

Synthesis and evaluation of chiral β -amino acid-based low-molecular-weight organogelators possessing a methyl/trifluoromethyl side chain

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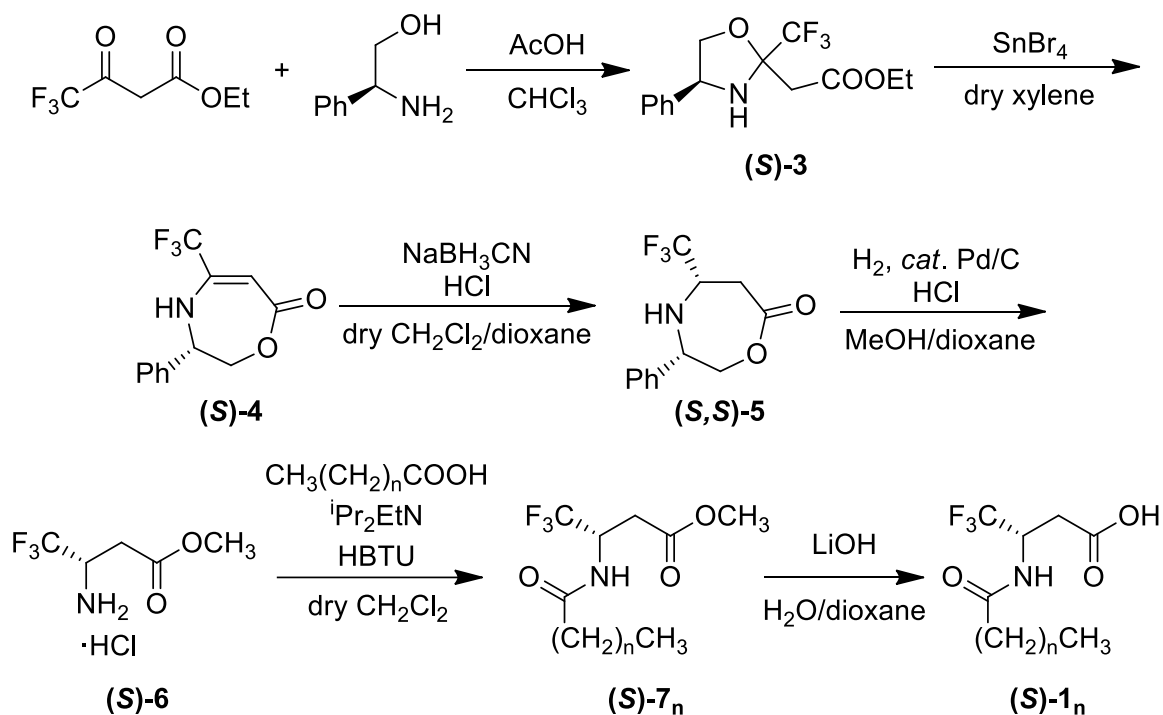
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Synthesis and characterization of the compounds

Compounds (*S*)-**1_n** were synthesized following the reactions shown in Scheme S1. The intermediate (*S*)-**6** was synthesized according to the literature.¹



Scheme S1 Synthesis of (*S*)-**1_n**

(*S*)-4-phenyl-2-trifluoromethyl-2-oxazolidineacetic acid ethyl ester ((*S*)-3**).** Under a nitrogen atmosphere, to a solution of (*S*)-phenylglycinol (2.96 g, 21.6 mmol) in CHCl₃ (50 ml) were added acetic acid (3.89 g, 64.8 mmol) and ethyl 4,4,4-trifluoroacetoacetate (4.02 g, 21.8 mmol) at room temperature. The solution was refluxed for 24 h. To the reaction mixture was added *sat.* Na₂CO₃ *aq.* and the aqueous layer was extracted with CHCl₃ three times. The organic layer was dried over anhydrous Na₂SO₄ and concentrated under reduced pressure. The residue was purified by Kugelrohr distillation (4.5 mmHg, 150 °C) to obtain (*S*)-**3** (5.10 g, 16.8 mmol, 78%) as colorless liquid. ¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.50-7.26 (m, 5H), 4.62-4.49 (m, 1H), 4.33-4.18 (m, 3H), 3.89 (d, 1H, *J* = 10.5 Hz), 3.72-3.66 (m, 1H), 3.03 (d, 1H, *J* = 15.3 Hz), 2.84 (d, 1H, *J* = 15.3 Hz), 1.30 (t, 3H, *J* = 7.2 Hz). ¹⁹F NMR (282 MHz, CDCl₃): δ (ppm) -83.7. IR (neat): ν (cm⁻¹) 2983, 1731, 1472, 1307, 1203, 1170, 1031, 702.

(*S*)-2,3,4,7-tetrahydro-3-phenyl-5-trifluoromethyl-1,4-oxazepine-7-one ((*S*)-4**).** Under a nitrogen atmosphere, to a solution of (*S*)-**3** (0.754 g, 2.49 mmol) in dry *o*-xylene (40 ml) was added freshly distilled SnBr₄ (0.334 g, 0.762 mmol) at room temperature. The solution was refluxed for 24 h. To

the reaction mixture was added water at 0 °C and the aqueous layer was extracted with CHCl₃ three times. The organic layer was dried over anhydrous Na₂SO₄ and concentrated under reduced pressure. The residue was purified by silica-gel column chromatography (eluent; hexane:EtOAc = 1 : 1) to obtain (*S*)-**4** (0.533 g, 2.07 mmol, 83%) as a white powder. Mp. 119.9-122.2 °C. ¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.50-7.41 (m, 3H), 7.35-7.29 (m, 2H), 5.31 (d, 1H, *J* = 2.4 Hz), 5.20 (s, 1H), 4.84 (d, 1H, *J* = 7.2 Hz), 4.60 (dd, 1H, *J*₁ = 12.9 Hz, *J*₂ = 7.2 Hz), 4.40 (d, 1H, *J* = 12.9 Hz). ¹⁹F NMR (282 MHz, CDCl₃): δ (ppm) -70.5. IR (KBr): ν (cm⁻¹) 3282, 3107, 3027, 2979, 1677, 1638, 1566, 1495, 1453, 1423, 1389, 1361.

(*S*)-2,3,4,5,6,7-hexahydro-3-phenyl-5-trifluoromethyl-1,4-oxazepine-7-one ((*S,S*)-5**).** Under a nitrogen atmosphere, to a solution of NaBH₃CN (1.05 g, 16.7 mmol) in CH₂Cl₂ (60 ml) was added a solution of (*S*)-**4** (3.42 g, 13.3 mmol) in 4M HCl / dioxane (30 ml) and CHCl₃ (30 ml) at -78 °C. The mixture was stirred at room temperature for 2 days. To the reaction mixture was added *sat.* NaHCO₃ aq. at 0 °C and extracted with CHCl₃. The organic layer was dried over anhydrous Na₂SO₄ and concentrated under reduced pressure. The residue was purified by silica-gel column chromatography (eluent; CHCl₃) to obtain (*S,S*)-**5** (2.33 g, 8.99 mmol, 68%) as a white powder. Mp 140.2-143.0 °C. ¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.44-7.32 (m, 5H), 4.36 (dd, 1H, *J*₁ = 13.2 Hz, *J*₂ = 8.7 Hz), 4.22-4.14 (m, 2H), 3.87-3.65 (m, 1H), 3.08-3.04 (m, 2H), 2.35 (br, 1H). ¹⁹F NMR (282 MHz, CDCl₃): δ (ppm) -78.7. IR (KBr): ν (cm⁻¹) 3332, 1739, 1602, 1491, 1470, 1454, 1432, 1394, 1321, 1187.

(*S*)-3-amino-4,4,4-trifluorobutyric acid methyl ester hydrochloride ((*S*)-6**).** To the solution of (*S,S*)-**5** (1.32 g, 5.09 mmol) in MeOH (30 ml) was added 10% Pd/C (0.557 g) and 4M HCl / dioxane (13 ml). The air inside the flask was replaced with H₂ and the mixture was stirred at room temperature for 1 day. After the solid Pd/C was filtered off by use of celite, the filtrate was concentrated under reduced pressure to obtain (*S*)-**6** (0.778 g, 3.75 mmol, 74%) as a white powder. Mp. 93.0-96.0 °C. ¹H NMR (300 MHz, CDCl₃/CD₃OD): δ (ppm) 4.44-4.24 (m, 1H), 3.80 (s, 3H), 3.59 (br, 3H), 3.16-2.92 (m, 2H). ¹⁹F NMR (282 MHz, CDCl₃): δ (ppm) -75.4. IR (KBr): ν (cm⁻¹) 3395, 2856, 1744, 1588, 1528, 1443, 1389, 1329, 1286, 1203, 1157, 1098, 1069, 908, 655.

***N*-octanoyl-(*S*)-3-amino-4,4,4-trifluorobutyric acid methyl ester ((*S*)-**7**₆).** Under a nitrogen atmosphere, to a solution of octanoic acid (0.198 g, 1.22 mmol) in CH₂Cl₂ (15 ml) was added *O*-(benzotriazol-1-yl)-*N,N,N',N'*-tetramethyluronium hexafluorophosphate (HBTU) (0.458 g, 1.21 mmol) and the mixture was stirred at 0 °C for 30 min. Then to the mixture was added (*S*)-**6** (0.251 g, 1.20 mmol) and ¹Pr₂NEt (0.778 g, 6.02 mmol) and stirred at room temperature for 3 days. Ethyl acetate was added to the reaction mixture and the organic layer was washed with 1 N HCl aq., *sat.* NaHCO₃ aq. and brine. The organic layer was dried over anhydrous Na₂SO₄ and concentrated under reduced pressure. The residue was purified by silica-gel column chromatography (eluent;

toluene:EtOAc = 7 : 1) to obtain (*S*)-**7₆** (0.108 g, 0.363 mmol, 30%) as a white powder. Mp: 65-68 °C. ¹H NMR (300 MHz, CDCl₃): δ (ppm) 6.32 (d, 1H, *J* = 8.7 Hz), 5.11-4.99 (m, 1H), 3.73 (s, 3H), 2.78-2.63 (m, 2H), 2.24 (t, 2H, *J* = 7.5 Hz), 1.71-1.58 (m, 2H), 1.38-1.22 (m, 8H), 0.88 (t, 3H, *J* = 6.6 Hz). ¹³C NMR (100 MHz, CDCl₃): δ (ppm) 172.8, 170.1, 124.6 (q, *J* = 280 Hz), 52.4, 47.2 (q, *J* = 32 Hz), 36.5, 32.9, 31.7, 29.0, 28.9, 25.4, 22.6, 14.0. ¹⁹F NMR (282 MHz, CDCl₃): δ (ppm) -76.7. IR (KBr) : ν (cm⁻¹) 3288, 3076, 2929, 2853, 1741, 1664, 1549, 1352, 1304, 1234, 1176, 1119, 665. MS(MALDI-TOF): *m/z* calcd for [C₁₃H₂₂F₃NO₃ + Na]⁺ 320.14, found 320.15.

***N*-nonanoyl-(*S*)-3-amino-4,4,4-trifluorobutyric acid methyl ester ((*S*)-**7₇**).** (*S*)-**7₇** was synthesized by the same procedure as (*S*)-**7₆** from nonanoic acid and obtained as a white solid (72%). Mp. 74.0-75.0 °C. ¹H NMR (500 MHz, CDCl₃): δ (ppm) 6.32 (d, 1H, *J* = 9.5 Hz), 5.11-4.99 (m, 1H), 3.73 (s, 3H), 2.78-2.63 (m, 2H), 2.24 (t, 2H, *J* = 8.0 Hz), 1.68-1.60 (m, 2H), 1.38-1.22 (m, 10H), 0.88 (t, 3H, *J* = 7.0 Hz). ¹³C NMR (100 MHz, CDCl₃): δ (ppm) 172.8, 170.1, 124.6 (q, *J* = 280 Hz), 52.4, 47.2 (q, *J* = 32 Hz), 36.5, 32.9, 31.8, 29.2, 29.1, 29.1, 25.4, 22.6, 14.1. ¹⁹F NMR (282 MHz, CDCl₃): δ (ppm) -76.7. IR (KBr): ν (cm⁻¹) 3293, 2934, 1739, 1666, 1549, 1351, 1303, 1238, 1179, 1119, 921, 665. MS(MALDI-TOF): *m/z* calcd for [C₁₄H₂₄F₃NO₃ + Na]⁺ 334.16, found 334.18.

***N*-decanoyl-(*S*)-3-amino-4,4,4-trifluorobutyric acid methyl ester ((*S*)-**7₈**).** (*S*)-**7₈** was synthesized by the same procedure as (*S*)-**7₆** from decanoic acid and obtained as a white solid (55%). Mp. 79.5-80.0 °C. ¹H NMR (500 MHz, CDCl₃): δ (ppm) 6.32 (d, 1H, *J* = 9.0 Hz), 5.11-4.99 (m, 1H), 3.73 (s, 3H), 2.78-2.63 (m, 2H), 2.24 (t, 2H, *J* = 7.5 Hz), 1.68-1.59 (m, 2H), 1.38-1.22 (m, 12H), 0.88 (t, 3H, *J* = 7.0 Hz). ¹³C NMR (100 MHz, CDCl₃): δ (ppm) 172.8, 170.1, 124.6 (q, *J* = 280 Hz), 52.4, 47.2 (q, *J* = 32 Hz), 36.5, 32.9, 31.9, 29.4, 29.3, 29.2, 29.1, 25.4, 22.7, 14.1. ¹⁹F NMR (282 MHz, CDCl₃): δ (ppm) -76.6. IR (KBr): ν (cm⁻¹) 3285, 2918, 2851, 1741, 1662, 1550, 1352, 1304, 1235, 1176, 1119, 924, 666. MS(MALDI-TOF): *m/z* calcd for [C₁₅H₂₆F₃NO₃ + Na]⁺ 348.18, found 348.21.

***N*-undecanoyl-(*S*)-3-amino-4,4,4-trifluorobutyric acid methyl ester ((*S*)-**7₉**).** (*S*)-**7₉** was synthesized by the same procedure as (*S*)-**7₆** from undecanoic acid and obtained as a white solid (68%). Mp. 80.0-82.0 °C. ¹H NMR (300 MHz, CDCl₃): δ (ppm) 6.32 (d, 1H, *J* = 9.0 Hz), 5.11-4.99 (m, 1H), 3.73 (s, 3H), 2.78-2.63 (m, 2H), 2.24 (t, 2H, *J* = 7.2 Hz), 1.71-1.58 (m, 2H), 1.38-1.18 (m, 14H), 0.88 (t, 3H, *J* = 6.6 Hz). ¹³C NMR (100 MHz, CDCl₃): δ (ppm) 172.8, 170.1, 124.6 (q, *J* = 280 Hz), 52.4, 47.2 (q, *J* = 32 Hz), 36.6, 32.9, 31.9, 29.5, 29.5, 29.3, 29.1, 25.4, 22.7, 14.1. ¹⁹F NMR (282 MHz, CDCl₃): δ (ppm) -76.6. IR (KBr): ν (cm⁻¹) 3292, 2917, 2850, 1742, 1666, 1550, 1352, 1300, 1181, 1119, 922, 665. MS(MALDI-TOF): *m/z* calcd for [C₁₆H₂₈F₃NO₃ + Na]⁺ 362.19, found 362.25.

***N*-dodecanoyl-(*S*)-3-amino-4,4,4-trifluorobutyric acid methyl ester ((*S*)-**7₁₀**).** (*S*)-**7₁₀** was synthesized by the same procedure as (*S*)-**7₆** from dodecanoic acid and obtained as a white solid

(66%). Mp. 88.0-89.5 °C. ¹H NMR (300 MHz, CDCl₃): δ (ppm) 6.32 (d, 1H, *J* = 9.3 Hz), 5.11-4.99 (m, 1H), 3.73 (s, 3H), 2.78-2.63 (m, 2H), 2.24 (t, 2H, *J* = 7.2 Hz), 1.71-1.58 (m, 2H), 1.38-1.20 (m, 16H), 0.88 (t, 3H, *J* = 6.6 Hz). ¹³C NMR (100 MHz, CDCl₃): δ (ppm) 172.8, 170.0, 124.6 (q, *J* = 280 Hz), 52.3, 47.2 (q, *J* = 32 Hz), 36.5, 32.9, 31.9, 29.6, 29.4, 29.3, 29.3, 29.1, 25.4, 22.7, 14.1. ¹⁹F NMR (282 MHz, CDCl₃): δ (ppm) -76.7. IR (KBr): ν (cm⁻¹) 3285, 2917, 2850, 1741, 1662, 1550, 1353, 1305, 1234, 1185, 1119, 922, 666. MS(MALDI-TOF): *m/z* calcd for [C₁₇H₃₀F₃NO₃ + Na]⁺ 376.21, found 376.24.

***N*-octanoyl-(*S*)-3-amino-4,4,4-trifluorobutyric acid ((*S*)-16).** To the solution of (*S*)-76 (52.8 mg, 0.178 mmol) in 1,4-dioxane (13 ml) and H₂O (9.0 ml) was added LiOH·H₂O (75.3 mg, 1.79 mmol) at 0 °C and the solution was stirred for 1 day. Ethyl acetate was added to the reaction mixture and the organic layer was washed with 1M HCl aq. The organic layer was dried over anhydrous Na₂SO₄ and then concentrated under reduced pressure to obtain (*S*)-16 (50.3 mg, 0.178 mmol, quant) as a white powder. Mp. 118.0-120.0 °C. ¹H NMR (300 MHz, CDCl₃/CD₃OD): δ (ppm) 5.11-4.95 (m, 1H), 2.74 (dd, 1H, *J*₁ = 16.0 Hz, *J*₂ = 4.7 Hz), 2.60 (dd, 1H, *J*₁ = 16.0 Hz, *J*₂ = 7.8 Hz), 2.23 (t, 2H, *J* = 7.7 Hz), 1.70-1.57 (m, 2H), 1.38-1.21 (m, 8H), 0.88 (t, 3H, *J* = 6.6 Hz). ¹³C NMR (100 MHz, CDCl₃): δ (ppm) 173.3, 172.2, 124.5 (q, *J* = 280 Hz), 47.2 (q, *J* = 32 Hz), 36.5, 32.7, 31.6, 29.0, 28.9, 25.4, 22.6, 14.0. ¹⁹F NMR (282 MHz, CDCl₃): δ (ppm) -77.0. IR (KBr): ν (cm⁻¹) 3297, 2914, 2849, 1707, 1666, 1548, 1372, 1328, 1204, 1125, 936, 652. MS(MALDI-TOF): *m/z* calcd for [C₁₂H₂₀F₃NO₃ + Na]⁺ 306.13, found 306.17.

***N*-nonanoyl-(*S*)-3-amino-4,4,4-trifluorobutyric acid ((*S*)-17).** (*S*)-17 was synthesized by the same procedure as (*S*)-16 from (*S*)-77 and obtained as a white solid (96%). Mp. 125.0-127.5 °C. ¹H NMR (500 MHz, CDCl₃): δ (ppm) 6.27 (d, 1H, *J* = 9.5 Hz), 5.15-5.04 (m, 1H), 2.84-2.66 (m, 2H), 2.25 (t, 2H, *J* = 7.5 Hz), 1.71-1.58 (m, 2H), 1.38-1.20 (m, 10H), 0.88 (t, 3H, *J* = 6.5 Hz). ¹³C NMR (100 MHz, CDCl₃/CD₃OD): δ (ppm) 173.4, 124.7 (q, *J* = 280 Hz), 47.3 (q, *J* = 32 Hz), 36.4, 31.8, 29.3, 29.1, 29.1, 25.5, 22.6, 14.1. ¹⁹F NMR (282 MHz, CDCl₃): δ (ppm) -76.9. IR (KBr): ν (cm⁻¹) 3295, 2914, 2849, 1705, 1667, 1543, 1372, 1255, 1205, 1124, 939, 651. MS(MALDI-TOF): *m/z* calcd for [C₁₃H₂₂F₃NO₃ + Na]⁺ 320.14, found 320.18.

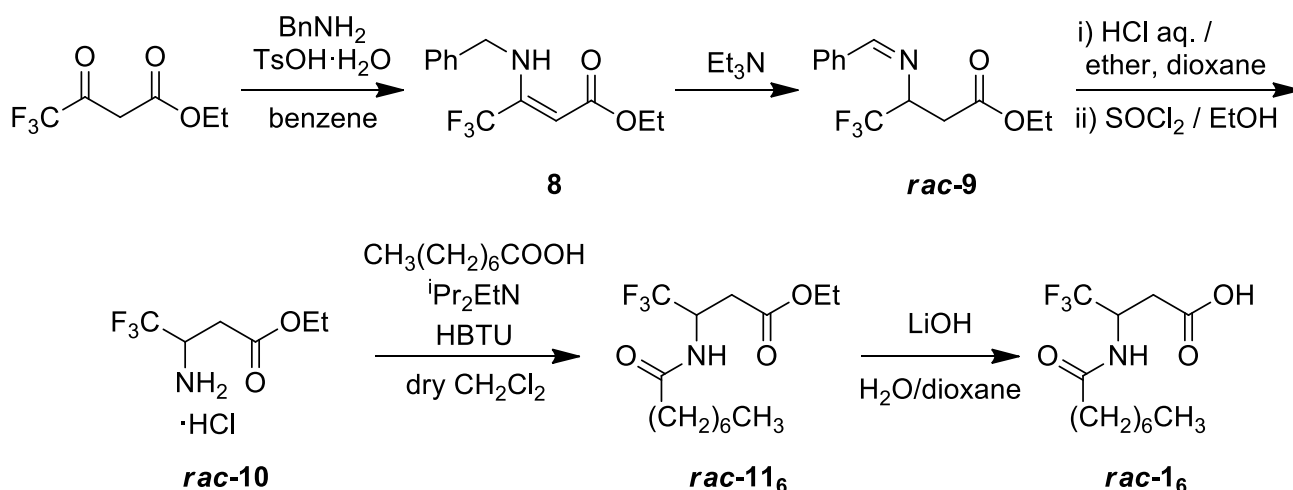
***N*-decanoyl-(*S*)-3-amino-4,4,4-trifluorobutyric acid ((*S*)-18).** (*S*)-18 was synthesized by the same procedure as (*S*)-16 from (*S*)-78 and obtained as a white solid (83%). Mp. 125.0-127.5 °C. ¹H NMR (500 MHz, CDCl₃): δ (ppm) 6.25 (d, 1H, *J* = 9.5 Hz), 5.15-5.04 (m, 1H), 2.84-2.66 (m, 2H), 2.25 (t, 2H, *J* = 7.0 Hz), 1.69-1.58 (m, 2H), 1.38-1.20 (m, 12H), 0.88 (t, 3H, *J* = 7.0 Hz). ¹³C NMR (100 MHz, CDCl₃/CD₃OD): δ (ppm) 173.3, 171.5, 124.7 (q, *J* = 280 Hz), 47.2 (q, *J* = 32 Hz), 36.5, 32.8, 31.9, 29.4, 29.3, 29.3, 29.1, 25.4, 22.7, 14.1. ¹⁹F NMR (282 MHz, CDCl₃): δ (ppm) -76.9. IR (KBr): ν (cm⁻¹) 3295, 2916, 2849, 1705, 1667, 1549, 1373, 1204, 1125, 936, 653. MS(MALDI-TOF): *m/z*

calcd for $[C_{14}H_{24}F_3NO_3 + Na]^+$ 334.16, found 334.22.

***N*-undecanoyl-(*S*)-3-amino-4,4,4-trifluorobutyric acid ((*S*)-19).** (*S*)-19 was synthesized by the same procedure as (*S*)-16 from (*S*)-79 and obtained as a white solid (82%). Mp. 127.0-130.0 °C. 1H NMR (400 MHz, $CDCl_3/CD_3OD$): δ (ppm) 5.10-4.95 (m, 1H), 2.77-2.57 (m, 2H), 2.23 (t, 2H, $J = 7.6$ Hz), 1.69-1.58 (m, 2H), 1.38-1.20 (m, 14H), 0.88 (t, 3H, $J = 6.8$ Hz). ^{13}C NMR (100 MHz, $CDCl_3/CD_3OD$): δ (ppm) 173.4, 171.5, 124.7 (q, $J = 280$ Hz), 47.3 (q, $J = 32$ Hz), 36.5, 32.9, 31.9, 29.6, 29.5, 29.3, 29.1, 25.5, 22.7, 14.1. ^{19}F NMR (282 MHz, $CDCl_3$): δ (ppm) -76.6. IR (KBr): ν (cm^{-1}) 3294, 2916, 2849, 1706, 1667, 1547, 1371, 1253, 1203, 1124, 936, 651. MS(MALDI-TOF): m/z calcd for $[C_{15}H_{26}F_3NO_3 + Na]^+$ 348.18, found 348.21.

***N*-dodecanoyl-(*S*)-3-amino-4,4,4-trifluorobutyric acid ((*S*)-110).** (*S*)-110 was synthesized by the same procedure as (*S*)-16 from (*S*)-710 and obtained as a white solid (quant.). Mp. 127.0-129.0 °C. 1H NMR (500 MHz, CD_3OD): δ (ppm) 5.10-4.95 (m, 1H), 2.78 (dd, 1H, $J_1 = 16.0$ Hz, $J_2 = 4.0$ Hz), 2.59 (dd, 1H, $J_1 = 16.5$ Hz, $J_2 = 10.5$ Hz), 2.21 (t, 2H, $J = 7.0$ Hz), 1.69-1.58 (m, 2H), 1.38-1.20 (m, 16H), 0.89 (t, 3H, $J = 7.0$ Hz). ^{13}C NMR (100 MHz, $CDCl_3/CD_3OD$): δ (ppm) 173.3, 171.5, 124.7 (q, $J = 280$ Hz), 47.2 (q, $J = 32$ Hz), 36.5, 32.8, 31.9, 29.6, 29.5, 29.4, 29.3, 29.1, 25.5, 22.7, 14.1. ^{19}F NMR (282 MHz, $CDCl_3$): δ (ppm) -76.6. IR (KBr): ν (cm^{-1}) 3294, 2916, 2849, 1705, 1667, 1543, 1373, 1206, 1125, 937, 652. MS(MALDI-TOF): m/z calcd for $[C_{16}H_{28}F_3NO_3 + Na]^+$ 362.19, found 362.24.

The compound *rac*-16 was synthesized following the reactions shown in Scheme S2. The intermediate *rac*-10 was synthesized according to the literature.²



Scheme S2 Synthesis of *rac*-16

3-benzylamino-4,4,4-trifluoro-but-2-enoic acid ethyl ester (8). Benzylamine (643 mg, 6.00 mmol)

was added dropwise to the solution of ethyl 4,4,4-trifluoroacetoacetate (1.00 g, 5.45 mmol) and *p*-TsOH·H₂O (47.2 mg / 0.274 mmol) in benzene (20 ml) at room temperature. The mixture was heated using the Dean-Stark apparatus for 1 day to remove water. After filtration, the solvent was removed under reduced pressure and the target product **8** (1.00 g, 3.66 mmol, 67%) was obtained as colorless liquid. ¹H NMR (300 MHz, CDCl₃): δ (ppm) 8.46 (s, 1H), 7.43-7.28 (m, 5H), 5.18 (s, 1H), 4.49 (d, 2H, *J* = 6.3 Hz), 4.16 (q, 2H, *J* = 7.2 Hz), 1.29 (t, 3H, *J* = 7.2 Hz). ¹⁹F NMR (282 MHz, CDCl₃): δ (ppm) -67.6. IR (neat): ν (cm⁻¹) 2983, 1675, 1635, 1296, 1208, 1139, 1040, 799, 734, 666.

***N*-benzylidene-3-amino-4,4,4-trifluorobutyric acid ethyl ester (*rac*-9).** Triethylamine (16 ml) was added dropwise to **8** (744 mg, 2.72 mmol) at room temperature and the solution was refluxed for 3 days. The mixture was purified by Kugelrohr distillation (9.0 mmHg, 130-135 °C) to obtain *rac*-**9** (550 mg, 2.01 mmol, 73%) as colorless liquid. ¹H NMR (300 MHz, CDCl₃): δ (ppm) 8.42 (s, 1H), 7.82-7.75 (m, 2H), 7.50-7.39 (m, 3H), 4.30-4.16 (m, 1H), 4.16-4.05 (m, 2H), 2.91 (d, 2H, *J* = 6.3 Hz), 1.20 (t, 3H, *J* = 7.2 Hz). ¹⁹F NMR (282 MHz, CDCl₃): δ (ppm) -76.1. IR (neat): ν (cm⁻¹) 2986, 2894, 1736, 1649, 1582, 1453, 1272, 1173, 1129, 1061, 1025, 885, 758, 694.

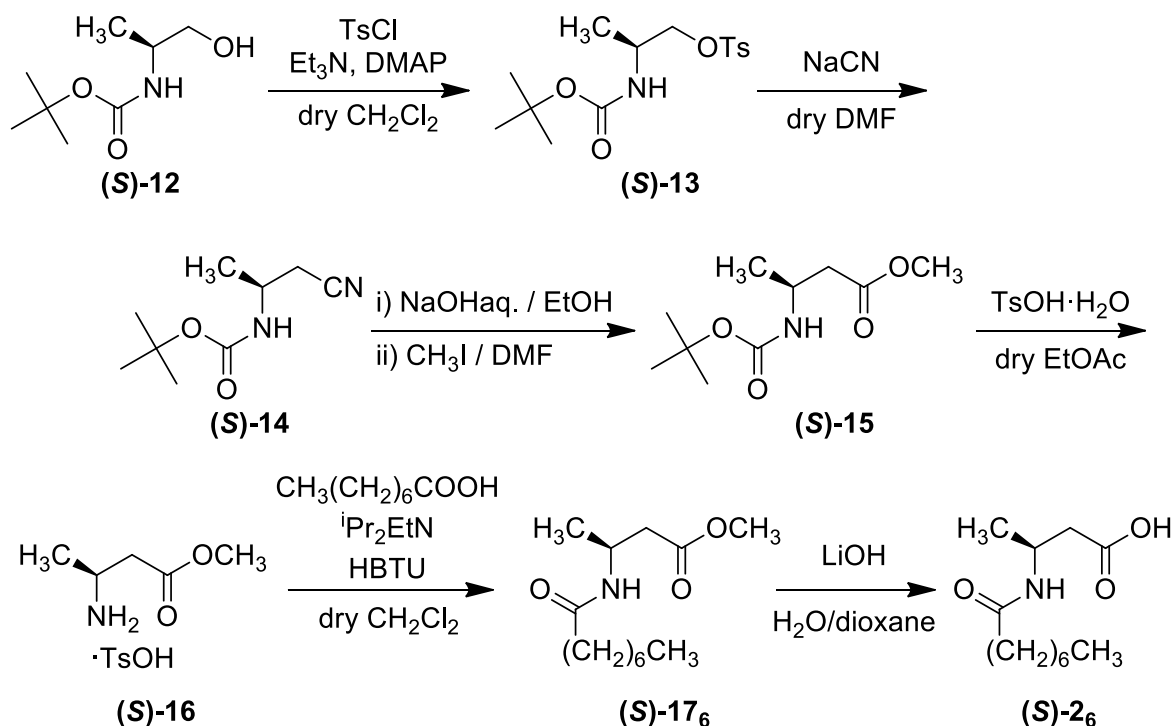
3-amino-4,4,4-trifluorobutyric acid ethyl ester hydrochloride (*rac*-10). The solution of *rac*-**9** (548 mg, 2.01 mmol) in diethyl ether (1.4 ml) was mixed with 1M HCl aq. (3.0 ml) and the solution was stirred for 1 h. Then 6M HCl aq. (0.3 ml) and dioxane (0.3 ml) were added dropwise to the reaction mixture at room temperature. The solution was refluxed for 2 days. The organic layer was removed and the aqueous layer was washed with ether (3 × 10 ml). The solvent was removed under reduced pressure to obtain crude carboxylic acid (377 mg). Thionyl chloride (247 mg, 2.08 mmol) was added dropwise to ethanol (2.0 ml) at -5 °C and stirred for 10 min. To the solution crude carboxylic acid (306 mg) was added and the mixture was stirred at room temperature for 14 h. The solvent and excess thionyl chloride were distilled off under reduced pressure and the residue was washed with ether to obtain *rac*-**10** (245 mg, 1.11 mmol, 68%) as a yellow solid. ¹H NMR (300 MHz, CDCl₃): δ (ppm) 8.91 (br, 3H), 4.64-4.46 (m, 1H), 4.19 (q, 2H, *J* = 7.2 Hz), 3.11-2.85 (m, 2H), 1.26 (t, 3H, *J* = 7.2 Hz). ¹⁹F NMR (282 MHz, CDCl₃): δ (ppm) -76.9. IR (KBr): ν (cm⁻¹) 3434, 2985, 2609, 1736, 1620, 1525, 1328, 1287, 1203, 1159, 1024, 870.

***N*-octanoyl-3-amino-4,4,4-trifluorobutyric acid ethyl ester (*rac*-11₆).** Under a nitrogen atmosphere, to a solution of octanoic acid (91.0 mg, 0.559 mmol) in CH₂Cl₂ (3.0 ml) was added *O*-(Benzotriazol-1-yl)-*N,N,N',N'*-tetramethyluronium hexafluorophosphate (HBTU) (211mg, 0.555 mmol) and the mixture was stirred at 0 °C for 30 min. Then to the mixture were added *rac*-**10** (121 mg, 0.547 mmol) and ⁱPr₂EtN (366 mg, 2.83 mmol) and the mixture was stirred at room temperature for 3 days. Ethyl acetate was added to the reaction mixture and the organic layer was washed with 1M HCl aq., *sat.* NaHCO₃ aq. and brine. The organic layer was dried over anhydrous Na₂SO₄ and concentrated under reduced pressure. The residue was purified by silica-gel column chromatography

(eluent; toluene:EtOAc = 7 : 1) to obtain *rac*-**11**6 (124 mg, 0.400 mmol, 74%) as a white solid. Mp. 79.5-80.0 °C. ¹H NMR (300 MHz, CDCl₃): δ (ppm) 6.36 (d, 1H, *J* = 9.0 Hz), 5.12-4.99 (m, 1H), 4.22-4.14 (m, 2H), 2.78-2.60 (m, 2H), 2.24 (t, 2H, *J* = 6.9 Hz), 1.72-1.55 (m, 2H), 1.35-1.22 (m, 11H), 0.88 (t, 3H, *J* = 6.6 Hz). ¹⁹F NMR (282 MHz, CDCl₃): δ (ppm) -76.6. IR (KBr): ν (cm⁻¹) 3294, 2928, 1736, 1666, 1549, 1421, 1308, 1236, 1121, 1030, 876, 662.

***N*-octanoyl-3-amino-4,4,4-trifluorobutyric acid (*rac*-**16**)**. To the solution of *rac*-**11**6 (56.7 mg, 0.182 mmol) in 1,4-dioxane (1.0 ml) and H₂O (0.7 ml) was added LiOH·H₂O (79.1 mg, 1.89 mmol) at room temperature and the solution was stirred for 1 day. Ethyl acetate was added to the reaction mixture and the organic layer was washed with 1M HCl aq. The organic layer was dried over anhydrous Na₂SO₄ and then concentrated under reduced pressure to obtain *rac*-**16** (50.7 mg, 1.79 mmol, 98%) as a white powder. Mp. 138.1-139.2 °C. ¹H NMR (500 MHz, CD₃OD): δ (ppm) 5.08-4.95 (m, 1H), 2.79 (dd, 1H, *J*₁ = 16.5 Hz, *J*₂ = 4.0 Hz), 2.60 (dd, 1H, *J*₁ = 16.5 Hz, *J*₂ = 6.5 Hz), 2.21 (t, 2H, *J* = 7.5 Hz), 1.65-1.55 (m, 2H), 1.40-1.25 (m, 8H), 0.90 (t, 3H, *J* = 7.0 Hz). ¹⁹F NMR (282 MHz, CDCl₃): δ (ppm) -76.9. IR (KBr): ν (cm⁻¹) 3354, 2937, 1728, 1627, 1556, 1419, 1302, 1225, 1186, 1122, 639.

The compound (*S*)-**26** was synthesized following the reactions shown in Scheme S3. The intermediate (*S*)-**14** was synthesized according to the literature.³



Scheme S3 Synthesis of (*S*)-**26**

(S)-2-[(*tert*-butoxycarbonyl)amino]propyl *p*-toluenesulfonate ((S)-13). Under a nitrogen atmosphere, to a solution of *N*-Boc-L-alaninol ((S)-12) (0.602 g, 3.43 mmol) in dry CH₂Cl₂ (4.0 ml) were added triethylamine (0.525 g, 5.18 mmol), *p*-toluenesulfonyl chloride (0.919 g, 4.82 mmol) and DMAP (0.126 g, 1.03 mmol) at 0 °C and the mixture was stirred at room temperature for 24 h. To the reaction mixture was added *sat.* NaHSO₄ aq. until pH = 2. The aqueous layer was washed with CH₂Cl₂ (3×10 ml) and the organic layer was dried over anhydrous Na₂SO₄ and concentrated under reduced pressure. The residue was purified by silica-gel column chromatography (eluent; hexane:EtOAc = 5 : 2) to obtain (S)-13 (0.884 g, 2.68 mmol, 78%) as a white solid. ¹H NMR (500 MHz, CDCl₃): δ (ppm) 7.79 (d, 2H, *J* = 8.0 Hz), 7.35 (d, 2H, *J* = 8.0 Hz), 4.57 (s, 1H), 4.10-3.80 (m, 3H), 2.37 (s, 3H), 1.40 (s, 9H), 1.15 (d, 3H, *J* = 6.5 Hz). IR (KBr): ν (cm⁻¹) 3426, 2968, 1726, 1500, 1349, 1232, 1189, 1162, 1080, 966, 820, 673, 555.

(S)-3-[(*tert*-butoxycarbonyl)amino]butanenitrile ((S)-14). Under a nitrogen atmosphere, a solution of sodium cyanide (0.273 g, 5.57 mmol) in dry DMF (1.0 ml) was added dropwise to a solution of (S)-13 (0.603 g, 1.83 mmol) in dry DMF (1.0 ml) and the mixture was stirred at room temperature. After 24 h, H₂O (10 ml) was added to the reaction mixture. The aqueous layer was washed with CH₂Cl₂ (3×10 ml). Then the organic layer was washed with *sat.* NaHCO₃ aq. and brine. The organic layer was combined and dried over anhydrous Na₂SO₄ and concentrated under reduced pressure. The residue was purified by silica-gel column chromatography (eluent; hexane:EtOAc = 4 : 1) to obtain (S)-14 (0.302 g, 1.51 mmol, 83%) as a white solid. ¹H NMR (300 MHz, CDCl₃): δ (ppm) 4.63 (s, 1H), 4.15-3.88 (m, 1H), 2.75 (dd, 1H, *J*₁ = 16.5 Hz, *J*₂ = 4.8 Hz), 2.53 (dd, 1H, *J*₁ = 16.5 Hz, *J*₂ = 4.2 Hz), 1.45 (s, 9H), 1.33 (d, 3H, *J* = 6.9 Hz). IR (KBr): ν (cm⁻¹) 3367, 2988, 1684, 1520, 1365, 1252, 1171, 785, 594.

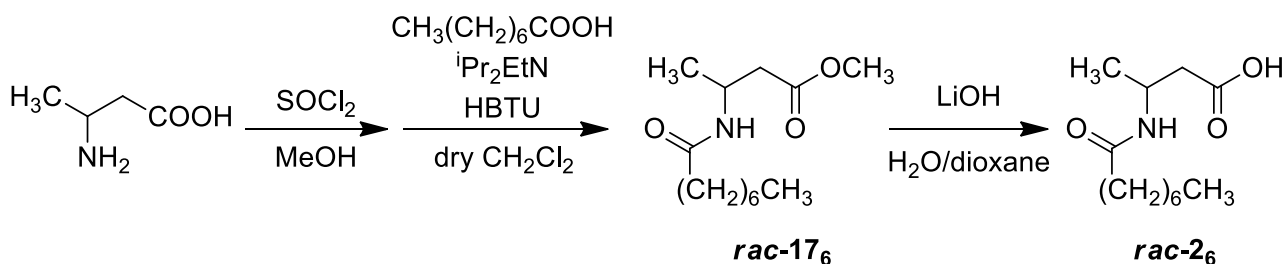
(S)-3-[(*tert*-butoxycarbonyl)amino]butyric acid methyl ester ((S)-15). To the solution of (S)-14 (0.100 g, 0.500 mmol) in EtOH (1.0 ml) was added dropwise to 2M NaOH aq. (1.0 ml) at room temperature and the solution was refluxed at 90 °C for 1 day. The reaction mixture was concentrated under reduced pressure to obtain crude sodium carboxylate as a white powder. To the solution of crude salt in DMF (1.0 ml) was added dropwise iodomethane (57.0 μl, 0.916 mmol) at room temperature and the solution was stirred for 3 days. The remaining solid was filtered off and H₂O was added to the filtrate. The aqueous layer was washed with EtOAc (20 ml × 3) and the organic layer was dried over anhydrous Na₂SO₄ and then concentrated under reduced pressure. The residue was purified by silica-gel column chromatography (eluent; hexane:EtOAc = 3 : 1) to obtain (S)-15 (48.0 mg, 0.206 mmol, 41%) as a white solid. ¹H NMR (300 MHz, CDCl₃): δ (ppm) 4.93 (s, 1H), 4.20-3.95 (m, 1H), 3.69 (s, 3H), 2.58-2.44 (m, 2H), 1.48 (s, 9H), 1.21 (d, 3H, *J* = 6.9 Hz). IR (KBr): ν (cm⁻¹) 3375, 2986, 1741, 1685, 1520, 1440, 1369, 1320, 1205, 1161, 1063, 851, 595.

(S)-3-aminobutyric acid methyl ester *p*-toluenesulfonate ((S)-16). To ethyl acetate (1.0 ml) were added (S)-15 (52.7 mg, 0.226 mmol) and TsOH·H₂O (43.6 mg, 0.229 mmol) at room temperature and the solution was stirred at 50 °C for 30 min. The mixture was stirred at room temperature for 1 day and the precipitate was collected by filtration to obtain (S)-16 (52.2 mg, 0.161 mmol, 71%) as a white powder. ¹H NMR (500 MHz, CD₃OD): δ (ppm) 7.71 (d, 2H, *J* = 8.5 Hz), 7.23 (d, 2H, *J* = 8.5 Hz), 3.74 (s, 3H), 3.74-3.65 (m, 1H), 2.80-2.65 (m, 2H), 2.37 (s, 3H), 1.35-1.32 (m, 3H). IR (KBr): ν (cm⁻¹) 3442, 3032, 2953, 1730, 1626, 1597, 1504, 1451, 1390, 1321, 1227, 1162, 1124, 1035, 1011, 818, 681, 568.

***N*-octanoyl-(S)-3-aminobutyric acid methyl ester ((S)-17₆).** Under a nitrogen atmosphere, to a solution of octanoic acid (91.0 mg, 0.559 mmol) in CH₂Cl₂ (3.0 ml) were added *O*-(Benzotriazol-1-yl)-*N,N,N',N'*-tetramethyluronium hexafluorophosphate (HBTU) (74.6 mg, 0.197 mmol) and the mixture was stirred at 0 °C for 30 min. Then to the mixture were added (S)-16 (52.2 mg, 0.161 mmol) and ¹Pr₂EtN (0.104 g, 0.807 mmol) and the mixture was stirred at room temperature for 12 h. Ethyl acetate was added to the reaction mixture and the organic layer was washed with 1M HCl aq., sat. NaHCO₃ aq. and brine. The organic layer was dried over anhydrous Na₂SO₄ and concentrated under reduced pressure. The residue was purified by silica-gel column chromatography (eluent; hexane:EtOAc = 2 : 1) to obtain (S)-17₆ (25.2 mg, 0.103 mmol, 64%) as a white solid. Mp. 45.5-48.0 °C. ¹H NMR (500 MHz, CDCl₃): δ (ppm) 6.02 (s, 1H), 4.50-4.30 (m, 1H), 3.69 (s, 3H), 2.59-2.48 (m, 2H), 2.14 (t, 2H, *J* = 7.5 Hz), 1.68-1.58 (m, 2H), 1.37-1.25 (m, 8H), 1.22 (d, 3H, *J* = 7.0 Hz), 0.88 (t, 3H, *J* = 7.0 Hz). ¹³C NMR (125 MHz, CDCl₃): δ (ppm) 172.3, 172.3, 51.6, 41.7, 39.7, 36.9, 31.7, 29.2, 29.0, 25.7, 22.6, 20.0, 14.0. IR (KBr): ν (cm⁻¹) 3304, 2926, 1730, 1636, 1550, 1464, 1433, 1377, 1304, 1207, 1144.

***N*-octanoyl-(S)-3-aminobutyric acid ((S)-2₆).** To the solution of (S)-17₆ (25.2 mg, 0.103 mmol) in 1,4-dioxane (10.0 ml) and H₂O (8.0 ml) was added LiOH·H₂O (46.7 mg, 1.11 mmol) at room temperature and the solution was stirred for 1 day. Ethyl acetate was added to the reaction mixture and the organic layer was washed with 1M HCl aq. The organic layer was dried over anhydrous Na₂SO₄ and then concentrated under reduced pressure to obtain (S)-2₆ (50.7 mg, 1.79 mmol, quant.) as a white powder. Mp. 82.6-84.3 °C. ¹H NMR (500 MHz, CD₃OD): δ (ppm) 4.28-4.21 (m, 1H), 2.53 (dd, 1H, *J*₁ = 15.5 Hz, *J*₂ = 6.5 Hz), 2.38 (dd, 1H, *J*₁ = 15.0 Hz, *J*₂ = 7.0 Hz), 2.14 (t, 2H, *J* = 7.5 Hz), 1.65-1.55 (m, 2H), 1.39-1.25 (m, 8H), 1.18 (d, 3H, *J* = 6.5 Hz), 0.90 (t, 3H, *J* = 6.5 Hz). ¹³C NMR (125 MHz, CDCl₃): δ (ppm) 175.3, 173.1, 41.9, 39.9, 36.9, 31.6, 29.2, 29.0, 25.7, 22.6, 20.0, 14.0. IR (KBr): ν (cm⁻¹) 3316, 2923, 1739, 1645, 1540, 1469, 1392, 1249, 1206, 696.

The compound *rac*-2₆ was synthesized following the reactions shown in Scheme S4.



Scheme S4 Synthesis of *rac-26*

***N*-octanoyl-*rac*-3-aminobutyric acid methyl ester (*rac-176*).** Thionyl chloride (425 μ l, 5.86 mmol) was added dropwise to methanol (7.0 ml) at -5 $^{\circ}$ C and stirred for 10 min. *Rac*-3-aminobutyric acid (0.500 g, 4.85 mmol) was added and the mixture was stirred at room temperature for 12 h. The solvent and excess thionyl chloride were distilled off under reduced pressure and the residue was washed with ether to obtain crude ester (0.740 g) as a colorless liquid. Under a nitrogen atmosphere, to a solution of octanoic acid (192 mg, 1.18 mmol) in CH_2Cl_2 (6.0 ml) was added *O*-(Benzotriazol-1-yl)-*N,N,N',N'*-tetramethyluronium hexafluorophosphate (HBTU) (451 mg, 1.19 mmol) and the mixture was stirred at 0 $^{\circ}$ C for 30 min. Then to the mixture were added crude ester (202 mg) and $i\text{Pr}_2\text{EtN}$ (759 mg, 5.87 mmol) and the mixture was stirred at room temperature for 12 h. Ethyl acetate was added to the reaction mixture and the organic layer was washed with 1M HCl aq., sat. NaHCO_3 aq. and brine. The organic layer was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was purified by silica-gel column chromatography (eluent; toluene:EtOAc = 7 : 1) to obtain *rac-176* (238 mg, 0.979 mmol, 74%) as a white solid. Mp. 44.1-46.8 $^{\circ}$ C. ^1H NMR (500 MHz, CDCl_3): δ (ppm) 6.02 (s, 1H), 4.42-4.30 (m, 1H), 3.69 (s, 3H), 2.58-2.47 (m, 2H), 2.14 (t, 2H, $J = 7.5$ Hz), 1.65-1.53 (m, 2H), 1.32-1.23 (m, 11H), 1.22 (d, 3H, $J = 7.0$ Hz), 0.88 (t, 3H, $J = 7.0$ Hz). ^{13}C NMR (125 MHz, CDCl_3): δ (ppm) 172.3, 172.2, 51.6, 41.7, 39.7, 36.9, 31.7, 29.2, 29.0, 25.7, 22.6, 20.0, 14.0. IR (KBr): ν (cm^{-1}) 3303, 2927, 2854, 1744, 1637, 1544, 1436, 1378, 1308, 1207, 1149, 999, 889, 723.

***N*-octanoyl-*rac*-3-aminobutyric acid (*rac-26*).** To the solution of *rac-176* (85.5 mg, 0.351 mmol) in 1,4-dioxane (2.0 ml) and H_2O (1.4 ml) was added $\text{LiOH}\cdot\text{H}_2\text{O}$ (154 mg, 3.66 mmol) at room temperature and the solution was stirred for 6 h. Ethyl acetate was added to the reaction mixture and the organic layer was washed with 1M HCl aq. The organic layer was dried over anhydrous Na_2SO_4 and then concentrated under reduced pressure to obtain *rac-26* (80.7 mg, quant.) as a white powder. Mp. 78.1-80.0 $^{\circ}$ C. ^1H NMR (500 MHz, CD_3OD): δ (ppm) 7.89 (d, 1H, $J = 3.9$ Hz), 4.30-4.20 (m, 1H), 2.51 (dd, 1H, $J_1 = 15.5$ Hz, $J_2 = 6.5$ Hz), 2.38 (dd, 1H, $J_1 = 15.5$ Hz, $J_2 = 7.0$ Hz), 2.14 (t, 2H, $J = 7.5$ Hz), 1.65-1.55 (m, 2H), 1.40-1.30 (m, 8H), 1.18 (d, 3H, $J = 6.5$ Hz), 0.91 (t, 3H, $J = 6.5$ Hz). ^{13}C NMR (125 MHz, CDCl_3): δ (ppm) 175.5, 173.3, 41.9, 39.8, 36.8, 31.6, 29.1, 28.9, 25.7, 22.6, 20.0, 14.0. IR (KBr): ν (cm^{-1}) 3296, 2931, 1703, 1645, 1551, 1405, 1241, 926.

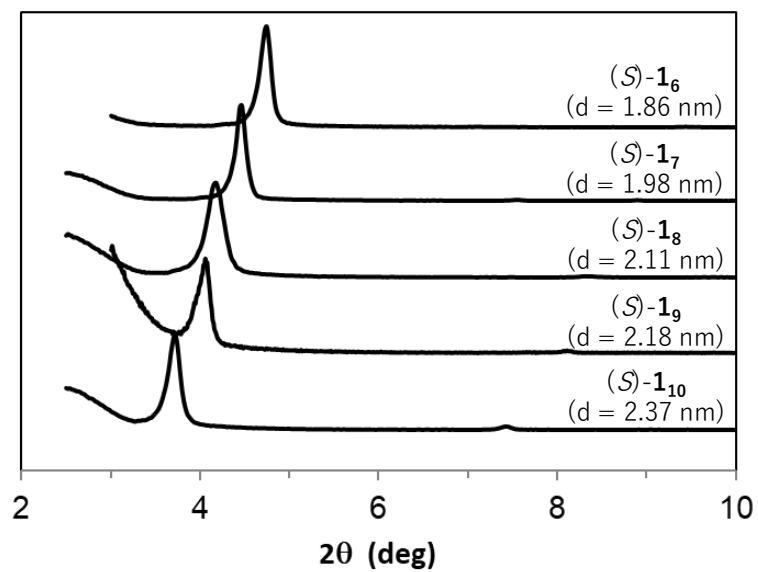


Figure S1. XRD patterns of the xerogels (S)-1_n (n = 6-10).

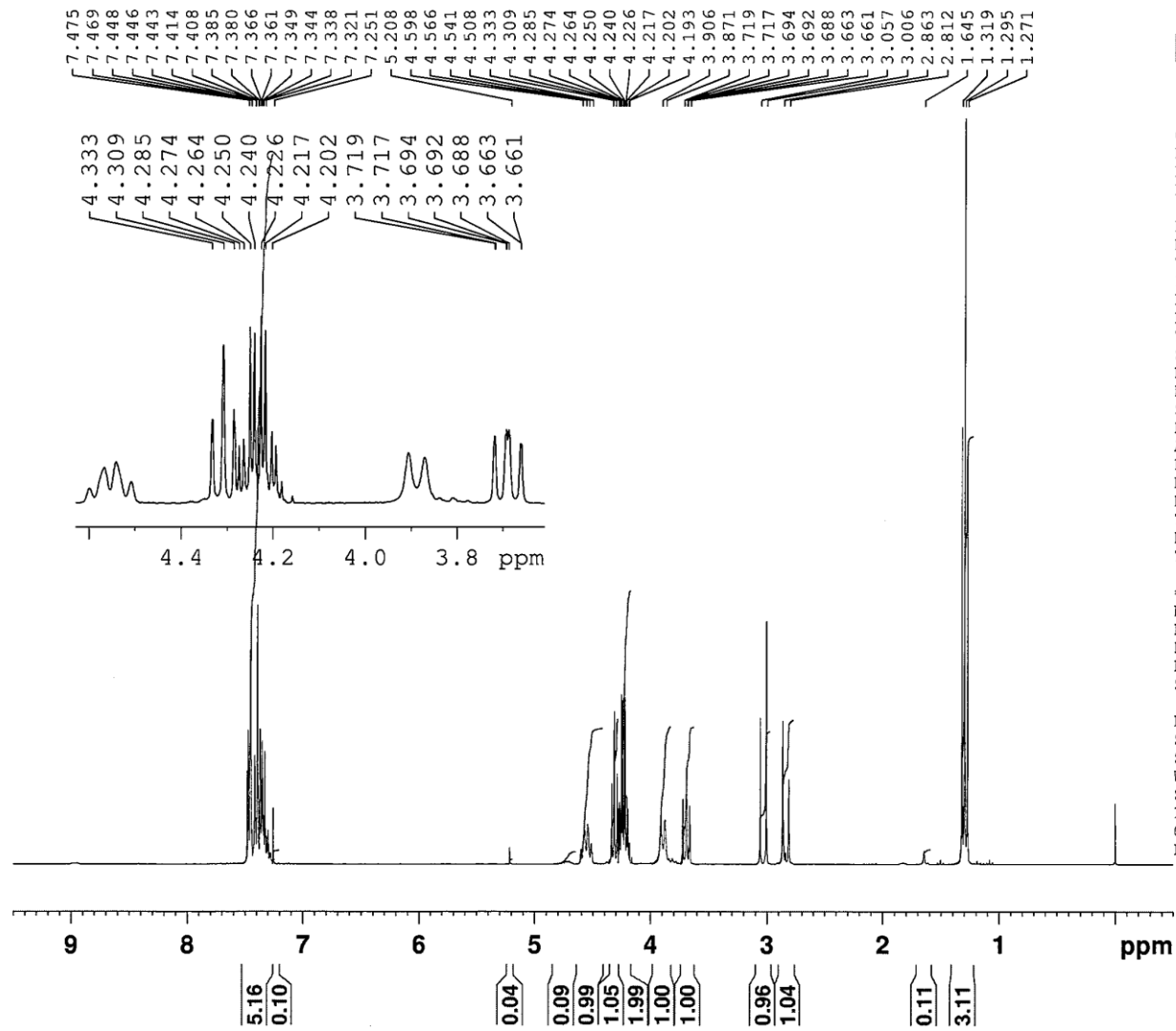
Table S1. Summary of crystallographic data.

	C₆-β-Ala (needle-like)	C₆-β-Ala (plate-like)	rac-1₆
empirical formula	C ₁₁ H ₂₁ NO ₃	C ₁₁ H ₂₁ NO ₃	C ₁₂ H ₂₀ FNO ₃
formula weight	215.29	215.29	283.29
temperature (K)	150	100	100
crystal size (mm)	0.33 × 0.08 × 0.03	0.17 × 0.14 × 0.01	0.33 × 0.05 × 0.02
crystal system	monoclinic	monoclinic	monoclinic
space group	<i>P2₁/c</i>	<i>P2₁</i>	<i>P2₁/n</i>
<i>a</i> (Å)	26.831(6)	5.288(3)	14.394(2)
<i>b</i> (Å)	4.8360(10)	7.448(5)	13.015(2)
<i>c</i> (Å)	9.328(2)	30.857(19)	22.744(4)
<i>α</i> (°)	90	90	90
<i>β</i> (°)	98.963(3)	92.940(7)	94.508(2)
<i>γ</i> (°)	90	90	90
<i>V</i> (Å ³)	1195.5(4)	1213.7(13)	4247.7(12)
<i>Z</i>	4	4	12
<i>D_c</i> (g/cm ³)	1.196	1.178	1.329
<i>μ</i> (MoK _α) (mm ⁻¹)	0.086	0.085	0.119
<i>θ</i> _{min/max} (°)	1.537/24.996	1.322/27.474	1.619/24.998
<i>R</i> 1 [<i>F</i> _o > 2σ(<i>F</i> _o)]	0.0465	0.0791	0.0538
<i>wR</i> 2 (all <i>F</i> _o ²)	0.1241	0.1206	0.1384
GOF	1.009	0.890	0.961
measured reflns	5245	6722	19960
independent reflns	2084	4270	7450
observed reflns	1618	1702	5455
reflns used	2084	4270	7450
parameters	145	279	532
CCDC number	1865320	1865321	1865322

References

- 1) Ishida, Y.; Iwahashi, N.; Nishizono, N.; Saigo, K. *Tetrahedron Lett.* **2009**, *50*, 1889.
- 2) Soloshonok, V. A.; Kukhar, V. P. *Tetrahedron* **1996**, *52*, 6953.
- 3) Sutherland, A.; Willis, C. L. *J. Org. Chem.* **1998**, *63*, 7764.

1H

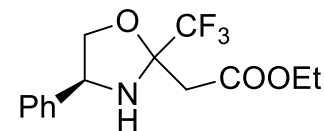


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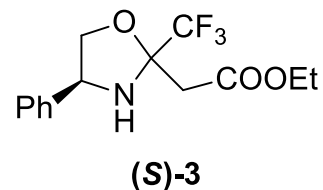
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(S)-3

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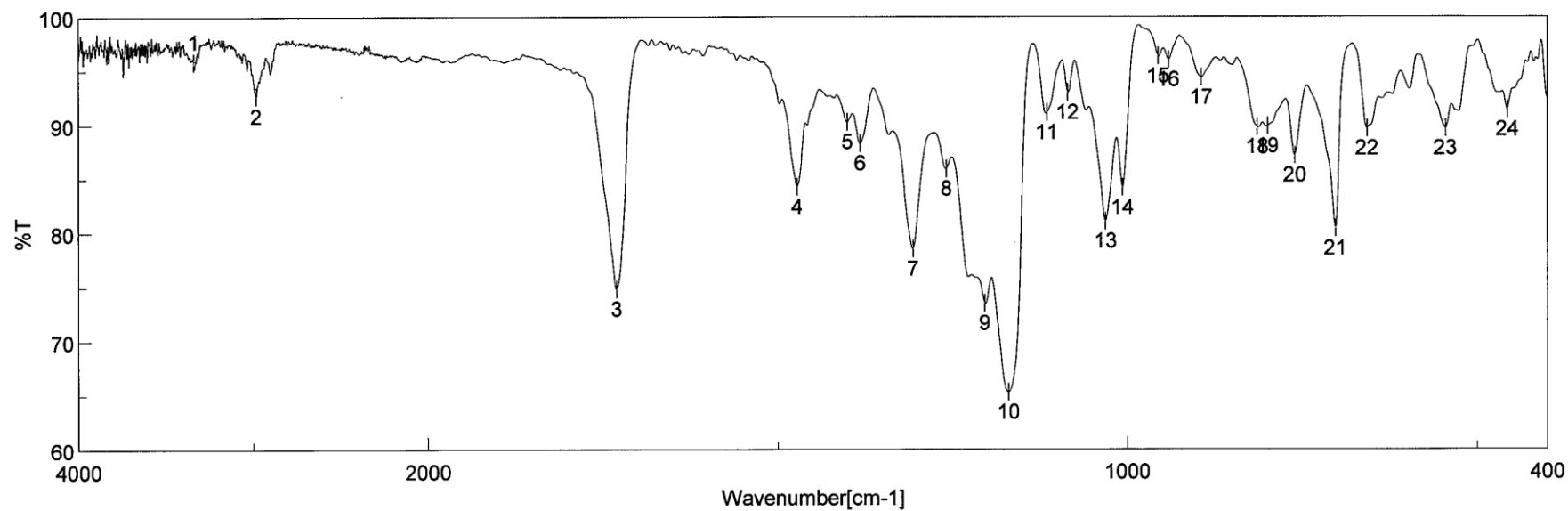
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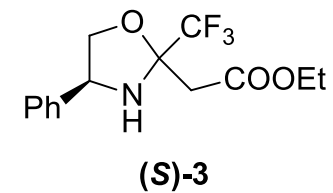


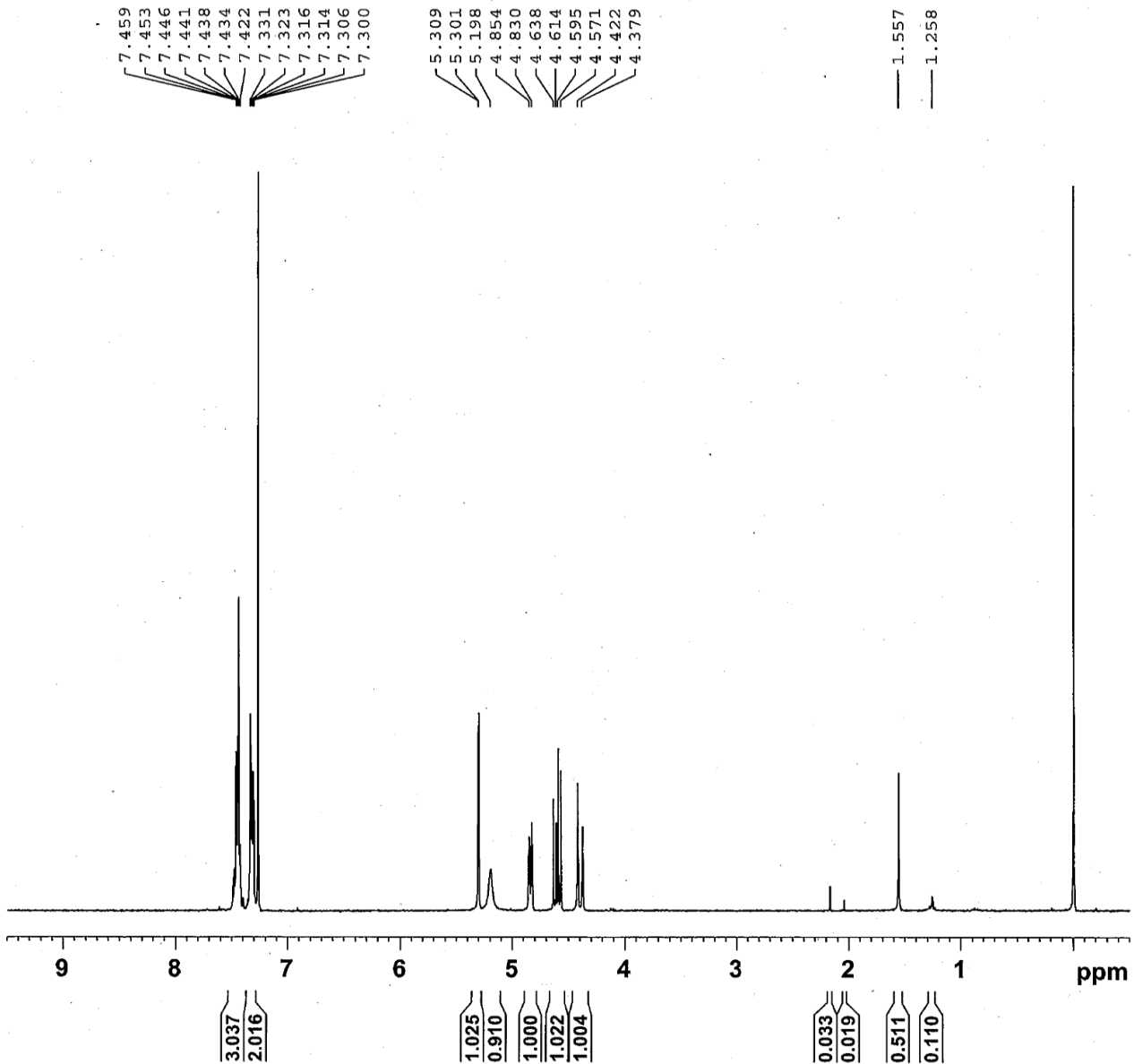


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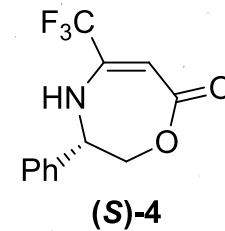
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 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 15.00 usec
 PL1 1.20 dB
 PL1W 8.19348145 W
 SFO1 300.1318534 MHz
 SI 32768
 SF 300.1300056 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



- ACCEPTANCE - System: AV300 OrderNo.: JH033009 Customer: Saitama University Engineer: IKD
 P/N Console: Z108356/162 Shim system: BOSS I original dataset: 104275_0150snf 3 1
 Probe: 5 mm PABBO BB-1H/D Z-GRD Z104275/0150 Sample depth:20 Gas: air
 Sensitivity test for 19F (additional test); Sample: 0,05% TFT in CDC13 (P/N: Z10234)

Sino= 243:1 (signal= -61 - -65 ppm noise= -59.08 - -60.08 ppm [1 ppm] noise range= 4.5 ppm)
 P1= 15usec PL1= -0.3dB



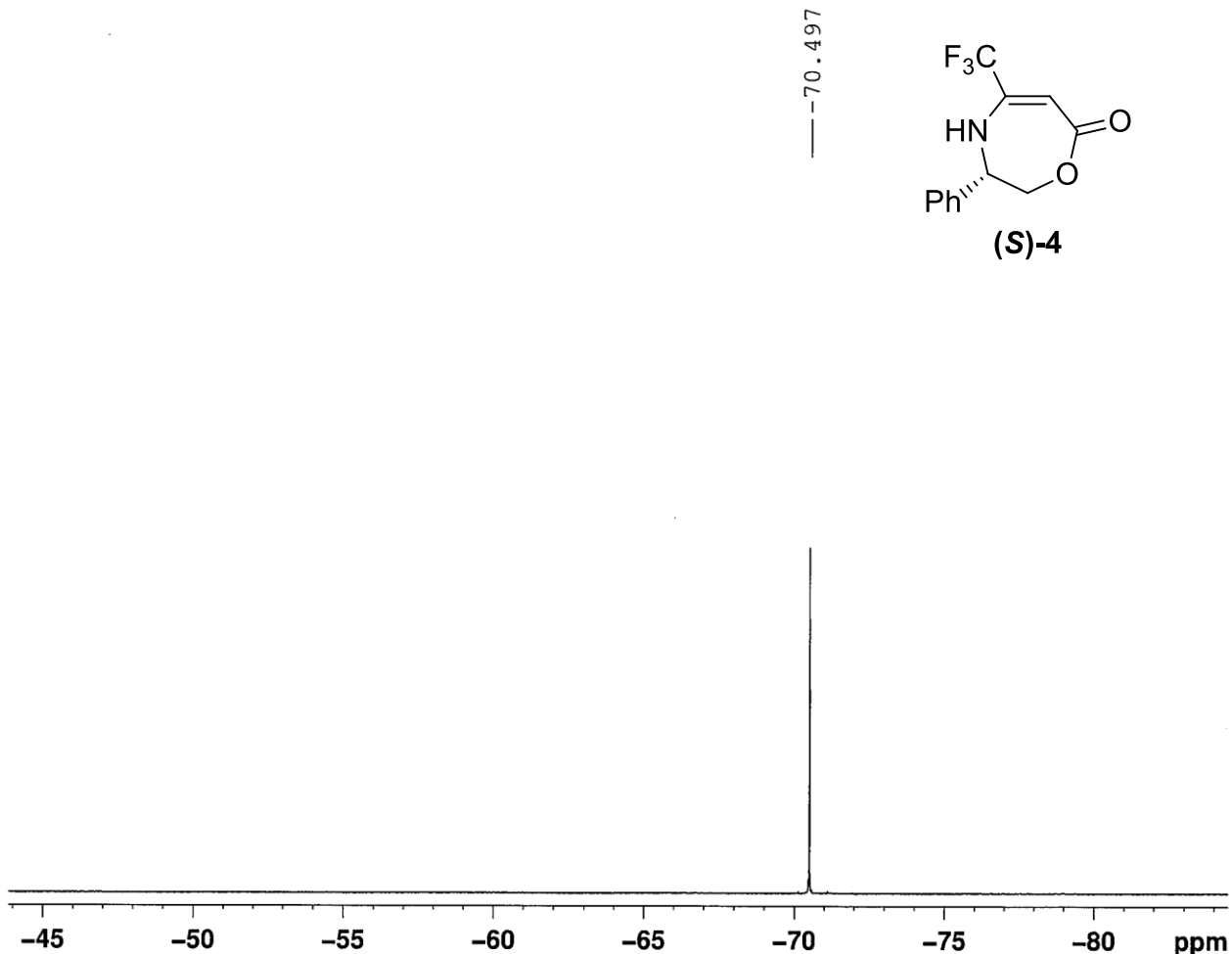
Current Data Parameters
 NAME A12ta020rk
 EXPNO 16011202
 PROCNO 1

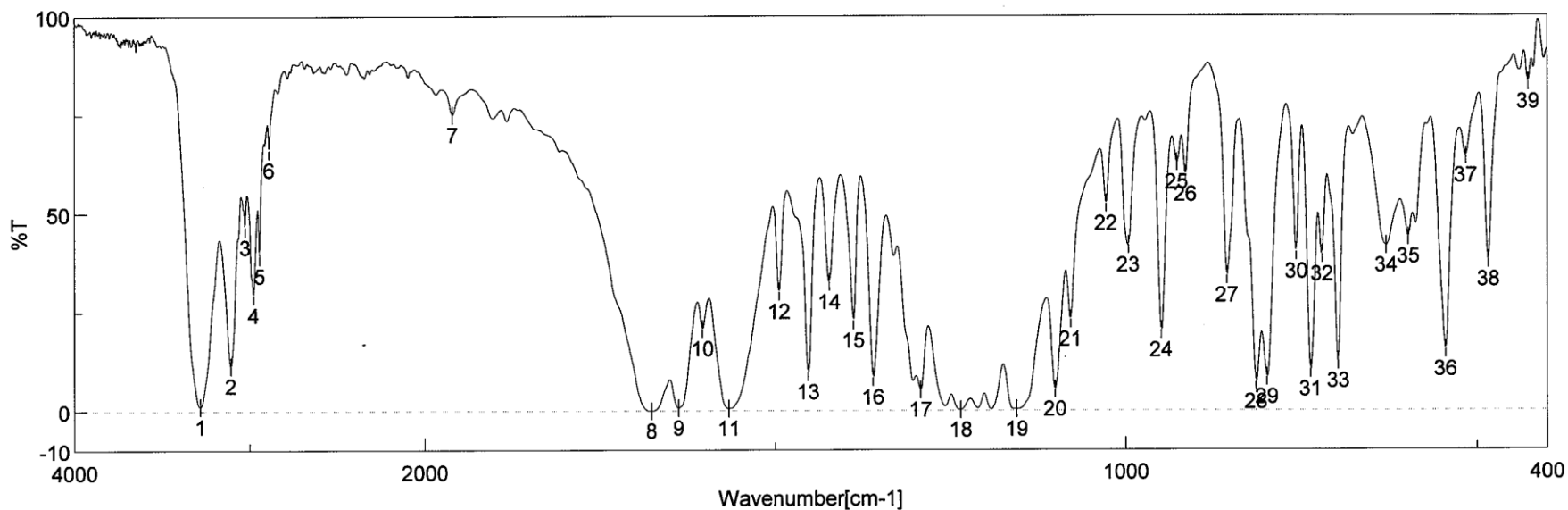
F2 - Acquisition Parameters
 Date_ 20160112
 Time_ 11.57
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgfhigqn
 TD 32768
 SOLVENT CDC13
 NS 2
 DS 0
 SWH 12019.230 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 203
 DW 41.600 usec
 DE 6.50 usec
 TE 297.3 K
 D1 10.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 19F
 P1 15.00 usec
 PL1 -0.30 dB
 PL1W 10.09325600 W
 SFO1 282.3865635 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.58 dB
 PL12 16.50 dB
 PL2W 9.45079708 W
 PL12W 0.24180678 W
 SFO2 300.1300000 MHz

F2 - Processing parameters
 SI 16384
 SF 282.4046280 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.00





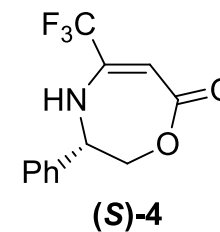
積算回数
ゼロフィリング
ゲイン
測定日時
測定者
ファイル名
サンプル名
コメント

16
ON
16
2016/02/28 15:12
kawamata
Memory#2
enamine (S)-7

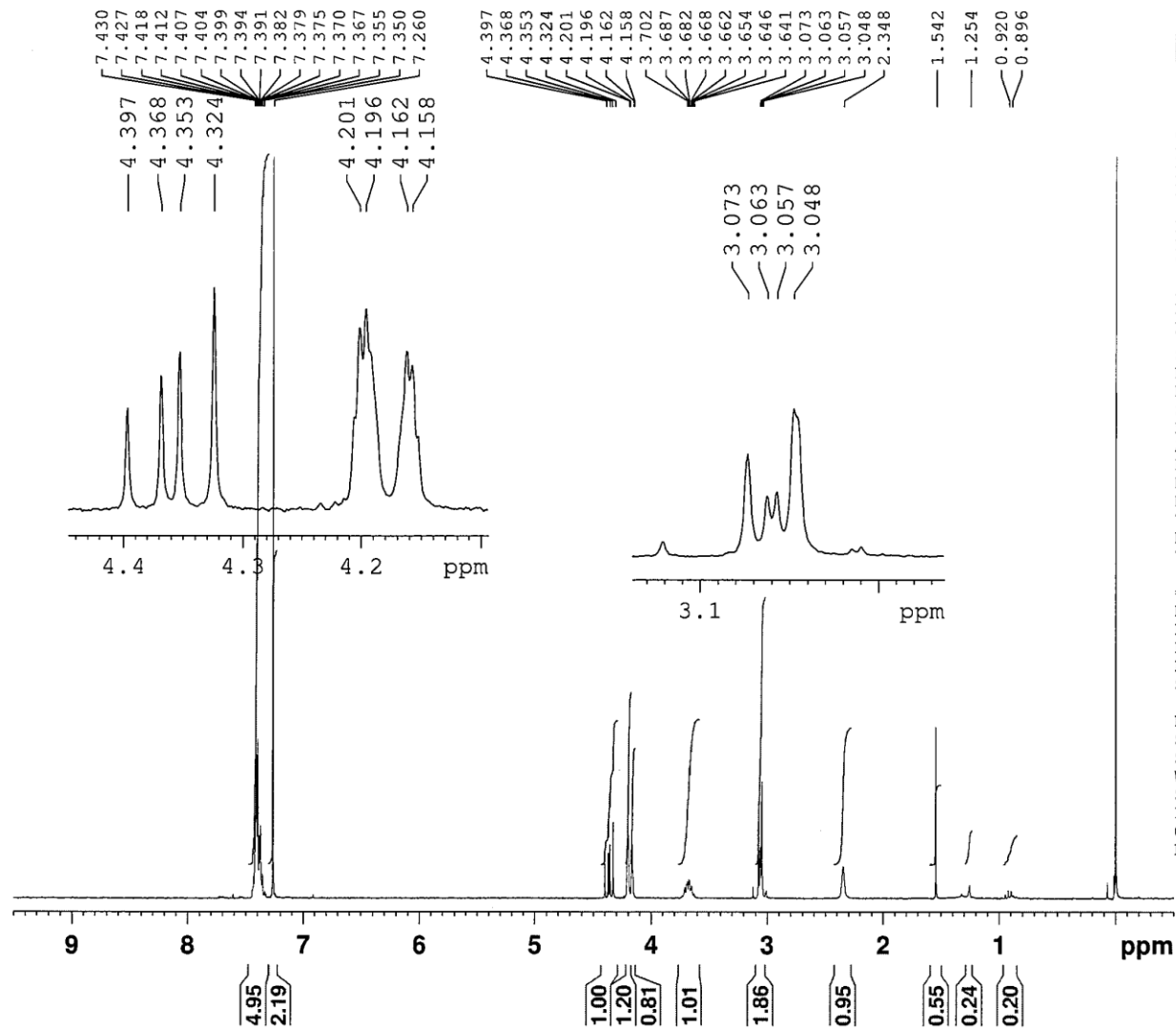
分解
アポダイゼーション
スキャンスピード
更新日時

4 cm-1
Cosine
2 mm/sec
2016/02/28 15:12

1:	3282.25,	1.12	2:	3106.76,	11.44	3:	3026.73,	46.58	4:	2978.52,	29.42
5:	2943.80,	39.26	6:	2888.84,	66.14	7:	1960.29,	75.02	8:	1676.80,	-0.05
9:	1638.23,	0.76	10:	1603.52,	20.77	11:	1565.92,	0.59	12:	1494.56,	30.13
13:	1453.10,	9.79	14:	1423.21,	32.58	15:	1388.50,	22.84	16:	1360.53,	8.48
17:	1293.04,	5.24	18:	1236.15,	0.25	19:	1156.12,	0.38	20:	1101.15,	5.45
21:	1078.98,	23.14	22:	1027.87,	52.44	23:	996.05,	41.92	24:	948.81,	20.40
25:	926.63,	62.88	26:	914.09,	59.81	27:	855.28,	34.25	28:	813.81,	7.23
29:	798.39,	8.52	30:	756.92,	40.24	31:	736.67,	10.45	32:	720.28,	39.55
33:	697.14,	12.53	34:	628.68,	41.76	35:	596.86,	44.02	36:	543.83,	15.49
37:	515.86,	64.48	38:	484.05,	38.21	39:	427.16,	83.22			



1H

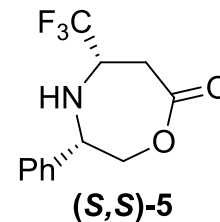


Current Data Parameters
NAME A12ta020rk
EXPNO 15100901
PROCNO 1

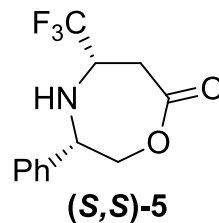
F2 - Acquisition Parameters
Date_ 20151009
Time 13.18
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 203
DW 80.800 usec
DE 6.50 usec
TE 296.8 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 15.00 usec
PL1 1.20 dB
PL1W 8.19348145 W
SFO1 300.1318534 MHz

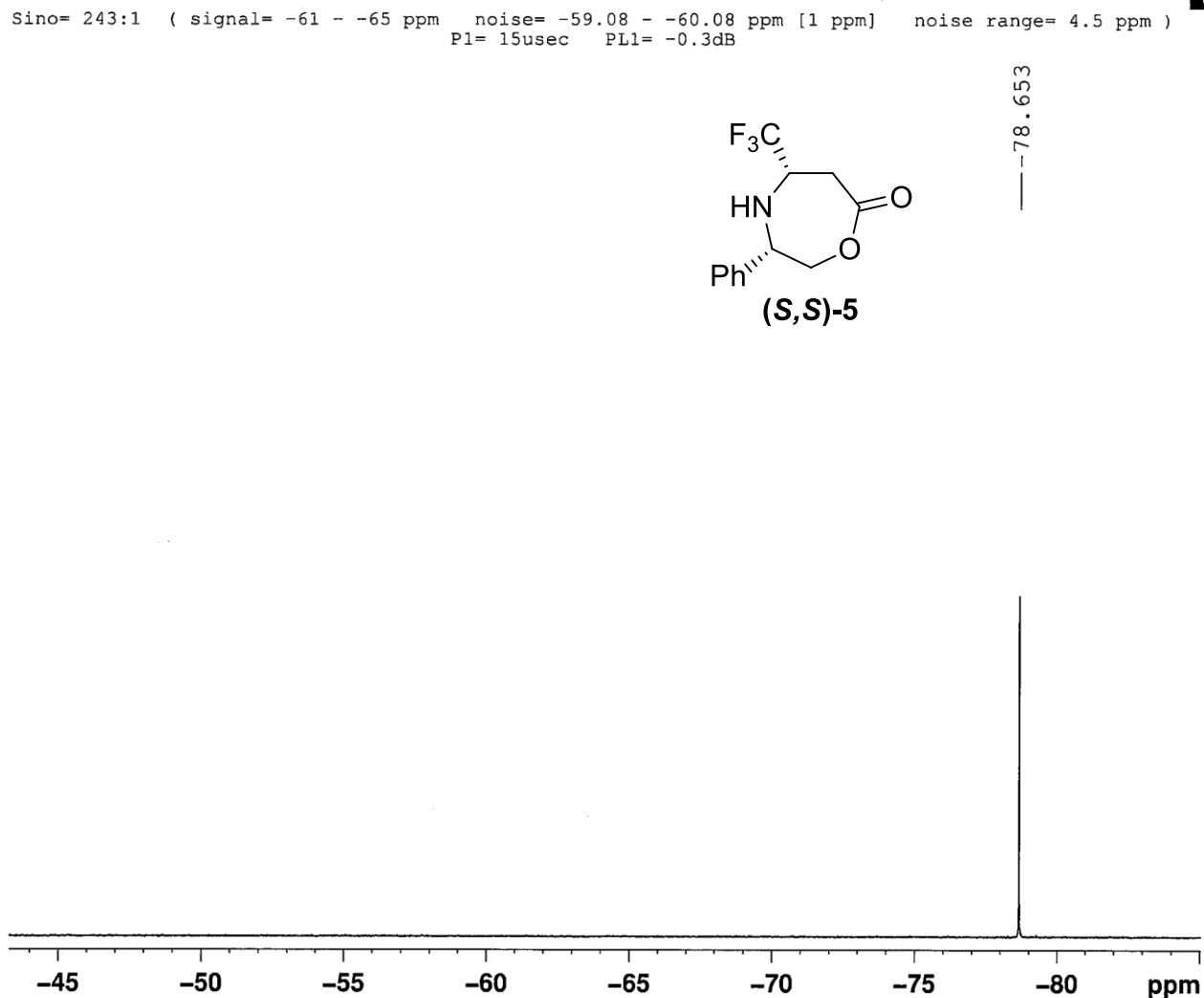
F2 - Processing parameters
SI 32768
SF 300.1300057 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



- ACCEPTANCE - System: AV300 OrderNo.: JH033009 Customer: Saitama University Engineer: IKD
 P/N Console: Z108356/162 Shim system: BOSS I original dataset: 104275_0150snf 3 1
 Probe: 5 mm PABBO BB-1H/D Z-GRD Z104275/0150 Sample depth:20 Gas: air
 Sensitivity test for 19F (additional test); Sample: 0,05% TFT in CDC13 (P/N: Z10234)
 Sino= 243:1 (signal= -61 - -65 ppm noise= -59.08 - -60.08 ppm [1 ppm] noise range= 4.5 ppm)
 P1= 15usec PL1= -0.3dB



---78.653



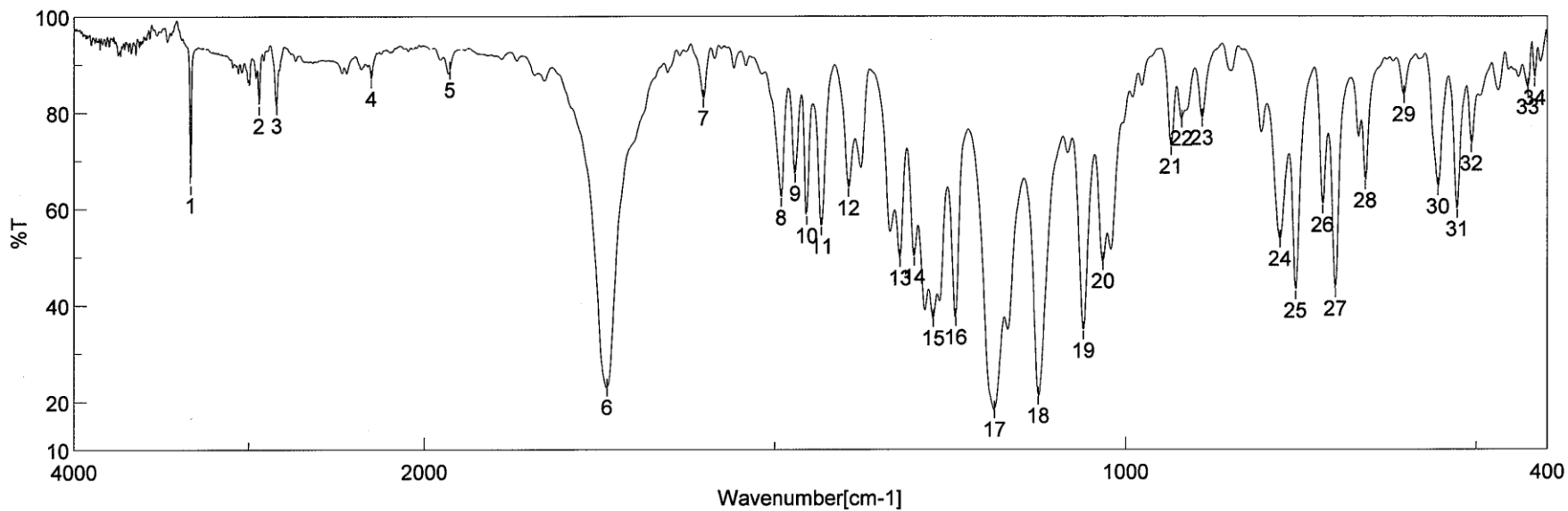
Current Data Parameters
 NAME A12ta020rk
 EXPNO 15100904
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20151009
 Time 14.48
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgfhigqn
 TD 32768
 SOLVENT CDC13
 NS 8
 DS 0
 SWH 12019.230 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 203
 DW 41.600 usec
 DE 6.50 usec
 TE 296.7 K
 D1 10.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 19F
 P1 15.00 usec
 PL1 -0.30 dB
 PL1W 10.09325600 W
 SFO1 282.3865635 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.58 dB
 PL12 16.50 dB
 PL2W 9.45079708 W
 PL12W 0.24180678 W
 SFO2 300.1300000 MHz

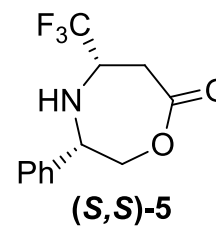
F2 - Processing parameters
 SI 16384
 SF 282.4046357 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.00



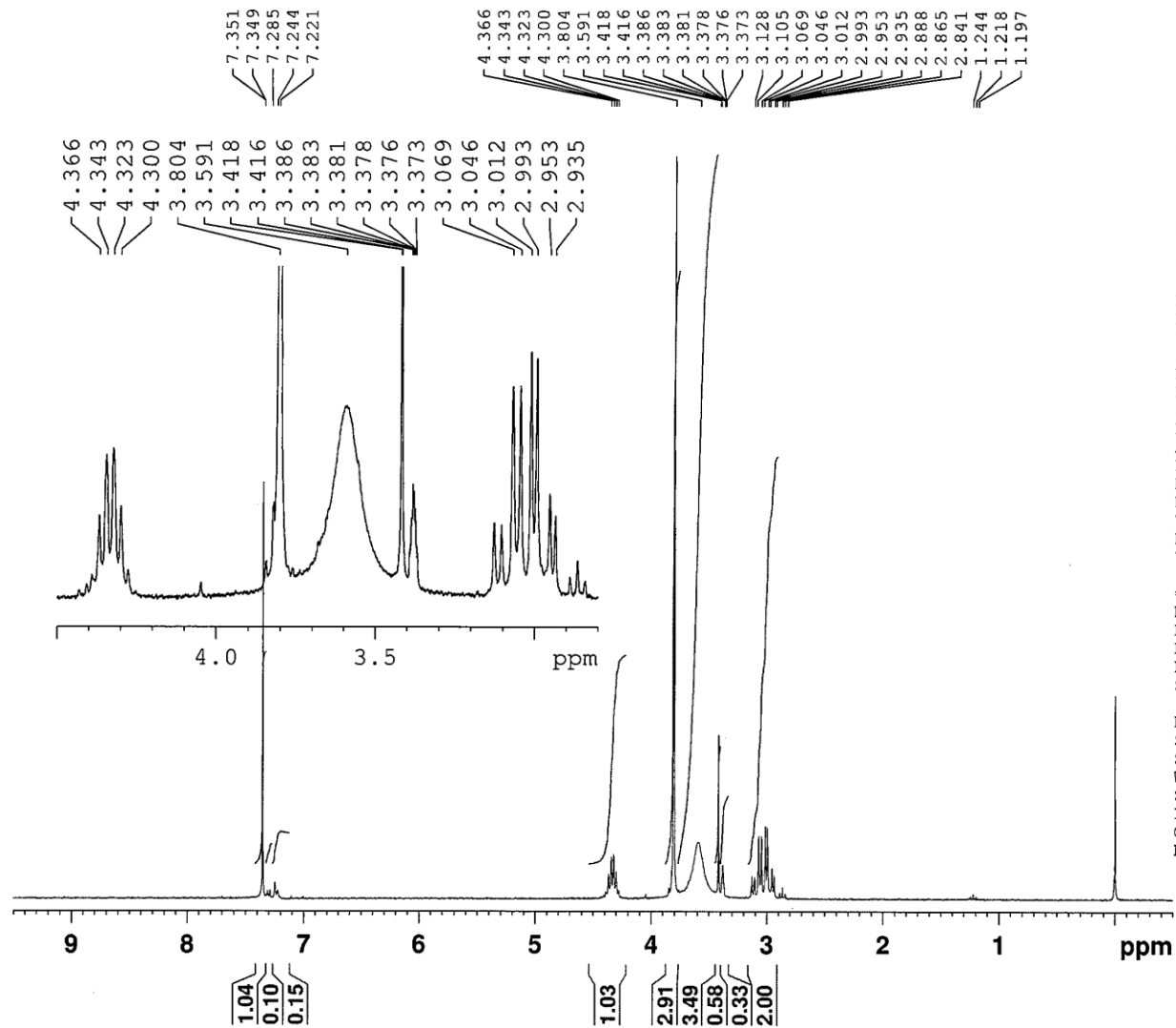
積算回数 16
 ゼロフィリング ON
 ゲイン 8
 測定日時 2016/02/28 15:23
 測定者 kawamata
 ファイル名 Memory#2
 サンプル名 lactone (3S, 5S)-8
 コメント

分解 4 cm-1
 アポダイゼーション Cosine
 スキャンスピード 2 mm/sec
 更新日時 2016/02/28 15:24

1:	3332.39,	64.87	2:	2941.88,	81.41	3:	2841.60,	81.46	4:	2300.66,	87.07
5:	1963.18,	88.86	6:	1739.48,	22.95	7:	1601.59,	82.98	8:	1490.70,	62.31
9:	1470.46,	67.31	10:	1454.06,	58.54	11:	1432.85,	56.32	12:	1394.28,	64.34
13:	1321.00,	49.77	14:	1300.75,	50.00	15:	1273.75,	37.25	16:	1241.93,	37.49
17:	1186.97,	18.29	18:	1124.30,	21.18	19:	1059.69,	34.70	20:	1031.73,	49.12
21:	935.31,	72.92	22:	919.88,	78.76	23:	890.95,	78.92	24:	779.10,	53.76
25:	756.92,	42.99	26:	718.35,	60.83	27:	700.03,	43.42	28:	657.61,	65.88
29:	602.65,	83.82	30:	554.43,	64.64	31:	527.44,	59.93	32:	507.19,	73.57
33:	428.12,	85.33	34:	418.48,	87.20						



1H

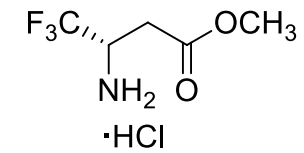


Current Data Parameters
NAME A12ta020rk
EXPNO 15112704
PROCNO 1

F2 - Acquisition Parameters
Date_ 20151127
Time 16.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 203
DW 80.800 usec
DE 6.50 usec
TE 297.0 K
D1 1.00000000 sec
TDO 1

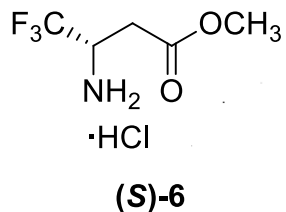
==== CHANNEL f1 =====
NUC1 1H
P1 15.00 usec
PL1 1.20 dB
PL1W 8.19348145 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1299784 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

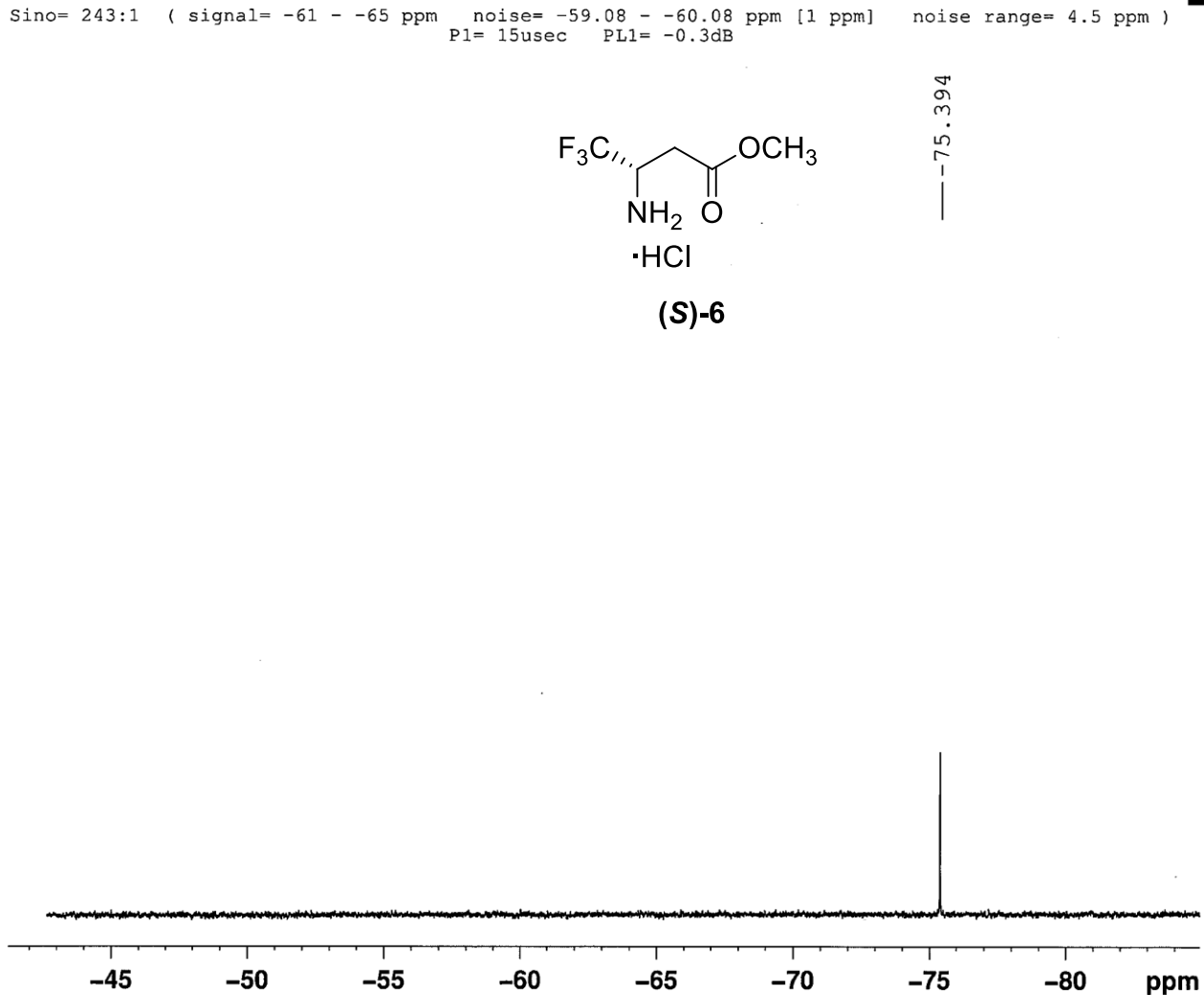


(S)-6

- ACCEPTANCE - System: AV300 OrderNo.: JH033009 Customer: Saitama University Engineer: IKD
 P/N Console: Z108356/162 Shim system: BOSS I original dataset: 104275_0150snf 3 1
 Probe: 5 mm PABBO BB-1H/D Z-GRD Z104275/0150 Sample depth:20 Gas: air
 Sensitivity test for 19F (additional test); Sample: 0,05% TFT in CDC13 (P/N: Z10234)
 Sino= 243:1 (signal= -61 - -65 ppm noise= -59.08 - -60.08 ppm [1 ppm] noise range= 4.5 ppm)
 P1= 15usec PL1= -0.3dB



---75.394



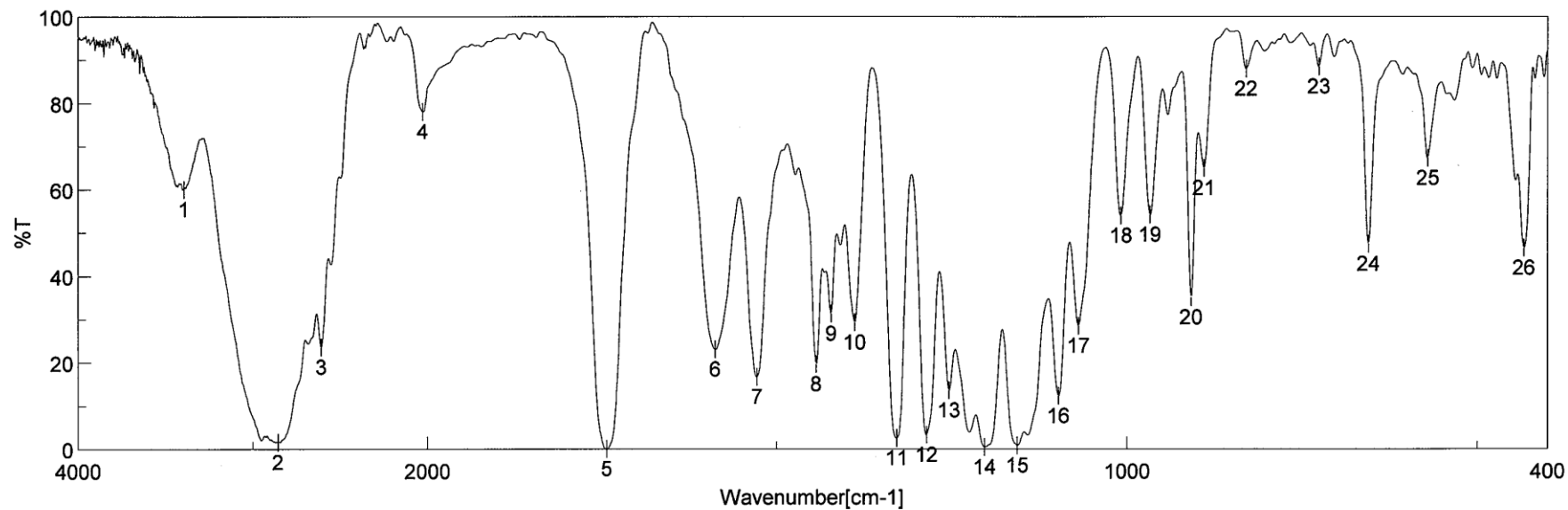
Current Data Parameters
 NAME A12ta020rk
 EXPNO 15101302
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20151013
 Time 13.07
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgfhigqn
 TD 32768
 SOLVENT CDC13
 NS 8
 DS 0
 SWH 12019.230 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 203
 DW 41.600 usec
 DE 6.50 usec
 TE 296.7 K
 D1 10.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 19F
 P1 15.00 usec
 PL1 -0.30 dB
 PL1W 10.09325600 W
 SFO1 282.3865635 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.58 dB
 PL12 16.50 dB
 PL2W 9.45079708 W
 PL12W 0.24180678 W
 SFO2 300.1300000 MHz

F2 - Processing parameters
 SI 16384
 SF 282.4046252 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.00



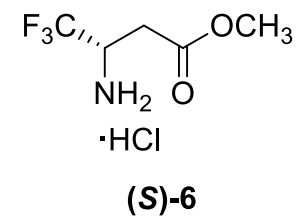
積算回数
ゼロフィリング
ゲイン
測定日時
測定者
ファイル名
サンプル名
コメント

16
ON
32
2016/02/28 15:39
kawamata
Memory#2
(S)-9

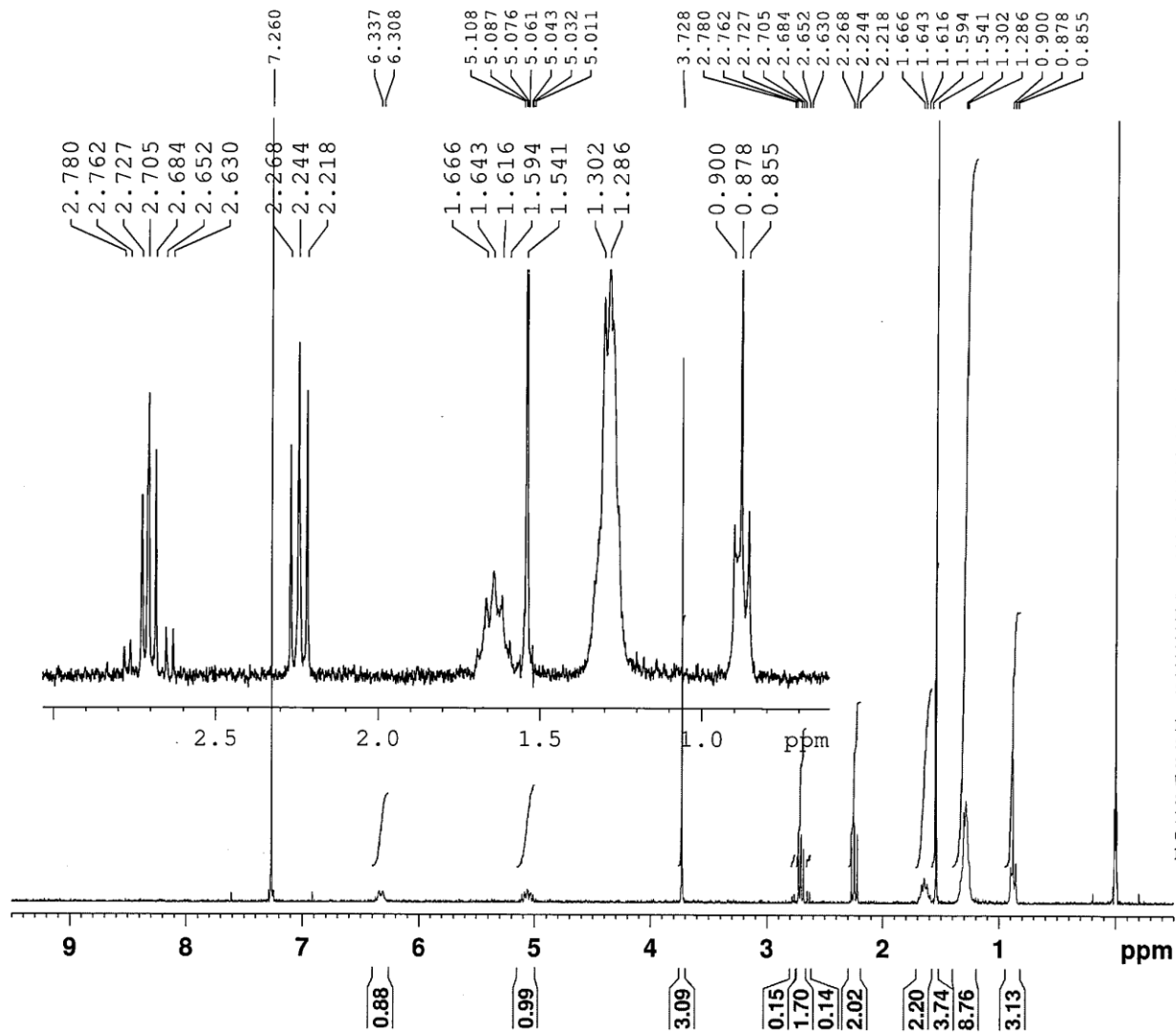
分解
アポダイゼーション
スキャンスピード
更新日時

4 cm-1
Cosine
2 mm/sec
2016/02/28 15:41

1:	3395.07,	60.07	2:	2856.06,	1.62	3:	2608.25,	23.62	4:	2026.82,	78.08
5:	1744.30,	0.10	6:	1588.09,	23.07	7:	1528.31,	16.80	8:	1443.46,	19.68
9:	1422.24,	31.37	10:	1388.50,	29.32	11:	1328.71,	2.62	12:	1286.29,	3.39
13:	1254.47,	13.63	14:	1203.36,	0.55	15:	1157.08,	0.95	16:	1098.26,	12.38
17:	1069.33,	28.57	18:	1008.59,	53.99	19:	967.13,	54.20	20:	908.31,	35.08
21:	889.99,	64.98	22:	830.21,	88.01	23:	726.07,	88.48	24:	654.71,	47.48
25:	569.86,	67.33	26:	433.91,	46.55						



1H

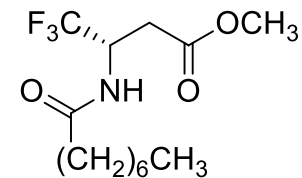


Current Data Parameters
 NAME A12ta020rk
 EXPNO 16020301
 PROCNO 1

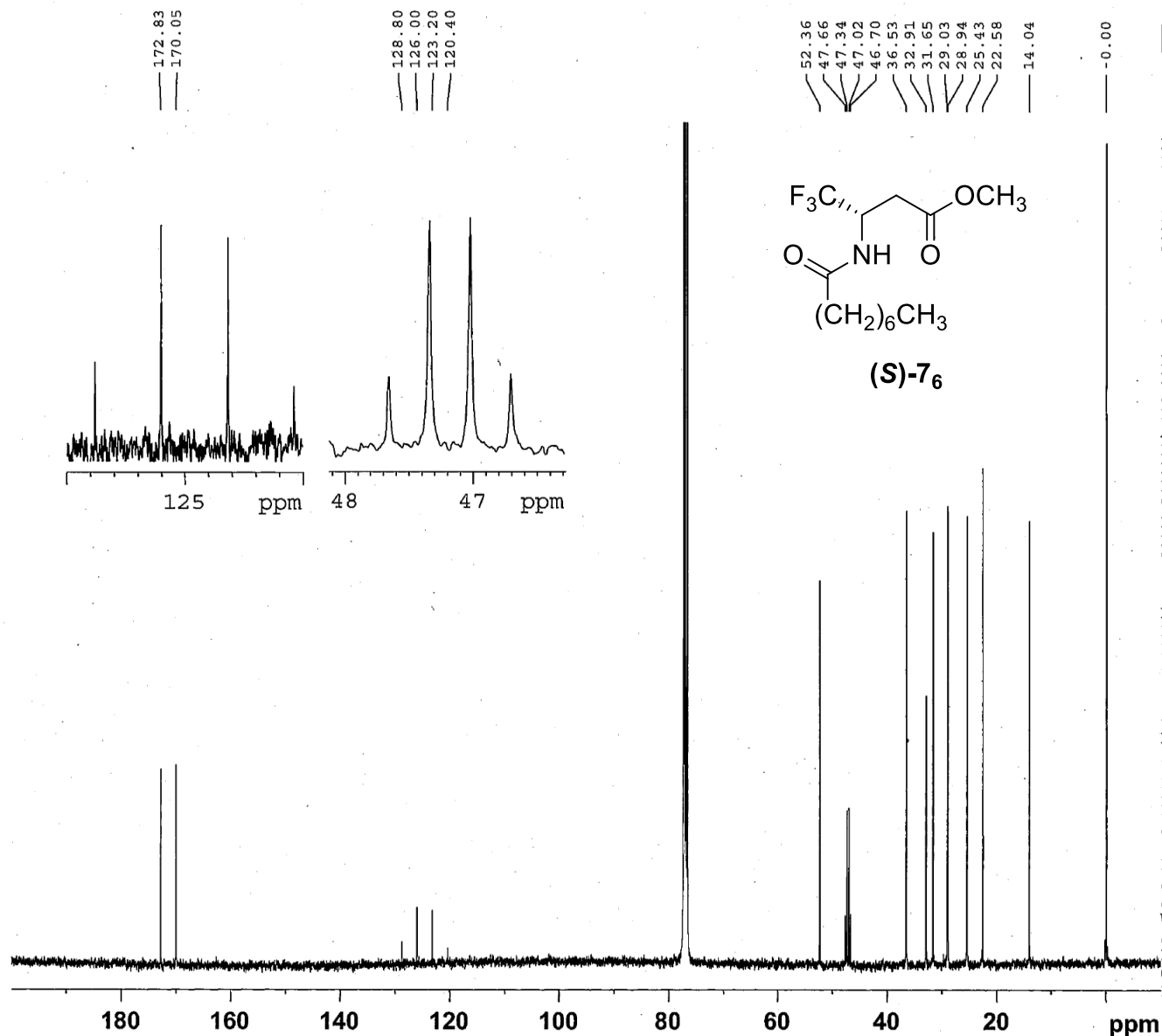
F2 - Acquisition Parameters
 Date_ 20160203
 Time 15.47
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 8
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953587 sec
 RG 203
 DW 80.800 usec
 DE 6.50 usec
 TE 297.2 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 15.00 usec
 PL1 1.20 dB
 PL1W 8.19348145 W
 SFO1 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300059 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



13C with dec. CPQNP



Current Data Parameters
 NAME kodama
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170807
 Time 18.39
 INSTRUM spect
 PROBHD 5 mm CPQNP 1H/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 2
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010548 sec
 RG 126.99
 DW 16.800 usec
 DE 18.00 usec
 TE 300.0 K
 D1 2.0000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 13C
 P1 12.00 usec
 PLW1 15.50000000 W
 SFO1 100.6248425 MHz

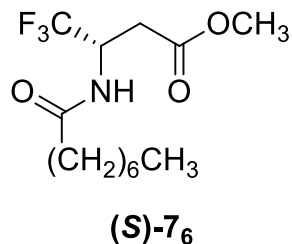
==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PLW2 5.19999981 W
 PLW12 0.14444000 W
 PLW13 0.11700000 W
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127668 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.40

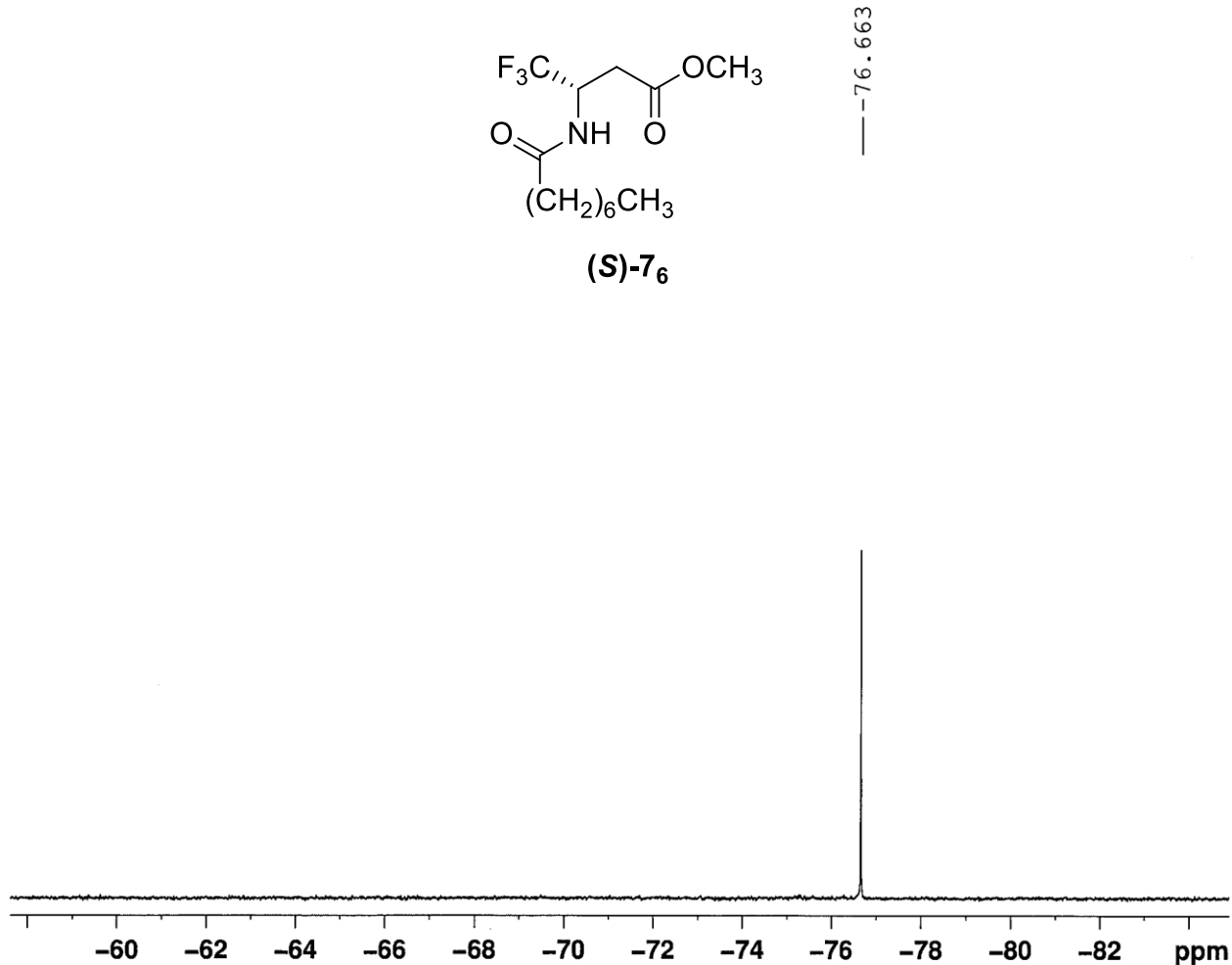
- ACCEPTANCE - System: AV300 OrderNo.: JH033009 Customer: Saitama University Engineer: IKD
 P/N Console: Z108356/162 Shim system: BOSS I original dataset: 104275_0150snf 3 1
 Probe: 5 mm PABBO BB-1H/D Z-GRD Z104275/0150 Sample depth:20 Gas: air
 Sensitivity test for 19F (additional test); Sample: 0,05% TFT in CDC13 (P/N: Z10234)



Sino= 243:1 (signal= -61 - -65 ppm noise= -59.08 - -60.08 ppm [1 ppm] noise range= 4.5 ppm)
 P1= 15usec PL1= -0.3dB



---76.663



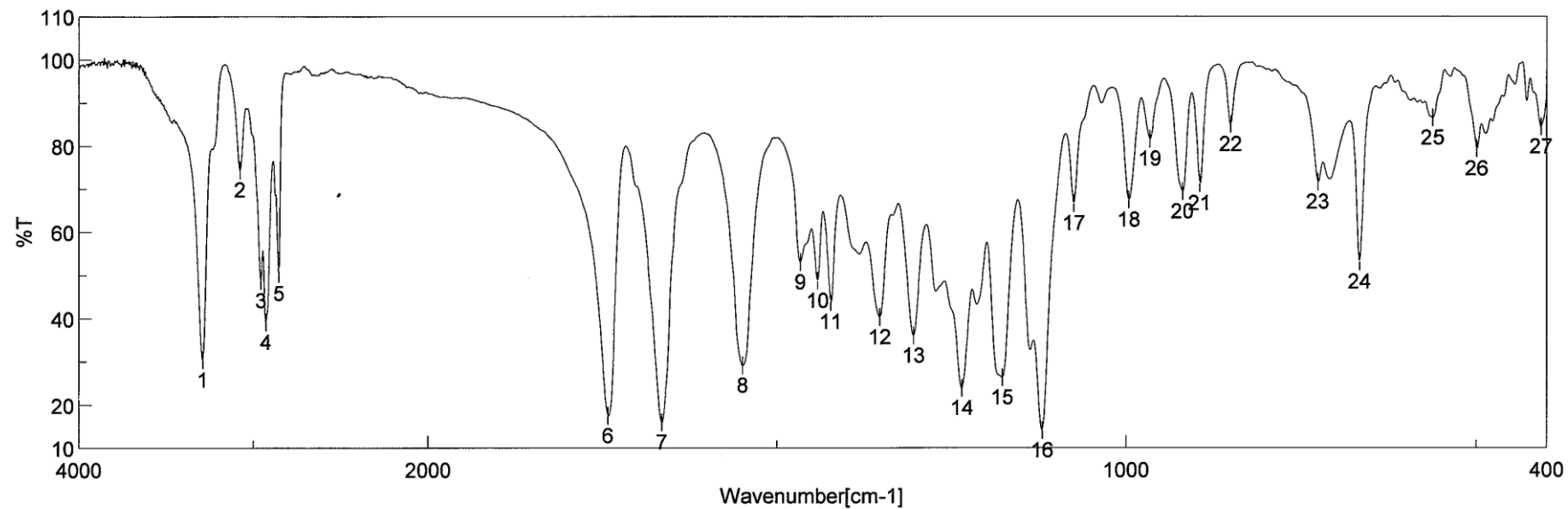
Current Data Parameters
 NAME A12ta020rk
 EXPNO 16020202
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160202
 Time_ 10.08
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgfhigqn
 TD 32768
 SOLVENT CDC13
 NS 1
 DS 0
 SWH 12019.230 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 203
 DW 41.600 usec
 DE 6.50 usec
 TE 297.2 K
 D1 10.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 19F
 P1 15.00 usec
 PL1 -0.30 dB
 PL1W 10.09325600 W
 SFO1 282.3865635 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.58 dB
 PL12 16.50 dB
 PL2W 9.45079708 W
 PL12W 0.24180678 W
 SFO2 300.1300000 MHz

F2 - Processing parameters
 SI 16384
 SF 282.4046312 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.00



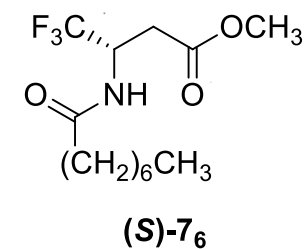
積算回数
ゼロフィリング
ゲイン
測定日時
測定者
ファイル名
サンプル名
コメント

16
ON
16
2016/02/04 17:07
wangxy kawamata
16020401
~~poly-phenol-methol~~
(s)-r0

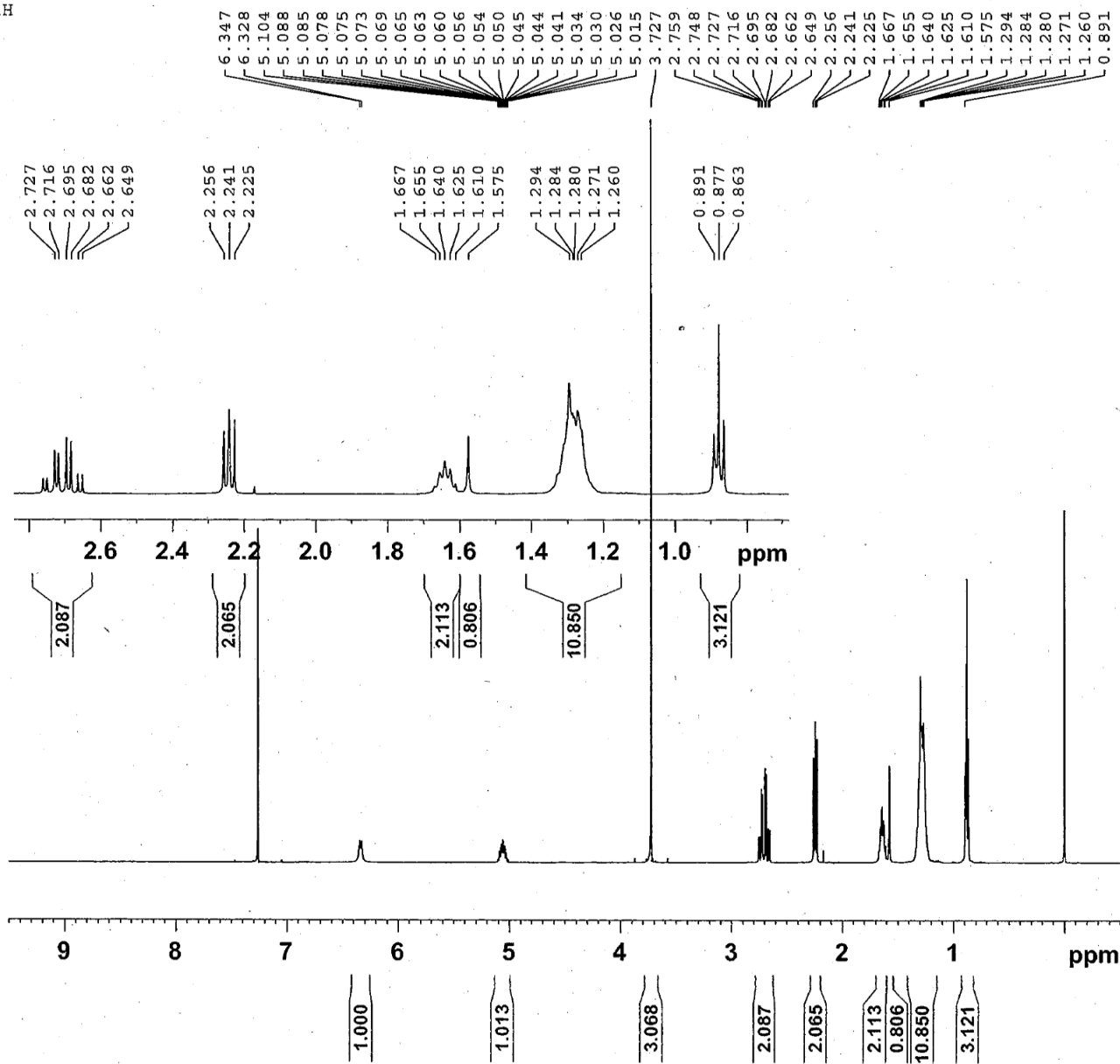
分解
アポダイゼーション
スキャンスピード
更新日時

4 cm-1
Cosine
2 mm/sec
2016/02/29 16:10

1:	3288.04,	30.44	2:	3075.90,	74.41	3:	2957.30,	48.79	4:	2929.34,	39.15
5:	2853.17,	50.45	6:	1741.41,	17.47	7:	1664.27,	15.95	8:	1548.56,	29.14
9:	1466.60,	53.07	10:	1441.53,	48.77	11:	1422.24,	43.88	12:	1351.86,	40.36
13:	1303.64,	36.06	14:	1234.22,	23.93	15:	1176.36,	26.37	16:	1119.48,	14.13
17:	1074.16,	66.73	18:	996.05,	67.49	19:	966.16,	81.70	20:	918.91,	69.45
21:	893.84,	71.37	22:	849.49,	85.02	23:	725.10,	71.68	24:	665.32,	53.20
25:	561.18,	86.57	26:	499.47,	79.43	27:	407.87,	84.54			

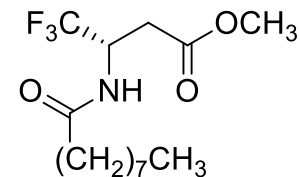


1H

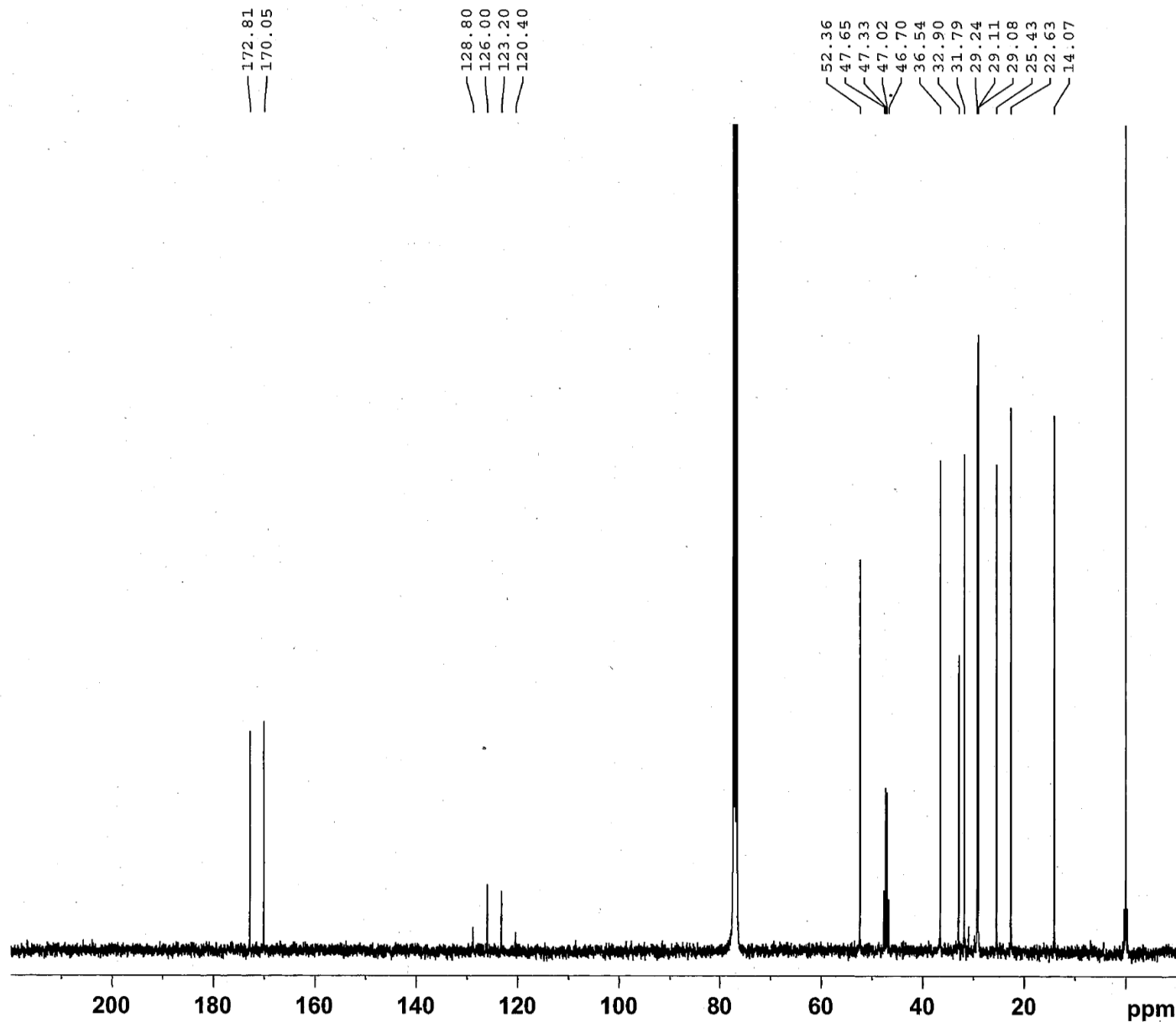


NAME A16mc211rk
 EXPNO 17091102
 PROCNO 1
 Date 20170911
 Time 15.49
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719923 sec
 RG 203
 DW 48.400 usec
 DE 6.50 usec
 TE 300.9 K
 D1 1.00000000 sec
 TD0 1

----- CHANNEL f1 -----
 NUC1 1H
 P1 11.80 usec
 PL1 2.40 dB
 PL1W 15.17711735 W
 SFO1 500.0330885 MHz
 SI 32768
 SF 500.0300102 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

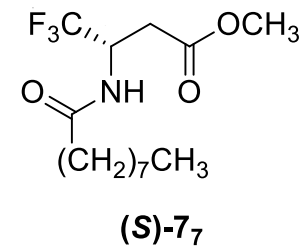


! with dec. CPQ

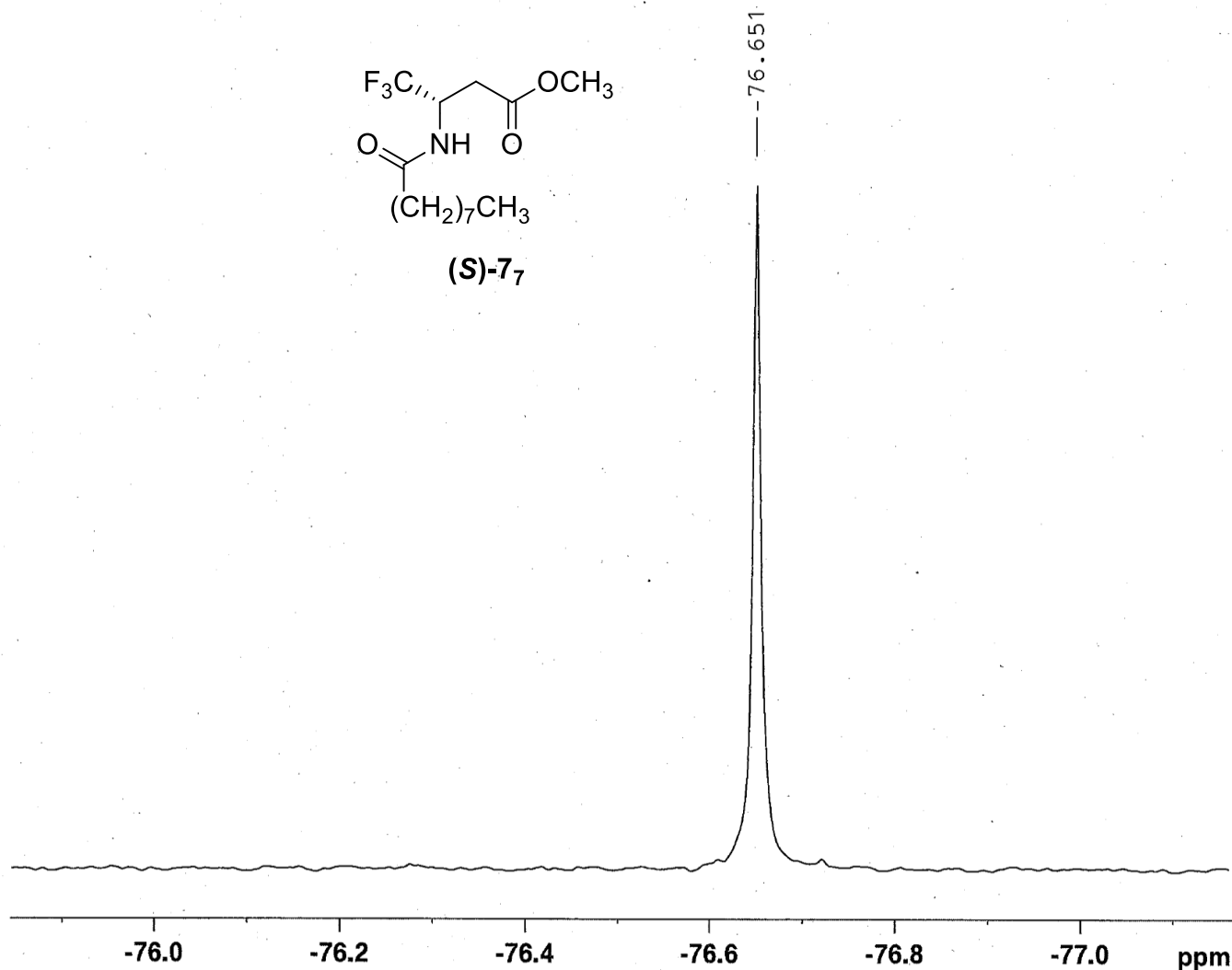
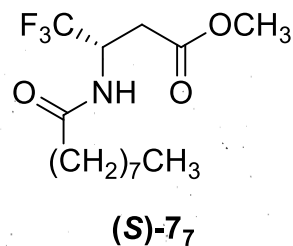


NAME kodama
EXPNO 3
PROCNO 1
Date_ 20170912
Time_ 18.16
INSTRUM spect
PROBHD 5 mm CPQNP 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 464
DS 2
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 126.99
DW 16.800 usec
DE 18.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

==== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
SI 32768
SF 100.6127670 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40



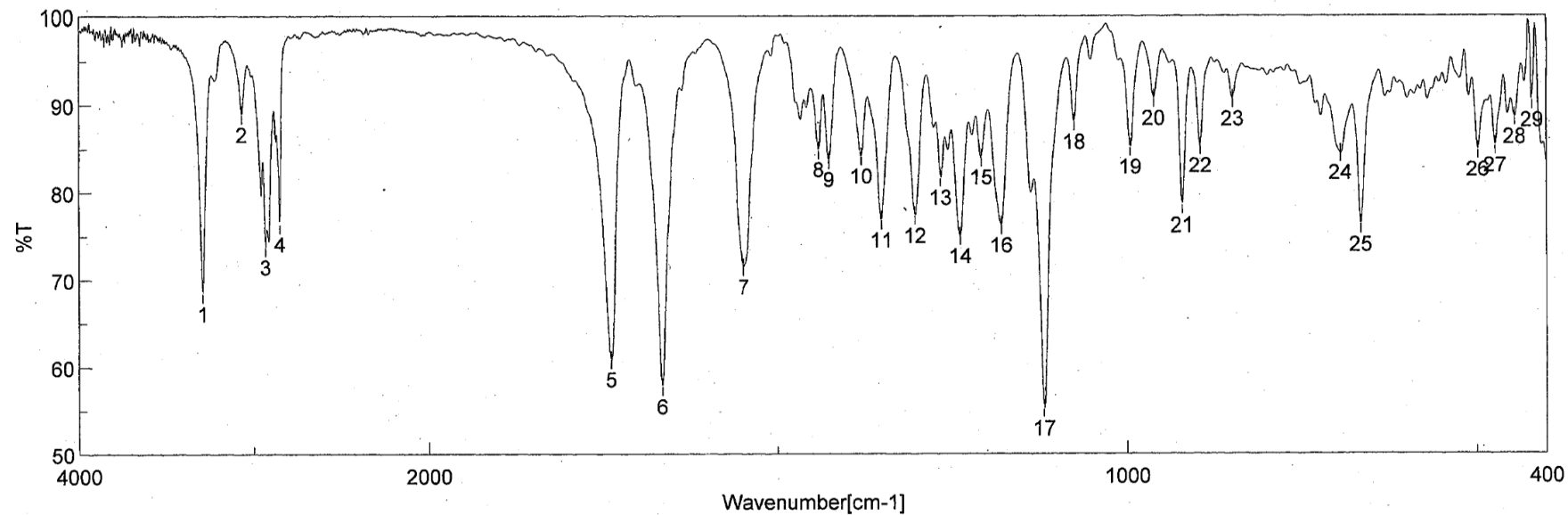
- ACCEPTANCE - System: AV300 OrderNo.: JH033009 Customer: Saitama University Engineer: IKD
 P/N Console: Z108356/162 Shim system: BOSS I original dataset: 104275_0150snf 3 1
 Probe: 5 mm PABBO BB-1H/D Z-GRD Z104275/0150 Sample depth:20 Gas: air
 Sensitivity test for 19F (additional test); Sample: 0,05% TFT in CDC13 (P/N: Z10234)
 Sino= 243:1 (signal= -61 - -65 ppm noise= -59.08 - -60.08 ppm [1 ppm] noise range= 4.5 ppm)
 P1= 15usec PL1= -0.3dB



NAME	A16mc211rk
EXPNO	16100405
PROCNO	1
Date_	20161004
Time	17.21
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgfhigqn
TD	32768
SOLVENT	CDC13
NS	1
DS	0
SWH	12019.230 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	41.600 usec
DE	6.50 usec
TE	296.7 K
D1	10.0000000 sec
D11	0.03000000 sec
D12	0.00002000 sec
TD0	1

===== CHANNEL f1 =====	
NUC1	19F
P1	15.00 usec
PL1	-0.30 dB
PL1W	10.09325600 W
SFO1	282.3865635 MHz

===== CHANNEL f2 =====	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.58 dB
PL12	16.50 dB
PL2W	9.45079708 W
PL12W	0.24180678 W
SFO2	300.1300000 MHz
SI	16384
SF	282.4046276 MHz
WDW	EM
SSB	0
LB	2.00 Hz
GB	0
PC	1.00



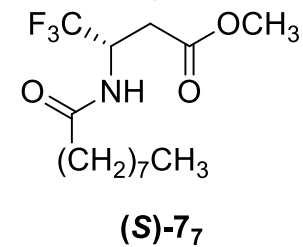
積算回数
ゼロフィリング
ゲイン
測定日時
測定者
ファイル名
サンプル名
コメント

16
ON
8
2016/11/22 12:40
kawamata
Memory#2
s-10-c9

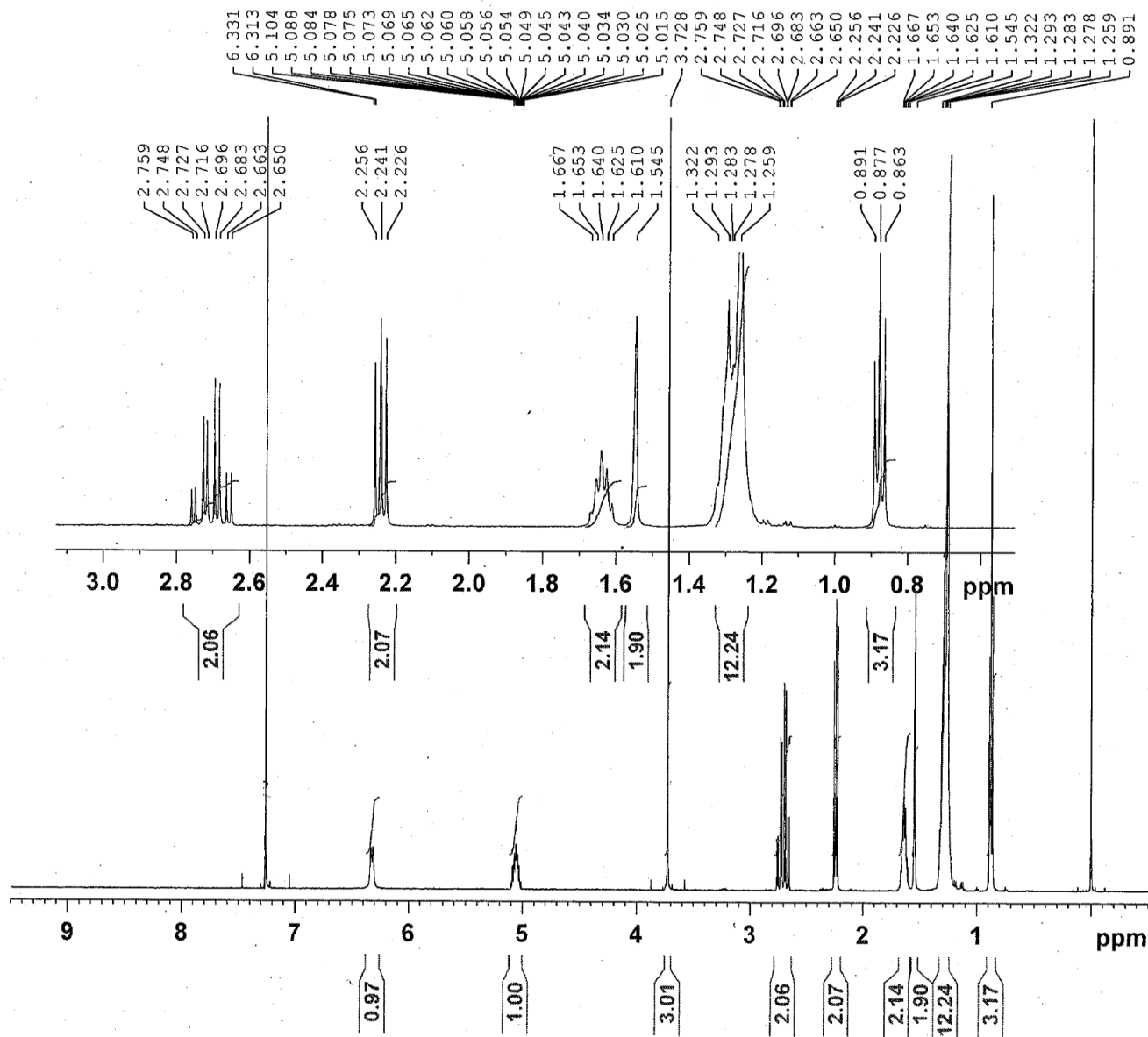
分解
アポダイゼーション
スキャンスピード
更新日時

4 cm-1
Cosine
2 mm/sec
2016/11/22 12:42

1:	3292.86,	68.41	2:	3069.16,	88.98	3:	2934.16,	73.75	4:	2851.24,	76.44
5:	1739.48,	60.88	6:	1666.20,	57.77	7:	1548.56,	71.48	8:	1440.56,	84.92
9:	1426.10,	83.74	10:	1379.82,	84.16	11:	1350.89,	76.88	12:	1302.68,	77.38
13:	1266.04,	81.67	14:	1238.08,	75.03	15:	1208.18,	84.02	16:	1179.26,	76.31
17:	1118.51,	55.24	18:	1075.12,	88.14	19:	995.09,	85.22	20:	961.34,	90.80
21:	920.84,	78.53	22:	894.81,	85.38	23:	848.53,	90.73	24:	694.25,	84.54
25:	665.32,	76.31	26:	498.51,	84.87	27:	473.44,	85.36	28:	445.48,	88.64
29:	420.41,	90.54									



1H

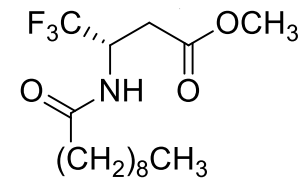


Current Data Parameters
 NAME Al6mc211rk
 EXPNO 17062002
 PROCNO 1

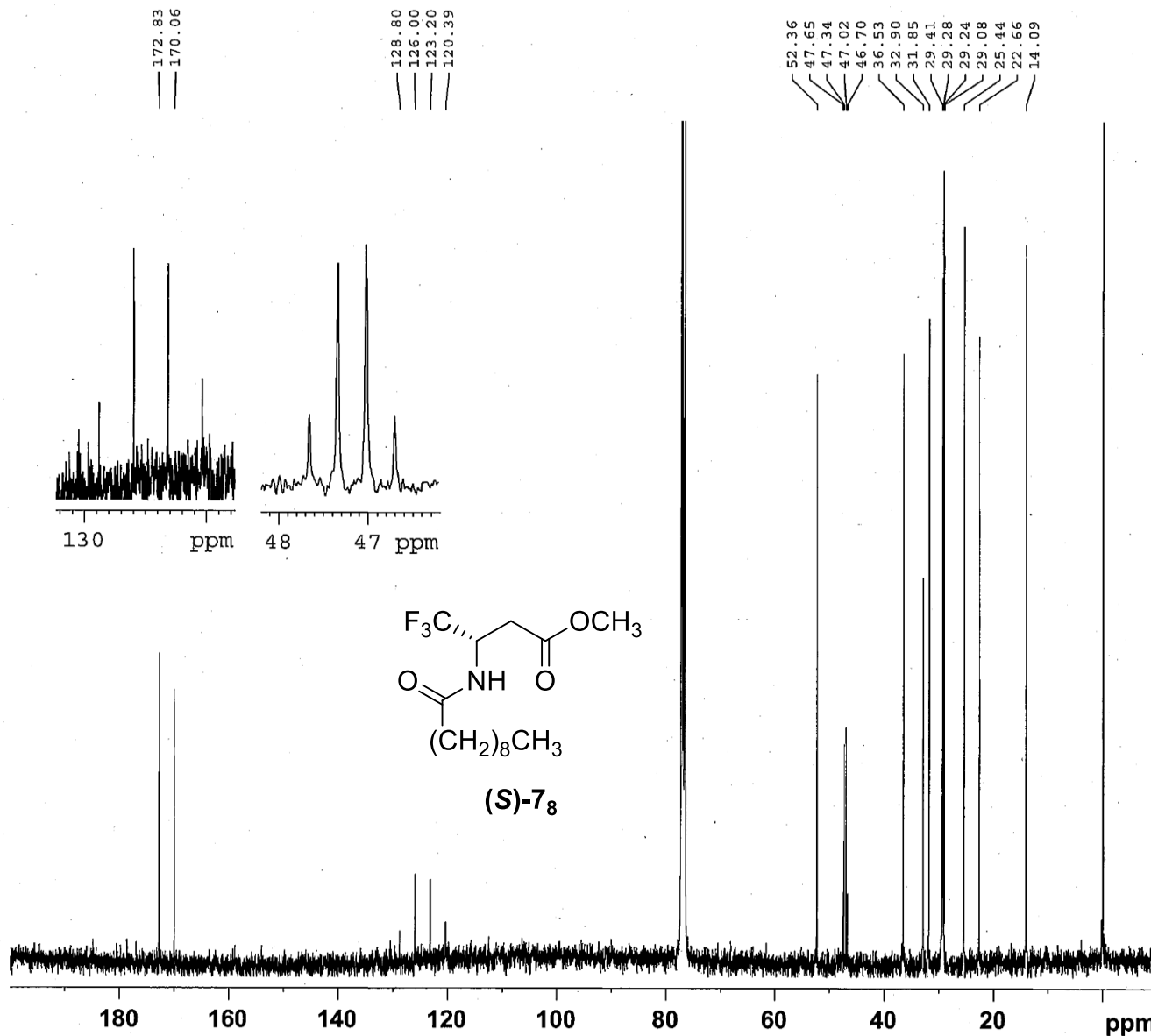
F2 - Acquisition Parameters
 Date_ 20170620
 Time 10.00
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719923 sec
 RG 203
 DW 48.400 usec
 DE 6.50 usec
 TE 299.9 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 11.80 usec
 PL1 2.40 dB
 PL1W 15.17711735 W
 SFO1 500.0330885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.0300109 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



13C with dec. CPQNP



Current Data Parameters
 NAME kodama
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170807
 Time 18.20
 INSTRUM spect
 PROBHD 5 mm CPQNP 1H/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 256
 DS 2
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010548 sec
 RG 126.99
 DW 16.800 usec
 DE 18.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

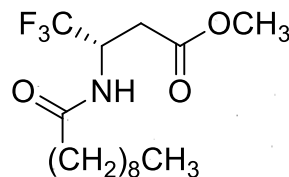
==== CHANNEL f1 =====
 NUC1 13C
 P1 12.00 usec
 PLW1 15.50000000 W
 SFO1 100.6248425 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PLW2 5.19999981 W
 PLW12 0.14444000 W
 PLW13 0.11700000 W
 SFO2 400.1316005 MHz

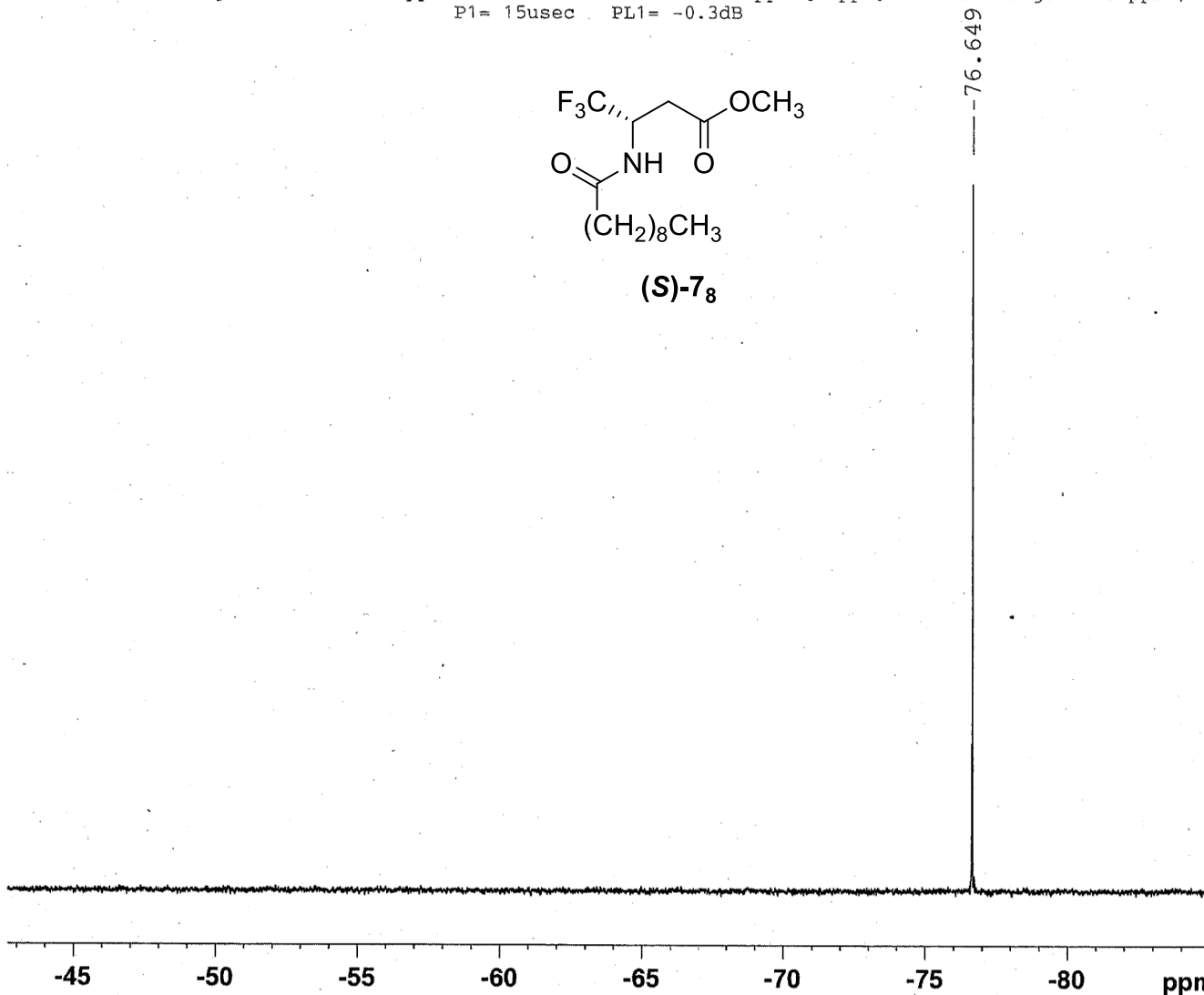
F2 - Processing parameters
 SI 32768
 SF 100.6127671 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.40

- ACCEPTANCE - System: AV300 OrderNo.: JH033009 Customer: Saitama University Engineer: IKD
 P/N Console: Z108356/162 Shim system: BOSS I original dataset: 104275_0150snf 3 1
 Probe: 5 mm PABBO BB-1H/D Z-GRD Z104275/0150 Sample depth:20 Gas: air
 Sensitivity test for 19F (additional test); Sample: 0,05% TFT in CDCl3 (P/N: Z10234)

Sino= 243:1 (signal= -61 - -65 ppm noise= -59.08 - -60.08 ppm [1 ppm] noise range= 4.5 ppm)
 P1= 15usec PL1= -0.3dB



(S)-7₈



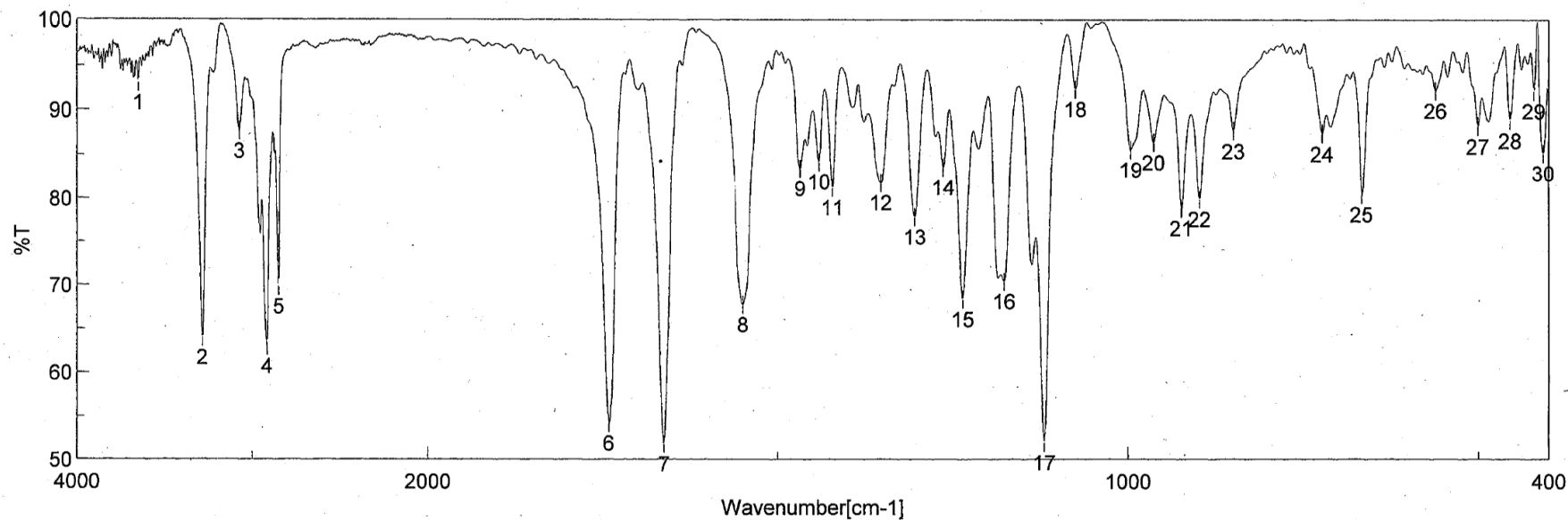
NAME	A16mc211rk
EXPNO	16100406
PROCNO	1
Date_	20161004
Time	17.25
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgfhigqn
TD	32768
SOLVENT	CDCl3
NS	1
DS	0
SWH	12019.230 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	41.600 usec
DE	6.50 usec
TE	296.6 K
D1	10.0000000 sec
D11	0.0300000 sec
D12	0.0000200 sec
TDO	1

==== CHANNEL f1 =====

NUC1	19F
P1	15.00 usec
PL1	-0.30 dB
PL1W	10.09325600 W
SFO1	282.3865635 MHz

==== CHANNEL f2 =====

CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.58 dB
PL12	16.50 dB
PL2W	9.45079708 W
PL12W	0.24180678 W
SFO2	300.1300000 MHz
SI	16384
SF	282.4046276 MHz
WDW	EM
SSB	0
LB	2.00 Hz
GB	0
PC	1.00



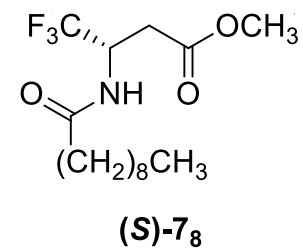
積算回数
ゼロフィリング
ゲイン
測定日時
測定者
ファイル名
サンプル名
コメント

16
ON
8
2016/11/22 12:58
kawamata
Memory#2
s-10-c10

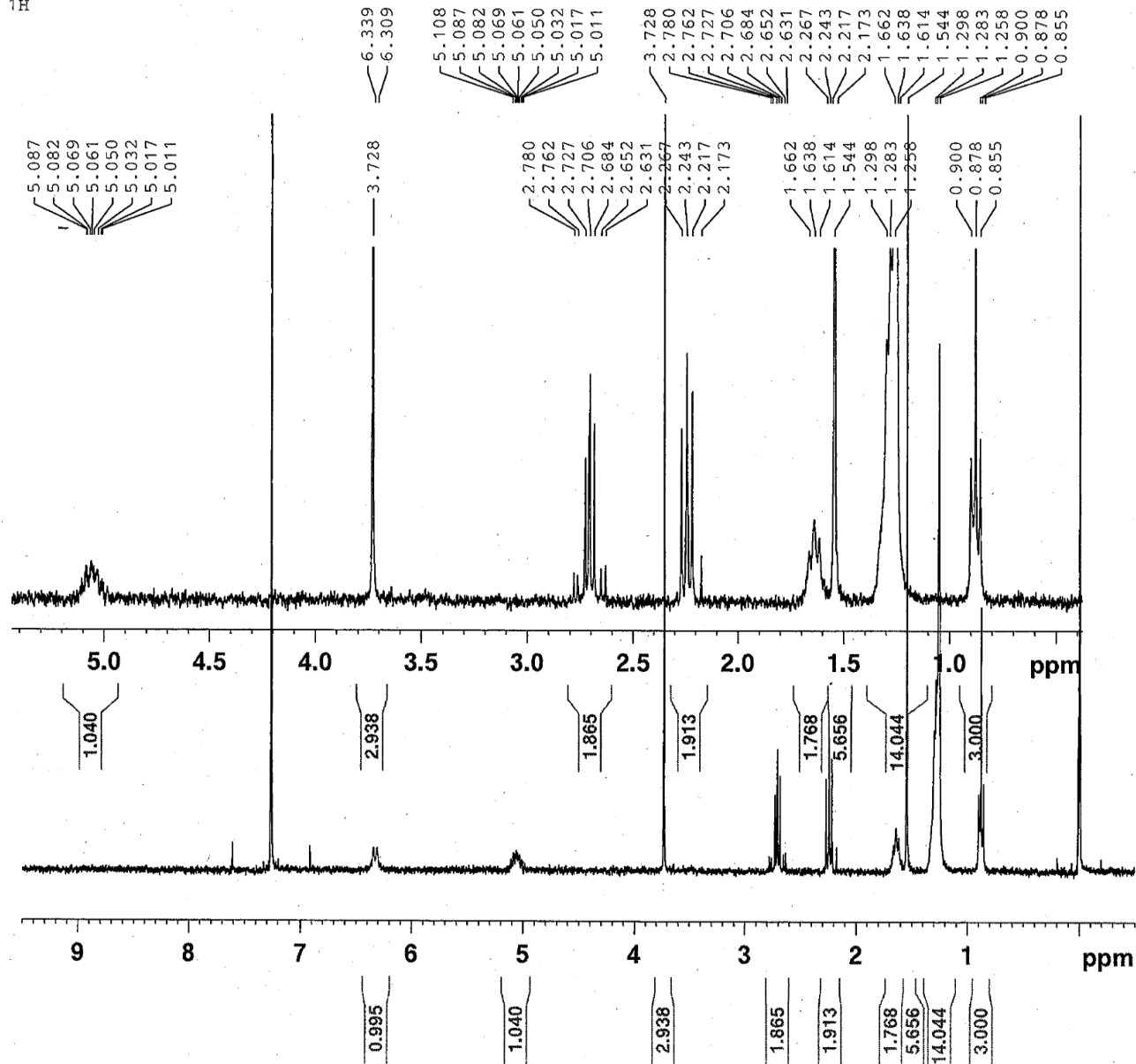
分解
アポダイゼーション
スキャンスピード
更新日時

4 cm-1
Cosine
2 mm/sec
2016/11/22 13:00

1:	3649.62,	93.03	2:	3285.14,	63.98	3:	3075.90,	87.70	4:	2917.77,	62.97
5:	2851.24,	69.78	6:	1741.41,	54.14	7:	1662.34,	51.76	8:	1549.52,	67.74
9:	1467.56,	83.36	10:	1440.56,	84.15	11:	1421.28,	81.18	12:	1351.86,	81.74
13:	1303.64,	77.82	14:	1263.15,	83.53	15:	1235.18,	68.33	16:	1176.36,	70.40
17:	1119.48,	51.92	18:	1075.12,	92.31	19:	996.05,	85.54	20:	963.27,	86.40
21:	923.74,	78.83	22:	897.70,	79.84	23:	849.49,	87.67	24:	723.18,	87.34
25:	666.29,	80.34	26:	561.18,	92.13	27:	501.40,	88.19	28:	455.12,	88.84
29:	421.37,	92.09	30:	407.87,	85.15						

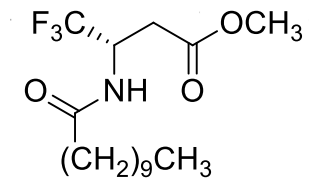


¹H

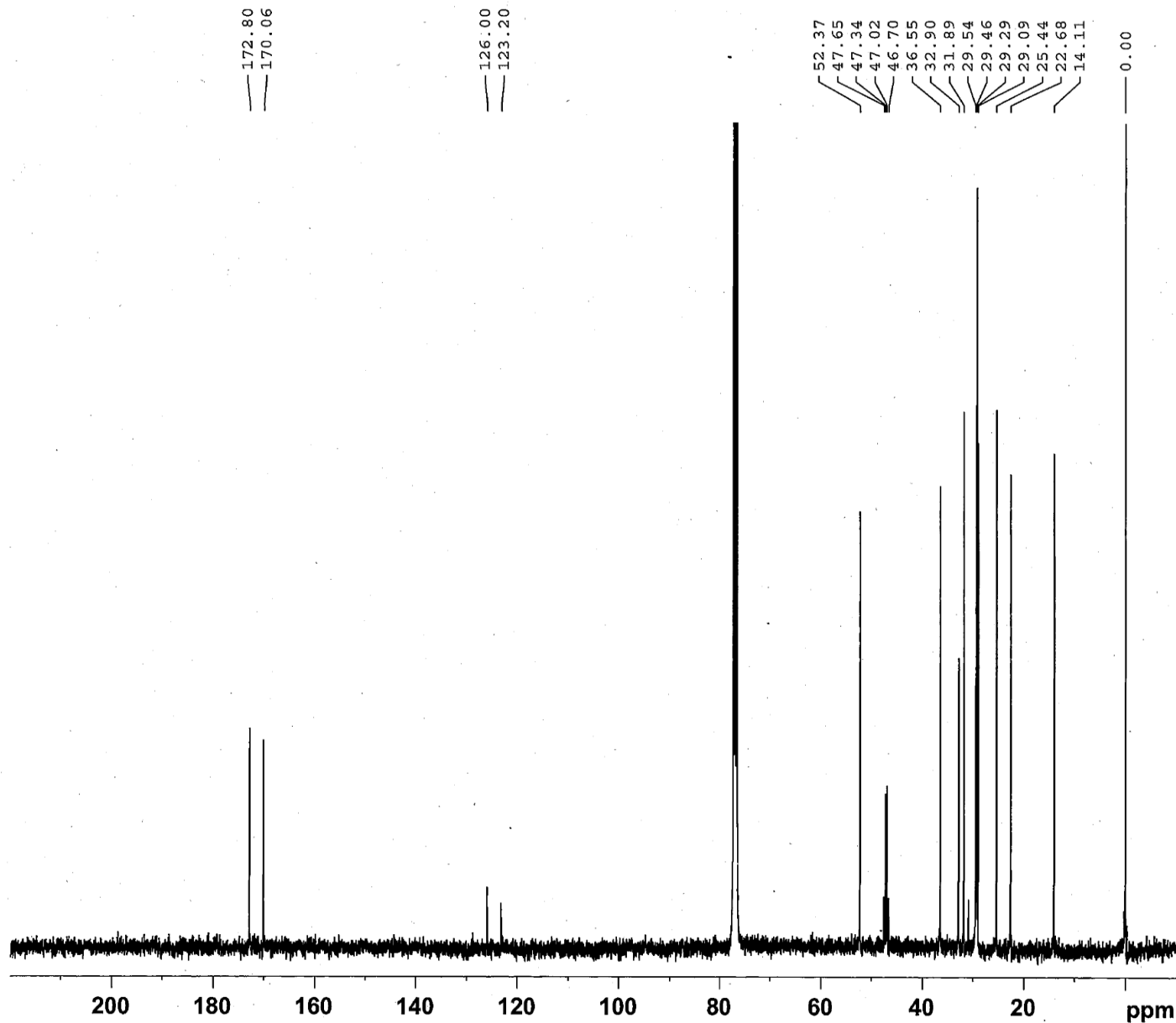


NAME A16mc211rk
 EXPNO 17060204
 PROCNO 1
 Date_ 20170602
 Time 16.06
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 8
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953587 sec
 RG 203
 DW 80.800 usec
 DE 6.50 usec
 TE 296.3 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 ¹H
 P1 15.00 usec
 PL1 1.20 dB
 PL1W 8.19348145 W
 SFO1 300.1318534 MHz
 SI 32768
 SF 300.1300057 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

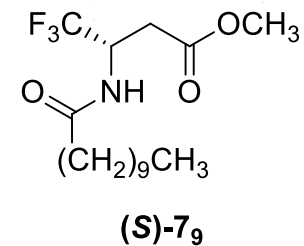


! with dec. CPQ



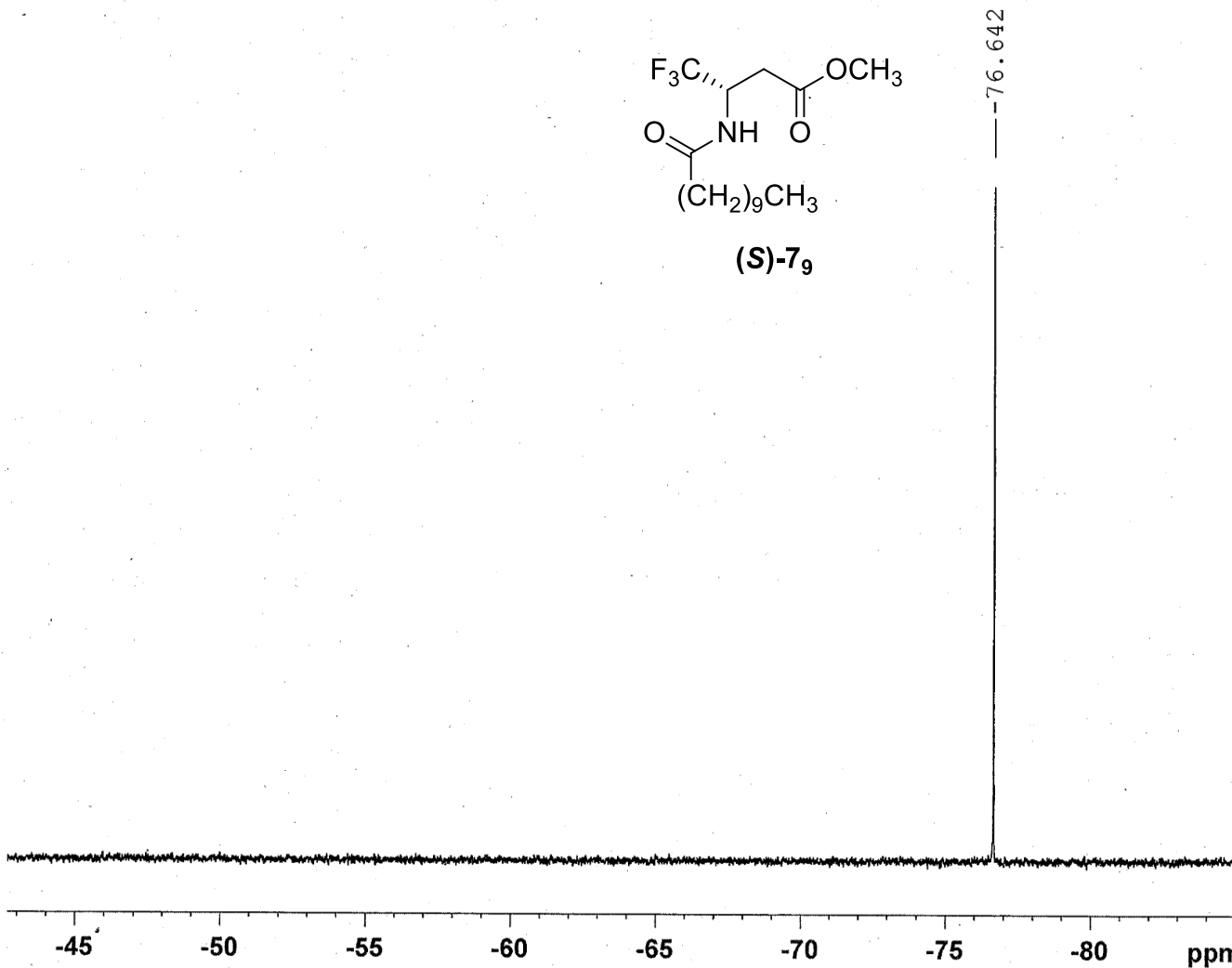
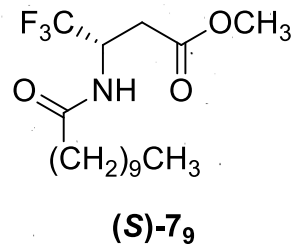
NAME kodama
EXPNO 4
PROCNO 1
Date_ 20170912
Time_ 18.40
INSTRUM spect
PROBHD 5 mm CPQNP 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 512
DS 2
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 126.99
DW 16.800 usec
DE 18.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
SI 32768
SF 100.6127666 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40



- ACCEPTANCE - System: AV300 OrderNo.: JH033009 Customer: Saitama University Engineer: IKD
 P/N Console: Z108356/162 Shim system: BOSS I original dataset: 104275_0150snf 3 1
 Probe: 5 mm PABBO BB-1H/D Z-GRD Z104275/0150 Sample depth:20 Gas: air
 Sensitivity test for 19F (additional test); Sample: 0,05% TFT in CDC13 (P/N: Z10234)

Sino= 243:1 (signal= -61 - -65 ppm noise= -59.08 - -60.08 ppm [1 ppm] noise range= 4.5 ppm)
 Pl= 15usec PL1= -0.3dB



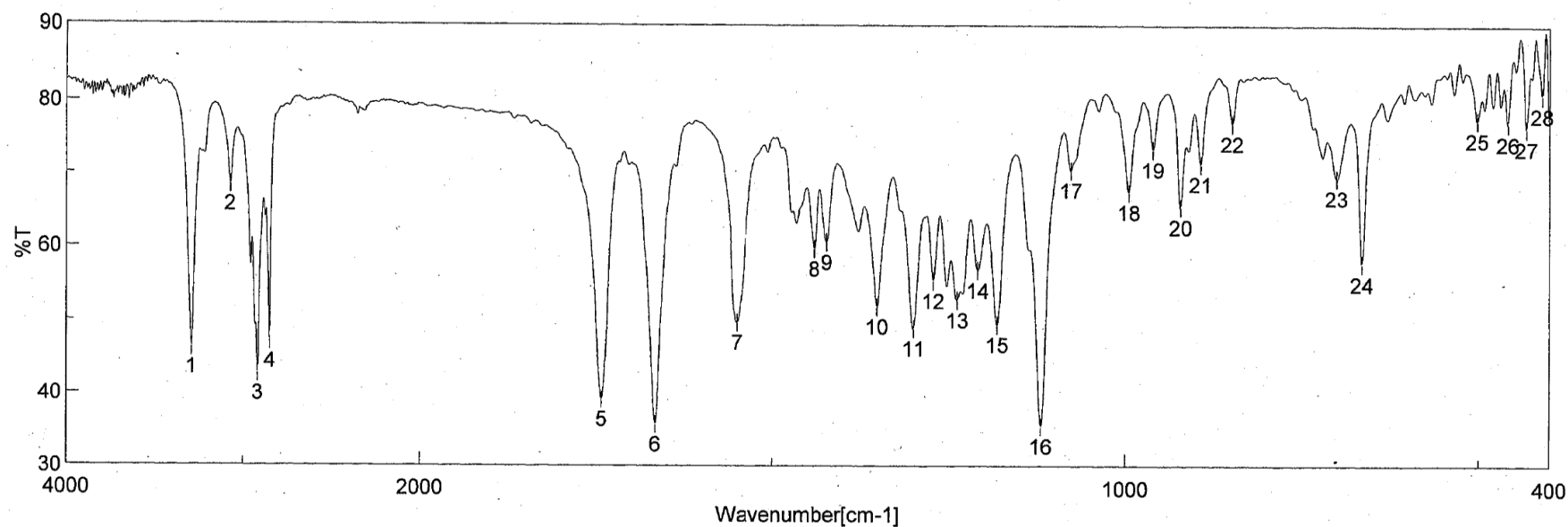
Current Data Parameters
 NAME Al6mc211rk
 EXPNO 16122002
 PROCNO 1

F2 - Acquisition Parameters
 Date 20161220
 Time 10.12
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgfhigqn
 TD 32768
 SOLVENT CDC13
 NS 1
 DS 0
 SWH 12019.230 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 203
 DW 41.600 usec
 DE 6.50 usec
 TE 296.7 K
 D1 10.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 19F
 P1 15.00 usec
 PL1 -0.30 dB
 PL1W 10.09325600 W
 SFO1 282.3865635 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.58 dB
 PL12 16.50 dB
 PL2W 9.45079708 W
 PL12W 0.24180678 W
 SFO2 300.1300000 MHz

F2 - Processing parameters
 SI 16384
 SF 282.4046271 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.00



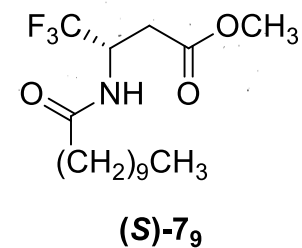
積算回数
ゼロファイリング
ゲイン
測定日時
測定者
ファイル名
サンプル名
コメント

16
ON
8
2017/09/19 14:37
kawamata
Memory#1
S-CF3-C10-COOMe

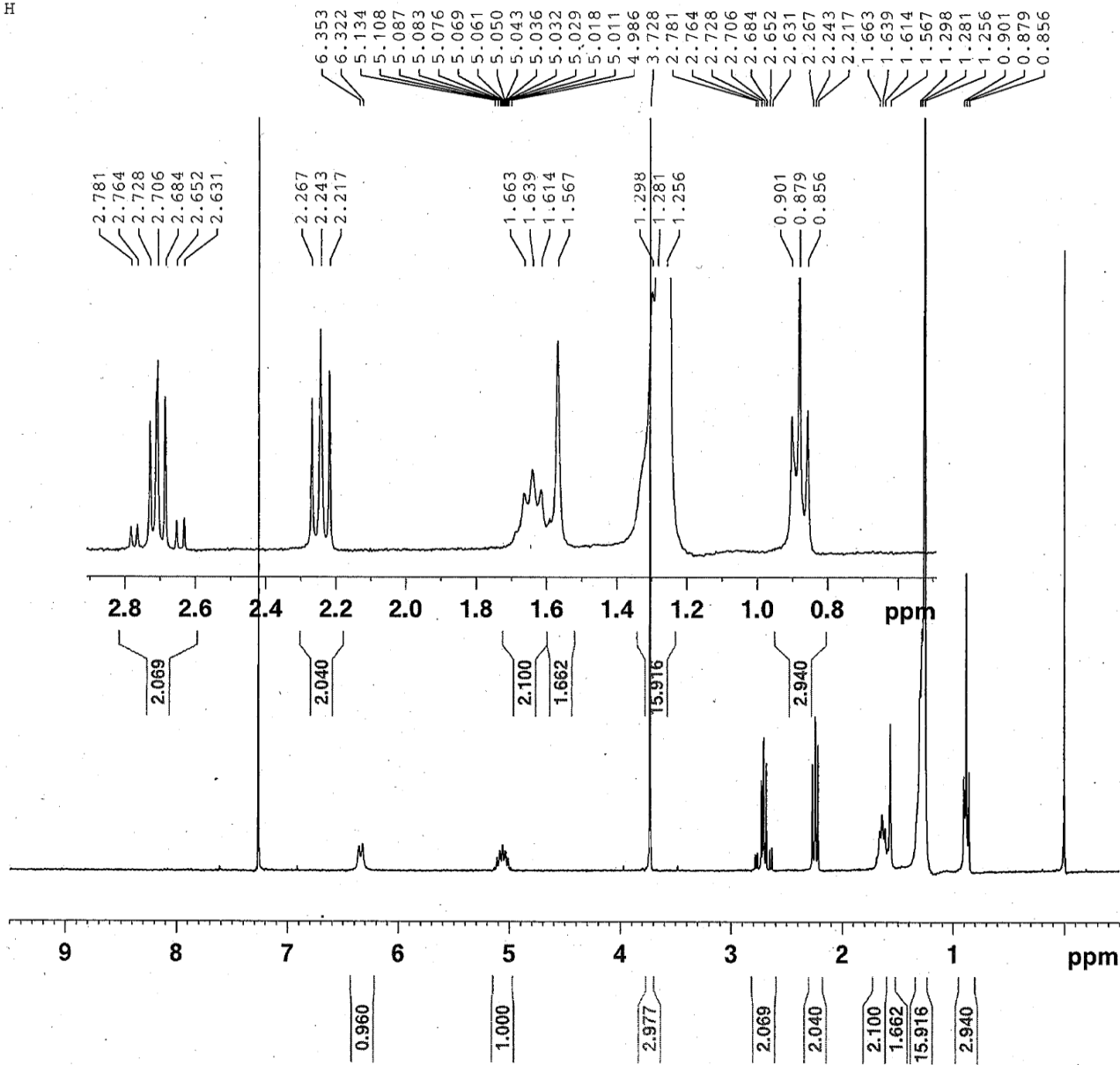
分解
アポダイゼーション
スキャンスピード
更新日時

4 cm-1
Cosine
2 mm/sec
2017/09/19 14:41

1:	3291.89,	46.20	2:	3073.01,	68.42	3:	2916.81,	42.64	4:	2850.27,	47.07
5:	1742.37,	39.14	6:	1666.20,	35.72	7:	1550.49,	49.69	8:	1440.56,	59.77
9:	1423.21,	60.66	10:	1351.86,	51.91	11:	1299.79,	48.89	12:	1271.82,	55.46
13:	1238.08,	52.81	14:	1209.15,	56.88	15:	1181.19,	49.45	16:	1119.48,	35.50
17:	1077.05,	70.58	18:	995.09,	67.49	19:	961.34,	73.46	20:	921.81,	65.43
21:	893.84,	71.44	22:	849.49,	77.06	23:	701.00,	69.51	24:	665.32,	57.81
25:	502.37,	77.56	26:	458.98,	77.08	27:	432.94,	76.41	28:	410.76,	81.02

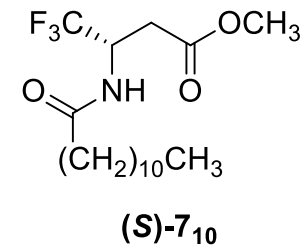


1H

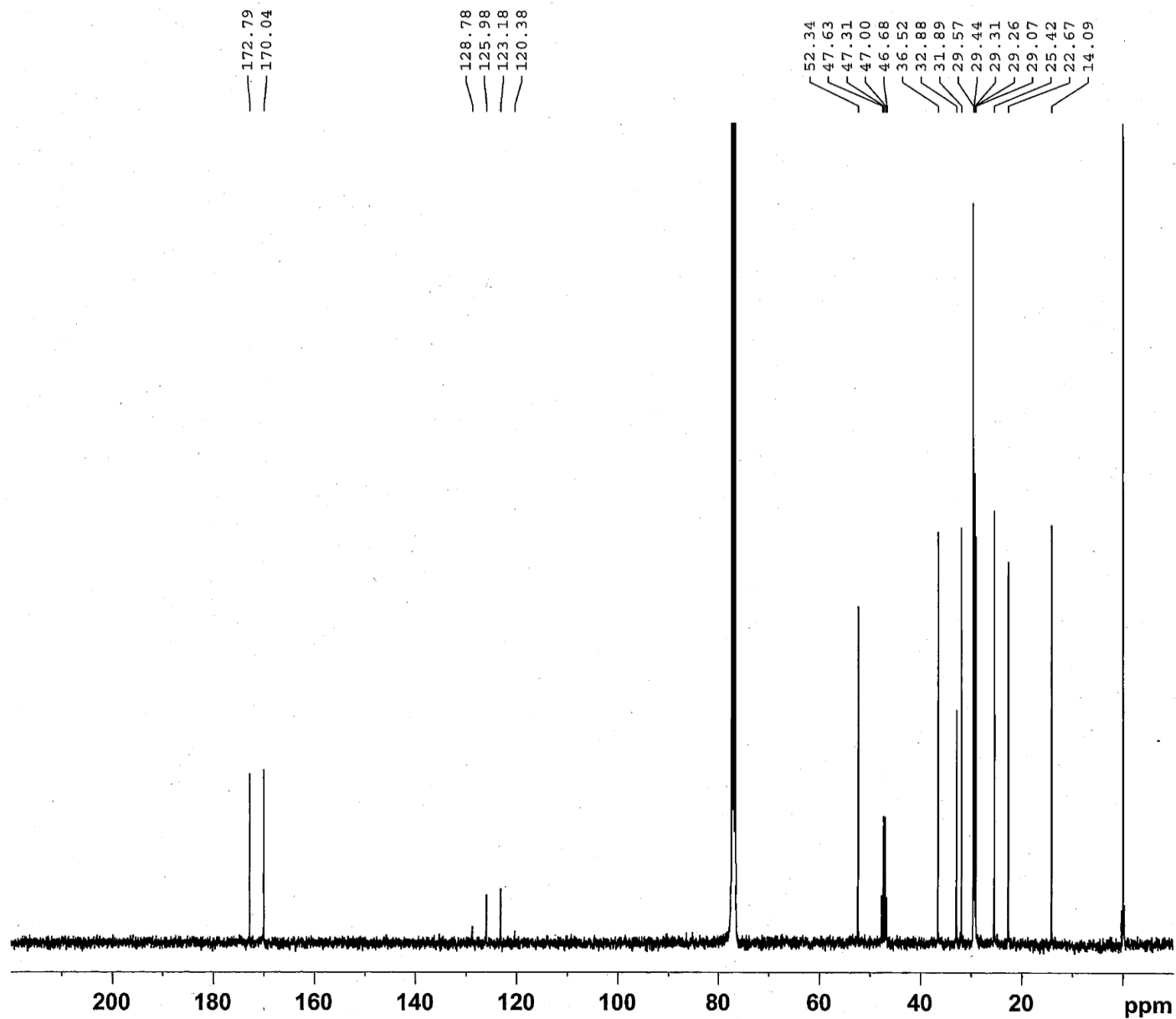


NAME A16mc211rk
 EXPNO 17061304
 PROCNO 1
 Date_ 20170613
 Time 11.40
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953587 sec
 RG 203
 DW 80.800 usec
 DE 6.50 usec
 TE 296.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 15.00 usec
 PL1 1.20 dB
 PL1W 8.19348145 W
 SFO1 300.1318534 MHz
 SI 32768
 SF 300.1300054 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

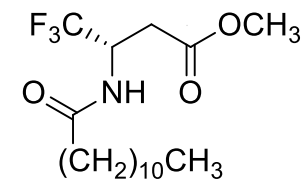


! with dec. CPD

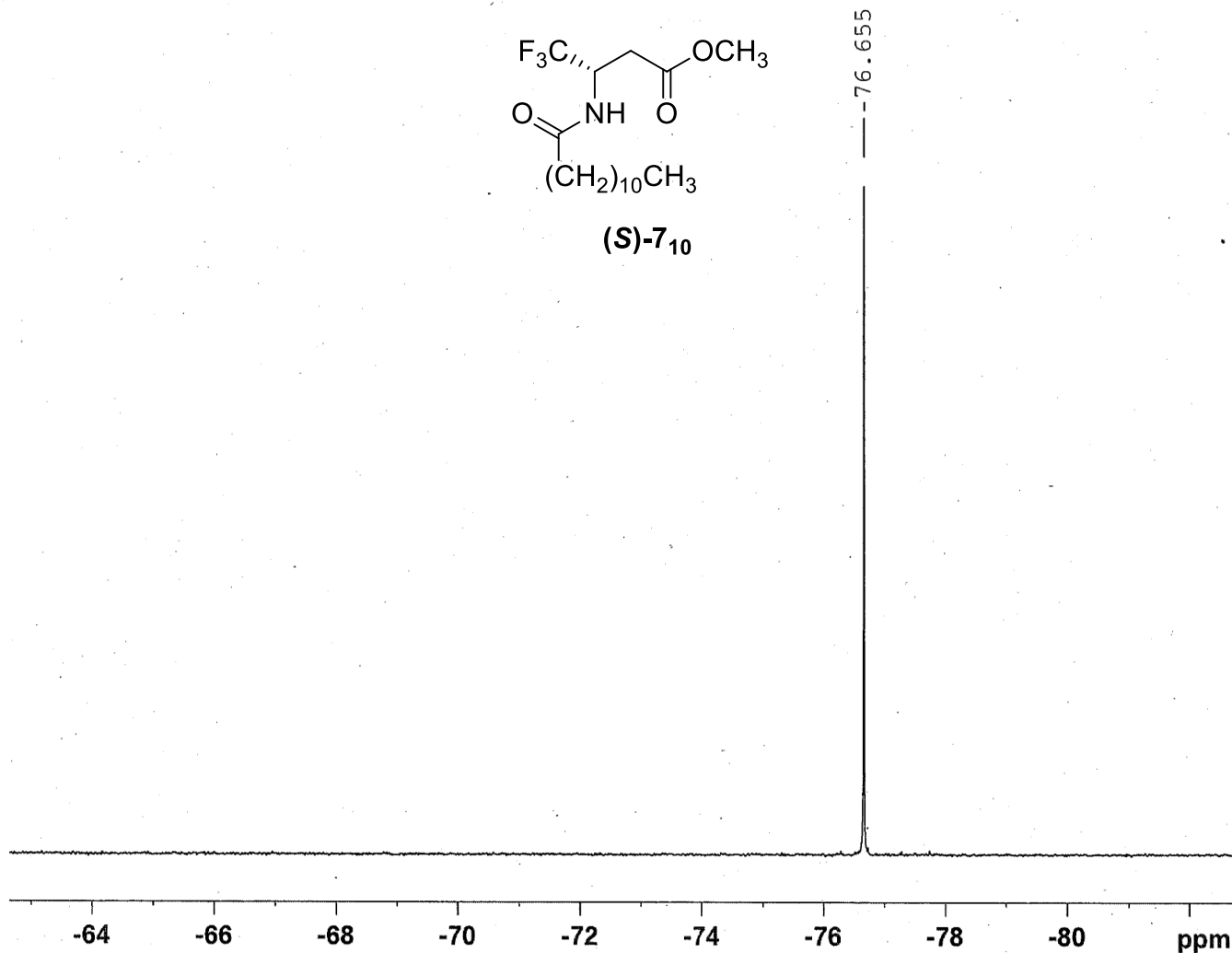
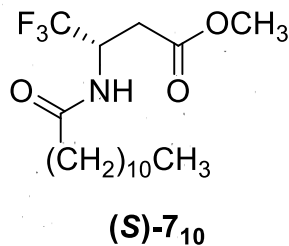


NAME kodama
EXPNO 2
PROCNO 1
Date_ 20170912
Time_ 16.45
INSTRUM spect
PROBHD 5 mm CPQNP 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 493
DS 2
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 126.99
DW 16.800 usec
DE 18.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40



- ACCEPTANCE - System: AV300 OrderNo.: JH033009 Customer: Saitama University Engineer: IKD
 P/N Console: Z108356/162 Shim system: BOSS I original dataset: 104275_0150snf 3 1
 Probe: 5 mm PABBO BB-1H/D Z-GRD Z104275/0150 Sample depth:20 Gas: air
 Sensitivity test for 19F (additional test); Sample: 0,05% TFT in CDCl3 (P/N: Z10234)
 Sino= 243:1 (signal= -61 - -65 ppm noise= -59.08 - -60.08 ppm [1 ppm] noise range= 4.5 ppm)
 P1= 15usec PL1= -0.3dB



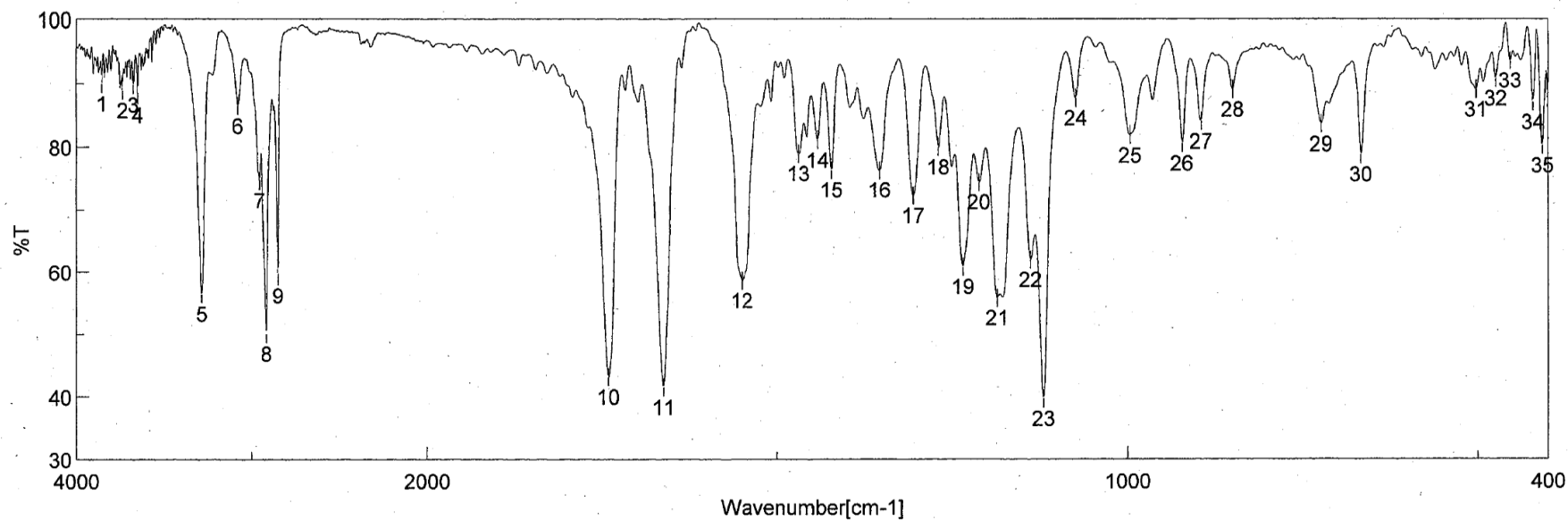
NAME	A16mc211rk
EXPNO	17061302
PROCNO	1
Date_	20170613
Time	11.33
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgfhigqn
TD	32768
SOLVENT	CDCl3
NS	1
DS	0
SWH	12019.230 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	41.600 usec
DE	6.50 usec
TE	296.0 K
D1	10.00000000 sec
D11	0.03000000 sec
D12	0.00002000 sec
TD0	1

==== CHANNEL f1 =====

NUC1	19F
P1	15.00 usec
PL1	-0.30 dB
PL1W	10.09325600 W
SFO1	282.3865635 MHz

==== CHANNEL f2 =====

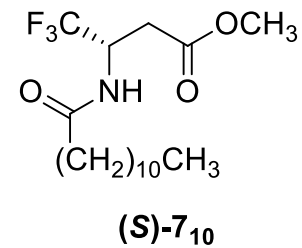
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.58 dB
PL12	16.50 dB
PL2W	9.45079708 W
PL12W	0.24180678 W
SFO2	300.1300000 MHz
SI	16384
SF	282.4046286 MHz
WDW	EM
SSB	0
LB	2.00 Hz
GB	0
PC	1.00



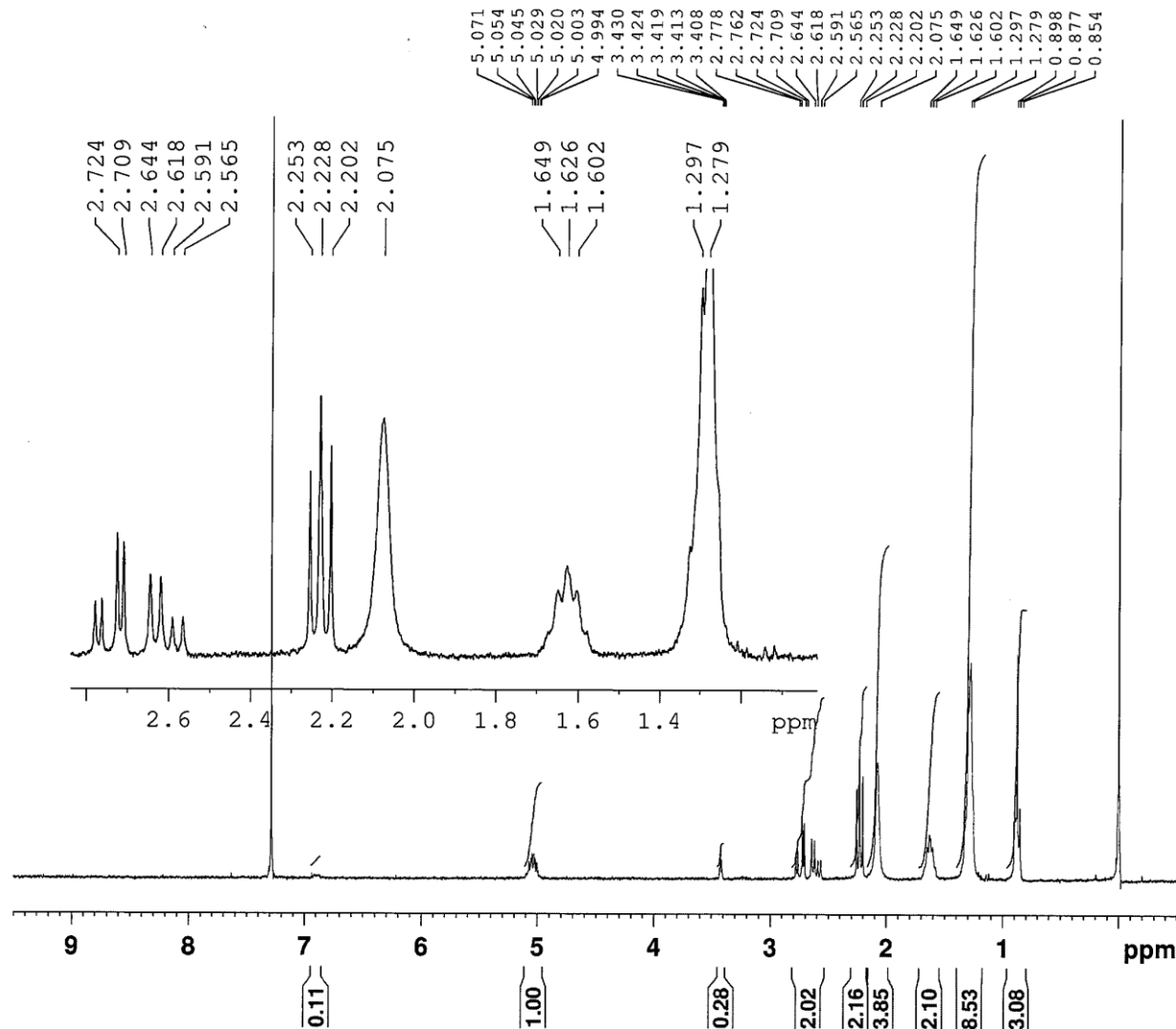
積算回数 16
 ゼロフィリング ON
 ゲイン 8
 測定日時 2016/11/22 14:06
 測定者 kawamata
 ファイル名 Memory#2
 サンプル名 s-10-c12
 コメント

分解 4 cm-1
 アポダイゼーション Cosine
 スキャンスピード 2 mm/sec
 更新日時 2016/11/22 14:08

1: 3853.08,	89.96	2: 3734.48,	88.90	3: 3673.73,	89.82	4: 3648.66,	88.17
5: 3285.14,	56.42	6: 3077.83,	86.46	7: 2955.38,	74.71	8: 2916.81,	50.01
9: 2850.27,	59.35	10: 1741.41,	43.15	11: 1662.34,	41.54	12: 1550.49,	58.62
13: 1468.53,	79.00	14: 1441.53,	81.13	15: 1421.28,	76.37	16: 1352.82,	76.34
17: 1304.61,	72.24	18: 1268.93,	80.07	19: 1234.22,	60.83	20: 1211.08,	74.39
21: 1185.04,	55.85	22: 1137.80,	61.98	23: 1119.48,	39.75	24: 1073.19,	87.68
25: 996.05,	81.89	26: 921.81,	80.63	27: 894.81,	84.02	28: 849.49,	89.04
29: 723.18,	83.61	30: 666.29,	78.84	31: 502.37,	89.03	32: 474.40,	90.75
33: 454.15,	93.57	34: 421.37,	87.00	35: 407.87,	80.24		



1H

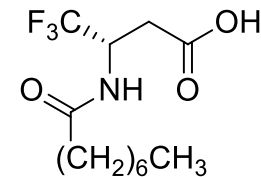


Current Data Parameters
 NAME A12ta020rk
 EXPNO 16021801
 PROCNO 1

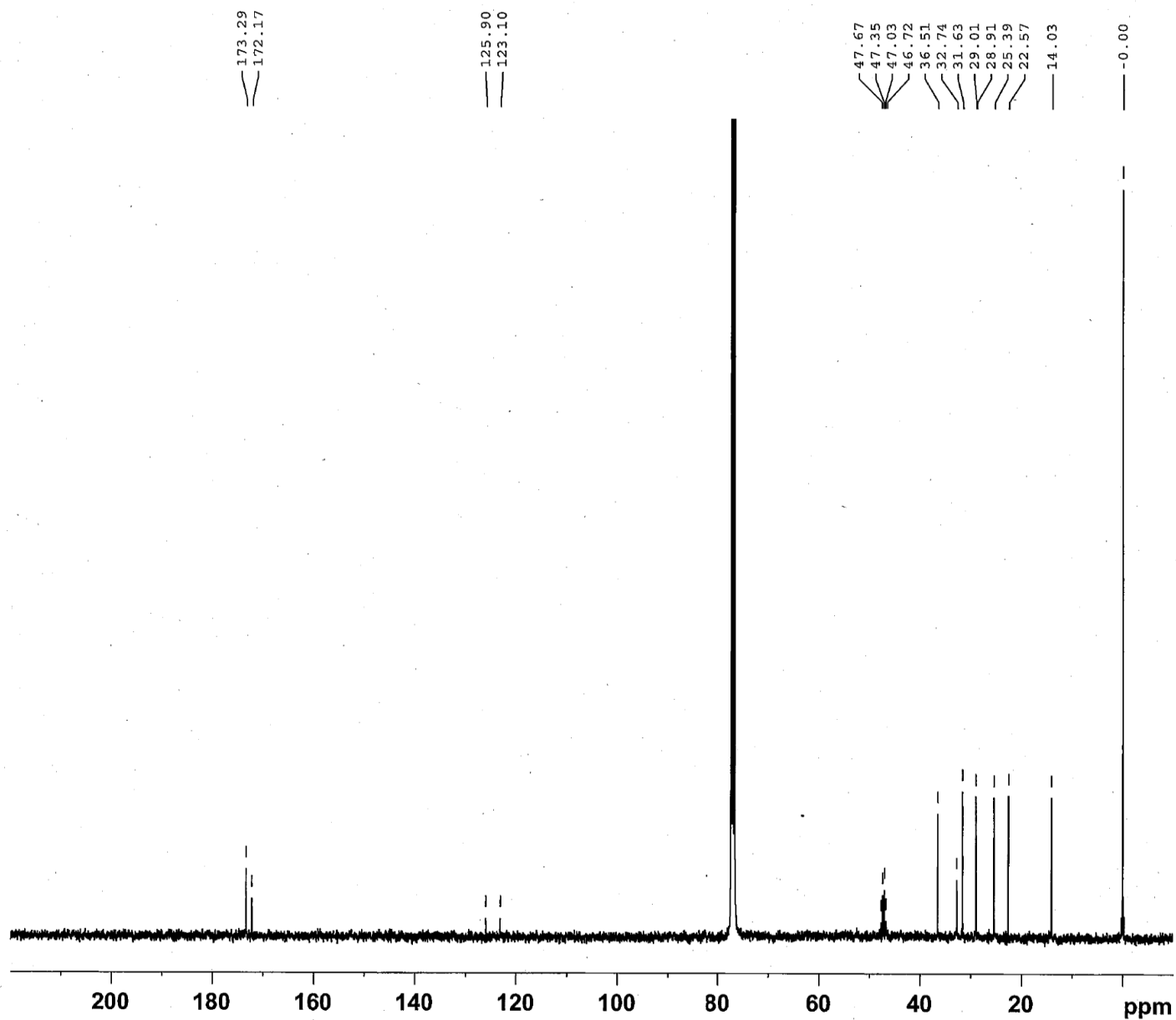
F2 - Acquisition Parameters
 Date_ 20160218
 Time 9.39
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 8
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953587 sec
 RG 203
 DW 80.800 usec
 DE 6.50 usec
 TE 297.7 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 15.00 usec
 PL1 1.20 dB
 PL1W 8.19348145 W
 SFO1 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1299978 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

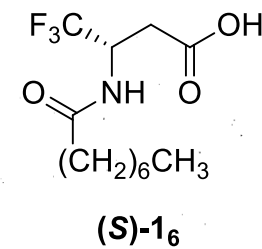


! with dec. CPQ

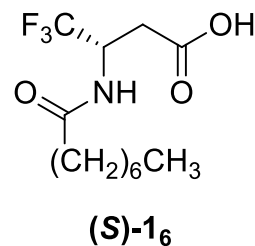


NAME kodama
EXPNO 1
PROCNO 1
Date_ 20170912
Time_ 16.13
INSTRUM spect
PROBHD 5 mm CPQNP 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 2
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 126.99
DW 16.800 usec
DE 18.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

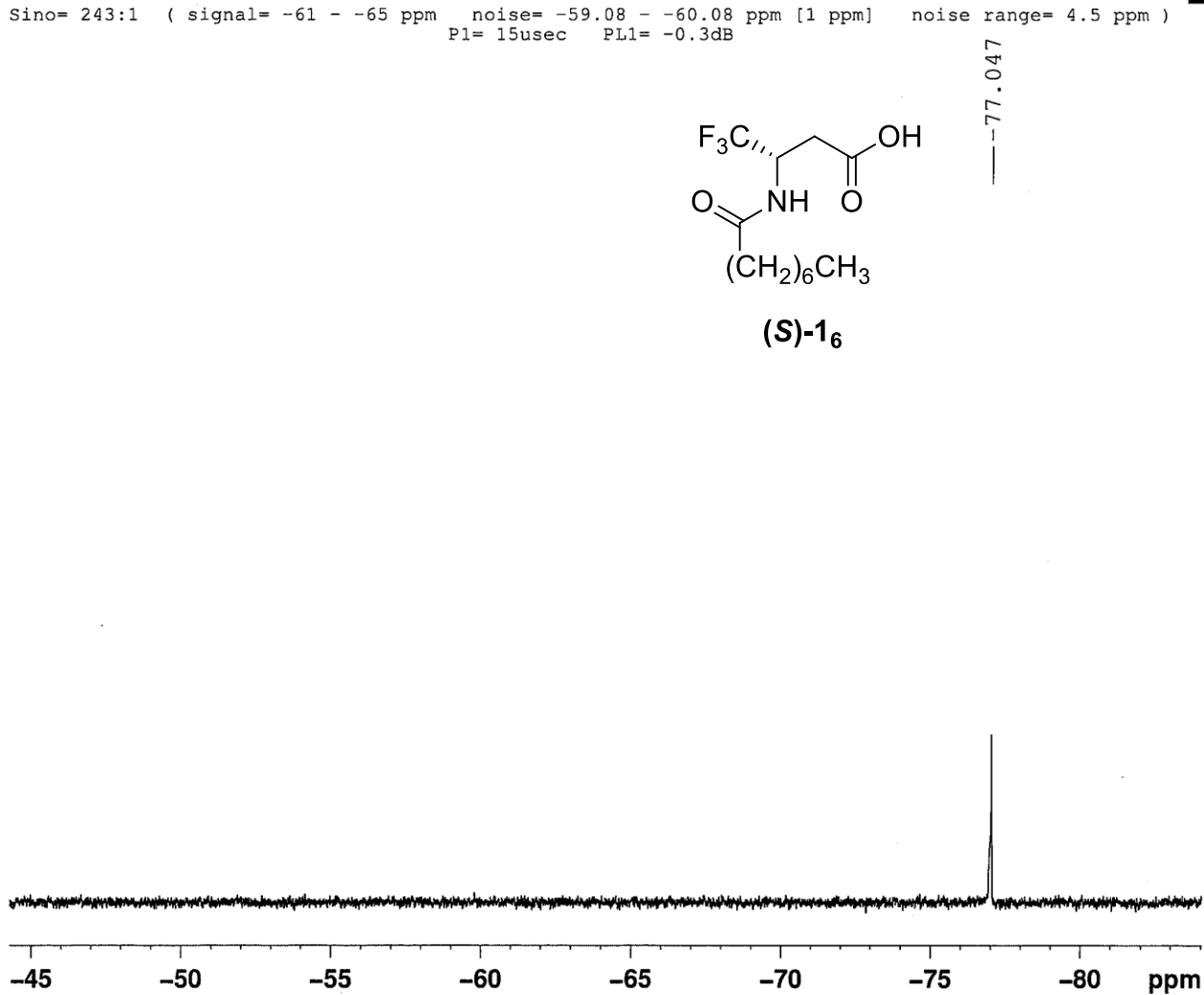
==== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
SI 32768
SF 100.6127674 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40



- ACCEPTANCE - System: AV300 OrderNo.: JH033009 Customer: Saitama University Engineer: IKD
 P/N Console: Z108356/162 Shim system: BOSS I original dataset: 104275_0150snf 3 1
 Probe: 5 mm PABBO BB-1H/D Z-GRD Z104275/0150 Sample depth:20 Gas: air
 Sensitivity test for 19F (additional test); Sample: 0,05% TFT in CDC13 (P/N: Z10234)
 Sino= 243:1 (signal= -61 - -65 ppm noise= -59.08 - -60.08 ppm [1 ppm] noise range= 4.5 ppm)
 P1= 15usec PL1= -0.3dB



---77.047



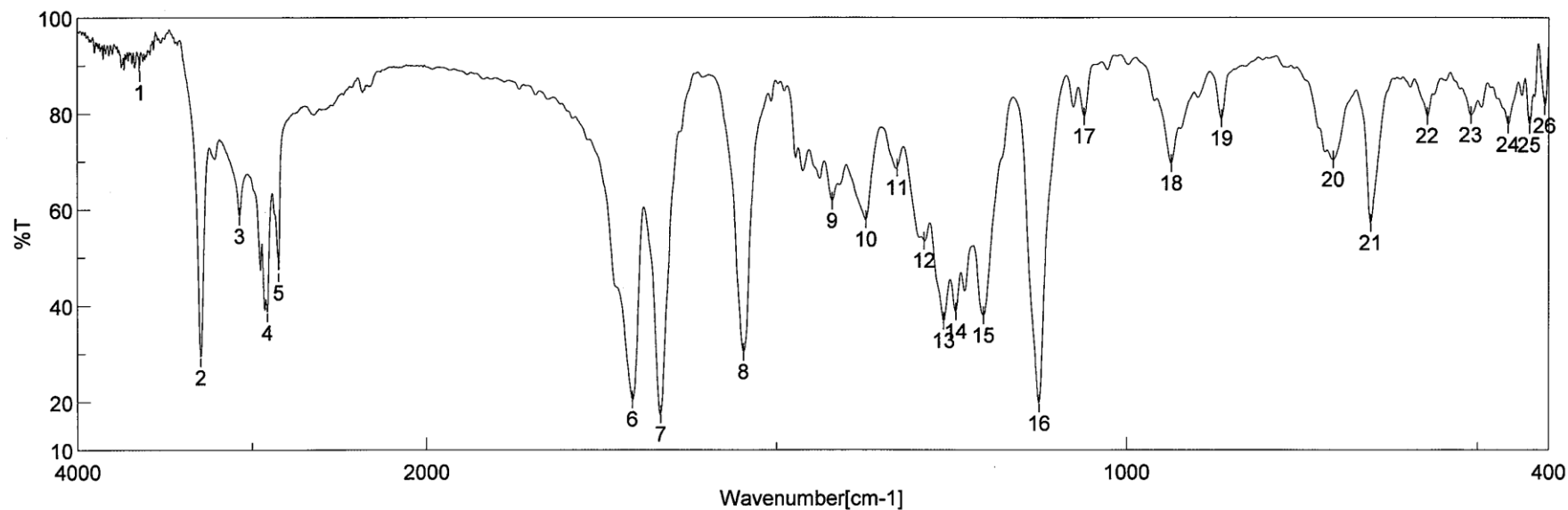
Current Data Parameters
 NAME A12ta020rk
 EXPNO 16020505
 PROCNO 2

F2 - Acquisition Parameters
 Date_ 20160205
 Time 13.47
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgfhigqn
 TD 32768
 SOLVENT CDC13
 NS 1
 DS 0
 SWH 12019.230 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 203
 DW 41.600 usec
 DE 6.50 usec
 TE 297.3 K
 D1 10.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 19F
 P1 15.00 usec
 PL1 -0.30 dB
 PL1W 10.09325600 W
 SFO1 282.3865635 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.58 dB
 PL12 16.50 dB
 PL2W 9.45079708 W
 PL12W 0.24180678 W
 SFO2 300.1300000 MHz

F2 - Processing parameters
 SI 16384
 SF 282.4046312 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.00



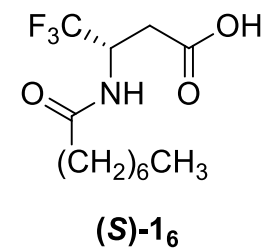
積算回数
ゼロフィリング
ゲイン
測定日時
測定者
ファイル名
サンプル名
コメント

16
ON
16
2016/02/28 15:54
kawamata
Memory#2
(S)-1-C8

分解
アポダイゼーション
スキャンスピード
更新日時

4 cm-1
Cosine
2 mm/sec
2016/02/28 15:55

1: 3648.66,	88.58	2: 3296.71,	29.21	3: 3074.94,	58.62	4: 2913.91,	38.53
5: 2849.31,	46.86	6: 1706.69,	20.56	7: 1666.20,	17.41	8: 1547.59,	30.44
9: 1420.32,	61.82	10: 1372.10,	57.95	11: 1327.75,	68.73	12: 1289.18,	53.55
13: 1261.22,	36.90	14: 1243.86,	38.83	15: 1204.33,	38.01	16: 1125.26,	19.71
17: 1060.66,	79.47	18: 936.27,	69.67	19: 864.92,	78.99	20: 705.82,	70.43
21: 651.82,	57.22	22: 570.83,	79.54	23: 510.08,	79.71	24: 458.01,	77.74
25: 428.12,	77.62	26: 405.94,	81.68				

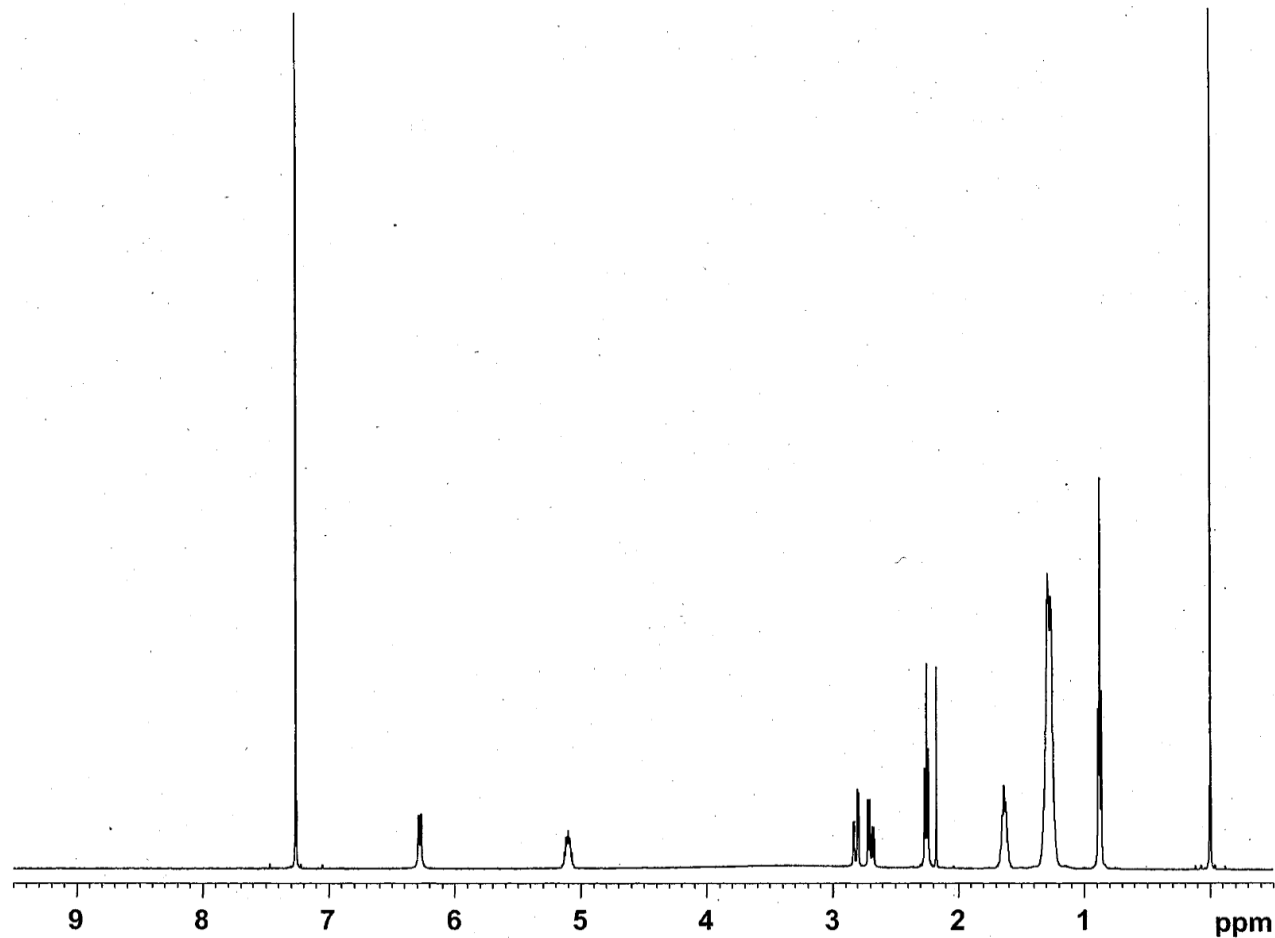


1H

6.287
6.268

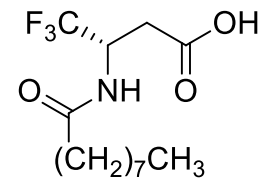
5.147
5.132
5.117
5.107
5.102
5.098
5.088
5.073
5.058

2.833
2.823
2.800
2.790
2.716
2.702
2.684
2.669
2.267
2.252
2.236
2.175
1.637
1.622
1.607
1.308
1.290
1.283
1.268
0.890
0.877
0.863

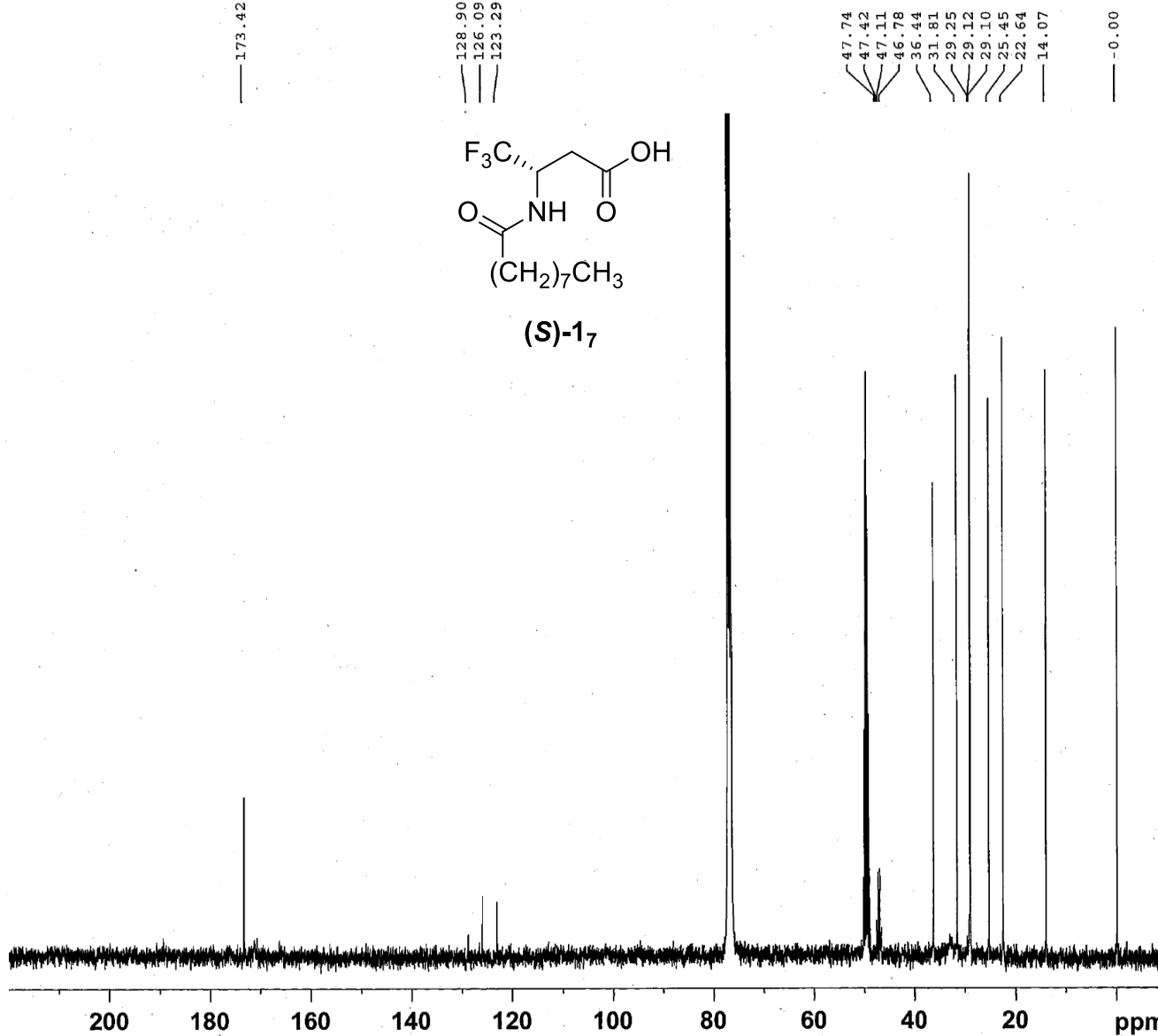
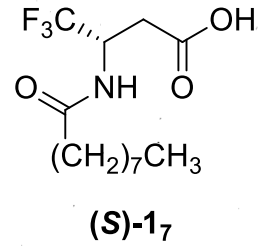


NAME A16mc211rk
 EXPNO 17091203
 PROCNO 1
 Date_ 20170912
 Time 18.05
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719923 sec
 RG 203
 DW 48.400 usec
 DE 6.50 usec
 TE 300.5 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 11.80 usec
 PL1 2.40 dB
 PL1W 15.17711735 W
 SFO1 500.0330885 MHz
 SI 32768
 SF 500.0300108 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



13C with dec. CPQNP



Current Data Parameters
 NAME kodama
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date 20170914
 Time 20.01
 INSTRUM spect
 PROBHD 5 mm CPQNP 1H/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1037
 DS 2
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010548 sec
 RG 126.99
 DW 16.800 usec
 DE 18.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 13C
 P1 12.00 usec
 PLW1 15.50000000 W
 SFO1 100.6248425 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PLW2 5.19999981 W
 PLW12 0.14444000 W
 PLW13 0.11700000 W
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127643 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.40

- ACCEPTANCE - System: AV300 OrderNo.: JH033009 Customer: Saitama University Engineer: IKD
 P/N Console: Z108356/162 Shim system: BOSS I original dataset: 104275_0150snf 3 1
 Probe: 5 mm PABBO BB-1H/D Z-GRD Z104275/0150 Sample depth:20 Gas: air
 Sensitivity test for 19F (additional test); Sample: 0,05% TFT in CDCl3 (P/N: Z10234)

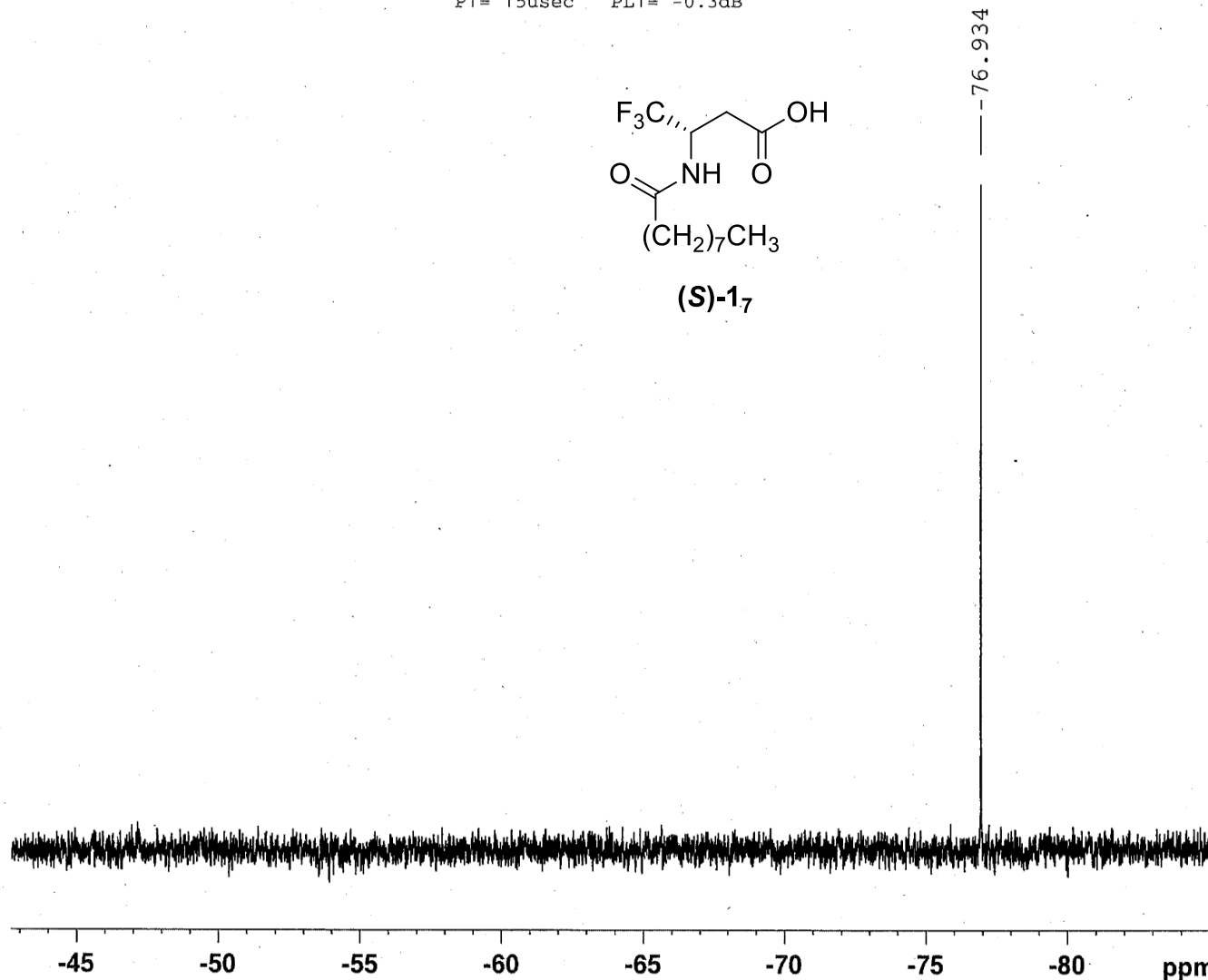
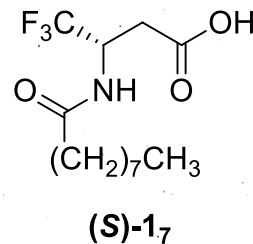
Sino= 243:1 (signal= -61 - -65 ppm noise= -59.08 - -60.08 ppm [1 ppm] noise range= 4.5 ppm)
 P1= 15usec PL1= -0.3dB

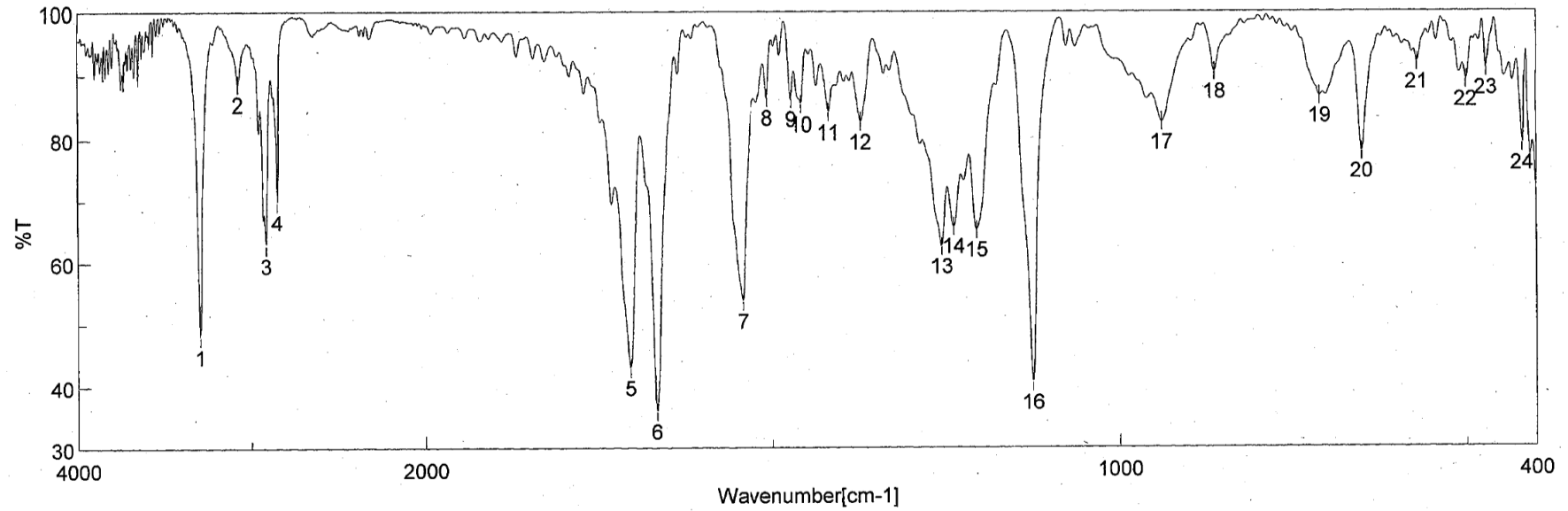


NAME A16mc211rk
 EXPNO 16101102
 PROCNO 1
 Date_ 20161011
 Time 12.47
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgfhigqn
 TD 32768
 SOLVENT CDCl3
 NS 1
 DS 0
 SWH 12019.230 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 203
 DW 41.600 usec
 DE 6.50 usec
 TE 296.3 K
 D1 10.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 19F
 P1 15.00 usec
 PL1 -0.30 dB
 PL1W 10.09325600 W
 SFO1 282.3865635 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.58 dB
 PL12 16.50 dB
 PL2W 9.45079708 W
 PL12W 0.24180678 W
 SFO2 300.1300000 MHz
 SI 16384
 SF 282.4046280 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.00



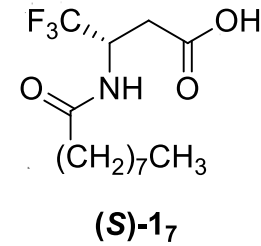


積算回数
ゼロフィリング
ゲイン
測定日時
測定者
ファイル名
サンプル名
コメント

16
ON
16
2016/11/22 14:42
kawata
Memory#2
s-F9

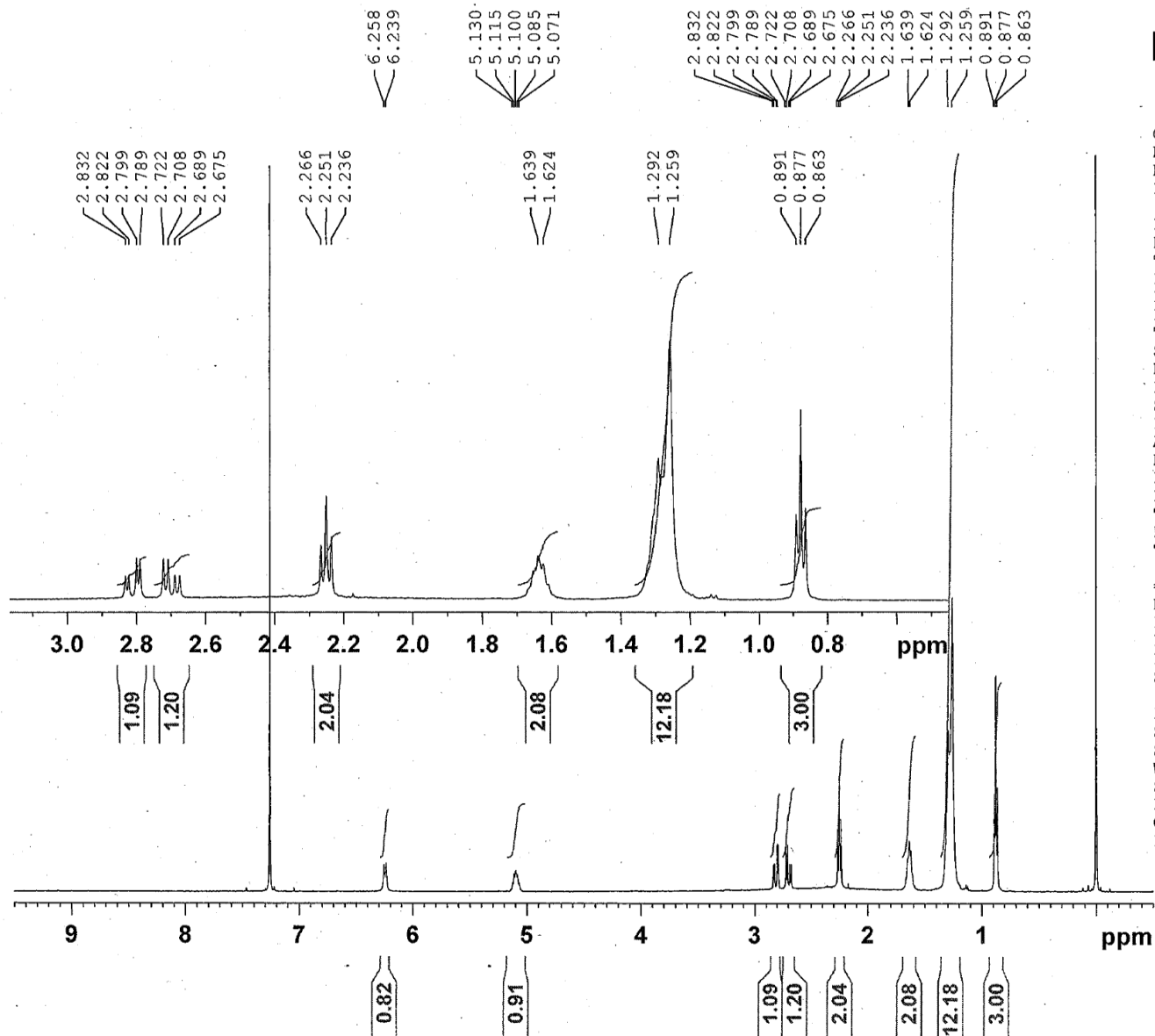
分解
アポダイゼーション
スキャンスピード
更新日時

4 cm-1
Cosine
2 mm/sec
2016/11/22 14:45



1:	3294.79,	47.99	2:	3074.94,	88.66	3:	2913.91,	62.70	4:	2849.31,	69.78
5:	1704.76,	42.92	6:	1667.16,	35.85	7:	1542.77,	53.64	8:	1507.10,	86.40
9:	1472.38,	86.19	10:	1457.92,	85.39	11:	1418.39,	84.12	12:	1372.10,	82.65
13:	1255.43,	62.50	14:	1238.08,	65.73	15:	1205.29,	65.20	16:	1124.30,	40.52
17:	939.16,	82.52	18:	862.99,	90.46	19:	711.60,	86.57	20:	650.86,	77.77
21:	570.83,	91.90	22:	500.44,	89.09	23:	471.51,	90.96	24:	420.41,	79.00

1H

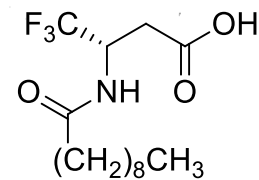


Current Data Parameters
 NAME Al6mc211rk
 EXPNO 17091201
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170912
 Time_ 16.23
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719923 sec
 RG 203
 DW 48.400 usec
 DE 6.50 usec
 TE 300.7 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 11.80 usec
 PL1 2.40 dB
 PL1W 15.17711735 W
 SF01 500.0330885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.0300109 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

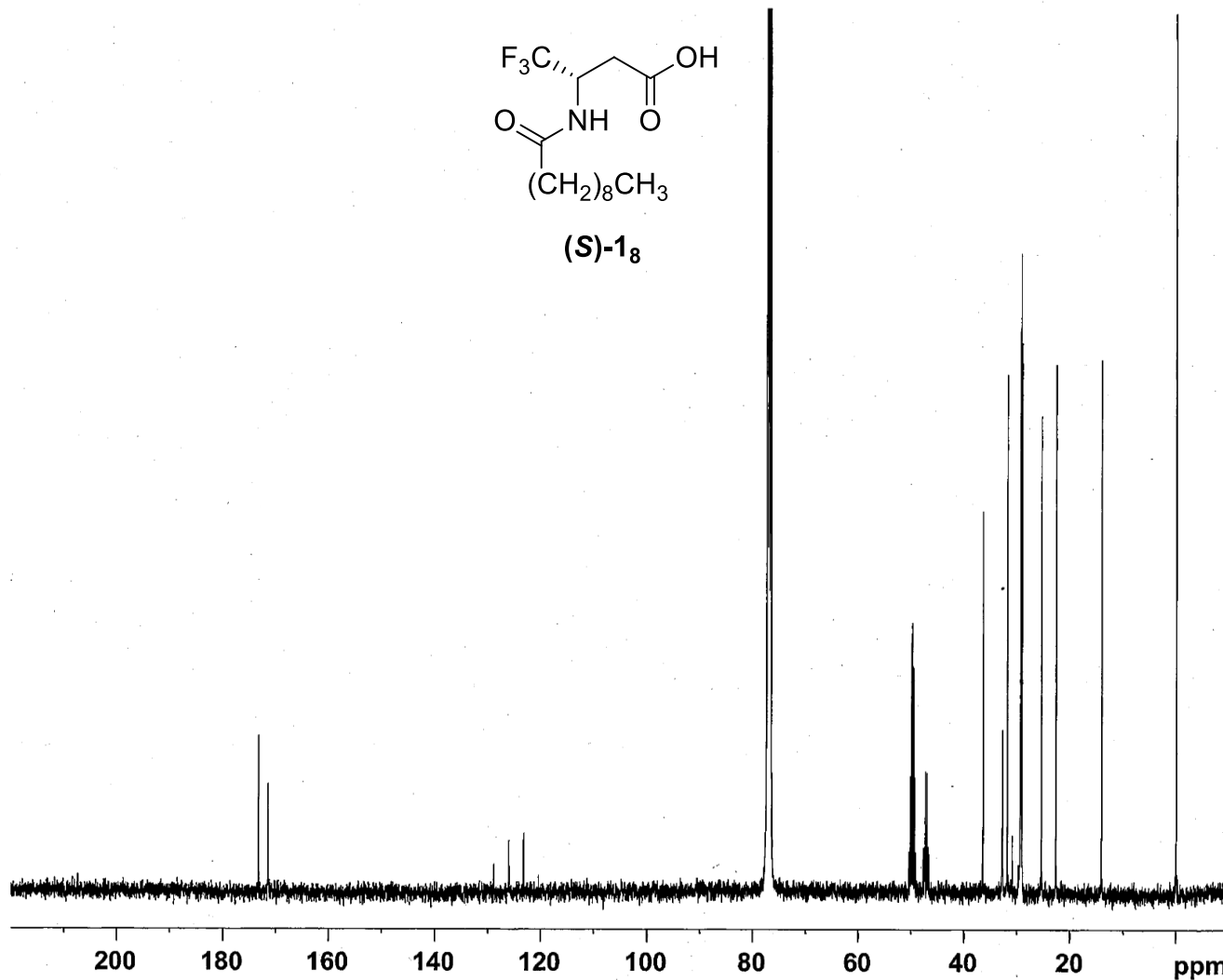
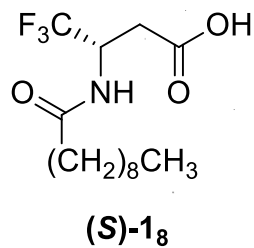


13C with dec. CPQNP

173.31
171.51

128.86
126.06
123.26
120.47

47.67
47.35
47.03
46.71
36.46
32.78
31.86
29.42
29.29
29.25
29.09
25.44
22.67
14.09



Current Data Parameters
NAME kodama
EXPNO 15
PROCNO 1

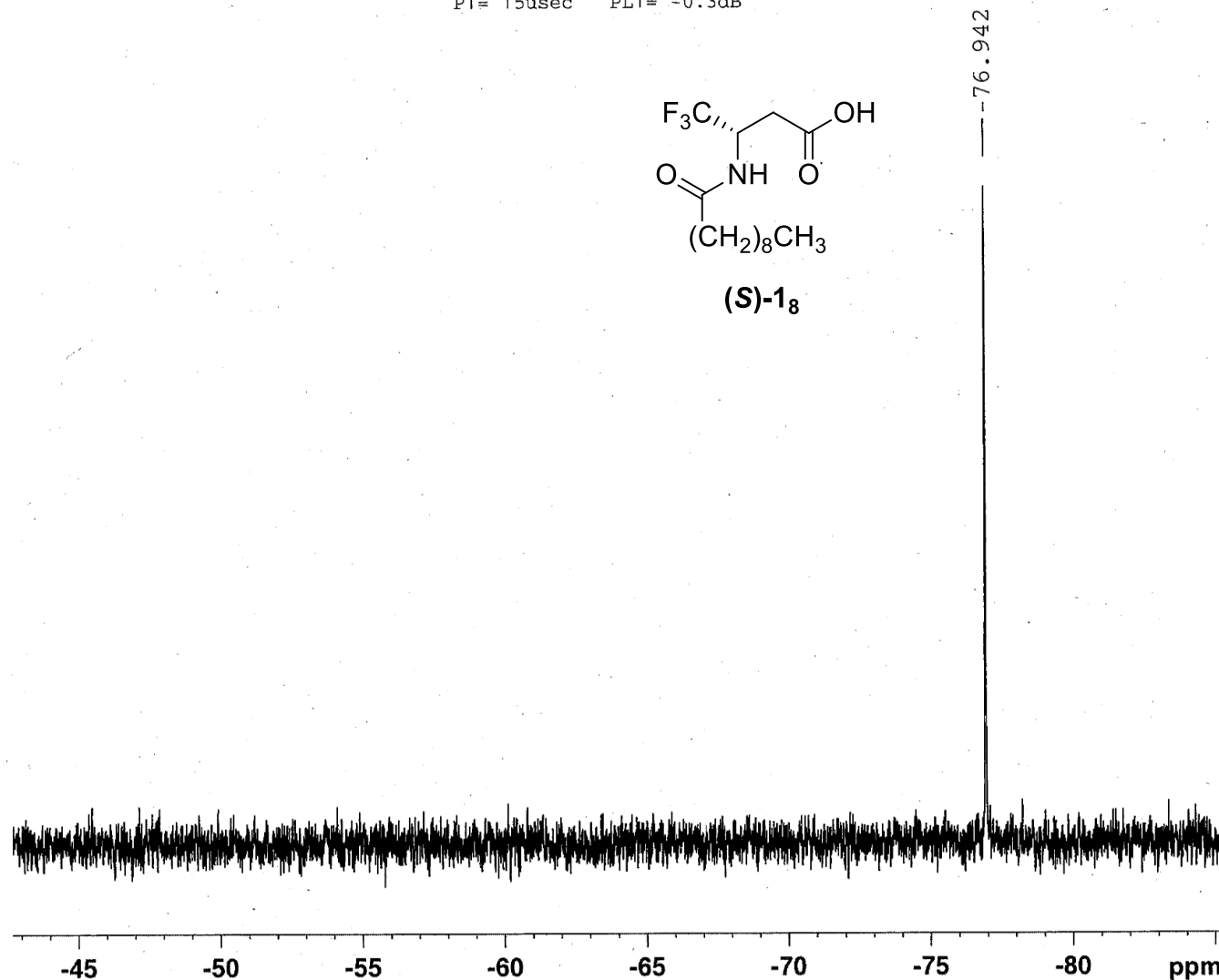
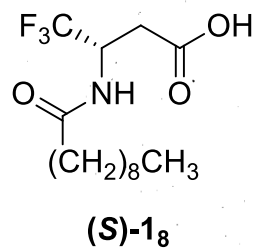
F2 - Acquisition Parameters
Date_ 20170914
Time_ 23.30
INSTRUM spect
PROBHD 5 mm CPQNP 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1027
DS 2
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 126.99
DW 16.800 usec
DE 18.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

==== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PLW1 15.50000000 W
SFO1 100.6248425 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 5.19999981 W
PLW12 0.14444000 W
PLW13 0.11700000 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127654 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

- ACCEPTANCE - System: AV300 OrderNo.: JH033009 Customer: Saitama University Engineer: IKD
 P/N Console: Z108356/162 Shim system: BOSS I original dataset: 104275_0150snf 3 1
 Probe: 5 mm PABBO BB-1H/D Z-GRD Z104275/0150 Sample depth:20 Gas: air
 Sensitivity test for 19F (additional test); Sample: 0,05% TFT in CDCl3 (P/N: Z10234)
 Sino= 243:1 (signal= -61 - -65 ppm noise= -59.08 - -60.08 ppm [1 ppm] noise range= 4.5 ppm)
 P1= 15usec PL1= -0.3dB



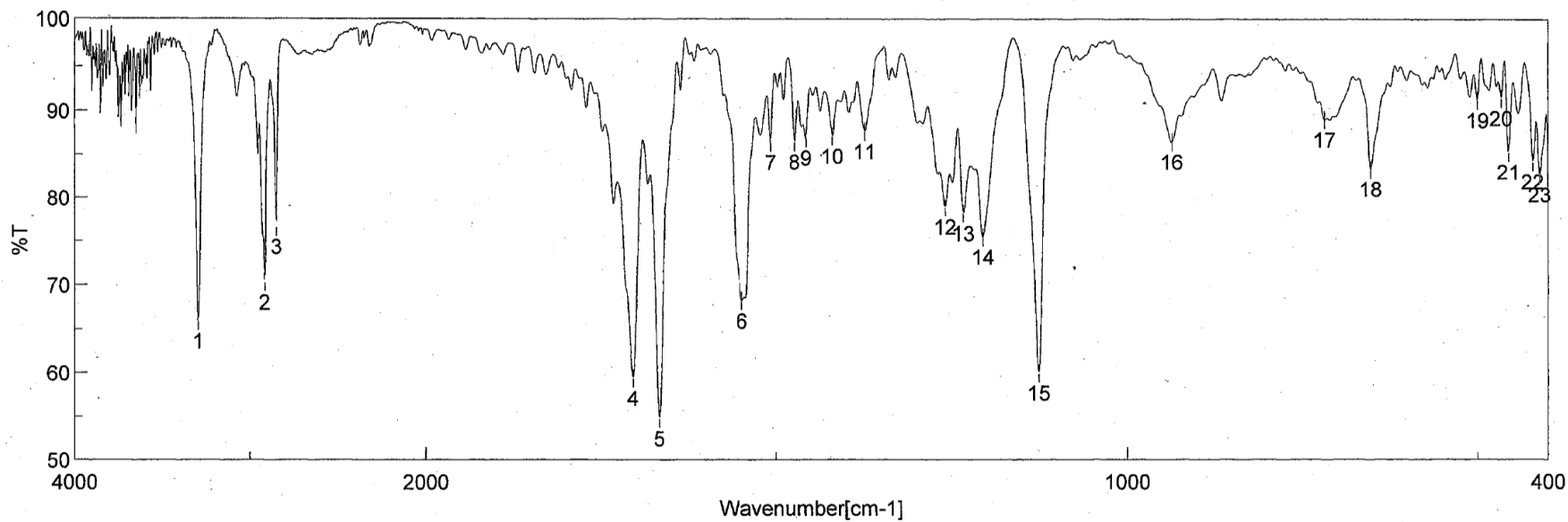
NAME	A16mc211rk
EXPNO	16101103
PROCNO	1
Date_	20161011
Time	12.50
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgfhigqn
TD	32768
SOLVENT	CDCl3
NS	1
DS	0
SWH	12019.230 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	41.600 usec
DE	6.50 usec
TE	296.4 K
D1	10.00000000 sec
D11	0.03000000 sec
D12	0.00002000 sec
TD0	1

===== CHANNEL f1 =====

NUC1	19F
P1	15.00 usec
PL1	-0.30 dB
PL1W	10.09325600 W
SFO1	282.3865635 MHz

===== CHANNEL f2 =====

CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.58 dB
PL12	16.50 dB
PL2W	9.45079708 W
PL12W	0.24180678 W
SFO2	300.1300000 MHz
SI	16384
SF	282.4046280 MHz
WDW	EM
SSB	0
LB	2.00 Hz
GB	0
PC	1.00



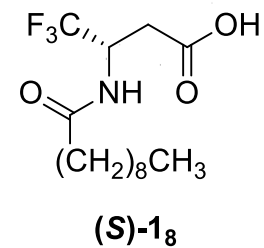
積算回数
ゼロフィリング
ゲイン
測定日時
測定者
ファイル名
サンプル名
コメント

16
ON
8
2016/11/22 14:25
kawamata
Memory#2
s-F10

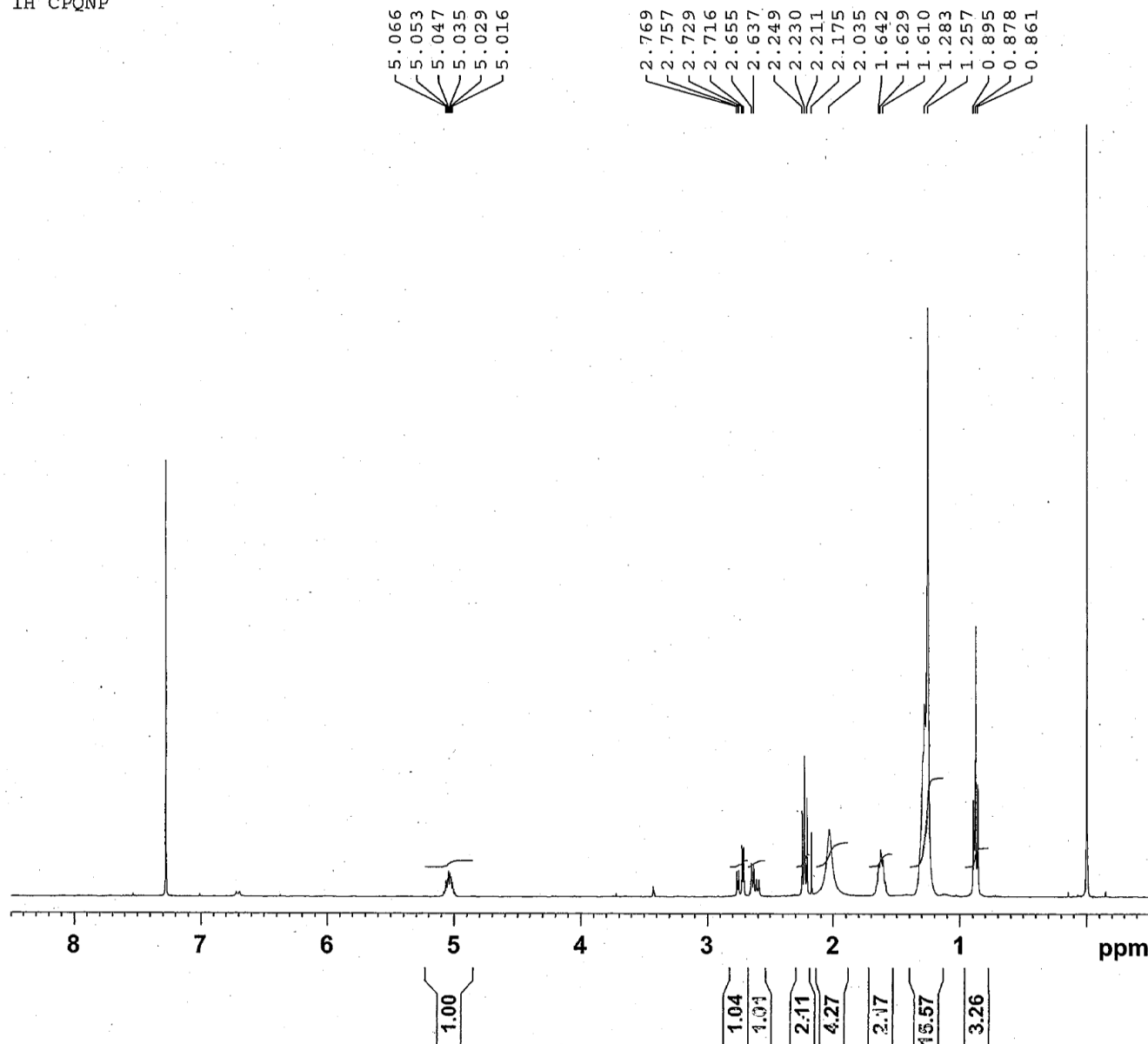
分解
アポダイゼーション
スキャンスピード
更新日時

4 cm-1
Cosine
2 mm/sec
2016/11/22 14:28

1: 3294.79,	65.91	2: 2915.84,	70.28	3: 2849.31,	76.60	4: 1704.76,	59.35
5: 1667.16,	54.71	6: 1548.56,	68.17	7: 1507.10,	86.37	8: 1473.35,	86.43
9: 1456.96,	86.88	10: 1419.35,	87.09	11: 1373.07,	87.61	12: 1258.32,	78.88
13: 1232.29,	78.12	14: 1204.33,	75.42	15: 1125.26,	59.92	16: 936.27,	86.42
17: 718.35,	88.94	18: 652.79,	83.22	19: 500.44,	91.17	20: 466.69,	91.42
21: 456.08,	85.25	22: 421.37,	84.13	23: 411.73,	82.60		



1H CPQNP

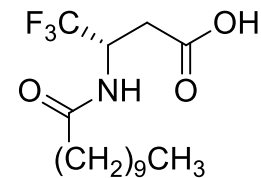


Current Data Parameters
NAME kodama
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170914
Time_ 21.01
INSTRUM spect
PROBHD 5 mm CPQNP 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 2
SWH 8305.647 Hz
FIDRES 0.126734 Hz
AQ 3.9453173 sec
RG 7.21
DW 60.200 usec
DE 10.00 usec
TE 300.0 K
D1 1.00000000 sec
TDO 1

----- CHANNEL f1 -----
NUC1 1H
P1 15.00 usec
PLW1 5.19999981 W
SFO1 400.1324708 MHz

F2 - Processing parameters
SI 32768
SF 400.1300025 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



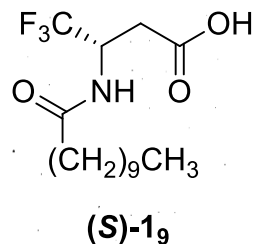
13C with dec. CPQNP

173.43
171.51

128.89
126.09
123.29
120.49

47.72
47.41
47.09
46.77
36.45
32.94
31.91
29.57
29.47
29.31
29.11
25.46
22.69
14.10

0.00



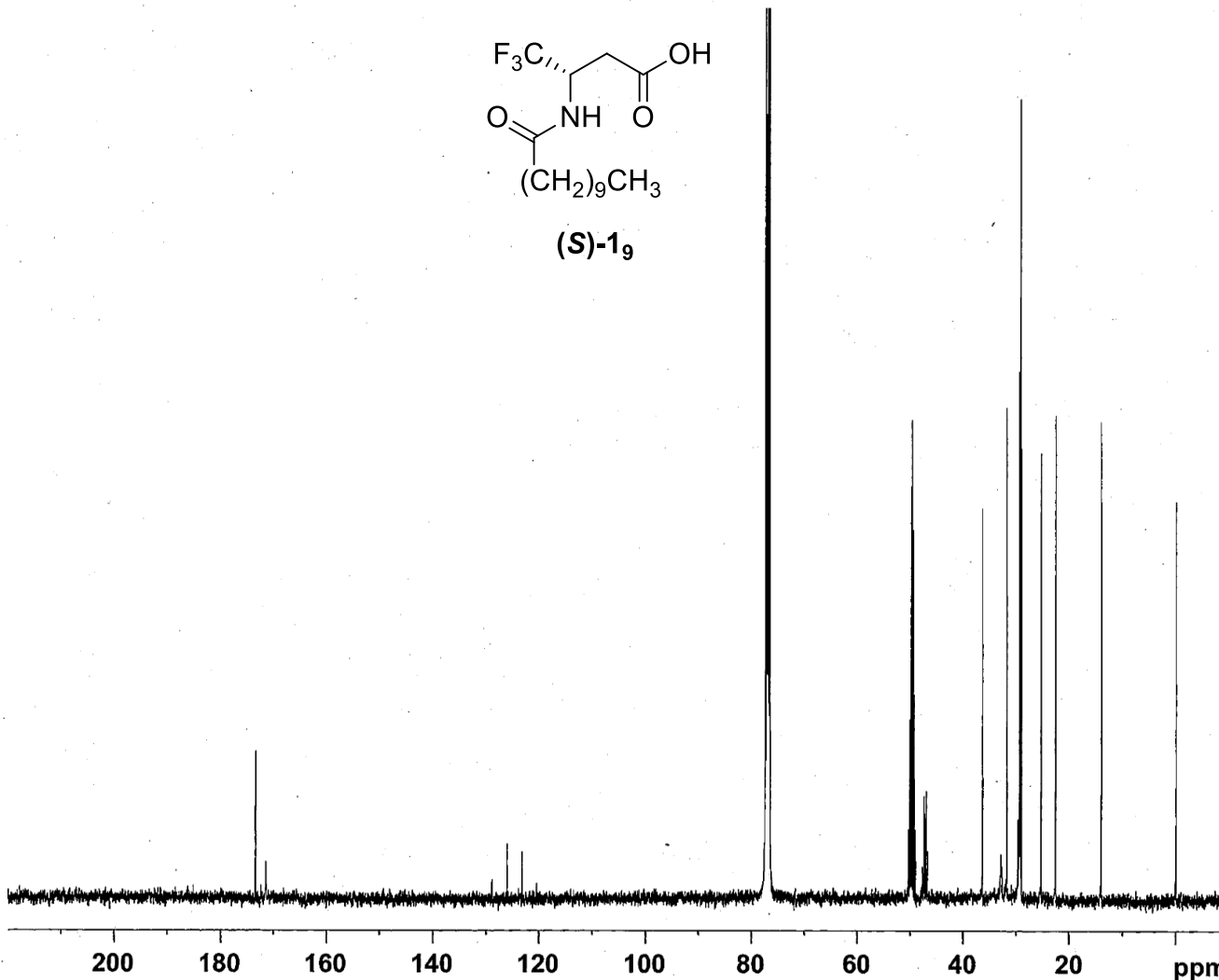
Current Data Parameters
NAME kodama
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170914
Time_ 21.15
INSTRUM spect
PROBHD 5 mm CPQNP 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 2
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 126.99
DW 16.800 usec
DE 18.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PLW1 15.50000000 W
SFO1 100.6248425 MHz

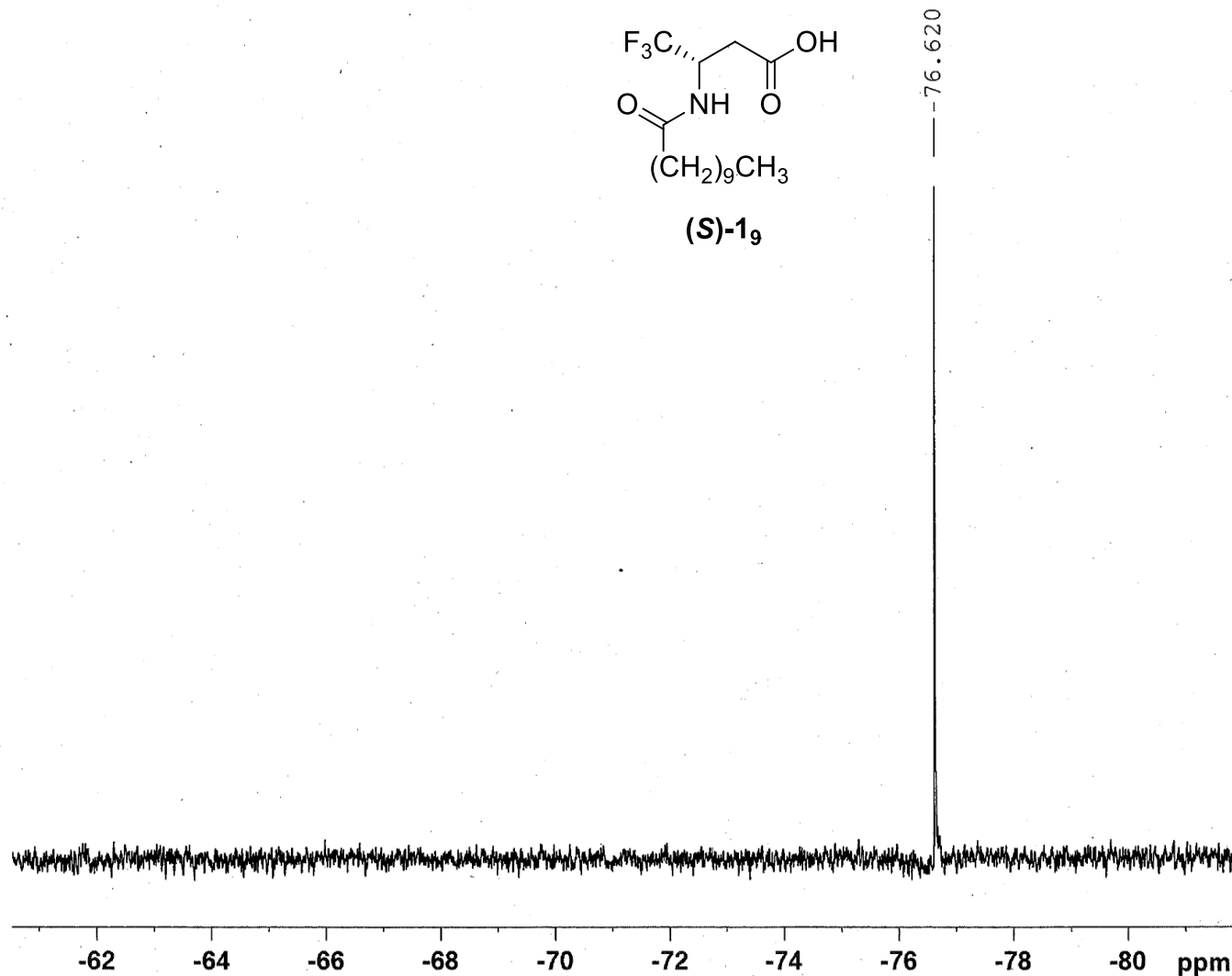
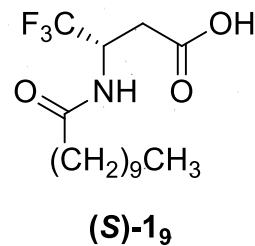
==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 5.19999981 W
PLW12 0.14444000 W
PLW13 0.11700000 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127639 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40



- ACCEPTANCE - System: AV300 OrderNo.: JH033009 Customer: Saitama University Engineer: IKD
 P/N Console: Z108356/162 Shim system: BOSS I original dataset: 104275_0150snf 3 1
 Probe: 5 mm PABBO BB-1H/D Z-GRD Z104275/0150 Sample depth:20 Gas: air
 Sensitivity test for 19F (additional test); Sample: 0.05% TFT in CDCl3 (P/N: Z10234)

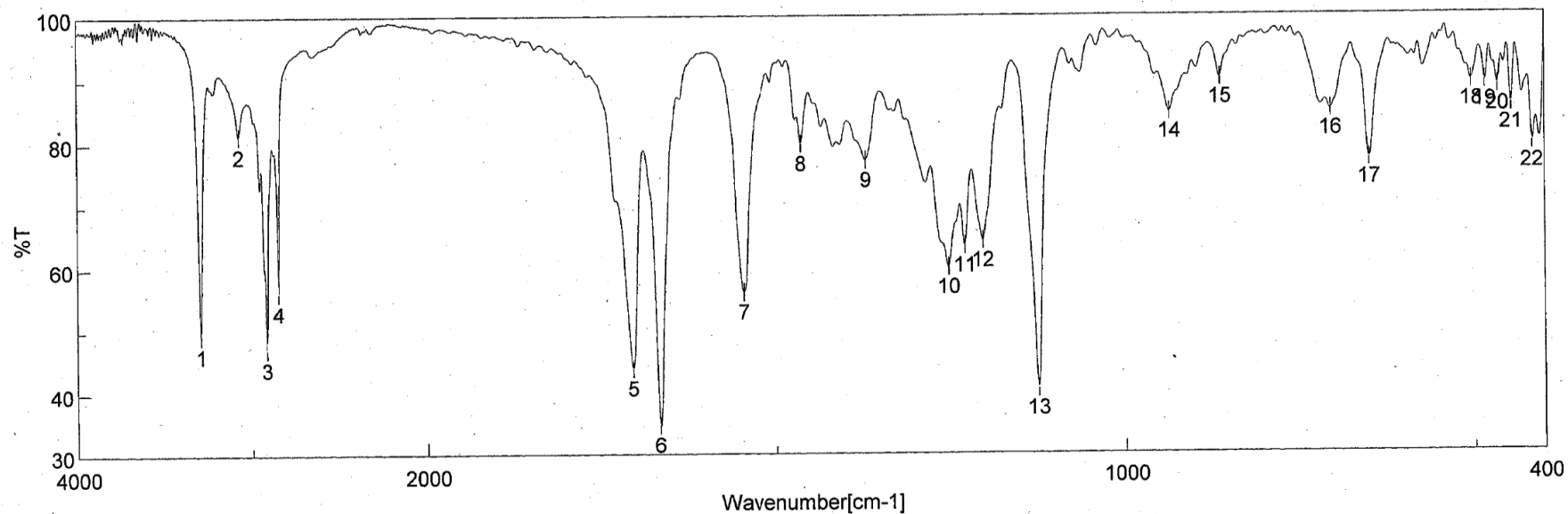
Sino= 243:1 (signal= -61 - -65 ppm noise= -59.08 - -60.08 ppm [1 ppm] noise range= 4.5 ppm)
 P1= 15usec PL1= -0.3dB



NAME A16mc211rk
 EXPNO 17091305
 PROCNO 1
 Date_ 20170913
 Time 13.48
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgfhigqn
 TD 32768
 SOLVENT CDCl3
 NS 1
 DS 0
 SWH 12019.230 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 203
 DW 41.600 usec
 DE 6.50 usec
 TE 297.0 K
 D1 10.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 19F
 P1 15.00 usec
 PL1 -0.30 dB
 PL1W 10.09325600 W
 SFO1 282.3865635 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.58 dB
 PL12 16.50 dB
 PL2W 9.45079708 W
 PL12W 0.24180678 W
 SFO2 300.1300000 MHz
 SI 16384
 SF 282.4046264 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.00



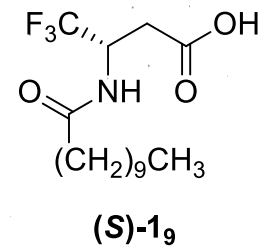
積算回数
ゼロフィリング
ゲイン
測定日時
測定者
ファイル名
サンプル名
コメント

16
ON
8
2017/09/19 14:53
kawamata
Memory#2
rac-CF3-C10-COOH
S

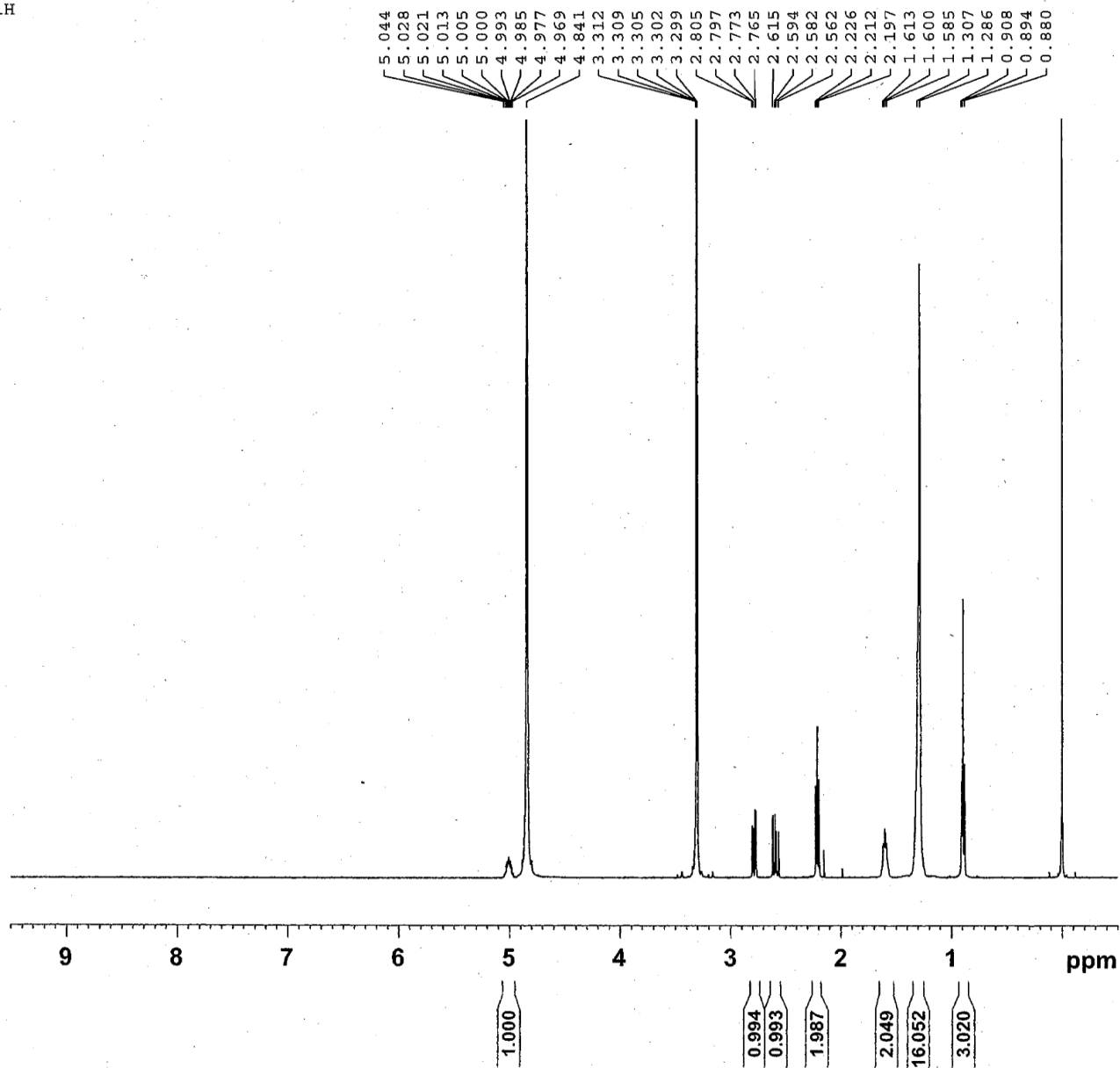
分解
アポダイゼーション
スキャンスピード
更新日時

4 cm-1
Cosine
2 mm/sec
2017/09/19 14:54

1: 3293.82,	49.33	2: 3073.98,	81.26	3: 2915.84,	47.16	4: 2849.31,	56.17
5: 1705.73,	43.92	6: 1667.16,	34.74	7: 1546.63,	56.14	8: 1463.71,	79.77
9: 1371.14,	77.14	10: 1252.54,	60.06	11: 1229.40,	63.50	12: 1203.36,	64.34
13: 1124.30,	40.57	14: 936.27,	84.67	15: 863.95,	90.22	16: 705.82,	85.03
17: 650.86,	77.19	18: 504.29,	89.58	19: 485.01,	89.46	20: 466.69,	88.75
21: 447.40,	85.75	22: 417.51,	79.57				

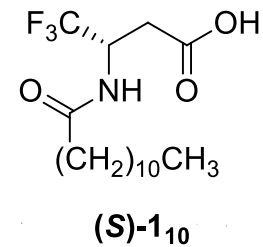


1H



NAME A16mc211rk
EXPNO 17091204
PROCNO 1
Date_ 20170912
Time 18.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 8
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 203
DW 48.400 usec
DE 6.50 usec
TE 300.5 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 11.80 usec
PL1 2.40 dB
PL1W 15.17711735 W
SFO1 500.0330885 MHz
SI 32768
SF 500.0300106 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

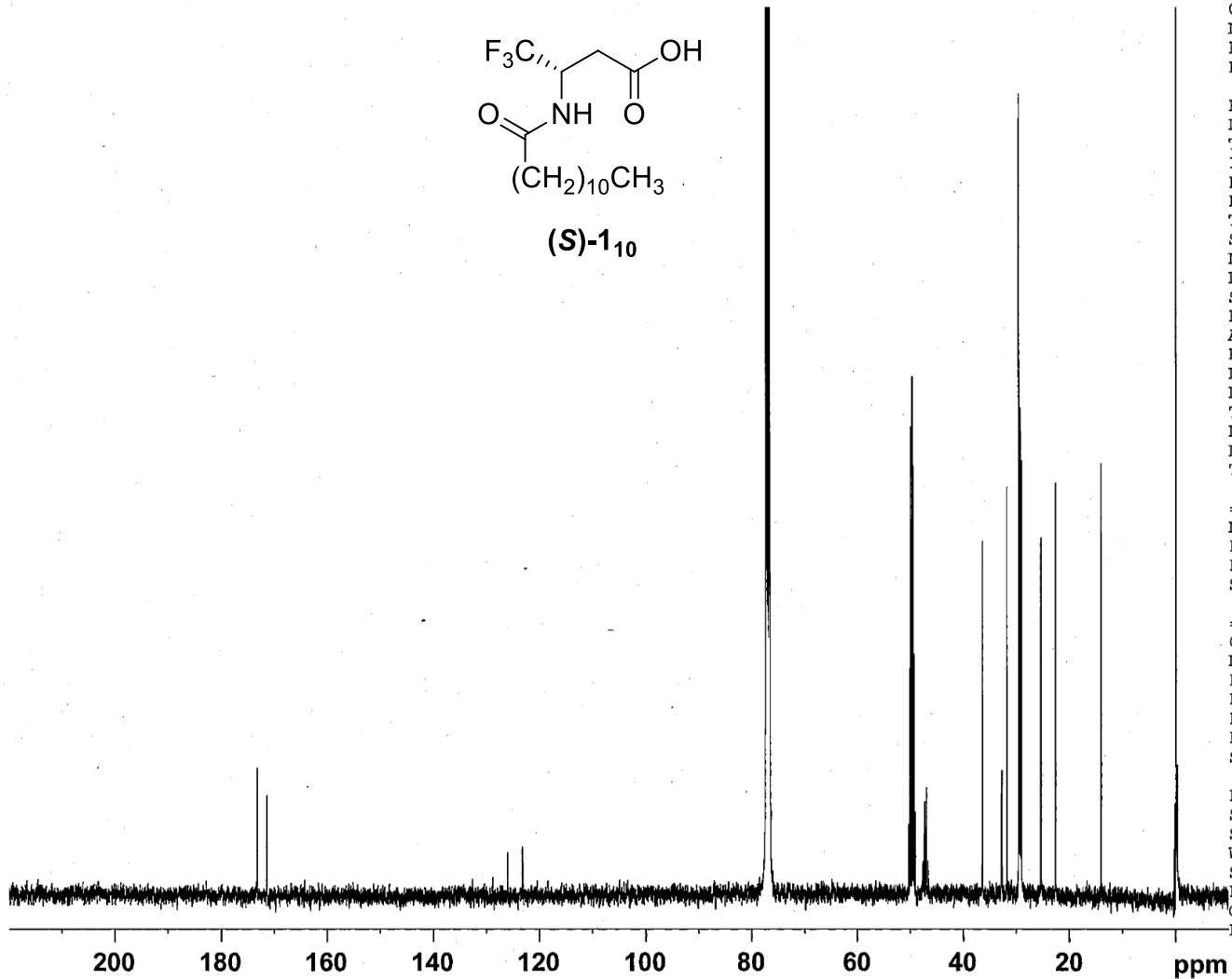
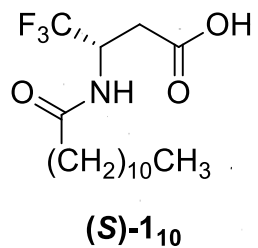


13C with dec. CPQNP

173.34
171.48

128.89
126.08
123.29
120.48

47.69
47.38
47.06
46.74
36.46
32.84
31.93
29.61
29.47
29.35
29.30
29.11
25.45
22.70
14.11



Current Data Parameters
NAME kodama
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170913
Time 20.17
INSTRUM spect
PROBHD 5 mm CPQNP 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 2
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 126.99
DW 16.800 usec
DE 18.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

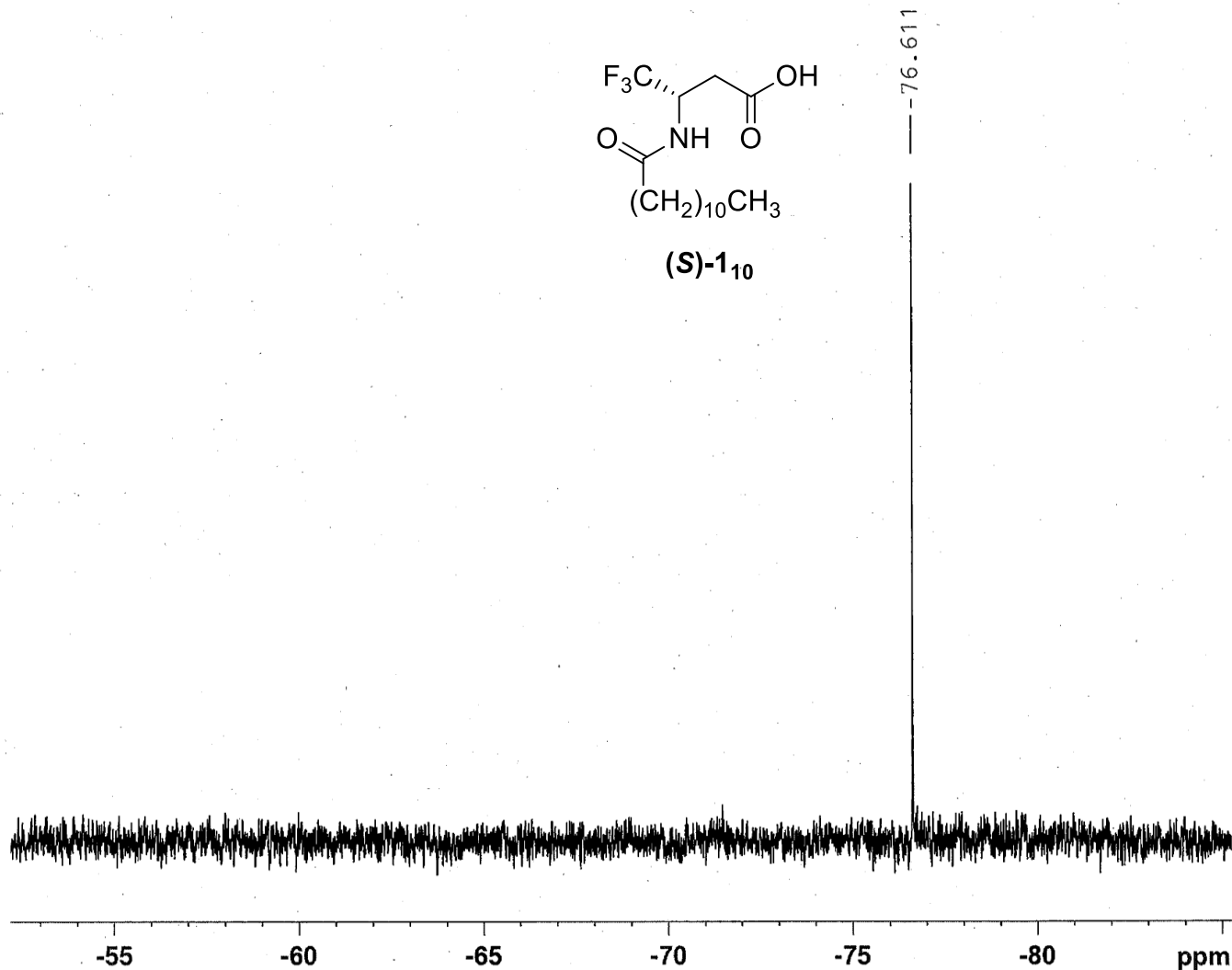
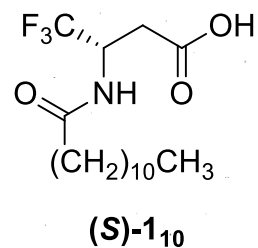
==== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PLW1 15.50000000 W
SFO1 100.6248425 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 5.199999981 W
PLW12 0.14444000 W
PLW13 0.11700000 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127642 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

- ACCEPTANCE - System: AV300 OrderNo.: JH033009 Customer: Saitama University Engineer: IKD
 P/N Console: Z108356/162 Shim system: BOSS I original dataset: 104275_0150snf 3 1
 Probe: 5 mm PABBO BB-1H/D Z-GRD Z104275/0150 Sample depth:20 Gas: air
 Sensitivity test for 19F (additional test); Sample: 0,05% TFT in CDCl3 (P/N: Z10234)

Sino= 243:1 (signal= -61 - -65 ppm noise= -59.08 - -60.08 ppm [1 ppm] noise range= 4.5 ppm)
 P1= 15usec PL1= -0.3dB



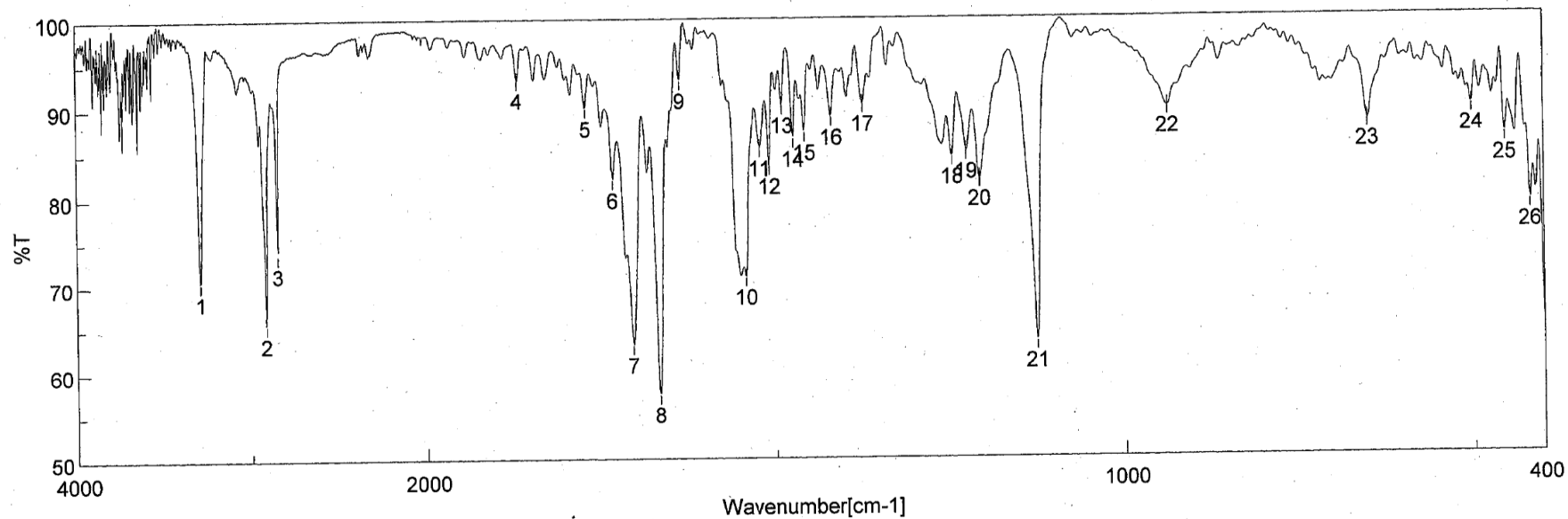
NAME	A16mc211rk
EXPNO	17091302
PROCNO	1
Date_	20170913
Time	12.40
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgfhigqn
TD	32768
SOLVENT	CDCl3
NS	1
DS	0
SWH	12019.230 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	41.600 usec
DE	6.50 usec
TE	297.0 K
D1	10.00000000 sec
D11	0.03000000 sec
D12	0.00002000 sec
TD0	1

==== CHANNEL f1 =====

NUC1	19F
P1	15.00 usec
PL1	-0.30 dB
PL1W	10.09325600 W
SFO1	282.3865635 MHz

==== CHANNEL f2 =====

CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.58 dB
PL12	16.50 dB
PL2W	9.45079708 W
PL12W	0.24180678 W
SFO2	300.1300000 MHz
SI	16384
SF	282.4046264 MHz
WDW	EM
SSB	0
LB	2.00 Hz
GB	0
PC	1.00



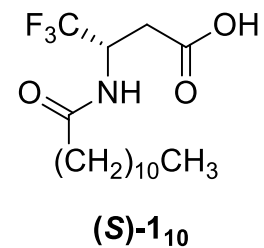
積算回数
ゼロフィリング
ゲイン
測定日時
測定者
ファイル名
サンプル名
コメント

16
ON
8
2016/11/22 14:57
kawamata
Memory#2
s-F12

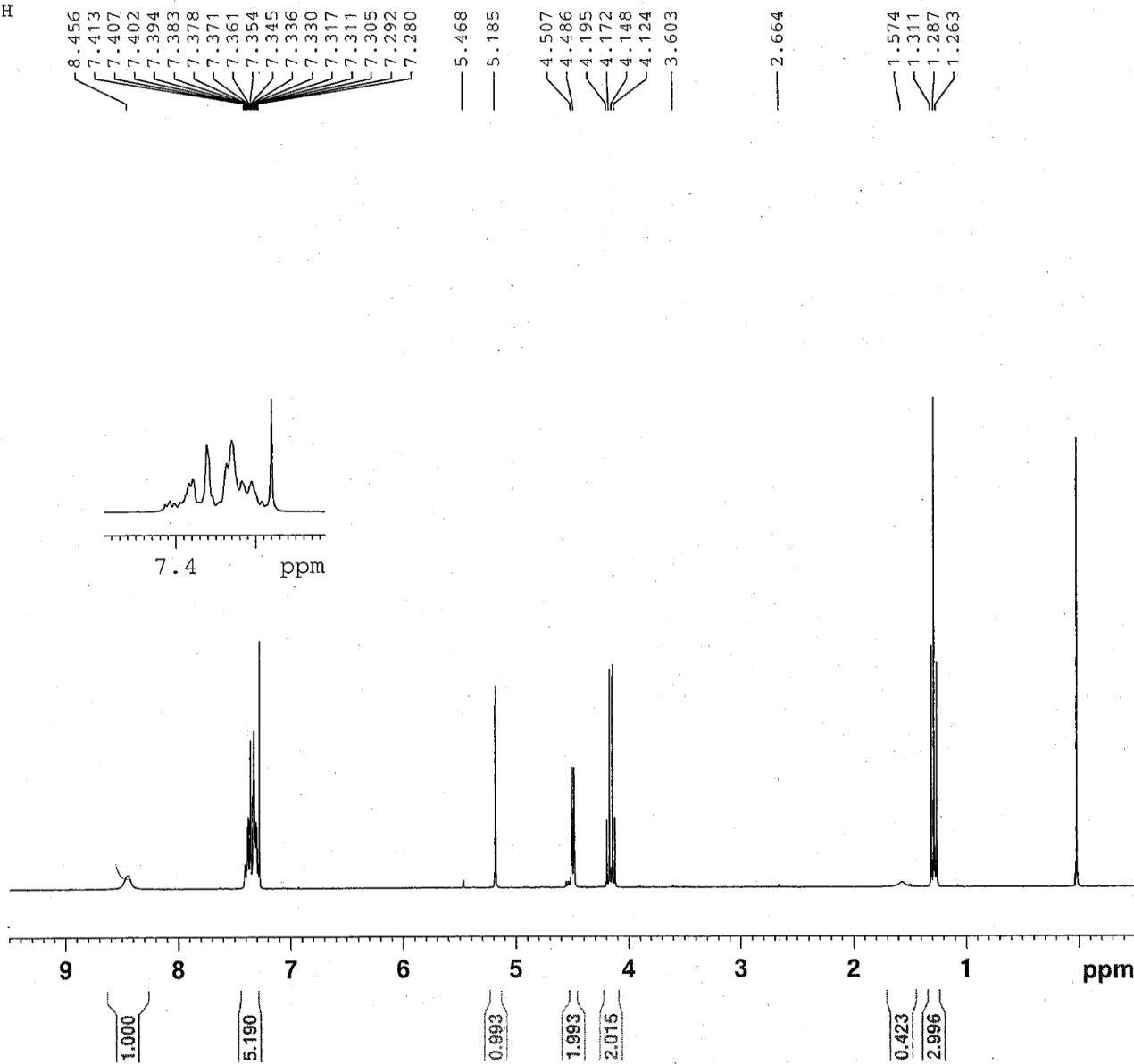
分解
アポダイゼーション
スキャンスピード
更新日時

4 cm-1
Cosine
2 mm/sec
2016/11/22 15:00

1: 3293.82,	70.39	2: 2915.84,	65.56	3: 2849.31,	73.56	4: 1868.68,	93.15
5: 1771.30,	89.91	6: 1732.73,	81.94	7: 1704.76,	63.06	8: 1667.16,	57.31
9: 1636.30,	92.96	10: 1542.77,	70.76	11: 1521.56,	85.38	12: 1507.10,	83.40
13: 1488.78,	90.09	14: 1473.35,	86.38	15: 1456.96,	87.08	16: 1418.39,	88.78
17: 1373.07,	90.24	18: 1245.79,	84.34	19: 1225.54,	84.90	20: 1206.26,	81.85
21: 1125.26,	63.28	22: 937.23,	89.72	23: 651.82,	88.02	24: 502.37,	89.63
25: 455.12,	86.28	26: 419.44,	78.83				

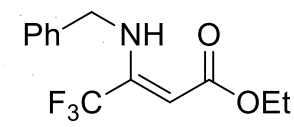


¹H



NAME A12TA020rk
EXPNO 16032804
PROCNO 1
Date_ 20160328
Time 18.00
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 203
DW 80.800 usec
DE 6.50 usec
TE 296.9 K
D1 1.00000000 sec
TDO 1

----- CHANNEL f1 -----
NUC1 1H
P1 15.00 usec
PL1 1.20 dB
PL1W 8.19348145 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

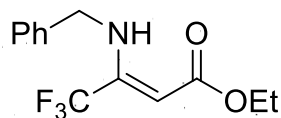


8

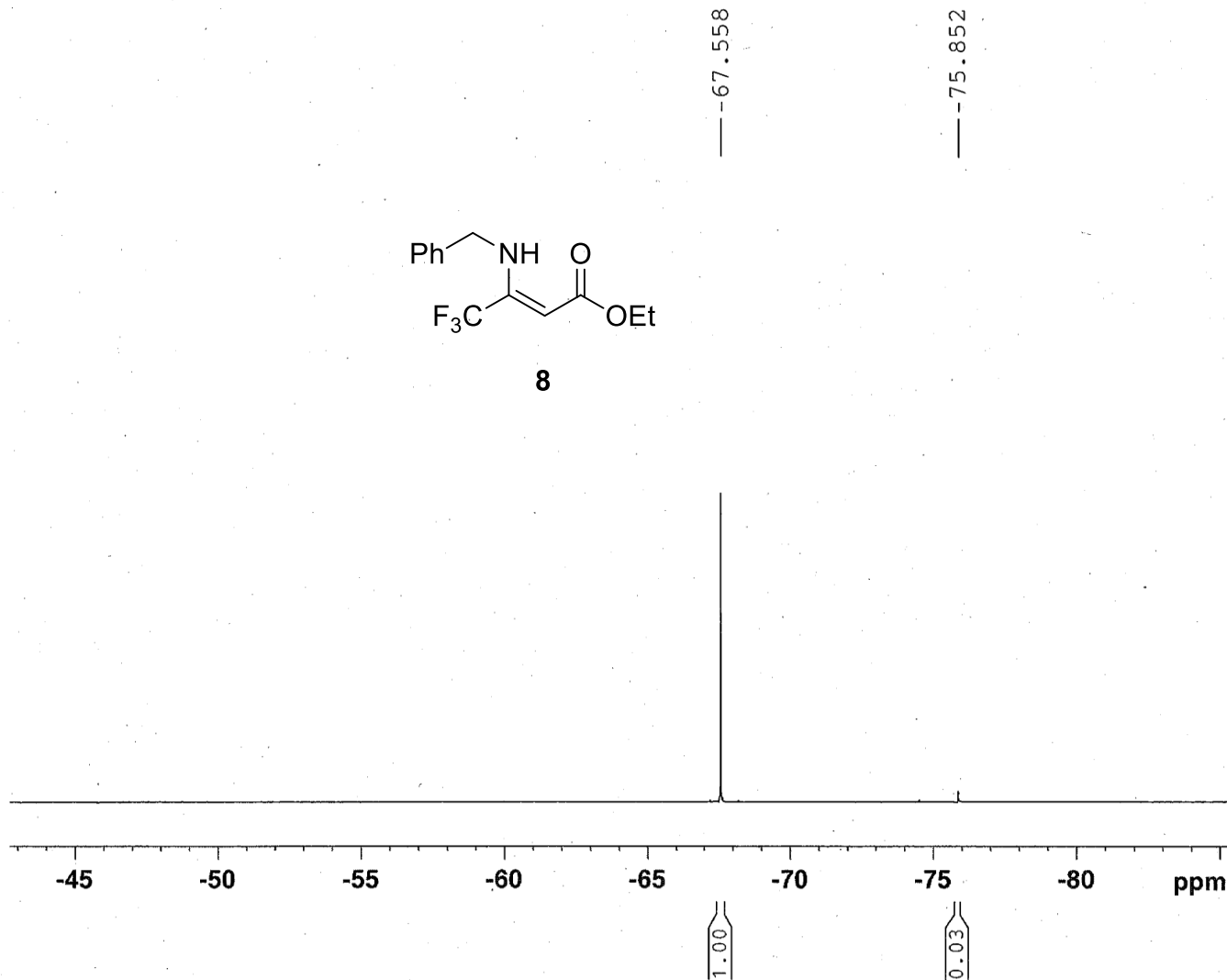
- ACCEPTANCE - System: AV300 OrderNo.: JH033009 Customer: Saitama University Engineer: IKD
 P/N Console: Z108356/162 Shim system: BOSS I original dataset: 104275_0150snf 3 1
 Probe: 5 mm PABBO BB-1H/D Z-GRD Z104275/0150 Sample depth:20 Gas: air
 Sensitivity test for 19F (additional test); Sample: 0,05% TFT in CDCl3 (P/N: Z10234)
 Sino= 243:1 (signal= -61 - -65 ppm noise= -59.08 - -60.08 ppm [1 ppm] noise range= 4.5 ppm)
 P1= 15usec PL1= -0.3dB



NAME A12TA020rk
 EXPNO 16032802
 PROCNO 1
 Date_ 20160328
 Time 17.52
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgfhigqn
 TD 32768
 SOLVENT CDCl3
 NS 1
 DS 0
 SWH 12019.230 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 203
 DW 41.600 usec
 DE 6.50 usec
 TE 297.1 K
 D1 10.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec
 TD0 1

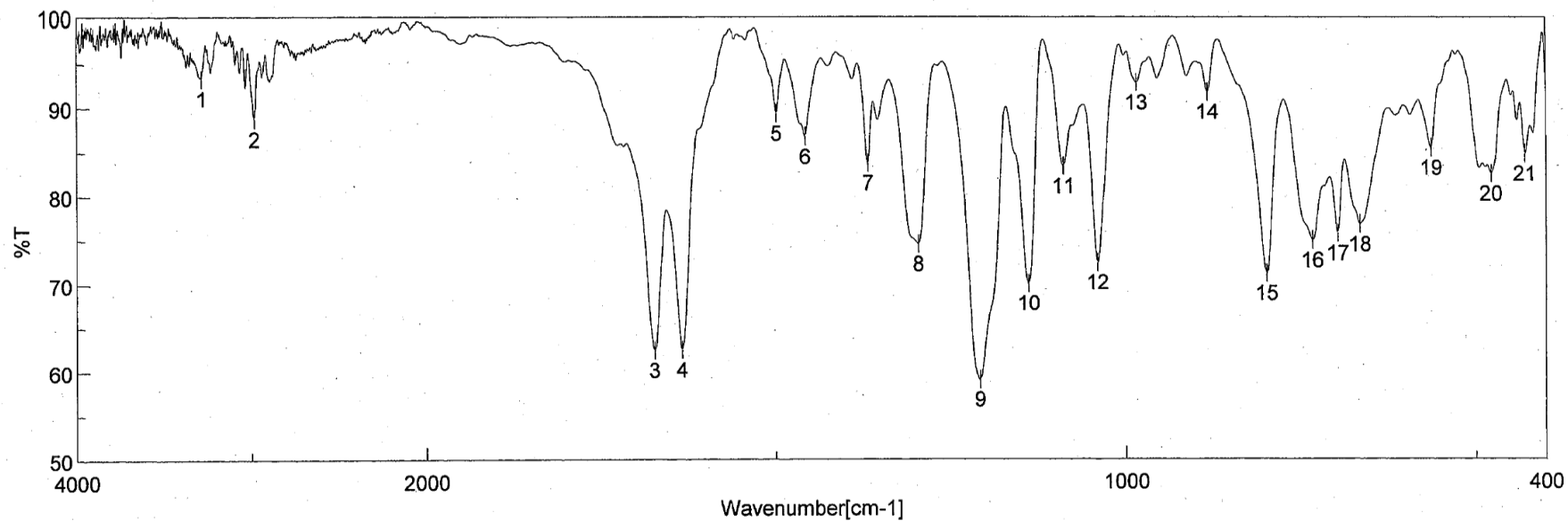


8



===== CHANNEL f1 =====
 NUC1 19F
 P1 15.00 usec
 PL1 -0.30 dB
 PL1W 10.09325600 W
 SFO1 282.3865635 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.58 dB
 PL12 16.50 dB
 PL2W 9.45079708 W
 PL12W 0.24180678 W
 SFO2 300.1300000 MHz
 SI 16384
 SF 282.4046330 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.00



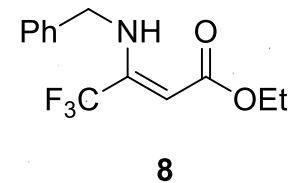
積算回数
ゼロフィリング
ゲイン
測定日時
測定者
ファイル名
サンプル名
コメント

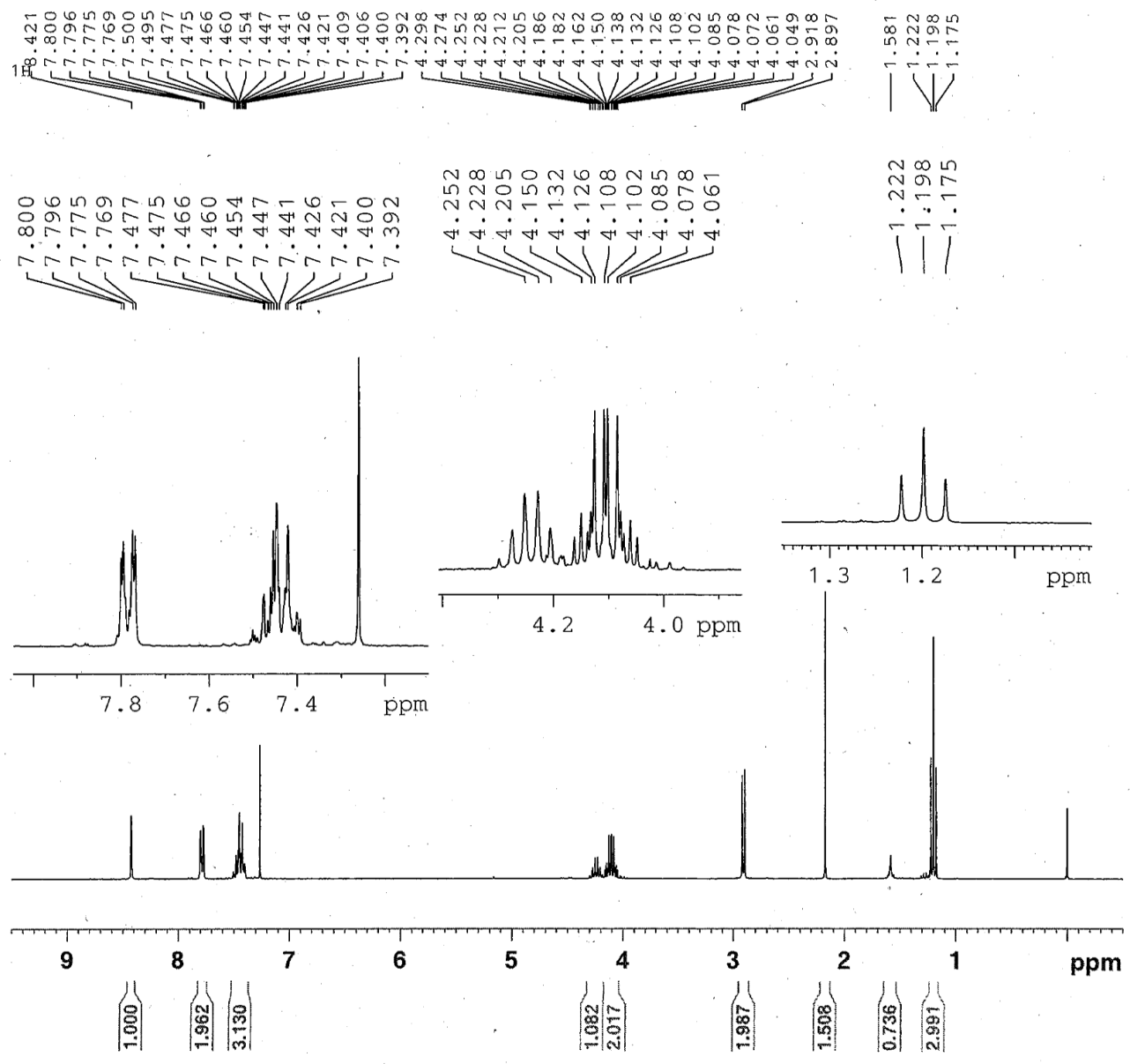
8
ON
8
2017/10/19 20:35
kawamata
no168
no168

分解
アポダイゼーション
スキャンスピード
更新日時

4 cm-1
Cosine
2 mm/sec
2018/01/25 19:46

1:	3286.11,	93.33	2:	2983.34,	88.80	3:	1674.87,	62.49	4:	1635.34,	62.56
5:	1498.42,	89.40	6:	1456.96,	86.81	7:	1367.28,	83.80	8:	1295.93,	74.72
9:	1208.18,	59.15	10:	1138.76,	70.23	11:	1088.62,	83.48	12:	1040.41,	72.63
13:	984.48,	92.92	14:	883.24,	91.85	15:	799.35,	71.42	16:	733.78,	75.20
17:	698.11,	75.98	18:	666.29,	76.96	19:	564.08,	85.57	20:	478.26,	82.64
21:	430.05,	84.90									



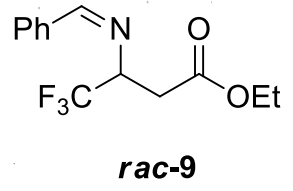


```

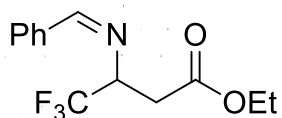
NAME      A16mc211rk
EXPNO     16042105
PROCNO    1
Date_     20160421
Time      17.31
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         8
DS         2
SWH       6188.119 Hz
FIDRES    0.094423 Hz
AQ         5.2953587 sec
RG         203
DW         80.800 usec
DE         6.50 usec
TE         296.4 K
D1         1.00000000 sec
TD0        1
  
```

```

===== CHANNEL f1 =====
NUC1      1H
P1        15.00 usec
PL1       1.20 dB
PL1W      8.19348145 W
SFO1      300.1318534 MHz
SI         32768
SF         300.1300059 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```

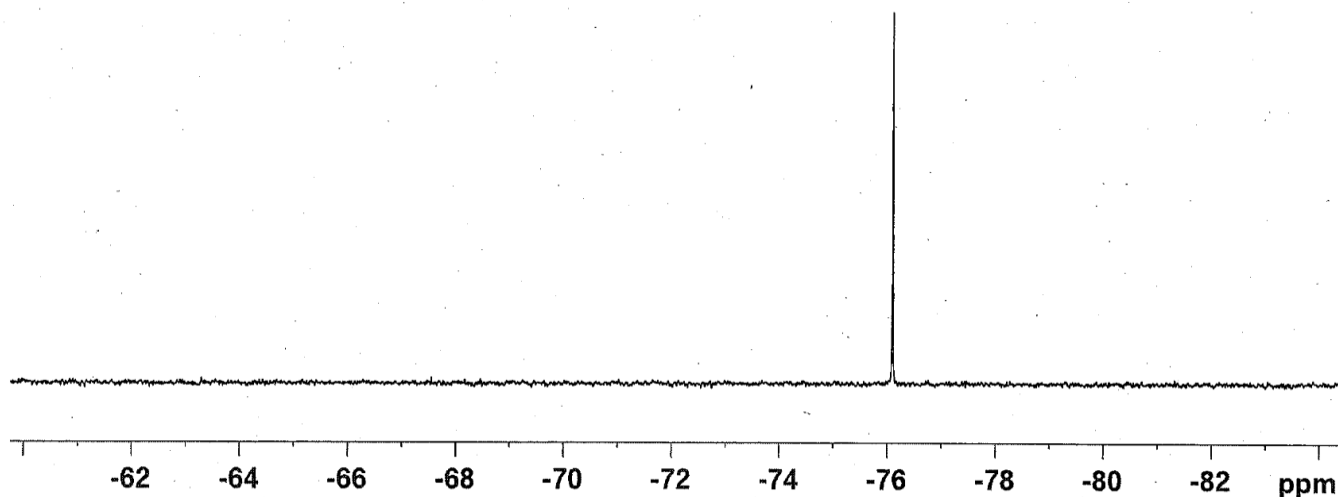


- ACCEPTANCE - System: AV300 OrderNo.: JH033009 Customer: Saitama University Engineer: IKD
 P/N Console: Z108356/162 Shim system: BOSS-I original dataset: 104275_0150snf 3 1
 Probe: 5 mm PABBO BB-1H/D Z-GRD Z104275/0150 Sample depth:20 Gas: air
 Sensitivity test for 19F (additional test); Sample: 0,05% TFT in CDCl3 (P/N: Z10234)
 Sino= 243:1 (signal= -61 - -65 ppm noise= -59.08 - -60.08 ppm [1 ppm] noise range= 4.5 ppm)
 P1= 15usec PL1= -0.3dB



rac-9

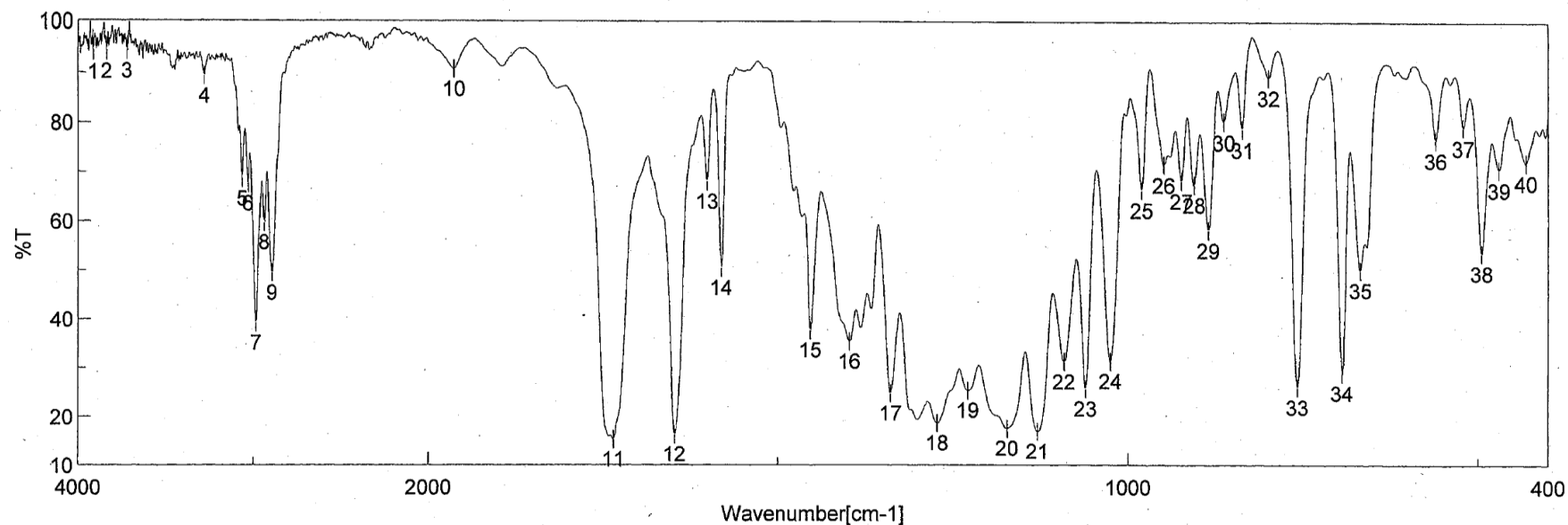
---76.095



NAME	A12TA020rk
EXPNO	16033002
PROCNO	1
Date_	20160330
Time	10.31
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgfhigqn
TD	32768
SOLVENT	CDCl3
NS	1
DS	0
SWH	12019.230 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	41.600 usec
DE	6.50 usec
TE	296.7 K
D1	10.00000000 sec
D11	0.03000000 sec
D12	0.00002000 sec
TD0	1

===== CHANNEL f1 =====
 NUC1 19F
 P1 15.00 usec
 PL1 -0.30 dB
 PL1W 10.09325600 W
 SFO1 282.3865635 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.58 dB
 PL12 16.50 dB
 PL2W 9.45079708 W
 PL12W 0.24180678 W
 SFO2 300.1300000 MHz
 SI 16384
 SF 282.4046286 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.00



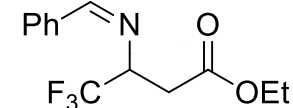
積算回数
ゼロフィリング
ゲイン
測定日時
測定者
ファイル名
サンプル名
コメント

16
ON
16
2016/03/30 16:44
kawamata
Memory#2
aldimine6

分解
アポダイゼーション
スキャンスピード
更新日時

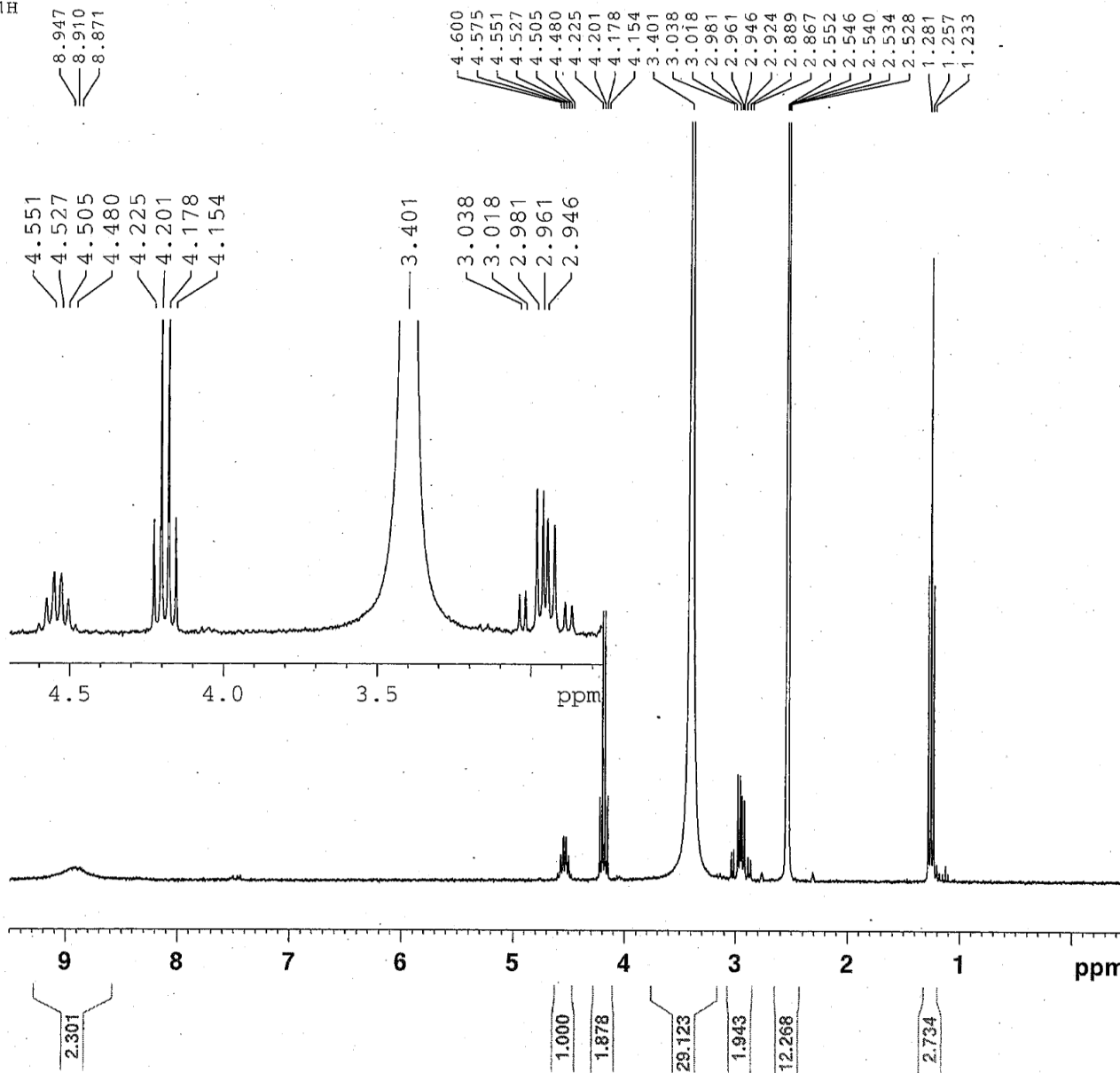
4 cm-1
Cosine
2 mm/sec
2016/03/30 16:44

1: 3912.86,	94.26	2: 3836.68,	94.34	3: 3720.98,	94.49	4: 3280.32,	89.41
5: 3065.30,	68.68	6: 3030.59,	67.66	7: 2986.23,	39.18	8: 2939.95,	59.72
9: 2893.66,	49.50	10: 1963.18,	90.82	11: 1735.62,	15.35	12: 1648.84,	16.39
13: 1602.56,	68.18	14: 1582.31,	50.66	15: 1453.10,	37.81	16: 1397.17,	35.49
17: 1338.36,	24.84	18: 1271.82,	18.70	19: 1228.43,	25.49	20: 1172.51,	17.63
21: 1129.12,	16.98	22: 1091.51,	31.38	23: 1060.66,	25.79	24: 1024.98,	31.47
25: 980.63,	66.50	26: 948.81,	71.62	27: 923.74,	68.38	28: 905.42,	67.61
29: 885.17,	58.48	30: 862.99,	80.19	31: 836.95,	78.75	32: 799.35,	89.11
33: 757.89,	26.07	34: 694.25,	29.00	35: 668.21,	50.40	36: 561.18,	76.70
37: 521.65,	79.18	38: 495.62,	53.99	39: 470.55,	70.77	40: 431.98,	72.23



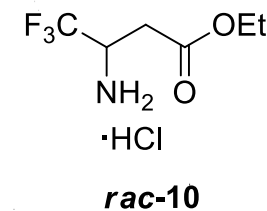
rac-9

¹H



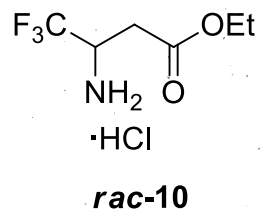
NAME A16mc211rk
 EXPNO 16042602
 PROCNO 1
 Date_ 20160426
 Time 18.29
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 8
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953587 sec
 RG 203
 DW 80.800 usec
 DE 6.50 usec
 TE 296.2 K
 D1 1.0000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 ¹H
 P1 15.00 usec
 PL1 1.20 dB
 PL1W 8.19348145 W
 SFO1 300.1318534 MHz
 SI 32768
 SF 300.1299890 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

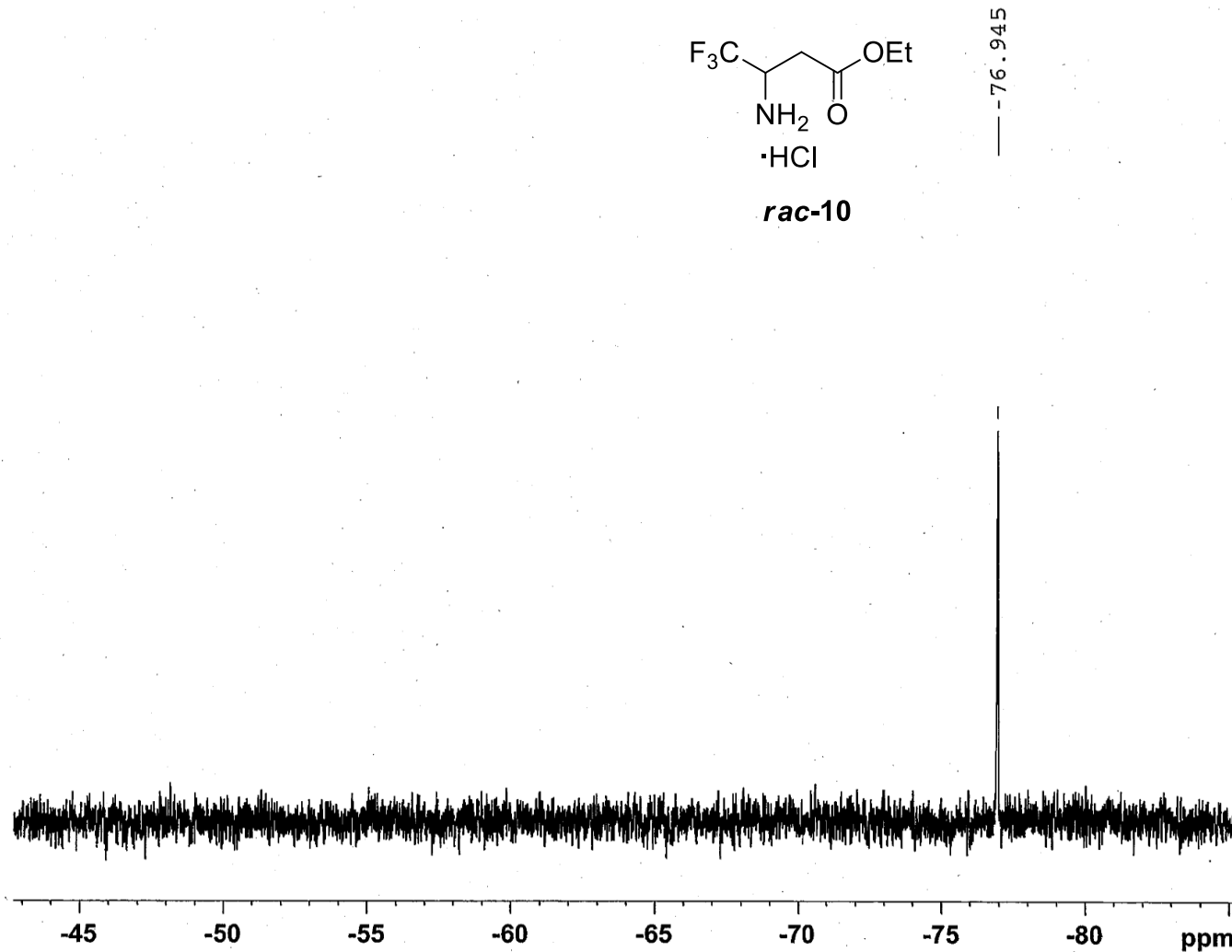


- ACCEPTANCE - System: AV300 OrderNo.: JH033009 Customer: Saitama University Engineer: IKD
 P/N Console: Z108356/162 Shim system: BOSS I original dataset: 104275_0150snf 3 1
 Probe: 5 mm PABBO BB-1H/D Z-GRD Z104275/0150 Sample depth:20 Gas: air
 Sensitivity test for 19F (additional test); Sample: 0,05% TFT in CDCl3 (P/N: Z10234)

Sino= 243:1 (signal= -61 - -65 ppm noise= -59.08 - -60.08 ppm [1 ppm] noise range= 4.5 ppm)
 P1= 15usec PL1= -0.3dB



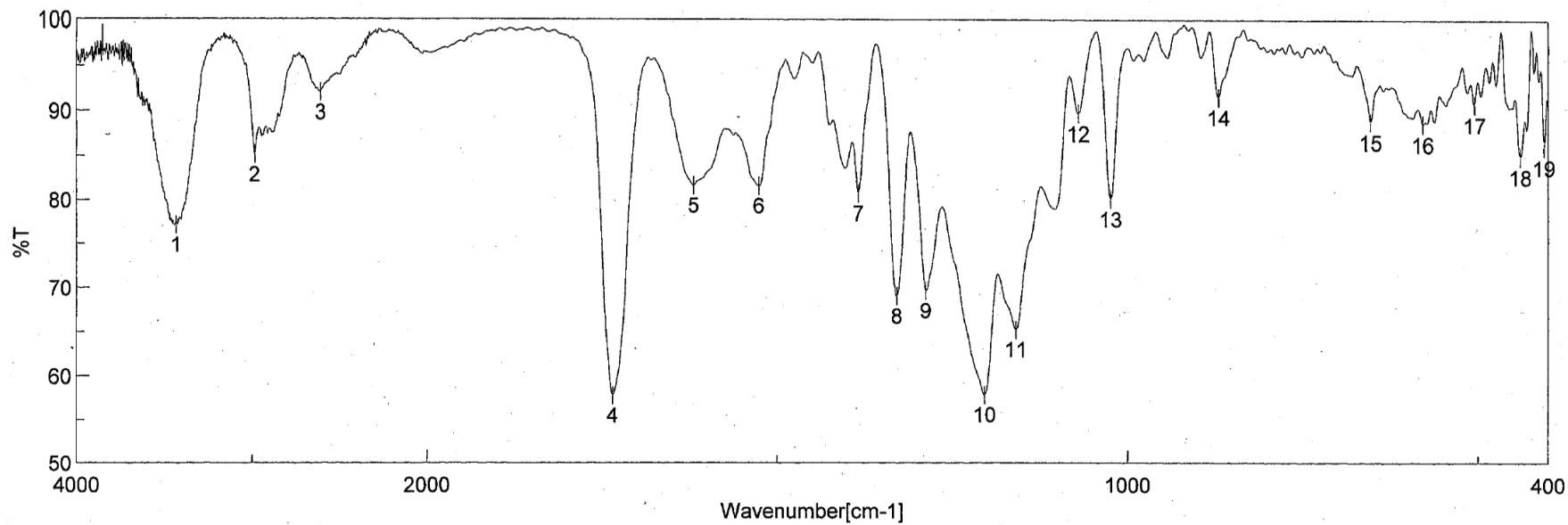
--- -76.945



NAME	A16mc211rk
EXPNO	16051005
PROCNO	1
Date_	20160510
Time_	13.22
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgfhigqn
TD	32768
SOLVENT	CDCl3
NS	1
DS	0
SWH	12019.230 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	41.600 usec
DE	6.50 usec
TE	296.3 K
D1	10.00000000 sec
D11	0.03000000 sec
D12	0.00002000 sec
TDO	1

===== CHANNEL f1 =====	
NUC1	19F
P1	15.00 usec
PL1	-0.30 dB
PL1W	10.09325600 W
SFO1	282.3865635 MHz

===== CHANNEL f2 =====	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.58 dB
PL12	16.50 dB
PL2W	9.45079708 W
PL12W	0.24180678 W
SFO2	300.1300000 MHz
SI	16384
SF	282.4046279 MHz
WPDW	EM
SSB	0
LB	2.00 Hz
GB	0
PC	1.00



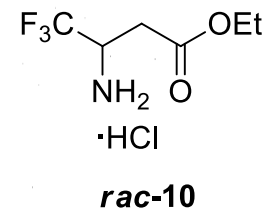
積算回数
ゼロフィリング
ゲイン
測定日時
測定者
ファイル名
サンプル名
コメント

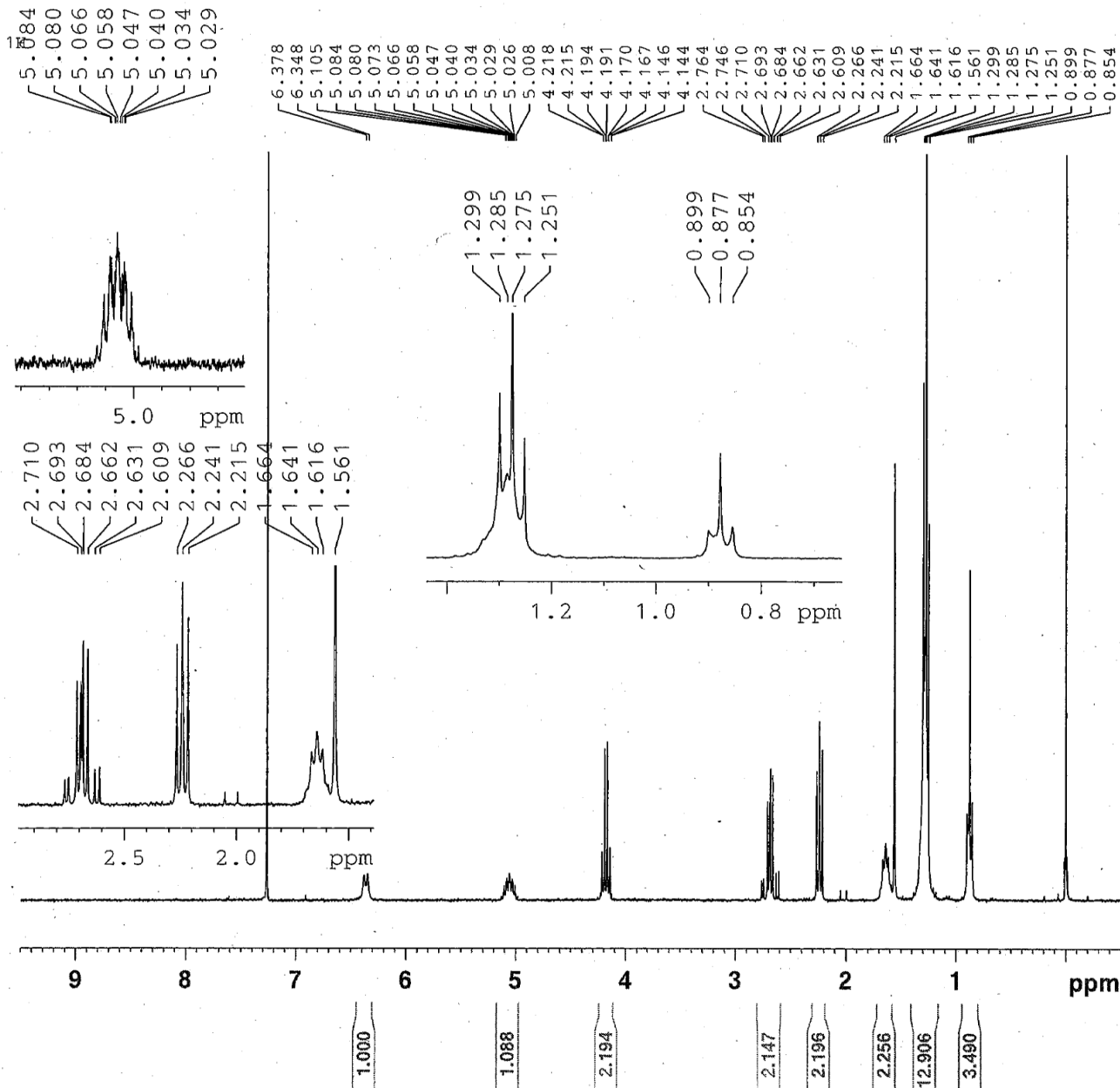
16
ON
16
2016/04/27 14:07
kawamata
Memory#2
ラセミ-9

分解
アポダイゼーション
スキャンスピード
更新日時

4 cm-1
Cosine
2 mm/sec
2016/04/27 14:10

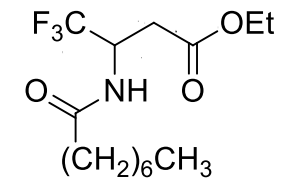
1:	3433.64,	77.13	2:	2985.27,	85.13	3:	2609.22,	92.09	4:	1735.62,	57.78
5:	1619.91,	81.73	6:	1525.42,	81.66	7:	1383.68,	80.81	8:	1328.71,	69.16
9:	1287.25,	69.79	10:	1203.36,	57.87	11:	1159.01,	65.35	12:	1069.33,	89.75
13:	1024.02,	80.21	14:	869.74,	91.59	15:	653.75,	88.86	16:	579.50,	88.63
17:	505.26,	90.80	18:	439.69,	85.05	19:	405.94,	86.12			





NAME A16mc211rk
 EXPNO 16050905
 PROCNO 1
 Date_ 20160509
 Time 11.36
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 8
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953587 sec
 RG 203
 DW 80.800 usec
 DE 6.50 usec
 TE 296.2 K
 D1 1.0000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 15.00 usec
 PL1 1.20 dB
 PL1W 8.19348145 W
 SFO1 300.1318534 MHz
 SI 32768
 SF 300.1300054 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



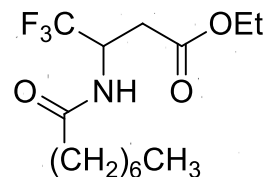
rac-11₆

- ACCEPTANCE - System: AV300 OrderNo.: JH033009 Customer: Saitama University Engineer: IKD
 P/N Console: Z108356/162 Shim system: BOSS I original dataset: 104275_0150snf 3 1
 Probe: 5 mm PABBO BB-1H/D Z-GRD Z104275/0150 Sample depth:20 Gas: air
 Sensitivity test for 19F (additional test); Sample: 0,05% TFT in CDC13 (P/N: Z10234)

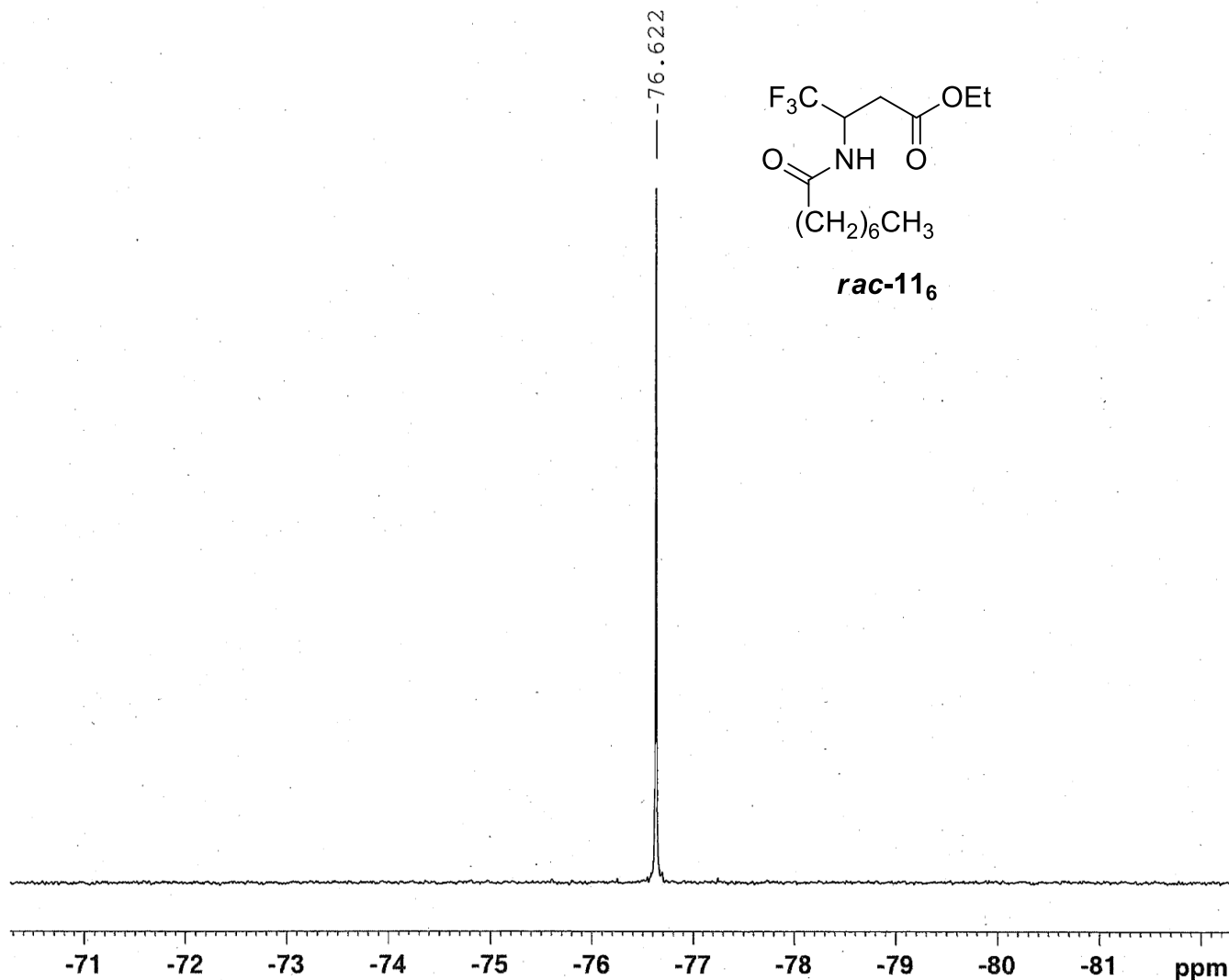
Sino= 243:1 (signal= -61 - -65 ppm noise= -59.08 - -60.08 ppm [1 ppm] noise range= 4.5 ppm)
 P1= 15usec PL1= -0.3dB



NAME	A16mc211rk
EXPNO	16050903
PROCNO	1
Date_	20160509
Time	11.31
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgfhigqn
TD	32768
SOLVENT	CDC13
NS	1
DS	0
SWH	12019.230 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	41.600 usec
DE	6.50 usec
TE	296.2 K
D1	10.00000000 sec
D11	0.03000000 sec
D12	0.00002000 sec
TD0	1

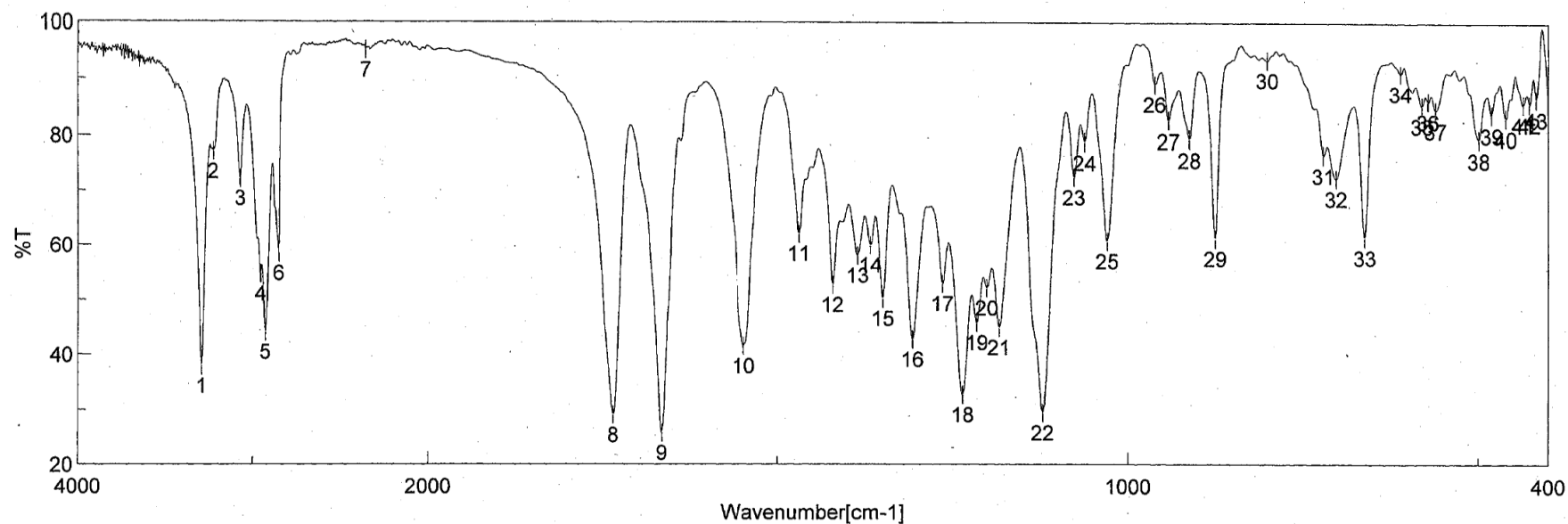


rac-11₆



==== CHANNEL f1 =====
 NUC1 19F
 P1 15.00 usec
 PL1 -0.30 dB
 PL1W 10.09325600 W
 SFO1 282.3865635 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.58 dB
 PL12 16.50 dB
 PL2W 9.45079708 W
 PL12W 0.24180678 W
 SFO2 300.1300000 MHz
 SI 16384
 SF 282.4046280 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.00



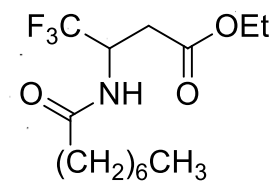
積算回数
ゼロフィリング
ゲイン
測定日時
測定者
ファイル名
サンプル名
コメント

16
ON
16
2016/05/10 9:51
kawamata
Memory#2
rac-10

分解
アポダイゼーション
スキャンスピード
更新日時

4 cm-1
Cosine
2 mm/sec
2016/05/10 9:53

1: 3293.82,	37.86	2: 3226.33,	77.11	3: 3073.01,	72.17	4: 2956.34,	54.74
5: 2928.38,	44.09	6: 2851.24,	58.48	7: 2354.66,	95.19	8: 1735.62,	29.01
9: 1666.20,	25.76	10: 1548.56,	41.59	11: 1469.49,	62.21	12: 1421.28,	52.82
13: 1385.60,	58.19	14: 1367.28,	60.11	15: 1349.93,	50.33	16: 1307.50,	42.85
17: 1265.07,	53.05	18: 1236.15,	32.75	19: 1215.90,	45.90	20: 1201.43,	52.29
21: 1184.08,	45.05	22: 1121.40,	29.48	23: 1077.05,	72.51	24: 1061.62,	78.72
25: 1029.80,	60.93	26: 961.34,	88.95	27: 942.06,	82.43	28: 912.16,	79.21
29: 875.52,	61.42	30: 801.28,	93.34	31: 721.25,	76.41	32: 702.93,	72.29
33: 662.43,	61.61	34: 611.32,	90.95	35: 580.47,	85.08	36: 571.79,	85.86
37: 561.18,	84.32	38: 499.47,	79.15	39: 481.15,	83.45	40: 460.90,	82.91



rac-11₆

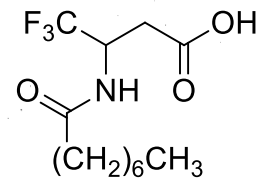
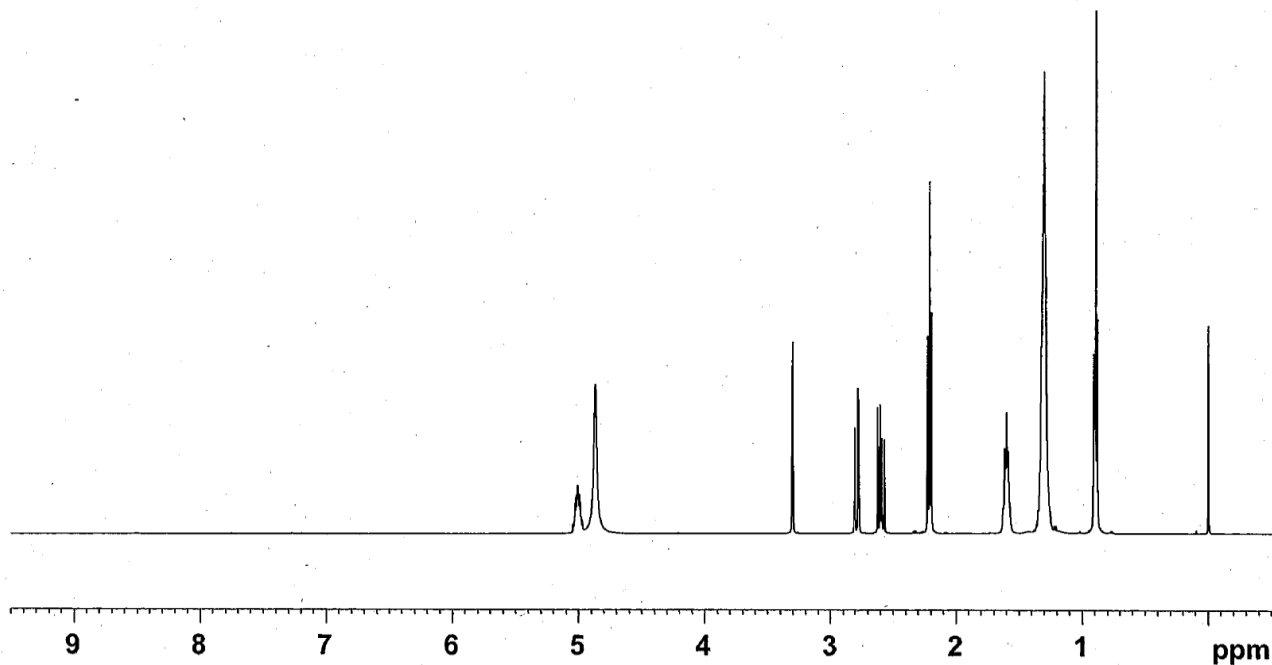
1H

5.046
5.038
5.030
5.023
5.015
5.009
5.002
4.994
4.987
4.979
4.971
4.870
4.870
3.313
3.309
3.306
3.303
3.300
2.813
2.805
2.780
2.772
2.624
2.604
2.591
2.571
2.228
2.213
2.198
2.163
1.615
1.601
1.587
1.573
1.312
1.308
1.301
0.910
0.896
0.882



NAME A16mc211rk
EXPNO 17092502
PROCNO 1
Date_ 20170925
Time 10.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 8
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 101
DW 48.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

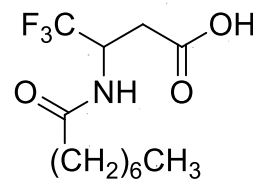
==== CHANNEL f1 =====
NUC1 1H
P1 11.80 usec
PL1 2.40 dB
PL1W 15.17711735 W
SFO1 500.0330885 MHz
SI 32768
SF 500.0300103 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



rac-1₆

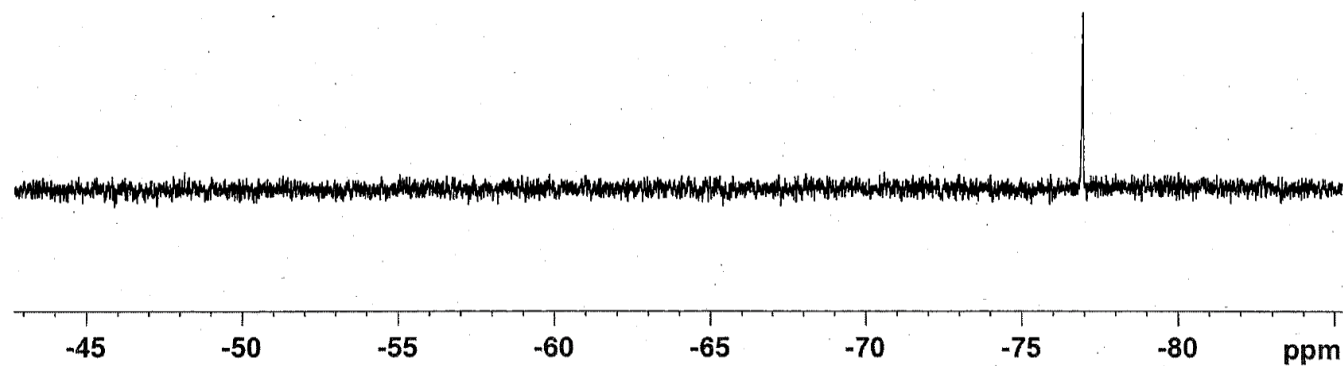
- ACCEPTANCE - System: AV300 OrderNo.: JH033009 Customer: Saitama University Engineer: IKD
 P/N Console: Z108356/162 Shim system: BOSS I original dataset: 104275_0150snf 3 1
 Probe: 5 mm PABBO BB-1H/D Z-GRD Z104275/0150 Sample depth:20 Gas: air
 Sensitivity test for 19F (additional test); Sample: 0,05% TFT in CDCl3 (P/N: Z10234)

Sino= 243:1 (signal= -61 - -65 ppm noise= -59.08 - -60.08 ppm [1 ppm] noise range= 4.5 ppm)
 P1= 15usec PL1= -0.3dB



rac-1₆

---76.945



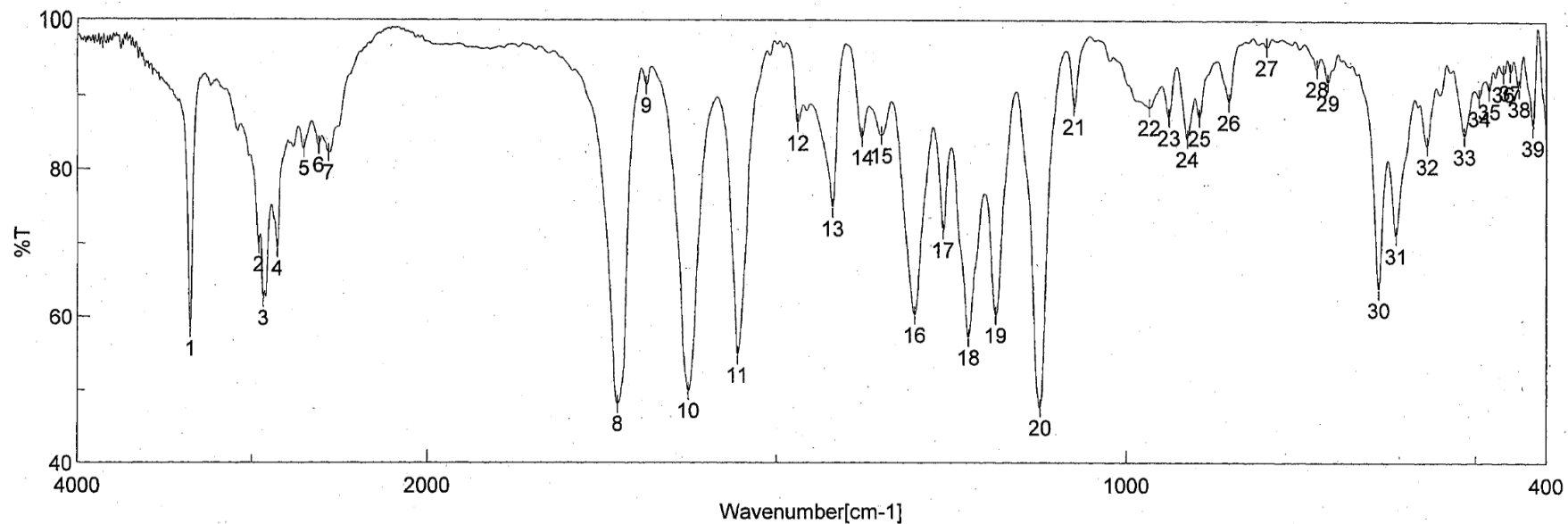
NAME	A16mc211rk
EXPNO	16051005
PROCNO	1
Date_	20160510
Time	13.22
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgfhigqn
TD	32768
SOLVENT	CDCl3
NS	1
DS	0
SWH	12019.230 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	41.600 usec
DE	6.50 usec
TE	296.3 K
D1	10.00000000 sec
D11	0.03000000 sec
D12	0.00002000 sec
TD0	1

==== CHANNEL f1 =====

NUC1	19F
P1	15.00 usec
PL1	-0.30 dB
PL1W	10.09325600 W
SFO1	282.3865635 MHz

==== CHANNEL f2 =====

CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.58 dB
PL12	16.50 dB
PL2W	9.45079708 W
PL12W	0.24180678 W
SFO2	300.1300000 MHz
SI	16384
SF	282.4046279 MHz
WDW	EM
SSB	0
LB	2.00 Hz
GB	0
PC	1.00



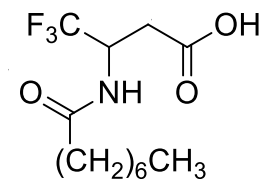
積算回数
ゼロフィリング
ゲイン
測定日時
測定者
ファイル名
サンプル名
コメント

16
ON
8
2016/05/10 10:13
kawamata
Memory#2
rac-1-C8

分解
アポダイゼーション
スキャンスピード
更新日時

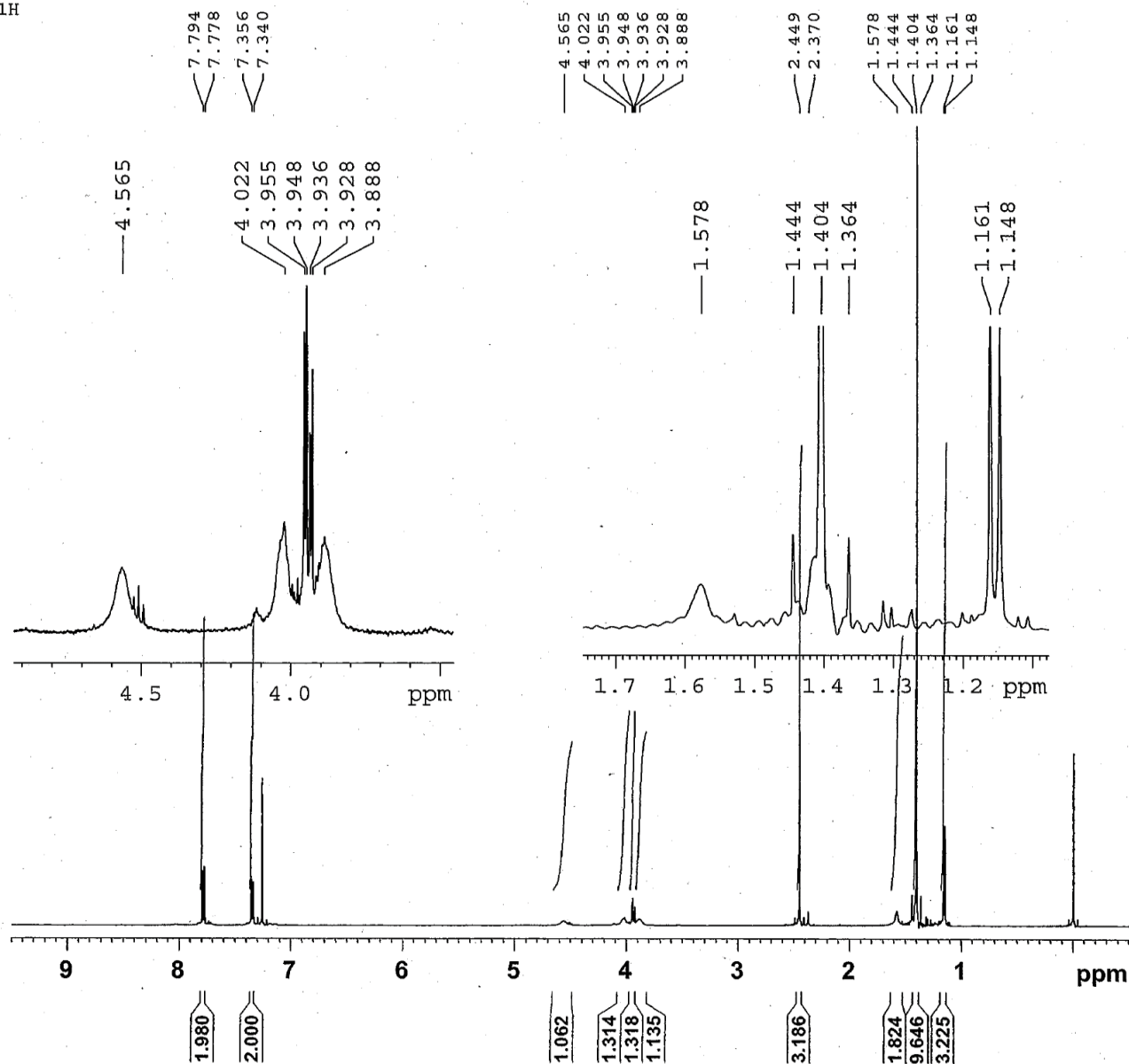
4 cm-1
Cosine
2 mm/sec
2016/05/10 10:14

1: 3353.60,	58.32	2: 2963.09,	69.89	3: 2937.06,	62.51	4: 2857.02,	69.36
5: 2704.67,	82.83	6: 2619.82,	83.30	7: 2564.86,	82.28	8: 1727.91,	48.05
9: 1686.44,	91.44	10: 1626.66,	49.86	11: 1556.27,	54.74	12: 1469.49,	86.34
13: 1419.35,	74.84	14: 1376.93,	84.40	15: 1348.96,	84.66	16: 1301.72,	60.28
17: 1261.22,	71.96	18: 1224.58,	57.18	19: 1186.01,	60.25	20: 1122.37,	47.51
21: 1074.16,	88.58	22: 967.13,	88.47	23: 939.16,	87.12	24: 913.13,	84.25
25: 895.77,	87.07	26: 853.35,	89.18	27: 799.35,	96.66	28: 727.03,	93.79
29: 711.60,	91.92	30: 639.29,	63.85	31: 614.22,	71.30	32: 569.86,	83.36
33: 516.83,	84.66	34: 495.62,	89.86	35: 481.15,	90.84	36: 460.90,	93.20
37: 451.26,	93.43	38: 438.73,	91.20	39: 419.44,	85.90		



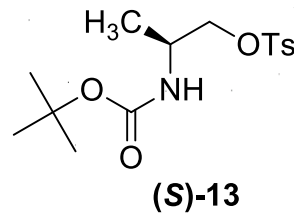
rac-1₆

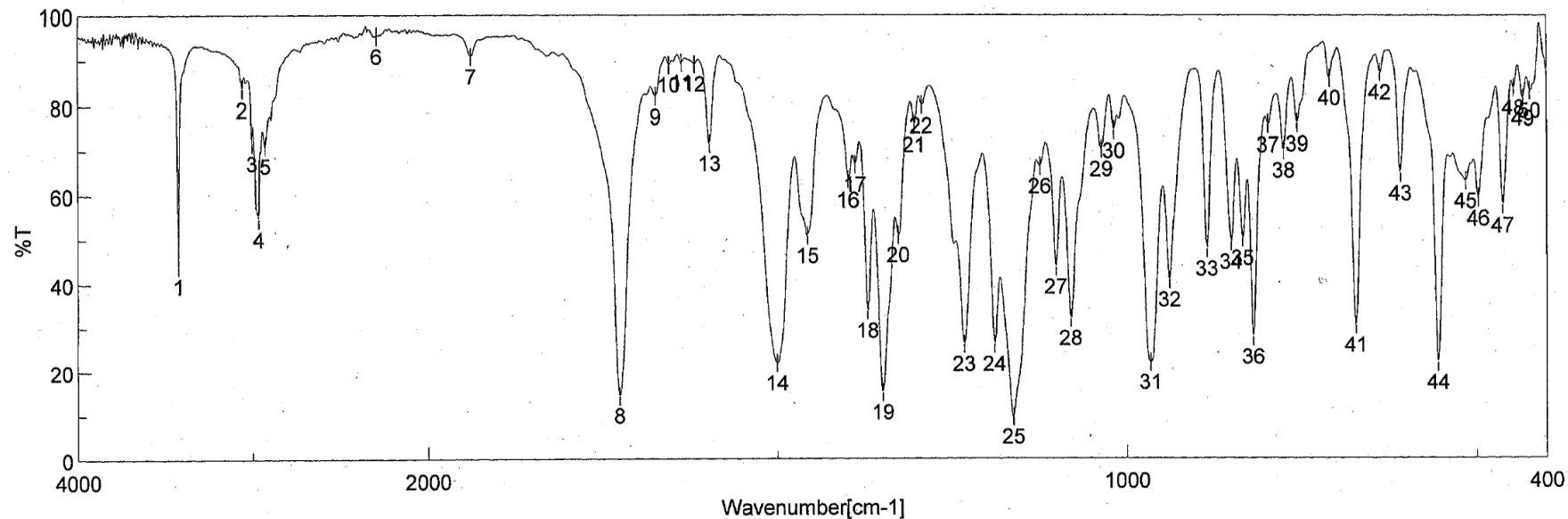
1H



NAME A16mc211rk
 EXPNO 16052301
 PROCNO 1
 Date 20160523
 Time 14.16
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719923 sec
 RG 203
 DW 48.400 usec
 DE 6.50 usec
 TE 300.3 K
 D1 1.00000000 sec
 TDO 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 11.80 usec
 PL1 2.40 dB
 PL1W 15.17711735 W
 SFO1 500.0330885 MHz
 SI 32768
 SF 500.0300109 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





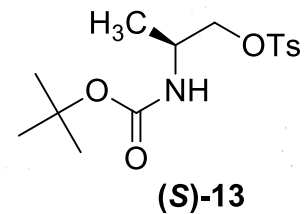
積算回数
ゼロフィリング
ゲイン
測定日時
測定者
ファイル名
サンプル名
コメント

16
ON
8
2016/06/03 14:25
kawamata
Memory#2
tosylate

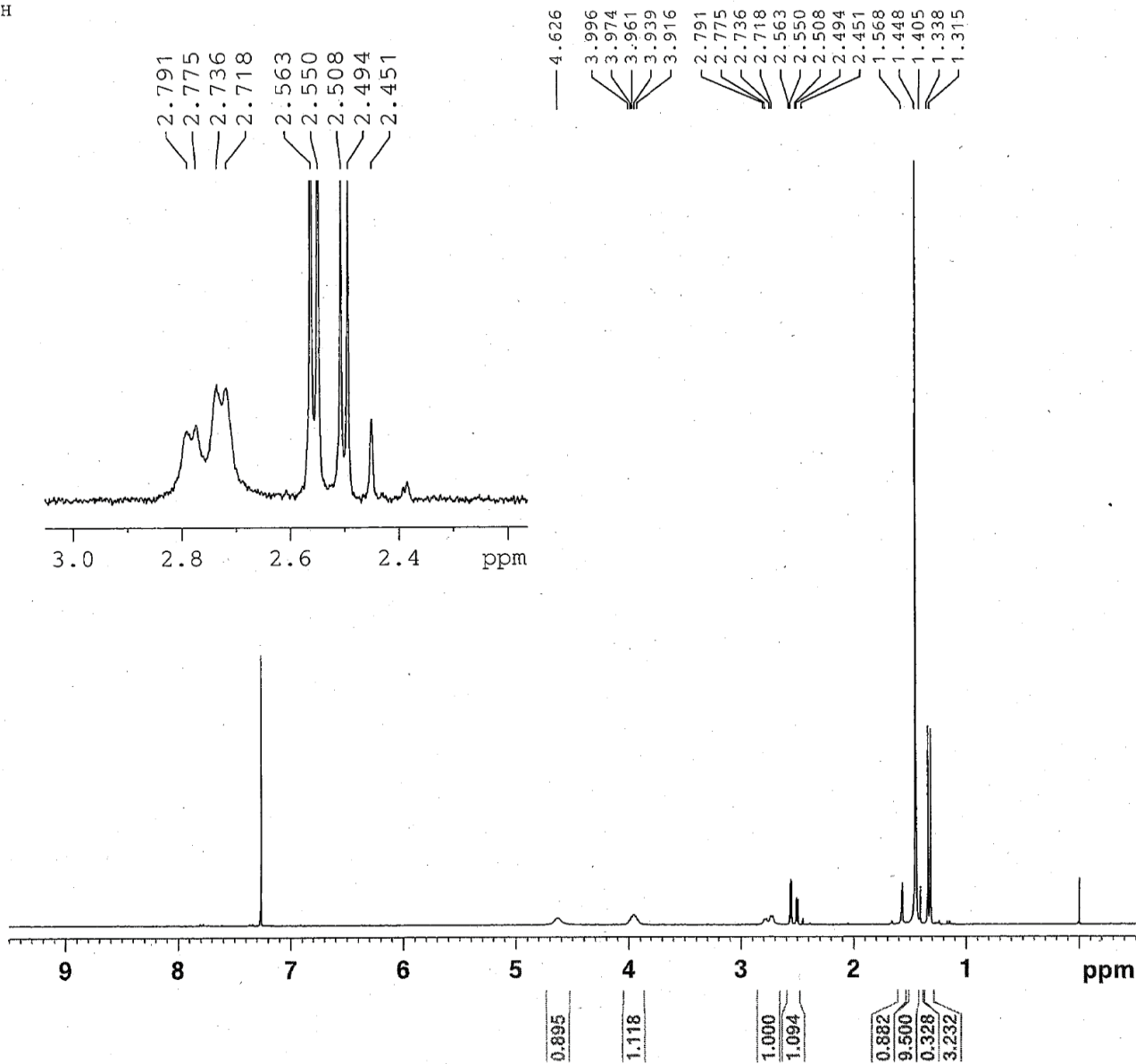
分解
アボダイゼーション
スキャンスピード
更新日時

4 cm-1
Cosine
2 mm/sec
2016/06/03 14:26

1: 3425.92,	44.11	2: 3060.48,	83.71	3: 3005.52,	71.70	4: 2967.91,	54.76
5: 2929.34,	71.09	6: 2292.95,	95.52	7: 1938.11,	90.97	8: 1725.98,	14.48
9: 1673.91,	82.01	10: 1654.62,	89.05	11: 1636.30,	89.56	12: 1617.98,	89.22
13: 1596.77,	71.64	14: 1500.35,	21.97	15: 1456.96,	51.09	16: 1398.14,	63.41
17: 1388.50,	66.85	18: 1371.14,	33.97	19: 1348.96,	15.23	20: 1326.79,	51.22
21: 1303.64,	75.79	22: 1293.04,	79.97	23: 1232.29,	26.28	24: 1188.90,	26.27
25: 1161.90,	9.51	26: 1123.33,	66.50	27: 1101.15,	44.03	28: 1079.94,	32.21
29: 1035.59,	70.32	30: 1018.23,	74.47	31: 966.16,	22.13	32: 939.16,	41.08
33: 886.13,	48.19	34: 851.42,	49.73	35: 835.03,	50.61	36: 819.60,	27.91
37: 798.39,	75.75	38: 776.21,	70.03	39: 756.92,	75.96	40: 710.64,	86.00

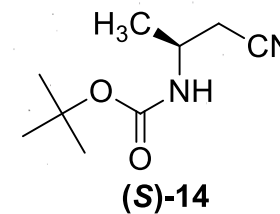


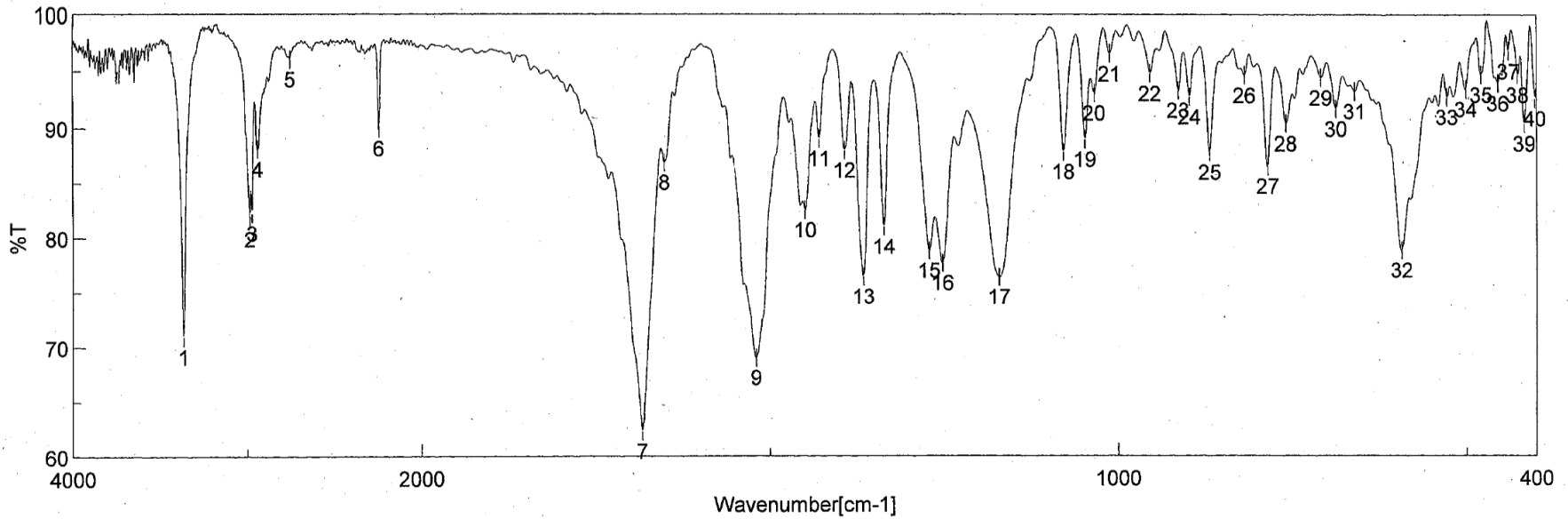
1H



NAME A16mc211rk
EXPNO 16062601
PROCNO 1
Date_ 20160526
Time 10.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 203
DW 80.800 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 15.00 usec
PL1 1.20 dB
PL1W 8.19348145 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1300052 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





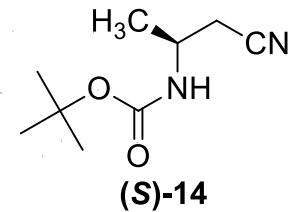
積算回数
ゼロフィリング
ゲイン
測定日時
測定者
ファイル名
サンプル名
コメント

16
ON
8
2016/06/03 14:38
kawamata
Memory#2
nitrile

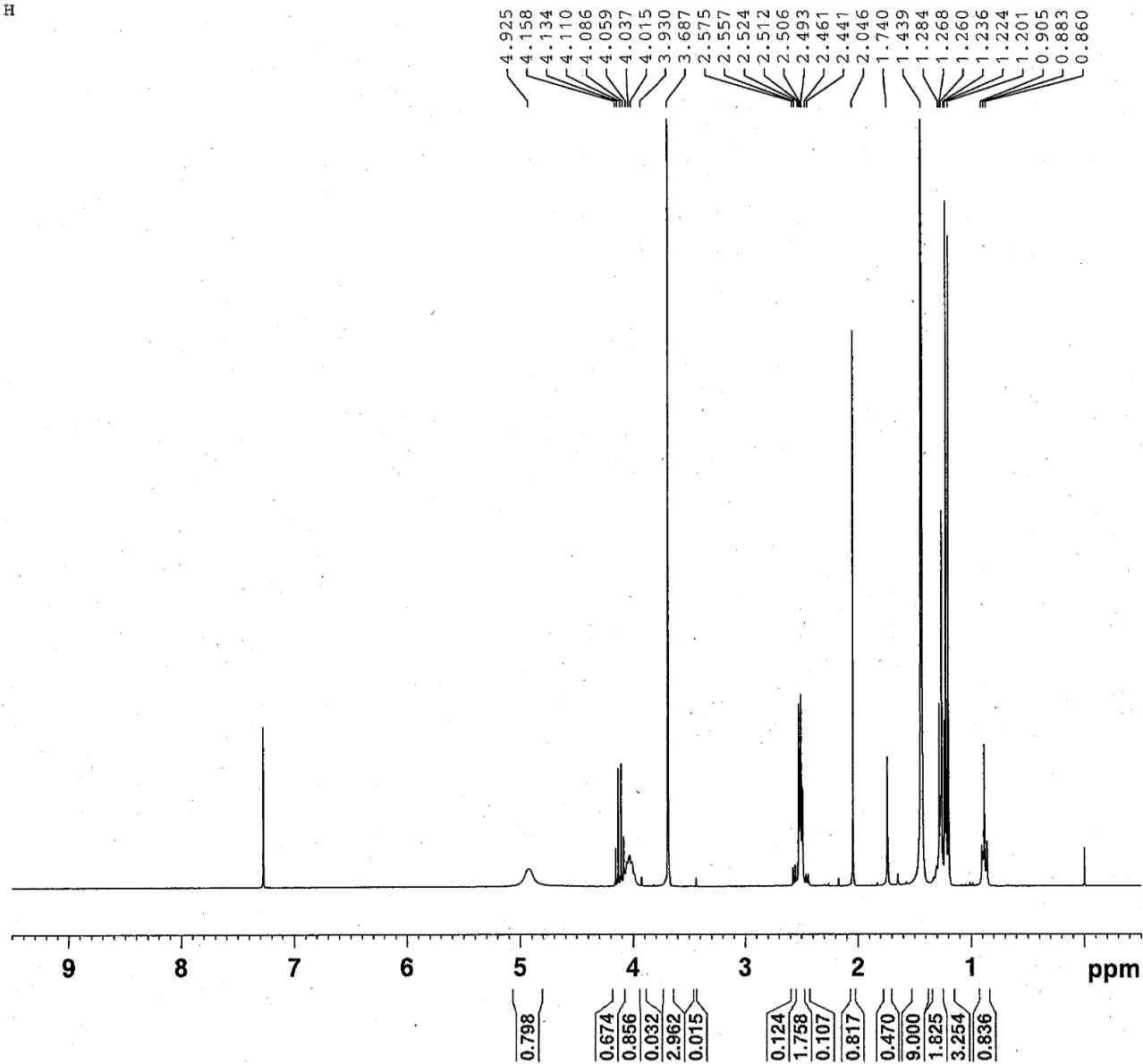
分解
アポダイゼーション
スキャンスピード
更新日時

4 cm-1
Cosine
2 mm/sec
2016/06/03 14:39

1:	3367.10,	70.93	2:	2988.16,	81.73	3:	2975.62,	82.27	4:	2943.80,	88.11
5:	2756.74,	96.10	6:	2245.70,	90.00	7:	1683.55,	62.29	8:	1651.73,	86.90
9:	1519.63,	69.06	10:	1449.24,	82.63	11:	1428.99,	89.04	12:	1392.35,	87.99
13:	1365.35,	76.51	14:	1335.46,	81.13	15:	1270.86,	78.93	16:	1251.58,	77.78
17:	1170.58,	76.51	18:	1078.01,	87.85	19:	1047.16,	88.98	20:	1033.66,	93.10
21:	1011.48,	96.61	22:	953.63,	94.87	23:	913.13,	93.36	24:	896.74,	92.79
25:	867.81,	87.80	26:	817.67,	94.71	27:	784.89,	86.55	28:	758.85,	90.38
29:	708.71,	94.49	30:	687.50,	91.70	31:	660.50,	93.26	32:	593.97,	79.01
33:	528.40,	92.75	34:	501.40,	93.49	35:	479.22,	94.77	36:	455.12,	94.02
37:	440.65,	96.86	38:	427.16,	94.77	39:	417.51,	90.38	40:	402.09,	92.64

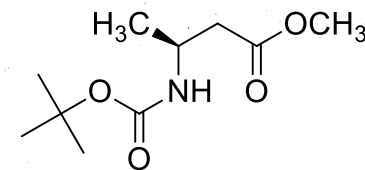


1H

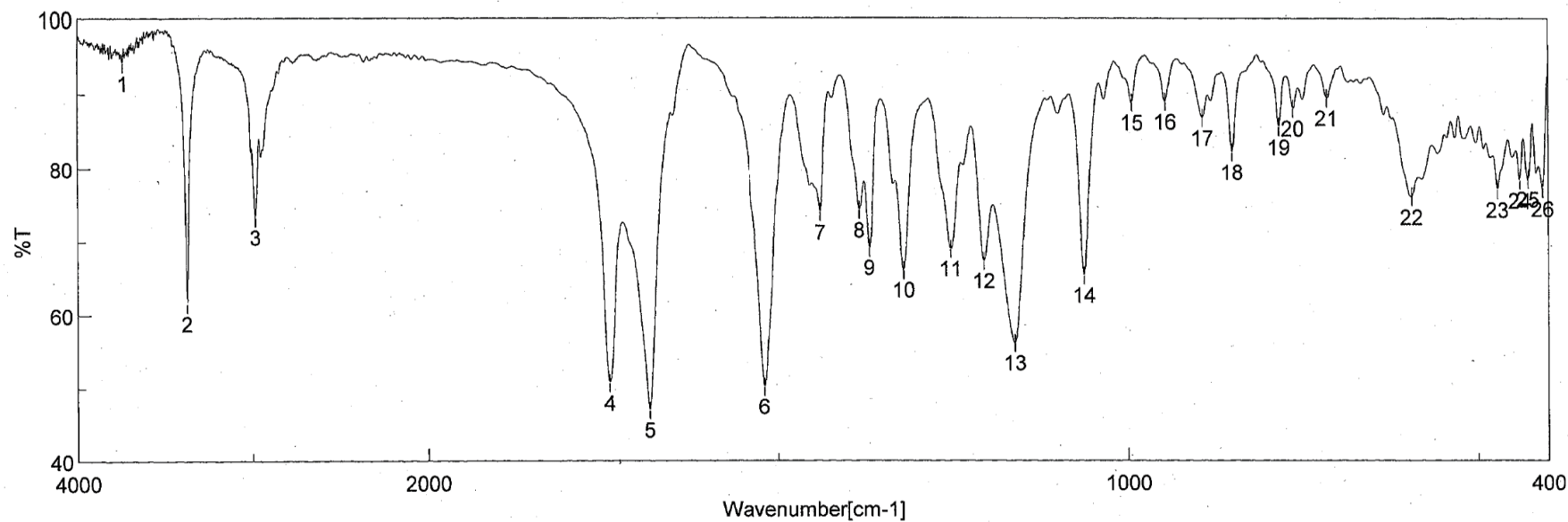


NAME A16mc211
EXPNO 16072901
PROCNO 1
Date_ 20160729
Time 14.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 114
DW 80.800 usec
DE 6.50 usec
TE 296.8 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 15.00 usec
PL1 1.20 dB
PL1W 8.19348145 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1300013 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



(S)-15



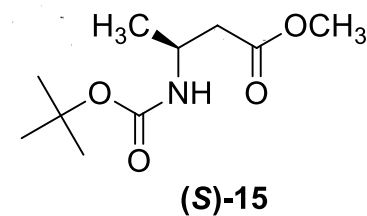
積算回数
ゼロフィリング
ゲイン
測定日時
測定者
ファイル名
サンプル名
コメント

12
ON
8
2016/08/02 17:28
kawamata
boc methyl ether
Boc Na

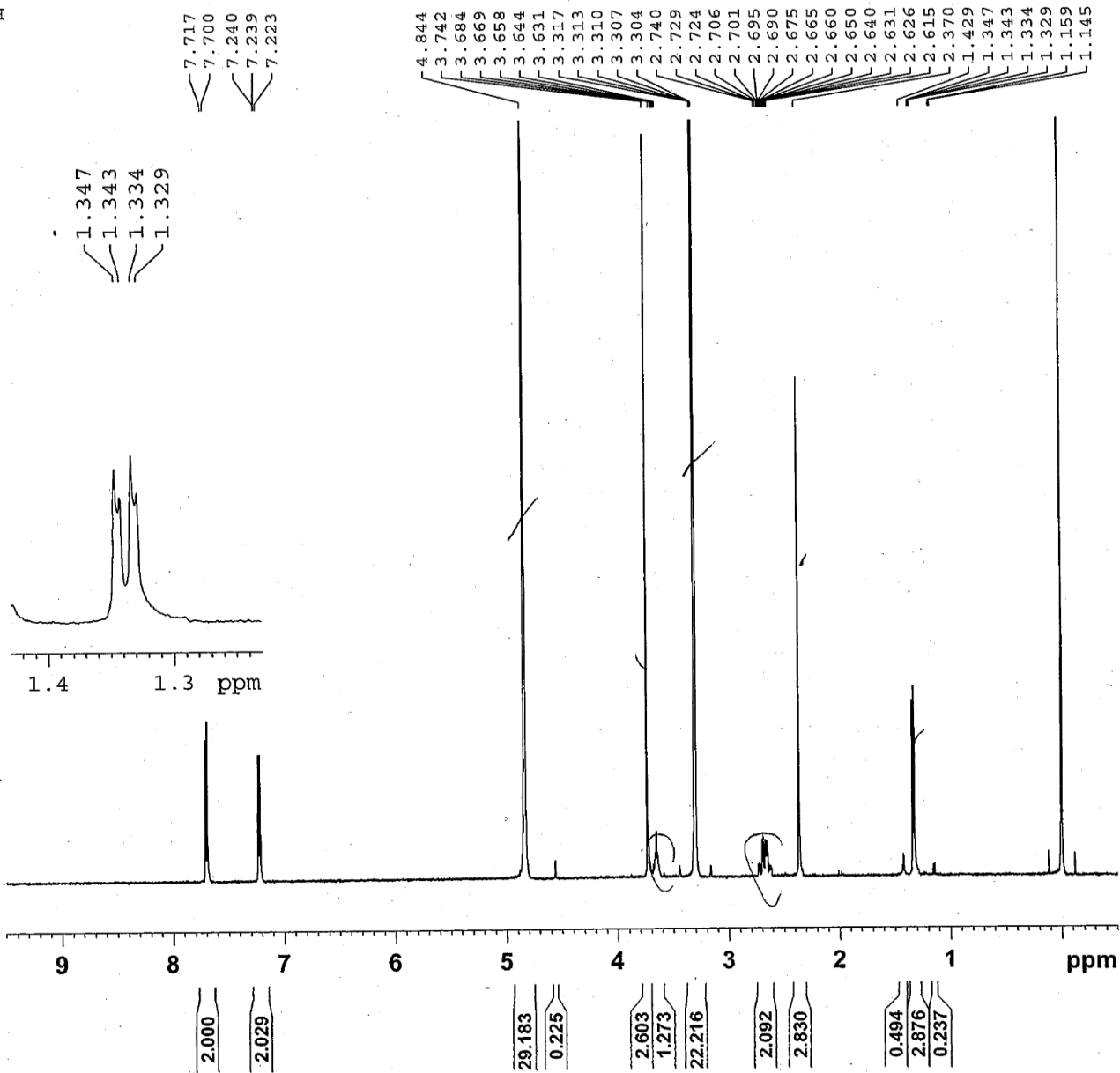
分解
アボダイゼーション
スキャンスピード
更新日時

4 cm-1
Cosine
2 mm/sec
2016/08/02 17:41

1: 3742.19,	94.19	2: 3374.82,	61.55	3: 2986.23,	73.38	4: 1741.41,	50.70
5: 1684.52,	46.93	6: 1519.63,	50.21	7: 1439.60,	74.12	8: 1383.68,	74.44
9: 1369.21,	69.28	10: 1320.04,	66.22	11: 1252.54,	69.15	12: 1205.29,	67.49
13: 1160.94,	56.19	14: 1062.59,	65.52	15: 994.12,	88.89	16: 946.88,	89.01
17: 893.84,	86.84	18: 851.42,	82.19	19: 784.89,	85.63	20: 764.64,	88.11
21: 716.43,	89.49	22: 594.93,	76.17	23: 472.47,	77.17	24: 440.65,	78.37
25: 429.08,	78.53	26: 407.87,	77.31				

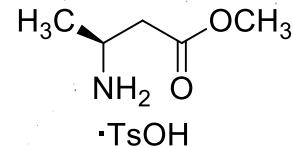


1H

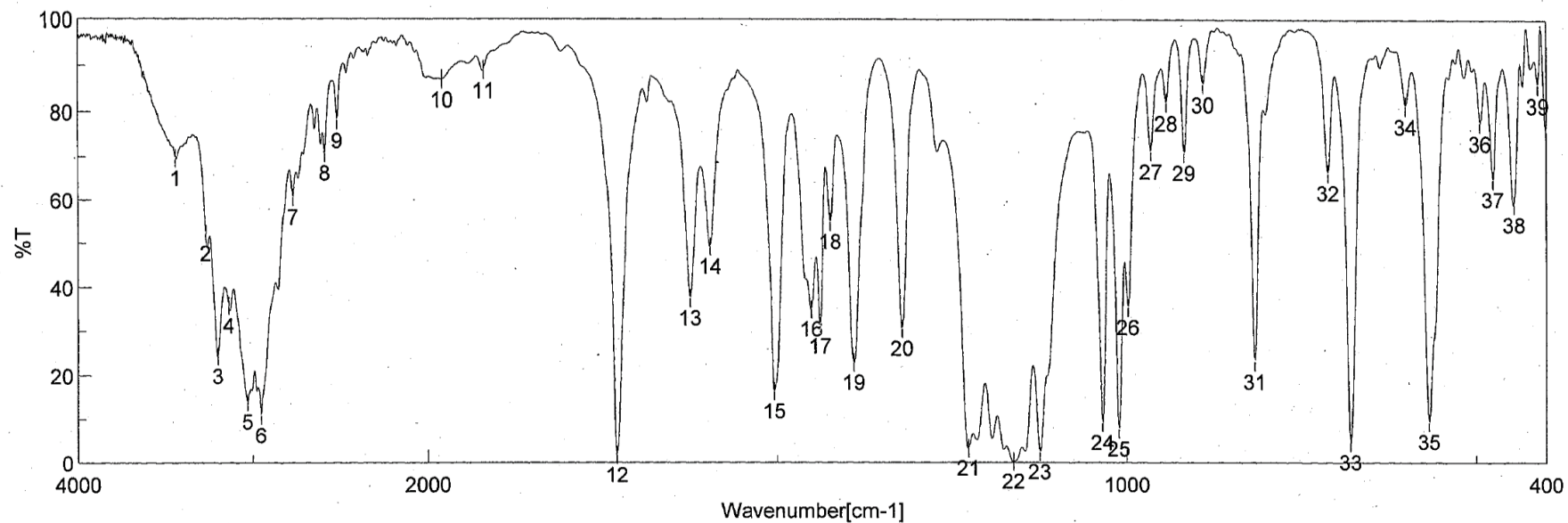


NAME 16mc211rk
 EXPNO 16080302
 PROCNO 1
 Date 20160803
 Time 11.22
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT MeOD
 NS 8
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719923 sec
 RG 203
 DW 48.400 usec
 DE 6.50 usec
 TE 300.7 K
 D1 1.00000000 sec
 TDO 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 11.80 usec
 PL1 2.40 dB
 PL1W 15.17711735 W
 SFO1 500.0330885 MHz
 SI 32768
 SF 500.0300083 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



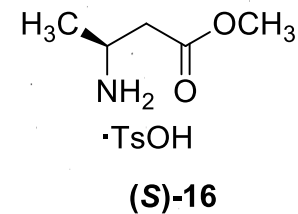
(S)-16



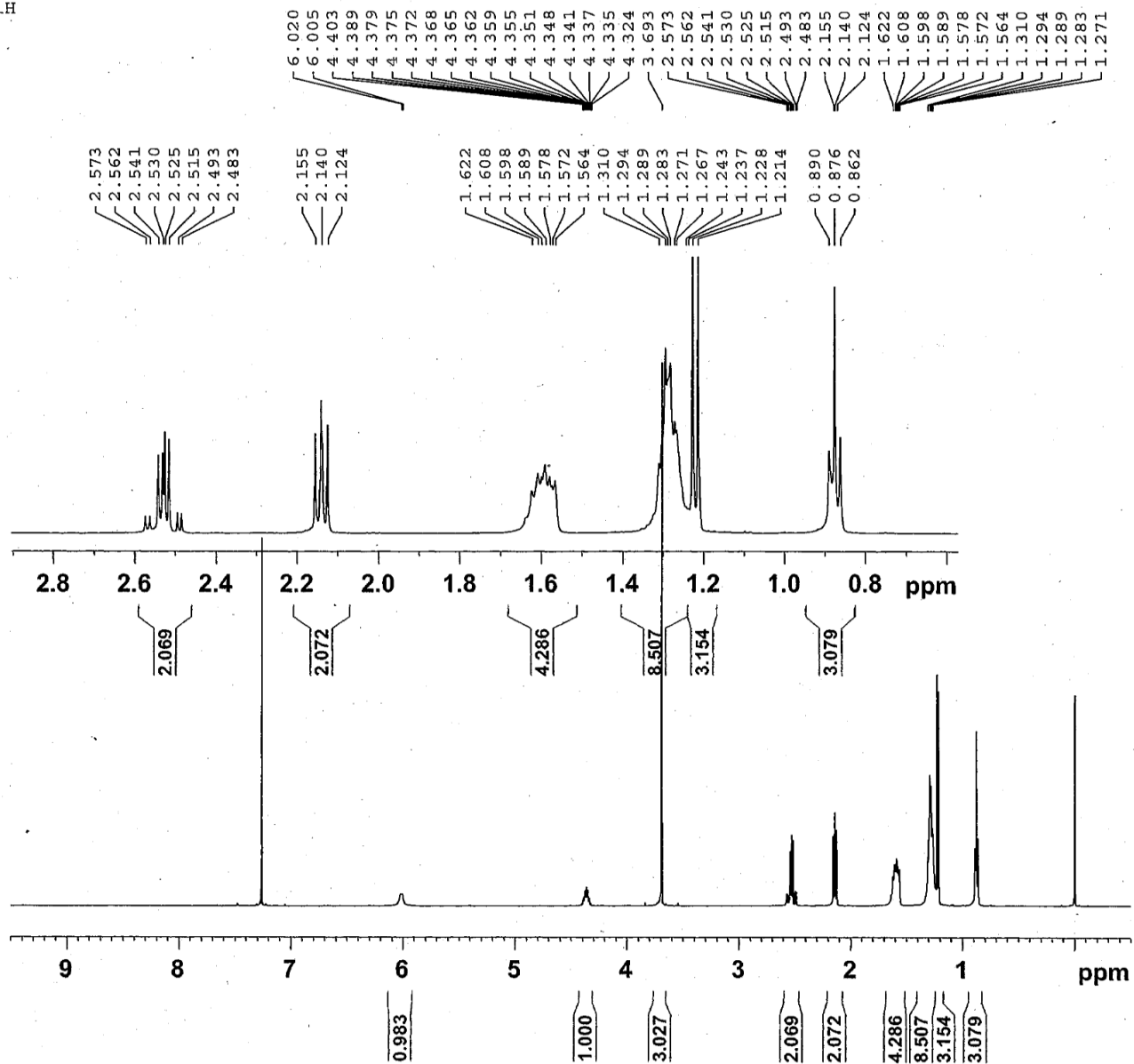
積算回数 12
 ゼロフィリング ON
 ゲイン 16
 測定日時 2016/08/08 10:28
 測定者 kawamata
 ファイル名 Memory#2
 サンプル名 TsOH methyl ester
 コメント

分解 4 cm-1
 アポダイゼーション Cosine
 スキャンスピード 2 mm/sec
 更新日時 2016/08/08 10:30

1: 3442.31,	69.61	2: 3270.68,	52.26	3: 3202.22,	24.36	4: 3139.54,	35.86
5: 3031.55,	13.92	6: 2953.45,	10.77	7: 2770.24,	60.66	8: 2587.04,	70.73
9: 2516.65,	78.12	10: 1979.57,	86.99	11: 1919.79,	89.06	12: 1729.83,	1.71
13: 1625.70,	37.63	14: 1596.77,	49.40	15: 1504.20,	16.44	16: 1451.17,	35.10
17: 1438.64,	31.20	18: 1424.17,	55.07	19: 1390.42,	22.96	20: 1321.00,	30.70
21: 1226.51,	3.32	22: 1161.90,	0.28	23: 1124.30,	2.49	24: 1034.62,	9.18
25: 1011.48,	7.74	26: 997.98,	35.57	27: 965.20,	71.19	28: 943.02,	81.87
29: 917.95,	70.91	30: 890.95,	85.97	31: 817.67,	23.13	32: 712.57,	66.31
33: 680.75,	4.65	34: 601.68,	81.22	35: 567.93,	9.32	36: 494.65,	77.55
37: 476.33,	64.96	38: 446.44,	59.14	39: 412.69,	85.78		

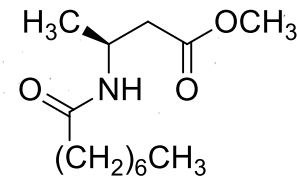


1H



NAME A16mc211rk
 EXPNO 17092901
 PROCNO 1
 Date 20170920
 Time 12.52
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719923 sec
 RG 203
 DW 48.400 usec
 DE 6.50 usec
 TE 299.8 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 11.80 usec
 PL1 2.40 dB
 PL1W 15.17711735 W
 SFO1 500.0330885 MHz
 SI 32768
 SF 500.0300101 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



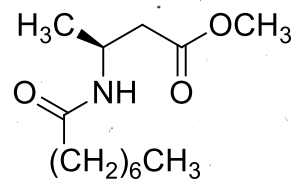
(S)-176

13C with Hdec

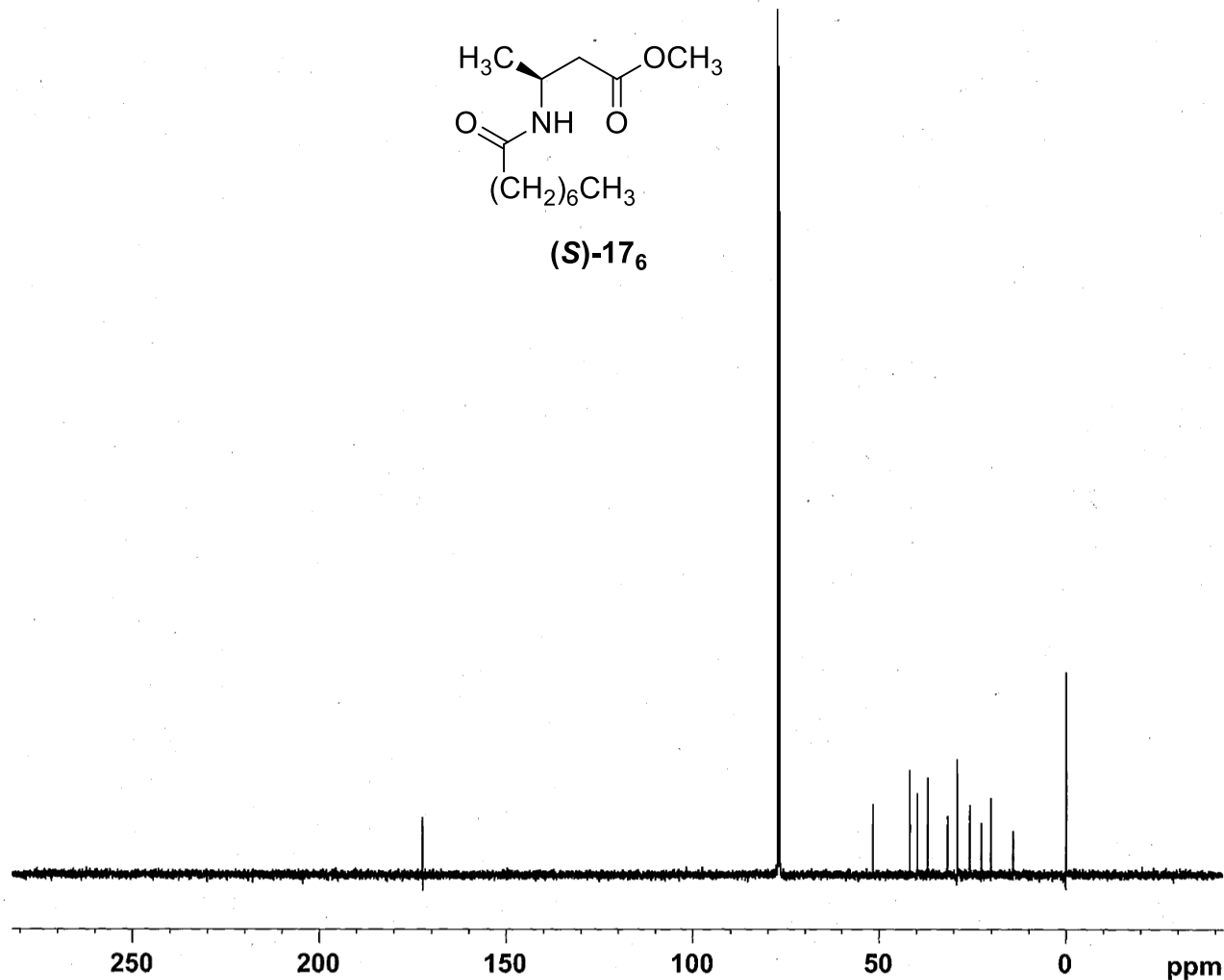


172.328
172.269

51.607
41.713
39.715
36.944
31.663
29.168
28.970
25.704
22.575
20.007
14.025



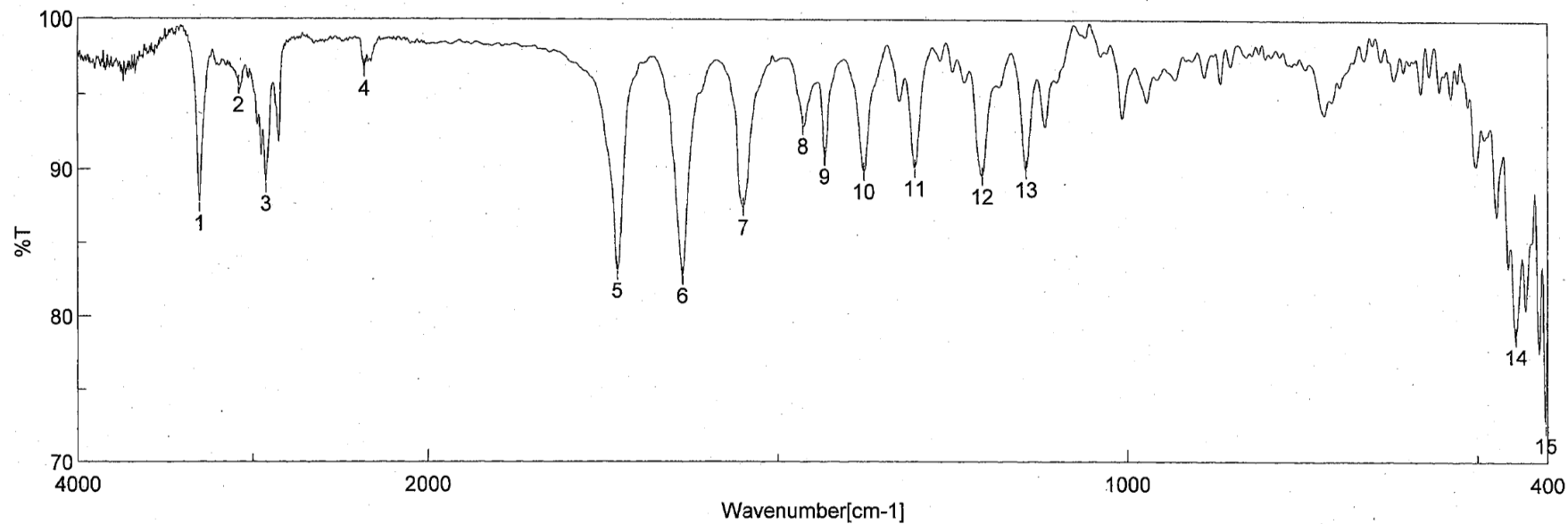
(S)-17₆



NAME A16mc211rk
EXPNO 17091401
PROCNO 1
Date_ 20170914
Time 19.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 632
DS 2
SWH 40760.871 Hz
FIDRES 0.621962 Hz
AQ 0.8039582 sec
RG 203
DW 12.267 usec
DE 6.50 usec
TE 302.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PL1 0.00 dB
PL1W 100.47545624 W
SFO1 125.7477319 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.40 dB
PL12 19.02 dB
PL13 22.02 dB
PL2W 15.17711735 W
PL12W 0.33051354 W
PL13W 0.16564916 W
SFO2 500.0316016 MHz
SI 16384
SF 125.7326440 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

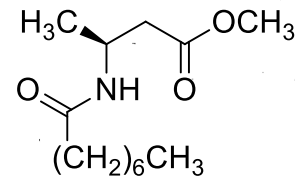


積算回数
ゼロフィリング
ゲイン
測定日時
測定者
ファイル名
サンプル名
コメント

12
ON
8
2016/08/08 10:43
kawamata
Memory#2
(S)-10C8 methyl ester (CH3)

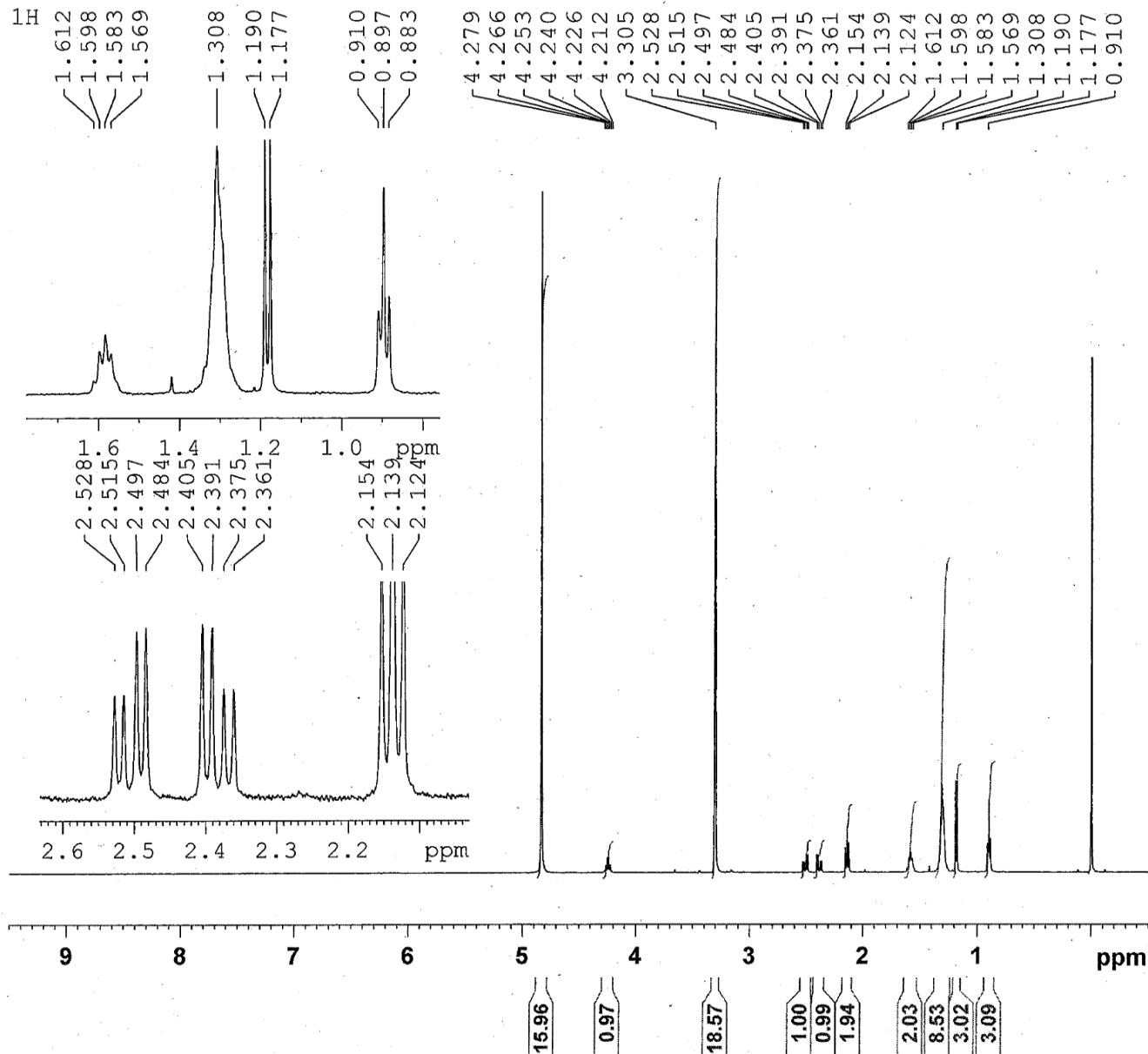
分解
アポダイゼーション
スキャンスピード
更新日時

4 cm-1
Cosine
2 mm/sec
2016/08/08 10:46



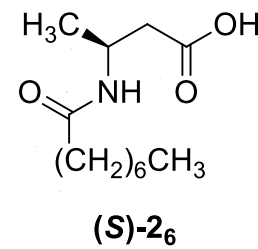
(S)-176

1:	3304.43,	87.71	2:	3081.69,	95.64	3:	2926.45,	89.02	4:	2361.41,	96.74
5:	1729.83,	83.15	6:	1636.30,	82.80	7:	1549.52,	87.46	8:	1463.71,	92.94
9:	1432.85,	90.90	10:	1376.93,	89.88	11:	1303.64,	90.11	12:	1207.22,	89.58
13:	1144.55,	90.06	14:	445.48,	78.76	15:	403.05,	72.58			



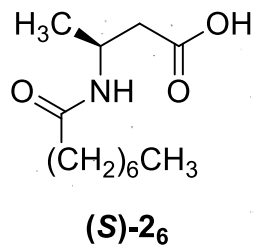
NAME A16mc211rk
 EXPNO 16083001
 PROCNO 1
 Date_ 20160830
 Time_ 9.54
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT MeOD
 NS 8
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719923 sec
 RG 203
 DW 48.400 usec
 DE 6.50 usec
 TE 301.9 K
 D1 1.00000000 sec
 TDO 1

==== CHANNEL f1 =====
 NUC1 ¹H
 P1 12.00 usec
 PL1 2.60 dB
 PL1W 15.32226563 W
 SF01 500.1330885 MHz
 SI 32768
 SF 500.1300129 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

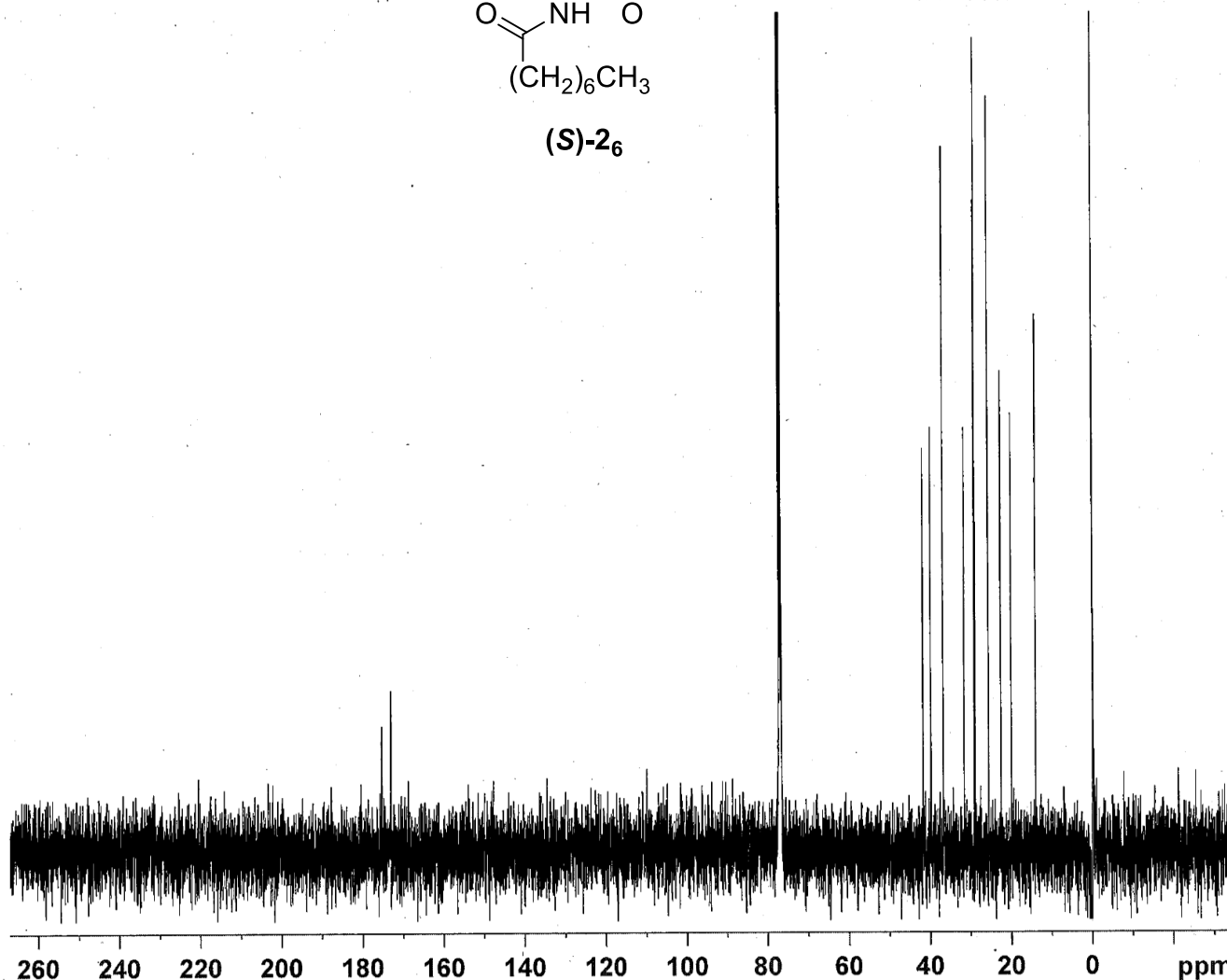


¹³C with Hdec

175.33
173.07



41.85
39.91
36.65
31.64
29.15
28.95
25.67
22.58
20.04
14.03



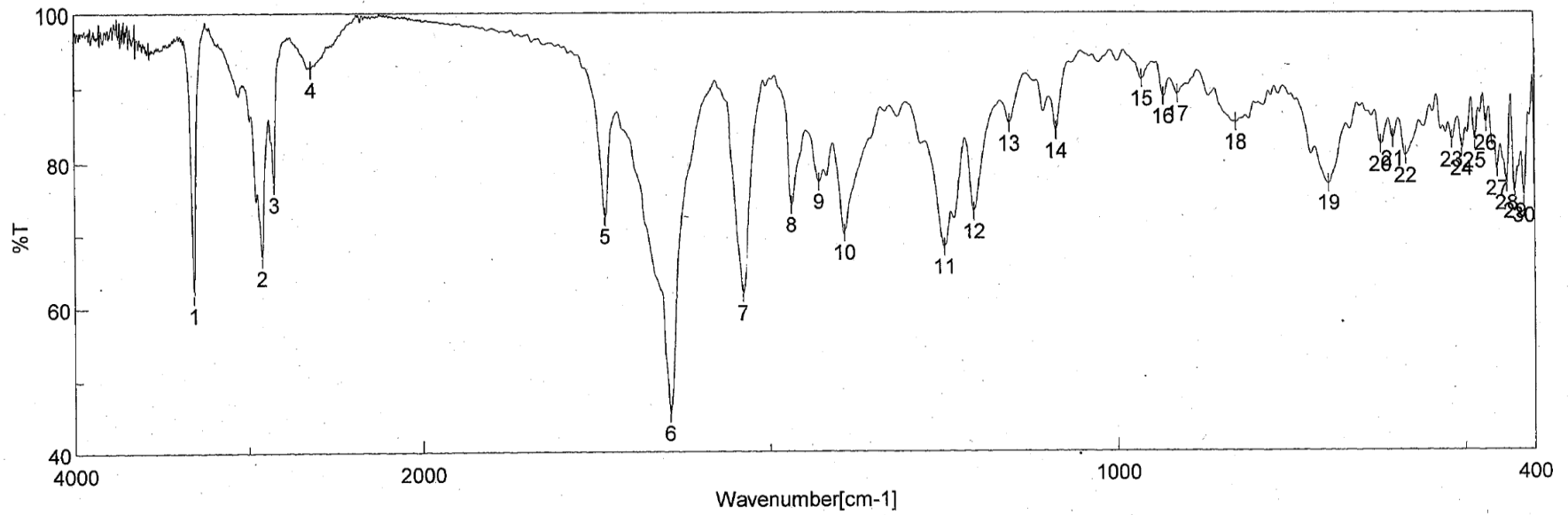
Current Data Parameters
NAME Al6mc211rk
EXPNO 17091501
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170915
Time 11.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 2
SWH 40760.871 Hz
FIDRES 0.621962 Hz
AQ 0.8039582 sec
RG 203
DW 12.267 usec
DE 6.50 usec
TE 301.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PL1 0 dB
PL1W 100.47545624 W
SFO1 125.7477319 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.40 dB
PL12 19.02 dB
PL13 22.02 dB
PL2W 15.17711735 W
PL12W 0.33051354 W
PL13W 0.16564916 W
SFO2 500.0316016 MHz

F2 - Processing parameters
SI 16384
SF 125.7326440 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



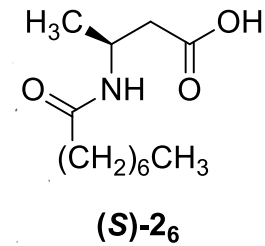
積算回数
ゼロフィリング
ゲイン
測定日時
測定者
ファイル名
サンプル名
コメント

16
ON
16
2016/09/05 12:09
kawamata
Memory#2
CH3 C8

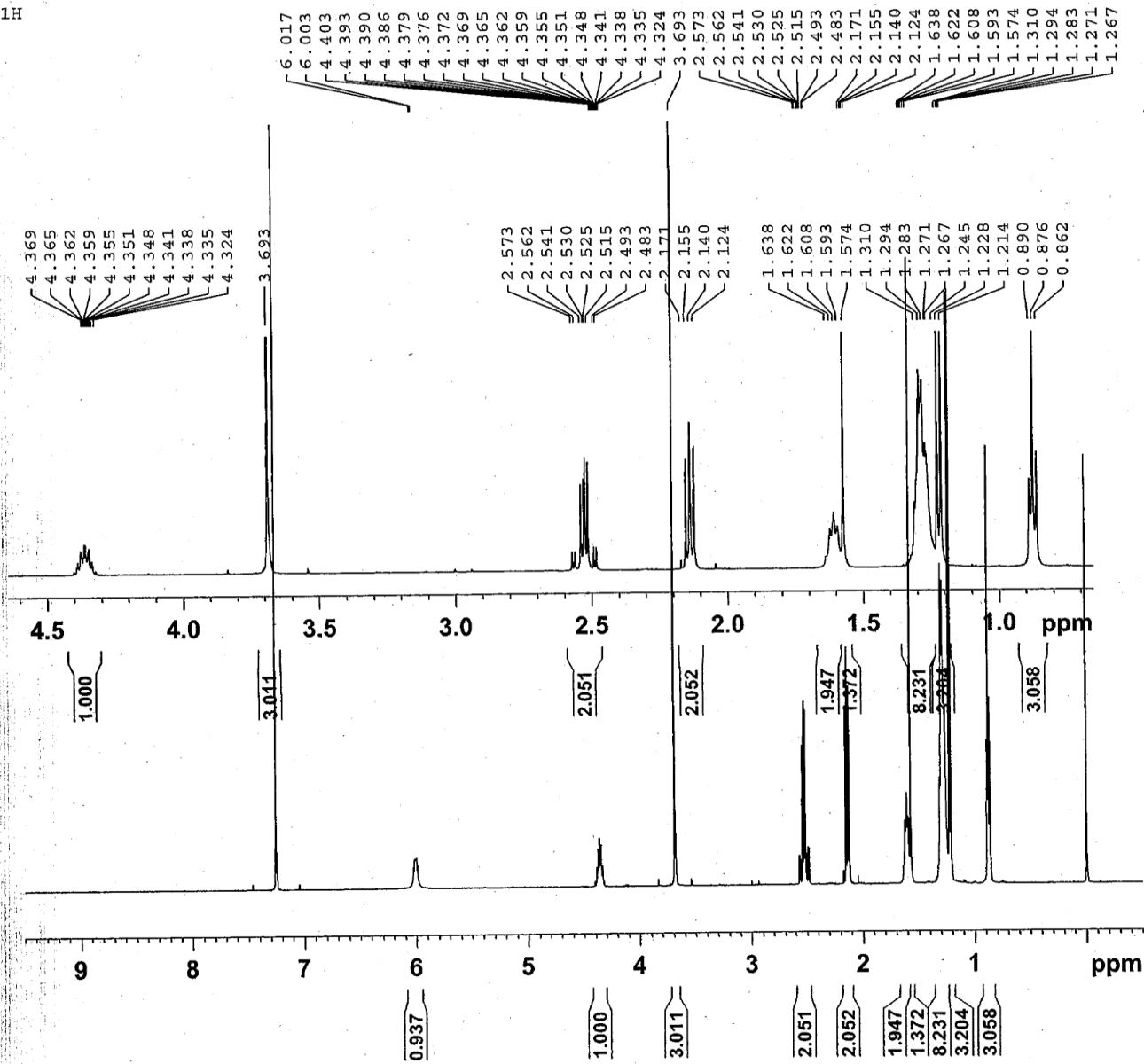
分解
アポダイゼーション
スキャンスピード
更新日時

4 cm-1
Cosine
2 mm/sec
2016/09/05 12:11

1:	3316.00,	61.78	2:	2922.59,	66.91	3:	2852.20,	77.10	4:	2637.18,	92.56
5:	1738.51,	72.61	6:	1644.98,	45.32	7:	1539.88,	61.93	8:	1468.53,	74.17
9:	1428.99,	77.30	10:	1392.35,	70.31	11:	1248.68,	68.35	12:	1206.26,	73.21
13:	1155.15,	85.17	14:	1087.66,	84.20	15:	964.23,	91.15	16:	933.38,	88.76
17:	913.13,	89.09	18:	829.24,	85.26	19:	696.18,	77.00	20:	620.97,	82.27
21:	603.61,	83.02	22:	585.29,	80.78	23:	518.76,	82.85	24:	504.29,	81.72
25:	485.97,	82.75	26:	469.58,	85.09	27:	453.19,	79.01	28:	439.69,	76.99
29:	428.12,	75.82	30:	415.58,	75.28						

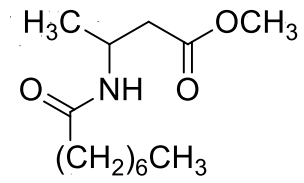


1H



NAME A16mc211rk
 EXPNO 16120102
 PROCNO 1
 Date 20161201
 Time 17.35
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719923 sec
 RG 203
 DW 48.400 usec
 DE 6.50 usec
 TE 299.8 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 11.80 usec
 PL1 2.40 dB
 PL1W 15.17711735 W
 SFO1 500.0330885 MHz
 SI 32768
 SF 500.0300105 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

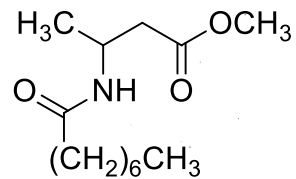


rac-17₆

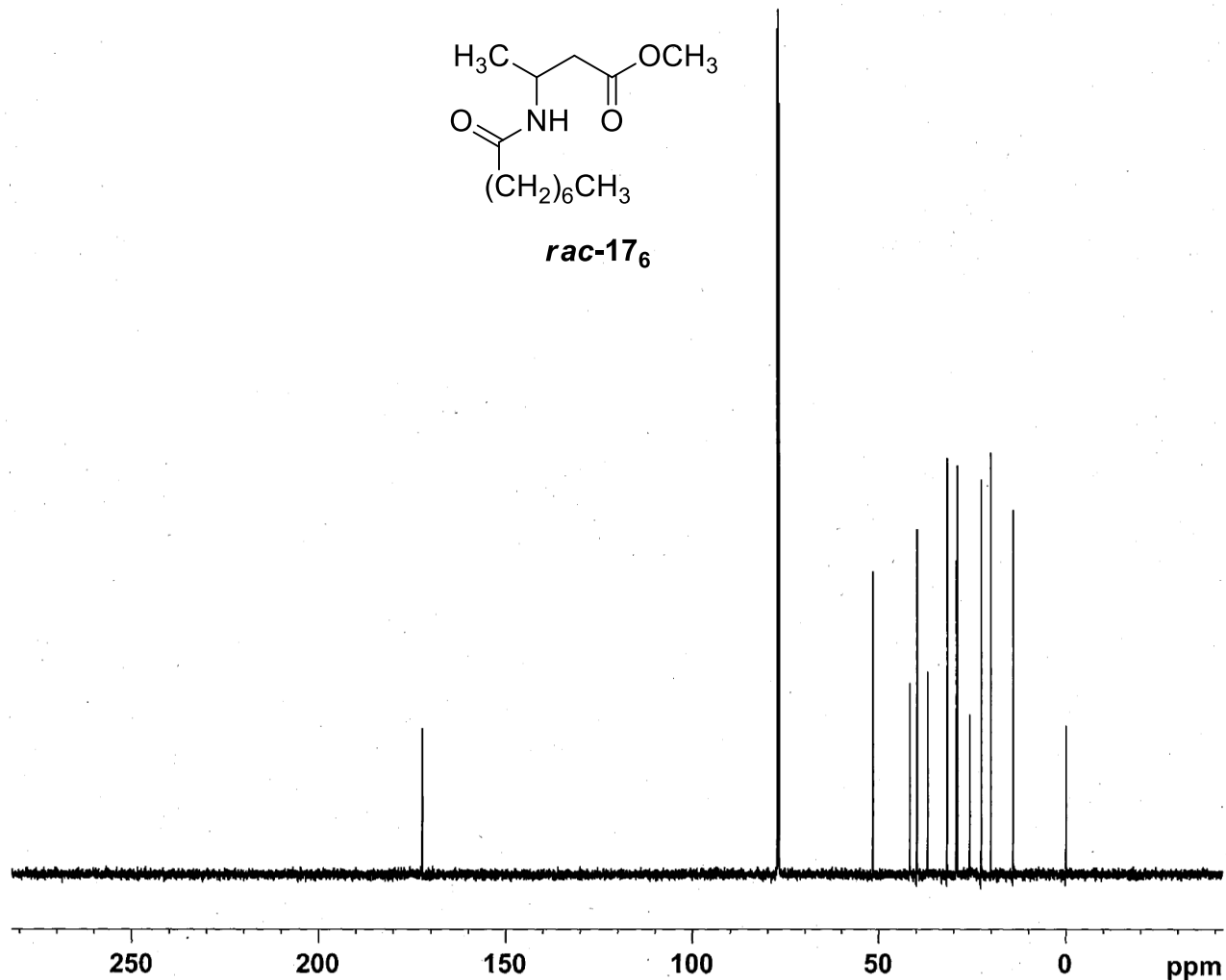
13C with Hdec

172.327
172.233

51.587
41.716
39.734
36.922
31.661
29.168
28.971
25.692
22.559
20.007
14.011



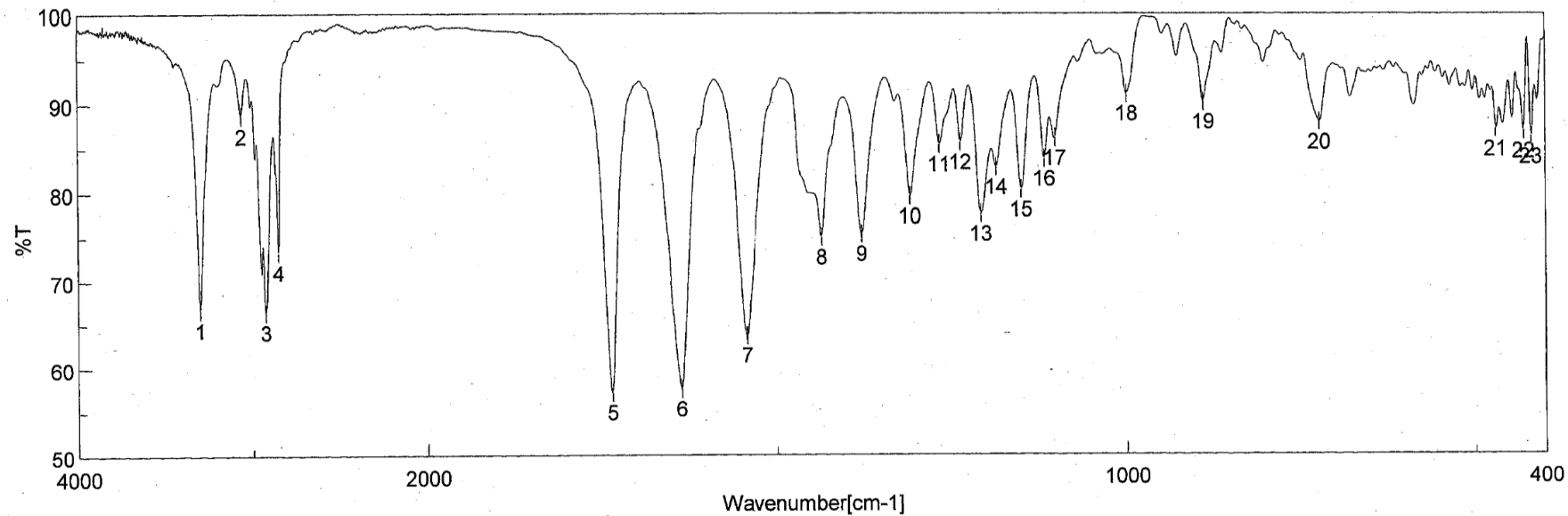
rac-17₆



NAME A16mc211rk
EXPNO 17091902
PROCNO 1
Date_ 20170919
Time_ 11.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 337
DS 2
SWH 40760.871 Hz
FIDRES 0.621962 Hz
AQ 0.8039582 sec
RG 203
DW 12.267 usec
DE 6.50 usec
TE 301.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PL1 0.00 dB
PL1W 100.47545624 W
SFO1 125.7477319 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.40 dB
PL12 19.02 dB
PL13 22.02 dB
PL2W 15.17711735 W
PL12W 0.33051354 W
PL13W 0.16564916 W
SFO2 500.0316016 MHz
SI 16384
SF 125.7326440 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



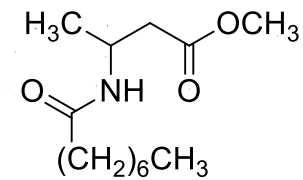
積算回数
ゼロフィリング
ゲイン
測定日時
測定者
ファイル名
サンプル名
コメント

16
ON
8
2017/09/19 13:55
kawamata
Memory#2
rac-ch3-C7-COOme

分解
アポダイゼーション
スキャンスピード
更新日時

4 cm-1
Cosine
2 mm/sec
2017/09/19 13:57

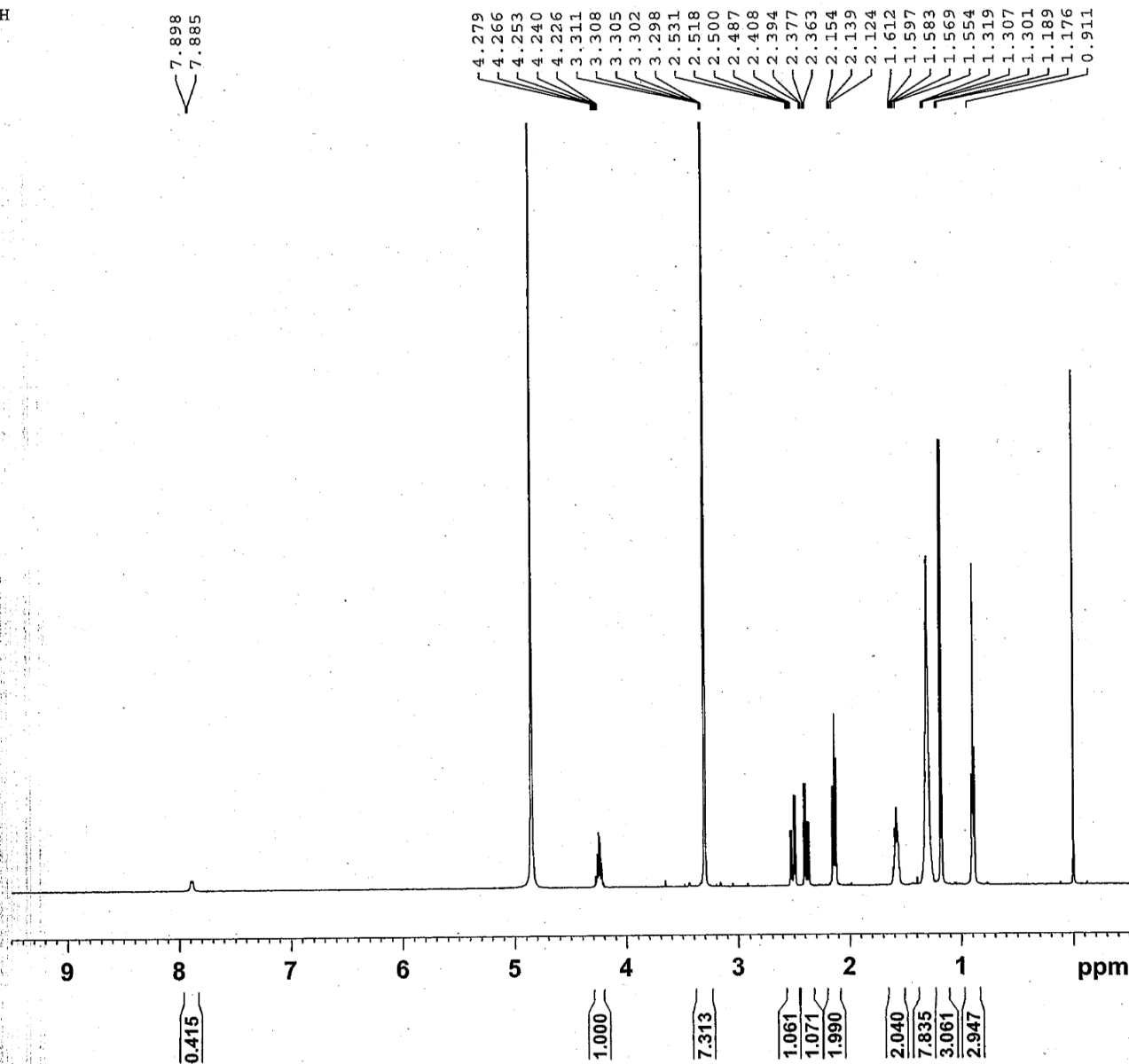
1: 3302.50,	66.68	2: 3065.30,	88.72	3: 2927.41,	66.43	4: 2854.13,	73.33
5: 1736.58,	57.17	6: 1637.27,	57.58	7: 1543.74,	63.69	8: 1435.74,	75.05
9: 1377.89,	75.42	10: 1308.46,	79.62	11: 1266.04,	85.43	12: 1236.15,	85.67
13: 1207.22,	77.70	14: 1185.04,	82.88	15: 1149.37,	80.37	16: 1116.58,	83.81
17: 1101.15,	86.14	18: 998.95,	91.06	19: 889.02,	90.14	20: 723.18,	87.86
21: 470.55,	87.09	22: 431.01,	86.85	23: 420.41,	86.22		



rac-17₆

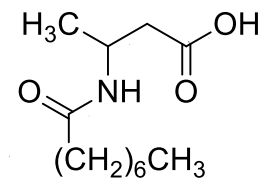
1H

7.898
7.885



NAME A16mc211rk
 EXPNO 16120203
 PROCNO 1
 Date_ 20161202
 Time 12.20
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT MeOD
 NS 8
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719923 sec
 RG 203
 DW 48.400 usec
 DE 6.50 usec
 TE 299.7 K
 D1 1.00000000 sec
 TDO 1

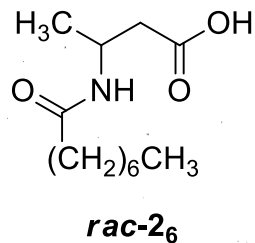
==== CHANNEL f1 =====
 NUC1 1H
 P1 11.80 usec
 PL1 2.40 dB
 PL1W 15.17711735 W
 SFO1 500.0330885 MHz
 SI 32768
 SF 500.0300109 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



rac-2₆

13C with Hdec

175.532
173.299



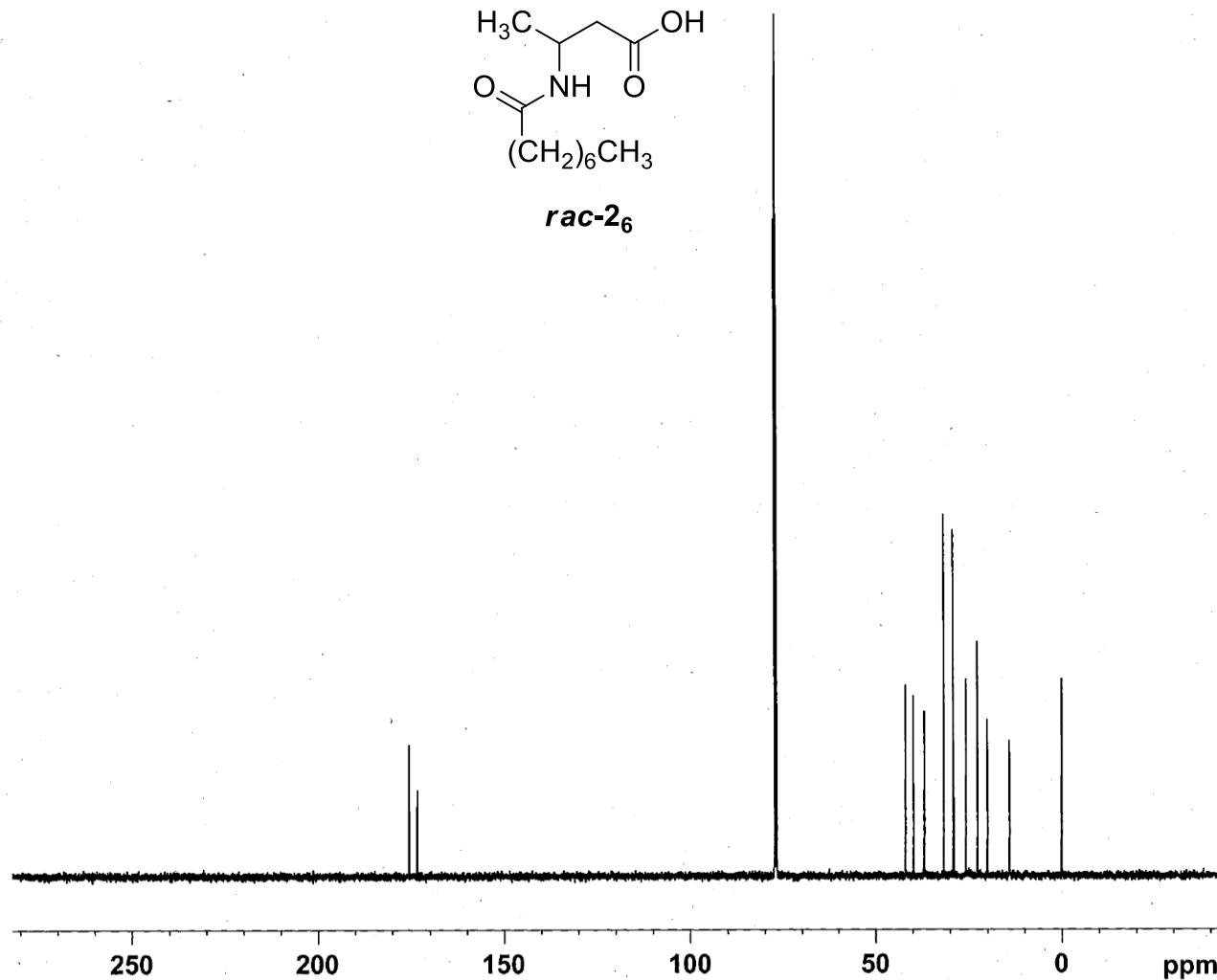
41.892
39.832
36.823
31.642
29.129
28.942
25.688
22.560
19.962
14.025

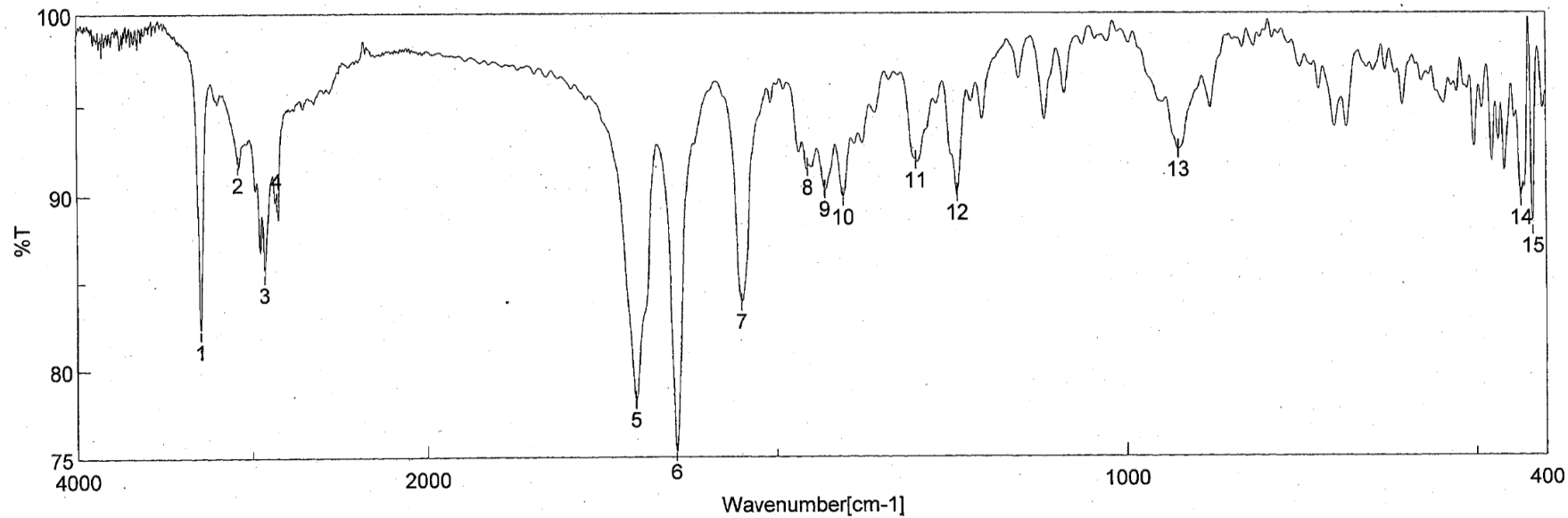


NAME A16mc211rk
EXPNO 17091901
PROCNO 1
Date 20170919
Time 10.21
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 662
DS 2
SWH 40760.871 Hz
FIDRES 0.621962 Hz
AQ 0.8039582 sec
RG 203
DW 12.267 usec
DE 6.50 usec
TE 301.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PL1 0.00 dB
PL1W 100.47545624 W
SFO1 125.7477319 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.40 dB
PL12 19.02 dB
PL13 22.02 dB
PL2W 15.17711735 W
PL12W 0.33051354 W
PL13W 0.16564916 W
SFO2 500.0316016 MHz
SI 16384
SF 125.7326440 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





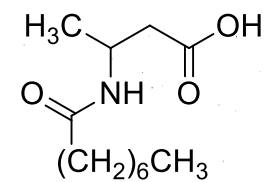
積算回数
ゼロフィリング
ゲイン
測定日時
測定者
ファイル名
サンプル名
コメント

16
ON
8
2017/09/19 14:09
kawamata
Memory#2
rac-ch3-C7-COOH

分解
アポダイゼーション
スキャンスピード
更新日時

4 cm-1
Cosine
2 mm/sec
2017/09/19 14:12

1: 3295.75,	82.22	2: 3081.69,	91.76	3: 2931.27,	85.47	4: 2860.88,	89.68
5: 1702.84,	78.28	6: 1644.98,	75.28	7: 1551.45,	83.87	8: 1455.03,	91.56
9: 1430.92,	90.32	10: 1404.89,	89.88	11: 1299.79,	91.95	12: 1240.97,	90.13
13: 925.66,	92.55	14: 435.83,	89.81	15: 419.44,	88.22		



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