Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Manganese-catalysed hydroperoxidation of carbon-carbon double bonds using molecular oxygen present in air and hydroxylamine under ambient conditions

Daisuke Yamamoto, Masayuki Soga, Hiromasa Ansai, and Kazuishi Makino*

Department of Pharmaceutical Sciences, Kitasato University, Tokyo 1088641, Japan

E-mail: yamamotod@pharm.kitasato-u.ac.jp
makinok@pharm.kitasato-u.ac.jp

Supporting Information

Table of contents

General information

IR spectra was obtained using a JASCO FT/IR 460-plus spectrophotometer. ^{1}H- and ^{13}C-NMR spectra were obtained on Agilent Technologies 400-MR DD2, 400-MR spectrometers. The chemical shifts are expressed in ppm downfield from internal solvent peaks $CDCl_3$ (7.26 ppm, ^{1}H NMR), $CDCl_3$ (77.0 ppm, ^{13}C NMR), and coupling constant (*J* values) are given in Hertz. The coupling patterns are expressed by s (singlet), d (doublet), dd (doublet of doublet), dq (doublet of quartet), t (triplet), dq (quartet of doublet), m (multiplet) and br (broad signal). MS spectra were measured with JEOL JMS-AX505HA, JMS-700V MStation and JEOL JMS-T100LP spectrometers. Melting points were measured on a Yanaco Micro Melting System MP-500P. Commercial reagents and solvents were used without further purification unless otherwise indicated. Flash column chromatography was carried out with Kanto Chemical silica gel (Kanto Chemical Co., Inc., silica gel 60N, spherical neutral, particle size 63–210 μm). TLC was performed on 0.25 mm E Merck silica gel 60 F254 plates.

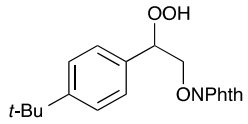
General procedure for the manganese-catalysed hydroperoxidation with NHPI

To a stirred solution of alkene (0.500 mmol) and *N*-hydroxyphthalimide (0.500 mmol) in MeCN (0.9 mL) at room temperature was added a solution of $Mn(acac)_3$ in MeCN (100 µl, 0.10 µmol, 0.020 mol%, 1.0 mM in MeCN [a]) under air (open flask). The progress of the reaction was monitored by TLC analysis. The reaction was quenched saturated aqueous NaCl solution (0.5 mL). The resulting mixture was extracted with ethyl acetate (3 x 1.0 mL). The combined organic phases were washed with brine (2 x 1.0 mL), dried (Na_2SO_4), filtered and concentrated under reduced pressure. The obtained crude material was purified by silica gel column chromatography using hexane and ethyl acetate as eluent.

[a] Preparation of a solution of $Mn(acac)_3$ in MeCN : A 10.0 mL measuring flask was charged with $Mn(acac)_3$ (3.5 mg, 0.010 mmol) and diluted to total volume of 10.0 mL with MeCN (1.0 mM in MeCN).

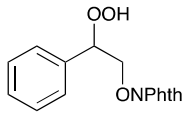
Analytical date for 5a-k, 7 and 9a-c

2-(2-(4-(*tert*-Butyl)phenyl)-2-hydroperoxyethoxy)isoindoline-1,3-dione (5a)



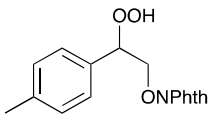
Prepared according to the general procedure to give **5a** in 92% yield; Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.37 (br s, O-O<u>H</u>), 7.89-7.84 (m, 2H), 7.80-7.75 (m, 2H), 7.39 (d, *J* = 8.8 Hz, 2H), 7.33 (d, *J* = 8.8 Hz, 2H), 5.40 (dd, *J* = 7.7, 3.8 Hz, 1H), 4.55 (dd, *J* = 11.6, 3.8 Hz, 1H), 4.50 (dd, *J* = 11.6, 7.7 Hz 1H), 1.30 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 163.8, 152.0, 134.7, 132.6, 128.7, 126.9, 125.7, 123.8, 85.3, 78.9, 34.6, 31.2; IR (neat) 3402, 3098, 3062, 3032, 2962, 1789, 1730, 1466, 1375, 1186, 1132, 1081, 1018, 997, 877, 701 cm^{-1}; HRMS (FAB, NBA) *m/z* calcd for $C_{20}H_{21}NO_5Na$ $[M+Na]^+$ 378.1317, found 378.1319.

2-(2-hydroperoxy-2-phenylethoxy)isoindoline-1,3-dione (5b)[1]



Prepared according to the general procedure to give **5b** in 64% yield; Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.47 (br s, O-O<u>H</u>), 7.90-7.85 (m, 2H), 7.81-7.77 (m, 2H), 7.43-7.34 (m, 5H), 5.42 (dd, *J* = 8.0, 3.2 Hz, 1H), 4.54 (dd, *J* = 11.6, 3.2 Hz, 1H), 4.49 (dd, *J* = 11.6, 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 163.8, 135.7, 134.8, 128.8, 128.7, 127.1, 123.8, 85.5, 78.9; IR (neat) 3387, 3064, 3030, 2918, 1787, 1729, 1375, 1186, 1019, 997, 877, 700 cm^{-1}; HRMS (FAB, NBA) *m/z* calcd for $C_{16}H_{13}NNaO_5$ $[M+Na]^+$ 322.0691, found 322.0682.

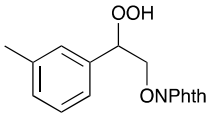
2-(2-hydroperoxy-2-(*p*-tolyl)ethoxy)isoindoline-1,3-dione (5c)[1]



Prepared according to the general procedure to give **5c** in 96% yield; White solid, mp. 85.5–89.6 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.44 (br s, O-O<u>H</u>), 7.88-7.83 (m, 2H), 7.79-7.74 (m, 2H), 7.28 (d, *J* = 7.6 Hz, 2H), 7.17 (d, *J* = 7.6 Hz, 2H), 5.38 (dd, *J* = 6.8,

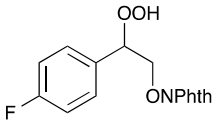
4.4 Hz, 1H), 4.51 (dd, *J* = 11.2, 4.4 Hz, 1H), 4.48 (dd, *J* = 11.2, 6.8 Hz 1H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 163.8, 138.7, 134.7, 132.6, 129.4, 128.7, 127.1, 123.8, 85.3, 78.9, 21.1; IR (KBr) 3369, 3031, 2940, 2923, 1786, 1718, 1652, 1373, 1187, 1119, 1084, 987, 943, 876, 817, 782, 699, 516 cm^{-1}; HRMS (FAB, NBA) *m/z* calcd for $C_{17}H_{15}NNaO_5$ $[M+Na]^+$ 336.0848, found 336.0856.

2-(2-Hydroperoxy-2-(*m*-tolyl)ethoxy)isoindoline-1,3-dione (5d)



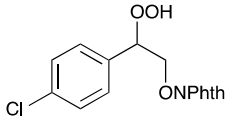
Prepared according to the general procedure except for the loading of $Mn(acac)_3$ (0.20 mol%) to give **5d** in quantitative yield; White solid, mp. 86.8–91.8 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.43 (br s, O-O<u>H</u>), 7.89-7.85 (m, 2H), 7.80-7.75 (m, 2H), 7.28-7.14 (m, 4H), 5.39 (dd, *J* = 8.0, 3.6 Hz, 1H), 4.52 (dd, *J* = 11.6, 3.6 Hz, 1H), 4.48 (dd, *J* = 11.6, 8.0 Hz, 1H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 163.7, 138.3, 135.6, 134.6, 129.4, 128.5, 127.7, 124.0, 123.6, 85.3, 78.8, 21.2; IR (KBr) 3394, 3056, 2913, 1783, 1725, 1610, 1465, 1376, 1187, 1141, 1082, 1016, 992, 880, 788, 700, 519 cm^{-1}; HRMS (FAB, NBA) *m/z* calcd for $C_{17}H_{15}NNaO_5$ $[M+Na]^+$ 336.0848, found 336.0852.

2-(2-(4-Fluorophenyl)-2-hydroeroxyethoxy)isoindoline-1,3-dione (5e)[1]



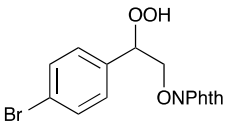
Prepared according to the general procedure except for the loading of $Mn(acac)_3$ (0.20 mol%) to give **5e** in 91% yield; White solid, mp. 85.4–88.8 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.57 (br s, O-O<u>H</u>), 7.89-7.84 (m, 2H), 7.80-7.76 (m, 2H), 7.42-7.37 (m, 2H), 7.09-7.03 (m, 2H), 5.38 (dd, *J* = 7.6, 3.6 Hz, 1H), 4.52 (dd, *J* = 11.2, 3.6 Hz, 1H), 4.48 (dd, *J* = 11.2, 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 163.7, 162.8, 134.7, 131.6, 129.0, 128.5, 123.7, 115.5, 84.5, 78.5; IR (KBr) 3449, 3065, 2912, 1785, 1719, 1601, 1509, 1466, 1377, 1220, 1186, 1135, 1081, 1063, 1018, 995, 876, 859, 830, 699, 544, 518 cm^{-1}; HRMS (FAB, NBA) *m/z* calcd for $C_{16}H_{12}FNNaO_5$ $[M+Na]^+$ 340.0597, found 340.0604.

2-(2-(4-chlorophenyl)-2-hydroperoxyethoxy)isoindoline-1,3-dione (5f)[1]



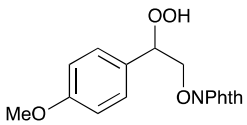
Prepared according to the general procedure except for the loading of $Mn(acac)_3$ (0.20 mol%) to give **5f** in 94% yield; White solid, mp. 112.9–116.2 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.56 (br s, O-OH), 7.88-7.83 (m, 2H), 7.80-7.75 (m, 2H), 7.37-7.31 (m, 4H), 5.38 (dd, *J* = 7.6, 3.6 Hz, 1H), 4.51 (dd, *J* = 11.6, 3.6 Hz, 1H), 4.46 (dd, *J* = 11.6, 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 163.8, 134.8, 134.7, 134.2, 128.9, 128.6, 128.5, 123.8, 84.7, 78.5; IR (KBr) 3366, 3037, 2937, 1784, 1717, 1491, 1465, 1375, 1190, 1122, 1081, 1018, 988, 876, 828, 784, 700, 580, 517 cm^{-1}; HRMS (FAB, NBA) *m/z* calcd for $C_{16}H_{12}ClNNaO_5$ $[M+Na]^+$ 356.0302, found 356.0303.

2-(2-(4-bromophenyl)-2-hydroperoxyethoxy)isoindoline-1,3-dione (5g)[1]



Prepared according to the general procedure except for the loading of $Mn(acac)_3$ (0.50 mol%) to give **5g** in 88% yield; White solid, mp. 112.1–115.6 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.48 (br s, O-OH), 7.90-7.86 (m, 2H), 7.82-7.77 (m, 2H), 7.52 (d, *J* = 8.0 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 5.37 (dd, *J* = 8.0, 3.6 Hz, 1H), 4.52 (dd, *J* = 11.6, 3.6 Hz, 1H), 4.45 (dd, *J* = 11.6, 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 163.7, 134.8, 131.7, 128.8, 128.5, 123.7, 122.8, 84.5, 78.3; IR (KBr) 3449, 3070, 2951, 2920, 1789, 1719, 1490, 1376, 1186, 1081, 1015, 996, 876, 821, 700, 518 cm^{-1}; HRMS (FAB, NBA) *m/z* calcd for $C_{16}H_{12}BrNNaO_5$ $[M+Na]^+$ 399.9797, found 399.9791.

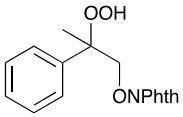
2-(2-hydroperoxy-2-(4-methoxyphenyl)ethoxy)isoindoline-1,3-dione (5h)



Prepared according to the general procedure except for the loading of $Mn(acac)_3$ (0.20 mol%) to give **5h** in 60% yield; White solid, mp. 104.7–107.8 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.36 (br s, O-OH), 7.90-7.85 (m, 2H), 7.80-7.75 (m, 2H), 7.33 (d, *J* = 8.8 Hz,

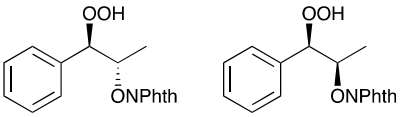
2H), 6.90 (d, *J* = 8.8 Hz, 2H), 5.36 (dd, *J* = 7.2, 4.2 Hz, 1H), 4.54 (dd, *J* = 11.4, 4.2 Hz, 1H), 4.50 (dd, *J* = 11.4, 7.2 Hz 1H), 3.80 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 163.8, 160.0, 134.8, 128.7, 128.6, 127.6, 123.8, 114.2, 85.0, 78.9, 55.3; IR (KBr) 3367, 2919, 2845, 1784, 1722, 1517, 1255, 1185, 1013, 993, 962, 880, 830, 699 cm^{-1}; HRMS (FAB, NBA) *m/z* calcd for $C_{17}H_{15}NNaO_6$ $[M+Na]^+$ 352.0797, found 352.0780.

2-(2-hydroperoxy-2-phenylpropoxy)isoindoline-1,3-dione (5i)[1]



Prepared according to the general procedure to give **5i** in quantitative yield; White solid, mp. 112.3–115.0 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.78 (br s, O-O<u>H</u>), 7.85-7.81 (m, 2H), 7.77-7.73 (m, *2*H), 7.49 (d, *J* = 7.2 Hz, 2H), 7.36 (t, *J* = 7.2 Hz, 2H), 7.29 (t, *J* = 7.2 Hz, 1H), 4.68 (d, *J* = 9.6 Hz, 1H), 4.62 (d, *J* = 9.6 Hz, 1H), 1.65 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 163.7, 140.7, 134.8, 128.5, 128.4, 127.8, 125.3, 123.7, 84.3, 79.7, 22.7; IR (KBr) 3367, 3009, 2965, 1782, 1720, 1492, 1459, 1378, 1186, 1141, 1081, 1019, 1002, 965, 878, 763, 700, 577, 517 cm^{-1}; HRMS (FAB, NBA) *m/z* calcd for $C_{17}H_{15}NNaO_5$ $[M+Na]^+$ 336.0848, found 336.0845.

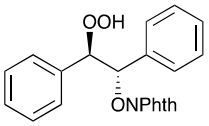
2-(((1*R,2*S**)-1-hydroperoxy-1-phenylpropan-2-yl)oxy)isoindoline-1,3-dione (*anti*-5j and *syn*-5j)**[1]



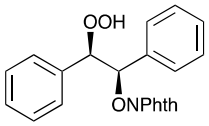
Prepared according to the general procedure to give *anti*-**5j** and *syn*-**5j** in 69% yield as a diastereomeric mixture (*anti*-**5j** : *syn*-**5j** = 4 : 1); The following physical data were measured as a diastereomeric mixture (*anti*-**5j** : *syn*-**5j** = 4 : 1). White solid, mp. 78.0–81.3 ˚C; Major diastereomer *anti*-**5j**: ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.97 (br s, O-O<u>H</u>), 7.88-7.84 (m, 2H), 7.80-7.76 (m, 2H), 7.44-7.42 (m, 2H), 7.39-7.31 (m, 3H), 5.16 (d, *J* = 3.4 Hz, 1H), 4.81 (qd, *J* = 6.6, 3.4 Hz, 1H), 1.28 (d, *J* = 6.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 164.6, 134.8, 128.7, 128.4, 128.1, 127.8, 123.8, 88.1, 84.3, 14.0; Minor diastereomer *syn*-**5j**: ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.71 (br s, O-O<u>H</u>), 7.88-7.84 (m, 2H), 7.80-7.76 (m, *2*H), 7.39-7.31 (m, 5H), 5.11 (d, *J* = 8.7 Hz, 1H), 4.62 (dq, *J* = 8.7,

6.6 Hz, 1H), 1.20 (d, J = 6.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 164.5, 136.8, 134.7, 128.8, 128.7, 128.6, 123.8, 91.0, 85.7, 16.9; IR (KBr) 3294, 3061, 2990, 2924, 1783, 1725, 1467, 1381, 1189, 1123, 1080, 978, 878, 761, 699, 518 cm^{-1}; HRMS (FAB, NBA) *m/z* calcd for $C_{17}H_{15}NNaO_5$ $[M+Na]^+$ 336.0848, found 336.0844.

2-((1*S,2*R**)-2-hydroperoxy-1,2-diphenylethoxy)isoindoline-1,3-dione (*anti*-5k and *syn*-5k)**



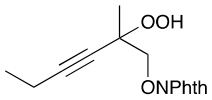
anti



syn

Prepared according to the general procedure except for the loading of $Mn(acac)_3$ (0.20 mol%) to give *anti*-**5k** and *syn*-**5k** in 80% yield as a diastereomeric mixture (*anti*-**5k** : *syn*-**5k** = 2 : 1); The diastereomeric mixture was partially separated by preparative TLC. Major diastereomer *anti*-**5k**: White solid, mp. 129.8–133.7 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.2 (br s, O-O<u>H</u>), 7.80-7.75 (m, 2H), 7.74-7.69 (m, 2H), 7.32-7.22 (m, 8H), 7.20-7.18 (m, 2H), 5.91 (d, J = 4.0 Hz, 1H), 5.23 (d, J = 4.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 164.1, 134.7, 133.9, 133.4, 128.9, 128.8, 128.6, 128.5, 127.9, 127.7, 123.7, 89.1, 87.9; IR (KBr) 3317, 3030, 2902, 1787, 1712, 1381, 1112, 1080, 1049, 977, 875, 732, 699 cm^{-1}; HRMS (FAB, NBA) *m/z* calcd for $C_{22}H_{17}NNaO_5$ $[M+Na]^+$ 398.1004, found 398.1014; Minor diastereomer *syn*-**5k**: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.83 (br s, O-O<u>H</u>), 7.81-7.77 (m, 2H), 7.75-7.71 (m, 2H), 7.27-7.24 (m, 2H), 7.22-7.20 (m, 8H), 5.57 (d, J = 9.2 Hz, 1H), 5.44 (d, J = 9.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 163.9, 135.8, 134.6, 134.5, 129.1, 128.7, 128.6, 128.5, 128.2, 128.1, 123.7, 90.7, 89.6; IR (neat) 3374, 3065, 3028, 2955, 2924, 2852, 1788, 1730, 1610, 1455, 1375, 1187, 1016, 980, 877, 760, 699, 518 cm^{-1}; HRMS (FAB, NBA) *m/z* calcd for $C_{22}H_{17}NNaO_5$ $[M+Na]^+$ 398.1004, found 398.0996.

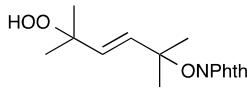
2-((2-hydroperoxy-2-methylhex-3-yn-1-yl)oxy)isoindoline-1,3-dione (7)



Prepared according to the general procedure to give **7** in 81% yield; White solid, mp. 67.6–70.3 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.44 (br s, O-O<u>H</u>), 7.88-7.84 (m, 2H), 7.80-7.75 (m, 2H), 4.50 (d, J = 10.1 Hz, 1H), 4.31 (d, J = 10.1 Hz, 1H), 2.22 (q, J = 7.6

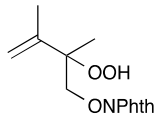
Hz, 2H), 1.62 (s, 3H), 1.12 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 163.5, 134.7, 128.5, 123.6, 89.0, 78.9, 77.8, 76.3, 21.5, 13.4, 12.2; IR (KBr) 3353, 2986, 2940, 2233, 1787, 1718, 1465, 1402, 1135, 1024, 1001, 879, 700, 617, 519 cm^{-1}; HRMS (FAB, NBA) *m/z* calcd for $C_{15}H_{15}NNaO_5$ $[M+Na]^+$ 312.0848, found 312.0848.

(*E*)-2-((5-hydroperoxy-2,5-dimethylhex-3-en-2-yl)oxy)isoindoline-1,3-dione (9a)



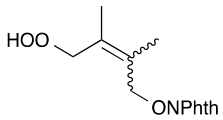
Prepared according to the general procedure except for the loading of $Mn(acac)_3$ (0.20 mol%) to give **9a** in 79% yield; White solid, mp. 79.0–82.2 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.08 (br s, O-O<u>H</u>), 7.83-7.79 (m, 2H), 7.76-7.71 (m, 2H), 6.08 (d, J = 16.4 Hz, 1H), 5.69 (d, J = 16.4 Hz, 1H), 1.54 (s, 6H), 1.29 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 165.7, 135.1, 134.5, 133.4, 129.0, 123.5, 87.1, 81.8, 24.9, 24.7; IR (KBr) 3360, 2984, 2929, 1787, 1726, 1683, 1466, 1375, 1257, 1122, 1079, 970, 879, 703, 518 cm^{-1}; HRMS (FAB, NBA) *m/z* calcd for $C_{16}H_{19}NNaO_5$ $[M+Na]^+$ 328.1161, found 328.1177.

2-((2-hydroperoxy-2,3-dimethylbut-3-en-1-yl)oxy)isoindoline-1,3-dione (9b)



Prepared according to the general procedure except for the loading of $Mn(acac)_3$ (0.20 mol%) to give **9b** in 61% yield; Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.68 (br s, O-O<u>H</u>), 7.85-7.80 (m, 2H), 7.78-7.73 (m, 2H), 4.97 (s, 1H), 4.93 (s, 1H), 4.46 (s, 2H), 1.86 (s, 3H), 1.39 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 163.8, 144.8, 134.8, 128.5, 123.7, 112.2, 84.1, 79.0, 20.0, 18.7; IR (neat) 3398, 2992, 2961, 2924, 1786, 1726, 1465, 1375, 1187, 1124, 1021, 878, 701, 519 cm^{-1}; HRMS (FAB, NBA) *m/z* calcd for $C_{14}H_{15}NNaO_5$ $[M+Na]^+$ 300.0848, found 300.0851.

(*E*/*Z*)-2-((4-hydroperoxy-2,3-dimethylbut-2-en-1-yl)oxy)isoindoline-1,3-dione (9c and 9c')



Prepared according to the general procedure except for the loading of $Mn(acac)_3$ (0.20 mol%) to give **9c** and **9c'** in 24% yield as a mixture of geometric isomers (**9c** : **9c'** = 3: 1); The following physical data were measured as a mixture of geometric isomers (**9c** : **9c'** = 3 : 1). White solid, mp. 75.6–79.7 ˚C; Major diastereomer **9c**: ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.44 (br s, O-OH), 7.85-7.80 (m, 2H), 7.78-7.71 (m, 2H), 4.74 (s, 2H), 4.53 (s, 2H), 2.02 (s, 3H), 1.82 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 164.0, 134.6, 133.9, 130.3, 129.9, 123.5, 78.5, 77.6, 17.7, 16.9; Minor diastereomer **9c'**: ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.35 (br s, O-OH), 7.85-7.80 (m, 2H), 7.78-7.71 (m, 2H), 4.78 (s, 2H), 4.57 (s, 2H), 1.99 (s, 3H), 1.81 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 164.0, 134.4, 134.0, 128.9, 128.8, 123.4, 77.2, 76.8, 18.2, 18.0; IR (KBr) 3334, 2924, 2855, 1784, 1719, 1706, 1464, 1397, 1187, 1143, 1079, 978, 878, 699, 515 cm^{-1}; HRMS (FAB, NBA) *m/z* calcd for $C_{14}H_{15}NNaO_5$ $[M+Na]^+$ 300.0848, found 300.0852.

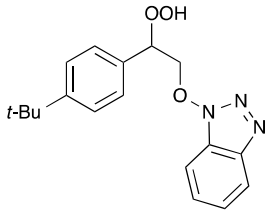
General procedure for the manganese-catalysed hydroperoxidation with HOBt

To a stirred solution of alkene (0.500 mmol) and 1-hydroxybenzotriazole monohydrate (0.500 mol) in MeCN (0.9 mL) at room temperature was added a solution of $Mn(acac)_3$ in MeCN (100 µl, 1.0 µmol, 0.20 mol% 10.0 mM in MeCN[b]) under air (open flask). The progress of the reaction was monitored by TLC analysis. The reaction was quenched saturated aqueous NaCl solution (0.5 mL). The resulting mixture was extracted with ethyl acetate (3 x 1.0 mL). The combined organic phases were washed with brine (2 x 1.0 mL), dried (Na_2SO_4), filtered, and concentrated under reduced pressure. The obtained crude material was purified by silica gel column chromatography using hexane and ethyl acetate as eluent.

[b] Preparation of MeCN solution of $Mn(acac)_3$: A 2.0 mL measuring flask was charged with $Mn(acac)_3$ (7.0 mg, 0.020 mmol) and diluted to total volume of 2.0 mL with MeCN (10.0 mM in MeCN).

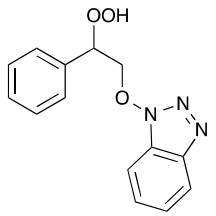
Analytical date for 10a, b, i, j, 12 and 14

1-(2-(4-(*tert*-butyl)phenyl)-2-hydroperoxyethoxy)-1*H*-benzo[*d*][1,2,3]triazole (10a)



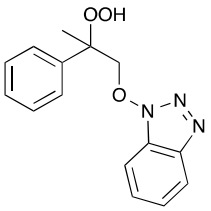
Prepared according to the general procedure to give **10a** in 52% yield; Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.74 (br s, O-O<u>H</u>), 8.00 (d, *J* = 8.4 Hz, 1H), 7.62-7.59 (m, 1H), 7.51 (t, *J* = 8.0 Hz, 1H), 7.43-7.37 (m, 3H), 7.33-7.31 (m, 2H), 5.39 (dd, *J* = 6.4, 5.2 Hz, 1H), 4.86-4.80 (m, 2H), 1.31 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 152.5, 132.1, 128.3, 127.0, 126.0, 125.9, 125.7, 124.8, 120.2, 109.0, 84.4, 80.1, 34.7, 31.2; IR (neat) 3250, 2962, 2905, 2872, 1913, 1701, 1617, 1509, 1443, 1363, 1267, 1240, 1099, 969, 832, 781, 766, 744, 588 cm^{-1}; HRMS (FAB, NBA) *m/z* calcd for $C_{18}H_{22}N_3O_3$ $[M+H]^+$ 328.1661, found 328.1667.

1-(2-hydroperoxy-2-phenylethoxy)-1*H*-benzo[*d*][1,2,3]triazole (10b)[1]



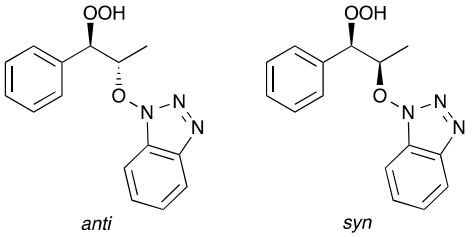
Prepared according to the general procedure to give **10b** in 90% yield; Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.59 (br s, O-O<u>H</u>), 8.02 (d, *J* = 8.4 Hz, 1H), 7.63 (d, *J* = 8.4 Hz, 1H), 7.53 (d, *J* = 8.4 Hz, 1H), 7.43-7.39 (m, 6H) 5.43 (dd, *J* = 6.4, 5.2 Hz, 1H), 4.83-4.81 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 143.2, 135.4, 129.1, 128.8, 128.3, 127.4, 127.2, 124.9, 120.0, 109.0, 84.3, 80.2; IR (neat) 3205, 2909, 2850, 1617, 1495, 1454, 1364, 1266, 1240, 1158, 1098, 969, 781, 744, 700 cm^{-1}; HRMS (FAB, NBA) *m/z* calcd for $C_{14}H_{13}N_3NaO_3$ $[M+Na]^+$ 294.0855, found 294.0851.

1-(2-hydroperoxy-2-phenylpropoxy)-1*H*-benzo[*d*][1,2,3]triazole (10i)



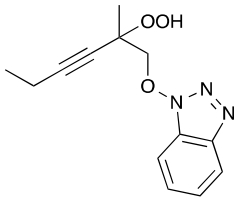
Prepared according to the general procedure to give **10i** in 96% yield; Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.00 (d, *J* = 8.4 Hz, 1H), 7.54-7.34 (m, 8H), 4.98 (d, *J* = 14.4 Hz, 1H), 4.94 (d, *J* = 14.4 Hz, 1H), 1.85 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 143.0, 140.2, 128.5, 128.0, 126.9, 125.5, 124.8, 119.7, 109.0, 84.1, 82.5, 21.7; IR (neat) 3222, 2989, 2852, 1608, 1446, 1374, 1240, 1099, 984, 744, 699 cm^{-1}; HRMS (FAB, NBA) *m/z* calcd for $C_{15}H_{15}N_3NaO_3$ $[M+Na]^+$ 308.1011, found 308.1010.

1-(((1*R,2*S**)-1-hydroperoxy-1-phenylpropan-2-yl)oxy)-1*H*-benzo[*d*][1,2,3]triazole (*anti*-10j and *syn*-10j)**



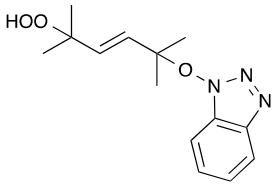
Prepared according to the general procedure to give *anti*-**10j** and *syn*-**10j** in 89% yield as a diastereomeric mixture (*anti*-**10j** : *syn*-**10j** = 5 : 1); The following physical data were measured as a diastereomeric mixture (*anti*-**10j** : *syn*-**10j** = 5 : 1). Colorless oil; Major diastereomer *anti*-**10j**: ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.73 (br s, O-O<u>H</u>), 8.02 (d, *J* = 8.4 Hz, 1H), 7.55-7.36 (m, 8H), 5.22 (d, *J* = 3.8 Hz, 1H), 5.09 (qd, *J* = 6.7, 3.8 Hz, 1H), 1.44 (d, *J* = 6.7 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 143.1, 135.3, 128.7, 128.5, 128.2, 128.1, 127.8, 124.8, 119.9, 109.1, 87.5, 87.4, 14.4; Minor diastereomer *syn*-**10j**: ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.51 (br s, O-O<u>H</u>), 8.03 (d, *J* = 8.4 Hz, 1H), 7.66 (d, *J* = 8.4 Hz, 1H), 7.55-7.36 (m, 7H), 5.30 (d, *J* = 8.0 Hz, 1H), 4.92 (dq, *J* = 8.0, 6.6 Hz, 1H), 1.30 (d, *J* = 6.6 Hz, 3H) ^{13}C NMR (100 MHz, $CDCl_3$) δ: 143.1, 136.3, 129.0, 128.4, 128.1, 128.0, 127.7, 124.8, 119.9, 109.3, 89.1, 87.4, 16.4; IR (neat) 3297, 3067, 3035, 2987, 2917, 2852, 1648, 1614, 1592, 1551, 1492, 1447, 1382, 1263, 1241, 1156, 1098, 1047, 781, 744, 700 cm^{-1}; HRMS (FAB, NBA) *m/z* calcd for $C_{15}H_{15}N_3NaO_3$ $[M+Na]^+$ 308.1011, found 308.1009.

1-((2-hydroperoxy-2-methylhex-3-yn-1-yl)oxy)-1*H*-benzo[*d*][1,2,3]triazole (12)



Prepared according to the general procedure except for the loading of $Mn(acac)_3$ (0.020 mol%) to give **12** in 80% yield; Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.37 (br s, O-O<u>H</u>), 8.02 (dt, *J* = 8.4 Hz, 1H), 7.71 (d, *J* = 8.4 Hz, 1H), 7.53 (t, *J* = 8.4 Hz, 1H), 7.40 (t, *J* = 8.4 Hz, 1H), 4.84 (d, *J* = 10.8, 1H), 4.64 (d, *J* = 10.8, 1H), 2.21 (q, *J* = 7.6 Hz, 2H), 1.70 (s, 3H), 1.12 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 143.3, 128.1, 127.3, 124.8, 120.1, 109.2, 90.0, 81.2, 78.4, 75.9, 21.8, 13.5, 12.3; IR (neat) 3219, 2985, 2942, 2245, 1616, 1445, 1372, 1243, 1098, 984, 784, 744 cm^{-1}; HRMS (FAB, NBA) *m/z* calcd for $C_{13}H_{15}N_3NaO_3$ $[M+Na]^+$ 284.1011, found 284.1015.

(*E*)-1-((5-hydroperoxy-2,5-dimethylhex-3-en-2-yl)oxy)-1*H*-benzo[*d*][1,2,3]triazole (14)



Prepared according to the general procedure to give **14** in 76% yield; Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.97 (br s, O-O<u>H</u>), 7.98 (d, *J* = 8.4 Hz, 1H), 7.56-7.48 (m, 2H), 7.36 (t, *J* = 6.4 Hz, 1H), 6.09 (d, *J* = 16.0 Hz, 1H), 5.64 (d, *J* = 16.0 Hz, 1H), 1.65 (s, 6H), 1.19 (s, 6H) ^{13}C NMR (100 MHz, $CDCl_3$) δ: 142.7, 137.3, 131.9, 129.7, 127.9, 124.4, 120.0, 109.7, 90.1, 81.3, 25.3, 24.1; IR (neat) 3237, 2982, 2934, 1720, 1617, 1445, 1371, 1298, 1267, 1242, 1144, 1120, 1093, 982, 849, 770, 745, 624, 580 cm^{-1}; HRMS (FAB, NBA) *m/z* calcd for $C_{14}H_{19}N_3NaO_3$ $[M+Na]^+$ 300.1324, found 300.1321.

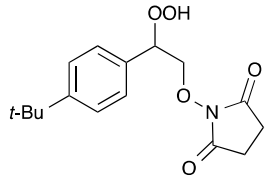
General procedure for the manganese-catalysed hydroperoxidation with NHS

To a stirred solution of alkene (0.500 mmol) and *N*-hydroxysuccinimide (0.500 mol) in MeCN (0.9 mL) at room temperature was added a solution of $Mn(acac)_3$ in MeCN (100 µl, 1.0 µmol, 0.20 mol%, 10.0 mM in MeCN[b]) under air (open flask). The progress of the reaction was monitored by TLC analysis. The reaction was quenched saturated aqueous NaCl solution (0.5 mL). The resulting mixture was extracted with ethyl acetate (3 x 1.0 mL). The combined organic phases were washed with brine (2 x 1.0 mL), dried (Na_2SO_4), filtered, and concentrated under reduced pressure. The obtained crude material was purified by silica gel column chromatography using hexane and ethyl acetate as eluent.

[b] Preparation of MeCN solution of $Mn(acac)_3$: A 2.0 mL measuring flask was charged with $Mn(acac)_3$ (7.0 mg, 0.020 mmol) and diluted to total volume of 2.0 mL with MeCN (10.0 mM in MeCN).

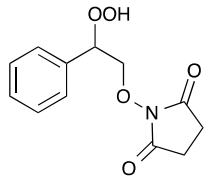
Analytical date for 11a, b, i, j, 13 and 15

1-(2-(4-(*tert*-butyl)phenyl)-2-hydroperoxyethoxy)pyrrolidine-2,5-dione (11a)



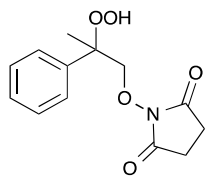
Prepared according to the general procedure to give **11a** in 69% yield; White solid, mp. 39.7–43.3 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.41 (br s, O-O<u>H</u>), 7.39 (d, *J* = 8.5 Hz, 2H), 7.30 (d, *J* = 8.5 Hz, 2H), 5.33 (dd, *J* = 8.1, 3.3 Hz, 1H), 4.47 (dd, *J* = 11.4, 3.3 Hz, 1H), 4.40 (dd, *J* = 11.4, 8.1 Hz, 1H), 2.76 (s, 4H), 1.31 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 171.7, 152.0, 132.4, 126.9, 125.7, 85.2, 77.7, 34.6, 31.2, 25.4; IR (KBr) 3293, 2963, 1777, 1719, 1509, 1364, 1208, 1078, 832, 651 cm^{-1}; HRMS (FAB, NBA) *m/z* calcd for $C_{16}H_{21}NNaO_5$ $[M+Na]^+$ 330.1317, found 330.1310.

1-(2-hydroperoxy-2-phenylethoxy)pyrrolidine-2,5-dione (11b)



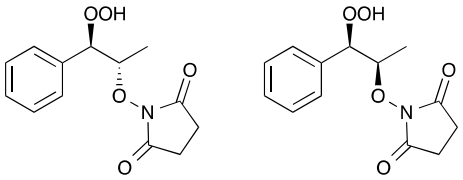
Prepared according to the general procedure to give **11b** in 80% yield; White solid, mp. 52.1–56.3 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.52 (br s, O-O<u>H</u>), 7.38-7.34 (m, 5H), 5.35 (dd, *J* = 8.2, 3.2 Hz, 1H), 4.47 (dd, *J* = 11.5, 3.2 Hz, 1H), 4.39 (dd, *J* = 11.5, 8.2 Hz, 1H), 2.76 (s, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 171.7, 135.5, 128.8, 128.7, 127.1, 85.3, 77.6, 25.4; IR (KBr) 3368, 2944, 1787, 1719, 1398, 1375, 1208, 1078, 993, 816, 765, 701, 653 cm^{-1}; HRMS (FAB, NBA) *m/z* calcd for $C_{12}H_{13}NNaO_5$ $[M+Na]^+$ 274.0691, found 274.0699.

1-(2-hydroperoxy-2-phenylpropoxy)pyrrolidine-2,5-dione (11i)



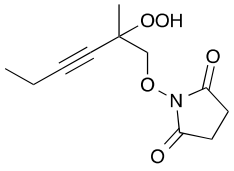
Prepared according to the general procedure to give **11i** in 92% yield; White solid, mp. 129.8–133.9 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.84 (br s, O-O<u>H</u>), 7.46 (d, *J* = 7.2, 2H), 7.37 (t, *J* = 7.2, 2H), 7.30 (t, *J* = 7.2, 1H), 4.59 (d, *J* = 9.4, 1H), 4.51 (d, *J* = 9.4 Hz, 1H), 2.74 (s, 4H), 1.60 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 171.6, 140.6, 128.5, 127.9, 125.3, 84.3, 78.5, 25.4, 22.9; IR (KBr) 3309, 2986, 1773, 1707, 1446, 1396, 1212, 1078, 980, 815, 785, 760, 695, 656, 579 cm^{-1}; HRMS (FAB, NBA) *m/z* calcd for $C_{13}H_{15}NNaO_5$ $[M+Na]^+$ 288.0848, found 288.0852.

1-(((1*R,2*S**)-1-hydroperoxy-1-phenylpropan-2-yl)oxy)pyrrolidine-2,5-dione (*anti*-11j and *syn*-11j)**



Prepared according to the general procedure to give *anti*-**11j** and *syn*-**11j** in 67% yield as a diastereomeric mixture (*anti*-**11j** : *syn*-**11j** = 3.5 : 1); The following physical data were measured as a diastereomeric mixture (*anti*-**11j** : *syn*-**11j** = 3.5 : 1). White solid, mp. 78.3–81.1 ˚C; Major diastereomer *anti*-**11j**: ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.0 (br s, O-O<u>H</u>), 7.42-7.30 (m, 5H), 5.03 (d, *J* = 3.5 Hz, 1H), 4.79 (qd, *J* = 6.6, 3.5 Hz, 1H), 2.76 (s, 4H), 1.21 (d, *J* = 6.6, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 172.4, 134.5, 128.7, 128.4, 128.3, 88.1, 83.0, 25.4, 14.4; Minor diastereomer *syn*-**11j**: ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.52 (O-O<u>H</u>), 7.42-7.30 (m, 5H), 5.06 (d, *J* = 8.8 Hz, 1H), 4.51 (dq, *J* = 8.8, 6.6 Hz, 1H), 2.79 (s, 4H), 1.13 (d, *J* = 6.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 172.4, 136.8, 128.8, 128.7, 127.7, 91.3, 84.5, 25.4, 16.8; IR (KBr) 3319, 3063, 2994, 2934, 1793, 1702, 1451, 1388, 1205, 1081, 814, 745, 698, 652 cm^{-1}; HRMS (FAB, NBA) *m/z* calcd for $C_{13}H_{15}NNaO_5$ $[M+Na]^+$ 288.0848, found 288.0841.

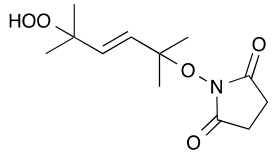
1-((2-hydroperoxy-2-methylhex-3-yn-1-yl)oxy)pyrrolidine-2,5-dione (13)



Prepared according to the general procedure except for the loading of $Mn(acac)_3$ (0.020

mol%) to give **13** in 20% yield; White solid, mp. 107.0–111.1 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.43 (br s, O-O<u>H</u>), 4.41 (d, *J* = 10.3 Hz, 1H), 4.15 (d, *J* = 10.3 Hz, 1H), 2.74 (s, 4H), 2.23 (q, *J* = 7.5 Hz, 2H), 1.57 (s, 3H), 1.13 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 171.4, 89.3, 78.0, 77.6, 76.2, 25.4, 21.5, 13.5, 12.3; IR (KBr) 3287, 2973, 2939, 2239, 1773, 1707, 1399, 1211, 1083, 984, 816, 774, 654 cm^{-1}; HRMS (FAB, NBA) *m/z* calcd for $C_{11}H_{15}NNaO_5$ $[M+Na]^+$ 264.0848, found 264.0850.

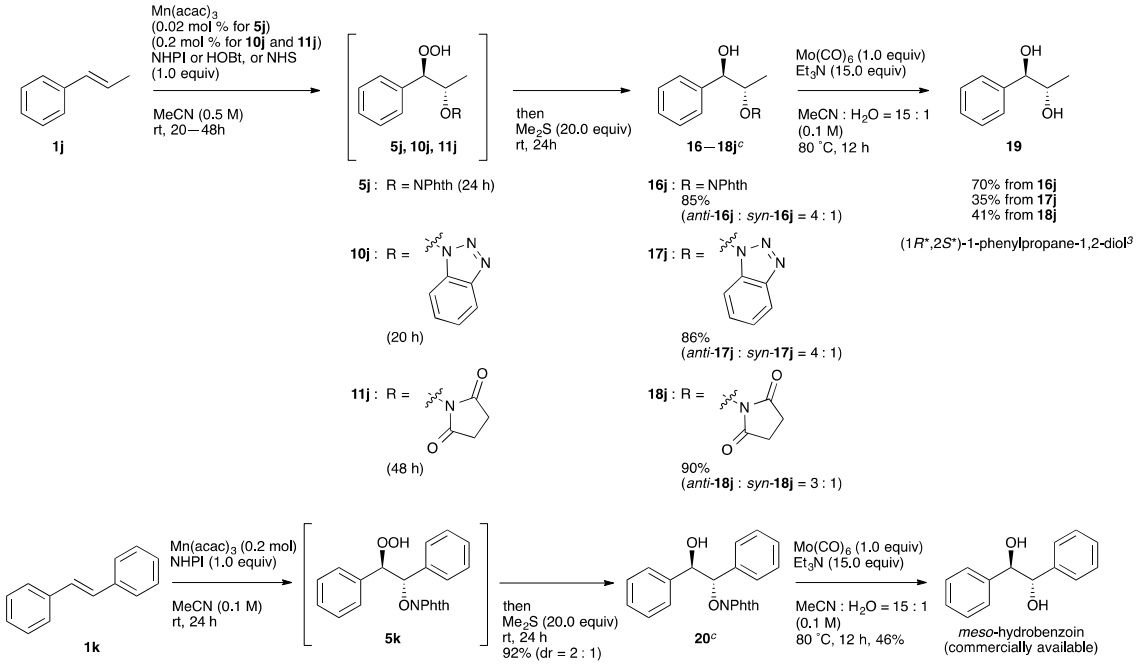
(*E*)-1-((5-hydroperoxy-2,5-dimethylhex-3-en-2-yl)oxy)pyrrolidine-2,5-dione (15)



Prepared according to the general procedure to give **15** in 51% yield; White solid, mp. 119.0–122.5 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.07 (br s, O-O<u>H</u>), 5.96 (d, *J* = 16.4 Hz, 1H), 5.68 (d, *J* = 16.4 Hz, 1H), 2.68 (s, 4H), 1.48 (s, 6H), 1.31 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 173.3, 135.4, 132.9, 87.6, 81.7, 25.5, 25.0, 24.7; IR (KBr) 3364, 2980, 2936, 1784, 1719, 1377, 1304, 1263, 1200, 1145, 1070, 996, 849, 816, 767, 655, 577 cm^{-1}; HRMS (FAB, NBA) *m/z* calcd for $C_{12}H_{19}NNaO_5$ $[M+Na]^+$ 280.1161, found 280.1165.

Determination of the relative configuration of the major diastereomer in 5j, 5k, 10j and 11j

After the manganese-catalysed hydroperoxidation of C–C double bond, peroxides **5j**, **5k**, **10j** and **11j** can be readily reduced by the addition of Me_2S in one-pot to afford the corresponding hydroxy compounds **16**–**18j** and **20**[c], respectively. In addition, treatment of these hydroxyl compounds **16**–**18j** and **20** with $Mo(CO)_6$[2] led to known synthetic-**19**[3] and synthetic-hydrobenzoin, respectively. By comparison of the chemical shifts in ^{1}H-NMR of synthetic-**19** and synthetic-hydrobenzoin with previous reported (1*R**, 2*S**)-1-phenylpropane-1,2-diol[3] and commercially available *meso*-hydrobenzoin, the relative configuration of the major diastereomer of **5j**, **5k**, **10j** and **11j** was determined to be *anti*-isomer.

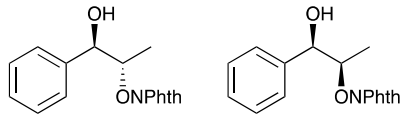


[c] The isolation yields of alcohols **16—18j** and **20** were improved than that of peroxides (**5j**, **5k**, **10j** and **11j**). These results indicated that the peroxides (**5j**, **5k**, **10j** and **11j**) were partially decomposed on silica gel for purification.

General procedure for the synthesis of alcohols 16–18j and 20[c]

After the manganese-catalysed hydroperoxidation reactions (5.0 mmol scale, 0.5 M in MeCN), the reaction mixture was treated with Me_2S (100.0 mmol, 20.0 equiv) at room temperature. After the reaction mixture was stirred for 24 h at room temperature, the saturated aqueous NaCl was added. The resultant mixture was extracted with $CHCl_3$ (3 × 10 mL) and successively washed with brine (1 × 20 mL). The organic phases were dried over Na_2SO_4 and concentrated under reduced pressure. The obtained crude material was purified on silica gel column chromatography using hexane and ethyl acetate as eluent.

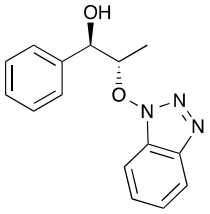
2-(((1*R,2*S**)-1-hydroxy-1-phenylpropan-2-yl)oxy)isoindoline-1,3-dione (*anti*-16j and *syn*-16j)**



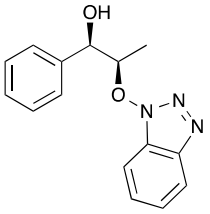
anti *syn*

Prepared according to the general procedure to give *anti*-**16j** and *syn*-**16j** in 85% yield as a diastereomeric mixture (*anti*-**16j** : *syn*-**16j** = 4 : 1); The diastereomeric mixture was partially separated by preparative TLC. Major diastereomer *anti*-**16j**: White solid, mp. 99.2–101.3 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.84-7.79 (m, 2H), 7.75-7.70 (m, 2H), 7.28-7.22 (m, 3H), 7.19-7.15 (m, 2H), 4.95-4.93 (m, 1H), 4.40 (qd, *J* = 6.8, 2.8 Hz, 1H), 3.94 (d, *J* = 3.6 Hz, O<u>H</u>), 1.13 (d, *J* = 6.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 164.9, 138.6, 134.8, 128.8, 128.2, 127.3, 125.8, 123.9, 88.1, 71.5, 11.1; IR (KBr) 3502, 3062, 3027, 2993, 2934, 1787, 1728, 1605, 1508, 1467, 1451, 1375, 1290, 1239, 1186, 1124, 1057, 976, 878, 748, 700, 518 cm^{-1}; HRMS (FAB, NBA) *m/z* calcd for $C_{17}H_{15}NNaO_4$ $[M+Na]^+$ 320.0899, found 320.0902; Minor diastereomer *syn*-**16j**: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.89-7.83 (m, 2H), 7.81-7.75 (m, 2H), 7.38-7.24 (m, 5H), 4.68 (dd, *J* = 8.4, 2.8 Hz, 1H), 4.60 (d, *J* = 2.8 Hz, 1H), 4.36 (dq, *J* = 8.4, 6.4 Hz, 1H), 1.25 (d, *J* = 6.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 164.9, 139.5, 134.8, 128.7, 128.5, 128.1, 127.0, 123.8, 91.0, 76.7, 16.4; IR (neat) 3470, 3062, 3030, 2983, 2927, 1788, 1730, 1608, 1496, 1468, 1453, 1382, 1328, 1234, 1187, 1120, 1025, 980, 878, 759, 700, 519 cm^{-1}; HRMS (FAB, NBA) *m/z* calcd for $C_{17}H_{15}NNaO_4$ $[M+Na]^+$ 320.0899, found 320.0895.

(1*R,2*S**)-2-((1*H*-benzo[*d*][1,2,3]triazol-1-yl)oxy)-1-phenylpropan-1-ol (*anti*-17j and *syn*-17j)**



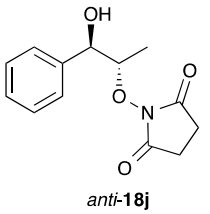
anti-**17j**



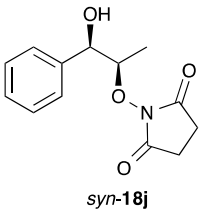
syn-**17j**

Prepared according to the general procedure to give *anti*-**17j** and *syn*-**17j** in 86% yield as a diastereomeric mixture (*anti*-**17j** : *syn*-**17j** = 4 : 1); The following physical data were measured as a diastereomeric mixture (*anti*-**17j** : *syn*-**17j** = 4 : 1). Light orange oil; Major diastereomer *anti*-**17j**: ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.97 (d, *J* = 8.0 Hz, 1H), 7.56-7.23 (m, 8H), 5.14 (d, *J* = 3.2 Hz, 1H), 4.86-4.80 (m, 1H), 3.38 (br s, O<u>H</u>), 1.36 (d, *J* = 6.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 143.4, 139.1, 128.7, 128.5, 128.1, 127.1, 126.2, 124.7, 120.3, 108.9, 90.5, 73.2, 12.3; Minor diastereomer *syn*-**17j**: ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.97 (d, *J* = 8.0 Hz, 1H), 7.56-7.23 (m, 8H), 4.97 (d, *J* = 7.6 Hz, 1H), 4.81-4.75 (m, 1H), 3.70 (br s, O<u>H</u>) 1.21 (d, *J* = 6.4 Hz, 3H) ^{13}C NMR (100 MHz, $CDCl_3$) δ: 143.4, 139.2, 128.6, 128.3, 128.2, 128.2, 128.0, 124.7, 120.2, 109.1, 91.4, 76.3, 15.8; IR (neat) 3378, 3064, 3027, 2957, 2922, 2867, 2848, 1724, 1616, 1491, 1447, 1382, 1326, 1262, 1240, 1195, 1157, 1099, 1047, 994, 744, 700 cm^{-1}; HRMS (FAB, NBA) *m/z* calcd for $C_{15}H_{16}N_3O_2$ $[M+H]^+$ 270.1243, found 270.1240

1-(((1*R,2*S**)-1-hydroxy-1-phenylpropan-2-yl)oxy)pyrrolidine-2,5-dione (*anti*-18j and *syn*-18j)**



anti-**18j**

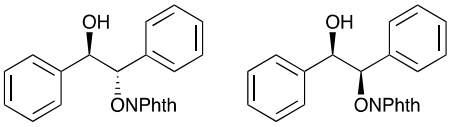


syn-**18j**

Prepared according to the general procedure to give *anti*-**18j** and *syn*-**18j** in 90% yield as a diastereomeric mixture (*anti*-**18j** : *syn*-**18j** = 3 : 1); The following physical data were measured as a diastereomeric mixture (*anti*-**18j** : *syn*-**18j** = 3 : 1). Colorless oil; Major diastereomer *anti*-**18j**: ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.35-7.25 (m, 5H), 4.85 (t, *J* = 3.2 Hz, 1H), 4.45-4.39 (m, 1H), 4.04 (d, *J* = 3.2 Hz, O<u>H</u>), 2.81 (s, 4H), 1.15 (d, *J* =

6.8, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 172.7, 138.4, 127.9, 127.1, 125.6, 86.8, 71.3, 25.1, 11.3; Minor diastereomer *syn*-**18j**: ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.35-7.25 (m, 5H), 4.65 (dd, *J* = 6.8, 4.0 Hz, 1H), 4.41-4.36 (m, 1H), 2.60 (s, 4H), 1.27 (d, *J* = 6.4, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 172.4, 139.5, 128.1, 127.7, 126.4, 89.3, 76.0, 24.9, 16.3; IR (neat) 3471, 3060, 3030, 2989, 2936, 2867, 1781, 1715, 1494, 1451, 1429, 1384, 1204, 1153, 1075, 1055, 994, 817, 735, 702, 651 cm^{-1}; HRMS (FAB, NBA) *m/z* calcd for $C_{13}H_{16}NO_4$ $[M+H]^+$ 250.1079, found 250.1085.

2-((1*S,2*R**)-2-hydroxy-1,2-diphenylethoxy)isoindoline-1,3-dione (*anti*-20 and *syn*-20)**



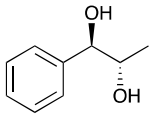
anti *syn*

Prepared according to the general procedure to give *anti*-**20** and *syn*-**20** in 92% yield as a diastereomeric mixture (*anti*-**20** : *syn*-**20** = 2 : 1); The diastereomeric mixture was partially separated by preparative TLC. Major diastereomer *anti*-**20**: White solid, mp. 138.0–140.0 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.88-7.82 (m, 2H), 7.79-7.74 (m, 2H), 7.30-7.18 (m, 8H), 7.14-7.10 (m, 2H), 5.37 (d, *J* = 4.0 Hz, 1H), 5.27-5.26 (m, 1H), 3.97 (br s, O<u>H</u>); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 164.4, 138.1, 134.8, 133.2, 128.9, 128.8, 128.8, 127.9, 127.7, 127.6, 126.6, 123.8, 92.5, 73.5; IR (KBr) 3496, 3067, 3032, 2922, 1786, 1727, 1605, 1494, 1468, 1453, 1375, 1326, 1186, 1123, 1080, 1059, 1016, 980, 877, 756, 700 cm^{-1}; HRMS (FAB, NBA) *m/z* calcd for $C_{22}H_{17}NNaO_4$ $[M+Na]^+$ 382.1055, found 382.1056; Minor diastereomer *syn*-**20**: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.79-7.75 (m, 2H), 7.73-7.69 (m, 2H), 7.24-7.20 (m, 5H), 7.16-7.10 (m, 5H), 5.21 (d, *J* = 8.8 Hz, 1H), 5.14 (d, *J* = 8.8 Hz, 1H), 4.28 (br s, O<u>H</u>); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 163.8, 138.4, 134.9, 134.6, 129.0, 128.7, 128.3, 128.0, 128.0, 127.9, 127.2, 123.7, 95.8, 76.8; IR (neat) 3480, 3064, 3030, 2925, 1788, 1730, 1608, 1496, 1468, 1455, 1375, 1187, 1129, 1079, 1062, 1016, 981, 877, 763, 699, 518 cm^{-1}; HRMS (FAB, NBA) *m/z* calcd for $C_{22}H_{17}NNaO_4$ $[M+Na]^+$ 382.1055, found 382.1055.

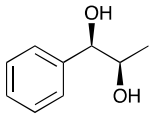
The synthesis of (1*R,2*S**)-1-phenylpropane-1,2-diol and *meso*-hydrobenzoin**

To a solution of **16–18j** or **20** (0.3 mmol) in CH_3CN/H_2O (15 : 1, 2.5 mL) at room temperature was added $Mo(CO)_6$ (0.3 mmol, 79.2 mg) and Et_3N (4.5 mmol, 0.6 mL). The reaction mixture was stirred at 80 °C for 12 h. The resultant mixture was filtered through a pad of celite with ethyl acetate. The filtrate was washed with brine, dried over Na_2SO_4 and concentrated under reduced pressure. The obtained crude material was purified on silica gel column chromatography using hexane and ethyl acetate as eluent.

(1*R,2*S**)-1-phenylpropane-1,2-diol (*anti*-19 and *syn*-19)**



anti

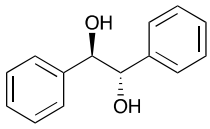


syn

The following physical data were measured as a diastereomeric mixture.

Major diastereomer *anti*-**19**: ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.39-7.34 (m, 5H), 4.68 (d, *J* = 4.4 Hz, 1H), 4.02 (qd, *J* = 6.4, 4.4 Hz, 1H), 2.41 (br s, O<u>H</u>), 1.92 (br s, O<u>H</u>), 1.09 (d, *J* = 6.4 Hz, 3H); Minor diastereomer *syn*-**19**: ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.33-7.28 (m, 5H), 4.38 (d, *J* = 7.2 Hz, 1H), 3.90-3.84 (m, 1H), 1.07 (d, *J* = 6.4 Hz, 3H).

***meso*-hydrobenzoin**



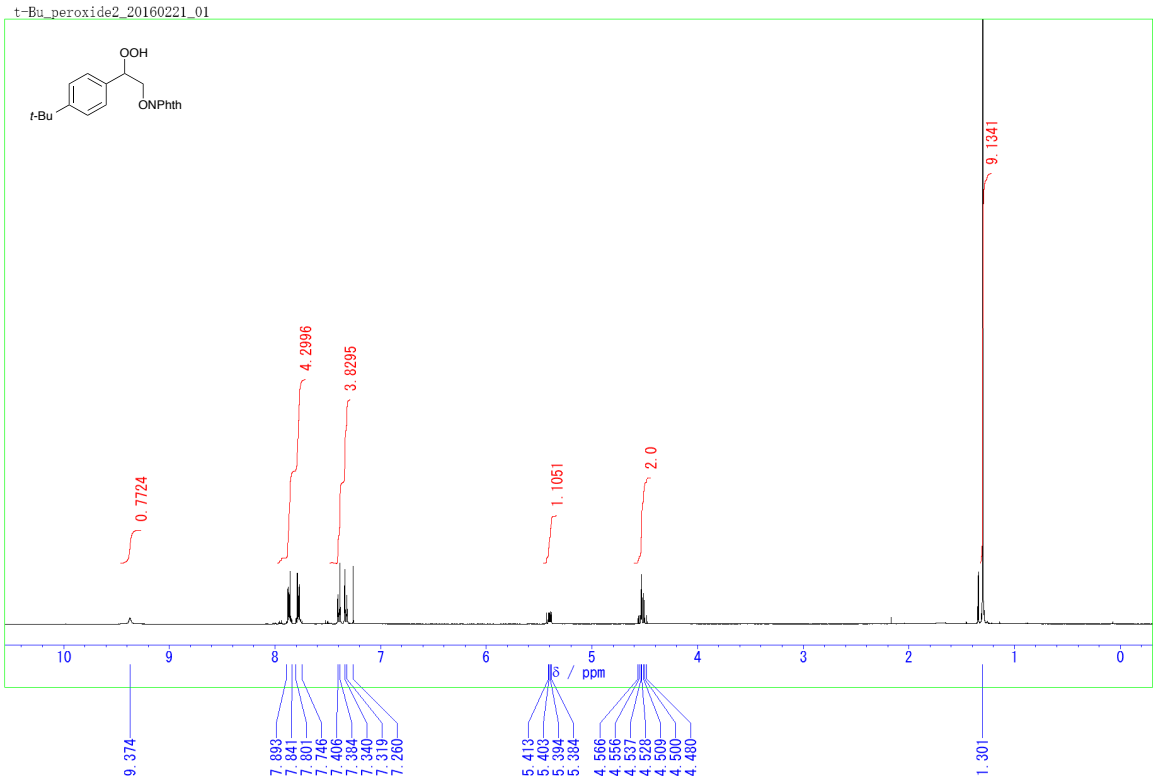
^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.34-7.25 (m, 5H), 4.84 (br s, 1H), 2.17 (br s, O<u>H</u>).

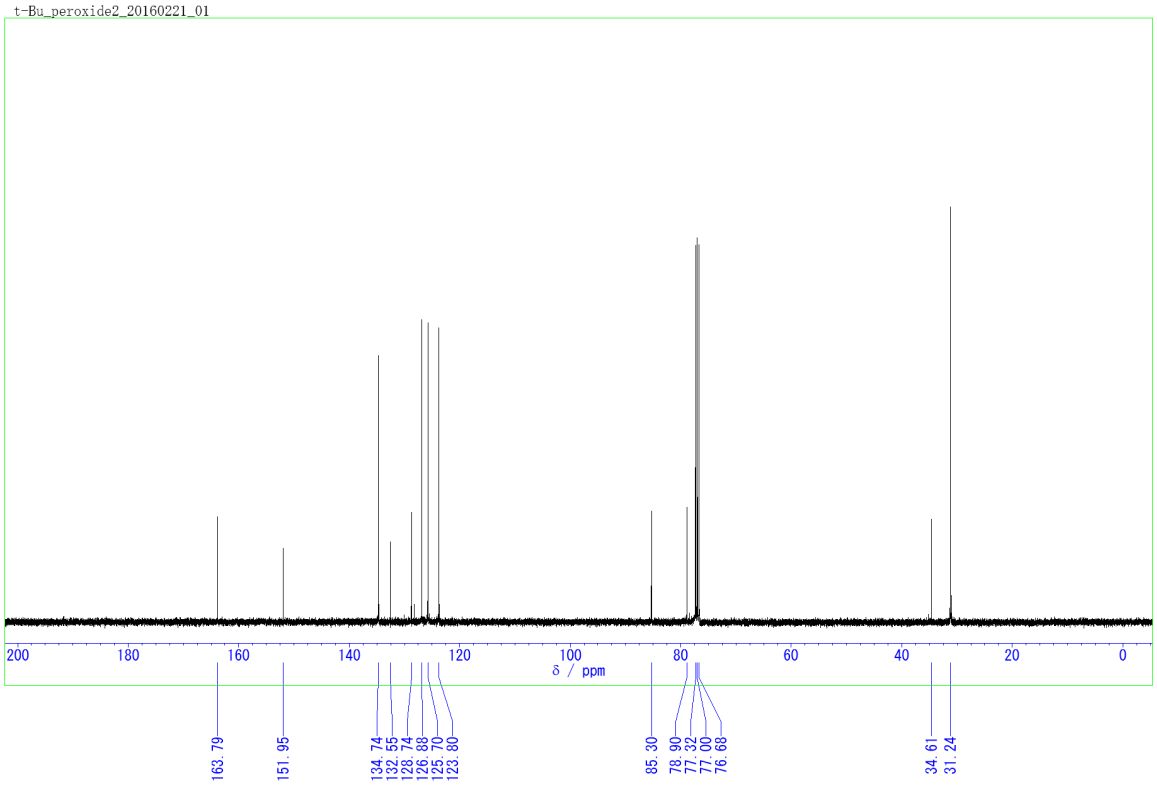
Reference:

1 R. Bag, D. Sar and T. Punniyamurthy, *Org. Biomol. Chem.*, 2016, **14**, 3246.

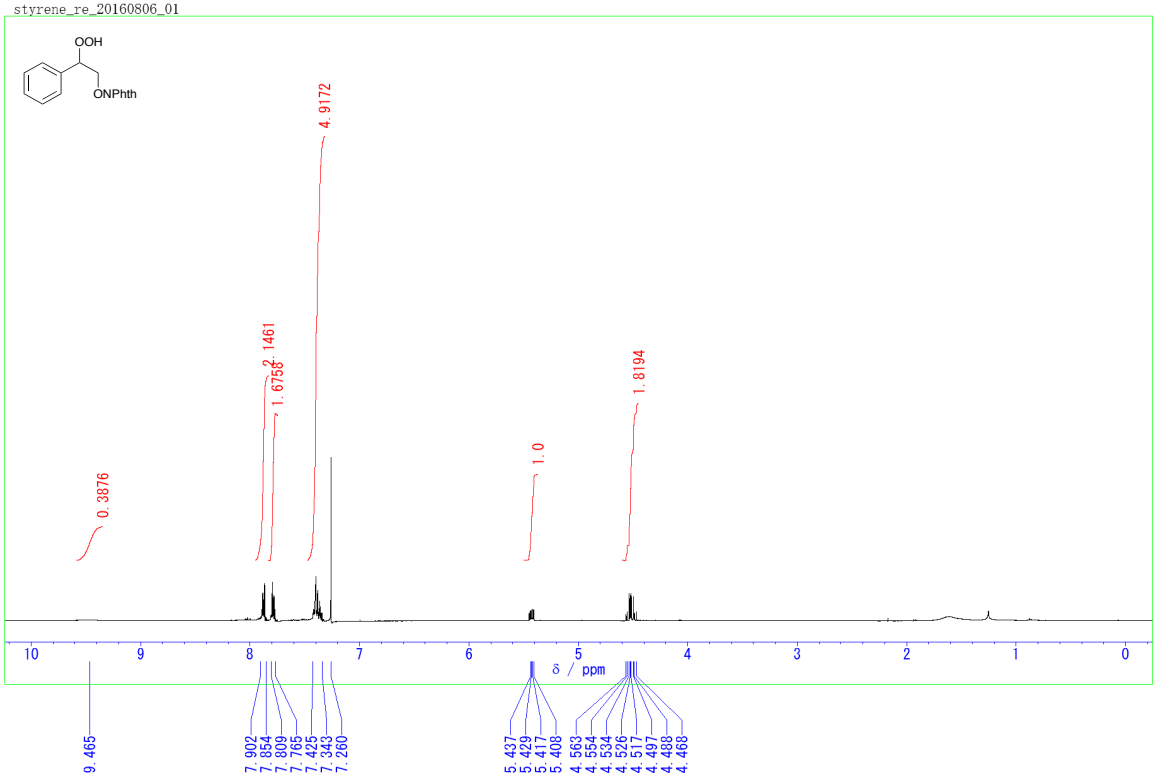
2 X.-F. Xia, S.-L. Zhu, Z. Gu, H. Wang, W. Li, X. Liu and Y.-M. Liang, *J. Org. Chem.*, 2015, **80**, 5572.

3 (a) C. Alamillo-Ferrer, S. C. Davidson, M. J. Rawling, N. H. Theodoulou, M. Campbell, P. G. Humphreys, A. R. Kennedy and N. C. O. Tomkinson, *Org. Lett.*, 2015, **17**, 5132; (b) S. M. Husain, T. Stillger, P. Dünkelmann, M. Lödige, L. Walter, E. Breitling, M. Pohl, M. Bürchner, I. Krossing, M. Müller, D. Romano and F. Molinari, *Adv. Synth. Catal.*, 2011, **353**, 2359.

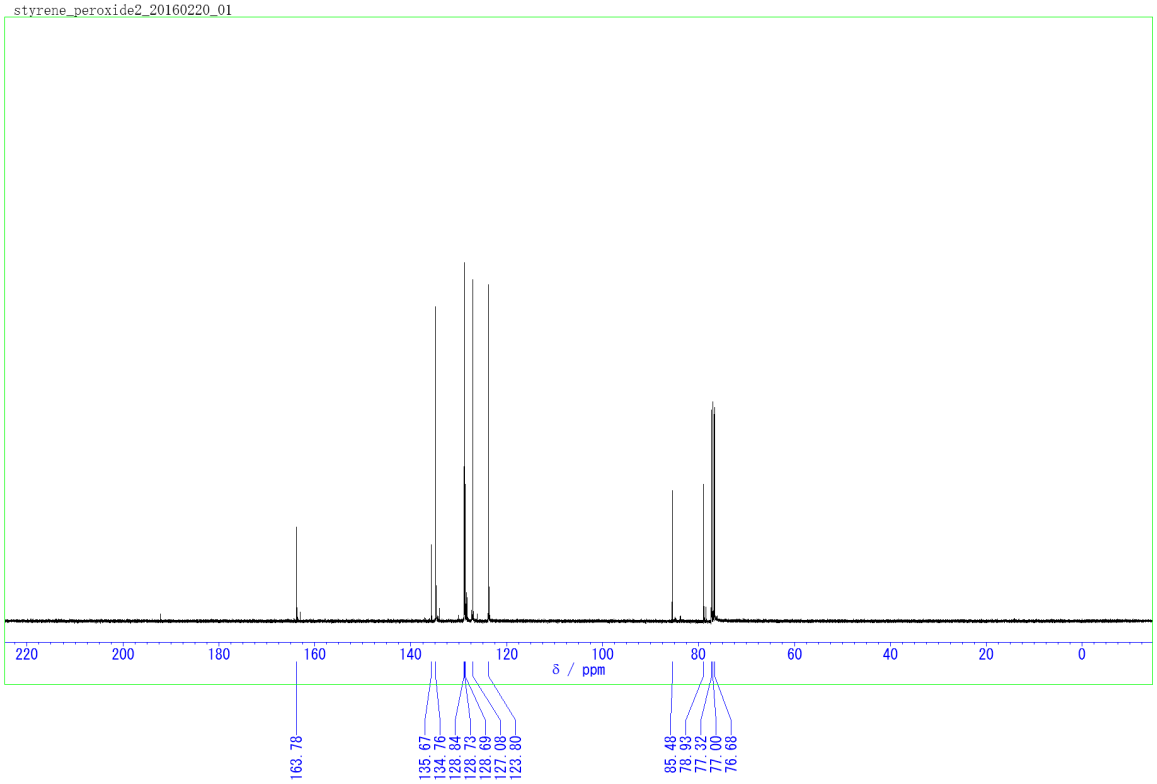

t-Bu_peroxide2_20160221_01
OOH
t-Bu
ONPhth
9.1341
4.2996
3.8295
2.0
1.1051
0.7724
δ / ppm
9.374
7.893
7.841
7.801
7.746
7.406
7.384
7.340
7.319
7.260
5.413
5.403
5.394
5.384
4.566
4.556
4.537
4.528
4.509
4.500
4.480
1.301

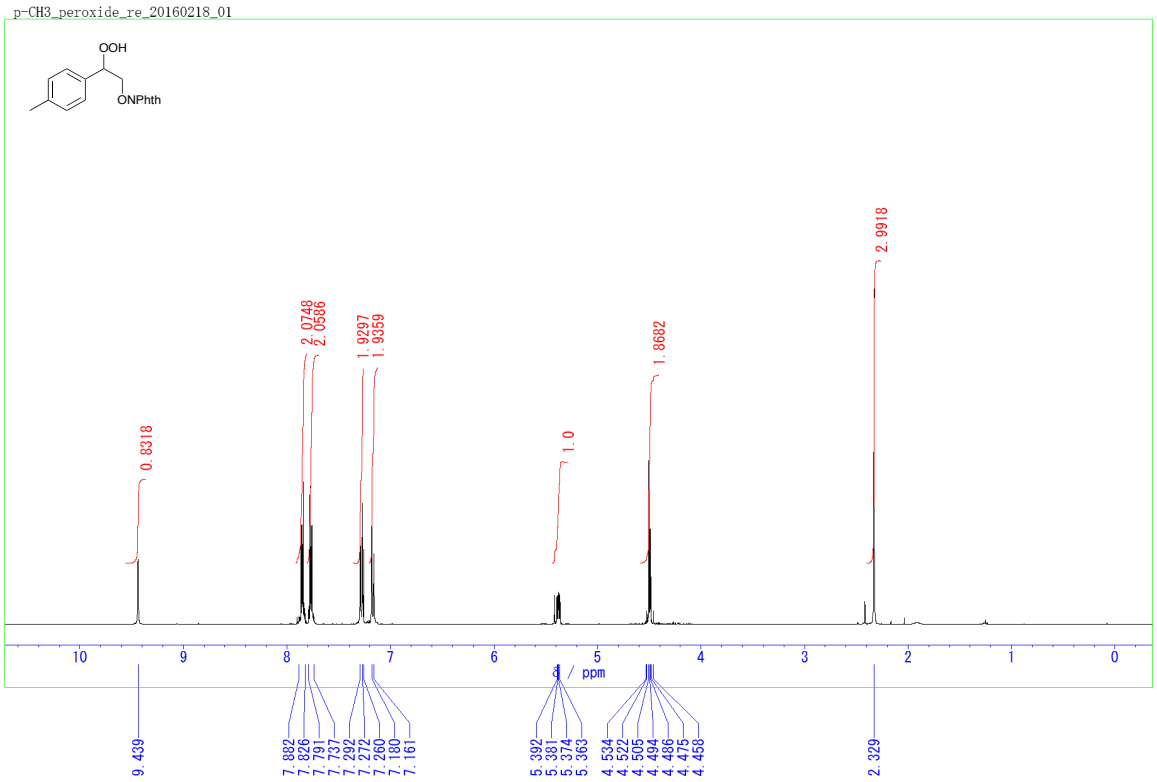

t-Bu_peroxide2_20160221_01
δ / ppm
163.79
151.95
134.74
132.55
128.74
126.88
125.70
123.80
85.30
78.90
77.32
77.00
76.68
34.61
31.24

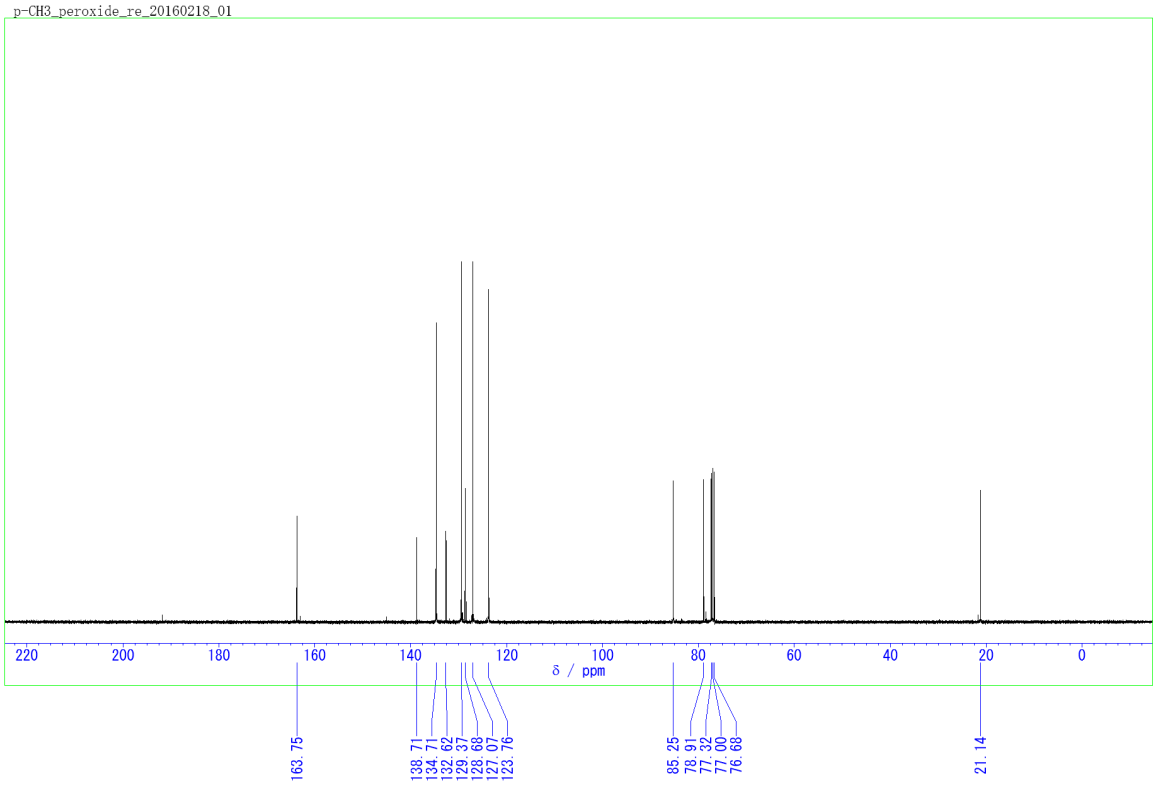
styrene_re_20160806_01

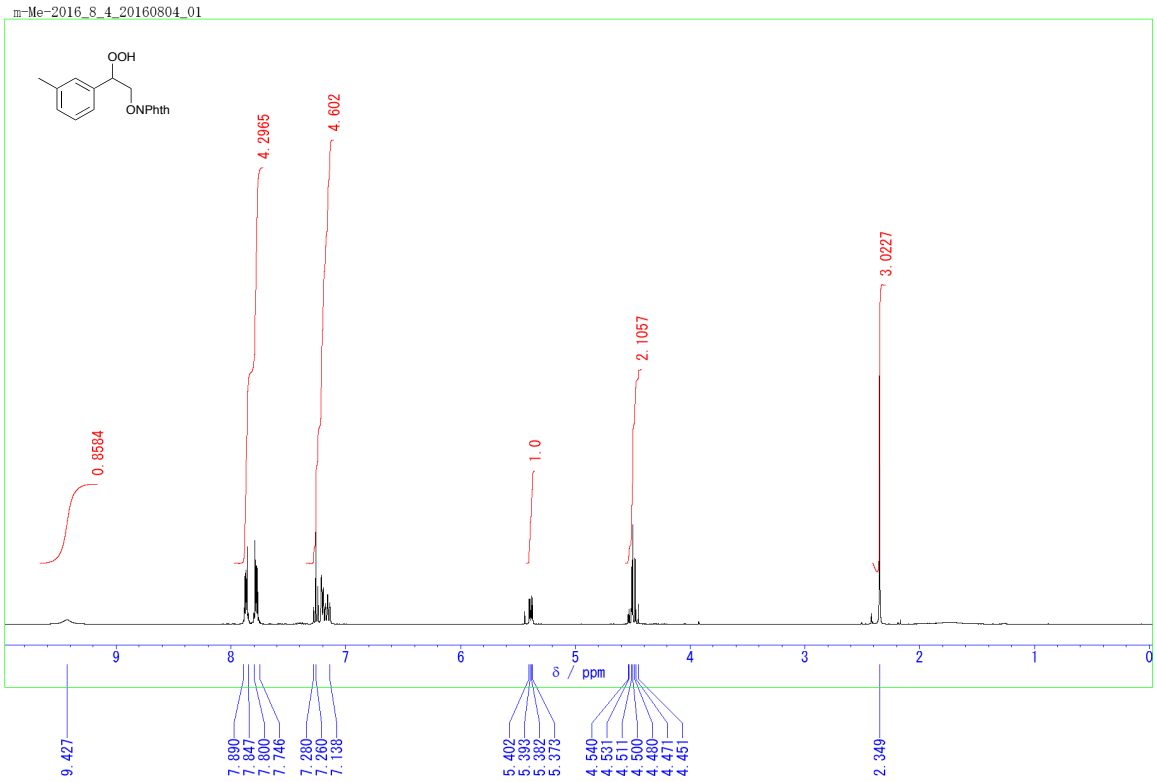


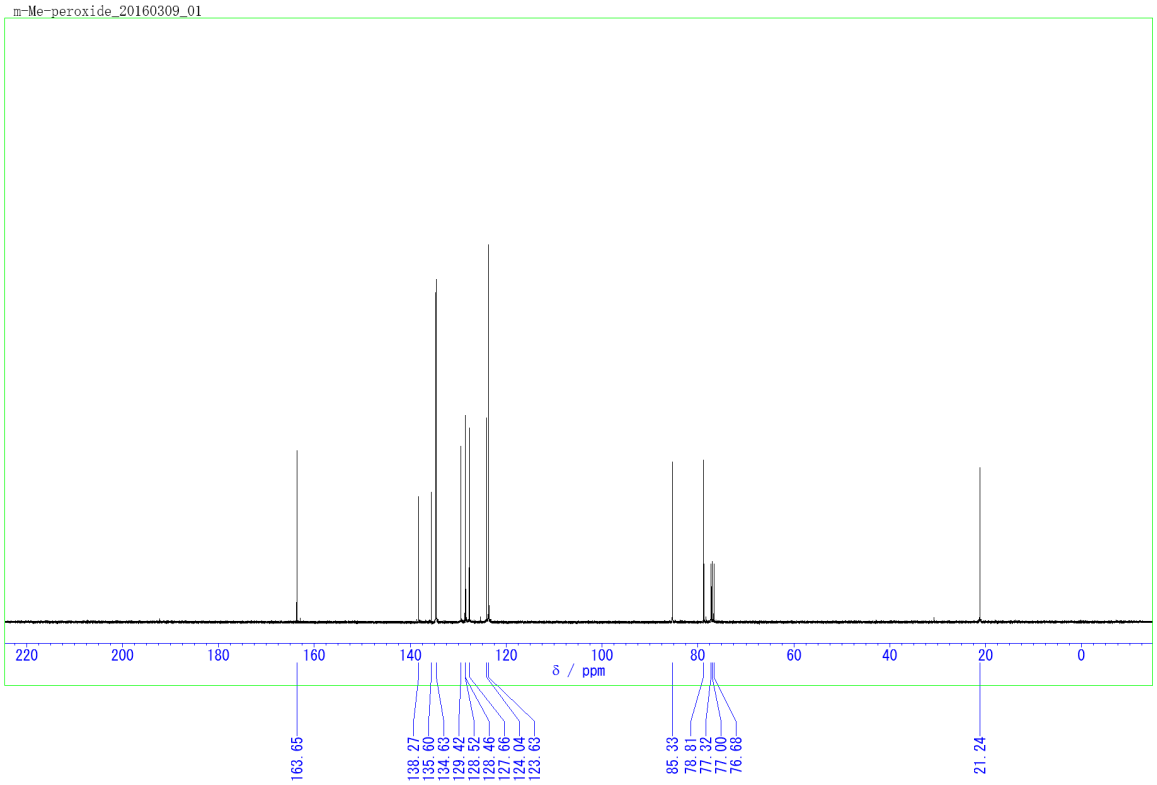
styrene_peroxide2_20160220_01



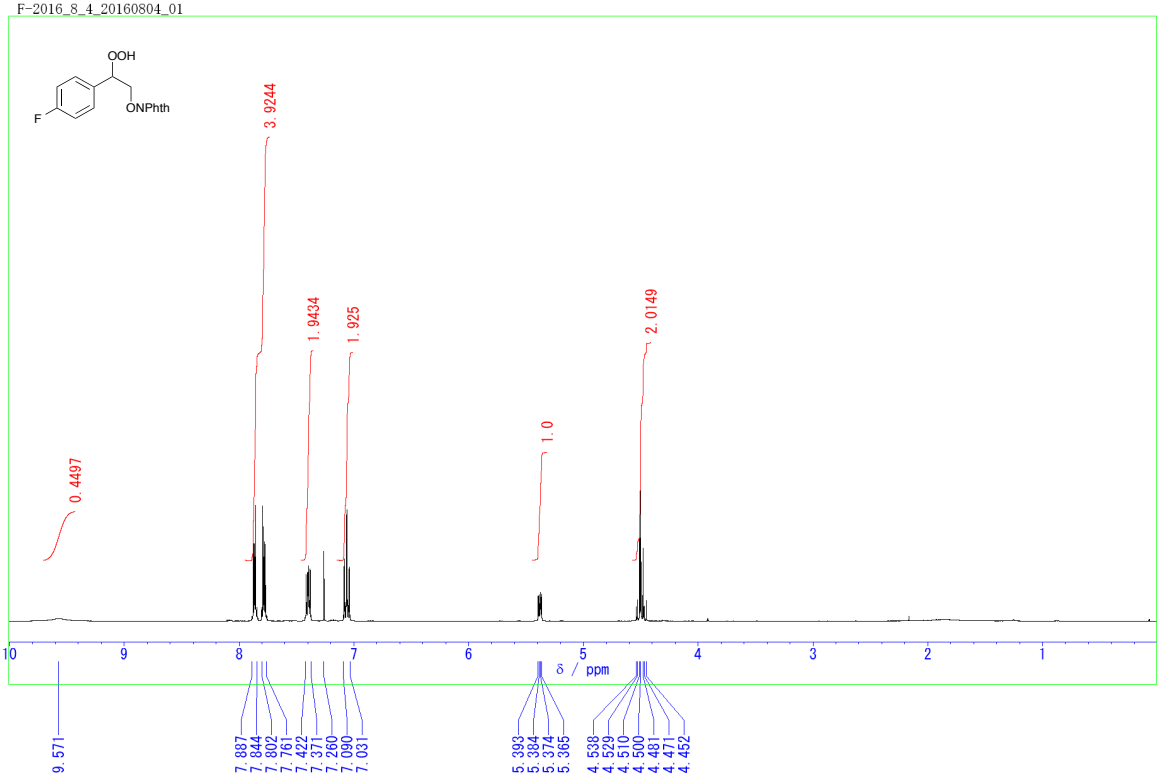

p-CH3_peroxide_re_20160218_01
OOH
ONPhth
0.8318
2.0748
2.0586
1.9297
1.9359
1.0
1.8682
2.9918
10
9
8
7
6
5
4
3
2
1
0
δ / ppm
9.439
7.882
7.826
7.791
7.737
7.292
7.272
7.260
7.180
7.161
5.392
5.381
5.374
5.363
4.534
4.522
4.505
4.494
4.486
4.475
4.458
2.329


p-CH3_peroxide_re_20160218_01
220
200
180
160
140
120
100
80
60
40
20
0
δ / ppm
163.75
138.71
134.71
132.62
129.37
128.68
127.07
123.76
85.25
78.91
77.32
77.00
76.68
21.14

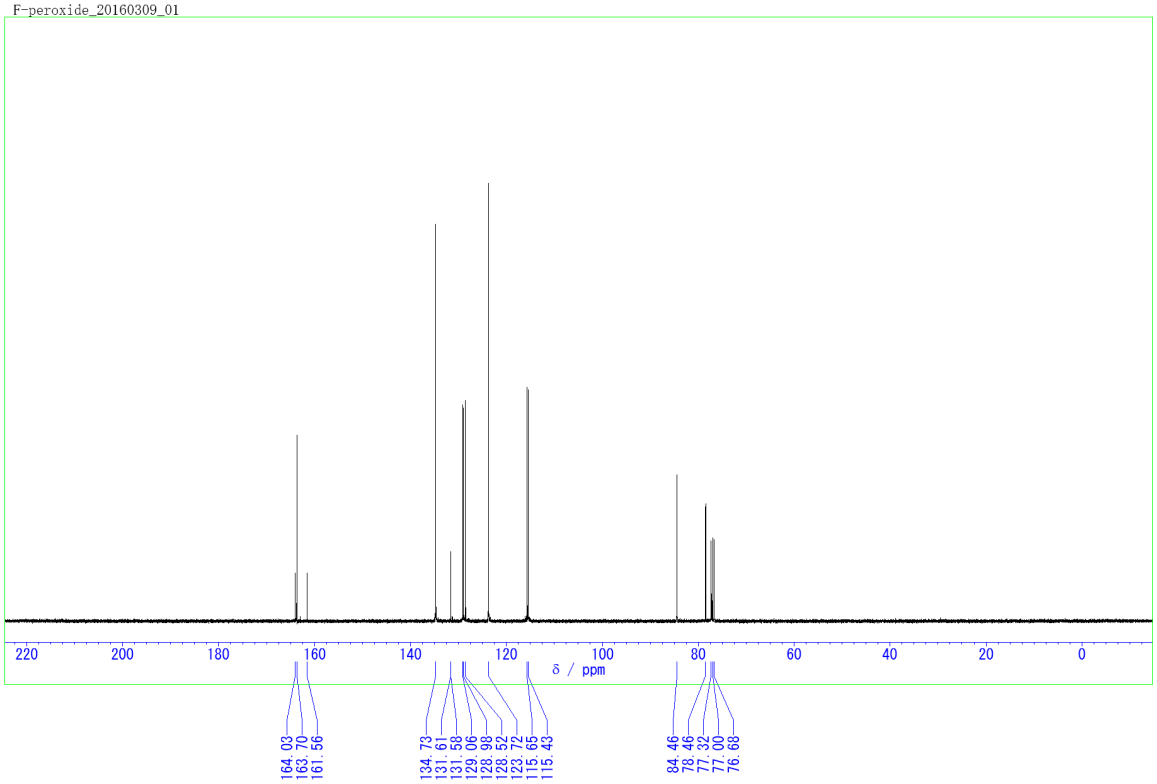

m-Me-2016_8_4_20160804_01
OOH
ONPhth
4.2965
4.602
3.0227
2.1057
0.8584
1.0
δ / ppm
9.427
7.890
7.847
7.800
7.746
7.280
7.260
7.138
5.402
5.393
5.382
5.373
4.540
4.531
4.511
4.500
4.480
4.471
4.451
2.349

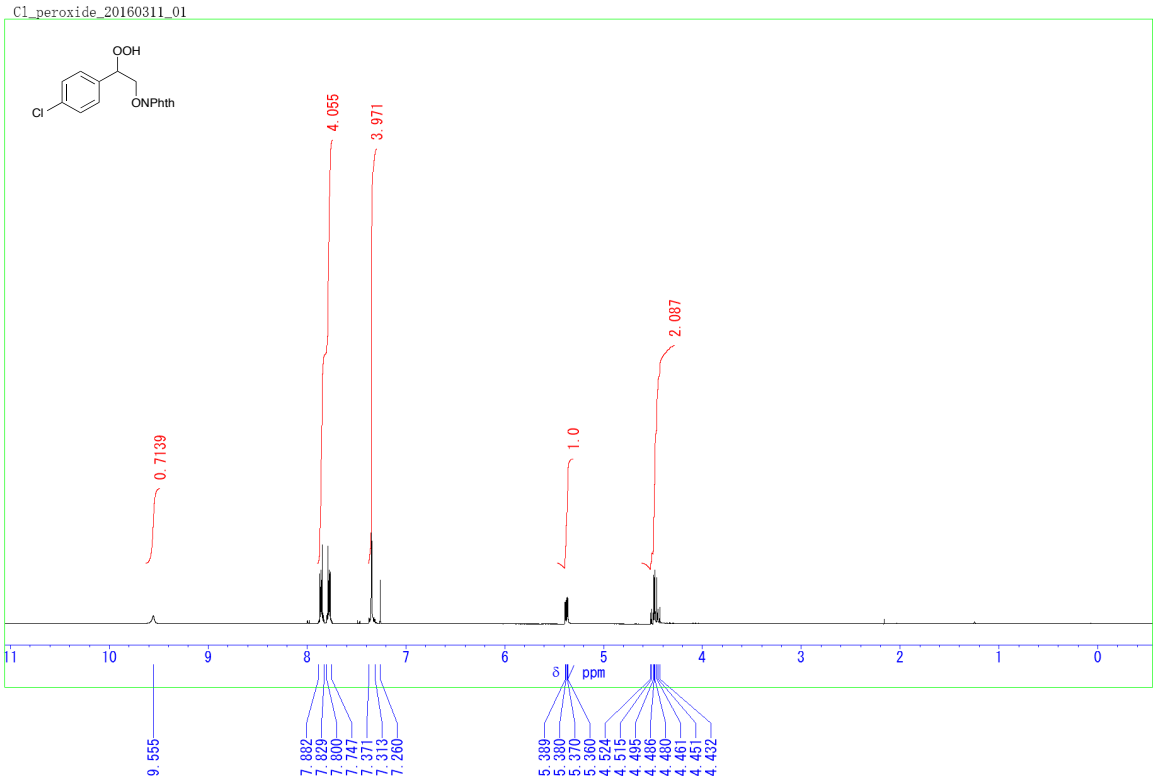

m-Me-peroxide_20160309_01
δ / ppm
163.65
138.27
135.60
134.63
129.42
128.52
128.46
127.66
124.04
123.63
85.33
78.81
77.32
77.00
76.68
21.24

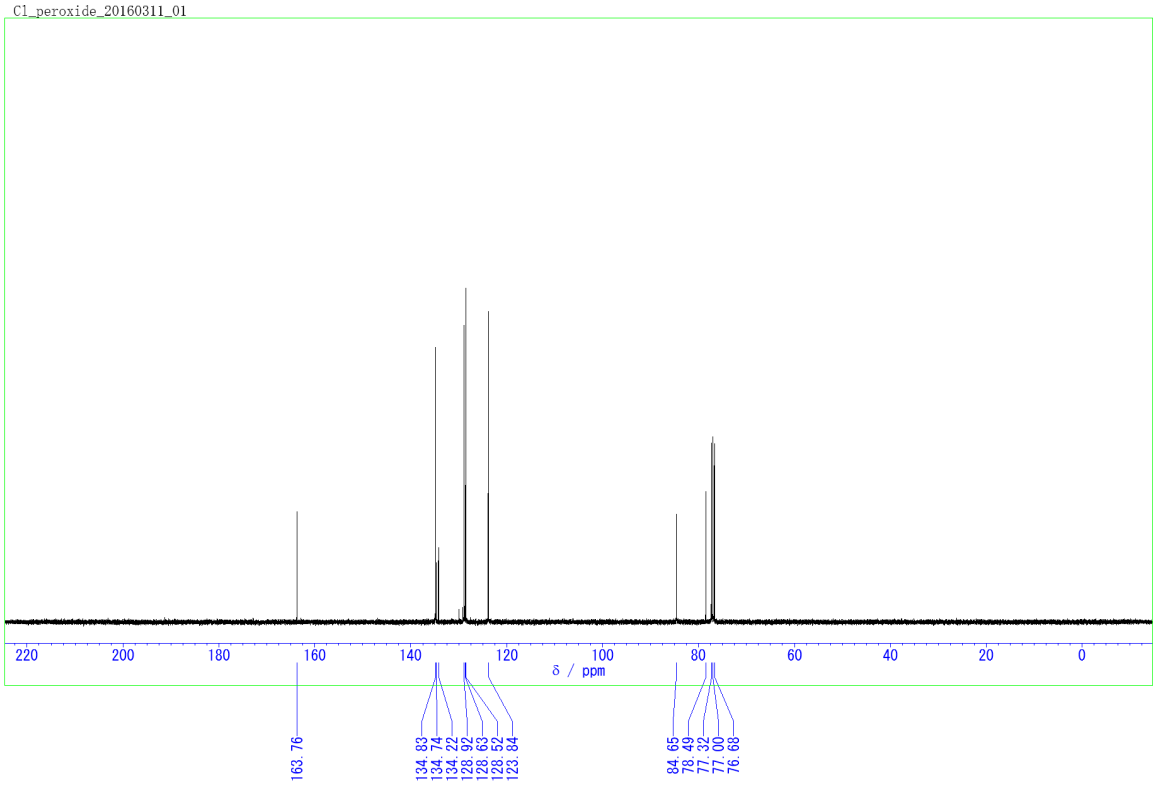
F-2016_8_4_20160804_01



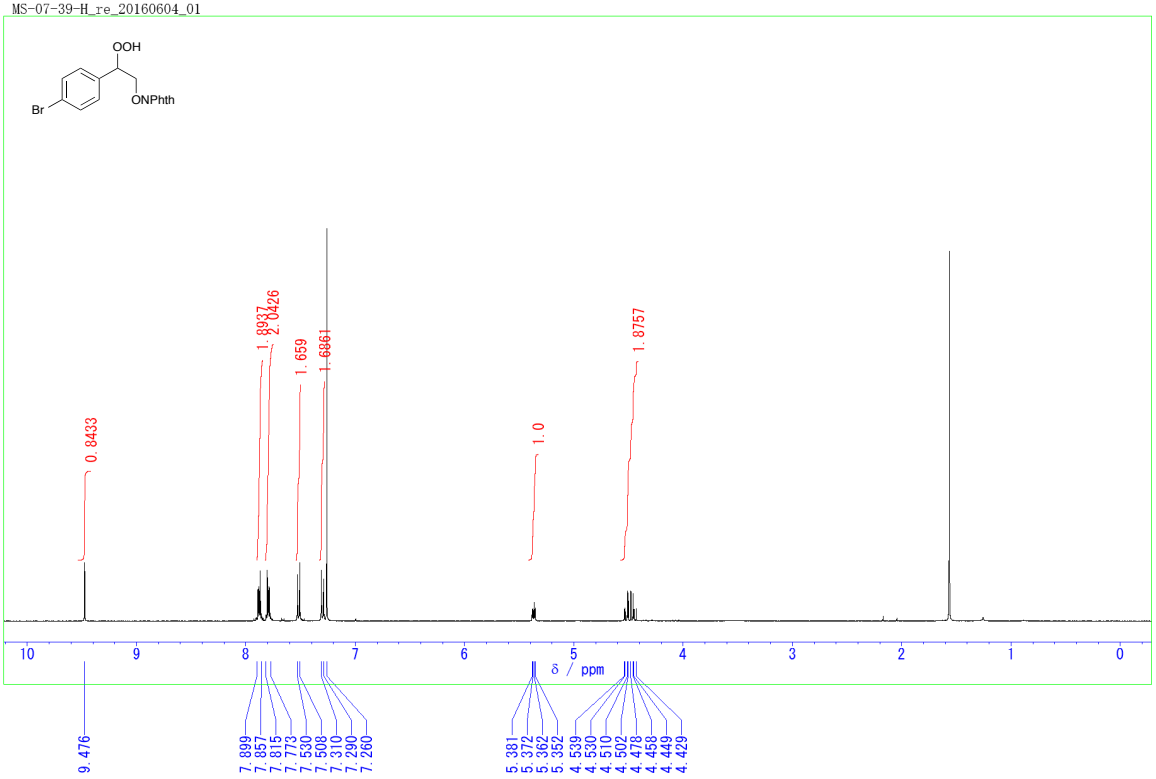
F-peroxide_20160309_01



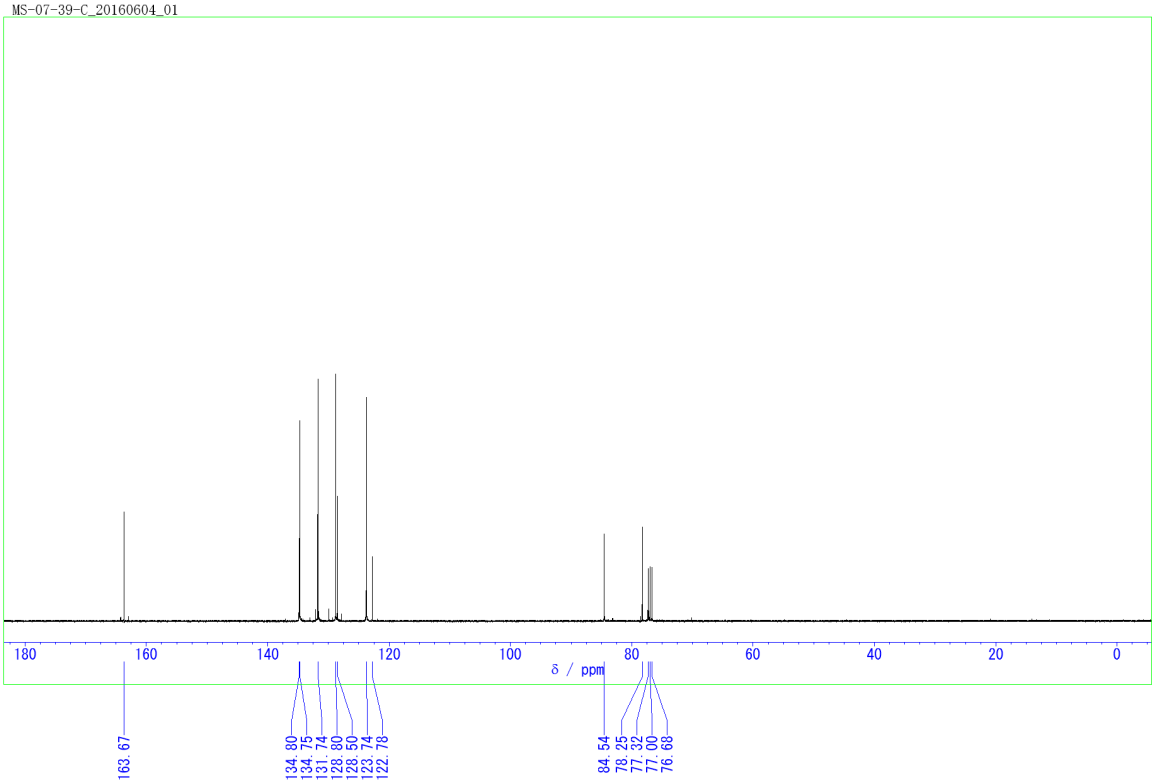

C1_peroxide_20160311_01
OOH
Cl
ONPhth
4.055
3.971
2.087
1.0
0.7139
δ / ppm
9.555
7.882
7.829
7.800
7.747
7.371
7.313
7.260
5.389
5.380
5.370
5.360
4.524
4.515
4.495
4.486
4.480
4.461
4.451
4.432


C1_peroxide_20160311_01
δ / ppm
163.76
134.83
134.74
134.22
128.92
128.63
128.52
123.84
84.65
78.49
77.32
77.00
76.68

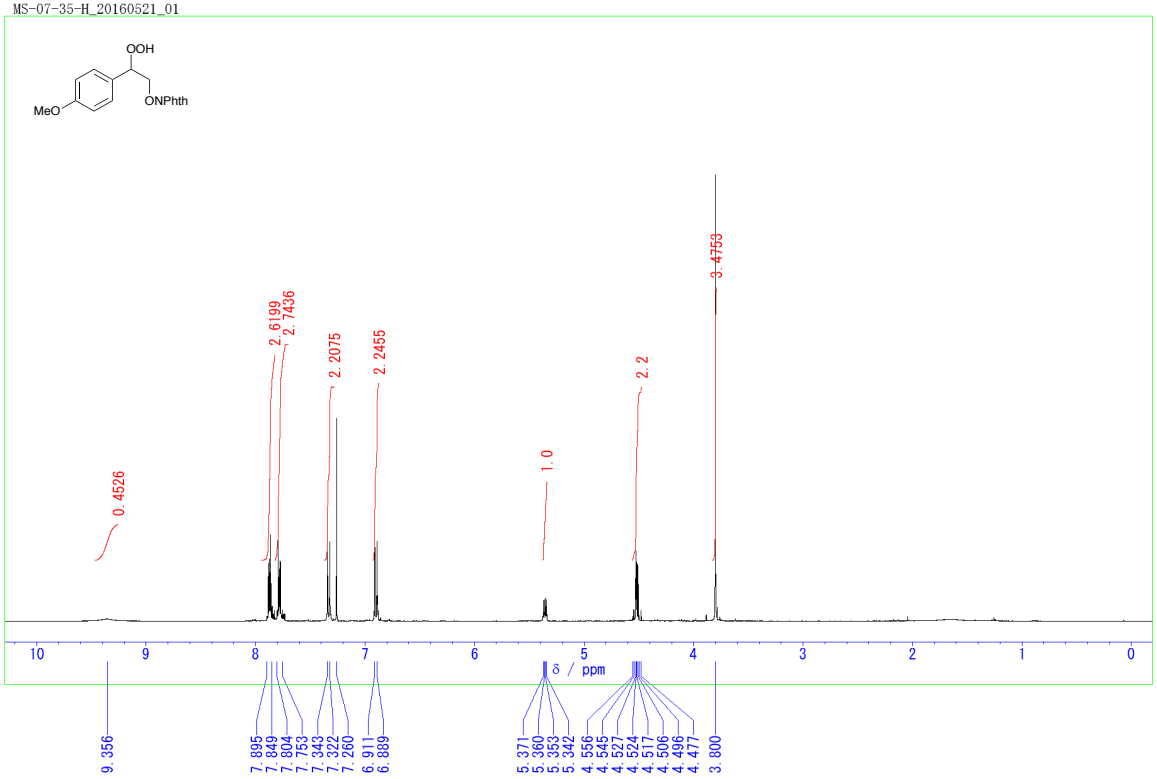
MS-07-39-H_re_20160604_01



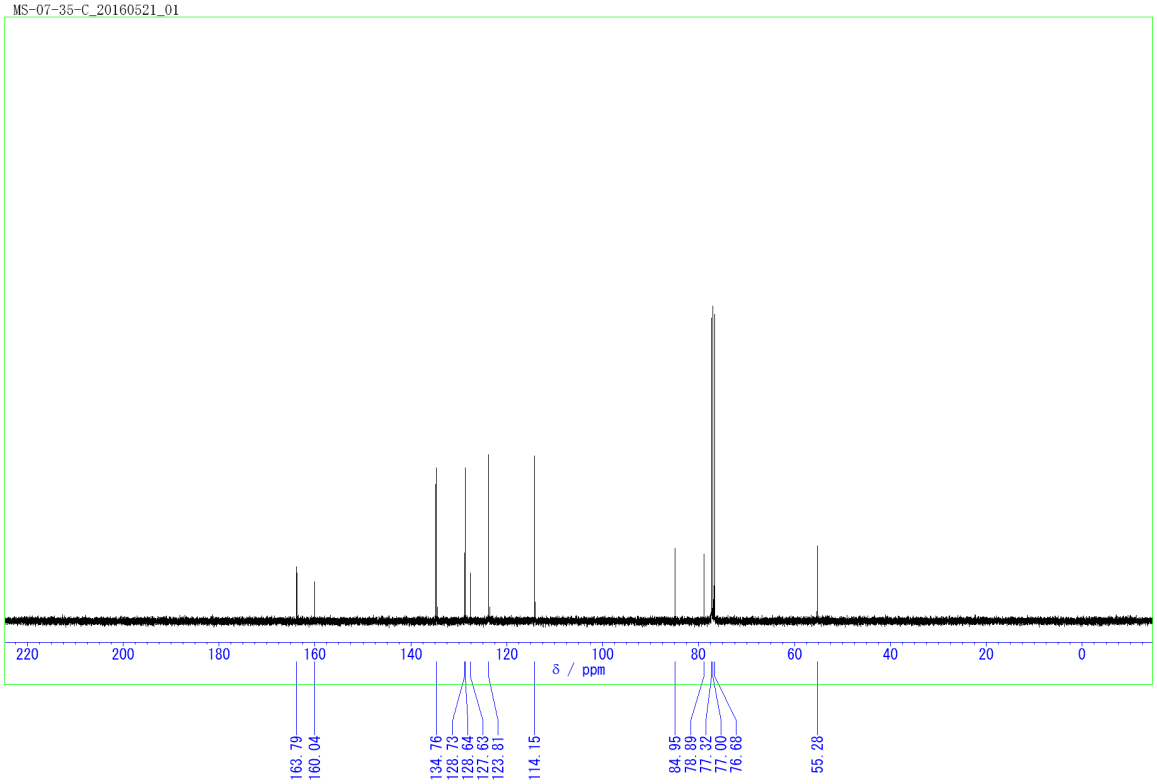
MS-07-39-C_20160604_01

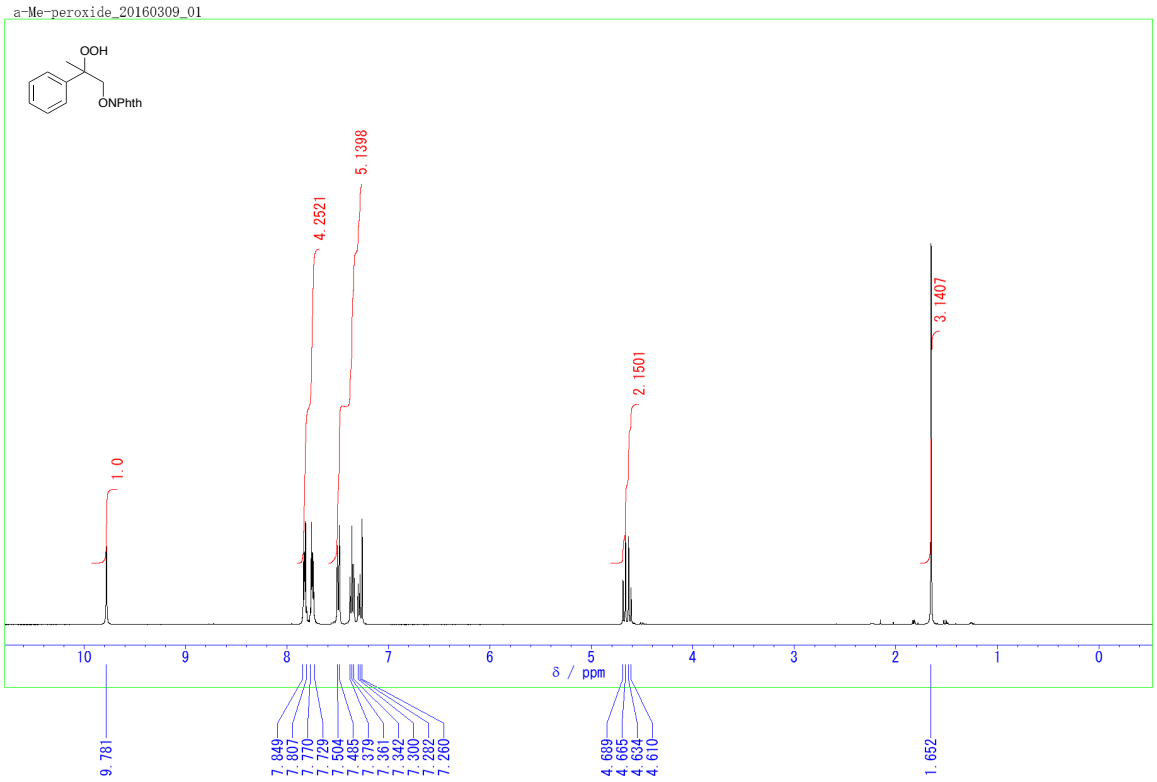


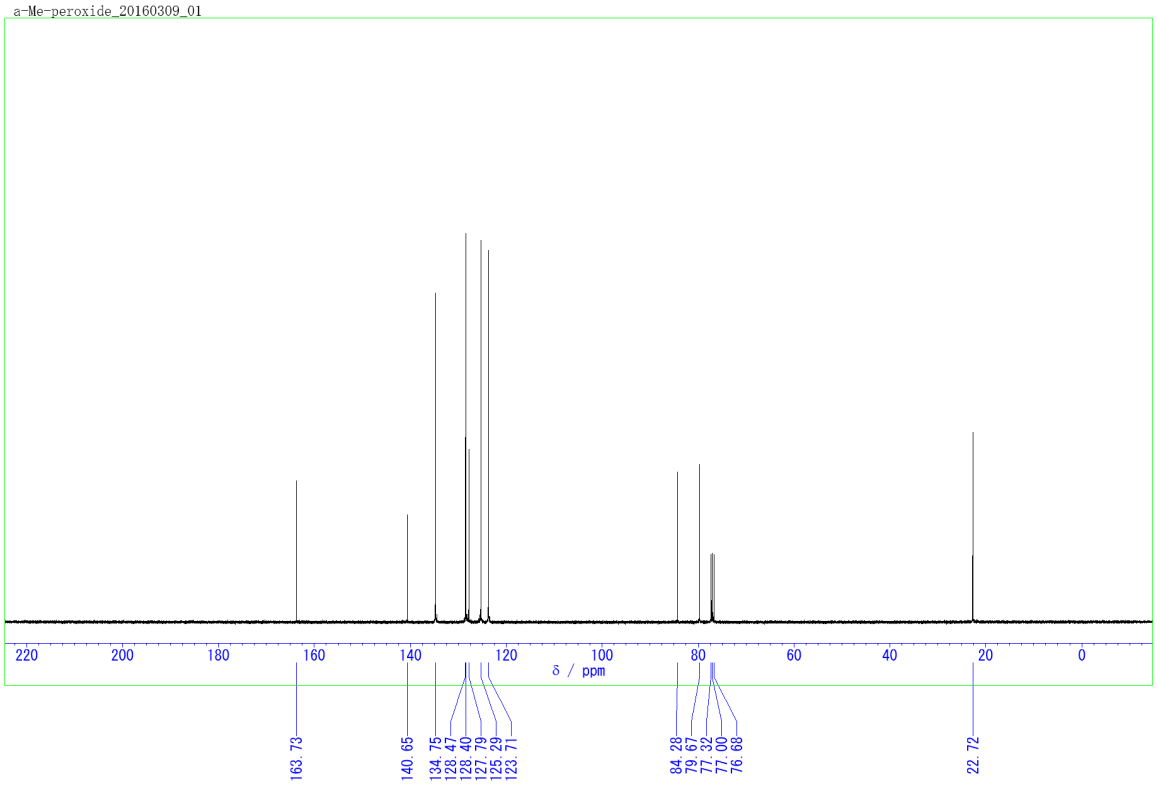
MS-07-35-H_20160521_01

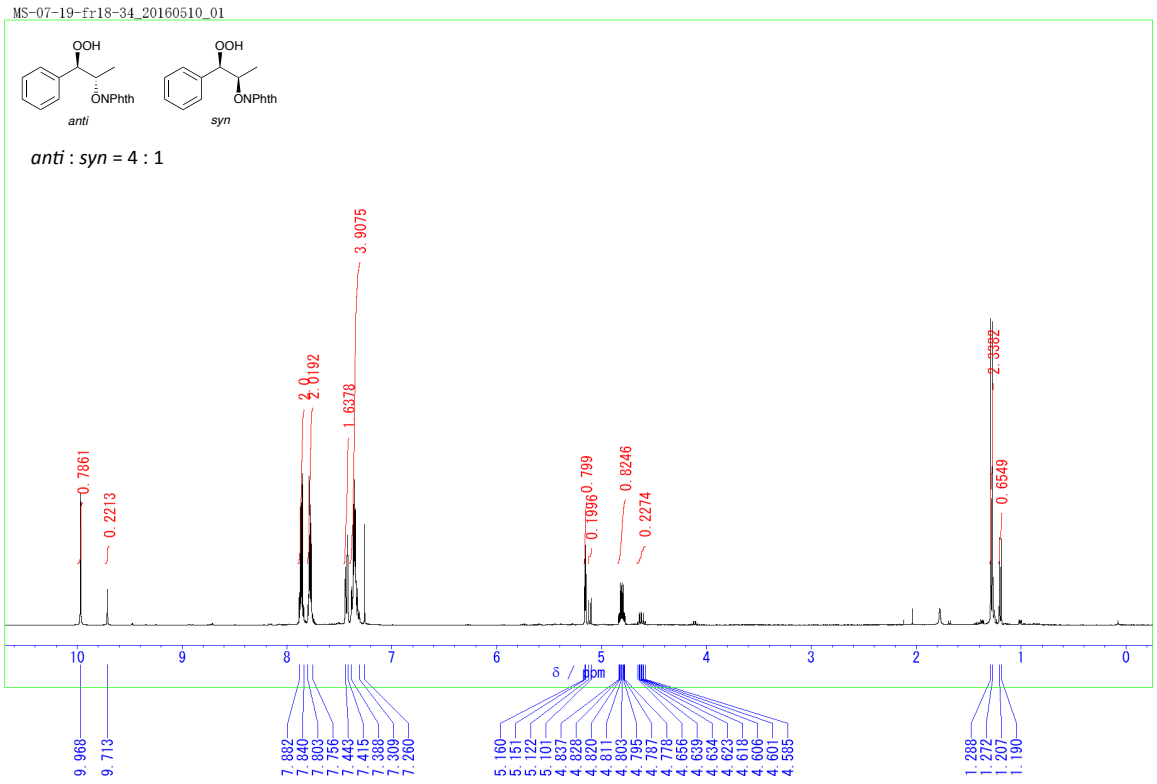


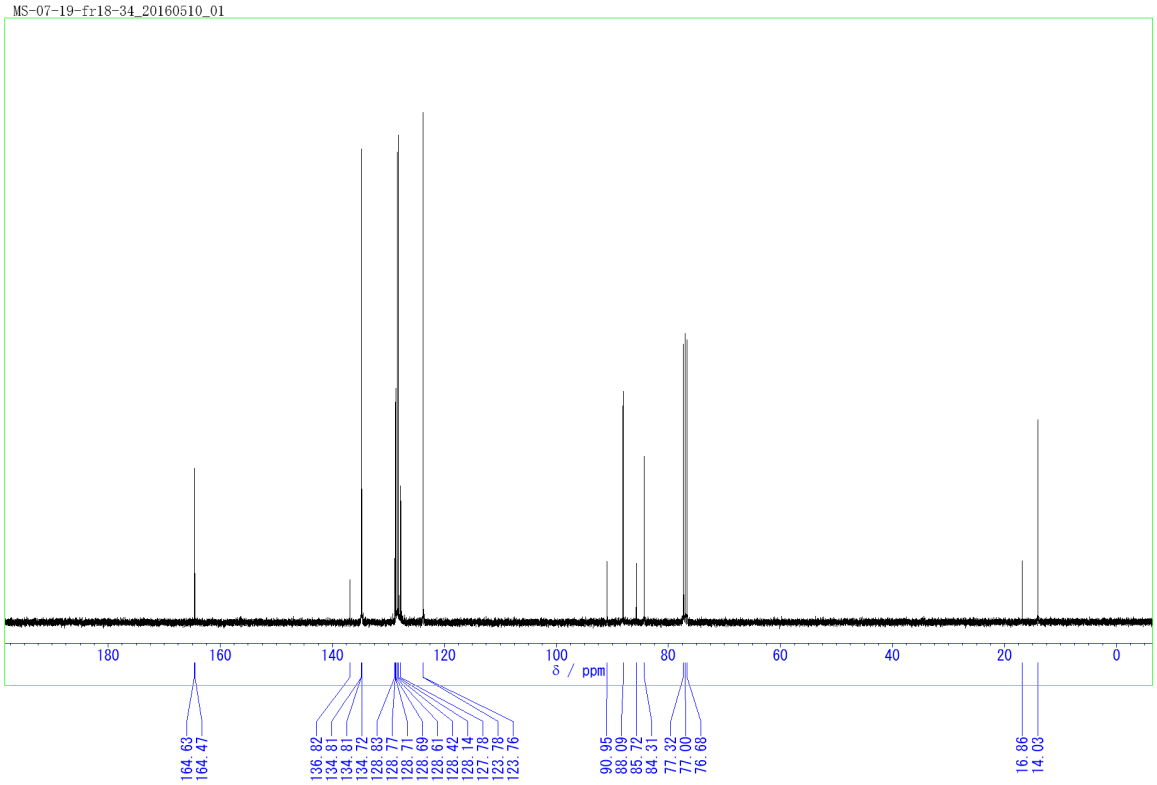
MS-07-35-C_20160521_01

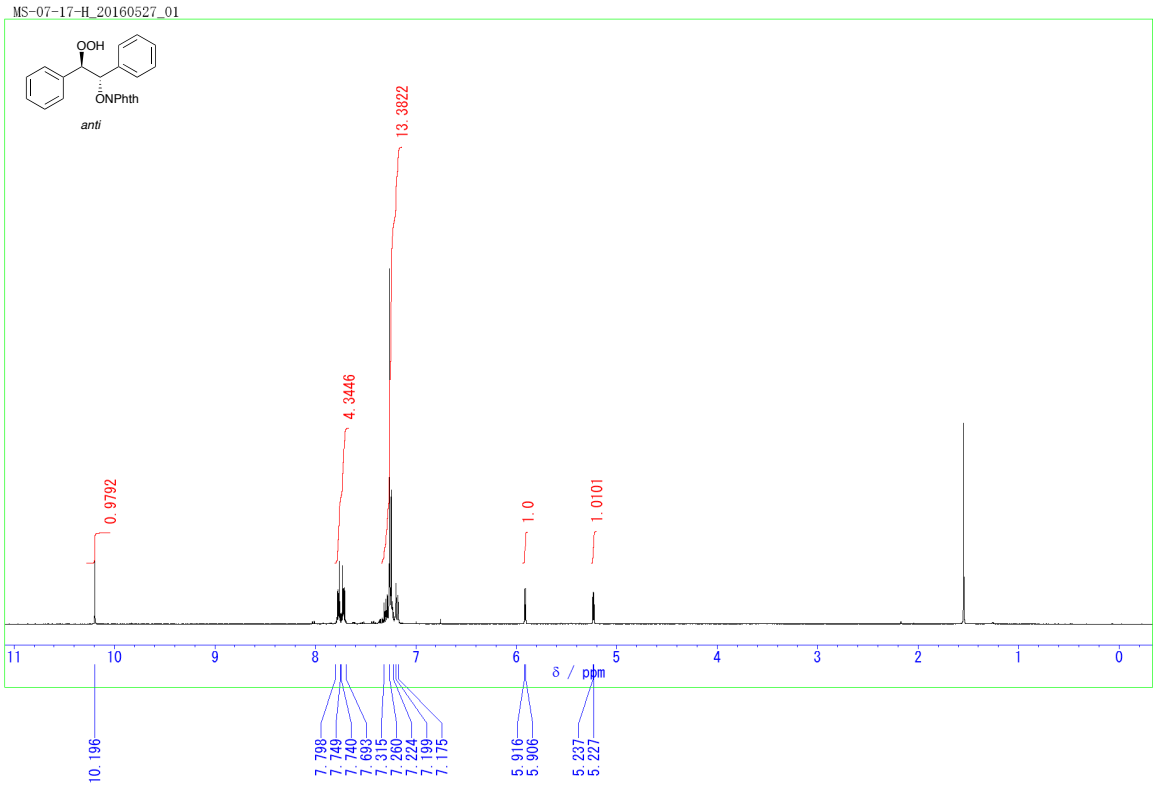


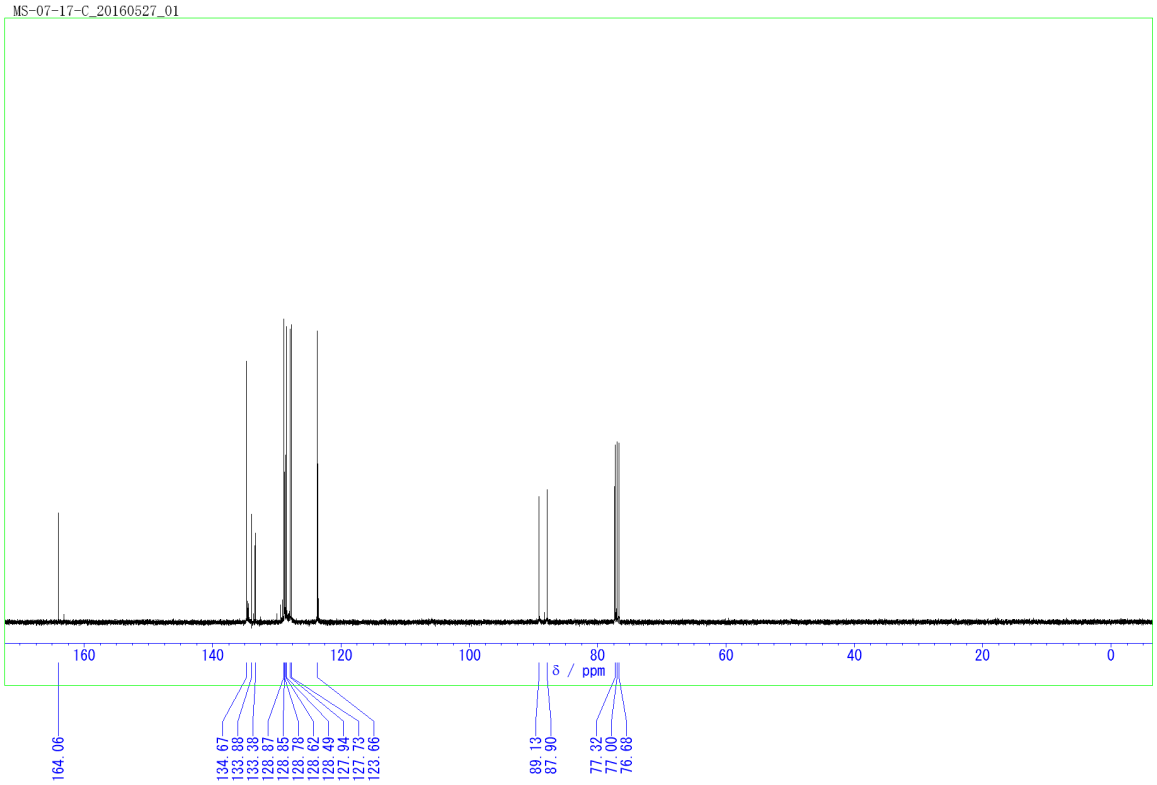

a-Me-peroxide_20160309_01
OOH
ONPhth
1.0
4.2521
5.1398
2.1501
3.1407
δ / ppm
9.781
7.849
7.807
7.770
7.729
7.504
7.485
7.379
7.361
7.342
7.300
7.282
7.260
4.689
4.665
4.634
4.610
1.652


a-Me-peroxide_20160309_01
δ / ppm
163.73
140.65
134.75
128.47
128.40
127.79
125.29
123.71
84.28
79.67
77.32
77.00
76.68
22.72

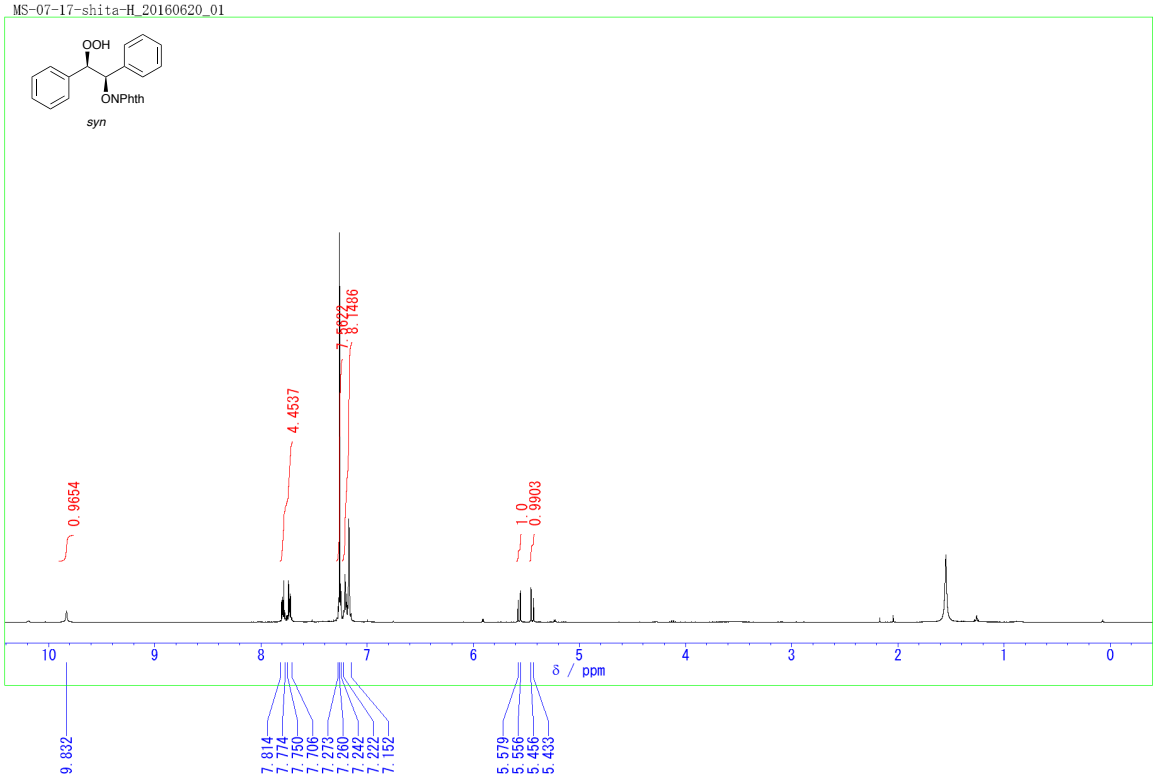

MS-07-19-fr18-34_20160510_01
OOH
ONPhth
anti
OOH
ONPhth
syn
anti : syn = 4 : 1
3.9075
2.0192
2.0
1.6378
0.7861
0.2213
0.7996
0.799
0.8246
0.2274
2.3382
0.6549
δ / ppm
9.968
9.713
7.882
7.840
7.803
7.756
7.443
7.415
7.388
7.309
7.260
5.160
5.151
5.122
5.101
4.837
4.828
4.820
4.811
4.803
4.795
4.787
4.778
4.656
4.639
4.634
4.623
4.618
4.606
4.601
4.585
1.288
1.272
1.207
1.190


MS-07-19-fr18-34_20160510_01
δ / ppm
164.63
164.47
136.82
134.81
134.81
134.72
128.83
128.77
128.71
128.69
128.61
128.42
128.14
127.78
123.78
123.76
90.95
88.09
85.72
84.31
77.32
77.00
76.68
16.86
14.03

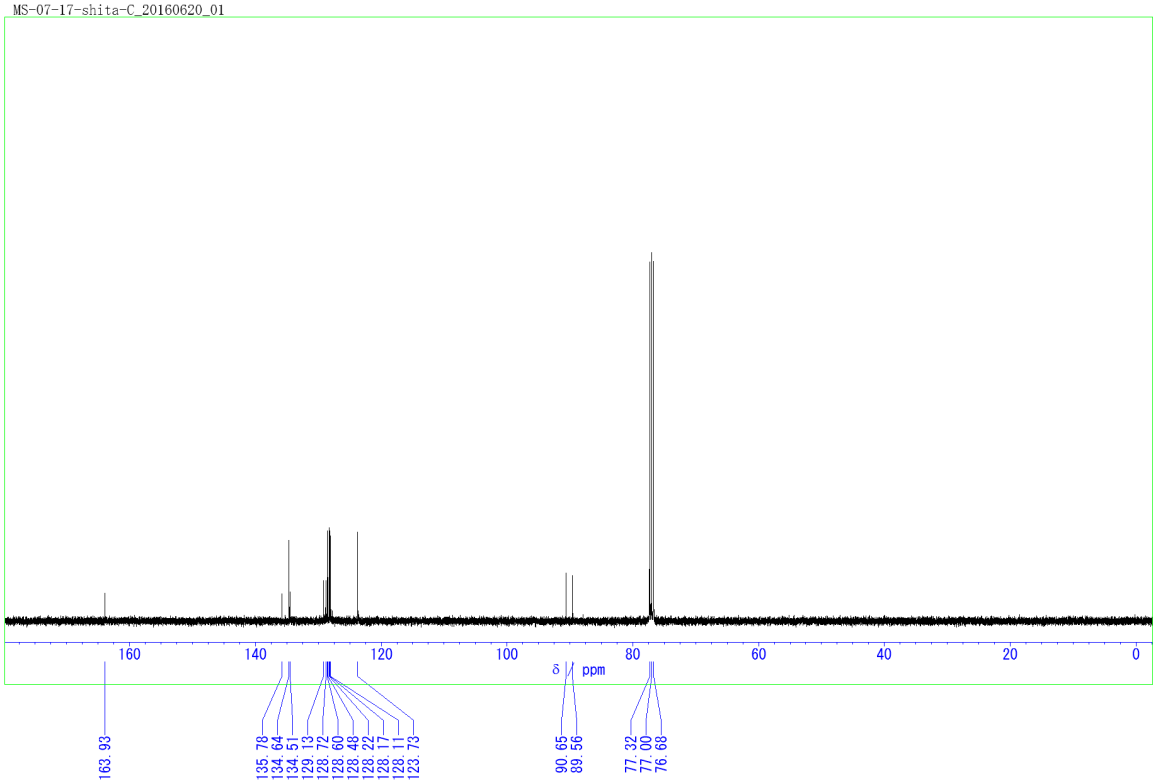

MS-07-17-H_20160527_01
OOH
ONPhth
anti
13.3822
4.3446
0.9792
1.0
1.0101
δ / ppm
10.196
7.798
7.749
7.740
7.693
7.315
7.260
7.224
7.199
7.175
5.916
5.906
5.237
5.227


MS-07-17-C_20160527_01
δ / ppm
164.06
134.67
133.88
133.38
128.87
128.85
128.78
128.62
128.49
127.94
127.73
123.66
89.13
87.90
77.32
77.00
76.68

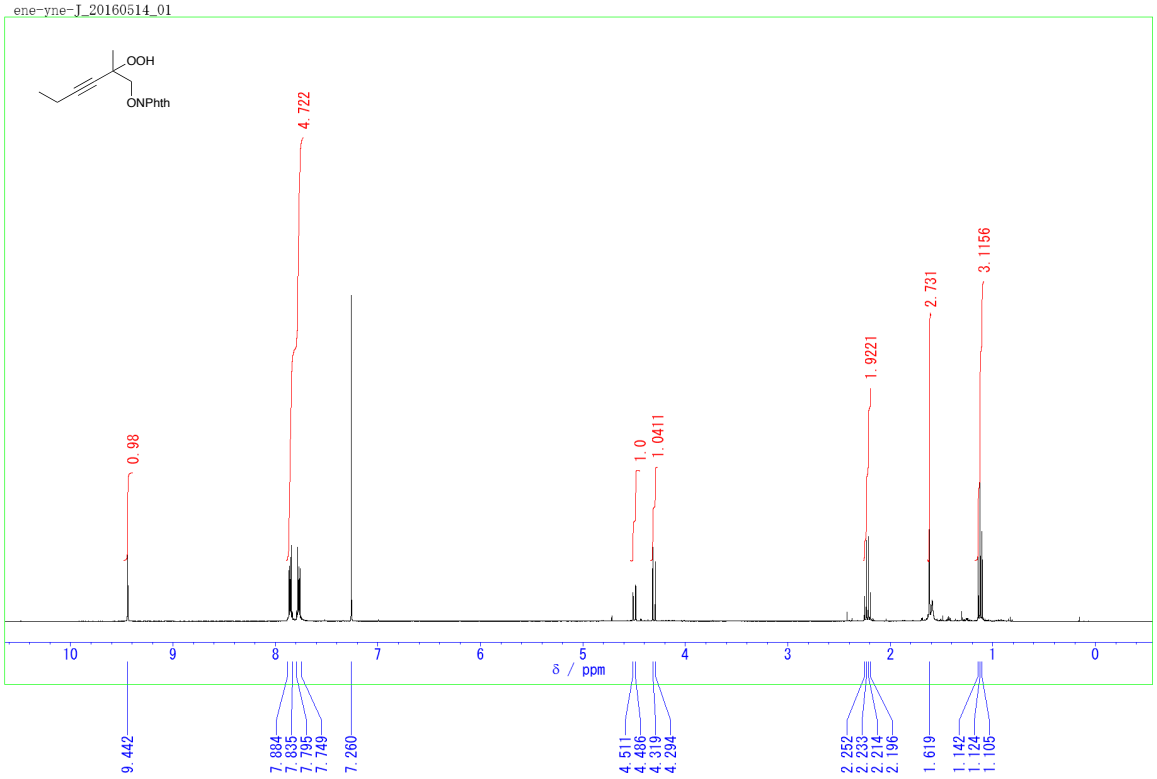
MS-07-17-shita-H_20160620_01



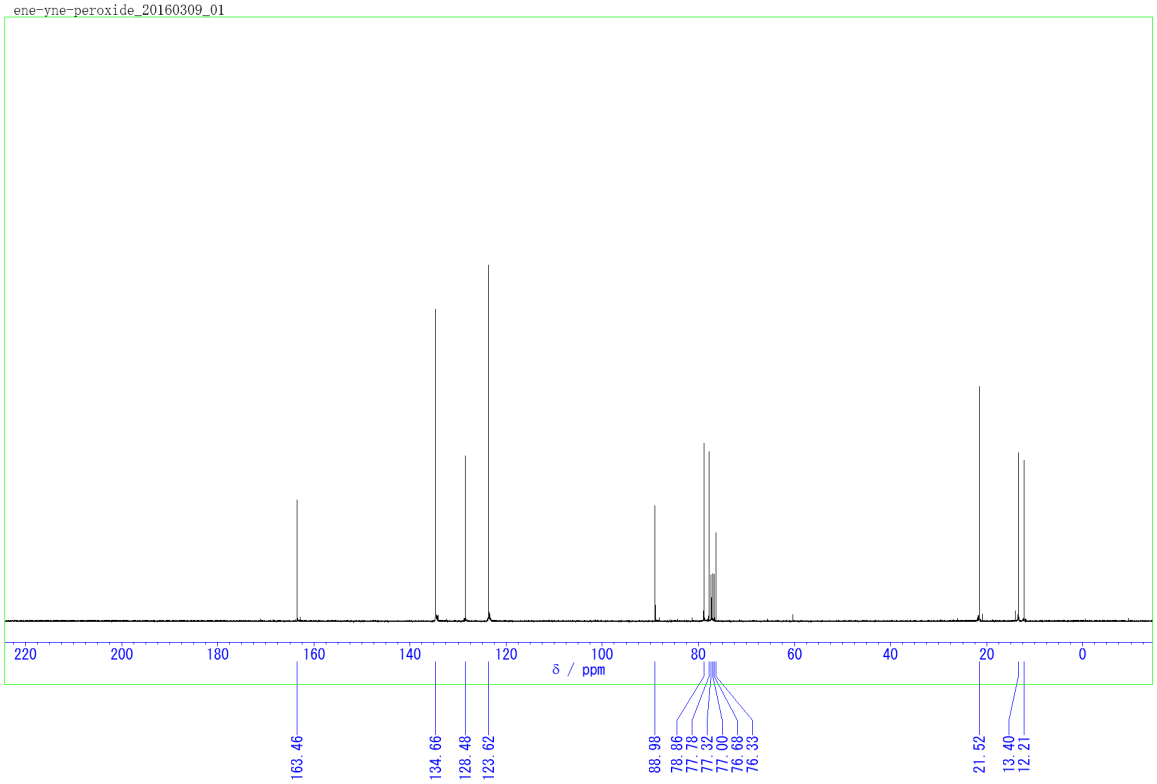
MS-07-17-shita-C_20160620_01

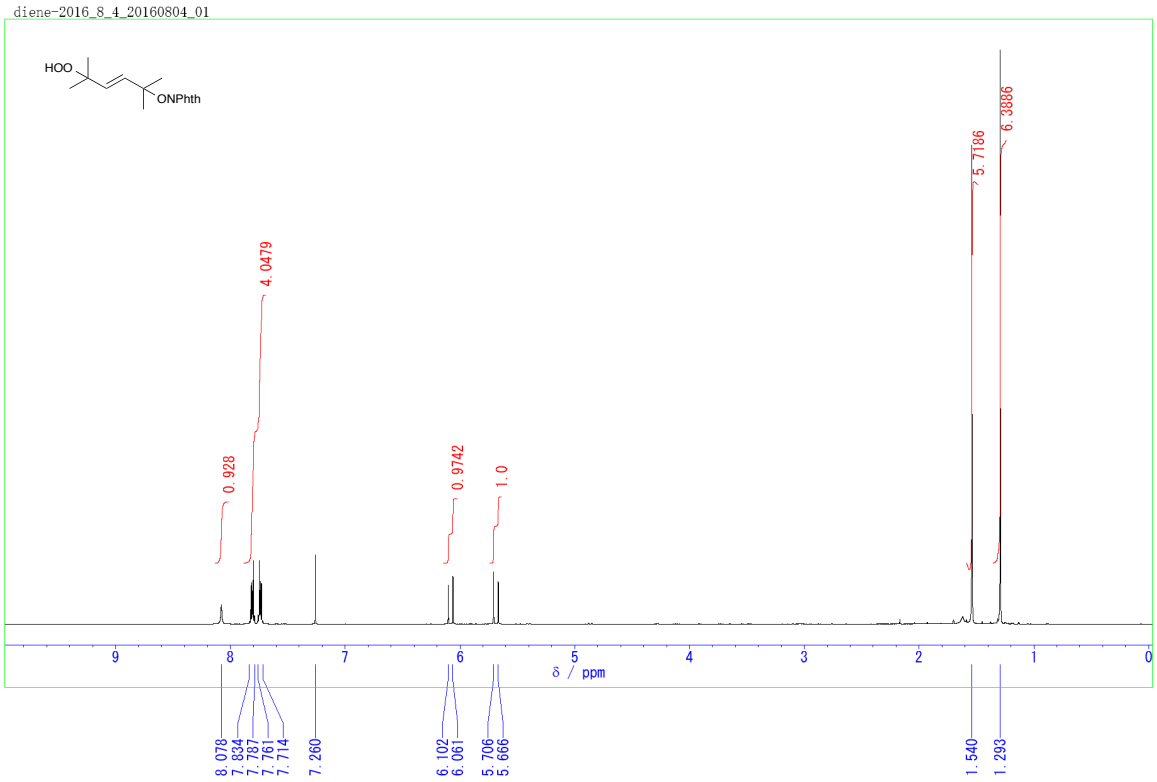


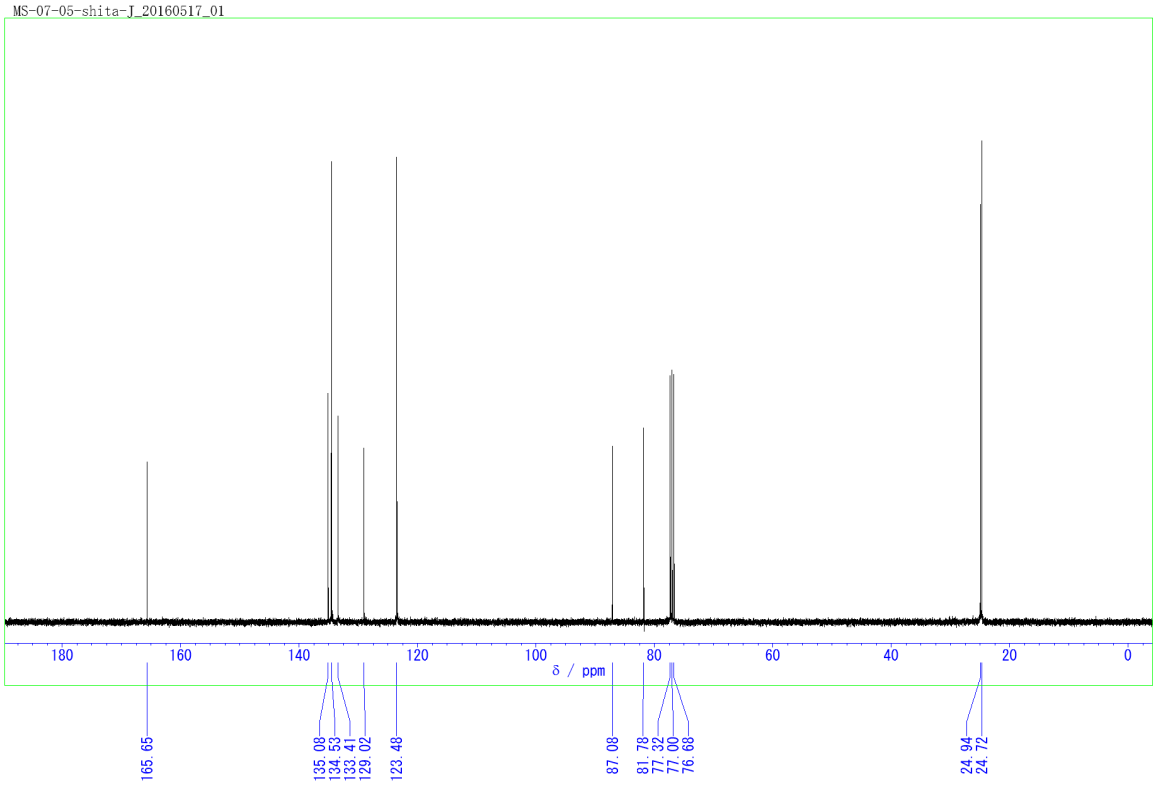
ene-yne-J_20160514_01

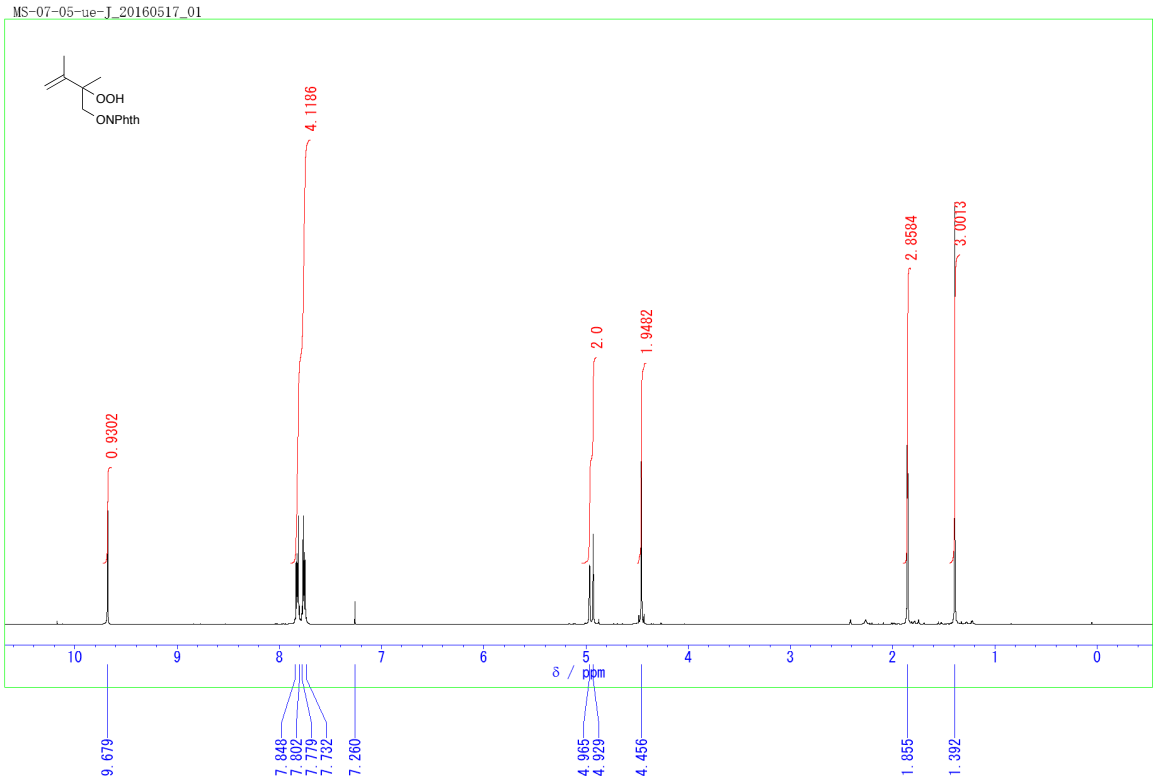


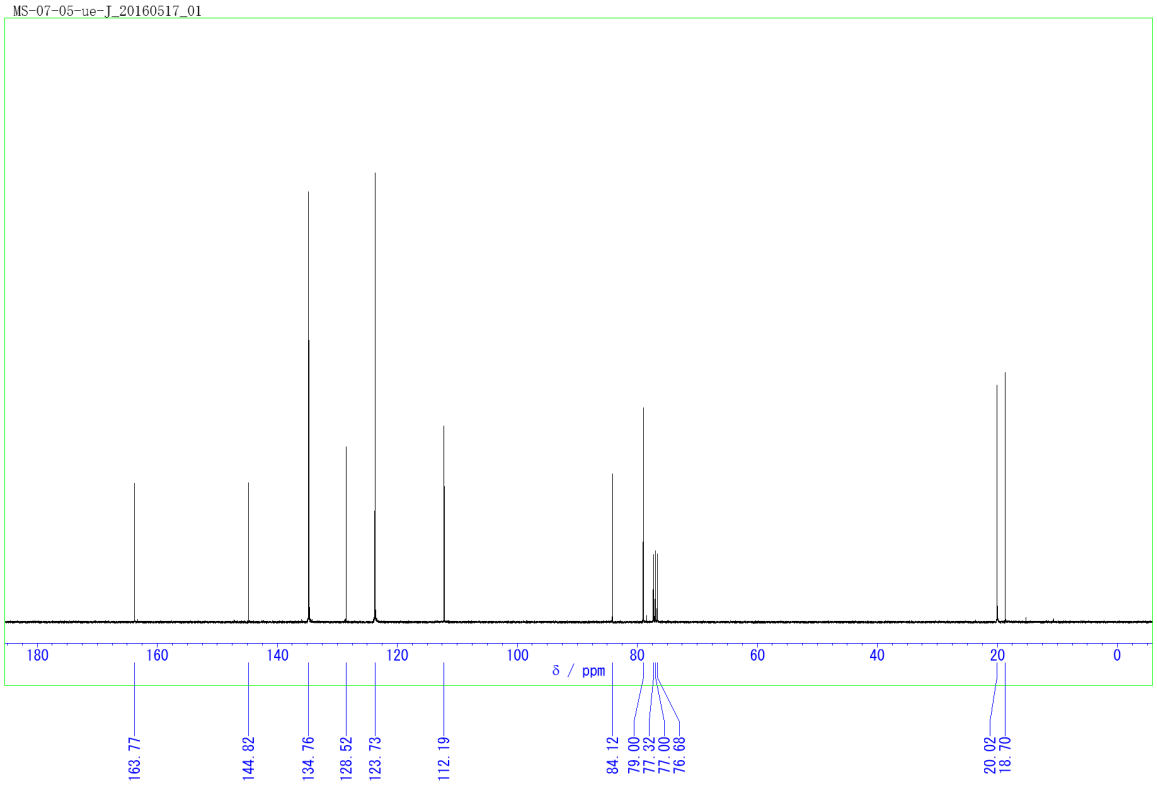
ene-yne-peroxide_20160309_01

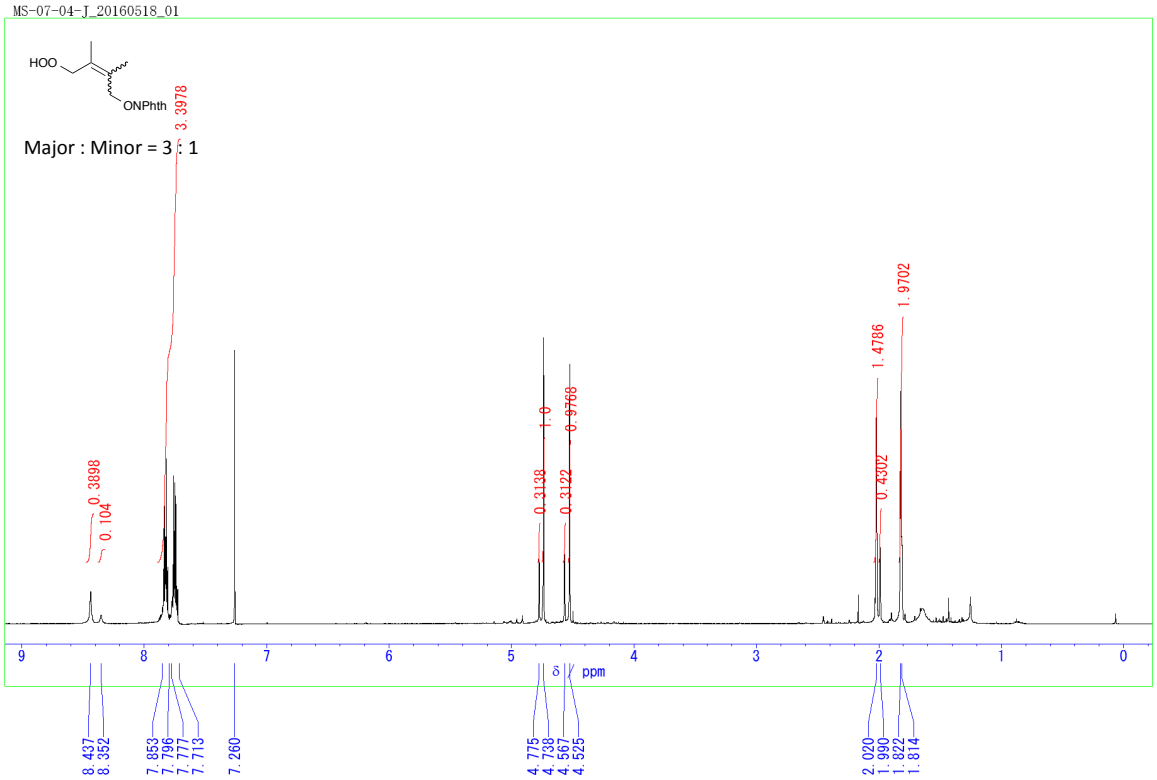


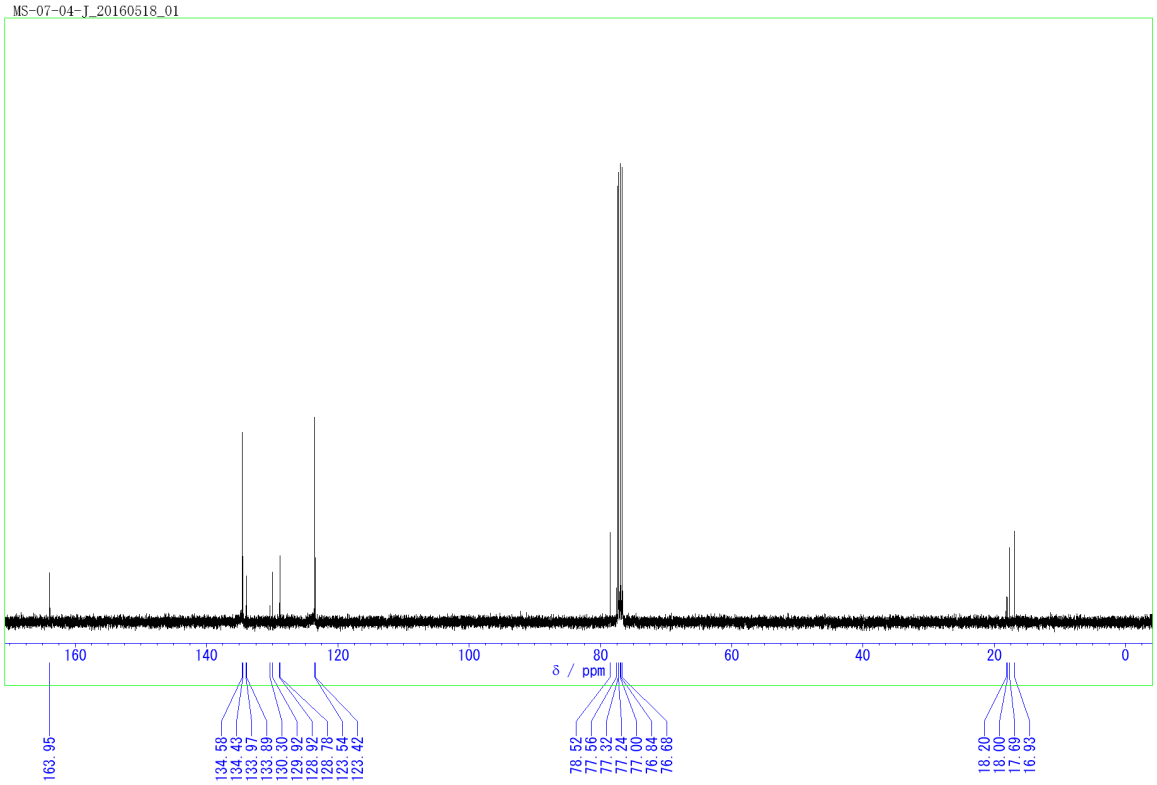

diene-2016_8_4_20160804_01
HOO
ONPhth
0.928
4.0479
0.9742
1.0
7.7186
6.3886
δ / ppm
8.078
7.834
7.787
7.761
7.714
7.260
6.102
6.061
5.706
5.666
1.540
1.293


MS-07-05-shita-J_20160517_01
δ / ppm
165.65
135.08
134.53
133.41
129.02
123.48
87.08
81.78
77.32
77.00
76.68
24.94
24.72

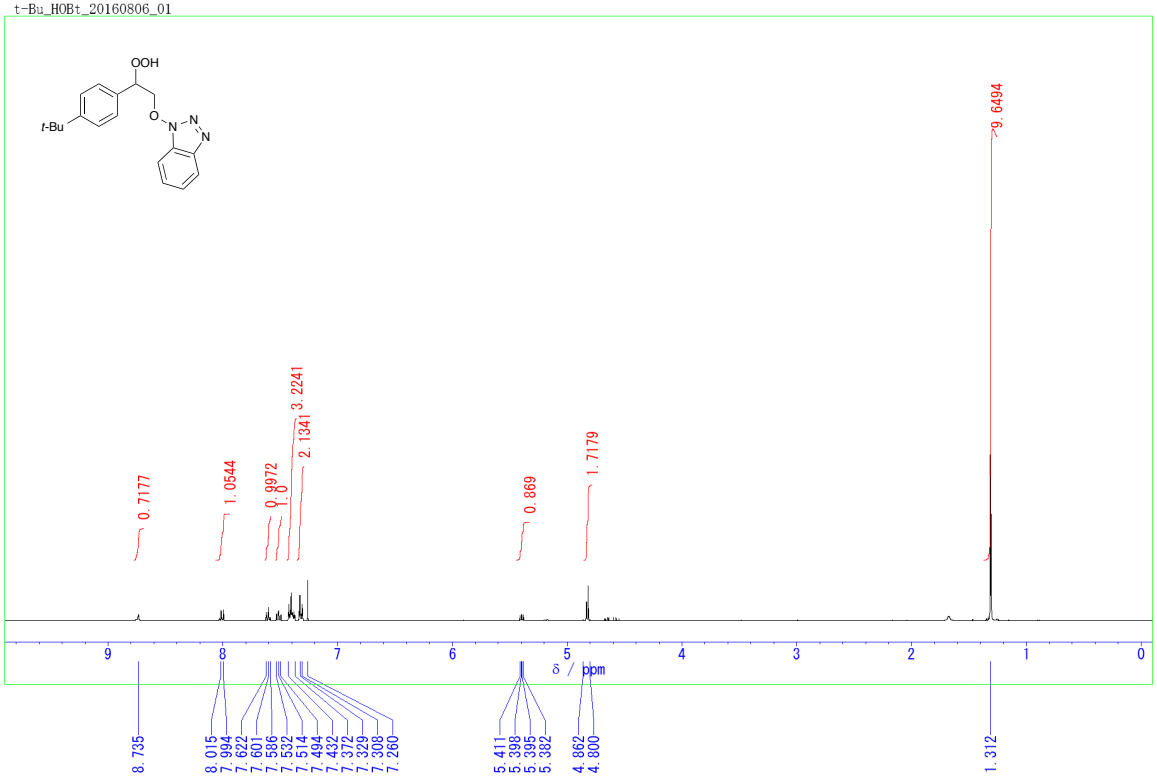

MS-07-05-ue-J_20160517_01
OOH
ONPhth
4.1186
2.8584
3.0073
2.0
1.9482
0.9302
δ / ppm
9.679
7.848
7.802
7.779
7.732
7.260
4.965
4.929
4.456
1.855
1.392


MS-07-05-ue-J_20160517_01
δ / ppm
163.77
144.82
134.76
128.52
123.73
112.19
84.12
79.00
77.32
77.00
76.68
20.02
18.70

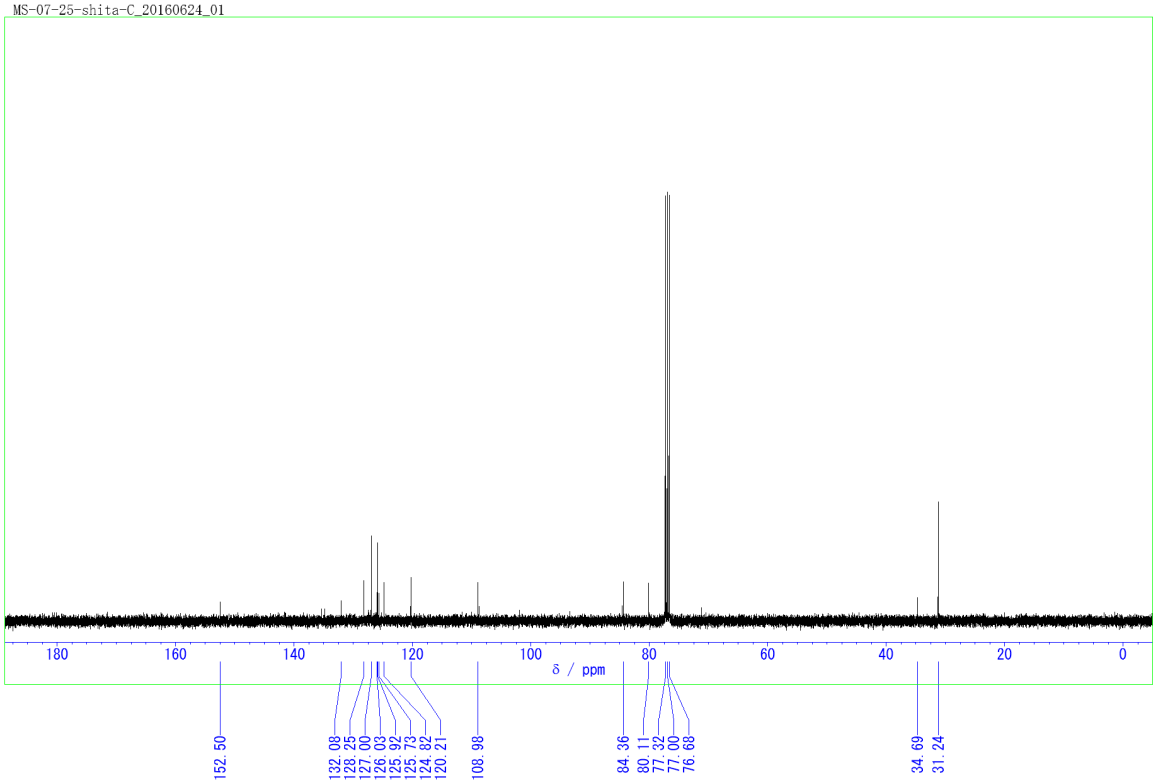

MS-07-04-J_20160518_01
HOO
ONPhth
Major : Minor = 3 : 1
3.3978
0.3898
0.104
1.0
0.3138
0.3122
0.9768
1.4786
0.4302
1.9702
9
8
7
6
5
4
3
2
1
0
δ
ppm
8.437
8.352
7.853
7.796
7.777
7.713
7.260
4.775
4.738
4.567
4.525
2.020
1.990
1.822
1.814

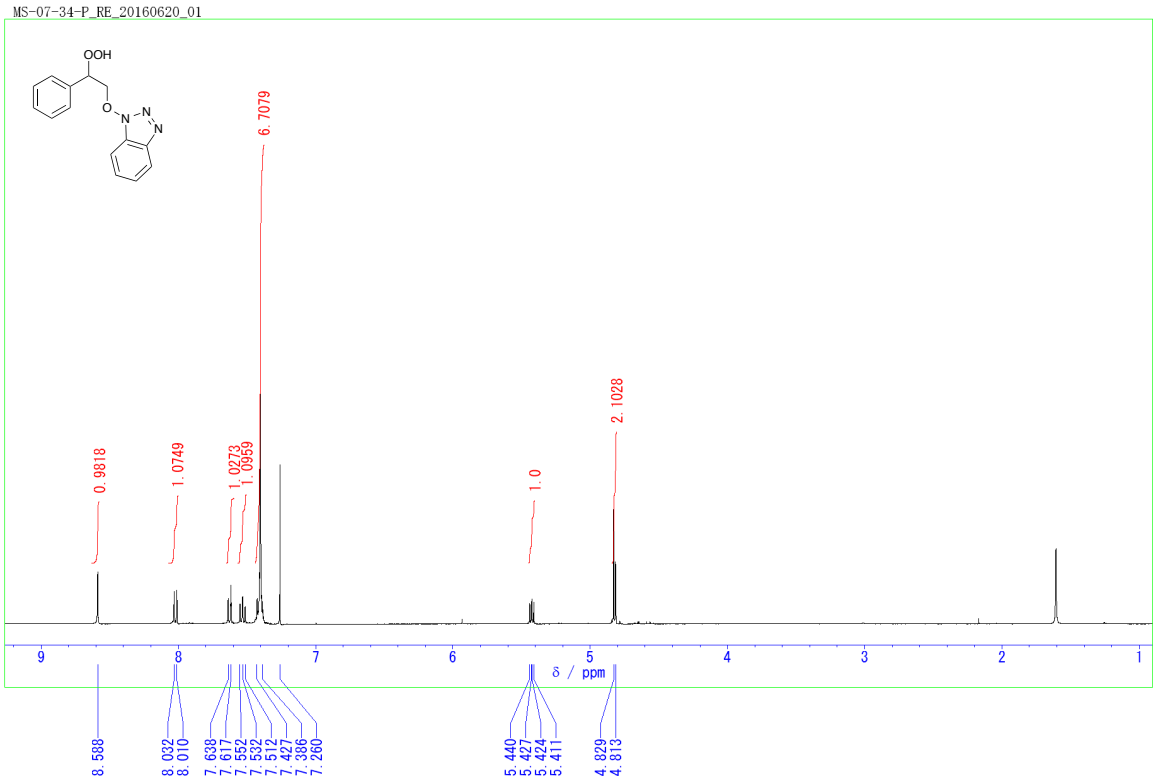

MS-07-04-J_20160518_01
160
140
120
100
80
60
40
20
0
δ / ppm
163.95
134.58
134.43
133.97
133.89
130.30
129.92
128.92
128.78
123.54
123.42
78.52
77.56
77.32
77.24
77.00
76.84
76.68
18.20
18.00
17.69
16.93

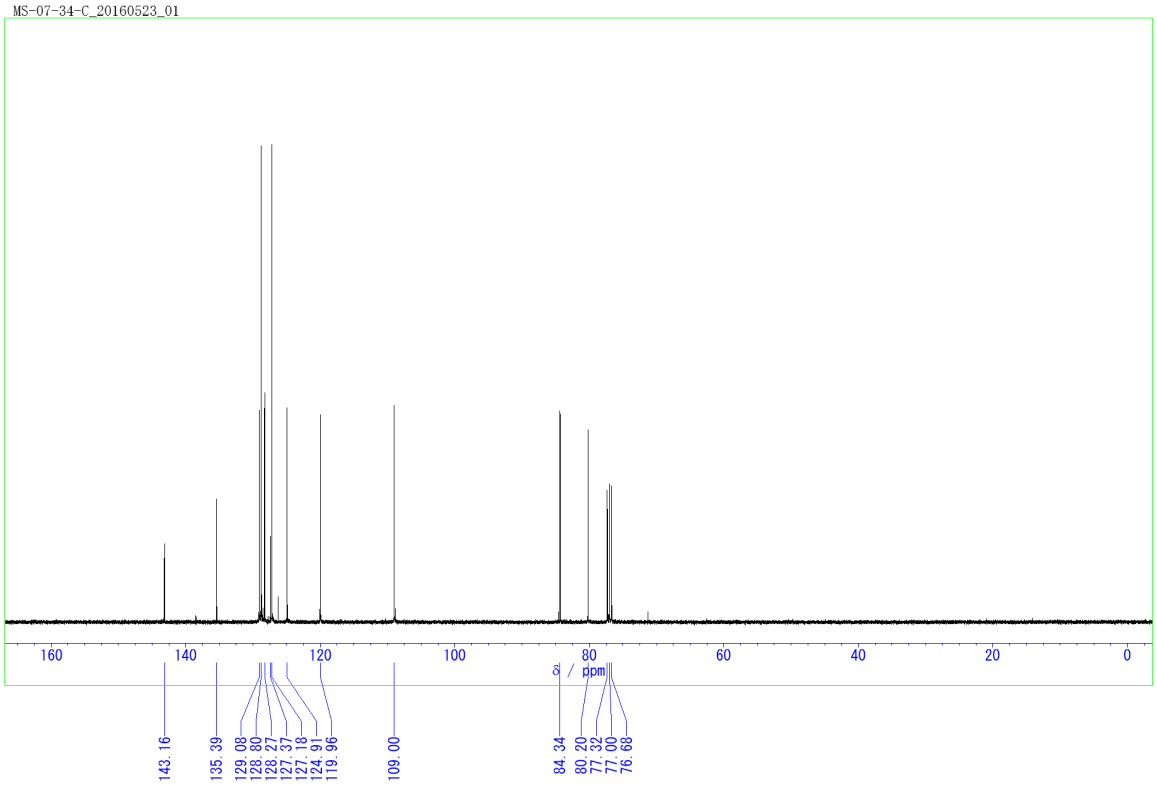
t-Bu_HOBt_20160806_01

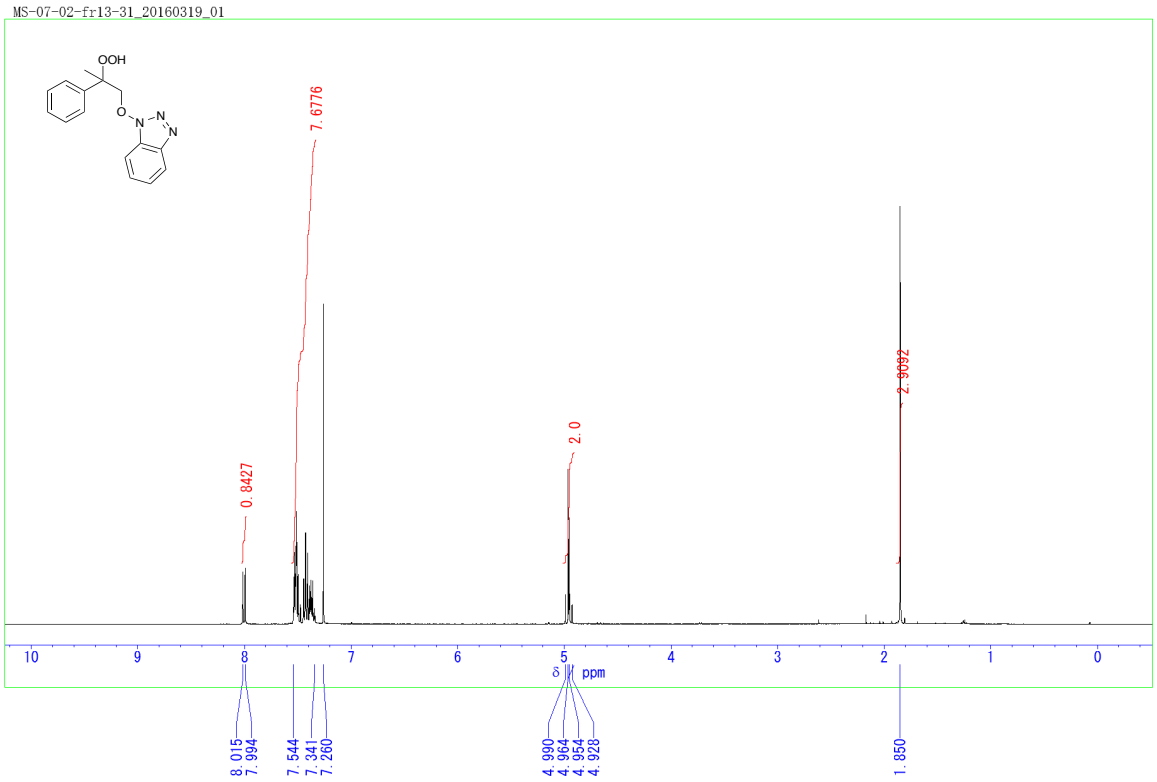


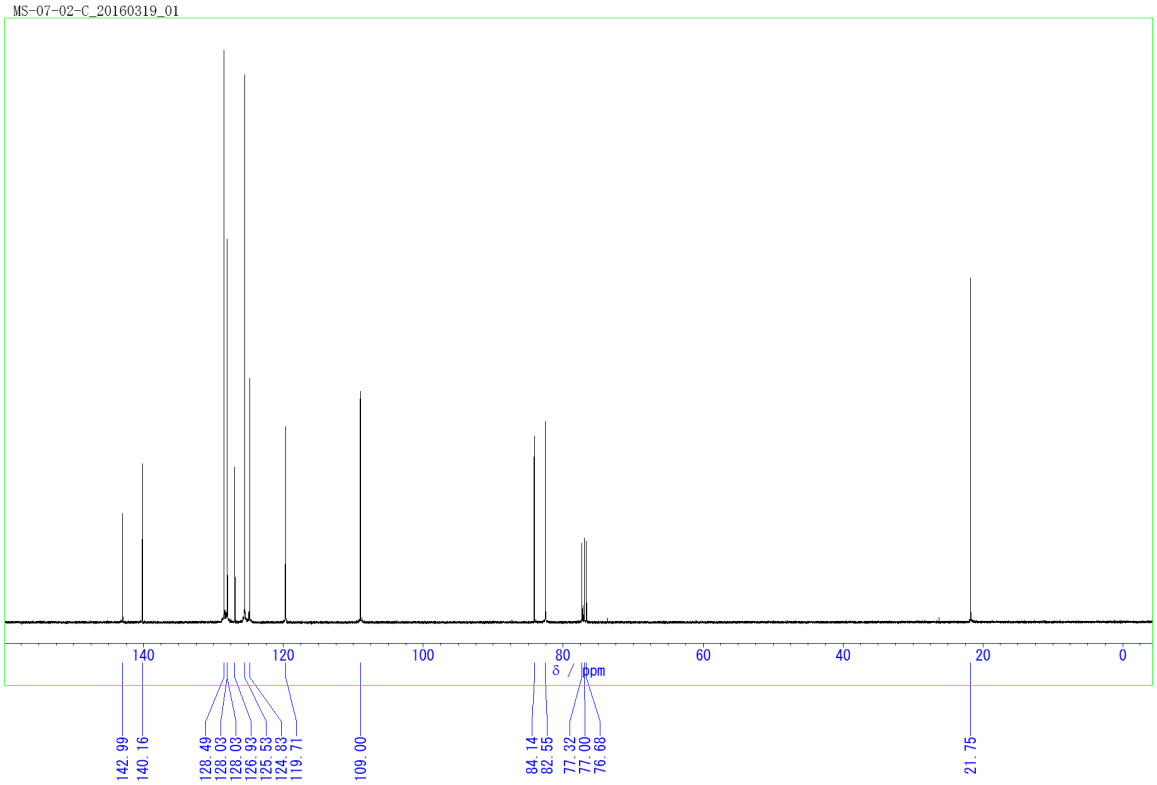
MS-07-25-shita-C_20160624_01

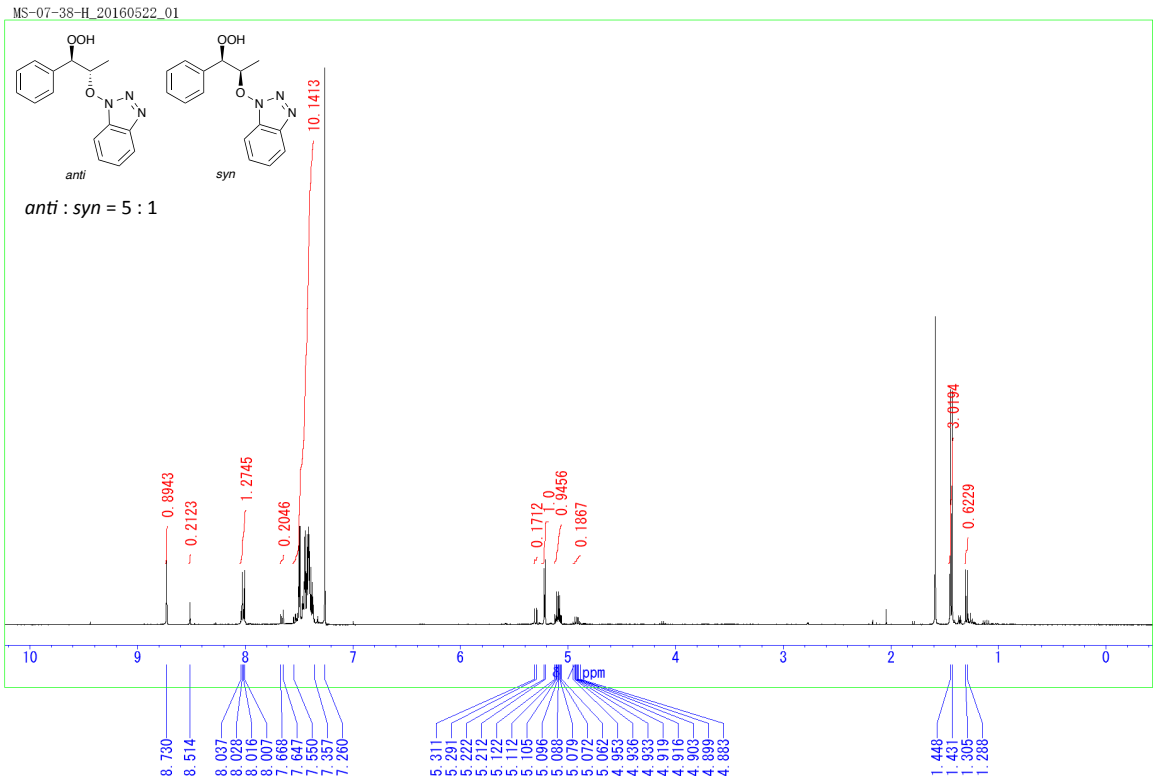


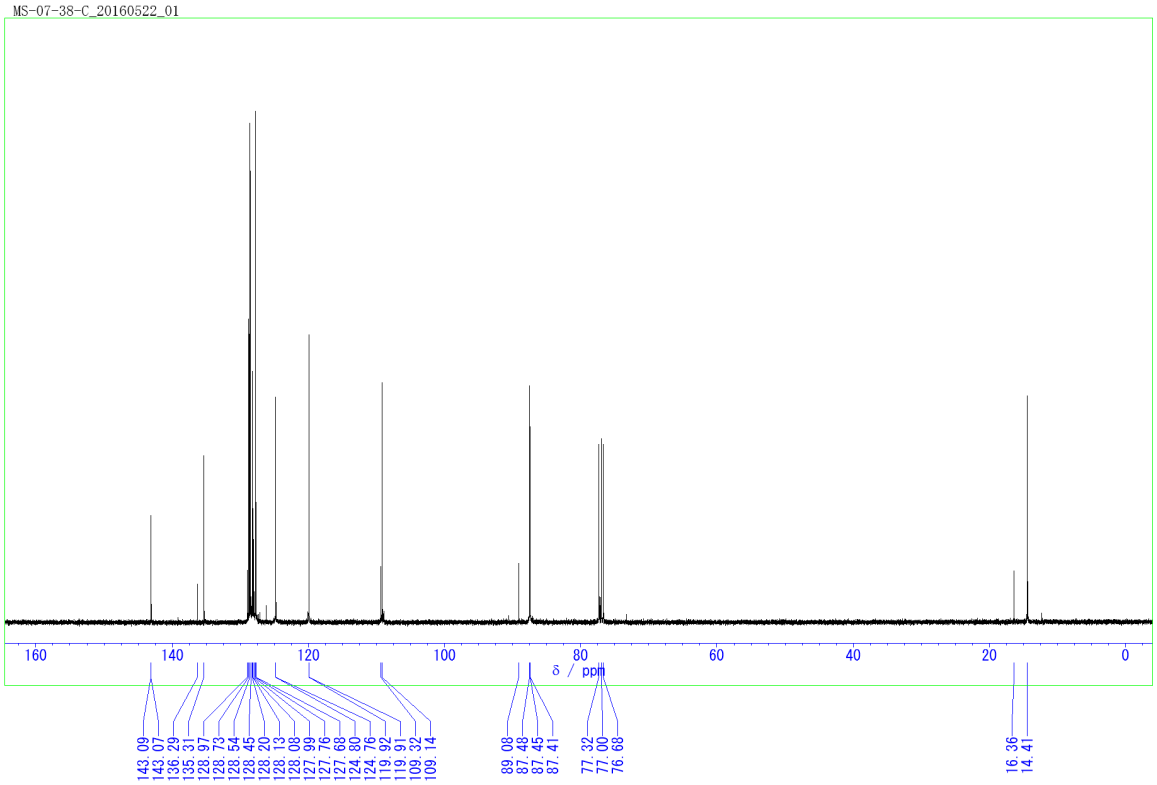

MS-07-34-P_RE_20160620_01
OOH
O
N
N
N
6.7079
2.1028
0.9818
1.0749
1.0273
1.0959
1.0
9
8
7
6
5
4
3
2
1
δ / ppm
8.588
8.032
8.010
7.638
7.617
7.552
7.532
7.512
7.427
7.386
7.260
5.440
5.427
5.424
5.411
4.829
4.813

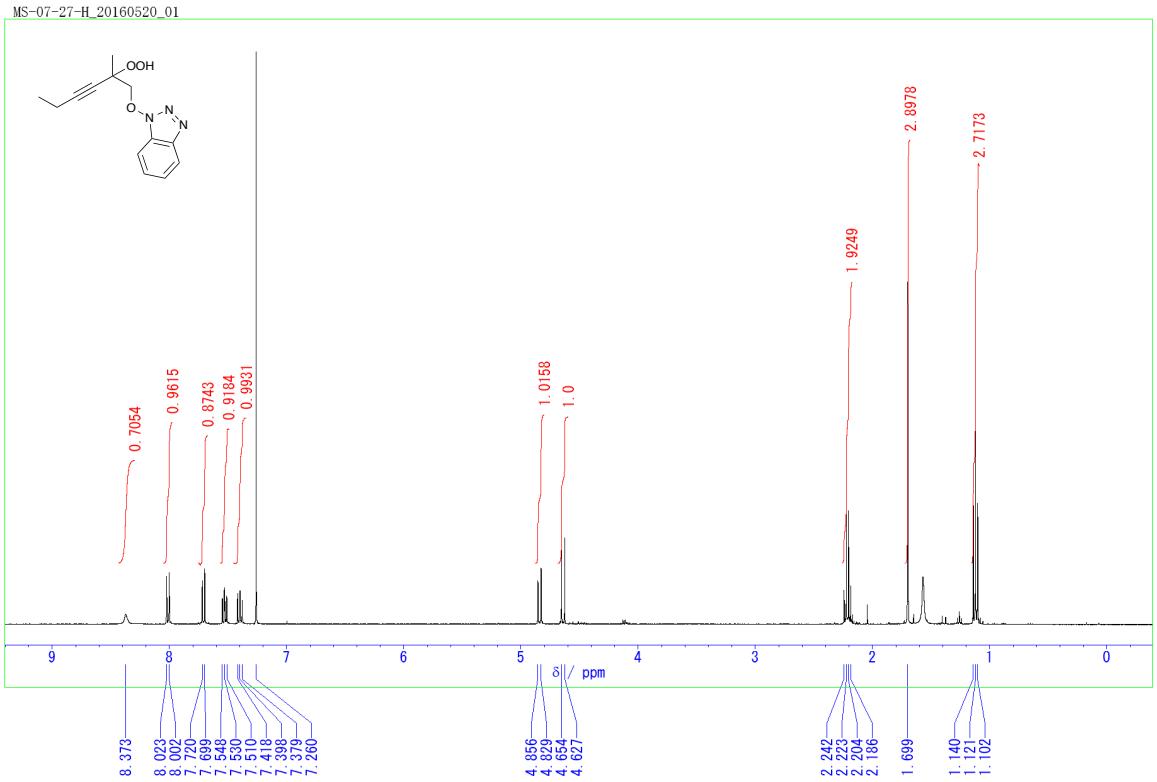

MS-07-34-C_20160523_01
160
140
120
100
80
60
40
20
0
δ / ppm
143.16
135.39
129.08
128.80
128.27
127.37
127.18
124.91
119.96
109.00
84.34
80.20
77.32
77.00
76.68

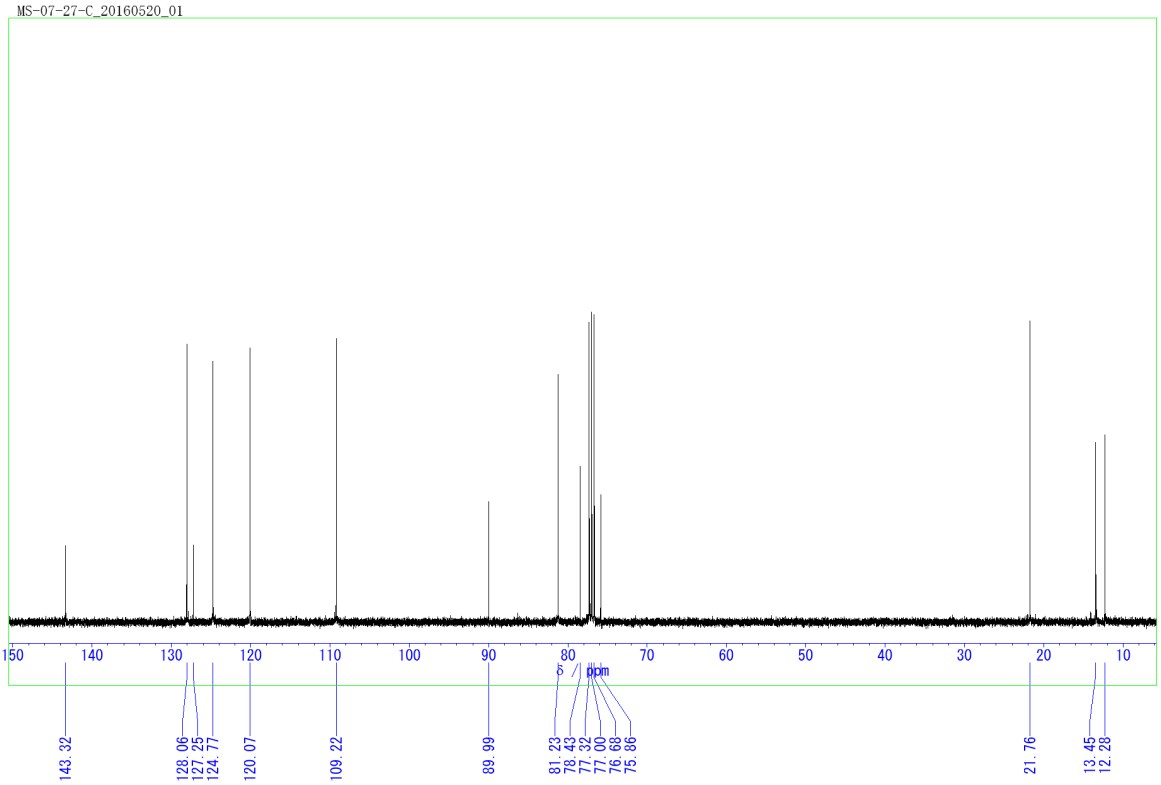

MS-07-02-fr13-31_20160319_01
OOH
O
N
N
N
7.6776
0.8427
2.0
2.9082
10
9
8
7
6
5
4
3
2
1
0
δ
ppm
8.015
7.994
7.544
7.341
7.260
4.990
4.964
4.954
4.928
1.850


MS-07-02-C_20160319_01
140
120
100
80
60
40
20
0
δ / ppm
142.99
140.16
128.49
128.03
128.03
126.93
125.53
124.83
119.71
109.00
84.14
82.55
77.32
77.00
76.68
21.75

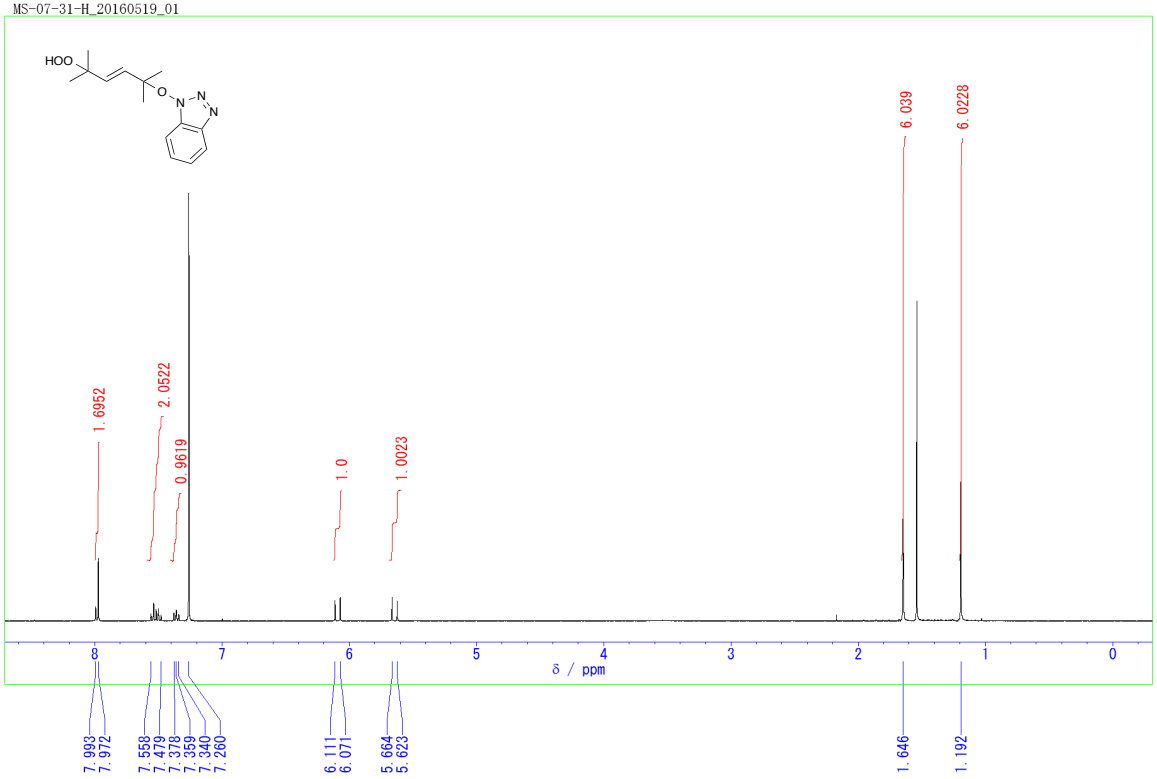

MS-07-38-H_20160522_01
OOH
anti
OOH
syn
anti : syn = 5 : 1
10.1413
0.8943
0.2123
1.2745
0.2046
0.1712
1.0
0.9456
0.1867
3.0194
0.6229
ppm
8.730
8.514
8.037
8.028
8.016
8.007
7.668
7.647
7.550
7.357
7.260
5.311
5.291
5.222
5.212
5.122
5.112
5.105
5.096
5.088
5.079
5.072
5.062
4.953
4.936
4.933
4.919
4.916
4.903
4.899
4.883
1.448
1.431
1.305
1.288


MS-07-38-C_20160522_01
δ / ppm
143.09
143.07
136.29
135.31
128.97
128.73
128.54
128.45
128.20
128.13
128.08
127.99
127.76
127.68
124.80
124.76
119.92
119.91
109.32
109.14
89.08
87.48
87.45
87.41
77.32
77.00
76.68
16.36
14.41

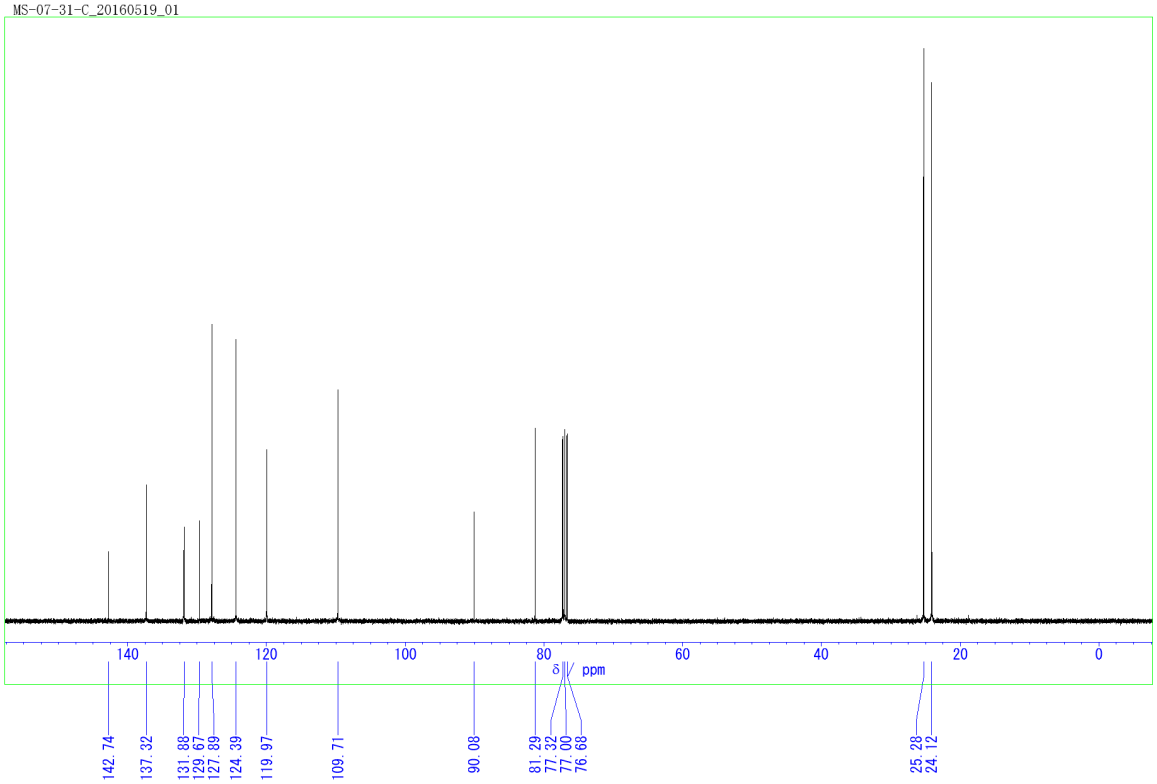

MS-07-27-H_20160520_01
OOH
O
N
N
N
0.7054
0.9615
0.8743
0.9184
0.9931
1.0158
1.0
1.9249
2.8978
2.7173
9
8
7
6
5
4
3
2
1
0
δ / ppm
8.373
8.023
8.002
7.720
7.699
7.648
7.530
7.510
7.418
7.398
7.379
7.260
4.856
4.829
4.654
4.627
2.242
2.223
2.204
2.186
1.699
1.140
1.121
1.102

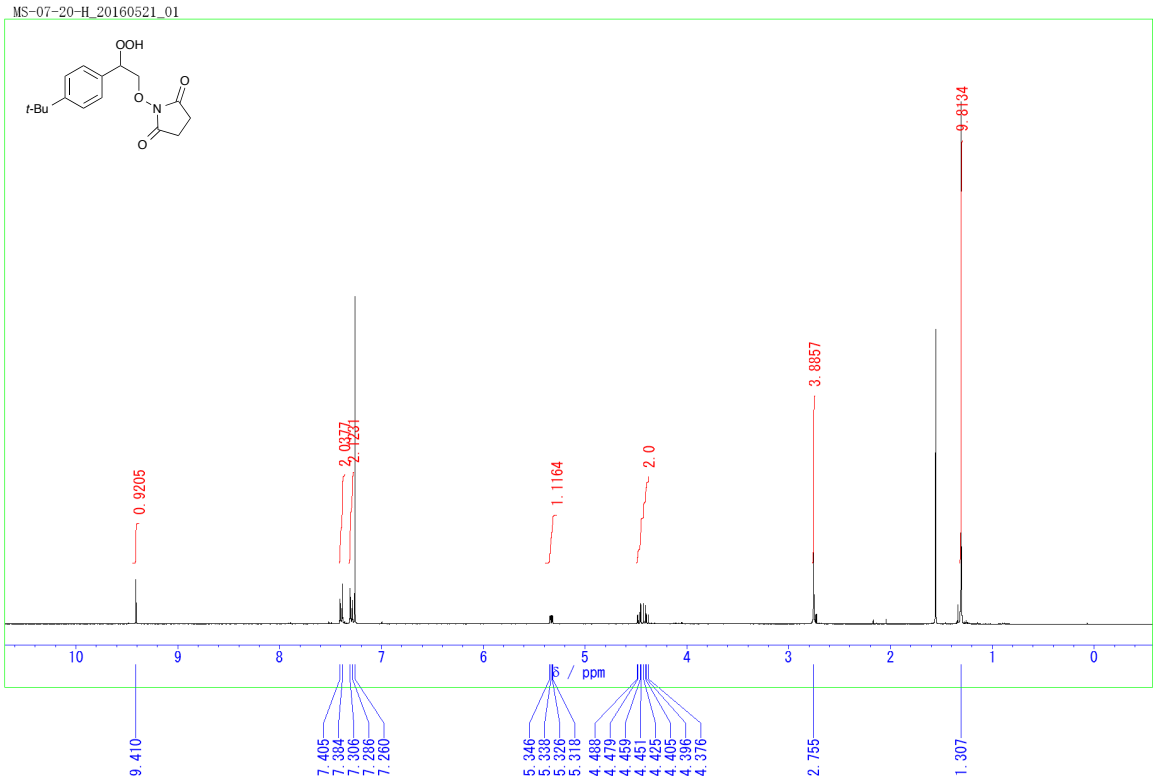

MS-07-27-C_20160520_01
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
δ / ppm
143.32
128.06
127.25
124.77
120.07
109.22
89.99
81.23
78.43
77.32
77.00
76.68
75.86
21.76
13.45
12.28

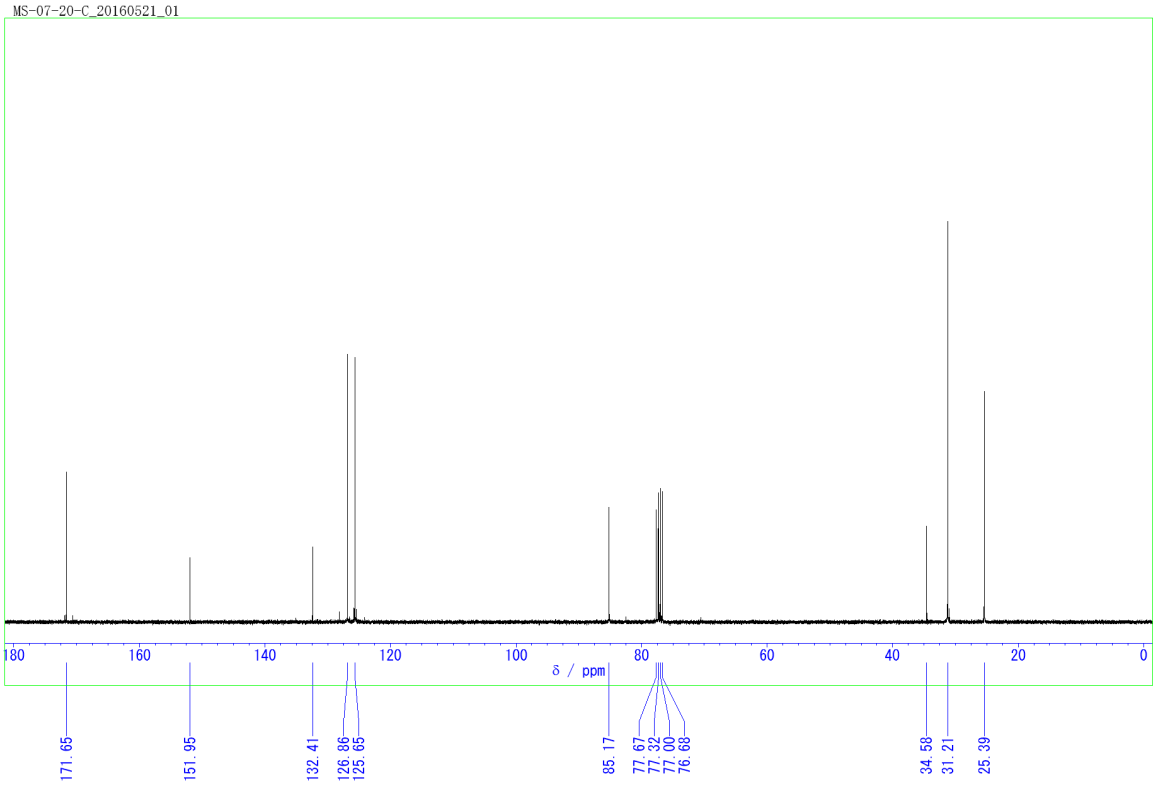
MS-07-31-H_20160519_01

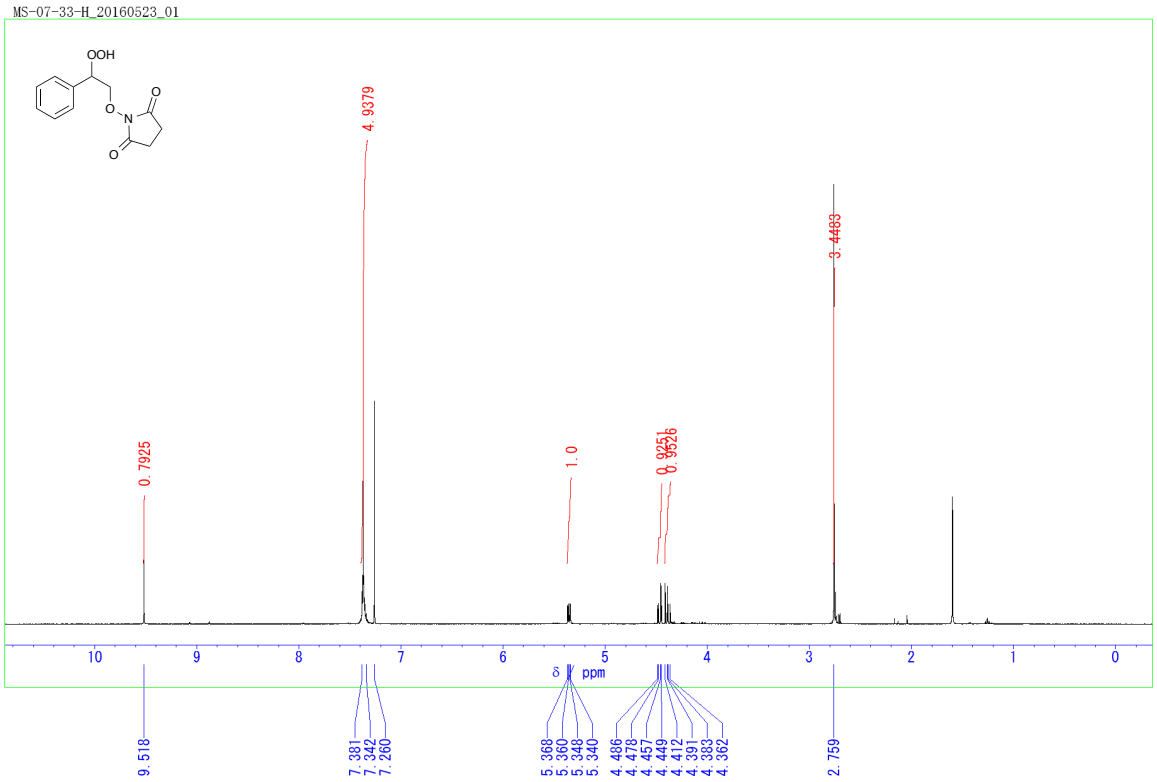


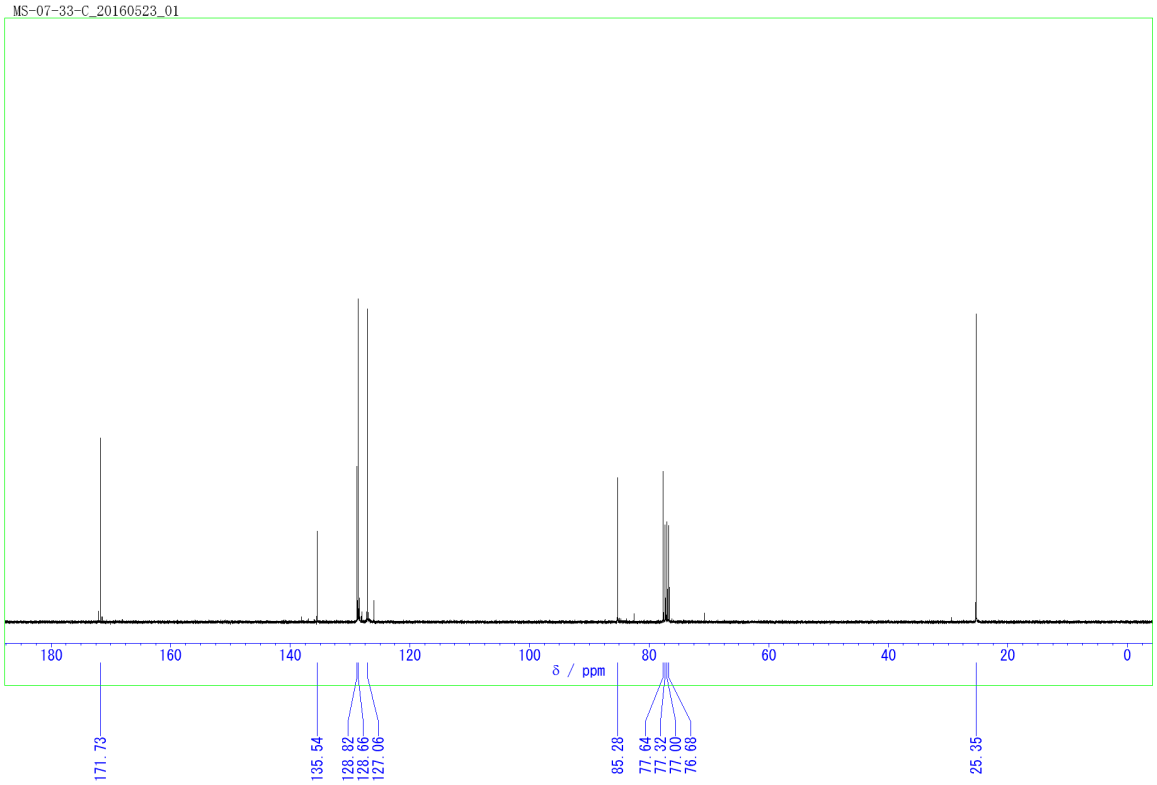
MS-07-31-C_20160519_01

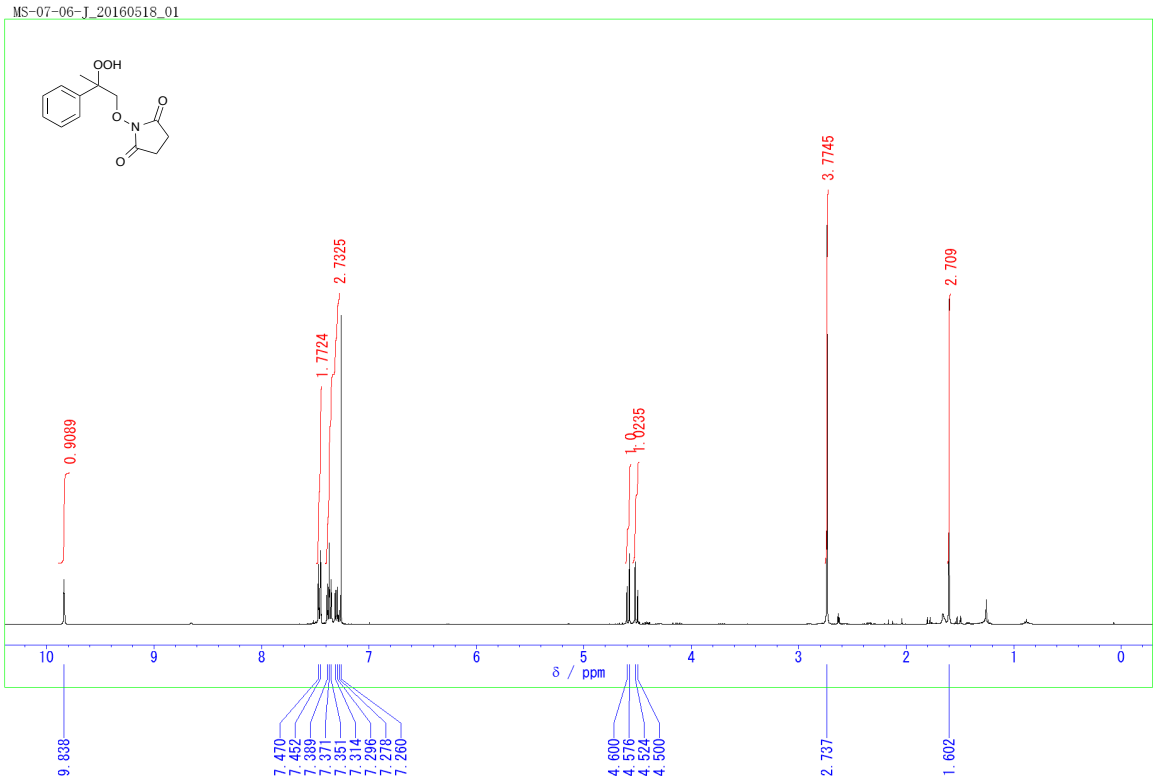


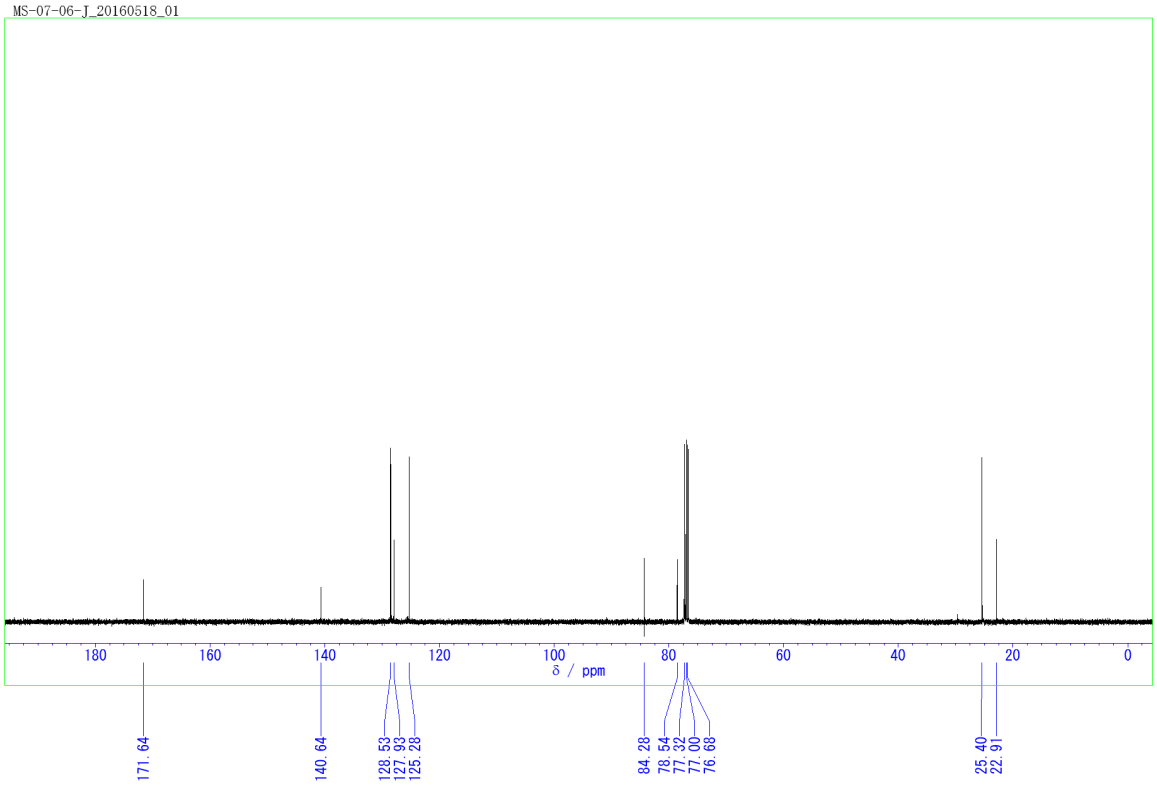

MS-07-20-H_20160521_01
OOH
t-Bu
O
N
O
O
9.0134
3.8857
2.0377
2.1231
2.0
1.1164
0.9205
δ / ppm
9.410
7.405
7.384
7.306
7.286
7.260
5.346
5.338
5.326
5.318
4.488
4.479
4.459
4.451
4.425
4.405
4.396
4.376
2.755
1.307


MS-07-20-C_20160521_01
δ / ppm
171.65
151.95
132.41
126.86
125.65
85.17
77.67
77.32
77.00
76.68
34.58
31.21
25.39

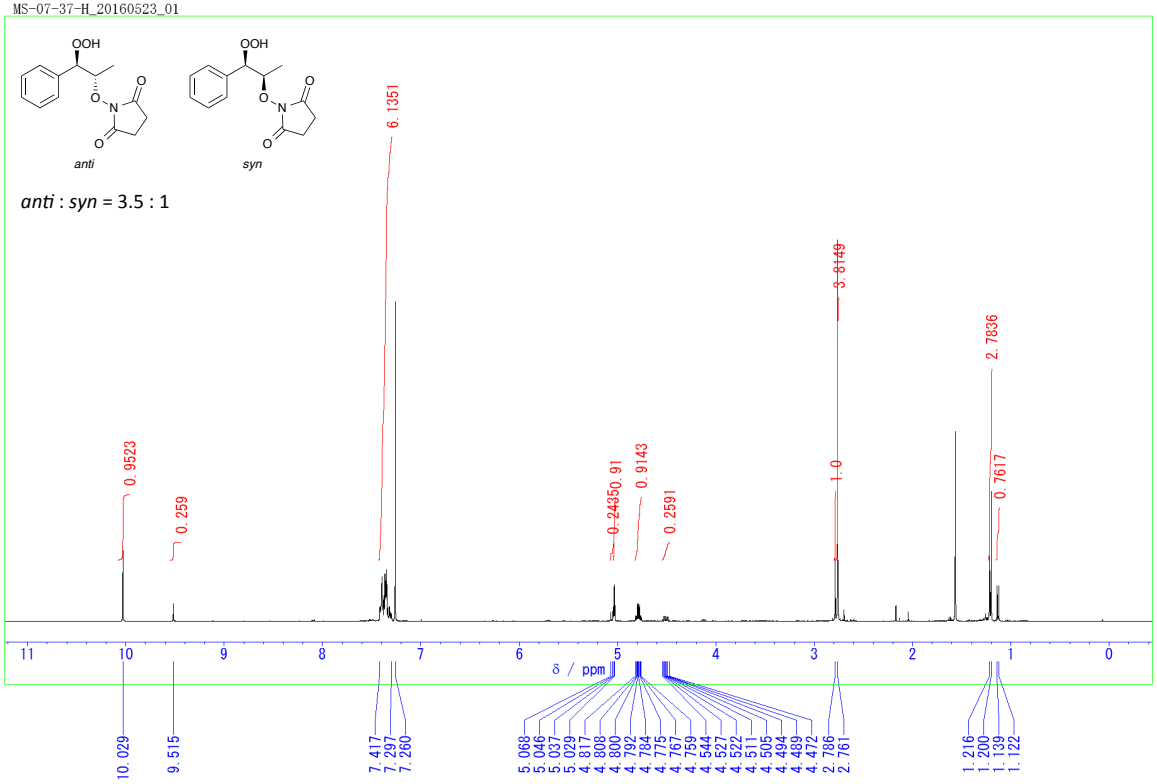

MS-07-33-H_20160523_01
OOH
O
O
N
O
4.9379
3.4483
0.7925
1.0
0.9551
0.9526
10
9
8
7
6
5
4
3
2
1
0
δ / ppm
9.518
7.381
7.342
7.260
5.368
5.360
5.348
5.340
4.486
4.478
4.457
4.449
4.412
4.391
4.383
4.362
2.759


MS-07-33-C_20160523_01
180
160
140
120
100
80
60
40
20
0
δ / ppm
171.73
135.54
128.82
128.66
127.06
85.28
77.64
77.32
77.00
76.68
25.35

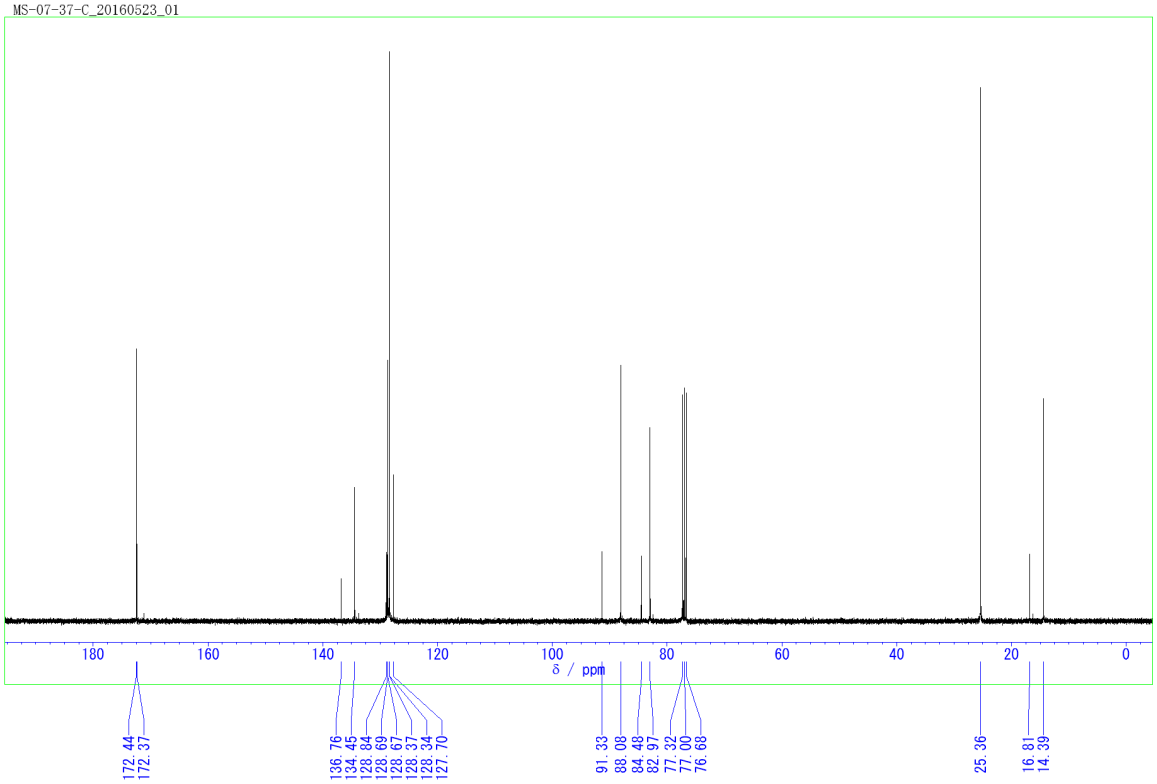

MS-07-06-J_20160518_01
OOH
O
O
N
O
0.9089
1.7724
2.7325
1.0235
3.7745
2.709
δ / ppm
9.838
7.470
7.452
7.389
7.371
7.351
7.314
7.296
7.278
7.260
4.600
4.576
4.524
4.500
2.737
1.602

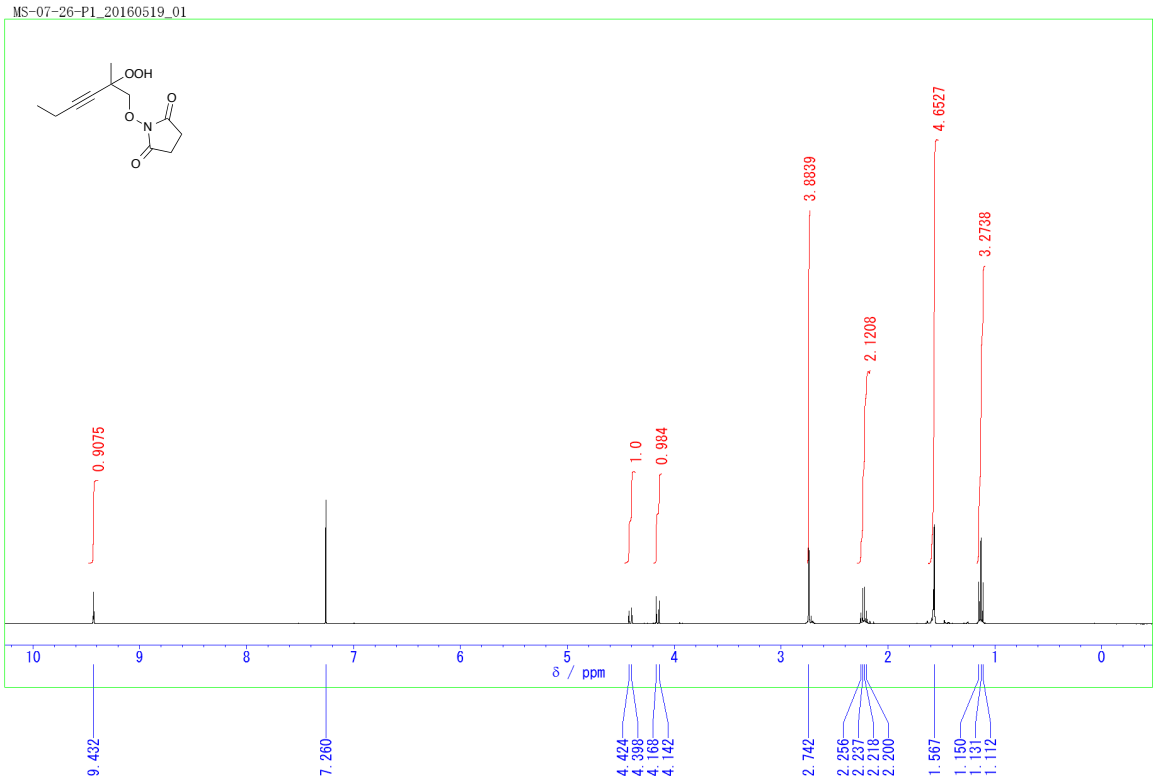

MS-07-06-J_20160518_01
δ / ppm
171.64
140.64
128.53
127.93
125.28
84.28
78.54
77.32
77.00
76.68
25.40
22.91

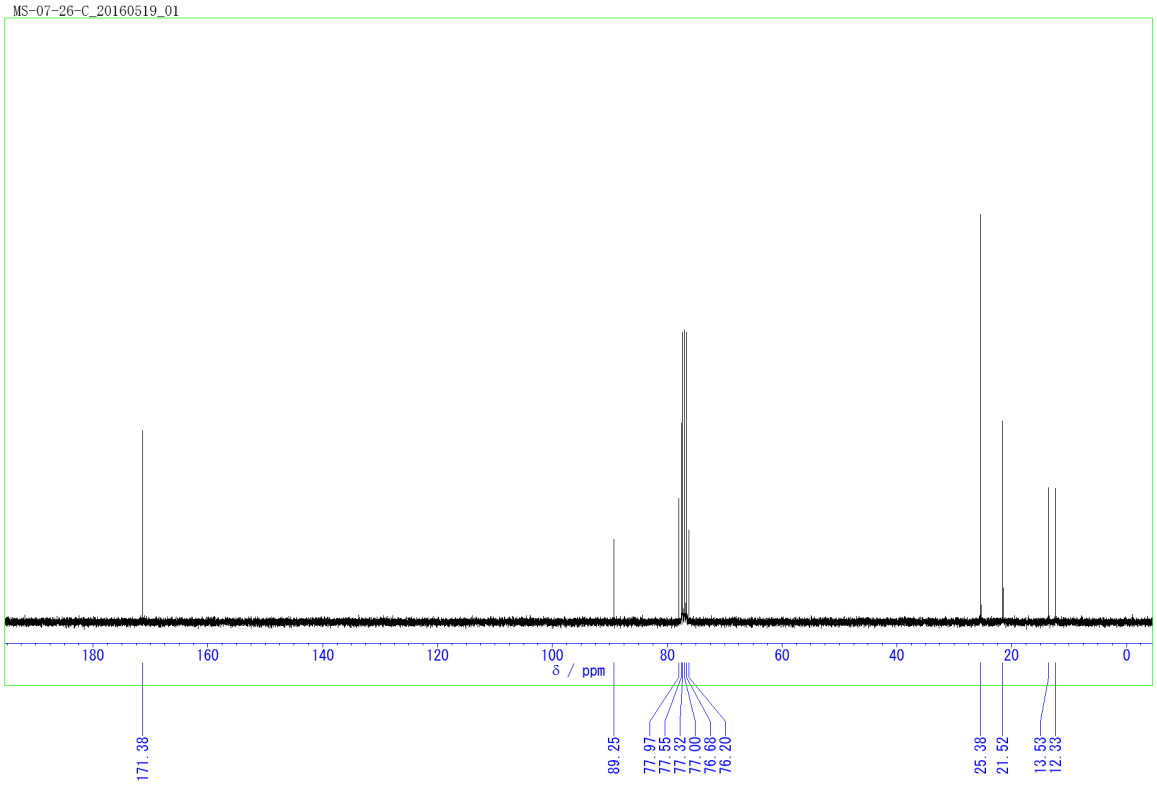
MS-07-37-H_20160523_01



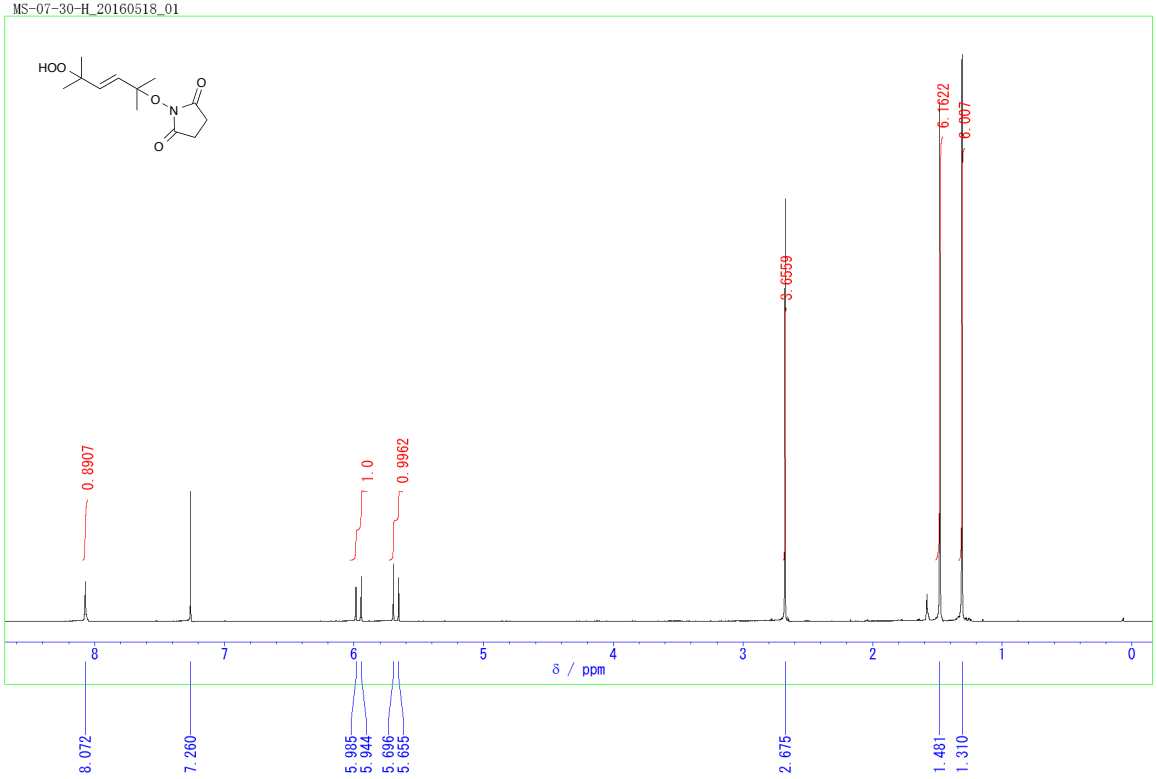
MS-07-37-C_20160523_01



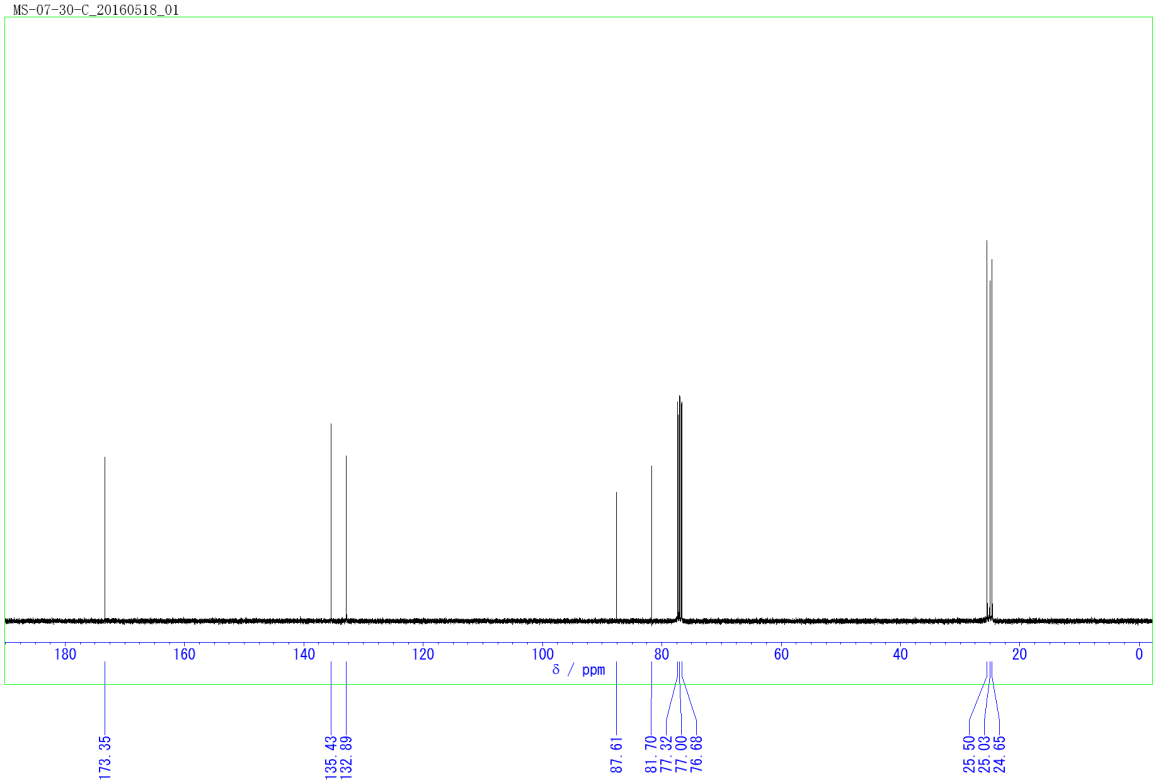

MS-07-26-P1_20160519_01
OOH
O
O
N
O
0.9075
1.0
0.984
3.8839
2.1208
4.6527
3.2738
10
9
8
7
6
5
4
3
2
1
0
δ / ppm
9.432
7.260
4.424
4.398
4.168
4.142
2.742
2.256
2.237
2.218
2.200
1.567
1.150
1.131
1.112


MS-07-26-C_20160519_01
180
160
140
120
100
80
60
40
20
0
δ / ppm
171.38
89.25
77.97
77.55
77.32
77.00
76.68
76.20
25.38
21.52
13.53
12.33

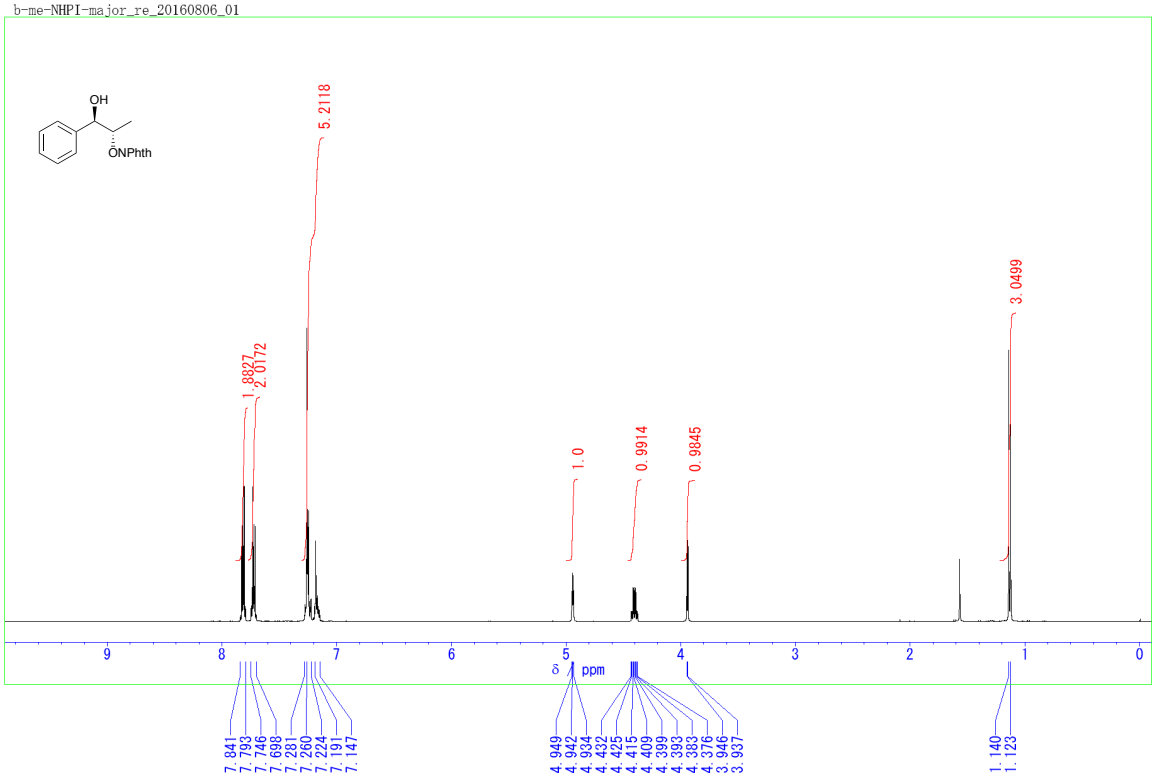
MS-07-30-H_20160518_01

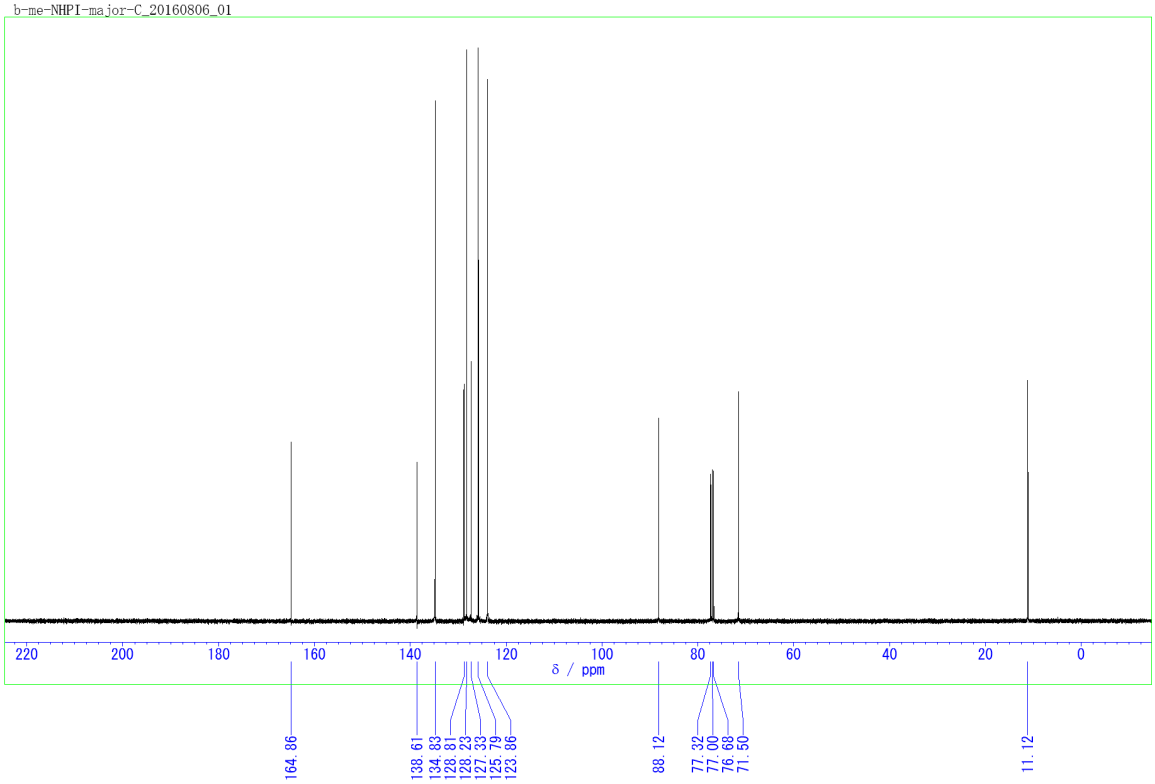


MS-07-30-C_20160518_01

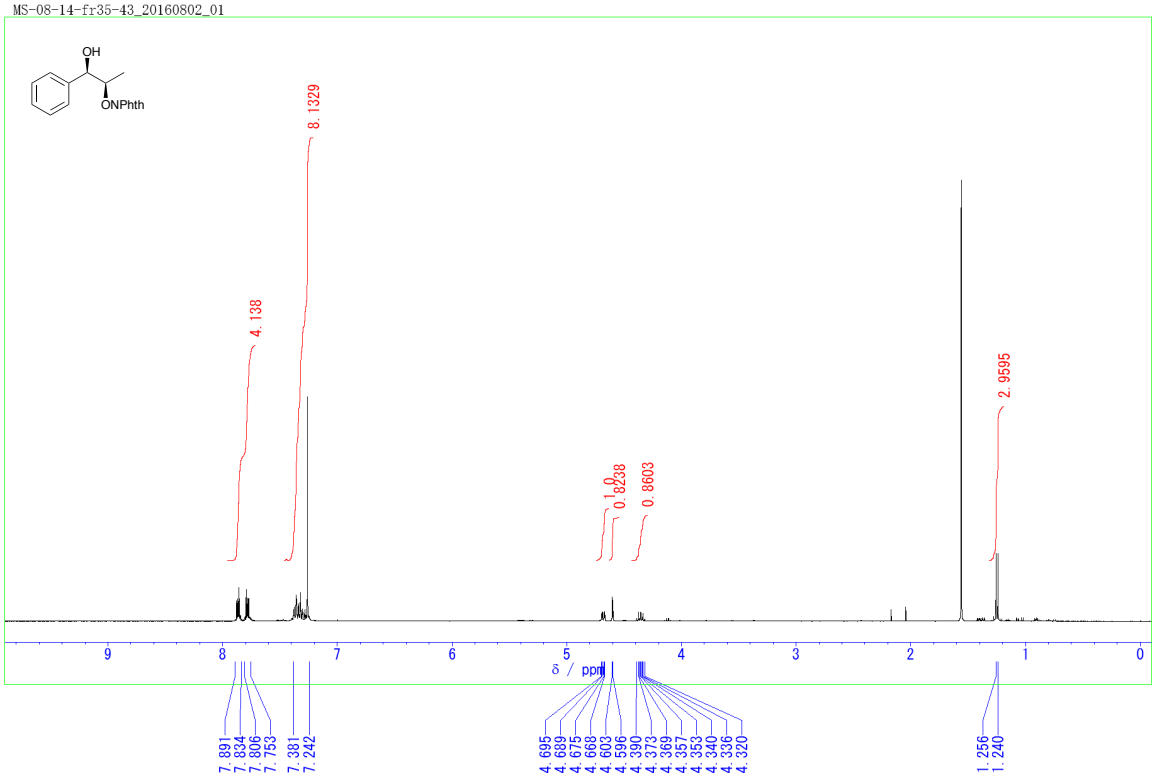


Determination of the relative configuration in 5j, 5k, 10j and 11j

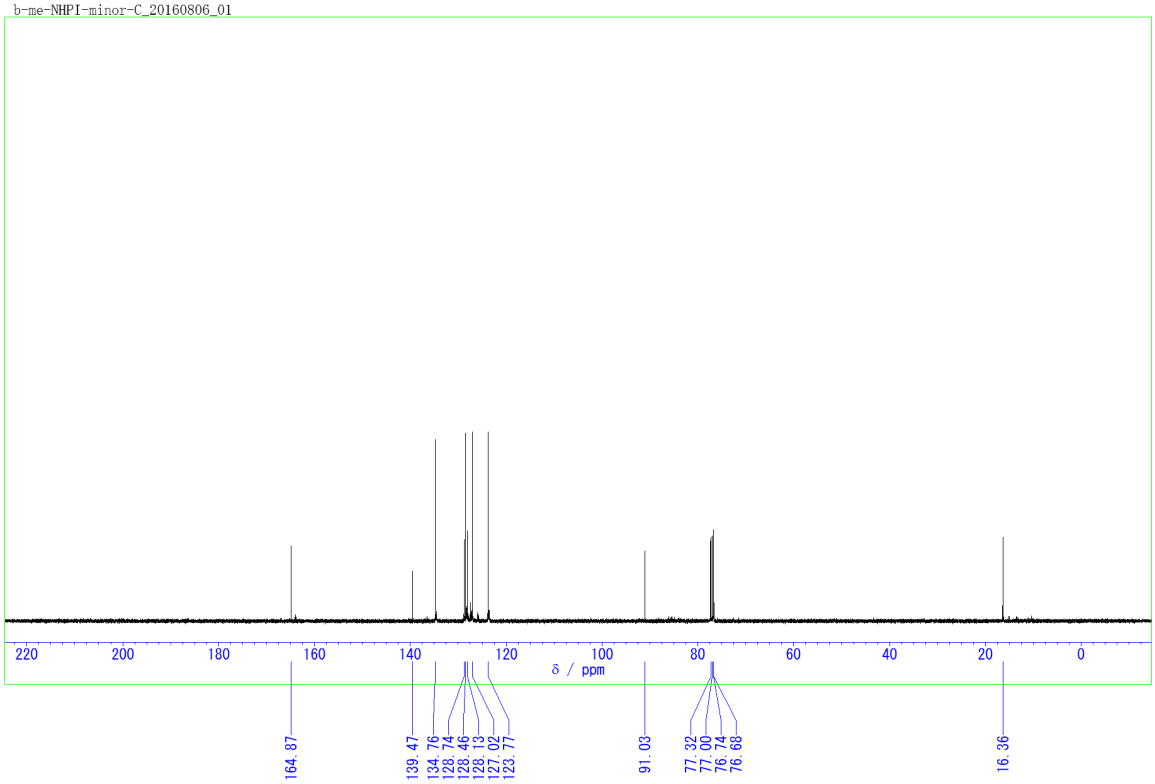


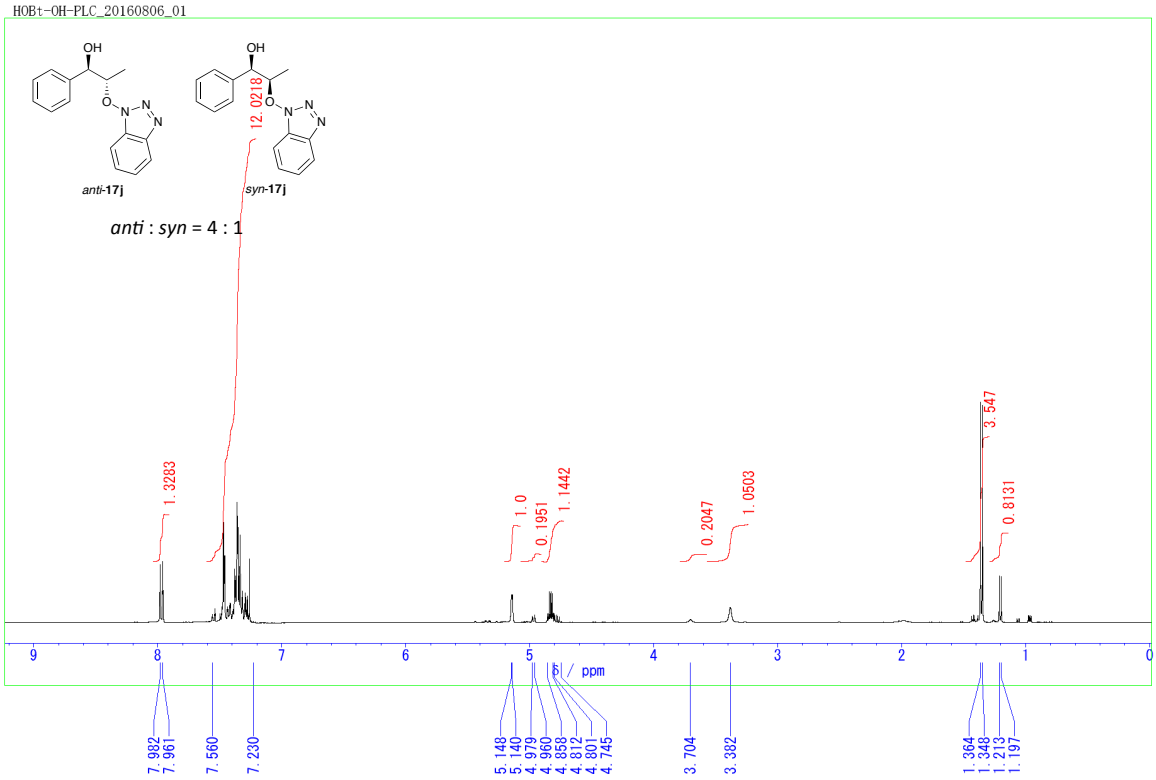


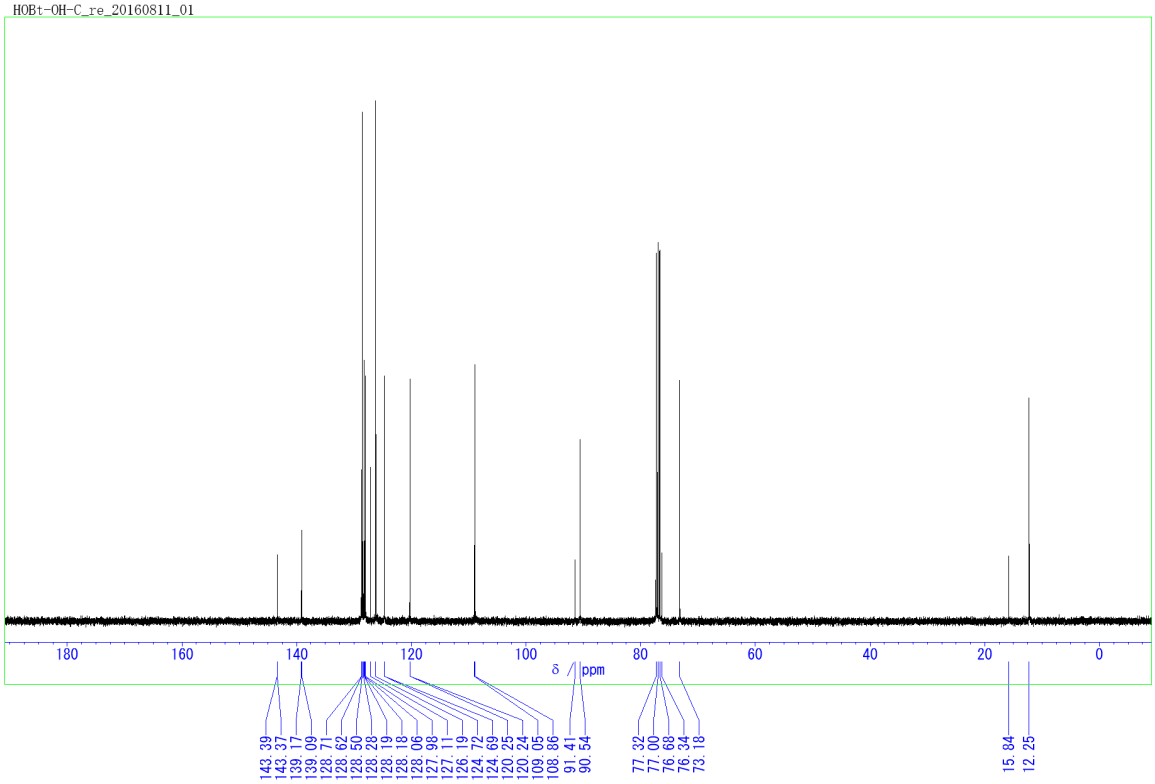
MS-08-14-fr35-43_20160802_01

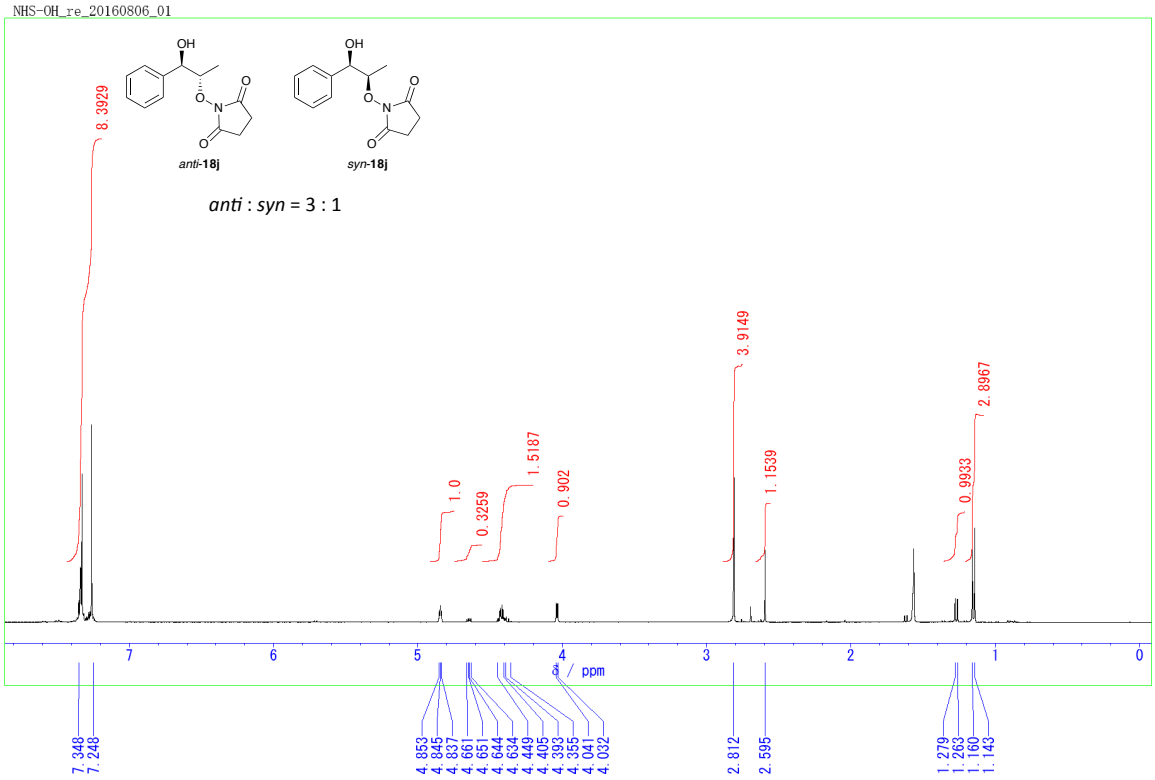


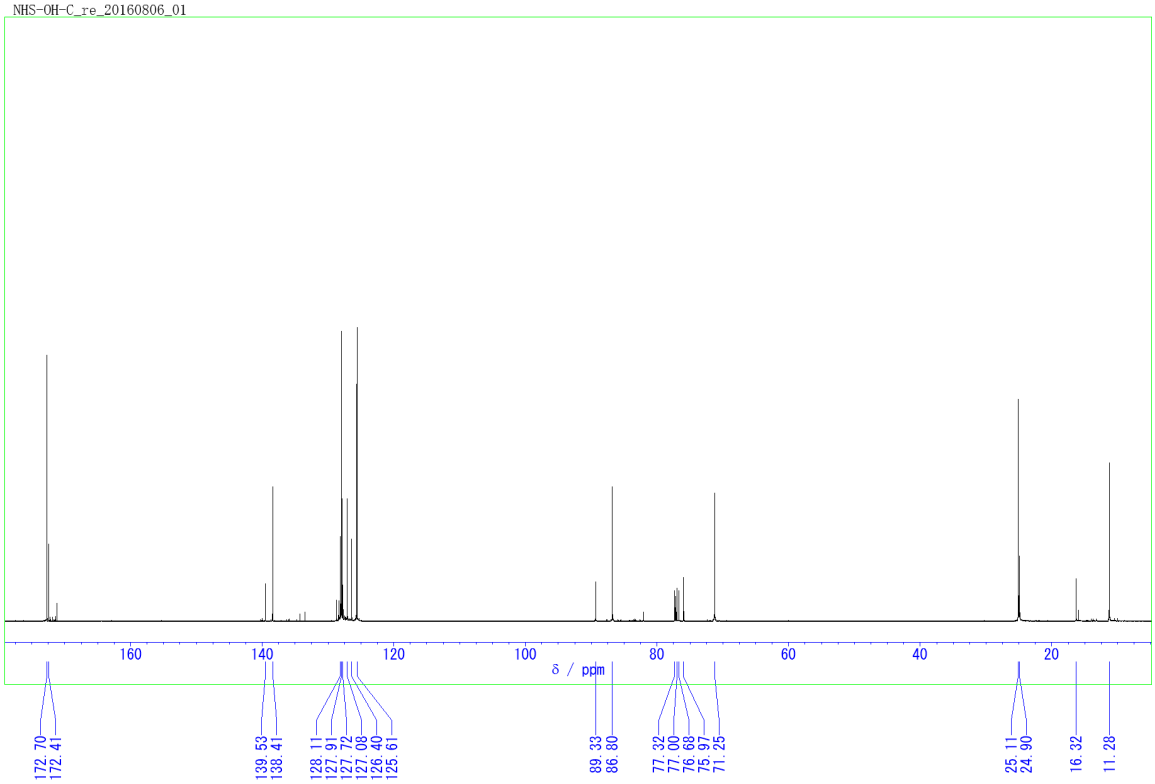
b-me-NHPI-minor-C_20160806_01

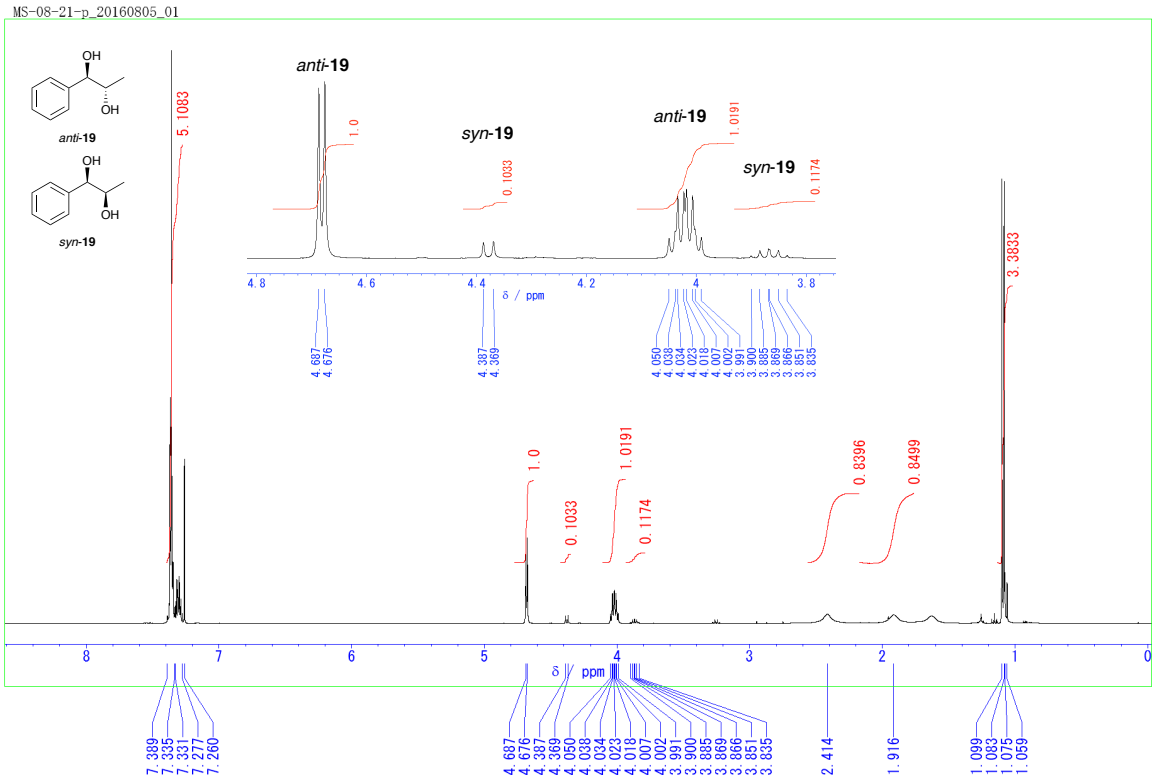


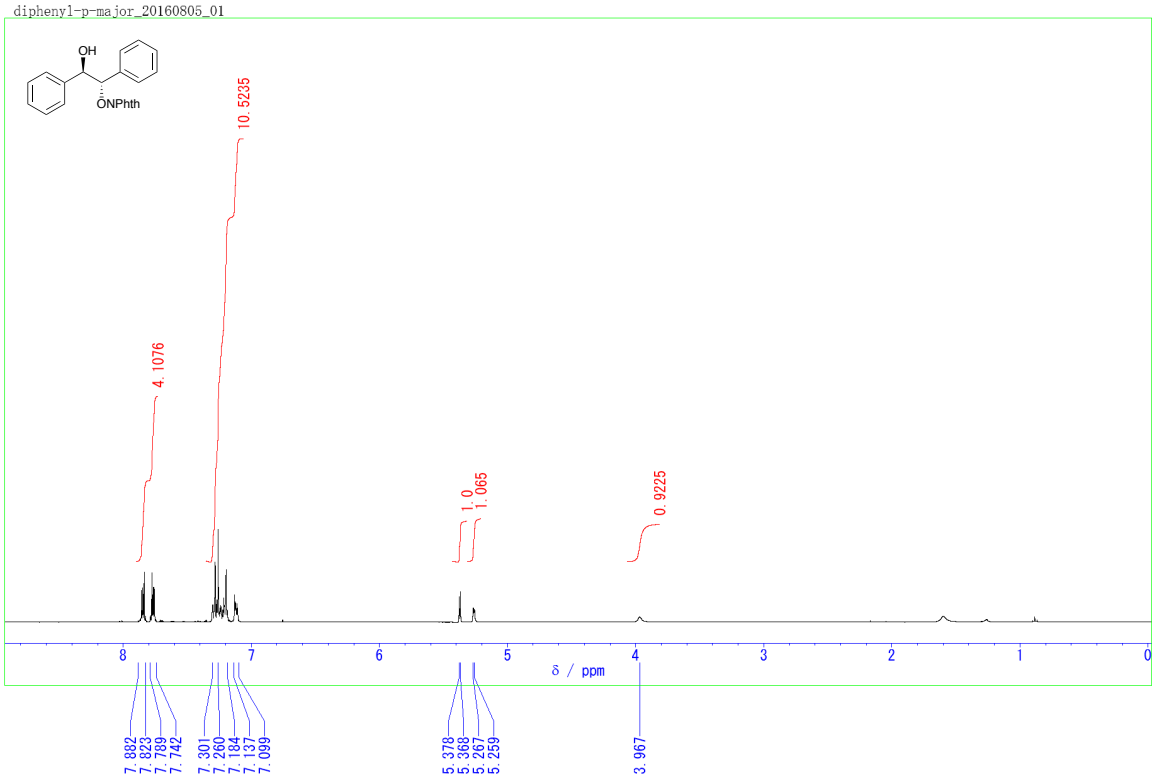

HOBt-OH-PLC_20160806_01
anti-17j
syn-17j
anti : syn = 4 : 1
12.0218
1.3283
1.0
0.1951
1.1442
0.2047
1.0503
3.547
0.8131
δ / ppm
7.982
7.961
7.560
7.230
5.148
5.140
4.979
4.960
4.858
4.812
4.801
4.745
3.704
3.382
1.364
1.348
1.213
1.197

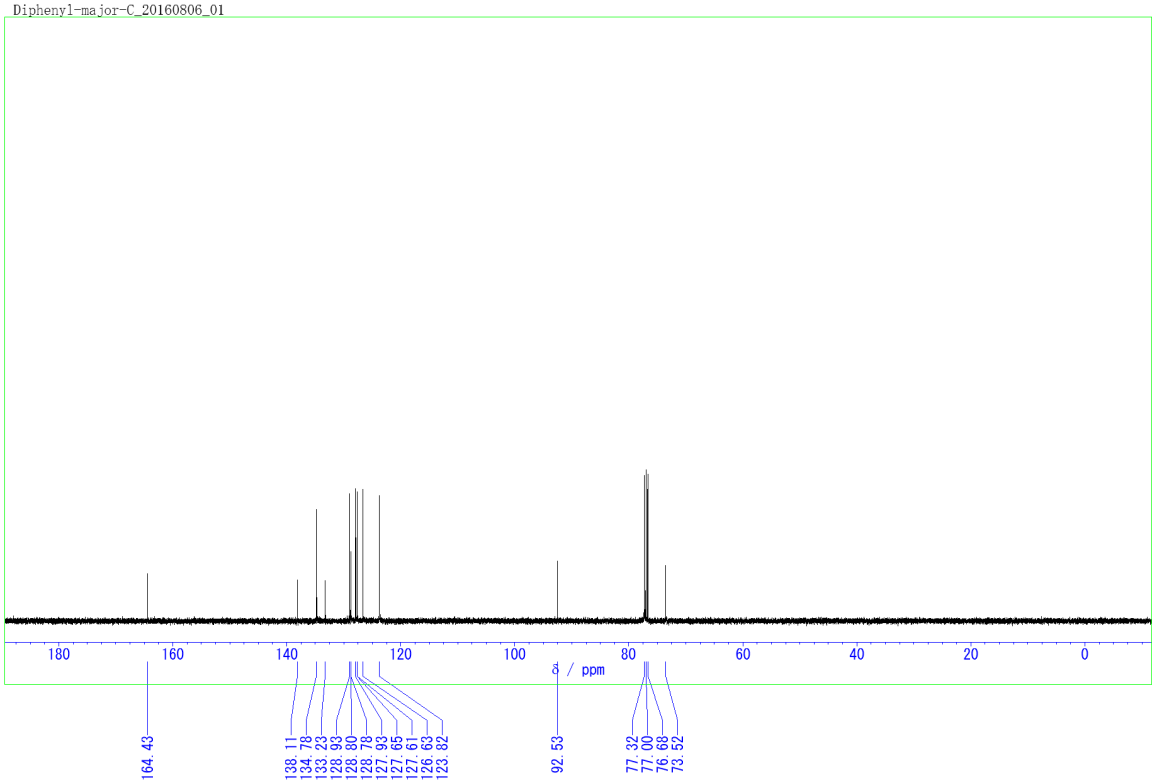

HOBt-OH-C_re_20160811_01
δ / ppm
143.39
143.37
139.17
139.09
128.71
128.62
128.50
128.28
128.19
128.18
128.06
127.98
127.11
126.19
124.72
124.69
120.25
120.24
109.05
108.86
91.41
90.54
77.32
77.00
76.68
76.34
73.18
15.84
12.25


NHS-OH_re_20160806_01
anti-18j
syn-18j
anti : syn = 3 : 1
8.3929
1.0
0.3259
1.5187
0.902
3.9149
1.1539
0.9933
2.8967
δ / ppm
7.348
7.248
4.853
4.845
4.837
4.661
4.651
4.644
4.634
4.449
4.405
4.393
4.355
4.041
4.032
2.812
2.595
1.279
1.263
1.160
1.143

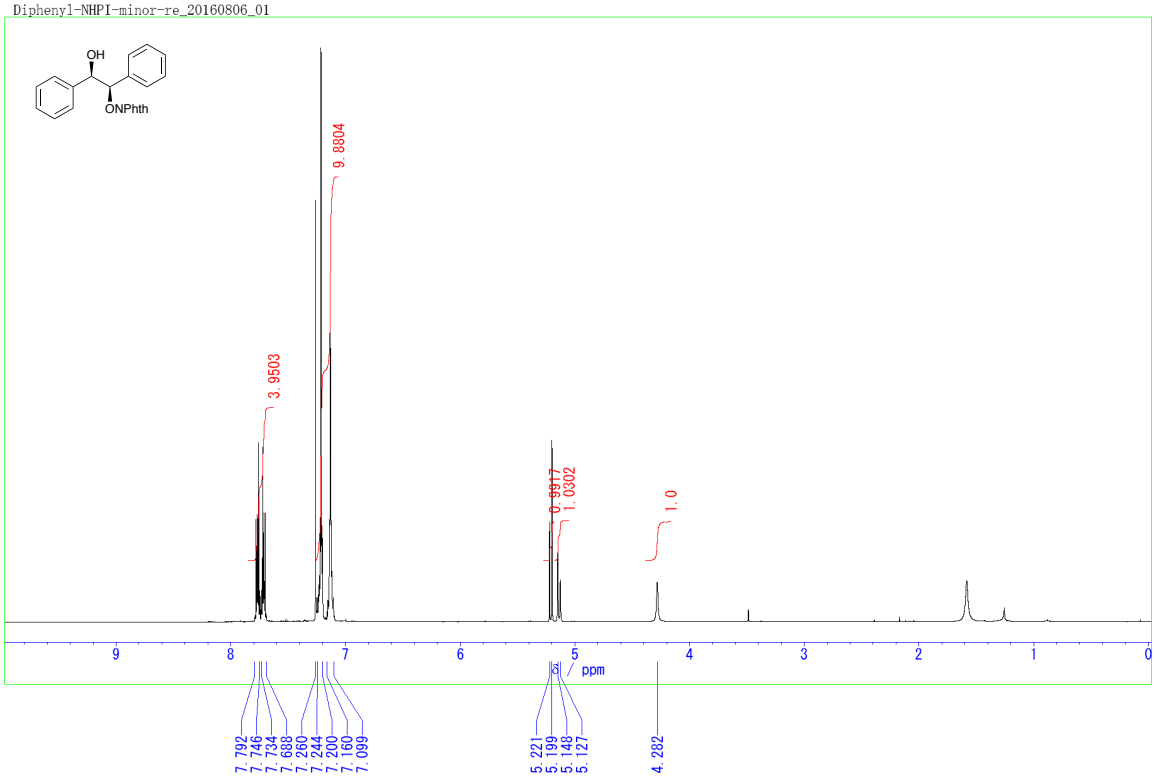

NHS-OH-C_re_20160806_01
δ / ppm
172.70
172.41
139.53
138.41
128.11
127.91
127.72
127.08
126.40
125.61
89.33
86.80
77.32
77.00
76.68
75.97
71.25
25.11
24.90
16.32
11.28


MS-08-21-p_20160805_01
anti-19
syn-19
anti-19
syn-19
anti-19
syn-19
δ / ppm
δ / ppm

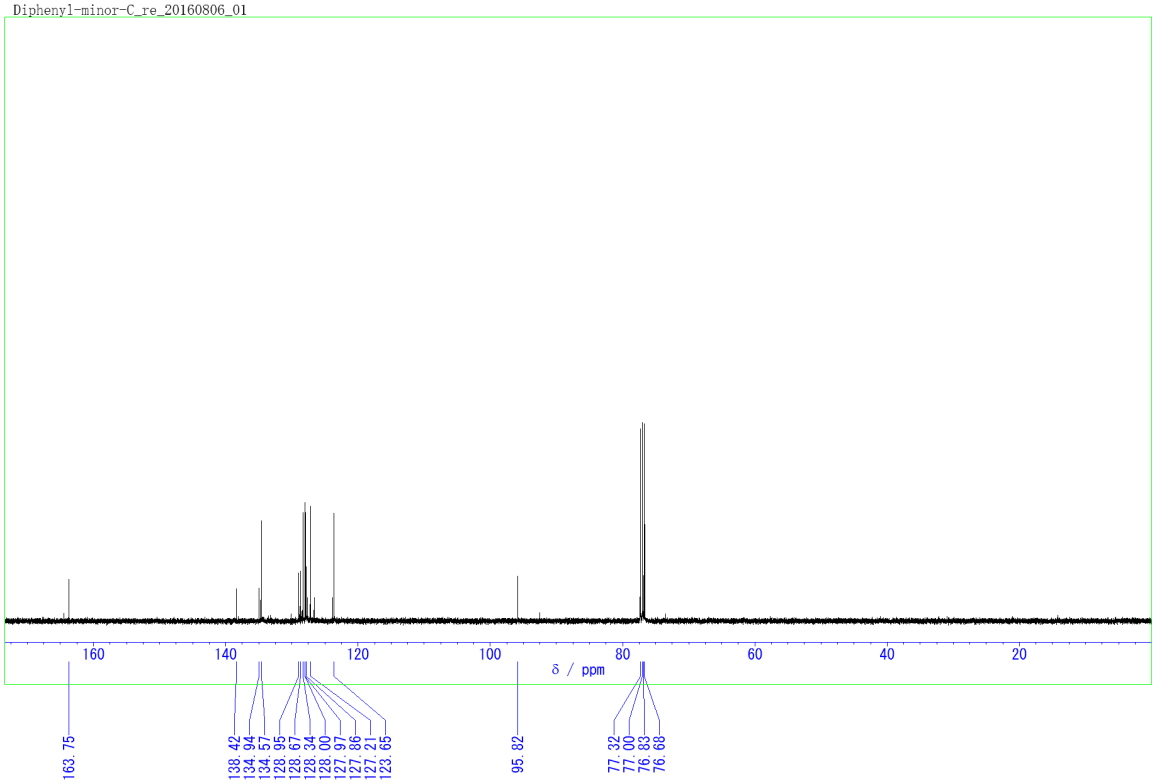

diphenyl-p-major_20160805_01
OH
ONPhth
10.5235
4.1076
1.0
1.065
0.9225
δ / ppm
7.882
7.823
7.789
7.742
7.301
7.260
7.184
7.137
7.099
5.378
5.368
5.267
5.259
3.967


Diphenyl-major-C_20160806_01
δ / ppm
164.43
138.11
134.78
133.23
128.93
128.80
128.78
127.93
127.65
127.61
126.63
123.82
92.53
77.32
77.00
76.68
73.52

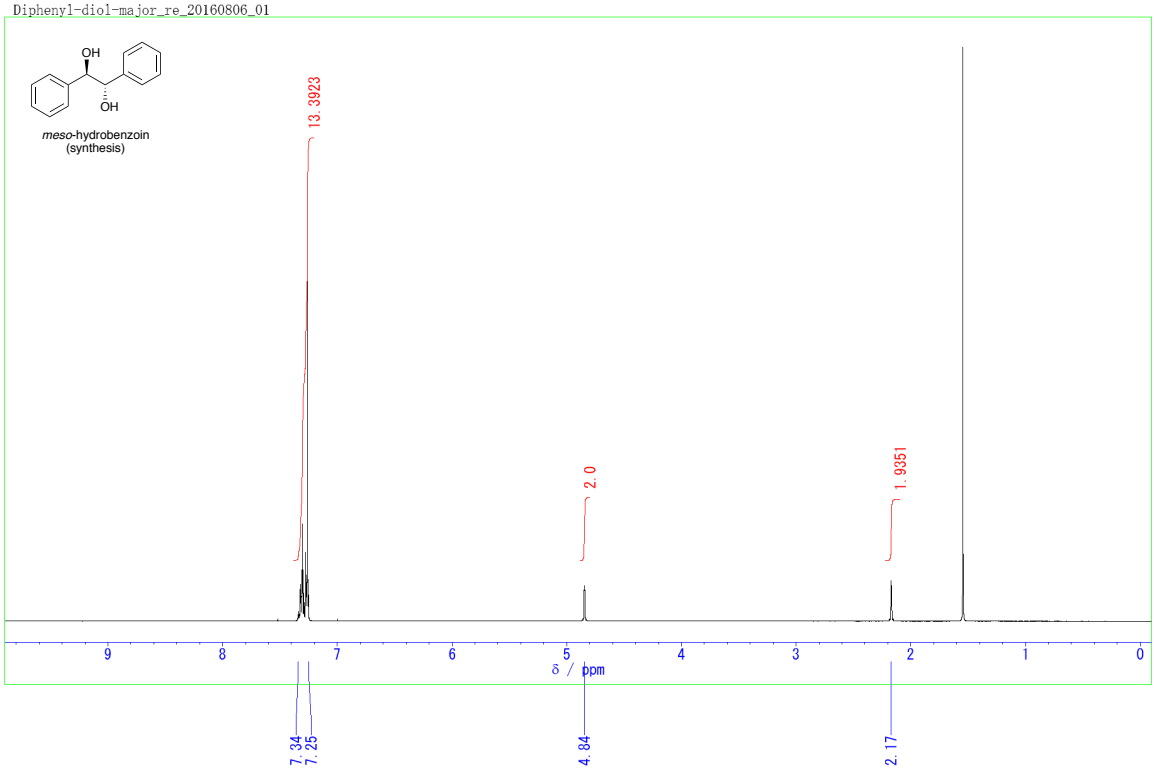
Diphenyl-NHPI-minor-re_20160806_01

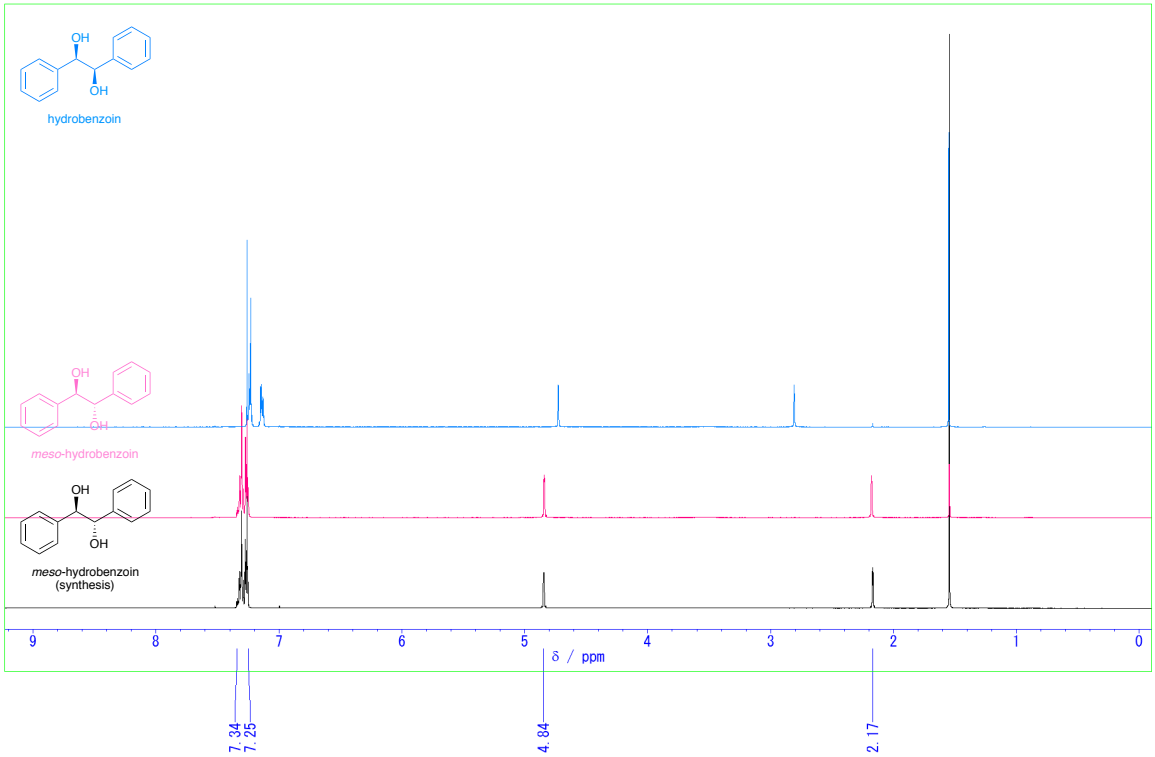


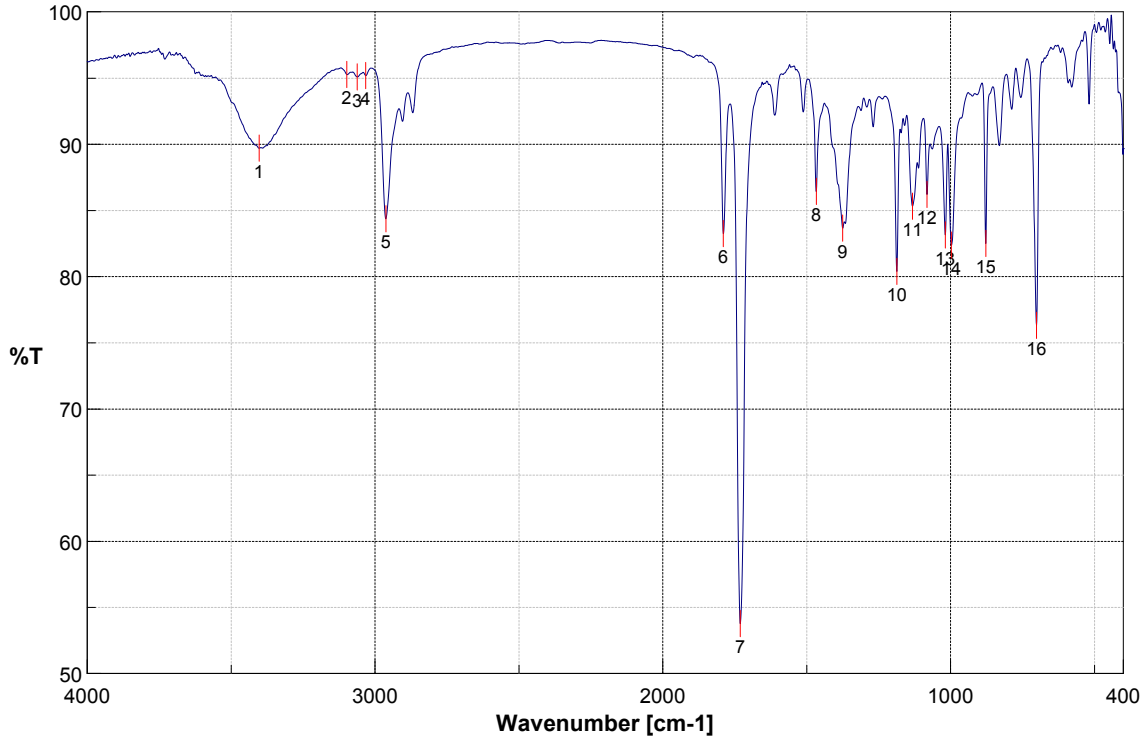
Diphenyl-minor-C_re_20160806_01



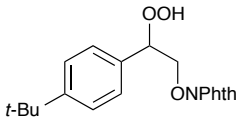
Diphenyl-diol-major_re_20160806_01



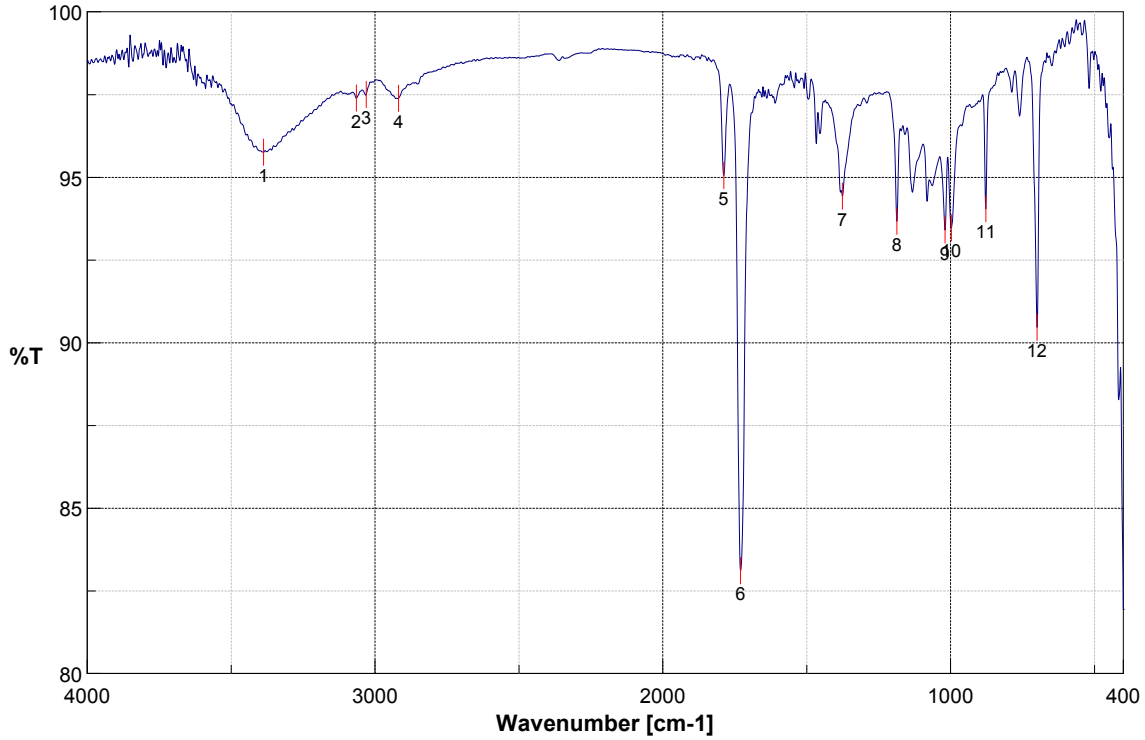




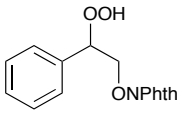
積算回数	16
分解	4 cm-1
ゼロフィリング	ON
アポダイゼーション	Cosine
ゲイン	Auto (2)
スキャンスピード	Auto (2 mm/sec)
測定日時	2016/05/30 14:04
更新日時	2016/08/05 14:57
測定者	yano
ファイル名	MS-05-33-pure.jws
サンプル名	momalcohol
コメント	



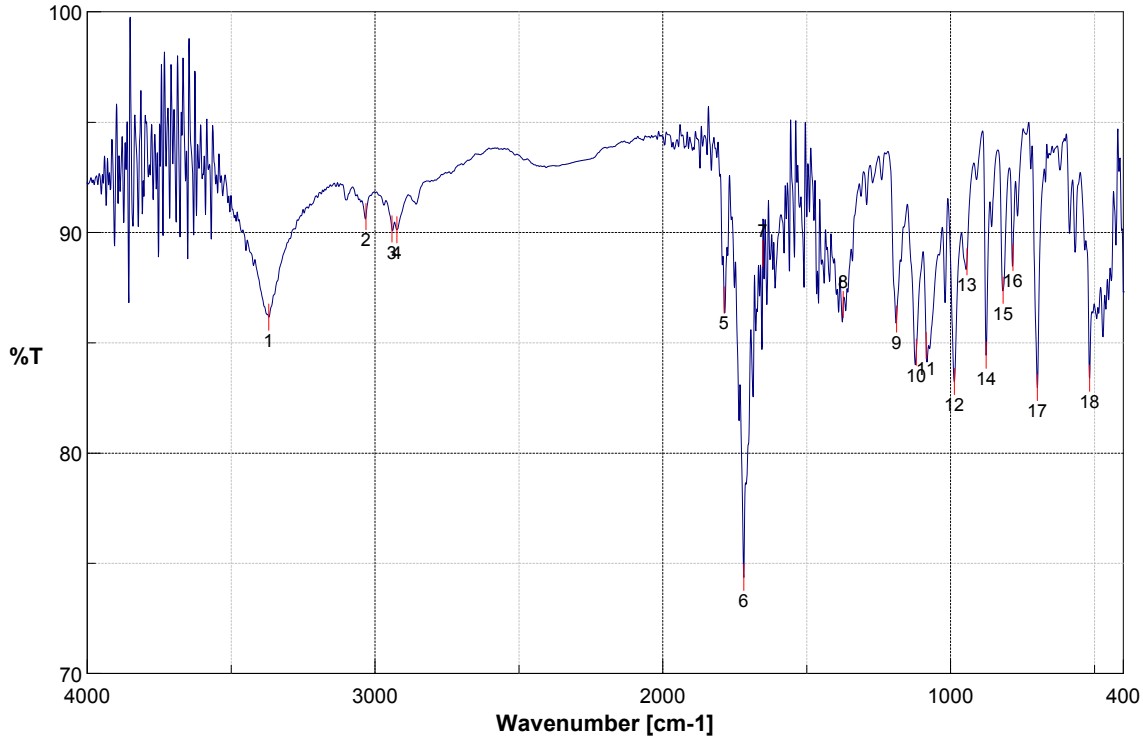
No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3402.78	89.7055	2	3098.08	95.2825	3	3062.41	95.0985
4	3032.51	95.1983	5	2962.13	84.3715	6	1789.62	83.2591
7	1730.8	53.7793	8	1466.6	86.4383	9	1375	83.6628
10	1186.97	80.4063	11	1132.97	85.3281	12	1081.87	86.2176
13	1018.23	83.1589	14	997.017	82.3851	15	877.452	82.5145
16	701.962	76.3333						



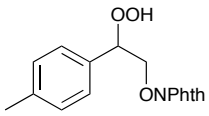
積算回数	16
分解	4 cm-1
ゼロフィリング	ON
アポダイゼーション	Cosine
ゲイン	Auto (2)
スキャンスピード	Auto (2 mm/sec)
測定日時	2016/05/30 14:49
更新日時	2016/08/05 15:02
測定者	yano
ファイル名	MS-07-32-pure.jws
サンプル名	momalcohol
コメント	



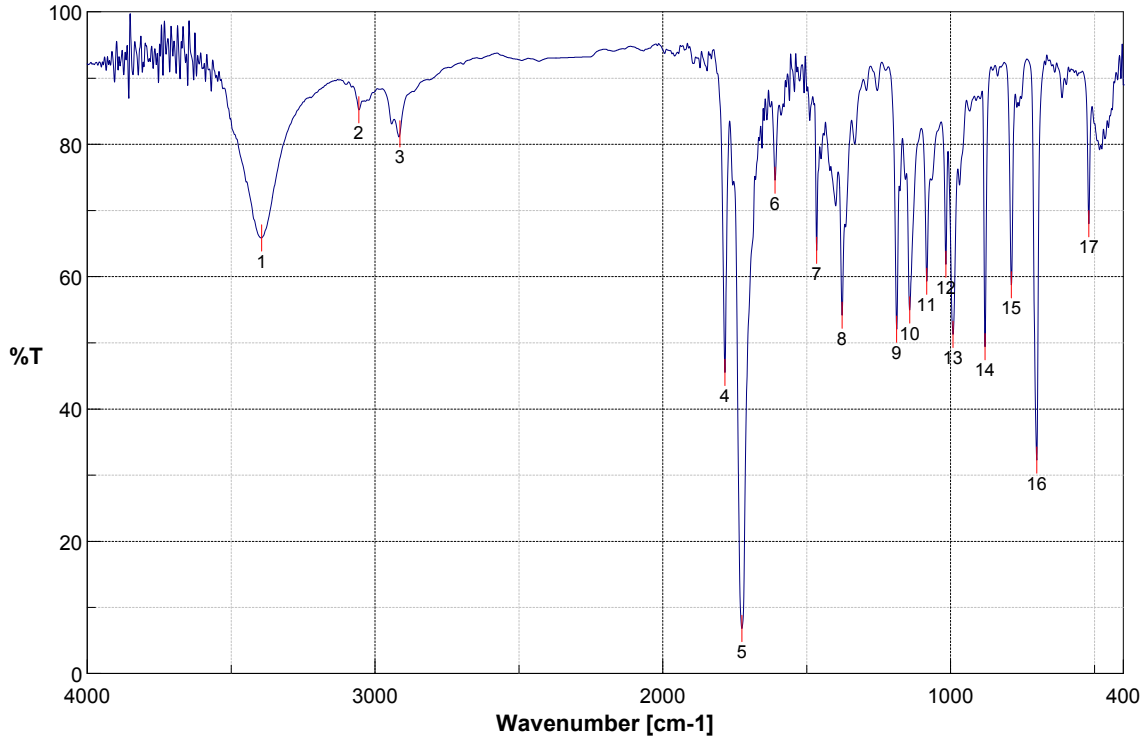
No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3387.35	95.7607	2	3064.33	97.3999	3	3030.59	97.5098
4	2918.73	97.3937	5	1787.69	95.057	6	1729.83	83.1115
7	1375.96	94.44	8	1186.97	93.6726	9	1019.19	93.4131
10	997.017	93.4786	11	877.452	94.0602	12	700.033	90.4713



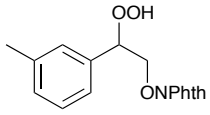
積算回数	16
分解	4 cm-1
ゼロフィリング	ON
アポダイゼーション	Cosine
ゲイン	Auto (4)
スキャンスピード	Auto (2 mm/sec)
測定日時	2016/05/30 15:00
更新日時	2016/08/05 15:03
測定者	yano
ファイル名	MS-05-39-pure.jws
サンプル名	momalcohol
コメント	



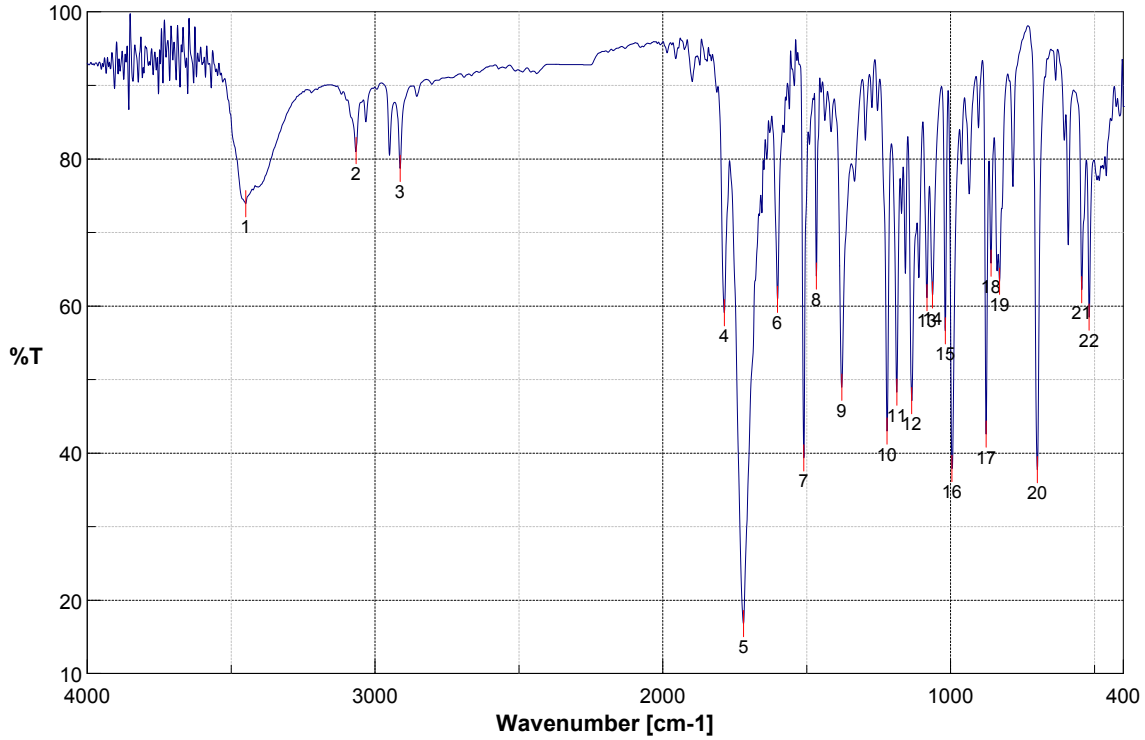
No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3369.03	86.1693	2	3031.55	90.7283	3	2940.91	90.161
4	2923.56	90.1228	5	1786.72	86.9474	6	1718.26	74.3754
7	1652.7	89.0451	8	1373.07	86.7381	9	1187.94	86.0863
10	1119.48	84.5834	11	1084.76	84.8743	12	987.375	83.2467
13	943.02	88.6706	14	876.488	84.4401	15	817.67	87.3868
16	782.958	88.8687	17	699.069	82.9742	18	516.829	83.3973



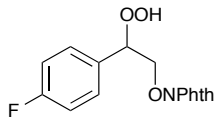
積算回数	16
分解	4 cm-1
ゼロフィリング	ON
アポダイゼーション	Cosine
ゲイン	Auto (4)
スキャンスピード	Auto (2 mm/sec)
測定日時	2016/05/30 14:38
更新日時	2016/08/05 15:04
測定者	yano
ファイル名	MS-05-34-pure.jws
サンプル名	momalcohol
コメント	



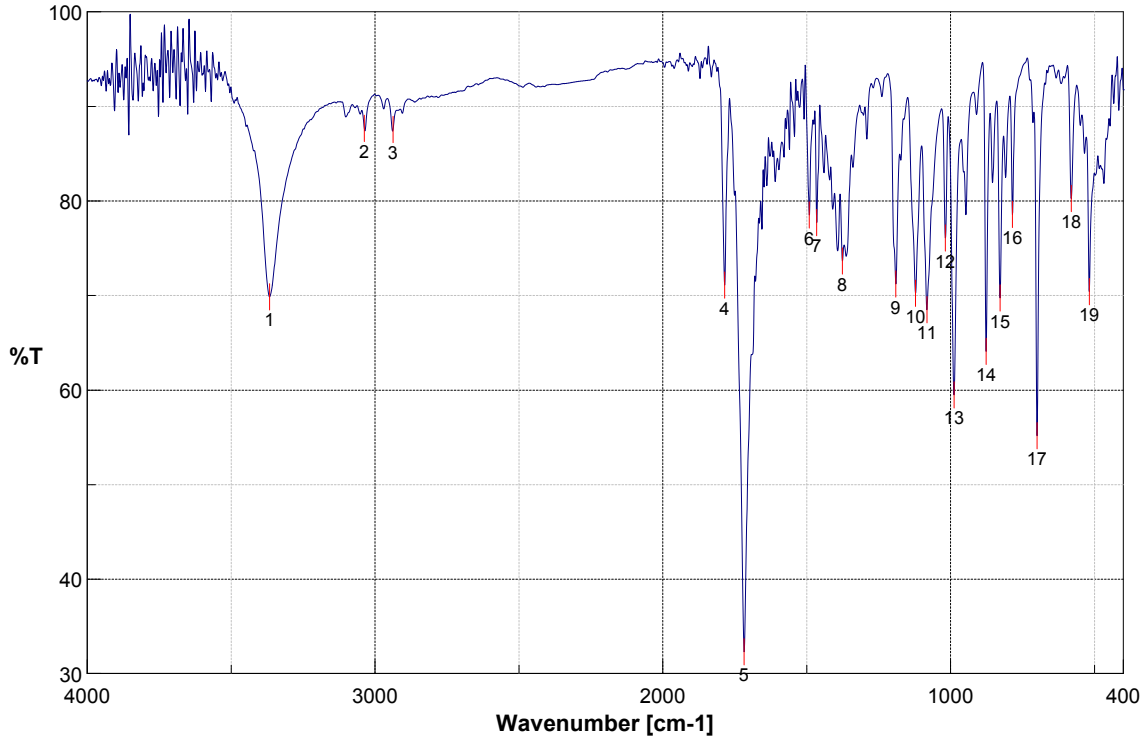
No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3394.1	65.8624	2	3056.62	85.2303	3	2913.91	81.5727
4	1783.83	45.538	5	1725.01	6.83102	6	1610.27	74.5791
7	1465.63	63.9776	8	1376.93	54.1716	9	1187.94	52.0876
10	1141.65	54.9487	11	1082.83	59.3045	12	1016.3	61.8614
13	992.196	51.2793	14	880.345	49.4371	15	788.743	58.7779
16	700.998	32.2845	17	519.722	68.0198			



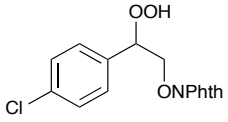
積算回数	16
分解	4 cm-1
ゼロフィリング	ON
アポダイゼーション	Cosine
ゲイン	Auto (4)
スキャンスピード	Auto (2 mm/sec)
測定日時	2016/05/30 15:22
更新日時	2016/08/05 15:07
測定者	yano
ファイル名	MS-05-27-pure.jws
サンプル名	momalcohol
コメント	



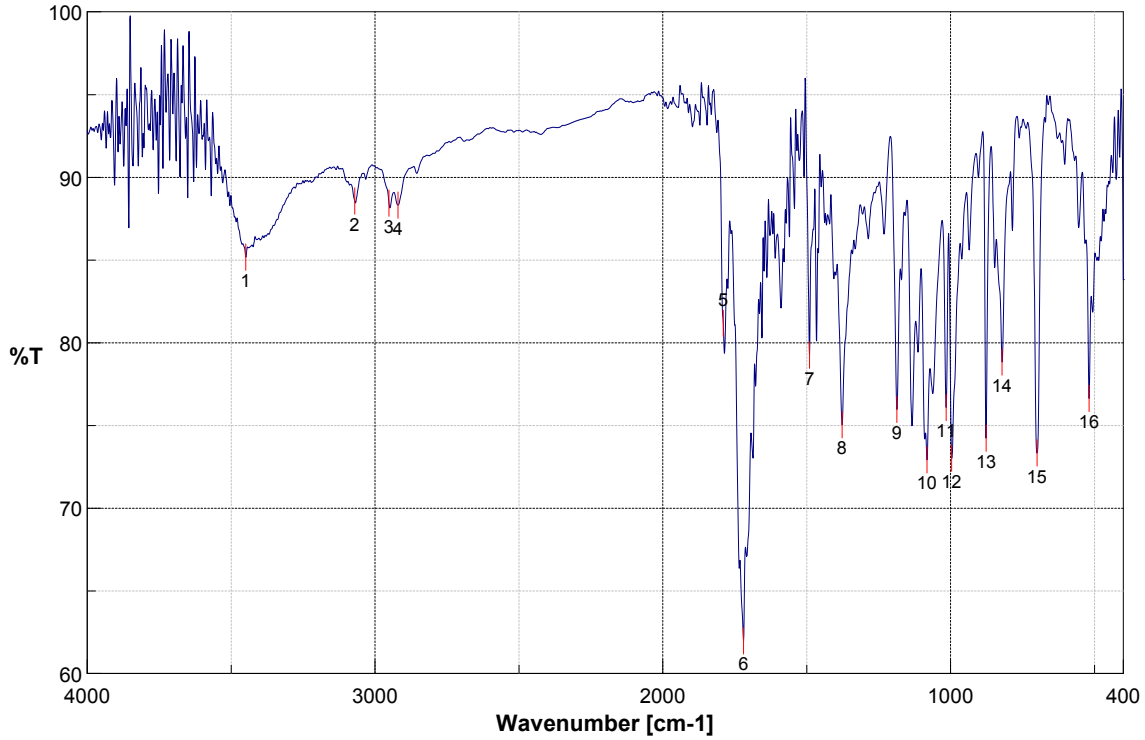
No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3449.06	73.914	2	3065.3	81.1557	3	2912.95	78.7165
4	1785.76	59.0997	5	1719.23	16.8057	6	1601.59	60.9213
7	1509.99	39.3718	8	1466.6	64.1025	9	1377.89	48.9761
10	1220.72	43.0015	11	1186.97	48.2857	12	1135.87	47.1398
13	1081.87	61.1526	14	1063.55	61.5084	15	1018.23	56.6387
16	995.089	37.901	17	876.488	42.5913	18	859.132	65.8366
19	830.205	63.3932	20	699.069	37.7571	21	544.792	62.2396
22	518.758	58.4967						



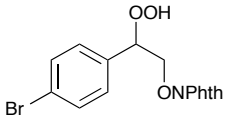
積算回数	16
分解	4 cm-1
ゼロフィリング	ON
アポダイゼーション	Cosine
ゲイン	Auto (4)
スキャンスピード	Auto (2 mm/sec)
測定日時	2016/05/30 15:28
更新日時	2016/08/05 15:09
測定者	yano
ファイル名	MS-06-01-pure.jws
サンプル名	momalcohol
コメント	



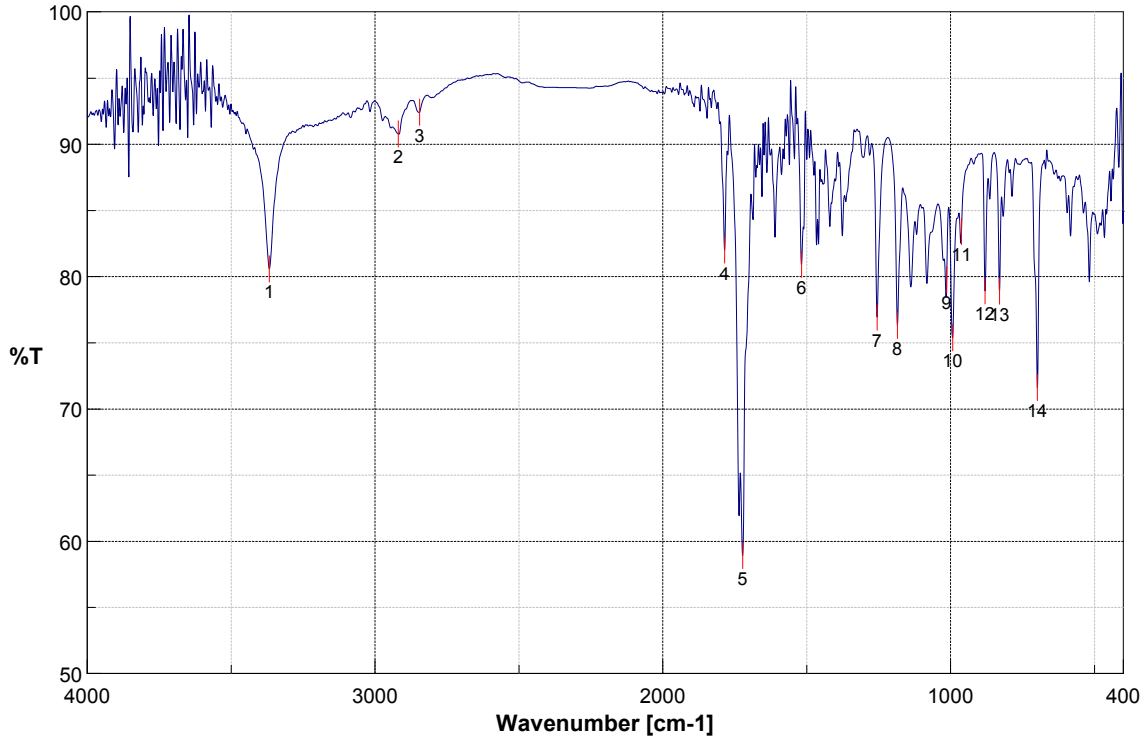
No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3366.14	69.8586	2	3037.34	87.6747	3	2937.06	87.5559
4	1784.8	71.1229	5	1717.3	32.3037	6	1491.67	78.5172
7	1465.63	77.7241	8	1375.96	73.6568	9	1190.83	71.234
10	1122.37	70.2341	11	1081.87	68.5166	12	1018.23	76.1013
13	988.339	59.4867	14	876.488	64.1072	15	828.277	69.7622
16	784.886	78.5956	17	700.033	55.1772	18	580.469	80.2644
19	517.793	70.4257						



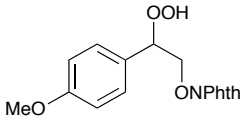
積算回数	16
分解	4 cm-1
ゼロフィリング	ON
アポダイゼーション	Cosine
ゲイン	Auto (4)
スキャンスピード	Auto (2 mm/sec)
測定日時	2016/05/30 15:36
更新日時	2016/08/05 15:10
測定者	yano
ファイル名	MS-06-04-pure.jws
サンプル名	momalcohol
コメント	



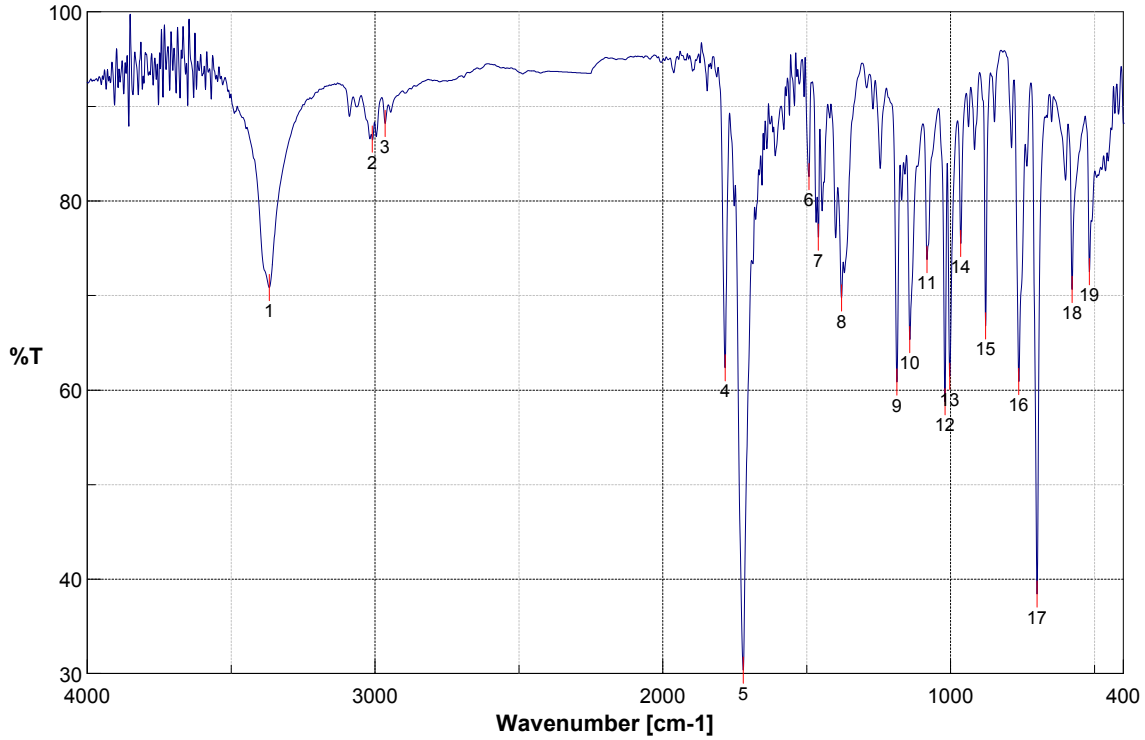
No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3449.06	85.1789	2	3070.12	88.577	3	2951.52	88.4482
4	2920.66	88.328	5	1789.62	81.1703	6	1719.23	61.9947
7	1490.7	79.2621	8	1376.93	75.0517	9	1186.97	75.9848
10	1081.87	72.9305	11	1015.34	76.0894	12	996.053	73.0296
13	876.488	74.2313	14	821.527	78.8409	15	700.033	73.3406
16	518.758	76.6373						



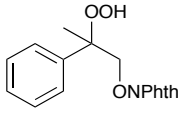
積算回数	16
分解	4 cm-1
ゼロフィリング	ON
アポダイゼーション	Cosine
ゲイン	Auto (4)
スキャンスピード	Auto (2 mm/sec)
測定日時	2016/05/30 14:19
更新日時	2016/08/05 15:12
測定者	yano
ファイル名	MS-07-35-pure.jws
サンプル名	momalcohol
コメント	



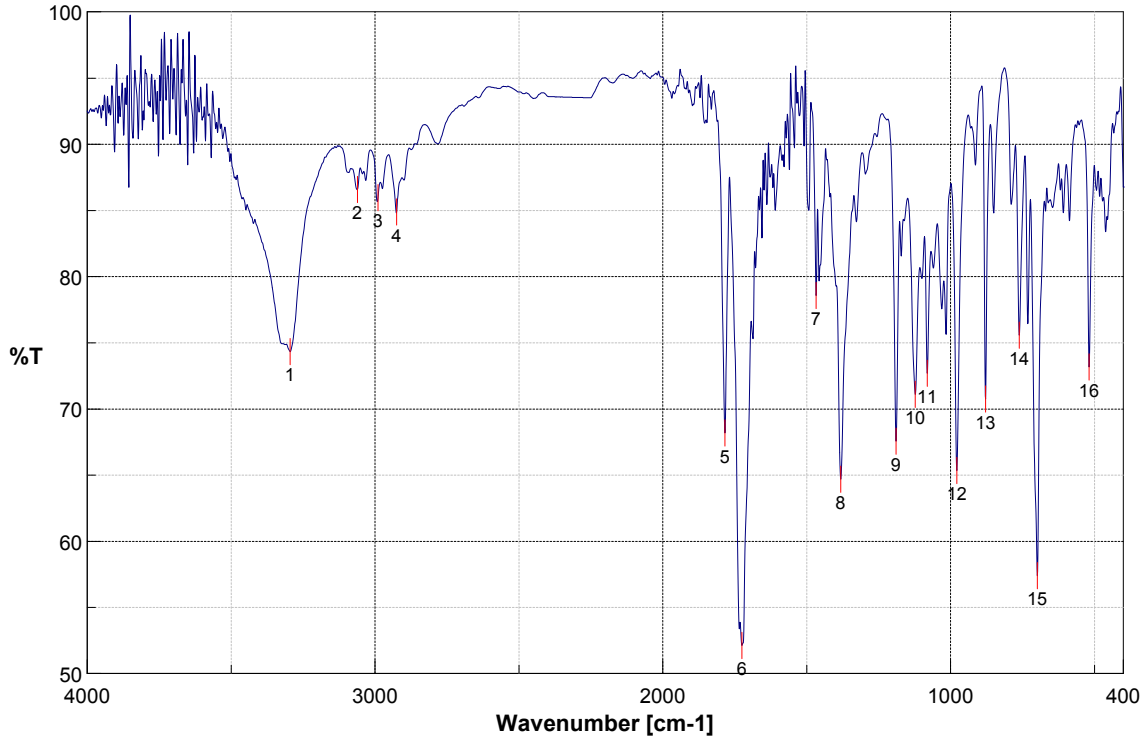
No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3367.1	80.5921	2	2919.7	90.7976	3	2845.45	92.4253
4	1784.8	82.0068	5	1722.12	58.9326	6	1517.7	80.9345
7	1255.43	76.9543	8	1185.04	76.3188	9	1013.41	79.7504
10	993.16	75.398	11	962.305	83.4213	12	880.345	78.9342
13	830.205	78.9107	14	699.069	71.6295			



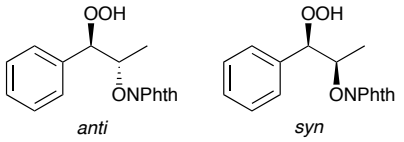
積算回数	16
分解	4 cm-1
ゼロフィリング	ON
アポダイゼーション	Cosine
ゲイン	Auto (4)
スキャンスピード	Auto (2 mm/sec)
測定日時	2016/05/30 15:07
更新日時	2016/08/05 15:13
測定者	yano
ファイル名	MS-06-05-pure.jws
サンプル名	momalcohol
コメント	



No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3367.1	70.8427	2	3009.37	86.564	3	2965.02	88.219
4	1782.87	62.3708	5	1720.19	30.3866	6	1492.63	82.598
7	1459.85	76.1932	8	1378.85	69.758	9	1186.97	60.8709
10	1141.65	65.3397	11	1081.87	73.8201	12	1019.19	58.7756
13	1002.8	61.4586	14	965.198	75.5167	15	878.417	66.8019
16	763.673	60.9254	17	700.033	38.4429	18	577.576	70.6428
19	517.793	72.5257						

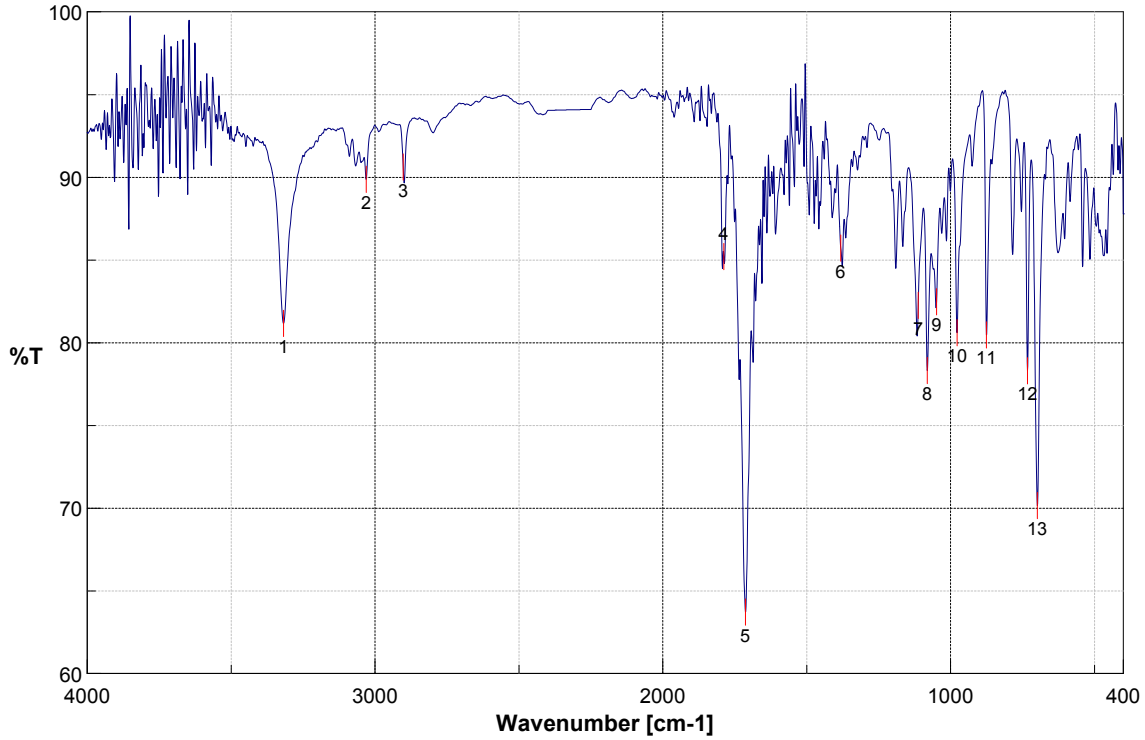


積算回数	16
分解	4 cm-1
ゼロフィリング	ON
アポダイゼーション	Cosine
ゲイン	Auto (4)
スキャンスピード	Auto (2 mm/sec)
測定日時	2016/05/30 15:14
更新日時	2016/08/05 15:17
測定者	yano
ファイル名	MS-07-19-pure.jws
サンプル名	momalcohol
コメント	

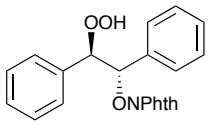


anti : *syn* = 4 : 1

No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3294.79	74.3452	2	3061.44	86.5954	3	2990.09	85.9631
4	2924.52	84.892	5	1783.83	68.1906	6	1725.01	52.1351
7	1467.56	78.5786	8	1381.75	64.6899	9	1189.86	67.5696
10	1123.33	71.1102	11	1080.91	72.6961	12	978.697	65.3541
13	878.417	70.758	14	761.744	75.577	15	699.069	57.4156
16	518.758	73.1889						

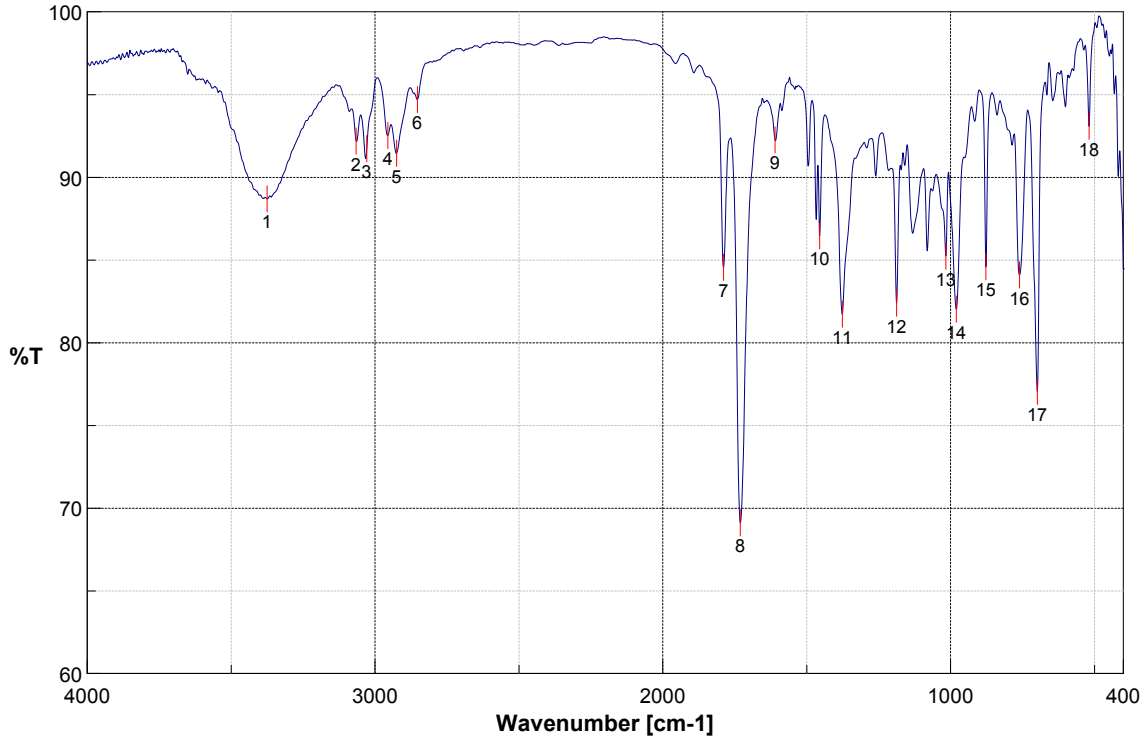


積算回数	16
分解	4 cm-1
ゼロフィリング	ON
アポダイゼーション	Cosine
ゲイン	Auto (4)
スキャンスピード	Auto (2 mm/sec)
測定日時	2016/05/30 15:45
更新日時	2016/08/05 15:21
測定者	yano
ファイル名	MS-07-17-pure.jws
サンプル名	momalcohol
コメント	

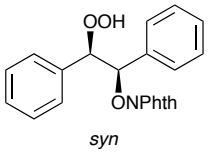


anti

No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3317.93	81.1752	2	3030.59	89.8769	3	2902.34	90.6238
4	1787.69	85.2228	5	1712.48	63.7207	6	1381.75	85.7227
7	1112.73	82.2707	8	1080.91	78.3254	9	1049.09	82.4763
10	977.733	80.605	11	875.524	80.4837	12	732.817	78.312
13	699.069	70.1701						

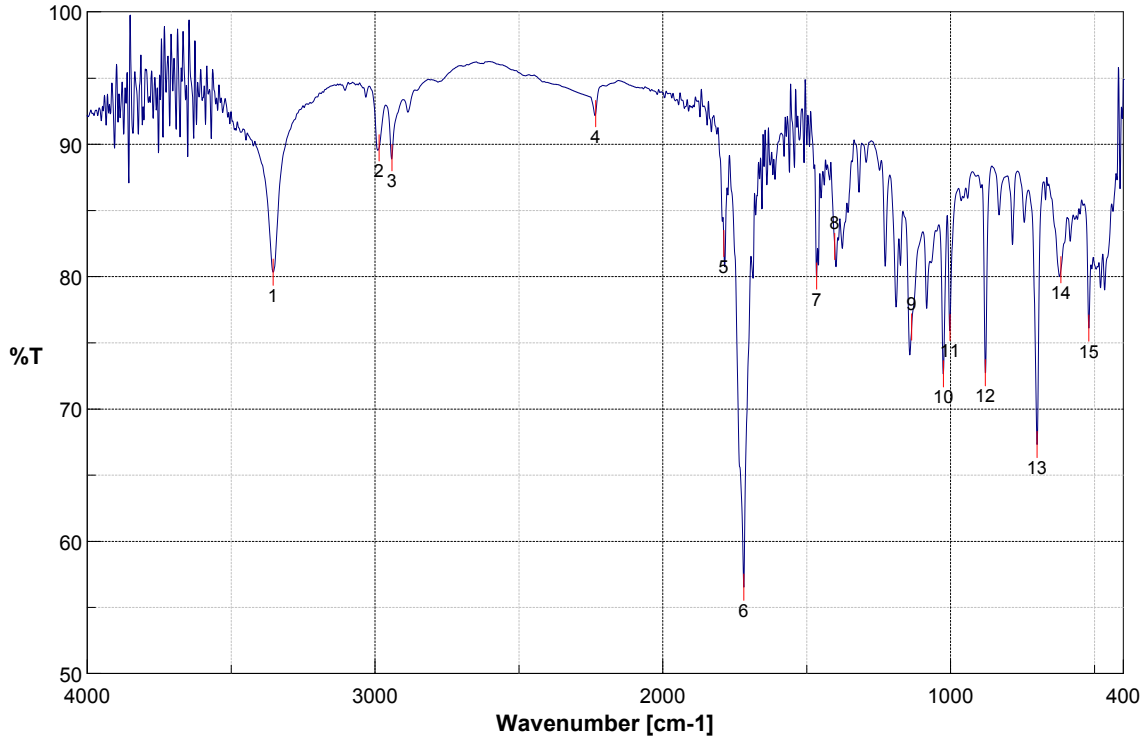


積算回数	16
分解	4 cm-1
ゼロフィリング	ON
アポダイゼーション	Cosine
ゲイン	Auto (2)
スキャンスピード	Auto (2 mm/sec)
測定日時	2016/06/25 14:10
更新日時	2016/08/05 15:22
測定者	yano
ファイル名	MS-07-17-shita.jws
サンプル名	momalcohol
コメント	

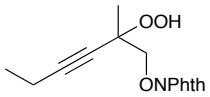


syn

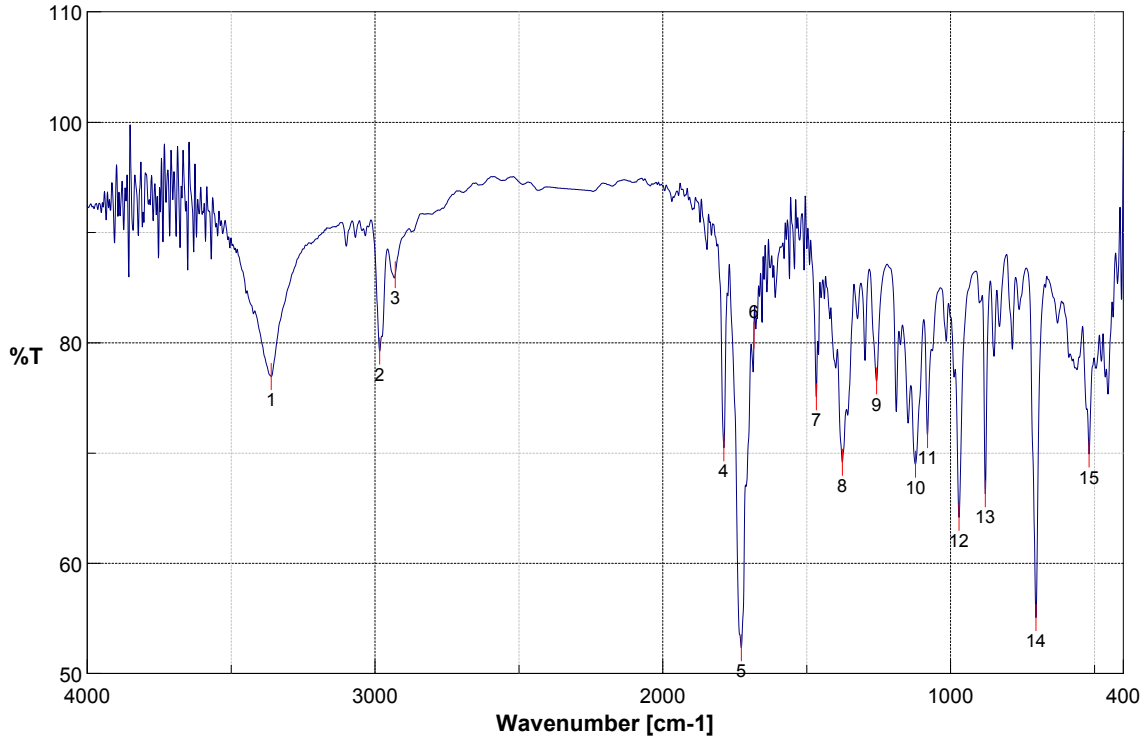
No					
1 3374.82	88.7096	2 3065.3	92.2078	3 3028.66	91.7392
4 2955.38	92.5388	5 2924.52	91.4603	6 2852.2	94.7008
7 1788.65	84.5685	8 1730.8	69.1262	9 1610.27	92.2715
10 1455.03	86.4653	11 1375.96	81.7326	12 1187.94	82.3924
13 1016.3	85.2476	14 980.625	82.0328	15 877.452	84.6031
16 760.78	84.101	17 699.069	77.0736	18 518.758	93.0902



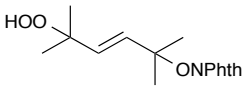
積算回数	16
分解	4 cm-1
ゼロフィリング	ON
アポダイゼーション	Cosine
ゲイン	Auto (4)
スキャンスピード	Auto (2 mm/sec)
測定日時	2016/05/30 16:45
更新日時	2016/08/05 15:25
測定者	yano
ファイル名	MS-06-09-pure.jws
サンプル名	momalcohol
コメント	



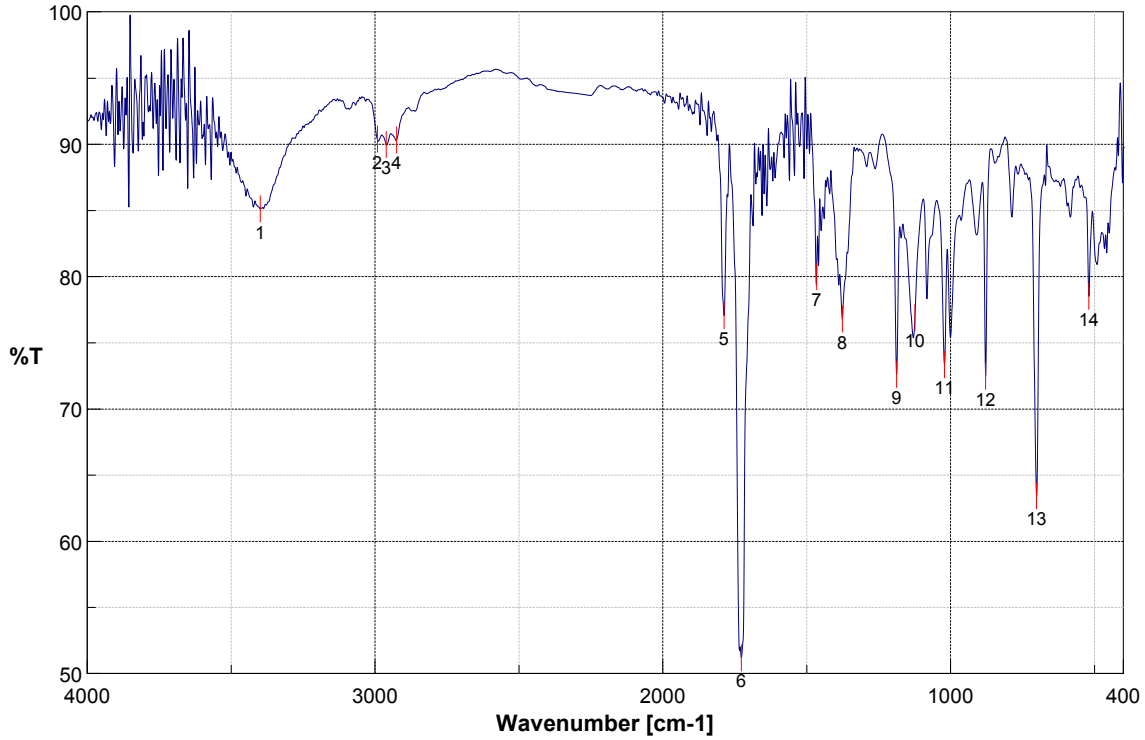
No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3353.6	80.3466	2	2986.23	89.7421	3	2940.91	88.9912
4	2233.16	92.3286	5	1787.69	82.5065	6	1718.26	56.5375
7	1465.63	80.0429	8	1402.96	82.276	9	1135.87	76.1931
10	1024.98	72.6603	11	1001.84	76.1527	12	879.381	72.7382
13	700.033	67.3127	14	617.109	80.5212	15	519.722	76.1273



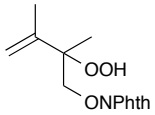
積算回数	16
分解	4 cm-1
ゼロフィリング	ON
アポダイゼーション	Cosine
ゲイン	Auto (8)
スキャンスピード	Auto (2 mm/sec)
測定日時	2016/05/30 16:53
更新日時	2016/08/05 15:26
測定者	yano
ファイル名	MS-07-04-pure.jws
サンプル名	momalcohol
コメント	



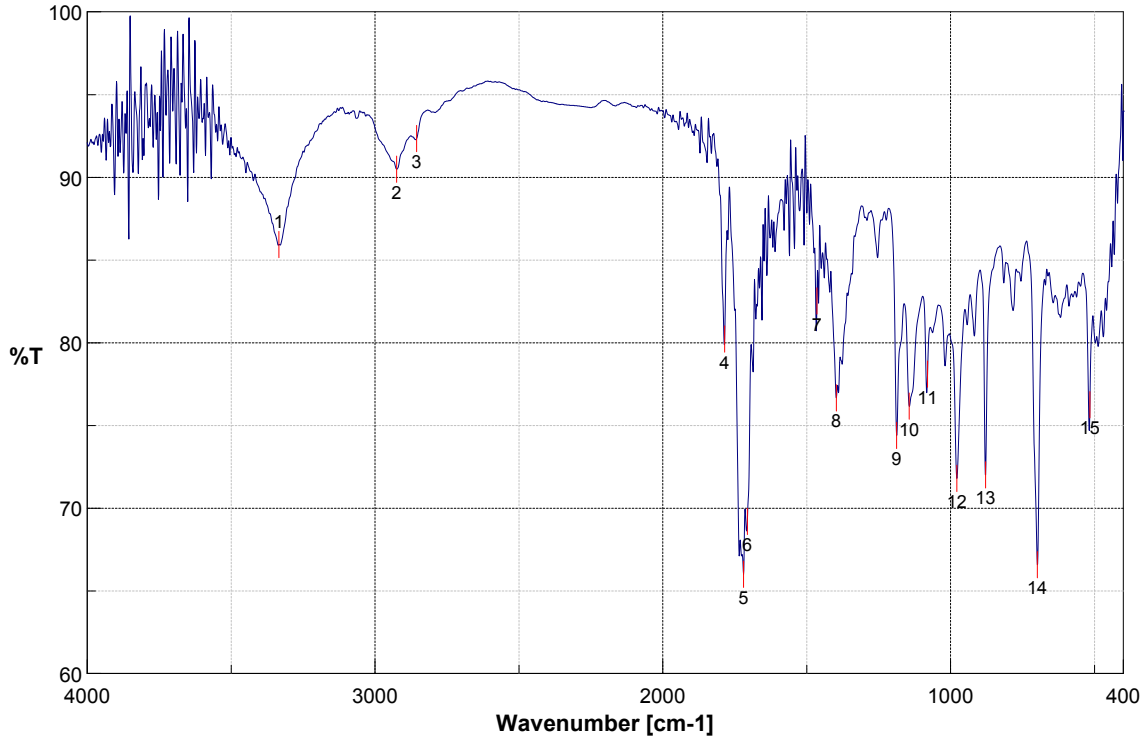
No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3360.35	76.9434	2	2984.3	79.2435	3	2929.34	86.1897
4	1787.69	70.4932	5	1726.94	52.355	6	1683.55	80.7053
7	1466.6	75.1048	8	1375.96	69.1749	9	1257.36	76.542
10	1122.37	68.9954	11	1079.94	71.6845	12	970.983	64.1885
13	879.381	66.3133	14	703.89	55.1005	15	518.758	69.9208



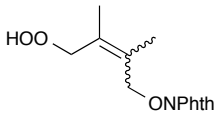
積算回数	16
分解	4 cm-1
ゼロフィリング	ON
アポダイゼーション	Cosine
ゲイン	Auto (4)
スキャンスピード	Auto (2 mm/sec)
測定日時	2016/05/30 17:11
更新日時	2016/08/05 15:28
測定者	yano
ファイル名	MS-07-05-fr29-47.jws
サンプル名	momalcohol
コメント	



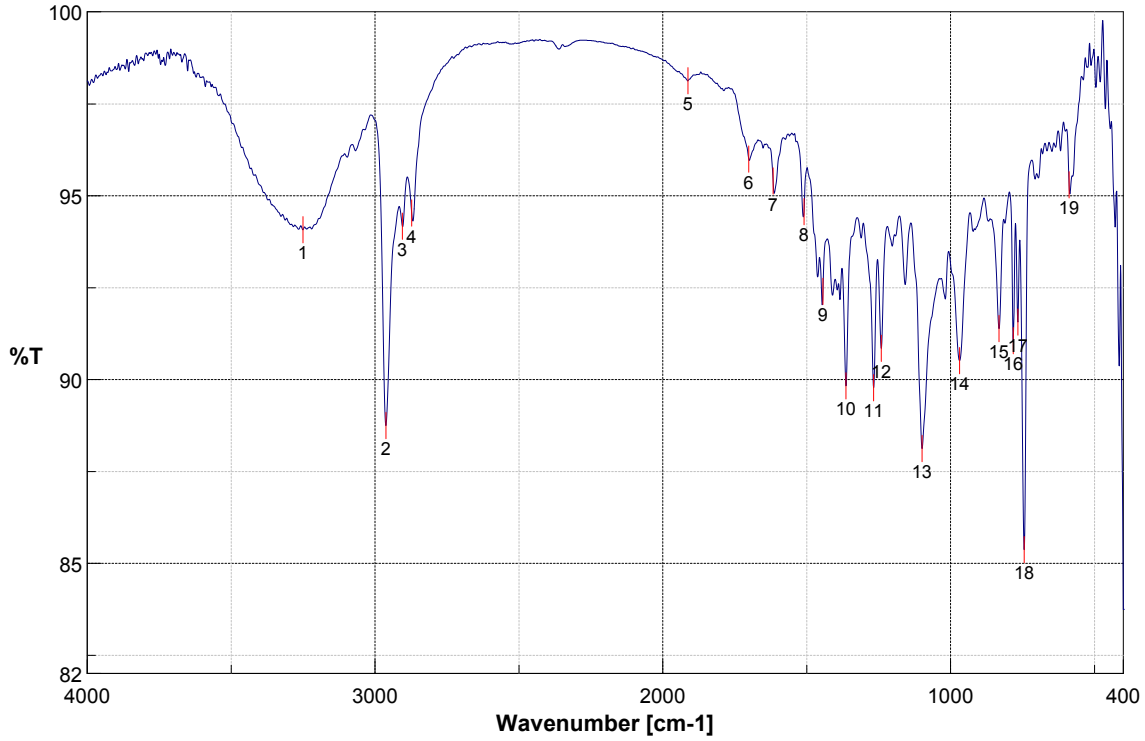
No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3398.92	85.1136	2	2992.02	90.3885	3	2961.16	89.9832
4	2924.52	90.3264	5	1786.72	77.071	6	1726.94	51.2014
7	1465.63	80.0047	8	1375.96	76.7994	9	1187.94	72.6179
10	1124.3	76.9174	11	1021.12	73.3468	12	878.417	72.4797
13	701.962	63.4505	14	519.722	78.508			



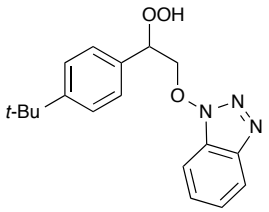
積算回数	16
分解	4 cm-1
ゼロフィリング	ON
アポダイゼーション	Cosine
ゲイン	Auto (4)
スキャンスピード	Auto (2 mm/sec)
測定日時	2016/05/30 17:24
更新日時	2016/08/05 15:29
測定者	yano
ファイル名	MS-07-05-fr59-90.jws
サンプル名	momalcohol
コメント	



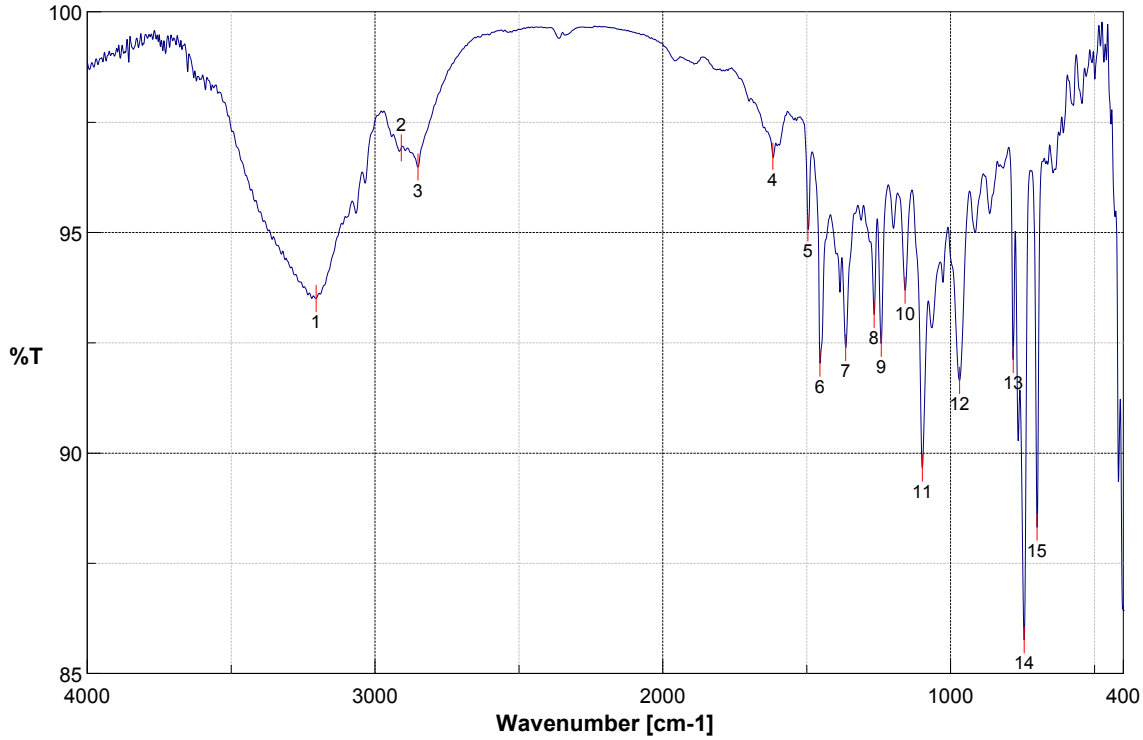
No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3334.32	85.9401	2	2924.52	90.4954	3	2855.1	92.3439
4	1784.8	80.2246	5	1719.23	66.0157	6	1706.69	69.2028
7	1464.67	82.5372	8	1397.17	76.6765	9	1187.94	74.3964
10	1143.58	76.1675	11	1079.94	78.1127	12	978.697	71.8083
13	878.417	72.0204	14	699.069	66.5955	15	515.865	76.2546



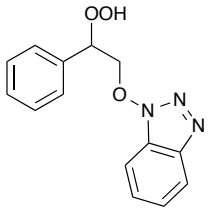
積算回数	16
分解	4 cm-1
ゼロフィリング	ON
アポダイゼーション	Cosine
ゲイン	Auto (2)
スキャンスピード	Auto (2 mm/sec)
測定日時	2016/05/30 18:29
更新日時	2016/08/05 15:56
測定者	yano
ファイル名	MS-07-25-pure.jws
サンプル名	momalcohol
コメント	



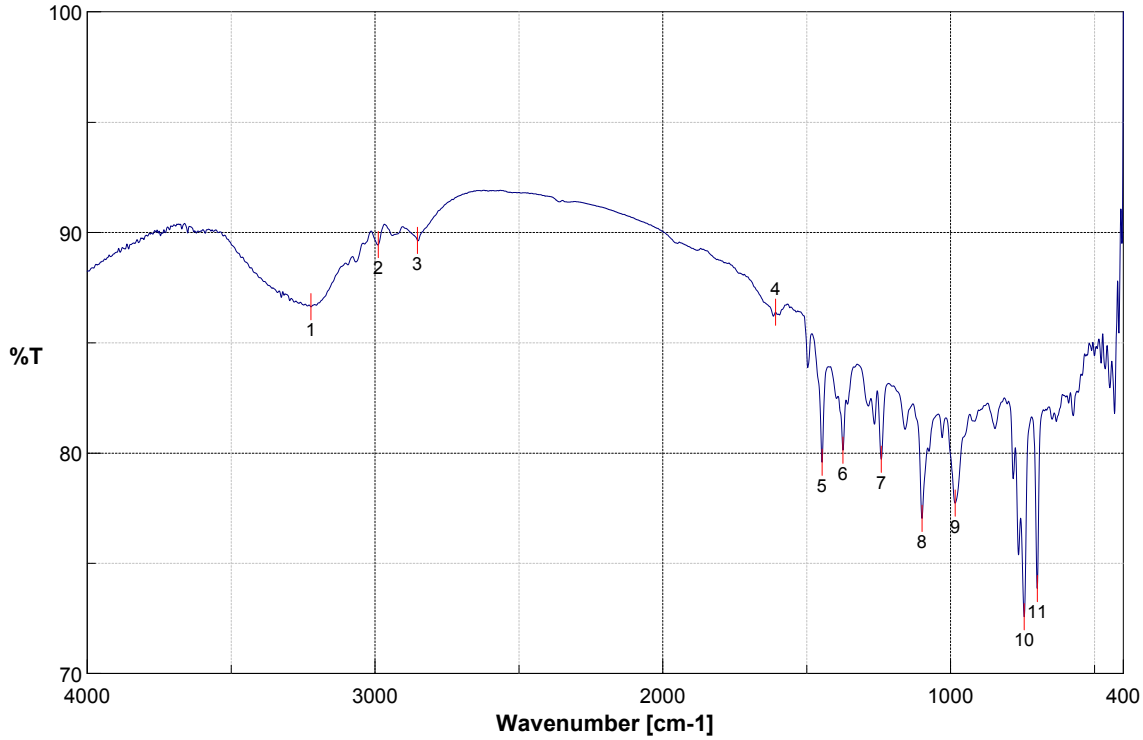
No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3250.43	94.0743	2	2962.13	88.7503	3	2905.24	94.1713
4	2872.45	94.5299	5	1913.04	98.1263	6	1701.87	96.0014
7	1617.02	95.4	8	1509.03	94.5671	9	1443.46	92.4
10	1363.43	89.8324	11	1267.97	89.7761	12	1240.97	90.853
13	1099.23	88.1217	14	969.055	90.5141	15	832.133	91.3909
16	781.993	91.0583	17	766.566	91.5658	18	744.388	85.3737
19	588.182	95.2969						



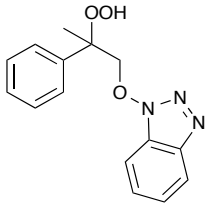
積算回数	16
分解	4 cm-1
ゼロフィリング	ON
アポダイゼーション	Cosine
ゲイン	Auto (2)
スキャンスピード	Auto (2 mm/sec)
測定日時	2016/05/30 18:25
更新日時	2016/08/05 15:59
測定者	yano
ファイル名	MS-07-34.jws
サンプル名	momalcohol
コメント	



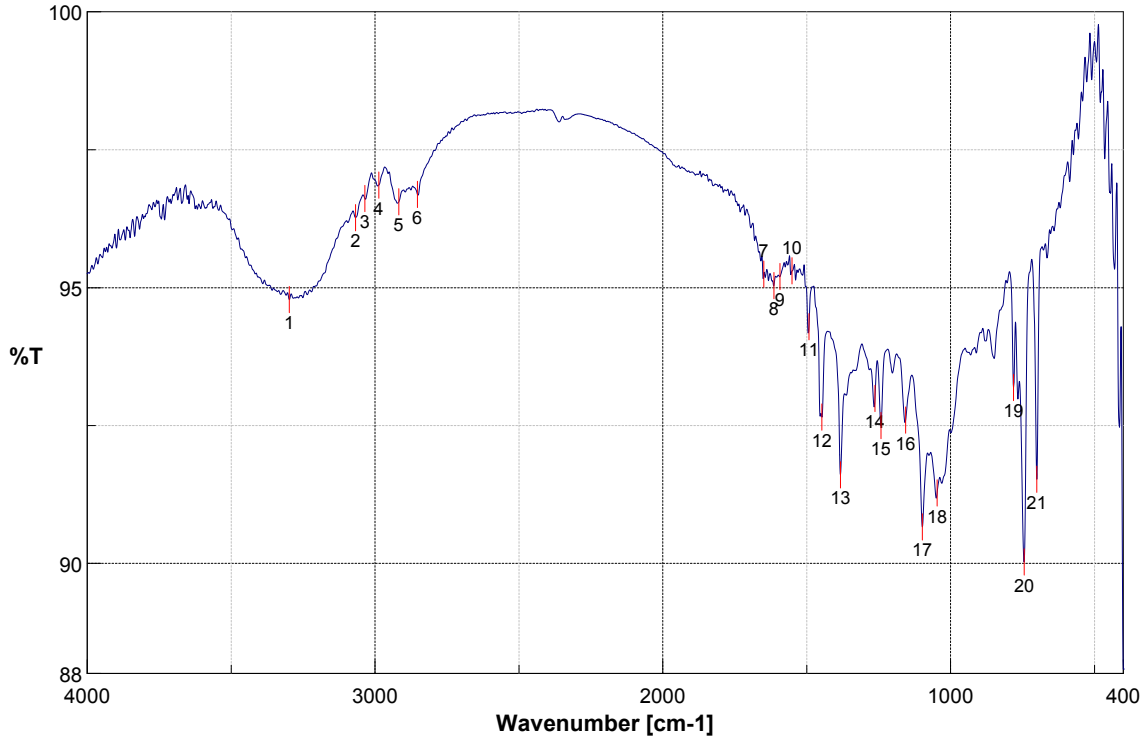
No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3205.11	93.5063	2	2909.09	96.919	3	2850.27	96.4876
4	1617.98	96.7271	5	1495.53	95.1077	6	1454.06	92.041
7	1364.39	92.3923	8	1266.04	93.1434	9	1240.97	92.4869
10	1158.04	93.6915	11	1098.26	89.6603	12	969.055	91.6485
13	781.993	92.1227	14	744.388	85.7715	15	700.033	88.3208



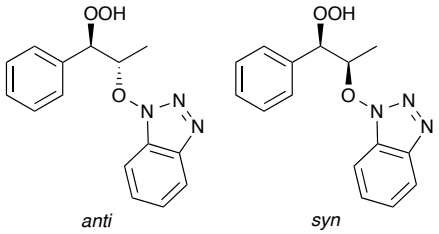
積算回数	16
分解	4 cm-1
ゼロフィリング	ON
アポダイゼーション	Cosine
ゲイン	Auto (2)
スキャンスピード	Auto (2 mm/sec)
測定日時	2016/05/30 18:38
更新日時	2016/08/05 16:09
測定者	yano
ファイル名	MS-07-02-pure.jws
サンプル名	momalcohol
コメント	



No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3222.47	86.6383	2	2989.12	89.454	3	2852.2	89.6494
4	1608.34	86.3905	5	1446.35	79.5871	6	1374.03	80.1385
7	1240.97	79.7175	8	1099.23	77.0465	9	984.482	77.7318
10	744.388	72.5777	11	699.069	73.8645			

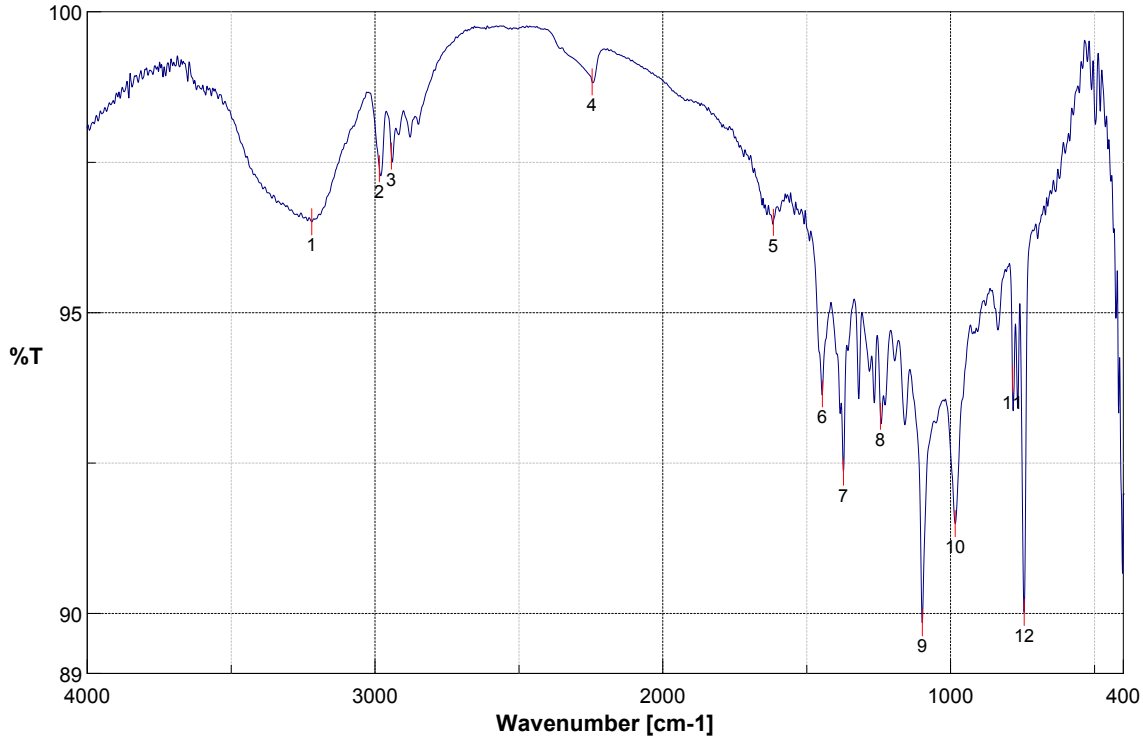


積算回数	16
分解	4 cm-1
ゼロフィリング	ON
アポダイゼーション	Cosine
ゲイン	Auto (2)
スキャンスピード	Auto (2 mm/sec)
測定日時	2016/05/30 18:42
更新日時	2016/08/05 16:07
測定者	yano
ファイル名	MS-07-38-pure.jws
サンプル名	momalcohol
コメント	

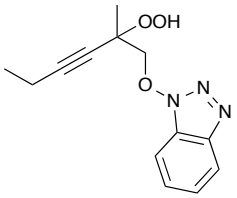


anti : *syn* = 5 : 1

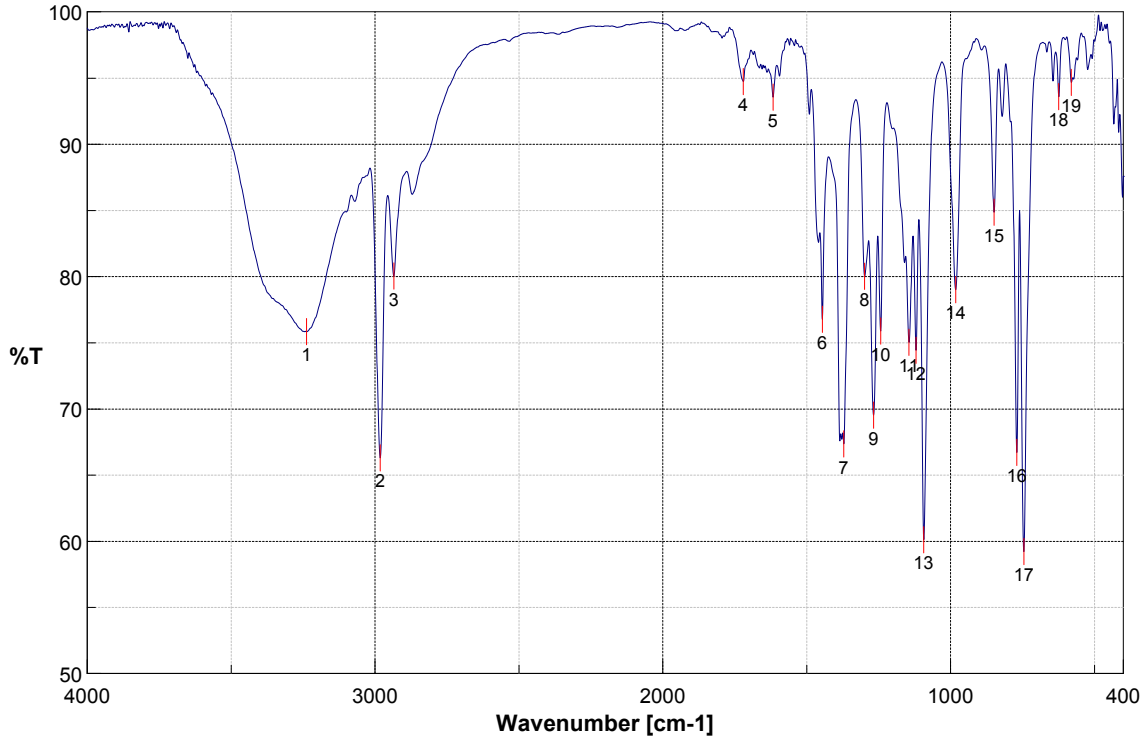
No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3297.68	94.7862	2	3067.23	96.2715	3	3035.41	96.617
4	2987.2	96.8632	5	2917.77	96.556	6	2852.2	96.6922
7	1648.84	95.2468	8	1614.13	95.0361	9	1592.91	95.1998
10	1551.45	95.306	11	1492.63	94.2941	12	1447.31	92.652
13	1382.71	91.6069	14	1263.15	92.9923	15	1241.93	92.5008
16	1156.12	92.5993	17	1098.26	90.6624	18	1047.16	91.2785
19	781.029	93.19	20	744.388	90.0284	21	700.998	91.5285



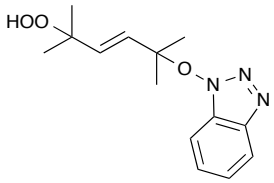
積算回数	16
分解	4 cm-1
ゼロフィリング	ON
アポダイゼーション	Cosine
ゲイン	Auto (2)
スキャンスピード	Auto (2 mm/sec)
測定日時	2016/05/30 15:56
更新日時	2016/08/05 17:01
測定者	yano
ファイル名	MS-07-27-pure.jws
サンプル名	momalcohol
コメント	



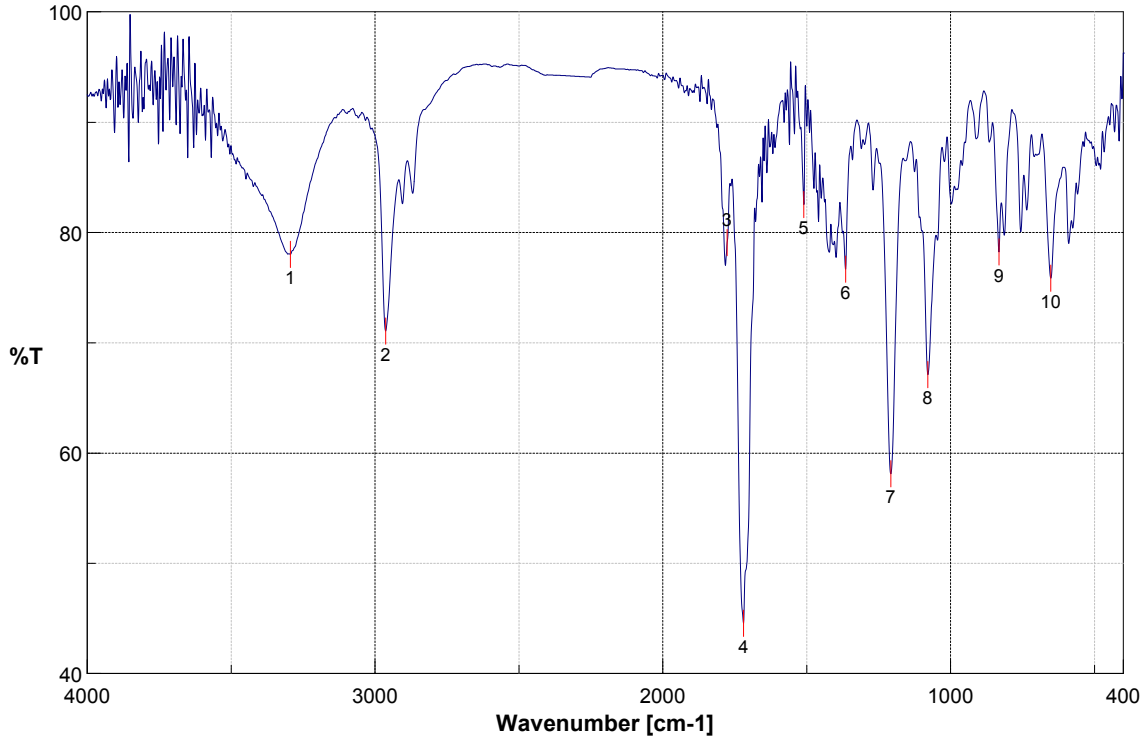
No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3219.58	96.513	2	2985.27	97.3951	3	2942.84	97.6052
4	2245.7	98.8394	5	1616.06	96.5016	6	1445.39	93.6528
7	1372.1	92.3521	8	1243.86	93.279	9	1098.26	89.8451
10	984.482	91.493	11	784.886	93.8984	12	744.388	90.0203



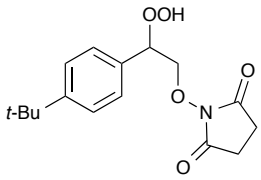
積算回数	16
分解	4 cm-1
ゼロフィリング	ON
アポダイゼーション	Cosine
ゲイン	Auto (2)
スキャンスピード	Auto (2 mm/sec)
測定日時	2016/05/30 18:17
更新日時	2016/08/05 16:11
測定者	yano
ファイル名	MS-07-31-pure.jws
サンプル名	momalcohol
コメント	



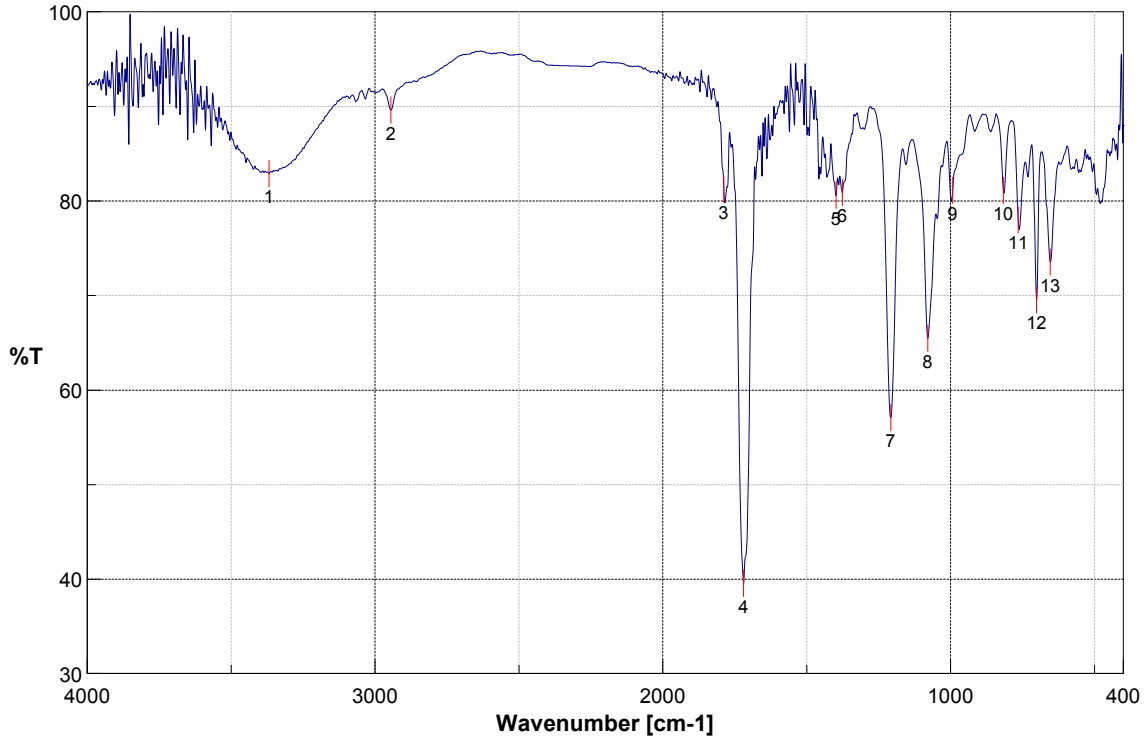
No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3237.9	75.8455	2	2982.37	66.3099	3	2934.16	80.0421
4	1720.19	94.7475	5	1617.02	93.5618	6	1445.39	76.7798
7	1371.14	67.3727	8	1298.82	80.0316	9	1267.97	69.5393
10	1242.9	75.8898	11	1144.55	75.0506	12	1120.44	74.4392
13	1093.44	60.1177	14	982.554	79.0153	15	849.49	84.8642
16	770.423	66.7241	17	745.352	59.2301	18	624.823	93.6065
19	580.469	94.6858						



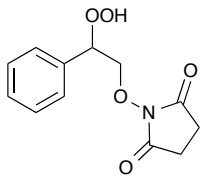
積算回数	16
分解	4 cm-1
ゼロフィリング	ON
アポダイゼーション	Cosine
ゲイン	Auto (4)
スキャンスピード	Auto (2 mm/sec)
測定日時	2016/05/30 17:57
更新日時	2016/08/05 16:31
測定者	yano
ファイル名	MS-07-20-pure.jws
サンプル名	momalcohol
コメント	



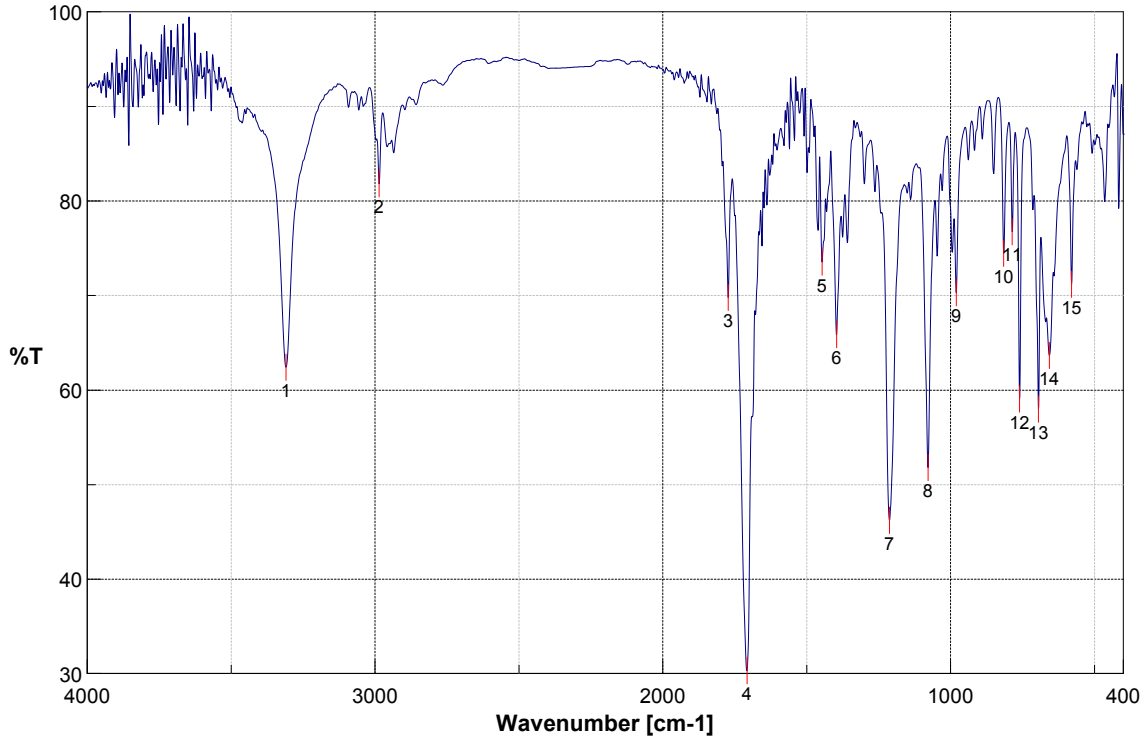
No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3293.82	78.0289	2	2963.09	71.08	3	1777.08	79.0913
4	1719.23	44.5739	5	1509.99	82.5413	6	1364.39	76.6895
7	1208.18	58.1396	8	1078.98	67.1277	9	832.133	78.2499
10	651.822	75.8661						



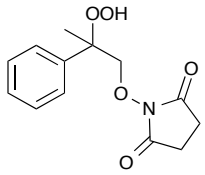
積算回数	16
分解	4 cm-1
ゼロフィリング	ON
アポダイゼーション	Cosine
ゲイン	Auto (4)
スキャンスピード	Auto (2 mm/sec)
測定日時	2016/05/30 17:50
更新日時	2016/08/05 16:38
測定者	yano
ファイル名	MS-07-33.jws
サンプル名	momalcohol
コメント	



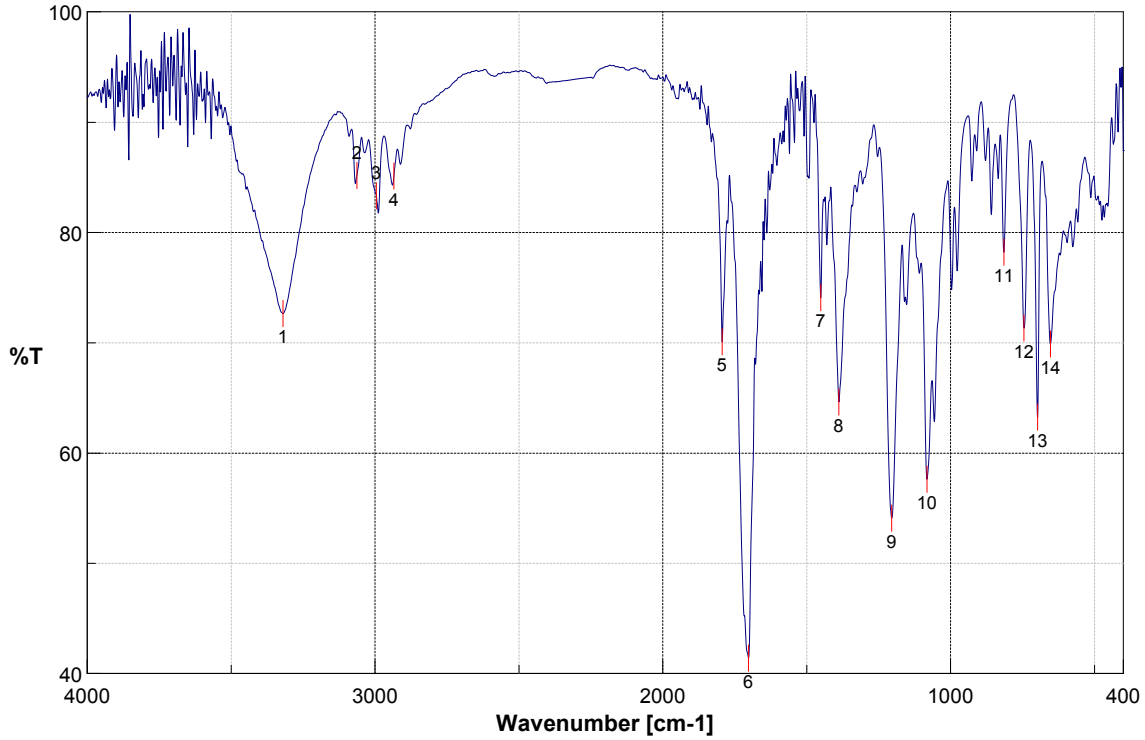
No					
1 3368.07	82.8952	2 2944.77	89.6315	3 1787.69	81.2337
4 1719.23	39.5642	5 1398.14	80.6063	6 1375.96	80.8993
7 1208.18	57.1039	8 1078.98	65.5022	9 993.16	81.1378
10 816.706	81.1081	11 765.601	78.0205	12 701.962	69.5511
13 653.75	73.5579				



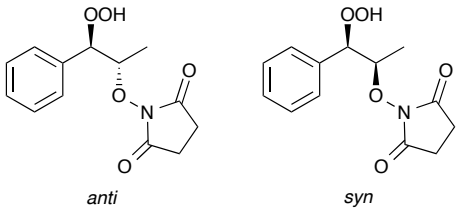
積算回数	16
分解	4 cm-1
ゼロフィリング	ON
アポダイゼーション	Cosine
ゲイン	Auto (4)
スキャンスピード	Auto (2 mm/sec)
測定日時	2016/05/30 18:03
更新日時	2016/08/05 16:40
測定者	yano
ファイル名	MS-07-06-pure.jws
サンプル名	momalcohol
コメント	



No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3309.25	62.4111	2	2986.23	81.8397	3	1773.23	69.8137
4	1707.66	30.3306	5	1446.35	73.5599	6	1396.21	65.858
7	1212.04	46.2236	8	1078.01	51.8217	9	980.625	70.304
10	815.742	74.466	11	785.85	76.7699	12	760.78	59.0484
13	695.212	57.9954	14	656.643	63.6533	15	579.504	71.2027

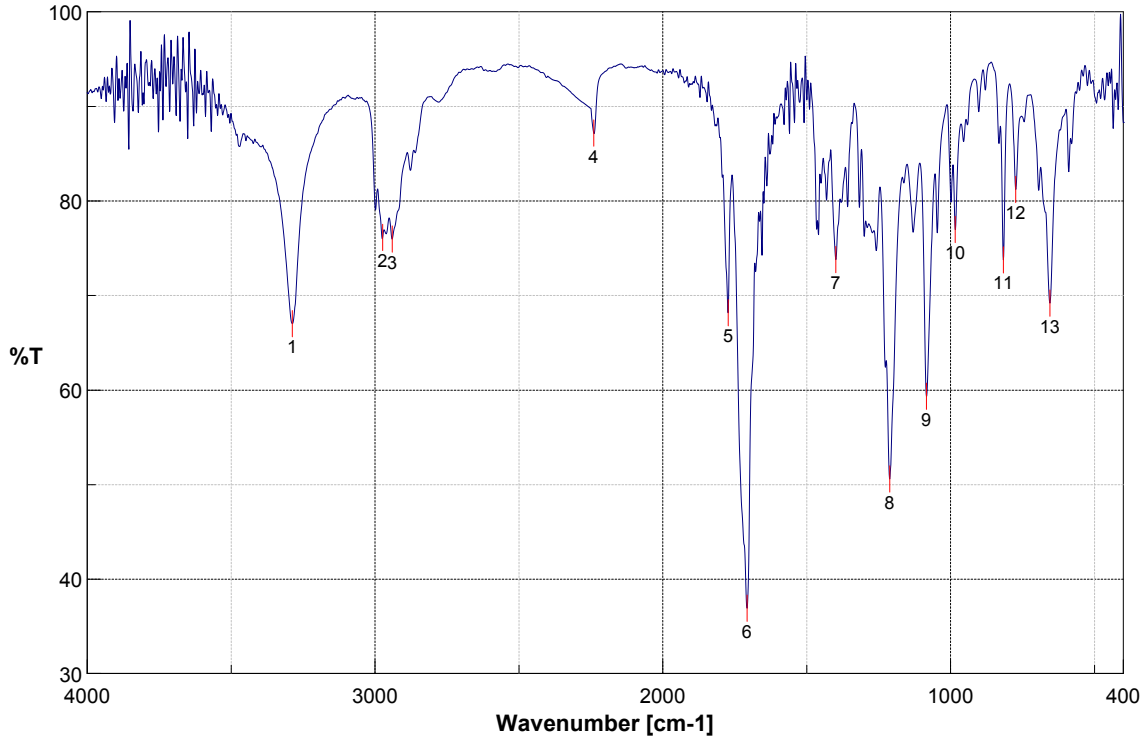


積算回数	16
分解	4 cm-1
ゼロフィリング	ON
アポダイゼーション	Cosine
ゲイン	Auto (4)
スキャンスピード	Auto (2 mm/sec)
測定日時	2016/05/30 18:09
更新日時	2016/08/05 16:42
測定者	yano
ファイル名	MS-07-37-pure.jws
サンプル名	momalcohol
コメント	

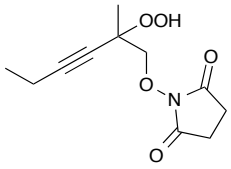


anti : *syn* = 3.5 : 1

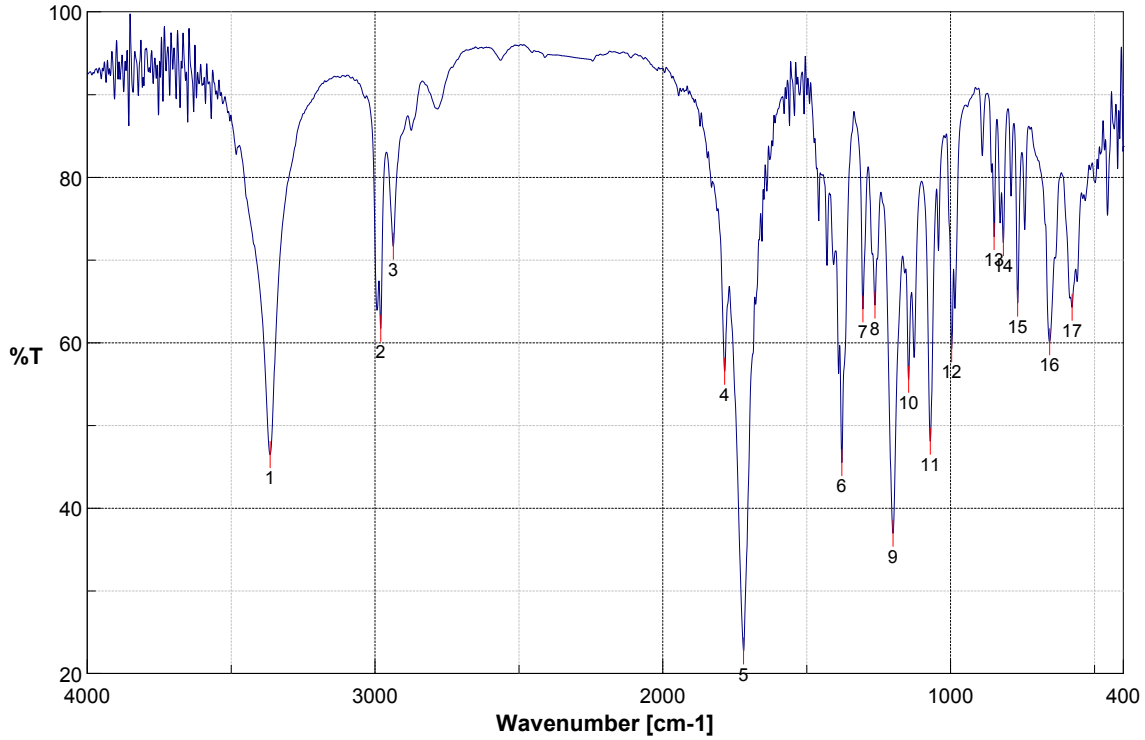
No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3319.86	72.6477	2	3063.37	85.174	3	2994.91	83.3253
4	2934.16	85.1315	5	1793.47	70.1084	6	1702.84	41.4174
7	1451.17	74.0883	8	1388.5	64.6347	9	1205.29	54.1117
10	1081.87	57.6272	11	814.777	78.2084	12	745.352	71.3463
13	698.105	63.281	14	652.786	69.8963			



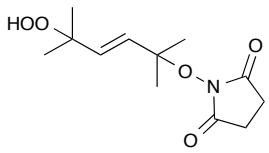
積算回数	16
分解	4 cm-1
ゼロフィリング	ON
アポダイゼーション	Cosine
ゲイン	Auto (8)
スキャンスピード	Auto (2 mm/sec)
測定日時	2016/05/30 17:32
更新日時	2016/08/05 16:43
測定者	yano
ファイル名	MS-07-26-pure.jws
サンプル名	momalcohol
コメント	



No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3287.07	67.0407	2	2973.7	76.151	3	2939.95	75.9885
4	2239.91	87.1921	5	1773.23	68.1808	6	1707.66	36.9155
7	1399.1	73.8173	8	1211.08	50.6047	9	1083.8	59.3437
10	984.482	76.9973	11	816.706	73.7736	12	774.279	81.2349
13	654.715	69.1994						

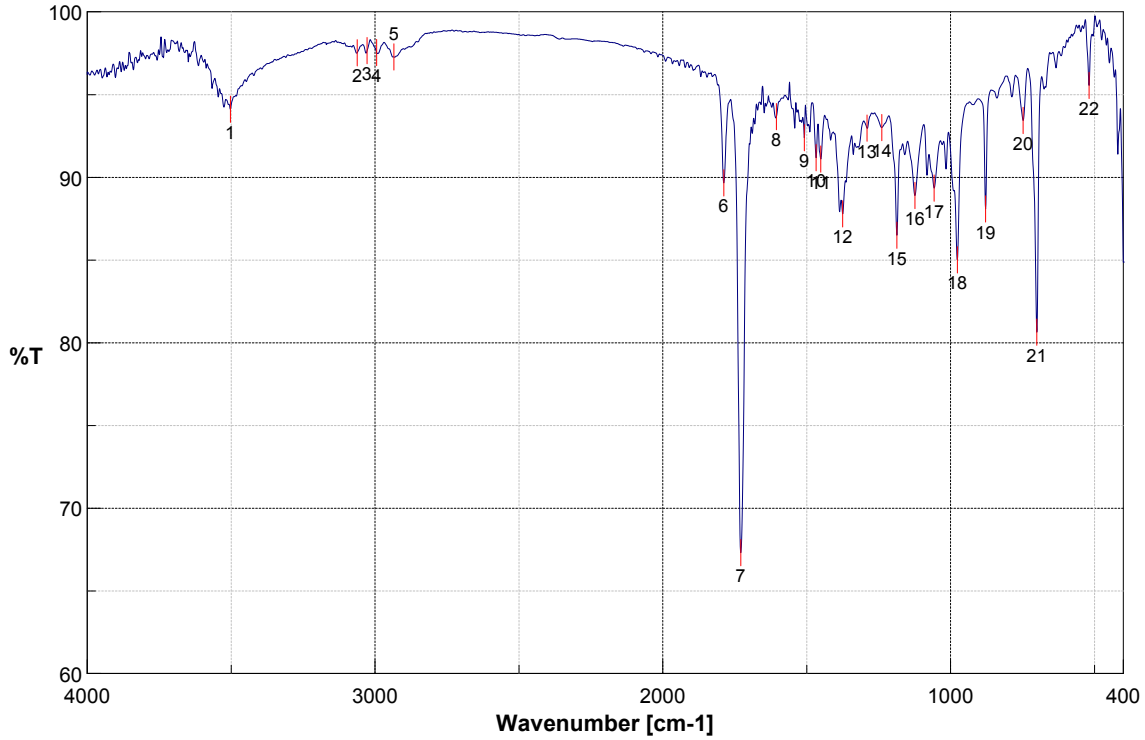


積算回数	16
分解	4 cm-1
ゼロフィリング	ON
アポダイゼーション	Cosine
ゲイン	Auto (8)
スキャンスピード	Auto (2 mm/sec)
測定日時	2016/05/30 17:38
更新日時	2016/08/05 16:45
測定者	yano
ファイル名	MS-07-30-pure.jws
サンプル名	momalcohol
コメント	

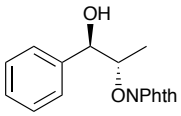


No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3364.21	46.483	2	2980.45	61.7514	3	2936.09	71.6745
4	1784.8	56.5465	5	1719.23	22.7504	6	1377.89	45.5165
7	1304.61	64.1196	8	1263.15	64.5734	9	1200.47	36.9717
10	1145.51	55.5848	11	1070.3	48.1238	12	996.053	59.2658
13	849.49	72.8452	14	816.706	72.113	15	767.53	64.7966
16	655.679	60.1164	17	577.576	64.3119			

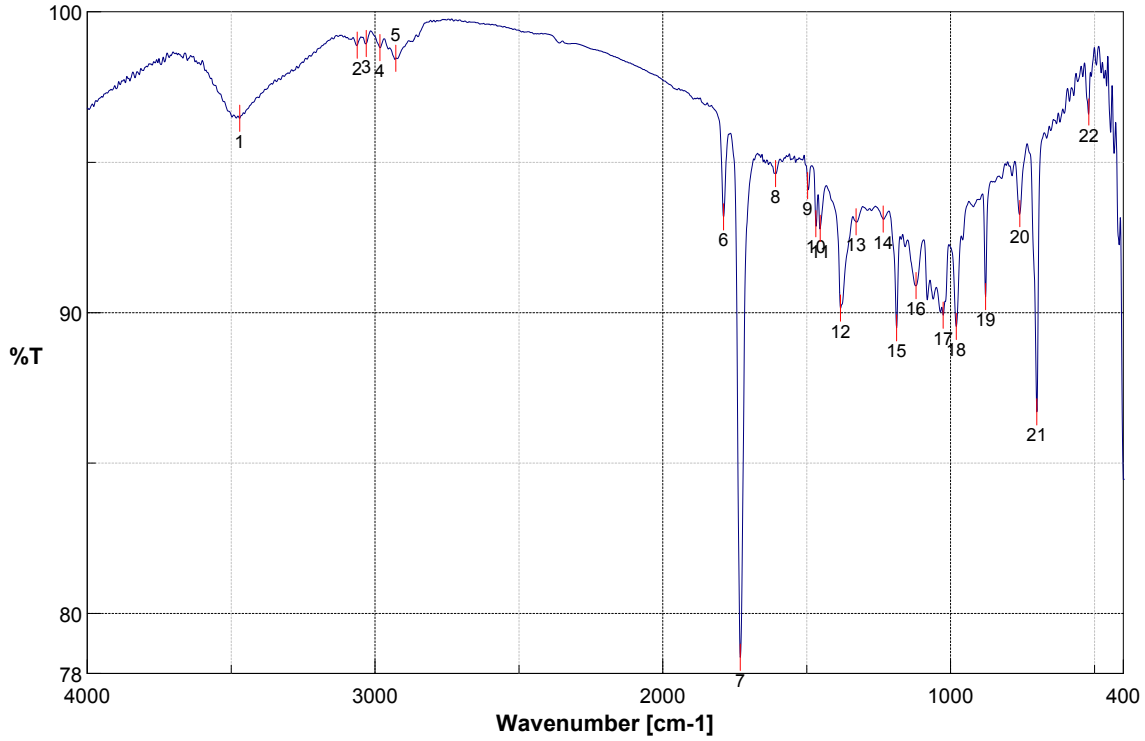
Determination of the relative configuration in 5j, 5k, 10j and 11j



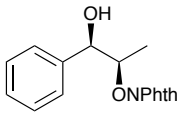
積算回数	16
分解	4 cm-1
ゼロフィリング	ON
アポダイゼーション	Cosine
ゲイン	Auto (2)
スキャンスピード	Auto (2 mm/sec)
測定日時	2016/08/06 22:17
更新日時	2016/08/11 17:48
測定者	yano
ファイル名	b-me-NHPI-major.jws
サンプル名	momalcohol
コメント	



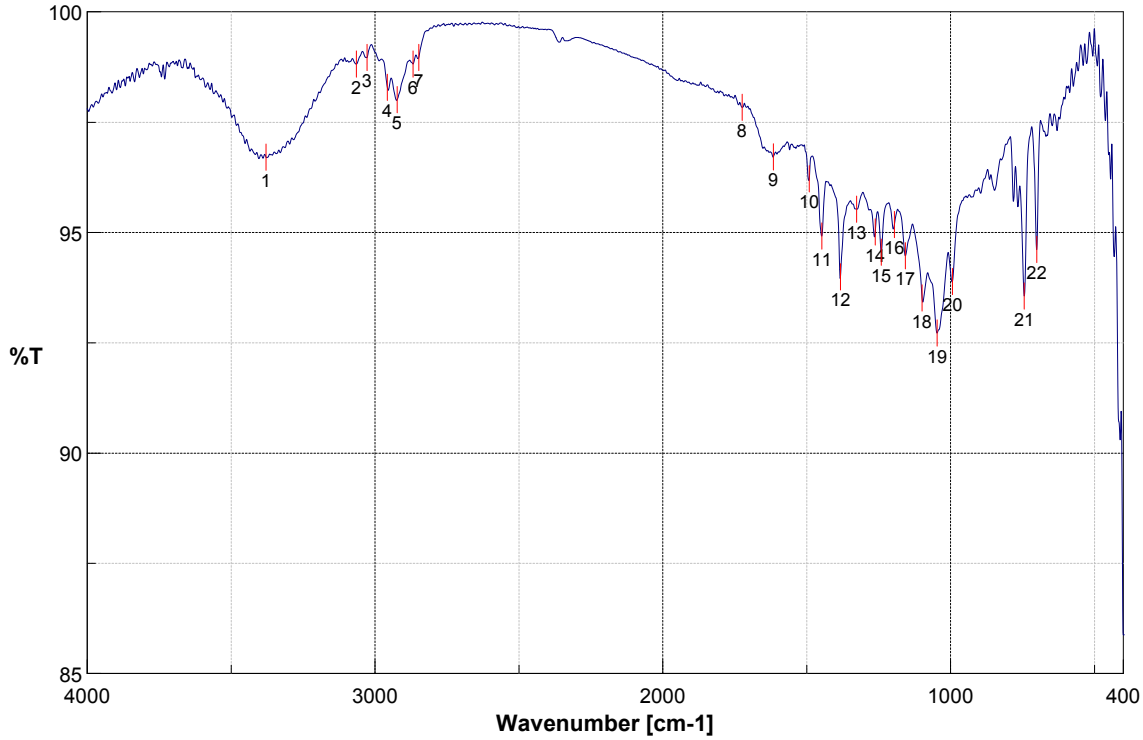
No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3502.1	94.1213	2	3062.41	97.5413	3	3027.69	97.6586
4	2993.94	97.5447	5	2934.16	97.2883	6	1787.69	89.6679
7	1728.87	67.3115	8	1605.45	93.6741	9	1508.06	92.4043
10	1467.56	91.1977	11	1451.17	91.1128	12	1375	87.7973
13	1290.14	92.9756	14	1239.04	93.0199	15	1186.97	86.5014
16	1124.3	88.9035	17	1057.76	89.3573	18	976.768	85.0234
19	878.417	88.0911	20	748.245	93.4492	21	700.998	80.6501
22	518.758	95.5601						



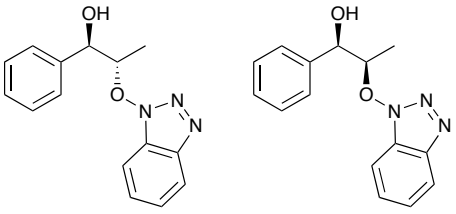
積算回数	16
分解	4 cm-1
ゼロフィリング	ON
アポダイゼーション	Cosine
ゲイン	Auto (2)
スキャンスピード	Auto (2 mm/sec)
測定日時	2016/08/06 20:33
更新日時	2016/08/11 18:06
測定者	yano
ファイル名	b-me-NHPI-minor.jws
サンプル名	momalcohol
コメント	



No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3470.28	96.4678	2	3062.41	98.8956	3	3030.59	98.9571
4	2983.34	98.8149	5	2927.41	98.458	6	1788.65	93.1875
7	1730.8	78.5447	8	1608.34	94.6276	9	1496.49	94.2263
10	1468.53	92.9581	11	1453.1	92.81	12	1382.71	90.1584
13	1328.71	93.0254	14	1234.22	93.1129	15	1187.94	89.4983
16	1120.44	90.9002	17	1025.94	89.9204	18	980.625	89.5506
19	878.417	90.5407	20	759.816	93.2935	21	700.998	86.706
22	519.722	96.6771						



積算回数	16
分解	4 cm-1
ゼロフィリング	ON
アポダイゼーション	Cosine
ゲイン	Auto (2)
スキャンスピード	Auto (2 mm/sec)
測定日時	2016/08/06 20:38
更新日時	2016/08/11 17:55
測定者	yano
ファイル名	b-me-HOBt.jws
サンプル名	momalcohol
コメント	

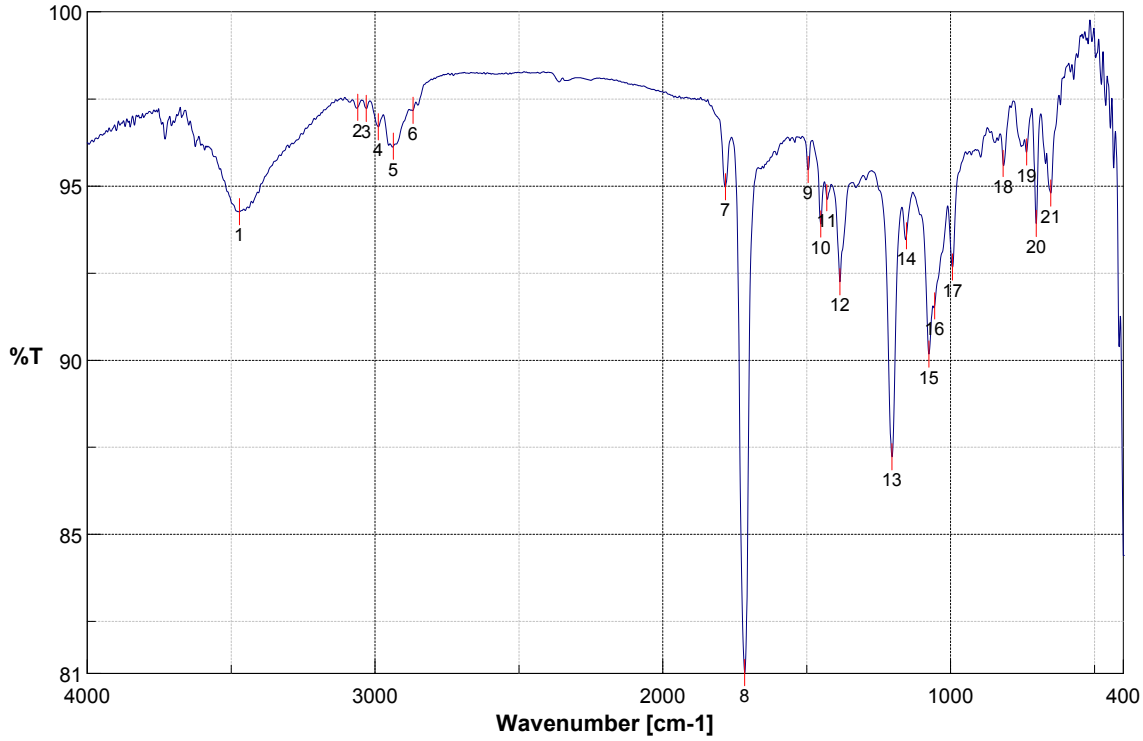


anti-**17j**

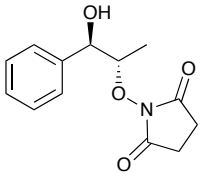
syn-**17j**

anti : *syn* = 4 : 1

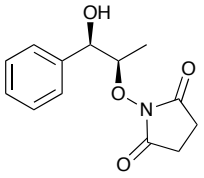
No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3378.67	96.7073	2	3064.33	98.8226	3	3027.69	98.9709
4	2957.3	98.2925	5	2922.59	98.0141	6	2867.63	98.8222
7	2848.35	98.9689	8	1724.05	97.8377	9	1616.06	96.718
10	1491.67	96.2185	11	1447.31	94.9202	12	1382.71	93.9954
13	1326.79	95.5322	14	1262.18	95.0146	15	1240.97	94.5572
16	1195.65	95.1843	17	1157.08	94.4732	18	1099.23	93.5207
19	1047.16	92.7222	20	994.125	93.8933	21	744.388	93.5602
22	700.998	94.6149						



積算回数	16
分解	4 cm-1
ゼロフィリング	ON
アポダイゼーション	Cosine
ゲイン	Auto (2)
スキャンスピード	Auto (2 mm/sec)
測定日時	2016/08/06 20:43
更新日時	2016/08/11 17:57
測定者	yano
ファイル名	b-me-NHS.jws
サンプル名	momalcohol
コメント	



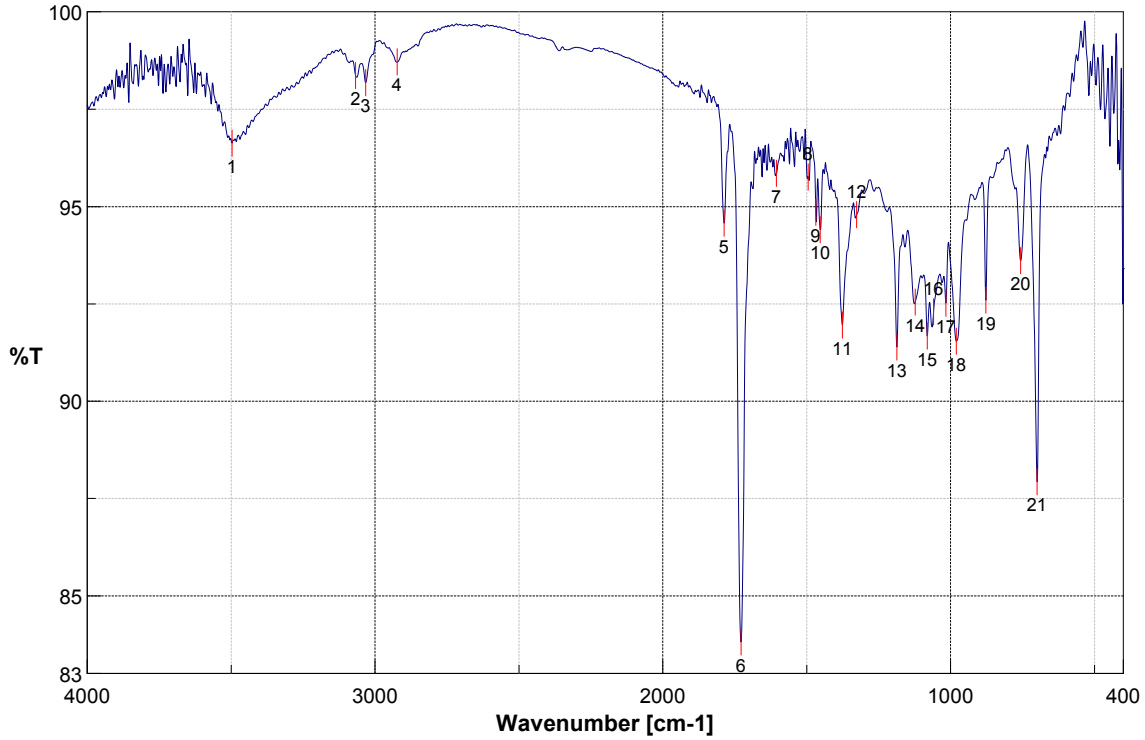
anti-**18j**



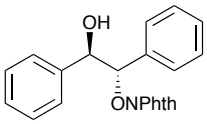
syn-**18j**

anti : *syn* = 3 : 1

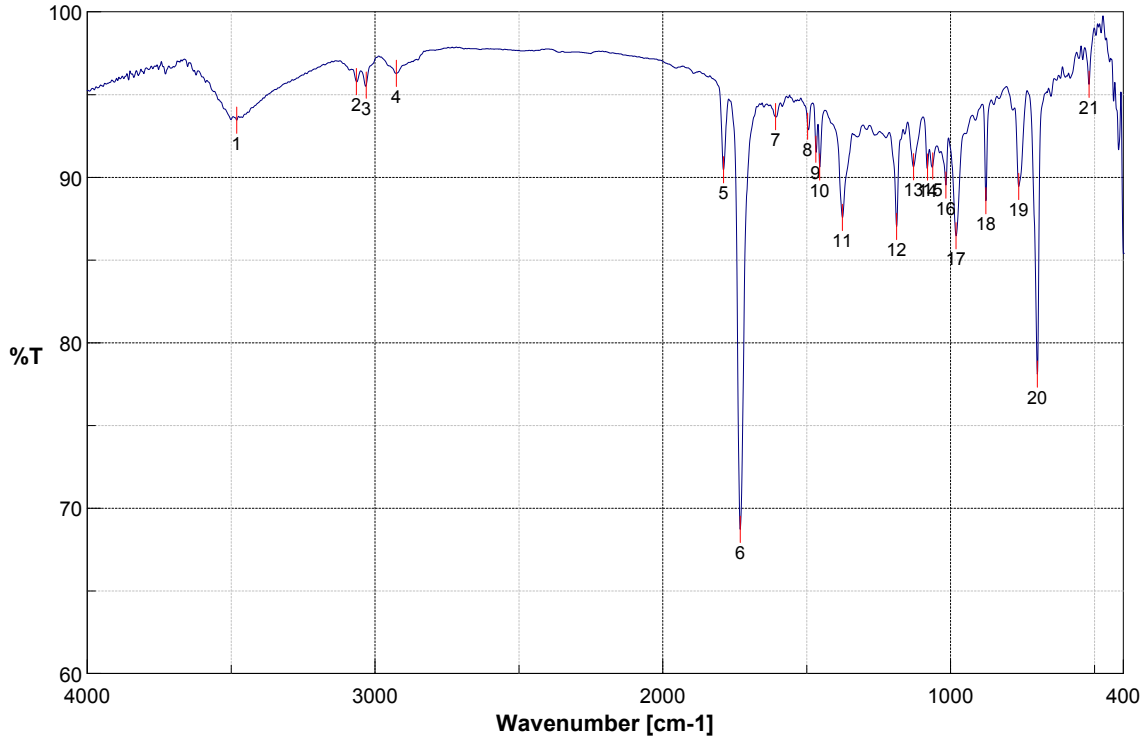
No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3471.24	94.265	2	3060.48	97.261	3	3030.59	97.2294
4	2989.12	96.705	5	2936.09	96.1441	6	2867.63	97.1739
7	1781.9	94.9855	8	1715.37	81.0335	9	1494.56	95.4743
10	1451.17	93.9123	11	1429.96	94.6649	12	1384.64	92.254
13	1204.33	87.2319	14	1153.22	93.5726	15	1075.12	90.1793
16	1055.84	91.5605	17	994.125	92.6745	18	817.67	95.6547
19	735.71	95.9818	20	702.926	93.9322	21	651.822	94.7993



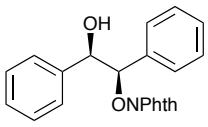
積算回数	16
分解	4 cm-1
ゼロフィリング	ON
アポダイゼーション	Cosine
ゲイン	Auto (2)
スキャンスピード	Auto (2 mm/sec)
測定日時	2016/08/06 22:21
更新日時	2016/08/11 17:58
測定者	yano
ファイル名	Diphenyl-NHPI-major.jws
サンプル名	momalcohol
コメント	



No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3496.31	96.6304	2	3067.23	98.3684	3	3032.51	98.1828
4	2922.59	98.7174	5	1786.72	94.5754	6	1727.91	83.8196
7	1605.45	95.8547	8	1494.56	95.7654	9	1468.53	94.8557
10	1453.1	94.4076	11	1375.96	91.9596	12	1326.79	94.7901
13	1186.97	91.393	14	1123.33	92.5478	15	1080.91	91.6731
16	1059.69	92.2948	17	1016.3	92.5175	18	980.625	91.5455
19	877.452	92.6006	20	756.923	93.6113	21	700.033	87.9309



積算回数	16
分解	4 cm-1
ゼロフィリング	ON
アポダイゼーション	Cosine
ゲイン	Auto (2)
スキャンスピード	Auto (2 mm/sec)
測定日時	2016/08/06 20:29
更新日時	2016/08/11 17:59
測定者	yano
ファイル名	diphenyl-NHPI-minor.jws
サンプル名	momalcohol
コメント	



No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3480.88	93.4639	2	3064.33	95.792	3	3030.59	95.5831
4	2925.48	96.2934	5	1788.65	90.4641	6	1730.8	68.7215
7	1608.34	93.6715	8	1496.49	93.104	9	1468.53	91.6989
10	1455.03	90.6273	11	1375.96	87.5818	12	1187.94	87.0311
13	1129.12	90.6478	14	1079.94	90.6226	15	1062.59	90.7012
16	1016.3	89.5404	17	981.59	86.4712	18	877.452	88.5862
19	763.673	89.4534	20	699.069	78.1145	21	518.758	95.6292