Supporting Information

Stereoinversion in Pd-Catalyzed Allylic Substitution Induced by Modification of Olefinic Moiety in Chiral Phosphine-Acrylamide Ligands

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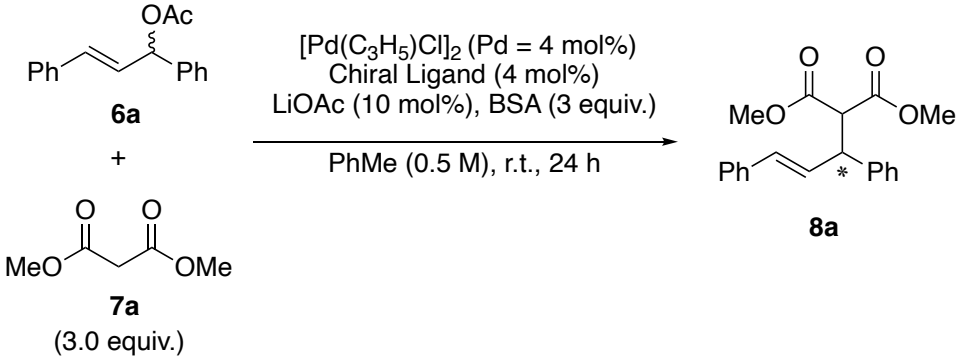
1. General information

Melting point was measured by an AS ONE micromelting point apparatus and are uncorrected. NMR spectra were recorded with 400 (Bruker AVANCE III-400M) and 500 MHz (Bruker AVANCE NEO 500) spectrometers in $CDCl_3$ as a solvent at room temperature unless otherwise noted. Chemical shifts (δ) are given in ppm relative to TMS (^1H), external 85% H_3PO_4 (^{31}P), or residual $CHCl_3$ (^{13}C) as a reference. All ^{13}C and ^{31}P NMR spectra recorded with the use of broadband proton decoupling. The coupling constants *J* are given in Hz, and the peak patterns are indicated as follows: s, singlet; d, doublet, t, triplet; q, quartet; m, multiplet. Optical rotation was measured on JASCO P-2100. HRMS was measured with an orbitrap mass spectrometer (Thermo Fisher Exactive). The ee value was determined by HPLC (JASCO GULLIVER 900 or 2000 system) equipped with a chiral column. Unless otherwise noted, all reagents were used without further purification. A high-power LED light source (Asahi spectra) CL-1501 was used for an irradiation source. Single-crystal X-ray data were collected on a Bruker AXS D8 VENTURE CCD using Cu Kα radiation. The structure was solved by the direct method of full matrix least-squares using SHELXS-97. All crystals for single-crystal X-ray diffraction analysis were obtained by slow evaporation in chloroform-hexane at room temperature.

2. Palladium-catalyzed allylic alkylation of dimethylmalonate with (*S*,a*S*)-ligands

We summarized the results of the palladium-catalyzed allylic alkylation of 1,3-diphenyl-2-propenyl acetate (**6a**) with dimethyl malonate (**7a**) using (*S*,a*S*)-ligands in **Table S1**. Although the yields and enantioselectivity varied, the product configuration trends were consistent with those observed using (*S*,a*R*)-ligands in **Table 1**, except for ligand (*S*,a*S*)-**4c**.

Table S1. Palladium-catalyzed asymmetric allylic alkylation with dimethyl malonate with (*S*,a*S*)-3 and 4a-f.[a]



Entry	Chiral ligand	Yield (%)[b]	ee (%)[c]
1	(*S*,a*S*)-**3**	62	71 (*S*)
2	(*S*,a*S*)-**4a**	86	58 (*S*)
3	(*S*,a*S*)-**4b**	37	81 (*S*)
4	(*S*,a*S*)-**4c**	61	74 (*S*)
5	(*S*,a*S*)-**4d**	72	47 (*R*)
6	(*S*,a*S*)-**4e**	15	67 (*R*)
7	(*S*,a*S*)-**4f**	82	48 (*R*)

[a] The reactions were carried out on a 0.2 mmol scale of 1,3-diphenyl-2-propenyl acetate (1.0 equiv.) in PhMe (0.5 M, 0.4 mL) at room temperature with 3.0 equiv. of dimethyl malonate and BSA in the presence of 10 mol% of LiOAc and chiral ligand (4 mol%) and $[Pd(\eta^3\text{-}C_3H_5)Cl]_2$ (2 mol%; Pd = 4 mol%).

[b] Isolated yield.

[c] Determined by HPLC analysis using a chiral column.

3. Experimental Section

3-1. Experimental Procedures and Product Characterization

Preparation of Amide (*S*,a*S*)-4a and (*S*,a*R*)-4a.

To the solution of aminophosphine (*S*)-**5** (158 mg, 0.4 mmol) in THF (1.5 mL) was added pyridine (0.1 mL, 1.2 mmol), DMAP (19.6 mg, 0.16 mmol) and *trans*-4-methoxycinnamoyl chloride (157 mg, 0.8 mmol) at room temperature. The reaction mixture was stirred at 60 °C (using an oil bath). After 24 h, the reaction mixture was diluted with ether and sat. $NaHCO_3$ aq. The organic layer was washed with brine and dried over $MgSO_4$. The filtrate was concentrated with a rotary evaporator, and the residue was purified by column chromatography (elution with *n*-hexane/ether = 4/1).

(*S*,a*S*)-*N*-(2-(Diphenylphosphanyl)-6-methylphenyl)-(*E*)-3-(4-methoxyphenyl)-*N*-(1-phenylethyl)acrylamide ((*S*,a*S*)-4a) (dr = >20:1). 24% yield (52.8 mg, 0.10 mmol) as a white solid; $[\alpha]^{20}_D$ = +384 (*c* 0.78, $CHCl_3$); mp 186-188 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46-7.42 (m, 2H), 7.37-7.13 (m, 13H), 7.05-7.01 (m, 4H), 6.90 (d, *J* = 8.8 Hz, 2H), 6.72 (d, *J* = 8.8 Hz, 2H), 5.36 (d, *J* = 15.5 Hz, 1H), 5.09 (q, *J* = 7.1 Hz, 1H), 3.77 (s, 3H), 2.03 (d, *J* = 7.1 Hz, 3H), 1.72 (s, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 167.0 (d, J_{CP} = 1.0 Hz), 160.4, 145.2 (d, J_{CP} = 25.0 Hz), 141.4, 140.4, 139.0 (d, J_{CP} = 14.0 Hz), 138.5 (d, J_{CP} = 3.0 Hz), 137.1 (d, J_{CP} = 14.0 Hz), 135.1 (d, J_{CP} = 12.0 Hz), 135.0 (d, J_{CP} = 22.0 Hz) × 2, 133.0, 132.9 (d, J_{CP} = 18.0 Hz) × 2, 132.1, 129.4 (d, J_{CP} = 3.0 Hz) × 2, 129.3 × 2, 129.2 (d, J_{CP} = 1.0 Hz), 128.5 (d, J_{CP} = 8.0 Hz) × 2, 128.3 (d, J_{CP} = 6.0 Hz) × 2, 128.1 (d, J_{CP} = 10.0 Hz) × 2, 128.0 × 2, 127.8, 127.3, 117.5, 113.6 × 2, 63.8 (d, J_{CP} = 5.0 Hz), 55.2, 21.5 (d, J_{CP} = 5.0 Hz), 18.3 (d, J_{CP} = 2.0 Hz); ^{31}P{^{1}H} NMR (162 MHz, $CDCl_3$) δ –15.5; HRMS (ESI-orbitrap-MS) *m*/*z* calcd for $C_{37}H_{34}O_2NP$ + H 556.2400 found 556.2390.

(*S*,a*R*)-*N*-(2-(Diphenylphosphanyl)-6-methylphenyl)-(*E*)-3-(4-methoxyphenyl)-*N*-(1-phenylethyl)acrylamide ((*S*,a*R*)-4a) (dr = >20:1). 53% yield (117.3 mg, 0.21 mmol) as a white solid; $[\alpha]^{20}_{D}$ = –136 (*c* 0.96, $CHCl_3$); mp 201-203 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, *J* = 15.3 Hz, 1H), 7.36-7.28 (m, 7H), 7.24-7.11 (m, 8H), 7.04-6.92 (m, 5H), 6.71 (d, *J* = 8.7 Hz, 2H), 5.99 (q, *J* = 7.1 Hz, 1H), 5.54 (d, *J* = 15.5 Hz, 1H), 3.76 (s, 3H), 1.77 (s, 3H), 1.70 (d, *J* = 7.1 Hz, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 166.9 (d, J_{CP} = 1.0 Hz), 160.4, 143.3 (d, J_{CP} = 27.0 Hz), 141.4, 141.2, 140.1 (d, J_{CP} = 15.0 Hz), 139.1 (d, J_{CP} = 3.0 Hz), 137.5 (d, J_{CP} = 12.0 Hz), 136.5 (d, J_{CP} = 13.0 Hz), 134.3 (d, J_{CP} = 22.0 Hz) × 2, 133.9 (d, J_{CP} = 2.0 Hz), 132.9 (d, J_{CP} = 18.0 Hz) × 2, 132.3, 129.4 × 2, 128.9 (d, J_{CP} = 1.0 Hz) × 2, 128.7, 128.4 (d, J_{CP} = 5.0 Hz) × 2, 128.3 (d, J_{CP} = 8.0 Hz) × 2, 128.2, 128.1, 127.8, 127.7 × 2, 127.2, 117.1 (d, J_{CP} = 1.0 Hz), 113.6 × 2, 57.6 (d, J_{CP} = 2.0 Hz), 55.2, 20.7 (d, J_{CP} = 10.0 Hz), 19.1 (d, J_{CP} = 4.0 Hz); ^{31}P{^{1}H} NMR (162 MHz, $CDCl_3$) δ –16.4; HRMS (ESI-orbitrap-MS) *m*/*z* calcd for $C_{37}H_{34}O_2NP$ + H 556.2400 found 556.2390.

Preparation of Amide (*S*,a*S*)-4b and (*S*,a*R*)-4b.

To the solution of aminophosphine (*S*)-**5** (395 mg, 1.0 mmol) in THF (3.75 mL) was added pyridine (0.25 mL, 3.0 mmol), DMAP (48.9 mg, 0.4 mmol) and *trans*-4-nitrocinnamoyl chloride (423 mg, 2.0 mmol) at room temperature. The reaction mixture was stirred at 60 °C (using an oil bath). After 24 h, the reaction mixture was diluted with ether and water. The organic layer was washed with brine and dried over $MgSO_4$. The filtrate was concentrated with a rotary evaporator, and the residue was purified by column chromatography (elution with *n*-hexane/ether = 2/1).

(*S*,a*S*)-*N*-(2-(Diphenylphosphanyl)-6-methylphenyl)-(*E*)-3-(4-nitrophenyl)-*N*-(1-phenylethyl)acrylamide ((*S*,a*S*)-4b) (dr = >20:1). 8% yield (46.8 mg, 0.08 mmol) as a yellow solid; $[\alpha]^{20}_{D}$ = +273 (*c* 0.54, $CHCl_3$); mp 235-236 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06-8.02 (m, 2H), 7.43-7.12 (m, 15H), 7.03-6.95 (m, 6H), 5.53 (d, *J* = 15.5 Hz, 1H), 5.20 (q, *J* = 7.0 Hz, 1H), 2.05 (d, *J* = 6.9 Hz, 3H), 1.77 (s, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 165.5 (d, J_{CP} = 0.7Hz), 147.6, 144.4 (d, J_{CP} = 24.8 Hz), 144.3, 140.9, 139.4 (d, J_{CP} = 13.9 Hz), 138.3 (d, J_{CP} = 3.1 Hz), 137.8, 136.9 (d, J_{CP} = 11.9 Hz), 135.3 (d, J_{CP} = 22.9 Hz) × 2, 134.7 (d, J_{CP} = 12.6 Hz), 132.9 (d, J_{CP} = 1.5 Hz), 132.7 (d, J_{CP} = 17.9 Hz) × 2, 132.3, 129.49 (d, J_{CP} = 2.2 Hz), 129.47 (d, J_{CP} = 3.0 Hz) × 2, 128.61 (d, J_{CP} = 8.0 Hz) × 2, 128.57, 128.3 (d, J_{CP} = 5.3 Hz) × 2, 128.2 × 2, 128.1, 128.0 × 2, 127.5, 123.9, 123.6 × 2, 63.9 (d, J_{CP} = 5.8 Hz), 21.6 (d, J_{CP} = 5.3 Hz), 18.3 (d, J_{CP} = 2.0 Hz); ^{31}P{^{1}H} NMR (162 MHz, $CDCl_3$) δ –15.7; HRMS (ESI-orbitrap-MS) *m*/*z* calcd for $C_{36}H_{31}O_3N_2P$ + H 571.2145 found 571.2140.

(*S*,a*R*)-*N*-(2-(Diphenylphosphanyl)-6-methylphenyl)-(*E*)-3-(4-nitrophenyl)-*N*-(1-phenylethyl)acrylamide ((*S*,a*R*)-4b) (dr = >20:1). 25% yield (144.4 mg, 0.25 mmol) as a yellow solid; $[\alpha]^{20}_{D}$ = –191 (*c* 0.54, $CHCl_3$); mp 178-180 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04-8.00 (m, 2H), 7.44-7.16 (m, 16H), 7.06-7.02 (m, 4H), 6.97-6.93 (m, 1H),

5.99 (q, J = 7.1 Hz, 1H), 5.70 (d, J = 15.5 Hz, 1H), 1.82 (s, 3H), 1.79 (d, J = 7.1 Hz, 3H); $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) δ 165.5 (d, J_{CP} = 1.1 Hz), 147.5, 142.5 (d, J_{CP} = 27.2 Hz), 141.1, 141.0, 140.2 (d, J_{CP} = 14.5 Hz), 138.8 (d, J_{CP} = 3.5 Hz), 138.4, 137.3 (d, J_{CP} = 12.6 Hz), 135.4 (d, J_{CP} = 12.8 Hz), 134.6 (d, J_{CP} = 1.8 Hz) × 2, 133.5 (d, J_{CP} = 1.8 Hz), 132.6 (d, J_{CP} = 18.0 Hz) × 2, 132.5, 129.0, 128.8 (d, J_{CP} = 1.5 Hz) × 2, 128.5 (d, J_{CP} = 9.7 Hz), 128.4 × 2, 128.3 (d, J_{CP} = 2.6 Hz) × 2, 128.2 × 2, 128.1, 127.8 × 2, 127.4, 123.43, 123.40 × 2, 58.0 (d, J_{CP} = 1.8 Hz), 20.5 (d, J_{CP} = 10.8 Hz), 19.0 (d, J_{CP} = 2.2 Hz); $^{31}P\{^{1}H\}$ NMR (121 MHz, $CDCl_3$) δ –16.2; HRMS (ESI-orbitrap-MS) m/z calcd for $C_{36}H_{31}O_3N_2P$ + H 571.2145 found 571.2139.

Preparation of Amide (*S*,a*S*)-4c and (*S*,a*R*)-4c.

To the solution of aminophosphine (*S*)-**5** (791 mg, 2.0 mmol) in THF (7.5 mL) was added pyridine (0.48 mL, 6.0 mmol), DMAP (97.7 mg, 0.80 mmol) and *trans*-crotonyl chloride (0.38 mL, 4.0 mmol) at room temperature. The reaction mixture was stirred at 40 °C (using an oil bath). After 24 h, the reaction mixture was diluted with ether and sat. $NaHCO_3$ aq. The organic layer was washed with brine and dried over $MgSO_4$. The filtrate was concentrated with a rotary evaporator, and the residue was purified by column chromatography (elution with *n*-hexane/ether = 3/1).

(*S*,a*S*)-*N*-(2-(Diphenylphosphanyl)-6-methylphenyl)-*N*-(1-phenylethyl)-(*E*)-2-butenamide ((*S*,a*S*)-4c) (dr = >20:1). 22% yield (207.7 mg, 0.45 mmol) as a light yellow solid; $[\alpha]^{20}_D$ = +93.8 (*c* 0.23, $CHCl_3$); mp 169-171 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39-7.15 (m, 15H), 7.01-6.95 (m, 3H), 6.59 (dq, J = 14.9 and 6.9 Hz, 1H), 5.03 (q, J = 7.0 Hz, 1H), 4.88 (dq, J = 14.9 and 1.6 Hz, 1H), 1.96 (d, J = 7.0 Hz, 3H), 1.74 (s, 3H), 1.34 (dd, J = 6.9 and 1.6 Hz, 3H); $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) δ 166.4, 145.1 (d, J_{CP} = 24.9 Hz), 141.4, 140.1, 138.9 (d, J_{CP} = 13.2 Hz), 138.2 (d, J_{CP} = 2.9 Hz), 137.0 (d, J_{CP} = 12.5 Hz), 135.15 (d, J_{CP} = 10.3 Hz), 135.08 (d, J_{CP} = 22.7 Hz) × 2, 132.9 (d, J_{CP} = 1.5 Hz), 132.8 (d, J_{CP} = 18.3 Hz) x 2, 132.0, 129.3 (d, J_{CP} = 2.2 Hz) × 2, 129.1, 128.3 (d, J_{CP} = 7.3 Hz) × 2, 128.2 (d, J_{CP} = 5.9 Hz) × 2, 128.0 , 127.9, 127.8 × 2, 127.2, 123.5, 63.3 (d, J_{CP} = 5.1 Hz), 21.5 (d, J_{CP} = 4.4 Hz), 18.3 (d, J_{CP} = 2.2 Hz), 17.6; $^{31}P\{^{1}H\}$ NMR (162 MHz, $CDCl_3$) δ –15.8; HRMS (ESI-orbitrap-MS) m/z calcd for $C_{31}H_{30}ONP$ + H 464.2138 found 464.2131.

(*S*,a*R*)-*N*-(2-(Diphenylphosphanyl)-6-methylphenyl)-*N*-(1-phenylethyl)-(*E*)-2-butenamide ((*S*,a*R*)-4c) (dr = >20:1). 22% yield (199.3 mg, 0.43 mmol) as a light yellow solid; $[\alpha]^{20}_D$ = –130 (*c* 0.20, $CHCl_3$); mp 156-158 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35-7.09 (m, 18H), 6.68 (dq, J = 15.0 and 6.9 Hz, 1H), 5.90 (q, J = 7.1 Hz, 1H), 5.04 (dq, J = 15.0 and 1.6 Hz, 1H), 1.75 (s, 3H), 1.66 (d, J = 7.2 Hz, 3H), 1.34 (dd, J = 6.9 and 1.6 Hz, 3H); $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) δ 166.4 (d, J_{CP} = 1.5 Hz), 143.2 (d, J_{CP} = 27.1 Hz), 141.5, 141.0, 140.0 (d, J_{CP} = 14.7 Hz), 138.9 (d, J_{CP} = 2.9 Hz), 137.6 (d, J_{CP} = 13.2 Hz), 136.3 (d, J_{CP} = 13.2 Hz), 134.4 (d, J_{CP} = 22.0 Hz) × 2, 133.7 (d, J_{CP} = 2.2 Hz), 132.8 (d, J_{CP} = 18.3 Hz) × 2, 132.2, 128.8 × (2 + 1), 128.3 (d, J_{CP} = 5.9 Hz) × 2, 128.2 (d,

J_{CP} = 8.1 Hz) × 2, 128.1, 128.0, 127.6 × 2, 127.1, 123.5, 57.4 (d, J_{CP} = 1.5 Hz), 20.7 (d, J_{CP} = 10.3 Hz), 19.0 (d, J_{CP} = 2.2 Hz), 17.6; $^{31}P\{^{1}H\}$ NMR (162 MHz, $CDCl_3$) δ –16.5; HRMS (ESI-orbitrap-MS) *m*/*z* calcd for $C_{31}H_{30}ONP$ + H 464.2138 found 464.2129.

Preparation of Amide (*S*,a*S*)-4d and (*S*,a*R*)-4d.

To the solution of aminophosphine (*S*)-**5** (158.2 mg, 0.4 mmol) in THF (1.5 mL) was added pyridine (0.1 mL, 1.2 mmol), DMAP (19.6 mg, 0.16 mmol) and 3-methylcrotonyl chloride (0.089 mL, 4.0 mmol) at room temperature. The reaction mixture was stirred at 60 °C (using an oil bath). After 24 h, the reaction mixture was diluted with ether and sat. $NaHCO_3$ aq. The organic layer was washed with brine and dried over $MgSO_4$. The filtrate was concentrated with a rotary evaporator, and the residue was purified by column chromatography (elution with *n*-hexane/ether = 4/1).

(*S*,a*S*)-*N*-(2-(Diphenylphosphanyl)-6-methylphenyl)-3-methyl-*N*-(1-phenylethyl)-2-butenamide ((*S*,a*S*)-4d) (dr = >20:1). 28% yield (54.1 mg, 0.11 mmol) as a white solid; $[\alpha]^{20}_{D}$ = +94.4 (*c* 0.34, $CHCl_3$); mp 134-136 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39-7.37 (m, 2H), 7.30-7.11 (m, 13H), 6.97-6.92 (m, 3H), 5.05 (q, *J* = 7.0 Hz, 1H), 4.77-4.76 (m, 1H), 1.91 (d, *J* = 1.3 Hz, 3H), 1.89 (d, *J* = 7.2 Hz, 3H), 1.81 (s, 3H), 1.30 (d, *J* = 1.0 Hz, 3H); $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) δ 167.6, 150.4, 145.9 (d, J_{CP} = 26.4 Hz), 141.7, 138.5 (d, J_{CP} = 12.7 Hz), 138.3 (d, J_{CP} = 3.9 Hz), 137.5 (d, J_{CP} = 12.7 Hz), 135.9 (d, J_{CP} = 13.7 Hz), 134.6 (d, J_{CP} = 22.5 Hz) × 2, 133.4 (d, J_{CP} = 1.0 Hz), 132.8 (d, J_{CP} = 18.6 Hz) × 2, 132.0, 129.3 (d, J_{CP} = 2.9 Hz) × 2, 128.9, 128.4 (d, J_{CP} = 7.8 Hz) × 2, 128.1 (d, J_{CP} = 4.9 Hz) × 2, 127.9, 127.8 × 2, 127.7, 127.0, 118.8, 62.6 (d, J_{CP} = 4.9 Hz), 27.0, 21.6 (d, J_{CP} = 6.8 Hz), 19.8, 18.4 (d, J_{CP} = 3.9 Hz); $^{31}P\{^{1}H\}$ NMR (162 MHz, $CDCl_3$) δ –15.9; HRMS (ESI-orbitrap-MS) *m*/*z* calcd for $C_{32}H_{32}ONP$ + H 478.2294 found 478.2288.

(*S*,a*R*)-*N*-(2-(Diphenylphosphanyl)-6-methylphenyl)-3-methyl-*N*-(1-phenylethyl)-2-butenamide ((*S*,a*R*)-4d) (dr = >20:1). 61% yield (116.8 mg, 0.24 mmol) as a light yellow oil; $[\alpha]^{20}_{D}$ = +161 (*c* 0.68, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32-7.11 (m, 18H), 5.87 (q, *J* = 7.1 Hz, 1H), 4.94-4.93 (m, 1H), 1.91 (d, *J* = 1.2 Hz, 3H), 1.82 (s, 3H), 1.56 (d, *J* = 7.2 Hz, 3H), 1.30 (d, *J* = 0.9 Hz, 3H); $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) δ 167.6 (d, J_{CP} = 1.0 Hz), 151.6, 144.2 (d, J_{CP} = 27.4 Hz), 142.1, 139.7 (d, J_{CP} = 13.7 Hz), 138.7 (d, J_{CP} = 2.9 Hz), 138.0 (d, J_{CP} = 13.7 Hz), 137.2 (d, J_{CP} = 13.7 Hz), 134.3 (d, J_{CP} = 2.0 Hz), 133.7 (d, J_{CP} = 20.5 Hz) × 2, 133.1 (d, J_{CP} = 19.6 Hz) × 2, 132.4, 128.5 (d, J_{CP} = 1.0 Hz) × 2, 128.4 (d, J_{CP} = 2.0 Hz) × 2, 128.3, 128.22, 128.18 (d, J_{CP} = 6.9 Hz) × 2, 127.72 (d, J_{CP} = 4.9 Hz) × 2, 127.69, 126.9, 118.7 (d, J_{CP} = 1.0 Hz), 57.0 (d, J_{CP} = 2.9 Hz), 27.1, 20.8 (d, J_{CP} = 8.8 Hz), 19.9, 19.2 (d, J_{CP} = 2.0 Hz); $^{31}P\{^{1}H\}$ NMR (162 MHz, $CDCl_3$) δ –16.9; HRMS (ESI-orbitrap-MS) *m*/*z* calcd for $C_{32}H_{32}ONP$ + H 478.2294 found 478.2285.

Preparation of Amide (*S*,a*S*)-4e and (*S*,a*R*)-4e.

To the solution of aminophosphine (*S*)-**5** (158 mg, 0.4 mmol) in THF (1.5 mL) was added triethylamine (0.33 mL, 2.4 mmol), DMAP (19.6 mg, 0.16 mmol) and 3-

chloropropionyl chloride (157 mg, 0.8 mmol) at room temperature. The reaction mixture was stirred at 40 °C (using an oil bath). After 72 h, the reaction mixture was diluted with ether and sat. $NaHCO_3$ aq. The organic layer was washed with brine and dried over $MgSO_4$. The filtrate was concentrated with a rotary evaporator. To the (1.5 mL) THF solution of residue without purification, ^{t}BuOK (179.54 mg, 1.6 mmol) was added. The reaction mixture was stirred at room temperature. After 18 h, the reaction mixture was diluted with ether and sat. $NaHCO_3$ aq. The organic layer was washed with brine and dried over $MgSO_4$. The filtrate was concentrated with a rotary evaporator, and the residue was purified by column chromatography (elution with *n*-hexane/ether = 3/1).

(*S*,a*S*)-*N*-(2-(Diphenylphosphanyl)-6-methylphenyl)-*N*-(1-phenylethyl)acrylamide ((*S*,a*S*)-4e) (dr = >20:1). 14% yield (24.5 mg, 0.055 mmol) as a light yellow solid; $[\alpha]^{20}_D$ = +59.0 (*c* 0.17, $CHCl_3$); mp 171-173 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39-6.96 (m, 18H), 6.02 (dd, *J* = 16.6 and 2.1 Hz, 1H), 5.22 (dd, *J* = 16.6 and 10.2 Hz, 1H), 4.95 (dd, *J* = 10.2 and 2.0 Hz, 1H), 4.93 (q, *J* = 7.2 Hz, 1H), 1.98 (d, *J* = 7.0 Hz, 3H), 1.67 (s, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 166.2 (d, J_{CP} = 0.6 Hz), 145.1 (d, J_{CP} = 25.1 Hz), 141.2, 138.7 (d, J_{CP} = 13.8 Hz), 138.3 (d, J_{CP} = 3.1 Hz), 136.8 (d, J_{CP} = 12.1 Hz), 135.06 (d, J_{CP} = 12.3 Hz), 135.05 (d, J_{CP} = 22.2 Hz) × 2, 133.13 (d, J_{CP} = 1.3 Hz), 133.07 (d, J_{CP} = 18.5 Hz) × 2, 132.1, 129.4 (d, J_{CP} = 2.6 Hz) × 2, 129.2, 129.0, 128.5 (d, J_{CP} = 7.9 Hz) × 2, 128.4 (d, J_{CP} = 5.9 Hz) × 2, 128.2, 128.1, 128.0 × 2, 127.4, 126.1, 63.9 (d, J_{CP} = 5.5 Hz), 21.2 (d, J_{CP} = 5.5 Hz), 18.2 (d, J_{CP} = 2.0 Hz); ^{31}P{^{1}H} NMR (162 MHz, $CDCl_3$) δ –15.4; HRMS (ESI-orbitrap-MS) *m*/*z* calcd for $C_{30}H_{28}ONP$ + H 450.1981 found 450.1982.

(*S*,a*R*)-*N*-(2-(Diphenylphosphanyl)-6-methylphenyl)-*N*-(1-phenylethyl)acrylamide ((*S*,a*R*)-4e) (dr = >20:1). 12% yield (21.0 mg, 0.047 mmol) as a light yellow solid; $[\alpha]^{20}_D$ = +159 (*c* 0.15, $CHCl_3$); mp 60-62 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36-7.08 (m, 18H), 6.08 (dd, *J* = 16.7 and 2.0 Hz, 1H), 5.86 (q, *J* = 7.1 Hz, 1H), 5.32 (dd, *J* = 16.6 and 10.2 Hz, 1H), 5.00 (dd, *J* = 10.2 and 2.0 Hz, 1H), 1.77 (s, 3H), 1.66 (d, *J* = 7.0 Hz, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 166.3 (d, J_{CP} = 0.9 Hz), 143.1 (d, J_{CP} = 27.3 Hz), 141.4, 140.1 (d, J_{CP} = 14.7 Hz), 138.9 (d, J_{CP} = 3.5 Hz), 137.3 (d, J_{CP} = 12.8 Hz), 136.0 (d, J_{CP} = 12.7 Hz), 134.7 (d, J_{CP} = 21.8 Hz) × 2, 133.7 (d, J_{CP} = 2.0 Hz), 133.1 (d, J_{CP} = 18.5 Hz) × 2, 132.3, 129.0, 128.90, 128.88, 128.7 (d, J_{CP} = 0.9 Hz), 128.5 (d, J_{CP} = 5.9 Hz) × 2, 128.4 (d, J_{CP} = 7.5 Hz) × 2, 128.3 (d, J_{CP} = 4.6 Hz) × 2, 127.8 × 2, 127.3, 126.9, 58.0 (d, J_{CP} = 2.0 Hz), 20.8 (d, J_{CP} = 10.3 Hz), 19.1 (d, J_{CP} = 2.2 Hz); ^{31}P{^{1}H} NMR (162 MHz, $CDCl_3$) δ –15.9; HRMS (ESI-orbitrap-MS) *m*/*z* calcd for $C_{30}H_{28}ONP$ + H 450.1981 found 450.1985.

Preparation of Amide (*S*,a*S*)-4f.

The $CHCl_3$ solution (2.0 mL) of aminophosphine (*S*,a*S*)-**3** (42.1 mg, 0.080 mmol) in pyrex glass test tube, which was deoxygenated by argon bubbling, was irradiated using a LED at 365 nm (Power: 50%, Distance: 20 cm) at room temperature. After 2 h, the

reaction mixture was concentrated with a rotary evaporator, and the residue was purified by preparative TLC (elution with *n*-hexane/ether = 3/1).

(*S*,a*S*)-*N*-(2-(Diphenylphosphanyl)-6-methylphenyl)-*N*-(1-phenylethyl)allocinnamamide ((*S*,a*S*)-4f). 28% yield (11.8 mg, 0.026 mmol) as a white solid; $[\alpha]^{20}_{D}$ = +161 (*c* 0.13, $CHCl_3$); mp 148-150 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60-6.96 (m, 23H), 6.07 (d, *J* = 12.8 Hz, 1H), 5.05 (d, *J* = 12.8 Hz, 1H), 4.88 (q, *J* = 7.0 Hz, 1H), 1.93 (d, *J* = 7.0 Hz, 3H), 1.75 (s, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 166.8, 145.8 (d, J_{CP} = 26.0 Hz), 141.6, 138.6 (d, J_{CP} = 3.5 Hz), 138.5 (d, J_{CP} = 13.4 Hz), 137.8, 137.0 (d, J_{CP} = 12.7 Hz), 135.9 (d, J_{CP} = 12.8 Hz), 134.9, 134.6 (d, J_{CP} = 21.6 Hz) × 2, 133.7 (d, J_{CP} = 1.7 Hz), 133.1 (d, J_{CP} = 18.5 Hz) × 2, 132.3, 130.1 (d, J_{CP} = 0.4 Hz)×2, 129.4 (d, J_{CP} = 2.4 Hz) × 2, 129.1, 128.6 (d, J_{CP} = 7.5 Hz) × 2, 128.4 (d, J_{CP} = 2.0 Hz) × 2, 128.3, 128.2, 127.99 × 2, 127.98, 127.8 × 2, 127.3, 123.3 (d, J_{CP} = 0.7 Hz), 63.6 (d, J_{CP} = 5.0 Hz), 21.3 (d, J_{CP} = 5.0 Hz), 18.6 (d, J_{CP} = 2.2 Hz); ^{31}P{^{1}H} NMR (162 MHz, $CDCl_3$) δ –16.3; HRMS (ESI-orbitrap-MS) *m*/*z* calcd for $C_{36}H_{32}ONP$ + H 526.2294 found 526.2294.

Preparation of Amide (*S*,a*R*)-4f.

The $CHCl_3$ solution (10 mL) of aminophosphine (*S*,a*R*)-**3** (210 mg, 0.40 mmol) in pyrex glass test tube, which was deoxygenated by argon bubbling, was irradiated using a LED at 365 nm (Power: 50%, Distance: 20 cm) at room temperature. After 2 h, the reaction mixture was concentrated with a rotary evaporator. This reaction was performed four more times, and the all of residue was purified by column chromatography (elution with *n*-hexane/ether = 2/1 and *n*-hexane/$CHCl_3$/ether = 25/8/1).

(*S*,a*R*)-*N*-(2-(Diphenylphosphanyl)-6-methylphenyl)-*N*-(1-phenylethyl)allocinnamamide ((*S*,a*R*)-4f). (rotamer ratio at C(=O)-N bond = 18:1) 9% yield (19.4 mg, 0.037 mmol) as a light yellow solid; $[\alpha]^{20}_{D}$ = +173 (*c* 0.18, $CHCl_3$); mp 50-52 °C; ^{1}H NMR (400 MHz, $CDCl_3$) (major rotamer) δ 7.59-7.08 (m, 23H), 6.11 (d, *J* = 12.8 Hz, 1H), 5.91 (q, *J* = 7.1 Hz, 1H), 5.14 (d, *J* = 12.8 Hz, 1H), 1.74 (s, 3H), 1.61 (d, *J* = 7.1 Hz, 3H); (minor rotamer) δ 7.67-7.65 (m, 2H), 7.59-7.08 (m, 19H), 6.77-6.74 (m, 2H), 6.75 (d, *J* = 12.8 Hz, 1H), 6.48 (d, *J* = 12.7 Hz, 1H), 5.91 (q, *J* = 7.1 Hz, 1H), 1.45 (s, 3H), 1.40 (d, *J* = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) (major rotamer) δ 166.9 (d, J_{CP} = 0.7 Hz), 143.6 (d, J_{CP} = 28.0 Hz), 141.4, 139.9 (d, J_{CP} = 14.0 Hz), 139.2 (d, J_{CP} = 3.7 Hz), 138.5, 137.5 (d, J_{CP} = 13.3 Hz), 136.8 (d, J_{CP} = 12.5 Hz), 135.0, 134.3 (d, J_{CP} = 2.2 Hz), 134.1 (d, J_{CP} = 21.4 Hz) × 2, 133.3 (d, J_{CP} = 18.4 Hz) × 2, 132.5 (d, J_{CP} = 0.5 Hz), 130.1 (d, J_{CP} = 1.5 Hz) × 2, 129.0 (d, J_{CP} = 1.5 Hz) × 2, 128.7, 128.5 (d, J_{CP} = 5.9 Hz) × 2, 128.40, 128.38 (d, J_{CP} = 7.4 Hz) × 2, 128.36, 128.0, 127.73 × 2, 127.72 × 2, 127.3, 122.7 (d, J_{CP} = 2.2 Hz), 57.4 (d, J_{CP} = 1.5 Hz), 20.7 (d, J_{CP} = 8.8 Hz), 19.2 (d, J_{CP} = 2.2 Hz); ^{31}P{^{1}H} NMR (162 MHz, $CDCl_3$) (major rotamer) δ –17.0; (minor rotamer) δ –15.5; HRMS (ESI-orbitrap-MS) *m*/*z* calcd for $C_{36}H_{32}ONP$ + H 526.2294 found 526.2286.

General Procedure for the Pd-Catalyzed Allylic Alkylation of Malonates.

To a mixture of $[Pd(\eta^3\text{-}C_3H_5)Cl]_2$ (1.48 mg, 4 μmol), (*S,*a*R*)-**4d** (3.82 mg, 8 μmol), and LiOAc (1.32 mg, 20 μmol) in a DCM (0.4 mL) was added BSA (0.15 mL, 0.60 mmol), allylic ester (0.20 mmol), and malonate (0.60 mmol) at room temperature under an Ar atmosphere. After the stirring was continued for 24 h at room temperature, the reaction mixture was diluted with ether and water. The organic layer was washed with brine and dried over $MgSO_4$. The filtrate was concentrated with a rotary evaporator, and the residue was purified by column chromatography (elution with *n*-hexane/EtOAc = 10/1).

(*S*)-(–)-Dimethyl (*E*)-2-(1,3-diphenylallyl)malonate ((*S*)-8a) (**Table 2**, entry 3).[1] Compound (*S*)-**8a** was obtained according to the general procedure in 99% yield (64.5 mg, 0.20 mmol) as a colorless oil; 95% ee; $[\alpha]^{20}_D$ –18.4 (*c* 0.24, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33-7.19 (m, 10H), 6.48 (d, *J* = 15.8 Hz, 1H), 6.33 (dd, *J* = 15.7 and 8.6 Hz, 1H), 4.27 (dd, *J* = 10.9 and 8.7 Hz, 1H), 3.96 (d, *J* = 10.9 Hz, 1H), 3.70 (s, 3H), 3.51 (s, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 168.1, 167.7, 140.1, 136.7, 131.7, 129.0, 128.7 × 2, 128.4 × 2, 127.8 × 2, 127.5, 127.1, 126.3 × 2, 57.6, 52.6, 52.4, 49.1; HPLC (Daicel CHIRALPAK® AD-3, 0.46 ϕ × 25 cm; Hexane:2-PrOH = 90:10, 0.50 mL/min, UV 254 nm) t_R = 25.8 min (minor) and 33.2 min (major).

(*S*)-(–)-Diethyl (*E*)-2-(1,3-diphenylallyl)malonate ((*S*)-8b) (**Table 2**, entry 11).[1] Compound (*S*)-**8b** was obtained according to the general procedure in 79% yield (56.0 mg, 0.16 mmol) as a yellow oil; 89% ee; $[\alpha]^{20}_D$ –16.3 (*c* 0.24, $CHCl_3$); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32-7.18 (m, 10H), 6.47 (d, *J* = 16.2 Hz, 1H), 6.33 (dd, *J* = 15.6 and 8.5 Hz, 1H), 4.26 (dd, *J* = 10.5 and 8.6 Hz, 1H), 4.17 (q, *J* = 7.1 Hz, 2H), 4.00-3.95 (m, 2H), 3.91 (d, *J* = 11.1 Hz, 1H), 1.21 (t, *J* = 7.1 Hz, 3H), 1.01 (t, *J* = 7.1 Hz, 3H); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 167.8, 167.4, 140.2, 136.8, 131.6, 129.3, 128.6 × 2, 128.4 × 2, 127.9 × 2, 127.5, 127.0, 126.3 × 2, 61.5, 61.3, 57.7, 49.2, 14.1, 13.7; HPLC (Daicel CHIRALPAK® AD-3, 0.46 ϕ × 25 cm; Hexane:2-PrOH = 90:10, 0.50 mL/min, UV 254 nm) t_R = 22.2 min (minor) and 29.3 min (major).

(*S*)-(–)-Dibenzyl (*E*)-2-(1,3-diphenylallyl)malonate ((*S*)-8d) (**Table 2**, entry 13).[1] Compound (*S*)-**8c** was obtained according to the general procedure in 88% yield (83.6 mg, 0.18 mmol) as a yellow oil; 89% ee; $[\alpha]^{20}_D$ –5.8 (*c* 0.22, $CHCl_3$); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34-7.19 (m, 18H), 7.06-7.04 (m, 2H), 6.41 (d, *J* = 16.0 Hz, 1H), 6.30 (dd, *J* = 15.7 and 8.5 Hz, 1H), 5.10 (q, *J* = 9.7 Hz, 2H), 4.93 (q, *J* = 9.8 Hz, 2H), 4.29 (dd, *J* = 10.6 and 8.6 Hz, 1H), 4.04 (d, *J* = 11.0 Hz, 1H); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 167.5, 167.1, 140.0, 136.6, 135.1, 135.0, 131.8, 128.9, 128.7 × 2, 128.5 × 2, 128.4 × (2+2), 128.3 × 2, 128.3, 128.1, 128.0 × 2, 127.9 × 2, 127.5, 127.1, 126.4 × 2, 67.3, 67.1, 57.7, 49.2; HPLC (Daicel CHIRALPAK® AD-H, 0.46 ϕ × 25 cm; Hexane:2-PrOH = 85:15, 0.50 mL/min, UV 254 nm) t_R = 39.1 min (minor) and 47.9 min (major).

(*R*)-(+)-Diethyl (*E*)-2-(1,3-diphenylallyl)-2-methylmalonate ((*R*)-8e) (**Table 2**, entry 14).[1] Compound (*R*)-**8e** was obtained according to the general procedure in 65% yield

(47.9 mg, 0.13 mmol) as a yellow oil; 86% ee; $[\alpha]^{20}_D$ +32.1 (*c* 0.25, $CHCl_3$); ^1H NMR (500 MHz, $CDCl_3$) δ 7.34-7.18 (m, 10H), 6.70 (dd, *J* = 15.9 and 9.1 Hz, 1H), 6.44 (d, *J* = 15.9 Hz, 1H), 4.29 (d, *J* = 9.2 Hz, 1H), 4.19-4.15 (m, 2H), 4.09-4.07 (m, 2H), 1.47 (s, 3H), 1.23 (t, *J* = 7.2 Hz, 3H), 1.16 (t, *J* = 7.2 Hz, 3H); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$) δ 171.2, 170.9, 139.4, 137.3, 132.5, 129.6 × 2, 128.8, 128.4 × 2, 128.2 × 2, 127.3, 127.1, 126.3 × 2, 61.3, 61.3, 58.8, 53.7, 18.7, 14.0, 13.9; HPLC (Daicel CHIRALPAK® AD-H, 0.46 ϕ × 25 cm+ AD-3, 0.46 ϕ × 25 cm; Hexane:2-PrOH = 99:1, 0.30 mL/min, UV 254 nm) t_R = 78.2 min (minor) and 95.7 min (major).

(*S*)-(–)-Dimethyl (*E*)-2-(1,3-di-*p*-chlorophenylallyl)malonate ((*S*)-8f) (**Table 2**, entry 15).[1] Compound (*S*)-**8f** was obtained according to the general procedure in 96% yield (75.2 mg, 0.19 mmol) as a yellow solid, mp 72-74 °C; 88% ee; $[\alpha]^{20}_D$ –3.9 (*c* 0.18, $CHCl_3$); ^1H NMR (500 MHz, $CDCl_3$) δ 7.31-7.21 (m, 8H), 6.40 (d, *J* = 15.7 Hz, 1H), 6.26 (dd, *J* = 15.6 and 8.7 Hz, 1H), 4.23 (dd, *J* = 10.8 and 8.5 Hz, 1H), 3.89 (d, *J* = 10.7 Hz, 1H), 3.71 (s, 3H), 3.55 (s, 3H); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$) δ 167.9, 167.5, 138.4, 135.0, 133.3, 133.0, 131.0, 129.2 × 2, 129.1, 128.9 × 2, 128.6 × 2, 127.5 × 2, 57.3, 52.7, 52.6, 48.3; HPLC (Daicel CHIRALPAK® AD-3, 0.46 ϕ × 25 cm; Hexane:2-PrOH = 85:15, 0.50 mL/min, UV 254 nm) t_R = 31.4 min (minor) and 46.0 min (major).

(*S*)-(–)-Dimethyl (*E*)-2-(1,3-diphenylallyl)malonate ((*S*)-8a) (**Table 2**, entry 16).[1] Compound (*S*)-**8a** was obtained according to the general procedure in 60% yield (38.8 mg, 0.12 mmol) as a yellow oil; 92% ee; $[\alpha]^{20}_D$ –14.4 (*c* 0.23, $CHCl_3$); ^1H NMR (500 MHz, $CDCl_3$) δ 7.33-7.19 (m, 10H), 6.48 (d, *J* = 15.8 Hz, 1H), 6.33 (dd, *J* = 15.9 and 8.8 Hz, 1H), 4.26 (dd, *J* = 10.9 and 8.7 Hz, 1H), 3.95 (d, *J* = 10.9 Hz, 1H), 3.71 (s, 3H), 3.52 (s, 3H); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$) δ 168.2, 167.7, 140.1, 136.8, 131.8, 129.0, 128.7 × 2, 128.4 × 2, 127.8 × 2, 127.5, 127.1, 126.3 × 2, 57.6, 52.6, 52.4, 49.2; HPLC (Daicel CHIRALPAK® AD-3, 0.46 ϕ × 25 cm; Hexane:2-PrOH = 90:10, 0.50 mL/min, UV 254 nm) t_R = 26.5 min (minor) and 34.3 min (major).

General Procedure for the Pd-Catalyzed Allylic Alkylation of Indoles.

To a mixture of indole or substituted indole (0.22 mmol), allylic ester (0.20 mmol), (*S*,a*R*)-**4d** (5.7 mg, 12 μmol), $[Pd(\eta^3\text{-}C_3H_5)Cl]_2$ (2.2 mg, 6 μmol), and K_2CO_3 (55.3 mg, 0.4 mol) was added DCM (0.2 mL) at room temperature under an Ar atmosphere. After stirring for 18 h at room temperature, the mixture was quenched with water and diluted with diethyl ether. The organic layer was washed with water and brine, and dried over $MgSO_4$. The filtrate was concentrated with a rotary evaporator and the residue was purified by column chromatography (elution with *n*-hexane/EtOAc/Et_3N = 20/4-2/1).

(*R*)-(–)-3-((*E*)-1,3-Diphenylallyl)-1*H*-indole ((*R*)-10a) (**Table 3**, entry 15).[2] Compound (*R*)-**10a** was obtained according to the general procedure in 90% yield (56.0 mg, 0.18 mmol) as a brown solid; mp 123-124 °C; 95% ee; $[\alpha]^{20}_D$ –38.6 (*c* 0.32, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.87 (s, 1H), 7.42 (d, *J* = 7.1 Hz , 1H), 7.36-7.14 (m, 12H),

7.03-6.99 (m, 1H), 6.84 (d, J = 2.3 Hz, 1H), 6.71 (dd, J = 7.4 and 15.8 Hz, 1H), 6.42 (d, J = 15.5 Hz, 1H), 5.11 (d, J = 7.3 Hz, 1H); $^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$) δ 143.3, 137.4, 136.6, 132.5, 130.5, 128.5 × (2 + 2), 128.4 × 2, 127.1, 126.8, 126.4, 126.3 × 2, 122.6, 122.0, 119.8, 119.4, 118.5, 111.1, 46.1; HPLC (Daicel CHIRALPAK® IB, 0.46 ϕ × 25 cm; Hexane:EtOH = 99:1, 1.0 mL/min, UV 254 nm) t_R = 36.7 min (major) and 41.2 min (minor).

(*R*)-(–)-3-((*E*)-1,3-Diphenylallyl)-6-methyl-1*H*-indole ((*R*)-10b) (**Table 4**, entry 2).[2] Compound (*R*)-**10b** was obtained according to the general procedure in 34% yield (21.7 mg, 0.067 mmol) as a brown solid; mp 138-140 °C; 92% ee; $[\alpha]^{20}_D$ –31.8 (*c* 0.27, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.83 (s, 1H), 7.37-7.14 (m, 12H), 6.86-6.81 (m, 2H), 6.71 (dd, J = 15.7 and 7.4 Hz, 1H), 6.43 (d, J = 15.8 Hz, 1H), 5.08 (d, J = 7.4 Hz, 1H), 2.42 (s, 3H); $^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$) δ 143.4, 137.5, 137.1, 132.6, 131.9, 130.4, 128.44 × (2 + 2), 128.36 × 2, 127.1, 126.3 × (2 + 1), 124.6, 121.9, 121.1, 119.5, 118.5, 111.0, 46.2, 21.7; HPLC (Daicel CHIRALPAK® IB, 0.46 ϕ × 25 cm; Hexane:EtOH = 99:1, 0.5 mL/min, UV 254 nm) t_R = 71.2 min (major) and 79.0 min (minor).

(*R*)-(–)-3-((*E*)-1,3-Diphenylallyl)-6-methoxy-1*H*-indole ((*R*)-10c) (**Table 4**, entry 3).[2] Compound (*R*)-**10c** was obtained according to the general procedure in 67% yield (45.7 mg, 0.13 mmol) as a brown solid; mp 150-152 °C; 97% ee; $[\alpha]^{20}_D$ –33.4 (*c* 0.25, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.83 (s, 1H), 7.37-7.17 (m, 11H), 6.82 (d, J = 2.2 Hz, 1H), 6.76 (dd, J = 2.3 and 1.0 Hz, 1H), 6.73-6.67 (m, 2H), 6.43 (d, J = 15.8 Hz, 1H), 5.06 (d, J = 7.5 Hz, 1H) 3.80 (s, 3H); $^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$) δ 156.4, 143.3, 137.4 × (1 + 1), 132.5, 130.4, 128.44 × 2, 128.42 × 2, 128.37 × 2, 127.1, 126.34, 126.27 × 2, 121.3, 121.1, 120.5, 118.6, 109.3, 94.5, 55.6, 46.2; HPLC (Daicel CHIRALPAK® IB, 0.46 ϕ × 25 cm; Hexane:EtOH = 99:1, 0.9 mL/min, UV 254 nm) t_R = 81.3 min (major) and 95.1 min (minor).

(*R*)-(–)-6-Benzyloxy-3-((*E*)-1,3-diphenylallyl)-1*H*-indole ((*R*)-10d) (**Table 4**, entry 4).[2] Compound (*R*)-**10d** was obtained according to the general procedure in 89% yield (73.6 mg, 0.18 mmol) as a brown solid; mp 131-133 °C; 95% ee; $[\alpha]^{20}_D$ –28.3 (*c* 0.15, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.86 (s, 1H), 7.43-7.16 (m, 16H), 6.81 (d, J = 2.1 Hz, 1H), 6.76 (dd, J = 8.7 and 2.3 Hz, 1H), 6.71-6.65 (m, 2H), 6.41 (d, J = 15.8 Hz, 1H), 5.04-5.03 (m, 3H); $^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$) δ 155.5, 143.3, 137.4, 137.3, 137.2, 132.5, 130.4, 128.51 × 2, 128.44 × 2, 128.40 × 2, 128.37 × 2, 127.8, 127.4 × 2, 127.1, 126.33, 126.25 × 2, 121.5, 121.3, 120.4, 118.5, 110.0, 95.9, 70.4, 46.2; HPLC (Daicel CHIRALPAK® IA-3, 0.46 ϕ × 25 cm; Hexane:EtOH = 99:1, 0.7 mL/min, UV 254 nm) t_R = 189.7 min (minor) and 208.0 min (major).

(*R*)-(–)-3-((*E*)-1,3-Diphenylallyl)-6-nitro-1*H*-indole ((*R*)-10e) (**Table 4**, entry 5).[2] Compound (*R*)-**10e** was obtained according to the general procedure in 56% yield (40.0 mg, 0.11 mmol) as a brown solid; mp 55-57 °C; 95% ee; $[\alpha]^{20}_D$ –46.7 (*c* 0.18, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 8.61 (s, 1H), 8.33 (d, J = 1.9 Hz, 1H), 7.90 (dd, J = 8.8

and 1.9 Hz, 1H), 7.43-7.20 (m, 12H), 6.69 (dd, J = 15.9 and 7.5 Hz, 1H), 6.42 (d, J = 15.7 Hz, 1H), 5.12 (d, J = 7.3 Hz, 1H); $^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$) δ 143.2, 142.4, 137.0, 135.1, 131.41, 131.38, 131.1, 128.64 × 2, 128.55 × (2+1), 128.3 × 2, 127.5, 126.8, 126.3 × 2, 119.7 (1+1), 114.9, 108.2, 45.9; HPLC (Daicel CHIRALPAK® IA-3, 0.46 ϕ × 25 cm; Hexane:EtOH = 98:2, 0.5 mL/min, UV 254 nm) t_R = 127.6 min (minor) and 136.5 min (major).

(*R*)-(–)-3-((*E*)-1,3-Diphenylallyl)-6-fluoro-1*H*-indole ((*R*)-10f) (**Table 4**, entry 6).[2] Compound (*R*)-**10f** was obtained according to the general procedure in 74% yield (48.7 mg, 0.15 mmol) as a brown solid; mp 51-53 °C; 96% ee; $[\alpha]^{20}_D$ –21.4 (*c* 0.12, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.87 (s, 1H), 7.36-7.17 (m, 11H), 6.99 (dd, J = 9.7 and 2.2 Hz, 1H), 6.83-6.65 (m, 3H), 6.42 (d, J = 15.8 Hz, 1H), 5.06 (d, J = 7.2 Hz, 1H); $^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$) δ 159.9 (d, $J_{C\text{-}F}$ = 238.1 Hz), 143.1, 137.3, 136.5 (d, $J_{C\text{-}F}$ = 12.5 Hz), 132.2, 130.7, 128.49 × 2, 128.45 × 2, 128.40 × 2, 127.2, 126.5, 126.3 × 2, 123.3, 122.8 (d, $J_{C\text{-}F}$ = 3.3 Hz), 120.6 (d, $J_{C\text{-}F}$ = 10.1 Hz), 118.7, 108.2 (d, $J_{C\text{-}F}$ = 24.2 Hz), 97.4 (d, $J_{C\text{-}F}$ = 26.0 Hz), 46.1; HPLC (Daicel CHIRALPAK® IA-3, 0.46 ϕ × 25 cm; Hexane:EtOH = 99:1, 0.6 mL/min, UV 254 nm) t_R = 75.1 min (minor) and 80.9 min (major).

(*R*)-(–)-6-Chloro-3-((*E*)-1,3-diphenylallyl)-1*H*-indole ((*R*)-10g) (**Table 4**, entry 7).[2] Compound (*R*)-**10g** was obtained according to the general procedure in 87% yield (59.8 mg, 0.17 mmol) as a brown solid; mp 55-57 °C; 96% ee; $[\alpha]^{20}_D$ –26.1 (*c* 0.13, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.93 (s, 1H), 7.36-7.18 (m, 12H), 6.97 (dd, J = 8.5 and 1.9 Hz, 1H), 6.85 (d, J = 1.4 Hz, 1H), 6.68 (dd, J = 15.8 and 7.4 Hz, 1H), 6.41 (d, J = 15.6 Hz, 1H), 5.06 (d, J = 7.4 Hz, 1H); $^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$) δ 142.9, 137.3, 137.0, 132.0, 130.7, 128.49 × 2, 128.47 × 2, 128.37 × 2, 128.0, 127.3, 126.5, 126.3 × 2, 125.3, 123.2, 120.7, 120.2, 118.8, 111.0, 46.0; HPLC (Daicel CHIRALPAK® IA-3, 0.46 ϕ × 25 cm; Hexane:EtOH = 99:1, 0.5 mL/min, UV 254 nm) t_R = 87.7 min (minor) and 93.1 min (major).

(*R*)-(–)-6-Bromo-3-((*E*)-1,3-diphenylallyl)-1*H*-indole ((*R*)-10h) (**Table 4**, entry 8).[2] Compound (*R*)-**10h** was obtained according to the general procedure in 86% yield (66.9 mg, 0.17 mmol) as a brown solid; mp 129-131 °C; 95% ee; $[\alpha]^{20}_D$ –20.3 (*c* 0.23, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.95 (s, 1H), 7.48 (d, J = 1.5 Hz, 1H), 7.37-7.19 (m, 11H), 7.11 (dd, J = 8.5 and 1.7 Hz, 1H), 6.86 (dd, J = 2.4 and 1.0 Hz, 1H), 6.68 (dd, J = 15.8 and 7.4 Hz, 1H), 6.41 (d, J = 15.8 Hz, 1H), 5.07 (d, J = 7.4 Hz, 1H); $^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$) δ 142.9, 137.3, 137.2, 132.0, 130.7, 128.49 × 2, 128.47 × 2, 128.36 × 2, 127.3, 126.5, 126.3 × 2, 125.6, 123.2, 122.7, 121.1, 118.8, 115.6, 114.0, 46.0; HPLC (Daicel CHIRALPAK® IA-3, 0.46 ϕ × 25 cm; Hexane:2-PrOH = 98:2, 0.9 mL/min, UV 254 nm) t_R = 52.5 min (minor) and 58.1 min (major).

(*R*)-(–)-3-((*E*)-1,3-Diphenylallyl)-5-methoxy-1*H*-indole ((*R*)-10j) (**Table 4**, entry 10).[2] Compound (*R*)-**10j** was obtained according to the general procedure in 73% yield

(49.7 mg, 0.15 mmol) as a brown solid; mp 55-57 °C; 93% ee; $[\alpha]^{20}_{D}$ –34.8 (*c* 0.11, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (s, 1H), 7.37-7.17 (m, 11H), 6.85-6.81 (m, 3H), 6.70 (dd, *J* = 15.8 and 7.4 Hz, 1H), 6.43 (d, *J* = 15.9 Hz, 1H), 5.06 (d, *J* = 7.2 Hz, 1H), 3.70 (s, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 153.7, 143.2, 137.4, 132.4, 131.7, 130.5, 128.46 × 2, 128.45 × 2 128.40 × 2, 127.13, 127.12, 126.4, 126.3 × 2, 123.4, 118.2, 112.1, 111.8, 101.6, 55.7, 46.1; HPLC (Daicel CHIRALPAK® IB, 0.46 ϕ × 25 cm; Hexane:EtOH = 99:1, 0.9 mL/min, UV 254 nm) t_R = 53.9 min (major) and 67.3 min (minor).

(*R*)-(–)-5-Bromo-3-((*E*)-1,3-diphenylallyl)-1*H*-indole ((*R*)-10k) (**Table 4**, entry 11).[2] Compound (*R*)-**10k** was obtained according to the general procedure in 82% yield (63.1 mg, 0.16 mmol) as a brown solid; mp 141-143 °C; 95% ee; $[\alpha]^{20}_{D}$ –25.1 (*c* 0.14, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (s, 1H), 7.53-7.52 (m, 1H) 7.38-7.19 (m, 12H), 6.93 (dd, *J* = 2.5 and 0.92 Hz, 1H), 6.69 (dd, *J* = 15.8 and 7.3 Hz, 1H), 6.40 (d, *J* = 15.8 Hz, 1H), 5.07 (d, *J* = 7.3 Hz, 1H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 142.8, 137.2, 135.2, 132.0, 130.7, 128.49 × (2+2), 128.47, 128.3 × 2, 127.2, 126.5, 126.3 × 2, 124.9, 123.8, 122.2, 118.4, 112.7, 112.6, 45.8; HPLC (Daicel CHIRALPAK® IB, 0.46 ϕ × 25 cm; Hexane:EtOH = 99:1, 0.9 mL/min, UV 254 nm) t_R = 62.6 min (major) and 71.8 min (minor).

(*R*)-(–)-4-Bromo-3-((*E*)-1,3-diphenylallyl)-1*H*-indole ((*R*)-10l) (**Table 4**, entry 12).[2] Compound (*R*)-**10l** was obtained according to the general procedure in 72% yield (55.5 mg, 0.14 mmol) as a brown solid; mp 81-83 °C; 82% ee; $[\alpha]^{20}_{D}$ –35.1 (*c* 0.015, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (s, 1H), 7.36-7.17 (m, 12H), 7.03-6.96 (m, 2H), 6.74 (dd, *J* = 15.8 and 6.5 Hz, 1H), 6.22 (dd, *J* = 15.8 and 1.3 Hz, 1H), 5.90 (d, *J* = 7.0 Hz, 1H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 143.9, 137.7, 137.6, 133.7 , 130.6, 128.9 × 2, 128.4 × 2, 128.2 × 2, 127.0, 126.2 × 2, 126.1, 124.9, 124.8, 124.3, 122.9, 119.0, 114.3, 110.5, 44.7; HPLC (Daicel CHIRALPAK® IA-3, 0.46 ϕ × 25 cm; Hexane:2-PrOH = 99:1, 0.5 mL/min, UV 254 nm) t_R = 80.4 min (minor) and 88.5 min (major).

(*R*)-(–)-3-((*E*)-1,3-Diphenylallyl)-2-phenyl-1*H*-indole ((*R*)-10m) (**Table 4**, entry 13).[2] Compound (*R*)-**10m** was obtained according to the general procedure in 72% yield (55.8 mg, 0.14 mmol) as a brown solid; mp 87-89 °C; 89% ee; $[\alpha]^{20}_{D}$ –58.3 (*c* 0.17, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (s, 1H), 7.55-7.15 (m, 18H), 7.02-6.98 (m, 1H), 6.89 (dd, *J* = 15.8 and 7.3 Hz, 1H), 6.41 (dd, *J* = 15.9 and 1.1 Hz, 1H), 5.28 (d, *J* = 7.1 Hz, 1H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 143.4, 137.4, 136.2, 135.6, 132.9, 132.2, 131.0, 128.8 × 2, 128.6 × 2, 128.4 × 2, 128.3 × 2, 128.2 × 2, 128.0, 127.9, 127.1, 126.3 × 2, 126.1, 122.1, 121.2, 119.7, 113.8, 110.9, 45.1; HPLC (Daicel CHIRALPAK® IB, 0.46 ϕ × 25 cm; Hexane:EtOH = 99:1, 0.9 mL/min, UV 254 nm) t_R = 20.9 min (major) and 23.0 min (minor).

3-2. References for Product Characterization

(1) Mino, T.; Takaya, K.; Koki, K.; Akimoto, N.; Yoshida, Y.; Kasashima, Y.; Sakamoto, M. Axially chiral *N*-alkyl-*N*-cinnamoyl amide type P,olefin ligands for Pd-catalyzed reactions. *Org. Biomol. Chem.* **2023**, *21*, 2775-2778.

(2) Tanaka, Y.; Mino, T.; Akita, K.; Sakamoto, M.; Fujita, T. Development of Chiral (*S*)-Prolinol-Derived Ligands for Palladium-Catalyzed Asymmetric Allylic Alkylation: Effect of a Siloxymethyl Group on the Pyrrolidine Backbone. *J. Org. Chem.* **2004**, *69*, 6679-6687.

4. DFT Calculations

4-1. General Information for DFT Calculations

All calculations were carried with the Gaussian 16 (revision C.01) program package.[1] The molecular structures and harmonic vibrational frequencies were obtained using ωB97X-D functional[2]/ SDD[3] (for Palladium atom) and 6-31+G*[4] basis sets (for other atoms) were used. Geometry optimization and vibrational analysis were performed at the same level. All stationary points were optimized without any symmetry assumptions and characterized by normal coordinate analysis at the same level of theory (number of imaginary frequencies, NIMAG, 0 for minima and 1 for TSs). The thermal corrections were computed at 298.15 K and 1 atm. Connectivity of the stationary points was the "pseudo" intrinsic reaction coordinate (IRC) method,[5] where IRC calculations were performed for 20 to 50 steps form the TS (in both forward and backward directions) and subsequent structures were optimized to obtain the corresponding local minima.[6] Single point energies were calculated at the ωB97X-D/def2-TZVPP[7] level of theory for the whole molecules and the self-consistent reaction field (SCRF) method based on the polarizable continuum model (smd)[8] was employed to evaluate the solvent reaction field (acetonitrile; e = 36.64). The reported energies are a sum of potential energies calculated at the ωB97X-D/SDD and 6-31+G* level of theory and the thermochemistry corrections. The Non-Covalent Interaction (NCI) analysis was performed by NCIPLOT version 4.2[9] and visualized by Visual Molecular Dynamics (VMD)[10].

4-2. Investigation of π-allyl-palladium complex with (*S*,a*R*)-4e and -4f

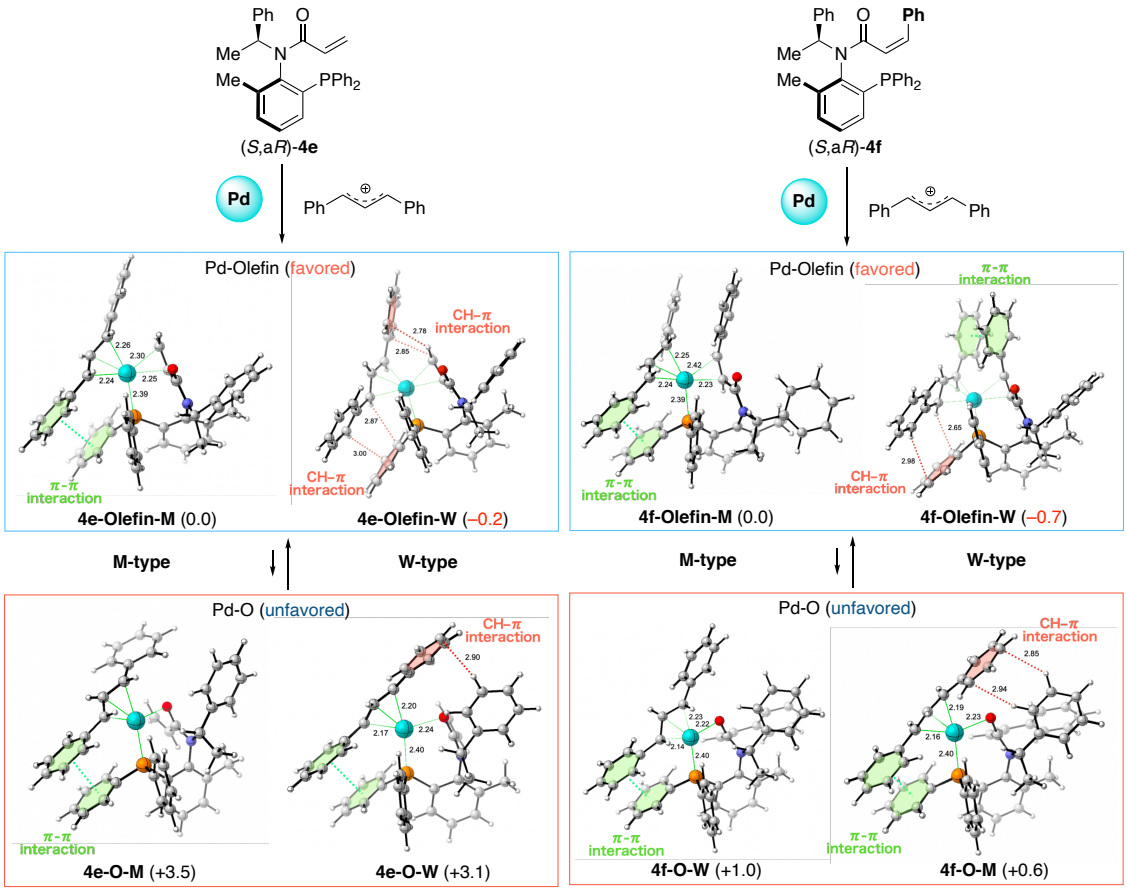


Figure S1. The comparison energy between the M- and W-type π-allyl palladium complexes with (*S*,a*R*)-**4e** and -**4f**. Energy changes and bond lengths at the ωB97X-D/def2-TZVPP/SMD(MeCN)//ωB97X-D/SDD (for palladium atom) and 6-31+G* (for the rest) are shown in kcal/mol and Å, respectively.

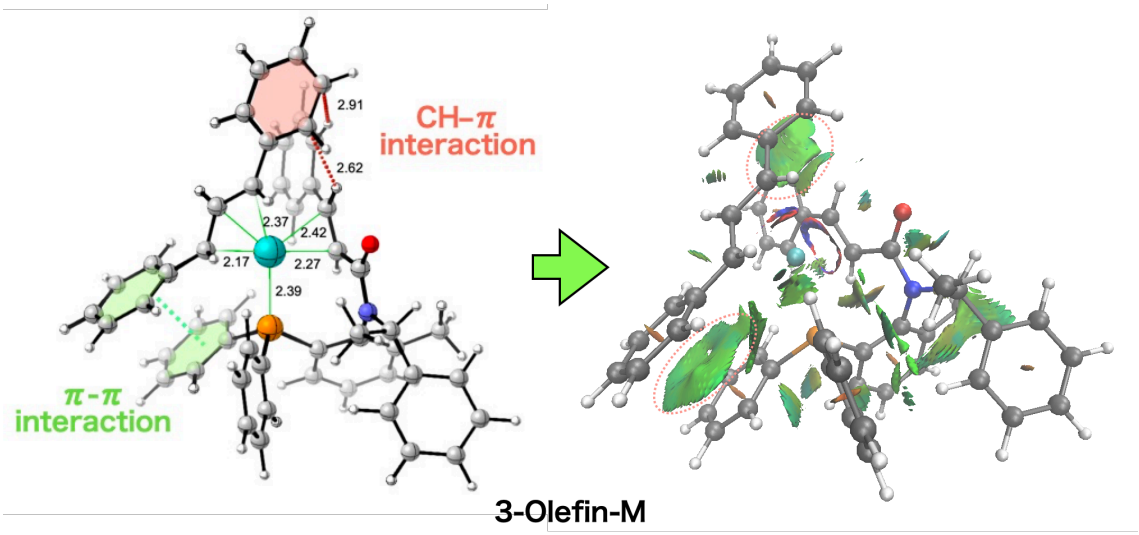
We also investigated the π-allyl complexes with ligands (*S*,a*R*)-**4e** and -**4f**, which yielded products with the opposite stereochemistry compared to (*S*,a*R*)-**3**. For the acrylamide ligand **4e**, olefin-coordinated palladium complexes were found to be more stable. In particular, the W-type complex (**4e-Olefin-W**) is slightly more stable than the M-type complex (**4e-Olefin-M**) due to two CH-π interactions of the aromatic ring on the π-allyl with acrylamide olefin and with benzene ring on phosphine atom.

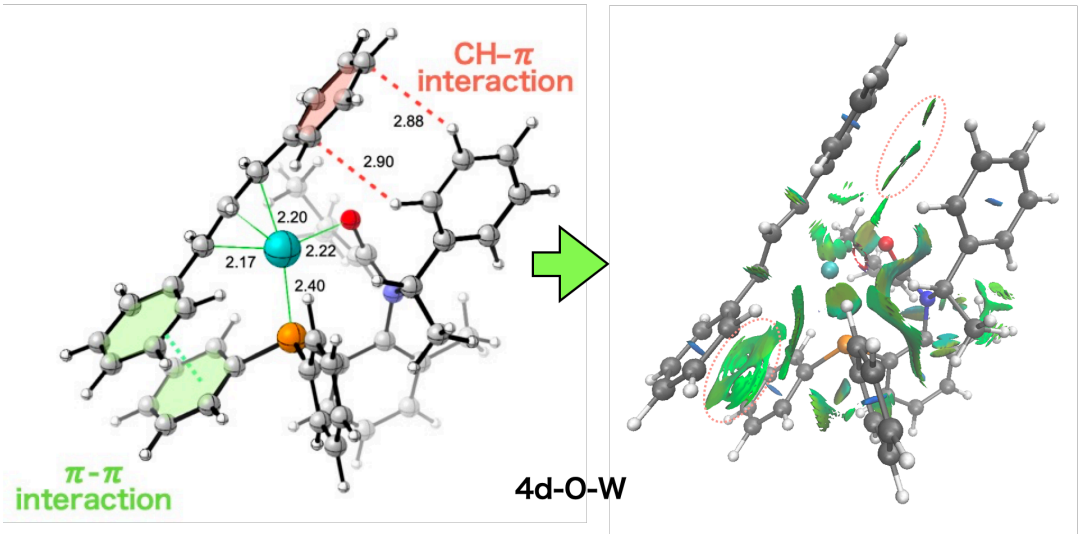
In the case of **4f**, the cis-isomer of **3**, olefin-coordinated palladium complexes were also preferred over oxygen-coordinated complexes, although the energy gap was small. Notably, the W-type complex (**4f-Olefin-W**) exhibited a π-π interaction between the benzene ring of the cis-cinnamoyl group and aromatic ring on the π-allyl. Additionally,

CH-π interaction between the hydrogen on π-allyl group and the aromatic ring on the phosphine further stabilized this W-type complex, making it the predominant species. These calculations suggest that palladium complexes with (*S*,a*R*)-**4e** and **4f** preferentially adopt a W-type conformation, though the underlying stabilizing interactions differ. These results align with experimental observations.

4-3. Visualization of non-covalent interactions using NCIPLOT

We visualized the non-covalent interactions (NCIs), such as π–π and CH–π interactions, in the stable complexes **3-Olefin-M**, **4d-O-W**, **4e-Olefin-W**, and **4f-Olefin-W** using NCIPLOT software[9] (**Figure S2**). The green patches indicate regions where positive van der Waals forces contribute to complex stabilization.





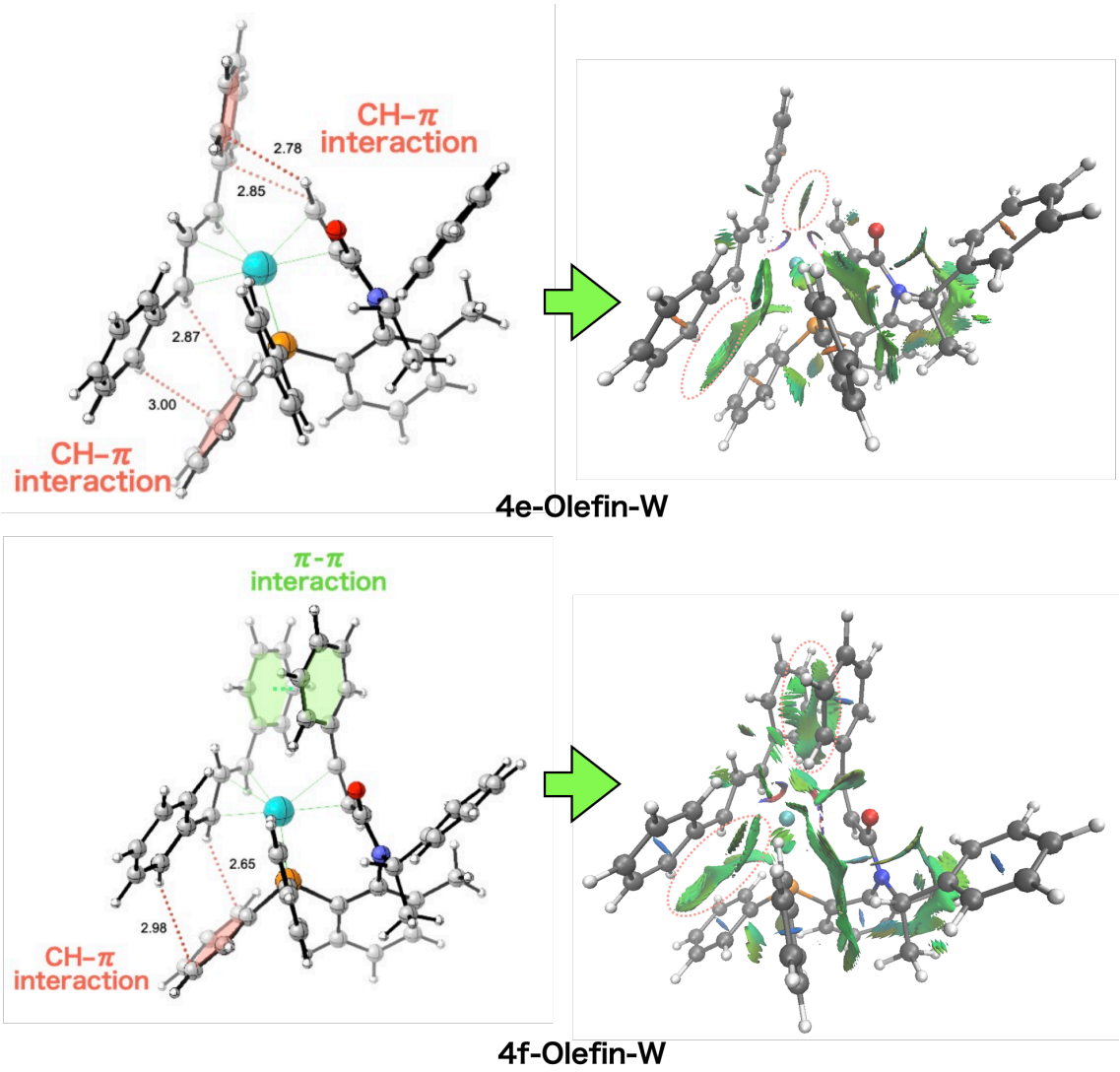


Figure S2. Visualization of π-π and CH-π interactions in the stable complexes **3-Olefin-M**, **4d-O-W**, **4e-Olefin-W**, and **4f-Olefin-W** using NCIPLOT.

4-4. References for DFT calculations

(1) Gaussian 16, Revision C.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.;

Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2016

(2) Chai, J. D.; Head-gordon, M. Long-range corrected double-hybrid density functionals. *J. Chem. Phys.* **2009**, *131*, 174105–174117.

(3) (a) Fuentealba, P.; Preuss, H.; Stoll, H.; Szentpaly, L. V. A proper account of core-polarization with pseudopotentials: single valence-electron alkali compounds. *Chem. Phys. Lett.* **1982**, *89*, 418–422. (b) Szentpaly, L. V.; Fuentealba, P.; Preuss, H.; Stoll, H. Pseudopotential calculations on Rb_2^+, Cs_2^+, RbH^+, CsH^+ and the mixed alkali dimer ions. *Chem. Phys. Lett.*, **1982**, *93*, 555–559.

(4) (a) Clark, T.; Chandrasekhar, J.; Spitznagel, G. W.; Schleyer, P. V. R. Efficient Diffuse Function-Augmented Basis Sets for Anion Calculations. III. The 3-21+G Basis Set for First-Row Elements, Li-F. *J. Comput. Chem*. **1983**, *4*, 294–301. (b) Krishnan, R.; Binkley, J. S.; Seeger, R.; Pople, J. A. Self‐consistent Molecular Orbital Methods. XX. A Basis Set for Correlated Wave Functions. *J. Chem. Phys*. **1980**, *72*, 650–654.

(5) (6) (a) Fukui, K. The path of chemical reactions - the IRC approach. *Acc. Chem. Res*. **1981**, *14*, 363–368. (b) Ishida, K.; Morokuma, K.; Komornicki, A. The intrinsic reaction coordinates. An ab initio calculation for HNC→HCN and $H^- + CH_4 \rightarrow CH_4 + H^-$. *J. Chem. Phys*. **1977**, *66*, 2153–2156. (c) Gonzalez, C.; Schlegel, H. B. An improved algorithm for reaction path following. *J. Chem. Phys*. **1989**, *90*, 2154–2161. (d) Gonzalez, C.; Schlegel, H. B. Reaction path following in mass-weighted internal coordinates. *J. Phys. Chem.* **1990**, *94*, 5523–5527.

(6) Isegawa, M.; Sameera, W. M. C.; Sharma, A. K.; Kitanosono, T.; Kato, M.; Kobayashi, S.; Morokuma, K. Copper-Catalyzed Enantioselective Boron Conjugate Addition: DFT and AFIR Study on Different Selectivities of Cu(I) and Cu(II) Catalysts. *ACS Catal*. **2017**, *7*, 5370–5380.

(7) Weigend, F.; Ahlrichs, R. Balanced Basis Sets of Split Valence, Triple Zeta Valence and Quadruple Zeta Valence Quality for H to Rn: Design and Assessment of Accuracy. *Phys. Chem. Chem. Phys*. **2005**, *7*, 3297–3305.

(8) Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions. *J. Phys. Chem. B* **2009**, *113*, 6378–6396.

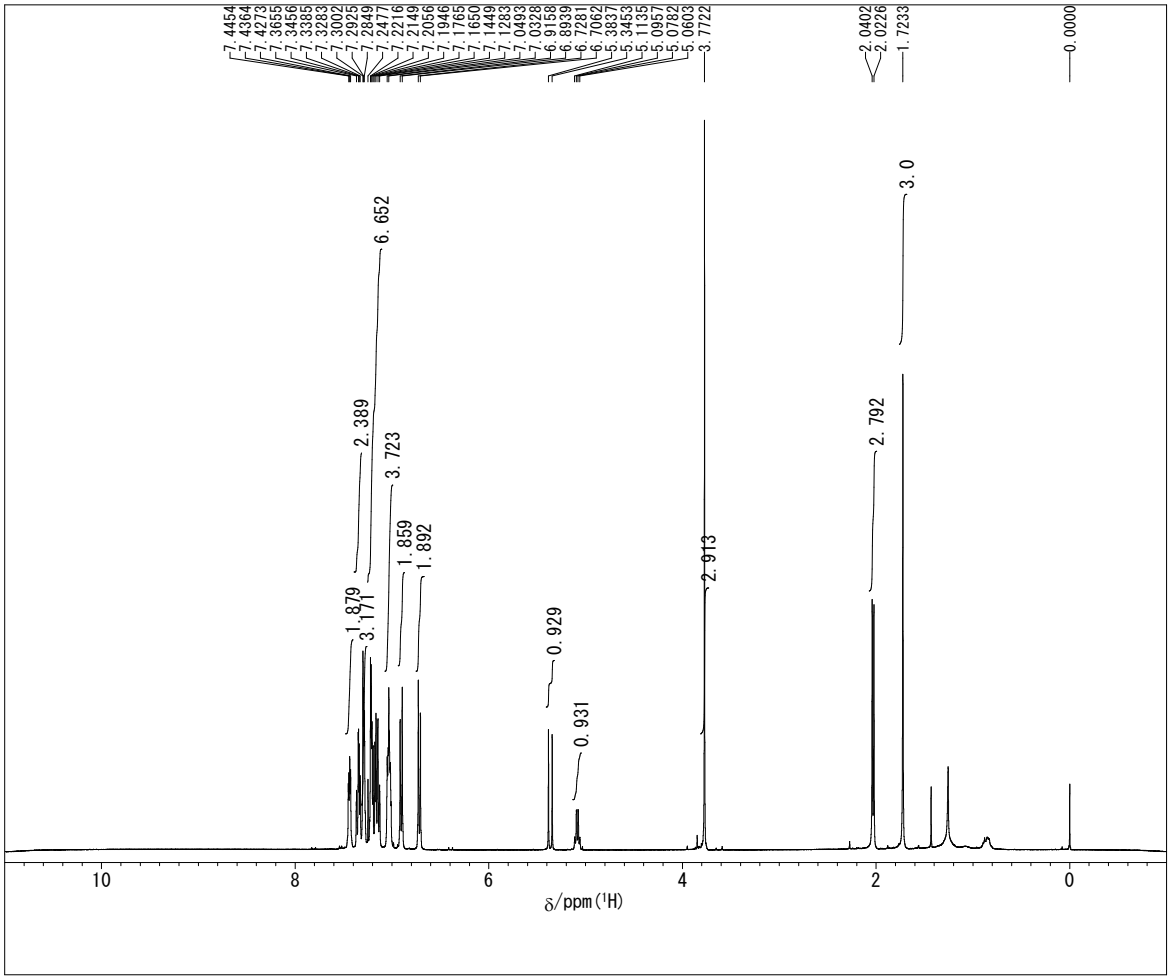
(9) (a) Boto, R. A.; Peccati, F.; Laplaza, R.; Quan, C.; Carbone, A.;Piquemal, J.-P.; Maday, Y.; Contreras-García, J. NCIPLOT4: Fast, robust, and quantitative analysis of noncovalent interactions. *J. Chem.Theory Comput.* **2020**, *16*, 4150−4158. (b) Contreras-García, J.; Johnson, E. R.; Keinan, S.; Chaudret, R.; Piquemal, J.-P.; Beratan, D. N.; Yang, W. NCIPLOT: program for plotting noncovalent interaction regions. *J. Chem. Theory Comput.* **2011**, *7*, 625−632. (c) Johnson, E. R.; Keinan, S.; Mori-Sanchez, P.; Contreras-García, J.; Cohen, A. J.; Yang, W. Revealing noncovalent interactions. *J. Am. Chem. Soc.* **2010**, *132*, 6498−6506.

(10) Humphrey, W.; Dalke, A.; Schulten, K. VMD: Visual molecular dynamics. *J. Molec. Graphics* **1996**, *14*, 33–38.

5. NMR Spectra and chiral phase HPLC chart

5-1. ^{1}H NMR, ^{13}C{^{1}H} NMR and ^{31}P{^{1}H} NMR of 4

^{1}H NMR, ^{13}C{^{1}H} NMR and ^{31}P{^{1}H} NMR of (*S*,a*S*)-**4a**



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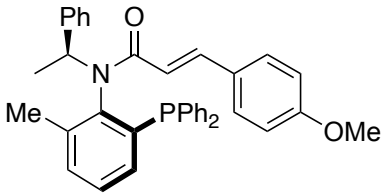
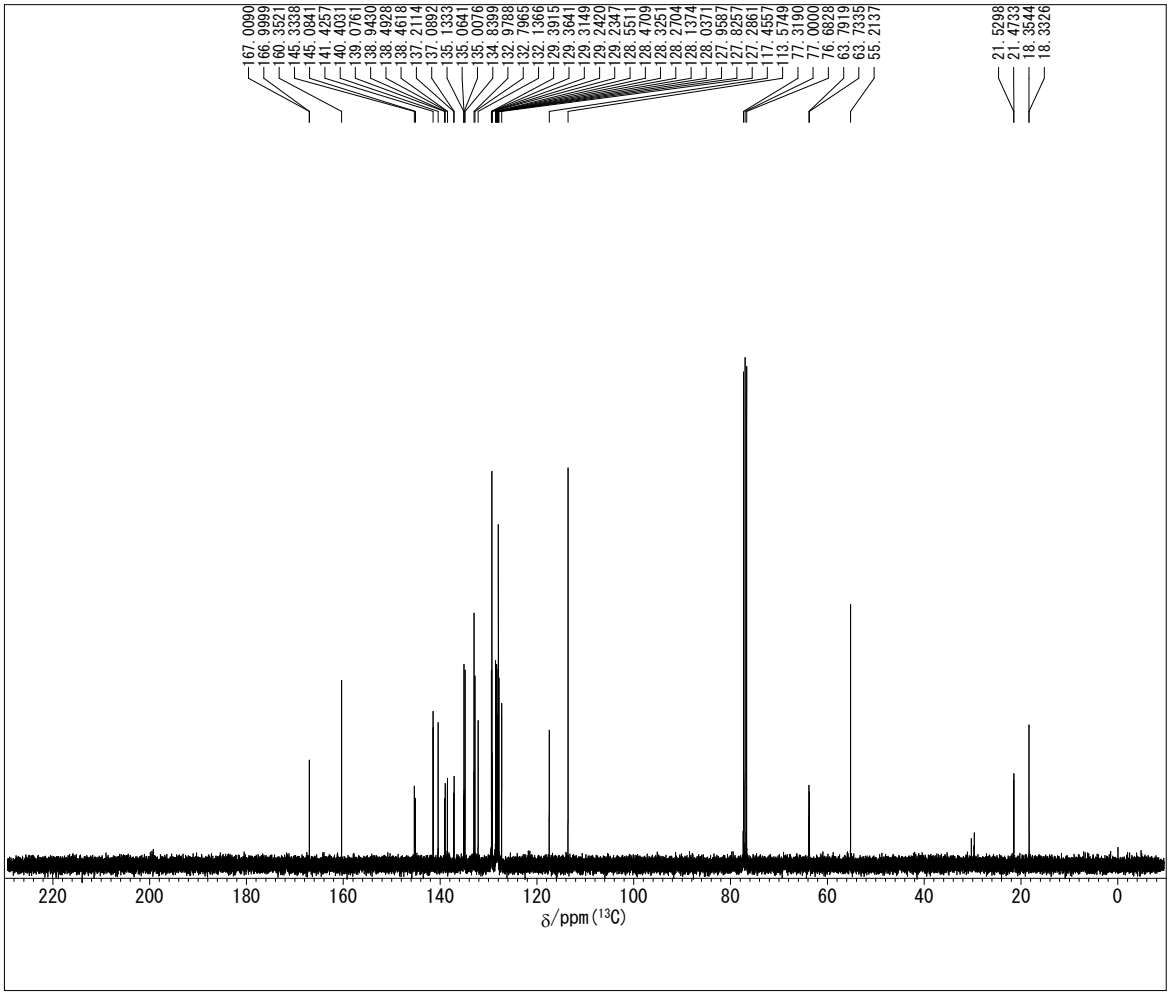
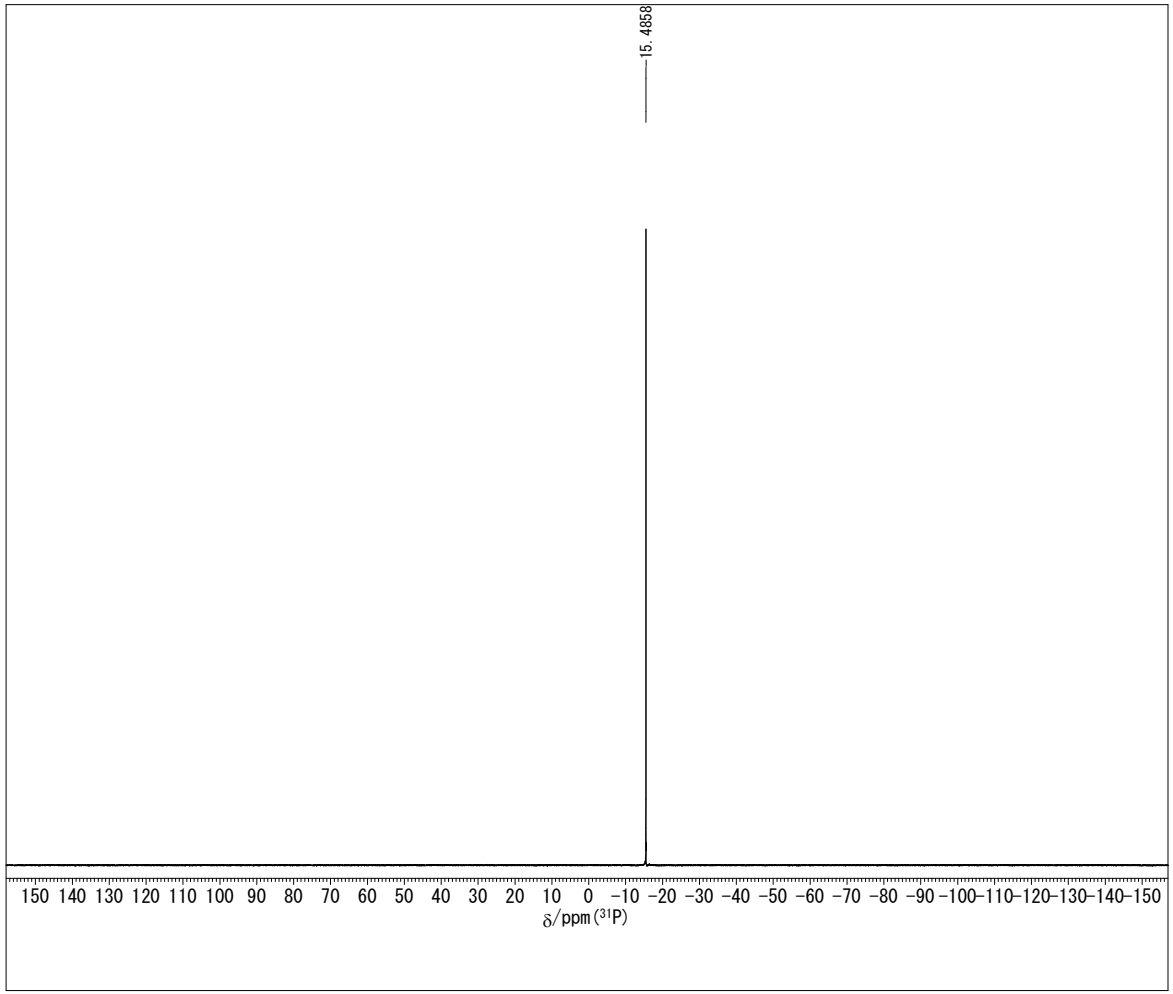
PRNT_DATE 2024/Apr/30 08:27:16
COMNT



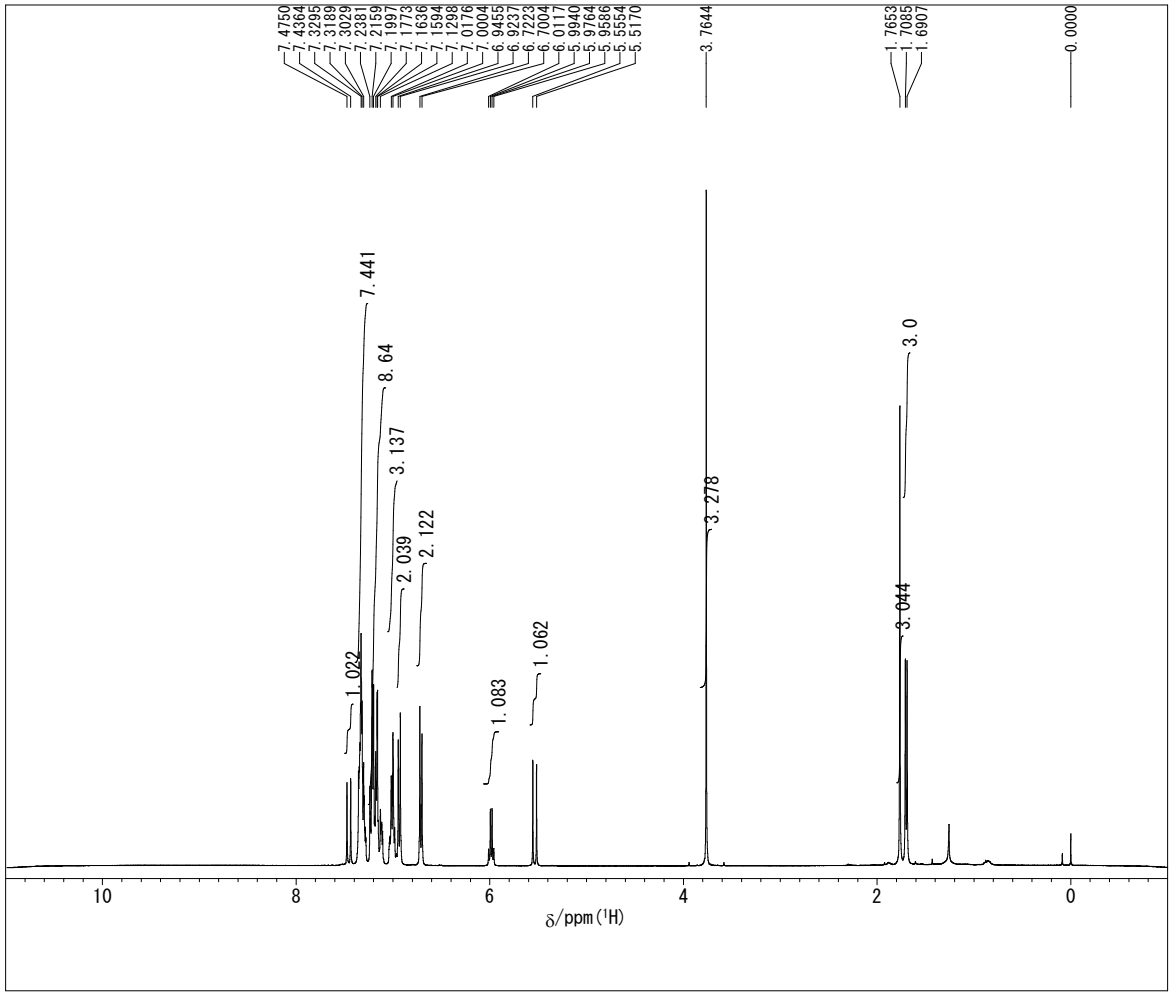


DATIM	14/Jan/2021 17:45:03
OBNUC	^{13}C
EXMOD	ZGPG30
OFR	100.61 MHz
OBSET	0.0 kHz
OBFIN	11067.71 Hz
POINT	131072(ZeroFill :×4)
FREQU	24038.46 Hz
SCANS	128
ACQTM	1.3631 s
PD	2.0 s
PW1	10.0 μs
CTEMP	17.25 °C
SLVNT	$CDCL_3$
EXREF	77.0 ppm
BF	0.25 Hz
RGAIN	2050
PRNT_DATE	2024/Apr/30 08:31:48
COMNT	

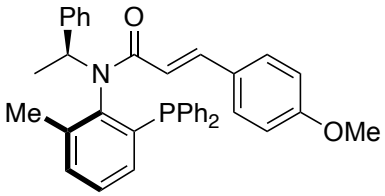


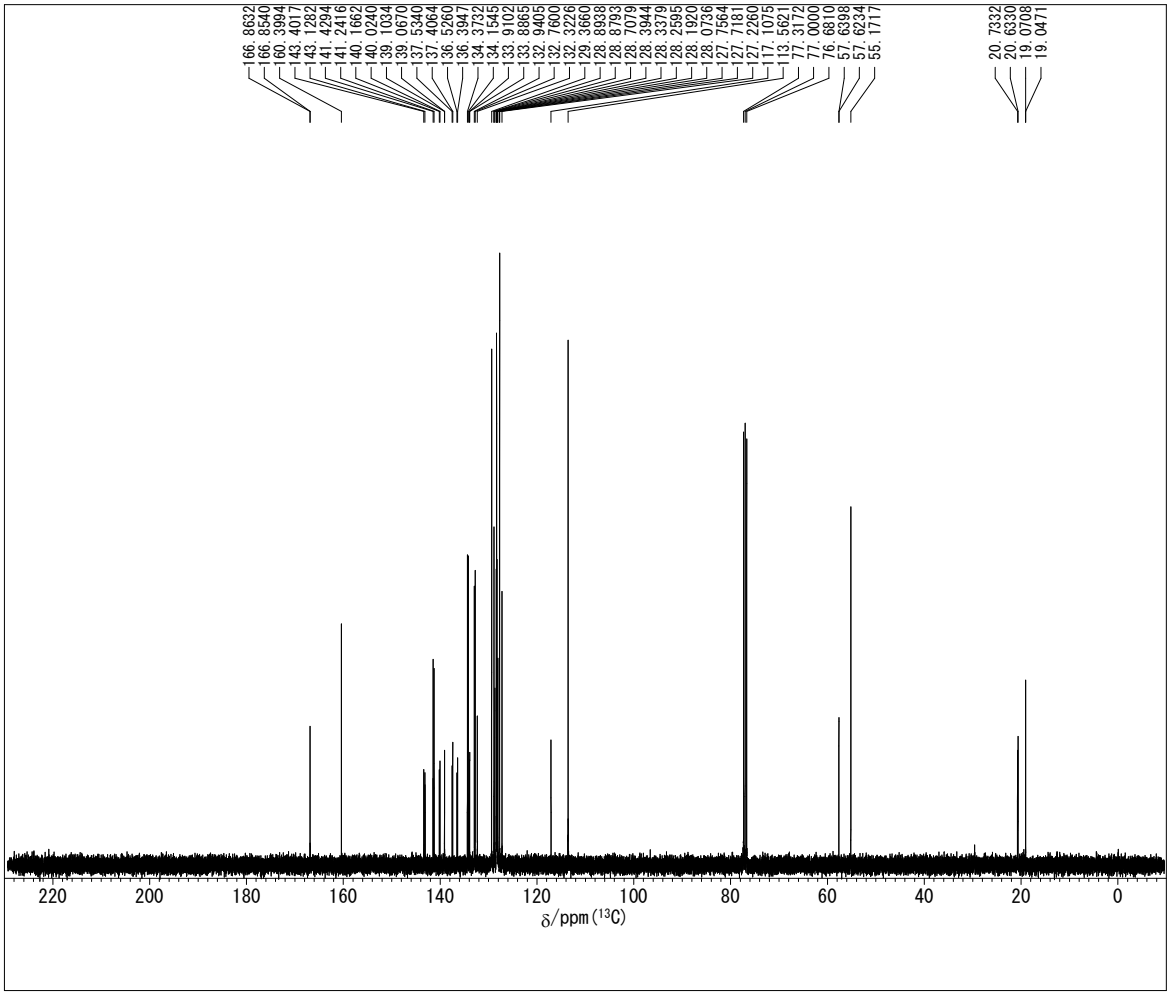
DATIM	14/Jan/2021 17:50:37
OBNUC	^{31}P
EXMOD	ZGPG30
OFR	161.98 MHz
OBSET	0.0 kHz
OBFIN	10001.57 Hz
POINT	32768
FREQU	51020.41 Hz
SCANS	32
ACQTM	0.6423 s
PD	2.0 s
PW1	10.0 μs
CTEMP	17.15 °C
SLVNT	$CDCL_3$
EXREF	157.9655 ppm
BF	0.25 Hz
RGAIN	2050
PRNT_DATE	2024/May/08 17:50:22
COMNT	

^{1}H NMR, ^{13}C{^{1}H} NMR and ^{31}P{^{1}H} NMR of (*S*,a*R*)-**4a**

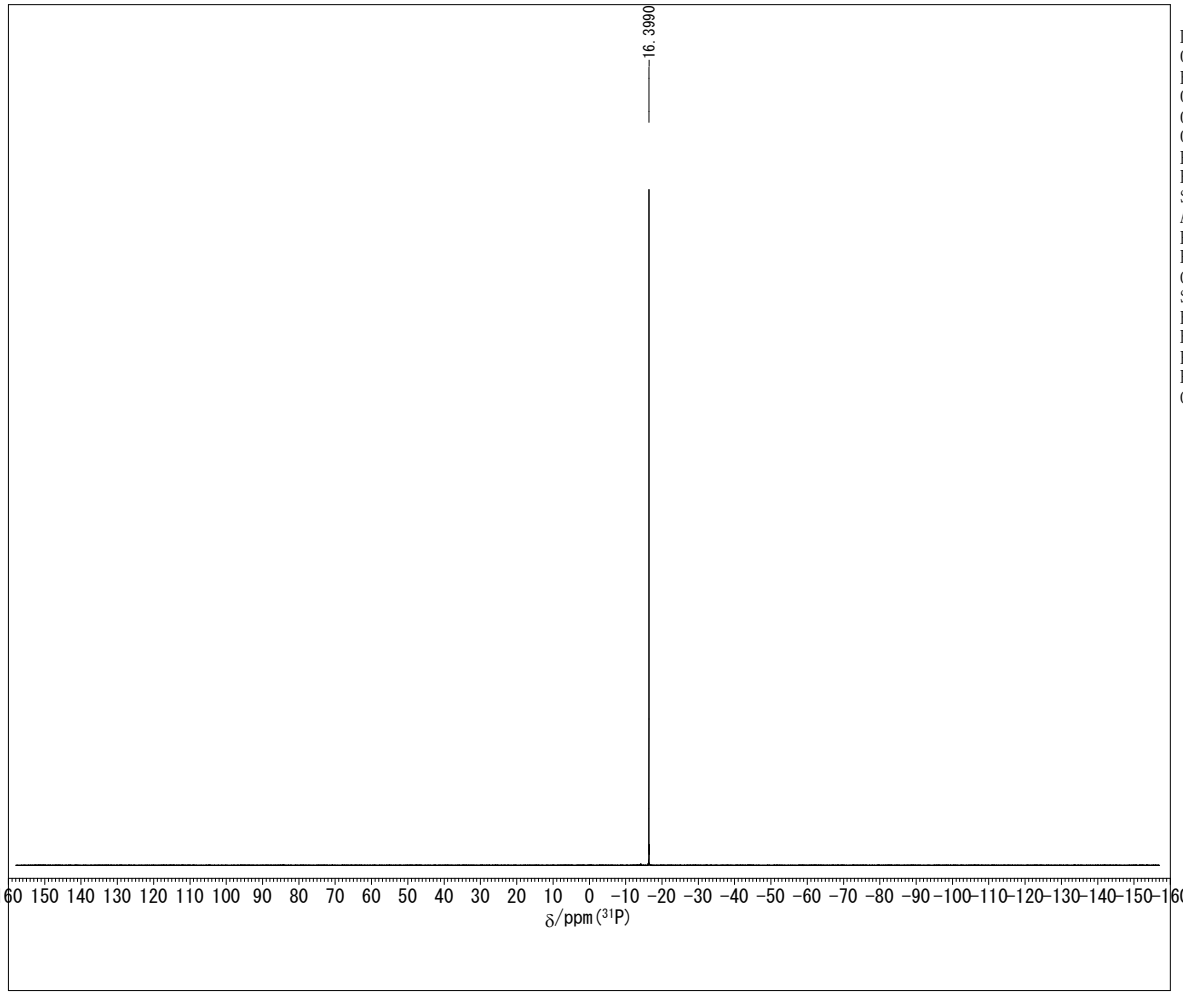


DATIM 14/Jan/2021 17:17:18
OBNUC ^{1}H
EXMOD ZG30
OFR 400.18 MHz
OBSET 0.0 kHz
OBFIN 2008.224 Hz
POINT 131072(ZeroFill :×4)
FREQU 4826.255 Hz
SCANS 8
ACQTM 6.7895 s
PD 1.0 s
PW1 14.0 μs
CTEMP 17.11 °C
SLVNT $CDCl_3$
EXREF 0.0 ppm
BF 0.25 Hz
RGAIN 144
PRNT_DATE 2024/Apr/30 08:48:06
COMNT



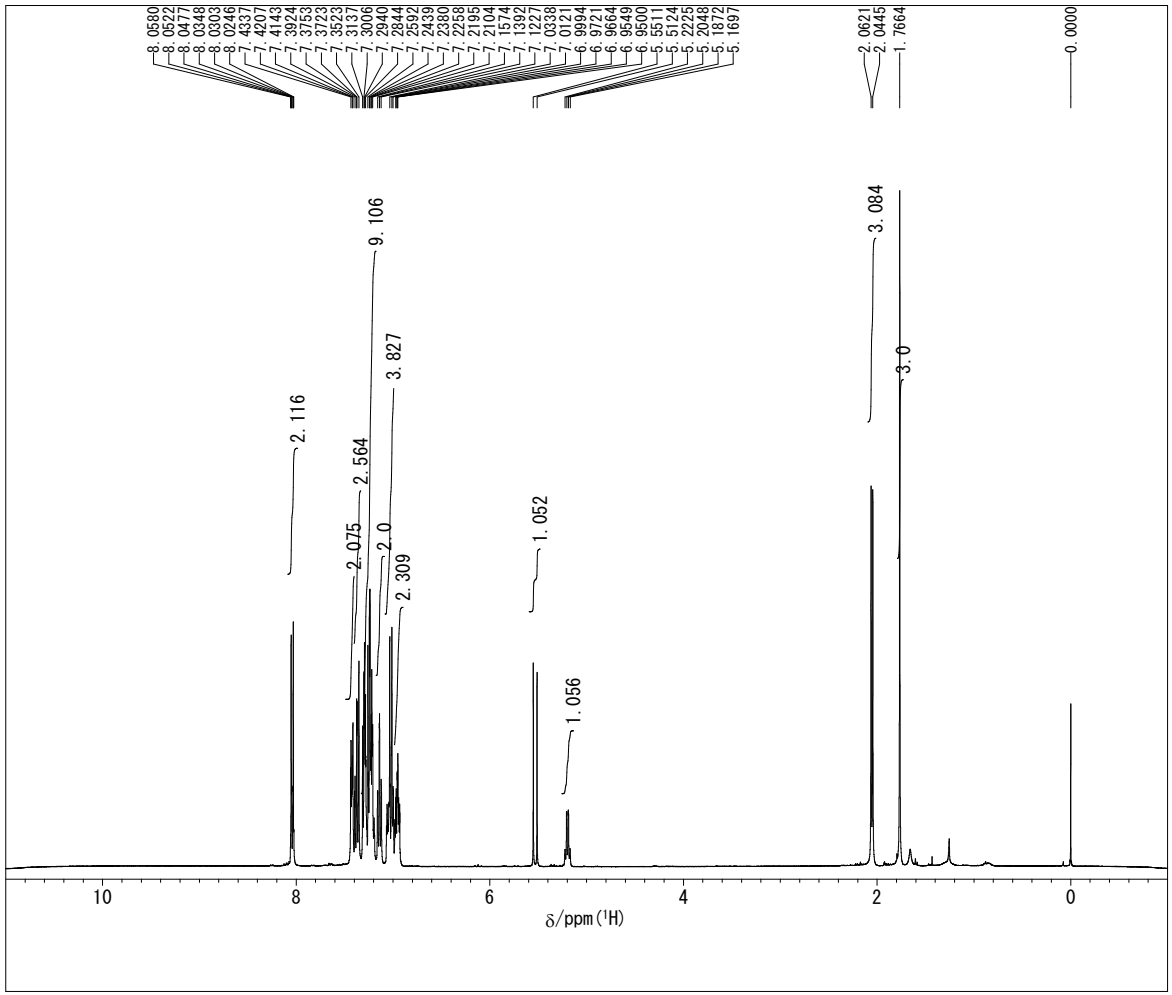


DATIM 14/Jan/2021 18:08:19
OBNUC ^{13}C
EXMOD ZGPG30
OFR 100.61 MHz
OBSET 0.0 kHz
OBFIN 11067.71 Hz
POINT 131072(ZeroFill :×4)
FREQU 24038.46 Hz
SCANS 77
ACQTM 1.3631 s
PD 2.0 s
PW1 10.0 μs
CTEMP 17.15 ℃
SLVNT $CDCL_3$
EXREF 77.0 ppm
BF 0.25 Hz
RGAIN 2050
PRNT_DATE 2024/Apr/30 08:49:32
COMNT

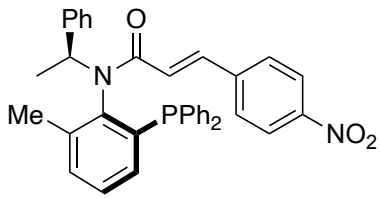


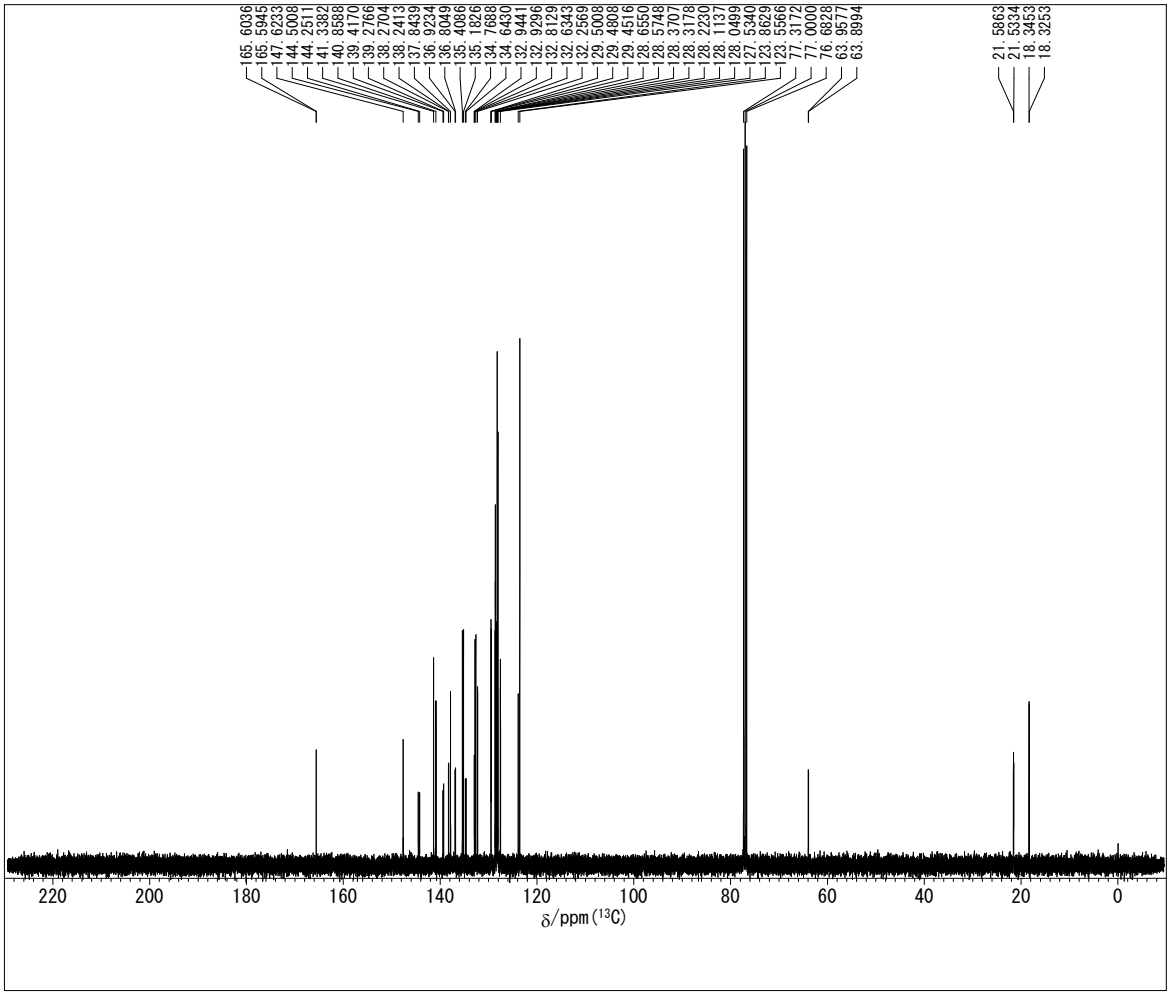
DATIM	14/Jan/2021 18:00:36
OBNUC	^{31}P
EXMOD	ZGPG30>
OFR	161.98 MHz
OBSET	0.0 kHz
OBFIN	10001.57 Hz
POINT	32768
FREQU	51020.41 Hz
SCANS	64
ACQTM	0.6423 s
PD	2.0 s
PW1	10.0 μs
CTEMP	17.15 °C
SLVNT	$CDCL_3$>
EXREF	157.9655 ppm
BF	0.25 Hz
RGAIN	2050
PRNT_DATE	2024/Apr/30 08:51:08
COMNT	

^{1}H NMR, ^{13}C{^{1}H} NMR and ^{31}P{^{1}H} NMR of (*S*,a*S*)-**4b**

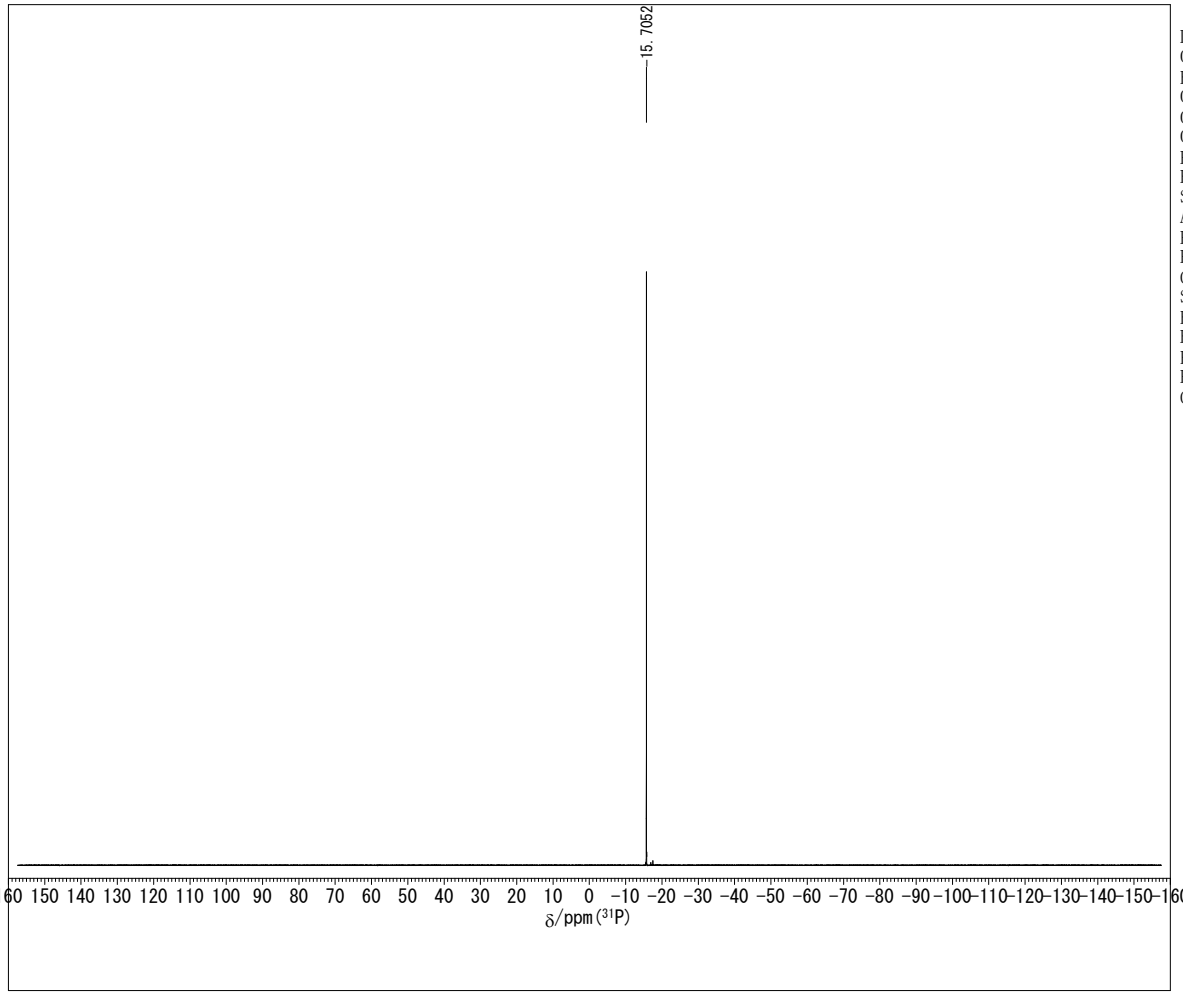


DATIM 11/Dec/2020 13:53:43
OBNUC ^{1}H
EXMOD ZG30
OFR 400.18 MHz
OBSET 0.0 kHz
OBFIN 2008.224 Hz
POINT 131072(ZeroFill :×4)
FREQU 4826.255 Hz
SCANS 16
ACQTM 6.7895 s
PD 1.0 s
PW1 14.0 μs
CTEMP 19.21 °C
SLVNT $CDCl_3$
EXREF 0.0 ppm
BF 0.25 Hz
RGAIN 203
PRNT_DATE 2024/Apr/30 08:58:20
COMNT



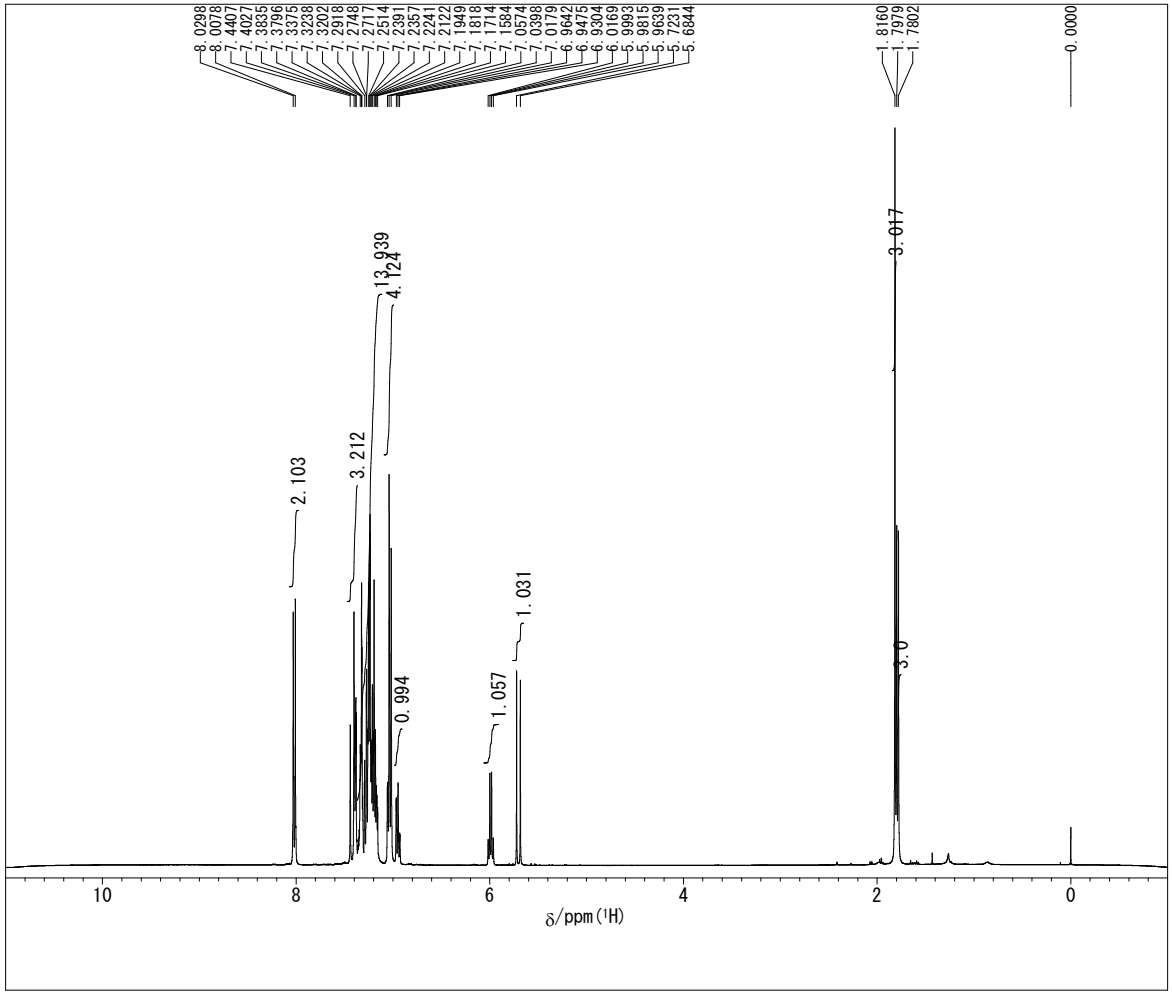


DATIM 11/Dec/2020 16:00:23
OBNUC ^{13}C
EXMOD ZGPG30
OFR 100.61 MHz
OBSET 0.0 kHz
OBFIN 11067.71 Hz
POINT 131072(ZeroFill :×4)
FREQU 24038.46 Hz
SCANS 256
ACQTM 1.3631 s
PD 2.0 s
PW1 10.0 μs
CTEMP 19.25 ℃
SLVNT $CDCL_3$
EXREF 77.0 ppm
BF 0.25 Hz
RGAIN 2050
PRNT_DATE 2024/Apr/30 09:02:02
COMNT

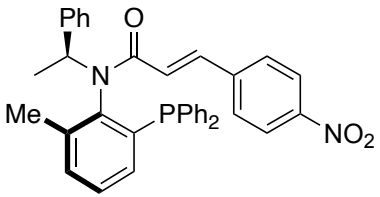


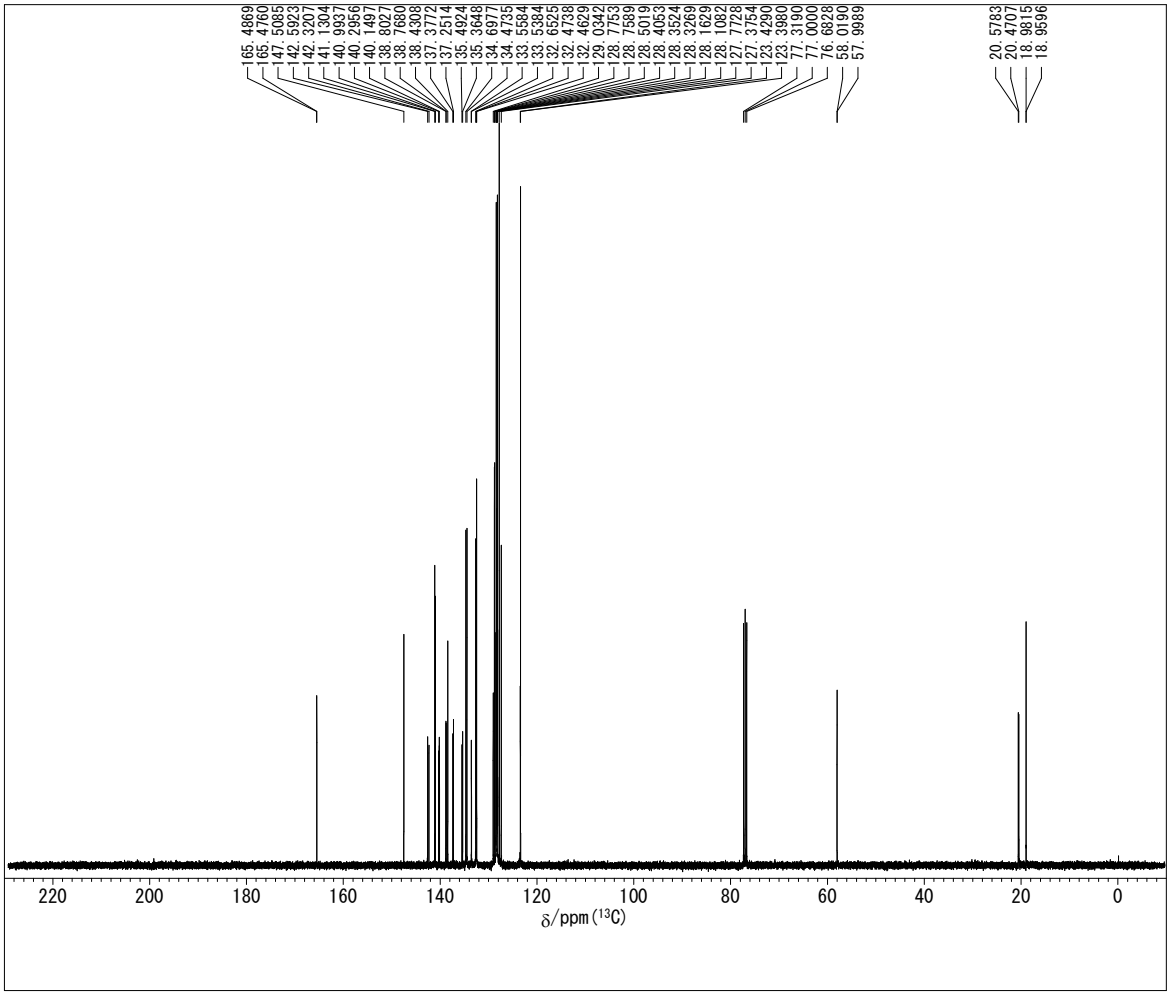
DATIM	11/Dec/2020 14:01:14
OBNUC	^{31}P
EXMOD	ZGPG30>
OFR	162.0 MHz
OBSET	0.0 kHz
OBFIN	9993.149 Hz
POINT	32768
FREQU	51020.41 Hz
SCANS	134
ACQTM	0.6423 s
PD	2.0 s
PW1	15.0 μs
CTEMP	19.81 °C
SLVNT	$CDCL_3$>
EXREF	157.4744 ppm
BF	0.25 Hz
RGAIN	203
PRNT_DATE	2024/Apr/30 09:03:11
COMNT	

^{1}H NMR, ^{13}C{^{1}H} NMR and ^{31}P{^{1}H} NMR of (*S*,a*R*)-**4b**

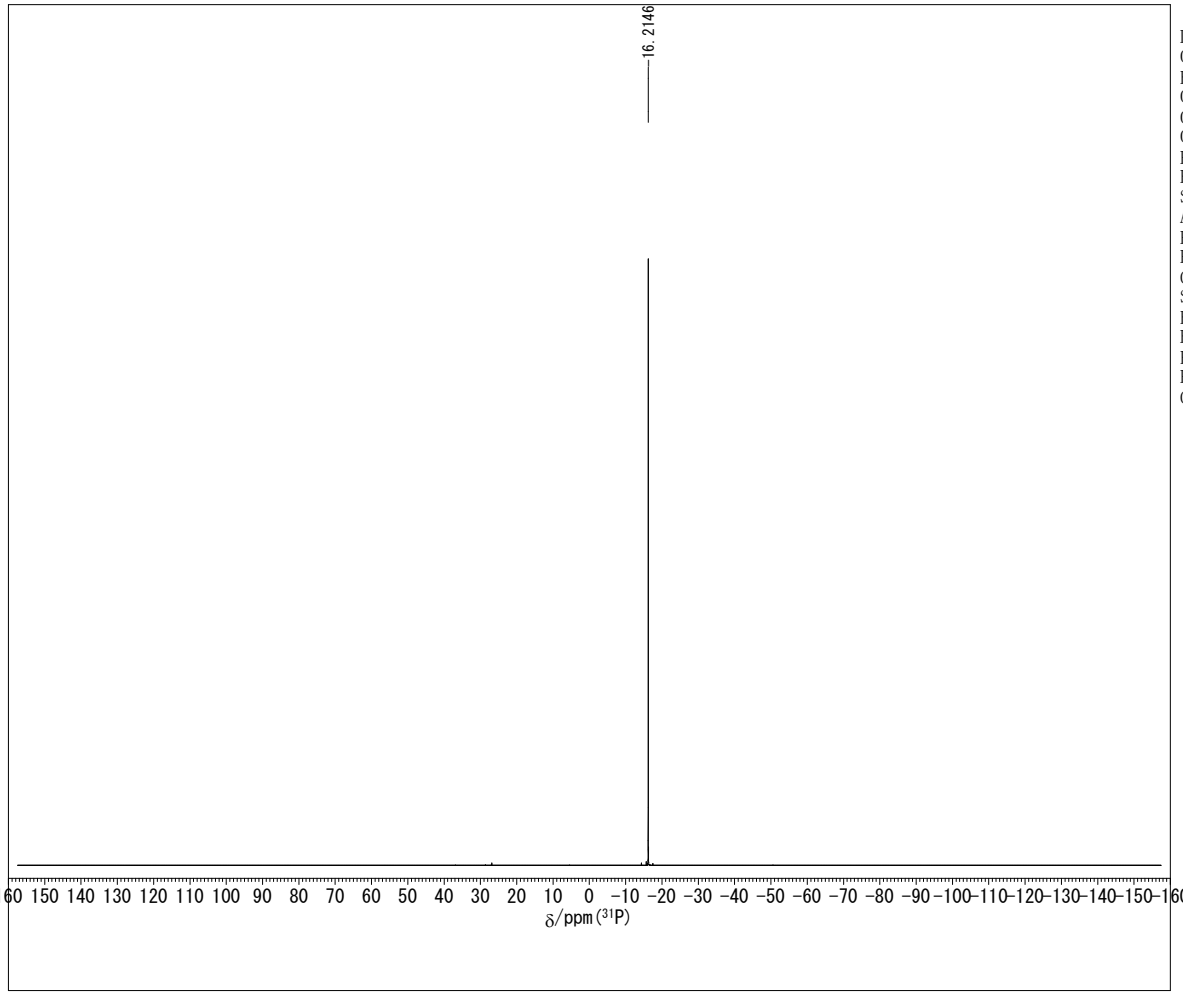


DATIM 11/Dec/2020 14:07:30
OBNUC ^{1}H
EXMOD ZG30
OFR 400.18 MHz
OBSET 0.0 kHz
OBFIN 2008.224 Hz
POINT 131072(ZeroFill :×4)
FREQU 4826.255 Hz
SCANS 16
ACQTM 6.7895 s
PD 1.0 s
PW1 14.0 μs
CTEMP 19.41 °C
SLVNT $CDCl_3$
EXREF 0.0 ppm
BF 0.25 Hz
RGAIN 51
PRNT_DATE 2024/Apr/30 09:09:16
COMNT



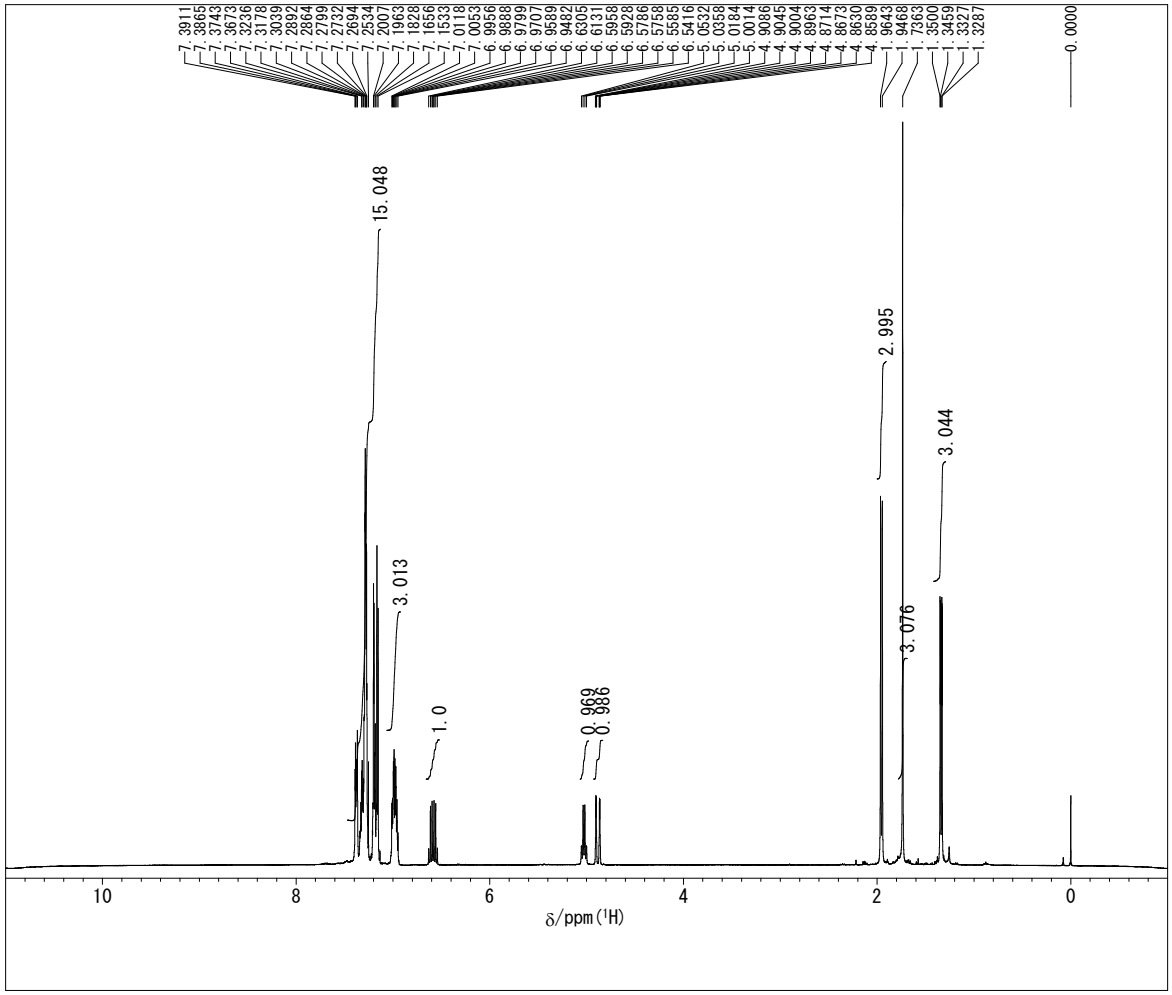


DATIM 11/Dec/2020 16:18:15
OBNUC ^{13}C
EXMOD ZGPG30
OFR 100.61 MHz
OBSET 0.0 kHz
OBFIN 11067.71 Hz
POINT 131072(ZeroFill :×4)
FREQU 24038.46 Hz
SCANS 256
ACQTM 1.3631 s
PD 2.0 s
PW1 10.0 μs
CTEMP 19.25 ℃
SLVNT $CDCL_3$
EXREF 77.0 ppm
BF 0.25 Hz
RGAIN 2050
PRNT_DATE 2024/Apr/30 09:10:18
COMNT

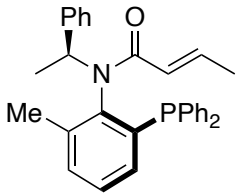


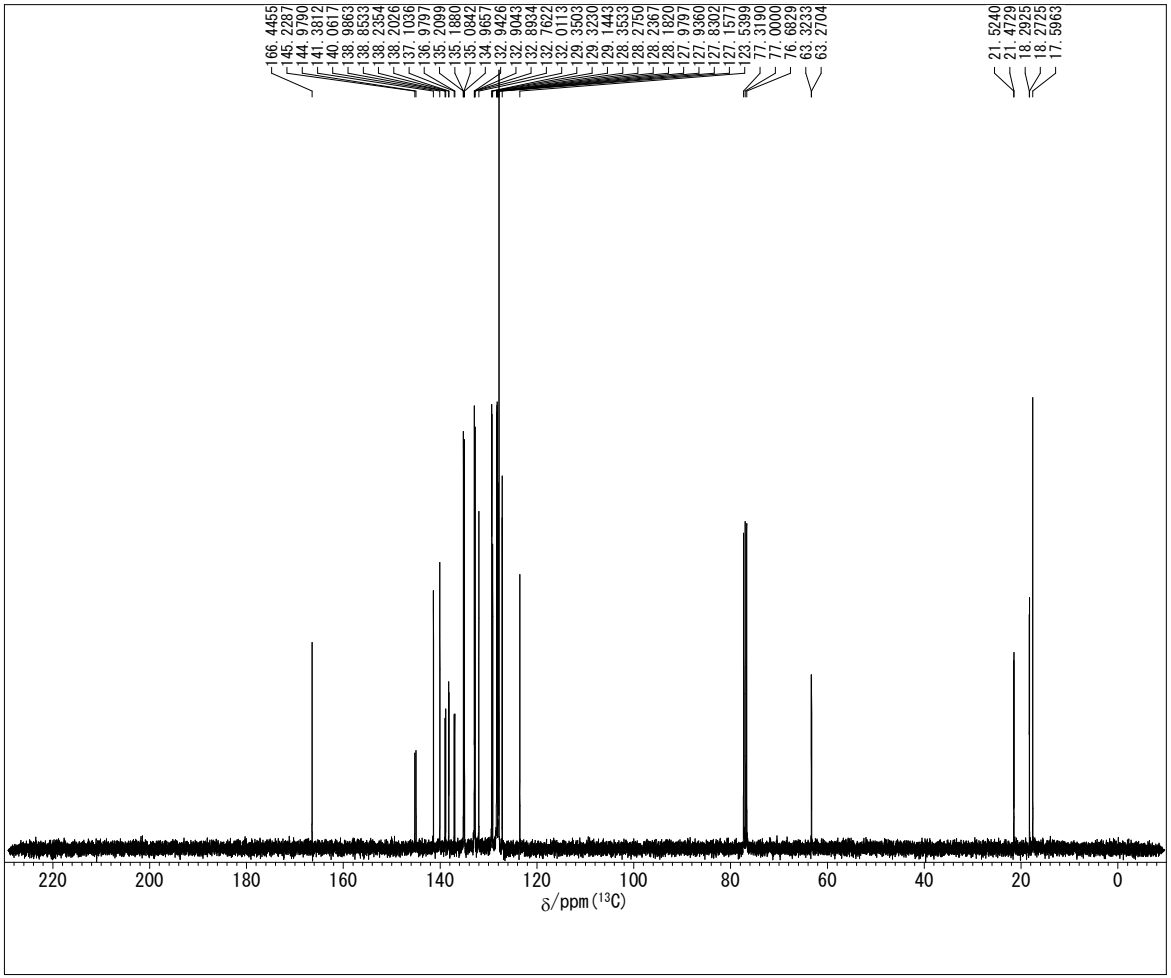
DATIM	11/Dec/2020 14:14:18
OBNUC	^{31}P
EXMOD	ZGPG30>
OFR	162.0 MHz
OBSET	0.0 kHz
OBFIN	9993.149 Hz
POINT	32768
FREQU	51020.41 Hz
SCANS	128
ACQTM	0.6423 s
PD	2.0 s
PW1	15.0 μs
CTEMP	19.81 °C
SLVNT	$CDCL_3$>
EXREF	157.4744 ppm
BF	0.25 Hz
RGAIN	203
PRNT_DATE	2024/Apr/30 09:11:39
COMNT	

^{1}H NMR, ^{13}C{^{1}H} NMR and ^{31}P{^{1}H} NMR of (*S*,a*S*)-**4c**

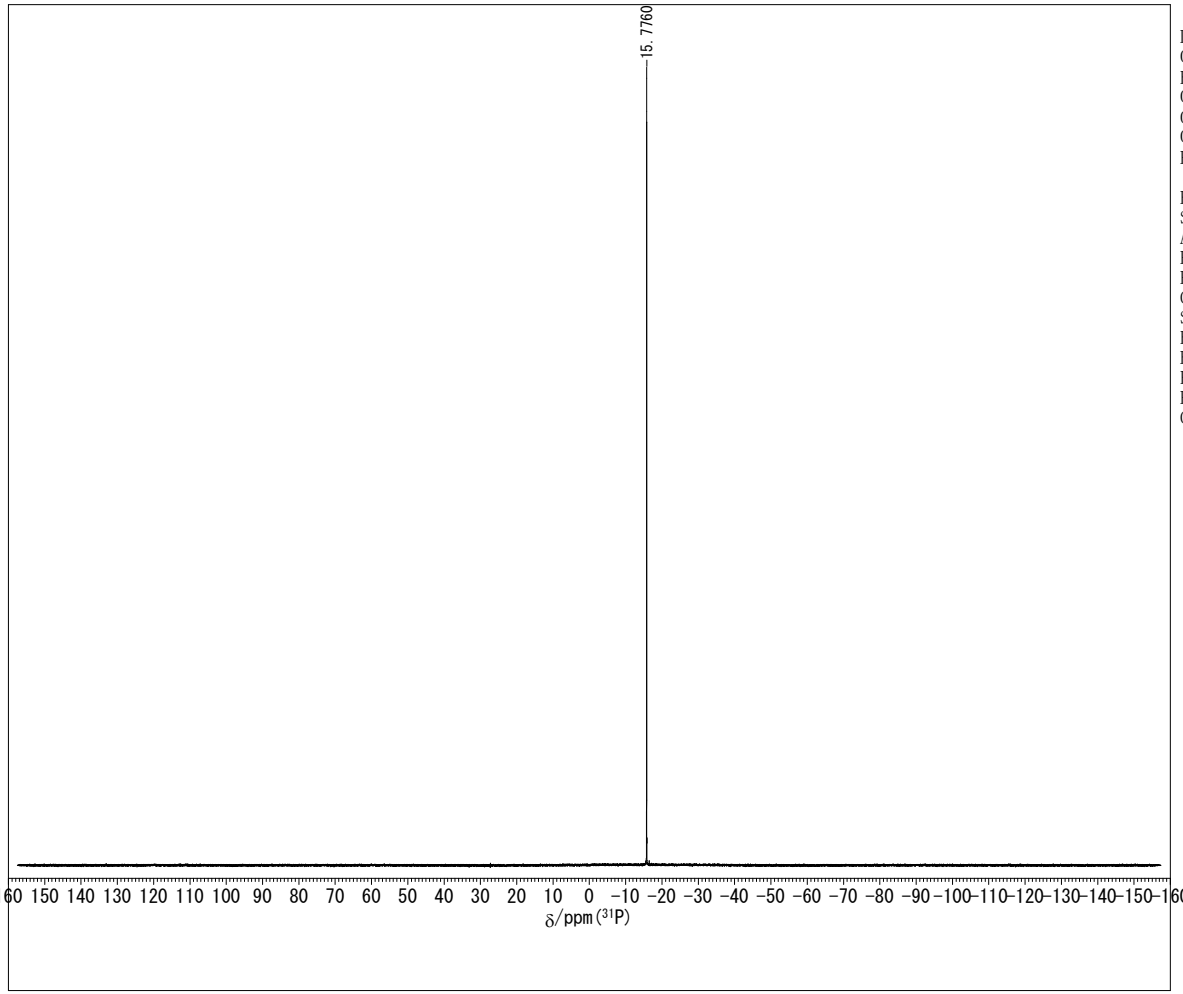


DATIM 25/Oct/2022 11:02:37
OBNUC ^{1}H
EXMOD ZG30>
OFR 400.18 MHz
OBSET 0.0 kHz
OBFIN 2008.224 Hz
POINT 131072(ZeroFill :×4)
FREQU 4826.255 Hz
SCANS 16
ACQTM 6.7895 s
PD 1.0 s
PW1 14.0 μs
CTEMP 20.81 ℃
SLVNT $CDCL_3$>
EXREF 0.0 ppm
BF 0.1473 Hz
RGAIN 81
PRNT_DATE 2024/Apr/30 11:41:21
COMNT



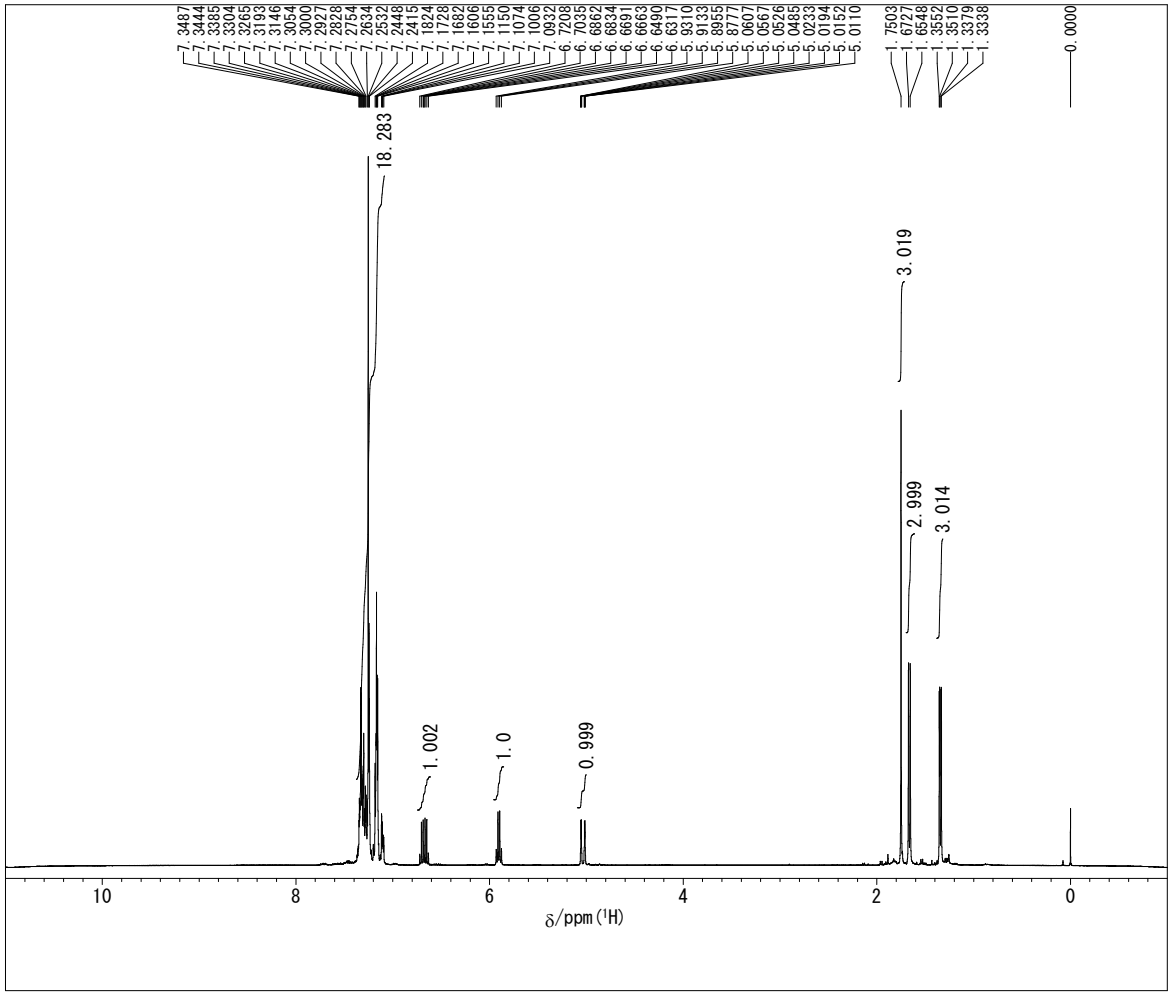


DATIM	07/Sep/2021 10:01:14
OBNUC	^{13}C
EXMOD	ZGPG30>
OFR	100.63 MHz
OBSET	0.0 kHz
OBFIN	11066.5 Hz
POINT	131072(ZeroFill :×4)
FREQU	24038.46 Hz
SCANS	64
ACQTM	1.3631 s
PD	2.0 s
PW1	10.0 μs
CTEMP	22.81 ℃
SLVNT	$CDCL_3$>
EXREF	77.0 ppm
BF	0.7336 Hz
RGAIN	203
PRNT_DATE	2024/May/21 17:47:08
COMNT	

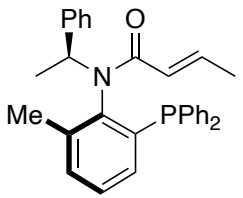


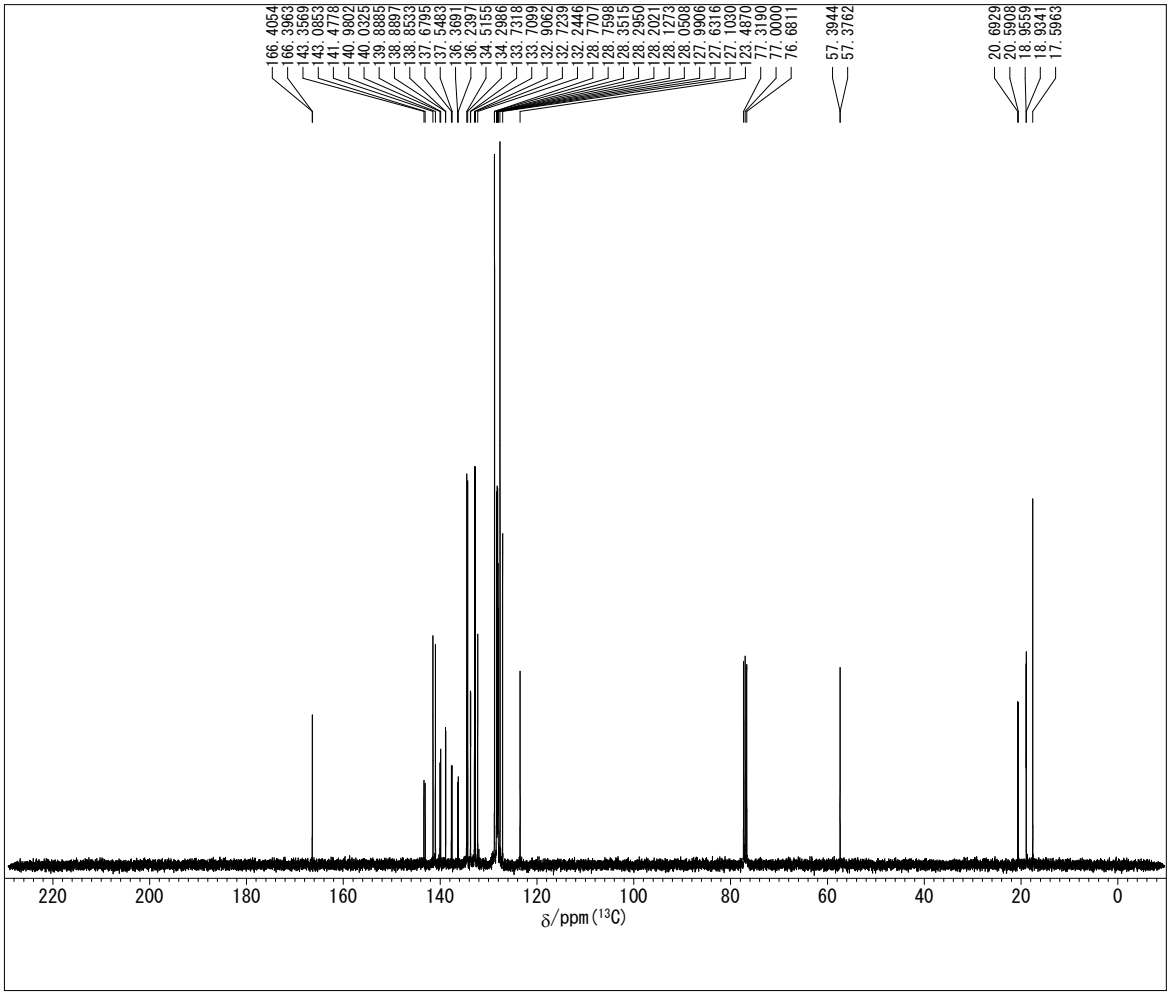
DATIM 01/Sep/2021 14:57:07
OBNUC ^{31}P
EXMOD ZGPG30>
OFR 162.0 MHz
OBSET 0.0 kHz
OBFIN -1.3506 Hz
POINT 131072(ZeroFill :×4)
FREQU 51020.41 Hz
SCANS 16
ACQTM 0.6423 s
PD 2.0 s
PW1 15.0 μs
CTEMP 24.11 ℃
SLVNT $CDCL_3$>
EXREF -15.8 ppm
BF 1.557 Hz
RGAIN 203
PRNT_DATE 2024/Apr/30 11:44:13
COMNT

^{1}H NMR, ^{13}C{^{1}H} NMR and ^{31}P{^{1}H} NMR of (*S*,a*R*)-**4c**

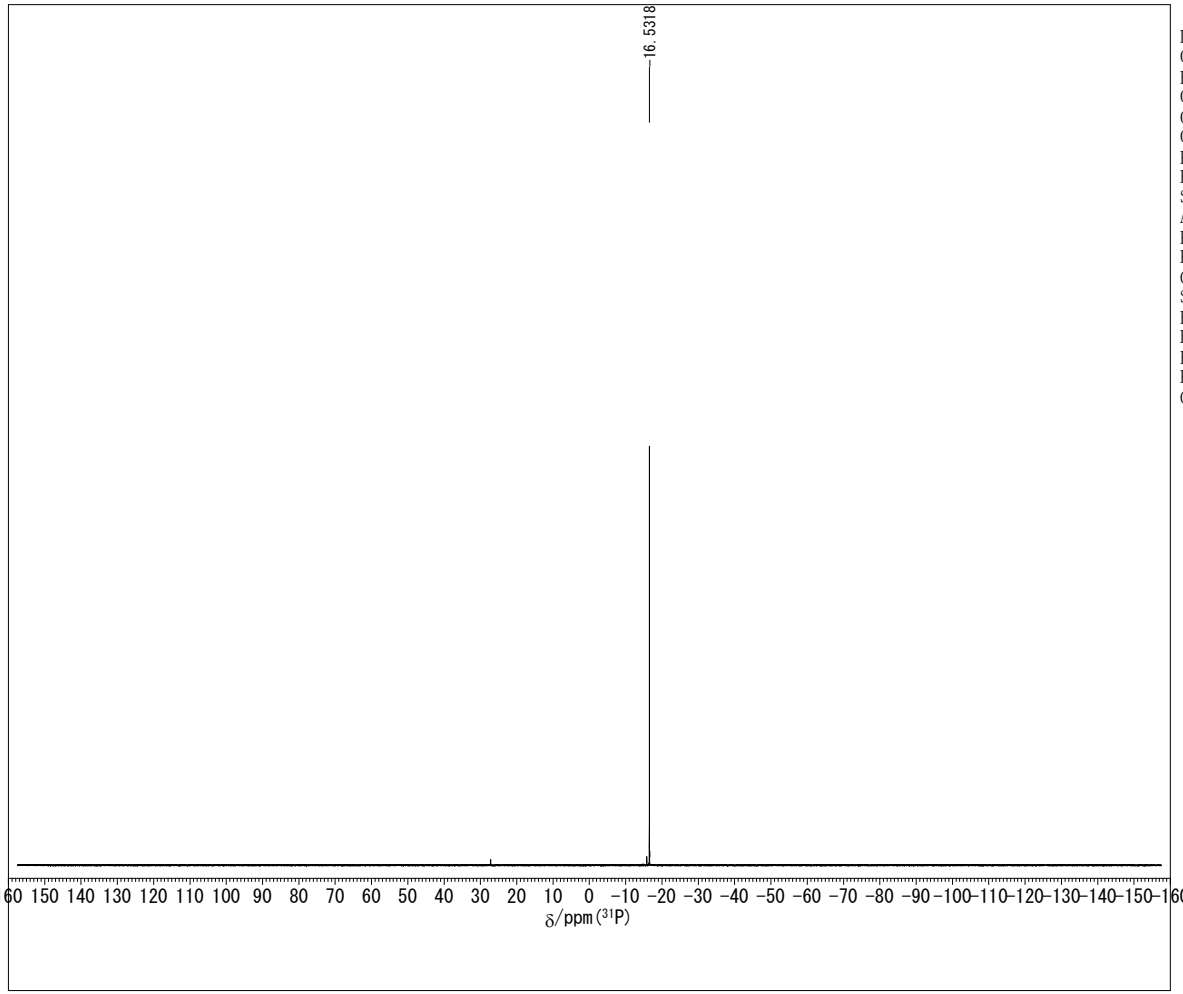


DATIM 25/Oct/2022 10:45:41
OBNUC ^{1}H
EXMOD ZG30>
OFR 400.18 MHz
OBSET 0.0 kHz
OBFIN 2008.224 Hz
POINT 131072(ZeroFill :×4)
FREQU 4826.255 Hz
SCANS 9
ACQTM 6.7895 s
PD 1.0 s
PW1 14.0 μs
CTEMP 20.81 °C
SLVNT $CDCL_3$>
EXREF 0.0 ppm
BF 0.1473 Hz
RGAIN 90
PRNT_DATE 2024/Apr/30 11:50:25
COMNT



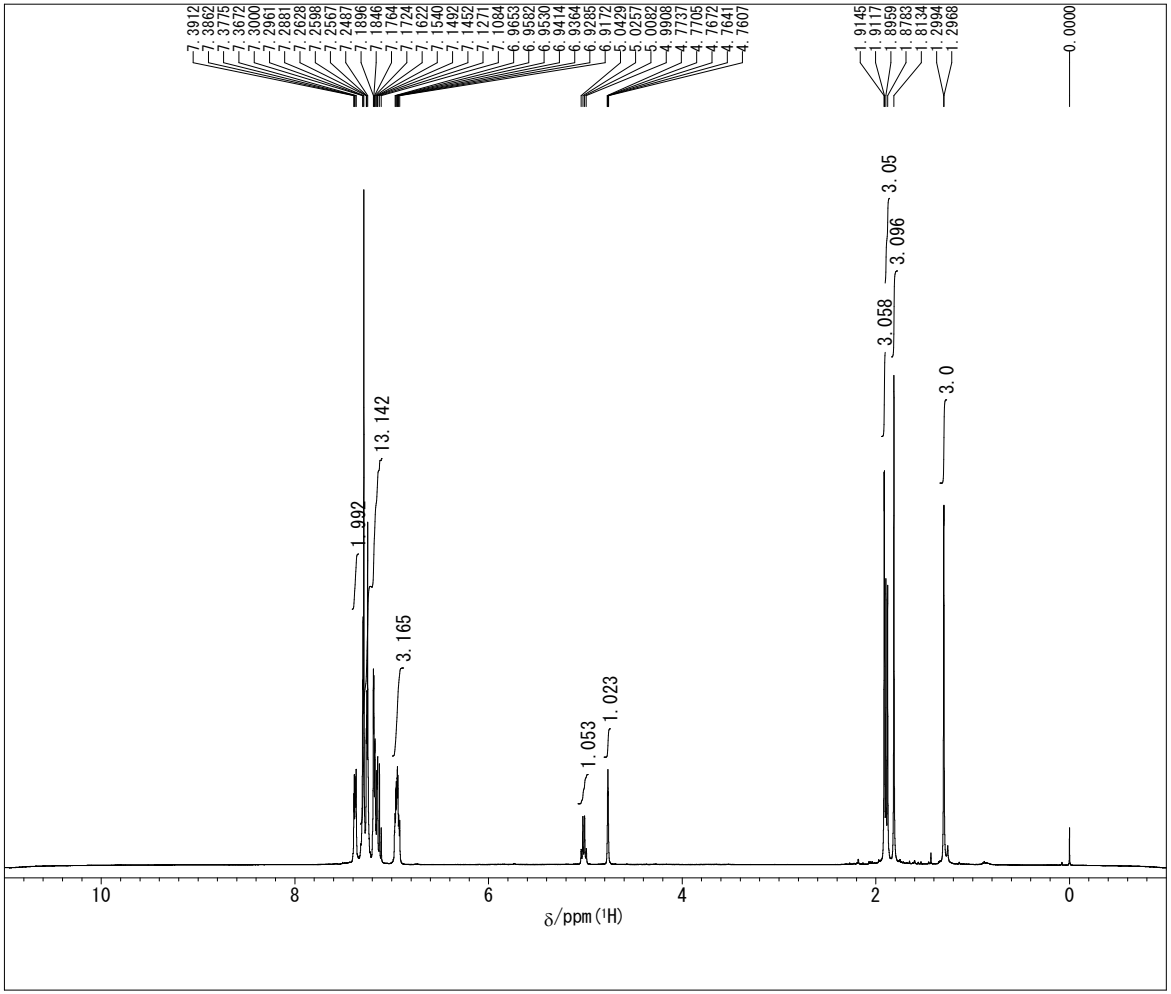


DATIM 07/Sep/2021 10:12:05
OBNUC ^{13}C
EXMOD ZGPG30>
OFR 100.63 MHz
OBSET 0.0 kHz
OBFIN 11066.5 Hz
POINT 131072(ZeroFill :×4)
FREQU 24038.46 Hz
SCANS 64
ACQTM 1.3631 s
PD 2.0 s
PW1 10.0 μs
CTEMP 22.71 ℃
SLVNT $CDCL_3$>
EXREF 77.0 ppm
BF 0.7336 Hz
RGAIN 203
PRNT_DATE 2024/Apr/30 11:53:30
COMNT

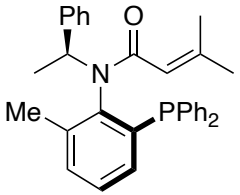


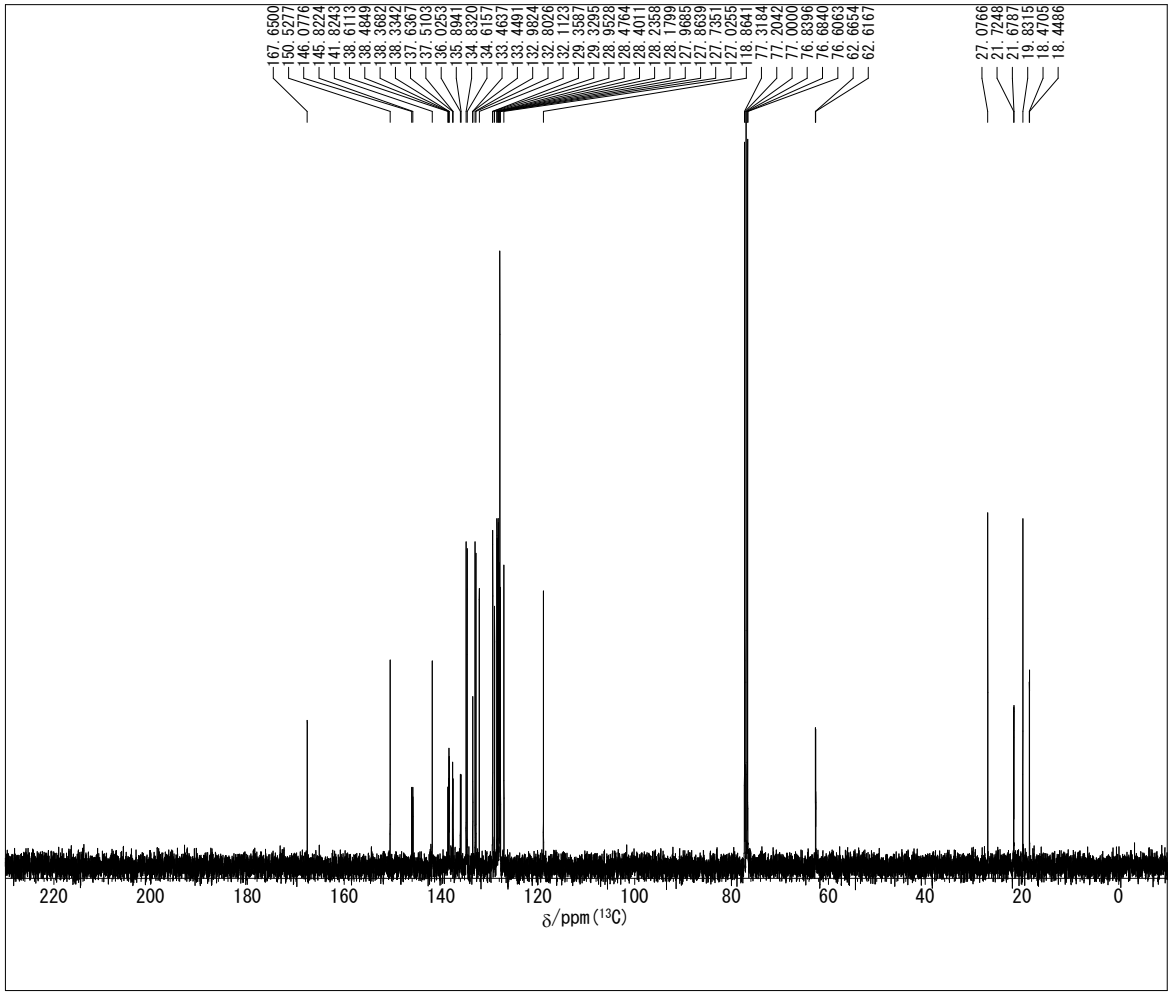
DATIM	01/Sep/2021 15:06:00
OBNUC	^{31}P
EXMOD	ZGPG30>
OFR	162.0 MHz
OBSET	0.0 kHz
OBFIN	9993.149 Hz
POINT	32768
FREQU	51020.41 Hz
SCANS	16
ACQTM	0.6423 s
PD	2.0 s
PW1	15.0 μs
CTEMP	24.11 °C
SLVNT	$CDCL_3$>
EXREF	157.4744 ppm
BF	0.25 Hz
RGAIN	203
PRNT_DATE	2024/Apr/30 11:54:55
COMNT	

^{1}H NMR, ^{13}C{^{1}H} NMR and ^{31}P{^{1}H} NMR of (*S*,a*S*)-**4d**

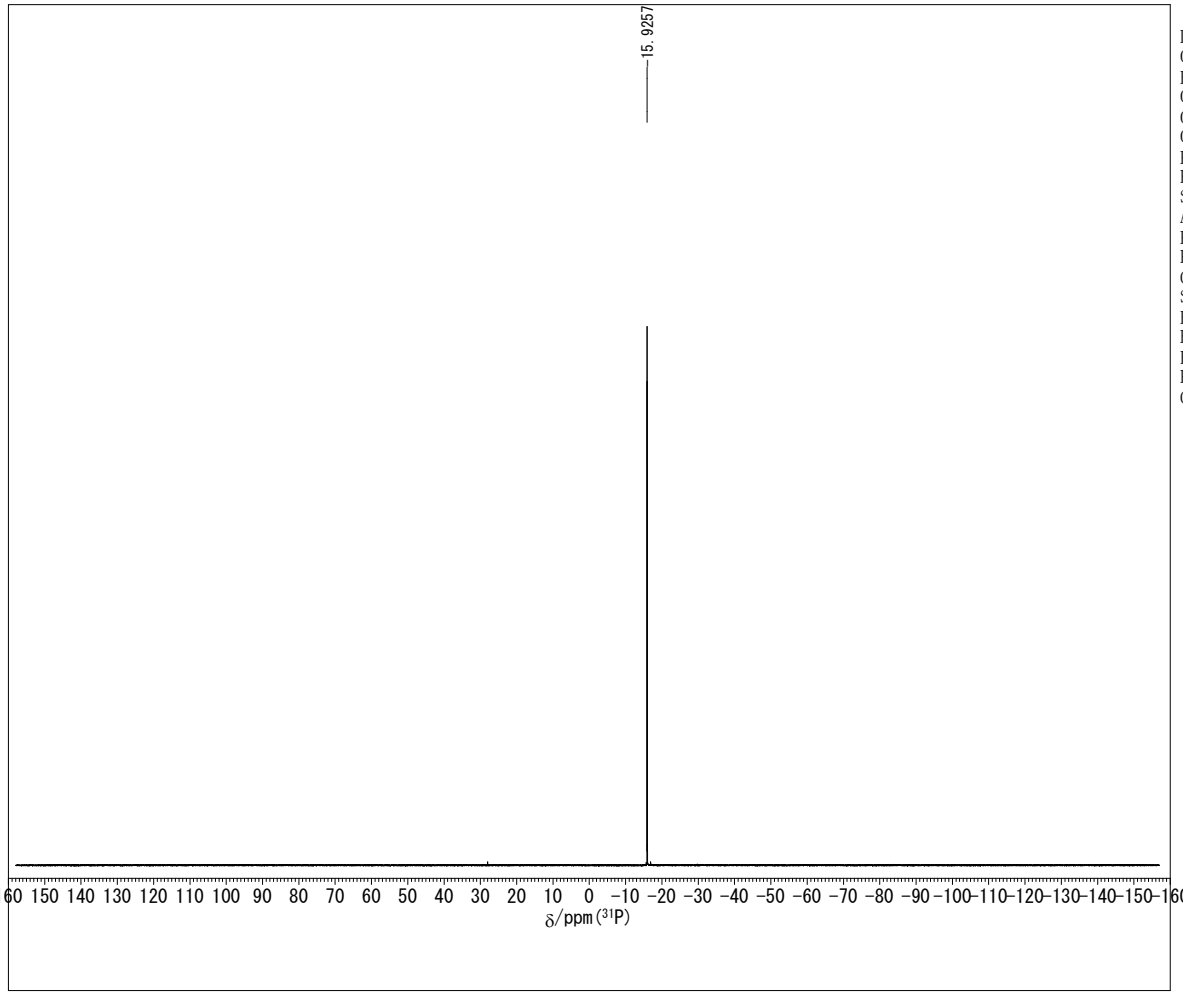


DATIM 05/Apr/2021 17:11:30
OBNUC ^{1}H
EXMOD ZG30>
OFR 400.18 MHz
OBSET 0.0 kHz
OBFIN 2008.224 Hz
POINT 131072(ZeroFill :×4)
FREQU 4826.255 Hz
SCANS 16
ACQTM 6.7895 s
PD 1.0 s
PW1 14.0 μs
CTEMP 22.21 °C
SLVNT $CDCl_3$>
EXREF 0.0 ppm
BF 0.1473 Hz
RGAIN 72
PRNT_DATE 2024/Apr/30 12:07:30
COMNT



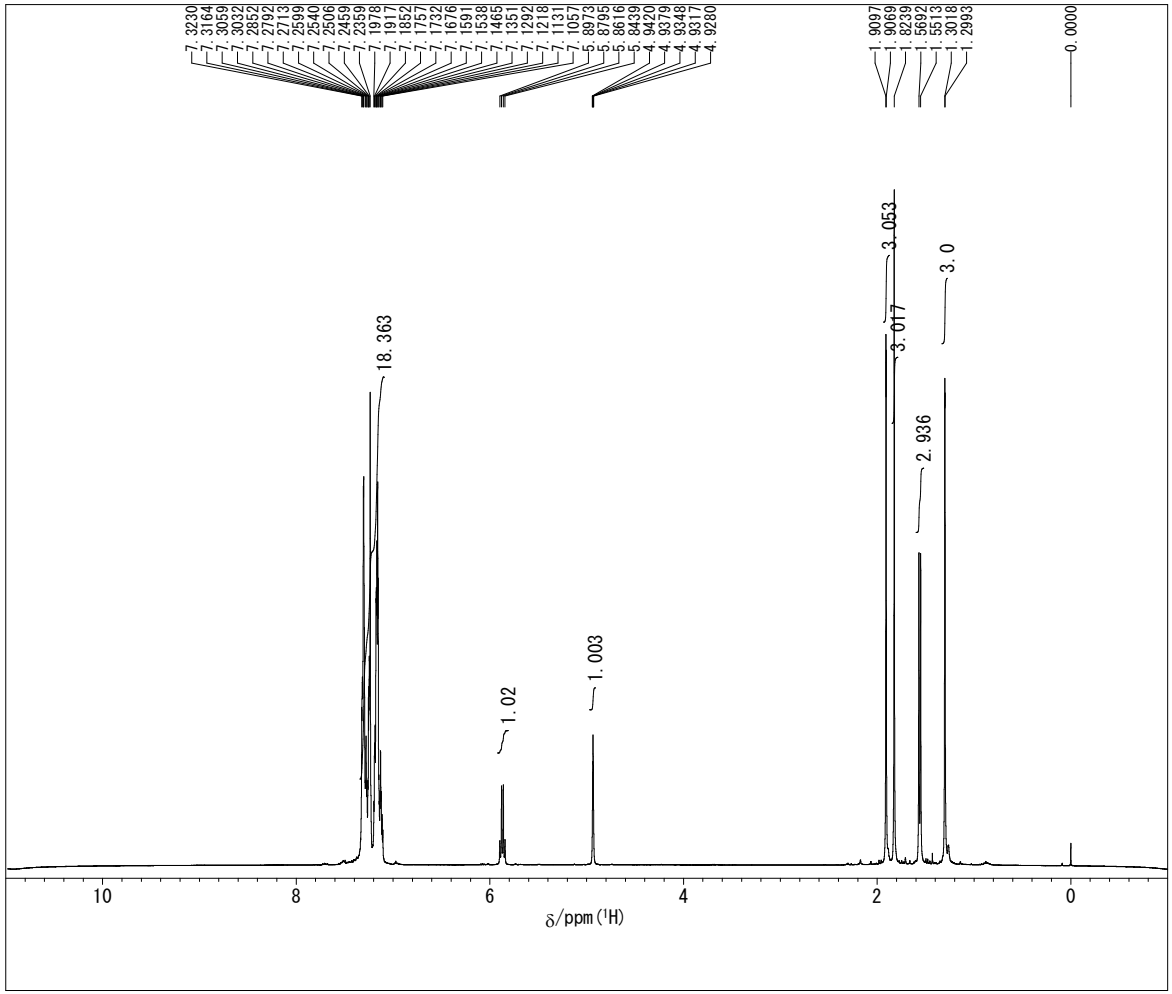


DATIM 05/Apr/2021 17:56:01
OBNUC ^{13}C
EXMOD ZGPG30>
OFR 100.61 MHz
OBSET 0.0 kHz
OBFIN 12705.91 Hz
POINT 131072(ZeroFill :×4)
FREQU 32051.28 Hz
SCANS 64
ACQTM 1.0224 s
PD 2.0 s
PW1 9.0 μs
CTEMP 20.65 °C
SLVNT $CDCL_3$>
EXREF 77.0 ppm
BF 0.9781 Hz
RGAIN 2050
PRNT_DATE 2024/Apr/30 12:08:23
COMNT

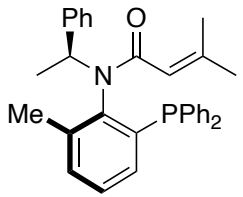


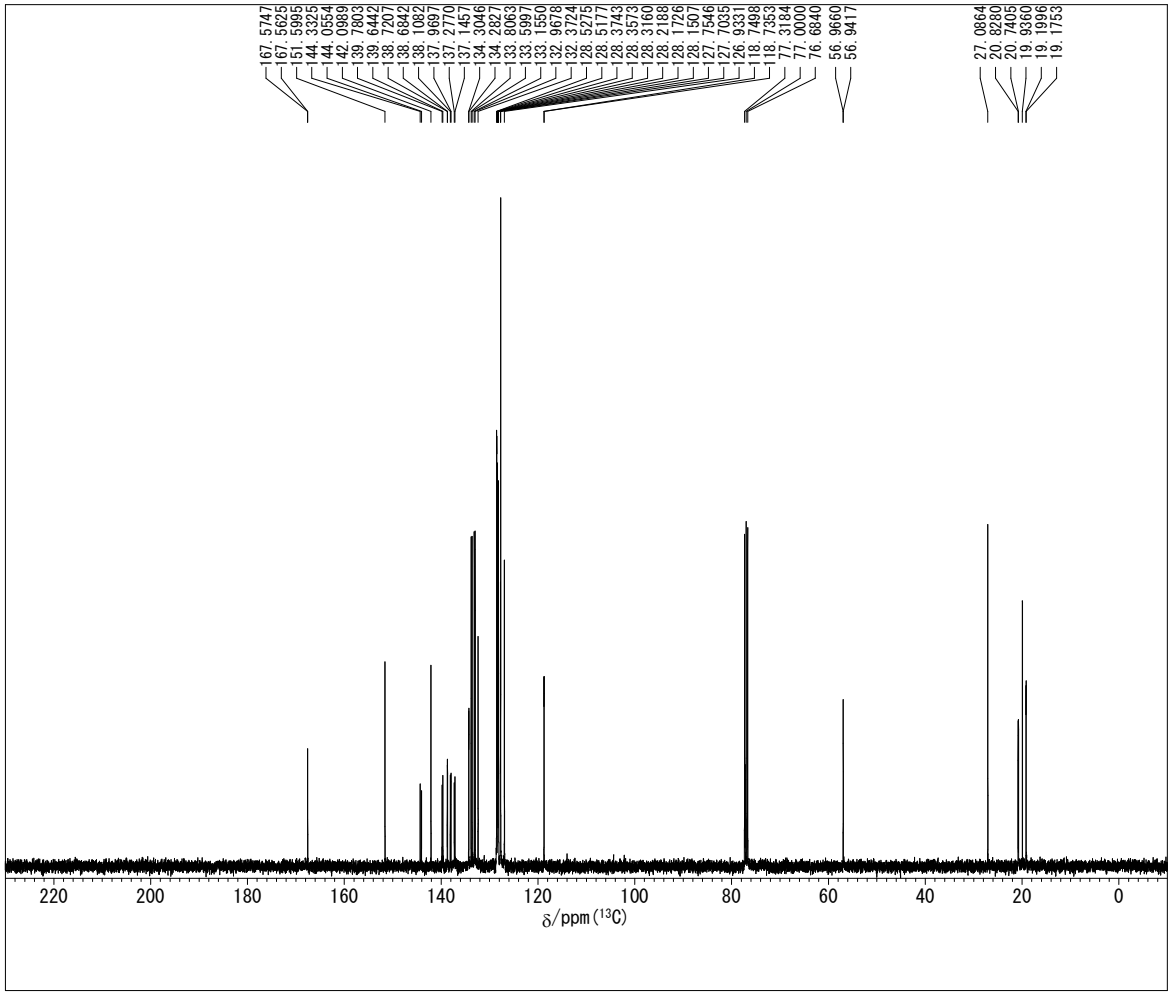
DATIM	05/Apr/2021 17:13:43
OBNUC	^{31}P
EXMOD	ZGPG30>
OFR	162.0 MHz
OBSET	0.0 kHz
OBFIN	9993.154 Hz
POINT	32768
FREQU	51020.41 Hz
SCANS	16
ACQTM	0.6423 s
PD	2.0 s
PW1	15.0 μs
CTEMP	22.61 °C
SLVNT	$CDCL_3$>
EXREF	157.9652 ppm
BF	0.25 Hz
RGAIN	203
PRNT_DATE	2024/Apr/30 12:09:07
COMNT	

^{1}H NMR, ^{13}C{^{1}H} NMR and ^{31}P{^{1}H} NMR of (*S*,a*R*)-**4d**

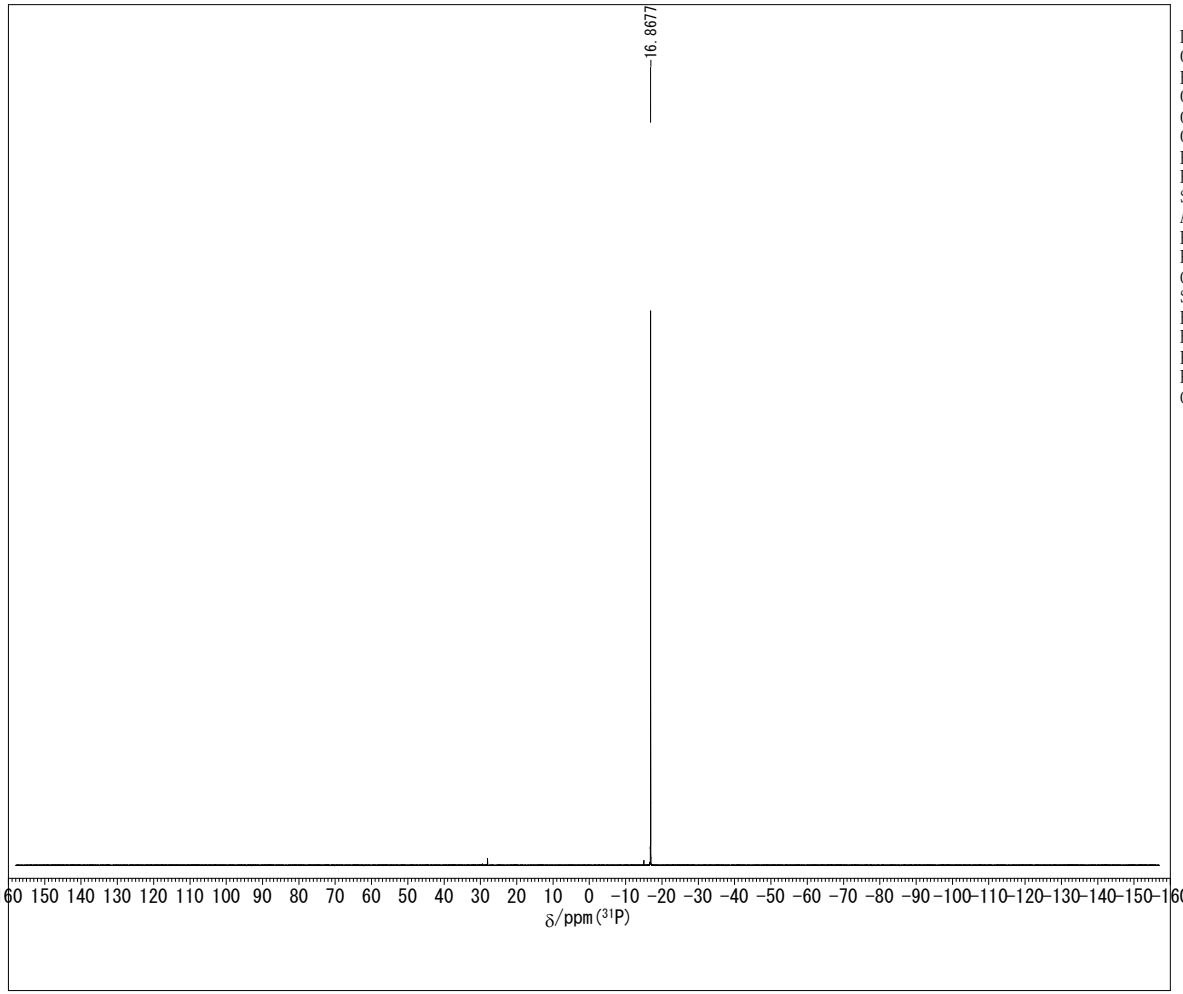


DATIM 05/Apr/2021 17:21:15
OBNUC ^{1}H
EXMOD ZG30>
OFR 400.18 MHz
OBSET 0.0 kHz
OBFIN 2008.224 Hz
POINT 131072(ZeroFill :×4)
FREQU 4826.255 Hz
SCANS 16
ACQTM 6.7895 s
PD 1.0 s
PW1 14.0 μs
CTEMP 22.21 ℃
SLVNT $CDCl_3$>
EXREF 0.0 ppm
BF 0.1473 Hz
RGAIN 25
PRNT_DATE 2024/Apr/30 12:19:30
COMNT



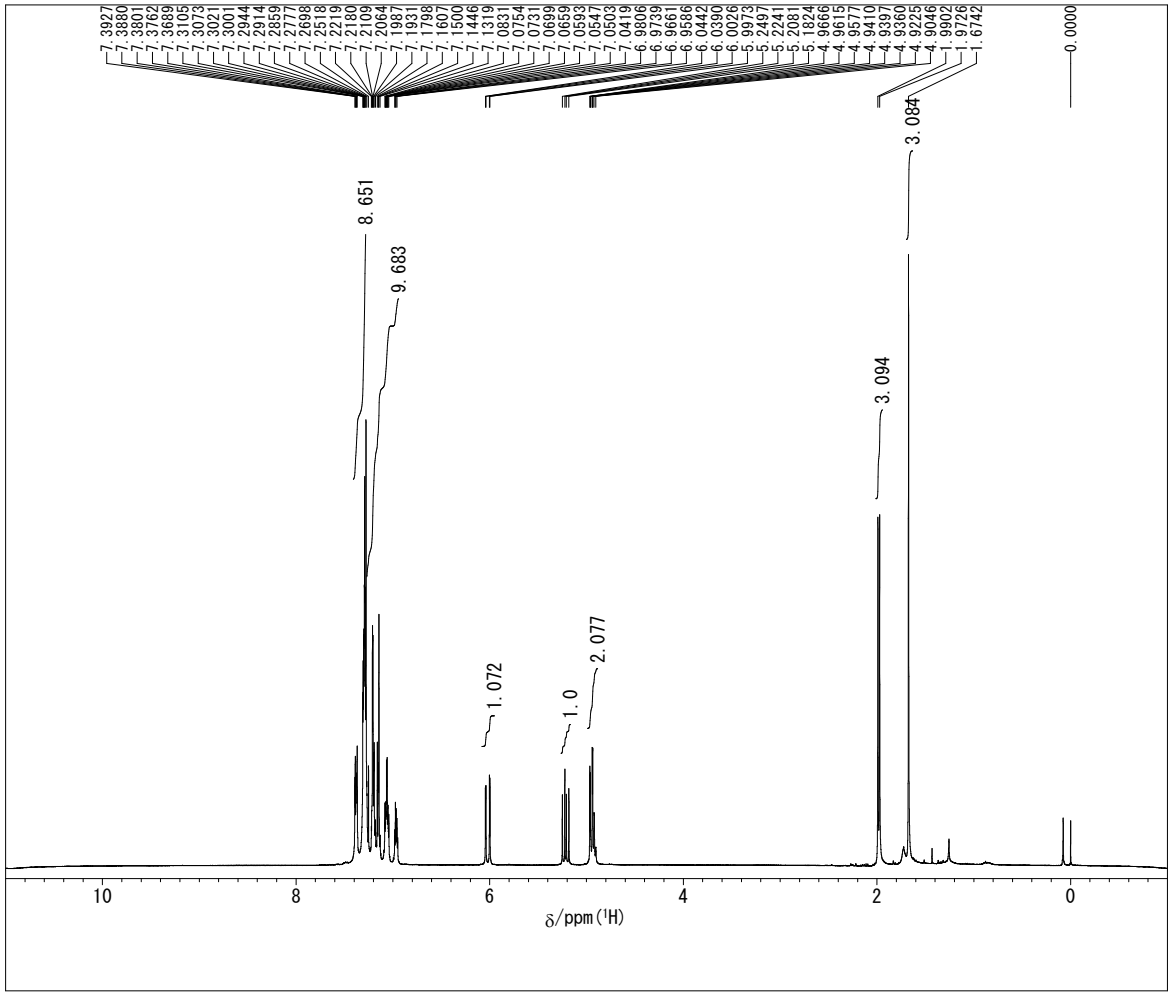


DATIM 05/Apr/2021 18:02:26
OBNUC ^{13}C
EXMOD ZGPG30>
OFR 100.61 MHz
OBSET 0.0 kHz
OBFIN 12705.91 Hz
POINT 131072(ZeroFill :×4)
FREQU 32051.28 Hz
SCANS 64
ACQTM 1.0224 s
PD 2.0 s
PW1 9.0 μs
CTEMP 20.65 ℃
SLVNT $CDCL_3$>
EXREF 77.0 ppm
BF 0.9781 Hz
RGAIN 2050
PRNT_DATE 2024/Apr/30 12:20:30
COMNT

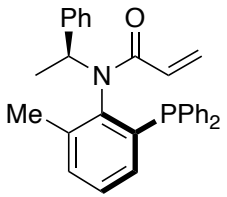


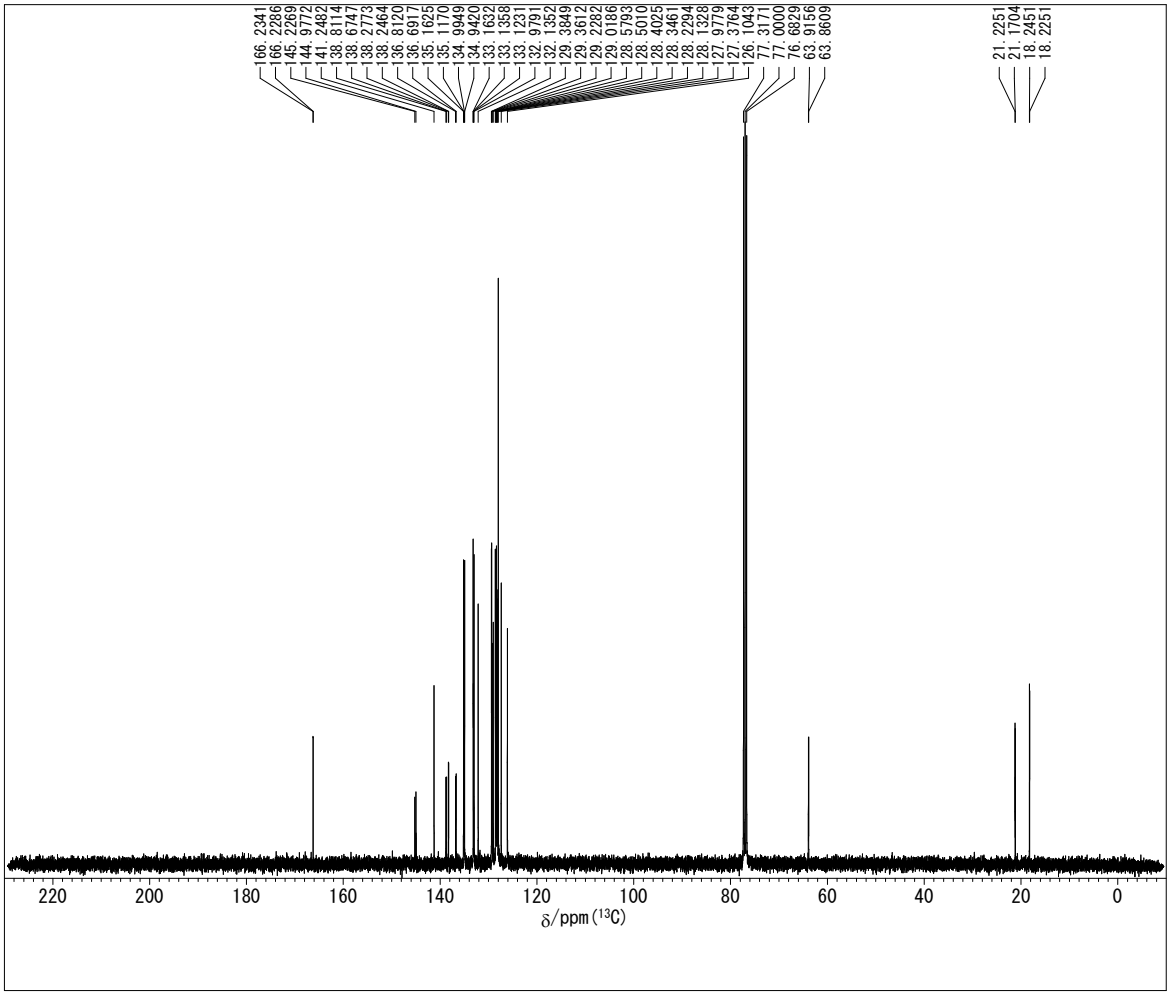
DATIM	05/Apr/2021 17:23:11
OBNUC	^{31}P
EXMOD	ZGPG30>
OFR	162.0 MHz
OBSET	0.0 kHz
OBFIN	9993.154 Hz
POINT	32768
FREQU	51020.41 Hz
SCANS	16
ACQTM	0.6423 s
PD	2.0 s
PW1	15.0 μs
CTEMP	22.61 °C
SLVNT	$CDCL_3$>
EXREF	157.9652 ppm
BF	0.25 Hz
RGAIN	203
PRNT_DATE	2024/Apr/30 12:21:38
COMNT	

^{1}H NMR, ^{13}C{^{1}H} NMR and ^{31}P{^{1}H} NMR of (*S*,a*S*)-**4e**

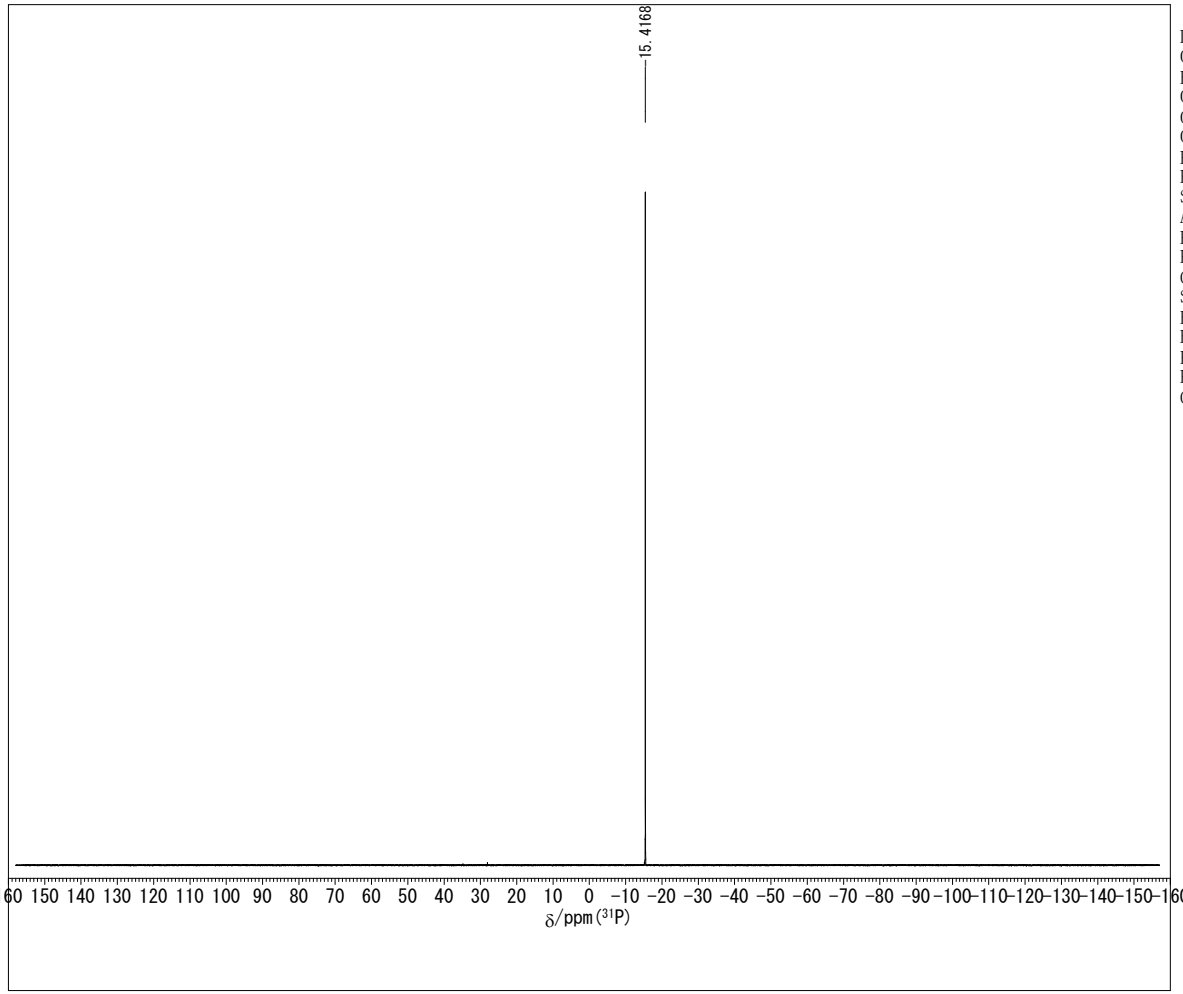


DATIM 03/Jun/2022 15:50:10
OBNUC ^{1}H
EXMOD ZG30>
OFR 400.18 MHz
OBSET 0.0 kHz
OBFIN 2008.224 Hz
POINT 131072(ZeroFill :×4)
FREQU 4826.255 Hz
SCANS 16
ACQTM 6.7895 s
PD 1.0 s
PW1 14.0 μs
CTEMP 22.81 °C
SLVNT $CDCl_3$>
EXREF 0.0 ppm
BF 0.1473 Hz
RGAIN 81
PRNT_DATE 2024/Apr/30 12:25:54
COMNT



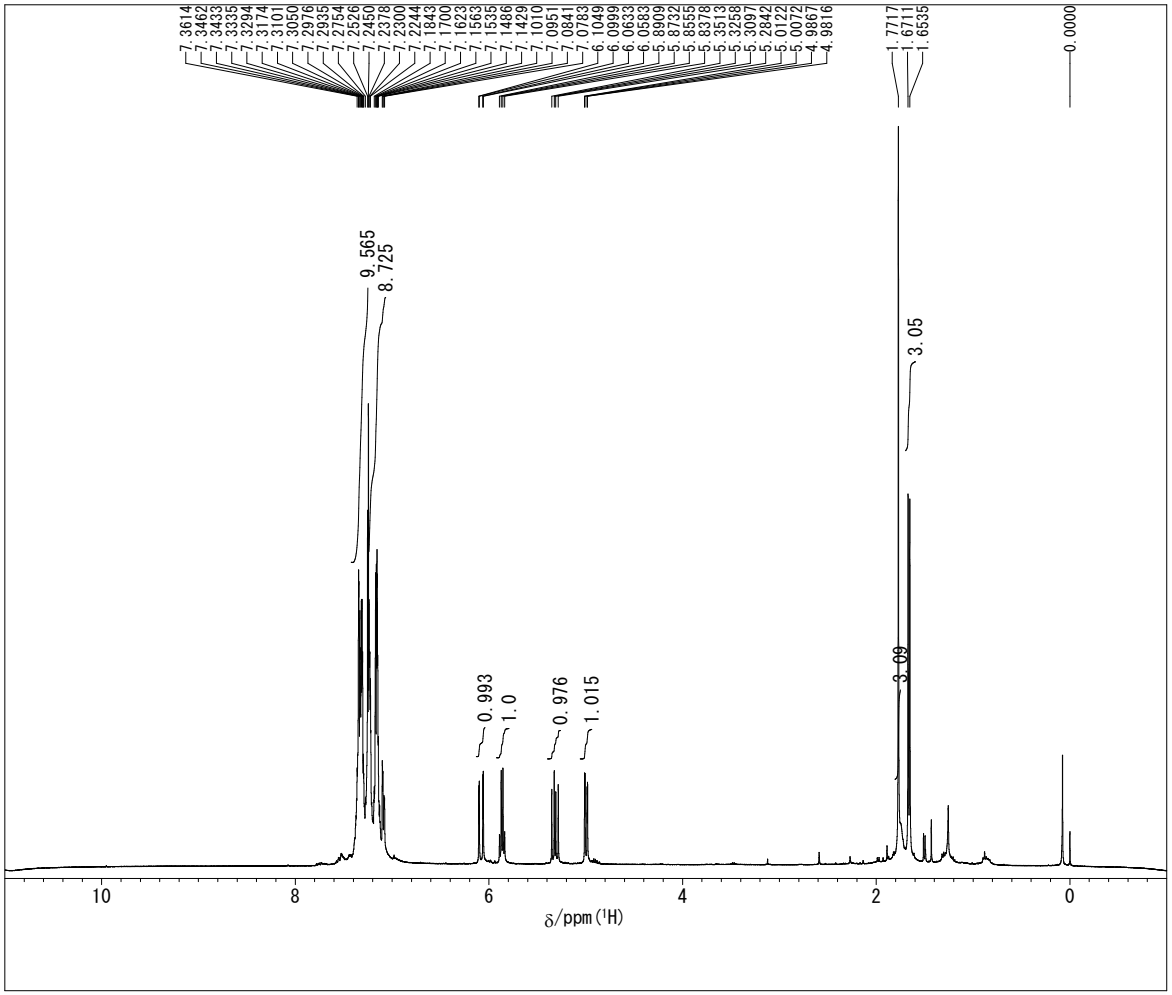


DATIM 03/Jun/2022 16:06:53
OBNUC ^{13}C
EXMOD ZGPG30>
OFR 100.63 MHz
OBSET 0.0 kHz
OBFIN 11066.5 Hz
POINT 131072(ZeroFill :×4)
FREQU 24038.46 Hz
SCANS 256
ACQTM 1.3631 s
PD 2.0 s
PW1 10.0 μs
CTEMP 23.61 °C
SLVNT $CDCL_3$>
EXREF 77.0 ppm
BF 0.7336 Hz
RGAIN 203
PRNT_DATE 2024/Apr/30 12:26:47
COMNT

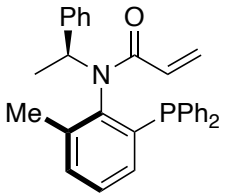


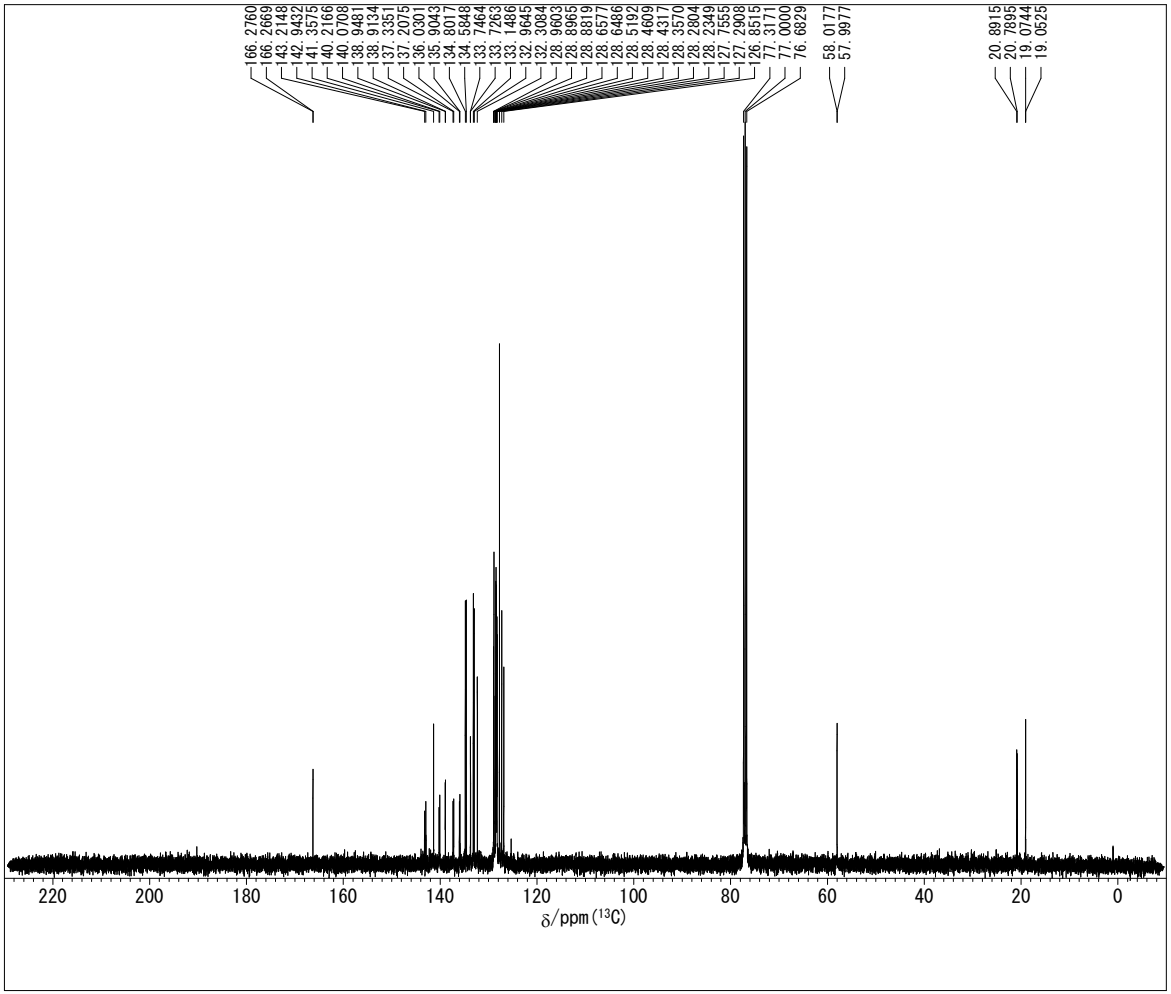
DATIM	03/Jun/2022 15:46:44
OBNUC	^{31}P
EXMOD	ZGPG30>
OFR	162.0 MHz
OBSET	0.0 kHz
OBFIN	9993.157 Hz
POINT	32768
FREQU	51020.41 Hz
SCANS	32
ACQTM	0.6423 s
PD	2.0 s
PW1	15.0 μs
CTEMP	23.31 °C
SLVNT	$CDCL_3$>
EXREF	157.9551 ppm
BF	0.25 Hz
RGAIN	203
PRNT_DATE	2024/Apr/30 12:27:36
COMNT	

^{1}H NMR, ^{13}C{^{1}H} NMR and ^{31}P{^{1}H} NMR of (*S*,a*R*)-**4e**

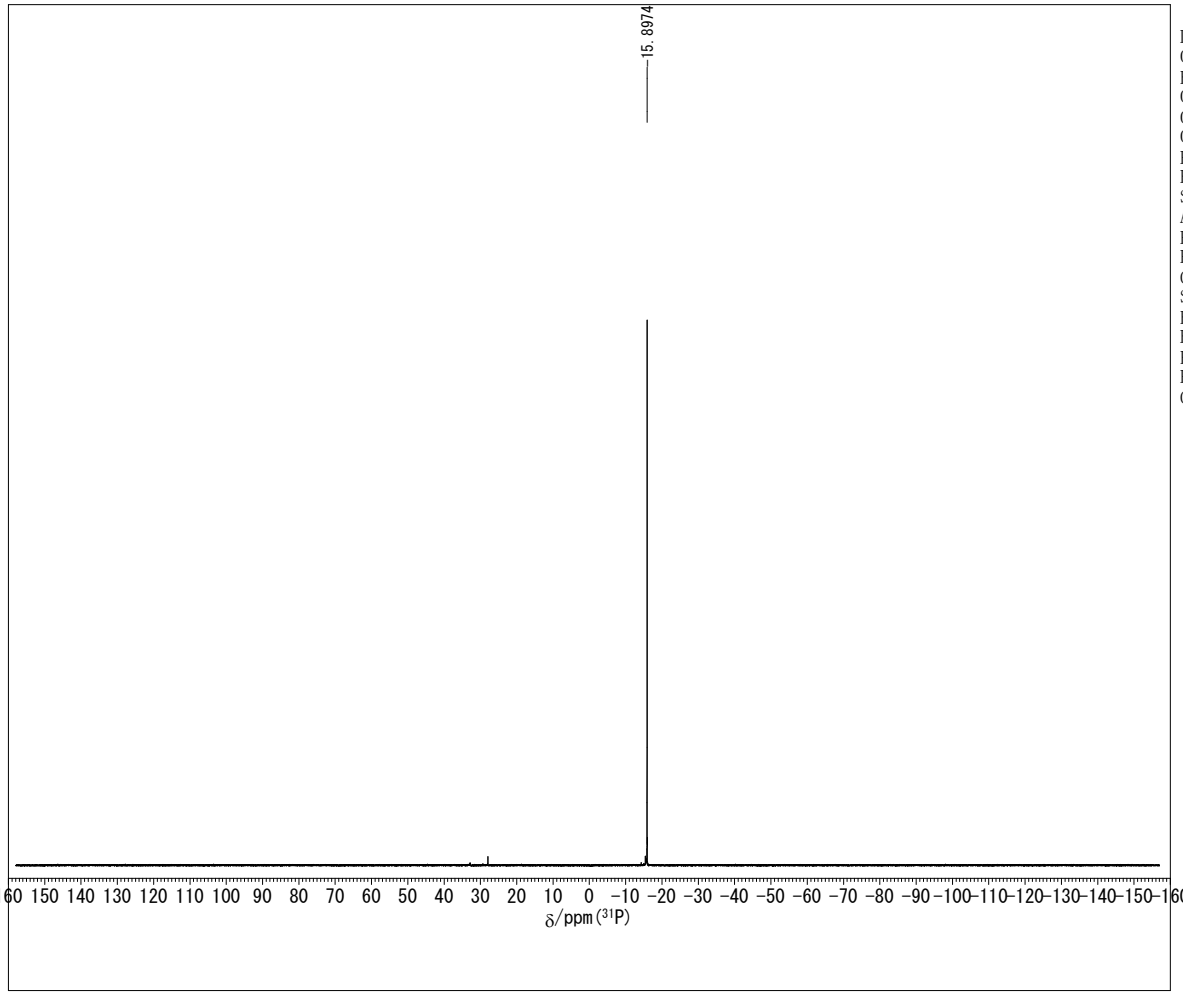


DATIM 03/Jun/2022 16:12:34
OBNUC ^{1}H
EXMOD ZG30>
OFR 400.18 MHz
OBSET 0.0 kHz
OBFIN 2008.224 Hz
POINT 131072(ZeroFill :×4)
FREQU 4826.255 Hz
SCANS 16
ACQTM 6.7895 s
PD 1.0 s
PW1 14.0 μs
CTEMP 22.91 °C
SLVNT $CDCl_3$>
EXREF 0.0 ppm
BF 0.1473 Hz
RGAIN 81
PRNT_DATE 2024/Apr/30 12:30:38
COMNT



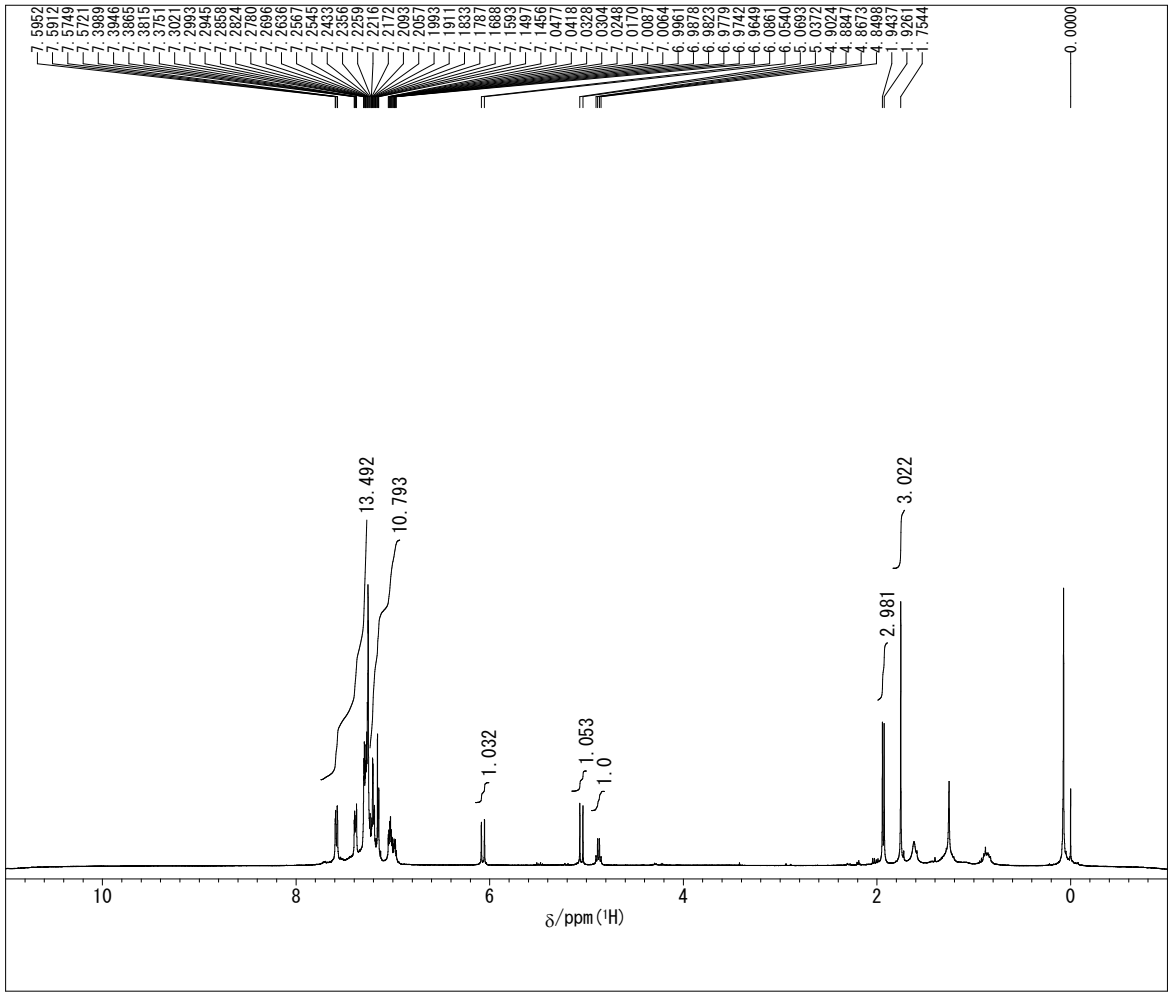


DATIM 03/Jun/2022 16:28:38
OBNUC ^{13}C
EXMOD ZGPG30>
OFR 100.63 MHz
OBSET 0.0 kHz
OBFIN 11066.5 Hz
POINT 131072(ZeroFill :×4)
FREQU 24038.46 Hz
SCANS 256
ACQTM 1.3631 s
PD 2.0 s
PW1 10.0 μs
CTEMP 23.61 ℃
SLVNT $CDCL_3$>
EXREF 77.0 ppm
BF 0.7336 Hz
RGAIN 203
PRNT_DATE 2024/Apr/30 12:31:34
COMNT

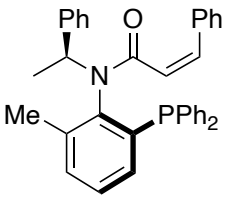


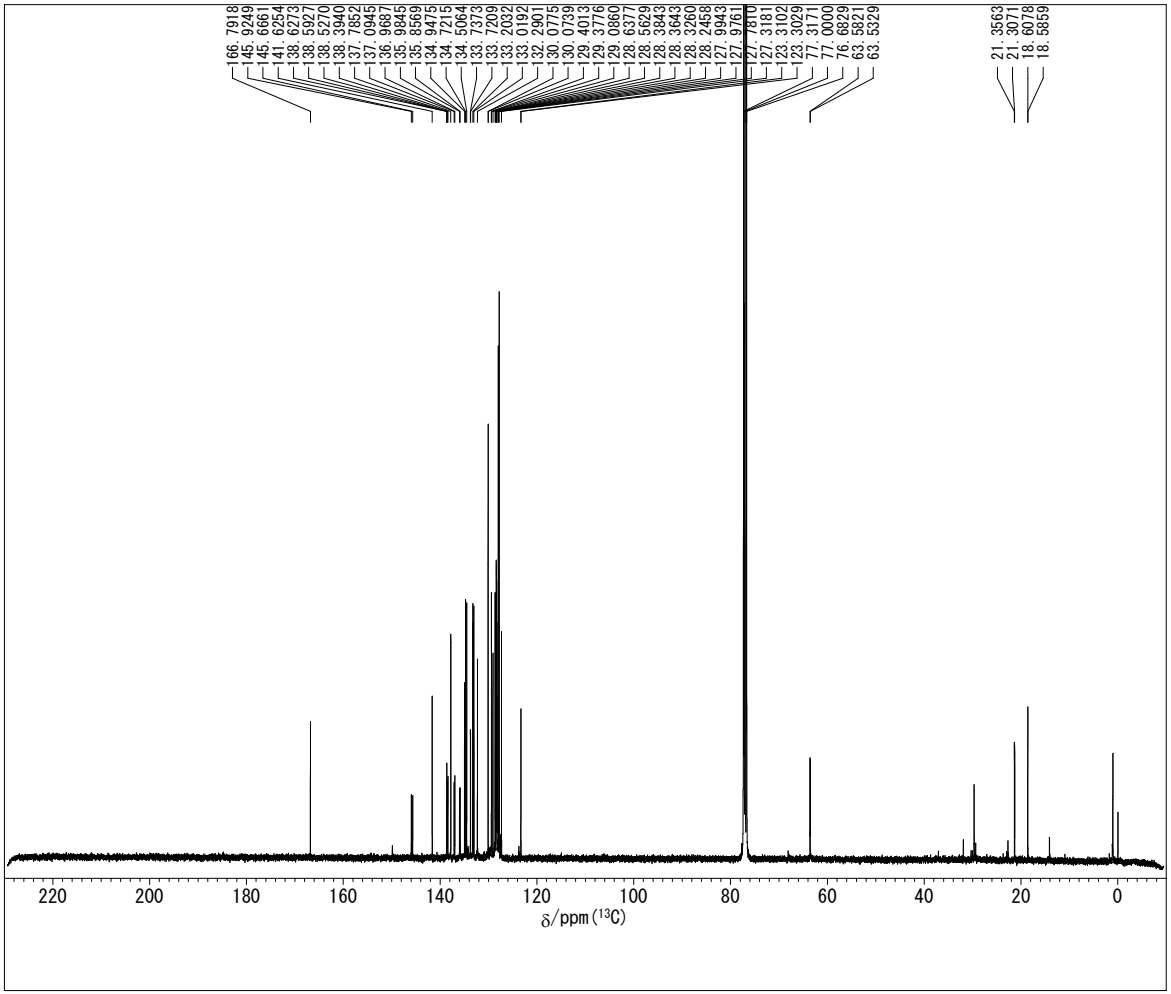
DATIM	03/Jun/2022 16:31:53
OBNUC	^{31}P
EXMOD	ZGPG30>
OFR	162.0 MHz
OBSET	0.0 kHz
OBFIN	9993.157 Hz
POINT	32768
FREQU	51020.41 Hz
SCANS	32
ACQTM	0.6423 s
PD	2.0 s
PW1	15.0 μs
CTEMP	23.51 °C
SLVNT	$CDCL_3$>
EXREF	157.9551 ppm
BF	0.25 Hz
RGAIN	203
PRNT_DATE	2024/Apr/30 12:32:39
COMNT	

^{1}H NMR, ^{13}C{^{1}H} NMR and ^{31}P{^{1}H} NMR of (*S*,a*S*)-**4f**

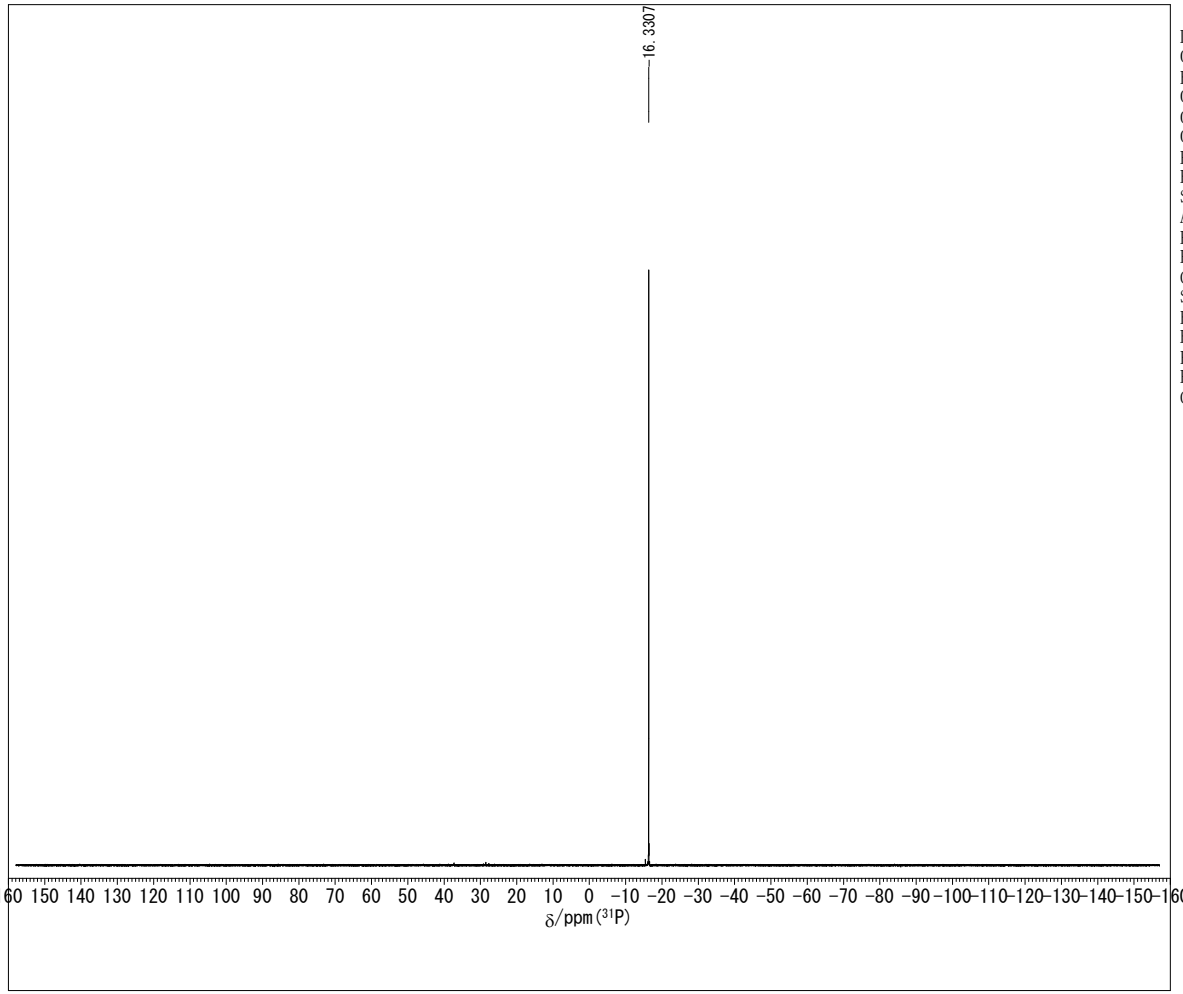


DATIM 30/May/2022 10:59:53
OBNUC ^{1}H
EXMOD ZG30>
OFR 400.18 MHz
OBSET 0.0 kHz
OBFIN 2008.224 Hz
POINT 131072(ZeroFill :×4)
FREQU 4826.255 Hz
SCANS 32
ACQTM 6.7895 s
PD 1.0 s
PW1 14.0 μs
CTEMP 22.51 °C
SLVNT $CDCL_3$>
EXREF 0.0 ppm
BF 0.1473 Hz
RGAIN 203
PRNT_DATE 2024/Apr/30 12:35:11
COMNT



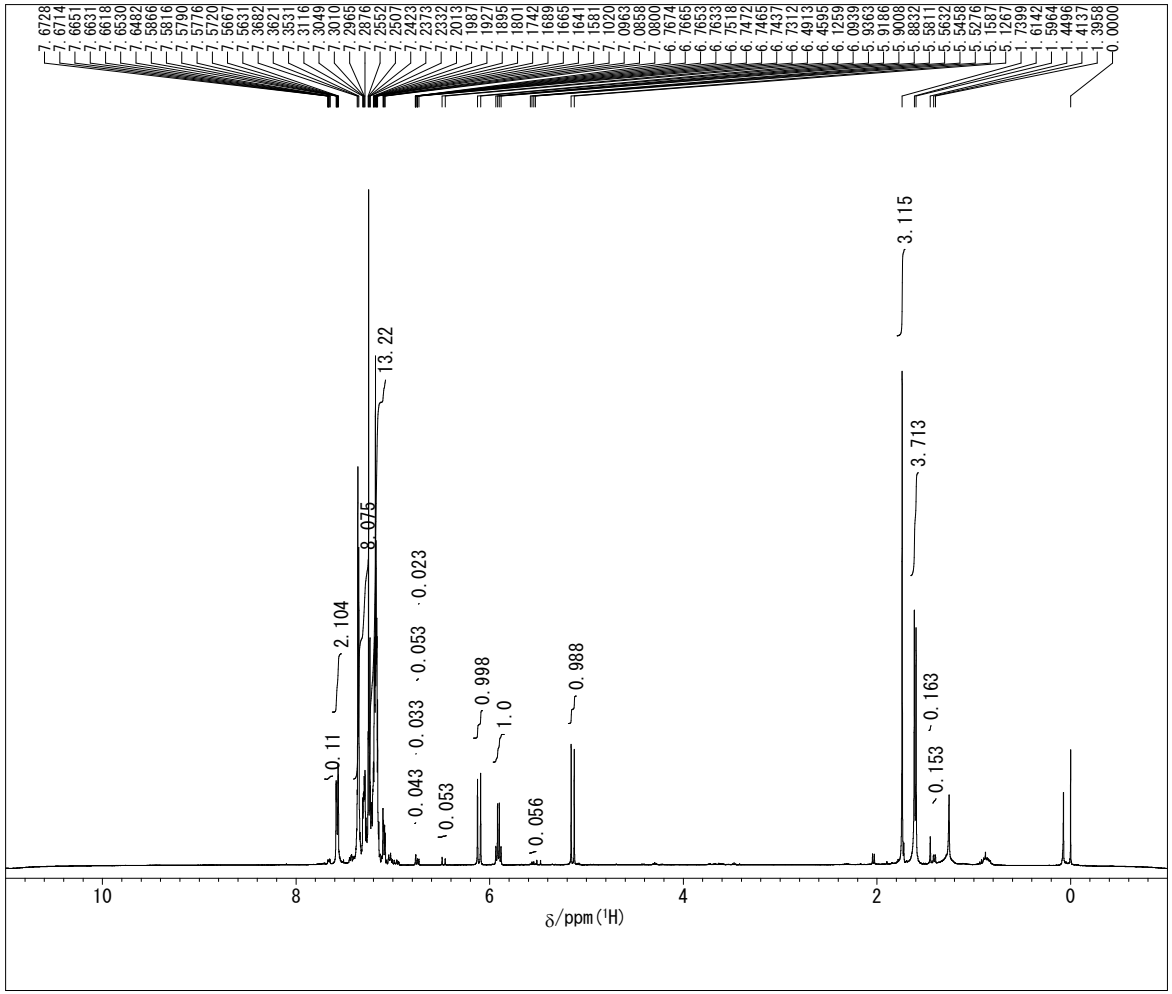


DATIM 22/Jan/2022 10:32:23
OBNUC ^{13}C
EXMOD ZGPG30>
OFR 100.63 MHz
OBSET 0.0 kHz
OBFIN 11066.5 Hz
POINT 131072(ZeroFill :×4)
FREQU 24038.46 Hz
SCANS 14424
ACQTM 1.3631 s
PD 2.0 s
PW1 10.0 μs
CTEMP 20.31 °C
SLVNT $CDCL_3$>
EXREF 77.0 ppm
BF 0.7336 Hz
RGAIN 203
PRNT_DATE 2024/Apr/30 12:38:10
COMNT

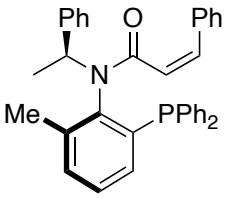


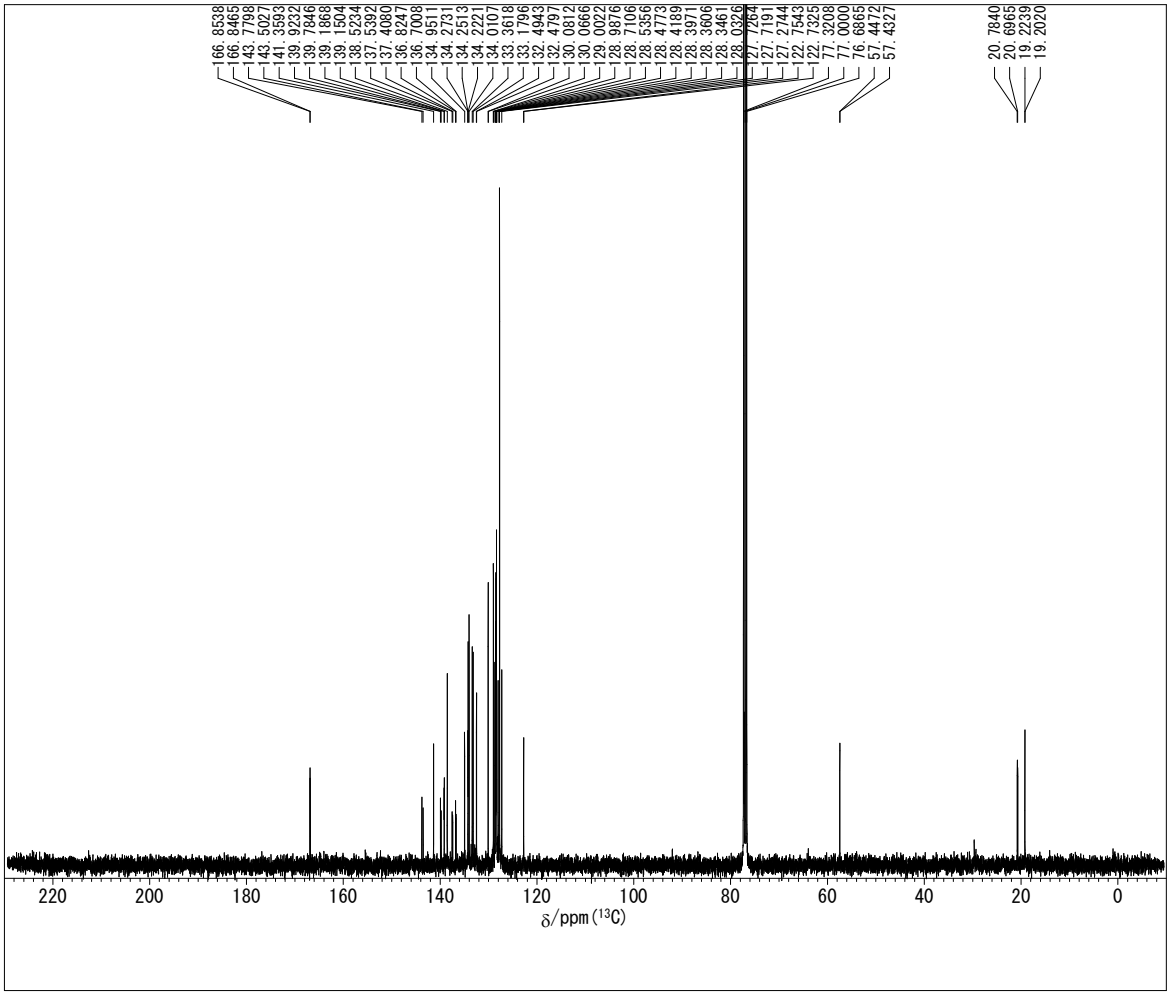
DATIM	21/Jan/2022 18:23:40
OBNUC	^{31}P
EXMOD	ZGPG30>
OFR	162.0 MHz
OBSET	0.0 kHz
OBFIN	9993.162 Hz
POINT	32768
FREQU	51020.41 Hz
SCANS	128
ACQTM	0.6423 s
PD	2.0 s
PW1	15.0 μs
CTEMP	20.71 °C
SLVNT	$CDCL_3$>
EXREF	157.9351 ppm
BF	0.25 Hz
RGAIN	203
PRNT_DATE	2024/Apr/30 12:39:02
COMNT	

^{1}H NMR, ^{13}C{^{1}H} NMR and ^{31}P{^{1}H} NMR of (*S*,a*R*)-**4f**

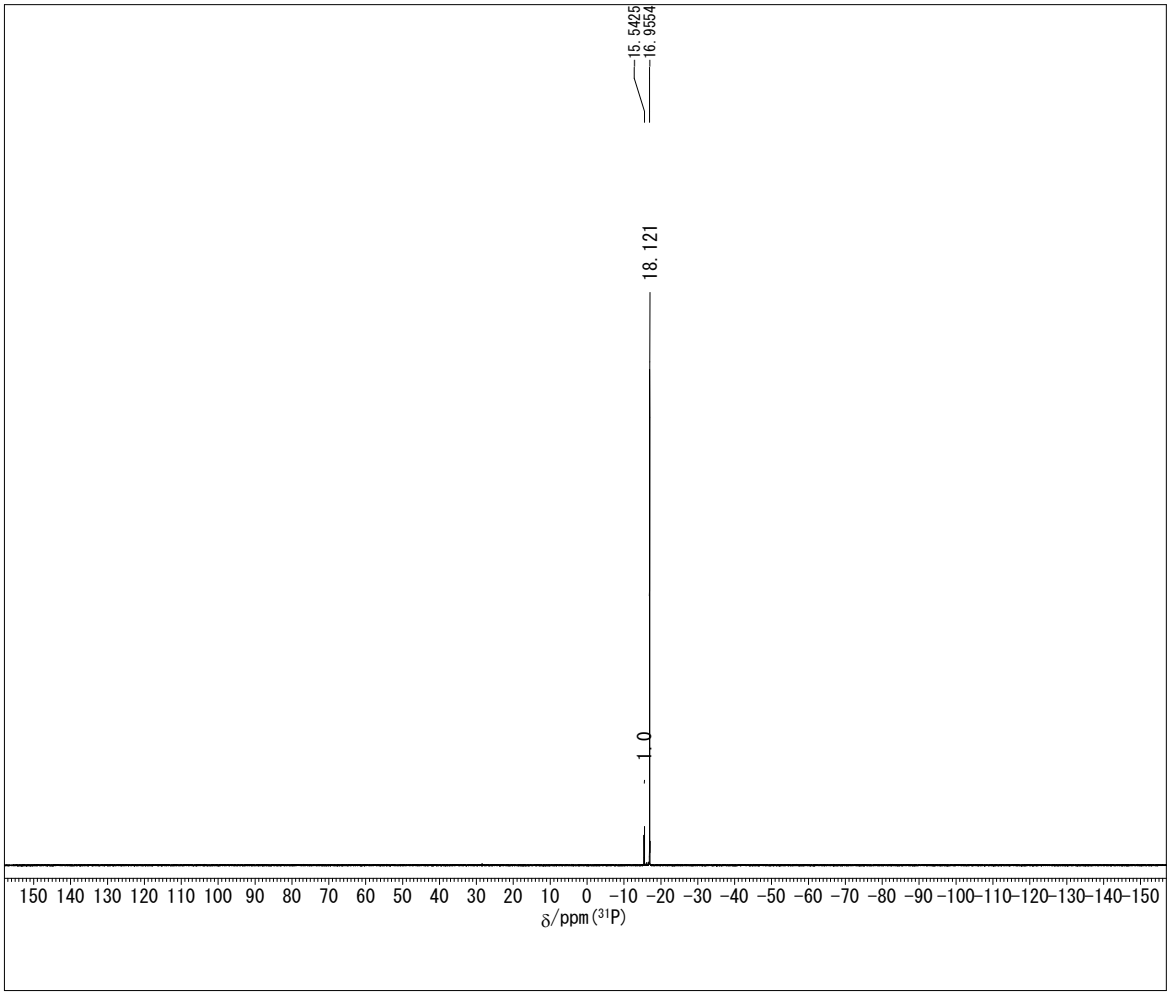


DATIM 19/Oct/2022 10:34:27
OBNUC ^{1}H
EXMOD ZG30>
OFR 400.18 MHz
OBSET 0.0 kHz
OBFIN 2008.224 Hz
POINT 131072(ZeroFill :×4)
FREQU 4826.255 Hz
SCANS 128
ACQTM 6.7895 s
PD 1.0 s
PW1 14.0 μs
CTEMP 22.01 °C
SLVNT $CDCL_3$>
EXREF 0.0 ppm
BF 0.1473 Hz
RGAIN 128
PRNT_DATE 2024/Apr/30 12:43:11
COMNT





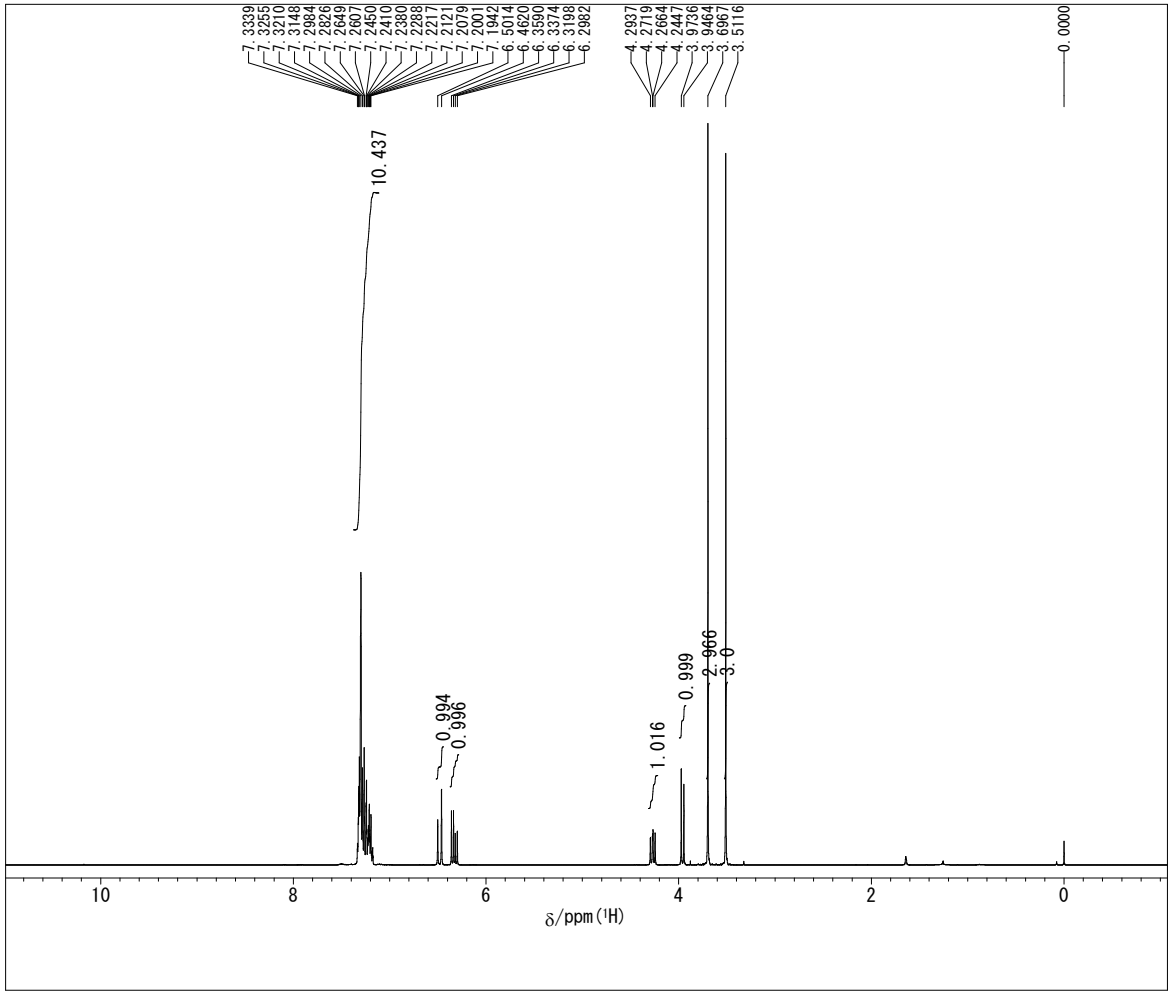
DATIM	25/Oct/2022 13:14:18
OBNUC	^{13}C
EXMOD	ZGPG30>
OFR	100.63 MHz
OBSET	0.0 kHz
OBFIN	9998.39 Hz
POINT	32768
FREQU	24038.46 Hz
SCANS	512
ACQTM	1.3631 s
PD	2.0 s
PW1	10.0 μs
CTEMP	21.61 °C
SLVNT	$CDCL_3$>
EXREF	77.0 ppm
BF	0.25 Hz
RGAIN	203
PRNT_DATE	2024/Apr/30 12:44:09
COMNT	



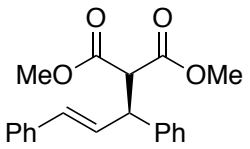
DATIM	19/Oct/2022 10:16:48
OBNUC	^{31}P
EXMOD	ZGPG30>
OFR	162.0 MHz
OBSET	0.0 kHz
OBFIN	9993.162 Hz
POINT	32768
FREQU	51020.41 Hz
SCANS	128
ACQTM	0.6423 s
PD	2.0 s
PW1	15.0 μs
CTEMP	22.61 °C
SLVNT	$CDCL_3$>
EXREF	157.9351 ppm
BF	0.25 Hz
RGAIN	203
PRNT_DATE	2024/Apr/30 12:47:08
COMNT	

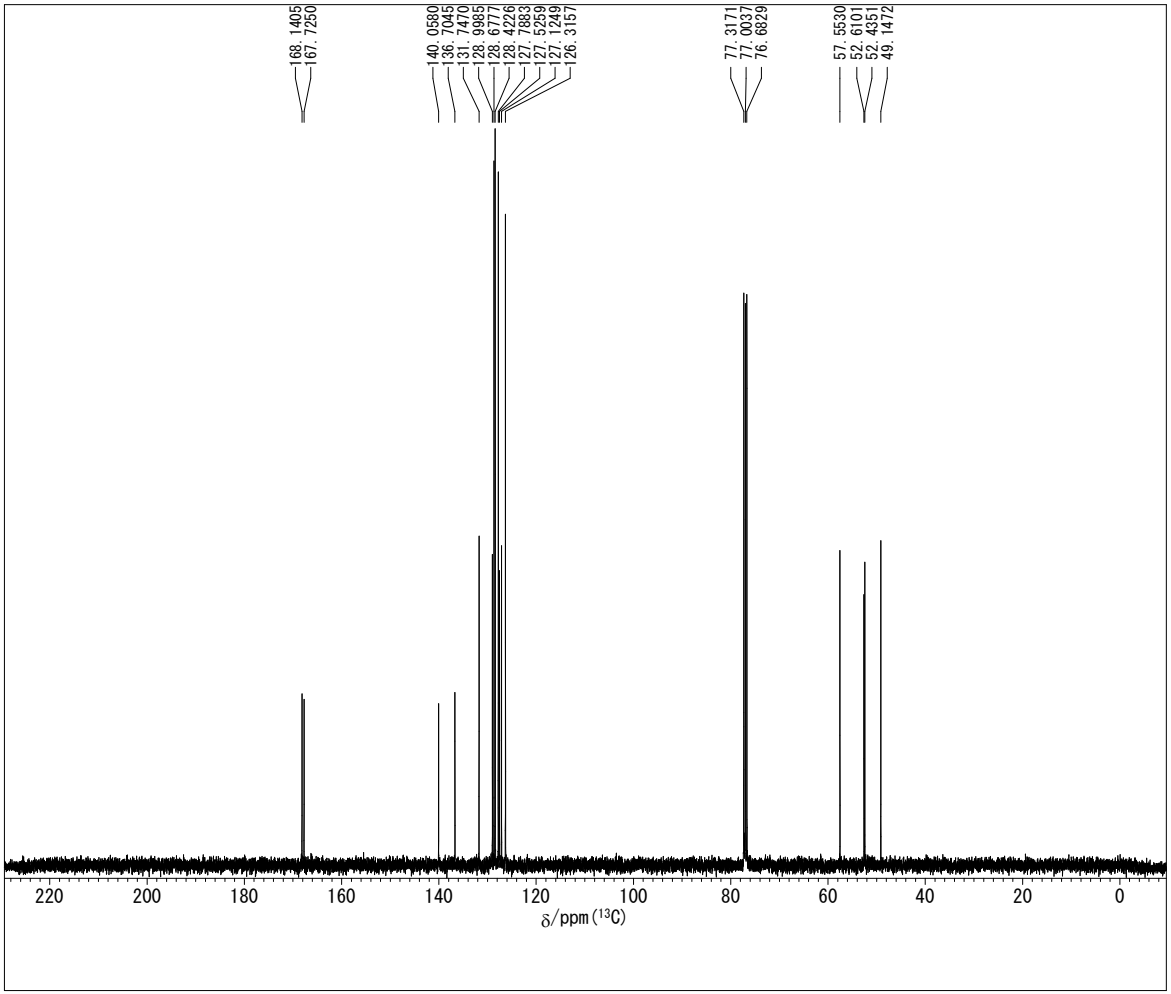
5-2. ^{1}H NMR, ^{13}C{^{1}H} NMR and chiral phase HPLC chart of 8

^{1}H NMR, ^{13}C{^{1}H} NMR and chiral phase HPLC chart of (*S*)-**8a** (**Table 2**, Entry 4)



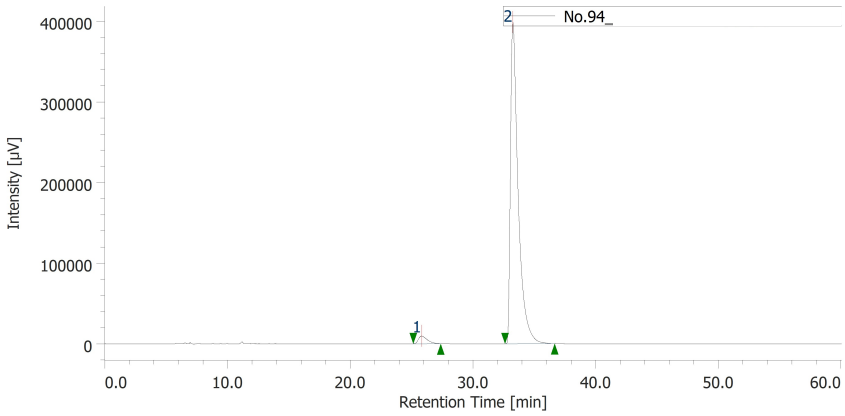
DATIM 20/Feb/2023 10:20:07
OBNUC ^{1}H
EXMOD ZG30>
OFR 400.18 MHz
OBSET 0.0 kHz
OBFIN 10003.83 Hz
POINT 65536
FREQU 4826.255 Hz
SCANS 8
ACQTM 13.5791 s
PD 1.0 s
PW1 14.0 μs
CTEMP 16.41 °C
SLVNT $CDCl_3$>
EXREF 0.0 ppm
BF 0.25 Hz
RGAIN 90
PRNT_DATE 2024/Apr/30 14:08:28
COMNT





DATIM	20/Feb/2023 10:24:44
OBNUC	^{13}C
EXMOD	ZGPG30>
OFR	100.63 MHz
OBSET	0.0 kHz
OBFIN	9998.39 Hz
POINT	32768
FREQU	24038.46 Hz
SCANS	64
ACQTM	1.3631 s
PD	2.0 s
PW1	10.0 μs
CTEMP	17.11 °C
SLVNT	$CDCL_3$>
EXREF	77.0 ppm
BF	0.25 Hz
RGAIN	203
PRNT_DATE	2024/Apr/30 14:09:36
COMNT	

Chromatogram

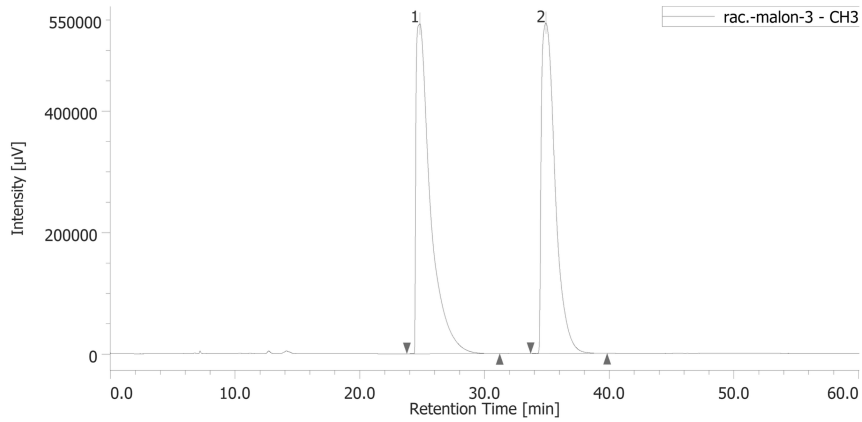


Chromatogram Information	
User Name	3385
Date Modified	2023/02/17 18:36:55
Description	AD-3, 0.5mL/min, Hex:2-PrOH=90:10
HPLC System Name	SYSTEM-3
Injection Date	2023/02/17 17:31:14
Volume	1.0 [μL]
Sample #	1
Project Name	2022system3
Acquisition Time	999.0 [min]
Acquisition Sequence	3-1615 kanda
Control Method	2019system3
Peak ID Table	
Calibration Method	
Additional Information	

Channel & Peak Information Table

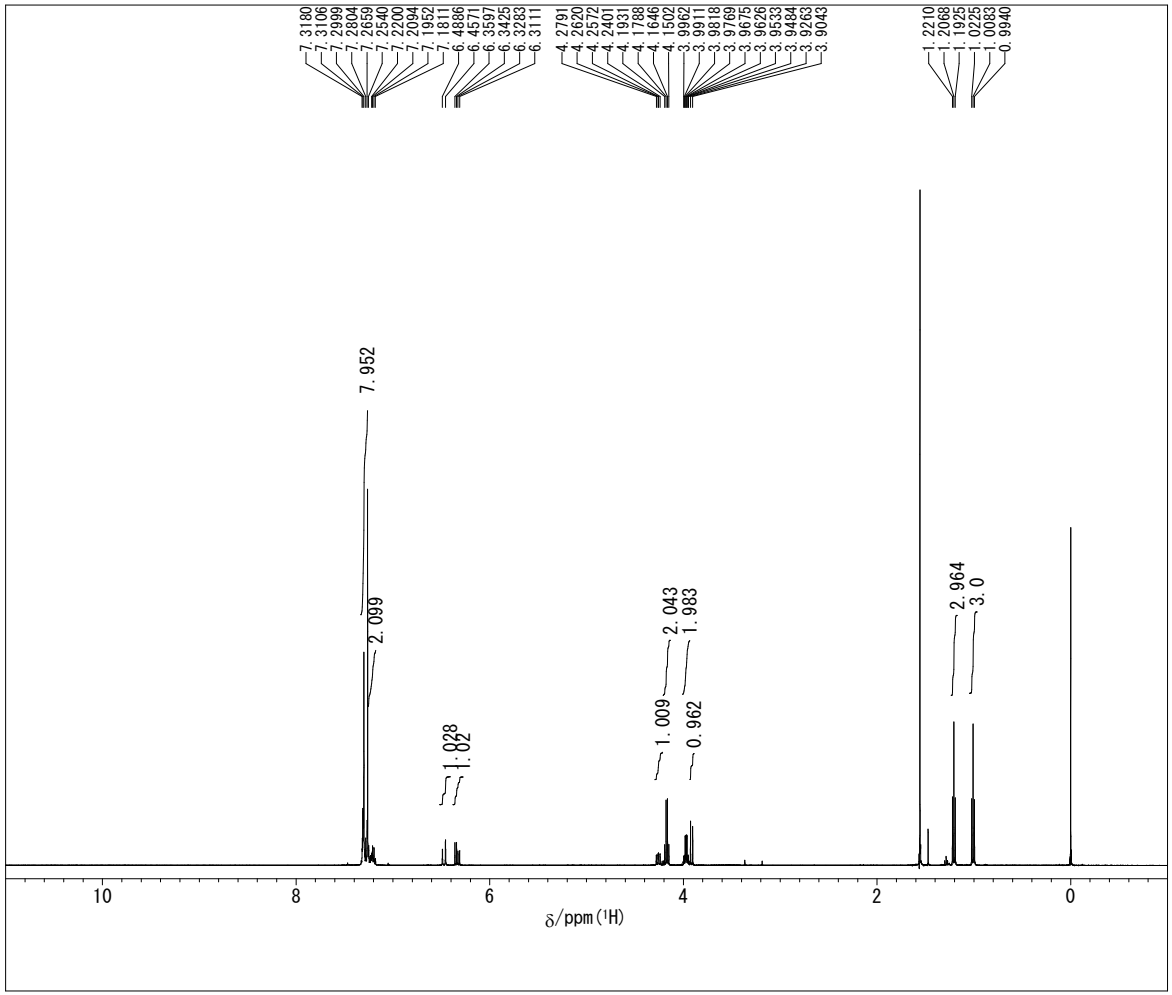
Chromatogram Name	
Sample Name	
Channel Name	UV-2075
Sampling Interval	500 [msec]
Peak Method	(Manual)

#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%
1	Unknown	3	25.82	481509	9620	2.679	2.356
2	Unknown	3	33.25	17492975	398663	97.321	97.644

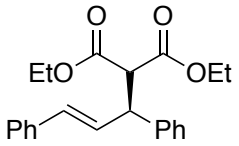


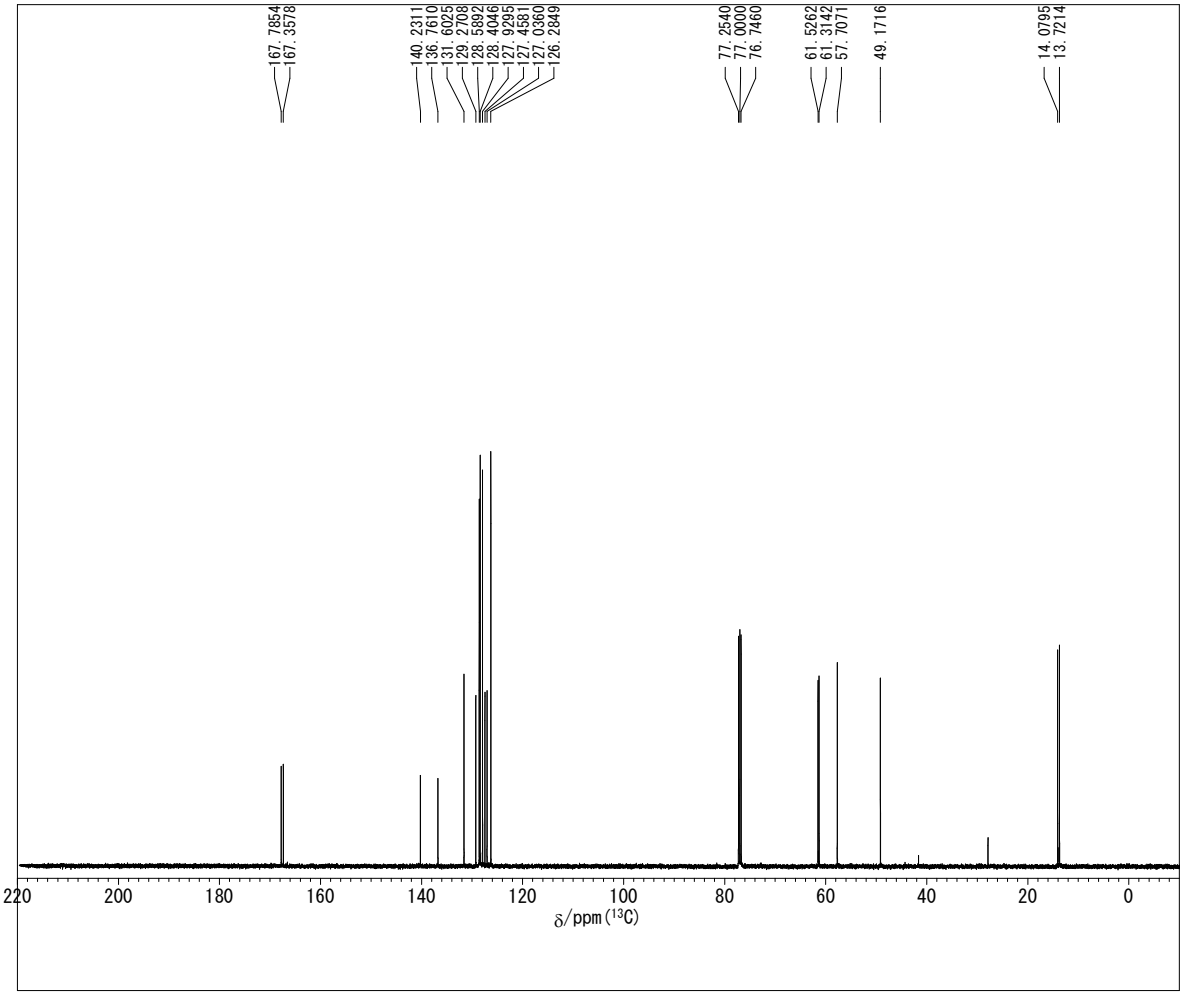
AD-3, 0.5 mL/min, Hex:2-PrOH=90:10

^{1}H NMR, ^{13}C{^{1}H} NMR and chiral phase HPLC chart of (*S*)-**8b** (**Table 2**, Entry 11)



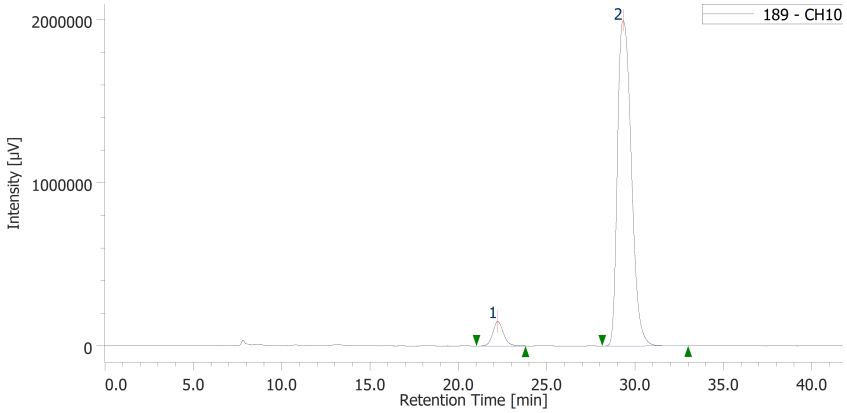

```
DATIM    10/Oct/2023 17:35:59
OBNUC                    1H
EXMOD                  ZG30
OFR                 500.13 MHz
OBSET                0.0 kHz
OBFIN             3083.419 Hz
POINT          131072(ZeroFill
    :×4)
FREQU             10000.0 Hz
SCANS                    8
ACQTM                3.2768 s
PD                   1.0 s
PW1                  2.6667 μs
CTEMP               22.2763 °C
SLVNT                CDCL3
EXREF                0.0 ppm
BF                   0.3052 Hz
RGAIN                  101
PRNT_DATE    2024/May/01 10:23:37
COMNT
```





DATIM	21/Nov/2023 13:54:59
OBNUC	^{13}C
EXMOD	ZGPG30
OFR	125.76 MHz
OBSET	0.0 kHz
OBFIN	12574.69 Hz
POINT	131072(ZeroFill :×4)
FREQU	30120.48 Hz
SCANS	128
ACQTM	1.0879 s
PD	2.0 s
PW1	3.0 μs
CTEMP	21.7051 °C
SLVNT	$CDCL_3$
EXREF	77.0 ppm
BF	0.9192 Hz
RGAIN	101
PRNT_DATE	2024/May/01 10:24:46
COMNT	

Chromatogram

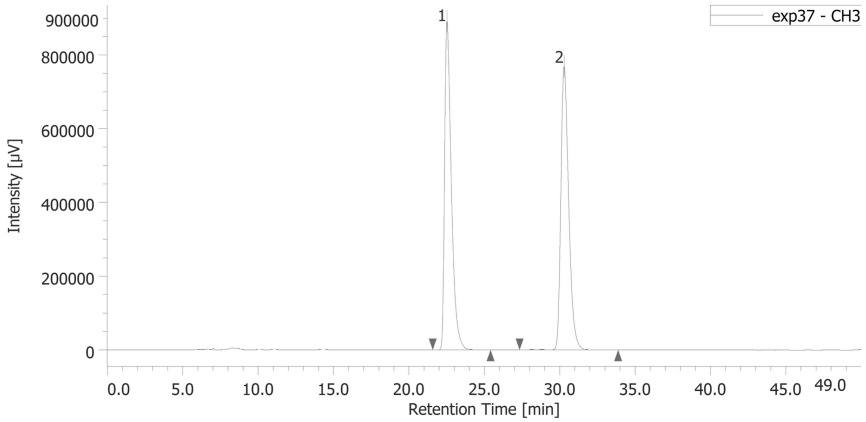


Chromatogram Information	
User Name	3385
Date Modified	2023/10/12 16:22:05
Description	AD-3, 0.5 mL/min, Hex:2pro=90:10
HPLC System Name	HPLC-1
Injection Date	2023/10/12 15:18:53
Volume	1.00 [μL]
Sample #	1
Project Name	2023system1
Acquisition Time	180.0 [min]
Acquisition Sequence	1-2463 mita
Control Method	system1_2017
Peak ID Table	
Calibration Method	
Additional Information	

Channel & Peak Information Table

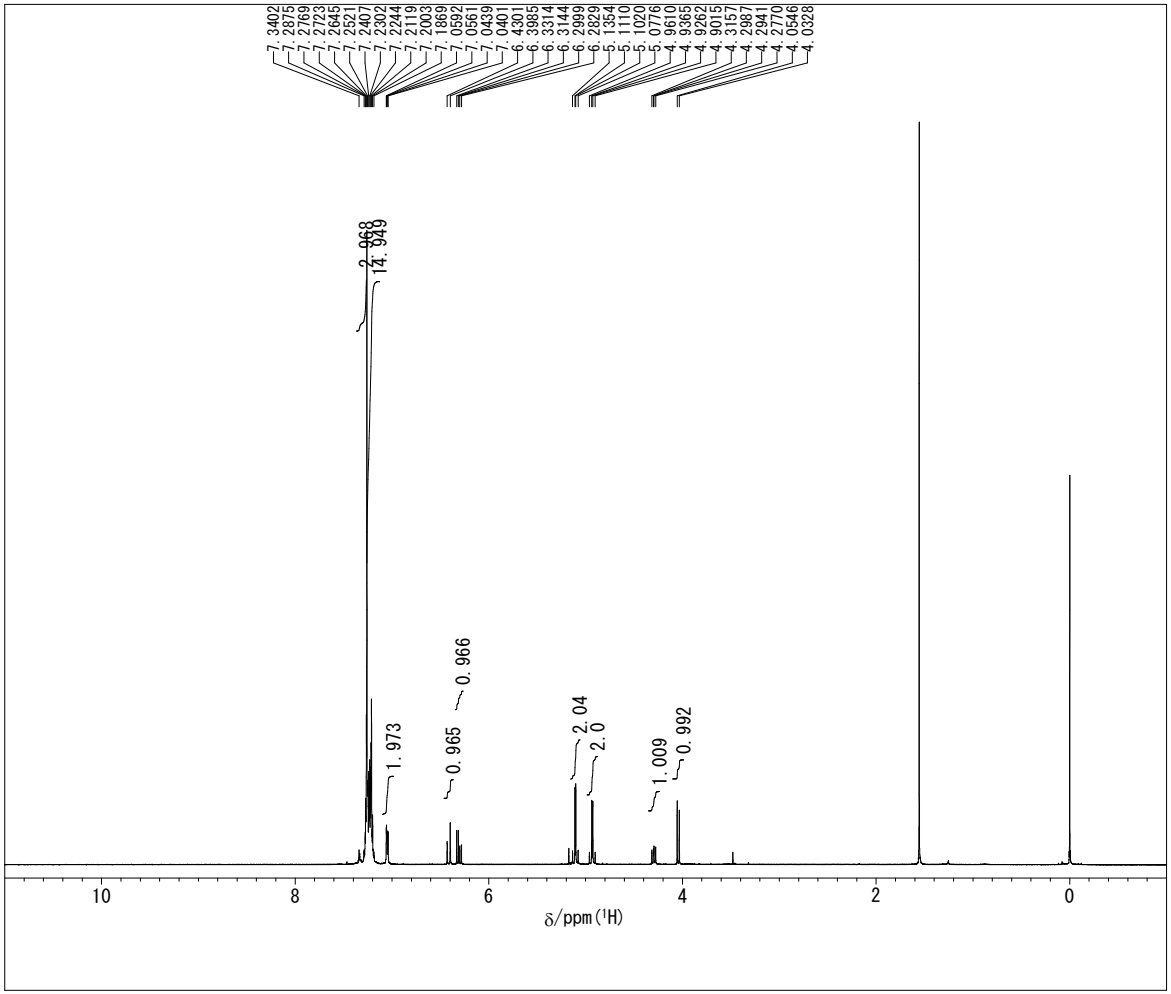
Chromatogram Name	189-CH10
Sample Name	
Channel Name	254.0nm
Sampling Interval	200 [msec]
Peak Method	(Manual)

#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%
1	Unknown	10	22.223	6253431	149542	5.437	6.97
2	Unknown	10	29.313	108762312	1995964	94.563	93.0

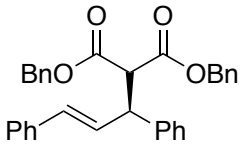


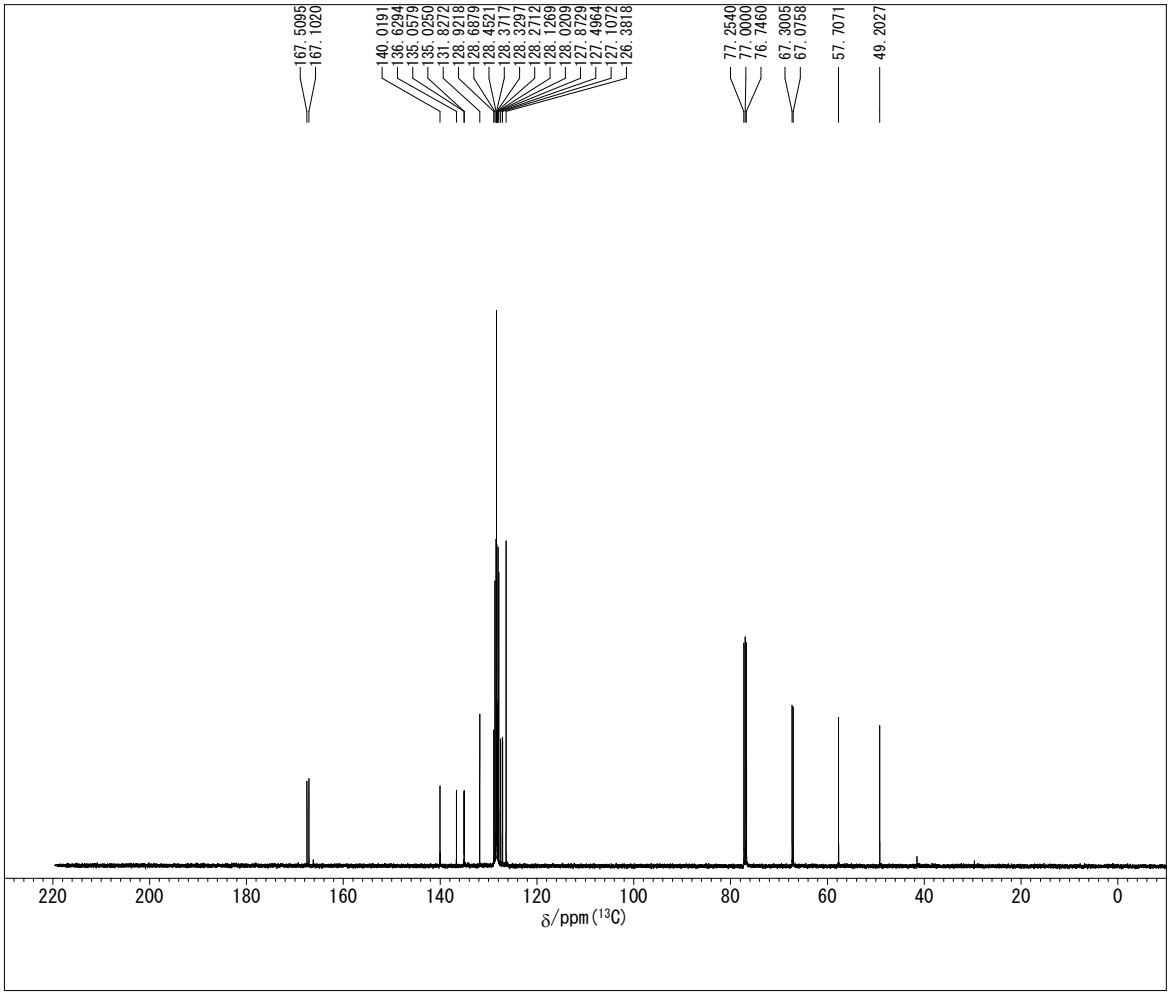
AD-3, 0.5 mL/min, hex:2-PrOH=90:10

^{1}H NMR, ^{13}C{^{1}H} NMR and chiral phase HPLC chart of (*S*)-**8d** (**Table 2**, Entry 13)



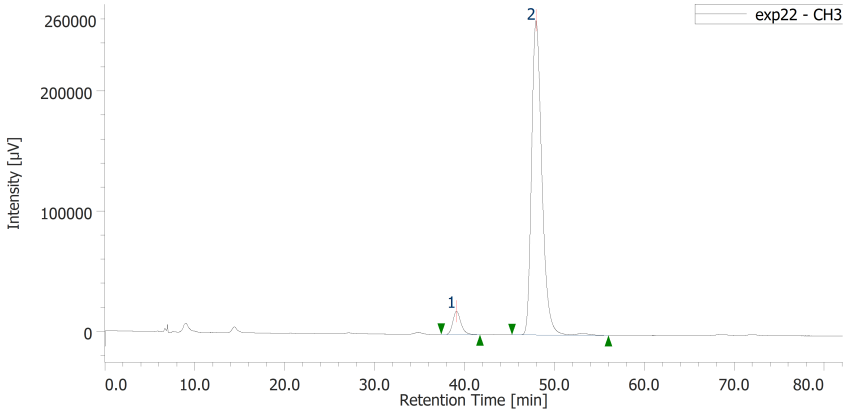

```
DATIM    23/Oct/2023 17:42:13
OBNUC                    1H
EXMOD                  ZG30
OFR                 500.13 MHz
OBSET                 0.0 kHz
OBFIN              3083.419 Hz
POINT          131072(ZeroFill
    :×4)
FREQU              10000.0 Hz
SCANS                     8
ACQTM                3.2768 s
PD                   1.0 s
PW1                  2.6667 μs
CTEMP               21.8189 °C
SLVNT                CDCl3
EXREF                0.0 ppm
BF                   0.3052 Hz
RGAIN                  101
PRNT_DATE    2024/May/01 10:27:58
COMNT
```





DATIM 21/Nov/2023 14:05:06
OBNUC ^{13}C
EXMOD ZGPG30
OFR 125.76 MHz
OBSET 0.0 kHz
OBFIN 12574.69 Hz
POINT 131072(ZeroFill :×4)
FREQU 30120.48 Hz
SCANS 128
ACQTM 1.0879 s
PD 2.0 s
PW1 3.0 μs
CTEMP 21.0435 °C
SLVNT $CDCL_3$
EXREF 77.0 ppm
BF 0.9192 Hz
RGAIN 101
PRNT_DATE 2024/May/01 16:25:03
COMNT

Chromatogram

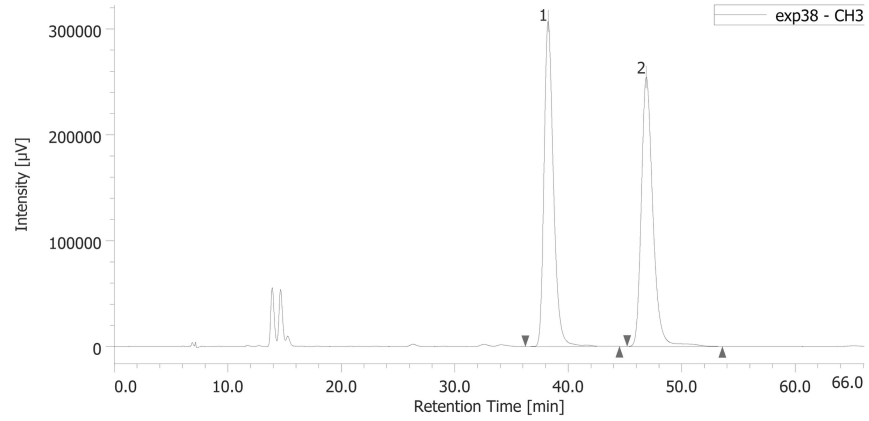


Chromatogram Information	
User Name	3385
Date Modified	2023/10/25 13:06:42
Description	AD-H, 0.5 mL/min, Hex:2pro=85:15
HPLC System Name	HPLC-1
Injection Date	2023/10/25 10:47:13
Volume	1.00 [μL]
Sample #	1
Project Name	2023system1
Acquisition Time	180.0 [min]
Acquisition Sequence	1-2483 mita
Control Method	system1_2017
Peak ID Table	
Calibration Method	
Additional Information	

Channel & Peak Information Table

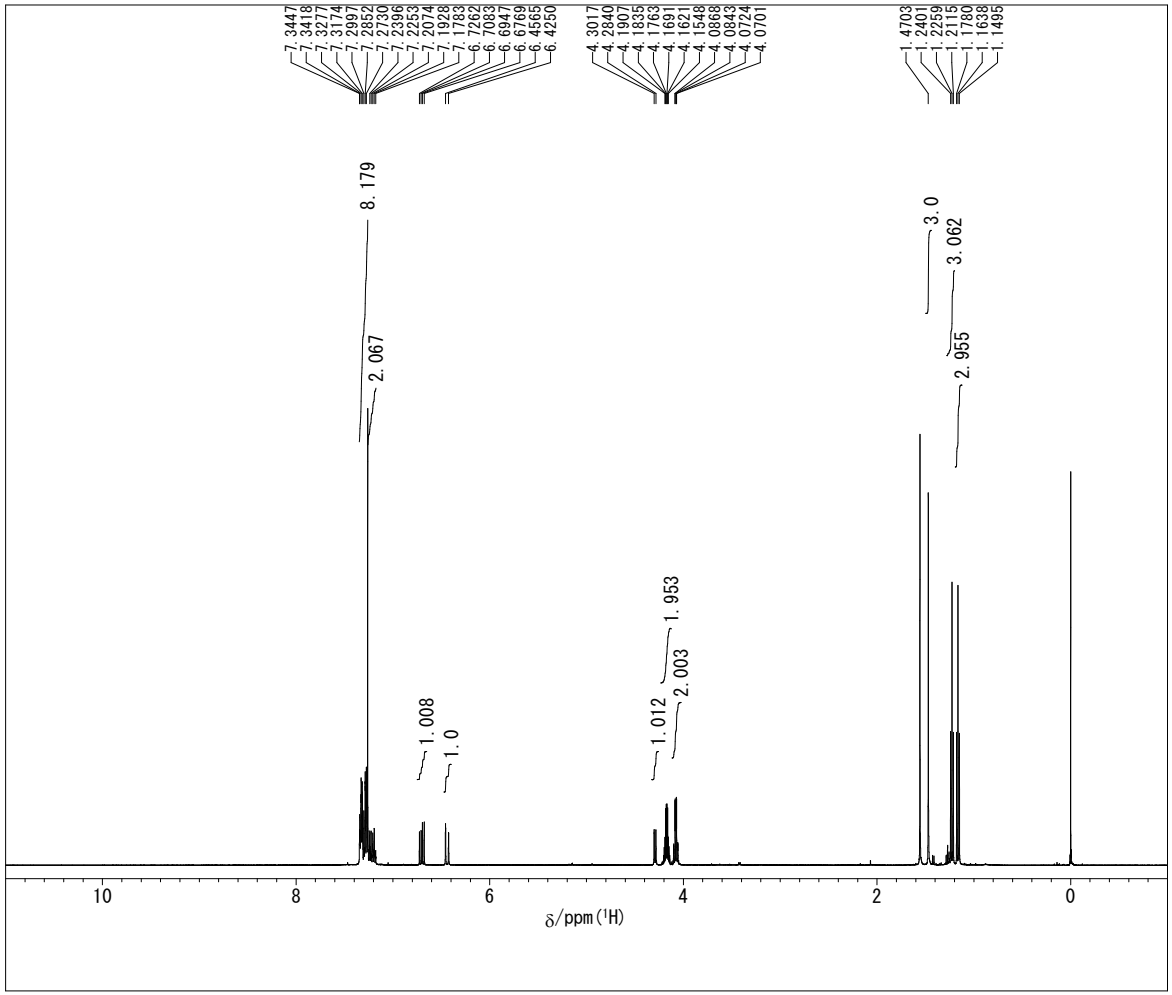
Chromatogram Name	exp22-CH3
Sample Name	
Channel Name	UV-2075
Sampling Interval	500 [msec]
Peak Method	(Manual)

#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%
1	Unknown	3	39.092	1207949	19369	5.468	6.89
2	Unknown	3	47.942	20883089	261812	94.532	93.1

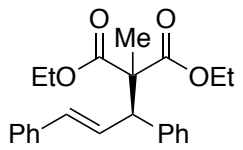


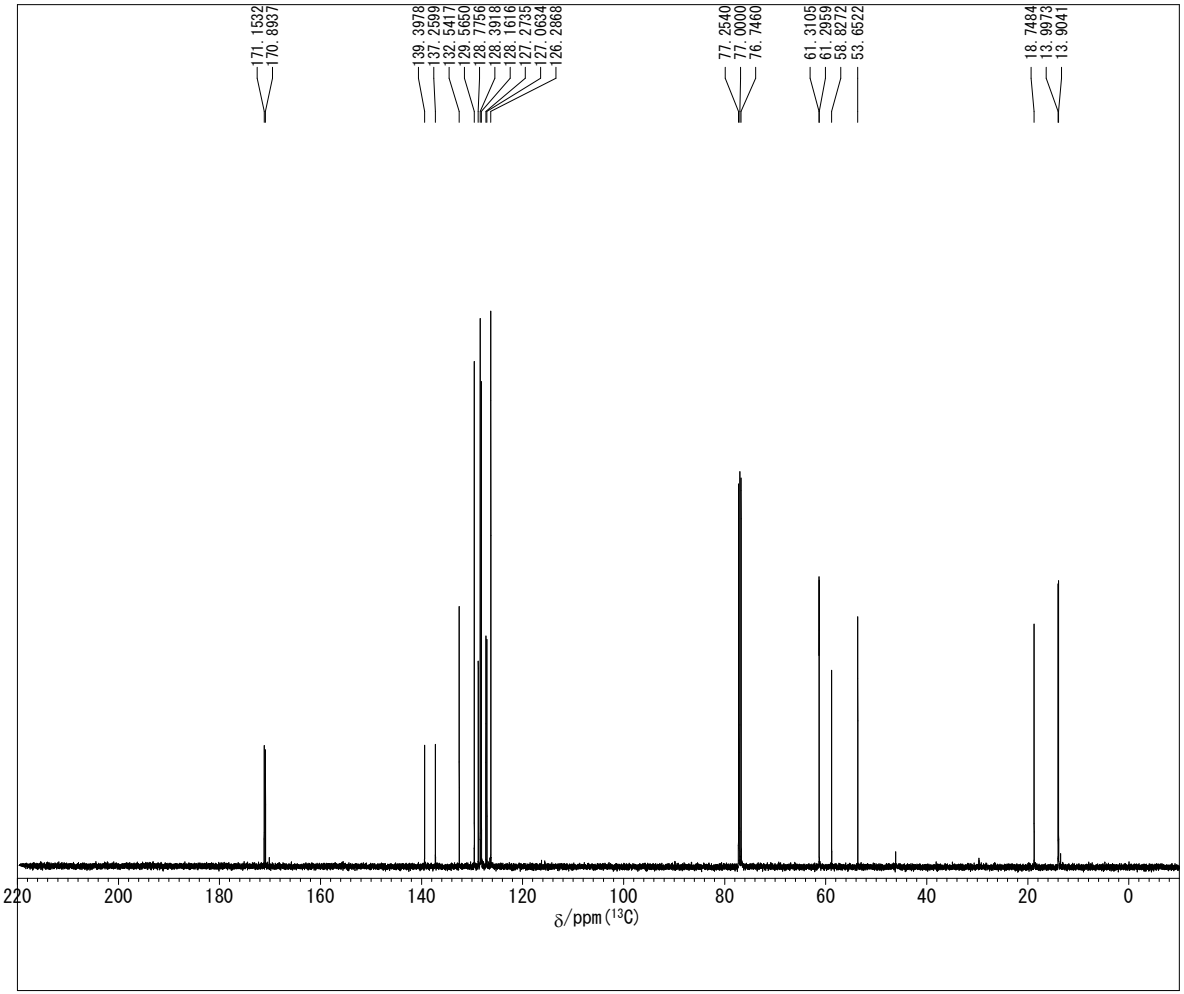
AD-H, 0.5 mL/min, hex:2-PrOH=85:15

^{1}H NMR, ^{13}C{^{1}H} NMR and chiral phase HPLC chart of (*R*)-**8e** (**Table 2**, Entry 14)



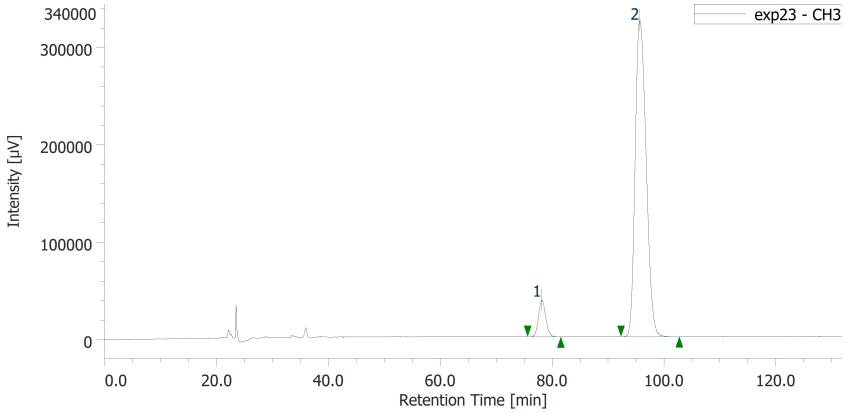
DATIM 18/Oct/2023 15:44:03
OBNUC ¹H
EXMOD ZG30
OFR 500.13 MHz
OBSET 0.0 kHz
OBFIN 3083.419 Hz
POINT 131072(ZeroFill :×4)
FREQU 10000.0 Hz
SCANS 8
ACQTM 3.2768 s
PD 1.0 s
PW1 2.6667 μs
CTEMP 22.164 °C
SLVNT $CDCl_3$
EXREF 0.0 ppm
BF 0.3052 Hz
RGAIN 101
PRNT_DATE 2024/May/01 10:34:47
COMNT





DATIM 21/Nov/2023 14:15:10
OBNUC ^{13}C
EXMOD ZGPG30
OFR 125.76 MHz
OBSET 0.0 kHz
OBFIN 12574.69 Hz
POINT 131072(ZeroFill :×4)
FREQU 30120.48 Hz
SCANS 128
ACQTM 1.0879 s
PD 2.0 s
PW1 3.0 μs
CTEMP 21.1555 °C
SLVNT $CDCL_3$
EXREF 77.0 ppm
BF 0.9192 Hz
RGAIN 101
PRNT_DATE 2024/May/01 10:35:41
COMNT

Chromatogram

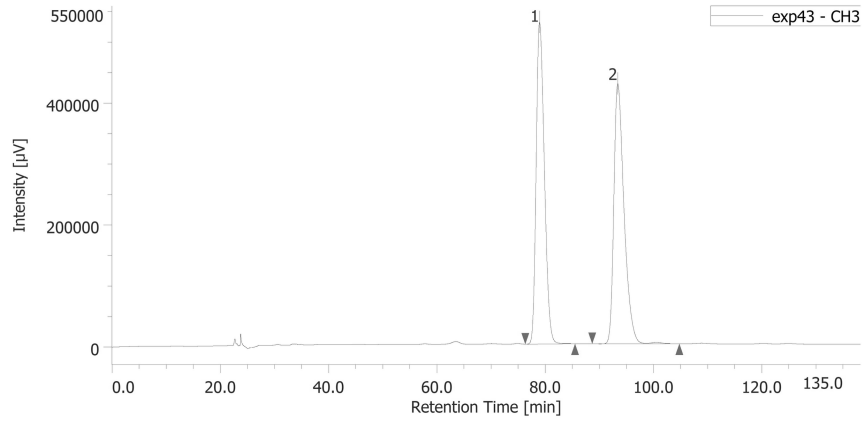


Chromatogram Information	
User Name	3385
Date Modified	2023/10/20 13:27:48
Description	AD-H,AD-3, 0.3 mL/min, hex:2-pr=99:1
HPLC System Name	SYSTEM-3
Injection Date	2023/10/20 10:51:01
Volume	1.0 [μL]
Sample #	1
Project Name	2023system3
Acquisition Time	180.0 [min]
Acquisition Sequence	3-1624 mita
Control Method	2019system3
Peak ID Table	
Calibration Method	
Additional Information	

Channel & Peak Information Table

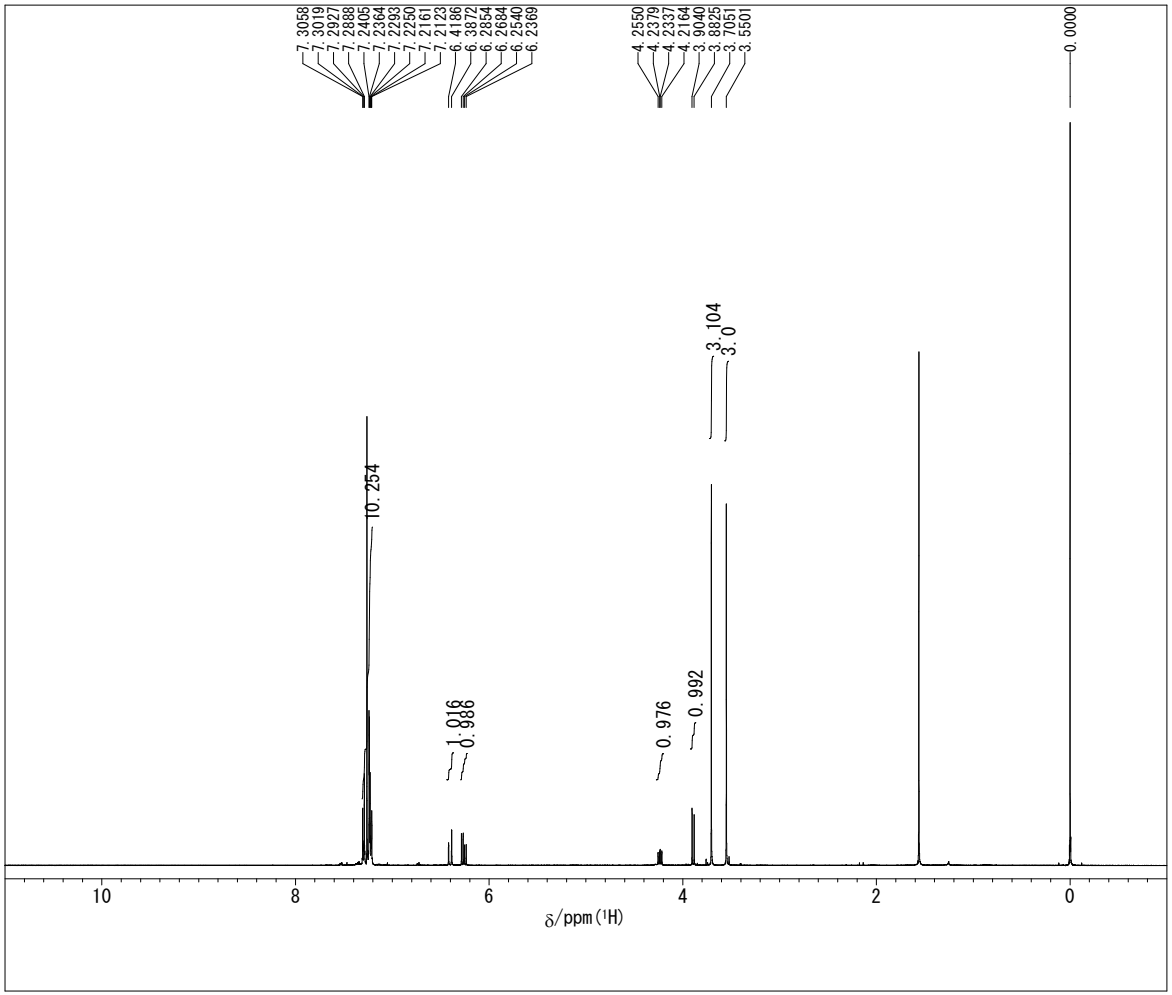
Chromatogram Name	exp23-CH3
Sample Name	
Channel Name	UV-2075
Sampling Interval	500 [msec]
Peak Method	(Manual)

#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%
1	Unknown	3	78.15	3318141	37591	6.984	10.377
2	Unknown	3	95.66	44194417	324651	93.016	89.623

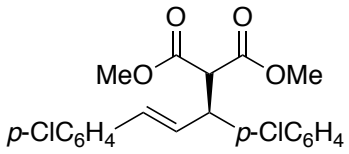


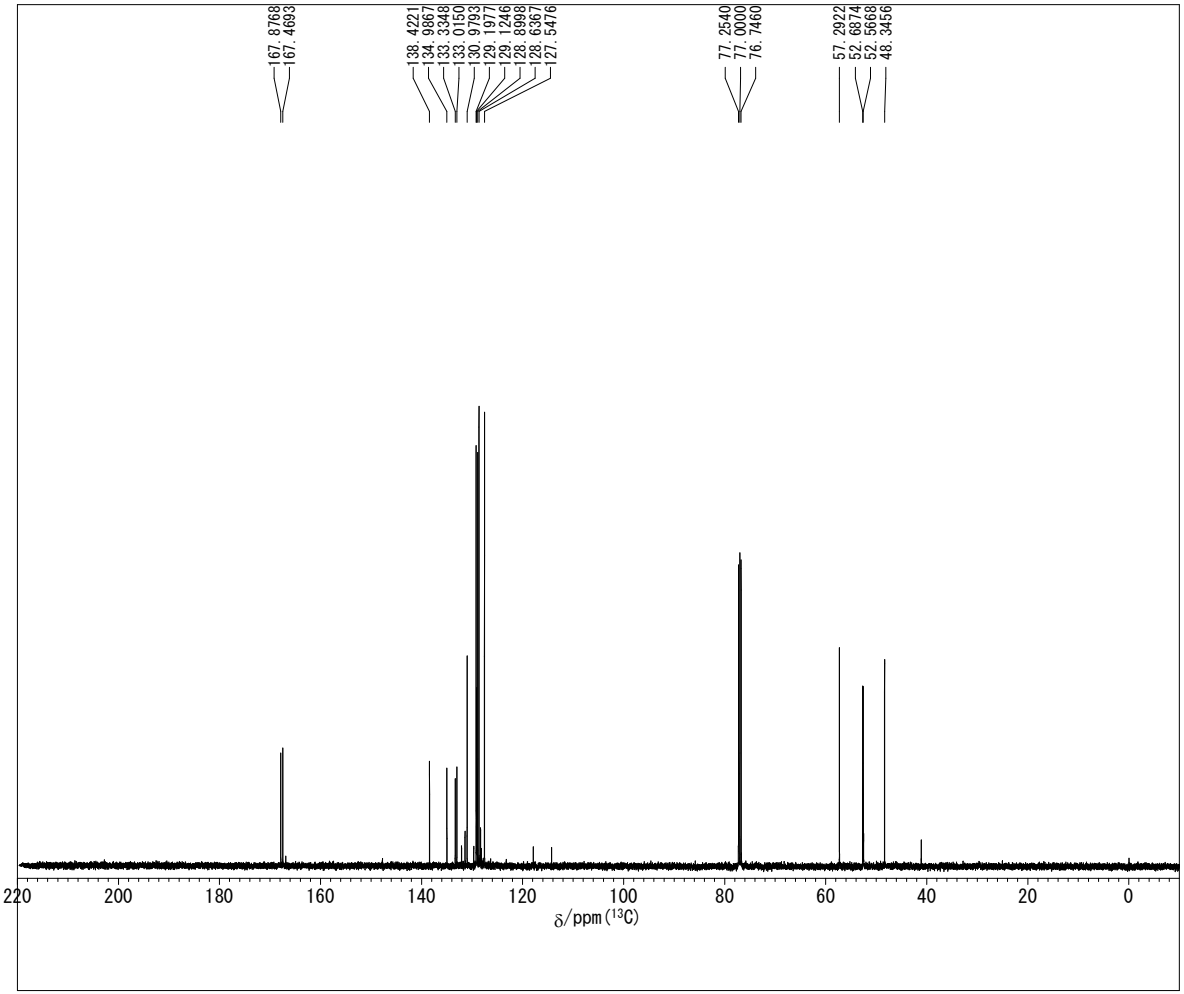
AD-H AD-3, 0.3 mL/min, hex:2-PrOH=99:1

^{1}H NMR, ^{13}C{^{1}H} NMR and chiral phase HPLC chart of (*S*)-**8f** (**Table 2**, Entry 15)



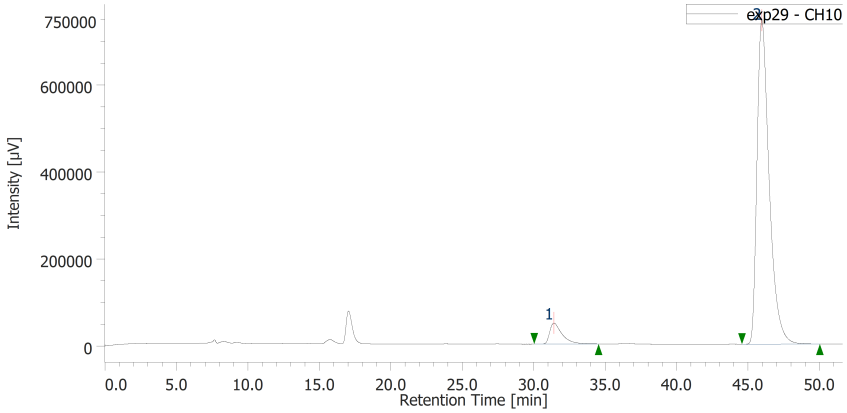
DATIM 12/Dec/2023 17:42:33
OBNUC ^{1}H
EXMOD ZG30
OFR 500.13 MHz
OBSET 0.0 kHz
OBFIN 3083.419 Hz
POINT 131072(ZeroFill :×4)
FREQU 10000.0 Hz
SCANS 8
ACQTM 3.2768 s
PD 1.0 s
PW1 2.6667 μs
CTEMP 20.5811 °C
SLVNT $CDCl_3$
EXREF 0.0 ppm
BF 0.3052 Hz
RGAIN 101
PRNT_DATE 2024/May/01 10:37:44
COMNT





DATIM 22/Nov/2023 11:15:04
OBNUC ^{13}C
EXMOD ZGPG30
OFR 125.76 MHz
OBSET 0.0 kHz
OBFIN 12574.69 Hz
POINT 131072(ZeroFill :×4)
FREQU 30120.48 Hz
SCANS 64
ACQTM 1.0879 s
PD 2.0 s
PW1 3.0 μs
CTEMP 21.7686 °C
SLVNT $CDCL_3$
EXREF 77.0 ppm
BF 0.9192 Hz
RGAIN 101
PRNT_DATE 2024/May/01 10:39:01
COMNT

Chromatogram

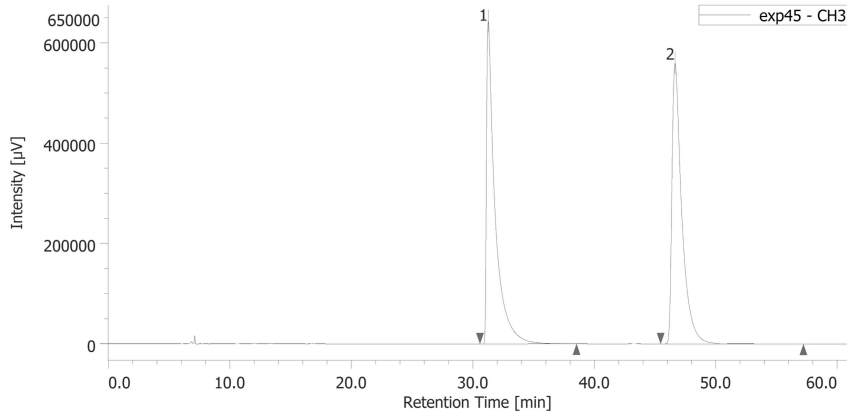


Chromatogram Information	
User Name	3385
Date Modified	2023/11/02 15:19:25
Description	AD-3, 0.5 mL/min, Hex:2pro=85:15
HPLC System Name	HPLC-1
Injection Date	2023/11/02 13:58:05
Volume	1.00 [μL]
Sample #	1
Project Name	2023system1
Acquisition Time	180.0 [min]
Acquisition Sequence	1-2498 mita
Control Method	system1_2017
Peak ID Table	
Calibration Method	
Additional Information	

Channel & Peak Information Table

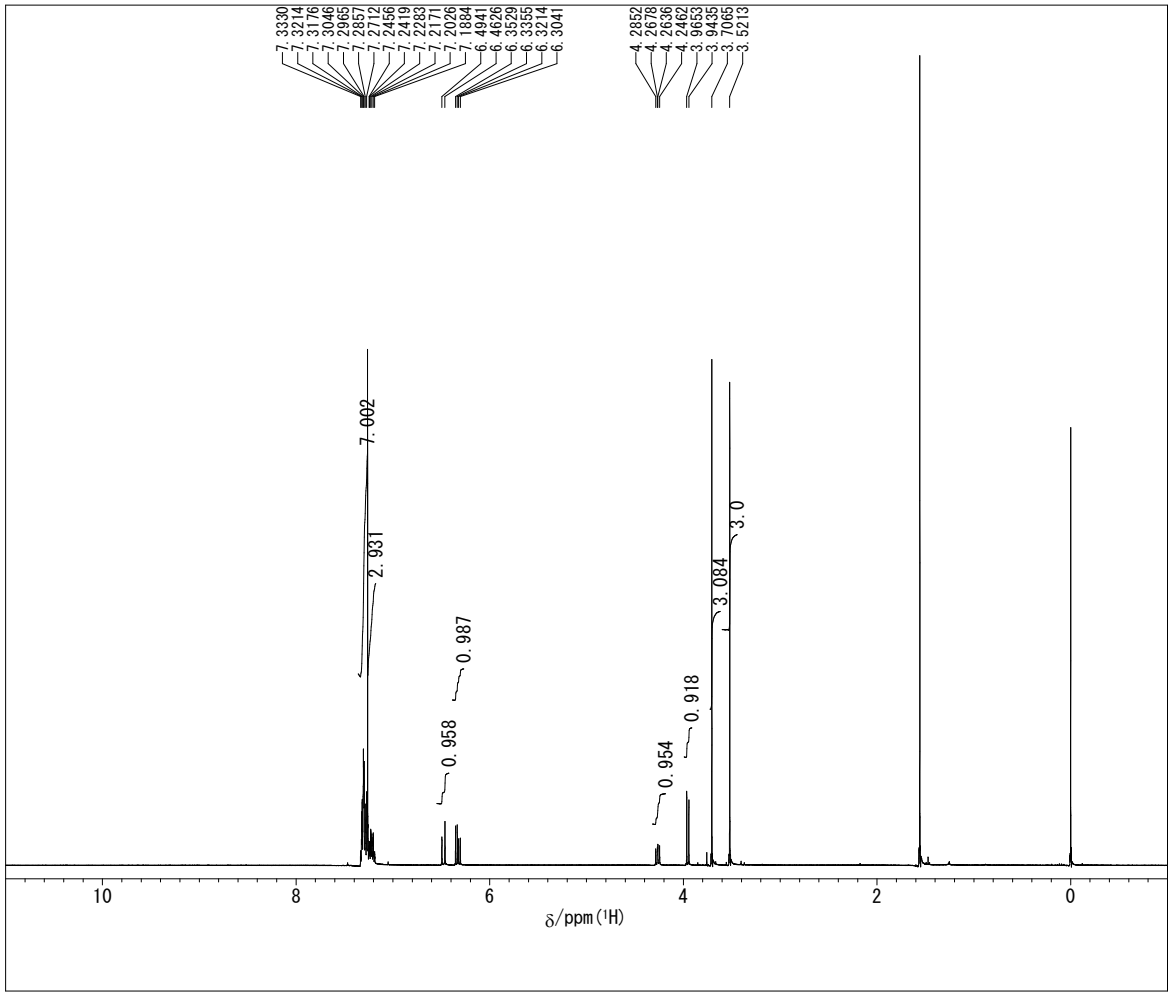
Chromatogram Name	exp29-CH10
Sample Name	
Channel Name	254.0nm
Sampling Interval	200 [msec]
Peak Method	(Manual)

#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%
1	Unknown	10	31.403	2901699	48200	6.163	6.08
2	Unknown	10	45.950	44179734	743930	93.837	93.9

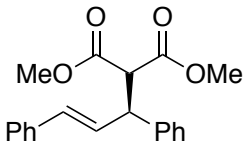


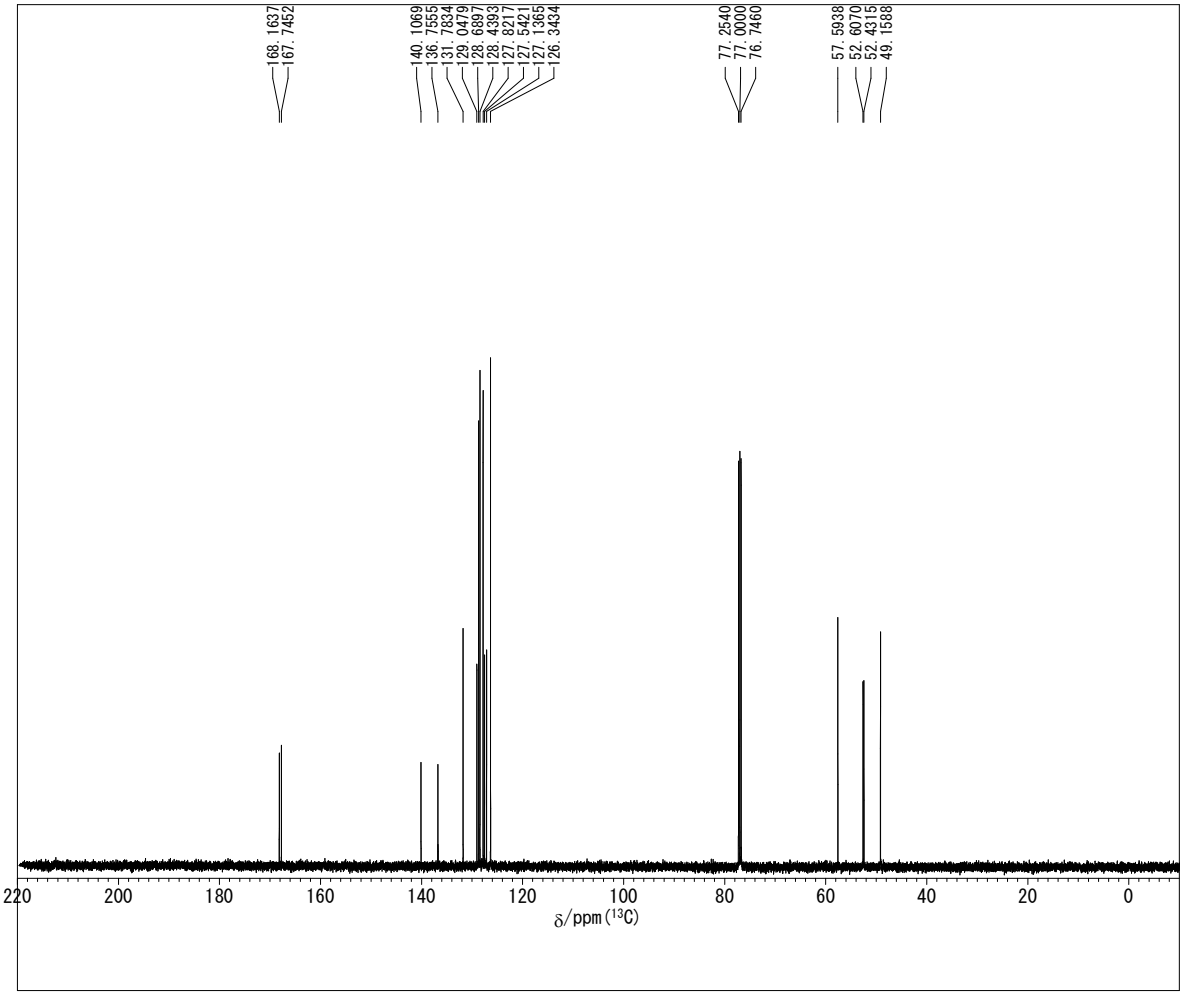
AD-3, 0.5 mL/min, hex:2-PrOH=85:15

^{1}H NMR, ^{13}C{^{1}H} NMR and chiral phase HPLC chart of (*S*)-**8a** (**Table 2**, Entry 16)



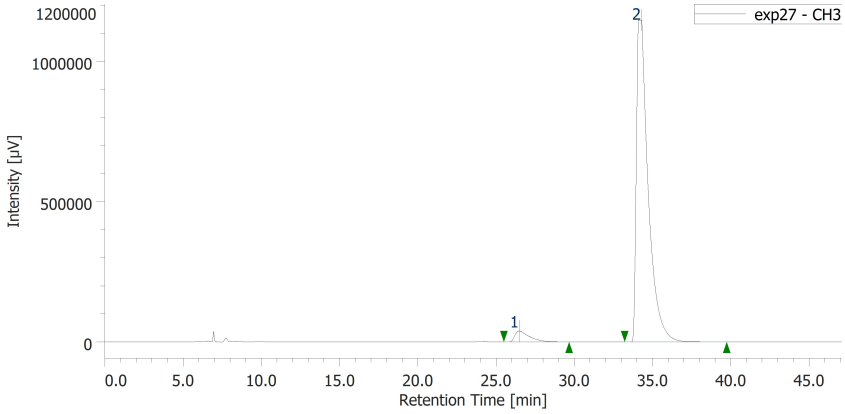
DATIM 25/Oct/2023 14:26:07
OBNUC ^{1}H
EXMOD ZG30
OFR 500.13 MHz
OBSET 0.0 kHz
OBFIN 3083.419 Hz
POINT 131072(ZeroFill :×4)
FREQU 10000.0 Hz
SCANS 8
ACQTM 3.2768 s
PD 1.0 s
PW1 2.6667 μs
CTEMP 21.6182 °C
SLVNT $CDCl_3$
EXREF 0.0 ppm
BF 0.3052 Hz
RGAIN 101
PRNT_DATE 2024/May/01 10:41:57
COMNT





DATIM 22/Nov/2023 11:08:04
OBNUC ^{13}C
EXMOD ZGPG30
OFR 125.76 MHz
OBSET 0.0 kHz
OBFIN 12574.69 Hz
POINT 131072(ZeroFill :×4)
FREQU 30120.48 Hz
SCANS 65
ACQTM 1.0879 s
PD 2.0 s
PW1 3.0 μs
CTEMP 21.3682 ℃
SLVNT $CDCL_3$
EXREF 77.0 ppm
BF 0.9192 Hz
RGAIN 101
PRNT_DATE 2024/May/01 10:42:47
COMNT

Chromatogram

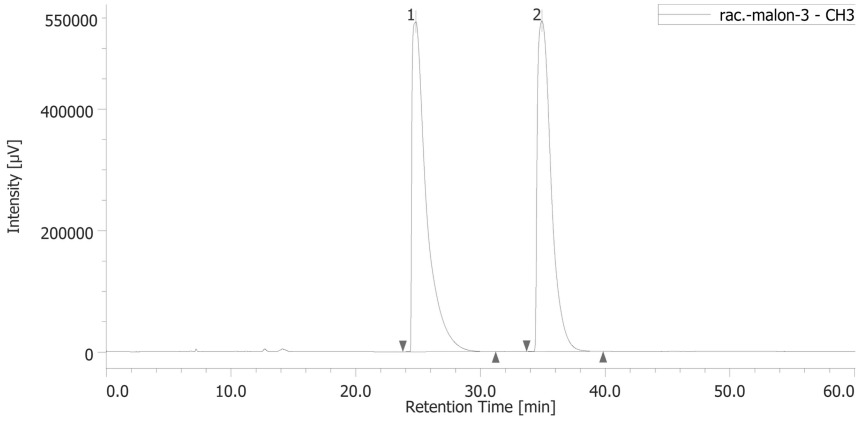


Chromatogram Information	
User Name	3385
Date Modified	2023/10/26 15:50:49
Description	AD-3, 0.5mL/min, hex:2pro=90:10
HPLC System Name	SYSTEM-3
Injection Date	2023/10/26 13:59:45
Volume	1.0 [μL]
Sample #	1
Project Name	2023system3
Acquisition Time	180.0 [min]
Acquisition Sequence	3-1645 mita
Control Method	2019system3
Peak ID Table	
Calibration Method	
Additional Information	

Channel & Peak Information Table

Chromatogram Name	exp27-CH3
Sample Name	
Channel Name	UV-2075
Sampling Interval	500 [msec]
Peak Method	(Manual)

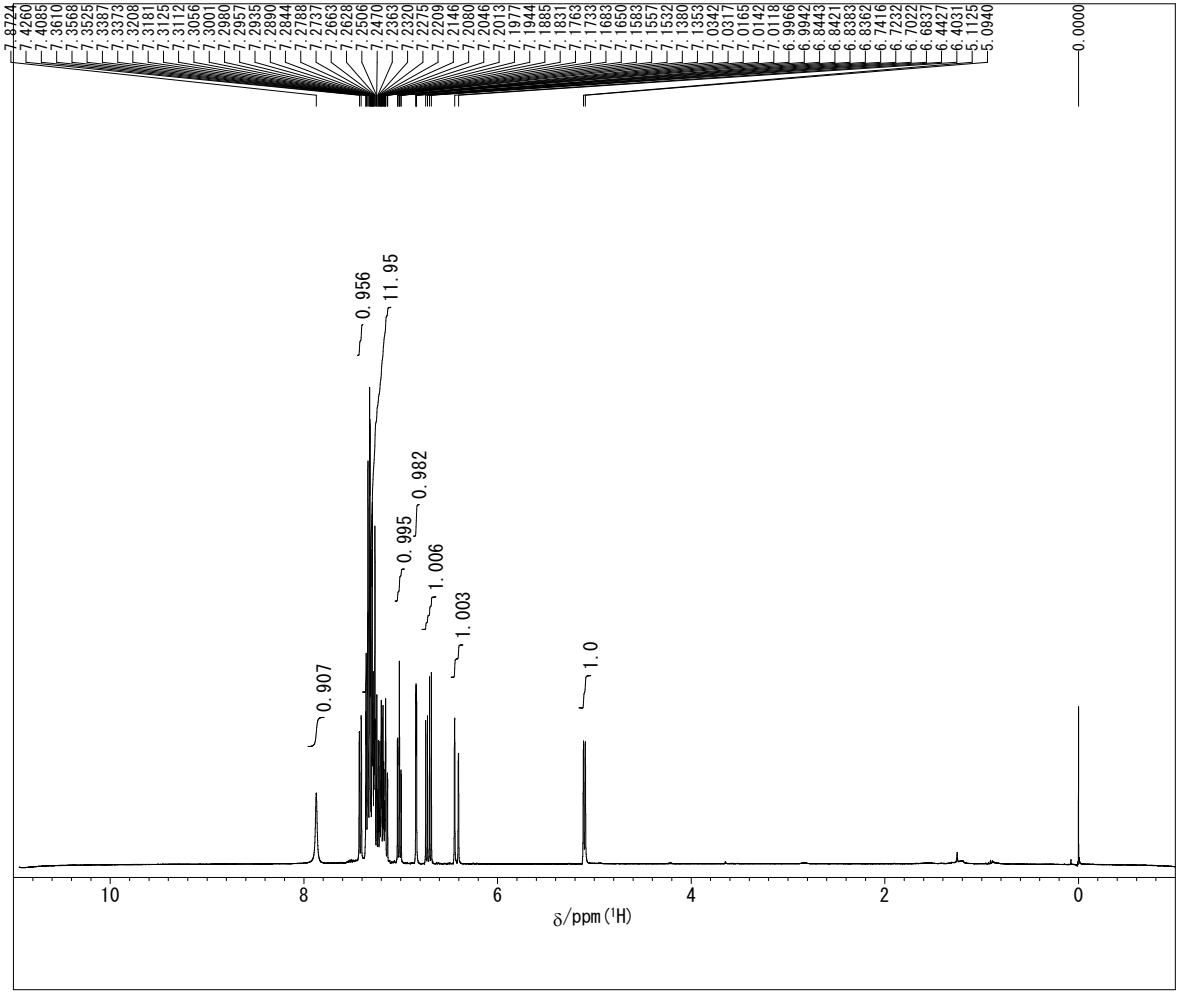
#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%
1	Unknown	3	26.48	2534316	39105	4.058	3.298
2	Unknown	3	34.27	59923876	1146577	95.942	96.702



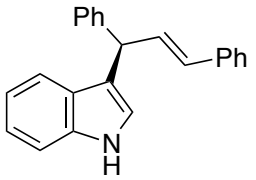
AD-3, 0.5 mL/min, Hex:2-PrOH=90:10

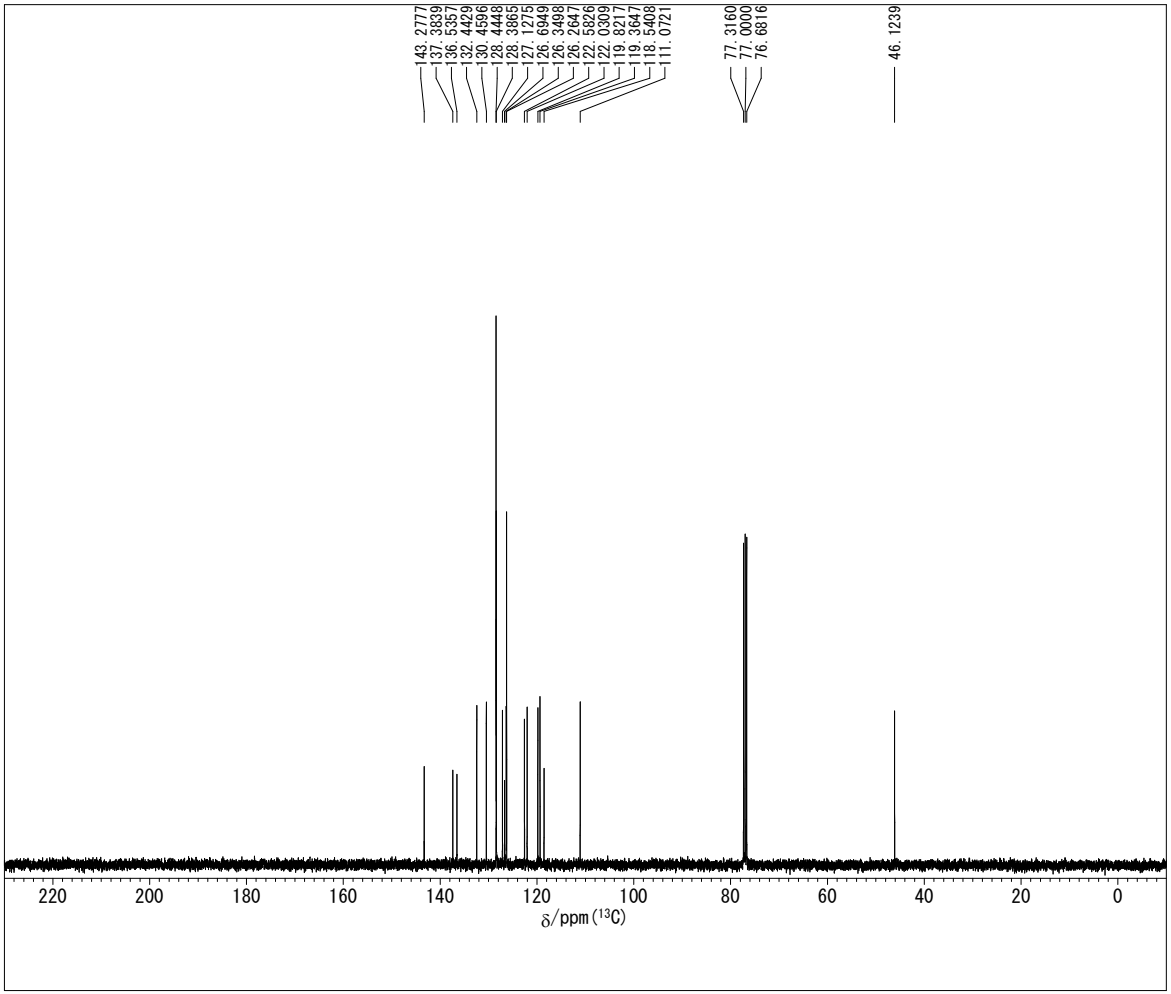
5-3. ^{1}H NMR, ^{13}C{^{1}H} NMR and chiral phase HPLC chart of 10

^{1}H NMR, ^{13}C{^{1}H} NMR and chiral phase HPLC chart of (*R*)-**10a** (**Table 3**, Entry 15 and **Table 4**, Entry 1)



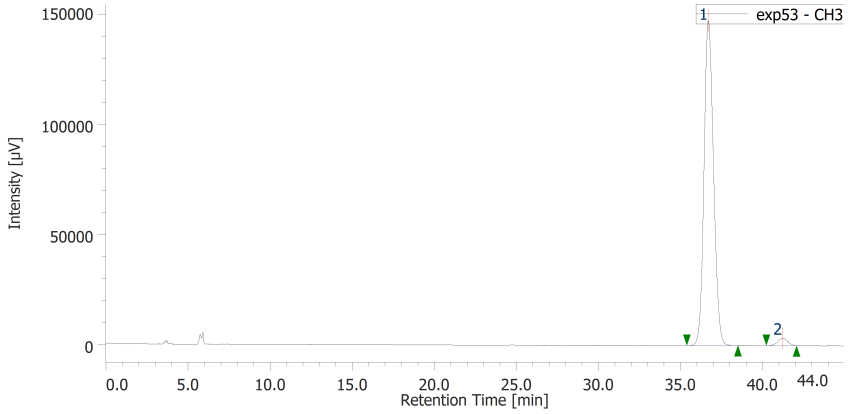
DATIM 15/Dec/2022 10:31:48
OBNUC ^{1}H
EXMOD ZG30>
OFR 400.13 MHz
OBSET 0.0 kHz
OBFIN 1996.017 Hz
POINT 131072(ZeroFill :×4)
FREQU 4826.255 Hz
SCANS 8
ACQTM 6.7895 s
PD 1.0 s
PW1 14.0 μs
CTEMP 16.01 ℃
SLVNT $CDCl_3$>
EXREF 0.0 ppm
BF 0.1473 Hz
RGAIN 128
PRNT_DATE 2024/May/02 07:50:48
COMNT





DATIM 15/Dec/2022 10:37:23
OBNUC ^{13}C
EXMOD ZGPG30>
OFR 100.61 MHz
OBSET 0.0 kHz
OBFIN 12705.91 Hz
POINT 131072(ZeroFill :×4)
FREQU 32051.28 Hz
SCANS 64
ACQTM 1.0224 s
PD 2.0 s
PW1 9.0 μs
CTEMP 16.51 ℃
SLVNT $CDCL_3$>
EXREF 77.0 ppm
BF 0.9781 Hz
RGAIN 2050
PRNT_DATE 2024/May/02 07:49:50
COMNT

Chromatogram



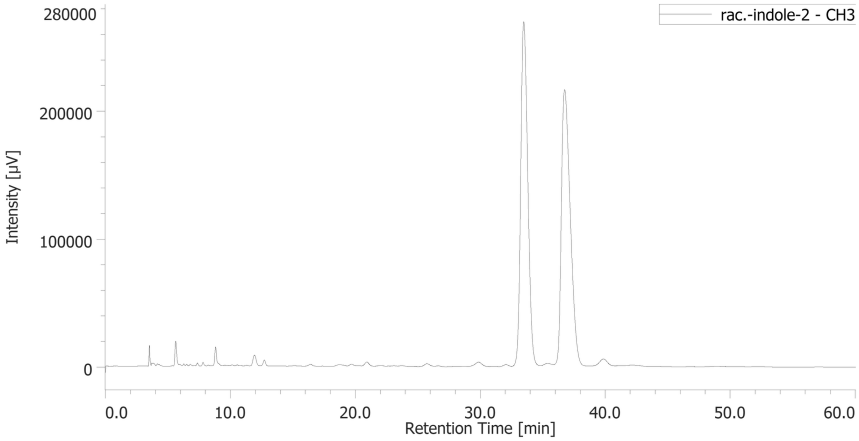
Chromatogram Information

User Name	3385
Date Modified	2022/12/15 14:57:18
Description	IB, 1.0 mL/min, Hex:EtOH=99:1, UV 254 nm, CD 254 nm
HPLC System Name	HPLC-1
Injection Date	2022/12/15 14:10:24
Volume	1.00 [μL]
Sample #	1
Project Name	2022system1
Acquisition Time	180.0 [min]
Acquisition Sequence	1-2215 toba
Control Method	system1_2017
Peak ID Table	
Calibration Method	
Additional Information	

Channel & Peak Information Table

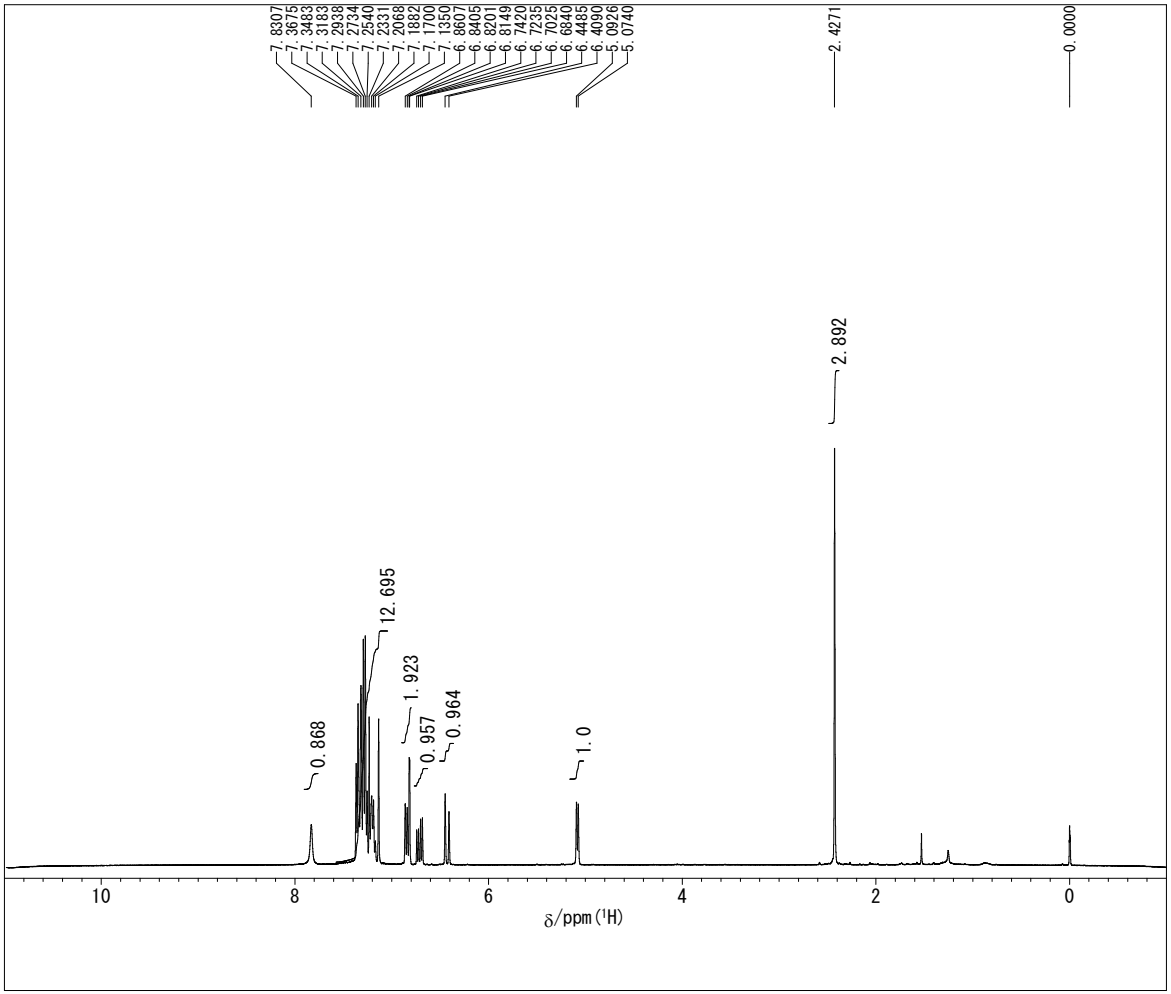
Chromatogram Name	exp53-CH3
Sample Name	
Channel Name	UV-2075
Sampling Interval	500 [msec]
Peak Method	(Manual)

#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%
1	Unknown	3	36.683	5916679	147477	97.660	97.8
2	Unknown	3	41.208	141774	3328	2.340	2.21

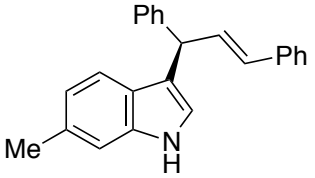


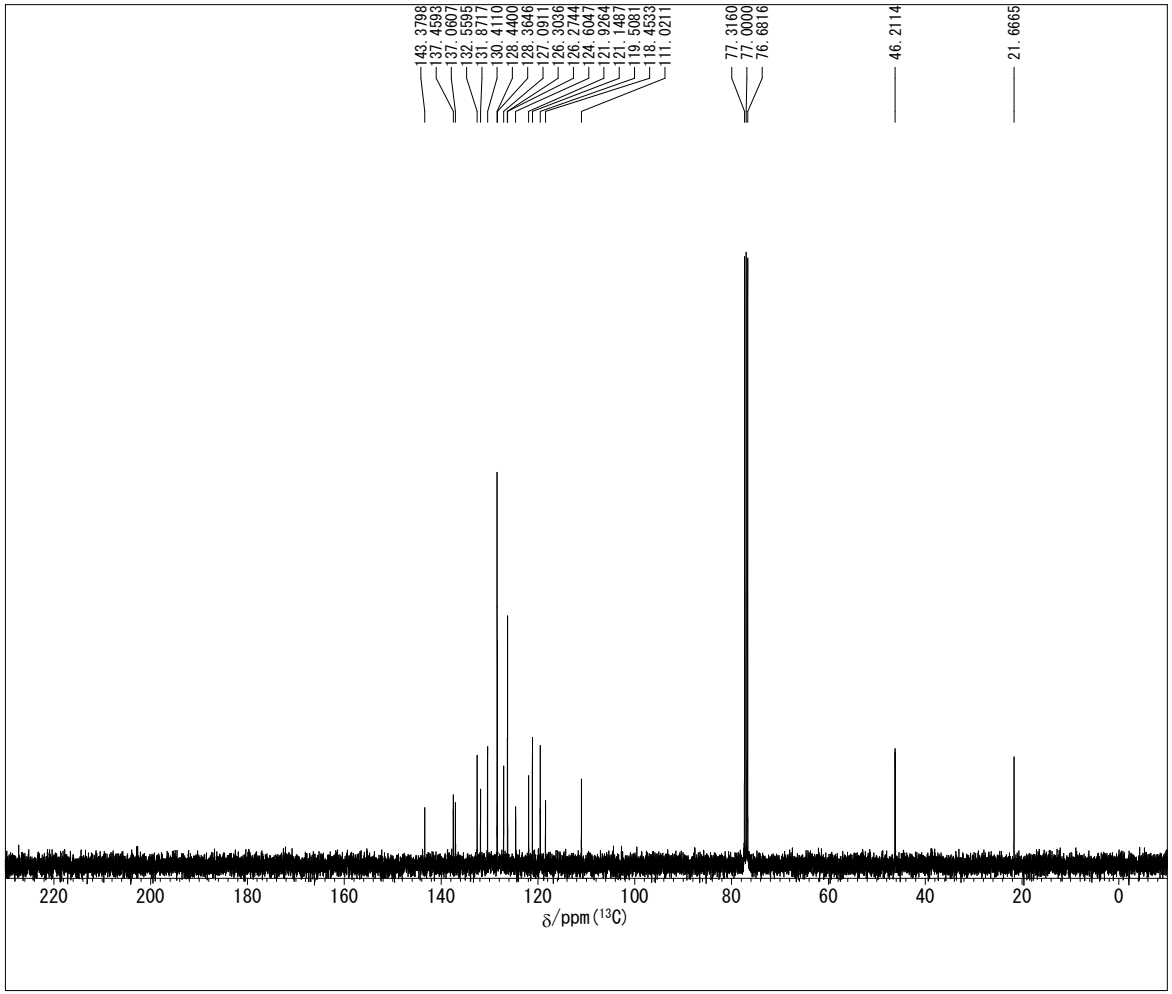
IB, 1.0 mL/min, Hex:EtOH=99:1, UV 254 nm, CD 254 nm

^{1}H NMR, ^{13}C{^{1}H} NMR and chiral phase HPLC chart of (*R*)-**10b** (**Table 4**, Entry 2)



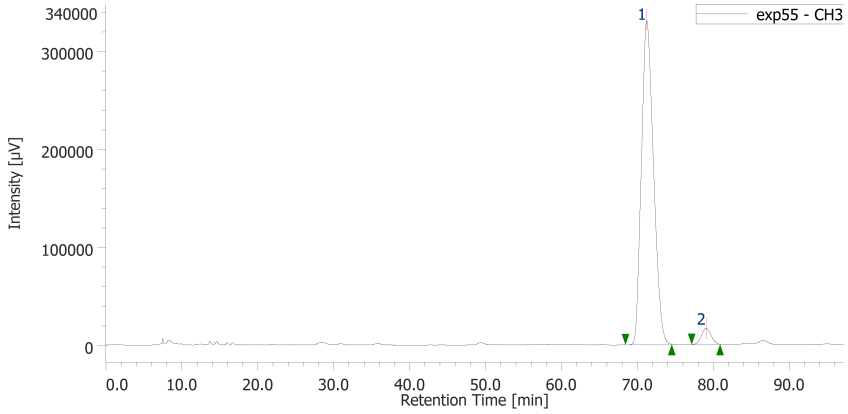
DATIM 10/Jan/2023 13:47:07
OBNUC ^{1}H
EXMOD ZG30>
OFR 400.13 MHz
OBSET 0.0 kHz
OBFIN 1996.017 Hz
POINT 131072(ZeroFill :×4)
FREQU 4826.255 Hz
SCANS 8
ACQTM 6.7895 s
PD 1.0 s
PW1 14.0 μs
CTEMP 17.81 °C
SLVNT $CDCl_3$>
EXREF 0.0 ppm
BF 0.1473 Hz
RGAIN 228
PRNT_DATE 2024/May/02 08:21:05
COMNT





DATIM 10/Jan/2023 13:51:29
OBNUC ^{13}C
EXMOD ZGPG30>
OFR 100.61 MHz
OBSET 0.0 kHz
OBFIN 12705.91 Hz
POINT 131072(ZeroFill :×4)
FREQU 32051.28 Hz
SCANS 64
ACQTM 1.0224 s
PD 2.0 s
PW1 9.0 μs
CTEMP 18.21 ℃
SLVNT $CDCL_3$>
EXREF 77.0 ppm
BF 0.9781 Hz
RGAIN 2050
PRNT_DATE 2024/May/02 08:21:42
COMNT

Chromatogram

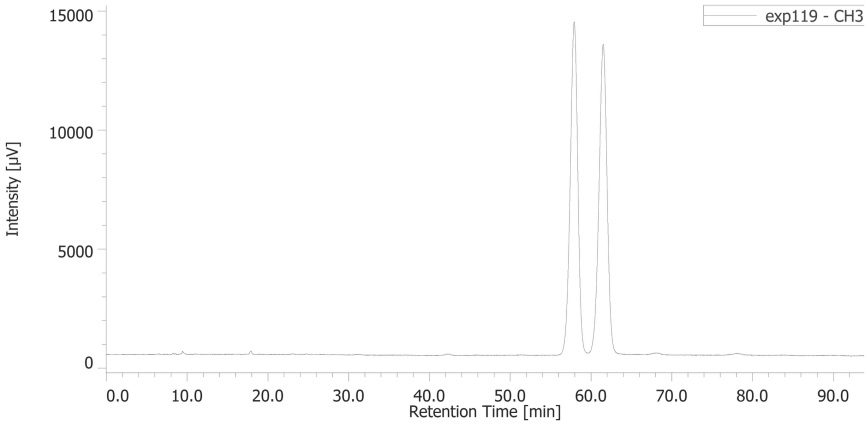


Chromatogram Information	
User Name	3385
Date Modified	2023/01/10 18:23:16
Description	IB, 0.5 mL/min, Hex:EtOH=99:1, UV 254 nm, CD 254 nm
HPLC System Name	HPLC-1
Injection Date	2023/01/10 16:07:54
Volume	1.00 [μL]
Sample #	1
Project Name	2022system1
Acquisition Time	180.0 [min]
Acquisition Sequence	1-2249 toba
Control Method	system1_2017
Peak ID Table	
Calibration Method	
Additional Information	

Channel & Peak Information Table

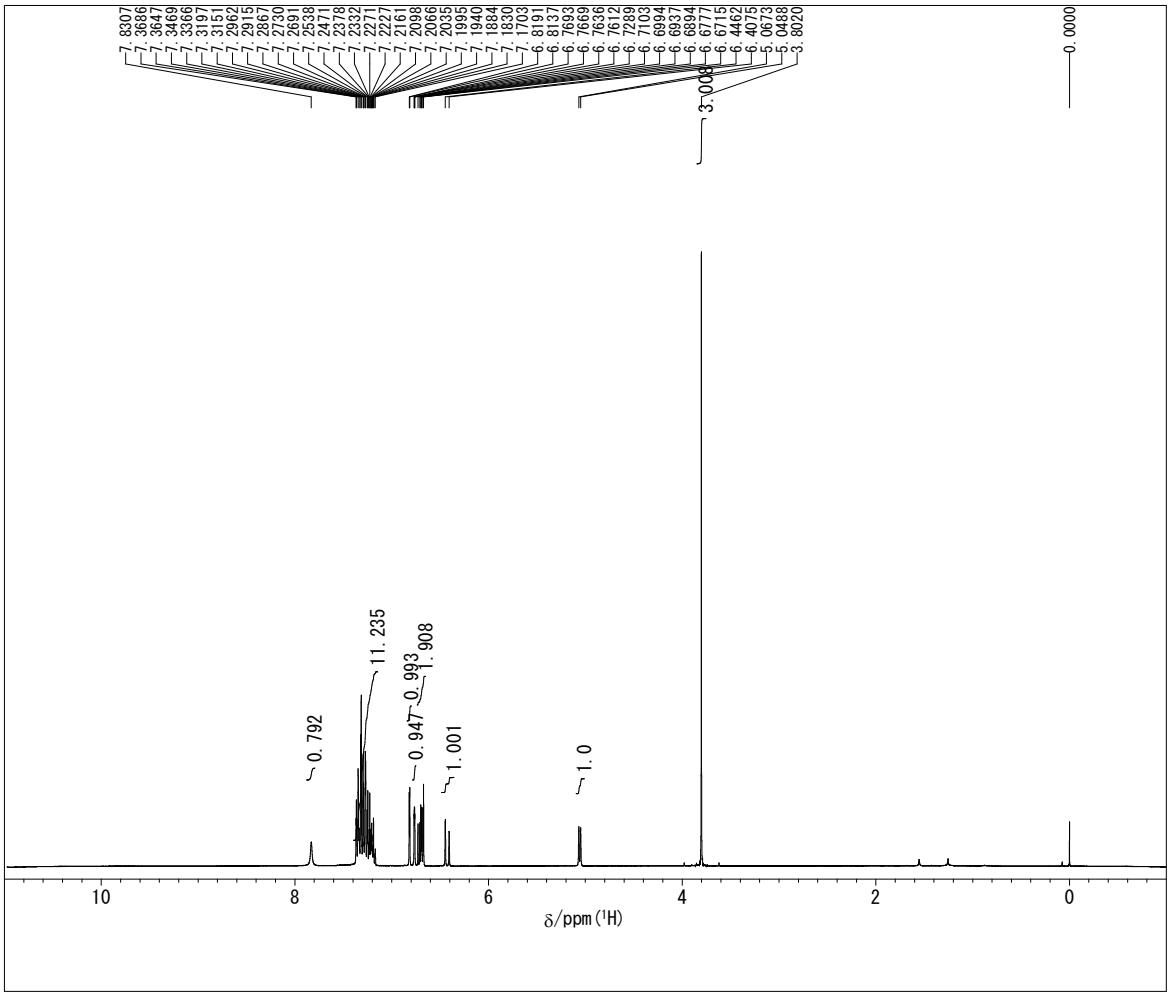
Chromatogram Name	exp55-CH3
Sample Name	
Channel Name	UV-2075
Sampling Interval	500 [msec]
Peak Method	(Manual)

#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%
1	Unknown	3	71.217	36600828	330636	96.211	95.2
2	Unknown	3	79.033	1441579	16538	3.789	4.76

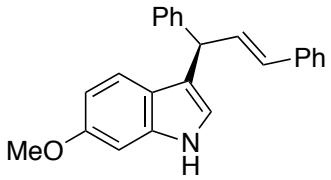


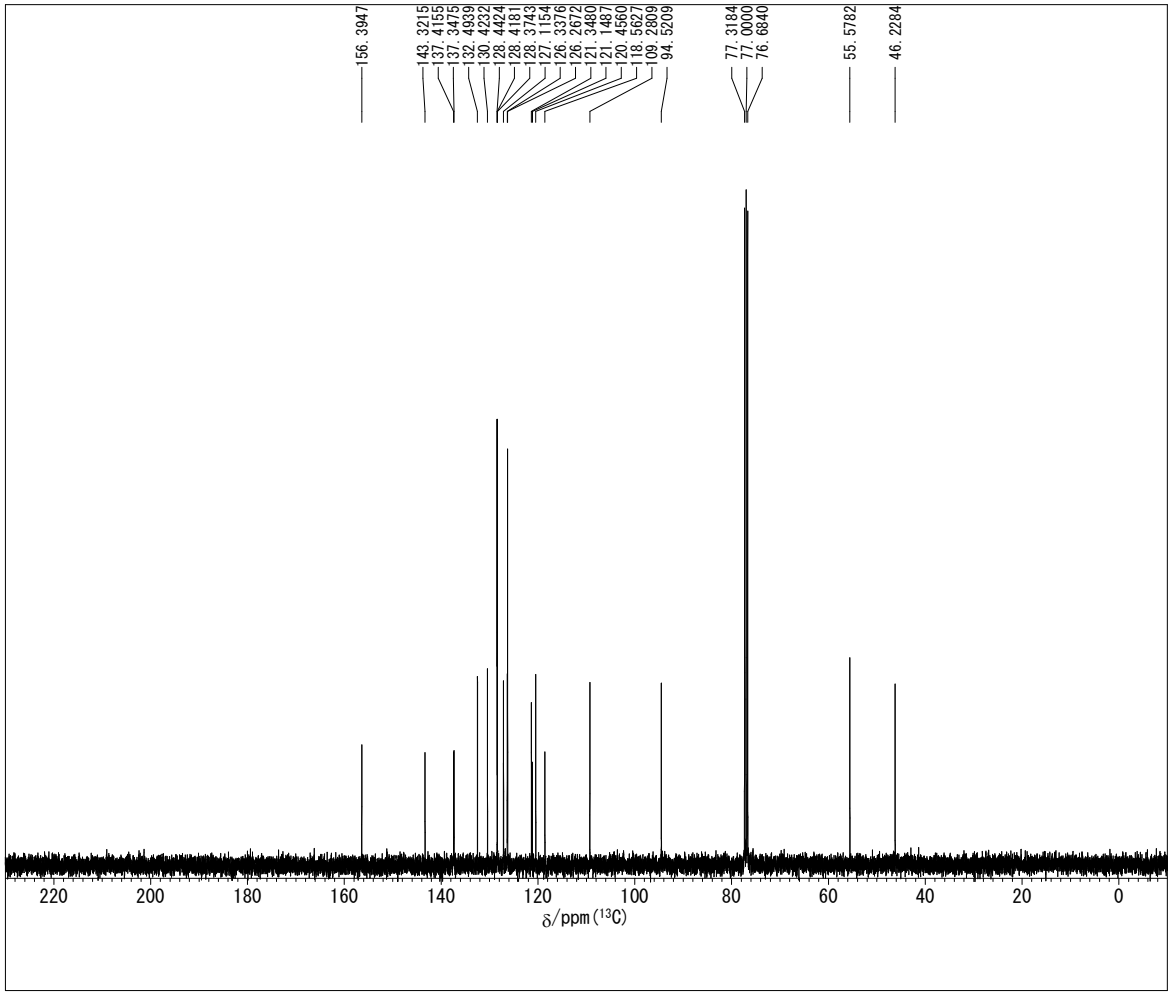
IB,flow0.5,Hex:EtOH=99:1

^{1}H NMR, ^{13}C{^{1}H} NMR and chiral phase HPLC chart of (*R*)-**10c** (**Table 4**, Entry 3)



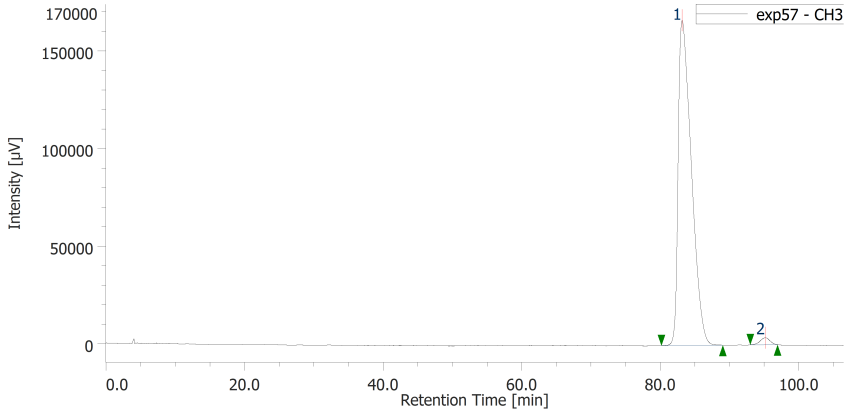
DATIM 18/Jan/2023 14:26:06
OBNUC ^{1}H
EXMOD ZG30>
OFR 400.13 MHz
OBSET 0.0 kHz
OBFIN 1996.017 Hz
POINT 131072(ZeroFill :×4)
FREQU 4826.255 Hz
SCANS 8
ACQTM 6.7895 s
PD 1.0 s
PW1 14.0 μs
CTEMP 17.61 °C
SLVNT $CDCl_3$>
EXREF 0.0 ppm
BF 0.1473 Hz
RGAIN 181
PRNT_DATE 2024/May/02 07:56:40
COMNT





DATIM 18/Jan/2023 14:30:28
OBNUC ^{13}C
EXMOD ZGPG30>
OFR 100.61 MHz
OBSET 0.0 kHz
OBFIN 12705.91 Hz
POINT 131072(ZeroFill :×4)
FREQU 32051.28 Hz
SCANS 64
ACQTM 1.0224 s
PD 2.0 s
PW1 9.0 μs
CTEMP 18.01 ℃
SLVNT $CDCL_3$>
EXREF 77.0 ppm
BF 0.9781 Hz
RGAIN 2050
PRNT_DATE 2024/May/02 07:57:40
COMNT

Chromatogram

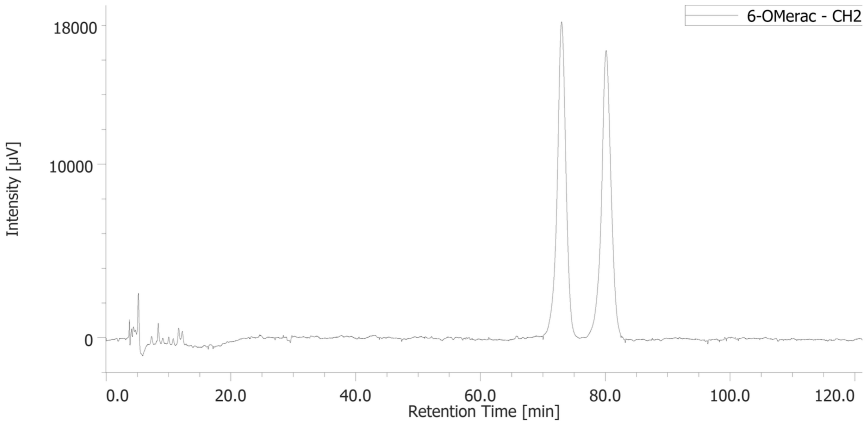


Chromatogram Information	
User Name	3385
Date Modified	2023/01/18 16:04:29
Description	IB, 0.9 mL/min, Hex:EtOH=99:1, UV 254 nm, CD 254 nm
HPLC System Name	HPLC-1
Injection Date	2023/01/18 14:16:16
Volume	1.00 [μL]
Sample #	1
Project Name	2022system1
Acquisition Time	180.0 [min]
Acquisition Sequence	1-2263 toba
Control Method	system1_2017
Peak ID Table	
Calibration Method	
Additional Information	

Channel & Peak Information Table

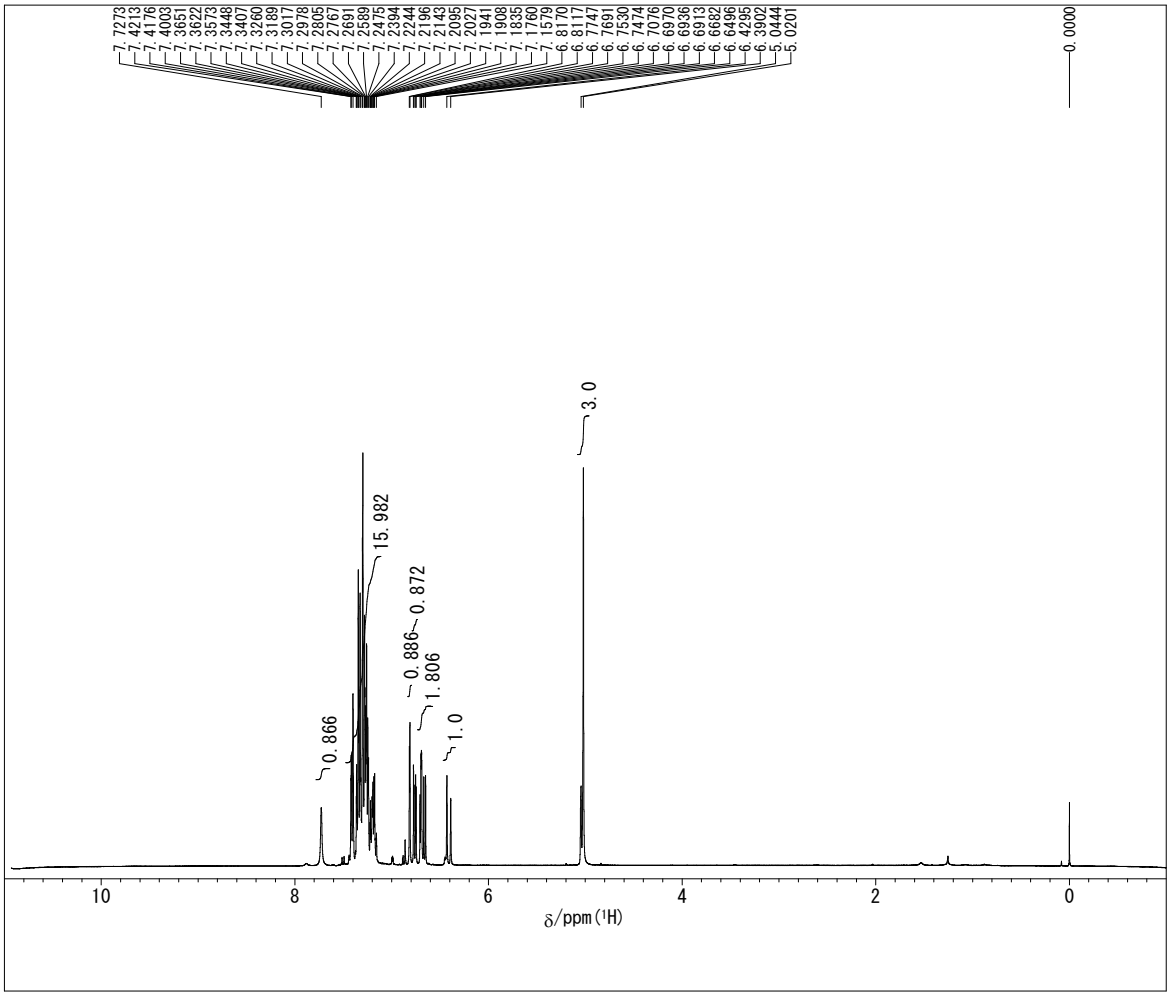
Chromatogram Name	exp57-CH3
Sample Name	
Channel Name	UV-2075
Sampling Interval	500 [msec]
Peak Method	(Manual)

#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%
1	Unknown	3	83.133	22003965	166343	98.445	97.9
2	Unknown	3	95.142	347593	3545	1.555	2.09

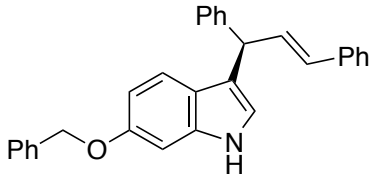


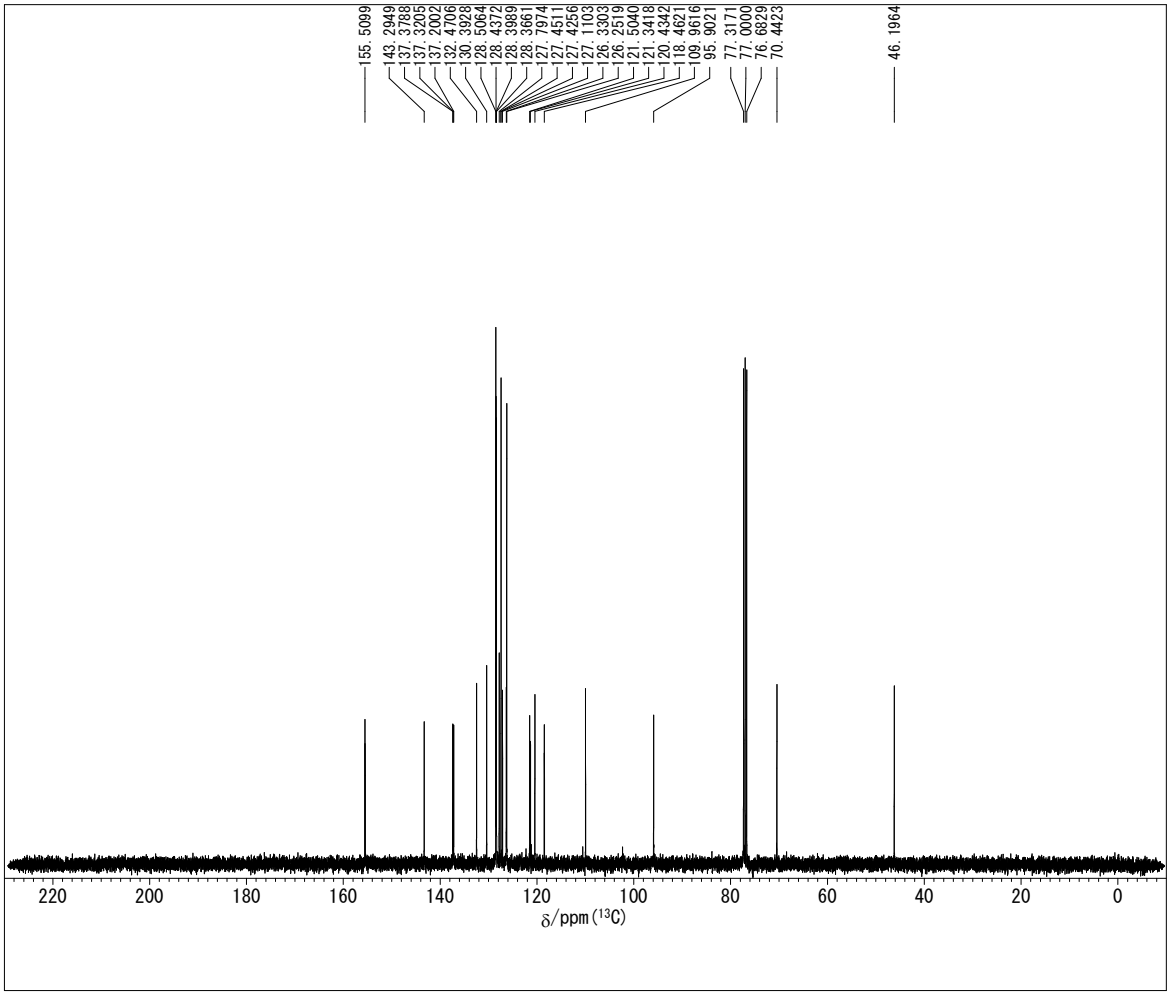
IB, 0.9mL/min, Hex:EtOH=99:1

^{1}H NMR, ^{13}C{^{1}H} NMR and chiral phase HPLC chart of (*R*)-**10d** (**Table 4**, Entry 4)



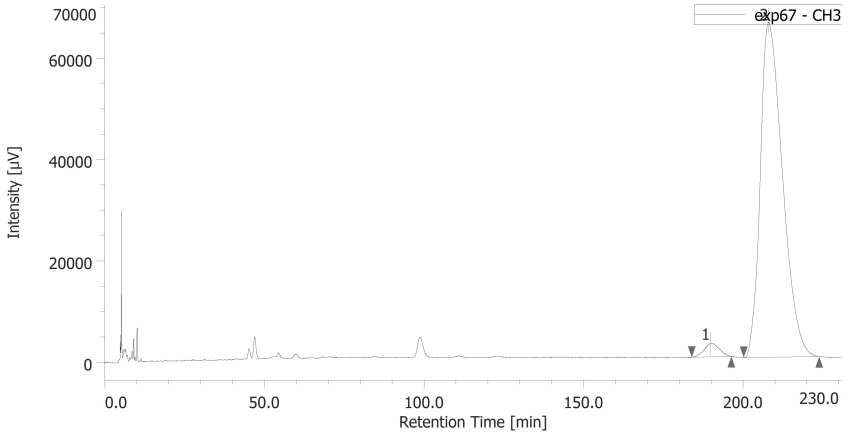
DATIM 07/Mar/2023 10:35:26
OBNUC ^{1}H
EXMOD ZG30>
OFR 400.18 MHz
OBSET 0.0 kHz
OBFIN 2008.224 Hz
POINT 131072(ZeroFill :×4)
FREQU 4826.255 Hz
SCANS 8
ACQTM 6.7895 s
PD 1.0 s
PW1 14.0 μs
CTEMP 16.61 °C
SLVNT $CDCL_3$>
EXREF 0.0 ppm
BF 0.1473 Hz
RGAIN 72
PRNT_DATE 2024/May/02 07:59:41
COMNT





DATIM 07/Mar/2023 10:40:56
OBNUC ^{13}C
EXMOD ZGPG30>
OFR 100.63 MHz
OBSET 0.0 kHz
OBFIN 11066.5 Hz
POINT 131072(ZeroFill :×4)
FREQU 24038.46 Hz
SCANS 64
ACQTM 1.3631 s
PD 2.0 s
PW1 10.0 μs
CTEMP 17.21 ℃
SLVNT $CDCL_3$>
EXREF 77.0 ppm
BF 0.7336 Hz
RGAIN 203
PRNT_DATE 2024/May/02 08:00:28
COMNT

Chromatogram

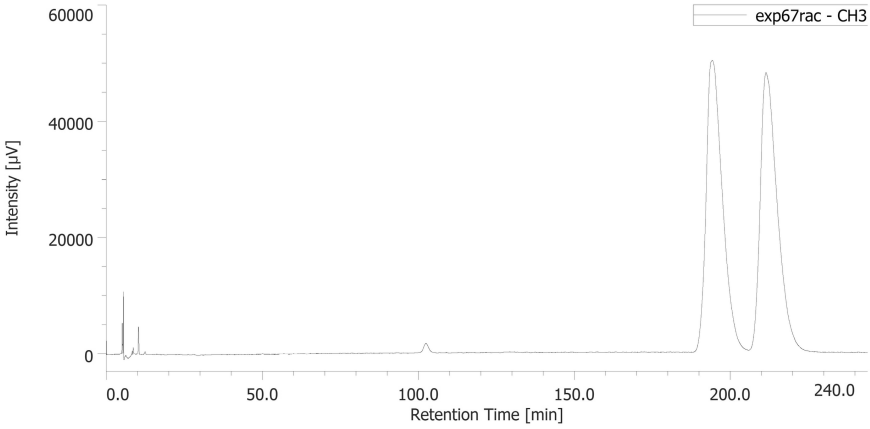


Chromatogram Information	
User Name	3385
Date Modified	2023/03/04 19:29:10
Description	IA-3,0.7mL/min, Hex:EtOH=99:1
HPLC System Name	SYSTEM-3
Injection Date	2023/03/04 15:38:16
Volume	1.0 [μL]
Sample #	1
Project Name	2022system3
Acquisition Time	999.0 [min]
Acquisition Sequence	3-1625 toba
Control Method	2019system3
Peak ID Table	
Calibration Method	
Additional Information	

Channel & Peak Information Table

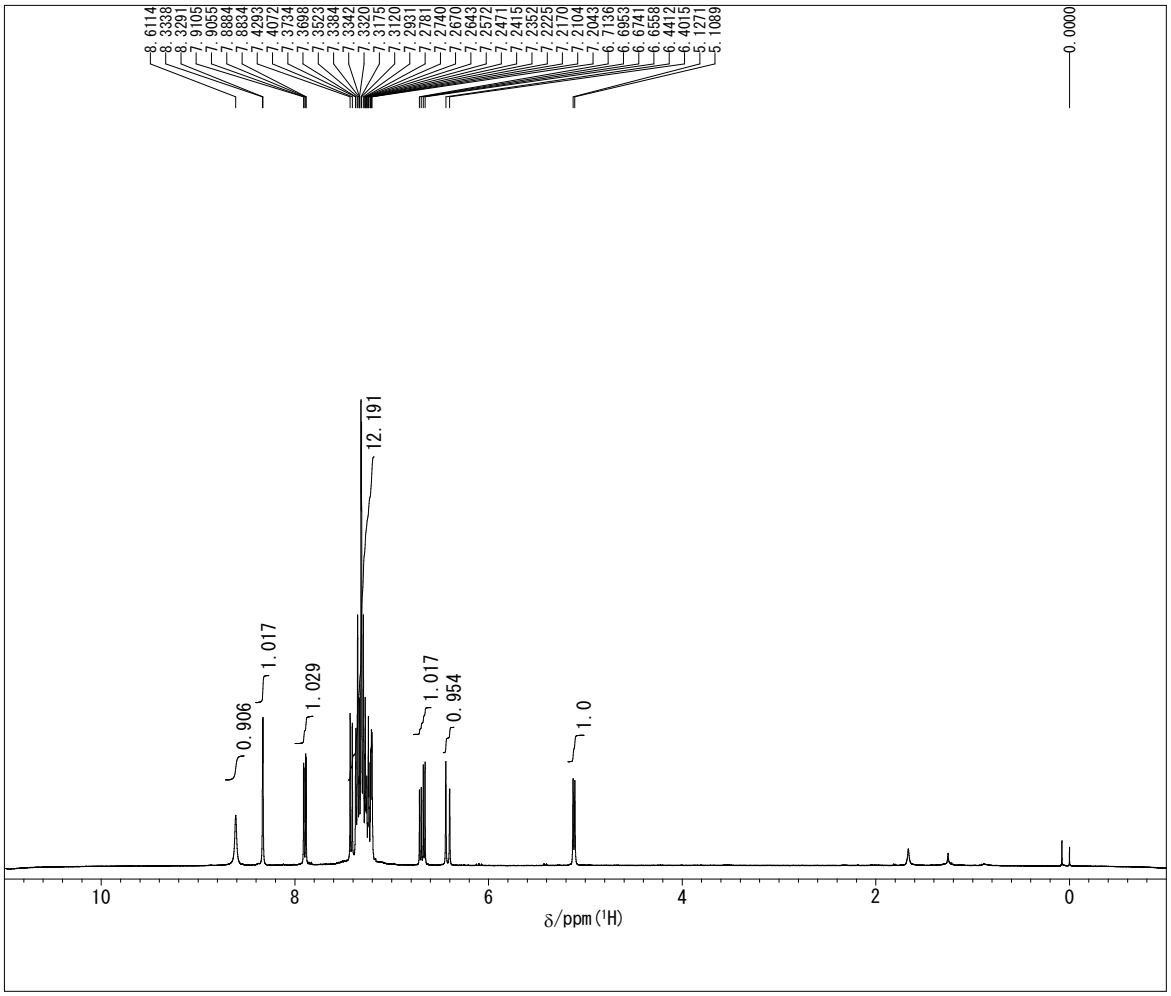
Chromatogram Name	exp67-CH3
Sample Name	
Channel Name	UV-2075
Sampling Interval	500 [msec]
Peak Method	(Manual)

#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%
1	Unknown	3	189.73	870528	2644	2.652	3.844
2	Unknown	3	208.03	31957143	66157	97.348	96.156

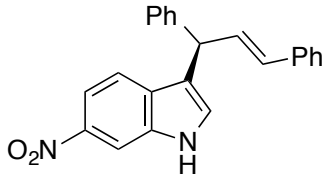


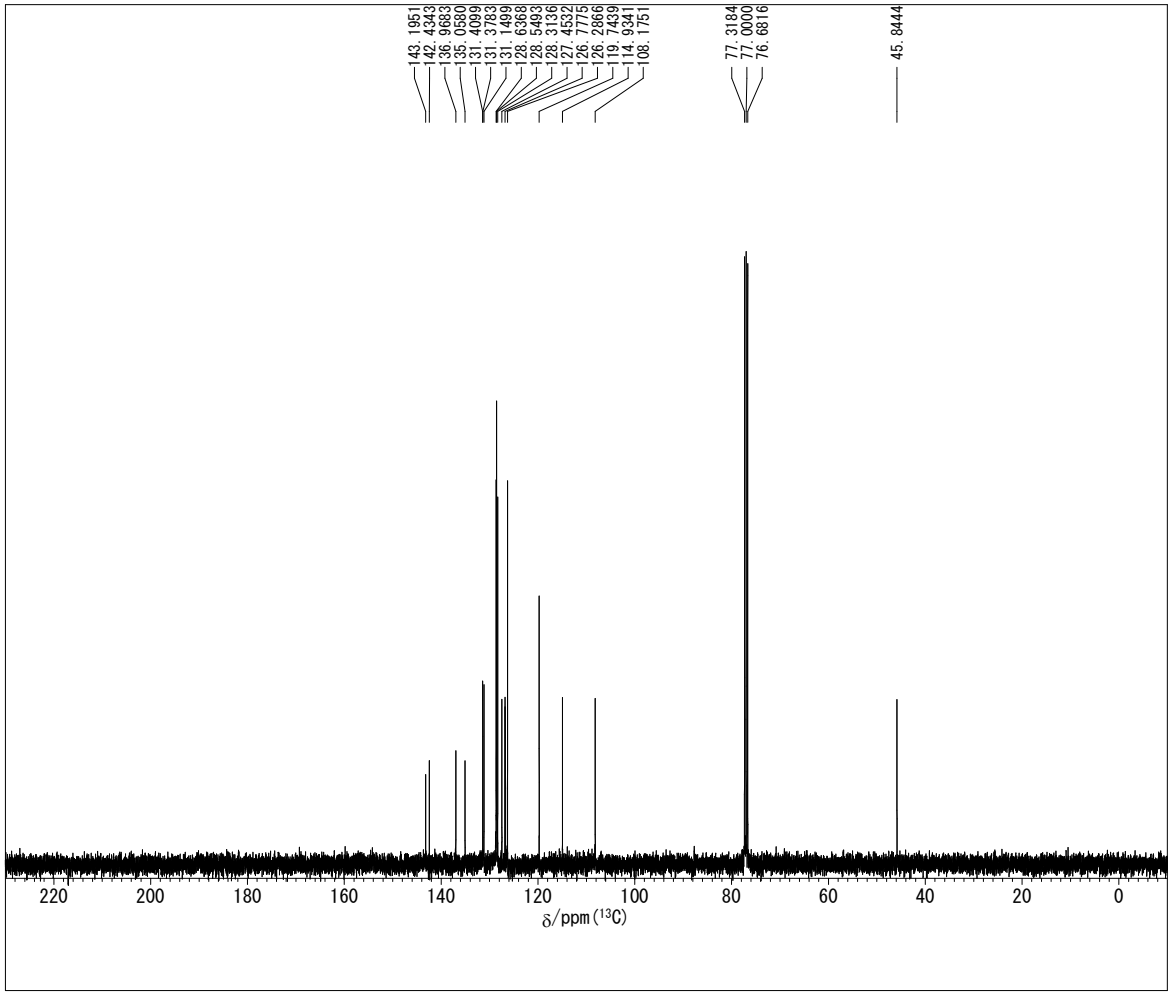
IA-3, 0.7 mL/min, hex:EtOH =99:1

^{1}H NMR, ^{13}C{^{1}H} NMR and chiral phase HPLC chart of (*R*)-**10e** (**Table 4**, Entry 5)



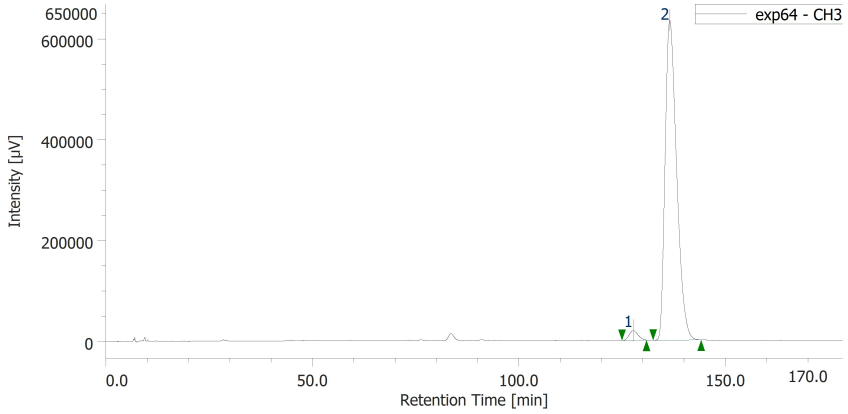
DATIM 07/Feb/2023 17:22:27
OBNUC ^{1}H
EXMOD ZG30>
OFR 400.13 MHz
OBSET 0.0 kHz
OBFIN 1996.017 Hz
POINT 131072(ZeroFill :×4)
FREQU 4826.255 Hz
SCANS 8
ACQTM 6.7895 s
PD 1.0 s
PW1 14.0 μs
CTEMP 17.81 ℃
SLVNT $CDCL_3$>
EXREF 0.0 ppm
BF 0.1473 Hz
RGAIN 181
PRNT_DATE 2024/May/02 08:02:07
COMNT





DATIM 07/Feb/2023 17:26:35
OBNUC ^{13}C
EXMOD ZGPG30>
OFR 100.61 MHz
OBSET 0.0 kHz
OBFIN 12705.91 Hz
POINT 131072(ZeroFill :×4)
FREQU 32051.28 Hz
SCANS 64
ACQTM 1.0224 s
PD 2.0 s
PW1 9.0 μs
CTEMP 18.21 ℃
SLVNT $CDCL_3$>
EXREF 77.0 ppm
BF 0.9781 Hz
RGAIN 2050
PRNT_DATE 2024/May/02 08:03:16
COMNT

Chromatogram

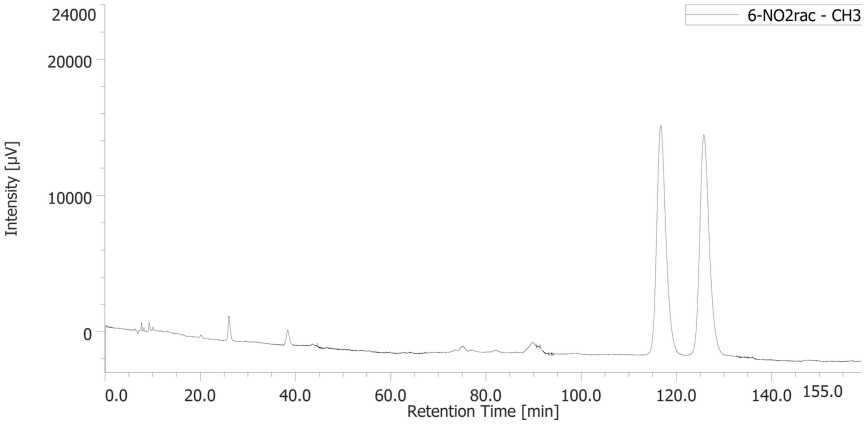


Chromatogram Information	
User Name	3385
Date Modified	2023/02/05 16:30:02
Description	IA-3,0.5mL/min, Hex:EtOH=98:2
HPLC System Name	SYSTEM-3
Injection Date	2023/02/05 13:03:15
Volume	1.0 [μL]
Sample #	1
Project Name	2022system3
Acquisition Time	999.0 [min]
Acquisition Sequence	3-1607 toba
Control Method	2019system3
Peak ID Table	
Calibration Method	
Additional Information	

Channel & Peak Information Table

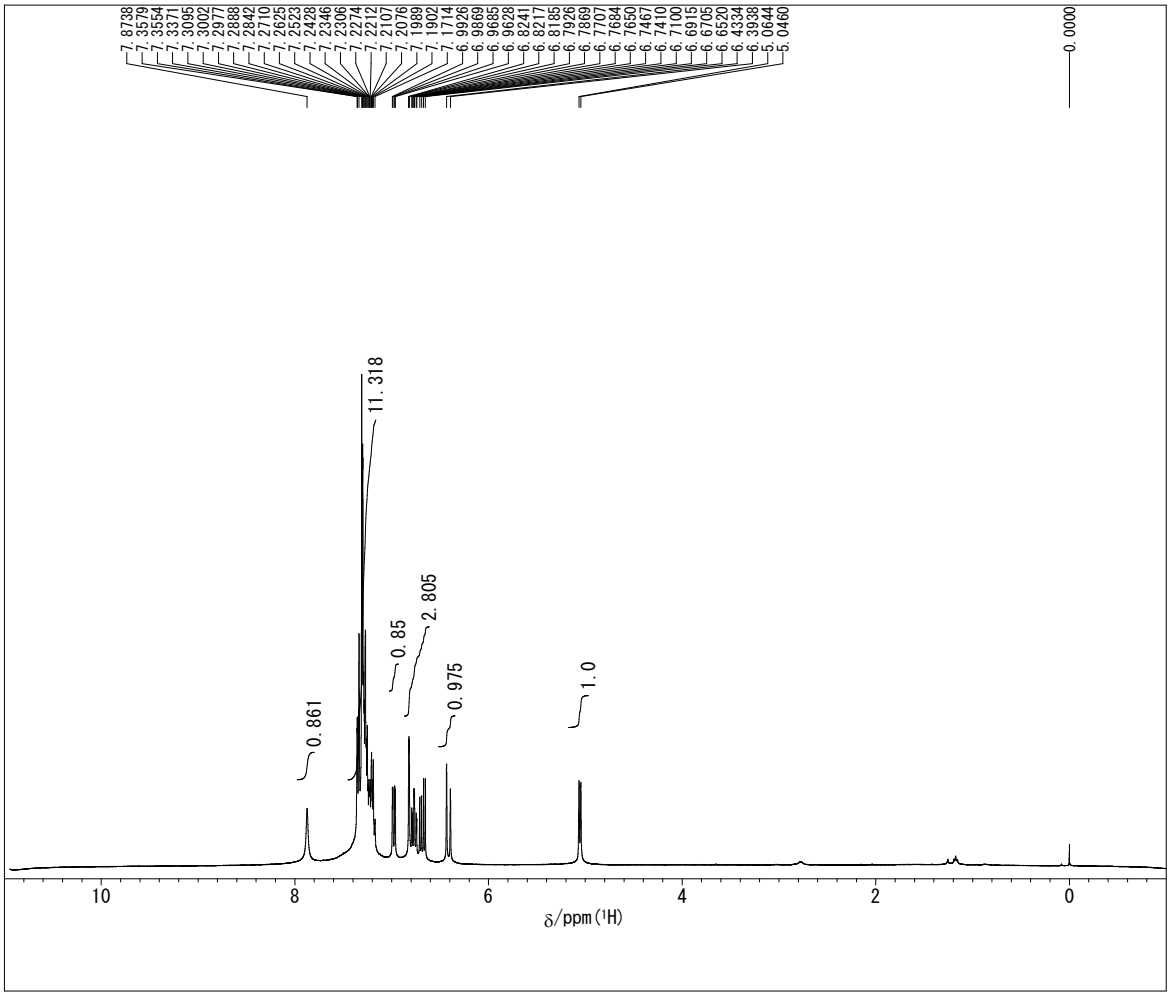
Chromatogram Name	exp64-CH3
Sample Name	
Channel Name	UV-2075
Sampling Interval	500 [msec]
Peak Method	(Manual)

#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%
1	Unknown	3	127.63	2909657	19507	2.309	2.983
2	Unknown	3	136.49	123078176	634489	97.691	97.017

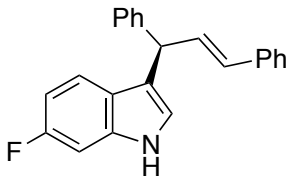


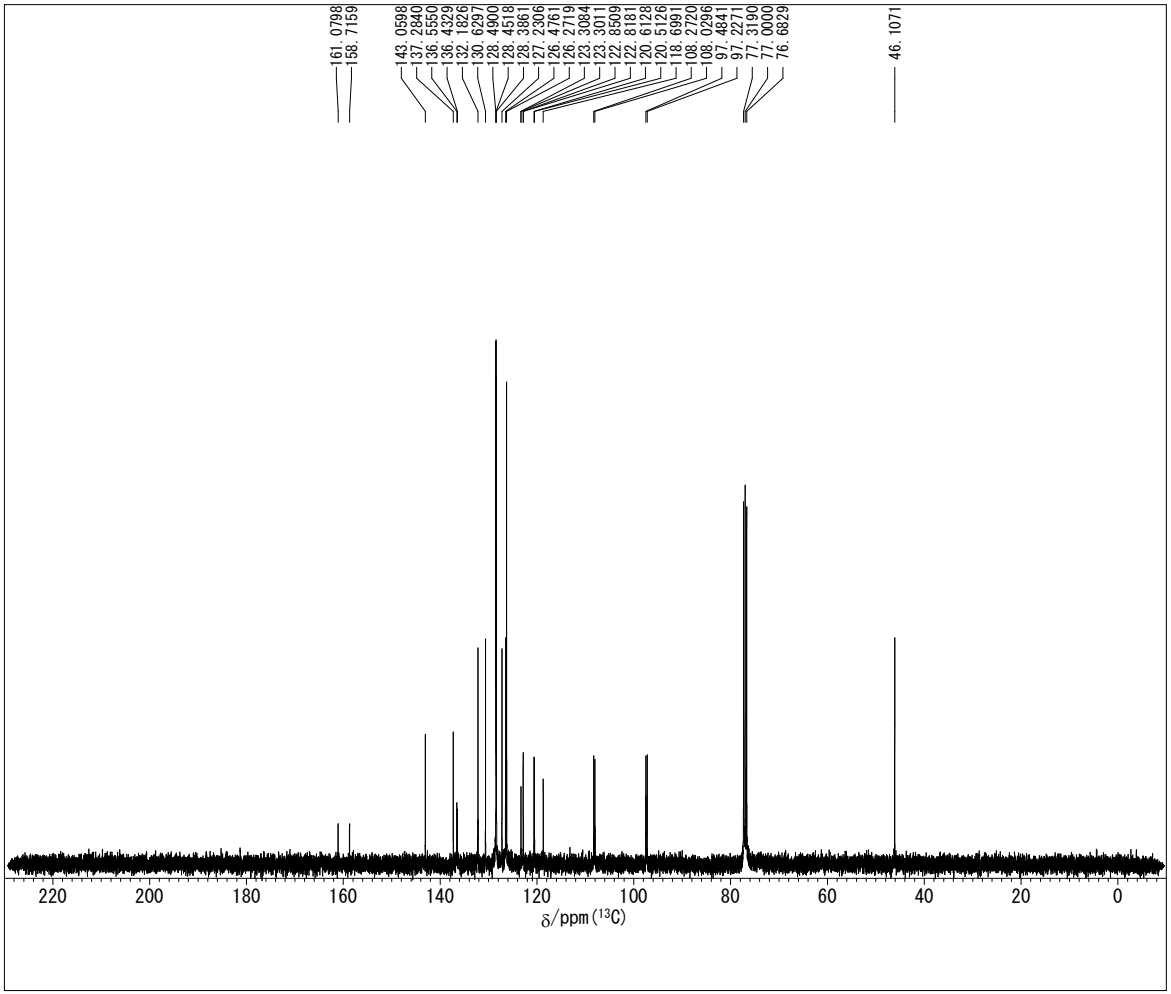
IA-3, 0.5 mL/min, Hex:EtOH=98:2, UV 254 nm, CD 254 nm

^{1}H NMR, ^{13}C{^{1}H} NMR and chiral phase HPLC chart of (*R*)-**10f** (**Table 4**, Entry 6)



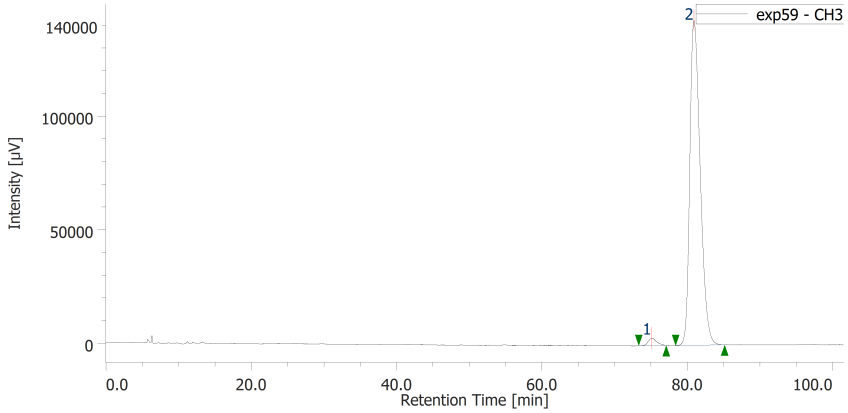
DATIM 20/Jan/2023 10:57:49
OBNUC ^{1}H
EXMOD ZG30>
OFR 400.18 MHz
OBSET 0.0 kHz
OBFIN 2008.224 Hz
POINT 131072(ZeroFill :×4)
FREQU 4826.255 Hz
SCANS 8
ACQTM 6.7895 s
PD 1.0 s
PW1 14.0 μs
CTEMP 19.11°C
SLVNT $CDCl_3$>
EXREF 0.0 ppm
BF 0.1473 Hz
RGAIN 81
PRNT_DATE 2024/May/02 08:04:49
COMNT





DATIM 20/Jan/2023 11:08:22
OBNUC ^{13}C
EXMOD ZGPG30>
OFR 100.63 MHz
OBSET 0.0 kHz
OBFIN 11066.5 Hz
POINT 131072(ZeroFill :×4)
FREQU 24038.46 Hz
SCANS 64
ACQTM 1.3631 s
PD 2.0 s
PW1 10.0 μs
CTEMP 19.81 ℃
SLVNT $CDCL_3$>
EXREF 77.0 ppm
BF 0.7336 Hz
RGAIN 203
PRNT_DATE 2024/May/02 08:05:30
COMNT

Chromatogram

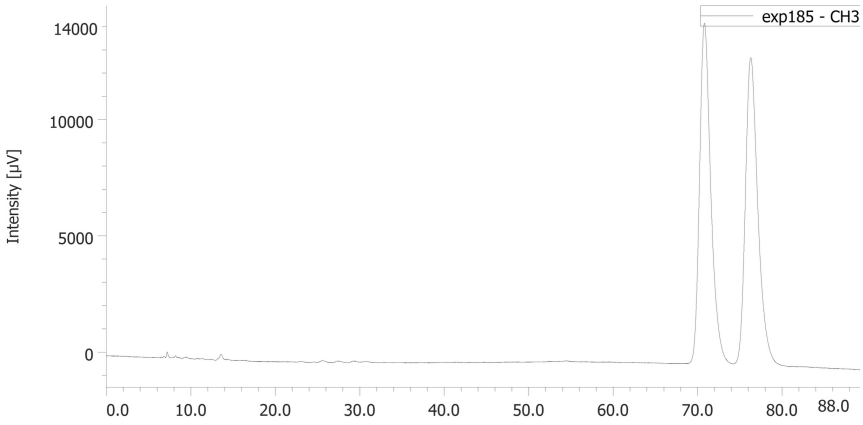


Chromatogram Information	
User Name	3385
Date Modified	2023/01/30 13:32:27
Description	IA-3, 0.6 mL/min, Hex:EtOH=99:1, UV 254 nm, CD 254 nm
HPLC System Name	HPLC-1
Injection Date	2023/01/30 11:29:40
Volume	1.00 [μL]
Sample #	1
Project Name	2022system1
Acquisition Time	180.0 [min]
Acquisition Sequence	1-2299 toba
Control Method	system1_2017
Peak ID Table	
Calibration Method	
Additional Information	

Channel & Peak Information Table

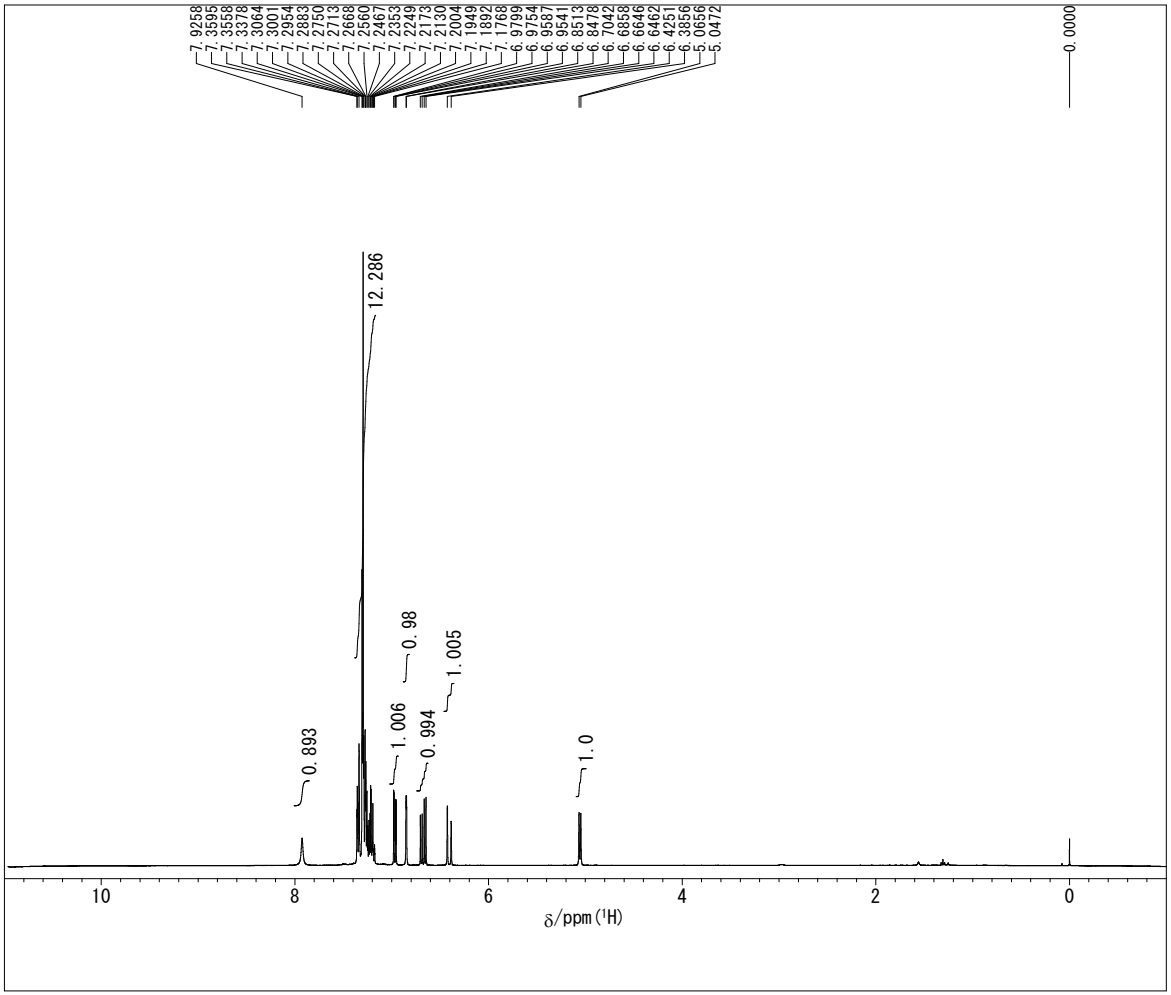
Chromatogram Name	exp59-CH3
Sample Name	
Channel Name	UV-2075
Sampling Interval	500 [msec]
Peak Method	(Manual)

#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%
1	Unknown	3	75.100	271229	3311	1.875	2.26
2	Unknown	3	80.908	14191542	142977	98.125	97.7

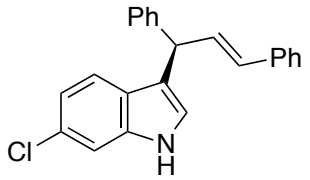


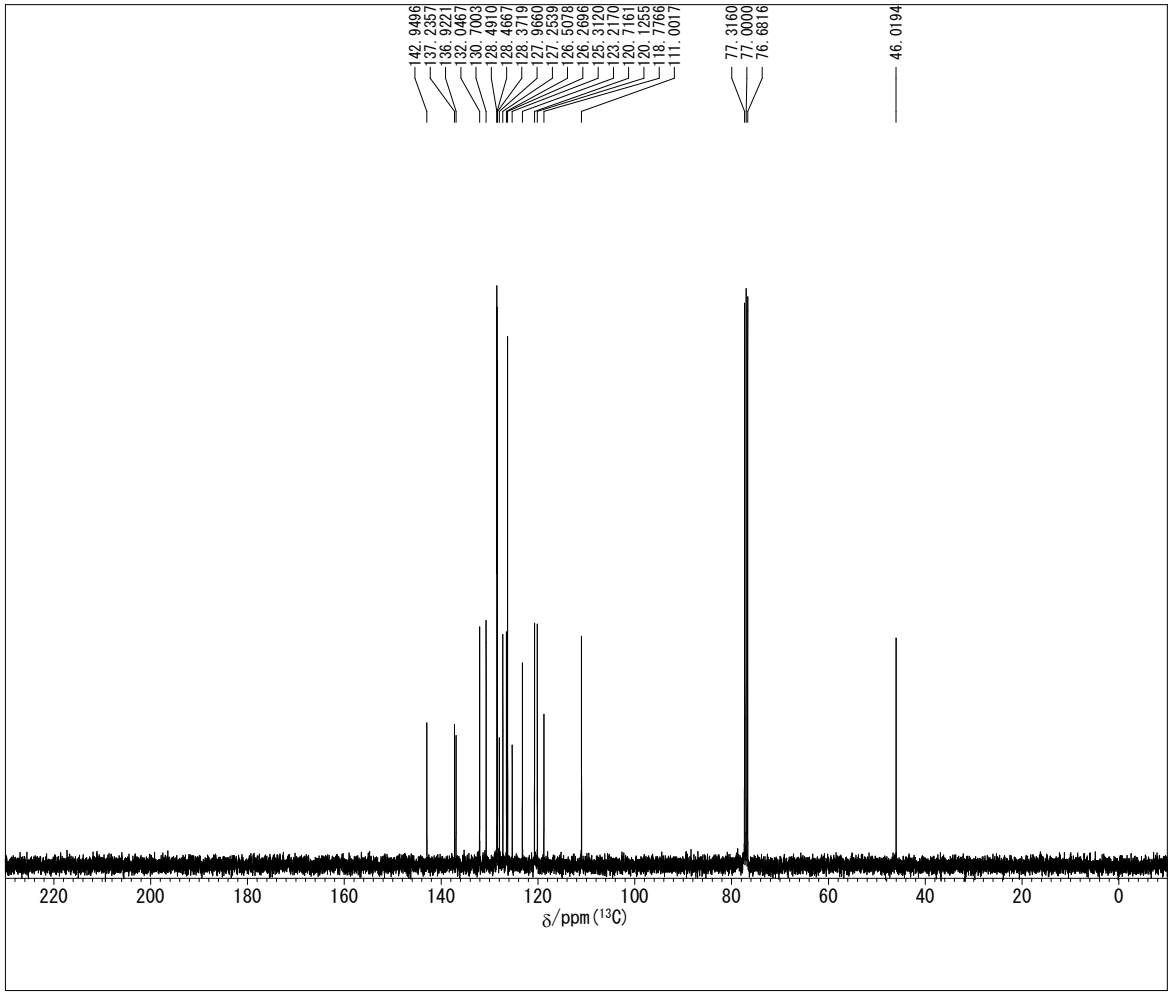
IA,flow0.5,Hex:EtOH=99:1

^{1}H NMR, ^{13}C{^{1}H} NMR and chiral phase HPLC chart of (*R*)-**10g** (**Table 4**, Entry 7)



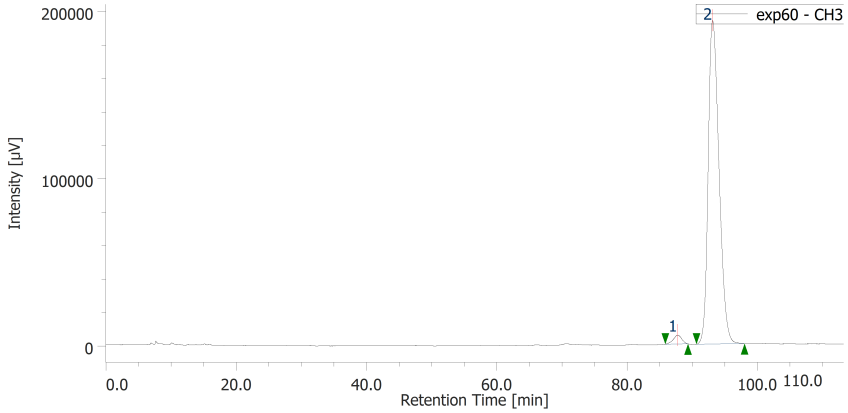
DATIM 20/Jan/2023 13:33:39
OBNUC ^{1}H
EXMOD ZG30>
OFR 400.13 MHz
OBSET 0.0 kHz
OBFIN 1996.017 Hz
POINT 131072(ZeroFill :×4)
FREQU 4826.255 Hz
SCANS 8
ACQTM 6.7895 s
PD 1.0 s
PW1 14.0 μs
CTEMP 18.41 ℃
SLVNT $CDCl_3$>
EXREF 0.0 ppm
BF 0.1473 Hz
RGAIN 181
PRNT_DATE 2024/May/02 08:07:01
COMNT





DATIM 20/Jan/2023 13:38:06
OBNUC ^{13}C
EXMOD ZGPG30>
OFR 100.61 MHz
OBSET 0.0 kHz
OBFIN 12705.91 Hz
POINT 131072(ZeroFill :×4)
FREQU 32051.28 Hz
SCANS 64
ACQTM 1.0224 s
PD 2.0 s
PW1 9.0 μs
CTEMP 18.91 ℃
SLVNT $CDCL_3$>
EXREF 77.0 ppm
BF 0.9781 Hz
RGAIN 2050
PRNT_DATE 2024/May/02 08:07:39
COMNT

Chromatogram

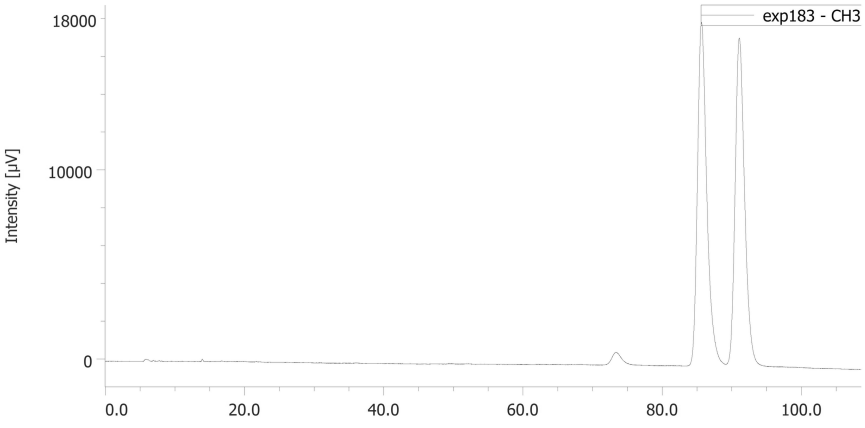


Chromatogram Information	
User Name	3385
Date Modified	2023/01/23 20:39:49
Description	IA-3, 0.5 mL/min, Hex:EtOH=99:1, UV 254 nm, CD 254 nm
HPLC System Name	HPLC-1
Injection Date	2023/01/23 14:05:46
Volume	1.00 [μL]
Sample #	1
Project Name	2022system1
Acquisition Time	180.0 [min]
Acquisition Sequence	1-2275 toba
Control Method	system1_2017
Peak ID Table	
Calibration Method	
Additional Information	

Channel & Peak Information Table

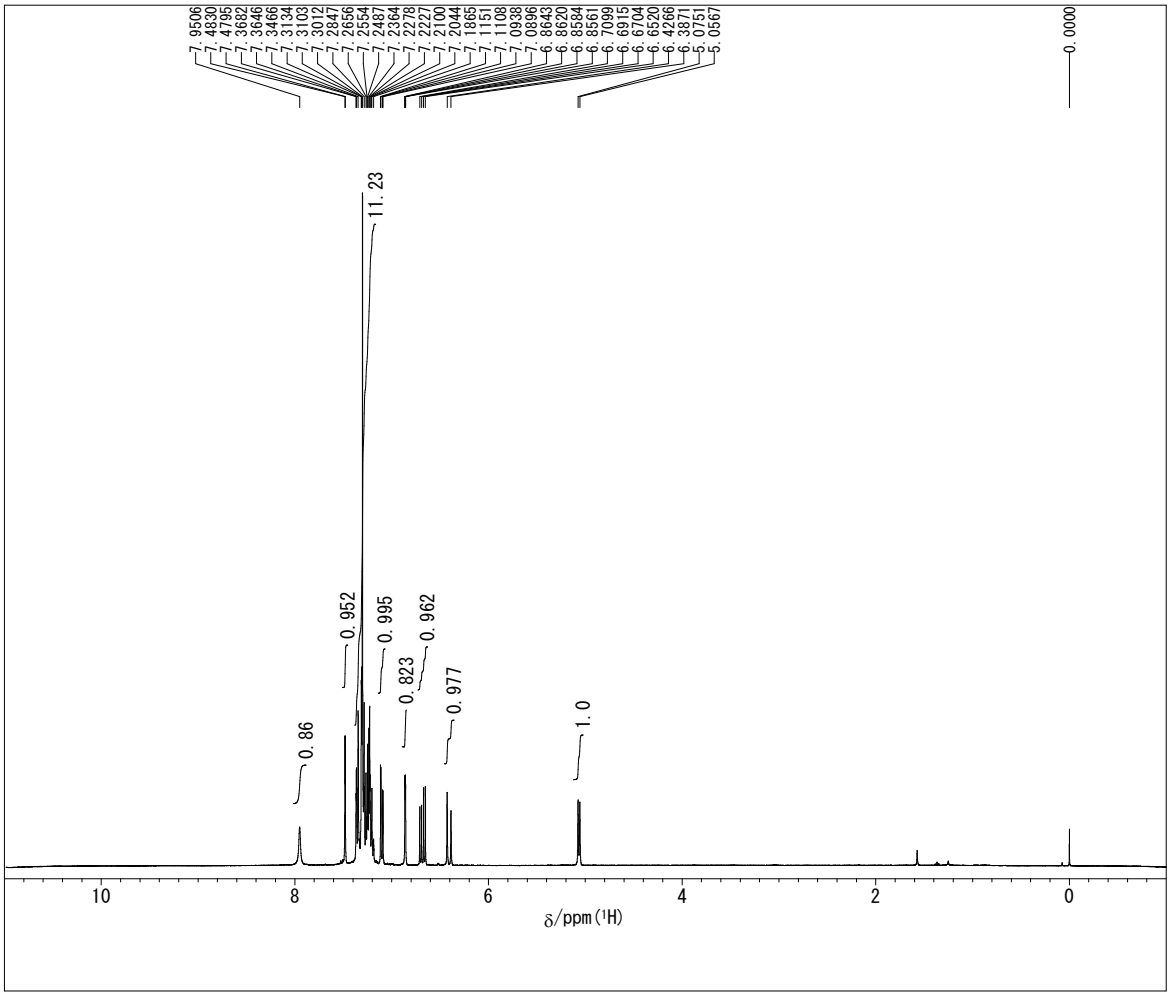
Chromatogram Name	exp60-CH3
Sample Name	
Channel Name	UV-2075
Sampling Interval	500 [msec]
Peak Method	(Manual)

#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%
1	Unknown	3	87.742	482026	5343	2.110	2.69
2	Unknown	3	93.100	22362252	193524	97.890	97.3

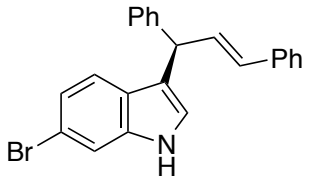


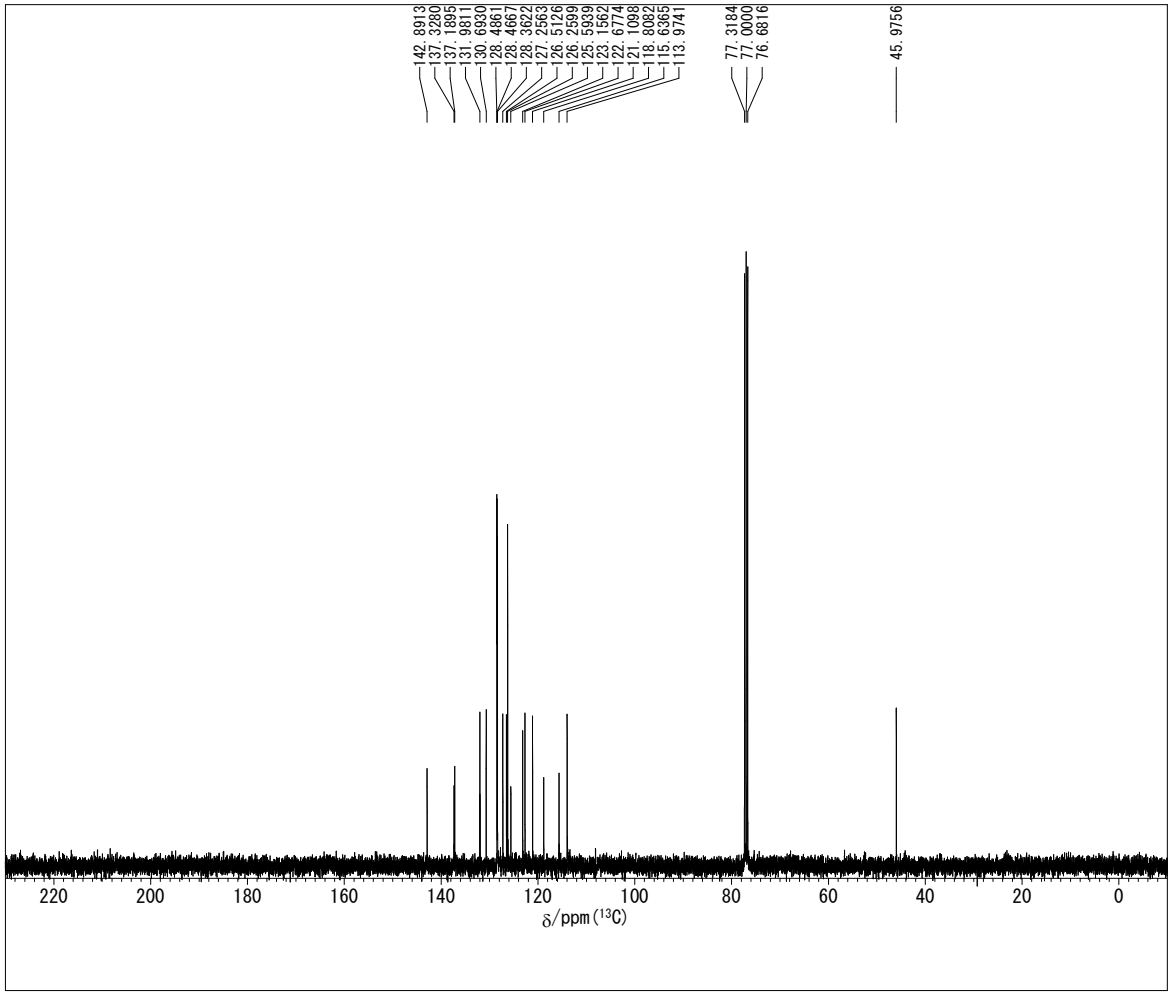
IA-3,flow0.5,Hex:EtOH=99:1

^{1}H NMR, ^{13}C{^{1}H} NMR and chiral phase HPLC chart of (*R*)-**10h** (**Table 4**, Entry 8)

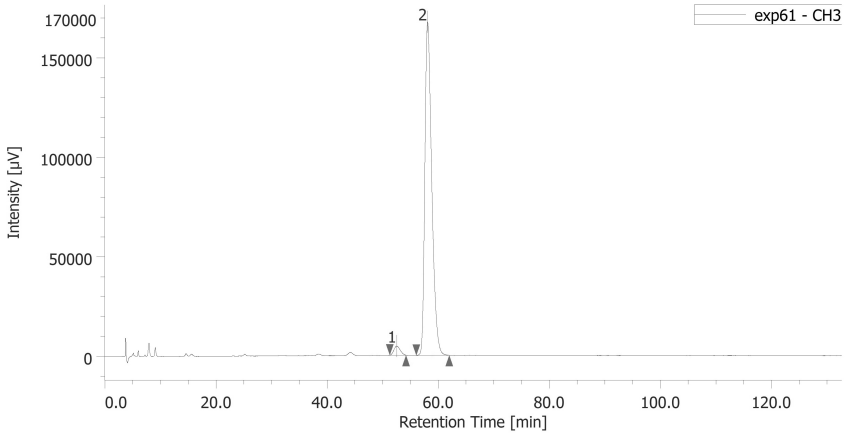


DATIM 31/Jan/2023 11:04:40
OBNUC ^{1}H
EXMOD ZG30>
OFR 400.13 MHz
OBSET 0.0 kHz
OBFIN 1996.017 Hz
POINT 131072(ZeroFill :×4)
FREQU 4826.255 Hz
SCANS 8
ACQTM 6.7895 s
PD 1.0 s
PW1 14.0 μs
CTEMP 11.51 °C
SLVNT $CDCL_3$>
EXREF 0.0 ppm
BF 0.1473 Hz
RGAIN 181
PRNT_DATE 2024/May/02 08:09:06
COMNT





DATIM 30/Jan/2023 14:05:52
OBNUC ^{13}C
EXMOD ZGPG30>
OFR 100.61 MHz
OBSET 0.0 kHz
OBFIN 12705.91 Hz
POINT 131072(ZeroFill :×4)
FREQU 32051.28 Hz
SCANS 64
ACQTM 1.0224 s
PD 2.0 s
PW1 9.0 μs
CTEMP 14.11 ℃
SLVNT $CDCL_3$>
EXREF 77.0 ppm
BF 0.9781 Hz
RGAIN 2050
PRNT_DATE 2024/May/02 08:09:42
COMNT



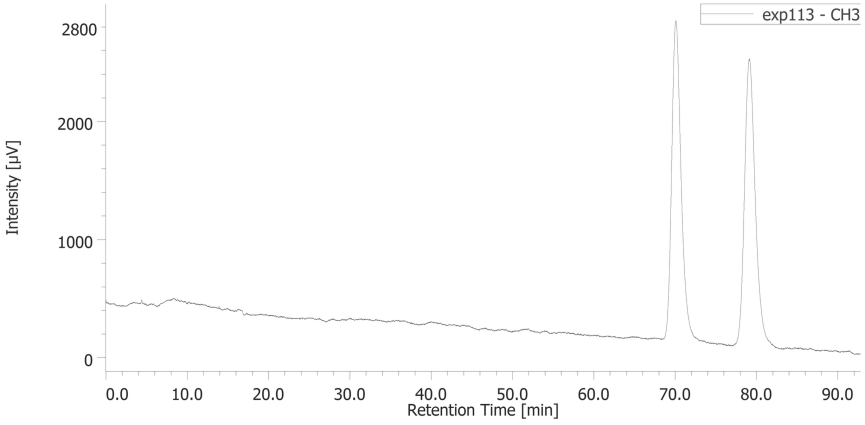
Chromatogram Information

User Name	3385
Date Modified	2023/01/28 14:47:45
Description	IA-3,0.9mL/min, Hex:2-PrOH=98:2
HPLC System Name	SYSTEM-3
Injection Date	2023/01/28 12:35:05
Volume	1.0 [μL]
Sample #	1
Project Name	2022system3
Acquisition Time	999.0 [min]
Acquisition Sequence	3-1599 toba
Control Method	2019system3
Peak ID Table	
Calibration Method	
Additional Information	

Channel & Peak Information Table

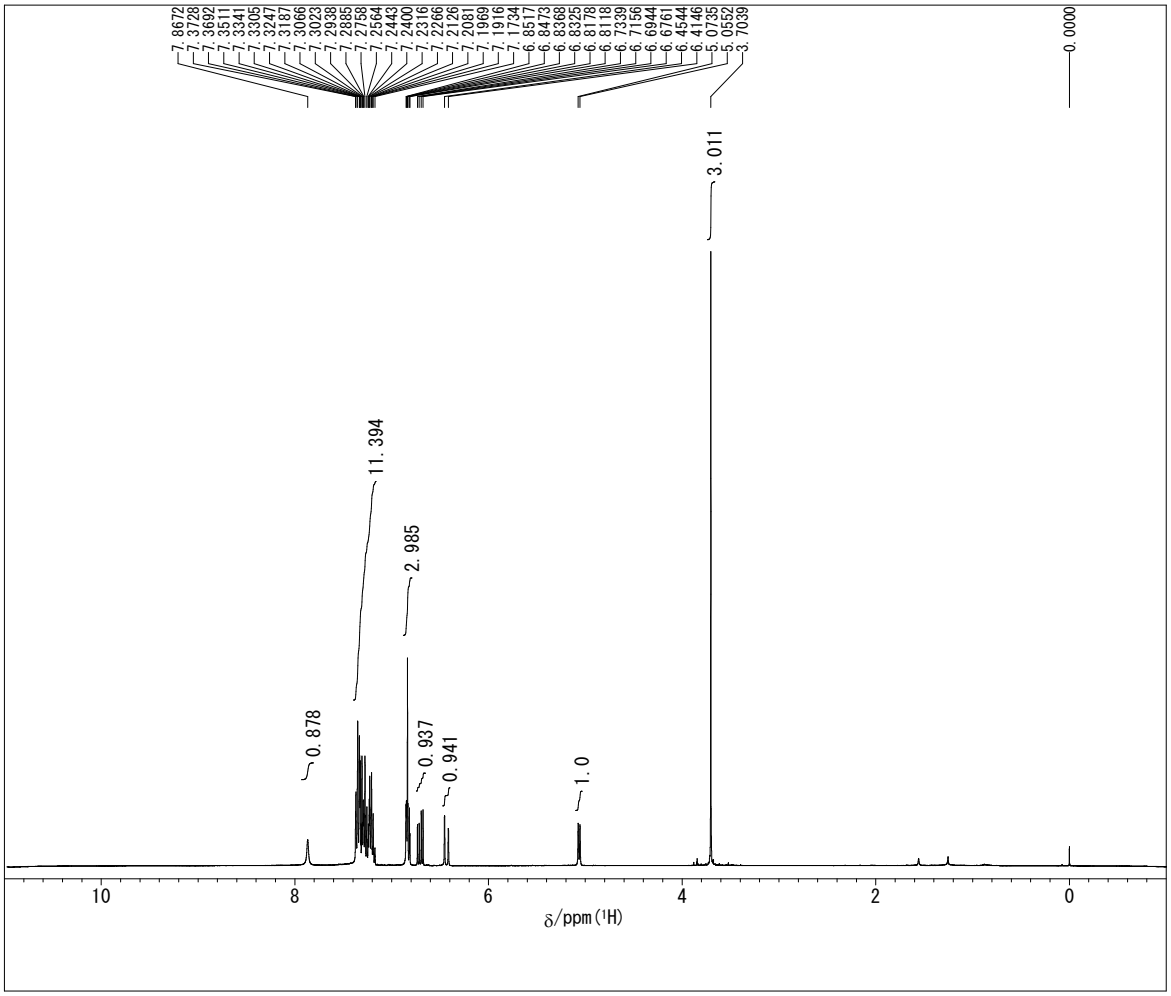
Chromatogram Name	exp61-CH3
Sample Name	
Channel Name	UV-2075
Sampling Interval	500 [msec]
Peak Method	(Manual)

#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%
1	Unknown	3	52.52	363539	4605	2.459	2.677
2	Unknown	3	58.08	14421636	167430	97.541	97.323

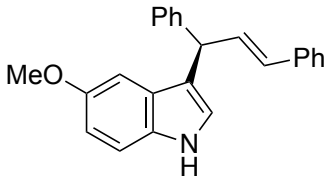


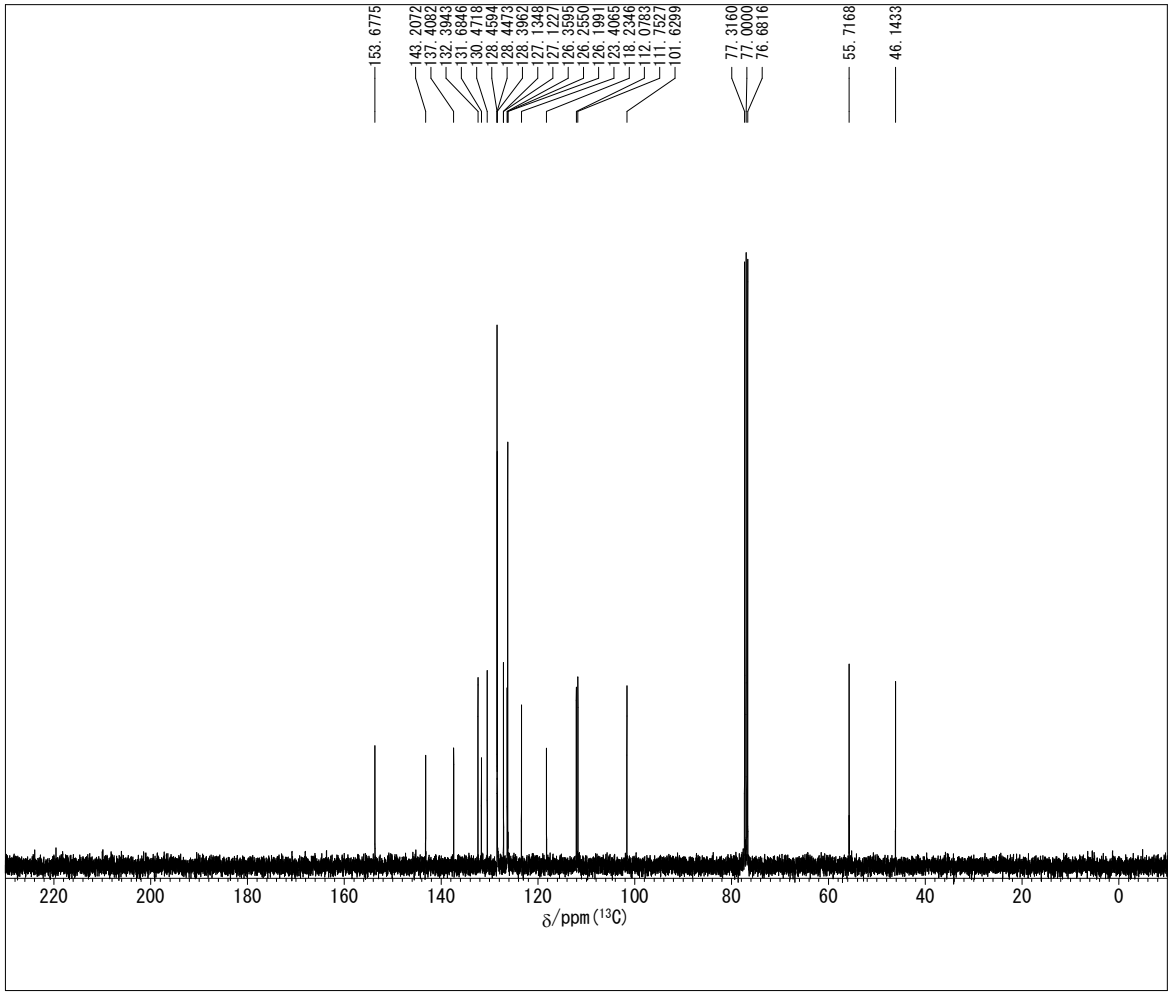
IA-3,flow0.9,Hex:2-pro=98:2

^{1}H NMR, ^{13}C{^{1}H} NMR and chiral phase HPLC chart of (*R*)-**10j** (**Table 4**, Entry 10)



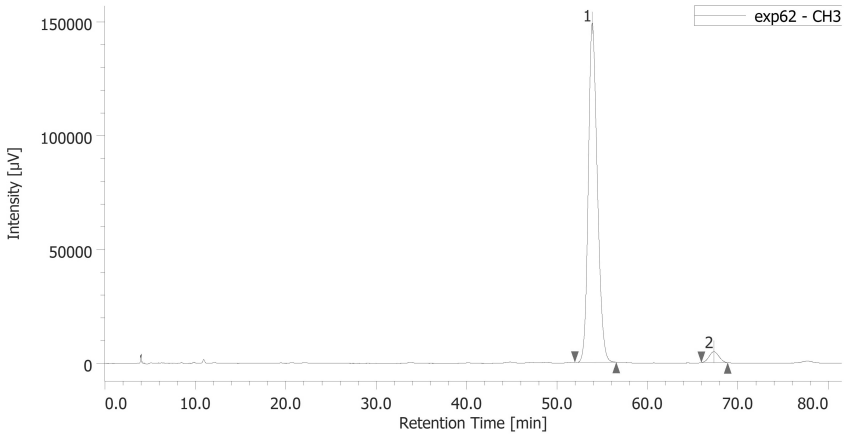
DATIM 30/Jan/2023 17:08:32
OBNUC ^{1}H
EXMOD ZG30>
OFR 400.13 MHz
OBSET 0.0 kHz
OBFIN 1996.017 Hz
POINT 131072(ZeroFill :×4)
FREQU 4826.255 Hz
SCANS 8
ACQTM 6.7895 s
PD 1.0 s
PW1 14.0 μs
CTEMP 16.51 °C
SLVNT $CDCl_3$>
EXREF 0.0 ppm
BF 0.1473 Hz
RGAIN 181
PRNT_DATE 2024/May/02 08:11:37
COMNT





DATIM 30/Jan/2023 17:12:47
OBNUC ^{13}C
EXMOD ZGPG30>
OFR 100.61 MHz
OBSET 0.0 kHz
OBFIN 12705.91 Hz
POINT 131072(ZeroFill :×4)
FREQU 32051.28 Hz
SCANS 64
ACQTM 1.0224 s
PD 2.0 s
PW1 9.0 μs
CTEMP 16.41 ℃
SLVNT $CDCL_3$>
EXREF 77.0 ppm
BF 0.9781 Hz
RGAIN 2050
PRNT_DATE 2024/May/02 08:12:23
COMNT

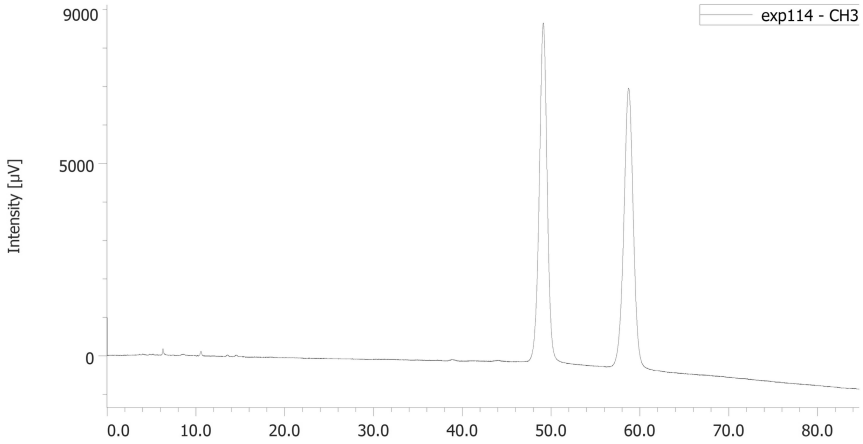
Chromatogram



Chromatogram Information	
User Name	3385
Date Modified	2023/01/27 19:37:52
Description	IB,0.9mL/min, Hex:EtOH=99:1
HPLC System Name	SYSTEM-3
Injection Date	2023/01/27 18:16:21
Volume	1.0 [μL]
Sample #	1
Project Name	2022system3
Acquisition Time	999.0 [min]
Acquisition Sequence	3-1598 toba
Control Method	2019system3
Peak ID Table	
Calibration Method	
Additional Information	

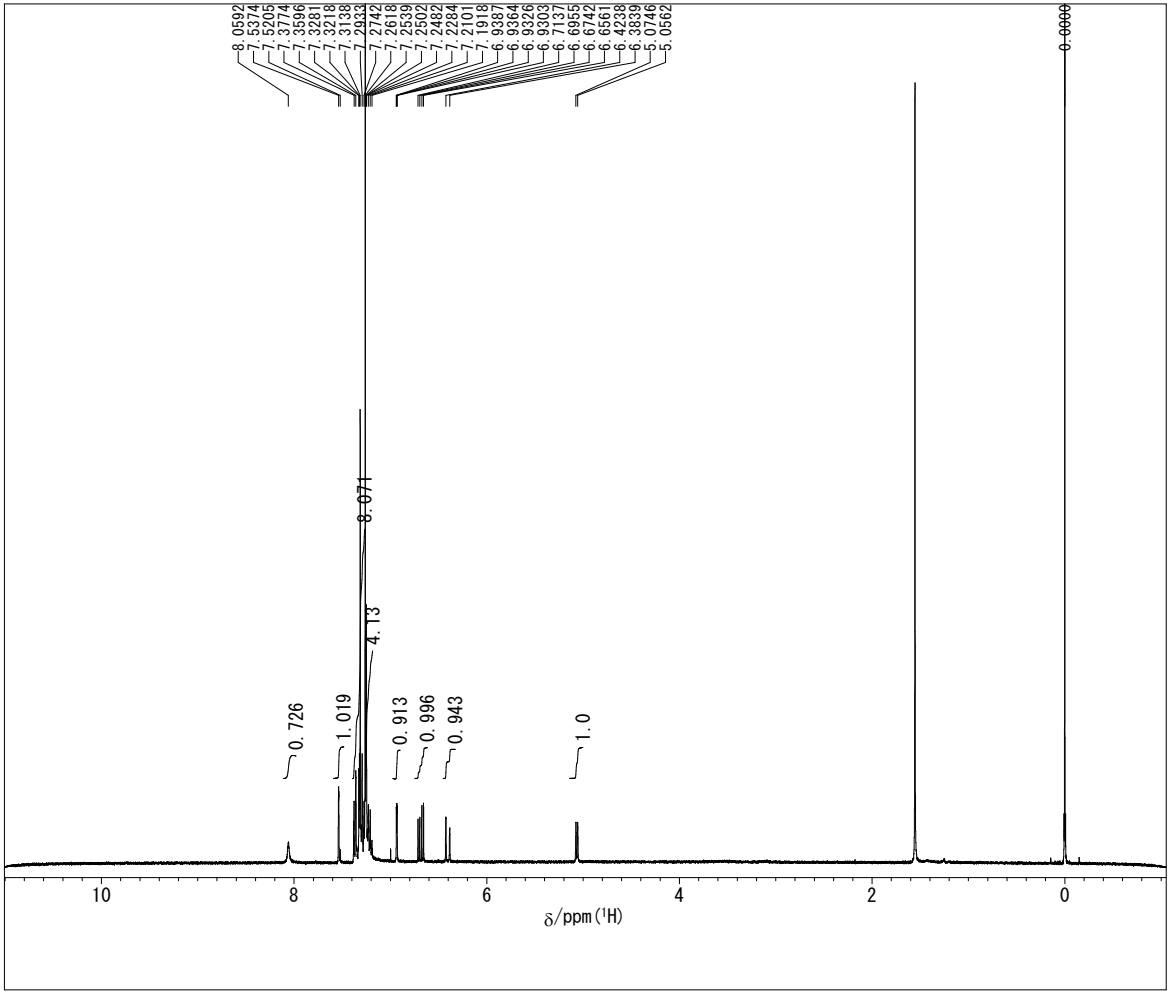
Channel & Peak Information Table	
Chromatogram Name	exp62-CH3
Sample Name	
Channel Name	UV-2075
Sampling Interval	500 [msec]
Peak Method	(Manual)

#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%
1	Unknown	3	53.88	10318260	149076	96.548	96.872
2	Unknown	3	67.33	368927	4814	3.452	3.128

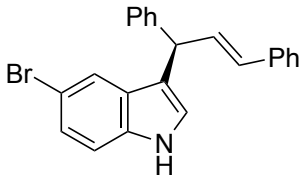


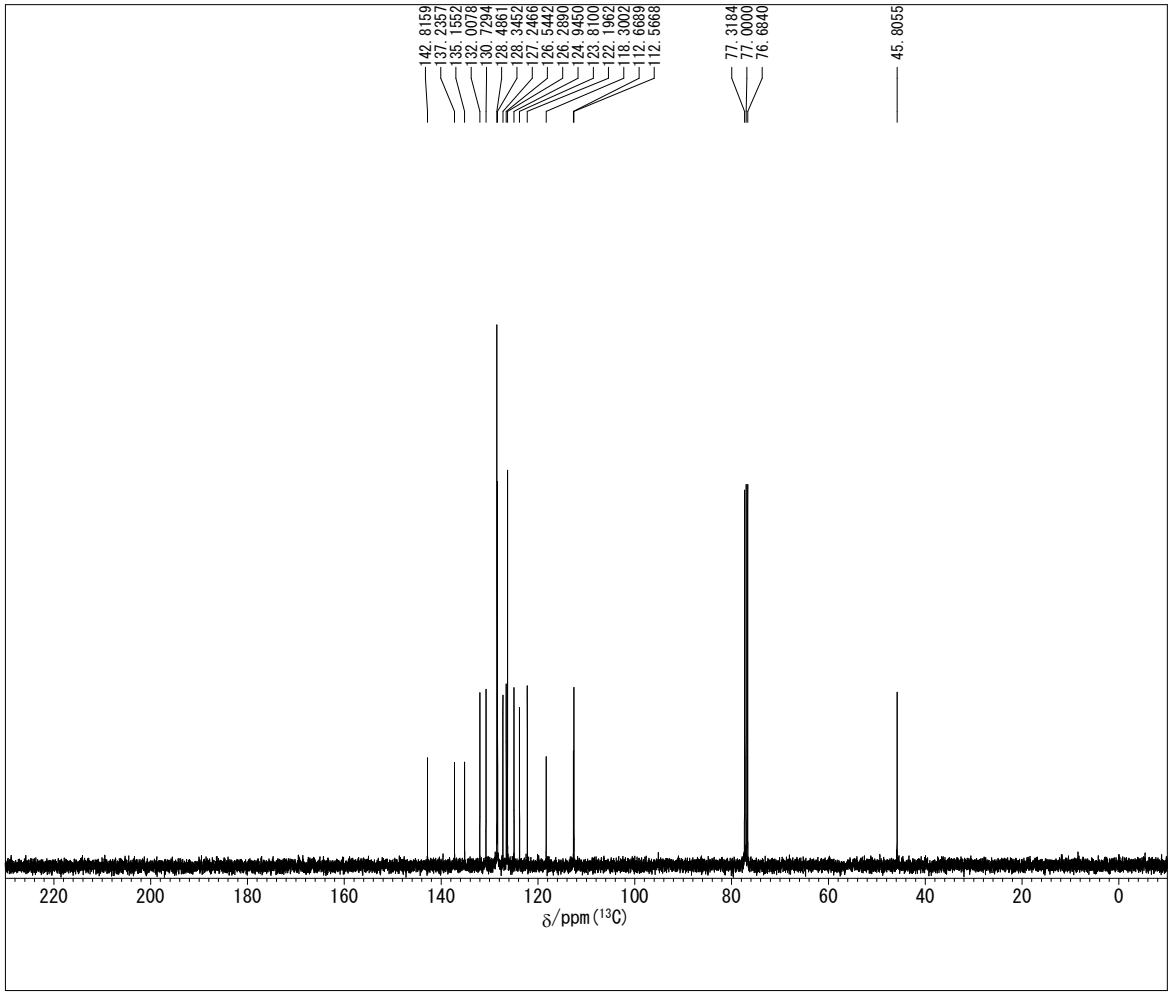
IB,flow0.9,Hex:EtOH=99:1

^{1}H NMR, ^{13}C{^{1}H} NMR and chiral phase HPLC chart of (*R*)-**10k** (**Table 4**, Entry 11)



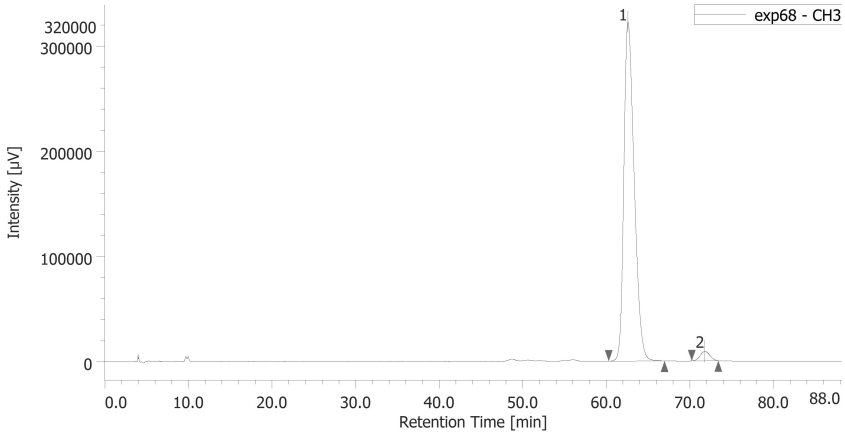
DATIM 14/Mar/2023 10:29:11
OBNUC ^{1}H
EXMOD ZG30>
OFR 400.18 MHz
OBSET 0.0 kHz
OBFIN 2008.224 Hz
POINT 131072(ZeroFill :×4)
FREQU 4826.255 Hz
SCANS 16
ACQTM 6.7895 s
PD 1.0 s
PW1 14.0 μs
CTEMP 18.81 °C
SLVNT $CDCl_3$>
EXREF 0.0 ppm
BF 0.1473 Hz
RGAIN 203
PRNT_DATE 2024/May/02 08:23:35
COMNT





DATIM 13/Mar/2023 14:26:50
OBNUC ^{13}C
EXMOD ZGPG30>
OFR 100.61 MHz
OBSET 0.0 kHz
OBFIN 12705.91 Hz
POINT 131072(ZeroFill :×4)
FREQU 32051.28 Hz
SCANS 64
ACQTM 1.0224 s
PD 2.0 s
PW1 9.0 μs
CTEMP 20.61 ℃
SLVNT $CDCL_3$>
EXREF 77.0 ppm
BF 0.9781 Hz
RGAIN 2050
PRNT_DATE 2024/May/02 08:24:13
COMNT

Chromatogram

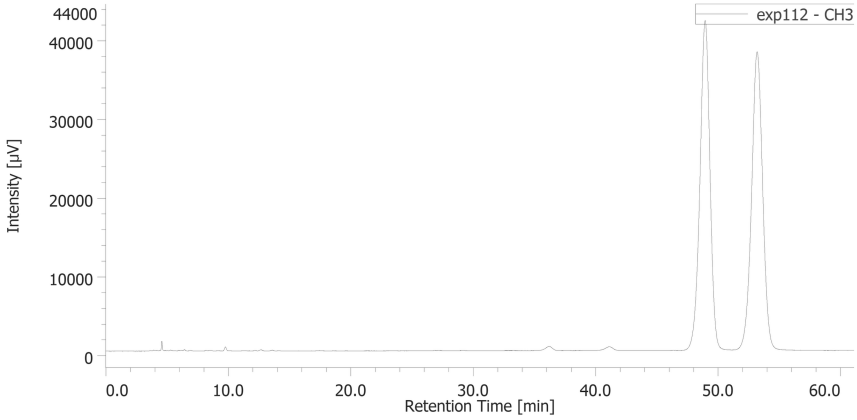


Chromatogram Information	
User Name	3385
Date Modified	2023/03/11 17:29:34
Description	IB,0.9mL/min, Hex:EtOH=99:1
HPLC System Name	SYSTEM-3
Injection Date	2023/03/11 16:01:22
Volume	1.0 [μL]
Sample #	1
Project Name	2022system3
Acquisition Time	999.0 [min]
Acquisition Sequence	3-1636 toba
Control Method	2019system3
Peak ID Table	
Calibration Method	
Additional Information	

Channel & Peak Information Table

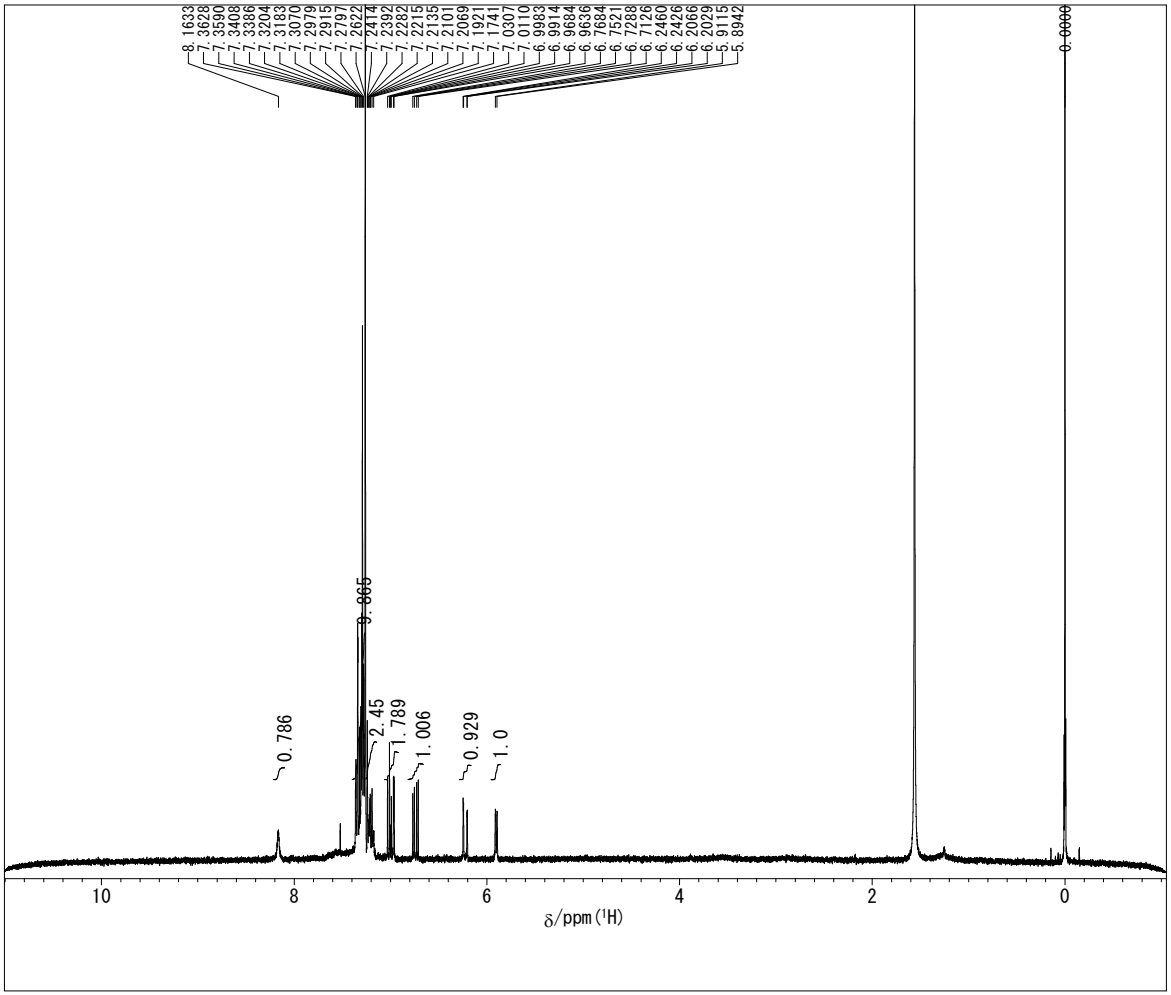
Chromatogram Name	exp68-CH3
Sample Name	
Channel Name	UV-2075
Sampling Interval	500 [msec]
Peak Method	(Manual)

#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%
1	Unknown	3	62.58	27636810	322117	97.428	97.271
2	Unknown	3	71.78	729538	9039	2.572	2.729

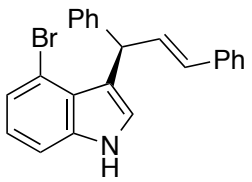


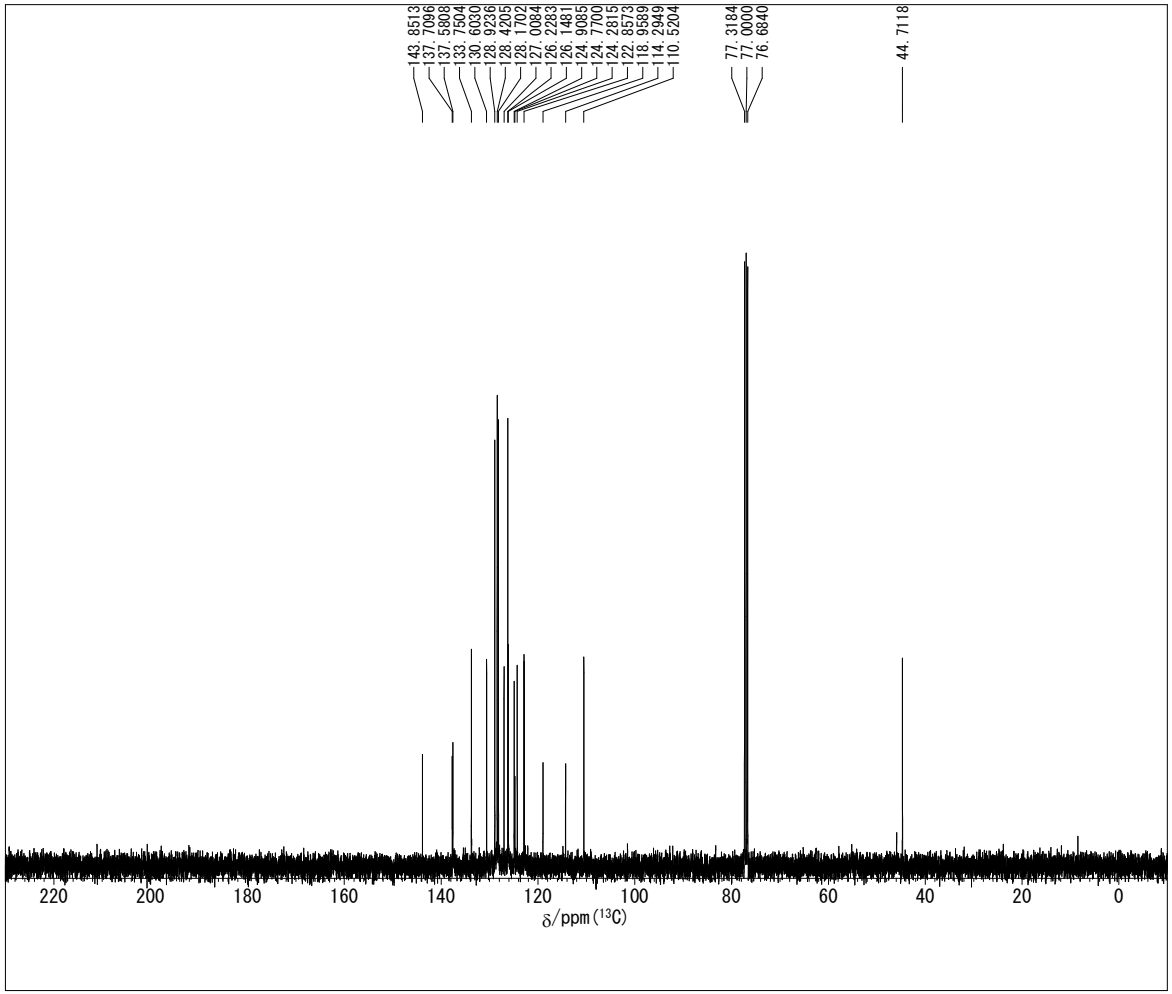
IB,flow0.9,Hex:EtOH=99:1

^{1}H NMR, ^{13}C{^{1}H} NMR and chiral phase HPLC chart of (*R*)-**10l** (**Table 4**, Entry 12)



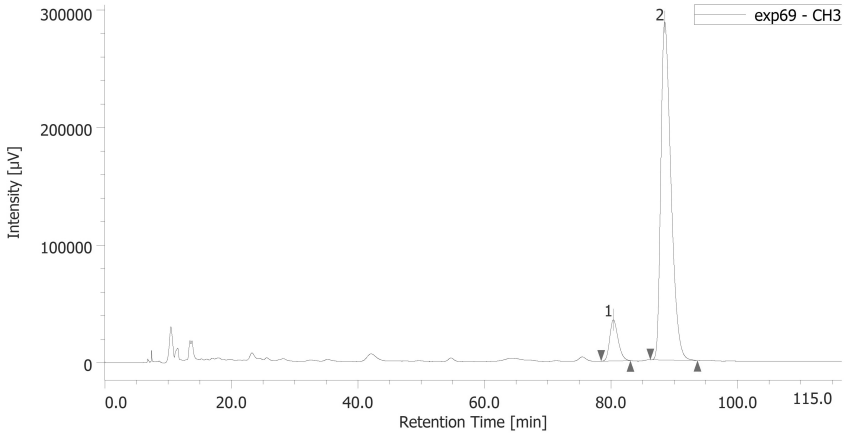
DATIM 14/Mar/2023 10:35:55
OBNUC ^{1}H
EXMOD ZG30>
OFR 400.18 MHz
OBSET 0.0 kHz
OBFIN 2008.224 Hz
POINT 131072(ZeroFill :×4)
FREQU 4826.255 Hz
SCANS 16
ACQTM 6.7895 s
PD 1.0 s
PW1 14.0 μs
CTEMP 18.81 °C
SLVNT $CDCl_3$>
EXREF 0.0 ppm
BF 0.1473 Hz
RGAIN 203
PRNT_DATE 2024/May/02 08:26:04
COMNT





DATIM 13/Mar/2023 18:02:37
OBNUC ^{13}C
EXMOD ZGPG30>
OFR 100.61 MHz
OBSET 0.0 kHz
OBFIN 12705.91 Hz
POINT 131072(ZeroFill :×4)
FREQU 32051.28 Hz
SCANS 64
ACQTM 1.0224 s
PD 2.0 s
PW1 9.0 μs
CTEMP 21.01 ℃
SLVNT $CDCL_3$>
EXREF 77.0 ppm
BF 0.9781 Hz
RGAIN 2050
PRNT_DATE 2024/May/02 08:26:40
COMNT

Chromatogram

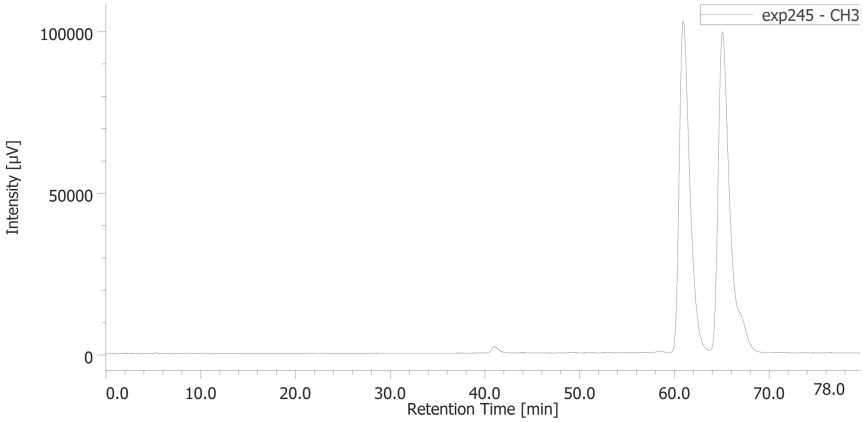


Chromatogram Information	
User Name	3385
Date Modified	2023/03/11 15:06:06
Description	IA-3,0.5mL/min, Hex:EtOH=99:1
HPLC System Name	SYSTEM-3
Injection Date	2023/03/11 13:09:35
Volume	1.0 [μL]
Sample #	1
Project Name	2022system3
Acquisition Time	999.0 [min]
Acquisition Sequence	3-1635 toba
Control Method	2019system3
Peak ID Table	
Calibration Method	
Additional Information	

Channel & Peak Information Table

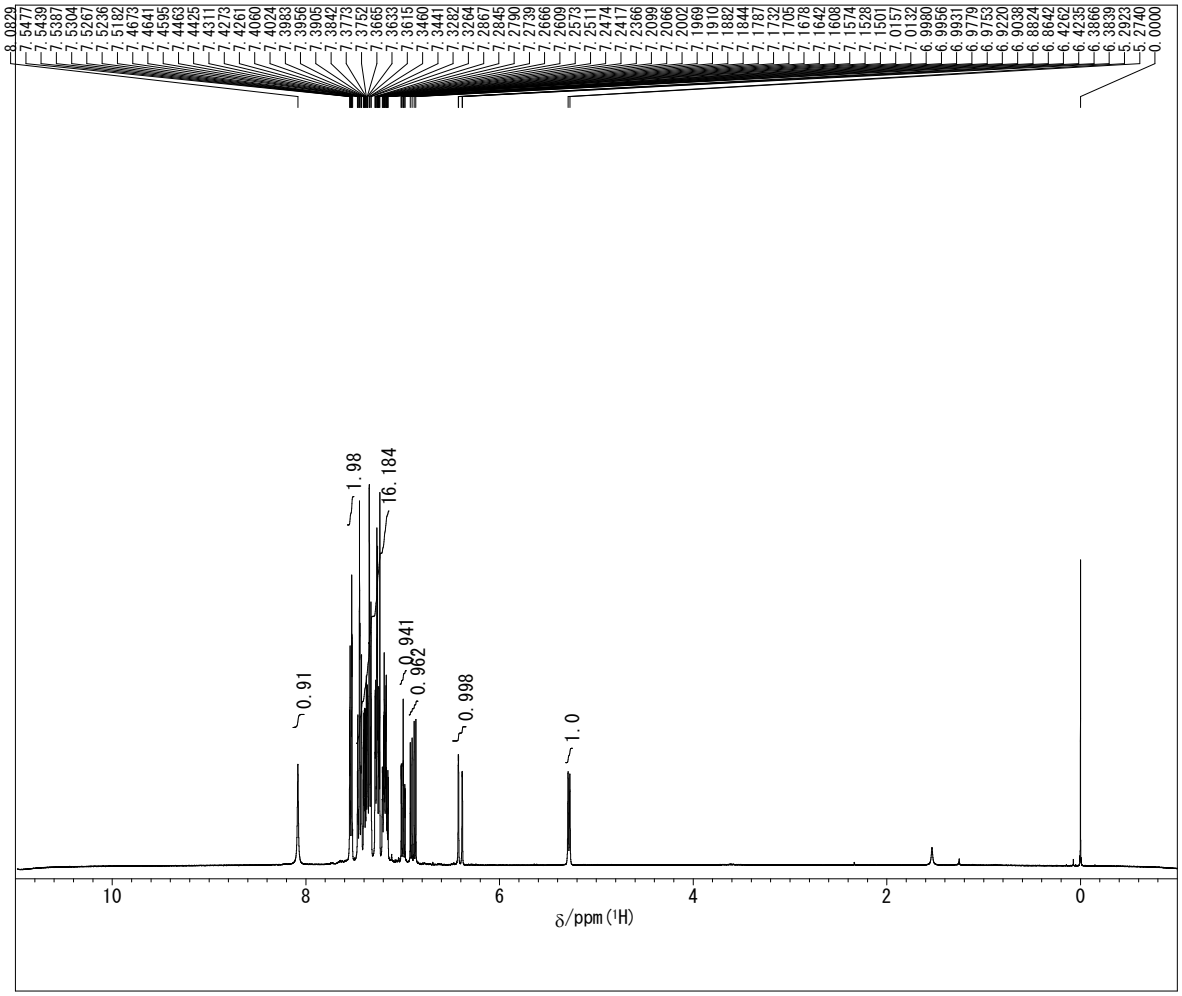
Chromatogram Name	exp69-CH3
Sample Name	
Channel Name	UV-2075
Sampling Interval	500 [msec]
Peak Method	(Manual)

#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%
1	Unknown	3	80.37	3223359	35013	9.145	10.853
2	Unknown	3	88.48	32025022	287602	90.855	89.147

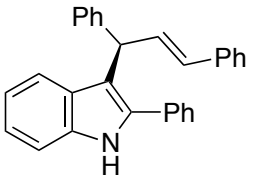


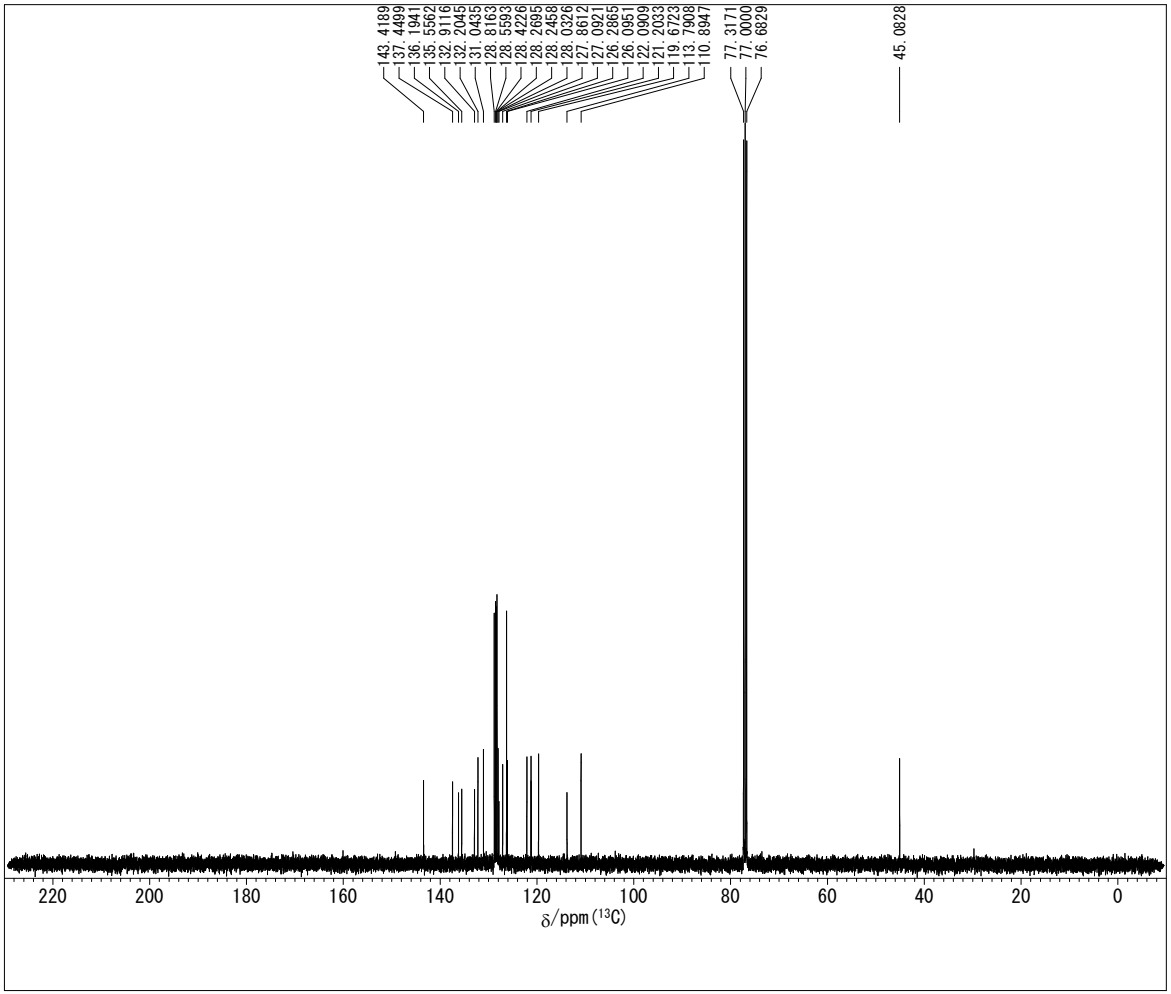
IA-3,0.7, Hex:EtOH=99:1

^{1}H NMR, ^{13}C{^{1}H} NMR and chiral phase HPLC chart of (*R*)-**10m** (**Table 4**, Entry 13)



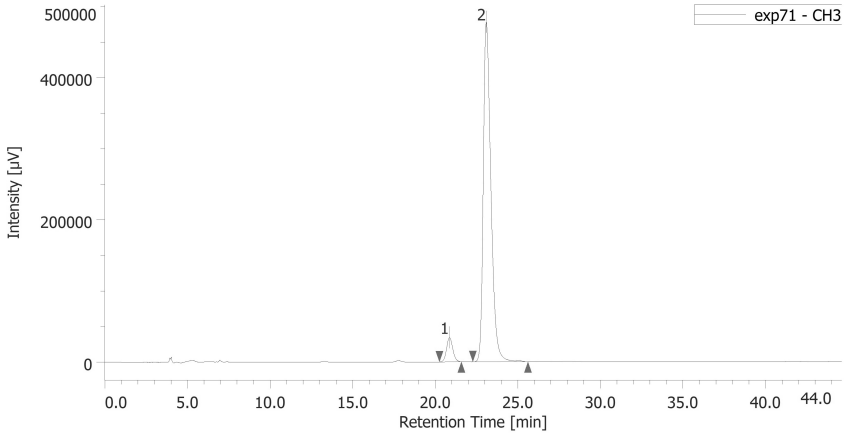
DATIM 20/Mar/2023 15:19:57
OBNUC ^{1}H
EXMOD ZG30>
OFR 400.18 MHz
OBSET 0.0 kHz
OBFIN 2008.224 Hz
POINT 131072(ZeroFill :×4)
FREQU 4826.255 Hz
SCANS 8
ACQTM 6.7895 s
PD 1.0 s
PW1 14.0 μs
CTEMP 18.51 °C
SLVNT $CDCL_3$>
EXREF 0.0 ppm
BF 0.1473 Hz
RGAIN 161
PRNT_DATE 2024/May/02 08:28:19
COMNT





DATIM 20/Mar/2023 15:30:30
OBNUC ^{13}C
EXMOD ZGPG30>
OFR 100.63 MHz
OBSET 0.0 kHz
OBFIN 11066.5 Hz
POINT 131072(ZeroFill :×4)
FREQU 24038.46 Hz
SCANS 128
ACQTM 1.3631 s
PD 2.0 s
PW1 10.0 μs
CTEMP 19.41 ℃
SLVNT $CDCL_3$>
EXREF 77.0 ppm
BF 0.7336 Hz
RGAIN 203
PRNT_DATE 2024/May/02 08:28:57
COMNT

Chromatogram

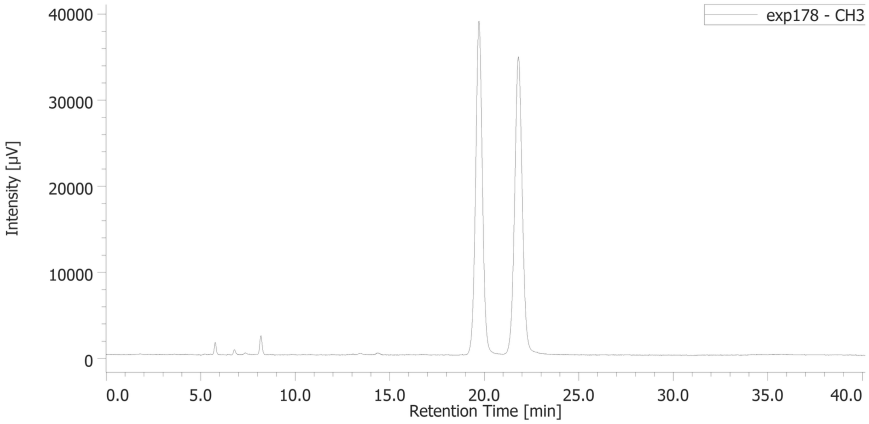


Chromatogram Information	
User Name	3385
Date Modified	2023/03/17 19:08:11
Description	IB,0.9mL/min, Hex:EtOH=99:1
HPLC System Name	SYSTEM-3
Injection Date	2023/03/17 18:23:33
Volume	1.0 [μL]
Sample #	1
Project Name	2022system3
Acquisition Time	999.0 [min]
Acquisition Sequence	3-1637 toba
Control Method	2019system3
Peak ID Table	
Calibration Method	
Additional Information	

Channel & Peak Information Table

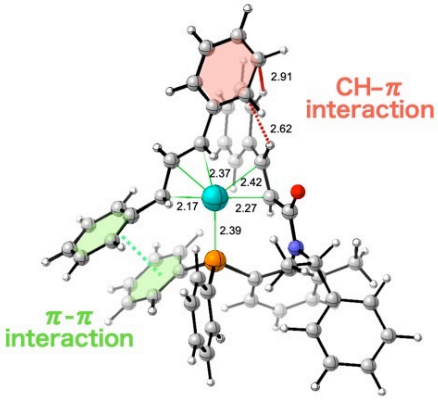
Chromatogram Name	exp71-CH3
Sample Name	
Channel Name	UV-2075
Sampling Interval	500 [msec]
Peak Method	(Manual)

#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%
1	Unknown	3	20.86	888045	34200	5.460	6.677
2	Unknown	3	23.08	15377481	478017	94.540	93.323



IB,flow0.9,Hex:EtOH=99:1

6. Cartesian Coordinates and Energies

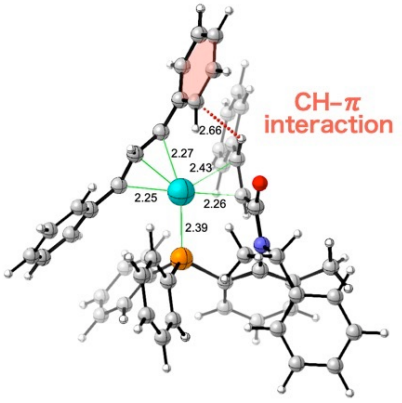


3-Olefin-M

at wb97xd/6-31+G* & SDD (for Pd)
Energy = -2569.005145 A.U.
Thermal correction to Gibbs Free Energy = 0.744763 A.U.
Sum of electronic and thermal Free Energies = -2568.260382 A.U.
at wb97xd/def2-TZVPP/smd(MeCN) Energy = -2569.87330545 A.U.

C	-2.90791400	-0.57839800	-1.95260700
C	-2.96569300	0.72535100	-1.46820800
H	-2.13104400	-0.81101600	-2.68396500
H	-3.78558200	1.03483600	-0.82502800
C	-1.86375000	1.60269400	-1.68322300
H	-1.31628800	1.43644200	-2.60983300
C	-3.96158400	-1.59119500	-1.84798800
C	-5.22646600	-1.31905200	-1.30800900
C	-3.70031700	-2.87460400	-2.35333900
C	-6.20756500	-2.30376900	-1.28551500
H	-5.46085400	-0.33414300	-0.91628300
C	-4.67655300	-3.86373200	-2.31314500
H	-2.72026100	-3.09644500	-2.77064800
C	-5.93515000	-3.57778700	-1.78304000
H	-7.18743400	-2.07647100	-0.87705700
H	-4.45990400	-4.85280700	-2.70454700
H	-6.70389700	-4.34444000	-1.76438200
Pd	-1.15899900	-0.03432000	-0.44792400
P	0.85263400	1.05451600	0.22856400
C	-0.42425700	-1.85522900	0.68552200
C	1.96707800	0.08428800	1.33573100
H	-0.06386900	-1.52130800	1.65171800
C	-1.74802100	-2.16977100	0.51492400
C	2.25615100	-1.27561700	1.08608300
C	2.45225200	0.67491800	2.50444900
N	1.86371400	-1.88793900	-0.15157400
H	-2.00045200	-2.75056900	-0.36888400
C	2.90423500	-2.05491500	2.05452000
C	3.18872900	-0.07019600	3.42195600
H	2.24980900	1.71957900	2.71487000
C	3.38196900	-1.42521500	3.20891000
H	3.57727600	0.40616800	4.31682300
H	3.90844400	-2.02100000	3.95026500
C	1.97096200	1.69617200	-1.06417100
C	1.59672100	1.70273100	-2.40773300
C	3.23466400	2.18527100	-0.70715100
C	2.45673700	2.20295600	-3.38204600
H	0.64821200	1.27332600	-2.70506600
C	4.09743700	2.68079900	-1.67921900
H	3.55060300	2.17486900	0.33285300
C	3.70807000	2.69357300	-3.01876900
H	2.15678500	2.18960500	-4.42558700
H	5.07657800	3.05184600	-1.39185400
H	4.38468700	3.07491000	-3.77743000
C	0.41733600	2.50409000	1.25510300
C	-0.41331800	2.28785100	2.36257900
C	0.86436100	3.79672100	0.98145300
C	-0.75654200	3.33662200	3.20579200
H	-0.78240100	1.28822700	2.57549600
C	0.50874100	4.85143100	1.82192900
H	1.48279500	3.99482000	0.11239800
C	-0.28951300	4.62396900	2.93800700
H	-1.38887500	3.15189500	4.06921100
H	0.85795600	5.85441700	1.59609000
H	-0.55654400	5.44724800	3.59390700
C	-2.80736400	-2.00683200	1.51825100
C	-3.99465800	-2.73082500	1.35824900
C	-2.67022200	-1.17247300	2.63908400
C	-5.01968400	-2.62803900	2.29539300
H	-4.11026800	-3.38629000	0.49953700
C	-3.69362000	-1.06468100	3.56984200
H	-1.75567400	-0.60470700	2.78339600
C	-4.87404200	-1.79328400	3.39936500
H	-5.93177000	-3.20117400	2.15911500
H	-3.57445800	-0.41679900	4.43321900
H	-5.67316100	-1.71037200	4.12984300
C	-1.85904200	3.00495800	-1.22446100
C	-2.54123200	3.41432000	-0.07079200
C	-1.18398900	3.96528100	-1.98660500
C	-2.57970700	4.75582000	0.28565600
H	-3.03151600	2.67990600	0.56348500
C	-1.21956900	5.30984200	-1.62765100
H	-0.64051100	3.66109200	-2.87784700
C	-1.92558600	5.70876200	-0.49587400
H	-3.11221400	5.05936300	1.18168500
H	-0.70286700	6.04487000	-2.23747600
H	-1.96055700	6.75753500	-0.21649300
C	3.08083800	-3.54566400	1.92261400
H	4.13836900	-3.80216900	1.80797400
H	2.71231100	-4.04045300	2.82774000
H	2.54144100	-3.95794200	1.06756000
C	2.85171000	-2.31249700	-1.19394300
H	2.57680100	-3.34443100	-1.43145800
C	0.57093400	-2.29489700	-0.34962900
O	0.22203600	-2.93782700	-1.33594000
C	4.29565800	-2.29935300	-0.73287100
C	5.03438700	-3.48338500	-0.76247700
C	4.94133300	-1.11751500	-0.35535100
C	6.38092900	-3.49662200	-0.40153000
H	4.55115600	-4.40991800	-1.06443900

C	6.28060700	-1.12689000	0.01968800
H	4.39253700	-0.18026300	-0.34483700
C	7.00521600	-2.31865500	0.00038500
H	6.93918200	-4.42769800	-0.43254600
H	6.76253400	-0.20150400	0.32246000
H	8.05235400	-2.32581300	0.28812800
C	2.69630900	-1.48185700	-2.47072200
H	1.64925100	-1.43430700	-2.78158800
H	3.08131700	-0.46997900	-2.32982700
H	3.27411300	-1.95258400	-3.27260000

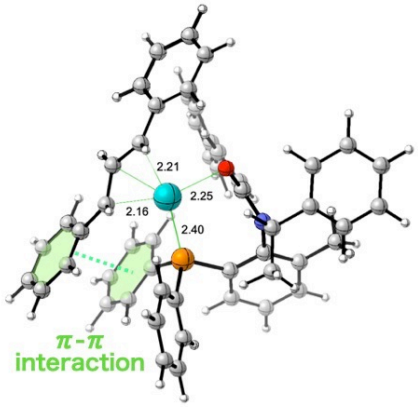


3-Olefin-W

at wb97xd/6-31+G* & SDD (for Pd)
Energy = -2569.003543 A.U.
Thermal correction to Gibbs Free Energy = 0.746302 A.U.
Sum of electronic and thermal Free Energies = -2568.257241 A.U.
at wb97xd/def2-TZVPP/smd(MeCN) Energy = -2569.87160499 A.U.

C	-3.52495300	0.04342600	-0.72281600
C	-2.90130800	1.19229700	-1.23762900
H	-3.95701000	0.09964400	0.27787800
H	-2.74892100	1.26022000	-2.31230900
C	-2.31847100	2.14083500	-0.37640100
H	-2.67863800	2.16049000	0.65445000
C	-4.08673600	-0.99429100	-1.60811300
C	-3.38312700	-1.46807100	-2.72406500
C	-5.35677100	-1.51233400	-1.33103900
C	-3.94647500	-2.43212300	-3.55168600
H	-2.36907700	-1.12316200	-2.91384500
C	-5.92558900	-2.46831400	-2.16882800
H	-5.90308900	-1.15989500	-0.45981600
C	-5.22146000	-2.93026700	-3.27902200
H	-3.38428300	-2.80621300	-4.40164500
H	-6.91679900	-2.85493600	-1.95164400
H	-5.66037300	-3.68308900	-3.92671700
Pd	-1.34837400	0.13532100	-0.07994500
P	0.79713800	0.97445900	0.55866600
C	-0.57763200	-1.89603800	0.53839800
C	1.91849600	-0.20195200	1.42699800
H	-0.16311900	-1.79102200	1.53509100
C	-1.91109000	-2.18205300	0.38332700
C	2.13744200	-1.50396000	0.92393300
C	2.44740200	0.14279400	2.67188600
N	1.68010400	-1.85395800	-0.39122500
H	-2.22374300	-2.54841300	-0.59250800
C	2.76392000	-2.47547700	1.71605700
C	3.16844100	-0.78899400	3.41543300
H	2.29310000	1.13696600	3.07706200
C	3.29488200	-2.08801500	2.95174900
H	3.59527300	-0.50350300	4.37197800
H	3.80644900	-2.83199900	3.55717000
C	1.80211800	1.69235200	-0.77442500
C	1.22871400	1.90813200	-2.02662600
C	3.14812900	2.01906500	-0.56631000
C	1.97958700	2.46294700	-3.05871000
H	0.19928000	1.61393000	-2.20207700
C	3.90198700	2.56451900	-1.60001200
H	3.61128200	1.83662300	0.40065900
C	3.31608500	2.79026500	-2.84666200
H	1.52550800	2.62339800	-4.03186500
H	4.94778900	2.80653400	-1.43679500
H	3.90729800	3.21147700	-3.65411100
C	0.55465600	2.30326800	1.79245400
C	-0.41525700	2.09509400	2.78208000
C	1.26969300	3.50173000	1.78270900
C	-0.65690100	3.06126100	3.75238600
H	-0.98973700	1.17097700	2.79275700
C	1.02635700	4.47173600	2.75476700
H	2.00324500	3.69977100	1.00824200
C	0.06669100	4.25510400	3.73950500
H	-1.40976000	2.88665400	4.51526700
H	1.58594000	5.40217700	2.73405600
H	-0.12182700	5.01325900	4.49363200
C	-2.88753100	-2.28810900	1.47767600
C	-4.04365900	-3.04833200	1.26590400
C	-2.69946300	-1.67309900	2.72515700
C	-4.98848400	-3.19778500	2.27881200
H	-4.19598600	-3.53263800	0.30552000
C	-3.64469900	-1.81617600	3.73215500
H	-1.81069500	-1.07384200	2.90794100
C	-4.79371800	-2.57960400	3.51093000
H	-5.87572200	-3.79871800	2.10369000
H	-3.48838700	-1.33541600	4.69328200
H	-5.53092400	-2.69233300	4.30002500
C	-1.70873000	3.40753600	-0.81941300
C	-1.46667500	3.70869500	-2.16842300
C	-1.41736100	4.37954300	0.14530400
C	-0.92758000	4.93411200	-2.53455500
H	-1.69990500	2.98918400	-2.94815700
C	-0.87492300	5.60746800	-0.22040400
H	-1.61786700	4.17294500	1.19346400
C	-0.62298300	5.88642500	-1.56046500

H	-0.74810900	5.15158800	-3.58309500
H	-0.65452200	6.34589400	0.54445500
H	-0.20277200	6.84489500	-1.84976300
C	2.85584600	-3.92532100	1.31649800
H	3.89342600	-4.20915900	1.11644800
H	2.48806100	-4.55435300	2.13437500
H	2.26838900	-4.15166700	0.42438200
C	2.61196700	-2.16626300	-1.52393100
H	2.25008000	-3.12007700	-1.91943300
C	0.35842600	-2.13952800	-0.61373300
O	-0.05770100	-2.54961100	-1.69203700
C	4.06259200	-2.34250000	-1.12145700
C	4.70883300	-3.54528900	-1.41306700
C	4.80622700	-1.30693700	-0.54718400
C	6.05954900	-3.72289800	-1.11800900
H	4.14873600	-4.35819000	-1.86988900
C	6.15063100	-1.48306800	-0.23625700
H	4.32963200	-0.35548400	-0.33197600
C	6.78199300	-2.69426300	-0.51862800
H	6.54431100	-4.66577000	-1.35359900
H	6.70918600	-0.67206900	0.22258500
H	7.83274100	-2.83087000	-0.28076400
C	2.50169300	-1.12945600	-2.64506800
H	1.45805600	-0.95505400	-2.91666500
H	2.96783200	-0.18511900	-2.35680500
H	3.02998800	-1.50920800	-3.52562800

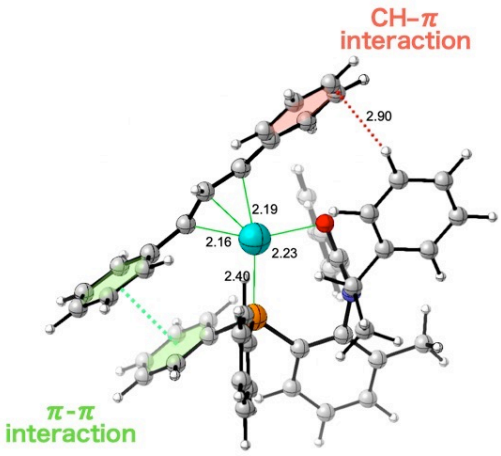


3-O-M

at wb97xd/6-31+G* & SDD (for Pd)
Energy = -2568.994407 A.U.
Thermal correction to Gibbs Free Energy = 0.74285 A.U.
Sum of electronic and thermal Free Energies = -2568.251557 A.U.
at wb97xd/def2-TZVPP/smd(MeCN) Energy = -2569.85984076 A.U.

C	0.14532500	1.84477100	-2.96247900
C	1.46660700	1.83034500	-2.49664500
H	-0.14446200	1.10270900	-3.70951000
H	1.86013800	2.68004000	-1.94617600
C	2.16848800	0.59624200	-2.47153200
H	1.92379400	-0.11457000	-3.26387800
C	-0.79953000	2.96198700	-2.78621800
C	-0.41560700	4.20891600	-2.27318300
C	-2.14478200	2.75415100	-3.11809400
C	-1.35560900	5.21937600	-2.09977100
H	0.62187200	4.41094000	-2.02308500
C	-3.08614100	3.76043700	-2.93284900
H	-2.45571400	1.78639000	-3.50173500
C	-2.69428900	4.99684200	-2.42228400
H	-1.04003000	6.18754800	-1.72136100
H	-4.12555300	3.58096300	-3.19012100
H	-3.42609300	5.78725700	-2.28524700
Pd	0.34518800	0.37543300	-1.32614000
P	1.05149900	-1.22284500	0.32484500
C	-1.59188500	0.99901500	1.33510000
C	-0.03701600	-1.74470500	1.74307200
H	-1.63344600	0.60264100	2.34304500
C	-1.31511800	2.29218100	1.09210900
C	-1.44292100	-1.75196100	1.66697300
C	0.56526700	-2.15788200	2.93500300
N	-2.05848900	-1.23212800	0.48031100
C	-2.23931200	-2.18062200	2.73611900
C	-0.20986500	-2.60552300	3.99988400
H	1.64420200	-2.11399700	3.04751100
C	-1.59516300	-2.62085300	3.89587000
H	0.27074800	-2.92713900	4.91884400
H	-2.19528000	-2.95290100	4.73884500
C	1.59714800	-2.81204500	-0.39992500
C	1.54256600	-2.96361500	-1.78897400
C	2.01823700	-3.89447900	0.38285400
C	1.91684500	-4.16292200	-2.38994200
H	1.18190800	-2.14427300	-2.40431700
C	2.39677100	-5.09184100	-0.21614000
H	2.04258000	-3.81421400	1.46510800
C	2.34917600	-5.22768200	-1.60357100
H	1.86133800	-4.26745100	-3.46949200
H	2.72215800	-5.92309600	0.40198000
H	2.63884300	-6.16547200	-2.06795600
C	2.47194300	-0.52351100	1.23600800
C	2.26313200	0.71484200	1.85878200
C	3.70759400	-1.15674400	1.36080600
C	3.26853000	1.29528000	2.62243300
H	1.30763000	1.22449300	1.75369100
C	4.71556000	-0.57002400	2.12585000
H	3.89864600	-2.09927000	0.85757000
C	4.49694900	0.64754700	2.76310400
H	3.09100400	2.25091700	3.10757700
H	5.67652800	-1.06780900	2.21540300
H	5.28372100	1.09715200	3.36176200
C	3.52479600	0.42537400	-1.91657700
C	4.11660000	1.36321600	-1.05907400
C	4.26325800	-0.70327100	-2.29187300
C	5.42463600	1.19384000	-0.62551200

H	3.55809800	2.22926200	-0.71652600
C	5.57010600	-0.88049700	-1.84640500
H	3.81552400	-1.44420600	-2.94962100
C	6.15765700	0.07463600	-1.02125400
H	5.87135600	1.93246900	0.03271400
H	6.13148000	-1.75691100	-2.15601000
H	7.18141500	-0.05274700	-0.68211500
C	-3.74254100	-2.14301000	2.66593700
H	-4.13750500	-3.02806700	2.15596900
H	-4.17324400	-2.11683500	3.67054600
H	-4.10078500	-1.27355000	2.10740600
C	-2.54789500	-2.13841100	-0.60398000
C	-4.07607900	-2.10852500	-0.67987100
C	-4.73243700	-0.89943700	-0.94359200
C	-4.85049500	-3.25590000	-0.49661100
C	-6.12165900	-0.83749100	-0.99447900
H	-4.15399400	0.00209300	-1.12049600
C	-6.24304900	-3.19735000	-0.55185300
H	-4.38083500	-4.21492700	-0.30247000
C	-6.88473200	-1.98700000	-0.79414900
H	-6.60979900	0.11140400	-1.19793400
H	-6.82383400	-4.10322300	-0.40404300
H	-7.96880200	-1.93989400	-0.83554400
C	-1.85207100	0.08167100	0.20915900
O	-1.87327100	0.50742700	-0.97519000
H	-1.35059800	2.63001600	0.05572500
C	-0.95317500	3.30150100	2.08797300
C	-0.98734900	4.65326700	1.71716400
C	-0.54380900	2.96620400	3.38877900
C	-0.64539900	5.64835800	2.62763800
H	-1.29639900	4.91796200	0.70891200
C	-0.19565400	3.96005700	4.29527100
H	-0.48030800	1.92410500	3.69128300
C	-0.24928900	5.30345800	3.91849000
H	-0.68721000	6.69212900	2.33119900
H	0.12048900	3.68916700	5.29829700
H	0.02124000	6.07790700	4.62998000
C	-1.96140300	-3.53834100	-0.46372800
H	-0.87085000	-3.51459600	-0.48009700
H	-2.27203800	-4.03627000	0.46004400
H	-2.28949100	-4.14824400	-1.30996800
H	-2.16151000	-1.69891800	-1.52948800

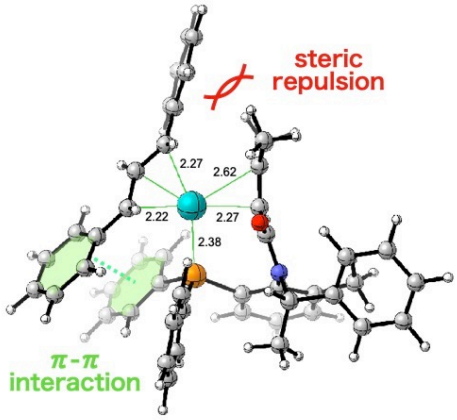


3-O-W

at wb97xd/6-31+G* & SDD (for Pd)
Energy = -2568.996333 A.U.
Thermal correction to Gibbs Free Energy = 0.739987 A.U.
Sum of electronic and thermal Free Energies = -2568.256346 A.U.
at wb97xd/def2-TZVPP/smd(MeCN) Energy = -2569.86576771 A.U.

C	-1.44878700	2.49082900	0.24383700
C	0.89745700	1.13286700	2.15254500
H	-1.30168900	3.14850700	1.09287800
C	-1.43652900	2.94967200	-1.01909000
C	-0.44718300	1.28189100	2.53696800
C	1.87573300	1.85724400	2.83915700
N	-1.45867500	0.59925200	1.77253800
C	-0.82047700	2.12561100	3.59014600
C	1.52171800	2.68898700	3.89643100
H	2.91807100	1.78377400	2.54431600
C	0.18853500	2.81583000	4.26746600
H	2.28893900	3.24719500	4.42426000
H	-0.08172000	3.47843200	5.08529100
C	-1.64968500	1.05535100	0.50085200
O	-1.96964800	0.26323500	-0.41607200
C	-1.76770300	-0.82988100	2.04233700
H	-1.15566000	-1.43159900	1.35668700
C	1.74958800	-1.57144000	1.80817600
C	1.19898400	-2.78861000	1.39734600
C	2.49444200	-1.53006100	2.99338000
C	1.39325900	-3.94648300	2.14604500
H	0.59667500	-2.82764000	0.49233000
C	2.69621500	-2.68729300	3.73912600
H	2.91169600	-0.59158500	3.34700000
C	2.14519000	-3.89725100	3.31724200
H	0.95127400	-4.88291700	1.81864000
H	3.27636500	-2.64262100	4.65583200
H	2.29589100	-4.79726300	3.90572300
C	3.01049600	0.62151100	0.29626600

C	2.96872800	1.80166100	-0.45862400
C	4.24022600	0.03326200	0.58901400
C	4.14735000	2.39917600	-0.89001900
H	2.01157800	2.26219700	-0.69905300
C	5.42053400	0.63419100	0.15171000
H	4.28874700	-0.89974600	1.14146300
C	5.37770100	1.81683100	-0.57981200
H	4.10726600	3.31930900	-1.46560500
H	6.37408300	0.16718400	0.37914200
H	6.29929300	2.28330500	-0.91516000
C	-2.26519800	2.32775400	3.96336600
H	-2.89504200	2.44947100	3.07691000
H	-2.65424900	1.47217300	4.52665300
H	-2.38093200	3.21442500	4.59225100
C	-1.39765300	-1.22780400	3.46991200
H	-1.98359200	-0.67378100	4.20893700
H	-1.62464400	-2.29012700	3.59392200
H	-0.33408200	-1.08244600	3.67867800
C	-3.21980100	-1.15176800	1.73989100
C	-3.52807000	-2.19817700	0.87115800
C	-4.25928300	-0.45683400	2.35938800
C	-4.85220300	-2.55870200	0.63850300
H	-2.72813600	-2.72429800	0.35396900
C	-5.58610900	-0.80474500	2.11789000
H	-4.03577300	0.36395700	3.03405200
C	-5.88579000	-1.86172800	1.26040900
H	-5.07465500	-3.37625900	-0.03992500
H	-6.38582100	-0.25443700	2.60518200
H	-6.91980200	-2.13867200	1.07687200
P	1.40571200	-0.06247500	0.82765800
Pd	0.00083900	-0.57473400	-1.04617100
C	1.48780300	-1.03450300	-2.54737800
C	0.33966200	-1.82970300	-2.79674400
H	1.50839600	-0.04217900	-3.00507400
C	2.82642600	-1.59068300	-2.26623700
C	-0.89776600	-1.18513300	-2.95341400
H	0.39329300	-2.90359500	-2.63626200
C	3.01182800	-2.79166900	-1.57001600
C	3.95035400	-0.89960100	-2.73073100
H	-0.89135800	-0.18035400	-3.38151500
C	-2.21510900	-1.84262600	-2.93154900
C	4.28942900	-3.29188200	-1.35037000
H	2.15580100	-3.33427800	-1.18066100
C	5.22948600	-1.40720800	-2.52551000
H	3.82311200	0.04296100	-3.25710300
C	-2.37331300	-3.23041200	-2.80874600
C	-3.35882000	-1.03921400	-3.02336900
C	5.40277200	-2.60335100	-1.83392100
H	4.41722100	-4.22093900	-0.80276600
H	6.09095100	-0.86178400	-2.89857400
C	-3.64300200	-3.79657000	-2.80049300
H	-1.50822000	-3.88407800	-2.74192300
C	-4.62862500	-1.60407900	-3.00446700
H	-3.24846400	0.03950100	-3.09227400
H	6.40067400	-2.99849800	-1.66862300
C	-4.77339200	-2.98542500	-2.90070100
H	-3.75094800	-4.87448700	-2.72342800
H	-5.50468800	-0.96644100	-3.06926500
H	-5.76407500	-3.43038900	-2.89620900
H	-1.61650900	2.22130700	-1.80955500
C	-1.20988500	4.32787500	-1.45521600
C	-0.75655000	5.33414100	-0.58698900
C	-1.44585900	4.65350400	-2.79863000
C	-0.56056600	6.62858500	-1.05066500
H	-0.54318600	5.10486400	0.45328400
C	-1.25375000	5.95131100	-3.26248300
H	-1.79476100	3.88274900	-3.48213400
C	-0.81137200	6.94158900	-2.38827200
H	-0.20851000	7.39789000	-0.37002700
H	-1.44933400	6.18927500	-4.30354400
H	-0.65849700	7.95516000	−2.74650100

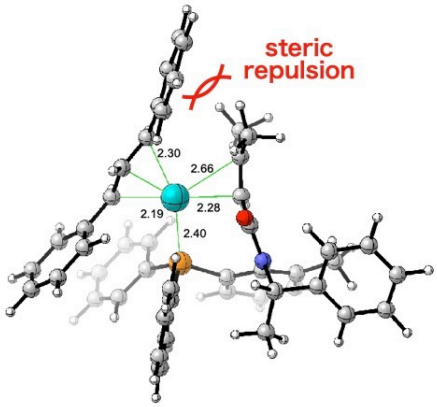


4d-Olefin-M

at wb97xd/6-31+G* & SDD (for Pd)
Energy = -2416.624574 A.U.
Thermal correction to Gibbs Free Energy = 0.722749 A.U.
Sum of electronic and thermal Free Energies = -2415.901825 A.U.
at wb97xd/def2-TZVPP/smd(MeCN) Energy = -2417.43975209 A.U.

C	2.46345900	2.36534500	-1.24782000
C	3.11186100	1.13145100	-1.07620500
H	1.85657200	2.50793200	-2.14346800
H	3.94862400	1.07373800	-0.38565500
C	2.58248000	-0.05327700	-1.62486100
H	1.94189900	0.05000600	-2.50316700
C	2.98048000	3.59435000	-0.61908300
C	3.61896800	3.57448400	0.63006700
C	2.85387600	4.81728300	-1.28916400
C	4.12495700	4.74349600	1.18624400
H	3.69220100	2.64422000	1.18856500

C	3.35577900	5.98993900	-0.73030200
H	2.37438600	4.84761900	-2.26465400
C	3.99280500	5.95609000	0.50832000
H	4.61376000	4.71242900	2.15536100
H	3.25427600	6.92870400	-1.26613400
H	4.38475600	6.86952700	0.94484600
Pd	1.08597800	0.85612100	-0.26467300
P	0.22673800	-1.24546500	0.46201800
C	-0.83038300	1.76135600	0.53705700
C	-1.14911900	-1.18728400	1.69481800
H	-0.84539500	1.42518500	1.56964400
C	-0.28537400	3.00840900	0.31929000
C	-2.31243900	-0.41607000	1.45484200
C	-0.98555900	-1.80191800	2.93629600
N	-2.56290300	0.10209900	0.13766600
C	-3.22610400	-0.16828100	2.48772300
C	-1.94123300	-1.63809000	3.93662000
H	-0.10875700	-2.40761600	3.13709300
C	-3.02699200	-0.80612800	3.71942100
H	-1.81346300	-2.13569300	4.89300900
H	-3.74184400	-0.63121900	4.51941300
C	-0.36579500	-2.35550000	-0.85294000
C	-0.59951600	-1.82365700	-2.12345900
C	-0.69126200	-3.69407200	-0.59784300
C	-1.12269100	-2.62487700	-3.13616800
H	-0.40477900	-0.77242800	-2.31891800
C	-1.18862700	-4.49989500	-1.61651000
H	-0.59317800	-4.10233300	0.40414700
C	-1.40246600	-3.96647600	-2.88806100
H	-1.31583600	-2.19714300	-4.11544500
H	-1.43245600	-5.53801900	-1.41216900
H	-1.80449000	-4.59323000	-3.67842400
C	1.58761400	-2.05838500	1.37278900
C	2.23258300	-1.27242900	2.34043800
C	2.02918500	-3.36351300	1.15720200
C	3.27112200	-1.79537900	3.10120400
H	1.90942400	-0.24685200	2.50999300
C	3.07095900	-3.88695700	1.92229900
H	1.59723500	-3.97475400	0.37391400
C	3.68756100	-3.11191000	2.89833500
H	3.75296700	-1.17893700	3.85436600
H	3.40678100	-4.90314600	1.73896700
H	4.49637300	-3.52517000	3.49348300
C	3.22624600	-1.37415400	-1.49868100
C	4.29651300	-1.61636400	-0.62559900
C	2.79173200	-2.41290600	-2.33219900
C	4.92714300	-2.85322600	-0.60910400
H	4.64598300	-0.84476400	0.05324300
C	3.41227900	-3.65807900	-2.30358200
H	1.96576100	-2.24255400	-3.01695900
C	4.48814700	-3.87856800	-1.44714500
H	5.75986600	-3.02102000	0.06688100
H	3.06397100	-4.44835500	-2.96170400
H	4.98578900	-4.84374300	-1.43311300
C	-4.38577700	0.78221200	2.34237600
H	-5.31289600	0.25409600	2.10011000
H	-4.54465900	1.31562600	3.28470100
H	-4.22077500	1.51430900	1.54907800
C	-3.60309900	-0.53547700	-0.73733400
C	-4.90762800	0.26676800	-0.78270200
C	-4.90655900	1.58368900	-1.26177600
C	-6.12699900	-0.28429000	-0.37956100
C	-6.07854900	2.33370700	-1.29742500
H	-3.98184800	2.02066100	-1.62235700
C	-7.30398300	0.46277100	-0.41997800
H	-6.18021000	-1.30565900	-0.01737500
C	-7.28388100	1.77904000	-0.87004800
H	-6.05161800	3.35281100	-1.67309900
H	-8.23742100	0.00981400	-0.09810800
H	-8.19921300	2.36264800	-0.90119400
C	-1.77339300	1.07915900	-0.40959000
O	-1.83341900	1.37632300	-1.60232500
C	-0.51019500	3.84987800	-0.90533300
H	0.29312000	4.58146800	-1.01956100
H	-1.44014100	4.41432900	-0.74862300
H	-0.63893900	3.26280200	-1.81191600
C	0.30826600	3.74192100	1.48917300
H	0.52593700	3.08325700	2.33430700
H	-0.41900600	4.49670700	1.81795600
H	1.21725900	4.28005500	1.20949500
C	-3.80713100	-1.99959600	-0.36874800
H	-2.86333000	-2.54039800	-0.40071200
H	-4.23735100	-2.13107600	0.62907200
H	-4.47993000	-2.46088500	-1.09699600
H	-3.16334700	-0.49535000	-1.73804400

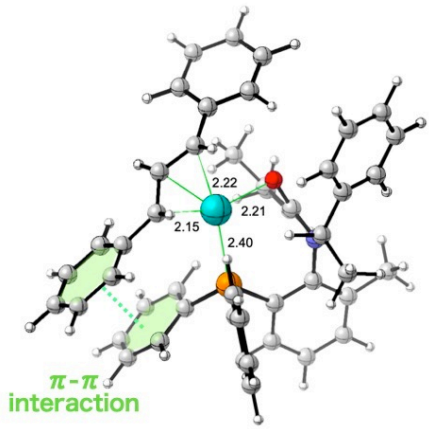


4d-Olefin-W

at wb97xd/6-31+G* & SDD (for Pd)
Energy = -2416.622911 A.U.
Thermal correction to Gibbs Free Energy = 0.722473 A.U.
Sum of electronic and thermal Free Energies = -2415.900438 A.U.

at wb97xd/def2-TZVPP/smd(MeCN) Energy = -2417.43849387 A.U.

C	-2.37389100	2.88035600	-0.41776900
C	-2.86344400	1.92515800	0.48042900
H	-2.64183700	2.76501200	-1.47000700
H	-2.85696200	2.13462700	1.54772500
C	-3.19507700	0.62564500	0.03642300
H	-3.51573800	0.51851900	-1.00197200
C	-1.98510700	4.23919400	-0.01360800
C	-1.51171000	4.53065300	1.27369200
C	-2.10580000	5.28300700	-0.94021900
C	-1.17189400	5.83145400	1.62277700
H	-1.37188900	3.73305100	1.99867700
C	-1.76208700	6.58638300	-0.59209600
H	-2.49222000	5.07678100	-1.93595600
C	-1.29254400	6.86289900	0.69025400
H	-0.80033800	6.04153900	2.62105300
H	-1.86728300	7.38553700	-1.31941200
H	-1.02279700	7.87814300	0.96429300
Pd	-1.07403500	0.98387300	-0.39525800
P	-0.54305800	-1.35409800	-0.42495000
C	1.05831200	1.32945800	-1.12033300
C	0.93618700	-1.85346200	-1.41961800
H	1.04830800	0.70400500	-2.00832200
C	0.76902200	2.66107500	-1.31473300
C	2.18925500	-1.21807100	-1.23953700
C	0.78808000	-2.77298800	-2.45854100
N	2.41284600	-0.40123700	-0.07890700
C	3.21888100	-1.39720300	-2.17306300
C	1.84485600	-3.03566900	-3.32745300
H	-0.15397100	-3.28900700	-2.60514100
C	3.02839600	-2.32737100	-3.20335500
H	1.72336800	-3.76800100	-4.11963700
H	3.83047100	-2.48485400	-3.91998600
C	-0.28948100	-2.09636700	1.21671000
C	-0.06952300	-1.24866700	2.30454100
C	-0.20394200	-3.48324500	1.39667400
C	0.20394400	-1.77753100	3.56372500
H	-0.08089100	-0.17044300	2.16545800
C	0.04437300	-4.01053800	2.65927600
H	-0.29360300	-4.15478500	0.54735500
C	0.24646900	-3.15756700	3.74495900
H	0.38907400	-1.10938700	4.39955600
H	0.10431400	-5.08649800	2.79181800
H	0.45414100	-3.57084000	4.72744700
C	-1.92364500	-2.21673300	-1.26218400
C	-2.29887300	-1.71352700	-2.51790000
C	-2.63944600	-3.28498700	-0.72283900
C	-3.34073800	-2.29120000	-3.23251900
H	-1.76166600	-0.86911800	-2.94633700
C	-3.68224500	-3.86873500	-1.44371600
H	-2.42383100	-3.65115900	0.27399000
C	-4.03145500	-3.38105100	-2.69761700
H	-3.61255200	-1.89592700	-4.20675700
H	-4.23039200	-4.69872800	-1.00808700
H	-4.84320300	-3.83815200	-3.25543300
C	-3.72693400	-0.40665300	0.94814000
C	-3.28400400	-0.53994100	2.27008800
C	-4.73563300	-1.25708600	0.48446400
C	-3.83088600	-1.50598100	3.10501800
H	-2.48851200	0.09830400	2.64363300
C	-5.29979500	-2.21145000	1.32563800
H	-5.07615200	-1.17523800	-0.54505800
C	-4.84488800	-2.34240800	2.63552800
H	-3.46445100	-1.60911100	4.12190400
H	-6.08822700	-2.85871300	0.95331800
H	-5.27708000	-3.09297300	3.29052300
C	4.49907700	-0.60290500	-2.14295800
H	5.31752000	-1.17111900	-1.69126800
H	4.79630100	-0.34997600	-3.16566600
H	4.39788300	0.32090300	-1.56989300
C	3.23758600	-0.92583100	1.06089600
C	4.66633800	-0.37390700	1.05756500
C	4.88699900	1.00136800	1.21142400
C	5.78002100	-1.20809900	0.92799100
C	6.17645600	1.52544000	1.19483600
H	4.04084100	1.66414900	1.35645800
C	7.07336500	-0.68654500	0.91751700
H	5.65813700	-2.28127900	0.82419700
C	7.27736100	0.68425600	1.04093000
H	6.32215400	2.59528900	1.31587900
H	7.92122100	-1.35768800	0.81348100
H	8.28376500	1.09230000	1.03216300
C	1.79243900	0.80889000	0.07860600
O	1.82394400	1.42809900	1.14126100
C	0.30662500	3.10729300	-2.67428300
H	1.12909700	3.65064600	-3.15827000
H	-0.52341500	3.81566500	-2.59240600
H	0.01405700	2.27405400	-3.31891600
C	1.16071100	3.76868700	-0.38044700
H	0.64847700	4.69938900	-0.63274500
H	2.24002000	3.93225300	-0.50893500
H	1.00340400	3.51955800	0.66596900
C	3.17917800	-2.44678200	1.12648000
H	3.70480700	-2.78524500	2.02371100
H	2.14907500	-2.79026800	1.19553500
H	3.63741500	-2.92847500	0.25701300
H	2.73782700	-0.52785700	1.94869600

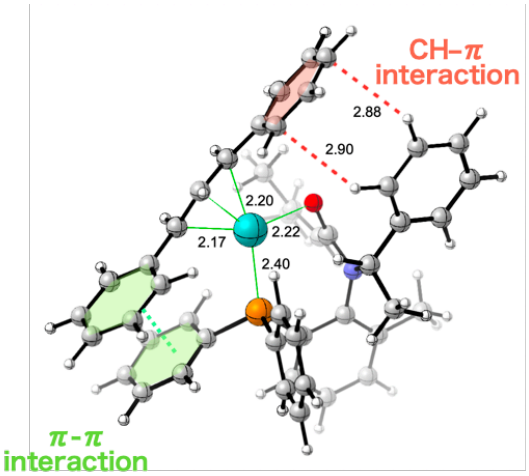


4d-O-M

at wb97xd/6-31+G* & SDD (for Pd)
Energy = -2416.629995 A.U.
Thermal correction to Gibbs Free Energy = 0.720187 A.U.
Sum of electronic and thermal Free Energies = -2415.909808 A.U.
at wb97xd/def2-TZVPP/smd(MeCN) Energy = -2417.44476538 A.U.

C	1.23303400	-2.74822600	-1.22642200
C	-0.08802100	-3.10311000	-0.92962300
H	1.42562100	-2.24118900	-2.17493000
H	-0.30084000	-3.78429600	-0.10962300
C	-1.14055800	-2.33064400	-1.49966600
H	-0.96222000	-1.95279400	-2.50826300
C	2.43192900	-3.24446700	-0.53116900
C	2.40585800	-4.35295400	0.32534300
C	3.63623400	-2.55159200	-0.71184400
C	3.55925000	-4.75461800	0.99013500
H	1.49136000	-4.92339300	0.46295100
C	4.78676900	-2.94891100	-0.03956500
H	3.66169200	-1.67535800	-1.35433300
C	4.75108000	-4.05068900	0.81370900
H	3.53109800	-5.62328000	1.64111900
H	5.70986700	-2.39526700	-0.18211300
H	5.65027300	-4.36659700	1.33423800
Pd	0.13995200	-1.00834000	-0.39145800
P	-1.38880200	0.77506900	0.09765200
C	1.76154300	0.75728300	2.54900400
C	-0.88989900	2.25781100	1.09965900
H	1.66765600	1.71165000	3.05693400
C	1.87495500	-0.36408700	3.29461900
C	0.42739000	2.74590000	1.10040100
C	-1.86247300	2.96131800	1.81729300
N	1.44847300	1.96205700	0.45934400
C	0.77777100	3.92692300	1.76568300
C	-1.53222000	4.13822800	2.48005100
H	-2.87976200	2.58556600	1.87349000
C	-0.22774300	4.61916100	2.44394000
H	-2.29486500	4.67750200	3.03353300
H	0.02220500	5.53592800	2.97099500
C	-2.03307000	1.55938400	-1.42955200
C	-1.59676400	1.09253900	-2.67284000
C	-2.91281500	2.64888500	-1.38951400
C	-2.03382000	1.68915800	-3.85326400
H	-0.89445200	0.26574800	-2.72076200
C	-3.35556900	3.24258700	-2.56724600
H	-3.25351500	3.04555900	-0.43821500
C	-2.91705900	2.76410400	-3.80181300
H	-1.67910700	1.31776800	-4.81016600
H	-4.03897100	4.08502200	-2.52057800
H	-3.25836300	3.23359600	-4.71942300
C	-2.82166900	0.16292000	1.04363400
C	-2.54883000	-0.39720100	2.29915200
C	-4.13722400	0.22369200	0.58641800
C	-3.58584400	-0.86280600	3.09836900
H	-1.52220500	-0.45418600	2.65795500
C	-5.17471700	-0.24804700	1.39008000
H	-4.36230700	0.62690200	-0.39570700
C	-4.90374600	-0.78276000	2.64547300
H	-3.36878200	-1.28533600	4.07503600
H	-6.19655800	-0.20075800	1.02596900
H	-5.71558400	-1.14385800	3.26988100
C	-2.56951300	-2.52262900	-1.18420400
C	-3.00591300	-3.10304100	0.01458900
C	-3.52361400	-2.13310200	-2.13123800
C	-4.35753800	-3.33186800	0.23490700
H	-2.29032000	-3.36889000	0.78791800
C	-4.87989500	-2.35548800	-1.90752500
H	-3.20027100	-1.66650200	-3.05905000
C	-5.29830200	-2.96693100	-0.72893800
H	-4.68099000	-3.78672300	1.16607600
H	-5.60628800	-2.06095300	-2.65906700
H	-6.35423400	-3.15158000	-0.55517400
C	2.20483700	4.40828000	1.79869200
H	2.57063900	4.66114900	0.79865400
H	2.29849700	5.29949600	2.42456500
H	2.87386100	3.63907100	2.20022000
C	1.60014300	2.02422500	-1.01219000
C	3.01337300	1.67835100	-1.44307500
C	3.19845600	0.90454200	-2.58927100
C	4.13155300	2.14897200	-0.75613000
C	4.47901800	0.59872500	-3.04307900
H	2.32977600	0.53170600	-3.13035100
C	5.41490300	1.83788300	-1.20090500
H	4.00182000	2.74796100	0.14090100
C	5.59314600	1.06161800	-2.34458500
H	4.60788100	-0.00410900	-3.93768000
H	6.27829800	2.20508100	-0.65356600
H	6.59374200	0.82238700	-2.69212600
C	1.76026100	0.78096500	1.08630400
O	2.04651600	-0.22872900	0.40425700
C	1.89930400	-0.25354400	4.79219700

H	2.82677700	-0.69096800	5.18241300
H	1.07531200	-0.83395100	5.22618900
H	1.82413400	0.77904400	5.14262700
C	1.97964900	-1.76211600	2.74848600
H	1.98358600	-2.49536200	3.55998700
H	2.88756800	-1.89021300	2.15106100
H	1.14414300	-1.99066900	2.07543000
C	1.16792200	3.37925900	-1.57263100
H	1.27550900	3.34758600	-2.66033000
H	0.12241600	3.60561500	-1.34352100
H	1.79992800	4.18984900	-1.19922200
H	0.93939500	1.26179300	-1.45218200

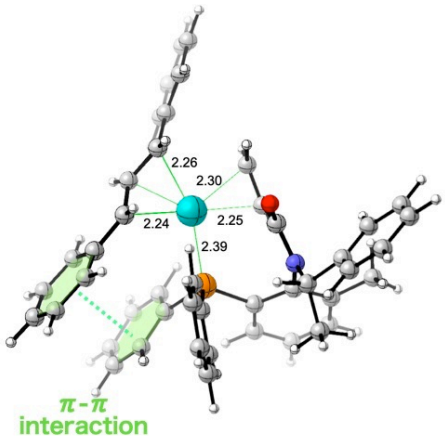


4d-O-W

at wb97xd/6-31+G* & SDD (for Pd)
Energy = -2416.626572 A.U.
Thermal correction to Gibbs Free Energy = 0.7176 A.U.
Sum of electronic and thermal Free Energies = -2415.908972 A.U.
at wb97xd/def2-TZVPP/smd(MeCN) Energy = -2417.44388481 A.U.

C	-0.90803300	-2.98638100	-1.14479300
C	0.28982100	-3.21436500	-0.44704000
H	-0.83957200	-2.82165000	-2.22136400
H	0.28275800	-3.67613500	0.53718800
C	1.47276300	-2.58748800	-0.91018800
H	1.55191000	-2.42100300	-1.98753700
C	-2.25176900	-3.33494800	-0.65643300
C	-2.49551800	-3.76013900	0.65763400
C	-3.33217000	-3.23193500	-1.54077000
C	-3.78021600	-4.10139000	1.06223300
H	-1.68269400	-3.83414100	1.37504200
C	-4.62042400	-3.56211500	-1.13374700
H	-3.15815000	-2.89405900	-2.55918600
C	-4.84604300	-4.00574400	0.16686500
H	-3.95202200	-4.44235200	2.07901400
H	-5.44667100	-3.47777900	-1.83277900
H	-5.84928100	-4.27390500	0.48467600
Pd	-0.02670200	-1.05915700	-0.55767200
P	1.37530400	0.74659600	0.16642900
C	-1.45224900	1.89184200	-2.42324000
C	0.92770600	2.52856900	-0.08531400
H	-1.36078100	2.97268700	-2.39513000
C	-1.41687900	1.27889700	-3.62473700
C	-0.41002200	2.96397800	-0.05565400
C	1.94272900	3.47963500	-0.22065700
N	-1.45243400	1.97318700	-0.00177400
C	-0.73757600	4.32319600	-0.13870300
C	1.63145100	4.83311300	-0.29762700
H	2.98126100	3.16778500	-0.27536000
C	0.30590300	5.24623500	-0.25037400
H	2.42647800	5.56493200	-0.40339300
H	0.06942900	6.30449300	-0.32209800
C	1.60275900	0.68027700	1.98388500
C	0.98183000	-0.33823400	2.71212200
C	2.32711400	1.66074300	2.67321100
C	1.08712800	-0.38740600	4.09972100
H	0.39424000	-1.09058000	2.19051800
C	2.44021000	1.60946000	4.05906500
H	2.79643100	2.47764900	2.13258000
C	1.81950400	0.58581600	4.77489800
H	0.59085600	-1.17984100	4.65222400
H	3.00515500	2.37536700	4.58165600
H	1.90050600	0.55315200	5.85720800
C	3.03404500	0.65956700	-0.58763100
C	3.09011100	0.70779800	-1.98685700
C	4.21475800	0.54158000	0.14464700
C	4.31546800	0.66725200	-2.64202200
H	2.17121100	0.79196300	-2.56515200
C	5.44240800	0.49853300	-0.51584300
H	4.18779400	0.46635800	1.22698400
C	5.49634000	0.56773600	-1.90429800
H	4.35161800	0.71613800	-3.72641200
H	6.35673700	0.40154400	0.06173400
H	6.45458700	0.53765200	-2.41438000
C	2.77637400	-2.68548700	-0.22419800
C	2.89070800	-2.78299200	1.16822900
C	3.94009000	-2.70957900	-1.00002500
C	4.13767700	-2.90916700	1.76820500
H	2.00387200	-2.74502300	1.79317500
C	5.18817000	-2.85217700	-0.40197600
H	3.86851300	-2.61759800	-2.08084000
C	5.29063100	-2.95108500	0.98324100
H	4.21032500	-2.97749100	2.84960000
H	6.08096800	-2.87683500	-1.01926500
H	6.26431200	-3.05807500	1.45206700
C	-2.16822600	4.79306700	-0.14843100
H	-2.57934700	4.83094600	0.86698700
H	-2.24063700	5.80033400	-0.56743800
H	-2.80682600	4.12728100	-0.73590500
C	-1.85774700	1.37118200	1.29502800

C	-3.33205600	1.00615800	1.28956100
C	-3.72342300	-0.30910000	1.53597700
C	-4.31454100	1.97700600	1.08688700
C	-5.07242500	-0.64869400	1.59316800
H	-2.96823000	-1.08179900	1.66173800
C	-5.66491200	1.64013000	1.13247100
H	-4.02781900	3.00567300	0.89221200
C	-6.04764700	0.32502300	1.39049900
H	-5.35938100	-1.67797000	1.78373200
H	-6.41826600	2.40611500	0.97267100
H	-7.10037300	0.06122700	1.43106100
C	-1.61994600	1.21693200	-1.13240500
O	-1.91698800	0.00305800	-1.03597700
C	-1.27097300	2.10071900	-4.87329300
H	-2.13532700	1.93940200	-5.52961500
H	-0.38664600	1.77783700	-5.43717600
H	-1.18395200	3.17043500	-4.66686500
C	-1.50265400	-0.20932200	-3.83749700
H	-0.63597300	-0.70800100	-3.38393800
H	-1.51463800	-0.44917700	-4.90450500
H	-2.39115300	-0.62711500	-3.35820700
C	-1.51787700	2.28432500	2.47155600
H	-1.81963500	1.77703400	3.39192200
H	-0.44734000	2.49624800	2.53730000
H	-2.06250900	3.23134200	2.41904500
H	-1.29431400	0.43633400	1.42080700

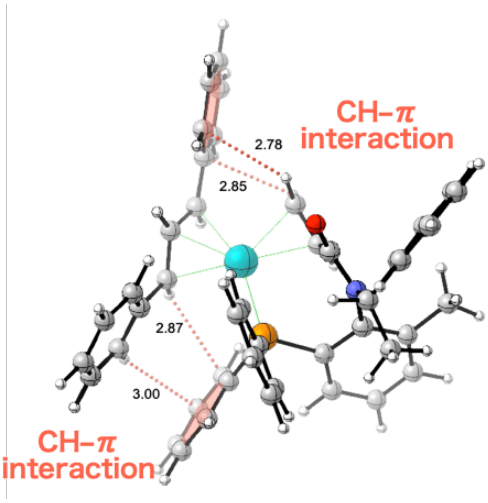


4e-Olefin-M

at wb97xd/6-31+G* & SDD (for Pd)
Energy = -2338.010142 A.U.
Thermal correction to Gibbs Free Energy = 0.670095 A.U.
Sum of electronic and thermal Free Energies = -2337.340047 A.U.
at wb97xd/def2-TZVPP/smd(MeCN) Energy = -2338.804468 A.U.

C	2.20650100	2.71243900	-1.15966200
C	2.98070400	1.54113200	-1.06752000
H	1.54364300	2.80278300	-2.02188700
H	3.85417000	1.52310900	-0.42137900
C	2.51062600	0.35046800	-1.65564400
H	1.81055300	0.46584400	-2.48522500
C	2.56506700	3.98747500	-0.51280000
C	3.33346400	4.04336600	0.65882000
C	2.10563400	5.18242200	-1.07854300
C	3.65042900	5.26720400	1.23555100
H	3.66936800	3.12687000	1.13802900
C	2.42429100	6.40901300	-0.50122900
H	1.50250200	5.15298400	-1.98312600
C	3.19829500	6.45405200	0.65568000
H	4.24664200	5.29797600	2.14249100
H	2.06765200	7.32803100	-0.95589200
H	3.44646000	7.40907500	1.10832300
Pd	1.03597300	1.07382000	-0.13870400
P	0.31091800	-1.11569700	0.48119700
C	-0.80139200	1.80554100	0.93738700
C	-0.89544600	-1.20638100	1.87662800
H	-0.71573200	1.49969600	1.97562000
C	-0.15499500	2.93144100	0.49952800
C	-2.11774500	-0.49994300	1.82663900
C	-0.56013500	-1.90193900	3.04061500
N	-2.54374300	0.11993600	0.60004800
H	-0.44233200	3.38494900	-0.44546600
C	-2.94036800	-0.41643800	2.95928600
C	-1.40937000	-1.88383100	4.14265300
H	0.36426200	-2.46537500	3.09597200
C	-2.57250600	-1.12984900	4.10501300
H	-1.14750700	-2.44297900	5.03554700
H	-3.21376200	-1.08509000	4.98093100
C	-0.47824600	-2.05613500	-0.86277800
C	-0.64038400	-1.46690000	-2.11927300
C	-0.99163000	-3.33909500	-0.63459500
C	-1.28024800	-2.15923300	-3.14475000
H	-0.31070000	-0.44636100	-2.28842500
C	-1.62343200	-4.03357200	-1.66087000
H	-0.91554400	-3.79059600	0.35176100
C	-1.76444700	-3.44553000	-2.91833400
H	-1.41508800	-1.68555800	-4.11240600
H	-2.01800800	-5.02806500	-1.47593900
H	-2.26499600	-3.98584000	-3.71628800
C	1.73985500	-2.06800000	1.09784900
C	2.55580200	-1.43268500	2.04508700
C	2.04165200	-3.37030400	0.69988300
C	3.62943300	-2.10577600	2.61613100
H	2.33778000	-0.41118300	2.35171000
C	3.12507200	-4.03971500	1.26715700
H	1.45139100	-3.86664900	-0.06270800
C	3.91116000	-3.41689200	2.23165800
H	4.24486700	-1.60948900	3.36065700
H	3.35448000	-5.05143300	0.94654100
H	4.74843700	-3.94625000	2.67660400
C	3.23038000	-0.93329400	-1.65814600
C	4.34374800	-1.18317100	-0.84392400

C	2.81657500	-1.92440900	-2.55745100
C	5.03660800	-2.38150000	-0.94863200
H	4.67779200	-0.44566800	-0.12064500
C	3.50569400	-3.12917100	-2.65626000
H	1.95418100	-1.74662700	-3.19445300
C	4.62267100	-3.35666300	-1.85689300
H	5.90081400	-2.55879600	-0.31614300
H	3.17671700	-3.88205900	-3.36604300
H	5.17100700	-4.29038500	-1.93879400
C	-4.17126500	0.45052800	2.98809500
H	-4.67890200	0.36171100	3.95197300
H	-3.90214700	1.50353100	2.84791800
H	-4.88867700	0.19839500	2.20364100
C	-3.51872500	-0.56743000	-0.29247600
H	-2.95931700	-0.82176900	-1.19920800
C	-1.84747700	1.16751400	0.05839300
O	-2.03010000	1.56251100	-1.08587400
C	-4.68206600	0.31636600	-0.73413000
C	-5.46525300	-0.14270300	-1.79818800
C	-5.01174400	1.53624400	-0.14778500
C	-6.56529200	0.58243500	-2.24509600
H	-5.20747800	-1.07671700	-2.29405700
C	-6.11283800	2.26730300	-0.59107700
H	-4.39799800	1.94180500	0.64866500
C	-6.89845400	1.79143400	-1.63649400
H	-7.15932300	0.20559900	-3.07265100
H	-6.34954300	3.21741400	-0.12063300
H	-7.75564900	2.36133900	-1.98207900
C	-4.03124000	-1.87540100	0.31916300
H	-3.21295300	-2.52929200	0.62861600
H	-4.68952800	-1.70530100	1.17482100
H	-4.61066300	-2.40585300	-0.44018200
H	0.46783800	3.51381000	1.17091400



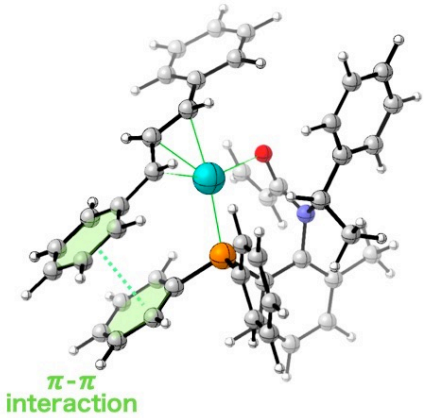
4e-Olefin-W

at wb97xd/6-31+G* & SDD (for Pd)
Energy = -2338.010115 A.U.

Thermal correction to Gibbs Free Energy = 0.669877 A.U.
Sum of electronic and thermal Free Energies = -2337.340238 A.U.
at wb97xd/def2-TZVPP/smd(MeCN) Energy = -2338.80458335 A.U.

C	-2.50716100	2.90256600	-0.51395200
C	-2.82848200	2.02154000	0.52471000
H	-2.89444100	2.66710500	-1.50730700
H	-2.68387100	2.33613100	1.55536600
C	-3.15090500	0.67211000	0.24753700
H	-3.60349200	0.45830300	-0.72252800
C	-2.09677700	4.30261400	-0.32278600
C	-1.48643800	4.75356200	0.85675400
C	-2.31936900	5.21412300	-1.36219000
C	-1.12871800	6.08834900	0.99719300
H	-1.26224900	4.05670900	1.66048500
C	-1.96367400	6.55267600	-1.21982900
H	-2.78745200	4.87635600	-2.28421400
C	-1.36923200	6.99215700	-0.03948000
H	-0.65305300	6.42488000	1.91315500
H	-2.15114700	7.25058000	-2.02992700
H	-1.08764200	8.03455200	0.07287000
Pd	-1.11481000	1.06539400	-0.50150700
P	-0.49768200	-1.24903200	-0.52395200
C	0.94084900	1.44799300	-1.36950700
C	0.80759000	-1.69327600	-1.75266100
H	0.95965500	0.99584700	-2.35698500
C	0.36066300	2.67435400	-1.18643900
C	2.08078200	-1.08203100	-1.71089800
C	0.50463100	-2.55750500	-2.80748800
N	2.46450900	-0.28995500	-0.57347100
H	0.54915000	3.23540700	-0.27468000
C	2.99251600	-1.25917000	-2.76184200
C	1.43570300	-2.79740800	-3.81329400
H	-0.45724300	-3.05511400	-2.85137200
C	2.65394400	-2.13505500	-3.79848100
H	1.19633500	-3.48614400	-4.61756600
H	3.36236900	-2.29230600	-4.60711100
C	0.12452100	-1.86434700	1.06900000
C	0.17146400	-1.00218500	2.16606100
C	0.62135000	-3.16810800	1.19372500
C	0.68801700	-1.44074500	3.38256600
H	-0.15295600	0.02780200	2.05924800
C	1.13278100	-3.60700700	2.40990700
H	0.62731200	-3.83567300	0.33524700
C	1.16324600	-2.74370300	3.50634200
H	0.73559600	-0.75789800	4.22520100
H	1.51914500	-4.61776300	2.49965600
H	1.56997400	-3.08588900	4.45334000
C	-1.92212100	-2.28295000	-1.01324400
C	-2.66494900	-1.86433000	-2.12669000
C	-2.30732000	-3.43858300	-0.33351000
C	-3.75745400	-2.60261200	-2.56681800

H	-2.37860400	-0.96036400	-2.66153500
C	-3.40549700	-4.17726700	-0.77430000
H	-1.77735200	-3.75976600	0.55653800
C	-4.12828700	-3.76612800	-1.88969900
H	-4.31872400	-2.27329700	-3.43618600
H	-3.69839200	-5.07235800	-0.23390500
H	-4.98157400	-4.34473500	-2.23051800
C	-3.49771100	-0.29646000	1.30699800
C	-3.00087000	-0.19600100	2.61389100
C	-4.38944300	-1.33112300	1.00478200
C	-3.38308400	-1.10830500	3.58844200
H	-2.30001900	0.59162800	2.87625500
C	-4.78105900	-2.24038800	1.98262700
H	-4.77800400	-1.42798700	-0.00605200
C	-4.27644700	-2.13412100	3.27574500
H	-2.98342100	-1.02137200	4.59421300
H	-5.47787300	-3.03391500	1.73013200
H	-4.57753100	-2.84445000	4.03976700
C	4.28958300	-0.49668500	-2.82746500
H	4.86296600	-0.79262600	-3.70968900
H	4.09724900	0.57996600	-2.89970600
H	4.91972600	-0.64837700	-1.94812300
C	3.30192000	-0.88102200	0.50763600
H	2.64787700	-0.95476800	1.38280400
C	1.82046000	0.88361300	-0.28256800
O	1.93141100	1.45207900	0.79460100
C	4.48124500	-0.00570000	0.92049800
C	5.10549100	-0.30871400	2.13469600
C	4.97685600	1.05606600	0.16717100
C	6.21310100	0.41103200	2.57137900
H	4.71465800	-1.11358300	2.75467700
C	6.08567500	1.78171900	0.60018300
H	4.48765500	1.34490500	-0.75644300
C	6.71297200	1.45888700	1.79977100
H	6.68253700	0.15721400	3.51742900
H	6.45329400	2.60815200	-0.00141200
H	7.57651500	2.02438200	2.13673900
C	3.77659000	-2.29600400	0.16080400
H	2.94866400	-2.94667900	-0.12922100
H	4.52438800	-2.30168400	-0.63603100
H	4.24210300	-2.72713800	1.05045800
H	-0.09018100	3.20582300	-2.01862200

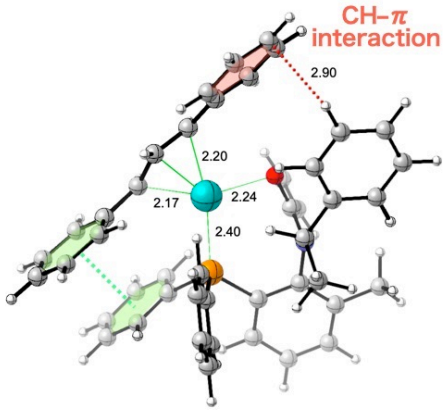


4e-O-M

at wb97xd/6-31+G* & SDD (for Pd)
Energy = -2338.006574 A.U.
Thermal correction to Gibbs Free Energy = 0.664797 A.U.
Sum of electronic and thermal Free Energies = -2337.341777 A.U.
at wb97xd/def2-TZVPP/smd(MeCN) Energy = -2338.79416412 A.U.

C	-1.16145700	-2.94704000	0.87305300
C	0.19947100	-3.19662200	0.64615600
H	-1.44680200	-2.54228900	1.84681800
H	0.51689100	-3.80965100	-0.19283900
C	1.14965200	-2.39145000	1.33309200
H	0.86655500	-2.07282000	2.33872600
C	-2.28122100	-3.43449300	0.05407600
C	-2.11117600	-4.30267900	-1.03346900
C	-3.56537700	-2.95584500	0.34573200
C	-3.20316800	-4.68650000	-1.80387700
H	-1.12958500	-4.69816900	-1.27899300
C	-4.65544900	-3.33383400	-0.42965000
H	-3.70372900	-2.25484200	1.16509200
C	-4.47728400	-4.20089800	-1.50605200
H	-3.06202400	-5.37078400	-2.63520500
H	-5.64243500	-2.94680600	-0.19566100
H	-5.32784000	-4.50210200	-2.11023900
Pd	-0.15958400	-1.09603600	0.21133600
P	1.26882900	0.79012600	-0.18195000
C	-1.82728700	0.52173200	-2.70919800
C	0.71076400	2.22743800	-1.21900200
H	-1.64040000	1.42672800	-3.27775800
C	-2.04849000	-0.64852100	-3.31260500
C	-0.63466400	2.62997300	-1.26965300
C	1.65777900	2.98347200	-1.91729300
N	-1.62090100	1.80053900	-0.62808200
C	-1.04198300	3.76900800	-1.97408600
C	1.27185300	4.12203300	-2.61644900
H	2.69982900	2.67834000	-1.92876700

C	-0.06267800	4.51222700	-2.63709900
H	2.01541600	4.70147700	-3.15506500
H	-0.35590000	5.39751900	-3.19465600
C	1.76806600	1.62048200	1.37363700
C	1.35538000	1.08211500	2.59584300
C	2.51587100	2.80489600	1.37471900
C	1.68620500	1.70471200	3.79713000
H	0.75502200	0.17706300	2.60949600
C	2.85187500	3.42565500	2.57372000
H	2.83416500	3.25404400	0.43877400
C	2.43735100	2.87712200	3.78730200
H	1.35172800	1.27736400	4.73784000
H	3.43272800	4.34290300	2.56017800
H	2.69442900	3.36723600	4.72143800
C	2.79939500	0.29340900	-1.03882500
C	2.65240800	-0.29658900	-2.30159600
C	4.07526000	0.47494600	-0.50633600
C	3.77266500	-0.66925800	-3.03476500
H	1.65864400	-0.45146300	-2.71841100
C	5.19651400	0.09394400	-1.24277600
H	4.20506100	0.90415300	0.48203800
C	5.04896300	-0.46809200	-2.50688300
H	3.65195700	-1.11446300	-4.01795800
H	6.18674600	0.23500700	-0.82024500
H	5.92533700	-0.75689500	-3.07956200
C	2.60793600	-2.45360700	1.12140600
C	3.18120300	-2.96780300	-0.04956900
C	3.45151800	-2.00249300	2.14341800
C	4.56044500	-3.06995200	-0.17166800
H	2.55187300	-3.28223300	-0.87742500
C	4.83486800	-2.09739900	2.01824000
H	3.02079100	-1.58772000	3.05200700
C	5.39150100	-2.64256700	0.86457900
H	4.99070000	-3.47513300	-1.08226500
H	5.47483200	-1.75597500	2.82632500
H	6.46966200	-2.72809300	0.76695700
C	-2.49501900	4.15681900	-2.05817900
H	-2.88384300	4.47281400	-1.08458600
H	-2.63458000	4.98554600	-2.75699800
H	-3.11297400	3.31805800	-2.39617400
C	-1.81277500	1.88859900	0.84137800
C	-3.21515900	1.47183100	1.24302700
C	-3.38439400	0.61879300	2.33366700
C	-4.34193700	1.95541900	0.57924100
C	-4.65857600	0.24959400	2.75667500
H	-2.50845400	0.23275500	2.85292700
C	-5.61877100	1.58121000	0.99263500
H	-4.22467500	2.61722000	-0.27443800
C	-5.78110200	0.72755000	2.08216600
H	-4.77636500	-0.41280300	3.60981900
H	-6.48894100	1.95985800	0.46433200
H	-6.77664900	0.43944600	2.40632300
C	-1.86575000	0.60063800	-1.22892700
O	-2.13680100	-0.40987800	-0.54894800
C	-1.47281300	3.27960900	1.37424300
H	-1.60717100	3.26906200	2.45929300
H	-0.43659500	3.56052300	1.16496400
H	-2.14059900	4.04209400	0.96331400
H	-1.11981400	1.17429700	1.30968600
H	-2.05648300	-0.72802200	-4.39515900
H	-2.23984200	-1.54774700	-2.73103700

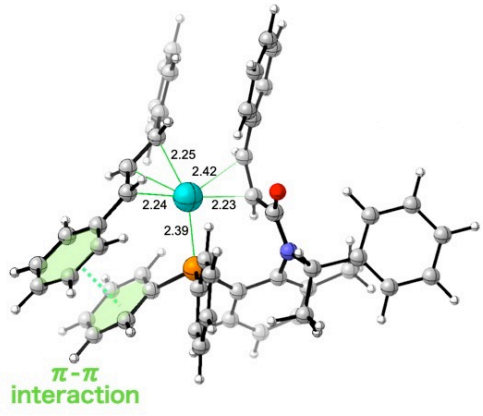


4e-O-W

at wb97xd/6-31+G* & SDD (for Pd)
Energy = -2338.00609 A.U.
Thermal correction to Gibbs Free Energy = 0.666049 A.U.
Sum of electronic and thermal Free Energies = -2337.340041 A.U.
at wb97xd/def2-TZVPP/smd(MeCN) Energy = -2338.79484193 A.U.

C	-0.99098300	-2.98188000	-1.20166400
C	0.16596300	-3.21279700	-0.44177700
H	-0.86798500	-2.84315800	-2.27802200
H	0.10023500	-3.61658500	0.56535000
C	1.38926400	-2.64438400	-0.88108600
H	1.52445900	-2.54262600	-1.96079700
C	-2.36987500	-3.25389000	-0.76367500
C	-2.67539000	-3.83323700	0.47633000
C	-3.42020700	-2.90996900	-1.62414100
C	-3.99612700	-4.08150500	0.83158400
H	-1.88577400	-4.11796100	1.16593900
C	-4.74170200	-3.14783600	-1.26432900
H	-3.19621300	-2.43918300	-2.57743100
C	-5.03221600	-3.74171900	-0.03853400
H	-4.21776100	-4.54842100	1.78676300
H	-5.54419200	-2.87061000	-1.94064900
H	-6.06311500	-3.93925500	0.24021400
Pd	-0.06717100	-1.05587500	-0.67333300
P	1.34814000	0.76301300	-0.01547700
C	-1.33880800	1.71322300	-2.80095800
C	0.93664300	2.52575500	-0.42467100
H	-1.14204500	2.77493000	-2.90652500
C	-1.36818000	0.90865400	-3.86445200

C	-0.39360600	2.98063400	-0.48291100
C	1.96886000	3.45185900	-0.59921500
N	-1.45444100	2.01087000	-0.38048700
C	-0.70089200	4.33012900	-0.69446400
C	1.67955100	4.79716600	-0.80259400
H	3.00418000	3.12516100	-0.58648000
C	0.35930600	5.22836400	-0.84399600
H	2.48845800	5.50850900	-0.93830000
H	0.14157900	6.27908400	-1.01514400
C	1.49423800	0.83599700	1.80981100
C	0.84140300	-0.12638500	2.58483000
C	2.19263100	1.86507200	2.45362500
C	0.88895200	-0.07226800	3.97542400
H	0.27415200	-0.91537200	2.09602800
C	2.24753400	1.91712000	3.84297100
H	2.68795500	2.63851400	1.87359400
C	1.59493500	0.94909300	4.60625900
H	0.36884500	-0.82220400	4.56408500
H	2.79260700	2.71972000	4.33043700
H	1.63110200	0.99684100	5.69042300
C	3.03843500	0.59548300	-0.67998100
C	3.16569400	0.53521600	-2.07413000
C	4.17814600	0.51390400	0.11965200
C	4.42176500	0.42490400	-2.65951700
H	2.27953900	0.58762300	-2.70457700
C	5.43631100	0.39926700	-0.47098500
H	4.09580800	0.52393500	1.20169700
C	5.56155200	0.36181000	-1.85605800
H	4.51331900	0.39006600	-3.74113900
H	6.31814100	0.33156400	0.15894200
H	6.54345200	0.27680900	-2.31209000
C	2.65477600	-2.73171400	-0.12598500
C	2.69734100	-2.75786600	1.27380700
C	3.85555300	-2.81340400	-0.83905300
C	3.91020200	-2.86979900	1.94241600
H	1.78086700	-2.67584700	1.85009500
C	5.06946400	-2.94120900	-0.17131900
H	3.83986600	-2.77826700	-1.92539400
C	5.10036300	-2.96835500	1.22058600
H	3.92741800	-2.88268600	3.02816400
H	5.99162100	-3.01081000	-0.74004700
H	6.04729500	-3.06369500	1.74353600
C	-2.12493100	4.80857100	-0.79978900
H	-2.59559900	4.87469800	0.18757400
H	-2.16517700	5.80414000	-1.24942000
H	-2.73390700	4.13228400	-1.40717100
C	-1.89866400	1.51683200	0.95040200
C	-3.36745400	1.13464600	0.93502800
C	-3.75407100	-0.13903400	1.35047200
C	-4.34959100	2.05501500	0.56638300
C	-5.10109800	-0.48400500	1.41476900
H	-2.99655600	-0.87640900	1.60846800
C	-5.69770400	1.70891400	0.61501700
H	-4.06420100	3.04984800	0.23770100
C	-6.07712000	0.43875200	1.04537300
H	-5.38538000	-1.47914400	1.74161900
H	-6.45217800	2.43397300	0.32385800
H	-7.12838100	0.16996300	1.09083500
C	-1.60010600	1.17242100	-1.44361100
O	-1.95405800	-0.01485200	-1.28198200
C	-1.60180600	2.52865300	2.05520000
H	-1.92257300	2.09394400	3.00571700
H	-0.53603000	2.76010400	2.13178300
H	-2.15822800	3.45902000	1.91013300
H	-1.32992500	0.60265700	1.16737500
H	-1.20699600	1.29311000	-4.86657700
H	-1.56748800	-0.15369200	-3.75206800

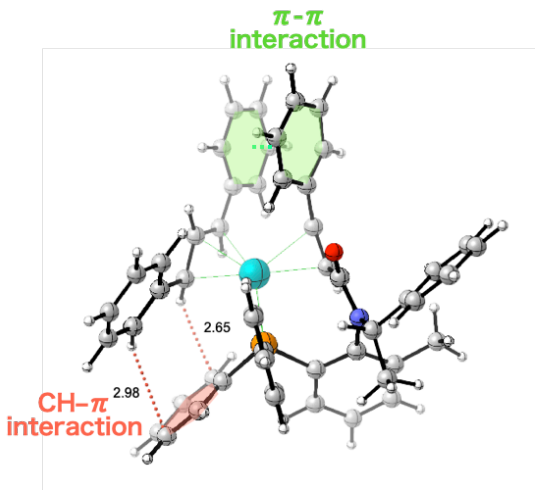


4f-Olefin-M

at wb97xd/6-31+G* & SDD (for Pd)
Energy = -2568.991937 A.U.
Thermal correction to Gibbs Free Energy = 0.746691 A.U.
Sum of electronic and thermal Free Energies = -2568.245246 A.U.
at wb97xd/def2-TZVPP/smd(MeCN) Energy = -2569.86149121 A.U.

C	2.25689100	2.53602600	-0.70128300
C	3.06154600	1.38358100	-0.67788700
H	1.70268900	2.75556400	-1.61435700
H	3.83662600	1.29640600	0.07861900
C	2.73629900	0.27543100	-1.48232200
H	2.10880300	0.46815800	-2.35519900
C	2.48108700	3.67752100	0.19902000
C	2.93307200	3.50561700	1.51557100
C	2.24192000	4.97176900	-0.27256400
C	3.15705000	4.60568100	2.33158600
H	3.08680800	2.50312700	1.90901000
C	2.47647000	6.07425100	0.54311900
H	1.86330700	5.11417000	-1.28121900
C	2.93420900	5.89444700	1.84423200
H	3.50264100	4.46188300	3.35049500
H	2.29065600	7.07316900	0.16186000
H	3.11206600	6.75383900	2.48289400

Pd	1.03175500	0.72129100	-0.08864400
P	0.49758300	-1.57452400	0.37990600
C	-1.00072700	1.22538900	0.75422700
C	-0.80775600	-1.84178400	1.65998800
H	-0.91557300	0.81710800	1.75668800
C	-0.55266400	2.52364300	0.61853600
C	-2.08047800	-1.22966000	1.54851100
C	-0.49023500	-2.53845000	2.82544500
N	-2.48375500	-0.64426000	0.30028800
C	-2.95914800	-1.21473400	2.63942600
C	-1.40030200	-2.60782800	3.87642700
H	0.47181300	-3.02736900	2.92570600
C	-2.60167000	-1.92609500	3.79130800
H	-1.14979600	-3.16760400	4.77171500
H	-3.28690800	-1.93101100	4.63446300
C	0.02084100	-2.60531700	-1.03865800
C	-0.31656700	-1.97120300	-2.23692100
C	-0.10739000	-3.99625200	-0.93511000
C	-0.75129900	-2.71944400	-3.32788400
H	-0.27246900	-0.88778000	-2.30814500
C	-0.51826600	-4.74322800	-2.03301700
H	0.08077500	-4.49470800	0.01131200
C	-0.83863900	-4.10525200	-3.23049600
H	-1.02620200	-2.21783200	-4.25026100
H	-0.61002100	-5.82129300	-1.94819600
H	-1.17259800	-4.68906300	-4.08244500
C	2.00483800	-2.26719400	1.14606100
C	2.57744400	-1.50336100	2.17492800
C	2.61752000	-3.46092600	0.76792200
C	3.71759200	-1.94448600	2.83324400
H	2.11457100	-0.56490700	2.47388800
C	3.76127400	-3.90147800	1.43102700
H	2.23590500	-4.04057600	-0.06357200
C	4.30838700	-3.15302900	2.46606900
H	4.14298300	-1.34953000	3.63545800
H	4.22981200	-4.83066900	1.12272400
H	5.19747400	-3.50264000	2.98140900
C	3.51415400	-0.96938800	-1.55966000
C	4.65089800	-1.20277100	-0.77406800
C	3.13701500	-1.93367500	-2.50335400
C	5.39581800	-2.36098500	-0.94386200
H	4.96919800	-0.48037100	-0.03002200
C	3.87262100	-3.10221700	-2.65942000
H	2.26109200	-1.76437700	-3.12258800
C	5.00956700	-3.31439700	-1.88470700
H	6.27962800	-2.52339300	-0.33565900
H	3.56591800	-3.83723700	-3.39660100
H	5.59719600	-4.21775000	-2.01567200
C	-4.24929100	-0.43715000	2.63512400
H	-5.10111800	-1.06866900	2.36708300
H	-4.43731000	-0.03081900	3.63336600
H	-4.22904400	0.38738400	1.91972000
C	-3.45815000	-1.36273700	-0.58724300
H	-3.08631500	-1.16319000	-1.59588800
C	-1.88959200	0.48589500	-0.19671000
O	-2.06361300	0.85750800	-1.35364600
C	-4.87105700	-0.77973900	-0.49510500
C	-5.10266400	0.55675700	-0.84368300
C	-5.96043200	-1.55134400	-0.08386300
C	-6.37473900	1.10976700	-0.74385800
H	-4.28223600	1.16544800	-1.20626200
C	-7.23686700	-1.00048900	0.01010900
H	-5.82963700	-2.59564000	0.17881000
C	-7.44805800	0.33547300	-0.31049300
H	-6.52884600	2.14959800	-1.01655600
H	-8.06591700	-1.62181000	0.33537800
H	-8.44138600	0.76698700	-0.23518900
C	-3.40898400	-2.86734900	-0.35449400
H	-2.39734000	-3.24567500	-0.48686800
H	-3.75001400	-3.15110400	0.64559000
H	-4.04941400	-3.36177700	-1.08965500
H	-0.06692200	2.89809000	1.51977900
C	-0.79990200	3.60268400	-0.35515200
C	-0.91868600	3.45445600	-1.74452400
C	-0.87416800	4.89276400	0.19079100
C	-1.11719900	4.56703500	-2.55232400
H	-0.86768300	2.46614400	-2.18027900
C	-1.10795900	6.00015700	-0.61590200
H	-0.74419200	5.03082800	1.26083300
C	-1.22322200	5.84022100	-1.99295500
H	-1.20139600	4.43786900	-3.62686600
H	-1.17906800	6.98681000	-0.16951700
H	-1.39027600	6.70283500	-2.63051400

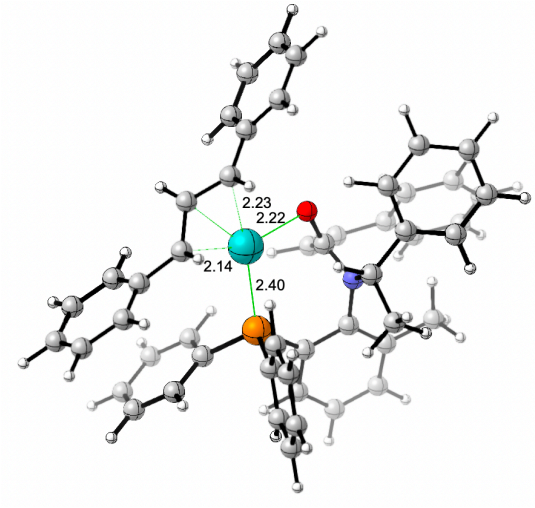


4f-Olefin-W

at wb97xd/6-31+G* & SDD (for Pd)
Energy = -2568.993711 A.U.
Thermal correction to Gibbs Free Energy = 0.745982 A.U.
Sum of electronic and thermal Free Energies = -2568.247729 A.U.
at wb97xd/def2-TZVPP/smd(MeCN) Energy =

-2569.86194255 A.U.

C	3.58250800	0.60479900	-0.80064000
C	3.15745400	1.20775700	0.37947900
H	3.37688100	1.12851500	-1.73632700
H	3.45283900	0.78114000	1.33445000
C	2.19037600	2.25279400	0.34849200
H	2.19758300	2.90719600	-0.52339700
C	4.55245500	-0.48708500	-0.90680200
C	5.21620300	-1.02372100	0.20560300
C	4.85048700	-0.99218700	-2.18139100
C	6.15848500	-2.03070700	0.04235500
H	5.00679100	-0.65981500	1.20613700
C	5.78375300	-2.00994200	-2.34265800
H	4.35021400	-0.57557900	-3.05346600
C	6.44303300	-2.52818900	-1.22876000
H	6.66746000	-2.43421700	0.91188800
H	6.00680500	-2.38862100	-3.33543500
H	7.18082800	-3.31534400	-1.35157200
Pd	1.23521900	0.48433200	-0.44360600
P	-0.92111600	1.51433900	-0.55059400
C	0.23387000	-1.39990600	-1.16635900
C	-1.95699400	0.81834100	-1.91130100
H	-0.02677000	-1.16548800	-2.19570500
C	1.53961400	-1.79780300	-0.95405900
C	-2.32827000	-0.54527800	-1.91040000
C	-2.26596100	1.60475300	-3.02336800
N	-2.15739300	-1.34218900	-0.72690800
C	-2.90152000	-1.12794600	-3.05018100
C	-2.90641500	1.04817300	-4.12634900
H	-2.01583100	2.65933400	-3.03628100
C	-3.19422800	-0.30831500	-4.14519000
H	-3.15921800	1.67386900	-4.97675300
H	-3.65579100	-0.74906000	-5.02454200
C	-1.94895000	1.42017200	0.94386400
C	-1.41919600	0.86749500	2.11012000
C	-3.28222500	1.85067200	0.92528100
C	-2.20714400	0.75346500	3.25271500
H	-0.40057600	0.49673300	2.11911400
C	-4.06785300	1.73745600	2.06625500
H	-3.71098600	2.26079600	0.01392400
C	-3.52924100	1.18865600	3.23172800
H	-1.79070600	0.30952700	4.15143000
H	-5.10204700	2.06766800	2.04484100
H	-4.14613800	1.09424300	4.12047600
C	-0.76278000	3.28825800	-0.96916200
C	0.11964600	3.64036600	-2.00072200
C	-1.43783500	4.29785200	-0.28106900
C	0.31106500	4.97285600	-2.34753200
H	0.65722300	2.86358800	-2.54186900
C	-1.24549800	5.63504000	-0.62908400
H	-2.09659100	4.05718500	0.54597700
C	-0.37458800	5.97573900	-1.65930600
H	0.99332800	5.23024300	-3.15220300
H	-1.77441600	6.41050400	-0.08319000
H	-0.22509300	7.01767700	-1.92567100
C	1.68434500	2.88492100	1.58433700
C	1.61449700	2.19515900	2.80343100
C	1.26706700	4.21965800	1.54171900
C	1.13613700	2.82339200	3.94575000
H	1.91615500	1.15161700	2.86116100
C	0.78382600	4.84907300	2.68537100
H	1.32374600	4.76981200	0.60577000
C	0.71476700	4.15276900	3.88926400
H	1.08524400	2.27547400	4.88196000
H	0.46469000	5.88579500	2.63441100
H	0.33806300	4.64225300	4.78221700
C	-3.16053700	-2.60879900	-3.13786200
H	-3.60629400	-2.86310200	-4.10299200
H	-2.22260700	-3.16792400	-3.04358300
H	-3.82609700	-2.97205200	-2.35118400
C	-3.30345200	-1.55503800	0.20011100
H	-3.05924100	-0.99685200	1.11044500
C	-0.91028800	-1.63361200	-0.22478300
O	-0.75751000	-2.05985500	0.90937600
C	-3.49009100	-3.00939600	0.62164700
C	-4.29827000	-3.25229100	1.73654500
C	-2.92230400	-4.09861400	-0.03530300
C	-4.55601100	-4.54990600	2.16716000
H	-4.72485800	-2.41390000	2.28442700
C	-3.17548500	-5.40096800	0.39231400
H	-2.25288200	-3.94013300	-0.87351900
C	-3.99836400	-5.63349400	1.49034700
H	-5.18755100	-4.71466600	3.03543100
H	-2.71787800	-6.23539900	-0.13159600
H	-4.19500400	-6.64813100	1.82344600
C	-4.61318000	-0.99005700	-0.35926200
H	-4.51404000	0.05356600	-0.66579800
H	-4.98822800	-1.56960400	-1.20650600
H	-5.36848700	-1.03559600	0.42918100
H	2.15519200	-1.79218000	-1.85387400
C	2.18742000	-2.50410100	0.17317900
C	2.04685600	-2.15498300	1.52249700
C	3.04023400	-3.56104900	-0.16477000
C	2.73642700	-2.85448900	2.50490700
H	1.38068200	-1.34624000	1.80181100
C	3.70383200	-4.28404600	0.82160400
H	3.18704600	-3.82041100	-1.21046300
C	3.55866000	-3.92807300	2.15933300
H	2.61621600	-2.57565600	3.54772700
H	4.34780600	-5.11206900	0.54132800
H	4.08303400	-4.48261100	2.93194600

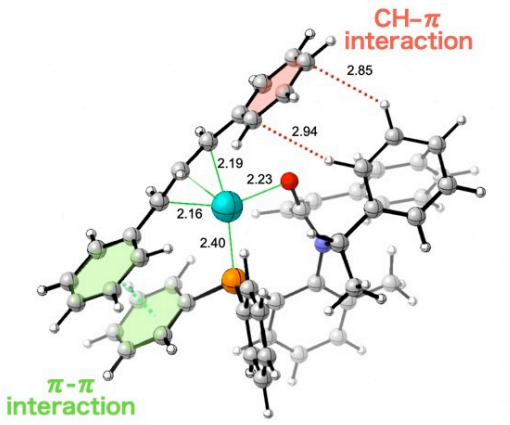


4f-O-M

at wb97xd/6-31+G* & SDD (for Pd)
Energy = -2568.987908 A.U.
Thermal correction to Gibbs Free Energy = 0.742683 A.U.
Sum of electronic and thermal Free Energies = -2568.245225 A.U.
at wb97xd/def2-TZVPP/smd(MeCN) Energy = -2569.8559255 A.U.

C	1.47403800	-0.55809500	-2.15334100
C	-0.42223900	-2.42558900	-0.31258100
H	0.53288400	-0.38266900	-2.66925600
C	2.53181400	-0.98883400	-2.84959600
C	0.96716200	-2.36347400	-0.08414200
C	-0.97134500	-3.62827400	-0.76256600
N	1.53550000	-1.08287300	0.25240400
C	1.78702100	-3.48744400	-0.21885800
C	-0.16344000	-4.74865300	-0.93418100
H	-2.03099700	-3.69580200	-0.98945500
C	1.19270800	-4.67934200	-0.64588800
H	-0.59851800	-5.67793900	-1.28920300
H	1.81616500	-5.56108900	-0.77019700
C	1.45987500	-0.14231600	-0.72178700
O	1.31536900	1.07037800	-0.45442000
C	1.62019400	-0.63286200	1.67539400
H	0.81336200	0.10206700	1.81803900
H	2.36602700	-1.22690600	-3.89937000
C	3.90849600	-1.17031100	-2.36273600
C	4.68269500	-2.21150800	-2.89263500
C	4.47527700	-0.32547200	-1.39913100
C	5.97503200	-2.43845300	-2.43201400
H	4.26011700	-2.85620200	-3.65992000
C	5.77314400	-0.54660100	-0.94770300
H	3.91871100	0.52574000	-1.01633600
C	6.52103600	-1.60856700	-1.45236400
H	6.56073100	-3.25539600	-2.84317500
H	6.19801400	0.11895300	-0.20317100
H	7.53426200	-1.77750200	-1.09966800
C	-2.10134700	-1.45577900	1.79604400
C	-1.99542700	-0.50952400	2.81937200
C	-2.56541900	-2.74035300	2.10809000
C	-2.35135600	-0.83151700	4.12739700
H	-1.60776800	0.48097600	2.59961500
C	-2.92663700	-3.06191800	3.41212800
H	-2.64210300	-3.49899500	1.33522500
C	-2.81980000	-2.10814500	4.42486300
H	-2.25488300	-0.08733600	4.91235500
H	-3.28621200	-4.06080100	3.63980800
H	-3.09567100	-2.36379900	5.44341800
C	-2.97680300	-1.32945800	-1.00033500
C	-2.75168700	-1.25150600	-2.38103600
C	-4.25751500	-1.61977300	-0.52997500
C	-3.78523800	-1.49386000	-3.27755200
H	-1.75864700	-1.02074300	-2.76001200
C	-5.29376000	-1.85807100	-1.43191400
H	-4.45876700	-1.65727100	0.53565500
C	-5.05978000	-1.80448800	-2.80206300
H	-3.59694400	-1.44424400	-4.34593400
H	-6.28767000	-2.08102100	-1.05615900
H	-5.86860200	-1.99700700	-3.50065500
C	3.26061700	-3.45551400	0.08707600
H	3.65257000	-2.43818900	0.11554700
H	3.45547500	-3.92970800	1.05738200
H	3.82621200	-4.01075000	-0.66622400
C	1.36848100	-1.78590300	2.64430300
H	2.10438700	-2.58697900	2.54046100
H	1.43775000	-1.39470800	3.66298800
H	0.37464800	-2.21987100	2.51486500
C	2.93634700	0.08448300	1.94960400
C	2.98859700	1.48067000	1.92135700
C	4.10150800	-0.62067900	2.26266400
C	4.17638800	2.15767900	2.18382700
H	2.09619500	2.04265300	1.66520200
C	5.28909100	0.05259700	2.53729900
H	4.09485200	-1.70522900	2.30305400
C	5.33230800	1.44457000	2.49460700
H	4.19599800	3.24310800	2.14417900
H	6.18252200	-0.51383700	2.78393000
H	6.25906000	1.96956300	2.70731400
P	-1.55802700	-1.01294100	0.10202900
Pd	-0.83995900	1.27729000	0.04946500
C	-2.66564300	2.28500500	0.53997600
C	-1.79739000	3.21465200	-0.10829300
H	-2.61815900	2.27158000	1.63071300
C	-3.97920000	1.88361500	0.00115300
C	-0.54594300	3.44428200	0.47377200
H	-2.01511500	3.56798800	-1.11354700
C	-4.24749400	1.85034700	-1.37392600
C	-5.00409500	1.56160500	0.89808400
H	-0.47435600	3.32711000	1.55796800
C	0.58515700	4.14598400	-0.14633800

C	-5.52252200	1.55098300	-1.83487900
H	-3.45335200	2.04695200	-2.08975300
C	-6.28257700	1.25983900	0.43615000
H	-4.80384500	1.56802800	1.96724000
C	0.75580200	4.20922900	-1.53561200
C	1.54577400	4.73716700	0.68370000
C	-6.54641600	1.26504400	-0.93077400
H	-5.71815800	1.53078300	-2.90255400
H	-7.07257000	1.02977000	1.14485600
C	1.85032400	4.86866300	-2.07963900
H	0.04823700	3.71339000	-2.19479800
C	2.64088300	5.39983000	0.13899500
H	1.42816900	4.68636800	1.76418300
H	-7.54403200	1.03728400	-1.29437000
C	2.79451700	5.46706000	-1.24415000
H	1.97621800	4.90736000	-3.15730700
H	3.37270000	5.86486400	0.79279600
H	3.65093600	5.97922500	-1.67211100



4f-O-W

at wb97xd/6-31+G* & SDD (for Pd)
Energy = -2568.9906730000002 A.U.
Thermal correction to Gibbs Free Energy = 0.743561 A.U.
Sum of electronic and thermal Free Energies = -2568.247112 A.U.
at wb97xd/def2-TZVPP/smd(MeCN) Energy = -2569.85745278 A.U.

C	1.47911800	-1.12910400	-2.08884400
C	-0.38417400	-2.45391800	0.19410000
H	0.52254500	-1.13723900	-2.60712000
C	2.53798000	-1.71279200	-2.66077200
C	1.00574000	-2.31162400	0.39012000
C	-0.92342700	-3.73956300	0.12587200
N	1.55902700	-0.98017800	0.36385200
C	1.83827700	-3.41993200	0.56750800
C	-0.10333300	-4.85424400	0.28105500
H	-1.98515100	-3.87942400	-0.05270200
C	1.25500900	-4.69064000	0.51165900
H	-0.53072400	-5.85065200	0.22279600
H	1.88979300	-5.56416100	0.63658500
C	1.48035000	-0.33631600	-0.82348000
O	1.35158700	0.90826200	-0.88610300
C	1.67003200	-0.15815300	1.61067000
H	0.88100000	0.60339600	1.54643400
H	2.36302400	-2.23840900	-3.59845600
C	3.92460100	-1.72882600	-2.16852800
C	4.71470400	-2.86040800	-2.41298600
C	4.48350600	-0.64826400	-1.47321200
C	6.01609400	-2.93384800	-1.92848300
H	4.29770600	-3.69398500	-2.97349500
C	5.79039300	-0.71815300	-0.99968500
H	3.91262600	0.26324700	-1.31908900
C	6.55495000	-1.86316300	-1.21454800
H	6.61413600	-3.82091200	-2.11549700
H	6.20816400	0.12845700	-0.46454500
H	7.57482800	-1.91446900	-0.84472700
C	-1.93745300	-0.78660900	1.92161300
C	-1.80601000	0.47278300	2.51244500
C	-2.30792000	-1.87664500	2.71922900
C	-2.04752500	0.64786000	3.87281700
H	-1.49032600	1.32033000	1.90786000
C	-2.55764100	-1.70211600	4.07659400
H	-2.38732100	-2.87003000	2.28643500
C	-2.42654700	-0.43960800	4.65580400
H	-1.93130000	1.63022600	4.32105300
H	-2.84437100	-2.55415700	4.68543100
H	-2.61178600	-0.30752300	5.71754000
C	-3.01116000	-1.66144700	-0.66898000
C	-2.91910100	-1.91468300	-2.04394300
C	-4.21394400	-1.90581200	-0.00645200
C	-4.00480000	-2.43509800	-2.73855000
H	-1.98938100	-1.71626000	-2.57378500
C	-5.30297500	-2.42469100	-0.70629900
H	-4.31880400	-1.68063000	1.04975300
C	-5.19984200	-2.69679200	-2.06657300
H	-3.91955500	-2.63864600	-3.80191500
H	-6.23632100	-2.60717000	-0.18233100
H	-6.04890800	-3.10479800	-2.60683100
C	3.31688300	-3.29241700	0.81944400
H	3.70141300	-2.31258700	0.53441600
H	3.53614600	-3.45505500	1.88232500
H	3.87130400	-4.04663000	0.25405200
C	1.41341300	-0.99774200	2.85961500
H	2.13937300	-1.80602000	2.97672100
H	1.49558000	-0.34250600	3.73101900
H	0.41478800	-1.43789700	2.85962600
C	3.00431400	0.57752600	1.67473400
C	3.08399300	1.91885500	1.28880200
C	4.15707400	-0.04731200	2.16003800
C	4.28862500	2.61318600	1.37446500
H	2.20212300	2.42369700	0.90583400

C	5.36051500	0.64599300	2.25308200
H	4.12798900	-1.08314600	2.48136800
C	5.43162400	1.97967100	1.85668200
H	4.32685700	3.65369100	1.06670200
H	6.24267700	0.14188600	2.63732200
H	6.36927000	2.52313100	1.93061000
P	-1.52514600	-0.98897700	0.14955100
Pd	-0.86994900	1.12191100	-0.77372600
C	-2.77257000	1.90644900	-1.44523700
C	-1.96287300	2.99198000	-1.02352500
H	-2.67017400	1.59139000	-2.48683600
C	-4.07691300	1.57014800	-0.84137300
C	-0.69056500	3.13911000	-1.60144600
H	-2.23396300	3.54012700	-0.12459100
C	-4.35449500	1.78022400	0.51537900
C	-5.07830600	1.03868600	-1.66091000
H	-0.56581500	2.82435400	-2.63957300
C	0.39206000	3.98229800	-1.06915700
C	-5.60632400	1.47623600	1.03613800
H	-3.58550700	2.16794300	1.17663200
C	-6.33693500	0.74783400	-1.14396600
H	-4.87218500	0.85449300	-2.71223000
C	0.33216700	4.58355800	0.19674900
C	1.54938800	4.14799300	-1.84001000
C	-6.60422000	0.96525800	0.20525500
H	-5.80475400	1.63963400	2.09125100
H	-7.10569700	0.34337700	-1.79523000
C	1.39187400	5.35167100	0.66423400
H	-0.54157500	4.45540000	0.82970800
C	2.61184700	4.91337200	-1.37111700
H	1.61897500	3.66502100	-2.81104200
H	-7.58490400	0.73525600	0.61103200
C	2.53271500	5.52252900	-0.12065100
H	1.32985800	5.81724500	1.64317700
H	3.50098500	5.03393900	-1.98237300
H	3.35712300	6.12817600	0.24440000