (CH_2); HRMS: m/z $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{11}\text{H}_9\text{F}_3\text{NO}$: 228.0631; found: 228.0647.

STEP 3: synthesis of *N*-((1-benzyl-1*H*-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).

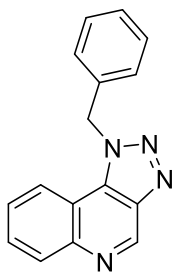


***N*-((1-benzyl-1*H*-1,2,3-triazol-4-yl)methyl)-*N*-(2-bromophenyl)-2,2,2-trifluoroacetamide, 2a:** 90% yield, 413.0 mg, 0.94 mmol; yellow solid; mp: 120-122 °C; R_f = 0.23 (*n*-hexane-EtOAc, 70:30); IR (neat): 3121, 3073, 1694, 1478, 1149, 719 cm^{-1} ; ^1H NMR (400.13 MHz, CDCl_3) δ 7.59 – 7.56 (m, 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, $J_{\text{C-F}}$ = 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, $J_{\text{C-F}}$ = 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 $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{18}\text{H}_{15}\text{BrF}_3\text{N}_4\text{O}$: 439.0354; found: 439.0377.

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

To a vial containing $\text{Pd}(\text{OAc})_2$ (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-

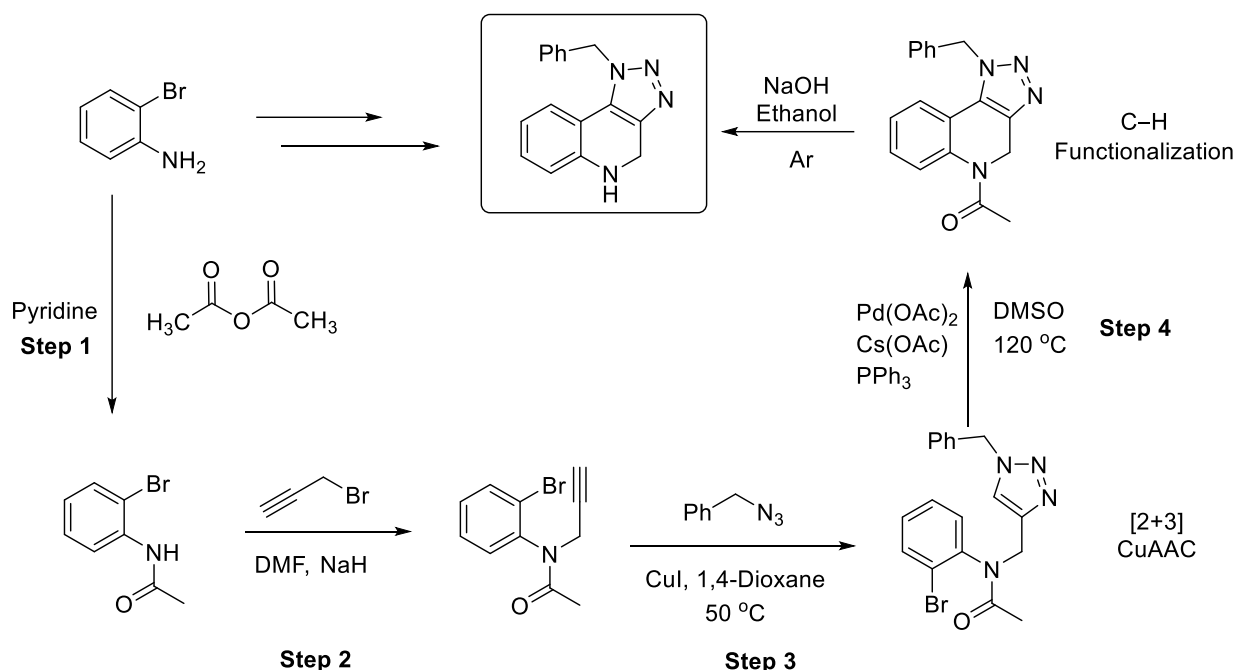
bromophenyl)-2,2,2-trifluoroacetamide (110.0 mg, 0.250 mmol, 1.00 equiv.), and Cs(OAc) (96.0 mg, 0.500 mmol, 2.00 equiv.). The mixture was stirred at 120 °C for 0.5 hours. Upon completion of reaction (monitored by TLC), an oxygen balloon was then applied. The reaction was monitored by TLC upon completion, the mixture was then diluted with diethyl ether, extracted with brine and dried over anhydrous Na₂SO₄. 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-1H-[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; ¹H NMR (400.13 MHz, CDCl₃) 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); ¹³C NMR (100.6 MHz, CDCl₃) 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 (CH₂); MS (EI, 70 eV): *m/z* (%) = 231 (100), 260 (M⁺, 100), 91 (100), 128 (90); HRMS: *m/z* [M + H]⁺ calcd for C₁₆H₁₃N₄: 261.1135; found: 261.1115.

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

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

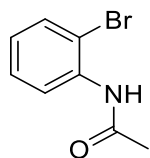


Scheme 2

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

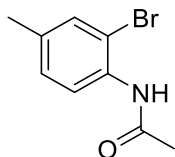
Following a slight modification of the literature procedure.⁵³

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 NaHCO₃ solution, and brine. The organic layer was dried over Na₂SO₄, 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. mp⁵³: 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, CDCl₃) 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); ¹³C NMR (100.6 MHz, CDCl₃) δ 168.2 (C), 135.7 (C), 132.2 (CH), 128.4 (CH), 125.1 (CH), 121.9 (CH), 113.2 (C), 24.8 (CH₃); HRMS: m/z [M + H]⁺ calcd for C₈H₉BrNO: 213.9862; found: 213.9855.

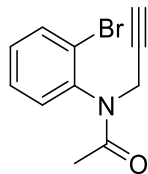


***N*-(2-bromo-4-methylphenyl)acetamide** : 94% yield, 2.15 g, 9.45 mmol; white solid; lit. mp ^{S3}: 86 - 88 °C; mp: 83 - 85 °C; R_f = 0.20 (*n*-hexane-EtOAc, 85:15); IR (neat): 3245, 1685, 1512, 1287, 754 cm⁻¹; ¹H NMR (400.13 MHz, CDCl₃) δ 8.05 (d, J = 8.4 Hz, 1H), 7.46 (bs, 1H), 7.26 (s, 1H), 7.01 (d, J = 8.3 Hz, 1H), 2.21 (s, 3H), 2.13 (s, 3H); ¹³C NMR (100.6 MHz, CDCl₃) δ 168.2 (C), 135.3 (C), 133.1 (C), 132.4 (CH), 128.9 (CH), 122.0 (CH), 113.3 (C), 24.7 (CH₃), 24.5 (CH₃); HRMS: m/z [M + H]⁺ calcd for C₉H₁₁BrNO: 228.0018; found: 228.0033.

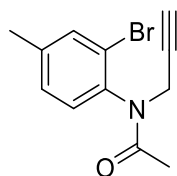
STEP 2: synthesis of N-(2-bromophenyl)-N-(prop-2-yn-1-yl)acetamide.

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 Na₂SO₄, 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; ¹HNMR (400.13 MHz, CDCl₃) 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); ¹³C NMR (100.6 MHz, CDCl₃) 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 (CH₂), 22.1 (CH₃); HRMS: m/z [M + H]⁺ calcd for C₁₁H₁₁BrNO: 252.0018; found: 252.0031.

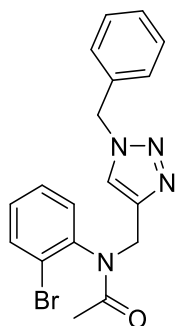


***N*-(2-bromo-4-methylphenyl)-*N*-(prop-2-yn-1-yl)acetamide:** 91% yield, 2.41 g, 9.1 mmol; white solid; mp: 46 - 48 °C; R_f = 0.22 (*n*-hexane-EtOAc, 95:5); IR (neat): 3258, 2901, 1738, 1352, 1277 cm⁻¹; ¹HNMR (400.13 MHz, CDCl₃) δ 7.50 (s, 1H), 7.33 – 7.25 (m, 1H), 7.23 – 7.13 (m, 1H), 5.04 (d, J = 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); ¹³C NMR (100.6 MHz, CDCl₃) 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 (CH₂), 22.1 (CH₃), 20.9 (CH₃); HRMS: m/z [M + H]⁺ calcd for C₁₂H₁₃BrNO: 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

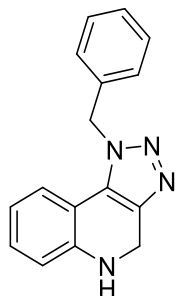
by flash column chromatography (70:30 *n*-hexane/EtOAc, R_f = 0.20) to afford the pure product as a yellow solid (366.2 mg, 0.95 mmol, 95% yield).



***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 [$\text{M} + \text{H}$] $^+$ calcd for $\text{C}_{18}\text{H}_{18}\text{BrN}_4\text{O}$: 385.0658; found: 385.0634.

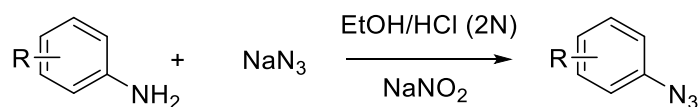
STEP 4: 1-benzyl-4,5-dihydro-1*H*-[1,2,3]triazolo[4,5-*c*]quinoline (4a)

To a vial containing $\text{Pd}(\text{OAc})_2$ (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 $\text{Cs}(\text{OAc})$ (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-1H-[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 [$\text{M} + \text{H}$] $^+$ calcd for $\text{C}_{16}\text{H}_{15}\text{N}_4$: 263.1291; found: 263.1276.

2.3. Typical procedure for the preparation of azides

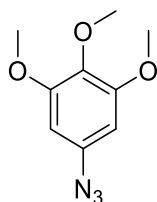


Scheme 3

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

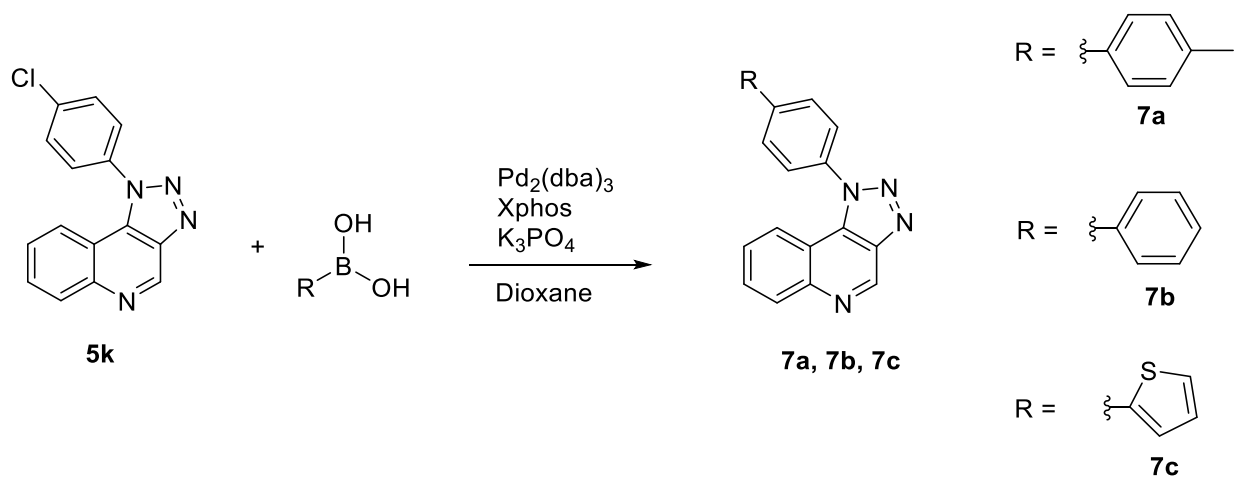
Following the same procedure reported in literature^{S6}, the 3,4,5-trimethoxyaniline (1.832 g, 10.0 mmol, 1.0 equiv.) was suspended in 17% hydrochloric acid at room temperature, and ethanol was added until a clear solution was obtained. The solution was then cooled to 0°C, and NaNO_2 (1.035 g, 15.0 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 Na₂SO₂, and concentrated under reduced pressure. The desired azide was obtained in quantitative yield without further purification.



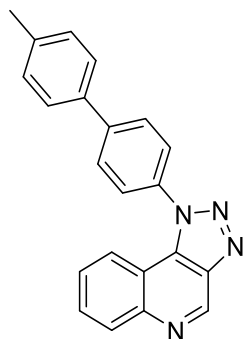
5-azido-1,2,3-trimethoxybenzene: 99% yield, 2.08 g, 9.9 mmol; brown solid; lit. mp ^{S7}: 42 – 43; mp: 45 - 47 °C; R_f = 0.20 (*n*-hexane-EtOAc, 75:25); IR (neat): 2910, 2485, 1461, 1135, 993 cm⁻¹; ¹H NMR (400.13 MHz, CDCl₃) δ 6.18 (s, 2H), 3.78 (s, 6H), 3.74 (s, 3H); ¹³C NMR (100.6 MHz, CDCl₃) δ 154.1 (C), 135.7 (C), 135.4 (C), 96.4 (CH), 61.0 (CH₃), 56.2 (CH₃). HRMS: *m/z* [M + H]⁺ calcd for C₉H₁₂N₃O₃:210.0873; found: 210.0888.

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

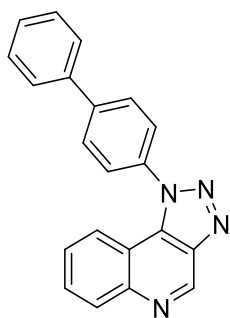


To a mixture of Pd₂(dba)₃ (4.6 mg, 0.005 mmol, 0.02 equiv.) and Xphos ligand (4.7 mg, 0.010 mmol, 0.04 equiv.) in dry dioxane (2 mL), compound **5k** (70.0 mg, 0.250 mmol, 1.00 equiv.), *p*-tolyl boronic acid (51.0 mg, 0.375 mmol, 1.50 equiv.), and K₃PO₄ (0.159 g, 0.750 mmol, 3.00 equiv.) were added. 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).

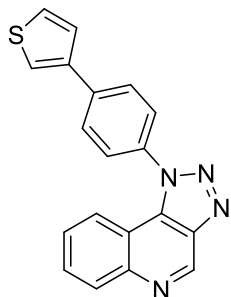


1-(4'-methyl-[1,1'-biphenyl]-4-yl)-1H-[1,2,3]triazolo[4,5-c]quinoline, 7a: 86% yield, 72.3 mg, 0.22 mmol; pale yellow solid; mp: 197-199 °C; R_f = 0.24 (*n*-hexane-EtOAc, 75:25); IR (neat): 3055, 1504, 992, 801, 767 cm^{-1} ; ^1H NMR (400.13 MHz, CDCl_3) δ 9.51 (s, 1H), 8.22 (d, J = 8.3 Hz, 1H), 7.83 – 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 [$\text{M} + \text{H}$] $^+$ calcd for $\text{C}_{22}\text{H}_{17}\text{N}_4$: 337.1448; found: 337.1463.



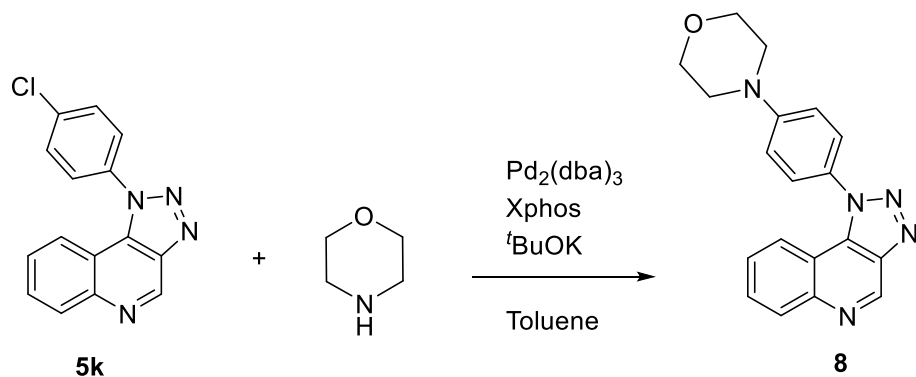
1-([1,1'-biphenyl]-4-yl)-1H-[1,2,3]triazolo[4,5-c]quinoline, 7b: 95% yield, 76.5 mg, 0.24 mmol; grey solid; mp: 178-180 °C; R_f = 0.22 (*n*-hexane-EtOAc, 75:25); IR (neat): 3063, 1527, 1087, 984, 758 cm^{-1} ; ^1H NMR (400.13 MHz, CDCl_3) δ 9.49 (s, 1H), 8.21 (d, J = 8.2, 1H), 7.85 – 7.81 (m, 3H), 7.80 – 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.

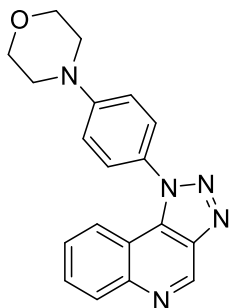


1-(4-(thiophen-3-yl)phenyl)-1H-[1,2,3]triazolo[4,5-c]quinoline, 7c: 85% yield, 69.7 mg, 0.22 mmol; pale yellow solid; mp: 230-232 °C; R_f = 0.18 (*n*-hexane-EtOAc, 70:30); IR (neat): 2967, 1535, 1267, 762, 567 cm^{-1} ; 1H NMR (400.13 MHz, $CDCl_3$) δ 9.60 (s, 1H), 8.41 – 8.38 (m, 1H), 7.91 – 7.85 (m, 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

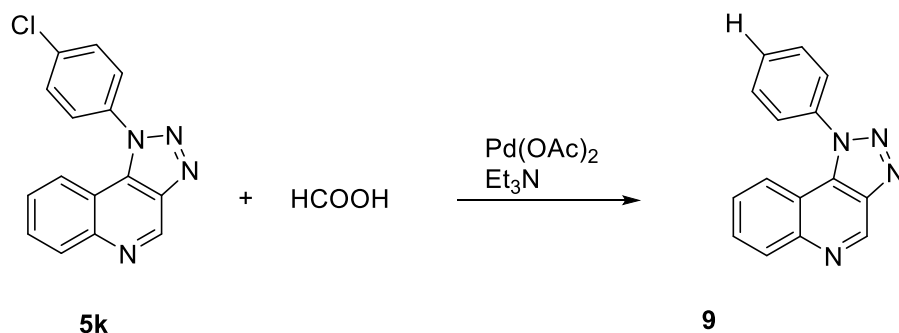


To a mixture of Pd(OAc)₂ (5.7 mg, 0.0063 mmol, 0.025 equiv.) and Xphos ligand (5.9 mg, 0.0125 mmol, 0.050 equiv.) in dry toluene (2.0 mL), compound **5k** (70.1 mg, 0.25 mmol, 1.0 equiv.), morpholine (32.7 mg, 0.37 mmol, 1.5 equiv.), and ^tBuOK (56.1 mg, 0.5 mmol, 2.0 equiv.) were added. The reaction 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).

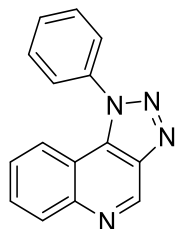


4-(4-(1H-[1,2,3]triazolo[4,5-c]quinolin-1-yl)phenyl)morpholine, 8: 52% yield, 43.2 mg, 0.13 mmol; grey solid; mp: 245–247 °C; *R*_f = 0.21 (*n*-hexane-EtOAc, 50:50); IR (neat): 2841, 1527, 1110, 754, 560 cm⁻¹; ¹H NMR (400.13 MHz, CDCl₃) δ 9.51 (s, 1H), 8.22 (d, *J* = 8.2 Hz, 1H), 7.75 – 7.66 (m, 2H), 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); ¹³C NMR (100.6 MHz, CDCl₃) 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 (CH₂), 48.4 (CH₂); MS (EI, 70 eV): *m/z* (%) = 300 (100), 115 (55), 207 (36), 331 (M⁺, 4); HRMS: *m/z* [M + H]⁺ calcd for C₁₉H₁₈N₅O: 332.1506; found: 332.1528.

2.6. Procedure for the synthesis of compound 9

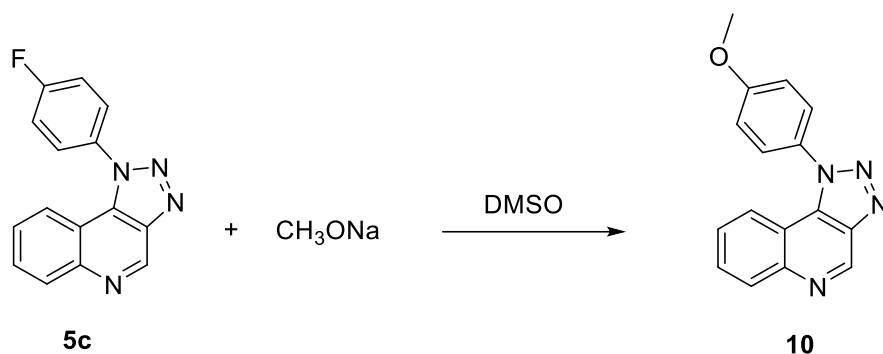


To a mixture of Pd(OAc)_2 (1.4 mg, 0.0062 mmol, 0.025 equiv.) and Et_3N (75.9 mg, 0.75 mmol, 3.0 equiv.) in dry DMSO (2.0 mL), compound **5k** (70 mg, 0.25 mmol, 1.0 equiv.) and formic acid (0.023 g, 0.50 mmol, 2.000 equiv.) were added. The reaction mixture was then stirred under argon at 120°C and monitored 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).

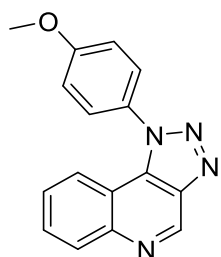


1-phenyl-1H-[1,2,3]triazolo[4,5-c]quinoline, 9: 71% yield, 43.8 mg, 0.1775 mmol; pale yellow solid; mp: $153\text{--}155^\circ\text{C}$; $R_f = 0.16$ (*n*-hexane- EtOAc , 60:40); IR (neat): 3073, 1504, 992, 767, 696 cm^{-1} ; ^1H NMR (400.13 MHz, CDCl_3) δ 9.52 (s, 1H), 8.23 (d, $J = 8.1$ Hz, 1H), 7.79 – 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 [$\text{M} + \text{H}$] $^+$ calcd for $\text{C}_{15}\text{H}_{11}\text{N}_4$: 247.0978; found: 247.0999.

2.7. Procedure for the synthesis compound 10

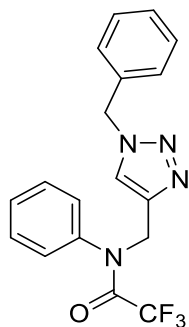


Compound **5c** (66 mg, 0.250 mmol, 1.000 equiv.) and sodium methoxide (20.2 mg, 0.375 mmol, 1.5 equiv.) were added to DMSO (2 mL). The reaction mixture was stirred at 140°C for 10 hours and monitored by TLC. Upon completion, the mixture was diluted with diethyl ether, extracted with brine, dried over anhydrous Na₂SO₄ 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).

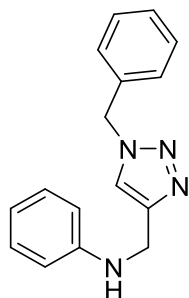


1-(4-methoxyphenyl)-1H-[1,2,3]triazolo[4,5-c]quinoline, 10: 78% yield, 54.0 mg, 0.195 mmol; brown solid; mp: 174-176 °C; *R*_f = 0.22 (*n*-hexane-EtOAc, 70:30); IR (neat): 2922, 1522, 1253, 843, 760 cm⁻¹; ¹H NMR (400.13 MHz, CDCl₃) δ 9.52 (s, 1H), 8.22 (d, *J* = 8.8 Hz, 1H), 7.73 – 7.63 (m, 2H), 7.53 – 7.46 (m, 2H), 7.44 – 7.38 (m, 1H), 7.14 – 7.07 (m, 2H), 3.89 (s, 3H); ¹³C NMR (100.6 MHz, CDCl₃) 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 (CH₃); MS (EI, 70 eV): *m/z* (%) = 205 (100), 233 (75), 151 (16), 276 (M⁺, 10); HRMS: *m/z* [M + H]⁺ calcd for C₁₆H₁₃N₄O: 277.1084; found: 277.1069.

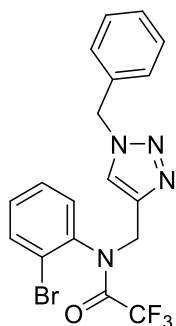
CHARACTERIZATION DATA OF COMPOUNDS 1a, 1a', 2a-q, 3a-h



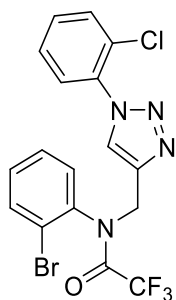
***N*-((1-benzyl-1*H*-1,2,3-triazol-4-yl)methyl)-2,2,2-trifluoro-*N*-phenylacetamide, 1a:** 91% yield, 327.6 mg, 0.91 mmol; white solid; mp: 100-102 °C; R_f = 0.21 (*n*-hexane-EtOAc, 80:20); IR (neat): 3118, 2359, 1685, 1455, 1074, 747 cm^{-1} ; ^1H NMR (400.13 MHz, CDCl_3) δ 7.58 (s, 1H), 7.42 – 7.32 (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, $J_{\text{C-F}}$ = 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, $J_{\text{C-F}}$ = 287.2 Hz) (C), 54.2 (CH_2), 47.3 (CH_2); HRMS: m/z $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{18}\text{H}_{16}\text{F}_3\text{N}_4\text{O}$: 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 $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{16}\text{H}_{17}\text{N}_4$: 265.1448; found: 265.1431.

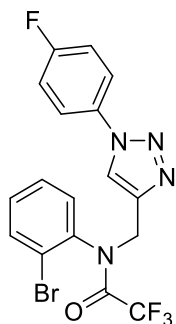


***N*-((1-benzyl-1*H*-1,2,3-triazol-4-yl)methyl)-*N*-(2-bromophenyl)-2,2,2-trifluoroacetamide, 2a:** 90% yield, 413.0 mg, 0.94 mmol; white solid; mp: 120-122 °C; R_f = 0.23 (*n*-hexane-EtOAc, 70:30); IR (neat): 3121, 3073, 1694, 1478, 1149, 719 cm^{-1} ; ^1H NMR (400.13 MHz, CDCl_3) δ 7.59 – 7.56 (m, 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, $J_{\text{C-F}}$ = 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, $J_{\text{C-F}}$ = 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 [$\text{M} + \text{H}$] $^+$ calcd for $\text{C}_{18}\text{H}_{15}\text{BrF}_3\text{N}_4\text{O}$: 439.0376; found: 439.0354.



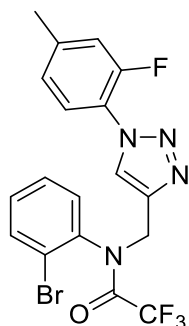
***N*-(2-bromophenyl)-*N*-((1-(2-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-2,2,2-trifluoroacetamide, 2b:** 93% yield, 425.0 mg, 0.93 mmol; white solid; mp: 121-123 °C; R_f = 0.19 (*n*-hexane-EtOAc, 70:30); IR (neat): 3144, 1698, 1481, 1153, 762 cm^{-1} ; ^1H NMR (400.13 MHz, CDCl_3) δ 8.09 (s, 1H), 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, $J_{\text{C-F}}$ = 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, $J_{\text{C-F}} = 288.1$ Hz) (C), 45.5 (CH₂); ¹⁹F NMR (376.5 MHz, CDCl₃) δ -68.9 (s); HRMS: m/z [M + H]⁺ calcd for C₁₇H₁₂BrClF₃N₄O: 458.9830; found: 458.9848.



***N*-(2-bromophenyl)-2,2,2-trifluoro-*N*-((1-(4-fluorophenyl)-1*H*-1,2,3-triazol-4-**

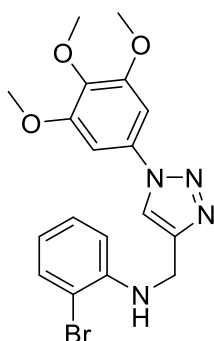
yl)methyl)acetamide, 2c: 85% yield, 376.5 mg, 0.85 mmol; brown solid; mp: 115-117 °C; $R_f = 0.25$ (*n*-hexane-EtOAc, 70:30); IR (neat): 3145, 3100, 1685, 1519, 1149, 833 cm⁻¹; ¹H NMR (400.13 MHz, CDCl₃) δ 8.05 (s, 1H), 7.68 – 7.61 (m, 3H), 7.27 – 7.19 (m, 2H), 7.18 – 7.07 (m, 3H), 5.41 (d, $J = 14.8$ Hz, 1H), 4.40 (d, $J = 14.8$ Hz, 1H); ¹³C NMR (100.6 MHz, CDCl₃) δ 162.5 (d, $J_{\text{C-F}} = 248.7$ Hz) (C), 157.0 (q, $J_{\text{C-F}} = 36.7$ Hz) (C), 142.5 (C), 137.8 (C), 133.6 (CH), 133.1 (d, $J_{\text{C-F}} = 2.9$ Hz) (C), 131.5 (CH), 131.1 (CH), 128.3 (CH), 123.3 (C), 122.5 (d, $J_{\text{C-F}} = 8.5$ Hz) (CH), 116.9 (CH), 116.7 (CH), 115.8 (q, $J_{\text{C-F}} = 288.4$ Hz) (C), 46.9 (CH₂); ¹⁹F NMR (376.5 MHz, CDCl₃) δ -68.9 (s), -111.8 (m); HRMS: m/z [M + H]⁺ calcd for C₁₇H₁₂BrF₄N₄O: 443.0125; found: 443.0145.



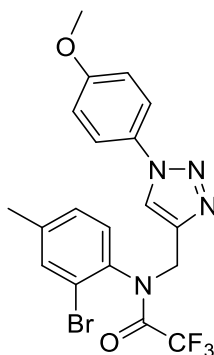
***N*-(2-bromophenyl)-2,2,2-trifluoro-*N*-((1-(2-fluoro-4-methylphenyl)-1*H*-1,2,3-triazol-4-**

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, CDCl₃) 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); ¹³C NMR (100.6 MHz, CDCl₃) δ 156.9 (q, $J_{\text{C-F}} = 36.6$

Hz), 153.2 (d, $J_{\text{C-F}} = 248.8$ Hz) (C), 141.8 (C), 141.5 (d, $J_{\text{C-F}} = 7.8$ Hz) (C), 137.6 (C), 133.6 (CH), 131.6 (CH), 131.0 (CH), 128.3 (CH), 125.8 (d, $J_{\text{C-F}} = 3.1$ Hz) (CH), 125.2 (d, $J_{\text{C-F}} = 7.6$ Hz) (CH), 124.5 (CH), 123.4 (C), 122.5 (d, $J_{\text{C-F}} = 10.4$ Hz) (C), 117.3 (d, $J_{\text{C-F}} = 19.6$ Hz) (CH), 116.1 (q, $J_{\text{C-F}} = 288.5$ Hz) (C), 45.6 (CH₂), 21.2 (CH₃); ¹⁹F NMR (376.5 MHz, CDCl₃) δ -68.9 (s), -124.4 (t, $J = 9.5$ Hz); HRMS: m/z [M + H]⁺ calcd for C₁₈H₁₄BrF₄N₄O: 457.0282; found: 457.0296.

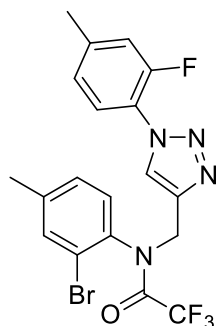


2-bromo-*N*-((1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)aniline, 2e: 81% yield, 337.8 mg, 0.81 mmol; pale yellow solid; mp: 138-140 °C; $R_f = 0.20$ (*n*-hexane-EtOAc, 70:30); IR (neat): 3346, 2938, 1595, 1508, 1126 cm⁻¹; ¹H NMR (400.13 MHz, CDCl₃) δ 7.90 (s, 1H), 7.48 (d, $J = 7.8$ Hz, 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); ¹³C NMR (100.6 MHz, CDCl₃) 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 (CH₃), 56.5 (CH₂), 40.1 (CH₃); HRMS: m/z [M + H]⁺ calcd for C₁₈H₂₀BrN₄O₃: 419.0713; found: 419.0708.

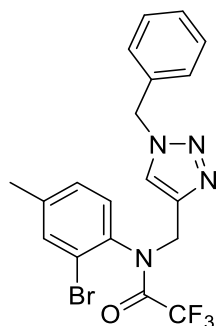


***N*-(2-bromo-4-methylphenyl)-2,2,2-trifluoro-*N*-((1-(4-methoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)acetamide, 2f:** 98% yield, 458.6 mg, 0.98 mmol; pale yellow solid; mp: 124-126 °C; R_f

= 0.24 (*n*-hexane-EtOAc, 60:40); IR (neat): 3153, 2962, 1677, 1151, 600 cm^{-1} ; ^1H 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, $J_{\text{C-F}} = 36.5$ 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, $J_{\text{C-F}} = 285.2$ 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 $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{19}\text{H}_{17}\text{BrF}_3\text{N}_4\text{O}_2$: 469.0481; found: 469.0497.

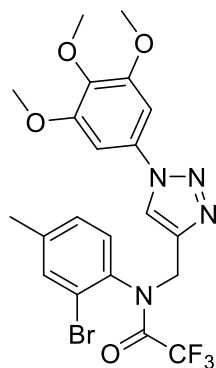


***N*-(2-bromo-4-methylphenyl)-2,2,2-trifluoro-*N*-((1-(2-fluoro-4-methylphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)acetamide, 2g:** 91% yield, 427.7 mg, 0.91 mmol; yellow solid; mp: 82–84 °C; R_f = 0.23 (*n*-hexane-EtOAc, 70:30); IR (neat): 3155, 1695, 1497, 1148, 823 cm^{-1} ; ^1H NMR (400.13 MHz, CDCl_3) 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, $J_{\text{C-F}} = 36.6$ Hz) (C), 153.0 (d, $J_{\text{C-F}} = 250.5$ Hz) (C), 141.9 (C), 141.7 (C), 141.4 (d, $J_{\text{C-F}} = 7.6$ Hz) (C), 134.9 (C), 133.9 (CH), 131.1 (CH), 128.9 (CH), 125.8 (d, $J_{\text{C-F}} = 3.3$ Hz) (CH), 125.2 (d, $J_{\text{C-F}} = 7.6$ Hz) (CH), 124.5 (CH), 122.9 (C), 122.5 (d, $J_{\text{C-F}} = 7.6$ Hz) (C), 117.3 (d, $J_{\text{C-F}} = 19.4$ Hz) (CH), 115.9 (q, $J_{\text{C-F}} = 285.2$ 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 $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{19}\text{H}_{16}\text{BrF}_4\text{N}_4\text{O}$: 471.0438; found: 471.0422.



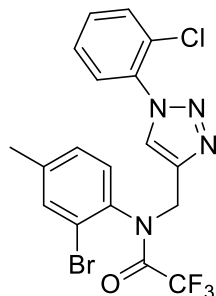
***N*-((1-benzyl-1*H*-1,2,3-triazol-4-yl)methyl)-*N*-(2-bromo-4-methylphenyl)-2,2,2-**

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, $J_{\text{C-F}}$ = 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, $J_{\text{C-F}}$ = 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 [$\text{M} + \text{H}$] $^+$ calcd for $\text{C}_{19}\text{H}_{17}\text{BrF}_3\text{N}_4\text{O}$: 453.0532; found: 453.0519.



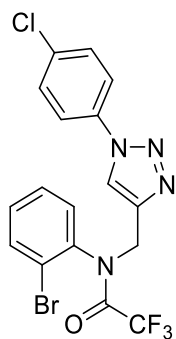
***N*-(2-bromo-4-methylphenyl)-2,2,2-trifluoro-*N*-((1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)acetamide, 2i:** 92% yield, 485.8 mg, 0.92 mmol; white solid; mp: 108-110 °C; R_f = 0.22 (*n*-hexane-EtOAc, 70:30); IR (neat): 3008, 1695, 1508, 1151, 774 cm^{-1} ; ^1H NMR (400.13 MHz, CDCl_3) δ 8.08 (bs, 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, $J_{\text{C-F}}$ = 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, $J_{C-F} = 287.5$ Hz) (C), 98.2 (CH), 61.1 (CH₃), 56.4 (CH₃), 46.1 (CH₂), 20.9 (CH₃); ¹⁹F NMR (376.5 MHz, CDCl₃) δ -68.9 (s); HRMS: m/z [M + H]⁺ calcd for C₂₁H₂₁BrF₃N₄O₄: 529.0693; found: 529.0675.



***N*-(2-bromophenyl)-*N*-((1-(2-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-2,2,2-**

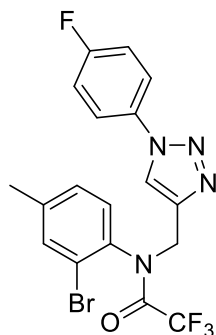
trifluoroacetamide, 2j: 89% yield, 419.3 mg, 0.89 mmol; pale brown solid; mp: 125-127 °C; R_f = 0.24 (*n*-hexane-EtOAc, 70:30); IR (neat): 3142, 1694, 1518, 1148, 840 cm⁻¹; ¹H NMR (400.13 MHz, CDCl₃) δ 8.09 (s, 1H), 7.67 – 7.56 (m, 2H), 7.53 (d, $J = 1.2$ Hz, 1H), 7.50 – 7.45 (m, 2H), 7.11 (dd, $J_1 = 8.1$ 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); ¹³C NMR (100.6 MHz, CDCl₃) δ 157.1 (q, $J_{C-F} = 35.2$ 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, $J_{C-F} = 288.0$ Hz) (C), 45.6 (CH₂), 20.9 (CH₃); ¹⁹F NMR (376.5 MHz, CDCl₃) δ -68.9 (s); HRMS: m/z [M + H]⁺ calcd for C₁₈H₁₄BrClF₃N₄O: 472.9986; found: 472.9966.



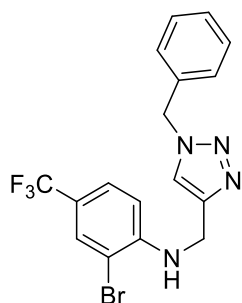
***N*-(2-bromophenyl)-*N*-((1-(4-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-2,2,2-**

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; ¹H NMR (400.13 MHz,

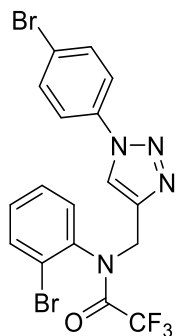
CDCl₃) δ 8.16 (s, 1H), 7.76 – 7.68 (m, 3H), 7.55 – 7.50 (m, 2H), 7.38 – 7.30 (m, 2H), 7.23 – 7.14 (m, 1H), 5.51 (d, J = 14.7 Hz, 1H), 4.50 (d, J = 14.7 Hz, 1H); ¹³C NMR (100.6 MHz, CDCl₃) δ 157 (q, J_{C-F} = 36.7 Hz) (C), 142.6 (C), 137.8 (C), 135.3 (C), 134.8 (C), 133.7 (CH), 131.5 (CH), 131.1 (CH), 130.0 (CH), 128.4 (CH), 123.3 (C), 122.2 (CH), 121.6 (CH), 115.9 (q, J_{C-F} = 285.8 Hz) (C), 46.0 (CH₂); ¹⁹F NMR (376.5 MHz, CDCl₃) δ -68.9 (s); HRMS: m/z [M + H]⁺ calcd for C₁₇H₁₂BrClF₃N₄O: 458.9830; found: 458.9848.



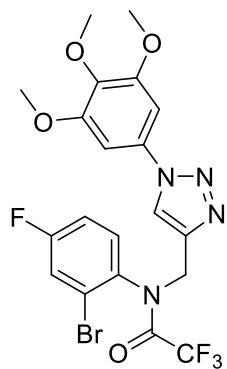
***N*-(2-bromo-4-methylphenyl)-2,2,2-trifluoro-*N*-((1-(4-fluorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)acetamide, 2l**: 94% yield, 428.6 mg, 0.94 mmol; yellow solid; mp: 128-130 °C; R_f = 0.19 (*n*-hexane-EtOAc, 70:30); IR (neat): 3138, 1695, 1518, 1144, 840 cm⁻¹; ¹H NMR (400.13 MHz, CDCl₃) δ 8.13 (s, 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); ¹³C NMR (100.6 MHz, CDCl₃) δ 162.5 (d, J_{C-F} = 248.5 Hz) (C), 157.2 (q, J_{C-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-F} = 3.7 Hz) (CH), 116.8 (d, J_{C-F} = 23.1 Hz) (CH), 115.8 (q, J_{C-F} = 288.2 Hz) (C), 46.1 (CH₂), 20.9 (CH₃); ¹⁹F NMR (376.5 MHz, CDCl₃) δ -68.9 (s), -111.8 (m); HRMS: m/z [M + H]⁺ calcd for C₁₈H₁₄BrF₄N₄O: 457.0282; found: 457.0275.



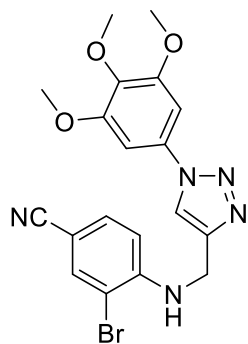
***N*-((1-benzyl-1*H*-1,2,3-triazol-4-yl)methyl)-2-bromo-4-(trifluoromethyl)aniline, 2m:** 70% yield, 287.7 mg, 0.70 mmol; yellow solid; mp: 118-120 °C; R_f = 0.16 (*n*-hexane-EtOAc, 75:25); IR (neat): 3378, 3068, 1324, 1109, 745 cm^{-1} ; ^1H NMR (400.13 MHz, CDCl_3) δ 7.67 (d, J = 1.2 Hz, 1H), 7.45 – 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, $J_{\text{C-F}}$ = 3.7 Hz) (CH), 129.2 (CH), 128.8 (CH), 128.0 (CH), 125.8 (q, $J_{\text{C-F}}$ = 3.7 Hz) (CH), 123.8 (q, $J_{\text{C-F}}$ = 271.8 Hz) (C), 121.6 (CH), 119.9 (q, $J_{\text{C-F}}$ = 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 $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{17}\text{H}_{15}\text{BrF}_3\text{N}_4$: 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, $J_{\text{C-F}}$ = 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, $J_{\text{C-F}}$ = 285.1 Hz), 46.0 (CH_2); ^{19}F NMR (376.5 MHz, CDCl_3) δ -68.9 (s); HRMS: m/z $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{17}\text{H}_{12}\text{Br}_2\text{F}_3\text{N}_4\text{O}$: 504.9304; found: 504.9327.

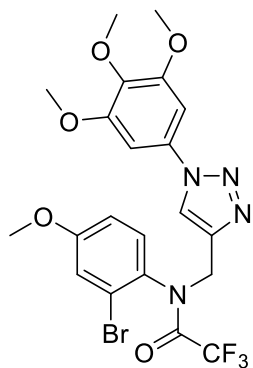


***N*-(2-bromo-4-fluorophenyl)-2,2,2-trifluoro-*N*-((1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)acetamide, 2o**: 73% yield, 389.3 mg, 0.73 mmol; white solid; mp: 118-120 °C; R_f = 0.22 (*n*-hexane-EtOAc, 60:40); IR (neat): 3723, 1705, 1504, 1151, 773 cm^{-1} ; ^1H NMR (400.13 MHz, CDCl_3) 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, $J_{\text{C-F}} = 255.5$ Hz) (C), 157.1 (q, $J_{\text{C-F}} = 36.7$ Hz) (C), 153.9 (C), 142.1 (C), 138.4 (C), 134.8 (d, $J_{\text{C-F}} = 3.4$ Hz) (C), 133.7 (d, $J_{\text{C-F}} = 9.0$ Hz) (CH), 132.6.0 (C), 124.2 (d, $J_{\text{C-F}} = 10.2$ Hz) (C), 122.3 (CH), 121.0 (d, $J_{\text{C-F}} = 25.6$ Hz) (CH), 115.8 (q, $J_{\text{C-F}} = 288.0$ Hz) (C), 115.5 (d, $J_{\text{C-F}} = 22.3$ 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 $[\text{M} + \text{H}]^+$ calcd $\text{C}_{20}\text{H}_{18}\text{BrF}_4\text{N}_4\text{O}_4$: 535.0442; found: 535.0463.

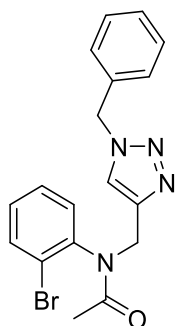


3-bromo-4-(((1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)amino)benzonitrile, 2p: 90% yield, 400,0 mg, 0.9 mmol; white solid; mp: 121-123 °C; R_f = 0.22 (*n*-hexane-EtOAc, 50:50); IR (neat): 3753, 3712, 3252, 2158, 2029, 1510, 1127, 826 cm^{-1} ; ^1H NMR (400.13 MHz, CDCl_3) δ 7.81 (s, 1H),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

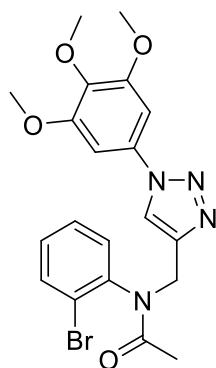
4.58 (s, 2H), 3.85 (s, 6H), 3.81 (s, 3H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 153.9 (C), 147.6 (C), 144.9 (C), 138.6 (C), 135.9 (CH), 133.0 (CH), 132.7 (C), 120.2 (CH), 118.7 (C), 110.8 (CH), 109.0 (C), 100.6 (C), 98.6 (CH), 61.1 (CH_3), 56.5 (CH_3), 39.4 (CH_2); HRMS: m/z $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{19}\text{H}_{19}\text{BrN}_5\text{O}_3$: 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} ; ^1H 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, $J_{\text{C-F}}$ = 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, $J_{\text{C-F}}$ = 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 $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{21}\text{H}_{21}\text{BrF}_3\text{N}_4\text{O}_5$: 545.0642; found: 545.0623.

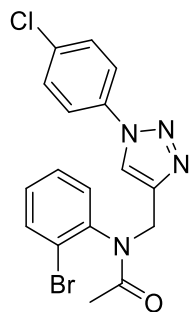


***N*-((1-benzyl-1*H*-1,2,3-triazol-4-yl)methyl)-*N*-(2-bromophenyl)acetamide, 3a:** 92% yield, 365.7 mg, 0.95 mmol; pale yellow solid; mp: 112-114 °C; R_f = 0.20 (*n*-hexane-EtOAc, 60:40); IR (neat): 3139, 2955, 1655, 1369, 1044, 709 cm^{-1} ; ^1H NMR (400.13 MHz, CDCl_3) δ 7.65 (dd, J_1 = 8.0 Hz, J_2 = 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 $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{18}\text{H}_{18}\text{BrN}_4\text{O}$: 385.0858; found: 385.0839.

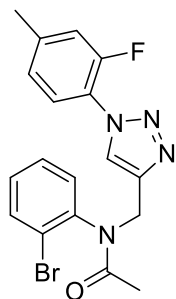


***N*-(2-bromophenyl)-*N*-((1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)acetamide, 3b:** 96% yield, 442.6 mg, 0.96 mmol; pale yellow solid; mp: 156-158 °C; R_f = 0.24 (*n*-hexane-EtOAc, 60:40); IR (neat): 3117, 2983, 1663, 1473, 763 cm^{-1} ; ^1H NMR (400.13 MHz, CDCl_3) δ 8.13 (s, 1H), 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 (CH₃), 56.4 (CH₃), 43.8 (CH₂), 22.3 (CH₃); HRMS: m/z [M + H]⁺ calcd for C₂₀H₂₂BrN₄O₄: 461.0819; found: 461.0833.

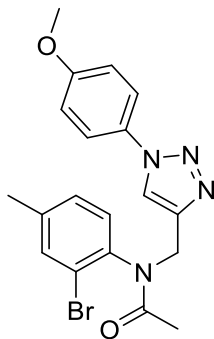


***N*-(2-bromophenyl)-*N*-((1-(2-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)acetamide, 3c:** 85% yield, 344.2 mg, 0.85 mmol; yellow liquid; R_f = 0.18 (*n*-hexane-EtOAc, 60:40); IR (neat): 3068, 1665, 1476, 1038, 759 cm⁻¹; ¹H NMR (400.13 MHz, CDCl₃) δ 7.61 (s, 1H), 7.59 (dd, J_1 = 8.0 Hz, J_2 = 1.2 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); ¹³C NMR (100.6 MHz, CDCl₃) 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 (CH₂), 22.3 (CH₃); HRMS: m/z [M + H]⁺ calcd for C₁₇H₁₅BrClN₄O: 405.0112; found: 405.0127.



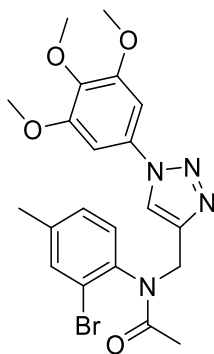
***N*-(2-bromophenyl)-*N*-((1-(2-fluoro-4-methylphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)acetamide, 3d:** 85% yield, 341.7 mg, 0.85 mmol; white oil; R_f = 0.25 (*n*-hexane-EtOAc, 50:50); IR (neat): 3178, 1657, 1046, 766, 562 cm⁻¹; ¹H NMR (400.13 MHz, CDCl₃) δ 8.16 (s, 1H), 7.78 (t, J = 7.9 Hz, 1H), 7.70 (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); ¹³C NMR (100.6 MHz, CDCl₃) 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, $J_{C-F} = 10.1$ Hz) (C), 117.3 (d, $J_{C-F} = 19.7$ Hz) (CH), 43.5 (CH₂), 22.3 (CH₃), 21.2 (CH₃); ¹⁹F NMR (376.5 MHz, CDCl₃) δ -124.30 (t, $J = 9.5$ Hz); HRMS: m/z [M + H]⁺ calcd for C₁₈H₁₇BrFN₄O: 403.0564; found: 403.0539.



***N*-(2-bromo-4-methylphenyl)-*N*-((1-(4-methoxyphenyl)-1*H*-1,2,3-triazol-4-**

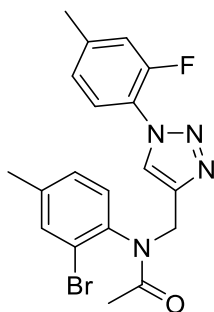
yl)methyl)acetamide, 3e: 98% yield, 405.7 mg, 0.98 mmol; white solid; mp: 120-122 °C; $R_f = 0.24$ (*n*-hexane-EtOAc, 60:40); IR (neat): 3144, 1649, 1431, 1042, 567 cm⁻¹; ¹H NMR (400.13 MHz, CDCl₃) δ 8.20 (bs, 1H), 7.66 (d, $J = 7.3$ Hz, 2H), 7.51 (s, 1H), 7.20 – 6.92 (m, 4H), 5.35 (bs, 1H), 4.46 (bs, 1H), 3.88 (s, 3H), 2.37 (s, 3H), 1.85 (s, 3H); ¹³C NMR (100.6 MHz, CDCl₃) 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 (CH₃), 43.8 (CH₂), 22.3 (CH₃), 20.8 (CH₃); HRMS: m/z [M + H]⁺ calcd for C₁₉H₂₀BrN₄O₂: 415.0764; found: 415.0776.



***N*-(2-bromo-4-methylphenyl)-*N*-((1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,3-triazol-4-**

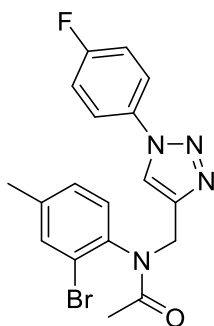
yl)methyl)acetamide, 3f: 83% yield, 394.2 mg, 0.83 mmol; white oil; mp: 138-140 °C; $R_f = 0.22$ (*n*-hexane-EtOAc, 60:40); IR (neat): 3415, 2967, 1656, 1127, 572 cm⁻¹; ¹H NMR (400.13 MHz, CDCl₃) δ 8.14 (s, 1H), 7.51 (s, 1H), 7.13 (d, $J = 7.8$ Hz, 1H), 7.04 (d, $J = 7.8$ Hz, 1H), 6.97 (s, 2H), 5.33

(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 $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{21}\text{H}_{24}\text{BrN}_4\text{O}_4$: 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} ; ^1H 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, $J_{\text{C-F}} = 60.3$ Hz) (C), 152.0 (C), 143.9 (C), 141.2 (d, $J_{\text{C-F}} = 7.3$ Hz) (C), 140.5 (C), 138.8 (C), 134.1 (CH), 130.5 (CH), 129.6 (CH), 125.7 (d, $J_{\text{C-F}} = 3.1$ Hz) (CH), 124.9 (d, $J_{\text{C-F}} = 7.5$ Hz) (C), 124.5 (CH), 123.2 (C), 117.30 (d, $J_{\text{C-F}} = 19.5$ 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 $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{19}\text{H}_{19}\text{BrFN}_4\text{O}$: 417.0721; found: 417.0740.



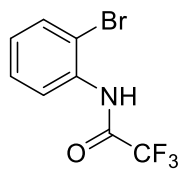
***N*-(2-bromo-4-methylphenyl)-*N*-((1-(4-fluorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)acetamide,**
3h: 93% yield, 374.8 mg, 0.93 mmol; white solid; mp: 155-157 °C; R_f = 0.23 (*n*-hexane-EtOAc, 60:40); IR (neat): 3140, 1653, 1515, 1042, 839 cm^{-1} ; ^1H NMR (400.13 MHz, CDCl_3) δ 8.12 (s, 1H), 7.76 – 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, $J_{\text{C-F}}$ = 250.1 Hz) (C), 144.7 (C), 140.6 (C), 139.0 (C), 134.2 (CH), 133.3 (d, $J_{\text{C-F}}$ = 3.0 Hz) (C), 130.4 (CH), 129.7 (CH), 123.1 (C), 122.4 (d, $J_{\text{C-F}}$ = 8.7 Hz) (CH), 122.1 (CH), 116.6 (d, $J_{\text{C-F}}$ = 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 $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{18}\text{H}_{17}\text{BrFN}_4\text{O}$: 403.0564; found: 403.0580.

References

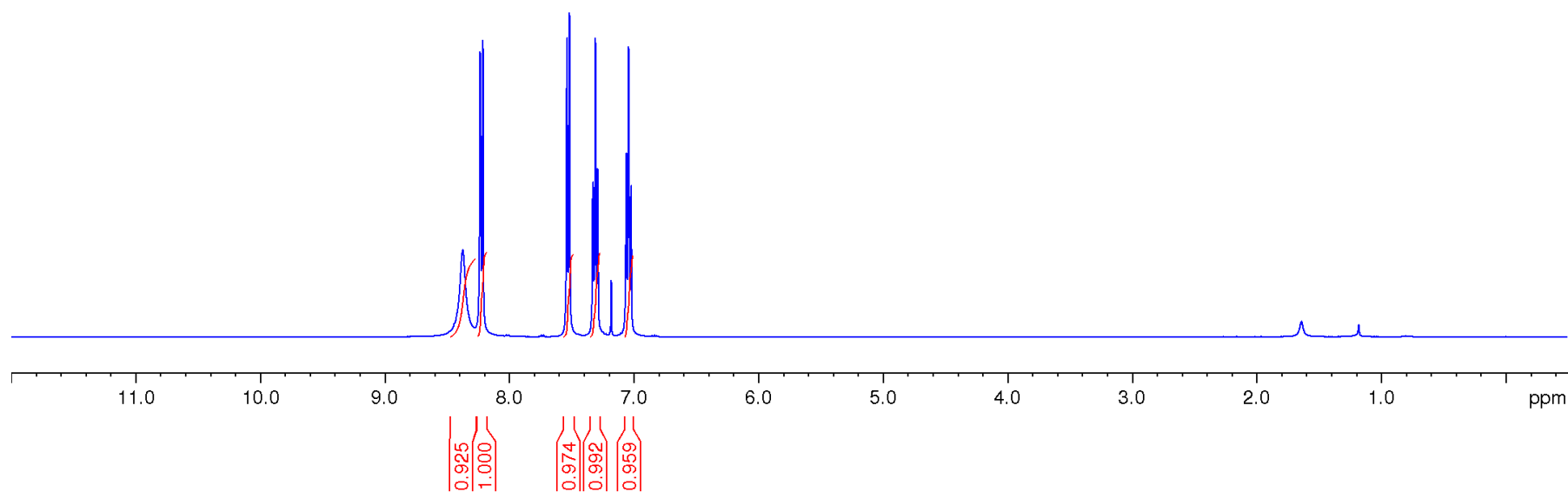
- S1.** Leggy, Arnold A.; Wenchen, Luo; and Kiplin, Guy R.; **Org. Lett.**, 2004, 6, 17, 3005 – 3007.
- S2.** Losa, Romain; Lorton, Charlotte; Retailleau, Pascal; Bignon, Jérôme; and Voituriez, Arnaud; **Org. Lett.**, 2023, 25, 27, 5140 – 5144.
- S3.** Benedí, Carolina; Bravo, Fernando; Uriz, Pedro; Fernández, Elena; Claver, Carmen; and Castellón, Sergio; **Tetrahedron Lett.**, 2003, 44, 6073 – 6077.
- S4.** Alcaide Benito, Almendros Pedro, Cembellín Sara, Martínez Teresa del Campo, Alejandro Muñoz; **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.

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

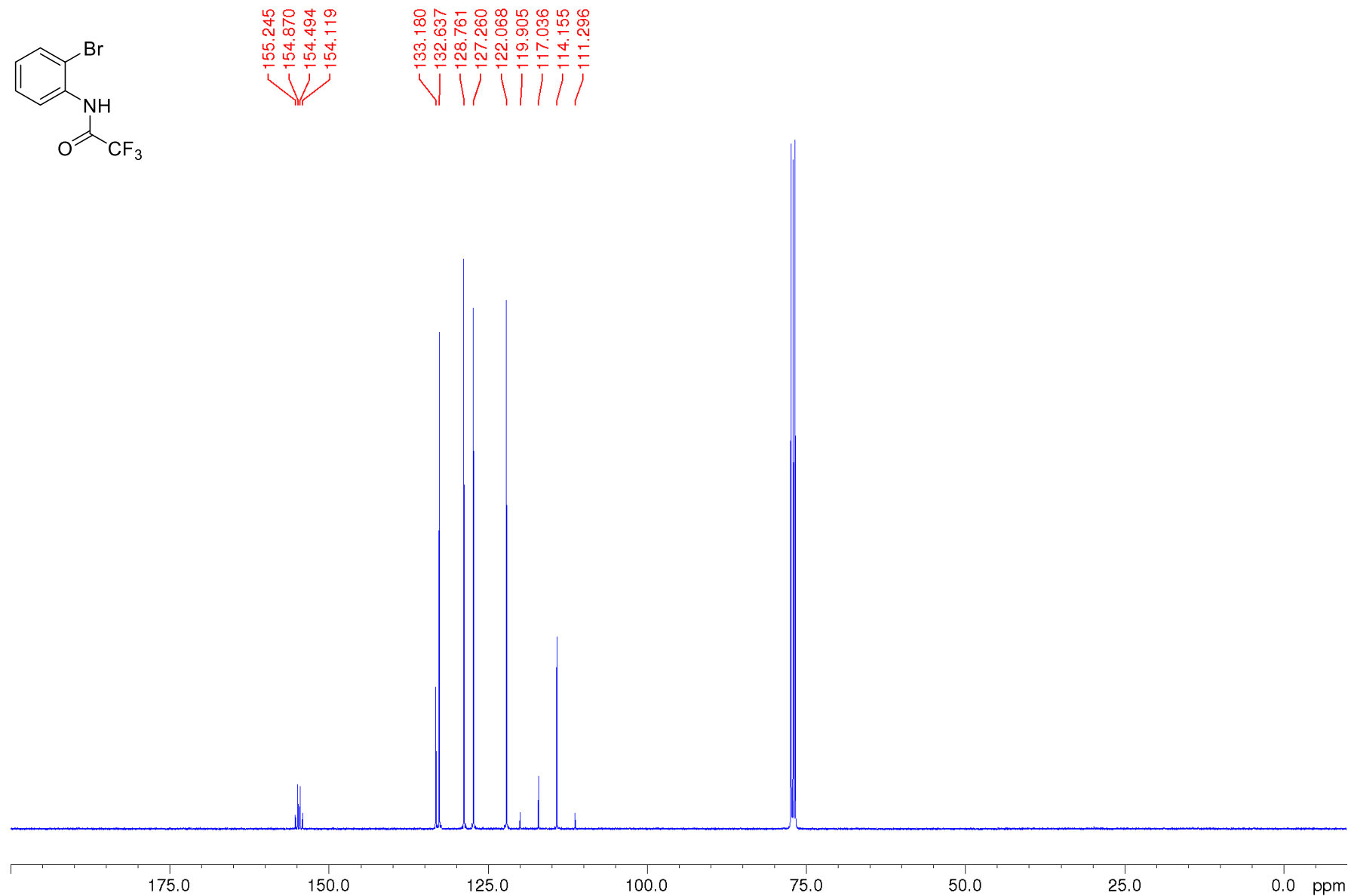
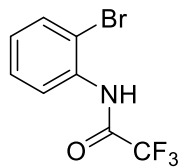
^1H NMR-spectrum (400 MHz, CDCl_3)



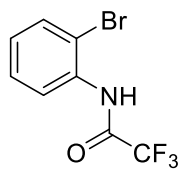
8.373
8.234
8.231
8.213
8.210
7.537
7.534
7.517
7.514
7.329
7.326
7.308
7.289
7.287
7.061
7.058
7.041
7.039
7.023
7.019



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



DEPT 135 NMR-spectrum (CDCl₃)



132.639
128.769
127.257
122.062

175.0

150.0

125.0

100.0

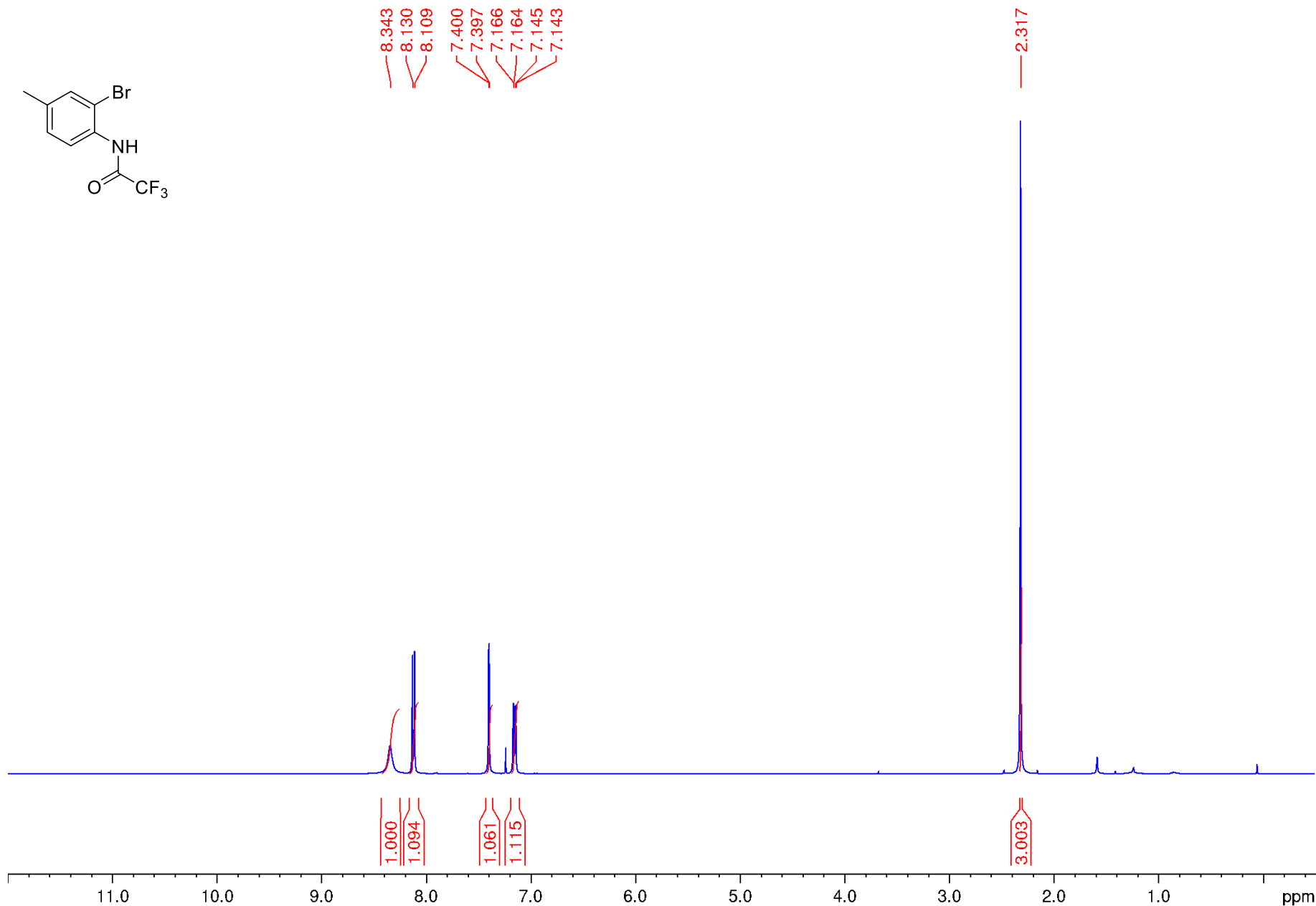
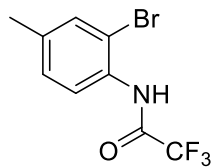
75.0

50.0

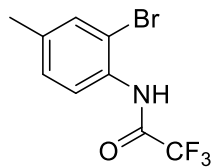
25.0

ppm

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



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



155.132
154.758
154.383
154.010

137.651
132.893
130.591
129.337

121.887
117.090
114.019

20.688

175.0

150.0

125.0

100.0

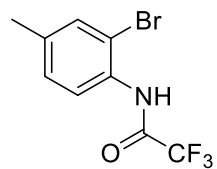
75.0

50.0

25.0

ppm

DEPT 135 NMR-spectrum (CDCl_3)



132.893
129.337
121.886

20.688

175.0

150.0

125.0

100.0

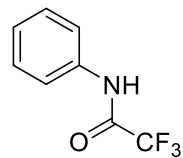
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50.0

25.0

ppm

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

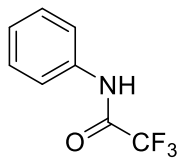


7.917
7.500
7.481
7.339
7.320
7.299
7.190
7.184
7.171
7.153

1.000
2.032
2.056
1.039

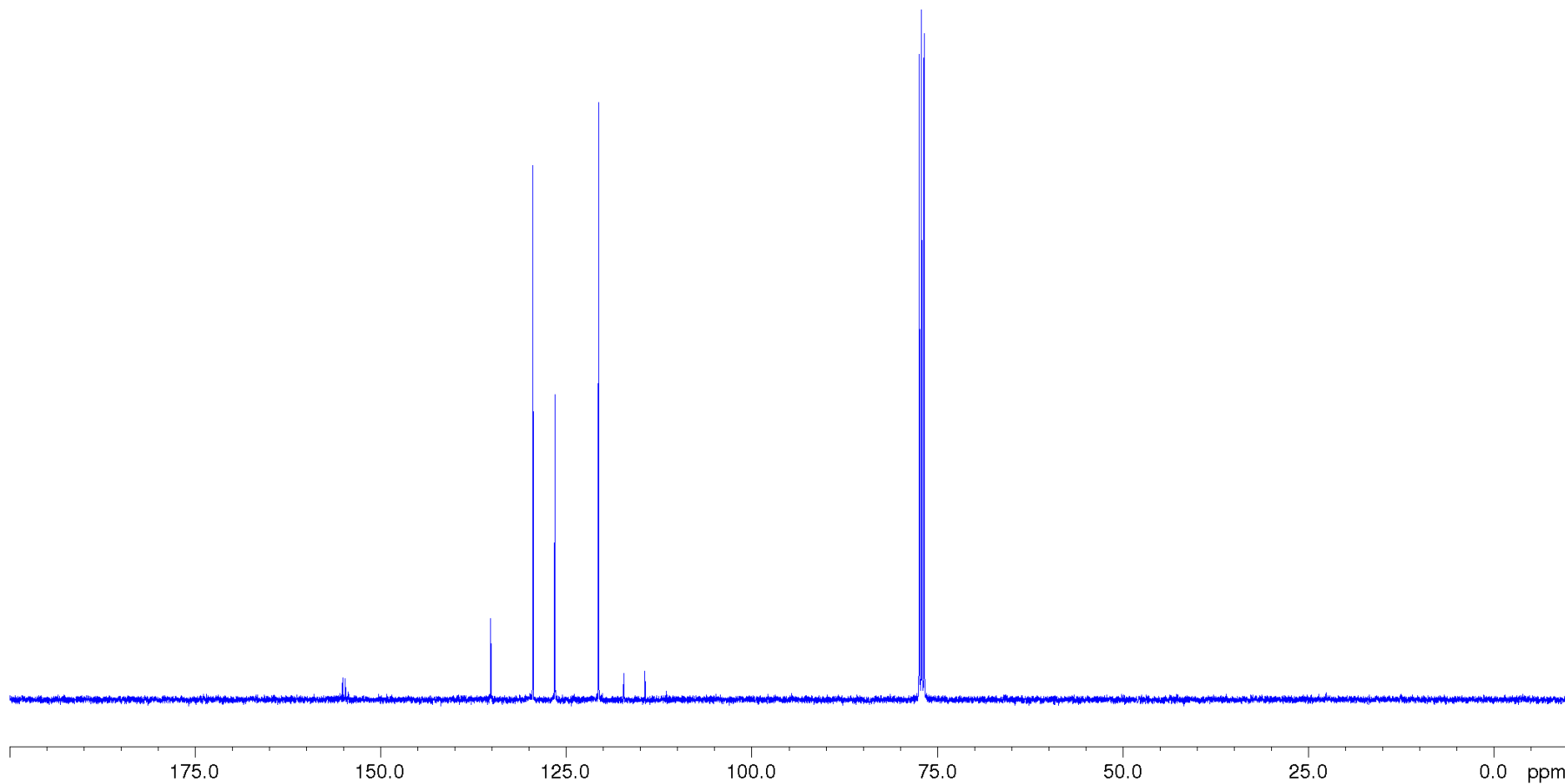
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 ppm

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

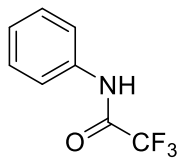


Chemical shift values (ppm) for the peaks in the spectrum:

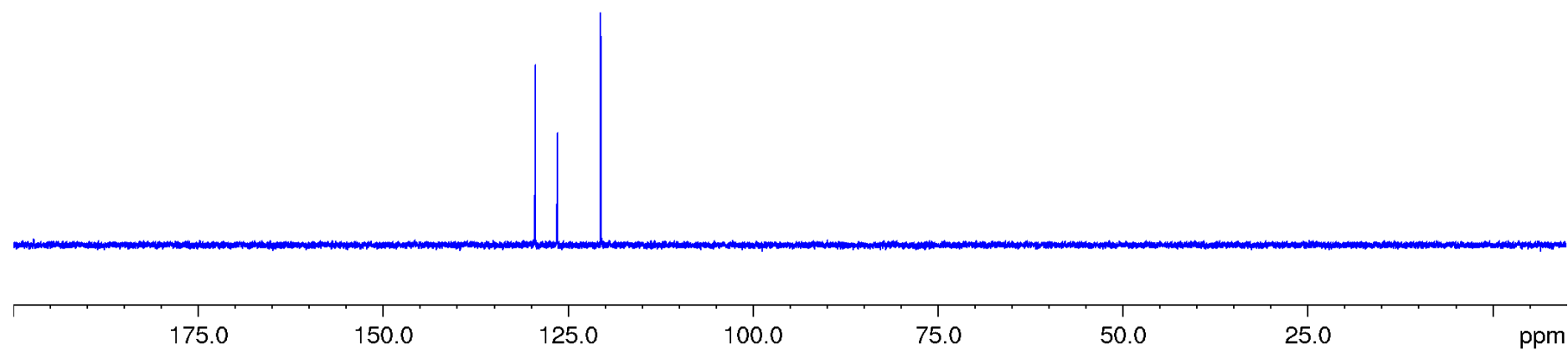
- 155.430
- 155.039
- 154.668
- 154.297
- 135.074
- 129.392
- 126.422
- 120.543
- 120.072
- 117.164
- 114.295
- 111.427
- 77.353
- 77.035
- 76.717



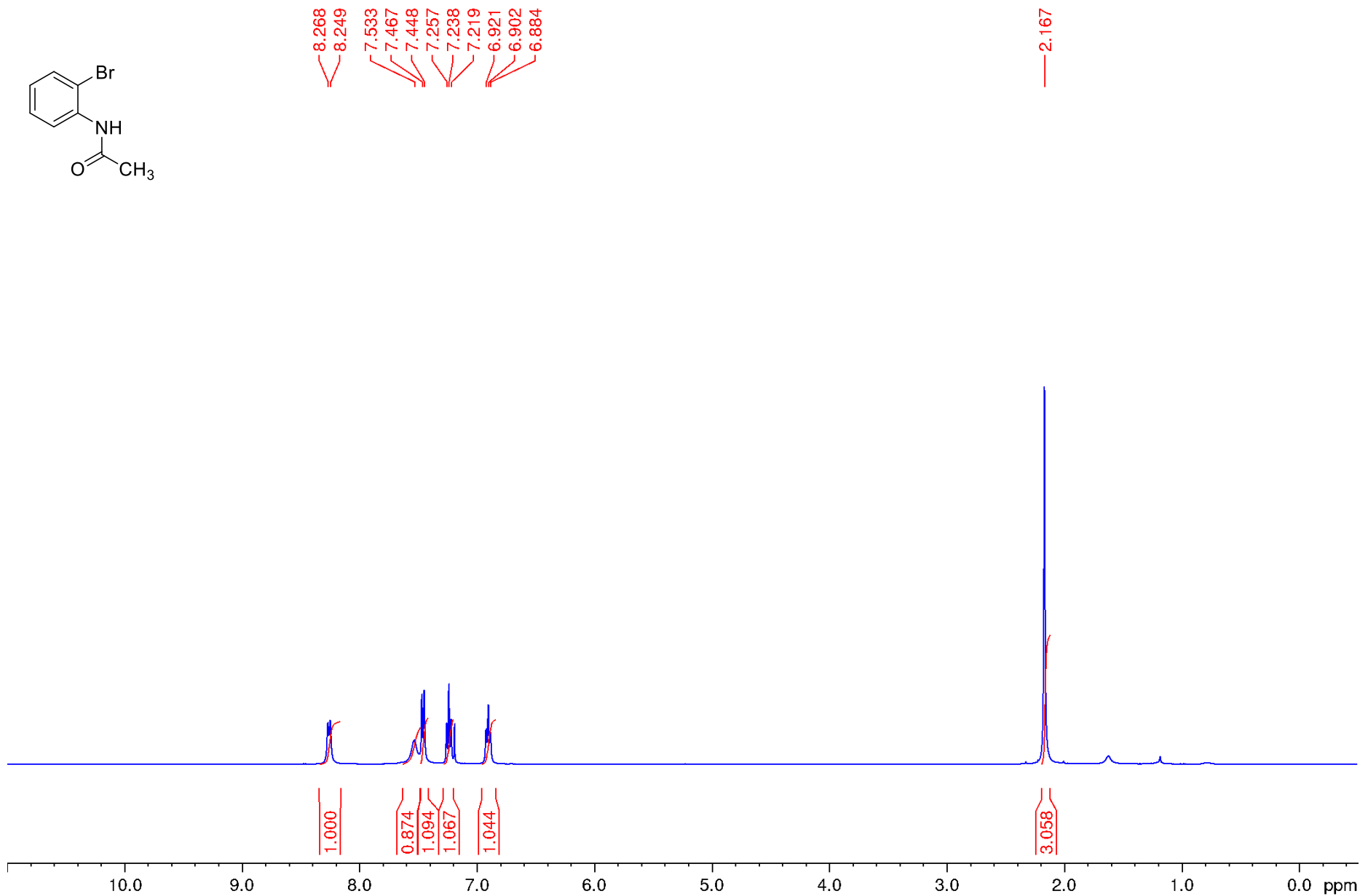
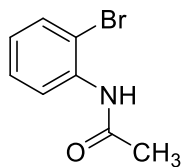
DEPT 135 NMR-spectrum (CDCl₃)



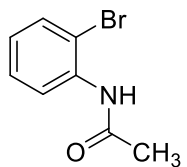
129.391
126.421
120.543



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



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



— 168.239

— 135.712

— 132.212

— 128.414

— 125.174

— 121.937

— 113.198

— 24.898

175.0

150.0

125.0

100.0

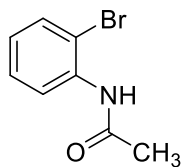
75.0

50.0

25.0

ppm

DEPT 135 NMR-spectrum (CDCl_3)



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125.172
121.936

24.898

175.0

150.0

125.0

100.0

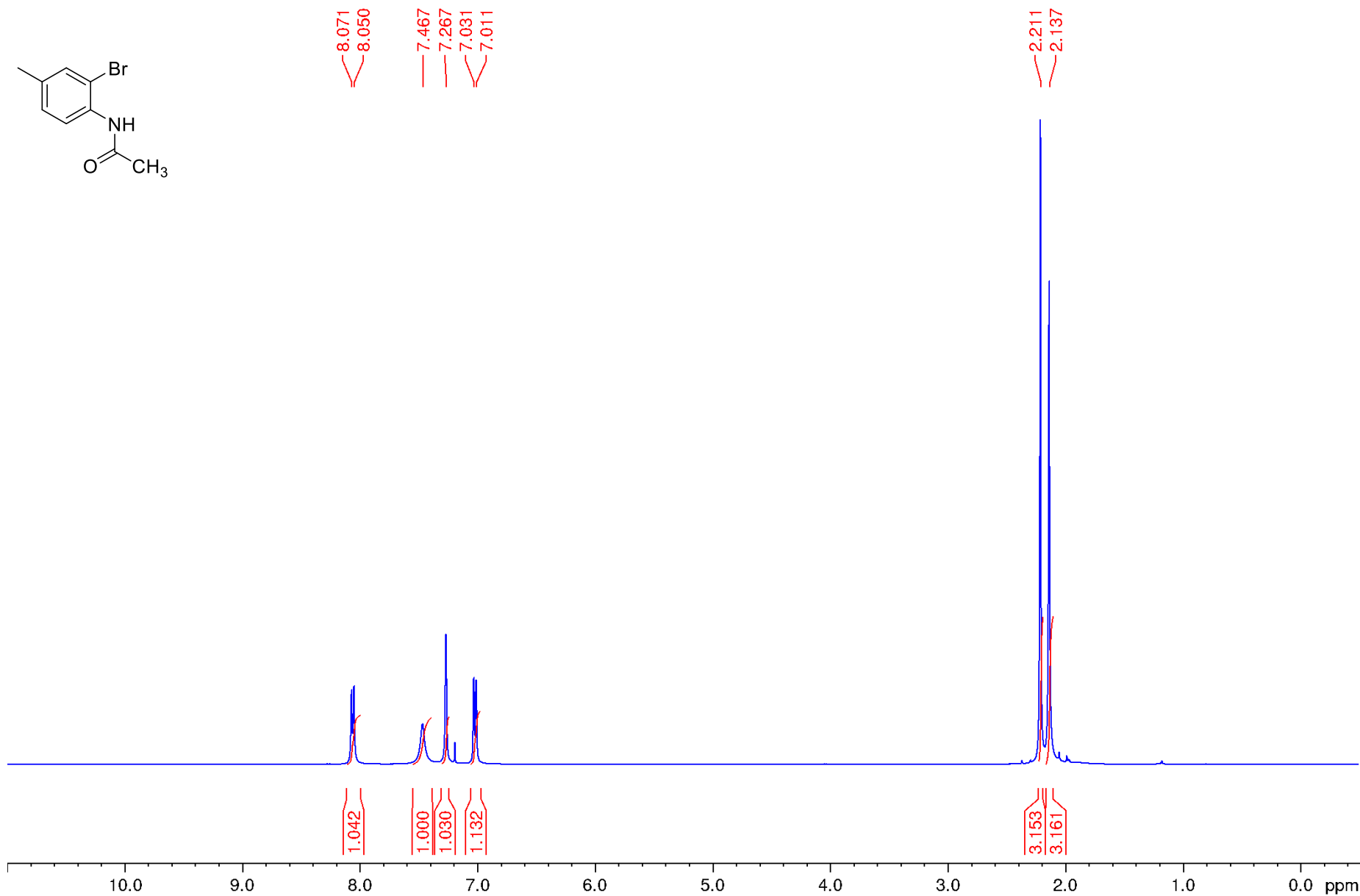
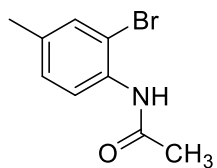
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50.0

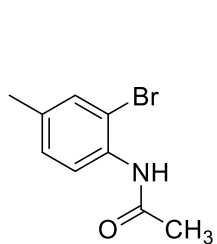
25.0

ppm

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



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



168.197

135.321

133.144

132.444

128.981

122.030

113.334

24.758

20.544

175.0

150.0

125.0

100.0

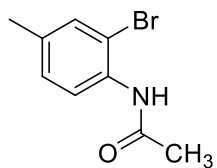
75.0

50.0

25.0

ppm

DEPT 135 NMR-spectrum (CDCl₃)



132.444
128.981
122.028

24.760
20.544

175.0

150.0

125.0

100.0

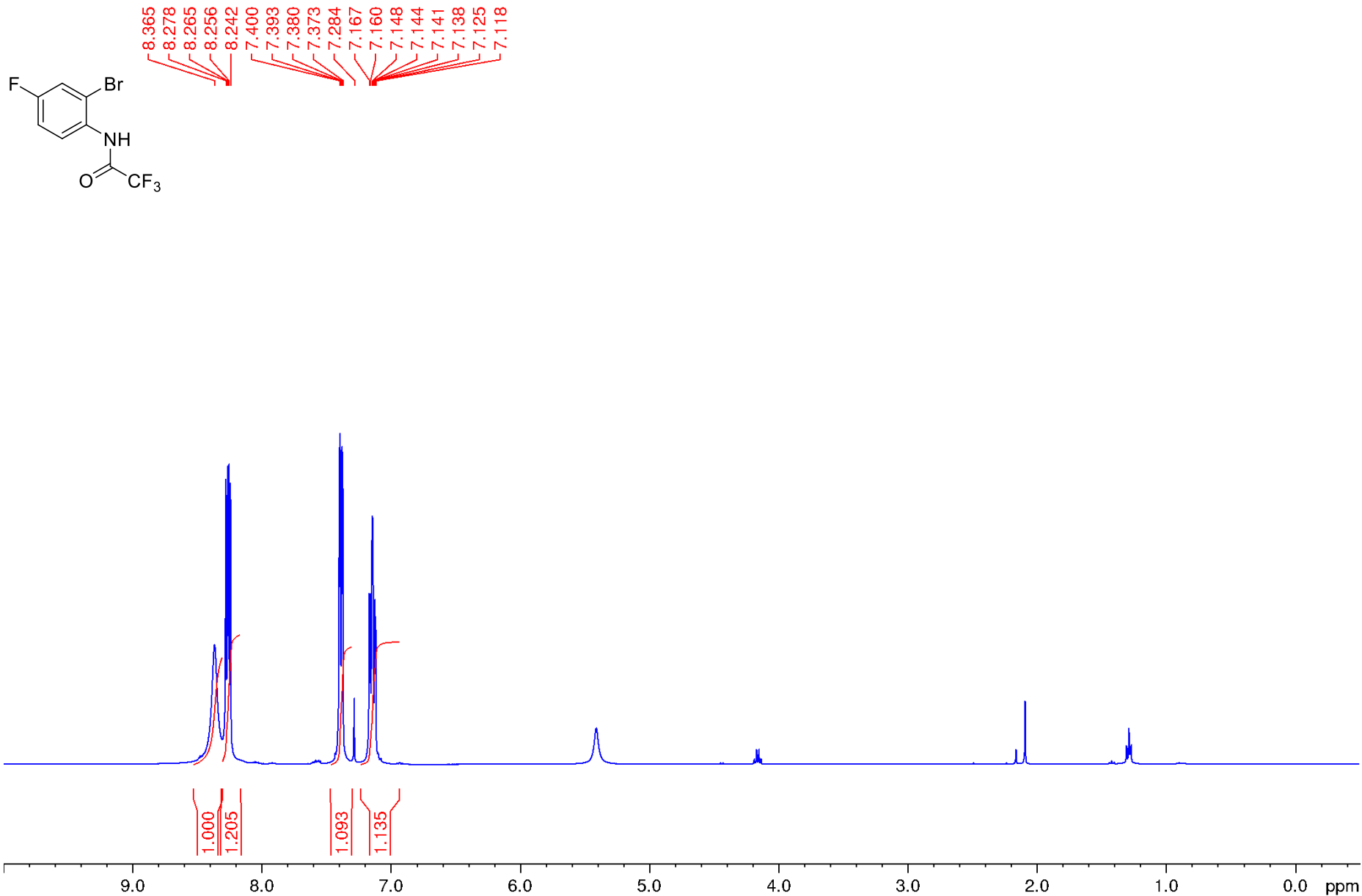
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50.0

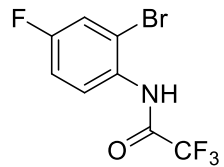
25.0

ppm

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



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



160.986
158.487
155.383
155.008
154.629
154.251

129.588
129.555
123.523
123.439
120.070
119.813
117.016
115.821
115.601
114.812
114.716
114.149
111.283

77.345
77.028
76.709

175.0

150.0

125.0

100.0

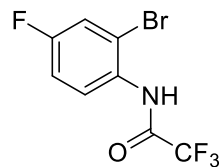
75.0

50.0

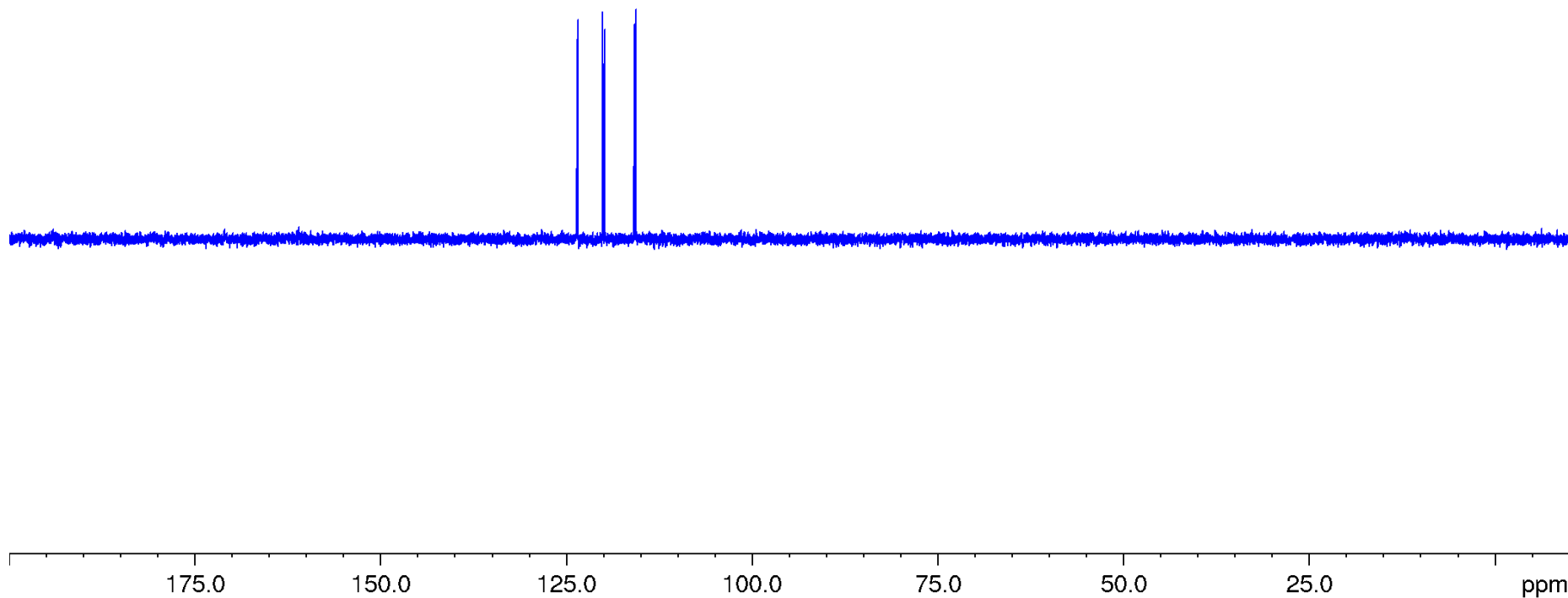
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ppm

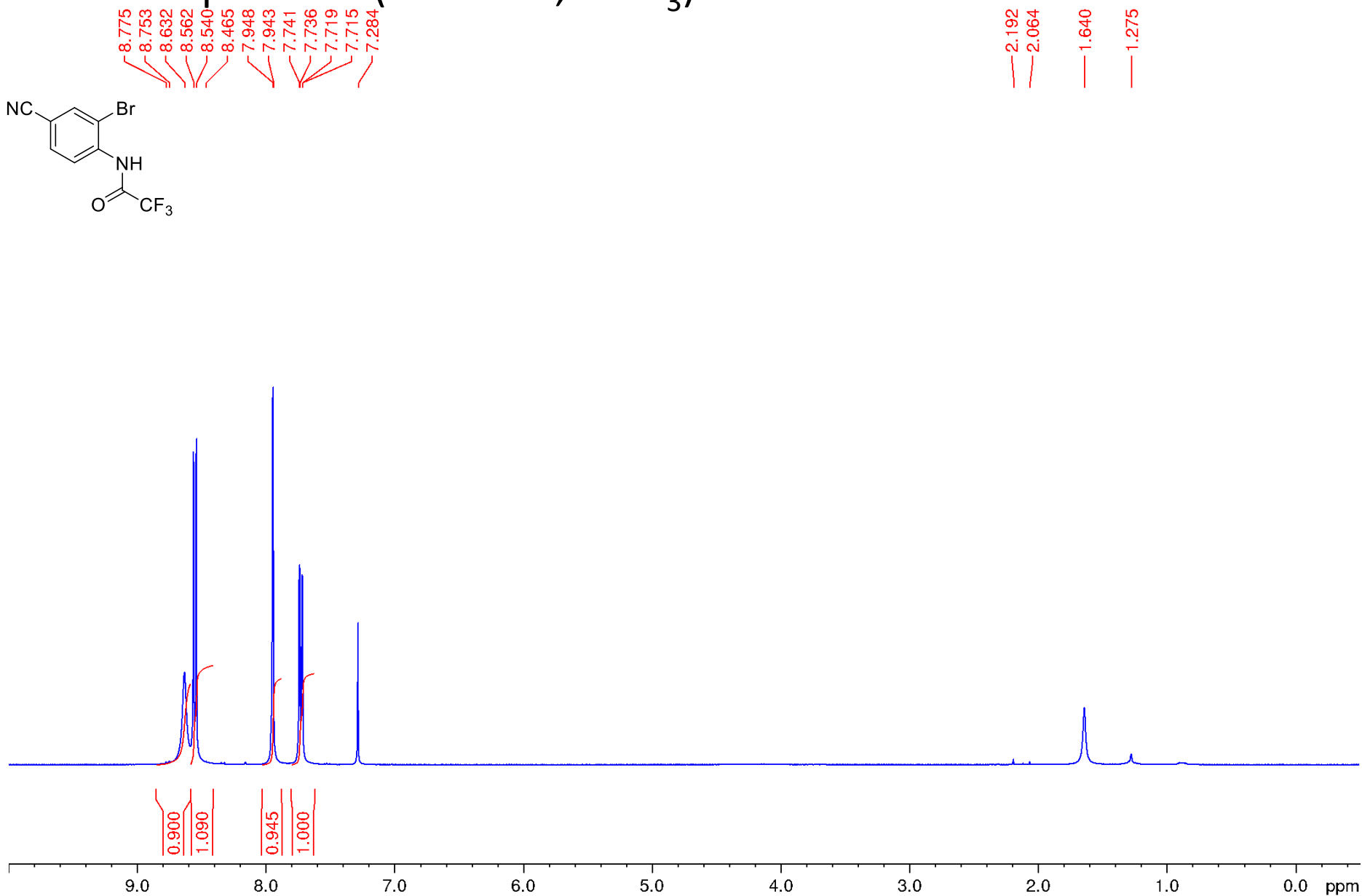
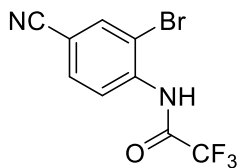
DEPT 135 NMR-spectrum (CDCl_3)



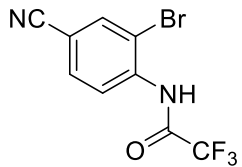
123.523
123.439
120.070
119.813
115.821
115.601



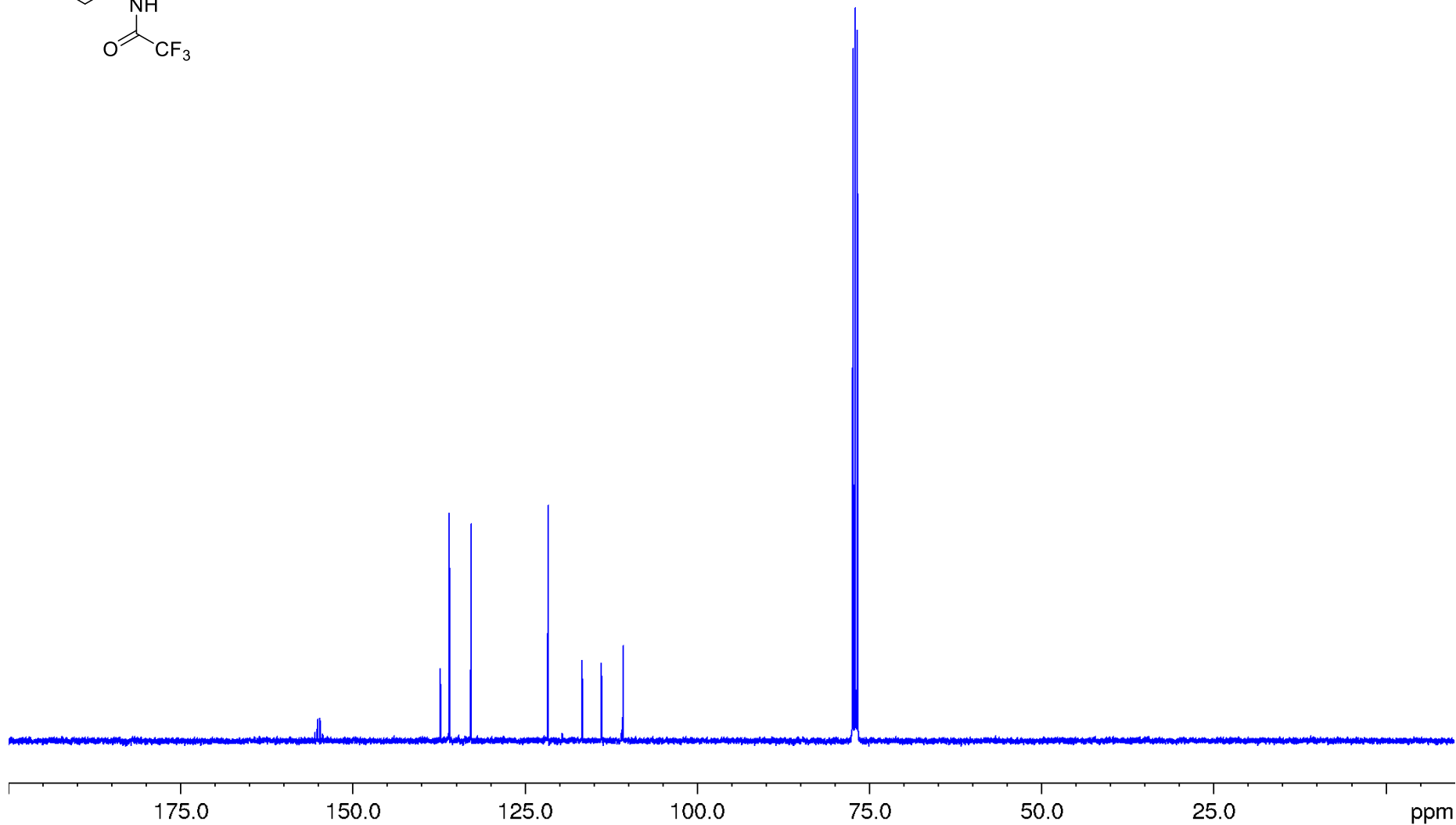
^1H NMR-spectrum (400 MHz, CDCl_3)



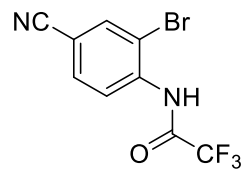
^{13}C NMR-spectrum (100 MHz, CDCl_3)



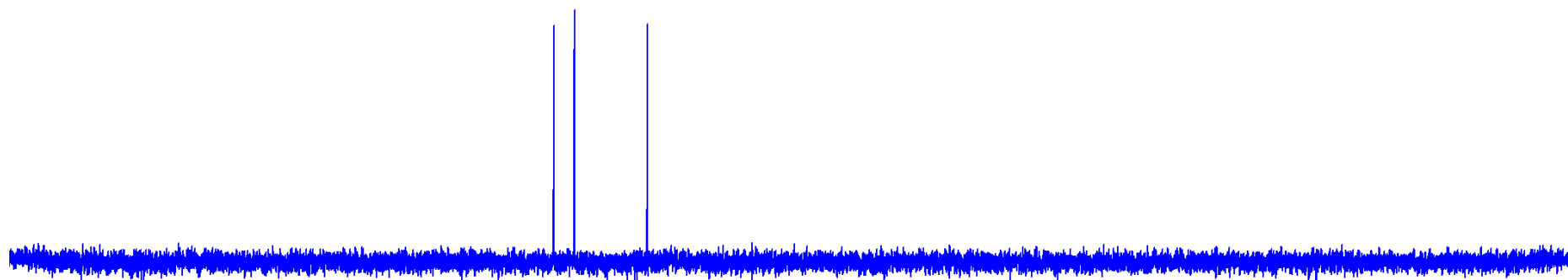
155.504
155.119
154.735
154.367
137.257
135.967
132.810
121.636
119.555
116.677
113.876
113.816
110.948
110.692



DEPT 135 NMR-spectrum (CDCl_3)



135.966
132.809
121.634



200.0

175.0

150.0

125.0

100.0

75.0

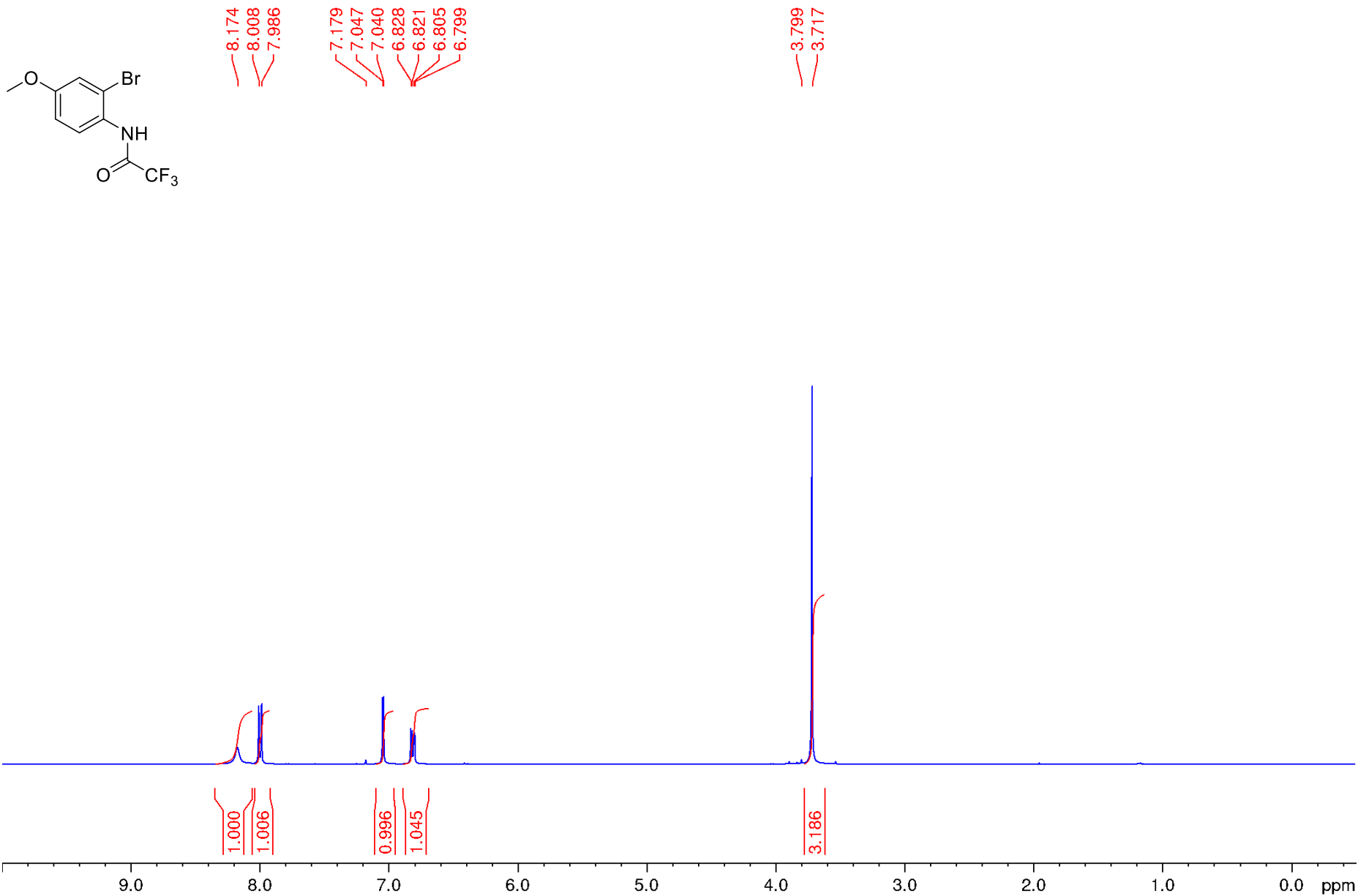
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25.0

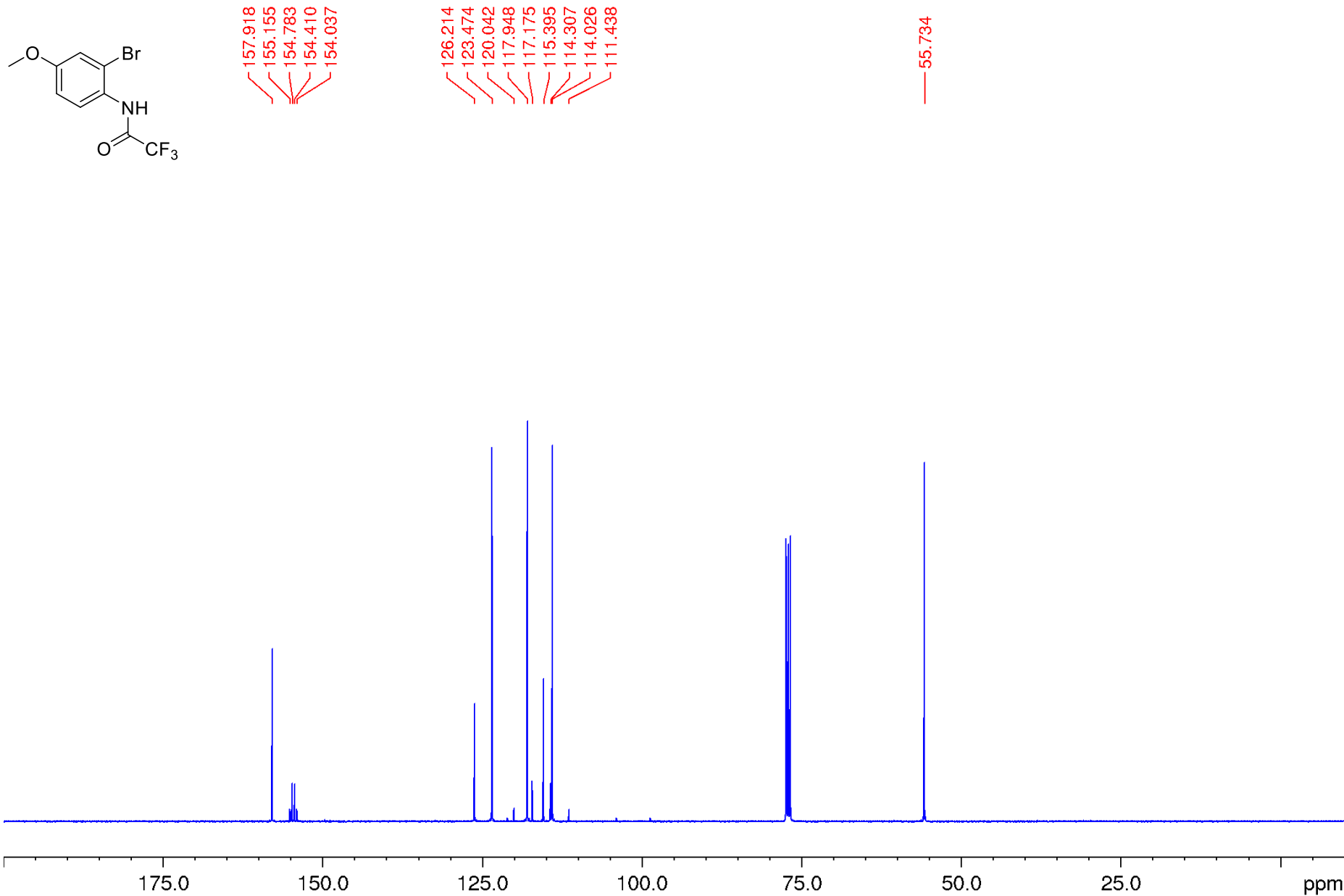
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ppm

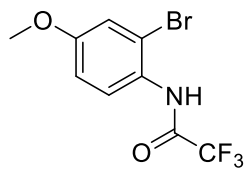
^1H NMR-spectrum (400 MHz, CDCl_3)



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



DEPT 135 NMR-spectrum (CDCl_3)



123.473

117.948

114.025

55.732

175.0

150.0

125.0

100.0

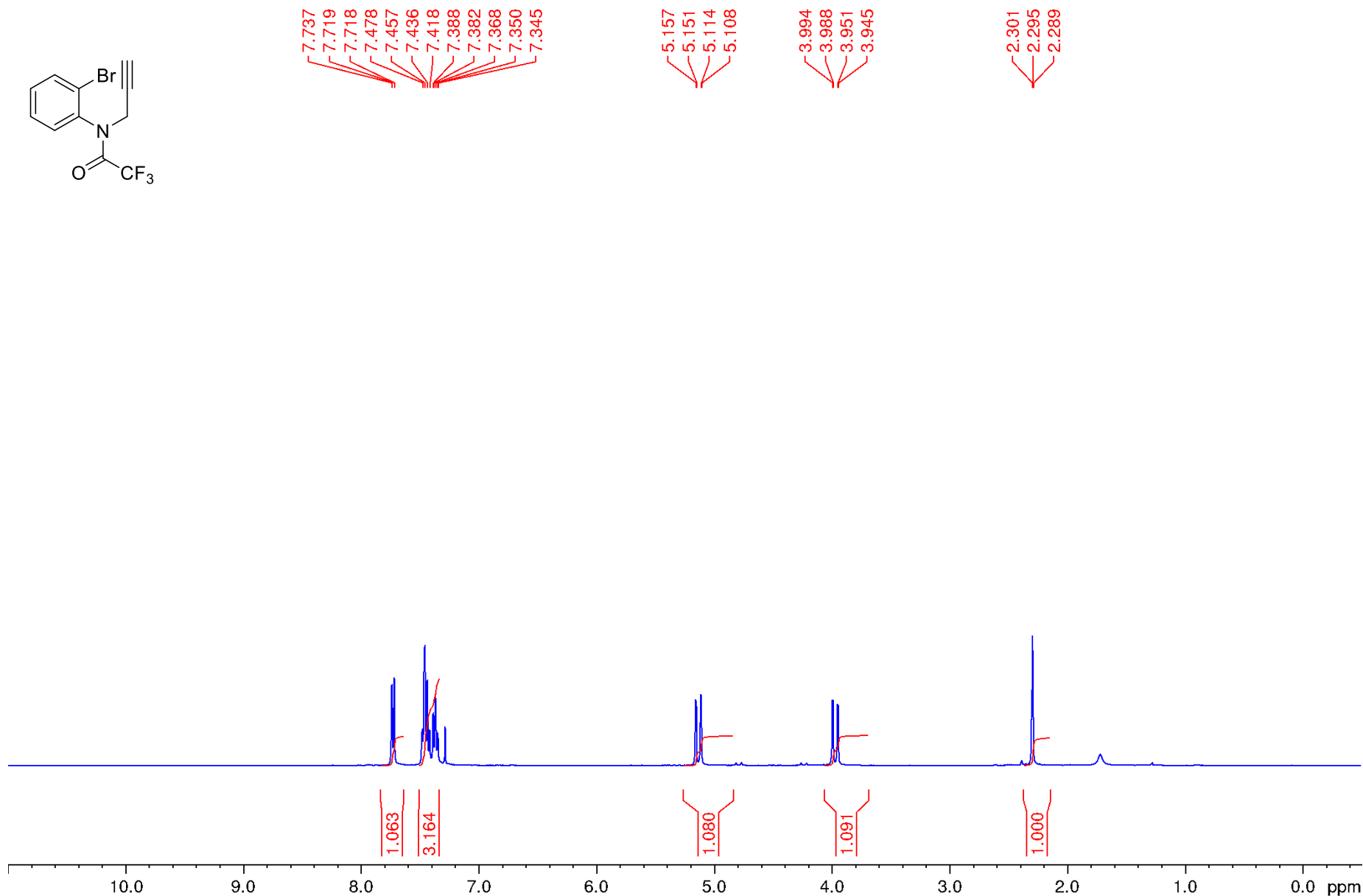
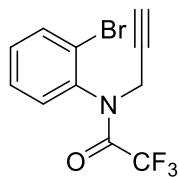
75.0

50.0

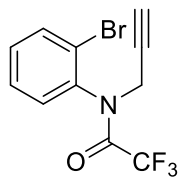
25.0

ppm

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



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



157.057
156.693
156.326
155.960

136.599
133.609
131.871
131.269
128.121
123.456
120.150
117.284
114.418
111.552

76.431
74.106

39.178

175.0

150.0

125.0

100.0

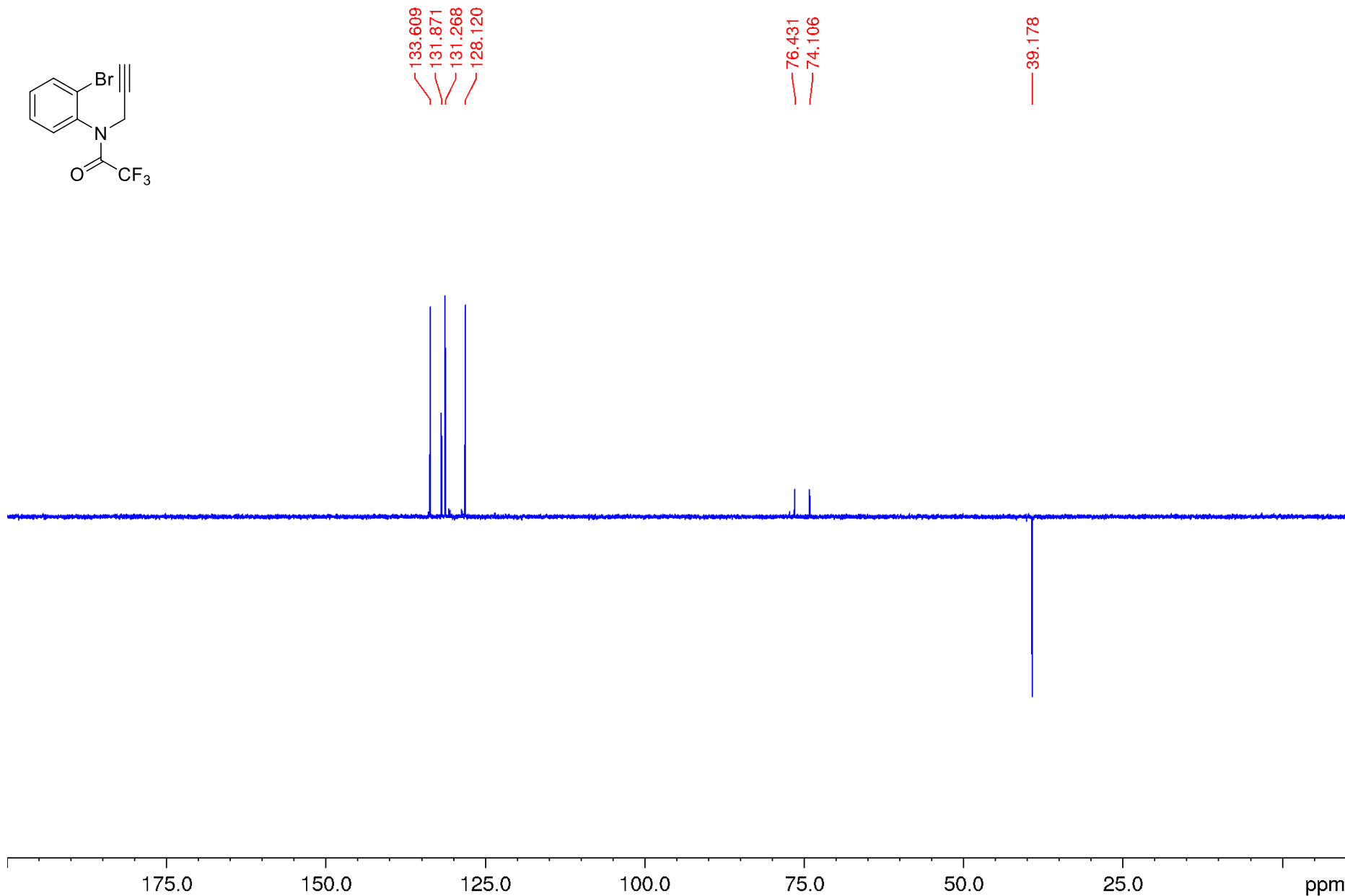
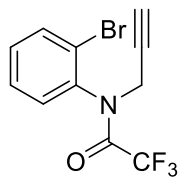
75.0

50.0

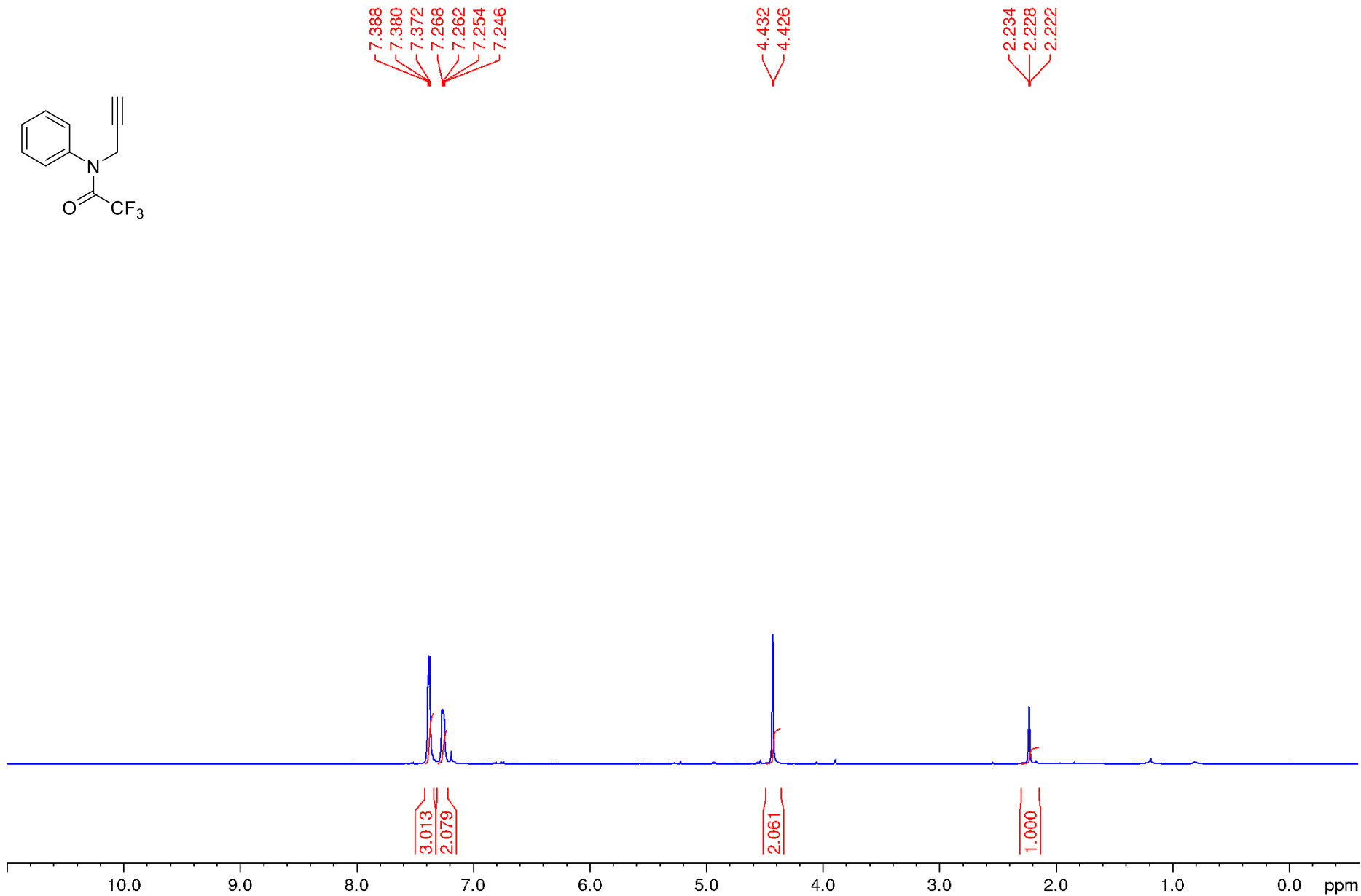
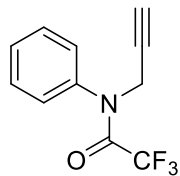
25.0

ppm

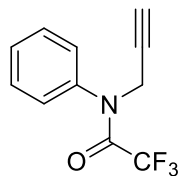
DEPT 135 NMR-spectrum (CDCl₃)



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



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



157.149
156.775
156.415
156.052

138.294

129.622
129.425
128.428

120.511

117.600

114.736

111.870

76.911

73.746

41.039

175.0

150.0

125.0

100.0

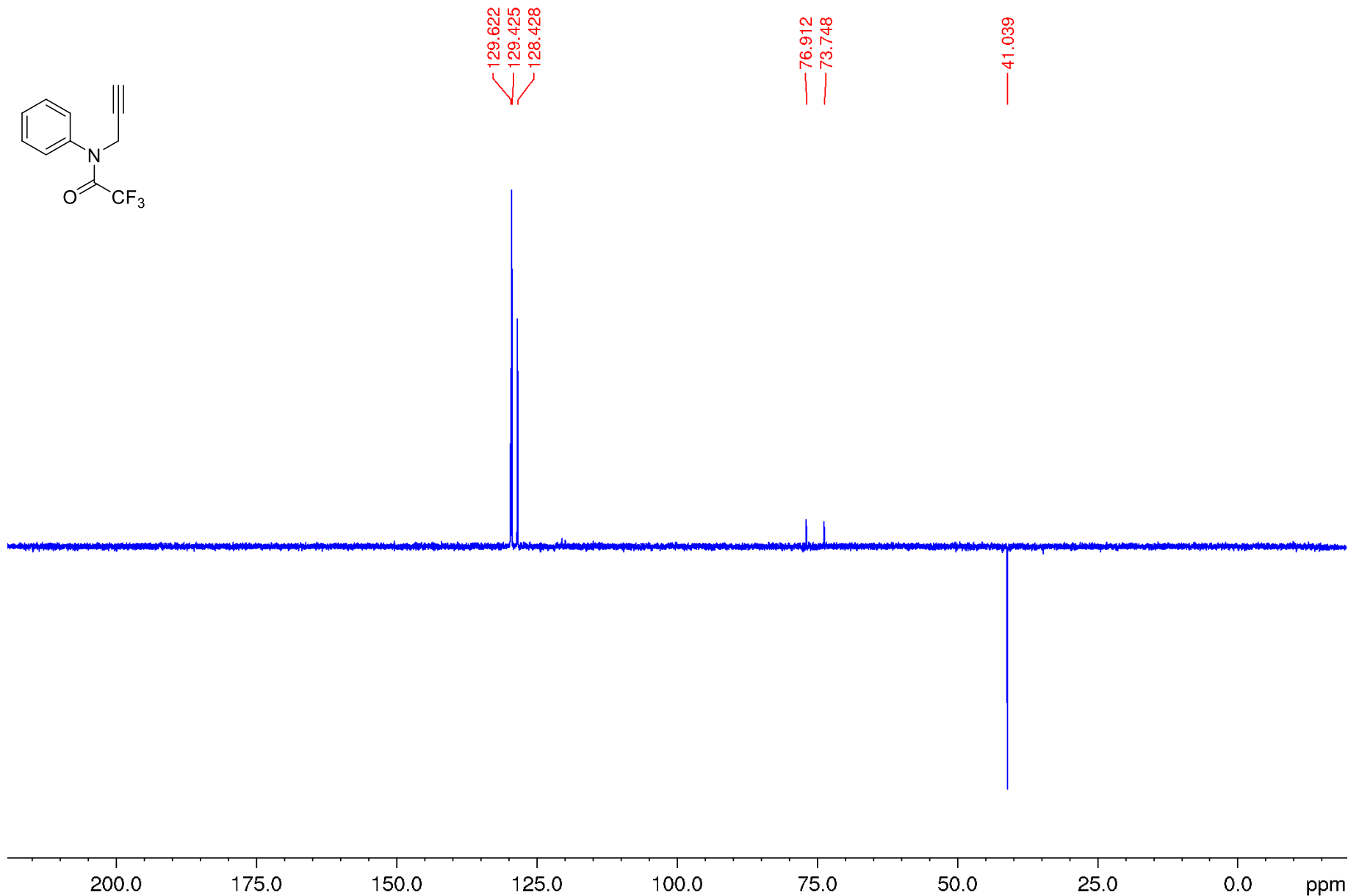
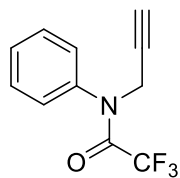
75.0

50.0

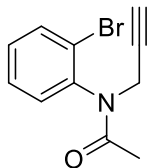
25.0

ppm

DEPT 135 NMR-spectrum (CDCl₃)



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

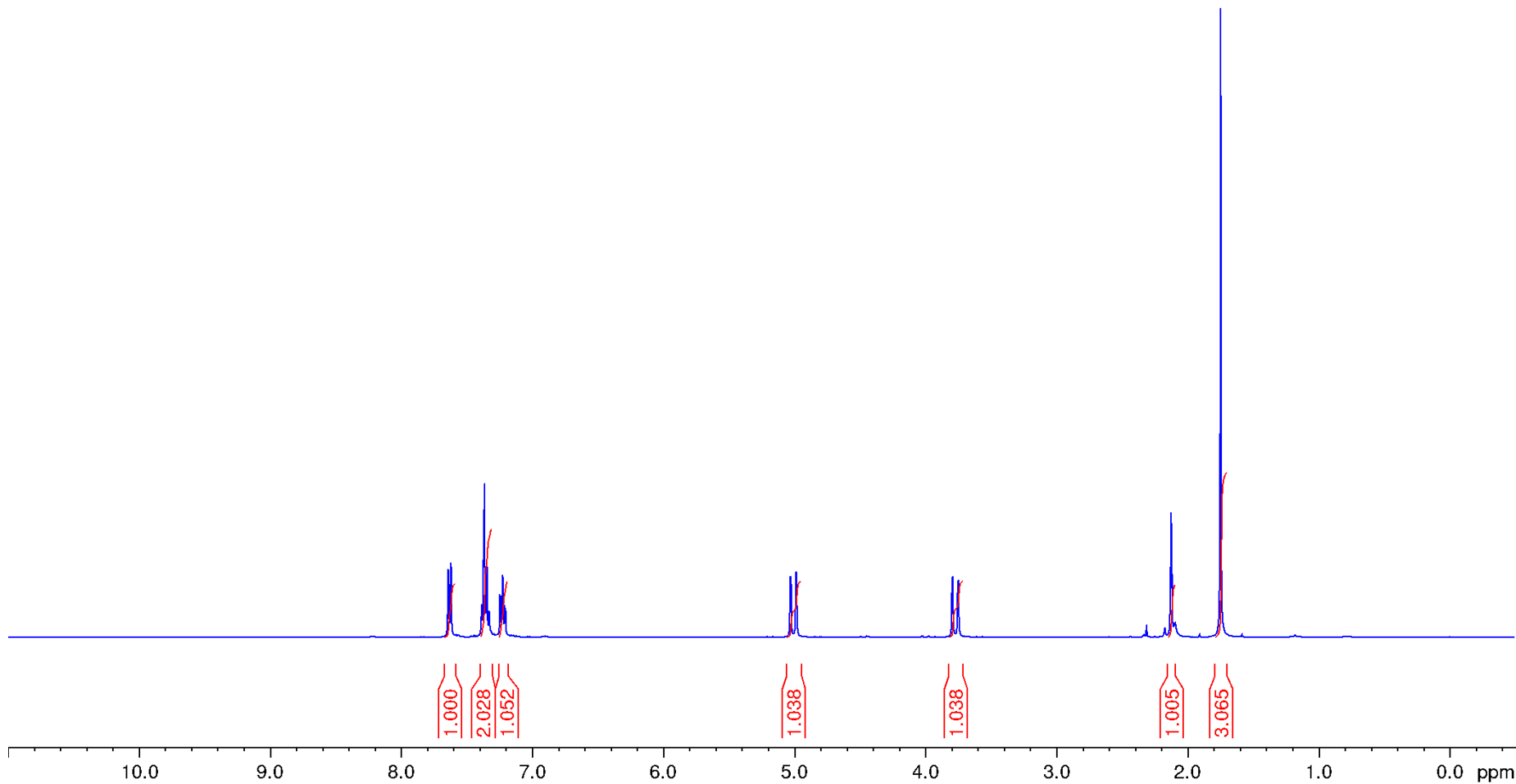


7.641
7.639
7.621
7.619
7.389
7.383
7.369
7.364
7.348
7.345
7.328
7.325
7.246
7.240
7.228
7.225
7.223
7.220
7.208
7.203

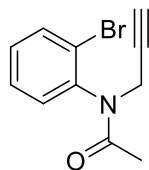
5.031
5.025
4.988
4.982

3.796
3.789
3.752
3.746

2.130
2.124
2.117
— 1.747



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



— 169.871

— 140.379

— 133.779

— 131.320

— 130.337

— 128.730

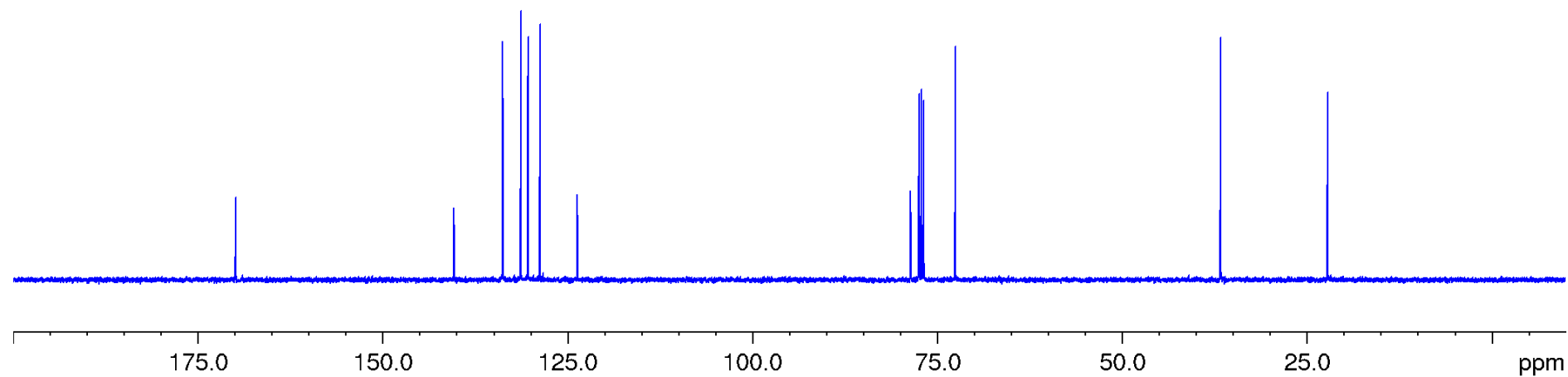
— 123.688

— 78.628

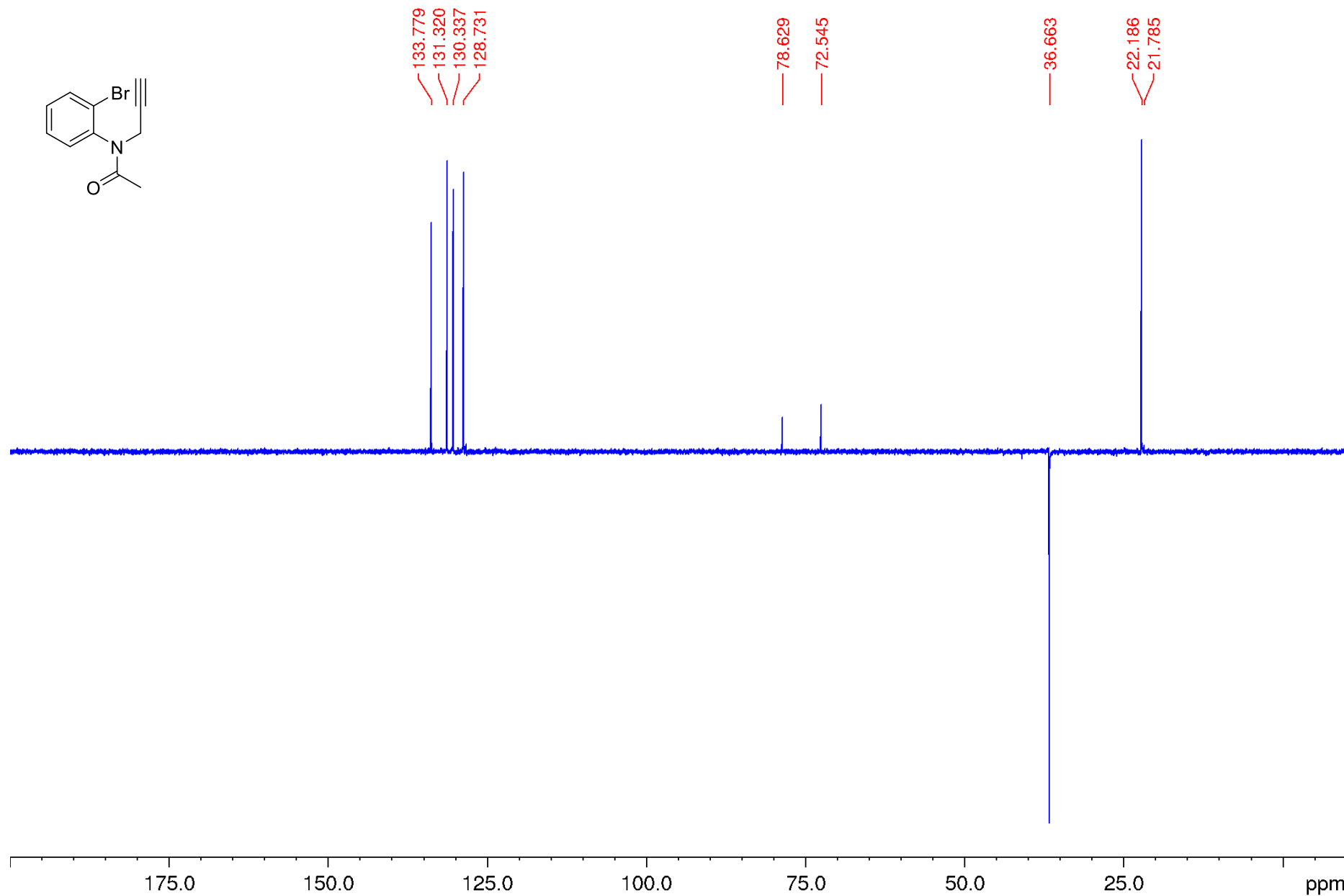
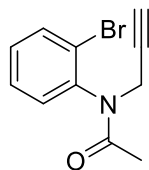
— 72.542

— 36.663

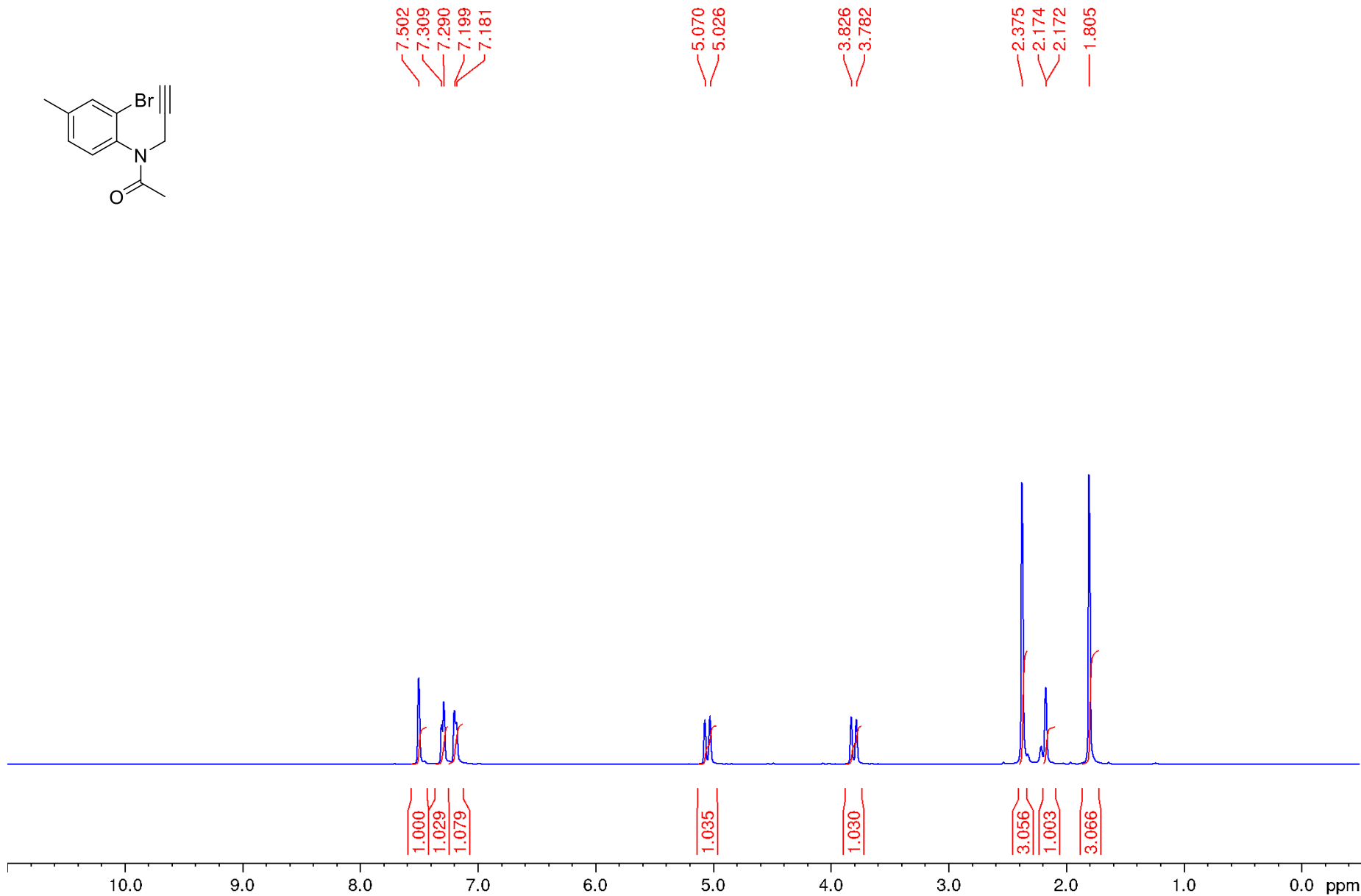
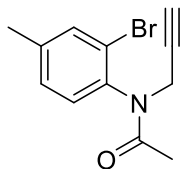
— 22.187



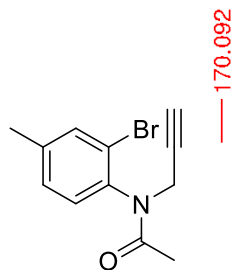
DEPT 135 NMR-spectrum (CDCl₃)



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



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



— 170.092

— 140.834

— 137.701

— 134.100

— 133.789

— 130.779

— 129.434

— 123.211

— 78.755

— 72.415

— 36.685

— 22.139

— 20.877

175.0

150.0

125.0

100.0

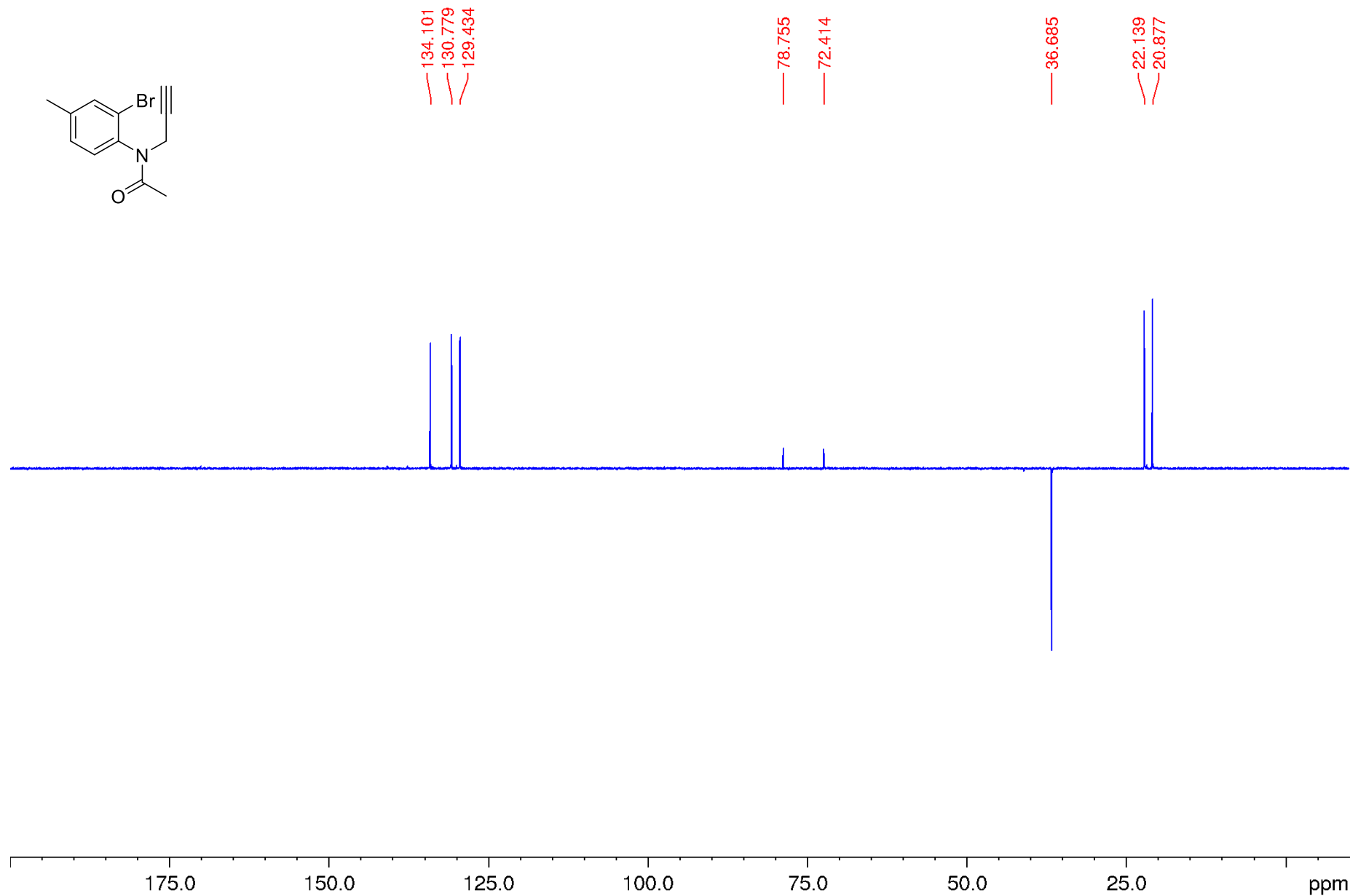
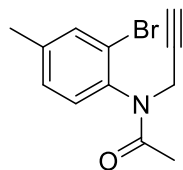
75.0

50.0

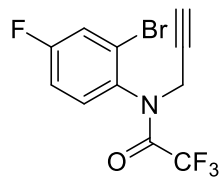
25.0

ppm

DEPT 135 NMR-spectrum (CDCl₃)



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

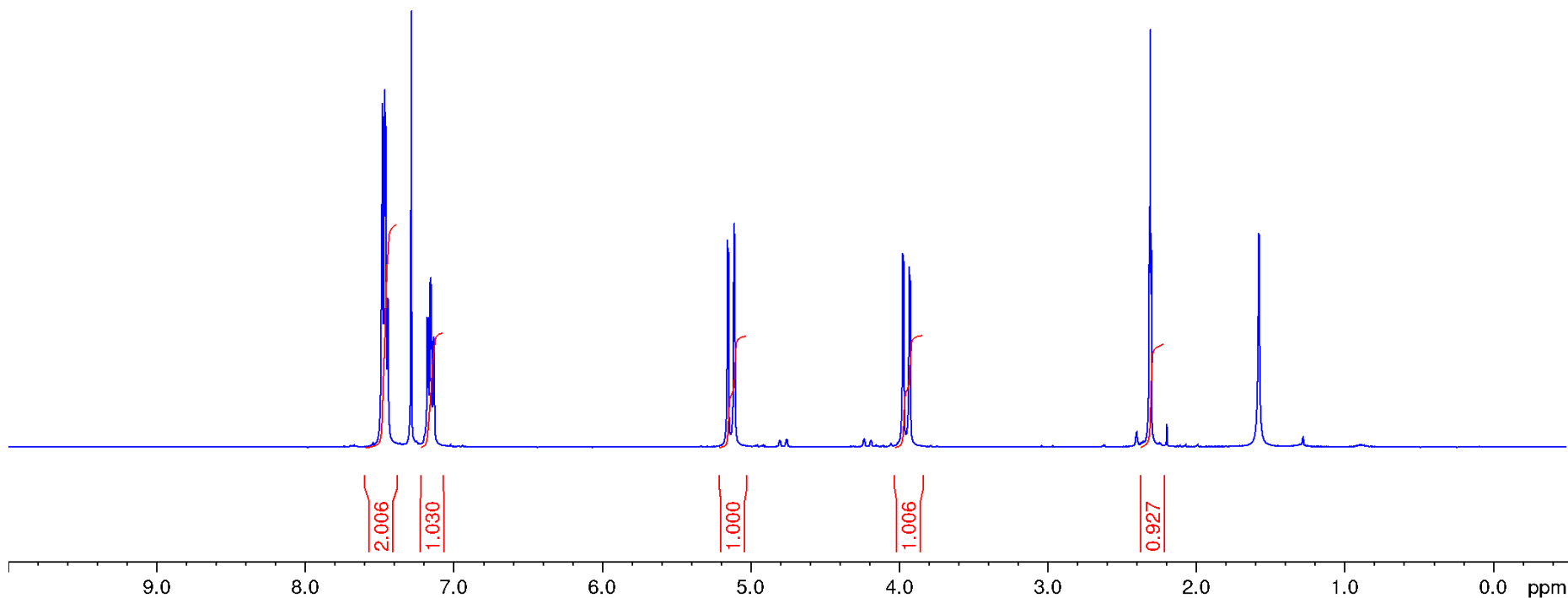


7.484
7.477
7.465
7.458
7.442
7.177
7.170
7.158
7.155
7.151
7.149
7.136
7.129

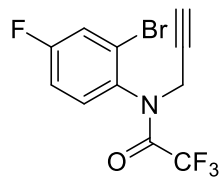
5.154
5.148
5.111
5.105

3.974
3.968
3.930
3.924

2.313
2.307
2.300



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



163.875
161.337
157.093
156.703
156.341
155.996

133.054
132.966
132.794
124.446
124.344
121.111
120.856
117.224
115.411
115.187
114.359

76.233
74.441

39.148

175.0

150.0

125.0

100.0

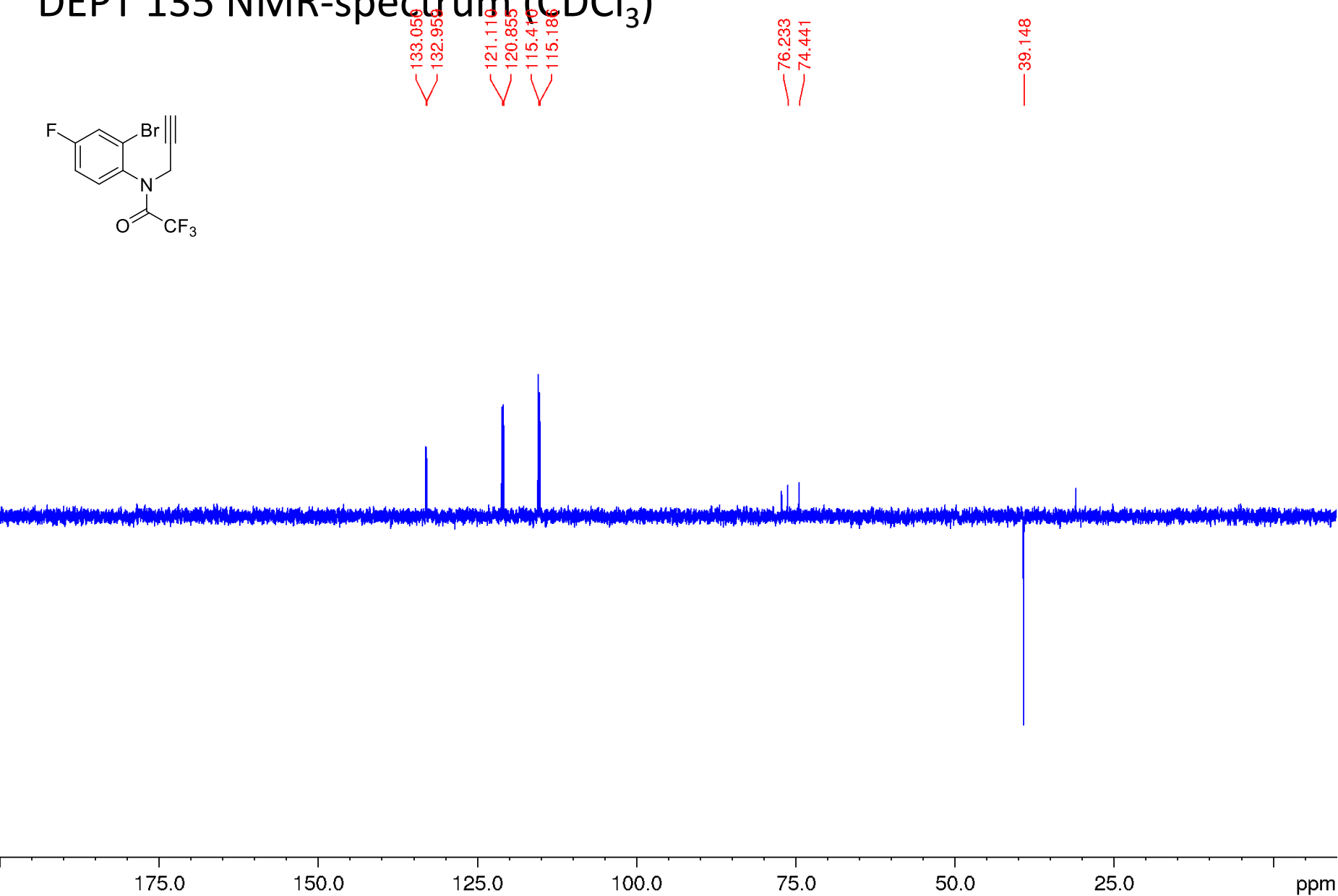
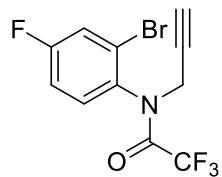
75.0

50.0

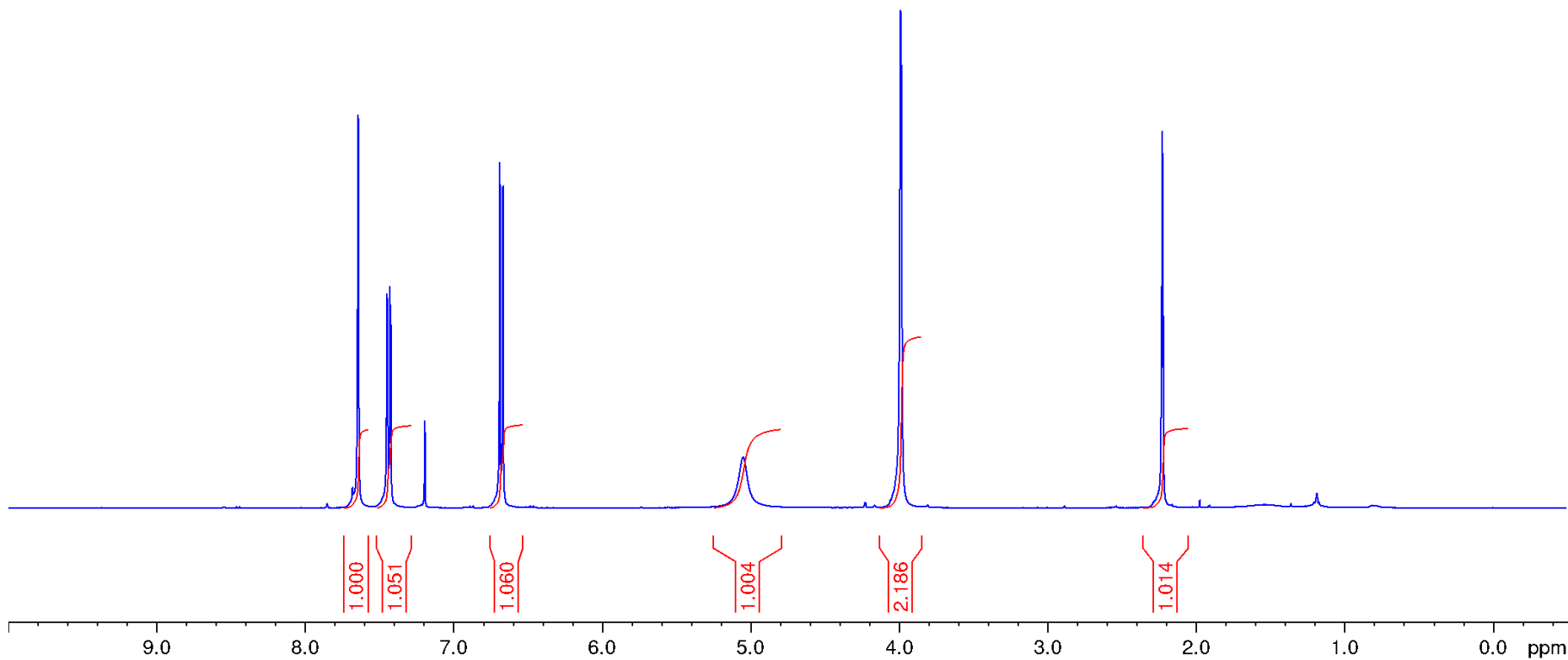
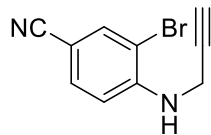
25.0

ppm

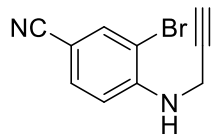
DEPT 135 NMR-spectrum (CDCl₃)



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



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



Chemical shifts (ppm) labeled above the spectrum:

- 147.112
- 135.866
- 132.895
- 118.662
- 111.070
- 109.133
- 101.029
- 78.648
- 72.560
- 33.084

175.0

150.0

125.0

100.0

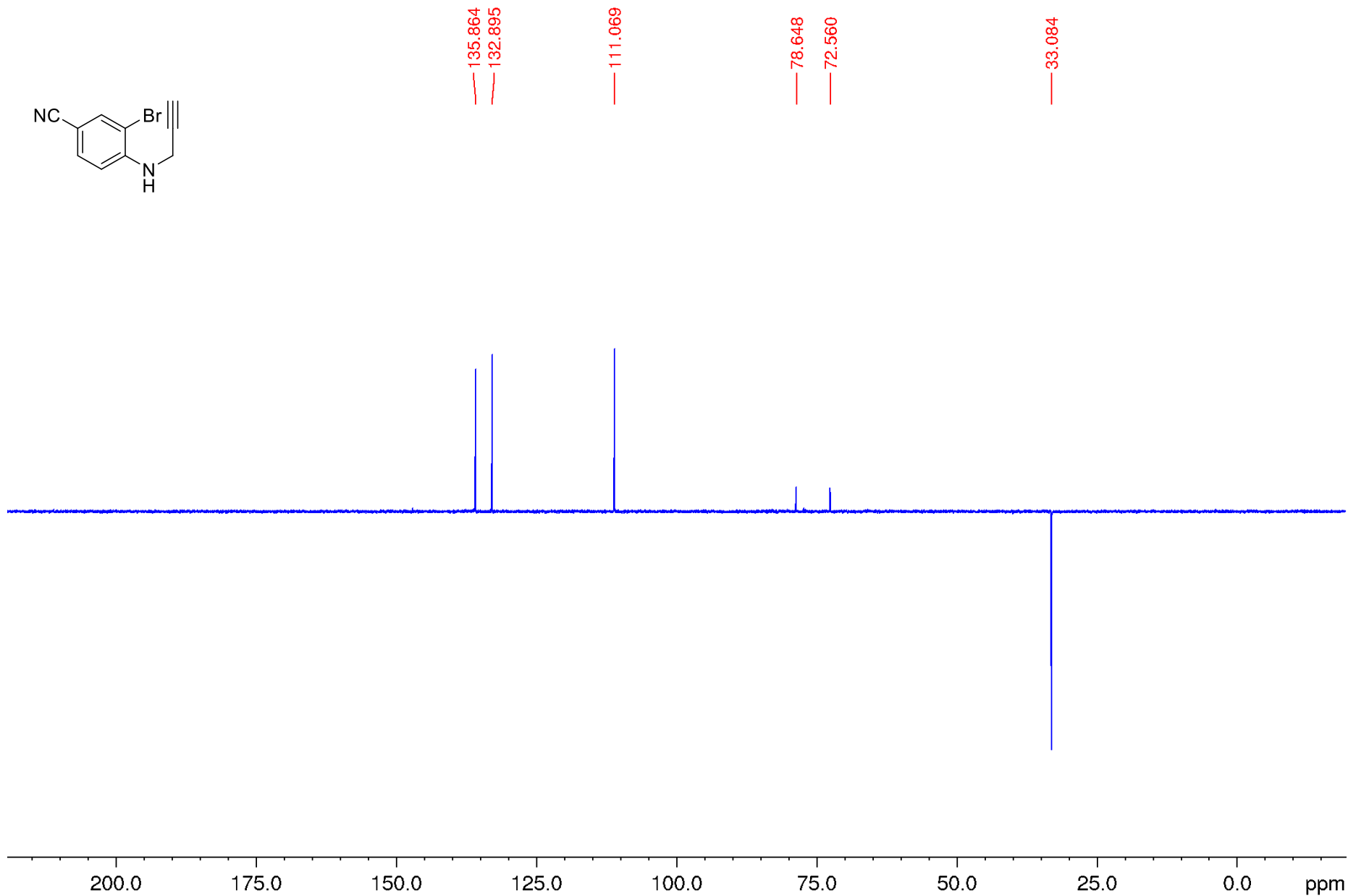
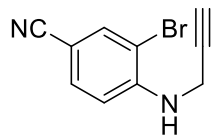
75.0

50.0

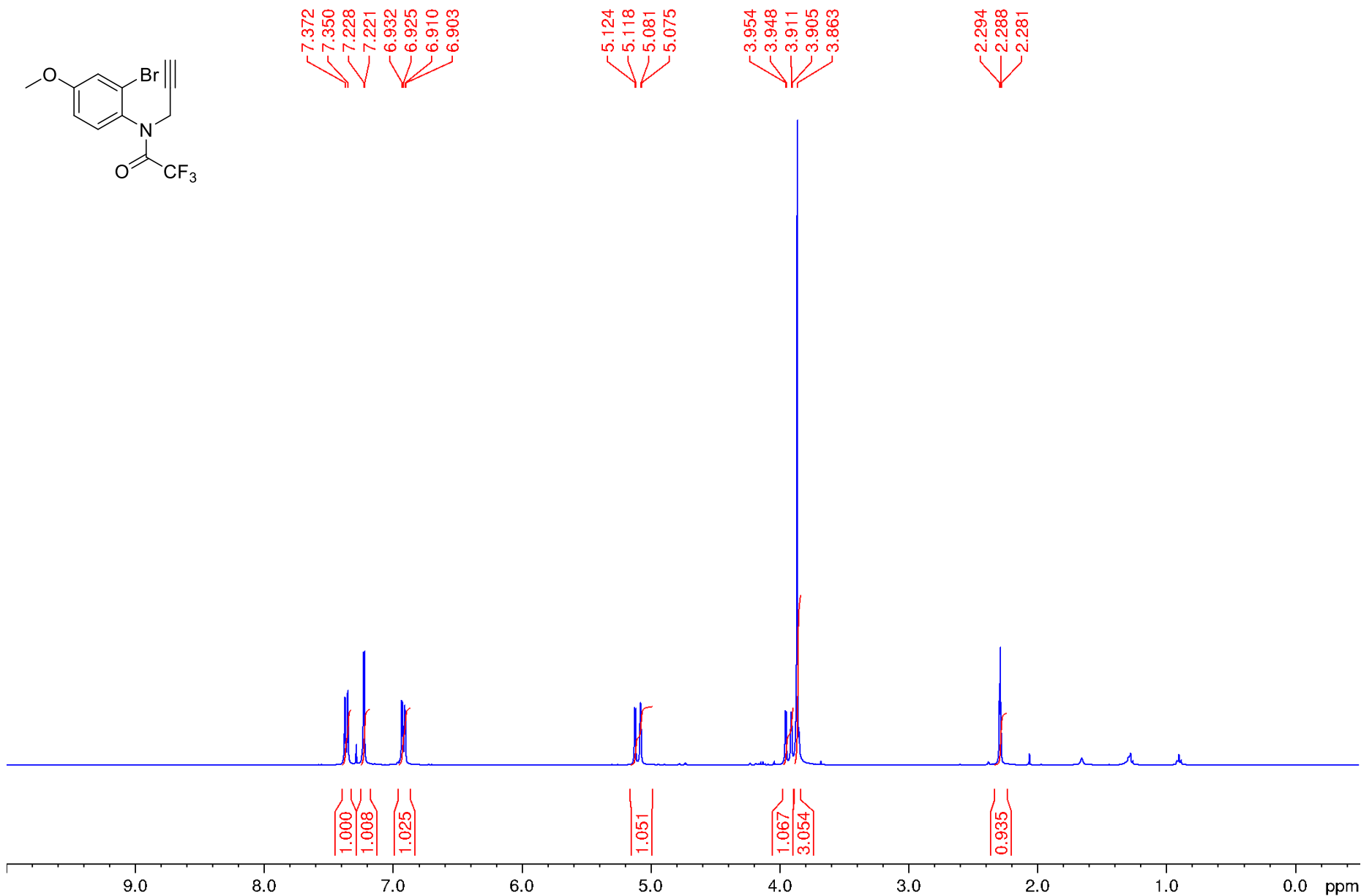
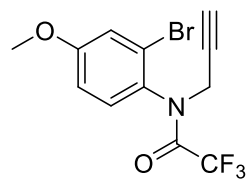
25.0

ppm

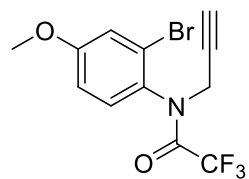
DEPT 135 NMR-spectrum (CDCl_3)



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



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



160.785
157.357
156.994
156.631
156.272

132.265
129.097
124.050
120.212
118.655
117.345
114.478
113.465
111.611

76.642
74.020

55.812

39.376

175.0

150.0

125.0

100.0

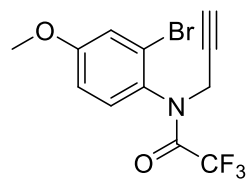
75.0

50.0

25.0

ppm

DEPT 135 NMR-spectrum (CDCl_3)



132.265

118.655

113.465

76.642

74.023

55.812

39.376

175.0

150.0

125.0

100.0

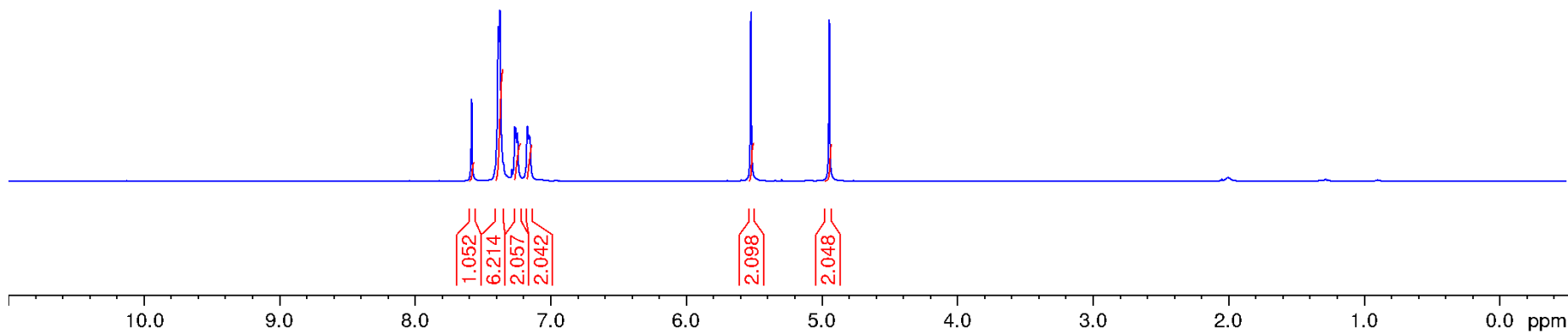
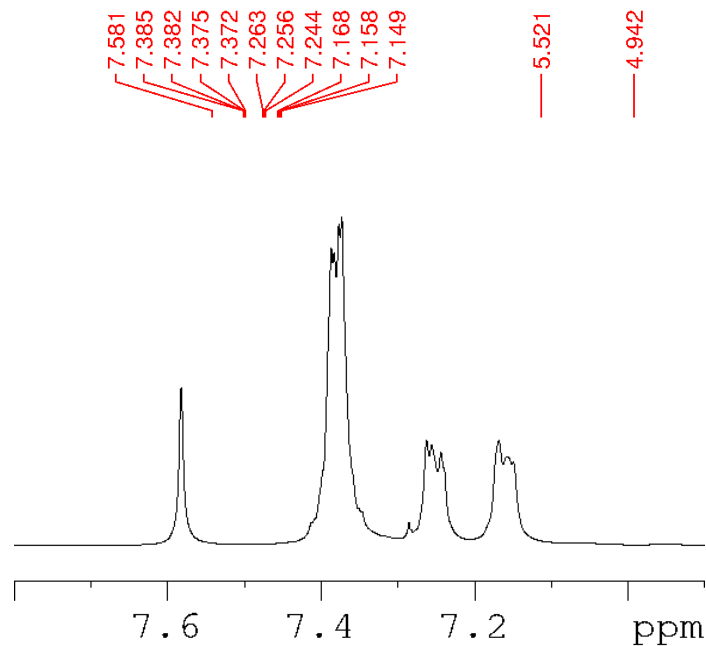
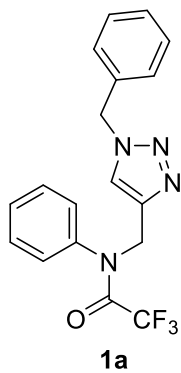
75.0

50.0

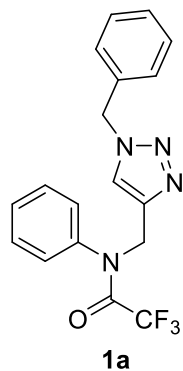
25.0

ppm

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



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



157.430
157.072
156.714
156.356
142.454
139.048
134.514
129.407
129.274
129.142
128.819
128.253
128.025
123.870
120.528
117.664
114.800
111.936

54.204
47.309

175.0

150.0

125.0

100.0

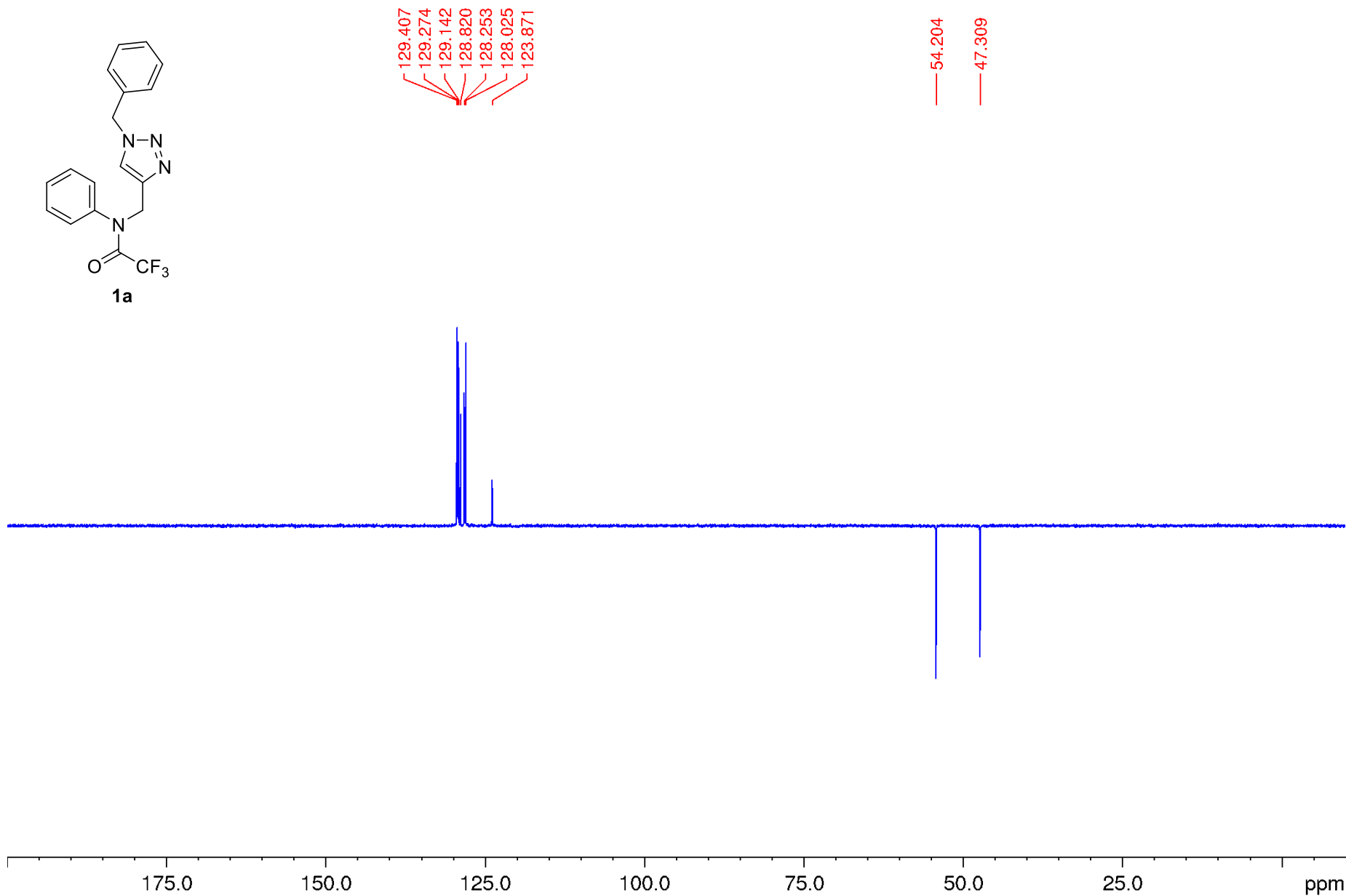
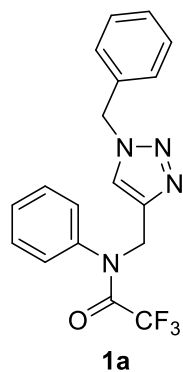
75.0

50.0

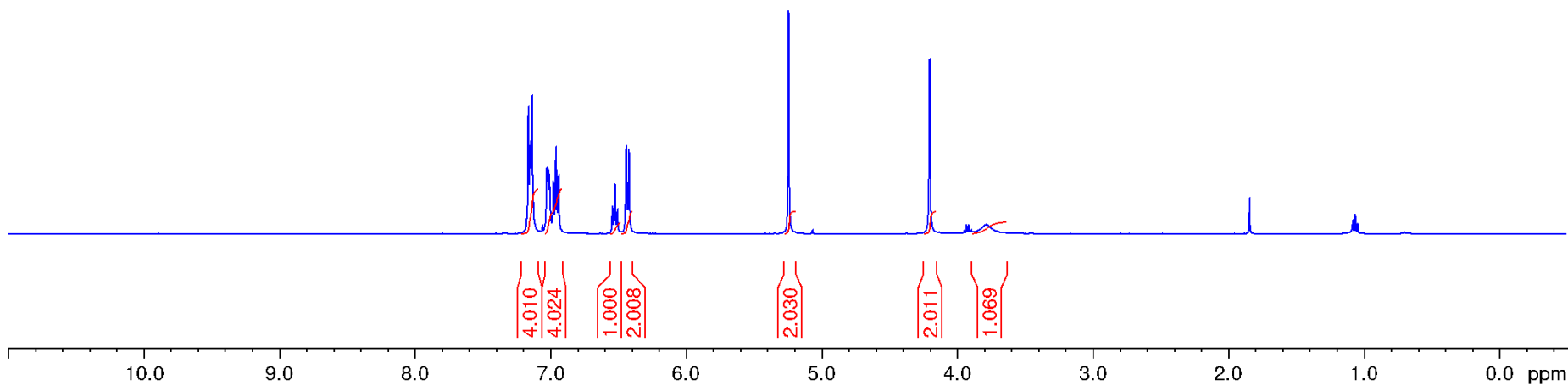
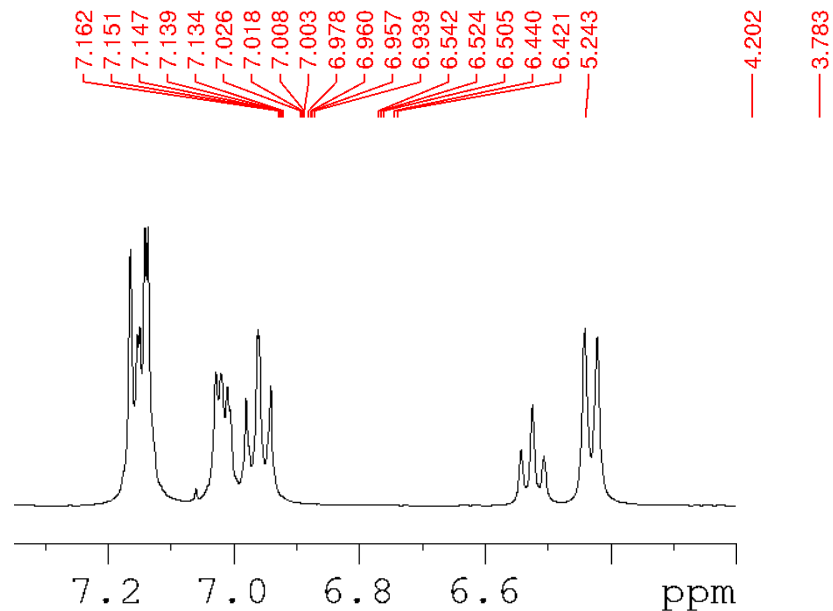
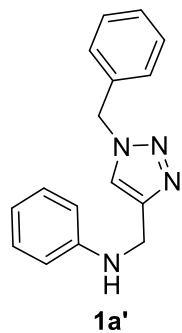
25.0

ppm

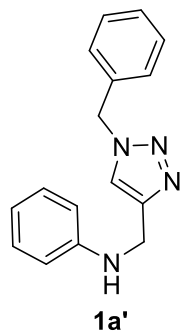
DEPT 135 NMR-spectrum (CDCl₃)



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



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



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

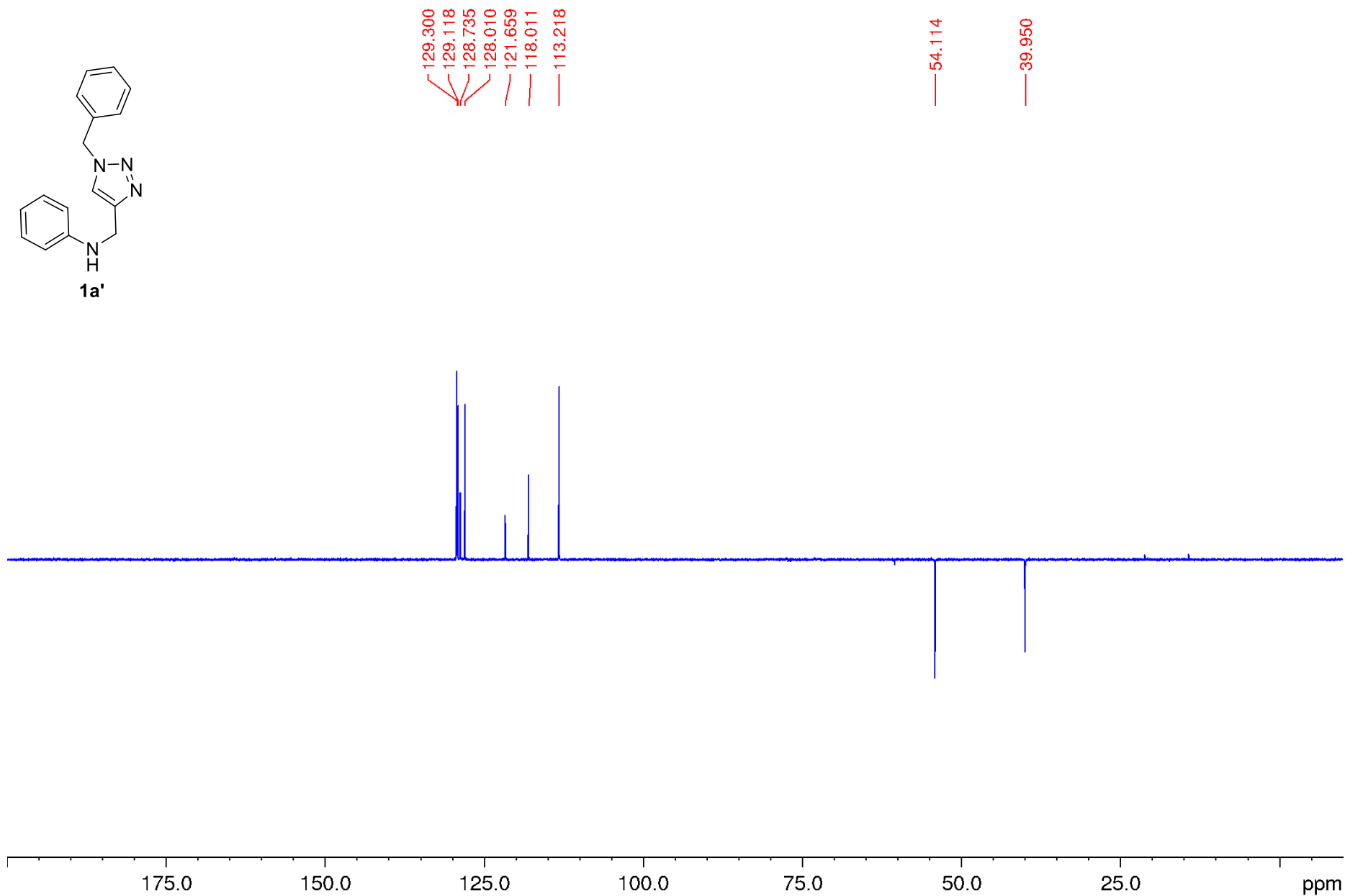
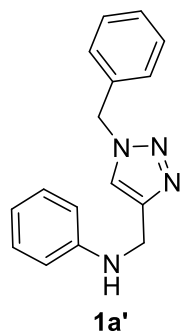
75.0

50.0

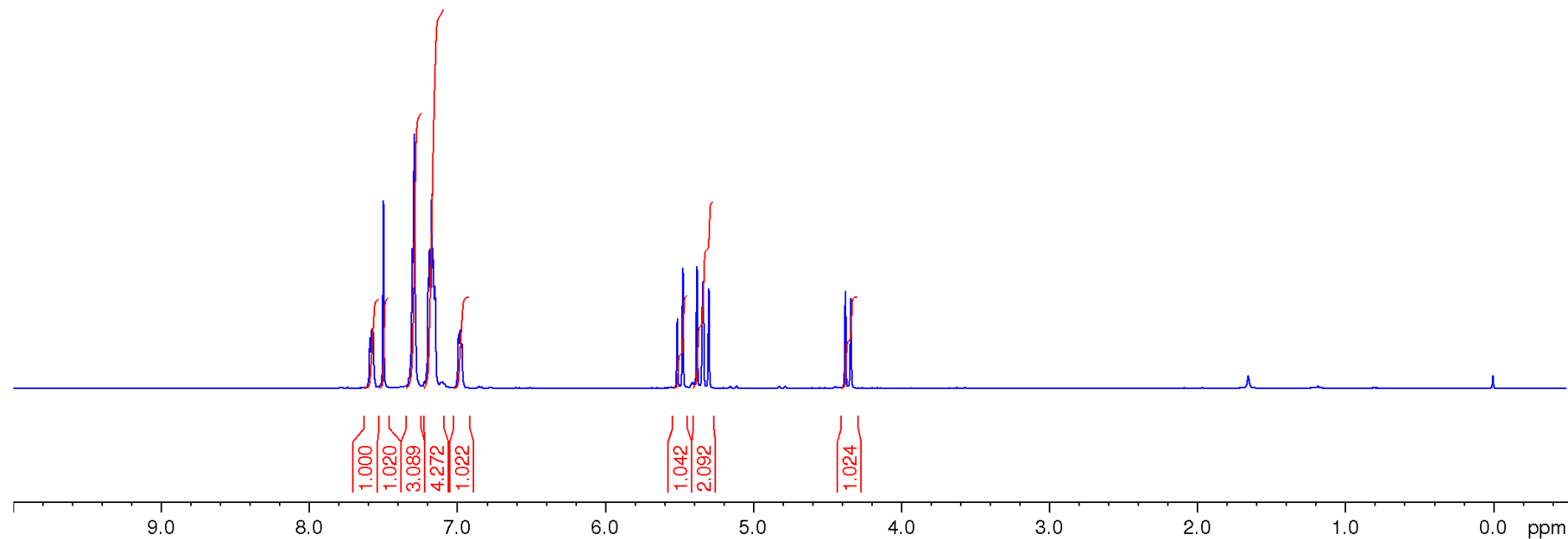
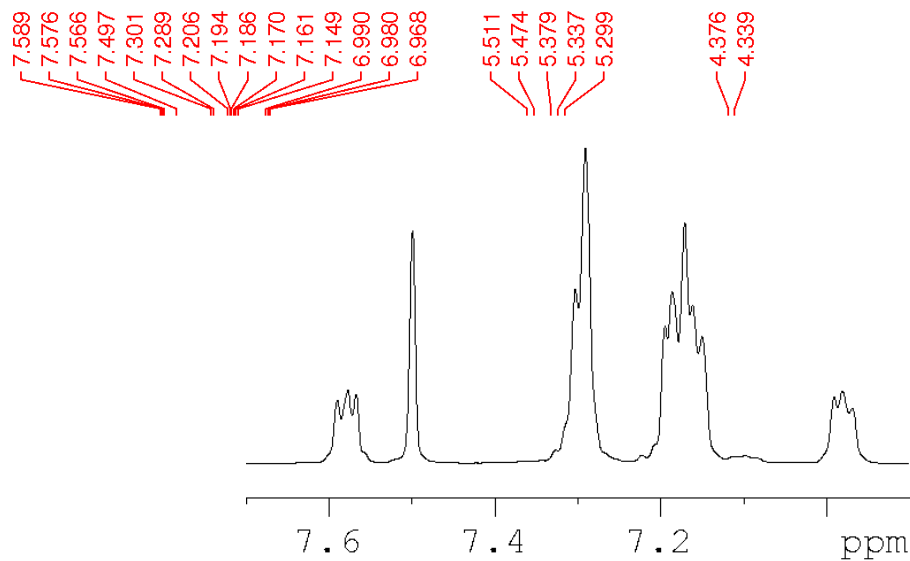
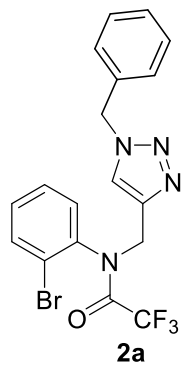
25.0

ppm

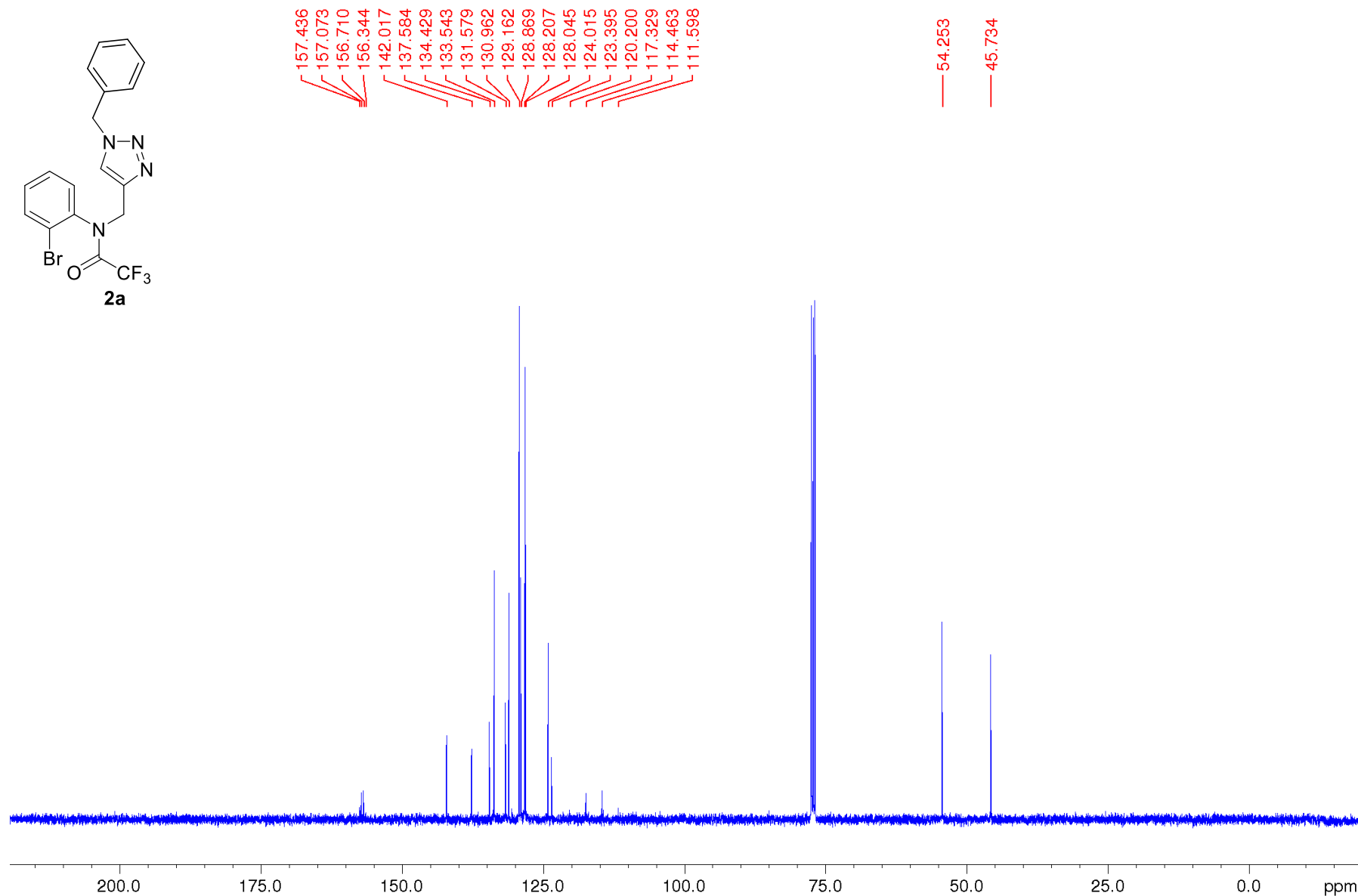
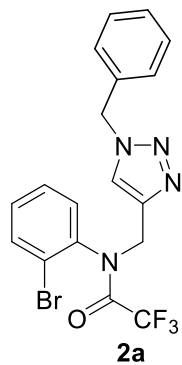
DEPT 135 NMR-spectrum (CDCl_3)



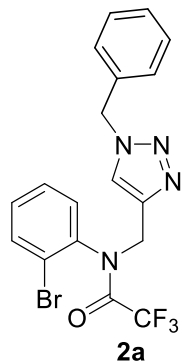
^1H NMR-spectrum (400 MHz, CDCl_3)



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



DEPT 135 NMR-spectrum (CDCl_3)



133.544
131.580
130.962
129.162
128.869
128.208
128.045
124.015

54.253

45.734

150.0

125.0

100.0

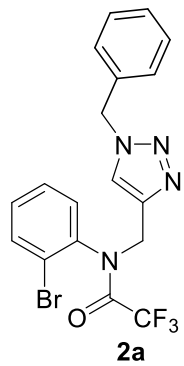
75.0

50.0

25.0

ppm

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



-68.995



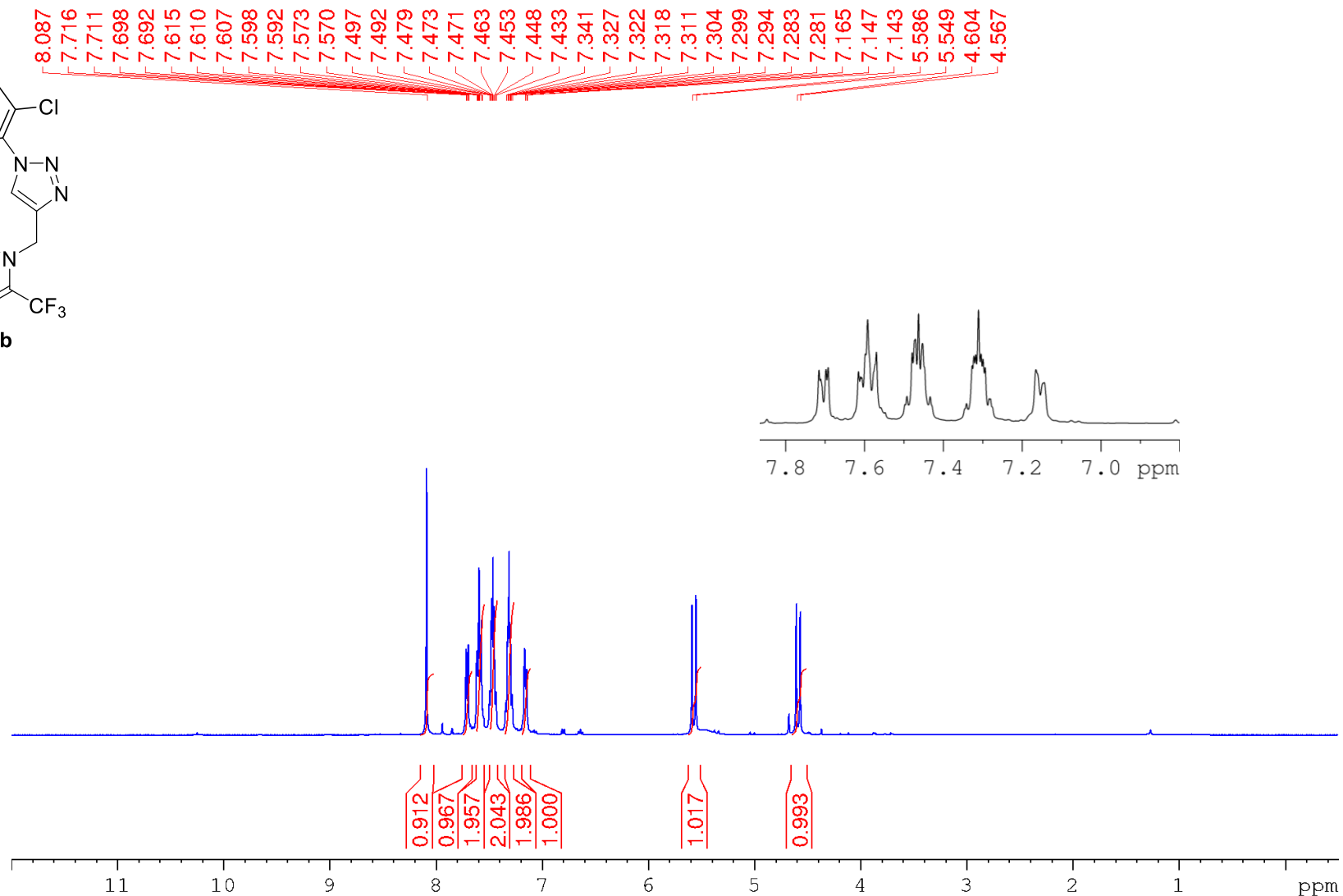
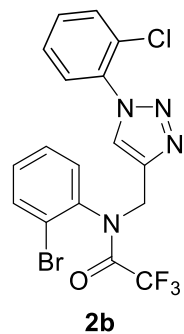
-75.0

-100.0

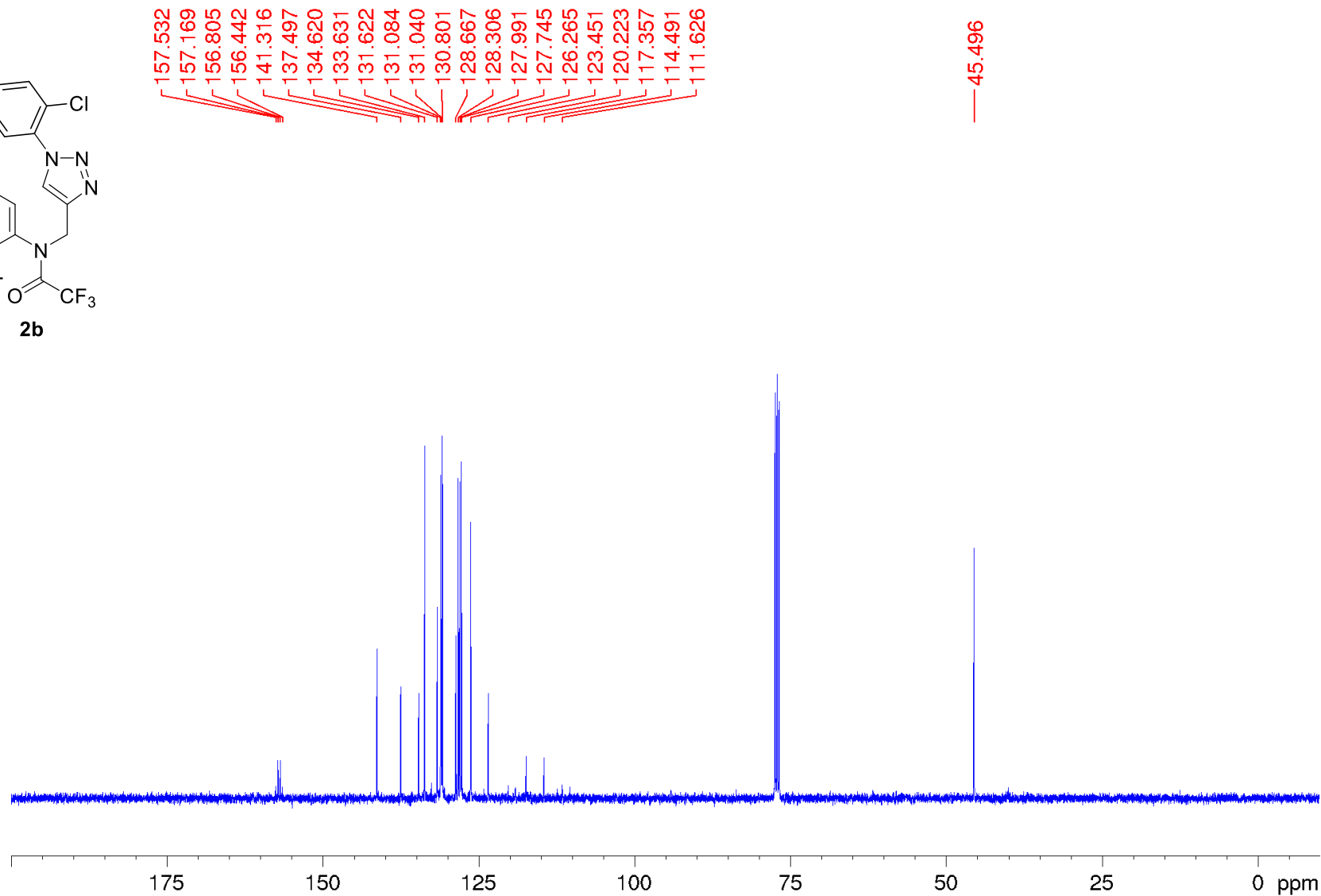
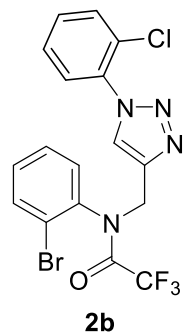
-125.0

ppm

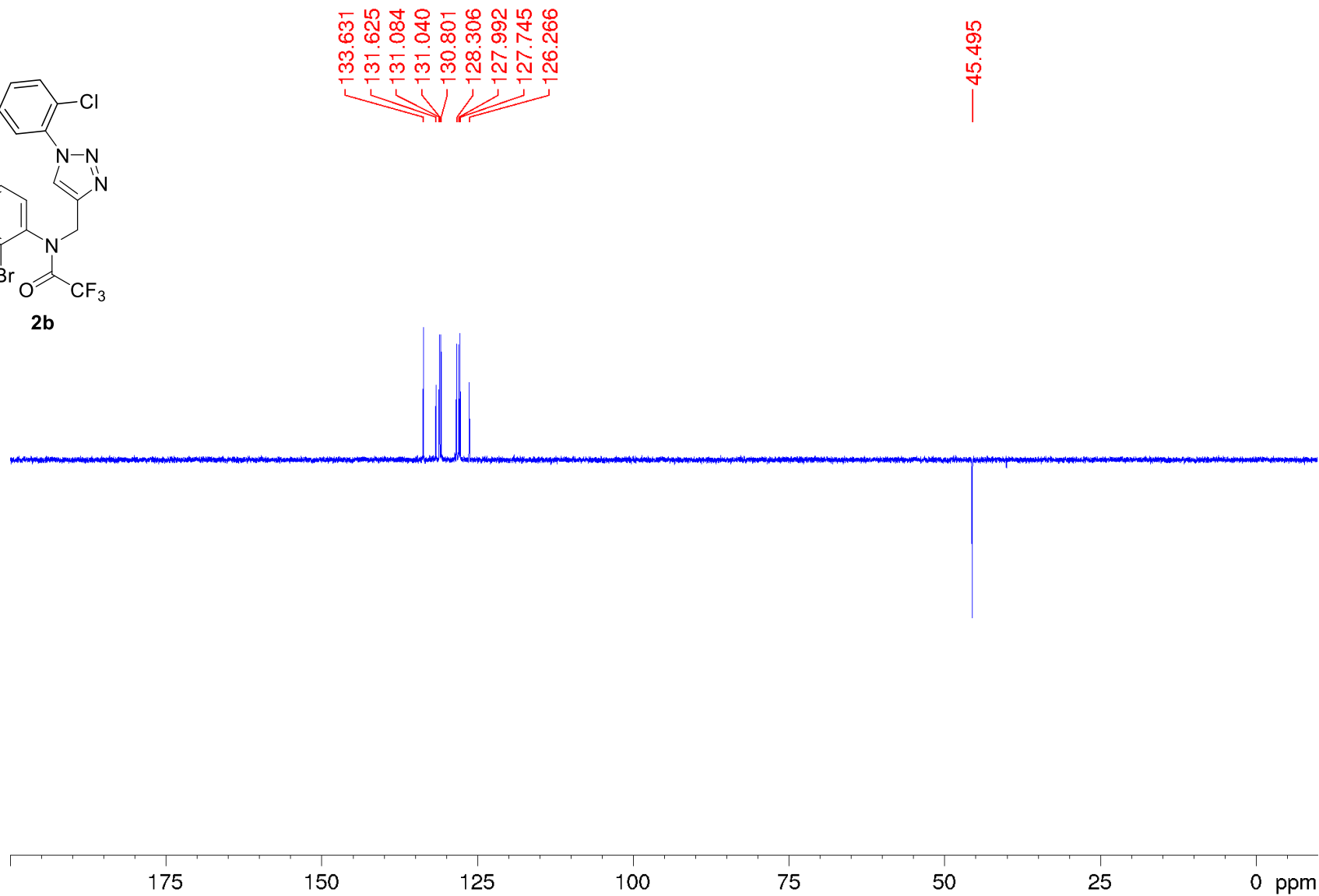
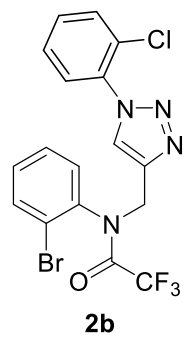
^1H NMR-spectrum (400 MHz, CDCl_3)



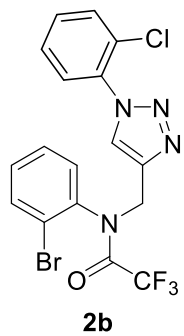
^{13}C NMR-spectrum (100 MHz, CDCl_3)



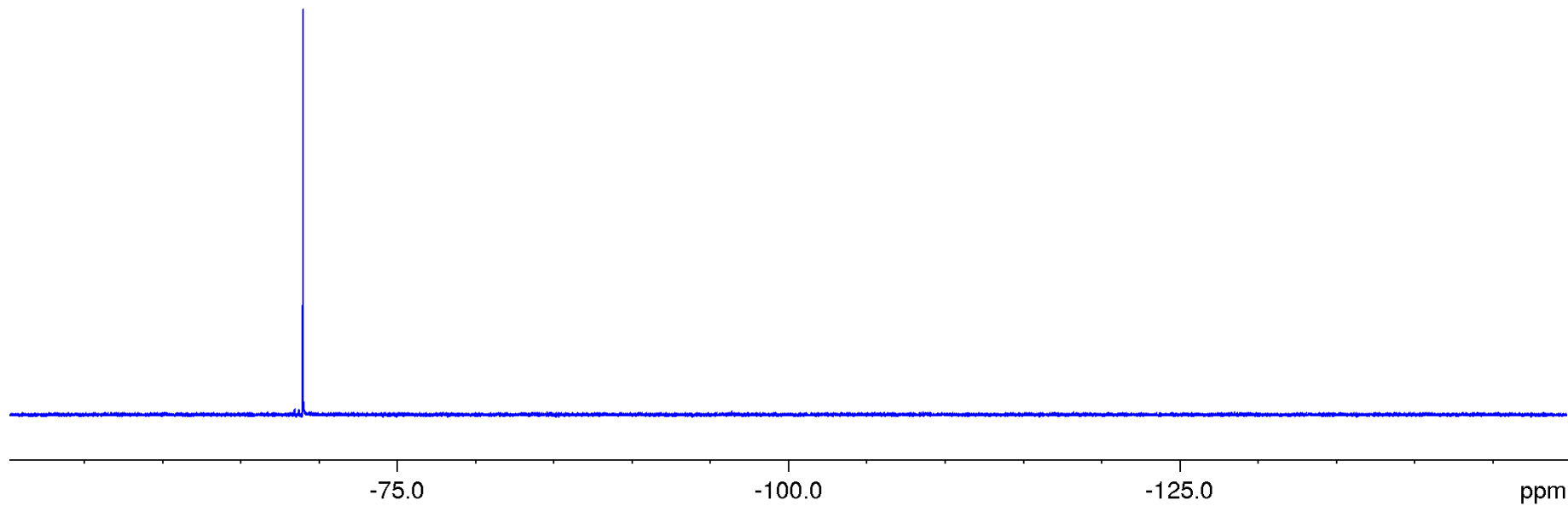
DEPT 135 NMR-spectrum (CDCl_3)



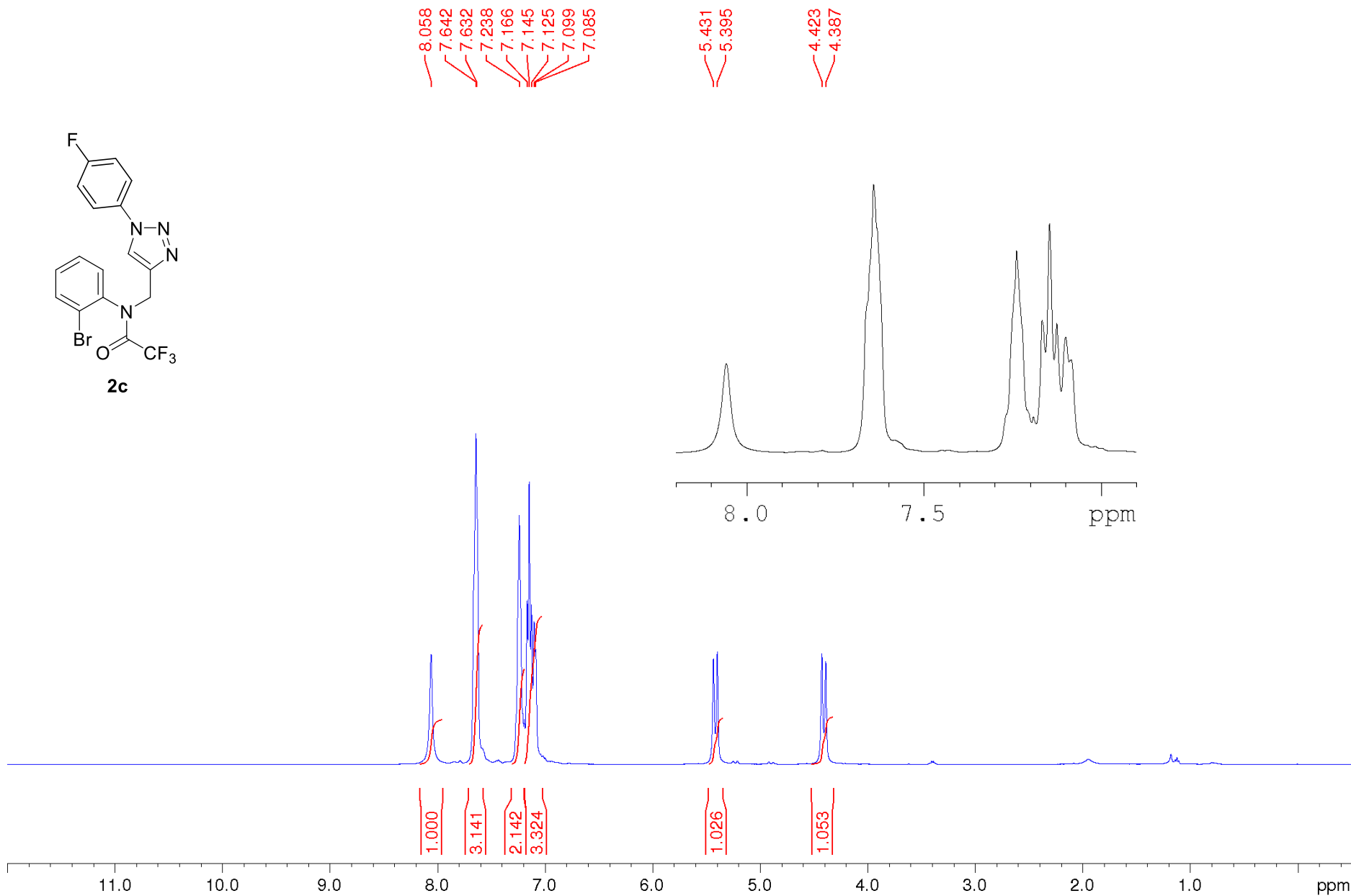
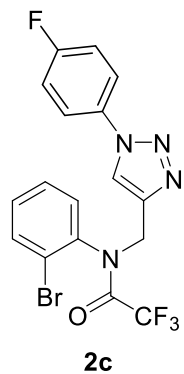
^{19}F NMR-spectrum (376.5 Hz, CDCl_3)



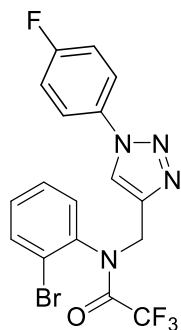
-68.985



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



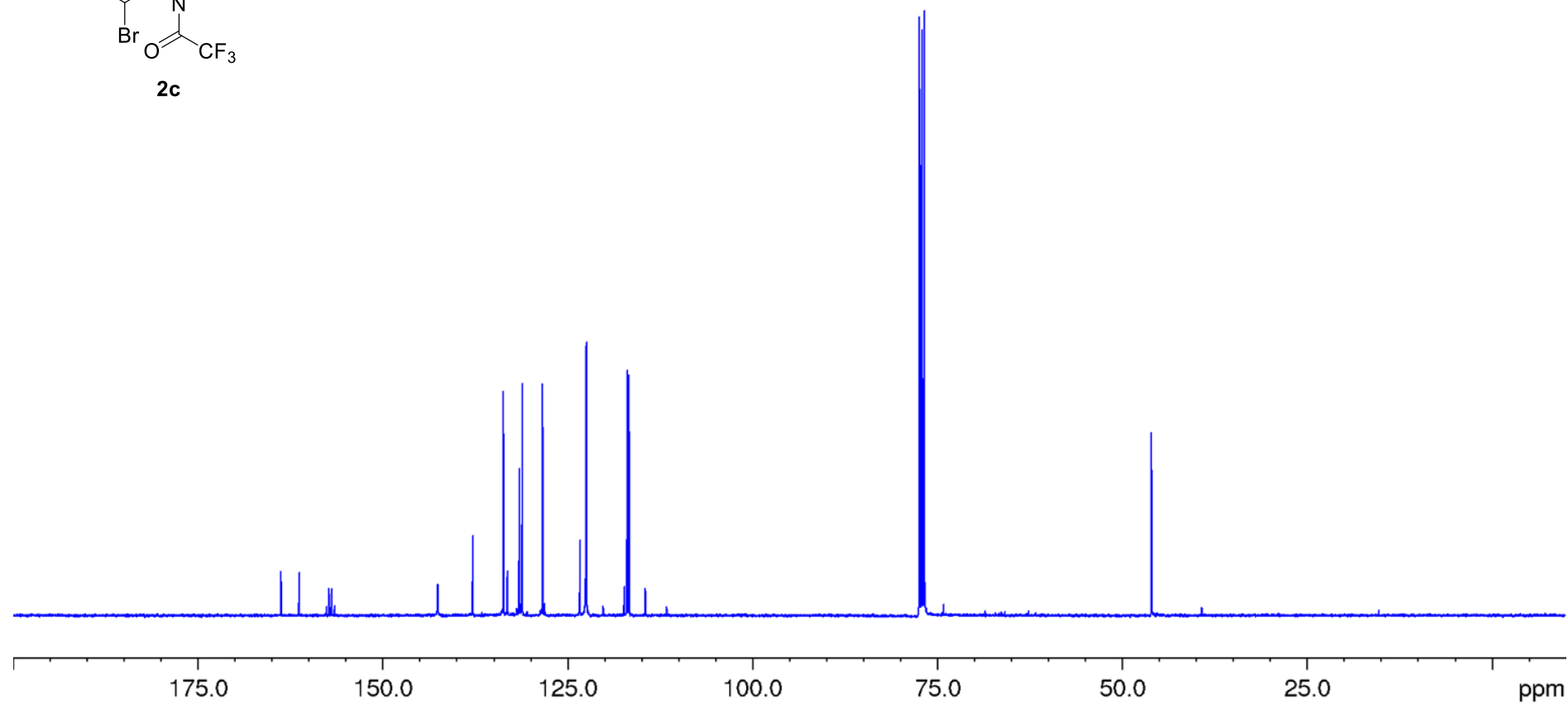
^{13}C NMR-spectrum (100 MHz, CDCl_3)



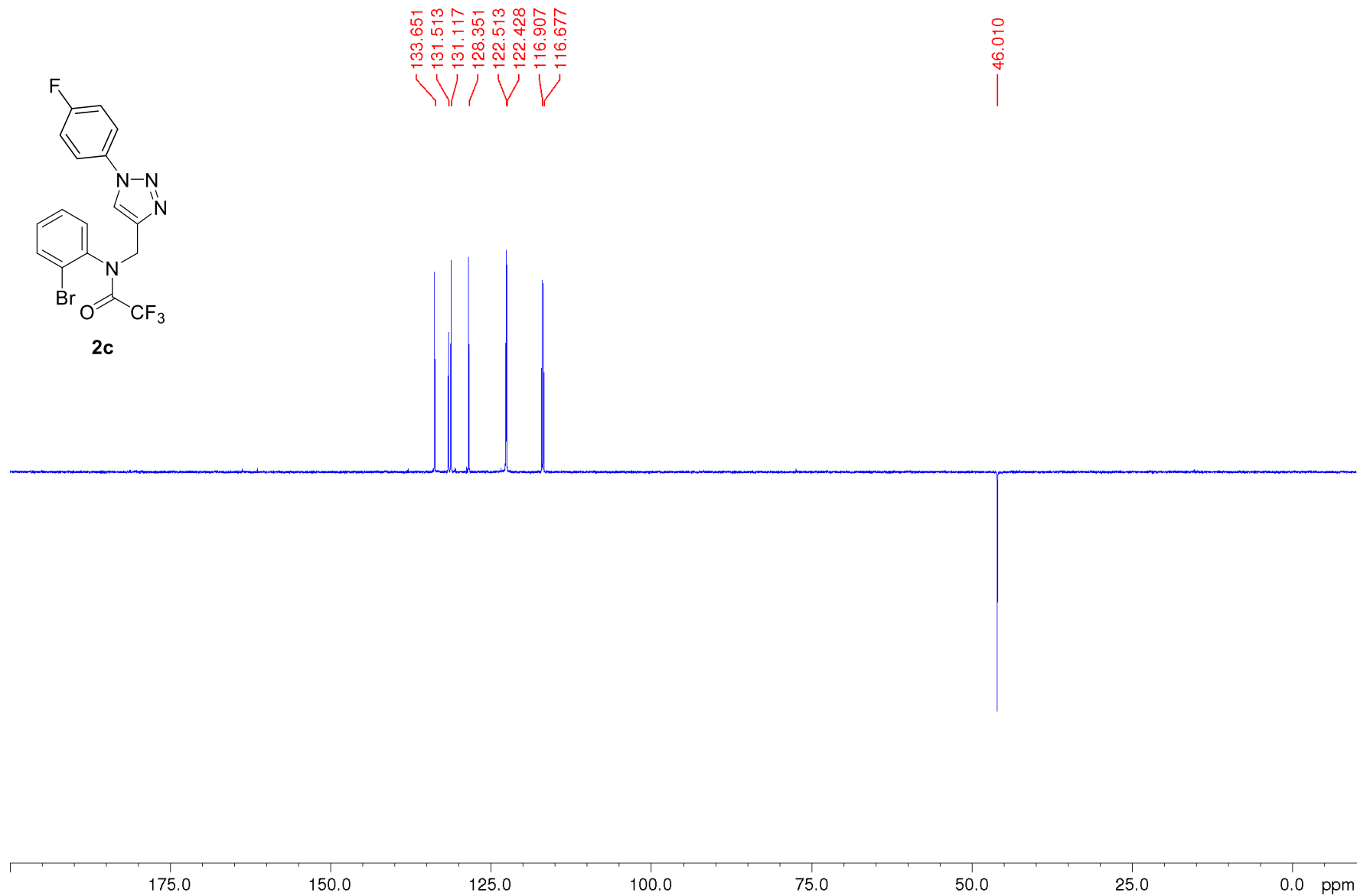
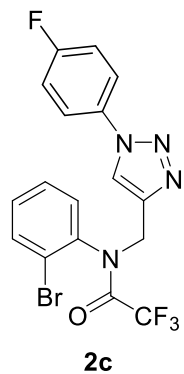
2c

163.765
161.285
157.614
157.249
156.885
156.520
142.537
137.814
133.657
133.135
133.106
131.506
131.121
128.354
123.302
122.513
122.428
120.187
117.322
116.911
116.680
114.457
111.594

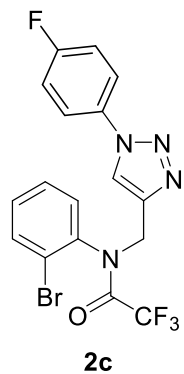
46.013



DEPT 135 NMR-spectrum (CDCl_3)



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



--68.98

--111.76
--111.77
--111.78
--111.80
--111.81
--111.82
--111.83

-60

-70

-80

-90

-100

-110

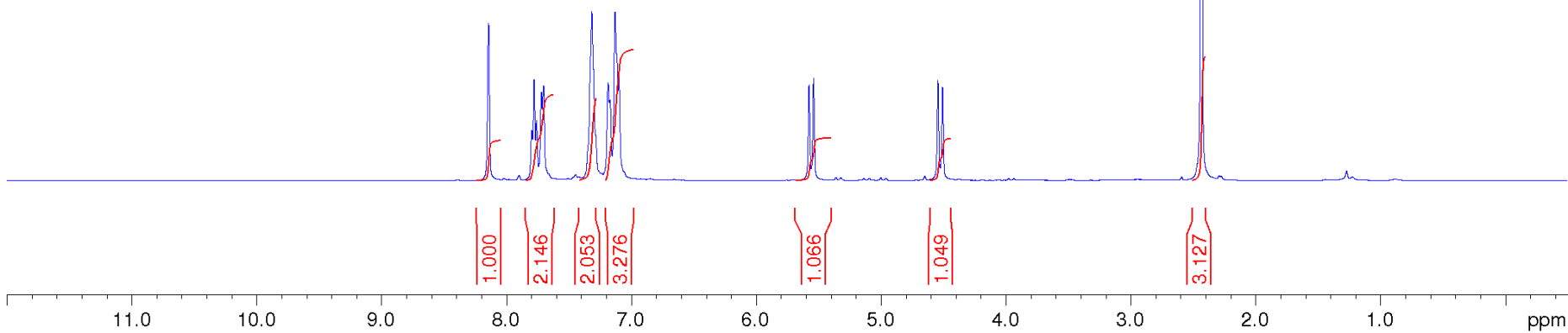
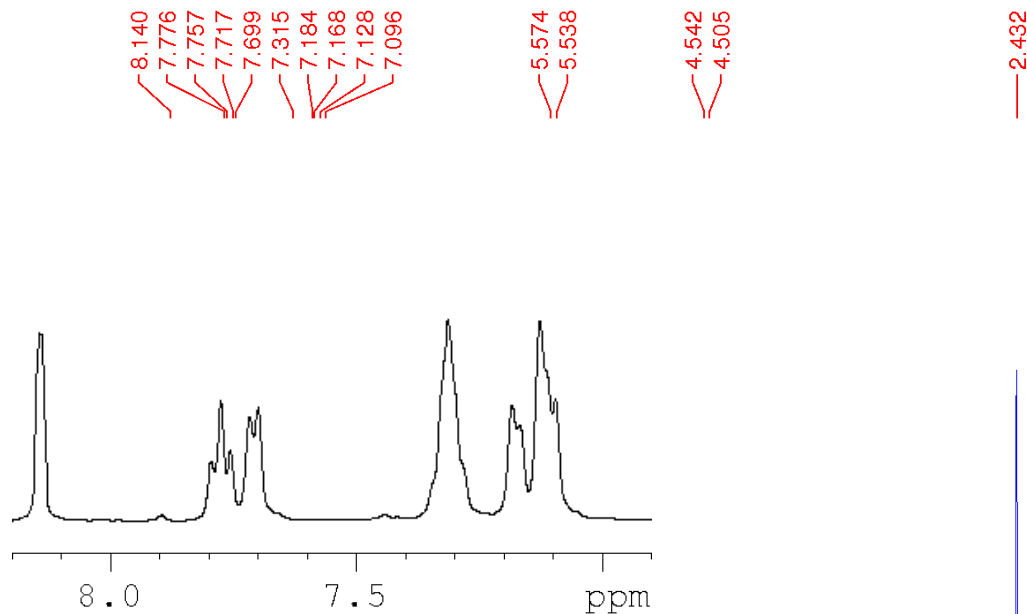
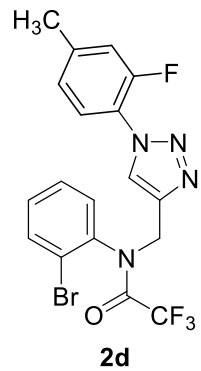
-120

-130

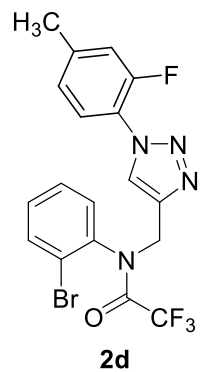
-140

ppm

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



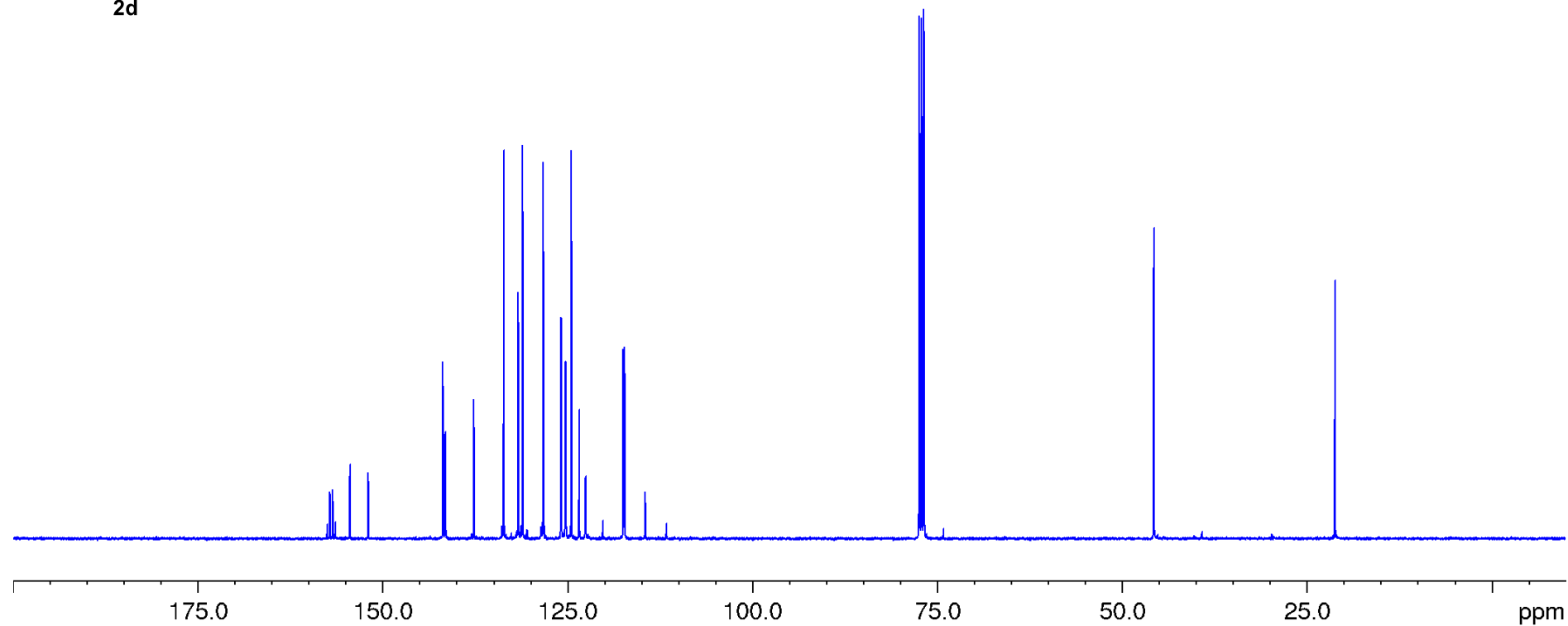
^{13}C NMR-spectrum (100 MHz, CDCl_3)



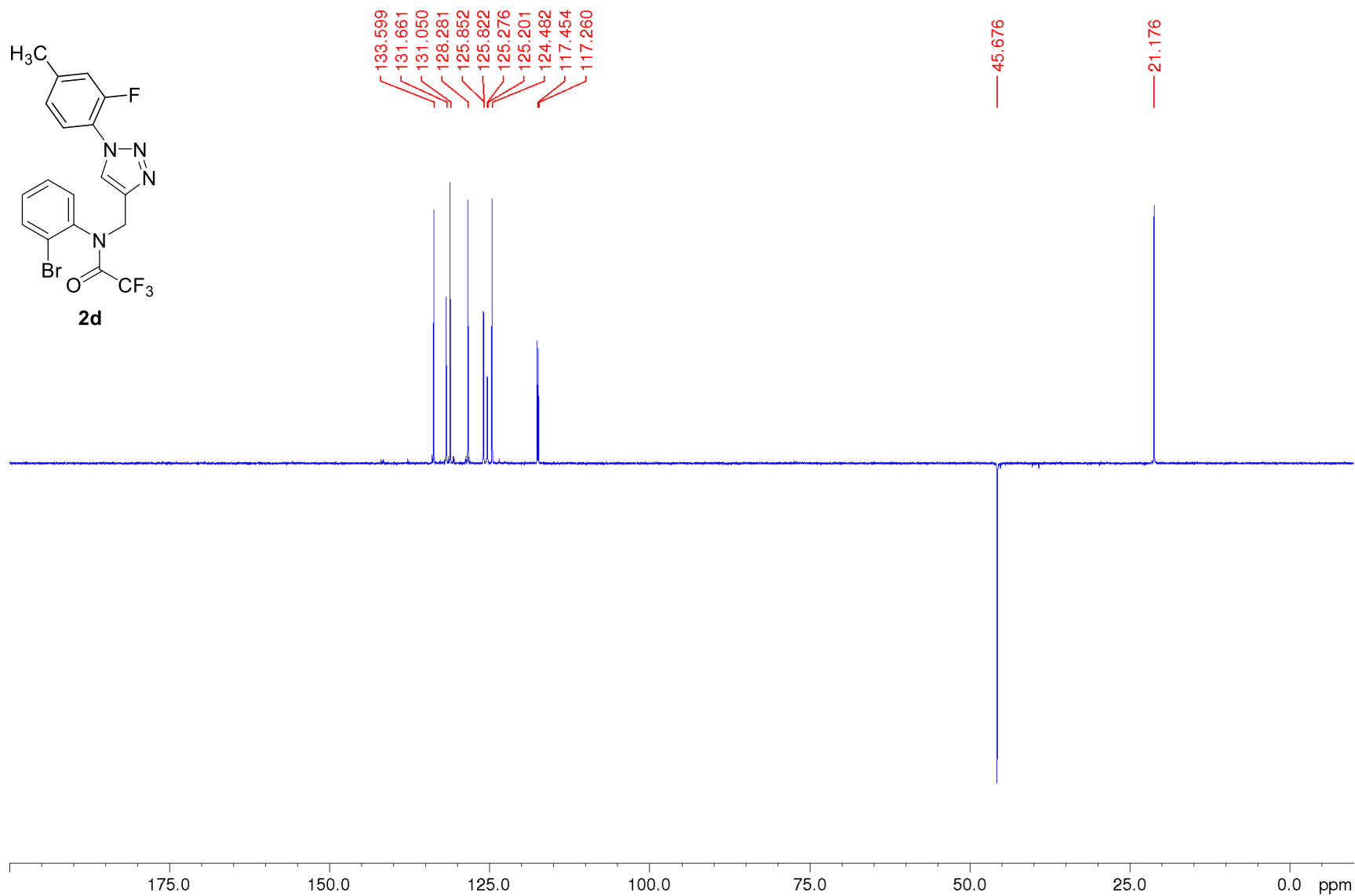
157.493
157.130
156.766
156.402
154.427
151.936
141.850
141.547
141.470
137.658
133.600
131.662
131.050
128.282
125.852
125.822
125.277
125.201
124.483
123.396
122.600
122.496
120.223
117.454
117.357
117.260
114.491
111.625

45.676

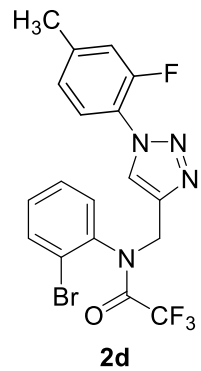
21.176



DEPT 135 NMR-spectrum (CDCl_3)



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



-68.959

-124.394
-124.423
-124.447

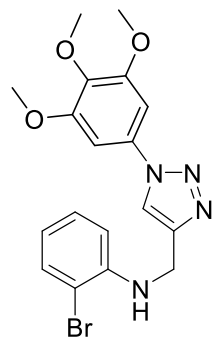
-75.0

-100.0

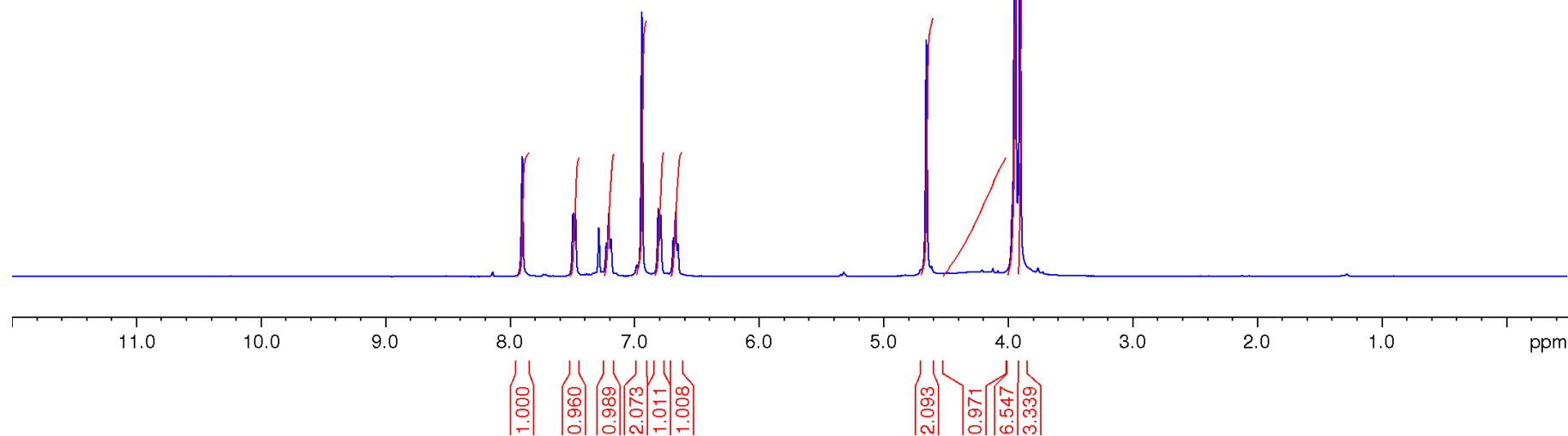
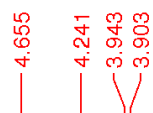
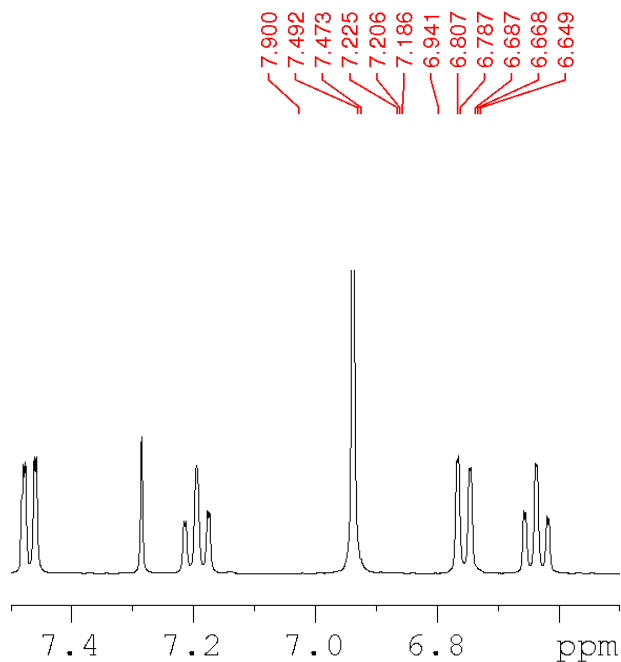
-125.0

ppm

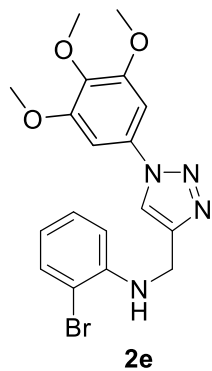
^1H NMR-spectrum (400 MHz, CDCl_3)



2e

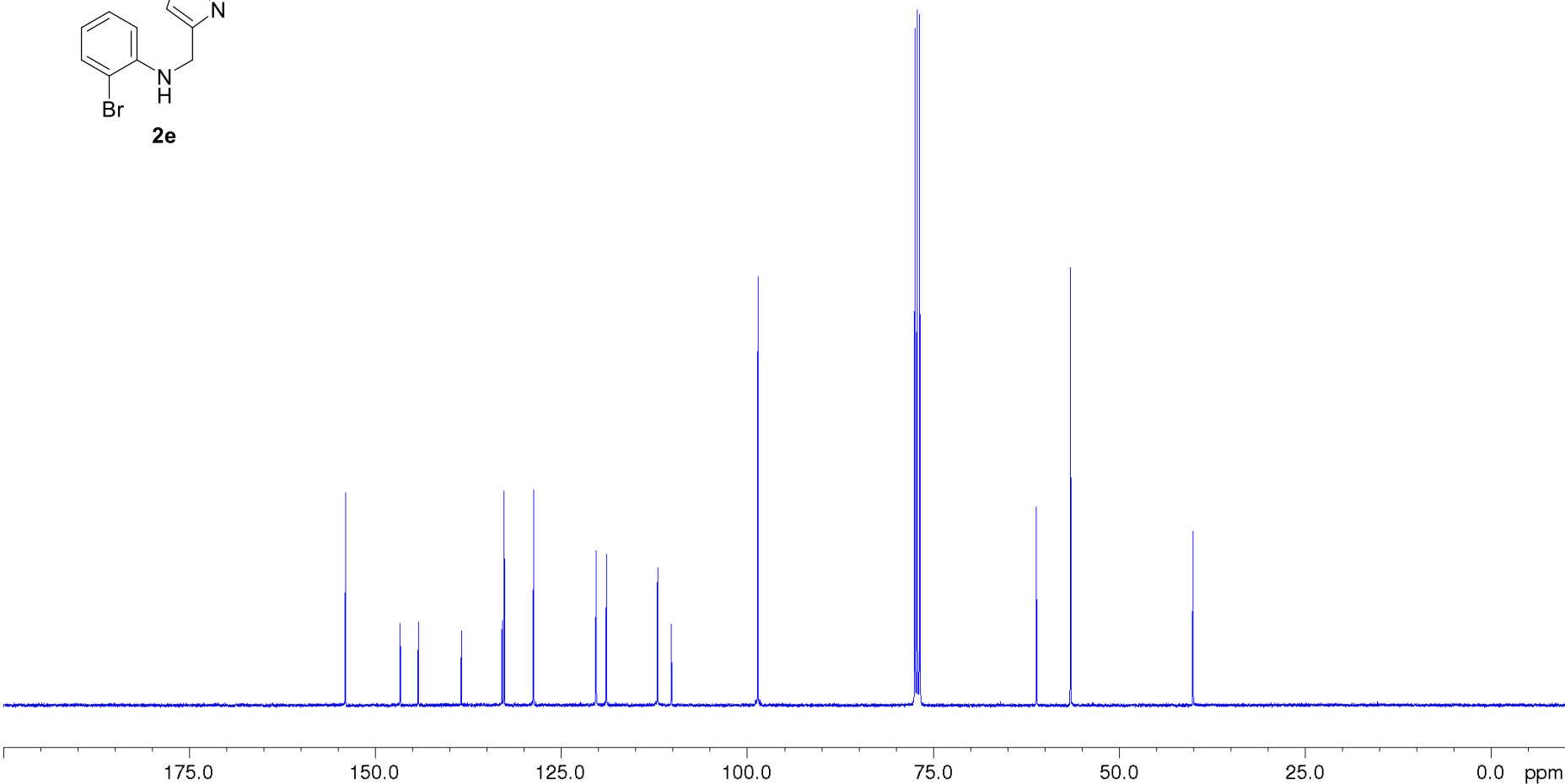


^{13}C NMR-spectrum (100 MHz, CDCl_3)

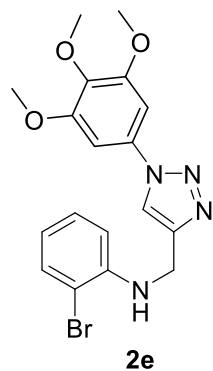


Chemical shift values (ppm) are listed above the spectrum:

- 153.905
- 146.567
- 144.139
- 138.347
- 132.866
- 132.580
- 128.630
- 120.237
- 118.857
- 111.982
- 110.131
- 98.493
- 61.067
- 56.481
- 40.114



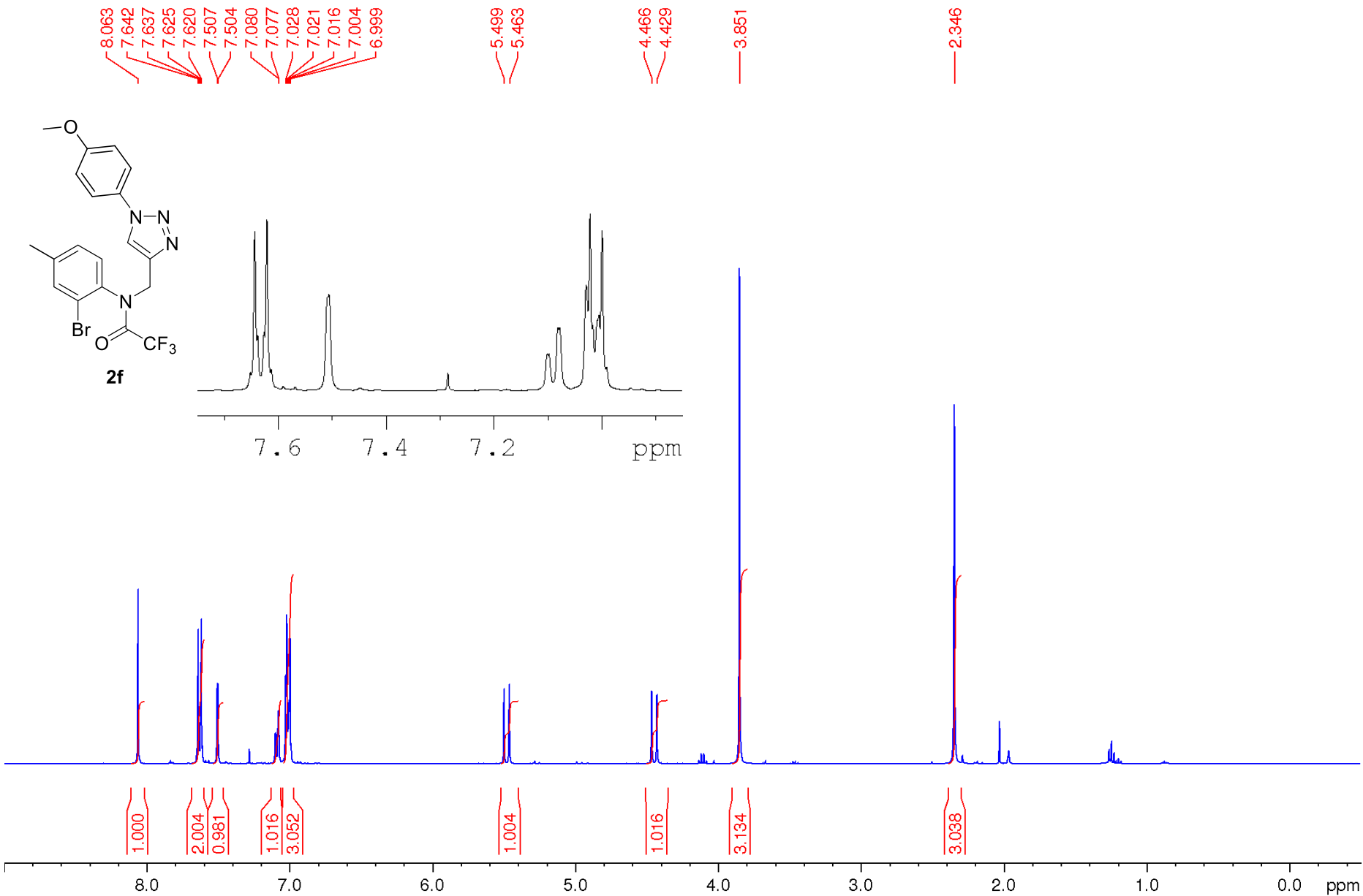
DEPT 135 NMR-spectrum (CDCl₃)



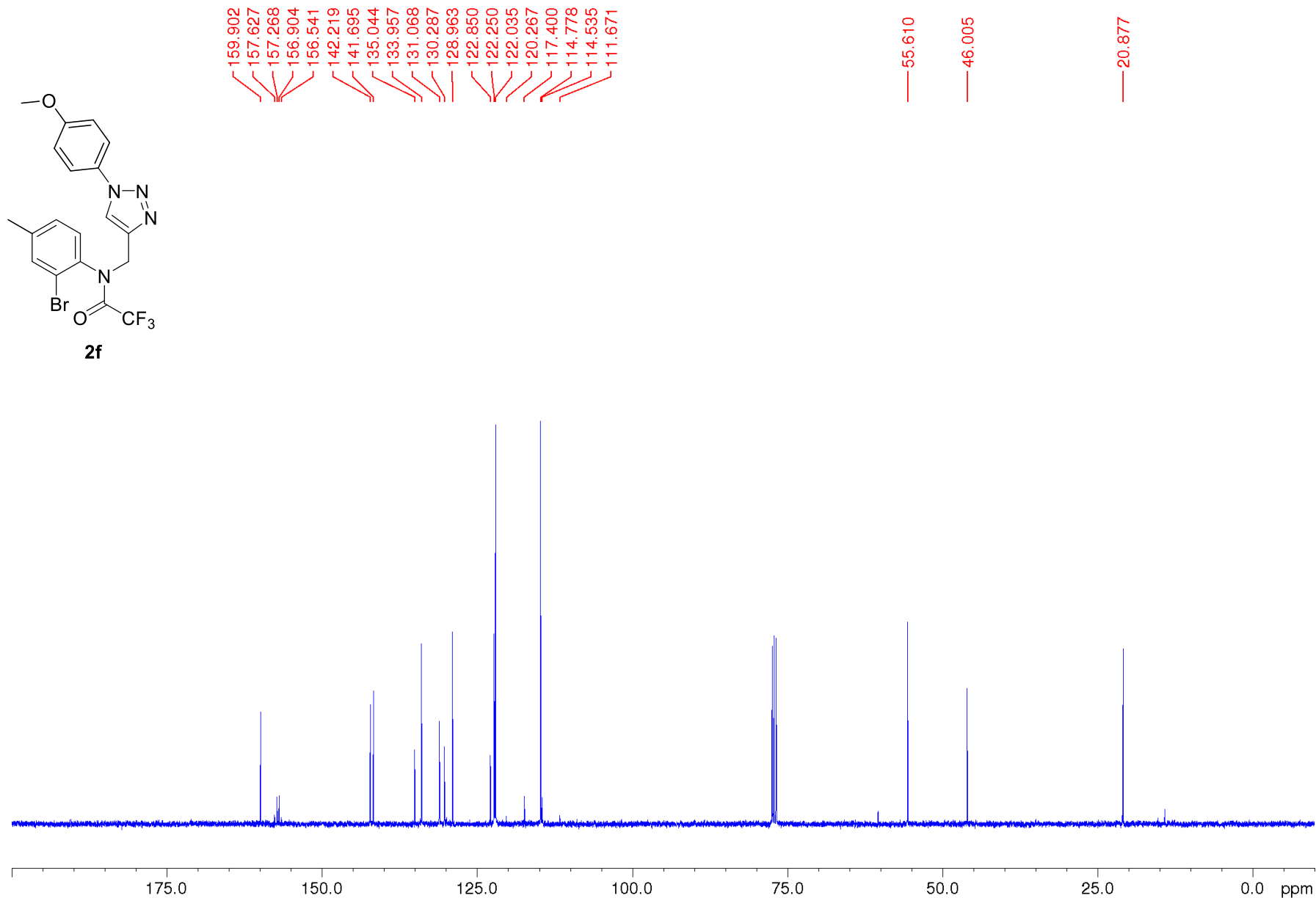
132.579
128.630
120.236
118.854
111.979
98.493
61.068
56.481
40.114

175.0 150.0 125.0 100.0 75.0 50.0 25.0 0.0 ppm

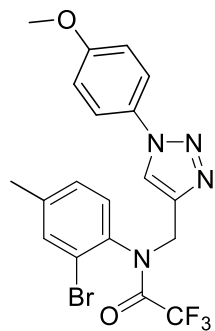
^1H NMR-spectrum (400 MHz, CDCl_3)



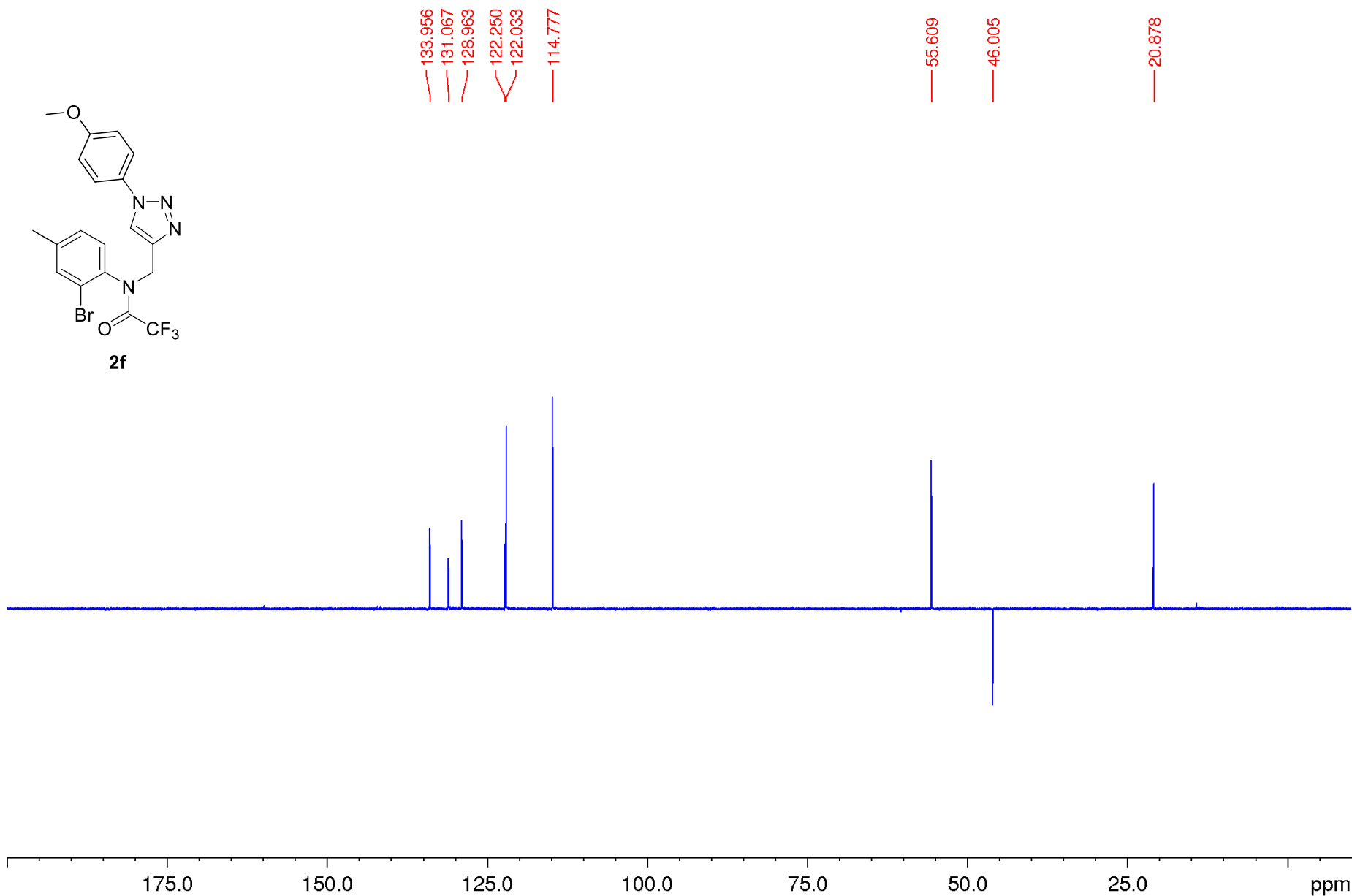
^{13}C NMR-spectrum (100 MHz, CDCl_3)



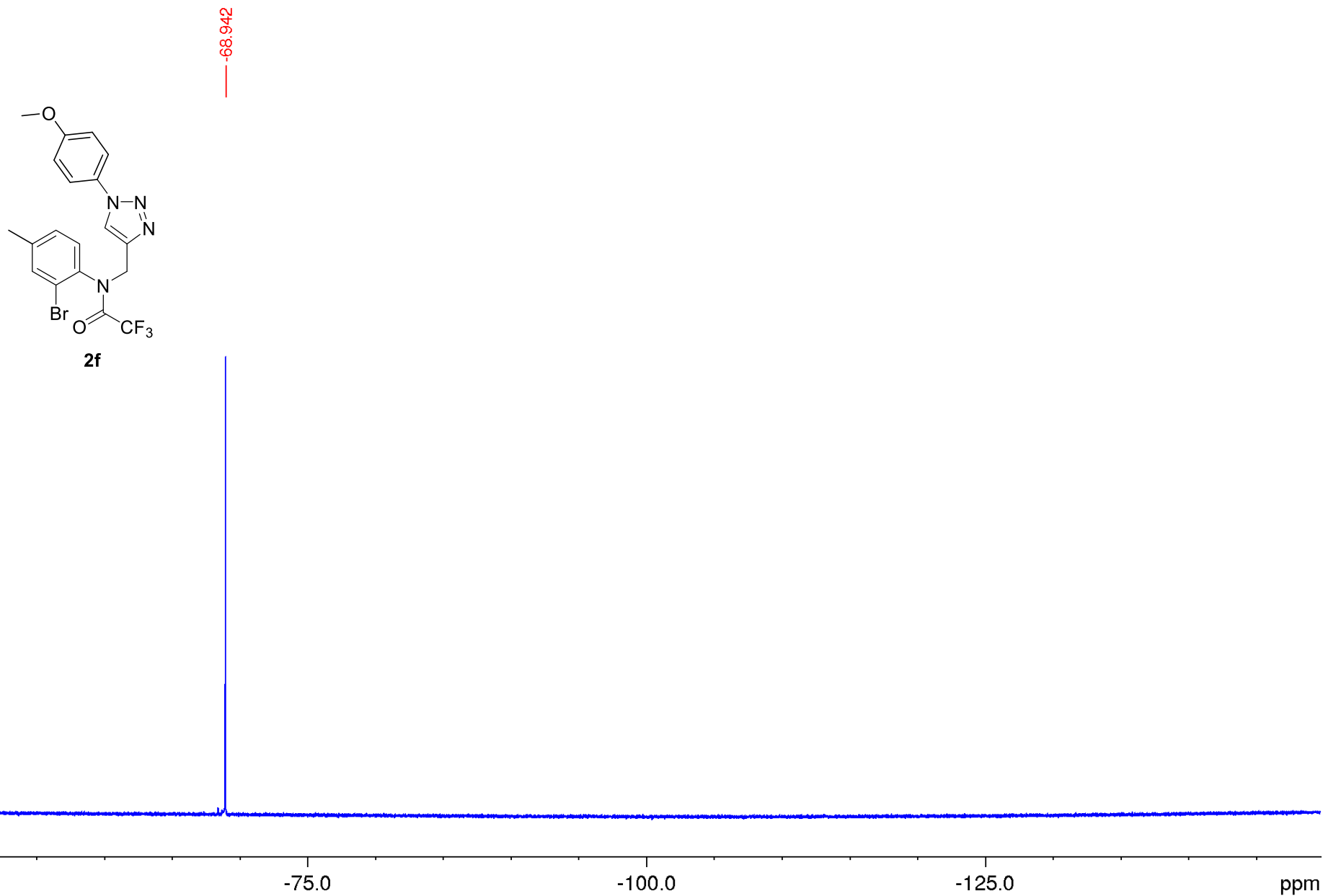
DEPT 135 NMR-spectrum (CDCl₃)



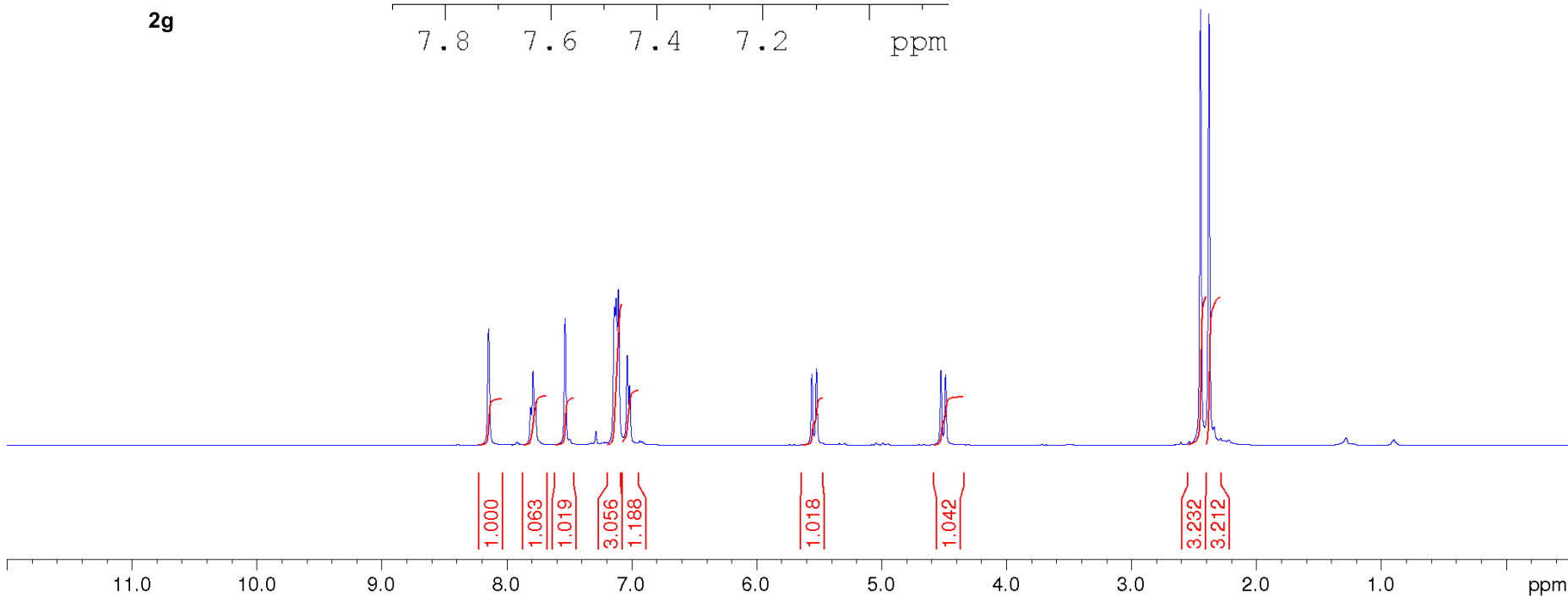
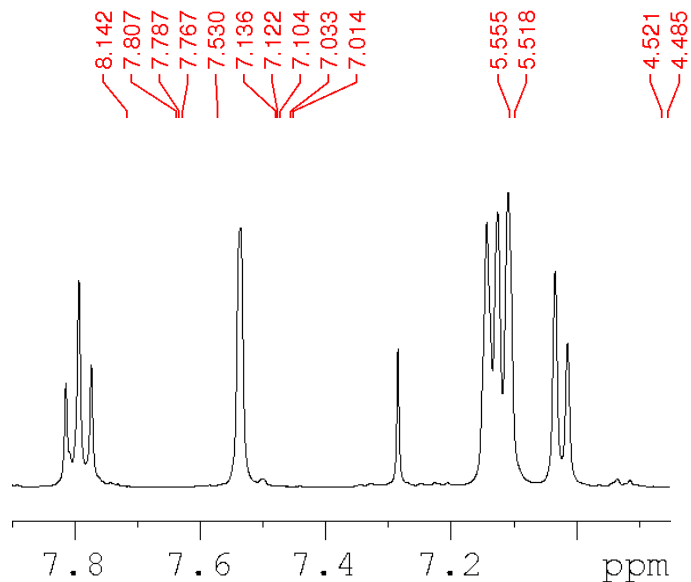
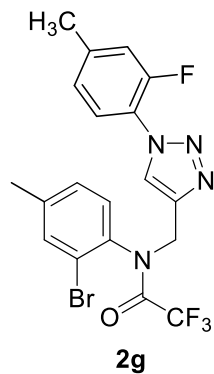
2f



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



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

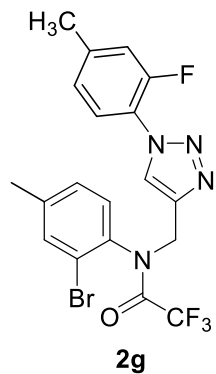


^{13}C NMR-spectrum (100 MHz, CDCl_3)

157.637
157.275
156.913
156.550
154.434
151.943
141.954
141.689
141.511
141.435
134.947
133.987
131.124
128.956
125.844
125.813
125.253
125.176
124.502
122.939
122.634
122.529
120.265
117.456
117.399
117.261
114.532
111.666

45.736

21.190
20.910



175.0

150.0

125.0

100.0

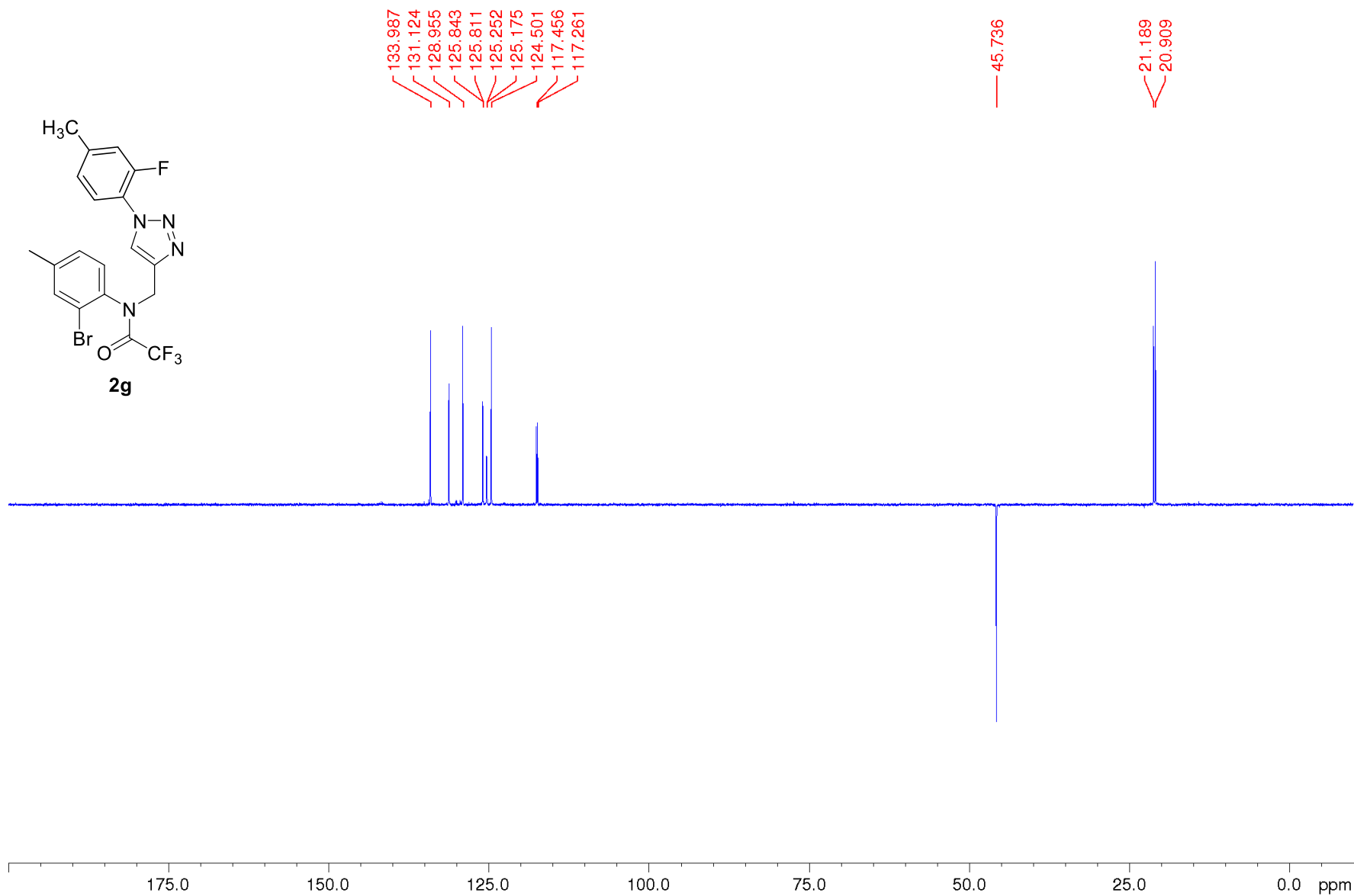
75.0

50.0

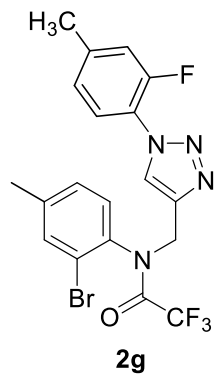
25.0

0.0 ppm

DEPT 135 NMR-spectrum (CDCl_3)



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



-68.928

-124.398
-124.423
-124.448

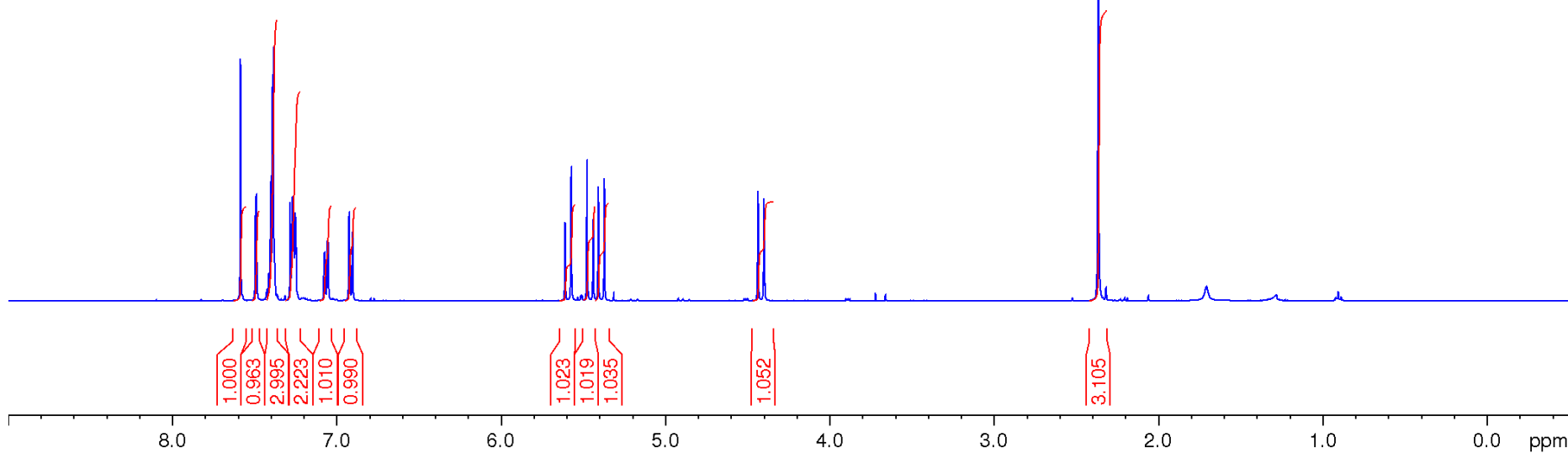
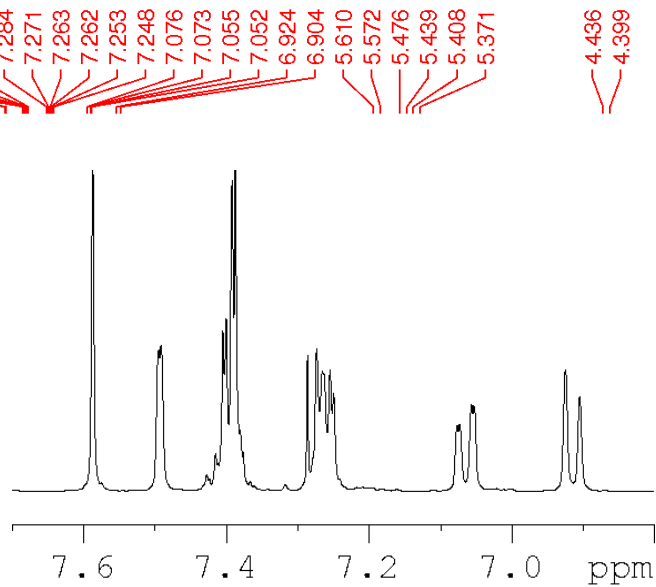
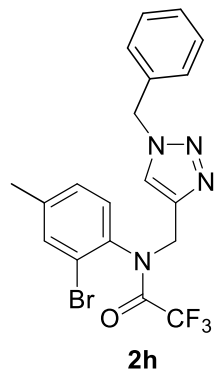
-75.0

-100.0

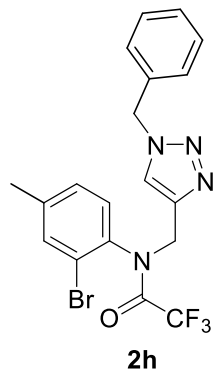
-125.0

ppm

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



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



157.563
157.211
156.844
156.484
142.117
141.586
134.870
134.459
133.934
131.046
131.030
129.149
128.858
128.045
123.953
122.922
120.238
117.371
114.506
111.665

54.235

45.800

20.911

175.0

150.0

125.0

100.0

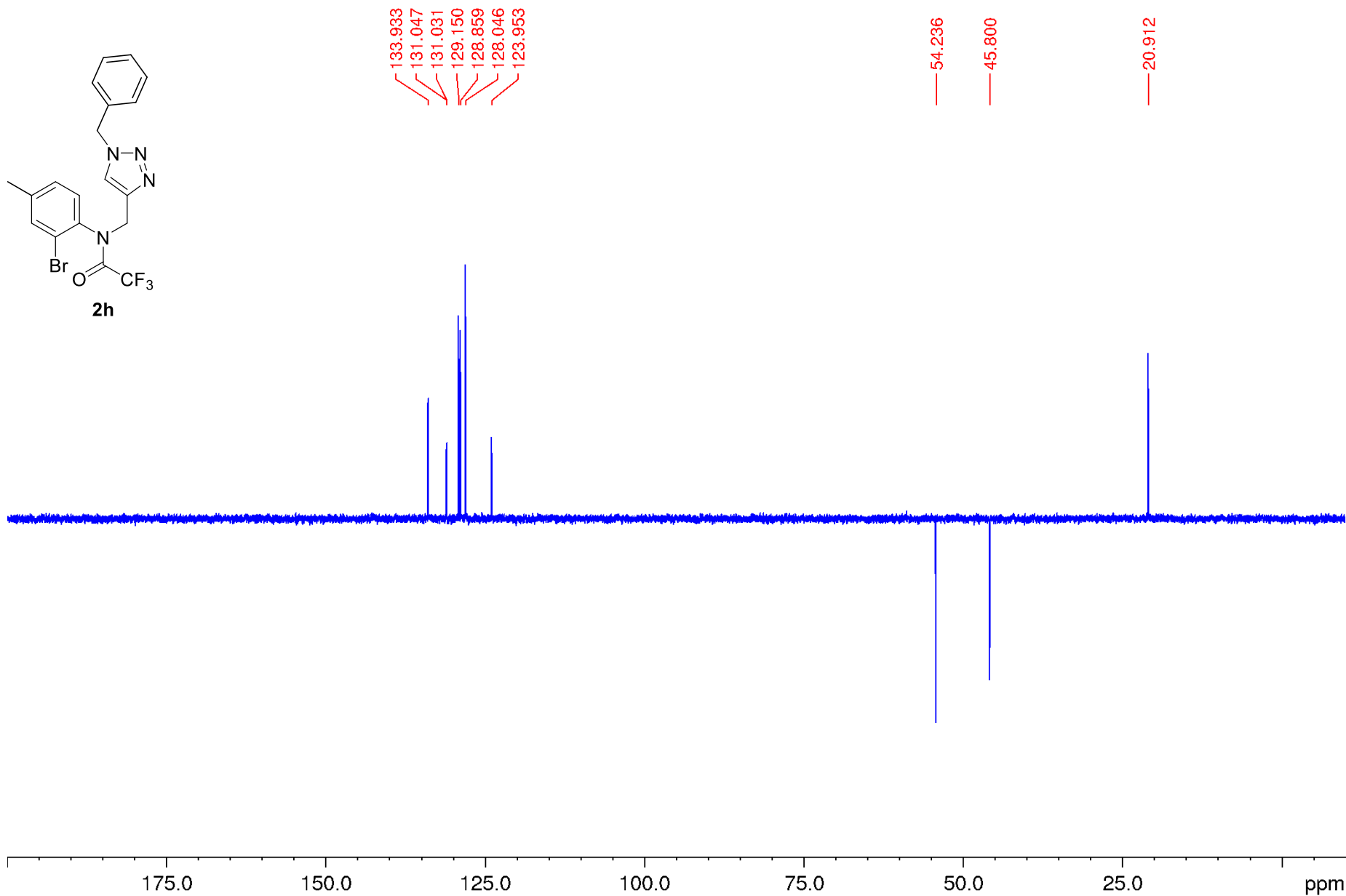
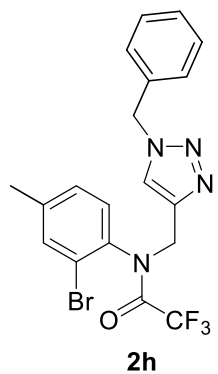
75.0

50.0

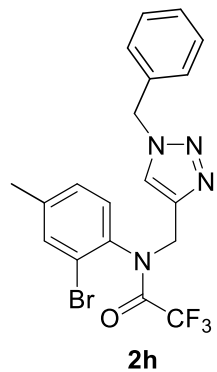
25.0

ppm

DEPT 135 NMR-spectrum (CDCl_3)



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



-68.965

—

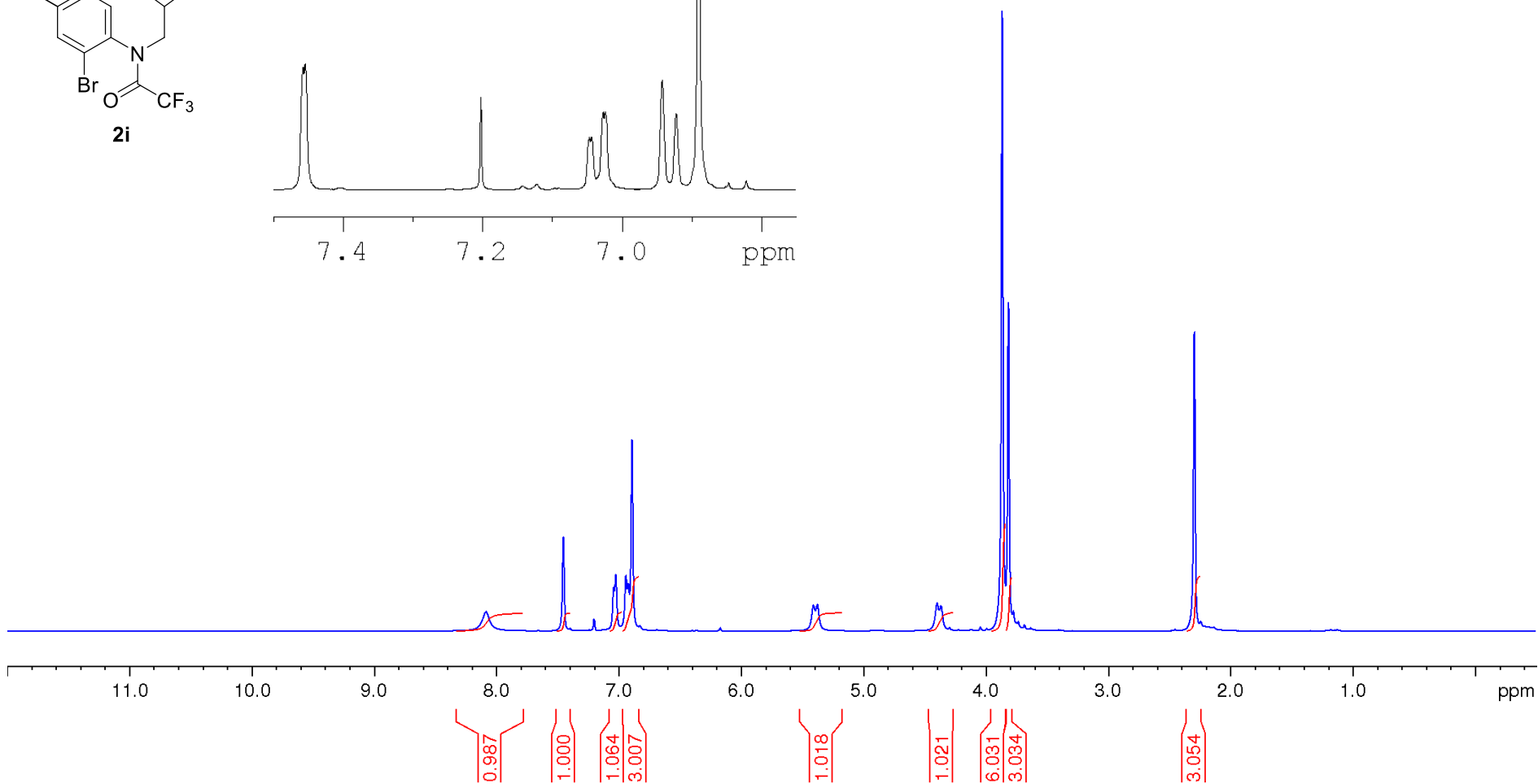
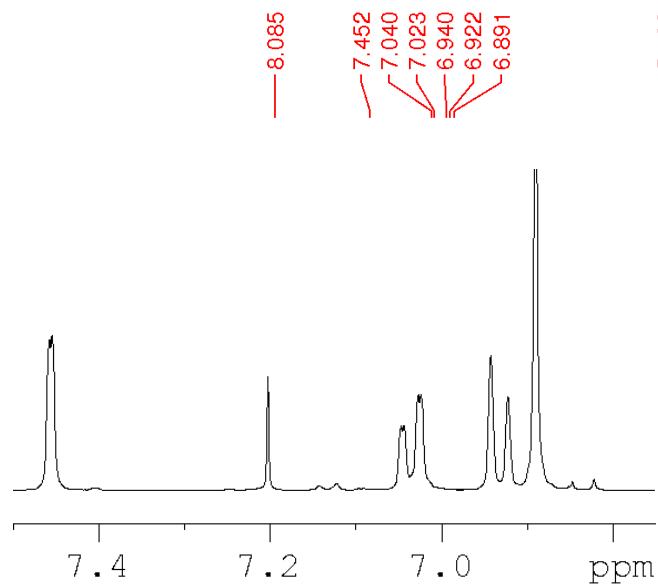
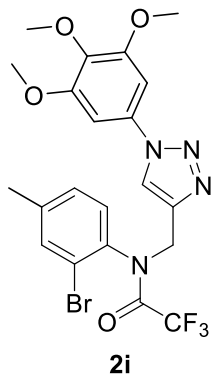
-75.0

-100.0

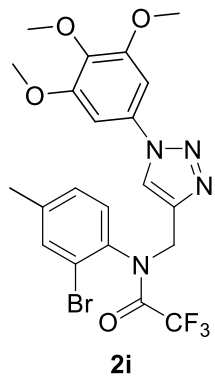
-125.0

ppm

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



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



157.758
157.387
157.024
156.668
153.957
142.442
141.768
138.405
135.074
134.026
132.692
130.980
128.990
122.833
122.338
117.377
114.514

98.246

61.061

56.495

46.114

20.921

175.0

150.0

125.0

100.0

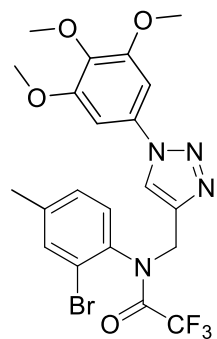
75.0

50.0

25.0

ppm

DEPT 135 NMR-spectrum (CDCl_3)



2i

134.026
130.973
128.990
122.337

98.245

61.061

56.494

46.113

20.922

175.0

150.0

125.0

100.0

75.0

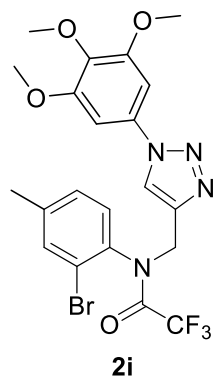
50.0

25.0

0.0

ppm

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



-68.943



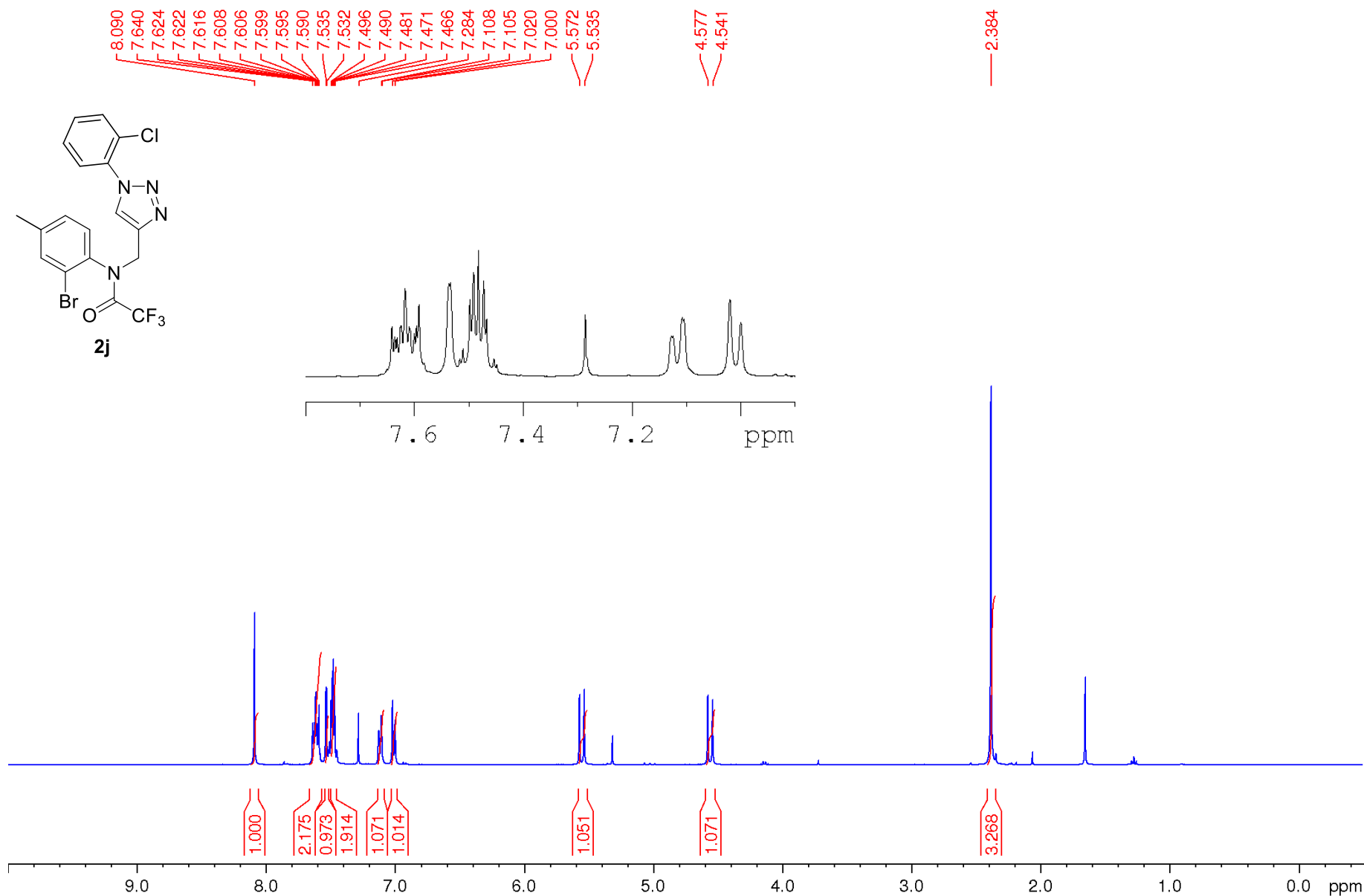
-75.0

-100.0

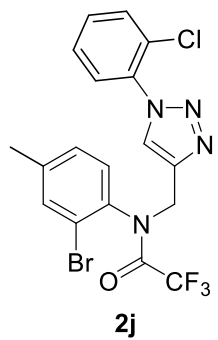
-125.0

ppm

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



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



157.681
157.319
156.956
156.593
141.709
141.482
134.833
134.716
134.008
131.119
130.951
130.797
128.975
128.680
127.961
127.764
126.164
123.002
120.267
117.401
114.535
111.669

45.644

20.924

175.0

150.0

125.0

100.0

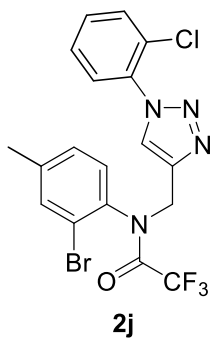
75.0

50.0

25.0

ppm

DEPT 135 NMR-spectrum (CDCl_3)



134.006
131.117
130.953
130.796
128.974
127.962
127.763
126.165

45.641

20.924

175.0

150.0

125.0

100.0

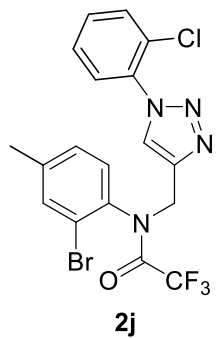
75.0

50.0

25.0

ppm

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



-68.943

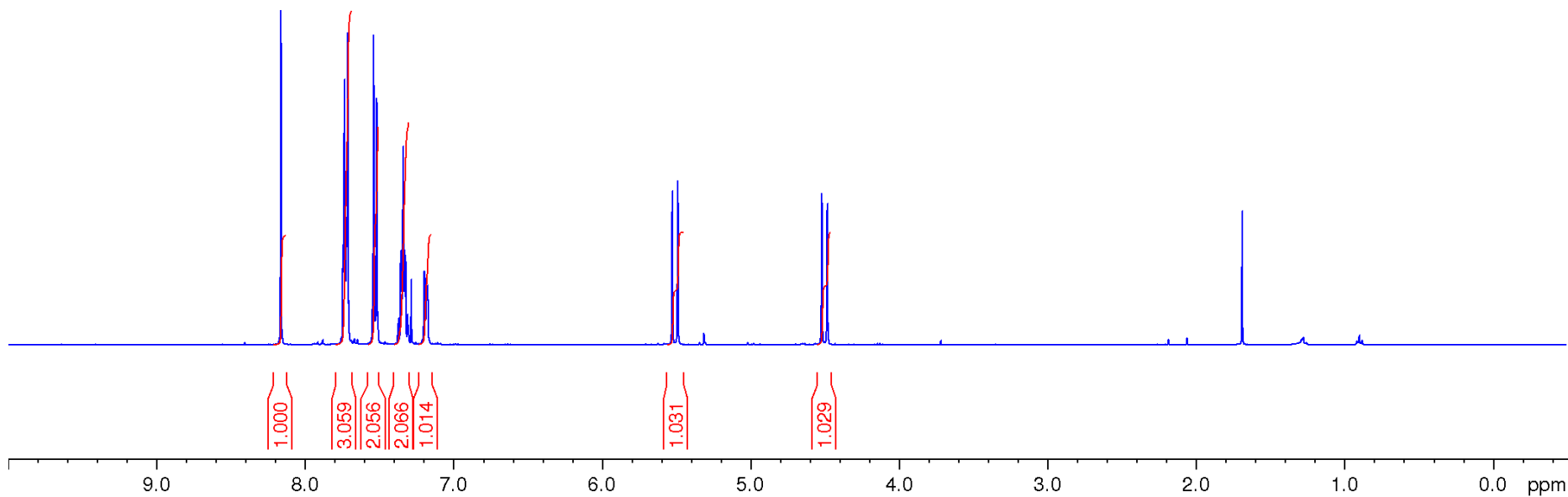
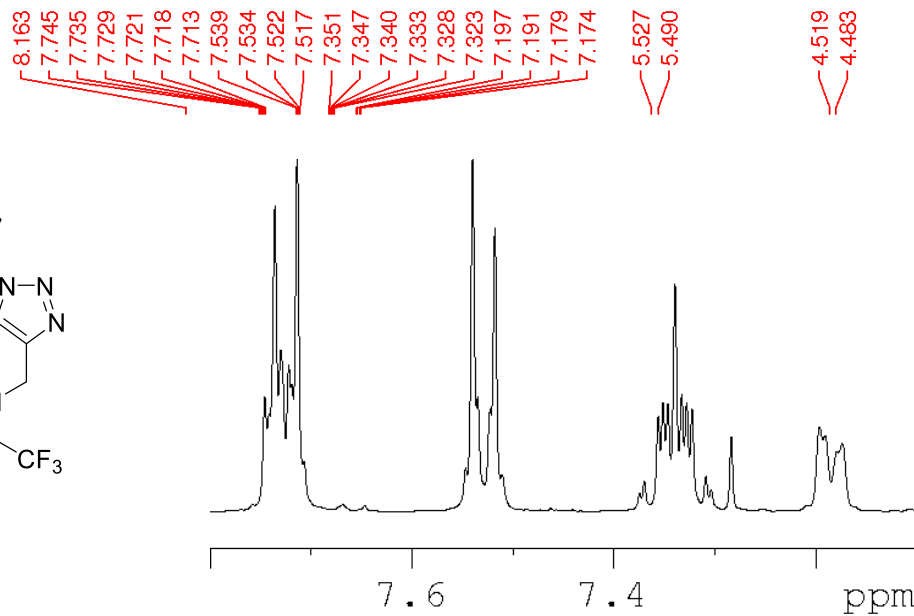
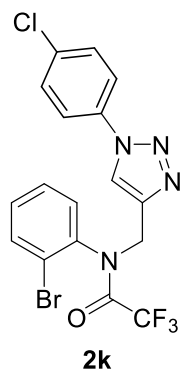
-75.0

-100.0

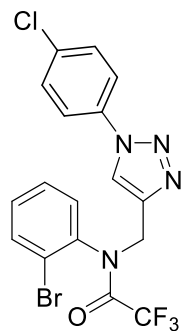
-125.0

ppm

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



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



2k

157.638
157.269
156.905
156.535
142.655
137.826
135.321
134.760
133.667
131.499
131.127
129.999
128.359
123.298
122.186
121.625
120.208
117.315
114.450
111.598

46.025

175.0

150.0

125.0

100.0

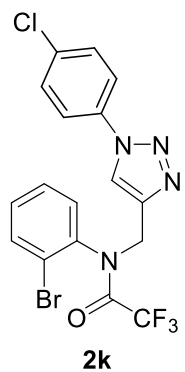
75.0

50.0

25.0

ppm

DEPT 135 NMR-spectrum (CDCl_3)



133.666
131.500
131.127
129.999
128.360
122.186
121.625

46.025

175.0

150.0

125.0

100.0

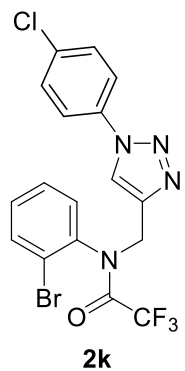
75.0

50.0

25.0

ppm

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



-68.983



-75.0

-100.0

-125.0

ppm

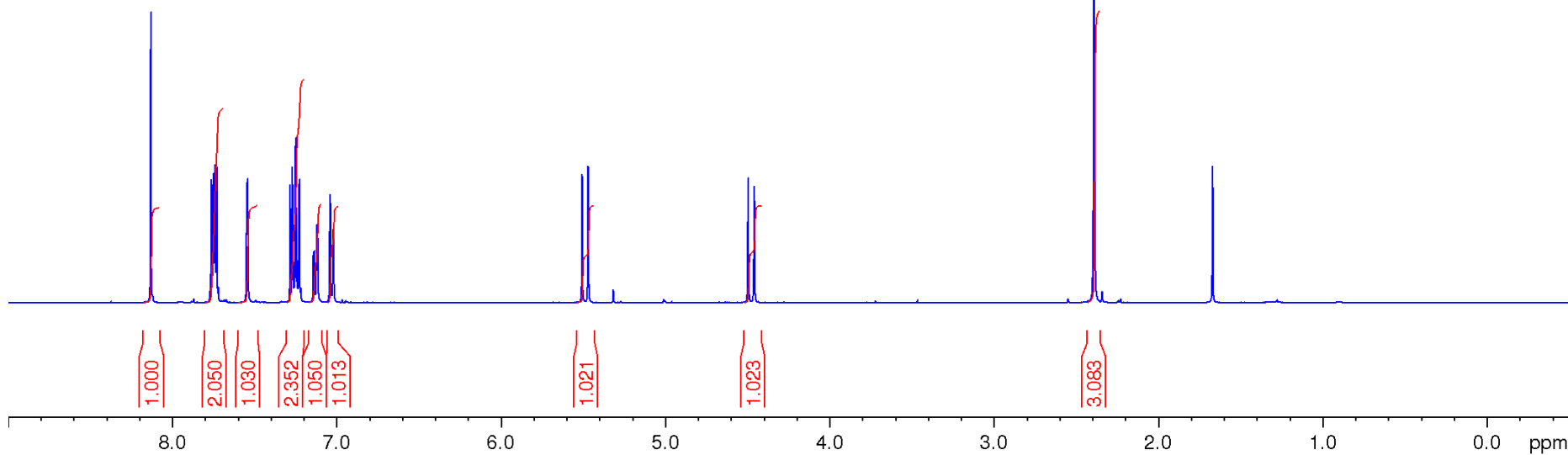
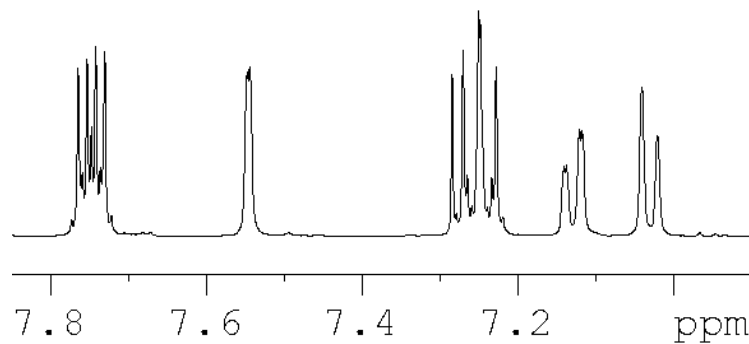
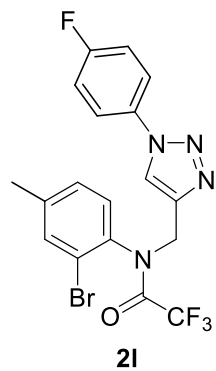
^1H NMR-spectrum (400 MHz, CDCl_3)

8.132
7.763
7.758
7.752
7.746
7.741
7.735
7.729
7.546
7.543
7.284
7.270
7.250
7.248
7.227
7.140
7.137
7.120
7.117
7.040
7.020

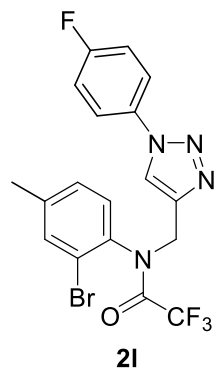
5.506
5.469

4.495
4.458

2.390



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



163.758
161.279
157.761
157.392
157.029
156.682
142.637
141.775
135.111
134.039
133.162
130.967
129.017
122.838
122.505
122.419
122.383
120.273
117.365
116.899
116.670
114.501
111.642

46.094

20.930

175.0

150.0

125.0

100.0

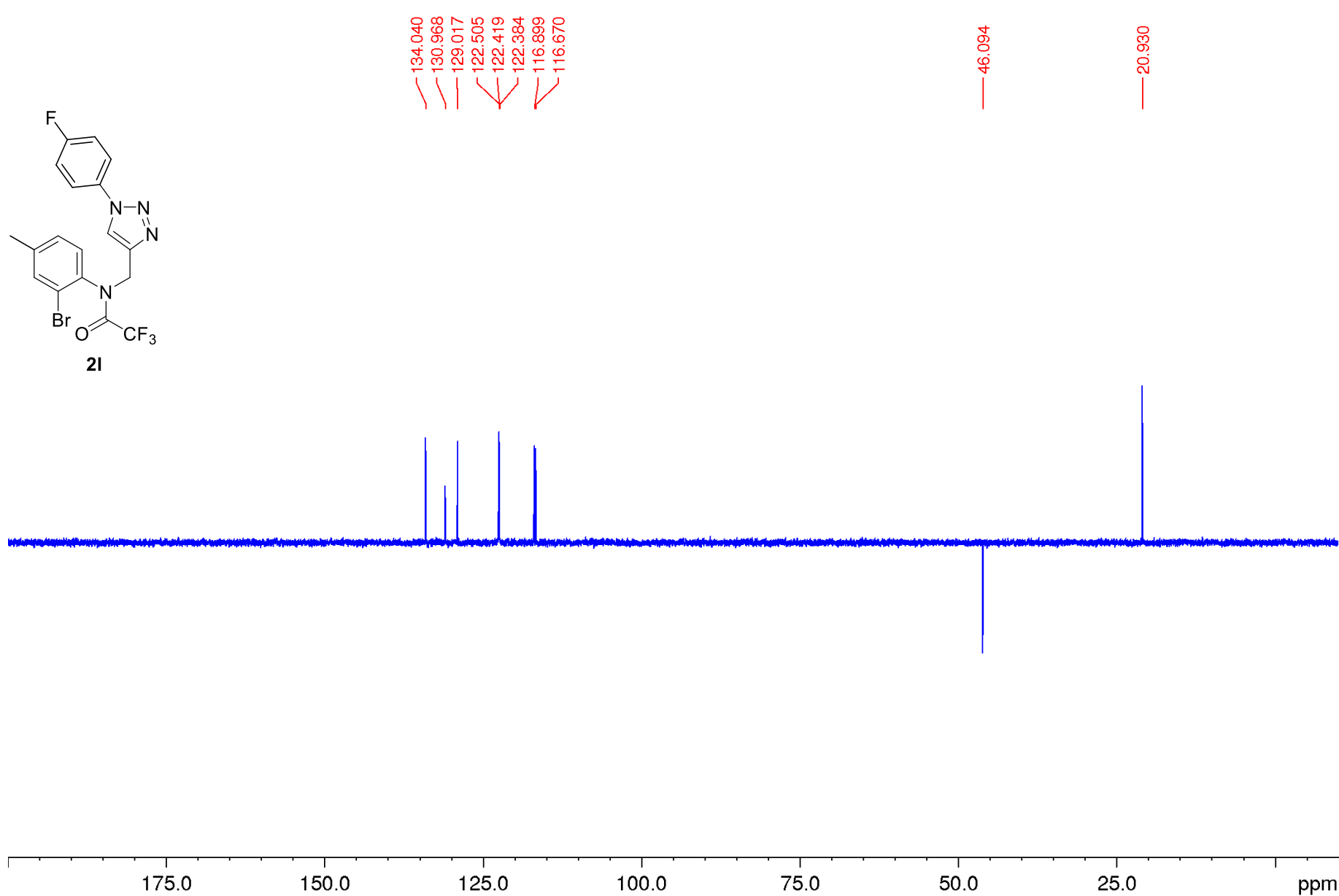
75.0

50.0

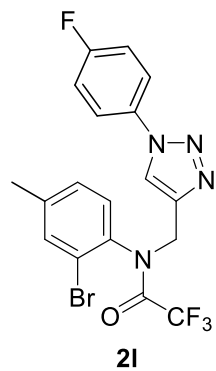
25.0

0.0 ppm

DEPT 135 NMR-spectrum (CDCl₃)



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



-68.957

-111.832
-111.844
-111.855
-111.865

-75.0

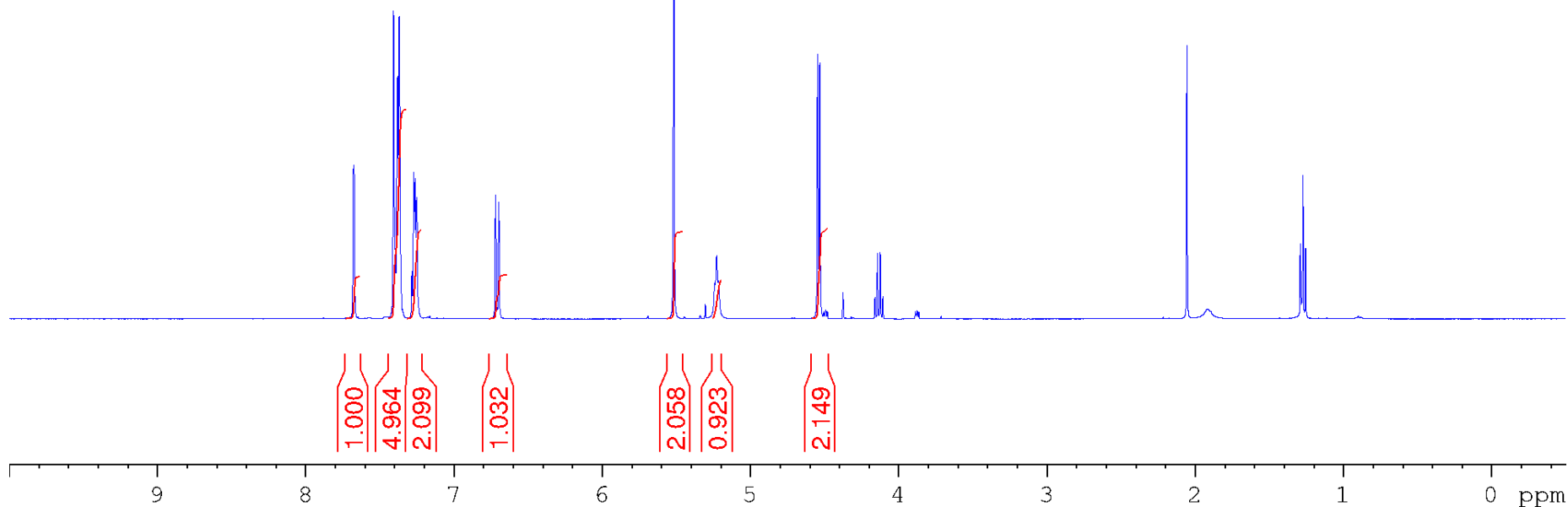
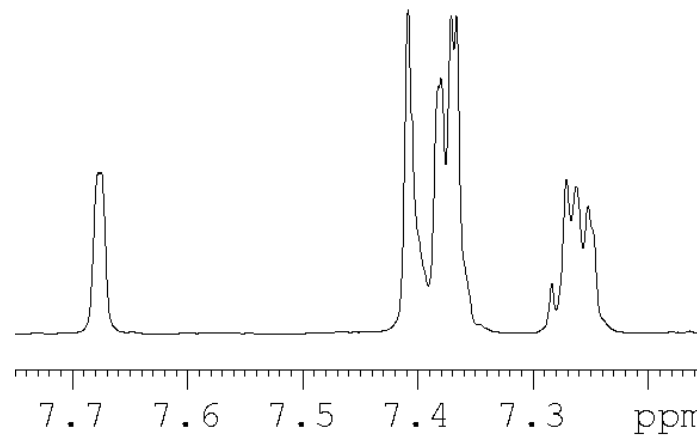
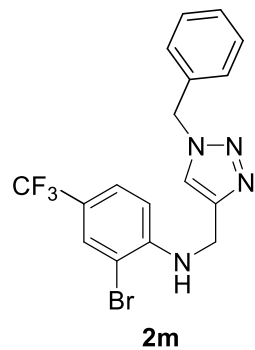
-100.0

-125.0

ppm

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

7.676
7.675
7.408
7.382
7.380
7.371
7.367
7.284
7.271
7.263
7.252
6.719
6.698
5.517
5.227
4.546
4.532

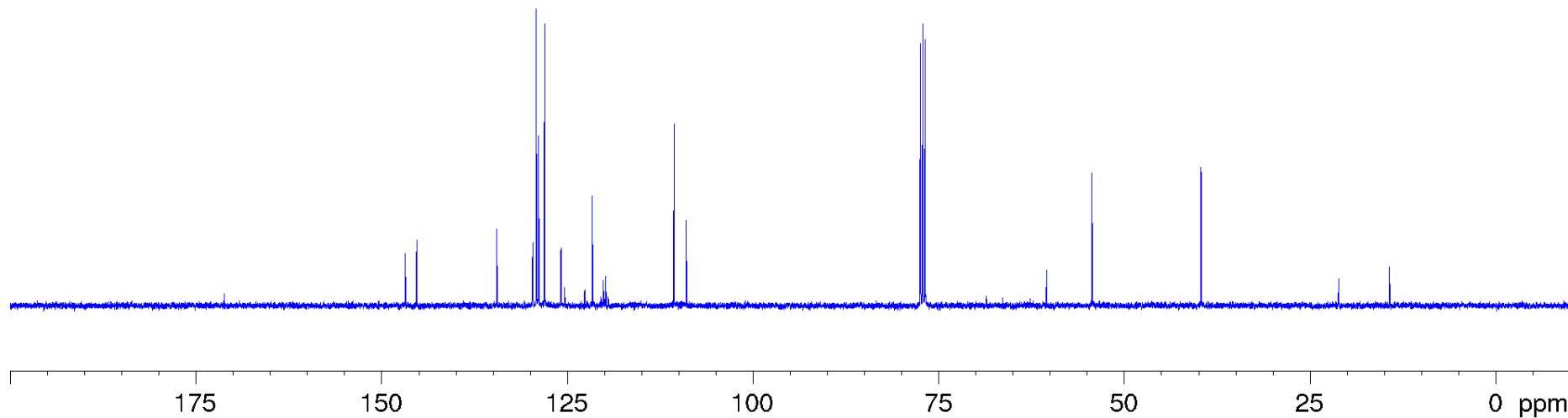
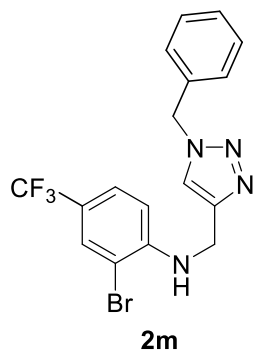


^{13}C NMR-spectrum (100 MHz, CDCl_3)

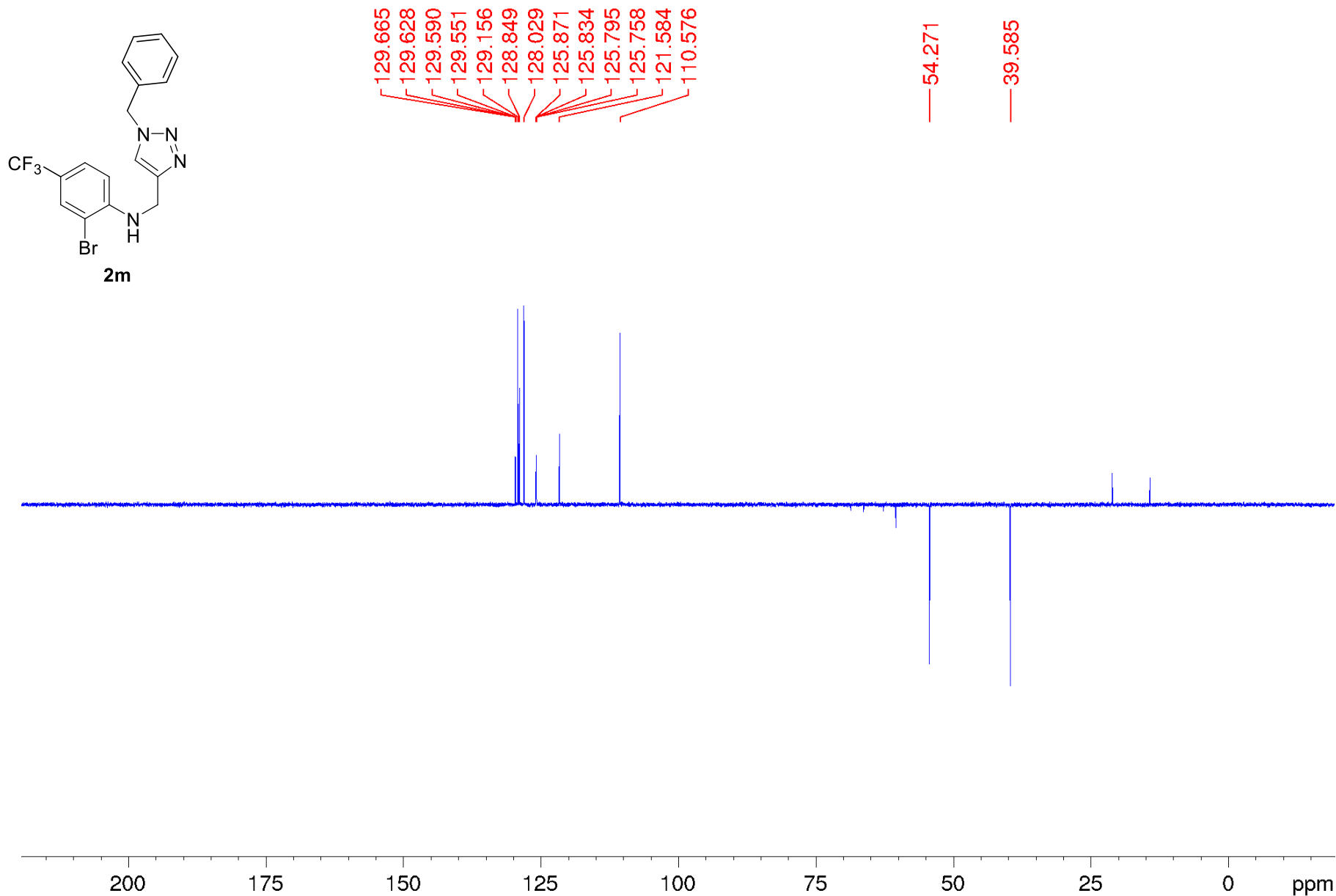
146.797
145.253
134.475
129.664
129.628
129.590
129.551
129.156
128.849
128.029
125.870
125.833
125.795
125.758
125.310
122.616
121.583
120.433
120.101
119.938
119.770
119.437
110.576
108.943

— 54.270

— 39.585

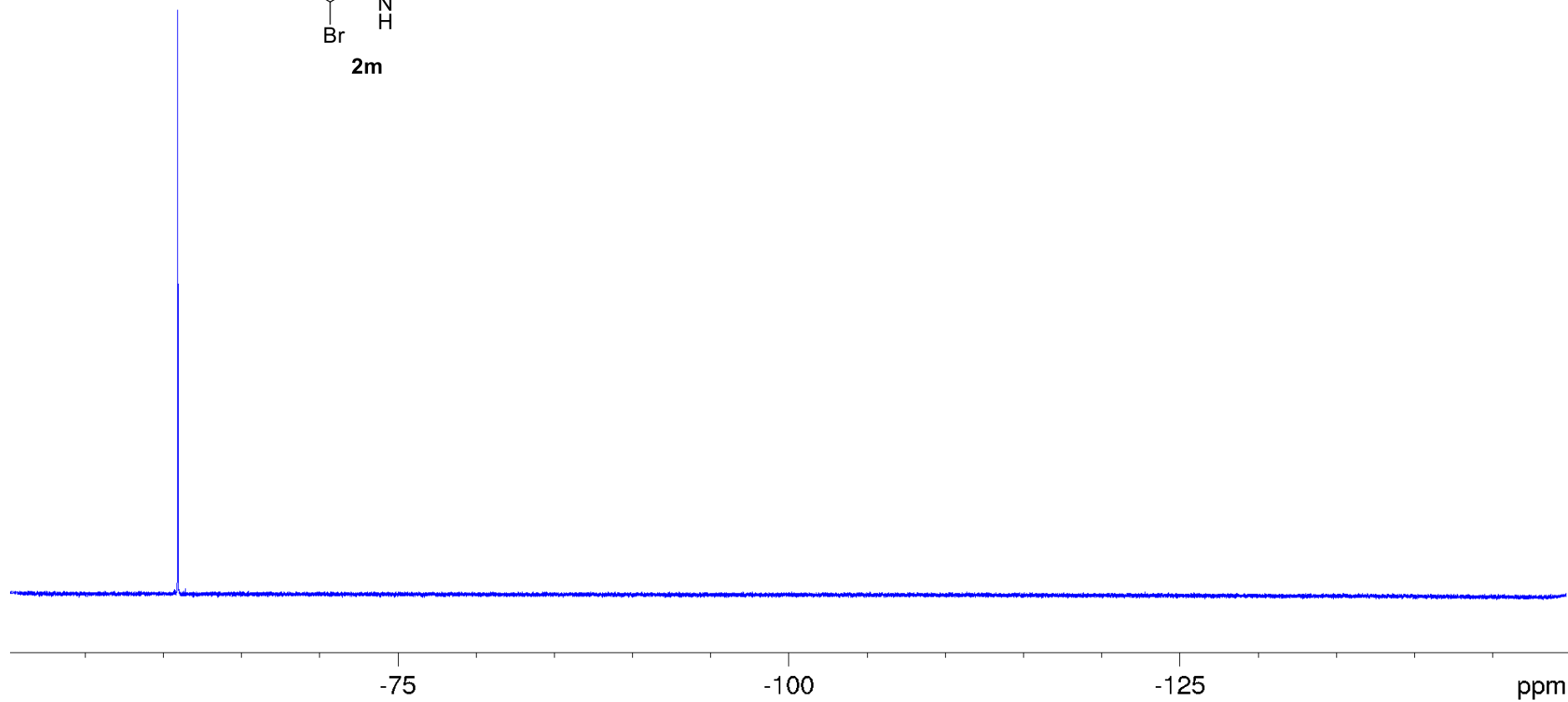
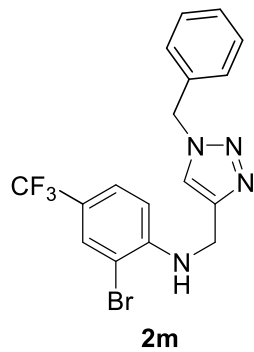


DEPT 135 NMR-spectrum (CDCl_3)

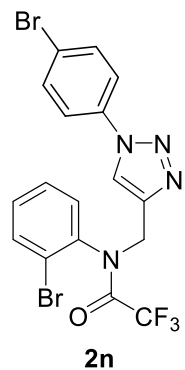


^{19}F NMR-spectrum (376.5 Hz, CDCl_3)

— -60.926



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

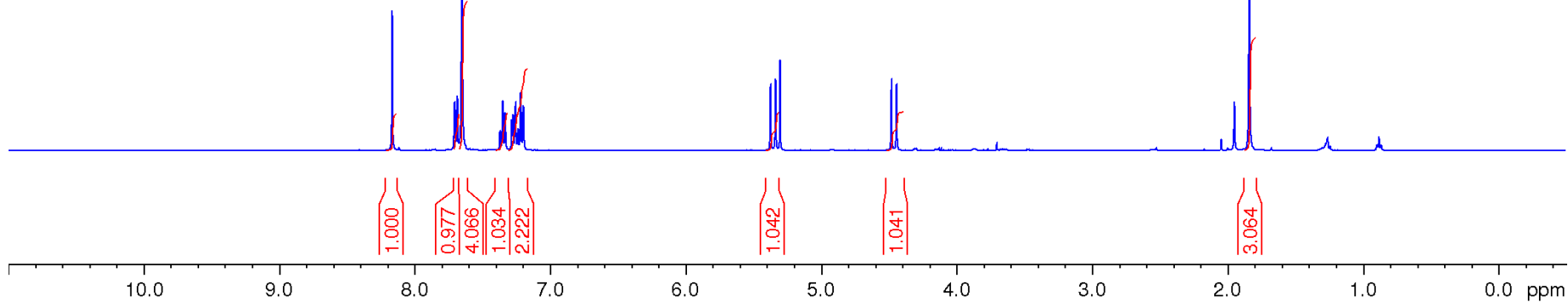
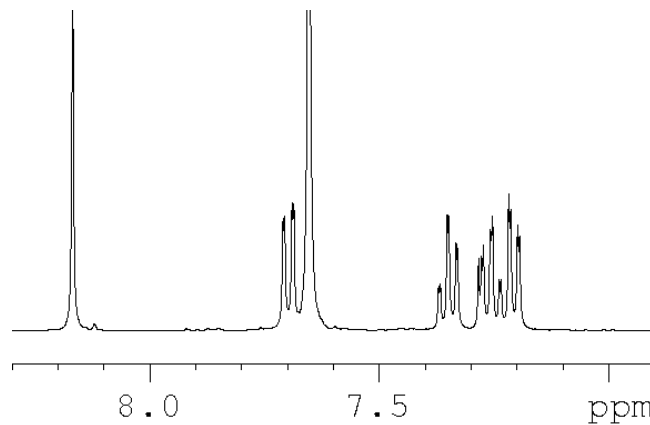


8.166
7.707
7.704
7.688
7.684
7.651
7.352
7.349
7.333
7.330
7.278
7.273
7.258
7.254
7.218
7.214
7.199
7.195

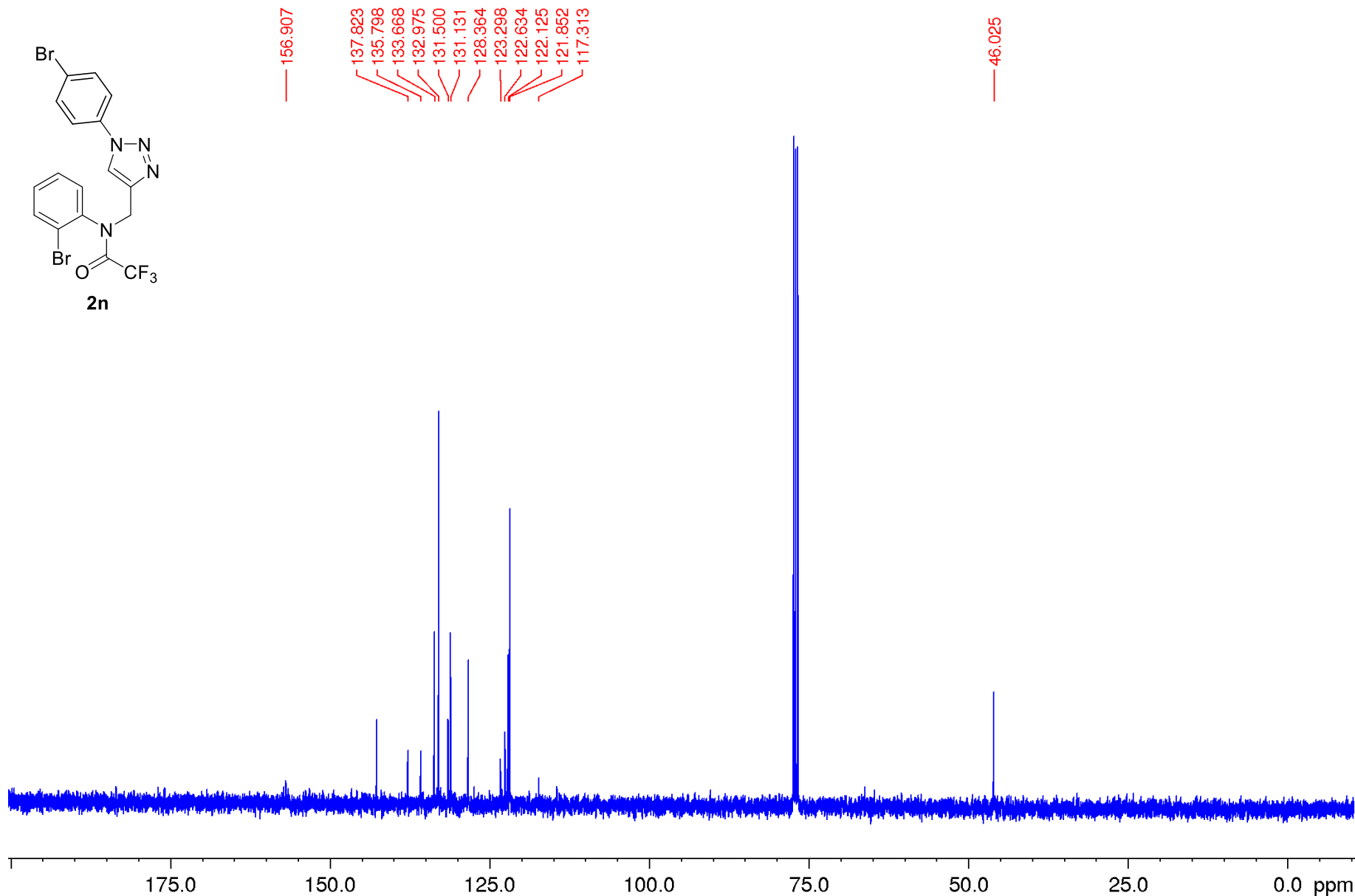
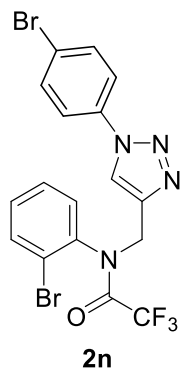
5.373
5.336

4.480
4.443

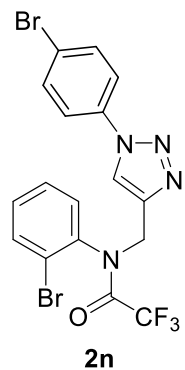
1.839



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



DEPT 135 NMR-spectrum (CDCl_3)



133.668
132.975
131.490
131.131
128.364
122.126
121.851

46.018

175.0

150.0

125.0

100.0

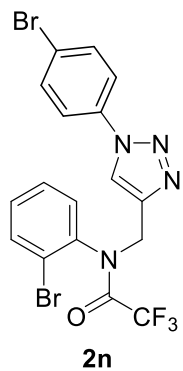
75.0

50.0

25.0

ppm

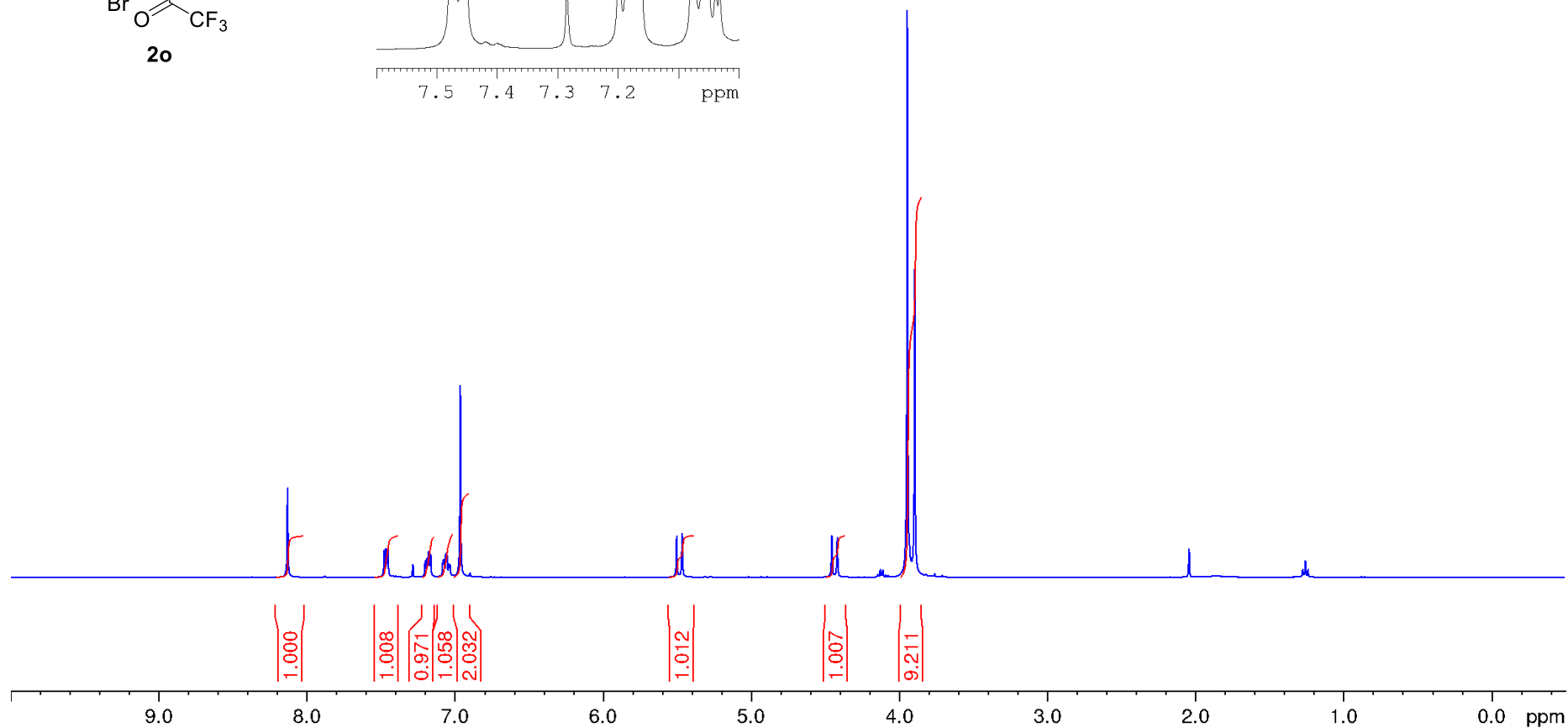
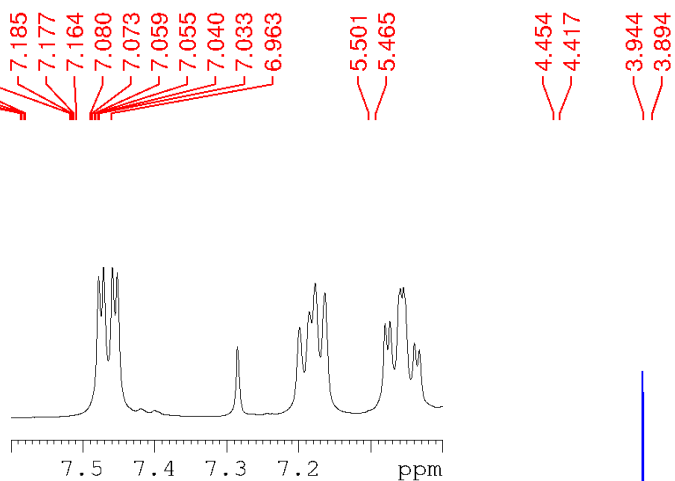
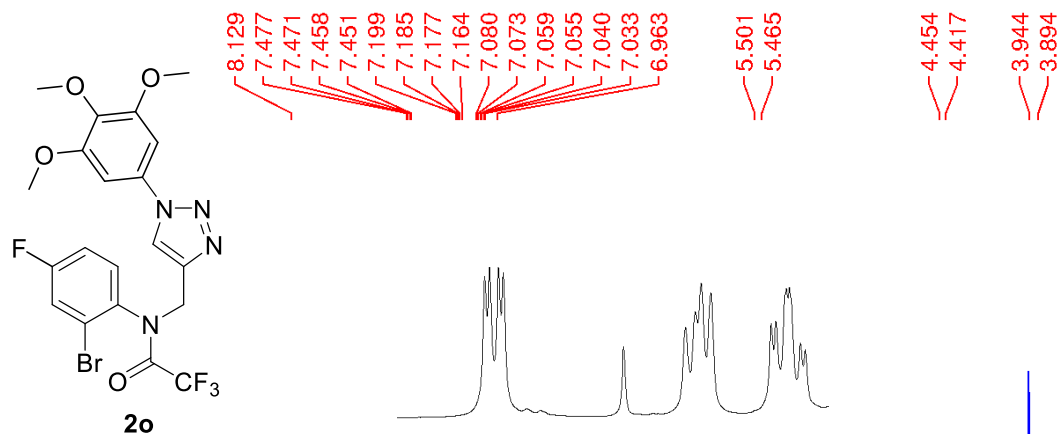
^{19}F NMR-spectrum (376.5 Hz, CDCl_3)



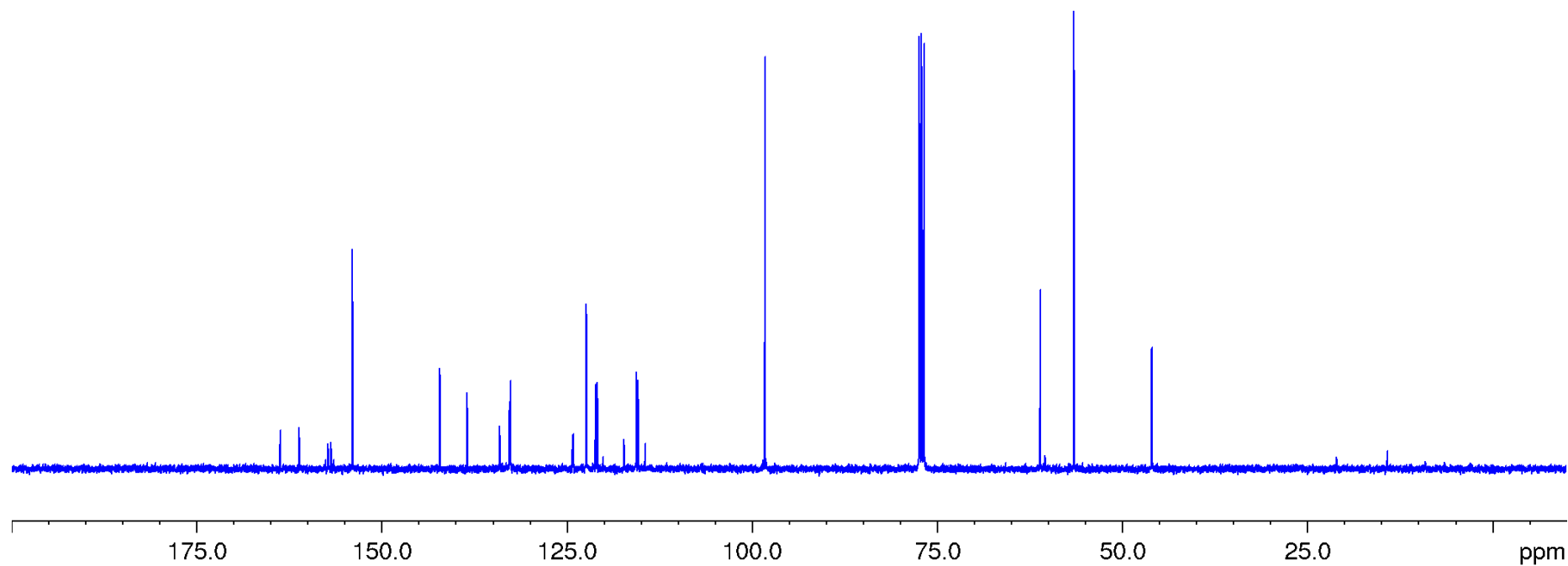
-68.982



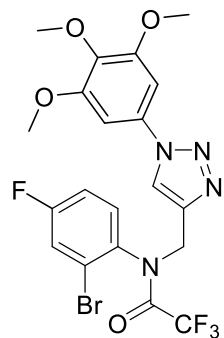
^1H NMR-spectrum (400 MHz, CDCl_3)



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



DEPT 135 NMR-spectrum (CDCl₃)



2o

132.754
132.660
122.352
121.118
120.861
115.594
115.372

98.225

61.057

56.482

45.985

175.0

150.0

125.0

100.0

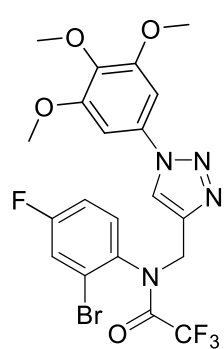
75.0

50.0

25.0

ppm

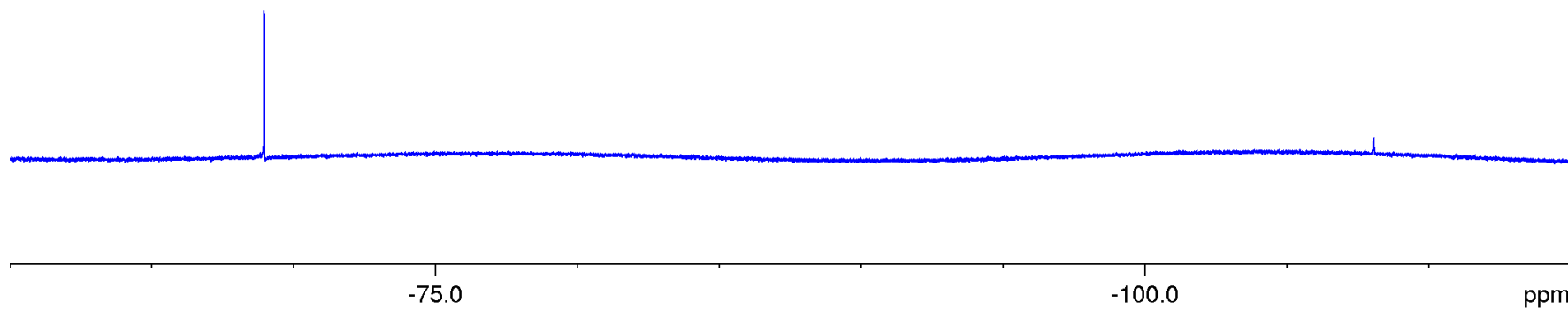
^{19}F NMR-spectrum (376.5 Hz, CDCl_3)



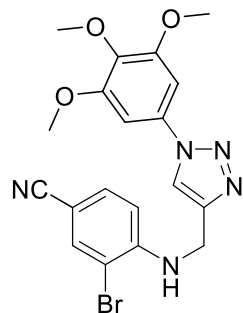
2o

-68.978

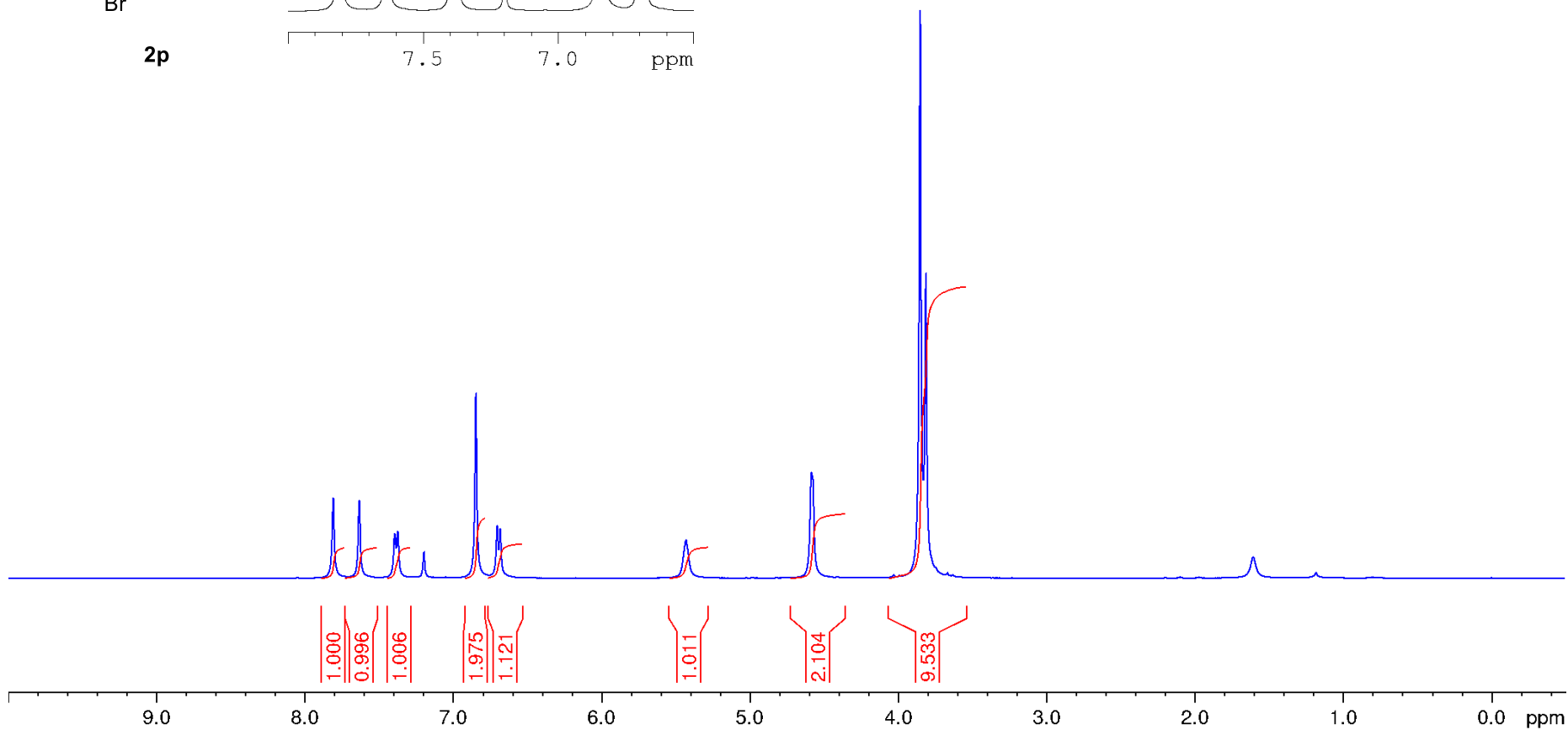
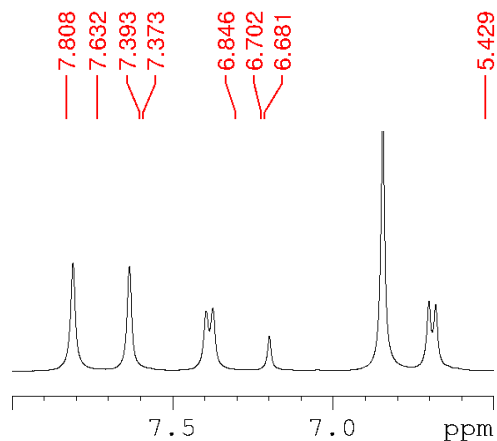
-108.049
-108.069
-108.083
-108.103



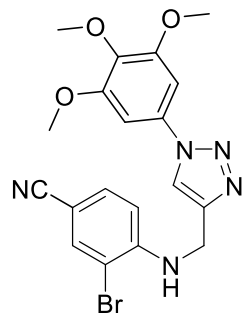
^1H NMR-spectrum (400 MHz, CDCl_3)



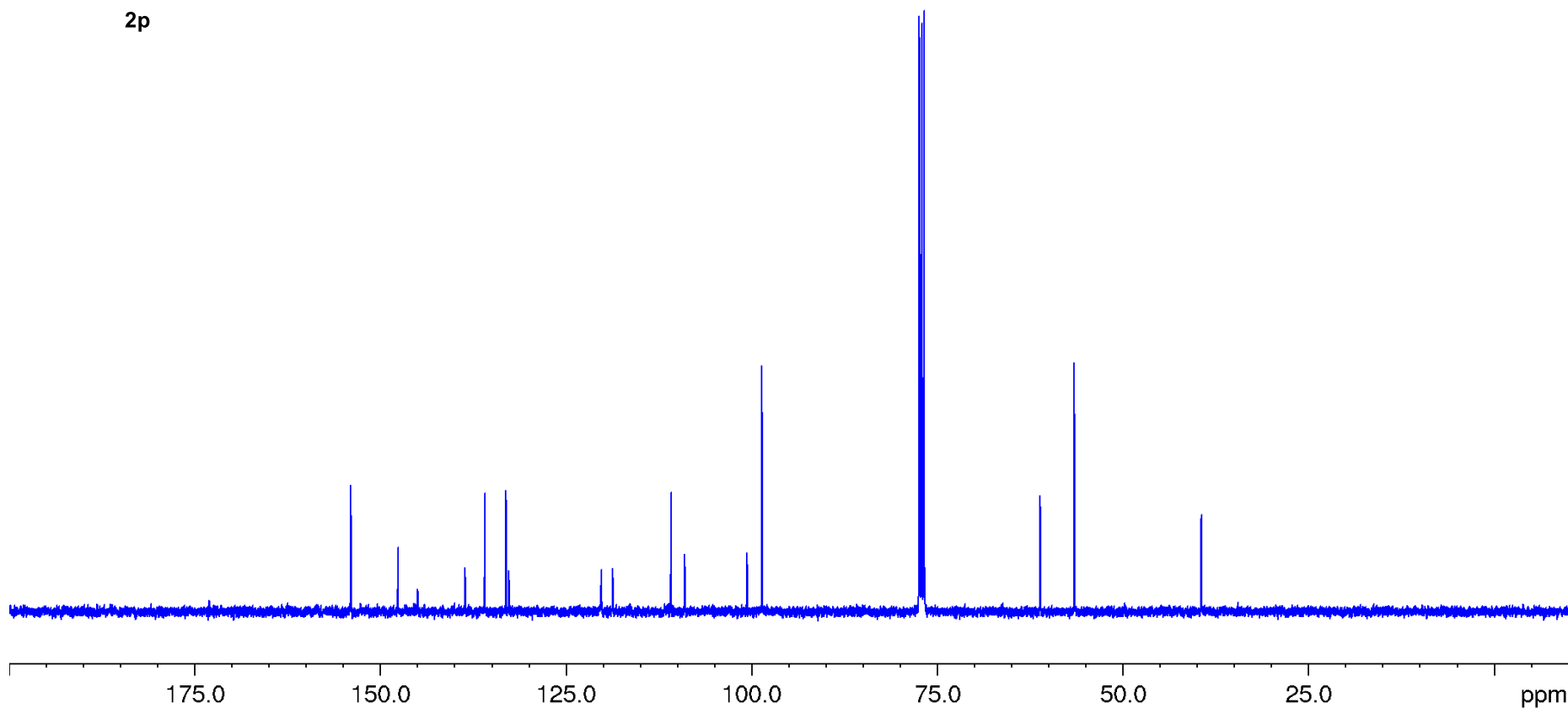
2p



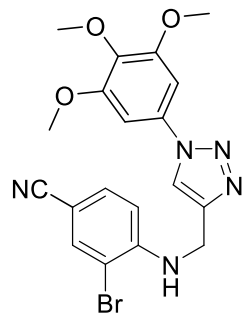
^{13}C NMR-spectrum (100 MHz, CDCl_3)



2p



DEPT 135 NMR-spectrum (CDCl₃)



2p

135.892
133.041
120.212
110.804
98.574
61.084
56.502
39.386

175.0

150.0

125.0

100.0

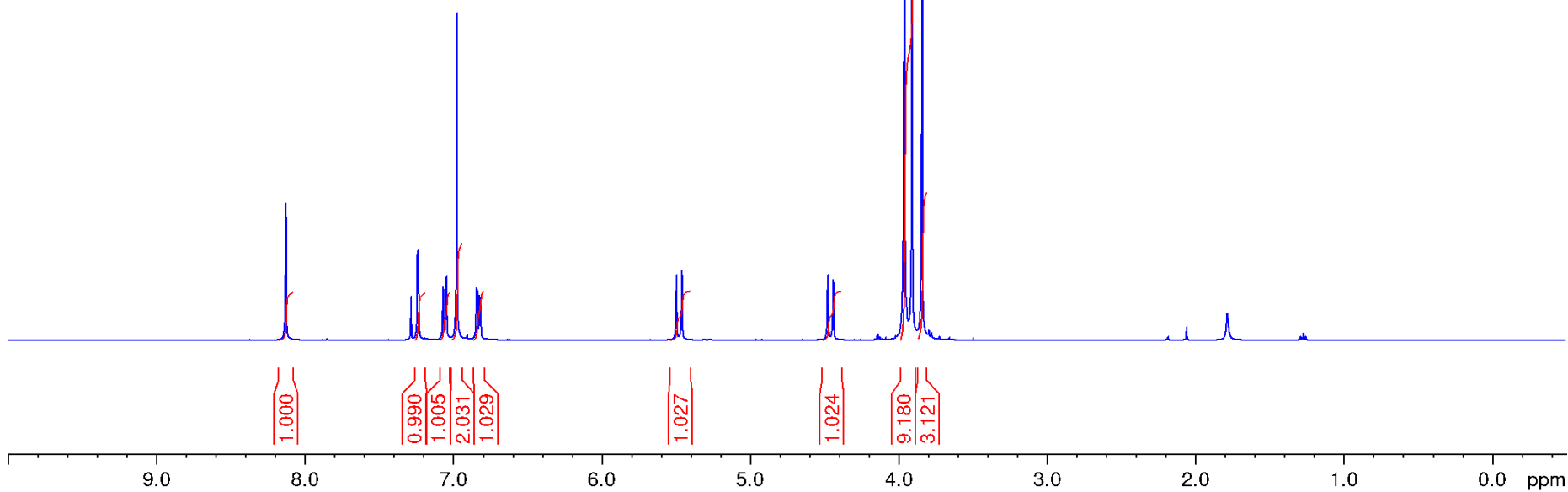
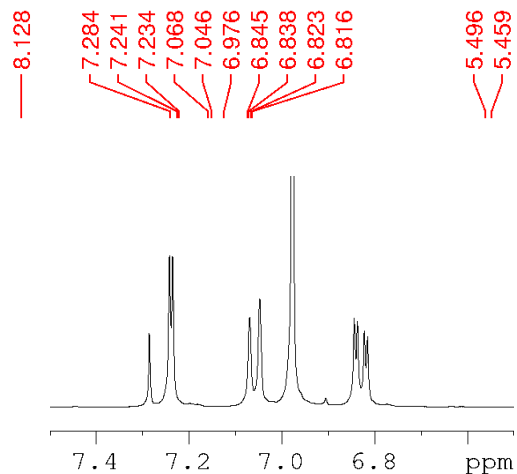
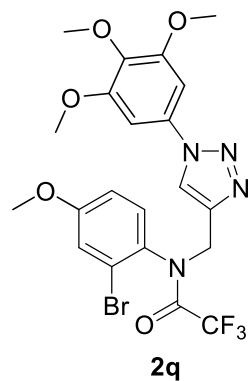
75.0

50.0

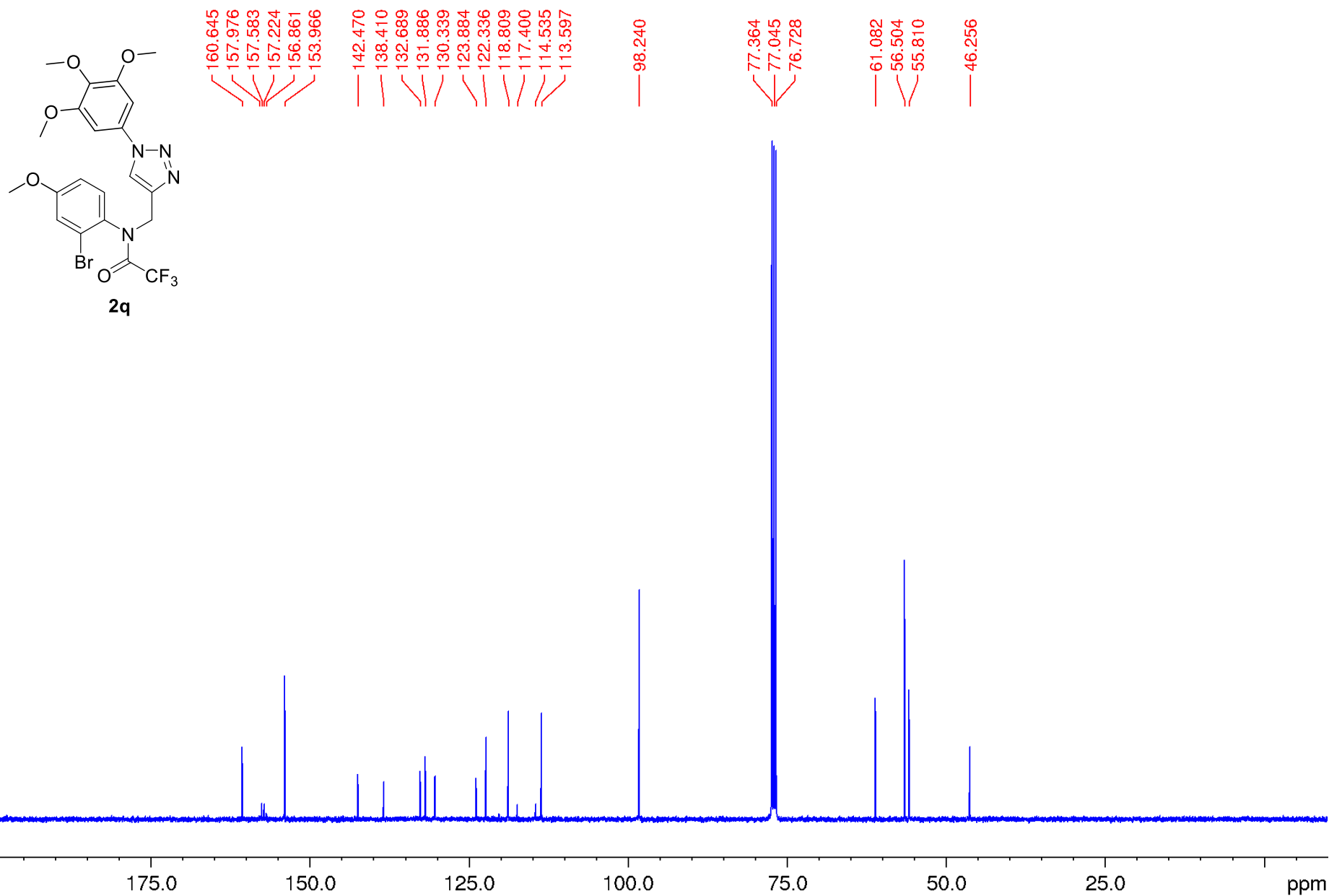
25.0

ppm

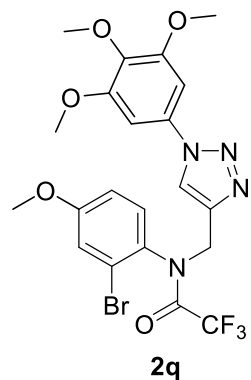
^1H NMR-spectrum (400 MHz, CDCl_3)



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



DEPT 135 NMR-spectrum (CDCl₃)



131.888
122.336
118.809
113.596
98.240
61.082
56.504
55.810
46.256

175.0

150.0

125.0

100.0

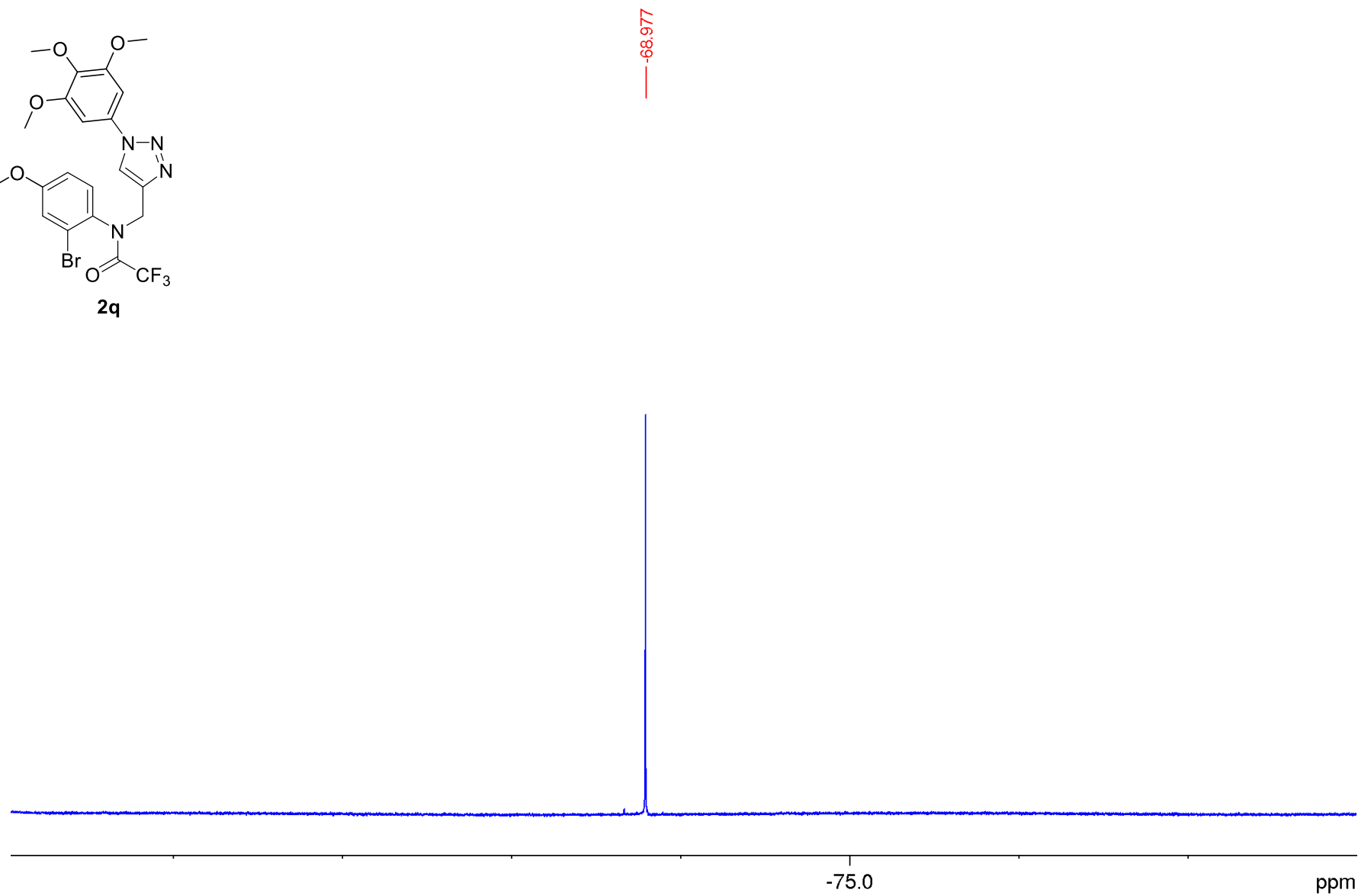
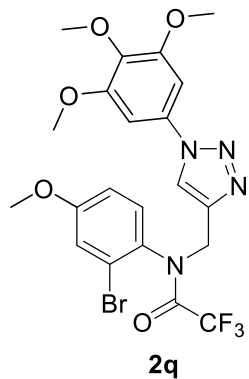
75.0

50.0

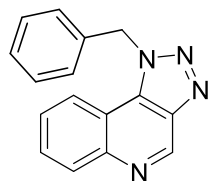
25.0

ppm

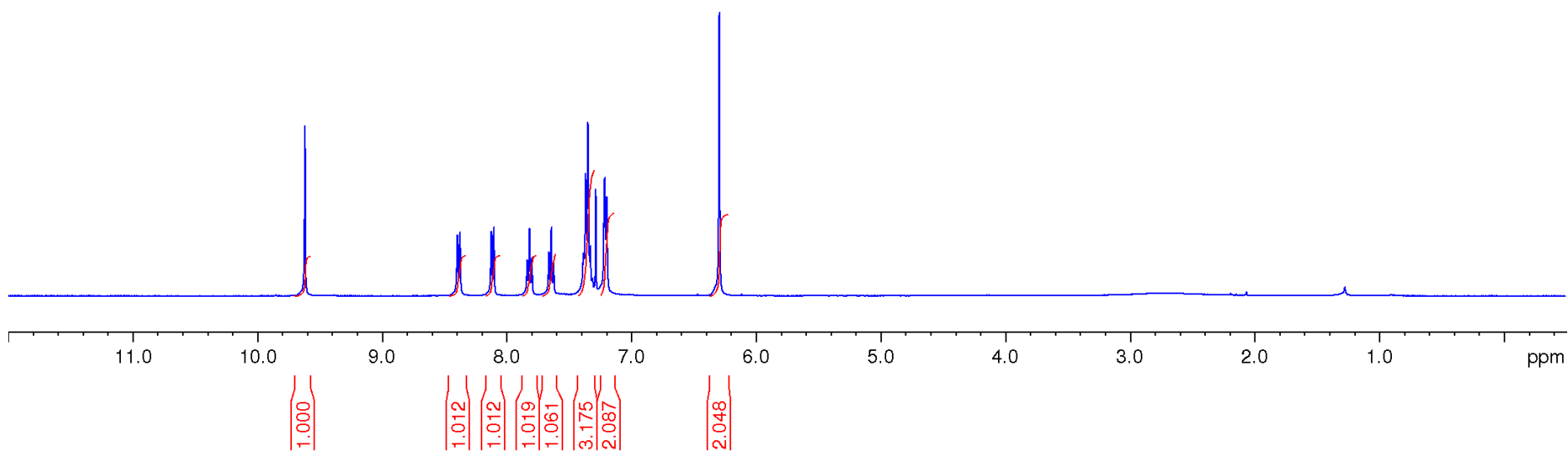
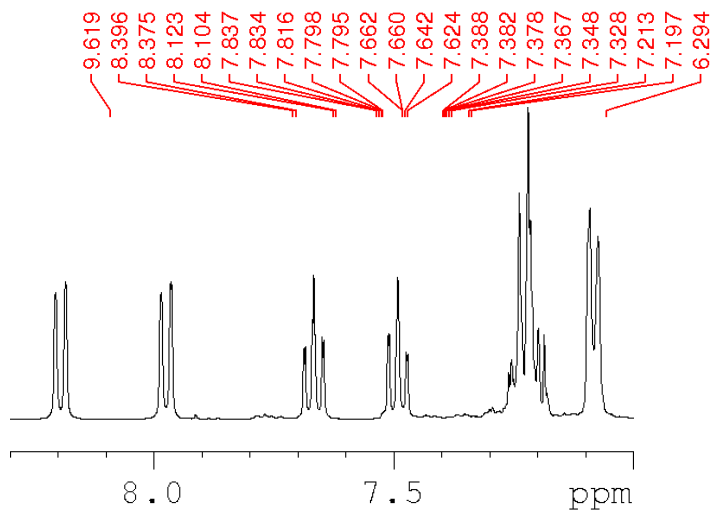
^{19}F NMR-spectrum (376.5 Hz, CDCl_3)



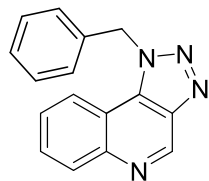
^1H NMR-spectrum (400 MHz, CDCl_3)



5a



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



5a

145.661
145.034
141.207
134.245
133.238
130.808
129.627
129.293
128.587
127.688
126.448
122.074
115.191

53.881

175.0

150.0

125.0

100.0

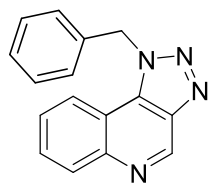
75.0

50.0

25.0

ppm

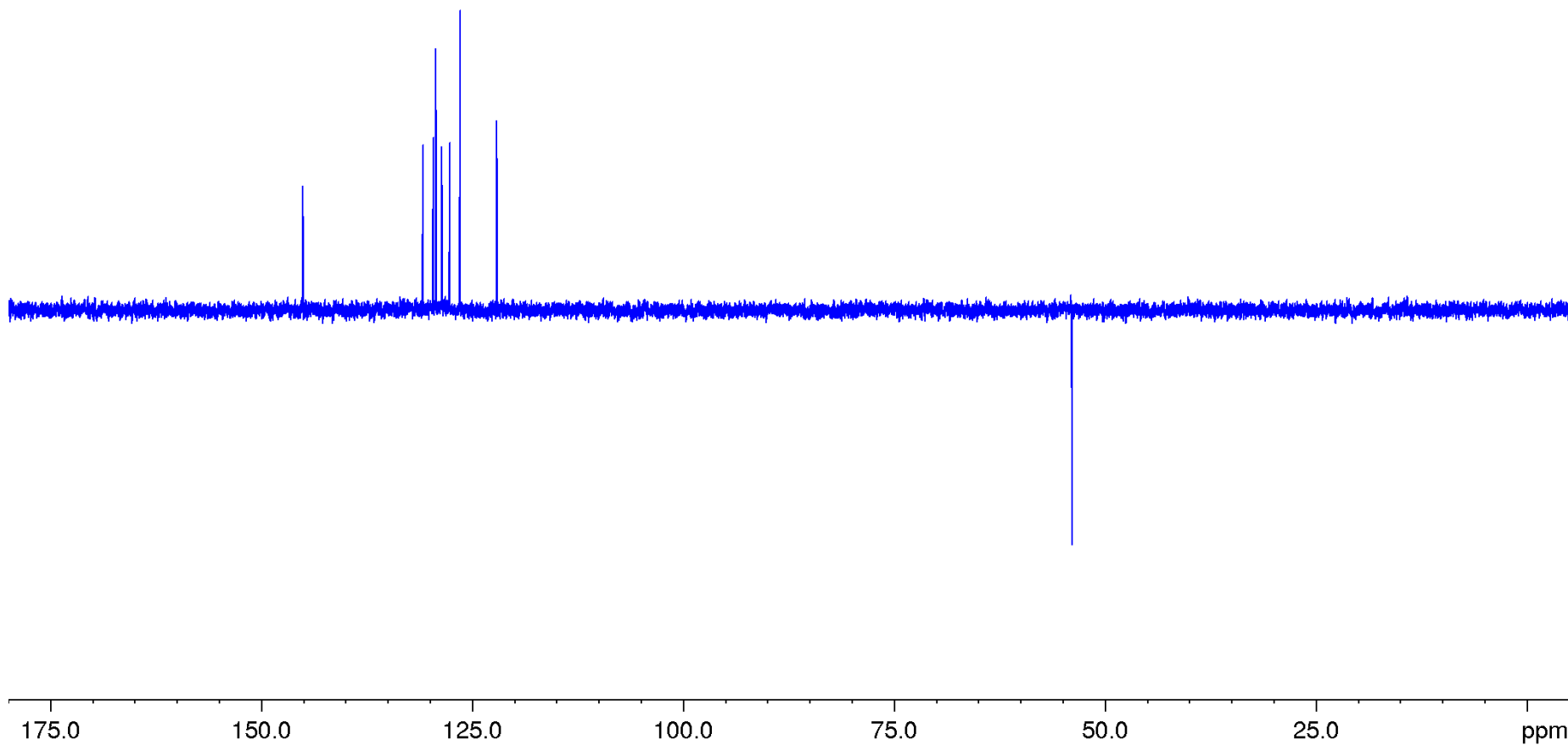
DEPT 135 NMR-spectrum (CDCl_3)



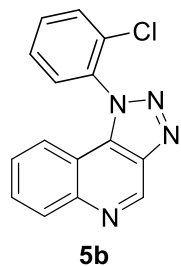
5a

145.079
130.861
129.628
129.305
128.600
127.682
126.456
122.074

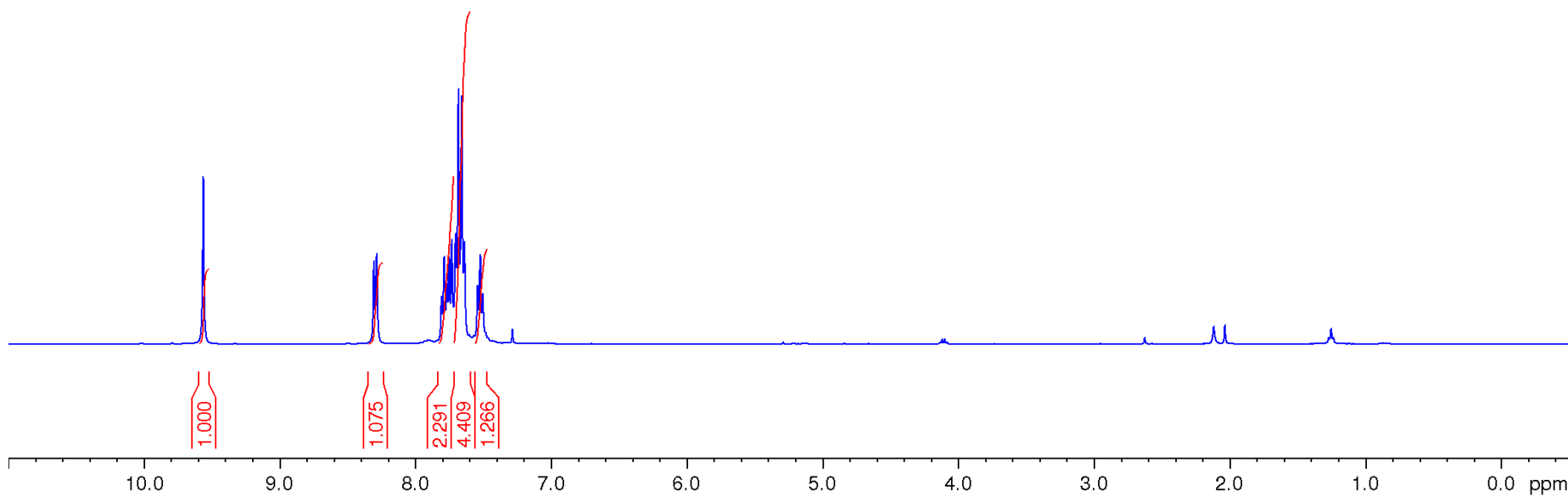
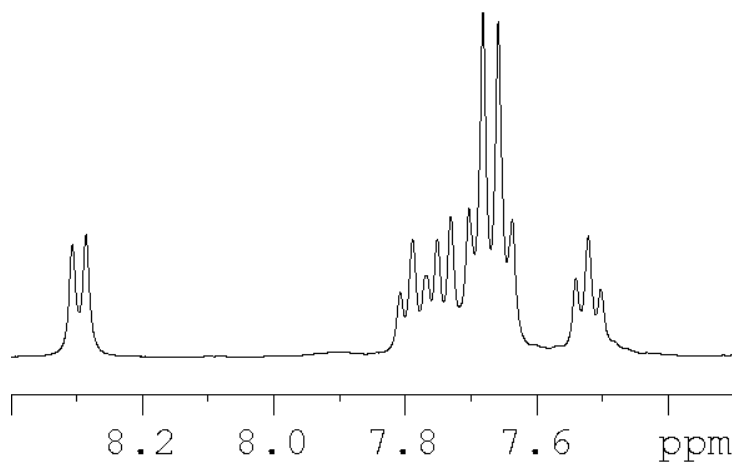
53.899



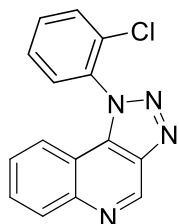
^1H NMR-spectrum (400 MHz, CDCl_3)



9.562
8.305
8.284
7.806
7.787
7.767
7.751
7.731
7.703
7.682
7.659
7.637
7.540
7.522
7.502

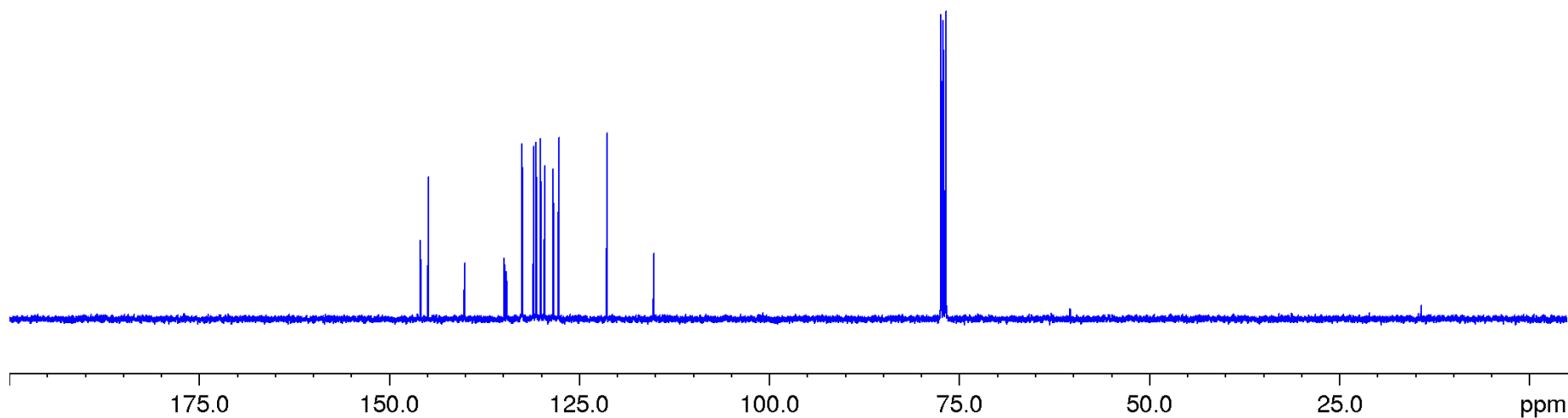


^{13}C NMR-spectrum (100 MHz, CDCl_3)

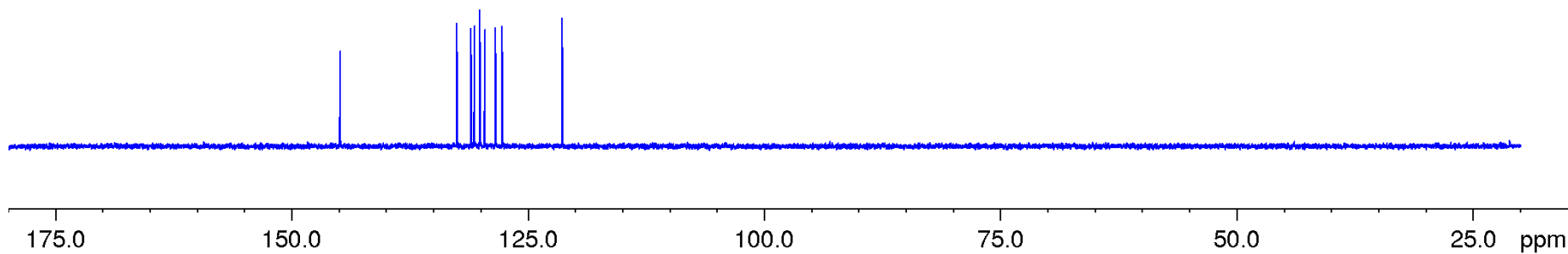
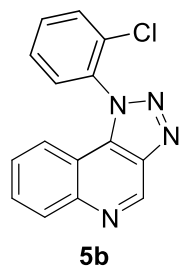


5b

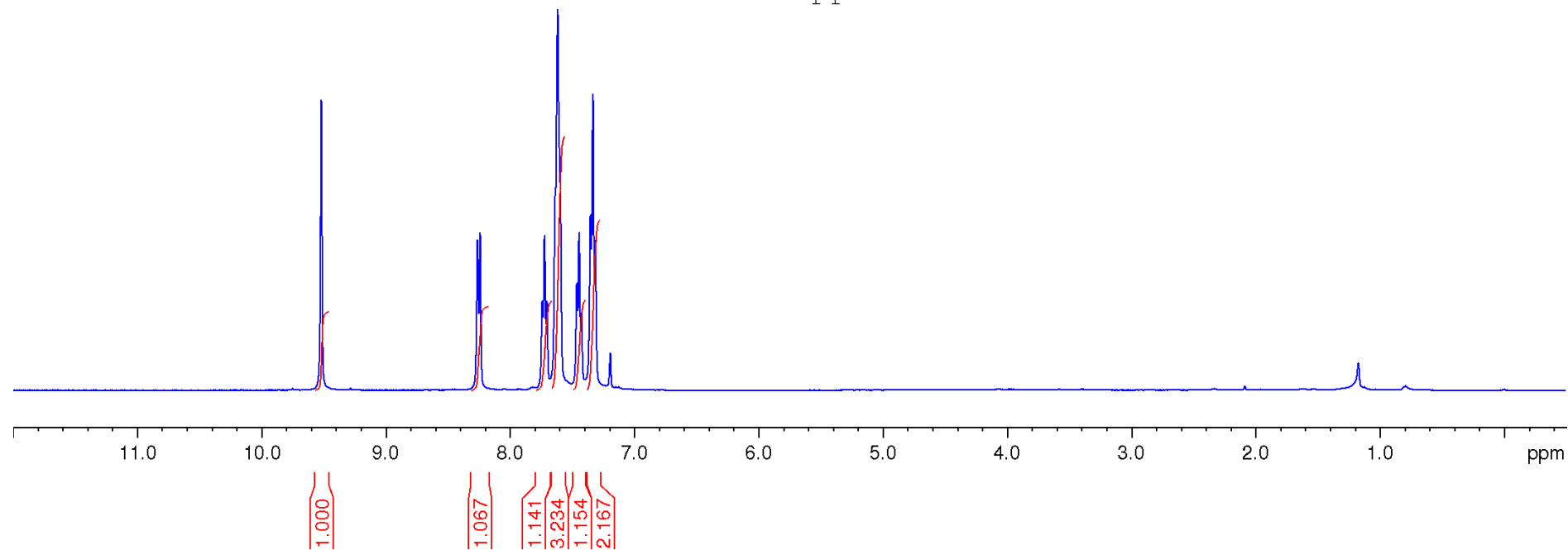
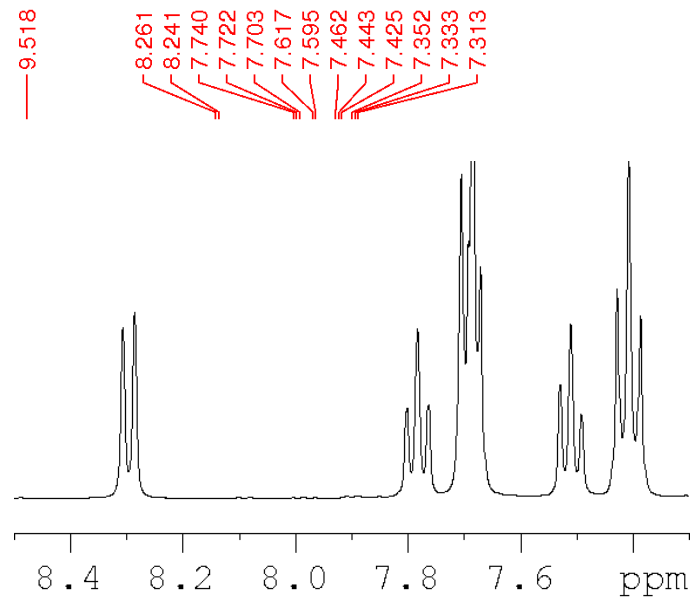
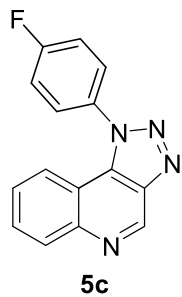
145.902
144.862
140.096
134.834
134.550
132.509
132.471
131.005
130.648
130.080
129.553
128.413
127.703
121.352
115.178



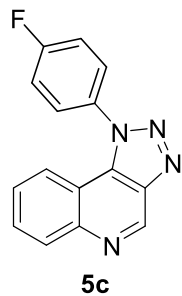
DEPT 135 NMR-spectrum (CDCl_3)



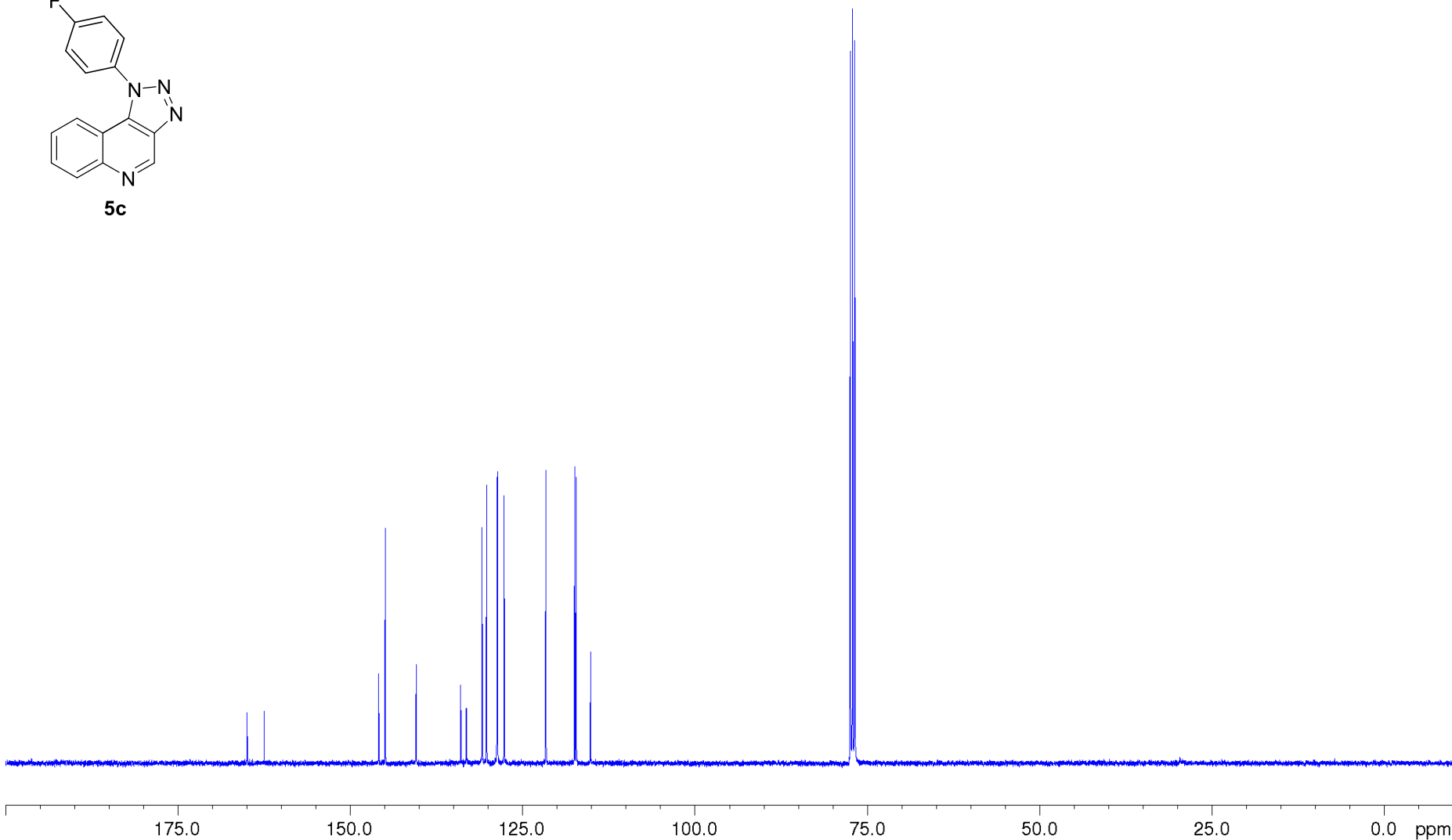
^1H NMR-spectrum (400 MHz, CDCl_3)



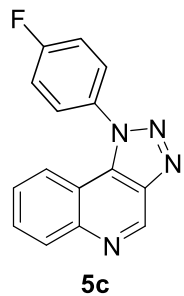
^{13}C NMR-spectrum (100 MHz, CDCl_3)



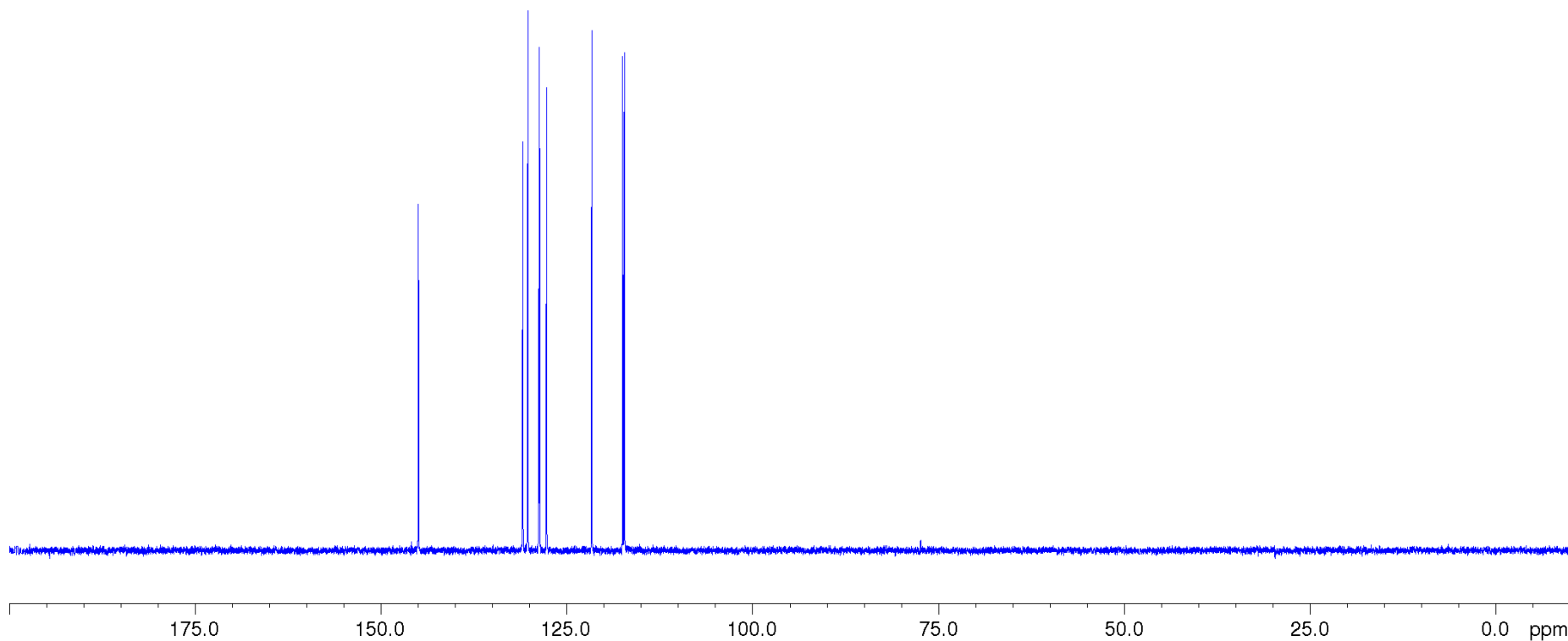
164.982
162.474
145.785
144.835
140.354
133.879
133.071
133.040
130.792
130.125
128.626
128.536
127.592
121.527
117.364
117.132
115.061



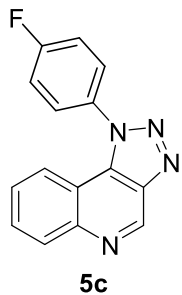
DEPT 135 NMR-spectrum (CDCl_3)



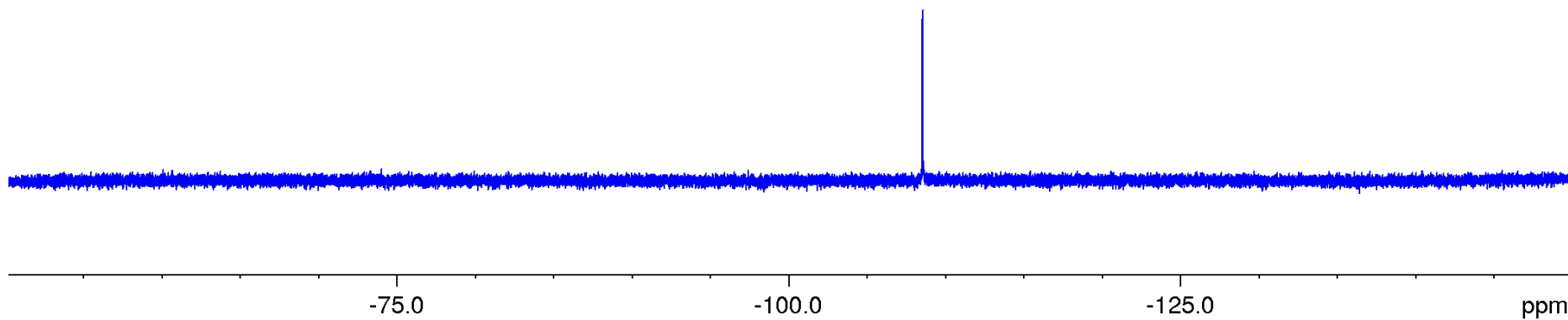
144.834
130.791
130.125
128.626
128.536
127.591
121.526
117.364
117.132



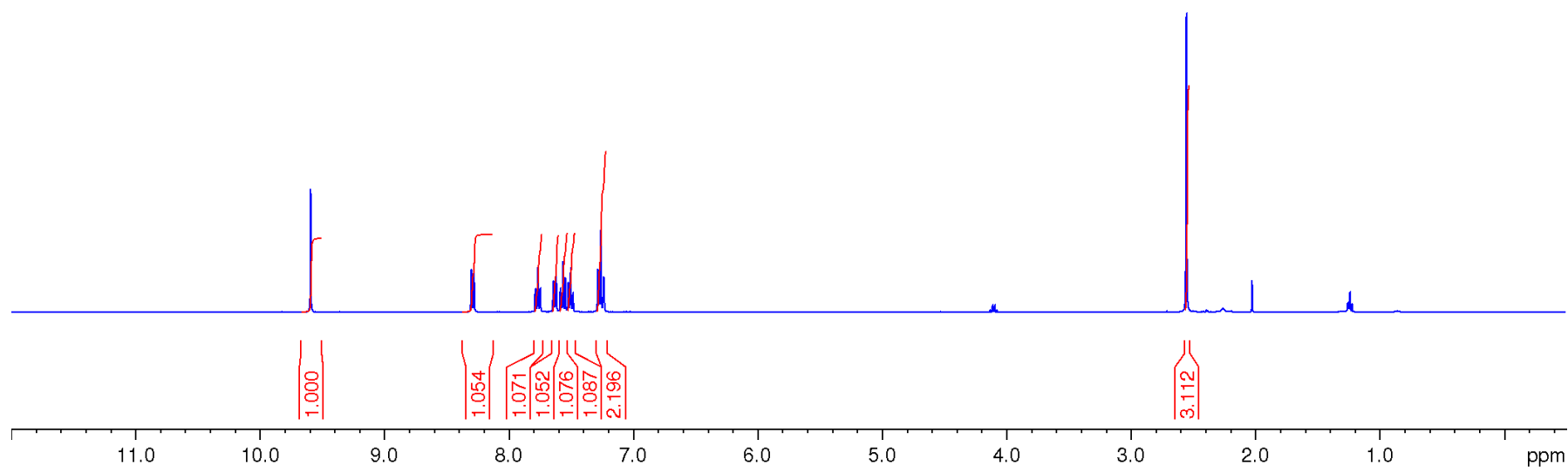
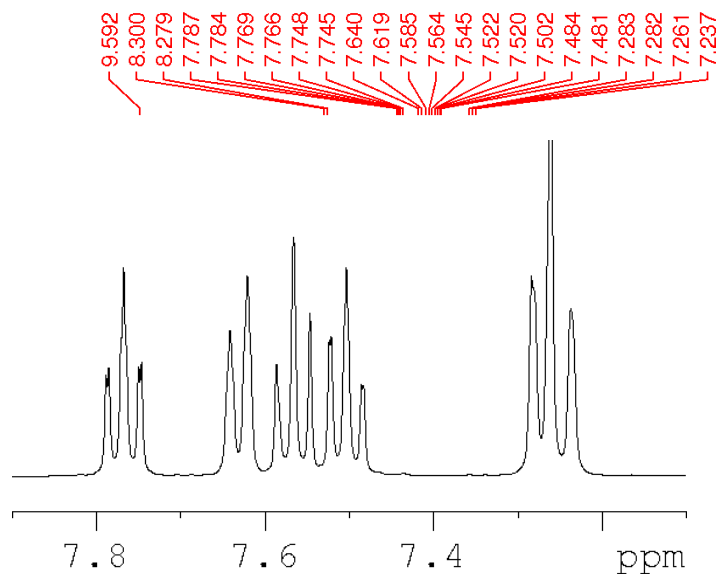
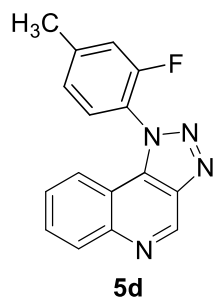
^{19}F NMR-spectrum (376.5 Hz, CDCl_3)



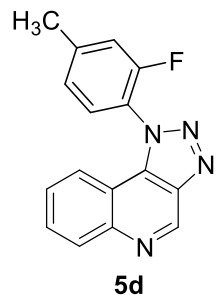
-108.547
-108.558
-108.569
-108.591



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

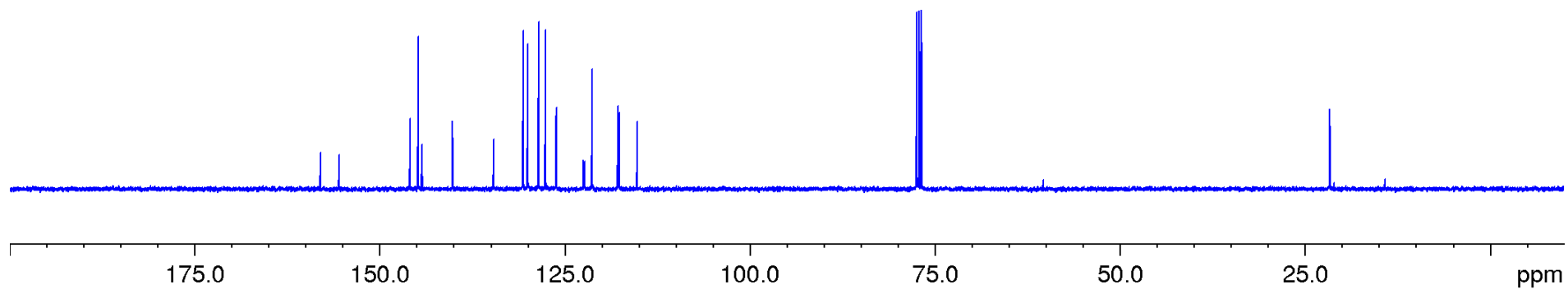


^{13}C NMR-spectrum (100 MHz, CDCl_3)

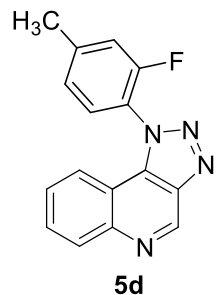


158.013
155.484
145.903
144.787
144.319
144.245
140.177
134.594
130.627
129.995
128.541
127.594
126.146
126.113
122.445
122.316
121.298
117.816
117.632
115.200

21.627

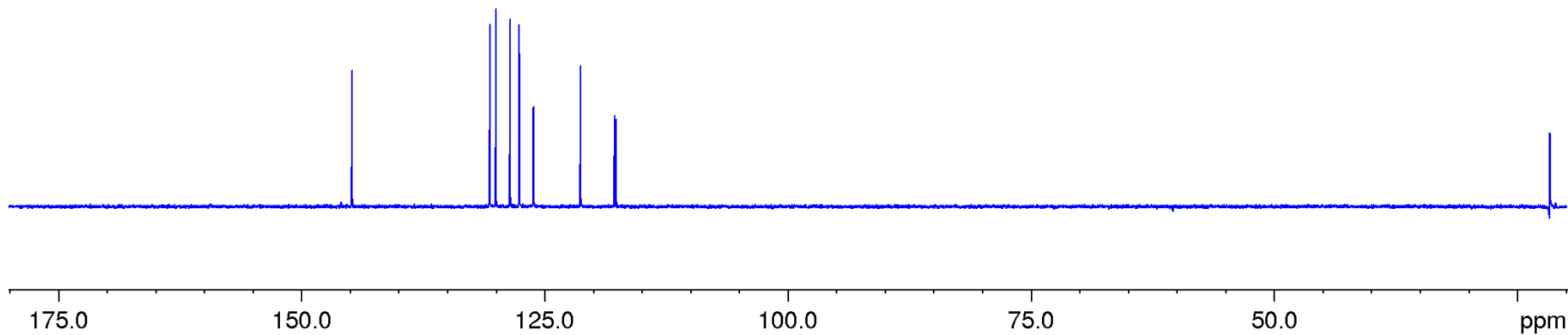


DEPT 135 NMR-spectrum (CDCl_3)

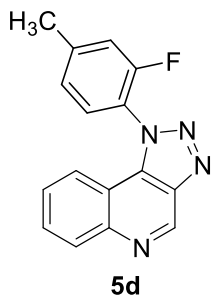


144.789
130.627
129.997
128.540
127.596
126.147
126.113
121.298
117.816
117.633

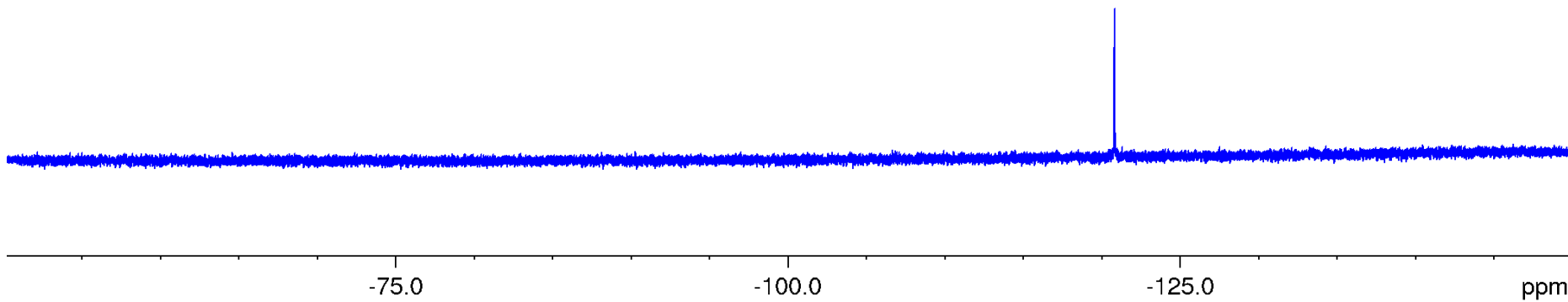
21.613



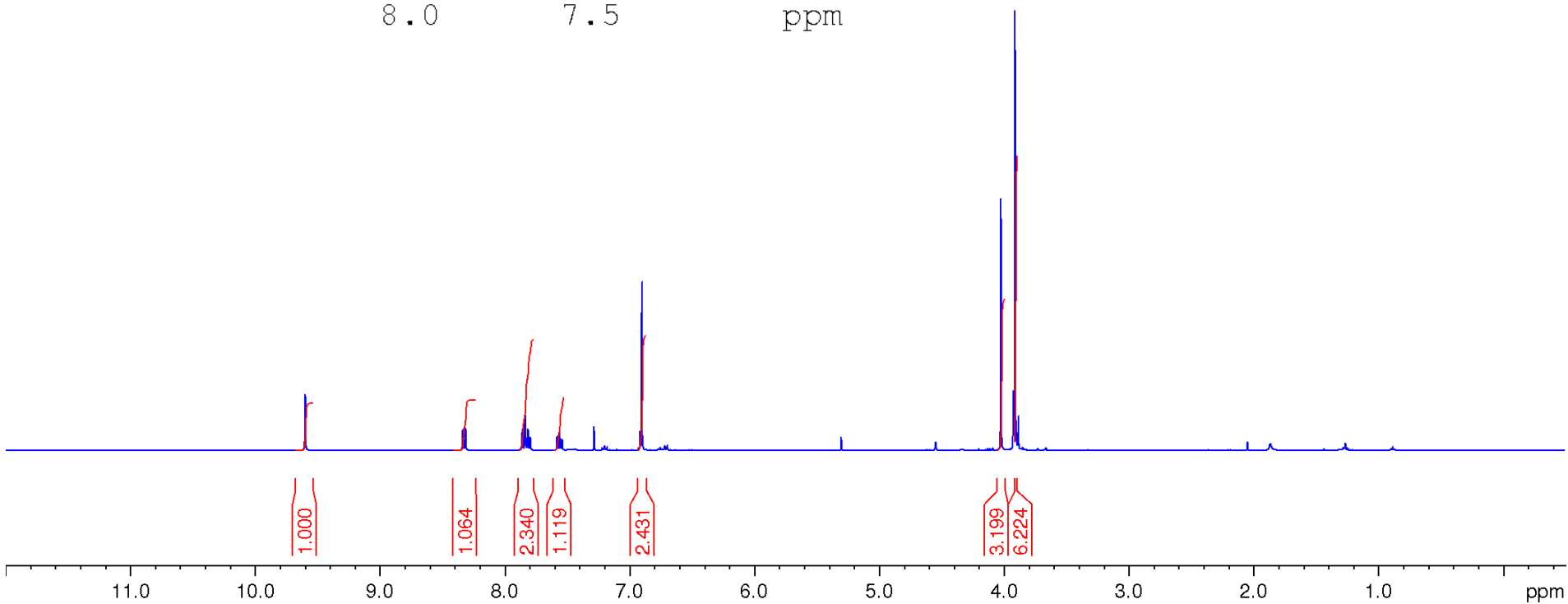
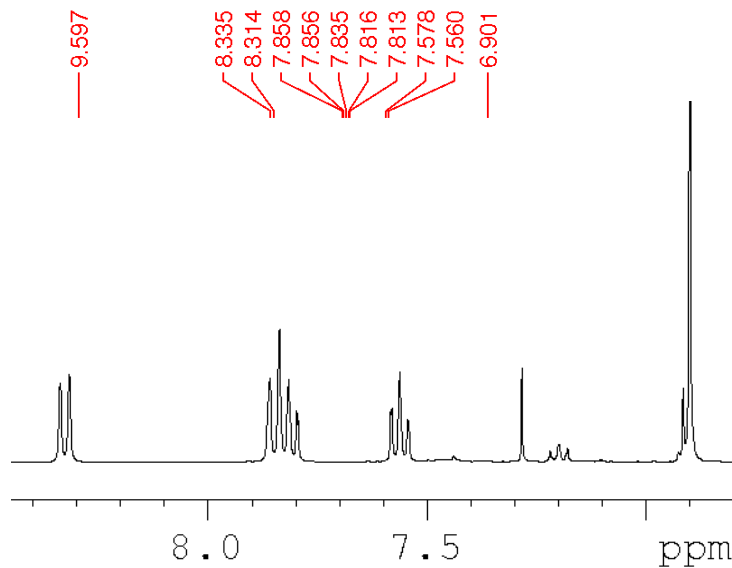
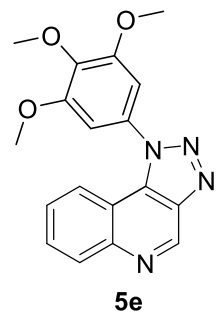
^{19}F NMR-spectrum (376.5 Hz, CDCl_3)



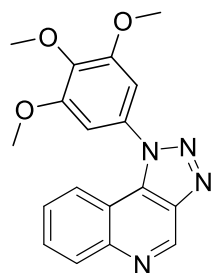
-120.823
-120.848
-120.870



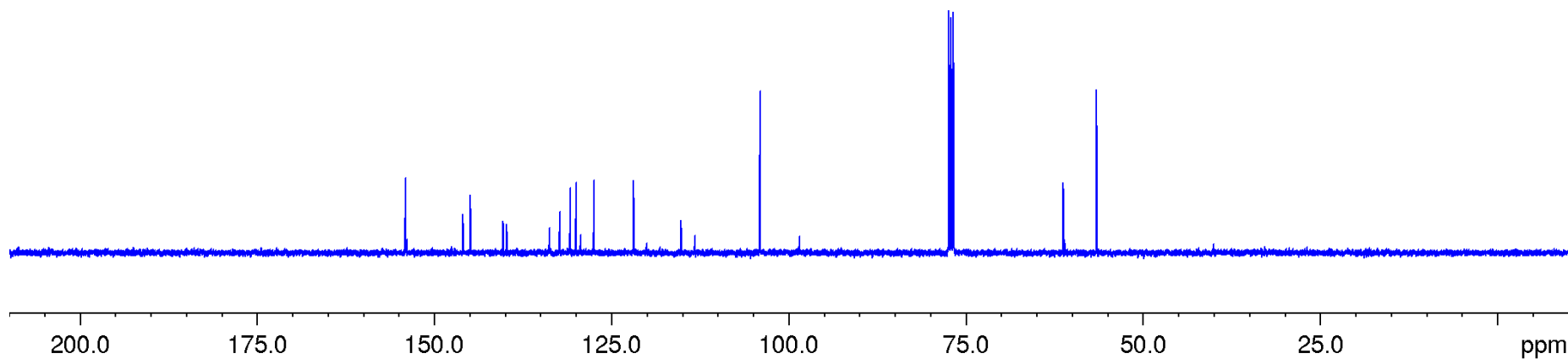
^1H NMR-spectrum (400 MHz, CDCl_3)



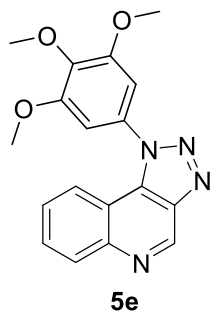
^{13}C NMR-spectrum (100 MHz, CDCl_3)



5e



DEPT 135 NMR-spectrum (CDCl_3)



144.917

130.817

129.997

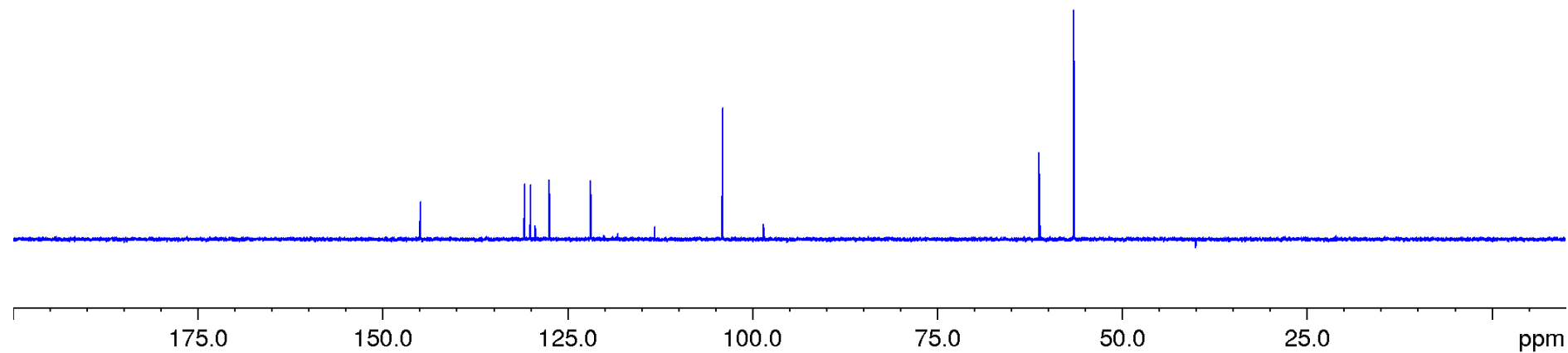
127.464

121.879

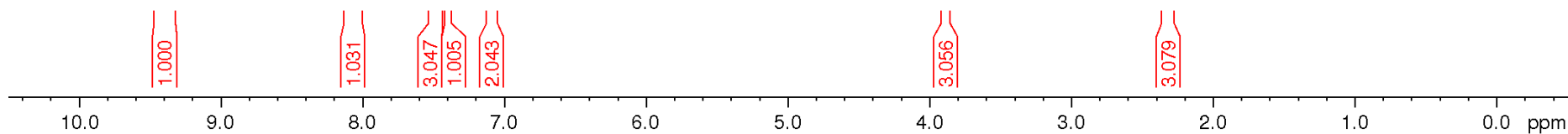
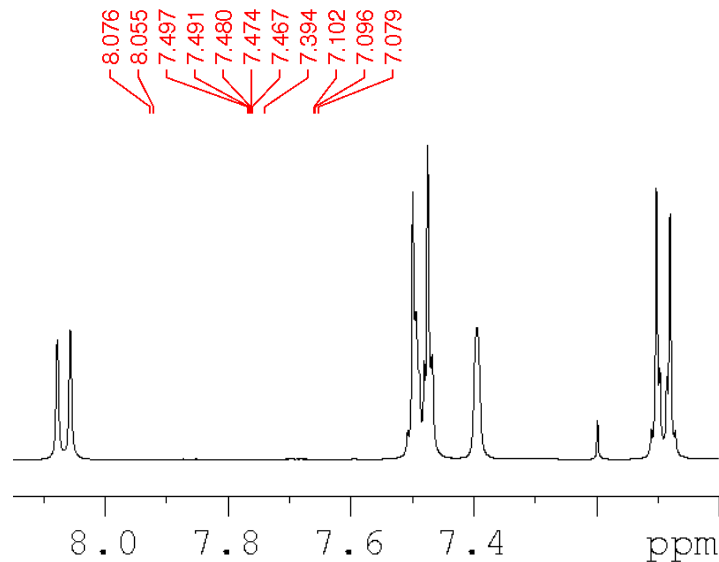
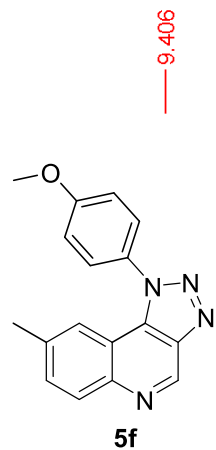
104.035

61.213

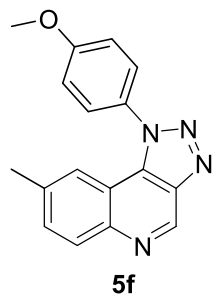
56.518



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



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



161.204

144.222

143.904

140.428

137.545

133.521

131.625

130.357

129.746

127.818

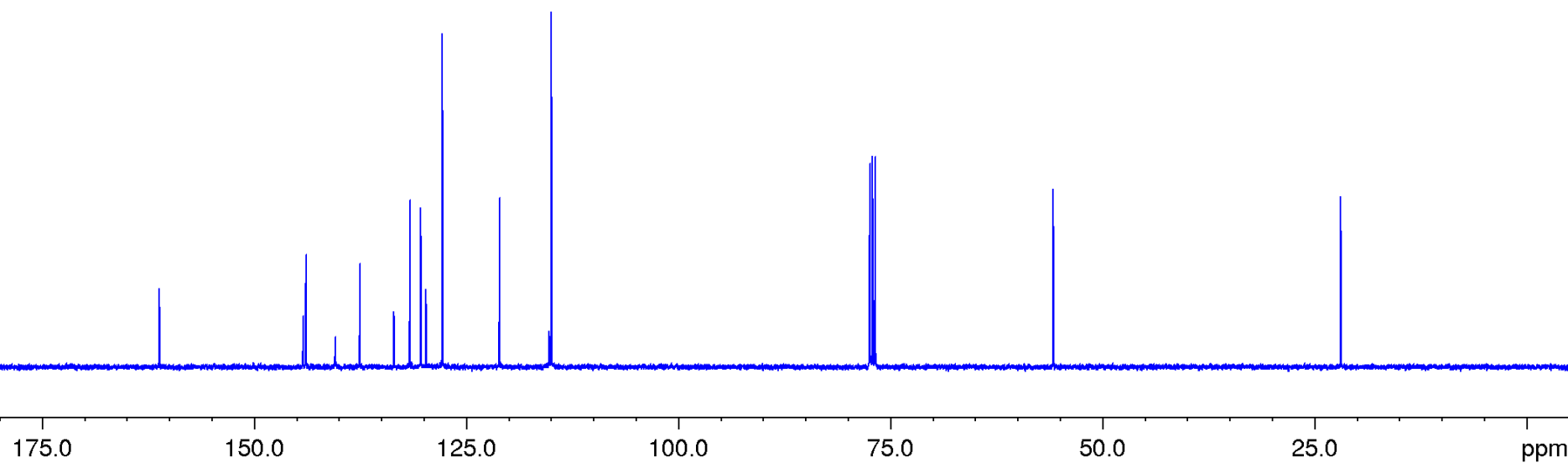
121.060

115.218

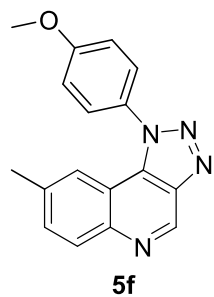
114.972

55.784

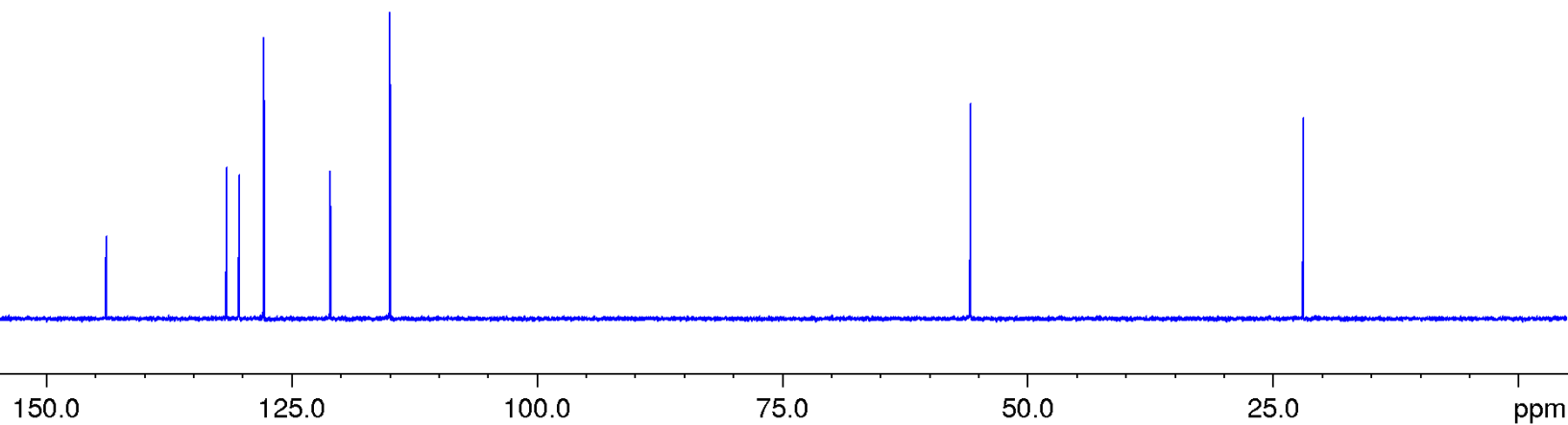
21.877



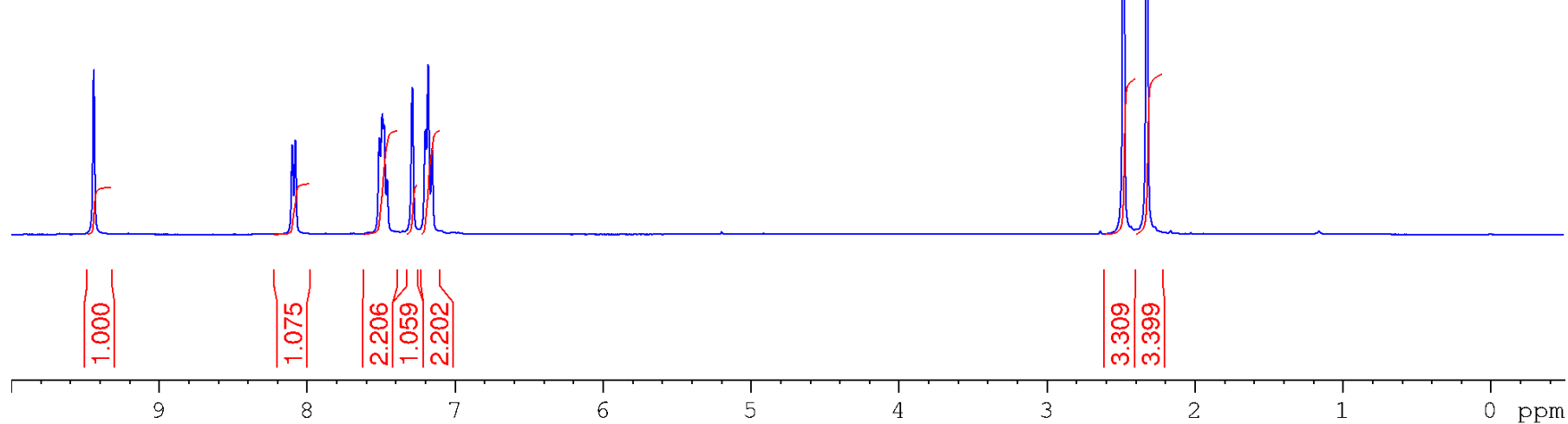
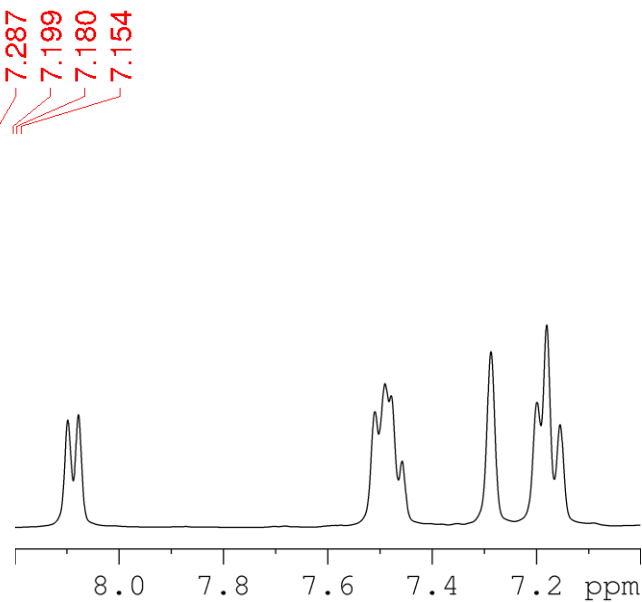
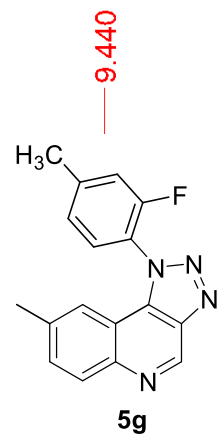
DEPT 135 NMR-spectrum (CDCl₃)



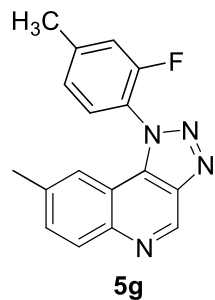
143.904
131.626
130.356
127.818
121.061
114.972
55.785
21.878



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

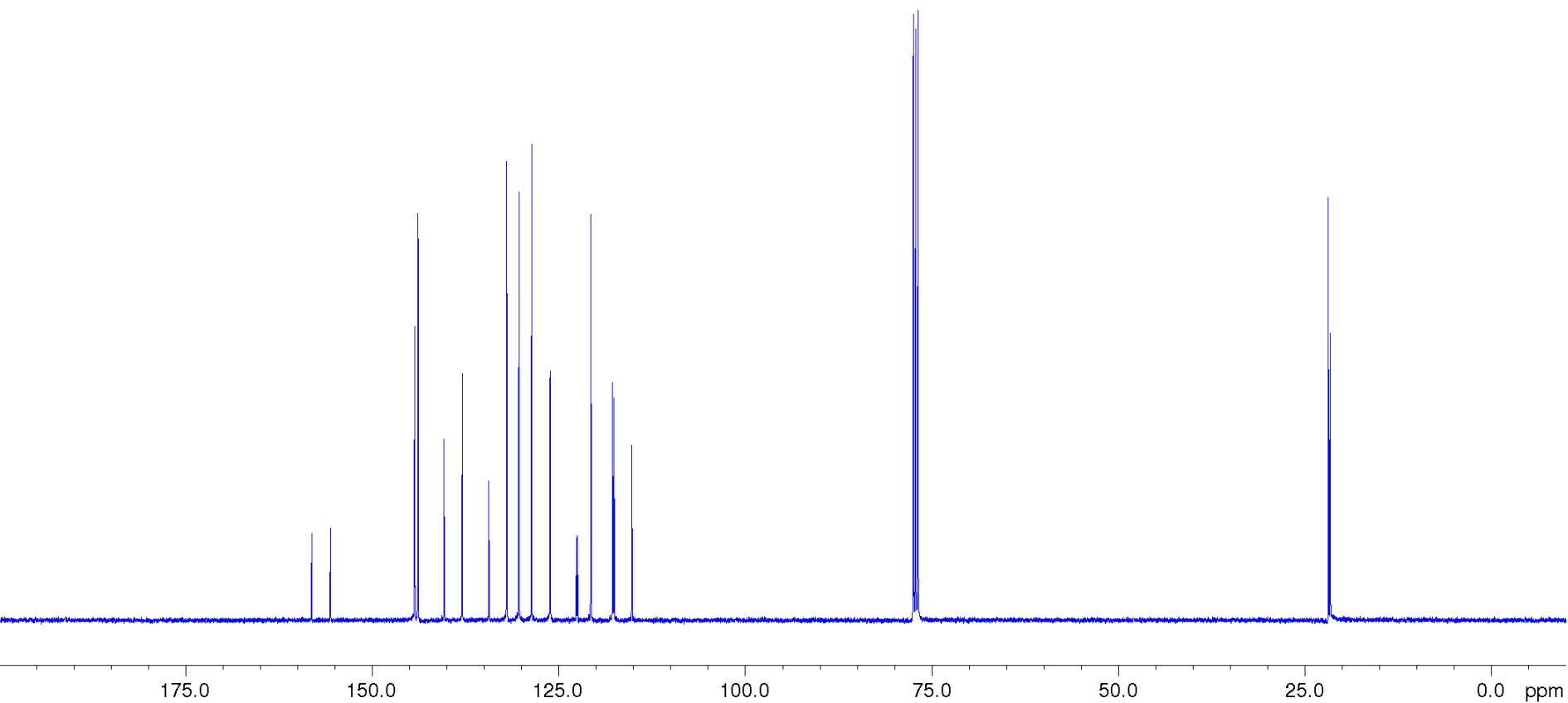


^{13}C NMR-spectrum (100 MHz, CDCl_3)

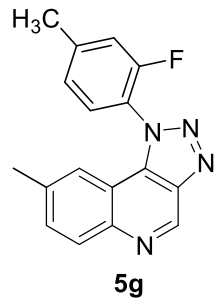


158.034
155.505
144.239
144.168
143.757
140.281
137.842
134.289
131.880
130.249
128.555
126.073
126.040
122.543
122.416
120.615
117.699
117.515
115.128

21.886
21.648

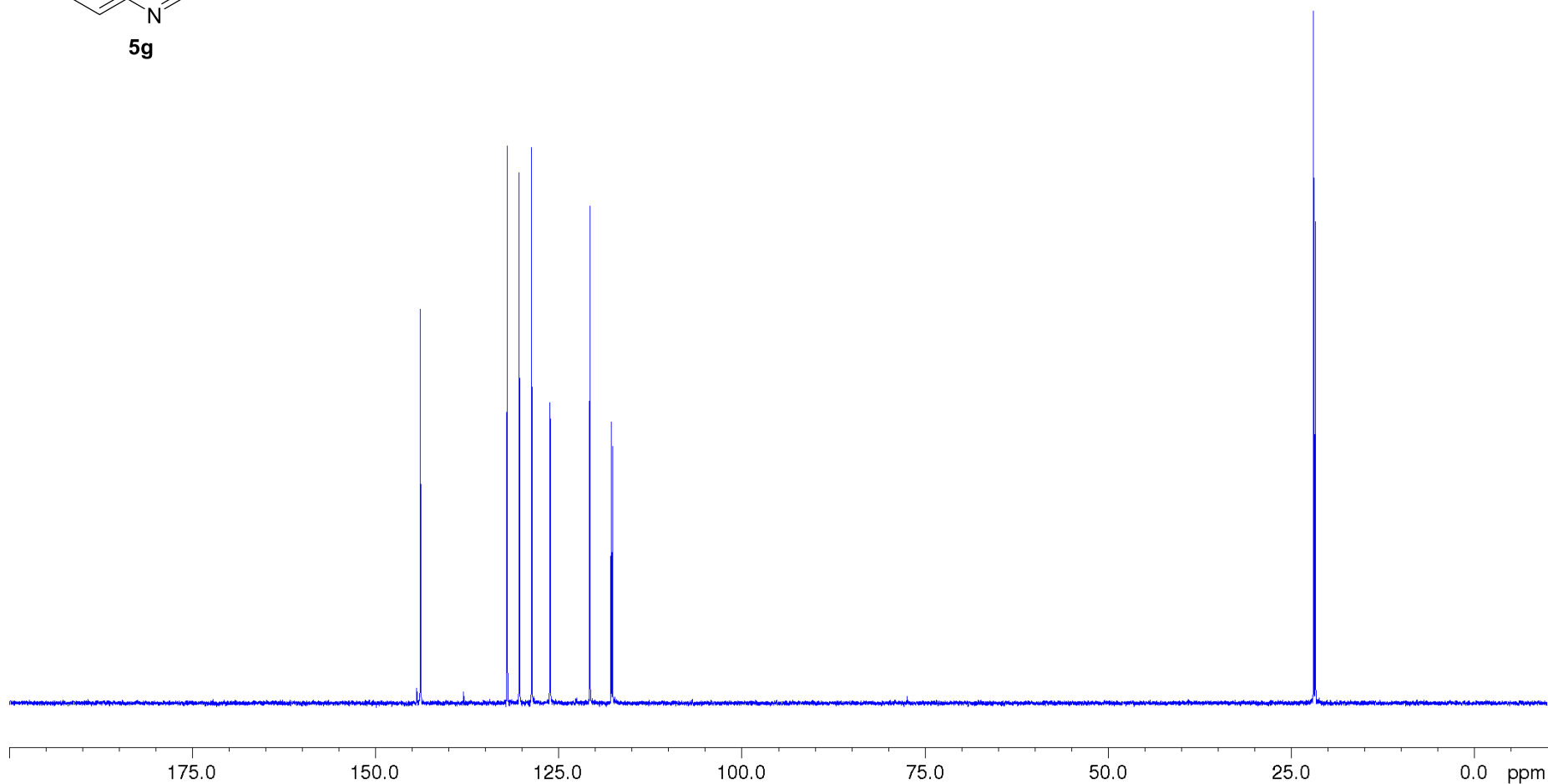


DEPT 135 NMR-spectrum (CDCl_3)

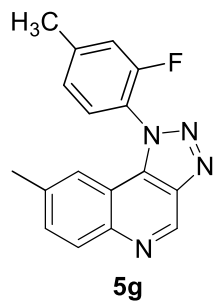


143.756
131.880
130.248
128.554
126.072
126.039
120.614
117.698
117.514

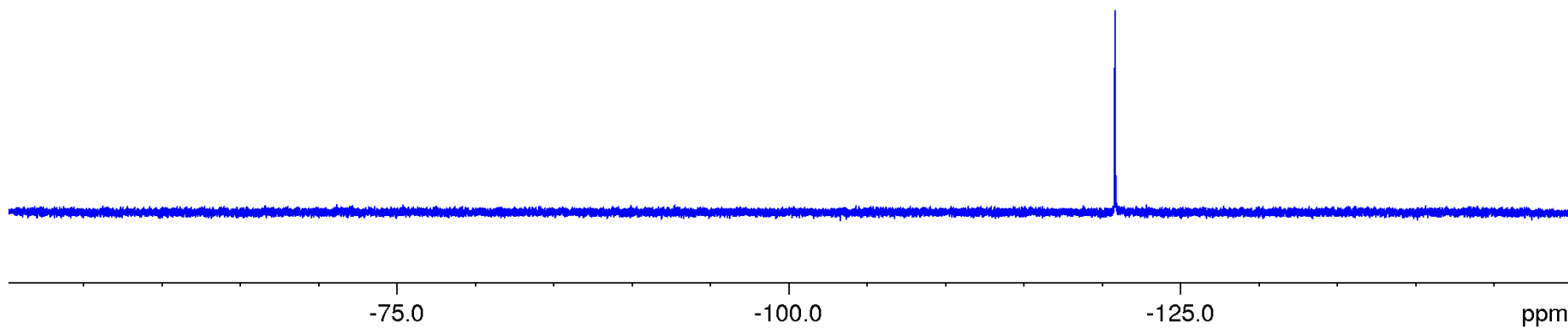
21.887
21.652



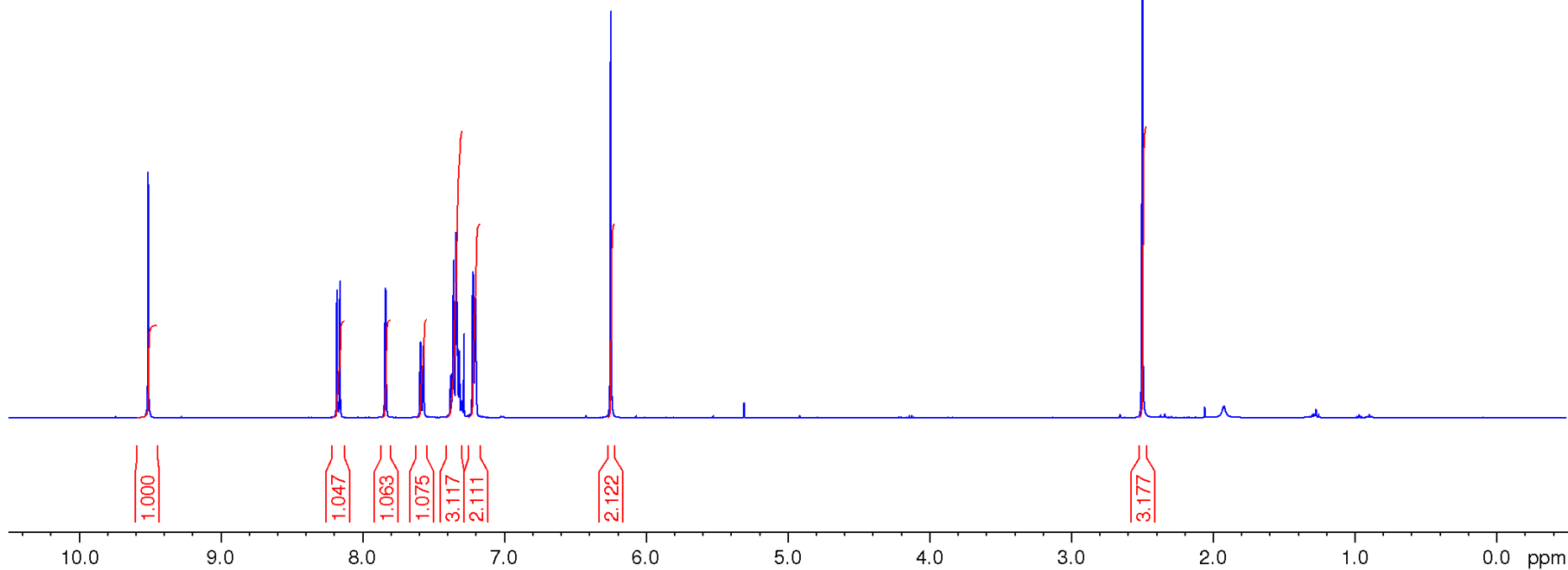
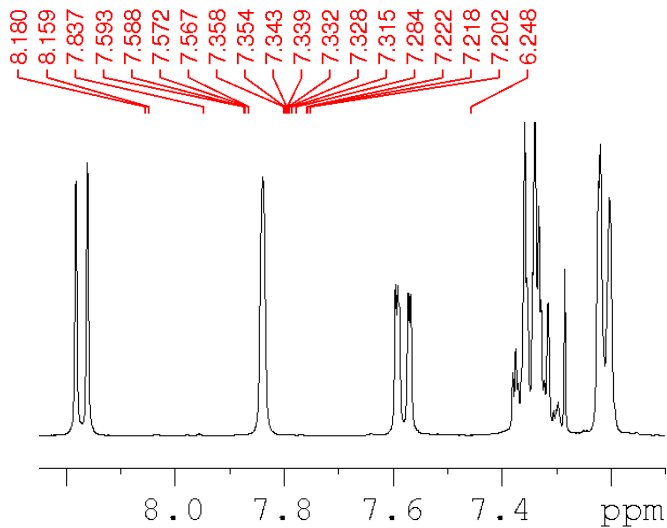
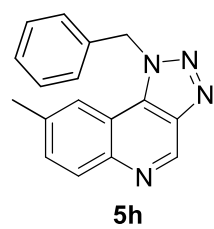
^{19}F NMR-spectrum (376.5 Hz, CDCl_3)



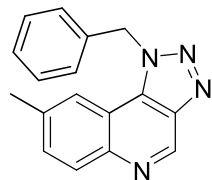
-120.825
-120.849
-120.872



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



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

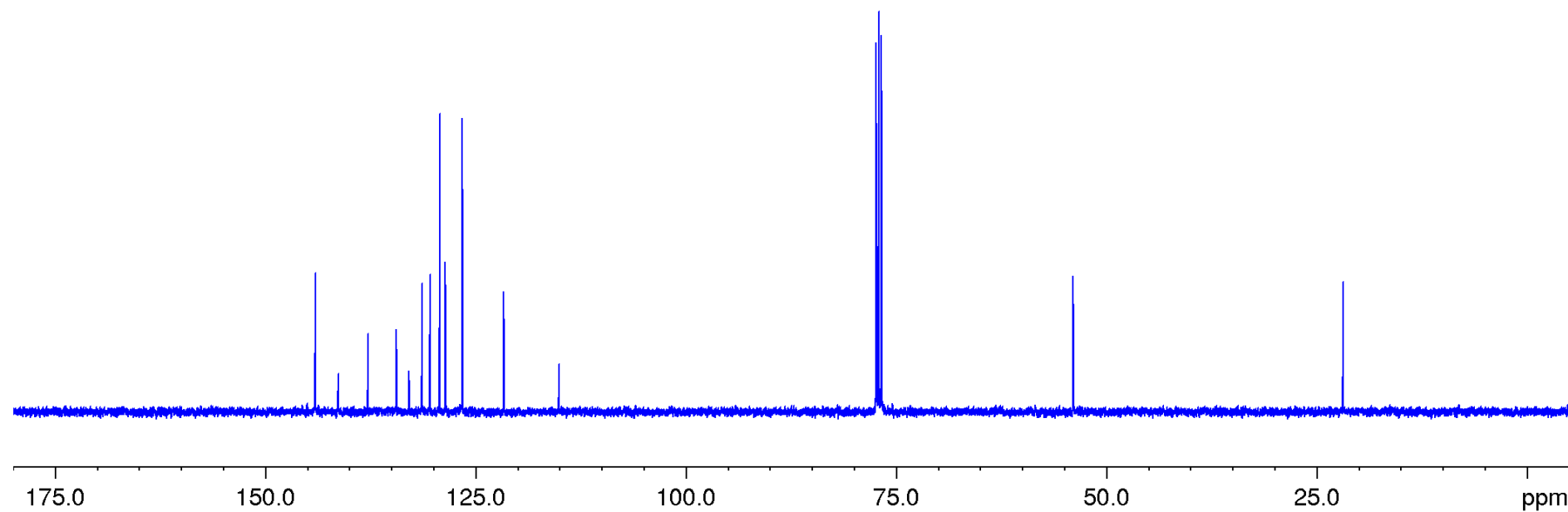


5h

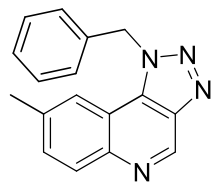
144.072
144.043
141.348
137.810
134.454
132.950
131.366
130.429
129.257
128.593
126.594
121.655
115.097

53.937

21.827



DEPT 135 NMR-spectrum (CDCl_3)



5h

144.072
131.366
130.428
129.257
128.593
126.594
121.655
53.938
21.827

150.0

125.0

100.0

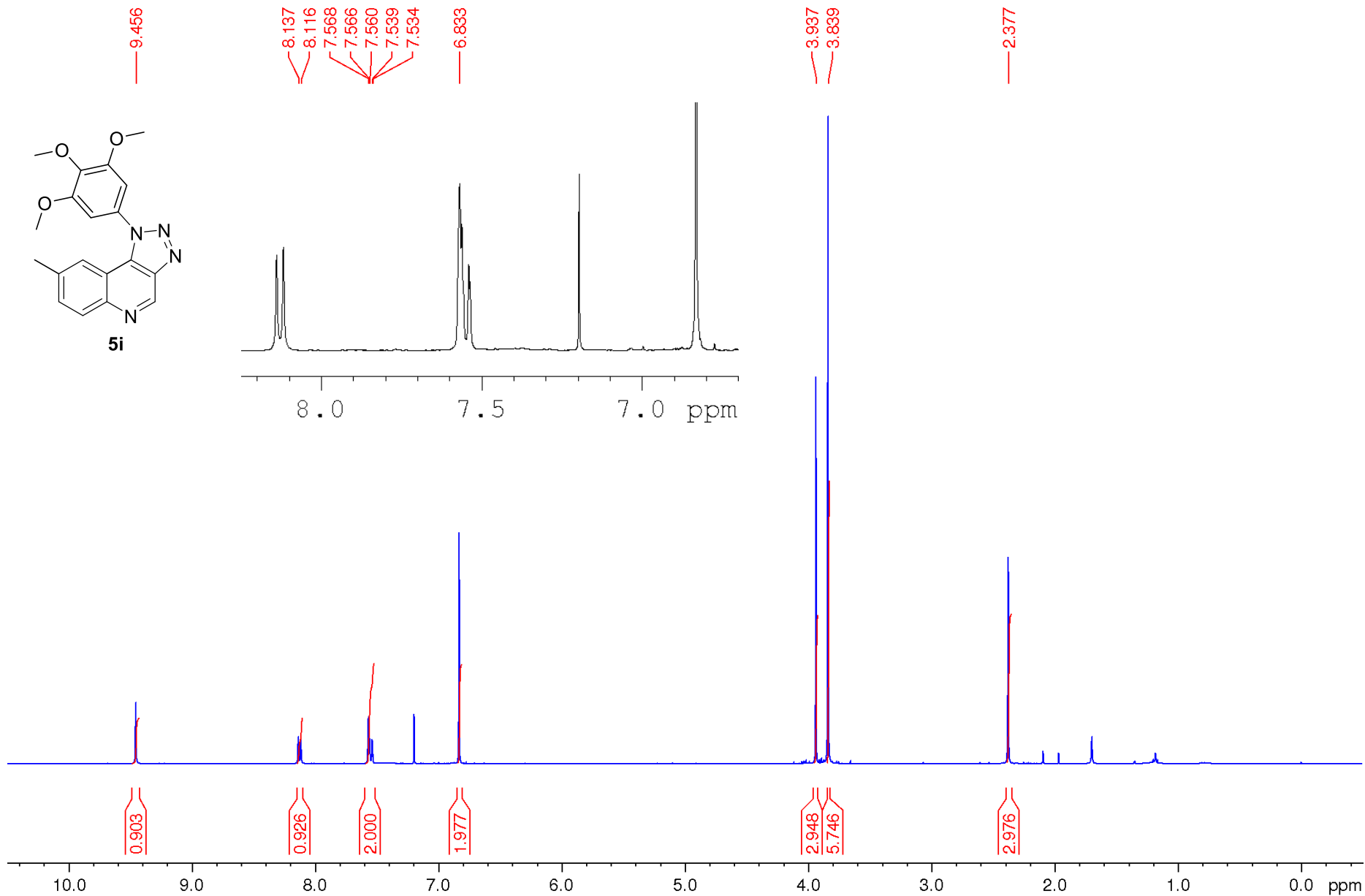
75.0

50.0

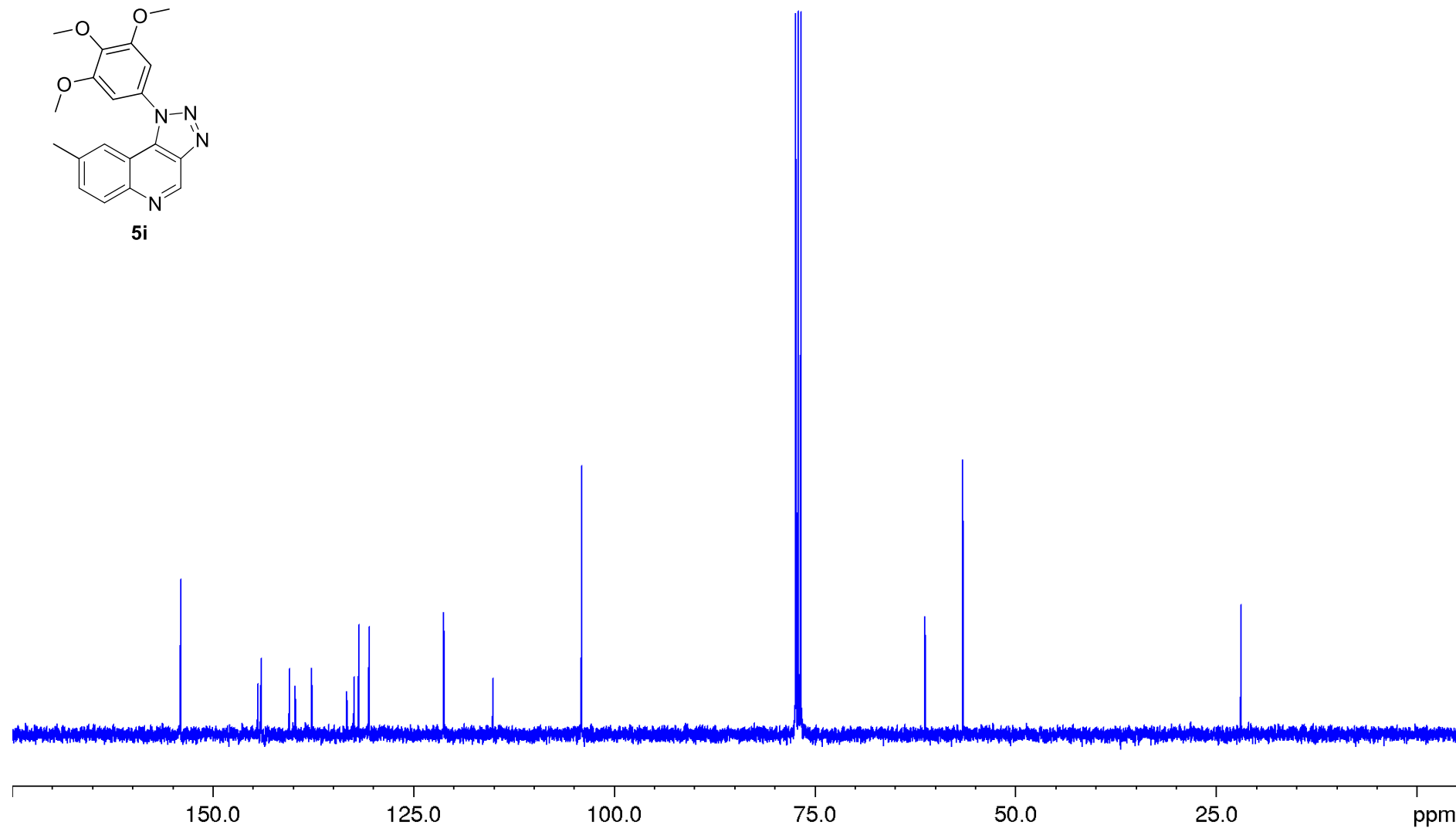
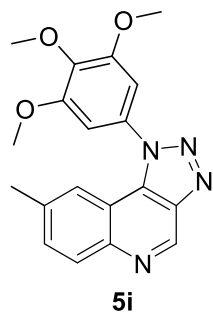
25.0

ppm

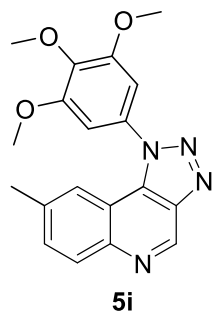
^1H NMR-spectrum (400 MHz, CDCl_3)



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



DEPT 135 NMR-spectrum (CDCl₃)



150.0

125.0

100.0

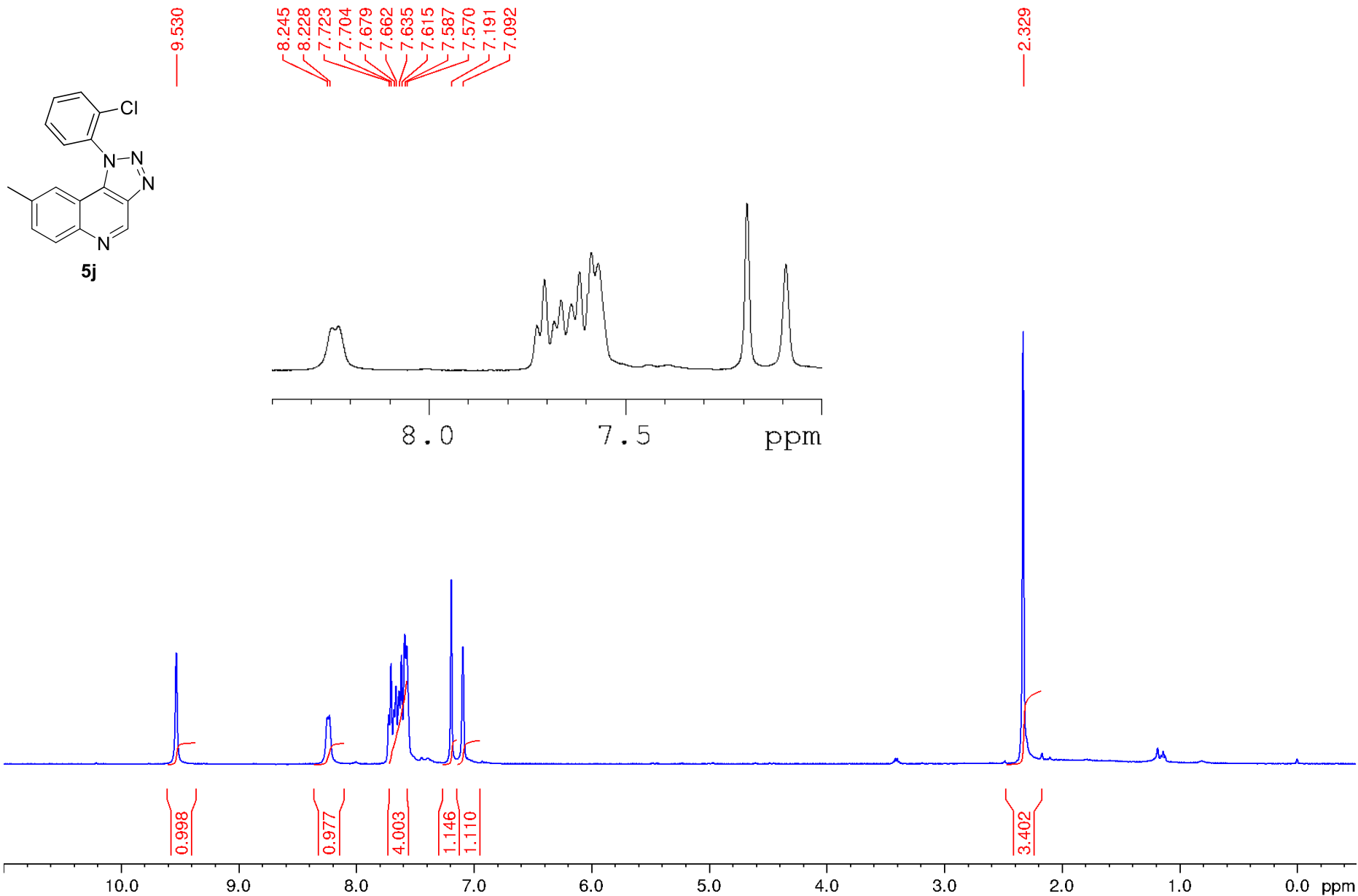
75.0

50.0

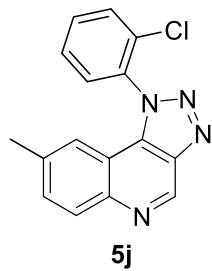
25.0

ppm

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

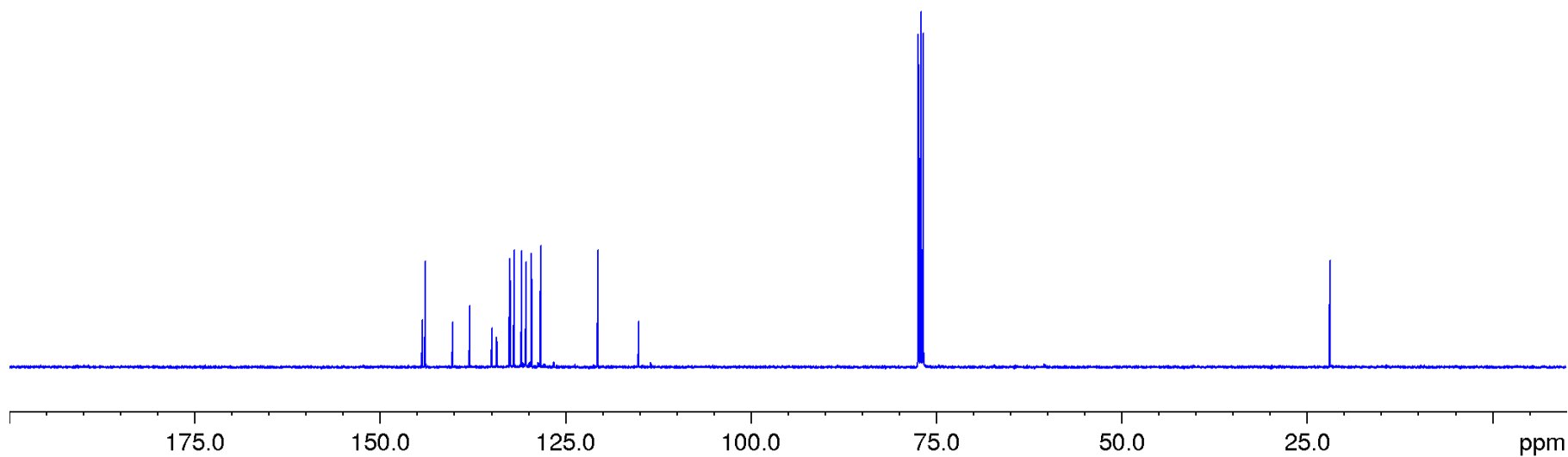


^{13}C NMR-spectrum (100 MHz, CDCl_3)

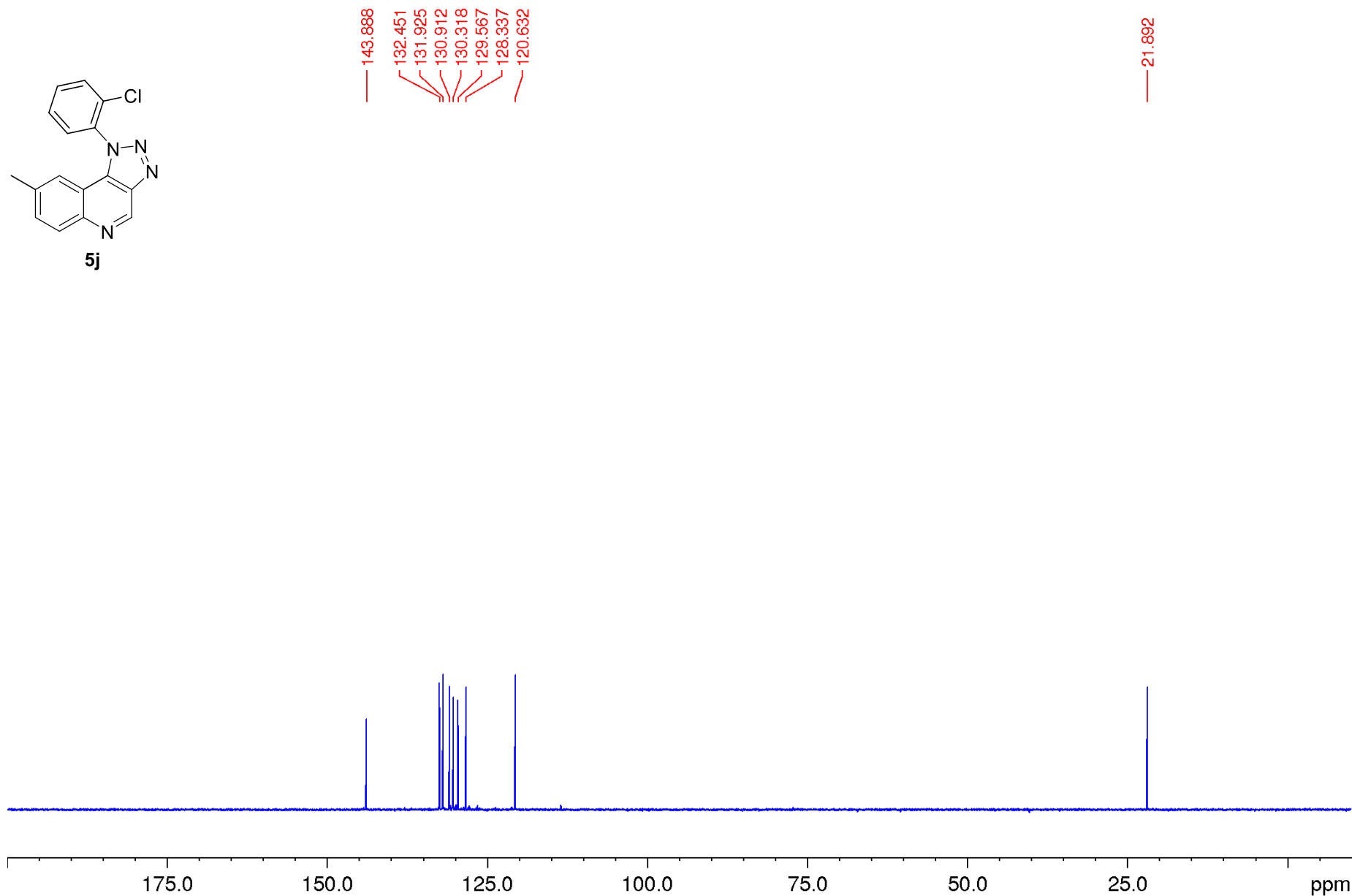
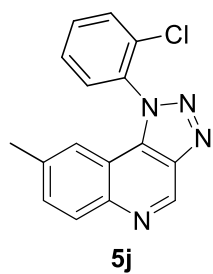


144.307
143.889
140.215
137.891
134.927
134.246
132.544
132.452
131.925
130.913
130.319
129.568
128.337
120.632
115.111

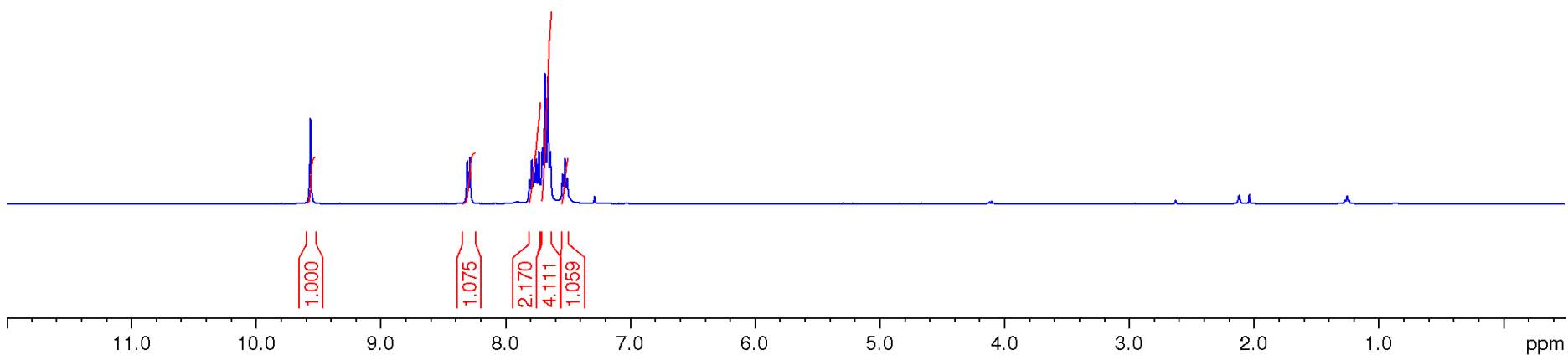
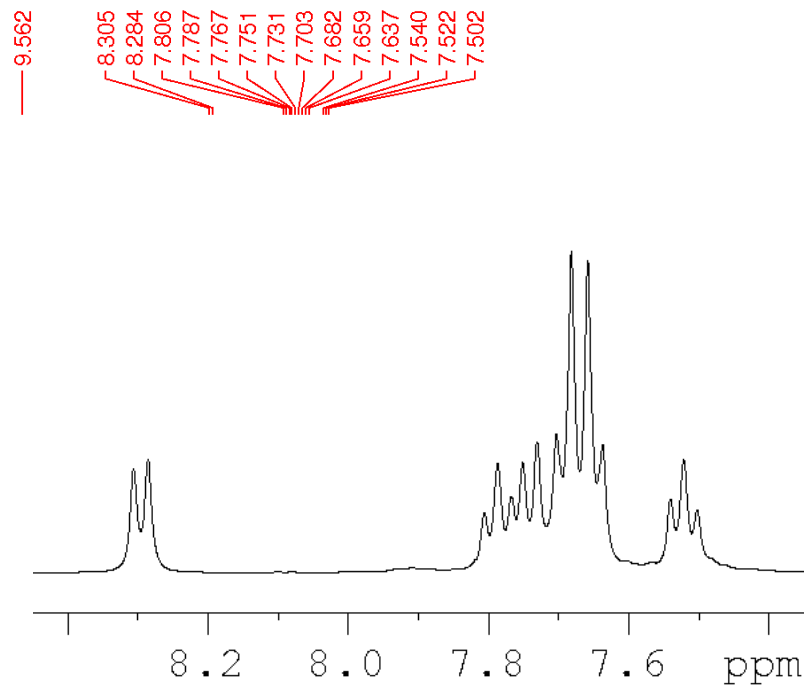
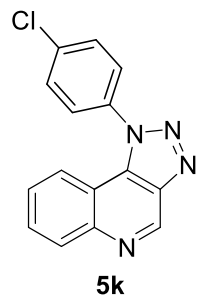
21.892



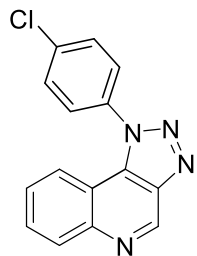
DEPT 135 NMR-spectrum (CDCl_3)



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

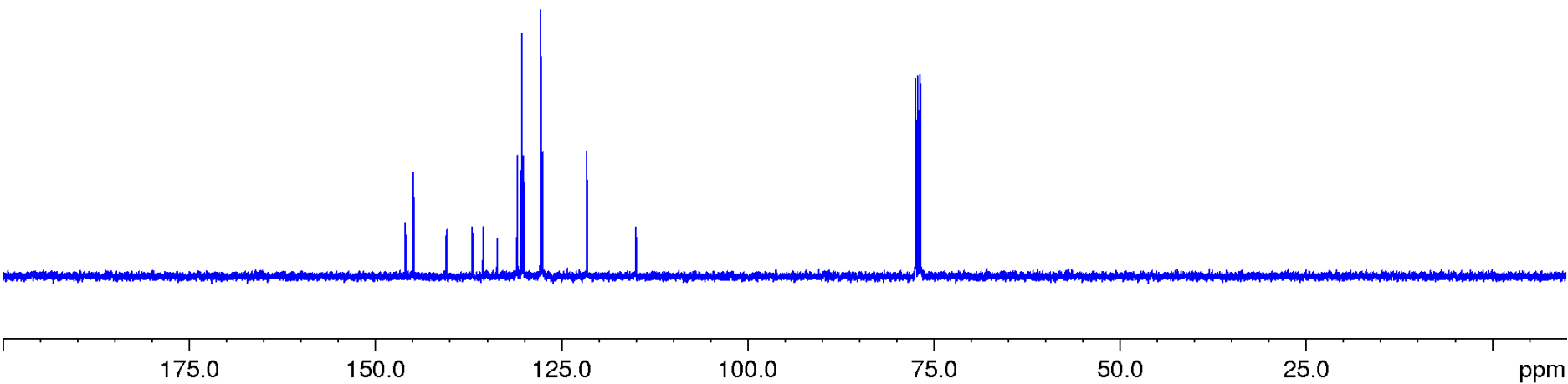


^{13}C NMR-spectrum (100 MHz, CDCl_3)

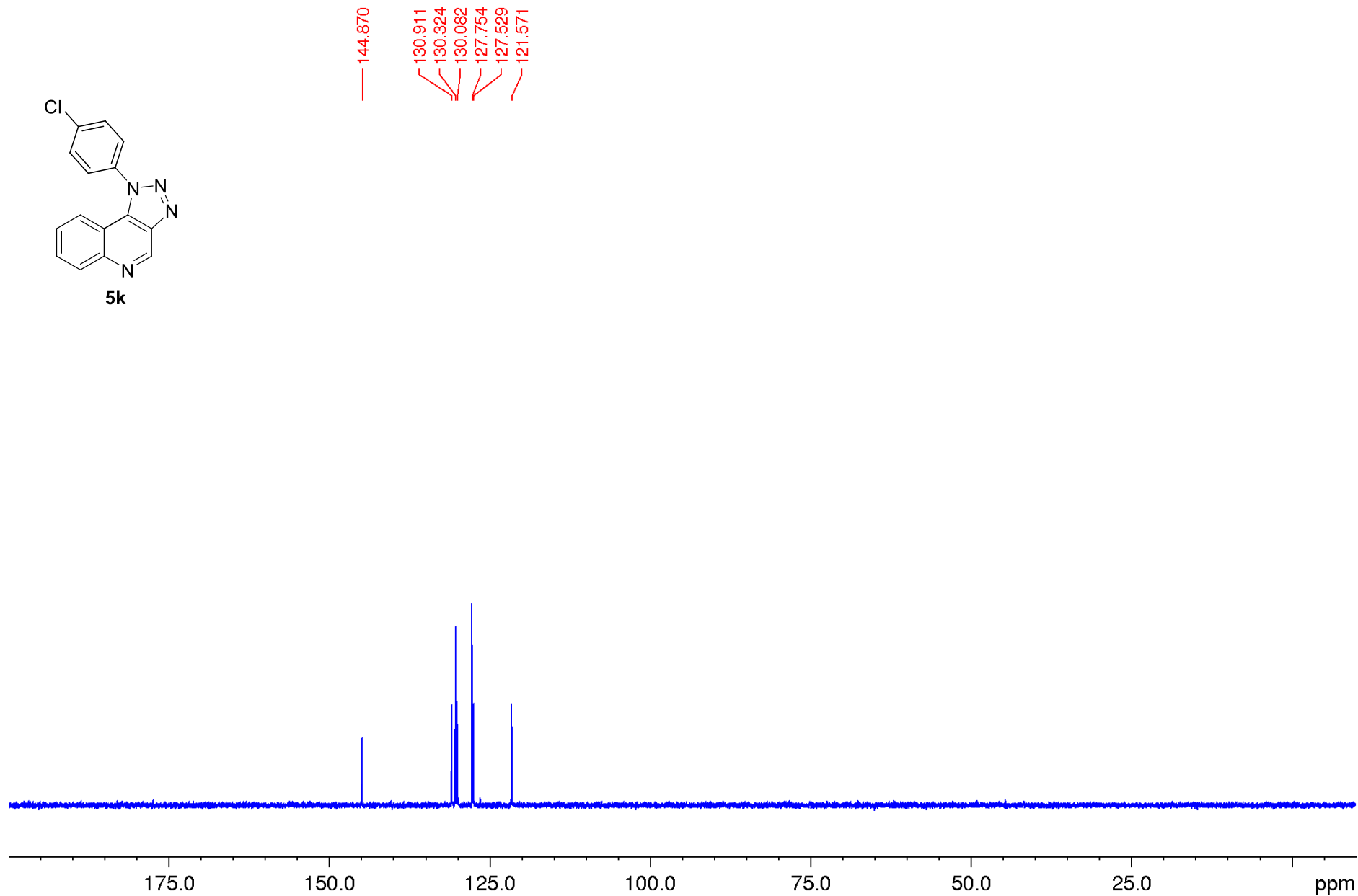
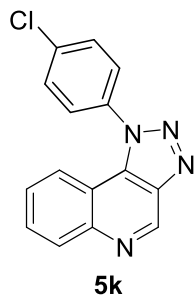


5k

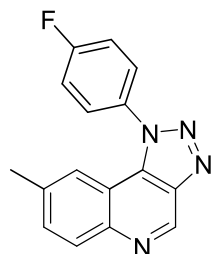
145.969
144.870
140.435
136.944
135.491
133.621
130.912
130.324
130.082
127.754
127.529
121.571
114.973



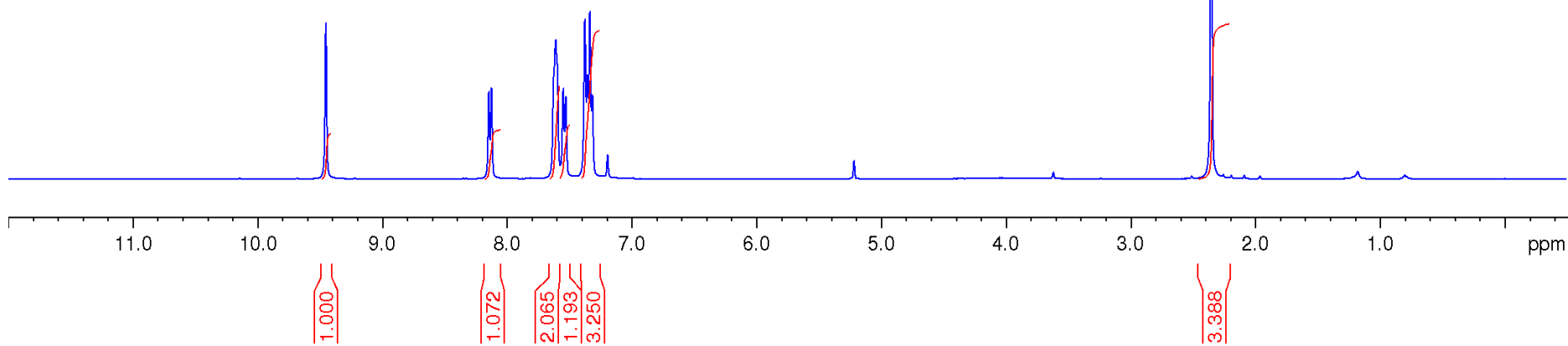
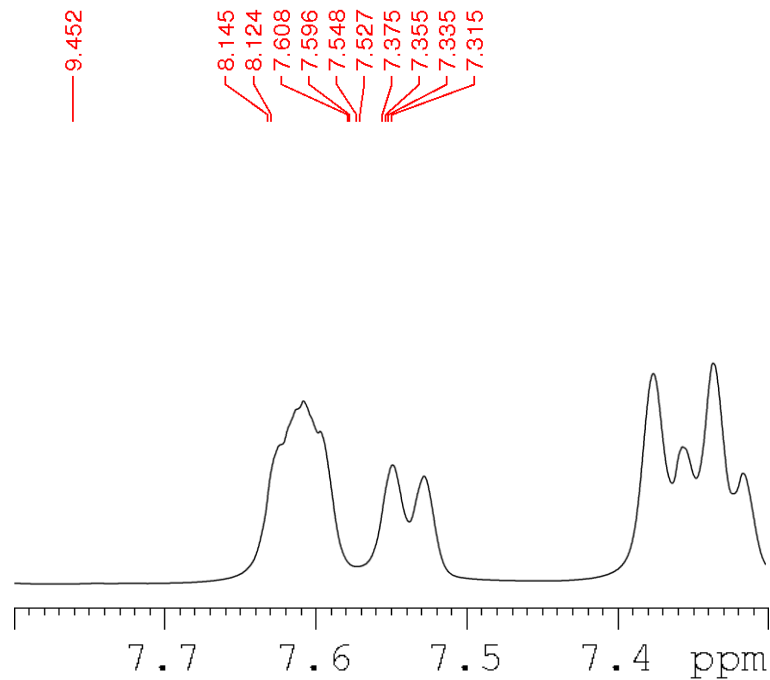
DEPT 135 NMR-spectrum (CDCl₃)



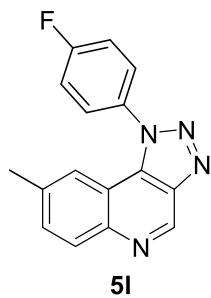
^1H NMR-spectrum (400 MHz, CDCl_3)



5I

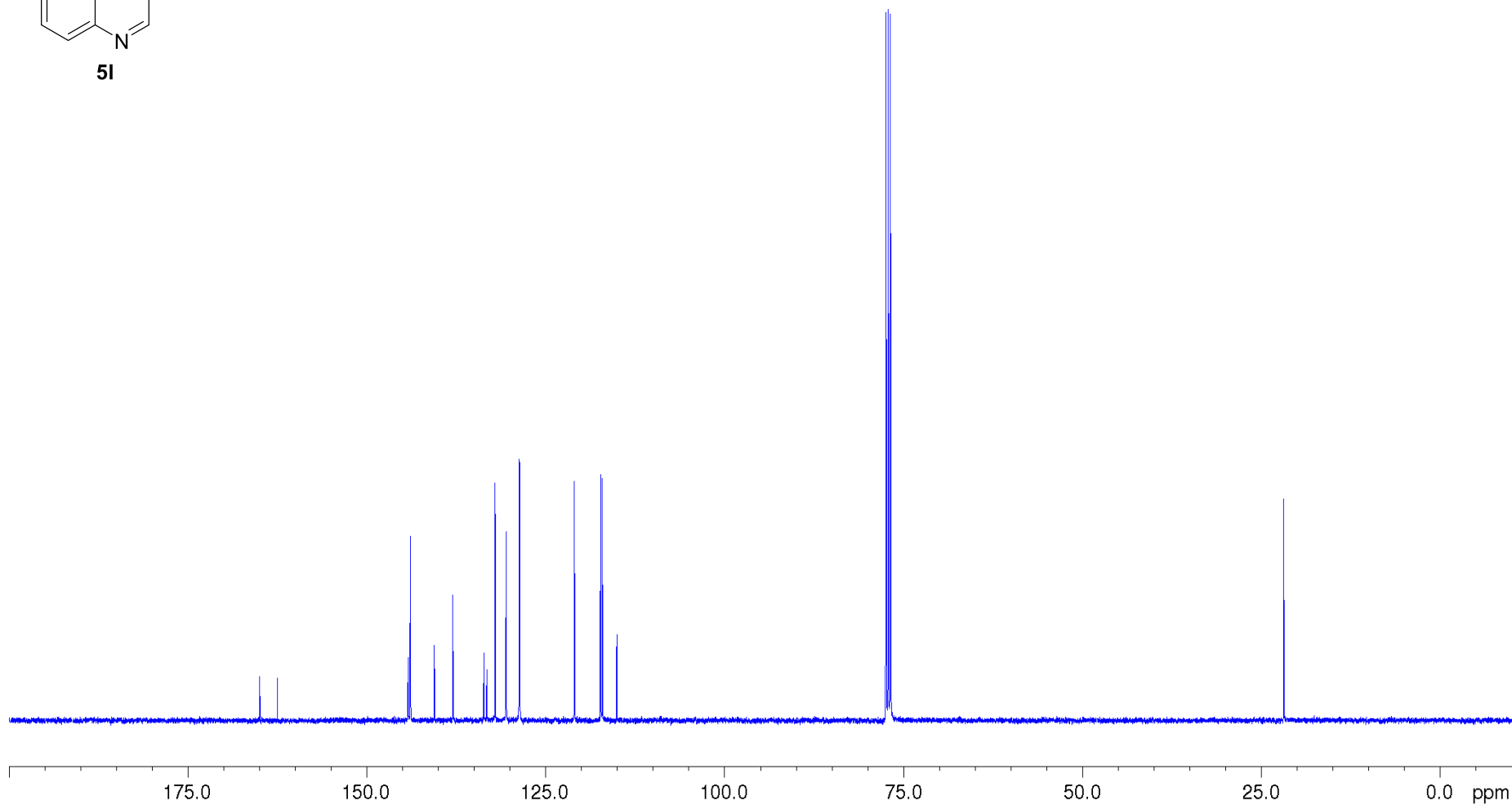


^{13}C NMR-spectrum (100 MHz, CDCl_3)

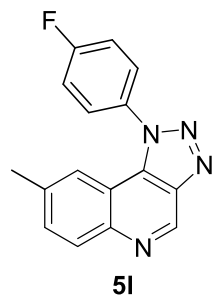


164.955
162.451
144.124
143.804
140.471
137.890
133.535
133.155
133.122
131.969
130.424
128.615
128.527
120.890
117.235
117.005
114.980

21.900

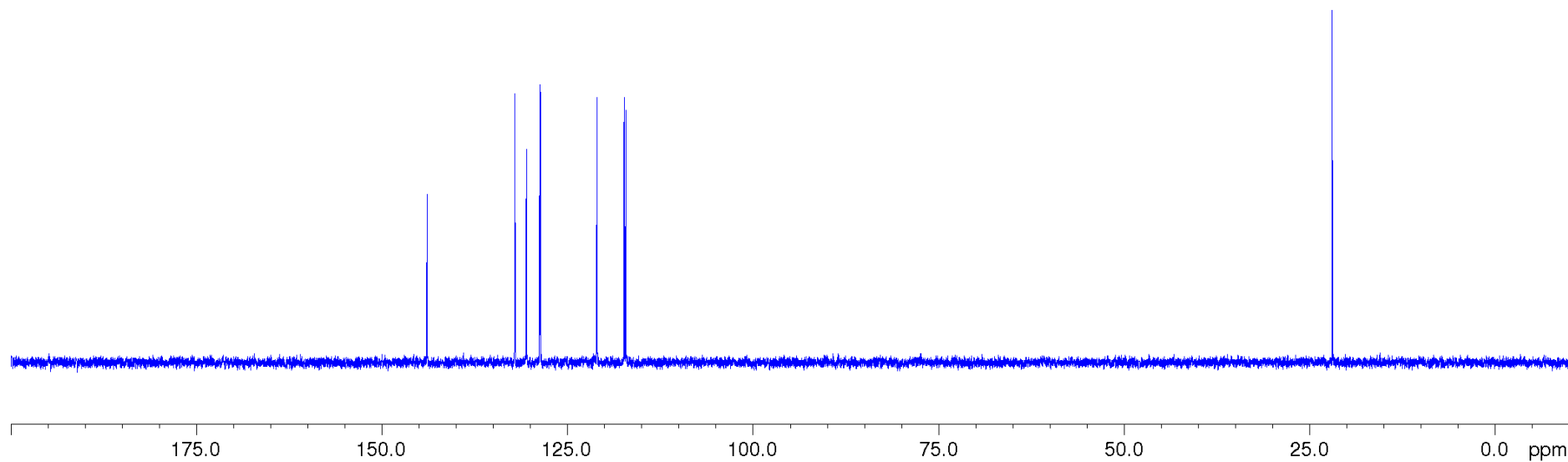


DEPT 135 NMR-spectrum (CDCl₃)

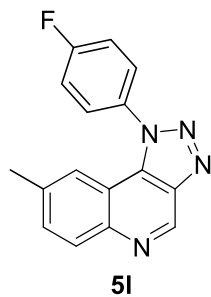


143.804
131.969
130.424
128.615
128.526
120.889
117.235
117.005

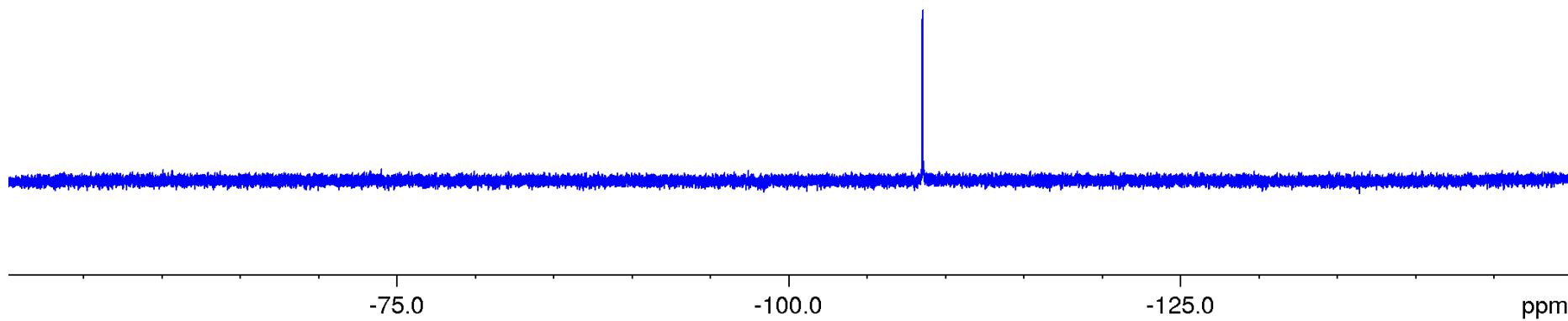
21.900



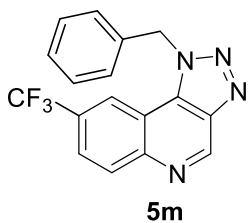
^{19}F NMR-spectrum (376.5 Hz, CDCl_3)



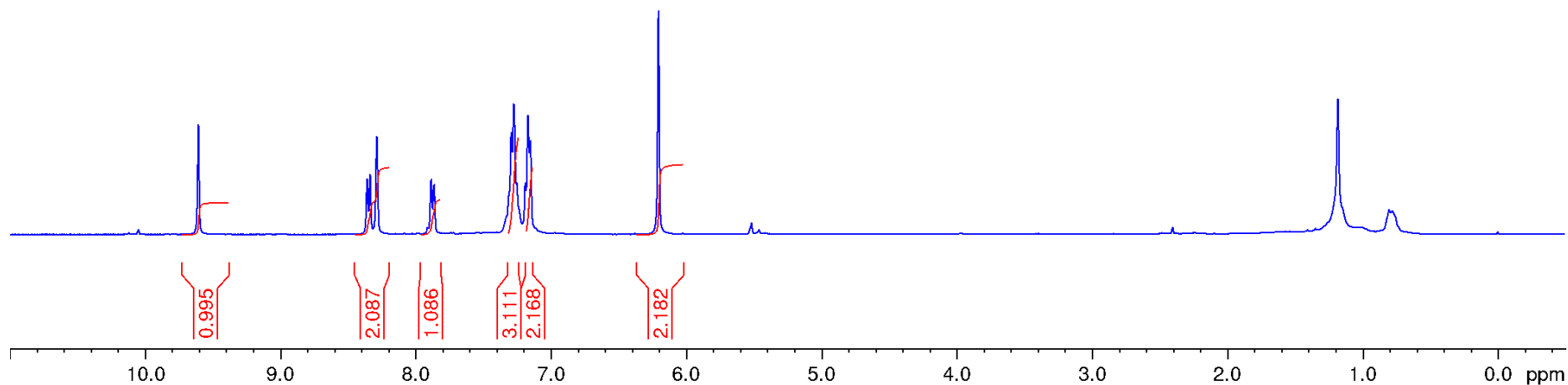
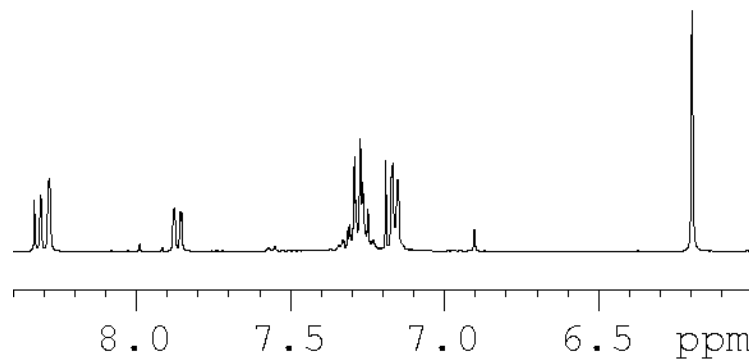
-108.547
-108.558
-108.569
-108.591



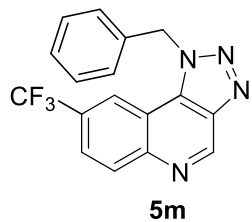
^1H NMR-spectrum (400 MHz, CDCl_3)



9.606
8.358
8.337
8.286
7.885
7.863
7.292
7.274
7.252
7.189
7.169
7.152
6.204

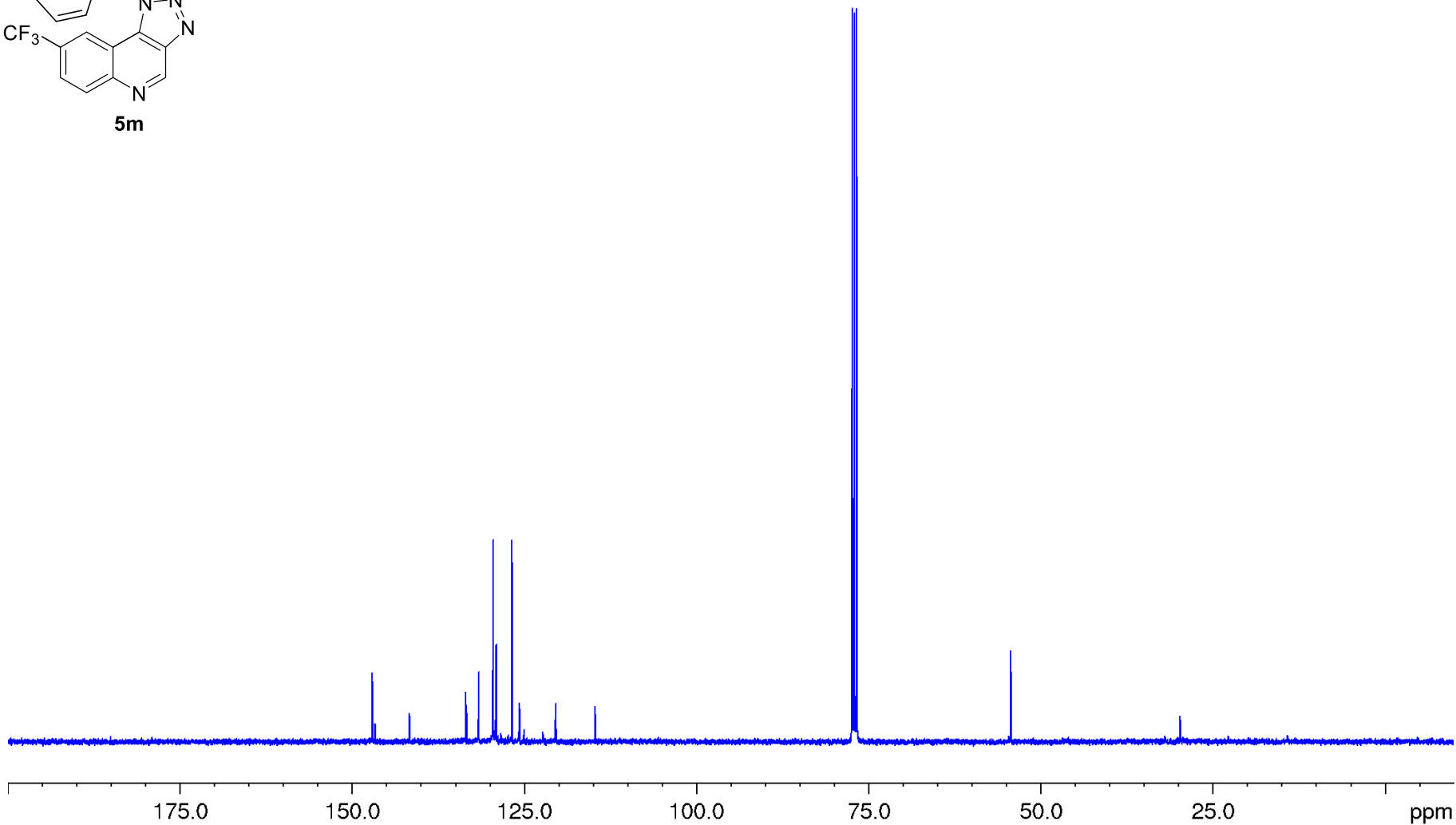


^{13}C NMR-spectrum (100 MHz, CDCl_3)

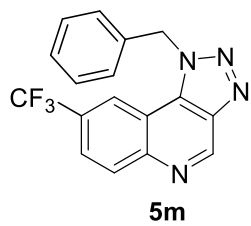


147.050
146.640
141.638
133.465
133.286
131.590
129.517
129.162
129.041
126.750
125.737
125.701
125.671
125.641
124.992
122.307
120.475
120.430
120.389
120.348
114.690

54.320

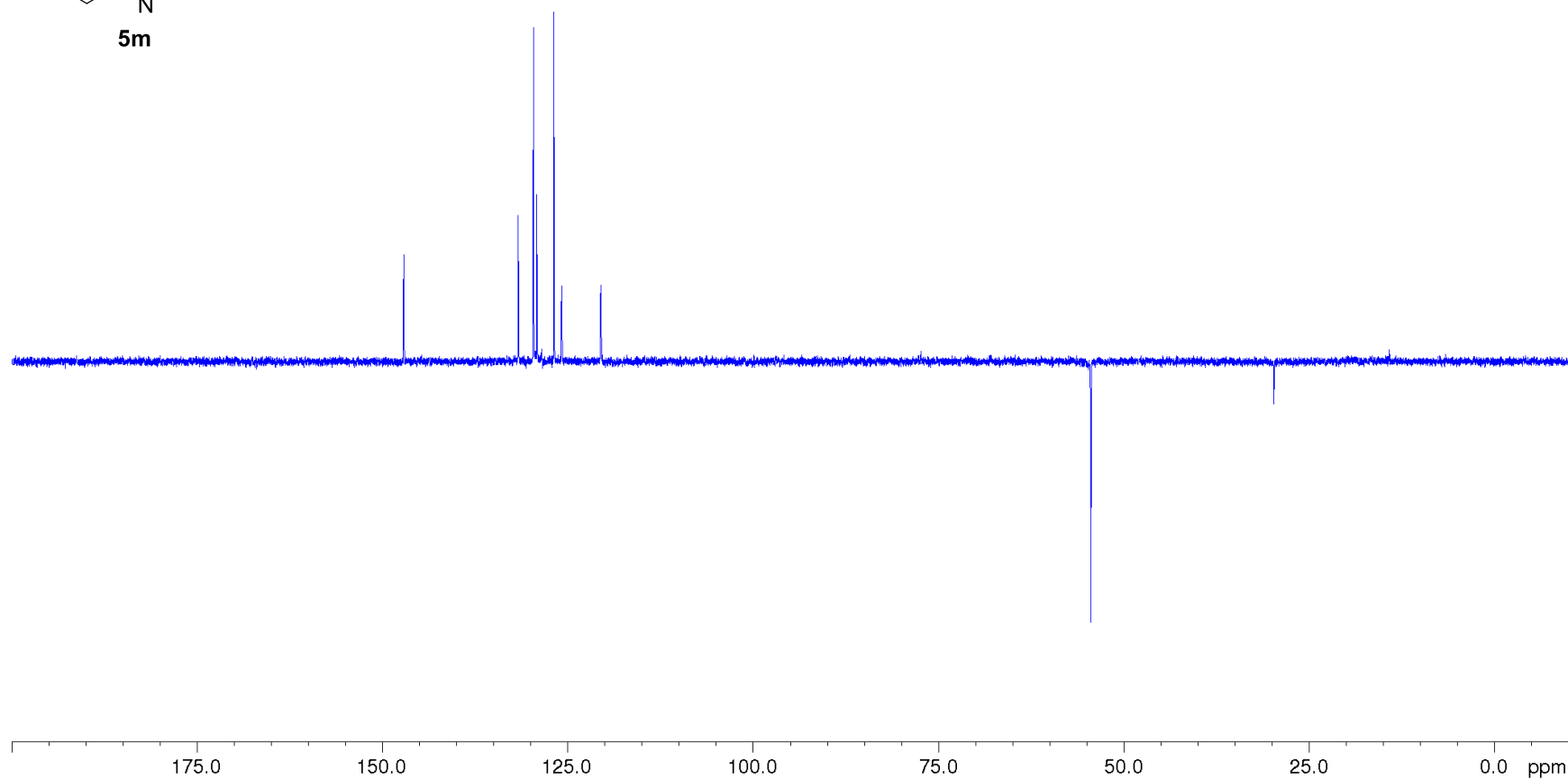


DEPT 135 NMR-spectrum (CDCl_3)

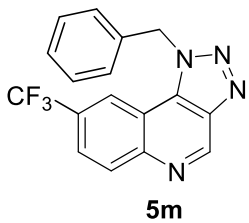


147.014
131.547
129.519
129.046
126.749
125.724
125.693
120.436
120.393

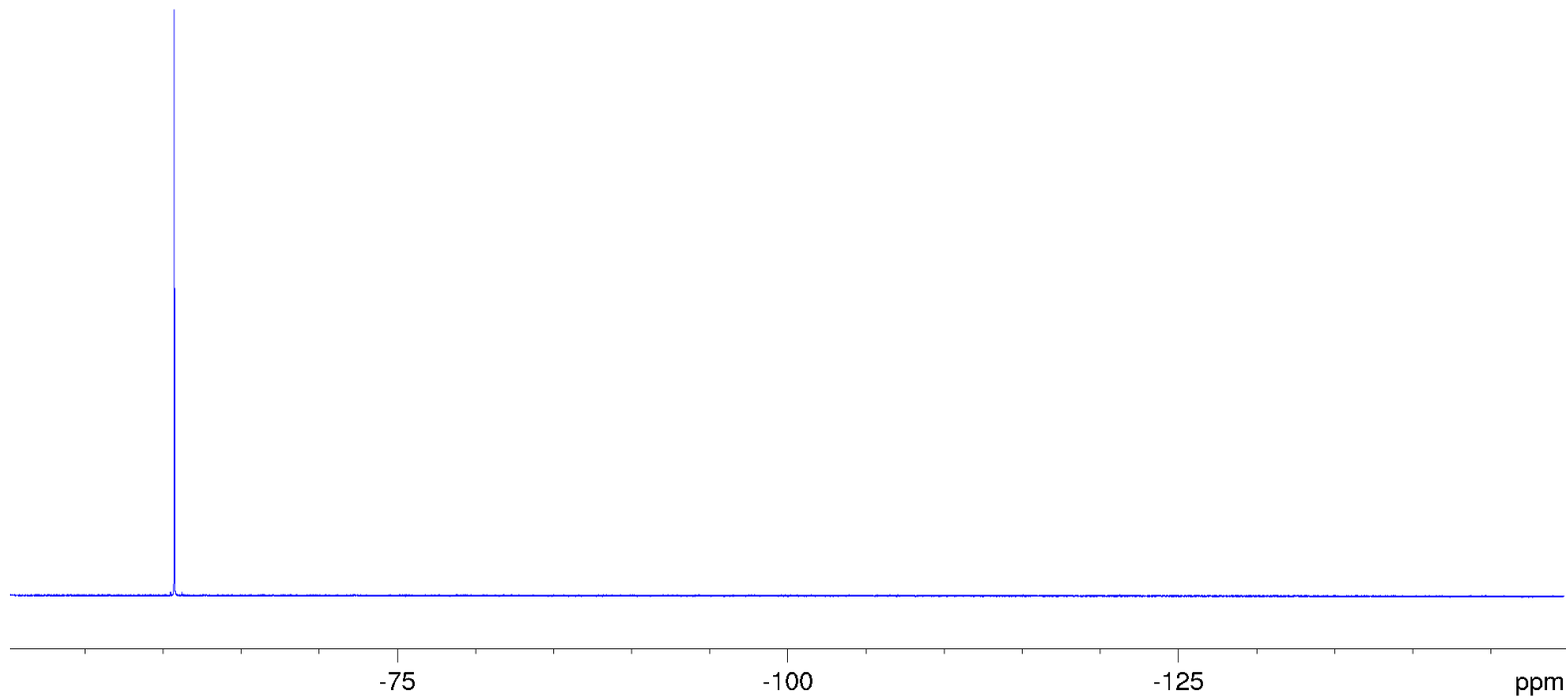
54.326



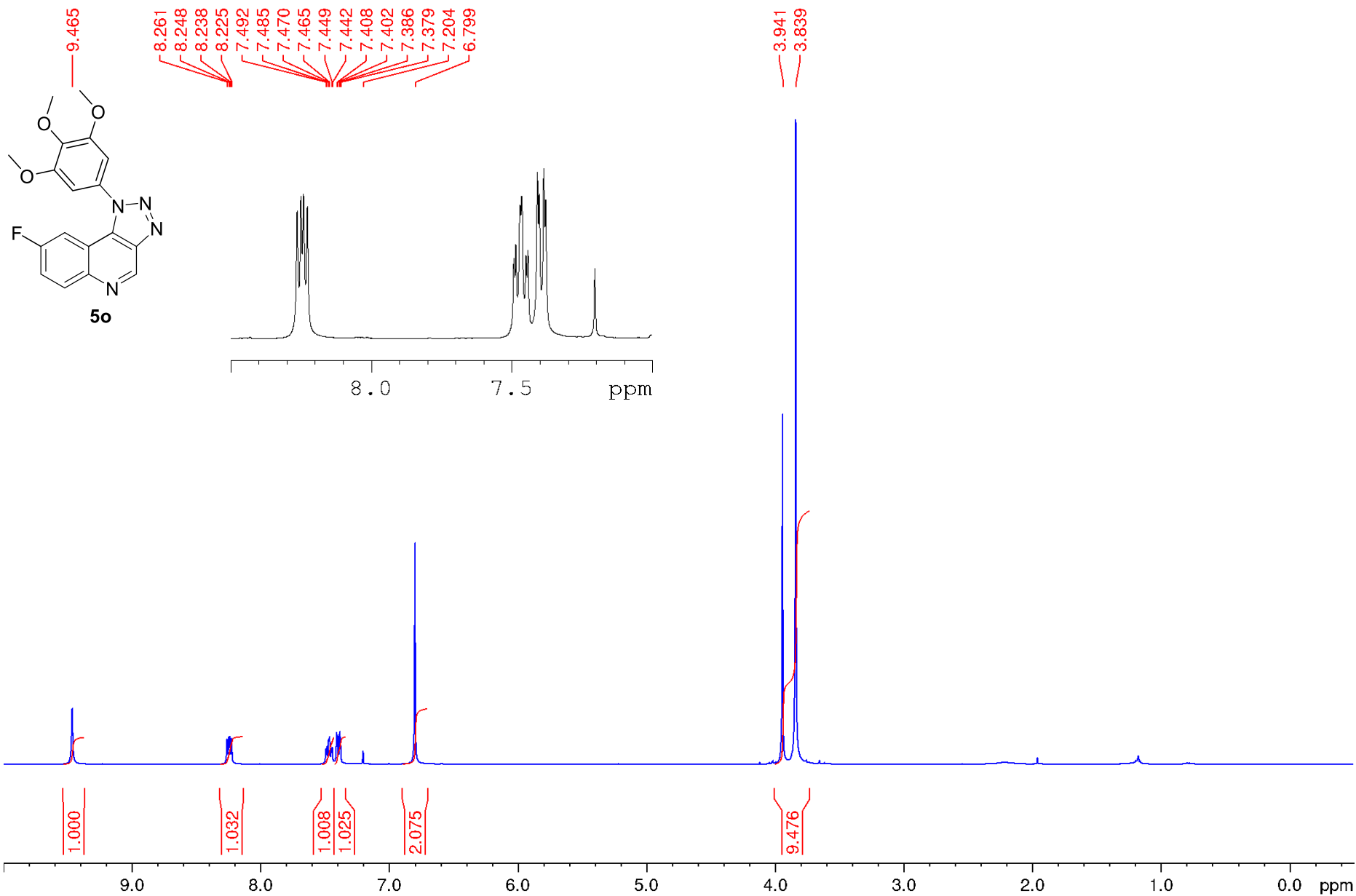
^{19}F NMR-spectrum (376.5 Hz, CDCl_3)



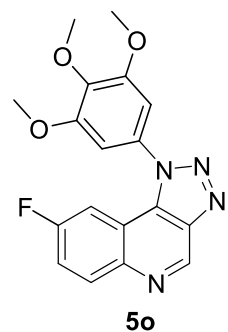
-60.720



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

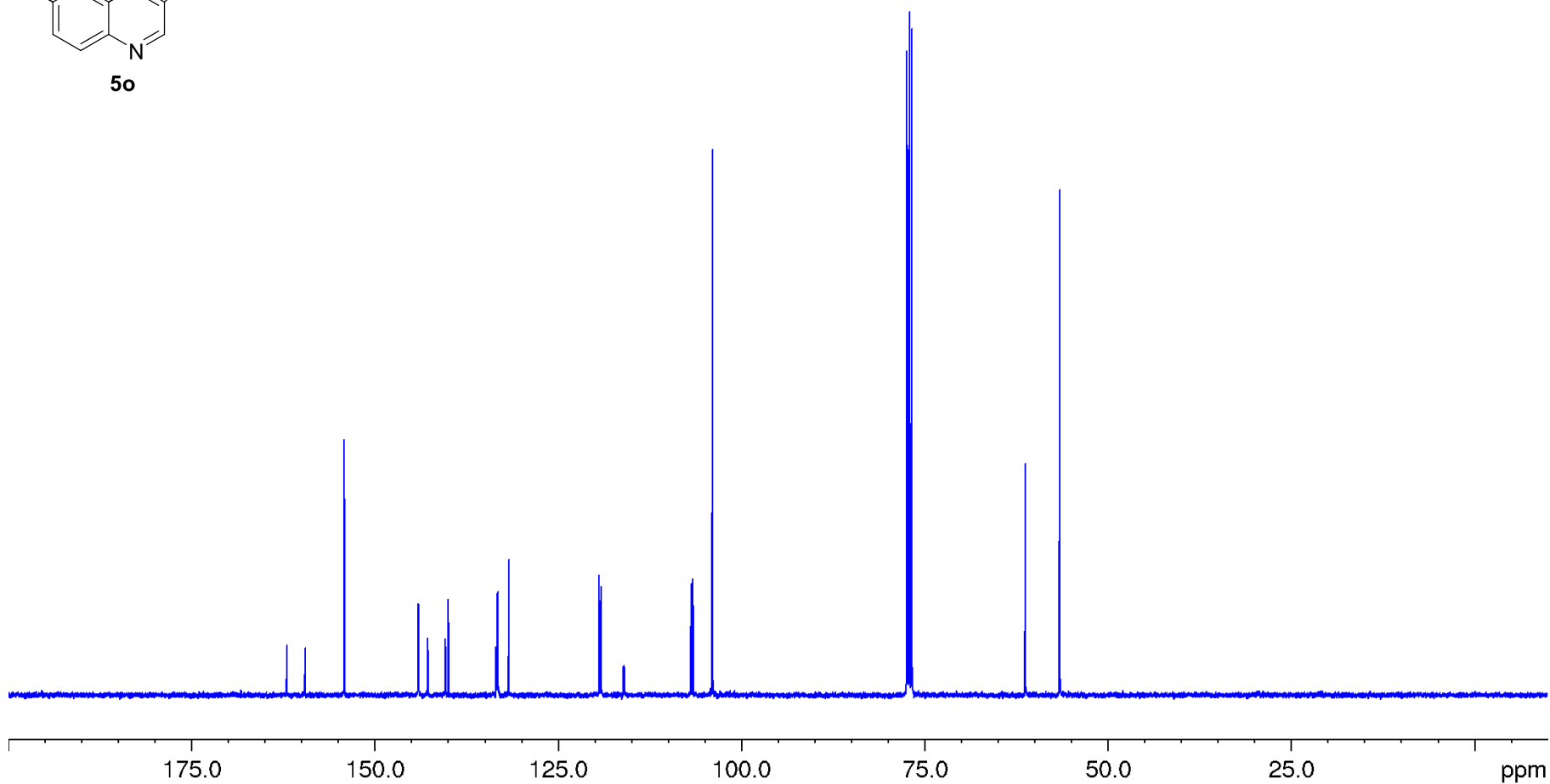


^{13}C NMR-spectrum (100 MHz, CDCl_3)

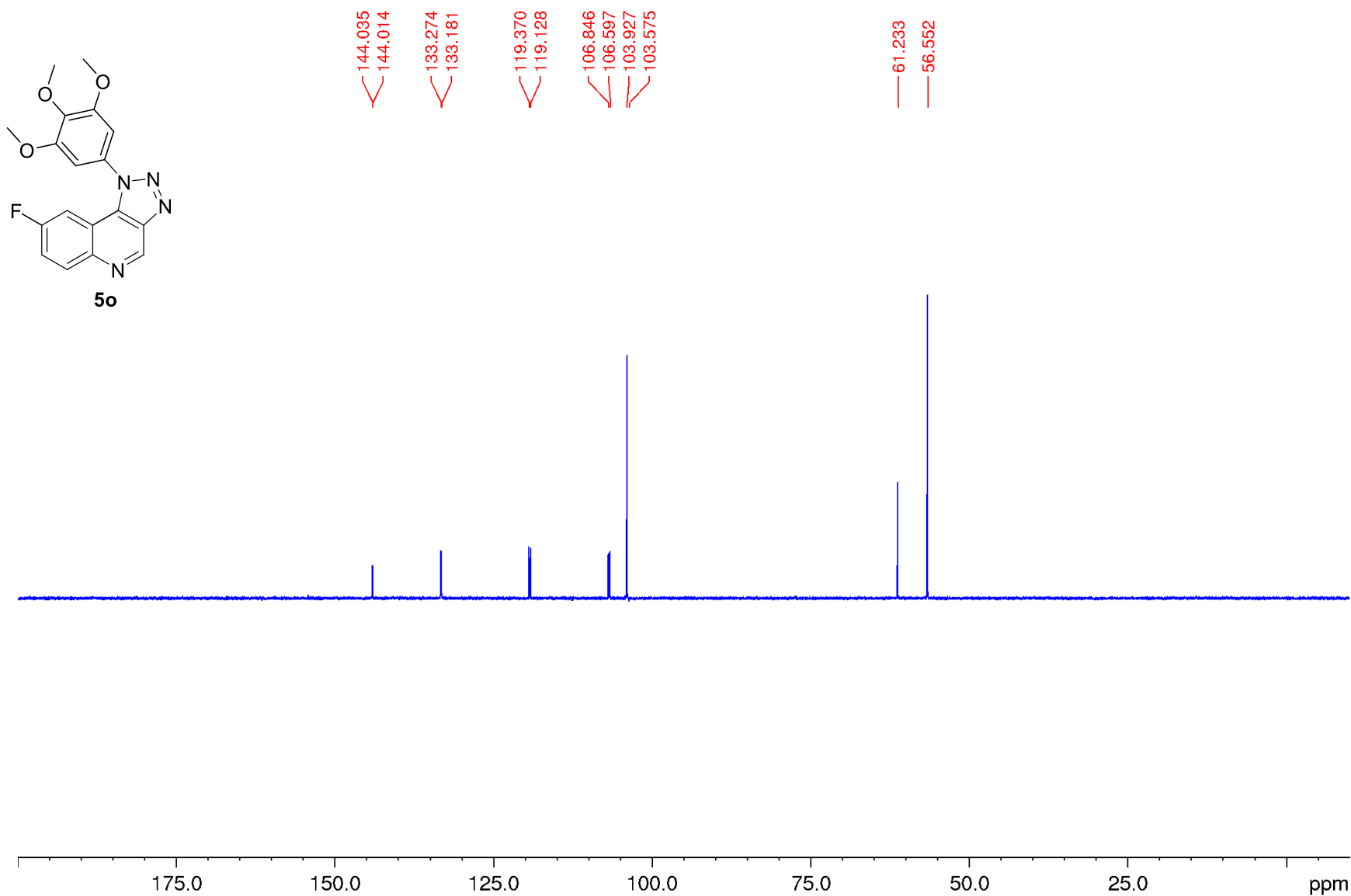


161.996
159.513
154.160
144.040
144.017
142.779
140.353
139.980
133.457
133.414
133.279
133.185
131.700
119.369
119.125
116.047
115.941
106.845
106.596
104.248
103.927

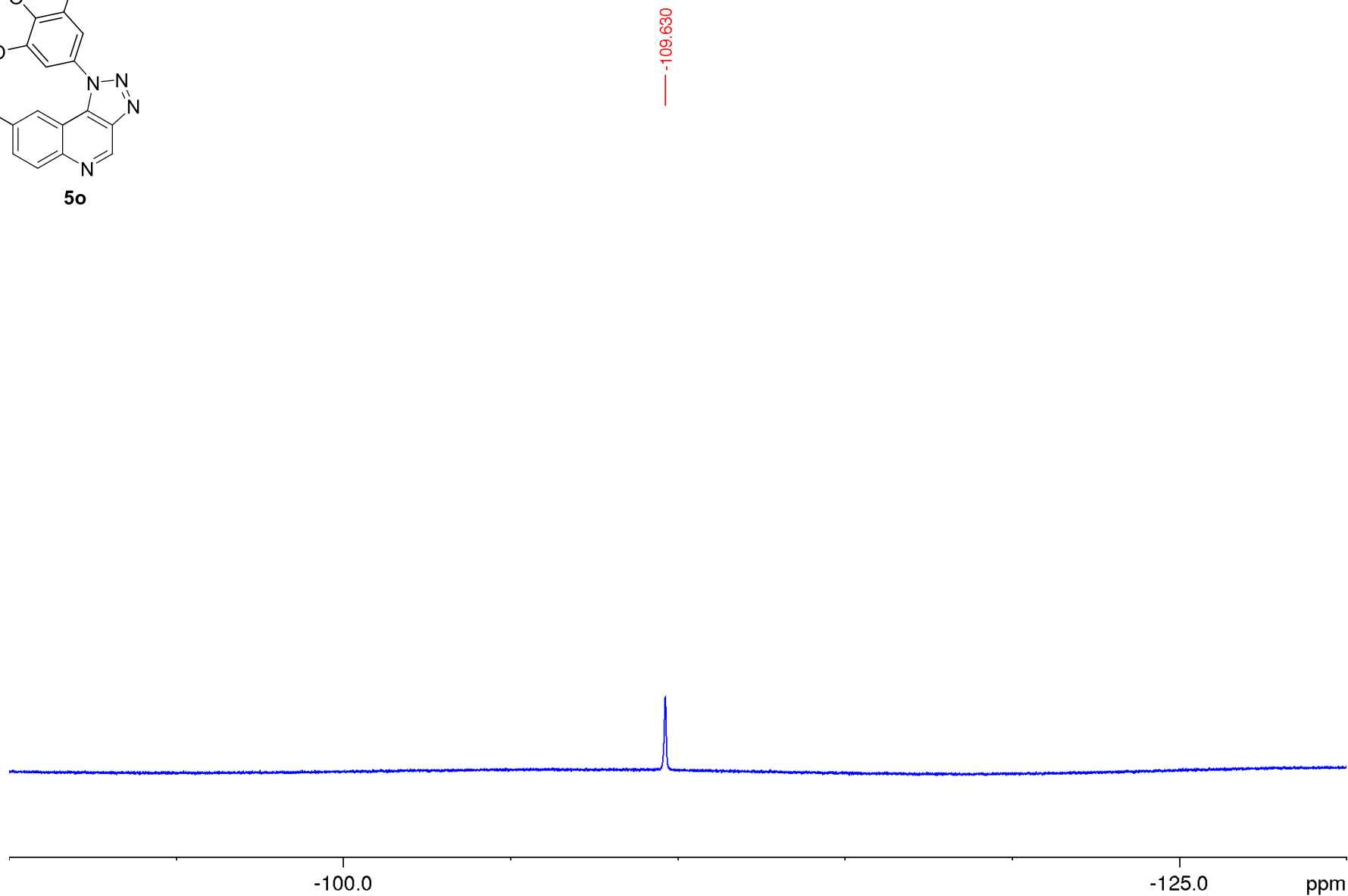
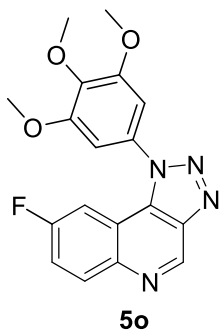
61.233
56.552



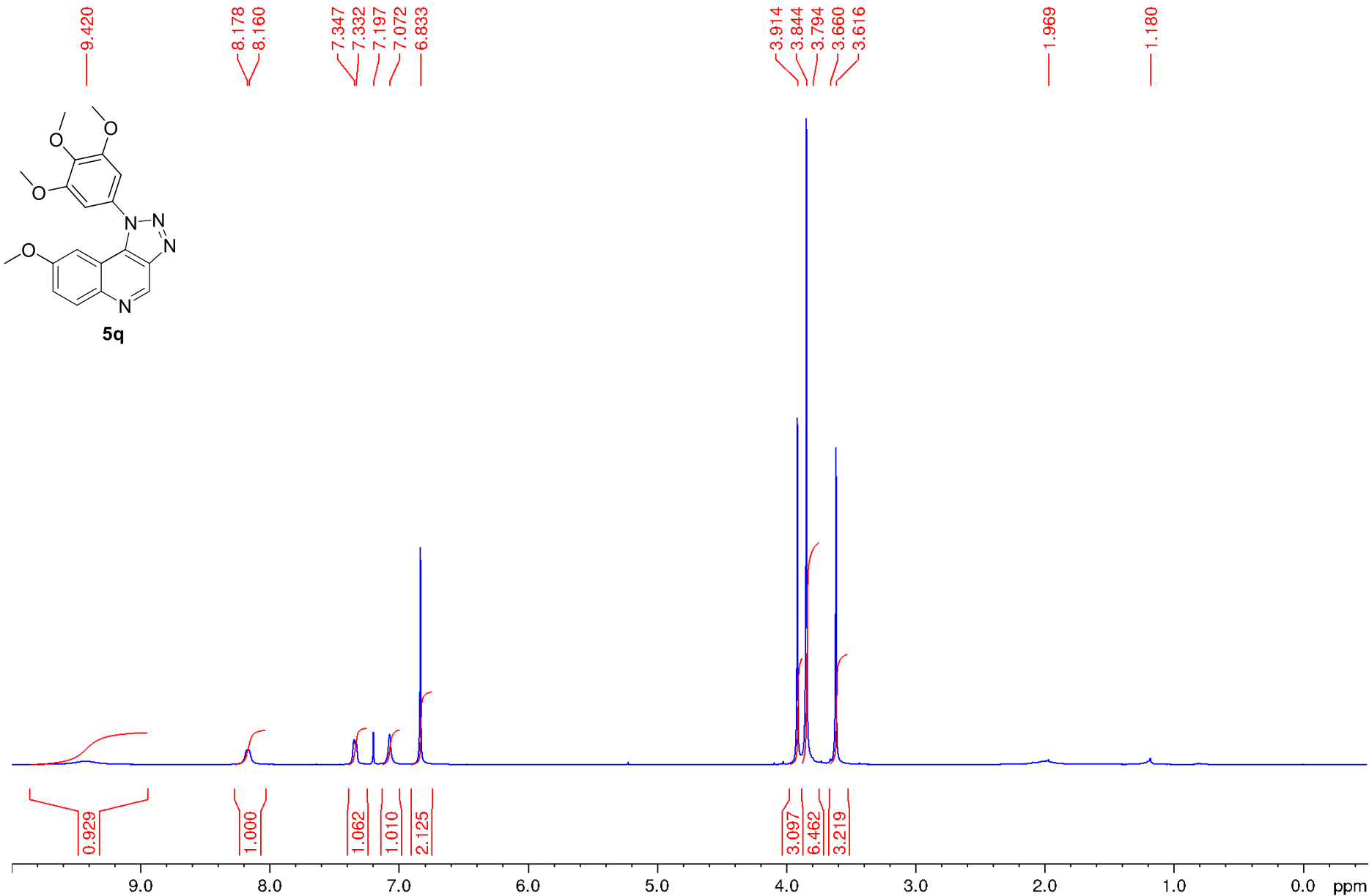
DEPT 135 NMR-spectrum (CDCl_3)



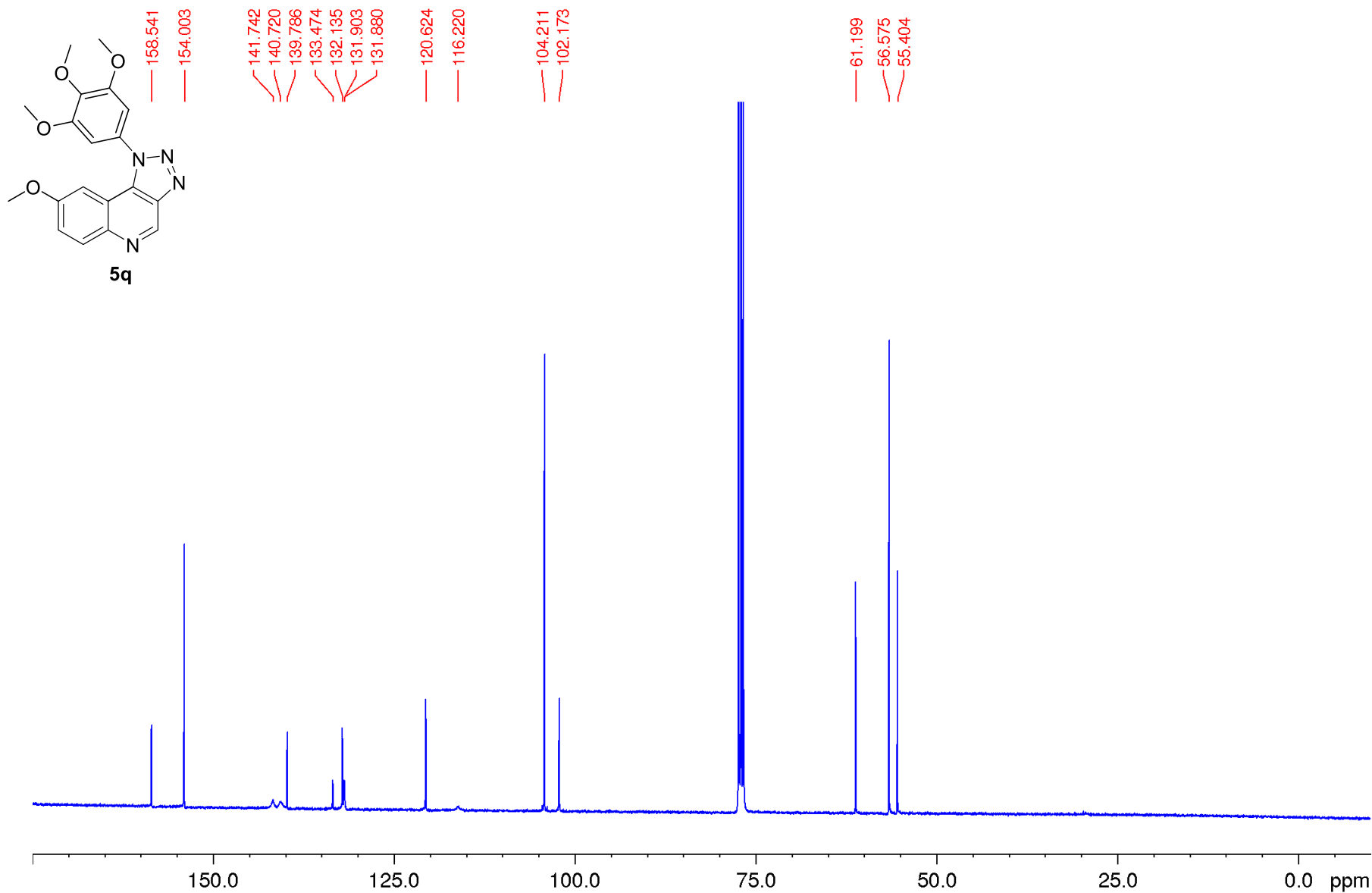
^{19}F NMR-spectrum (376.5 Hz, CDCl_3)



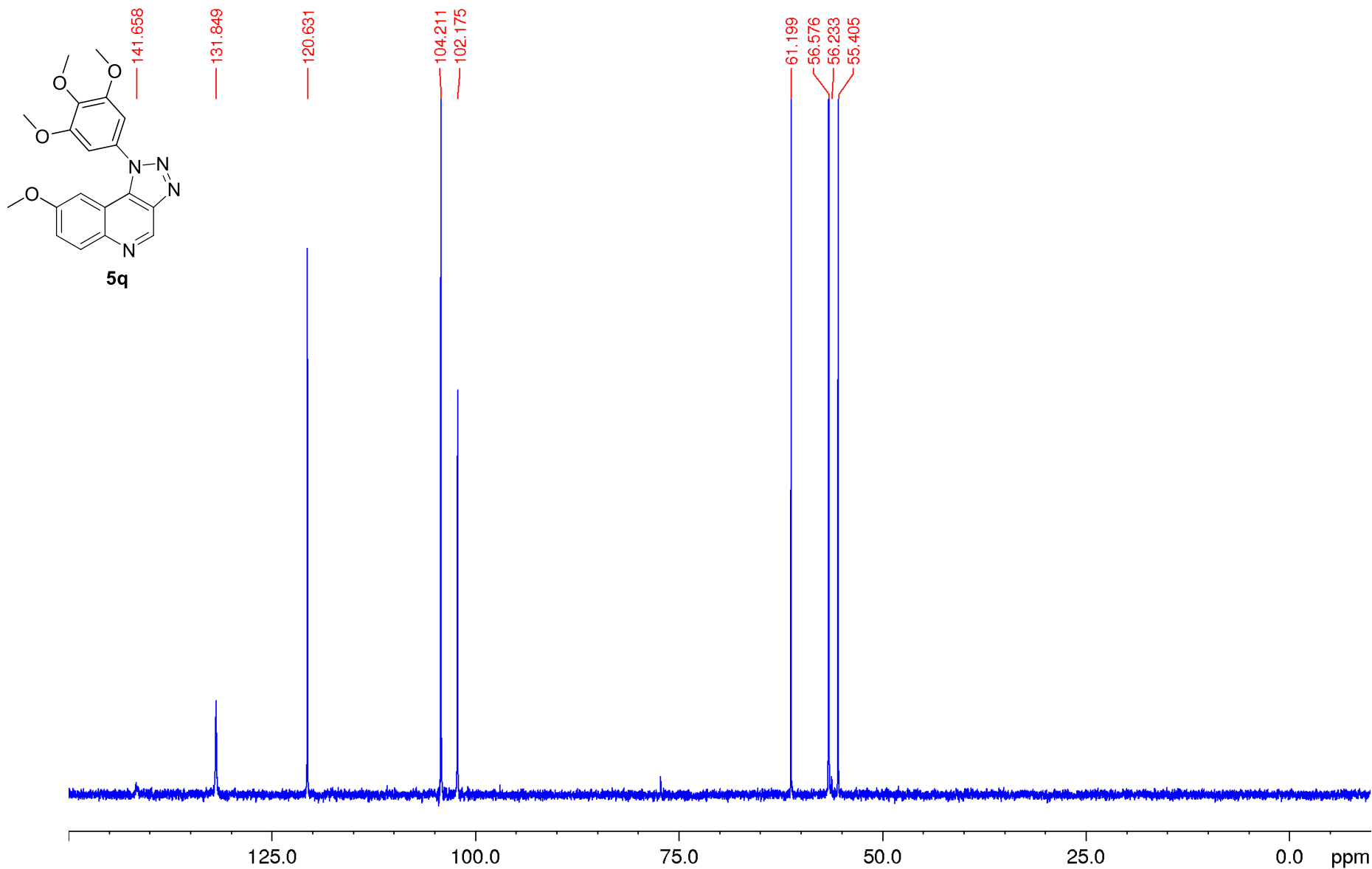
^1H NMR-spectrum (400 MHz, CDCl_3)



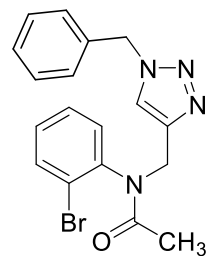
^{13}C NMR-spectrum (100 MHz, CDCl_3)



DEPT 135 NMR-spectrum (CDCl_3)



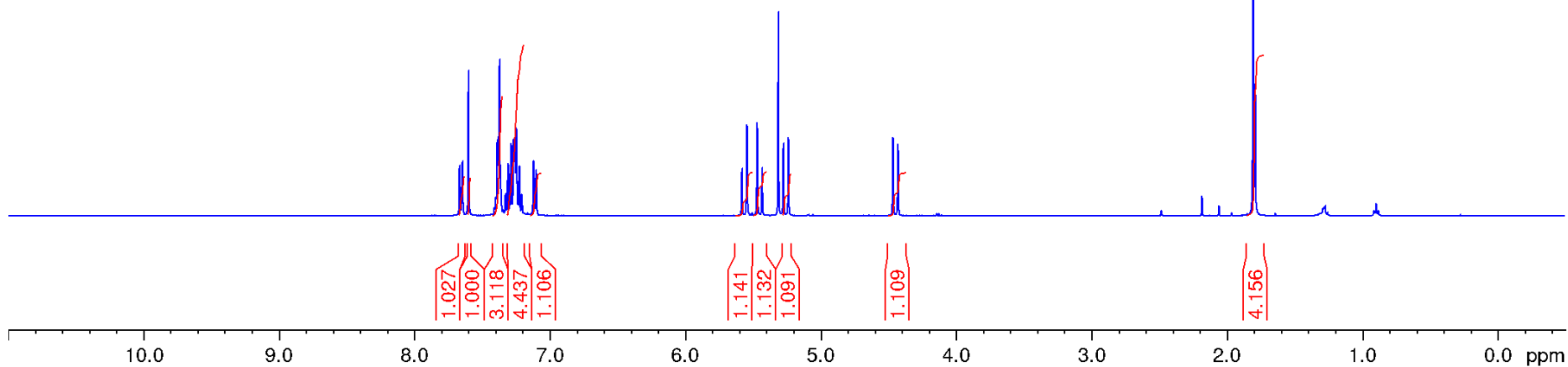
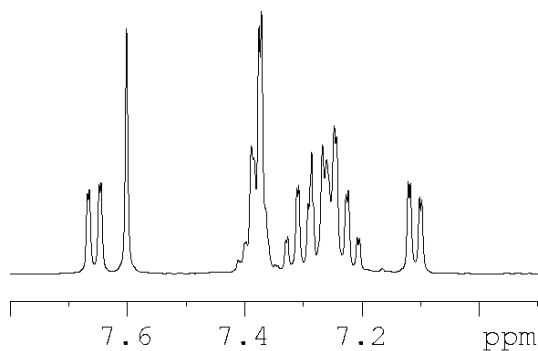
^1H NMR-spectrum (400 MHz, CDCl_3)



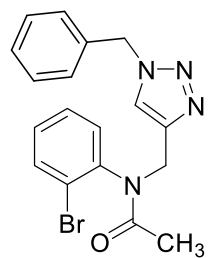
3a

7.667, 7.663, 7.647, 7.644, 7.600, 7.387, 7.383, 7.374, 7.370, 7.310, 7.306, 7.291, 7.284, 7.267, 7.260, 7.247, 7.243, 7.227, 7.223, 7.121, 7.117, 7.102, 7.098, 5.581, 5.544, 5.468, 5.431, 5.312, 5.274, 5.237, 4.465, 4.428

1.805



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



3a

170.385

144.117

141.497

134.689

133.754

130.990

129.964

129.080

128.833

128.721

128.048

123.713

123.663

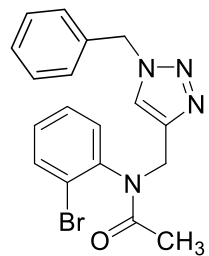
54.142

43.616

22.317

ppm

DEPT 135 NMR-spectrum (CDCl_3)



3a

133.755
130.990
129.964
129.080
128.833
128.722
128.049
123.714

54.142

43.615

22.316

150.0

125.0

100.0

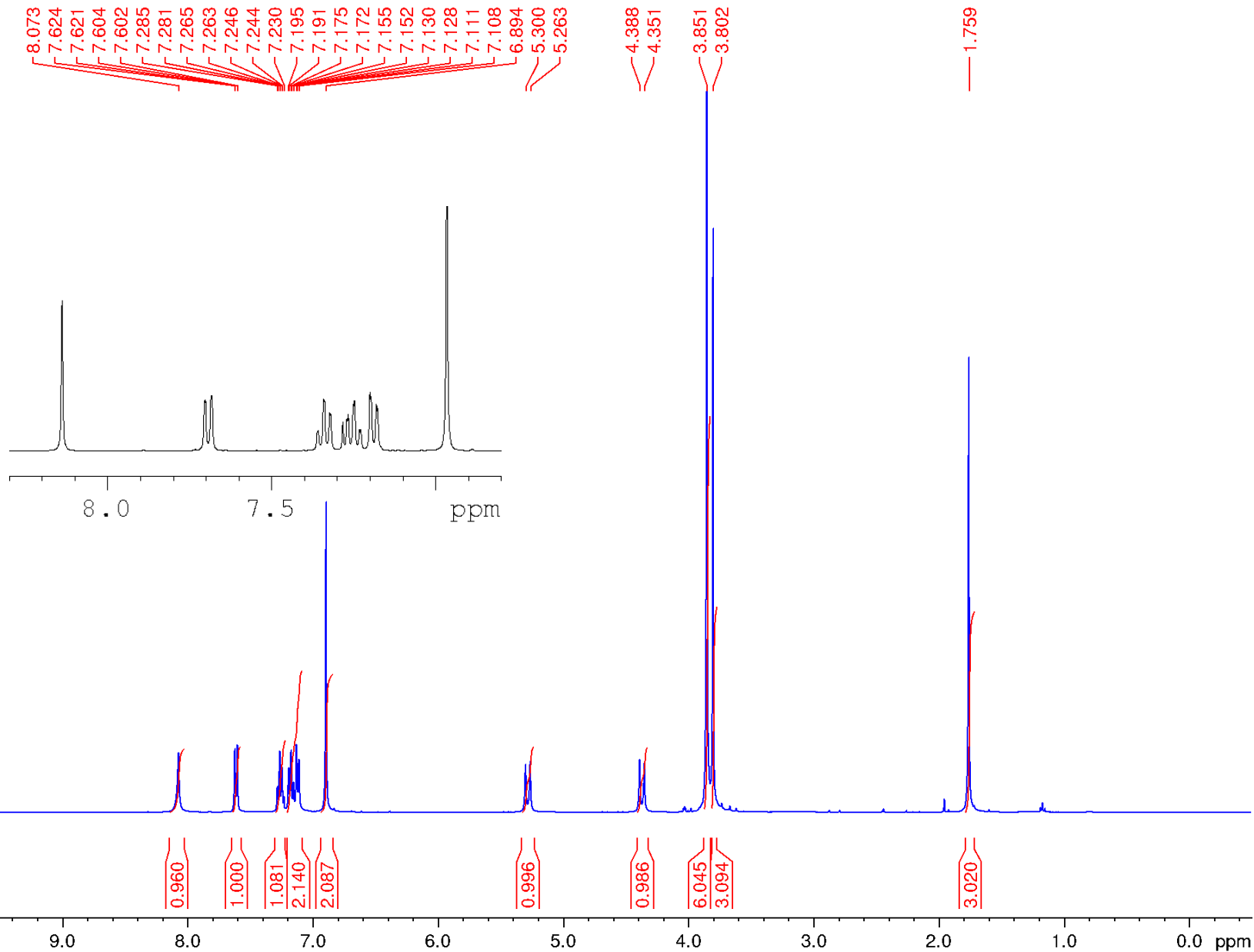
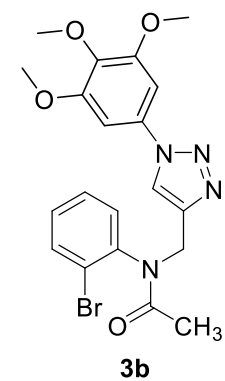
75.0

50.0

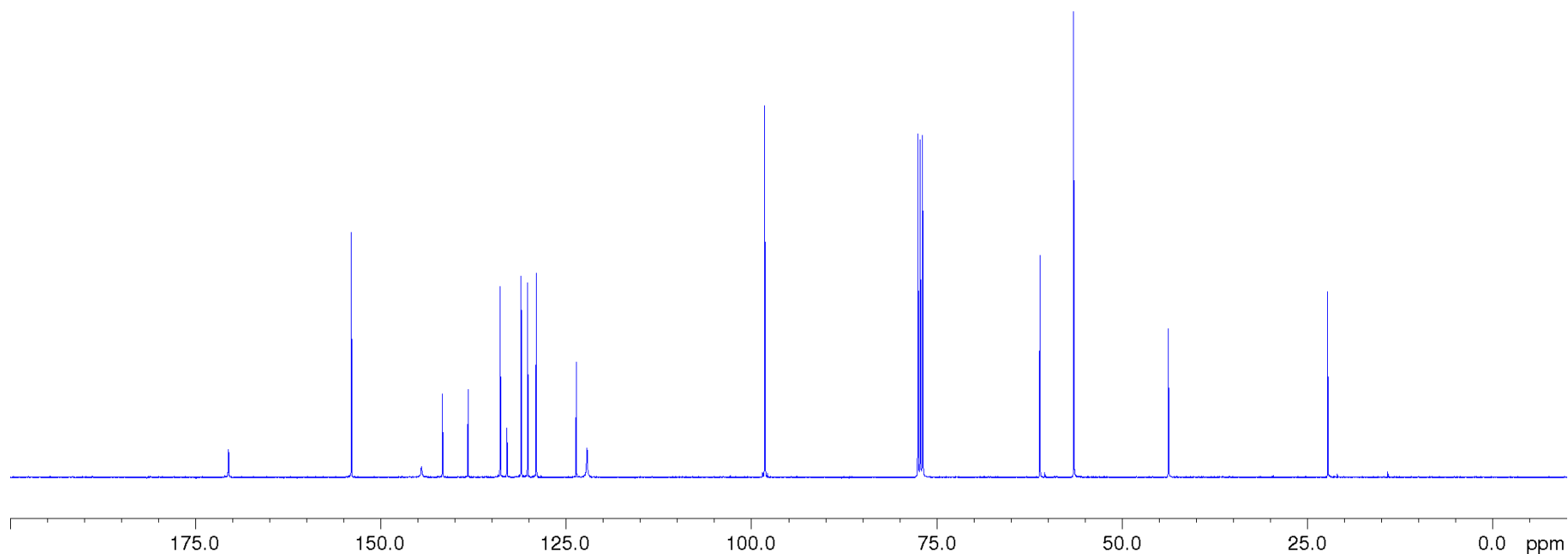
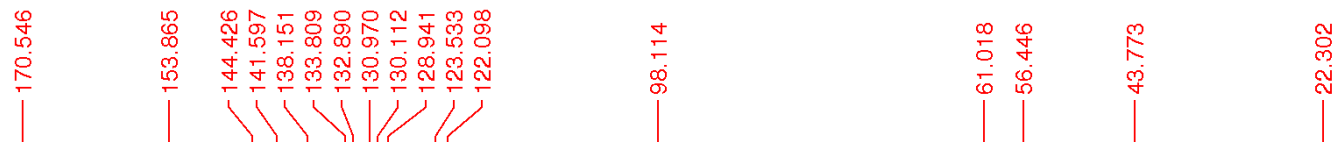
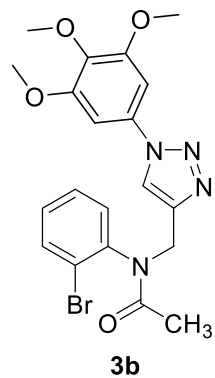
25.0

ppm

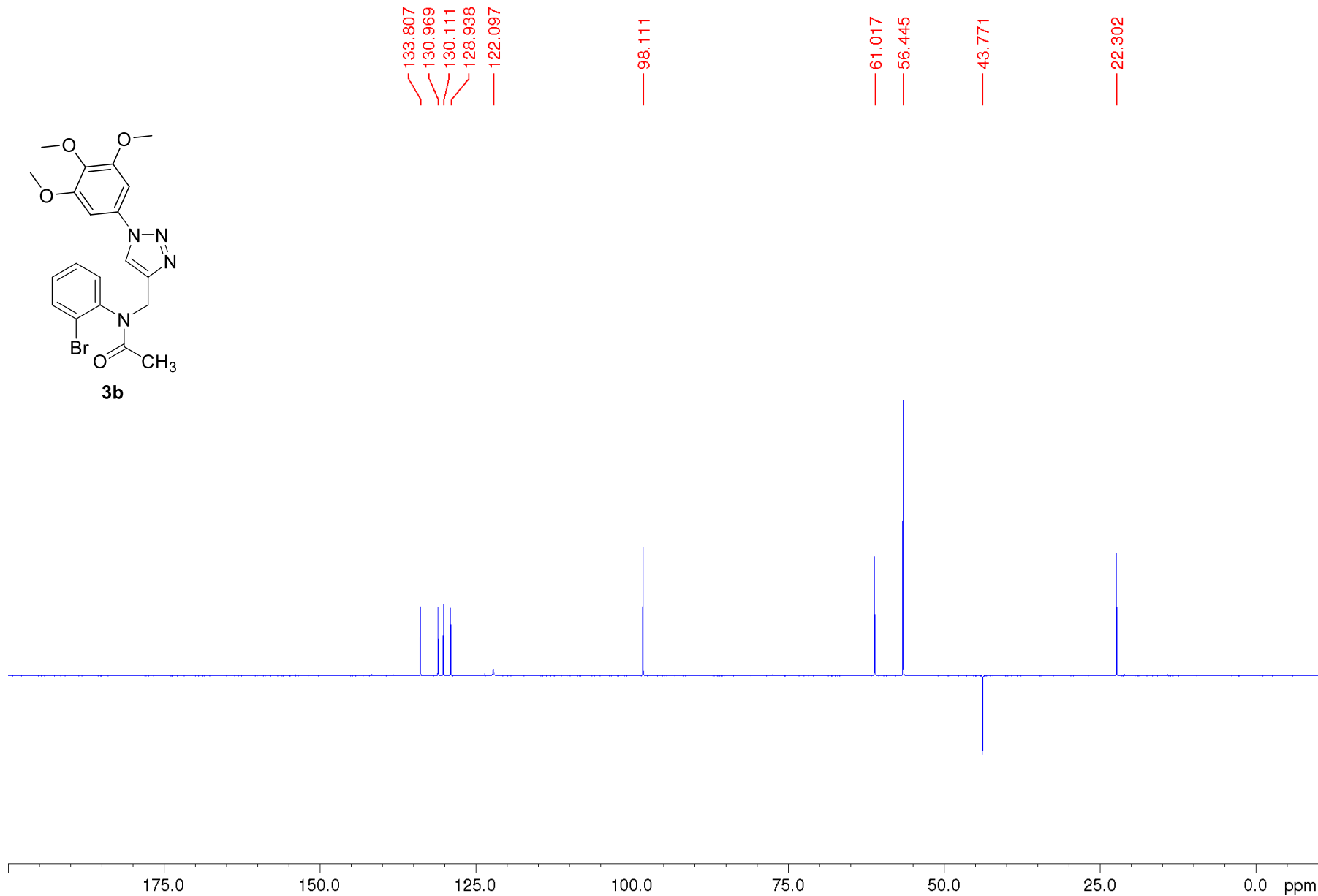
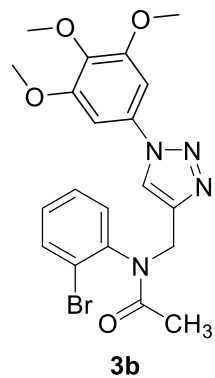
^1H NMR-spectrum (400 MHz, CDCl_3)



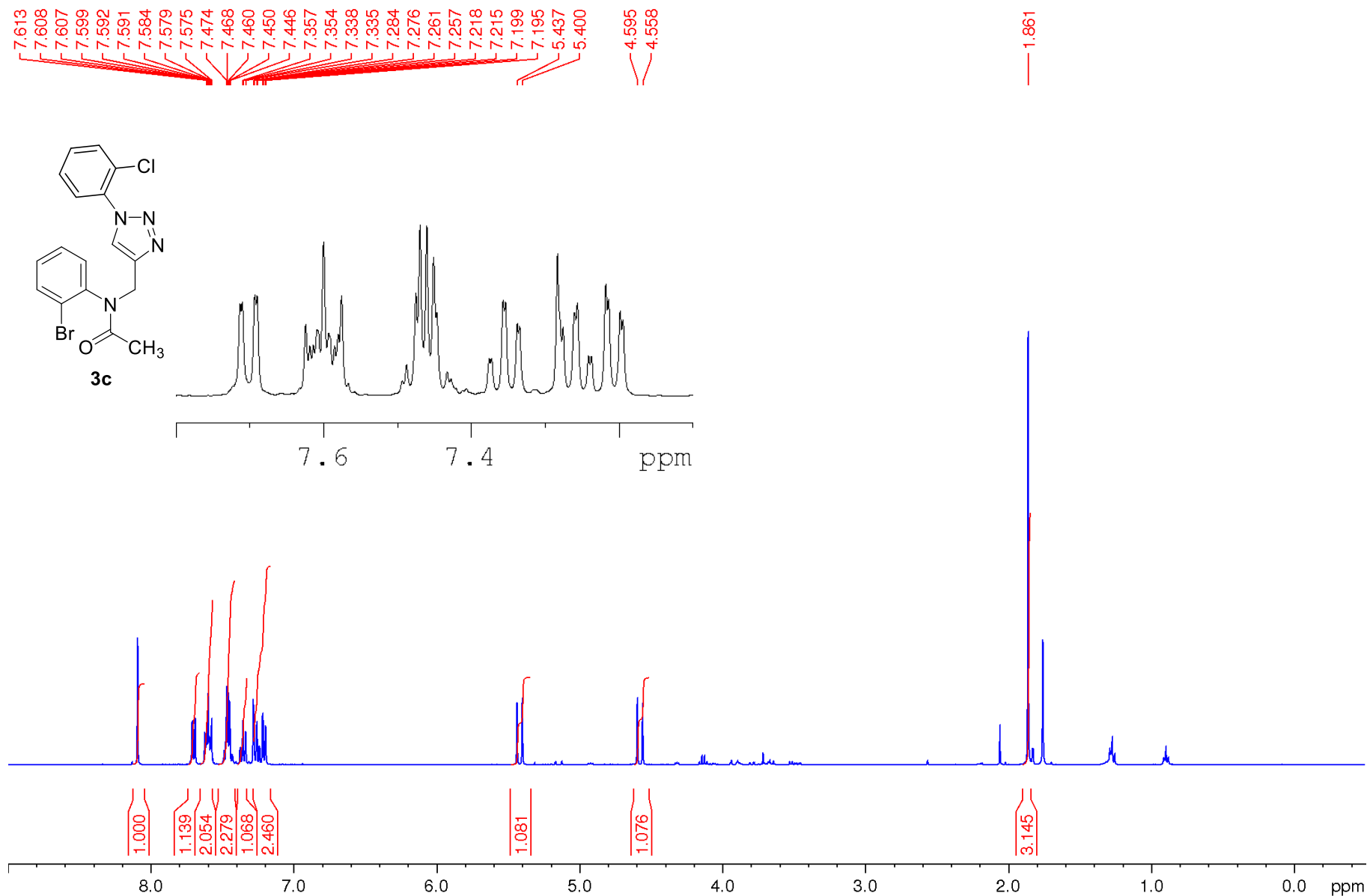
^{13}C NMR-spectrum (100 MHz, CDCl_3)



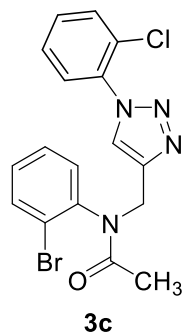
DEPT 135 NMR-spectrum (CDCl₃)



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



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



170.487

143.450

141.468

133.834

131.086

130.748

130.071

128.922

128.703

127.872

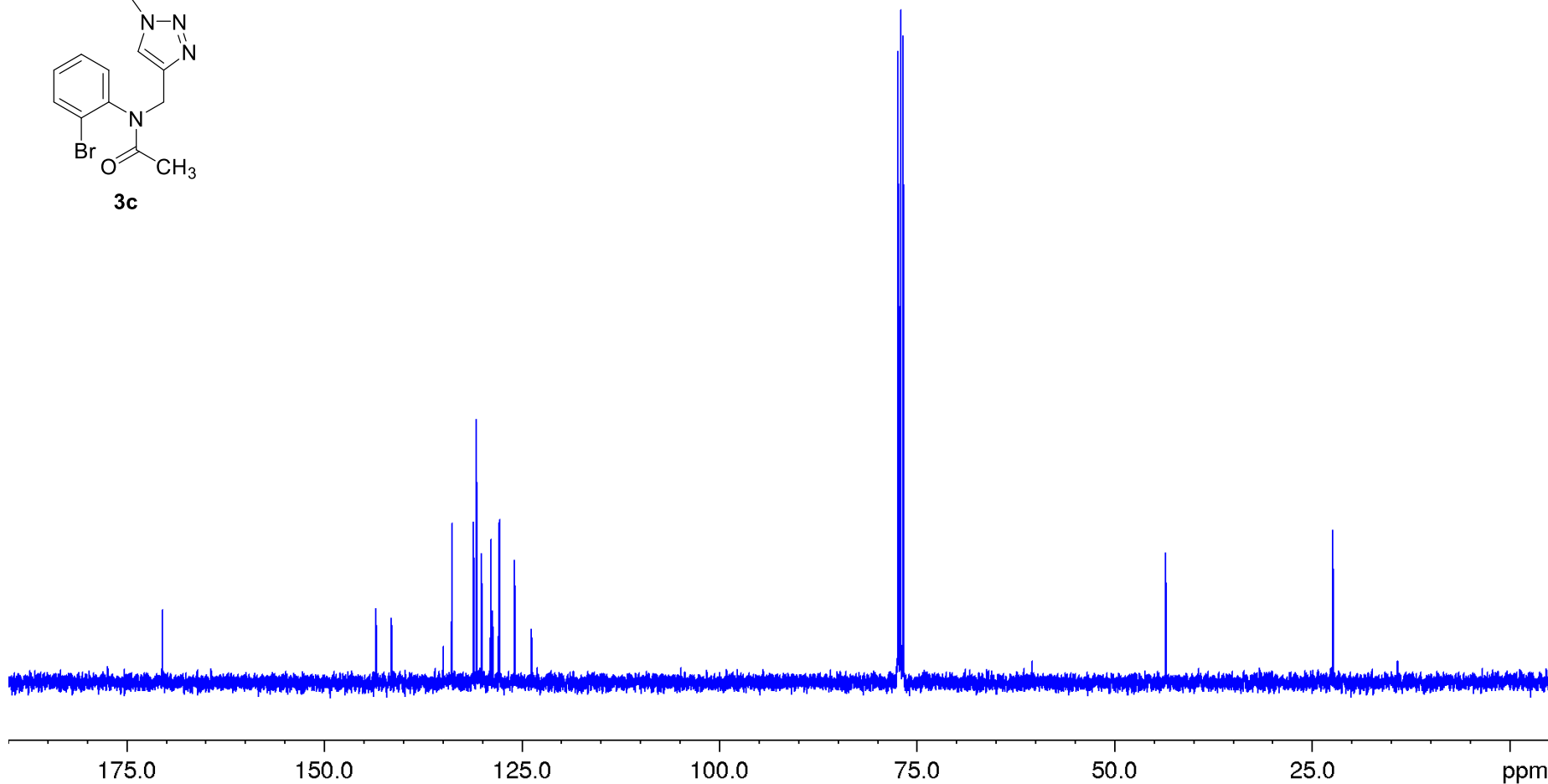
127.790

125.889

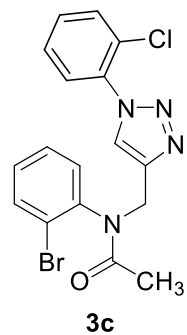
123.746

43.476

22.344



DEPT 135 NMR-spectrum (CDCl_3)



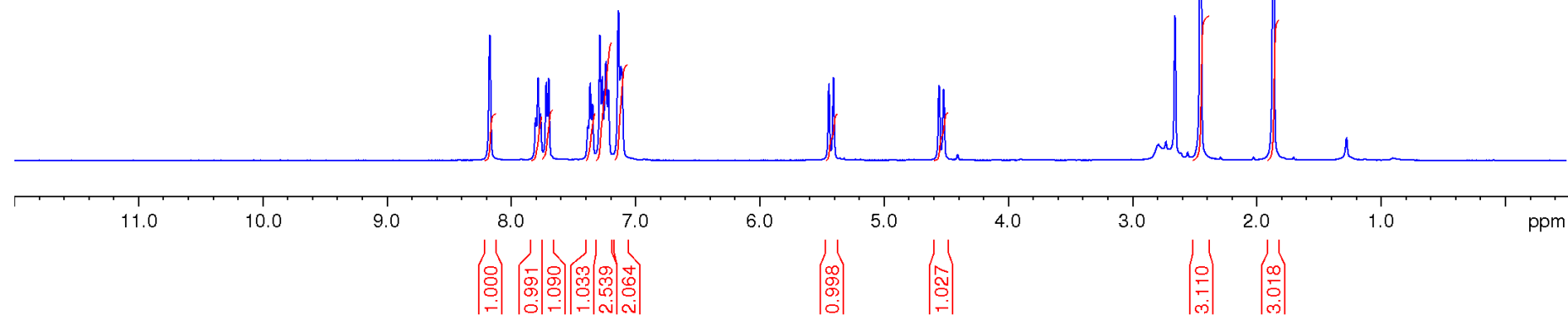
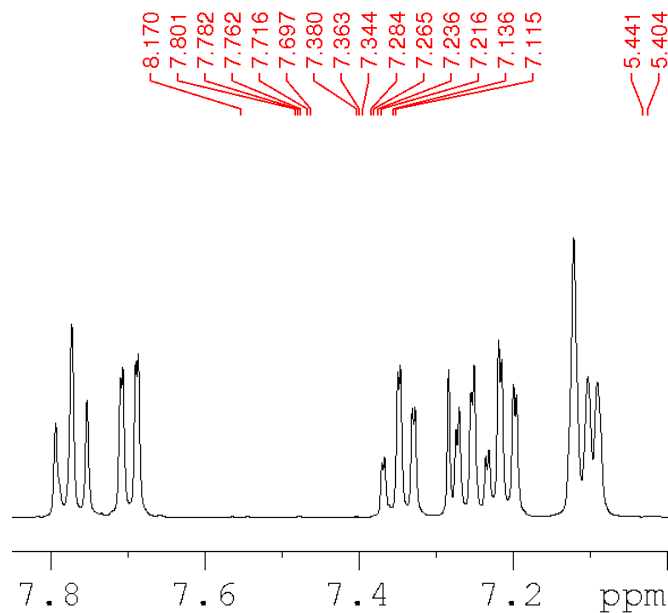
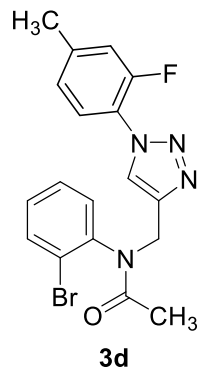
133.834
131.086
130.747
130.071
128.922
127.790
125.889

43.475

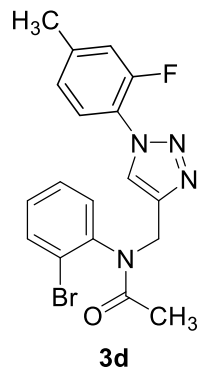
22.344

175.0 150.0 125.0 100.0 75.0 50.0 25.0 ppm

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



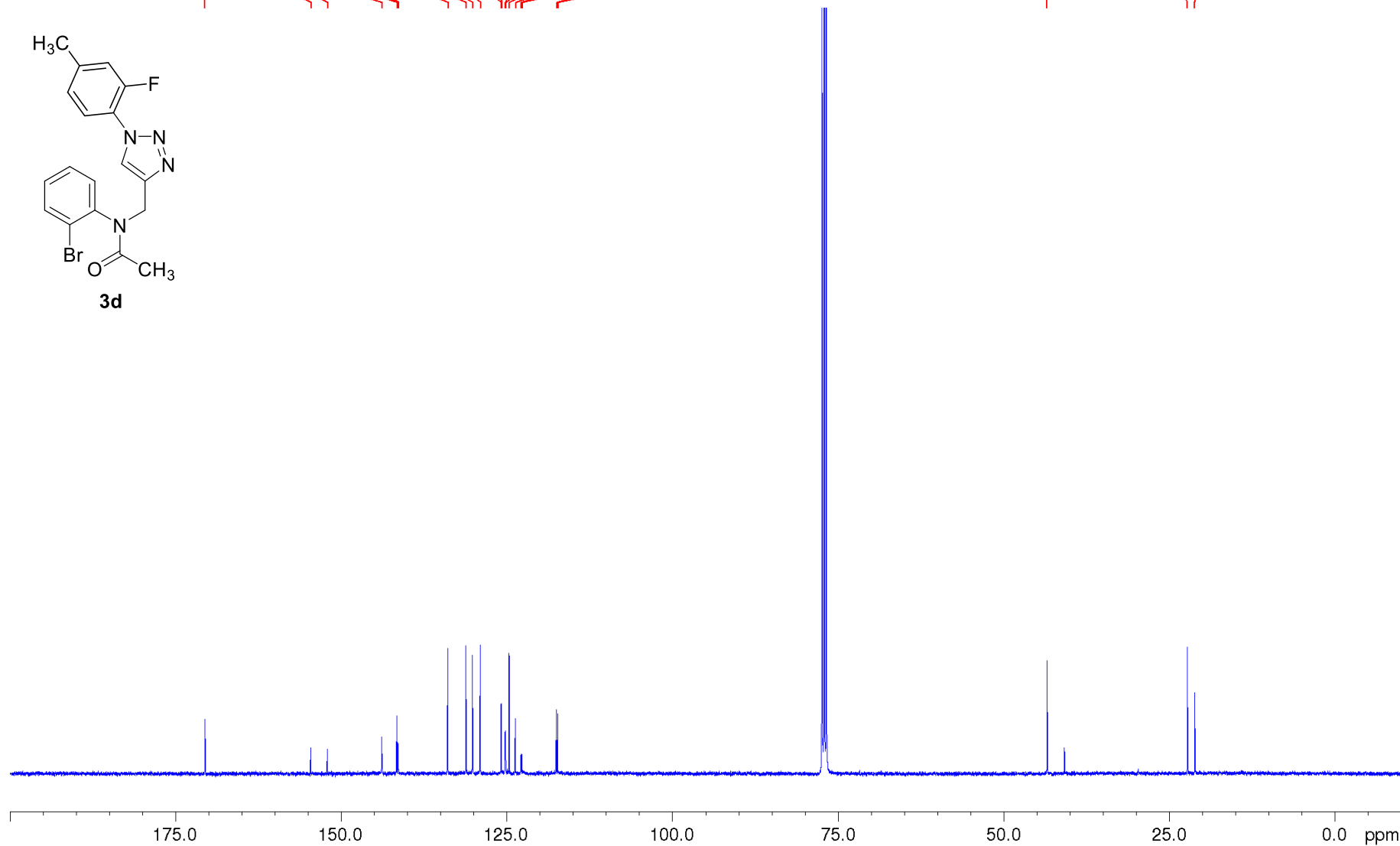
^{13}C NMR-spectrum (100 MHz, CDCl_3)



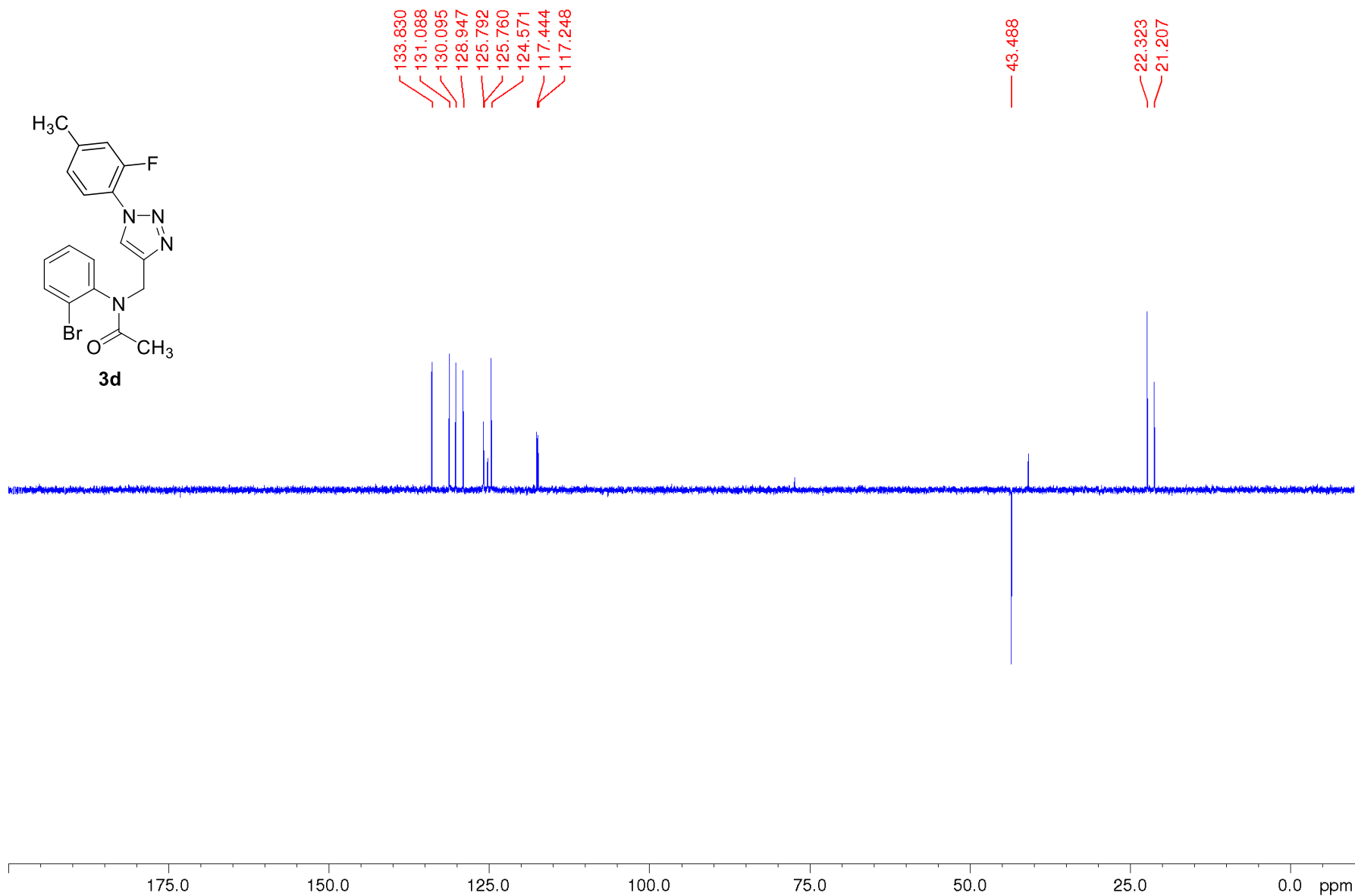
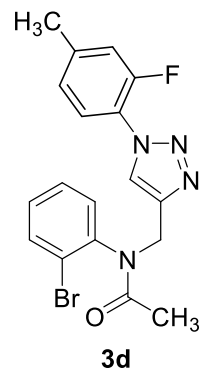
170.548
154.506
152.012
143.797
141.523
141.374
141.298
133.832
131.087
130.098
128.950
125.794
125.763
125.177
125.104
124.572
123.662
122.776
122.670
117.445
117.250

43.484

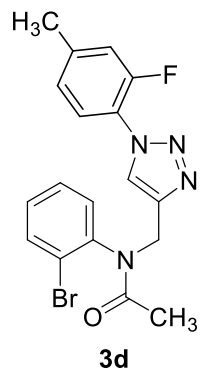
22.322
21.205



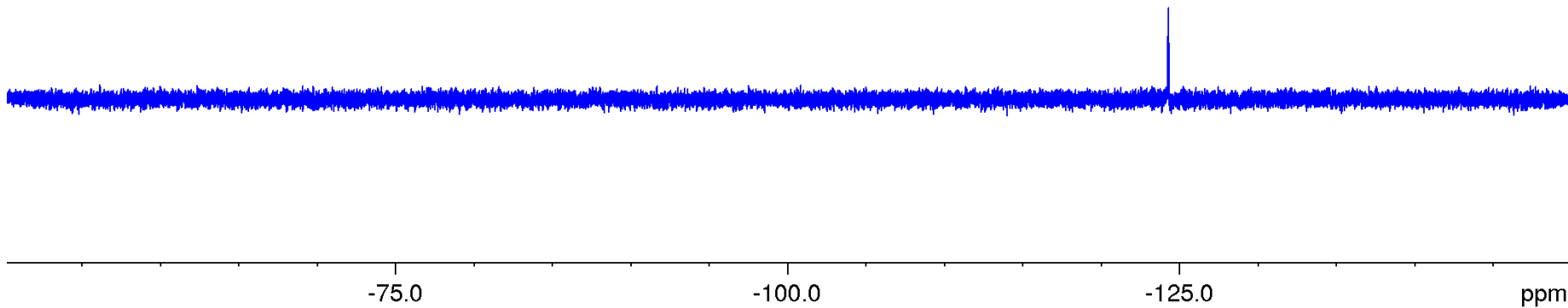
DEPT 135 NMR-spectrum (CDCl_3)



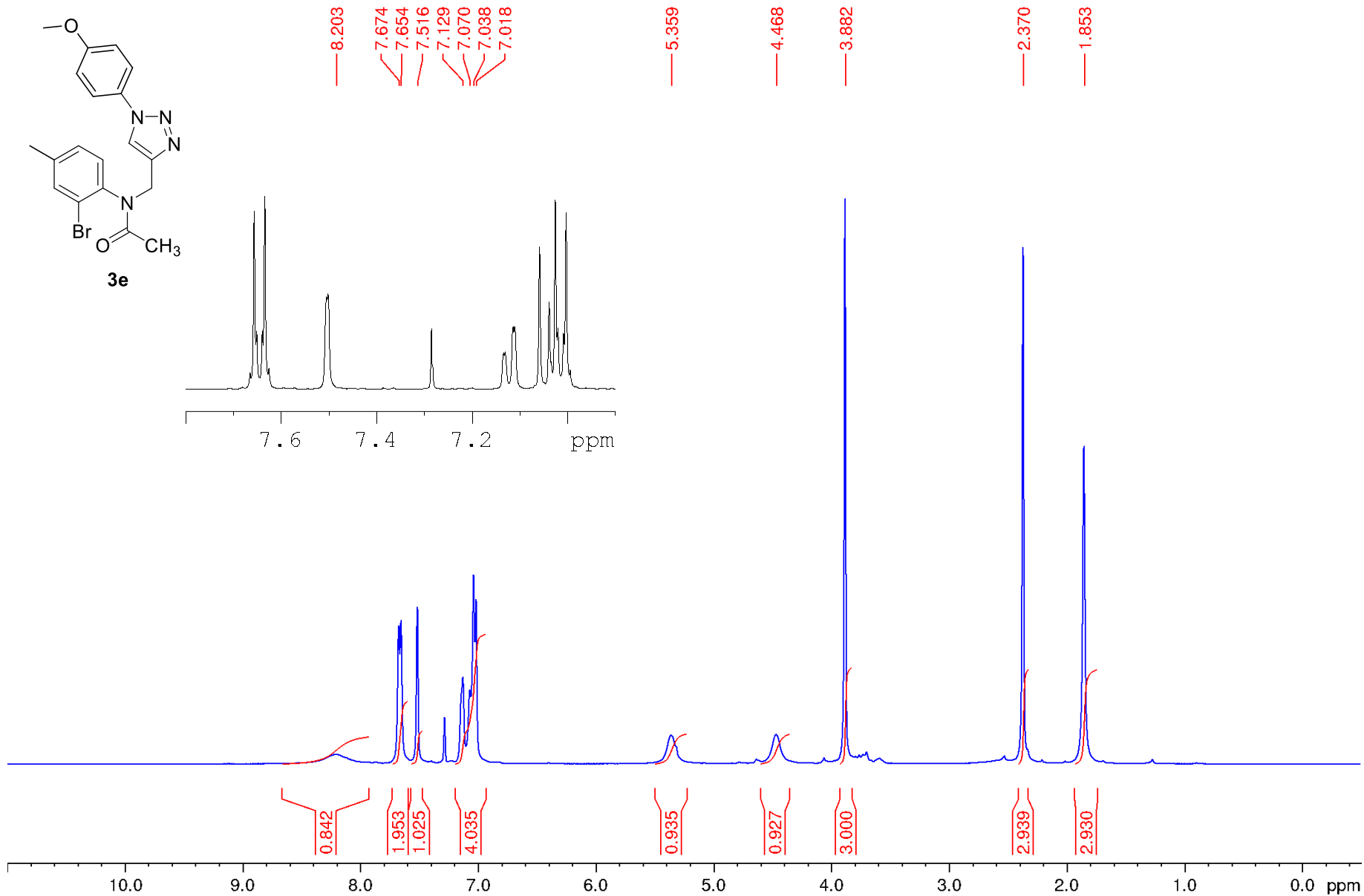
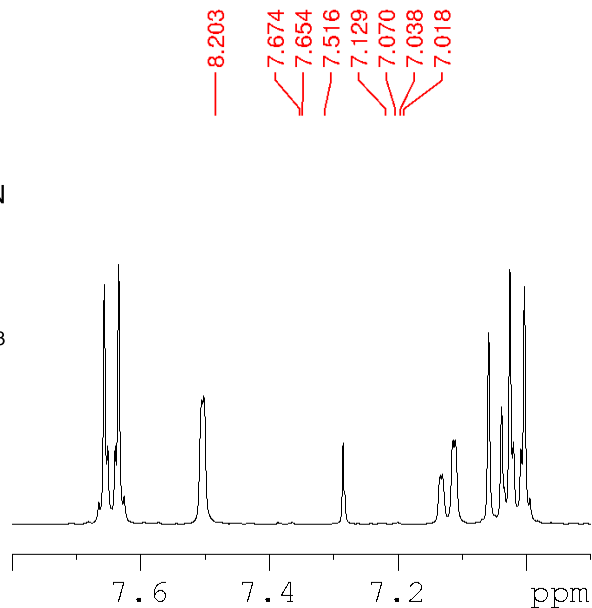
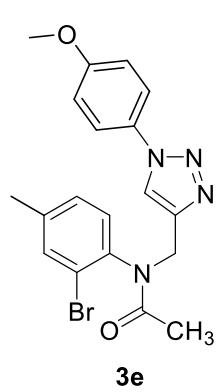
^{19}F NMR-spectrum (376.5 Hz, CDCl_3)



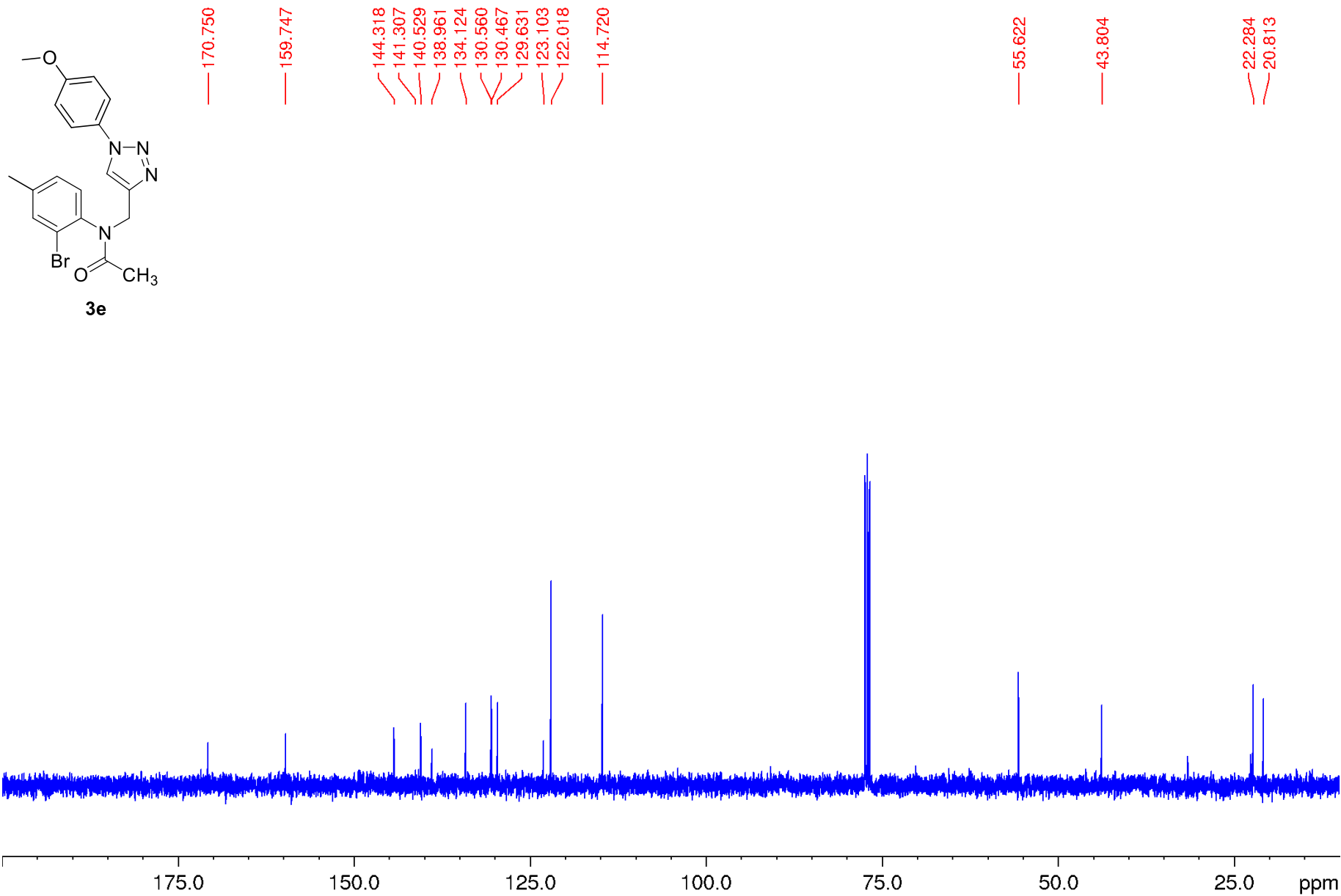
-124.298
-124.327
-124.351



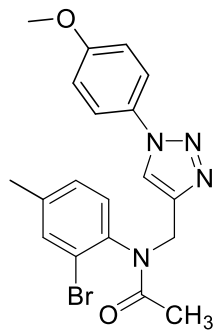
^1H NMR-spectrum (400 MHz, CDCl_3)



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



DEPT 135 NMR-spectrum (CDCl₃)



3e

134.134
130.458
129.643
122.060
122.030
114.724

55.630

43.796

22.293
20.827

175.0

150.0

125.0

100.0

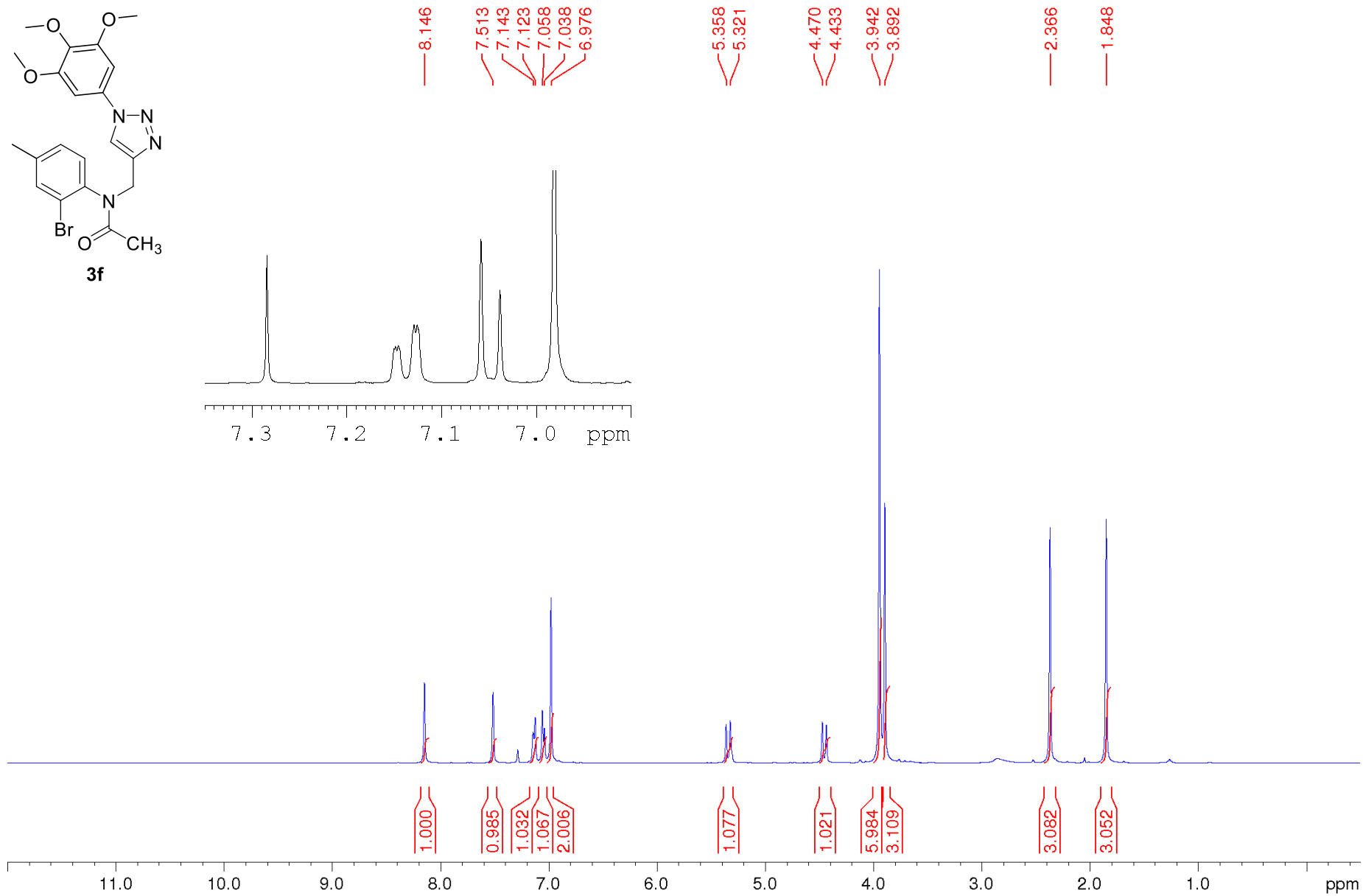
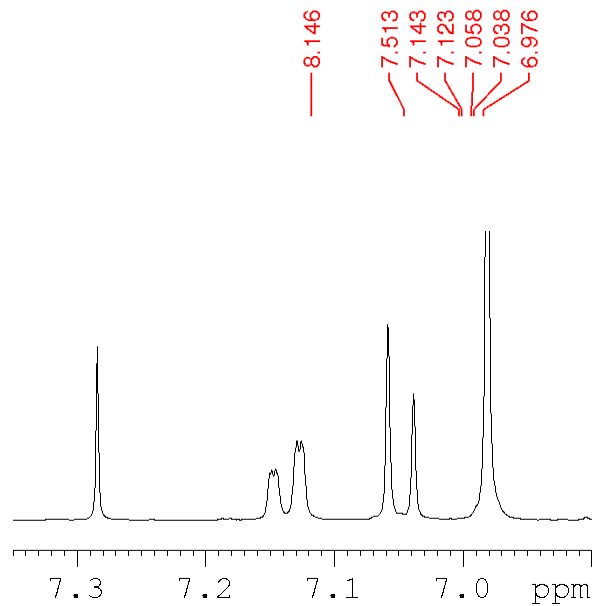
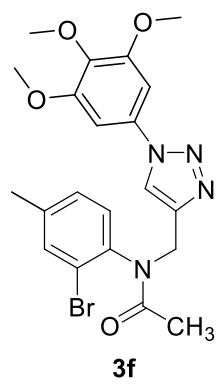
75.0

50.0

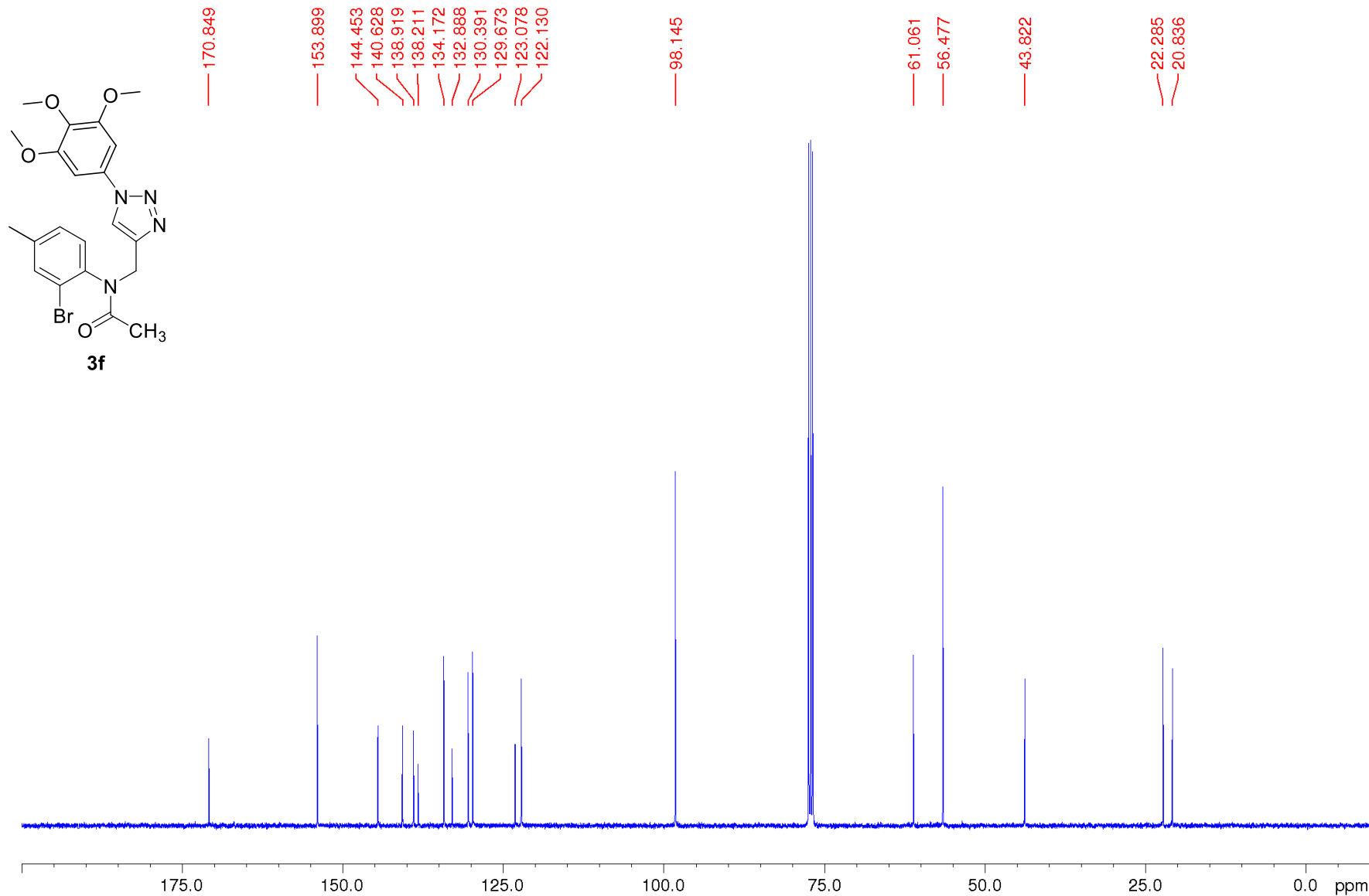
25.0

ppm

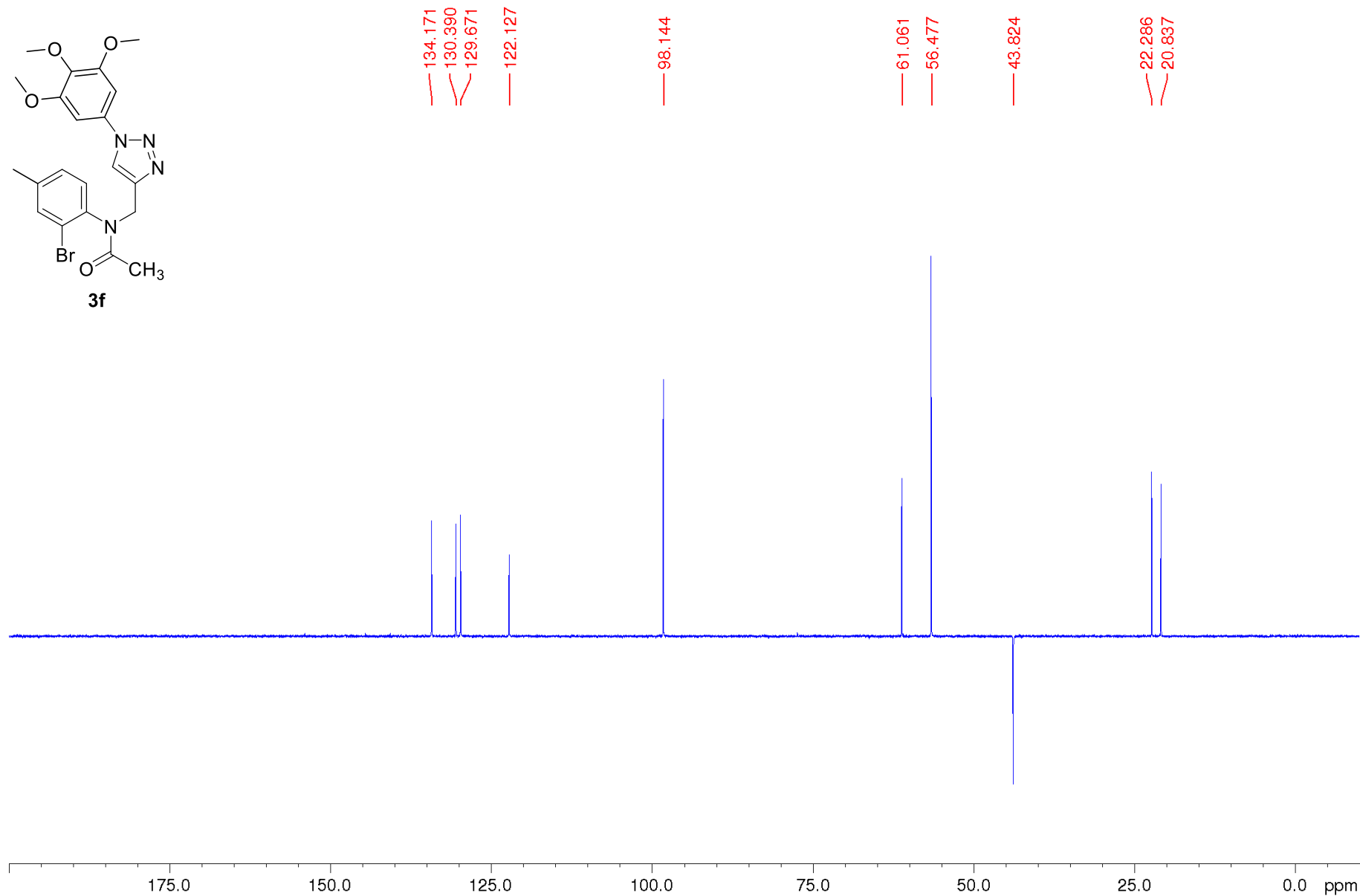
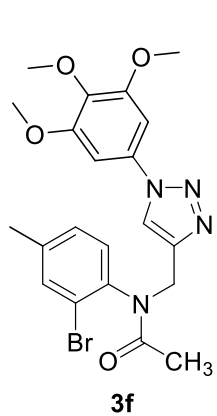
^1H NMR-spectrum (400 MHz, CDCl_3)



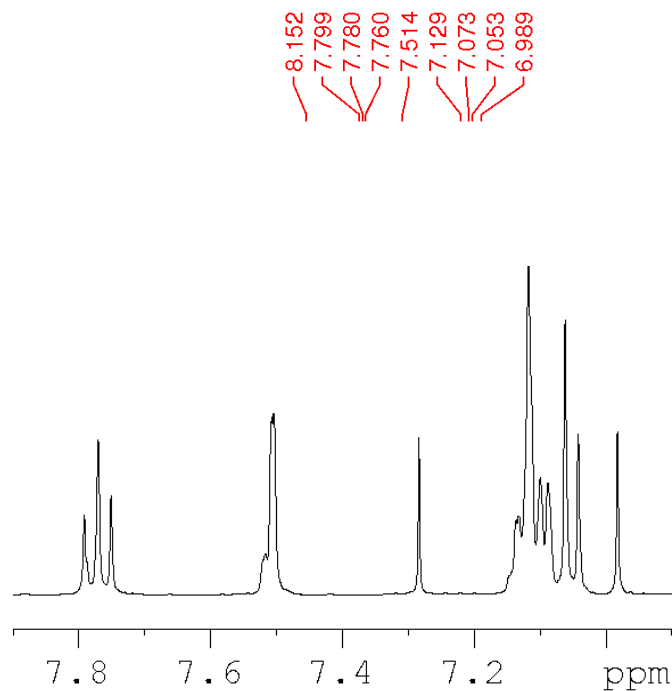
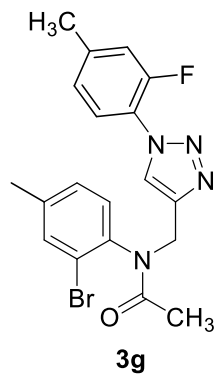
^{13}C NMR-spectrum (100 MHz, CDCl_3)



DEPT 135 NMR-spectrum (CDCl_3)



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

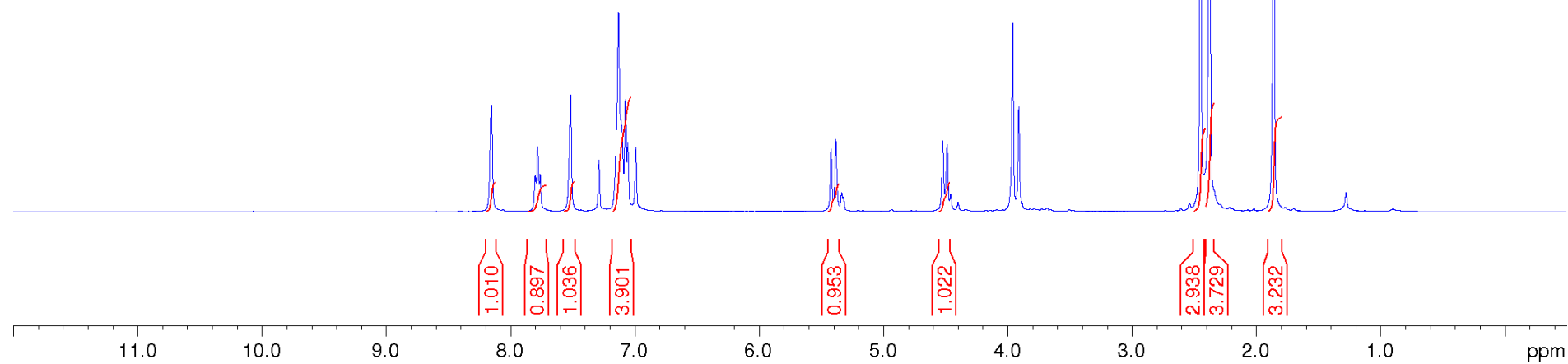


5.418
5.380

4.520
4.484

2.445
2.372

1.856



1.010

0.897

1.036

3.901

0.953

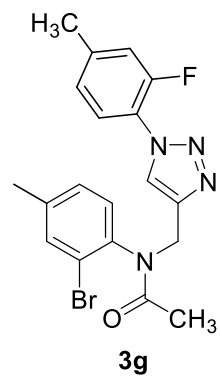
1.022

2.938

3.729

3.232

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



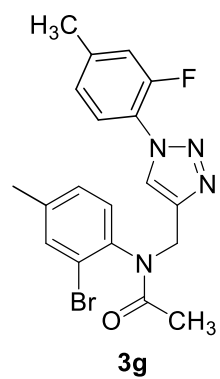
170.715
154.497
153.918
152.004
143.962
141.260
141.185
140.540
138.843
134.150
130.530
129.627
125.762
125.730
125.049
124.975
124.575
123.190
117.424
117.230
98.166

43.518

22.292
21.195
20.833

ppm

DEPT 135 NMR-spectrum (CDCl_3)



134.149
130.530
129.625
125.760
125.728
124.574
117.423
117.228

43.519

22.293
21.195
20.833

175.0

150.0

125.0

100.0

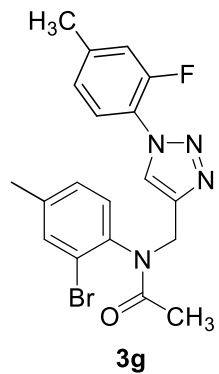
75.0

50.0

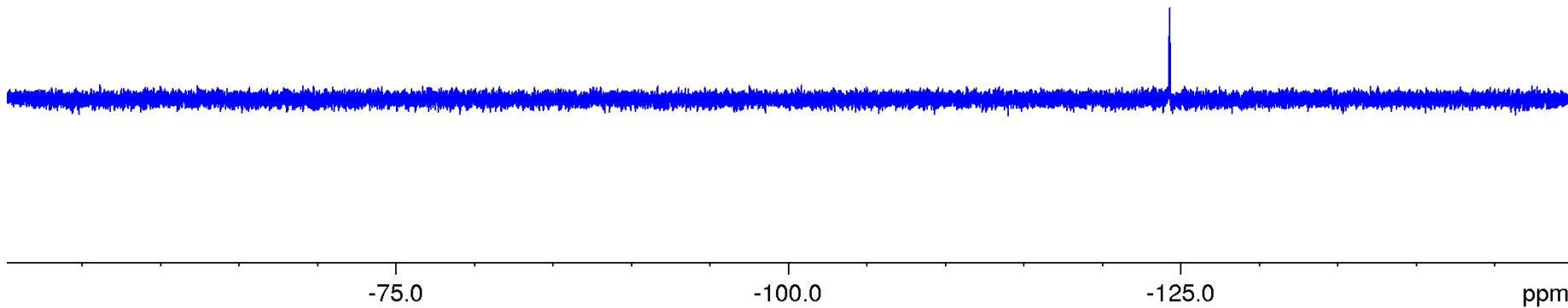
25.0

ppm

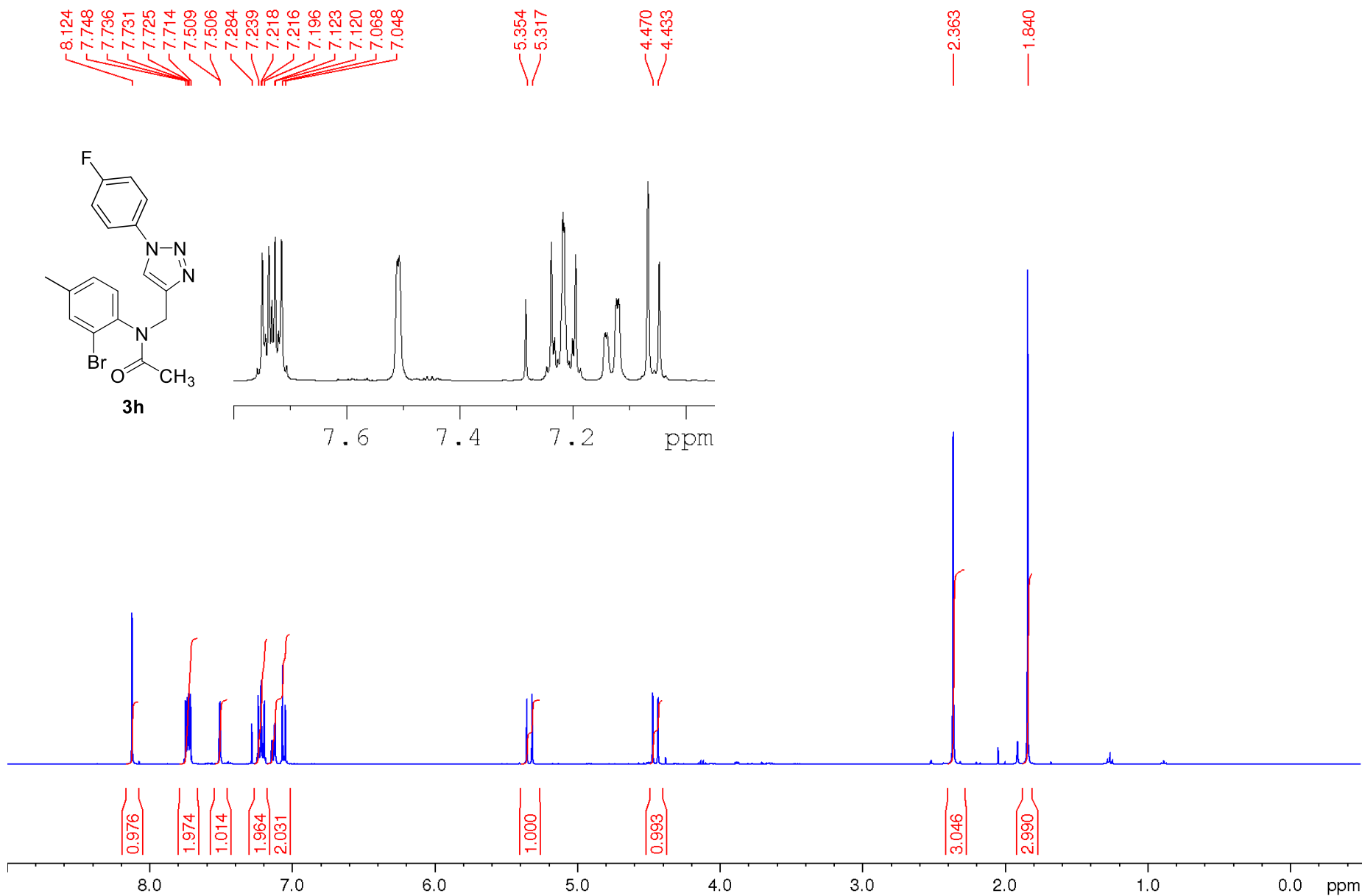
^{19}F NMR-spectrum (376.5 Hz, CDCl_3)



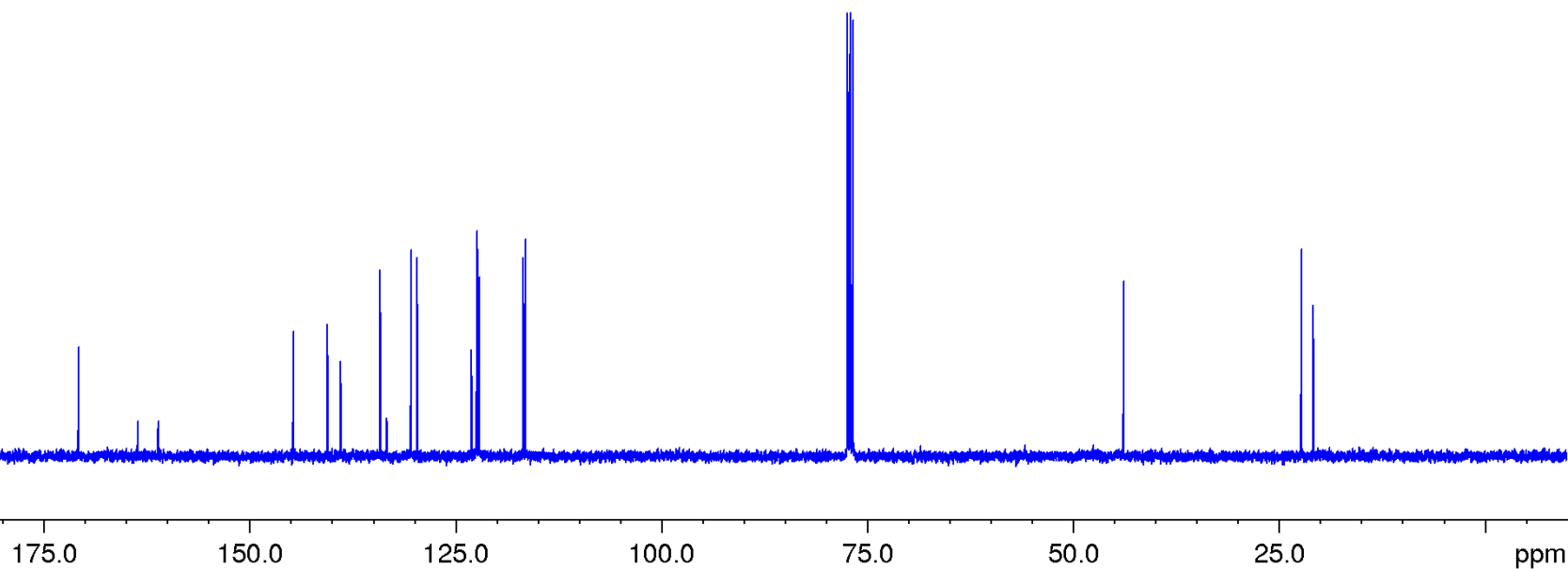
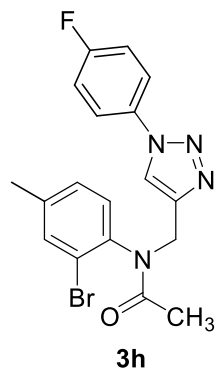
-124.298
-124.327
-124.351



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



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

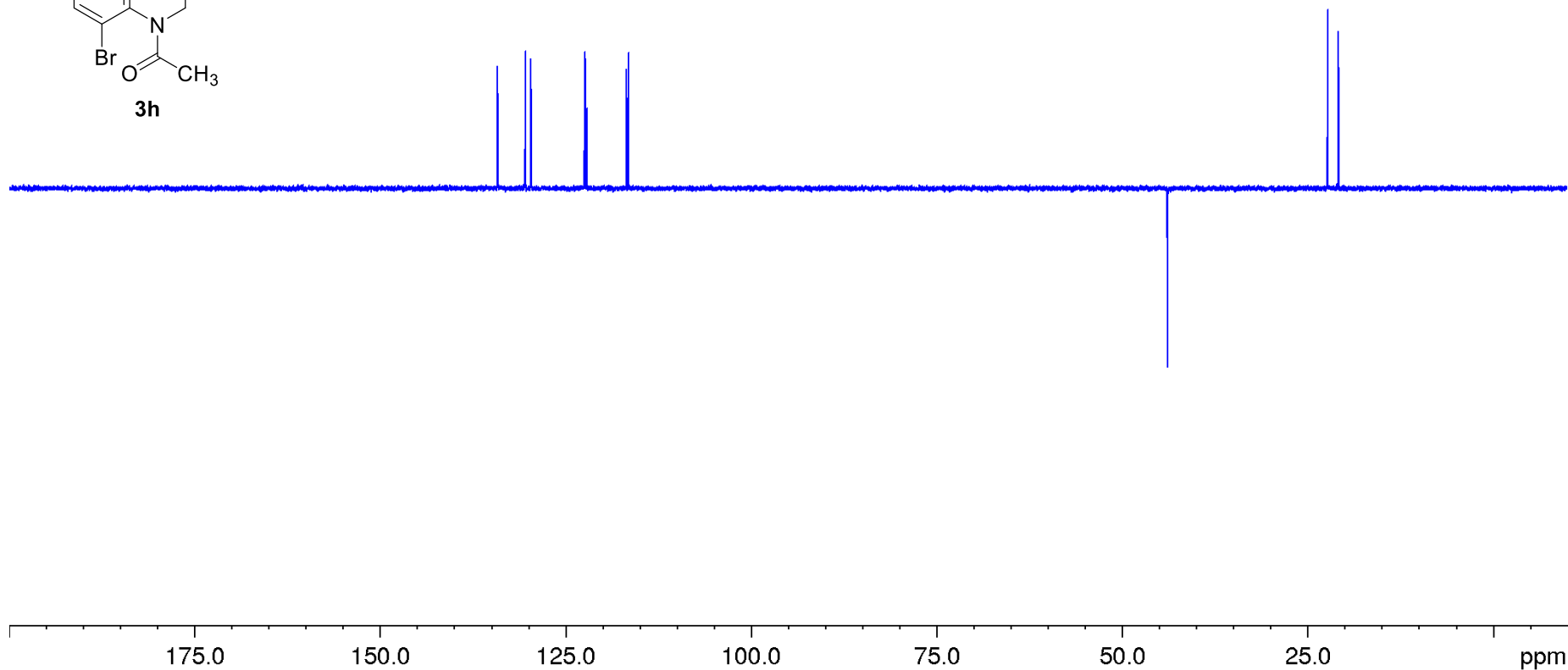
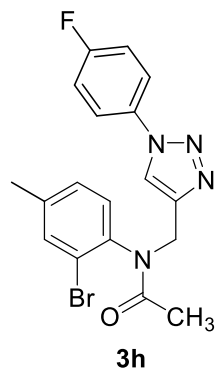


DEPT 135 NMR-spectrum (CDCl_3)

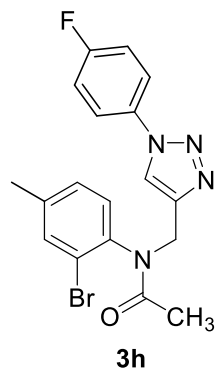
134.158
130.401
129.664
122.410
122.323
122.119
116.772
116.541

43.838

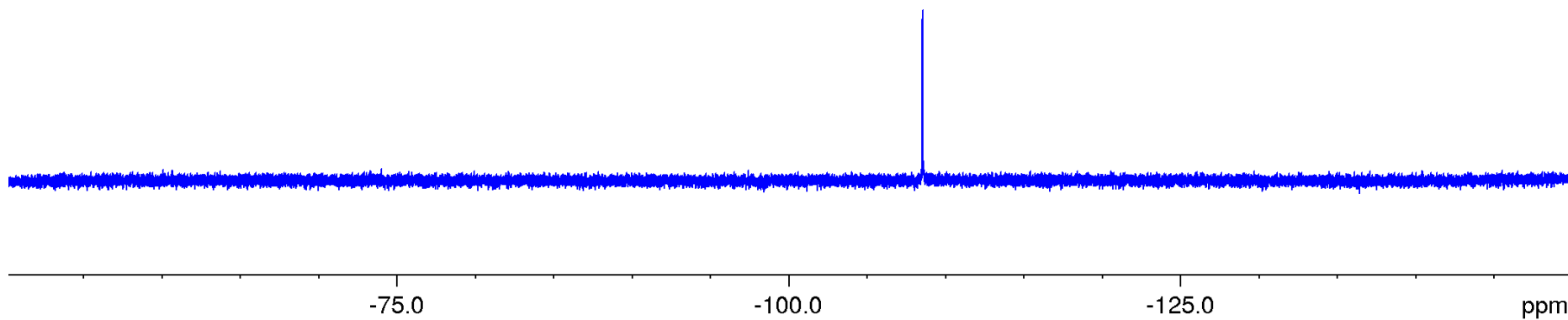
22.271
20.819



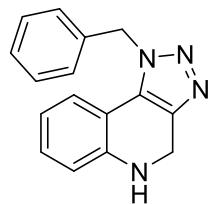
^{19}F NMR-spectrum (376.5 Hz, CDCl_3)



-108.547
-108.558
-108.569
-108.591

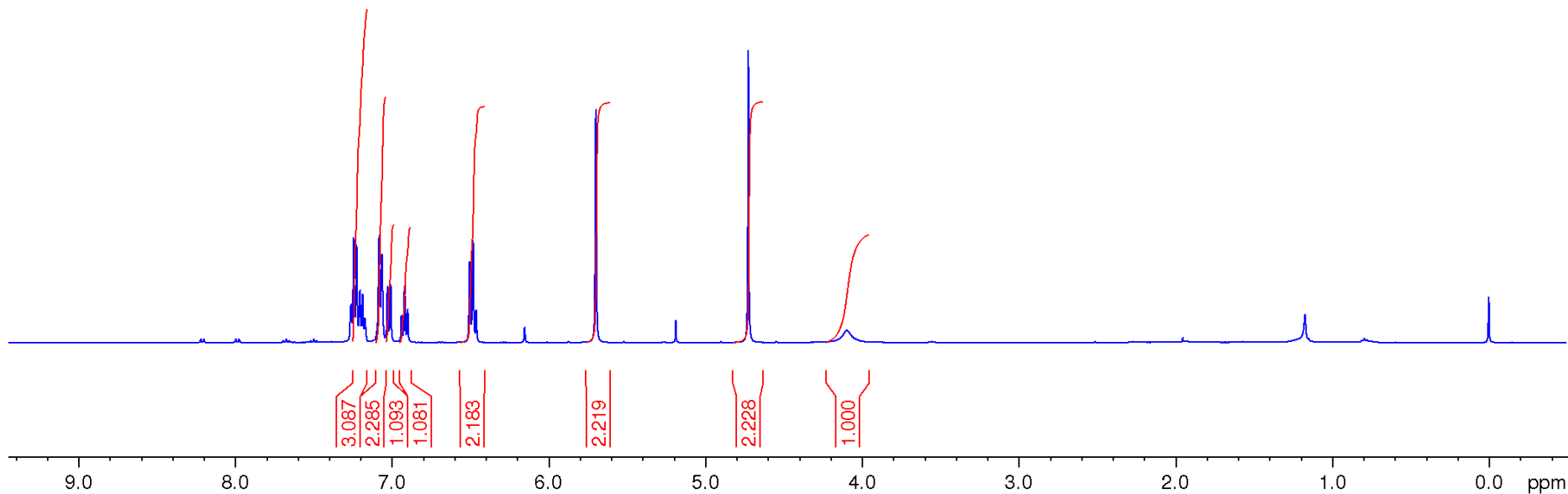
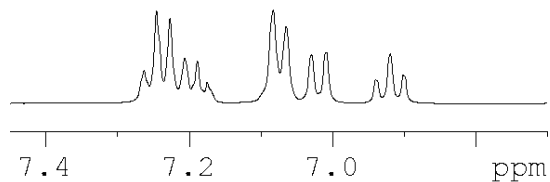


^1H NMR-spectrum (400 MHz, CDCl_3)

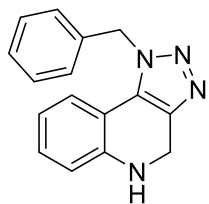


4a

7.262
7.244
7.225
7.205
7.187
7.173
7.081
7.063
7.028
7.008
6.940
6.937
6.919
6.901
6.504
6.482
6.462
5.699
— 4.725
— 4.096



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

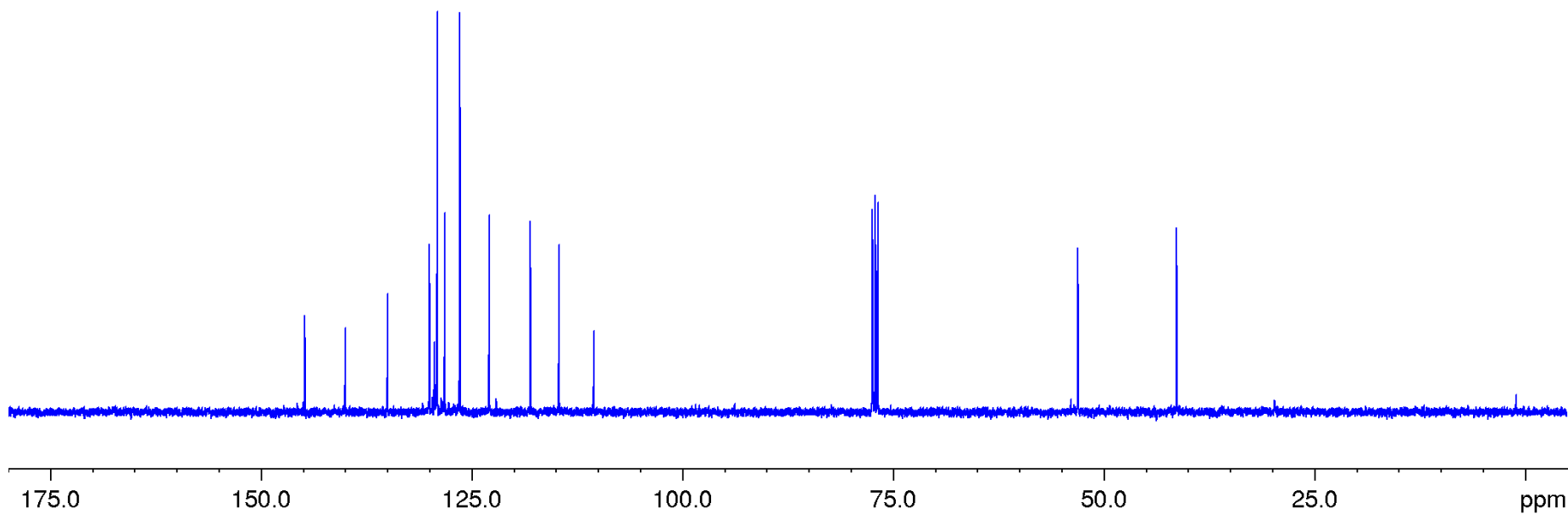


4a

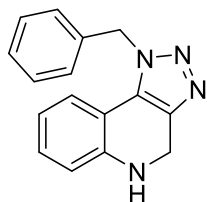
144.813
140.005
134.987
130.026
129.431
129.095
128.177
126.414
122.920
118.051
114.626
110.505

53.063

41.344



DEPT 135 NMR-spectrum (CDCl₃)

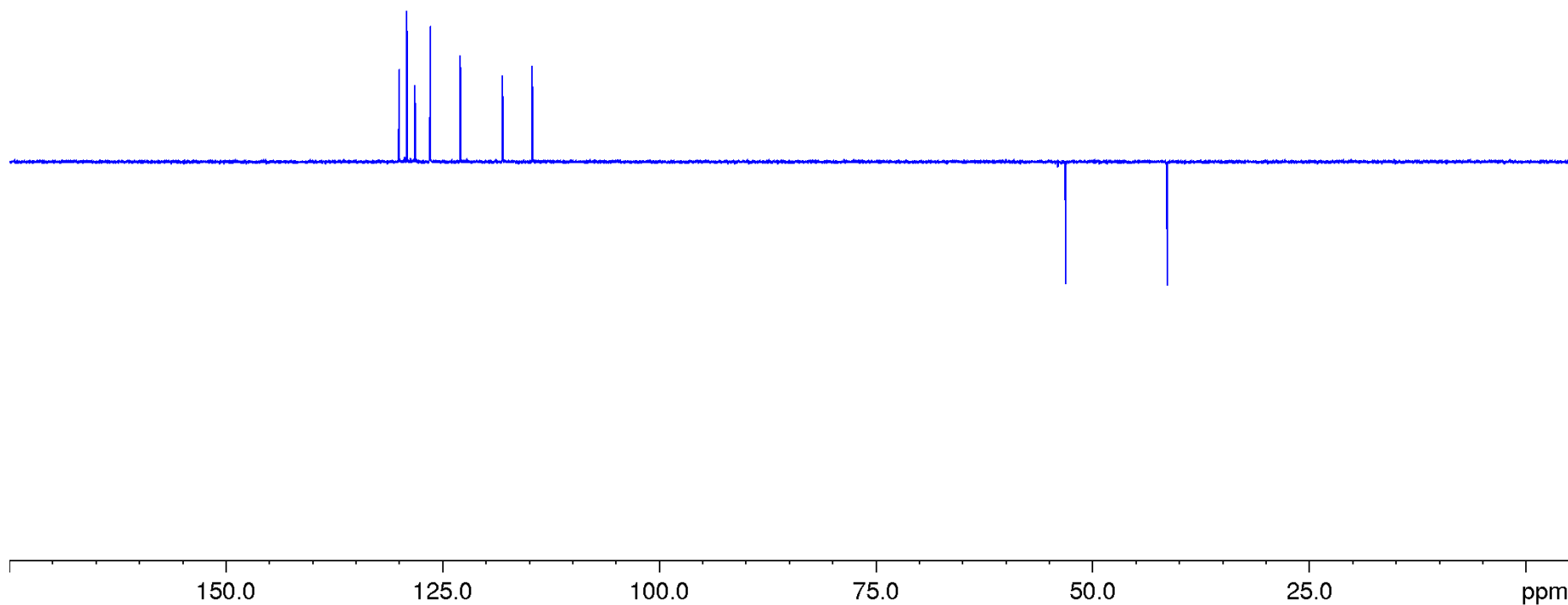


4a

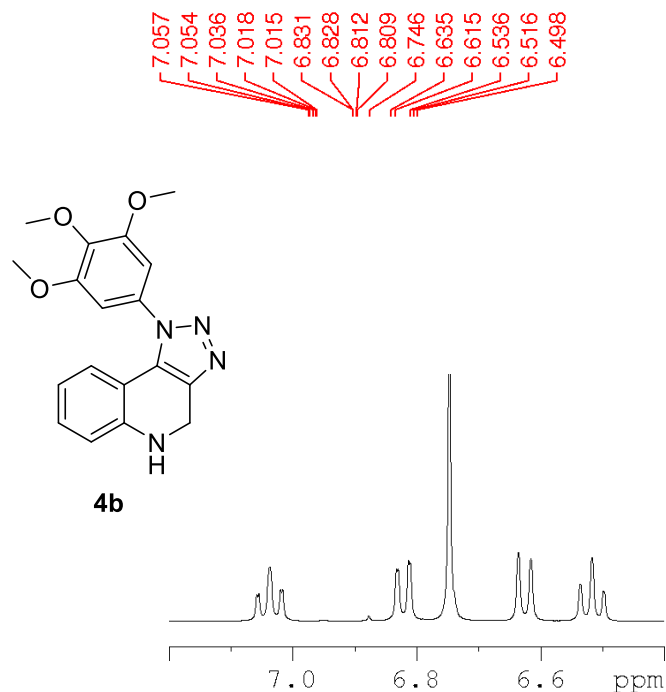
130.014
129.089
128.171
126.414
122.920
118.073
114.622

53.068

41.351



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



4.869

3.937
3.844

8.0

7.0

6.0

5.0

4.0

3.0

2.0

1.0

0.0

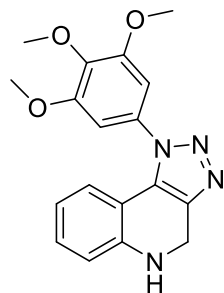
ppm

1.000
0.994
1.979
1.015
1.001

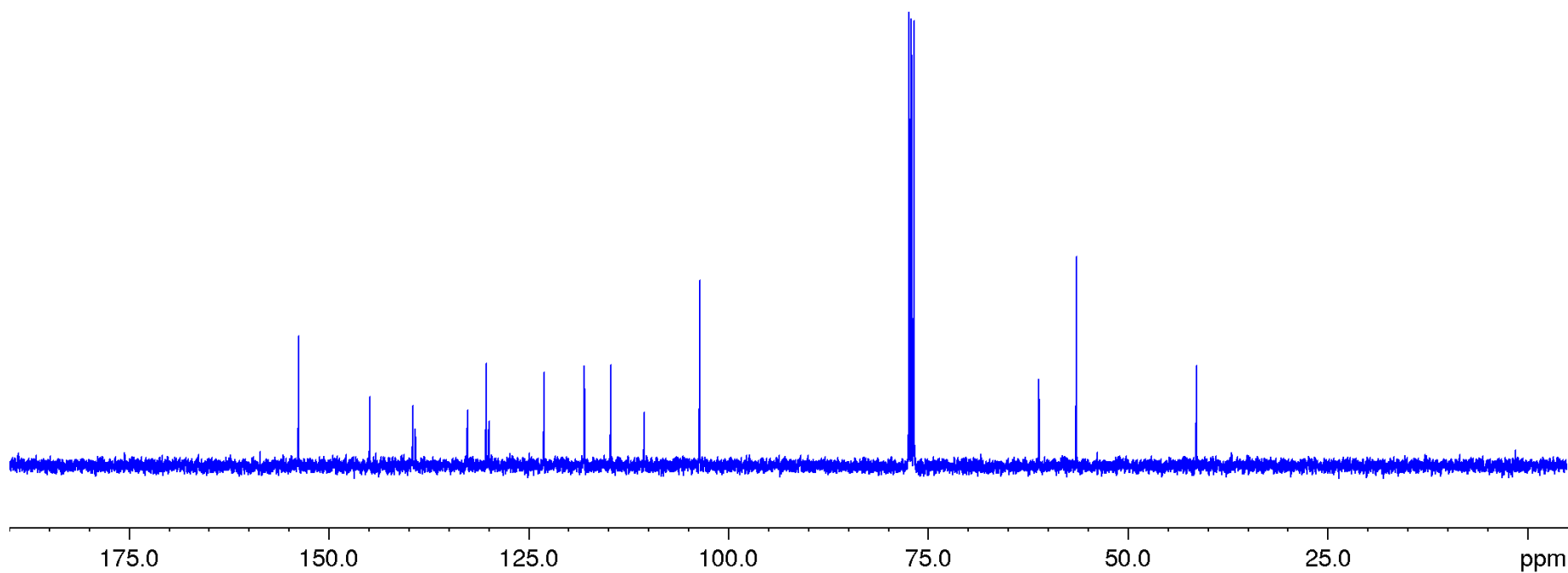
2.001

0.863
3.063
5.989

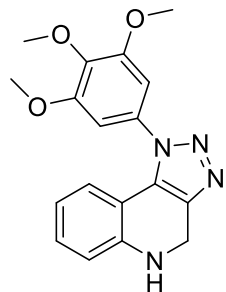
^{13}C NMR-spectrum (100 MHz, CDCl_3)



4b

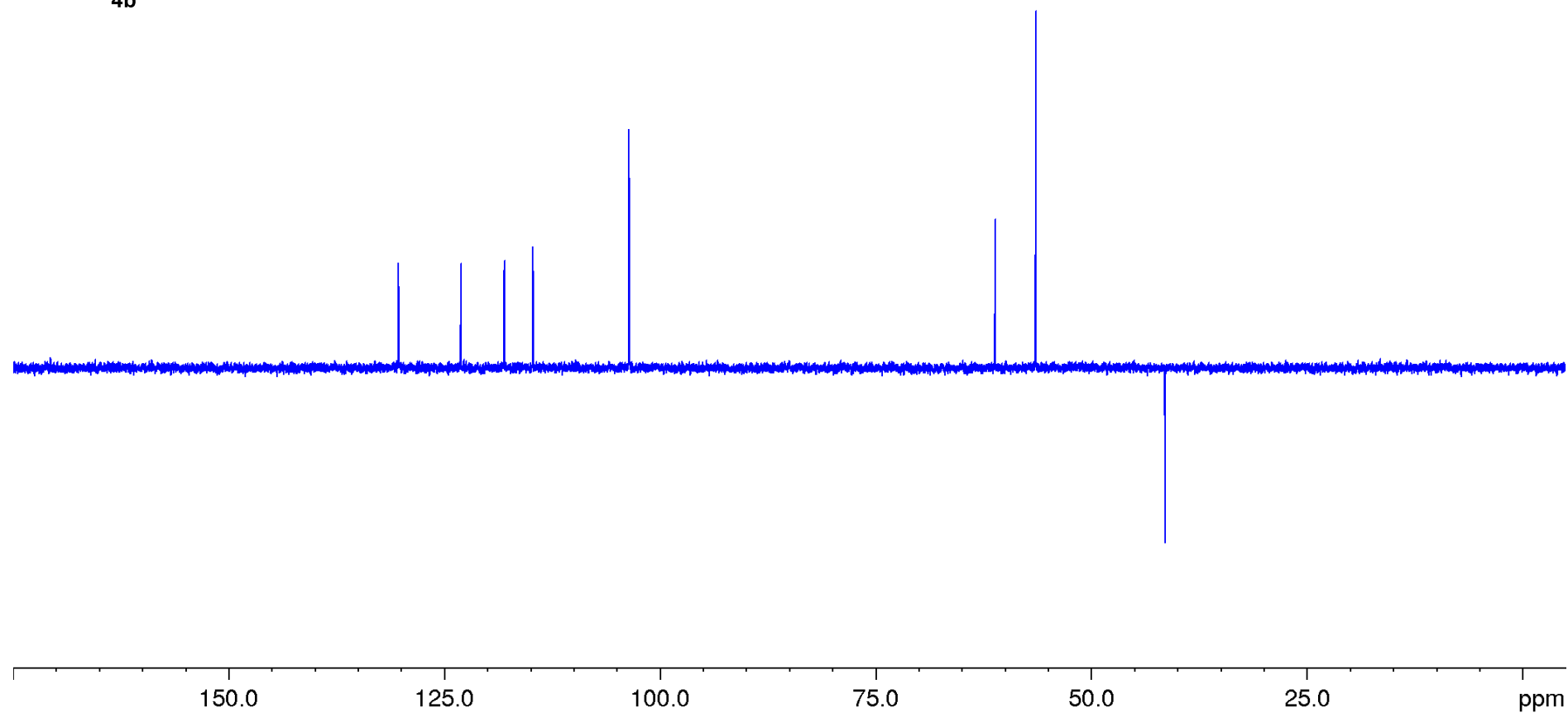


DEPT 135 NMR-spectrum (CDCl₃)

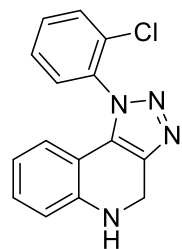


4b

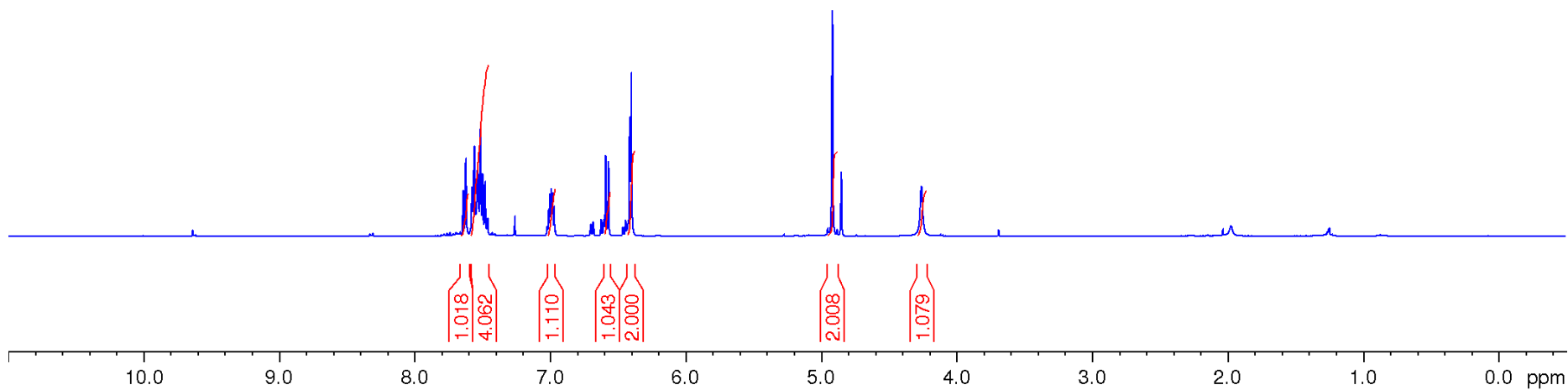
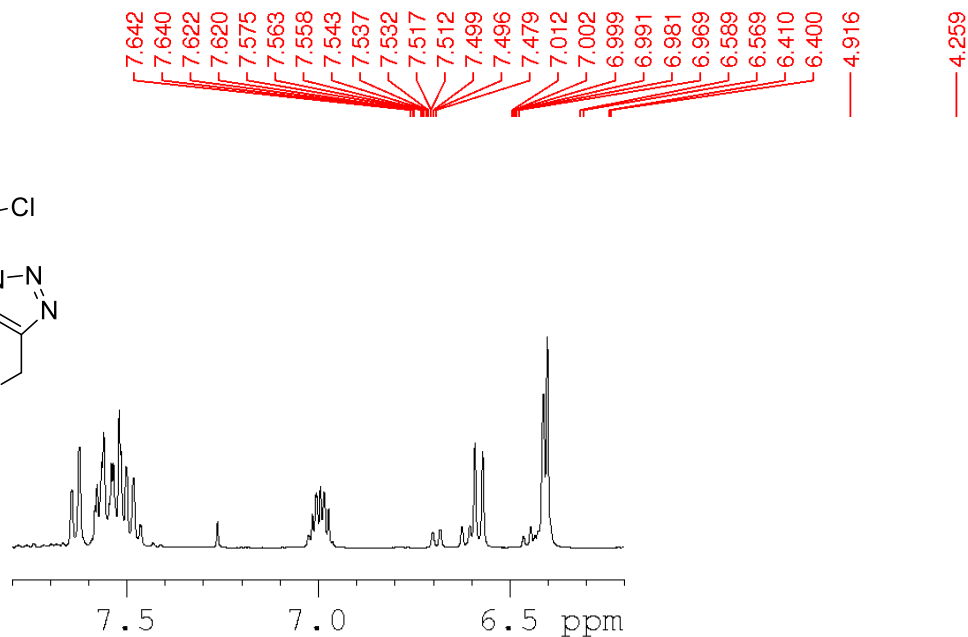
130.295
123.071
118.030
114.703
103.562
61.133
56.415
41.404



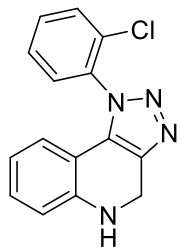
^1H NMR-spectrum (400 MHz, CDCl_3)



4c



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



4c

144.735
138.572
135.178
131.890
130.737
130.435
129.671
129.263
128.086
126.063
122.076
117.845
114.455
110.056

41.372

175.0

150.0

125.0

100.0

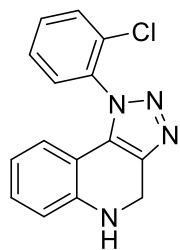
75.0

50.0

25.0

ppm

DEPT 135 NMR-spectrum (CDCl_3)



4c

131.894
130.737
130.437
129.262
128.089
122.076
117.845
114.456

41.372

175.0

150.0

125.0

100.0

75.0

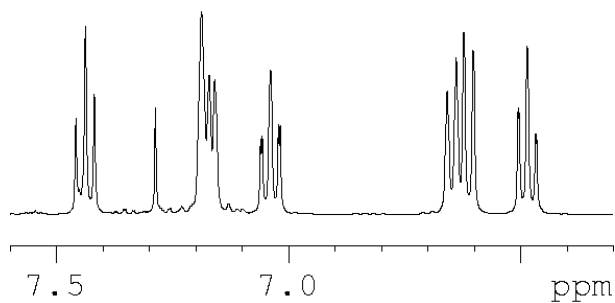
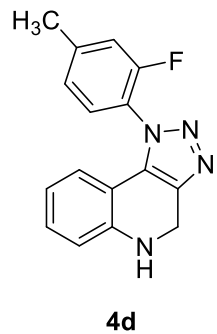
50.0

25.0

ppm

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

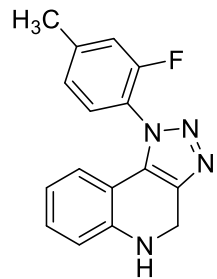
7.456
7.435
7.416
7.185
7.168
7.157
7.057
7.054
7.037
7.036
7.019
7.015
6.657
6.638
6.622
6.620
6.602
6.600
6.504
6.502
6.485
6.467
6.464
4.932
4.930
4.155
2.516



8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 ppm

0.990
2.010
1.005
1.997
1.017
2.039
1.000
3.001

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



4d

157.862
155.396
144.715
143.460
143.386
138.781
131.045
130.321
128.374
125.743
125.709
122.817
122.688
122.089
117.887
117.595
117.408
114.475
110.305

41.391

21.527

150.0

125.0

100.0

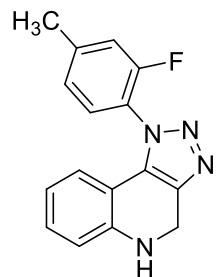
75.0

50.0

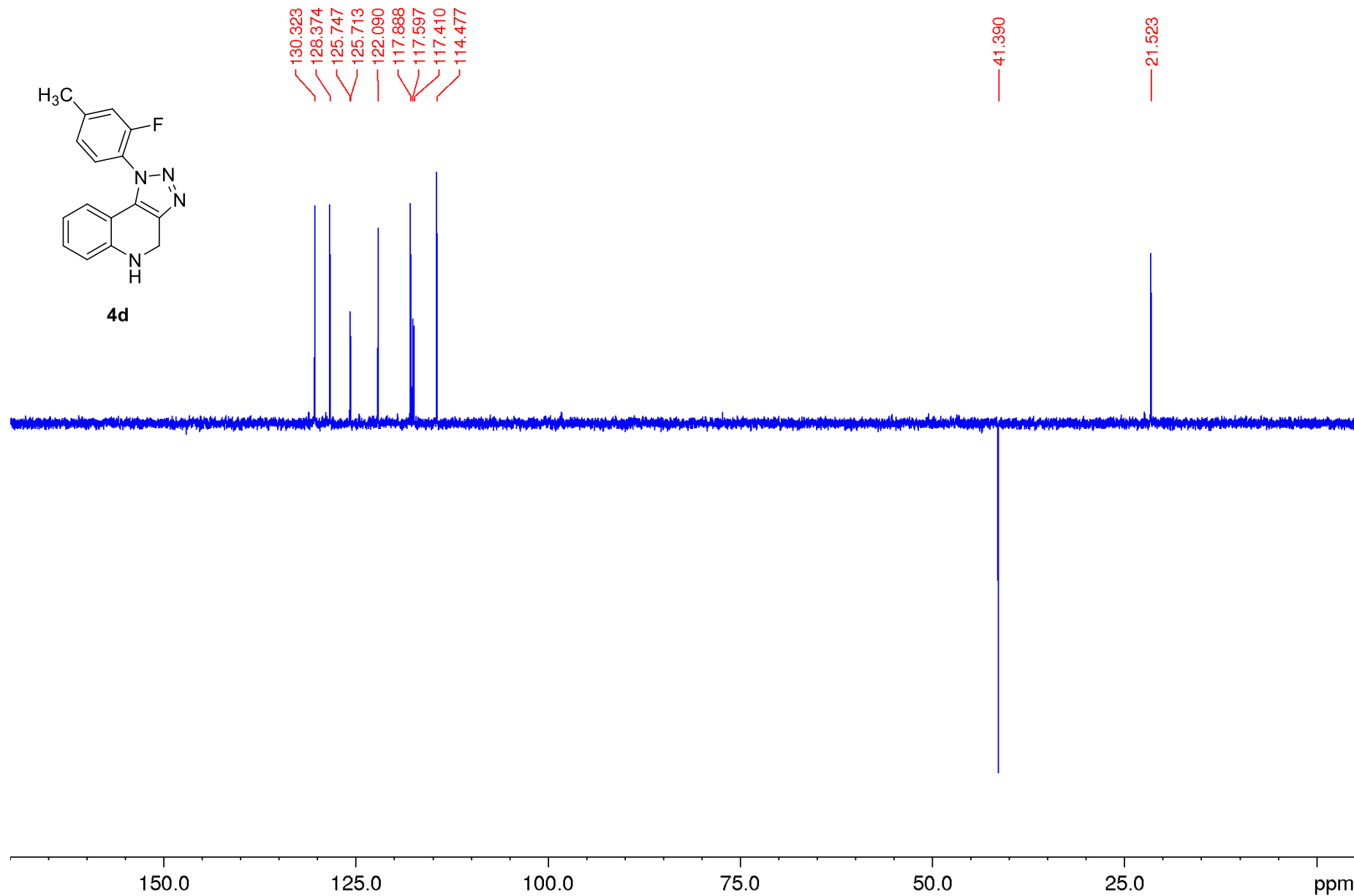
25.0

ppm

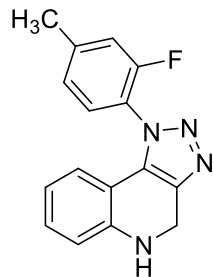
DEPT 135 NMR-spectrum (CDCl_3)



4d

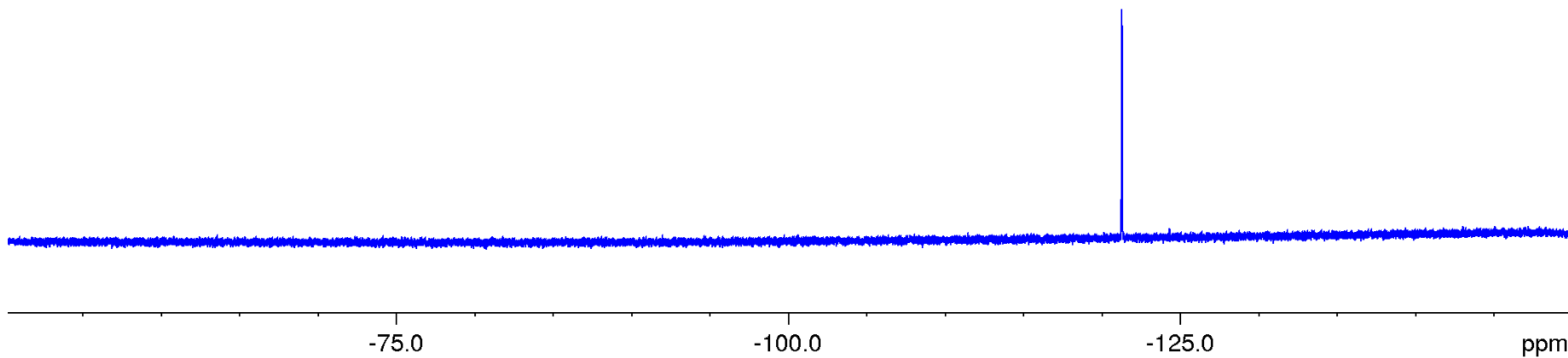


^{19}F NMR-spectrum (376.5 Hz, CDCl_3)

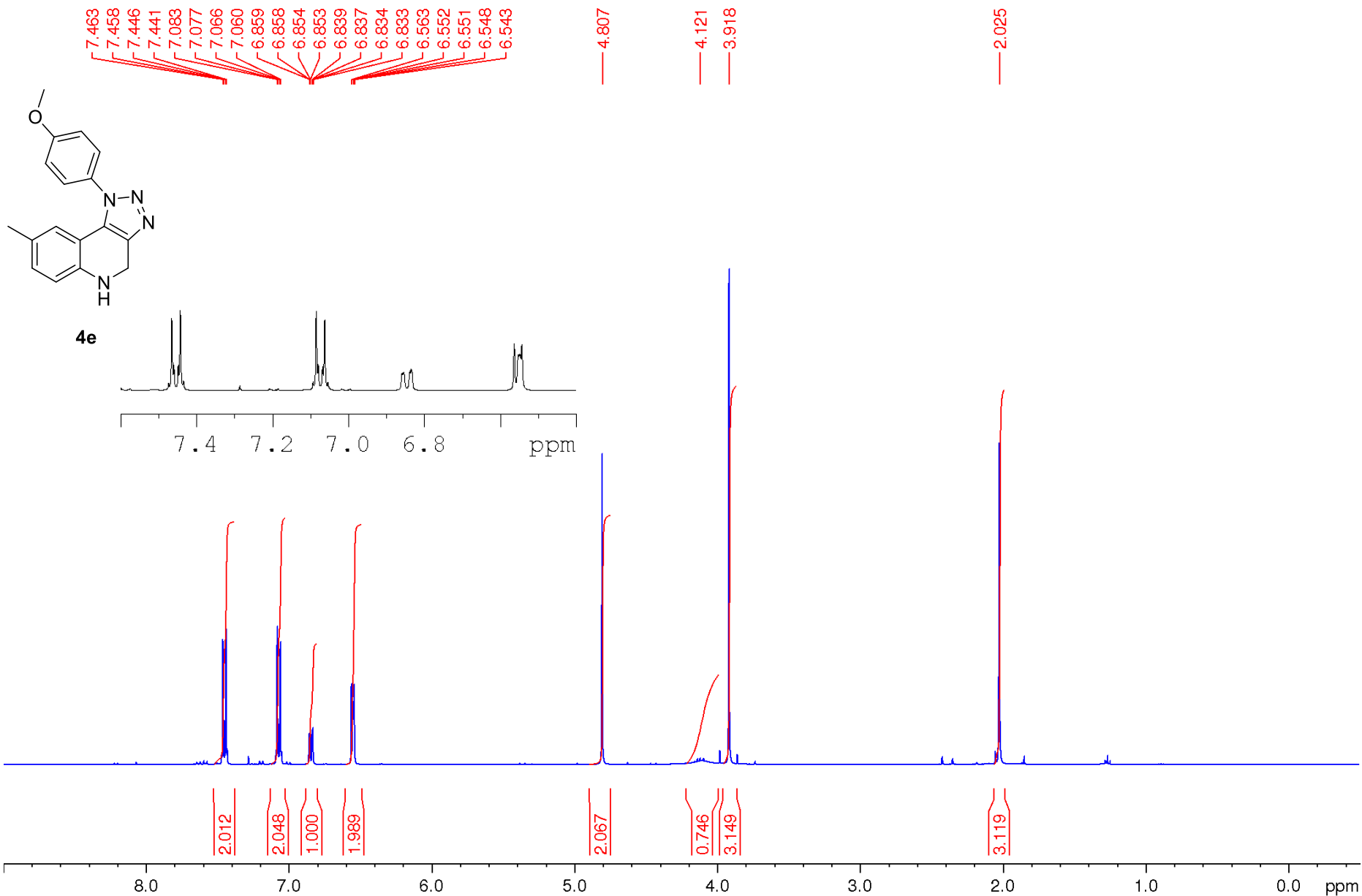


4d

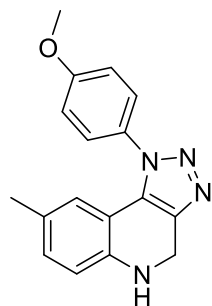
-121.270
-121.294
-121.318



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



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



4e

160.682
142.599
139.784
130.736
130.130
127.331
127.119
123.125
115.011
114.732
114.615
110.816

55.681

41.395

20.540

175.0

150.0

125.0

100.0

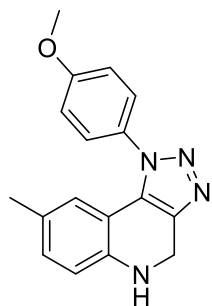
75.0

50.0

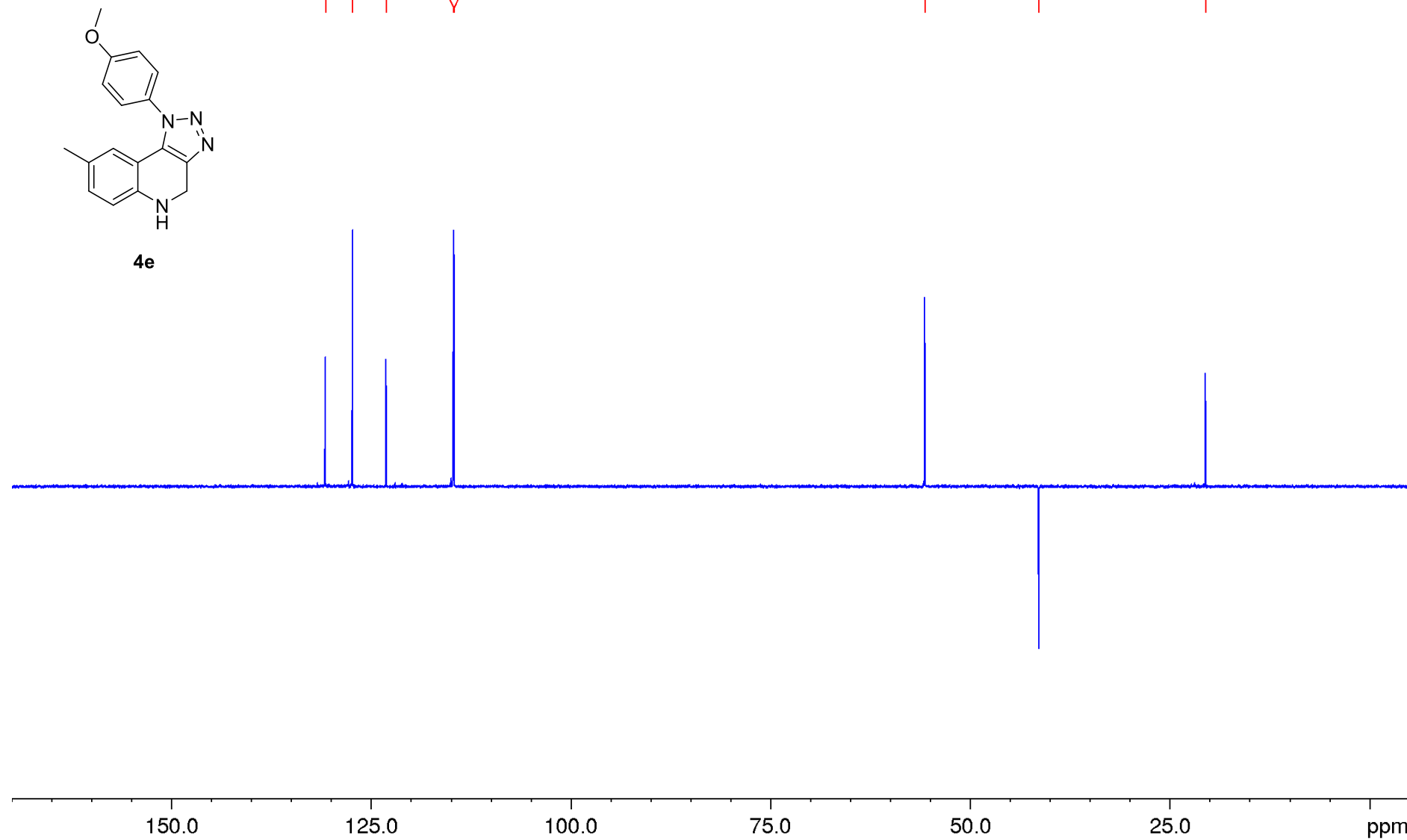
25.0

ppm

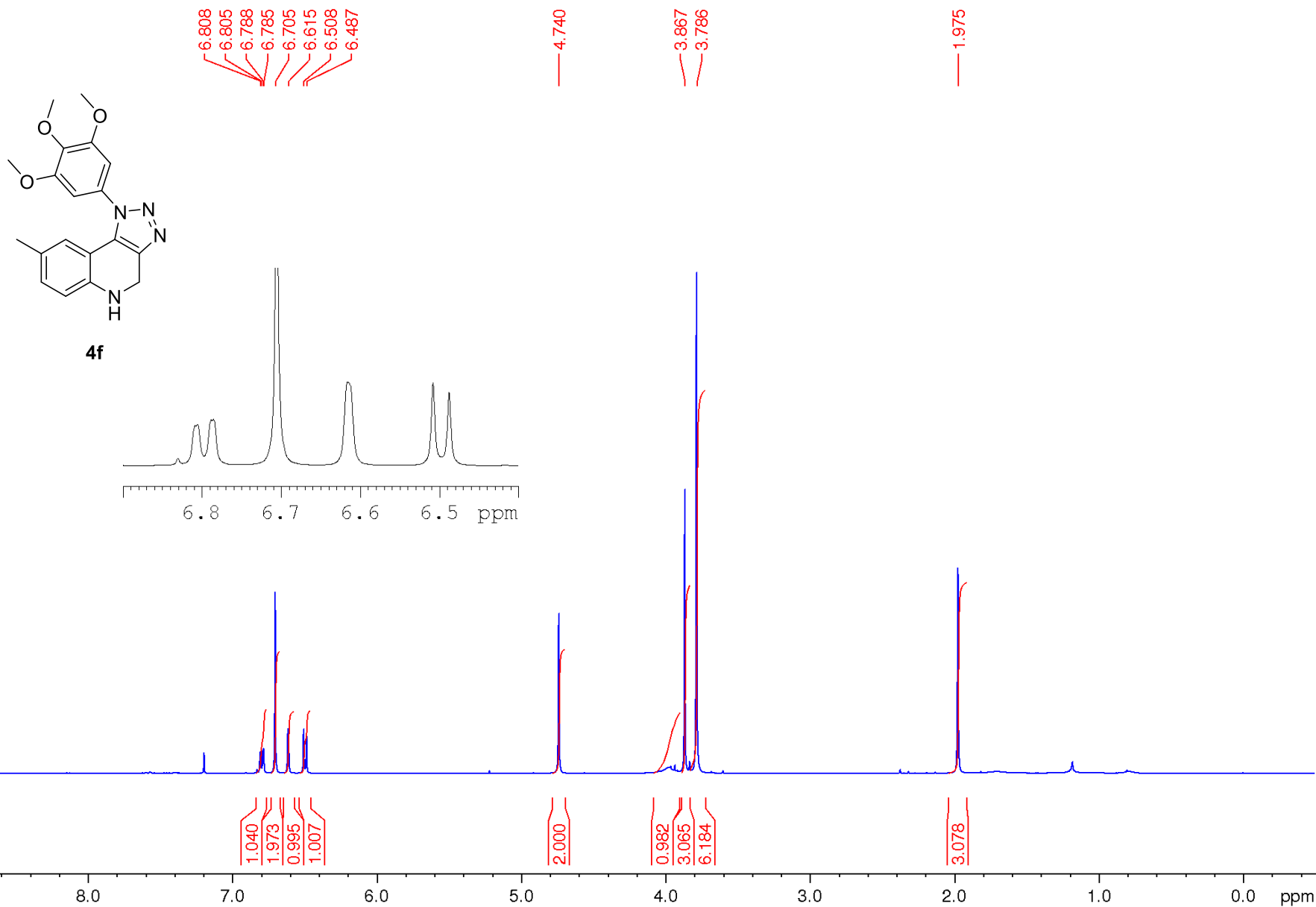
DEPT 135 NMR-spectrum (CDCl₃)



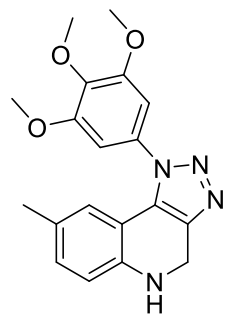
4e



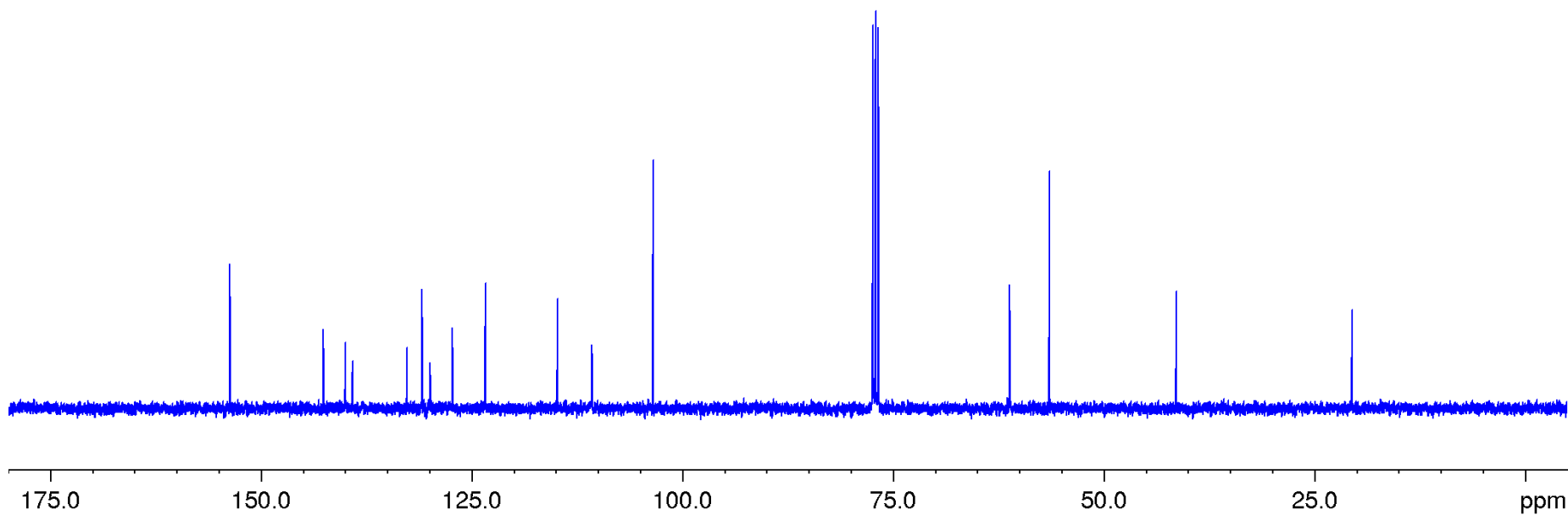
^1H NMR-spectrum (400 MHz, CDCl_3)



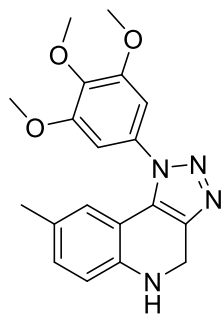
^{13}C NMR-spectrum (100 MHz, CDCl_3)



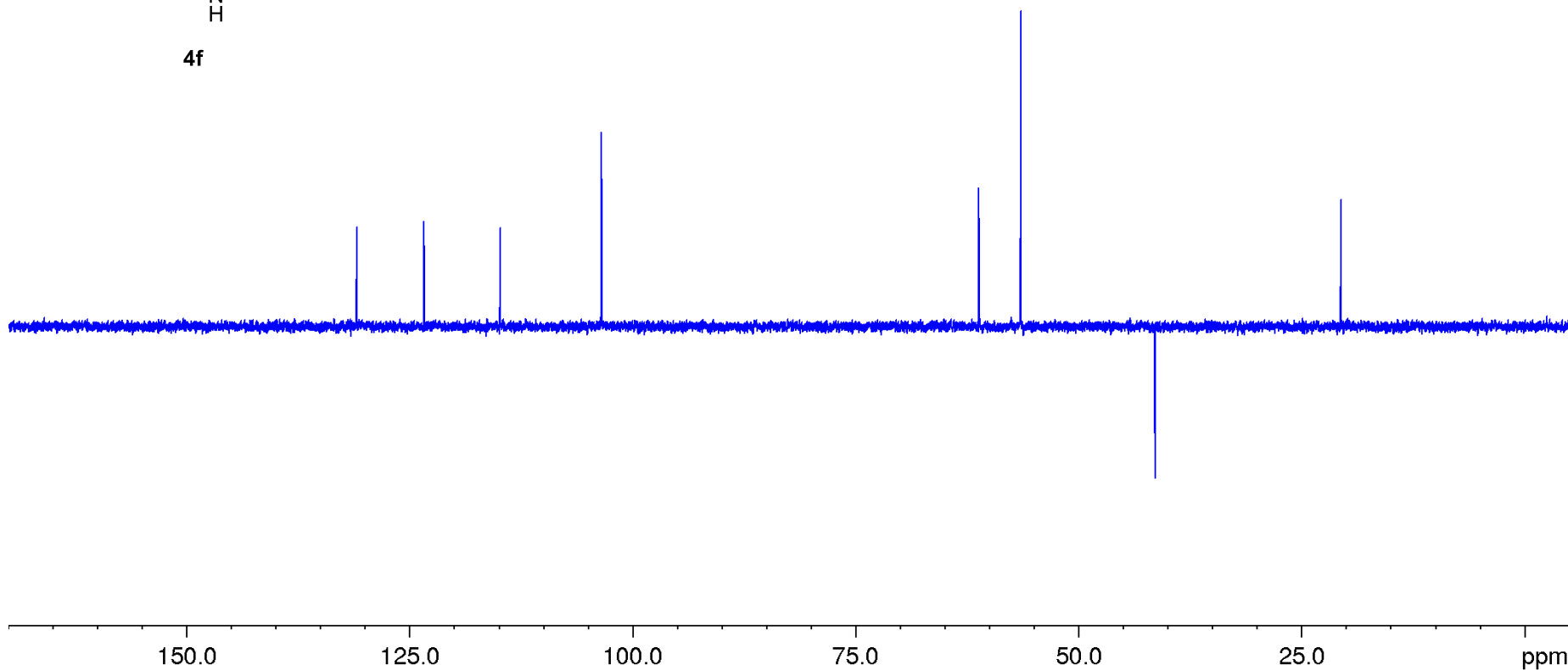
4f



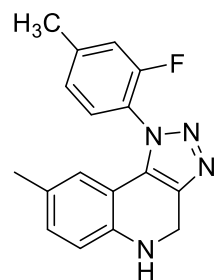
DEPT 135 NMR-spectrum (CDCl₃)



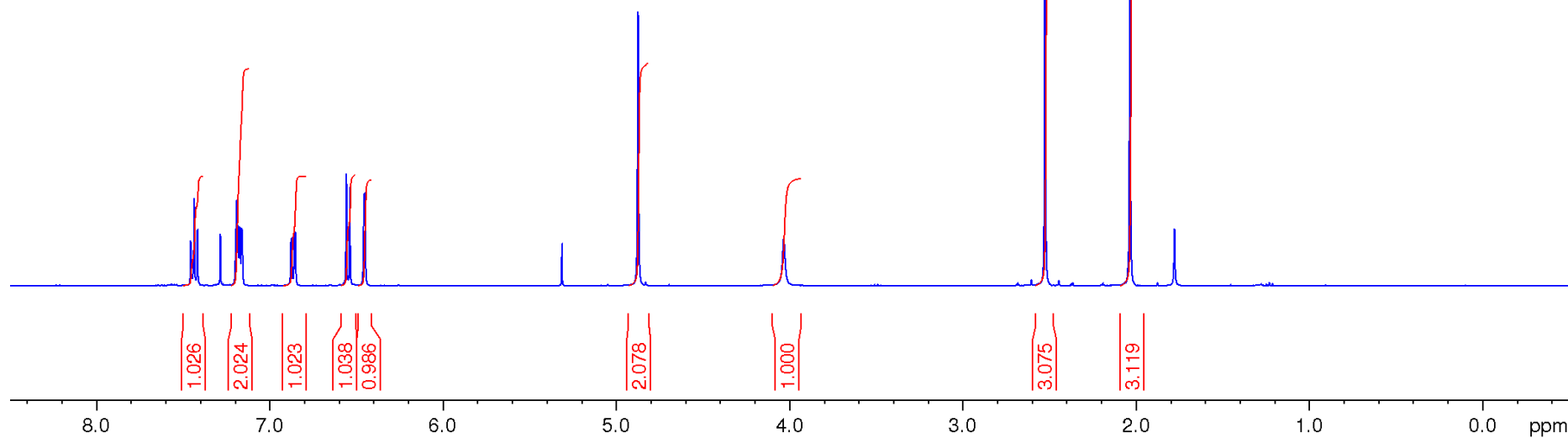
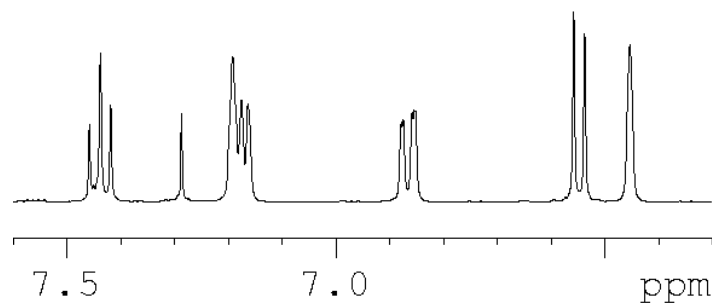
4f



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



4g

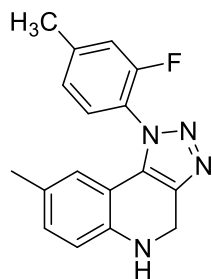


^{13}C NMR-spectrum (100 MHz, CDCl_3)

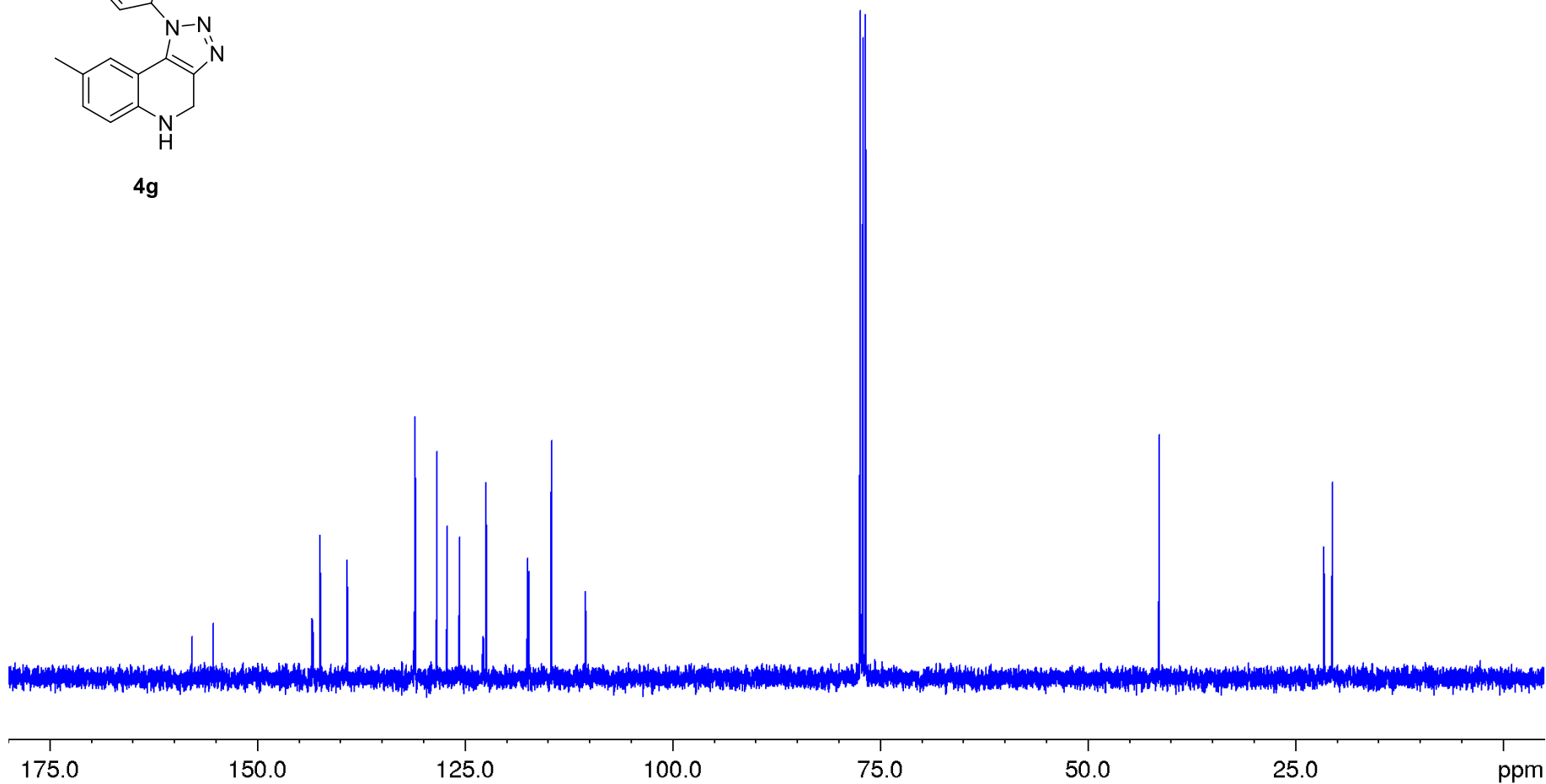
157.859
155.330
143.387
143.314
142.453
139.172
131.127
130.991
128.372
127.157
125.669
125.634
122.859
122.731
122.443
117.473
117.286
114.580
110.478

41.383

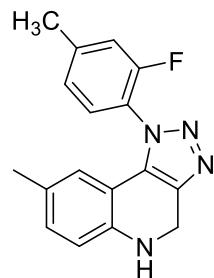
21.541
20.542



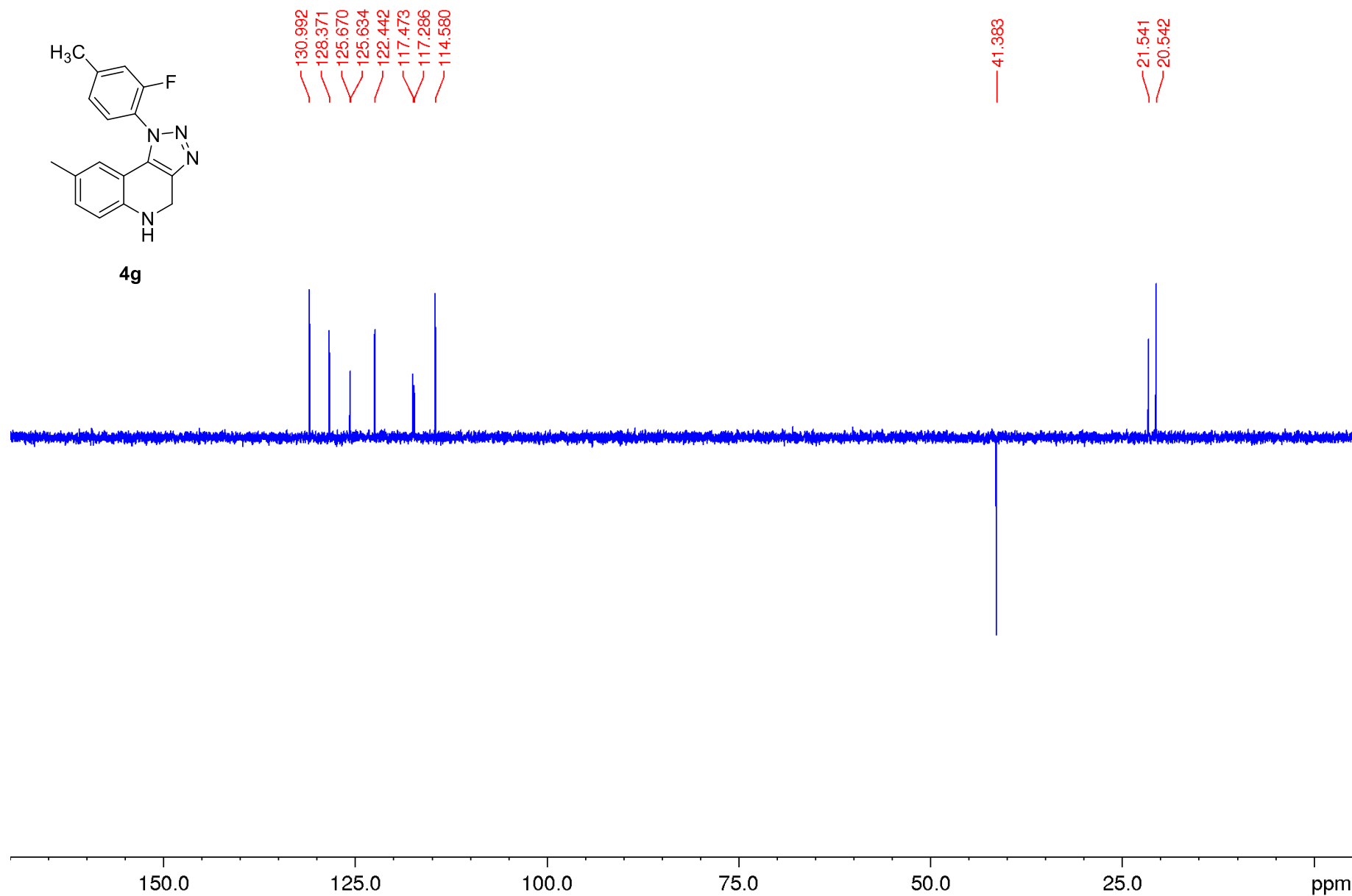
4g



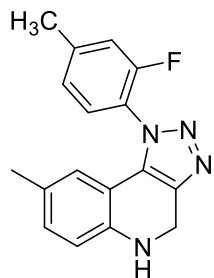
DEPT 135 NMR-spectrum (CDCl₃)



4g

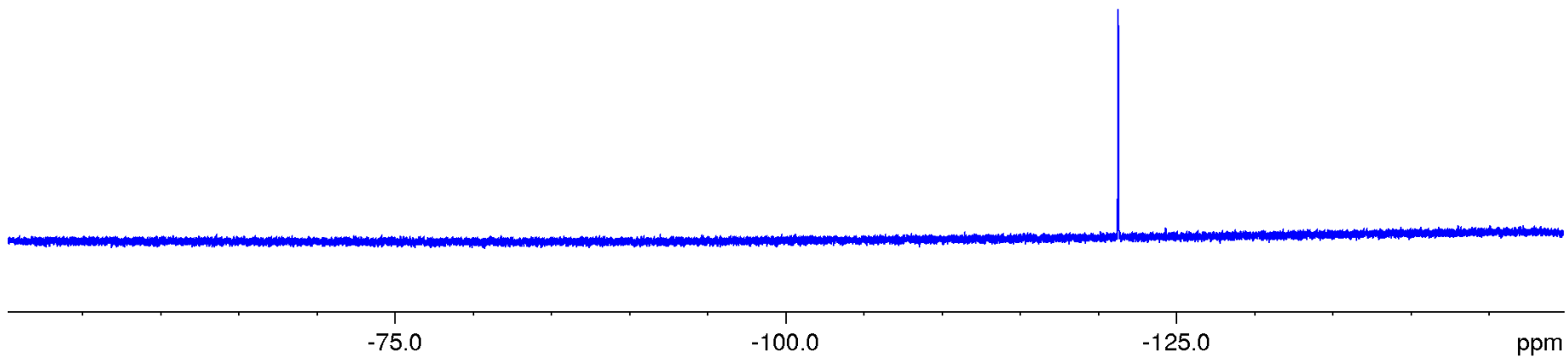


^{19}F NMR-spectrum (376.5 Hz, CDCl_3)

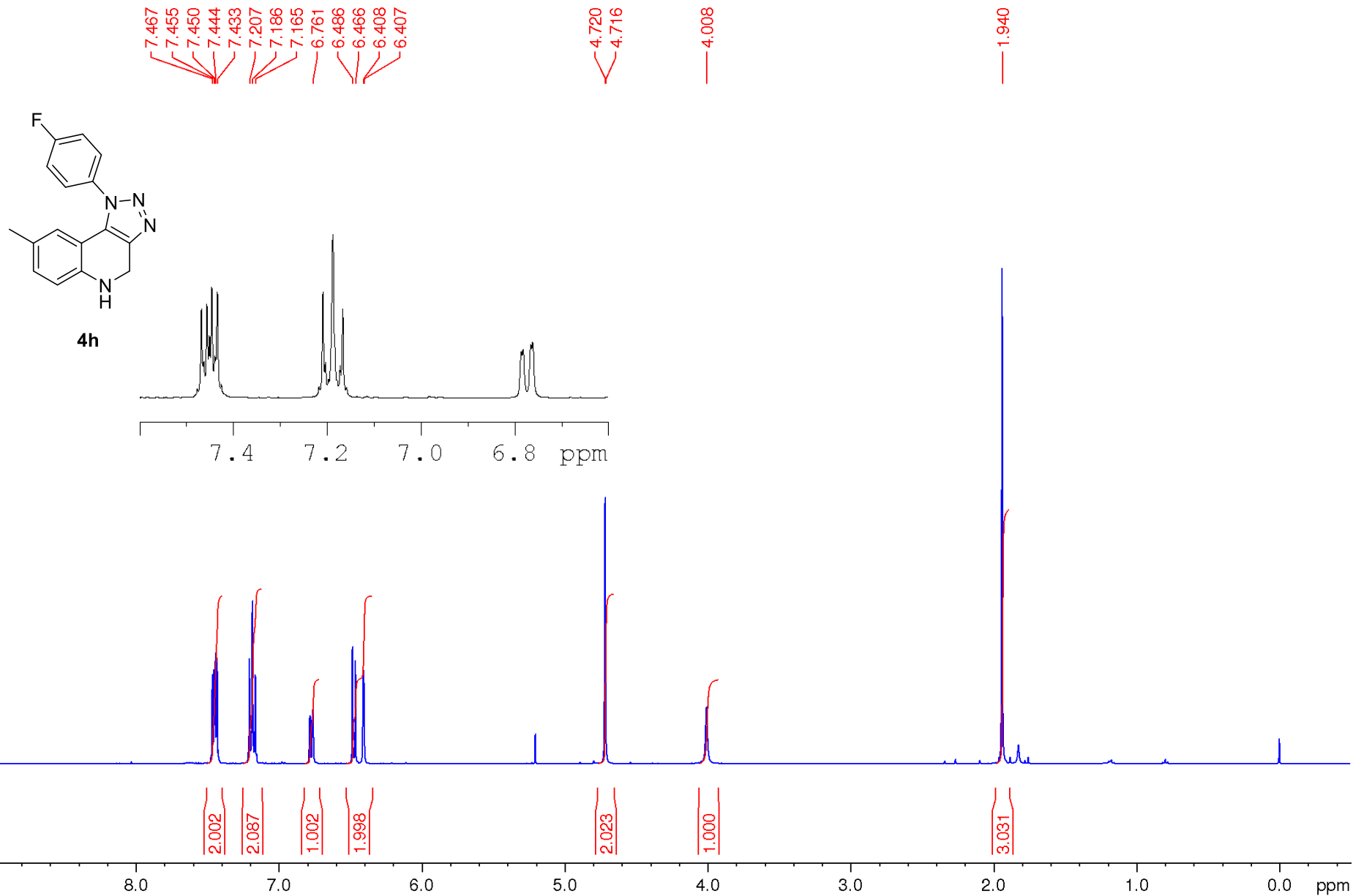


4g

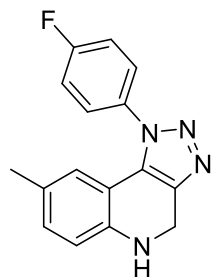
-121.270
-121.294
-121.318



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



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

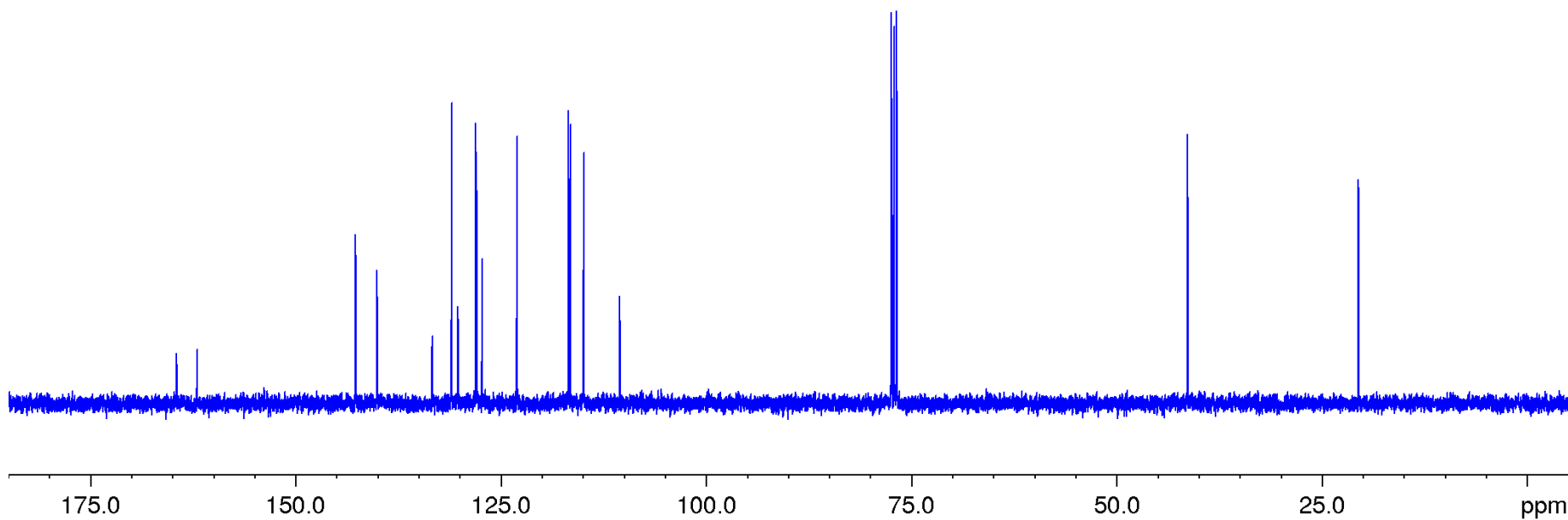


4h

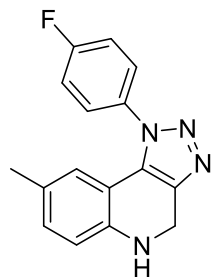
164.497
162.007
142.686
140.071
133.392
133.361
130.985
130.204
128.037
127.948
127.277
123.039
116.745
116.517
114.912
110.520

41.340

20.512



DEPT 135 NMR-spectrum (CDCl₃)



4h

130.985
128.037
127.947
123.040
116.746
116.518
114.912

41.339

20.512

150.0

125.0

100.0

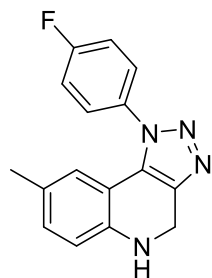
75.0

50.0

25.0

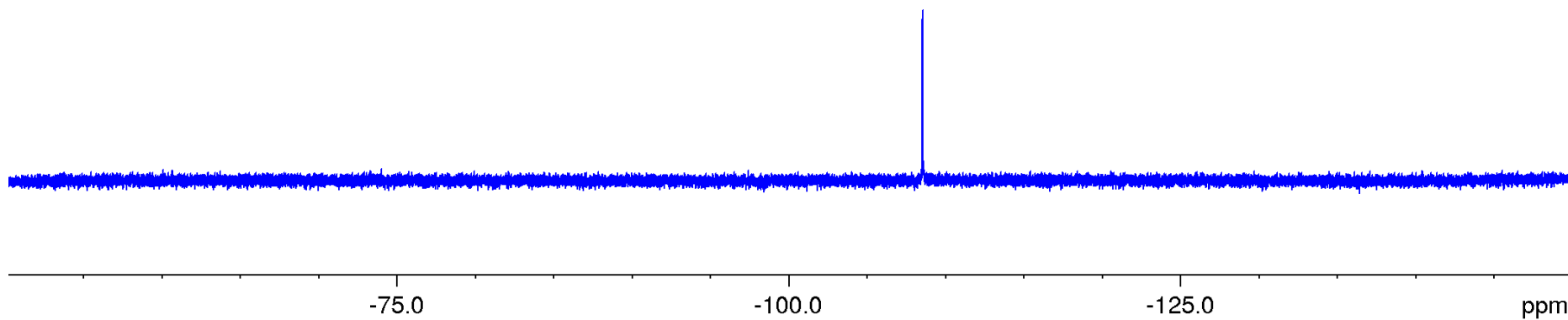
ppm

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

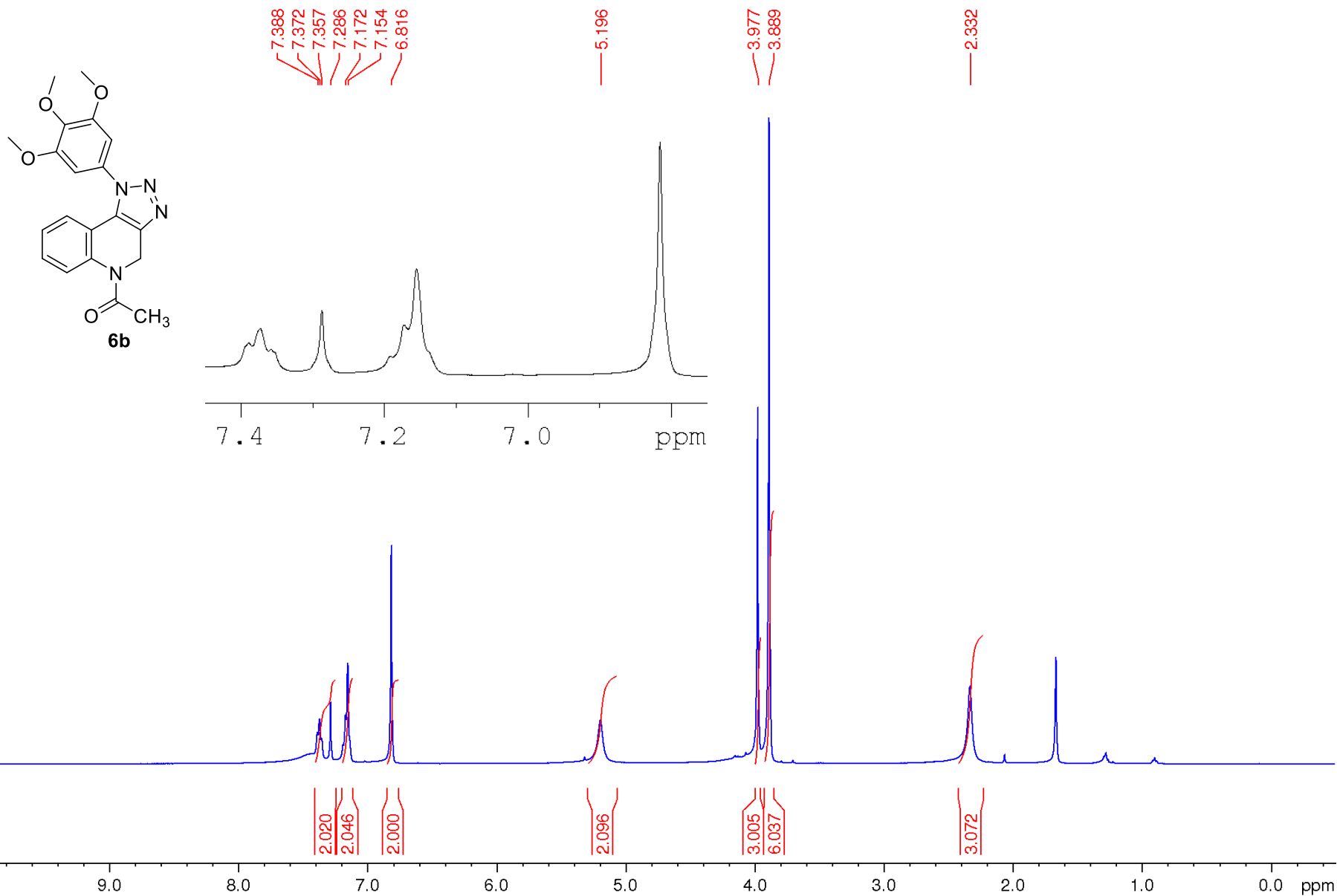


4h

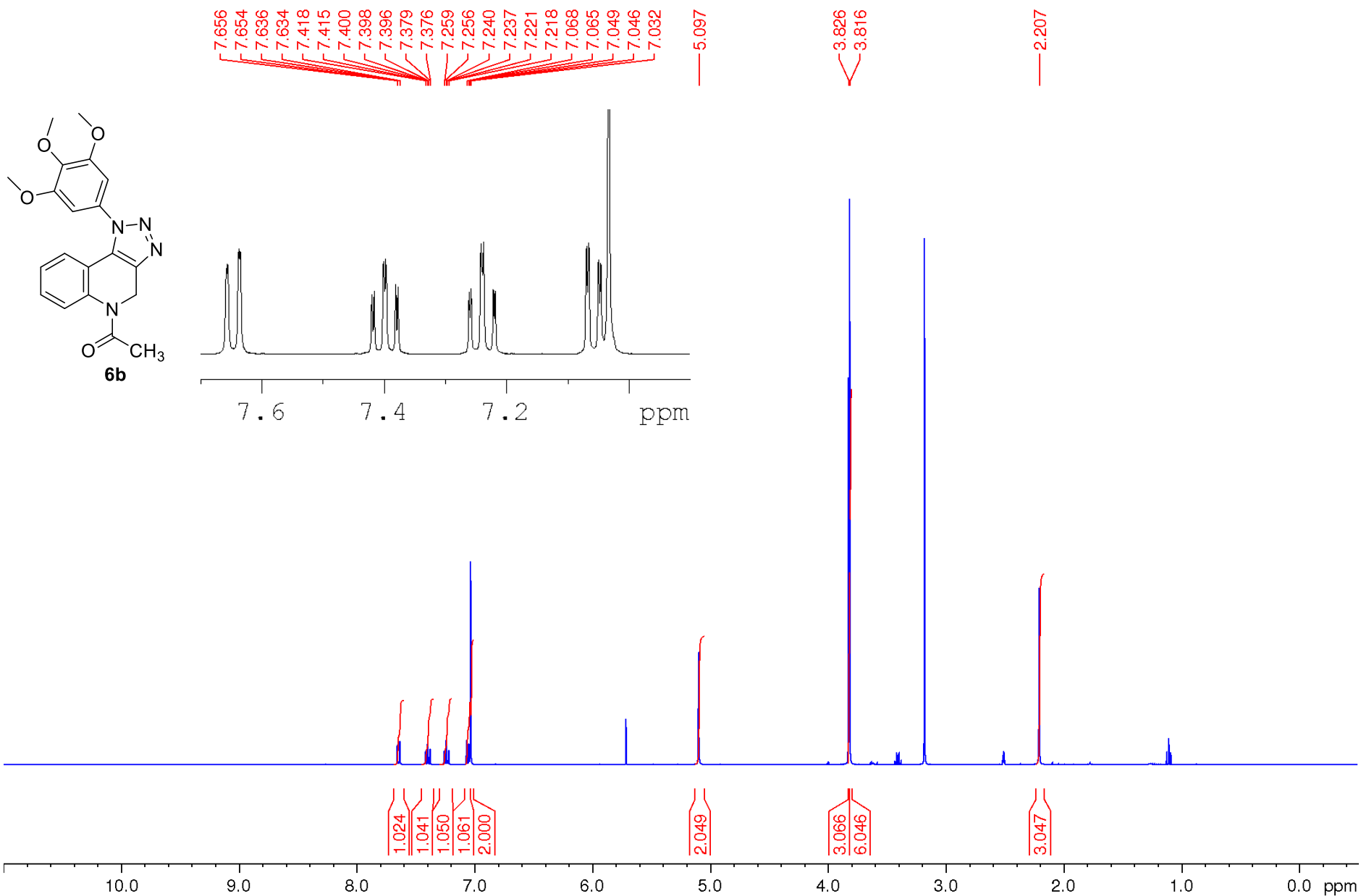
-108.547
-108.558
-108.569
-108.591



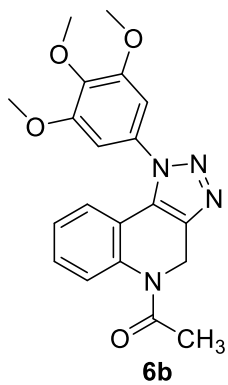
^1H NMR-spectrum at 25 °C (400 MHz, CDCl_3)



^1H NMR-spectrum at 60 °C(400 MHz, DMSO)

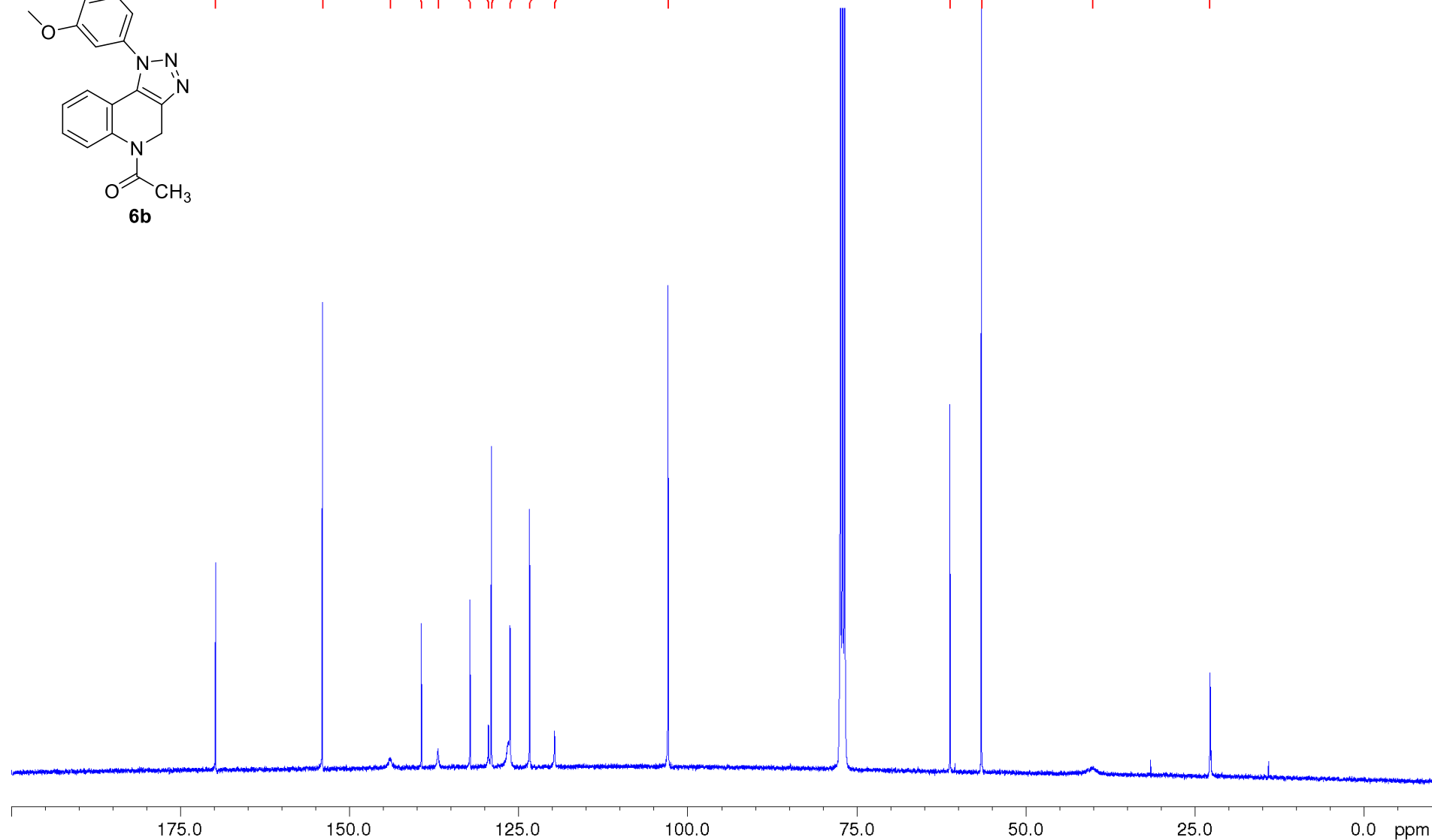


^{13}C NMR-spectrum, 10 thousands scans (100 MHz, CDCl_3)

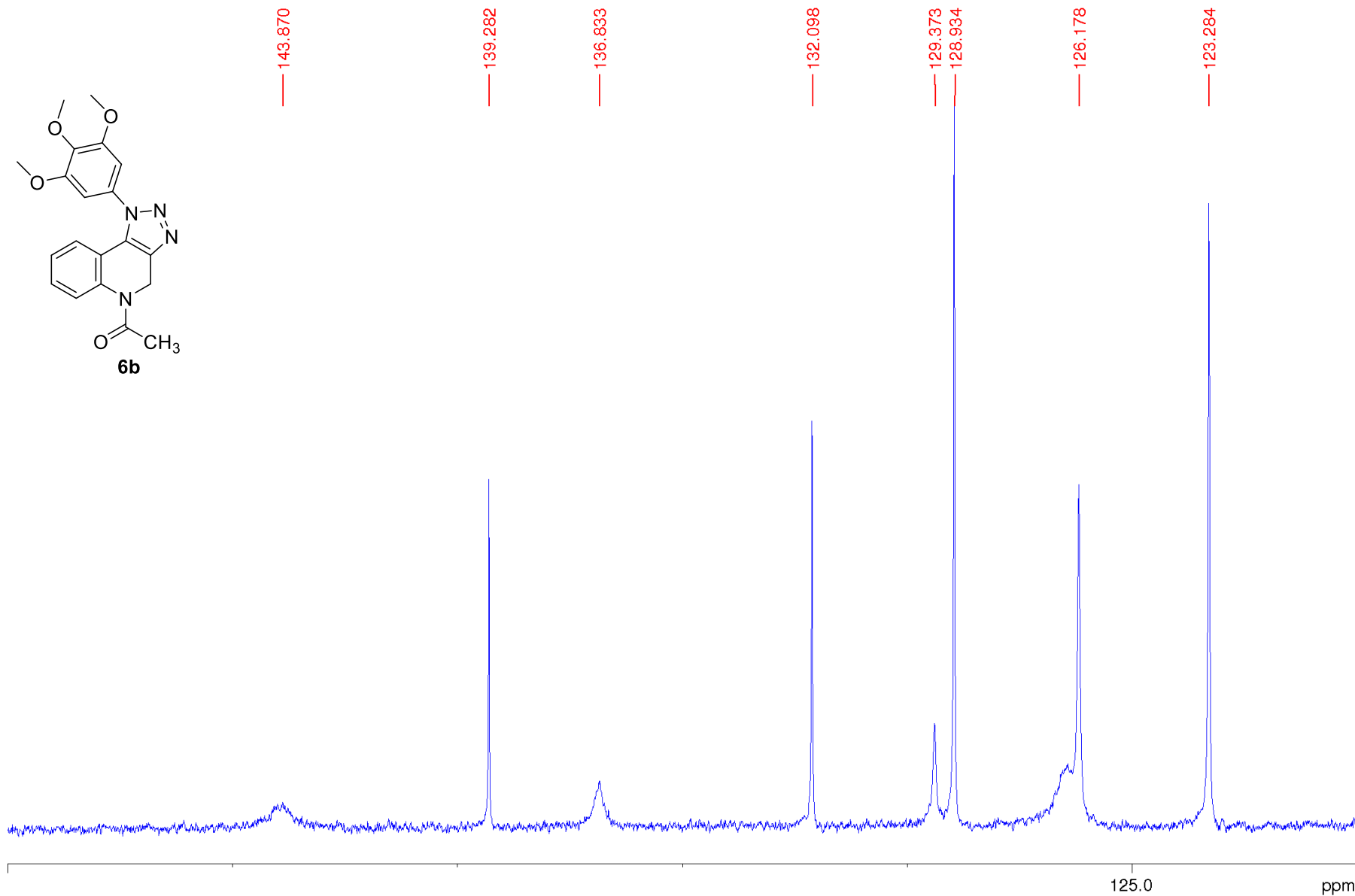
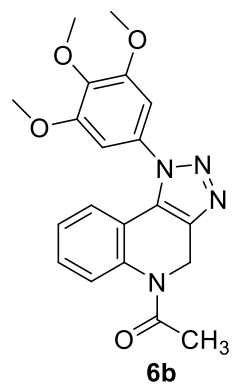


Chemical shift values (ppm) for the peaks in the spectrum:

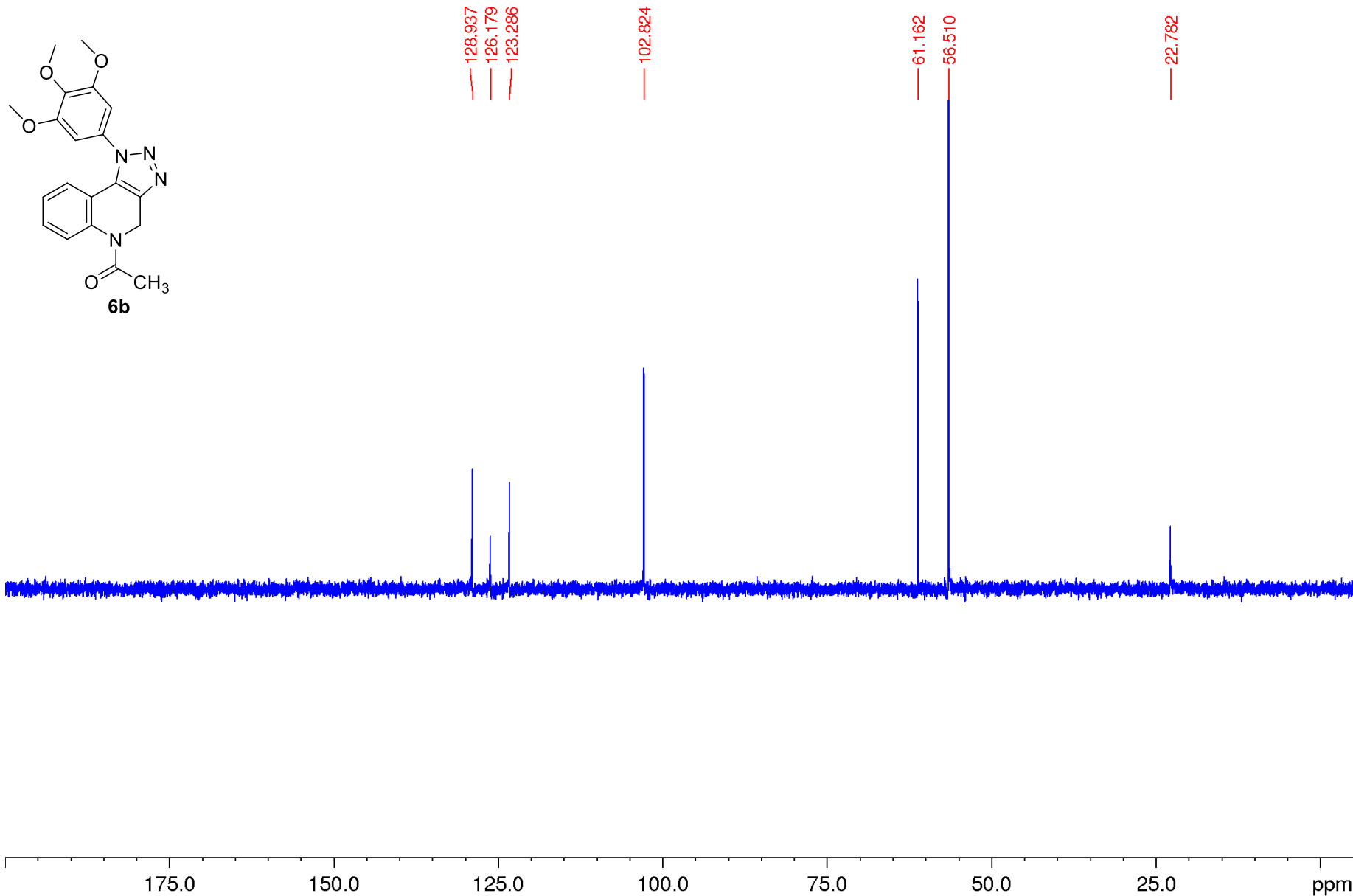
- 169.820
- 153.923
- 143.870
- 139.282
- 136.833
- 132.098
- 129.373
- 128.934
- 126.178
- 123.284
- 119.614
- 102.822
- 61.160
- 56.508
- 40.093
- 22.782



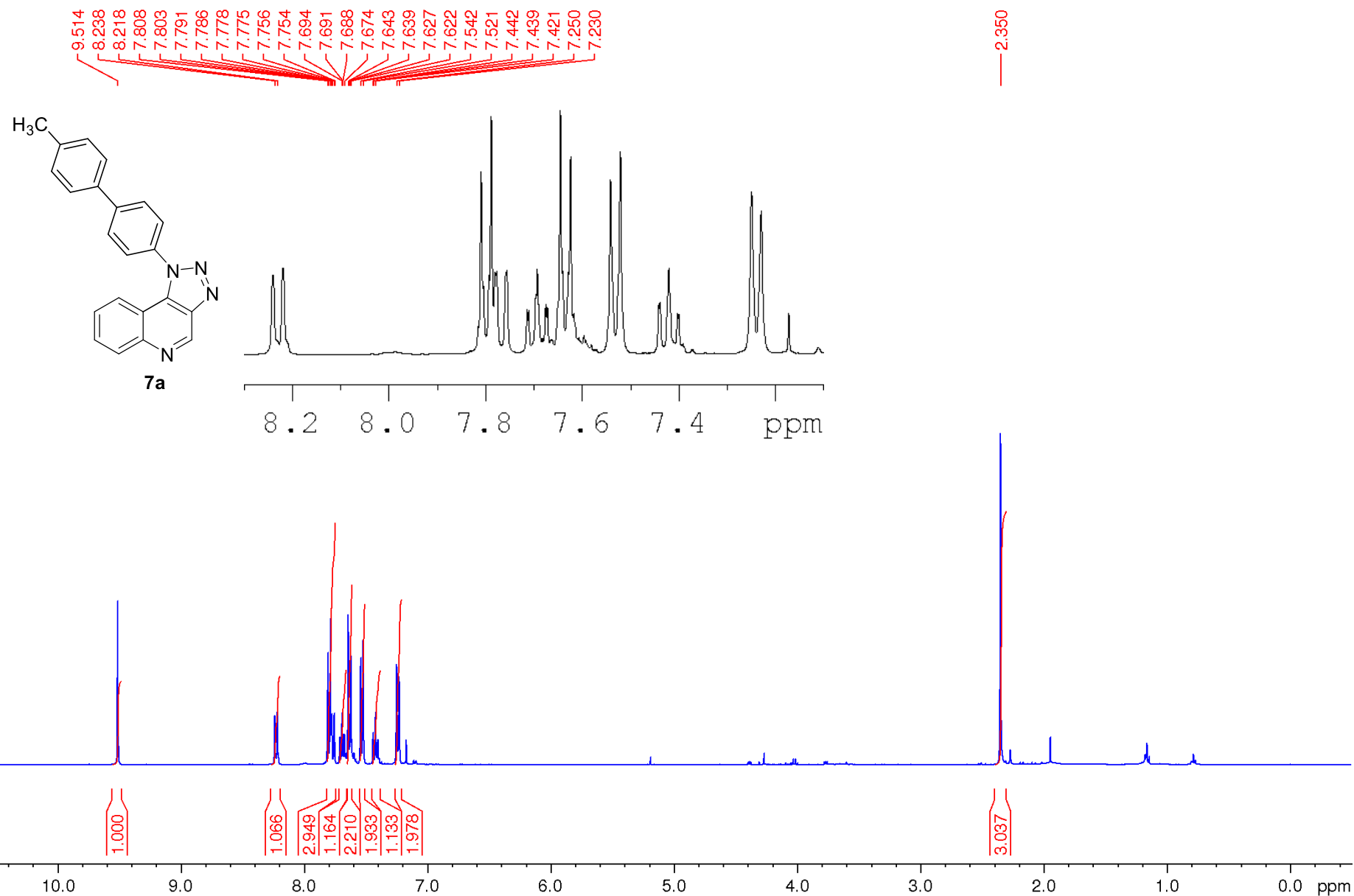
^{13}C NMR-spectrum, 10 thousand scans (100 MHz, CDCl_3)



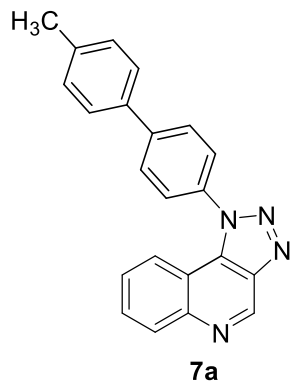
DEPT 135 NMR-spectrum (CDCl₃)



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

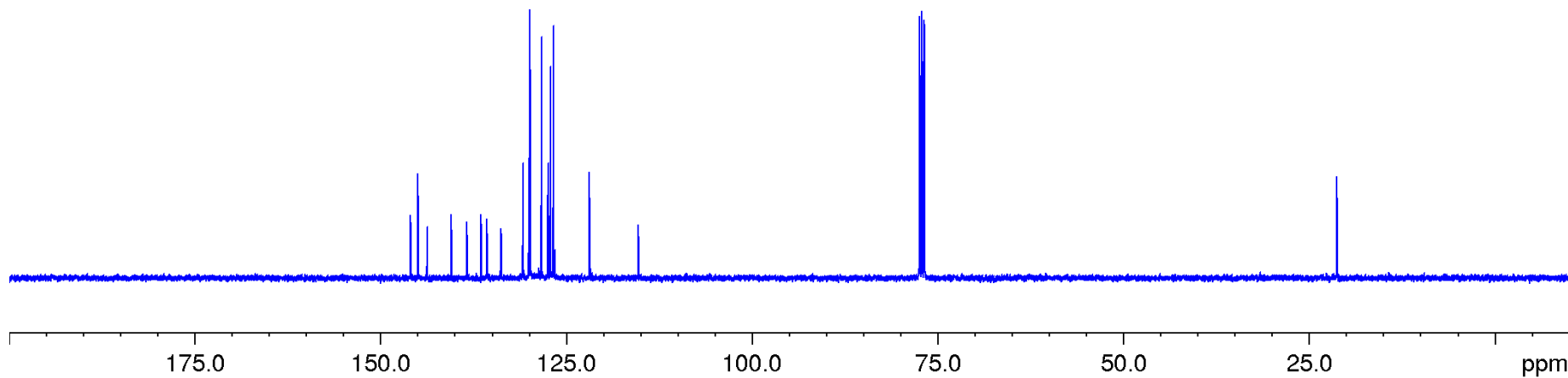


^{13}C NMR-spectrum (100 MHz, CDCl_3)

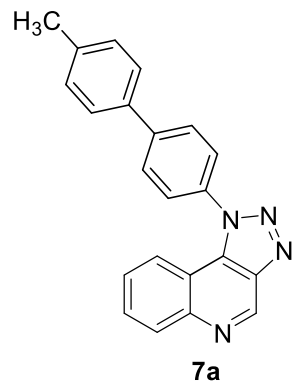


145.938
144.961
143.711
140.492
138.381
136.446
135.694
133.740
130.788
129.955
129.862
128.317
127.441
127.116
126.711
121.871
115.274

21.212



DEPT 135 NMR-spectrum (CDCl_3)



144.961

130.788

129.956

129.862

128.317

127.442

127.117

126.712

121.871

21.213

150.0

125.0

100.0

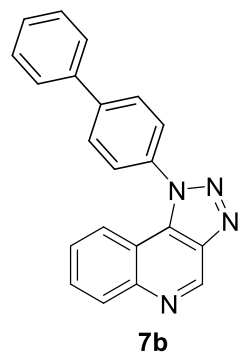
75.0

50.0

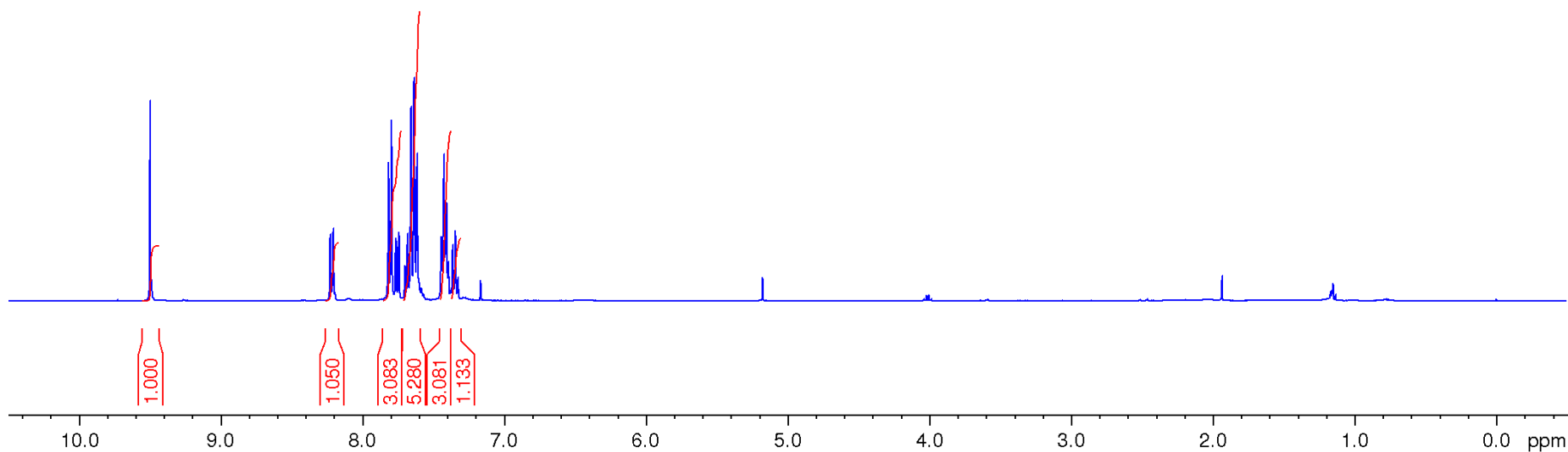
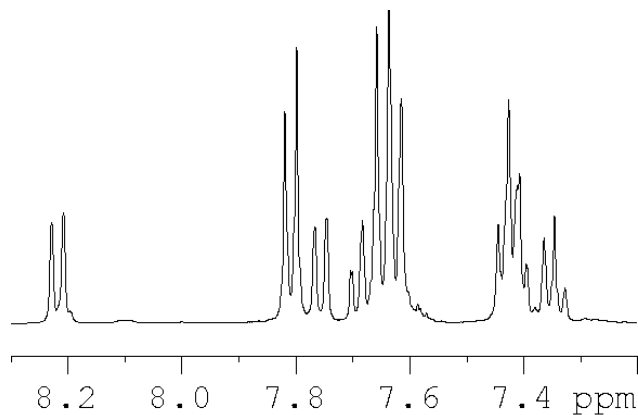
25.0

ppm

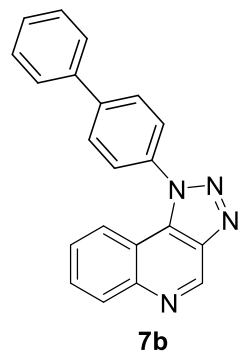
^1H NMR-spectrum (400 MHz, CDCl_3)



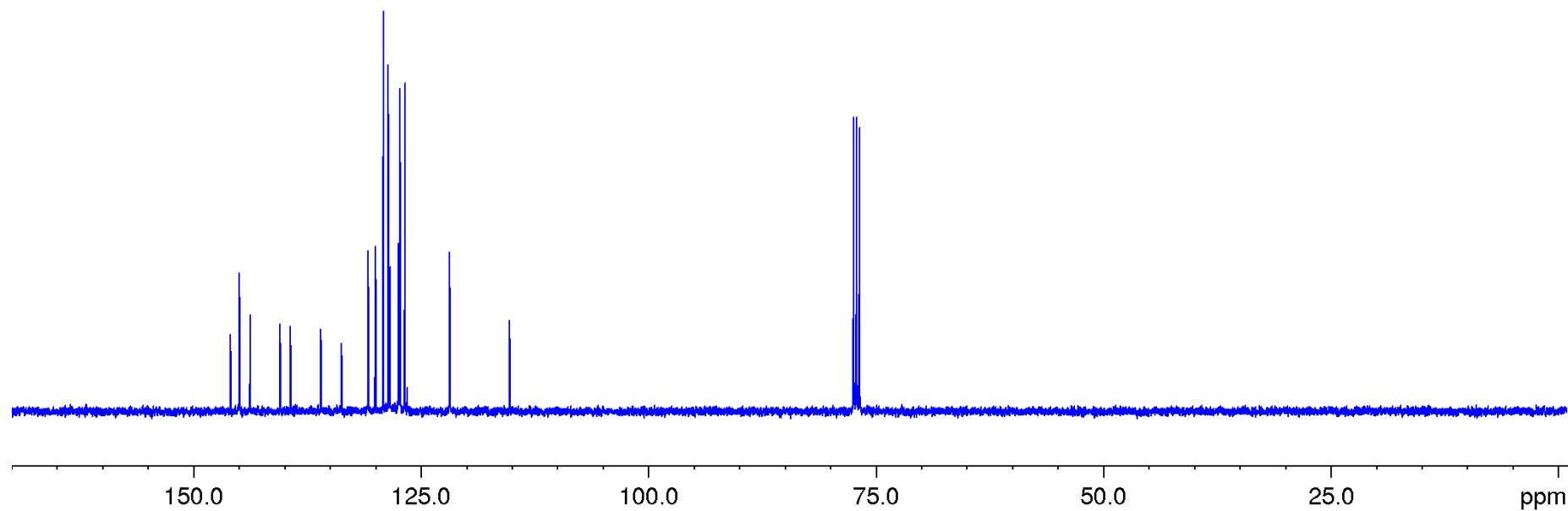
9.499
8.227
8.206
7.817
7.796
7.764
7.743
7.701
7.698
7.681
7.662
7.657
7.636
7.444
7.426
7.412
7.410
7.406
7.395
7.363
7.345
7.326



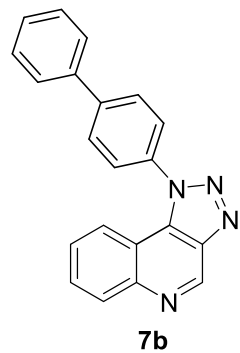
^{13}C NMR-spectrum (100 MHz, CDCl_3)



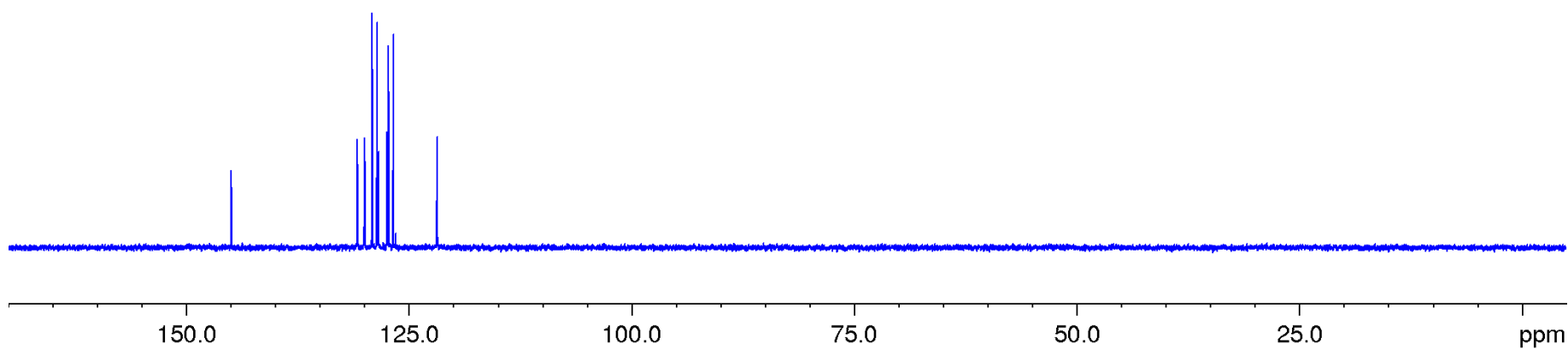
145.943
144.952
143.766
140.493
139.346
135.988
133.720
130.809
129.973
129.147
128.580
128.399
127.449
127.298
126.758
121.848
115.243



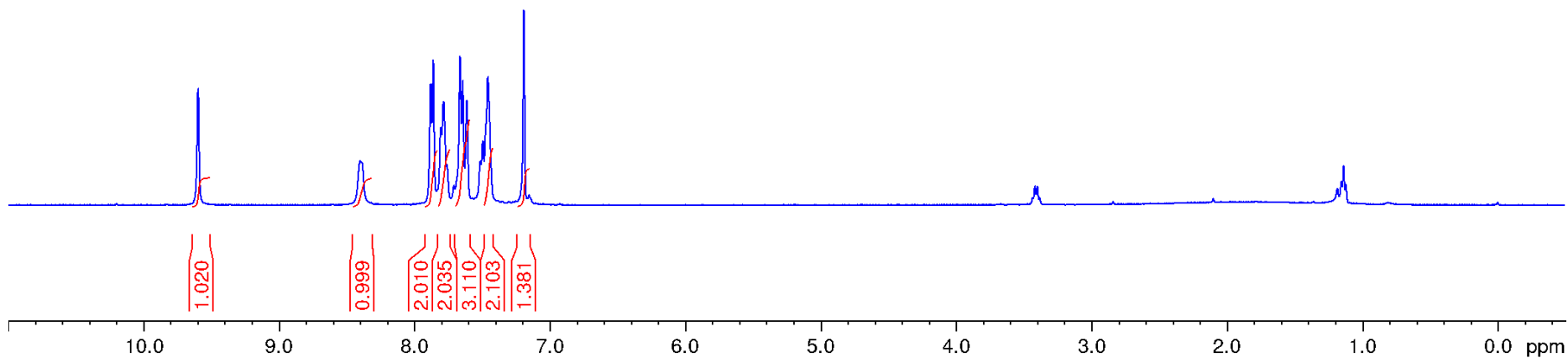
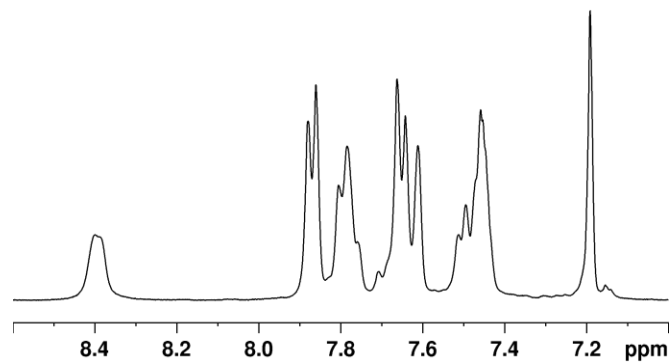
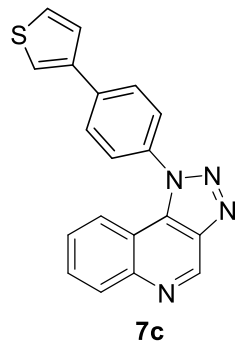
DEPT 135 NMR-spectrum (CDCl_3)



144.952
130.809
129.973
129.147
128.580
128.399
127.449
127.298
126.758
121.848

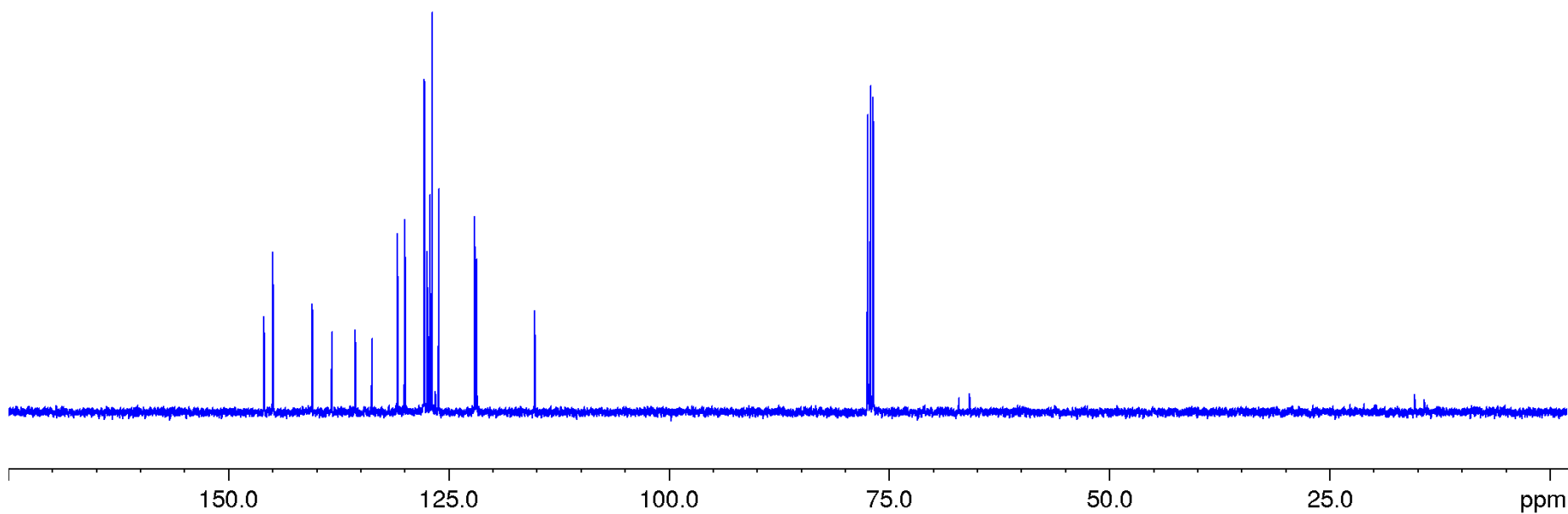
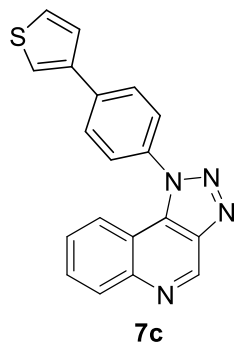


^1H NMR-spectrum (400 MHz, CDCl_3)

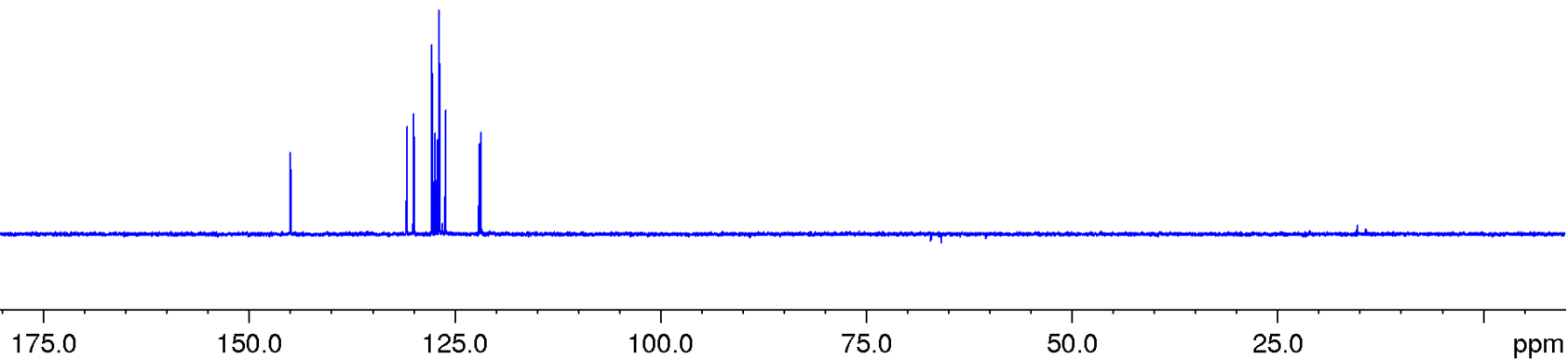
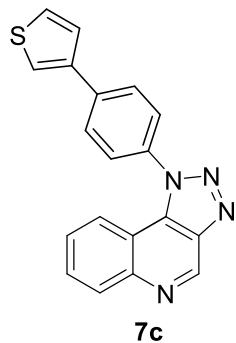


^{13}C NMR-spectrum (100 MHz, CDCl_3)

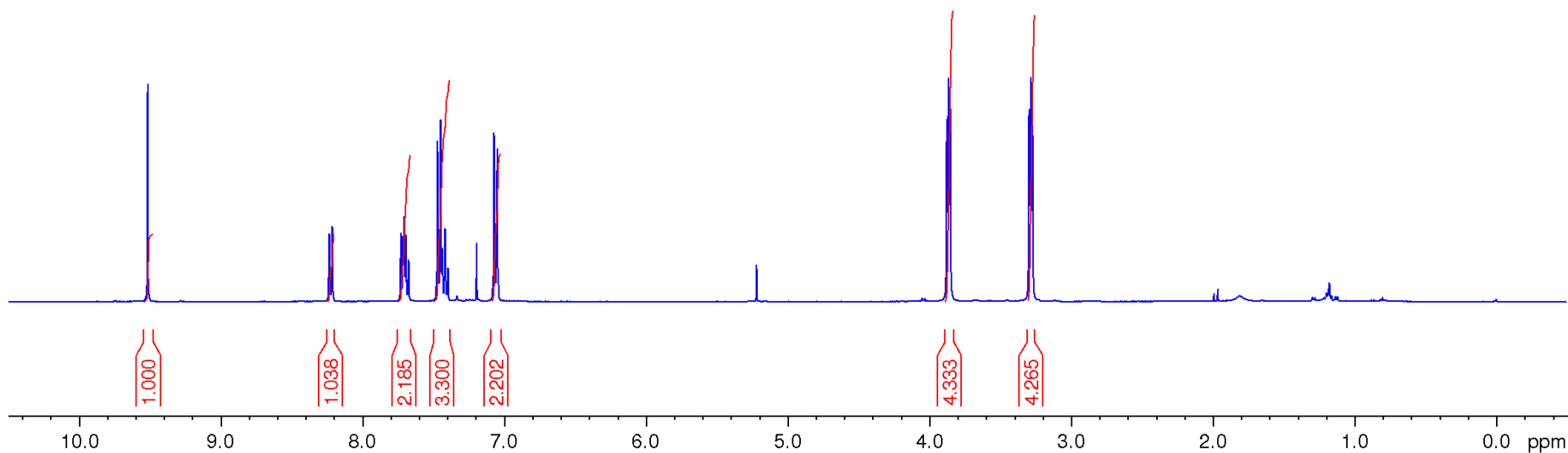
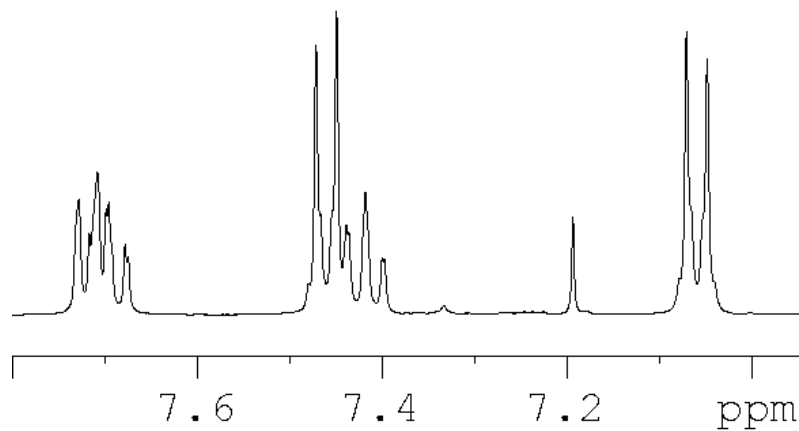
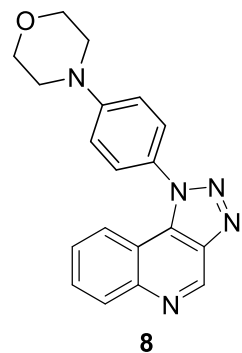
145.947
144.941
140.500
140.466
138.266
135.587
133.712
130.810
129.949
127.744
127.429
127.134
126.872
126.121
122.024
121.815
115.229



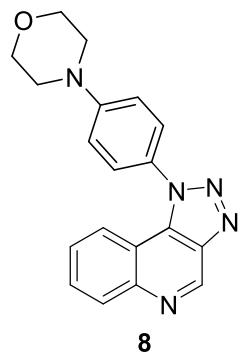
DEPT 135 NMR-spectrum (CDCl_3)



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



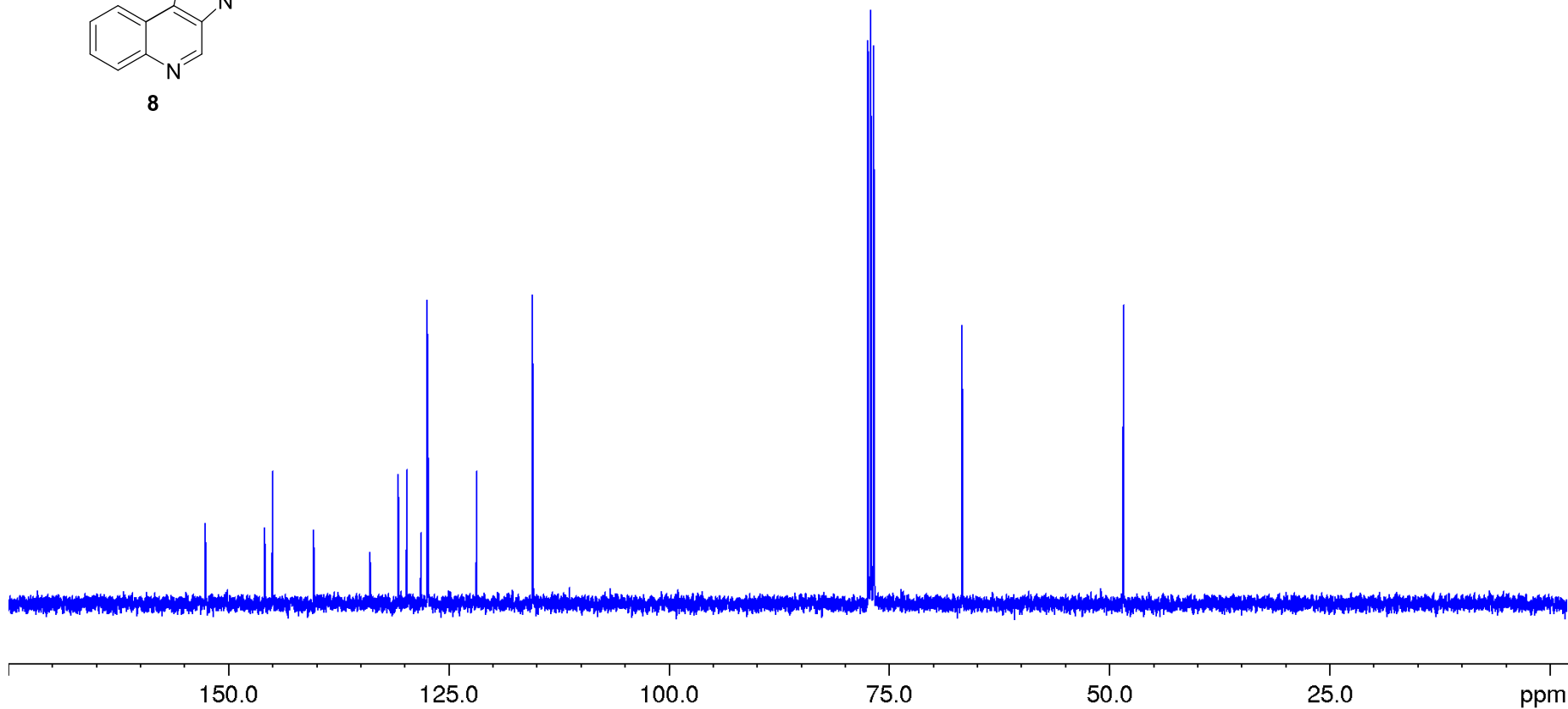
^{13}C NMR-spectrum (100 MHz, CDCl_3)



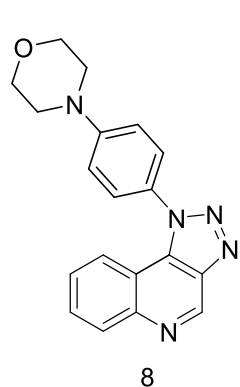
152.640
145.873
145.005
140.346
133.916
130.708
129.750
128.141
127.411
127.288
121.812
115.464

66.699

48.381



DEPT 135 NMR-spectrum (CDCl₃)



145.006

130.709

129.751

127.412

127.289

121.813

115.467

66.699

48.381

150.0

125.0

100.0

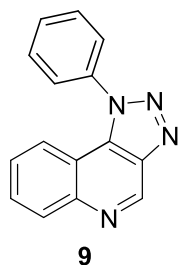
75.0

50.0

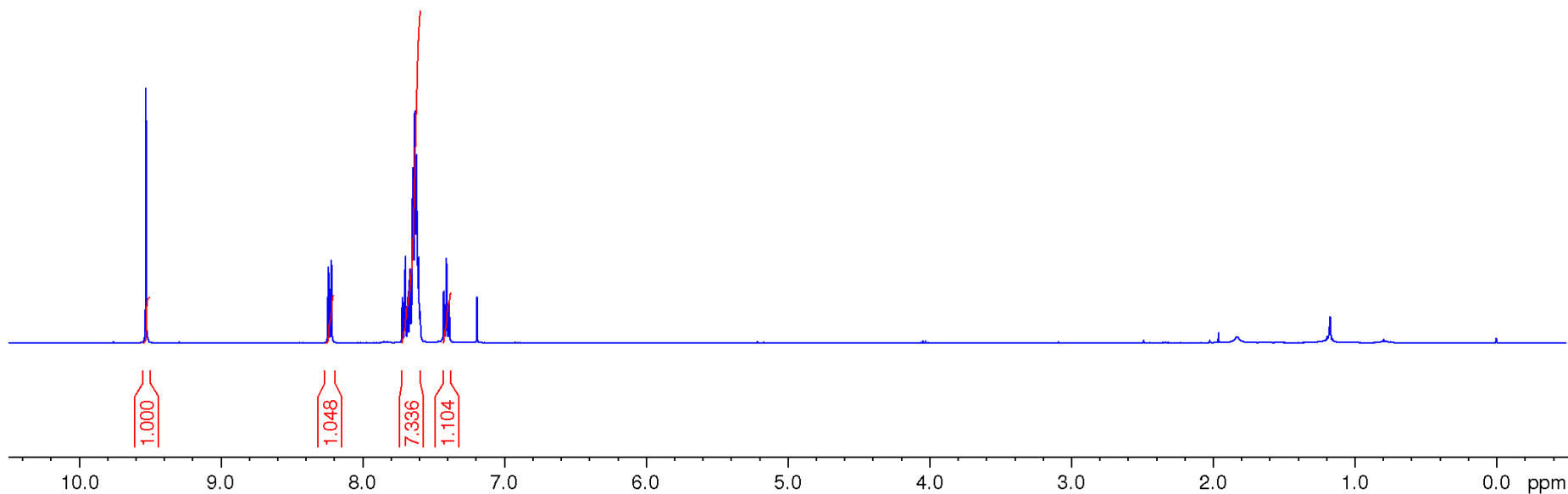
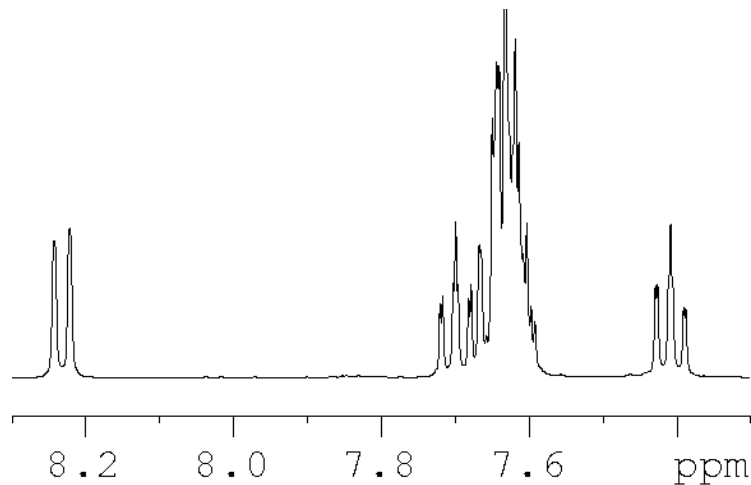
25.0

ppm

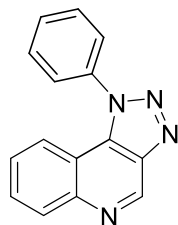
^1H NMR-spectrum (400 MHz, CDCl_3)



9.528
8.241
8.220
7.702
7.699
7.695
7.678
7.666
7.664
7.649
7.643
7.640
7.631
7.618
7.613
7.607
7.602
7.428
7.425
7.407

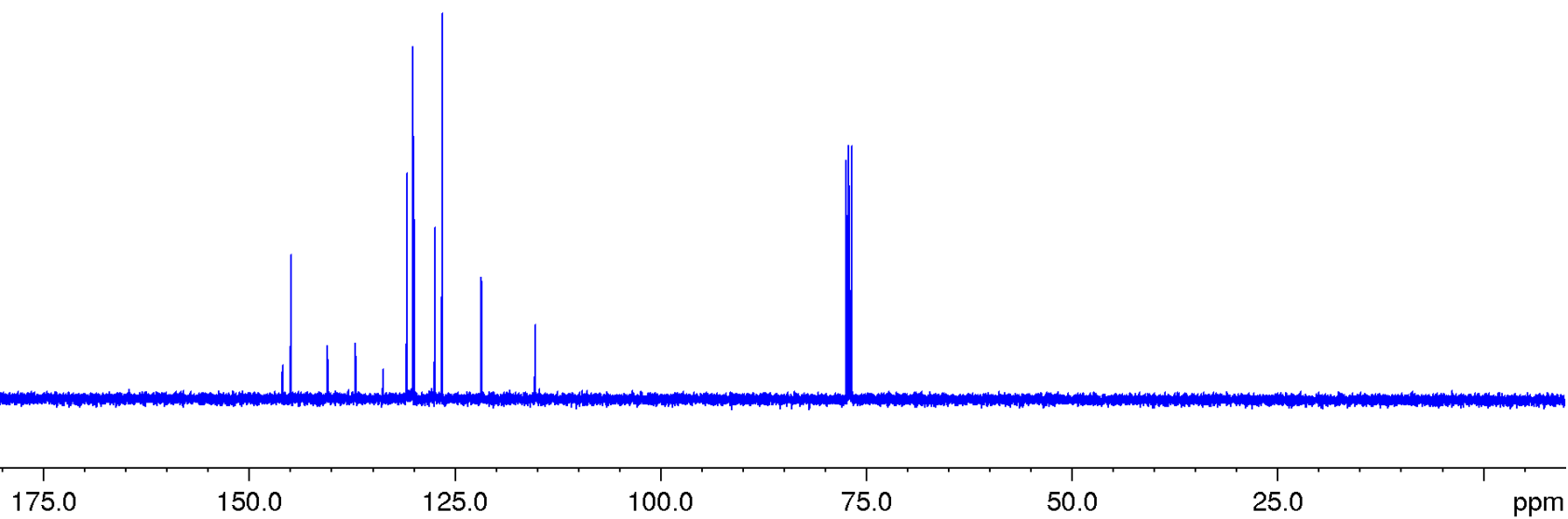


^{13}C NMR-spectrum (100 MHz, CDCl_3)

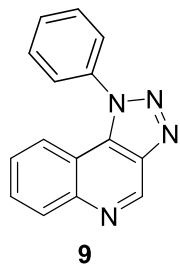


9

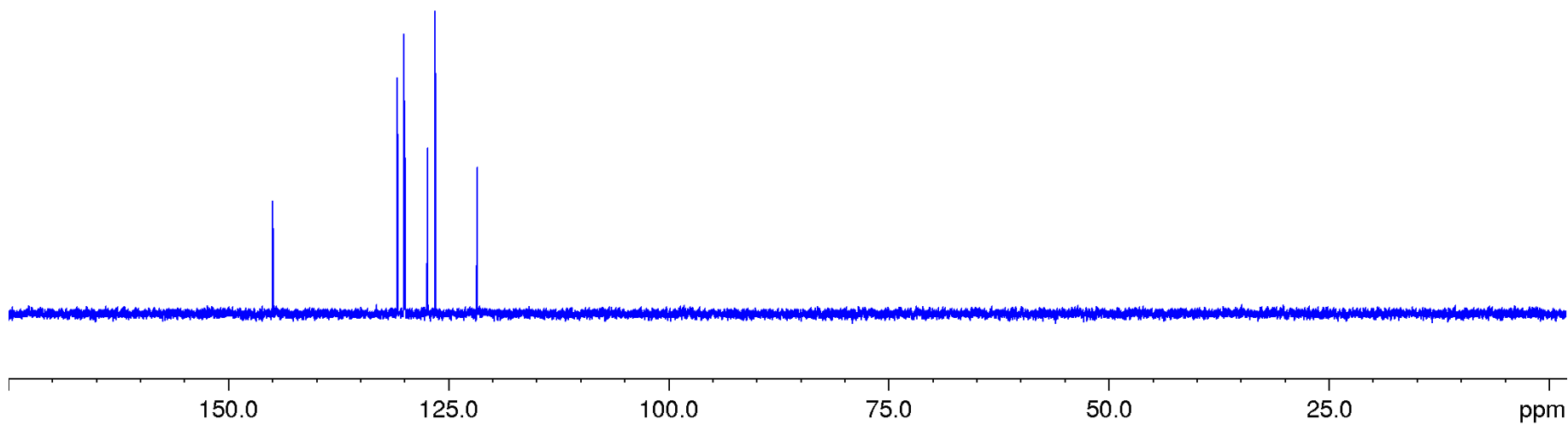
145.934
144.933
140.448
137.053
130.818
130.796
130.050
129.942
129.909
127.384
126.484
121.743
115.208



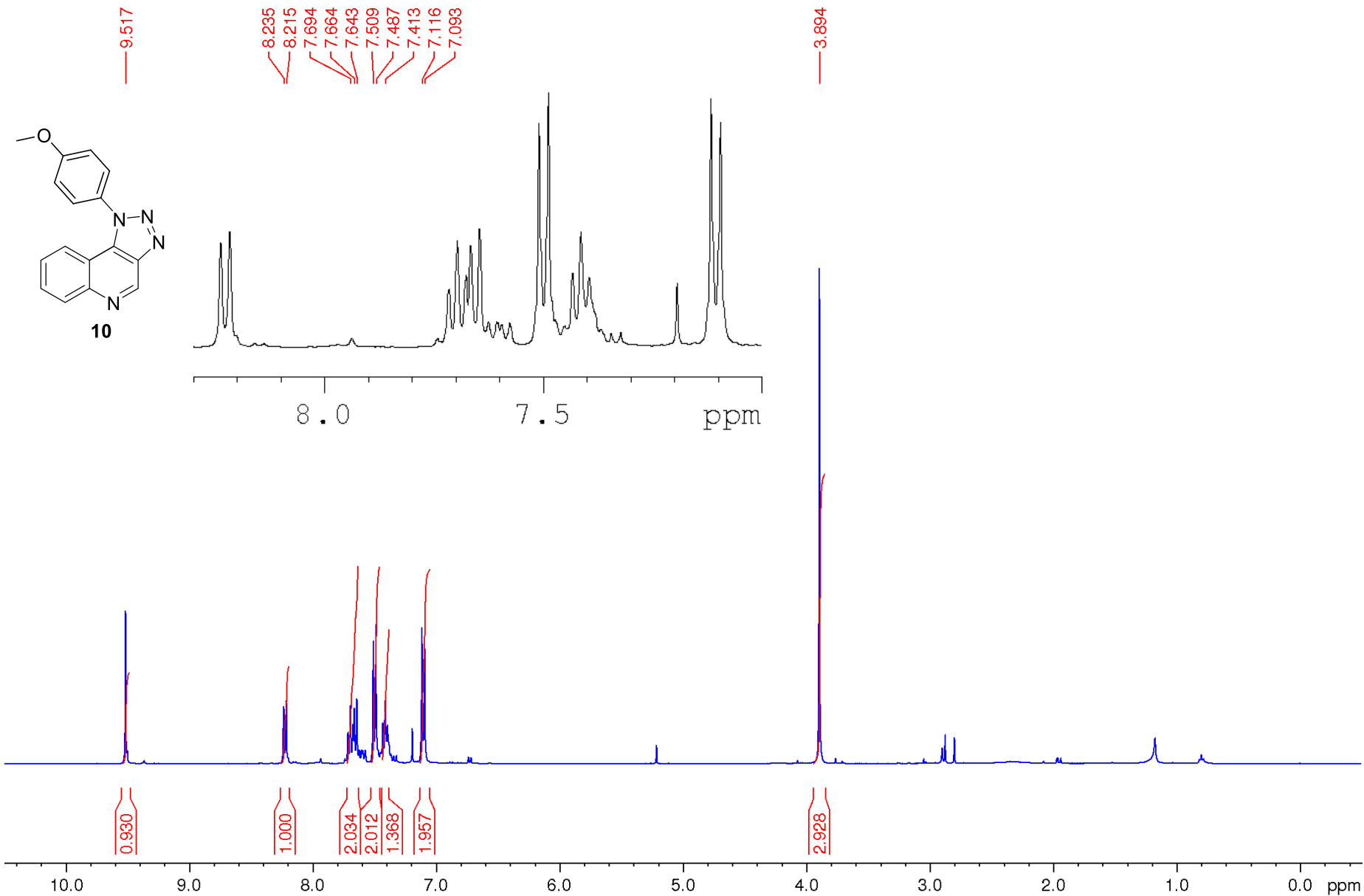
DEPT 135 NMR-spectrum (CDCl₃)



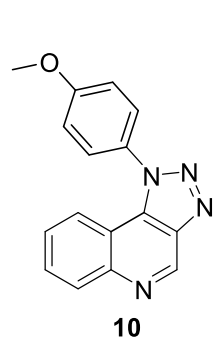
144.962
130.820
130.052
129.918
127.390
126.493
121.748



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

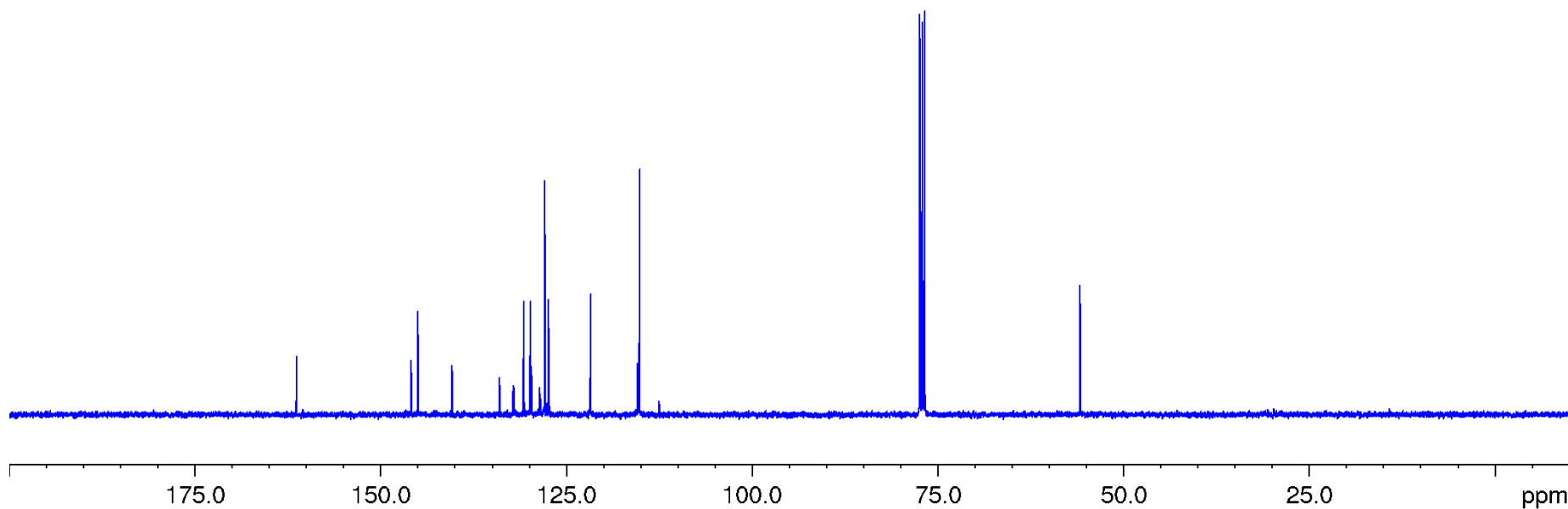


^{13}C NMR-spectrum (100 MHz, CDCl_3)

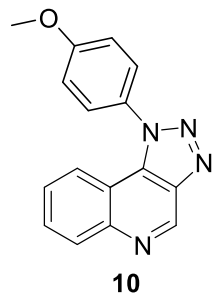


Chemical shift values (ppm) for the peaks in the spectrum:

- 161.278
- 145.881
- 144.964
- 140.339
- 133.959
- 130.730
- 129.834
- 129.666
- 127.869
- 127.367
- 121.709
- 115.353
- 115.120
- 55.783



DEPT 135 NMR-spectrum (CDCl₃)



144.964

130.730

129.834

127.869

127.367

121.709

115.120

55.784

150.0

125.0

100.0

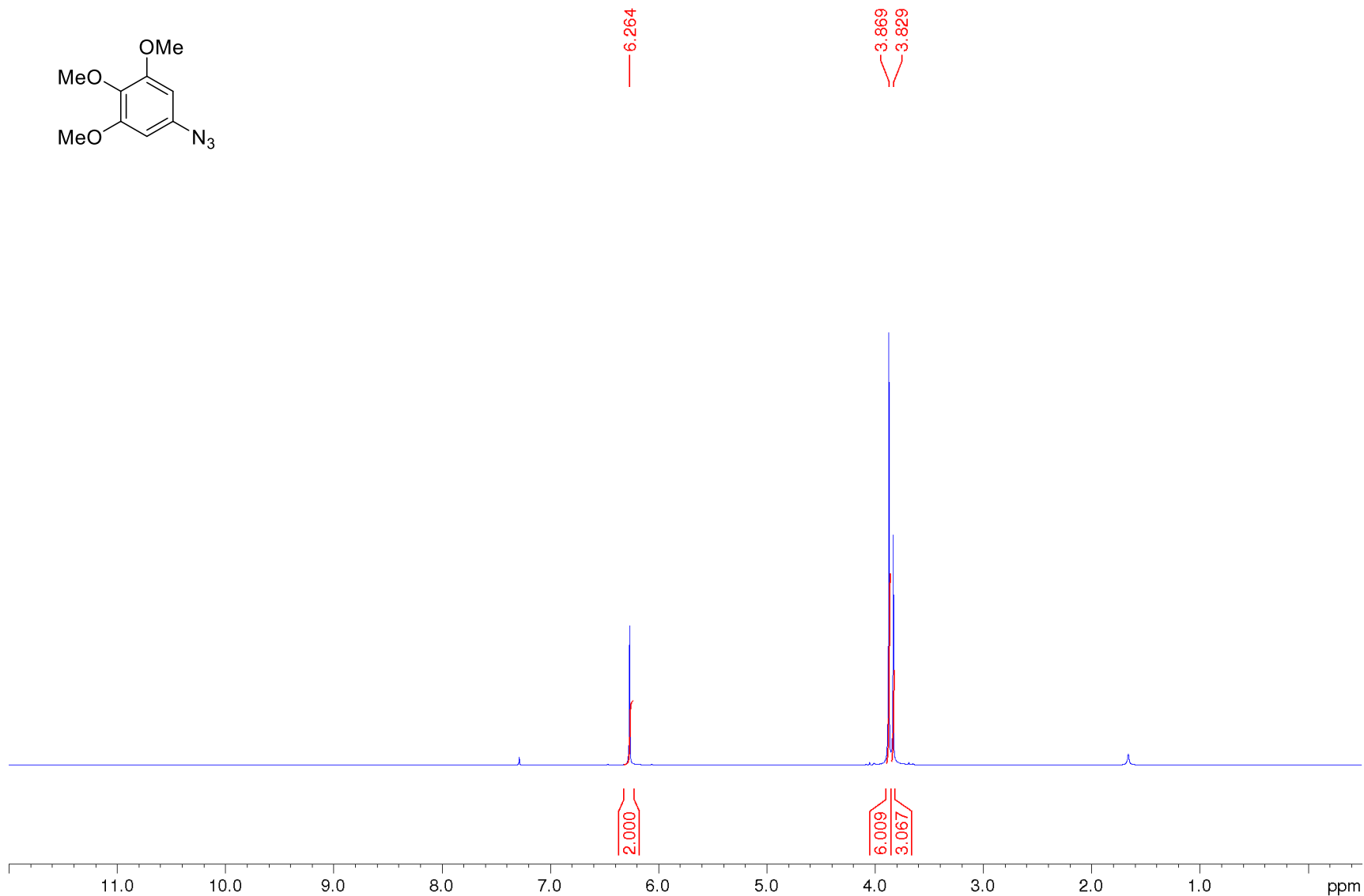
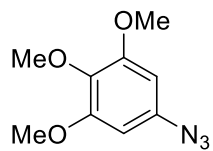
75.0

50.0

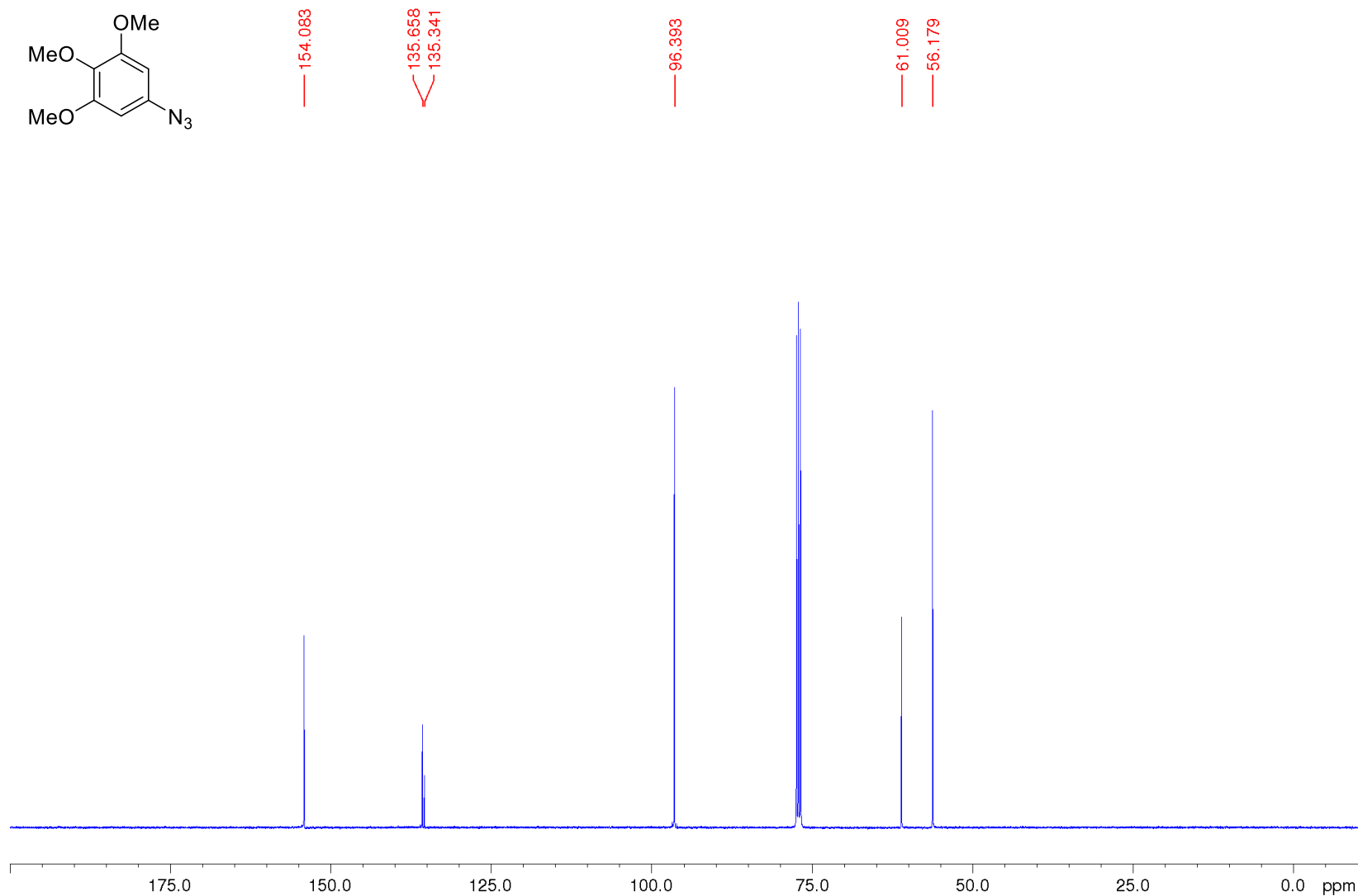
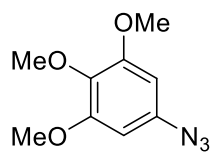
25.0

ppm

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



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



DEPT 135 NMR-spectrum (CDCl_3)

