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$SnCl_4$ or $TiCl_4$: Highly efficient catalysts for detetrahydropyranylation and demethoxymethylation of phenolic ethers and sequel one-pot asymmetric synthesis of 3-aryl-2-hydroxy-2,3-dihydroindan-1-ones from chalcone epoxides

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1. Selected spectral data of THP and MOM deprotected products

2.2.6 3-(4-fluorophenyl)-2,5-dihydroxy-2,3-dihydroinden-1-one (1):

Light yellow solid; Yield: 495 mg (96%); m.p = 145-147°C; IR ν_{max} (KBr, cm^{-1}): 3405 (OH str), 2922, 2875 (aromatic C-H str), 1688 (C=O str), 1595 (aromatic, C=C str), 1266, 1089, 858, 731; ^{1}H NMR ($CDCl_3$, 500 MHz) δ ppm 7.87 (d, *J* = 8.5 Hz, 2H), 7.54 (d, *J* = 8.5 Hz, 1H), 7.06 (d, *J* = 9 Hz, 2H),6.95 (d, *J* = 9 Hz, 2H), 6.4 (s, 1H) 5.29 (t, *J* = 7 Hz, 1H), 5.22 (d, *J* = 1.5 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ ppm 195.55, 161.83, 137.36, 131.82, 131.42, 129.79, 125.99, 123.01, 116.23, 75.01, 63.53; MS (EI, 70eV): m/z (%) = 258 [$M^{+\cdot}$,$C_{15}H_{11}FO_3$]; HRMS (ESI-TOF) calcd for $C_{15}H_{11}FO_3$ 258.0692, found 258.0694; The absolute configuration was determined by comparison with the optical rotation reported for the $[\alpha]_D^{25}$ = -10.4 (c 0.25, $CHCl_3$).

2.2.7 3-(4-chlorophenyl)-2,5-dihydroxy-2,3-dihydroinden-1-one (2):

Light yellow solid; Yield: 538mg (98%); m.p = 155-157°C IR ν_{max} (KBr, cm^{-1}): 3415 (OH str), 2931, 2873 (aromatic C-H str), 1681 (C=O str), 1597 (aromatic, C=C str), 1263, 1081, 860, 737; ^{1}H NMR ($CDCl_3$, 500 MHz) δ ppm 7.88 (d, *J* = 8.5 Hz , 2H), 7.56-7.53 (m, 1H), 7.07 (t, *J* = 7 Hz, 2H), 6.96 (d, *J* = 9 Hz, 2H), 6.45 (s, 1H), 5.30 (t, *J* =7 Hz,1H), 5.23 (d, *J* = 1.5 Hz,1H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ ppm 195.72, 162.00, 137.53, 131.99, 131.59, 129.96, 126.16, 123.18, 116.40, 76.23, 63.70; MS (EI, 70eV): m/z (%) = 274 [$M^{+\cdot}$, $C_{15}H_{11}ClO_3$]; HRMS (ESI-TOF) calcd for $C_{15}H_{11}\mathbf{Cl}O_3$ 274.0397, found 274.0396; The absolute configuration was determined by comparison with the optical rotation reported for the $[\alpha]_D^{25}$ = -10.5 (c 0.26, $CHCl_3$)**.**

2.2.8 3-(4-bromophenyl)-2,5-dihydroxy-2,3-dihydroinden-1-one (3):

Light yellow solid; Yield: 606mg (95%); m.p = 162-168°C; IR ν_{max} (KBr, cm^{-1}): 3425 (OH str), 2935, 2877 (aromatic C-H str), 1687 (C=O str), 1585 (aromatic, C=C str), 1266, 1088, 862, 733; ^{1}H NMR ($CDCl_3$, 500 MHz) δ ppm 7.86 (d, *J* = 8.5 Hz, 2H), 7.54-7.52 (m, 1H), 7.05 (t, *J* = 7 Hz, 2H), 6.95 (d, *J* = 9 Hz, 2H), 6.42 (s, 1H), 5.29 (t, *J* = 7 Hz, 1H), 5.22 (d, *J* = 1.5 Hz,1H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ ppm 195.57, 161.85, 137.38, 131.84, 131.45, 129.81, 126.01, 123.04, 116.25, 75.40, 63.55; MS (EI, 70eV): m/z (%) = 318 [$M^{+\cdot}$, $C_{15}H_{11}BrO_3$], 320 [M+2]; HRMS (ESI-TOF) calcd for $C_{15}H_{11}BrO_3$ 317.9892, found 317.9894; The absolute configuration was determined by comparison with the optical rotation reported for the $[\alpha]_D^{25}$ = -9.4 (c 0.56, $CHCl_3$).

2. Spectral data of selected indanone derivatives

2.3.1 3-Phenyl-2-hydroxy-2, 3-dihydroindan-1-one (2a):

Light yellow solid; Yield: 439 mg (98%); m.p = 178-180 °C,IR ν_{max} (KBr, cm^{-1}): 3452 (OH str), 2963 (aromatic C-H str), 1686 (C=O str), 1599 (aromatic, C=C str), 1451, 1419, 1262, 1021, 933, 868, 799 and 704,^{1}H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 7.89 (m, 2 H, H_{Ar}), 7.66 (m, 1 H, H_{Ar}), 7.54 (m, 3 H, H_{Ar}), 7.37-7.30 (m, 3 H, H_{Ar}), 5.39 (d, *J* = 2.0 Hz, 1 H, H2), 5.24 (d, *J* = 2.0 Hz, 1 H, H3), 4.05 (s, br, D_2O exchangeable, 1 H),^{13}C-NMR ($CDCl_3$, 125 MHz) δ (ppm): 197.8 (C=O), 138.1, 134.3, 133.6, 129.2, 128.8, 128.6, 127.9, 76.1 (C2), 63.8 (C3),MS (EI, 70eV): m/z (%) = 224(35) [M^+, $C_{15}H_{12}O_2$], 207(25), 195(29), 178(37), 165(40), 152(33), 121(64), 105(100), 91(62), 77(74) and 51(69); HRMS (ESI-TOF) calcd for $C_{15}H_{12}O_2$ 224.0837, found 224.0838; The absolute configuration was determined by comparison with the optical rotation reported for the $[\alpha]_D^{25}$ = -8.5 (c 1.1, $CHCl_3$).

2.3.2 3-(4-Chlorophenyl) -2-hydroxy-2, 3-dihydroindan-1-one (2b):

Light yellow solid; Yield: 745 mg (98%); m.p = 188-190°C,IR ν_{max} (KBr, cm^{-1}): 3408 (OH str), 2917 (aromatic C-H str), 1689 (C=O str), 1589 (aromatic, C=C str), 1489, 1415, 1288, 1177, 1091, 1014, 929 and 701,^{1}H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 7.83 (d, *J* = 7.5 Hz, 2 H, H_{Ar}), 7.59 (t, *J* = 7.0 Hz, 1 H, H_{Ar}), 7.48-7.45 (m, 2 H, H_{Ar}), 7.40 (dd, J=6.0, 2.0Hz, 2 H, H_{Ar}), 7.25 (m, 1 H, H_{Ar}), 5.27 (d, *J* = 2.0 Hz, 1 H, H2), 5.12 (d, *J* = 2.0 Hz, 1 H, H3), 4.02 (s, br, D_2O exchangeable, 1 H),^{13}C-NMR ($CDCl_3$, 125 MHz) δ (ppm): 197.4 (C=O), 136.6, 134.8, 134.4, 133.5, 129.4, 129.2, 128.7, 128.5, 75.9 (C2), 62.9 (C3), MS (EI, 70eV): m/z (%) = 258(17) [M^+, $C_{15}H_{11}ClO_2$], 242(28), 207(36), 179(43), 165(32), 135(57), 130(61), 105(100), 89(49), 77(61), 75(55) and 51(62); HRMS (ESI-TOF) calcd for $C_{15}H_{11}ClO_2$ 258.0448, found 258.0450; The absolute configuration was determined by comparison with the optical rotation reported for the $[\alpha]_D^{25}$ = -8.8 (c 1.2, $CHCl_3$).

2.3.3 2-Hydroxy-3-p-tolyl-2,3-dihydroinden-1-one (2c):

Light yellow solid; Yield: 434mg (91%); m.p = 144-146°C,IR ν_{max} (KBr, cm^{-1}): 3391 (OH str), 2951 (aromatic C-H str), 1693 (C=O str), 1577 (aromatic, C=C str), 1468, 1401, 1271, 1152, 1084, 1002, 910 and 725, ^{1}H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 7.81 (d, *J* = 5.5 Hz, 2 H, H_{Ar}), 7.55 (m, 1 H, H_{Ar}), 7.44 (m, 1 H, H_{Ar}), 7.34 (d, *J* = 6.0 Hz, 2 H, H_{Ar}), 7.07(d, *J* = 5.0 Hz, 2 H, H_{Ar}), 5.28 (d, *J* = 2.0 Hz, 1 H, H2), 5.14 (d, *J* = 2.0 Hz, 1 H, H3), 4.05 (s, br, D_2O exchangeable, 1 H), 2.24 (s, 3 H), ^{13}C-NMR ($CDCl_3$, 125 MHz) δ (ppm): 197.9 (C=O), 138.7, 135.2, 134.3, 133.7, 129.2, 129.2, 128.6, 127.9, 76.2 (C2), 63.8 (C3), 21.2, MS (EI, 70eV): m/z (%) = 238(21) [M^+, $C_{16}H_{14}O_2$], 212(28), 203(16), 159(43), 145(32), 125(57), 105(100), 79(49), and 55(42); HRMS (ESI-TOF) calcd for $C_{16}H_{14}O_2$ 238.0994, found 238.0995; The absolute configuration was determined by comparison with the optical rotation reported for the $[\alpha]_D^{25}$ = -9.0 (c 1.3, $CHCl_3$).

2.3.4 3-(3-Nitrophenyl)-2-hydroxy-2,3-dihydroindan-1-one (2e):

Light yellow solid; Yield 442mg (82%); m.p = 196-198°C;IR ν_{max} (KBr, cm^{-1}): 3369 (OH str), 2923 (aromatic C-H str), 1680 (C=O str), 1613 (aromatic, C=C str), 1528 (N─O str), 1393, 1348 (N─O bending), 1259, 1094, 986, 911, 840, 728, 687; ^{1}H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 8.14 (d, *J* = 7.5 Hz, I H, H_{Ar}), 7.99 (m, 1 H, H_{Ar}), 7.86 (m, 2 H, H_{Ar}), 7.70 (t, *J* = 7.5 Hz, 1 H, H_{Ar}), 7.61-7.58 (m, 2 H, H_{Ar}), 7.45 (m, 1 H, H_{Ar}), 5.57 (d, J = 2.0 Hz, 1 H, H2), 5.32 (d, *J* = 2.0 Hz, 1 H, H3), 3.82 (s, br, D_2O exchangeable, 1 H).^{13}C-NMR ($CDCl_3$, 125 MHz) δ (ppm): 197.4 (C=O), 147.8, 137.7, 134.9, 134.2, 129.4, 129.2, 128.7, 123.8, 123.2, 76.5 (C2), 61.75 (C3);MS (EI, 70eV): m/z (%) = 269(13) [M^+, $C_{15}H_{11}NO_4$], 241(21), 196(61), 176(32), 165(48), 136(43), 105(100), 89(64), 77(44), 63(39) and 51(60); HRMS (ESI-TOF) calcd for $C_{15}H_{11}NO_4$ 269.0688, found 269.0690; The absolute configuration was determined by comparison with the optical rotation reported for the $[\alpha]_D^{25}$ = -16.4 (c 1.0, $CHCl_3$).

2.3.5 3-Phenyl-5-chloro-2-hydroxy-2,3-dihydroinden-1-one (2f):

Light yellow solid; Yield: 502 mg (97%); m.p = 180-182°C;IR ν_{max} (KBr, cm^{-1}): 3449 (OH str), 2950 (aromatic C-H str), 1682 (C=O str), 1582 (aromatic, C=C str), 1389, 1275, 1059, 854, 723 (C-Cl, str).^{1}H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 7.92 (d, *J* = 8.5 Hz,2 H, H_{Ar}), 7.78 (d, *J* = 8.5 Hz, 2 H, H_{Ar}), 7.45 (m, 2 H, H_{Ar}), 7.17 (m, 2 H, H_{Ar}), 5.23 (d, *J* = 4.0 Hz, 1 H, H2), 5.10 (d, *J* = 4.0 Hz, 1 H, H3), 3.92 (s, br, D_2O exchangeable, 1 H);^{13}C-NMR ($CDCl_3$, 125 MHz) δ (ppm): 196.7 (C=O), 140.8, 137.7, 132.0, 130.0, 129.5, 128.9, 128.6, 127.9, 76.1 (C2), 63.7 (C3);MS (EI, 70eV): m/z (%) = 258(35) [$M^{+\cdot}$, $C_{15}H_{11}ClO_2$], 139 (100); HRMS (ESI-TOF) calcd for $C_{15}H_{11}ClO_2$ 258.0448, found 258.0450; The absolute configuration was determined by comparison with the optical rotation reported for the $[\alpha]_D^{25}$ = -10.5 (c 1.5, $CHCl_3$).

2.3.6 3-(4-Chlorophenyl)-5-chloro-2-hydroxy-2,3-dihydro-indan-1-one (2g):

Light yellow solid; Yield: 574 mg (98%); m.p = 202-204°C;IR ν_{max} (KBr, cm^{-1}): 3438 (OH str), 2922 (aromatic C-H str), 1674 (C=O str), 1591 (aromatic, C=C str), 1396, 1282, 1173, 1091, 756 (C-Cl, str);^{1}H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 8.06 (d, *J* = 8.5 Hz, 1 H, H_{Ar}), 7.89 (m, 1 H, H_{Ar}), 7.53 (d, *J* = 8.5 Hz, 1 H, H_{Ar}), 7.47 (d, *J* = 8.5 Hz, 1 H, H_{Ar}), 7.28 (m, 2 H, H_{Ar}), 7.16 (d, *J* = 8.5 Hz, 1 H, H_{Ar}), 5.48 (d, *J* = 3.5 Hz, 1 H, H2), 5.21 (d, *J* = 3.5 Hz, 1 H, H3), 3.72 (s, br, D_2O exchangeable, 1 H);^{13}C-NMR ($CDCl_3$, 125MHz) δ (ppm): 196.4 (C=O), 141.0, 136.3, 134.3, 131.8, 131.6, 129.9, 129.6, 129.4, 128.9, 128.8, 75.9 (C2), 62.8 (C3);MS (EI, 70eV): m/z (%) = 292(10) [$M^{+\cdot}$, $C_{15}H_{10}Cl_2O_2$], 245(25), 139(100); HRMS (ESI-TOF) calcd for $C_{15}H_{10}Cl_2O_2$ 292.0058, found 292.0060; The absolute configuration was determined by comparison with the optical rotation reported for the $[\alpha]_D^{25}$ = -10.2 (c 1.4, $CHCl_3$).

2.3.7 5-Chloro-2-hydroxy-3-p-tolyl-2,3-dihydroindan-1-one (2h):

Light yellow solid; Yield: 744mg (91%); m.p = 182-184°C;IR ν_{max} (KBr, cm^{-1}): 3439 (OH str), 2922 (aromatic C-H str), 1670 (C=O str), 1594 (aromatic, C=C str), 1491, 1399, 1296, 1095, 760 (C-Cl, str);^{1}H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 8.01 (dd, *J* = 8.0, 2.0 Hz,2 H, H_{Ar}), 7.74 (m,1 H, H_{Ar}), 7.54 (m, 2 H, H_{Ar}), 7.21 (m, 2 H, H_{Ar}), 5.02 (d, *J* = 3.0 Hz, 1 H, H2), 4.95 (d, *J* = 3.0 Hz, 1 H, H3), 3.68 (s, br, D_2O exchangeable, 1 H), 2.49 (s, 3H); ^{13}C-NMR ($CDCl_3$, 125 MHz) δ (ppm): 193.4 (C=O), 146.5, 141.5, 131.4, 131.2, 130.3, 130.1, 129.8, 129.4, 128.9, 76.2 (C2), 62.3 (C3), 22.3;MS (EI, 70eV): m/z (%) = 272(25) [$M^{+\cdot}$, $C_{16}H_{13}ClO_2$], 160(55), 141(72), 139(100), 111(62), 105(73); HRMS (ESI-TOF) calcd for $C_{16}H_{13}ClO_2$ 272.0604, found 272.0606; The absolute configuration was determined by comparison with the optical rotation reported for the $[\alpha]_D^{25}$ = -9.5 (c 0.57, $CHCl_3$).

2.3.8 3-(4-Bromophenyl)-5-chloro-2-hydroxy-2,3-dihydro indan-1-one (2i):

Light yellow solid; Yield: 641 mg (95%); m.p = 210-212°C;IR ν_{max} (KBr, cm^{-1}): 3426 (OH str), 2923 (aromatic C-H str), 1678 (C=O str), 1591 (aromatic, C=C str), 1417, 1395, 1282, 1170, 1092, 757 (C-Cl, str);^{1}H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 7.88 (m, 2 H, H_{Ar}), 7.55-7.49 (m, 3 H, H_{Ar}), 7.40 (m, 2 H, H_{Ar}), 5.31 (d, *J* = 2.5 Hz, 1 H, H2), 5.15, (d, *J* = 2.5 Hz, 1 H, H3), 4.05 (s, br, D_2O exchangeable, 1 H);^{13}C-NMR ($CDCl_3$, 125 MHz) δ(ppm): 196.3 (C=O), 141.1, 136.8, 131.8, 131.8, 129.9, 129.6, 129.6, 123.1 75.8 (C2), 62.8 (C3);MS (EI, 70eV): m/z (%) = 336(18) [$M^{+\cdot}$, $C_{15}H_{10}ClBrO_2$], 139 (100), 111(53); HRMS (ESI-TOF) calcd for $C_{15}H_{10}ClBrO_2$ 335.9553, found 335.9554; The absolute configuration was determined by comparison with the optical rotation reported for the $[\alpha]_D^{25}$ = -9.8 (c 0.59, $CHCl_3$).

2.3.9 3-(3, 4, 5-Trimethoxyphenyl)-5-chloro-2-hydroxy-2,3-dihydroindan-1-one (2j):

Light yellow solid; Yield: 837 mg (80%); m.p = 220-222°C;IR ν_{max} (KBr, cm^{-1}): 3440 (OH str), 2920 (aromatic C-H str), 1666 (C=O str), 1592 (aromatic, C=C str), 1406, 1336, 1233, 1125(C-O-C, str), 1091, 771 (C-Cl, str); ^{1}H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 7.84 (d, *J* = 6.5 Hz, 2 H, H_{Ar}), 7.51 (d, *J* = 7.0 Hz, 1 H, H_{Ar}), 6.74 (s, 2 H, H_{Ar}), 5.35 (d, *J* = 2.5 Hz, 1 H, H2), 5.10 (d, *J* = 2.5 Hz, 1 H, H3), 4.10 (s, br, D_2O exchangeable, 1 H), 3.87 (s, OMe, 9H);^{13}C-NMR ($CDCl_3$, 125 MHz) δ (ppm): 191.2 (C=O), 153.6, 132.3, 131.6, 131.5, 129.8, 129.3, 128.9, 127.6, 107.4, 75.2(C2), 61.0(C3), 60.8, 56.3.MS (EI, 70eV): m/z (%) = 348(29) [$M^{+\cdot}$, $C_{18}H_{17}ClO_5$], 181(69), 139 (100), 111(59); HRMS (ESI-TOF) calcd for $C_{18}H_{17}ClO_5$ 348.0765, found 348.0767; The absolute configuration was determined by comparison with the optical rotation reported for the $[\alpha]_D^{25}$ = -10.1 (c 0.26, $CHCl_3$).

2.3.10 3-Phenyl-5-bromo-2-hydroxy-2,3-dihydroindan-1-one (2k):

Light yellow solid; Yield: 594 mg (98%); m.p = 192-194°C;IR ν_{max} (KBr, cm^{-1}): 3466 (OH str), 2920 (aromatic C-H str), 1678 (C=O str), 1593 (aromatic, C=C str), 1398, 1281, 1095, 843, 713 (C-Br, str);^{1}H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 7.99 (dd, *J* = 8.5 Hz, 1.5 Hz, 1 H, H_{Ar}), 7.87 (dd, *J* = 8.5 Hz, 1.5 Hz, 2 H, H_{Ar}), 7.69 (m, 3 H, H_{Ar}), 7.54 (m, 2 H, H_{Ar}), 5.48 (d, *J* = 2.5 Hz, 1 H, H2), 5.15 (d, *J* = 2.5 Hz, 1 H, H3), 3.51 (s, br, D_2O exchangeable, 1 H);^{13}C-NMR ($CDCl_3$, 125 MHz) δ (ppm): 196.9 (C=O), 137.7, 132.5, 132.4, 131.7, 130.6, 130.4, 129.6, 128.9, 128.6, 128.6, 127.9, 76.1 (C2), 63.7 (C3);MS (EI, 70eV): m/z (%) = 302(18) [$M^{+\cdot}$, $C_{15}H_{11}BrO_2$], 185(69), 183(53), 91(100); HRMS (ESI-TOF) calcd for $C_{15}H_{11}BrO_2$ 301.9942, found 301.9943; The absolute configuration was determined by comparison with the optical rotation reported for the $[\alpha]_D^{25}$ = -15.4 (c 0.92, $CHCl_3$).

2.3.11 3-(4-Bromophenyl)-5-bromo-2-hydroxy-2,3-dihydro indan-1-one (2m):

Light yellow solid; Yield = 734mg (96%); m.p = 198-200°C;IR ν_{max} (KBr, cm^{-1}): 3441 (OH str), 2921, 2853 (aromatic C-H str), 1676 (C=O str), 1588 (aromatic, C=C str), 1276, 1066, 820, 746 (C-Br, str);^{1}H-NMR ($CDCl_3$, 500MHz) δ (ppm): 7.79 (d, *J* = 8.5 Hz, 1 H, H_{Ar}), 7.71 (d, *J* = 7.0 Hz, 2 H, H_{Ar}), 7.50 (d, *J* = 7.0 Hz, 2 H, H_{Ar}), 7.40 (m, 2 H, H_{Ar}), 5.30 (d, *J* = 4.5 Hz, 1 H, H2), 5.15 (d, *J* = 4.5 Hz, 1 H, H3), 4.05 (s, br, D_2O exchangeable, 1 H);^{13}C-NMR ($CDCl_3$, 125 MHz) δ (ppm): 196.5 (C=O), 136.8, 132.6, 132.2, 131.8, 130.0, 129.8, 129.6, 123.1, 75.9 (C2), 62.8 (C3);MS (EI, 70eV): m/z (%) = 380(32) [$M^{+\cdot}$, $C_{15}H_{10}Br_2O_2$], 185(75), 183 (100); HRMS (ESI-TOF) calcd for $C_{15}H_{10}Br_2O_2$ 379.9048, found 379.9047; The absolute configuration was determined by comparison with the optical rotation reported for the $[\alpha]_D^{25}$ = -16.0 (c 0.98, $CHCl_3$).

2.3.12 3-p-Tolyl-5-bromo-2-hydroxy-2,3-dihydroindan-1-one (2n):

Light yellow solid; Yield: 282 mg (89%); m.p = 181-183°C;IR ν_{max} (KBr, cm^{-1}): 3464 (OH str), 2917, 2849 (aromatic C-H str), 1685 (C=O str), 1586 (aromatic, C=C str), 1279, 1071, 815, 757 (C-Br, str). ^{1}H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 7.69 (m, 2 H, H_{Ar}), 7.69 (m, 1 H, H_{Ar}), 7.32 (d, *J* = 8.0 Hz, 2 H, H_{Ar}), 7.10 (m, 2 H, H_{Ar}), 5.23 (d, *J* = 2.5 Hz, 1 H, H2), 5.10 (d, *J* = 2.5 Hz, 1 H, H3), 3.98 (s, br, D_2O exchangeable, 1 H), 2.26 (s, 3 H);^{13}C-NMR ($CDCl_3$, 125 MHz) δ (ppm): 195.99 (C=O), 137.84, 133.76, 131.41, 129.00, 128.24, 126.79, 75.23 (C2), 62.68 (C3), 20.12;MS (EI, 70eV): m/z (%) = 316(14) [$M^{+\cdot}$, $C_{16}H_{13}BrO_2$], 219(59), 185 (100), 183(82); HRMS (ESI-TOF) calcd for $C_{16}H_{13}BrO_2$ 316.0099, found 316.0100; The absolute configuration was determined by comparison with the optical rotation reported for the $[\alpha]_D^{25}$ = -10.2 (c 0.26, $CHCl_3$).

2.3.13 2-Hydroxy-5,6-dimethyl-3-phenyl-2,3-dihydroinden-1-one (2o):

Light yellow solid; Yield: 464 mg (92%); m.p = 112-114°C;IR ν_{max} (KBr, cm^{-1}): 3420 (OH str), 2959, 2869 (aromatic C-H str), 1688 (C=O str), 1583 (aromatic, C=C str), 1253, 1063, 835;^{1}H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 7.71 (m, 1 H, H_{Ar}), 7.63 (dd, *J* = 7.0, 1.5 Hz, 1 H, H_{Ar}), 7.54 (d, *J* = 7.5 Hz, 2 H, H_{Ar}), 7.36 (t, *J* = 7.0 Hz, 1 H, H_{Ar}), 7.32 (d, *J* = 7.0 Hz, 1 H, H_{Ar}), 7.27 (d, *J* = 8.0 Hz, 1 H, H_{Ar}), 5.35 (d, *J* = 2.5 Hz, 1 H, H2), 5.25 (d, *J* = 2.5 Hz, 1 H, H3), 3.95 (s, br, D_2O exchangeable, 1 H), 2.34 (s, 3 H), 2.33 (s, 3 H); ^{13}C-NMR ($CDCl_3$, 125 MHz) δ (ppm): 197.4 (C=O), 144.2, 138.4, 137.8, 131.3, 130.3, 129.8, 128.7, 128.5, 127.9, 126.2, 75.8 (C2), 64.1 (C3), 20.2, 19.8; MS (EI, 70eV): m/z (%) = 252(07) [$M^{+\cdot}$, $C_{17}H_{16}O_2$], 234(15),105 (25), 88(100); HRMS (ESI-TOF) calcd for $C_{17}H_{16}O_2$ 252.1150, found 252.1151; The absolute configuration was determined by comparison with the optical rotation reported for the $[\alpha]_D^{25}$ = -16.8 (c 1.1, $CHCl_3$).

2.3.14 2-Hydroxy-5,6-dimethyl-3-(3-nitrophenyl)-2,3-dihydro inden-1-one (2r):

Light yellow solid; Yield: 469 mg (79%); m.p = 142-144°C;IR ν_{max} (KBr, cm^{-1}): 3381 (OH str), 2943 (aromatic C-H str), 1674 (C=O str), 1620 (aromatic, C=C str), 1504 (N─O str), 1371, 1353 (N─O bending), 1241, 1061, 916, 832, 783, 675;^{1}H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 8.14 (m, 1 H, H_{Ar}), 7.94 (m, 1 H, H_{Ar}), 7.59 (m, 2 H, H_{Ar}), 7.44 (d, *J* = 8.0 Hz, 1 H, H_{Ar}), 7.29 (d, *J* = 8.0 Hz, 1 H, H_{Ar}), 5.54 (d, *J* = 4.0 Hz, 1 H, H2), 5.34 (d, *J* = 4.0 Hz, 1 H, H3), 3.82 (s, br, D_2O exchangeable, 1 H), 2.35(s, 3 H), 2.30 (s, 3 H);^{13}C-NMR ($CDCl_3$, 125 MHz) δ (ppm): 196.9(C=O), 147.7, 145.1, 138.1, 137.7, 134.3, 131.7, 130.5, 129.6, 129.1, 126.4, 123.7, 123.2, 76.5 (C2), 62.0 (C3), 20.2, 19.8;MS (EI, 70eV): m/z (%) = 297(14) [$M^{+\cdot}$, $C_{17}H_{15}NO_4$], 280 (10), 133 (100); HRMS (ESI-TOF) calcd for $C_{17}H_{15}NO_4$ 297.1001, found 297.1003; The absolute configuration was determined by comparison with the optical rotation reported for the $[\alpha]_D^{25}$ = -10.1 (c 0.57, $CHCl_3$).

2.3.15 3-(4-Chlorophenyl)-2-hydroxy-2,3-dihydrocyclopenta[b] naphthalen-1-one (2t):

Light yellow solid; Yield: 562 mg (91%); m.p = 108-110°C; IR ν_{max} (KBr, cm^{-1}): 3415 (OH str), 2931, 2873 (aromatic C-H str), 1681 (C=O str), 1597 (aromatic, C=C str), 1263, 1081, 860, 737;^{1}H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 8.41 (m, 1H, H_{Ar}), 7.97 (t, *J* = 8.0 Hz, 2 H, H_{Ar}), 7.92 (t, *J* = 8.0 Hz, 2 H, H_{Ar}), 7.62 (dd, *J* = 2.0, 7.5 Hz, 2 H, H_{Ar}), 7.50 (d, *J* = 7.0 Hz, 2 H, H_{Ar}), 7.33 (d, *J* = 7.5 Hz, 1H, H_{Ar}), 5. 49 (d, *J* = 2.0 Hz, 1H, H2), 5.27 (d, *J* = 2.0 Hz, 1H, H3), 4.15 (s, br, D_2O exchangeable, 1 H);^{13}C-NMR ($CDCl_3$, 125 MHz) δ (ppm): 197.4 (C=O), 136.7, 136.0, 134.8, 132.4, 130.8, 130.5, 129.7, 129.4, 129.3, 129.3, 128.8, 128.0, 127.4, 123.8, 75.9 (C2), 63.1 (C3);MS (EI, 70eV): m/z (%) = 308 (11) [$M^{+\cdot}$, $C_{19}H_{13}ClO_2$], 290 (23), 144 (100), 65 (45); HRMS (ESI-TOF) calcd for $C_{19}H_{13}ClO_2$ 308.0604, found 308.0606; The absolute configuration was determined by comparison with the optical rotation reported for the $[\alpha]_D^{25}$ = -3.8 (c 0.14, $CHCl_3$).

2.3.16 3-(4-Bromophenyl)-2-hydroxy-2,3-dihydrocyclopenta[b] naphthalen-1-one (2u):

Light yellow solid; Yield: 537 mg (92%); m.p = 112-114°C;IR ν_{max} (KBr, cm^{-1}): 3409 (OH str), 2925, 2870 (aromatic C-H str), 1685 (C=O str), 1590 (aromatic, C=C str), 1258, 1080, 865, 730; ^{1}H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 8.42 (m, 1 H, H_{Ar}), 7.98 (t, *J* = 8.0 Hz, 2 H, H_{Ar}), 7.93 (t, *J* = 8.0 Hz, 2 H, H_{Ar}), 7.65 (dd, *J* = 2.0, 7.5 Hz, 2 H, H_{Ar}), 7.50 (d, *J* = 7.0 Hz, 2 H, H_{Ar}), 7.43 (d, *J* = 7.5 Hz, 1 H, H_{Ar}), 5. 50 (d, *J* = 2.0 Hz, 1 H, H2), 5.27 (d, *J* = 2.0 Hz, 1 H, H3), 4.20 (s, br, D_2O exchangeable, 1 H);^{13}C-NMR ($CDCl_3$, 125 MHz) δ (ppm): 197.3 (C=O), 137.2, 136.0, 132.4, 131.7, 130.8, 130.5, 129.7, 129.7, 129.3, 129.3, 128.0, 127.4, 123.7, 123.0, 75.9 (C2), 63.2 (C3).MS (EI, 70eV): m/z (%) = 352 (09), 354 (09) [$M^{+\cdot}$, $C_{19}H_{13}BrO_2$], 155 (100); HRMS (ESI-TOF) calcd for $C_{19}H_{13}BrO_2$ 352.0099, found 352.0101; The absolute configuration was determined by comparison with the optical rotation reported for the $[\alpha]_D^{25}$ = -4.4 (c 0.20, $CHCl_3$).

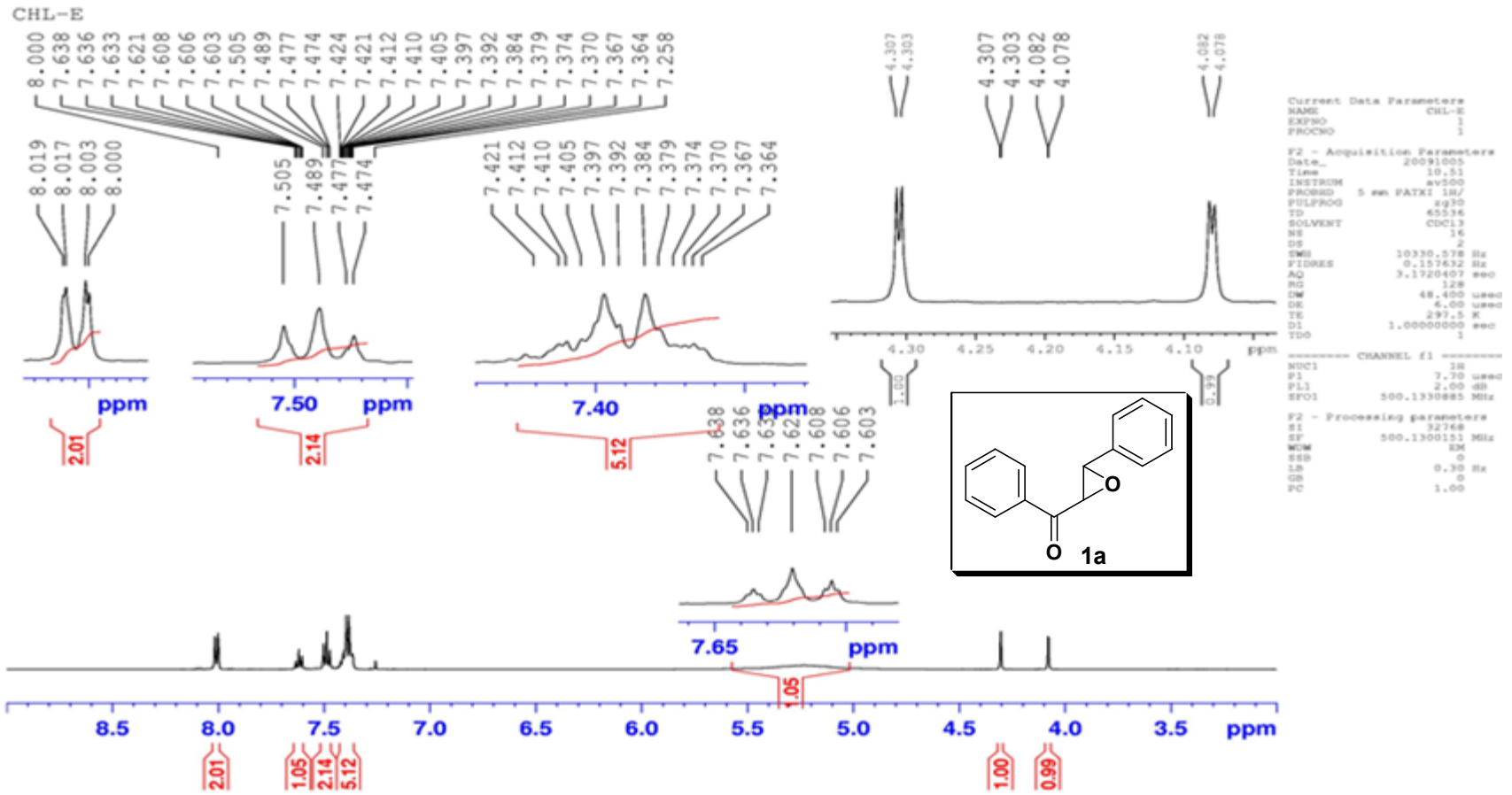
2.3.17 2-Hydroxy-3-p-tolyl-2,3-dihydrocyclopenta[b]naphth-alen-1-one (2v):

Light yellow solid; Yield: 496 mg (86%); m.p = 125-127°C;IR ν_{max} (KBr, cm^{-1}): 3429 (OH str), 2951, 2880 (aromatic C-H str), 1692 (C=O str), 1607 (aromatic, C=C str), 1271, 1107, 843, 729; ^{1}H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 8.41 (m, 1 H, H_{Ar}), 7.98-7.87 (m, 3 H, H_{Ar}), 7.63 (m, 2 H, H_{Ar}), 7.45 (d, *J* = 8.0 Hz, 2 H, H_{Ar}), 7.17 (d, *J* = 8.0 Hz, 2 H, H_{Ar}), 5. 52 (d, *J* = 2.0 Hz, 1 H, H2), 5.29 (d, *J* = 2.0 Hz, 1 H, H3), 4.09 (s, br, D_2O exchangeable, 1 H), 2.32 (s, 3H); ^{13}C-NMR ($CDCl_3$, 125 MHz) δ (ppm): 197.8 (C=O), 138.8, 136.0, 135.3, 132.4, 130.9, 130.5, 129.7, 129.3, 129.2, 128.6, 128.3, 127.9, 127.3, 123.9, 76.3 (C2), 64.0 (C3), 21.2; MS (EI, 70eV): m/z (%) = 288 (08) [$M^{+\cdot}$, $C_{20}H_{16}O_2$], 270 (28), 133 (100); HRMS (ESI-TOF) calcd for $C_{18}H_{18}O_2$ 266.1307, found 266.1308; The absolute configuration was determined by comparison with the optical rotation reported for the $[\alpha]_D^{25}$ = -10.5 (c 0.32, $CHCl_3$).

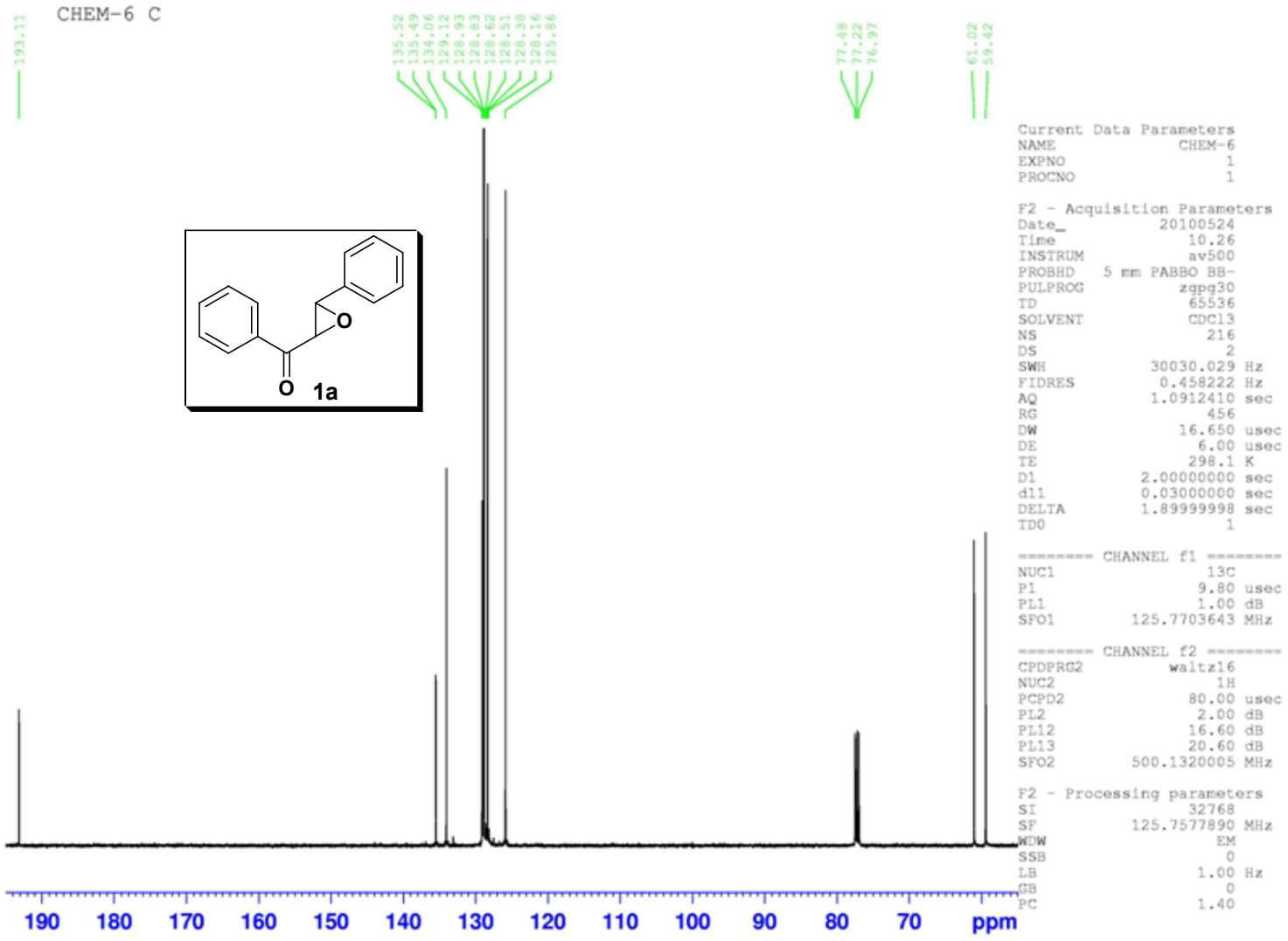
2.3.18 2-Hydroxy-3-(3-nitrophenyl)-2,3-dihydrocyclopenta[b] naphthalen-1-one (2w):

Light yellow solid; Yield: 728 mg (76%); m.p =138-140°C;IR ν_{max} (KBr, cm^{-1}): 3382 (OH str), 2992, 2886 (aromatic C-H str), 1695 (C=O str), 1620 (aromatic, C=C str), 1262, 1095, 860, 743;^{1}H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 8.54 (m, 1 H, H_{Ar}), 8.14 (m, 1 H, H_{Ar}), 7.97-7.87 (m, 3 H, H_{Ar}), 7.70 (m, 1 H, H_{Ar}), 7.62 (m, 1 H, H_{Ar}), 7.59 (m, 1 H, H_{Ar}), 7.43 (m, 1 H, H_{Ar}), 7.25 (m, 1 H, H_{Ar}), 5.72 (d, *J* = 2.0 Hz, 1 H, H2), 5.40 (d, *J* = 2.0 Hz, 1 H, H3), 3.84 (s, br, D_2O exchangeable, 1 H);^{13}C-NMR ($CDCl_3$, 125 MHz) δ (ppm): 197.2 (C=O), 137.8, 136.2, 134.2, 132.3, 131.2, 130.9, 129.8, 129.7, 129.5, 129.2, 128.0, 127.6, 123.8, 123.6, 123.2, 76.6 (C2), 61.9 (C3);MS (EI, 70eV): m/z (%) = 319 (09) [$M^{+\cdot}$, $C_{19}H_{13}NO_4$], 302 (12), 189 (20), 155 (100), 127 (50); HRMS (ESI-TOF) calcd for $C_{19}H_{13}NO_4$ 319.0845, found 319.0847; The absolute configuration was determined by comparison with the optical rotation reported for the $[\alpha]_D^{25}$ = -9.8 (c 0.60, $CHCl_3$).

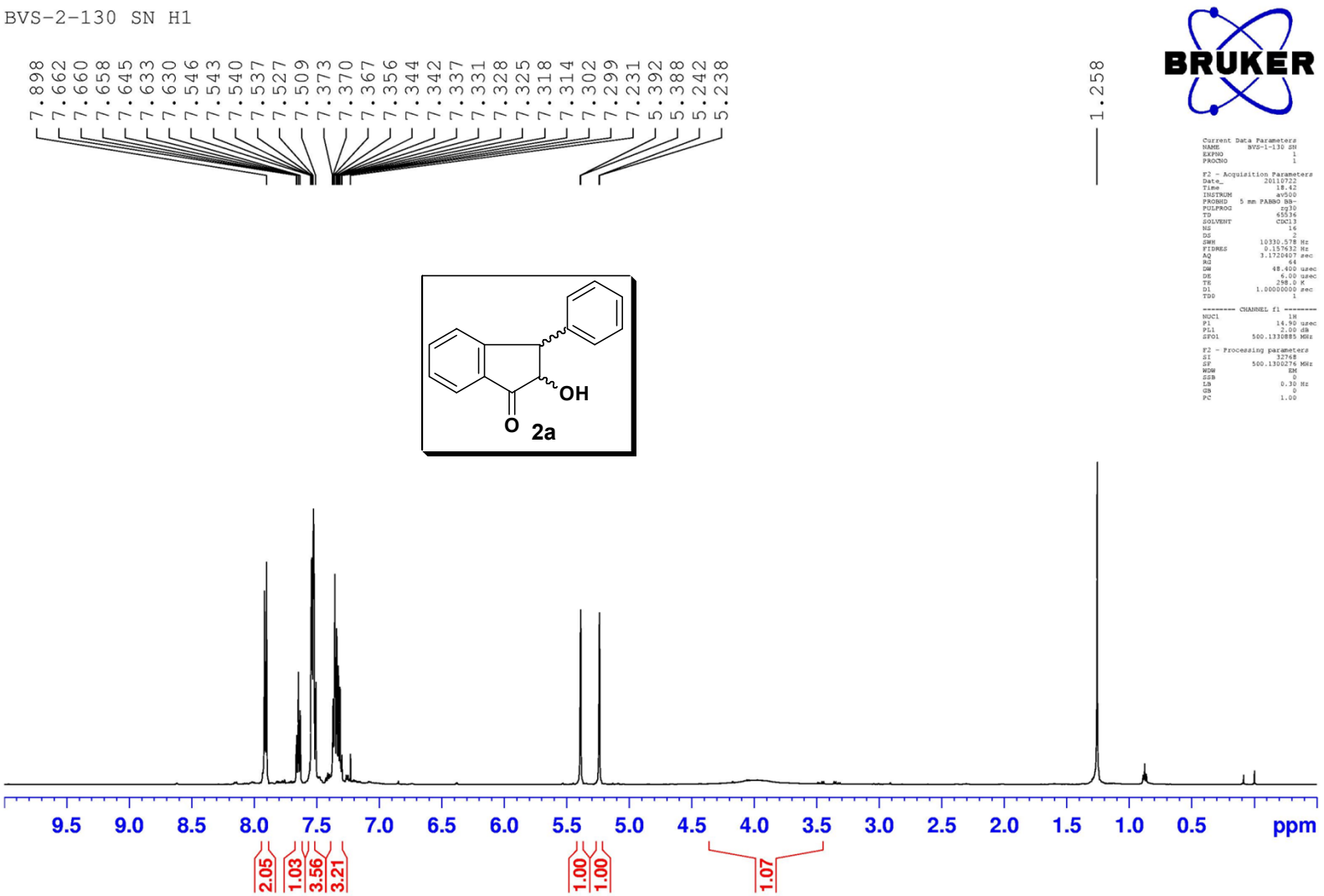
3. ^{1}H & ^{13}C-NMR spectrum of Epoxy chalcones and 2-hydroxy-Indanone derivatives



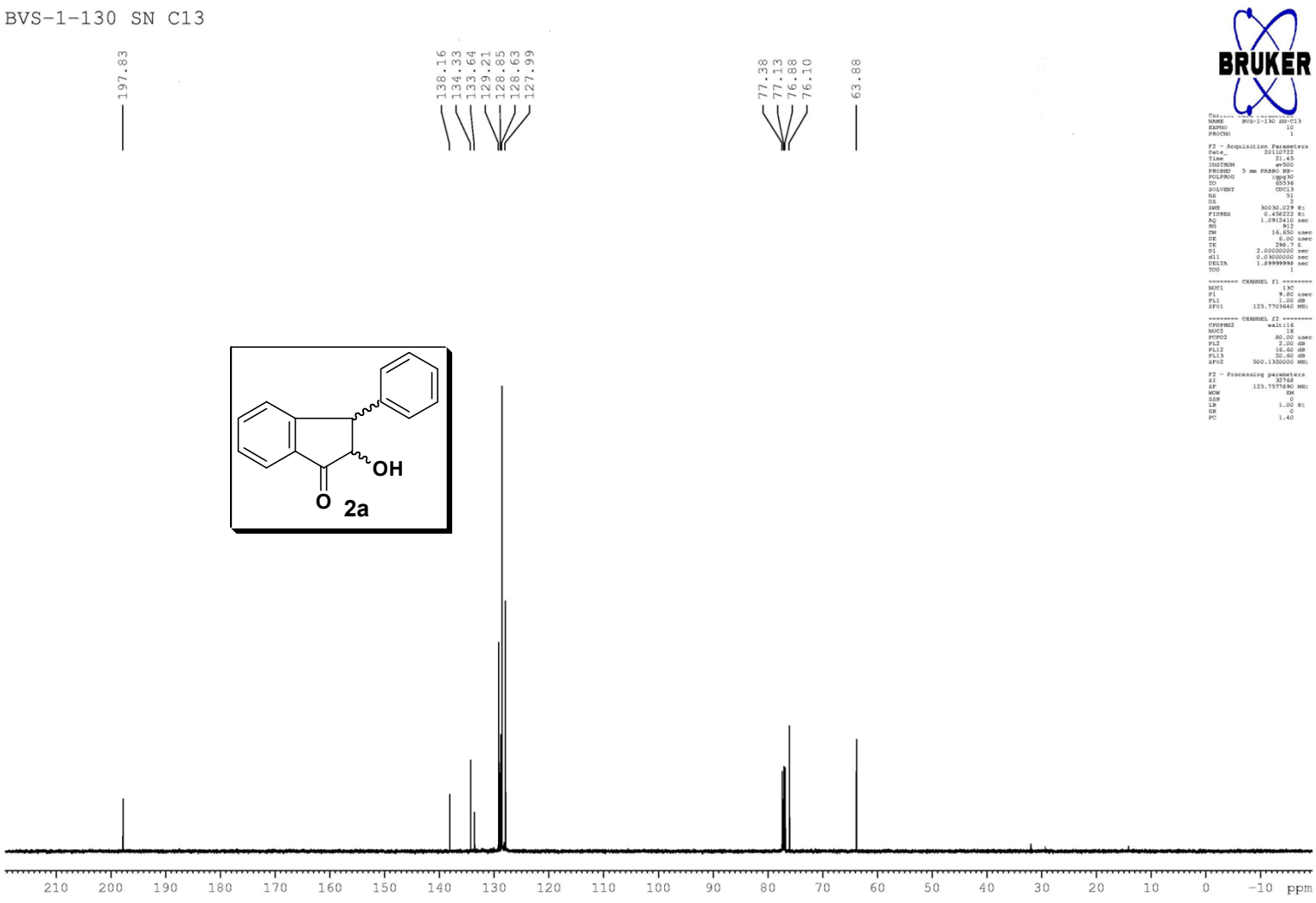
^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of **1a**



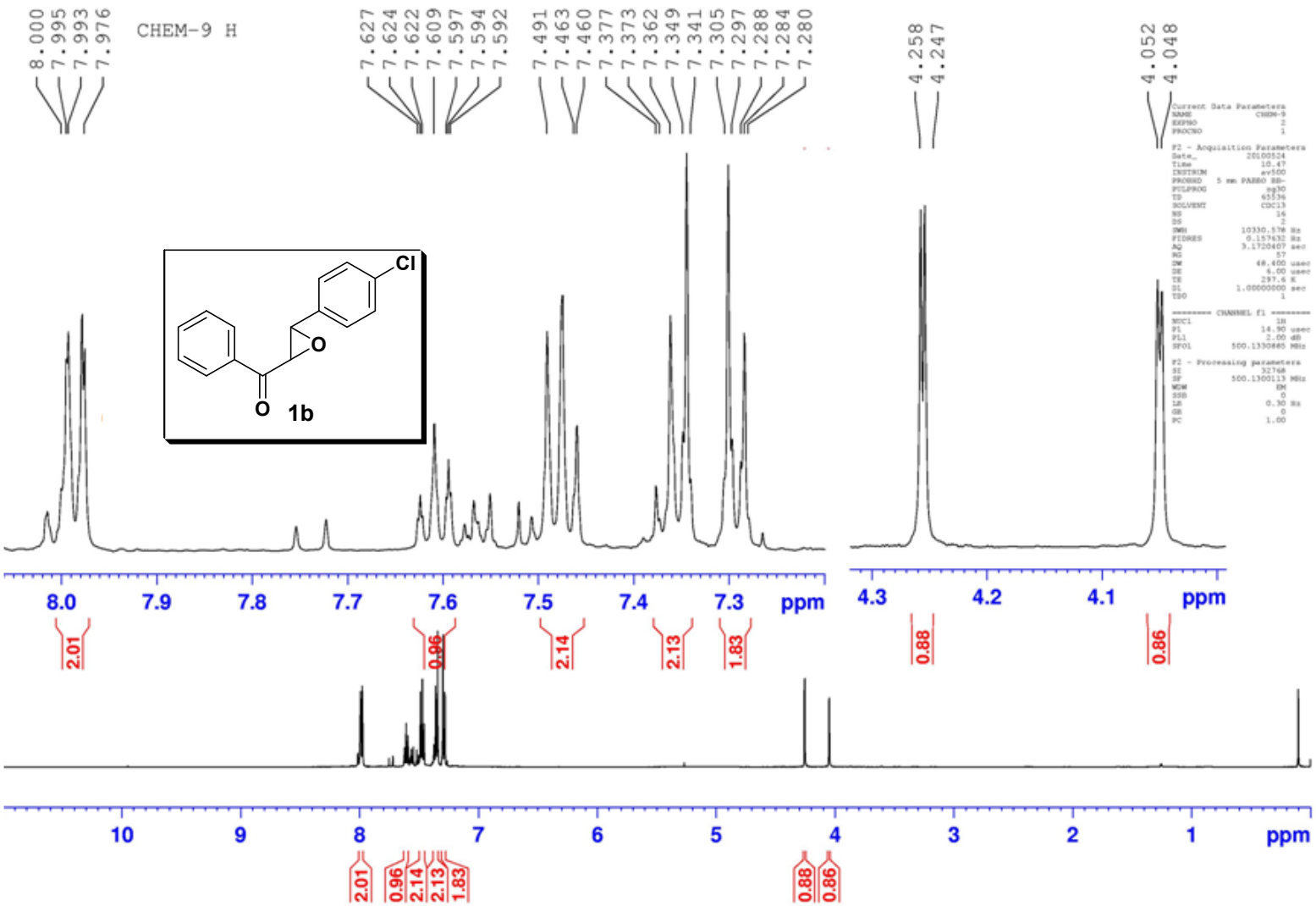
^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **1a**



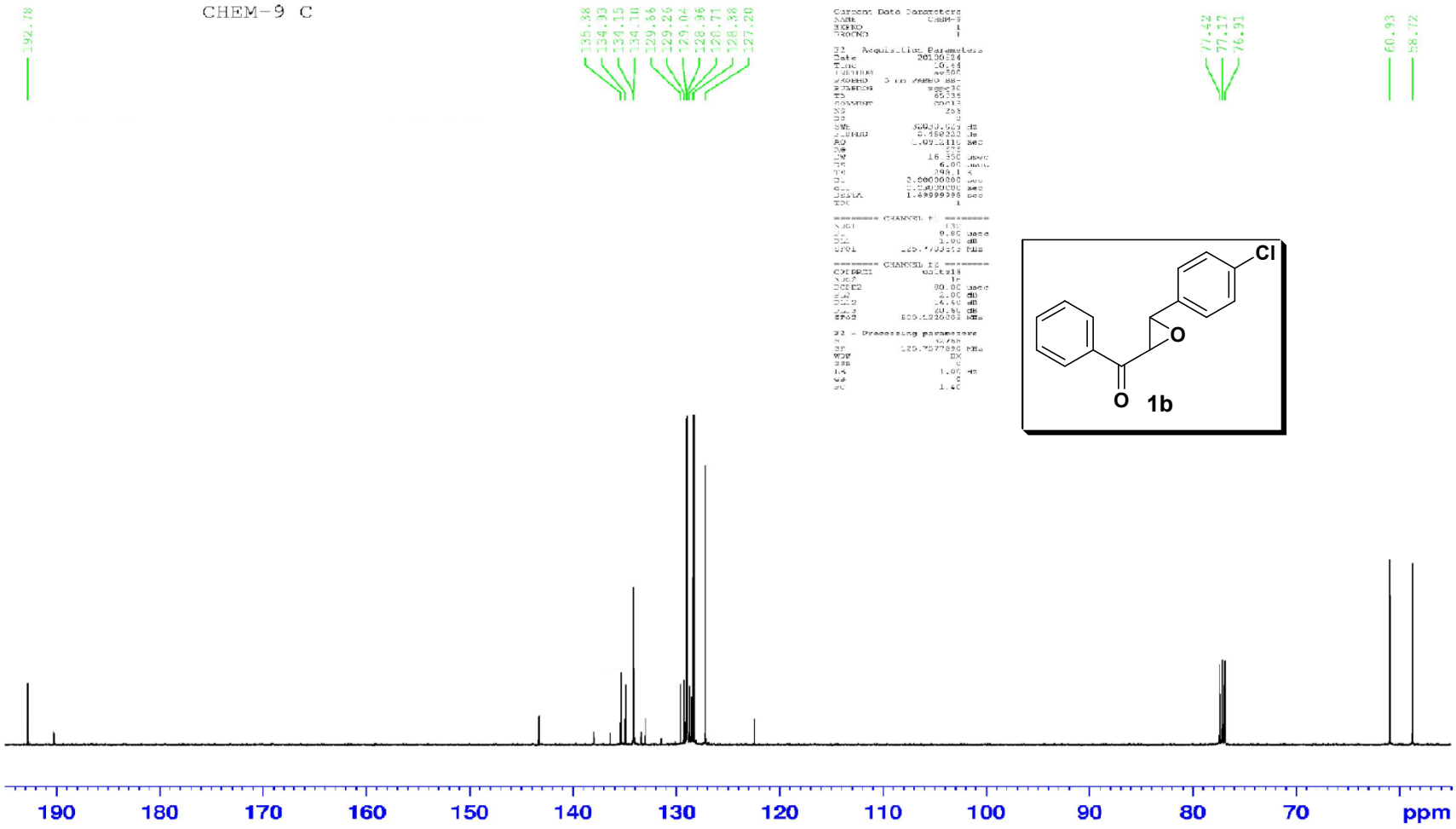
^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of **2a**



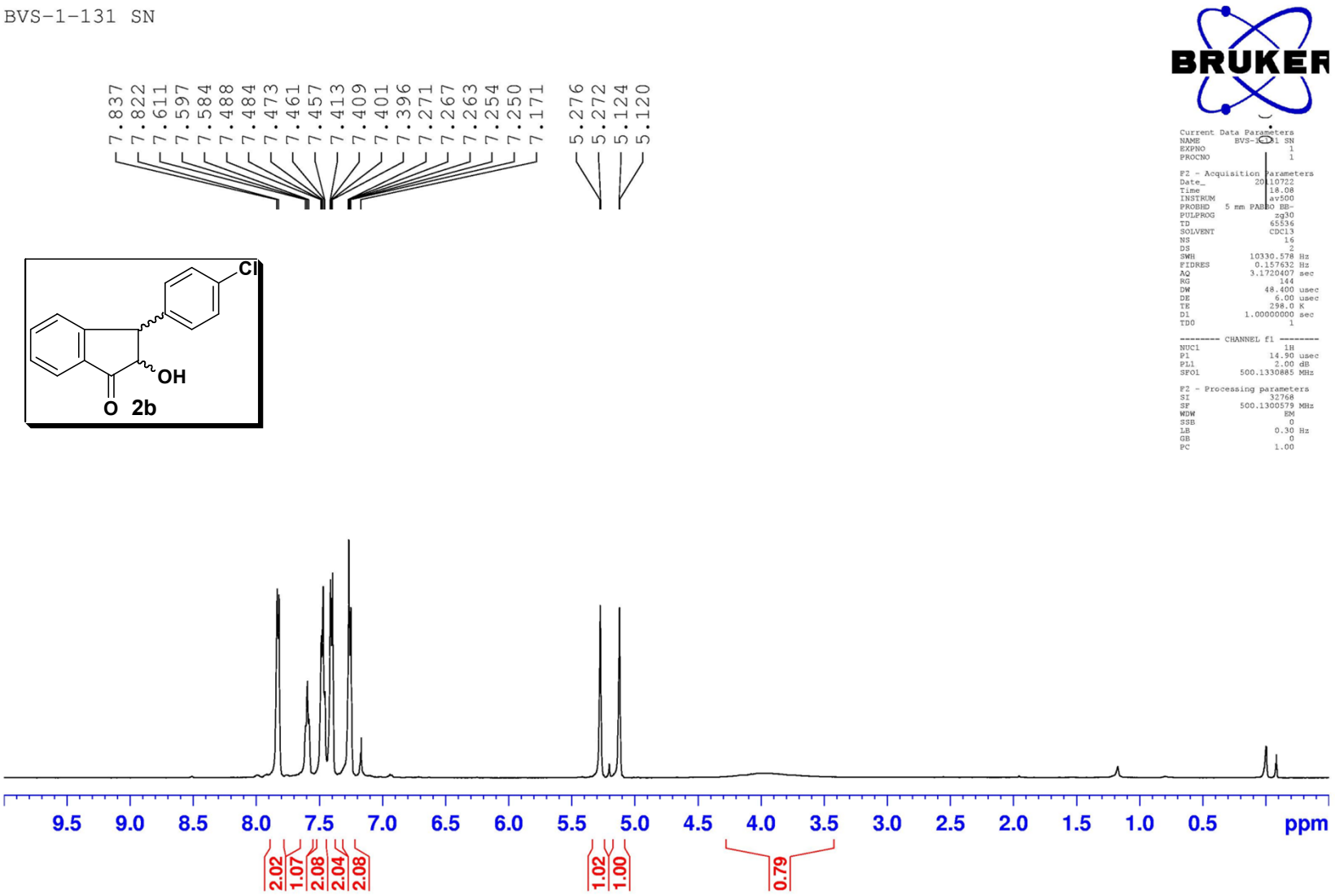
^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **2a**



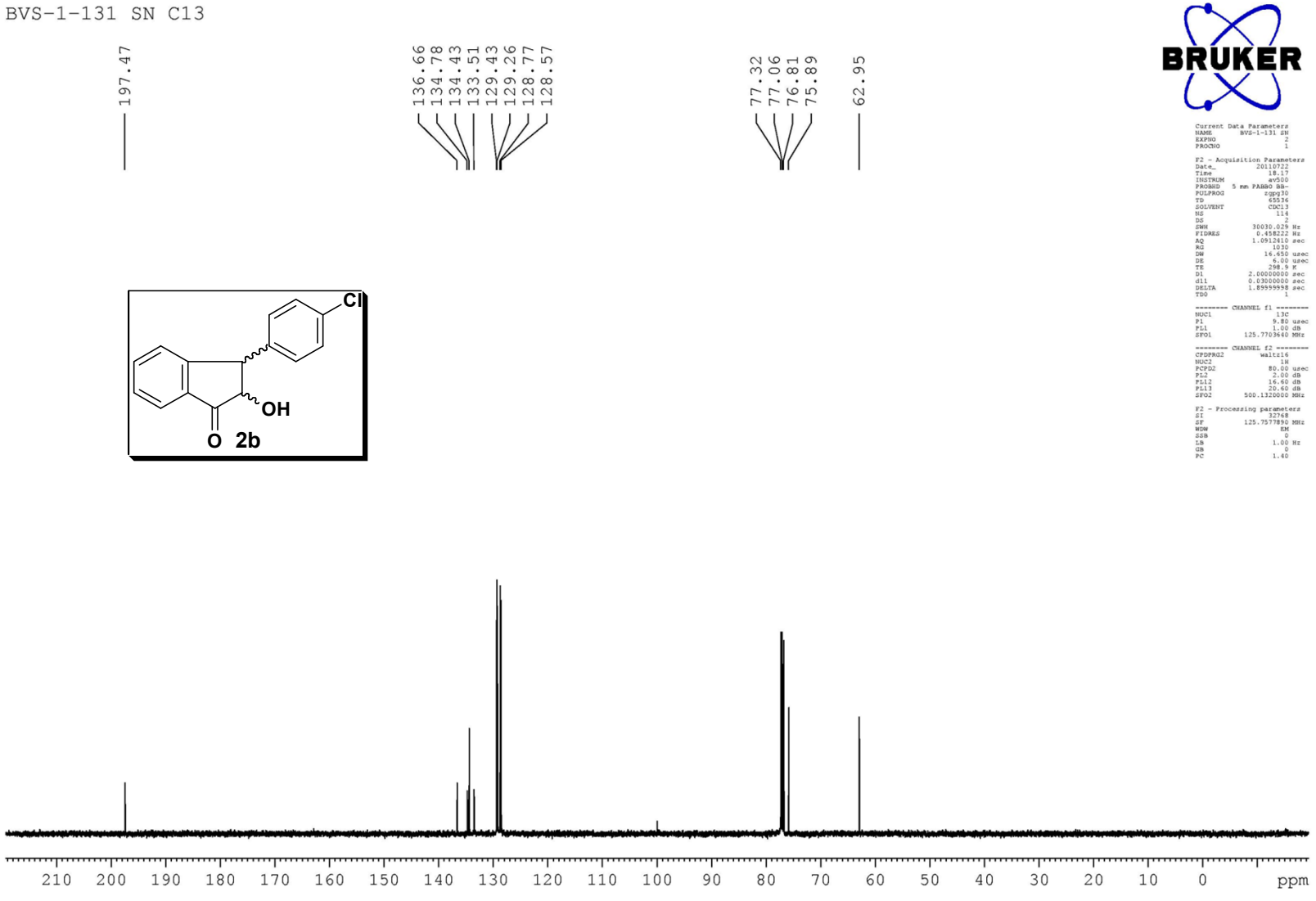
^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of **1b**



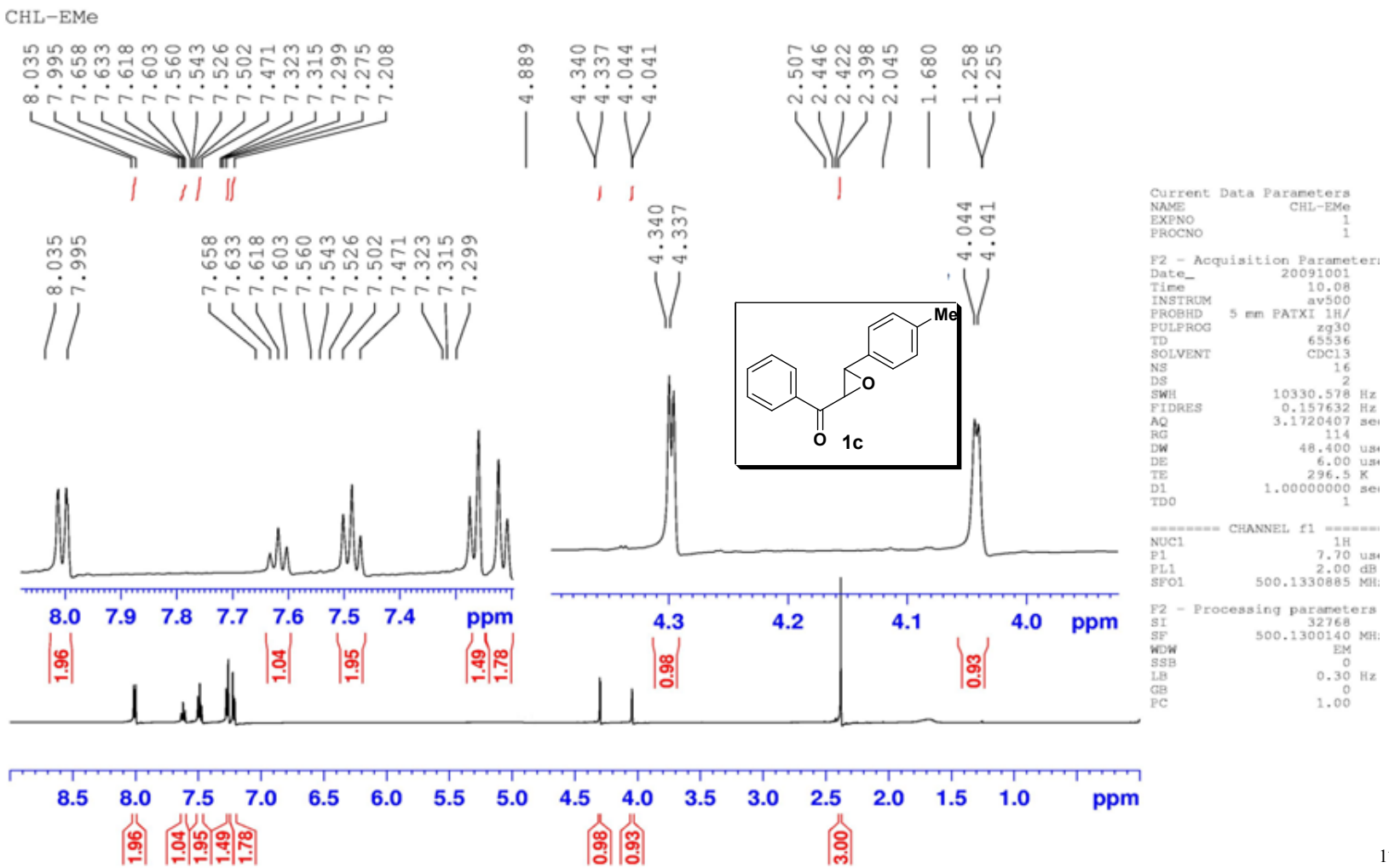
^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **1b**



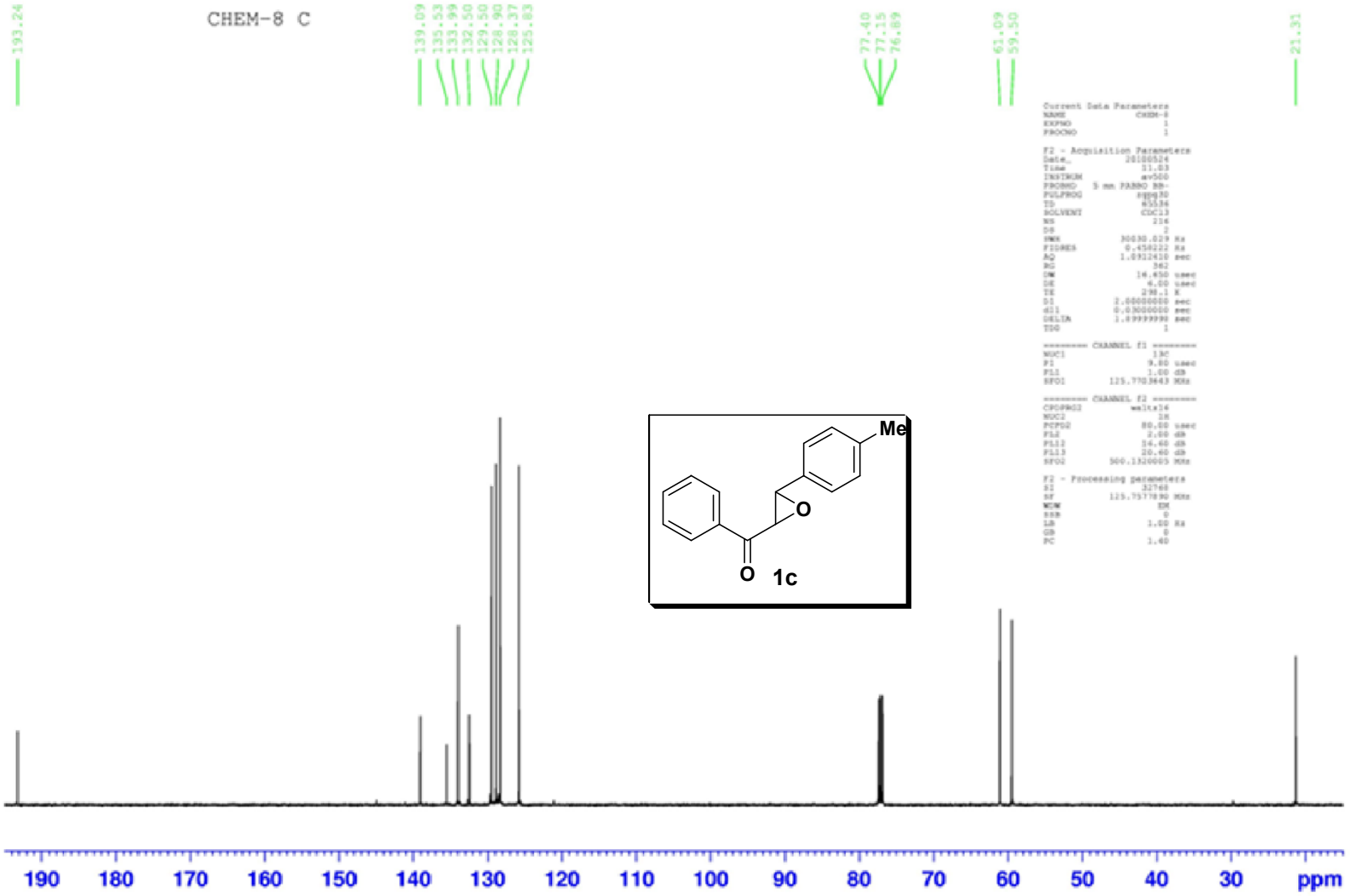
^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of **2b**



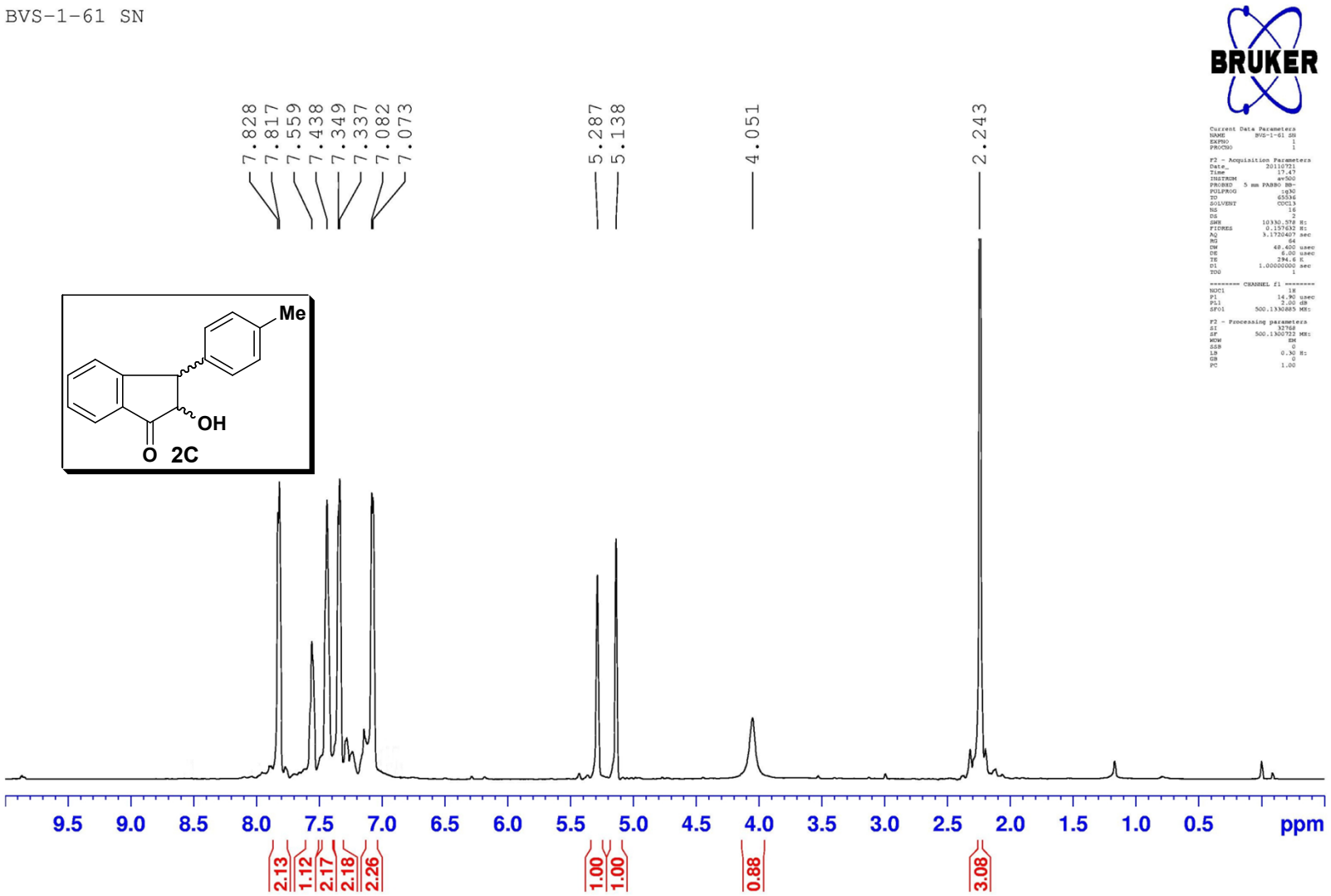
^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **2b**



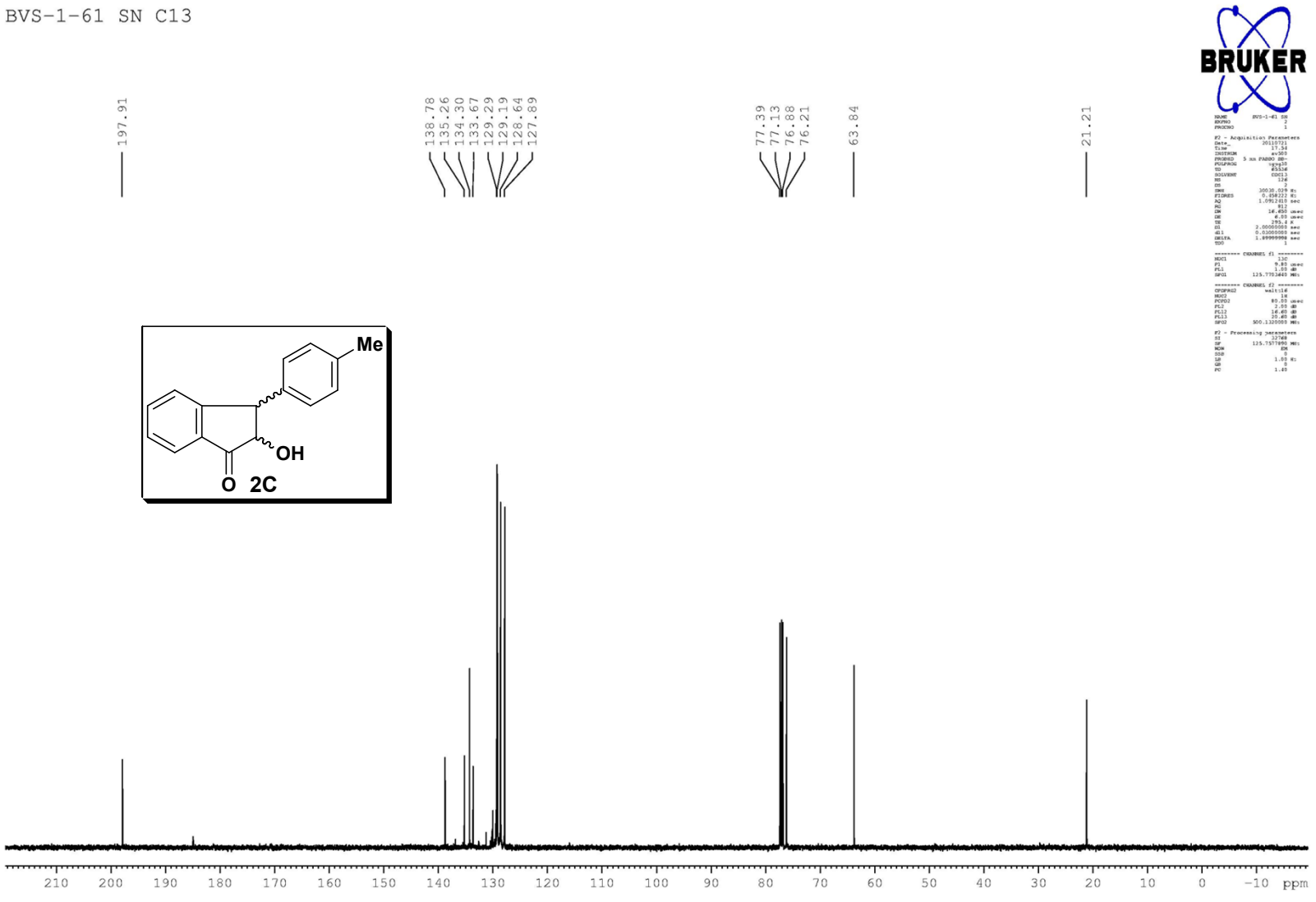
^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of **1c**



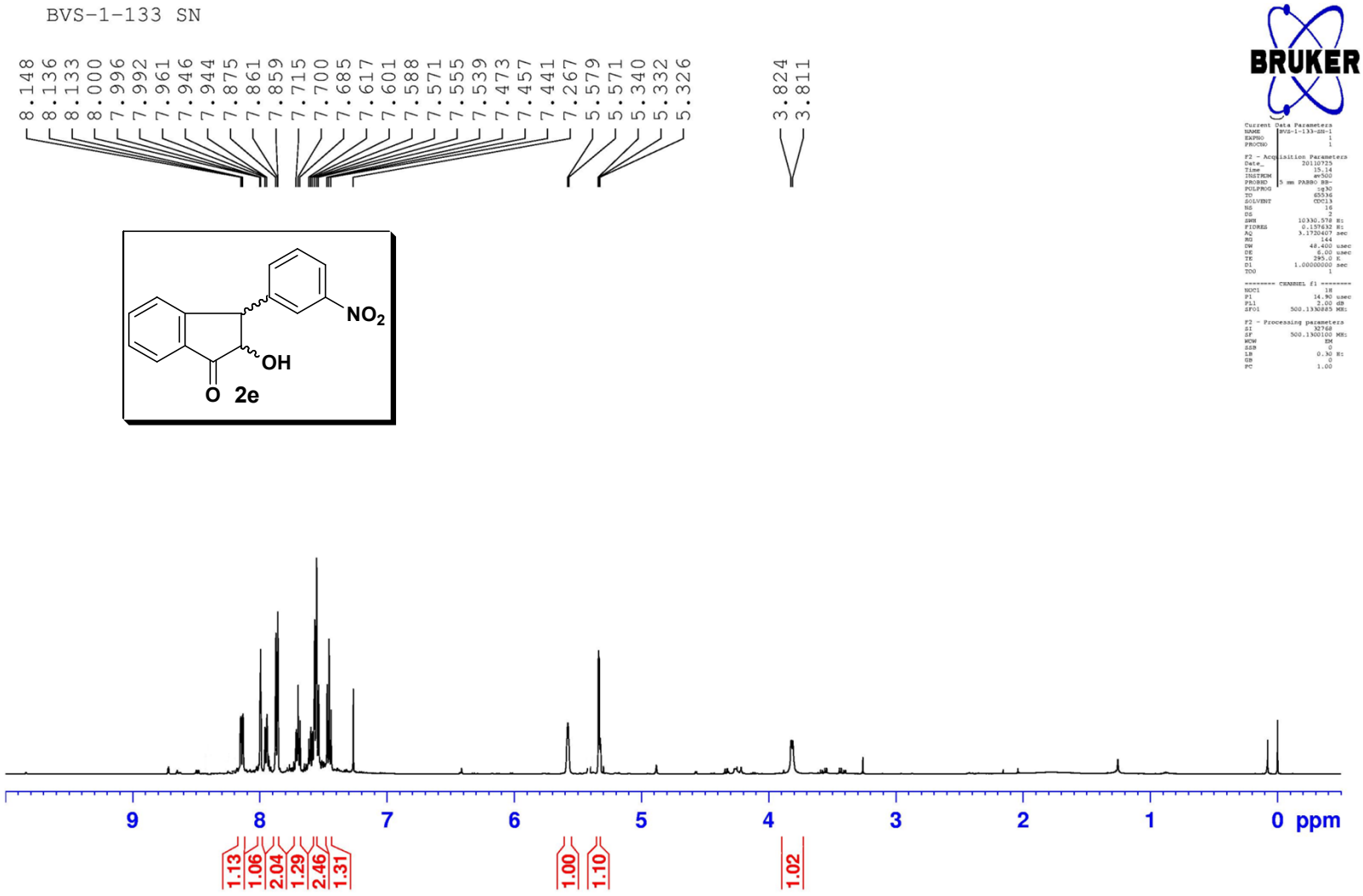
^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of **1c**



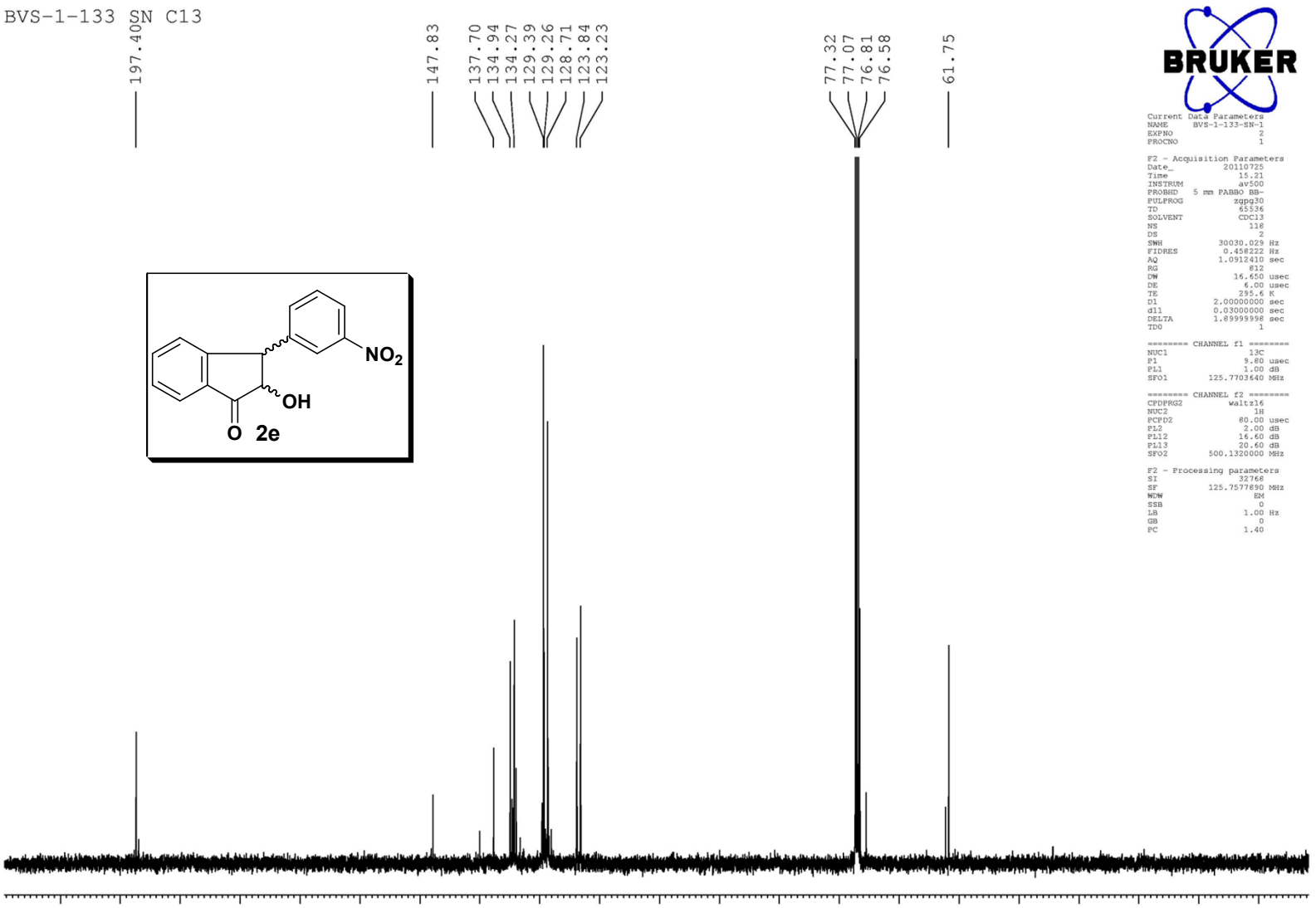
^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of **2c**



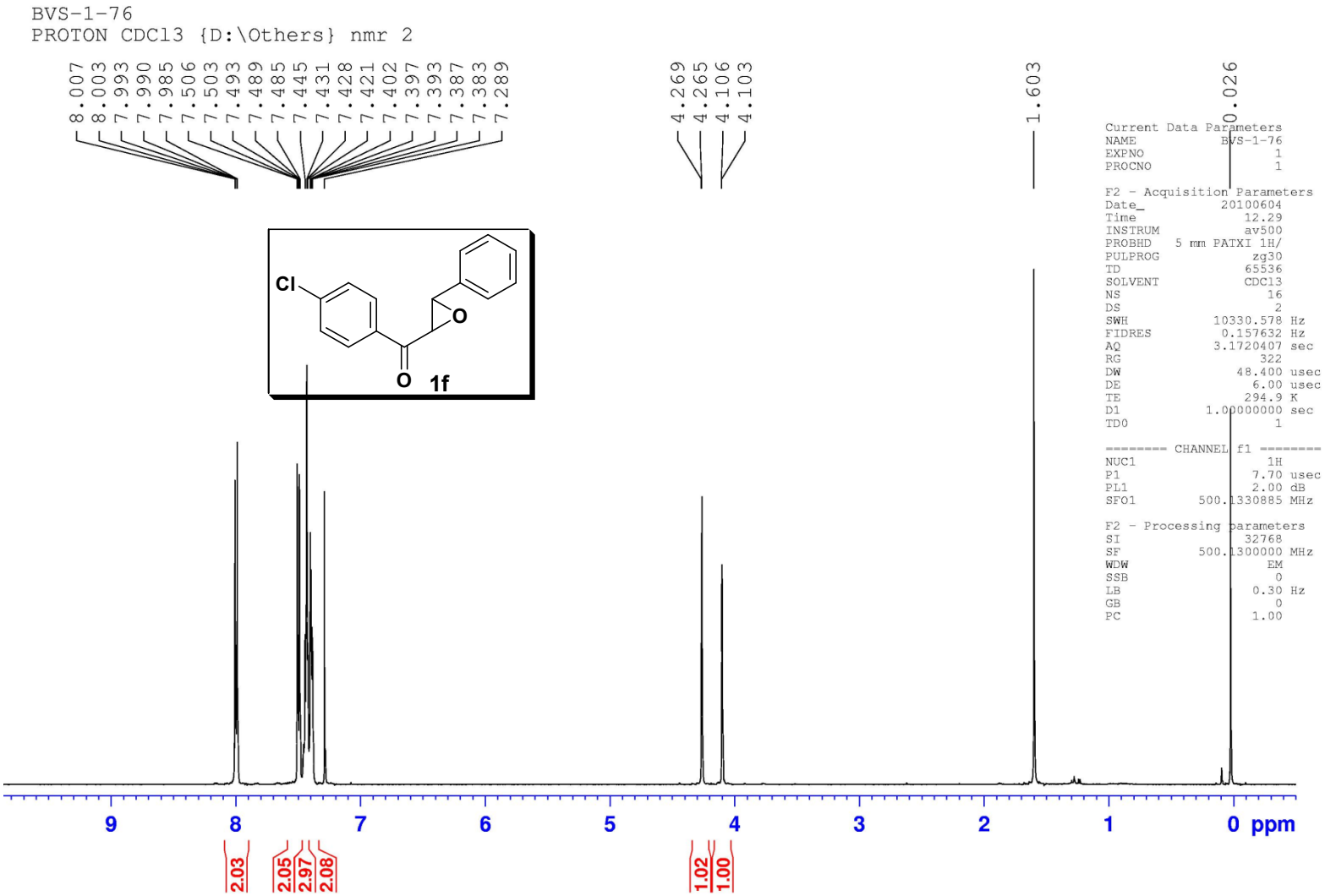
^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **2c**



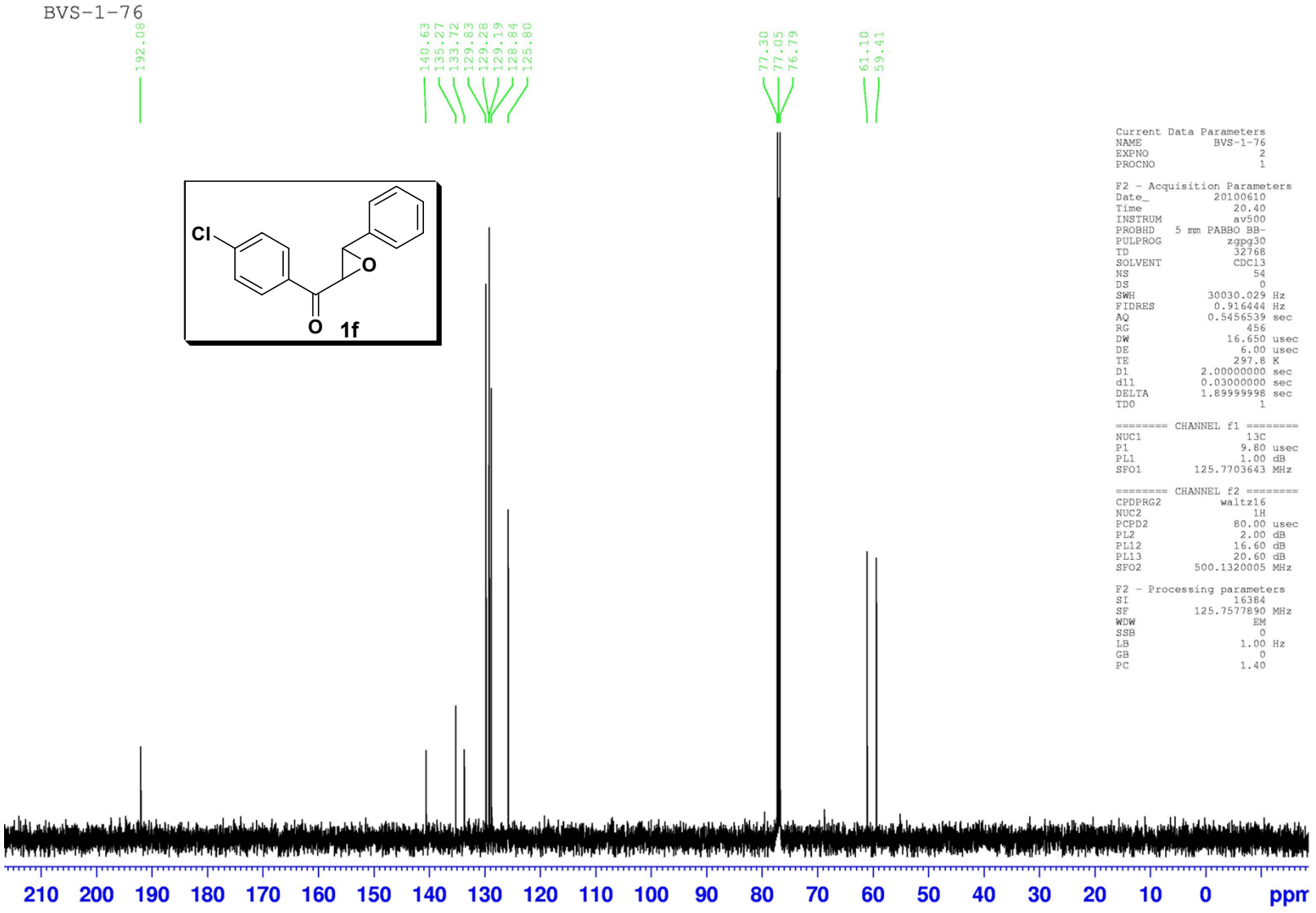
^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of **2e**



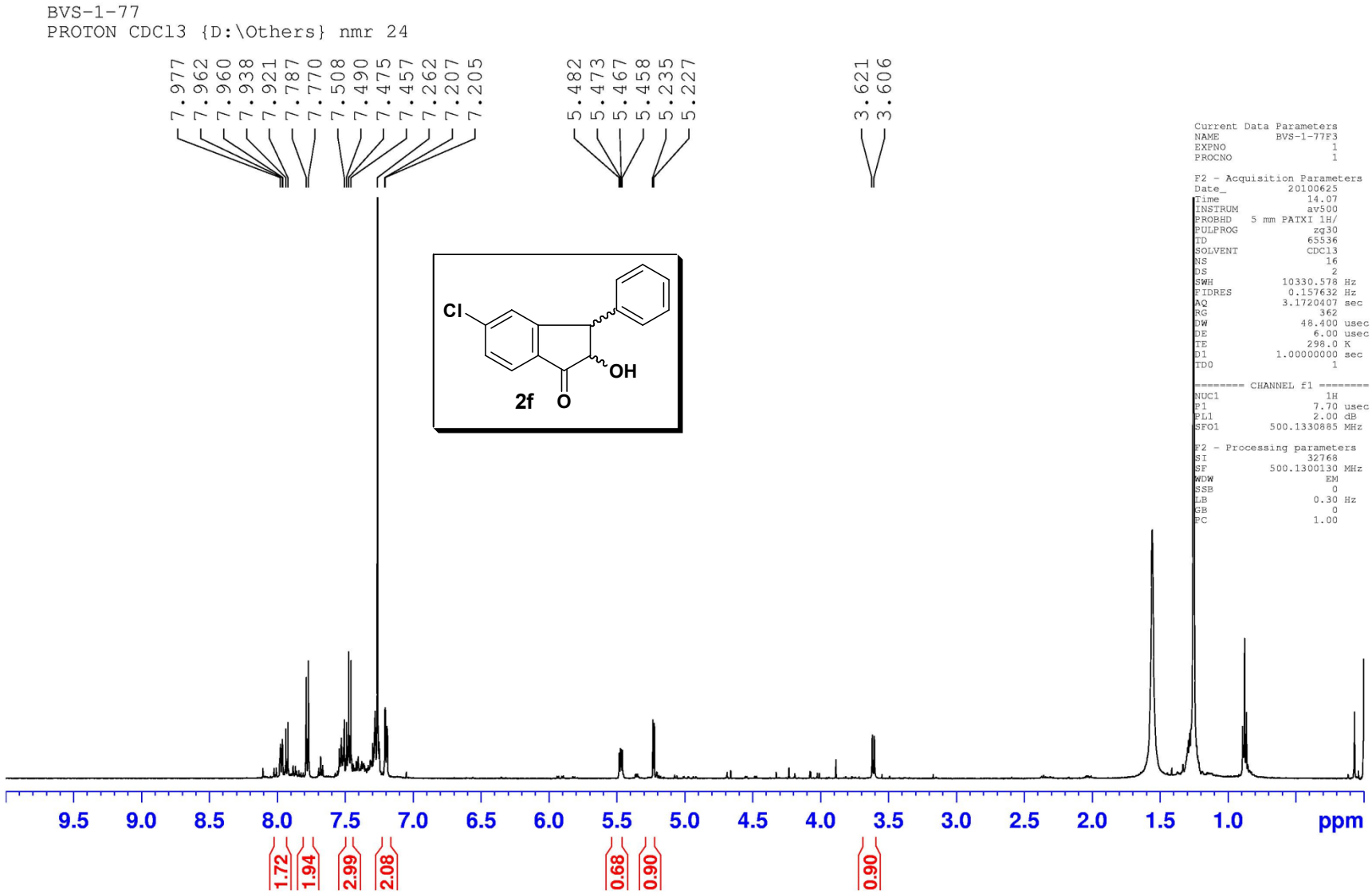
^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **2e**



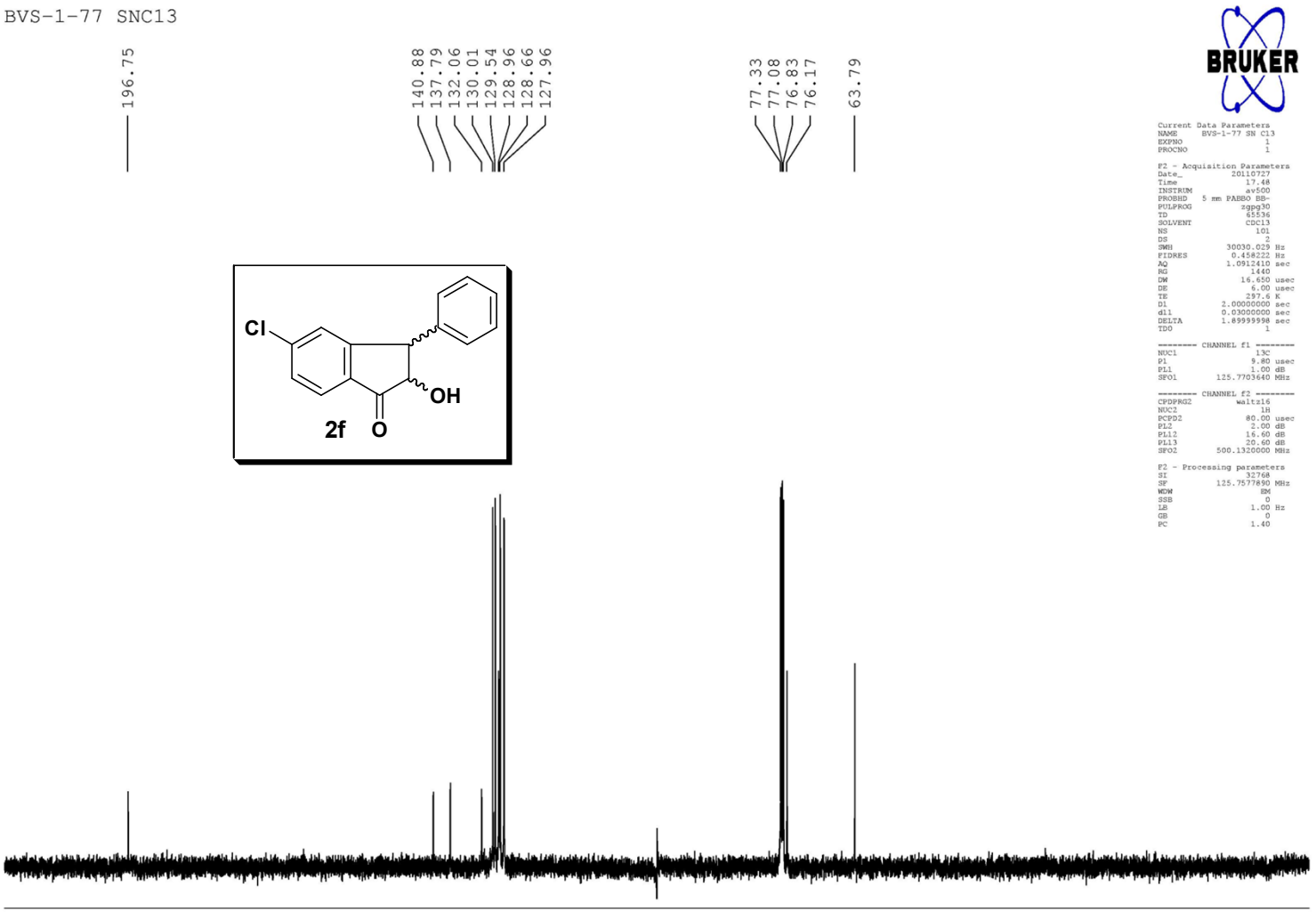
^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of **1f**



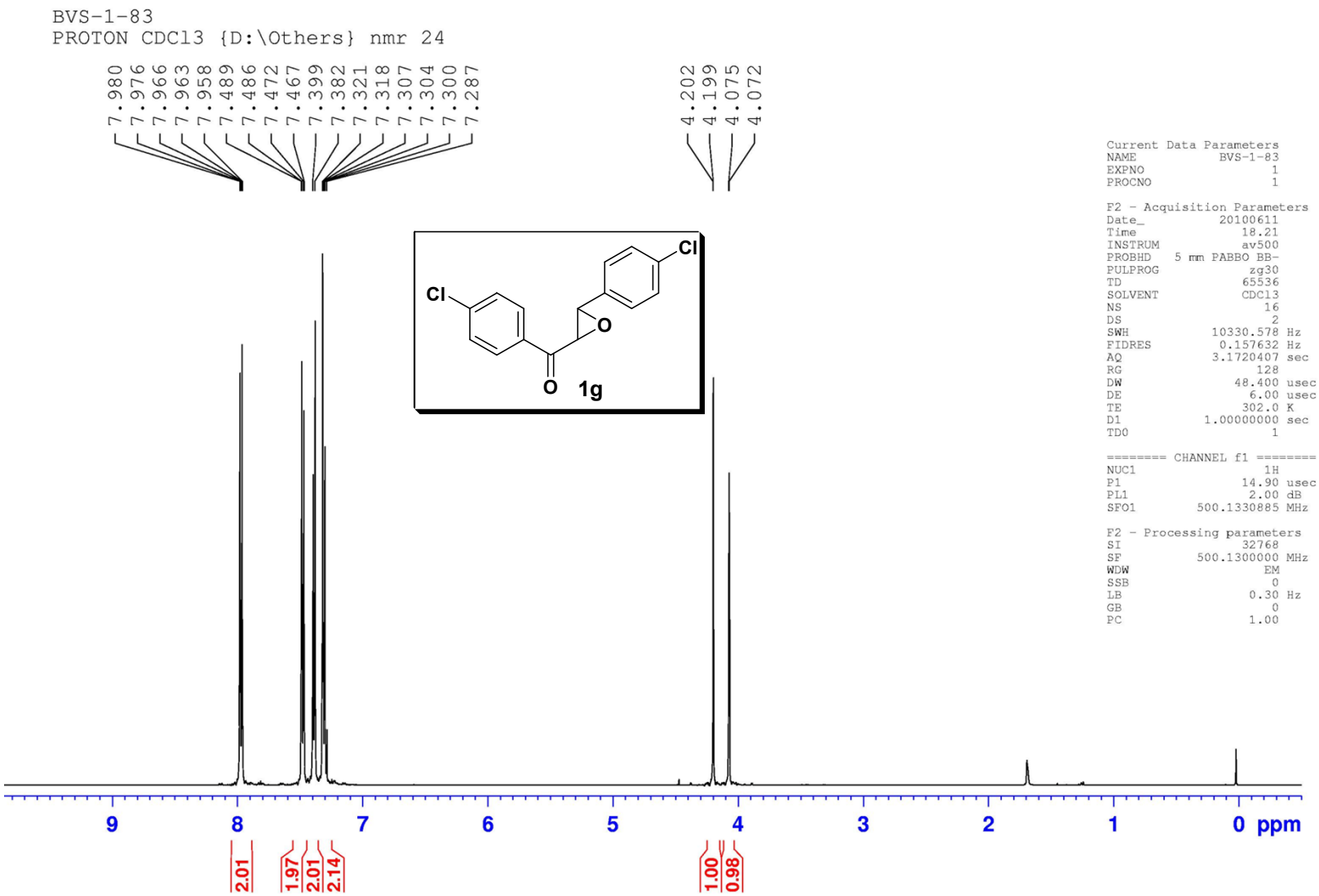
^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **1f**



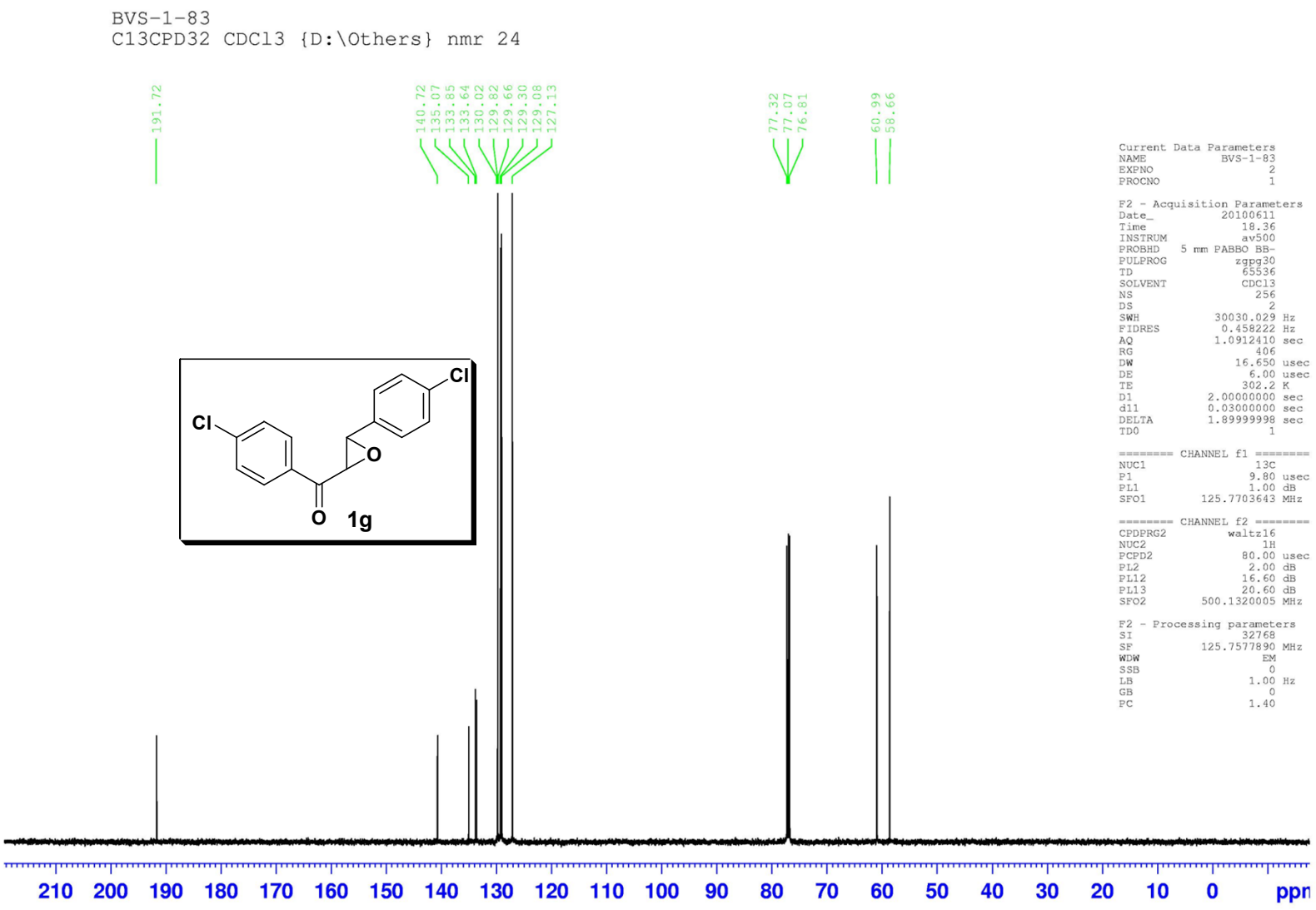
^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of 2**f**



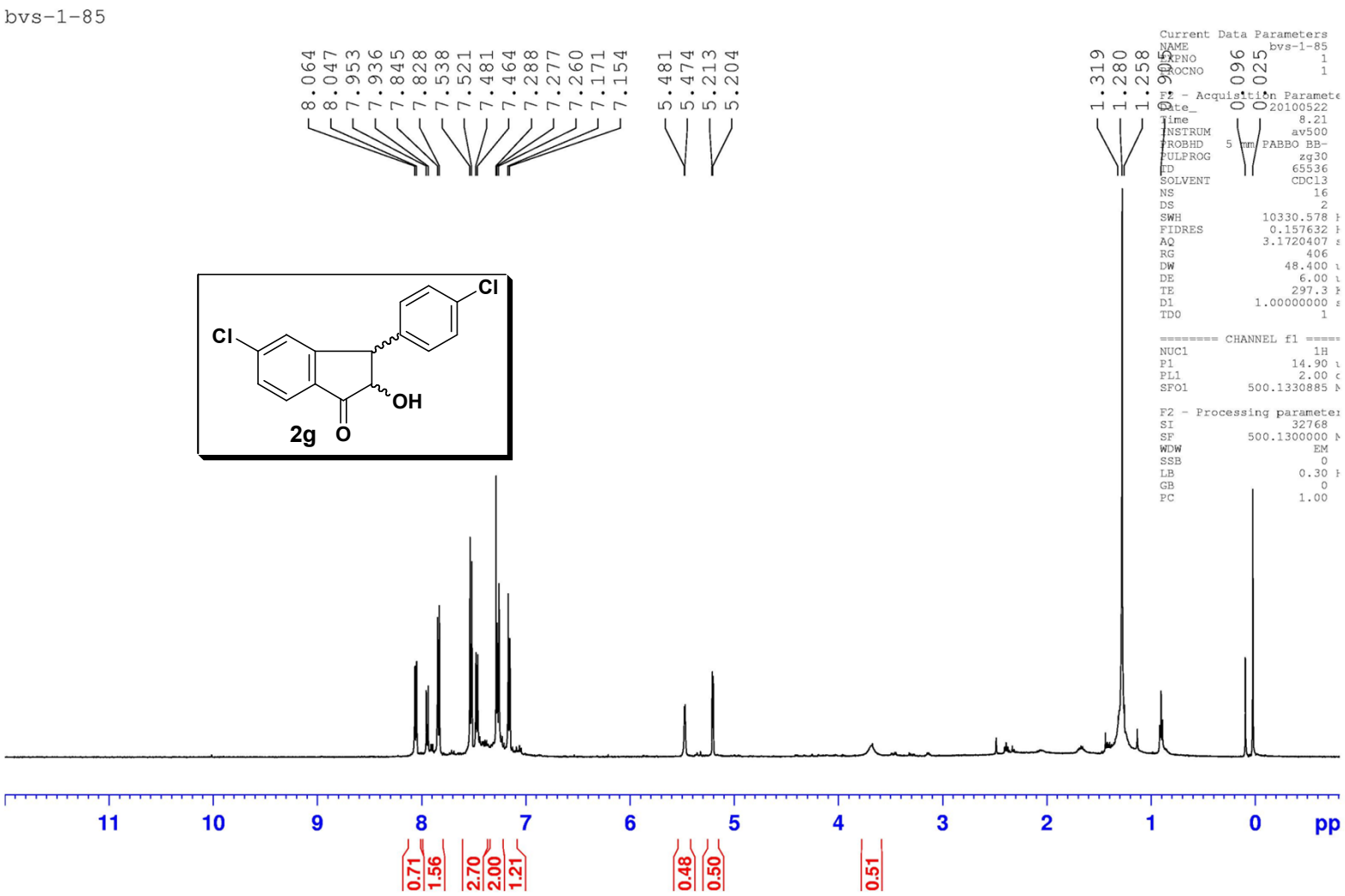
^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **2f**



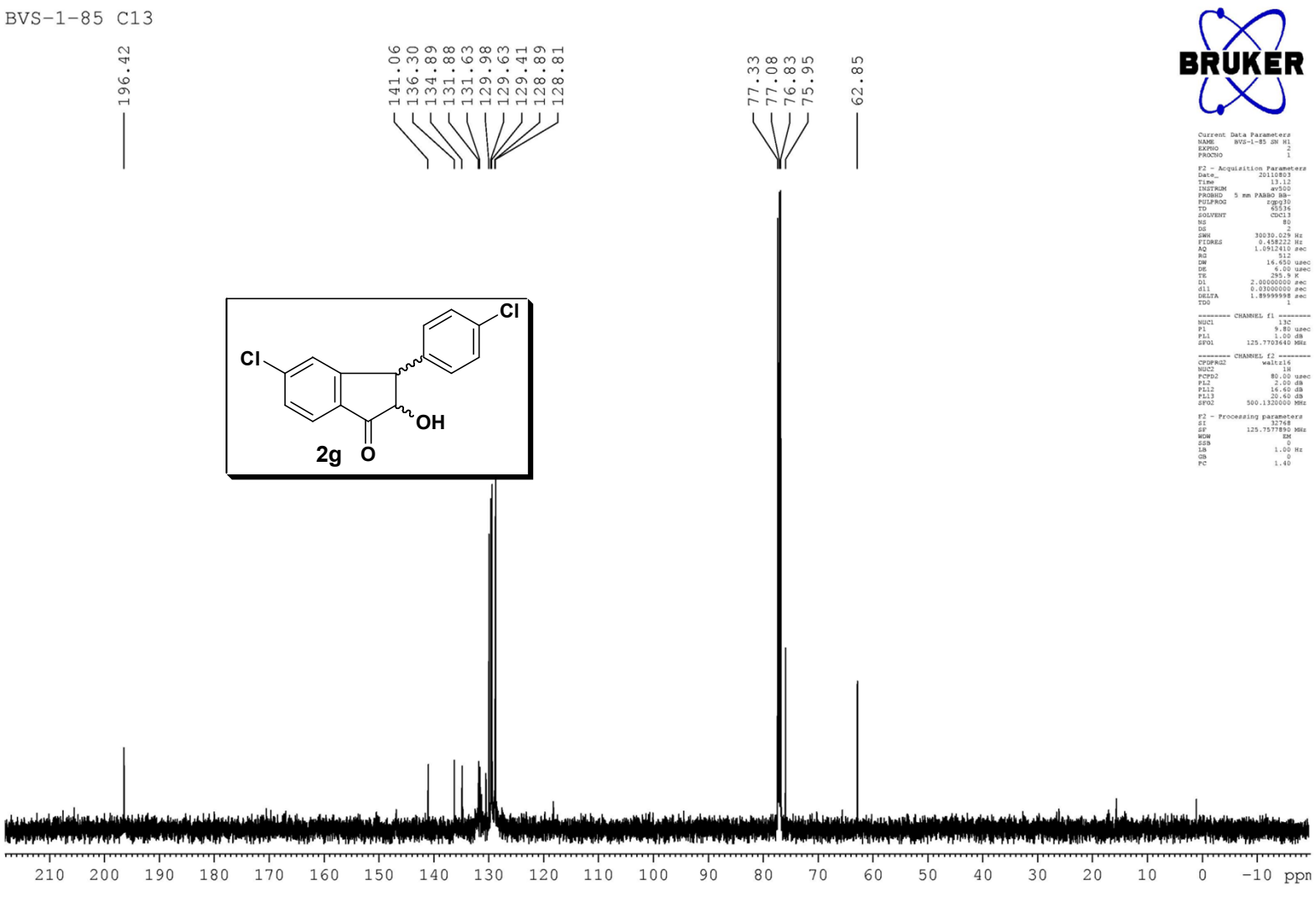
^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of **1g**



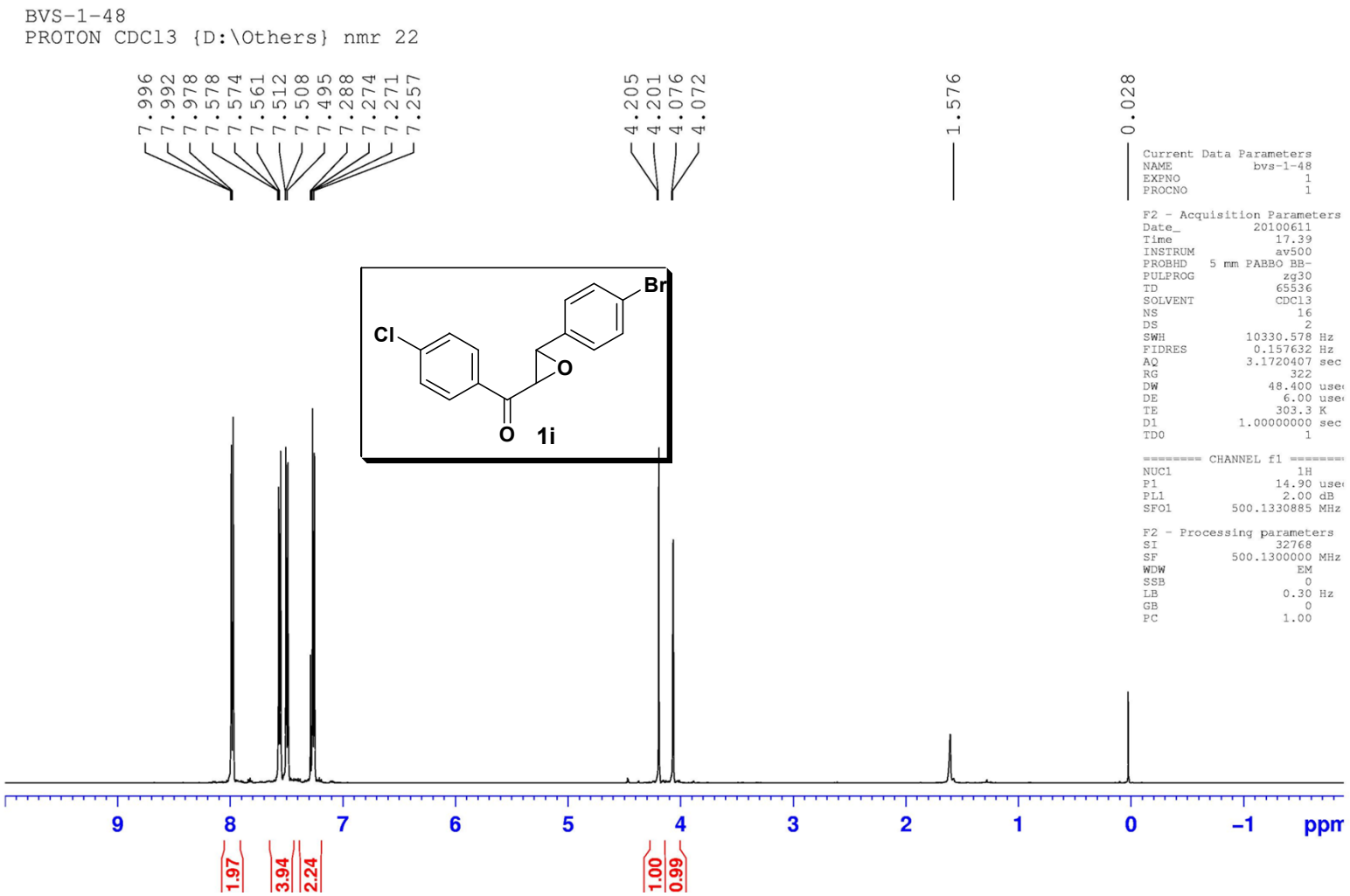
^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **1g**



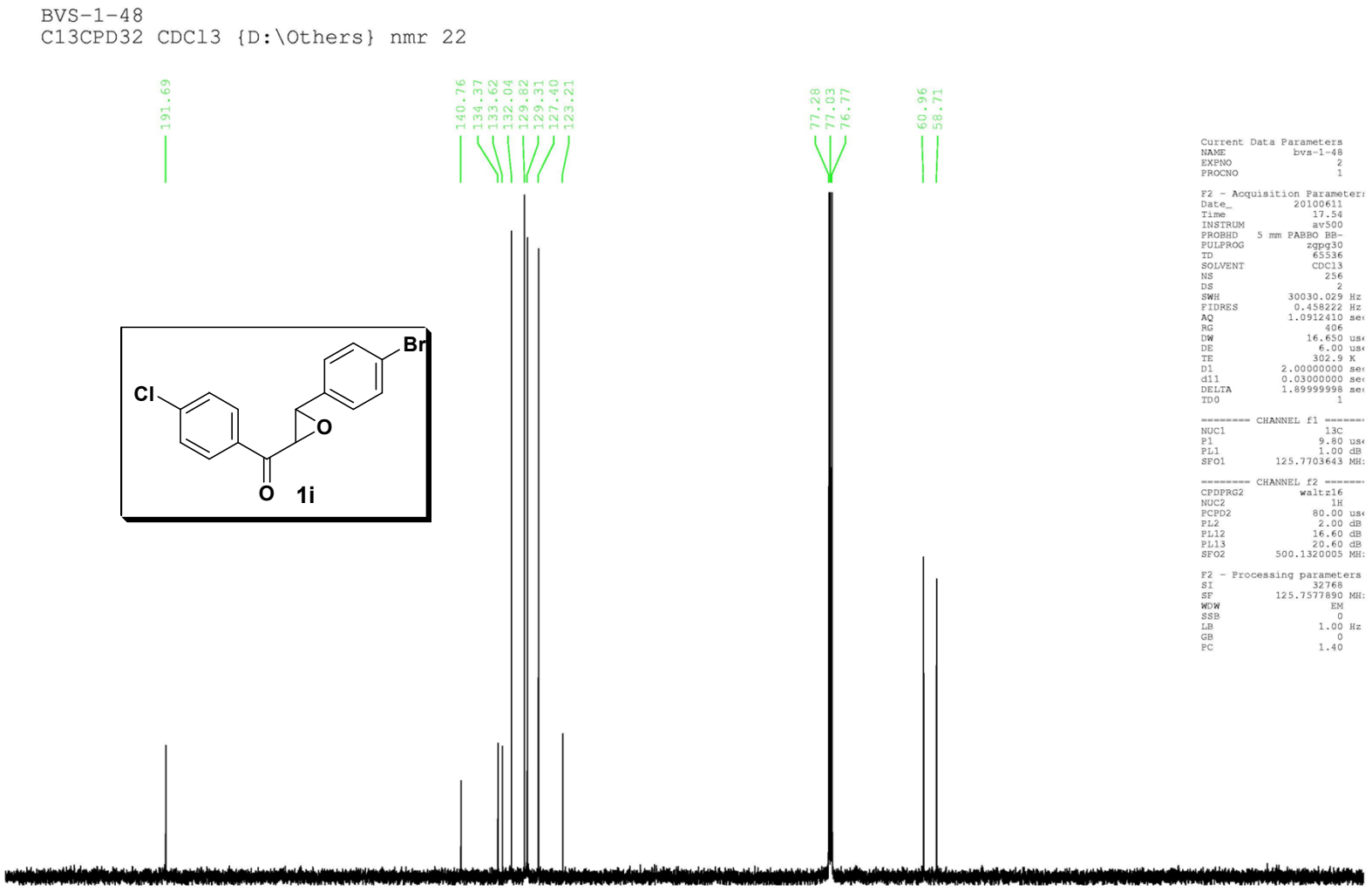
^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of **2g**



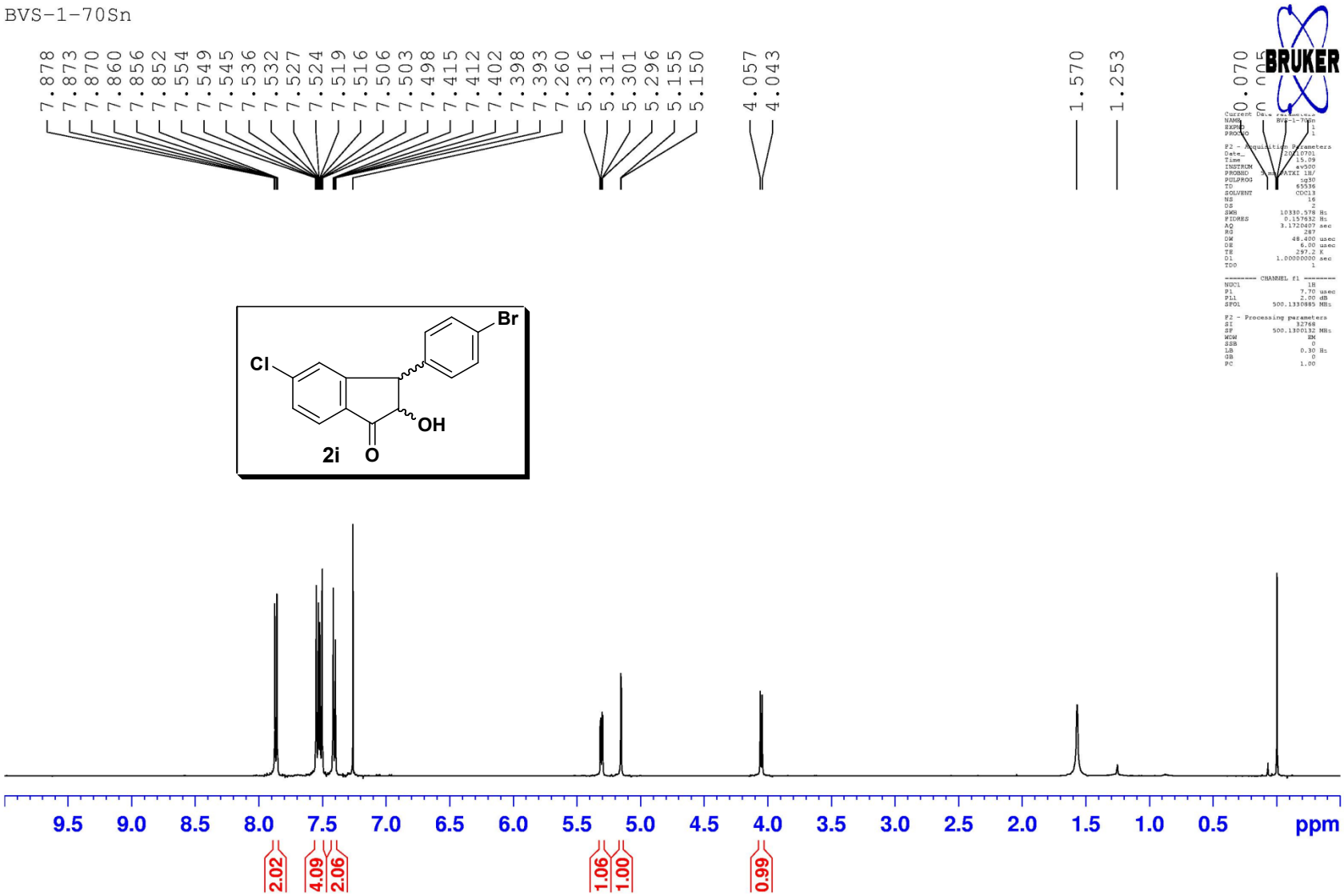
^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **2g**



^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of **1i**

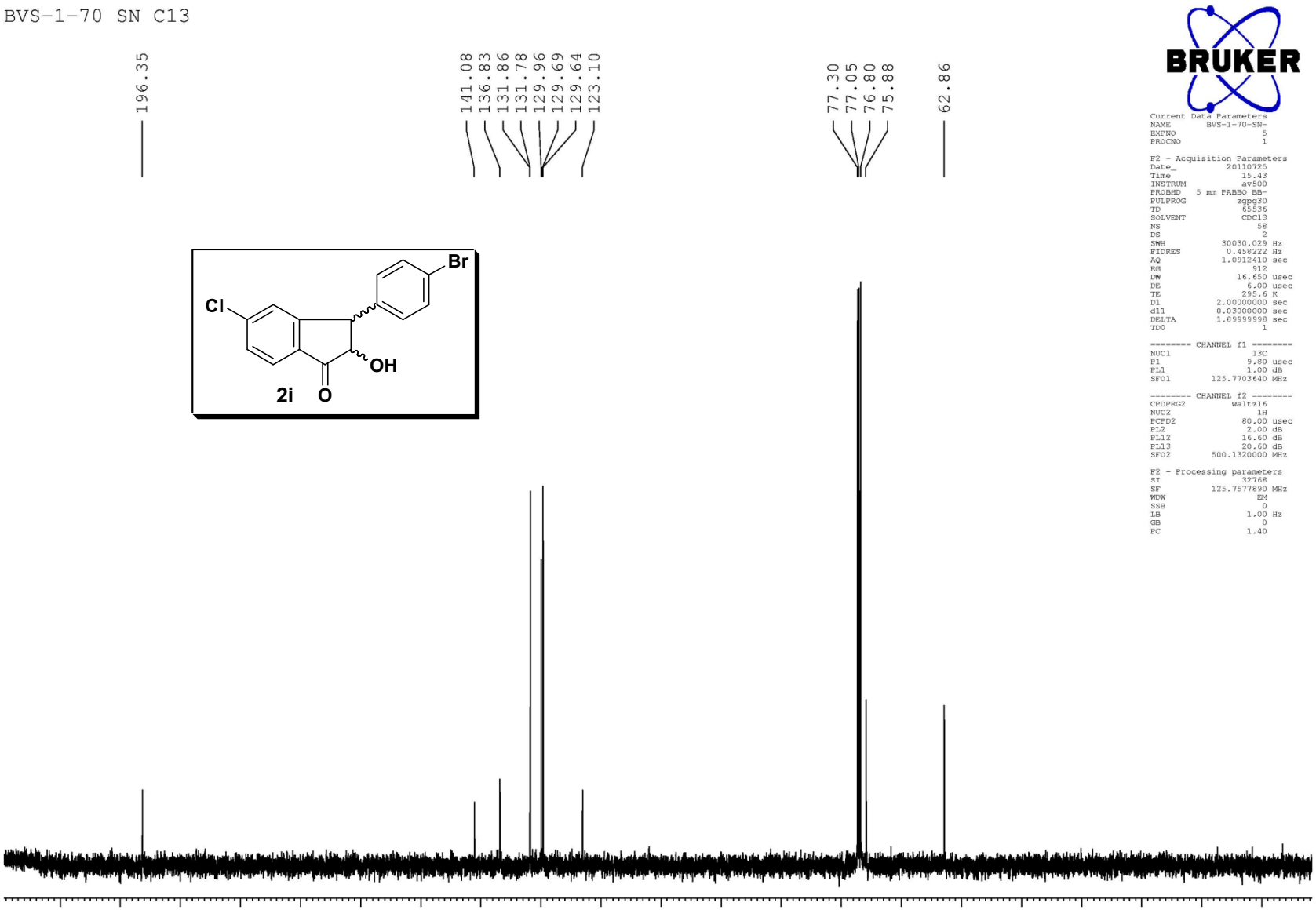


^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **1i**



^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of **2i**

BVS-1-70 SN C13



BRUKER

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PROCNO 1

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DW 16.650 usec
DE 6.00 usec
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DELTA 1.89999998 sec
TD0 1

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PL1 1.00 dB
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======== CHANNEL f2 ========
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PL12 16.60 dB
PL13 20.60 dB
SFO2 500.1320000 MHz

F2 - Processing parameters
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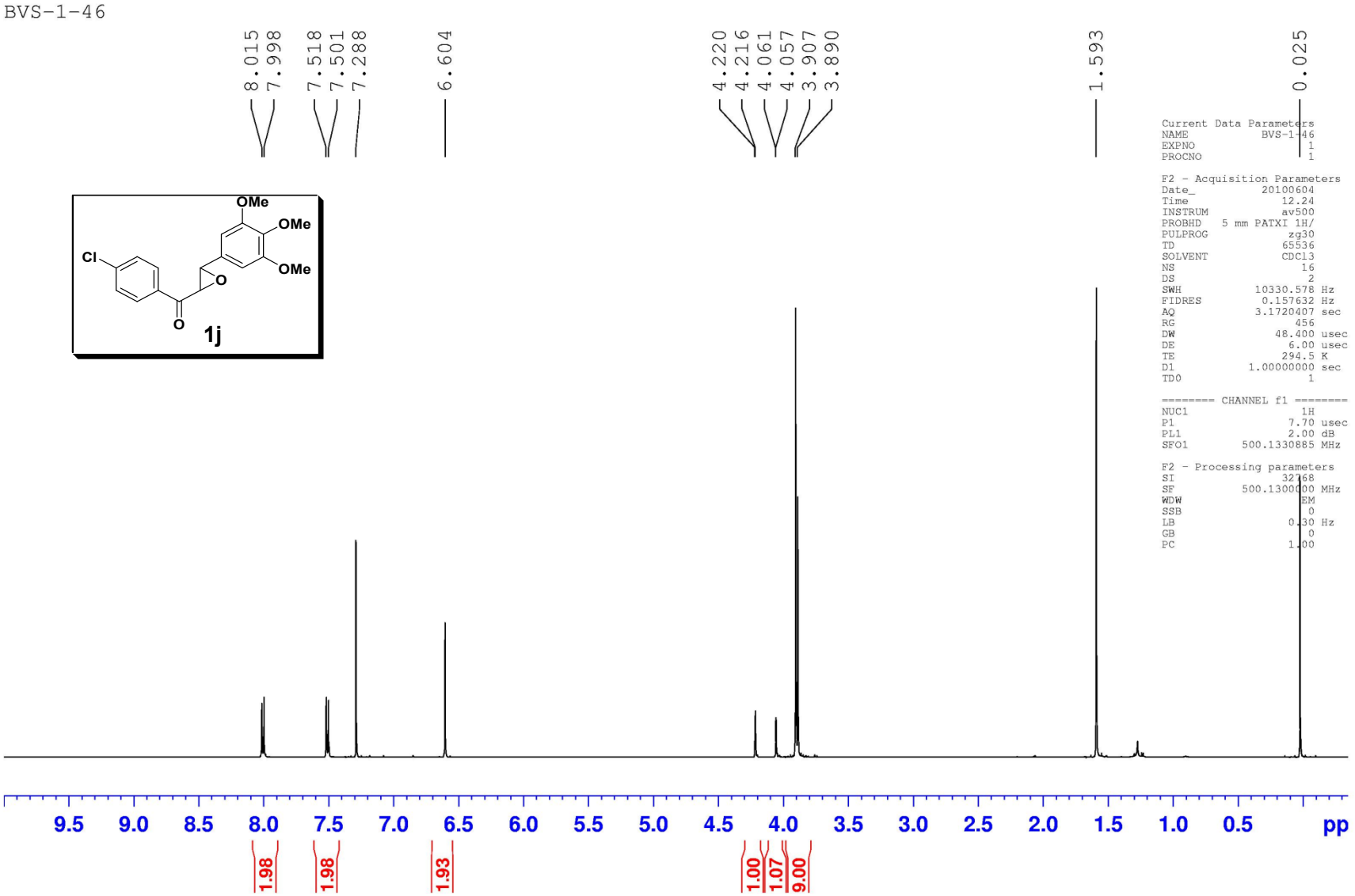
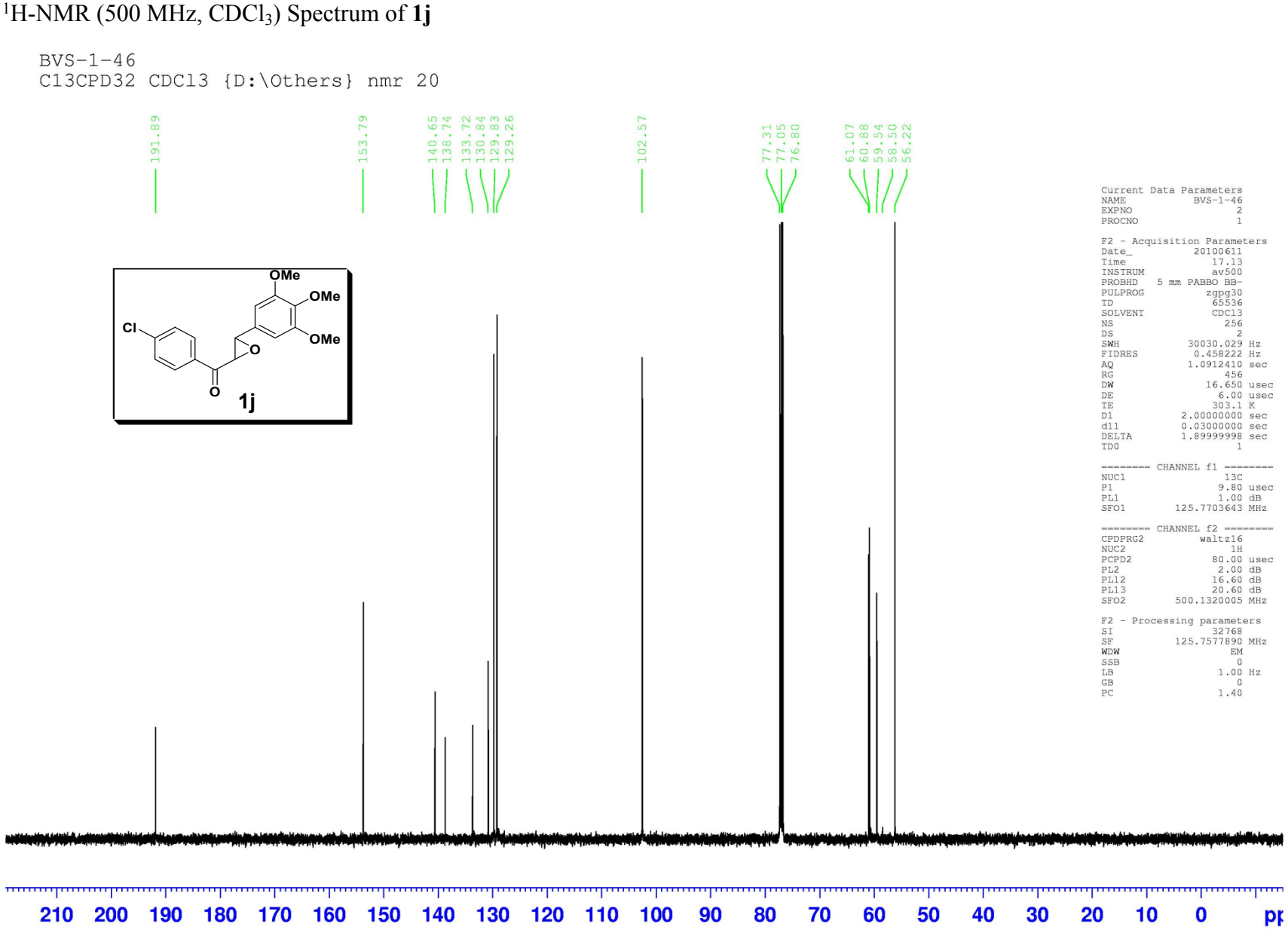
LB 1.00 Hz
GB 0
PC 1.40

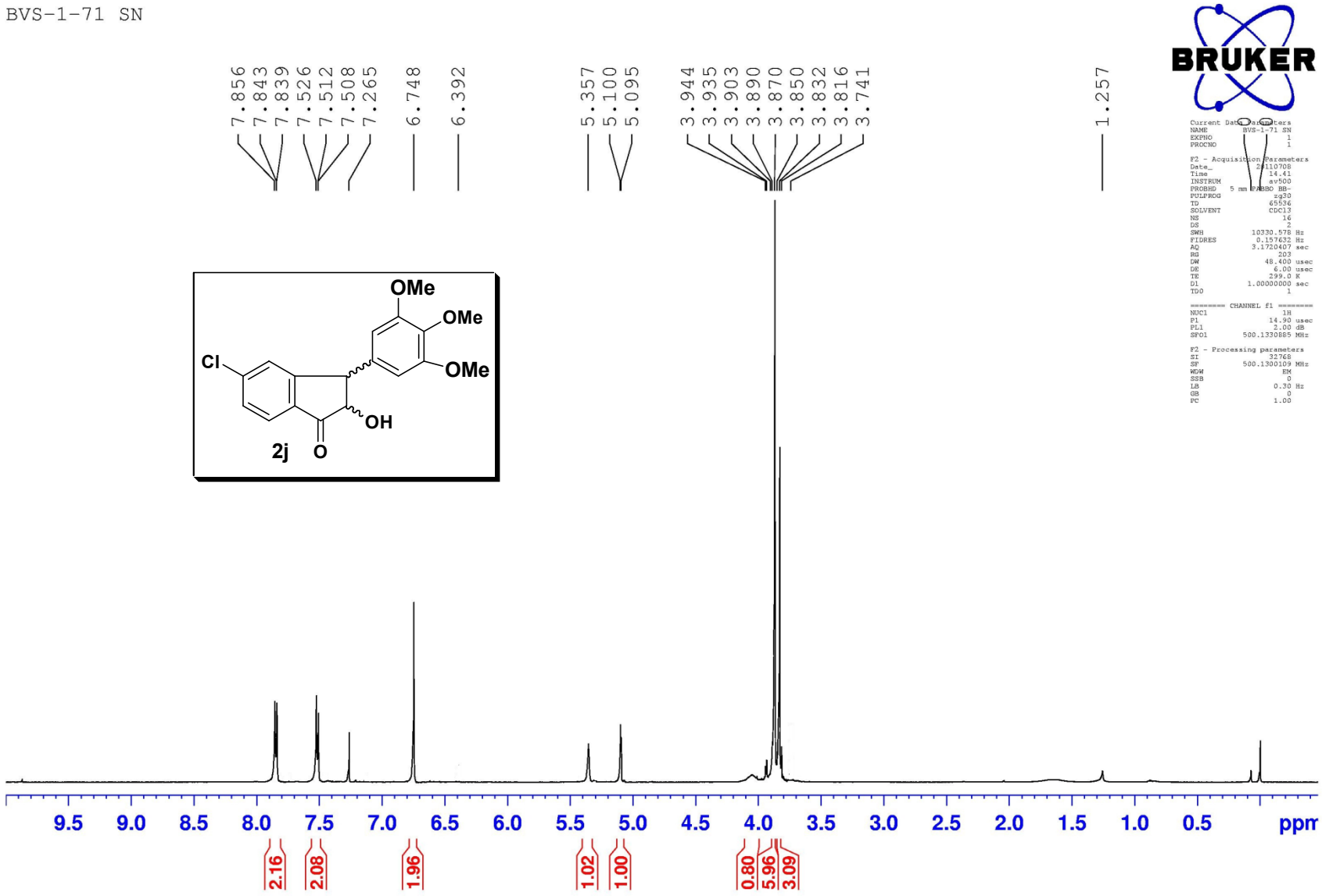
^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **2i**



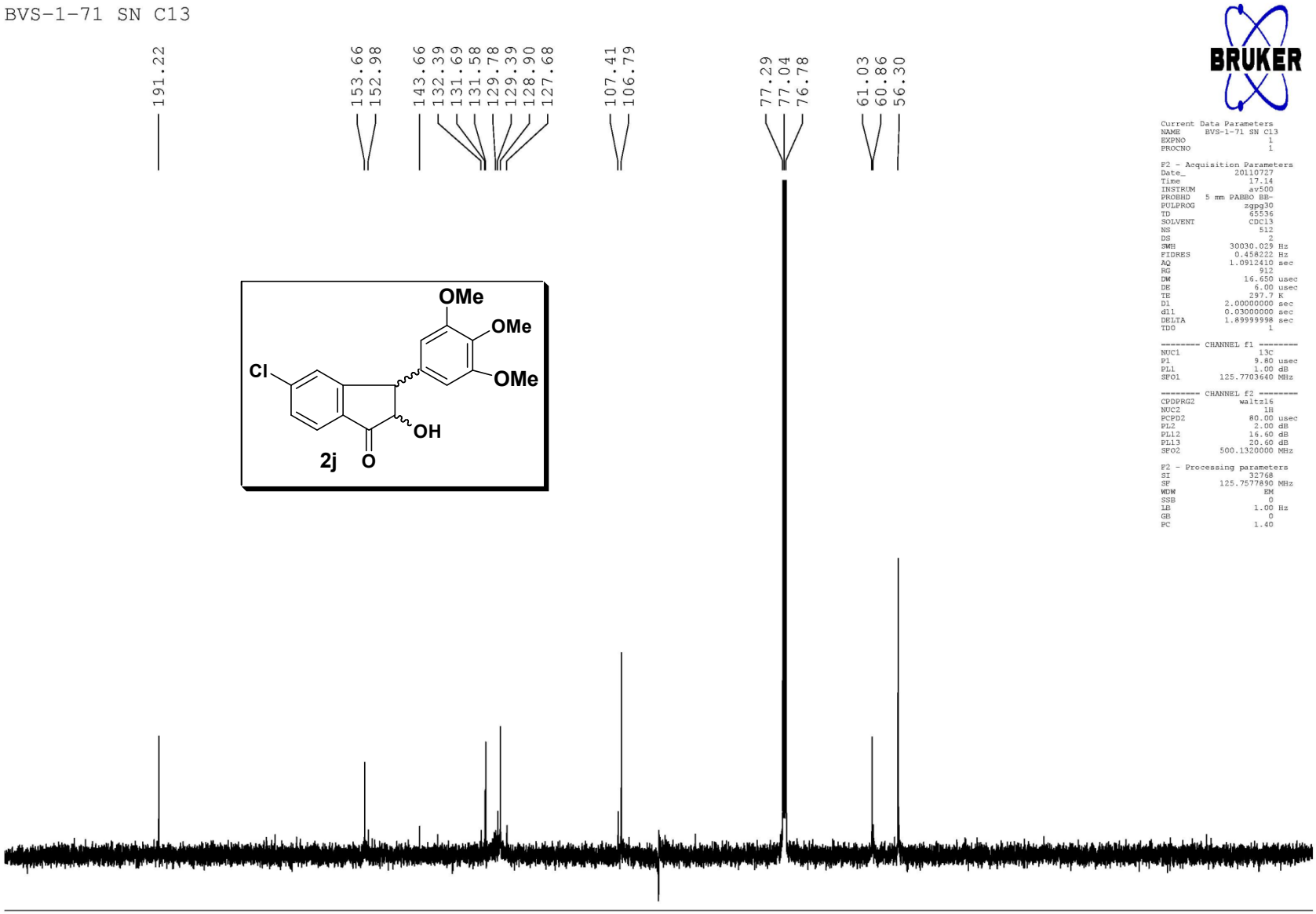
^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of **1j**



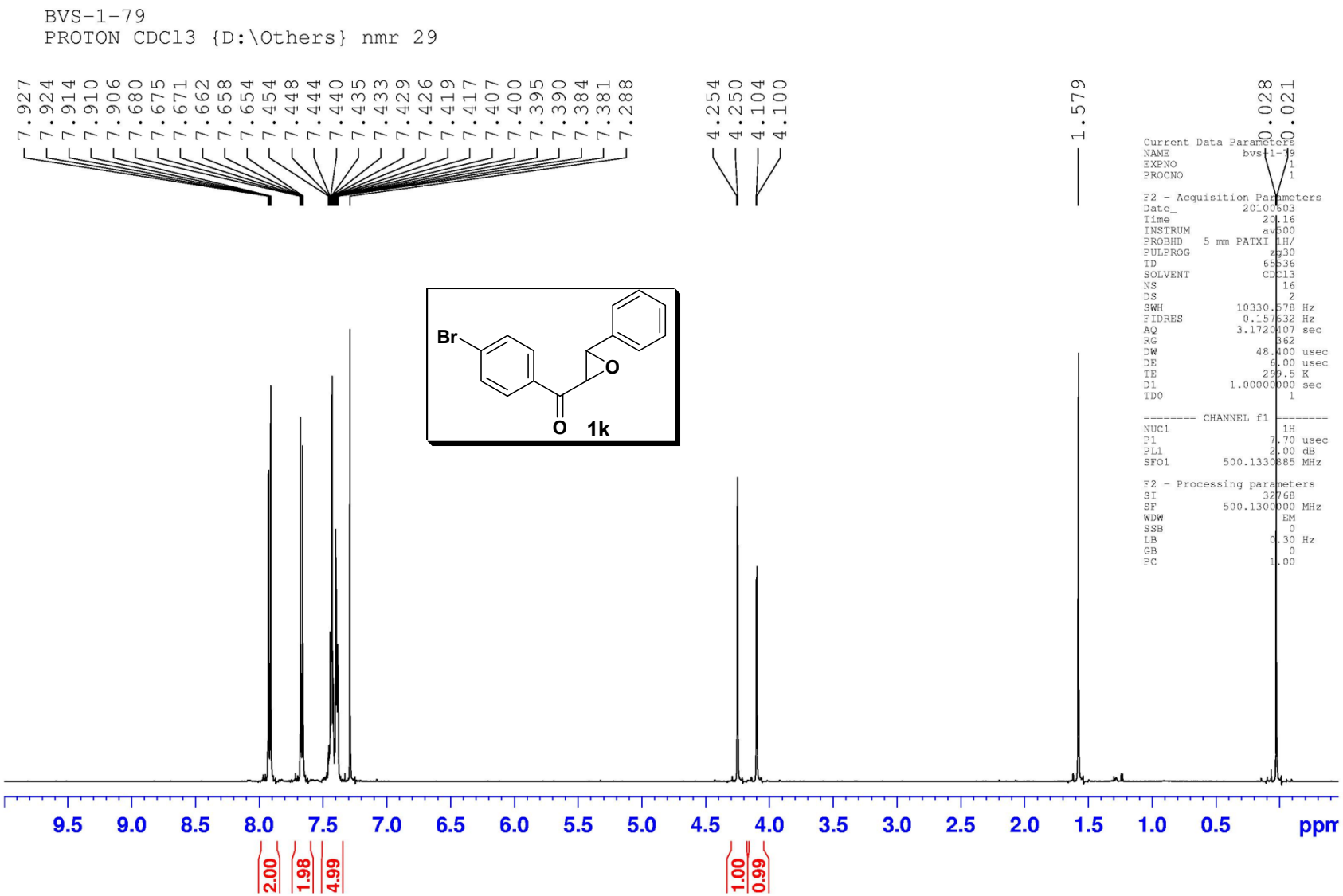
^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **1j**



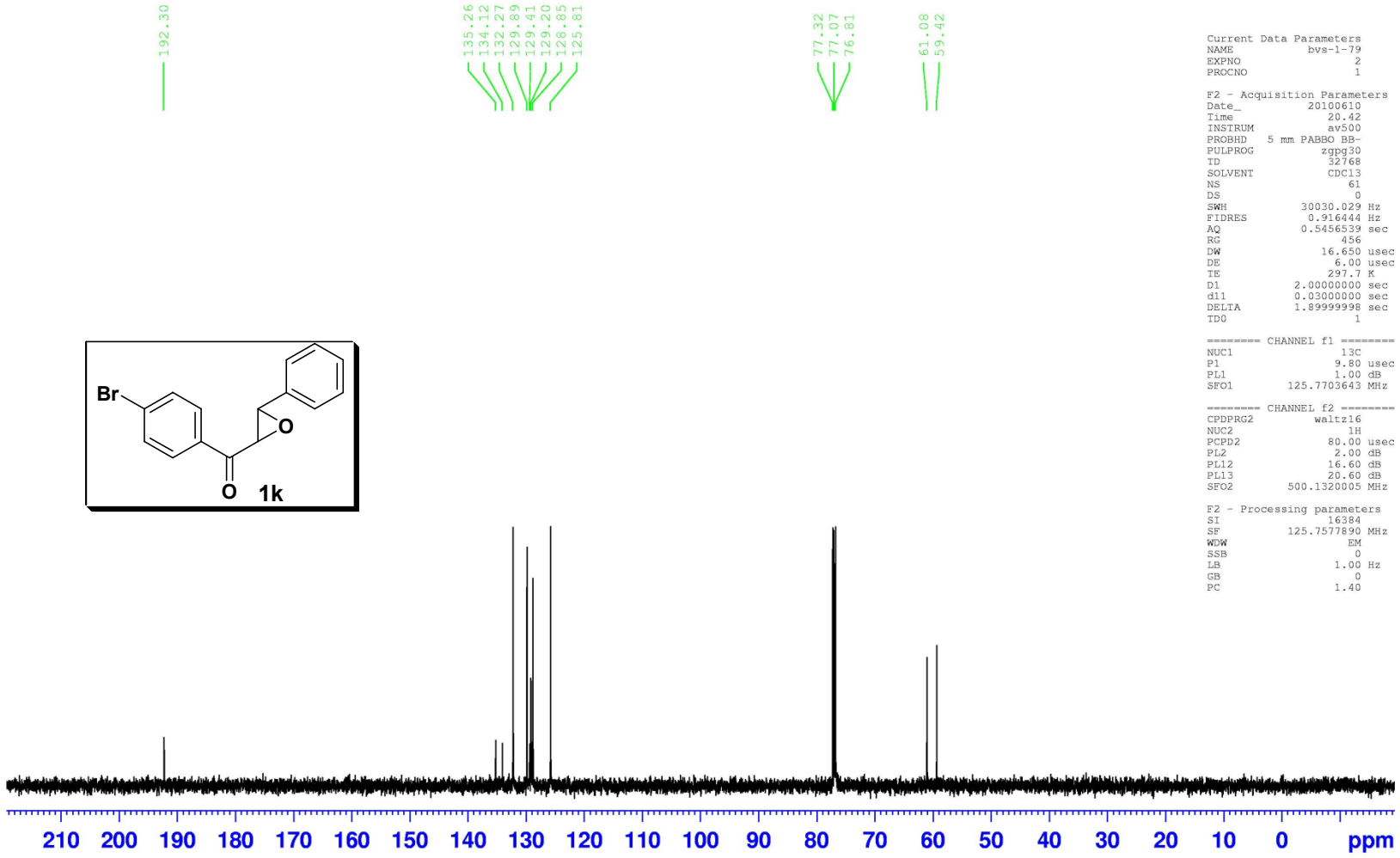
^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of **2j**



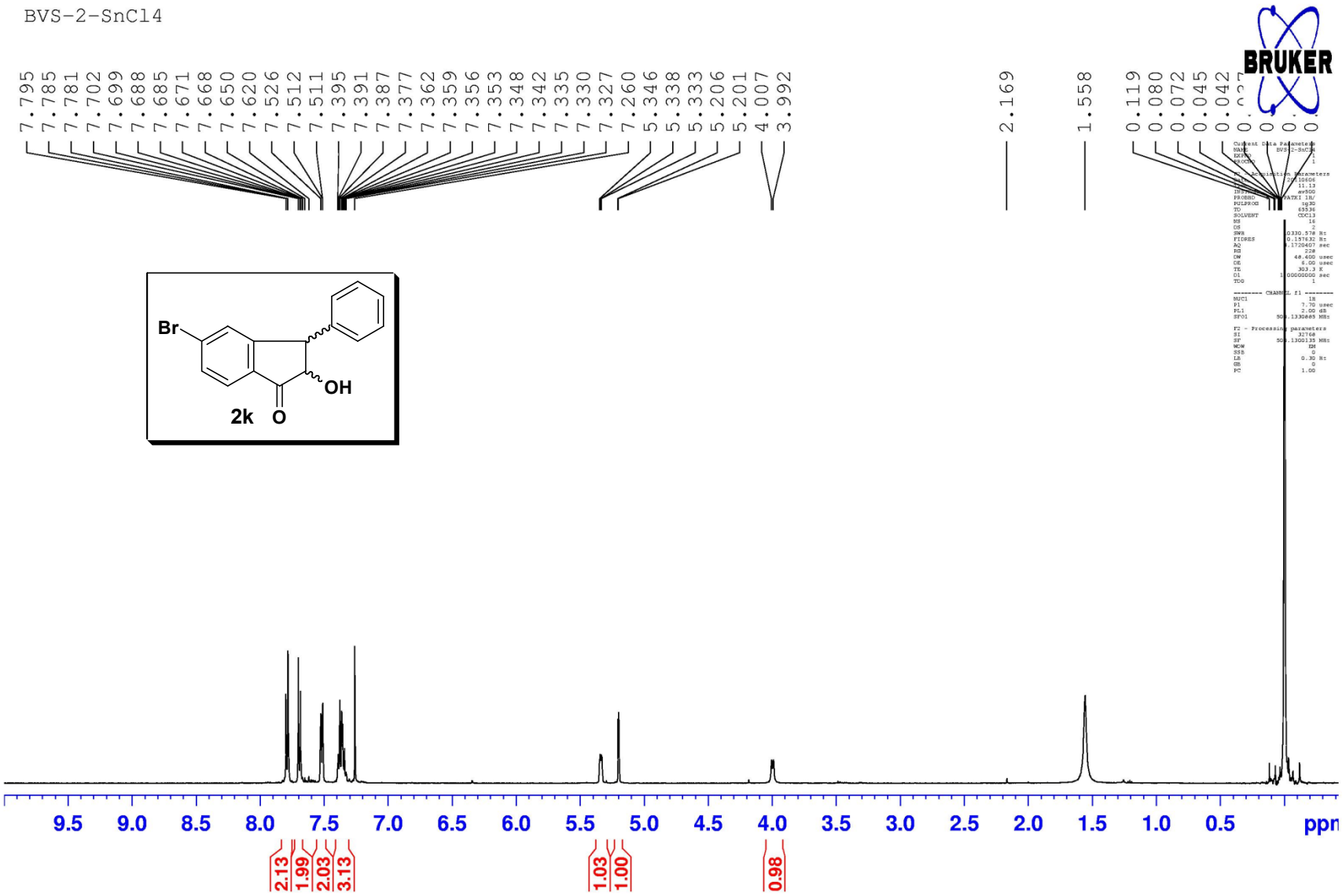
^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **2j**



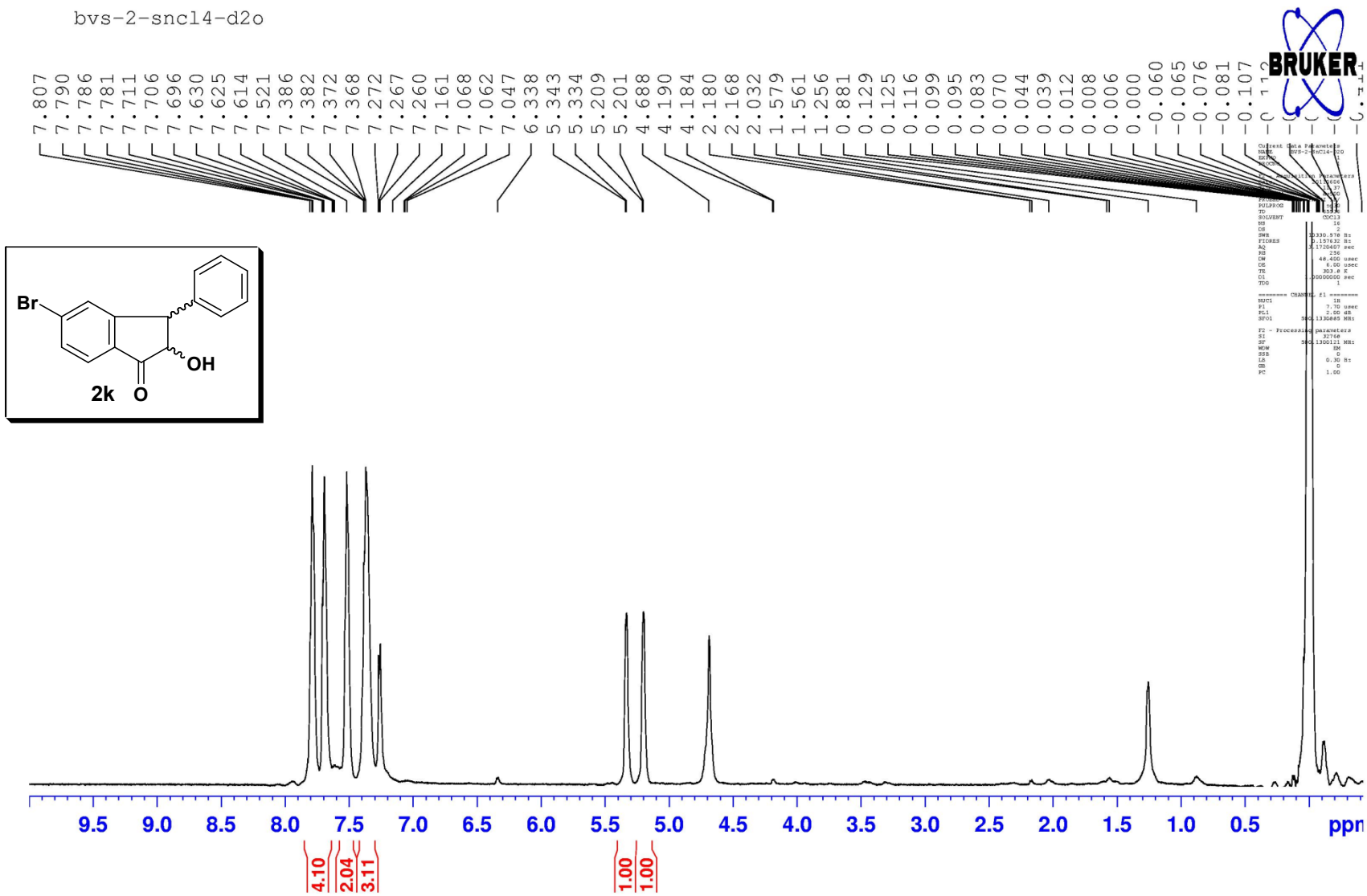
^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of **1k**



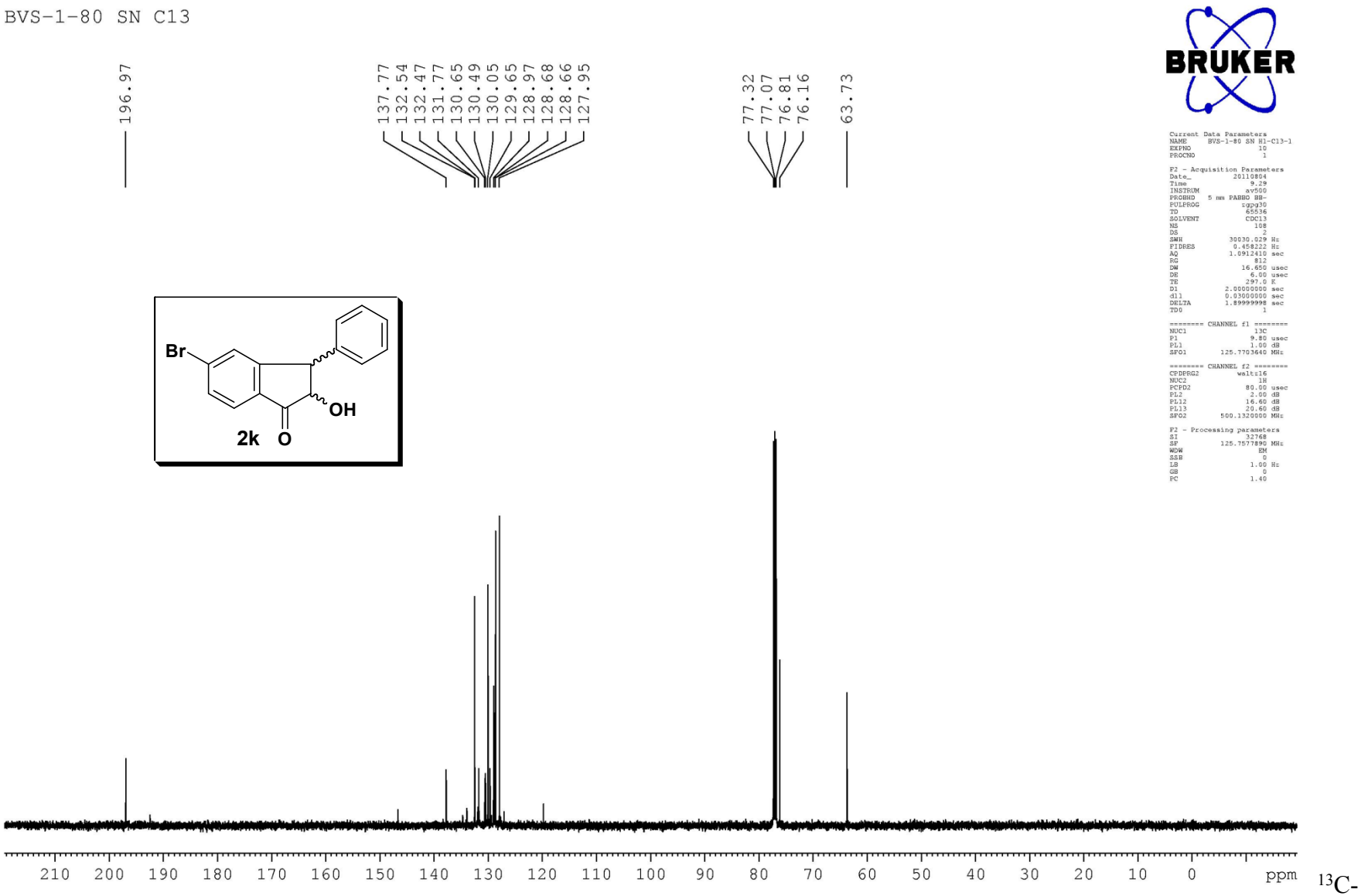
^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **1k**



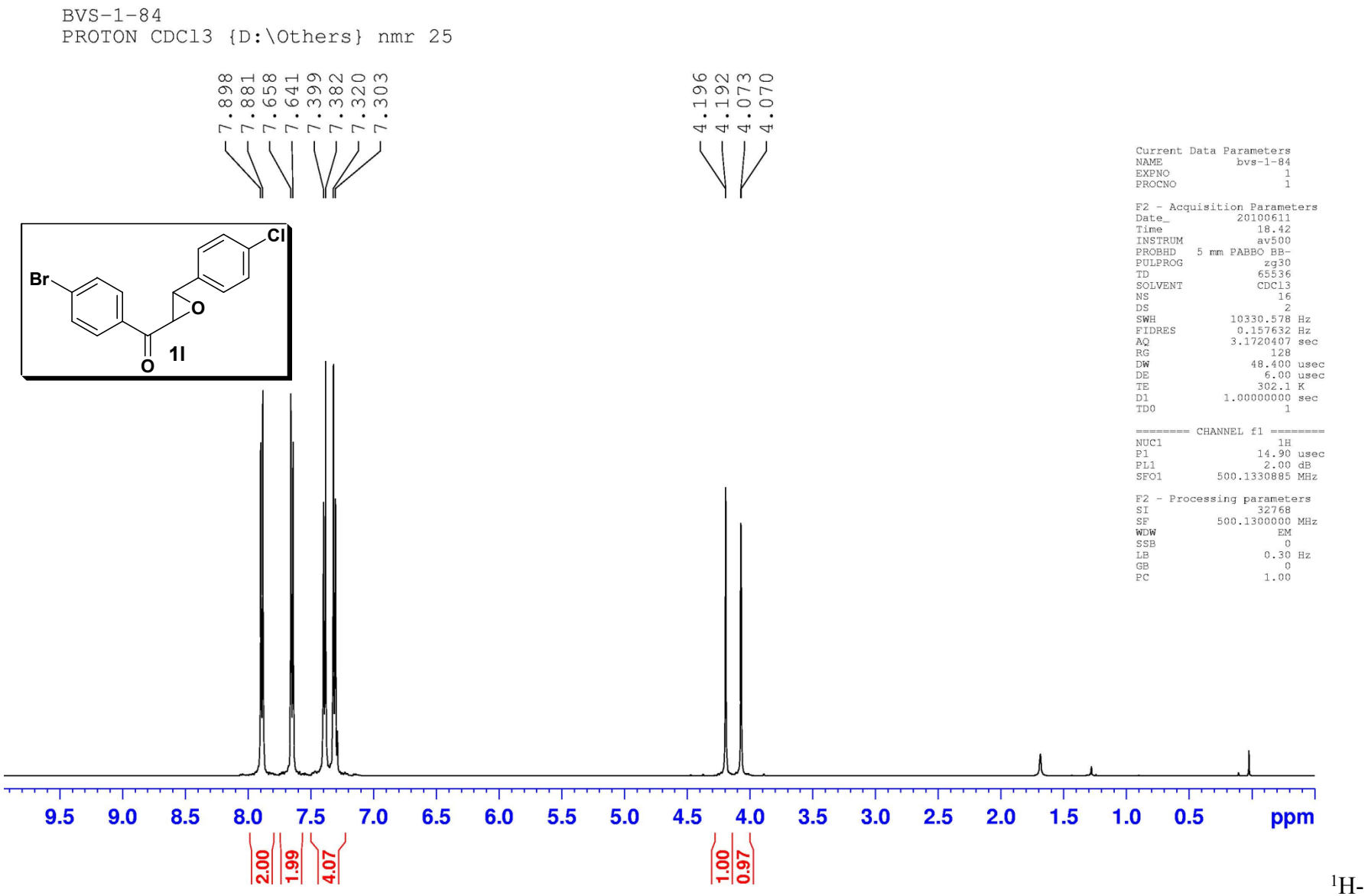
^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of **2k**



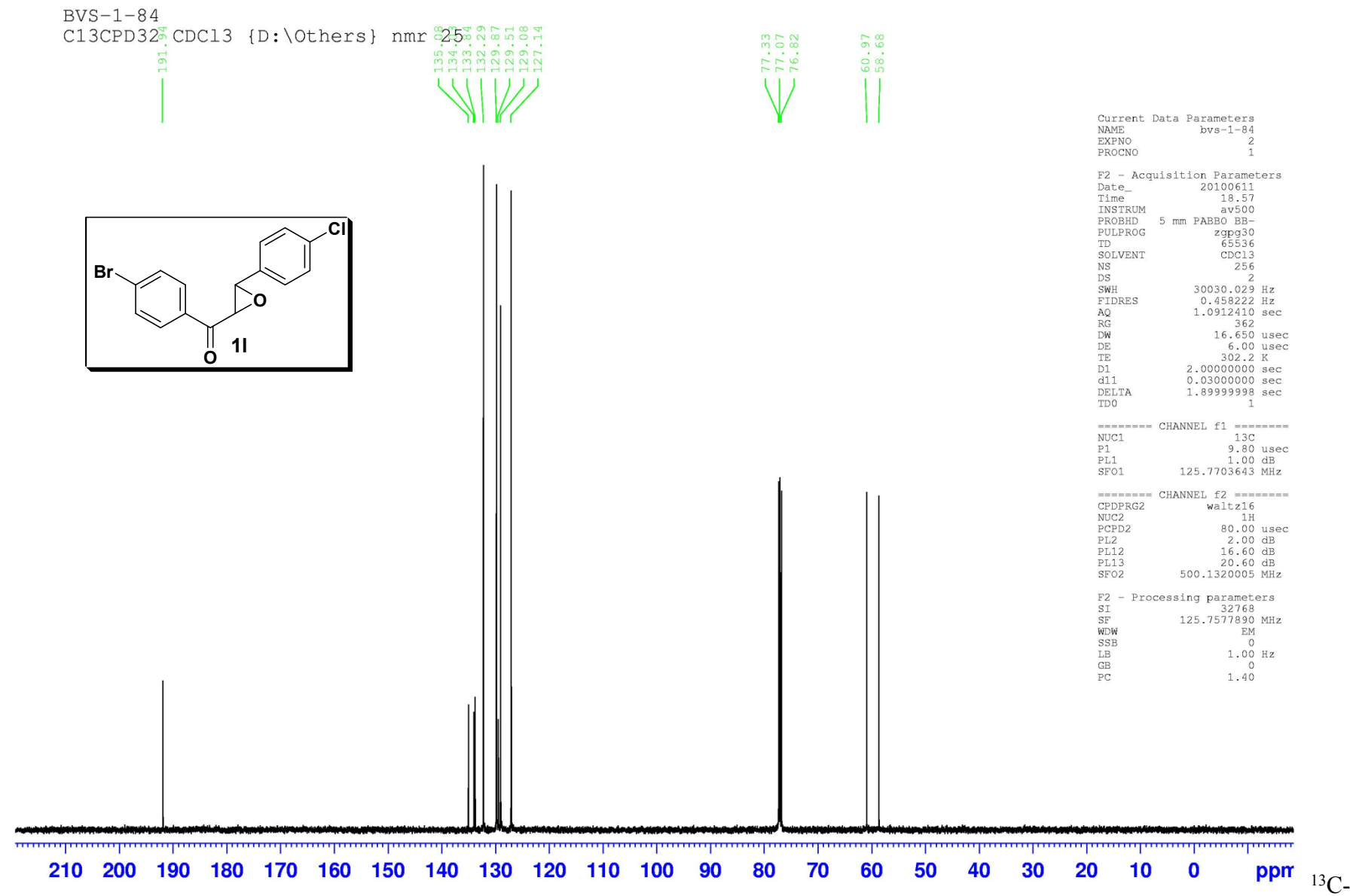
^{1}H-NMR D_2O Exchangeable (500 MHz, $CDCl_3$) Spectrum of **2k**



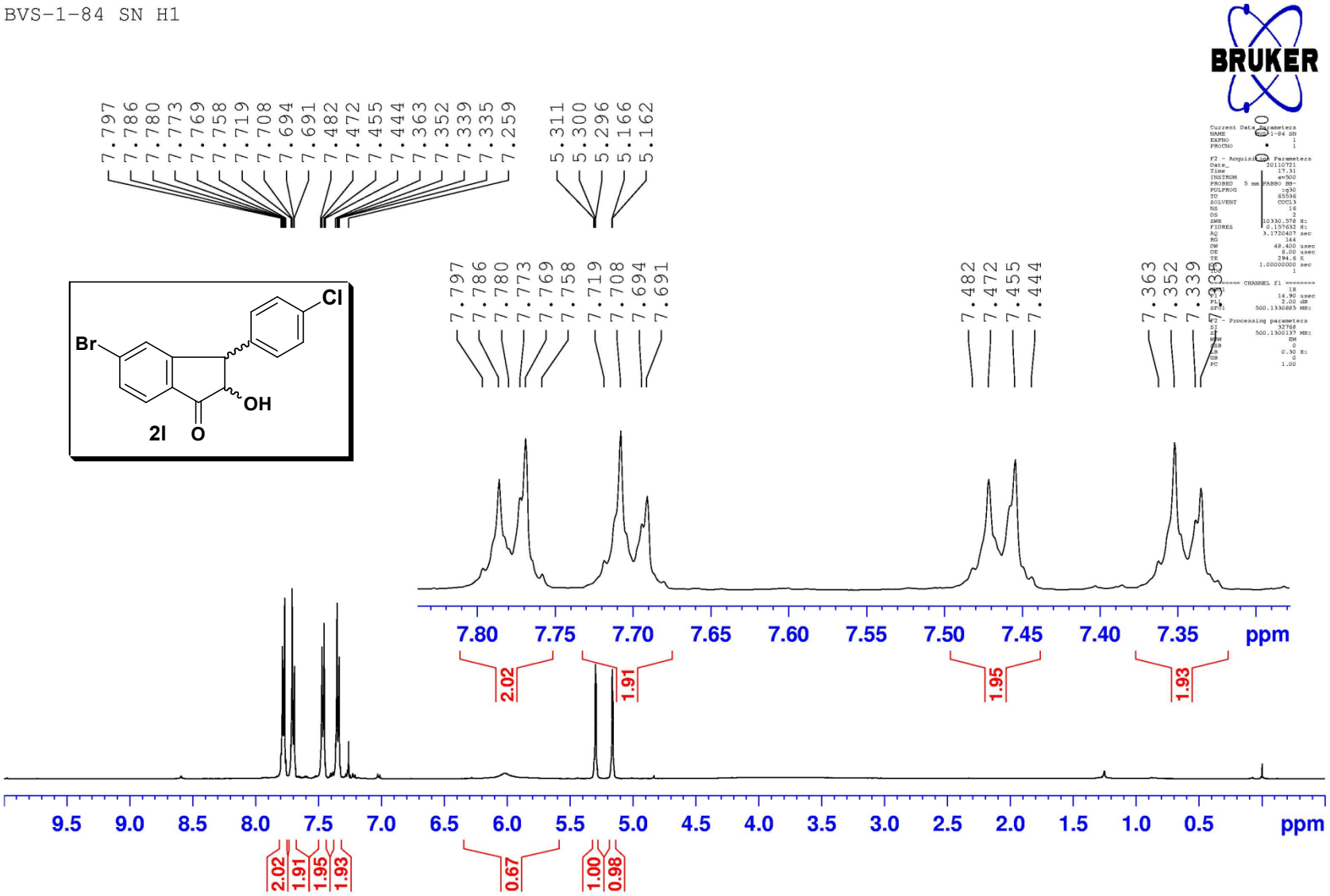
^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **2k**



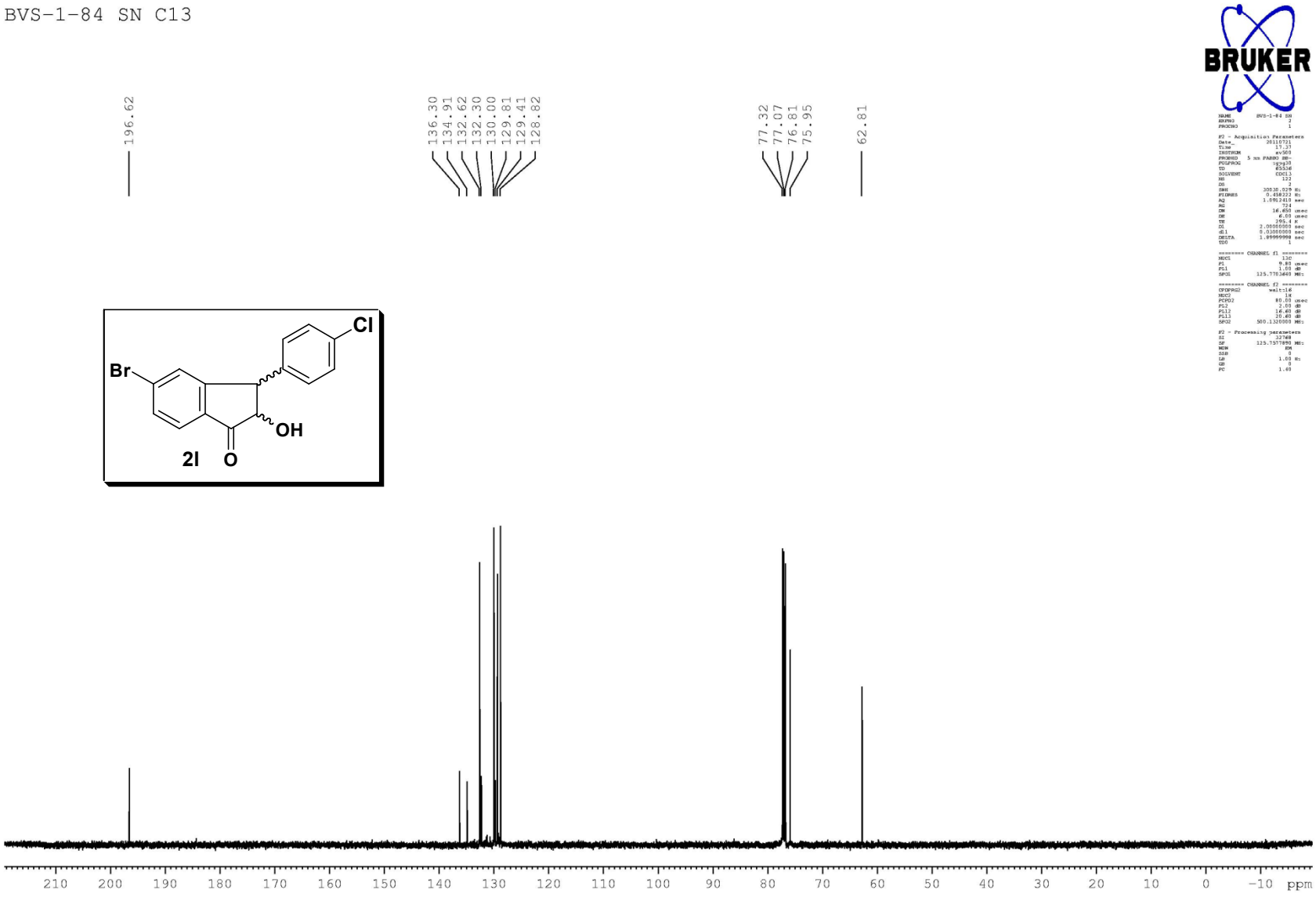
^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of **1l**



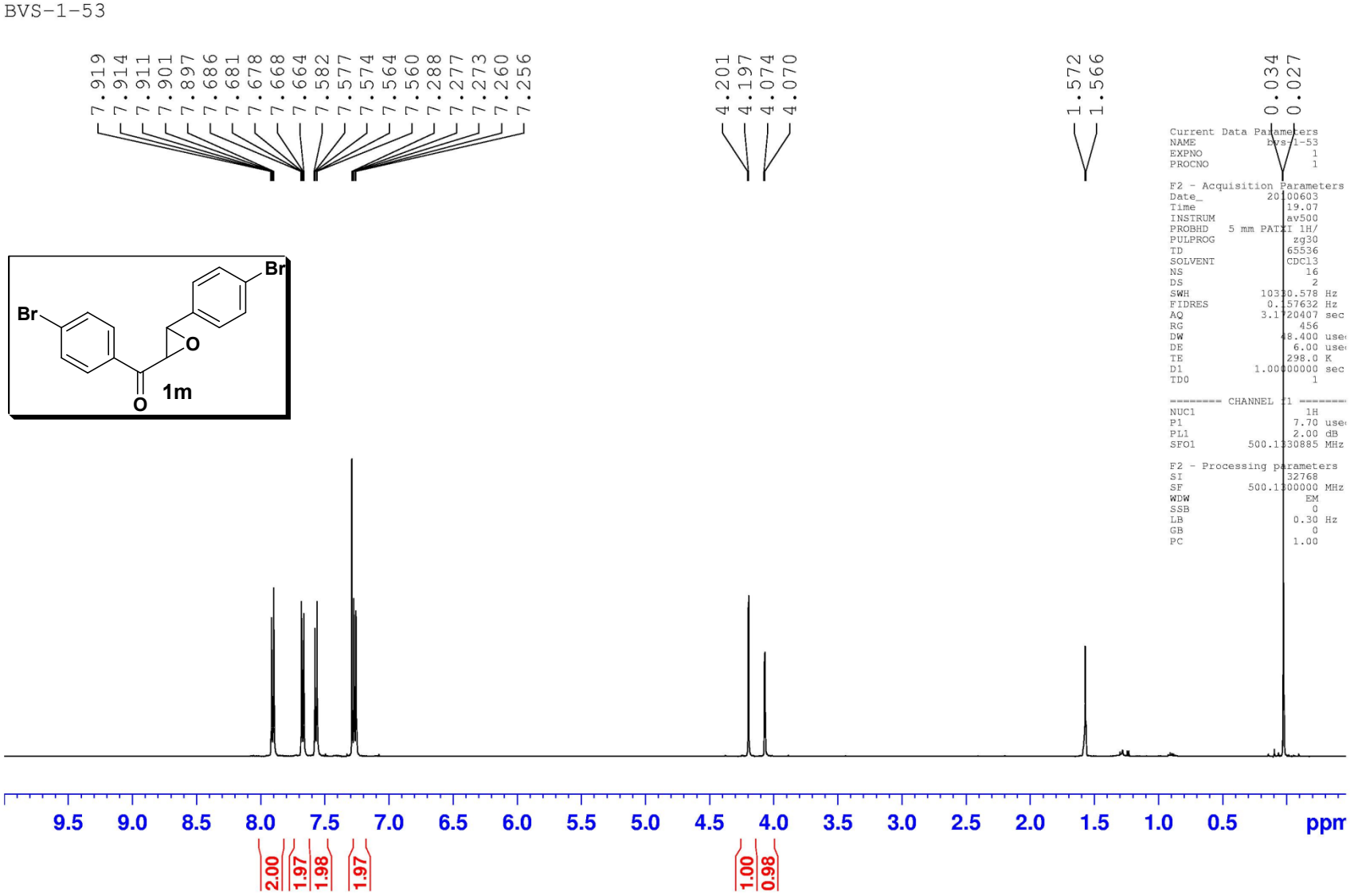
^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **1l**



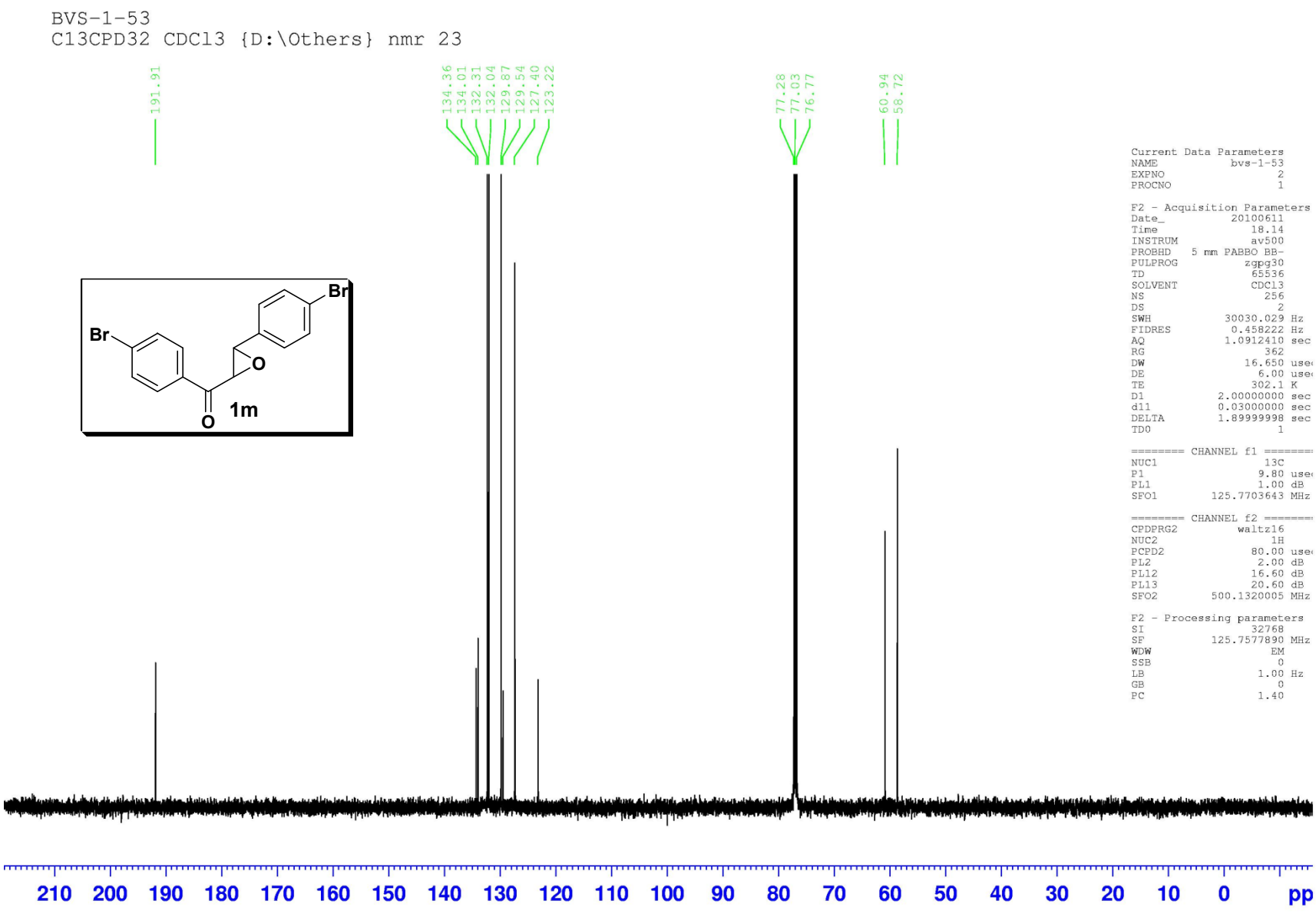
^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of **2l**



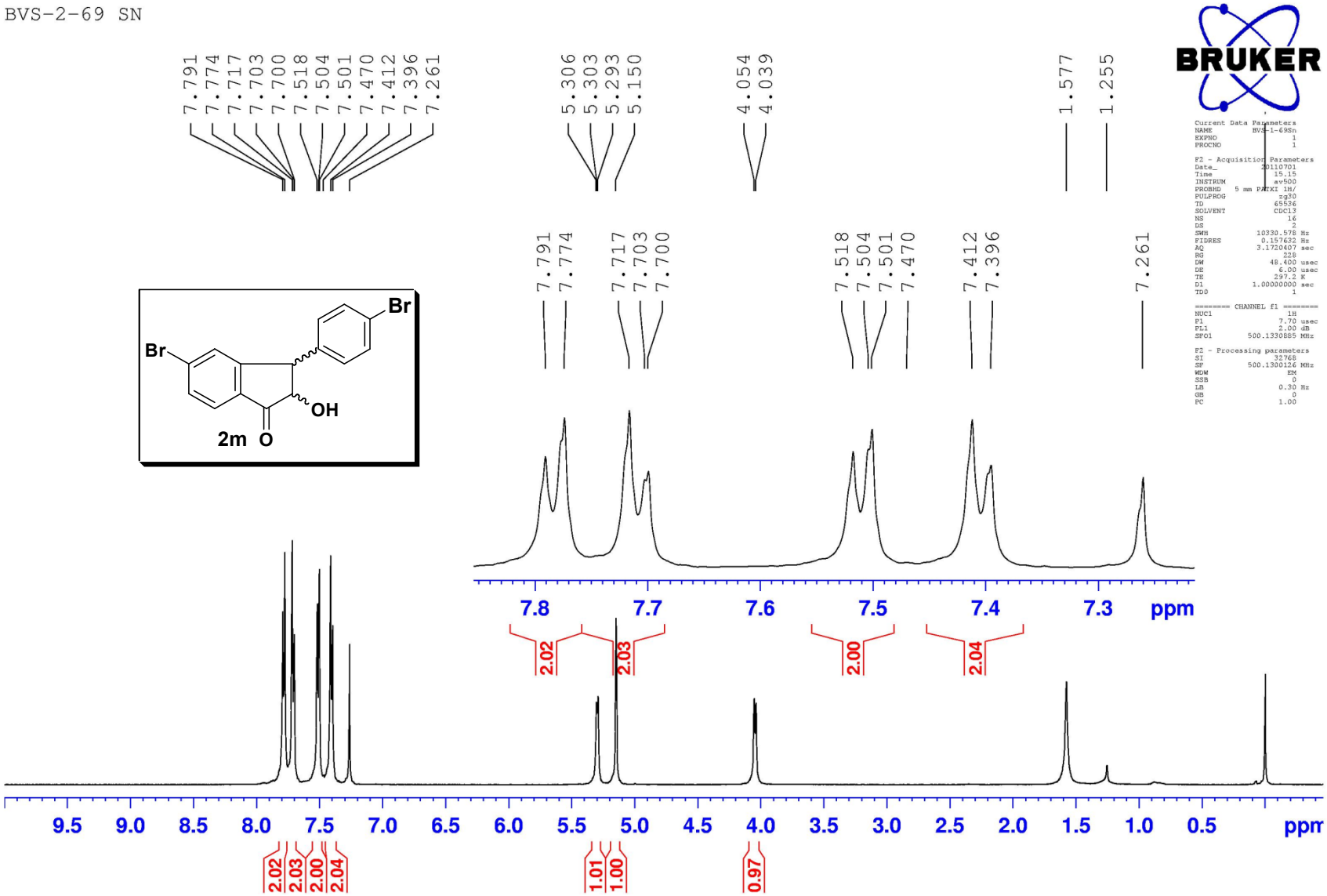
^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **2l**



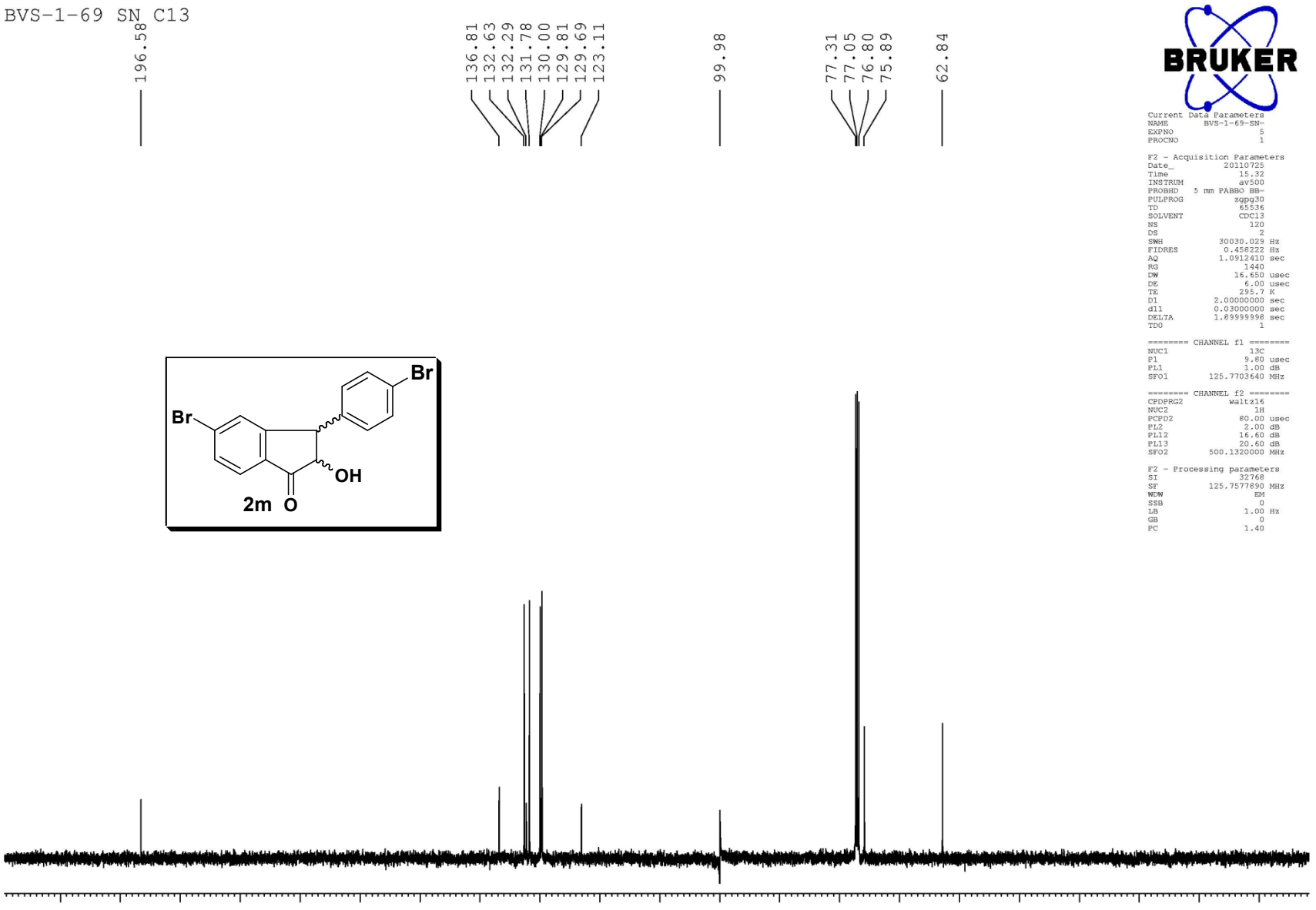
^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of **1m**



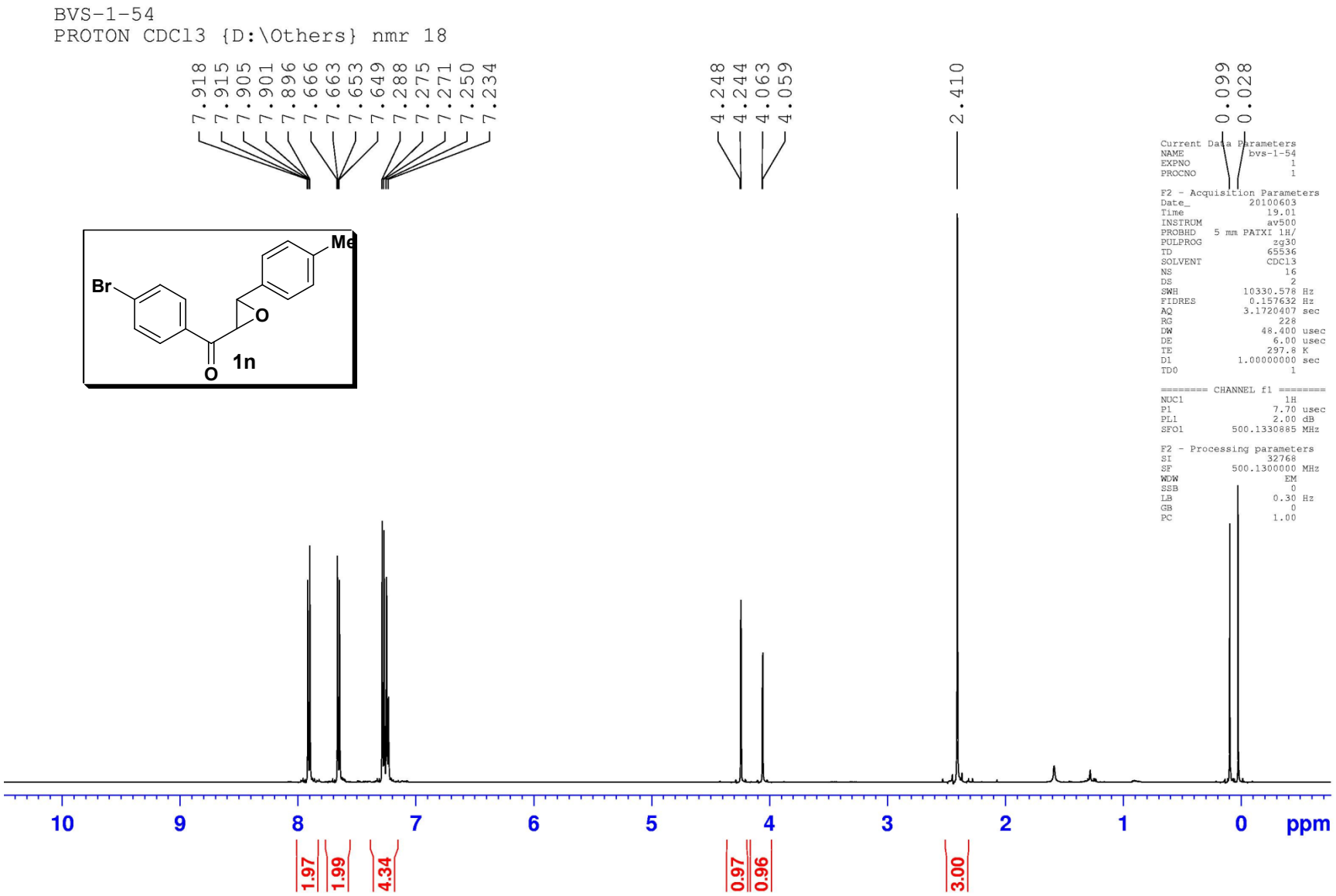
^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **1m**



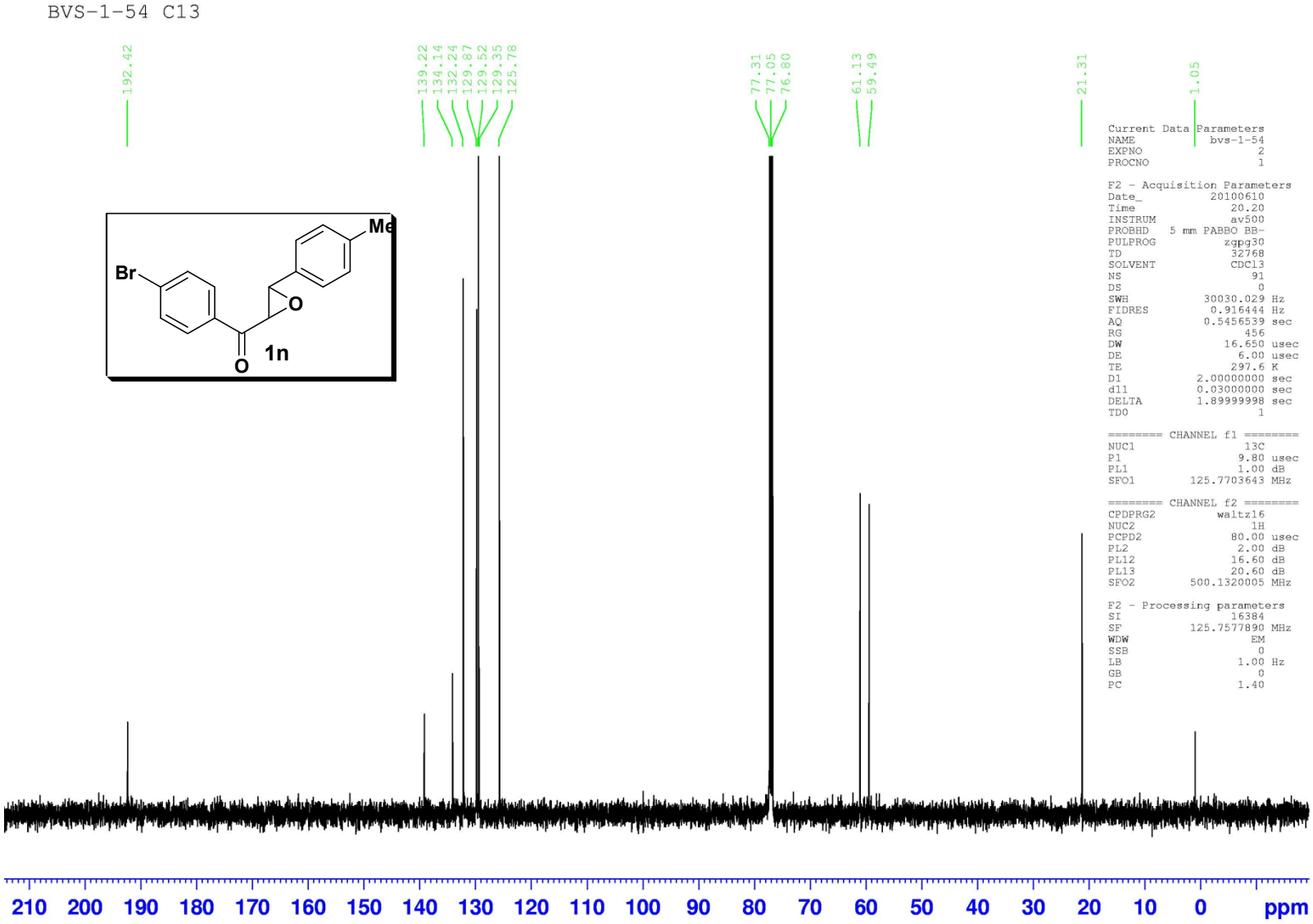
^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of **2m**



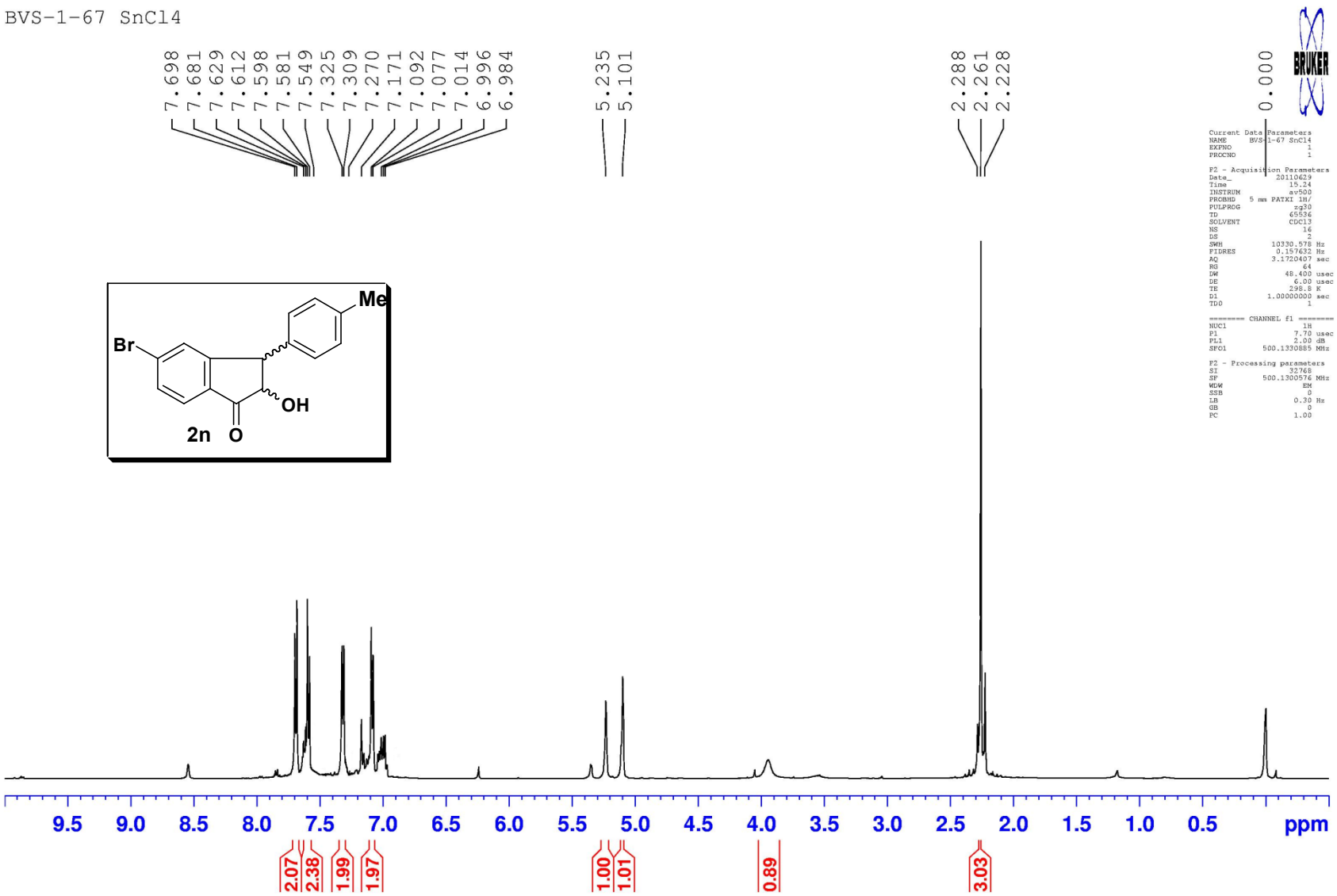
^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **2m**



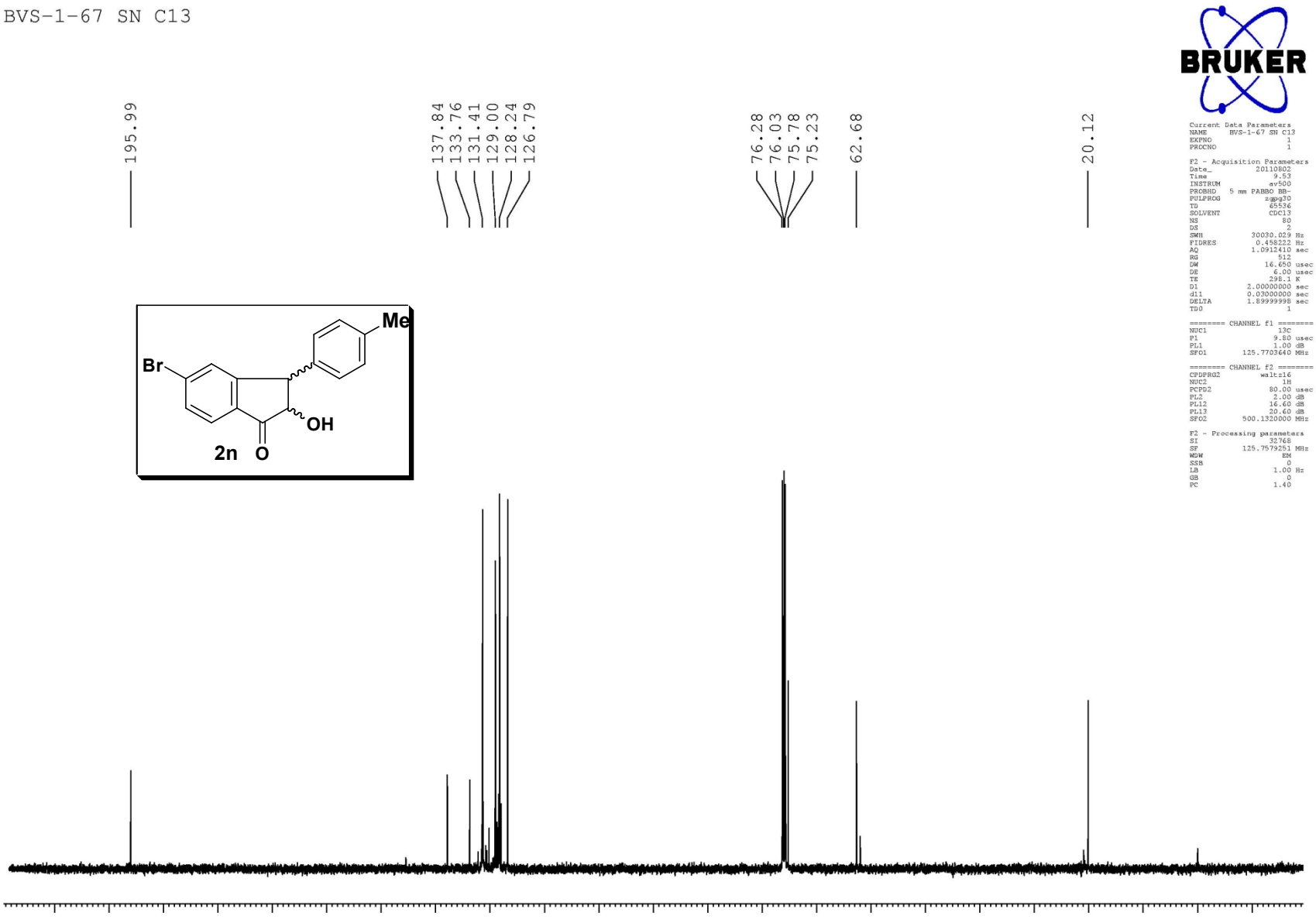
^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of **1n**



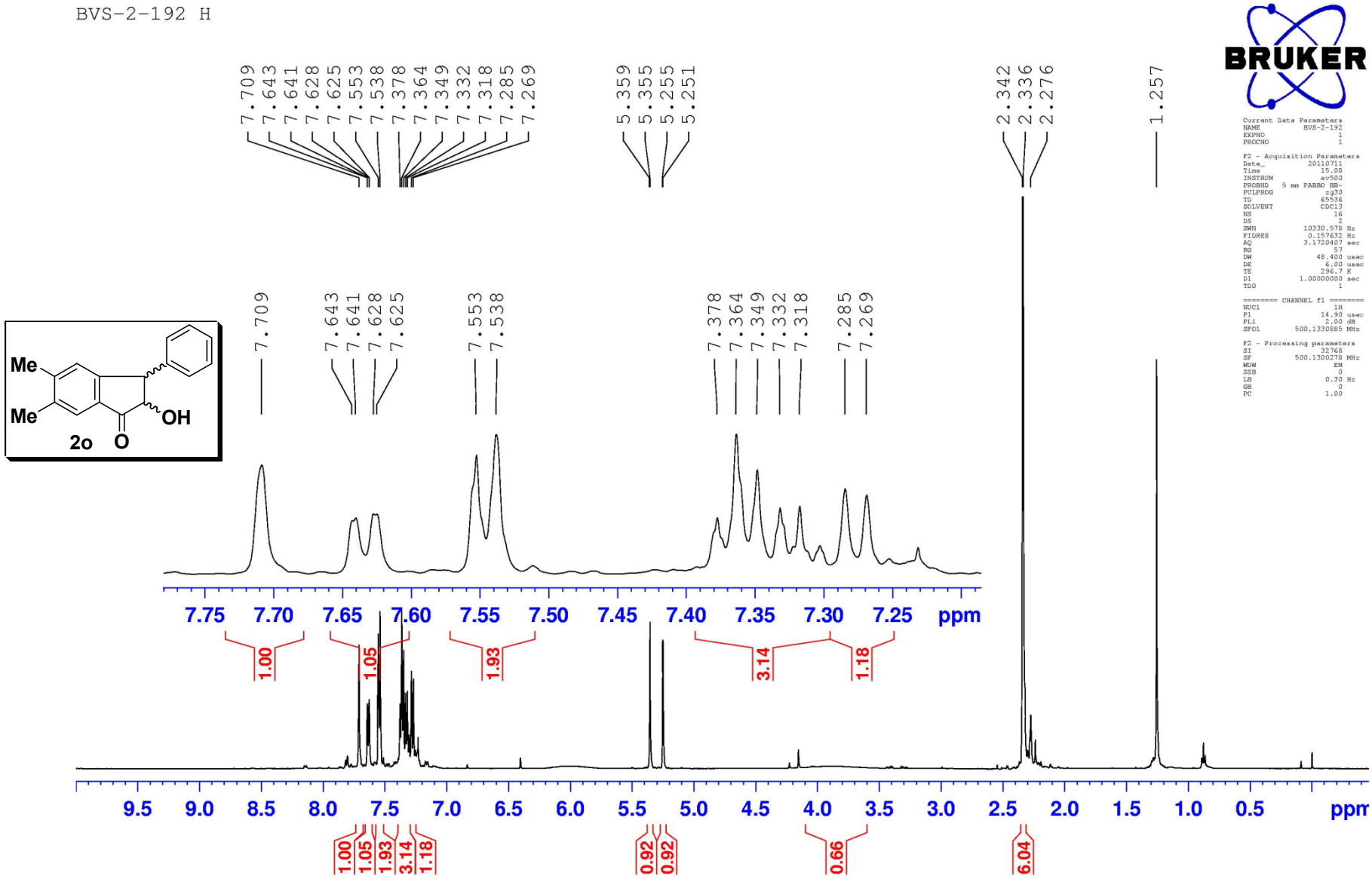
^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **1n**



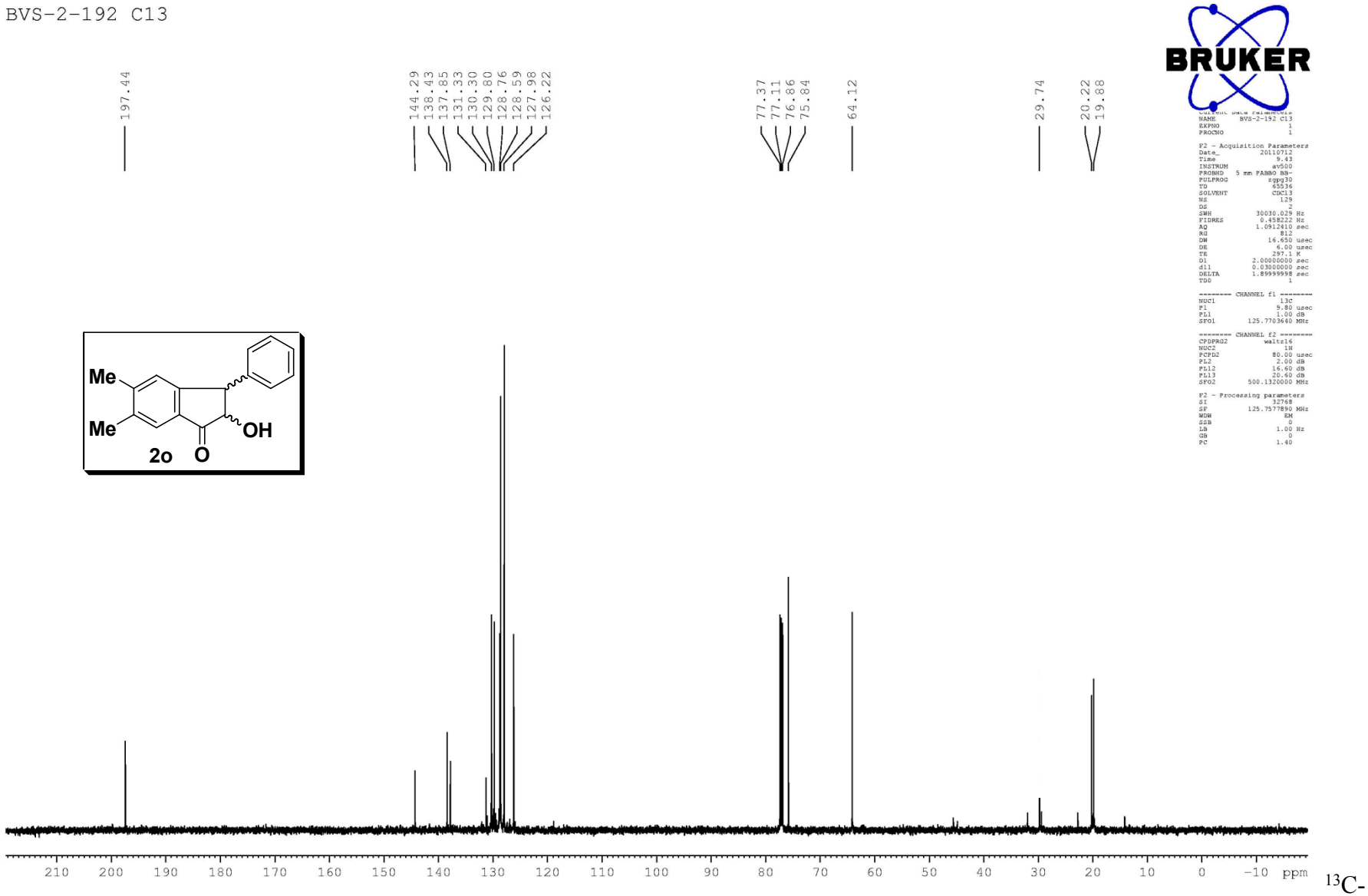
^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of **2n**



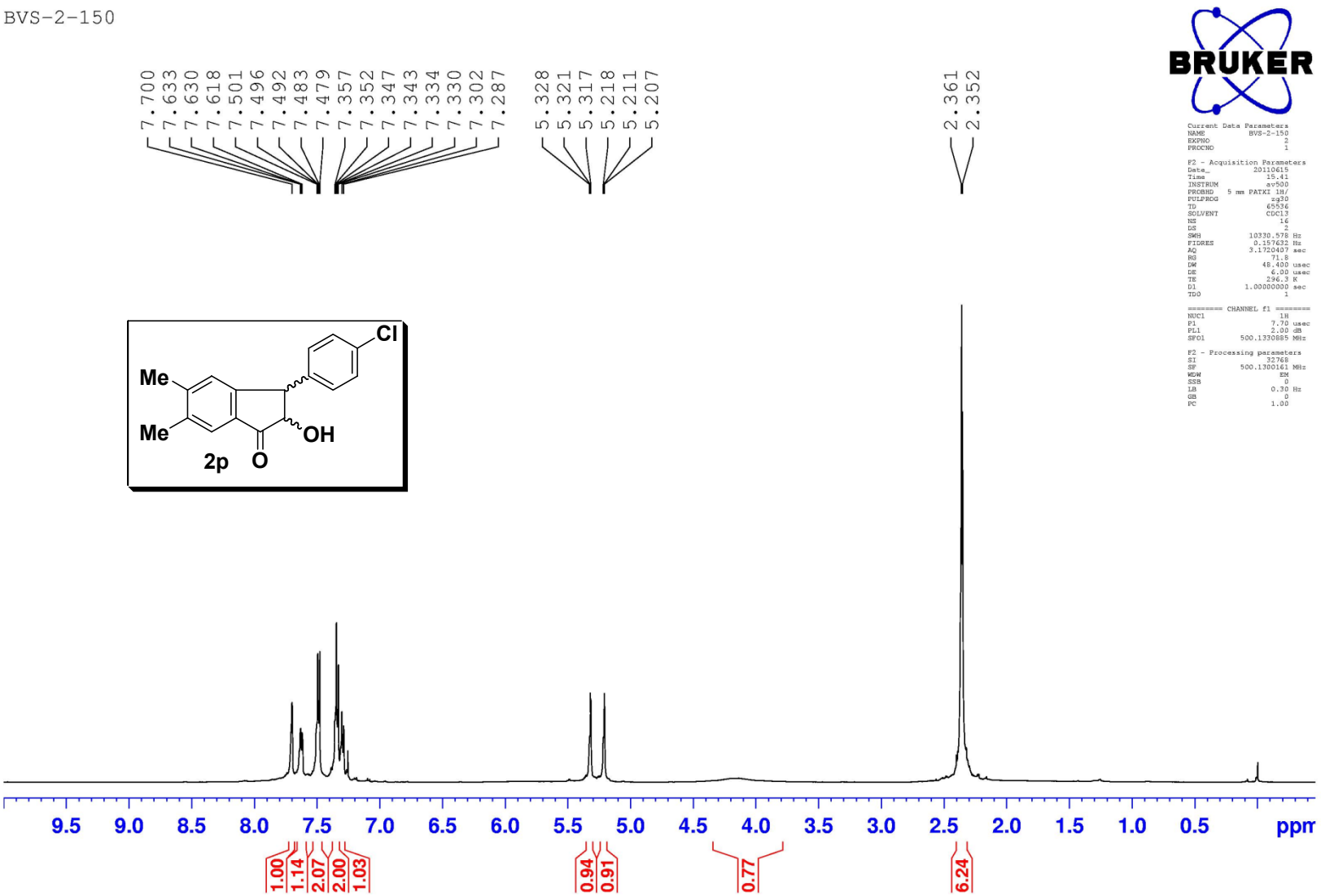
^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **2n**



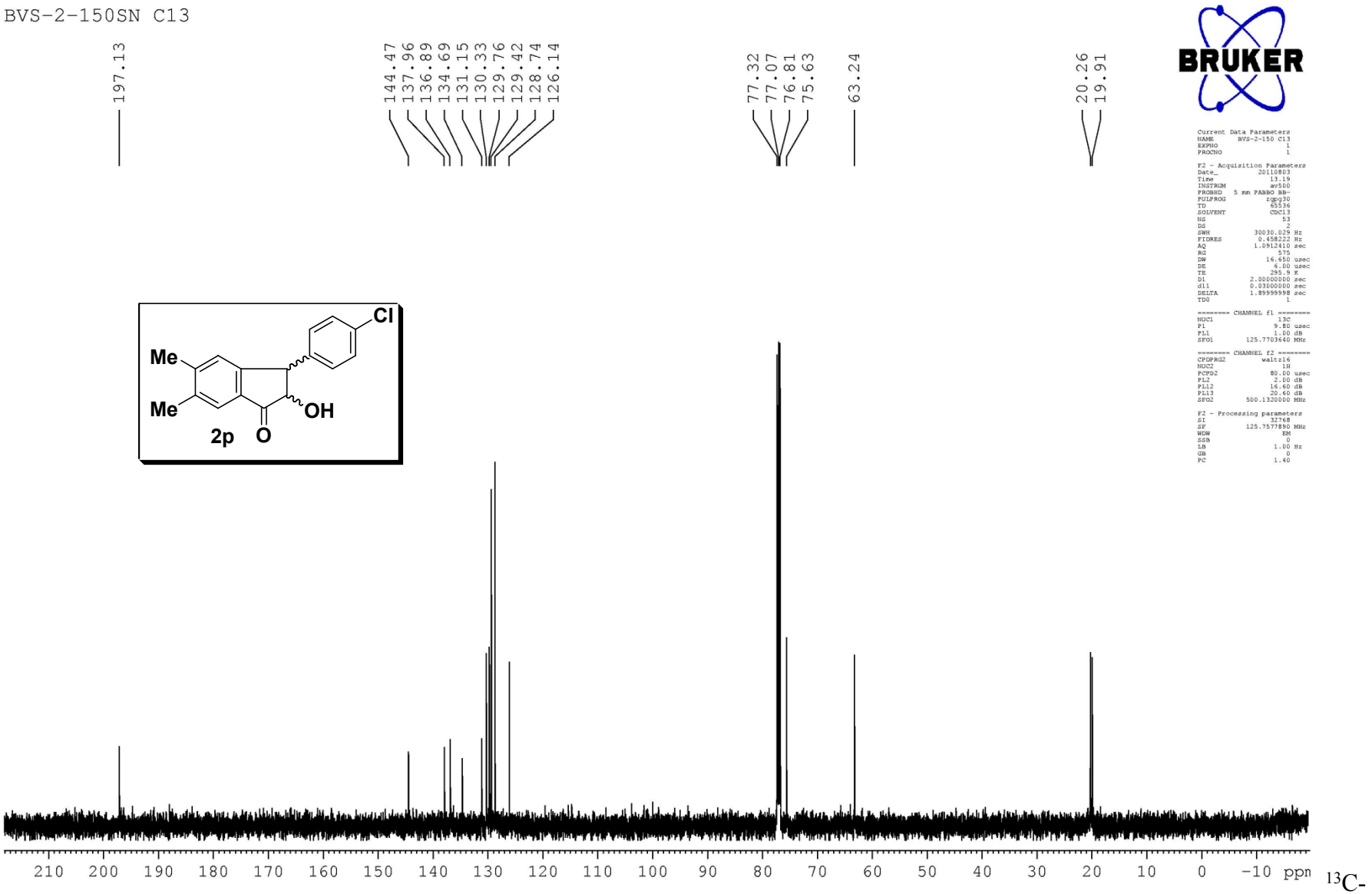
^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of **2o**



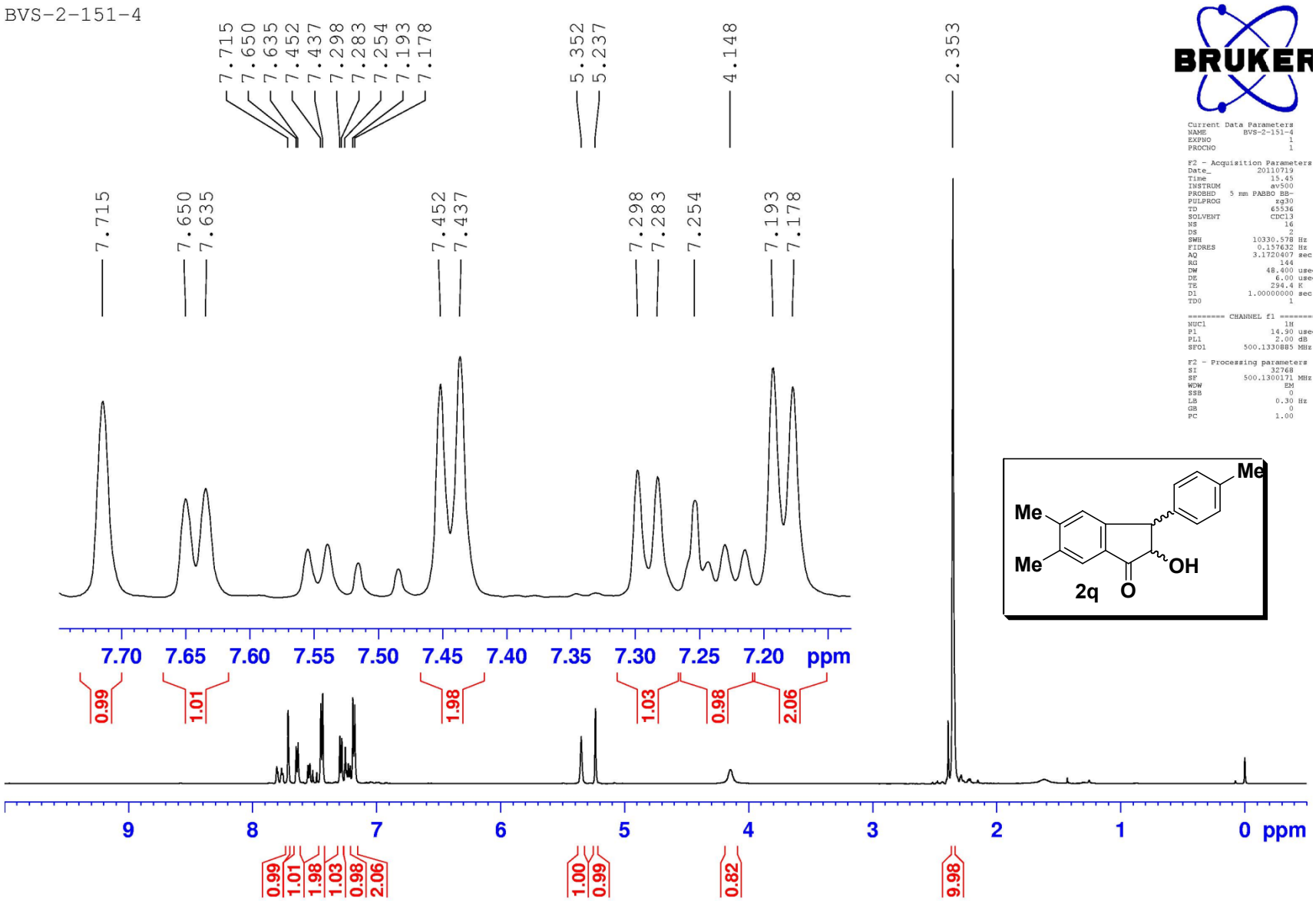
^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **2o**



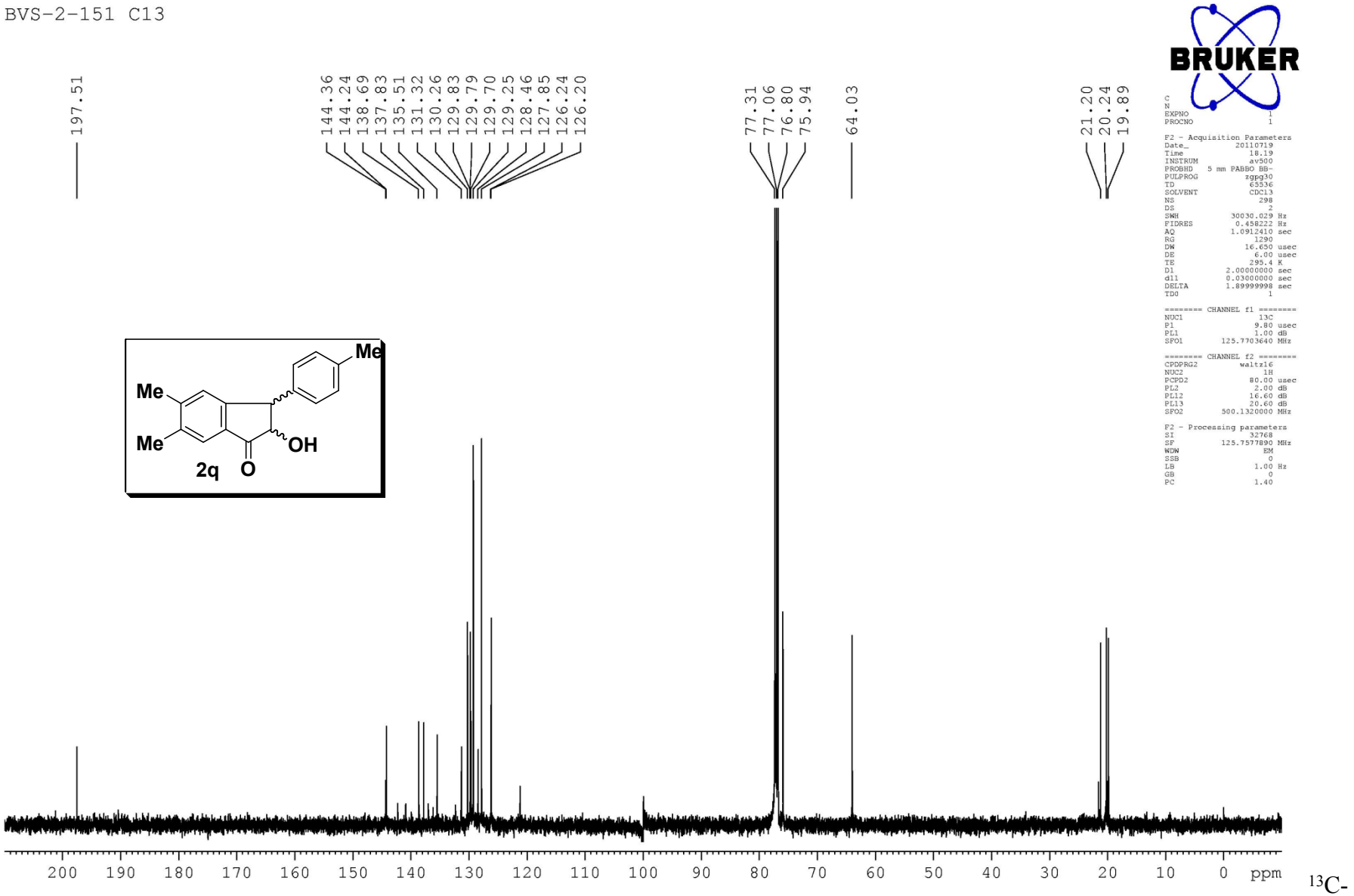
^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of **2p**



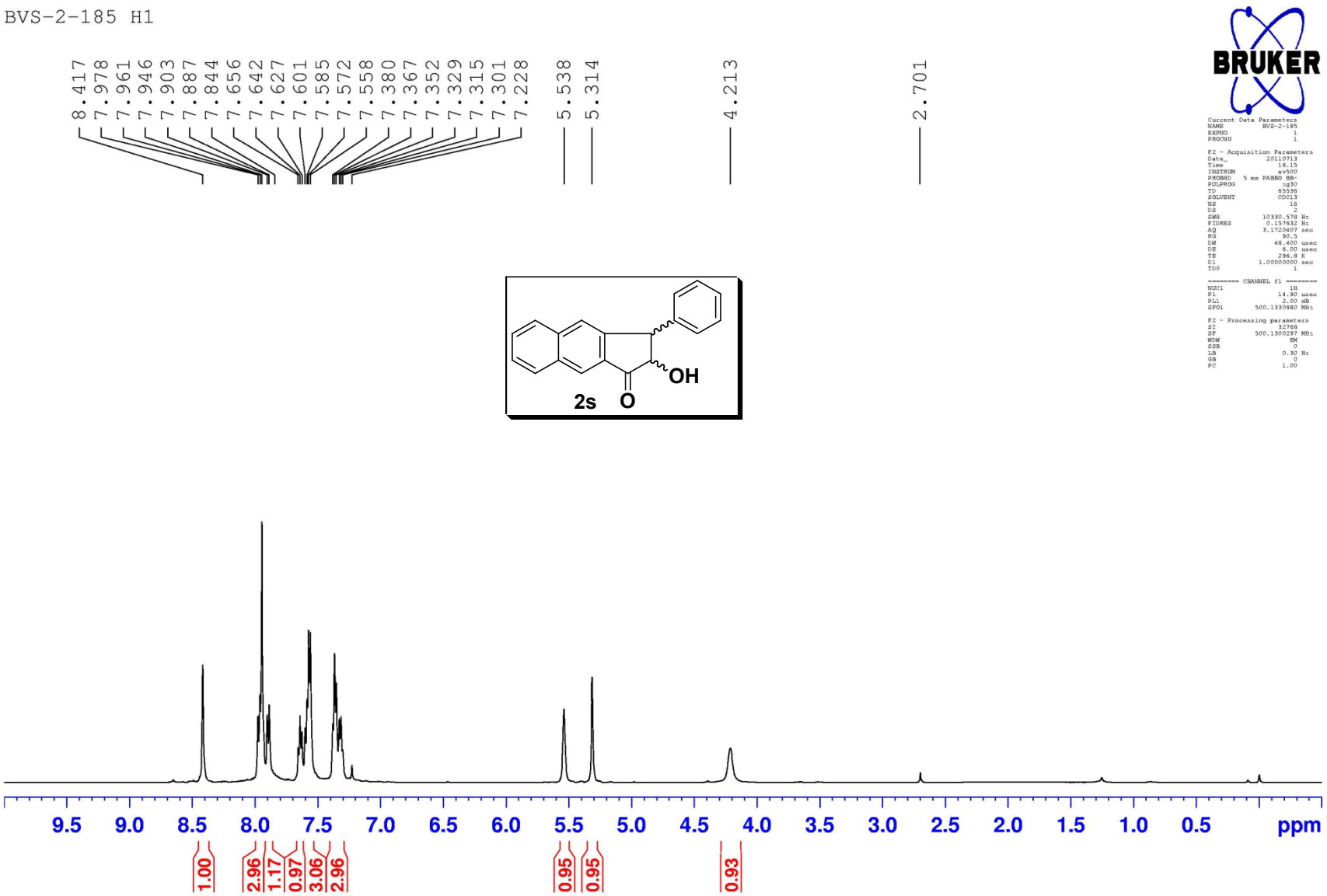
^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **2p**



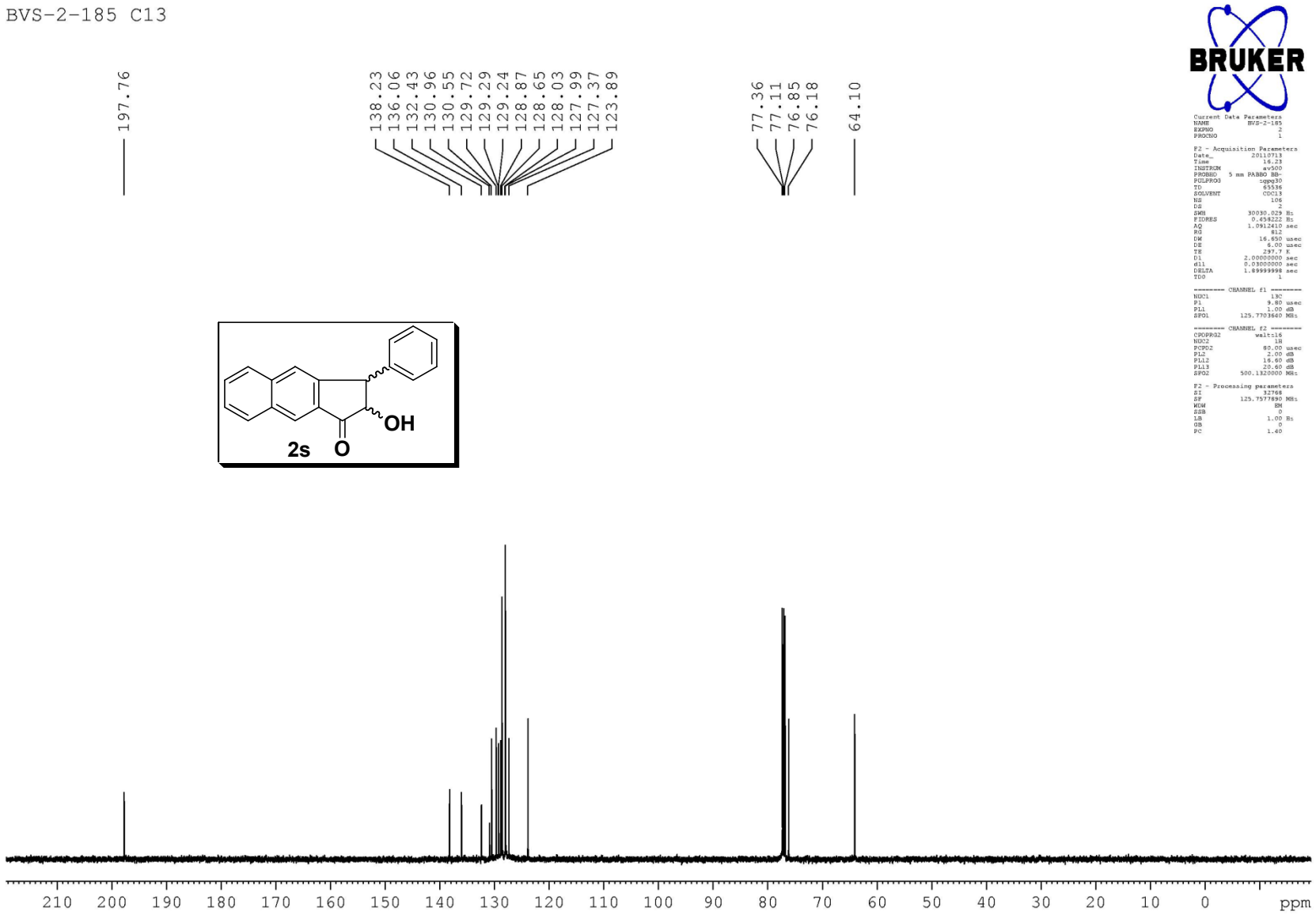
^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of **2q**



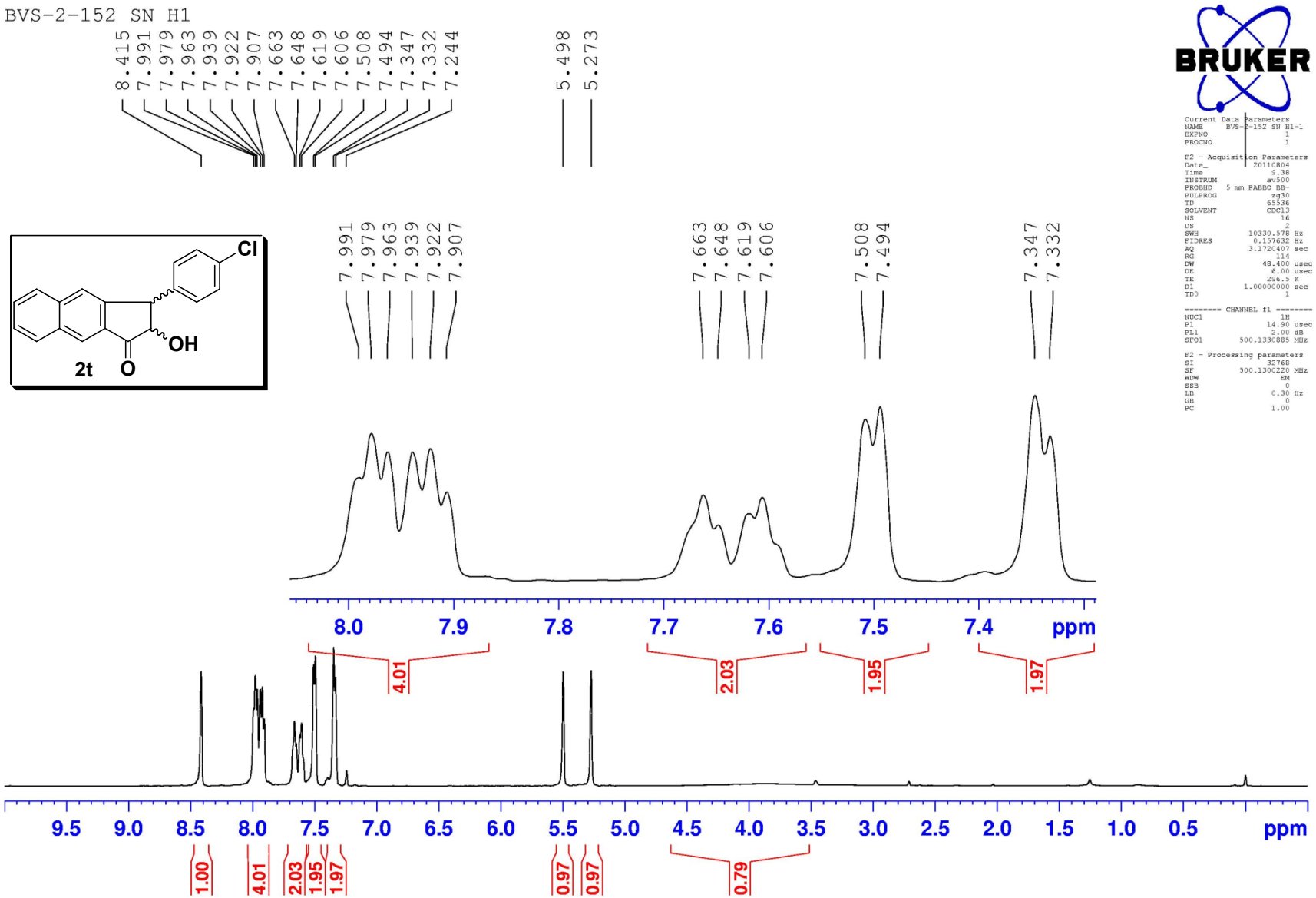
^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **2q**



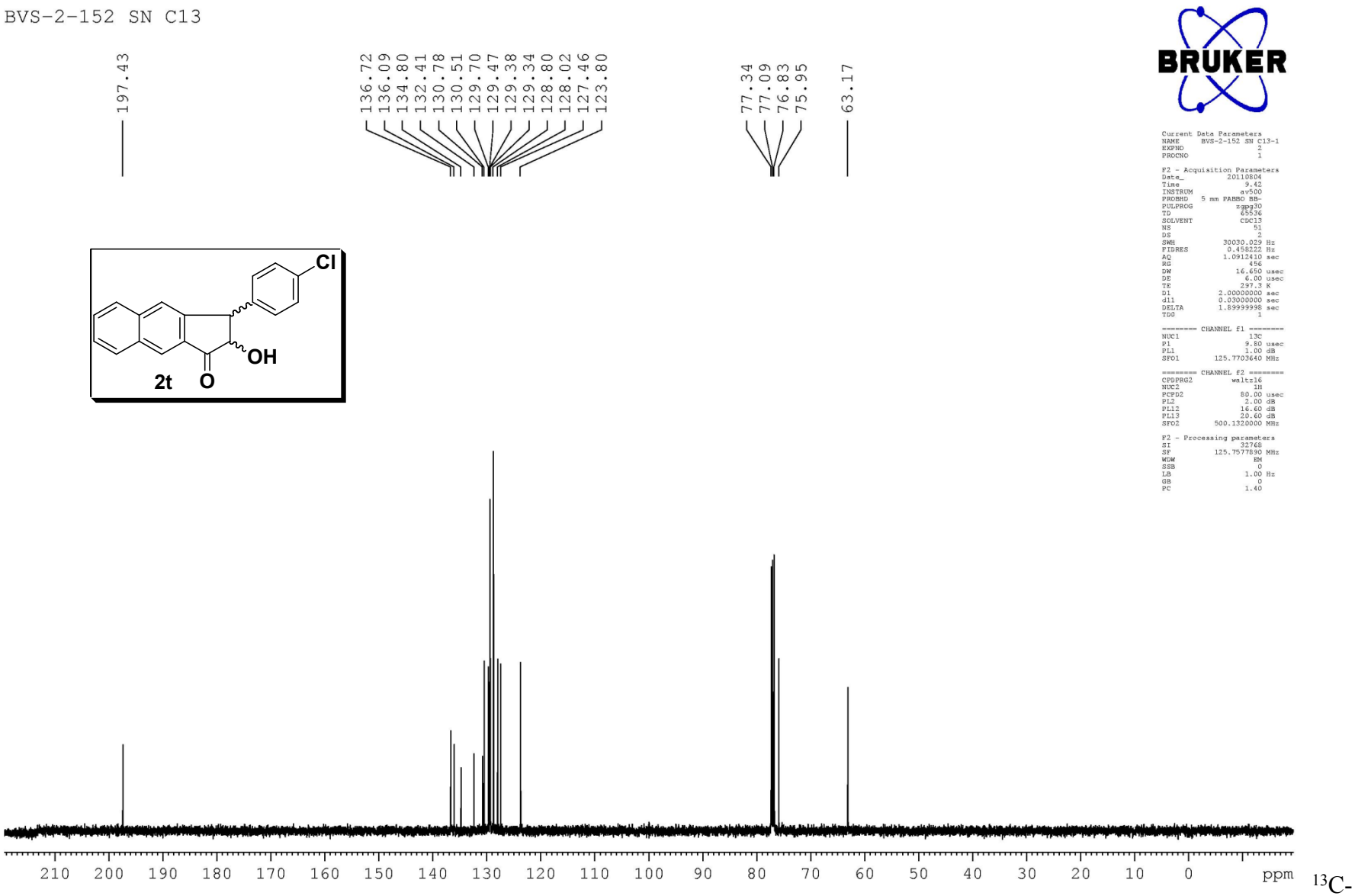
^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of **2s**



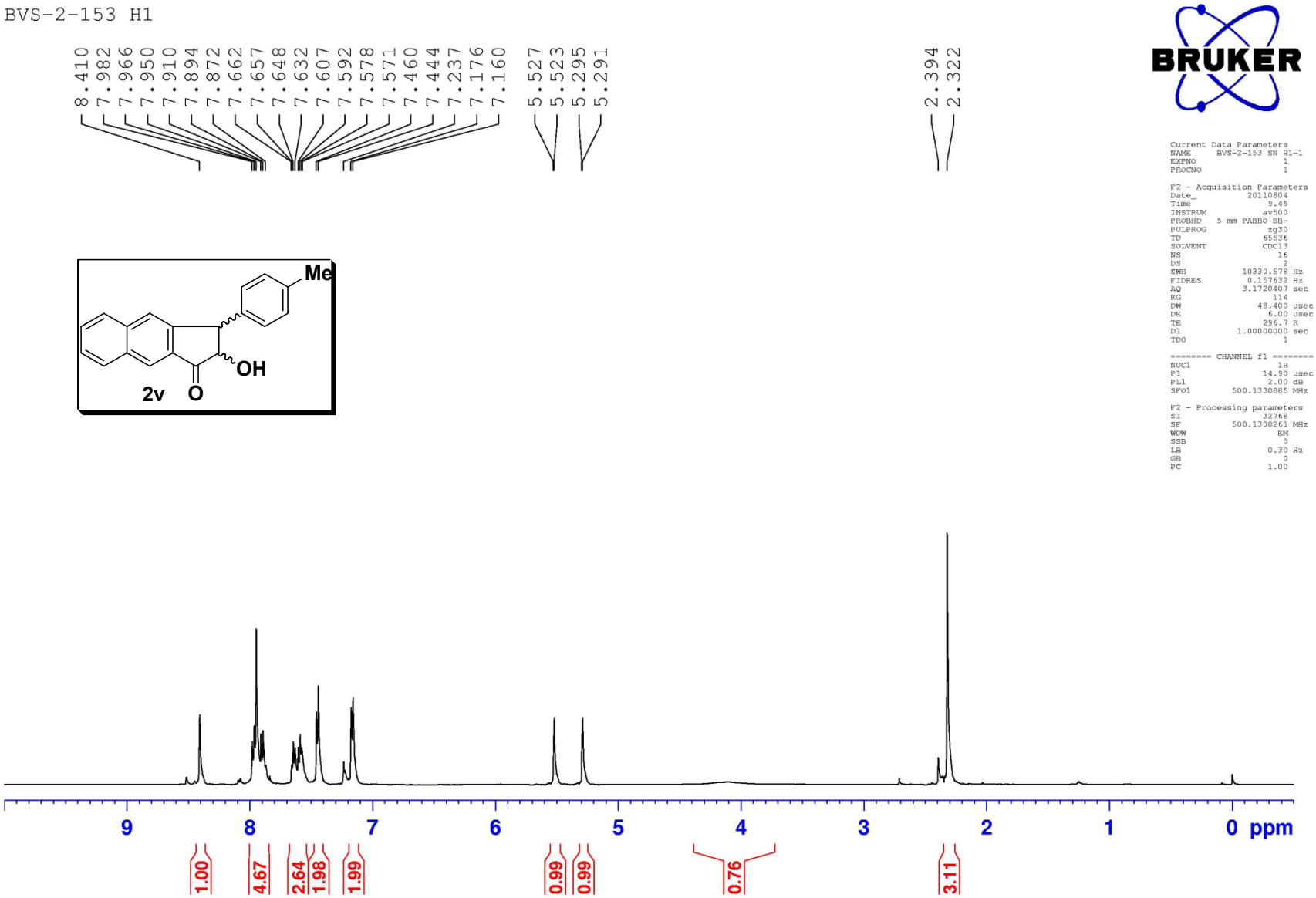
^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **2s**



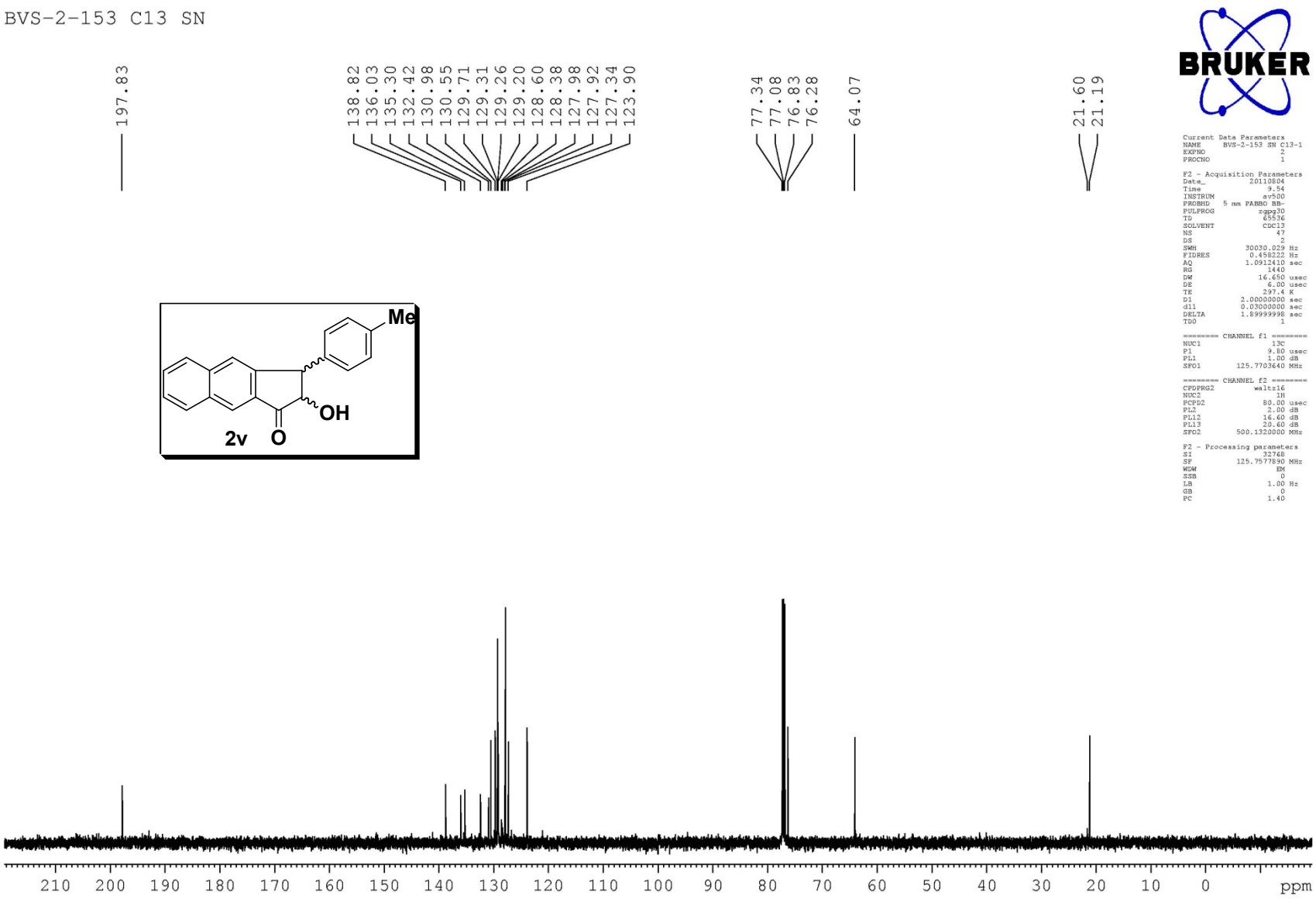
^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of **2t**



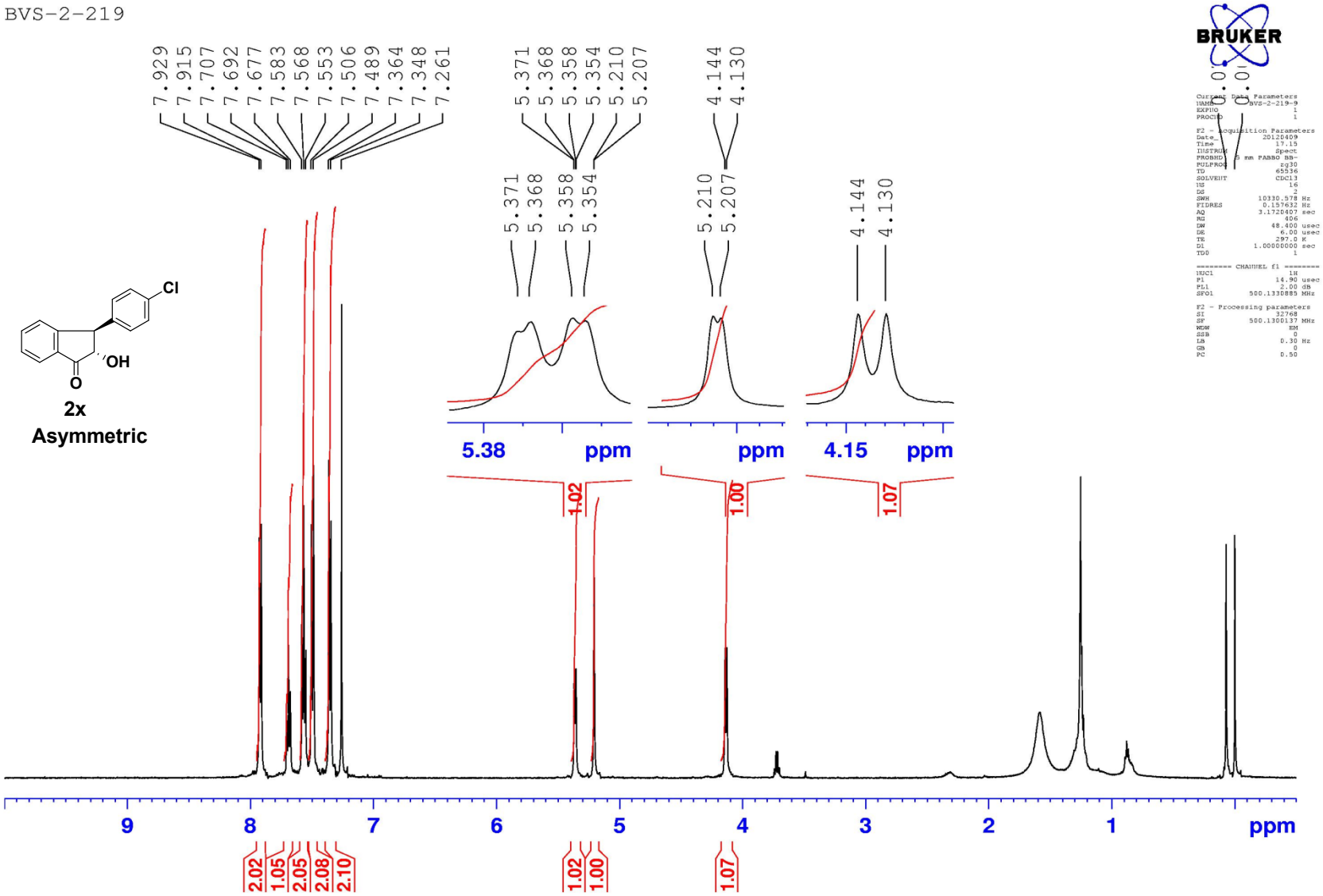
^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **2t**



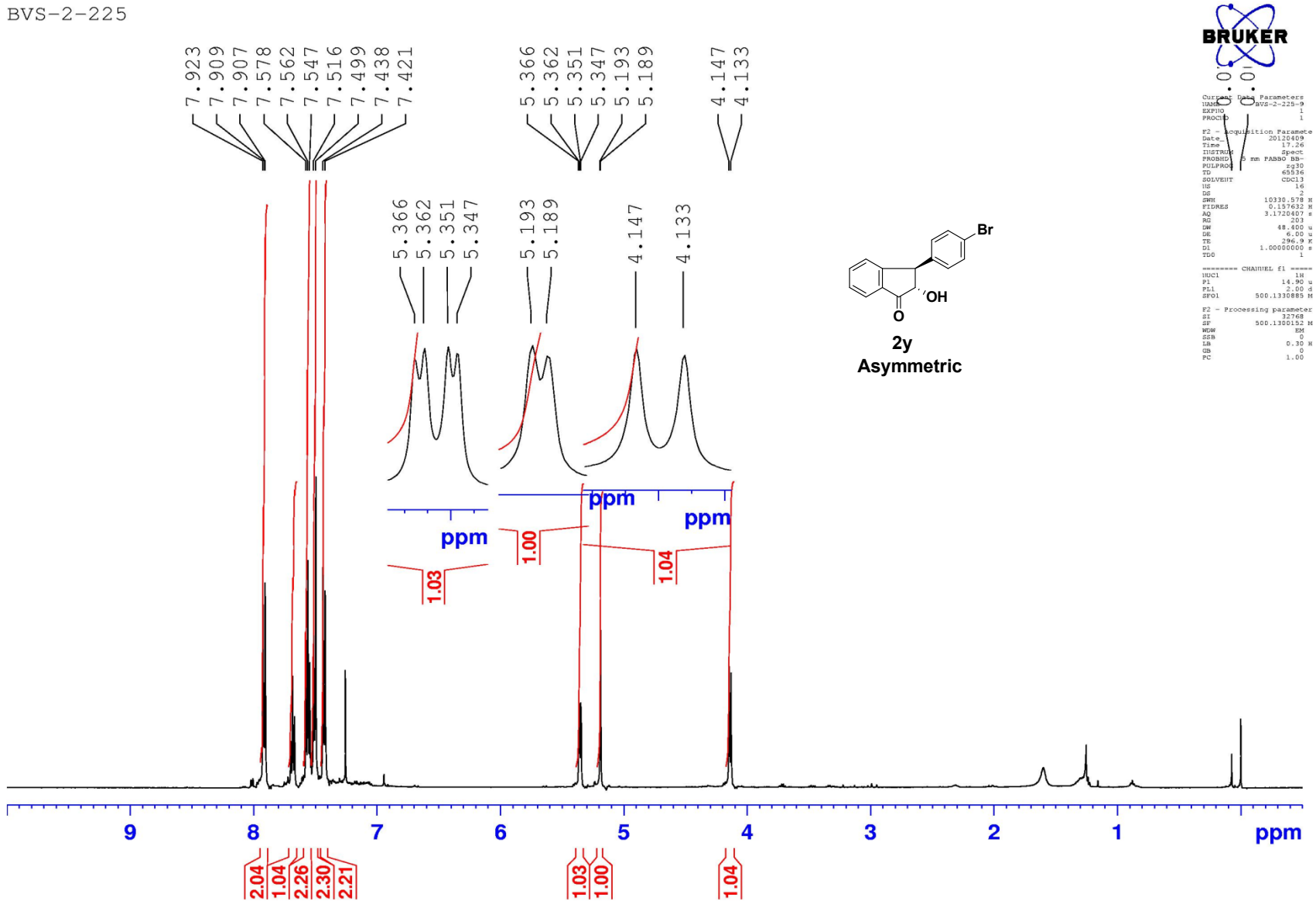
^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of **2v**



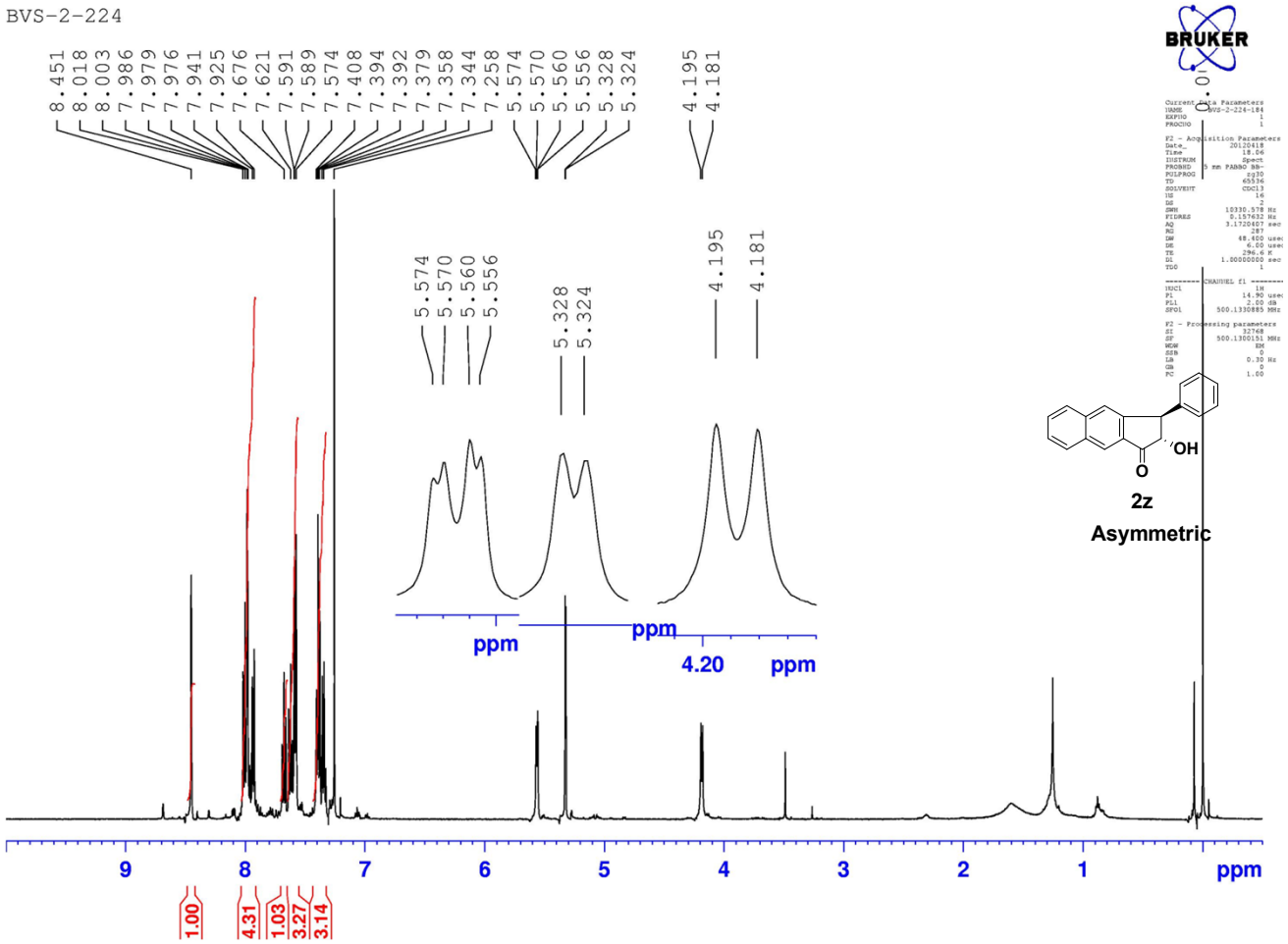
^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **2v**



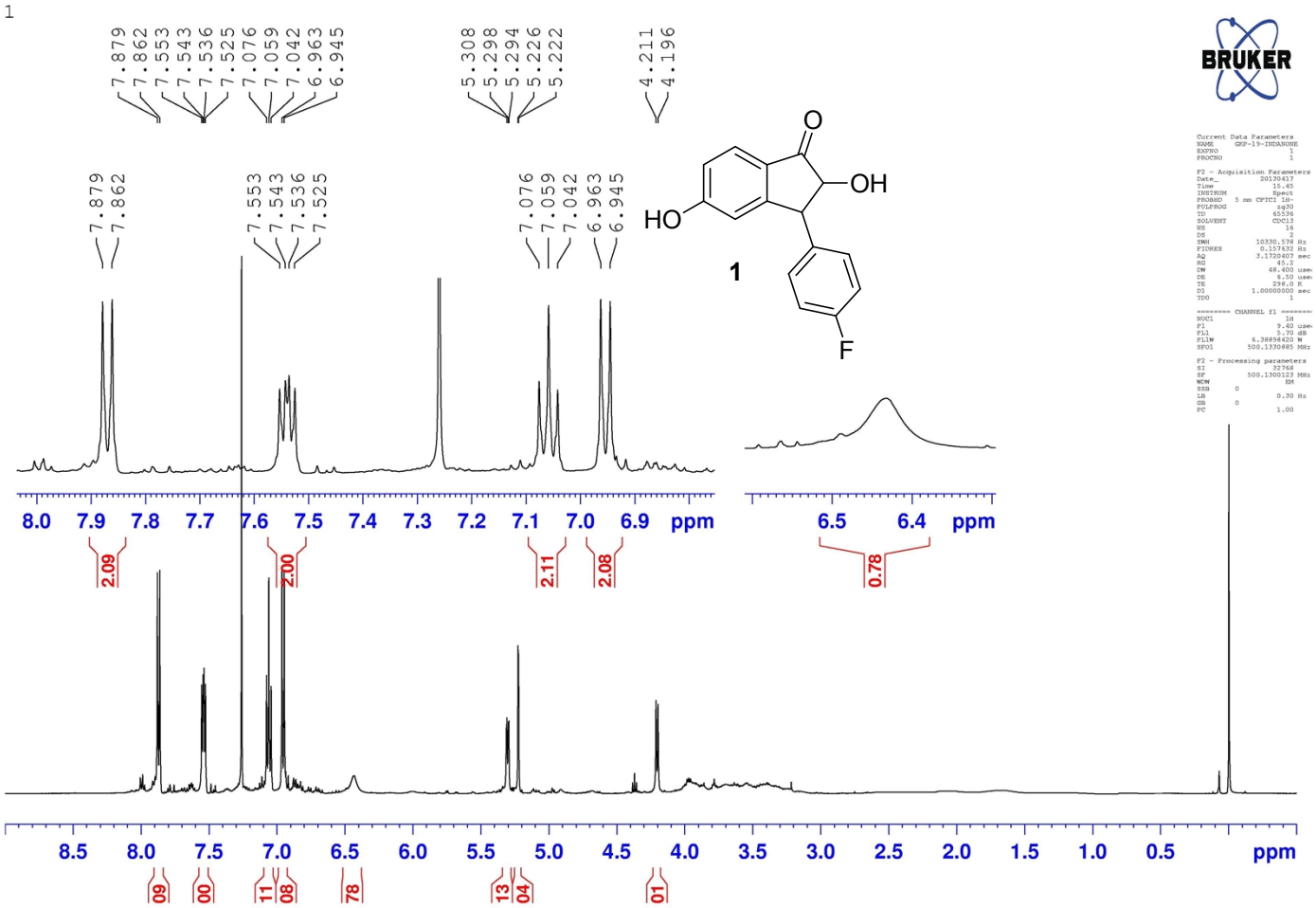
^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of **4a**

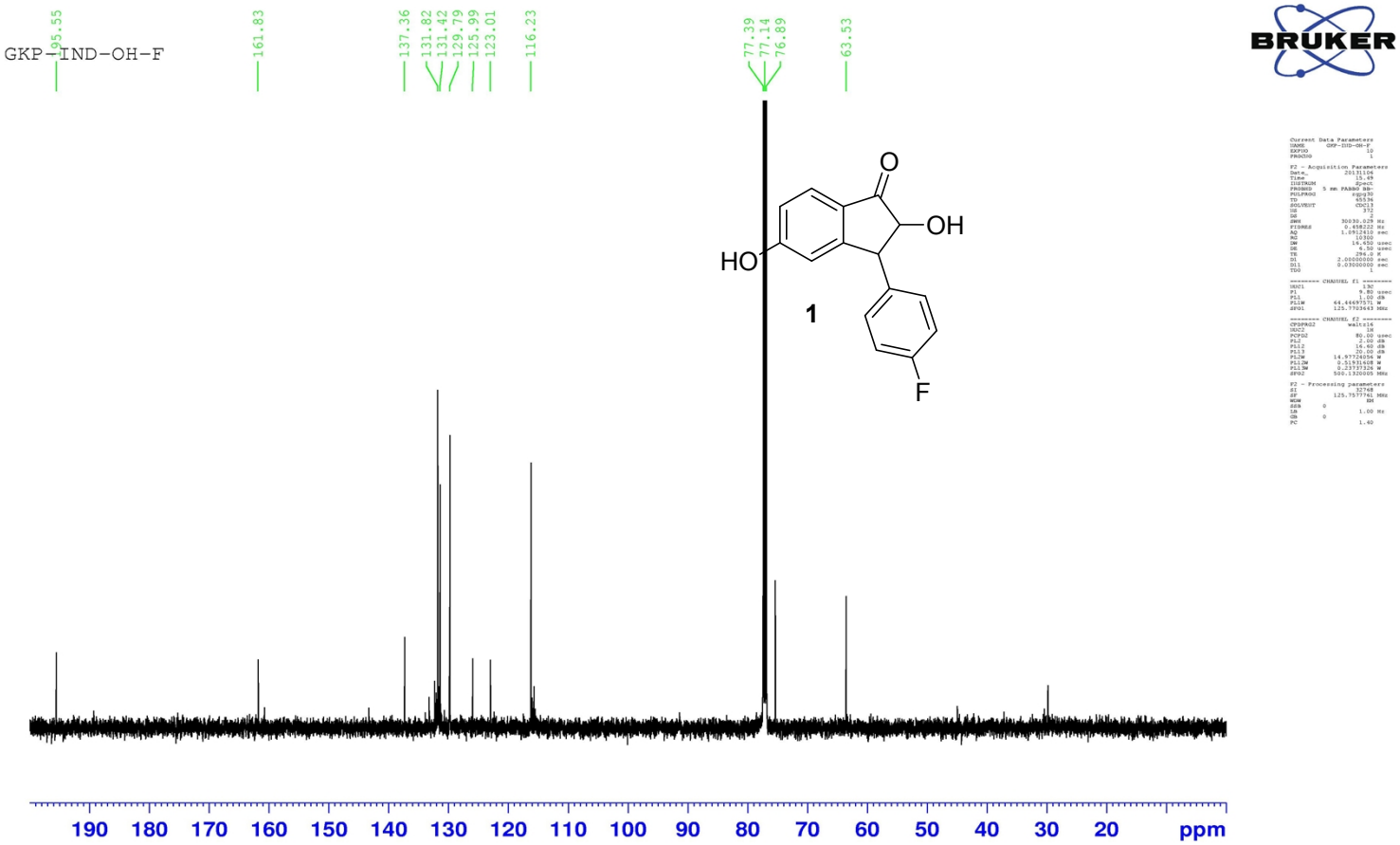


^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of **4b**



^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of **4c**


1
7.879
7.862
7.553
7.543
7.536
7.525
7.076
7.059
7.042
6.963
6.945
5.308
5.298
5.294
5.226
5.222
4.211
4.196
HO
OH
O
F
1
8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 ppm
6.5 6.4 ppm
2.09
2.00
2.11
2.08
0.78
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
09
00
11
08
78
13
04
01


GKP-IND-OH-F
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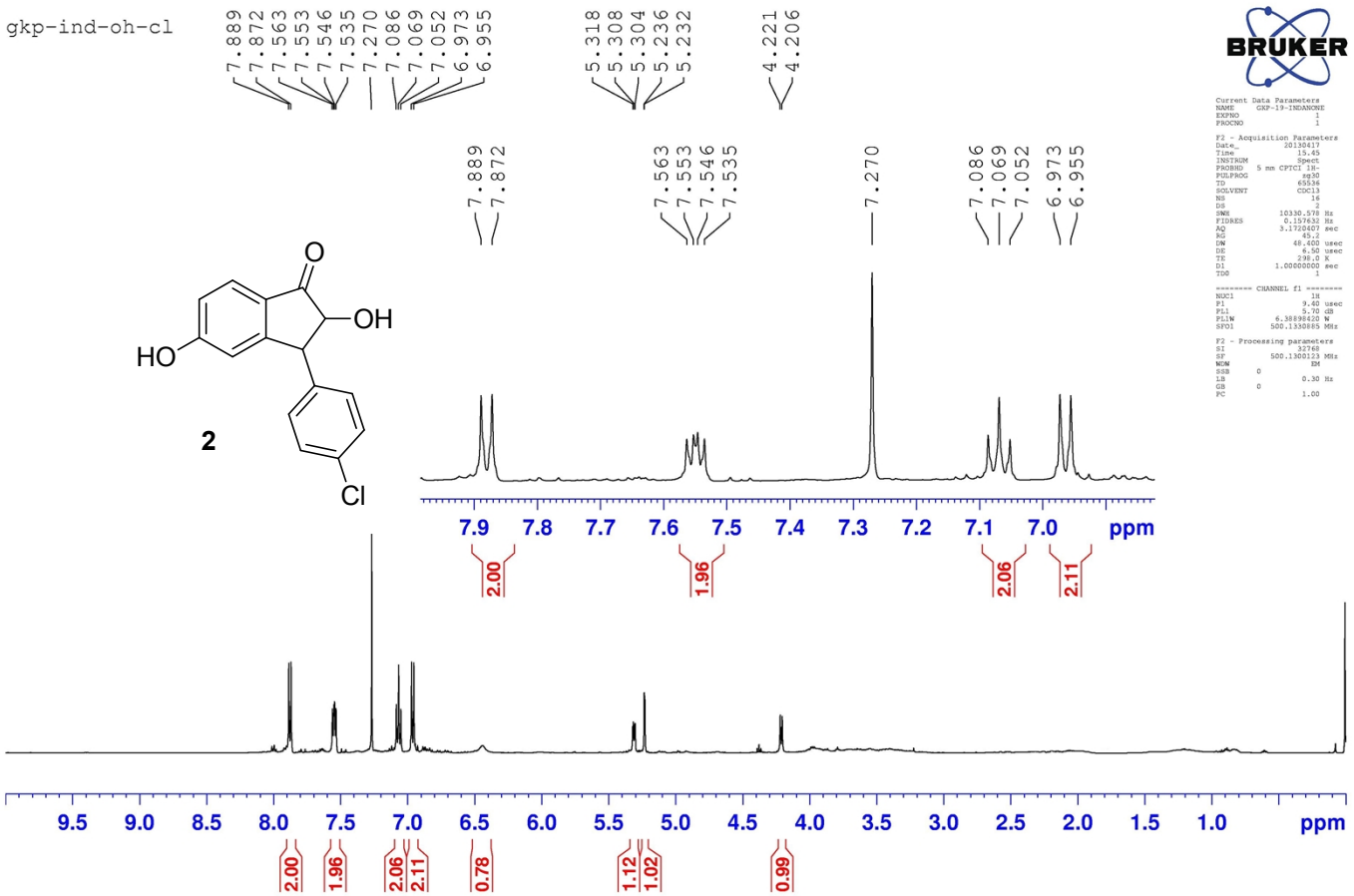
161.83
137.36
131.82
131.42
129.79
125.99
123.01
116.23
77.39
77.14
76.89
63.53
BRUKER
O
OH
HO
1
F
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


gkp-ind-oh-cl
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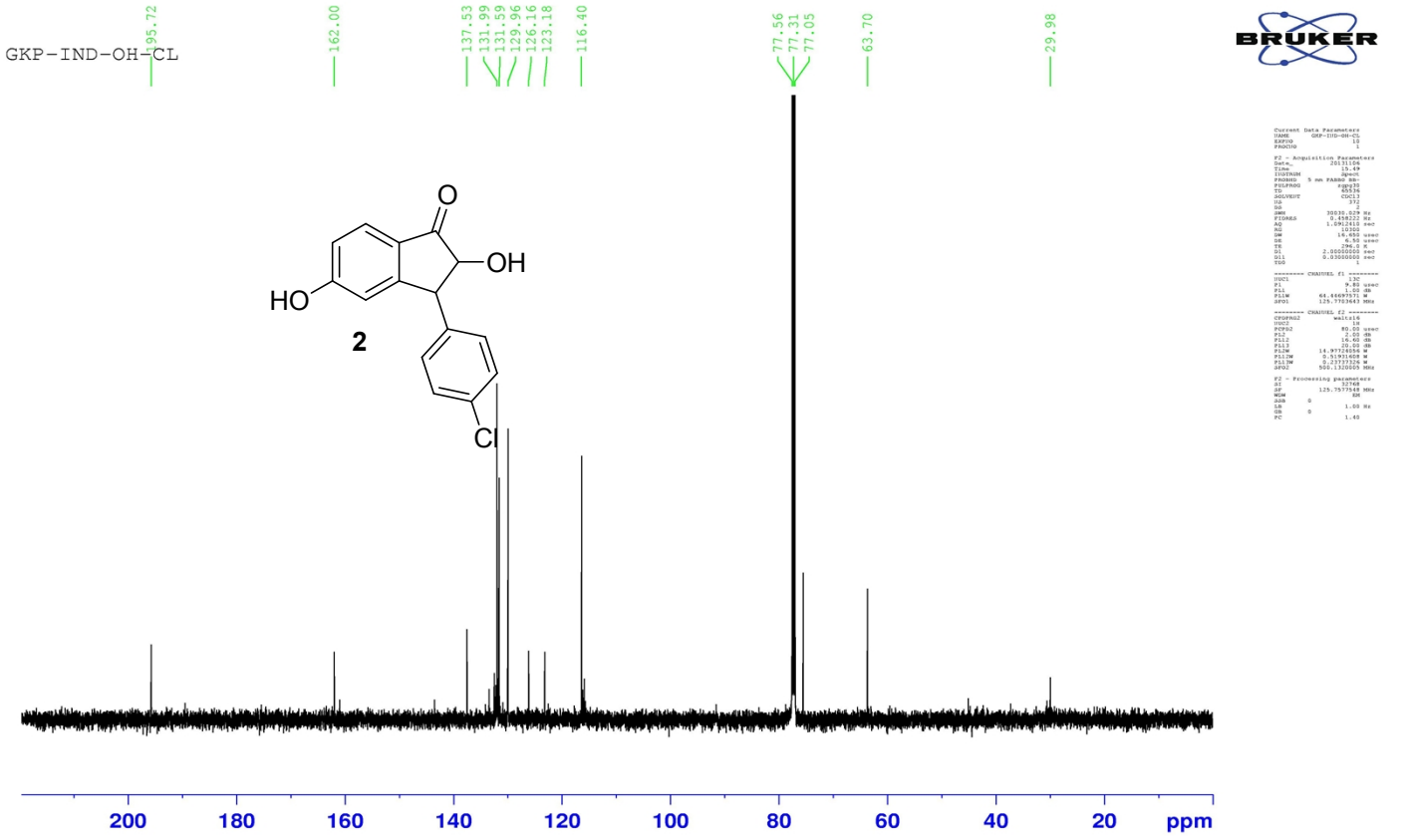
7.872
7.563
7.553
7.546
7.535
7.270
7.086
7.069
7.052
6.973
6.955
5.318
5.308
5.304
5.236
5.232
4.221
4.206
BRUKER
O
OH
HO
Cl
2
ppm
2.00
1.96
2.06
2.11
0.78
1.12
1.02
0.99


GKP-IND-OH-CL
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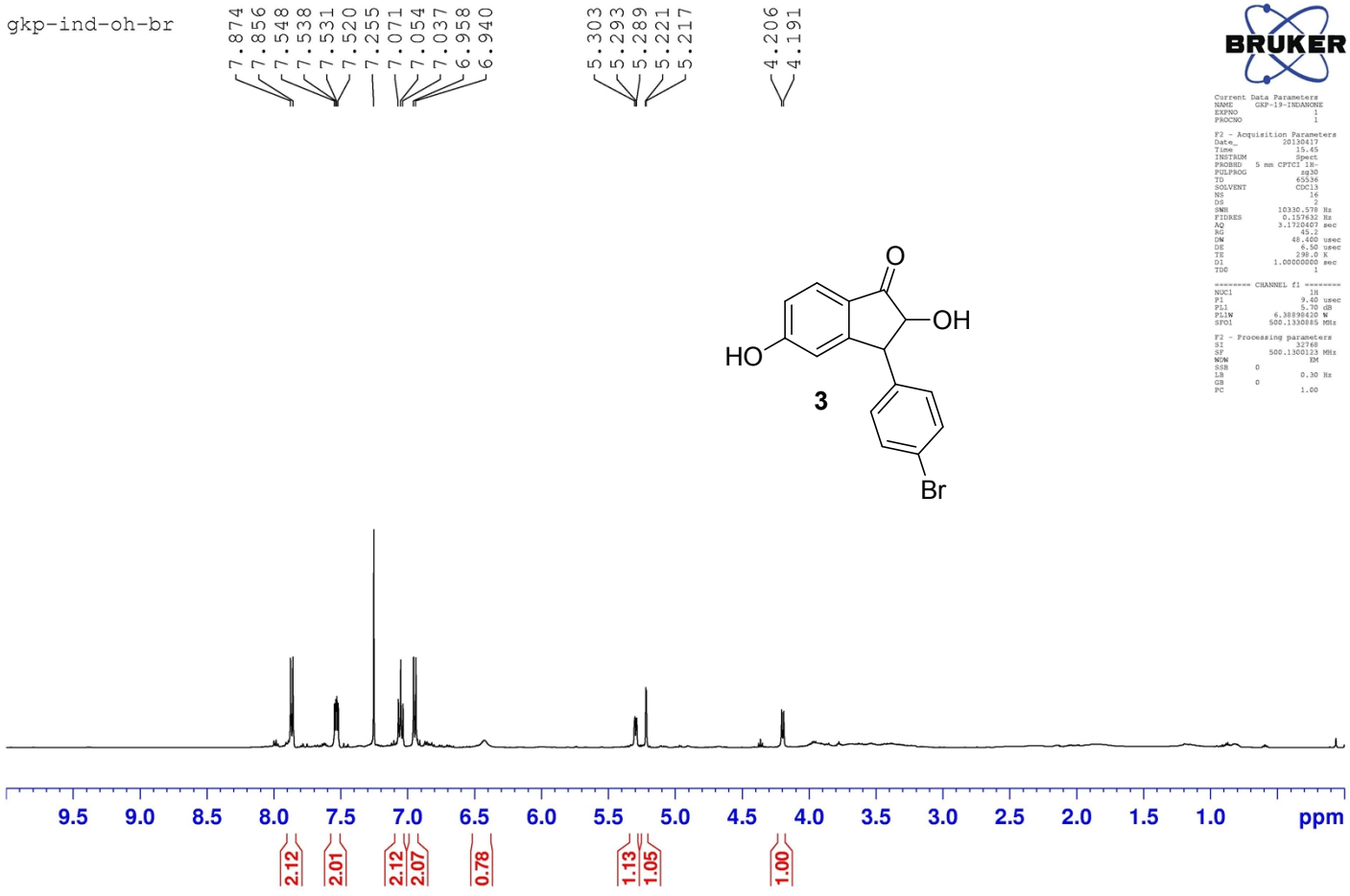
162.00
137.53
131.99
131.59
129.96
126.16
123.18
116.40
77.56
77.31
77.05
63.70
29.98
BRUKER
O
OH
HO
2
Cl
200
180
160
140
120
100
80
60
40
20
ppm


gkp-ind-oh-br
7.874
7.856
7.548
7.538
7.531
7.520
7.255
7.071
7.054
7.037
6.958
6.940
5.303
5.293
5.289
5.221
5.217
4.206
4.191
BRUKER
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NAME GKP-19-INDANONE
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130417
Time 15.45
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PULPROG zg30
TD 65536
SOLVENT CDCl3
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DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 45.2
DW 48.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 9.40 usec
PL1 5.70 dB
PL1W 6.38898420 W
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300123 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
OH
HO
3
Br
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
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1.0
ppm
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2.12
2.07
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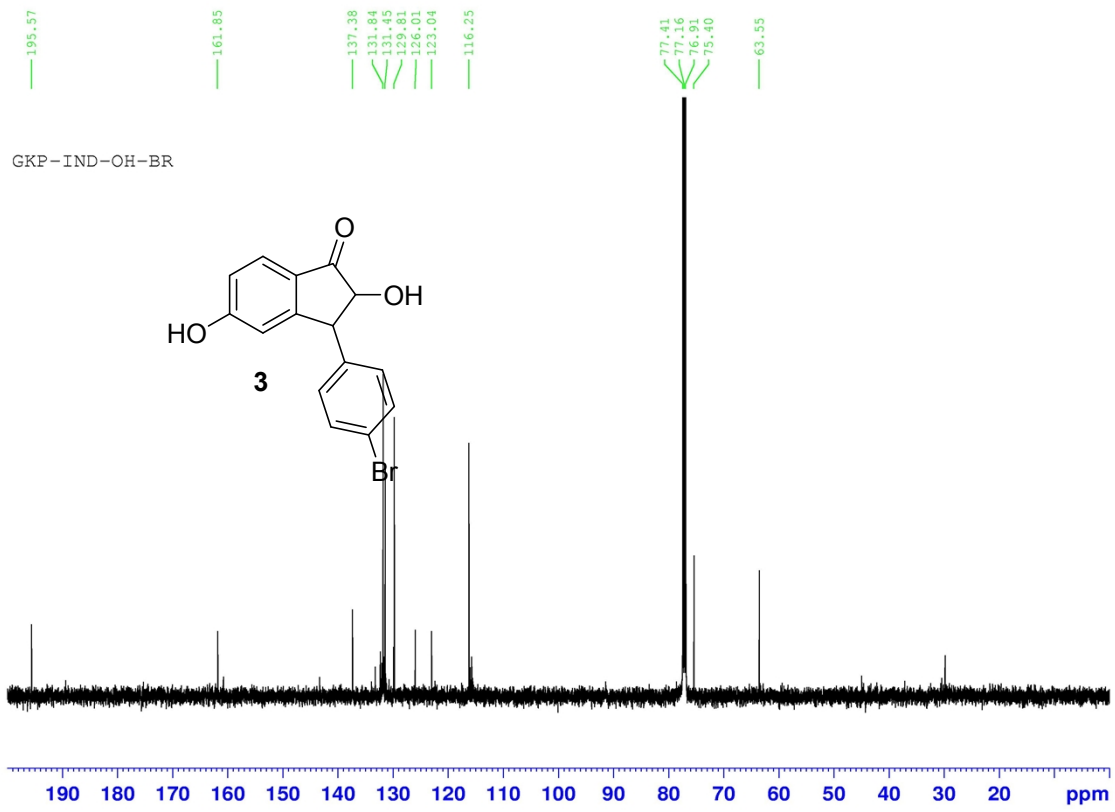
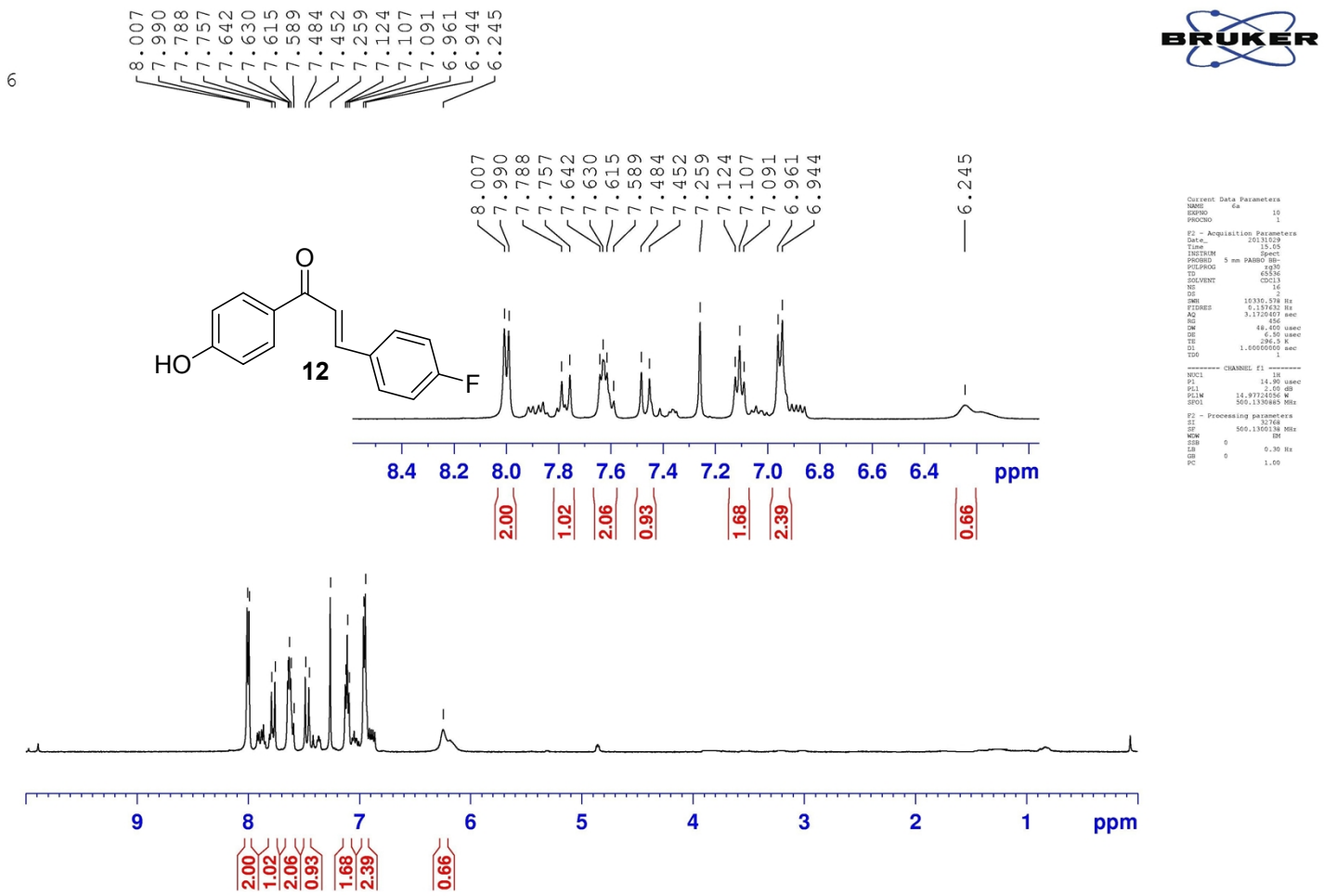
1.13
1.05
1.00


195.57
161.85
137.38
131.84
131.45
129.81
126.01
123.04
116.25
77.41
77.16
76.91
75.40
63.55
GKP-IND-OH-BR
O
OH
HO
3
Br
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm



Current Data Parameters
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EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
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TD 65536
SOLVENT CDCl3
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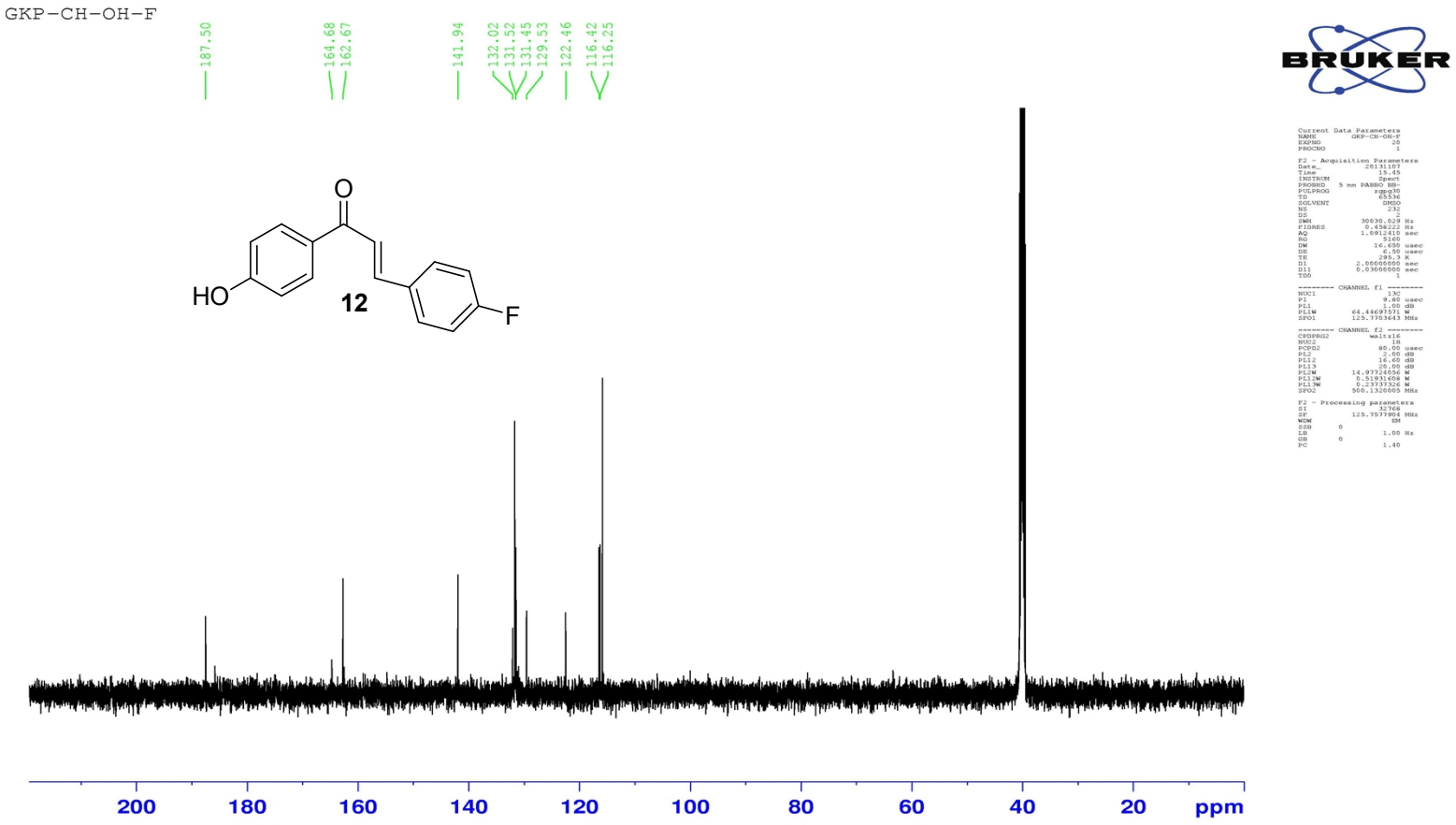
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 456
DW 48.400 usec
DE 6.50 usec
TE 296.5 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.90 usec
PL1 2.00 dB
PL1W 14.97240596 W
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300138 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00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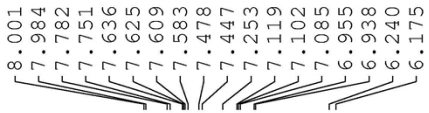
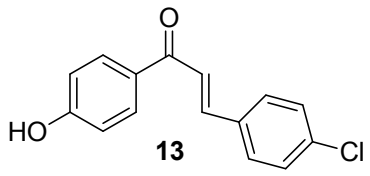
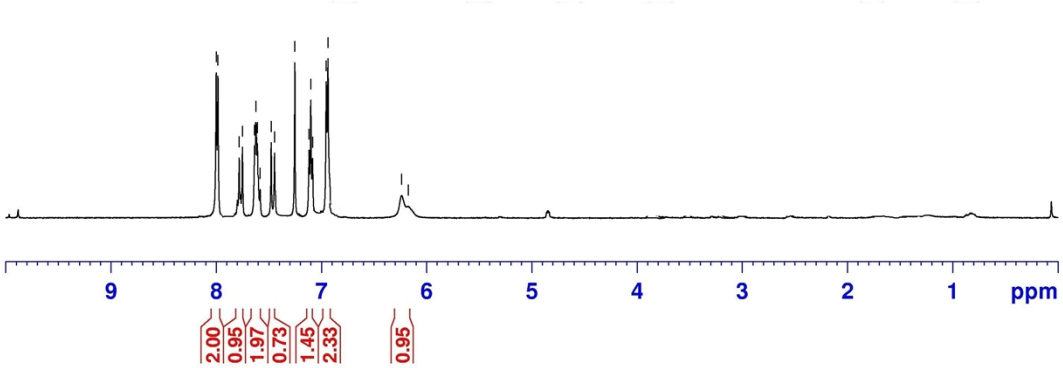
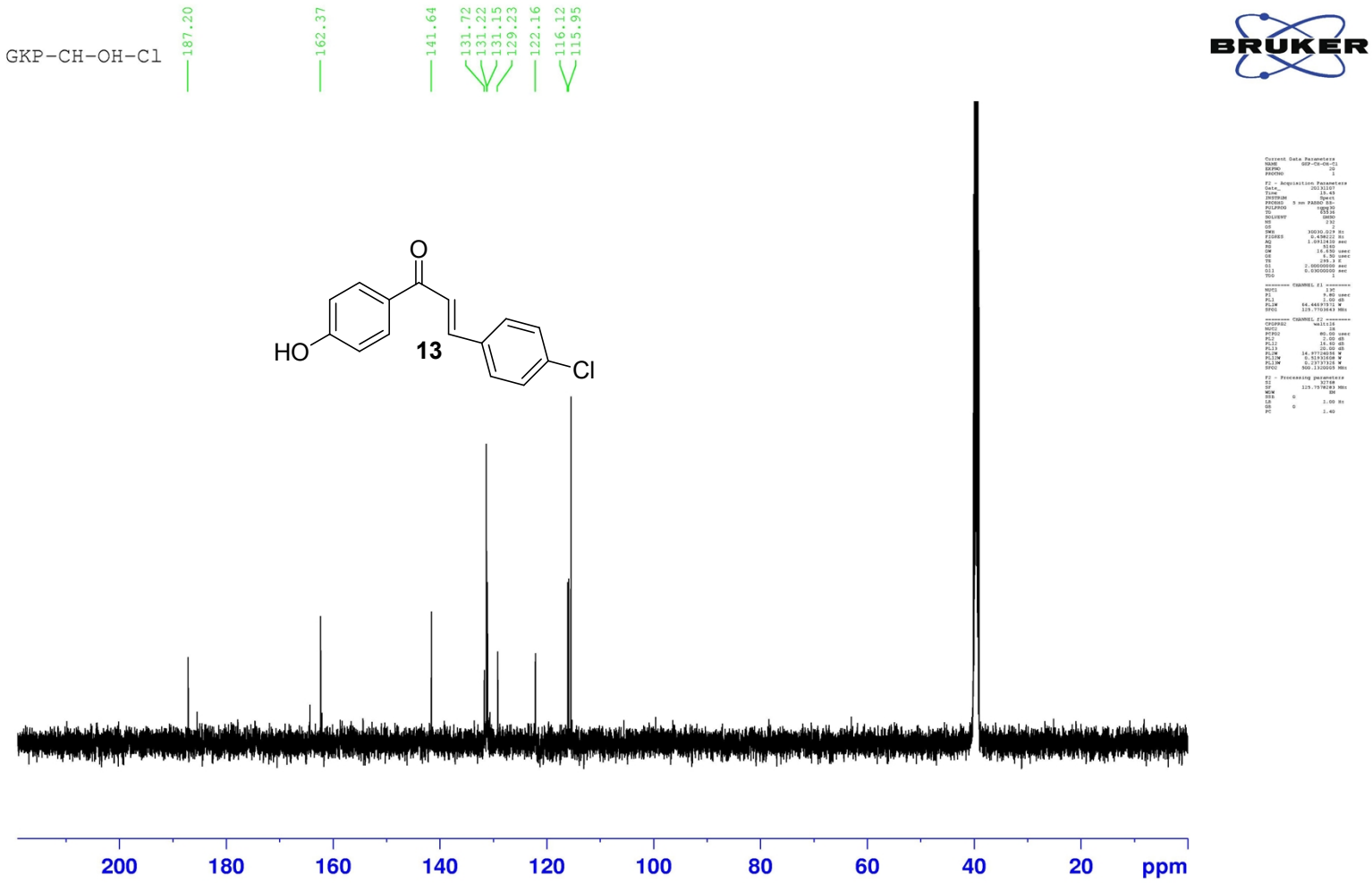
187.50
164.68
162.67
141.94
132.02
131.52
131.45
129.53
122.46
116.42
116.25
BRUKER
HO
O
F
12
200
180
160
140
120
100
80
60
40
20
ppm


8.001
7.984
7.782
7.751
7.636
7.625
7.609
7.583
7.478
7.447
7.253
7.119
7.102
7.085
6.955
6.938
6.240
6.175


O
HO
Cl

13


9
8
7
6
5
4
3
2
1
ppm
2.00
0.95
1.97
0.73
1.45
2.33
0.95


GKP-CH-OH-Cl
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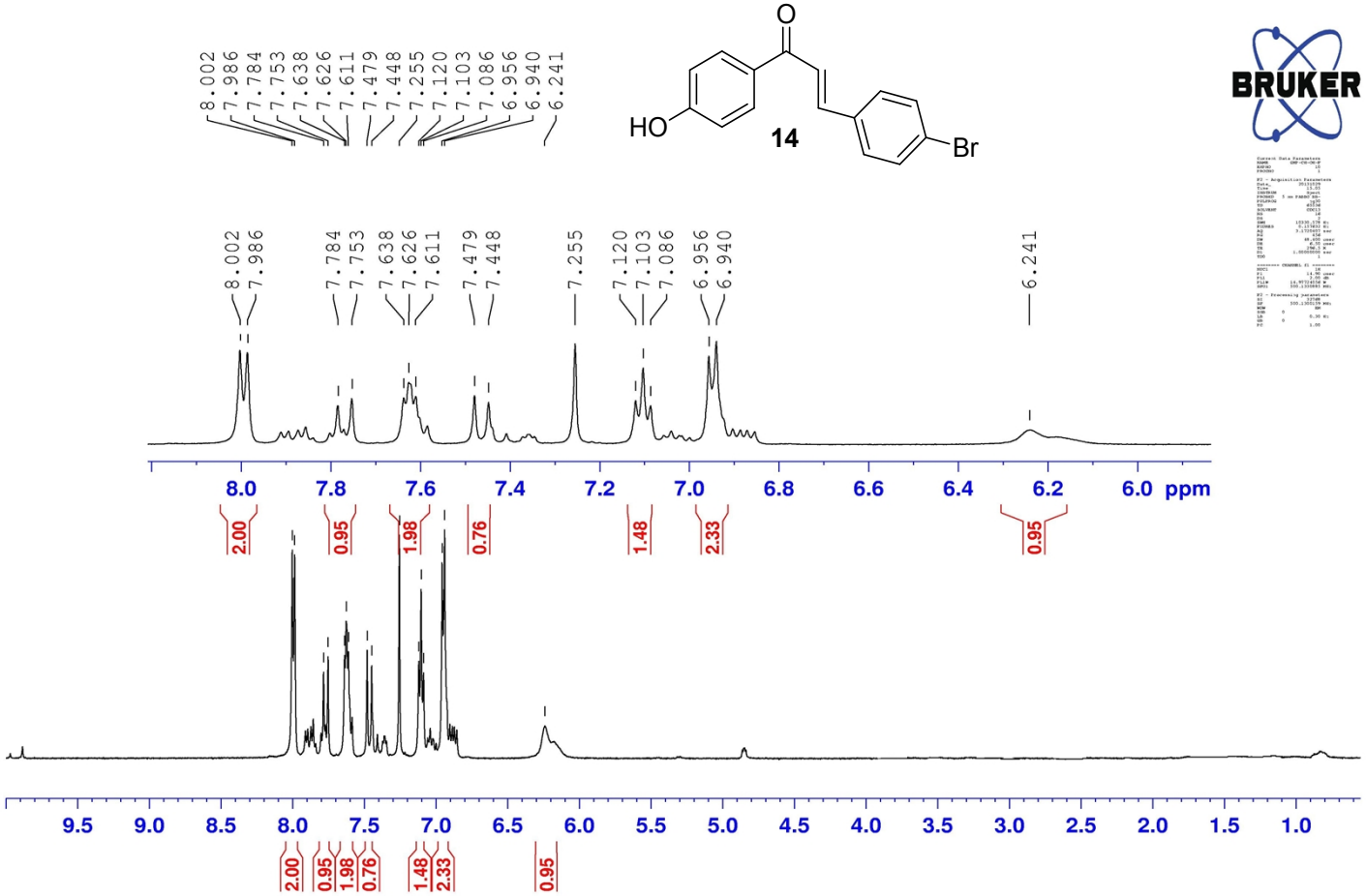
141.64
131.72
131.22
131.15
129.23
122.16
116.12
115.95
BRUKER
O
HO
13
Cl
200
180
160
140
120
100
80
60
40
20
ppm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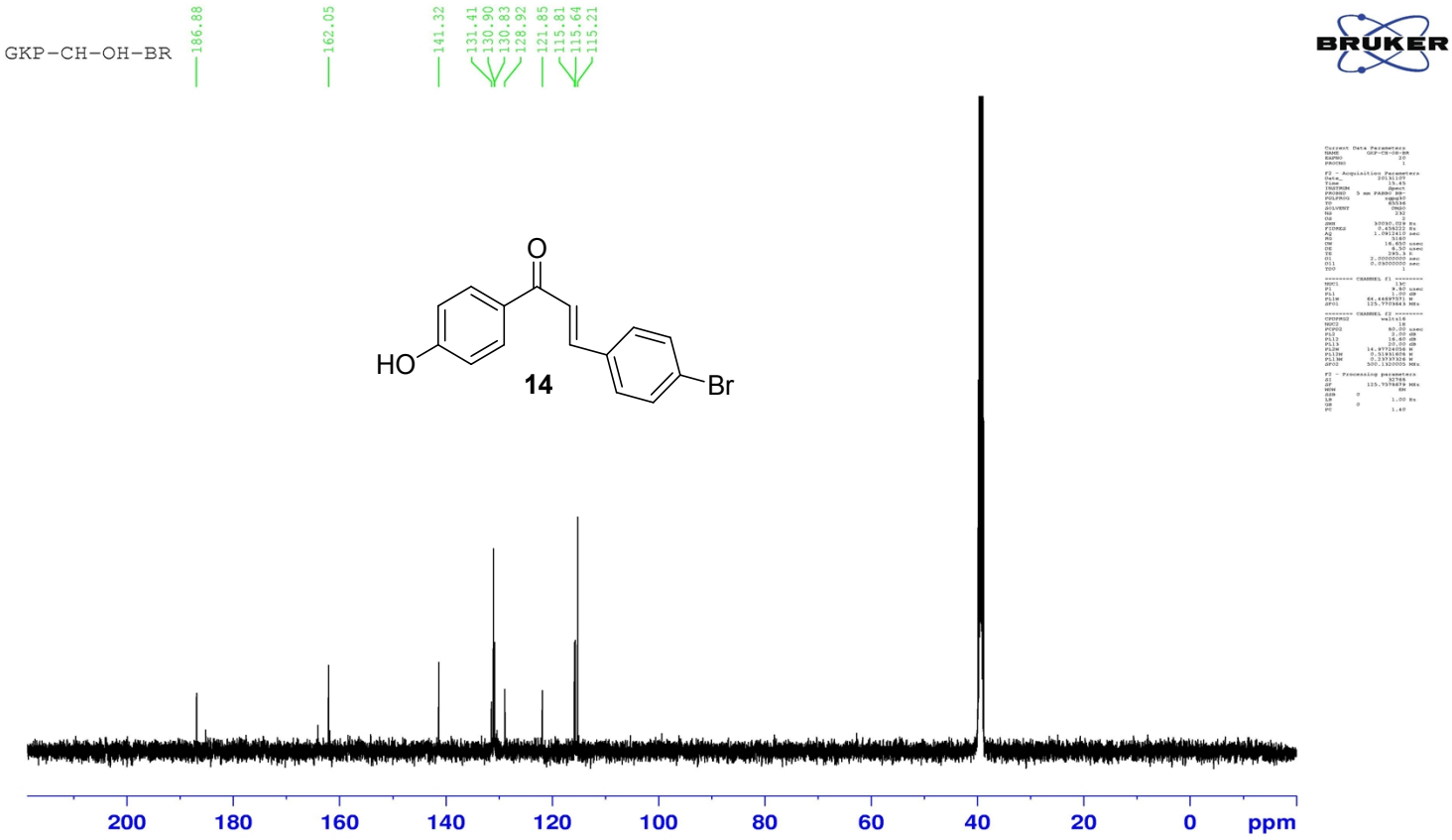
7.986
7.784
7.753
7.638
7.626
7.611
7.479
7.448
7.255
7.120
7.103
7.086
6.956
6.940
6.241
HO
O
Br
14
BRUKER
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6
6.4
6.2
6.0 ppm
2.00
0.95
1.98
0.76
1.48
2.33
0.95
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0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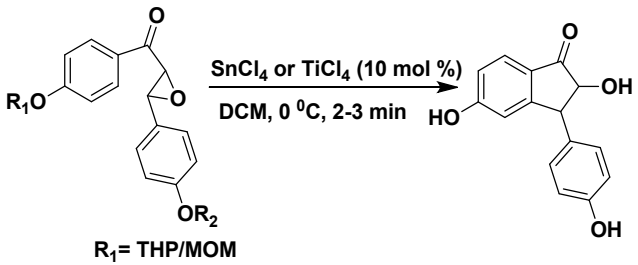
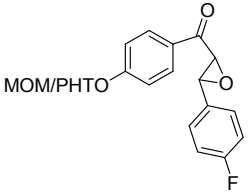
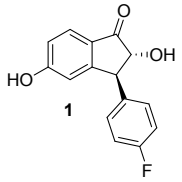
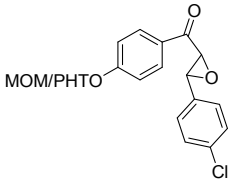
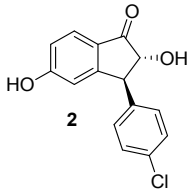
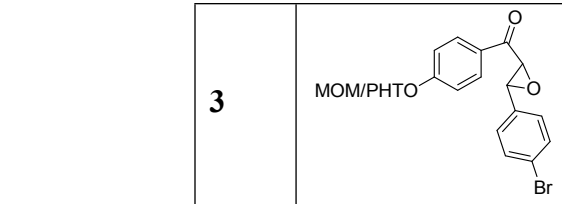
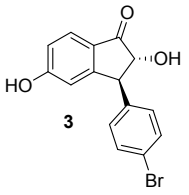
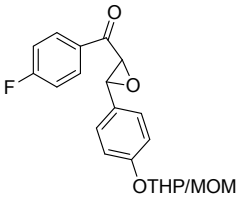
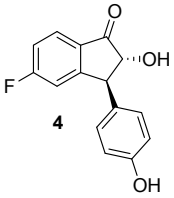
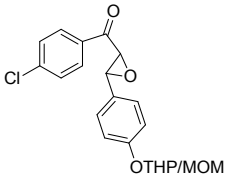
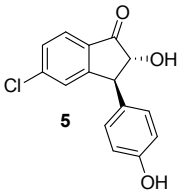
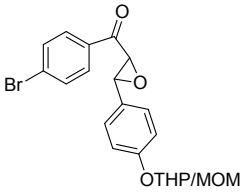
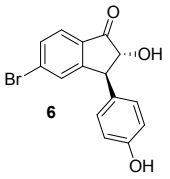
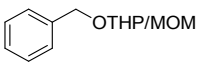
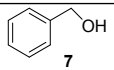
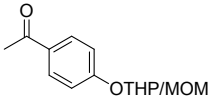
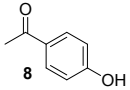
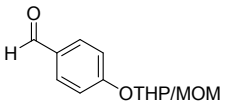
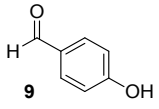
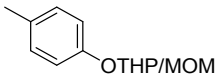
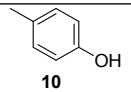
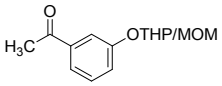
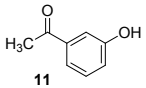
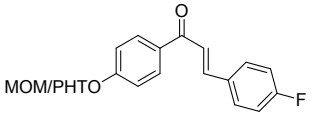
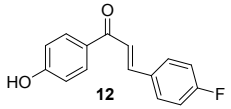
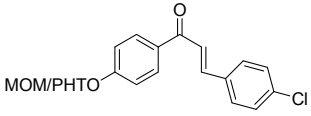
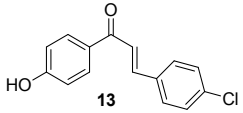
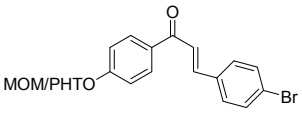
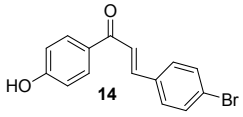
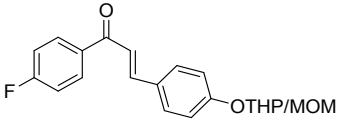
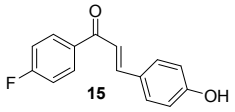
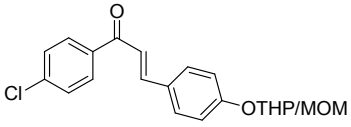
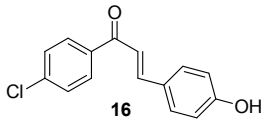
141.32
131.41
130.90
130.83
128.92
121.85
115.81
115.64
115.21
BRUKER
HO
O
Br
14
200
180
160
140
120
100
80
60
40
20
0
ppm

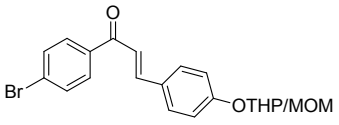
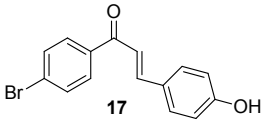
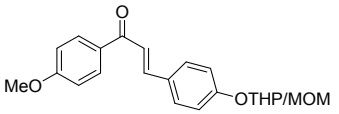
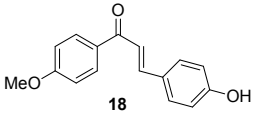
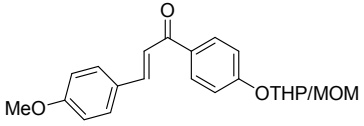
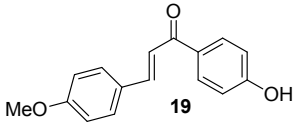
Table 3 Examples of the THP and MOM ethers deprotection and sequel cyclization reaction



Entry	ROTHP/MOM	ROH	Time (min)	Yield (%)[a]	Yield (%)[b]
1			3	96	93
2			2	98	98

3			**2**	**95**	**94**
4			**3**	**96**	**93**
5			**3**	**95**	**92**
6			**2**	**92**	**92**
7			**2**	**10**	**25**
8			**2**	**95**	**92**

9			**2**	**96**	**95**
10			**2**	**92**	**95**
11			**2**	**90**	**92**
12			**3**	**98**	**94**
13			**3**	**96**	**98**
14			**2**	**97**	**94**
15			**2**	**96**	**93**
16			**3**	**95**	**92**

17			**3**	**96**	**95**
18			**2**	**90**	**92**
19			**3**	**95**	**95**

[a] yield (1-19) from R-OTHP and [b] yield (1-19) from R-OMOM ethers deprotection.

Table 6. HPLC conditions and retention times of racemic and enantiomeric excess of the indanone derivatives.[a]

Entry	Indanone[a]	Chiral Column	Eluent (hexane:Isopropanol)	Flow rate (ml/min)	Retention time (min) & Area (%)	ee [a] (config)[a]
1	**2x**	Chiralcel-OD-H	97.5/2.5	0.5	26.9(13.9) 36.9(86.1)	72.2% (2*R*,3*S*)
2	**2y**	Chiralcel-OD-H	92.5/7.5	0.8	38.8(12.5) 53.1(87.5)	75% (2*R*,3*S*)
3	**2z**	Chiralpak-AD-H	92.5/7.5	1	28.6 82.4) 32.5(17.6)	64.8%(2*R*,3*S*)

4	**2za**	Chiralpak-AD-H	92.5/7.5	1	5.3(>99.9)	>99.9%(2*R*,3*S*)
5	**2zb**	Chiralcel-AD-H	92.5/7.5	0.5	28.8(16.5) 42.5(83.5)	66.8% (2*R*,3*S*)

[a]-Detection at 254 nm. Configuration determined based on HPLC data analysis

Table 7 HPLC conditions and retention times of racemic and enantiomeric excess of the epoxide derivatives.[a]

S.No	Indanone[a]	Chiral Column	Eluent (hexane:Isopropanol)	Flow rate (ml/min)	Retention time (min) & Area (%)	ee (config)[a]
1	**1x**	Chiralcel-OD-H	55/1	0.5	54.7(13) 58.7 (87)	**74% (2*R*,3*S*)**
2	**1y**	Chiralcel-OD-H	95/5	0.8	22.4(11.2) 22.4(88.8)	**77.6% (2*R*,3*S*)**
3	**1z**	Chiralpak-AD-H	95/5	1	20.8(17.6) 23.5(82.4)	**64.8% (2*R*,3*S*)**
4	**1za**	Chiralpak-AD-	95/5	0.5	54.0(>99.9)	**>99.9% (2*R*,3*S*)**

		H				
5	**1zb**	Chiralcel-AD-H	95/5	0.8	20.5 16.6) 22.9(83.4)	**66.8% (2*R*,3*S*)**

[a]-Detection at 254 nm. Configuration determined ased on HPLC data analysis.

4. HPLC chromatograms of Epoxy chalcones and 2-hydroxy-Indanone derivatives

12/1/2011 4:16 PM Chromatogram F:\Shrinivaslvenkat.b\BVS-2-221 RACEMIC.prm Page 1 of 1

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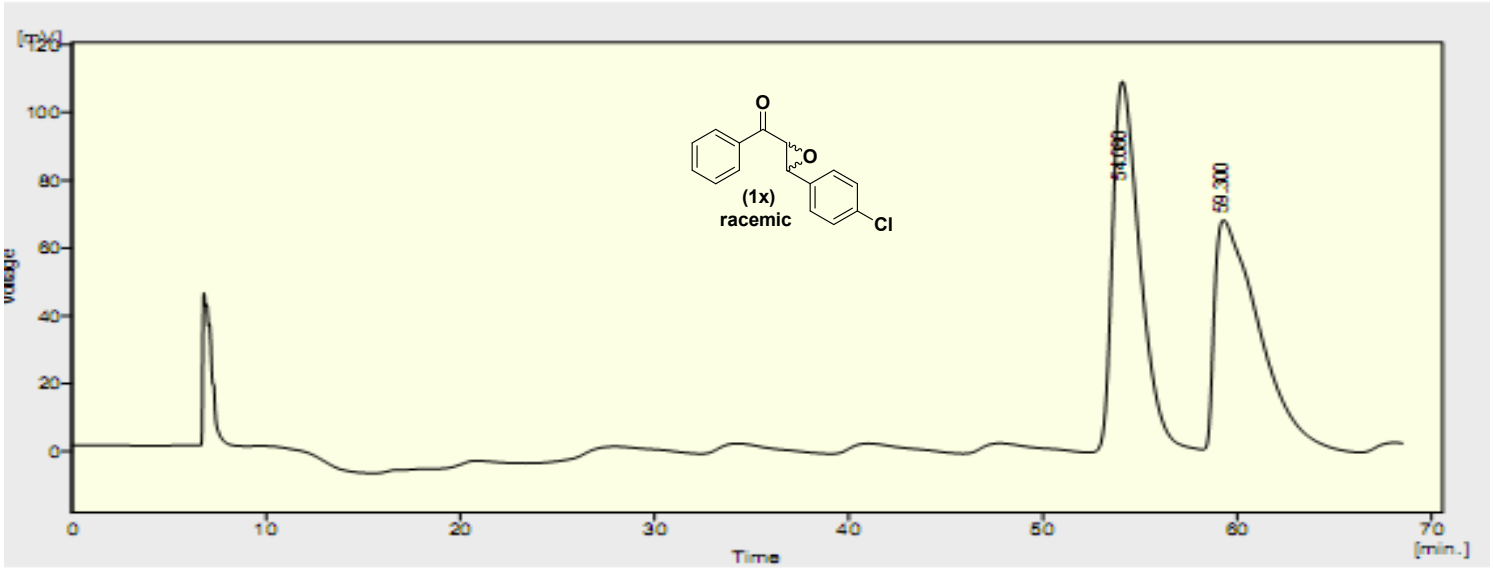
Sample Info:

Sample ID	: BVS-2-221 RACEMIC	Amount	: 0
Sample	: BVS-2-221 RACEMIC	ISTD Amount	: 0
Inj. Volume [ml]	: 0	Dilution	: 1



Result Table (Uncal - F:\Shrinivaslvenkat.b\BVS-2-221 RACEMIC)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	54.080	10830.192	109.358	49.6	61.5	1.51
2	59.300	11013.546	68.494	50.4	38.5	2.49
	Total	21843.738	177.853	100.0	100.0	

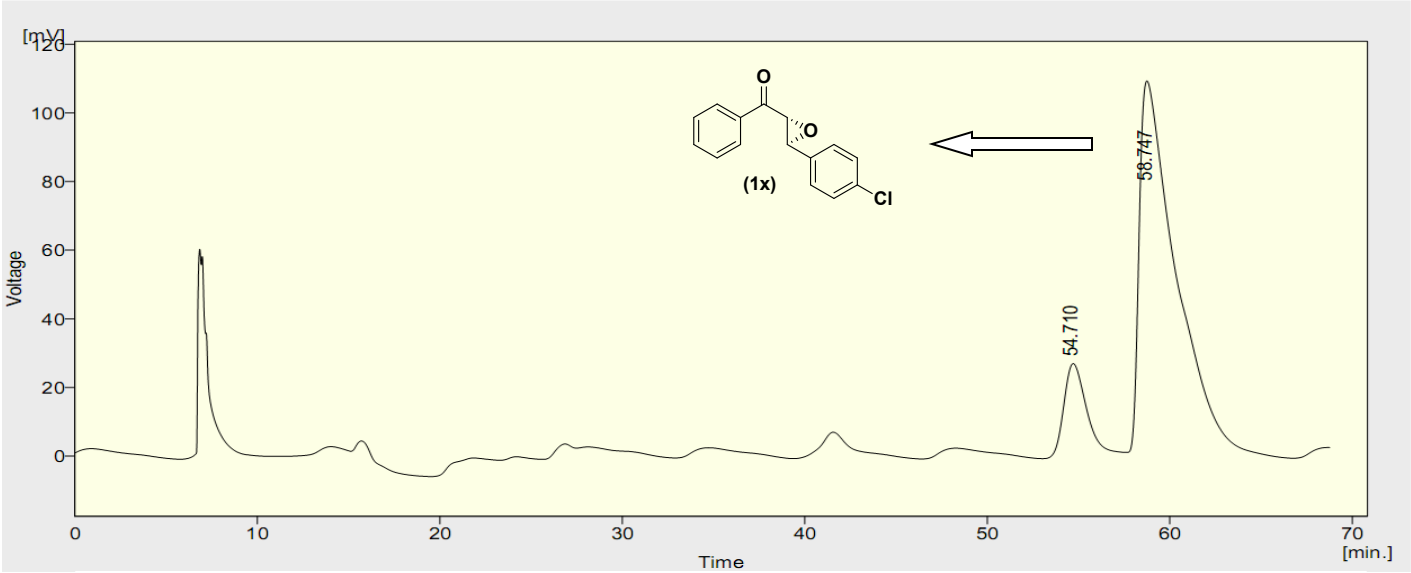
Chromatogram of **1x**(racemic).

DEPT. OF CHEMISTRY

IIT ROORKEE

Sample Info:

Sample ID	: BVS-2-221 chairal-1	Amount	: 0
Sample	: BVS-2-221 chairal-1	ISTD Amount	: 0
Inj. Volume [ml]	: 0	Dilution	: 1



Result Table (Uncal - F:\Shrinivas\venkat.b\BVS-2-221 chairal-1)

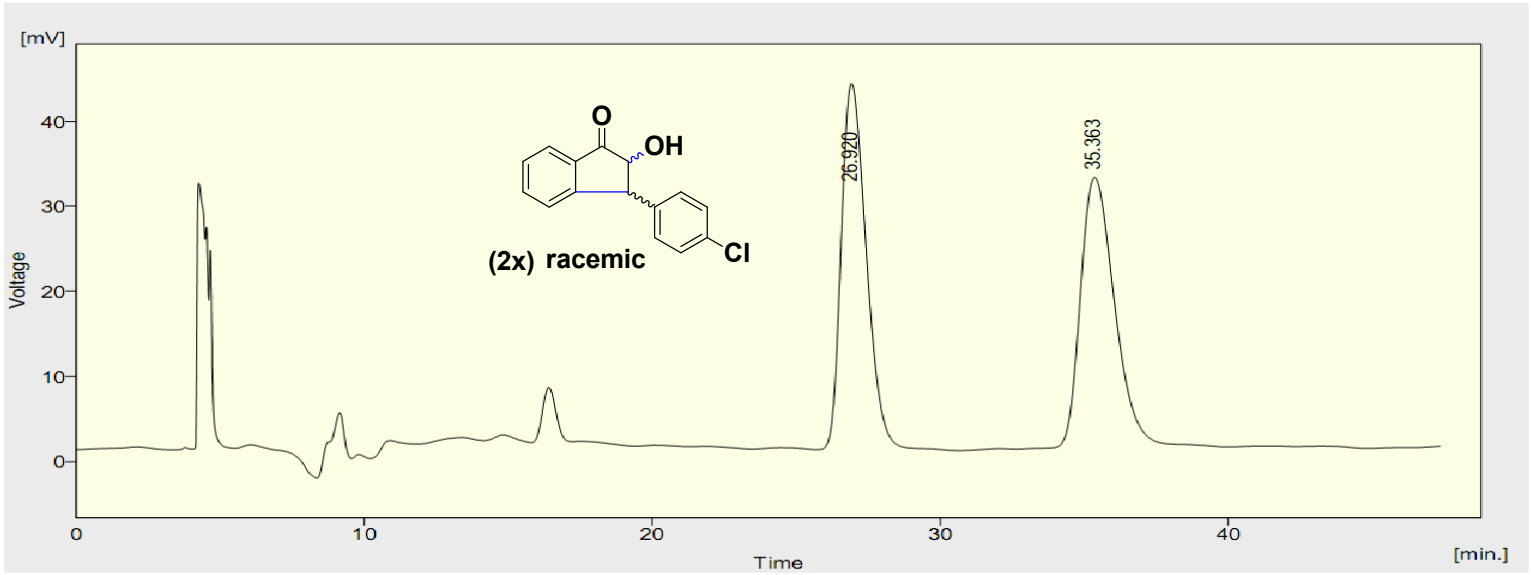
	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	54.710	2269.937	26.611	13.0	19.6	1.29
2	58.747	15224.951	109.040	87.0	80.4	2.00
	Total	17494.889	135.651	100.0	100.0	

Chromatogram of **1x** (asymmetric).

DEPT. OF CHEMISTRY
IIT ROORKEE

Sample Info:

Sample ID	: BVS-2-214 Racemic	Amount	: 0
Sample	: BVS-2-214 Racemic	ISTD Amount	: 0
Inj. Volume [ml]	: 0	Dilution	: 1



Result Table (Uncal - F:\Shrinivas\venkat.b\BVS-2-214 Racemic)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	26.920	2576.361	42.957	50.0	57.5	0.94
2	35.363	2580.839	31.704	50.0	42.5	1.27
	Total	5157.201	74.661	100.0	100.0	

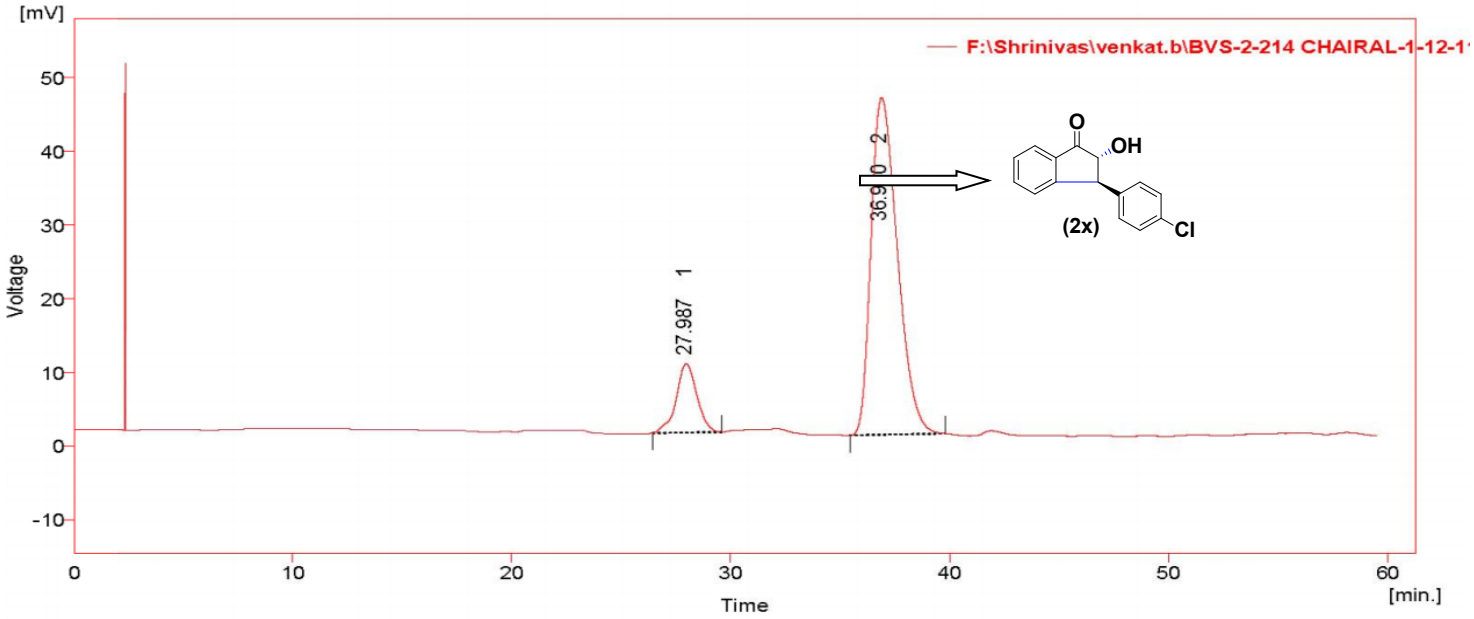
Chromatogram of **2x** (racemic).

DEPT. OF CHEMISTRY

IIT ROORKEE

Sample Info:

Sample ID	: BVS-2-214 CHAIRAL-1	Amount	: 0
Sample	: BVS-2-214 CHAIRAL-1	ISTD Amount	: 0
Inj. Volume [ml]	: 0	Dilution	: 1



Result Table (Uncal - F:\Shrinivas\venkat.b\BVS-2-214 CHAIRAL-1-12-11)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	27.987	615.855	9.368	13.9	17.0	0.98
2	36.900	3829.838	45.782	86.1	83.0	1.31
	Total	4445.692	55.150	100.0	100.0	

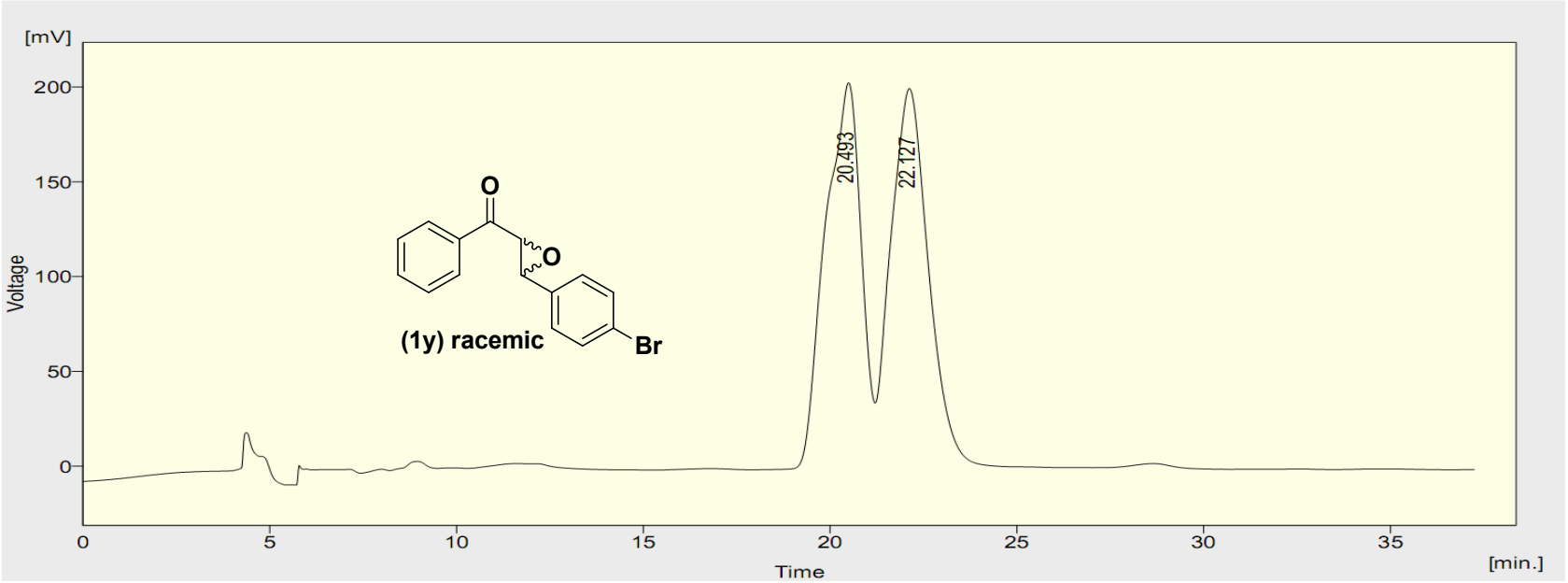
Chromatogram of **2x** (asymmetric).

DEPT. OF CHEMISTRY

IIT ROORKEE

Sample Info:

Sample ID	: BVS-2- 221 (RACEMIC EPOXIDE SINGLE BROMO)	Amount	: 0
Sample	: BVS-2- 221 (RACEMIC EPOXIDE SINGLE BROMO)	ISTD Amount	: 0
Inj. Volume [ml]	: 0	Dilution	: 1



Result Table (Uncal - F:\Shrinivas\venkat.b\BVS-2- 221 (RACEMIC EPOXIDE SINGLE BROMO))

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	20.493	11127.669	178.922	49.9	50.3	1.06
2	22.127	11182.367	176.941	50.1	49.7	1.03
	Total	22310.036	355.863	100.0	100.0	

Chromatogram of **1y** (racemic).

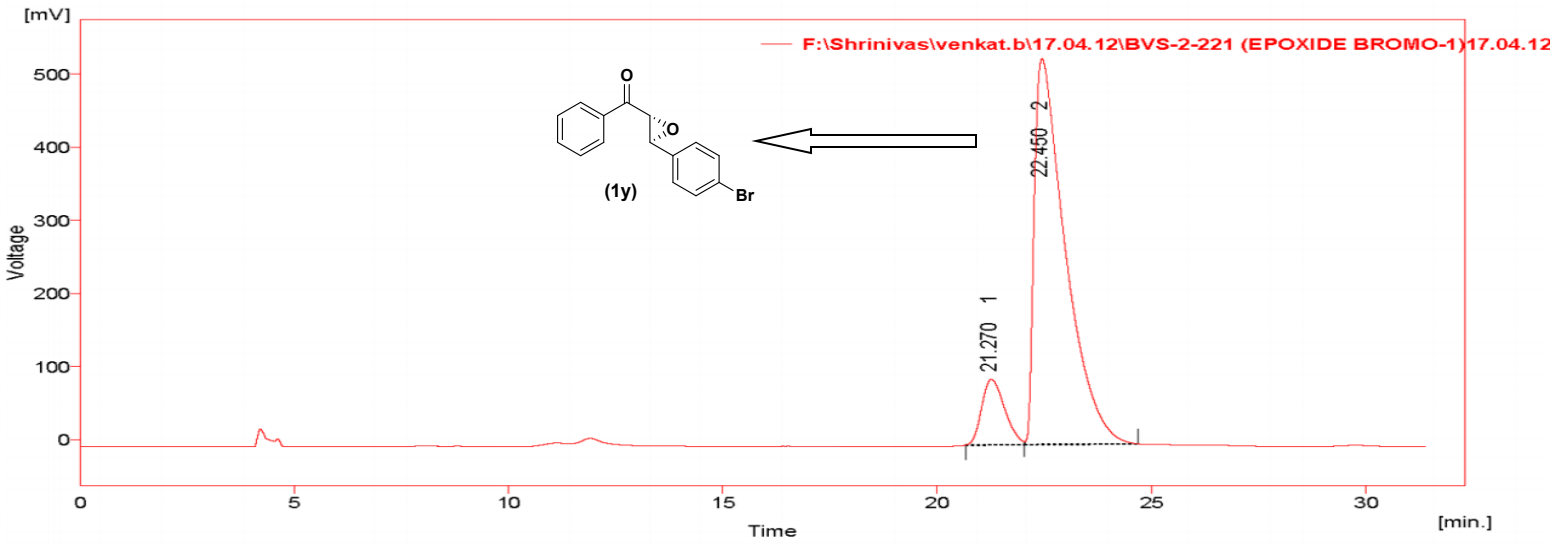
5/1/2012 11:18 AM Chromatogram F:\Shrinivas\venkat.b\17.04.12\BVS-2-221 (EPOXIDE BROMO-1)17.04.12..PRM Page 1 of 1

DEPT. OF CHEMISTRY

IIT ROORKEE

Sample Info:

Sample ID	: BVS-2-221 (EPOXIDE BROMO-1)17.04.12.	Amount	: 0
Sample	: BVS-2-221 (EPOXIDE BROMO-1)17.04.12.	ISTD Amount	: 0
Inj. Volume [ml]	: 0	Dilution	: 1



Result Table (Uncal - F:\Shrinivas\venkat.b\17.04.12\BVS-2-221 (EPOXIDE BROMO-1)17.04.12.)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	21.270	3345.229	89.675	11.2	14.5	0.59
2	22.450	26653.670	527.569	88.8	85.5	0.76
	Total	29998.898	617.244	100.0	100.0	

Chromatogram of **1y** (asymmetric).

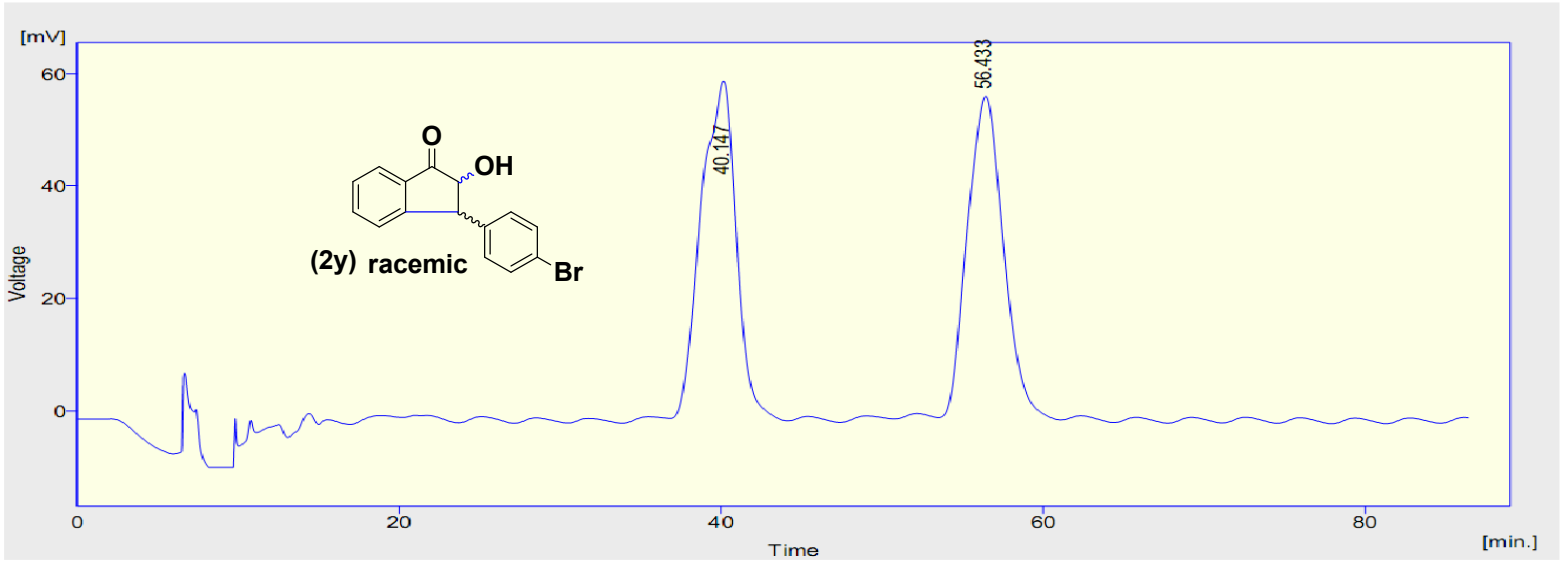
4/21/2012 3:45 PM Chromatogram F:\Shrinivas\venkat.b\17.04.12\BVS-2-225 (RACEMIC SINGLEBROMO -2).prm Page 1 of 1

DEPT. OF CHEMISTRY

IIT ROORKEE

Sample Info:

Sample ID	: BVS-2-225 (RACEMIC SINGLEBROMO -2)	Amount	: 0
Sample	: BVS-2-225 (RACEMIC SINGLEBROMO -2)	ISTD Amount	: 0
Inj. Volume [ml]	: 0	Dilution	: 1



Result Table (Uncal - F:\Shrinivas\venkat.b\17.04.12\BVS-2-225 (RACEMIC SINGLEBROMO -2))

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	40.147	8771.229	59.125	50.1	51.0	2.46
2	56.433	8744.352	56.862	49.9	49.0	2.46
	Total	17515.581	115.988	100.0	100.0	

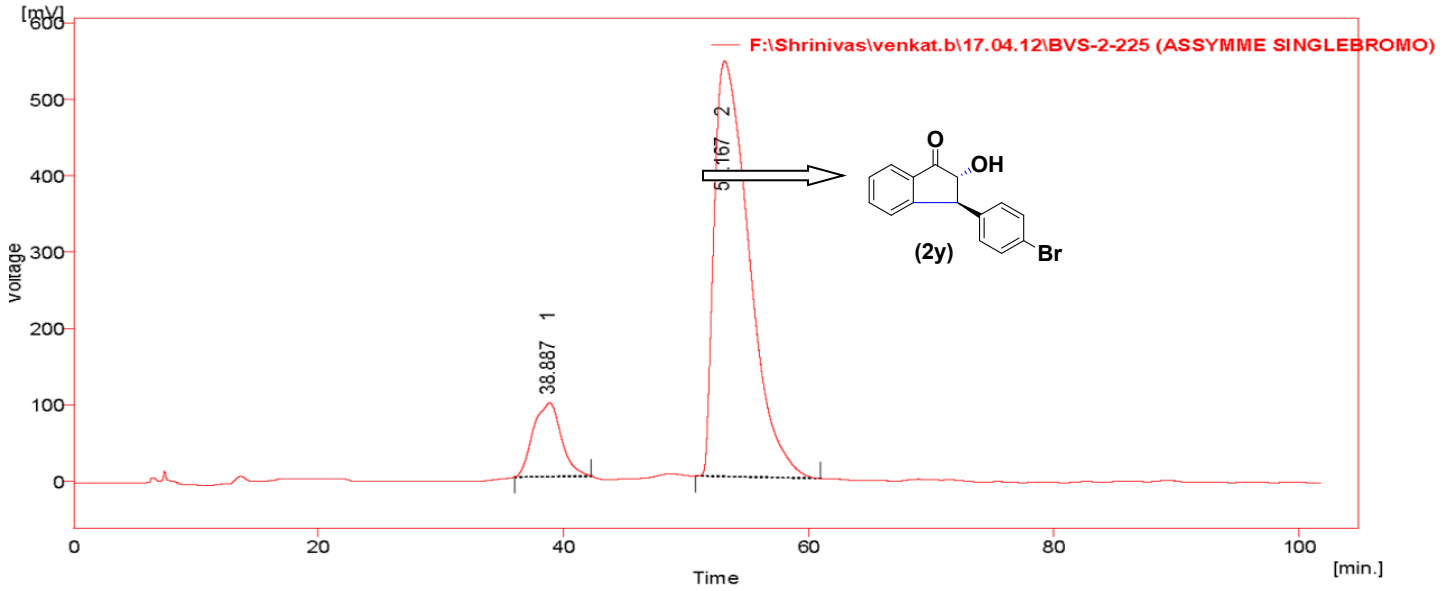
Chromatogram of 2y (racemic).

DEPT. OF CHEMISTRY

IIT ROORKEE

Sample Info:

Sample ID	: BVS-2-225 (ASSYMME SINGLEBROMO)	Amount	: 0
Sample	: BVS-2-225 (ASSYMME SINGLEBROMO)	ISTD Amount	: 0
Inj. Volume [ml]	: 0	Dilution	: 1



Result Table (Uncal - F:\Shrinivas\venkat.b\17.04.12\BVS-2-225 (ASSYMME SINGLEBROMO))

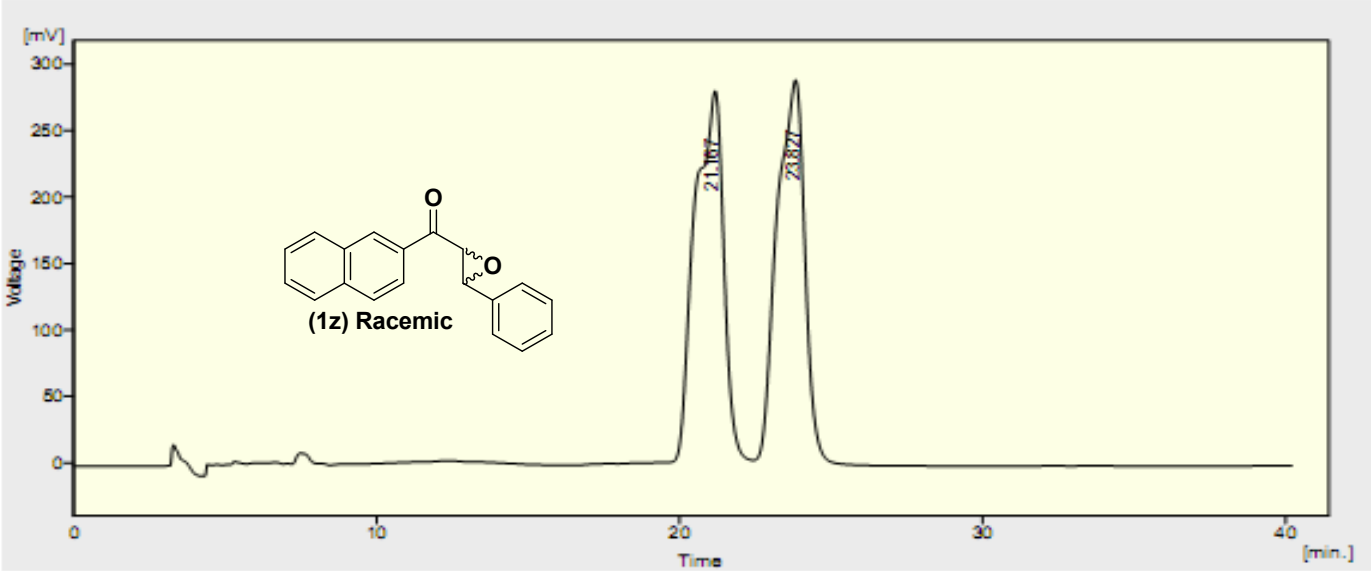
	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	38.887	15400.980	96.525	12.5	15.1	2.55
2	53.167	107678.977	543.640	87.5	84.9	3.10
	Total	123079.957	640.165	100.0	100.0	

Chromatogram of **2y** (asymmetric).

DEPT. OF CHEMISTRY
IIT ROORKEE

Sample Info:

Sample ID	: BVS-2-224 (RACEMIC NAPTHYL EPOXIDE-1)	Amount	: 0
Sample	: BVS-2-224 (RACEMIC NAPTHYL EPOXIDE-1)	ISTD Amount	: 0
Inj. Volume [ml]	: 0	Dilution	: 1



Result Table (Uncal - F:\Shrinivas\venkat.b\17.04.12\BVS-2-224 (RACEMIC NAPTHYL EPOXIDE-1))

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	21.167	18093.244	277.249	50.2	49.2	1.15
2	23.827	17944.839	286.252	49.8	50.8	1.07
	Total	36038.083	563.501	100.0	100.0	

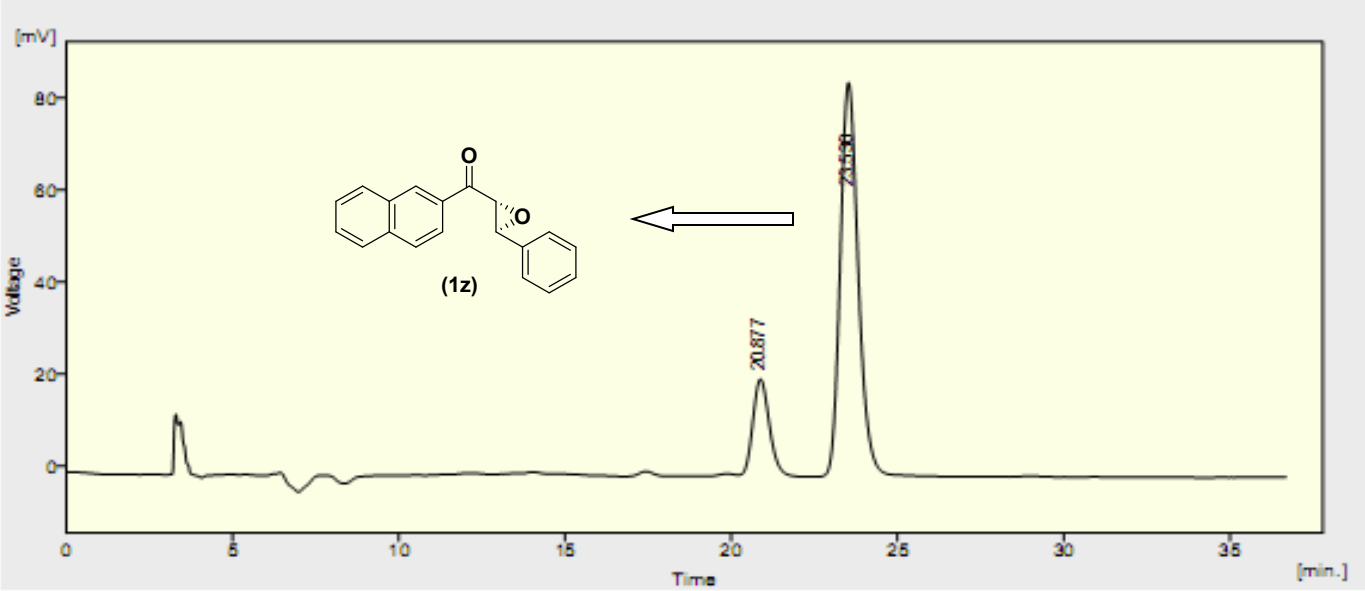
Chromatogram of 1z (racemic).

DEPT. OF CHEMISTRY

IIT ROORKEE

Sample Info:

Sample ID	: BVS-2-224 (ASSY NAPTHYEPOXIDE)	Amount	: 0
Sample	: BVS-2-224 (ASSY NAPTHYEPOXIDE)	ISTD Amount	: 0
Inj. Volume [ml]	: 0	Dilution	: 1



Result Table (Uncal - F:\Shrinivasvenkat.b\17.04.12\BVS-2-224 (ASSY NAPTHYEPOXIDE))

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	20.877	679.543	20.522	17.6	19.4	0.53
2	23.530	3177.613	85.345	82.4	80.6	0.57
	Total	3857.157	105.866	100.0	100.0	

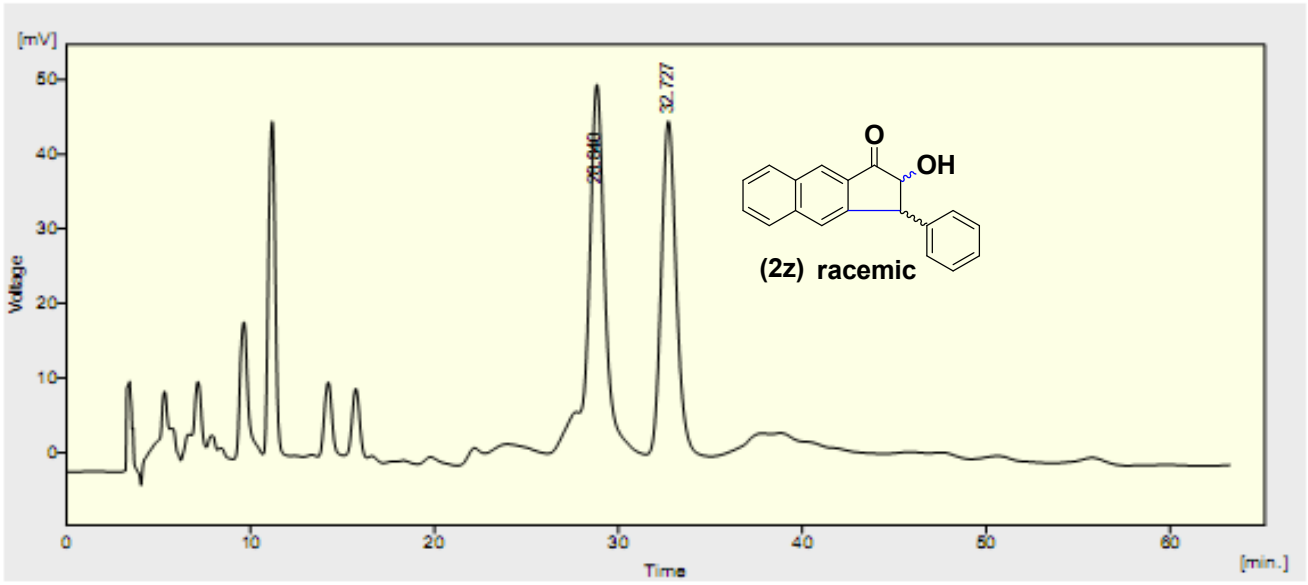
Chromatogram of **1z** (asymmetric).

DEPT. OF CHEMISTRY

IIT ROORKEE

Sample Info:

Sample ID	: BVS-2-224 (RACEMIC NAPTHYL-1)	Amount	: 0
Sample	: BVS-2-224 (RACEMIC NAPTHYL-1)	ISTD Amount	: 0
Inj. Volume [ml]	: 0	Dilution	: 1



Result Table (Uncal - F:\Shrinivas\venkat.b\17.04.12\BVS-2-224 (RACEMIC NAPTHYL-1))

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	28.840	2292.942	45.597	48.6	50.7	0.77
2	32.727	2428.293	44.260	51.4	49.3	0.85
	Total	4721.235	89.857	100.0	100.0	

Chromatogram of **2z** (racemic).

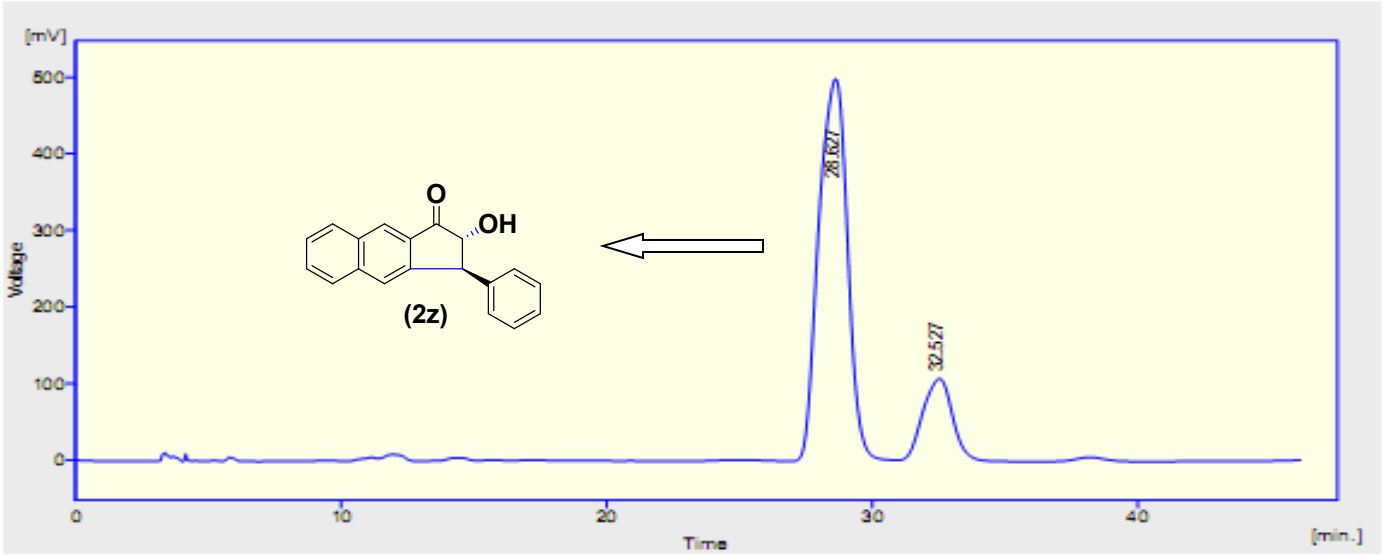
4/24/2012 2:52 PM Chromatogram F:\Shrinivasvenkat.b\17.04.12\BVS-2-224 (ASSYM NAPTHYL-1).prn Page 1 of 1

DEPT. OF CHEMISTRY

IIT ROORKEE

Sample Info:

Sample ID	: BVS-2-224 (ASSYM NAPTHYL-1)	Amount	: 0
Sample	: BVS-2-224 (ASSYM NAPTHYL-1)	ISTD Amount	: 0
Inj. Volume [ml]	: 0	Dilution	: 1



Result Table (Uncal - F:\Shrinivasvenkat.b\17.04.12\BVS-2-224 (ASSYM NAPTHYL-1))

	Retan. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	28.627	37020.422	496.811	82.8	82.7	1.23
2	32.527	7684.838	103.845	17.2	17.3	1.22
	Total	44705.260	600.656	100.0	100.0	

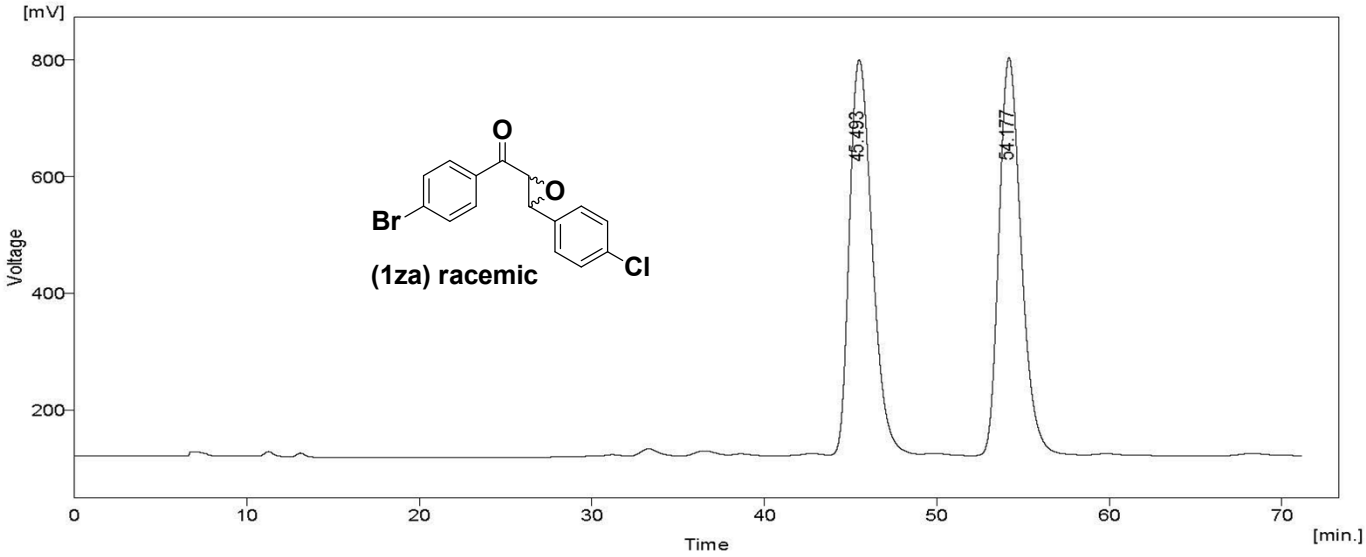
Chromatogram of **2z**(asymmetric).

DEPT. OF CHEMISTRY

IIT ROORKEE

Sample Info:

Sample ID	:	Amount	: 0
Sample	:	ISTD Amount	: 0
Inj. Volume [ml]	: 0	Dilution	: 1



Result Table (Uncal - F:\Shrinivas\venkat.b\17.04.12\BVS-2-220 RACEMIC))

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	45.493	61170.539	675.588	50.2	49.8	1.42
2	54.177	60604.715	680.828	49.8	50.2	1.37
	Total	121775.253	1356.416	100.0	100.0	

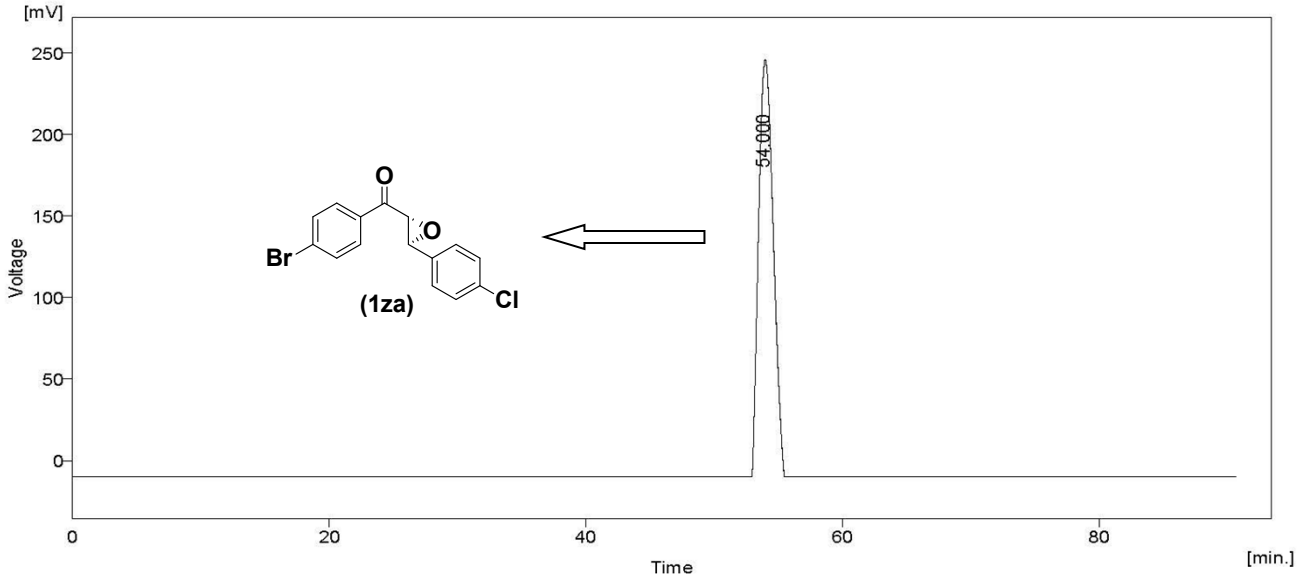
Chromatogram of 1za (racemic).

DEPT. OF CHEMISTRY

IIT ROORKEE

Sample Info:

Sample ID	: bvs-2-220	Amount	: 0
Sample	: bvs-2-220	ISTD Amount	: 0
Inj. Volume [ml]	: 0	Dilution	: 1



Result Table (Uncal - F:\Shrinivas\venkat.b\17.04.12\bvs-2-220 Assymetric).)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	54.000	20271.442	255.949	100.0	100.0	1.31
	Total	20271.442	255.949	100.0	100.0	

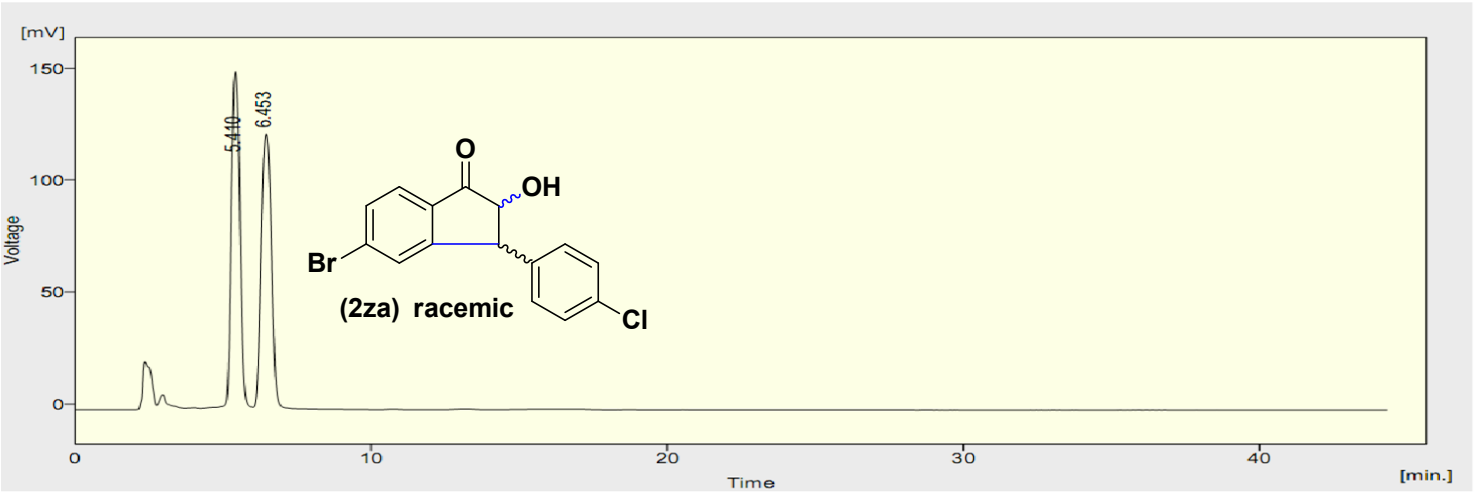
Chromatogram of **1za** (asymmetric).

4/24/2012 12:56 PM Chromatogram F:\Shrinivas\venkat.b\17.04.12\BVS-2-225 (Cl- Br-RACEMI -1).prm Page 1 of 1

DEPT. OF CHEMISTRY
IIT ROORKEE

Sample Info:

Sample ID	: BVS-2-225 (Cl- Br-RACEMI -1)	Amount	: 0
Sample	: BVS-2-225 (Cl- Br-RACEMI -1)	ISTD Amount	: 0
Inj. Volume [ml]	: 0	Dilution	: 1



Result Table (Uncal - F:\Shrinivas\venkat.b\17.04.12\BVS-2-225 (Cl- Br-RACEMI -1))

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	5.410	2888.319	148.652	50.1	55.0	0.32
2	6.453	2877.132	121.811	49.9	45.0	0.39
	Total	5765.451	270.463	100.0	100.0	

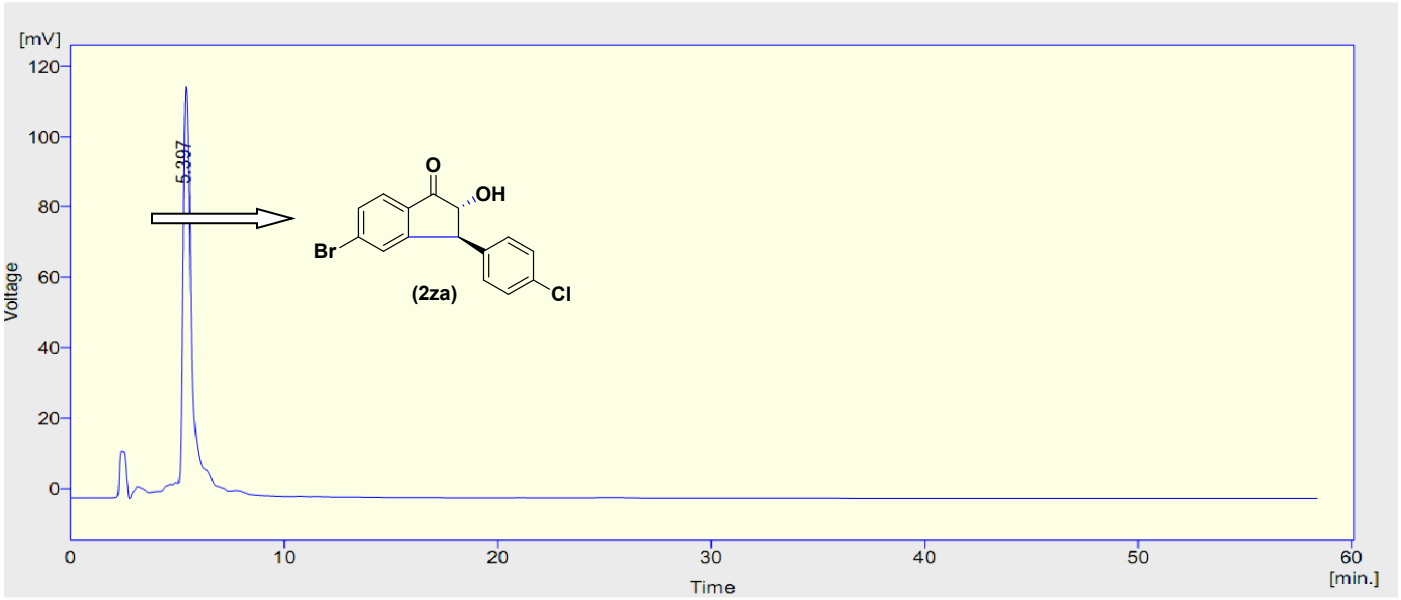
Chromatogram of **2za** (racemic).

DEPT. OF CHEMISTRY

IIT ROORKEE

Sample Info:

Sample ID	: BVS-2-225 (Cl-Br ASSYMETRIC-1)	Amount	: 0
Sample	: BVS-2-225 (Cl-Br ASSYMETRIC-1)	ISTD Amount	: 0
Inj. Volume [ml]	: 0	Dilution	: 1



Result Table (Uncal - F:\Shrinivas\venkat.b\17.04.12\BVS-2-225 (Cl-Br ASSYMETRIC-1))

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	5.397	2502.042	109.822	100.0	100.0	0.36
	Total	2502.042	109.822	100.0	100.0	

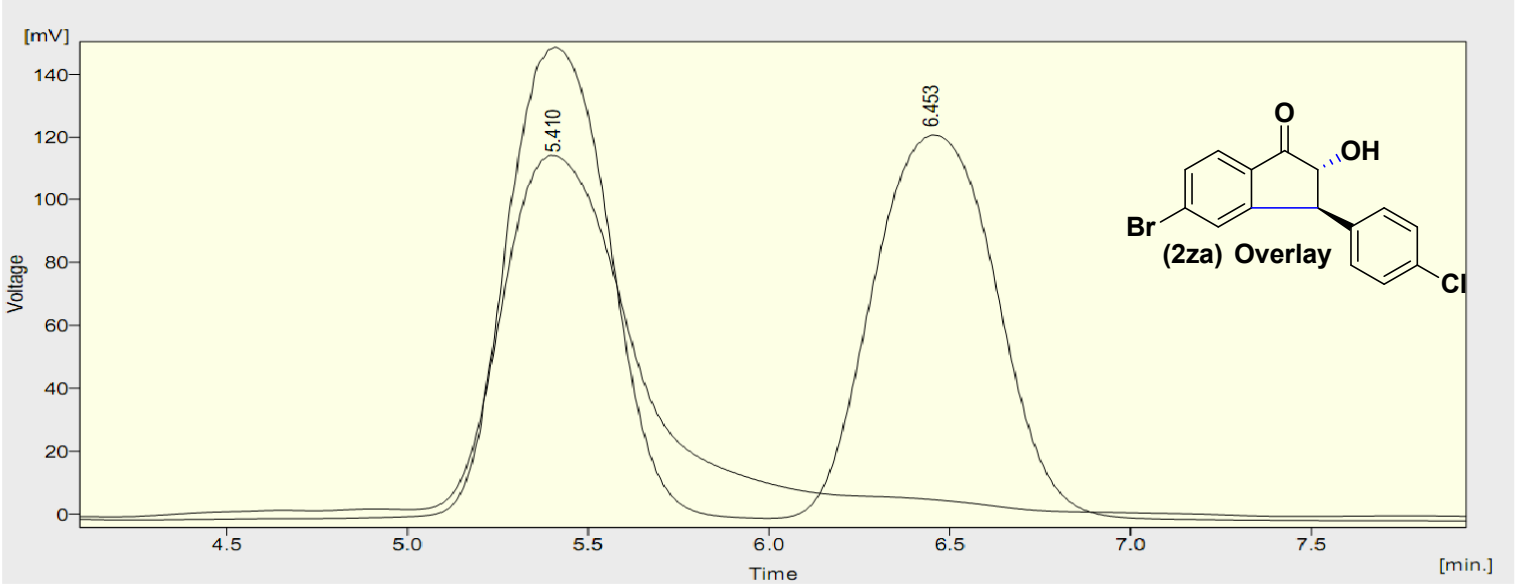
Chromatogram of **2za** (asymmetric).

DEPT. OF CHEMISTRY

IIT ROORKEE

Sample Info:

Sample ID	: BVS-2-225 (Cl- Br-RACEMI -1)	Amount	: 0
Sample	: BVS-2-225 (Cl- Br-RACEMI -1)	ISTD Amount	: 0
Inj. Volume [ml]	: 0	Dilution	: 1



Result Table (Uncal - F:\Shrinivas\venkat.b\17.04.12\BVS-2-225 (Cl-Br RACEMIC-ASSYMETRIC-1))

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	5.410	2888.319	148.652	50.1	55.0	0.32
2	6.453	2877.132	121.811	49.9	45.0	0.39
	Total	5765.451	270.463	100.0	100.0	

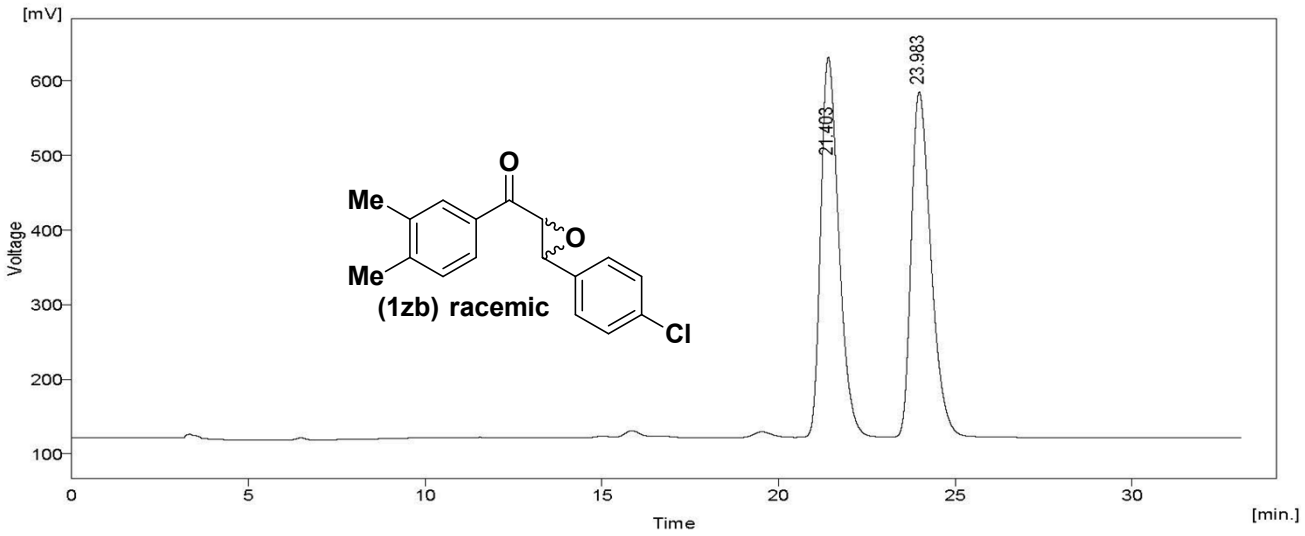
Overlay Chromatogram of **2za** this showing >99.9% ee

DEPT. OF CHEMISTRY

IIT ROORKEE

Sample Info:

Sample ID	:	Amount	: 0
Sample	:	ISTD Amount	: 0
Inj. Volume [ml]	: 0	Dilution	: 1



Result Table (Uncal - F:\Shrinivas\venkat.b\17.04.12\bvs-2-226 racemic))

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	21.403	17888.474	507.610	50.3	52.4	0.55
2	23.983	17698.435	461.609	49.7	47.6	0.60
	Total	35586.909	969.220	100.0	100.0	

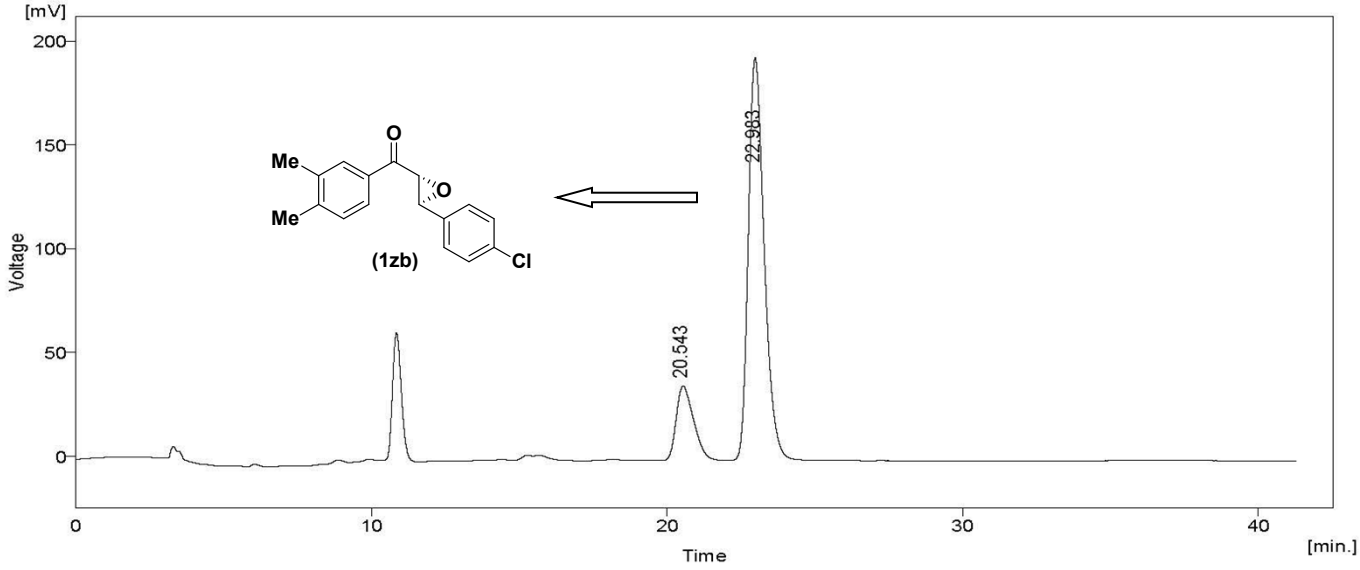
Chromatogram of **1zb** (racemic).

DEPT. OF CHEMISTRY

IIT ROORKEE

Sample Info:

Sample ID	: bvs-2-226	Amount	: 0
Sample	: bvs-2-226	ISTD Amount	: 0
Inj. Volume [ml]	: 0	Dilution	: 1



Result Table (Uncal - F:\Shrinivas\venkat.b\17.04.12\bvs-2-226 assymetric-new))

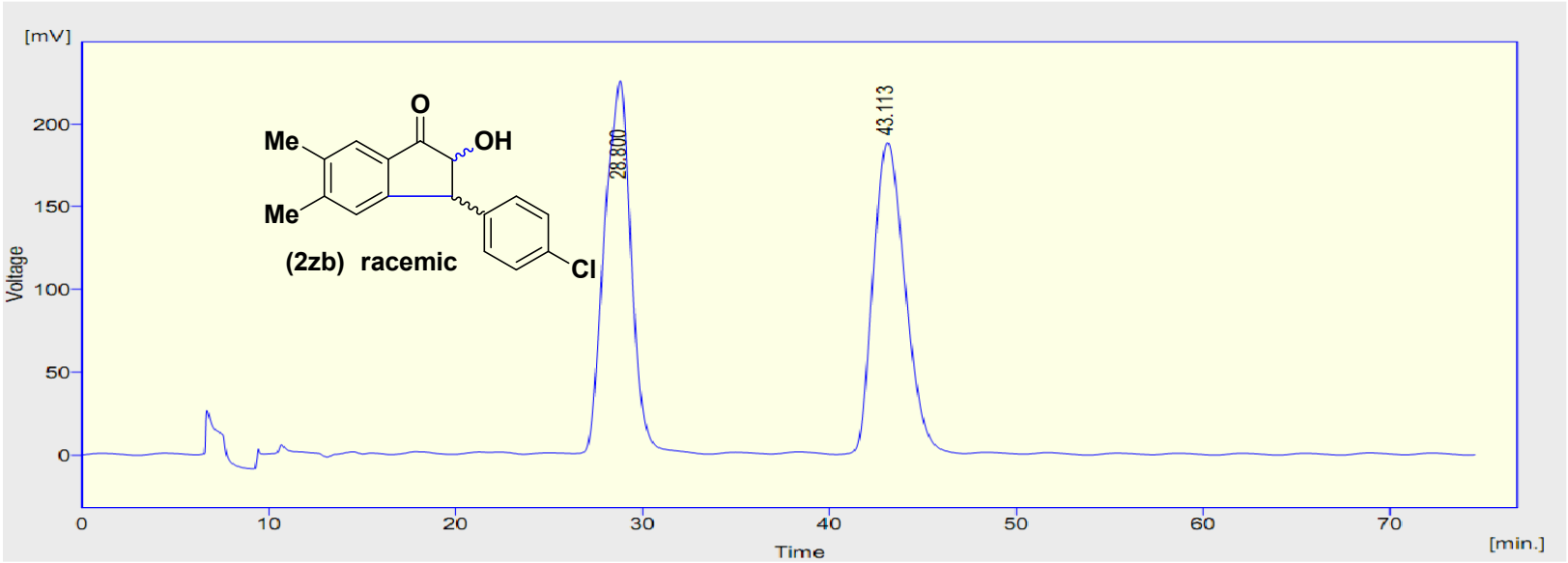
	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	20.543	1428.218	35.693	16.6	15.6	0.64
2	22.983	7171.592	193.583	83.4	84.4	0.57
	Total	8599.809	229.276	100.0	100.0	

Chromatogram of **1zb** (asymmetric).

DEPT. OF CHEMISTRY
IIT ROORKEE

Sample Info:

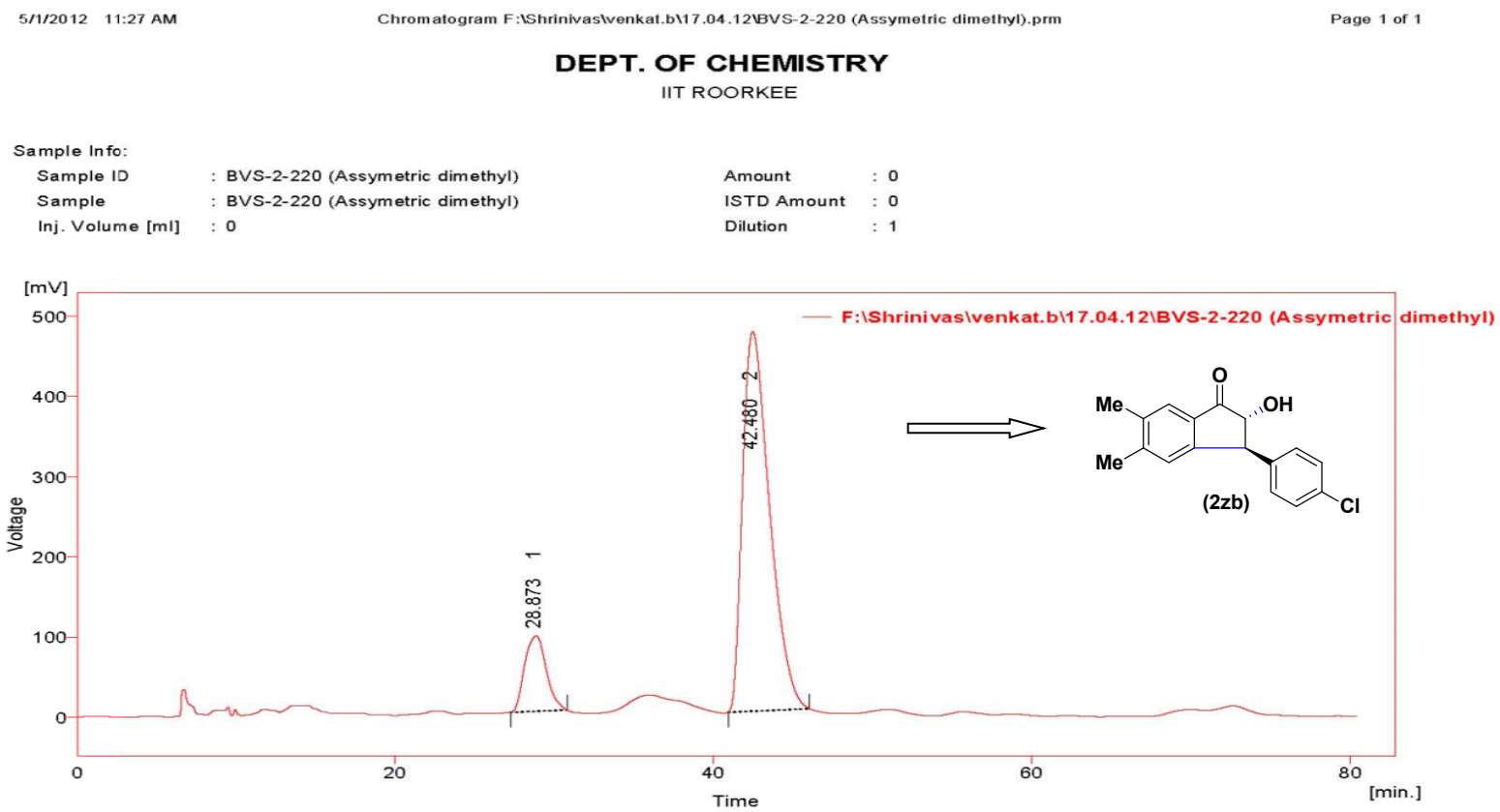
Sample ID	: BVS-2-220 (RACEMIC DIMETHYL)	Amount	: 0
Sample	: BVS-2-220 (RACEMIC DIMETHYL)	ISTD Amount	: 0
Inj. Volume [ml]	: 0	Dilution	: 1



Result Table (Uncal - F:\Shrinivas\venkat.b\17.04.12\BVS-2-220 (RACEMIC DIMETHYL))

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	28.800	21658.163	223.452	49.8	54.4	1.57
2	43.113	21871.282	187.194	50.2	45.6	1.86
	Total	43529.445	410.646	100.0	100.0	

Chromatogram of **2zb** (racemic)



Result Table (Uncal - F:\Shrinivas\venkat.b\17.04.12\BVS-2-220 (Assymetric dimethyl))

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	28.873	8927.666	93.840	13.8	16.5	1.53
2	42.480	55931.965	473.345	86.2	83.5	1.85
	Total	64859.632	567.185	100.0	100.0	

Chromatogram of **2zb** (asymmetric).

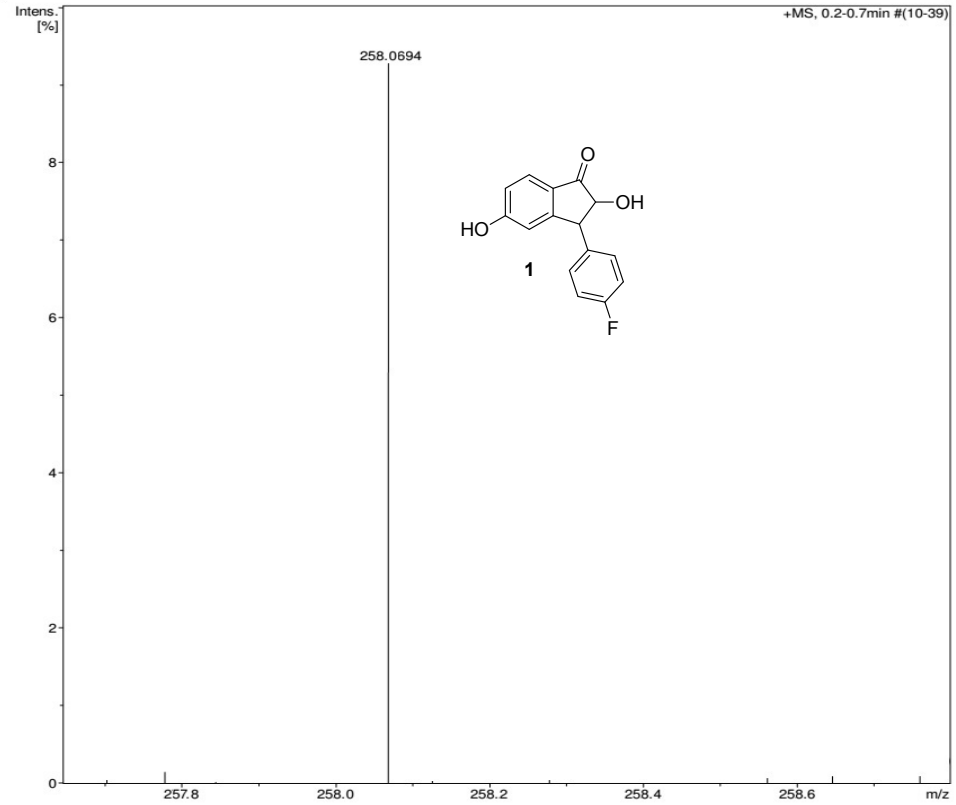
Display Report

Analysis Info

Analysis Name	D:\Data\DR.Naseem\GKP-42.d	Acquisition Date	8/22/2013 5:14:31 PM
Method	tune_wide.m	Operator	IIT ROORKEE
Sample Name	GKP-42	Instrument	micrOTOF-Q II 10328
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



Display Report

Analysis Info

Analysis Name	D:\Data\DR.Naseem\GKP-29.d	Acquisition Date	8/21/2013 4:44:46 PM
Method	tune_wide.m	Operator	IIT ROORKEE
Sample Name	GKP-29	Instrument	micrOTOF-Q II 10328
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source