Multinuclear Zinc Bisamidinate Catalyzed Asymmetric Alkylation of α-Ketoesters and Its Unique Chemoselectivity

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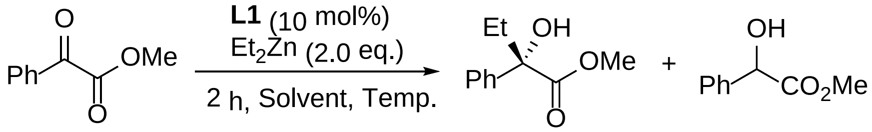
Supporting Information

Table S1 Optimization of reaction condition



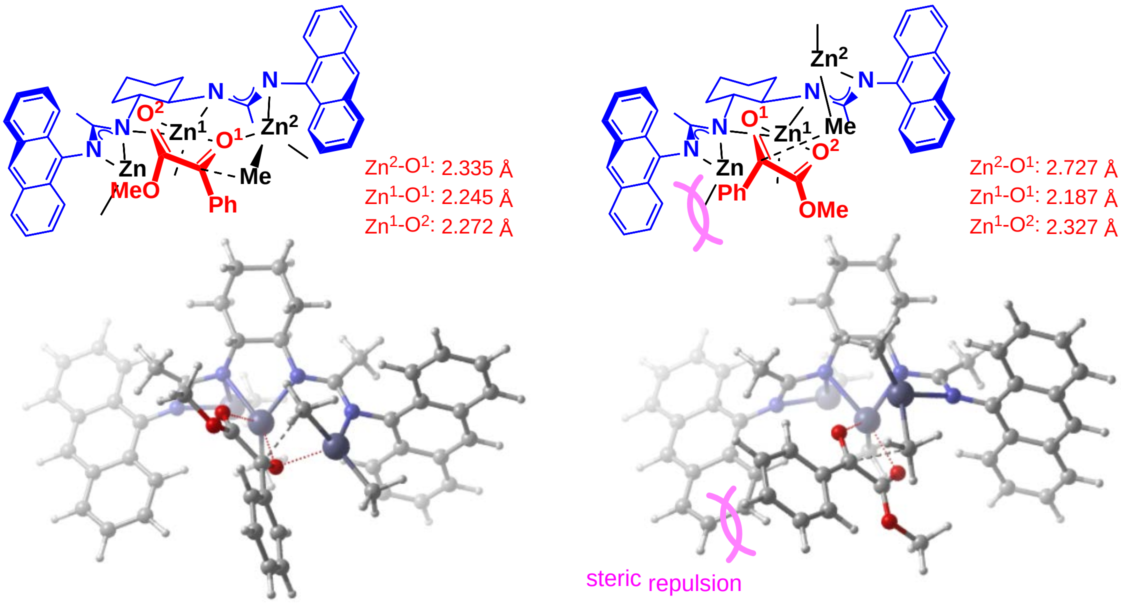
1a 2a 3a

Entry	Temp. (°C)	Solvent	2a Yield (%)[a]	2a ee (%)[b]	3a Yield (%)[a]
1	0	toluene	44	18	56
2	-20	toluene	50	15	49
3	-45	toluene	74	20	24
4[c]	-78	toluene	29	7	5
5	-45	DCM	62	5	27
6	-45	hexane	63	0	24
7	-45	THF	<1	n.d.	0

[a]Determined by ^{1}H NMR analysis. [b]Determined by chiral HPLC analysis. Absolute configuration was assigned to be *S* by comparison to literature. [c]8 h.

Computational Details

All calculations were performed with the Gaussian 03 package.[1] On the basis of the stoichiometric experiments and the relationship between ee values of **L4** and **1g**, DFT calculation was conducted for the trimetallic TS model consisting of Zn species, bisamidine ligand, and α-ketoester in a ratio of 3 : 1 : 1 (Fig. S1). **TS$_{\mathbf{major}}$** and **TS$_{\mathbf{minor}}$** provide *R* and *S* configuration products, respectively. The relative energy difference between was verified using B3LYP/6-311+G* for C, H, N, O, SDD for Zn//B3LYP/6-31G* for C, H, N, O, LANL2DZ for Zn.



TS$_{\textbf{major}}$ (0.0 kcal mol^{-1}) **TS**$_{\textbf{minor}}$ (+1.2 kcal mol^{-1})

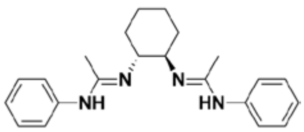
Fig. S1 Chemical models and 3D structures of **TS**$_{\textbf{major}}$ and **TS**$_{\textbf{minor}}$

General information

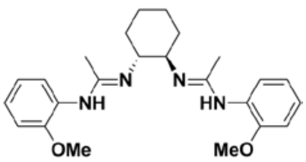
All reactions were performed under nitrogen atmosphere with magnetic stirring in dried glassware. Diethylzinc 1.0 M in hexane solution was purchased from Aldrich. All dehydrated solvents are purchased from Kanto Chemical co., Inc. and used without purification. Enantiomeric excess was determined by SHIMAZU HPLC system with UV detection at 254 nm and Daicel chiralpac AD-H, AS-H, OD-H, or OJ-H columns, or SHIMAZU GC system with a cyclodex β column. ^{1}H NMR and ^{13}C NMR spectra were recorded on a JEOL JNM-ECX400 spectrometer. Chemical shifts in $CDCl_3$ were reported in ppm from Me_4Si as the internal standard ($CDCl_3$: δ = 0) for ^{1}H NMR and from the solvent resonance ($CDCl_3$: δ = 77.0) for ^{13}C NMR. Data were reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, br = broad, m = multiplet), coupling constant, and number of protons. Infrared (IR) spectra were recorded on a JASCO FT/IR-230 Fourier transform infrared spectrophotometer. Elemental analyses were performed by Elementar vario MICRO cube. High resolution mass was performed by Waters micromass LTC ESI-TOF and JEOL JMS-GC mate II. Purification of the products was performed by column chromatography on silica gel 60N (spherical, neutral, Kanto Chemical Co., Inc), Wakogel

$50NH_2$ (Wako Pure Chemical Industries, Ltd) or activated alumina (about 75μm, Wako Pure Chemical Industries, Ltd).

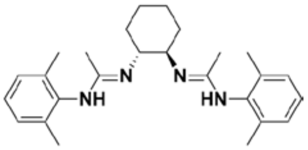
Synthesis of bisamidine ligands



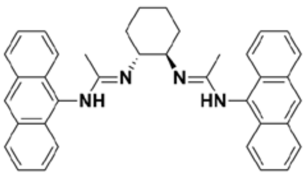
General procedure for synthesis of **L1:** To a suspension of the N-(2-Acetylamino-cyclohexyl)-acetamide[3] (198.3 mg, 1.0 mmol) in toluene was added phosphoryl chloride (0.19 ml, 2.0 mmol). The mixture was allowed to stir at room temperature for 15 h. Pyridine(0.17 ml, 2.0 mmol) followed by aniline (0.18 ml, 2.0 mmol) was added to the solution. The flask was heated to 110 ˚C and stirred for 6 h. After cooling to room temperature, the separated colorless viscous liquid was treated with 1 N NaOH aqueous solution, and extracted by CH_2Cl_2. The combined organic layers were washed with brine, dried over Na_2SO_4, and concentrated under reduced pressure. The residue was purified by recrystallization from AcOEt to afford **L1** as a colorless crystal (216 mg, 62% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.23 (t, *J* = 7.6 Hz, 4H), 6.96 (t, *J* = 7.2 Hz, 2H), 6.75 (d, *J* = 7.6 Hz, 4H), 5.64 (br, 2H), 3.87-3.85 (m, 2H), 2.32-2.30 (m, 2H), 1.80 (s, 6H), 1.75-1.73 (m, 2H), 1.40-1.24 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 156.3, 151.6, 128.7, 122.4, 121.7, 55.7, 32.3, 24.8, 18.1; IR (KBr) 3367.1 (s), 3051.8 (m), 2937.1 (s), 2858.0 (m), 1621.8 (s), 1539.9 (s), 1487.8 (s) cm^{-1}; Anal. Calcd for $C_{22}H_{28}N_4$: 75.82% C, 8.10% H, 16.08% N; found: 75.46% C, 8.22% H, 15.95% N.



L2: Obtained according to the general procedure using *p*-anisidine. Purification by column chromatography on activated alumina (Et_2O) followed by recrystallization from Et_2O afforded **L2** as a colorless crystal (19% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.96-6.92 (m, 2H), 6.88-6.83 (m, 4H), 6.74 (d, *J* = 8.0 Hz, 2H), 5.42 (br, 2H), 3.96 (br, 2H), 3.76 (s , 6H), 2.34-2.31 (m, 2H), 1.75 (s, 6H), 1.64 (br, 2H), 1.42-1.37 (m, 2H), 1.29-1.26 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 157.4, 151.5, 140.8, 123.4, 122.4, 120.7, 111.2, 55.29, 55.26, 32.4, 24.9, 18.1; IR (KBr) 3242.7 (s), 3027.7 (m), 2931.3 (s), 2859.1 (m), 1625.7 (s), 1535.1 (s), 1490.7 (s) cm^{-1}; HRMS Calcd for $C_{24}H_{32}N_4O_2$: 408.2525; found: 408.2513.



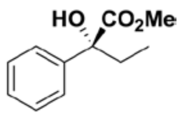
L3: Obtained according to the general procedure using 2,6-dimethylaniline. Purification by column chromatography on activated alumina (AcOEt/ hexane = 1/3) afforded **L3** as a white powder (52% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.00-6.98 (m, 4H), 6.83-6.80 (m, 2H), 5.03 (br, 2H), 3.99 (br, 2H), 2.38-2.34 (m, 2H), 2.08 (s, 6H), 2.06 (s, 6H), 1.78-1.76 (m, 2H), 1.58 (s, 6H), 1.44-1.39 (m, 2H), 1.30-1.27 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 154.9, 148.9, 129.1, 128.4, 127.7, 127.6, 121,5, 54.8, 33.2, 25.0, 18.3.; IR (KBr) 3317.0 (s), 3062.4 (m), 2929.3 (s), 2857.0 (m), 1635.3 (s), 1552.4 (s), 1467.6 (m) cm^{-1}; Anal. Calcd for $C_{26}H_{36}N_4$: 77.18% C, 8.97% H, 13.85% N; found: 77.18% C, 8.97% H, 13.71% N.



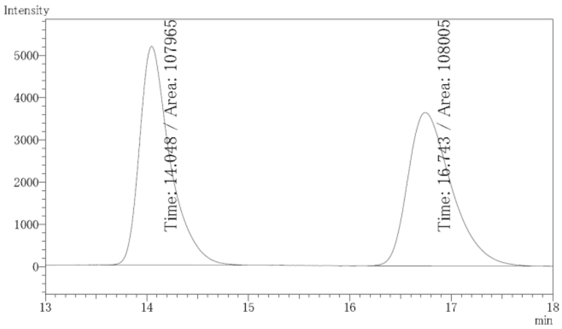
L4: Obtained according to the general procedure using 9-anthrylamine[4] and DMAP instead of pyridine. Purification by column chromatography on Wakogel 50NH_2 (AcOEt/hexane = 1/5) followed by recrystallization from MeOH afforded **L4** as a yellow crystal (42% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.10-8.05 (m, 6H), 7.96-7.93 (m, 4H), 7.45-7.29 (m, 8H), 5.82 (br, 2H), 4.38 (br, 2H), 2.67-2.64 (m, 2H), 1.88 (br, 2H), 1.59 (s, 6H), 1.55-1.53 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.3, 144.8, 132.29, 132.27, 128.5, 128.3, 125.3, 125.1, 124.5, 124.3, 124.1, 123.5, 119.6, 56.0, 33.1, 25.0, 19.3; IR (KBr) 3411.5 (s), 3047.0 (s), 2924.5 (s), 1641.1 (s), 1514.8 (s) cm^{-1}; Anal. Calcd for $C_{38}H_{36}N_4$: 83.18% C, 6.61% H, 10.21% N; found: 83.28% C, 6.82% H, 10.23% N.

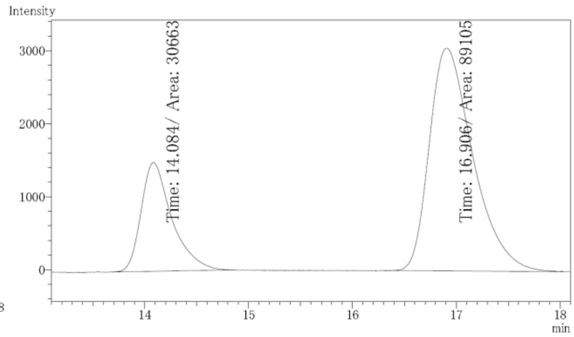
Typical experimental procedure for asymmetric alkylation of α-ketoesters and characterization of products

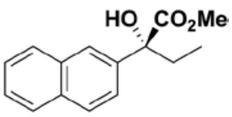
The chiral bisamidine ligand (0.01 mmol, 10 mol%) was dissolved in toluene (0.5 ml) under an atmosphere of N_2 and diethyl zinc (1.0 M in hexane, 0.2 ml, 0.2 mmol) was added. The mixture was allowed to stir at room temperature for 10 min. After cooling the solution to -45 ˚C, methyl phenylglyoxylate (16.4 mg, 0.1 mmol) was added with stirring. The mixture was stirred at -45 ˚C for 2 h, quenched by 1N HCl aqueous solution at -45 ˚C, and then extracted with CH_2Cl_2. The combined organic layers were washed with brine, dried over Na_2SO_4, and then concentrated under reduced pressure. The crude mixture was purified by flash column chromatography on silica gel 60N. Compound data of catalytic reaction product are below.



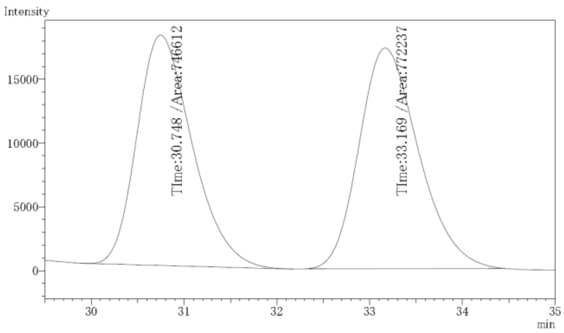
Methyl-2-hydroxy-2-phenylbutanoate (2a): Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.57 (d, *J* = 8.4 Hz, 2H), 7.37-7.33 (m, 2H), 7.29 (d, *J* = 7.2 Hz, 1H), 3.79 (s, 1H), 3.73 (s, 3H), 2.23 (dq, *J* = 14.3 Hz, *J* = 7.2 Hz, 1H), 2.04 (dq, *J* = 14.3 Hz, *J* = 7.2 Hz, 1H), 0.95 (t, *J* = 7.2 Hz, 3H). The ^{1}H and ^{13}C NMR spectra of **2a** were identical to reported values.[5] The absolute configuration was assigned based on comparison with reported GC analysis.[6] Chiral HPLC analysis: Daicel chiral column AD-H, 2-propanol/hexane = 1/99, 1.0 ml/min.

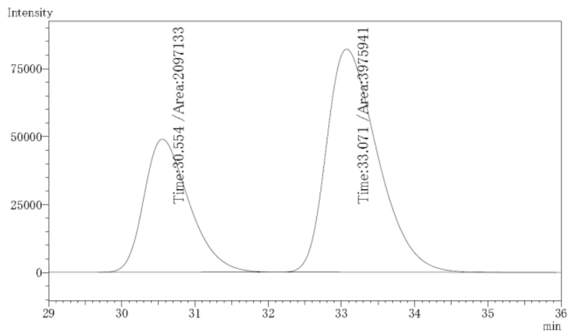


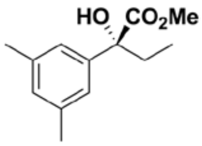




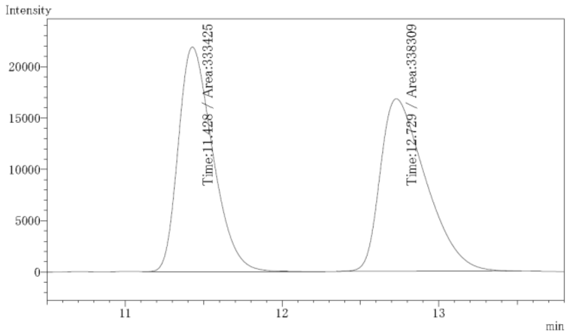
Methyl-2-hydroxy-2-(2-naphthyl)-butanoate (2b): Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.08 (s, 1H), 7.86-7.81 (m, 3H), 7.68 (dd, *J* = 8.8 Hz, *J* = 2.0 Hz, 1H), 7.49-7.45 (m, 2H), 3.88 (s, 1H), 3.78 (s, 3H), 2.32 (dq, *J* = 14.4 Hz, *J* = 7.2 Hz, 1H), 2.15 (dq, *J* = 14.4 Hz, *J* = 7.2 Hz, 1H), 0.95 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 175.8, 138.9, 133.0, 132.7, 128.3, 127.9, 127.4, 126.1, 124.6, 123.7, 78.9, 53.3, 32.5, 8.04; IR (neat) 3250.4 (s), 3057.6 (m), 2960.2 (s), 2880.2 (m), 1732.7 (s) cm^{-1}; HRMS Calcd for $C_{15}H_{16}O_3$ (M+Na): 267.0997; Found: 267.1022; Chiral HPLC analysis: Daicel chiral column AD-H, 2-propanol/hexane = 1/99, 1.0 ml/min.

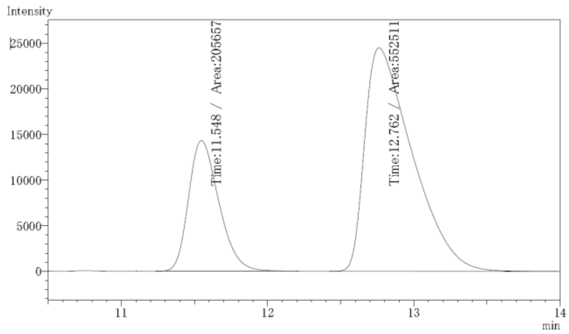


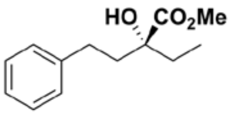




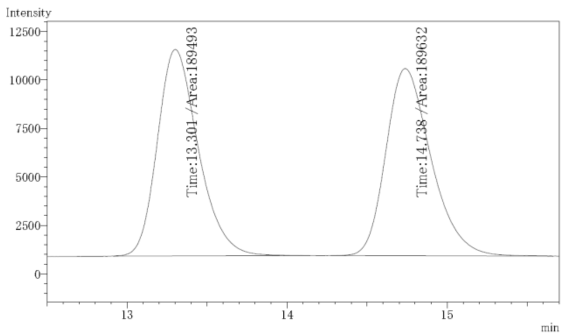
Methyl-2-hydroxy-2-(3,5-dimethylphenyl)-butanoate (2c): Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.17 (s, 2H), 6.92 (s, 1H), 3.78 (s, 3H), 3.66 (s, 1H), 2.32 (s, 3H), 2.21 (dq, J = 14.4 Hz, J = 7.2 Hz, 1H), 2.02 (dq, J = 14.4 Hz, J = 7.2 Hz, 1H), 0.91 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 175.9, 141.6, 137.7, 129.3, 123.2, 78.7, 53.2, 32.4, 21.5, 8.08; IR (neat) 3504 (s), 2960 (m), 1728 (s) cm^{-1}; HRMS Calcd for $C_{13}H_{18}O_3$ (M+Na): 245.1154; Found: 245.1185; Chiral HPLC analysis: Daicel chiral column AD-H, 2-propanol/hexane = 1/99, 1.0 ml/min.

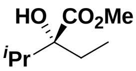




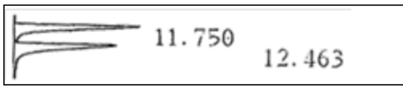


Methyl-2-ethyl-2-hydroxy-4-pehnyl butanoate (2d): Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.29-7.25 (m, 2H), 7.19-7.16 (m, 3H), 3.73 (s, 3H), 3.31 (s, 1H), 2.85-2.77 (m, 1H), 2.46-2.38 (m, 1H), 2.10-1.95 (m, 2H), 1.18-1.68 (m, 2H), 0.86 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 177.1, 141.6, 128.4, 128.3, 125.9, 77.6, 52.7, 40.6, 40.6, 32.4, 30.0, 7.81; IR (neat) 3523.3 (s), 3025.7 (m), 2959.2 (s), 1730.8 (s) cm^{-1}; HRMS Calcd for $C_{13}H_{18}O_3$: 222.1256; Found: 222.1179; Chiral HPLC analysis: Daicel chiral column AD-H, 2-propanol/hexane = 1/99, 1.0 ml/min.





Methyl 2-hydroxy-2-isopropyl-butanoate (2e): Colorless oil. [1]H NMR (400 MHz, CDCl3) : δ 3.79 (s, 3H), 3.09 (s, 1H), 2.00-1.90 (m, 1H), 1.81-1.63 (m, 2H), 0.94 (d, *J* = 6.8 Hz, 3H), 0.83 (d, *J* = 6.8 Hz, 3H), 0.82 (t, *J* = 7.2 Hz, 3H); [13]C NMR (100 MHz, $CDCl_3$) δ = 177.5, 80.5, 52.5, 35.2, 29.6, 17.6, 15.9, 8.19; IR (neat) 3532.0 (s), 2923.6 (s), 2856.1 (s), 1731.8 (s) cm^{-1}; HRMS Calcd for $C_8H_{16}O_3$ (M+Na): 160.1100; Found: 160.1014 ; Chiral GC analysis: 95 ˚C



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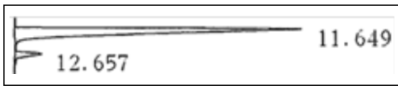

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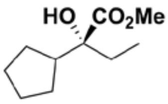
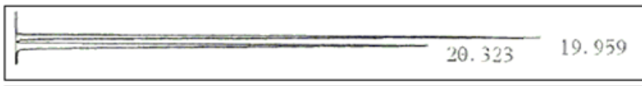


Methyl-2-cyclopentyl-2-hydroxybutanoate (2f): Colorless oil. [1]H NMR (400 MHz, $CDCl_3$): δ 3.78 (s, 3H), 3.14 (s, 1H), 2.23-2.14 (m, 1H), 1.76-1.32 (m, 10H), 0.82 (t, *J* = 7.2, 3H); [13]C NMR (100 MHz, $CDCl_3$): δ 177.5, 78.9, 52.6, 47.2, 30.9, 26.7, 26.0, 25.6, 25.5, 8.18; IR (neat) 3530.1 (s), 2954.4 (s), 2871.5 (m), 1729.8 (s) cm^{-1}; HRMS Calcd for $C_{10}H_{18}O_3$ (M+Na): 209.1154; Found: 209.1155; Chiral GC analysis: 100 ˚C (10 min), 5 ˚C /min, 150 ˚C (20 min)



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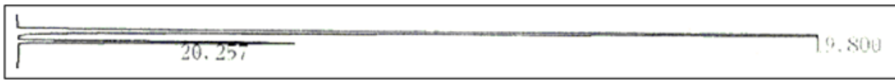

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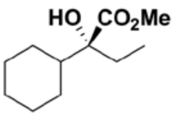
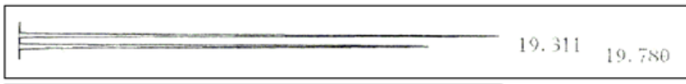


Methyl-2-cyclohexyl-2-hydroxybutanoate (2g): Colorless oil. [1]H NMR (400 MHz, $CDCl_3$): δ 3.78 (s, 3H), 3.12 (s, 1H), 1.83-1.57 (m, 7H), 1.29-1.05 (m, 6H), 0.81 (t, *J* = 7.6 Hz, 3H); [13]C NMR (100 MHz, $CDCl_3$): δ 177.5, 80.6, 52.5, 45.1, 29.0, 27.6, 26.3, 25.8, 8.09; IR (neat) 3530.1 (s), 2930.3 (s), 2857.0 (m), 1731.7 (s) cm^{-1}; HRMS Calcd for $C_{11}H_{20}O_3$ (M+Na): 223.1310; Found: 223.1270; Chiral GC analysis: 100 ˚C (5 min), 5 ˚C /min, 150 ˚C (20 min)



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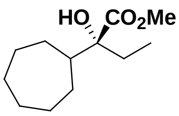

Methyl 2-cycloheptyl-2-hydroxy-butanoate (2h): Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.78 (s, 3H), 3.12 (s, 1H), 1.86-1.64 (m, 6H), 1.53-1.30 (m, 9H), 0.80 (t, *J* = 8.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 177.6, 81.7, 52.5, 46.3, 29.7, 29.5, 28.3, 28.2, 27.3, 27.1, 27.0, 8.15; IR (neat) 3529.1 (s), 2926.4 (s), 2858.0 (s), 1729.8 (s) cm^{-1}; HRMS Calcd for $C_{12}H_{22}O_3$ (M+Na): 214.1569; Found: 214.1526 ; Chiral GC analysis: 100˚C (10 min), 5˚C /min, 150 ˚C (30 min)

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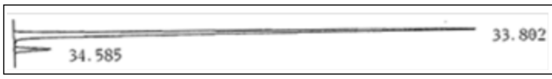

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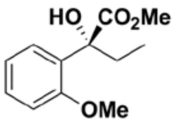
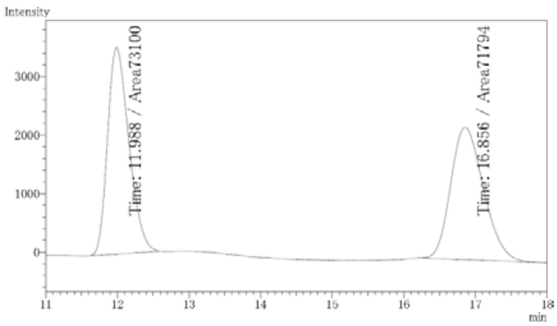
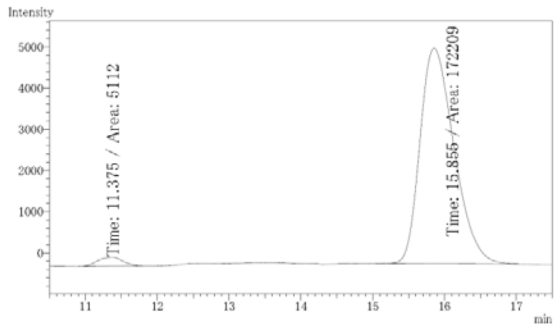
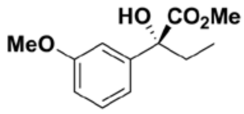


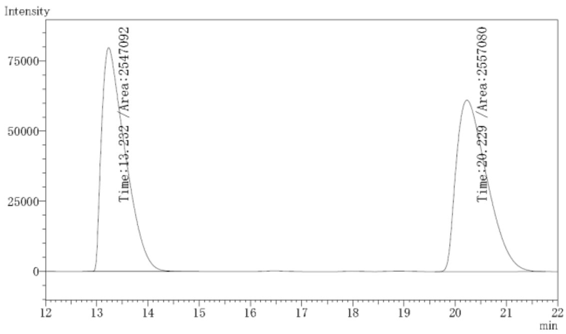
Methyl-2-hydroxy-2-*o*-methoxyphenylbutanoate (2i): Colorless crystal. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.46 (d, *J* = 7.7 Hz, 1H), 7.30 (dd, *J* = 8.1 Hz, *J* = 7.7 Hz, 1H), 6.99 (dd, *J* = 7.7 Hz, *J* = 7.7 Hz, 1H), 6.89 (d, *J* = 8.1 Hz, 1H), 4.04 (s, 1H), 3.81 (s, 3H), 3.70 (s, 3H), 2.26-2.16 (m, 2H), 0.98 (t, *J* = 7.3 Hz, 3H). The ^{1}H and ^{13}C NMR spectra of **2g** were identical to reported values. [5]

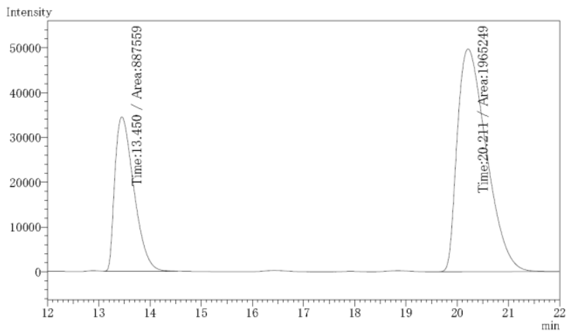


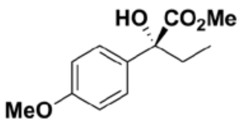




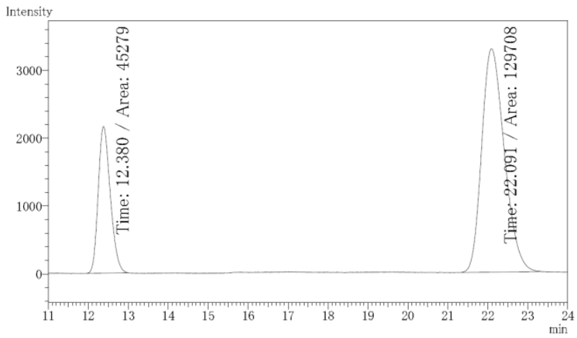
Methyl-2-hydroxy-2-*m*-methoxyphenylbutanoate (2j): Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.26 (t, *J* = 7.6 Hz, 1H), 7.17-7.15 (m, 2H), 6.84-6.82 (m, 1H), 3.81 (s, 3H), 3.79 (s, 3H), 3.72 (s, 1H), 2.20 (dq, *J* = 14.4 Hz, *J* = 7.2 Hz, 1H), 2.03 (dq, *J* = 14.4 Hz, *J* = 7.2 Hz, 1H), 0.91 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 175.7, 159.5, 143.4, 129.2, 117.9, 112.9, 111.5, 78.7, 55.2, 53.2, 32.6, 8.05; IR (neat) 3499.2 (s), 2958.3 (m), 2842.6 (w), 1729.8 (s) cm^{-1}; HRMS Calcd for $C_{12}H_{16}O_4$ (M+Na): 247.0946; Found: 247.0946; Chiral HPLC analysis: Daicel chiral column OJ-H, 2-propanol/hexane = 10/90, 1.0 ml/min.

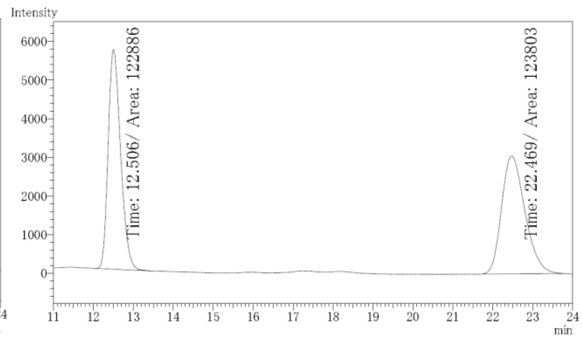


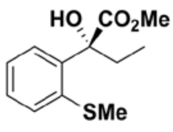




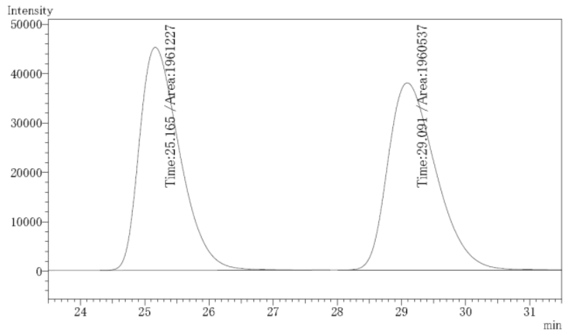
Methyl-2-hydroxy-2-*p*-methoxyphenylbutanoate (2k): Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.49 (d, *J* = 9.0 Hz, 2H), 6.88 (d, *J* = 9.0 Hz, 2H), 3.80 (s, 3H), 3.78 (s, 3H), 3.69 (s, 1H), 2.21 (dq, *J* = 14.6 Hz, *J* = 7.3 Hz, 1H), 2.00 (dq, *J* = 14.6 Hz, *J* = 7.3 Hz, 1H), 0.91 (t, *J* = 7.3 Hz, 3H). The ^{1}H and ^{13}C NMR spectra of **2i** were identical to reported values. [5]

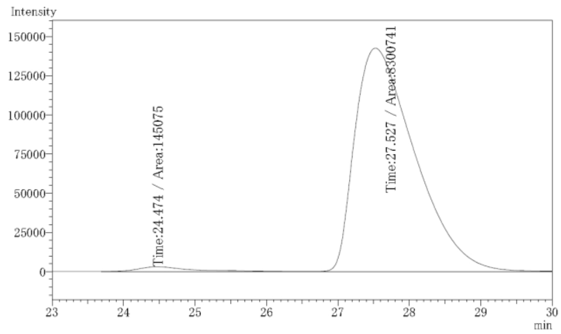






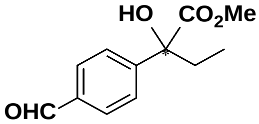
Methyl-2-hydroxy-2-*o*-thiomethylphenylbutanoate (2l): Colorless crystal. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.50 (d, *J* = 7.6 Hz, 1H), 7.39 (d, J = 8.0, 1H), 7.31-7.19 (m, 2H), 4.01 (s, 1H), 3.75 (s, 3H), 2.42 (s, 3H), 2.26 (q, *J* = 7.2 Hz, 2H), 0.98 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 175.6, 140.8, 137.7, 130.1, 128.5, 126.8, 125.7, 78.6, 52.9, 31.0, 18.2, 7.93; IR (KBr) 3486.7 (s), 3049.9 (m), 2967.9 (s), 2630.4 (s) cm^{-1}; Anal. Calcd for $C_{12}H_{16}O_3S$: 59.97% C, 6.71% H, 13.34% S; found: 59.97% C, 6.86% H, 13.58% S; Chiral HPLC analysis: Daicel chiral column OJ-H, 2-propanol/hexane = 5/95, 1.0 ml/min.



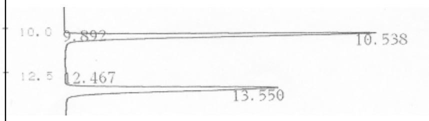


Typical experimental procedure for competing asymmetric alkylation of α-ketoesters in the presence of aldehydes and characterization of products

To a stirred solution of chiral bisamidine ligand (0.01 mmol, 10 mol%) in toluene (0.5 ml) was added diethyl zinc 1.0 M hexane solution (0.4 ml, 0.4 mmol) at room temperature. After 10 min reaction tube was cooled to -45 ^{o}C, and then a mixture of phenylglyoxylate (16.4 mg, 0.1 mmol) and benzaldehyde (10.6 mg, 0.1 mmol) in 0.5 ml of toluene was added dropwise. The reaction mixture was stirred at -45 ^{o}C for 2 h. The mixture was stirred at -45 ˚C for 2 h, quenched by 1N HCl aqueous solution at -45 ˚C, and then extracted with CH_2Cl_2. The combined organic layers were washed with brine, dried over Na_2SO_4, and then concentrated under reduced pressure. The crude mixture was purified by flash column chromatography on silica gel 60N. Compound data of catalytic reaction product are below.



Methyl 2-hydroxy-2-(4-formylphenyl)-butanoate (*p*-7): colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 10.02 (s, 1H), 7.87 (d, *J* = 8.4 Hz, 2H), 7.80 (d, *J* = 8.4 Hz, 2H), 3.84 (s, 1H), 3.82 (s, 3H), 2.25 (dq, *J* = 14.2 Hz, 7.2 Hz, 1H), 2.05 (dq, *J* = 14.2 Hz, 7.2 Hz, 1H), 0.92 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 191.9, 175.1, 148.2, 135.7, 129.6, 126.5, 78.8, 53.6, 32.9, 7.94; Chiral HPLC analysis: Daicel chiral column AD-H, 2-propanol/hexane = 10/90, 1.0 ml/min.



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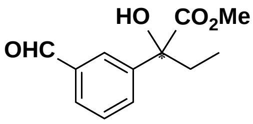
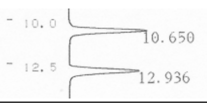


Methyl 2-hydroxy-2-(3-formylphenyl)-butanoate (*m*-7): colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 10.04 (s, 1H), 8.14 (t, *J* = 1.6 Hz, 1H), 7.92-7.89 (m, 1.6 Hz, 1H), 7.83 (d, *J* = 8.0 Hz, 1H), 7.53 (t, *J* = 8.0 Hz, 1H), 3.87 (s, 1H), 3.81 (s, 3H), 2.27 (dq, *J* = 14.4 Hz, 7.2 Hz, 1H), 2.05 (dq, *J* = 14.4 Hz, 7.2 Hz, 1H), 0.92 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 192.3, 175.3, 142.8, 136.4, 131.9, 129.0, 128.9, 127.4, 78.4, 53.6, 32.9, 7.95; Chiral HPLC analysis: Daicel chiral column AD-H, 2-propanol/hexane = 10/90, 1.0 ml/min.



#	Time	Area
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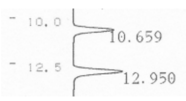

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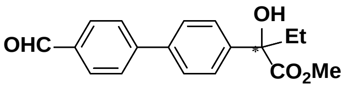
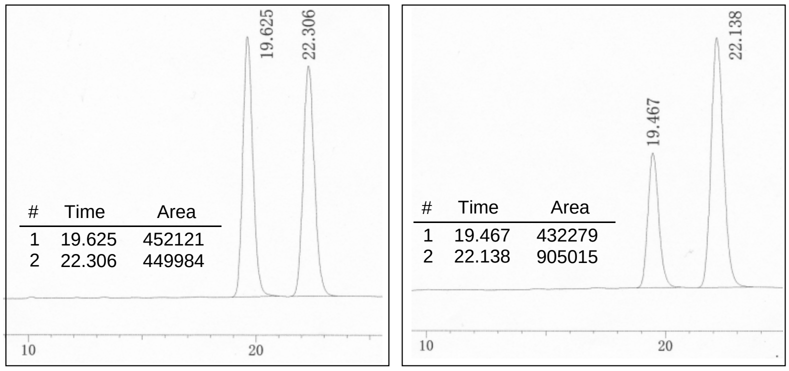


Methyl-2-hydroxy-2-(4-(4-formylphenyl) phenyl)-butanoate (10): colorless oil. [1]H NMR (400 MHz, $CDCl_3$) δ = 10.06 (s, 1H), 7.96 (d, *J* = 8.2 Hz, 2H), 7.77-7.70 (m, 4H), 7.63 (d, *J* = 8.4 Hz, 2H), 3.82 (s, 3H), 3.81 (s, 1H), 2.27 (dq, *J* = 14.4 Hz, 7.2 Hz, 1H), 2.07 (dq, *J* = 14.4 Hz, 7.2 Hz, 1H), 0.95 (t, *J* = 7.2 Hz, 3H); [13]C NMR (100 MHz, $CDCl_3$) δ = 191.9, 175.6, 146.6, 142.0, 139.0, 135.2, 130.3, 127.6, 127.2, 126.4, 78.6, 53.4, 32.8, 8.04; Chiral HPLC analysis: Daicel chiral column AD-H, 2-propanol/hexane = 10/90, 1.3 ml/min.



Cartesian coordinates, Harmonic frequencies, and absolute electronic energies of TS_{major} and TS_{minor}

The Cartesian coordinates of all stationary points are listed. For each structure, absolute electronic energies are shown in parentheses. For the located transition state structures, the number of negative eigenvalues of the Hessian at the converged structures are also indicated (nimag = 1).

TS_{major}

```
SCF Done: E(RB3LYP) = -3102.65831275 a.u.
---------------------------------------------------------------------
 Center     Atomic     Atomic             Coordinates (Angstroms)
 Number     Number      Type             X           Y           Z
---------------------------------------------------------------------
      1          6           0        0.870181   -2.966266   -2.874265
      2          6           0        0.182908   -2.516779   -1.564428
      3          6           0       -1.241261   -2.014779   -1.907476
      4          6           0       -1.359029   -3.673791   -3.847972
      5          6           0        0.094753   -4.084897   -3.584936
      6          1           0        0.039145   -3.404042   -0.924689
      7          1           0        0.957739   -2.089078   -3.531133
      8          1           0        1.892631   -3.298398   -2.668309
      9          1           0       -1.927967   -4.513429   -4.266762
     10          1           0       -1.378913   -2.875484   -4.604728
     11          1           0        0.108558   -4.989189   -2.959037
     12          1           0        0.595120   -4.350513   -4.524774
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Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

		1			2			3		
		A			A			A		
Frequencies --		-158.2162			9.5042			12.1316		
Red. masses --		7.0496			5.9331			5.8511		
Frc consts --		0.1040			0.0003			0.0005		
IR Inten --		62.2618			0.0454			0.0617		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
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3	6	0.00	0.00	0.00	-0.01	0.04	-0.01	0.01	-0.05	0.03
4	6	0.00	0.00	0.00	0.00	0.05	-0.02	0.02	-0.08	0.05
5	6	0.00	0.00	0.00	-0.01	0.04	-0.01	0.01	-0.08	0.07
6	1	0.00	0.01	0.00	-0.02	0.03	-0.01	0.01	-0.03	0.05
7	1	0.00	-0.01	-0.01	0.00	0.03	0.00	0.01	-0.07	0.03
8	1	0.00	-0.01	0.00	-0.01	0.03	0.00	0.01	-0.06	0.05
9	1	0.00	0.00	0.00	-0.01	0.06	-0.02	0.02	-0.09	0.06
10	1	0.00	0.00	0.00	0.00	0.06	-0.01	0.02	-0.09	0.04
11	1	0.00	0.00	0.00	-0.02	0.04	-0.02	0.01	-0.07	0.08
12	1	0.00	-0.01	0.00	-0.01	0.04	-0.01	0.02	-0.09	0.07
13	1	0.00	0.00	0.00	0.00	0.05	0.00	0.01	-0.06	0.02
14	7	0.00	0.00	0.00	-0.01	0.03	0.00	0.00	-0.03	0.02

15	7	0.01	0.01	-0.02	-0.01	0.03	0.00	0.01	-0.03	0.02
16	6	0.00	0.00	0.00	-0.01	0.02	0.01	0.01	-0.02	0.00
17	6	0.00	0.00	-0.01	-0.01	0.01	0.01	0.01	-0.01	0.02
18	7	0.00	0.00	0.00	-0.01	0.01	0.01	0.00	0.00	-0.01
19	7	0.01	0.01	-0.03	0.00	0.01	0.00	0.01	0.00	0.00
20	6	0.00	0.00	0.00	-0.01	0.03	0.01	0.02	-0.04	-0.01
21	1	0.00	0.00	0.00	0.00	0.03	0.00	0.03	-0.05	-0.02
22	1	0.00	0.00	0.00	-0.03	0.02	0.03	0.01	-0.04	-0.03
23	1	0.00	0.00	0.00	-0.01	0.06	0.02	0.04	-0.03	0.00
24	6	-0.01	0.01	0.01	-0.03	0.01	0.02	0.02	-0.01	0.04
25	1	0.00	0.00	0.02	-0.04	-0.01	0.02	0.02	-0.02	0.04
26	1	-0.02	0.01	0.01	-0.03	0.02	0.02	0.02	0.01	0.04
27	1	-0.01	0.01	0.01	-0.04	0.02	0.03	0.02	-0.01	0.06
28	6	0.00	0.00	0.00	-0.01	0.05	-0.02	0.01	-0.06	0.04
29	1	0.00	0.00	0.00	-0.01	0.05	-0.02	0.01	-0.06	0.03
30	1	0.00	0.00	0.00	-0.01	0.04	-0.02	0.01	-0.05	0.05
31	6	0.01	0.00	0.00	0.00	0.04	0.00	0.02	-0.05	0.02
32	1	0.01	0.00	0.00	-0.01	0.02	0.00	0.03	-0.05	0.04
33	1	0.01	0.00	-0.02	-0.02	0.05	0.00	0.02	-0.05	0.02
34	30	0.00	0.03	-0.01	0.00	0.03	0.00	0.00	-0.03	0.01
35	8	-0.03	0.02	0.00	-0.01	0.04	0.02	-0.02	-0.03	0.02
36	8	0.14	-0.10	-0.10	0.03	0.02	-0.01	-0.01	-0.03	0.02
37	6	0.02	-0.01	-0.04	0.01	0.03	0.00	-0.03	-0.02	0.02
38	6	0.21	-0.13	-0.19	0.03	0.02	-0.02	-0.03	-0.02	0.02
39	6	0.06	0.02	-0.11	0.06	-0.01	-0.10	-0.01	0.01	-0.03
40	1	0.13	0.06	-0.10	0.09	0.01	-0.10	0.01	0.01	-0.03
41	1	0.06	0.04	-0.14	0.05	-0.03	-0.12	-0.01	0.02	-0.06
42	6	0.00	0.00	0.00	0.04	0.02	-0.01	-0.06	0.00	0.03
43	1	0.00	0.00	0.00	0.05	0.02	-0.03	-0.07	-0.03	0.03
44	1	0.00	0.00	0.00	0.06	0.02	0.00	-0.06	0.01	0.02
45	30	-0.03	-0.02	0.17	0.02	0.00	-0.04	-0.01	0.00	-0.01
46	30	0.01	0.01	0.00	0.01	0.01	-0.01	-0.02	-0.01	0.02
47	6	-0.30	0.24	0.04	-0.02	-0.02	-0.04	-0.04	0.00	0.00
48	1	-0.10	0.08	-0.01	-0.04	-0.01	-0.02	-0.04	0.00	0.00
49	1	-0.23	0.15	-0.15	0.01	-0.03	-0.04	-0.05	0.00	0.00
50	8	-0.02	0.00	-0.03	0.00	0.03	0.00	-0.05	-0.01	0.03
51	6	-0.07	0.02	0.01	-0.02	0.05	0.02	-0.05	-0.01	0.04
52	1	-0.05	0.04	0.04	-0.02	0.06	0.04	-0.05	-0.02	0.04
53	1	-0.08	0.02	0.01	-0.03	0.05	0.02	-0.06	-0.01	0.04
54	1	-0.10	0.02	0.00	-0.04	0.04	0.02	-0.04	-0.01	0.03
55	1	-0.20	0.30	0.46	-0.03	-0.06	-0.05	-0.04	0.01	-0.01
56	1	0.01	0.00	-0.14	0.06	-0.02	-0.12	-0.03	0.01	-0.03
57	1	0.00	0.00	0.00	0.04	0.01	0.01	-0.08	0.01	0.03
58	1	0.01	0.00	0.00	0.01	0.04	-0.01	0.03	-0.05	0.00
59	6	0.09	-0.06	-0.09	0.06	0.01	-0.03	-0.04	-0.02	0.03
60	6	0.01	-0.07	-0.07	0.08	0.01	-0.04	-0.03	-0.02	0.03
61	6	0.06	-0.01	-0.05	0.07	0.00	-0.04	-0.05	-0.01	0.03
62	6	-0.05	-0.05	-0.02	0.12	0.00	-0.06	-0.04	-0.02	0.04
63	1	0.01	-0.09	-0.09	0.08	0.02	-0.03	-0.03	-0.03	0.02
64	6	-0.01	0.00	0.00	0.10	-0.01	-0.06	-0.06	-0.01	0.04
65	1	0.09	0.01	-0.06	0.05	0.00	-0.03	-0.05	-0.01	0.03
66	6	-0.05	-0.02	0.01	0.12	-0.01	-0.06	-0.06	-0.01	0.04
67	1	-0.09	-0.07	0.00	0.13	0.01	-0.06	-0.04	-0.03	0.04
68	1	-0.03	0.03	0.02	0.11	-0.02	-0.06	-0.07	0.00	0.05
69	1	-0.08	-0.01	0.05	0.15	-0.01	-0.08	-0.07	-0.01	0.05
70	6	0.01	0.00	-0.01	-0.01	0.00	0.01	0.02	0.02	-0.01
71	6	0.00	0.00	-0.01	-0.01	0.03	0.01	0.04	0.04	-0.02
72	6	0.01	0.00	-0.01	-0.01	-0.04	0.02	0.01	0.01	-0.03
73	6	0.00	0.00	-0.01	-0.01	0.08	0.00	0.05	0.05	0.00
74	6	0.00	0.00	-0.01	-0.02	0.02	0.02	0.05	0.06	-0.03
75	6	0.01	0.00	0.00	-0.02	-0.05	0.03	0.02	0.02	-0.04
76	6	0.01	0.00	-0.01	0.00	-0.07	0.02	-0.01	-0.02	-0.03
77	6	0.00	0.00	-0.01	-0.02	0.11	0.00	0.07	0.08	-0.01
78	1	0.00	0.00	-0.01	0.00	0.08	-0.01	0.04	0.04	0.01
79	6	0.00	0.00	-0.01	-0.03	0.06	0.02	0.07	0.09	-0.03

80	6	0.00	0.00	0.00	-0.02	-0.02	0.03	0.04	0.05	-0.04
81	6	0.01	0.00	0.00	-0.02	-0.10	0.04	0.01	0.01	-0.05
82	1	0.01	-0.01	-0.01	0.00	-0.06	0.01	-0.02	-0.03	-0.02
83	6	0.01	0.00	0.00	0.00	-0.11	0.03	-0.02	-0.03	-0.04
84	6	0.00	0.00	-0.01	-0.02	0.10	0.01	0.08	0.10	-0.02
85	1	0.00	0.00	-0.01	-0.01	0.14	-0.01	0.08	0.09	0.00
86	1	0.00	0.00	-0.01	-0.03	0.05	0.03	0.08	0.11	-0.04
87	1	0.00	0.00	0.00	-0.03	-0.03	0.04	0.05	0.06	-0.05
88	6	0.01	0.00	0.00	-0.01	-0.13	0.04	-0.01	-0.02	-0.05
89	1	0.01	0.00	0.00	-0.03	-0.11	0.05	0.01	0.02	-0.07
90	1	0.01	0.00	0.00	0.00	-0.13	0.03	-0.04	-0.05	-0.04
91	1	0.00	0.00	-0.01	-0.03	0.12	0.01	0.10	0.13	-0.02
92	1	0.01	0.00	0.00	-0.01	-0.16	0.05	-0.02	-0.02	-0.06
93	6	0.00	0.00	0.00	-0.02	-0.02	0.02	0.01	0.02	-0.02
94	6	0.00	0.00	0.00	-0.01	-0.04	-0.02	0.00	0.05	-0.08
95	6	0.00	0.00	0.00	-0.05	-0.04	0.06	0.03	0.01	0.02
96	6	0.00	0.00	0.00	0.02	-0.02	-0.07	-0.02	0.06	-0.12
97	6	0.00	0.00	0.00	-0.02	-0.07	-0.01	0.01	0.07	-0.10
98	6	0.00	0.00	0.00	-0.06	-0.07	0.08	0.03	0.03	0.01
99	6	0.00	0.00	0.00	-0.07	-0.03	0.10	0.04	-0.03	0.08
100	6	0.00	0.00	0.00	0.03	-0.04	-0.11	-0.03	0.10	-0.18
101	1	0.00	0.00	0.00	0.03	0.00	-0.08	-0.03	0.04	-0.10
102	6	0.00	0.00	0.00	-0.01	-0.08	-0.05	0.00	0.11	-0.16
103	6	0.00	0.00	0.00	-0.05	-0.09	0.04	0.02	0.06	-0.05
104	6	0.00	0.00	0.00	-0.09	-0.09	0.13	0.05	0.01	0.06
105	1	0.00	0.00	0.00	-0.06	0.00	0.08	0.03	-0.04	0.09
106	6	0.00	0.00	0.00	-0.09	-0.04	0.15	0.05	-0.04	0.13
107	6	0.00	0.00	0.00	0.02	-0.07	-0.10	-0.02	0.12	-0.21
108	1	0.00	0.00	0.00	0.06	-0.03	-0.14	-0.04	0.11	-0.21
109	1	0.00	0.00	0.00	-0.02	-0.10	-0.04	0.00	0.13	-0.18
110	1	0.00	0.00	0.00	-0.06	-0.11	0.05	0.03	0.07	-0.06
111	6	0.00	0.00	0.00	-0.11	-0.08	0.17	0.06	-0.02	0.12
112	1	0.00	0.00	0.00	-0.10	-0.12	0.15	0.06	0.02	0.05
113	1	0.00	0.00	0.00	-0.11	-0.03	0.17	0.06	-0.07	0.17
114	1	0.00	0.00	0.00	0.03	-0.08	-0.13	-0.03	0.15	-0.26
115	1	0.00	0.00	0.00	-0.13	-0.09	0.21	0.07	-0.03	0.16

TS$_{minor}$

SCF Done: E(RB3LYP) = -3102.65646909 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.360693	-3.351401	-2.074523
2	6	0	0.541628	-2.676471	-0.950686
3	6	0	-0.826703	-2.232781	-1.521665
4	6	0	-0.744563	-4.135590	-3.233129
5	6	0	0.630513	-4.549483	-2.697324
6	1	0	0.330753	-3.431820	-0.171477
7	1	0	1.566464	-2.598703	-2.846217
8	1	0	2.333385	-3.674885	-1.688081
9	1	0	-1.290453	-5.007161	-3.615550
10	1	0	-0.612221	-3.449749	-4.082348
11	1	0	0.504840	-5.338131	-1.940766
12	1	0	1.242691	-4.981122	-3.499010
13	1	0	-0.604972	-1.504096	-2.316329
14	7	0	-1.618171	-1.609353	-0.459392
15	7	0	1.233340	-1.499499	-0.380502
16	6	0	-2.780005	-0.960449	-0.719560
17	6	0	2.511271	-1.646114	0.069510
18	7	0	-3.579911	-0.850641	0.330487
19	7	0	3.295489	-0.599251	-0.092341

20	6	0	-3.161883	-0.404357	-2.073479
21	1	0	-4.053037	-0.916780	-2.452613
22	1	0	-3.417466	0.654583	-1.972312
23	1	0	-2.357967	-0.502725	-2.803337
24	6	0	3.018157	-2.917348	0.727312
25	1	0	3.947721	-3.257443	0.259640
26	1	0	3.245608	-2.707811	1.778268
27	1	0	2.282349	-3.721218	0.693307
28	6	0	-1.564335	-3.440143	-2.138881
29	1	0	-2.529905	-3.109462	-2.541075
30	1	0	-1.790849	-4.153689	-1.333070
31	6	0	-0.852440	-0.713246	2.802755
32	1	0	-0.542264	-1.630547	3.321254
33	1	0	-1.876840	-0.475456	3.131784
34	1	0	-0.246590	0.089586	3.242064
35	30	0	-0.157322	-0.413124	0.807371
36	8	0	-0.301821	1.298171	-0.547266
37	8	0	1.142916	1.328367	1.638258
38	6	0	0.265779	2.403118	-0.290685
39	6	0	1.017086	2.389611	1.030090
40	6	0	1.865067	0.219916	-3.579500
41	1	0	2.199259	1.098810	-4.144893
42	1	0	2.451323	-0.642653	-3.923306
43	1	0	0.815421	0.033174	-3.838481
44	6	0	-2.739278	-3.909264	2.564991
45	1	0	-3.314812	-4.629558	1.970733
46	1	0	-1.802982	-4.394843	2.866472
47	1	0	-3.312637	-3.695700	3.475420
48	30	0	2.117308	0.543027	-1.555519
49	30	0	-2.384058	-2.204337	1.518651
50	6	0	2.795847	2.649522	-1.184197
51	1	0	2.485059	3.174200	-2.090674
52	1	0	2.858231	3.345584	-0.350453
53	1	0	3.801020	2.222672	-1.327708
54	8	0	1.414876	3.554339	1.532962
55	6	0	2.115484	3.494359	2.797065
56	1	0	2.408075	4.522573	3.007007
57	1	0	1.448891	3.114667	3.574708
58	1	0	2.989241	2.845429	2.714051
59	6	0	4.621651	-0.534962	0.395845
60	6	0	4.898274	-0.290041	1.764651
61	6	0	5.688004	-0.644470	-0.534751
62	6	0	3.863854	-0.134998	2.740687
63	6	0	6.270494	-0.190180	2.208809
64	6	0	7.052429	-0.523154	-0.075899
65	6	0	5.465602	-0.889502	-1.926678
66	6	0	4.159367	0.073261	4.065004
67	1	0	2.831940	-0.155040	2.414865
68	6	0	6.532439	0.025765	3.598979
69	6	0	7.310152	-0.305683	1.281474
70	6	0	8.113669	-0.640427	-1.027489
71	1	0	4.447428	-0.993816	-2.284113
72	6	0	6.512853	-0.992680	-2.807313
73	6	0	5.512300	0.147444	4.504438
74	1	0	3.354122	0.185982	4.786345
75	1	0	7.569195	0.090936	3.921033
76	1	0	8.340153	-0.226315	1.622450
77	6	0	7.856431	-0.865872	-2.353797
78	1	0	9.136413	-0.546107	-0.669971
79	1	0	6.317095	-1.174693	-3.860542
80	1	0	5.729051	0.307282	5.557284
81	1	0	8.674371	-0.951060	-3.064149
82	6	0	-4.809353	-0.154617	0.327575
83	6	0	-6.013907	-0.896647	0.236646
84	6	0	-4.852152	1.250213	0.506857

85	6	0	-6.023181	-2.316374	0.062074
86	6	0	-7.283016	-0.211266	0.313237
87	6	0	-6.130177	1.921393	0.577460
88	6	0	-3.667087	2.043293	0.618315
89	6	0	-7.200664	-3.014089	-0.028913
90	1	0	-5.074570	-2.838759	0.004790
91	6	0	-8.486710	-0.977437	0.211854
92	6	0	-7.310182	1.177331	0.479974
93	6	0	-6.153062	3.341836	0.747327
94	1	0	-2.704155	1.548718	0.567053
95	6	0	-3.733554	3.404497	0.776458
96	6	0	-8.451170	-2.336668	0.046042
97	1	0	-7.182748	-4.092940	-0.157949
98	1	0	-9.436891	-0.451641	0.270786
99	1	0	-8.268722	1.688827	0.536043
100	6	0	-4.993778	4.064867	0.842208
101	1	0	-7.119956	3.837141	0.798868
102	1	0	-2.819341	3.987294	0.847476
103	1	0	-9.375066	-2.903987	-0.027944
104	1	0	-5.029342	5.143618	0.968540
105	6	0	-0.102960	3.607101	-1.066145
106	6	0	0.349478	4.913787	-0.793317
107	6	0	-0.985036	3.411952	-2.149722
108	6	0	-0.078108	5.983327	-1.577784
109	1	0	1.029899	5.093765	0.026099
110	6	0	-1.401788	4.483007	-2.931275
111	1	0	-1.329176	2.407202	-2.362647
112	6	0	-0.951446	5.775574	-2.646756
113	1	0	0.278900	6.984518	-1.353077
114	1	0	-2.080451	4.311668	-3.761997
115	1	0	-1.278218	6.614138	-3.255711

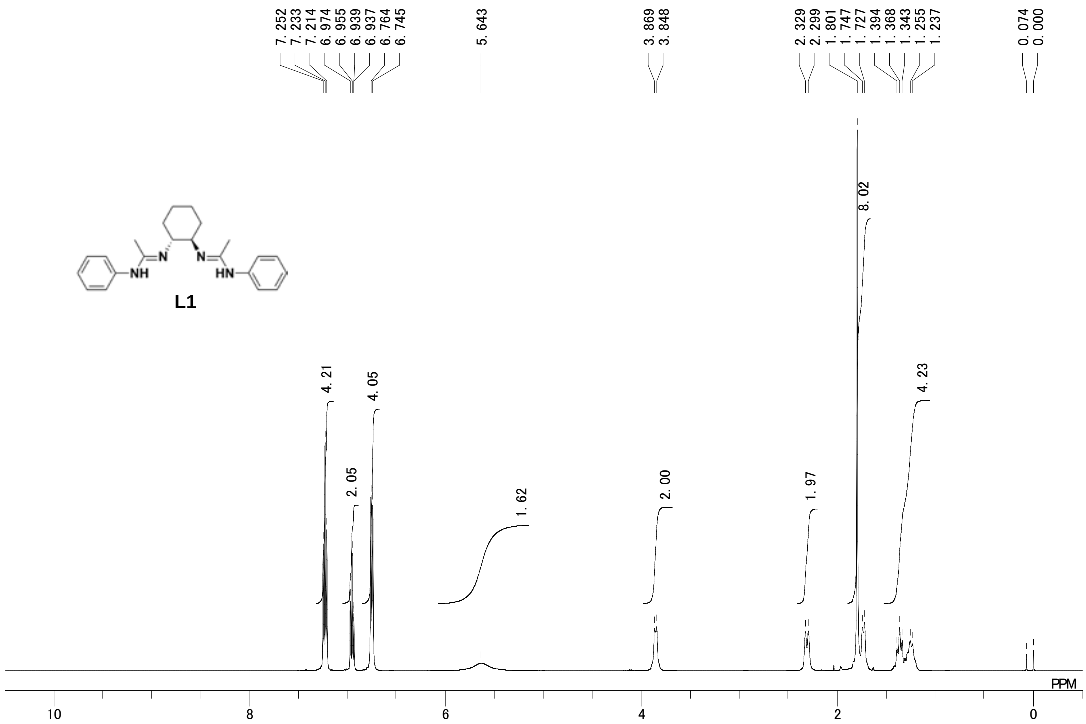
Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

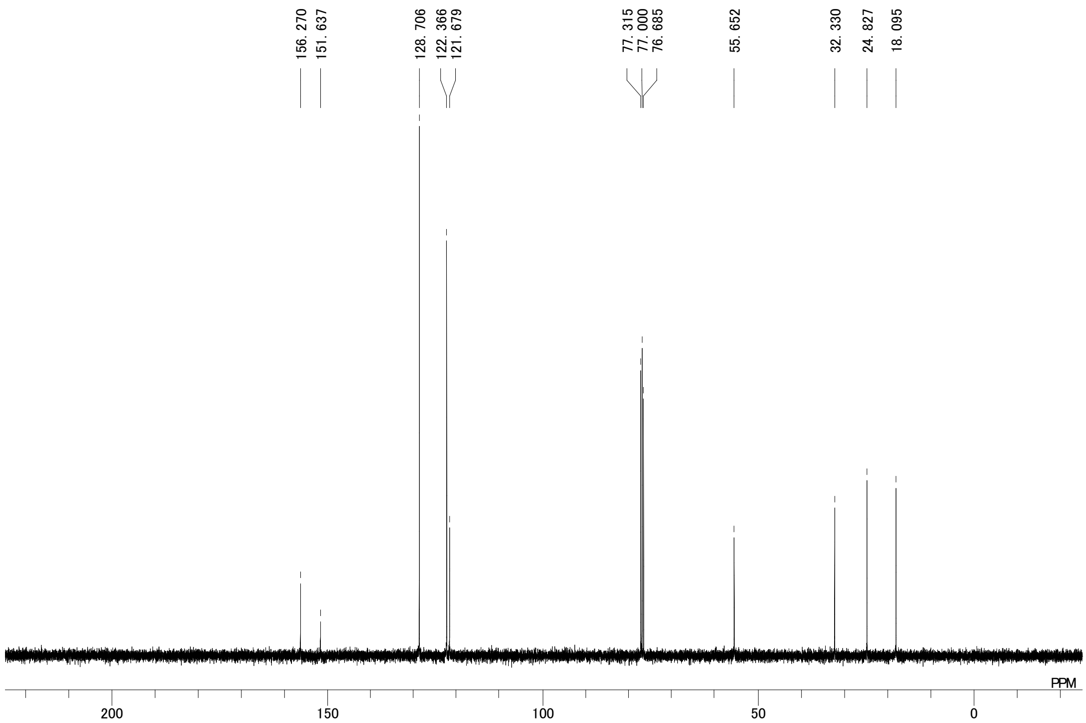
		1			2			3		
		A			A			A		
Frequencies --		-80.9670			9.5470			13.0746		
Red. masses --		6.9583			5.8351			6.0445		
Frc consts --		0.0269			0.0003			0.0006		
IR Inten --		28.3588			0.0258			0.1410		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.01	0.00	0.01	0.01	-0.04	0.05	-0.03	-0.06	-0.02
2	6	-0.01	-0.01	0.01	0.01	-0.03	0.05	-0.01	-0.05	-0.01
3	6	-0.01	-0.01	0.01	0.01	-0.03	0.04	-0.02	-0.05	0.00
4	6	0.00	0.00	0.01	0.01	-0.05	0.06	-0.04	-0.05	0.00
5	6	0.00	0.00	0.01	0.01	-0.05	0.07	-0.04	-0.05	-0.01
6	1	-0.01	-0.02	0.01	0.01	-0.02	0.06	-0.01	-0.05	-0.01
7	1	-0.01	0.01	0.02	0.00	-0.05	0.04	-0.03	-0.05	-0.02
8	1	-0.01	0.00	0.01	0.01	-0.03	0.05	-0.02	-0.06	-0.03
9	1	0.00	0.00	0.00	0.01	-0.06	0.07	-0.05	-0.05	0.01
10	1	0.00	0.00	0.01	0.01	-0.06	0.05	-0.05	-0.05	0.00
11	1	0.00	0.00	0.00	0.01	-0.04	0.07	-0.03	-0.05	-0.01
12	1	0.00	0.01	0.00	0.01	-0.05	0.07	-0.05	-0.05	-0.02
13	1	-0.01	-0.01	0.01	0.01	-0.04	0.03	-0.02	-0.05	0.00
14	7	-0.01	-0.01	0.01	0.01	-0.02	0.03	0.00	-0.04	0.00
15	7	-0.02	-0.01	0.02	0.00	-0.02	0.03	-0.01	-0.06	-0.02
16	6	-0.01	-0.01	0.01	0.02	-0.01	0.02	0.00	-0.02	0.01
17	6	-0.01	-0.01	0.00	0.01	0.00	0.02	0.00	-0.04	-0.03
18	7	-0.01	0.00	0.01	0.01	0.01	0.01	0.01	0.00	0.01
19	7	0.00	-0.01	0.00	0.00	0.00	0.00	-0.03	-0.02	-0.01
20	6	-0.01	-0.02	0.01	0.03	-0.01	0.01	0.00	-0.02	0.01
21	1	0.02	-0.06	-0.02	0.08	-0.06	-0.03	0.01	-0.03	0.01

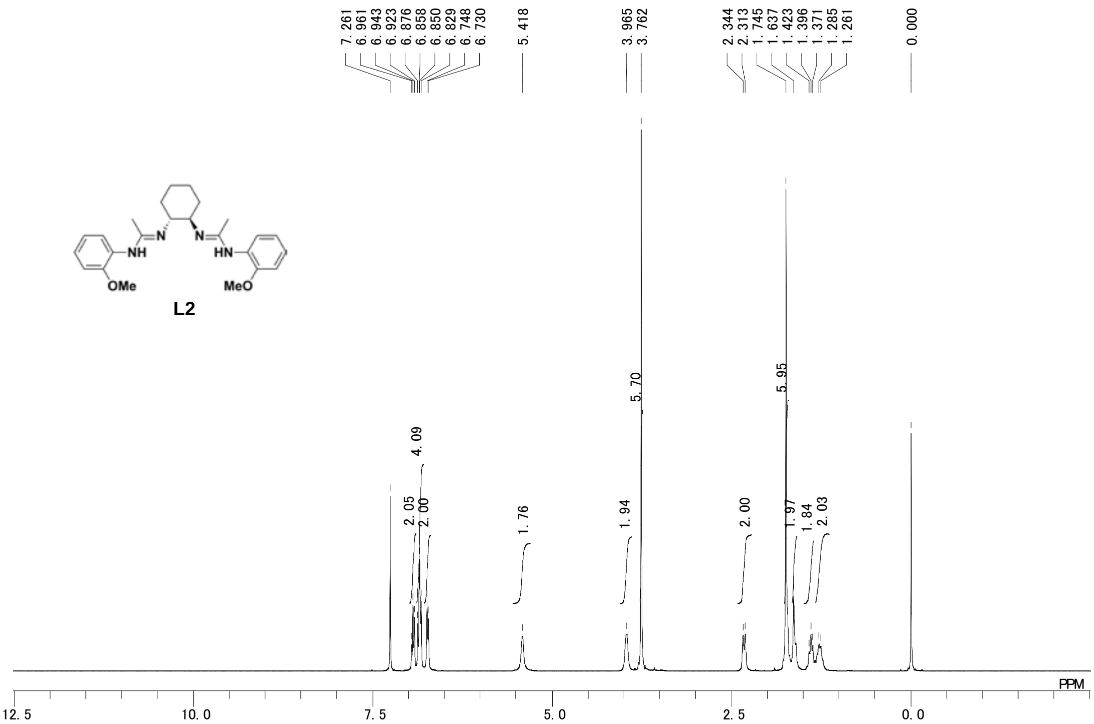
22	1	-0.07	-0.03	0.01	-0.03	-0.03	0.01	0.00	-0.02	0.01
23	1	0.01	0.02	0.02	0.07	0.04	0.04	0.00	-0.02	0.01
24	6	0.00	-0.01	-0.02	0.02	0.01	0.03	0.03	-0.04	-0.07
25	1	-0.01	-0.02	-0.04	0.02	0.00	0.02	0.02	-0.03	-0.11
26	1	0.02	-0.02	-0.02	0.04	0.02	0.02	0.07	-0.06	-0.07
27	1	-0.01	-0.01	-0.01	0.03	0.00	0.05	0.04	-0.05	-0.06
28	6	-0.01	-0.01	0.01	0.01	-0.04	0.05	-0.03	-0.05	0.01
29	1	-0.01	-0.01	0.01	0.01	-0.04	0.05	-0.03	-0.04	0.02
30	1	0.00	-0.01	0.00	0.00	-0.03	0.06	-0.02	-0.05	0.02
31	6	0.00	-0.01	0.02	0.01	-0.02	0.03	0.04	-0.03	-0.01
32	1	-0.01	-0.01	0.02	0.00	-0.03	0.02	0.02	-0.04	-0.02
33	1	0.00	0.00	0.01	0.02	0.00	0.04	0.05	0.00	0.00
34	1	0.00	-0.01	0.02	0.04	-0.03	0.03	0.07	-0.05	-0.01
35	30	0.00	-0.04	0.02	0.01	-0.02	0.03	0.02	-0.03	-0.02
36	8	-0.23	0.06	0.11	-0.01	-0.02	0.02	0.03	-0.04	-0.04
37	8	-0.01	-0.02	-0.03	0.00	-0.01	0.01	0.00	-0.01	-0.02
38	6	-0.23	0.03	0.08	-0.01	-0.02	0.02	0.01	-0.03	-0.04
39	6	-0.06	0.00	0.00	-0.01	-0.01	0.01	0.00	-0.01	-0.03
40	6	-0.01	-0.13	0.00	-0.04	-0.02	0.01	-0.01	-0.03	0.00
41	1	-0.05	-0.17	-0.10	-0.03	-0.03	0.01	-0.01	-0.05	-0.02
42	1	-0.01	-0.14	0.04	-0.05	-0.03	0.01	-0.02	-0.04	0.01
43	1	-0.02	-0.17	0.07	-0.04	-0.01	0.02	-0.01	-0.03	0.01
44	6	-0.01	0.00	0.01	-0.05	0.02	0.05	-0.01	0.00	0.02
45	1	-0.01	0.00	0.01	-0.09	0.04	0.07	-0.04	0.01	0.04
46	1	-0.01	0.00	0.01	-0.06	-0.01	0.02	-0.02	-0.02	0.01
47	1	-0.01	0.00	0.01	-0.02	0.05	0.06	0.01	0.01	0.03
48	30	0.16	0.12	-0.04	-0.02	-0.01	0.01	0.01	0.00	-0.01
49	30	-0.01	-0.01	0.01	-0.02	0.01	0.03	0.01	-0.02	0.01
50	6	0.19	-0.05	-0.09	-0.03	-0.01	0.00	0.02	-0.01	-0.02
51	1	0.01	0.20	0.12	-0.04	-0.01	0.00	0.02	-0.01	-0.02
52	1	0.21	-0.30	0.12	-0.02	-0.01	-0.01	0.01	-0.01	-0.02
53	1	0.25	0.17	-0.39	-0.03	-0.01	-0.01	0.02	0.00	-0.01
54	8	-0.03	-0.01	-0.02	-0.01	-0.01	0.00	-0.01	-0.01	-0.03
55	6	0.05	-0.02	-0.06	0.00	0.00	0.00	-0.02	0.00	-0.03
56	1	0.07	-0.03	-0.07	-0.01	0.00	0.00	-0.02	0.00	-0.03
57	1	0.10	-0.03	-0.02	0.01	0.00	0.01	-0.03	0.00	-0.03
58	1	0.04	-0.03	-0.12	0.00	0.01	0.00	-0.02	0.00	-0.02
59	6	0.00	-0.02	0.00	0.01	0.01	-0.02	-0.03	0.01	0.01
60	6	0.00	-0.02	0.00	0.03	0.03	-0.03	-0.06	-0.02	0.02
61	6	0.00	-0.02	0.00	0.00	0.00	-0.03	-0.02	0.08	0.02
62	6	0.00	-0.02	0.00	0.04	0.04	-0.01	-0.07	-0.08	0.01
63	6	0.00	-0.01	0.00	0.03	0.04	-0.05	-0.07	0.02	0.04
64	6	0.00	-0.01	0.00	0.00	0.01	-0.05	-0.03	0.12	0.03
65	6	0.00	-0.02	0.00	-0.02	-0.02	-0.03	0.01	0.11	0.01
66	6	-0.01	-0.01	0.00	0.06	0.05	-0.02	-0.10	-0.11	0.02
67	1	0.00	-0.03	0.00	0.04	0.03	0.00	-0.07	-0.11	0.00
68	6	0.00	0.00	0.00	0.05	0.06	-0.05	-0.09	-0.01	0.05
69	6	0.00	0.00	0.00	0.02	0.03	-0.06	-0.05	0.09	0.04
70	6	0.00	0.00	0.00	-0.01	0.01	-0.07	-0.01	0.20	0.04
71	1	0.00	-0.03	0.00	-0.03	-0.02	-0.01	0.02	0.07	-0.01
72	6	0.00	-0.01	0.00	-0.04	-0.02	-0.04	0.02	0.18	0.01
73	6	-0.01	0.00	0.00	0.06	0.07	-0.04	-0.10	-0.08	0.04
74	1	-0.01	-0.01	0.00	0.07	0.06	-0.01	-0.11	-0.16	0.01
75	1	-0.01	0.01	0.00	0.06	0.07	-0.07	-0.10	0.02	0.06
76	1	0.00	0.01	0.00	0.02	0.04	-0.08	-0.06	0.12	0.06
77	6	0.00	0.00	0.00	-0.03	-0.01	-0.06	0.01	0.23	0.03
78	1	0.00	0.01	0.00	-0.01	0.02	-0.08	-0.02	0.23	0.06
79	1	0.00	-0.02	0.00	-0.05	-0.04	-0.03	0.04	0.21	0.01
80	1	-0.01	0.01	0.00	0.08	0.08	-0.05	-0.12	-0.10	0.04
81	1	0.00	0.00	0.00	-0.04	-0.02	-0.07	0.02	0.29	0.04
82	6	-0.01	0.00	0.01	0.01	0.02	-0.01	0.03	0.02	0.02
83	6	-0.01	0.00	0.00	0.01	0.03	-0.09	0.01	0.04	0.02
84	6	-0.01	0.00	0.01	0.02	0.01	0.04	0.05	0.02	0.03
85	6	-0.01	0.00	0.00	0.01	0.04	-0.15	-0.01	0.04	0.01
86	6	-0.01	0.00	0.00	0.01	0.04	-0.12	0.03	0.07	0.03

87	6	-0.01	0.00	0.00	0.02	0.02	0.01	0.07	0.04	0.04
88	6	-0.01	0.00	0.02	0.02	0.00	0.11	0.07	0.00	0.04
89	6	-0.01	0.00	0.00	0.01	0.05	-0.23	-0.03	0.07	0.00
90	1	-0.01	0.00	0.00	0.01	0.03	-0.12	-0.02	0.03	0.00
91	6	-0.01	0.00	-0.01	0.01	0.05	-0.21	0.01	0.09	0.02
92	6	-0.01	0.00	-0.01	0.02	0.03	-0.06	0.05	0.06	0.04
93	6	-0.01	0.00	0.00	0.02	0.01	0.07	0.09	0.04	0.06
94	1	-0.02	-0.01	0.04	0.01	-0.01	0.12	0.06	-0.02	0.03
95	6	-0.01	0.00	0.02	0.02	-0.01	0.16	0.09	-0.01	0.05
96	6	-0.01	0.00	-0.01	0.01	0.06	-0.26	-0.01	0.09	0.01
97	1	0.00	0.00	0.00	0.01	0.06	-0.27	-0.05	0.07	-0.01
98	1	-0.01	0.00	-0.01	0.01	0.06	-0.23	0.02	0.11	0.03
99	1	-0.01	0.00	-0.01	0.02	0.04	-0.08	0.06	0.08	0.05
100	6	-0.01	0.00	0.01	0.02	0.00	0.14	0.11	0.02	0.06
101	1	-0.01	0.00	-0.01	0.02	0.02	0.05	0.10	0.06	0.06
102	1	-0.01	0.00	0.04	0.02	-0.02	0.22	0.10	-0.02	0.05
103	1	-0.01	0.00	-0.01	0.01	0.07	-0.32	-0.02	0.11	0.01
104	1	-0.01	0.00	0.00	0.03	-0.01	0.18	0.13	0.02	0.07
105	6	-0.10	0.01	0.03	-0.03	-0.02	0.02	0.00	-0.04	-0.05
106	6	0.00	-0.01	-0.01	-0.03	-0.02	0.01	-0.02	-0.03	-0.04
107	6	-0.11	0.04	0.02	-0.04	-0.03	0.03	0.02	-0.05	-0.06
108	6	0.07	-0.01	-0.04	-0.04	-0.02	0.01	-0.02	-0.04	-0.05
109	1	0.01	-0.04	-0.02	-0.02	-0.01	0.00	-0.03	-0.02	-0.04
110	6	-0.02	0.04	-0.01	-0.05	-0.03	0.03	0.01	-0.06	-0.06
111	1	-0.18	0.05	0.05	-0.04	-0.03	0.04	0.03	-0.06	-0.06
112	6	0.06	0.02	-0.04	-0.06	-0.03	0.02	-0.01	-0.06	-0.06
113	1	0.14	-0.02	-0.07	-0.04	-0.02	0.00	-0.04	-0.03	-0.05
114	1	-0.03	0.07	-0.01	-0.06	-0.04	0.04	0.03	-0.07	-0.07
115	1	0.12	0.02	-0.06	-0.07	-0.03	0.02	-0.01	-0.06	-0.07

Scanned images of ^{1}H-, ^{13}C-NMR of new compounds



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MeO
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6.829
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6.730
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3.762
2.344
2.313
1.745
1.637
1.423
1.396
1.371
1.285
1.261
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2.05
4.09
2.00
1.76
1.94
5.70
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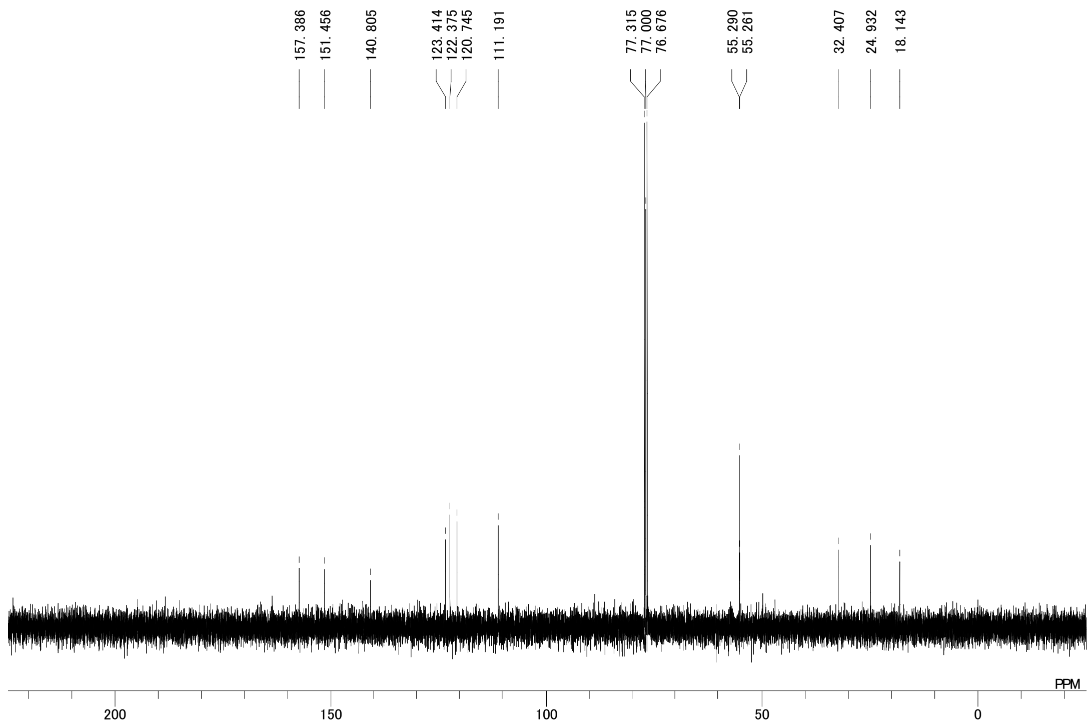
10.0
7.5
5.0
2.5
0.0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18.143
PPM
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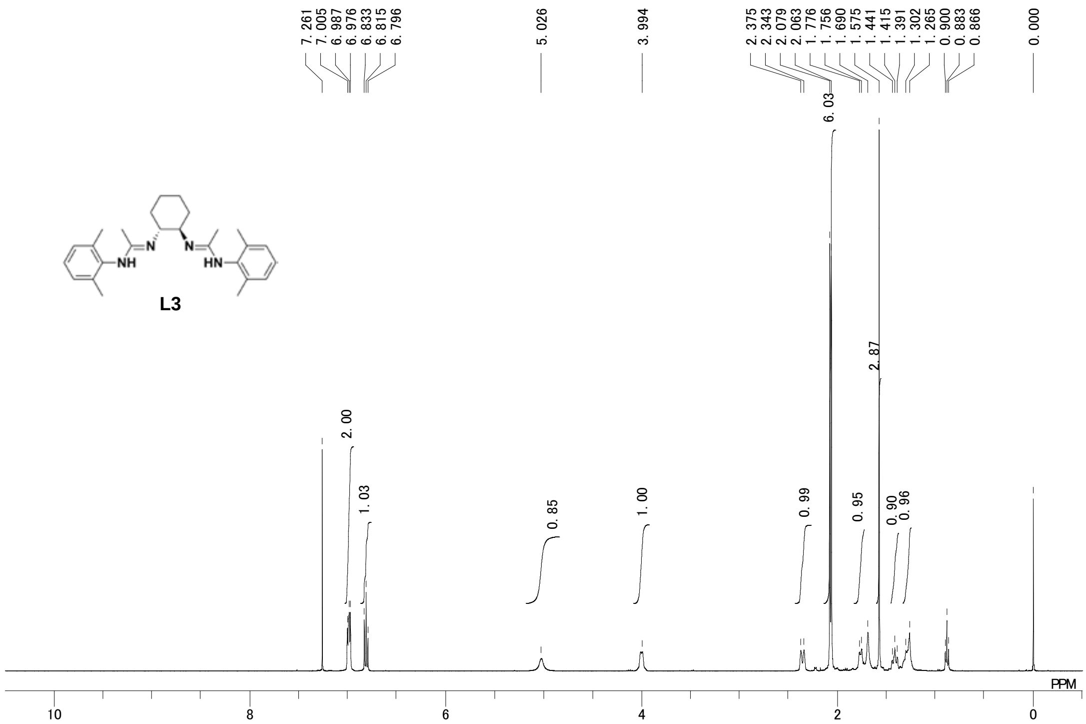
150
100
50
0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2.063
1.776
1.756
1.690
1.575
1.441
1.415
1.391
1.302
1.265
0.900
0.883
0.866
0.000
NH
N
N
HN
L3
6.03
2.87
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1.00
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PPM
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8
6
4
2
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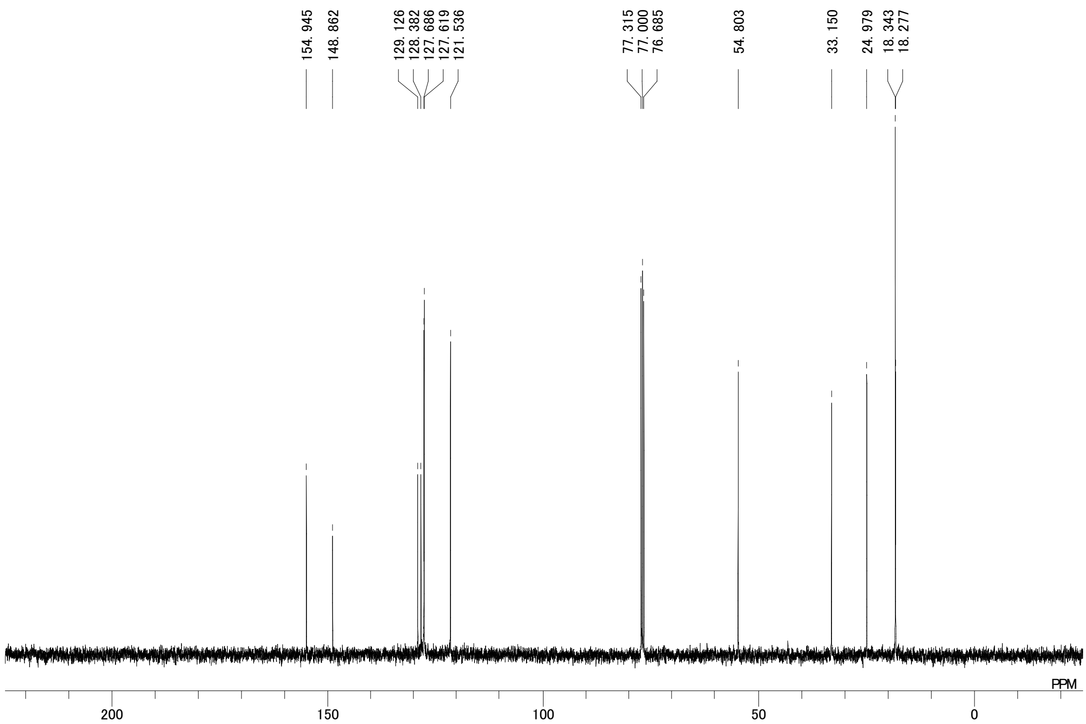
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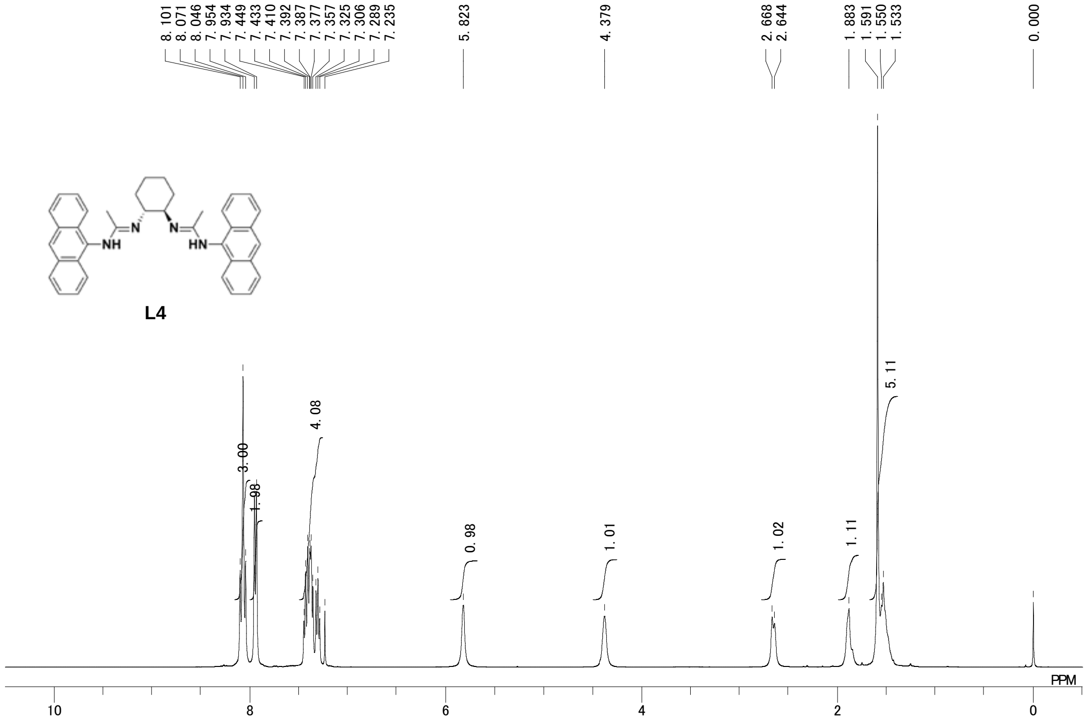
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7.289
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4.379
2.668
2.644
1.883
1.591
1.550
1.533
0.000
L4
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PPM
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6
4
2
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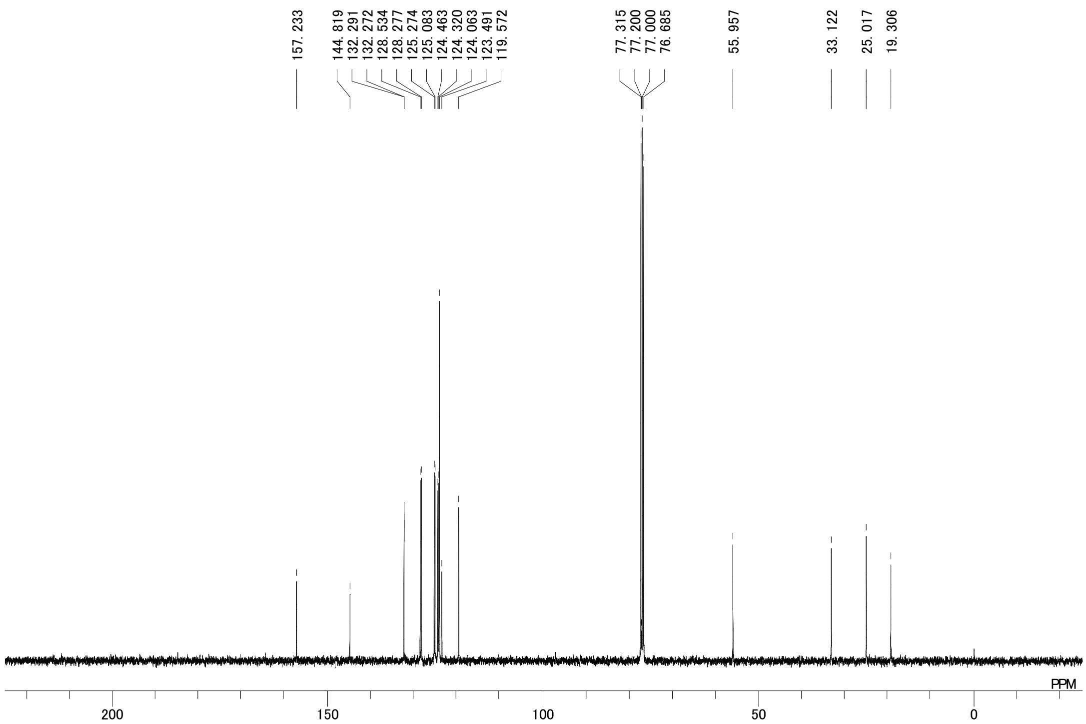
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PPM
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50
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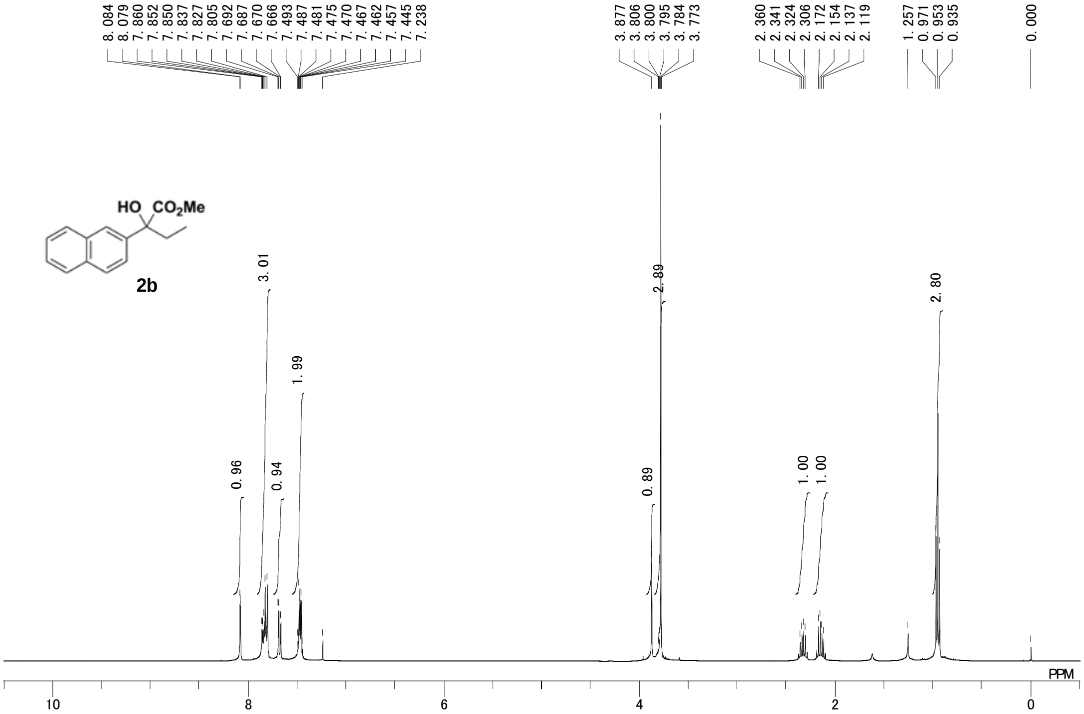
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3.877 3.806 3.800 3.795 3.784 3.773
2.360 2.341 2.324 2.306 2.172 2.154 2.137 2.119
1.257 0.971 0.953 0.935
0.000
HO CO2Me
2b
0.96
3.01
0.94
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0.89
2.89
1.00
1.00
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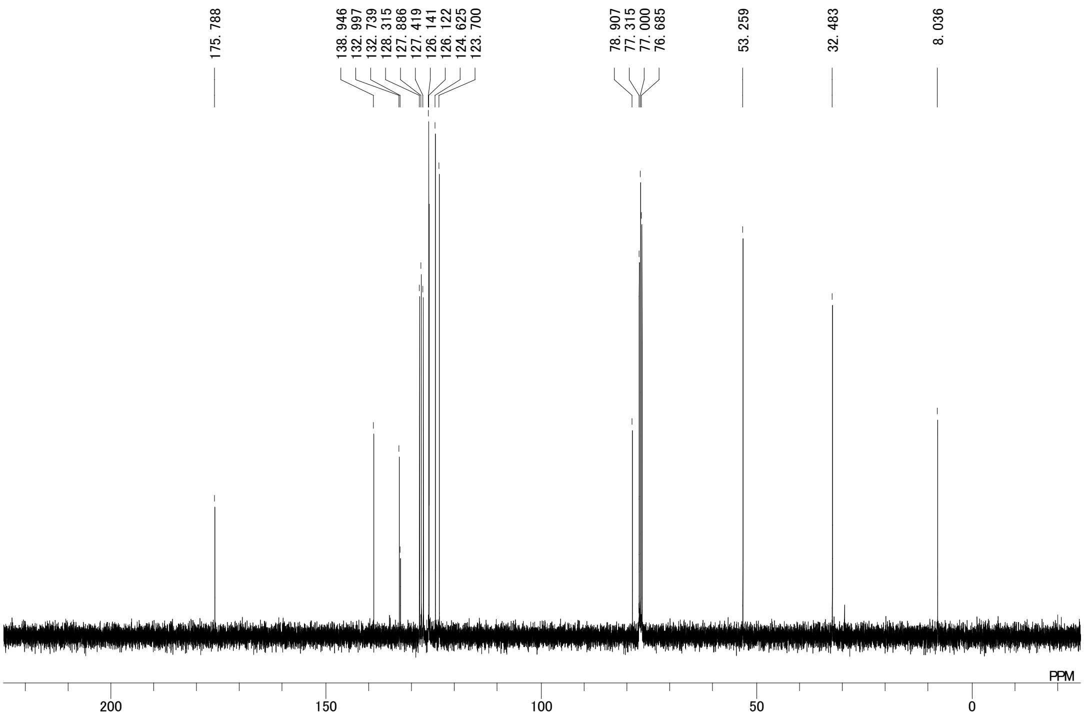
PPM
10
8
6
4
2
0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78.907 77.315 77.000 76.685
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150
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50
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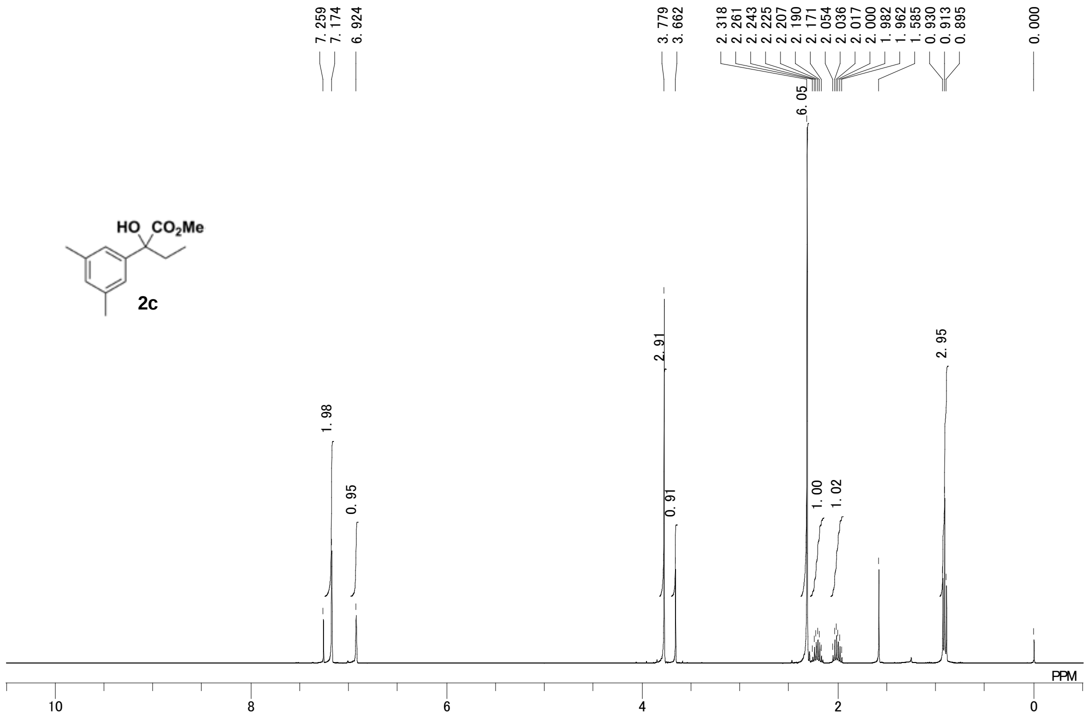
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2.190
2.171
2.054
2.036
2.017
2.000
1.982
1.962
1.585
0.930
0.913
0.895
0.000
6.05
2.91
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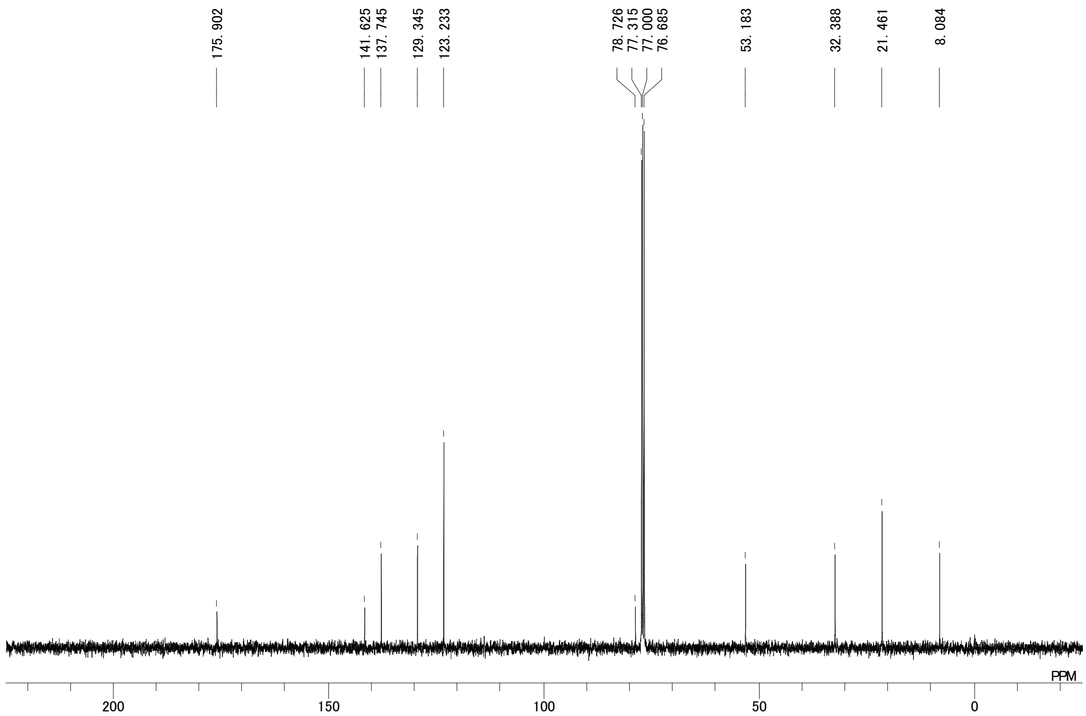
1.98
0.95
0.91
1.00
1.02
PPM
10
8
6
4
2
0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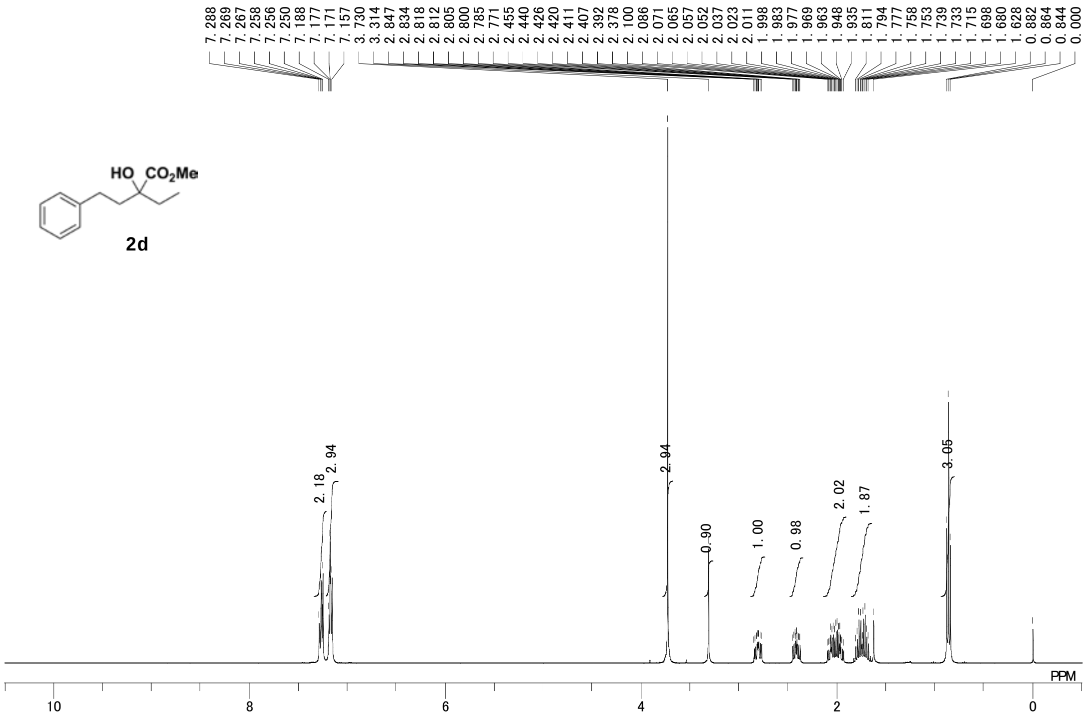
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2.818
2.812
2.805
2.800
2.785
2.771
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2.440
2.426
2.420
2.411
2.407
2.392
2.378
2.100
2.086
2.071
2.065
2.057
2.052
2.037
2.023
2.011
1.998
1.983
1.977
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1.794
1.777
1.758
1.753
1.739
1.733
1.715
1.698
1.680
1.628
0.882
0.864
0.844
0.000
HO
CO2Me
2d
2.18
2.94
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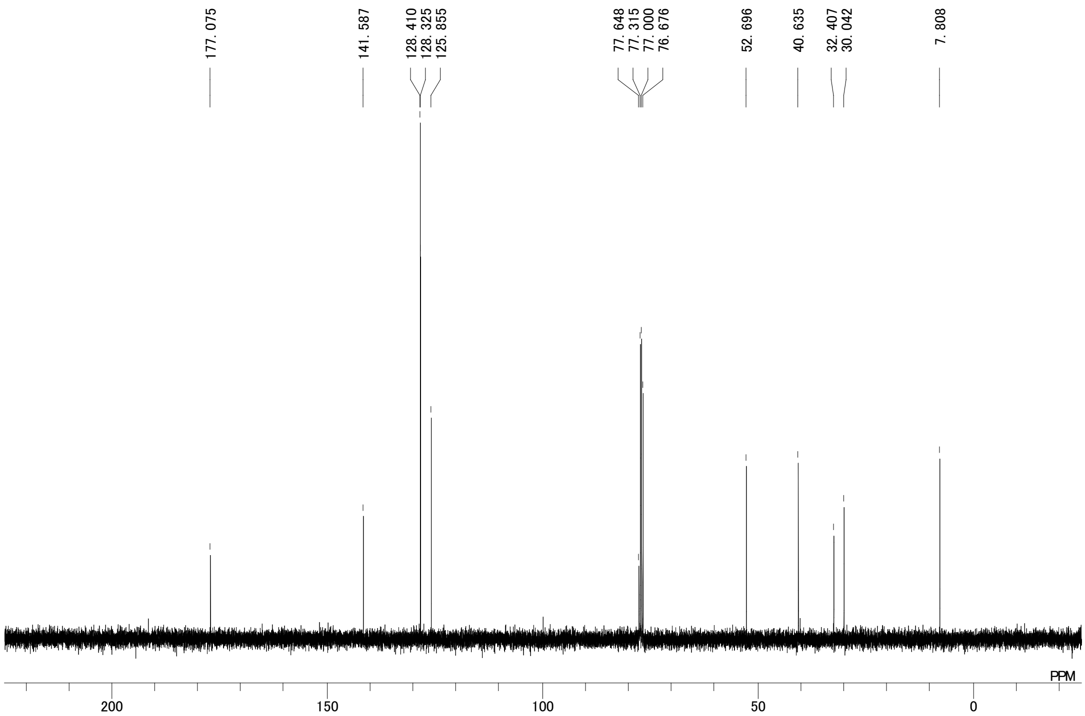
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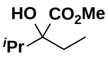

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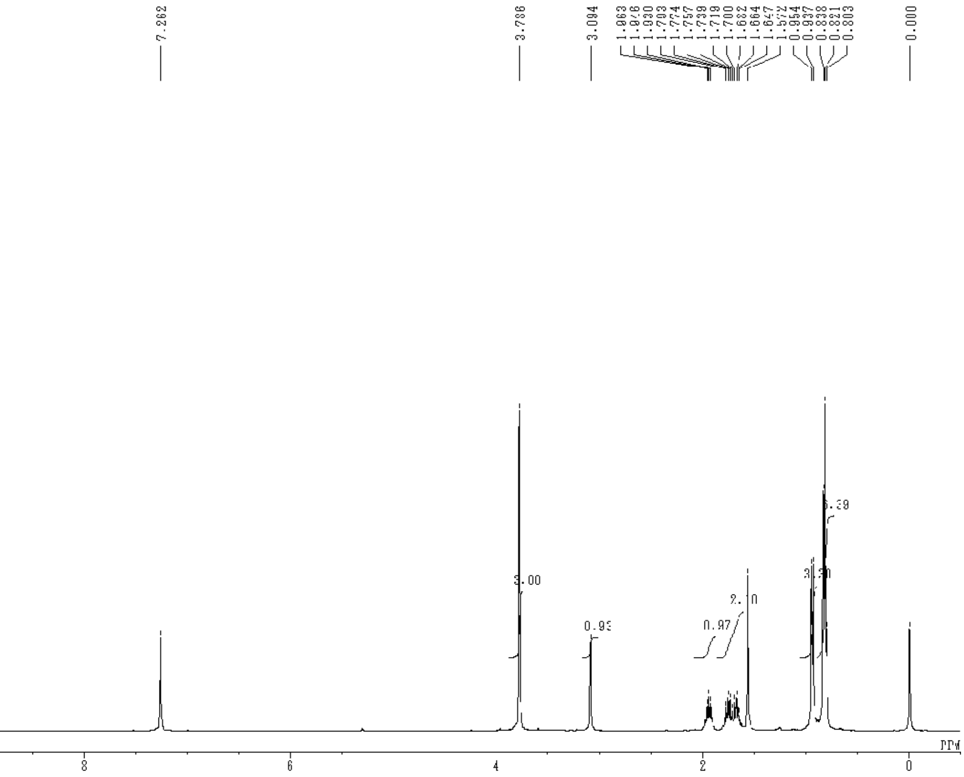
CO2Me
iPr

2e



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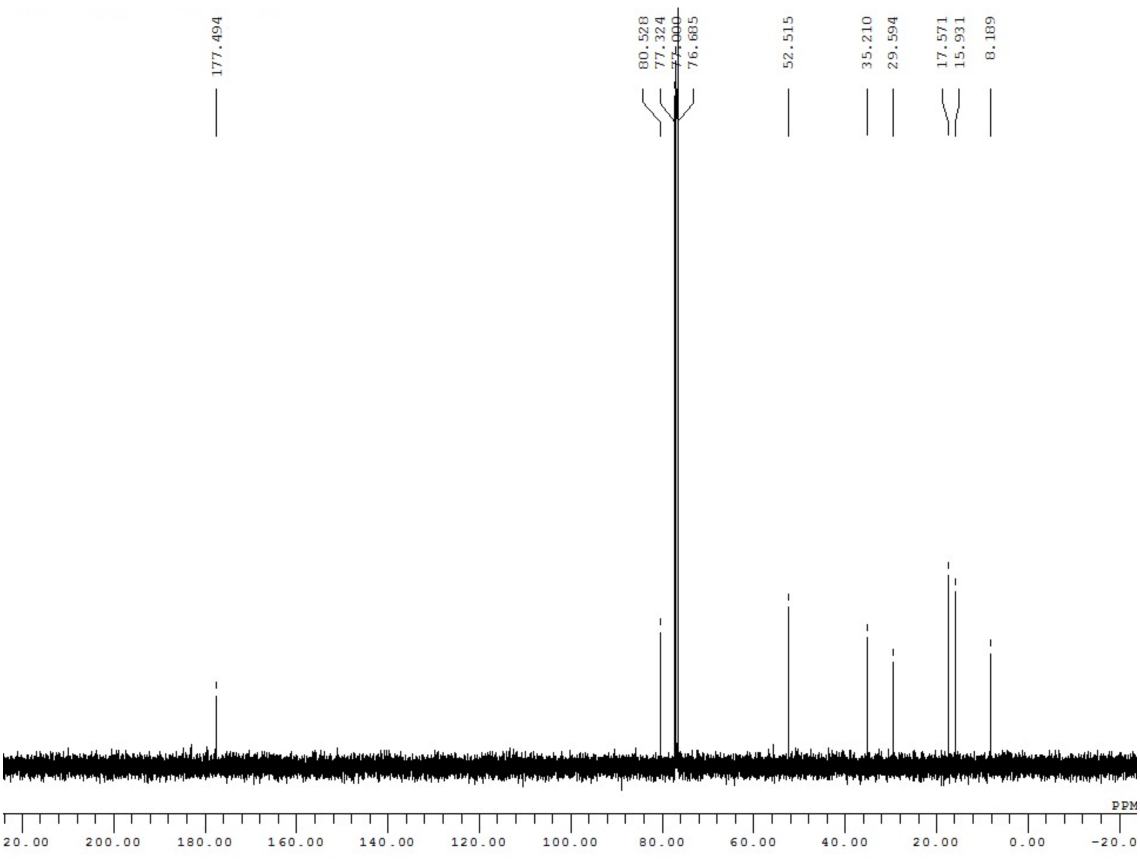
0.000



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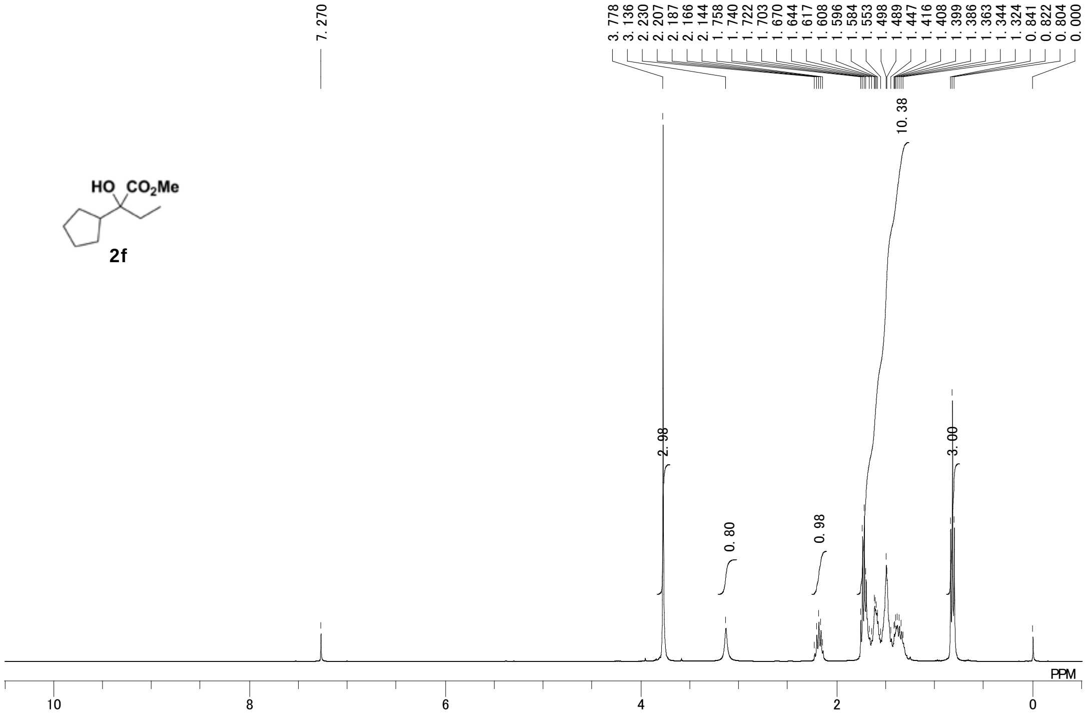
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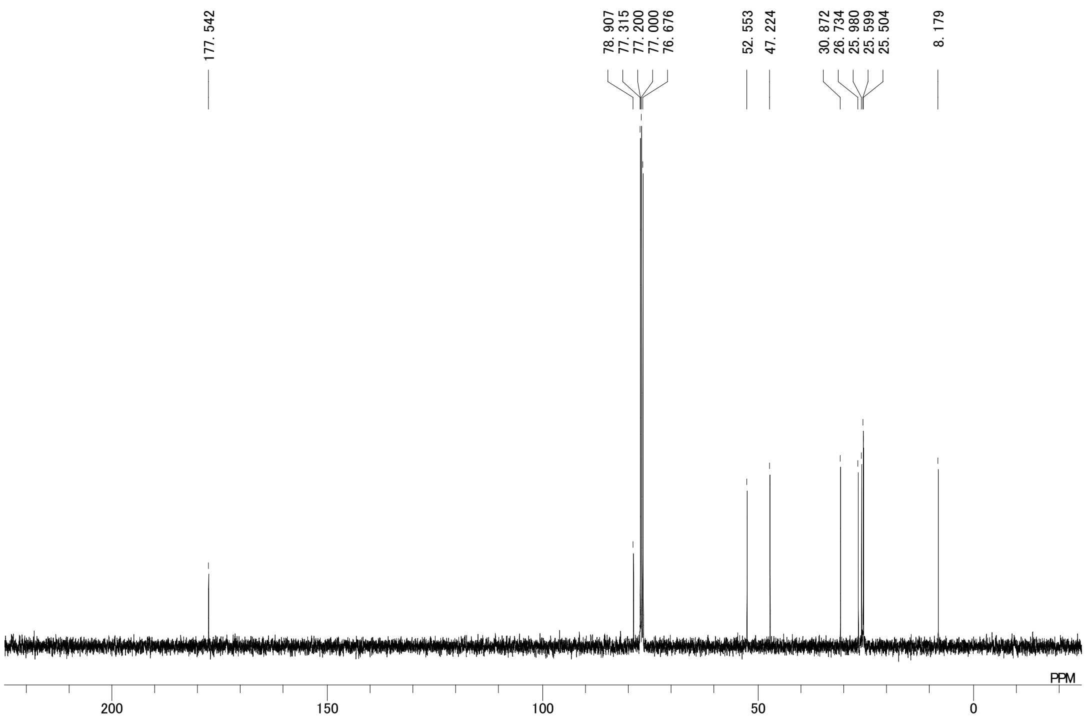
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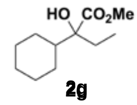
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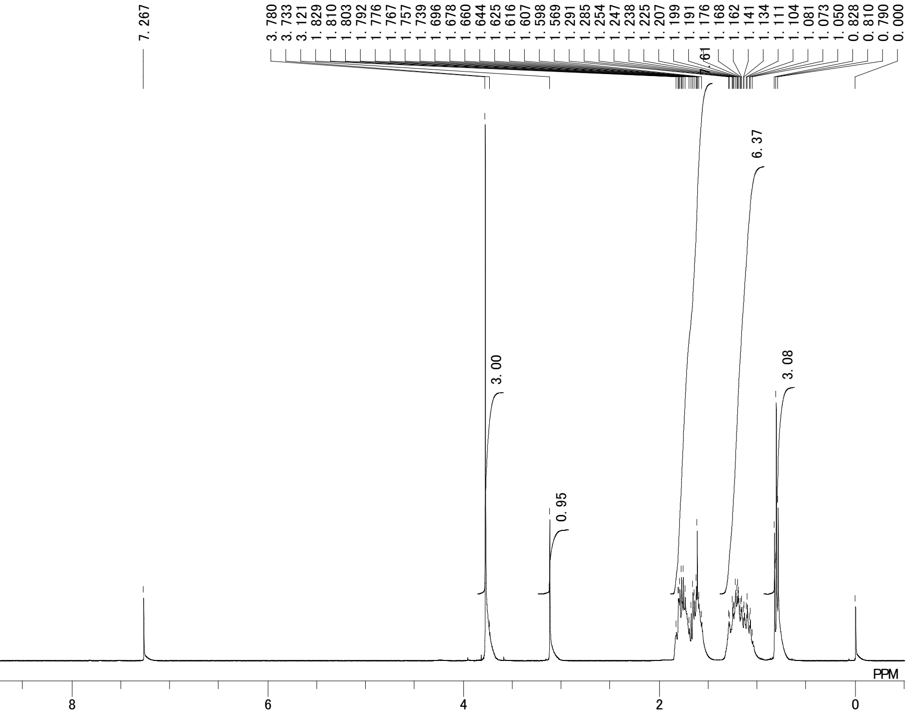
CO2Me
2g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1.696
1.678
1.660
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1.616
1.607
1.598
1.569
1.291
1.285
1.254
1.247
1.238
1.225
1.207
1.199
1.191
1.176
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1.162
1.141
1.134
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PPM
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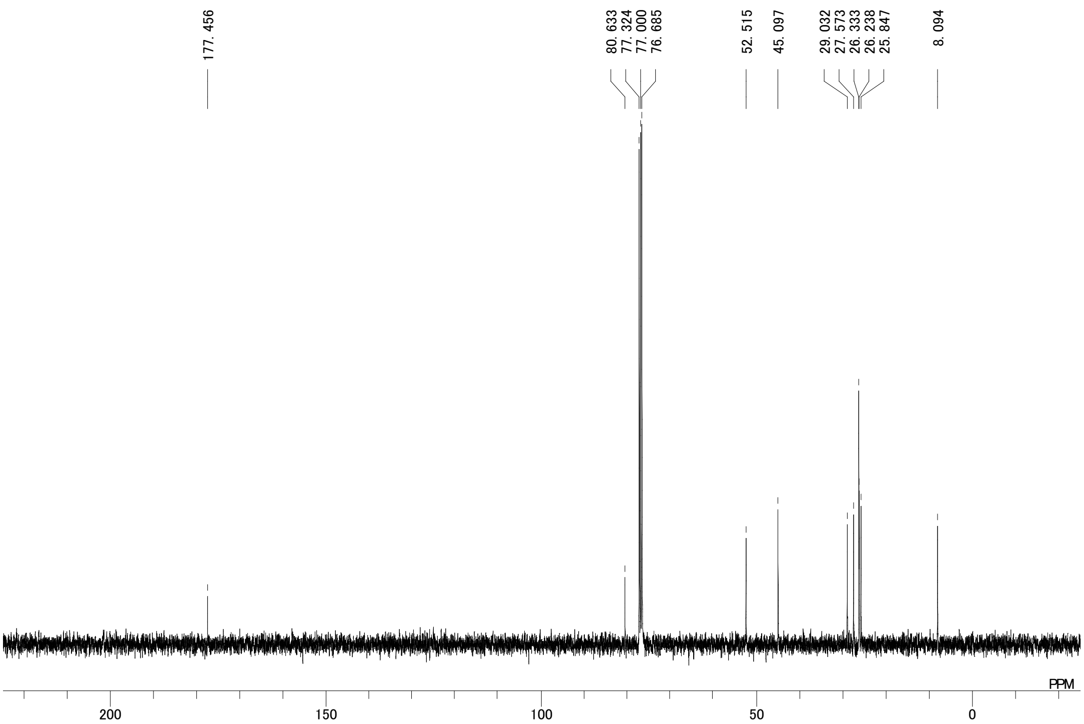
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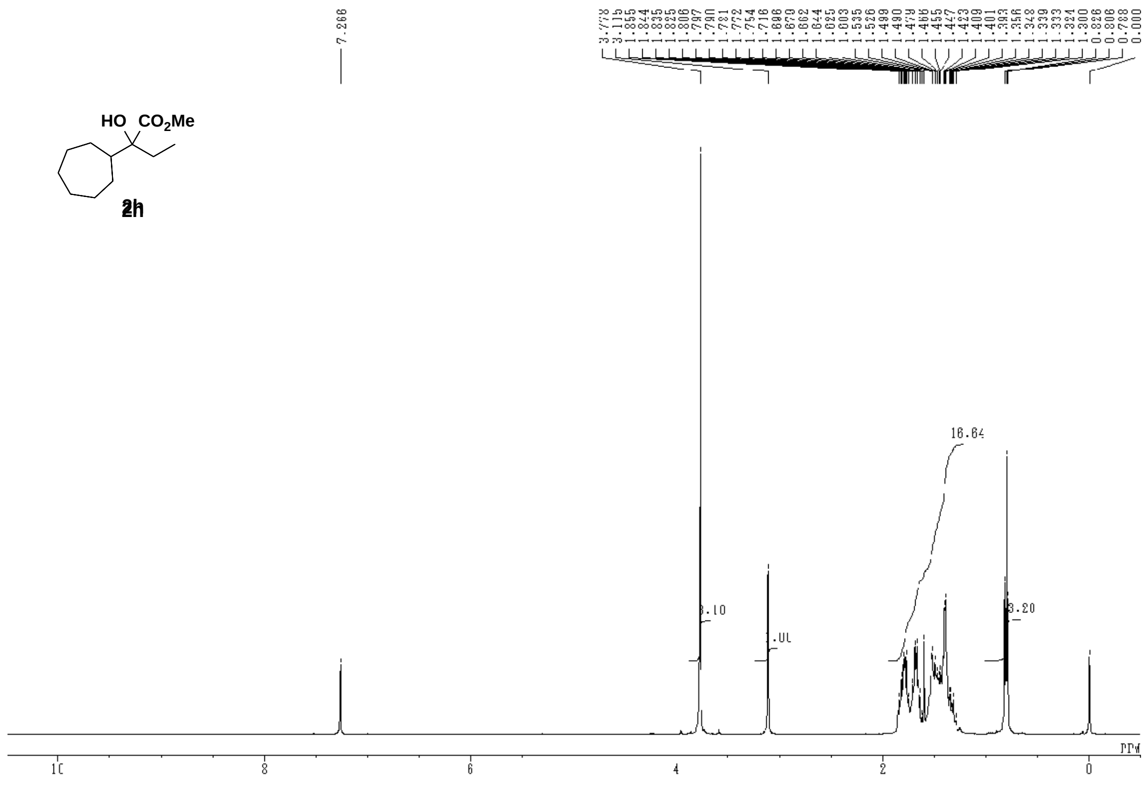
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8
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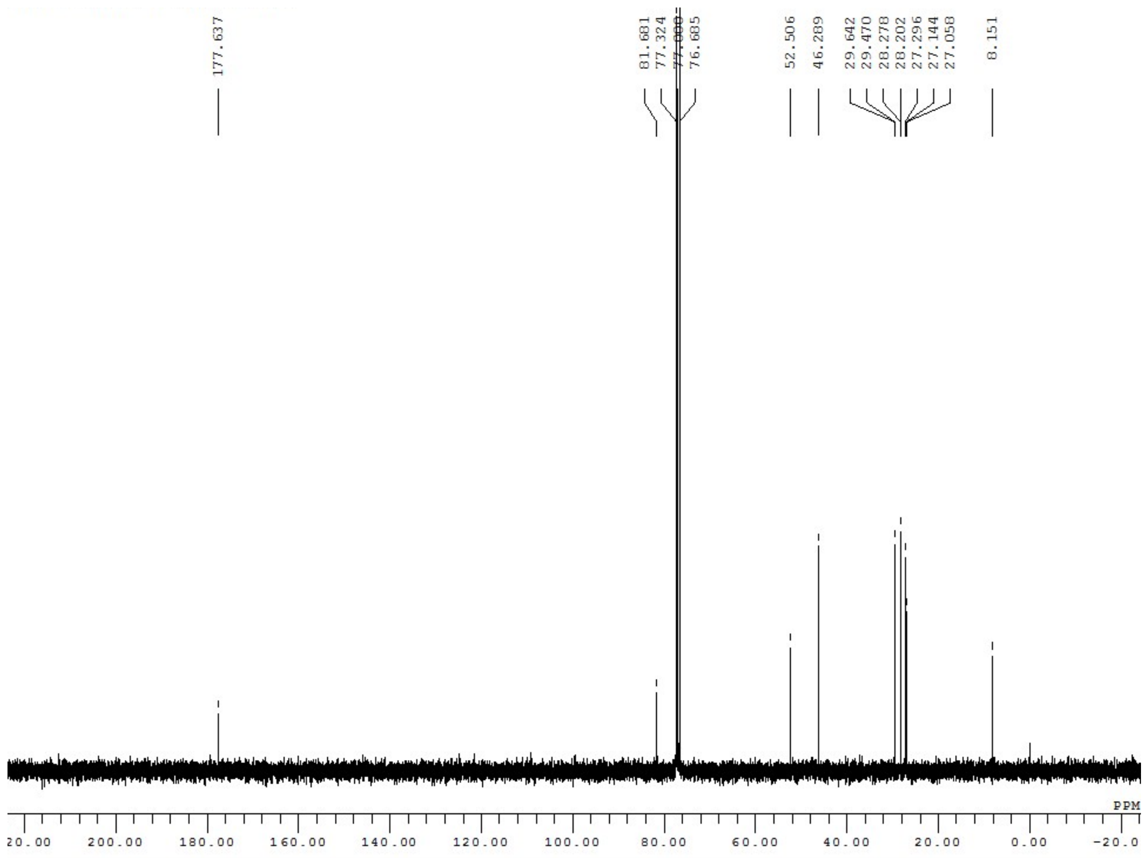
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28.202
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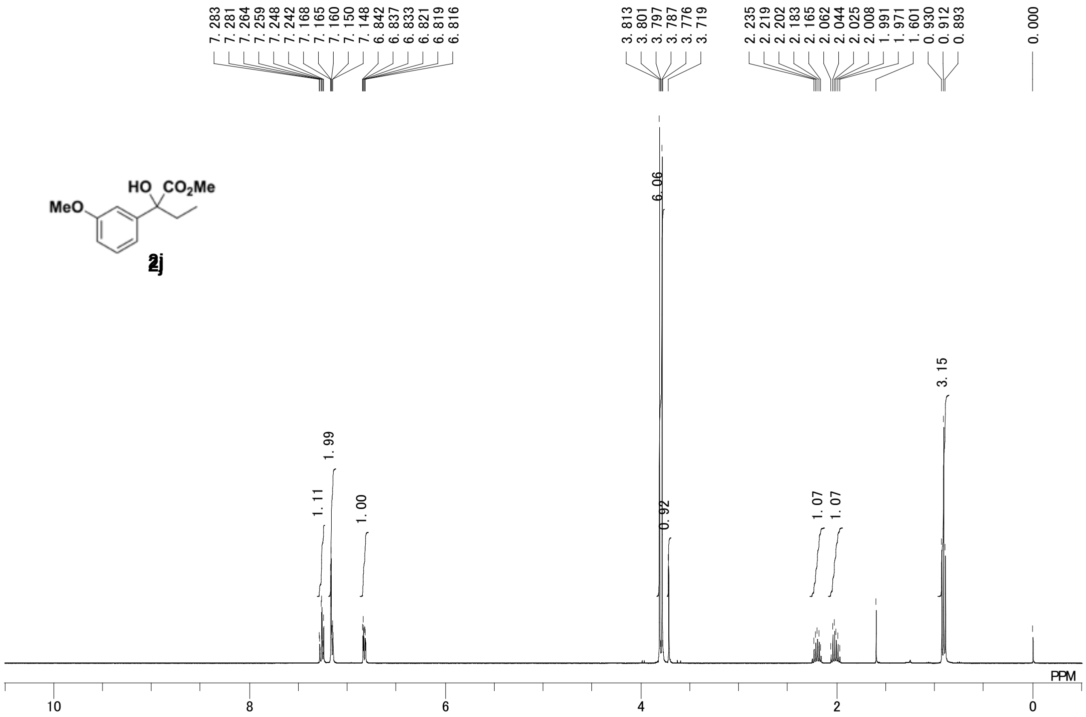
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2.235 2.219 2.202 2.183 2.165 2.062 2.044 2.025 2.008 1.991 1.971 1.601 0.930 0.912 0.893
0.000
MeO
HO CO2Me
2j
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1.00
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PPM
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8
6
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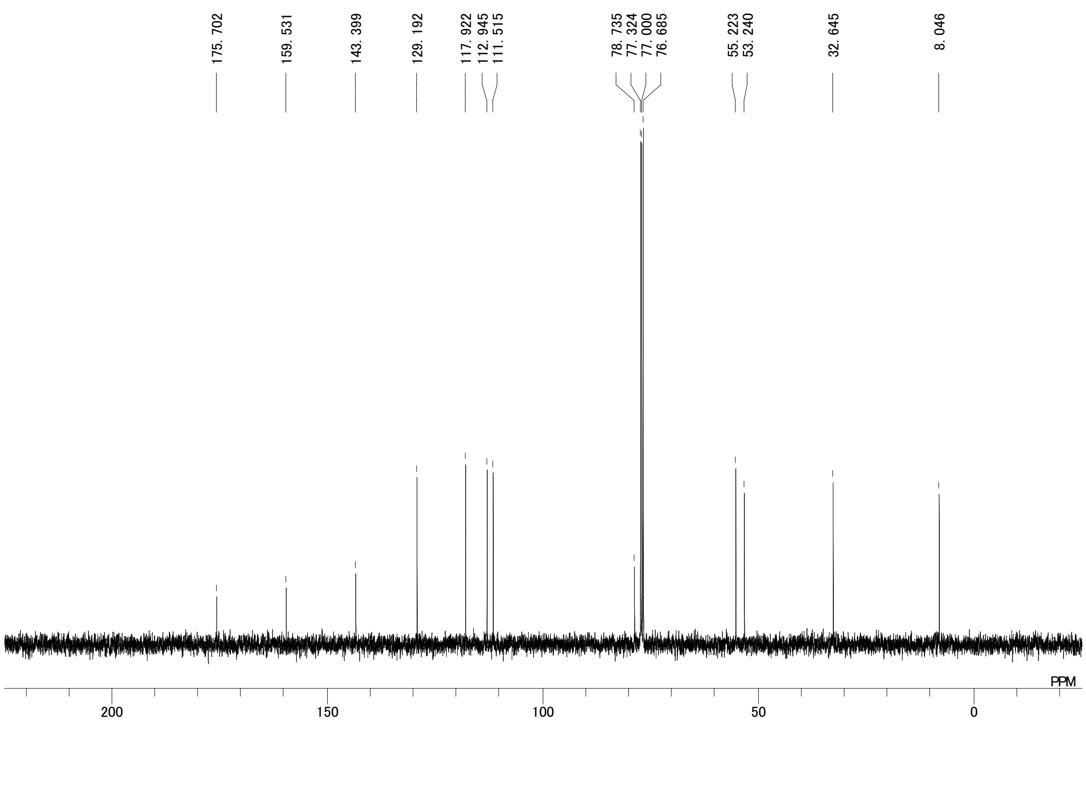
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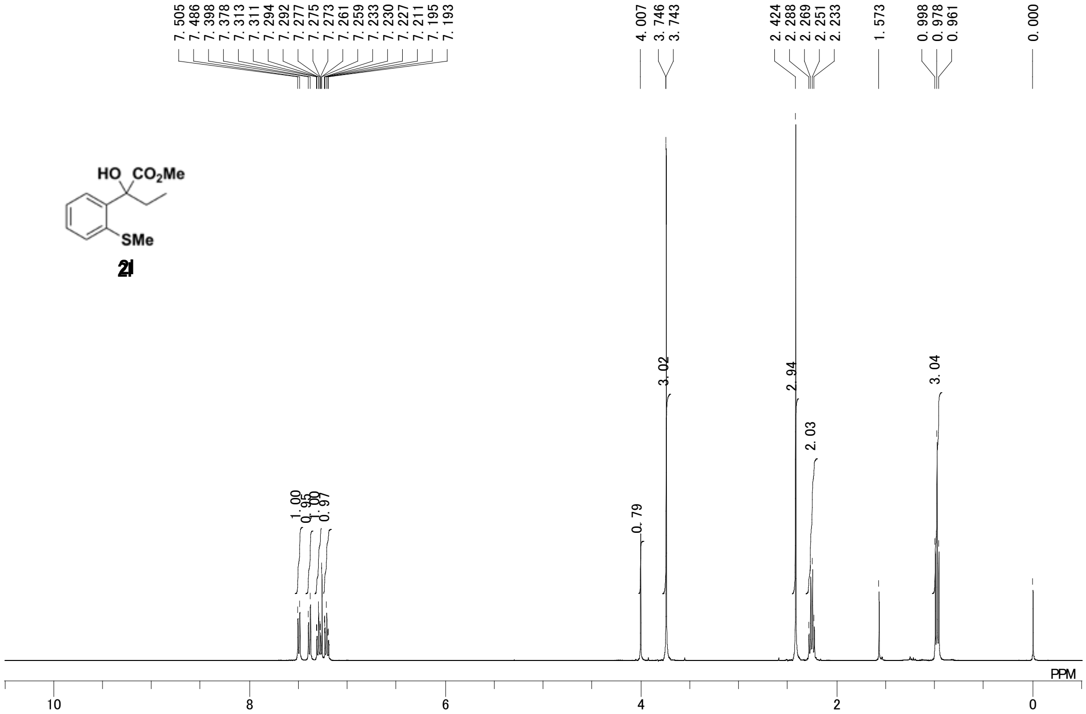
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7.273
7.261
7.259
7.233
7.230
7.227
7.211
7.195
7.193
4.007
3.746
3.743
2.424
2.288
2.269
2.251
2.233
1.573
0.998
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2.03
3.04
PPM
10
8
6
4
2
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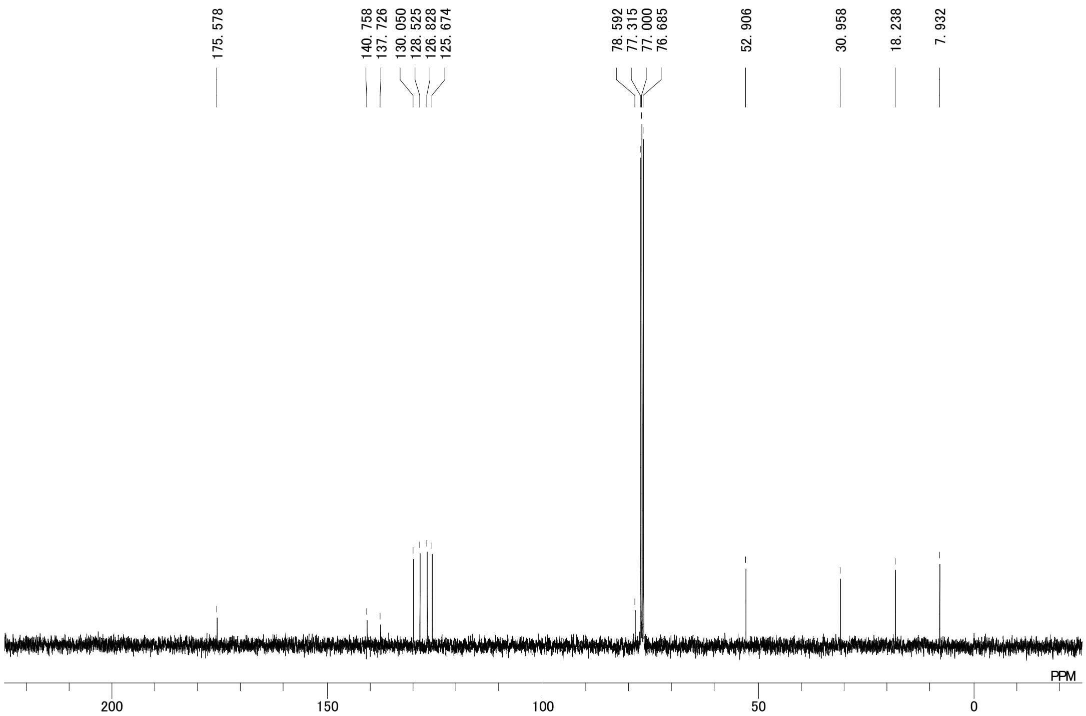
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PPM
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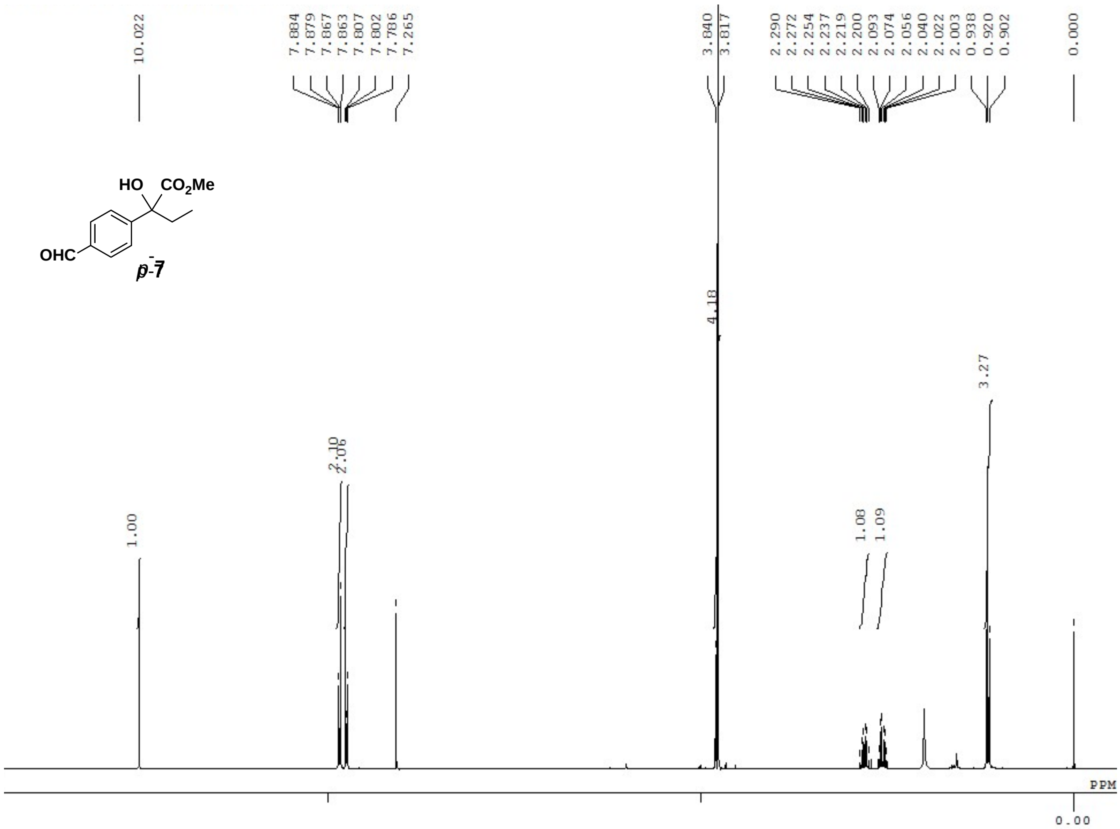
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p-7
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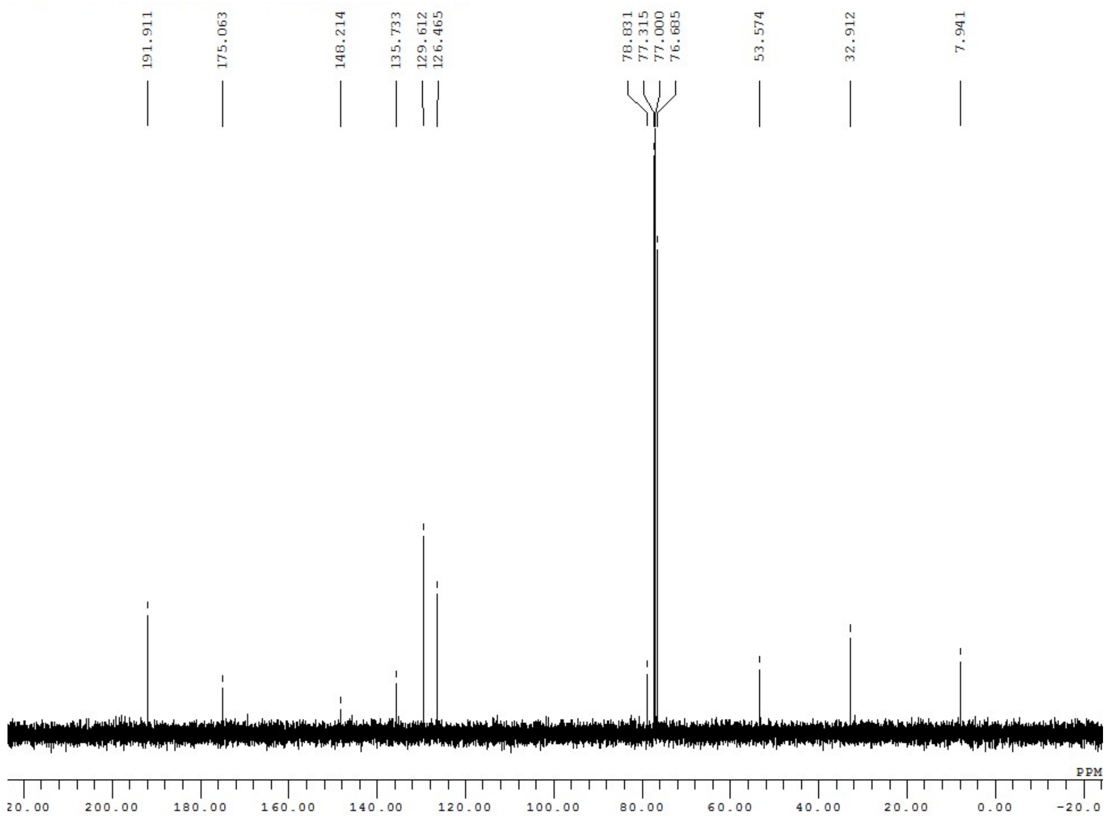
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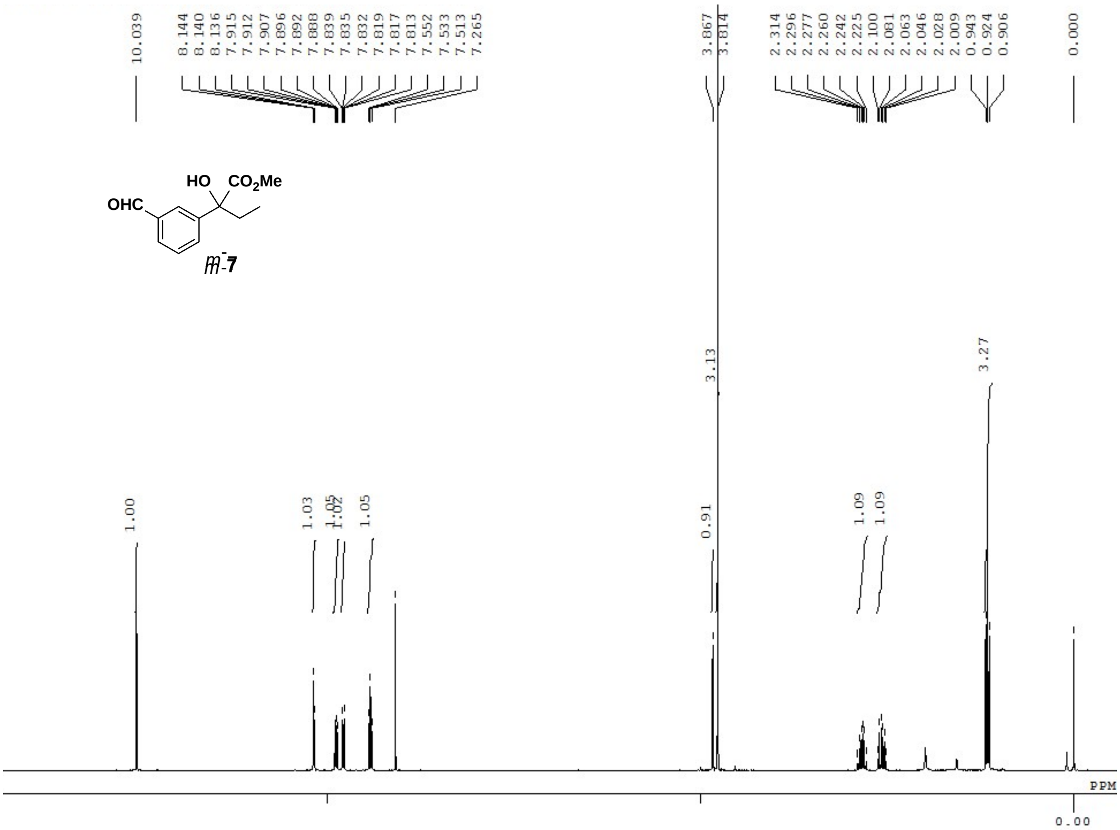
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3.867 3.814
2.314 2.296 2.277 2.260 2.242 2.225 2.100 2.081 2.063 2.046 2.028 2.009 0.943 0.924 0.906
0.000
HO CO2Me
OHC
m-7
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0.91
1.09
1.09
PPM
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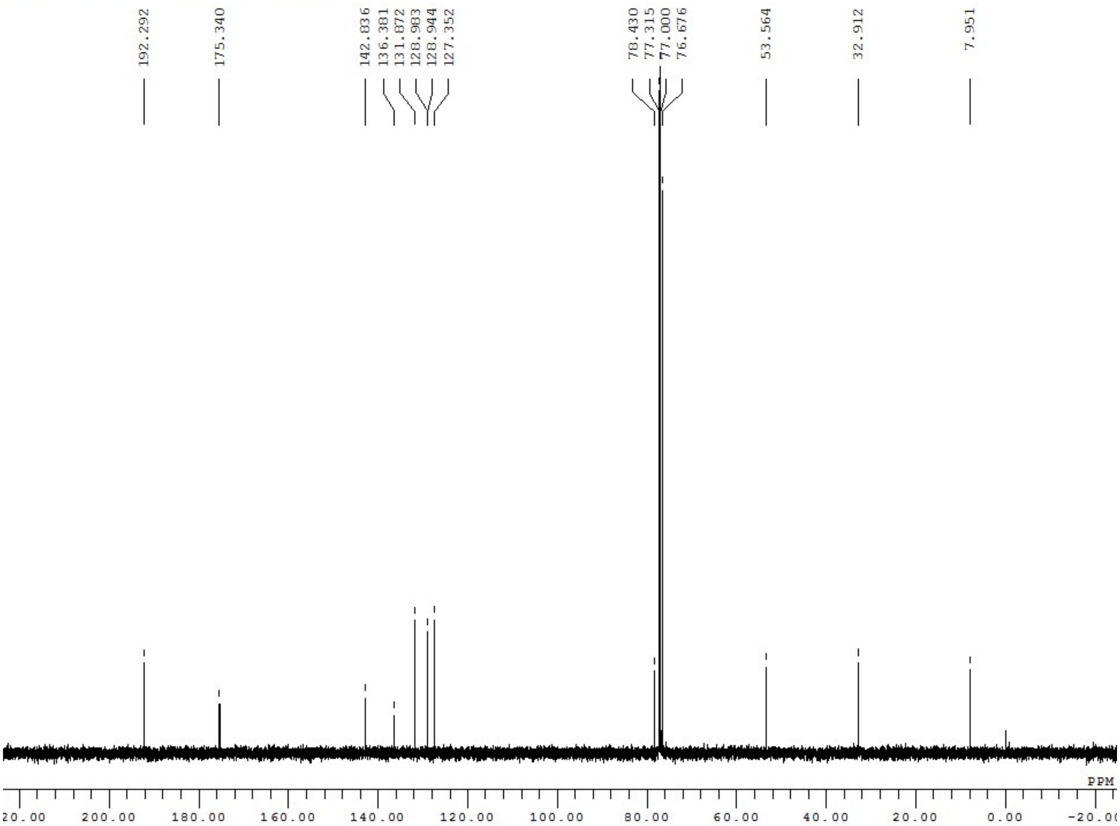
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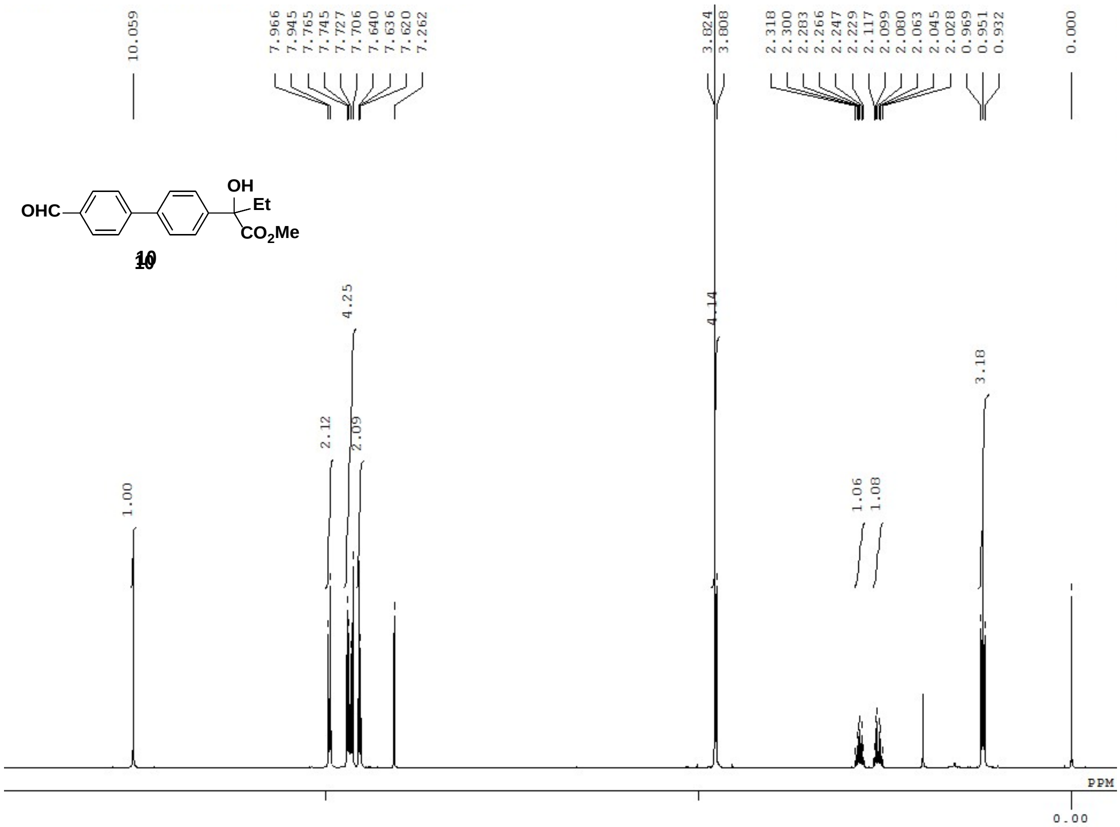
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2.318 2.300 2.283 2.266 2.247 2.229 2.117 2.099 2.080 2.063 2.045 2.028 0.969 0.951 0.932
0.000
OH
Et
OHC
CO2Me
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1.06
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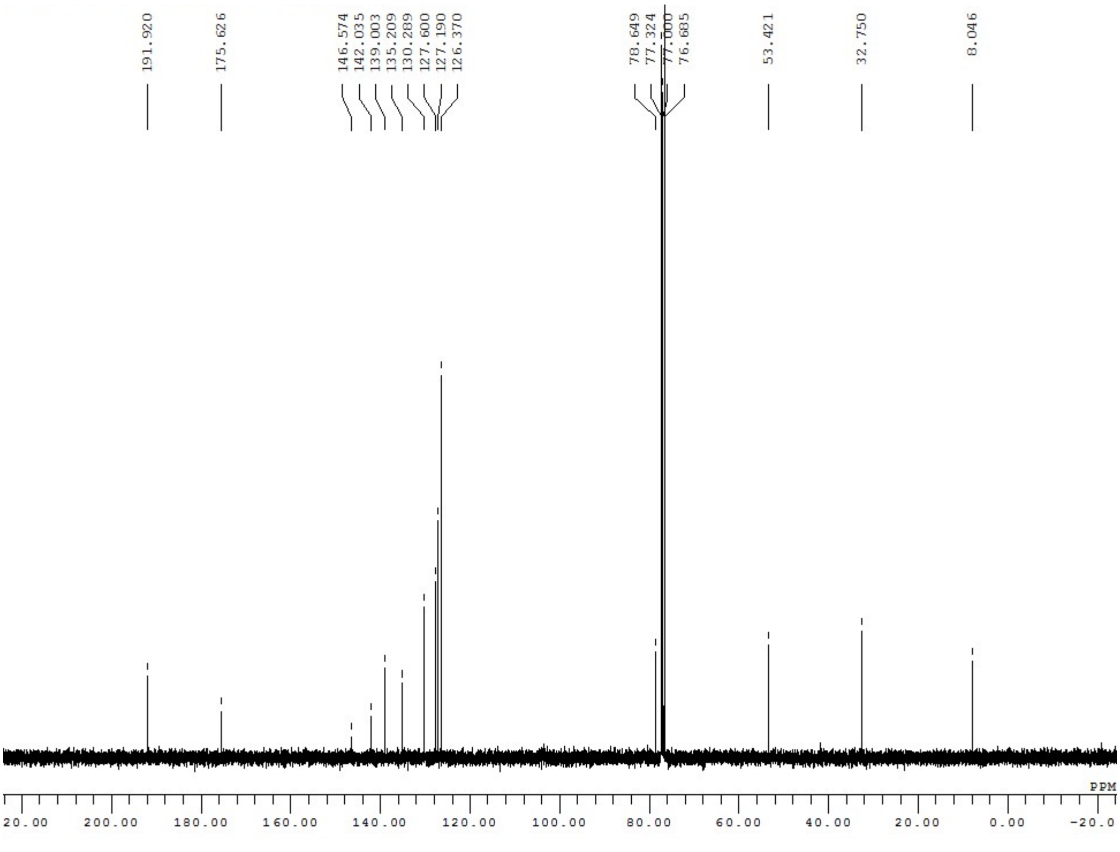
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