Supplementary Material (ESI) for Chemical Communications

N-Heterocyclic Carbene Catalysed Asymmetric Cross-Benzoin Reactions of Heteroaromatic Aldehydes with Trifluoromethyl Ketones

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1. General Methods

Preparative column chromatography: Merck silica gel 60, particle size 0.040-0.063 mm (230-240 mesh, flash).

Analytical TLC: SIL G-25 UV254 from MACHEREY-NAGEL. Visualization of the developed TLC plates was performed with ultraviolet irradiation (254 nm) or by staining with basic potassium permanganate solution.

Optical rotation values were measured on a Perkin-Elmer 241 polarimeter.

Microanalyses were performed with a Vario EL element analyser.

Mass spectra were acquired on a Finnigan SSQ7000 (EI 70 eV) spectrometer and high resolution mass spectra on a Thermo Fisher Scientific Orbitrap XL.

IR spectra were taken on a Perkin-Elmer FT-IR Spectrum 100 using an ATR-Unit.

^{1}H-, ^{13}C- and ^{19}F-NMR spectra were recorded at ambient temperature on Varian Mercury 300 or Inova 400 instruments with tetramethylsilane as an internal standard.

Analytical HPLC was performed on a Hewlett-Packard 1100 Series instrument using chiral stationary phases (Daicel AS, Daicel OJ, Daicel AD, Daicel IA).

2. Materials

Unless otherwise noted, all commercially available compounds were used without further purification. The ketones which are not commercially available were prepared according to the procedure reported in the literature.[1]

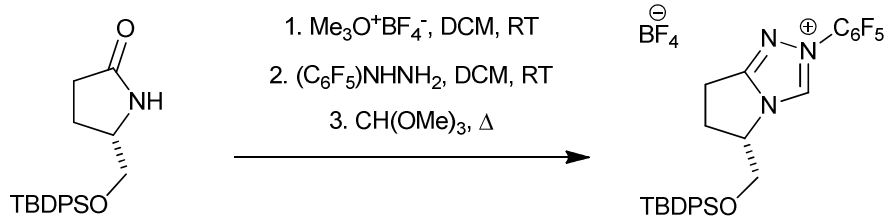
The **racemic products** were prepared using the general procedure with 2-(Perfluorophenyl)-6,7-dihydro-5H-pyrrolo[2,1-c][1,2,4]triazol-2-ium tetrafluoroborate as catalyst precursor[2].

Absolute **THF** was freshly distilled from Solvona® under argon.

Absolute **CH_2Cl_2** was washed with conc. H_2SO_4, $NaHCO_3$, dried with $MgSO_4$ and freshly distilled from calcium hydride under argon.

[1] R. P. Singh, G. Cao, R. L. Kirchmeier, J. M. Shreeve, *J. Org. Chem.*, 1999, **64**, 2873-2876.
[2] M. S. Kerr, J. R. Alaniz, T. Rovis, *J. Org. Chem.*, 2005, **70**, 5725-5728.

*3. Synthesis of the Catalyst Precursor **5***



10 **5**

Catalyst precursor **5** was prepared with a modified procedure reported in the literature.[3]

A 50 mL dry Schlenk flask was charged with the lactam **10** (2.55 g, 7.21 mmol) in absolute CH_2Cl_2 (30 mL). Trimethyloxonium tetrafluoroborate (1.07 g, 7.21 mmol) was added and the reaction mixture stirred for 24 h at room temperature. Afterwards (perfluorophenyl)hydrazine (1.43 g, 7.21 mmol) was added and the solution was again stirred for 18 hours. The solvent was removed in vacuo and the residue was redissolved in trimethyl orthoformate (30 mL). The reaction mixture was refluxed for 24 hours. The solvent was removed in vacuo and the residue was recrystallised from *i*-propanol affording a brown solid. The mother liquor was concentrated in vacuo and the residue redissolved in trimethyl orthoformate (15 mL) and stirred at 80 °C for further 24 h. The solvent was removed in vacuo and the residue was recrystallised from *i*-propanol affording a brown solid. Both precipitates were combined and recrystallised first from ethyl acetate and then from *i*-propanol. (*S*)-2-perfluorophenyl-5-((tertbutyldiphenylsilyloxy)methyl)-6,7-dihydro-5H-pyrrolo[2,1-c][1,2,4]triazol-2-ium tetrafluoroborate (**5**) (1.18 g, 26%) was isolated as analytically pure colorless solid.

M.p. 194-197 °C (from *i*-propanol); $[\alpha]_D^{22}$ = -15.3 (*c* = 1.00, $CHCl_3$); IR (ATR): 3071, 2958, 2863, 2107, 1662, 1602, 1529, 1490, 1427, 1372, 1294, 1263, 1219, 1188, 1108, 1059, 1006, 857, 822, 782, 742, 704 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ = 0.94 (s, 9H), 2.52-2.62 (m, 1H), 3.00-3.10 (m, 1H), 3.22-3.28 (m, 2H), 3.81 (dd, 1H, *J* = 11.9 Hz, 2.5 Hz), 4.26 (dd, 1H, *J* = 2.5 Hz, 11.9 Hz), 5.18-5.24 (m, 1H), 7.32-7.54 (m, 10H), 9.96 (s, 1H) ppm; ^{13}C NMR[4] (101 MHz, $CDCl_3$): δ = 19.1, 22.5, 26.7, 30.0, 62.9, 64.7, 128.0, 128.1, 130.1, 130.2, 131.2, 132.0, 135.2, 135.3, 142.8, 164.0 ppm; MS (EI, 70 eV): *m/z* 486 (25%), 389 (20), 334 (31), 298 (10), 258 (11); HRMS (ESI+) calcd for $C_{28}H_{27}F_5N_3OSi^+$, 544.1838. Found 544.1844.

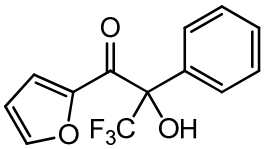
[3] D. Enders, J. Han, A. Henseler, *Chem. Commun*., 2008, 3989-3991.
[4] The carbons of the perfluoro substituent were not observed.

4. General Procedure for the Asymmetric Cross-Benzoin Condensation

A 4 mL screw cap tube was evacuated three times and refilled with argon without heating. Then it was charged with 1 mmol aldehyde (1 equiv.), 2 mmol ketone (2 equiv.), 0.1 mmol catalyst precursor **5** (0.1 equiv.) and 1 mL dry THF. This mixture was cooled to 0 °C. Finally, 1 mmol Hünig's base was added dropwise[5] and the solution was stirred at 0 °C for 24-48 h[6]. Once no aldehyde and no benzoin intermediate was monitored by TLC anymore the raw mixture was directly purified by column chromatography.

5. Analytical Data

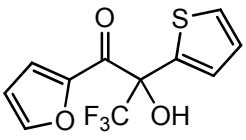
3,3,3-Trifluoro-1-(furan-2-yl)-2-hydroxy-2-phenylpropan-1-one **(3a)**[7] was purified by flash chromatography (*n*-pentane:ether = 4:1; R_f = 0.51 in *n*-pentane:ether = 1:1) yielding an off-white solid (232 mg, 86%). The product was recrystallised from *n*-hexane:*i*-propanol (50:1) affording colourless crystals (116 mg, 43%). The *ee* (99%) was determined by HPLC on a chiral stationary phase (Daicel AS, *n*-heptane:*i*-propanol = 9:1, 1.5 mL/min), t_R = 4.38 min (minor), 6.66 min (major). M.p. 106-109 °C (from *n*-hexane:*i*-propanol = 50:1); $[\alpha]_D^{22}$ = -37.7 (*c* = 1.00, $CHCl_3$); IR (ATR): 3354, 3144, 2925, 2853, 2776, 2108, 2002, 1978, 1640, 1556, 1494, 1455, 1390, 1303, 1268, 1232, 1173, 1088, 1072, 1020, 935, 883, 824, 766, 750, 714, 670 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ = 5.08 (br s, 1H), 6.42 (ddd, 1H, *J* = 3.8 Hz, 1.7 Hz, 0.7 Hz), 6.98 (d, 1H, *J* = 3.7 Hz), 7.37-7.43 (m, 3H), 7.52-7.57 (m, 3H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ = 81.2 (q, *J* = 28.6 Hz), 112.6, 123.2 (q, *J* = 286.0 Hz), 124.0, 126.8, 126.9, 128.7, 129.4, 134.2, 148.3, 181.0 ppm; ^{19}F NMR (377 MHz, $CDCl_3$): -72.9 ppm; MS (EI, 70 eV): *m/z* 270 (M^+, 44%), 253 (33), 175 (10), 105 (29), 95 (100), 77 (14); Calcd. for $C_{13}H_9F_3O_3$: C, 57.79; H, 3.36. Found: C, 57.85; H, 3.36.



3a

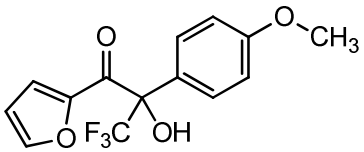
[5] Under the reaction conditions the benzoin intermediate is easily oxidised to the diketone, lowering the yield. Any contact to oxygen should be avoided after the addition of base.
[6] For time specification, see Table 2 in the main text.
[7] D. Enders, A. Henseler, *Adv. Synth. Catal.*, 2009, **351**, 1749.

3,3,3-Trifluoro-1-(furan-2-yl)-2-hydroxy-2-(thiophen-2-yl)propan-1-one **(3b)** was purified by flash chromatography (*n*-pentane:ether = 9:1; R_f = 0.44 in *n*-pentane:ether = 1:1) yielding an yellow oil which solidified over night in the fridge (196 mg, 71%). The *ee* (61%) was determined by HPLC on a chiral stationary phase (Daicel AS, *n*-heptane:ethanol = 9:1, 0.7 mL/min), t_R = 8.70 min (minor), 10.32 min (major). M.p. 83 °C (from *n*-pentane:ether = 9:1); $[\alpha]_D^{22}$ = -30.2 (*c* = 1.00, $CHCl_3$); IR (ATR): 3324, 3122, 2729, 2111, 1744, 1640, 1552, 1453, 1390, 1293, 1269, 1138, 1089, 1074, 1021, 923, 883, 844, 803, 776, 735, 709 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ = 5.43 (br s, 1H), 6.52 (dd, 1H, *J* = 3.8 Hz, 1.7 Hz), 7.04 (dd, 1H, *J* = 5.0 Hz, 3.8 Hz), 7.26 (d, 1H, *J* = 3.7 Hz), 7.36-7.42 (m, 2H), 7.67 (dd, 1H, *J* = 1.6 Hz, 0.6 Hz) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ = 79.6 (q, *J* = 30.7 Hz), 113.0, 122.8 (q, *J* = 286.6 Hz), 124.5, 127.1, 127.6, 127.8, 127.9, 137.3, 148.9, 179.6 ppm; ^{19}F NMR (282 MHz, $CDCl_3$): -74.4 ppm; MS (EI, 70 eV): *m/z* 276 (M^+, 9%), 259 (3), 181 (22), 111 (41), 95 (100); Calcd. for $C_{11}H_7F_3O_3S$: C, 47.83; H, 2.55. Found: C, 47.89; H, 2.50.



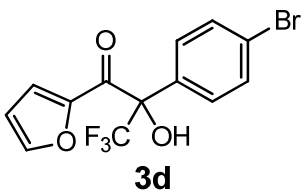
3b

3,3,3-Trifluoro-1-(furan-2-yl)-2-hydroxy-2-(4-methoxyphenyl)propan-1-one **(3c)** was purified by flash chromatography (*n*-pentane:ether = 4:1; R_f = 0.50 in *n*-pentane:ether = 1:1) yielding an off-white solid (207 mg, 69%). The *ee* (82%) was determined by HPLC on a chiral stationary phase (Daicel AS, *n*-heptane:*i*-propanol = 9:1, 1.5 mL/min), t_R = 6.18 min (minor), 9.88 min (major). M.p. 103 °C (from *n*-pentane:ether = 4:1); $[\alpha]_D^{22}$ = -6.2 (*c* = 1.00, $CHCl_3$); IR (ATR): 3360, 3145, 2965, 2841, 2052, 1642, 1610, 1555, 1511, 1456, 1390, 1303, 1256, 1164, 1089, 1019, 932, 884, 811, 773, 753, 696 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ = 3.80 (s, 3H), 5.05 (br s, 1H), 6.42 (dd, 1H, *J* = 1.6 Hz, 3.7 Hz), 6.87-6.93 (m, 2H), 6.98 (d, 1H, *J* = 3.7 Hz), 7.46 (d, 2H, *J* = 8.5 Hz), 7.57 (d, 1H, J = 1.0 Hz) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ = 55.2, 81.0 (q, *J* = 28.8 Hz), 112.6, 114.1, 123.4 (q, *J* = 286.4 Hz), 124.0, 126.2, 128.3, 148.3, 148.7, 160.2, 181.4 ppm; ^{19}F NMR (282 MHz, $CDCl_3$): -73.2 ppm; MS (EI, 70 eV): *m/z* 300 (M^+, 7%), 205 (100), 135 (68), 108 (11), 95 (31), 77 (9); Calcd. for $C_{14}H_{11}F_3O_4$: C, 56.01; H, 3.69. Found: C, 55.96; H, 3.63.



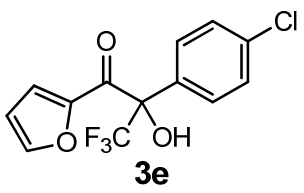
3c

2-(4-Bromophenyl)-3,3,3-trifluoro-1-(furan-2-yl)-2-hydroxypropan-1-one **(3d)** was purified by flash chromatography (*n*-pentane:ether = 4:1; R_f = 0.50 in *n*-pentane:ether = 1:1) yielding an off-white solid (311 mg, 89%). The product was recrystallised from *n*-hexane:*i*-propanol (50:1) affording colourless crystals (171 mg, 49%). The *ee* (99%) was determined by HPLC on a chiral stationary phase (Daicel AS, *n*-heptane:ethanol = 9:1, 0.7 mL/min), t_R = 7.79 min (minor), 8.90 min (major). M.p. 133-136 °C (from *n*-hexane:*i*-propanol = 50:1); $[\alpha]_D^{22}$ = -51.1 (*c* = 1.00, $CHCl_3$); IR (ATR): 3339, 3153, 2322, 2110, 1654, 1556, 1458, 1394, 1361, 1280, 1256, 1175, 1129, 1075, 1015, 932, 885, 834, 799, 770, 726, 683 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ = 5.05 (br s, 1H), 6.47 (dd, 1H, *J* = 1.7 Hz, 3.7 Hz), 7.09 (d, 1H, *J* = 3.7 Hz), 7.44 (d, 2H, *J* = 8.7 Hz), 7.55 (d, 2H, *J* = 8.6 Hz), 7.59 (d, 1H, *J* = 1.6 Hz) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ = 81.0 (q, *J* = 29.2 Hz), 112.8, 123.1 (q, *J* = 286.6 Hz), 124.0, 124.1, 128.7, 128.7, 132.0, 133.3, 148.6, 180.5 ppm; ^{19}F NMR (282 MHz, $CDCl_3$): -73.1 ppm; MS (CI, 100 eV): *m/z* 249 ($M+H^+$, 14%), 331 (18), 280 (17), 252 (100), 95 (34); Calcd. for $C_{13}H_8BrF_3O_3$: C, 44.73; H, 2.31. Found: C, 45.03; H, 2.32.



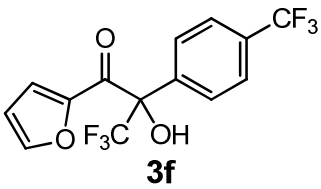
3d

2-(4-Chlorophenyl)-3,3,3-trifluoro-1-(furan-2-yl)-2-hydroxypropan-1-one **(3e)** was purified by flash chromatography (*n*-pentane:ether = 4:1; R_f = 0.50 in *n*-pentane:ether = 1:1) yielding an off-white solid (274 mg, 90%). The product was recrystallised from *n*-hexane:*i*-propanol (50:1) affording colourless crystals (140 mg, 46%). The *ee* (81%) was determined by HPLC on a chiral stationary phase (Daicel OJ, *n*-heptane:ethanol = 9:1, 1.0 mL/min), t_R = 9.74 min (major), 14.97 min (minor). M.p. 109-111 °C (from *n*-hexane:*i*-propanol = 50:1); $[\alpha]_D^{22}$ = -42.5 (*c* = 1.00, $CHCl_3$); IR (ATR): 3337, 2040, 2000, 1740, 1653, 1558, 1493, 1459, 1396, 1363, 1281, 1257, 1202, 1177, 1128, 1109, 1091, 1076, 1017, 937, 926, 886, 835, 801, 771, 758, 738, 688 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ = 5.03 (br s, 1H), 6.47 (dd, 1H, *J* = 1.4 Hz, 3.7 Hz), 7.08 (d, 1H, *J* = 3.7 Hz), 7.38 (d, 2H, *J* = 8.6 Hz), 7.50 (d, 2H, *J* = 8.8 Hz), 7.57-7.61 (m, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ = 80.9 (q, *J* = 29.2 Hz), 112.8, 123.1 (q, *J* = 286.6 Hz), 124.1, 128.5, 128.5, 129.0, 132.8, 135.7, 148.6, 180.6 ppm; ^{19}F NMR (282 MHz, $CDCl_3$): -73.0 ppm; MS (CI, 100 eV): *m/z* 305 ($M+H^+$, 100%), 287 (4), 191 (1), 95 (2); Calcd. for $C_{13}H_8ClF_3O_3$: C, 51.25; H, 2.65. Found: C, 51.32; H, 2.13.



3e

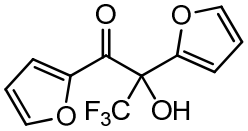
3,3,3-Trifluoro-1-(furan-2-yl)-2-hydroxy-2-(4-(trifluoromethyl)phenyl)propan-1-one **(3f)**



3f

was purified by flash chromatography (*n*-pentane:ether = 4:1; R_f = 0.38 in *n*-pentane:ether = 1:1) yielding an off-white solid (325 mg, 96%). The product was recrystallised from *n*-hexane:*i*-propanol (50:1) affording colourless crystals (139 mg, 41%). The *ee* (96%) was determined by HPLC on a chiral stationary phase (Daicel AS, *n*-heptane:ethanol = 9:1, 1.3 mL/min), t_R = 3.79 min (minor), 5.34 min (major). M.p. 112-113 °C (from *n*-hexane:*i*-propanol = 50:1); $[\alpha]_D^{22}$ = -65.2 (*c* = 1.00, $CHCl_3$); IR (ATR): 3377, 3149, 2111, 1946, 1647, 1552, 1453, 1420, 1393, 1321, 1300, 1265, 1169, 1125, 1103, 1067, 1019, 965, 934, 884, 852, 816, 769, 710, 681 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ = 5.11 (br s, 1H), 6.49 (dd, 1H, *J* = 1.6 Hz, 3.7 Hz), 7.14 (d, 1H, *J* = 3.7 Hz), 7.58-7.60 (m, 1H), 7.67 (d, 2H, *J* = 8.7 Hz), 7.72 (d, 2H, *J* = 8.7 Hz) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ = 81.0 (q, *J* = 28.8 Hz), 112.9, 123.1 (q, *J* = 286.7 Hz), 123.6 (q, *J* = 272.5 Hz), 124.2, 125.7, 125.7, 127.6, 131.6 (q, *J* = 32.8 Hz), 138.1, 148.8, 180.2 ppm; ^{19}F NMR (282 MHz, $CDCl_3$): -63.0, -73.0 ppm; MS (CI, 100 eV): *m/z* 339 ($M+H^+$, 20%), 321 (32), 293 (19), 173 (11), 145 (9), 95 (100); Calcd. for $C_{14}H_8F_6O_3$: C, 49.72; H, 2.38. Found: C, 49.84; H, 2.31.

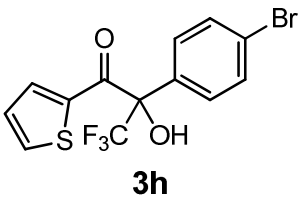
3,3,3-Trifluoro-1,2-di(furan-2-yl)-2-hydroxypropan-1-one **(3g)** was purified by flash chromatography (*n*-pentane:ether = 4:1; R_f = 0.65 in *n*-pentane:ether = 1:1) yielding an yellow oil which solidified over night in the fridge (224 mg, 86%). The *ee* (39%) was determined by HPLC on a chiral stationary phase (Daicel AD, *n*-heptane:ethanol = 4:1, 1.0 mL/min), t_R = 7.70 min (major), 8.96 min (minor). M.p. 54-58 °C (from *n*-pentane:ether = 9:1); $[\alpha]_D^{22}$ = +4.2 (*c* = 1.00, $CHCl_3$); IR (ATR): 3411, 3145, 2920, 2852, 1672, 1560, 1495, 1459, 1387, 1277, 1186, 1112, 1087, 1032, 971, 938, 889, 849, 809, 753, 693, 590, 530, 482 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ = 5.36 (br s, 1H), 6.48 (dd, 1H, *J* = 1.8 Hz, 3.3 Hz), 6.52 (dd, 1H, *J* = 1.6 Hz, 3.7 Hz), 6.74 (d, 1H, *J* = 3.0 Hz) ppm 6.98 (d, 1H, *J* = 3.7 Hz), 7.43 (d, 1H, *J* = 1.0 Hz), 7.69 (d, 1H, *J* = 0.8 Hz) ppm; ^{13}C NMR[8] (101 MHz, $CDCl_3$): δ = 110.9, 111.1, 113.0, 122.3 (q, *J* = 285.7 Hz), 124.3, 143.8, 146.5, 148.4, 149.2, 178.0 ppm; ^{19}F NMR (377 MHz, $CDCl_3$): -74.2 ppm; MS (CI, 100 eV): *m/z* 261 ($M+H^+$, 6%), 243 (100), 215 (19), 165 (13), 149 (19), 109 (13), 95 (42), 81 (21); Calcd. for $C_{11}H_7F_3O_4$: C, 50.78; H, 2.71. Found: C, 51.13; H, 3.10.



3g

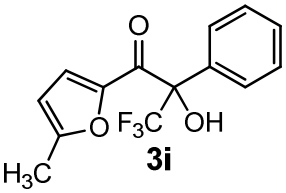
[8] One of the quaternary carbons was not observed.

2-(4-Bromophenyl)-3,3,3-trifluoro-2-hydroxy-1-(thiophen-2-yl)propan-1-one **(3h)** was purified by flash chromatography (*n*-pentane:ether = 4:1; R_f = 0.27 in *n*-pentane:ether = 4:1) yielding an yellow oil which solidified over night in the fridge (340 mg, 93%). The *ee* (65%) was determined by HPLC on a chiral stationary phase (Daicel AS, *n*-heptane:ethanol = 9:1, 1.0 mL/min), t_R = 5.88 min (minor), 7.68 min (major). M.p. 86-91 °C (from *n*-pentane:ether = 4:1); $[\alpha]_D^{22}$ = -43.6 (*c* = 1.17, $CHCl_3$); IR (ATR): 3068, 2815, 2323, 2061, 1988, 1792, 1626, 1602, 1554, 1516, 1457, 1414, 1328, 1275, 1192, 1164, 1068, 1003, 943, 861, 835, 766, 732, 701, 666 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ = 4.94 (br s, 1H), 6.99 (dd, 1H, *J* = 4.0 Hz, 4.9 Hz), 7.44 (d, 2H, *J* = 8.3 Hz), 7.49 (d, 1H, *J* = 3.9 Hz), 7.55 (d, 2H, *J* = 8.8 Hz), 7.67 (dd, 1H, *J* = 1.1 Hz, 4.9 Hz) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ = 81.5 (q, *J* = 28.3 Hz), 123.0 (q, *J* = 286.3 Hz), 124.1, 128.4, 128.6, 132.0, 133.1, 136.6, 137.0, 138.1, 185.5 ppm; ^{19}F NMR (377 MHz, $CDCl_3$): -73.4 ppm; MS (CI, 100 eV): *m/z* 367 ($M+H^+$, 9%), 347 (16), 296 (14), 268 (100), 111 (81), 85 (28); Calcd. for $C_{13}H_8BrF_3O_2S$: C, 42.76; H, 2.21. Found: C, 42.83; H, 2.14.



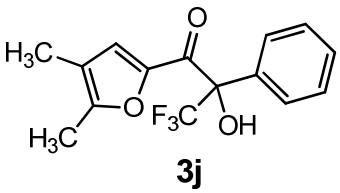
3h

3,3,3-Trifluoro-2-hydroxy-1-(5-methylfuran-2-yl)-2-phenylpropan-1-one **(3i)** was purified by flash chromatography (*n*-pentane:ether = 4:1; R_f = 0.53 in *n*-pentane:ether = 1:1) yielding an off-white solid (267 mg, 94%). The product was recrystallised from *n*-hexane:*i*-propanol (50:1) affording colourless crystals (176 mg, 62%). The *ee* (99%) was determined by HPLC on a chiral stationary phase (Daicel AS, *n*-heptane:*i*-propanol = 9:1, 1.3 mL/min), t_R = 4.36 min (minor), 6.83 min (major). M.p. 107 °C (from *n*-hexane:*i*-propanol = 50:1); $[\alpha]_D^{22}$ = +31.4 (*c* = 1.00, $CHCl_3$); IR (ATR): 3348, 2327, 2118, 1651, 1500, 1452, 1310, 1268, 1166, 1070, 1028, 992, 971, 940, 818, 770, 745, 713, 674, 656 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ = 2.33 (s, 3H), 5.27 (br s, 1H), 6.05 (dd, 1H, *J* = 3.7 Hz, 0.8 Hz), 6.82 (d, 1H, *J* = 3.6 Hz), 7.35-7.42 (m, 3H), 7.50-7.55 (m, 2H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ = 14.0, 80.9 (q, *J* = 28.9 Hz), 109.9, 123.4 (q, *J* = 286.6 Hz), 126.6, 127.0, 128.7, 129.3, 135.0, 147.3, 160.6, 180.1 ppm; ^{19}F NMR (282 MHz, $CDCl_3$): -72.5 ppm; MS (CI, 100 eV): *m/z* 285 (M^+, 46%), 267 (99), 239 (79), 175 (8), 109 (100); Calcd. for $C_{14}H_{11}F_3O_3$: C, 59.16; H, 3.90. Found: C, 59.15; H, 3.73.



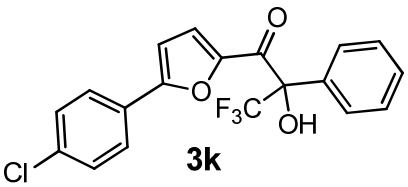
3i

1-(4,5-Dimethylfuran-2-yl)-3,3,3-trifluoro-2-hydroxy-2-phenylpropan-1-one **(3j)** was purified by flash chromatography (*n*-pentane:ether = 4:1; R_f = 0.59 in *n*-pentane:ether = 1:1) yielding an off-white solid (268 mg, 90%). The *ee* (85%) was determined by HPLC on a chiral stationary phase (Daicel AS, *n*-heptane:*i*-propanol = 9:1, 1.0 mL/min), t_R = 5.40 min (minor), 10.75 min (major). M.p. 151 °C (from *n*-pentane:ether = 4:1); $[\alpha]_D^{22}$ = +20.1 (*c* = 1.00, $CHCl_3$); IR (ATR): 3326, 2929, 2110, 1637, 1505, 1453, 1326, 1262, 1165, 1132, 1070, 987, 954, 934, 833, 767, 706, 671 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ = 1.86, (s, 3H), 2.24 (s, 3H), 5.32 (br s, 1H), 6.69 (s, 1H), 7.37-7.42 (m, 3H), 7.50-7.55 (m, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ = 9.6, 12.2, 80.8 (q, *J* = 28.7 Hz), 118.8, 123.3 (q, *J* = 286.2 Hz), 127.0, 128.1, 128.6, 129.2, 135.1, 145.9, 157.0, 179.5 ppm; ^{19}F NMR (377 MHz, $CDCl_3$): -72.4 ppm; MS (CI, 100 eV): *m/z* 299 ($M+H^+$, 100%), 281 (34), 253 (86), 235 (11), 151 (12), 123 (85); Calcd. for $C_{15}H_{13}F_3O_3$: C, 60.40; H, 4.39. Found: C, 60.42; H, 4.51.



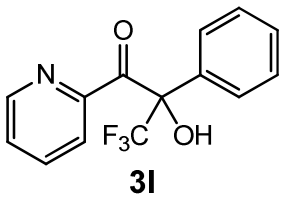
3j

1-(5-(4-Chlorophenyl)furan-2-yl)-3,3,3-trifluoro-2-hydroxy-2-phenylpropan-1-one **(3k)** was purified by flash chromatography (*n*-pentane:ether = 4:1; R_f = 0.58 in *n*-pentane:ether = 1:1) yielding an yellow oil (286 mg, 75%). The oil was dissolved in hot *n*-hexane:*i*-propanol (50:1), layered with *n*-pentane and kept over night in the fridge. The yellow cristals were filtered off and the solvent was removed from mother liquor affording a yellow oil (190 mg, 50%). The *ee* (94%) was determined by HPLC on a chiral stationary phase (Daicel AS, *n*-heptane:*i*-propanol = 9:1, 1.3 mL/min), t_R = 5.47 min (minor), 7.88 min (major). M.p. 127-128 °C (from *n*-pentane: *n*-hexane:*i*-propanol 500:50:1); $[\alpha]_D^{22}$ = -78.2 (*c* = 1.05, $CHCl_3$); IR (ATR): 3280, 2808, 2086, 1603, 1516, 1465, 1411, 1311, 1277, 1157, 1097, 1031, 959, 943, 922, 823, 795, 714, 673 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ = 5.24 (br s, 1H), 6.64 (d, 1H, *J* = 3.9 Hz), 7.11 (d, 1H, *J* = 3.8 Hz), 7.32-7.44 (m, 5H), 7.51-7.61 (m, 4H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ = 81.2 (q, *J* = 29.0 Hz), 108.2, 123.4 (q, *J* = 287.0 Hz), 126.3, 126.5, 127.0, 127.1, 128.8, 129.3, 129.4, 134.5, 136.0, 147.9, 158.7, 180.4 ppm; ^{19}F NMR (282 MHz, $CDCl_3$): -72.3 ppm; MS (CI, 100 eV): *m/z* 381 ($M+H^+$, 26%), 363 (13), 335 (38), 205 (100), 149 (40), 105 (21), 77 (11); Calcd. for $C_{19}H_{12}ClF_3O_3$: C, 59.94; H, 3.18. Found: C, 59.91; H, 3.05.



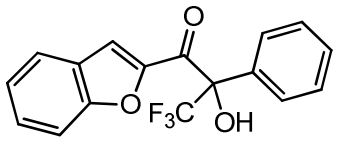
3k

3,3,3-Trifluoro-2-hydroxy-2-phenyl-1-(pyridin-2-yl)propan-1-one **(3l)** was purified by flash chromatography (*n*-pentane:ether = 4:1; R_f = 0.36 in *n*-pentane:ether = 4:1) yielding an colourless oil which solidified over night in the fridge (205 mg, 73%). The *ee* (62%) was determined by HPLC on a chiral stationary phase (Daicel IA, *n*-heptane:ethanol = 9:1, 1.0 mL/min), t_R = 7.34 min (minor), 9.01 min (major). M.p. 69-72 °C (from *n*-pentane:ether = 4:1); $[\alpha]_D^{22}$ = -136.1 (*c* = 1.00, $CHCl_3$); IR (ATR): 3125, 3064, 2923, 1718, 1586, 1488, 1467, 1448, 1251, 1184, 1157, 1136, 1066, 1004, 944, 925, 850, 803, 764, 753, 703, 674 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ = 7.30-740 (m, 3H), 7.46 (ddd, 1H, *J* = 7.7 Hz, 4.9 Hz, 1.2 Hz), 7.68 (d, 2H, *J* = 7.3 Hz), 7.90 (dt, 1H, *J* = 7.8 Hz, 1.7 Hz), 8.16 (dt, 1H, *J* = 7.9 Hz, 1.1 Hz), 8.41 (ddd, 1H, *J* = 4.8 Hz, 1.6 Hz, 0.8 Hz), 8.76 (br s, 1H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ = 84.1 (q, *J* = 27.5 Hz), 123.0 (q, *J* = 284.7 Hz), 124.6, 126.4, 127.9, 128.4, 129.1, 134.3, 138.4, 147.0, 151.7, 189.0 ppm; ^{19}F NMR (377 MHz, $CDCl_3$): -76.4 ppm; MS (CI, 100 eV): *m/z* 282 ($M+H^+$, 100%), 264 (62), 242 (14), 175 (10), 107 (11), 83 (37); Calcd. for $C_{14}H_{10}F_3NO_2$: C, 59.79; H, 3.58; N, 4.98. Found: C, 59.88; H, 3.56; N, 4.96.



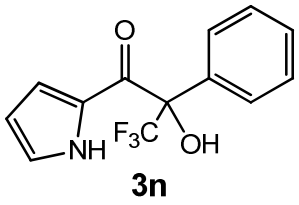
3l

1-(Benzofuran-2-yl)-3,3,3-trifluoro-2-hydroxy-2-phenylpropan-1-one **(3m)** was purified by flash chromatography (*n*-pentane:ether = 4:1; R_f = 0.68 in *n*-pentane:ether = 1:1) yielding an off-white solid (272 mg, 85%). The *ee* (67%) was determined by HPLC on a chiral stationary phase (Daicel AS, *n*-heptane:*i*-propanol = 9:1, 1.3 mL/min), t_R = 4.68 min (minor), 10.64 min (major). M.p. 130-134 °C (from *n*-pentane:ether = 4:1); $[\alpha]_D^{22}$ = -67.3 (*c* = 1.00, $CHCl_3$); IR (ATR): 3358, 2157, 1992, 1664, 1546, 1286, 1262, 1169, 1062, 939, 843, 749, 707, 671 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ = 4.96 (br s, 1H), 7.20-7.31 (m, 2H), 7.40-7.65 (m, 8H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ = 81.7 (q, *J* = 28.8 Hz), 112.5, 119.7, 123.2 (q, *J* = 286.7 Hz), 123.8, 124.3, 126.4, 126.9, 128.9, 129.6, 129.7, 134.0, 148.4, 155.8, 183.2 ppm; ^{19}F NMR (282 MHz, $CDCl_3$): -73.1 ppm; MS (CI, 100 eV): *m/z* 321 ($M+H^+$, 51%), 303 (100), 275 (47), 175 (12), 145 (93), 105 (18), 89 (24); Calcd. for $C_{17}H_{11}F_3O_3$: C, 63.75; H, 3.46%. Found: C, 63.70; H, 3.33.



3m

3,3,3-Trifluoro-2-hydroxy-2-phenyl-1-(1H-pyrrol-2-yl)propan-1-one **(3n)** was purified by flash chromatography (*n*-pentane:ether = 4:1; R_f = 0.37 in *n*-pentane:ether = 1:1) yielding an off-white oil (229 mg, 85%). The raw product was dissolved in hot *n*-hexane:*i*-propanol (50:1), layered with *n*-pentane and kept over night in the fridge. The colourless cristals were filtered off and the solvent was removed from mother liquor affording a yellowish oil (110 mg, 41%). The *ee* (93%) was determined by HPLC on a chiral stationary phase (Daicel AS, *n*-heptane:*i*-propanol = 9:1, 1.3 mL/min), t_R = 6.73 min (minor), 9.99 min (major). M.p. 108-109 °C (from *n*-pentane: *n*-hexane:*i*-propanol 500:50:1); $[\alpha]_D^{22}$ = +16.3 (*c* = 1.00, $CHCl_3$); IR (ATR): 3346, 2112, 1623, 1542, 1453, 1425, 1375, 1272, 1214, 1162, 1130, 1091, 1058, 1046, 1025, 943, 883, 853, 820, 758, 712, 691, 669, 658 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ = 5.32 (br s, 1H), 6.14 (td, 1H, *J* = 4.1 Hz, 2.5 Hz), 6.54 (br s, 1H), 7.03 (ddd, 1H, *J* = 3.1 Hz, 2.5 Hz, 1.3 Hz), 7.35-7.41 (m, 3H), 7.51-7.57 (m, 2H), 9.67 (br s, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ = 80.8 (q, *J* = 28.4 Hz), 112.0, 122.2, 123.5 (q, *J* = 286.6 Hz), 126.9, 127.0, 127.1, 128.7, 129.3, 135.5, 182.4 ppm; ^{19}F NMR (282 MHz, $CDCl_3$): -72.6 ppm; MS (CI, 100 eV): *m/z* 270 ($M+H^+$, 98%), 252 (60), 224 (100), 175 (12), 94 (70); Calcd. for $C_{13}H_{10}F_3NO_2$: C, 58.00; H, 3.74; N, 5.20. Found: C, 57.93; H, 3.86; N, 5.17.



3n

6. NMR-Spectra and HPLC-Chromatogram of New Compounds

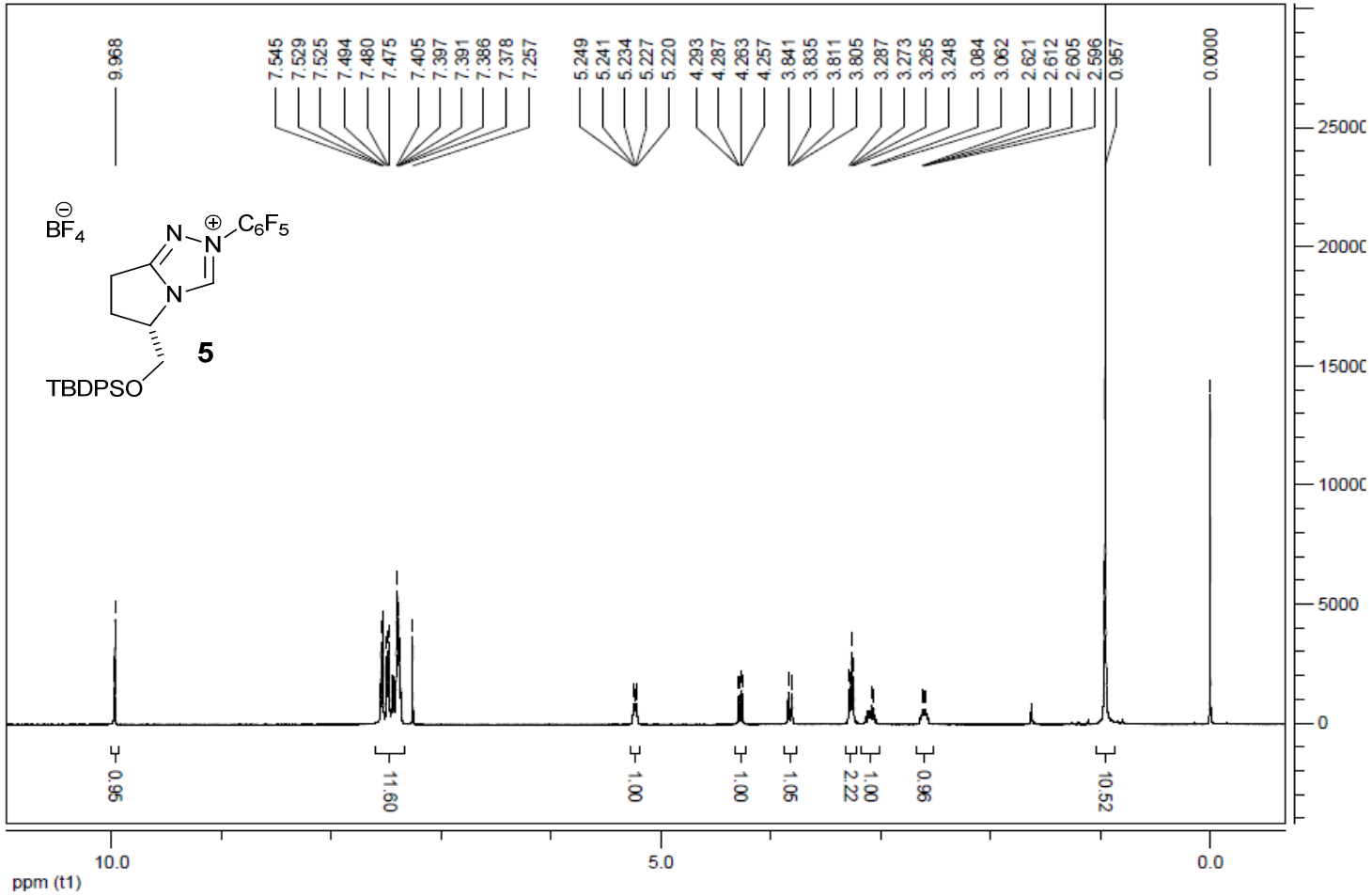


Figure S1 ^{1}H-NMR spectrum (400 MHz, $CDCl_3$) of (*S*)-2-perfluorophenyl-5-((tertbutyldiphenylsilyloxy)methyl)-6,7-dihydro-5H-pyrrolo[2,1-c][1,2,4]triazol-2-ium tetrafluoroborate (**5**).

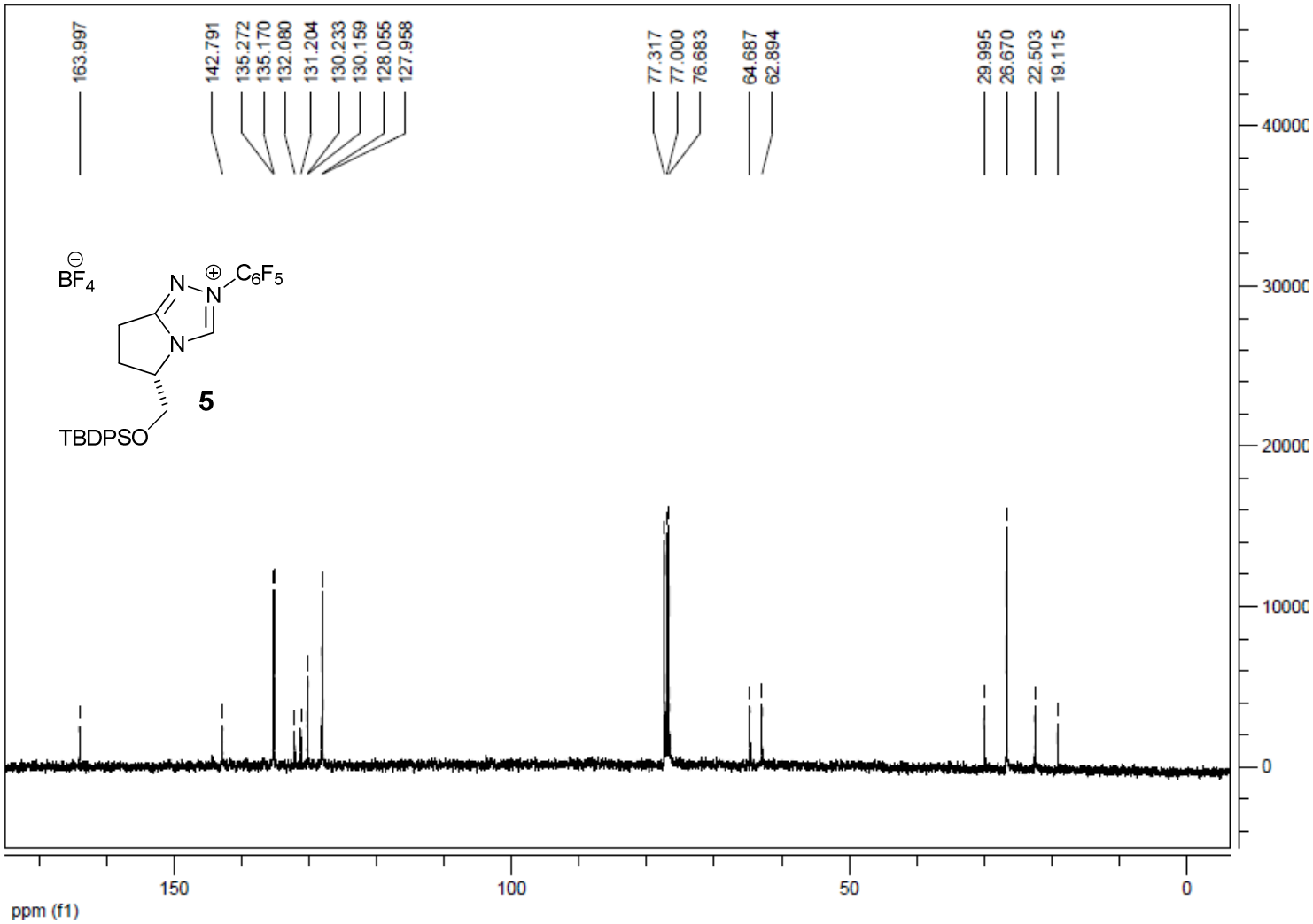


Figure S2 ^{13}C-NMR spectrum (400 MHz, $CDCl_3$) of (*S*)-2-perfluorophenyl-5-((tertbutyldiphenylsilyloxy)methyl)-6,7-dihydro-5H-pyrrolo[2,1-c][1,2,4]triazol-2-ium tetrafluoroborate (**5**).

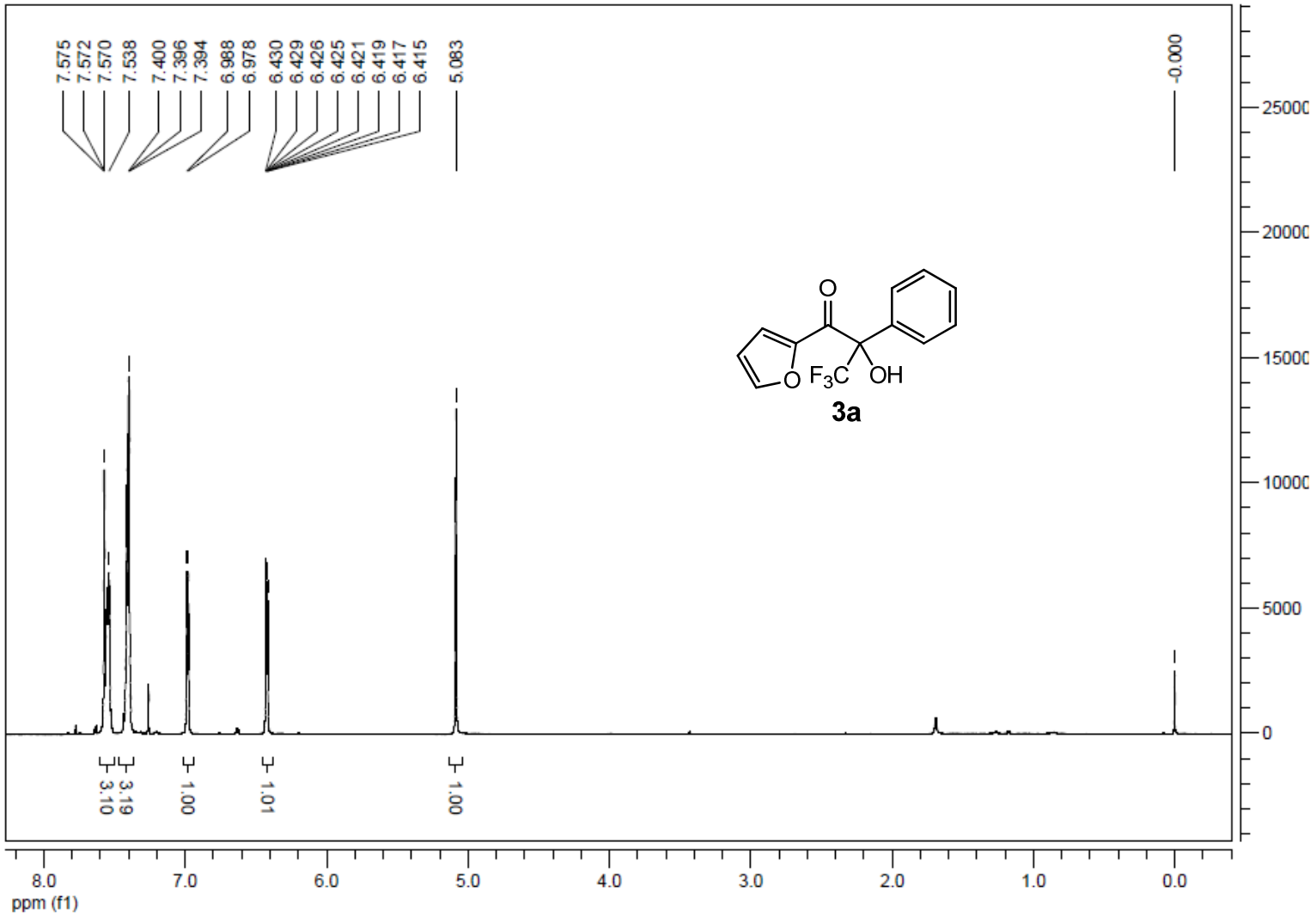


Figure S3 ^{1}H-NMR spectrum (400 MHz, $CDCl_3$) of 3,3,3-trifluoro-1-(furan-2-yl)-2-hydroxy-2-phenylpropan-1-one (**3a**).

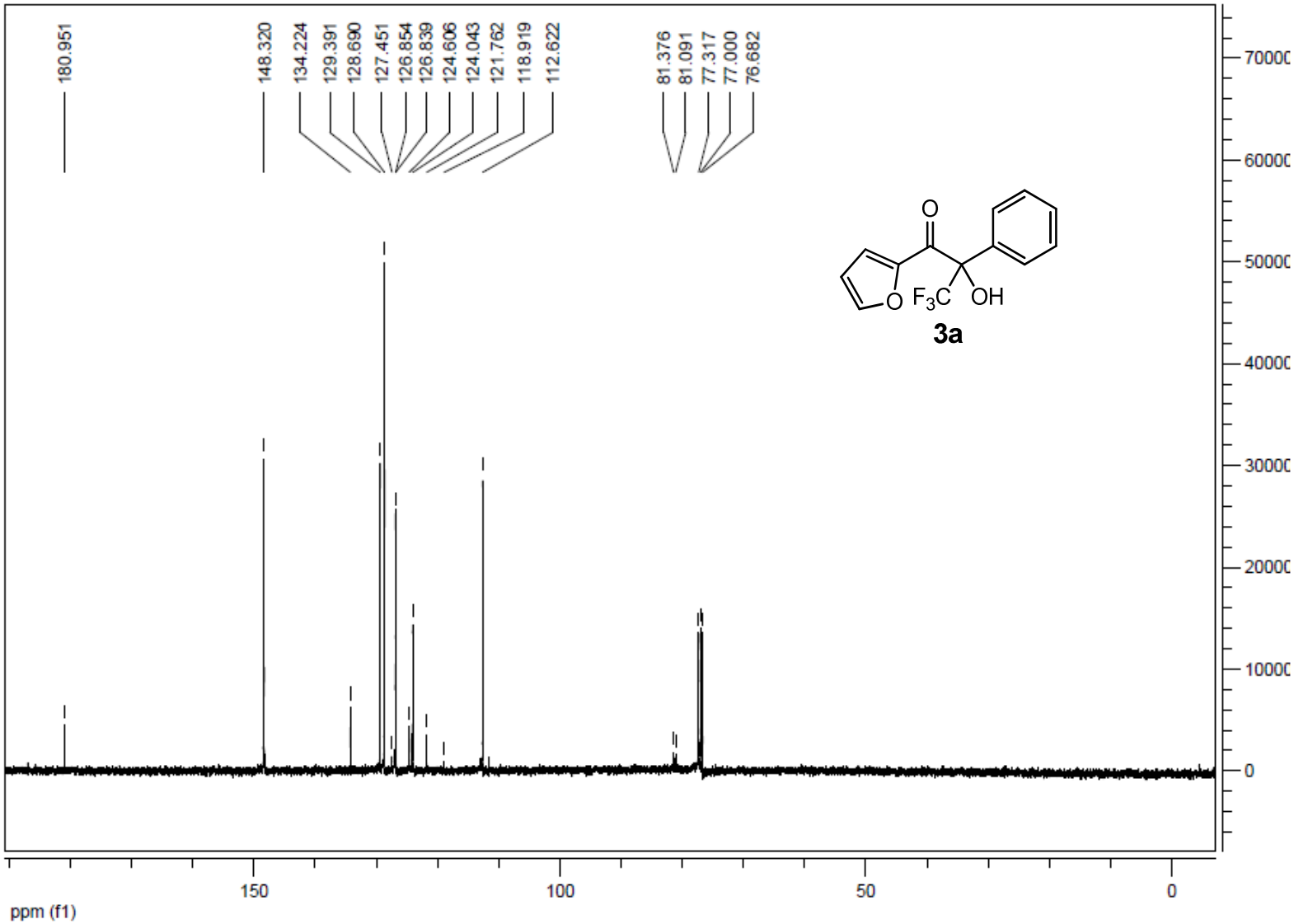
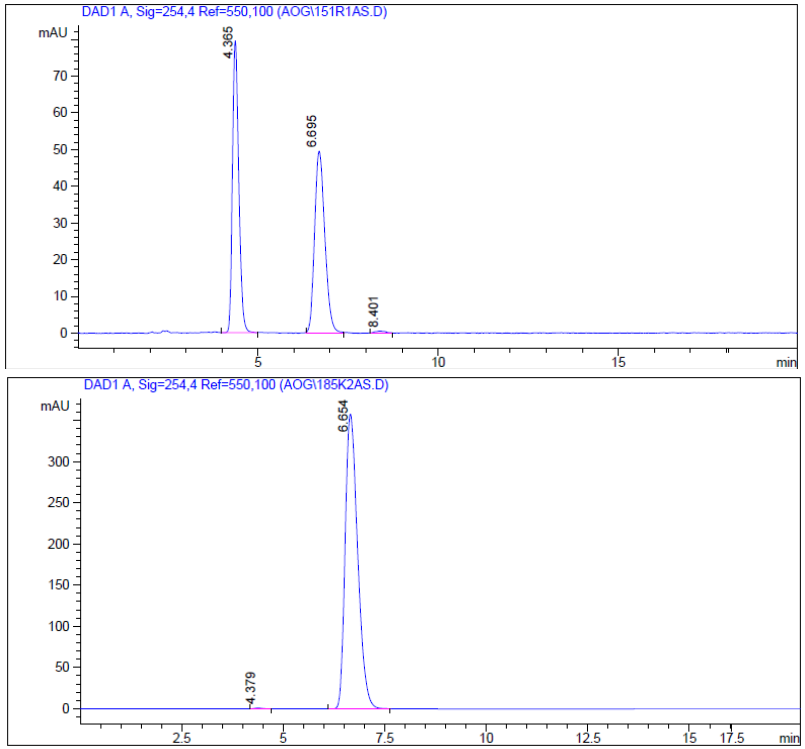


Figure S4 ^{1}H-NMR spectrum (400 MHz, $CDCl_3$) of 3,3,3-trifluoro-1-(furan-2-yl)-2-hydroxy-2-phenylpropan-1-one (**3a**).



Sample Name: AOG 185 K2
Data file: D:\BERT\AOG\185K2AS.D
Sample Info: Laufmittel: n-Heptan/IP 9:1;
Die Probe ist im LM gelöst

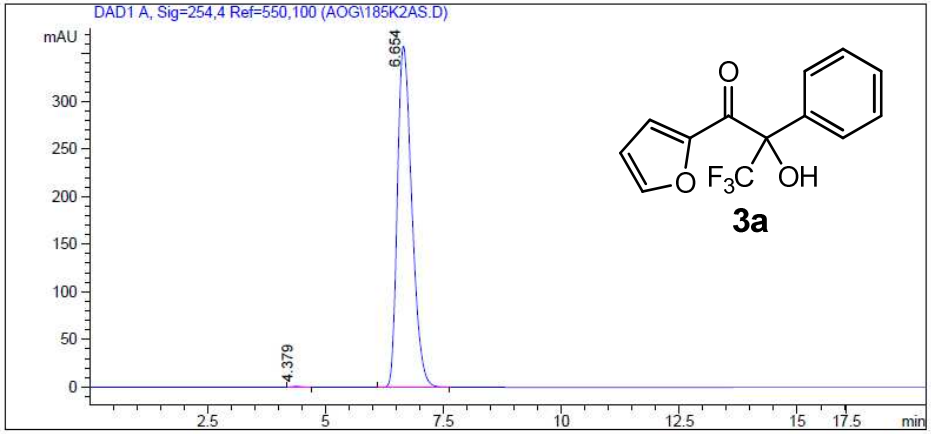
Agilent Technologies

Säule: DAICELAS.M
Säuleninfo: (250x4,6)mm

Operator: Analytik Labor AKEN

Injektion Time: 09:24:23
Injektion Date: 26.04.2010

Instrument Conditions:	At Start	At Stop
Temperature in°C:	30.0	30.0
Pressure in bar:	46.7	46.9
Flow in ml/min:	1.5	1.5



3a

#	Ret. Time (min)	Width	Height (mAU)	Area (mAU*s)	Area %
1	4.38	0.19	1.06	13.53	0.18
2	6.65	0.33	358.17	7645.73	99.82
Total				7659.26	100.00

Figure S5 HPLC chromatogram of **3a**; comparison of racemic and non-racemic (left); non-racemic (right).

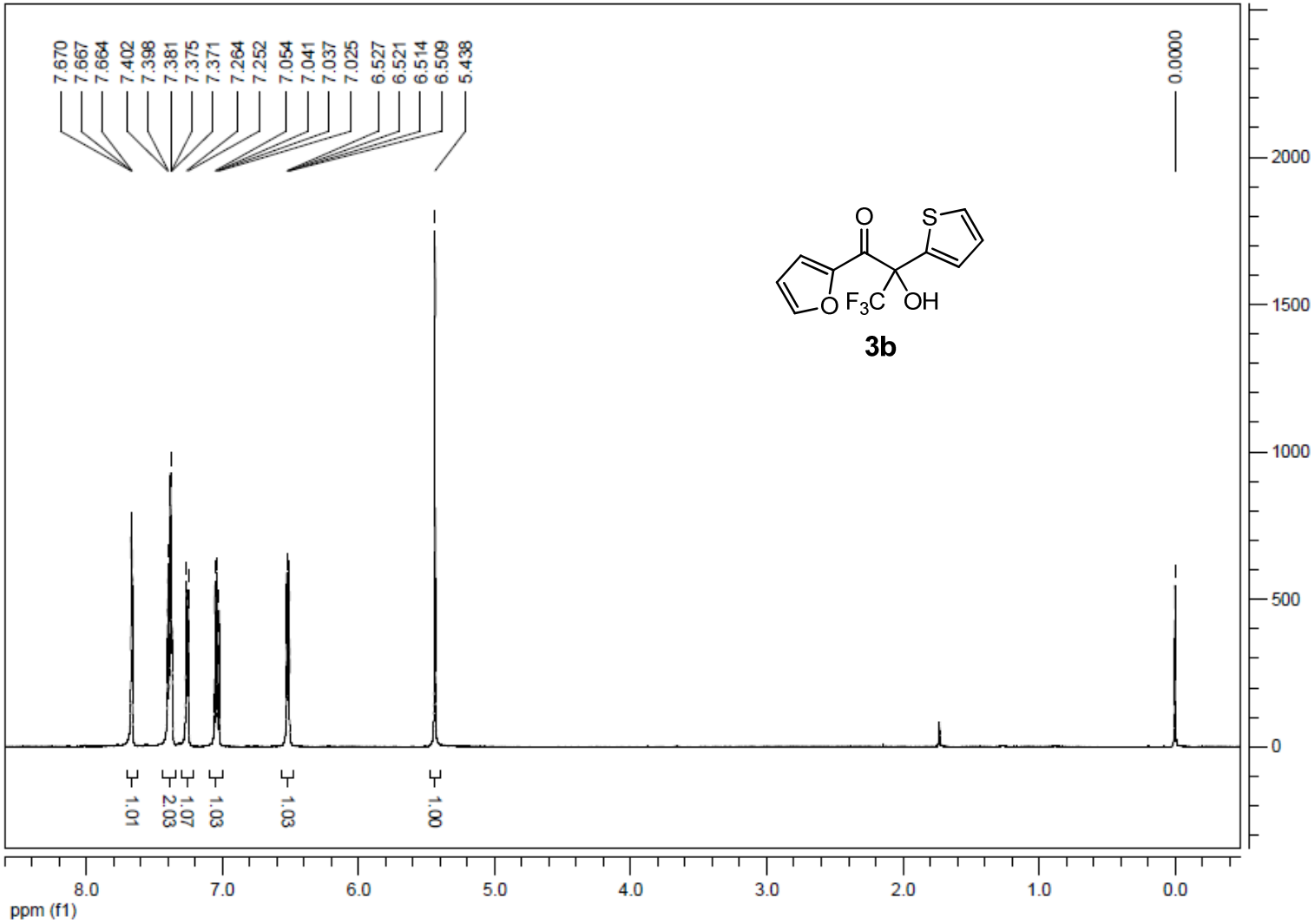


Figure S6 ^{1}H-NMR spectrum (300 MHz, $CDCl_3$) of 3,3,3-trifluoro-1-(furan-2-yl)-2-hydroxy-2-(thiophen-2-yl)propan-1-one (**3b**).

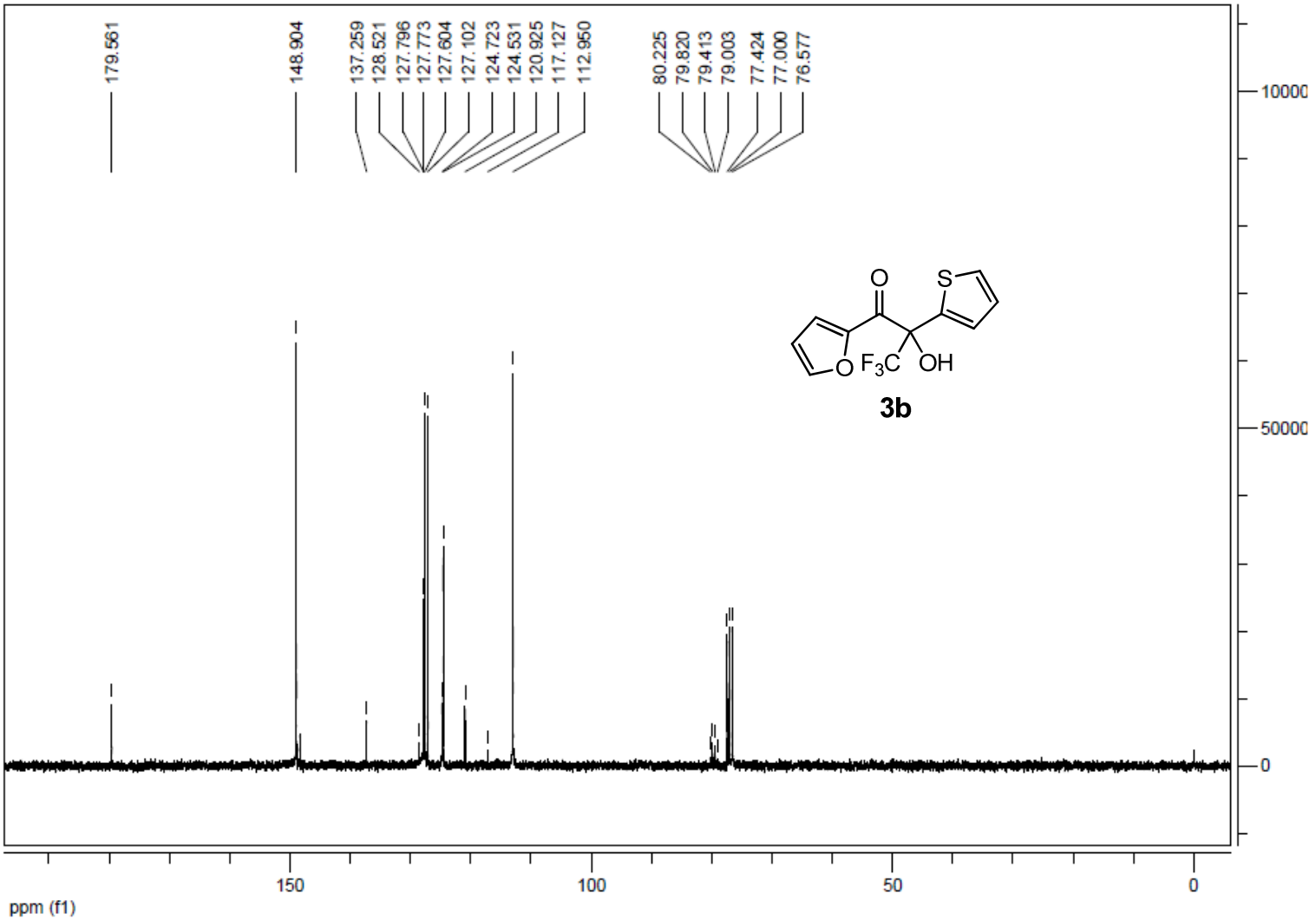
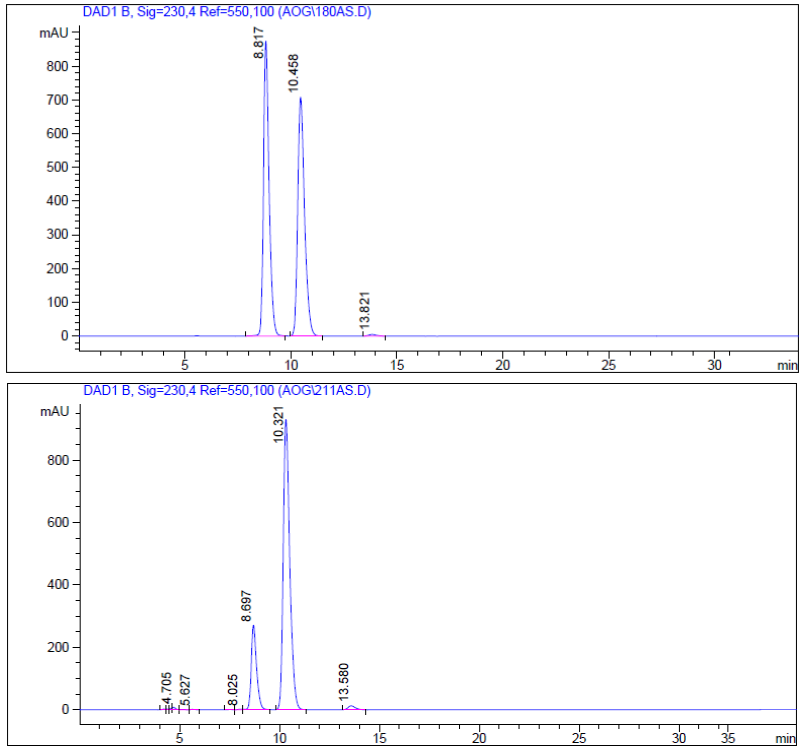


Figure S7 ^{13}C-NMR spectrum (300 MHz, $CDCl_3$) of 3,3,3-trifluoro-1-(furan-2-yl)-2-hydroxy-2-(thiophen-2-yl)propan-1-one (**3b**).



Sample Name: AOG 211
Data file: D:\BERT\AOG\211AS.D
Sample Info: Laufmittel: n-Heptan/EtOH 9:1; Die Probe ist in LM/DCM gelöst

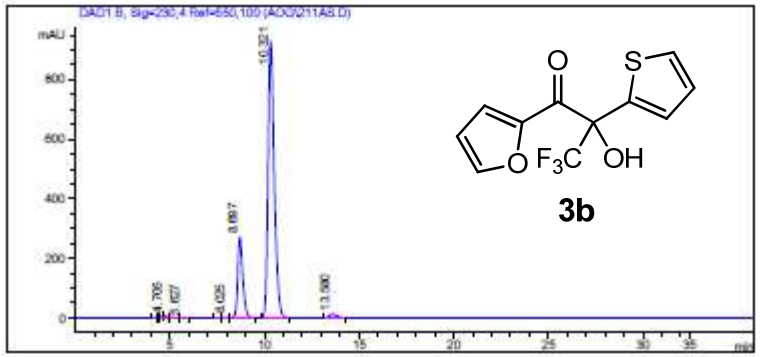
Agilent Technologies

Säule: DAICELAS.M
Säuleninfo: (250x4,6)mm

Operator: Analytik Labor AKEN

Injektion Time: 13:26:13
Injektion Date: 06.05.2010

Instrument Conditions:	At Start	At Stop
Temperature in°C:	30.0	30.0
Pressure in bar:	21.0	21.2
Flow in ml/min:	0.7	0.7



3b

#	Ret. Time (min)	Width	Height (mAU)	Area (mAU*s)	Area %
1	4.20	0.14	2.24	22.44	0.08
2	4.37	0.10	2.43	16.53	0.06
3	4.57	0.10	5.24	34.49	0.13
4	4.70	0.15	8.38	89.62	0.34
5	5.12	0.20	1.47	21.36	0.08
6	5.63	0.18	1.45	17.73	0.07
7	7.51	0.16	0.70	9.11	0.03
8	8.02	0.19	1.88	26.10	0.10
9	8.70	0.28	271.23	5019.78	18.84
10	10.32	0.34	931.67	21061.28	79.03
11	13.58	0.39	12.76	331.44	1.24
Total				26649.86	100.00

Figure S8 HPLC chromatogram of **3b**; comparison of racemic and non-racemic (left); non-racemic (right).

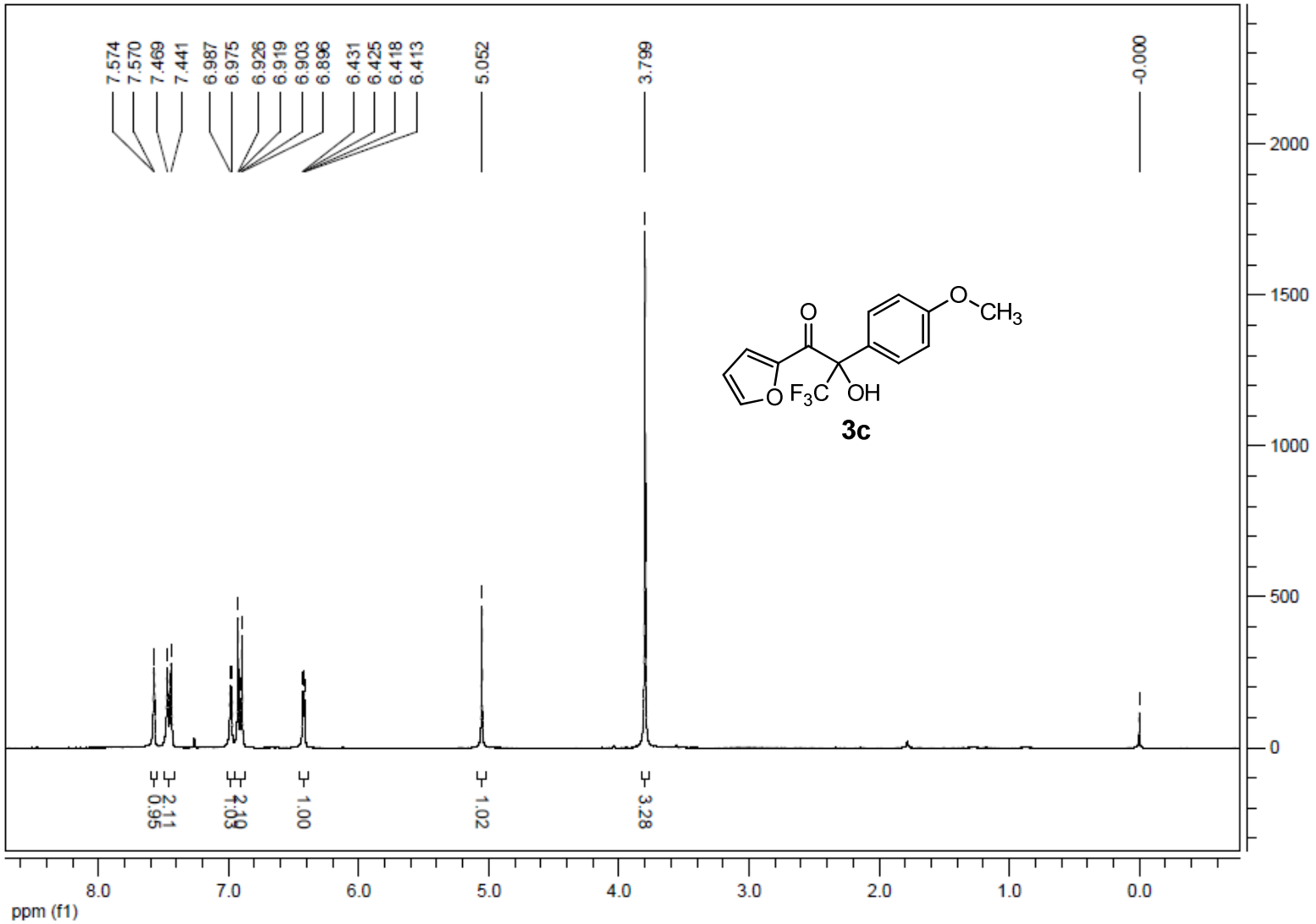


Figure S9 ^{1}H-NMR spectrum (300 MHz, $CDCl_3$) of 3,3,3-trifluoro-1-(furan-2-yl)-2-hydroxy-2-(4-methoxyphenyl)propan-1-one (**3c**).

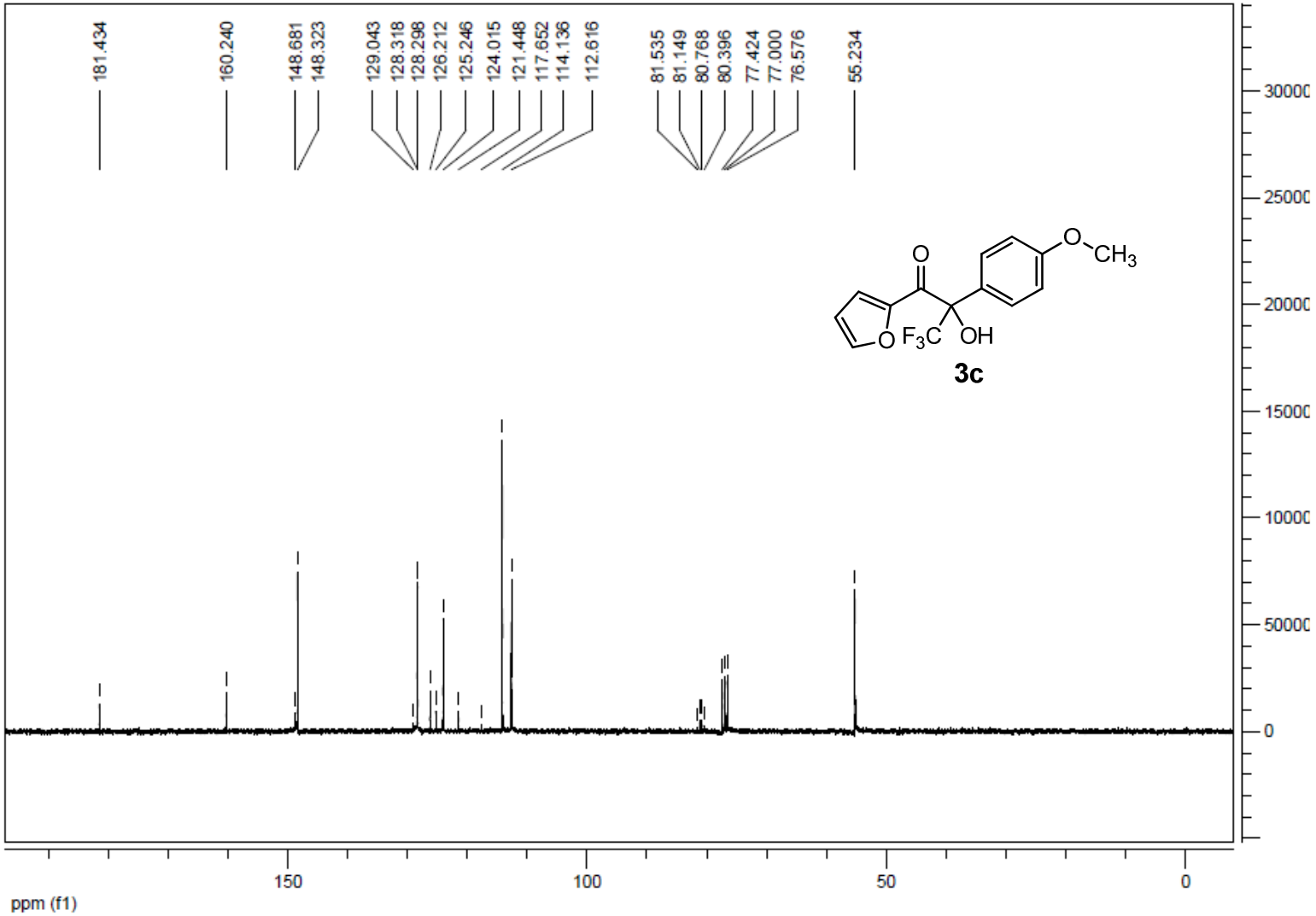
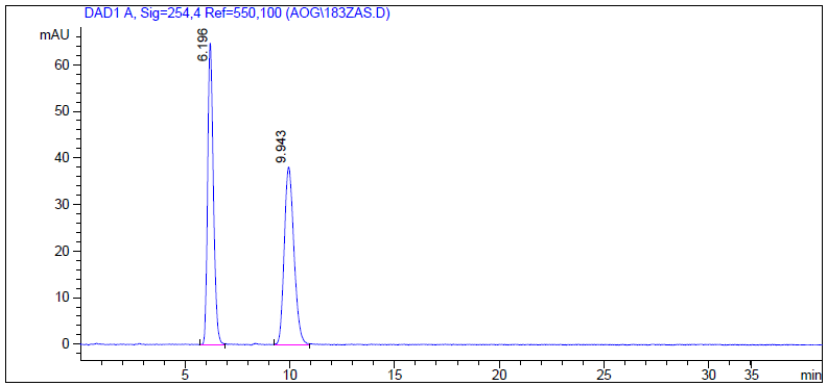


Figure S10 ^{13}C-NMR spectrum (300 MHz, $CDCl_3$) of 3,3,3-trifluoro-1-(furan-2-yl)-2-hydroxy-2-(4-methoxyphenyl)propan-1-one (**3c**).



Sample Name: AOG 223 CKI
Data file: D:\BERT\AOG\223CKIAS.D
Sample Info: Laufmittel: n-Heptan/IP 9:1;
Die Probe ist im LM gelöst

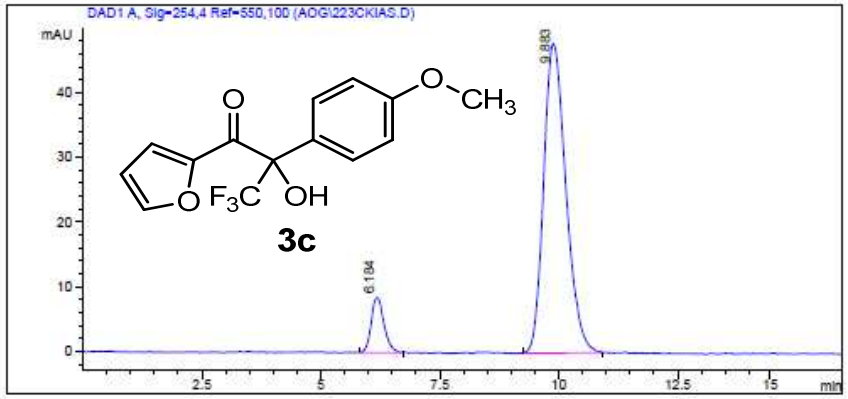
Agilent Technologies

Säule: DAICELAS.M
Säuleninfo: (250x4,6)mm

Operator: Analytik Labor AKEN

Injektion Time: 10:04:58
Injektion Date: 18.05.2010

Instrument Conditions:	At Start	At Stop
Temperature in °C:	30.0	30.0
Pressure in bar:	45.8	45.8
Flow in ml/min:	1.5	1.5



#	Ret. Time (min)	Width	Height (mAU)	Area (mAU*s)	Area %
1	6.18	0.28	8.51	160.11	9.32
2	9.88	0.47	47.87	1556.93	90.68
Total				1717.03	100.00

Figure S11 HPLC chromatogram of **3c**; comparison of racemic and non-racemic (left); non-racemic (right).

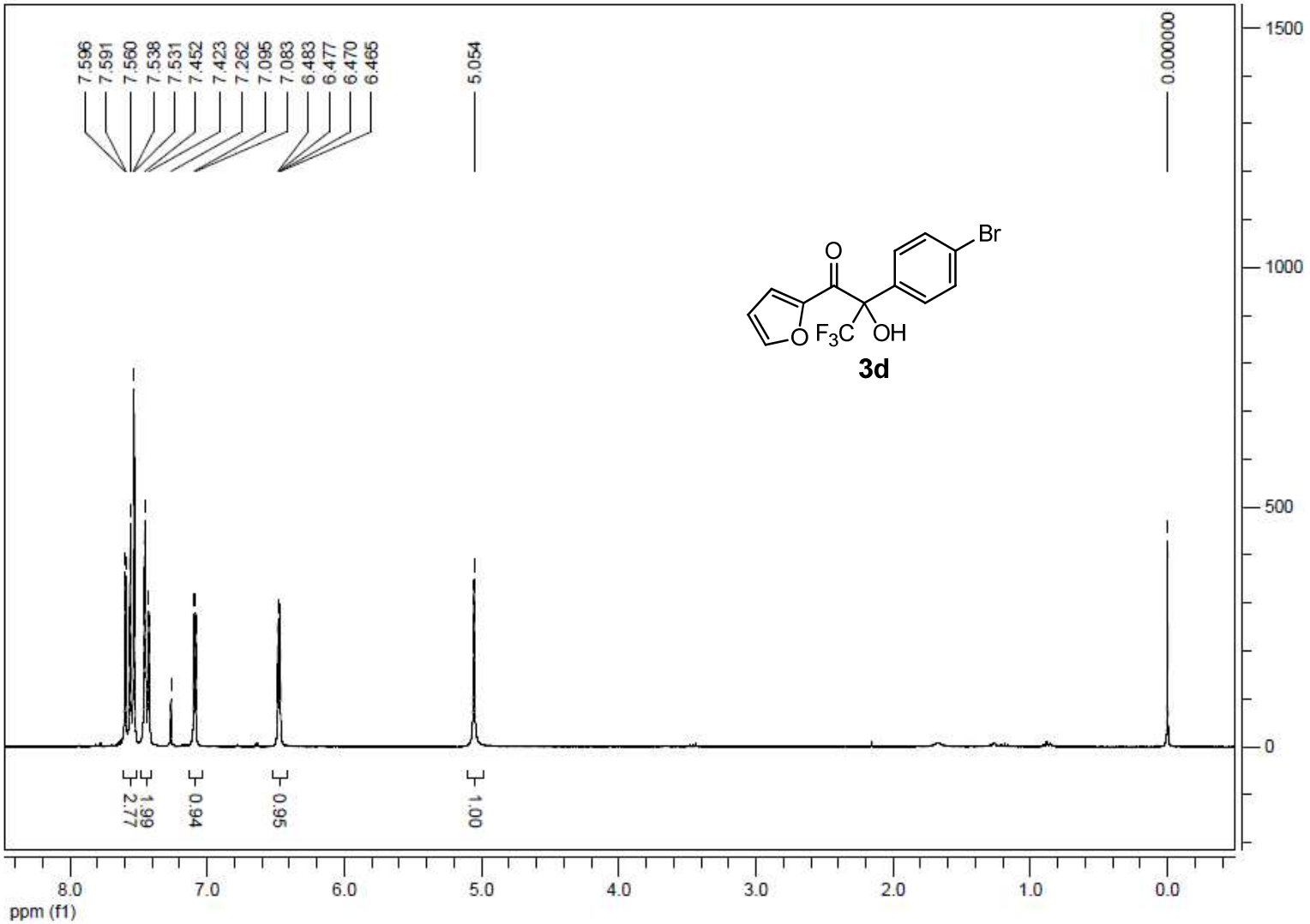


Figure S12 ^{1}H-NMR spectrum (300 MHz, $CDCl_3$) of 2-(4-bromophenyl)-3,3,3-trifluoro-1-(furan-2-yl)-2-hydroxypropan-1-one (**3d**).

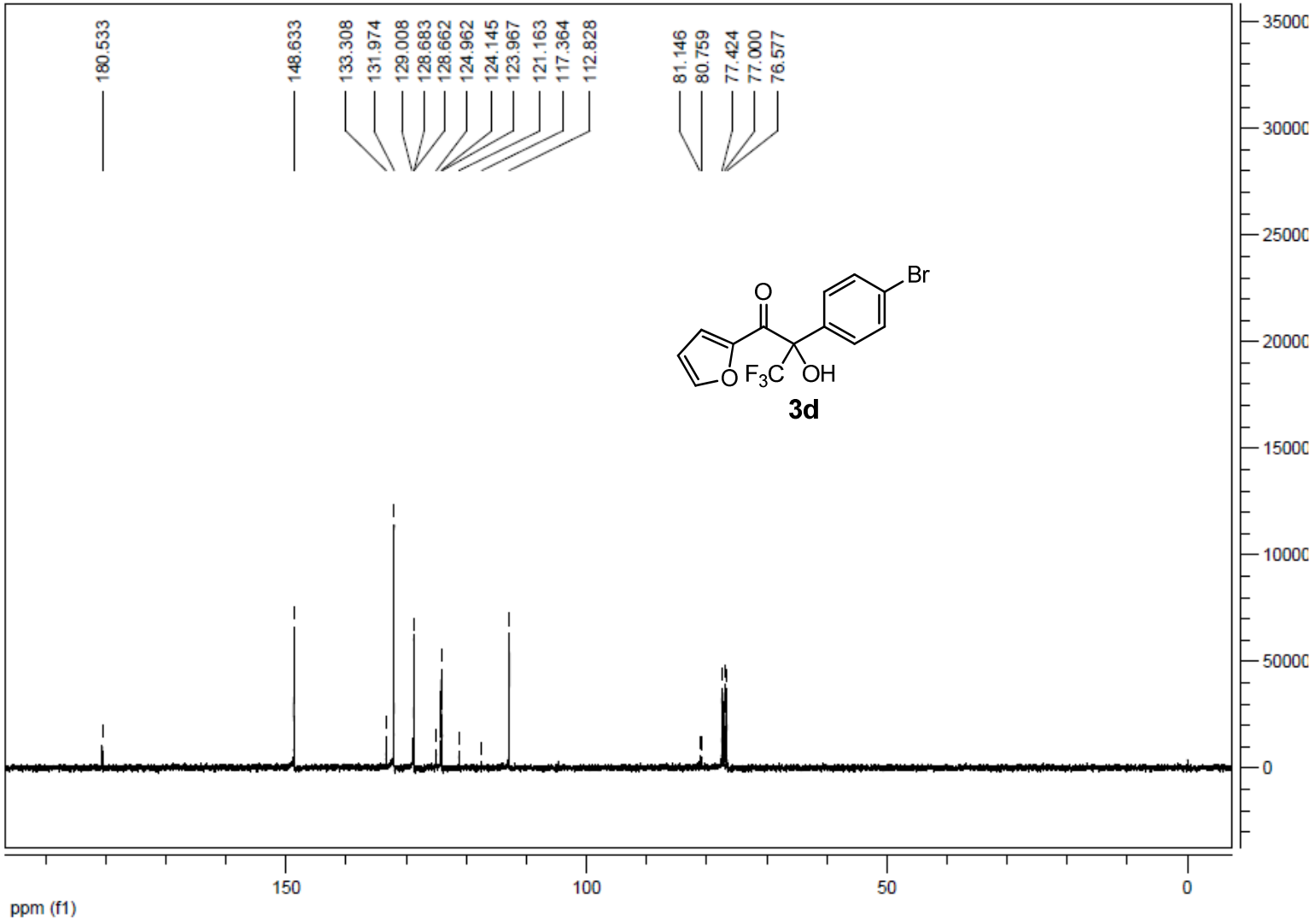
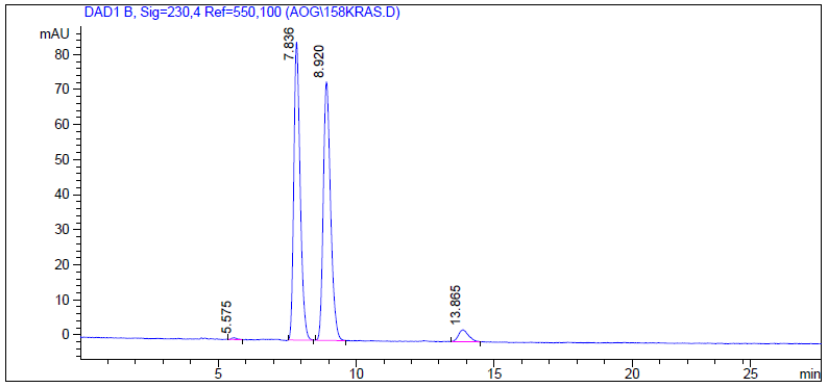


Figure S13 ^{13}C-NMR spectrum (300 MHz, $CDCl_3$) of 2-(4-bromophenyl)-3,3,3-trifluoro-1-(furan-2-yl)-2-hydroxypropan-1-one (**3d**).



Sample Name: AOG 191 K
Data file: D:\BERT\AOG\191KAS.D
Sample Info: Laufmittel: n-Heptan/EtOH 9:1;
Die Probe ist in DCM/LM gelöst

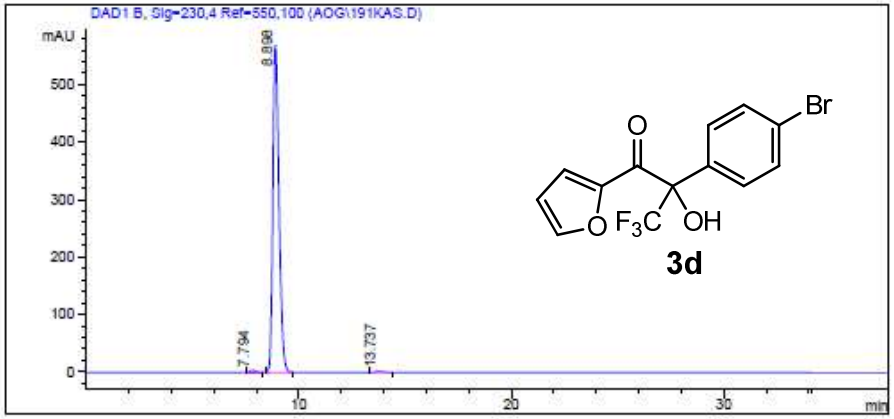
Agilent Technologies

Säule: DAICELAS.M
Säuleninfo: (250x4,6)mm

Operator: Analytik Labor AKEN

Injektion Time: 12:43:45
Injektion Date: 16.04.2010

Instrument Conditions:	At Start	At Stop
Temperature in°C:	30.0	30.0
Pressure in bar:	21.0	20.6
Flow in ml/min:	0.7	0.7



#	Ret. Time (min)	Width	Height (mAU)	Area (mAU*s)	Area %
1	7.79	0.23	3.99	69.73	0.60
2	8.90	0.31	569.43	11403.73	98.94
3	13.74	0.33	1.91	52.03	0.45
Total				11525.49	100.00

Figure S14 HPLC chromatogram of **3d**; comparison of racemic and non-racemic (left); non-racemic (right).

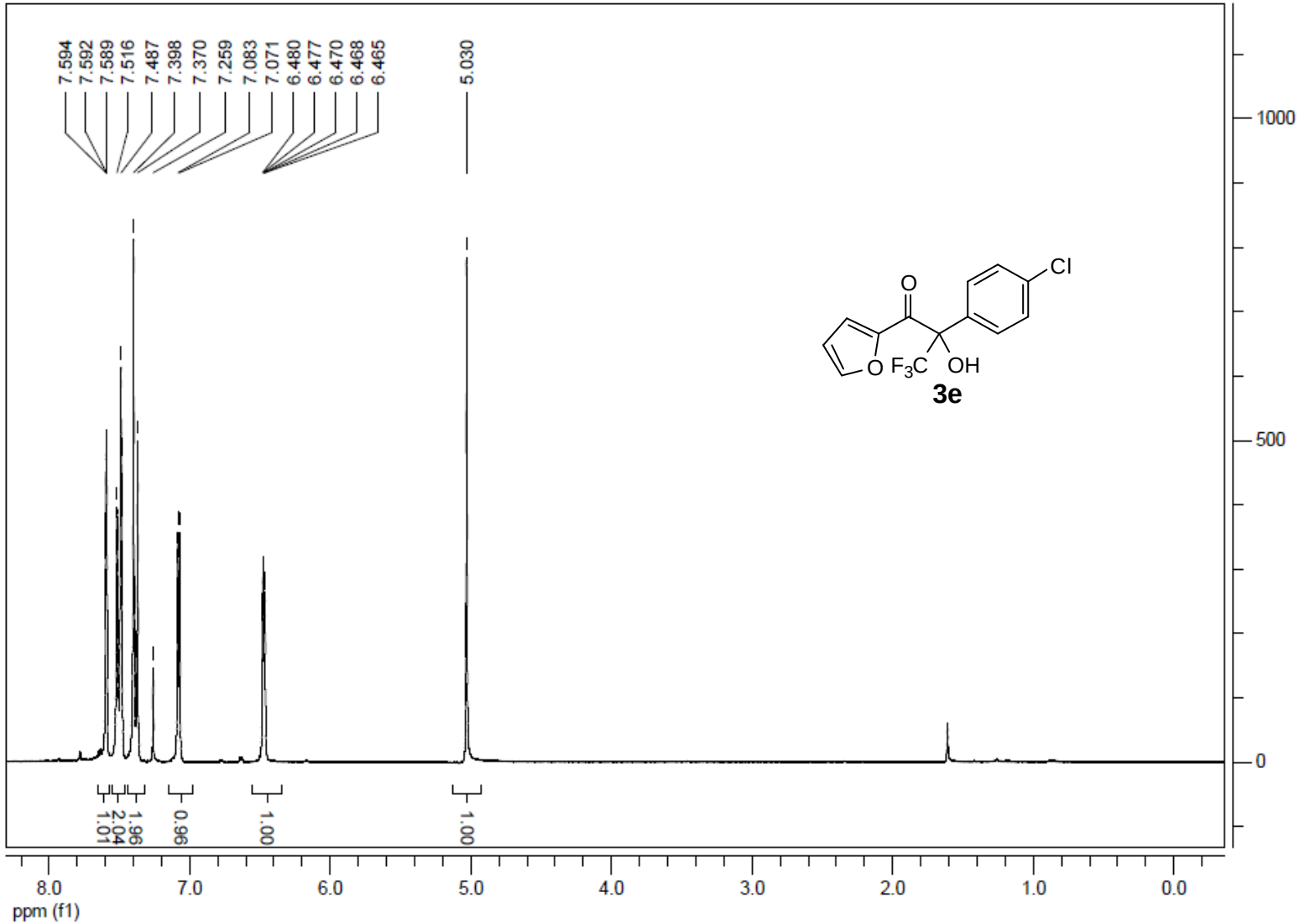


Figure S15 ^{1}H-NMR spectrum (300 MHz, $CDCl_3$) of 2-(4-chlorophenyl)-3,3,3-trifluoro-1-(furan-2-yl)-2-hydroxypropan-1-one (**3e**).

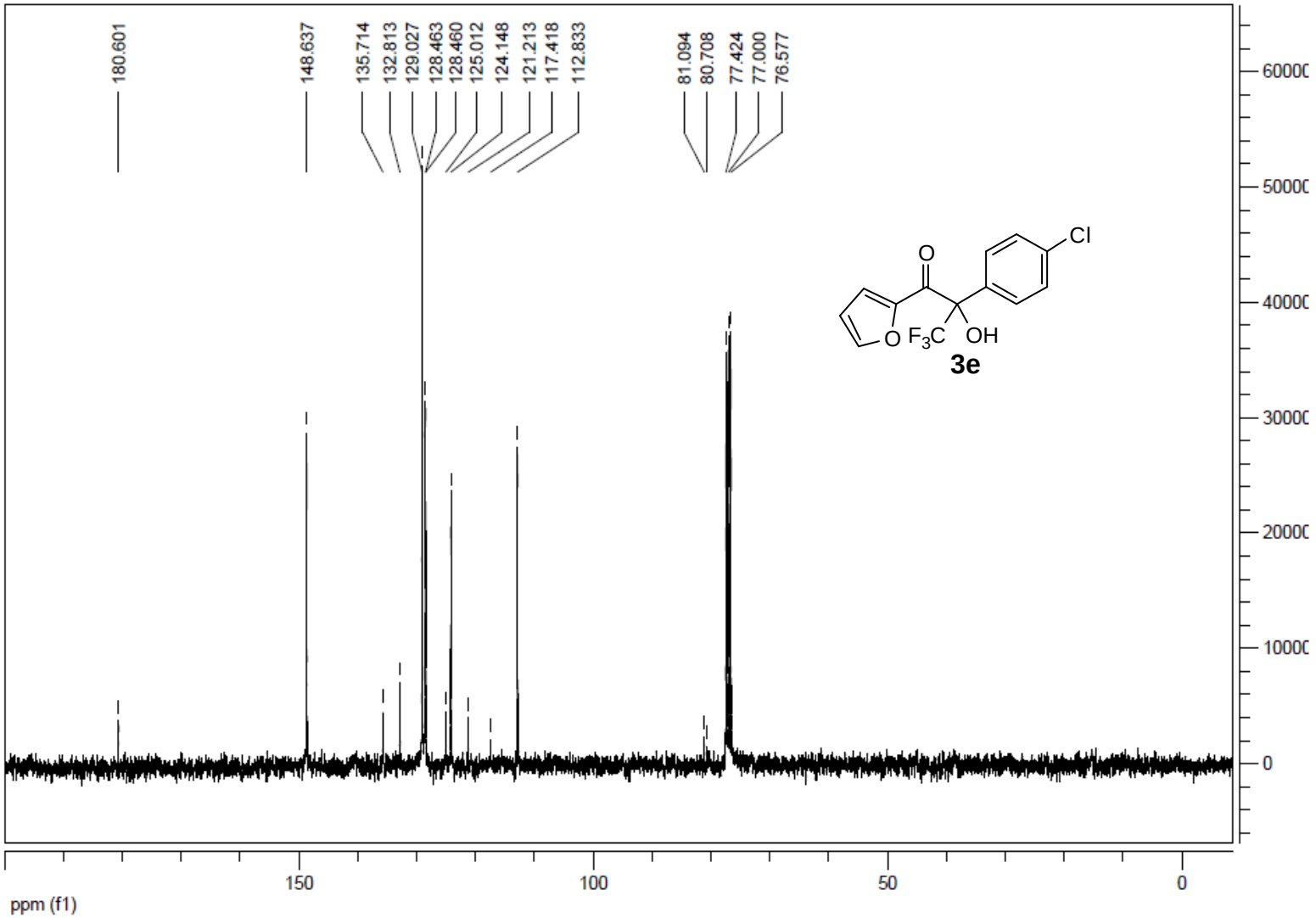
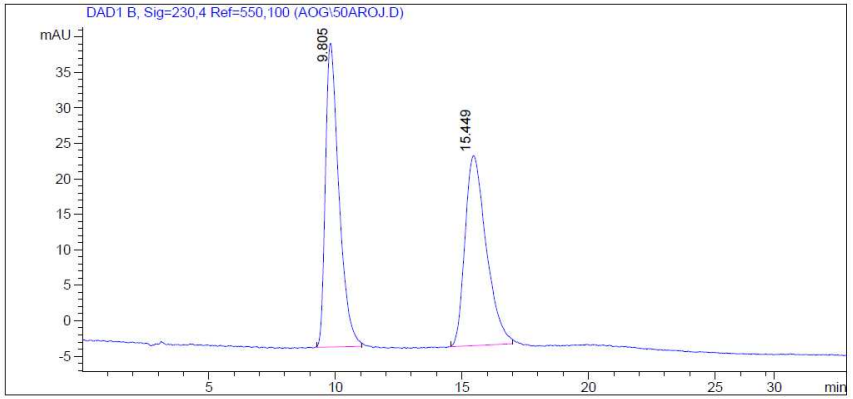
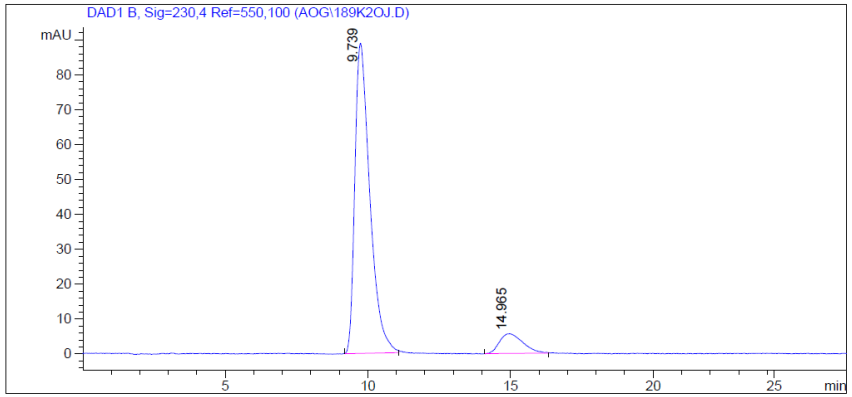


Figure S16 ^{13}C-NMR spectrum (300 MHz, $CDCl_3$) of 2-(4- chlorophenyl)-3,3,3-trifluoro-1-(furan-2-yl)-2-hydroxypropan-1-one (**3e**).





Sample Name: AOG 189 K2
Data file: D:\BERT\AOG\189K2OJ.D
Sample Info: Laufmittel: n-Heptan/IP 9:1;
Die Probe ist im LM/DCM gelöst

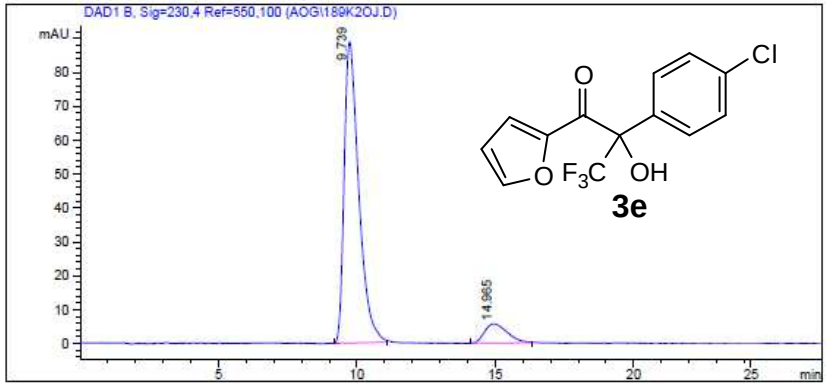
Agilent Technologies

Säule: DAICELOJ.M
Säuleninfo: (250x4,6)mm

Operator: Analytik Labor AKEN

Injektion Time: 14:42:55
Injektion Date: 11.05.2010

Instrument Conditions:	At Start	At Stop
Temperature in°C:	30.0	30.0
Pressure in bar:	38.9	38.2
Flow in ml/min:	1.0	1.0



#	Ret. Time (min)	Width	Height (mAU)	Area (mAU*s)	Area %
1	9.74	0.51	88.96	3247.43	90.90
2	14.97	0.68	5.67	325.23	9.10
Total				3572.65	100.00

Figure S17 HPLC chromatogram of **3e**; comparison of racemic and non-racemic (left); non-racemic (right).

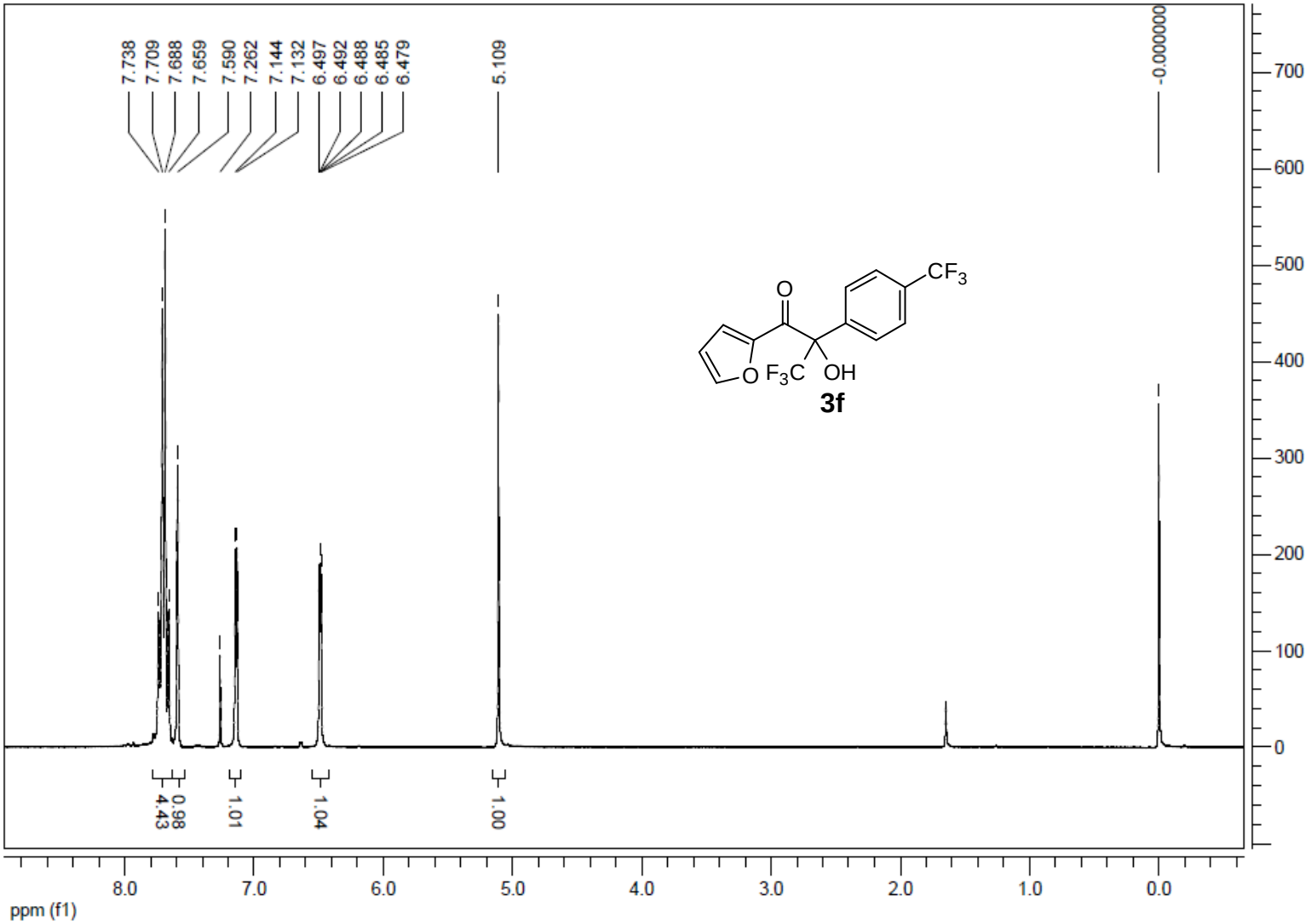


Figure S18 ^{1}H-NMR spectrum (300 MHz, $CDCl_3$) of 3,3,3-trifluoro-1-(furan-2-yl)-2-hydroxy-2-(4-(trifluoromethyl)phenyl)propan-1-one (**3f**).

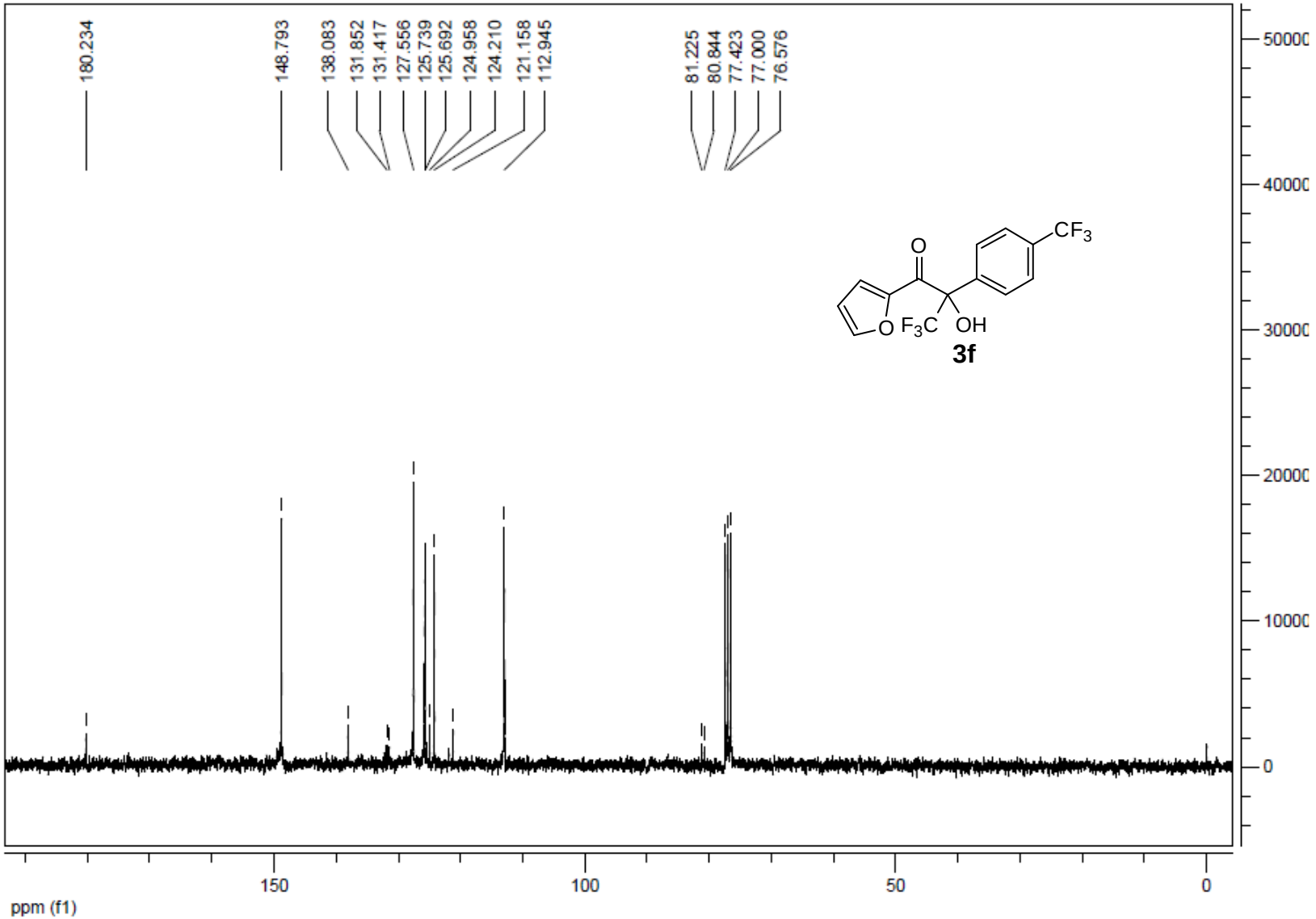
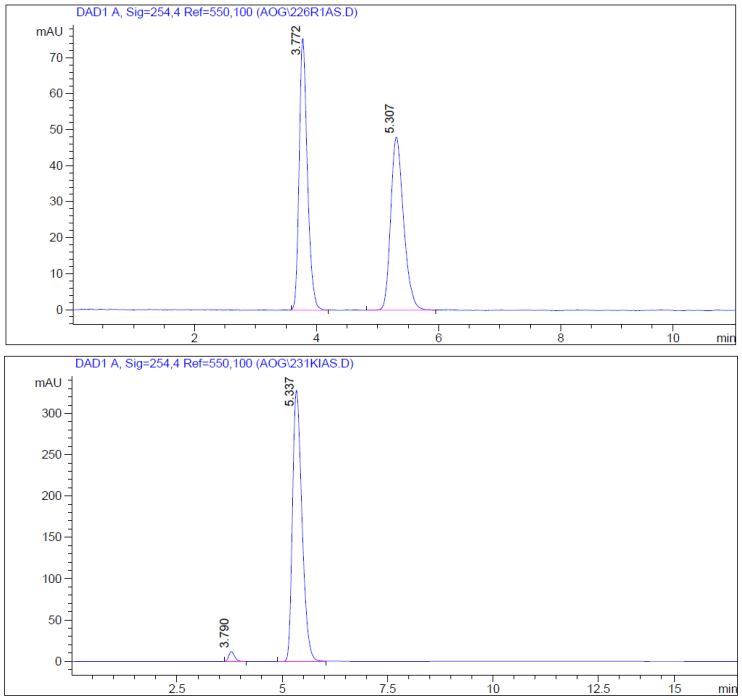


Figure S19 ^{13}C-NMR spectrum (300 MHz, $CDCl_3$) of 3,3,3-trifluoro-1-(furan-2-yl)-2-hydroxy-2-(4-(trifluoromethyl)phenyl)propan-1-one (**3f**).



Sample Name: AOG 231 KI
Data file: D:\BERT\AOG\231KIAS.D
Sample Info: Laufmittel: n-Heptan/IP 9:1;
Die Probe ist im DCM/LM gelöst

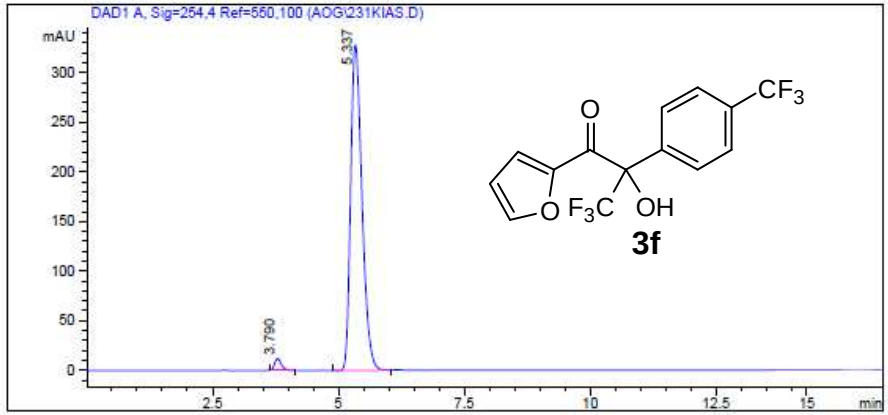
Agilent Technologies

Säule: DAICELAS.M
Säuleninfo: (250x4,6)mm

Operator: Analytik Labor AKEN

Injektion Time: 14:30:46
Injektion Date: 20.05.2010

Instrument Conditions:	At Start	At Stop
Temperature in°C:	30.0	30.0
Pressure in bar:	38.7	38.8
Flow in ml/min:	1.3	1.3



#	Ret. Time (min)	Width	Height (mAU)	Area (mAU*s)	Area %
1	3.79	0.15	12.16	116.19	2.21
2	5.34	0.24	328.55	5133.65	97.79
Total				5249.84	100.00

Figure S20 HPLC chromatogram of **3f**; comparison of racemic and non-racemic (left); non-racemic (right).

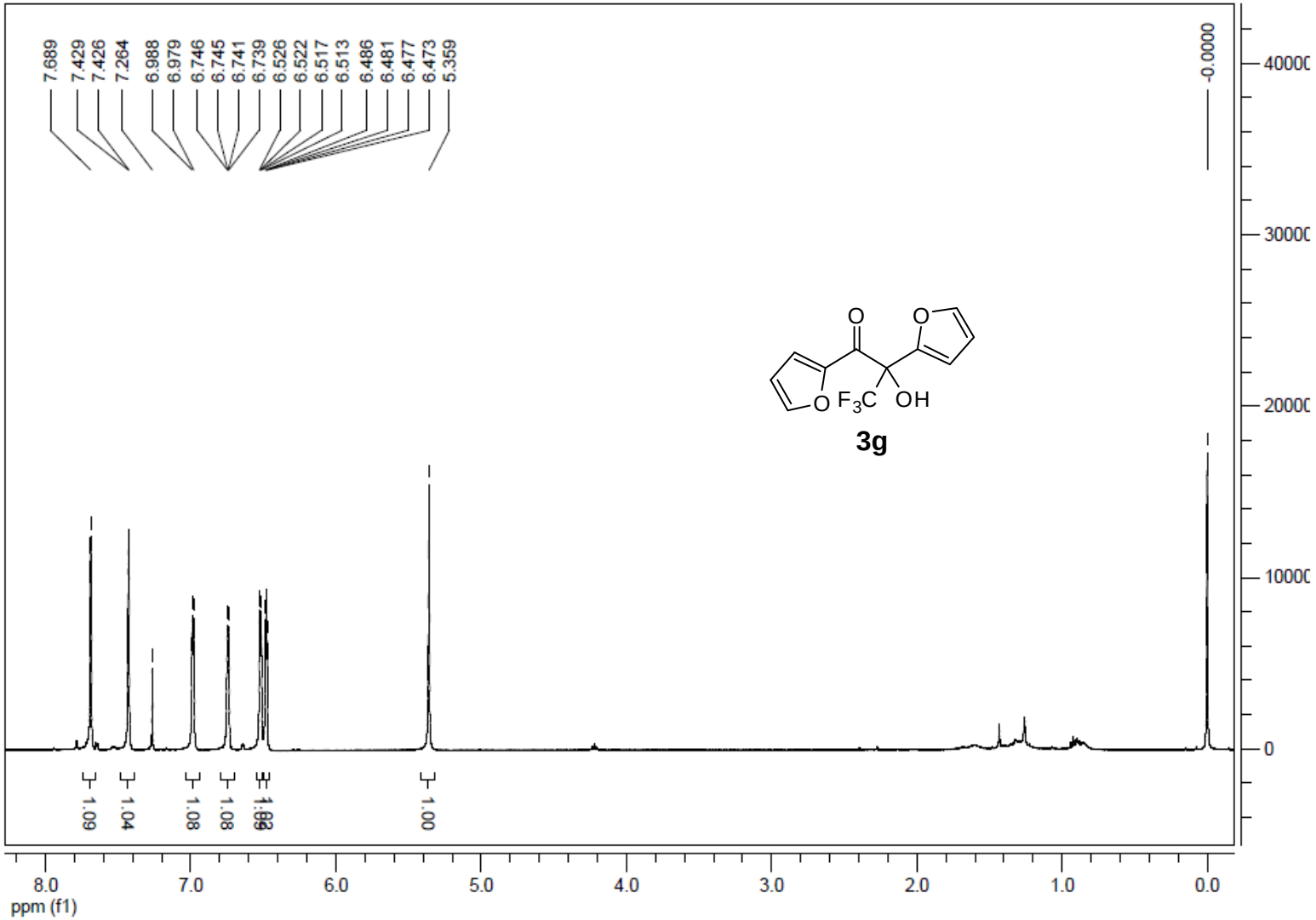


Figure S21 ^{1}H-NMR spectrum (400 MHz, $CDCl_3$) of 3,3,3-Trifluoro-1,2-di(furan-2-yl)-2-hydroxypropan-1-one (**3g**).

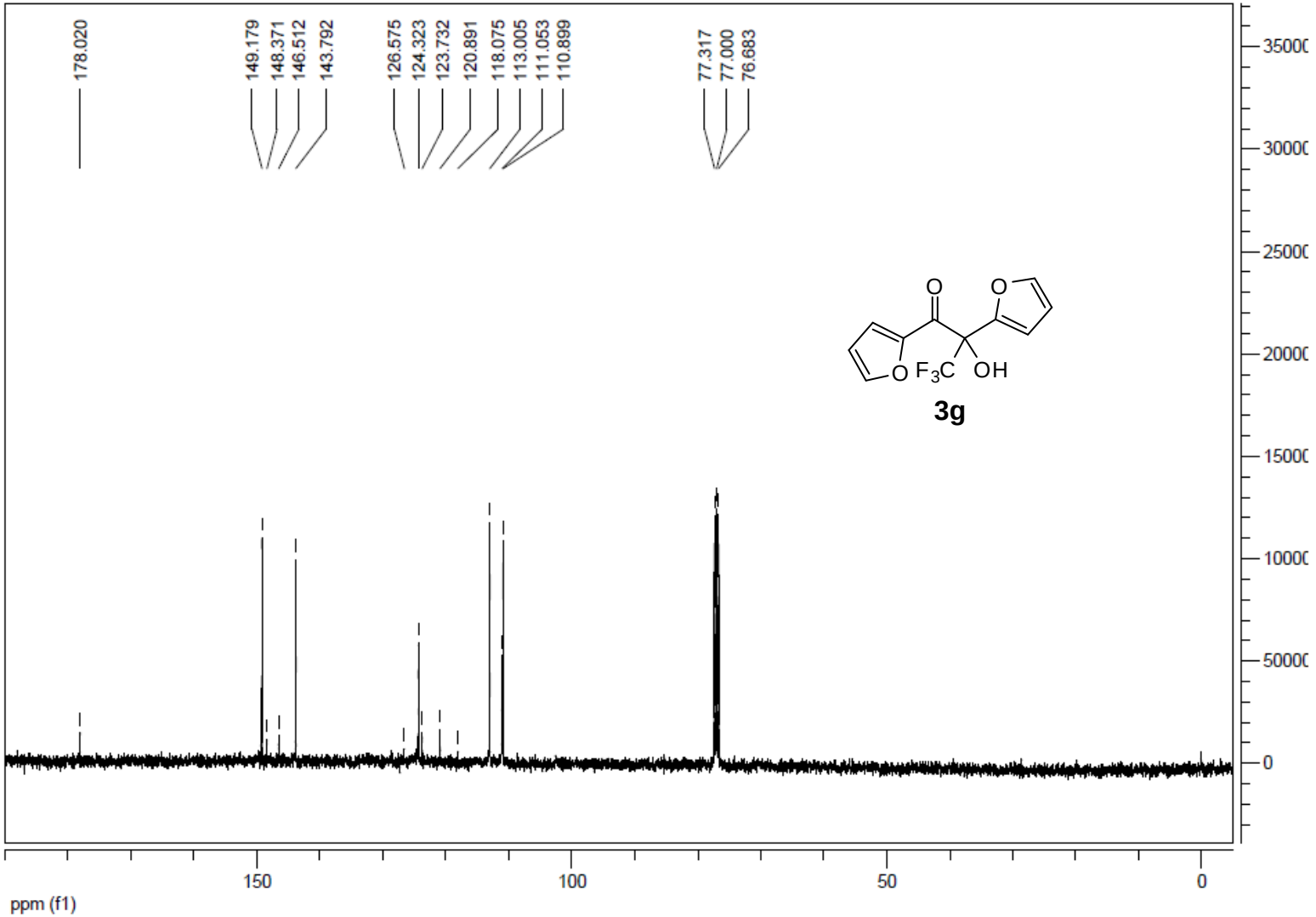
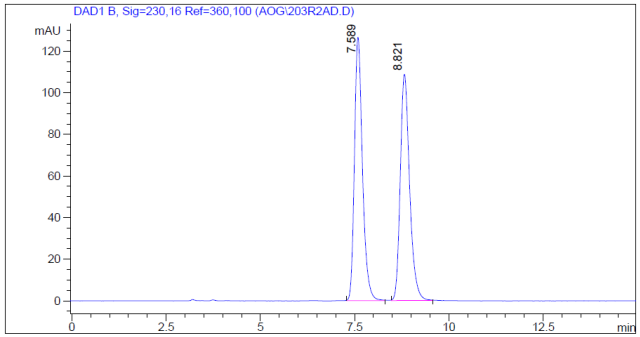


Figure S22 ^{13}C-NMR spectrum (400 MHz, $CDCl_3$) of 3,3,3-Trifluoro-1,2-di(furan-2-yl)-2-hydroxypropan-1-one (**3g**).

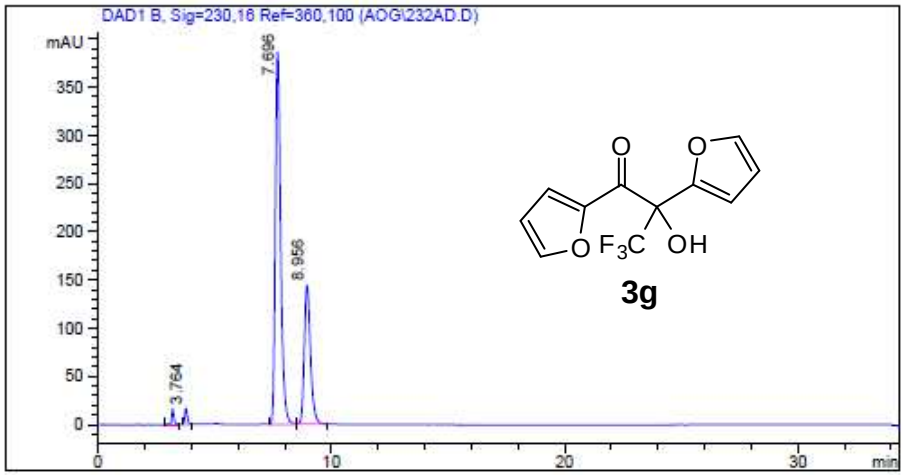



```
Sample Name:          AOG 232
Data file:            D:\GONZO\AOG\232AD.D
Sample Info:          Laufmittel: n-Heptan/IP 9:1;
                      Die Probe ist im LM gelöst

Säule:                DAICELAD.M
Säuleninfo:           (250x4,6)mm
Operator:             Analytik Labor AKEN

Injektion Time:       12:52:22
Injektion Date:       19.05.2010

Instrument Conditions:   At Start          At Stop
Temperature in°C:          30.0°C           30.0°C
Pressure in bar:           31.5             32.0
Flow in ml/min:            1.0              1.0
```



#	Ret. Time (min)	Width	Height (mAU)	Area (mAU*s)	Area %
1	3.20	0.10	16.59	115.55	1.28
2	3.76	0.12	16.81	132.13	1.46
3	7.70	0.24	386.31	6118.05	67.59
4	8.96	0.28	144.27	2686.17	29.68
Total				9051.89	100.00

Figure S23 HPLC chromatogram of **3g**; comparison of racemic and non-racemic (left); non-racemic (right).

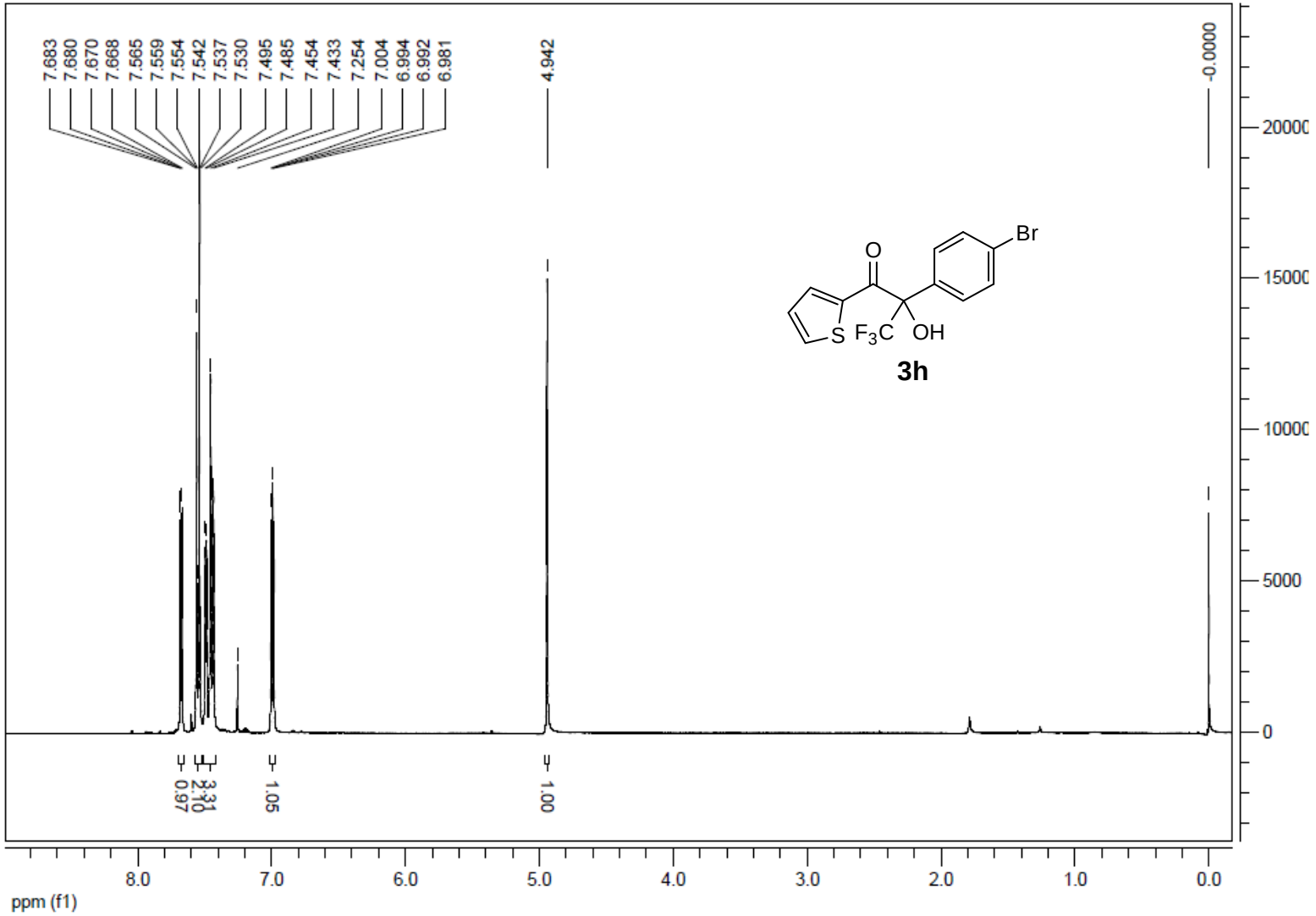


Figure S24 ^{1}H-NMR spectrum (400 MHz, $CDCl_3$) of 2-(4-bromophenyl)-3,3,3-trifluoro-2-hydroxy-1-(thiophen-2-yl)propan-1-one (**3h**).

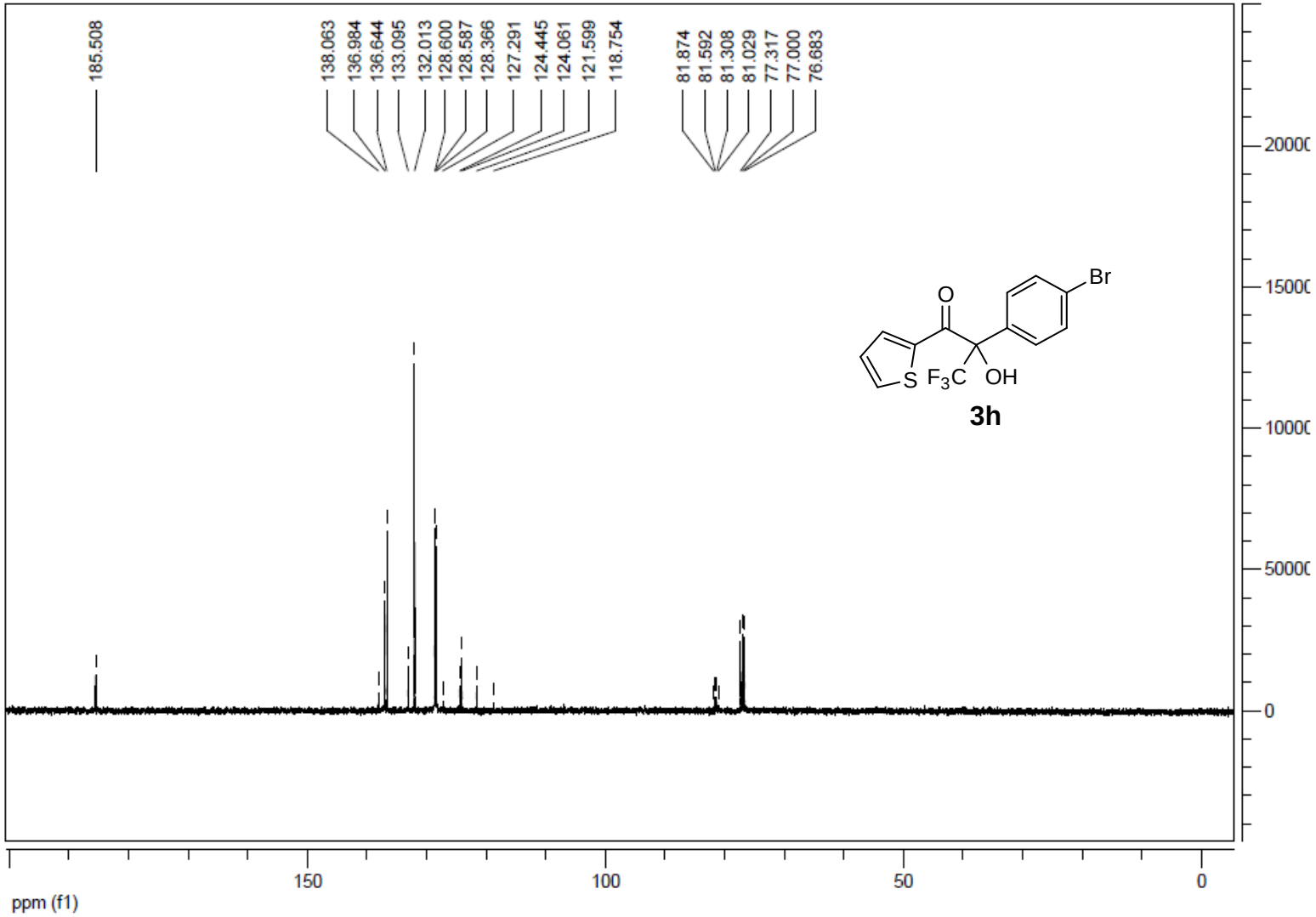
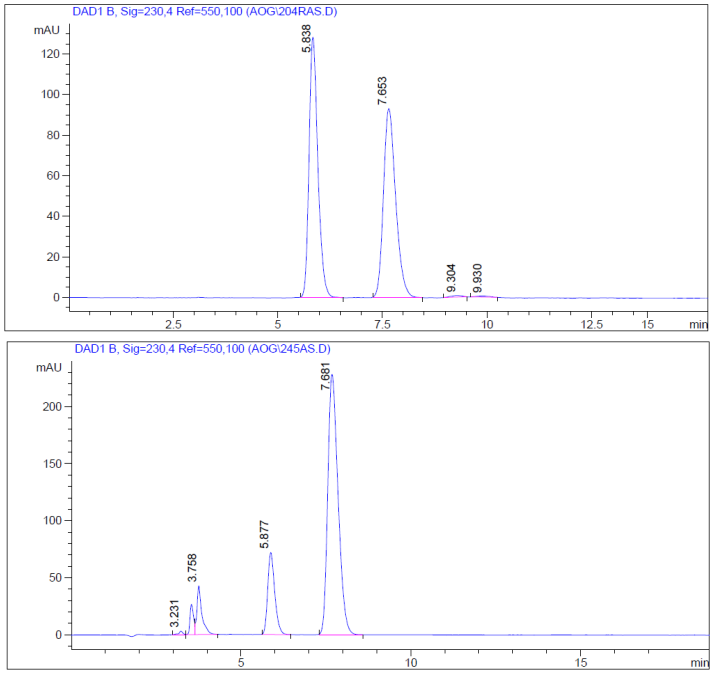


Figure S25 ^{13}C-NMR spectrum (400 MHz, $CDCl_3$) of 2-(4-bromophenyl)-3,3,3-trifluoro-2-hydroxy-1-(thiophen-2-yl)propan-1-one (**3h**).



Sample Name: AOG 245
Data file: D:\BERT\AOG\245AS.D
Sample Info: Laufmittel: n-Heptan/IP 9:1;
Die Probe ist im DCM/LM gelöst

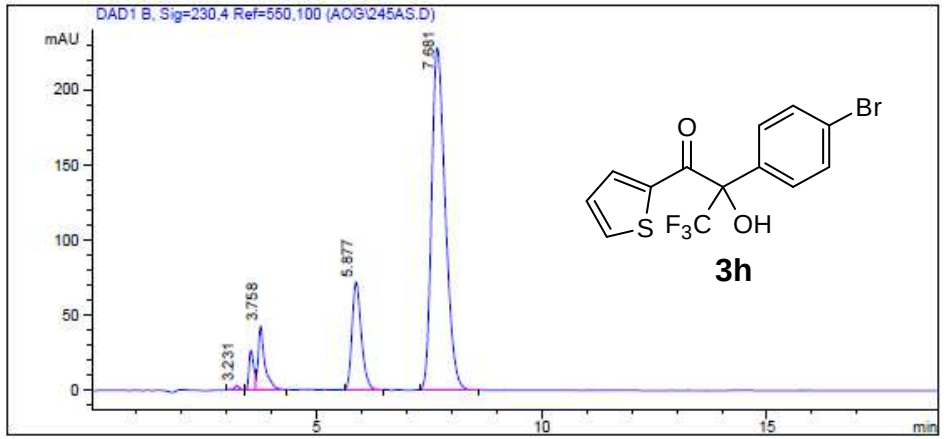
Agilent Technologies

Säule: DAICELAS.M
Säuleninfo: (250x4,6)mm

Operator: Analytik Labor AKEN

Injektion Time: 11:09:23
Injektion Date: 28.05.2010

Instrument Conditions:	At Start	At Stop
Temperature in°C:	30.0	30.0
Pressure in bar:	29.2	29.1
Flow in ml/min:	1.0	1.0



#	Ret. Time (min)	Width	Height (mAU)	Area (mAU*s)	Area %
1	3.23	0.12	3.12	24.53	0.38
2	3.54	0.11	26.64	193.95	2.98
3	3.76	0.15	42.87	436.51	6.70
4	5.88	0.22	72.02	1036.91	15.93
5	7.68	0.32	228.26	4818.53	74.01
Total				6510.43	100.00

Figure S26 HPLC chromatogram of **3h**; comparison of racemic and non-racemic (left); non-racemic (right).

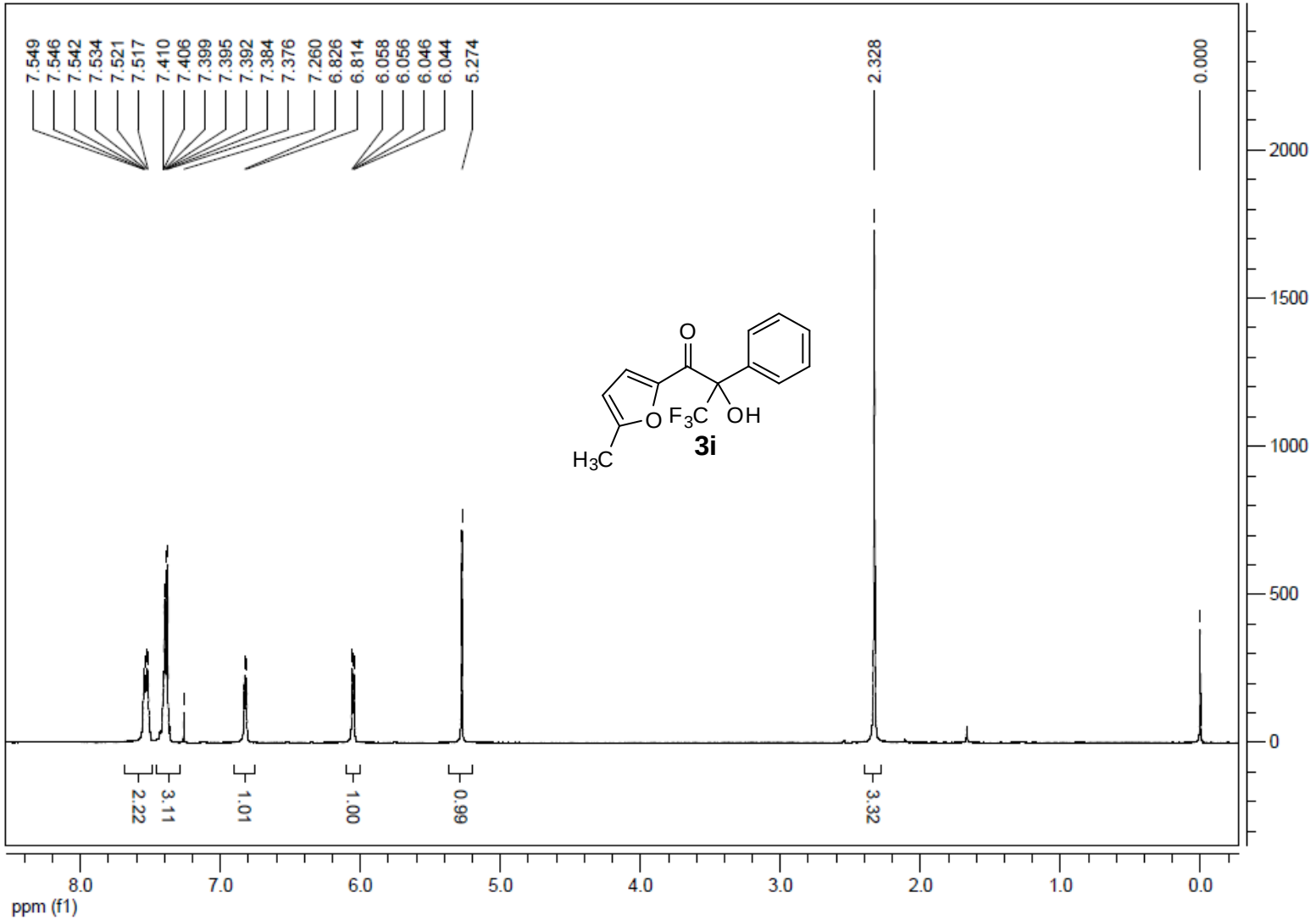


Figure S27 ^{1}H-NMR spectrum (300 MHz, $CDCl_3$) of 3,3,3-trifluoro-2-hydroxy-1-(5-methylfuran-2-yl)-2-phenylpropan-1-one (**3i**).

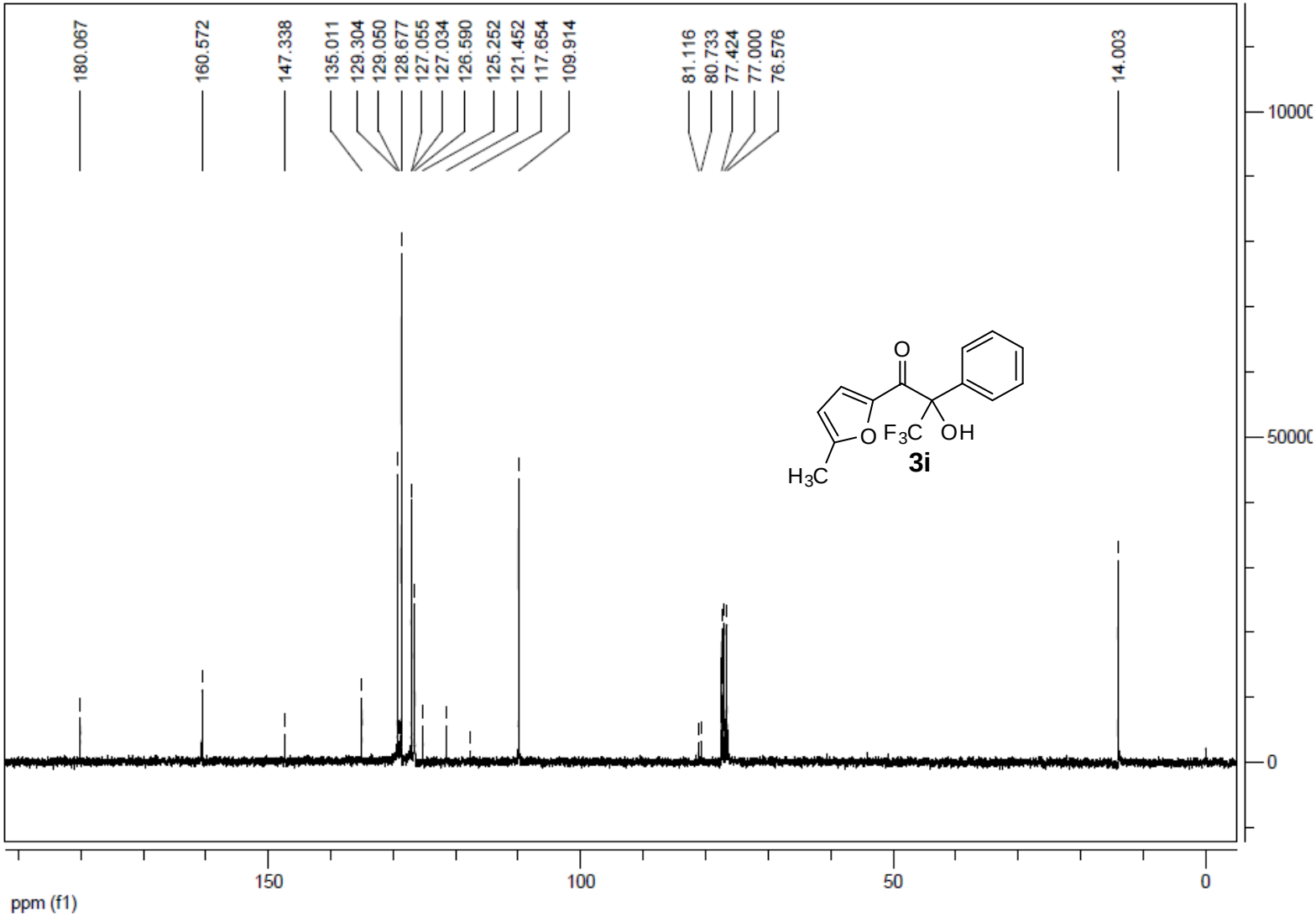
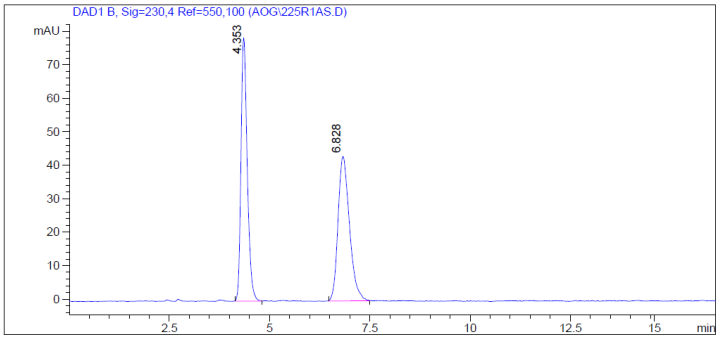
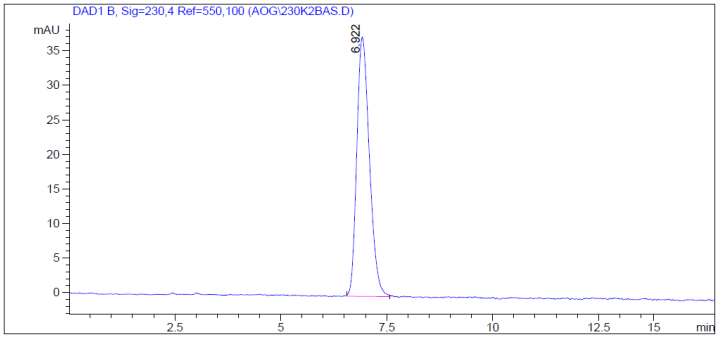


Figure S28 ^{13}C-NMR spectrum (300 MHz, $CDCl_3$) of 3,3,3-trifluoro-2-hydroxy-1-(5-methylfuran-2-yl)-2-phenylpropan-1-one (**3i**).





Sample Name: AOG 230 K2B
Data file: D:\BERT\AOG\230K2BAS.D
Sample Info: Laufmittel: n-Heptan/IP 9:1;
Die Probe ist im DCM/LM gelöst

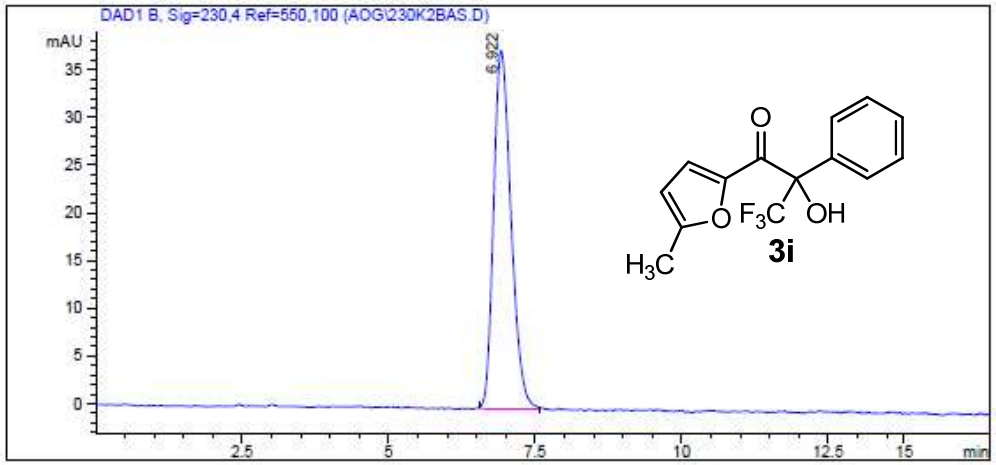
Agilent Technologies

Säule: DAICELAS.M
Säuleninfo: (250x4,6)mm

Operator: Analytik Labor AKEN

Injektion Time: 08:22:15
Injektion Date: 21.05.2010

Instrument Conditions:	At Start	At Stop
Temperature in°C:	30.0	30.0
Pressure in bar:	39.7	39.6
Flow in ml/min:	1.3	1.3



#	Ret. Time (min)	Width	Height (mAU)	Area (mAU*s)	Area %
1	6.92	0.31	37.57	777.50	100.00
Total				777.50	100.00

Figure S29 HPLC chromatogram of **3i** ; comparison of racemic and non-racemic (left); non-racemic (right).

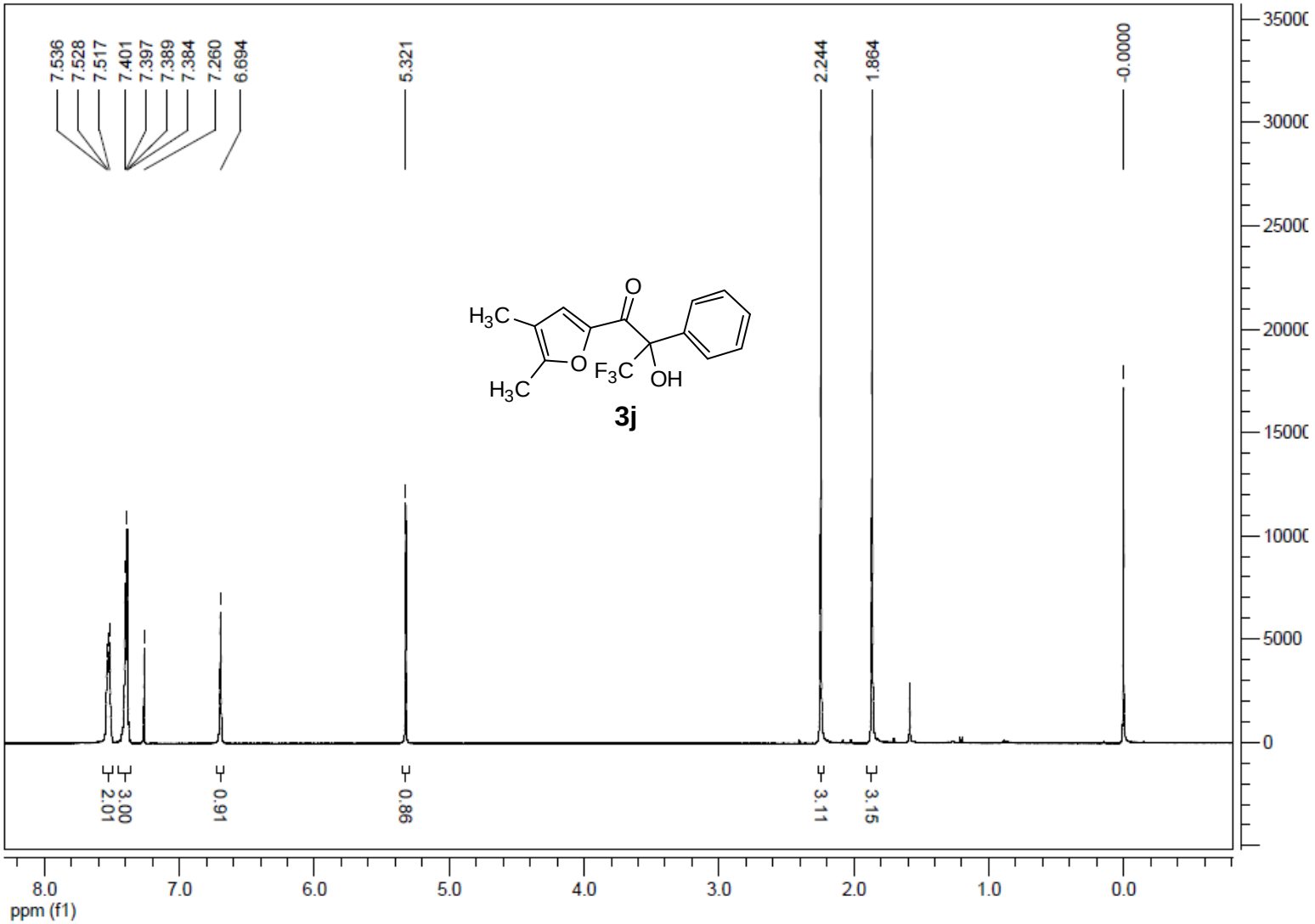


Figure S30 ^{1}H-NMR spectrum (400 MHz, $CDCl_3$) of 1-(4,5-dimethylfuran-2-yl)-3,3,3-trifluoro-2-hydroxy-2-phenylpropan-1-one (**3j**).

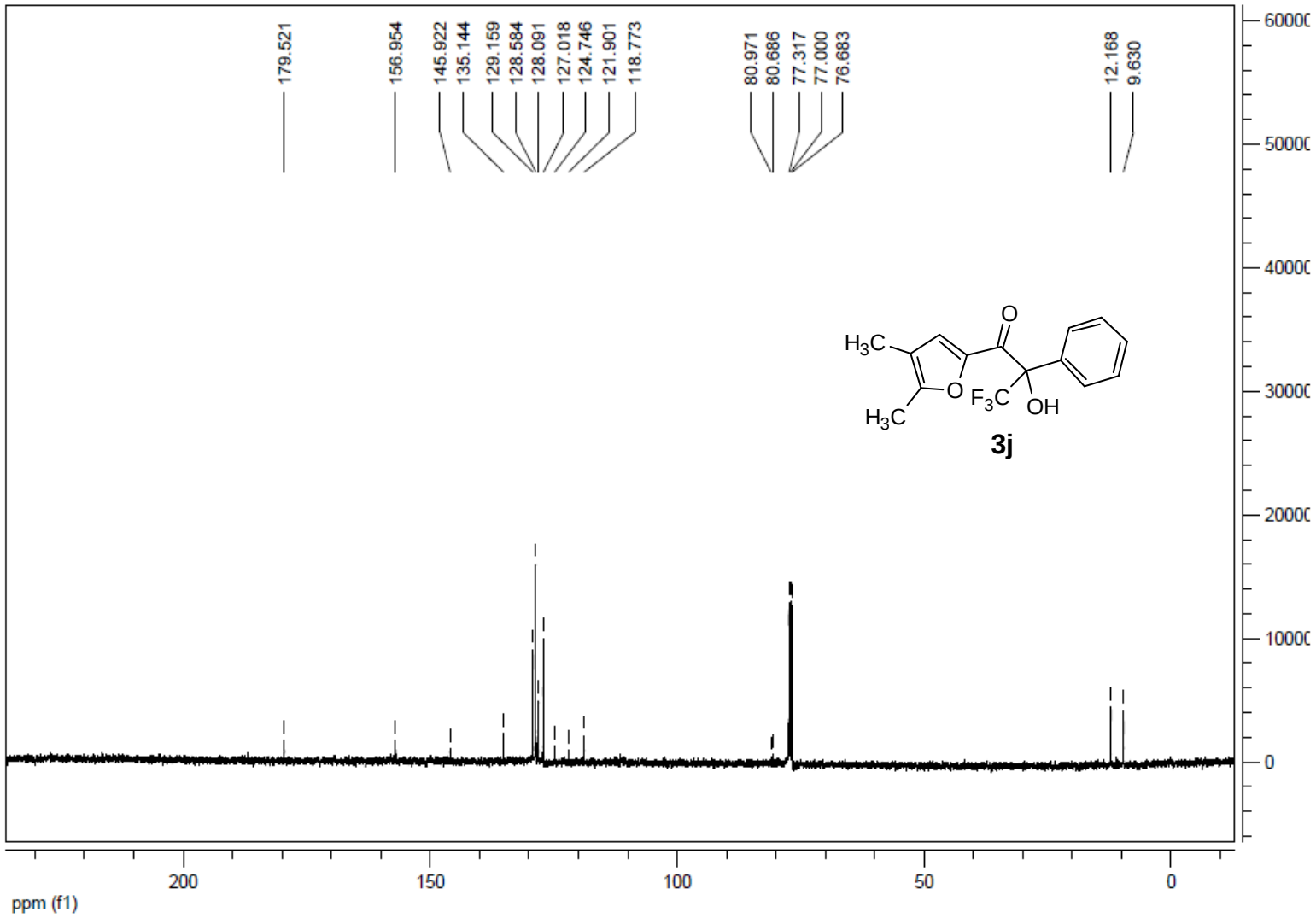
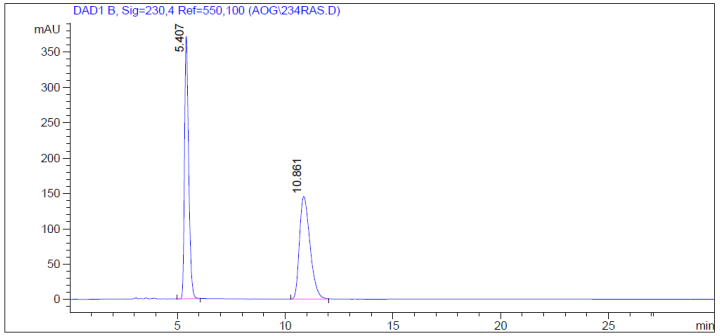


Figure S31 ^{13}C-NMR spectrum (400 MHz, $CDCl_3$) of 1-(4,5-dimethylfuran-2-yl)-3,3,3-trifluoro-2-hydroxy-2-phenylpropan-1-one (**3j**).



Sample Name: AOG 252
Data file: D:\BERT\AOG\252AS.D
Sample Info: Laufmittel: n-Heptan/IP 9:1;
Die Probe ist im DCM/LM gelöst

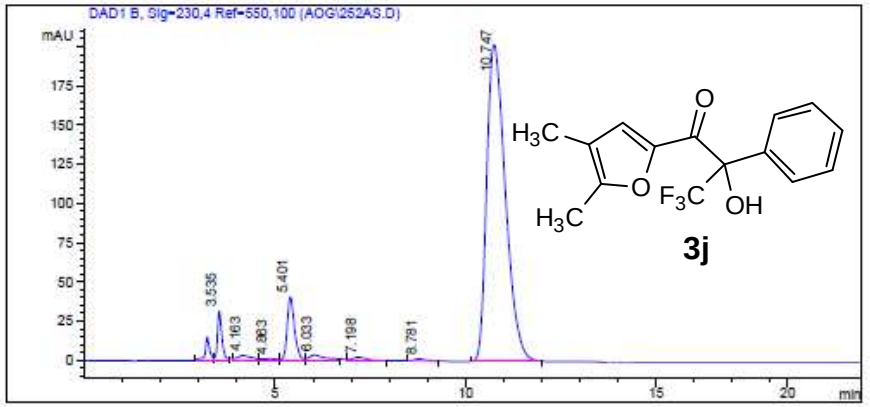
Agilent Technologies

Säule: DAICELAS.M
Säuleninfo: (250x4,6)mm

Operator: Analytik Labor AKEN

Injektion Time: 08:18:45
Injektion Date: 01.06.2010

Instrument Conditions:	At Start	At Stop
Temperature in°C:	30.0	30.0
Pressure in bar:	31.8	30.3
Flow in ml/min:	1.0	1.0



#	Ret. Time (min)	Width	Height (mAU)	Area (mAU*s)	Area %
1	3.22	0.12	15.07	126.98	1.55
2	3.54	0.12	31.73	264.20	3.23
3	4.16	0.36	3.35	94.56	1.16
4	4.86	0.33	1.41	38.63	0.47
5	5.40	0.20	40.56	549.27	6.72
6	6.03	0.42	3.69	120.98	1.48
7	7.20	0.36	2.37	64.66	0.79
8	8.78	0.23	1.39	27.03	0.33
9	10.75	0.51	202.03	6889.73	84.27
Total				8176.02	100.00

Figure S32 HPLC chromatogram of **3j**; comparison of racemic and non-racemic (left); non-racemic (right).

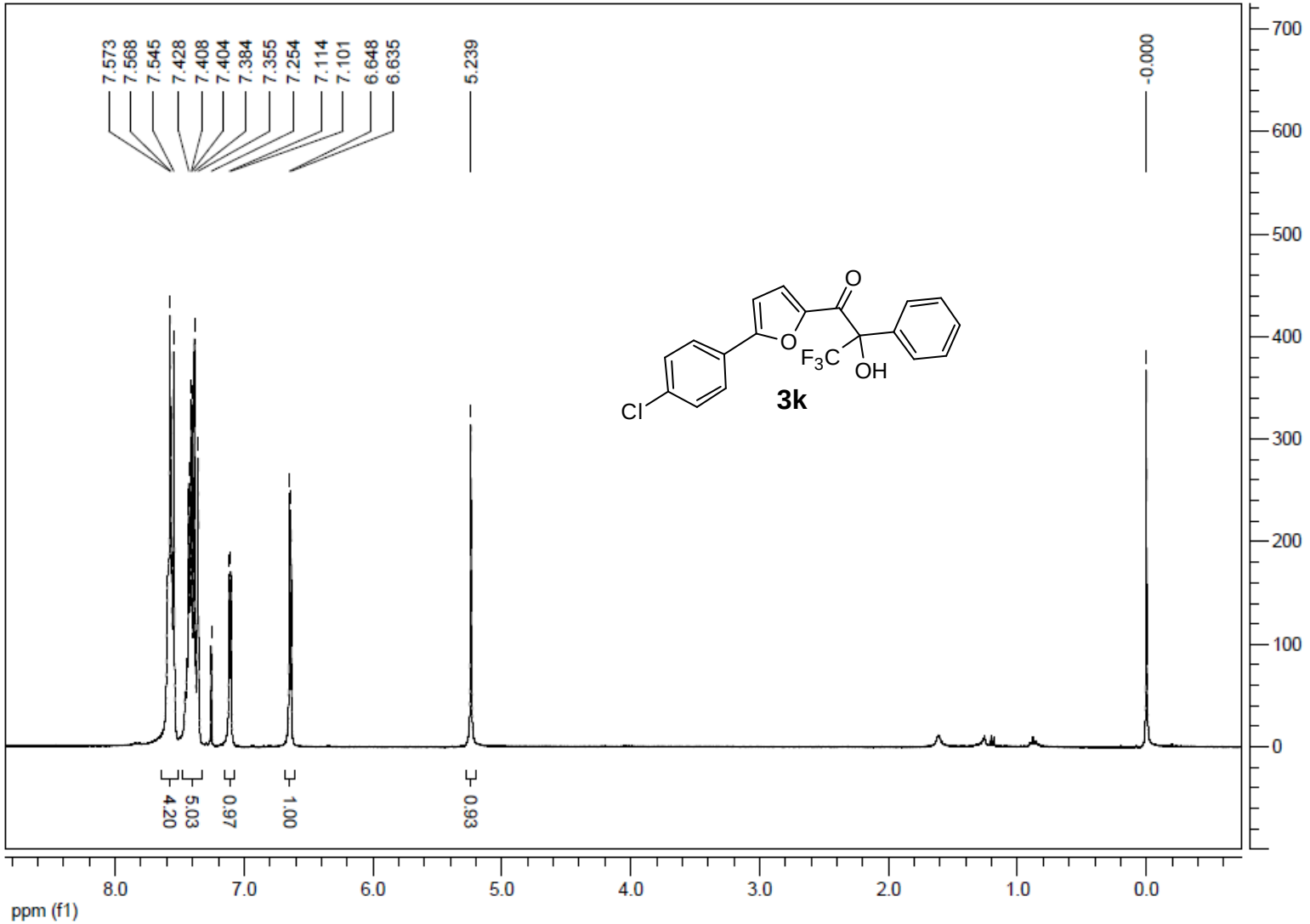


Figure S33 ^{1}H-NMR spectrum (300 MHz, $CDCl_3$) of 1-(5-(4-chlorophenyl)furan-2-yl)-3,3,3-trifluoro-2-hydroxy-2-phenylpropan-1-one (**3k**).

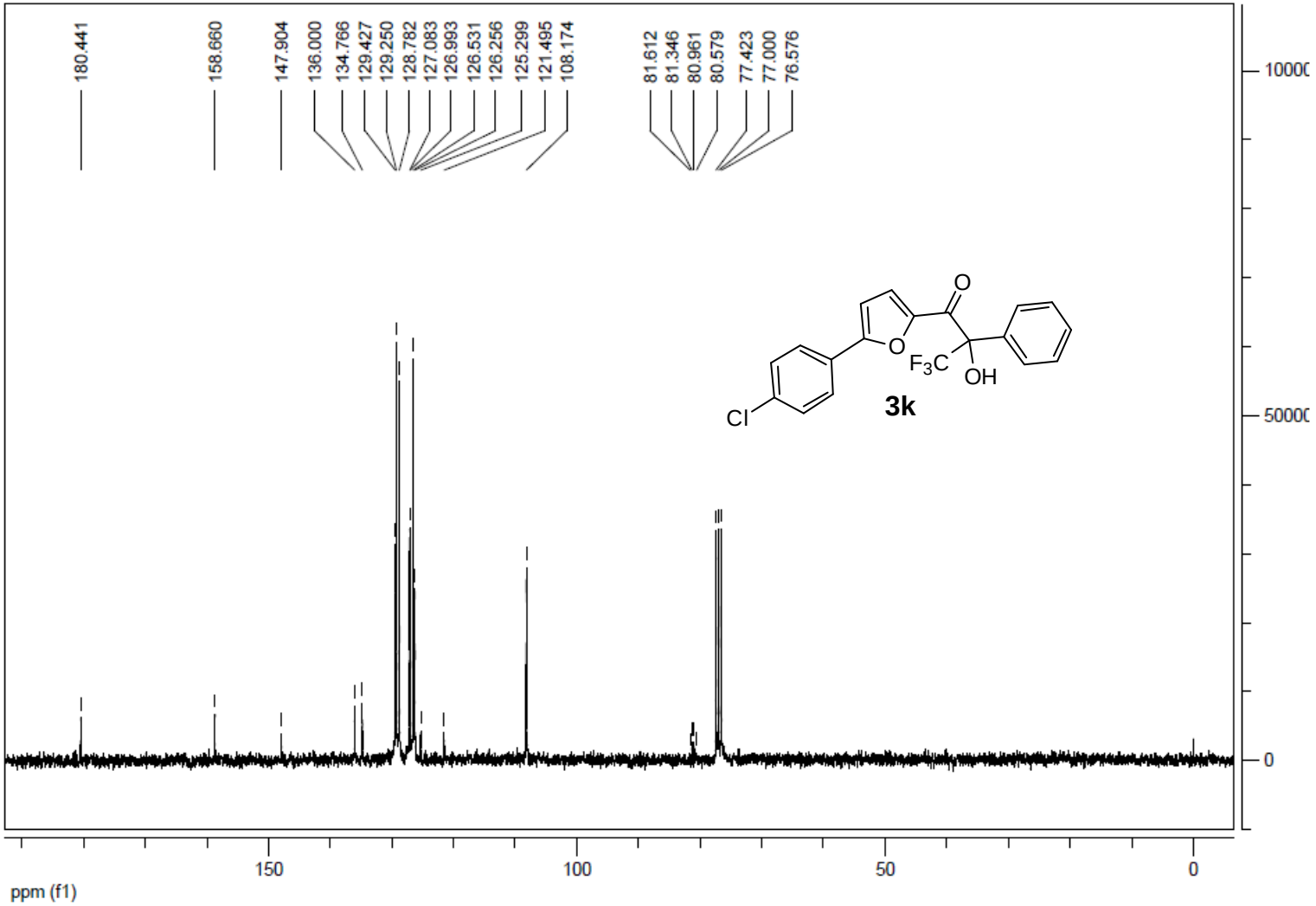
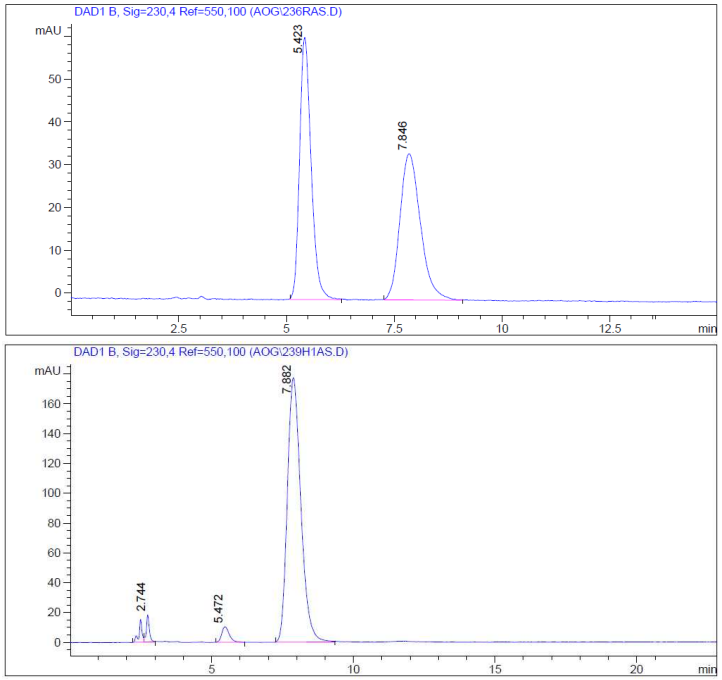


Figure S34 ^{13}C-NMR spectrum (300 MHz, $CDCl_3$) of 1-(5-(4-chlorophenyl)furan-2-yl)-3,3,3-trifluoro-2-hydroxy-2-phenylpropan-1-one (**3k**).



Sample Name: AOG 239 H1
Data file: D:\BERT\AOG\239H1AS.D
Sample Info: Laufmittel: n-Heptan/IP 9:1;
Die Probe ist im DCM/LM gelöst

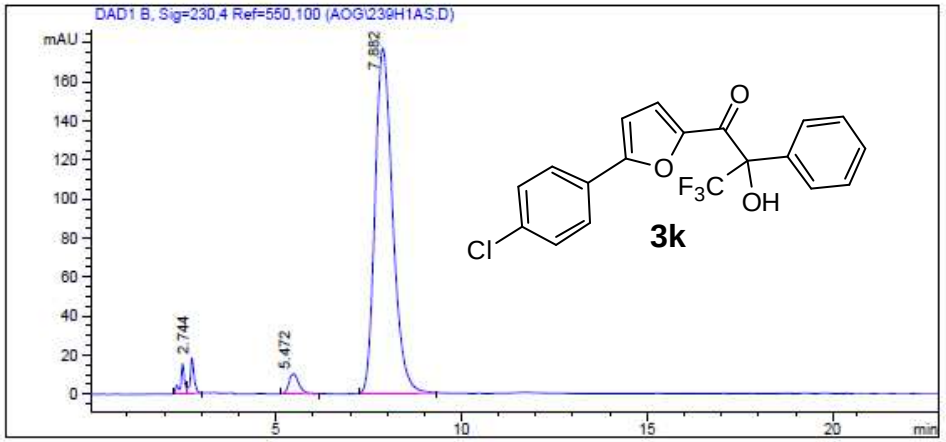
Agilent Technologies

Säule: DAICELAS.M
Säuleninfo: (250x4,6)mm

Operator: Analytik Labor AKEN

Injektion Time: 14:13:48
Injektion Date: 31.05.2010

Instrument Conditions:	At Start	At Stop
Temperature in°C:	30.0	30.0
Pressure in bar:	40.2	39.9
Flow in ml/min:	1.3	1.3



#	Ret. Time (min)	Width	Height (mAU)	Area (mAU*s)	Area %
1	2.49	0.11	15.30	114.66	1.81
2	2.74	0.11	18.25	134.00	2.12
3	5.47	0.29	10.39	194.23	3.07
4	7.88	0.51	177.26	5876.62	92.99
Total				6319.51	100.00

Figure S35 HPLC chromatogram of **3k**; comparison of racemic and non-racemic (left); non-racemic (right).

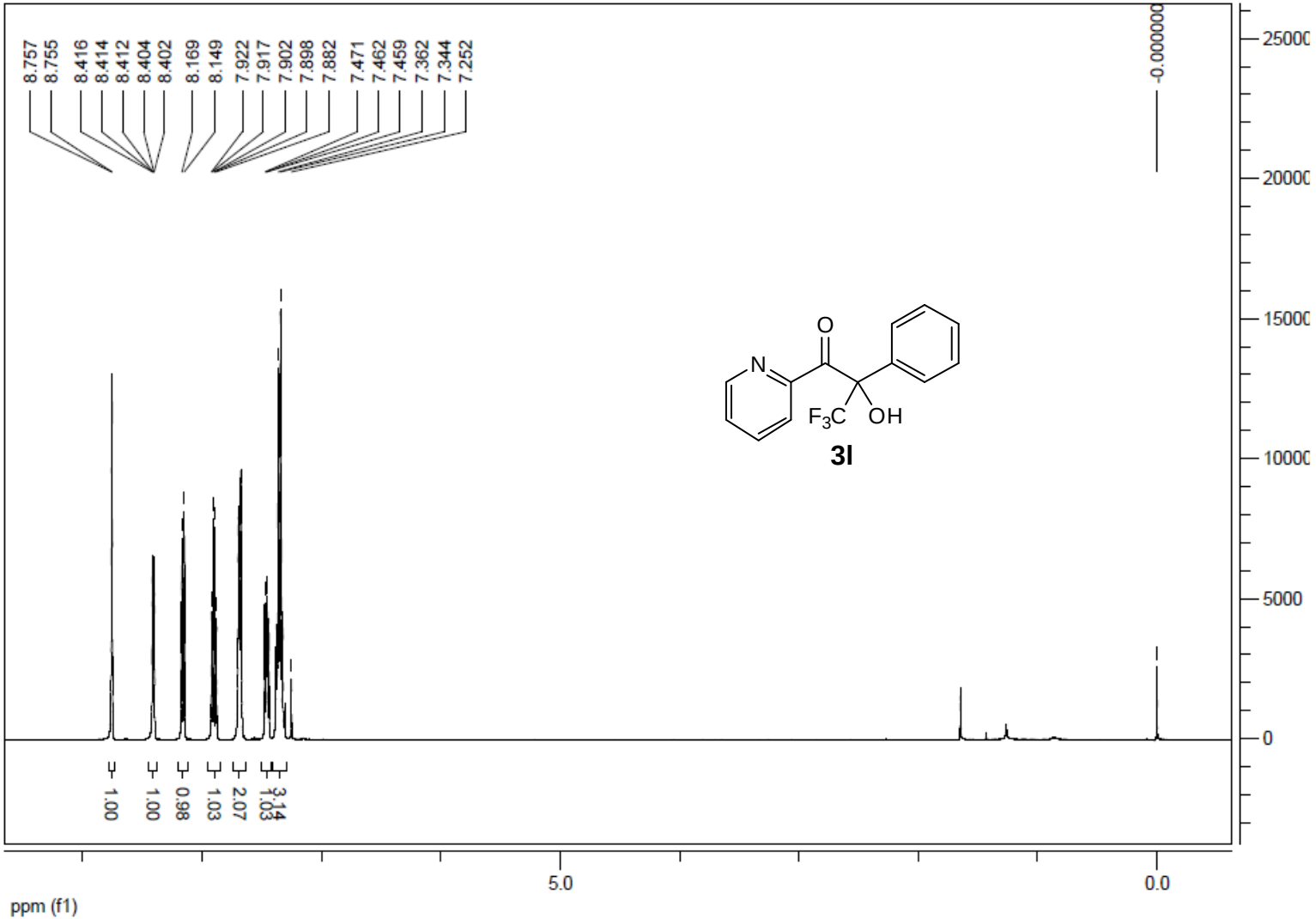


Figure S36 ^{1}H-NMR spectrum (400 MHz, $CDCl_3$) of 3,3,3-trifluoro-2-hydroxy-2-phenyl-1-(pyridin-2-yl)propan-1-one (**3l**).

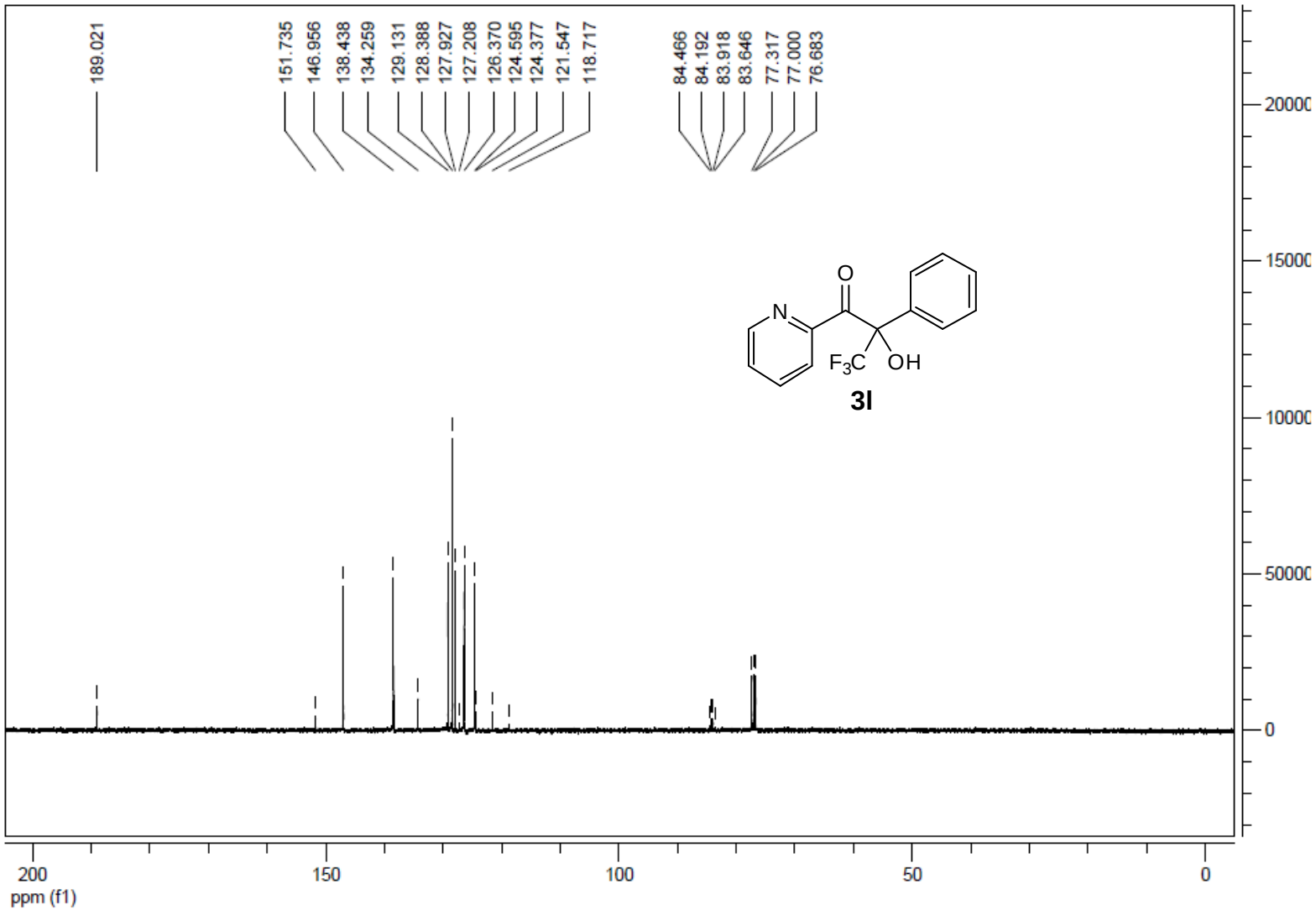
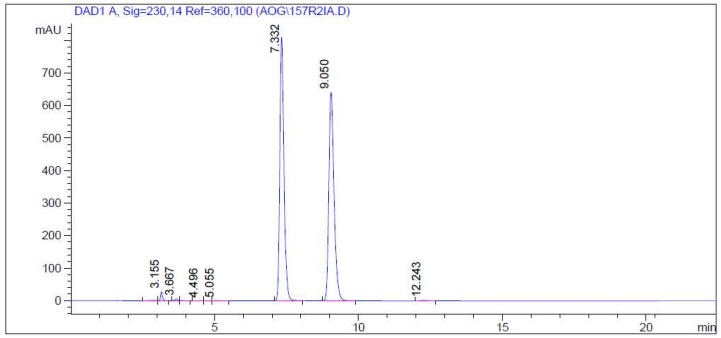


Figure S37 ^{13}C-NMR spectrum (400 MHz, $CDCl_3$) of 3,3,3-trifluoro-2-hydroxy-2-phenyl-1-(pyridin-2-yl)propan-1-one (**3l**).



Sample Name: AOG 218
Data file: D:\BERT\AOG\218IA.D
Sample Info: Laufmittel: n-Heptan/EtOH 9:1;
Die Probe ist im LM gelöst

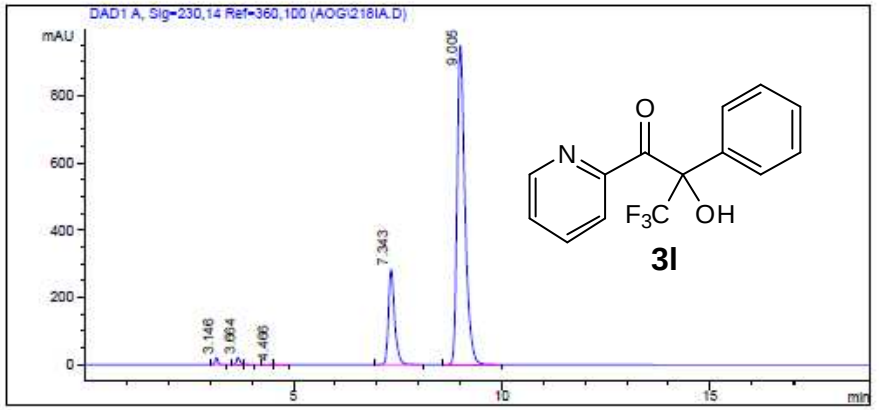
Agilent Technologies

Säule: DAICELIA.M
Säuleninfo: (250x4,6)mm

Operator: Analytik Labor AKEN

Injektion Time: 15:04:18
Injektion Date: 10.05.2010

Instrument Conditions:	At Start	At Stop
Temperature in°C:	30.0	30.0
Pressure in bar:	49.6	48.9
Flow in ml/min:	1.0	1.0



#	Ret. Time (min)	Width	Height (mAU)	Area (mAU*s)	Area %
1	3.15	0.08	21.27	109.77	0.70
2	3.66	0.09	21.56	125.98	0.80
3	3.86	0.14	1.30	13.29	0.08
4	4.47	0.15	1.25	14.13	0.09
5	4.67	0.17	1.22	15.86	0.10
6	7.34	0.16	289.62	2955.27	18.80
7	9.00	0.20	949.53	12485.34	79.43
Total				15719.65	100.00

Figure S38 HPLC chromatogram of **3l**; comparison of racemic and non-racemic (left); non-racemic (right).

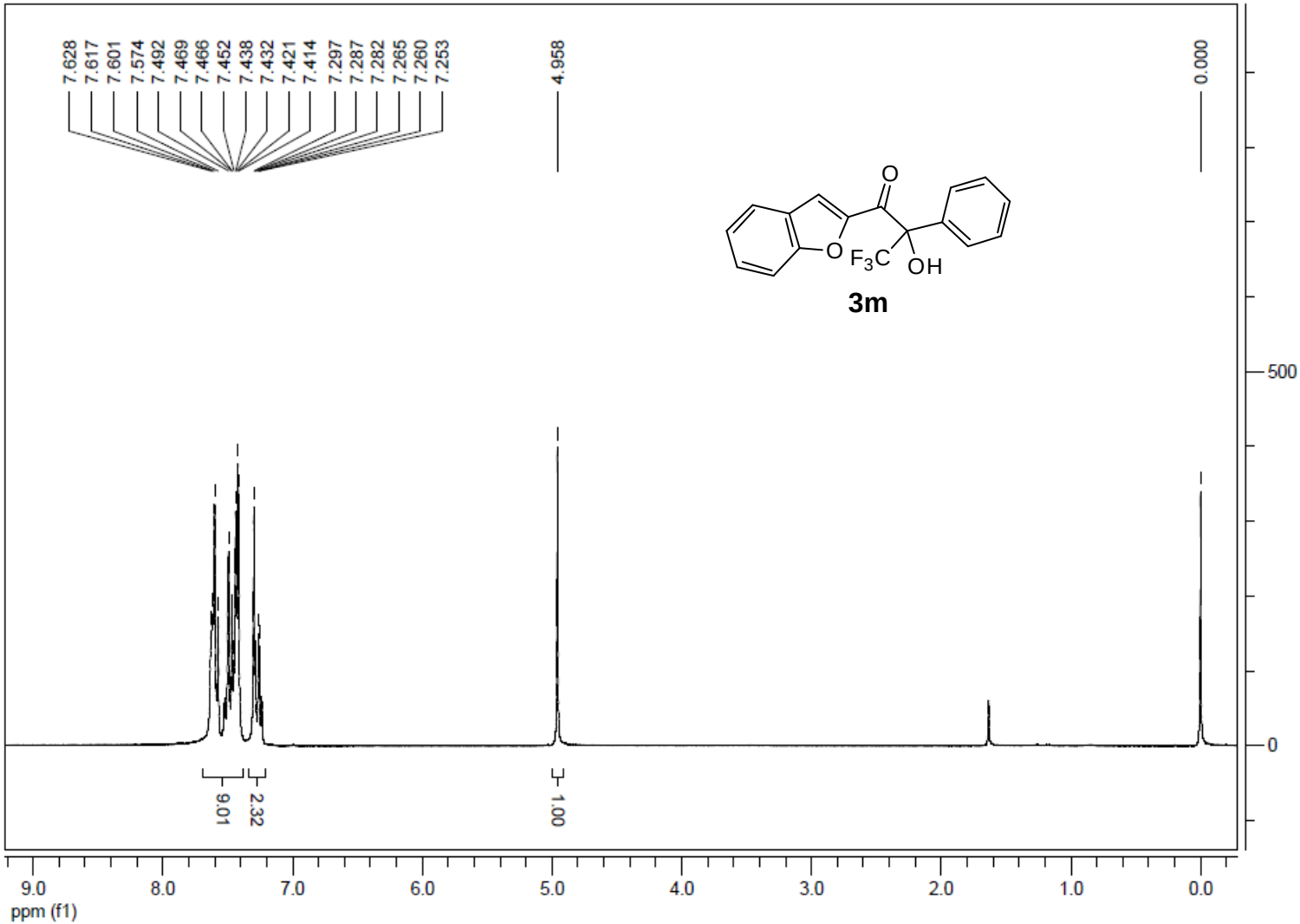


Figure S39 ^{1}H-NMR spectrum (300 MHz, $CDCl_3$) of 1-(benzofuran-2-yl)-3,3,3-trifluoro-2-hydroxy-2-phenylpropan-1-one (**3m**).

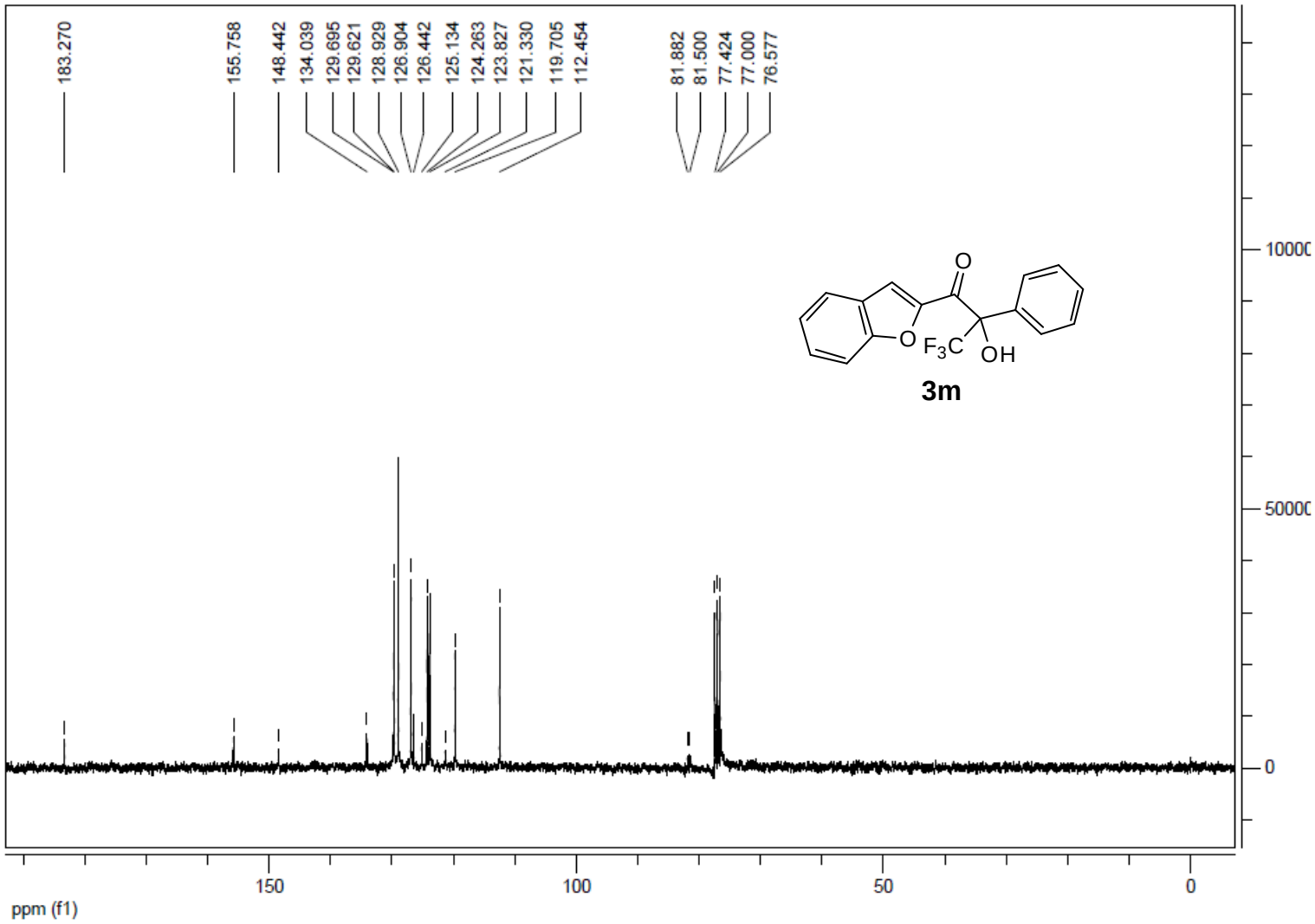
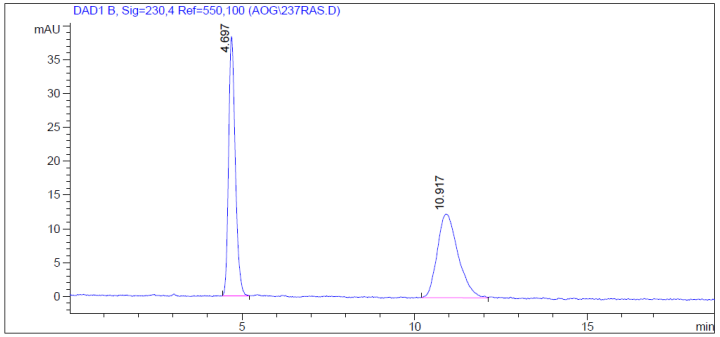


Figure S40 ^{13}C-NMR spectrum (300 MHz, $CDCl_3$) of 1-(benzofuran-2-yl)-3,3,3-trifluoro-2-hydroxy-2-phenylpropan-1-one (**3m**).



Sample Name: AOG 240
Data file: D:\BERT\AOG\240AS.D
Sample Info: Laufmittel: n-Heptan/IP 9:1;
Die Probe ist im DCM/LM gelöst

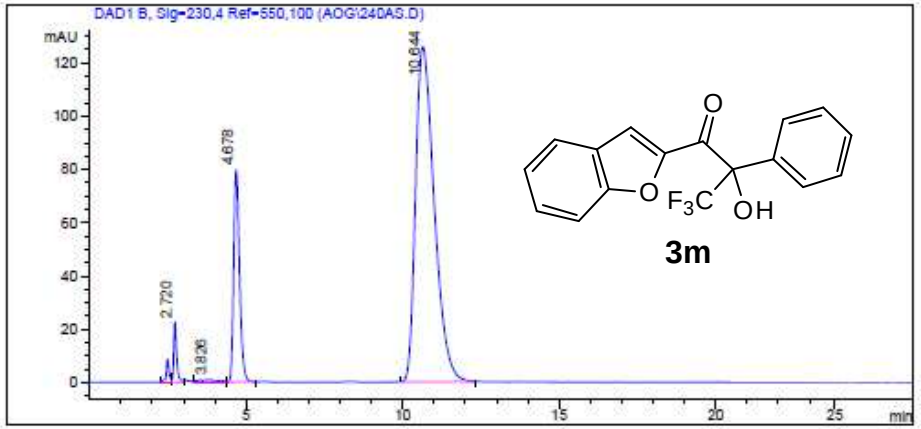
Agilent Technologies

Säule: DAICELAS.M
Säuleninfo: (250x4,6)mm

Operator: Analytik Labor AKEN

Injektion Time: 11:28:21
Injektion Date: 27.05.2010

Instrument Conditions:	At Start	At Stop
Temperature in°C:	30.0	30.0
Pressure in bar:	38.8	38.9
Flow in ml/min:	1.3	1.3



#	Ret. Time (min)	Width	Height (mAU)	Area (mAU*s)	Area %
1	2.48	0.10	8.72	56.50	0.87
2	2.72	0.10	22.49	148.68	2.28
3	3.83	0.44	0.96	33.70	0.52
4	4.68	0.20	79.75	1035.59	15.91
5	10.64	0.64	125.90	5232.70	80.41
Total				6507.18	100.00

Figure S41 HPLC chromatogram of **3m**; comparison of racemic and non-racemic (left); non-racemic (right).

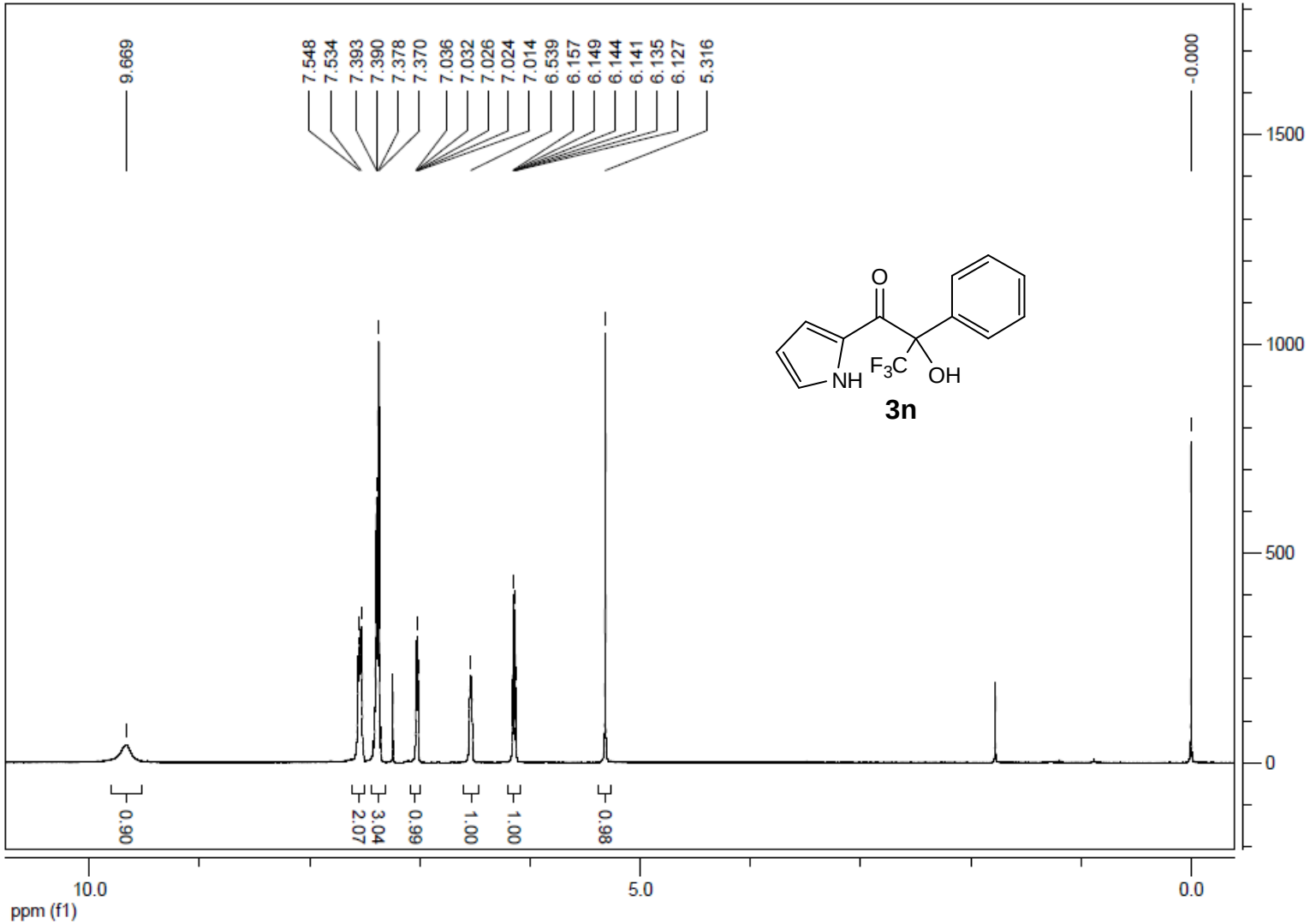


Figure S42 ^{1}H-NMR spectrum (300 MHz, $CDCl_3$) of 3,3,3-trifluoro-2-hydroxy-2-phenyl-1-(1H-pyrrol-2-yl)propan-1-one (**3n**).

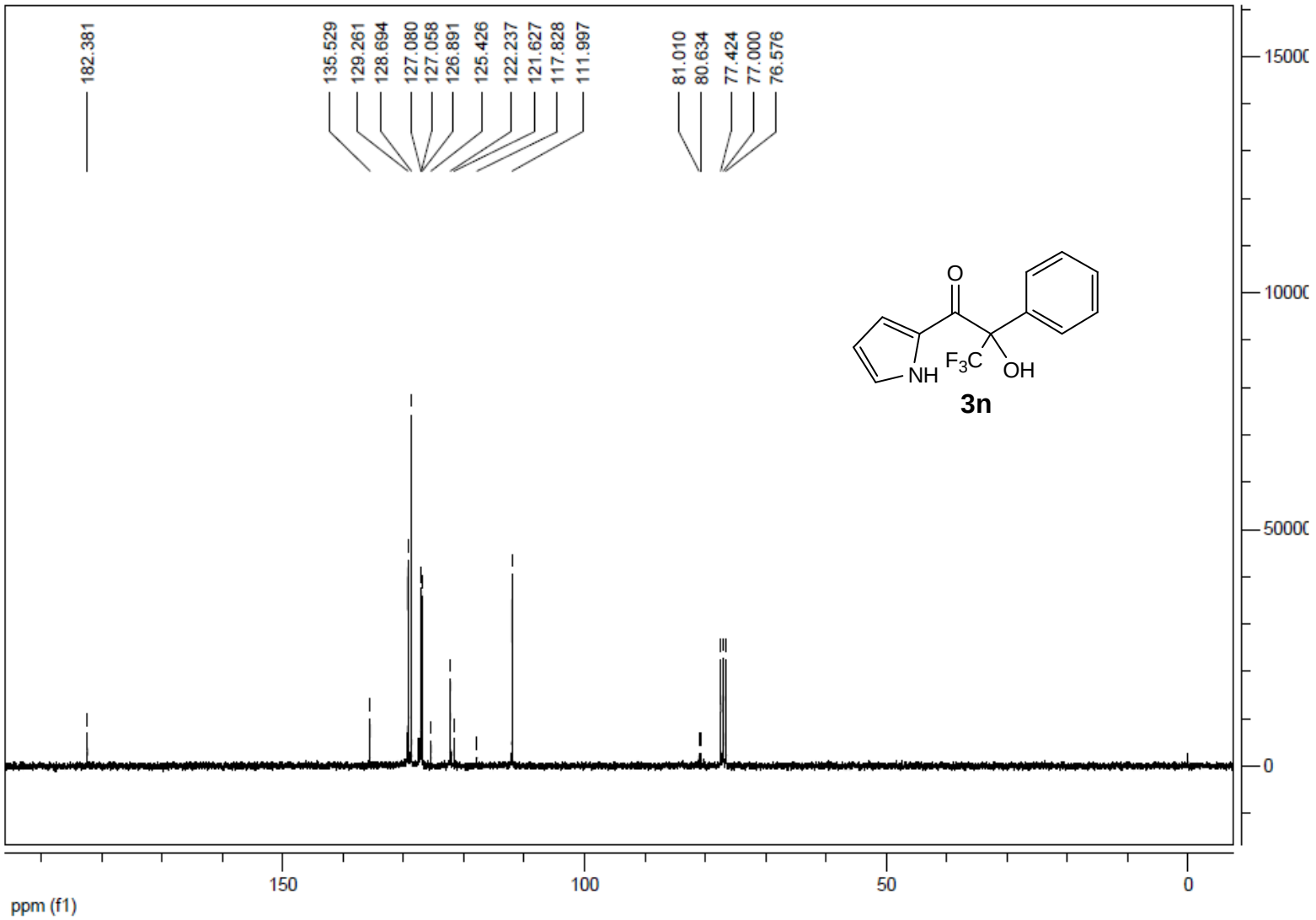
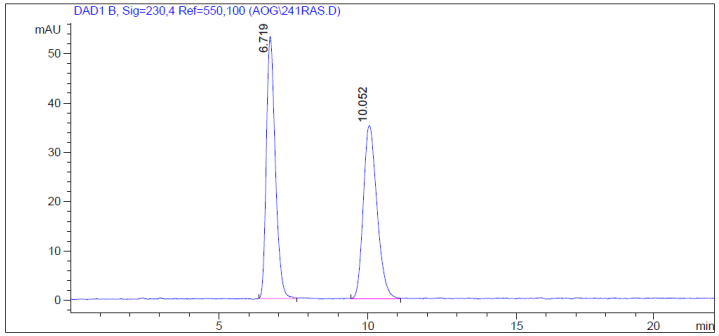
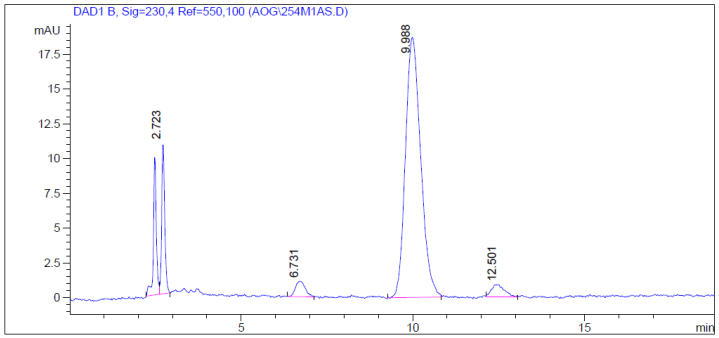


Figure S43 ^{13}C-NMR spectrum (300 MHz, $CDCl_3$) of 3,3,3-trifluoro-2-hydroxy-2-phenyl-1-(1H-pyrrol-2-yl)propan-1-one (**3n**).





Sample Name: AOG 254 M1
Data file: D:\BERT\AOG\254M1AS.D
Sample Info: Laufmittel: n-Heptan/IP 9:1;
Die Probe ist im DCM/LM gelöst

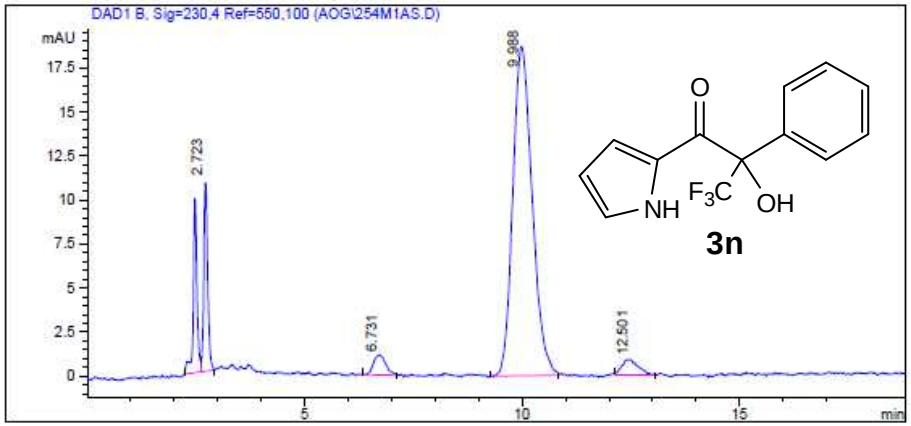
Agilent Technologies

Säule: DAICELAS.M
Säuleninfo: (250x4,6)mm

Operator: Analytik Labor AKEN

Injektion Time: 13:15:42
Injektion Date: 02.06.2010

Instrument Conditions:	At Start	At Stop
Temperature in°C:	30.0	30.0
Pressure in bar:	40.0	39.6
Flow in ml/min:	1.3	1.3



#	Ret. Time (min)	Width	Height (mAU)	Area (mAU*s)	Area %
1	2.48	0.08	10.07	58.46	7.80
2	2.72	0.10	10.86	66.58	8.89
3	6.73	0.26	1.12	22.34	2.98
4	9.99	0.41	18.69	578.30	77.19
5	12.50	0.33	0.89	23.47	3.13
Total				749.15	100.00

Figure S44 HPLC chromatogram of **3n**; comparison of racemic and non-racemic (left); non-racemic (right).