

Supporting Information

Enantio- and diastereo-selective synthesis of piperidines by coupling of four components
in a “one-pot” sequence involving diphenylprolinol silyl ether-mediated Michael reaction

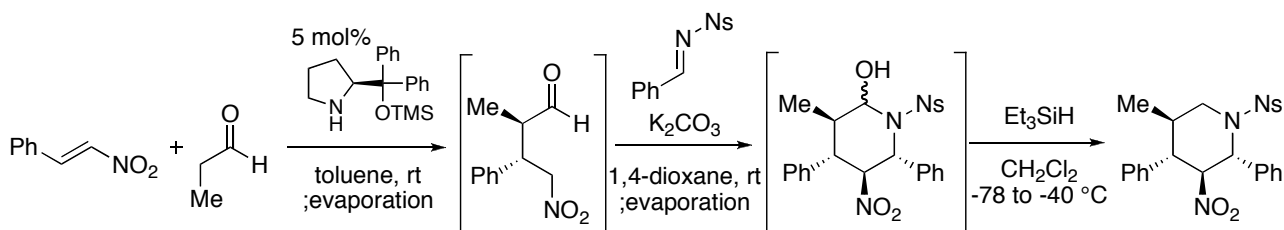
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General Remarks

All reactions were carried out under argon atmosphere and monitored by thin-layer chromatography using Merck 60 F254 precoated silica gel plates (0.25 mm thickness). FT-IR spectra were recorded on a JASCO FT/IR-410 spectrometer. ^1H and ^{13}C NMR spectra were recorded on a Bruker AM400 (400 MHz for ^1H NMR, 100 MHz for ^{13}C NMR) instrument. Data for ^1H NMR are reported as chemical shift (δ ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constant (Hz), integration, and assignment. Data for ^{13}C NMR are reported as chemical shift. High-resolution mass spectral analyses (HRMS) were carried out using Bruker ESI-TOF MS. All liquid aldehydes and solvents were distilled before use. Preparative thin layer chromatography was performed using Wakogel B-5F purchased from Wako Pure Chemical Industries, Tokyo, Japan. Flash chromatography was performed using silica gel 60N of Kanto Chemical Co. Int., Tokyo, Japan. HPLC analysis was performed on a HITACHI Elite LaChrom Series HPLC, UV detection monitored at appropriate wavelength respectively, using CHIRALCEL OB-H (0.46 cm x 25 cm), CHIRALPAK IA (0.46 cm x 25 cm) and CHIRALPAK IB (0.46 cm x 25 cm).

Typical procedure of synthesis for tetrasubstituted piperidine



To a mixture of nitroalkene (0.2 mmol) and aldehyde (0.24 mmol) in toluene (160 μL) was added toluene solution of diphenylprolinol trimethylsilyl ether (0.25 M, 40.0 μL). After the reaction mixture was stirred at 23 °C until complete consumption of nitroalkene, Ns-imine (0.24 mmol), K_2CO_3 (27.6 mg, 0.2 mmol) and 1,4-dioxane (200 μL) were added to the reaction mixture. After the reaction mixture was stirred for 7 hours, domino aza-Henry reaction/acetalization reaction was quenched by silica gel pad with 10% $\text{MeOH}/\text{CHCl}_3$, and concentrated in vacuo. To the mixture of residue

and triethylsilane (159.3 μ L, 1.0 mmol) in CH_2Cl_2 (2.0 mL) was added trifluoroacetic acid (76.5 mL, 1.0 mmol) at -78°C . The reaction mixture was stirred for 7 hours while increasing temperature until -20°C . The reaction was quenched by addition of aq NaHCO_3 and extracted with CHCl_3 (3 x 10 mL). Combined organic layer was concentrated in vacuo. Purification by preparative thin layer chromatography (EtOAc : hexane = 1:2) gave corresponding piperidine derivative in 74% yield as a single diastereomer. Enantiomeric excess of piperidine derivative was determined by HPLC equipped with CHIRALPAK AD-H.

(3*R*, 4*S*, 5*S*, 6*R*)-3-methy-5-nitro-1-(*p*-nitrobenzenesulfonyl)-4,6-diphenylpiperidine (compound 3)

^1H NMR (CDCl_3 , 400 MHz): δ 0.88 (3H, d, $J = 6.4$ Hz), 2.27-2.43 (1H, m), 3.00 (1H, t, $J = 10.8$ Hz), 3.09 (1H, t, $J = 12.8$ Hz), 4.38 (1H, dd, $J = 4.0, 13.2$ Hz), 4.86 (1H, d, $J = 10.0$ Hz), 5.40 (1H, t, $J = 10.4$ Hz), 7.04 (2H, t, $J = 7.2$ Hz), 7.10-7.24 (5H, m), 7.25-7.38 (3H, m), 7.44 (2H, d, $J = 8.8$ Hz), 8.05 (2H, d, $J = 8.8$ Hz); ^{13}C NMR (CDCl_3 , 100 MHz): δ 16.7, 35.8, 54.0, 54.7, 65.0, 92.3, 123.5, 127.7, 128.2, 128.3, 129.1, 129.4, 129.9, 132.2, 136.7, 145.6, 149.4; IR (neat): ν 1555, 1530, 1349, 1157, 1090, 854, 797, 744, 700, 606 cm^{-1} ; HRMS (ESI): $[\text{M}+\text{Na}]$ calcd for $[\text{C}_{24}\text{H}_{23}\text{N}_3\text{O}_6\text{SNa}]$: 504.1200, found: 504.1216; $[\alpha]_{\text{D}}^{23^\circ\text{C}}$ -48.0 (c 1.0, CHCl_3); Enantiomeric excess was determined by HPLC with a CHIRALPAK AD-H column (i PrOH : hexane = 1 : 4), 1.0 mL/min, minor enantiomer $\text{rt} = 7.7$ min, major enantiomer $\text{rt} = 13.1$ min; White solid (mp: 207°C).

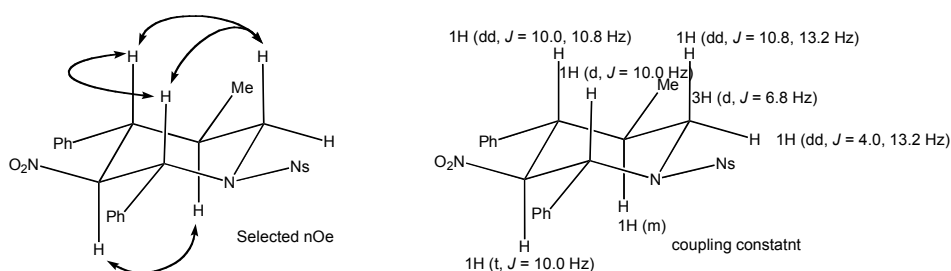
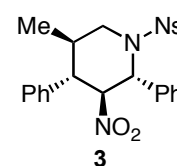
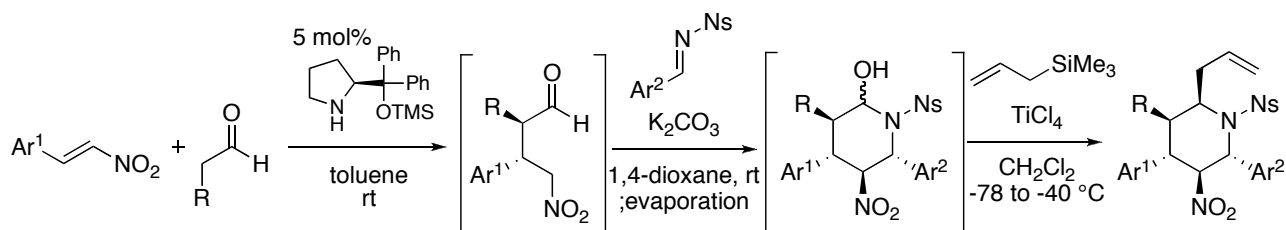


Figure 1. Determination of relative configuration

Typical procedure for one-pot synthesis of 2-allyl piperidine



To a mixture of nitroalkene (0.2 mmol) and aldehyde (0.24 mmol) in toluene (160 μ L) was added toluene solution of diphenylprolinol trimethylsilyl ether (0.25 M, 40.0 μ L). After the reaction mixture was stirred at 23 °C until complete consumption of nitroalkene, Ns-imine (0.24 mmol), K₂CO₃ (5.5 mg, 0.04 mmol) and 1,4-dioxane (200 μ L) were added to the reaction mixture. After the reaction mixture was stirred for 12 hours, solvents were removed under reduced pressure. To the mixture of residue and allyltrimethylsilane (127.0 μ L, 0.8 mmol) in CH₂Cl₂ (2 mL) was added TiCl₄ (43.8 μ L, 0.4 mmol) at -78 °C. The reaction mixture was stirred for 7 hours while increasing temperature until -40 °C. The reaction was quenched by addition of aq NaHCO₃ and extracted with CHCl₃ (3 x 10 mL). Combined organic layer was concentrated in vacuo. Purification by column chromatography (EtOAc : hexane = 1:9) gave corresponding piperidine derivative in 79% yield as a single diastereomer. Enantiomeric excess of piperidine derivative was determined by HPLC equipped with CHIRALPAK AD-H.

(2R, 3R, 4S, 5S, 6R)-2-allyl-3-methyl-5-nitro-1-(p-nitrobenzenesulfonyl)-4,6-diphenylpiperidine (compound 4)

¹H NMR (CDCl₃, 400 MHz): δ 0.83 (3H, d, *J* = 6.8 Hz), 2.58-2.78 (2H, m), 2.93 (1H, dt, *J* = 9.2, 14.8 Hz), 3.32 (1H, t, *J* = 11.6 Hz), 4.83 (1H, dt, *J* = 12.4, 4.4 Hz), 5.05 (1H, d, *J* = 11.2 Hz), 5.38 (1H, d, *J* = 10.0 Hz), 5.46 (1H, d, *J* = 17.2 Hz), 5.93 (1H, t, *J* = 11.2 Hz), 5.92-6.06 (1H, m), 6.50-7.80 (12H, m), 7.91 (2H, d, *J* = 8.8 Hz); ¹³C NMR (CDCl₃, 100 MHz): δ 16.3, 29.6, 39.7, 51.0, 57.5, 59.7, 89.0, 118.8, 123.0, 128.0, 128.1, 128.4, 129.3, 130.2, 134.5, 137.0, 147.0, 148.9; IR (neat): ν 1553, 1529, 1349, 1312, 1160, 794, 742, 698, 609 552 cm⁻¹; HRMS (ESI): [M+Na] calcd for [C₂₇H₂₇N₃O₆NaS]: 544.1513, found: 544.1492; [α]_D^{20°C} -187.7 (c 1.82, CHCl₃); Enantiomeric excess was determined by HPLC with a CHIRALPAK AD-H column (iPrOH : hexane = 1 : 80), 1.0 mL/min, minor enantiomer rt = 27.9 min, major enantiomer rt = 31.8 min; White solid (mp: 241 °C).

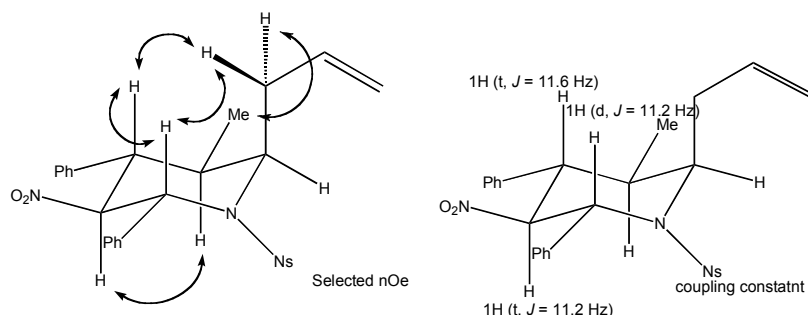
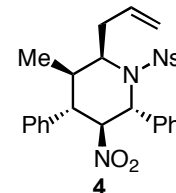
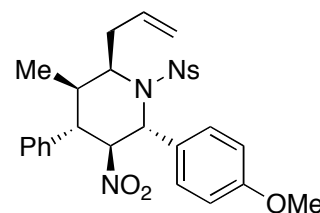


Figure 2. Determination of relative configuration

(2R, 3R, 4S, 5S, 6R)-2-allyl-6-(p-methoxyphenyl)-3-methyl-5-nitro-1-(p-nitrobenzenesulfonyl)-4-phenyl piperidine

(Table 2, entry 2)

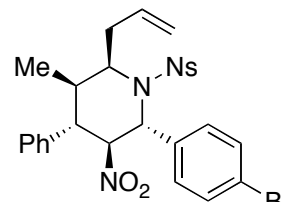
¹H NMR (CDCl₃, 400 MHz): δ 0.82 (3H, d, *J* = 6.8 Hz), 2.56-2.75 (2H, m), 2.92 (1H, br-q, *J* = 12 Hz), 3.32 (1H, t, *J* = 11.6 Hz), 3.63 (3H, s), 4.82 (1H, dt, *J* = 12.0, 4.4 Hz), 4.98 (1H, d, *J* = 11.2 Hz), 5.36 (1H, d, *J* = 9.6 Hz), 5.44 (1H, d, *J* = 17.2 Hz), 5.87 (1H, t, *J* = 10.8 Hz), 5.92-6.07 (1H, m), 6.20-7.70 (11H, m), 7.93 (2H, d, 8.8 Hz); ¹³C NMR (CDCl₃, 100 MHz): δ 16.2, 29.5, 39.6, 50.9, 55.2, 57.0, 59.4, 89.2, 113.2, 118.6, 121.8, 122.8, 128.1, 128.3, 134.7, 137.0, 146.9, 148.9, 160.3; IR (neat): ν 1553, 1529, 1348, 1259, 1160, 1030, 834, 742, 608, 547 cm⁻¹; HRMS (ESI): [M+Na] calcd for [C₂₈H₂₉N₃O₇NaS]: 574.1618, found: 574.1590; [α]_D^{24°C} -200.9 (c 1.0, CHCl₃); Enantiomeric excess was determined by HPLC with a CHIRALPAK AD-H column (iPrOH : hexane = 1 : 20), 1.0 mL/min, minor enantiomer rt = 18.6 min, major enantiomer rt = 12.0 min; Yellow solid (mp: 185 °C).



(2R, 3R, 4S, 5S, 6R)-2-allyl-6-(p-bromophenyl)-3-methyl-5-nitro-1-(p-nitrobenzenesulfonyl)-4-phenyl piperidine

(Table 2, entry 3)

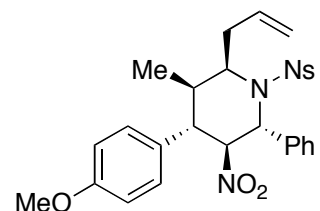
¹H NMR (CDCl₃, 400 MHz): δ 0.82 (3H, d, *J* = 6.8 Hz), 2.57-2.67 (1H, m), 2.67-2.77 (1H, m), 2.90 (1H, ddd, *J* = 9.6, 12.0, 14.0 Hz), 3.31 (1H, t, *J* = 11.2 Hz), 4.82 (1H, dt, *J* = 12.0, 4.8 Hz), 4.98 (1H, d, *J* = 11.2 Hz), 5.36 (1H, d, *J* = 10.4 Hz), 5.44 (1H, d, *J* = 17.2 Hz), 5.87 (1H, t, *J* = 11.2 Hz), 5.91-6.04 (1H, m), 6.50-7.72 (12H, m), 8.01 (2H, d, *J* = 8.8 Hz); ¹³C NMR (CDCl₃, 100 MHz): δ 16.3, 29.6, 39.6, 50.9, 57.0, 59.6, 88.8, 118.8, 123.2, 124.2, 128.1, 128.5, 129.2, 131.1, 134.6, 136.7, 146.7, 149.1; IR (neat): ν 1553, 1530, 1490, 1349, 1161, 1088, 1012, 829, 742, 610, 418 cm⁻¹; HRMS (ESI): [M+Na] calcd for [C₂₇H₂₆N₃O₆NaSBr]: 624.0601, found: 624.0617; [α]_D^{24°C} -202.9 (c 1.0, CHCl₃); Enantiomeric excess was determined by HPLC with a CHIRALPAK AD-H column (iPrOH : hexane = 1 : 20), 1.0 mL/min, minor enantiomer rt = 11.7 min, major enantiomer rt = 10.0 min; White solid (mp: 203 °C).



(2R, 3R, 4S, 5S, 6R)-2-allyl-4-(p-methoxyphenyl)-3-methyl-5-nitro-1-(p-nitrobenzenesulfonyl)-6-phenyl piperidine

(Table 2, entry 4)

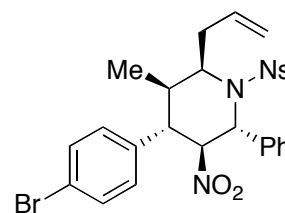
¹H NMR (CDCl₃, 400 MHz): δ 0.82 (3H, d, *J* = 6.8 Hz), 2.53-2.65 (1H, m), 2.70 (1H, br-d, *J* = 14.8), 2.91 (1H, br-q, *J* = 11.6 Hz), 3.27 (1H, t, *J* = 11.2 Hz), 3.80 (3H, s), 4.82 (1H, dt, *J* = 12.0, 6.0 Hz), 5.03 (1H, d, *J* = 11.2 Hz), 5.36 (1H, d, *J* = 10.0 Hz), 5.44 (1H, d, *J* = 16.8 Hz), 5.87 (1H, t, *J* = 11.2 Hz), 5.92-6.05 (1H, m), 6.30-7.70 (11H, m), 7.90 (2H, d, *J* = 8.8 Hz); ¹³C NMR (CDCl₃, 100 MHz): δ 16.3, 29.5, 39.8, 50.2, 55.2, 57.6, 59.7, 89.2, 118.7, 123.0, 127.9, 128.0, 128.9, 129.3, 130.2, 134.6, 147.0, 148.9, 159.4; IR (neat): ν 1552, 1530, 1348, 1253, 1160, 1031, 794, 742, 618, 414 cm⁻¹; HRMS (ESI): [M+Na] calcd for [C₂₈H₂₉N₃O₇NaS]: 574.1618 found 574.1646; [α]_D^{23°C} -165.9 (c 1.0, CHCl₃); Enantiomeric excess was determined by HPLC with a CHIRALPAK AD-H column (iPrOH : hexane = 1 : 20), 1.0 mL/min, minor enantiomer rt = 11.4 min, major enantiomer rt = 14.8 min; White solid (mp: 210 °C).



(2R, 3R, 4S, 5S, 6R)-2-allyl-4-(p-bromophenyl)-3-methyl-5-nitro-1-(p-nitrobenzenesulfonyl)-6-phenyl piperidine

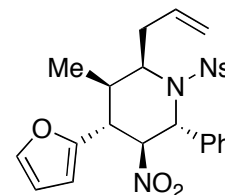
(Table 2, entry 5 & 6)

¹H NMR (CDCl₃, 400 MHz): δ 0.75 (3H, d, *J* = 6.4 Hz), 2.46-2.58 (1H, m), 2.63 (1H, br-d, *J* = 14.8 Hz), 2.82 (1H, br-q, *J* = 12 Hz), 3.23 (1H, t, *J* = 11.2 Hz), 4.74 (1H, dt, *J* = 12.0, 5.6 Hz), 4.95 (1H, d, *J* = 10.8 Hz), 5.30 (1H, d, *J* = 10.0 Hz), 5.38 (1H, d, *J* = 17.2 Hz), 5.80 (1H, t, *J* = 10.8 Hz), 5.84-5.98 (1H, m), 6.3-7.70 (11H, m), 7.83 (2H, d, *J* = 8.4 Hz); ¹³C NMR (CDCl₃, 100 MHz): δ 16.3, 29.5, 39.6, 50.5, 57.4, 59.6, 88.7, 118.9, 122.4, 123.0, 128.0, 129.4, 130.0, 134.3, 136.0, 146.8, 149.0; IR (neat): ν 1556, 1529, 1348, 1160, 793, 742, 612, 406 cm⁻¹; HRMS (ESI): [M+Na] calcd for [C₂₇H₂₆N₃O₆NaSBr]: 624.0601, found 624.0584; [α]_D^{23°C} -173.9 (c 1.0, CHCl₃); Enantiomeric excess was determined by HPLC with a CHIRALPAK AD-H column (*i*PrOH : hexane = 1 : 20), 1.0 mL/min, minor enantiomer rt = 10.1 min, major enantiomer rt = 13.1 min; White solid (mp: 256 °C).



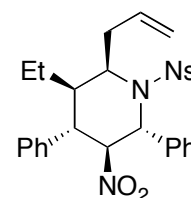
(2R, 3R, 4S, 5S, 6R)-2-allyl-4-(2-furyl)-3-methyl-5-nitro-1-(p-nitrobenzenesulfonyl)-6-phenyl piperidine (Table 2, entry 7)

¹H NMR (CDCl₃, 400 MHz): δ 0.91 (3H, d, *J* = 6.8 Hz), 2.63-2.90 (3H, m), 3.48 (1H, t, *J* = 11.2 Hz), 4.81 (1H, dt, *J* = 12.0, 4.8 Hz), 4.98 (1H, d, *J* = 11.2 Hz), 5.35 (1H, d, *J* = 10.4 Hz), 5.43 (1H, d, *J* = 17.2 Hz), 5.95 (1H, t, *J* = 10.8 Hz), 5.94-6.03 (1H, m), 6.22 (1H, d, *J* = 3.2 Hz), 6.30-6.35 (1H, m), 6.60-7.40 (7H, m), 7.46 (1H, s), 7.90 (2H, d, *J* = 8.8 Hz); ¹³C NMR (CDCl₃, 100 MHz): δ 16.2, 29.5, 38.1, 44.6, 57.4, 59.4, 86.9, 109.3, 110.3, 118.8, 123.0, 127.96, 128.02, 129.4, 130.1, 134.4, 143.1, 147.0, 148.9, 149.6; IR (neat): ν 1555, 1530, 1348, 1312, 1160, 1088, 1030, 794, 742, 612 cm⁻¹; HRMS (ESI): [M+Na] calcd for [C₂₅H₂₅N₃O₇NaS]: 534.1305, found 534.1288; [α]_D^{23°C} -159.9 (c 1.0, CHCl₃); Enantiomeric excess was determined by HPLC with a CHIRALPAK AD-H column (*i*PrOH : hexane = 1 : 20), 1.0 mL/min, minor enantiomer rt = 11.3 min, major enantiomer rt = 12.5 min; White solid (mp: 235 °C).



(2R, 3R, 4S, 5S, 6R)-2-allyl-3-ethyl-5-nitro-1-(p-nitrobenzenesulfonyl)-4,6-diphenylpiperidine (Table 2, entry 8)

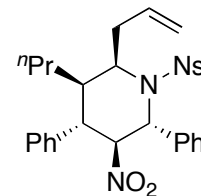
¹H NMR (CDCl₃, 400 MHz): δ 0.93 (3H, t, *J* = 7.6 Hz), 1.04-1.16 (1H, m), 1.16-1.29 (1H, m), 2.42 (1H, tt, *J* = 4.4, 10.8 Hz), 2.65 (1H, br-d, *J* = 14.8 Hz), 2.93 (1H, dt, *J* = 9.6, 14.4 Hz), 3.36 (1H, t, *J* = 11.2 Hz), 4.99 (1H, dt, *J* = 12.0, 4.8 Hz), 5.05 (1H, d, *J* = 11.2 Hz), 5.37 (1H, d, *J* = 10.0 Hz), 5.46 (1H, d, *J* = 17.2 Hz), 5.93 (1H, t, *J* = 10.8 Hz), 5.95-6.07 (1H, m), 6.30-7.80 (12H, m), 7.91 (2H, d, *J* = 8.8 Hz); ¹³C NMR (CDCl₃, 100 MHz): δ 10.8, 23.0, 29.1, 46.0, 50.4, 56.8, 57.4, 89.3, 118.7, 123.0, 127.9, 128.0, 128.3, 129.3, 130.2, 134.5, 137.2, 147.0, 148.9; IR (neat): ν 1553, 1530, 1348, 1161, 1088, 994, 792, 741, 700, 609 cm⁻¹; HRMS (ESI): [M+Na] calcd for [C₂₈H₂₉N₃O₆NaS]: 558.1669, found 558.1684; [α]_D^{25°C} -171.2 (c 1.0, CHCl₃); Enantiomeric excess was determined by HPLC with a



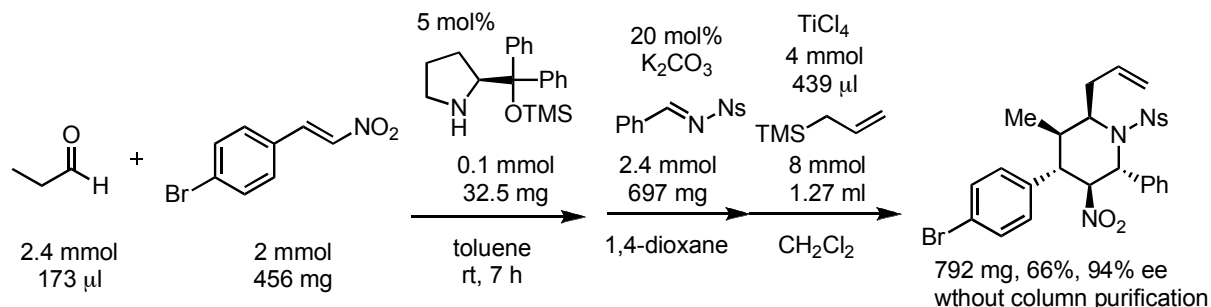
CHIRALPAK AD-H column (*i*PrOH : hexane = 1 : 10), 1.0 mL/min, minor enantiomer *rt* = 8.8 min, major enantiomer *rt* = 10.4 min; White solid (mp: 237 °C).

(2*R*, 3*R*, 4*S*, 5*S*, 6*R*)-2-allyl-3-*n*-propyl-5-nitro-1-(*p*-nitrobenzenesulfonyl)-4,6-diphenylpiperidine (Table 2, entry 9)

¹H NMR (CDCl₃, 400 MHz): δ 0.86 (3H, t, *J* = 7.6 Hz), 1.03-1.16 (2H, m), 1.21-1.33 (1H, m), 1.38-1.50 (1H, m), 2.53 (1H, dq, *J* = 17.2, 5.2 Hz), 2.66 (1H, br-d, *J* = 14.8 Hz), 2.85-3.00 (1H, m), 3.36 (1H, t, *J* = 11.6 Hz), 4.94 (1H, dt, *J* = 12.0, 4.8 Hz), 5.05 (1H, d, *J* = 11.6 Hz), 5.38 (1H, d, *J* = 10.0 Hz), 5.47 (1H, d, *J* = 17.2 Hz), 5.92 (1H, t, *J* = 11.2 Hz), 5.95-6.07 (1H, m), 6.50-7.70 (13H, m), 7.91 (2H, d, *J* = 8.8 Hz); ¹³C NMR (CDCl₃, 100 MHz): δ 13.7, 19.2, 29.3, 31.9, 43.8, 50.4, 58.1, 57.4, 89.4, 118.8, 123.0, 127.95, 128.02, 128.3, 129.3, 130.3, 134.5, 137.2, 147.0, 148.9; IR (neat): ν 1553, 1530, 1348, 1161, 1088, 794, 740, 699, 610, 551 cm⁻¹; HRMS (ESI): [M+Na] calcd for [C₂₉H₃₁N₃O₆NaS]: 572.1826, found 572.1807; [α]_D²⁴ -137.1 (c 1.0, CHCl₃); Enantiomeric excess was determined by HPLC with a CHIRALPAK AD-H column (*i*PrOH : hexane = 1 : 20), 1.0 mL/min, minor enantiomer *rt* = 6.5 min, major enantiomer *rt* = 13.4 min; White solid (mp: 178 °C).

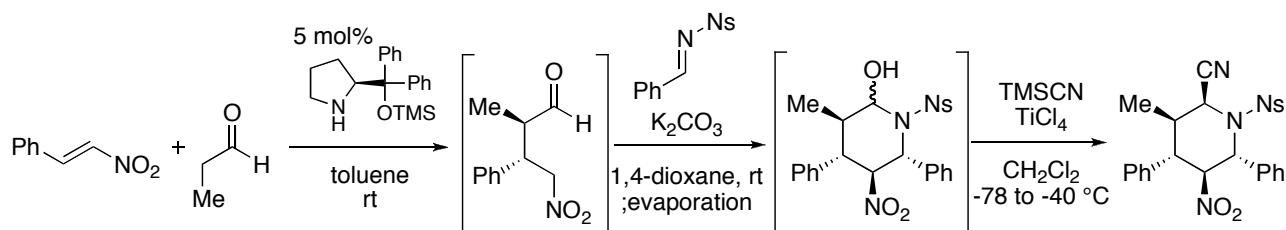


Large scale synthesis of 2-allyl piperidine



To a mixture of *p*-bromonitrostyrene (456 mg, 2.0 mmol) and propanal (173 µL, 2.4 mmol) in toluene (1.2 mL) was added diphenylprolinol trimethylsilyl ether (33 mg, 0.1 mmol). After the reaction mixture was stirred at 23 °C until complete consumption of nitroalkene, Ns-imine (697 mg, 2.4 mmol), K₂CO₃ (55 mg, 0.4 mmol) and 1,4-dioxane (2 mL) were added to the reaction mixture. After the reaction mixture was stirred for 12 hours, solvents were removed under reduced pressure. To the mixture of residue and allyltrimethylsilane (1.27 mL, 8.0 mmol) in CH₂Cl₂ (20 mL) was added TiCl₄ (439 µL, 4.0 mmol) at -78 °C. The reaction mixture was stirred for 7 hours while increasing temperature until -40 °C. The reaction was quenched by addition of aq NaHCO₃ and extracted with CHCl₃ (3 x 10 mL). Combined organic layer was concentrated in vacuo. Purification by recrystallization (MeOH) gave corresponding piperidine derivative in 66% yield as a single diastereomer with 94% ee.

Typical procedure for one-pot synthesis of 2-cyano piperidine

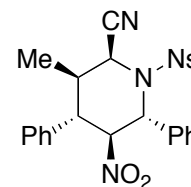


To a mixture of nitroalkene (0.2 mmol) and aldehyde (0.24 mmol) in toluene (160 μ L) was added toluene solution of diphenylprolinol trimethylsilyl ether (0.25 M, 40.0 μ L). After the reaction mixture was stirred at 23 $^{\circ}$ C until complete consumption of nitroalkene, Ns-imine (0.24 mmol), K_2CO_3 (5.5 mg, 0.04 mmol) and 1,4-dioxane (200 μ L) were added to the reaction mixture. After the reaction mixture was stirred for 12 hours, solvents were removed under reduced pressure. To the mixture of residue and trimethylsilyl cyanide (100.0 μ L, 0.8 mmol) in CH_2Cl_2 (200 μ L) was added $TiCl_4$ (43.8 μ L, 0.4 mmol) at -78 $^{\circ}$ C. The reaction mixture was stirred for 7 hours while increasing temperature until -40 $^{\circ}$ C. The reaction was quenched by addition of aq $NaHCO_3$ and extracted with $CHCl_3$ (3 x 10 mL). Combined organic layer was concentrated in vacuo. Purification by column chromatography (EtOAc : hexane = 1:5) gave corresponding piperidine derivative in 80% yield as a single diastereomer. Enantiomeric excess of piperidine derivative was determined by HPLC equipped with CHIRALPAK AD-H.

(2S, 3R, 4S, 5S, 6R)-2-cyano-3-*n*-propyl-5-nitro-1-(*p*-nitrobenzenesulfonyl)-4,6-diphenylpiperidine (Table 2, entry10)

1H NMR ($CDCl_3$, 400 MHz): δ 1.07 (3H, d, J = 6.8 Hz), 2.54-2.66 (1H, m), 3.39 (1H, t, J = 11.2

Hz), 5.15 (1H, d, J = 10.8 Hz), 5.42 (1H, t, J = 10.8 Hz), 5.62 (1H, d, J = 4.8 Hz), 6.95-7.06 (2H, m), 7.12-7.25 (4H, m), 7.35 (2H, d, J = 8.8 Hz), 7.33-7.43 (3H, m), 8.05 (2H, d, J = 8.8 Hz); ^{13}C



NMR ($CDCl_3$, 100 MHz): δ 15.8, 38.3, 51.6, 53.6, 62.6, 90.7, 114.6, 123.7, 128.3, 128.5, 129.0, 129.2, 129.5, 130.2, 131.1, 134.8, 144.9, 149.8; IR (neat): ν 1558, 1532, 1350, 1170, 1088, 744, 701, 615, 552 cm^{-1} ; HRMS (ESI): $[M+Na]$ calcd for $[C_{25}H_{22}N_4O_6NaS]$: 529.1152, found: 529.1148; $[\alpha]_D^{20} -82.3$ (c 0.80, $CHCl_3$); Enantiomeric excess was determined by HPLC with a CHIRALPAK AD-H column (i PrOH : hexane = 1 : 10), 1.0 mL/min, minor enantiomer rt = 25.8 min, major enantiomer rt = 43.5 min; White solid (mp: 248 $^{\circ}$ C).

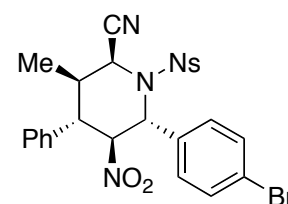
(2R, 3R, 4S, 5S, 6R)-6-(*p*-bromophenyl)-2-cyano-3-methyl-5-nitro-1-(*p*-nitrobenzenesulfonyl)-4-phenyl piperidine (Table 2, entry 11)

1H NMR ($CDCl_3$, 400 MHz): δ 1.06 (3H, d, J = 6.8 Hz), 2.53-2.65 (1H, m), 3.38 (1H, t, J

= 11.2 Hz), 5.11 (1H, d, J = 10.8 Hz), 5.37 (1H, t, J = 10.8 Hz), 5.60 (1H, d, J = 4.8 Hz),

7.02 (2H, d, J = 8.4 Hz), 7.15 (2H, d, J = 8.4 Hz), 7.20-7.28 (2H, m), 7.30-7.44 (5H, m),

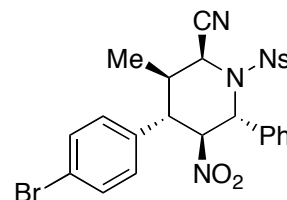
8.14 (2H, d, J = 8.8 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 15.8, 38.2, 51.4, 53.5, 62.0, 90.4, 114.5, 123.8, 125.0, 128.3, 128.5, 129.0, 129.5, 131.4, 132.5, 134.6, 144.6, 150.0; IR (neat): ν 1556, 1531, 1348, 1167, 1091, 1011, 828, 744, 606,



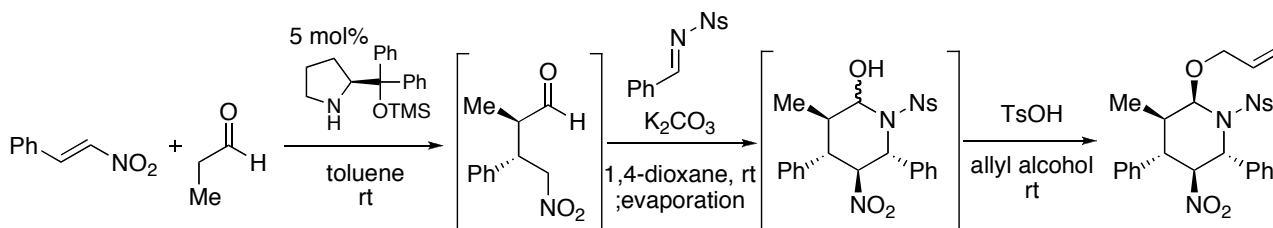
552 cm^{-1} ; HRMS (ESI): $[M+Na]$ calcd for $[C_{25}H_{21}N_4O_6NaSBr]$: 609.0240, found: 609.0215; $[\alpha]_D^{20^\circ\text{C}}$ -105.3 (c 0.2, CHCl_3); Enantiomeric excess was determined by HPLC with a CHIRALPAK AD-H column ($i\text{-PrOH}$: hexane = 1 : 10), 1.0 mL/min, minor enantiomer r_t = 30.5 min, major enantiomer r_t = 44.6 min; White solid (mp: 213 $^\circ\text{C}$).

(2R, 3R, 4S, 5S, 6R)-4-(p-broophenyl)-2-cyano-3-methyl-5-nitro-1-(p-nitrobenzenesulfonyl)-4-phenyl piperidine
(Table 2, entry 12)

^1H NMR (CDCl_3 , 400 MHz): δ 1.06 (3H, d, J = 6.8 Hz), 2.50-2.62 (1H, m), 3.37 (1H, t, J = 11.6 Hz), 5.14 (1H, d, J = 10.4 Hz), 5.37 (1H, t, J = 10.4 Hz), 5.61 (1H, d, J = 4.4 Hz), 7.02 (2H, t, J = 7.2 Hz), 7.06-7.23 (4 H, m), 7.34 (2H, d, J = 8.4 Hz), 7.53 (2H, d, J = 7.6 Hz), 8.04 (2H, d, J = 8.4 Hz); ^{13}C NMR (CDCl_3 , 100 MHz): δ 15.8, 38.2, 51.0, 53.5, 62.5, 90.4, 114.5, 123.1, 123.7, 128.3, 128.5, 129.1, 130.2, 131.0, 132.7, 133.9, 144.7, 149.8; IR (neat): ν 1557, 1532, 1350, 1170, 1088, 1011, 795, 745, 617, 552 cm^{-1} ; HRMS (ESI): $[M+Na]$ calcd for $[C_{25}H_{21}N_4O_6NaSBr]$: 609.0240, found: 609.0217; $[\alpha]_D^{23^\circ\text{C}}$ -126.7 (c 0.35, CHCl_3); Enantiomeric excess was determined after removing Ns group by HPLC with a CHIRALPAK AD-H column ($i\text{-PrOH}$: hexane = 1 : 10), 1.0 mL/min, minor enantiomer r_t = 12.7 min, major enantiomer r_t = 14.9 min; White solid (mp: 284 $^\circ\text{C}$).



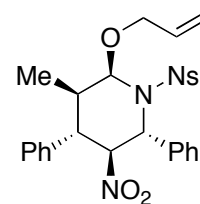
Typical procedure for one-pot synthesis of 2-allyloxy piperidine



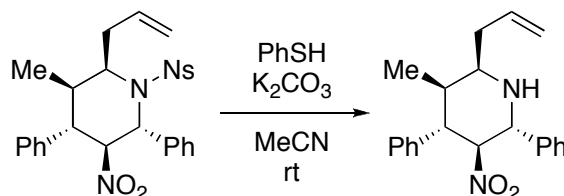
To a mixture of nitroalkene (0.2 mmol) and aldehyde (0.24 mmol) in toluene (160 μL) was added toluene solution of diphenylprolinol trimethylsilyl ether (0.25 M, 40.0 μL). After the reaction mixture was stirred at 23 $^\circ\text{C}$ until complete consumption of nitroalkene, Ns-imine (0.24 mmol), K_2CO_3 (27.6 mg, 0.2 mmol) and 1,4-dioxane (200 μL) were added to the reaction mixture. After the reaction mixture was stirred for 12 hours, solvents were removed under reduced pressure. To the mixture of residue was added *p*-toluenesulfonic acid (79.9 mg, 0.42 mmol) and allyl alcohol (2 mL) at room temperature. The reaction mixture was stirred for 24 hours. The reaction was quenched by addition of aq NaHCO_3 and extracted with CHCl_3 (3 x 10 mL). Combined organic layer was concentrated in vacuo. Purification by column chromatography (EtOAc : hexane = 1 : 7) gave corresponding piperidine derivative in 67% yield as a single diastereomer. Enantiomeric excess of piperidine derivative was determined by HPLC equipped with CHIRALPAK IA.

(2R, 3R, 4S, 5S, 6R)-2-allyloxy-3-methyl-5-nitro-1-(p-nitrobenzenesulfonyl)-4,6-diphenylpiperidine (equation 5)

¹H NMR (CDCl₃, 400 MHz): δ 0.92 (3H, d, *J* = 6.8 Hz), 2.43-2.54 (1H, m), 3.56 (1H, t, *J* = 11.6 Hz), 4.22 (1H, dd, *J* = 6.0, 12.8 Hz), 4.46 (1H, dd, *J* = 5.2, 12.4 Hz), 5.32 (1H, d, *J* = 11.2 Hz), 5.41 (1H, dd, *J* = 1.2, 10.4 Hz), 5.50 (1H, dd, *J* = 1.2, 17.2 Hz), 5.63 (1H, d, *J* = 3.2 Hz), 5.75 (1H, t, *J* = 10.8 Hz), 6.02-6.14 (1H, m), 7.00 (2H, t, *J* = 7.6 Hz), 7.11-7.18 (3H, m), 7.25-7.41 (5H, m), 7.98 (2H, d, *J* = 8.8 Hz); ¹³C NMR (CDCl₃, 100 MHz): δ 15.2, 41.3, 49.8, 57.7, 70.1, 88.2, 89.7, 118.6, 123.4, 127.9, 128.2, 128.3, 129.2, 129.4, 130.5, 131.0, 133.0, 136.8, 146.6, 149.2; IR (neat): ν 2931, 1555, 1531, 1349, 1165, 1011, 805, 745, 700 cm⁻¹; HRMS (ESI): [M+Na] calcd for [C₂₇H₂₇N₃O₇NaSBr]: 560.1462, found: 560.1442; [α]_D^{22°C} -91.3 (c 1.1, CHCl₃); Enantiomeric excess was determined after removing Ns group by HPLC with a CHIRALPAK IA column (*i*PrOH : hexane = 1 : 80), 1.0 mL/min, minor enantiomer rt = 26.9 min, major enantiomer rt = 23.3 min; White solid (mp: 237 °C).



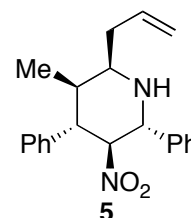
Typical procedure of removing Ns-group

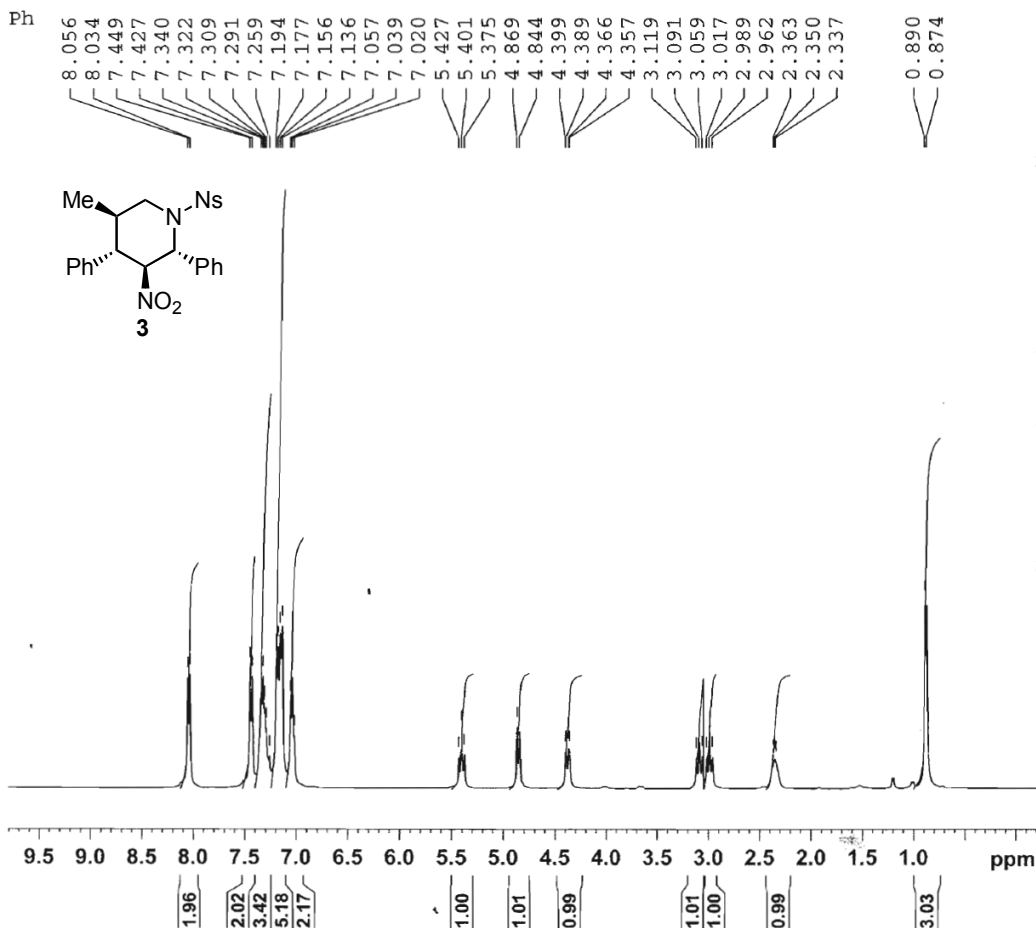


To a mixture of (2R, 3R, 4S, 5S, 6R)-2-allyl-3-methyl-5-nitro-1-(p-nitrobenzenesulfonyl)-4,6-diphenylpiperidine (31.3 mg, 0.06 mmol) and benzenethiol (30.8 μL, 0.3 mmol) in MeCN (600 μL) was added K₂CO₃ (41.5 mg, 0.3 mmol) at room temperature. After the reaction mixture was stirred for 7 hours, the reaction was quenched by addition of saturated NaHCO₃ aq and extracted with EtOAc (3 x 10 mL). Combined organic layer was dried over Na₂SO₄ and concentrated in vacuo. Purification by column chromatography (EtOAc : hexane = 1:9) gave corresponding piperidine derivative in quantitative yield.

(2R, 3R, 4S, 5S, 6R)-2-allyl-3-methyl-5-nitro-4,6-diphenylpiperidine (compound 5)

¹H NMR (CDCl₃, 400 MHz): δ 0.73 (3H, d, *J* = 7.2 Hz), 2.33 (1H, br-d, *J* = 14.0 Hz), 2.47-2.59 (1H, m), 2.78 (1H, dt, *J* = 13.6, 9.6 Hz), 3.17 (1H, dt, *J* = 11.6, 4.4 Hz), 3.24 (1H, t, *J* = 11.2 Hz), 4.36 (1H, d, *J* = 9.6 Hz), 4.78 (1H, t, *J* = 10.8 Hz), 5.19 (1H, d, *J* = 10.0 Hz), 5.29 (1H, d, *J* = 17.2 Hz), 5.69-5.82 (1H, m), 7.18-8.43 (10 H, m); ¹³C NMR (CDCl₃, 100 MHz): δ 16.3, 29.5, 38.2, 49.5, 56.6, 57.8, 96.1, 118.6, 127.5, 127.8, 128.8, 128.9, 135.1, 137.9, 138.5; IR (neat): ν 3064, 3031, 2925, 1549, 1495, 1456, 1371, 756, 738, 700 cm⁻¹; [α]_D^{24°C} +75.9 (c 0.53, CHCl₃); White solid (mp: 120 °C).



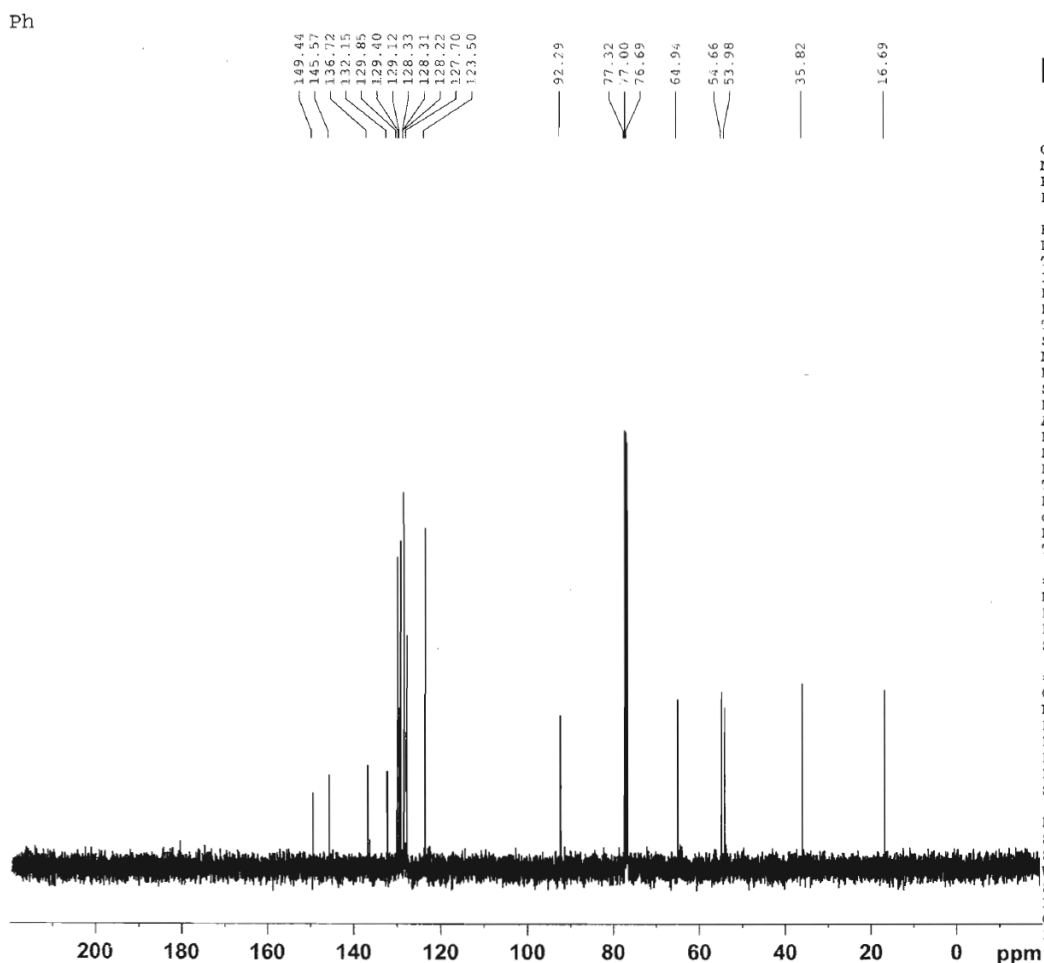


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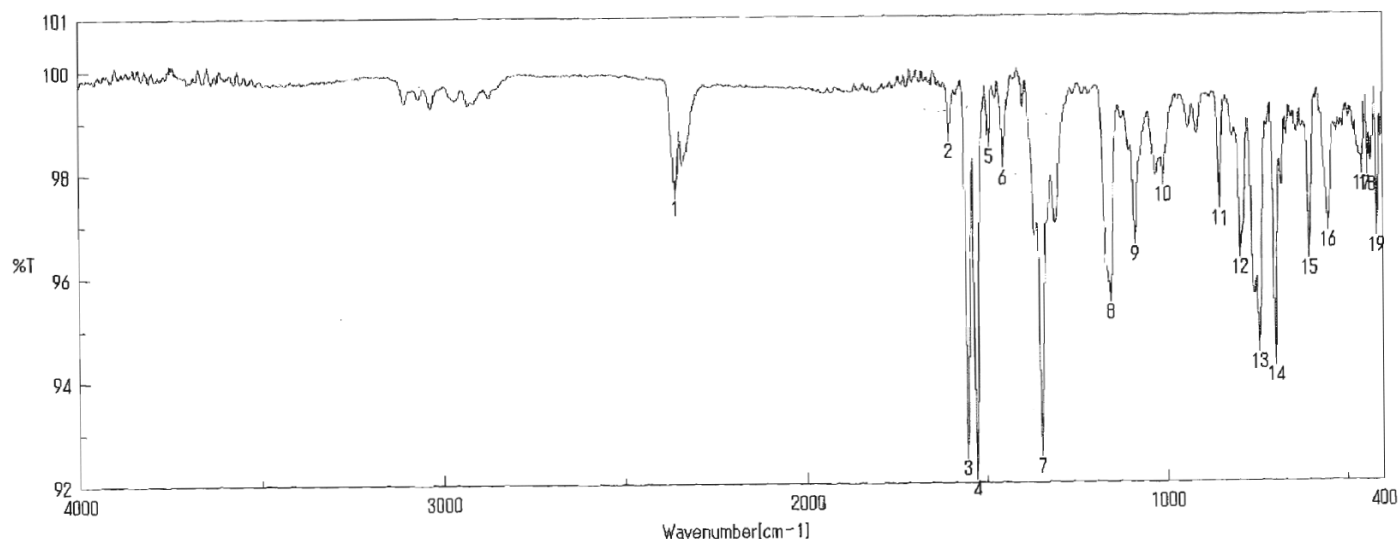
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 測定者
 ファイル名 Memory#3
 サンプル名 background
 コメント

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 アポダイゼーション Cosine
 スキャンスピード 2 mm/sec

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9: 1089.58, 96.7665	10: 1011.48, 97.8945	11: 854.31, 97.4254	12: 797.42, 96.4867
13: 744.39, 94.6752	14: 700.03, 94.4217	15: 605.54, 96.4697	16: 553.47, 96.9961
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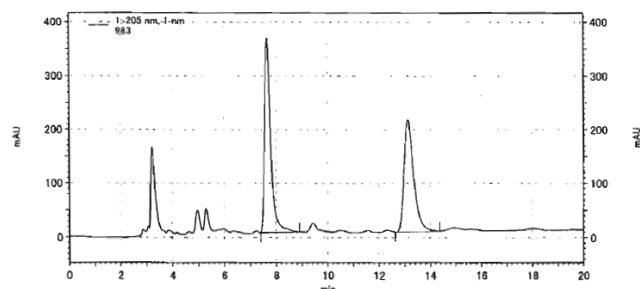
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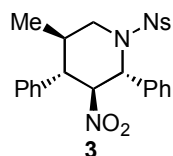
面積%レポート

ページ 1/1

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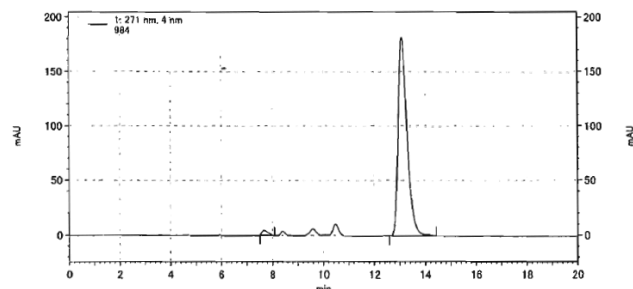
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面積%レポート

ページ 1/1

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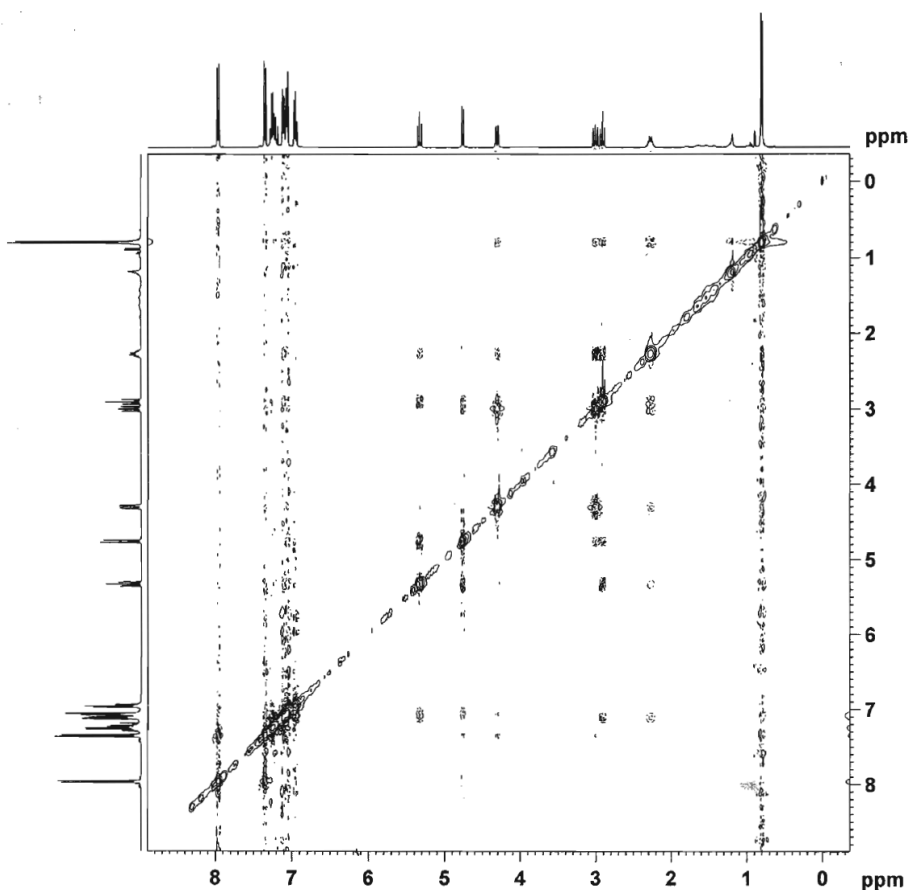
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保持時間 = retention time

面積 = area

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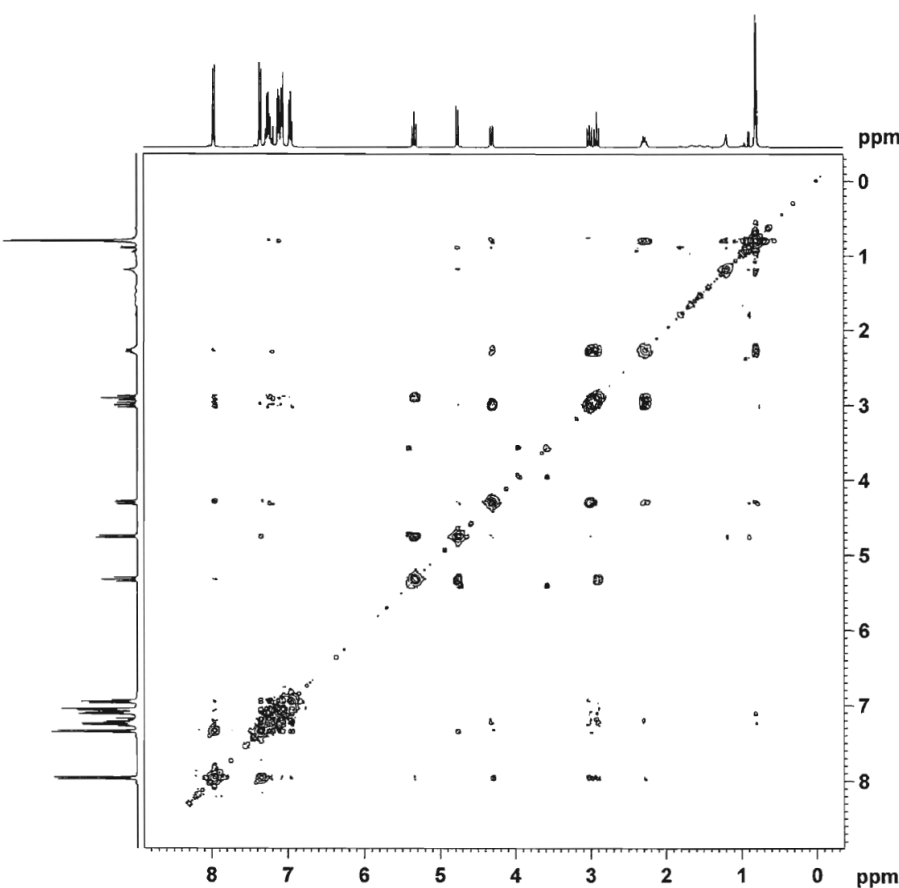
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Current Data Parameters
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EXPNO 72
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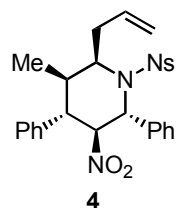
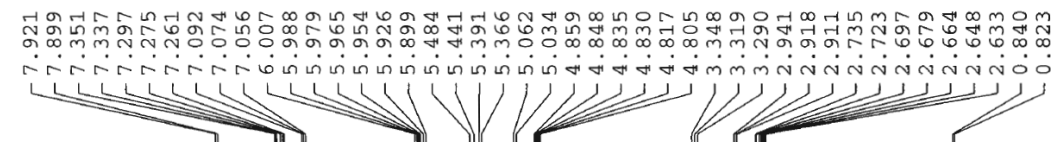
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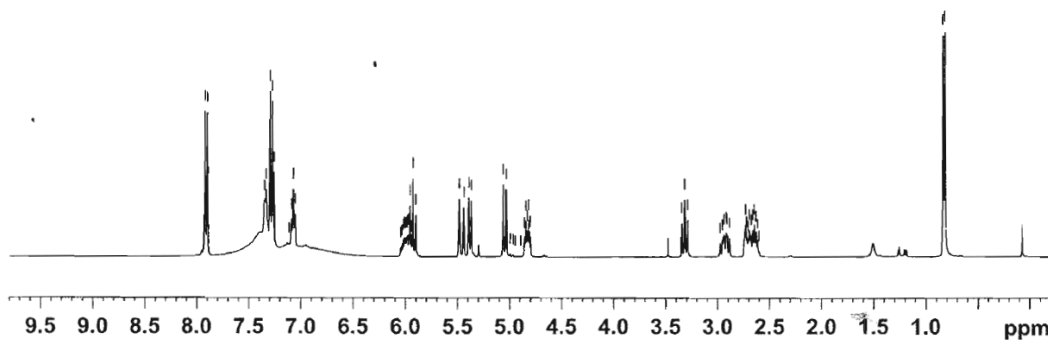


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COSYGS



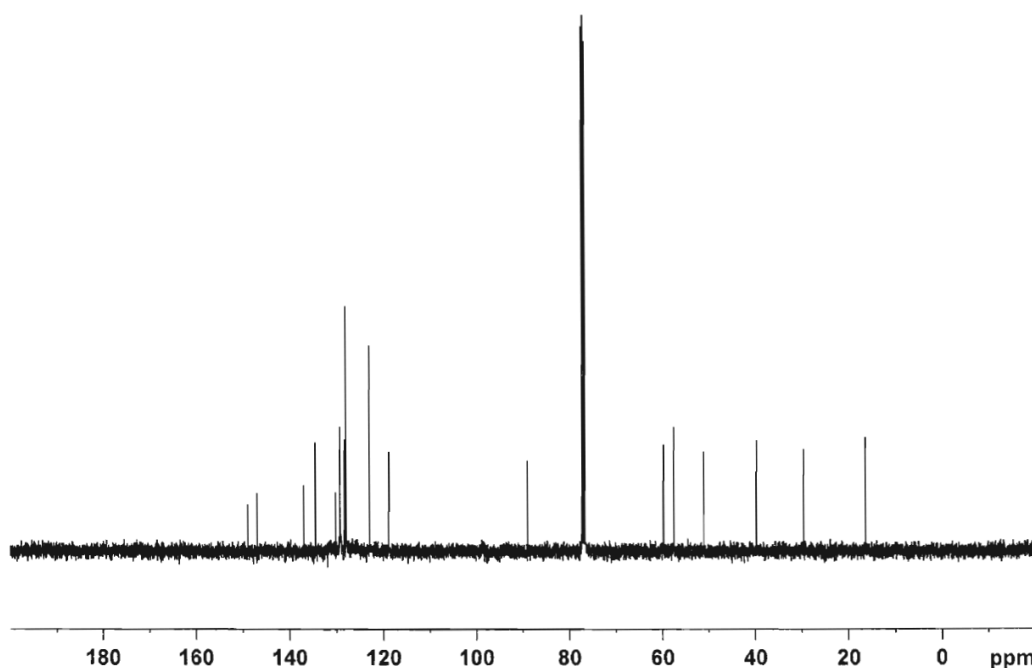
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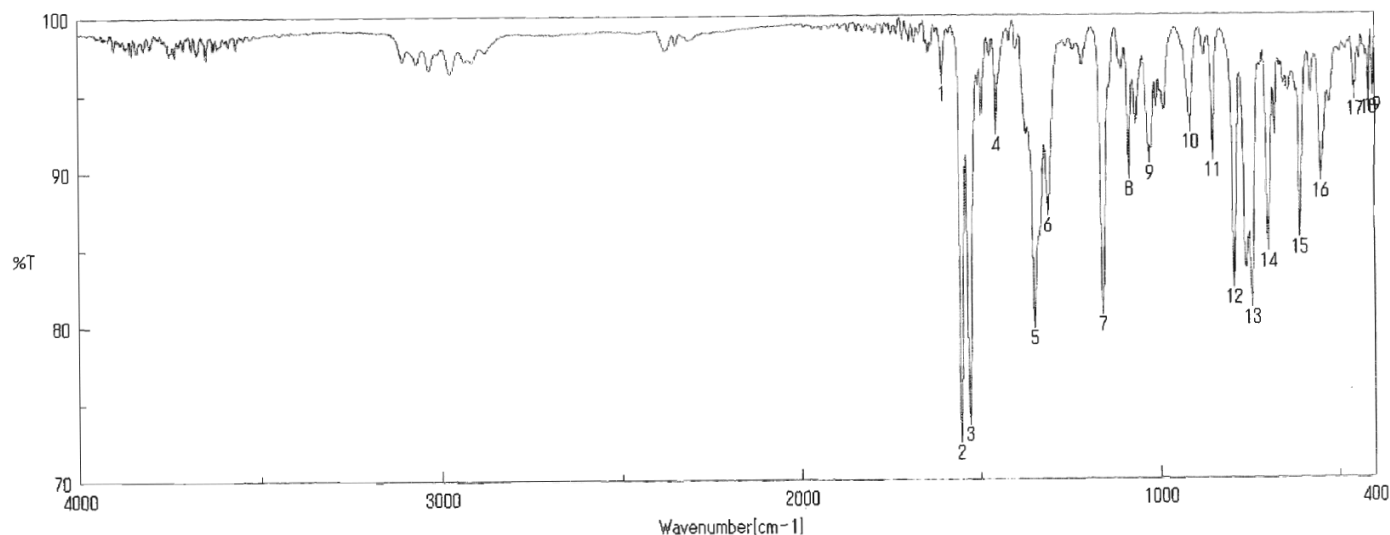
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SSB 0
LB 1.00 Hz
GB 0
PC 1.40





積算回数 16
 ゼロフィリング ON
 ゲイン 1
 日時 110/04/27 13:23
 測定者
 ファイル名 2010_04_27-allyl.JWS
 サンプル名 buckground
 コメント

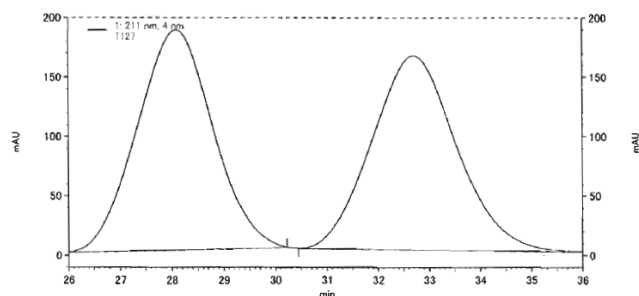
分解 4 cm-1
 アポダイゼーション Cosine
 スキャンスピード 2 mm/sec

1: 1606.41, 96.1311	2: 1553.38, 72.9201	3: 1529.27, 74.1024	4: 1456.96, 92.8416
5: 1348.96, 80.3523	6: 1312.32, 87.6079	7: 1159.97, 81.1898	8: 1087.66, 89.9178
9: 1029.80, 90.9515	10: 916.99, 92.9750	11: 854.31, 91.1159	12: 793.56, 82.8749
13: 742.46, 81.5547	14: 698.11, 85.2260	15: 609.40, 86.0848	16: 551.54, 89.7190
17: 456.08, 95.0007	18: 417.51, 95.0963	19: 404.98, 95.2344	

面積%レポート

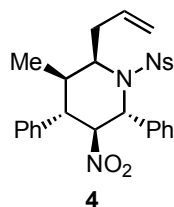
ページ 1/1

データファイル名: \\Server\Enterprise\Projects\Default\Data\2010-04-18 skmt allyl rac
 AD-H 80 vs 1 ml 2kaim.dat
 メソッドファイル名: \\Server\Enterprise\Projects\Default\Method\80vs1 ml.met
 ユーザー名: System
 分析日時: 2010/04/19 20:09:19
 印刷日時: 2010/04/19 22:35:07



1: 211 nm, 4

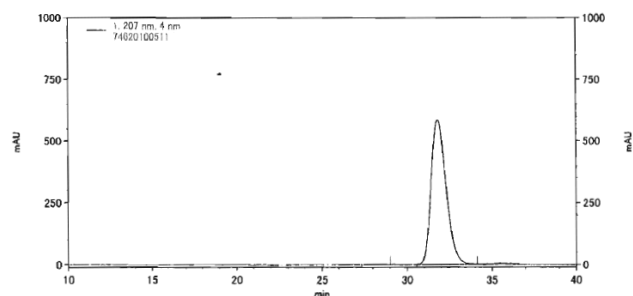
名前	保持時間	面積	面積%	ピークコード
	28.09	75461105	49.953	MM
	32.69	75604229	50.047	MM
トータル		151065334	100.000	



面積%レポート

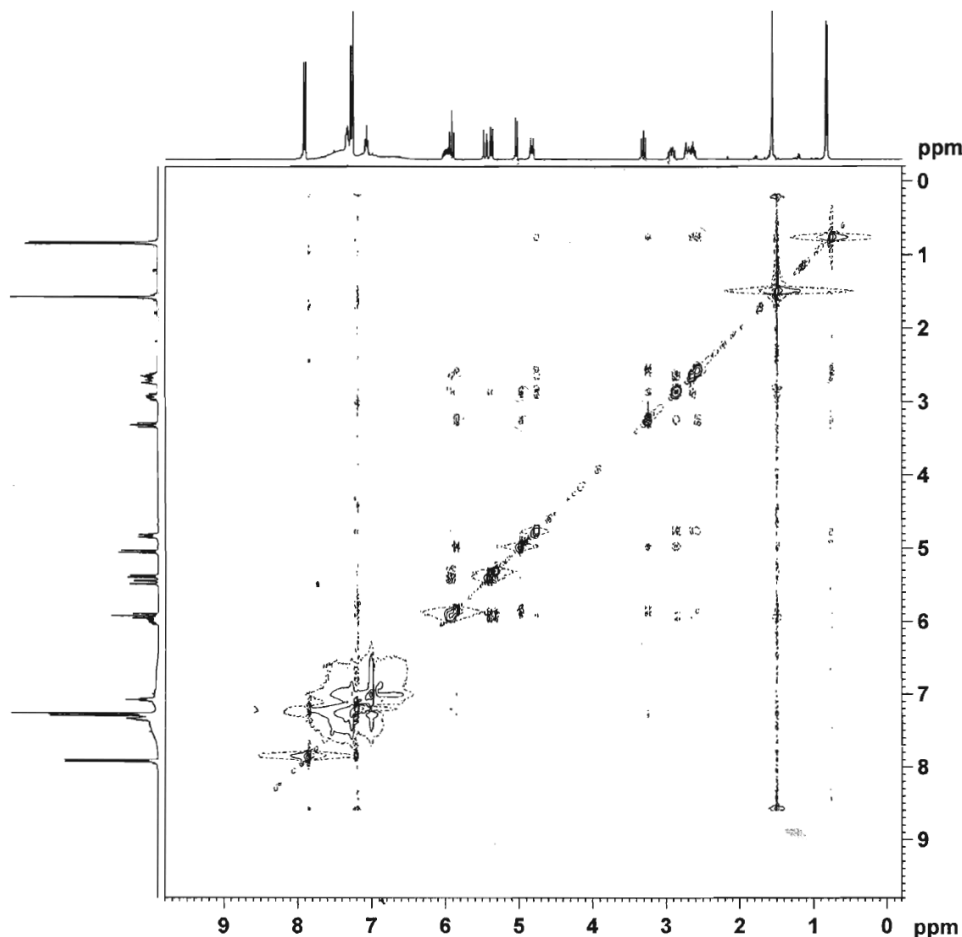
ページ 1/1

データファイル名: \\Server\Enterprise\Projects\Default\Data\2010-05-29-skmt allyl normal
 chi-AD-H-80 vs 1 ml
 メソッドファイル名: \\Server\Enterprise\Projects\Default\Method\80vs1 ml.met
 ユーザー名: System
 分析日時: 2010/05/31 20:37:21
 印刷日時: 2010/05/31 21:28:44



1: 207 nm, 4

名前	保持時間	面積	面積%	ピークコード
	27.93	328751	0.229	MM
	31.80	143455303	99.771	MM
トータル		143784054	100.000	



Current Data Parameters
NAME May25-2010-hayashi
EXPNO 352
PROCNO 1

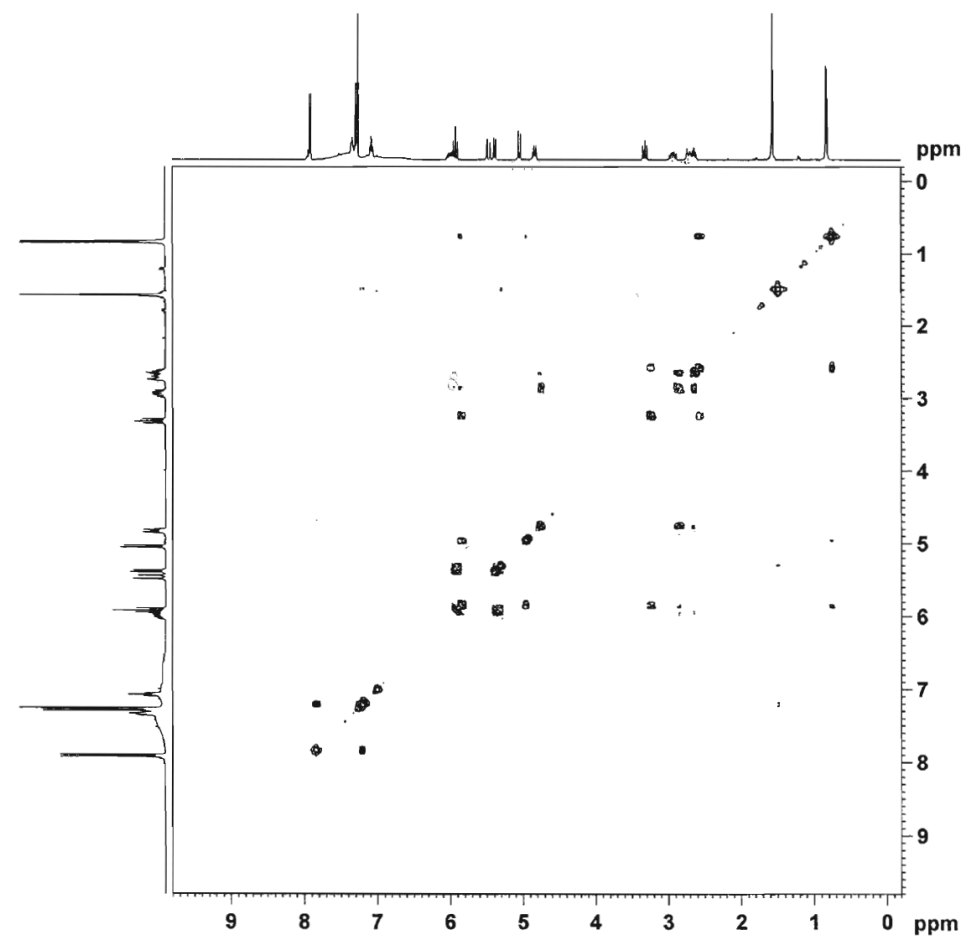
F2 - Acquisition Parameters
Date_ 20100525
Time 22.26
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG noesyph
TD 2048
SOLVENT CDCl3
NS 16
DS 4
SWH 3378.378 Hz
FIDRES 1.649599 Hz
AQ 0.3031540 sec
RG 228
DW 148.000 usec
DE 6.00 usec
TE 295.9 K
d0 0.00013272 sec
D1 1.94757104 sec
D8 0.30000001 sec
IN0 0.00029600 sec
STICNT 128

***** CHANNEL f1 *****
NUC1 1H
P1 12.00 usec
PL1 -4.00 dB
SFO1 400.1817897 MHz

F1 - Acquisition parameters
ND0 1
TD 256
SFO1 400.1818 MHz
FIDRES 13.195791 Hz
SW 8.442 ppm
FMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 400.1800348 MHz
WDW QSI
SSB 2
LB 0.00 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 States-TPPI
SF 400.1800348 MHz
WDW QSI
SSB 2
LB 0.00 Hz
GB 0



Current Data Parameters
NAME May25-2010-hayashi
EXPNO 351
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100525
Time 22.21
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG cosyppg
TD 2048
SOLVENT CDCl3
NS 1
DS 8
SWH 3378.378 Hz
FIDRES 1.649599 Hz
AQ 0.3031540 sec
RG 203
DW 148.000 usec
DE 6.00 usec
TE 295.8 K
d0 0.00000300 sec
D1 1.37548101 sec
D15 0.00000400 sec
IN0 0.00029600 sec

***** CHANNEL f1 *****
NUC1 1H
P0 12.00 usec
P1 12.00 usec
PL1 -4.00 dB
SFO1 400.1817897 MHz

***** GRADIENT CHANNEL *****
GPRAM1 SINE.100
GPRAM2 SINE.100
GPZ1 10.00 %
GPZ2 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
ND0 1
TD 128
SFO1 400.1818 MHz
FIDRES 26.393581 Hz
SW 8.442 ppm
FMODE QF

F2 - Processing parameters
SI 1024
SF 400.1800348 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 400.1800348 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

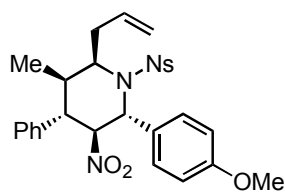
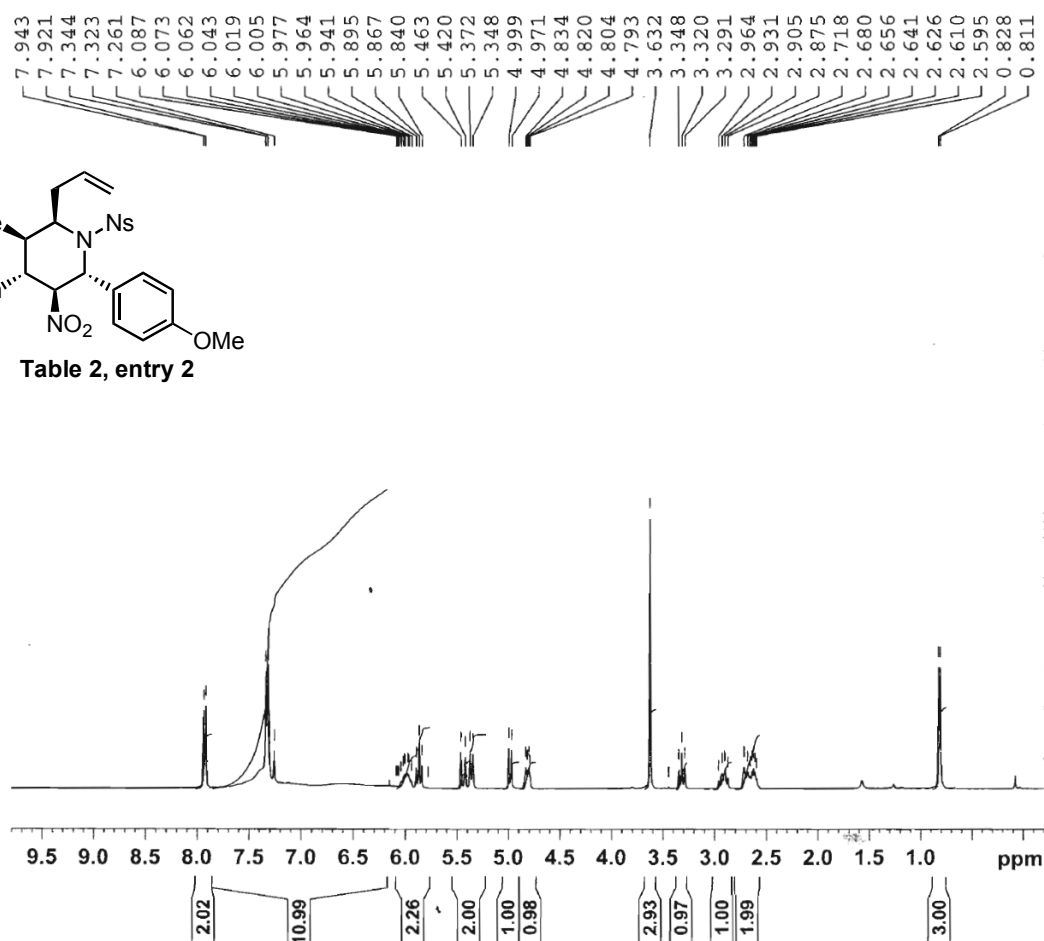


Table 2, entry 2



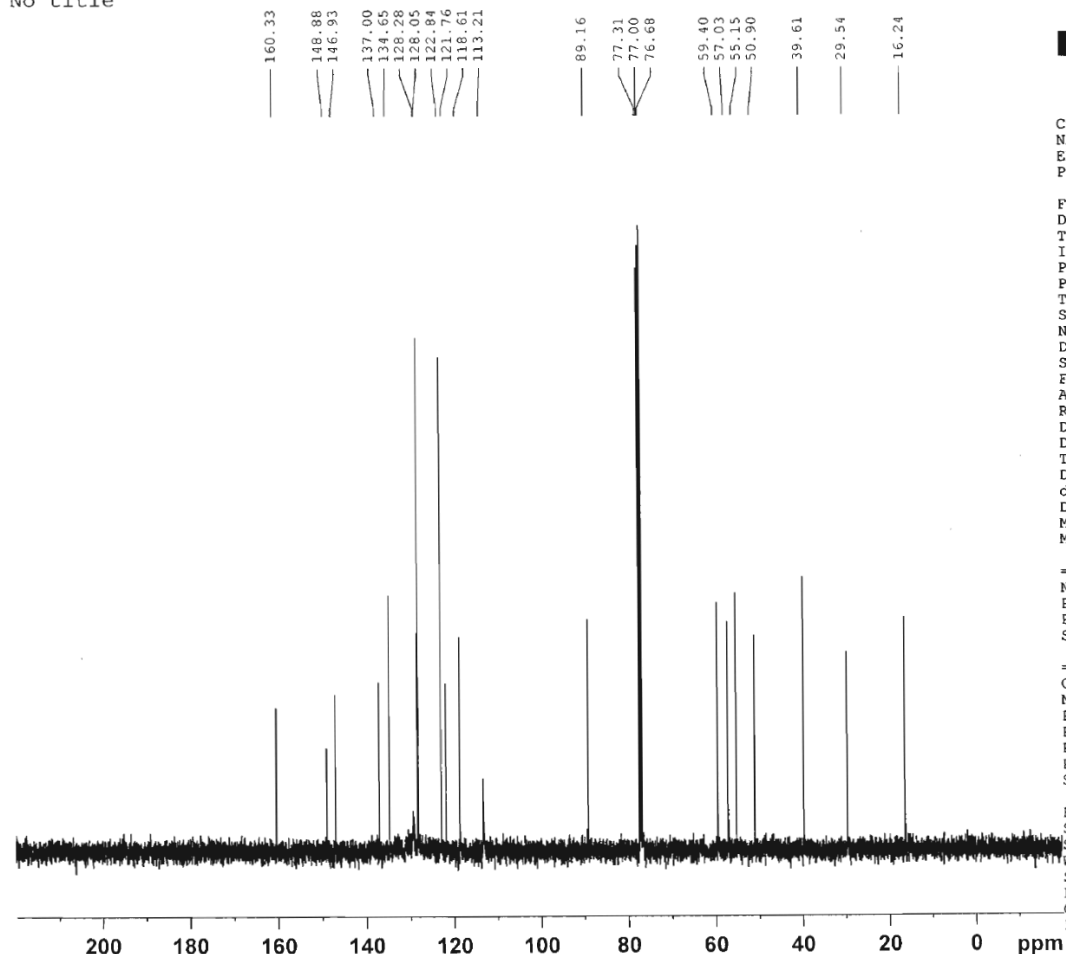
Current Data Parameters
NAME May19-2010
EXPNO 53
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100519
Time 16.08
INSTRUM dpx400
PROBHD 5 mm QNP 1H/29
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 6
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 161.3
DW 60.800 usec
DE 6.00 usec
TE 303.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.90 usec
PL1 3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 16384
SF 400.1300087 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

No title



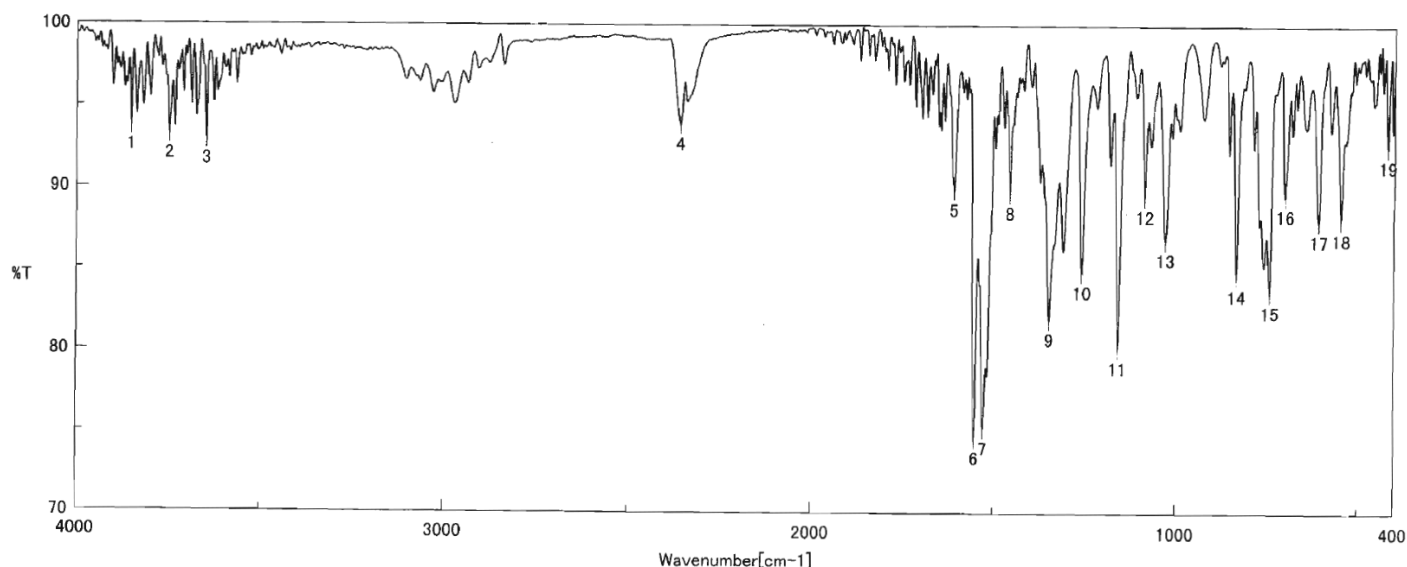
Current Data Parameters
NAME May19-2010
EXPNO 64
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100519
Time 22.06
INSTRUM dpx400
PROBHD 5 mm QNP 1H/29
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 101
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289652 sec
RG 23170.5
DW 15.700 usec
DE 6.00 usec
TE 303.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.30 usec
PL1 3.00 dB
SFO1 100.6254358 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 3.00 dB
PL12 22.00 dB
PL13 22.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127747 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



積算回数 16
 ゼロフィリング ON
 ゲイン 2
 日時 110/05/27 17:10
 測定者
 ファイル名 2010.05.27-allyl-imineOMe. JWS
 サンプル名 background
 コメント

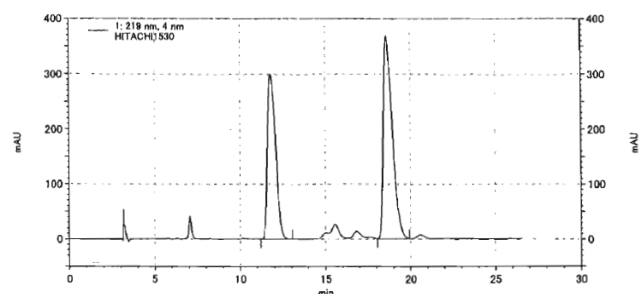
分解 4 cm⁻¹
 アポダイゼーション Cosine
 スキャンスピード 2 mm/sec

1: 3853.08, 93.7394	2: 3749.90, 93.2463	3: 3648.66, 92.9315	4: 2360.44, 93.8917
5: 1610.27, 89.8905	6: 1553.38, 74.6261	7: 1529.27, 75.2592	8: 1456.96, 89.7022
9: 1348.00, 81.9604	10: 1259.29, 84.8547	11: 1159.97, 80.1854	12: 1087.66, 89.4953
13: 1029.80, 86.8608	14: 834.06, 84.6133	15: 742.46, 83.6215	16: 701.00, 89.5553
17: 608.43, 88.0103	18: 546.72, 88.1051	19: 419.44, 92.5722	

面積%レポート

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データファイル名: \\KServer\Enterprise\Projects\Default\Data\2010.05.10 skmt allyl imine
 OMe racem AD-H 20 vs 1 1ml.dat
 メソッドファイル名: \\KServer\Enterprise\Projects\Default\Method\20vs1 1ml.met
 ユーザー名: System
 分析日時: 2010/05/10 15:51:51
 印刷日時: 2010/05/10 16:20:27

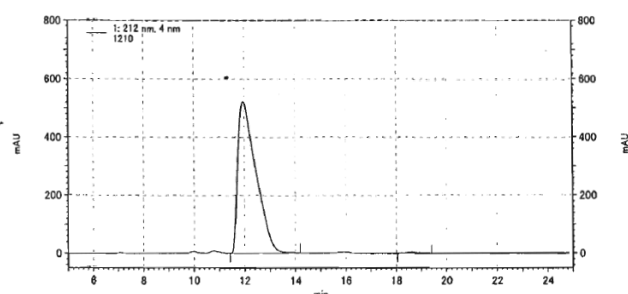


1: 219 nm, 4 nm結果	保持時間	面積	面積%	ピーク番号
Pk #	名前			
1		11.77	40218837	42.528
2		18.59	54351102	57.472
トータル			94569939	100.000

面積%レポート

ページ 1/1

データファイル名: \\KServer\Enterprise\Projects\Default\Data\2010-05-19 skmt allyl imine
 OMe rac 20vs1 AD-H 1ml 2nd try.dat
 メソッドファイル名: \\KServer\Enterprise\Projects\Default\Method\20vs1 1ml.met
 ユーザー名: System
 分析日時: 2010/05/19 22:40:35
 印刷日時: 2010/05/19 23:15:14



1: 212 nm, 4 nm結果	保持時間	面積	面積%	ピーク番号
Pk #	名前			
1		11.96	104100716	99.414
2		18.61	613479	0.586
トータル			104714195	100.000

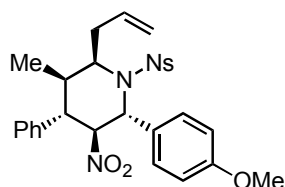


Table 2, entry 2

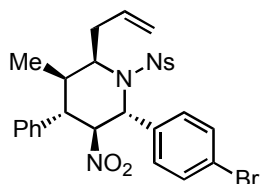
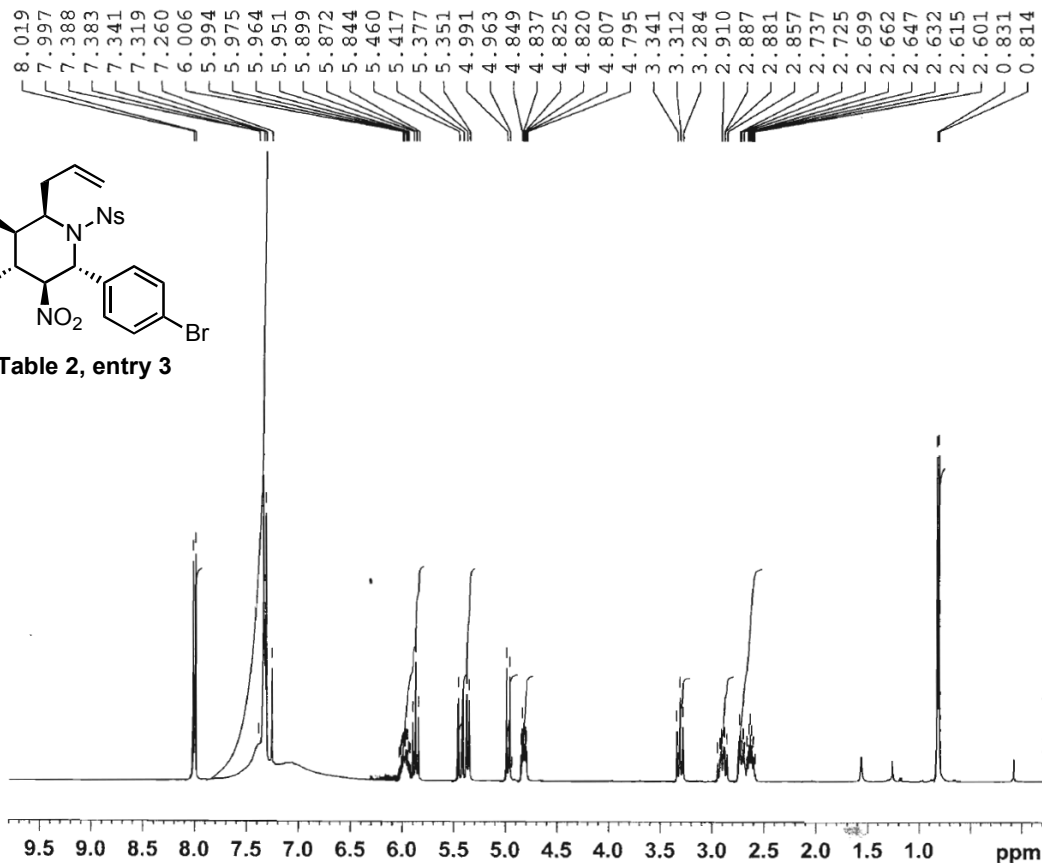


Table 2, entry 3



Current Data Parameters
NAME May19-2010
EXPNO 50
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100519
Time 15.56
INSTRUM dpx400
PROBHD 5 mm QNP 1H/29
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 5
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 1448.2
DW 60.800 usec
DE 6.00 usec
TE 303.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.90 usec
PL1 3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 16384
SF 400.1300092 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



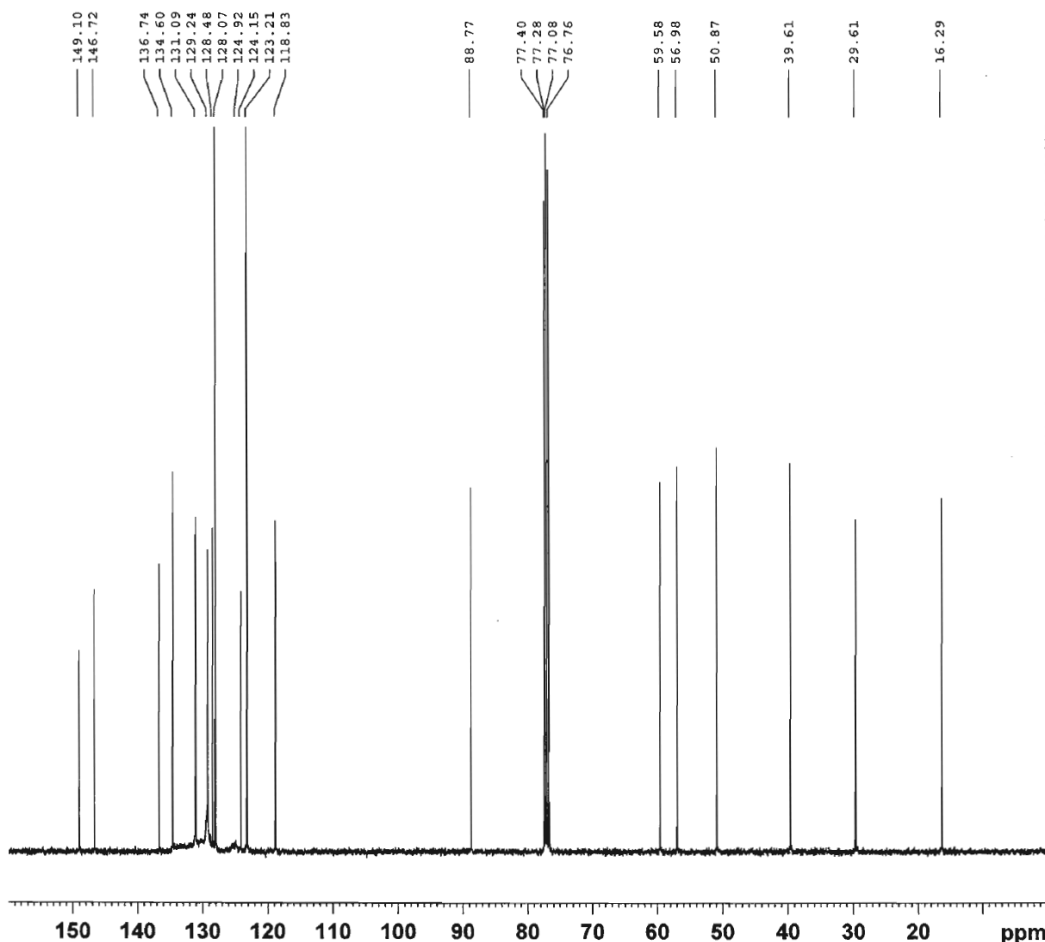
Current Data Parameters
NAME May19-2010-hayashi
EXPNO 80
PROCNO 1

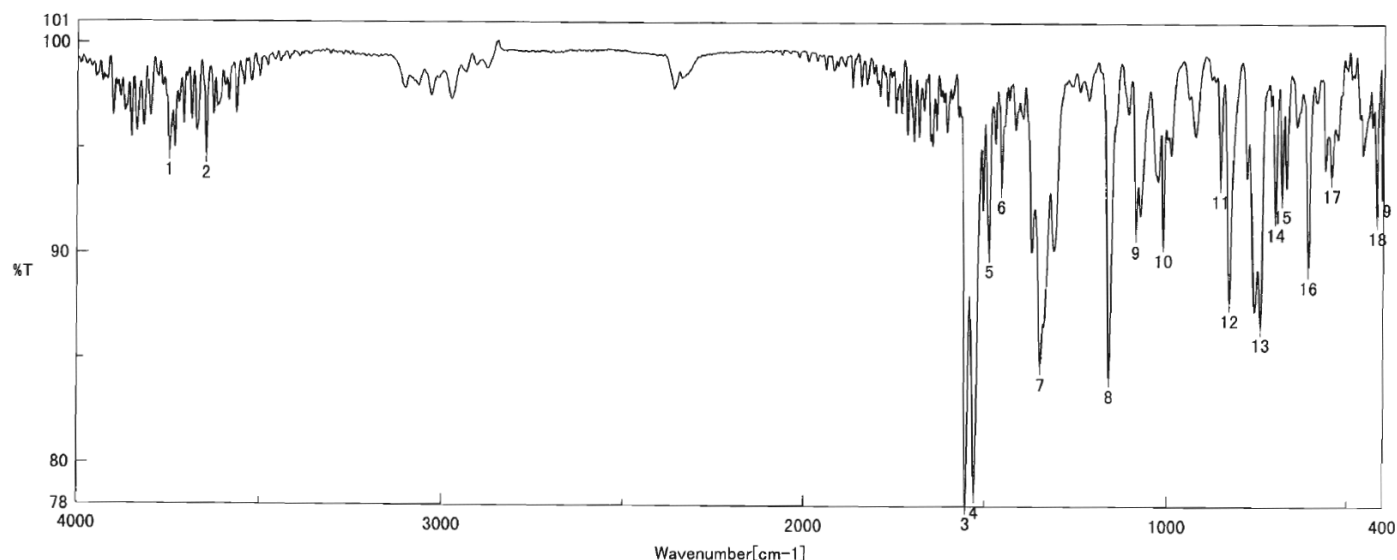
F2 - Acquisition Parameters
Date_ 20100520
Time 0.21
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 50.8
DW 20.800 usec
DE 6.00 usec
TE 298.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 7.20 usec
PL1 -3.50 dB
SFO1 100.6354036 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -4.00 dB
PL12 14.00 dB
PL13 14.00 dB
SFO2 400.1816007 MHz

F2 - Processing parameters
SI 32768
SF 100.6253410 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





積算回数 16
 ゼロフィリング ON
 ゲイン 2
 日時 110/05/27 10:59
 測定者
 ファイル名 2010.05.27-allyl-imineBr. JWS
 サンプル名 background
 コメント

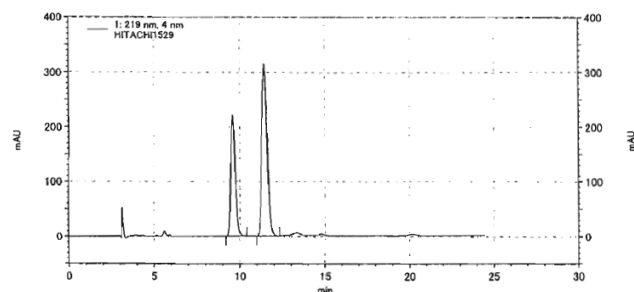
分解 4 cm-1
 アポダイゼーション Cosine
 スキャンスピード 2 nm/sec

1: 3749.90, 94.8610	2: 3648.66, 94.7281	3: 1553.38, 78.1020	4: 1530.24, 78.6454
5: 1489.74, 90.1372	6: 1456.96, 93.2077	7: 1348.96, 84.7673	8: 1160.94, 84.2000
9: 1087.66, 91.0814	10: 1012.45, 90.6651	11: 854.31, 93.4744	12: 829.24, 87.7931
13: 742.46, 86.6691	14: 701.96, 91.9087	15: 683.64, 92.7759	16: 610.36, 89.3769
17: 544.79, 93.7563	18: 418.48, 91.7539	19: 404.01, 93.0943	

面積%レポート

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データファイル名: \\Server\Enterprise\Projects\Default\Data\2010.05.10 skmt allyl imine
 Br racem AD-H 20 vs 1 lml.dat
 メソッドファイル名: \\Server\Enterprise\Projects\Default\Method\20vs1 lml.met
 ユーザー名: System
 分析日時: 2010/05/10 14:06:09
 印刷日時: 2010/05/10 14:33:58

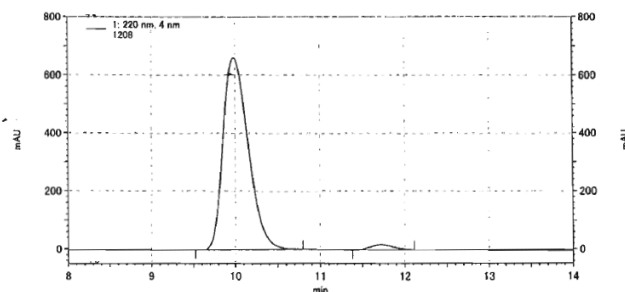


1: 219 nm, 4 nm結果	名前	保持時間	面積	面積%	ピークタイプ
PK #					
1		9.57	15756675	37.291	MM
2		11.41	26496239	62.709	MM
	トータル		42252914	100.000	

面積%レポート

ページ 1/1

データファイル名: \\Server\Enterprise\Projects\Default\Data\2010-05-19 skmt allyl imine
 Br rac 20vs1 AD-H 1ml.dat
 メソッドファイル名: \\Server\Enterprise\Projects\Default\Method\20vs1 lml.met
 ユーザー名: System
 分析日時: 2010/05/19 21:02:37
 印刷日時: 2010/05/19 21:21:42



1: 220 nm, 4 nm結果	名前	保持時間	面積	面積%	ピークタイプ
PK #					
1		9.98	55055385	97.571	MM
2		11.71	1370690	2.429	MM
	トータル		56426075	100.000	

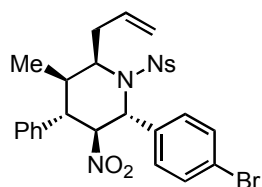
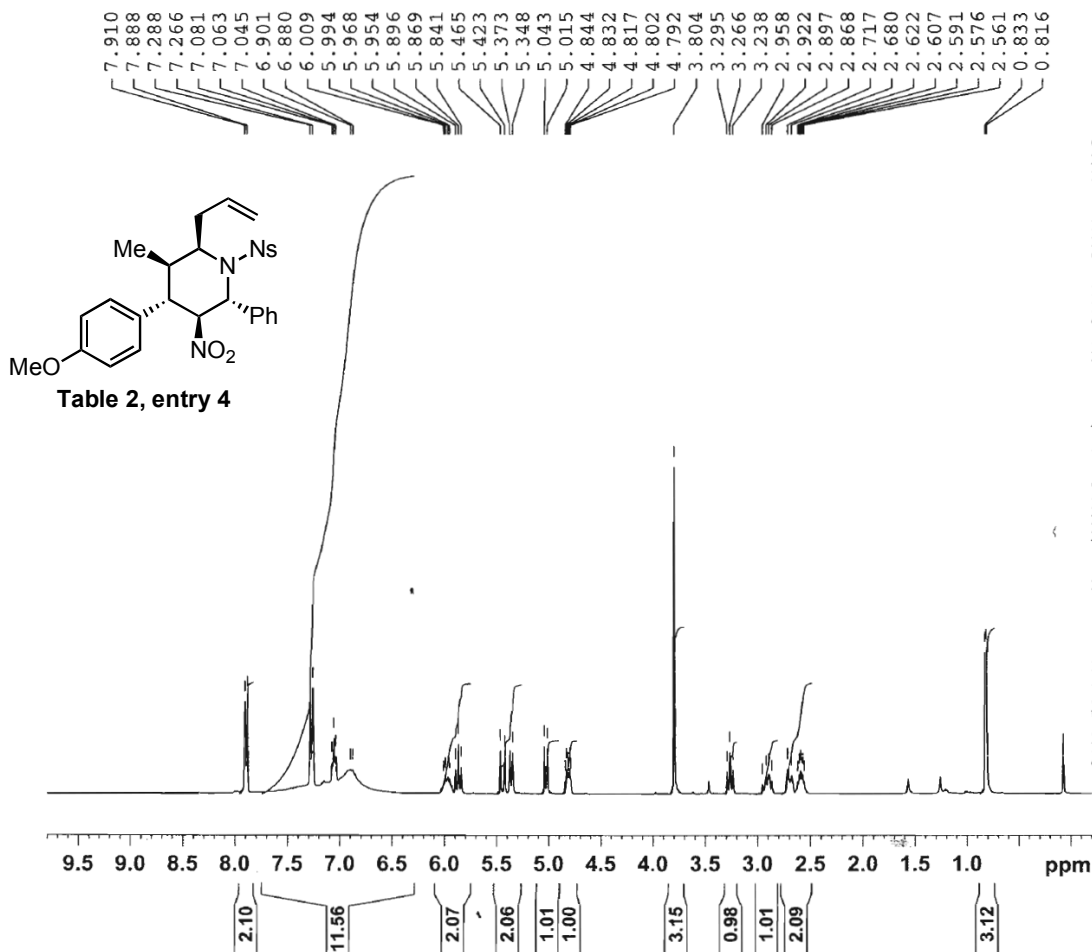


Table 2, entry 3



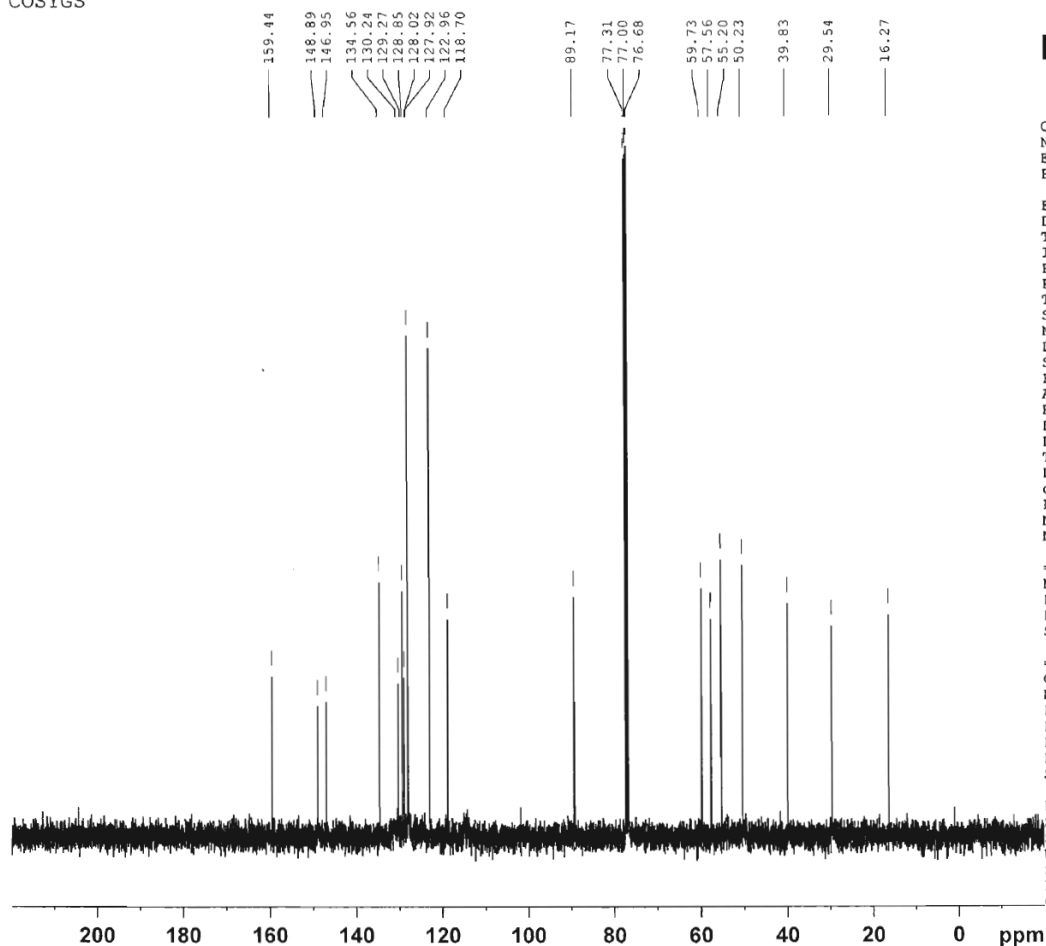
Current Data Parameters
NAME May22-2010
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100522
Time 0.23
INSTRUM dpx400
PROBHD 5 mm QNP 1H/29
PULPROG zg30
TD 32768
SOLVENT CDCl₃
NS 6
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 1625.5
DW 60.800 usec
DE 6.00 usec
TE 303.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.90 usec
PL1 3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 16384
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

COSYGS



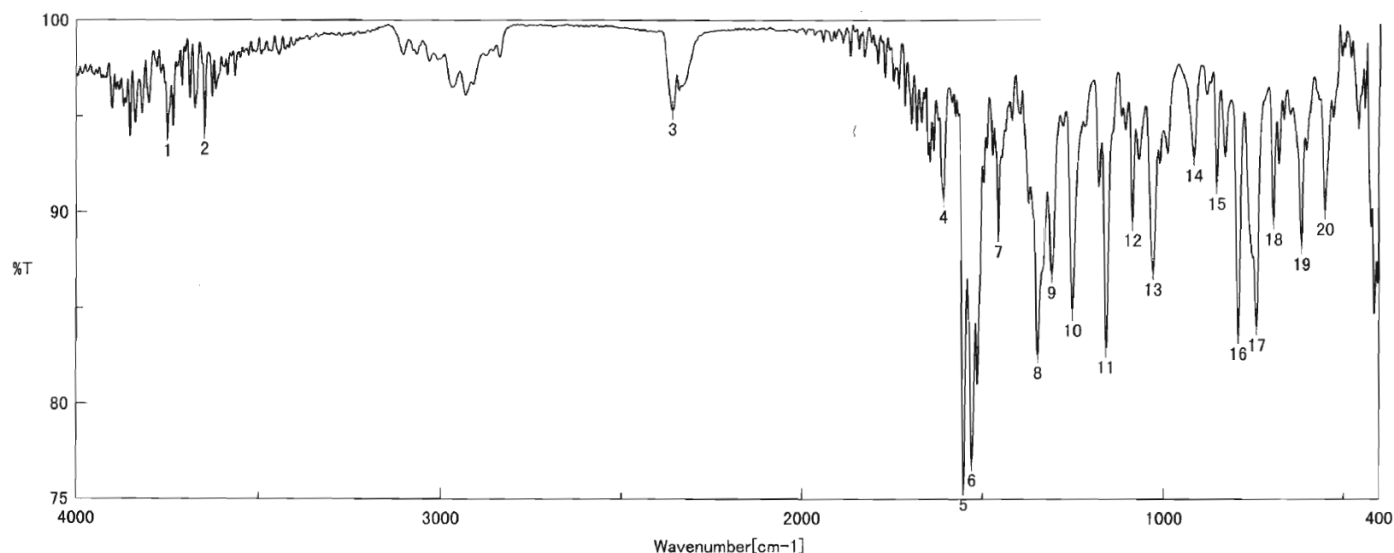
Current Data Parameters
NAME May22-2010
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100522
Time 0.29
INSTRUM dpx400
PROBHD 5 mm QNP 1H/29
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 100
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289652 sec
RG 32768
DW 15.700 usec
DE 6.00 usec
TE 303.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.30 usec
PL1 3.00 dB
SFO1 100.6254358 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 3.00 dB
PL12 22.00 dB
PL13 22.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127737 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00



積算回数 16
 ゼロフィリング ON
 ゲイン 2
 日時 110/05/27 17:25
 測定者
 ファイル名 2010.05.27-allyl-styOMe. JWS
 サンプル名 background
 コメント

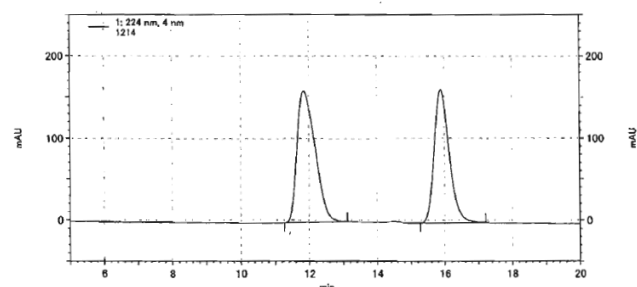
分解 4 cm-1
 アポダイゼーション Cosine
 スキャンスピード 2 mm/sec

1: 3749.90, 94.1972	2: 3648.66, 94.3187	3: 2360.44, 95.3286	4: 1609.31, 90.7759
5: 1552.42, 75.7095	6: 1530.24, 77.0027	7: 1456.96, 88.9749	8: 1348.00, 82.6352
9: 1309.43, 86.8220	10: 1252.54, 84.8333	11: 1159.97, 82.9342	12: 1087.66, 89.5625
13: 1030.77, 86.9818	14: 917.95, 92.9194	15: 854.31, 91.4462	16: 793.56, 83.6304
17: 742.46, 84.0869	18: 696.18, 89.6073	19: 618.07, 88.3015	20: 552.51, 90.1462

面積%レポート

ページ 1/1

データファイル名: \\Server\Enterprise\Projects\Default\Data\2010-05-21 skat allyl sty OMe
 rac 20vs1 AD-H 1ml.dat
 プリントファイル名: \\Server\Enterprise\Projects\Default\Method\20vs1 1ml.met
 ユーザー名: System
 分析日時: 2010/05/21 14:06:03
 印刷日時: 2010/05/21 14:37:34

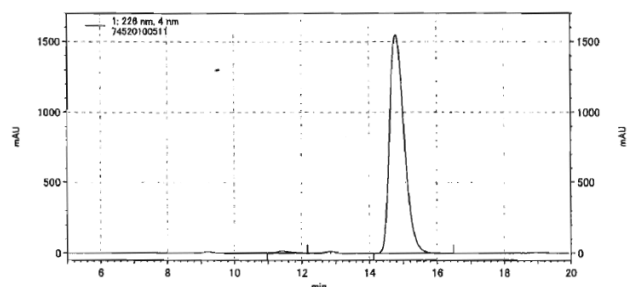


1: 224 nm, 4 nm結果	保持時間	面積	面積%	ピークコード
PK #	名前			
1		11.84	23549631	53.999
2		15.89	20061343	46.001
	トータル		43610974	100.000

面積%レポート

ページ 1/1

データファイル名: \\Server\Enterprise\Projects\Default\Data\2010.05.29-skatallyl sty OMe
 ch1-AD-H-20 vs 1-1ml
 プリントファイル名: \\Server\Enterprise\Projects\Default\Method\20vs1 1ml.met
 ユーザー名: System
 分析日時: 2010/05/31 18:05:33
 印刷日時: 2010/05/31 19:14:02



1: 226 nm, 4 nm結果	保持時間	面積	面積%	ピークコード
PK #	名前			
1		11.42	1578893	0.843
2		14.79	185763769	99.157
	トータル		187342662	100.000

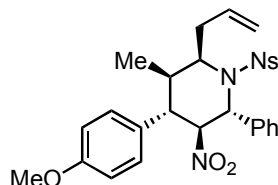


Table 2, entry 4

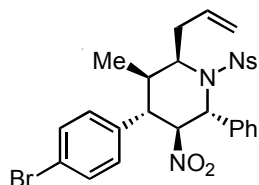
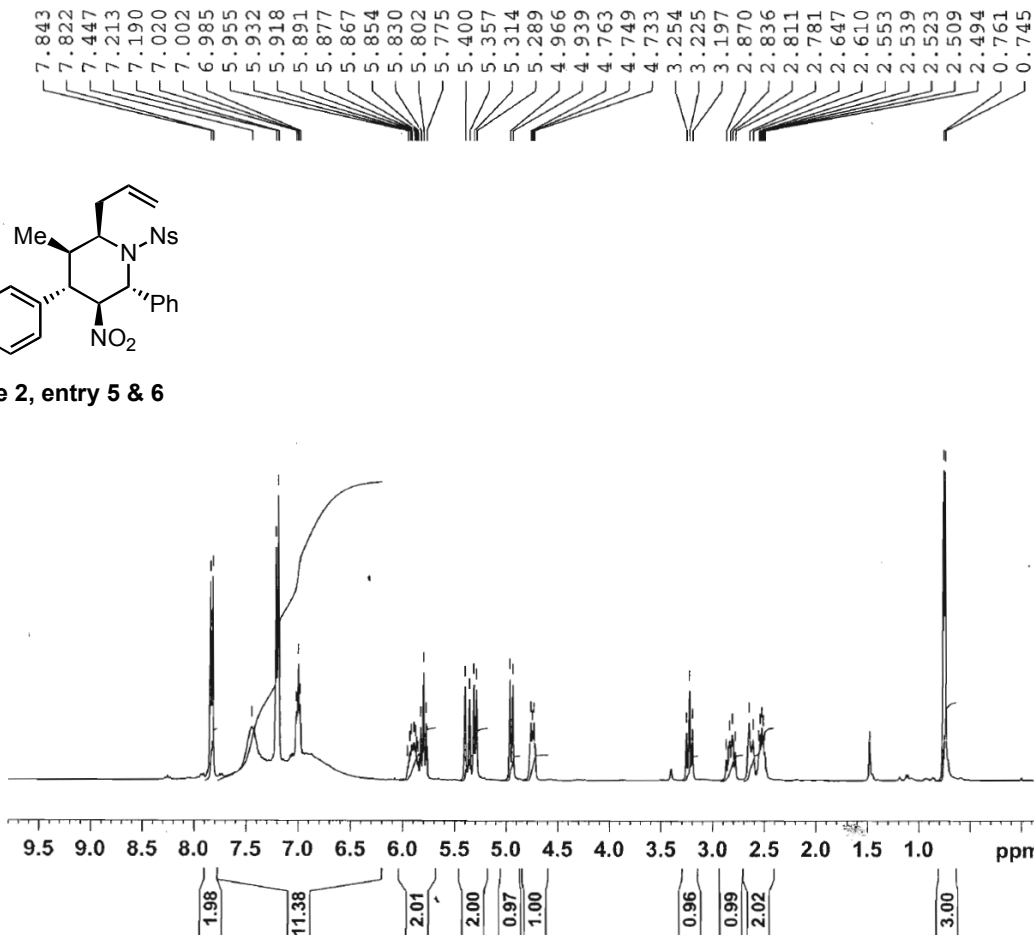


Table 2, entry 5 & 6



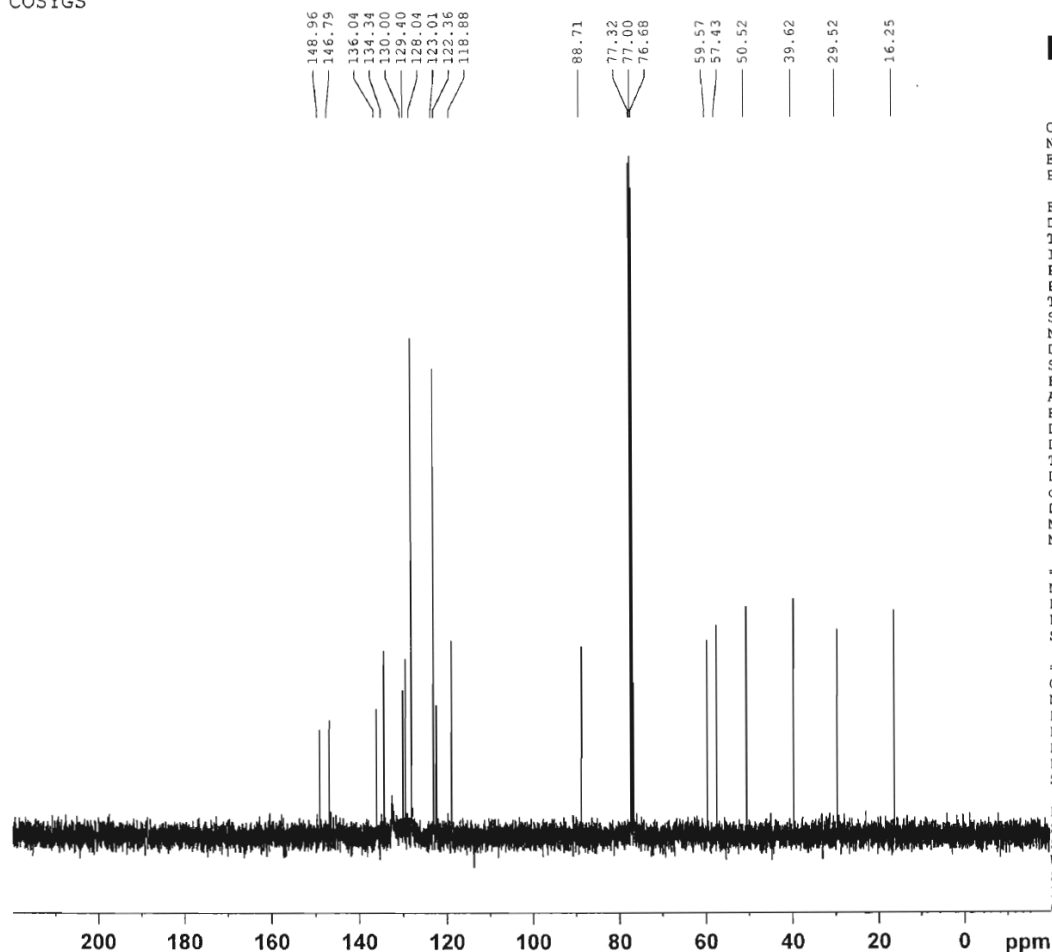
Current Data Parameters
NAME May22-2010
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100522
Time_ 0.06
INSTRUM dpx400
PROBHD 5 mm QNP 1H/29
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 5
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 2580.3
DW 60.800 usec
DE 6.00 usec
TE 303.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.70 usec
PL1 4.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 16384
SF 400.1300377 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

COSYGS



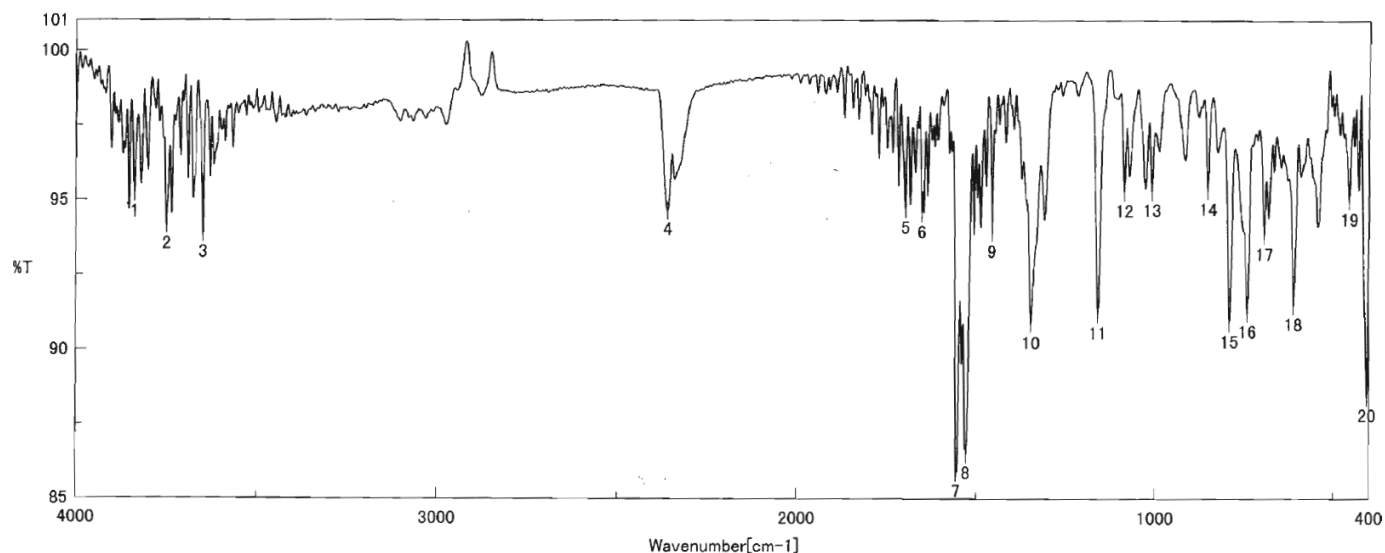
Current Data Parameters
NAME May22-2010
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100522
Time_ 0.14
INSTRUM dpx400
PROBHD 5 mm QNP 1H/29
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 129
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289652 sec
RG 13004
DW 15.700 usec
DE 6.00 usec
TE 303.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.30 usec
PL1 3.00 dB
SFO1 100.6254358 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 3.00 dB
PL12 22.00 dB
PL13 22.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127718 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00



積分回数 16
 ゼロフィリング ON
 ゲイン 2
 日時 110/05/27 17:17
 測定者
 ファイル名 2010.05.27-allyl-styBr. JWS
 サンプル名 background
 コメント

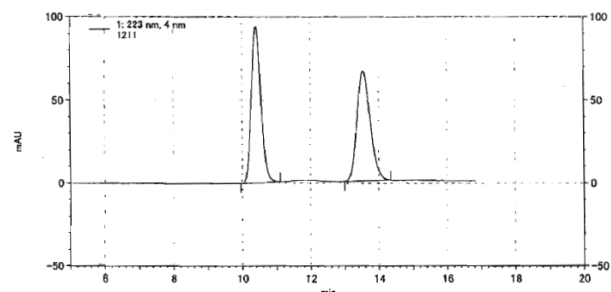
分解 4 cm⁻¹
 アポダイゼーション Cosine
 スキャンスピード 2 mm/sec

1: 3838.61, 95.2464	2: 3749.90, 94.1900	3: 3648.66, 93.9087	4: 2361.41, 94.6747
5: 1698.02, 94.7411	6: 1652.70, 94.5939	7: 1556.27, 85.9142	8: 1529.27, 86.5276
9: 1456.96, 93.9444	10: 1348.00, 90.8893	11: 1159.97, 91.2120	12: 1087.66, 95.2967
13: 1010.52, 95.3166	14: 854.31, 95.3512	15: 792.60, 90.9266	16: 742.46, 91.2651
17: 696.18, 93.8525	18: 612.29, 91.5110	19: 457.05, 95.0180	20: 405.94, 88.4548

面積%レポート

ページ 1/1

データファイル名: \\Server\Enterprise\Projects\Default\Data\2010-05-19 skmt allyl stylen
 Br rac 20vs1 AD-H 1ml.dat
 メソッドファイル名: \\Server\Enterprise\Projects\Default\Method\20vs1 1ml.met
 ユーザー名: System
 分析日時: 2010/05/20 13:26:43
 印刷日時: 2010/05/20 13:48:13

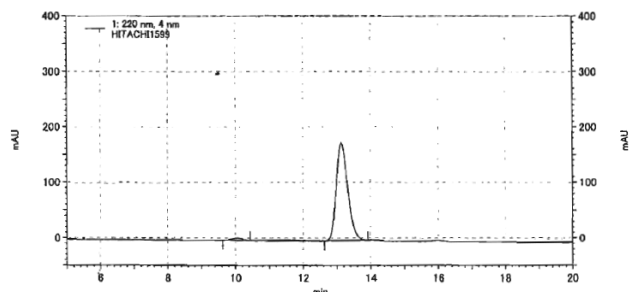


1: 223 nm, 4 nm結果	PK #	名前	保持時間	面積	面積%	ピークタイプ
	1		10.40	7218084	49.875	MM
	2		13.53	7254157	50.125	MM
				14472241	100.000	

面積%レポート

ページ 1/1

データファイル名: \\Server\Enterprise\Projects\Default\Data\2010-05-22 skmt chi allyl sty
 Br AD-H 20 vs 1. 1 ml.dat
 メソッドファイル名: \\Server\Enterprise\Projects\Default\Method\20vs1 1ml.met
 ユーザー名: System
 分析日時: 2010/05/22 15:51:01
 印刷日時: 2010/05/22 16:25:45



1: 220 nm, 4 nm結果	PK #	名前	保持時間	面積	面積%	ピークタイプ
	1		10.05	403014	2.359	MM
	2		13.13	16681730	97.641	MM
				17084744	100.000	

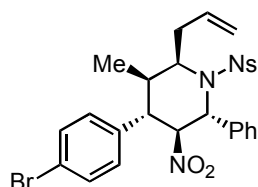


Table 2, entry 5 & 6

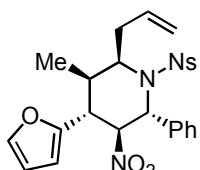
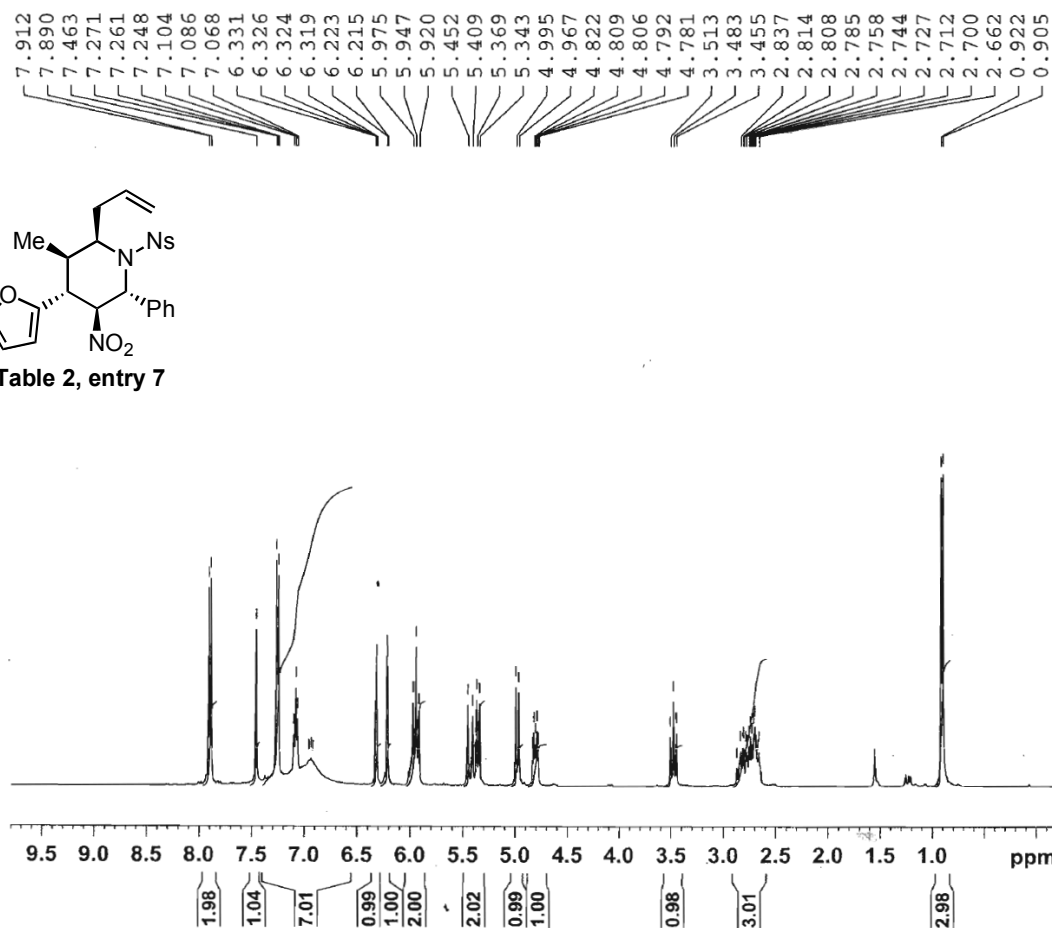


Table 2, entry 7



Current Data Parameters
NAME May22-2010
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100522
Time_ 0.31
INSTRUM dpx400
PROBHD 5 mm QNP 1H/29
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 5
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 2298.8
DW 60.800 usec
DE 6.00 usec
TE 303.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.90 usec
PL1 3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 16384
SF 400.1300090 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



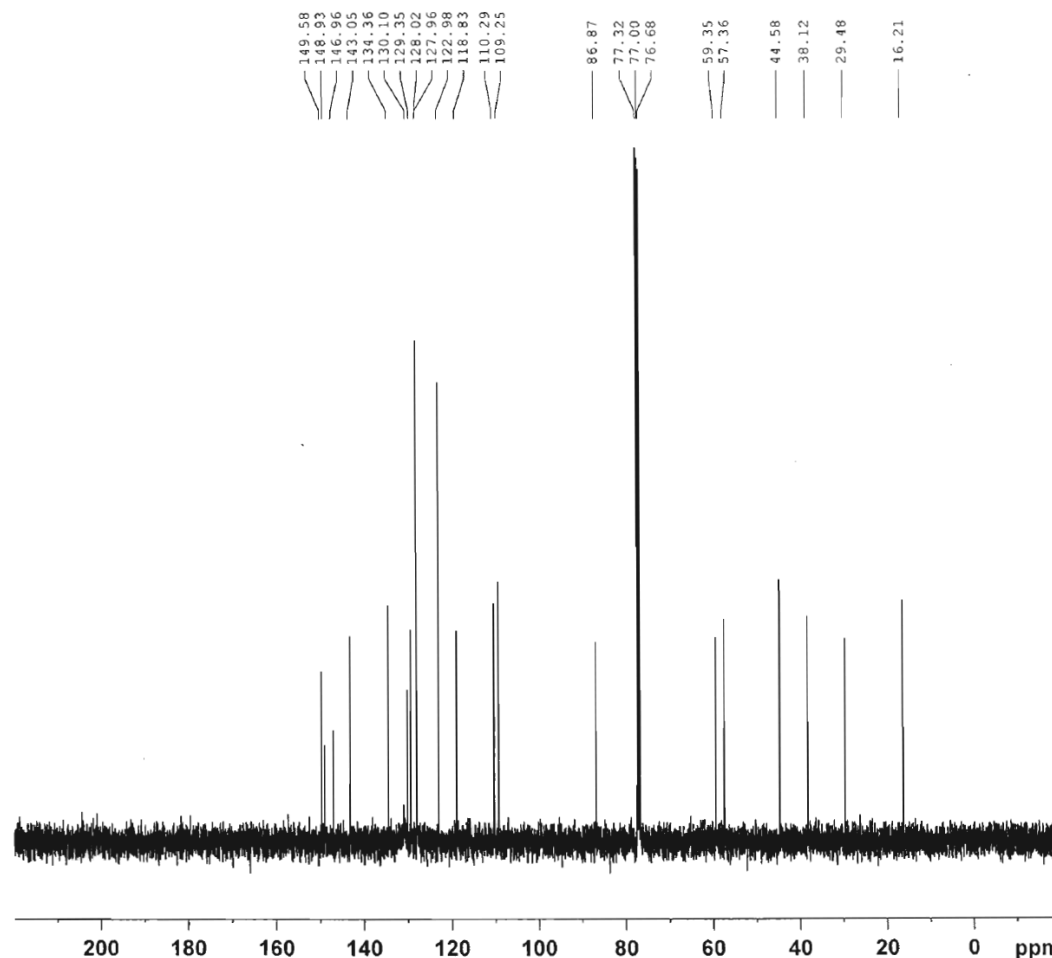
Current Data Parameters
NAME May22-2010
EXPNO 15
PROCNO 1

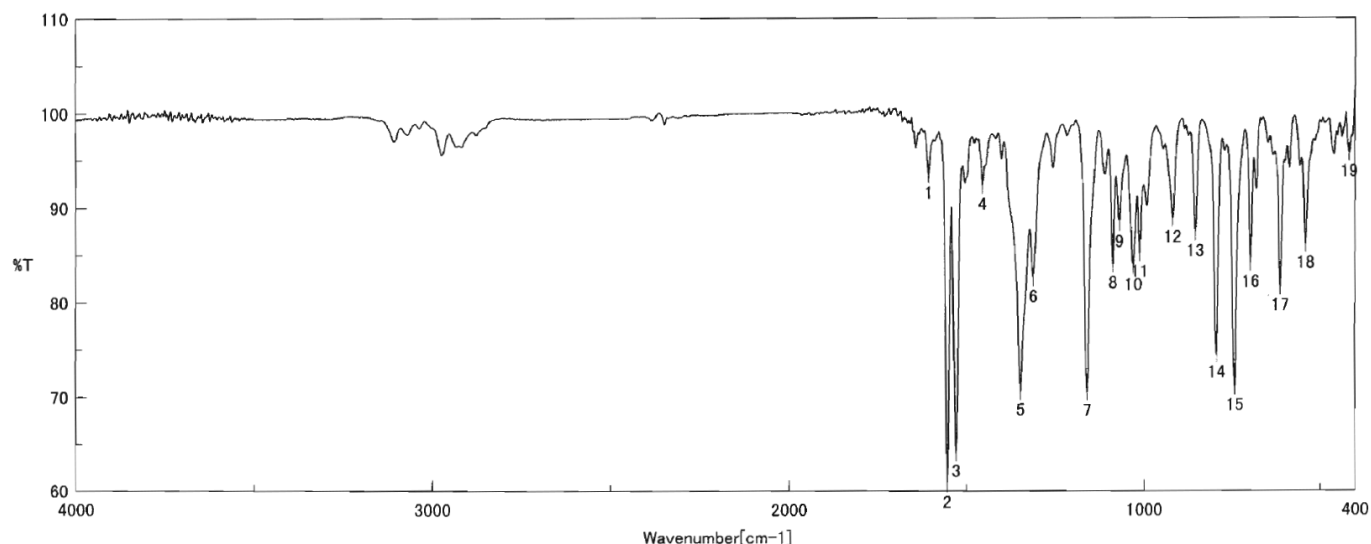
F2 - Acquisition Parameters
Date_ 20100522
Time_ 0.38
INSTRUM dpx400
PROBHD 5 mm QNP 1H/29
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 101
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289652 sec
RG 46341
DW 15.700 usec
DE 6.00 usec
TE 303.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.30 usec
PL1 3.00 dB
SFO1 100.6254358 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 3.00 dB
PL12 22.00 dB
PL13 22.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127718 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00





積算回数 16
 ゼロフィリング ON
 ゲイン 2
 日時 110/06/14 18:33
 測定者
 ファイル名 Memory#3
 サンプル名 background
 コメント

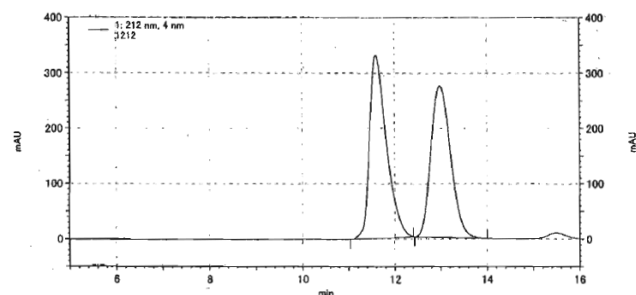
分解 4 cm-1
 アポダイゼーション Cosine
 スキャンスピード 2 mm/sec

1: 1607.38, 93.5819	2: 1555.31, 60.8342	3: 1530.24, 64.1437	4: 1455.99, 92.4149
5: 1348.00, 70.6667	6: 1312.32, 82.6566	7: 1160.94, 70.5792	8: 1087.66, 84.1166
9: 1068.37, 88.4483	10: 1029.80, 83.9016	11: 1011.48, 85.2906	12: 918.91, 88.9383
13: 854.31, 87.4751	14: 793.56, 74.6394	15: 742.46, 71.1517	16: 696.18, 84.2057
17: 612.29, 81.7224	18: 540.93, 86.2149	19: 416.55, 95.8081	

面積%レポート

ページ 1/1

データファイル名: \\Server\Enterprise\Projects\Default\Data\2010-05-19 skmt allyl stylen
 Run rac 20vs1 AD-H 1ml.dat
 メソッドファイル名: \\Server\Enterprise\Projects\Default\Method\20vs1 1ml.met
 ユーザー名: System
 分析日時: 2010/05/20 14:31:18
 印刷日時: 2010/05/20 14:53:09

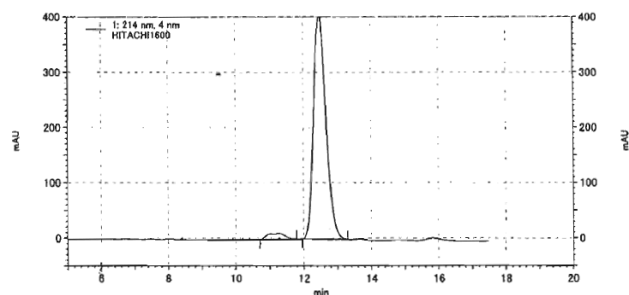


1: 212 nm, 4 nm結果	名前	保持時間	面積	面積%	ピークコメント
PK #					
1		11.59	33401138	50.563	BI
2		12.98	32657777	49.437	BI
			66058915	100.000	

面積%レポート

ページ 1/1

データファイル名: \\Server\Enterprise\Projects\Default\Data\2010-05-22 skmt chi allyl sty
 Run AD-H 20 vs 1. 1 ml.dat
 メソッドファイル名: \\Server\Enterprise\Projects\Default\Method\20vs1 1ml.met
 ユーザー名: System
 分析日時: 2010/05/22 16:53:10
 印刷日時: 2010/05/22 17:14:44



1: 214 nm, 4 nm結果	名前	保持時間	面積	面積%	ピークコメント
PK #					
1		11.25	1568578	3.652	BI
2		12.47	41381501	96.348	BI
			42950079	100.000	

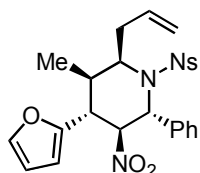


Table 2, entry 7

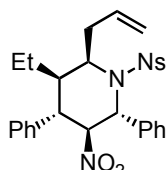
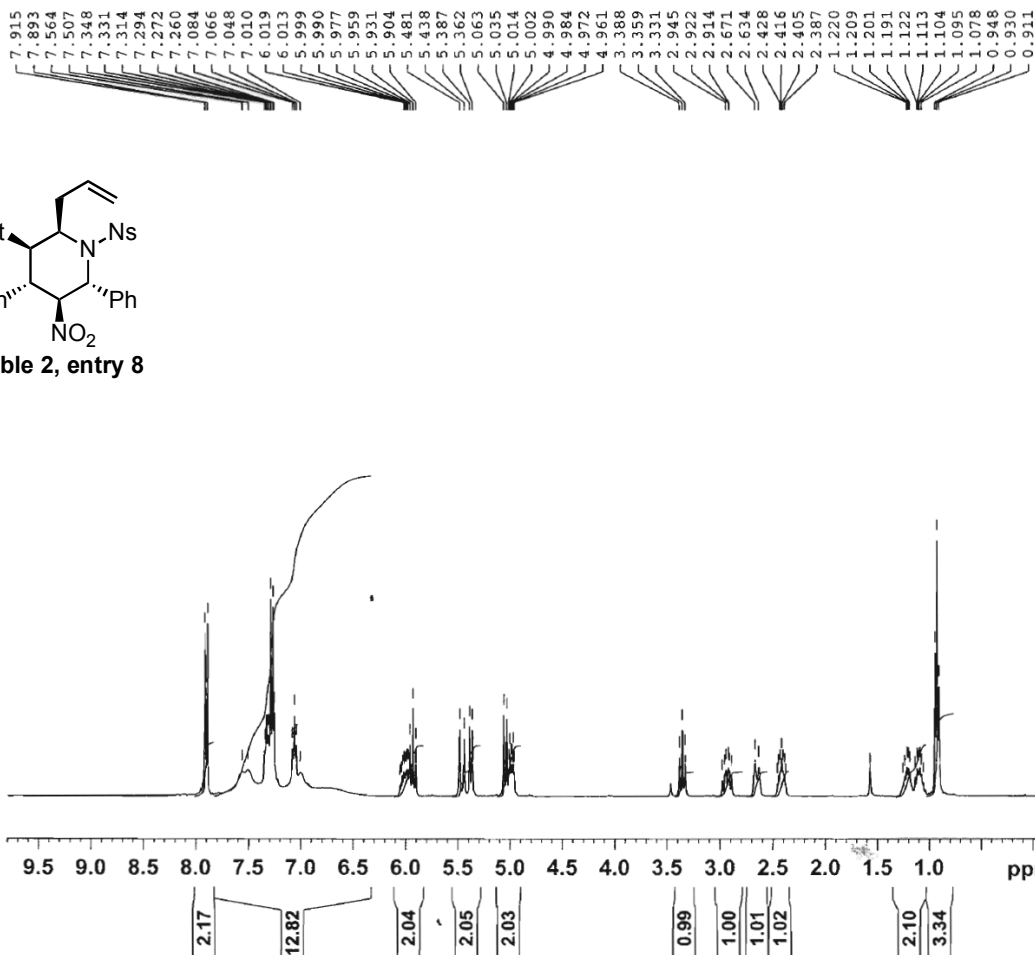


Table 2, entry 8



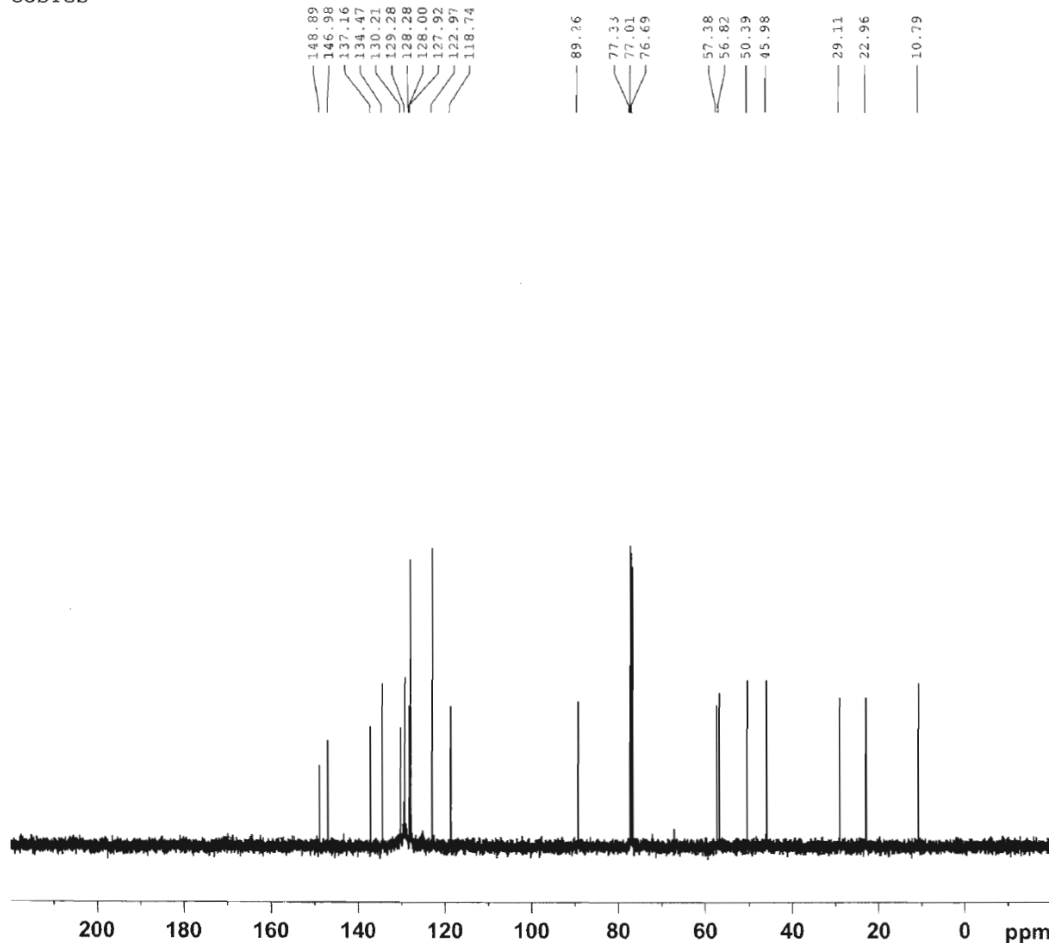
Current Data Parameters
NAME May28-2010
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100528
Time 13.57
INSTRUM dpx400
PROBHD 5 mm QNP 1H/29
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 1149.4
DW 60.400 usec
DE 6.00 usec
TE 303.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.70 usec
PL1 4.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

COSYGS



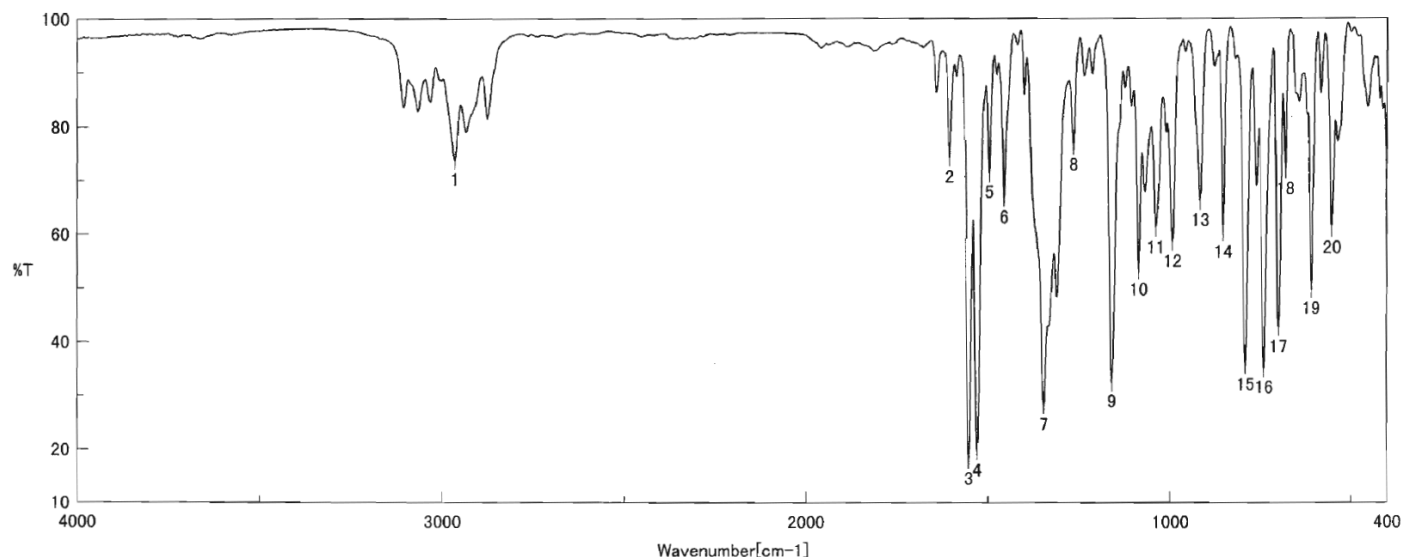
Current Data Parameters
NAME May28-2010
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100528
Time 14.03
INSTRUM dpx400
PROBHD 5 mm QNP 1H/29
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 100
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289652 sec
RG 32768
DW 15.700 usec
DE 6.00 usec
TE 303.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999999 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.30 usec
PL1 3.00 dB
SFO1 100.6254358 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 3.00 dB
PL12 22.00 dB
PL13 22.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127742 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



積分回数 16
 ゼロフィリング ON
 ゲイン 1
 日時 110/06/14 17:52
 測定者
 ファイル名 Memory#7
 サンプル名 background
 コメント

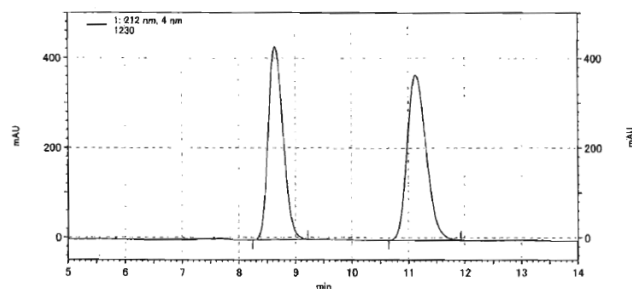
分解 4 cm-1
 アポダイゼーション Cosine
 スキャンスピード 2 mm/sec

1: 2965.98, 73.7347	2: 1606.41, 74.2693	3: 1553.38, 18.1710	4: 1530.24, 19.7254
5: 1497.45, 71.4268	6: 1456.96, 66.8368	7: 1348.00, 28.2683	8: 1266.04, 76.5163
9: 1160.94, 32.5631	10: 1087.66, 53.4146	11: 1040.41, 61.2402	12: 994.12, 58.6781
13: 917.95, 66.2408	14: 854.31, 60.3928	15: 791.64, 35.6850	16: 740.53, 35.1338
17: 700.03, 42.7354	18: 681.71, 72.0539	19: 609.40, 49.8858	20: 552.51, 61.1717

面積%レポート

ページ 1/1

データファイル名: \\Server\Enterprise\Projects\Default\Data\2010-05-24 skmt allyl sokusa
 Et rac AD-H 28vs1 1ml.dat
 メソッドファイル名: \\Server\Enterprise\Projects\Default\Method\20vs1 1ml.met
 ユーザー名: System
 分析日時: 2010/05/25 20:44:44
 印刷日時: 2010/05/25 21:09:07

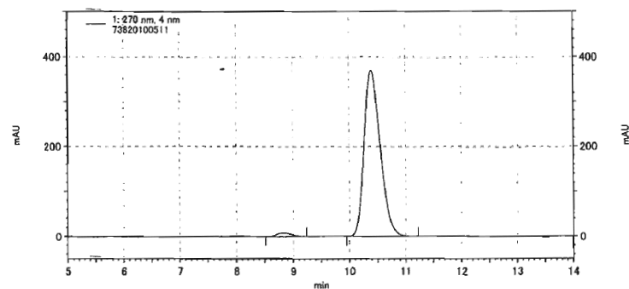


1: 212 nm, 4 nm結果	名前	保持時間	面積	面積%	ピークコード
2		8.65	31416535	47.553	■
		11.13	34649151	52.447	■
			66065686	100.000	

面積%レポート

ページ 1/1

データファイル名: \\Server\Enterprise\Projects\Default\Data\2010.05.29-skmt-allyl sokusa
 Et chi AD-H 10 vs. 1 1ml.dat
 メソッドファイル名: \\Server\Enterprise\Projects\Default\Method\20vs1 1ml.met
 ユーザー名: System
 分析日時: 2010/05/29 15:59:25
 印刷日時: 2010/05/29 16:52:48



1: 270 nm, 4 nm結果	名前	保持時間	面積	面積%	ピークコード
2		8.83	581820	1.942	■
		10.39	29382466	98.058	■
			29964286	100.000	

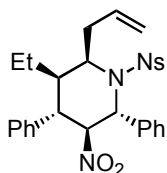


Table 2, entry 8

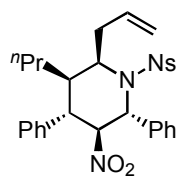
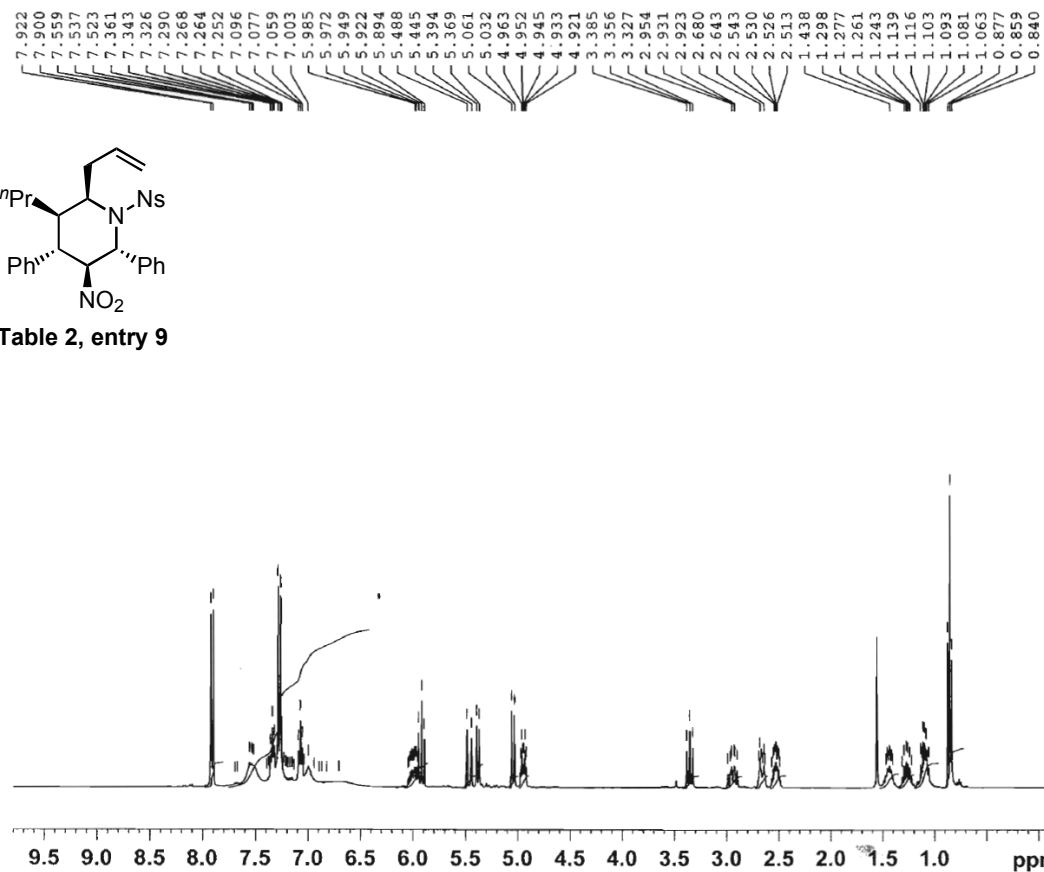


Table 2, entry 9



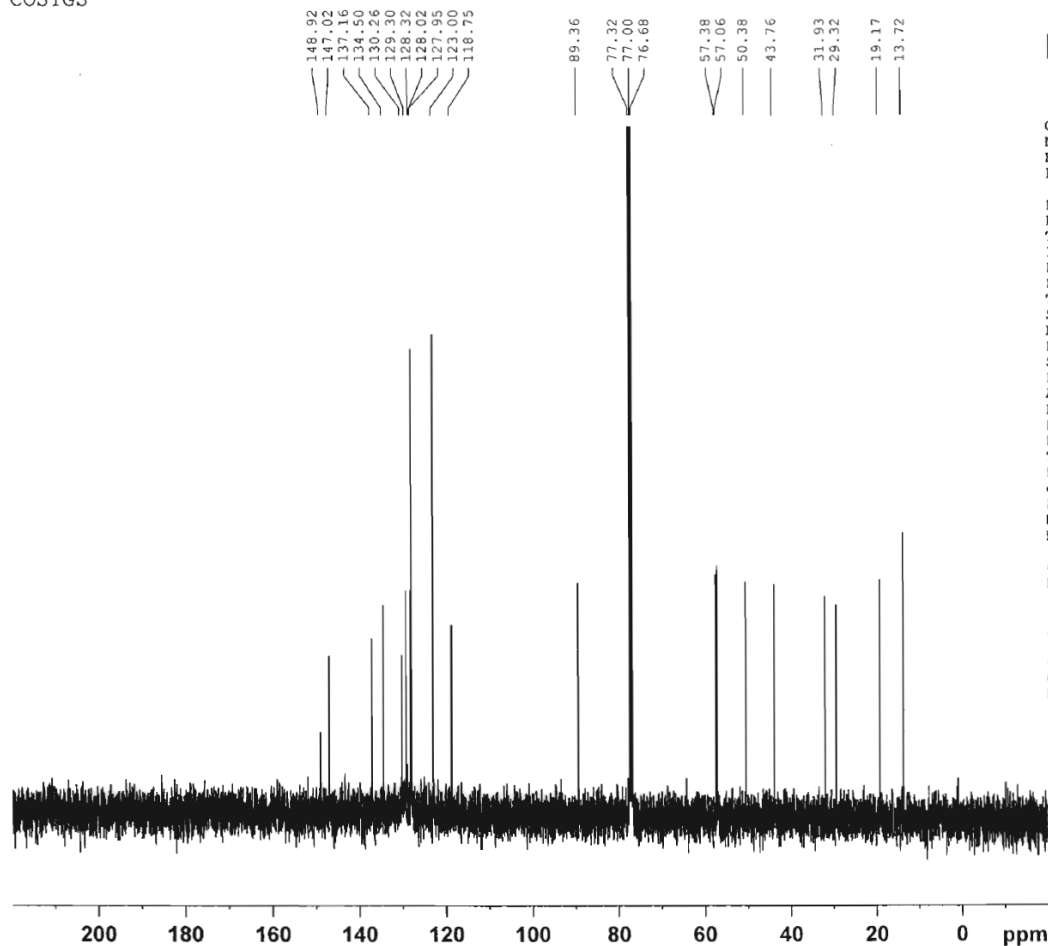
Current Data Parameters
NAME Jun10-2010
EXPNO 132
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100610
Time 14.25
INSTRUM dpx400
PROBHD 5 mm QNP 1H/29
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 5
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 3649.1
DW 60.800 usec
DE 6.00 usec
TE 303.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.70 usec
PL1 4.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 16384
SF 400.1300077 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

COSYGS



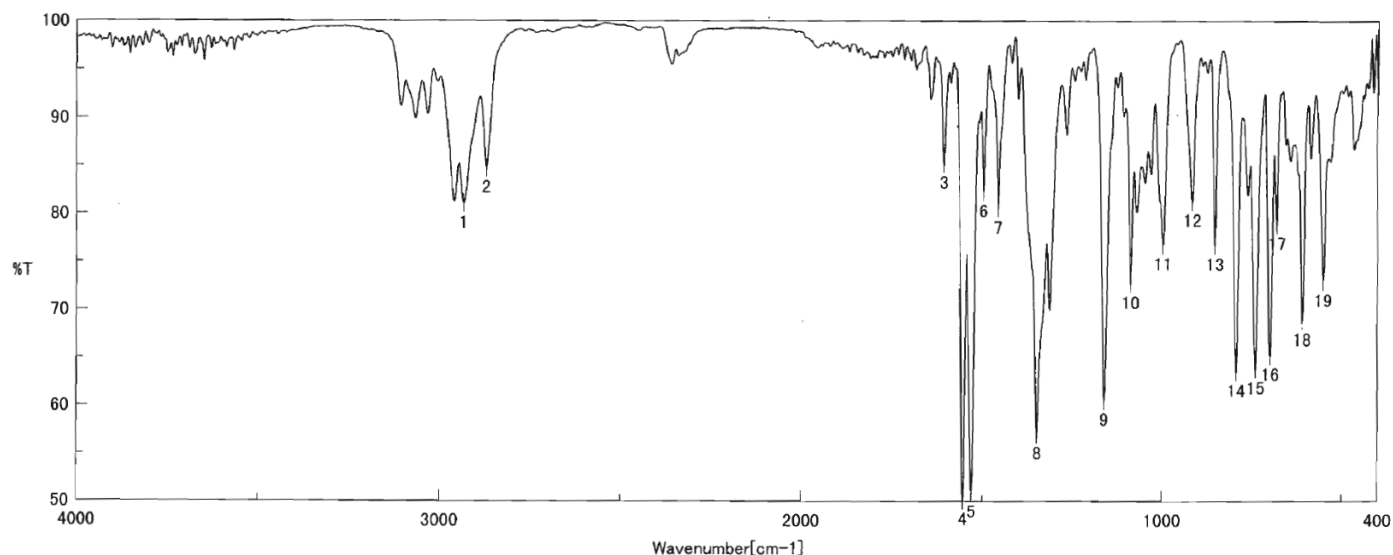
Current Data Parameters
NAME Jun10-2010
EXPNO 133
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100610
Time 14.33
INSTRUM dpx400
PROBHD 5 mm QNP 1H/29
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 151
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289652 sec
RG 32768
DW 15.700 usec
DE 6.00 usec
TE 303.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.30 usec
PL1 3.00 dB
SFO1 100.6254358 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 3.00 dB
PL12 22.00 dB
PL13 22.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127708 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



積算回数 16
 ゼロフィリング ON
 ゲイン 2
 日時 110/06/14 18:02
 測定者
 ファイル名 Memory#10
 サンプル名 background
 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 nm/sec

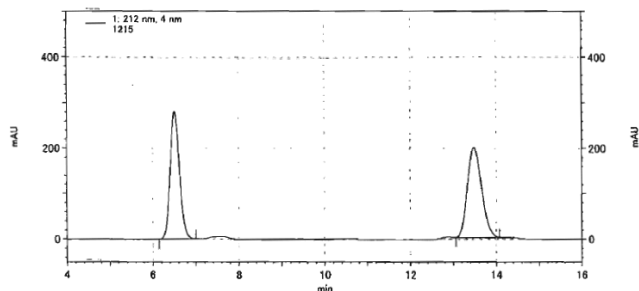
1: 2934.16, 81.0877	2: 2872.45, 84.7693	3: 1606.41, 85.2503	4: 1553.38, 50.1605
5: 1530.24, 50.9511	6: 1497.45, 82.2895	7: 1456.96, 80.5819	8: 1348.00, 57.0850
9: 1160.94, 60.5678	10: 1087.66, 72.7407	11: 997.98, 76.8001	12: 916.99, 81.3162
13: 854.31, 76.7396	14: 793.56, 63.5758	15: 739.57, 63.8382	16: 699.07, 65.2761
17: 681.71, 78.9093	18: 610.36, 68.8981	19: 551.54, 72.9877	

面積%レポート

ページ 1/1

データファイル名: \\Server\Enterprise\Projects\Default\Data\2010-05-21 skmt allyl sokusa
 nPr rac 20vs1 AD-H 1ml.dat
 メソッドファイル名: \\Server\Enterprise\Projects\Default\Method\20vs1 1ml.met
 ユーザー名: System
 分析日時: 2010/05/21 15:15:02
 印刷日時: 2010/05/21 15:54:59

VVX

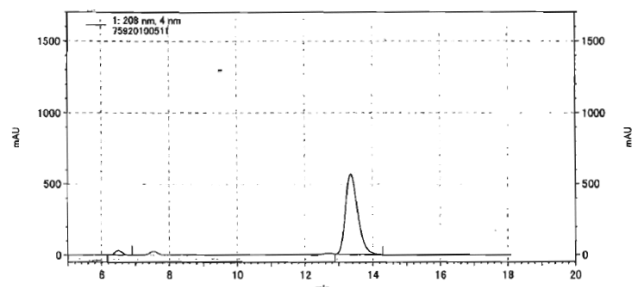


1: 212 nm, 4 nm結果	PK #	名前	保持時間	面積	面積%	ピークタイプ
	1		6.51	17061914	48.250	■
	2		13.49	18299457	51.750	■
				35361371	100.000	

面積%レポート

ページ 1/1

データファイル名: \\Server\Enterprise\Projects\Default\Data\2010.06.02-skmt-allyl sokusa
 nPr AD-H 20 vs. 1 1ml.dat
 メソッドファイル名: \\Server\Enterprise\Projects\Default\Method\20vs1 1ml.met
 ユーザー名: System
 分析日時: 2010/06/03 2:25:42
 印刷日時: 2010/06/03 2:46:14



1: 208 nm, 4 nm結果	PK #	名前	保持時間	面積	面積%	ピークタイプ
	1		6.49	1892111	3.204	■
	2		13.35	57154602	96.796	■
				59046713	100.000	

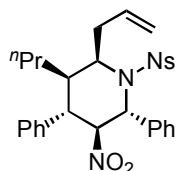
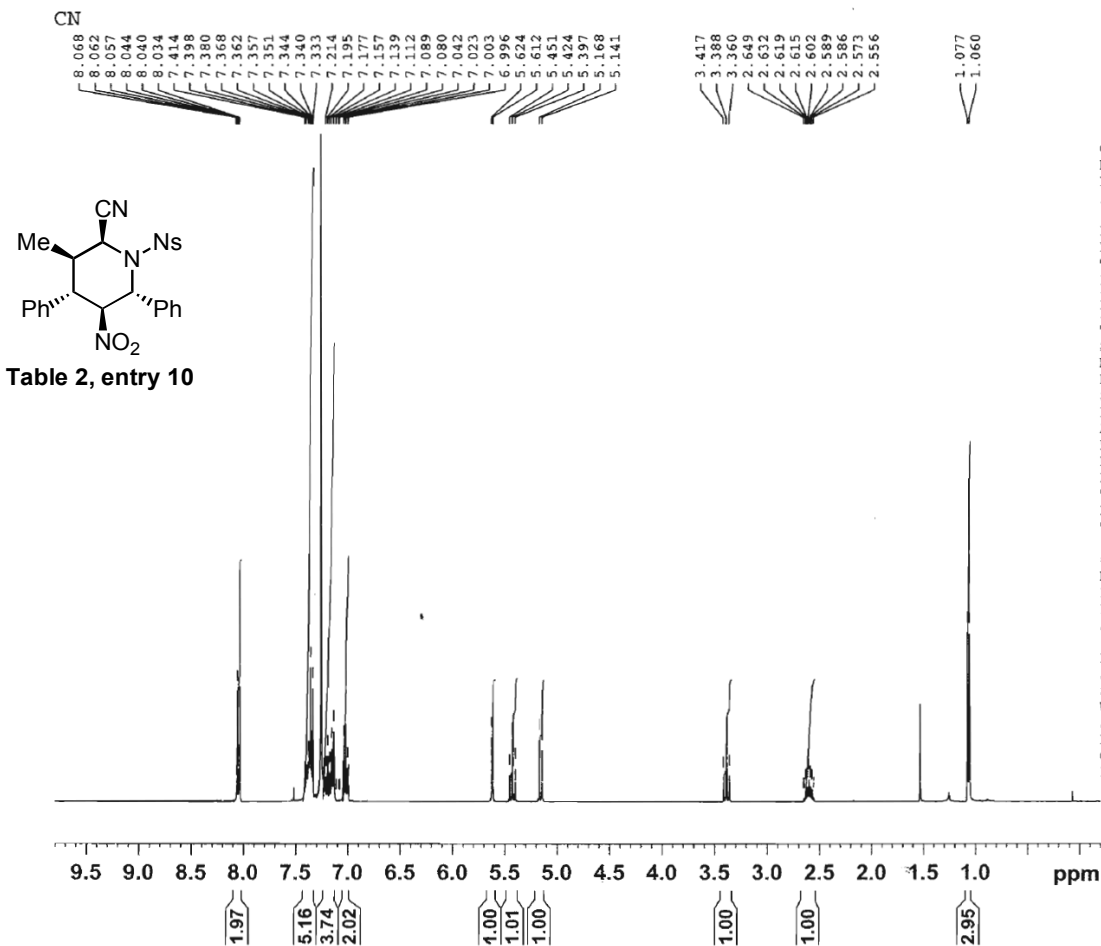


Table 2, entry 9

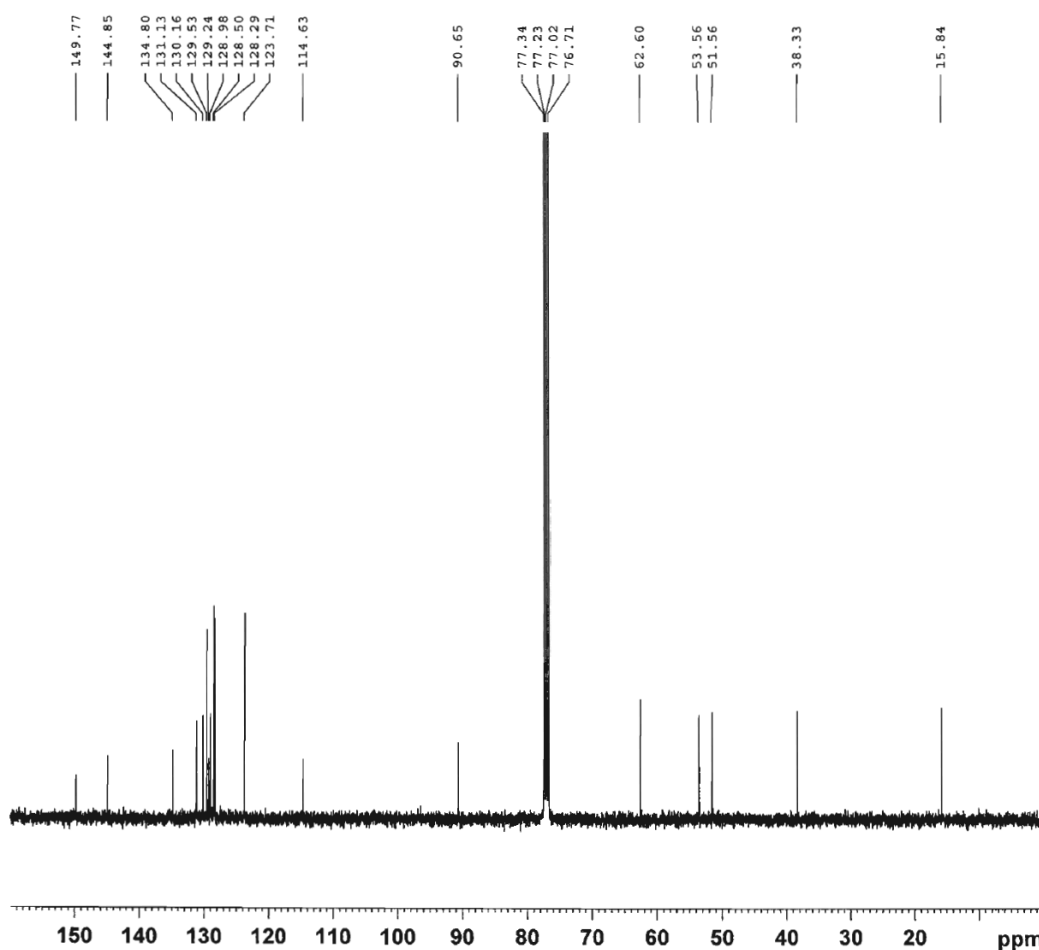


Current Data Parameters
 NAME Apr14-2010-user1
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100414
 Time 21.59
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 512
 DW 60.800 usec
 DE 6.00 usec
 TE 297.3 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 12.00 usec
 PL1 -4.00 dB
 SFO1 400.1824713 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1800078 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



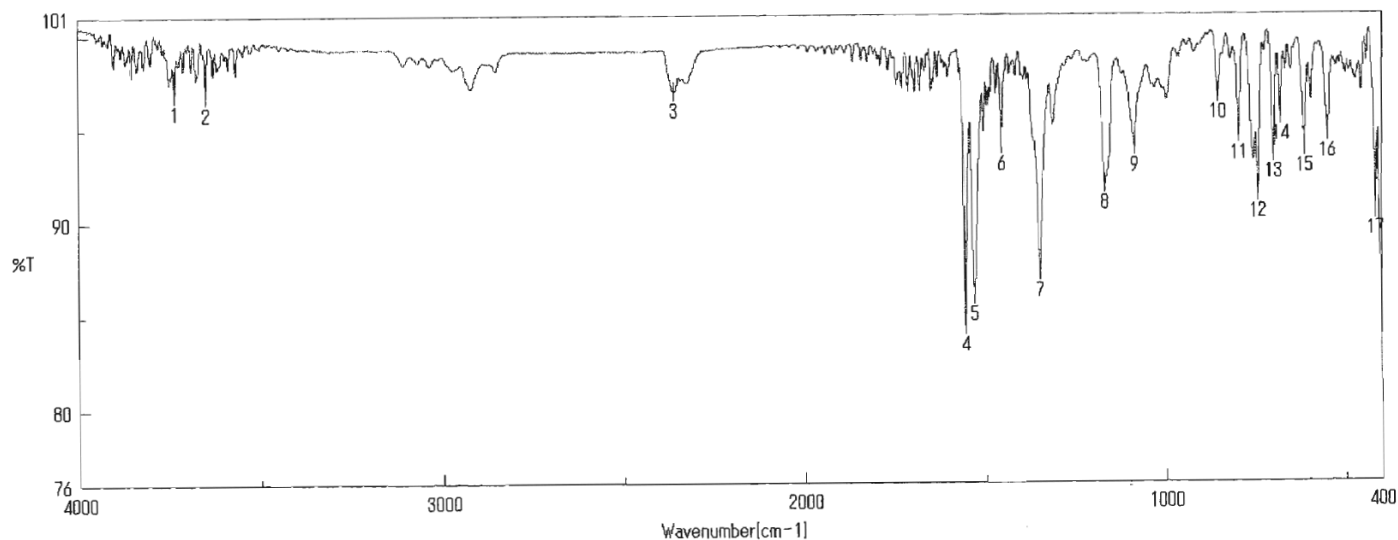
Current Data Parameters
 NAME Apr16-2010-hayashi
 EXPNO 150
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100416
 Time 23.57
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 181
 DW 20.800 usec
 DE 6.00 usec
 TE 298.4 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 7.20 usec
 PL1 -3.50 dB
 SFO1 100.6354036 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -4.00 dB
 PL12 14.00 dB
 PL13 14.00 dB
 SFO2 400.1816007 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6253410 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



積算回数 16
 ゼロフィリング ON
 ゲイン 1
 日時 110/04/18 18:39
 測定者
 ファイル名 Memory#4
 サンプル名 background
 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

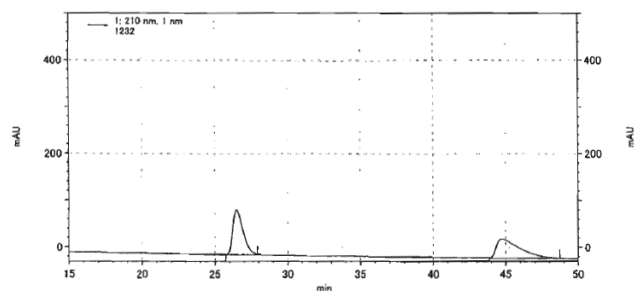
1: 3734.48, 96.9382	2: 3648.66, 96.8322	3: 2361.41, 96.9632	4: 1558.20, 84.4362
5: 1532.17, 86.0705	6: 1456.96, 94.0423	7: 1349.93, 87.3148	8: 1169.62, 91.9946
9: 1087.66, 93.9600	10: 855.28, 96.7861	11: 797.42, 94.5983	12: 744.39, 91.4742
13: 701.00, 93.8006	14: 681.71, 95.6174	15: 615.18, 93.8878	16: 551.54, 94.6752
17: 417.51, 90.5264			

面積%レポート

ページ 1/1

データファイル名: \\Server\Enterprise\Projects\Default\Data\2010-05-26 skmt allyl normal
 rac AD-H 10vs1 1ml.dat
 メソッドファイル名: \\Server\Enterprise\Projects\Default\Method\10vs1. 1ml.met
 ユーザー名: System
 分析日時: 2010/05/26 10:01:29
 印刷日時: 2010/05/26 10:57:42

VVM



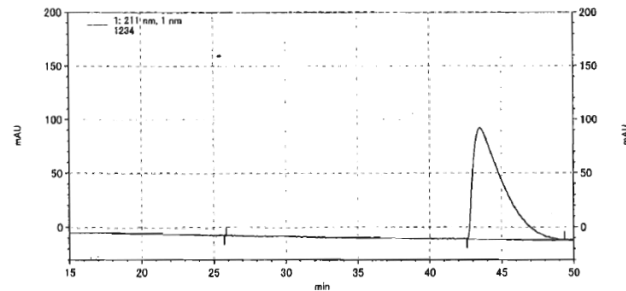
1: 210 nm, 1 nm結果	名前	保持時間	面積	面積%	ピーク番号
Pk #					
1		26.49	18682677	50.325	1
2		44.73	18441017	49.675	2
	トータル		37123694	100.000	

面積%レポート

ページ 1/1

データファイル名: \\Server\Enterprise\Projects\Default\Data\2010-05-26 skmt allyl normal
 ch1 AD-H 10vs1 1ml.dat
 メソッドファイル名: \\Server\Enterprise\Projects\Default\Method\10vs1. 1ml.met
 ユーザー名: System
 分析日時: 2010/05/26 11:00:40
 印刷日時: 2010/05/26 12:09:08

VVM



1: 211 nm, 1 nm結果	名前	保持時間	面積	面積%	ピーク番号
Pk #					
1		25.80	28192	0.048	1
2		43.54	58825228	99.952	2
	トータル		58853420	100.000	

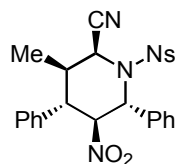


Table 2, entry 10

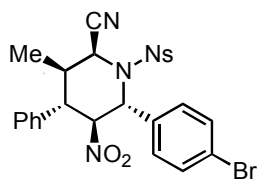
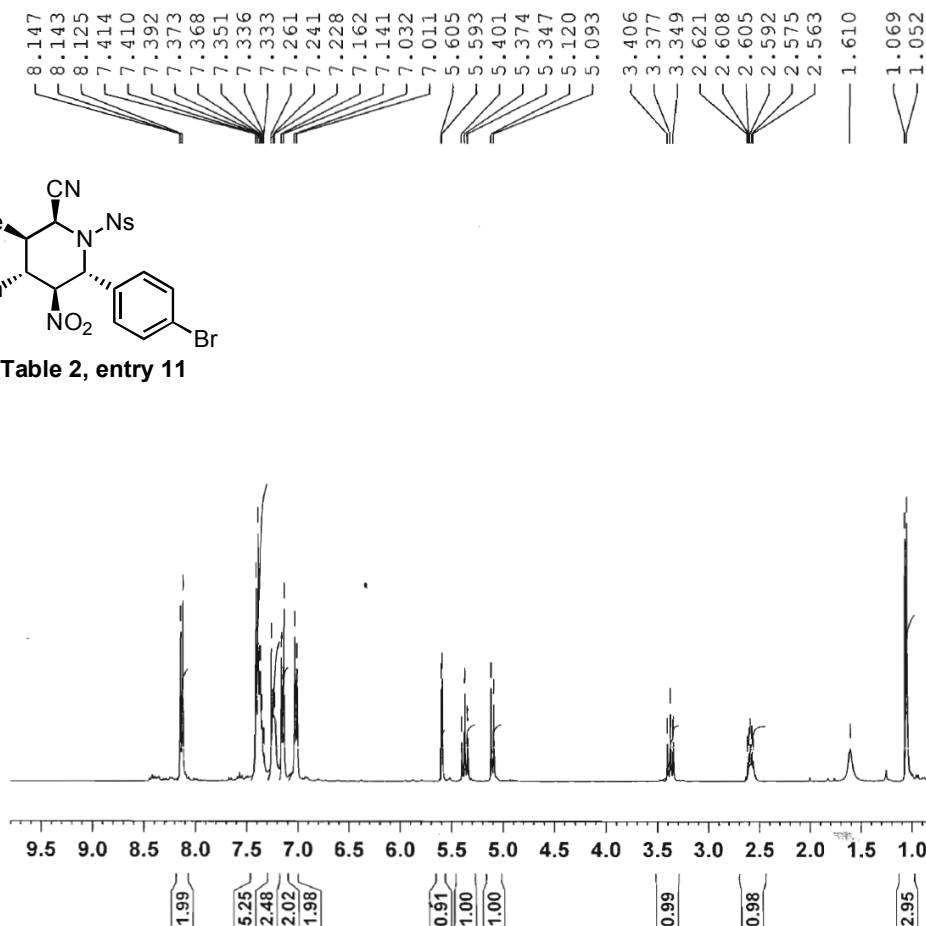


Table 2, entry 11

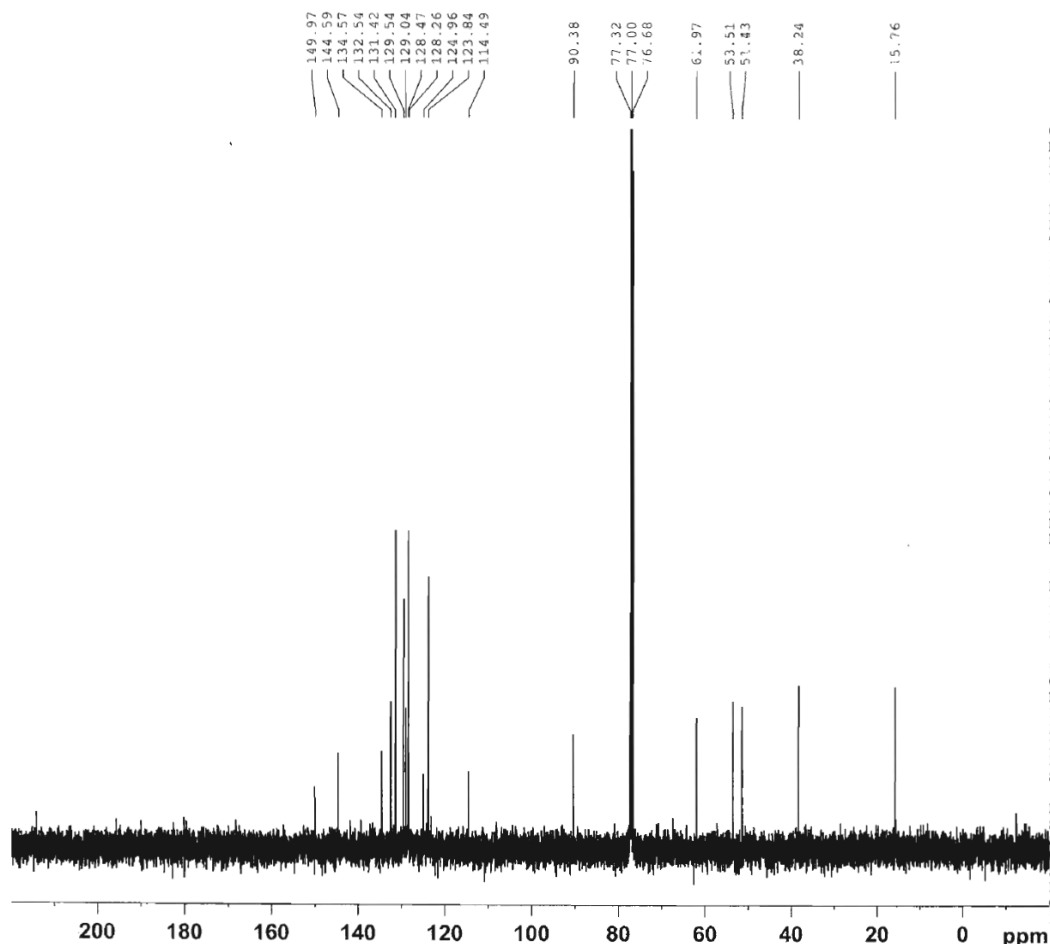


Current Data Parameters
NAME May27-2010
EXPNO 62
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100527
Time 16.36
INSTRUM dpx400
PROBHD 5 mm QNP 1H/29
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 3649.1
DW 60.800 usec
DE 6.00 usec
TE 303.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.70 usec
PL1 4.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 16384
SF 400.1300092 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



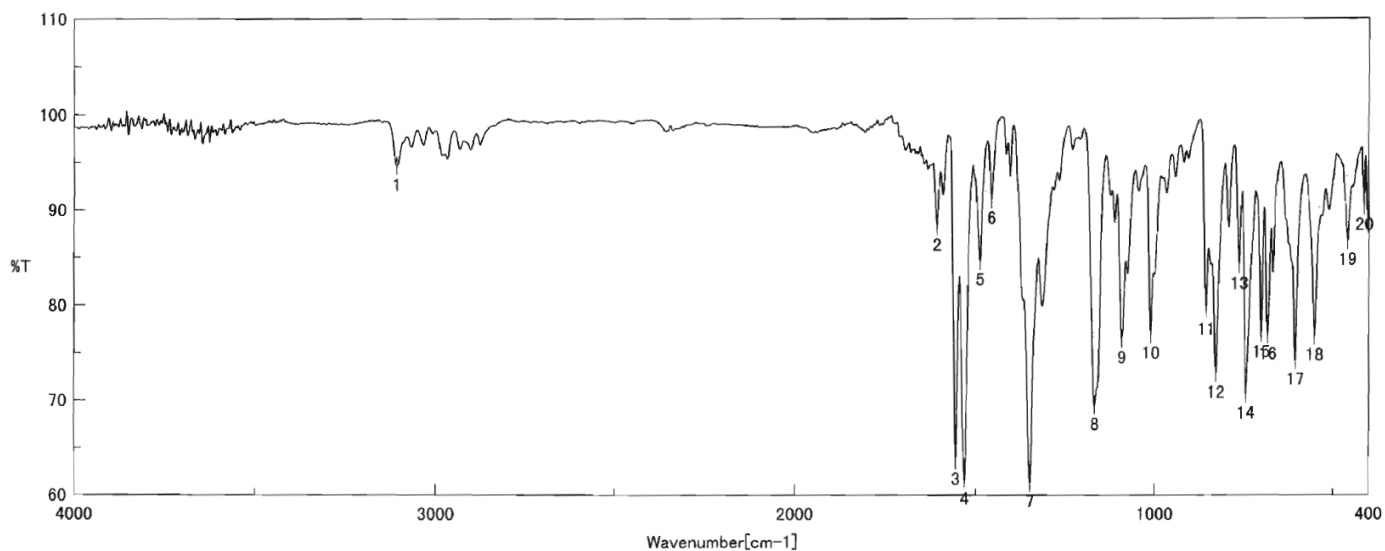
Current Data Parameters
NAME May27-2010
EXPNO 63
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100527
Time 16.41
INSTRUM dpx400
PROBHD 5 mm QNP 1H/29
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 100
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289652 sec
RG 41285.1
DW 15.700 usec
DE 6.00 usec
TE 303.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.30 usec
PL1 3.00 dB
SFO1 100.6254358 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 3.00 dB
PL12 22.00 dB
PL13 22.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127708 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



積算回数 16
 ゼロフィリング ON
 ゲイン 2
 日時 110/06/14 17:35
 測定者
 ファイル名 Memory#16
 サンプル名 background
 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

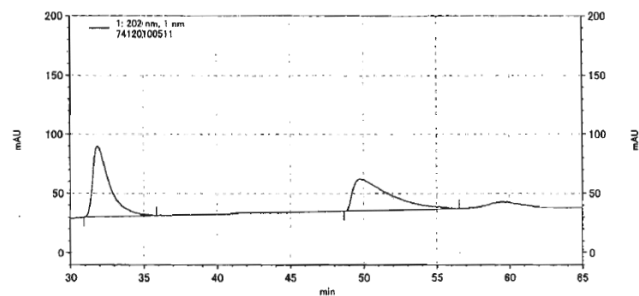
1: 3107.72, 94.5962	2: 1607.38, 88.3293	3: 1556.27, 63.7332	4: 1531.20, 61.6338
5: 1487.81, 84.6973	6: 1455.99, 91.1635	7: 1348.00, 61.3532	8: 1166.72, 69.4989
9: 1090.55, 76.5136	10: 1010.52, 77.0015	11: 855.28, 79.4824	12: 828.28, 72.8439
13: 762.71, 84.2619	14: 744.39, 70.6882	15: 701.00, 77.0998	16: 682.68, 76.9000
17: 605.54, 74.2207	18: 551.54, 76.7844	19: 459.94, 86.7585	20: 413.66, 90.4452

面積%レポート

ページ 1/1

データファイル名: \\Server\Enterprise\Projects\Default\Data\2010.05.29-skmt CN imine Br
 rac-AD-H-10 vs 1- 1ml
 メソッドファイル名: \\Server\Enterprise\Projects\Default\Method\10vs1. 1ml.met
 ユーザー名: System
 分析日時: 2010/05/30 15:06:30
 印刷日時: 2010/05/30 16:19:18

VVM



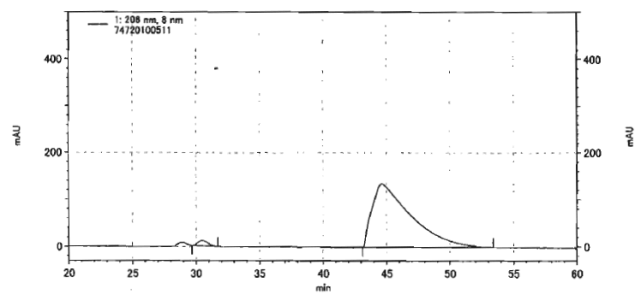
1: 202 nm, 1 nm結果	名前	保持時間	面積	面積%	ピークコード
PK #					
1		31.87	18695505	50.349	1
2		49.80	18436283	49.651	2
トータル			37131788	100.000	

面積%レポート

ページ 1/1

データファイル名: \\Server\Enterprise\Projects\Default\Data\2010.05.29-skmt CN imine Br
 chi-AD-H-10 vs 1- 1ml
 メソッドファイル名: \\Server\Enterprise\Projects\Default\Method\10vs1. 1ml.met
 ユーザー名: System
 分析日時: 2010/06/01 13:29:15
 印刷日時: 2010/06/01 14:34:46

VVX



1: 206 nm, 8 nm結果	名前	保持時間	面積	面積%	ピークコード
PK #					
1		30.47	2388260	2.038	1
2		44.61	114727199	97.962	2
トータル			117113459	100.000	

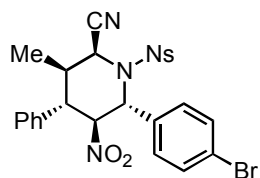


Table 2, entry 11

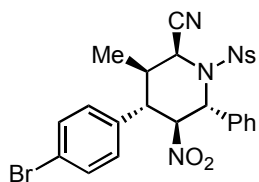
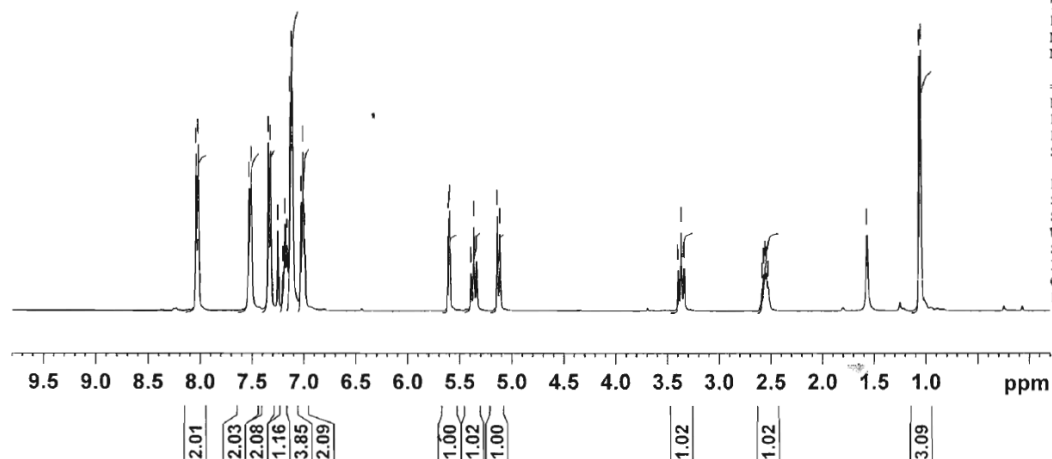


Table 2, entry 12



Current Data Parameters
NAME May27-2010
EXPNO 64
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100527
Time 16.46
INSTRUM dpx400
PROBHD 5 mm QNP 1H/29
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 4096
DW 60.800 usec
DE 6.00 usec
TE 303.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.90 usec
PL1 3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 16384
SF 400.1300092 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40



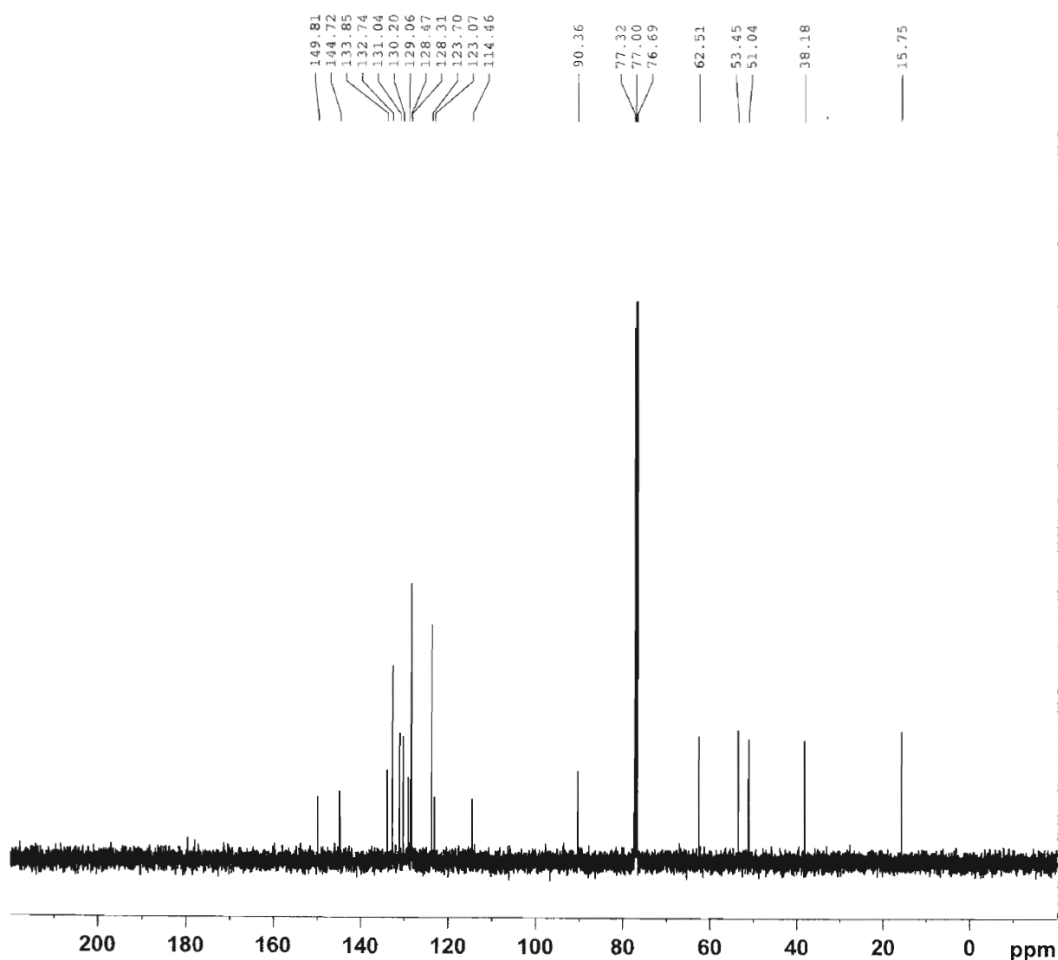
Current Data Parameters
NAME May27-2010
EXPNO 65
PROCNO 1

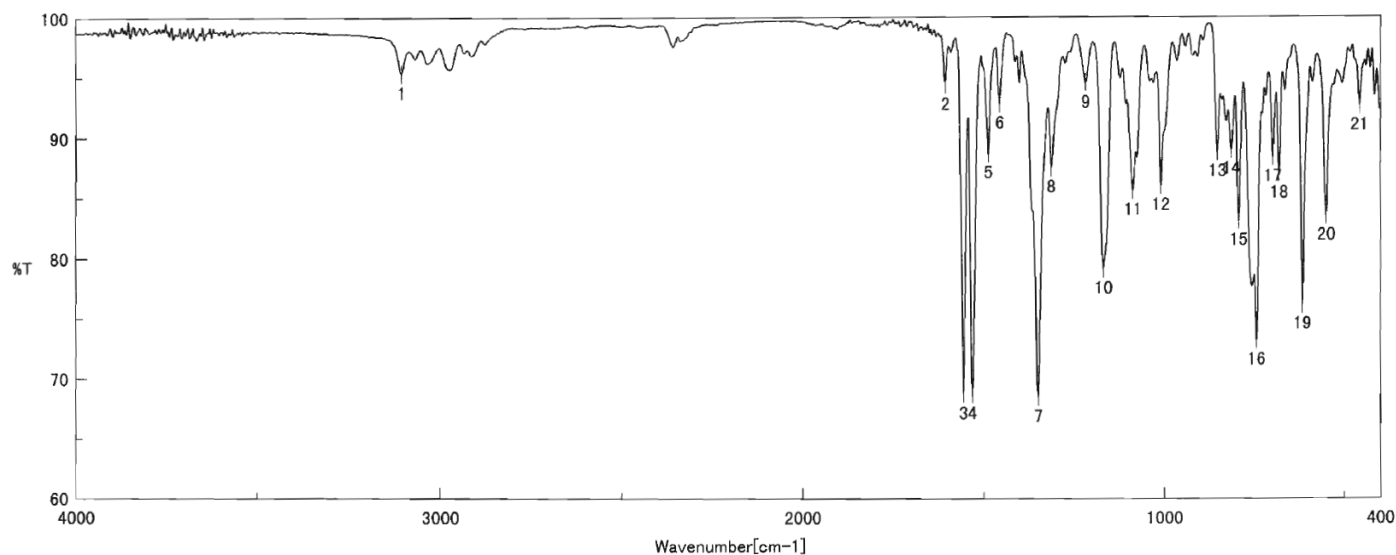
F2 - Acquisition Parameters
Date_ 20100527
Time 16.53
INSTRUM dpx400
PROBHD 5 mm QNP 1H/29
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 122
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289652 sec
RG 23170.5
DW 15.700 usec
DE 6.00 usec
TE 303.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.30 usec
PL1 3.00 dB
SFO1 100.6254358 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 3.00 dB
PL12 22.00 dB
PL13 22.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127713 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





積算回数 16
 ゼロフィリング ON
 ゲイン 2
 日時 110/06/15' 13:23
 測定者
 ファイル名 Memory#3
 サンプル名 background
 コメント

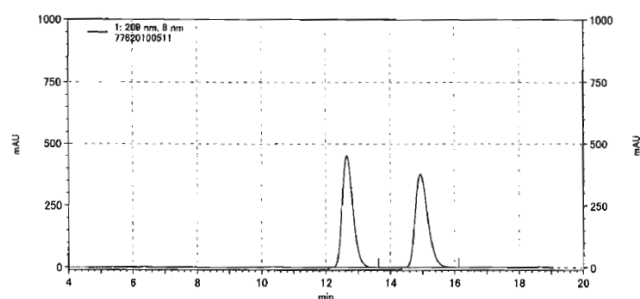
分解 4 cm-1
 アポダイゼーション Cosine
 スキャンスピード 2 mm/sec

1: 3105.80, 95.3425	2: 1607.38, 94.4681	3: 1557.24, 68.7705	4: 1532.17, 68.7658
5: 1488.78, 88.7740	6: 1457.92, 92.9211	7: 1349.93, 68.5338	8: 1314.25, 87.6051
9: 1218.79, 94.6198	10: 1169.62, 79.2183	11: 1087.66, 85.7008	12: 1010.52, 86.1135
13: 854.31, 88.9193	14: 815.74, 89.1193	15: 794.53, 83.1792	16: 745.35, 73.2796
17: 700.03, 88.5048	18: 682.68, 87.1034	19: 617.11, 76.2598	20: 551.54, 83.6058

面積%レポート

ページ 1/1

データファイル名: \\Server\Enterprise\Projects\Default\Data\20100607 skmt -cn sty br dens
 rac 10vsl 1ml.dat
 メソッドファイル名: \\Server\Enterprise\Projects\Default\Method\10vsl 1ml.met
 ユーザー名: System
 分析日時: 2010/06/07 22:06:42
 印刷日時: 2010/06/07 22:28:21
 VVX

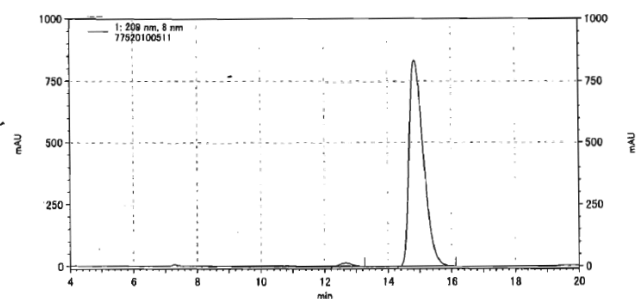


PK #	名前	保持時間	面積	面積%	ピークサインコート
1		12.65	41825327	50.427	■
2		14.93	41117121	49.573	■
トータル			82942448	100.000	

面積%レポート

ページ 1/1

データファイル名: \\Server\Enterprise\Projects\Default\Data\20100607 skmt -cn sty br dens
 rac 10vsl 1ml.dat
 メソッドファイル名: \\Server\Enterprise\Projects\Default\Method\10vsl 1ml.met
 ユーザー名: System
 分析日時: 2010/06/07 20:23:49
 印刷日時: 2010/06/07 22:33:59
 VVX



PK #	名前	保持時間	面積	面積%	ピークサインコート
1		12.66	1385037	1.317	■
2		14.85	103808400	98.683	■
トータル			105191437	100.000	

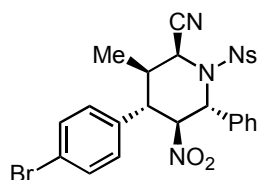
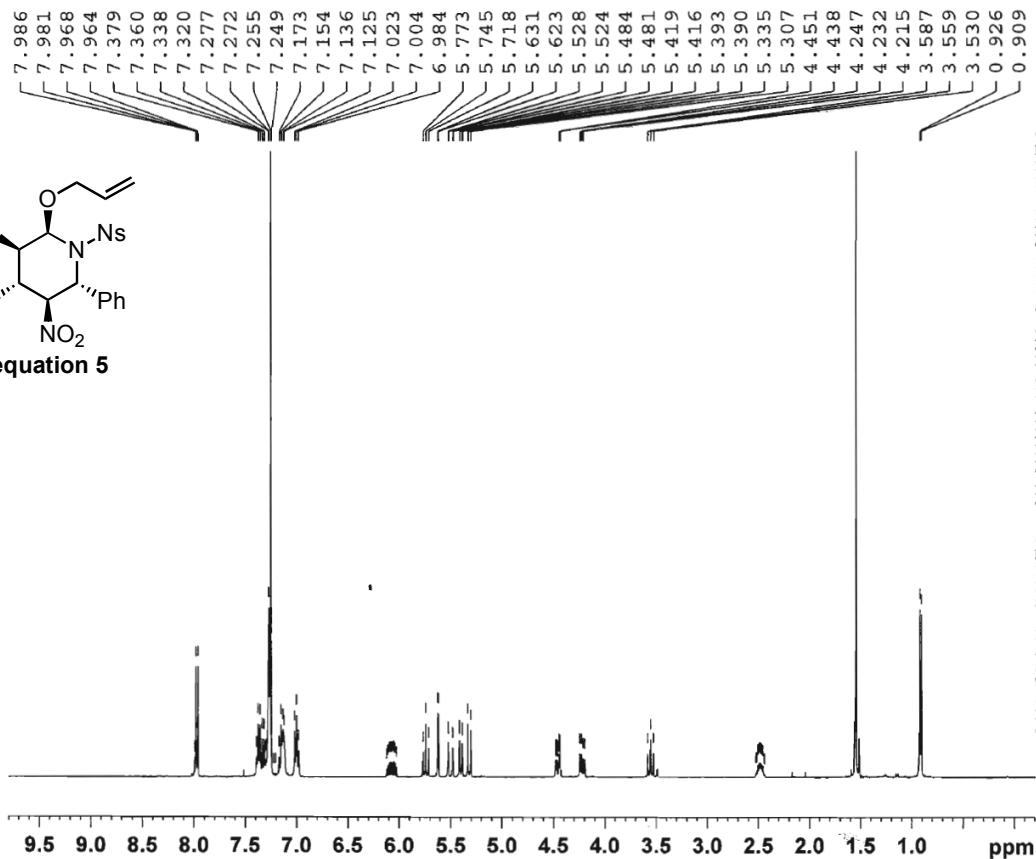
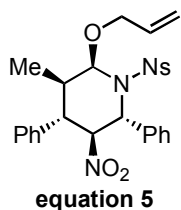


Table 2, entry 12

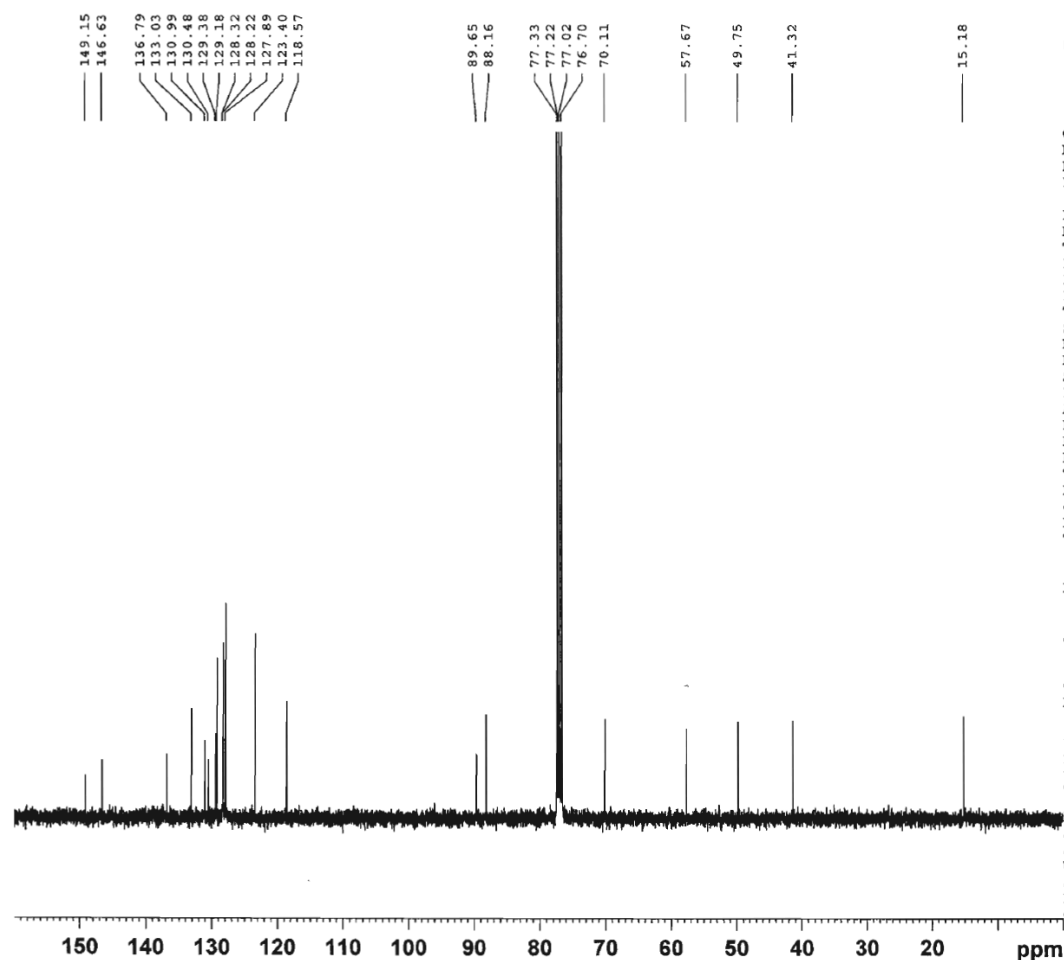


Current Data Parameters
NAME Apr25-2010-hayashi
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100425
Time 13.50
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 456
DW 60.800 usec
DE 6.00 usec
TE 296.9 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.00 usec
PL1 -4.00 dB
SFO1 400.1824713 MHz

F2 - Processing parameters
SI 32768
SF 400.1800076 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



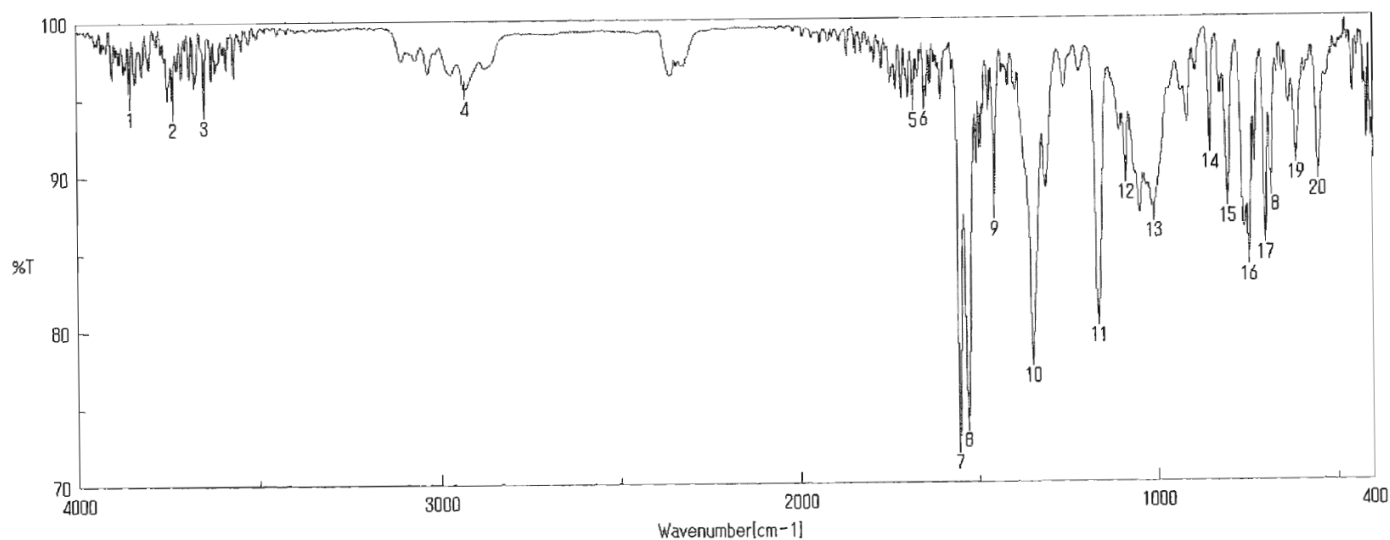
Current Data Parameters
NAME Apr25-2010-hayashi
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100425
Time 15.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 181
DW 20.800 usec
DE 6.00 usec
TE 298.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 7.20 usec
PL1 -3.50 dB
SFO1 100.6354036 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -4.00 dB
PL12 14.00 dB
PL13 14.00 dB
SFO2 400.1816007 MHz

F2 - Processing parameters
SI 32768
SF 100.6253410 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



積算回数 16
 ゼロフィリング ON
 ゲイン 1
 日時 110/04/27 14:19
 測定者
 ファイル名 Memory#6
 サンプル名 background
 コメント

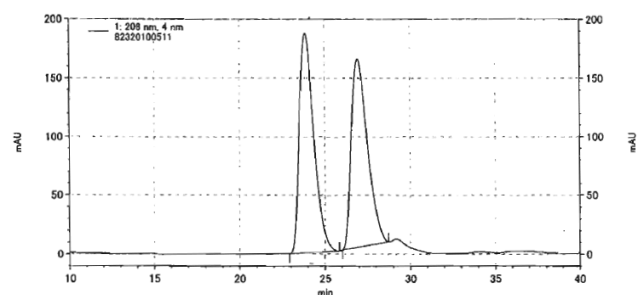
分解 4 cm⁻¹
 アポダイゼーション Cosine
 スキャンスピード 2 mm/sec

1: 3852.11, 95.0523	2: 3734.48, 94.3275	3: 3648.66, 94.4703	4: 2931.27, 95.5866
5: 1683.55, 94.6548	6: 1652.70, 94.7148	7: 1555.31, 72.4886	8: 1531.20, 73.9118
9: 1456.96, 87.5470	10: 1348.96, 78.1091	11: 1164.79, 80.6703	12: 1088.62, 89.8855
13: 1010.52, 87.4015	14: 854.31, 91.7762	15: 805.13, 88.3263	16: 745.35, 84.5702
17: 700.03, 85.9594	18: 684.61, 89.0377	19: 615.18, 91.0708	20: 553.47, 90.0238

面積%レポート

ページ 1/1

データファイル名: \\Server\Enterprise\Projects\Default\Data\2010-06-15
 skant-Dalyl-rac-1A-80vs1.dat
 プラットフォーム名: \\Server\Enterprise\Projects\Default\Method\80vs1 1ml.met
 ユーザー名: System
 分析日時: 2010/06/16 20:46:12
 印刷日時: 2010/06/16 21:36:03

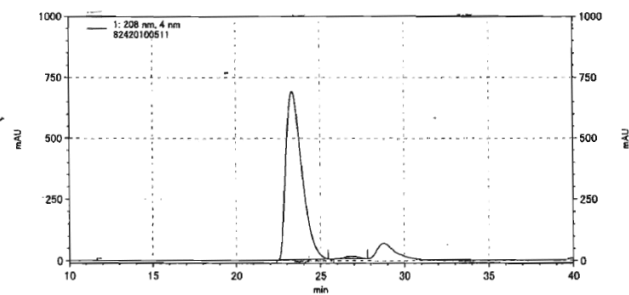


名前	保持時間	面積	面積%	ピークコード
1: 208 nm, 4	23.86	44205271	51.033	MM
2: 208 nm, 4	26.93	42415123	48.967	MM
トータル		86620394	100.000	

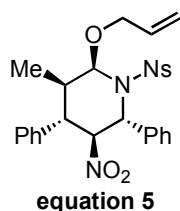
面積%レポート

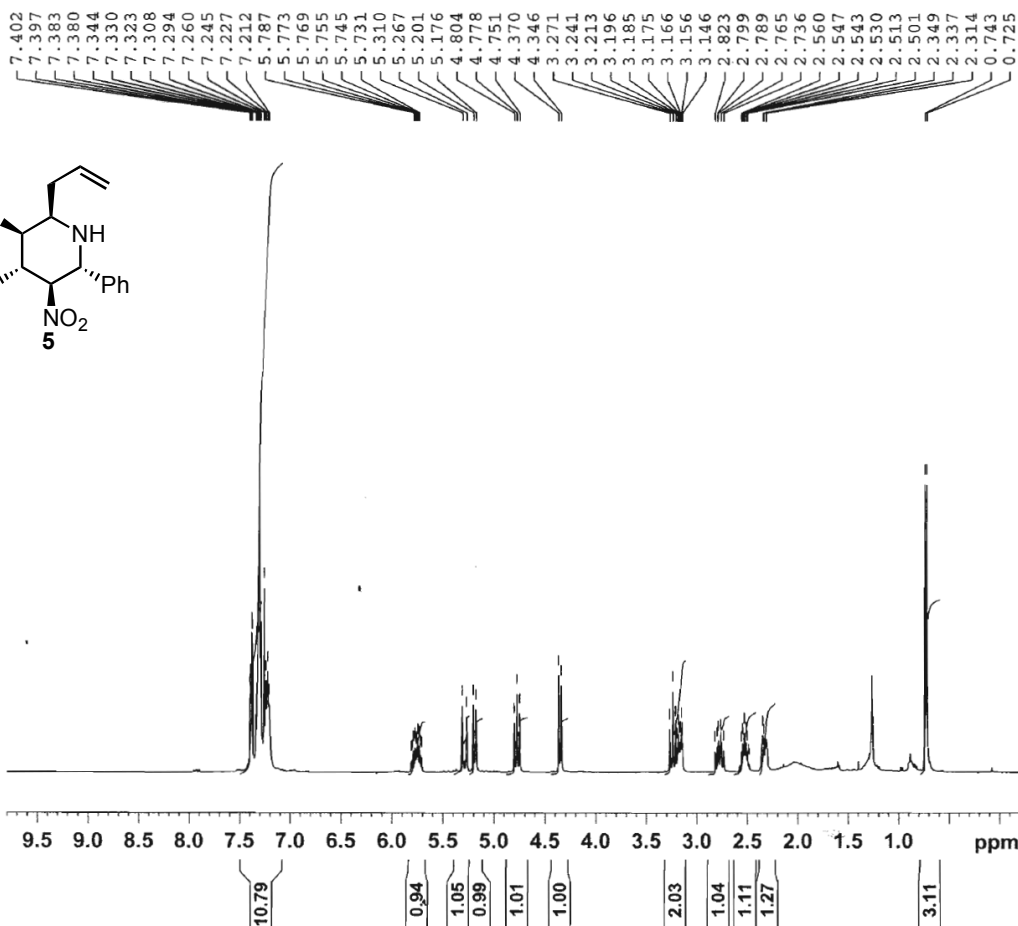
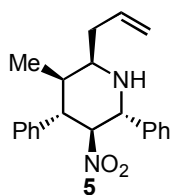
ページ 1/1

データファイル名: \\Server\Enterprise\Projects\Default\Data\2010-06-15
 skant-Dalyl-rac-1A-80vs1.dat
 プラットフォーム名: \\Server\Enterprise\Projects\Default\Method\80vs1 1ml.met
 ユーザー名: System
 分析日時: 2010/06/16 21:46:24
 印刷日時: 2010/06/16 22:49:48



名前	保持時間	面積	面積%	ピークコード
1: 208 nm, 4	23.33	180980246	98.678	MM
2: 208 nm, 4	26.85	2428380	1.324	MM
トータル		183408626	100.000	





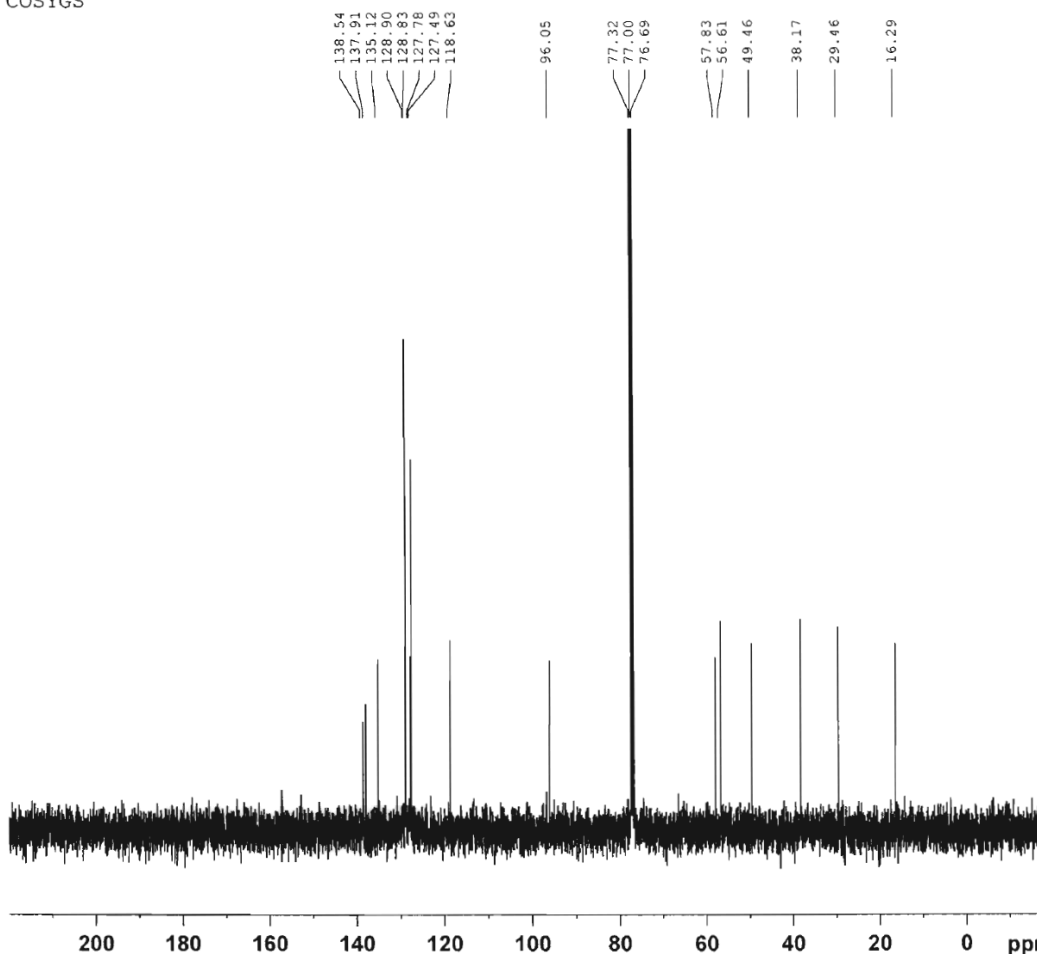
Current Data Parameters
NAME May29-2010
EXPNO 86
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100529
Time 18.55
INSTRUM dpx400
PROBHD 5 mm QNP 1H/29
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.992344 sec
RG 3251
DW 60.800 usec
DE 6.00 usec
TE 303.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.70 usec
PL1 4.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 16384
SF 400.1300092 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

COSYGS



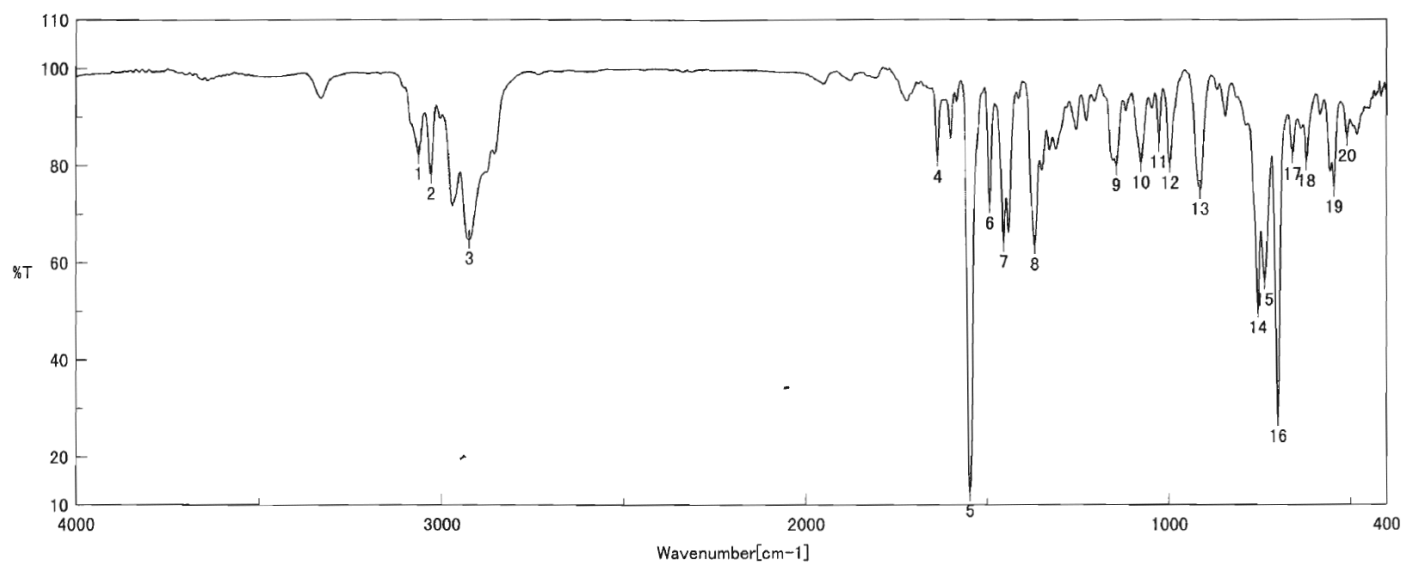
Current Data Parameters
NAME May29-2010
EXPNO 87
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100529
Time 19.00
INSTRUM dpx400
PROBHD 5 mm QNP 1H/29
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 101
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289652 sec
RG 20642.5
DW 15.700 usec
DE 6.00 usec
TE 303.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.30 usec
PL1 3.00 dB
SFO1 100.6254358 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 3.00 dB
PL12 22.00 dB
PL13 22.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127698 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00



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

16
ON
2
110/06/14 17:44
Memory#5
background

分解
アポダイゼーション
スキャンスピード

4 cm-1
Cosine
2 mm/sec

1: 3064.33, 82.3288	2: 3030.59, 78.2336	3: 2924.52, 64.9168	4: 1639.20, 81.6557
5: 1548.56, 12.7935	6: 1494.56, 72.1405	7: 1455.99, 64.2195	8: 1371.14, 63.6569
9: 1146.47, 79.9904	10: 1078.98, 80.5164	11: 1029.80, 84.6565	12: 998.95, 80.4762
13: 916.02, 75.0801	14: 755.96, 50.6008	15: 737.64, 56.3262	16: 700.03, 28.2570
17: 660.50, 82.2213	18: 622.89, 80.8433	19: 545.76, 75.5402	20: 510.08, 85.9245

