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Supporting Information

Organocatalytic Enantioselective Synthesis of Csp^2–N Atropisomers via Formal Csp^2–O Bond Amination

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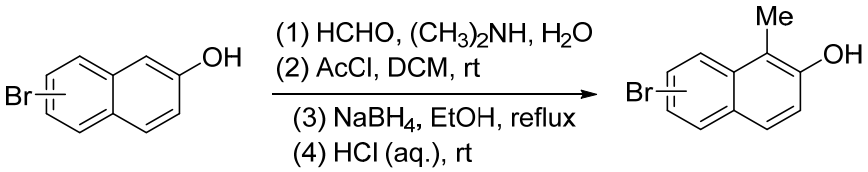
I. General Information

Flash column chromatography was performed over silica gel (200-300 mesh). All air or moisture sensitive reactions were conducted in oven-dried glassware under argon atmosphere using anhydrous solvents. Anhydrous dichloromethane, tetrahydrofuran and common solvents were purchased from Energy Chemical, China. Reagents were purchased at the highest commercial quality and used without further purification, unless otherwise stated. All heating was achieved by oil bath. All crystals were obtained by slowly volatilizing of saturated CD_2Cl_2 solution at room temperature. ^{1}H, ^{13}C, ^{19}F, and ^{31}P NMR spectra were collected on a Bruker AV 400 MHz or 500MHz NMR spectrometer using residue solvent peaks as an internal standard (^{1}H NMR: $CDCl_3$ at 7.26 ppm, CD_2Cl_2 at 5.32 ppm, DMSO-d_6 at 2.50 ppm, acetone-d_6 at 2.05 ppm, CD_3CN at 1.94 ppm; ^{13}C NMR: $CDCl_3$ at 77.16 ppm, CD_2Cl_2 at 53.84, DMSO-d_6 at 39.52 ppm, acetone-d_6 at 29.84 ppm, CD_3CN at 118.26 ppm). The enantiomeric excess values were determined by chiral HPLC using an Agilent 1200 LC instrument with Daicel CHIRALPAK® IA-3, IB, IC-3, IE-3, IF-3. The HRMS measurements were collected on Orbitrap, Thermo Scientific Q Exactive. The instrumentation type used for the crystal measurement was Bruker D8 VENTURE.

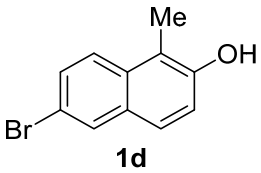
II. Substrate Preparation

The 1-methylnaphthalen-2-ol **1a** was commercially available.

General Procedure A.



The Br-substituted 1-methylnaphthalen-2-ols **1b,1d** were prepared using the previously reported procedures.[1] The procedure is described using **1d** as an example.



1d

6-Bromo-1-methylnaphthalen-2-ol (**1d**). To solution of 6-bromonaphthalen-2-ol (2.0 g, 1.0 equiv, 8.96 mmol) in EtOH (12 mL) was added 40% aqueous dimethylamine solution (2.48 mL, 2.2 equiv, 19.72 mmol) and 37% aqueous formaldehyde solution (1.32 mL, 2.0 equiv, 17.92 mmol) at room temperature. The resulting reaction mixture was stirred for 2 h and concentrated under vacuum to yield a dry-solid. The crude product was used in next step without further purification. Acetyl chloride (1.28 mL, 2.0 equiv, 17.92 mmol) was added to the solution of the above crude product in 50 mL of DCM at room temperature. The resulting reaction mixture was stirred for 2 h and the solvent was removed by vacuum. The residue was redissolved in ethanol (20 ml), cooled to 0 °C, and sodium borohydride (520 mg, 1.5 equiv, 13.66 mmol) was added portion wise.

The resulting reaction mixture was heated at reflux for 3 h then cooled to room

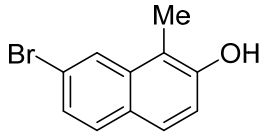
[1] Kusuma, B. R.; Khandelwal, A.; Gu, W.; Brown, D.; Liu, W.; Vielhauer, G.; Holzbeierlein, J.; Blagg, B. S. Synthesis and Biological Evaluation of Coumarin Replacements of Novobiocin as Hsp90 Inhibitors. *Bioorg. Med. Chem.* **2014**, 22, 1441-1449.

temperature, treated with 18 mL of water, and stirred for 30 min. After 30 min the reaction mixture was acidified with 3M HCl (10 mL), ethanol was removed, extracted with ethyl acetate (3 × 25 mL). The combined organic layers were washed with brine, dried over anhydrous sodium sulfate, filtered, and concentrated. The residue was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 5:1) to give **1d** (1.16 g, 55% yield) as a pale brown amorphous solid, mp 122.3-123.5 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.91 (d, *J* = 2.1 Hz, 1H), 7.77 (d, *J* = 9.1 Hz, 1H), 7.56 – 7.50 (m, 2H), 7.07 (d, *J* = 8.8 Hz, 1H), 4.95 (br, 1H), 2.51 (s, 3H) ppm.

^{13}C NMR (101 MHz, Chloroform-*d*) δ 150.9, 132.5, 130.5, 130.4, 129.6, 126.6, 125.2, 118.8, 117.1, 115.8, 10.6 ppm.

HRMS (CI-) Calcd for $C_{11}H_8BrO^-$ [M-H$^+$]: 234.9764, Found: 234.9761.



1b

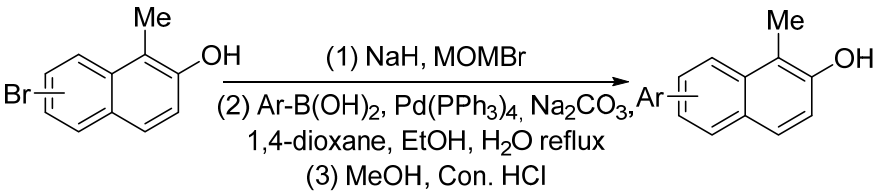
7-Bromo-1-methylnaphthalen-2-ol (**1b**) was prepared as a pale yellow amorphous solid from 7-bromonaphthalen-2-ol (2.0 g, 1.0 equiv, 8.96 mmol) according to the General Procedure A (eluent for flash column chromatography: petroleum ether/ethyl acetate = 5:1, 1.0 g, 47% yield), mp 150.0-151.1 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.06 (s, 1H), 7.60 (dd, *J* = 17.4, 8.7 Hz, 2H), 7.41 (d, *J* = 8.7 Hz, 1H), 7.06 (d, *J* = 8.8 Hz, 1H), 4.98 (br, 1H), 2.49 (s, 3H) ppm.

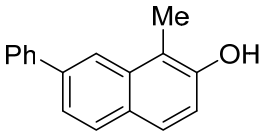
^{13}C NMR (101 MHz, Chloroform-*d*) δ 151.4, 135.3, 130.2, 127.7, 127.5, 126.6, 125.7, 121.0, 118.1, 114.8, 10.6 ppm.

HRMS (CI-) Calcd for $C_{11}H_8BrO^-$ [M-H$^+$]: 234.9764, Found: 234.9762.

General Procedure B.



The substituted 1-methylnaphthalen-2-ols **1c,1e-1h** were prepared using the following procedures. The procedure is described using **1c** as an example.



1c

1-Methyl-7-phenylnaphthalen-2-ol (**1c**). To solution of 7-bromo-1-methylnaphthalen-2-ol **1b** (0.2 g, 1.0 equiv, 0.85 mmol) in dry-THF (5 mL) was slowly added NaH (50 mg, 60% dispersion in mineral oil, 1.5 equiv, 1.3 mmol) at 0°C. The resulting reaction mixture was stirred for 1 h, then bromomethyl methyl ether (0.1 mL, 1.5 equiv, 1.3 mmol) was added slowly. The resulting reaction mixture was stirred for other 3 h then quenched by water (2 mL), extracted with ethyl acetate (3 × 3 mL). The combined organic layers were washed with brine, dried over anhydrous sodium sulfate, filtered, and concentrated. The crude product was used in next step without further purification.

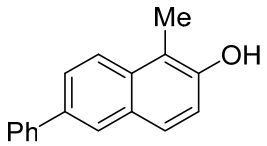
To a solution of the crude product from last step and phenylboronic acid (207 mg, 2.0 equiv, 1.7 mmol) in in a mixed solvent of 1,4-dioxane, EtOH, and H_2O (v/v/v = 4:1:1, 6 mL) were added $Pd(PPh_3)_4$ (49.1 mg, 5 mol%, 0.043 mmol) and Na_2CO_3 (450 mg, 5.0 equiv, 4.3 mmol). After degassing with Ar for 20 min, the mixture was heated to refluxed for 16 h. After cooling to room temperature, the mixture was filtered through celite. The residue was redissolved in MeOH (5 mL) and conc. HCl aq. (35%, 0.2 mL) was added. After stirring for 1 h at 50°C in an oil bath, the reaction mixture was extracted with ethyl acetate (3 × 3 mL). The combined organic layers were washed with brine, dried over anhydrous

sodium sulfate, filtered, and concentrated. The residue was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 5:1) to give **1c** (110 mg, 55% yield over three steps) as a yellow amorphous solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.10 (s, 1H), 7.85 (d, *J* = 8.4 Hz, 1H), 7.74 (d, *J* = 8.2 Hz, 2H), 7.66 (d, *J* = 8.7 Hz, 1H), 7.61 (d, *J* = 8.4 Hz, 1H), 7.51 (t, *J* = 7.6 Hz, 2H), 7.40 (t, *J* = 7.4 Hz, 1H), 7.08 (d, *J* = 8.7 Hz, 1H), 4.91 (br, 1H), 2.60 (s, 3H) ppm.

^{13}C NMR (101 MHz, Chloroform-*d*) δ 151.0, 141.9, 139.3, 134.2, 129.1, 129.0, 128.5, 127.7, 127.5, 127.2, 123.1, 121.5, 117.8, 115.6, 10.7 ppm.

HRMS (CI+) Calcd for $C_{17}H_{15}O^{+}$ [M+H^{+}]: 235.1117, Found: 235.1118.



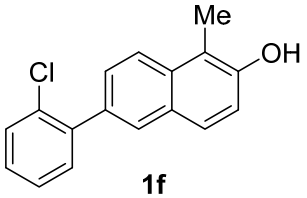
1e

1-Methyl-6-phenylnaphthalen-2-ol (**1e**) was prepared as a white amorphous solid from 6-bromo-1-methylnaphthalen-2-ol **1d** (0.2 g, 1.0 equiv, 0.85 mmol) and phenylboronic acid (207 mg, 2.0 equiv, 1.7 mmol) according to the General Procedure B (eluent for flash column chromatography: petroleum ether/ethyl acetate = 5:1, 127 mg, 64% yield), mp 117.3-118.2 ^{o}C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.02 – 7.97 (m, 2H), 7.78 (dd, *J* = 8.8, 2.0 Hz, 1H), 7.74 – 7.71 (m, 2H), 7.69 (d, *J* = 8.8 Hz, 1H), 7.49 (t, *J* = 7.8 Hz, 2H), 7.37 (td, *J* = 7.2, 1.3 Hz, 1H), 7.10 (d, *J* = 8.8 Hz, 1H), 4.88 (br, 1H), 2.57 (s, 3H) ppm.

^{13}C NMR (101 MHz, Chloroform-*d*) δ 150.7, 141.2, 135.9, 133.2, 129.6, 129.0, 127.8, 127.3, 127.2, 126.5, 126.1, 123.9, 118.2, 115.3, 10.7 ppm.

HRMS (CI+) Calcd for $C_{17}H_{15}O^{+}$ [M+H^{+}]: 235.1117, Found: 235.1116.



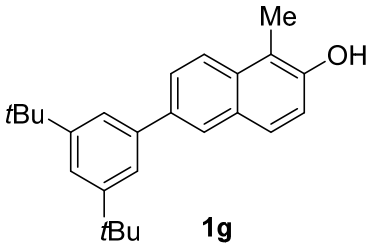
1f

6-(2-Chlorophenyl)-1-methylnaphthalen-2-ol (**1f**) was prepared as a white amorphous solid from 6-bromo-1-methylnaphthalen-2-ol **1d** (0.2 g, 1.0 equiv, 0.85 mmol) and 2-chlorophenylboronic acid (266 mg, 2.0 equiv, 1.7 mmol) according to the General Procedure B (eluent for flash column chromatography: petroleum ether/ethyl acetate = 5:1, 150 mg, 66% yield), mp 124.7-126.1 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.98 (d, *J* = 8.7 Hz, 1H), 7.82 (d, *J* = 1.9 Hz, 1H), 7.67 (d, *J* = 8.8 Hz, 1H), 7.62 (dd, *J* = 8.8, 1.9 Hz, 1H), 7.51 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.44 (dd, *J* = 7.3, 2.0 Hz, 1H), 7.37 – 7.28 (m, 2H), 7.11 (d, *J* = 8.8 Hz, 1H), 4.94 (br, 1H), 2.58 (s, 3H) ppm.

^{13}C NMR (101 MHz, Chloroform-*d*) δ 151.0, 140.6, 134.4, 133.2, 132.9, 131.7, 130.1, 129.1, 129.0, 128.6, 128.1, 127.8, 127.0, 122.9, 118.1, 115.4, 10.7 ppm.

HRMS (CI+) Calcd for $C_{17}H_{14}ClO^{+}$ [M+H^{+}]: 269.0728, Found: 269.0728.



1g

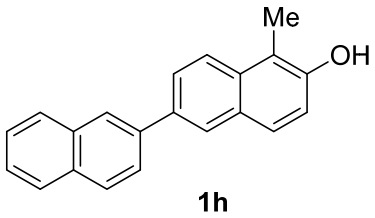
6-(3,5-Di-*tert*-butylphenyl)-1-methylnaphthalen-2-ol (**1g**) was prepared as a yellow amorphous solid from 6-bromo-1-methylnaphthalen-2-ol **1d** (0.2 g, 1.0 equiv, 0.85 mmol) and (3,5-di-*tert*-butylphenyl)boronic acid (398 mg, 2.0 equiv, 1.7 mmol) according to the General Procedure B (eluent for flash column chromatography: petroleum ether/ethyl acetate = 8:1, 240 mg, 82% yield), mp 96.3-97.3 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.00 (d, *J* = 8.8 Hz, 1H), 7.96 (s, 1H), 7.78 (d, *J* = 8.8 Hz, 1H), 7.71 (d, *J* = 8.8 Hz, 1H), 7.54 (s, 2H), 7.47 (s, 1H), 7.10 (d, *J* =

8.8 Hz, 1H), 4.97 (br, 1H), 2.58 (s, 3H), 1.42 (s, 18H) ppm.

^{13}C NMR (101 MHz, Chloroform-*d*) δ 151.3, 150.6, 140.6, 137.2, 133.0, 129.6, 127.7, 126.6, 123.7, 121.9, 121.4, 118.1, 115.3, 109.8, 35.2, 31.7, 10.7 ppm.

HRMS (CI-) Calcd for $C_{25}H_{29}O^-$ [M-H$^+$]: 345.2224, Found: 345.2213.



1h

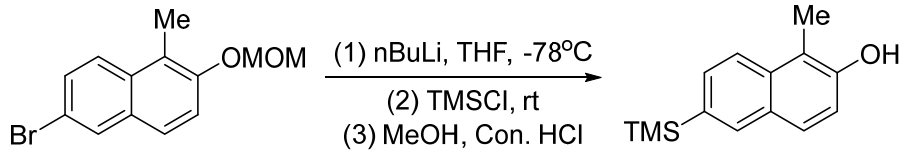
5-Methyl-[2,2'-binaphthalen]-6-ol (**1h**) was prepared as a brown amorphous solid from 6-bromo-1-methylnaphthalen-2-ol **1d** (0.2 g, 1.0 equiv, 0.85 mmol) and naphthalen-2-ylboronic acid (292 mg, 2.0 equiv, 1.7 mmol) according to the General Procedure B (eluent for flash column chromatography: petroleum ether/ethyl acetate = 5:1, 160 mg, 67% yield), mp 177.5-178.3 °C.

^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 9.61 (s, 1H), 8.33 (s, 1H), 8.25 (s, 1H), 8.06 – 7.92 (m, 6H), 7.75 (d, *J* = 8.8 Hz, 1H), 7.58 – 7.49 (m, 2H), 7.22 (d, *J* = 8.8 Hz, 1H), 2.46 (s, 3H) ppm.

^{13}C NMR (101 MHz, DMSO-*d*$_6$) δ 152.6, 137.5, 133.5, 133.4, 133.1, 132.1, 128.5, 128.4, 128.1, 127.5, 127.3, 126.4, 126.1, 125.9, 125.1, 125.1, 124.9, 123.7, 118.6, 114.6, 10.5 ppm.

HRMS (CI+) Calcd for $C_{21}H_{17}O^+$ [M+H$^+$]: 285.1274, Found: 285.1273.

Synthesis of **1-methyl-6-(trimethylsilyl)naphthalen-2-ol** (**1i**).



To solution of 6-bromo-2-(methoxymethoxy)-1-methylnaphthalene (0.28 g, 1.0 equiv, 1 mmol) in dry-THF (10 mL) was slowly added nBuLi (0.8 mL, 2.5 M in *n*-hexane, 2.0 equiv, 2.0 mmol) at -78°C. The resulting reaction mixture was

stirred for 30 min at room temperature then cooled down to -78°C again. Chlorotrimethylsilane (0.25 mL, 2.0 equiv, 2.0 mmol) was added to the mixture slowly at -78°C. The resulting reaction mixture was stirred for other 3 h at room temperature then quenched by water (5 mL), extracted with ethyl acetate (3 × 5 mL). The combined organic layers were washed with brine, dried over anhydrous sodium sulfate, filtered, and concentrated. The crude product was used in next step without further purification.

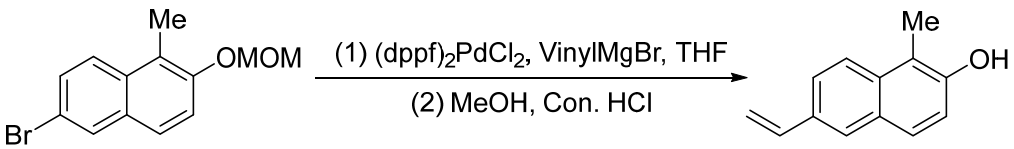
The crude product was redissolved in MeOH (20 mL) and conc. HCl aq. (35%, 1 mL) was added at room temperature. After stirring for 3 h, the reaction mixture was extracted with ethyl acetate (3 × 20 mL). The combined organic layers were washed with brine, dried over anhydrous sodium sulfate, filtered, and concentrated. The residue was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 5:1) to give **1i** (160 mg, 69% yield over three steps) as a white solid, mp 77.4-78.9 °C.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.96 – 7.87 (m, 2H), 7.67 – 7.59 (m, 2H), 7.06 (d, *J* = 8.7 Hz, 1H), 4.98 (br, 1H), 2.53 (s, 3H), 0.34 (s, 9H) ppm.

^{13}C NMR (126 MHz, Chloroform-*d*) δ 150.9, 134.5, 134.5, 134.2, 130.5, 128.9, 127.7, 122.4, 117.6, 115.2, 10.5, -0.9 ppm.

HRMS (CI-) Calcd for $C_{14}H_{17}OSi^-$ [M-H$^+$]: 229.1054, Found: 229.1052.

Synthesis of **1-methyl-6-vinylnaphthalen-2-ol** (**1j**).



To solution of 6-bromo-2-(methoxymethoxy)-1-methylnaphthalene (0.28 g, 1.0 equiv, 1 mmol) and 1,1'-Bis(diphenylphosphino)ferrocene palladium dichloride (36.3 mg, 5 mol%, 0.05 mmol) in dry-THF (10 mL) was slowly added Vinylmagnesium bromide (4 mL, 1 M in THF, 4.0 equiv, 4.0 mmol) at room temperature. The resulting reaction mixture was refluxed for 12 h at 80 °C. The

reaction mixture was cooled down to room temperature then quenched by water (5 mL), extracted with ethyl acetate (3 × 5 mL). The combined organic layers were washed with brine, dried over anhydrous sodium sulfate, filtered, and concentrated. The crude product was used in next step without further purification.

The crude product was redissolved in MeOH (20 mL) and conc. HCl aq. (35%, 1 mL) was added at room temperature. After stirring for 3 h, the reaction mixture was extracted with ethyl acetate (3 × 20 mL). The combined organic layers were washed with brine, dried over anhydrous sodium sulfate, filtered, and concentrated. The residue was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 5:1) to give **1j** (150 mg, 82% yield over two steps) as a yellow solid, mp 127.1-129.0 °C.

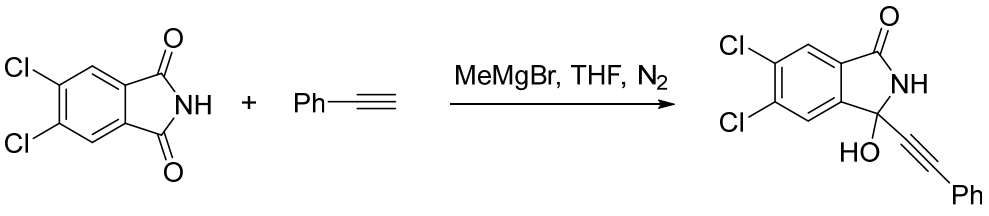
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.87 (d, *J* = 8.8 Hz, 1H), 7.69 – 7.63 (m, 2H), 7.59 (d, *J* = 8.8 Hz, 1H), 7.05 (d, *J* = 8.7 Hz, 1H), 6.86 (dd, *J* = 17.6, 10.9 Hz, 1H), 5.83 (d, *J* = 17.6 Hz, 1H), 5.29 (d, *J* = 10.9 Hz, 1H), 4.93 (br, 1H), 2.53 (s, 3H) ppm.

^{13}C NMR (101 MHz, Chloroform-*d*) δ 150.9, 136.9, 133.7, 132.5, 129.3, 127.7, 127.1, 123.8, 123.6, 118.0, 115.6, 113.3, 10.6 ppm.

HRMS (CI-) Calcd for $C_{13}H_{11}O^-$ [M-H$^+$]: 183.0815, Found: 183.0809.

The propargylic alcohols **2a-2h** were prepared using the reaction according to a reported procedure.[2]

Synthesis of **5,6-Dichloro-3-hydroxy-3-(phenylethynyl)isoindolin-1-one** (**2i**).



To a solution of phenylacetylene (1.5 g, 3.0 equiv, 15.0 mmol) in dry-THF (5 mL)

[2] Qian, C.; Liu, M.; Sun, J.; Li, P. Chiral Phosphoric Acid-catalyzed Regio- and Enantioselective Reactions of Functionalized Propargylic Alcohols. *Org. Chem. Front*. **2022**, *9*, 1234-1240.

was slowly added methyl magnesium bromide (5 mL, 3 M in Et_2O, 3.0 equiv, 15.0 mmol) under argon atmosphere at 0 °C. The mixture was stirred at room temperature for 3 h and then cooled to 0 °C. The 5,6-dichlorophthalimide (1.07 g, 1.0 equiv, 5 mmol) was dispersed to 5 mL dry-THF, then added to reaction mixture. Next, the mixture was stirred at room temperature for other 24 h. Upon completion, a solution of saturated aqueous solution of NH_4Cl (15 mL) was added. The layers were separated, and the aqueous layer was extracted with ethyl acetate (20 mL × 3).

The combined organic layers were dried with anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure to give the residue. The residue was purified by column chromatography on silica gel (eluent: DCM/ethyl acetate = 2:1 to 1:2) to afford the pure propargylic alcohol **2i** as a yellow solid (1.15 g, 73% yield), mp 245.4-247.1 °C.

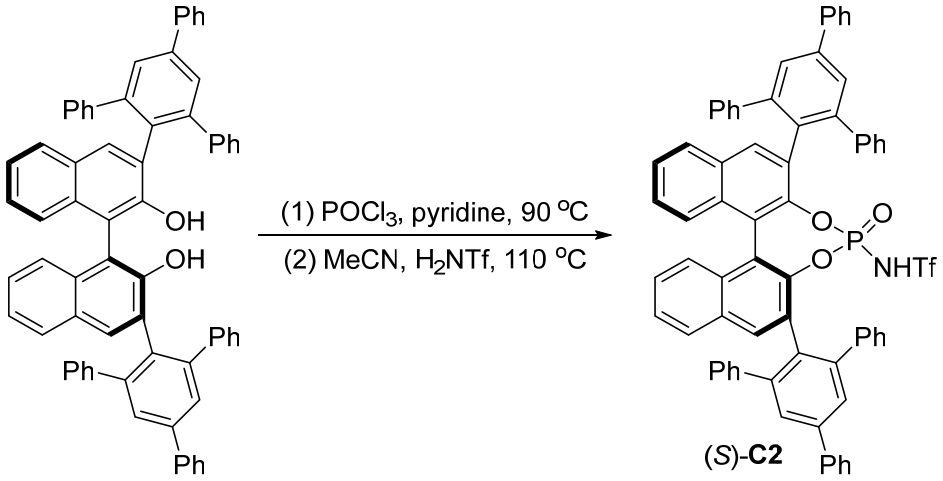
^{1}H NMR (400 MHz, Acetone-d_6) δ 8.86 (br, 1H), 7.99 (s, 1H), 7.84 (s, 1H), 7.48 – 7.44 (m, 2H), 7.38 (q, J = 6.9, 6.4 Hz, 3H), 6.61 (br, 1H) ppm.

^{13}C NMR (101 MHz, Acetone-d_6) δ 166.2, 148.8, 137.3, 134.7, 132.6, 131.4, 130.1, 129.5, 126.1, 125.8, 122.3, 87.0, 84.2, 80.0 ppm.

HRMS (CI+) Calcd for $C_{16}H_{10}Cl_2NO_2^+$ [M+H$^+$]: 318.0083, Found: 318.0082.

III. Preparation of Catalyst C2

The catalyst (*S*)-**C2** was prepared using the following procedure.



1,1,1-Trifluoro-N-((2s,11bS)-4-oxido-2-(5'-phenyl-[1,1':3',1''-terphenyl]-2'-yl)-6-(5'-phenyl-[1,1':3',1''-terphenyl]-4'-yl)dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepin-4-yl)methanesulfonamide (**(*S*)-C2**). At 0 °C, to a solution of (1'S,3s)-3-(5'-phenyl-[1,1':3',1''-terphenyl]-2'-yl)-3'-(5'-phenyl-[1,1':3',1''-terphenyl]-4'-yl)-[1,1'-binaphthalene]-2,2'-diol[3](2.25 g, 1.0 equiv, 2.5 mmol) in anhydrous pyridine (20 mL) was added $POCl_3$ (1.2 mL, 5 equiv, 12.5 mmol) under Ar. The mixture was heated to 90 °C and stirred for 24 h then the pyridine was removed by vacuum. The residue was filtered with a short layer of silica gel (eluent: petroleum ether/DCM = 2:1) to remove the residual pyridine and $POCl_3$. The filter was concentrated. The crude product was used in next step without further purification.

At Ar atmosphere, the crude product and trifluoromethylsulfonamide (745 mg, 2.0 equiv, 5.0 mmol) were dissolved by dry-MeCN (20 mL) in 35 mL sealed tube. The reaction mixture was stirred at 110 °C for 24 h then was concentrated by vacuum, and the residue was purified by flash column chromatography on silica gel (eluent: DCM/ethyl acetate = 2:1) to afford the desired products **C2** as white solid (2.0 g, 74% yield over two steps).

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[3] Denmark, S. E.; Burk, M. T. Development and Mechanism of an Enantioselective Bromocycloetherification Reaction via Lewis Base/Chiral Brønsted Acid Cooperative Catalysis. *Chirality* **2014**, 26, 344–355.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.77 (s, 1H), 7.71 (s, 1H), 7.64 (d, *J* = 7.7 Hz, 6H), 7.50 – 7.28 (m, 16H), 7.23 – 7.06 (m, 12H), 6.93 (t, *J* = 7.5 Hz, 2H), 6.84 (t, *J* = 7.6 Hz, 2H), 6.78 (t, *J* = 7.5 Hz, 1H), 6.66 (dd, *J* = 14.3, 8.3 Hz, 3H), 4.68 (br, 1H) ppm.

^{13}C NMR (126 MHz, Chloroform-*d*) δ 144.7, 144.6, 144.2, 144.2, 144.1, 143.6, 143.5, 143.4, 142.0, 141.5, 141.4, 141.3, 141.2, 141.2, 140.5, 140.2, 134.7, 134.4, 132.0, 131.8, 131.4, 131.0, 130.7, 130.7, 130.6, 130.3, 129.8, 129.6, 129.0, 129.0, 128.9, 128.3, 128.1, 128.0, 127.9, 127.8, 127.7, 127.4, 127.3, 127.0, 126. 8, 126.7, 126.6, 126.4, 126.1, 126.1, 125.7, 125.6, 121.4 (q, *J* = 315.0 Hz) ppm.

^{31}P NMR (202 MHz, Chloroform-*d*) δ -0.68 ppm.

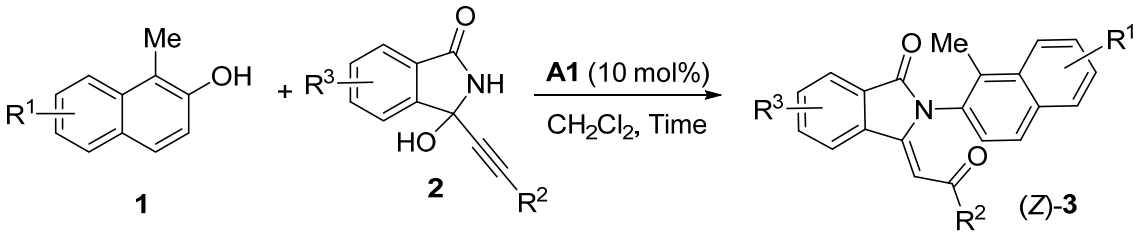
^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.91 ppm.

$[\alpha]_D^{25}$: +311.0 (*c* = 1.0, CH_2Cl_2).

HRMS (CI-) Calcd for $C_{69}H_{44}F_3NO_5PS^-$ [M-H$^+$]: 1086.2635, Found: 1086.2638.

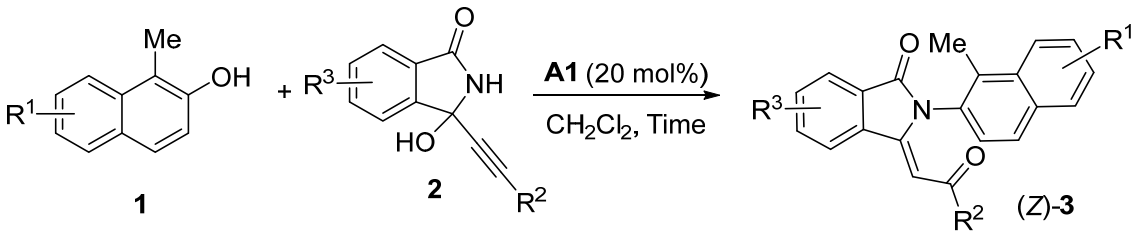
IV. Synthesis of Racemic (*Z*)-Products

General Procedure C.

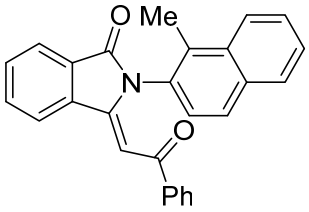


To a 10 mL-vial charged with naphthalene-2-sulfonic acid (**A1**, 4.2 mg, 10 mol%, 0.02 mmol) and the 1-methylnaphthalen-2-ol **1** (0.2 mmol), propargylic alcohol **2** (0.4 mmol) was added the solvent DCM (4.8 mL). The mixture was stirred at room temperature for noted time under Ar. Upon completion (10~36 h), the reaction was quenched by addition of a Et_3N (14 μL, 50 mol%, 0.1 mmol). Next, the mixture was concentrated by vacuum. The residue was subjected to silica gel column chromatography to afford the pure product.

General Procedure D.



To a 10 mL-vial charged with naphthalene-2-sulfonic acid (**A1**, 8.4 mg, 20 mol%, 0.04 mmol) and the 1-methylnaphthalen-2-ol **1** (0.2 mmol), propargylic alcohol **2** (0.4 mmol) was added the solvent DCM (6.0 mL). The mixture was stirred at 30°C for noted time under Ar. Upon completion (10~36 h), the reaction was quenched by addition of a Et_3N (14 μL, 50 mol%, 0.1 mmol). Next, the mixture was concentrated by vacuum. The residue was subjected to silica gel column chromatography to afford the pure product.



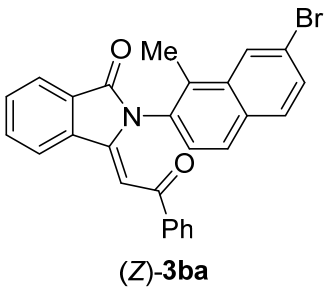
(*Z*)-**3aa**

(*Z*)-2-(1-Methylnaphthalen-2-yl)-3-(2-oxo-2-phenylethylidene)isoindolin-1-one ((*Z*)-**3aa**) was prepared as a yellow amorphous solid from 1-methylnaphthalen-2-ol **1a** (31.6 mg, 1.0 equiv, 0.2 mmol) and 3-hydroxy-3-(phenylethynyl)isoindolin-1-one **2a** (99.6 mg, 2.0 equiv, 0.4 mmol) according to the General Procedure C (24 h, eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 60.0 mg, 77% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.99 (d, *J* = 7.5 Hz, 1H), 7.89 (d, *J* = 7.7 Hz, 1H), 7.86 – 7.81 (m, 1H), 7.77 – 7.70 (m, 2H), 7.67 (t, *J* = 7.6 Hz, 1H), 7.50 – 7.43 (m, 3H), 7.34 – 7.28 (m, 3H), 7.08 (t, *J* = 7.7 Hz, 2H), 7.03 (d, *J* = 8.6 Hz, 1H), 6.55 (s, 1H), 2.33 (s, 3H) ppm.

^{13}C NMR (101 MHz, Chloroform-*d*) δ 191.8, 167.6, 142.2, 138.0, 137.4, 133.2, 133.2, 133.1, 132.9, 132.8, 131.3, 131.0, 128.4, 128.1, 128.0, 127.1, 127.0, 126.8, 126.2, 125.8, 124.8, 124.3, 120.4, 102.7, 14.4 ppm.

HRMS (CI+) Calcd for $C_{27}H_{20}NO_2^+$ [M+H$^+$]: 390.1489, Found: 390.1487.



(*Z*)-**3ba**

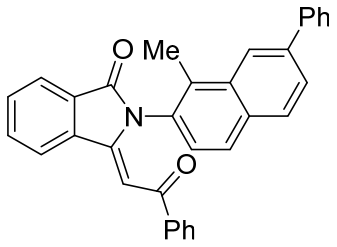
(*Z*)-2-(7-Bromo-1-methylnaphthalen-2-yl)-3-(2-oxo-2-phenylethylidene)isoindolin-1-one ((*Z*)-**3ba**) was prepared as a yellow amorphous solid from 7-bromo-1-methylnaphthalen-2-ol **1b** (47.4 mg, 1.0 equiv, 0.2 mmol) and 3-hydroxy-3-(phenylethynyl)isoindolin-1-one **2a** (99.6 mg, 2.0

equiv, 0.4 mmol) according to the General Procedure D (36 h, eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 59.0 mg, 63% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.01 – 7.96 (m, 2H), 7.88 (d, *J* = 7.7 Hz, 1H), 7.74 (t, *J* = 7.6 Hz, 1H), 7.67 (t, *J* = 7.4 Hz, 1H), 7.60 – 7.52 (m, 2H), 7.43 (d, *J* = 8.6 Hz, 1H), 7.39 – 7.34 (m, 3H), 7.13 (t, *J* = 7.5 Hz, 2H), 7.06 (d, *J* = 8.6 Hz, 1H), 6.59 (s, 1H), 2.31 (s, 3H) ppm.

^{13}C NMR (101 MHz, Chloroform-*d*) δ 191.4, 167.6, 142.3, 137.9, 137.4, 134.1, 133.2, 133.0, 132.5, 132.5, 131.6, 131.1, 130.0, 129.6, 128.2, 128.2, 128.1, 127.3, 127.0, 126.3, 124.4, 120.6, 120.5, 102.6, 14.5 ppm.

HRMS (CI+) Calcd for $C_{27}H_{19}BrNO_2^+$ [M+H$^+$]: 468.0594, Found: 468.0595.



(*Z*)-**3ca**

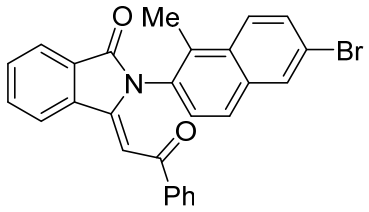
(*Z*)-2-(1-Methyl-7-phenylnaphthalen-2-yl)-3-(2-oxo-2-phenylethylidene)isoindolin-1-one ((*Z*)-**3ca**) was prepared as a yellow amorphous solid from 1-methyl-7-phenylnaphthalen-2-ol **1c** (46.8 mg, 1.0 equiv, 0.2 mmol) and 3-hydroxy-3-(phenylethynyl)isoindolin-1-one **2a** (99.6 mg, 2.0 equiv, 0.4 mmol) according to the General Procedure D (18 h, eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 62.3 mg, 67% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.02 – 7.98 (m, 2H), 7.90 (d, *J* = 7.6 Hz, 1H), 7.81 (d, *J* = 8.5 Hz, 1H), 7.77 – 7.67 (m, 5H), 7.53 – 7.48 (m, 3H), 7.41 – 7.35 (m, 3H), 7.29 (d, *J* = 7.3 Hz, 1H), 7.11 (t, *J* = 7.6 Hz, 2H), 7.05 (d, *J* = 8.6 Hz, 1H), 6.58 (s, 1H), 2.39 (s, 3H) ppm.

^{13}C NMR (101 MHz, Chloroform-*d*) δ 191.7, 167.6, 142.3, 141.5, 138.9, 138.0, 137.5,

133.5, 133.1, 133.1, 132.9, 132.4, 131.9, 131.1, 129.0, 129.0, 128.4, 128.2, 128.0, 127.7, 127.5, 126.9, 126.0, 125.9, 124.4, 123.0, 120.4, 102.7, 14.5 ppm.

HRMS (CI+) Calcd for $C_{33}H_{24}NO_2^+$ [M+H$^+$]: 466.1802, Found: 466.1802.



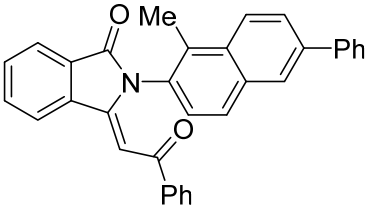
(*Z*)-**3da**

(*Z*)-2-(6-Bromo-1-methylnaphthalen-2-yl)-3-(2-oxo-2-phenylethylidene)isoindolin-1-one ((*Z*)-**3da**) was prepared as a yellow amorphous solid from 6-bromo-1-methylnaphthalen-2-ol **1d** (47.4 mg, 1.0 equiv, 0.2 mmol) and 3-hydroxy-3-(phenylethynyl)isoindolin-1-one **2a** (99.6 mg, 2.0 equiv, 0.4 mmol) according to the General Procedure D (36 h, eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 80.5 mg, 86% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.99 (d, *J* = 7.4 Hz, 1H), 7.92 – 7.86 (m, 2H), 7.77 – 7.66 (m, 3H), 7.52 (d, *J* = 9.0 Hz, 1H), 7.40 – 7.32 (m, 4H), 7.14 (t, *J* = 7.1 Hz, 2H), 7.05 (d, *J* = 8.6 Hz, 1H), 6.59 (s, 1H), 2.33 (s, 3H) ppm.

^{13}C NMR (101 MHz, Chloroform-*d*) δ 191.4, 167.6, 142.3, 137.9, 137.4, 134.3, 133.5, 133.2, 133.0, 131.9, 131.3, 131.1, 130.3, 129.5, 128.2, 128.1, 128.1, 127.0, 126.7, 126.1, 124.4, 120.5, 120.5, 102.6, 14.4 ppm.

HRMS (CI+) Calcd for $C_{27}H_{19}BrNO_2^+$ [M+H$^+$]: 468.0594, Found: 468.0593.



(*Z*)-**3ea**

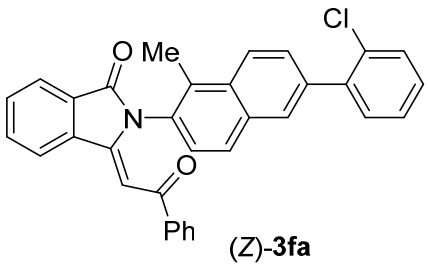
(*Z*)-2-(1-Methyl-6-phenylnaphthalen-2-yl)-3-(2-oxo-2-

phenylethylidene)isoindolin-1-one ((*Z*)-**3ea**) was prepared as a yellow amorphous solid from 1-methyl-6-phenylnaphthalen-2-ol **1e** (46.8 mg, 1.0 equiv, 0.2 mmol) and 3-hydroxy-3-(phenylethynyl)isoindolin-1-one **2a** (99.6 mg, 2.0 equiv, 0.4 mmol) according to the General Procedure D (18 h, eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 79.1 mg, 85% yield).

^{1}H NMR (500 MHz, Acetone-d_6) δ 8.28 (d, *J* = 7.7 Hz, 1H), 8.12 – 8.07 (m, 2H), 7.94 (d, *J* = 7.5 Hz, 1H), 7.89 – 7.85 (m, 2H), 7.82 (d, *J* = 8.4 Hz, 2H), 7.80 – 7.76 (m, 1H), 7.60 (d, *J* = 8.6 Hz, 1H), 7.57 – 7.49 (m, 4H), 7.45 – 7.39 (m, 2H), 7.26 (t, *J* = 7.8 Hz, 2H), 7.17 (d, *J* = 8.6 Hz, 1H), 7.04 (s, 1H), 2.45 (s, 3H) ppm.

^{13}C NMR (126 MHz, Acetone-d_6) δ 190.8, 168.0, 143.7, 141.3, 139.2, 139.0, 138.9, 134.3, 134.1, 133.7, 133.5, 133.4, 132.8, 131.9, 129.8, 129.0, 129.0, 129.0, 128.4, 128.0, 127.7, 127.2, 126.7, 126.3, 126.2, 124.4, 122.0, 103.5, 14.5 ppm.

HRMS (CI+) Calcd for $C_{33}H_{24}NO_2^+$ [M+H$^+$]: 466.1802, Found: 466.1802.



(*Z*)-**3fa**

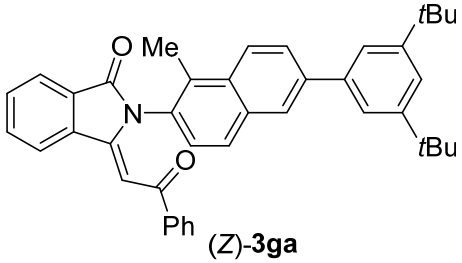
(*Z*)-2-(6-(2-Chlorophenyl)-1-methylnaphthalen-2-yl)-3-(2-oxo-2-phenylethylidene)isoindolin-1-one ((*Z*)-**3fa**) was prepared as a yellow amorphous solid from 6-(2-chlorophenyl)-1-methylnaphthalen-2-ol **1f** (53.7 mg, 1.0 equiv, 0.2 mmol) and 3-hydroxy-3-(phenylethynyl)isoindolin-1-one **2a** (99.6 mg, 2.0 equiv, 0.4 mmol) according to the General Procedure D (18 h, eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 74.0 mg, 74% yield).

^{1}H NMR (400 MHz, Acetone-d_6) δ 8.26 (d, *J* = 7.7 Hz, 1H), 8.07 (d, *J* = 8.8 Hz, 1H), 7.93 (d, *J* = 7.4 Hz, 1H), 7.88 – 7.83 (m, 2H), 7.76 (td, *J* = 7.5, 0.9 Hz, 1H), 7.63 (dd,

J = 8.7, 1.9 Hz, 1H), 7.60 – 7.56 (m, 2H), 7.56 – 7.52 (m, 3H), 7.47 – 7.39 (m, 3H), 7.24 (t, *J* = 7.7 Hz, 2H), 7.20 (d, *J* = 8.6 Hz, 1H), 7.03 (s, 1H), 2.47 (s, 3H) ppm.

^{13}C NMR (101 MHz, Acetone-d_6) δ 190.9, 167.9, 143.6, 141.0, 139.0, 138.8, 137.9, 134.1, 133.8, 133.7, 133.7, 133.5, 133.0, 132.8, 132.6, 131.9, 130.8, 130.0, 129.5, 129.0, 128.9, 128.9, 128.4, 128.2, 127.6, 127.2, 125.3, 124.4, 122.0, 103.5, 14.6 ppm.

HRMS (CI+) Calcd for $C_{33}H_{23}ClNO_2^+$ [M+H$^+$]: 500.1412, Found: 500.1409.



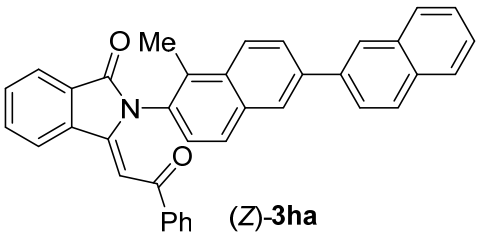
(*Z*)-**3ga**

(*Z*)-2-(6-(3,5-Di-*tert*-butylphenyl)-1-methylnaphthalen-2-yl)-3-(2-oxo-2-phenylethylidene)isoindolin-1-one ((*Z*)-**3ga**) was prepared as a yellow amorphous solid from 6-(3,5-di-*tert*-butylphenyl)-1-methylnaphthalen-2-ol **1g** (69.3 mg, 1.0 equiv, 0.2 mmol) and 3-hydroxy-3-(phenylethynyl)isoindolin-1-one **2a** (99.6 mg, 2.0 equiv, 0.4 mmol) according to the General Procedure D (18 h, eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 72.8 mg, 63% yield).

^{1}H NMR (500 MHz, Acetone-d_6) δ 8.28 (d, *J* = 7.7 Hz, 1H), 8.12 (d, *J* = 2.0 Hz, 1H), 8.09 (d, *J* = 8.7 Hz, 1H), 7.94 (d, *J* = 7.5 Hz, 1H), 7.90 – 7.85 (m, 2H), 7.78 (t, *J* = 7.5 Hz, 1H), 7.67 (d, *J* = 1.8 Hz, 2H), 7.61 – 7.54 (m, 4H), 7.45 (t, *J* = 7.4 Hz, 1H), 7.27 (t, *J* = 7.8 Hz, 2H), 7.17 (d, *J* = 8.6 Hz, 1H), 7.04 (s, 1H), 2.45 (s, 3H), 1.42 (s, 18H) ppm.

^{13}C NMR (126 MHz, Acetone-d_6) δ 190.7, 168.0, 152.1, 143.8, 140.8, 140.4, 139.0, 138.9, 134.3, 134.1, 133.7, 133.5, 133.2, 132.7, 131.9, 129.0, 129.0, 129.0, 127.6, 127.0, 126.8, 126.7, 126.0, 124.4, 122.5, 122.4, 122.0, 103.5, 35.6, 31.8, 14.5 ppm.

HRMS (CI+) Calcd for $C_{41}H_{40}NO_2^+$ [M+H$^+$]: 578.3054, Found: 578.3054.



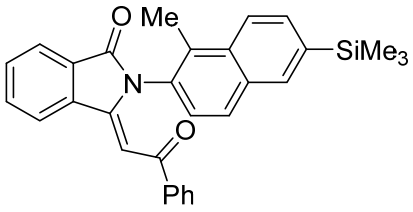
(*Z*)-**3ha**

(*Z*)-2-(5-Methyl-[2,2'-binaphthalen]-6-yl)-3-(2-oxo-2-phenylethylidene)isoindolin-1-one ((*Z*)-**3ha**) was prepared as a yellow amorphous solid from 5-methyl-[2,2'-binaphthalen]-6-ol **1h** (56.9 mg, 1.0 equiv, 0.2 mmol) and 3-hydroxy-3-(phenylethynyl)isoindolin-1-one **2a** (99.6 mg, 2.0 equiv, 0.4 mmol) according to the General Procedure D (20 h, eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 91.8 mg, 89% yield).

^{1}H NMR (400 MHz, Acetone-d_6) δ 8.33 (s, 1H), 8.26 (d, J = 7.7 Hz, 1H), 8.22 (d, J = 1.8 Hz, 1H), 8.11 (d, J = 8.8 Hz, 1H), 8.04 – 7.92 (m, 6H), 7.87 – 7.83 (m, 1H), 7.79 – 7.75 (m, 1H), 7.62 (d, J = 8.6 Hz, 1H), 7.58 – 7.52 (m, 4H), 7.45 – 7.41 (m, 1H), 7.25 (t, J = 7.8 Hz, 2H), 7.18 (d, J = 8.6 Hz, 1H), 7.03 (s, 1H), 2.46 (s, 3H) ppm.

^{13}C NMR (101 MHz, Acetone-d_6) δ 190.8, 168.0, 143.7, 139.0, 138.9, 138.8, 138.6, 134.8, 134.3, 134.1, 133.8, 133.5, 133.4, 132.9, 131.9, 129.6, 129.5, 129.2, 129.0, 129.0, 128.9, 128.5, 127.7, 127.3, 127.2, 127.1, 127.0, 126.7, 126.4, 126.3, 126.2, 124.4, 122.0, 103.5, 14.6 ppm.

HRMS (CI+) Calcd for $C_{37}H_{26}NO_2^+$ [M+H$^+$]: 516.1958, Found: 516.1962.



(*Z*)-**3ia**

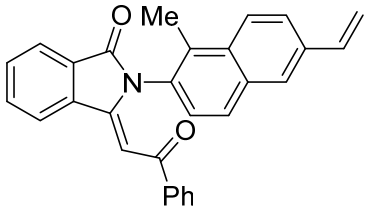
(*Z*)-2-(1-Methyl-6-(trimethylsilyl)naphthalen-2-yl)-3-(2-oxo-2-phenylethylidene)isoindolin-1-one ((*Z*)-**3ia**) was prepared as a yellow amorphous solid from 1-methyl-6-(trimethylsilyl)naphthalen-2-ol **1i** (46.1 mg,

1.0 equiv, 0.2 mmol) and 3-hydroxy-3-(phenylethynyl)isoindolin-1-one **2a** (99.6 mg, 2.0 equiv, 0.4 mmol) according to the General Procedure D (24 h, eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 39.7 mg, 43% yield).

^{1}H NMR (400 MHz, Acetone-d_6) δ 8.25 (d, J = 7.7 Hz, 1H), 8.01 – 7.97 (m, 2H), 7.92 (dt, J = 7.5, 1.0 Hz, 1H), 7.86 – 7.82 (m, 1H), 7.75 (td, J = 7.5, 0.9 Hz, 1H), 7.68 (dd, J = 8.4, 1.3 Hz, 1H), 7.57 – 7.51 (m, 3H), 7.44 – 7.40 (m, 1H), 7.27 – 7.21 (m, 2H), 7.15 (d, J = 8.6 Hz, 1H), 7.03 (s, 1H), 2.43 (s, 3H), 0.36 (s, 9H) ppm.

^{13}C NMR (101 MHz, Acetone-d_6) δ 190.6, 168.0, 143.9, 138.9, 138.8, 138.6, 135.0, 134.1, 133.9, 133.6, 133.4, 133.4, 133.3, 131.9, 130.9, 129.5, 129.0, 128.9, 127.5, 126.5, 124.5, 124.3, 122.0, 103.4, 14.4, -1.0 ppm.

HRMS (CI+) Calcd for $C_{30}H_{28}NO_2Si^+$ [M+H$^+$]: 462.1884, Found: 462.1885.



(*Z*)-**3ja**

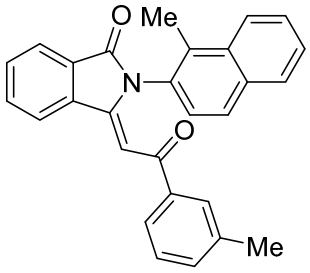
(*Z*)-2-(1-Methyl-6-vinylnaphthalen-2-yl)-3-(2-oxo-2-phenylethylidene)isoindolin-1-one ((*Z*)-**3ja**) was prepared as a yellow amorphous solid from 1-methyl-6-vinylnaphthalen-2-ol **1j** (36.8 mg, 1.0 equiv, 0.2 mmol) and 3-hydroxy-3-(phenylethynyl)isoindolin-1-one **2a** (99.6 mg, 2.0 equiv, 0.4 mmol) according to the General Procedure C (24 h, eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 33.2 mg, 40% yield).

^{1}H NMR (400 MHz, Acetone-d_6) δ 8.26 (d, J = 7.7 Hz, 1H), 7.96 (d, J = 8.8 Hz, 1H), 7.92 (d, J = 7.5 Hz, 1H), 7.86 (t, J = 7.6 Hz, 1H), 7.79 – 7.72 (m, 3H), 7.55 – 7.51 (m, 2H), 7.48 (d, J = 8.6 Hz, 1H), 7.43 (t, J = 7.4 Hz, 1H), 7.24 (t, J = 7.8 Hz, 2H), 7.12 (d, J = 8.7 Hz, 1H), 7.01 (s, 1H), 6.93 (dd, J = 17.6, 11.0 Hz, 1H), 5.97 (d, J = 18.1

Hz, 1H), 5.35 (d, *J* = 11.5 Hz, 1H), 2.40 (s, 3H) ppm.

^{13}C NMR (101 MHz, Acetone-d_6) δ 190.9, 167.9, 143.6, 138.9, 138.8, 137.6, 136.1, 134.1, 134.1, 133.8, 133.5, 133.4, 133.3, 131.9, 129.0, 129.0, 128.9, 127.5, 127.5, 127.2, 125.8, 124.4, 124.2, 122.0, 114.9, 103.6, 14.5 ppm.

HRMS (CI+) Calcd for $C_{29}H_{22}NO_2^+$ [M+H$^+$]: 416.1645, Found: 416.1647.



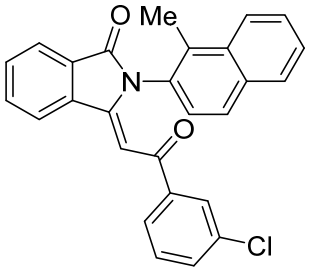
(*Z*)-**3ab**

(*Z*)-2-(1-Methylnaphthalen-2-yl)-3-(2-oxo-2-(*m*-tolyl)ethylidene)isoindolin-1-one ((*Z*)-**3ab**) was prepared as a yellow amorphous solid from 1-methylnaphthalen-2-ol **1a** (31.6 mg, 1.0 equiv, 0.2 mmol) and 3-hydroxy-3-(*m*-tolylethynyl)isoindolin-1-one **2b** (105.3 mg, 2.0 equiv, 0.4 mmol) according to the General Procedure C (24 h, eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 66.2 mg, 82% yield).

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.99 (d, *J* = 7.5 Hz, 1H), 7.89 (d, *J* = 7.7 Hz, 1H), 7.84 – 7.80 (m, 1H), 7.77 – 7.73 (m, 2H), 7.67 (t, *J* = 7.5 Hz, 1H), 7.49 – 7.45 (m, 3H), 7.20 (d, *J* = 7.6 Hz, 1H), 7.08 (d, *J* = 7.5 Hz, 1H), 7.01 (dd, *J* = 8.1, 6.9 Hz, 2H), 6.91 (s, 1H), 6.52 (s, 1H), 2.28 (s, 3H), 2.01 (s, 3H) ppm.

^{13}C NMR (126 MHz, Chloroform-*d*) δ 192.5, 167.5, 141.8, 138.2, 138.1, 137.4, 133.5, 133.2, 133.1, 133.0, 132.7, 131.3, 130.9, 128.3, 128.3, 127.9, 127.7, 127.1, 126.2, 126.1, 125.8, 125.7, 124.7, 124.2, 120.4, 103.0, 21.0, 14.4 ppm.

HRMS (CI+) Calcd for $C_{28}H_{22}NO_2^+$ [M+H$^+$]: 404.1645, Found: 404.1643.



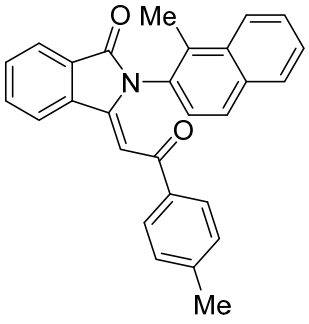
(*Z*)-**3ac**

(*Z*)-3-(2-(3-Chlorophenyl)-2-oxoethylidene)-2-(1-methylnaphthalen-2-yl)isoindolin-1-one ((*Z*)-**3ac**) was prepared as a yellow amorphous solid from 1-methylnaphthalen-2-ol **1a** (31.6 mg, 1.0 equiv, 0.2 mmol) and 3-((3-chlorophenyl)ethynyl)-3-hydroxyisoindolin-1-one **2c** (113.5 mg, 2.0 equiv, 0.4 mmol) according to the General Procedure C (24 h, eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 53.4 mg, 63% yield).

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.99 (d, *J* = 7.5 Hz, 1H), 7.89 (d, *J* = 7.7 Hz, 1H), 7.87 – 7.84 (m, 1H), 7.77 – 7.74 (m, 2H), 7.68 (td, *J* = 7.5, 1.0 Hz, 1H), 7.51 – 7.46 (m, 3H), 7.25 – 7.16 (m, 3H), 7.03 – 6.95 (m, 2H), 6.46 (s, 1H), 2.34 (s, 3H) ppm.

^{13}C NMR (126 MHz, Chloroform-*d*) δ 190.7, 167.5, 142.8, 139.6, 137.2, 134.3, 133.3, 133.2, 133.2, 132.7, 132.5, 131.2, 131.1, 129.2, 128.5, 128.3, 127.9, 127.2, 126.5, 126.4, 126.1, 125.6, 124.6, 124.4, 120.5, 101.7, 14.4 ppm.

HRMS (CI+) Calcd for $C_{27}H_{19}ClNO_2^+$ [M+H$^+$]: 424.1099, Found: 424.1097.



(*Z*)-**3ad**

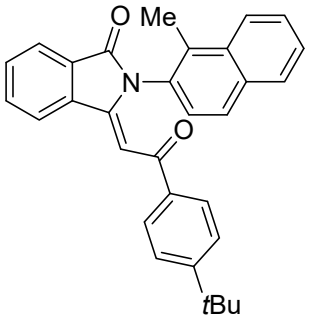
(*Z*)-2-(1-Methylnaphthalen-2-yl)-3-(2-oxo-2-(*p*-tolyl)ethylidene)isoindolin-1-one ((*Z*)-**3ad**) was prepared as a yellow amorphous solid from 1-

methylnaphthalen-2-ol **1a** (31.6 mg, 1.0 equiv, 0.2 mmol) and 3-hydroxy-3-(*p*-tolylethynyl)isoindolin-1-one **2d** (105.3 mg, 2.0 equiv, 0.4 mmol) according to the General Procedure C (24 h, eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 52.5 mg, 65% yield).

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.99 (d, *J* = 7.5 Hz, 1H), 7.88 (d, *J* = 7.7 Hz, 1H), 7.84 – 7.79 (m, 1H), 7.77 – 7.71 (m, 2H), 7.67 (td, *J* = 7.5, 0.9 Hz, 1H), 7.50 – 7.43 (m, 3H), 7.22 (d, *J* = 8.2 Hz, 2H), 7.03 (d, *J* = 8.7 Hz, 1H), 6.84 (d, *J* = 7.9 Hz, 2H), 6.54 (s, 1H), 2.32 (s, 3H), 2.24 (s, 3H) ppm.

^{13}C NMR (126 MHz, Chloroform-*d*) δ 191.6, 167.6, 143.7, 141.8, 137.5, 135.6, 133.2, 133.2, 133.0, 132.8, 131.4, 130.9, 128.6, 128.5, 128.4, 128.3, 127.1, 126.2, 126.0, 125.8, 124.7, 124.3, 120.4, 103.1, 21.7, 14.5 ppm.

HRMS (CI+) Calcd for $C_{28}H_{22}NO_2^+$ [M+H$^+$]: 404.1645, Found: 404.1643.



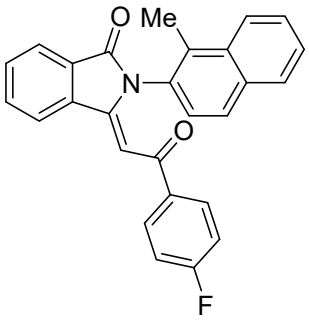
(*Z*)-**3ae**

(*Z*)-3-(2-(4-(*tert*-Butyl)phenyl)-2-oxoethylidene)-2-(1-methylnaphthalen-2-yl)isoindolin-1-one ((*Z*)-**3ae**) was prepared as a yellow amorphous solid from 1-methylnaphthalen-2-ol **1a** (31.6 mg, 1.0 equiv, 0.2 mmol) and 3-((4-(*tert*-butyl)phenyl)ethynyl)-3-hydroxyisoindolin-1-one **2e** (122.2 mg, 2.0 equiv, 0.4 mmol) according to the General Procedure C (24 h, eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 49.0 mg, 55% yield).

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.99 (d, *J* = 7.3 Hz, 1H), 7.89 (d, *J* = 7.7 Hz, 1H), 7.80 (d, *J* = 8.2 Hz, 1H), 7.77 – 7.70 (m, 2H), 7.67 (t, *J* = 7.7 Hz, 1H), 7.48 – 7.43 (m, 3H), 7.22 (d, *J* = 8.4 Hz, 2H), 7.04 (dd, *J* = 11.7, 8.6 Hz, 3H), 6.52 (s, 1H), 2.29 (s, 3H), 1.24 (s, 9H) ppm.

^{13}C NMR (126 MHz, Chloroform-*d*) δ 192.0, 167.6, 156.5, 141.6, 137.4, 135.5, 133.2, 133.2, 133.0, 132.7, 131.3, 130.9, 128.4, 128.3, 128.0, 127.1, 126.2, 126.1, 125.9, 124.9, 124.8, 124.3, 120.4, 103.1, 35.1, 31.1, 14.5 ppm.

HRMS (CI+) Calcd for $C_{31}H_{28}NO_2^+$ [M+H$^+$]: 446.2115, Found: 446.2114.



(*Z*)-**3af**

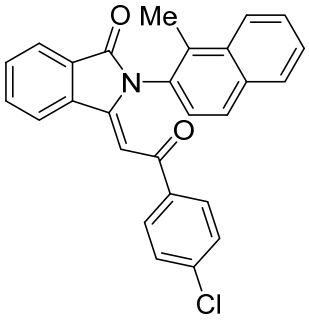
(*Z*)-3-(2-(4-Fluorophenyl)-2-oxoethylidene)-2-(1-methylnaphthalen-2-yl)isoindolin-1-one ((*Z*)-**3af**) was prepared as a yellow amorphous solid from 1-methylnaphthalen-2-ol **1a** (31.6 mg, 1.0 equiv, 0.2 mmol) and 3-((4-fluorophenyl)ethynyl)-3-hydroxyisoindolin-1-one **2f** (106.9 mg, 2.0 equiv, 0.4 mmol) according to the General Procedure C (24 h, eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 60.3 mg, 74% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.99 (dt, *J* = 7.5, 1.0 Hz, 1H), 7.90 – 7.83 (m, 2H), 7.78 – 7.66 (m, 3H), 7.52 – 7.45 (m, 3H), 7.35 – 7.28 (m, 2H), 7.01 (d, *J* = 8.6 Hz, 1H), 6.72 (t, *J* = 8.7 Hz, 2H), 6.48 (s, 1H), 2.33 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 190.5, 167.6, 165.5 (d, *J* = 254.5 Hz), 142.2, 137.3, 134.5 (d, *J* = 3.8 Hz), 133.2, 133.2, 133.1, 132.8, 131.3, 131.1, 130.7, 130.7, 128.4, 127.1, 126.5, 126.4, 125.9, 124.7, 124.4, 120.4, 115.0 (d, *J* = 22.3 Hz), 102.3, 14.5 ppm.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -105.25 ppm.

HRMS (CI+) Calcd for $C_{27}H_{19}FNO_2^+$ [M+H$^+$]: 408.1394, Found: 408.1396.



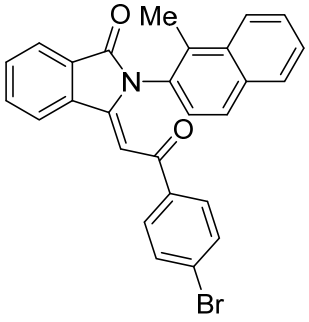
(*Z*)-**3ag**

(*Z*)-3-(2-(4-Chlorophenyl)-2-oxoethylidene)-2-(1-methylnaphthalen-2-yl)isoindolin-1-one ((*Z*)-**3ag**) was prepared as a yellow amorphous solid from 1-methylnaphthalen-2-ol **1a** (31.6 mg, 1.0 equiv, 0.2 mmol) and 3-((4-chlorophenyl)ethynyl)-3-hydroxyisoindolin-1-one **2g** (113.5 mg, 2.0 equiv, 0.4 mmol) according to the General Procedure C (24 h, eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 76.3 mg, 90% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.98 (d, *J* = 7.4 Hz, 1H), 7.89 – 7.83 (m, 2H), 7.77 – 7.72 (m, 2H), 7.67 (t, *J* = 7.4 Hz, 1H), 7.52 – 7.47 (m, 3H), 7.24 – 7.18 (m, 2H), 7.00 (dd, *J* = 8.6, 6.7 Hz, 3H), 6.47 (s, 1H), 2.32 (s, 3H) ppm.

^{13}C NMR (101 MHz, Chloroform-*d*) δ 190.8, 167.5, 142.5, 139.1, 137.3, 136.4, 133.2, 133.2, 133.1, 132.7, 131.3, 131.2, 129.3, 128.4, 128.3, 128.1, 127.2, 126.5, 126.4, 125.7, 124.7, 124.4, 120.4, 102.0, 14.5 ppm.

HRMS (CI+) Calcd for $C_{27}H_{19}ClNO_2^+$ [M+H$^+$]: 424.1099, Found: 424.1102.



(*Z*)-**3ah**

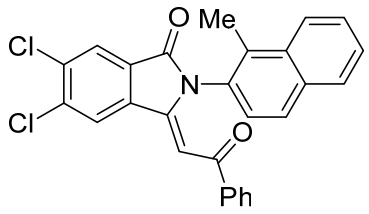
(*Z*)-3-(2-(4-Bromophenyl)-2-oxoethylidene)-2-(1-methylnaphthalen-2-yl)isoindolin-1-one ((*Z*)-**3ah**) was prepared as a yellow amorphous solid from 1-methylnaphthalen-2-ol **1a** (31.6 mg, 1.0 equiv, 0.2 mmol) and 3-((4-

bromophenyl)ethynyl)-3-hydroxyisoindolin-1-one **2h** (131.3 mg, 2.0 equiv, 0.4 mmol) according to the General Procedure C (24 h, eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 79.6 mg, 85% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.98 (d, *J* = 7.6 Hz, 1H), 7.89 – 7.83 (m, 2H), 7.77 – 7.72 (m, 2H), 7.67 (td, *J* = 7.5, 1.0 Hz, 1H), 7.53 – 7.47 (m, 3H), 7.18 – 7.09 (m, 4H), 7.00 (d, *J* = 8.6 Hz, 1H), 6.46 (s, 1H), 2.32 (s, 3H) ppm.

^{13}C NMR (101 MHz, Chloroform-*d*) δ 191.1, 167.5, 142.5, 137.3, 136.8, 133.2, 133.2, 133.1, 132.8, 131.2, 131.2, 131.1, 129.4, 128.4, 128.3, 128.0, 127.2, 126.5, 126.4, 125.7, 124.7, 124.4, 120.5, 102.0, 14.5 ppm.

HRMS (CI+) Calcd for $C_{27}H_{19}BrNO_2^+$ [M+H$^+$]: 468.0594, Found: 468.0594.



(*Z*)-**3ai**

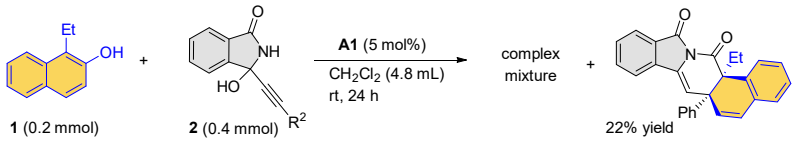
(*Z*)-5,6-Dichloro-2-(1-methylnaphthalen-2-yl)-3-(2-oxo-2-phenylethylidene)isoindolin-1-one ((*Z*)-**3ai**) was prepared as a yellow amorphous solid from 1-methylnaphthalen-2-ol **1a** (31.6 mg, 1.0 equiv, 0.2 mmol) and 5,6-dichloro-3-hydroxy-3-(phenylethynyl)isoindolin-1-one **2i** (127.3 mg, 2.0 equiv, 0.4 mmol) according to the General Procedure C (10 h, eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 47.7 mg, 52% yield).

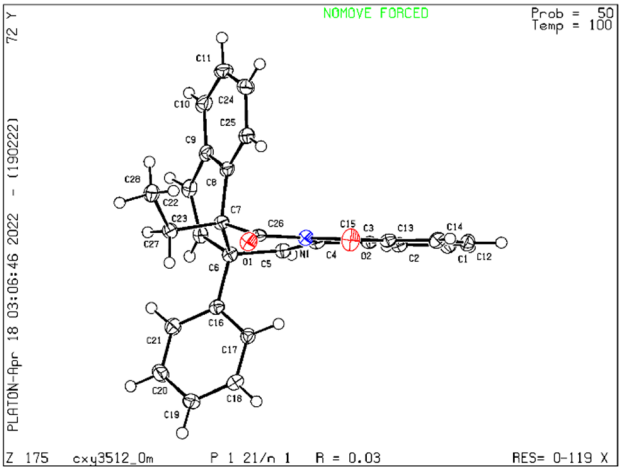
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.05 (s, 1H), 7.97 (s, 1H), 7.82 (dd, *J* = 7.6, 2.1 Hz, 1H), 7.73 – 7.70 (m, 1H), 7.49 – 7.43 (m, 3H), 7.30 (dt, *J* = 8.6, 2.3 Hz, 3H), 7.09 (t, *J* = 7.7 Hz, 2H), 6.98 (d, *J* = 8.6 Hz, 1H), 6.51 (s, 1H), 2.29 (s, 3H) ppm.

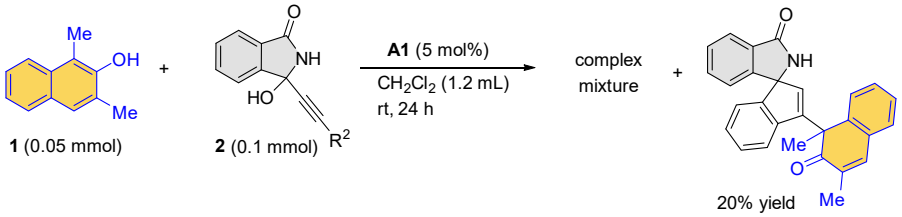
^{13}C NMR (101 MHz, Chloroform-*d*) δ 191.1, 165.5, 140.1, 137.9, 137.5, 136.5, 135.7, 133.3, 133.3, 133.2, 132.7, 130.74, 128.4, 128.1, 128.1, 127.9, 127.3, 126.5, 126.4, 126.1, 125.6, 124.8, 122.6, 104.3, 14.4 ppm.

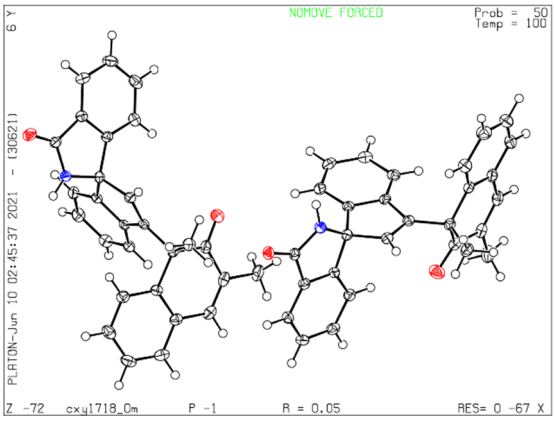
HRMS (CI+) Calcd for $C_{27}H_{18}Cl_2NO_2^+$ [M+H$^+$]: 458.0709, Found: 458.0705.

Further investigations



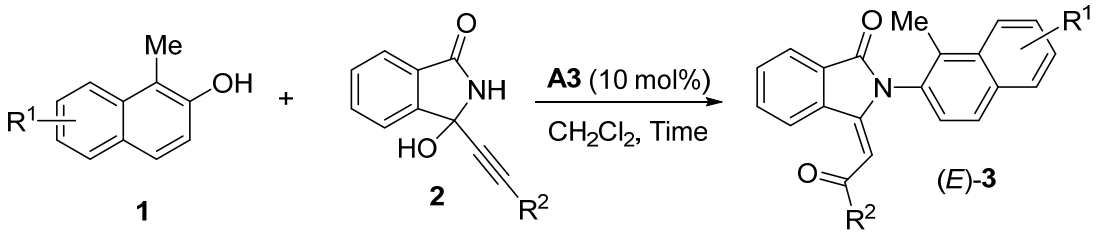




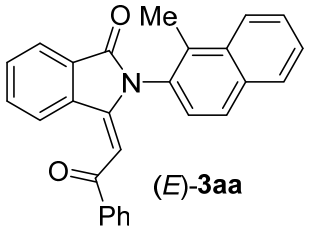


V. Synthesis of (*E*)-Products

General Procedure E



At room temperature, to a 10 mL-vial charged with 4-nitrobenzenesulfonic acid (**A3**, 4.1 mg, 10 mol%, 0.02 mmol) and the 1-methylnaphthalen-2-ol **1** (0.2 mmol), propargylic alcohol **2** (0.4 mmol) was added the solvent DCM (4.8 mL). The mixture was stirred for noted time under Ar. Upon completion (24 h), the reaction was quenched by addition of a Et_3N (14 μL, 50 mol%, 0.1 mmol). Next, the mixture was concentrated by vacuum. The residue was subjected to silica gel column chromatography to afford the pure product.

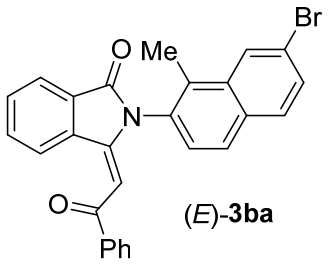


(*E*)-2-(1-methylnaphthalen-2-yl)-3-(2-oxo-2-phenylethylidene)isoindolin-1-one ((*E*)-**3aa**) was prepared as a yellow amorphous solid from 1-methylnaphthalen-2-ol **1a** (31.6 mg, 1.0 equiv, 0.2 mmol) and 3-hydroxy-3-(phenylethynyl)isoindolin-1-one **2a** (99.6 mg, 2.0 equiv, 0.4 mmol) according to the General Procedure E (24 h, eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 63.8 mg, 82% yield), mp 170.5-171.7 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.04 (d, *J* = 7.8 Hz, 1H), 8.19 – 8.14 (m, 1H), 8.02 (d, *J* = 7.4 Hz, 1H), 7.97 – 7.94 (m, 1H), 7.92 (d, *J* = 8.6 Hz, 1H), 7.79 – 7.75 (m, 3H), 7.71 (t, *J* = 7.8 Hz, 1H), 7.67 – 7.59 (m, 2H), 7.49 (t, *J* = 7.4 Hz, 1H), 7.41 – 7.34 (m, 3H), 6.36 (s, 1H), 2.57 (s, 3H) ppm.

^{13}C NMR (101 MHz, Chloroform-*d*) δ 189.9, 167.3, 149.7, 139.1, 134.3, 134.2, 133.8, 133.3, 133.0, 132.1, 130.2, 129.6, 128.9, 128.8, 128.7, 128.3, 128.3, 127.7, 127.0, 126.9, 126.2, 125.0, 123.9, 105.6, 14.0 ppm.

HRMS (CI+) Calcd for $C_{27}H_{20}NO_2^+$ [M+H$^+$]: 390.1489, Found: 390.1487.



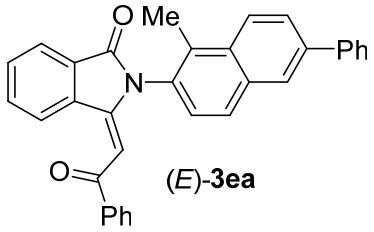
(*E*)-**3ba**

(*E*)-2-(7-Bromo-1-methylnaphthalen-2-yl)-3-(2-oxo-2-phenylethylidene)isoindolin-1-one ((*E*)-**3ba**) was prepared as a yellow amorphous solid from 7-bromo-1-methylnaphthalen-2-ol **1b** (47.4 mg, 1.0 equiv, 0.2 mmol) and 3-hydroxy-3-(phenylethynyl)isoindolin-1-one **2a** (99.6 mg, 2.0 equiv, 0.4 mmol) according to the General Procedure E (24 h, eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 77.7 mg, 83% yield), mp 175.2-176.0 °C.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 9.02 (d, *J* = 7.8 Hz, 1H), 8.30 (d, *J* = 2.0 Hz, 1H), 8.01 (d, *J* = 7.4 Hz, 1H), 7.87 (d, *J* = 8.6 Hz, 1H), 7.81 (d, *J* = 8.7 Hz, 1H), 7.76 (d, *J* = 7.5 Hz, 3H), 7.73 – 7.67 (m, 2H), 7.50 (t, *J* = 7.4 Hz, 1H), 7.38 (dt, *J* = 7.6, 3.4 Hz, 3H), 6.31 (s, 1H), 2.52 (s, 3H) ppm.

^{13}C NMR (126 MHz, Chloroform-*d*) δ 189.8, 167.2, 149.4, 139.0, 134.5, 134.2, 133.9, 133.6, 133.0, 132.2, 132.1, 130.6, 130.4, 130.4, 130.0, 128.8, 128.3, 128.2, 127.7, 127.5, 126.7, 123.9, 121.4, 105.6, 14.1 ppm.

HRMS (CI+) Calcd for $C_{27}H_{19}BrNO_2^+$ [M+H$^+$]: 468.0594, Found: 468.0595.



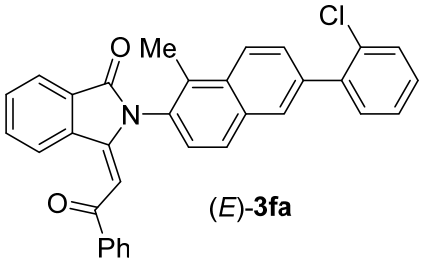
(*E*)-**3ea**

(*E*)-2-(1-Methyl-6-phenylnaphthalen-2-yl)-3-(2-oxo-2-phenylethylidene)isoindolin-1-one ((*E*)-**3ea**) was prepared as a yellow amorphous solid from 1-methyl-6-phenylnaphthalen-2-ol **1e** (46.8 mg, 1.0 equiv, 0.2 mmol) and 3-hydroxy-3-(phenylethynyl)isoindolin-1-one **2a** (99.6 mg, 2.0 equiv, 0.4 mmol) according to the General Procedure E (24 h, eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 88.4 mg, 95% yield), mp 162.5-163.1 °C.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 9.07 (d, *J* = 7.9 Hz, 1H), 8.23 (d, *J* = 8.8 Hz, 1H), 8.16 (s, 1H), 8.04 (d, *J* = 7.4 Hz, 1H), 7.98 (d, *J* = 8.6 Hz, 1H), 7.91 (dd, *J* = 8.8, 2.0 Hz, 1H), 7.81 – 7.77 (m, 5H), 7.72 (td, *J* = 8.6, 7.6, 1.1 Hz, 1H), 7.51 (dt, *J* = 18.6, 7.7 Hz, 3H), 7.45 – 7.37 (m, 4H), 6.41 (s, 1H), 2.60 (s, 3H) ppm.

^{13}C NMR (126 MHz, Chloroform-*d*) δ 189.9, 167.3, 149.7, 140.5, 139.6, 139.1, 134.2, 134.1, 133.8, 132.9, 132.4, 132.1, 130.1, 129.6, 129.1, 128.9, 128.7, 128.5, 128.3, 127.8, 127.7, 127.5, 126.6, 126.5, 126.5, 125.6, 123.9, 105.6, 14.0 ppm.

HRMS (CI+) Calcd for $C_{33}H_{24}NO_2^+$ [M+H$^+$]: 466.1802, Found: 466.1802.



(*E*)-**3fa**

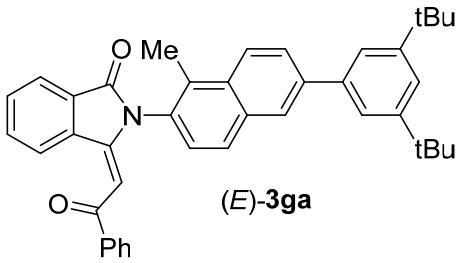
(*E*)-2-(6-(2-Chlorophenyl)-1-methylnaphthalen-2-yl)-3-(2-oxo-2-phenylethylidene)isoindolin-1-one ((*E*)-**3fa**) was prepared as a yellow amorphous solid from 6-(2-chlorophenyl)-1-methylnaphthalen-2-ol **1f** (53.7 mg, 1.0 equiv, 0.2 mmol) and 3-hydroxy-3-(phenylethynyl)isoindolin-1-one **2a** (99.6

mg, 2.0 equiv, 0.4 mmol) according to the General Procedure E (24 h, eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 71.0 mg, 71% yield), mp 158.7-159.5 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.06 (d, *J* = 7.6 Hz, 1H), 8.23 (d, *J* = 8.7 Hz, 1H), 8.05 – 8.00 (m, 2H), 7.97 (d, *J* = 8.6 Hz, 1H), 7.83 – 7.75 (m, 4H), 7.72 (t, *J* = 7.4 Hz, 1H), 7.56 – 7.53 (m, 1H), 7.52 – 7.46 (m, 2H), 7.44 – 7.35 (m, 5H), 6.42 (s, 1H), 2.61 (s, 3H) ppm.

^{13}C NMR (101 MHz, Chloroform-*d*) δ 189.9, 167.3, 149.6, 140.0, 139.1, 138.1, 134.3, 134.2, 133.8, 133.6, 132.9, 132.8, 132.5, 132.1, 131.6, 130.2, 130.1, 129.9, 129.2, 129.1, 128.7, 128.6, 128.5, 128.3, 127.7, 127.1, 126.6, 124.7, 123.8, 105.6, 14.0 ppm.

HRMS (CI+) Calcd for $C_{33}H_{23}ClNO_2^+$ [M+H$^+$]: 500.1412, Found: 500.1412.



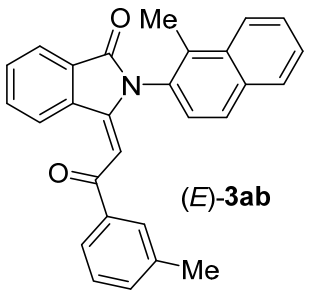
(*E*)-**3ga**

(*E*)-2-(6-(3,5-Di-*tert*-butylphenyl)-1-methylnaphthalen-2-yl)-3-(2-oxo-2-phenylethylidene)isoindolin-1-one ((*E*)-**3ga**) was prepared as a yellow amorphous solid from 6-(3,5-di-*tert*-butylphenyl)-1-methylnaphthalen-2-ol **1g** (69.3 mg, 1.0 equiv, 0.2 mmol) and 3-hydroxy-3-(phenylethynyl)isoindolin-1-one **2a** (99.6 mg, 2.0 equiv, 0.4 mmol) according to the General Procedure E (24 h, eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 84.4 mg, 73% yield), mp 140.2-141.6 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.11 (d, *J* = 7.7 Hz, 1H), 8.28 (d, *J* = 8.8 Hz, 1H), 8.19 (s, 1H), 8.06 (t, *J* = 9.0 Hz, 2H), 7.97 (d, *J* = 8.7 Hz, 1H), 7.84 (d, *J* = 8.1 Hz, 2H), 7.80 (d, *J* = 7.8 Hz, 1H), 7.74 (t, *J* = 7.4 Hz, 1H), 7.65 (s, 2H), 7.58 (s, 1H), 7.52 (t, *J* = 7.4 Hz, 1H), 7.47 – 7.39 (m, 3H), 6.45 (s, 1H), 2.65 (s, 3H), 1.49 (s, 18H) ppm.

^{13}C NMR (101 MHz, Chloroform-*d*) δ 189.9, 167.3, 151.5, 149.7, 140.9, 140.1, 139.1, 134.2, 134.2, 134.1, 133.8, 132.9, 132.3, 132.1, 130.1, 129.4, 128.7, 128.5, 128.3, 127.7, 127.0, 126.7, 126.6, 125.5, 123.8, 122.1, 122.0, 105.6, 35.2, 31.7, 14.0 ppm.

HRMS (CI+) Calcd for $C_{41}H_{40}NO_2^+$ [M+H$^+$]: 578.3054, Found: 578.3051.



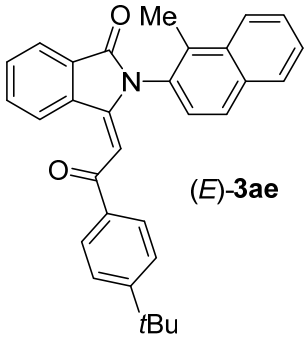
(*E*)-**3ab**

(*E*)-2-(1-Methylnaphthalen-2-yl)-3-(2-oxo-2-(m-tolyl)ethylidene)isoindolin-1-one ((*E*)-**3ab**) was prepared as a yellow amorphous solid from 1-methylnaphthalen-2-ol **1a** (31.6 mg, 1.0 equiv, 0.2 mmol) and 3-hydroxy-3-(*m*-tolylethynyl)isoindolin-1-one **2b** (105.3 mg, 2.0 equiv, 0.4 mmol) according to the General Procedure E (24 h, eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 69.4 mg, 86% yield), mp 158.2-159.4 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.03 (d, *J* = 7.9 Hz, 1H), 8.16 (dd, *J* = 8.3, 1.6 Hz, 1H), 8.04 (d, *J* = 7.2 Hz, 1H), 7.98 – 7.91 (m, 2H), 7.77 (td, *J* = 7.7, 1.4 Hz, 1H), 7.72 (d, *J* = 8.1 Hz, 1H), 7.68 (d, *J* = 3.3 Hz, 1H), 7.66 – 7.59 (m, 2H), 7.53 (d, *J* = 7.6 Hz, 1H), 7.40 (d, *J* = 8.6 Hz, 1H), 7.31 (d, *J* = 7.8 Hz, 1H), 7.27 – 7.23 (m, 1H), 6.38 (s, 1H), 2.59 (s, 3H), 2.35 (s, 3H) ppm.

^{13}C NMR (101 MHz, Chloroform-*d*) δ 190.2, 167.3, 149.3, 139.0, 138.5, 134.2, 134.2, 133.7, 133.7, 133.2, 132.0, 130.1, 129.6, 128.8, 128.8, 128.5, 128.2, 127.6, 127.0, 126.9, 126.8, 126.1, 125.5, 124.9, 123.8, 105.9, 21.4, 14.0 ppm.

HRMS (CI+) Calcd for $C_{28}H_{22}NO_2^+$ [M+H$^+$]: 404.1645, Found: 404.1643.



(*E*)-**3ae**

(*E*)-3-(2-(4-(*tert*-Butyl)phenyl)-2-oxoethylidene)-2-(1-methylnaphthalen-2-yl)isoindolin-1-one ((*E*)-**3ae**) was prepared as a yellow amorphous solid from 1-methylnaphthalen-2-ol **1a** (31.6 mg, 1.0 equiv, 0.2 mmol) and 3-((4-(*tert*-butyl)phenyl)ethynyl)-3-hydroxyisoindolin-1-one **2e** (122.2 mg, 2.0 equiv, 0.4 mmol) according to the General Procedure E (24 h, eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 58.8 mg, 66% yield), mp 131.2-132.5 °C.

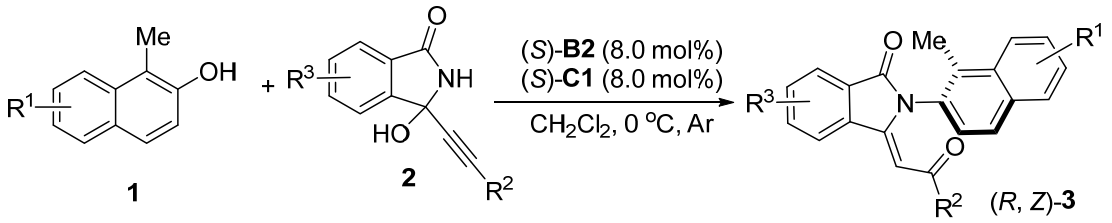
^{1}H NMR (500 MHz, Chloroform-*d*) δ 9.04 (d, *J* = 7.7 Hz, 1H), 8.16 (d, *J* = 7.5 Hz, 1H), 8.01 (d, *J* = 7.3 Hz, 1H), 7.96 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.91 (d, *J* = 8.6 Hz, 1H), 7.76 (td, *J* = 7.7, 1.3 Hz, 1H), 7.73 – 7.68 (m, 3H), 7.66 – 7.60 (m, 2H), 7.38 (dd, *J* = 12.2, 8.6 Hz, 3H), 6.36 (s, 1H), 2.56 (s, 3H), 1.28 (s, 9H) ppm.

^{13}C NMR (126 MHz, Chloroform-*d*) δ 189.6, 167.4, 156.8, 149.3, 136.5, 134.3, 134.3, 133.8, 133.8, 133.3, 132.0, 130.2, 129.6, 128.8, 128.3, 128.3, 127.7, 127.0, 126.9, 126.2, 125.7, 125.0, 123.8, 105.9, 35.2, 31.1, 14.0 ppm.

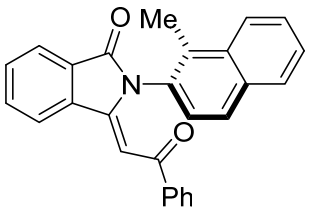
HRMS (CI+) Calcd for $C_{31}H_{28}NO_2^+$ [M+H$^+$]: 446.2115, Found: 446.2114.

VI. Enantioselective Synthesis of (*Z*)-Atropisomers

General Procedure F



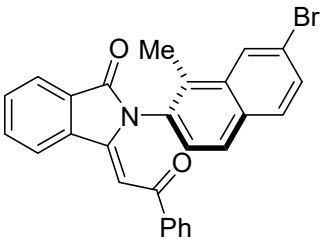
At room temperature, to a 20 mL-vial charged with (*S*)-**B2** (15.3 mg, 8.0 mol%, 0.016 mmol), (*S*)-**C1** (14.1 mg, 8.0 mol%, 0.016 mmol), the 1-methylnaphthalen-2-ol **1** (0.2 mmol) and propargylic alcohol **2** (0.4 mmol) was added the solvent DCM (8.0 mL). The mixture was stirred for 5 minutes at room temperature then cooled down to 0°C for other 6 days under Ar. Upon completion, the reaction was directly subjected to silica gel column chromatography to afford the desired product.



(*R*, *Z*)-**3aa**

(*R*)-(*Z*)-2-(1-Methylnaphthalen-2-yl)-3-(2-oxo-2-phenylethylidene)isoindolin-1-one ((*R*, *Z*)-**3aa**) was prepared as a yellow amorphous solid from 1-methylnaphthalen-2-ol **1a** (31.6 mg, 1.0 equiv, 0.2 mmol) and 3-hydroxy-3-(phenylethynyl)isoindolin-1-one **2a** (99.6 mg, 2.0 equiv, 0.4 mmol) according to the General Procedure F (eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 43.6 mg, 91% ee, 56% yield), mp 168.8-170.0 °C.

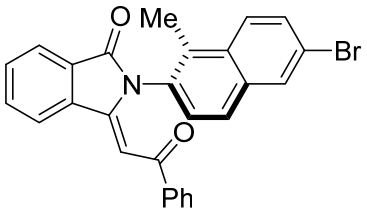
$[\alpha]_D^{25}$: -4.60 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK IE-3 column; 30% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 26.2 min (major), 32.5 min (minor).



(*R*, *Z*)-**3ba**

(*R*)-(*Z*)-2-(7-Bromo-1-methylnaphthalen-2-yl)-3-(2-oxo-2-phenylethylidene)isoindolin-1-one ((*R*, *Z*)-**3ba**) was prepared as a yellow amorphous solid from 7-bromo-1-methylnaphthalen-2-ol **1b** (47.4 mg, 1.0 equiv, 0.2 mmol) and 3-hydroxy-3-(phenylethynyl)isoindolin-1-one **2a** (99.6 mg, 2.0 equiv, 0.4 mmol) according to the General Procedure F (eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 53.2 mg, 79% ee, 57% yield), mp 177.6-178.8 °C.

$[\alpha]_D^{25}$: +37.3 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK IE-3 column; 30% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 23.6 min (minor), 25.4 min (major).

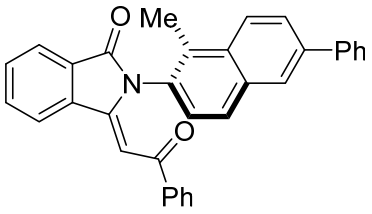


(*R*, *Z*)-**3da**

(*R*)-(*Z*)-2-(6-Bromo-1-methylnaphthalen-2-yl)-3-(2-oxo-2-phenylethylidene)isoindolin-1-one ((*R*, *Z*)-**3da**) was prepared as a yellow amorphous solid from 6-bromo-1-methylnaphthalen-2-ol **1d** (47.4 mg, 1.0 equiv, 0.2 mmol) and 3-hydroxy-3-(phenylethynyl)isoindolin-1-one **2a** (99.6 mg, 2.0 equiv, 0.4 mmol) according to the General Procedure F (eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 29.9 mg, 90% ee, 32% yield), mp 168.7-169.9 °C.

$[\alpha]_D^{25}$: -10.2 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK

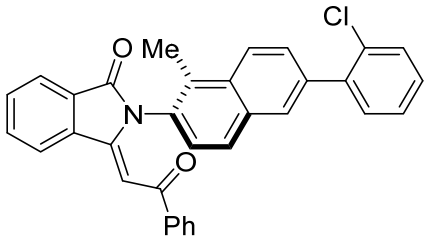
IE-3 column; 30% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 24.1 min (major), 29.4 min (minor).



(*R*, *Z*)-**3ea**

(*R*)-(*Z*)-2-(1-Methyl-6-phenylnaphthalen-2-yl)-3-(2-oxo-2-phenylethylidene)isoindolin-1-one ((*R*, *Z*)-**3ea**) was prepared as a yellow amorphous solid from 1-methyl-6-phenylnaphthalen-2-ol **1e** (46.8 mg, 1.0 equiv, 0.2 mmol) and 3-hydroxy-3-(phenylethynyl)isoindolin-1-one **2a** (99.6 mg, 2.0 equiv, 0.4 mmol) according to the General Procedure F (eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 63.2 mg, 92% ee, 68% yield) , mp 160.1-161.2 °C.

$[\alpha]_D^{25}$: -14.6 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK IE-3 column; 30% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 36.9 min (major), 53.3 min (minor).

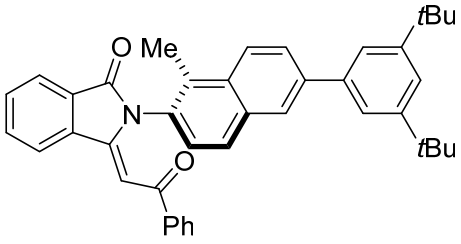


(*R*, *Z*)-**3fa**

(*R*)-(*Z*)-2-(6-(2-Chlorophenyl)-1-methylnaphthalen-2-yl)-3-(2-oxo-2-phenylethylidene)isoindolin-1-one ((*R*, *Z*)-**3fa**) was prepared as a yellow amorphous solid from 6-(2-chlorophenyl)-1-methylnaphthalen-2-ol **1f** (53.7 mg, 1.0 equiv, 0.2 mmol) and 3-hydroxy-3-(phenylethynyl)isoindolin-1-one **2a** (99.6 mg, 2.0 equiv, 0.4 mmol) according to the General Procedure F (eluent for flash

column chromatography: petroleum ether/DCM = 1:1 to DCM, 46.9 mg, 88% ee, 47% yield), mp 161.4-163.1 °C.

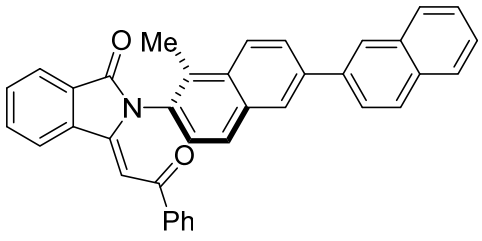
$[\alpha]_D^{25}$: +2.4 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK IE-3 column; 30% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 35.9 min (major), 43.7 min (minor).



(*R*, *Z*)-**3ga**

(*R*)-(*Z*)-2-(6-(3,5-Di-*tert*-butylphenyl)-1-methylnaphthalen-2-yl)-3-(2-oxo-2-phenylethylidene)isoindolin-1-one ((*R*, *Z*)-**3ga**) was prepared as a yellow amorphous solid from 6-(3,5-di-*tert*-butylphenyl)-1-methylnaphthalen-2-ol **1g** (69.3 mg, 1.0 equiv, 0.2 mmol) and 3-hydroxy-3-(phenylethynyl)isoindolin-1-one **2a** (99.6 mg, 2.0 equiv, 0.4 mmol) according to the General Procedure F (eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 36.9 mg, 76% ee, 32% yield), mp 143.2-144.7 °C.

$[\alpha]_D^{25}$: -5.7 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK IE-3 column; 30% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 16.3 min (major), 25.6 min (minor).

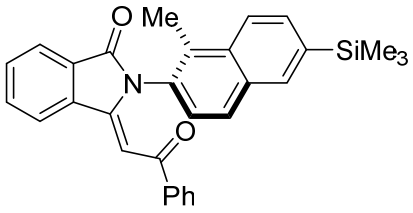


(*R*, *Z*)-**3ha**

(*R*)-(*Z*)-2-(5-Methyl-[2,2'-binaphthalen]-6-yl)-3-(2-oxo-2-phenylethylidene)isoindolin-1-one ((*R*, *Z*)-**3ha**) was prepared as a yellow

amorphous solid from 5-methyl-[2,2'-binaphthalen]-6-ol **1h** (56.9 mg, 1.0 equiv, 0.2 mmol) and 3-hydroxy-3-(phenylethynyl)isoindolin-1-one **2a** (99.6 mg, 2.0 equiv, 0.4 mmol) according to the General Procedure F (eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 65.9 mg, 94% ee, 64% yield), mp 170.5-171.8 °C.

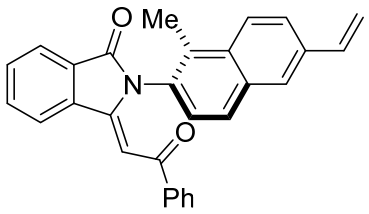
$[\alpha]_D^{25}$: -12.6 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK IE-3 column; 50% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 29.1 min (major), 46.0 min (minor).



(*R*, *Z*)-**3ia**

(*R*)-(*Z*)-2-(1-Methyl-6-(trimethylsilyl)naphthalen-2-yl)-3-(2-oxo-2-phenylethylidene)isoindolin-1-one ((*R*, *Z*)-**3ia**) was prepared as a yellow amorphous solid from 1-methyl-6-(trimethylsilyl)naphthalen-2-ol **1i** (46.1 mg, 1.0 equiv, 0.2 mmol) and 3-hydroxy-3-(phenylethynyl)isoindolin-1-one **2a** (99.6 mg, 2.0 equiv, 0.4 mmol) according to the General Procedure F (eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 41.5 mg, 85% ee, 45% yield), mp 117.6-119.2 °C.

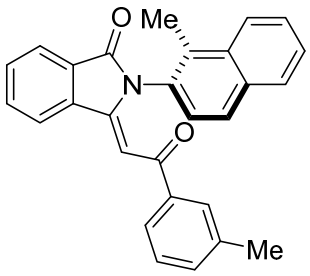
$[\alpha]_D^{25}$: -2.9 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK IE-3 column; 30% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 19.3 min (major), 28.7 min (minor).



(*R*, *Z*)-**3ja**

(*R*)-(*Z*)-2-(1-Methyl-6-vinylnaphthalen-2-yl)-3-(2-oxo-2-phenylethylidene)isoindolin-1-one ((*R*, *Z*)-**3ja**) was prepared as a yellow amorphous solid from 1-methyl-6-vinylnaphthalen-2-ol **1j** (36.8 mg, 1.0 equiv, 0.2 mmol) and 3-hydroxy-3-(phenylethynyl)isoindolin-1-one **2a** (99.6 mg, 2.0 equiv, 0.4 mmol) according to the General Procedure F (eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 33.2 mg, 94% ee, 40% yield), mp 154.2-155.7 °C.

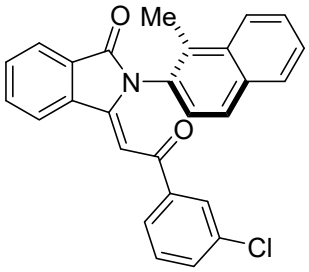
$[\alpha]_D^{25}$: +8.6 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK IE-3 column; 40% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 20.5 min (major), 26.4 min (minor).



(*R*, *Z*)-**3ab**

(*R*)-(*Z*)-2-(1-Methylnaphthalen-2-yl)-3-(2-oxo-2-(*m*-tolyl)ethylidene)isoindolin-1-one ((*R*, *Z*)-**3ab**) was prepared as a yellow amorphous solid from 1-methylnaphthalen-2-ol **1a** (31.6 mg, 1.0 equiv, 0.2 mmol) and 3-hydroxy-3-(*m*-tolylethynyl)isoindolin-1-one **2b** (105.3 mg, 2.0 equiv, 0.4 mmol) according to the General Procedure F (eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 25.8 mg, 91% ee, 32% yield), mp 159.1-160.3 °C.

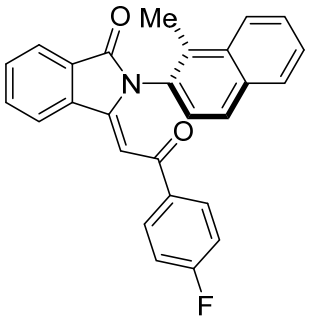
$[\alpha]_D^{25}$: -8.4 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK IE-3 column; 30% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 27.3 min (major), 33.8 min (minor).



(*R*, *Z*)-**3ac**

(*R*)-(*Z*)-3-(2-(3-Chlorophenyl)-2-oxoethylidene)-2-(1-methylnaphthalen-2-yl)isoindolin-1-one ((*R*, *Z*)-**3ac**) was prepared as a yellow amorphous solid from 1-methylnaphthalen-2-ol **1a** (31.6 mg, 1.0 equiv, 0.2 mmol) and 3-((3-chlorophenyl)ethynyl)-3-hydroxyisoindolin-1-one **2c** (113.5 mg, 2.0 equiv, 0.4 mmol) according to the General Procedure F (eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 40.6 mg, 90% ee, 48% yield), mp 170.5-172.4 °C.

$[\alpha]_D^{25}$: -9.6 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK IE-3 column; 30% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 19.9 min (major), 23.2 min (minor).

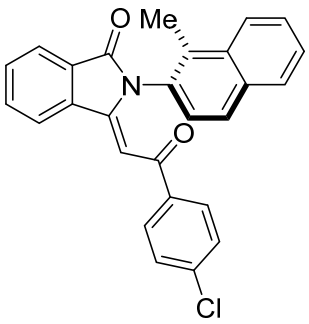


(*R*, *Z*)-**3af**

(*R*)-(*Z*)-3-(2-(4-Fluorophenyl)-2-oxoethylidene)-2-(1-methylnaphthalen-2-yl)isoindolin-1-one ((*R*, *Z*)-**3af**) was prepared as a yellow amorphous solid from 1-methylnaphthalen-2-ol **1a** (31.6 mg, 1.0 equiv, 0.2 mmol) and 3-((4-fluorophenyl)ethynyl)-3-hydroxyisoindolin-1-one **2f** (106.9 mg, 2.0 equiv, 0.4 mmol) according to the General Procedure F (eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 47.2 mg, 88% ee, 58%

yield), mp 197.4-198.8 °C.

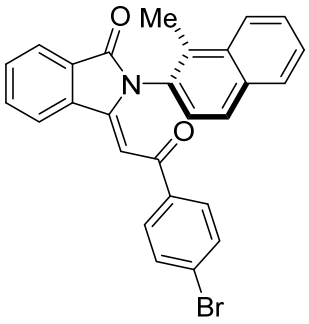
$[\alpha]_D^{25}$: -3.4 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK IE-3 column; 30% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 20.3 min (major), 23.8 min (minor).



(*R*, *Z*)-**3ag**

(*R*)-(*Z*)-3-(2-(4-Chlorophenyl)-2-oxoethylidene)-2-(1-methylnaphthalen-2-yl)isoindolin-1-one ((*R*, *Z*)-**3ag**) was prepared as a yellow amorphous solid from 1-methylnaphthalen-2-ol **1a** (31.6 mg, 1.0 equiv, 0.2 mmol) and 3-((4-chlorophenyl)ethynyl)-3-hydroxyisoindolin-1-one **2g** (113.5 mg, 2.0 equiv, 0.4 mmol) according to the General Procedure F (eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 56.7 mg, 90% ee, 67% yield), mp 160.1-161.3 °C.

$[\alpha]_D^{25}$: -3.6 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK IE-3 column; 30% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 20.1 min (major), 24.1 min (minor).



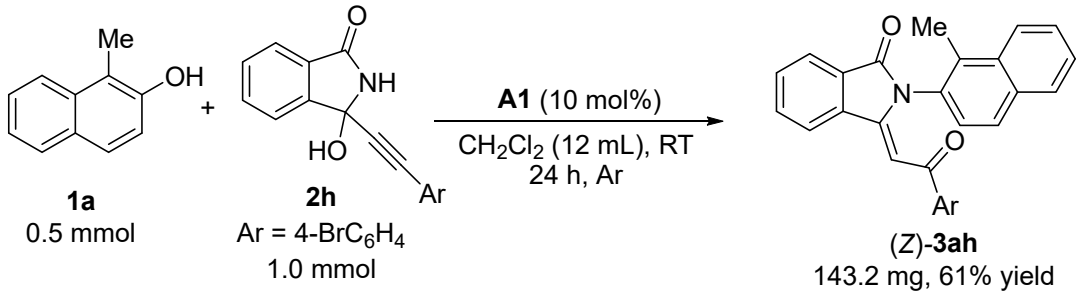
(*R*, *Z*)-**3ah**

(*R*)-(*Z*)-3-(2-(4-Bromophenyl)-2-oxoethylidene)-2-(1-methylnaphthalen-2-

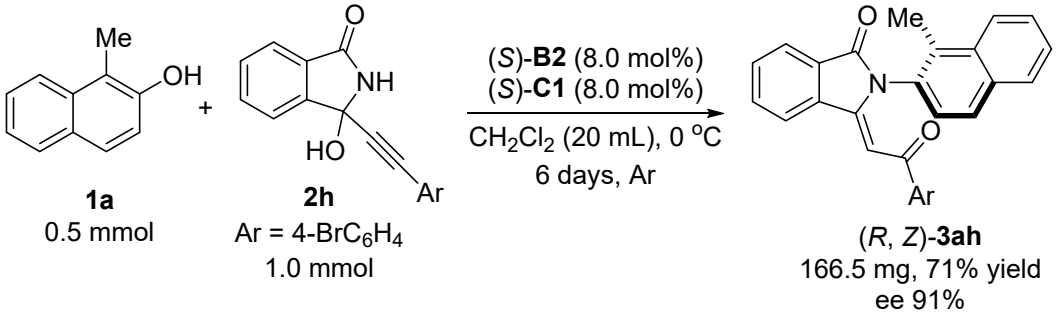
yl)isoindolin-1-one ((*R*, *Z*)-**3ah**) was prepared as a yellow amorphous solid from 1-methylnaphthalen-2-ol **1a** (31.6 mg, 1.0 equiv, 0.2 mmol) and 3-((4-bromophenyl)ethynyl)-3-hydroxyisoindolin-1-one **2h** (131.3 mg, 2.0 equiv, 0.4 mmol) according to the General Procedure F (eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 67.2 mg, 91% ee, 72% yield), mp 175.7-176.2 °C.

$[\alpha]_D^{25}$: -3.9 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK IE-3 column; 30% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 21.0 min (major), 25.4 min (minor).

VII. Scale up of Reactions



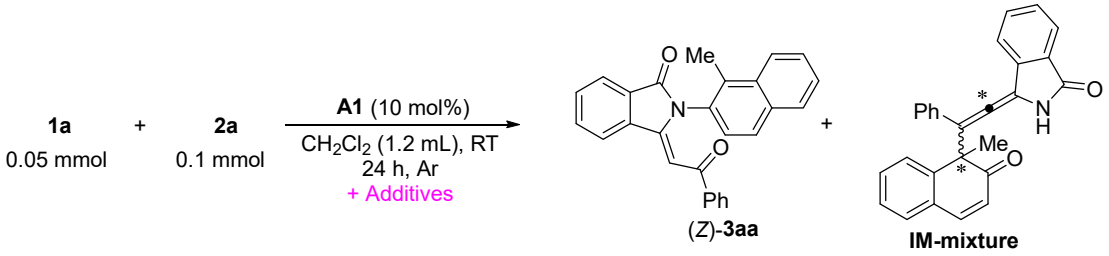
(*Z*)-3-(2-(4-Bromophenyl)-2-oxoethylidene)-2-(1-methylnaphthalen-2-yl)isoindolin-1-one ((*Z*)-**3ah**) was prepared as a yellow amorphous solid from 1-methylnaphthalen-2-ol **1a** (79.0 mg, 1.0 equiv, 0.5 mmol) and 3-((4-bromophenyl)ethynyl)-3-hydroxyisoindolin-1-one **2h** (329.0 mg, 2.0 equiv, 1.0 mmol) according to the General Procedure C (24 h, eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 143.2 mg, 61% yield).



(*R*)-(*Z*)-3-(2-(4-Bromophenyl)-2-oxoethylidene)-2-(1-methylnaphthalen-2-yl)isoindolin-1-one ((*R, Z*)-**3ah**) was prepared as a yellow amorphous solid from 1-methylnaphthalen-2-ol **1a** (79.0 mg, 1.0 equiv, 0.5 mmol) and 3-((4-bromophenyl)ethynyl)-3-hydroxyisoindolin-1-one **2h** (329.0 mg, 2.0 equiv, 1.0 mmol) according to the General Procedure F (eluent for flash column chromatography: petroleum ether/DCM = 1:1 to DCM, 166.5 mg, 91% ee, 71% yield).

VIII. Mechanistic Study

(1) Controlled experiment-H_2O



Entry	**Additives**	(*Z*)-**3aa**/%	**IM**/%
1	4Å MS (25 mg)	<5	90% (Mixture of diastereoisomers)
2	Na_2SO_4 (1 equiv.)	74%	<5
3	$+H_2{}^{18}O$ (10 equiv.)	80% (^{18}O-3aa major)	<5

Entry 1:

At room temperature, to a 4 mL-vial charged with naphthalene-2-sulfonic acid (**A1**, 1.1 mg, 10 mol%, 0.005 mmol), 4Å molecular sieve (25 mg) and 1-methylnaphthalen-2-ol **1a** (7.9 mg, 1.0 equiv, 0.05 mmol), 3-hydroxy-3-(phenylethynyl)isoindolin-1-one **2a** (24.9 mg, 2.0 equiv, 0.1 mmol) was added the solvent DCM (1.2 mL). The mixture was stirred for 24 h under Ar. Upon completion, the reaction was quenched by addition of a Et_3N (3.5 μL, 50 mol%, 0.025 mmol). Next, the mixture was concentrated by vacuum. CH_2Br_2 (3.5 μL, 0.05 mmol) was added to the mixture as internal standard, the composition of products was observed by ^{1}H NMR analysis.

Target product **3aa** was not observed, but an unknown intermediate **IM** was observed. Through the isolation and analysis, it was determined that the structure was tetrasubstituted allene, and was a mixture of diastereoisomers. This phenomenon (mixture of diastereoisomers) may be due to the equilibrium between **IM** and the starting material **1a**, **2a**. The characterization of **IM** would be discussed later in the supporting information.

The reason for the absence of **3aa** may be that the molecular sieve removed water or inhibited acid as a base, resulting in the inability of the rearrangement

reaction in the latter step.

Entry 2:

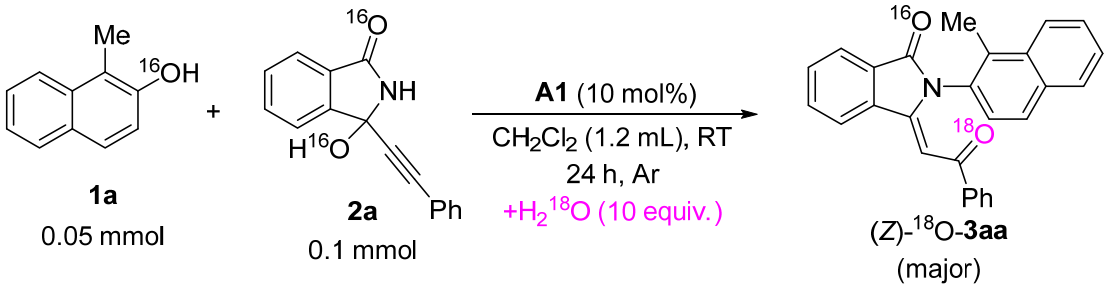
At room temperature, to a 4 mL-vial charged with naphthalene-2-sulfonic acid (**A1**, 1.1 mg, 10 mol%, 0.005 mmol), anhydrous Na_2SO_4 (7.1 mg, 1.0 equiv, 0.05 mmol) and 1-methylnaphthalen-2-ol **1a** (7.9 mg, 1.0 equiv, 0.05 mmol), 3-hydroxy-3-(phenylethynyl)isoindolin-1-one **2a** (24.9 mg, 2.0 equiv, 0.1 mmol) was added the solvent DCM (1.2 mL). The mixture was stirred for 24 h under Ar. Upon completion, the reaction was quenched by addition of a Et_3N (3.5 μL, 50 mol%, 0.025 mmol). Next, the mixture was concentrated by vacuum. CH_2Br_2 (3.5 μL, 0.05 mmol) was added to the mixture as internal standard, the composition of products was observed by ^1H NMR analysis.

The product **3aa** was obtained in 74% yield (slightly lower), probably because the crystalline water in Na_2SO_4 was still reactive.

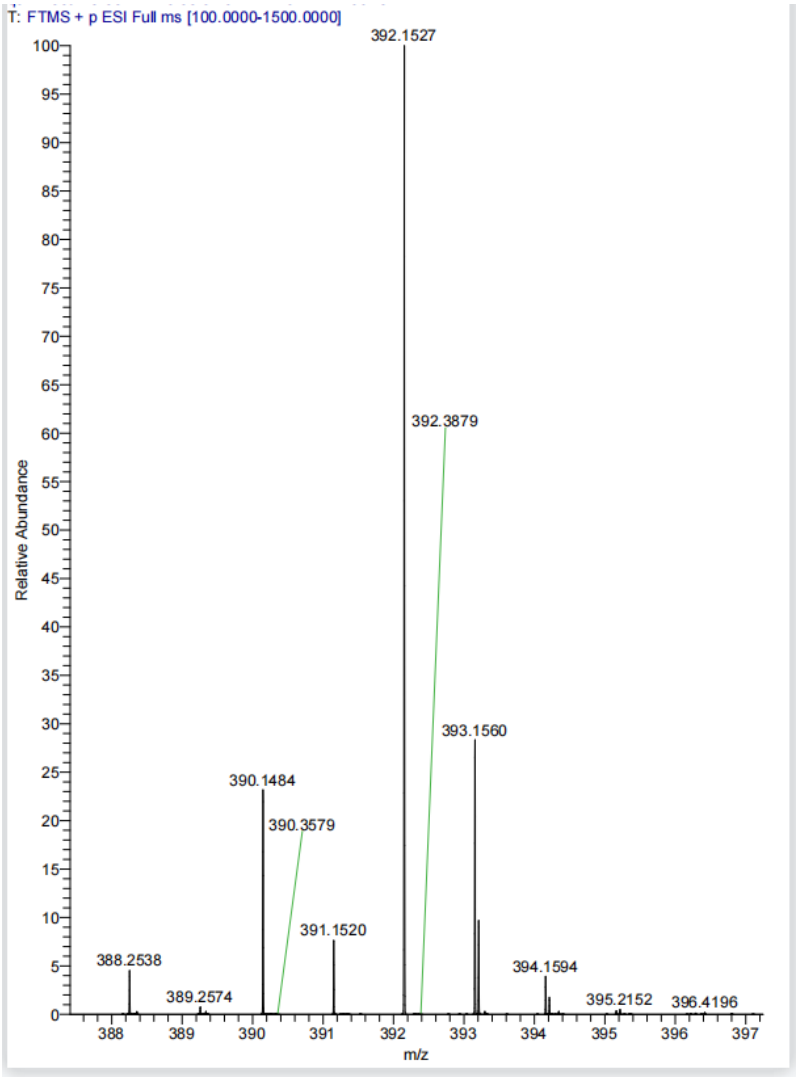
Entry 3:

At room temperature, to a 4 mL-vial charged with naphthalene-2-sulfonic acid (**A1**, 1.1 mg, 10 mol%, 0.005 mmol), $H_2{}^{18}O$ (10.0 mg, 10.0 equiv, 0.5 mmol) and 1-methylnaphthalen-2-ol **1a** (7.9 mg, 1.0 equiv, 0.05 mmol), 3-hydroxy-3-(phenylethynyl)isoindolin-1-one **2a** (24.9 mg, 2.0 equiv, 0.1 mmol) was added the solvent DCM (1.2 mL). The mixture was stirred for 24 h under Ar. Upon completion, the reaction was quenched by addition of a Et_3N (3.5 μL, 50 mol%, 0.025 mmol). Next, the mixture was concentrated by vacuum. CH_2Br_2 (3.5 μL, 0.05 mmol) was added to the mixture as internal standard, the composition of products was observed by ^1H NMR analysis.

The product **3aa** was obtained in 80% yield in NMR. The pure **3aa** was isolated by prepared TLC, then analyzed by mass spectrometry and NMR.

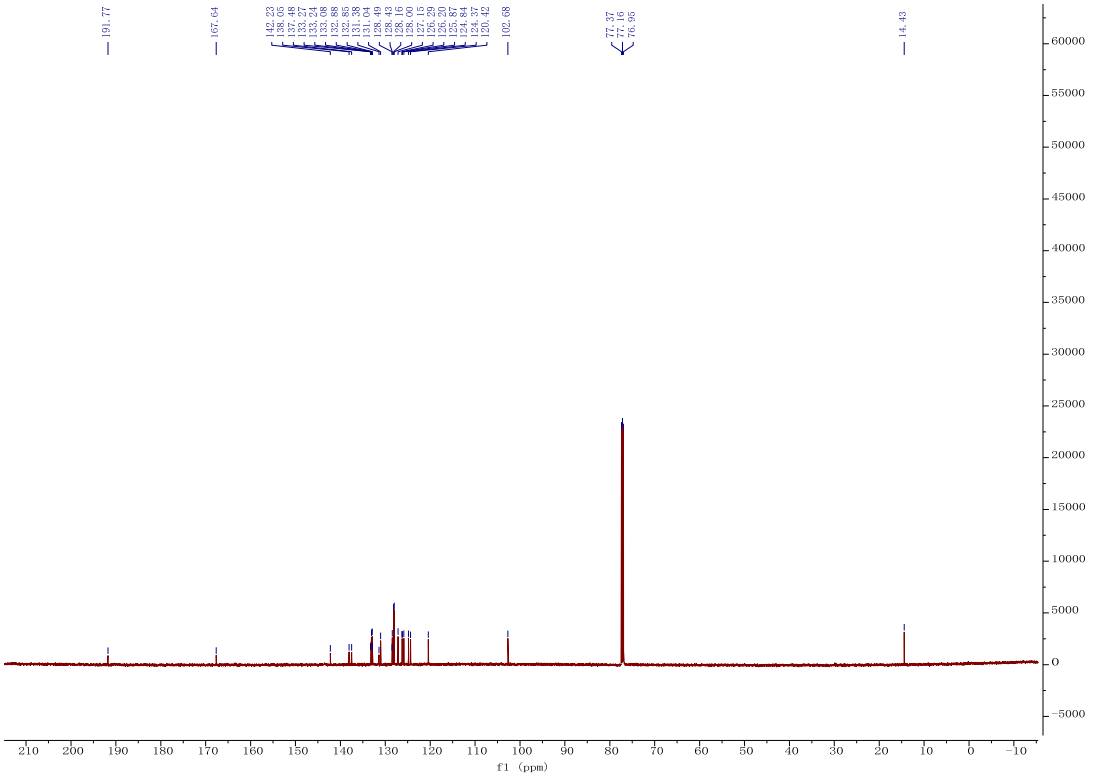


HRMS (CI+) Calcd for $C_{27}H_{20}NO^{16}O^{+}$ [M+H^{+}]: 390.1489, Calcd for $C_{27}H_{20}NO^{18}O^{+}$ [M+H^{+}]: 392.1531. Found: 390.1484 (minor) and 392.1527 (major).



^{13}C NMR of (Z)-**3aa**: (carbon of ketone 191.84 ppm).

^{13}C NMR of (Z)-^{18}O-**3aa**: (carbon of ketone 191.77 ppm).



In conclusion, the experiment proved that the oxygen atoms on the structure of the product ketone were not entirely derived from the phenolic hydroxyl group of **1a** in a catalytic cycle. Combined with the discovery of the intermediate allene **IM**, the existence of a process of adding water with the system.

(2) Controlled experiment-Ar

1) **1a** (0.05 mmol) + **2a** (0.1 mmol) → **A1** (10 mol%), CH_2Cl_2 (1.2 mL), RT, 24 h, Air → (*Z*)-**3aa** <5% yield + (*E*)-**3aa** 40% yield

2) **1a** (0.05 mmol) + **2a** (0.1 mmol) → (*S*)-**B2** (8.0 mol%), (*S*)-**C1** (8.0 mol%), CH_2Cl_2 (2.0 mL), RT, 24 h, Air → Messy

Entry 1:

At room temperature, to a 4 mL-vial charged with naphthalene-2-sulfonic acid (**A1**, 1.1 mg, 10 mol%, 0.005 mmol) and 1-methylnaphthalen-2-ol **1a** (7.9 mg, 1.0 equiv, 0.05 mmol), 3-hydroxy-3-(phenylethynyl)isoindolin-1-one **2a** (24.9 mg, 2.0 equiv, 0.1 mmol) was added the solvent DCM (1.2 mL). The mixture was

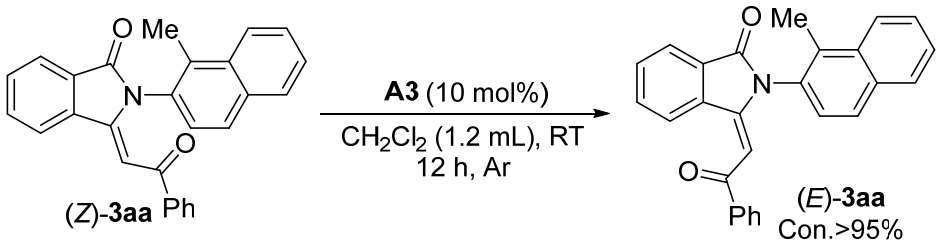
stirred for 24 h under air. Upon completion, the reaction was quenched by addition of a Et_3N (3.5 μL, 50 mol%, 0.025 mmol). Next, the mixture was concentrated by vacuum. CH_2Br_2 (3.5 μL, 0.05 mmol) was added to the mixture as internal standard, the composition of products was observed by ^1H NMR analysis.

Entry 2:

At room temperature, to a 4 mL-vial charged with (*S*)-**B2** (3.8 mg, 8.0 mol%, 0.004 mmol), (*S*)-**C1** (3.5 mg, 8.0 mol%, 0.004 mmol) and 1-methylnaphthalen-2-ol **1a** (7.9 mg, 1.0 equiv, 0.05 mmol), 3-hydroxy-3-(phenylethynyl)isoindolin-1-one **2a** (24.9 mg, 2.0 equiv, 0.1 mmol) was added the solvent DCM (1.2 mL). The mixture was stirred for 24 h under air. Upon completion, the reaction system was monitored by TLC.

Both experiments showed complex products, possibly due to the intermediates could be oxidized by oxygen. **A1** catalyzed the reaction faster, which allowed the reaction to obtain partial thermodynamic product (*E*)-**3aa**.

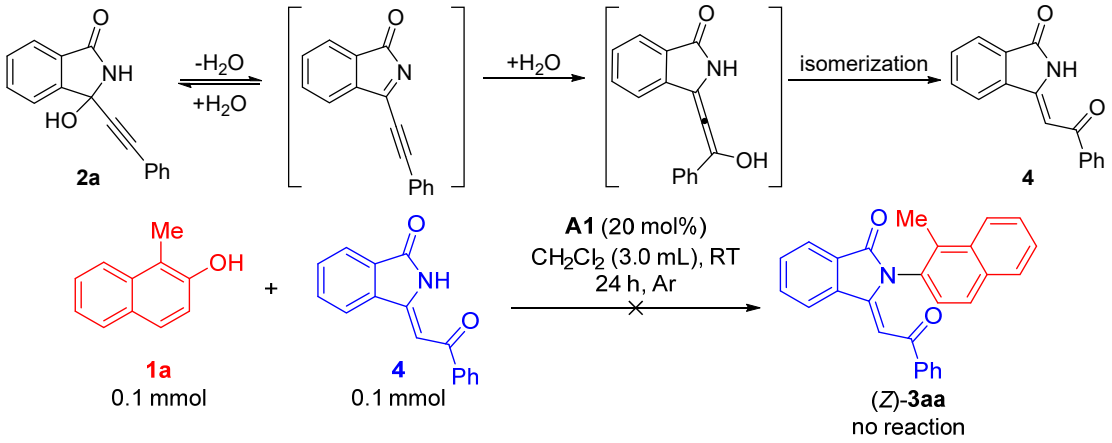
(3) Products transformation of (*Z*)-**3aa to** (*E*)-**3aa**



At room temperature, to a 4 mL-vial charged with 4-nitrobenzenesulfonic acid (**A3**, 2.1 mg, 10 mol%, 0.01 mmol) and (*Z*)-**3aa** (38.9 mg, 1.0 equiv, 0.1 mmol) was added the solvent DCM (1.2 mL). The mixture was stirred for 12 h under Ar. Upon completion, the reaction was quenched by addition of a Et_3N (7.0 μL, 50 mol%, 0.05 mmol). Next, the mixture was concentrated by vacuum. CH_2Br_2 (3.5 μL, 0.05 mmol) was added to the mixture as internal standard, the composition of products was observed by ^1H NMR analysis.

This experiment proved that (*E*)-**3aa** could be formed from (*Z*)-**3aa** catalyzed by a stronger acid. In General Procedure D, we did find the formation of (*Z*)-**3aa** in the process then went to (*E*)-**3aa**. It indicated that (*Z*)-**3aa** was the kinetics product, (*E*)-**3aa** was the more stable thermodynamics product because of the steric hindrance.

(4) Reaction of 4 with 1a

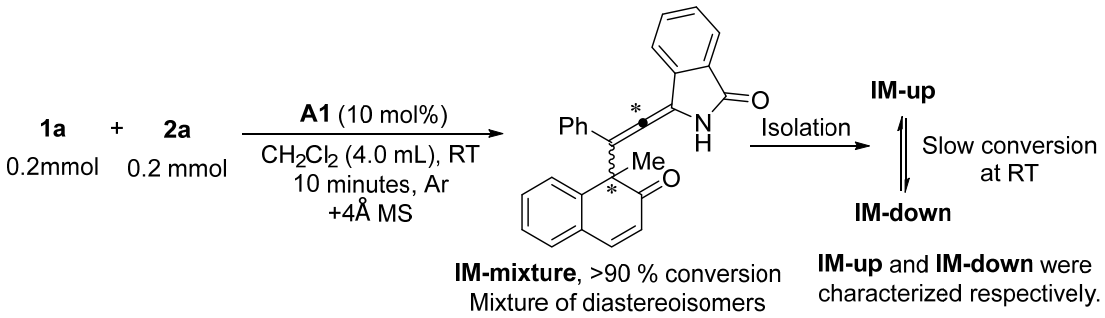


Based on our previous research, **2a** could be isomerized to form 3-(2-oxo-2-phenylethylidene)isoindolin-1-one (**4**) in the presence of Lewis acids.

At room temperature, to a 4 mL-vial charged with naphthalene-2-sulfonic acid (**A1**, 4.2 mg, 20 mol%, 0.01 mmol) and 3-(2-oxo-2-phenylethylidene)isoindolin-1-one (**4**) (24.9 mg, 1.0 equiv, 0.1 mmol) was added the solvent DCM (3.0 mL). The mixture was stirred for 24 h under Ar. Upon completion, the reaction was quenched by addition of a Et_3N (7.0 μL, 50 mol%, 0.05 mmol). Next, the mixture was concentrated by vacuum. CH_2Br_2 (3.5 μL, 0.05 mmol) was added to the mixture as internal standard, the composition of products was observed by ^1H NMR analysis. It was still a mixture of starting materials.

The experimental result showed that the two starting materials could not react to form the target product (*Z*)-**3aa** by a simple dehydration.

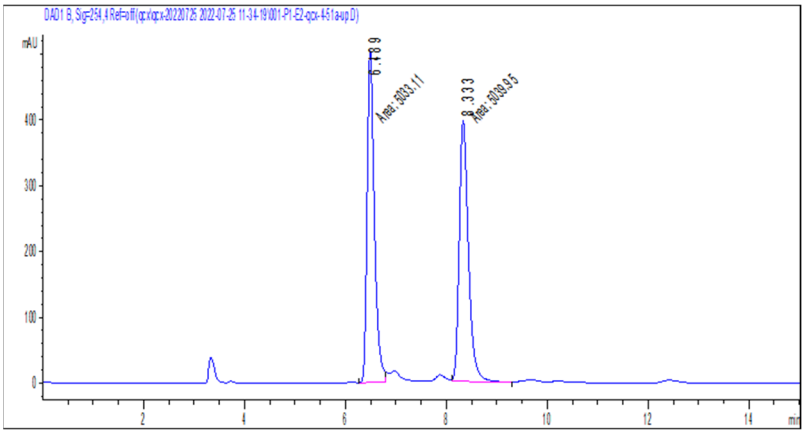
(5) Isolation of the intermediate



At room temperature, to a 10 mL-vial charged with naphthalene-2-sulfonic acid (**A1**, 4.2 mg, 10 mol%, 0.02 mmol), 4Å molecular sieve (50 mg) and 1-methylnaphthalen-2-ol **1a** (31.6 mg, 1.0 equiv, 0.2 mmol), 3-hydroxy-3-(phenylethynyl)isoindolin-1-one **2a** (49.8 mg, 1.0 equiv, 0.2 mmol) was added the solvent DCM (4.0 mL). The mixture was stirred at room temperature, monitored by TLC. Upon completion (10 minutes), 2 products were formed (Con.>90%). The products were isolated by prepared TLC (eluent for flash column chromatography: petroleum ether/ethyl acetate = 2:1), then characterized by NMR analysis quickly. Through subsequent research, it was found that the two products were mixture of diastereoisomers (dr~1:2). Since they could convert to each other at room temperature, we could not determine their absolute configurations separately, but their enantiomers could be separated separately by HPLC. The less polar one was named **IM-up**, the other one was named **IM-down**.

IM-up:

HPLC analysis of the product: Daicel CHIRALPAK IA-3 column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 6.5 min, 8.3 min.



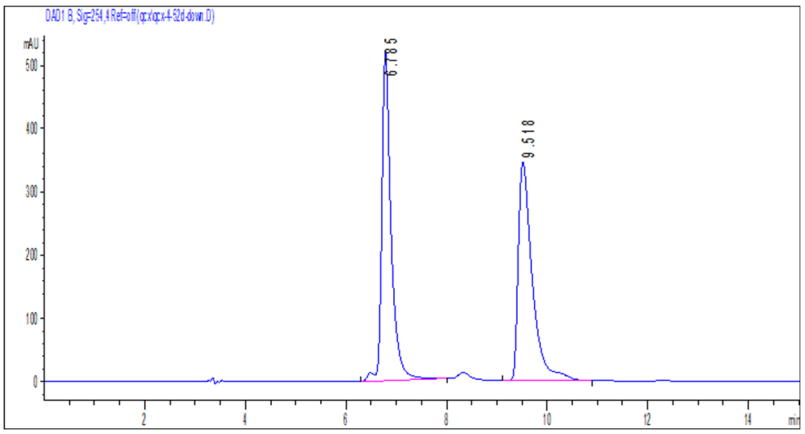
#	Time	Type	Area	Height	Width	Area%	Symmetry
1	6.489	MF	5033.1	505.1	0.1661	49.966	0.675
2	8.333	FM	5039.9	397.2	0.2115	50.034	0.713

^{1}H NMR (500 MHz, DMSO-d_6) δ 10.74 (s, 1H), 7.94 (d, J = 9.9 Hz, 1H), 7.86 (d, J = 7.6 Hz, 1H), 7.81 – 7.75 (m, 2H), 7.67 (dd, J = 7.5, 1.5 Hz, 1H), 7.65 – 7.60 (m, 2H), 7.45 (td, J = 7.5, 1.5 Hz, 1H), 7.40 (td, J = 7.4, 1.4 Hz, 1H), 7.17 – 7.10 (m, 3H), 6.84 (dd, J = 8.0, 1.6 Hz, 2H), 6.37 (d, J = 9.8 Hz, 1H), 1.36 (s, 3H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 199.6, 193.6, 166.6, 145.7, 145.1, 137.1, 134.0, 132.5, 130.8, 130.4, 129.5, 129.2, 128.6, 128.4, 127.9, 127.6, 127.1, 126.9, 124.3, 123.4, 121.9, 121.6, 113.4, 56.1, 30.7 ppm.

IM-down:

HPLC analysis of the product: Daicel CHIRALPAK IA-3 column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 6.8 min, 9.5 min.

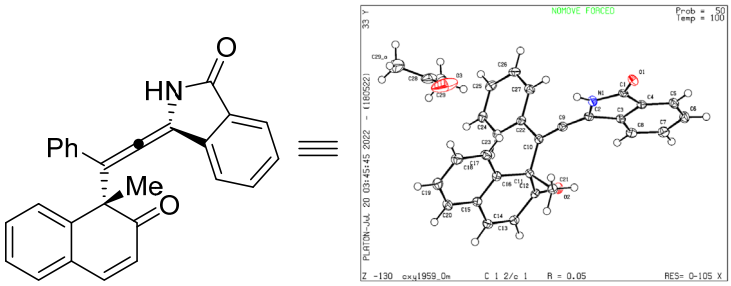


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	6.785	VB R	6723.1	520	0.188	49.986	0.636
2	9.518	BB	6727	345.2	0.2893	50.014	0.447

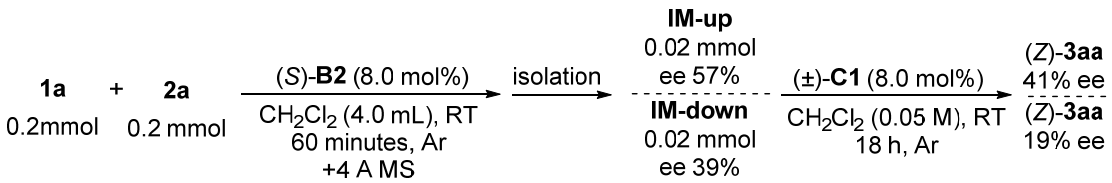
^{1}H NMR (400 MHz, DMSO-d_6) δ 10.73 (s, 1H), 7.91 (d, J = 9.9 Hz, 1H), 7.89 – 7.84 (m, 2H), 7.78 (td, J = 7.4, 1.2 Hz, 1H), 7.67 – 7.61 (m, 2H), 7.60 – 7.50 (m, 2H), 7.40 (td, J = 7.4, 1.5 Hz, 1H), 7.16 – 7.09 (m, 3H), 6.85 (dd, J = 8.0, 1.7 Hz, 2H), 6.36 (d, J = 9.8 Hz, 1H), 1.42 (s, 3H) ppm.

^{13}C NMR (126 MHz, DMSO-d_6) δ 199.6, 194.0, 166.6, 145.6, 144.7, 137.0, 134.0, 132.7, 131.1, 130.5, 129.5, 129.4, 128.6, 127.9, 127.6, 127.0, 126.9, 126.8, 124.2, 123.5, 122.1, 121.7, 113.8, 56.2, 30.7 ppm.

The structures were stable at low temperatures, but there still was a conversion of diastereoisomers and enantiomers. We determined the connection of chemical bond by X-ray crystallography, but we did not confirm which isomer it was.



(6) Reaction of chiral intermediates to products catalyzed by racemic acid



At room temperature, to a 10 mL-vial charged with catalyst ((*S*)-**B2**, 15.3 mg, 8.0 mol%, 0.016 mmol), 4Å molecular sieve (50 mg) and 1-methylnaphthalen-2-ol **1a** (31.6 mg, 1.0 equiv, 0.2 mmol), 3-hydroxy-3-(phenylethynyl)isoindolin-1-one **2a** (49.8 mg, 1.0 equiv, 0.2 mmol) was added the solvent DCM (4.0 mL). The

mixture was stirred at room temperature for 60 minutes, 2 products were formed (Con.>80%, dr ~1:1). The products were isolated by prepared TLC (eluent for flash column chromatography: petroleum ether/ethyl acetate = 2:1). The ee of two diastereoisomers was analyzed by HPLC separately.

The intermediates would racemize during separation and HPLC, so the **IMs** formed in the system should have higher ee. The proportion of diastereomers depended on the acid catalysts.

IM-up: 59% ee, HPLC analysis of the product: Daicel CHIRALPAK IA-3 column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 6.5 min (major), 8.4 min (minor).

IM-down: 39% ee, HPLC analysis of the product: Daicel CHIRALPAK IA-3 column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 6.8 min (major), 9.7 min (minor).

At room temperature, to a 4 mL-vial charged with (±)-**C1** (1.4 mg, 8.0 mol%, 0.0016 mmol) and **IM** (7.8 mg, 1.0 equiv, 0.02 mmol) the solvent DCM (0.4 mL). The mixture was stirred at room temperature under Ar. Upon completion (about 18 h), target product (*Z*)-**3aa** was formed. The product was isolated by prepared TLC (petroleum ether/DCM = 1:3), then analyzed by HPLC.

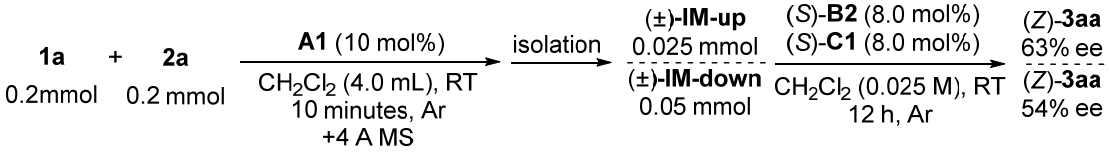
(*Z*)-**3aa** could be obtained from two diastereoisomers **IM** separately.

(*Z*)-**3aa** from **IM-up** (59% ee): 41% ee, 60% isolated yield.

(*Z*)-**3aa** from **IM-down** (39% ee): 19% ee, 40% isolated yield.

The results indicated that the chiral intermediates could convert in part to chiral target products by racemic acid. It proved that two **IM**s were intermediates in the reaction process. The decreasing of ee due to the equilibrium between **IM**s and the starting materials, and the ee of **IM**s would keep decreasing in presence of racemic acid.

(7) Reaction of racemic intermediates to products catalyzed by chiral acid



At room temperature, to a 10 mL-vial charged with naphthalene-2-sulfonic acid (**A1**, 4.2 mg, 10 mol%, 0.02 mmol), 4Å molecular sieve (50 mg) and 1-methylnaphthalen-2-ol **1a** (31.6 mg, 1.0 equiv, 0.2 mmol), 3-hydroxy-3-(phenylethynyl)isoindolin-1-one **2a** (49.8 mg, 1.0 equiv, 0.2 mmol) was added the solvent DCM (4.0 mL). The mixture was stirred at room temperature, monitored by TLC. Upon completion (10 minutes), 2 products were formed (Con.>90%, dr ~1:2). The products were isolated by prepared TLC (eluent for flash column chromatography: petroleum ether/ethyl acetate = 2:1).

At room temperature, to a 10 mL-vial charged with (*S*)-**B2** (1.9 mg, 8.0 mol%, 0.002 mmol), (*S*)-**C1** (1.8 mg, 8.0 mol%, 0.002 mmol) and **IM-up** (9.8 mg, 1.0 equiv, 0.025 mmol) the solvent DCM (1.0 mL). The mixture was stirred at room temperature under Ar. Upon completion (about 12 h), target product (*Z*)-**3aa** was formed. The product was isolated by prepared TLC (petroleum ether/DCM = 1:3), then analyzed by HPLC.

At room temperature, to a 10 mL-vial charged with (*S*)-**B2** (3.8 mg, 8.0 mol%, 0.004 mmol), (*S*)-**C1** (3.6 mg, 8.0 mol%, 0.004 mmol) and **IM-down** (19.5 mg, 1.0 equiv, 0.05 mmol) the solvent DCM (2.0 mL). The mixture was stirred at room temperature under Ar. Upon completion (about 12 h), target product (*Z*)-**3aa** was formed. The product was isolated by prepared TLC (petroleum ether/DCM = 1:3), then analyzed by HPLC.

(*Z*)-**3aa** from racemic **IM-up**: 63% ee, 60% isolated yield.

(*Z*)-**3aa** from racemic **IM-down**: 54% ee, 50% isolated yield.

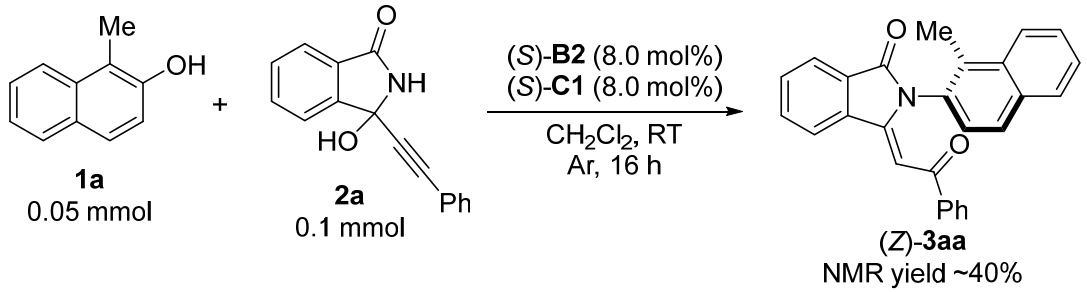
The results indicated that the racemic intermediates could convert to chiral target products by chiral acid. It further proved the equilibrium between **IM**s

and the starting materials, and the ee of **IM**s would keep increasing in presence of chiral acid.

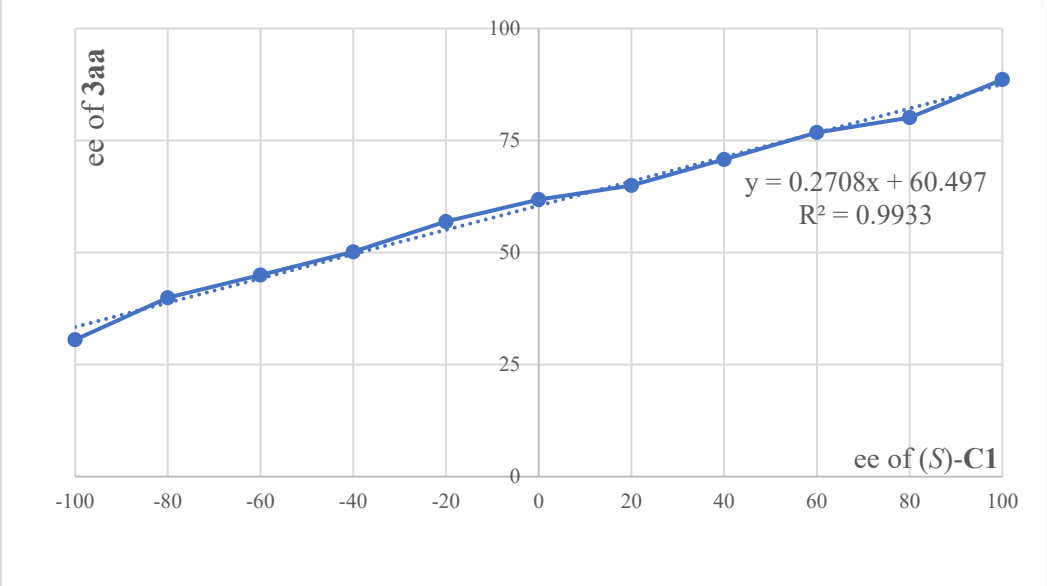
(8) Non-linear effect

a) With 100% ee (*S*)-**B2**

At room temperature, to a 4 mL-vial charged with (*S*)-**B2** (3.8 mg, 8.0 mol%, 0.004 mmol), and 1-methylnaphthalen-2-ol **1a** (7.9 mg, 1.0 equiv, 0.05 mmol), 3-hydroxy-3-(phenylethynyl)isoindolin-1-one **2a** (24.9 mg, 2.0 equiv, 0.1 mmol) was added the corresponding ee value DCM solution of **C1** (1.2 mL, 0.0033 M, 8.0 mol%). The mixture was stirred for 16 h under air. Upon completion, the mixture was directly subjected to short silica gel column chromatography to afford the desired product, then analyzed by HPLC.

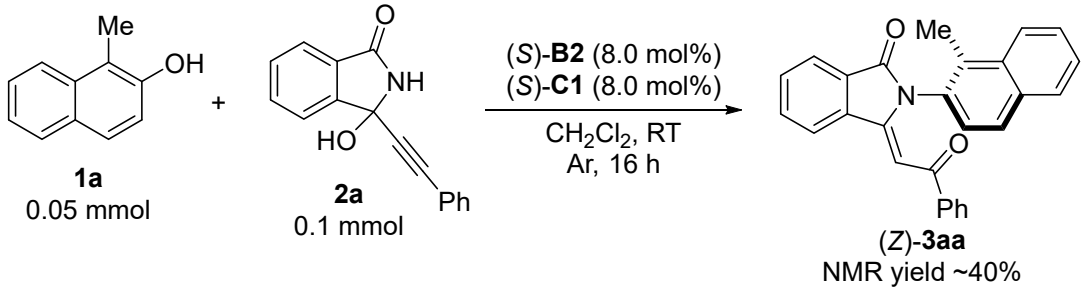


Entry	ee of (*S*)-**C1** (%)	ee of (*Z*)-**3aa** (%)
1	+100	88.61
2	+80	80.09
3	+60	76.78
4	+40	70.76
5	+20	64.95
6	0	61.81
7	-20	56.90
8	-40	50.15
9	-60	44.98
10	-80	39.91
11	-100	30.53



b) With 100% ee (*S*)-**C1**

At room temperature, to a 4 mL-vial charged with (*S*)-**C1** (3.5 mg, 8.0 mol%, 0.004 mmol), and 1-methylnaphthalen-2-ol **1a** (7.9 mg, 1.0 equiv, 0.05 mmol), 3-hydroxy-3-(phenylethynyl)isoindolin-1-one **2a** (24.9 mg, 2.0 equiv, 0.1 mmol) was added the corresponding ee value DCM solution of **B2** (1.2 mL, 0.0033 M, 8.0 mol%). The mixture was stirred for 16 h under air. Upon completion, the mixture was directly subjected to short silica gel column chromatography to afford the desired product, then analyzed by HPLC.



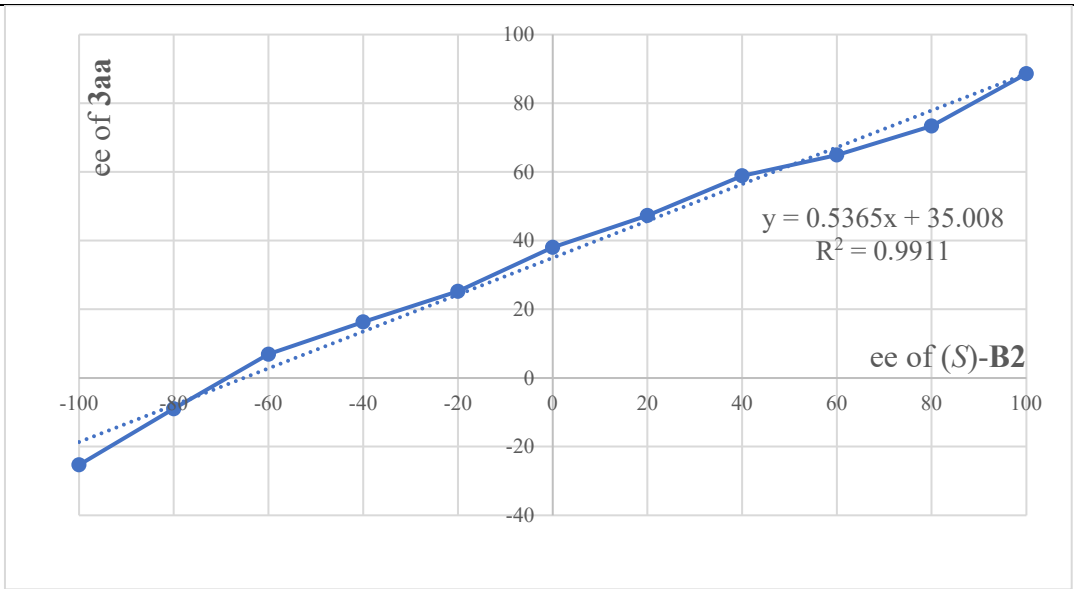
1a
0.05 mmol

2a
0.1 mmol

(*Z*)-**3aa**
NMR yield ~40%

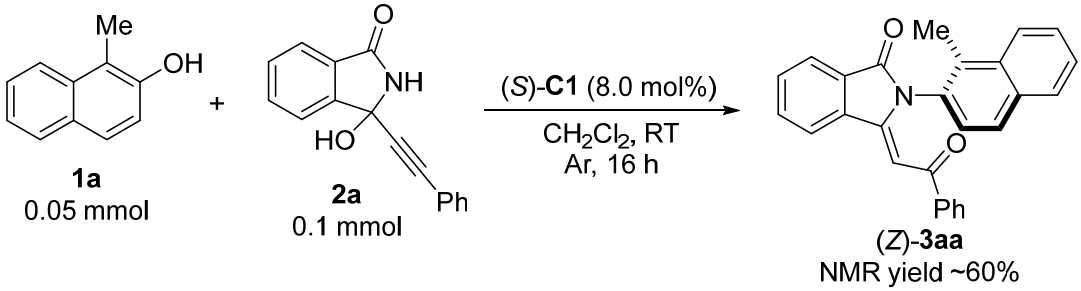
Entry	ee of (*S*)-**B2** (%)	ee of (*Z*)-**3aa** (%)
1	+100	88.61
2	+80	73.34
3	+60	64.91
4	+40	58.84
5	+20	47.29

6	0	38.01
7	-20	25.22
8	-40	16.29
9	-60	6.89
10	-80	-9.00
11	-100	-25.31



c) Only (*S*)-**C1**

At room temperature, to a 4 mL-vial charged with 1-methylnaphthalen-2-ol **1a** (7.9 mg, 1.0 equiv, 0.05 mmol), 3-hydroxy-3-(phenylethynyl)isoindolin-1-one **2a** (24.9 mg, 2.0 equiv, 0.1 mmol) was added the corresponding ee value DCM solution of **C1** (1.2 mL, 0.0033 M, 8.0 mol%). The mixture was stirred for 16 h under air. Upon completion, the mixture was directly subjected to short silica gel column chromatography to afford the desired product, then analyzed by HPLC.

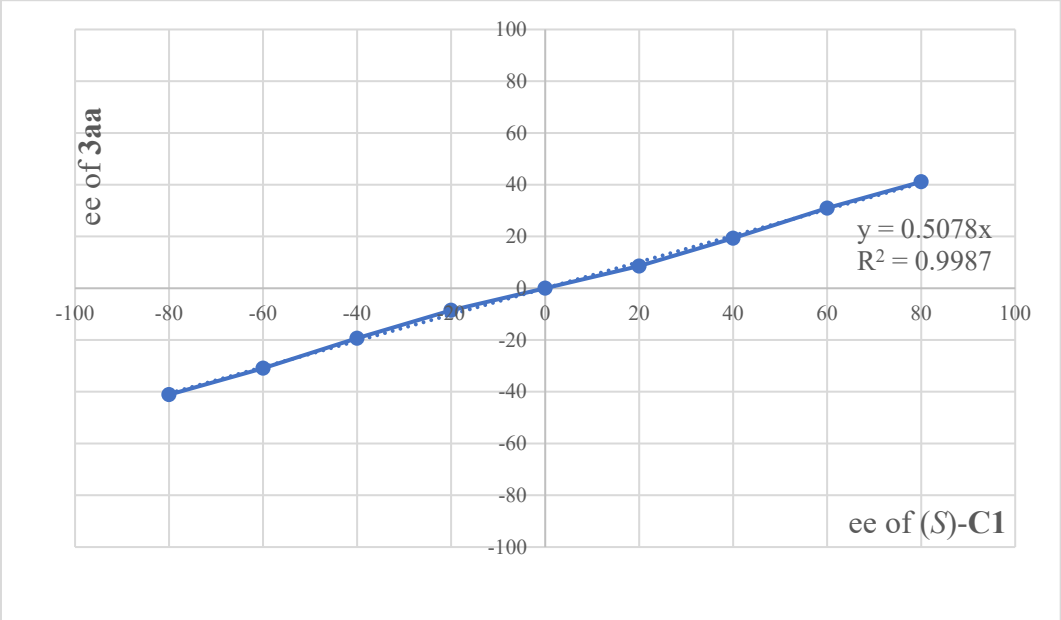


1a
0.05 mmol

2a
0.1 mmol

(*Z*)-**3aa**
NMR yield ~60%

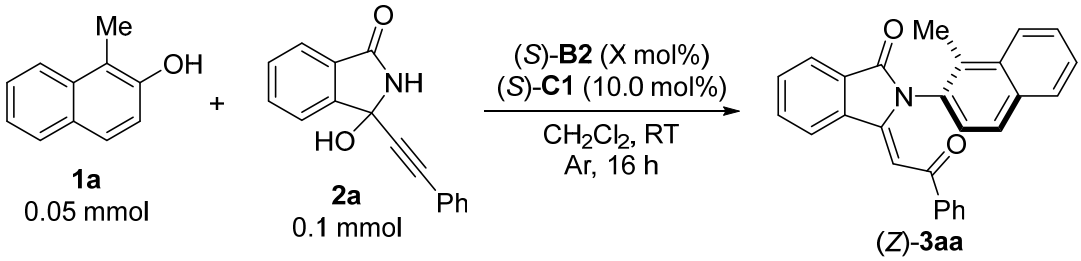
Entry	ee of (*S*)-**C1** (%)	ee of (*Z*)-**3aa** (%)
1	+80	41.16
2	+60	30.94
3	+40	19.33
4	+20	8.564
5	0	0
6	-20	-8.564
7	-40	-19.33
8	-60	-30.94
9	-80	-41.16



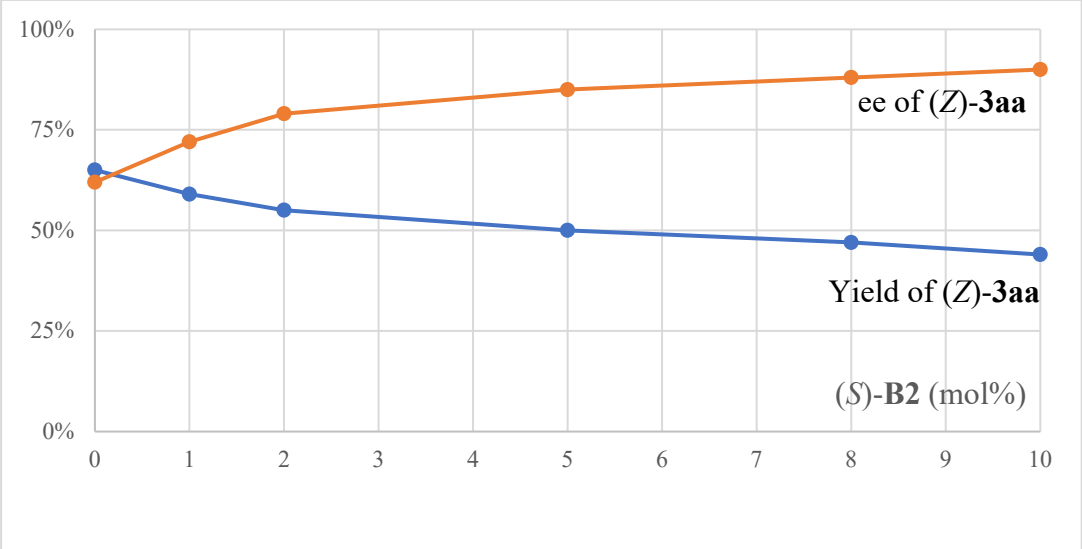
(9) Influence of addition of (*S*)-B2.

At room temperature, to a 4 mL-vial charged with (*S*)-**C1** (4.4 mg, 10.0 mol%, 0.005 mmol), (*S*)-**B2** (0 - 10 mol%) and 1-methylnaphthalen-2-ol **1a** (7.9 mg, 1.0 equiv, 0.05 mmol), 3-hydroxy-3-(phenylethynyl)isoindolin-1-one **2a** (24.9 mg, 2.0 equiv, 0.1 mmol) was added the solvent DCM (1.2 mL). The mixture was stirred for 16 h under air. Upon completion, the mixture was directly subjected to short silica gel column chromatography to remove catalysts, then was concentrated by vacuum. CH_2Br_2 (3.5 μL, 0.05 mmol) was added to the mixture as internal standard, yield of the product was observed by ^1H NMR analysis.

The ee of the product was analyzed by HPLC.



Entry	Usage of (*S*)-**B2** (mol%)	NMR yield of **3aa** (%)	ee of (*Z*)-**3aa**
1	0	65	62
2	1	59	72
3	2	55	79
4	5	50	85
5	8	47	88
6	10	44	90



IX. DFT Calculations

All DFT calculations were performed with Gaussian 16.[4] All molecular geometries optimizations were carried out with the M06-2X method including solvent effect in dichloromethane with SMD model.[5] The 6-31G(d) basis set was used for all atoms.[6] Signal point energies were calculated at the M06-2X/6-311G(d,p) level. The GD3 dispersion correction was used to simulate long-range dispersion interactions.[7] The reported free energies and electronic energies were obtained from the above-mentioned single-point SMD calculations combined with the liquid-phase free-energy and ZPE corrections, respectively. Frequency analysis was performed on the optimized structure. Each transition state was connected to its respective reactant and product by intrinsic reaction coordinate (IRC) calculations.[8] All energies of the optimized structures are Gibbs free relative energies and under standard conditions (298.15K and 1atm in Kcal mol^{-1}). 3D structures shown in figures were generated by CYLview.[9]

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[4] 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.; 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 16 Revision A.03*, Gaussian, Inc., Wallingford CT, **2016**.

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[7] Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. A Consistent and Accurate Ab Initio Parametrization of Density Functional Dispersion Correction (DFT-D) for the 94 Elements H-Pu. *J. Chem. Phys.* **2010**, *132* (15), 154104-154119.

[8] Gonzalez, C.; Schlegel, H. B. An improved algorithm for reaction path following. *J. Chem. Phys.* **1989**, 90, 2154–2161.

[9] CYLview, 1.0b; Legault, C. Y., Université de Sherbrooke, 2009 (http://www.cylview.org).

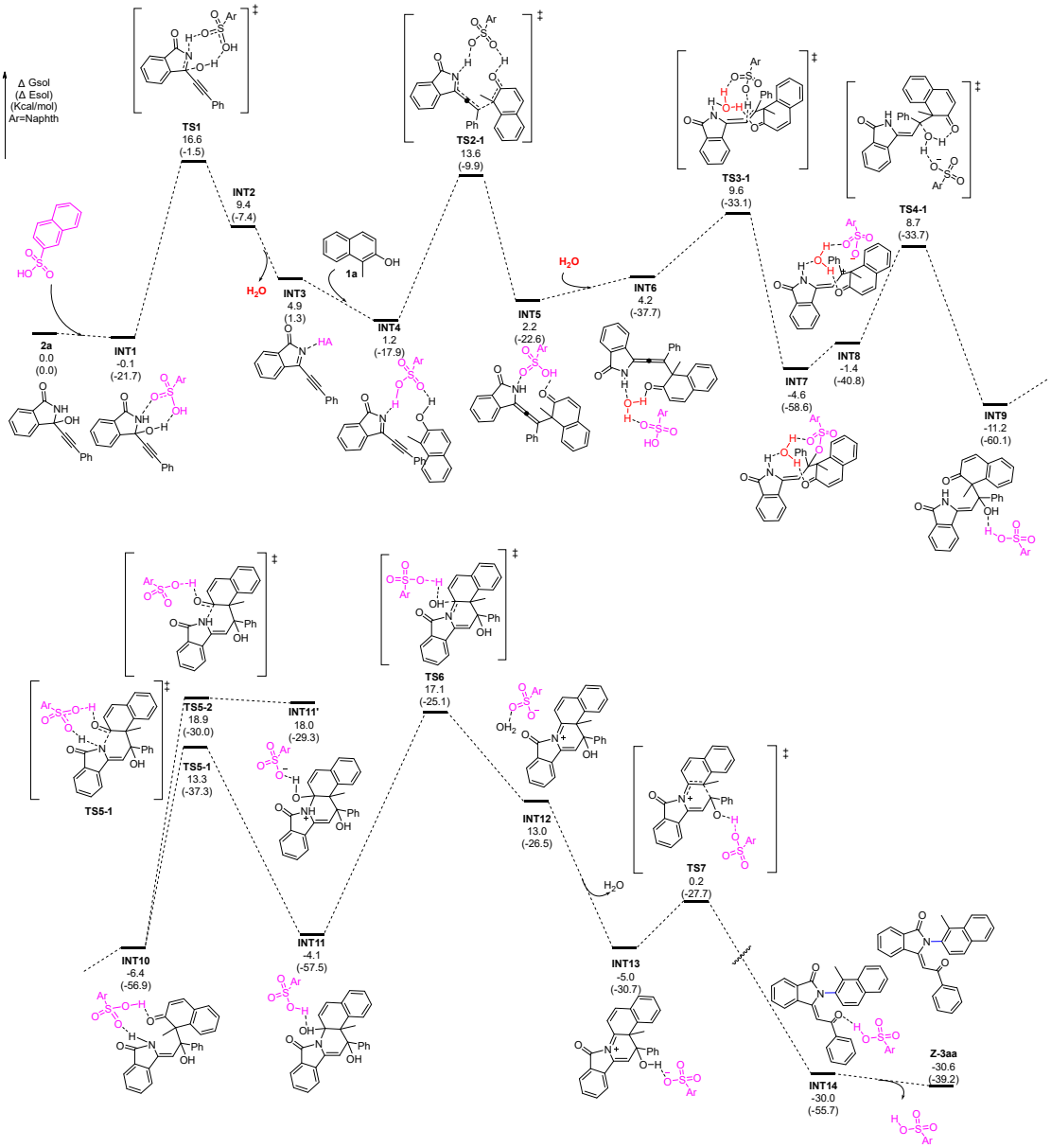
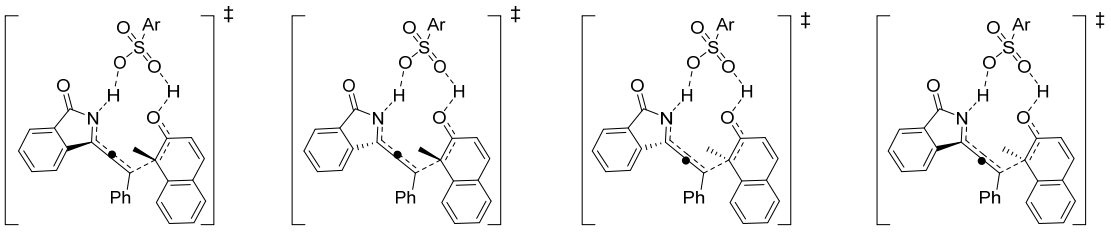


Figure S1. Complete energetic profiles at the M06-2X-D3/6-311G(d,p)-SMD(DCM)//M06-2X-D3/6-31G(d) level of theory (kcal/mol).



TS2-1
13.6
(-9.9)

TS2-2
22.2
(-2.1)

TS2-3
13.8
(-9.3)

TS2-4
20.2
(-2.1)

Scheme S1. Different isomers of TS2 at the M06-2X-D3/6-311G(d,p)-

SMD(DCM)//M06-2X-D3/6-31G(d) level of theory.

DFT calculation shows that the distribution of diastereoisomers of INT5 intermediate formed through TS2 is uneven, which is consistent with the control experiment (7).

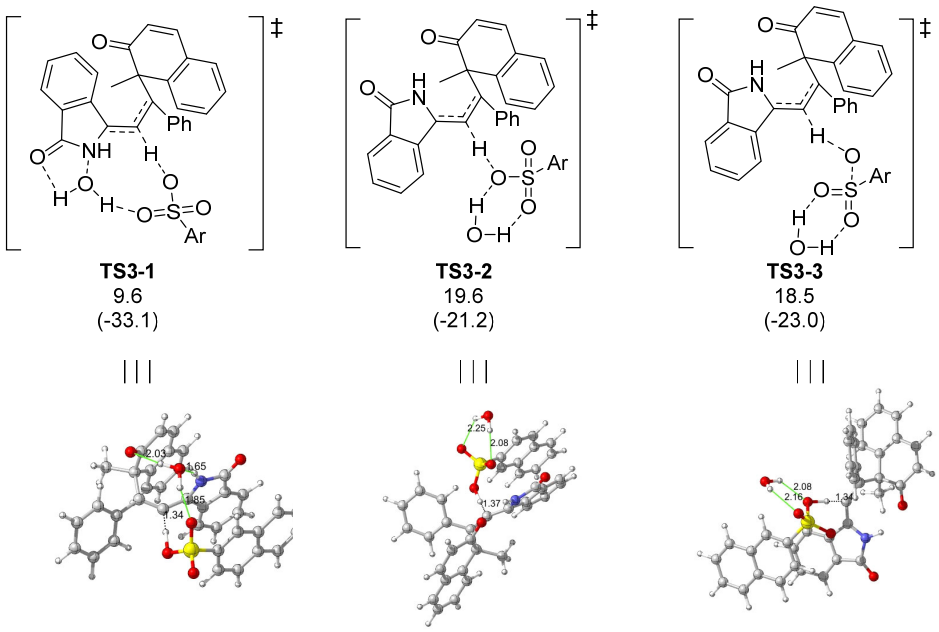


Figure S2. Different conformations of TS3 at the M06-2X-D3/6-311G(d,p)-SMD(DCM)//M06-2X-D3/6-31G(d) level of theory.

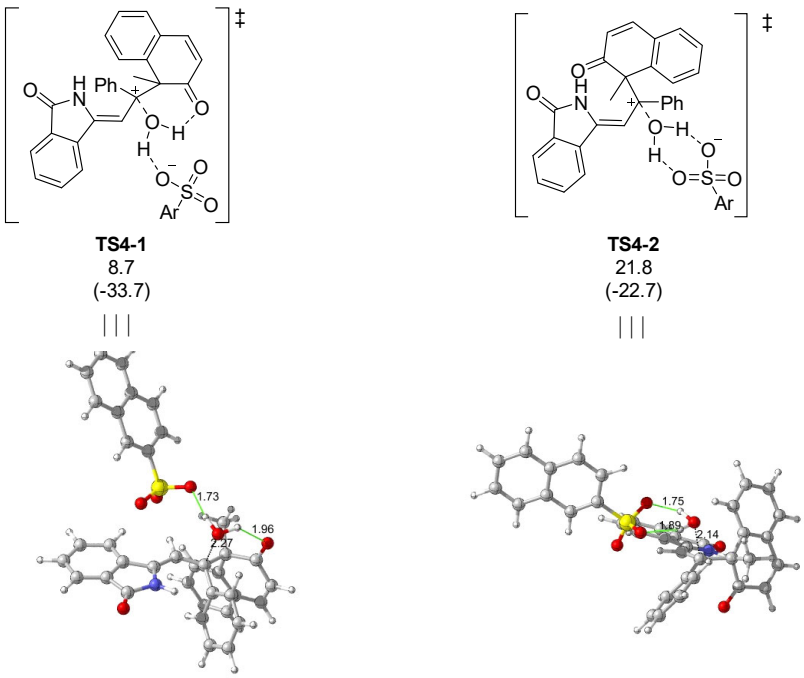


Figure S3. Different conformations of TS4 at the M06-2X-D3/6-311G(d,p)-SMD(DCM)//M06-2X-D3/6-31G(d) level of theory.

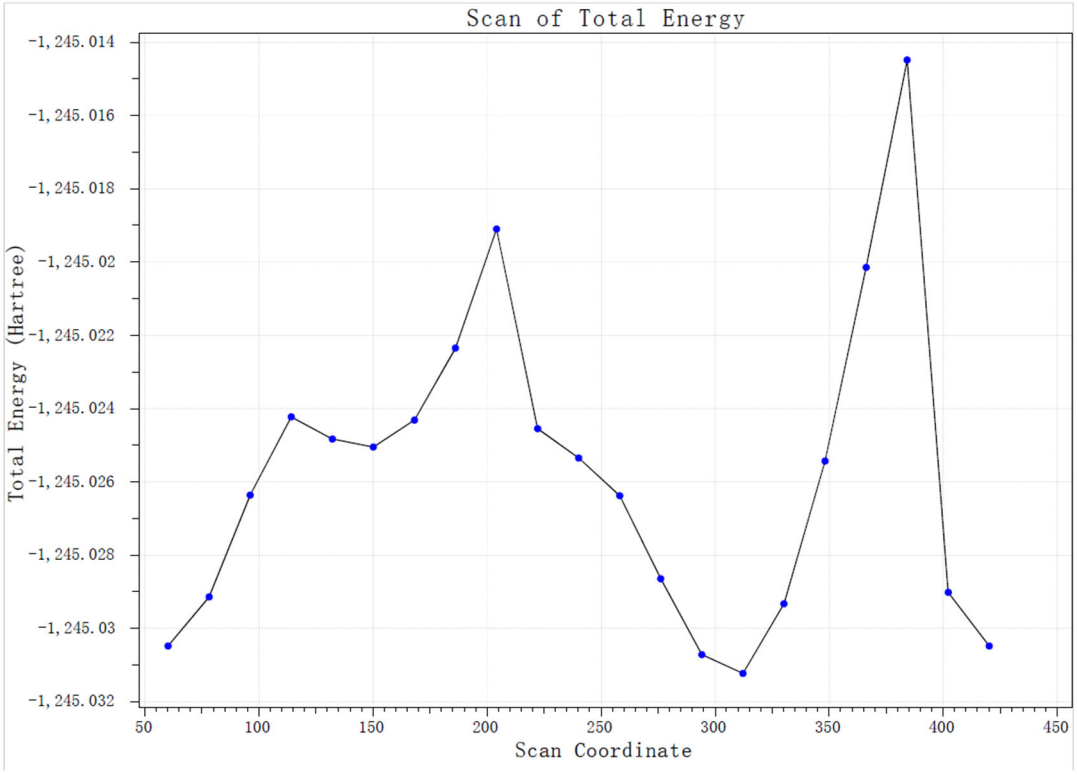


Figure S4. Energy change of carbonyl group rotation at the M06-2X-D3/6-31G(d) level of theory (kcal/mol).

Scanning shows that the rotational energy barrier of carbonyl groups is approximately 10kcal/mol.

Energies

Table S1. Absolute electronic energies, thermal corrections to energies and free energies at 298.15 K (in Hartree) of all stationary points. Geometries were optimized in the level of M06-2X/6-31G(d). Free energies were obtained from the single point SMD(DCM) calculation at the level of M06-2X/6-311G(d,p) combined with the liquid-phase free-energy correction mentioned above.

	E	E+ZPE	G
2-Naphthalenesulfonic acid	-1009.266662	-1009.6149229	-1009.489543
1a	-500.056206	-500.3599209	-500.2127329
2a	-820.946373	-821.3899307	-821.2038577
H_2O	-76.368377	-76.4196877	-76.4158407
INT1	-1830.224626	-1831.031122	-1830.693592
TS1	-1830.190652	-1831.002691	-1830.666944
INT2	-1830.204295	-1831.010274	-1830.678482
INT3	-2330.271688	-2331.397854	-2330.890876
INT4	-2253.90136	-2254.96998	-2254.488452
TS2-1	-2253.88561	-2254.952946	-2254.468559
TS2-2	-2253.875498	-2254.936006	-2254.454894
TS2-3	-2253.885017	-2254.952579	-2254.468234
TS2-4	-2253.875206	-2254.938658	-2254.458135
INT5	-2253.910146	-2254.96968	-2254.486857

INT6	-2330.282349	-2331.408876	-2330.899518
TS3-1	-2330.271688	-2331.397854	-2330.890876
TS3-2	-2330.256128	-2331.379106	-2330.874879
TS3-3	-2330.258631	-2331.381468	-2330.876677
INT7	-2330.308393	-2331.433139	-2330.915498
INT8	-2330.289349	-2331.416674	-2330.908365
TS4-1	-2330.274764	-2331.403315	-2330.892234
TS4-2	-2330.257678	-2331.381945	-2330.871365
INT9	-2330.316669	-2331.436656	-2330.923916
INT10	-2330.309242	-2331.430685	-2330.916315
TS5-1	-2330.273954	-2331.400554	-2330.884896
TS5-2	-2330.260415	-2331.394802	-2330.876026
INT11	-2330.306469	-2331.431891	-2330.912606
INT11’	-2330.259853	-2331.397989	-2330.877378
TS6	-2330.254098	-2331.396346	-2330.878895
INT12	-2330.259109	-2331.401152	-2330.885363
INT13	-2253.916341	-2254.988622	-2254.498322
TS7	-2253.910499	-2254.978518	-2254.489927
INT14	-2253.961991	-2255.021984	-2254.538069
Z-3aa	-1244.689362	-1245.385573	-1245.049577

Table S2. Relative electronic energies, thermal corrections to energies and free

energies at 298.15 K (in kcal/mol) of all stationary points. Geometries were optimized in the level of M06-2X/6-31G(d). Free energies were obtained from the single point SMD(DCM) calculation at the level of M06-2X/6-311G(d,p) combined with the liquid-phase free-energy correction mentioned above.

	E	E+ZPE	G
INT1	-7.3	-16.5	-0.1
TS1	14.0	1.4	16.6
INT2	5.5	-3.4	9.4
INT3	5.7	2.0	4.9
INT4	-0.3	-15.6	1.2
TS2-1	9.6	-4.9	13.6
TS2-2	15.9	5.7	22.2
TS2-3	9.9	-4.7	13.8
TS2-4	16.1	4.0	20.2
INT5	-14.6	-5.8	-15.4
INT6	-8.2	-27.7	4.2
TS3-1	-1.5	-20.8	9.6
TS3-2	8.2	-9.0	19.6
TS3-3	6.7	-10.5	18.5
INT7	-24.6	-42.9	-5.9
INT8	-12.6	-32.6	-1.4
TS4-1	-3.5	-24.2	8.7
TS4-2	7.3	-10.8	21.8

INT9	-29.8	-45.1	-11.2
INT10	-25.1	-41.4	-6.4
TS5-1	-3.0	-22.5	13.3
TS5-2	5.5	-18.8	18.9
INT11	-23.4	-42.1	-4.1
INT11′	5.9	-20.8	18.0
TS6	9.5	-19.8	17.1
INT12	6.4	-22.8	13.0
INT13	-9.7	-27.3	-5.0
TS7	-6.0	-21.0	0.2
INT14	-38.4	-48.3	-30.0
Z-3aa	-34.6	-34.8	-30.6

Cartesian Coordinates (Å)

2-Naphthalenesulfonic acid

C	4.19459300	0.11777500	0.04819100
C	3.26149100	1.12286000	0.02453900
C	1.87575800	0.82119800	-0.01033900
C	1.47049200	-0.54328100	-0.02085000
C	2.45789500	-1.56245800	0.00242100
C	3.78981200	-1.23932200	0.03686600
H	1.20772600	2.88061300	-0.04463000
H	5.25222800	0.35966300	0.07516900
H	3.56984500	2.16450400	0.03175800
C	0.88647200	1.84304400	-0.04159100
C	0.08572300	-0.85022100	-0.05526400
H	2.13745100	-2.60032400	-0.00700700
H	4.54022500	-2.02280900	0.05528500
C	-0.82690500	0.16981700	-0.07703800
C	-0.44562600	1.53347600	-0.07630000
H	-0.24978900	-1.88299200	-0.07059200
H	-1.20783900	2.30401600	-0.12089200
S	-2.54775900	-0.22719200	-0.11218500
O	-2.70038000	-1.63578000	-0.39165900
O	-3.27130700	0.77695700	-0.87143400
O	-2.93447300	0.02988300	1.44363300
H	-3.73466200	0.58658500	1.44773400

1a

C	-3.11162000	-0.24215300	-0.00002100
C	-2.17397700	-1.24211800	-0.00000800
C	-0.78789300	-0.94242600	-0.00000100
C	-0.36055500	0.41703300	-0.00000300
C	-1.35930800	1.42931100	-0.00002100
C	-2.69377700	1.10893300	-0.00002800
H	-0.12920500	-3.00561700	0.00000600
H	-4.16991700	-0.48190000	-0.00002800
H	-2.47844500	-2.28567600	-0.00000600
C	0.19107900	-1.96753300	0.00000600

C	1.03062800	0.73513200	0.00001400
H	-1.05835400	2.47169800	-0.00003400
H	-3.43714900	1.90015800	-0.00004300
C	1.94071600	-0.30112600	0.00000800
C	1.52203100	-1.65511300	0.00000100
H	2.27260900	-2.44268800	-0.00001500
O	3.27327200	0.00174300	-0.00002100
H	3.78336700	-0.81969500	0.00025500
C	1.49918100	2.16566000	0.00003600
H	1.13220900	2.70055800	-0.88284500
H	1.13197500	2.70059800	0.88279400
H	2.58771700	2.21503500	0.00017500

2a

C	-1.03380900	-0.90850400	0.67280700
C	-2.78611800	-1.41988300	-0.85365800
O	-3.49815300	-2.06650100	-1.58700300
N	-1.62283200	-1.84847100	-0.24748600
H	-1.33316900	-2.81599400	-0.26757800
O	-1.17294500	-1.43412500	1.97992600
H	-0.60054800	-0.91748100	2.56714700
C	0.38769400	-0.62968400	0.38340100
C	1.55505300	-0.37251600	0.20319600
C	2.93648400	-0.06490900	-0.02983900
C	3.93826900	-0.95647400	0.37682900
C	3.29224200	1.13211600	-0.66629500
C	5.27483600	-0.65183300	0.14902500
H	3.65653700	-1.88250800	0.86696900
C	4.63098000	1.42912400	-0.89073100
H	2.51141200	1.81652000	-0.98095600
C	5.62364100	0.53963300	-0.48396300
H	6.04632700	-1.34652000	0.46507900
H	4.90066600	2.35664300	-1.38538500
H	6.66834800	0.77425300	-0.66125100
C	-2.94386800	0.00082000	-0.42009000
C	-1.90991700	0.32300800	0.44413300
C	-1.80176700	1.59092100	0.99092300
C	-2.77820000	2.52834700	0.64816100
C	-3.82379100	2.19994500	-0.22042500
C	-3.91748100	0.92259200	-0.77118900

H	-0.98260400	1.85462000	1.65430400
H	-2.72374700	3.53125400	1.05983400
H	-4.56524000	2.95209600	-0.46976000
H	-4.71486400	0.64521300	-1.45311600

H_2O

O	0.00000000	0.00000000	0.11830700
H	0.00000000	-0.76308600	-0.47322800
H	0.00000000	0.76308600	-0.47322800

INT1

C	0.82710200	-0.51113000	-0.00528900
C	-0.59026100	-1.15669400	1.78244100
O	-1.26442500	-1.06951700	2.78900600
N	0.28214800	-0.21161500	1.30066500
H	0.35847700	0.71877400	1.70768200
O	0.32241100	0.37606500	-1.00879700
H	-0.63932700	0.22567400	-1.07006600
C	2.28863000	-0.39674500	-0.05693500
C	3.49148600	-0.30249300	-0.09812400
C	4.91952700	-0.18355700	-0.14800200
C	5.51082000	1.05325400	-0.43831800
C	5.72930600	-1.30156800	0.09227000
C	6.89491600	1.16539100	-0.48787800
H	4.87713800	1.91483300	-0.62032300
C	7.11256600	-1.17995300	0.04143800
H	5.26392400	-2.25507700	0.31873000
C	7.69718400	0.05129200	-0.24875900
H	7.34857100	2.12525500	-0.71224200
H	7.73617100	-2.04792800	0.22957100
H	8.77792700	0.14294200	-0.28730500
C	-0.54955300	-2.27529800	0.79387900
C	0.30656000	-1.92463200	-0.23879900
C	0.52518100	-2.76835900	-1.31531100
C	-0.14841200	-3.99140400	-1.31710400
C	-1.01465800	-4.34461900	-0.27676300
C	-1.22883500	-3.48357800	0.79870200
H	1.19536400	-2.48758000	-2.12190000

H	-0.00006700	-4.68103600	-2.14192500
H	-1.52421200	-5.30203500	-0.31133800
H	-1.89824400	-3.73445700	1.61537200
C	-5.38420900	-1.63573600	-0.71534800
C	-4.96390000	-0.61685300	-1.53193500
C	-4.01461000	0.33042600	-1.06978800
C	-3.50963900	0.20811400	0.25655300
C	-3.95974300	-0.85831600	1.08087100
C	-4.87621200	-1.75890600	0.60076000
H	-3.94568800	1.48033700	-2.90456100
H	-6.11080500	-2.35602400	-1.07775700
H	-5.35037700	-0.52040900	-2.54265000
C	-3.54914400	1.39098200	-1.89720200
C	-2.54560500	1.14596700	0.71724000
H	-3.54683700	-0.95292400	2.08086200
H	-5.21755500	-2.57336000	1.23168700
C	-2.10949300	2.13510600	-0.12604600
C	-2.61359100	2.28163800	-1.44389600
H	-2.14571000	1.05471900	1.72387200
H	-2.24317500	3.08405100	-2.07355200
S	-0.81947900	3.23266900	0.40635500
O	-1.27043500	4.60168100	0.38631400
O	0.21299800	3.09524800	-0.80633700
O	-0.22180300	2.66412100	1.60708700
H	0.49862400	2.14809900	-0.88061500

TS1

C	-0.59902800	1.45763900	0.32093000
C	1.32714500	1.54832500	1.55488400
O	2.16409600	1.19693300	2.34176700
N	0.09998800	0.87955900	1.31553400
H	-0.17680000	-0.05219900	1.72181800
O	-0.16049800	0.41056400	-1.33120300
H	0.77585600	0.13911100	-1.30337000
C	-1.99163100	1.24275100	0.19216700
C	-3.14218600	0.89368100	0.05007700
C	-4.46478300	0.38337800	-0.10307900

C	-4.62849800	-1.01089600	-0.12411200
C	-5.56761000	1.23732600	-0.23725400
C	-5.90492500	-1.53786200	-0.27647300
H	-3.74954700	-1.64452900	-0.04101300
C	-6.83712800	0.69393300	-0.38039900
H	-5.42032100	2.31213400	-0.22123800
C	-7.00512600	-0.69062400	-0.40002400
H	-6.04005500	-2.61404500	-0.29726200
H	-7.69672200	1.34861400	-0.47857400
H	-7.99966700	-1.11023900	-0.51440900
C	1.30167100	2.73977000	0.65590300
C	0.12061800	2.69852900	-0.07642200
C	-0.19934100	3.67112500	-1.00484300
C	0.71836600	4.71270500	-1.17017900
C	1.90665200	4.75728500	-0.43574500
C	2.21948100	3.76176100	0.49428500
H	-1.11692800	3.61850100	-1.58136700
H	0.50731400	5.50009000	-1.88609500
H	2.59671900	5.57957900	-0.59285400
H	3.13784200	3.78200200	1.07147900
C	5.86566800	-0.76914900	-0.92556500
C	4.89851700	-1.36235300	-1.69680300
C	3.62164800	-1.65726900	-1.15287700
C	3.36027500	-1.33057100	0.20736100
C	4.37764700	-0.71250900	0.98120100
C	5.60201300	-0.43898800	0.42610900
H	2.79900900	-2.51324300	-2.96514200
H	6.84020500	-0.54955500	-1.35019400
H	5.09635100	-1.61683400	-2.73456600
C	2.59201900	-2.26162500	-1.92842700
C	2.07685600	-1.61288000	0.75178900
H	4.16004500	-0.45478500	2.01336300
H	6.37639100	0.03205600	1.02309700
C	1.10614300	-2.17881900	-0.03125300
C	1.36024500	-2.51708000	-1.38667700
H	1.86644600	-1.36261200	1.78817500
H	0.56468100	-2.96016700	-1.97774600

S	-0.55827700	-2.41147500	0.59222800
O	-0.82656500	-3.83553300	0.69754400
O	-1.37396200	-1.72349300	-0.46735800
O	-0.59061700	-1.65759700	1.87525000
H	-0.67619400	-0.43966900	-1.11392600

INT2

C	-0.74115400	1.58616700	0.69678600
C	1.30881500	1.64187800	1.52748300
O	2.27393400	1.27400200	2.14546200
N	0.06975800	0.91949400	1.46904100
H	-0.19510400	-0.57849600	1.95021400
O	-0.12826000	0.30840800	-1.62710900
H	0.73456000	-0.10526900	-1.77146800
C	-2.05844300	1.17125400	0.41559000
C	-3.16847400	0.77214600	0.13524300
C	-4.44411500	0.21363500	-0.16950500
C	-4.60561400	-1.17887400	-0.09085800
C	-5.51786600	1.03284200	-0.54676100
C	-5.84219600	-1.73787900	-0.38708200
H	-3.75194200	-1.79176200	0.18142600
C	-6.75013800	0.46083000	-0.83232600
H	-5.37520100	2.10671300	-0.60670000
C	-6.91220400	-0.92215400	-0.75257000
H	-5.97151100	-2.81365800	-0.33202200
H	-7.58493500	1.09156600	-1.11952500
H	-7.87681800	-1.36547100	-0.97904000
C	1.15068200	2.87768300	0.69882700
C	-0.13562700	2.83833400	0.17545700
C	-0.61193900	3.82341700	-0.66671600
C	0.26083500	4.87686200	-0.96564600
C	1.55238000	4.91970600	-0.43849400
C	2.02266000	3.90747300	0.40789900
H	-1.61192300	3.77515700	-1.08506800
H	-0.07025200	5.67299600	-1.62439400
H	2.20297700	5.74962300	-0.69422700
H	3.02750400	3.92438400	0.81715200

C	5.83067900	-0.70002800	-1.32508100
C	4.81866700	-1.36554200	-1.96945700
C	3.60136300	-1.64764600	-1.29848700
C	3.44935800	-1.23381000	0.05416200
C	4.50880500	-0.53980000	0.69456200
C	5.67350100	-0.28025000	0.01818800
H	2.64642600	-2.63673100	-2.97427500
H	6.75907000	-0.48898100	-1.84628100
H	4.93419500	-1.68523500	-3.00139500
C	2.52514600	-2.32242900	-1.94141100
C	2.23213000	-1.51137300	0.73260100
H	4.36834300	-0.20993300	1.71929800
H	6.48135200	0.25106800	0.51084700
C	1.21711100	-2.14595900	0.06945200
C	1.35095500	-2.56466800	-1.28049200
H	2.11407300	-1.19131600	1.76296400
H	0.51905200	-3.05703500	-1.77460500
S	-0.35450900	-2.43692700	0.84376800
O	-0.49687200	-3.82690700	1.21154900
O	-1.34507900	-1.85342300	-0.06733700
O	-0.27586900	-1.59050600	2.16243300
H	-0.68078100	-0.41672100	-1.28462900

INT3

C	0.52029200	0.23630100	1.51973100
C	2.31399100	-1.01558700	1.84260300
O	2.95400000	-2.00719400	2.05683600
N	0.86987200	-0.98253800	1.80202200
H	-0.01959400	-2.49406100	1.48106500
C	-0.82282100	0.63732900	1.33342600
C	-1.96329600	0.96347100	1.07959600
C	-3.31315100	1.27378000	0.74000700
C	-4.18276100	0.22834600	0.38834400
C	-3.76122500	2.60353600	0.73430300
C	-5.49358400	0.52587000	0.03569000
H	-3.81017200	-0.79161200	0.38285400
C	-5.07539400	2.88371400	0.38692800

H	-3.07552400	3.39904000	1.00724100
C	-5.94033500	1.84627000	0.03756900
H	-6.16839000	-0.27719200	-0.24114400
H	-5.42739500	3.91001600	0.38652600
H	-6.96673300	2.06993100	-0.23577800
C	2.80835800	0.37090900	1.55466100
C	1.67921100	1.15598700	1.35084900
C	1.76917000	2.49262700	1.01324600
C	3.05733000	3.03113400	0.89787100
C	4.19146300	2.24655200	1.10710400
C	4.08205400	0.88848500	1.43753200
H	0.88290500	3.09269200	0.83254300
H	3.17574200	4.07679600	0.63232800
H	5.17414100	2.69603800	1.00678300
H	4.95693300	0.26557700	1.59439000
C	2.47077900	2.28532700	-2.49004600
C	2.90566000	1.02363900	-2.17061100
C	1.97793000	0.00246000	-1.84100300
C	0.58817700	0.30776000	-1.85239500
C	0.16625900	1.62072900	-2.18506200
C	1.08750400	2.58889500	-2.49652500
H	3.46315300	-1.52863700	-1.45428200
H	3.18977100	3.06104800	-2.73489700
H	3.96692500	0.79074500	-2.15494200
C	2.40013900	-1.30335800	-1.46185600
C	-0.34074300	-0.69315800	-1.46053000
H	-0.89771400	1.84313600	-2.17875900
H	0.75971100	3.59218400	-2.74988700
C	0.11332200	-1.91965500	-1.06426100
C	1.49211100	-2.25221700	-1.07555700
H	-1.40167900	-0.46512600	-1.41141200
H	1.81002300	-3.23454200	-0.74035600
S	-1.03613000	-3.06720500	-0.34296200
O	-0.32781600	-3.34851800	1.05106400
O	-1.02852700	-4.32132100	-1.06020400
O	-2.28587800	-2.35145100	-0.13753600

INT4

C	-2.82155800	-0.42150600	0.94989800
C	-4.34656900	-1.99675800	0.35912400
O	-4.75915000	-3.07657200	0.05372600
N	-2.97380800	-1.70067000	0.65822600
H	-2.15576800	-2.42059700	0.59966900
C	-1.62001500	0.19324100	1.26636500
C	-0.58559800	0.82706400	1.40644200
C	0.66493100	1.46629100	1.57586200
C	0.75175600	2.83566100	1.88314800
C	1.83152400	0.70896200	1.37820200
C	1.99812400	3.42739100	2.00646000
H	-0.15673200	3.41644200	2.00743300
C	3.07522600	1.31067000	1.50529400
H	1.74006400	-0.33500500	1.10288900
C	3.15556800	2.66685700	1.81956800
H	2.07312500	4.48681400	2.22629900
H	3.97327300	0.72042800	1.34513800
H	4.12721000	3.14304400	1.90867700
C	-5.07093800	-0.70314900	0.53577100
C	-4.13391200	0.25551700	0.91180500
C	-4.49786400	1.56379700	1.18018900
C	-5.85108200	1.88701700	1.04431200
C	-6.78912200	0.92717600	0.65706800
C	-6.40971300	-0.39486000	0.39734700
H	-3.76176900	2.30355200	1.47723900
H	-6.17937100	2.90185000	1.24196200
H	-7.83091000	1.21363200	0.55840500
H	-7.12915700	-1.15058000	0.10029500
C	2.71534300	4.71659700	-1.16366900
C	2.79569300	3.37519300	-1.44961100
C	1.63211800	2.57357900	-1.52601100
C	0.35334600	3.16391500	-1.30368400
C	0.30447600	4.55489600	-1.00986200
C	1.45176500	5.30867800	-0.94259400
H	2.67418900	0.72493000	-1.98228400
H	3.61458000	5.32226900	-1.11080700

H	3.76009800	2.90244700	-1.62004600
C	1.70231300	1.18393400	-1.81438400
C	-0.82398500	2.36127000	-1.34493500
H	-0.65789300	5.02897500	-0.84375000
H	1.38725200	6.37028200	-0.72295700
C	-0.70345000	1.00799400	-1.62365100
C	0.57010500	0.42356300	-1.87034800
H	0.61082600	-0.63574400	-2.09492800
O	-1.81328200	0.23884900	-1.63908600
H	-1.55042100	-0.71111300	-1.71755000
C	-2.17537300	2.95919700	-1.06701100
H	-2.20441600	3.42102100	-0.07091800
H	-2.42440900	3.74267400	-1.79172100
H	-2.94953900	2.19251800	-1.11794500
C	5.90759900	-1.52165200	1.10737600
C	5.36536100	-1.65664400	-0.14694700
C	4.02675500	-2.09679200	-0.31525000
C	3.25090200	-2.39675500	0.83908500
C	3.83628900	-2.24520000	2.12336700
C	5.13457800	-1.82001600	2.25593200
H	4.04307500	-2.04537600	-2.48178200
H	6.93418100	-1.18852900	1.22338800
H	5.95623600	-1.43278000	-1.03121800
C	3.43782100	-2.25027200	-1.60252500
C	1.89564600	-2.79907800	0.67687000
H	3.23486700	-2.47230200	2.99950100
H	5.57376900	-1.70991800	3.24228900
C	1.35643100	-2.90039400	-0.57610600
C	2.13645400	-2.65253800	-1.73531400
H	1.27601100	-3.00479500	1.54546000
H	1.68071200	-2.77208900	-2.71404000
S	-0.35277600	-3.37362200	-0.79812900
O	-0.93788500	-3.27927400	0.58145000
O	-0.35034400	-4.70830800	-1.37341900
O	-0.92980100	-2.32300500	-1.67788500

TS2-1

C	-3.04420400	-0.67441100	0.63652000
C	-4.14711200	-2.68694400	0.53354900
O	-4.32022900	-3.87428400	0.44191700
N	-2.90905600	-2.02462300	0.51138600
H	-1.98036200	-2.45738100	0.39973600
C	-2.04084000	0.21891200	0.67568400
C	-1.12818400	1.07838700	0.59820900
C	-0.02034100	1.70757300	1.27060500
C	-0.09449700	3.02592500	1.74358900
C	1.17137600	0.97887300	1.39374300
C	1.02348600	3.61299000	2.31660300
H	-1.02341700	3.57797000	1.64611000
C	2.28885300	1.57694900	1.96905500
H	1.19697700	-0.04136900	1.02083100
C	2.21659300	2.89298900	2.41934800
H	0.97134500	4.63517500	2.67715900
H	3.21469100	1.01550400	2.05471100
H	3.09139300	3.36155900	2.85969100
C	-5.15902800	-1.59816900	0.69693900
C	-4.48517100	-0.38131900	0.76695200
C	-5.16859600	0.81514400	0.92800300
C	-6.55957400	0.75136700	1.01364300
C	-7.23552500	-0.47136900	0.93932900
C	-6.53806000	-1.67063000	0.78024900
H	-4.63860100	1.76074300	0.98895700
H	-7.12906600	1.66628500	1.14051600
H	-8.31832700	-0.48415800	1.00800900
H	-7.04545200	-2.62808700	0.72292600
C	1.34111100	5.27089900	-0.94567100
C	1.90347300	4.02614100	-1.14221100
C	1.09070700	2.89785600	-1.35733000
C	-0.32135800	3.02714600	-1.35087900
C	-0.87099300	4.31172200	-1.16827400
C	-0.05528600	5.41102700	-0.97167500
H	2.75326800	1.52452600	-1.62840400
H	1.97223300	6.13800000	-0.78151800
H	2.98261500	3.89855500	-1.13636500

C	1.66910300	1.61015600	-1.61238000
C	-1.14910200	1.84031200	-1.45384100
H	-1.94754800	4.44433300	-1.18205500
H	-0.50112200	6.39153400	-0.83649500
C	-0.51914000	0.61080200	-1.82000100
C	0.90784100	0.51253000	-1.85969600
H	1.35102500	-0.44368800	-2.10734700
O	-1.28168100	-0.41179800	-2.09156700
H	-0.72726900	-1.28193100	-2.15091000
C	-2.63047100	1.97107900	-1.69786500
H	-3.09786000	2.64745000	-0.97792700
H	-2.81113900	2.36289900	-2.70513100
H	-3.11358200	0.99629600	-1.62523600
C	6.67679400	-0.87490000	1.25500800
C	6.23516900	-1.19781100	-0.00255300
C	4.90362100	-1.64365700	-0.21235300
C	4.03036300	-1.75116600	0.90655100
C	4.51741700	-1.41663000	2.19879000
C	5.80850500	-0.98580800	2.36934400
H	5.08942000	-1.90723100	-2.35287000
H	7.69730200	-0.53640600	1.40333800
H	6.89973800	-1.11907300	-0.85880000
C	4.41518700	-1.98171500	-1.50383600
C	2.69230300	-2.17553600	0.69840700
H	3.84552700	-1.51051600	3.04833100
H	6.17296800	-0.73467100	3.36038000
C	2.25288500	-2.47254100	-0.56468900
C	3.12018700	-2.39405200	-1.68182500
H	2.00610600	-2.24442900	1.53899000
H	2.73267800	-2.64206200	-2.66499200
S	0.55343200	-2.97978600	-0.80172700
O	-0.19304300	-2.22055400	0.23800900
O	0.49079400	-4.42805800	-0.69063900
O	0.21415800	-2.46200900	-2.17321500

TS2-2

C	1.01830200	-2.08729300	1.01272100

C	-0.67362300	-3.64109700	1.16760400
O	-1.72109300	-4.12727600	1.49736000
N	-0.21480500	-2.35049600	1.52352100
H	-0.83726600	-1.62550800	1.88505700
C	1.80551100	-1.00348900	1.22327800
C	2.57898100	-0.03378000	1.09694800
C	3.63317300	0.82562200	1.56027000
C	3.35338600	1.82363600	2.50435700
C	4.92673500	0.70955300	1.03067600
C	4.36085400	2.69021900	2.91500700
H	2.35102000	1.89955200	2.91392400
C	5.92226700	1.58662900	1.43836200
H	5.13011000	-0.06085000	0.29387000
C	5.64160700	2.57710800	2.37960500
H	4.14366100	3.45607300	3.65254600
H	6.91874900	1.50127700	1.01735900
H	6.42340900	3.26031000	2.69595100
C	0.43924700	-4.22885200	0.36624700
C	1.46449700	-3.29024900	0.28945800
C	2.64757700	-3.55942400	-0.38274000
C	2.76193900	-4.80805000	-0.99524700
C	1.72983200	-5.74996700	-0.92251700
C	0.54835800	-5.47150900	-0.23201200
H	3.44298800	-2.82170800	-0.43242500
H	3.66946000	-5.05626900	-1.53622100
H	1.85329300	-6.71128900	-1.41042800
H	-0.26077800	-6.19117000	-0.16359100
C	5.43783800	3.30789400	-1.76673600
C	5.19151200	2.05684800	-2.29434100
C	4.00742600	1.36261700	-1.98490700
C	3.03766100	1.95180100	-1.13035300
C	3.31079400	3.23989500	-0.61651100
C	4.48493100	3.89924200	-0.92207700
H	4.51522500	-0.38255600	-3.17964100
H	6.35653800	3.83355000	-2.00635200
H	5.91409800	1.58544900	-2.95591700
C	3.76400800	0.05065500	-2.52313700

C	1.85863400	1.20890400	-0.74435500
H	2.58961500	3.72367700	0.03195200
H	4.67003400	4.88443300	-0.50529900
C	1.59189500	-0.03599500	-1.40552400
C	2.62422700	-0.62137900	-2.24258900
H	2.40279400	-1.59687900	-2.66383700
O	0.53118200	-0.71247500	-1.21494700
H	-0.71695500	-0.12346200	-1.11017600
C	0.75472800	1.89120400	0.02065400
H	1.15979000	2.49278500	0.83984500
H	0.17910200	2.55939100	-0.63213800
H	0.06854500	1.16523000	0.45633300
C	-8.71617500	2.26505600	-0.29475100
C	-7.52119000	2.88540500	-0.03168000
C	-6.31387400	2.14176500	0.01034100
C	-6.36325700	0.73919000	-0.22558400
C	-7.61327700	0.12406100	-0.49423300
C	-8.76382200	0.86938700	-0.52850900
H	-5.03548900	3.82942400	0.46572500
H	-9.63370500	2.84412300	-0.32467800
H	-7.48178100	3.95617500	0.14860400
C	-5.06078000	2.75872500	0.28365200
C	-5.15753500	-0.00959000	-0.18654200
H	-7.63930500	-0.94731800	-0.67195000
H	-9.71642300	0.39242400	-0.73501300
C	-3.97849400	0.63033000	0.07724100
C	-3.90816500	2.02352600	0.32167900
H	-5.16435900	-1.08149100	-0.36235300
H	-2.94778500	2.48051800	0.53704000
S	-2.49192900	-0.32206500	0.14011700
O	-2.80434900	-1.72639800	-0.06456400
O	-1.77874300	0.02192300	1.38121900
O	-1.71880300	0.27785500	-1.07372200

TS2-3

C	-3.15826100	0.67917600	0.49362000
C	-4.25883000	2.68552400	0.29366600

O	-4.43009900	3.87105500	0.17743500
N	-3.01993400	2.02870800	0.36406500
H	-2.08565500	2.46130700	0.31877300
C	-2.15323900	-0.20544600	0.60832200
C	-1.22128300	-1.04718000	0.60628100
C	-0.14880500	-1.63699200	1.36725600
C	1.00110900	-0.86304200	1.58118800
C	-0.21585800	-2.95223100	1.84947500
C	2.08591200	-1.41466200	2.25556000
H	1.02023300	0.15751600	1.20767400
C	0.87032800	-3.49221000	2.52170500
H	-1.11248900	-3.53948200	1.68160400
C	2.02435600	-2.72826800	2.71455000
H	2.97848500	-0.81540400	2.40908000
H	0.82436900	-4.51193600	2.88995700
H	2.87508900	-3.16054400	3.23236100
C	-5.27545500	1.59359500	0.39791700
C	-4.60333600	0.38044300	0.52672200
C	-5.29167500	-0.81728600	0.65378600
C	-6.68552200	-0.75889800	0.64332900
C	-7.35940900	0.45992200	0.50977600
C	-6.65722600	1.66064100	0.38592700
H	-4.76381000	-1.75973400	0.76285200
H	-7.25888300	-1.67494400	0.74141100
H	-8.44442600	0.46859200	0.50446800
H	-7.16324400	2.61516700	0.28441700
C	1.26419200	-5.29799800	-0.70662200
C	1.87539500	-4.07161800	-0.86573300
C	1.11398500	-2.92231600	-1.14943900
C	-0.29694800	-3.01237400	-1.25803800
C	-0.89584100	-4.27951200	-1.11073100
C	-0.12989600	-5.39868600	-0.84082900
H	2.83014800	-1.59561000	-1.27912500
H	1.85508100	-6.18133300	-0.48836100
H	2.95379300	-3.97358800	-0.77499700
C	1.74666000	-1.65251300	-1.35651800
C	-1.08089700	-1.80499200	-1.44033700

H	-1.97123000	-4.38219200	-1.20940800
H	-0.61296900	-6.36493300	-0.73376100
C	-0.38768300	-0.59531100	-1.74984900
C	1.03738900	-0.53627000	-1.66843000
H	1.51975400	0.41141000	-1.86762700
O	-1.09315000	0.45178500	-2.08769100
H	-0.51202200	1.29533700	-2.08616900
C	-2.53588400	-1.89976100	-1.82131500
H	-2.63064100	-2.30599800	-2.83451700
H	-3.08961800	-2.54852300	-1.13830900
H	-2.99504900	-0.91096000	-1.81168900
C	6.96043400	0.75970200	0.50871500
C	5.98663700	1.12521400	1.40333700
C	4.72510800	1.59163600	0.95111400
C	4.48397000	1.67680200	-0.44893700
C	5.51122000	1.29434900	-1.35091900
C	6.72037200	0.84525700	-0.88425600
H	3.88658100	1.91626600	2.92222500
H	7.92241800	0.40579800	0.86574500
H	6.16813300	1.06565000	2.47332600
C	3.69252500	1.97041400	1.85386500
C	3.21541600	2.12618700	-0.90495500
H	5.32092500	1.36750700	-2.41831600
H	7.50034200	0.55667800	-1.58160100
C	2.23709900	2.45208400	-0.00499500
C	2.47343300	2.38980200	1.39209500
H	3.01329900	2.19648500	-1.97094100
H	1.67177800	2.65740700	2.07338200
S	0.61061000	2.95584300	-0.55182300
O	0.51218700	4.39959300	-0.40752600
O	-0.29482600	2.16835700	0.33133100
O	0.51244200	2.46377500	-1.96724400

TS2-4

C	0.84649100	2.02937600	1.02312200
C	-0.85294900	3.52395900	1.42451200
O	-1.88538700	3.95444400	1.85892200

N	-0.34148000	2.22369600	1.65584300
H	-0.95992700	1.44358400	1.90021600
C	1.62442600	0.92858600	1.03000600
C	2.42813700	-0.02346500	0.86217100
C	3.51347300	-0.75750100	1.48223900
C	3.22084200	-1.69596900	2.47980600
C	4.83708200	-0.57819000	1.06057200
C	4.24494200	-2.44909500	3.04552500
H	2.19301300	-1.81777500	2.80758700
C	5.85153000	-1.34235700	1.62165200
H	5.05376500	0.15272200	0.28802200
C	5.55724800	-2.27985600	2.61180900
H	4.01590400	-3.16989400	3.82372900
H	6.87467500	-1.20737000	1.28602000
H	6.35359800	-2.87446300	3.04799400
C	0.19106600	4.20417400	0.60262800
C	1.22432500	3.30062200	0.37607600
C	2.34768200	3.64811400	-0.35879800
C	2.39851400	4.94548100	-0.86889400
C	1.35970500	5.85520500	-0.64161100
C	0.23637400	5.49433500	0.10481100
H	3.14815500	2.93363600	-0.52898900
H	3.25843700	5.25711300	-1.45303400
H	1.43101600	6.85582100	-1.05531700
H	-0.57909400	6.18617900	0.28795000
C	5.54435500	-3.43038000	-1.49271500
C	5.34263800	-2.20981900	-2.10387400
C	4.14401700	-1.49919100	-1.91163000
C	3.11615600	-2.03539900	-1.09658000
C	3.34199200	-3.29099000	-0.49852200
C	4.53204300	-3.96981900	-0.68640300
H	4.75599900	0.18781900	-3.14149300
H	6.47402600	-3.97064800	-1.63785900
H	6.11136600	-1.77547700	-2.73781700
C	3.95341700	-0.21320900	-2.52721300
C	1.90993000	-1.25866300	-0.81884200
H	2.57755700	-3.73817600	0.12517500

H	4.67975700	-4.93126600	-0.20485200
C	1.71079800	-0.07563700	-1.60406500
C	2.80127000	0.47774800	-2.36991100
H	2.61667900	1.43084000	-2.85386200
O	0.63274500	0.62651100	-1.59123500
H	-0.33813000	0.15618200	-1.38766300
C	0.73248800	-1.94843600	-0.16882600
H	0.24475600	-2.63141900	-0.87311700
H	1.06320200	-2.52917200	0.69633500
H	-0.01389300	-1.23968300	0.18522500
C	-8.43256800	-2.59428400	0.07467000
C	-7.91076800	-1.71889400	-0.84352300
C	-6.59370000	-1.21232400	-0.69542600
C	-5.81999900	-1.62751400	0.42433700
C	-6.38635500	-2.53291600	1.35887100
C	-7.66215500	-3.00641000	1.18895100
H	-6.63038600	0.01743300	-2.47710300
H	-9.44156100	-2.97490700	-0.04908100
H	-8.49945400	-1.39907400	-1.69912800
C	-6.02908700	-0.29992200	-1.62961700
C	-4.50099200	-1.12334300	0.57667100
H	-5.78833300	-2.84246400	2.21160400
H	-8.08751000	-3.69852100	1.90870700
C	-3.99862100	-0.25189200	-0.34932800
C	-4.75766400	0.17740100	-1.46559400
H	-3.89121600	-1.41980300	1.42489100
H	-4.32103700	0.88482000	-2.16278900
S	-2.34942600	0.37591700	-0.17166800
O	-1.59039600	-0.31640900	-1.28805600
O	-1.85499000	-0.06717000	1.15303600
O	-2.39155700	1.82465200	-0.36740600

INT5

C	1.97284000	-0.91625600	-1.19086500
C	1.12722100	-2.87366800	-2.10589300
O	0.33813800	-3.67381600	-2.55906700
N	0.85002500	-1.57808500	-1.70278400

H	-0.07257800	-1.15527700	-1.72171400
C	2.01190400	0.29258700	-0.67468600
C	2.06595400	1.37414900	0.05666600
C	2.20930000	2.73428000	-0.53517200
C	3.38231600	3.47864100	-0.37878400
C	1.14819700	3.27049800	-1.26805300
C	3.48750500	4.74623300	-0.94165000
H	4.21984900	3.05152200	0.16704700
C	1.25241700	4.54193500	-1.82521200
H	0.24882600	2.67835400	-1.40150000
C	2.42013900	5.28212400	-1.66046300
H	4.40507700	5.31428600	-0.82434400
H	0.42027900	4.94851700	-2.39085100
H	2.50289800	6.27246800	-2.09690700
C	2.58531400	-3.05479800	-1.83249700
C	3.09003600	-1.87659900	-1.28762000
C	4.41533300	-1.78035400	-0.88401100
C	5.22354800	-2.90170700	-1.06002800
C	4.71919700	-4.08301500	-1.61932900
C	3.38446500	-4.17405400	-2.00977500
H	4.79788600	-0.86756500	-0.43622700
H	6.26482300	-2.86082400	-0.75530700
H	5.37765500	-4.93690700	-1.74256200
H	2.96888700	-5.08272000	-2.43377600
C	4.44691500	-2.01105800	2.77942900
C	3.10763600	-2.25991600	2.51264100
C	2.23985200	-1.21351400	2.18127000
C	2.71970400	0.10555300	2.10451700
C	4.06547600	0.34212600	2.37926800
C	4.92229100	-0.70291800	2.71927600
H	0.51611800	-2.53011400	1.95978800
H	5.11504800	-2.82810200	3.03015600
H	2.71909000	-3.27397200	2.55253400
C	0.83080900	-1.48918200	1.92407100
C	1.81783100	1.22310900	1.60877000
H	4.46162500	1.35086600	2.31611000
H	5.96628700	-0.49262200	2.92964500

C	0.32507600	0.87699000	1.62721300
C	-0.07357600	-0.52873200	1.66802300
H	-1.11987900	-0.75111300	1.49231200
O	-0.50682200	1.77998600	1.55084000
C	2.02327200	2.53777800	2.36783000
H	1.83427900	2.37499500	3.43293500
H	3.03654900	2.92379300	2.25042500
H	1.32737400	3.29094600	1.99734200
C	-3.75544400	0.51019600	-0.26417200
C	-4.83471500	0.01152800	-0.94101000
C	-5.89597100	-0.59028800	-0.21519900
C	-5.81263800	-0.65641800	1.20395400
C	-4.67302500	-0.11354700	1.86031200
C	-3.65543000	0.46173600	1.14913100
H	-7.08876800	-1.07068500	-1.95337100
H	-4.88002100	0.08202300	-2.02392000
C	-7.03517400	-1.12569300	-0.86987600
C	-6.87542500	-1.25804800	1.92525800
H	-4.62584700	-0.15553600	2.94480400
H	-2.79028200	0.89178400	1.64670500
C	-7.96491000	-1.76893500	1.26664600
C	-8.04638800	-1.70264400	-0.14544000
H	-6.81057600	-1.30658200	3.00865500
H	-8.77252200	-2.22803500	1.82771600
H	-8.91453400	-2.11146400	-0.65193900
S	-2.41215900	1.18285200	-1.20016500
O	-1.23671400	0.33880300	-0.99514300
O	-2.86587100	1.48147100	-2.53697700
O	-2.12745100	2.56605600	-0.46473700
H	-1.50453400	2.40421700	0.29179200

INT6

C	0.01941400	0.44148100	0.42765900
C	1.81019600	1.02576700	1.75657100
O	2.51127900	1.14130400	2.73851500
N	0.58934600	0.37065800	1.69011600
H	0.06041800	-0.00027300	2.48908900

C	-1.17149200	-0.01987800	0.06186600
C	-2.46298100	0.03438200	-0.17900300
C	-3.20883300	-1.09232700	-0.80729900
C	-4.20967600	-1.78402200	-0.11445000
C	-2.86530200	-1.49529600	-2.10150400
C	-4.84744000	-2.86472700	-0.71290500
H	-4.46351500	-1.47617400	0.89584900
C	-3.50737200	-2.57792000	-2.69681300
H	-2.08322400	-0.95735500	-2.63185800
C	-4.49959700	-3.26324300	-2.00301900
H	-5.61267000	-3.40585100	-0.16553500
H	-3.22799800	-2.88713200	-3.69887000
H	-4.99744000	-4.11104400	-2.46248000
C	2.05806700	1.53247500	0.37260400
C	0.99374500	1.14273400	-0.43598000
C	0.96719000	1.44741700	-1.78883200
C	2.04604400	2.16485000	-2.30548400
C	3.11107900	2.56422500	-1.48952800
C	3.12910100	2.25236600	-0.13013900
H	0.13428900	1.14176700	-2.41507800
H	2.06032900	2.42016600	-3.36065600
H	3.93727500	3.11722400	-1.92526600
H	3.95147400	2.54027400	0.51669700
C	-0.82087600	4.54383600	-1.42662700
C	-0.78267700	4.29535700	-0.06235100
C	-1.57553100	3.28845900	0.50303900
C	-2.41451100	2.51279000	-0.31315500
C	-2.44529300	2.77369500	-1.68284600
C	-1.66101100	3.78145700	-2.23723500
H	-0.83620700	3.65146200	2.52255900
H	-0.19822000	5.32059200	-1.85772900
H	-0.12926700	4.87592800	0.58340700
C	-1.51985100	3.03728200	1.93981700
C	-3.20410700	1.34424500	0.25715300
H	-3.07345400	2.16743500	-2.33002600
H	-1.69922800	3.96487100	-3.30657900
C	-3.17230100	1.24089900	1.79201400

C	-2.25834400	2.09679400	2.55165500
H	-2.20276400	1.91551700	3.61988700
O	-3.85048700	0.38857100	2.35020700
C	-4.66854300	1.38482300	-0.20366400
H	-5.08716500	2.37533800	-0.00419800
H	-4.75404300	1.17811100	-1.27313700
H	-5.25423100	0.64076600	0.33725800
O	-1.33725300	-0.86157700	3.31888300
H	-2.27898900	-0.68681600	3.16011300
H	-1.14443700	-1.73140800	2.93020900
C	5.85878700	0.21151100	0.71194500
C	4.78223900	-0.48036100	1.20536900
C	3.86044600	-1.09688800	0.31847000
C	4.05219000	-0.97352400	-1.08671700
C	5.17284800	-0.24618700	-1.56403300
C	6.05734800	0.32693500	-0.68611500
H	2.55251800	-1.88332400	1.86985200
H	6.56164600	0.67907600	1.39399500
H	4.60551900	-0.55004900	2.27412000
C	2.73269700	-1.81071000	0.80038000
C	3.11791300	-1.57661800	-1.97175200
H	5.31660100	-0.15311800	-2.63712200
H	6.91478000	0.87745600	-1.06077400
C	2.04499500	-2.28005700	-1.49387000
C	1.86228600	-2.37968000	-0.09258500
H	3.27045500	-1.47218900	-3.04230700
H	1.32867500	-2.74473100	-2.16279600
S	0.51088700	-3.33529500	0.54010700
O	-0.64683000	-3.01852100	-0.52120100
H	-0.94812900	-2.08974400	-0.39395200
O	0.77973000	-4.74579800	0.40718700
O	0.13260000	-2.77406600	1.82978100

TS3-1

C	-0.01688900	0.36687000	0.23127000
C	1.62250400	1.25020700	1.56013300
O	2.16632700	1.58534300	2.57715500

N	0.37422500	0.56780300	1.49217400
H	-0.19475400	0.23285200	2.31404600
C	-1.18291100	-0.31033100	-0.15244500
C	-2.46113900	0.08132600	-0.19897900
C	-3.49798000	-0.87777700	-0.67416300
C	-4.63301600	-1.19414700	0.08285700
C	-3.30829100	-1.51173600	-1.90659100
C	-5.55498400	-2.12010300	-0.39259900
H	-4.76590100	-0.73535500	1.05708800
C	-4.23480600	-2.43430200	-2.38179600
H	-2.41750800	-1.28238900	-2.48521600
C	-5.36350500	-2.73754500	-1.62703500
H	-6.42288200	-2.36840200	0.21025800
H	-4.06871900	-2.92081200	-3.33755600
H	-6.08645100	-3.45955000	-1.99327100
C	2.03476300	1.44055900	0.13946400
C	1.05595900	0.85559700	-0.66213300
C	1.18431100	0.81019300	-2.03915600
C	2.32905300	1.39300200	-2.59292800
C	3.29621800	1.99747700	-1.78743800
C	3.16338300	2.02910300	-0.39459800
H	0.42864900	0.33435300	-2.65682100
H	2.47072200	1.37149500	-3.66872700
H	4.17560400	2.43452700	-2.24956900
H	3.92128100	2.46847700	0.24507900
C	-0.03348100	4.23504500	-1.68955400
C	-0.17373500	4.24000800	-0.31017900
C	-1.09589700	3.39047800	0.31863500
C	-1.87019800	2.50677100	-0.44991100
C	-1.73196400	2.52456300	-1.83889600
C	-0.82778400	3.38057800	-2.45638500
H	-0.61580600	4.11649300	2.31961600
H	0.68715500	4.89005800	-2.16769200
H	0.43318500	4.90265000	0.30132500
C	-1.23114500	3.40599100	1.77138500
C	-2.85215600	1.53673100	0.19072200
H	-2.31978700	1.83354700	-2.43880500

H	-0.72828700	3.37063100	-3.53744700
C	-2.86727000	1.58484500	1.72691000
C	-2.05244600	2.57676100	2.43677700
H	-2.12768400	2.57266100	3.51907800
O	-3.56466500	0.79342500	2.34541500
C	-4.27585900	1.93129800	-0.26364500
H	-4.44310200	2.99244000	-0.05561700
H	-4.39441800	1.76314300	-1.33715200
H	-5.02706400	1.34515500	0.26596900
O	-1.21931700	-0.62382100	3.29064600
H	-2.16299400	-0.42449100	3.17792700
H	-1.06857800	-1.50608300	2.89445400
C	5.64510100	0.07260600	1.07572800
C	4.49765700	-0.55386900	1.49250100
C	3.69451200	-1.27570100	0.57002300
C	4.09029700	-1.33874200	-0.79620700
C	5.28511000	-0.68551900	-1.19421500
C	6.04447400	0.00340000	-0.28181100
H	2.15507700	-1.85574500	2.00152000
H	6.25349400	0.62156700	1.78747500
H	4.18002800	-0.49745900	2.53000700
C	2.48659600	-1.90760100	0.96725400
C	3.27313600	-2.04277200	-1.72292800
H	5.58716800	-0.74052300	-2.23702400
H	6.95874700	0.49709000	-0.59678600
C	2.11181200	-2.64562400	-1.32022700
C	1.72063300	-2.56171100	0.03924800
H	3.58527500	-2.08851000	-2.76305100
H	1.47281000	-3.17224100	-2.02166600
S	0.18211500	-3.32282000	0.53113200
O	-0.76916800	-2.84245600	-0.57271600
H	-0.93991000	-1.59537300	-0.42695200
O	0.33758200	-4.76349600	0.49045600
O	-0.16064900	-2.69965400	1.81800000

TS3-2

C	0.19635600	-1.37503100	-0.52318500

C	-0.83220800	-2.52720600	-2.23465300
O	-0.96729900	-3.01863500	-3.32179400
N	0.33403300	-1.86383200	-1.77693200
H	1.16062800	-1.67152500	-2.34404000
C	1.00897400	-0.40696900	0.02814600
C	2.30977800	-0.10111100	0.10682100
C	2.69897300	1.33911100	0.02622000
C	2.09417400	2.08080700	-1.00174500
C	3.60031200	1.98719600	0.88175700
C	2.38133200	3.42860200	-1.17481900
H	1.38895200	1.58500900	-1.66453800
C	3.88451900	3.33839200	0.70409800
H	4.05536600	1.46158900	1.71202200
C	3.28271600	4.06073500	-0.32235300
H	1.88920600	3.98168700	-1.96773200
H	4.57288500	3.83019300	1.38428000
H	3.50665500	5.11516500	-0.44995700
C	-1.76692800	-2.47770900	-1.07416300
C	-1.12965000	-1.79777900	-0.03614800
C	-1.76611300	-1.56226700	1.17032100
C	-3.07315200	-2.04110200	1.30986200
C	-3.71007800	-2.71499700	0.26670300
C	-3.05921600	-2.94650000	-0.95090800
H	-1.28022400	-1.00026600	1.96233500
H	-3.61444800	-1.86113500	2.23349500
H	-4.73385800	-3.04892800	0.40212800
H	-3.54791600	-3.45598700	-1.77475300
C	6.35626900	-0.42379600	3.13777000
C	6.72082800	-0.33830600	1.80135500
C	5.78536500	-0.58471500	0.78876000
C	4.46605500	-0.92034400	1.12651200
C	4.11131800	-1.01175100	2.47191800
C	5.04542100	-0.76388300	3.47294700
H	7.20147800	-0.18615400	-0.81823900
H	7.08610700	-0.22590100	3.91559500
H	7.73792200	-0.07161300	1.52690100
C	6.17047800	-0.46631200	-0.61305500

C	3.41494500	-1.17307800	0.06025800
H	3.08364100	-1.24611500	2.73725900
H	4.74929300	-0.82897600	4.51493500
C	3.93167500	-1.06389500	-1.39541000
C	5.32386000	-0.68279300	-1.63369300
H	5.62558900	-0.59337800	-2.67152200
O	3.16877400	-1.29796400	-2.31937500
H	0.13614000	0.61744700	0.25916300
C	2.89063100	-2.61165300	0.23144100
H	3.73743400	-3.29846700	0.31624300
H	2.28460800	-2.69659000	1.13726800
H	2.29026400	-2.91280100	-0.62690900
C	-7.15945100	-0.19672700	2.52762400
C	-6.87818600	-0.22301300	1.18540700
C	-5.64594300	0.28080300	0.69148500
C	-4.70722400	0.82197800	1.61441100
C	-5.02881400	0.84429900	2.99769000
C	-6.22456300	0.34375900	3.44527100
H	-6.04989000	-0.14385100	-1.39212200
H	-8.10367200	-0.58745300	2.89354300
H	-7.59500000	-0.63186000	0.47817300
C	-5.31789600	0.24761900	-0.69073400
C	-3.45448000	1.27933300	1.13256300
H	-4.30727200	1.26387000	3.69380200
H	-6.46222300	0.36299600	4.50406300
C	-3.16733500	1.19075800	-0.20396500
C	-4.10289300	0.69156800	-1.14328400
H	-2.71079700	1.66132700	1.82629200
H	-3.85146200	0.69855300	-2.20051800
S	-1.56915800	1.70064200	-0.80143600
O	-1.64562700	3.08896500	-1.24063200
O	-1.16549500	0.71941700	-1.82466900
O	-0.67086400	1.54341000	0.43627200
O	-2.80311500	2.01125200	-3.80697400
H	-2.06975700	1.42542700	-3.56020500
H	-2.64143800	2.77856000	-3.23546000

TS3-3

C	0.18228300	-1.56057300	-0.17376100
C	-0.76015800	-3.35969900	-1.26630000
O	-0.84805500	-4.26879400	-2.04690100
N	0.34772400	-2.48529500	-1.14994800
H	1.19347300	-2.52513300	-1.72058900
C	0.98948000	-0.46394100	0.02812900
C	2.29173800	-0.14191100	0.03151600
C	2.67634700	1.20327500	-0.49033100
C	2.06624600	1.58819700	-1.69621400
C	3.56364100	2.09565400	0.12851100
C	2.33507900	2.82444700	-2.26980100
H	1.36815800	0.90804500	-2.17743900
C	3.82903900	3.33287000	-0.45171100
H	4.01909600	1.85947700	1.08169600
C	3.22226300	3.70010400	-1.64943000
H	1.83814200	3.10260500	-3.19315900
H	4.50457000	4.01946400	0.04874000
H	3.42997500	4.67017000	-2.08992000
C	-1.71367400	-2.89446700	-0.21764700
C	-1.14341800	-1.79629300	0.42620600
C	-1.82302400	-1.10708900	1.41973800
C	-3.09583400	-1.57088400	1.76266800
C	-3.65429100	-2.68484800	1.13133600
C	-2.96707900	-3.36647000	0.12113700
H	-1.39854600	-0.22205800	1.88269700
H	-3.67149600	-1.04398700	2.51719800
H	-4.65100600	-3.00723500	1.41610200
H	-3.39844600	-4.22021500	-0.39124100
C	6.30482900	0.60256200	3.03035100
C	6.67519700	0.24810200	1.74055900
C	5.74948300	-0.33587900	0.86689300
C	4.43428300	-0.56432900	1.29707600
C	4.07411100	-0.21336900	2.59764700
C	4.99852200	0.36811000	3.45998900
H	7.16611500	-0.46150700	-0.78346000
H	7.02670900	1.06000100	3.69854000

H	7.68895600	0.42729800	1.39264400
C	6.14031200	-0.68088900	-0.49516200
C	3.39132000	-1.16674300	0.37235200
H	3.04974600	-0.36460500	2.92765600
H	4.69761300	0.64583200	4.46492000
C	3.92239400	-1.56242200	-1.02838600
C	5.30559900	-1.24620800	-1.38352300
H	5.61267000	-1.50423900	-2.39106700
O	3.17684300	-2.12626900	-1.81374500
H	0.12925300	0.56803700	-0.02223600
C	2.85577500	-2.45630500	1.02348800
H	3.69702100	-3.06707800	1.36254100
H	2.22817900	-2.22180200	1.88709700
H	2.27408800	-3.04127100	0.31183300
C	-7.47510600	0.27750700	1.67078500
C	-6.89177000	-0.36317100	0.60799300
C	-5.64134100	0.07373100	0.09543300
C	-5.00174000	1.19207700	0.70289700
C	-5.63477000	1.84119000	1.79730800
C	-6.84030500	1.39342500	2.27209500
H	-5.49689100	-1.43558500	-1.44939000
H	-8.43059600	-0.06560000	2.05507800
H	-7.37830900	-1.21542800	0.14042700
C	-5.00234200	-0.58433700	-0.98826000
C	-3.73795700	1.61806500	0.22011100
H	-5.14037100	2.69760000	2.24734400
H	-7.31641400	1.89362000	3.10932500
C	-3.14842000	0.92896300	-0.80940700
C	-3.77139800	-0.17684400	-1.43183400
H	-3.23869800	2.48005800	0.66427300
H	-3.25629300	-0.68560300	-2.23951000
S	-1.53017200	1.41313100	-1.37395100
O	-1.61674400	2.73887100	-1.97675400
O	-1.02607100	0.31115300	-2.19642200
O	-0.71059800	1.49392300	-0.06054100
O	-1.70797900	4.10715900	0.62000300
H	-1.81429800	4.14356800	-0.34476600

H	-1.05477400	3.39455400	0.70768300

INT7

C	0.36578800	-0.88144700	0.27021700
C	-1.05684400	0.63401900	-0.84058600
O	-1.62807300	1.20183100	-1.74808300
N	-0.05351800	-0.30943200	-0.97105800
H	0.20052400	-0.69019200	-1.90005800
C	1.85091700	-0.94084300	0.55498800
C	2.86521700	-0.15746400	0.16989200
C	4.21782100	-0.55844300	0.66908500
C	5.18492600	-1.05331700	-0.21330800
C	4.51733200	-0.47864000	2.03092300
C	6.42863600	-1.45257600	0.26379200
H	4.93672500	-1.13554300	-1.26784400
C	5.76612800	-0.87388700	2.50660500
H	3.76152900	-0.10972600	2.72015600
C	6.72495500	-1.35913600	1.62312100
H	7.16808700	-1.84506900	-0.42735900
H	5.98625300	-0.80452200	3.56736900
H	7.69781900	-1.66920100	1.99126000
C	-1.27041100	0.79836800	0.62591000
C	-0.42644000	-0.07597900	1.29134200
C	-0.41588800	-0.15355700	2.67414800
C	-1.29301300	0.68181600	3.37070500
C	-2.15514900	1.55288400	2.69724300
C	-2.15602500	1.61936800	1.30345200
H	0.23935600	-0.84356900	3.19776300
H	-1.31299400	0.64747900	4.45571900
H	-2.83343800	2.17949100	3.26804100
H	-2.82353600	2.27813500	0.75470000
C	0.06711800	4.11072800	0.82106700
C	0.09909400	3.83623100	-0.53805300
C	0.94413400	2.84123100	-1.04645300
C	1.75561200	2.10157400	-0.17173100
C	1.71983800	2.39073400	1.19267000
C	0.87981800	3.38139300	1.68947100

H	0.26284600	3.10791900	-3.09846100
H	-0.59625000	4.87779200	1.20747400
H	-0.54648600	4.37625700	-1.22514800
C	0.92289800	2.51729100	-2.46845600
C	2.74887500	1.09005900	-0.72157800
H	2.34395300	1.81818900	1.87419300
H	0.85107500	3.57700200	2.75675900
C	2.46950900	0.64965200	-2.16136000
C	1.62282600	1.49997800	-3.00004100
H	1.53833000	1.22164800	-4.04489200
O	3.01777200	-0.35290500	-2.60129200
C	4.09549900	1.86335300	-0.82924900
H	3.93813200	2.77433200	-1.41389500
H	4.44589700	2.14257800	0.16798300
H	4.86007300	1.25543000	-1.31604500
O	0.58522600	-1.39873000	-3.48972200
H	1.55678700	-1.42408900	-3.46595100
H	0.26923500	-2.28002600	-3.23248700
C	-5.80619800	1.30014100	-1.16497100
C	-4.80781300	0.43475500	-1.53309400
C	-4.25292900	-0.46261000	-0.58522700
C	-4.72545700	-0.44585800	0.75646900
C	-5.76637800	0.45235000	1.10326600
C	-6.29421000	1.30307400	0.16451400
H	-2.79462900	-1.34133900	-1.94486800
H	-6.22257600	1.99141300	-1.89024600
H	-4.40539600	0.43860500	-2.54137500
C	-3.18857800	-1.33516800	-0.93233600
C	-4.11721200	-1.29713200	1.72205400
H	-6.13122800	0.46081000	2.12674000
H	-7.08722300	1.99089600	0.44096200
C	-3.07465900	-2.11320200	1.38212000
C	-2.61653100	-2.10929500	0.03995900
H	-4.48429600	-1.27436000	2.74420300
H	-2.59175400	-2.75614600	2.11068700
S	-1.18810600	-3.07175200	-0.34439700
O	0.00145700	-2.30966500	0.43504100

H	2.09665800	-1.78607600	1.19308300
O	-1.26542300	-4.34589300	0.32976300
O	-0.94575900	-3.01047800	-1.77572300

INT8

C	0.52984700	1.61195100	0.22614800
C	-0.19228300	3.39315400	-0.99111800
O	-0.38660800	4.04571600	-1.97350800
N	0.56157700	2.16407700	-0.96991300
H	0.68962900	1.53926900	-1.80241100
C	1.11207700	0.33290200	0.54175100
C	2.20283200	-0.17858900	-0.06841600
C	3.09517500	0.65053400	-0.93326400
C	3.26738500	0.41994400	-2.30351500
C	3.78966000	1.70727800	-0.32884000
C	4.11600700	1.23903600	-3.04431300
H	2.70554700	-0.35953500	-2.80292900
C	4.64391000	2.51308200	-1.07182400
H	3.65877700	1.88848600	0.73445200
C	4.80908600	2.28029900	-2.43474800
H	4.22306000	1.06394200	-4.10983000
H	5.17715300	3.32375600	-0.58575000
H	5.46928200	2.91230100	-3.01994200
C	-0.62176800	3.59692800	0.42018100
C	-0.19817300	2.48887100	1.15263100
C	-0.50709700	2.34175200	2.49355800
C	-1.24065000	3.37302100	3.08955000
C	-1.64427500	4.49218700	2.36045600
C	-1.34261600	4.62037100	0.99820600
H	-0.23670600	1.44710500	3.04217200
H	-1.51606600	3.29310900	4.13559300
H	-2.21918900	5.26823100	2.85504100
H	-1.67235200	5.47406900	0.41581200
C	6.46518100	-1.56645900	2.31123700
C	6.28396100	-2.39367700	1.21187600
C	5.06989200	-2.40049300	0.51452900
C	4.02242100	-1.56375800	0.92881300

C	4.21088500	-0.74733600	2.04258500
C	5.42189200	-0.74129400	2.72807900
H	5.71923500	-3.93110800	-0.89574000
H	7.41047600	-1.56577900	2.84346900
H	7.08625100	-3.04687700	0.87924600
C	4.88884600	-3.27716200	-0.63785000
C	2.66636600	-1.59970700	0.23442500
H	3.39644300	-0.10832800	2.37662000
H	5.54994000	-0.09442600	3.59004600
C	2.66094900	-2.37520000	-1.09605800
C	3.76913500	-3.29305000	-1.37919500
H	3.65170900	-3.92979700	-2.24935800
O	1.72352700	-2.26076400	-1.86596100
C	1.67732500	-2.39154100	1.12415700
H	2.03895000	-3.41878300	1.23298100
H	1.62845100	-1.94958000	2.12364800
H	0.68066300	-2.39568000	0.66946200
O	0.09629800	0.04748700	-2.51097900
H	0.42205100	-0.81151200	-2.18128400
H	-0.78120200	0.12286200	-2.08174300
C	-8.24433800	-0.37883100	-1.13780800
C	-6.93349000	0.02503500	-1.14053300
C	-5.94249600	-0.72422600	-0.45472200
C	-6.32543700	-1.90595300	0.23875600
C	-7.68880600	-2.29843500	0.22375900
C	-8.62606700	-1.55432800	-0.44713900
H	-4.26111100	0.57092800	-0.96426700
H	-8.99479100	0.20055400	-1.66637700
H	-6.63129400	0.92502300	-1.66927000
C	-4.57833200	-0.32689400	-0.44218200
C	-5.33138800	-2.65824400	0.92459800
H	-7.97715300	-3.20214000	0.75433400
H	-9.66618400	-1.86505500	-0.45199400
C	-4.02321900	-2.25841700	0.92333400
C	-3.65503500	-1.07835900	0.23002300
H	-5.63136700	-3.56083700	1.45037300
H	-3.25827700	-2.82709400	1.44220000

S	-1.94206200	-0.59297600	0.25643300
O	-1.60858000	-0.36444800	1.67932400
H	0.55723200	-0.22860400	1.28797600
O	-1.18005900	-1.70097300	-0.35399900
O	-1.85975000	0.65276000	-0.56347700

TS4-1

C	-0.91204000	1.70597400	0.01445400
C	-1.08266500	3.86810100	0.80885800
O	-1.45917100	4.75264500	1.52730700
N	-1.47164100	2.50421600	0.94591500
H	-2.07848200	2.18692300	1.69319100
C	-1.11806200	0.34194800	-0.19479600
C	-2.06832300	-0.43003700	0.45475900
C	-3.24764000	0.21944600	1.10873100
C	-3.54427600	0.12981700	2.47337600
C	-4.12902400	0.90153100	0.25582300
C	-4.70748500	0.71611300	2.96850800
H	-2.85253300	-0.37182500	3.13738800
C	-5.29525900	1.46807000	0.75764900
H	-3.89574100	0.97532100	-0.80295500
C	-5.58755200	1.37713300	2.11646900
H	-4.92183500	0.65301000	4.03039500
H	-5.96993100	1.98838700	0.08556800
H	-6.49266800	1.82784800	2.51042100
C	-0.17591700	3.87570900	-0.36632000
C	-0.04977600	2.56442400	-0.82106700
C	0.78077600	2.24541500	-1.88551800
C	1.45723800	3.30364000	-2.49627100
C	1.31453400	4.62057100	-2.05050000
C	0.49395900	4.92785300	-0.96206700
H	0.94680900	1.21448000	-2.18619000
H	2.12582000	3.09431900	-3.32464600
H	1.86307600	5.41334900	-2.54864300
H	0.38573500	5.94126200	-0.59039800
C	-4.48277000	-1.44428100	-3.69667100
C	-5.15289500	-1.80347000	-2.53585200

C	-4.45813500	-1.97998200	-1.33348700
C	-3.06713200	-1.78156700	-1.28991300
C	-2.40170600	-1.43920800	-2.46869800
C	-3.10050000	-1.27316300	-3.66138700
H	-6.25737600	-2.52487400	-0.22790800
H	-5.02961400	-1.30957800	-4.62396700
H	-6.22797600	-1.96149500	-2.54887900
C	-5.17834000	-2.41759800	-0.14226200
C	-2.28566600	-1.90208100	0.03111800
H	-1.32466600	-1.30299200	-2.46615200
H	-2.55940300	-1.01025700	-4.56442600
C	-3.10489200	-2.59846300	1.14858500
C	-4.55974100	-2.72818200	1.00586900
H	-5.08883700	-3.10151000	1.87587100
O	-2.54939600	-3.00432400	2.15489900
C	-0.99293000	-2.70691600	-0.18046500
H	-1.25586100	-3.66022300	-0.64884400
H	-0.26436900	-2.19210200	-0.80877400
H	-0.50606000	-2.90316000	0.77232300
O	-0.86437900	-0.86080000	2.33331100
H	-1.07454200	-1.77863200	2.58152500
H	0.04538900	-0.90911200	1.93555700
C	8.44150700	0.27550800	0.78660700
C	7.11354800	0.61799000	0.81353300
C	6.11635200	-0.31394500	0.42515000
C	6.51122400	-1.61463900	0.00475800
C	7.89224200	-1.93953000	-0.01300900
C	8.83499000	-1.01857300	0.36822100
H	4.40529100	1.00169900	0.76000400
H	9.19665000	0.99515100	1.08683200
H	6.80221900	1.60836200	1.13454700
C	4.73441800	0.01587900	0.44434900
C	5.51177300	-2.54895500	-0.38610200
H	8.18988500	-2.93426000	-0.33430100
H	9.88864700	-1.27925100	0.35121200
C	4.18647500	-2.21070600	-0.36122900
C	3.80705000	-0.91258800	0.06160300

H	5.82201300	-3.53971300	-0.70741500
H	3.41714100	-2.91406100	-0.66291800
S	2.07468600	-0.50210000	0.09643900
O	1.57544200	-0.80302000	-1.27291900
H	-0.40723600	-0.12610000	-0.86726600
O	1.47917900	-1.41001500	1.11530300
O	1.97642600	0.91997400	0.46429600

TS4-2

C	1.89229700	1.24207900	-0.72275000
C	3.42015300	2.97630400	-0.93353400
O	4.49970000	3.50818800	-0.93733100
N	3.20753600	1.60393900	-0.66434000
H	3.99566600	1.00319900	-0.46605800
C	1.26248800	0.02921600	-0.59982000
C	1.71569000	-1.26109400	-0.20761800
C	1.03785700	-2.38919600	-0.91348100
C	0.59764100	-2.16238200	-2.22479300
C	0.78869200	-3.64606800	-0.33823700
C	-0.05537400	-3.15741400	-2.94063100
H	0.78937000	-1.20554800	-2.69550200
C	0.12556600	-4.63379000	-1.05107900
H	1.05272200	-3.83871000	0.69403900
C	-0.29594400	-4.39549000	-2.35695700
H	-0.38596500	-2.95455400	-3.95345500
H	-0.08185400	-5.58620000	-0.57485600
H	-0.82143600	-5.16775800	-2.90943000
C	2.06361800	3.52189200	-1.18700300
C	1.14919100	2.47582500	-1.06920700
C	-0.21437500	2.68405600	-1.23308100
C	-0.61865900	3.98812000	-1.53235200
C	0.29954400	5.03482600	-1.65401000
C	1.66771100	4.81436000	-1.47853700
H	-0.93681700	1.87601500	-1.13695100
H	-1.67570100	4.19114400	-1.66912900
H	-0.05799500	6.03296400	-1.88521400
H	2.39586800	5.61427300	-1.56278600

C	4.58126900	1.35741600	3.39496000
C	5.44034900	0.78636800	2.46803200
C	4.95803800	-0.08535600	1.48548300
C	3.58289800	-0.40568900	1.42000900
C	2.73826700	0.16697800	2.36909500
C	3.22802500	1.04427000	3.33584900
H	6.94027000	-0.33500600	0.61133100
H	4.96031400	2.03943400	4.14830700
H	6.50087800	1.02211300	2.48248000
C	5.88947800	-0.58206300	0.47798600
C	3.11610200	-1.44724200	0.38851000
H	1.68584400	-0.06135600	2.37167900
H	2.53472900	1.48109500	4.04714000
C	4.06265300	-1.52325800	-0.85416600
C	5.49009700	-1.25411200	-0.61301600
H	6.17007800	-1.55283100	-1.40343700
O	3.66484000	-1.85428400	-1.94944500
C	3.33797600	-2.81958700	1.08470000
H	4.35642800	-2.85031500	1.47856800
H	2.63602300	-2.91030400	1.91652000
H	3.20984000	-3.64759900	0.38578600
O	0.51766300	-1.54365300	1.54464500
H	0.00228100	-0.69098600	1.56343900
H	-0.20801500	-2.11369800	1.19319300
C	-8.39476500	0.83998700	-0.68632500
C	-7.08403400	0.64093800	-1.03792000
C	-6.11303000	0.30990900	-0.05730700
C	-6.51577500	0.18698800	1.30173500
C	-7.87853500	0.39948500	1.63485500
C	-8.79612500	0.71774200	0.66599200
H	-4.41522800	0.19069700	-1.42434100
H	-9.13042800	1.09184500	-1.44362300
H	-6.76734800	0.73160600	-2.07343400
C	-4.74921600	0.09906300	-0.39489100
C	-5.54205900	-0.14150200	2.28563800
H	-8.18237500	0.30473100	2.67402800
H	-9.83616700	0.87733000	0.93275800

C	-4.23359400	-0.34044800	1.93959600
C	-3.84654700	-0.21700900	0.58230900
H	-5.85714200	-0.22855300	3.32201400
H	-3.48155400	-0.58003200	2.68415600
S	-2.14458600	-0.51543900	0.15706100
O	-1.34985200	0.32031500	1.10942900
H	0.21881500	0.06573900	-0.89746400
O	-1.90436900	-1.96119700	0.38200200
O	-1.97746900	-0.08237300	-1.24437100

INT9

C	1.11179900	1.73347400	-0.12018800
C	1.47016300	3.80734200	-1.11476900
O	1.87718100	4.62523200	-1.90738000
N	1.70010500	2.43492100	-1.16886000
H	2.23983600	2.01290500	-1.91142200
C	1.16728300	0.42075800	0.16159400
C	1.82188500	-0.63577600	-0.68969700
C	3.14454000	-0.15583100	-1.29326800
C	3.44557800	-0.38875100	-2.63692300
C	4.08904900	0.49287400	-0.48950500
C	4.67865900	-0.00428200	-3.16167000
H	2.71373600	-0.86758300	-3.27813100
C	5.32097300	0.86902700	-1.01301900
H	3.84782500	0.71587200	0.54603500
C	5.62239600	0.61668400	-2.35021000
H	4.89565200	-0.18943000	-4.20885900
H	6.04117100	1.37415600	-0.37720300
H	6.58102700	0.91852900	-2.75984500
C	0.63987300	4.00243600	0.10552100
C	0.41181300	2.75910900	0.68858200
C	-0.36233800	2.64563600	1.83675000
C	-0.88288500	3.81808600	2.38131700
C	-0.64149600	5.06737100	1.79719100
C	0.12579900	5.17347300	0.63957100
H	-0.58513200	1.67812400	2.27671400
H	-1.49762900	3.76035900	3.27410800

H	-1.06587200	5.95832700	2.24889700
H	0.31960200	6.12791500	0.16075700
C	4.54172600	-1.14625900	3.60631400
C	5.09802000	-1.75385100	2.48977500
C	4.30924400	-2.06396500	1.37643500
C	2.93808100	-1.74238000	1.36197700
C	2.38527600	-1.17906400	2.51470700
C	3.17603700	-0.87564000	3.62074500
H	5.97611300	-2.97895300	0.31214800
H	5.16021700	-0.90449800	4.46421400
H	6.15499100	-2.00581100	2.47096300
C	4.90928800	-2.77428100	0.25426000
C	2.08671200	-2.00145300	0.12780700
H	1.32118000	-0.97815100	2.56862400
H	2.71738400	-0.42837700	4.49661800
C	2.77330400	-2.90700700	-0.90940200
C	4.19747600	-3.20991600	-0.79703800
H	4.63544800	-3.77018300	-1.61561800
O	2.12955100	-3.29685200	-1.88039300
C	0.75111100	-2.66337400	0.51903500
H	0.95225800	-3.52726000	1.15943800
H	0.09145000	-1.98125200	1.05993700
H	0.22163600	-3.01291900	-0.36820200
O	0.88028600	-0.92855700	-1.73196200
H	1.07880900	-1.82679700	-2.08083900
H	-0.70189600	-0.85592000	-1.22689600
C	-8.57667500	0.04742300	-0.98838700
C	-7.28157100	0.49763800	-0.98776600
C	-6.24111300	-0.30180100	-0.44732600
C	-6.55487600	-1.57858900	0.09794100
C	-7.90440900	-2.01586200	0.08302000
C	-8.89026200	-1.22307300	-0.44716300
H	-4.62394500	1.10932200	-0.84530600
H	-9.36760800	0.66313600	-1.40408300
H	-7.03092600	1.47047700	-1.40108900
C	-4.89208400	0.13931400	-0.43657400
C	-5.51329300	-2.37820800	0.64571800

H	-8.14241100	-2.99067900	0.49954200
H	-9.91936400	-1.56781000	-0.45381400
C	-4.21825700	-1.93777000	0.65511400
C	-3.92692100	-0.66890400	0.09844700
H	-5.76551700	-3.34835100	1.06425500
H	-3.41714800	-2.53161600	1.08209200
S	-2.25643300	-0.09559400	0.11571600
O	-1.67132900	-0.43205200	1.41246800
H	0.57632400	0.09824500	1.00770400
O	-1.66062300	-1.06646000	-0.99232500
O	-2.20312200	1.28064200	-0.33836800

INT10

C	-2.24348300	-0.81698800	1.06316300
C	-0.23699900	-1.92831200	1.38417200
O	0.95628700	-2.16608400	1.34393600
N	-0.84858800	-0.76163200	0.96569600
C	-3.14781000	0.00178600	0.51488900
C	-2.99098100	1.14484200	-0.47908400
C	-2.64194500	2.46869400	0.20336700
C	-1.84337000	2.51392900	1.34562100
C	-3.11121300	3.66869300	-0.34065400
C	-1.46761500	3.73378900	1.89977100
H	-1.48764300	1.60115700	1.80897900
C	-2.75534500	4.88786200	0.22658700
H	-3.74346000	3.64700100	-1.22278200
C	-1.92042700	4.92509300	1.34055000
H	-0.81348500	3.74511400	2.76593300
H	-3.12198900	5.81110400	-0.21130200
H	-1.62664000	5.87656700	1.77201200
C	-1.33936300	-2.79975300	1.86687200
C	-2.54222000	-2.11243400	1.71181800
C	-3.74248300	-2.71011000	2.07954800
C	-3.69326900	-3.99370100	2.61972500
C	-2.48030000	-4.67623000	2.77419000
C	-1.28092100	-4.08221000	2.39056200
H	-4.69199400	-2.19715300	1.96144600
H	-4.61579800	-4.47611500	2.92720700

H	-2.48042400	-5.67585000	3.19619900
H	-0.32719400	-4.58976500	2.49398800
C	-2.28140100	-3.49538200	-2.56742300
C	-1.04062800	-2.90944900	-2.37738300
C	-0.93054500	-1.53871400	-2.10400300
C	-2.08356900	-0.73854900	-2.00623600
C	-3.32567500	-1.34041600	-2.22470200
C	-3.42529700	-2.70063300	-2.49686500
H	1.25136100	-1.60326200	-2.04929300
H	-2.36036900	-4.55757000	-2.77326900
H	-0.13379100	-3.50521300	-2.43764000
C	0.38837100	-0.94939800	-1.93841100
C	-1.99962700	0.75483700	-1.69623100
H	-4.22418800	-0.73655800	-2.15261600
H	-4.40422200	-3.14358000	-2.65124000
C	-0.56349700	1.25349700	-1.48352300
C	0.57068500	0.35304800	-1.66284800
H	1.56048000	0.78701100	-1.56479300
O	-0.37356800	2.44988600	-1.26860900
C	-2.41971000	1.52816800	-2.97626700
H	-1.71216600	1.29988300	-3.78000100
H	-3.41933600	1.23210500	-3.28967000
H	-2.39103700	2.60251400	-2.78181000
O	-4.26604600	1.28884500	-1.11027400
H	-4.84020100	1.74138000	-0.47235600
H	-4.18720400	-0.25499900	0.69971700
C	6.31734400	-2.64925300	-0.95194500
C	6.52577500	-1.29303700	-0.91975900
C	5.51629900	-0.42049600	-0.43869000
C	4.28733700	-0.97977600	0.00808400
C	4.09672500	-2.38615100	-0.02936400
C	5.09328400	-3.20212200	-0.50216500
H	6.63947600	1.41043700	-0.72386900
H	7.09691700	-3.30785300	-1.32203400
H	7.46620400	-0.86945600	-1.26158700
C	5.69489300	0.99135400	-0.38869300
C	3.26286700	-0.11801700	0.47988900

H	3.15266100	-2.78621200	0.33192800
H	4.95053300	-4.27771900	-0.52975200
C	3.47869200	1.23316900	0.49397500
C	4.70151600	1.81248800	0.07123900
H	2.32454700	-0.54638400	0.82368900
H	4.83053900	2.88910100	0.11342300
S	2.17675000	2.29126700	1.05725800
O	2.67582000	3.15463500	2.10264500
O	0.99766000	1.46126900	1.30214100
O	1.90171800	3.18273000	-0.22378700
H	1.01993800	2.93050600	-0.65373700
H	-0.29093700	0.07400600	0.80013900

TS5-1

C	1.58918400	0.66005700	1.35119100
C	-0.21626700	1.48725800	0.10876900
O	-1.03462800	1.56742100	-0.76458600
N	0.71552200	0.36033000	0.23841800
C	2.74499900	0.02324900	1.52428700
C	3.30417400	-0.93611100	0.49797400
C	2.78965800	-2.37075000	0.68765100
C	1.60406600	-2.65782300	1.36470300
C	3.54187300	-3.43184600	0.17113900
C	1.13562000	-3.96366600	1.45566600
H	1.00484600	-1.86800800	1.79990600
C	3.08957100	-4.74345800	0.28895400
H	4.47765500	-3.23310600	-0.34301900
C	1.87689800	-5.01159000	0.91635300
H	0.17681800	-4.14865400	1.92808600
H	3.68213400	-5.55320700	-0.12544300
H	1.50975200	-6.03055200	0.98326500
C	0.03340500	2.37917400	1.25485500
C	1.07227300	1.85808900	2.02345200
C	1.48696000	2.51651300	3.17784900
C	0.82345800	3.68769100	3.53181600
C	-0.22310100	4.20418500	2.75414400
C	-0.63075100	3.55101300	1.59715300

H	2.29363000	2.12788800	3.79100000
H	1.12073500	4.21345400	4.43367500
H	-0.71778900	5.11820300	3.06472100
H	-1.43982100	3.92400600	0.97769500
C	4.33469700	3.84119100	-1.43655300
C	3.24009500	3.35189100	-2.13186600
C	2.79511100	2.03769200	-1.94338300
C	3.46118800	1.17673000	-1.04485900
C	4.57484600	1.68280000	-0.36864800
C	4.99911300	2.99660100	-0.55272000
H	1.24448600	2.21906800	-3.47984700
H	4.66820600	4.86304600	-1.58415100
H	2.70486800	3.98741000	-2.83232100
C	1.62417800	1.58034700	-2.68679000
C	3.01393200	-0.29434500	-0.94039300
H	5.12238000	1.04598700	0.31243800
H	5.86213500	3.35579200	-0.00082700
C	1.52810800	-0.41616200	-1.29354400
C	1.00236000	0.44072700	-2.37891900
H	0.09243600	0.10307500	-2.86323700
O	1.10903700	-1.65787600	-1.30100800
C	3.77122200	-1.07787300	-2.03597600
H	3.60539300	-0.60440500	-3.00750900
H	4.83858000	-1.05739800	-1.80984700
H	3.41762600	-2.10898800	-2.08525700
O	4.72319900	-0.96862000	0.63189200
H	4.93165600	-1.70039200	1.23265900
H	3.39336100	0.29529800	2.35200300
C	-7.61931800	1.64307300	-0.47725100
C	-7.38454600	0.43691100	0.13095500
C	-6.10687900	-0.17808600	0.05435000
C	-5.07187400	0.47855700	-0.66961700
C	-5.34422600	1.72734900	-1.28906900
C	-6.58710300	2.29738000	-1.19491800
H	-6.63076000	-1.92744900	1.21560100
H	-8.60013100	2.10358700	-0.41142300
H	-8.17378100	-0.06757900	0.68203200

C	-5.83273800	-1.42678100	0.67407800
C	-3.79286400	-0.12810300	-0.75130800
H	-4.54380400	2.21988000	-1.83463400
H	-6.78742300	3.25241700	-1.67029900
C	-3.57131600	-1.32792600	-0.12879600
C	-4.58959100	-1.99675500	0.58963300
H	-2.99337300	0.35504800	-1.30481300
H	-4.36624200	-2.95537300	1.04524300
S	-1.94206000	-2.04073500	-0.15867900
O	-2.08066900	-3.46831300	0.09783400
O	-1.16907800	-1.31632800	0.90627100
O	-1.39592400	-1.67922000	-1.50991500
H	0.10752600	-1.73292800	-1.52720000
H	0.04922000	-0.46641000	0.46539600

TS5-2

C	-1.06749100	-0.25393100	1.51757100
C	0.72538700	-1.18407800	0.27555400
O	1.26695200	-1.72521000	-0.64207000
N	-0.75764400	-1.01683400	0.32426600
H	-1.15103100	-1.96348300	0.40227500
C	-2.25176500	0.33192200	1.67205300
C	-3.33581800	0.43117900	0.61788900
C	-3.40891000	1.91448900	0.17356700
C	-2.30676600	2.77233200	0.25099900
C	-4.64135400	2.43852700	-0.23399200
C	-2.43448300	4.11371100	-0.09273400
H	-1.32882600	2.39334800	0.53079400
C	-4.76612700	3.78332800	-0.57709400
H	-5.51133700	1.79209500	-0.30175000
C	-3.66209500	4.62570700	-0.50703500
H	-1.55732200	4.75136000	-0.04865600
H	-5.72912000	4.16579900	-0.90098400
H	-3.75547100	5.67279700	-0.77771100
C	1.22426300	-0.68762100	1.56344500
C	0.16498200	-0.17286100	2.31315500
C	0.40477900	0.38222600	3.56352000

C	1.71936100	0.40252800	4.02652700
C	2.77589500	-0.10577900	3.26121000
C	2.53860000	-0.65962400	2.00737900
H	-0.40010000	0.79670500	4.16185600
H	1.93023800	0.83232700	5.00067600
H	3.78950500	-0.05629100	3.64465500
H	3.34240200	-1.03916000	1.38238100
C	-3.75183700	-4.86967000	0.27919700
C	-2.99526900	-4.44118100	-0.80231600
C	-2.75651600	-3.08032000	-1.01995300
C	-3.31383300	-2.10168000	-0.15366400
C	-4.05577000	-2.55898100	0.93971600
C	-4.26435600	-3.92145800	1.15580400
H	-1.55615800	-3.46284400	-2.81510800
H	-3.92717500	-5.92802600	0.44146000
H	-2.55891200	-5.16245900	-1.48795900
C	-1.84146700	-2.69783100	-2.09814200
C	-3.12240200	-0.61720300	-0.54778400
H	-4.48385500	-1.84937200	1.63054100
H	-4.84258200	-4.23408000	2.01948600
C	-1.70782200	-0.45396200	-1.14630900
C	-1.29675100	-1.47996100	-2.14548800
H	-0.54311300	-1.18156500	-2.86671100
O	-1.40072600	0.77507600	-1.41433100
C	-4.12941800	-0.32557900	-1.68326300
H	-4.05596800	-1.08677500	-2.46236100
H	-5.13893000	-0.35039000	-1.26674200
H	-3.93826900	0.65473100	-2.12374600
O	-4.60275300	0.12213400	1.19931200
H	-4.92375600	0.93543200	1.61856700
H	-2.42088700	0.92131300	2.57052200
C	7.24129500	-1.61794900	-0.25346900
C	6.82908400	-0.45084400	0.33850200
C	5.59143700	0.14560400	-0.01765400
C	4.78342900	-0.48545500	-1.00537300
C	5.23430400	-1.69368100	-1.59806000
C	6.43426200	-2.24802300	-1.23157800

H	5.75565700	1.83342300	1.33113000
H	8.19028600	-2.06429900	0.02677000
H	7.44628600	0.03638400	1.08888000
C	5.12999600	1.34979900	0.58539200
C	3.53683300	0.09919600	-1.35968200
H	4.60573600	-2.17016000	-2.34517100
H	6.77065100	-3.17259200	-1.68987300
C	3.12266100	1.24673600	-0.74254700
C	3.92257800	1.89080800	0.23623000
H	2.90179500	-0.37347400	-2.10155400
H	3.56050700	2.80619900	0.69363800
S	1.51525000	1.94835100	-1.06259200
O	1.72022300	3.34236200	-1.43429400
O	0.75570700	1.72685700	0.18760500
O	0.93714000	1.08720500	-2.16624200
H	-0.43648900	0.89735800	-1.83297200

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C	-0.97355500	-0.58849600	1.28762500
C	0.62072700	-1.06779600	-0.33217600
O	1.14333900	-1.16761600	-1.42384300
N	-0.69827800	-0.69517500	-0.09036700
C	-2.14691800	-0.16266600	1.76365700
C	-3.23254500	0.32057900	0.82953900
C	-3.18969800	1.86212300	0.72075200
C	-2.10991000	2.61452900	1.18521300
C	-4.31442700	2.54840300	0.24314600
C	-2.11368200	4.00467200	1.10295200
H	-1.24770500	2.11826700	1.61601700
C	-4.32540600	3.93778600	0.16920200
H	-5.18891400	1.99090000	-0.07428200
C	-3.21888500	4.67267700	0.58678400
H	-1.24509800	4.55877800	1.44441900
H	-5.20369300	4.44554200	-0.21728400
H	-3.22319700	5.75587500	0.51990000
C	1.21887800	-1.28506300	1.01054100
C	0.26075200	-0.99035800	1.98056100

C	0.57314900	-1.08663300	3.33128700
C	1.86546900	-1.48240400	3.67314600
C	2.81963800	-1.78313100	2.69401600
C	2.50241400	-1.69266800	1.34050600
H	-0.15987200	-0.86023400	4.09934800
H	2.13678800	-1.56173700	4.72121700
H	3.81681600	-2.09054000	2.99277200
H	3.22390200	-1.93396300	0.56623600
C	-3.70302900	-4.79800100	-0.33098300
C	-3.03538100	-4.20329000	-1.39378500
C	-2.80222600	-2.82723000	-1.41391300
C	-3.27028600	-1.99856800	-0.36848200
C	-3.92836800	-2.61744500	0.69540000
C	-4.13559000	-3.99761600	0.71758400
H	-1.85514700	-2.85625200	-3.39923600
H	-3.87413700	-5.86964500	-0.31957500
H	-2.66584500	-4.80753900	-2.21819000
C	-2.01486200	-2.25534100	-2.50827000
C	-3.08536500	-0.46544000	-0.53452900
H	-4.29478700	-2.02596800	1.52064900
H	-4.64753700	-4.43978100	1.56670100
C	-1.64965400	-0.25673000	-1.11148200
C	-1.45705500	-1.05507300	-2.38434900
H	-0.81204400	-0.62976200	-3.14635500
O	-1.44651500	1.12124800	-1.39119500
C	-4.13131600	0.02021000	-1.55025400
H	-4.11956300	-0.61186700	-2.43937100
H	-5.12164900	-0.04787400	-1.09441500
H	-3.93384900	1.05015500	-1.85381200
O	-4.52938800	0.00636300	1.34019200
H	-4.78066900	0.72855600	1.93529500
H	-2.30945100	-0.08352200	2.83448000
C	6.71569400	-1.76521400	0.00675500
C	6.31491000	-0.66874100	0.72860700
C	5.23471600	0.13504000	0.28221300
C	4.58313700	-0.20810700	-0.93534200
C	5.02036500	-1.34401800	-1.66428800

C	6.06096500	-2.10900300	-1.20113100
H	5.27639200	1.50801000	1.95782300
H	7.53864200	-2.37753200	0.36165700
H	6.81426600	-0.40485600	1.65696900
C	4.76689300	1.24898400	1.03416900
C	3.46660800	0.55615600	-1.36352600
H	4.50001900	-1.60411200	-2.58147600
H	6.38516200	-2.98272900	-1.75691700
C	3.04024900	1.59920000	-0.58989300
C	3.68796300	1.97572200	0.61332900
H	2.92972300	0.28779400	-2.26650500
H	3.31898100	2.82456500	1.17921900
S	1.60035600	2.49600900	-1.07457700
O	1.86655300	3.91283600	-0.96541300
O	0.60055600	2.07054900	0.10188000
O	1.06574200	1.94538100	-2.31859700
H	-0.78815900	1.20996000	-2.11049100
H	-0.27562200	1.80721600	-0.30067800

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C	1.09840600	0.35327900	1.43584300
C	-0.69222100	1.12618400	0.03909700
O	-1.20909100	1.47476300	-0.97225600
N	0.83180200	0.98043500	0.13901800
H	1.16618200	1.95557600	0.19928700
C	2.25519500	-0.25595400	1.66673200
C	3.33362200	-0.47536600	0.62581300
C	3.33723400	-1.97887000	0.25718300
C	2.19901200	-2.78071100	0.38628100
C	4.54070200	-2.57575900	-0.13610100
C	2.26108900	-4.14082600	0.10380800
H	1.24185700	-2.34513600	0.65503600
C	4.60054900	-3.93977700	-0.41517600
H	5.43769200	-1.97323200	-0.24594900
C	3.46014800	-4.72655300	-0.29630500
H	1.35451300	-4.73253700	0.18159600
H	5.54147800	-4.38063500	-0.72955100

H	3.50336200	-5.78800700	-0.51954700
C	-1.17342900	0.91785900	1.40612300
C	-0.12860100	0.48878800	2.22779900
C	-0.37450500	0.19555700	3.56270500
C	-1.68011400	0.33308800	4.03234600
C	-2.72286000	0.74386200	3.19395300
C	-2.48012900	1.04057500	1.85646900
H	0.41950500	-0.14138000	4.22102300
H	-1.89456900	0.10538700	5.07163000
H	-3.73101100	0.81984800	3.58701000
H	-3.27493300	1.33448500	1.17619400
C	3.91728200	4.78713400	0.10766200
C	3.17033300	4.34388300	-0.97554500
C	2.89366700	2.98501600	-1.15068300
C	3.40074400	2.02113900	-0.23837000
C	4.13340400	2.49378700	0.85440200
C	4.38190600	3.85599500	1.02753000
H	1.79876900	3.30770000	-3.02976800
H	4.12307400	5.84472900	0.23602500
H	2.77398900	5.05360200	-1.69671100
C	2.00235400	2.58279400	-2.24637900
C	3.15372400	0.52894800	-0.58191300
H	4.52632300	1.79630200	1.57804400
H	4.95302900	4.18098800	1.89138900
C	1.69885300	0.41778000	-1.12457400
C	1.40385100	1.39187100	-2.23738200
H	0.68687400	1.06831600	-2.98440400
O	1.39866200	-0.84596000	-1.40974500
C	4.13079600	0.14599400	-1.70819400
H	4.09552100	0.88019400	-2.51476300
H	5.14378800	0.13013100	-1.29926100
H	3.88250200	-0.83742000	-2.11155100
O	4.60956400	-0.19378000	1.19910400
H	4.91100400	-1.01083300	1.62549500
H	2.40939900	-0.73601100	2.63014900
C	-7.32259100	1.53213500	-0.34793400
C	-6.84058100	0.49621600	0.41178300

C	-5.60837900	-0.12946300	0.08817400
C	-4.87779100	0.33440500	-1.04231700
C	-5.40132600	1.40816600	-1.80906600
C	-6.59455000	1.99431800	-1.47104900
H	-5.64700100	-1.56114700	1.71380100
H	-8.26710000	2.00155000	-0.09122000
H	-7.39821700	0.13608800	1.27250500
C	-5.07892200	-1.20252900	0.85920600
C	-3.63580900	-0.27811900	-1.36462000
H	-4.83489200	1.75561900	-2.66862300
H	-6.98665000	2.81454500	-2.06398000
C	-3.15343400	-1.29429800	-0.58684500
C	-3.87880300	-1.77436800	0.53376500
H	-3.05563000	0.06895800	-2.21384300
H	-3.46527300	-2.59117600	1.11702800
S	-1.53659100	-1.99445300	-0.87706500
O	-1.70231300	-3.44067800	-0.96725700
O	-0.74827000	-1.53473400	0.29715100
O	-1.03492700	-1.32574000	-2.12174200
H	0.46730000	-0.97635400	-1.79451500

TS6

C	0.66220600	-0.58532700	-0.83744000
C	0.38911500	-1.81903700	1.18732200
O	0.68494500	-2.25339700	2.25780500
N	1.24065600	-0.86894300	0.43961400
C	1.20850100	0.31586100	-1.65006400
C	2.34005000	1.19744200	-1.17689200
C	1.75044500	2.50902400	-0.61093200
C	0.47513200	2.56722700	-0.05286200
C	2.49831100	3.69130200	-0.69515100
C	-0.03328900	3.76187100	0.44869100
H	-0.12566700	1.67224800	0.04359500
C	1.98394600	4.89078600	-0.21226000
H	3.49653800	3.67516800	-1.12202600
C	0.71711300	4.93003200	0.36553200
H	-1.01439200	3.76089600	0.91444000

H	2.58099300	5.79472900	-0.28202300
H	0.32206300	5.86418000	0.75187300
C	-0.72443800	-2.09956900	0.27204700
C	-0.54475600	-1.41141500	-0.92920000
C	-1.49060200	-1.50835600	-1.94153800
C	-2.61904500	-2.29188000	-1.70442300
C	-2.79987100	-2.96214900	-0.48921500
C	-1.84752100	-2.87319300	0.52339600
H	-1.38271400	-0.96422900	-2.87472500
H	-3.39150100	-2.35139600	-2.46553800
H	-3.70773700	-3.53302900	-0.32689700
H	-1.98142600	-3.33604200	1.49485000
C	5.86450800	-2.77938600	-1.61471200
C	5.55354700	-2.64851600	-0.26481100
C	4.66263500	-1.66900200	0.16872800
C	4.08894800	-0.75884500	-0.75292700
C	4.39225900	-0.91785200	-2.10278900
C	5.26545600	-1.92424400	-2.52711500
H	4.82562900	-2.23126400	2.29425000
H	6.55321500	-3.54950900	-1.94579700
H	5.98325300	-3.32825600	0.46587000
C	4.24768900	-1.65491000	1.57738700
C	3.23197300	0.40434300	-0.14770900
H	3.96060000	-0.25532700	-2.83663200
H	5.47359600	-2.02521200	-3.58748900
C	2.38410600	-0.36975800	0.85737800
C	3.12329900	-1.03857200	1.95275900
H	2.69632400	-1.10908500	2.94163400
O	1.67447000	1.22892500	2.18373700
C	4.21132900	1.37513600	0.53740200
H	4.91364000	0.83704000	1.17379300
H	4.77825600	1.88157800	-0.24720400
H	3.66897000	2.10747000	1.13600600
O	3.19155300	1.55313000	-2.25864400
H	2.79315100	2.32665800	-2.68645500
H	0.76400800	0.52579200	-2.61814800
C	-6.05638400	0.04733700	-3.00946800

C	-6.23967700	-0.48865400	-1.75953600
C	-5.28642300	-0.27552700	-0.72927300
C	-4.13701000	0.51334500	-1.01087200
C	-3.97786600	1.06305100	-2.30975600
C	-4.91147300	0.83392400	-3.28837200
H	-6.31229300	-1.44402000	0.77800900
H	-6.79081800	-0.12597700	-3.78973700
H	-7.11825100	-1.09006800	-1.54058100
C	-5.42771000	-0.84937400	0.56443100
C	-3.15185900	0.68316400	-0.00289400
H	-3.09650200	1.66700200	-2.51279400
H	-4.77986700	1.25717700	-4.27933000
C	-3.30337000	0.08721700	1.21902500
C	-4.45810200	-0.68080200	1.51631100
H	-2.25782800	1.26149000	-0.22135300
H	-4.53357900	-1.14656900	2.49362100
S	-2.04145900	0.23381800	2.48573700
O	-2.02032900	-1.08174100	3.13423500
O	-2.38715400	1.37859000	3.32495800
O	-0.78970600	0.48223000	1.67583000
H	1.89888500	1.06499400	3.11226500
H	0.68493500	1.08502800	2.12287000

INT12

C	0.60643400	-0.52083200	-0.85584300
C	0.41823200	-1.94122300	1.07060700
O	0.76989000	-2.46305100	2.07887600
N	1.22683000	-0.87689300	0.38628800
C	1.11622300	0.45118400	-1.60804500
C	2.24519700	1.31156000	-1.09190200
C	1.64746800	2.53201300	-0.35667600
C	0.47478500	2.43218800	0.39077400
C	2.28882000	3.77450800	-0.43569300
C	-0.04187400	3.53717300	1.06425500
H	-0.04344400	1.48807500	0.49960200
C	1.76633700	4.88384800	0.22459200
H	3.21481600	3.87576300	-0.99345300

C	0.60069700	4.76967800	0.97907300
H	-0.94468600	3.41185000	1.65645200
H	2.27942900	5.83775000	0.15385000
H	0.19888800	5.63443600	1.49731700
C	-0.69390600	-2.18398700	0.14503100
C	-0.56506000	-1.38761800	-0.99382700
C	-1.52065000	-1.44023900	-2.00022300
C	-2.60886600	-2.29149800	-1.81869400
C	-2.73904600	-3.07288400	-0.66469600
C	-1.77551300	-3.03047100	0.33984700
H	-1.45389100	-0.81073500	-2.88201500
H	-3.38827300	-2.32107900	-2.57400000
H	-3.61678600	-3.69808700	-0.54200500
H	-1.87374600	-3.58154100	1.26792700
C	5.94220900	-2.47321900	-1.88655700
C	5.62609900	-2.47107400	-0.53045400
C	4.70045600	-1.56657600	-0.01655600
C	4.09479800	-0.60604300	-0.86540000
C	4.40822000	-0.62886900	-2.22093300
C	5.31865900	-1.56289100	-2.72597100
H	4.92345200	-2.24372200	2.07235100
H	6.65821100	-3.18752000	-2.27920000
H	6.08327400	-3.19313400	0.14042100
C	4.30347900	-1.66034100	1.39769500
C	3.18855300	0.46033600	-0.16562000
H	3.95400300	0.08249200	-2.89343400
H	5.53517000	-1.56382800	-3.78942400
C	2.39499600	-0.44159200	0.76302400
C	3.15814300	-1.11640300	1.82559300
H	2.75260500	-1.19921100	2.82269800
O	1.61480200	0.98550700	2.68508000
C	4.12578300	1.41059600	0.60900700
H	4.89629900	0.85380400	1.13980500
H	4.60768000	2.06607100	-0.12023800
H	3.56469900	2.00866600	1.32717300
O	3.04363100	1.79144100	-2.16137300
H	2.56875000	2.53905000	-2.55683200

H	0.65393100	0.71789000	-2.55360700
C	-5.77459400	0.58141300	-3.19558900
C	-6.05475700	-0.12474800	-2.05269000
C	-5.16421500	-0.10374000	-0.94730100
C	-3.97586100	0.67229300	-1.03903000
C	-3.71536200	1.39882700	-2.23014700
C	-4.59004200	1.35315000	-3.28609000
H	-6.31933400	-1.43998900	0.30557800
H	-6.46240400	0.55466800	-4.03491300
H	-6.96417800	-0.71548800	-1.97826100
C	-5.40612000	-0.85435600	0.23639100
C	-3.05743300	0.65977700	0.04332100
H	-2.80500900	1.99166100	-2.28667200
H	-4.38191900	1.91185700	-4.19330200
C	-3.30611300	-0.09909200	1.15407200
C	-4.49853300	-0.85962100	1.26172800
H	-2.13703000	1.23352700	-0.03178400
H	-4.65290000	-1.45658100	2.15495100
S	-2.13964400	-0.15718800	2.51796000
O	-2.18852800	-1.54805600	2.98277200
O	-2.54300300	0.87536500	3.46991400
O	-0.82564800	0.17007500	1.85123000
H	1.52299300	1.94874100	2.70887100
H	0.68089800	0.67024200	2.61633100

INT13

C	-0.86276200	2.02743400	0.20256800
C	-0.05016000	2.37469100	-2.00169900
O	-0.05253300	2.32524600	-3.19692600
N	-0.93636800	1.58574700	-1.15040400
C	-1.49395900	1.37720100	1.17539900
C	-2.28718000	0.10828600	0.91517200
C	-3.46368900	0.04828800	1.88653300
C	-4.25280200	1.17157500	2.14830300
C	-3.73911100	-1.14478700	2.55850100
C	-5.32980100	1.09301700	3.02766000
H	-4.01790300	2.11969300	1.67121200

C	-4.81187200	-1.22117000	3.44234800
H	-3.10456300	-2.00341200	2.37369000
C	-5.61651500	-0.10751600	3.67236700
H	-5.93535300	1.97367100	3.21744200
H	-5.01650900	-2.15491700	3.95696900
H	-6.45231600	-0.16947700	4.36218500
C	0.62257500	3.29434300	-1.06803500
C	0.12214900	3.11243700	0.22006600
C	0.59479000	3.88705100	1.27363900
C	1.57455200	4.83557100	0.99365200
C	2.07258800	5.01275900	-0.30405300
C	1.59523300	4.24056300	-1.35763000
H	0.21928600	3.75541100	2.28314500
H	1.96414000	5.44975600	1.79915900
H	2.84127100	5.75683100	-0.48323600
H	1.96787900	4.35019100	-2.37034700
C	-4.37495800	-3.81655200	-1.59362000
C	-3.22179500	-3.36533600	-2.21163000
C	-2.71904800	-2.08648900	-1.92506600
C	-3.35122400	-1.25839000	-0.97744300
C	-4.54091100	-1.70823000	-0.40426900
C	-5.04103400	-2.97320400	-0.70407800
H	-1.10462500	-2.25691800	-3.36489700
H	-4.76627500	-4.80399900	-1.81277200
H	-2.70016100	-3.98407200	-2.93594900
C	-1.60547800	-1.57927600	-2.67877000
C	-2.76202100	0.09149100	-0.62142600
H	-5.08834800	-1.08204800	0.28984000
H	-5.96274500	-3.30128800	-0.23402700
C	-1.58170200	0.46686000	-1.49133700
C	-1.14715900	-0.29700000	-2.59032800
H	-0.29625200	0.03763400	-3.16713200
C	-3.81513400	1.18791300	-0.95188500
H	-4.03455900	1.17613100	-2.02334000
H	-4.74023900	0.99176900	-0.40897000
H	-3.44828700	2.18058200	-0.67975200
O	-1.49480200	-1.01067400	1.15349900

H	-0.57684700	-0.86947300	0.79177800
H	-1.32761300	1.65145300	2.21179200
C	7.65718800	-1.78892700	2.02571100
C	7.33135200	-1.66457900	0.69890100
C	5.99030900	-1.42930600	0.29919200
C	4.98338900	-1.32316200	1.29876200
C	5.35027400	-1.45491300	2.66347000
C	6.65491700	-1.68281500	3.02025200
H	6.39890500	-1.36799200	-1.82606200
H	8.68662800	-1.96984400	2.31898200
H	8.09729300	-1.74534400	-0.06807100
C	5.62346300	-1.29218000	-1.06833000
C	3.63918200	-1.08764900	0.90366500
H	4.57439600	-1.37330900	3.42001200
H	6.92470100	-1.78362700	4.06687400
C	3.32802000	-0.96518800	-0.42218700
C	4.32293500	-1.06384700	-1.42670800
H	2.85475400	-0.99682600	1.64908300
H	4.03509400	-0.94308700	-2.46604900
S	1.64249000	-0.70661900	-0.93982600
O	1.18720500	-1.96400000	-1.55060900
O	1.69285100	0.43681900	-1.87641700
O	0.90669800	-0.35559200	0.31451000

TS7

C	0.87201800	-1.94469300	0.50060200
C	0.26560000	-2.77927000	-1.60747400
O	0.23461200	-2.87835100	-2.80471300
N	1.14961600	-1.91805100	-0.89118600
C	1.32963700	-1.01376500	1.33699700
C	2.16432400	0.17368600	0.91760500
C	3.33113500	0.45792000	1.82712300
C	3.94939300	-0.55446400	2.56729000
C	3.78099500	1.77548500	1.95963400
C	5.02147700	-0.25982600	3.40439600
H	3.58353200	-1.57470500	2.49233800
C	4.84861400	2.06823600	2.80179700

H	3.27806500	2.55800000	1.40216000
C	5.47587100	1.05204300	3.51972500
H	5.49316000	-1.05348000	3.97484000
H	5.18865300	3.09428000	2.90063400
H	6.30804700	1.28286000	4.17735800
C	-0.45663800	-3.52927300	-0.55386600
C	-0.09165100	-3.03503900	0.69718800
C	-0.65221900	-3.55794700	1.85513600
C	-1.58306700	-4.58602600	1.71791100
C	-1.94590100	-5.07721000	0.45869100
C	-1.38278600	-4.54860900	-0.70053800
H	-0.38044300	-3.18036800	2.83566000
H	-2.03845900	-5.01276500	2.60576200
H	-2.67876300	-5.87414100	0.38866200
H	-1.65748400	-4.90301000	-1.68837300
C	4.66650300	3.31642700	-2.08320200
C	3.41022300	2.92571500	-2.49764700
C	2.88388000	1.68411900	-2.09014100
C	3.61511500	0.84147800	-1.22086200
C	4.89440500	1.25475300	-0.82157800
C	5.41064300	2.46780300	-1.25149100
H	1.03536100	1.90912000	-3.20887900
H	5.07905500	4.26800700	-2.40056800
H	2.81542000	3.55830600	-3.15004000
C	1.63255000	1.22971300	-2.60650300
C	2.97827600	-0.38214600	-0.70067200
H	5.48788800	0.63744300	-0.15672300
H	6.40346800	2.76573500	-0.92910000
C	1.77840400	-0.80304000	-1.39973900
C	1.14347100	-0.03425300	-2.37687400
H	0.19836400	-0.35899400	-2.79093900
C	3.92975800	-1.54062700	-0.39161700
H	4.36143700	-1.90673800	-1.32800900
H	4.74318100	-1.22738000	0.26107400
H	3.40908200	-2.36748700	0.09247500
O	1.47086300	1.28693000	0.66077200
H	0.46627700	1.11374400	0.51070200

H	0.97497000	-0.99682400	2.36320200
C	-7.95506900	2.11928800	1.27611700
C	-7.53369500	1.36979100	0.20745000
C	-6.15053100	1.16229500	-0.03373700
C	-5.20297200	1.74545100	0.85338300
C	-5.66865600	2.51472900	1.95184000
C	-7.01160200	2.69885000	2.15919300
H	-6.41371700	-0.06500200	-1.79744600
H	-9.01576100	2.27184200	1.44965700
H	-8.25408500	0.92276400	-0.47264800
C	-5.68423300	0.38524600	-1.12944800
C	-3.81773000	1.54170300	0.61646300
H	-4.93777200	2.95643400	2.62382700
H	-7.35768200	3.29025700	3.00104100
C	-3.41161400	0.79076500	-0.45245500
C	-4.34462500	0.19818200	-1.33848800
H	-3.07786400	1.97028800	1.28587400
H	-3.97669100	-0.40910800	-2.15894200
S	-1.67848400	0.57419500	-0.80047500
O	-1.31725200	1.53690700	-1.85124000
O	-1.52793300	-0.83942000	-1.19896000
O	-1.00586800	0.86958400	0.51027200

INT14

C	-2.27501400	1.89097500	0.38132600
C	-3.33465300	2.22670200	-1.66254600
O	-3.75238100	1.98970700	-2.76838700
N	-2.57166300	1.35004900	-0.87320400
C	-1.59413300	1.30481700	1.38374200
C	-0.80303700	0.04901500	1.25229400
C	-1.09880200	-1.10325300	2.14562900
C	-2.04036200	-0.99693400	3.17468700
C	-0.46948900	-2.33172400	1.90743900
C	-2.34077800	-2.10160600	3.96564500
H	-2.54809100	-0.05287400	3.34848400
C	-0.78236800	-3.43571600	2.68855500
H	0.23871600	-2.43057600	1.09148400

C	-1.71310400	-3.32066900	3.72111900
H	-3.06834800	-2.01252000	4.76573900
H	-0.30934200	-4.39001400	2.48186600
H	-1.95598200	-4.18573900	4.33037500
C	-3.51648900	3.44337100	-0.82399100
C	-2.90411000	3.22905000	0.40836500
C	-2.92796700	4.21331000	1.38857900
C	-3.59457900	5.40335300	1.09904200
C	-4.21113500	5.60958700	-0.14012000
C	-4.17597600	4.62392800	-1.12493100
H	-2.44673200	4.06983100	2.35123700
H	-3.63430100	6.18687800	1.84894400
H	-4.71851000	6.54909300	-0.33290900
H	-4.64225100	4.76088200	-2.09518100
C	-1.74394700	-5.00452300	-0.81064400
C	-1.14595800	-4.02731200	-1.56548900
C	-1.60251800	-2.68547000	-1.50924200
C	-2.69418700	-2.35405400	-0.65845000
C	-3.30115700	-3.39031400	0.09906000
C	-2.83531200	-4.68014700	0.02794900
H	-0.13672300	-1.91689700	-2.91584100
H	-1.38146100	-6.02673400	-0.85381100
H	-0.29983100	-4.25764300	-2.20691000
C	-0.95912100	-1.66160000	-2.25568000
C	-3.09893500	-0.98634700	-0.52598900
H	-4.12461900	-3.15460800	0.76522500
H	-3.30205500	-5.45628600	0.62685000
C	-2.36590900	-0.02761600	-1.19387300
C	-1.32244900	-0.35531600	-2.09122000
H	-0.77855700	0.44016800	-2.58821100
C	-4.26272400	-0.63109800	0.36051200
H	-5.13982900	-1.22545800	0.08623300
H	-4.04141800	-0.83795400	1.41435200
H	-4.53354100	0.42197600	0.26797100
O	0.08764000	-0.00336300	0.41103200
H	-1.56214300	1.81535900	2.34182600
H	1.15130000	-1.11827600	-0.26813600

C	7.42493900	2.31879200	1.60784300
C	6.09675200	2.60921000	1.42619000
C	5.26607500	1.74982500	0.66160400
C	5.83507000	0.57942900	0.08524900
C	7.21260700	0.30499700	0.28842200
C	7.98993900	1.15435200	1.03297400
H	3.46435700	2.92770800	0.89305300
H	8.05119100	2.98339800	2.19450100
H	5.66088600	3.50287300	1.86441600
C	3.88659300	2.02809700	0.45403200
C	5.00748200	-0.28435900	-0.67875200
H	7.63717500	-0.59024300	-0.15711800
H	9.04249100	0.93809700	1.18457700
C	3.68600300	0.02622800	-0.84814700
C	3.10096600	1.19049500	-0.29026600
H	5.41604000	-1.18343400	-1.13112200
H	2.04918400	1.39975500	-0.46055100
S	2.65903800	-1.06235800	-1.79814300
O	1.78705100	-0.24047600	-2.61844500
O	1.78090000	-1.77750600	-0.67095600
O	3.47380700	-2.10264000	-2.38451100

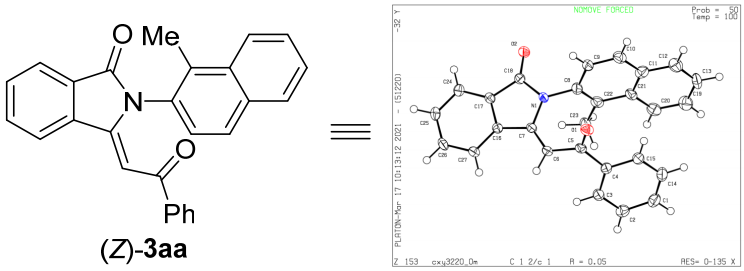
***Z*-3aa**

C	1.93572800	0.48574200	0.46984500
C	2.72875100	-1.59413800	-0.22016500
O	2.72156500	-2.76369200	-0.52125900
N	1.61950500	-0.85919100	0.21993300
C	1.10774000	1.45240400	0.89707000
C	-0.28242100	1.23147700	1.41548400
C	-1.42182300	1.92246900	0.73476200
C	-1.22739900	2.86562100	-0.27697200
C	-2.72069100	1.55571700	1.10153100
C	-2.32362500	3.44368700	-0.91267500
H	-0.21965800	3.13818300	-0.57823200
C	-3.81262300	2.12360800	0.45909600
H	-2.84467800	0.80413800	1.87481600
C	-3.61467100	3.07101100	-0.54610500

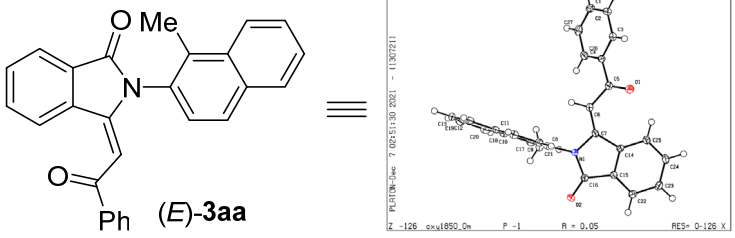
H	-2.17005900	4.17916200	-1.69591500
H	-4.81852700	1.82100400	0.73203800
H	-4.46860300	3.51493300	-1.04864600
C	3.85230400	-0.61919500	-0.24914900
C	3.36969500	0.62801300	0.14047700
C	4.22126400	1.72490600	0.19847200
C	5.55503900	1.53366700	-0.15876000
C	6.03108200	0.27803200	-0.55379700
C	5.17746100	-0.82206500	-0.60059500
H	3.86756400	2.70283300	0.51048400
H	6.23960600	2.37537100	-0.12807800
H	7.07612300	0.16459600	-0.82282400
H	5.52133300	-1.80717100	-0.89892500
C	-4.69235000	-1.88038200	-0.39453800
C	-3.77800400	-2.39607300	0.48870400
C	-2.39696700	-2.09785000	0.36482400
C	-1.95781500	-1.26466100	-0.70184200
C	-2.92745100	-0.75115100	-1.60286000
C	-4.25979500	-1.04551600	-1.45001900
H	-1.78832200	-3.24561100	2.09931100
H	-5.74763900	-2.10980500	-0.28529700
H	-4.09844800	-3.03608400	1.30645600
C	-1.44783400	-2.59549500	1.29878900
C	-0.57165600	-0.92035200	-0.81144600
H	-2.61341900	-0.09330900	-2.40646600
H	-4.98752400	-0.63096100	-2.14069800
C	0.28388700	-1.35811800	0.17634200
C	-0.13777100	-2.22284700	1.21458300
H	0.59351800	-2.54053300	1.94932500
C	-0.09434800	-0.08326000	-1.96815100
H	-0.42519800	-0.52550600	-2.91309500
H	-0.49810400	0.93437900	-1.91917100
H	0.99452300	-0.01876300	-1.99356700
O	-0.47467700	0.50518000	2.37036900
H	1.50163900	2.46407700	0.94864300

X. Determination of the Stereochemistry

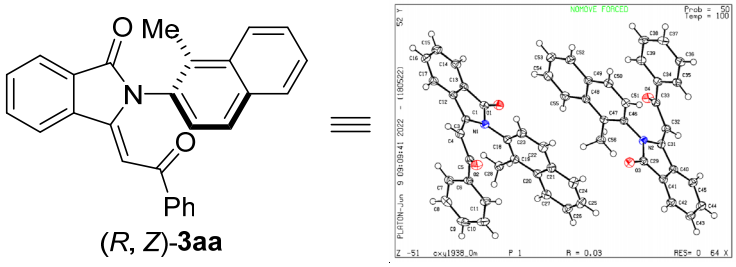
The absolute stereochemistry of products (*Z*)-**3aa**, (*E*)-**3aa**, (*R*, *Z*)-**3aa** and **IM** was determined by X-ray diffraction (shown below). The X-ray data have been deposited at the Cambridge Crystallographic Data Center (CCDC 2294518 for (*Z*)-**3aa**, CCDC 2294530 for (*E*)-**3aa,** CCDC 2294540 for (*R*, *Z*)-**3aa,** CCDC 2294537 for **IM**). The stereochemistry of other products was assumed by analogy.



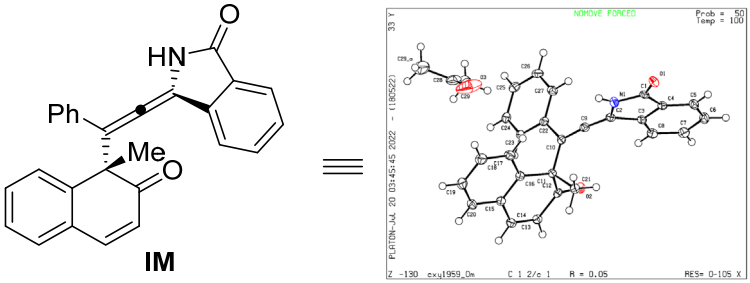
(*Z*)-**3aa**



(*E*)-**3aa**



(*R*, *Z*)-**3aa**



IM

Crystal data and structure refinement for (*Z*)-3aa.

Identification code	(*Z*)-**3aa**
Empirical formula	$C_{27}H_{19}NO_2$
Formula weight	389.43
Temperature/K	100.0
Crystal system	monoclinic
Space group	C2/c
a/Å	25.101(3)
b/Å	11.6276(15)
c/Å	14.0265(14)
α/°	90
β/°	108.344(5)
γ/°	90
Volume/Å^3	3885.9(8)
Z	8
ϱ_{calc}g/cm^3	1.331
μ/mm^{-1}	0.663
F(000)	1632.0
Crystal size/mm^3	0.31 × 0.28 × 0.24
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	7.42 to 136.8
Index ranges	-30 ≤ h ≤ 30, -13 ≤ k ≤ 13, -14 ≤ l ≤ 16
Reflections collected	19156
Independent reflections	3555 [R_{int} = 0.0560, R_{sigma} = 0.0376]
Data/restraints/parameters	3555/0/272
Goodness-of-fit on F^2	1.050
Final R indexes [I>=2σ (I)]	R_1 = 0.0517, wR_2 = 0.1249
Final R indexes [all data]	R_1 = 0.0595, wR_2 = 0.1292
Largest diff. peak/hole / e Å^{-3}	0.70/-0.33

Crystal data and structure refinement for (*E*)-3aa.

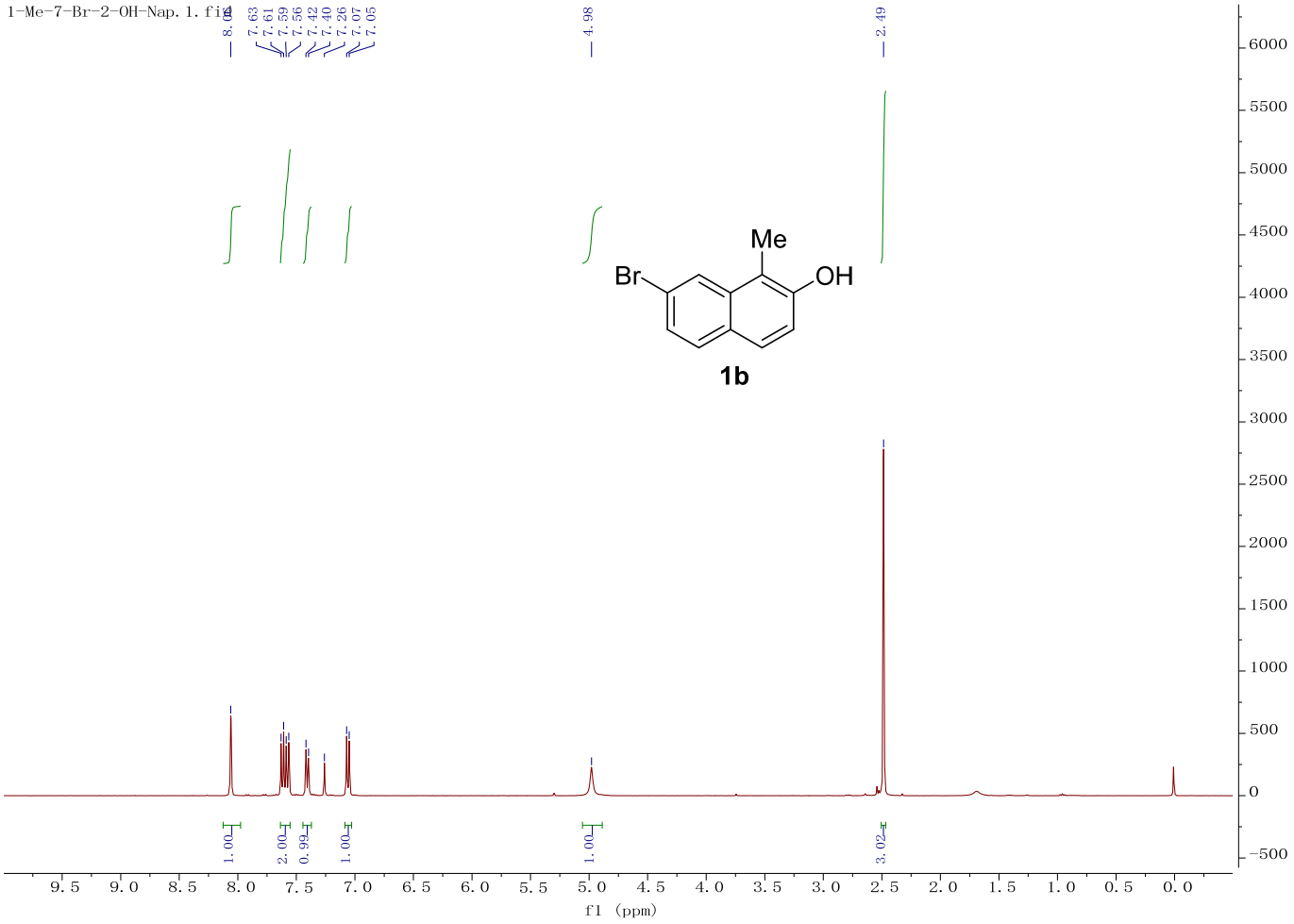
Identification code	(*E*)-**3aa**
Empirical formula	$C_{27}H_{19}NO_2$
Formula weight	389.43
Temperature/K	100.0
Crystal system	triclinic
Space group	P-1
a/Å	8.0198(3)
b/Å	9.4799(4)
c/Å	13.7043(6)
α/°	103.446(2)
β/°	97.519(2)
γ/°	102.443(2)
Volume/Å^3	971.41(7)
Z	2
ϱ_{calc}g/cm^3	1.331
μ/mm^{-1}	0.084
F(000)	408.0
Crystal size/mm^3	0.32 × 0.28 × 0.28
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.568 to 54.982
Index ranges	-10 ≤ h ≤ 10, -12 ≤ k ≤ 12, -17 ≤ l ≤ 17
Reflections collected	18544
Independent reflections	4454 [R_{int} = 0.0575, R_{sigma} = 0.0499]
Data/restraints/parameters	4454/0/273
Goodness-of-fit on F^2	1.038
Final R indexes [I>=2σ (I)]	R_1 = 0.0514, wR_2 = 0.1162
Final R indexes [all data]	R_1 = 0.0786, wR_2 = 0.1274
Largest diff. peak/hole / e Å^{-3}	0.56/-0.29

Crystal data and structure refinement for (*R*, *Z*)-3aa.

Identification code	(*R*, *Z*)-**3aa**
Empirical formula	$C_{27}H_{19}NO_2$
Formula weight	389.43
Temperature/K	100.0(2)
Crystal system	triclinic
Space group	P1
a/Å	7.8226(5)
b/Å	9.8700(6)
c/Å	13.4677(8)
α/°	72.435(2)
β/°	82.536(2)
γ/°	83.621(2)
Volume/Å^3	980.10(10)
Z	2
ϱ_{calc}g/cm^3	1.320
μ/mm^{-1}	0.657
F(000)	408.0
Crystal size/mm^3	0.32 × 0.22 × 0.19
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	6.92 to 149.452
Index ranges	$-8 \le h \le 9$, $-12 \le k \le 12$, $-16 \le l \le 16$
Reflections collected	38301
Independent reflections	7748 [R_{int} = 0.0353, R_{sigma} = 0.0243]
Data/restraints/parameters	7748/3/544
Goodness-of-fit on F^2	1.031
Final R indexes [I>=2σ (I)]	R_1 = 0.0301, wR_2 = 0.0783
Final R indexes [all data]	R_1 = 0.0317, wR_2 = 0.0797
Largest diff. peak/hole / e Å^{-3}	0.24/-0.17
Flack parameter	0.04(6)

Crystal data and structure refinement for IM.

Identification code	**IM**
Empirical formula	$C_{28.5}H_{22}NO_{2.5}$
Formula weight	418.47
Temperature/K	100.0(2)
Crystal system	monoclinic
Space group	C2/c
a/Å	28.218(2)
b/Å	10.8756(7)
c/Å	17.0557(12)
α/°	90
β/°	124.150(2)
γ/°	90
Volume/Å^3	4331.7(5)
Z	8
ϱ_{calc}g/cm^3	1.283
μ/mm^{-1}	0.082
F(000)	1760.0
Crystal size/mm^3	0.39 × 0.35 × 0.28
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.444 to 55.122
Index ranges	-36 ≤ h ≤ 36, -14 ≤ k ≤ 13, -22 ≤ l ≤ 20
Reflections collected	23405
Independent reflections	4998 [R_{int} = 0.0602, R_{sigma} = 0.0565]
Data/restraints/parameters	4998/0/292
Goodness-of-fit on F^2	1.025
Final R indexes [I>=2σ (I)]	R_1 = 0.0489, wR_2 = 0.1048
Final R indexes [all data]	R_1 = 0.0861, wR_2 = 0.1219
Largest diff. peak/hole / e Å^{-3}	0.31/-0.29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7.59
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7.40
7.26
7.07
7.05
4.98
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Me
Br
OH
1b
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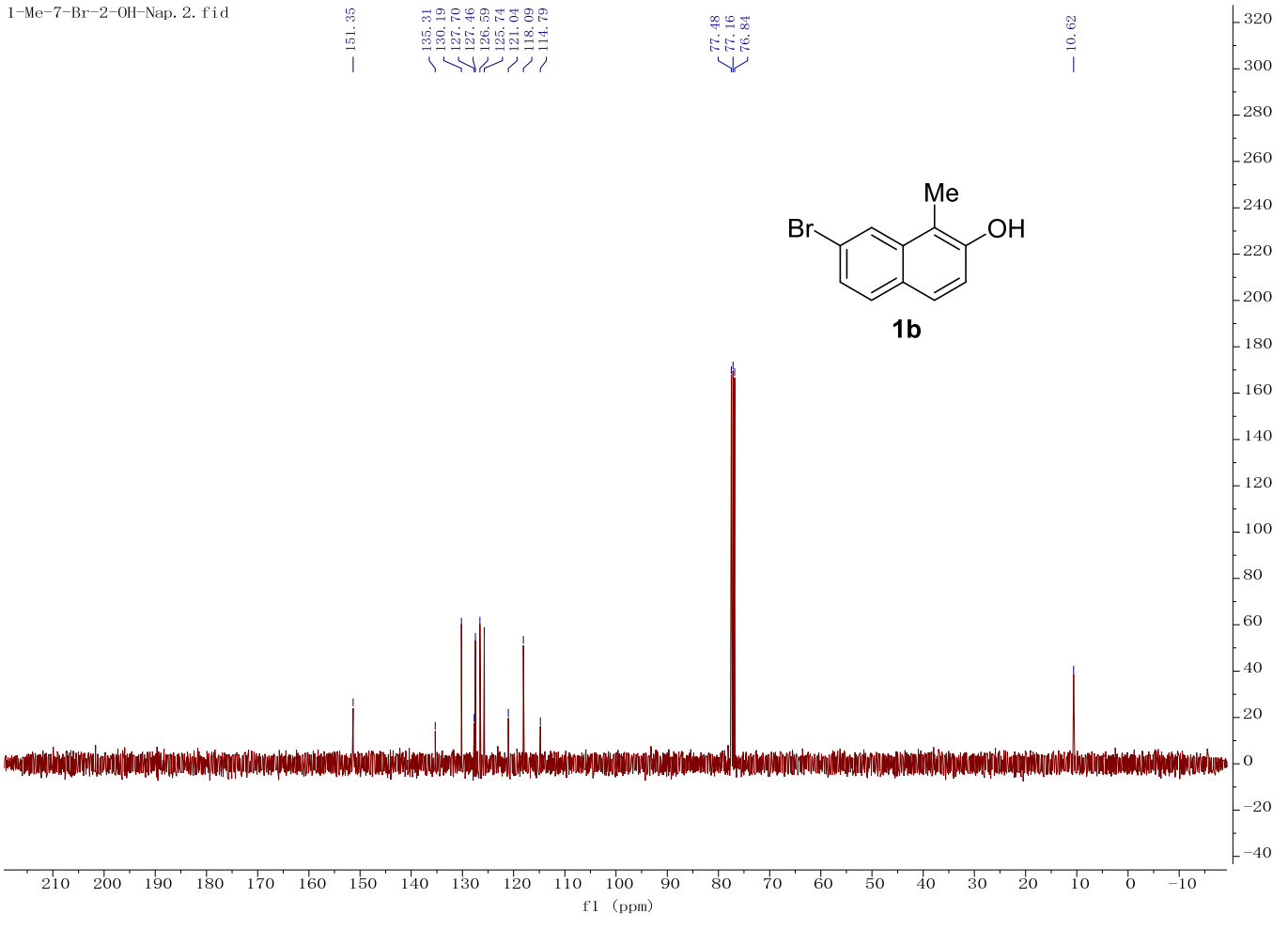
2.00
0.99
1.00
1.00
3.02
f1 (ppm)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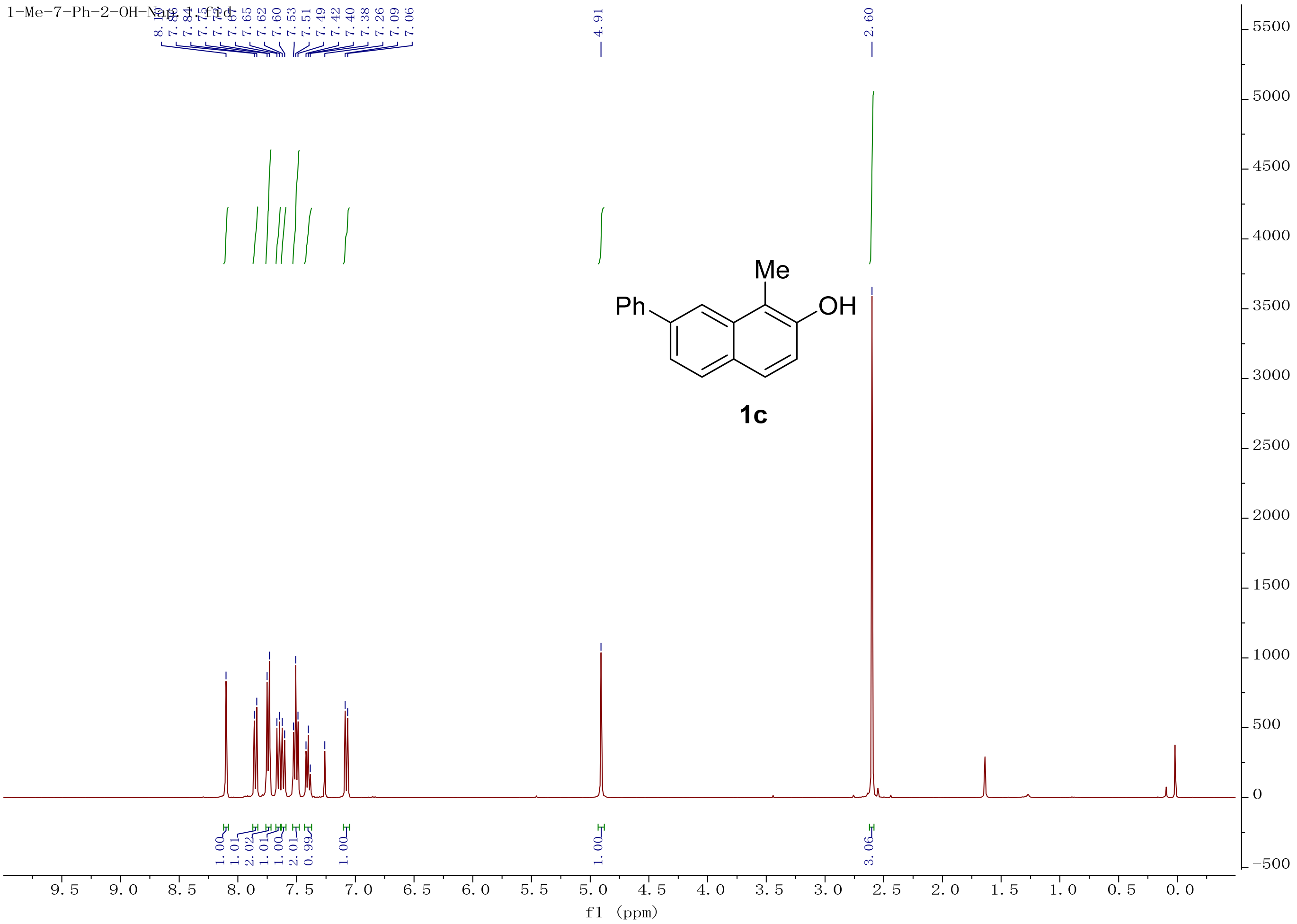
127.46
126.59
125.74
121.04
118.09
114.79
77.48
77.16
76.84
10.62
Me
Br
OH
1b
f1 (ppm)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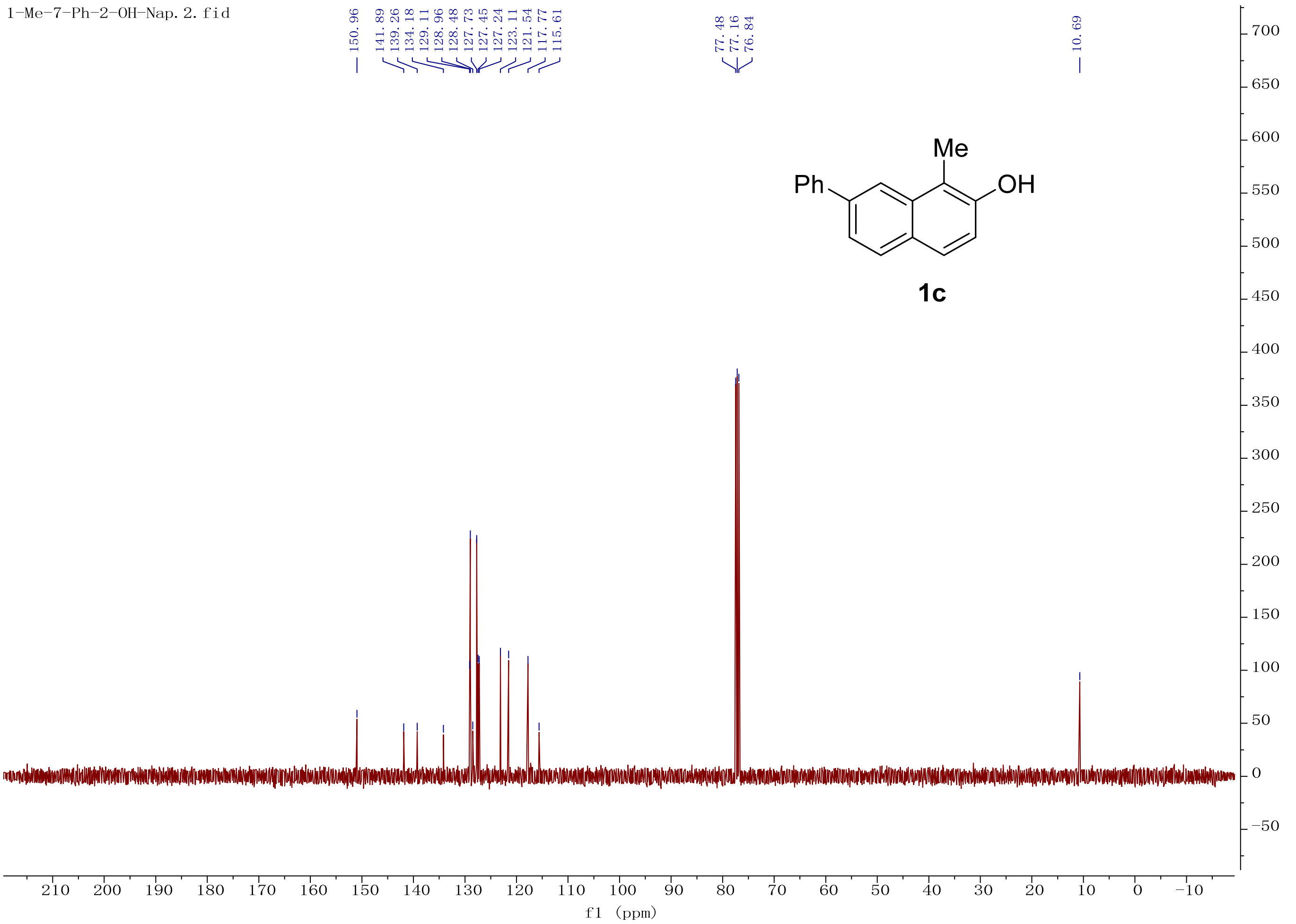
4.91
2.60
Me
Ph
OH
1c
1.00 1.01 2.02 1.01 1.00 2.01 0.99 1.00
1.00
3.06
f1 (ppm)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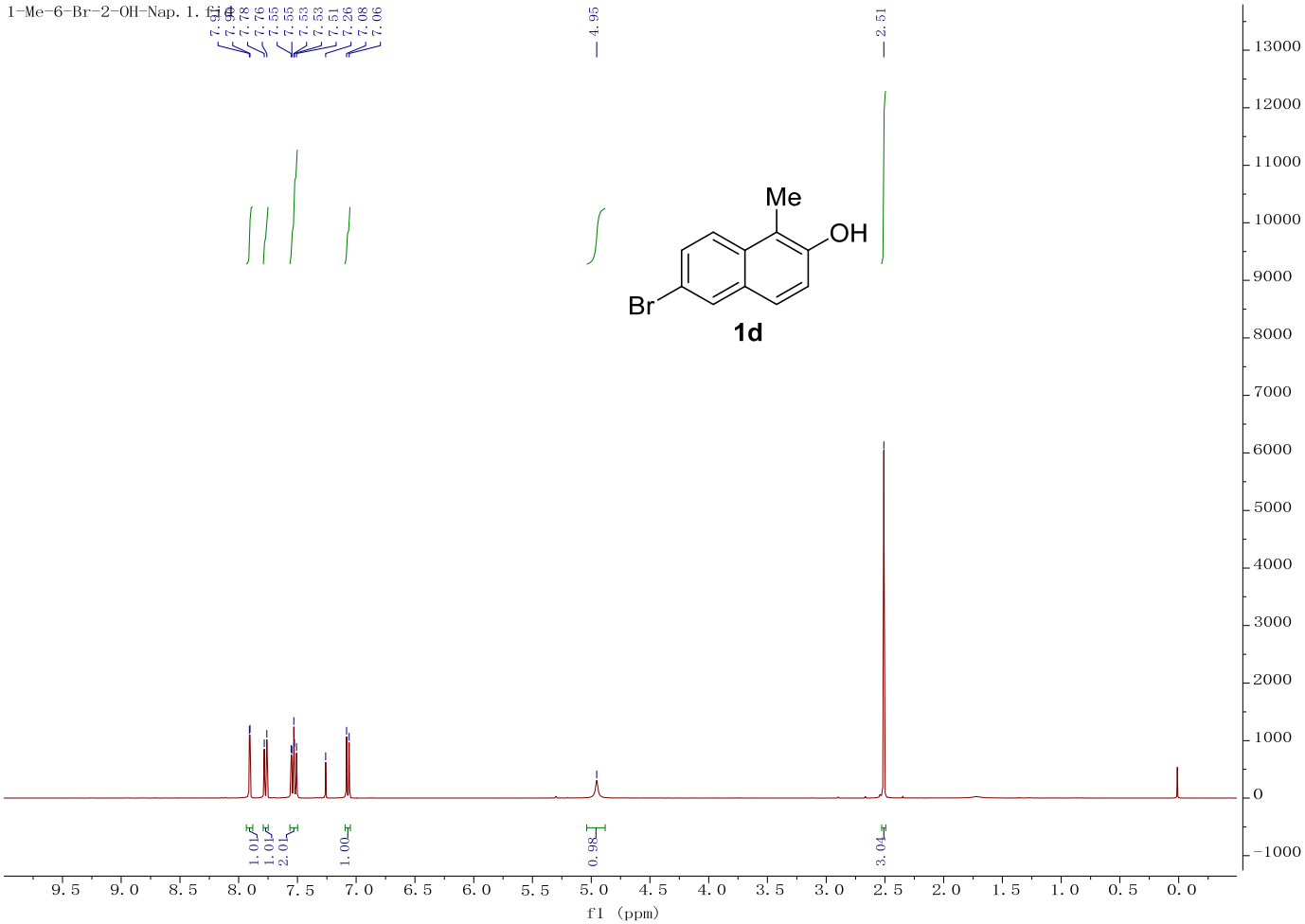
141.89 139.26 134.18 129.11 128.96 128.48 127.73 127.45 127.24 123.11 121.54 117.77 115.61
77.48 77.16 76.84
10.69
Me
Ph
OH
1c
f1 (ppm)

1-Me-6-Br-2-OH-Nap. 1. fid



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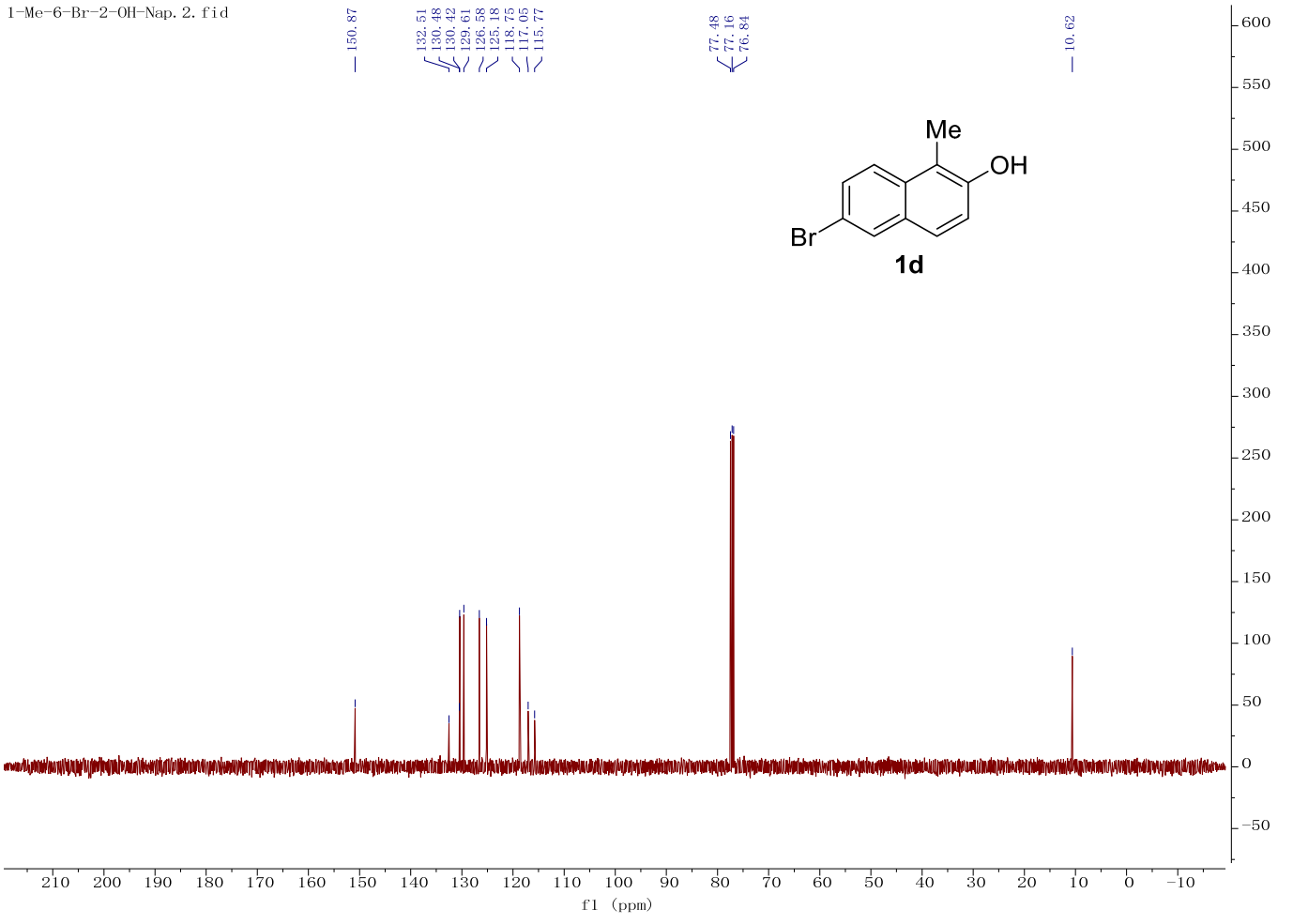

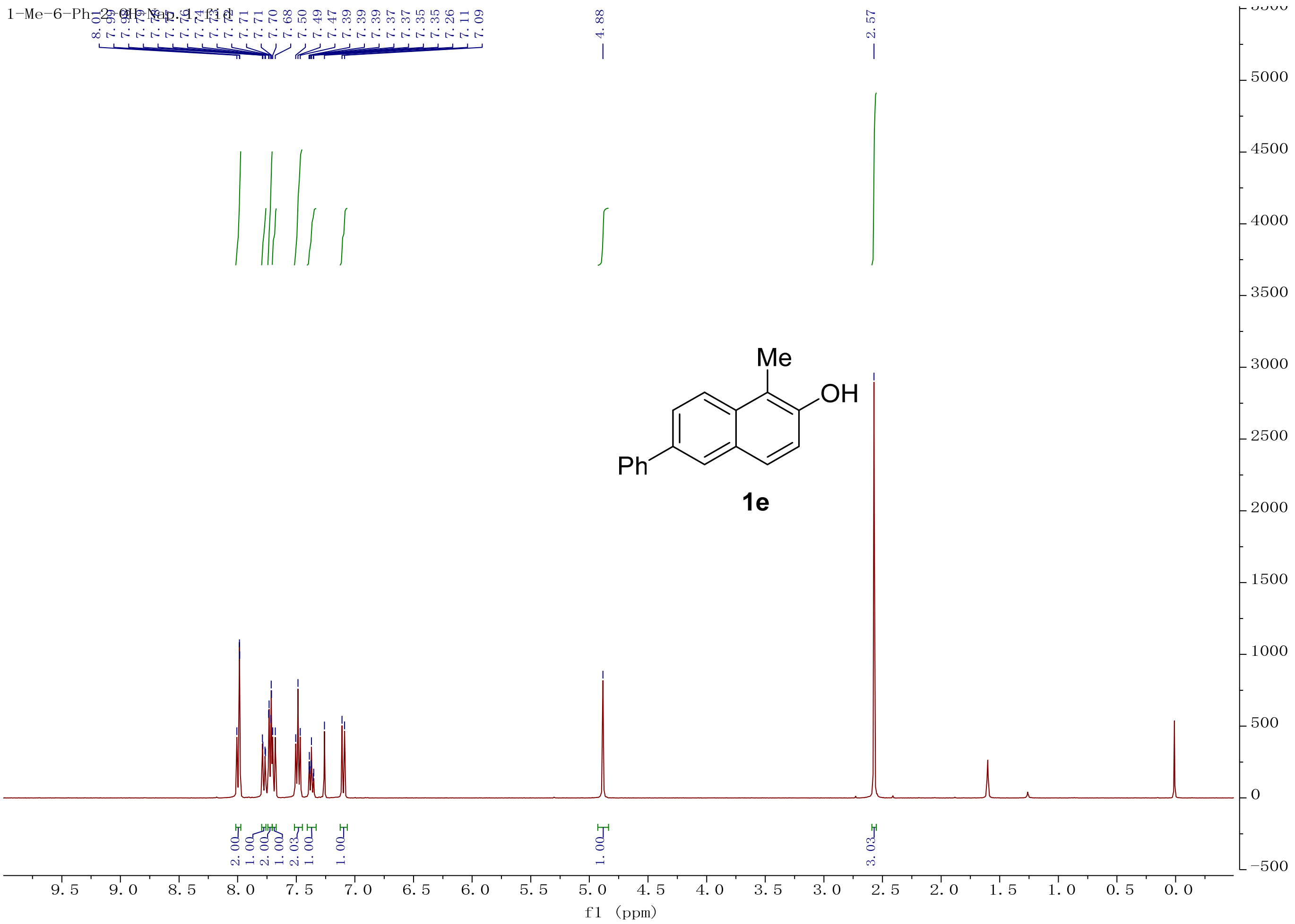
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OH
Ph
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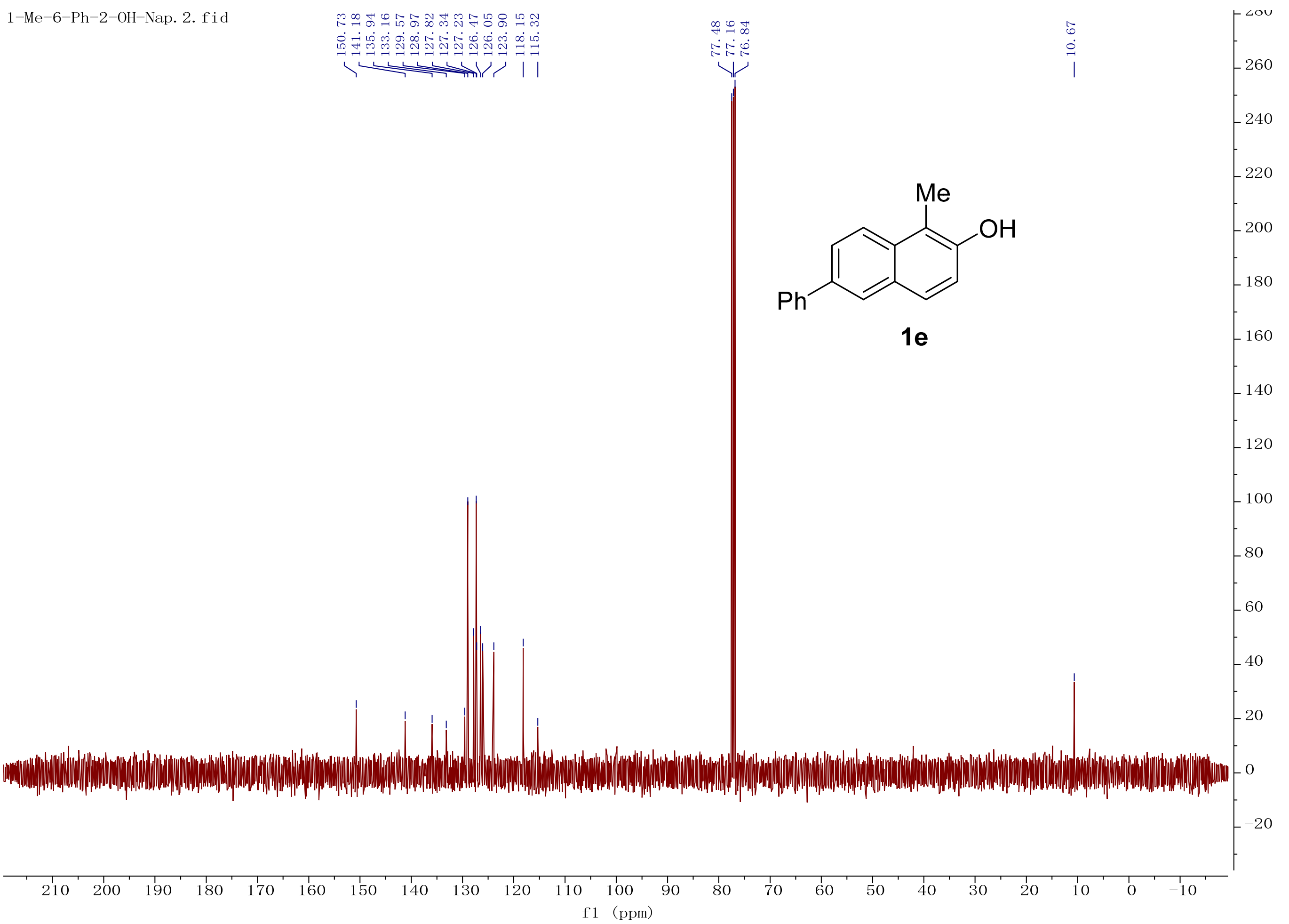
1.00
1.00
1.00
3.03
f1 (ppm)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127.23
126.47
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115.32
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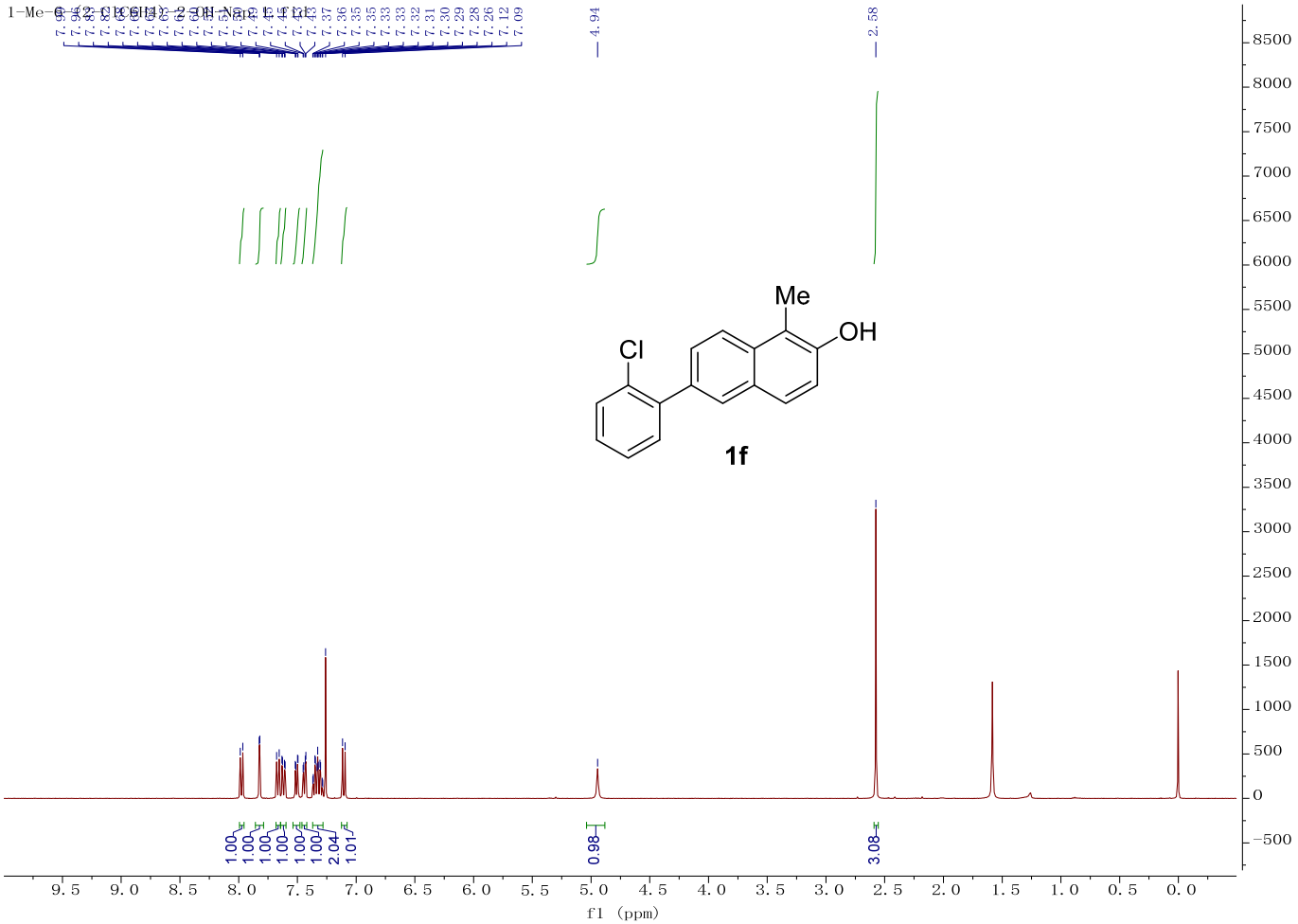
77.16
76.84
10.67
Me
OH
Ph
1e
f1 (ppm)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Cl
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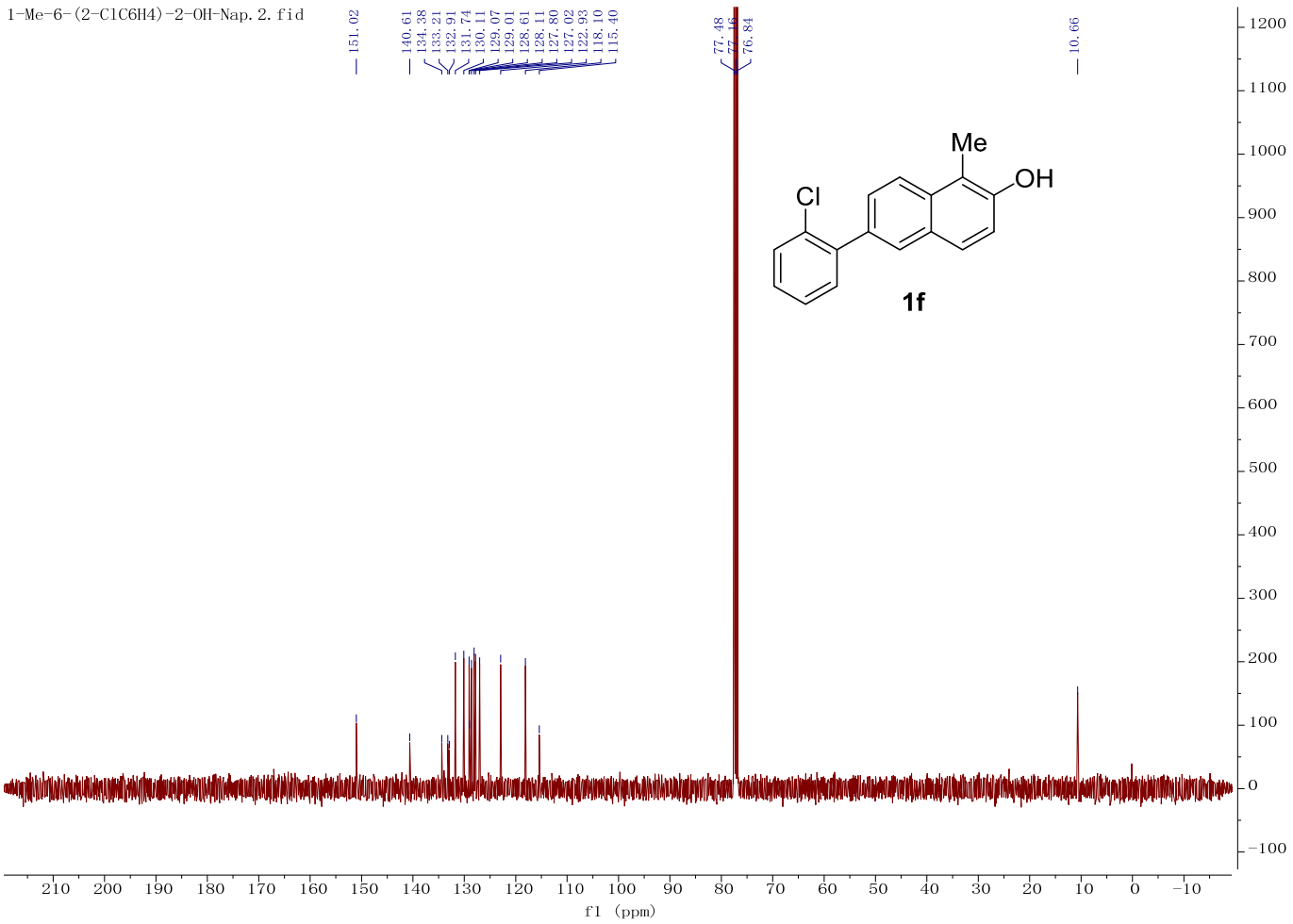
1.01
0.98
3.08
f1 (ppm)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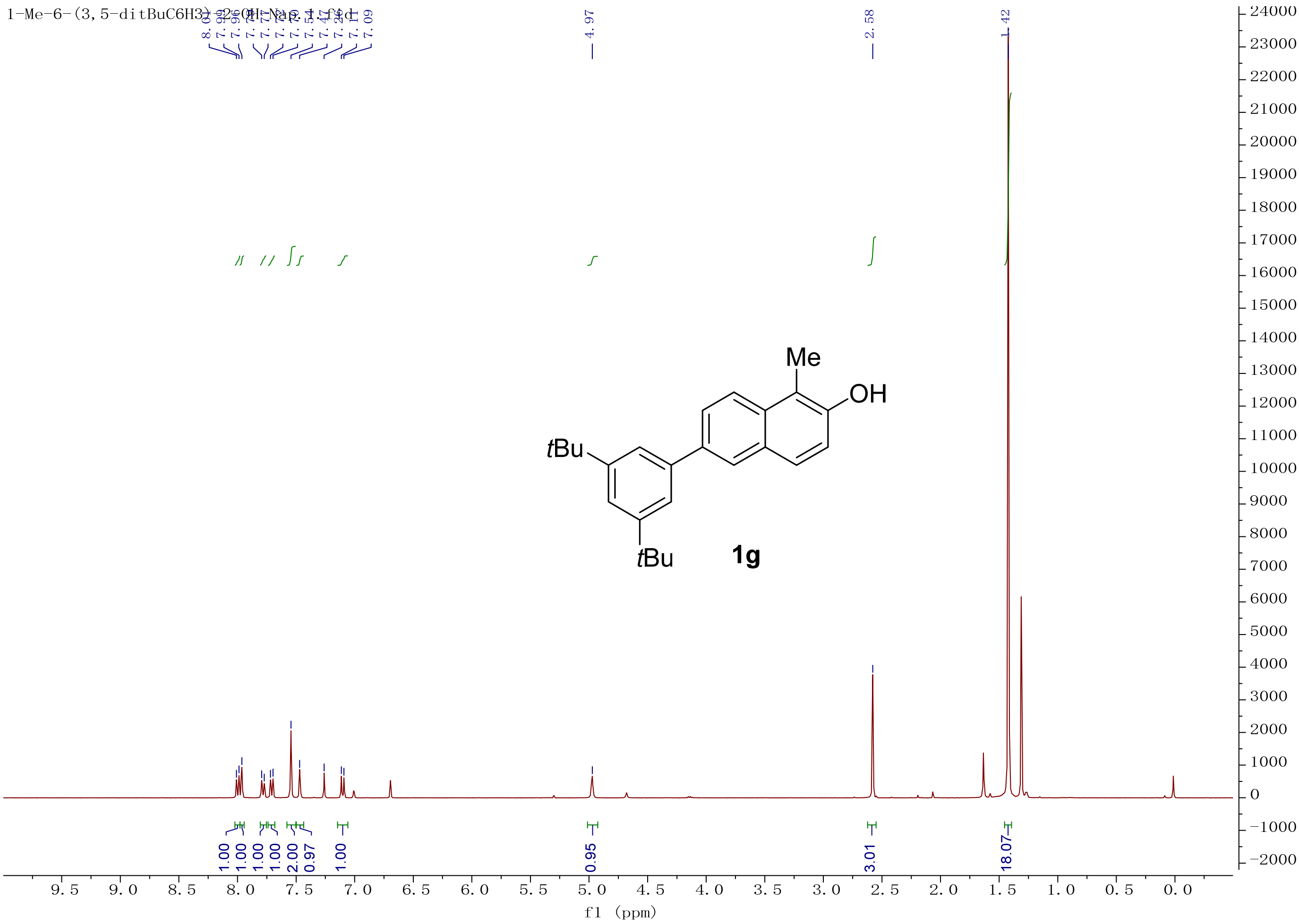
76.84
10.66
Me
OH
Cl
1f
f1 (ppm)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Me
OH
tBu
tBu
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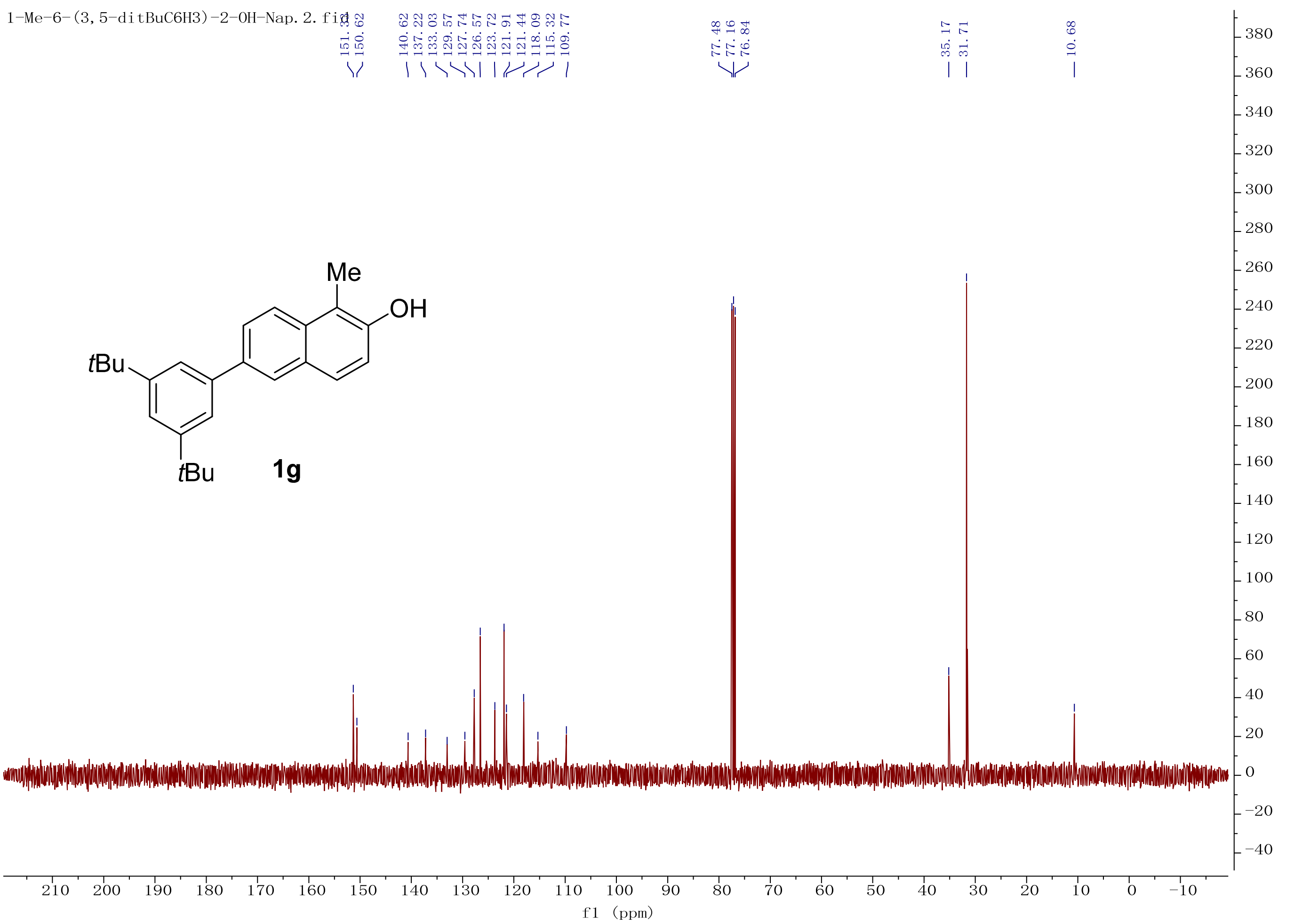
1.00
2.00
0.97
1.00
0.95
3.01
18.07
f1 (ppm)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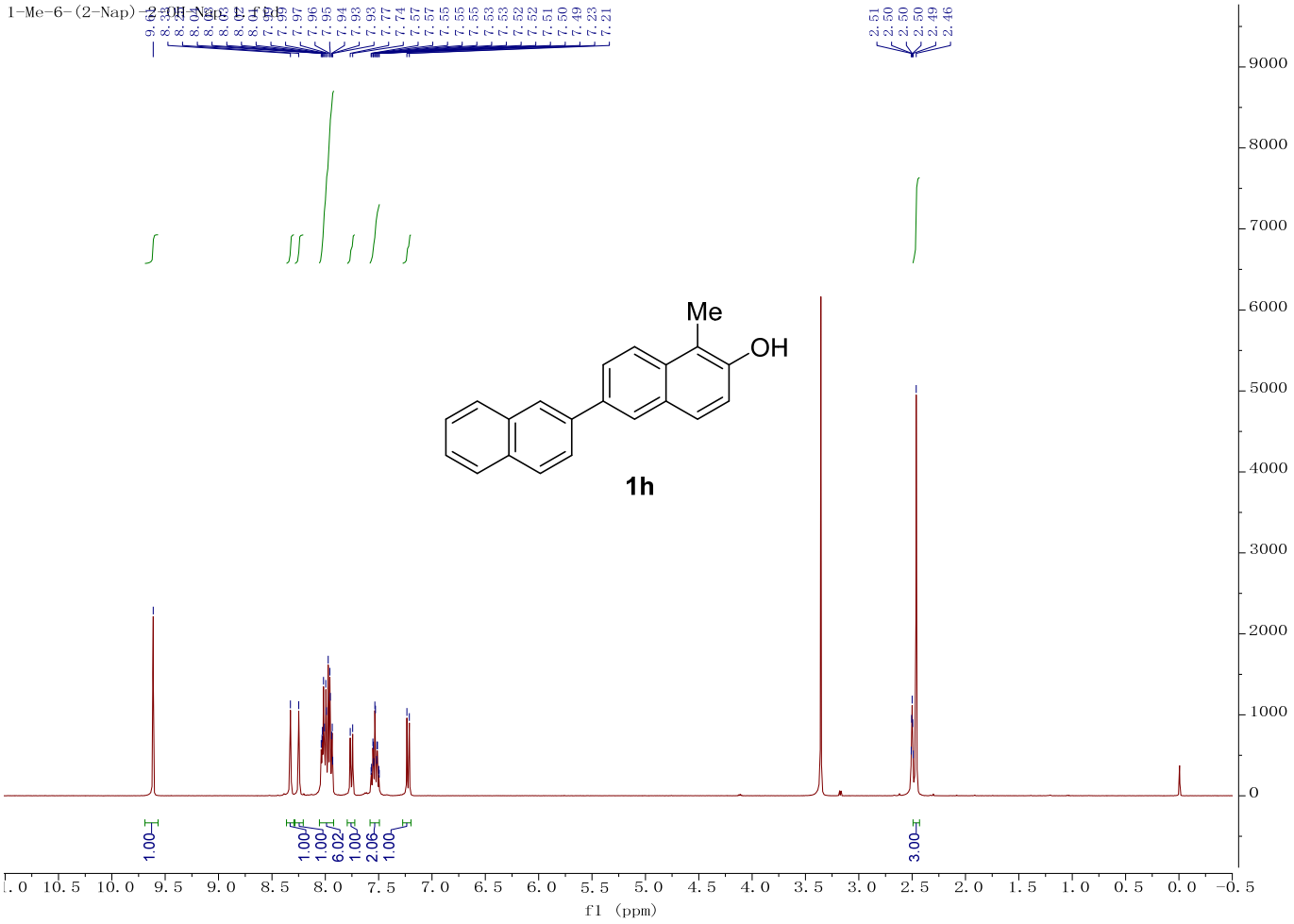
123.72
121.91
121.44
118.09
115.32
109.77
77.48
77.16
76.84
35.17
31.71
10.68
Me
OH
tBu
tBu
1g
f1 (ppm)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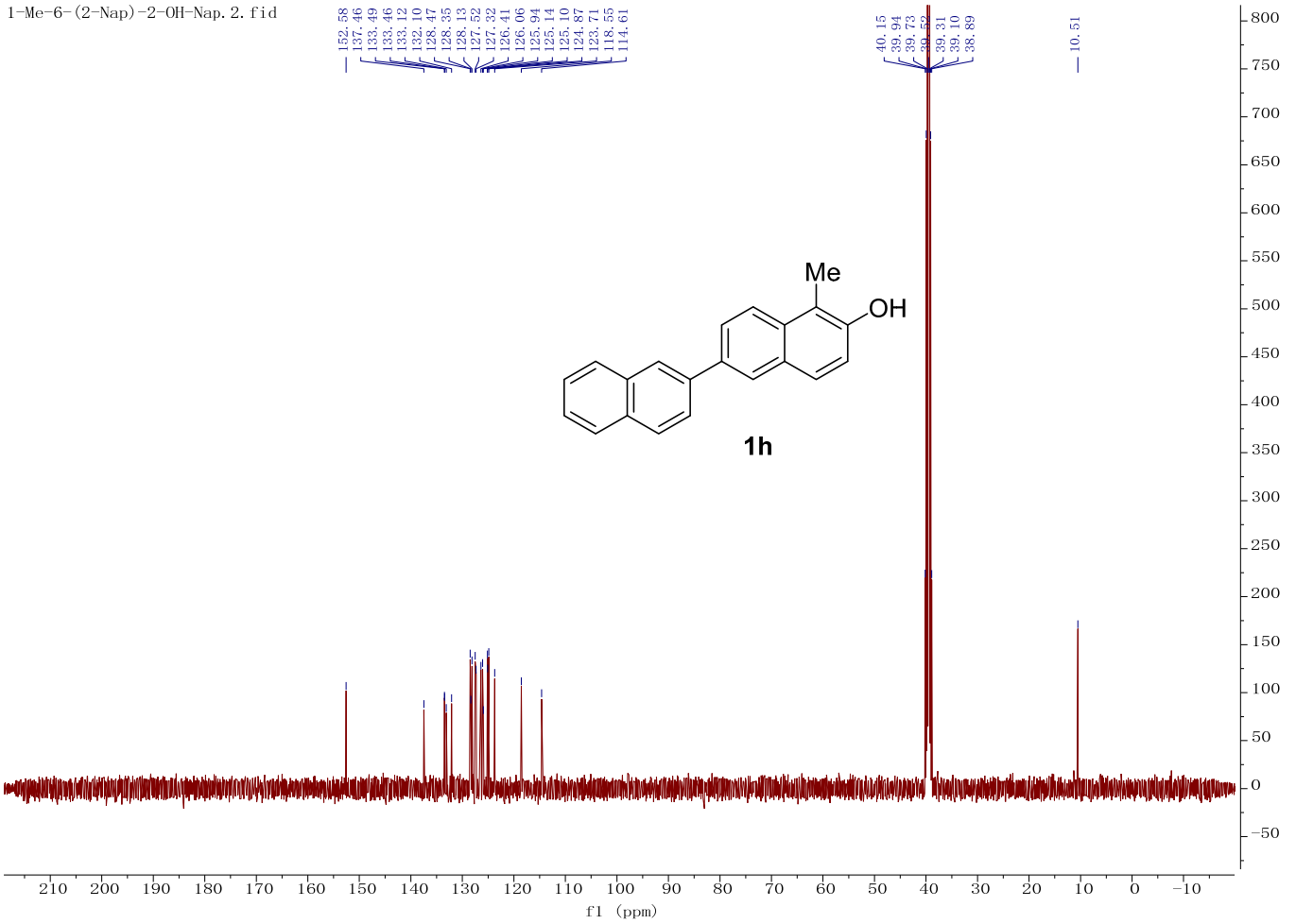
OH
1h
f1 (ppm)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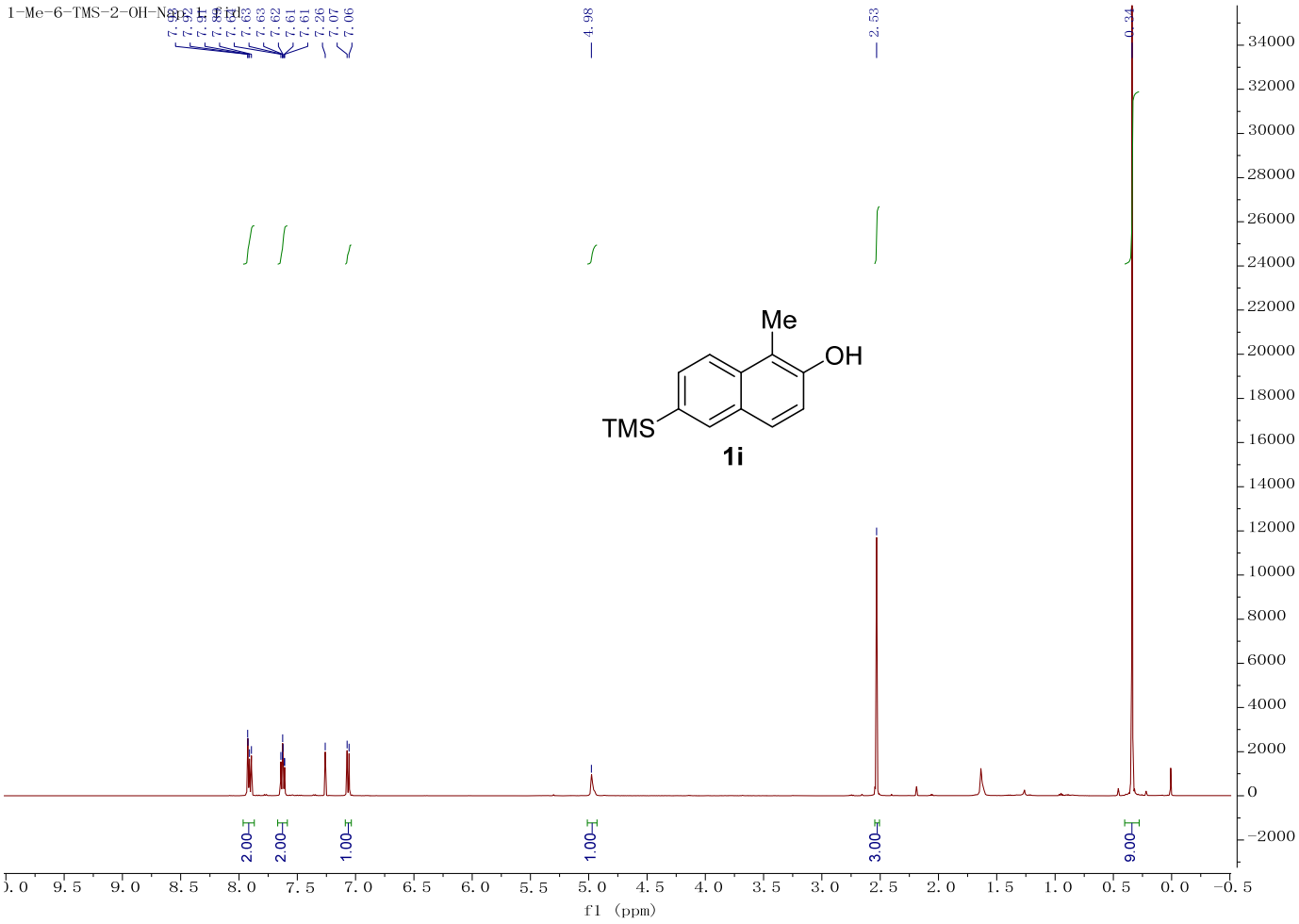
Me
OH
1h
f1 (ppm)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7.63
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7.61
7.26
7.07
7.06
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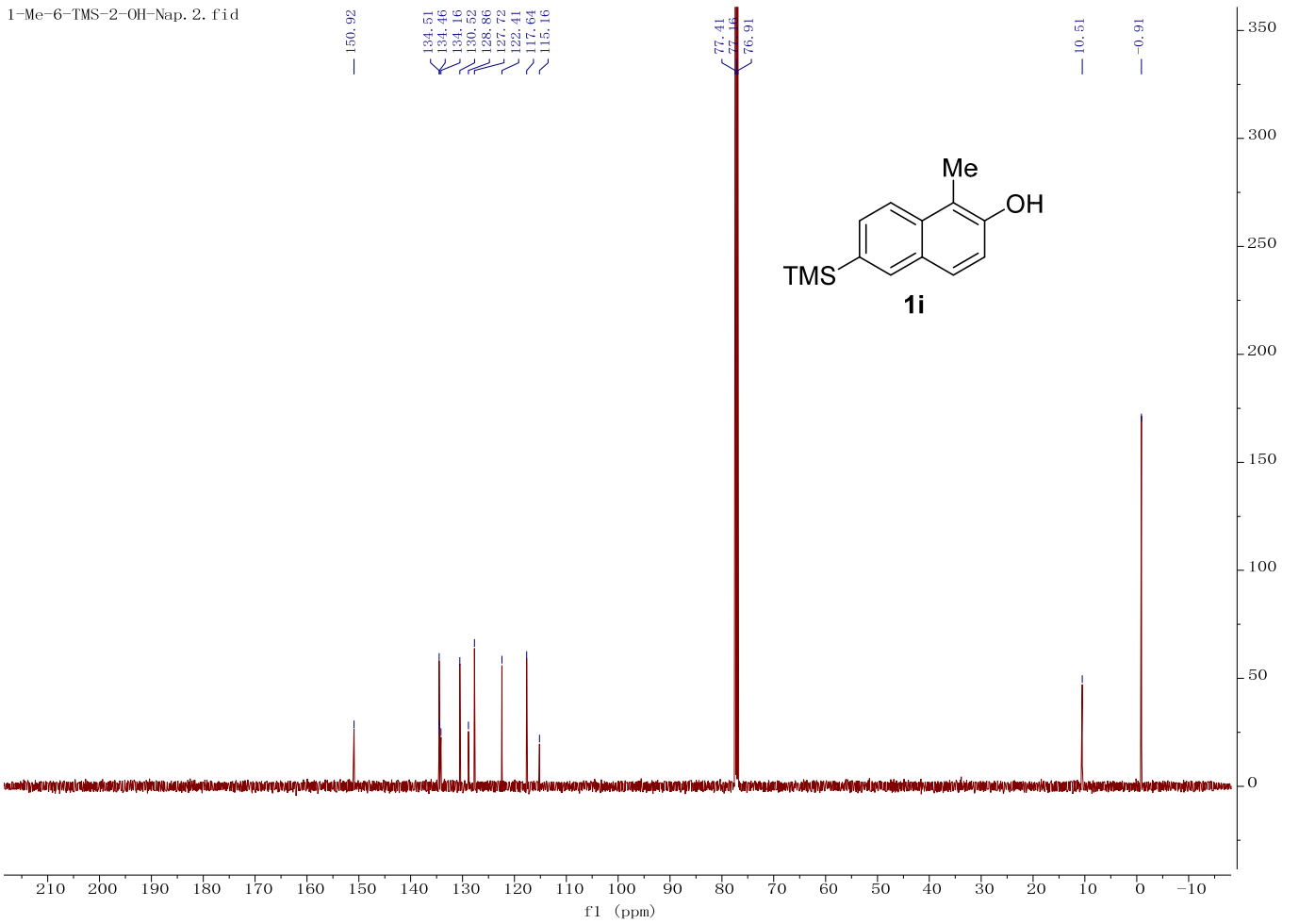
2.53
0.34
Me
OH
TMS
1i
2.00
2.00
1.00
1.00
3.00
9.00
f1 (ppm)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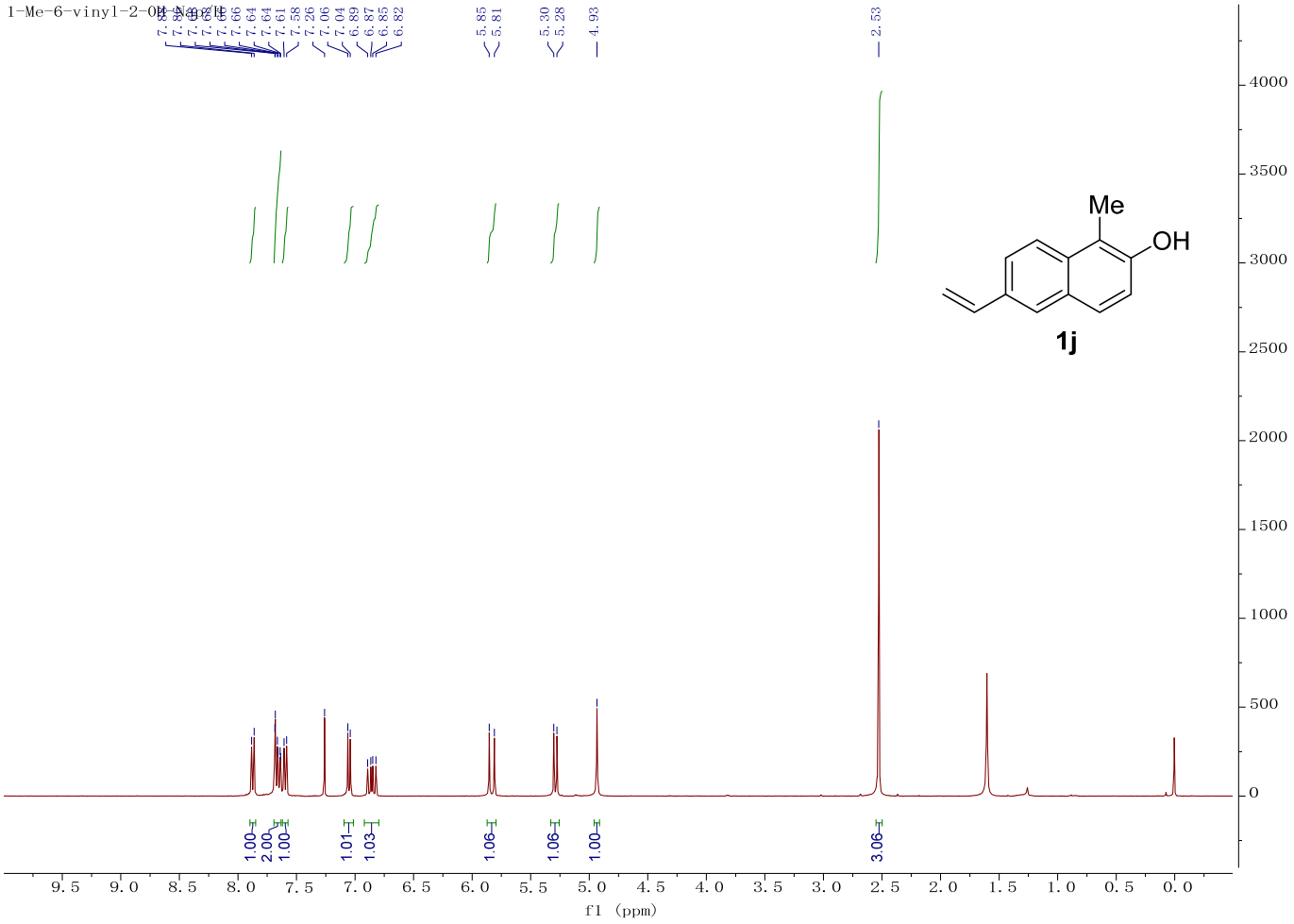
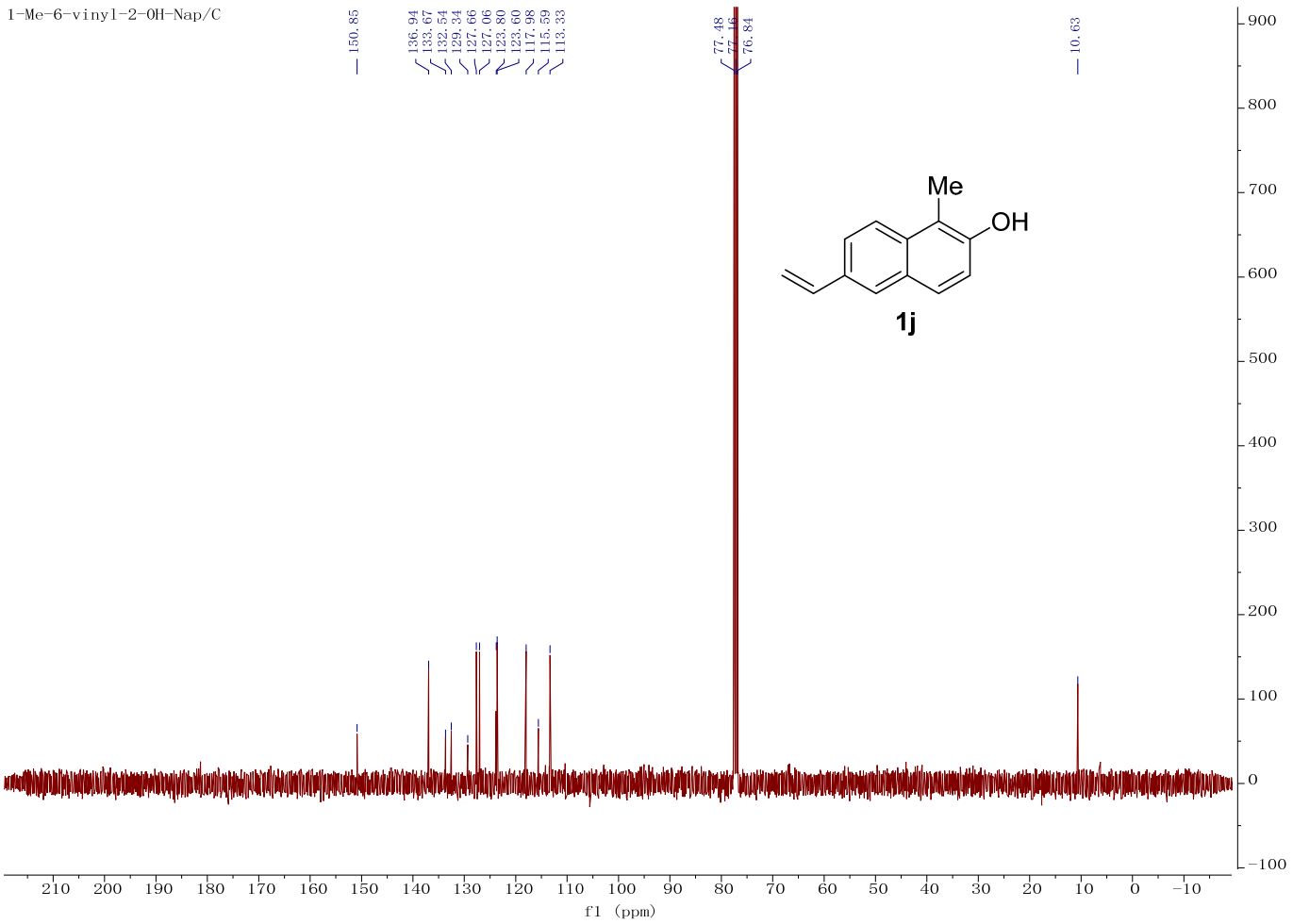
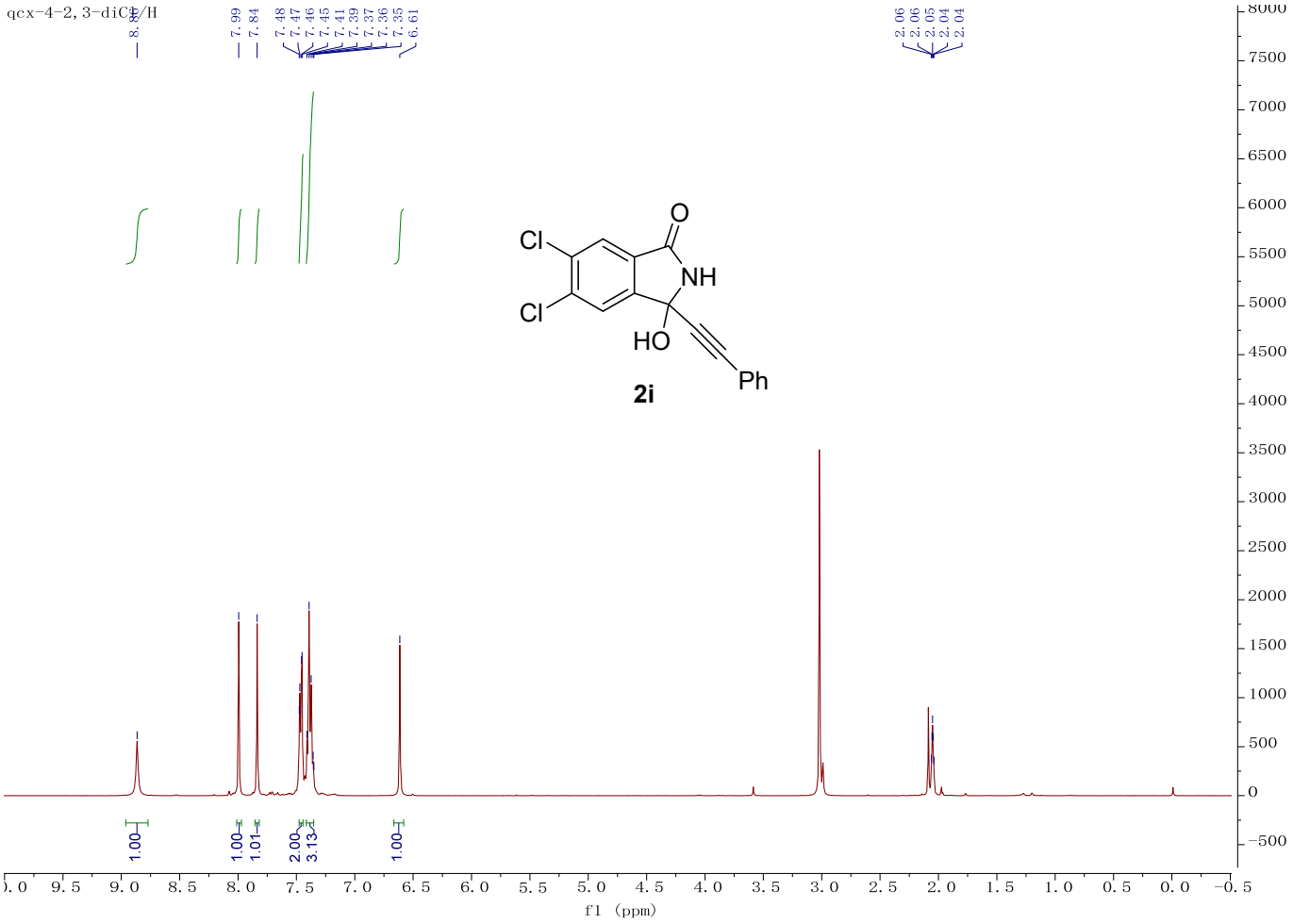
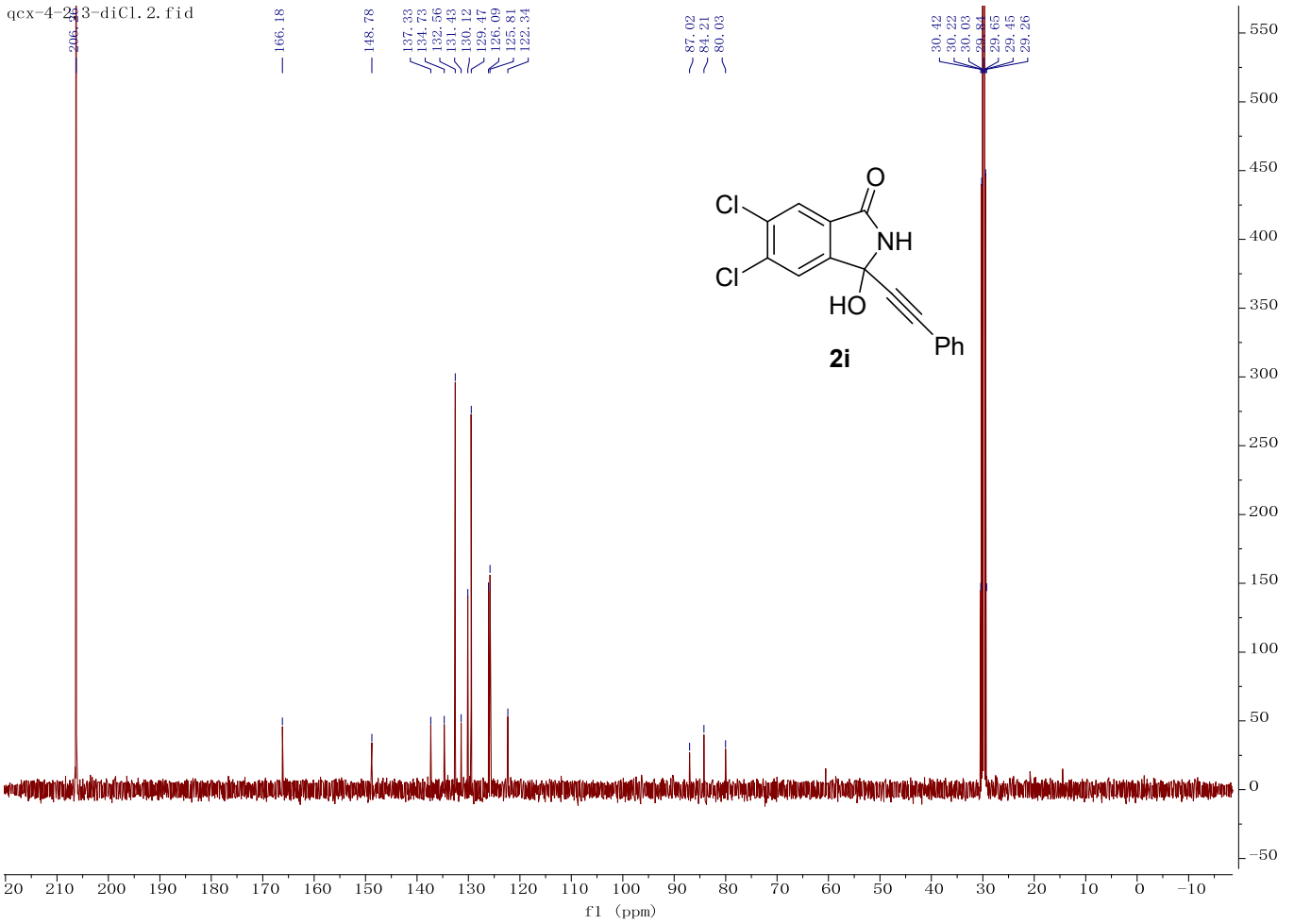
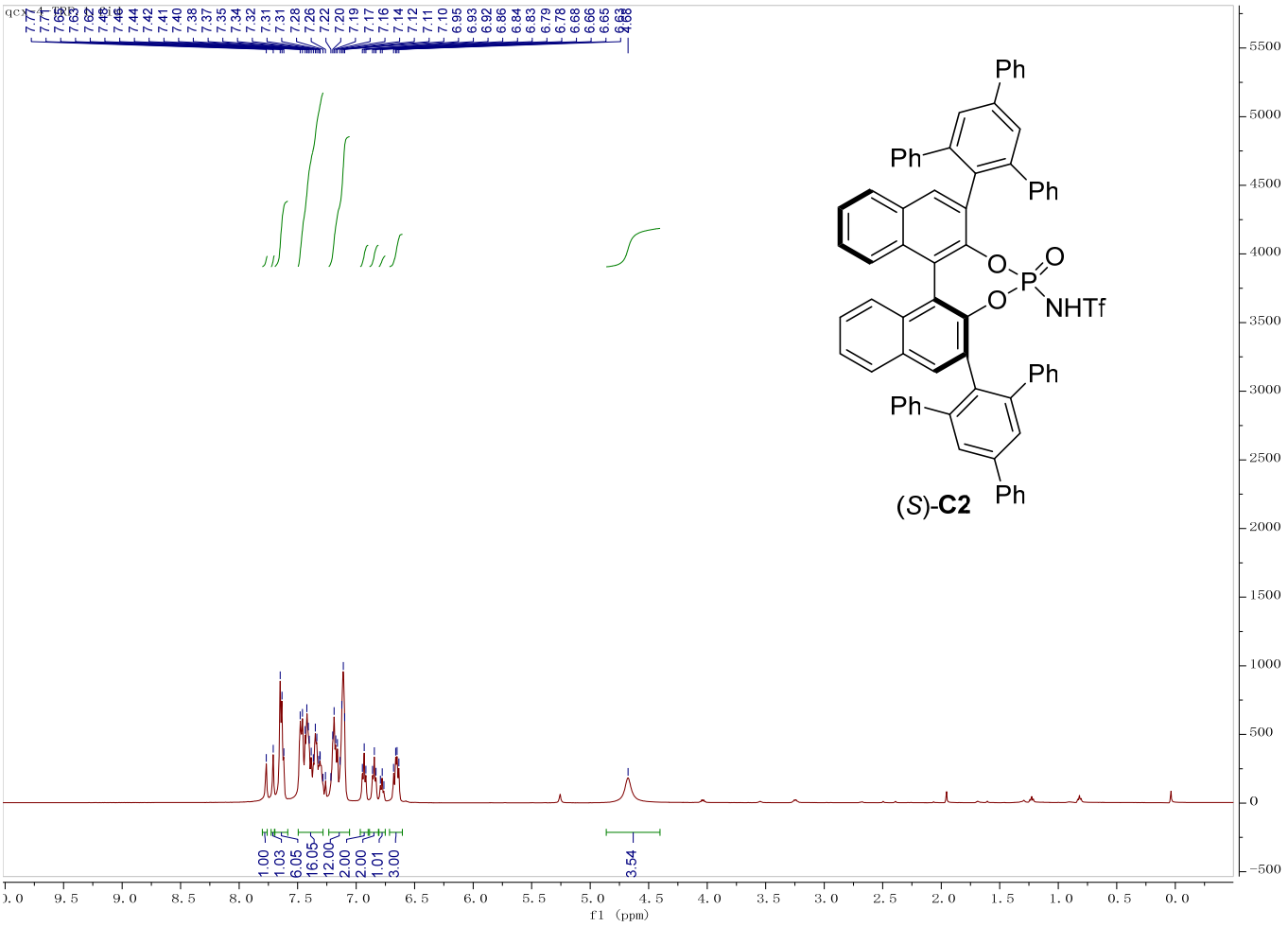
117.64
115.16
77.41
77.16
76.91
10.51
-0.91
Me
OH
TMS
1i
f1 (ppm)

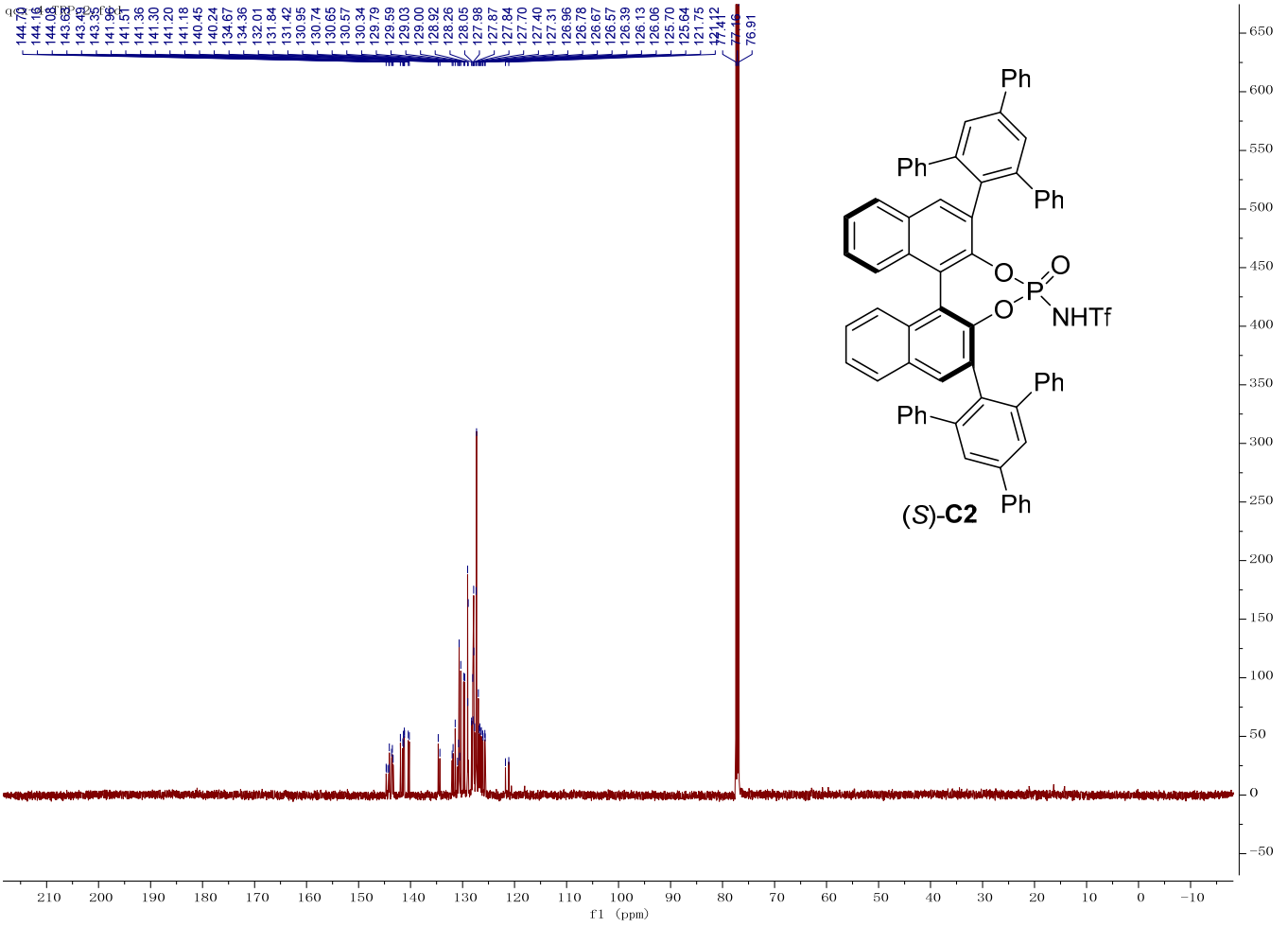

1-Me-6-vinyl-2-OH-Nap/H
7.66
7.64
7.64
7.61
7.58
7.26
7.06
7.04
6.89
6.87
6.85
6.82
5.85
5.81
5.30
5.28
4.93
2.53
Me
OH
1j
1.00
2.00
1.00
1.01
1.03
1.06
1.06
1.00
3.06
f1 (ppm)


1-Me-6-vinyl-2-OH-Nap/C
150.85
136.94
133.67
132.54
129.34
127.66
127.06
123.80
123.60
117.98
115.59
113.33
77.48
77.16
76.84
10.63
Me
OH
1j
f1 (ppm)


qcx-4-2,3-diCl-H
8.32
7.99
7.84
7.48
7.47
7.46
7.45
7.41
7.39
7.37
7.36
7.35
6.61
2.06
2.06
2.05
2.04
2.04
Cl
Cl
O
NH
HO
Ph
2i
1.00
1.00
1.01
2.00
3.13
1.00
f1 (ppm)

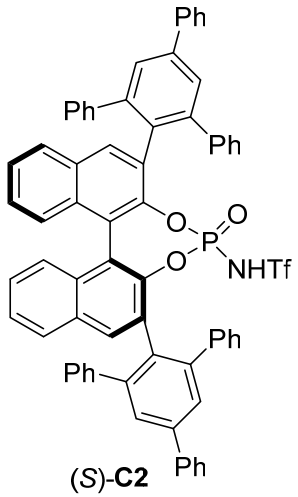

qcx-4-2,3-diCl.2.fid
206.43
166.18
148.78
137.33
134.73
132.56
131.43
130.12
129.47
126.09
125.81
122.34
87.02
84.21
80.03
30.42
30.22
30.03
29.84
29.65
29.45
29.26
Cl
Cl
O
NH
HO
Ph
2i
f1 (ppm)


Ph
Ph
Ph
O
P
O
O
NHTf
Ph
Ph
Ph
(S)-C2
1.00
1.03
6.05
16.05
12.00
2.00
2.00
1.01
3.00
3.54
f1 (ppm)


Ph
Ph
Ph
O
P
O
O
NHTf
Ph
Ph
Ph
(S)-C2
f1 (ppm)

qcx-3-68.2.fid

-0.68

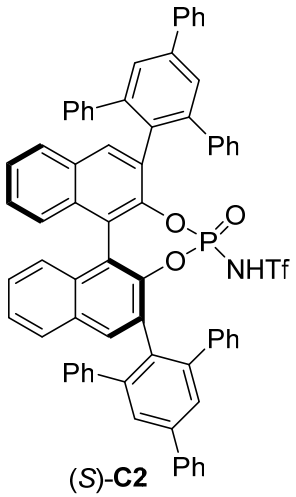


(*S*)-**C2**

f1 (ppm)

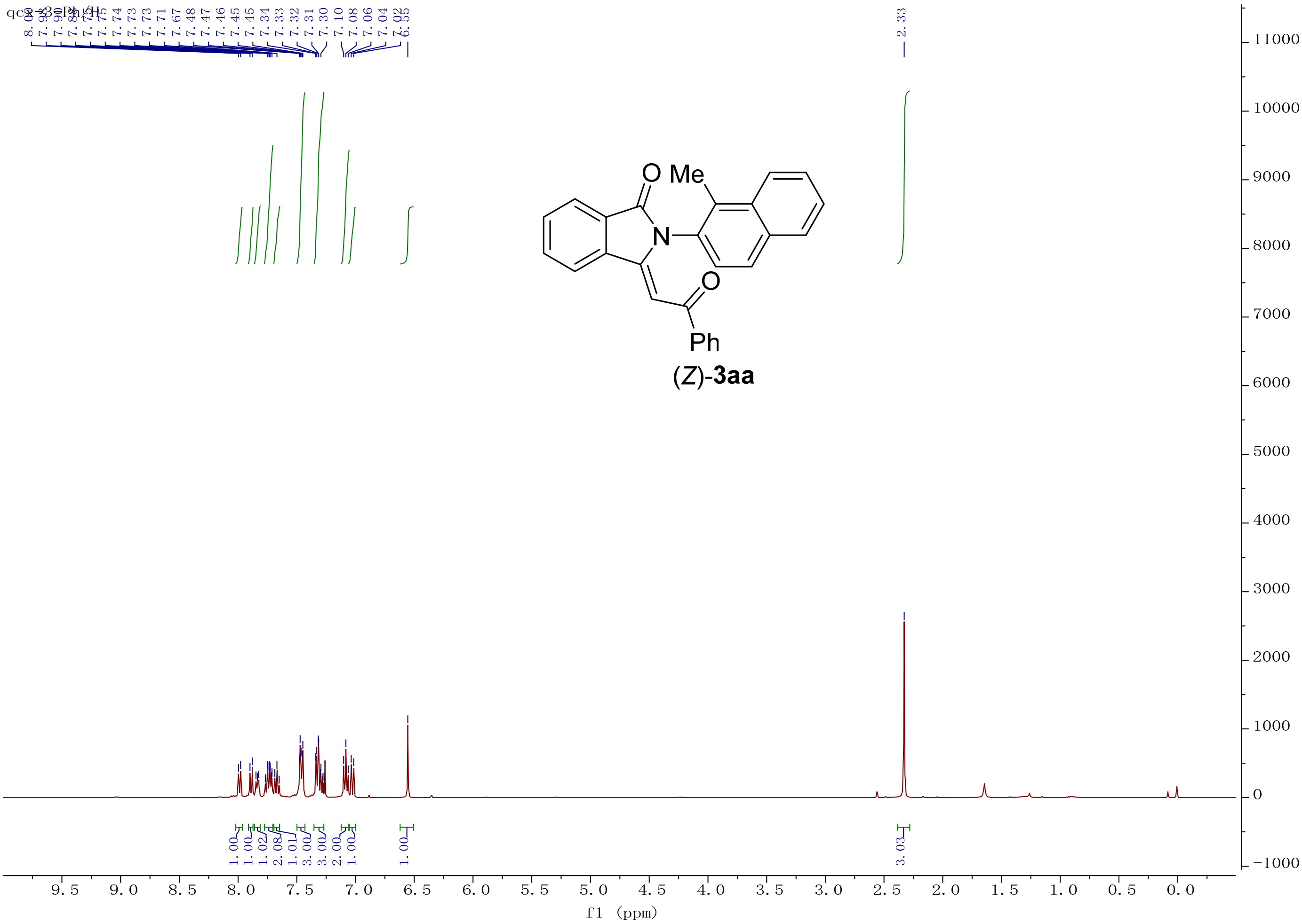
催化剂核磁/F

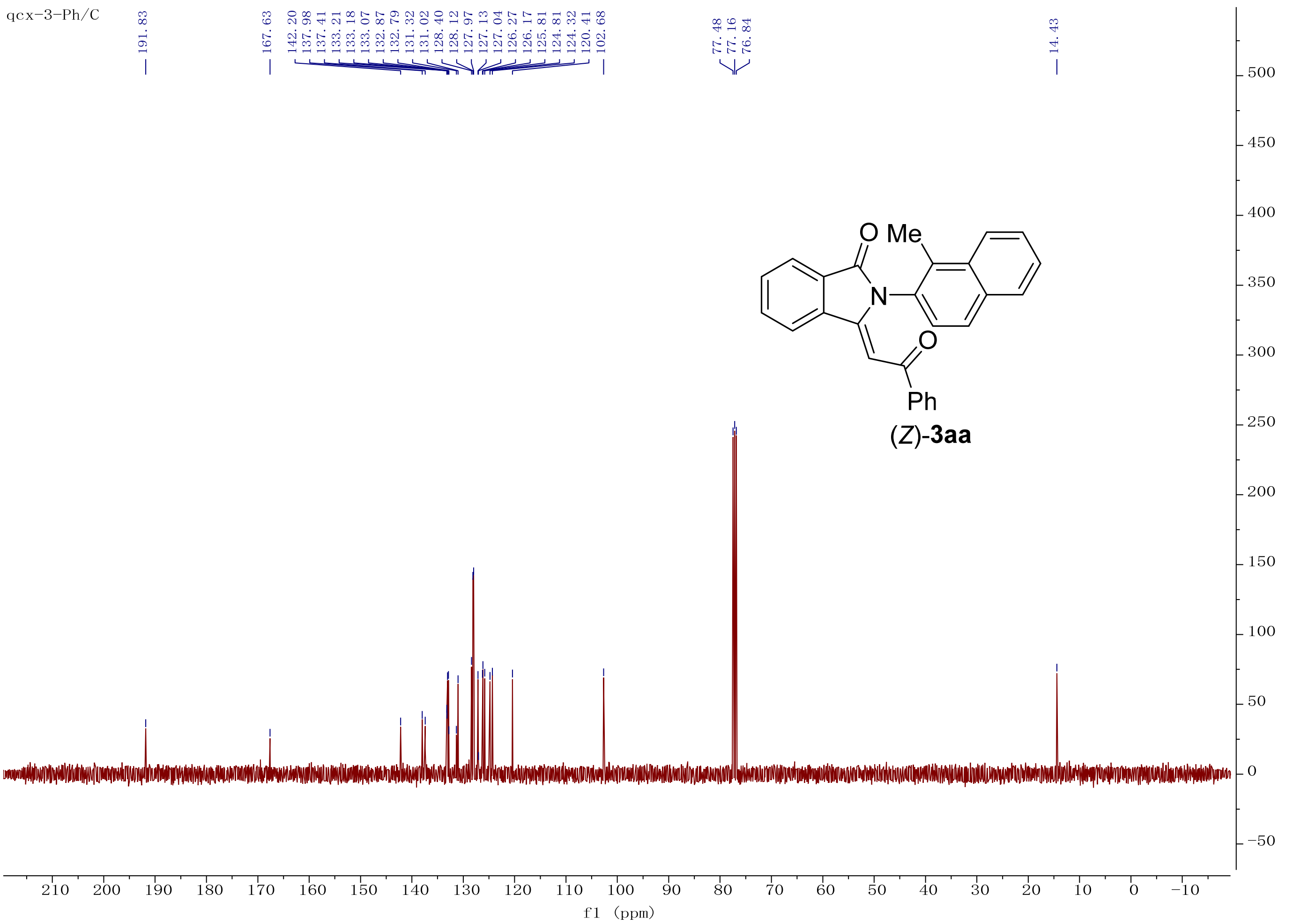
-78.91

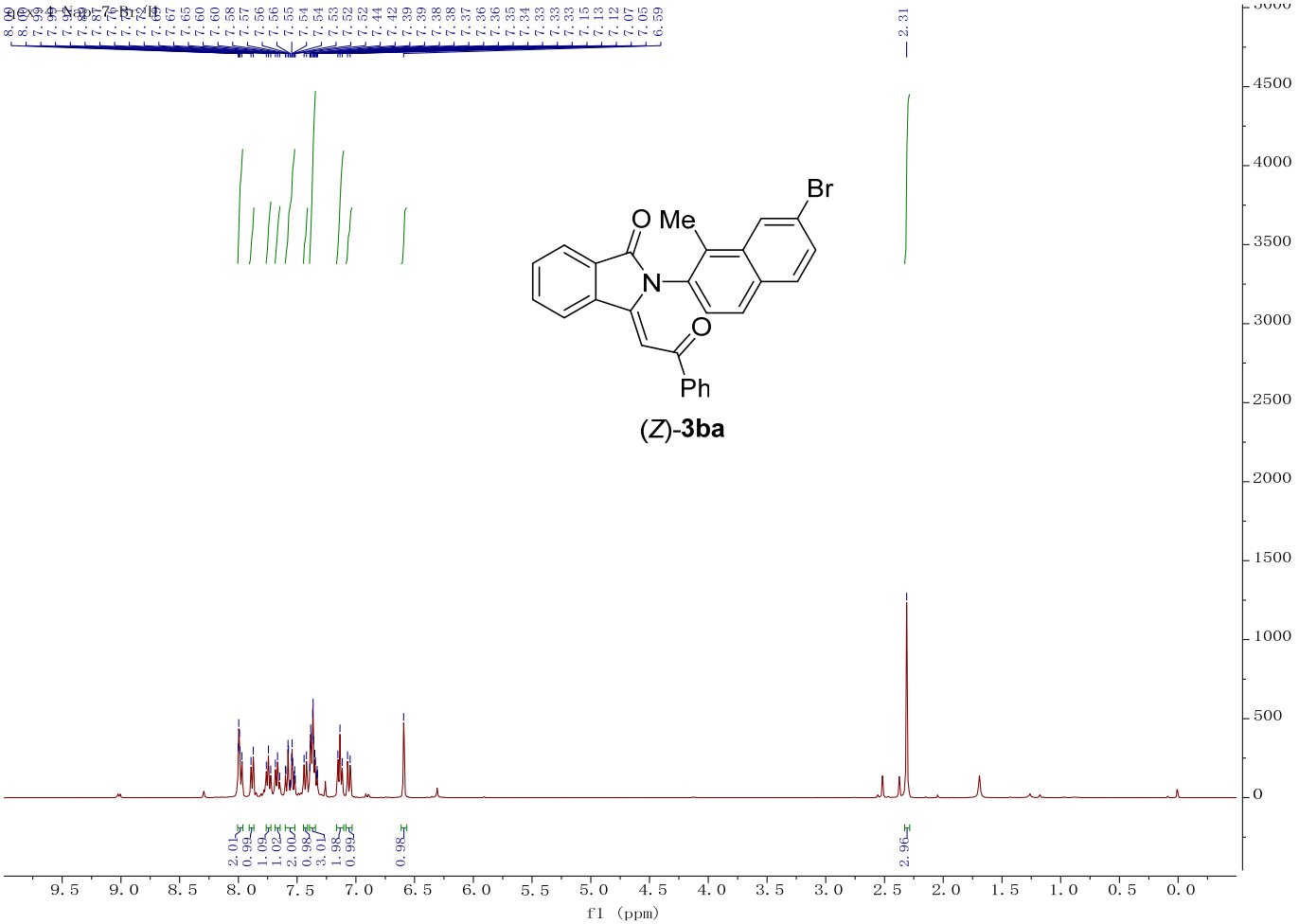


(*S*)-**C2**

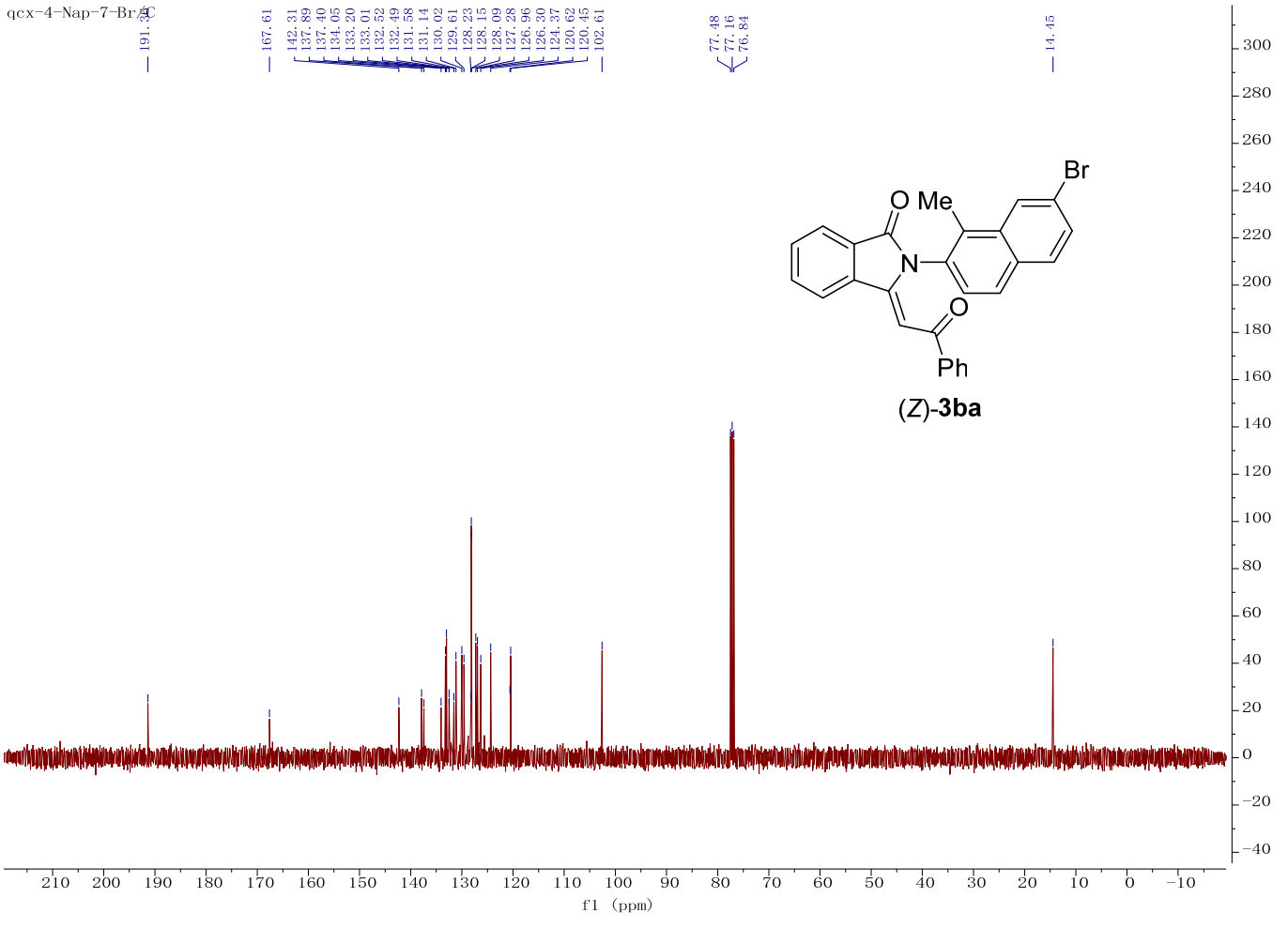
f1 (ppm)


7.73
7.71
7.67
7.48
7.47
7.46
7.45
7.45
7.34
7.33
7.32
7.31
7.30
7.10
7.08
7.06
7.04
6.55
2.33
O Me
N
O
Ph
(Z)-3aa
1.00
1.00
1.02
2.08
1.01
3.00
3.00
2.00
1.00
1.00
3.03
f1 (ppm)

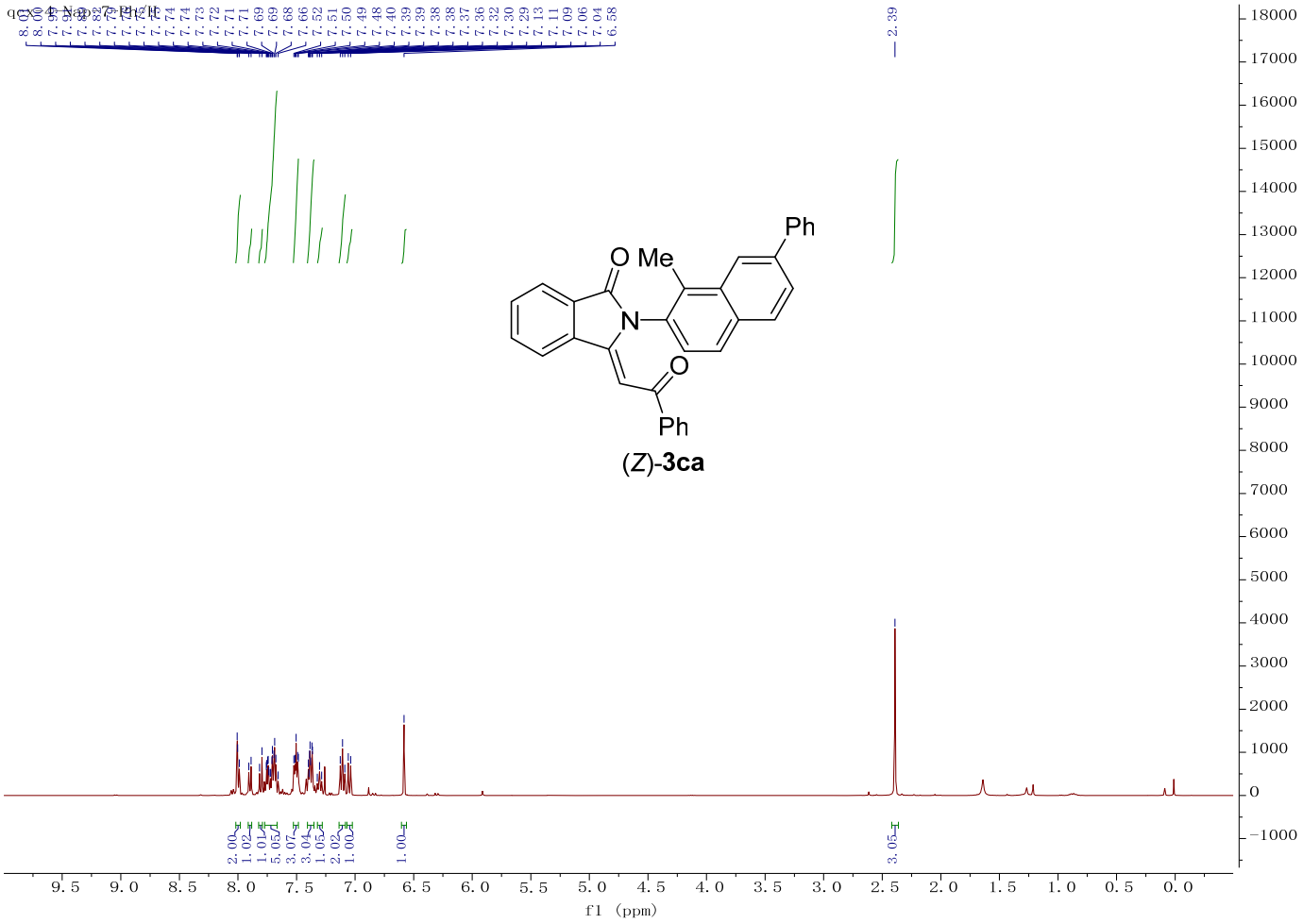

qcx-3-Ph/C
191.83
167.63
142.20
137.98
137.41
133.21
133.18
133.07
132.87
132.79
131.32
131.02
128.40
128.12
127.97
127.13
127.04
126.27
126.17
125.81
124.81
124.32
120.41
102.68
77.48
77.16
76.84
14.43
O Me
N
O
Ph
(Z)-3aa
f1 (ppm)



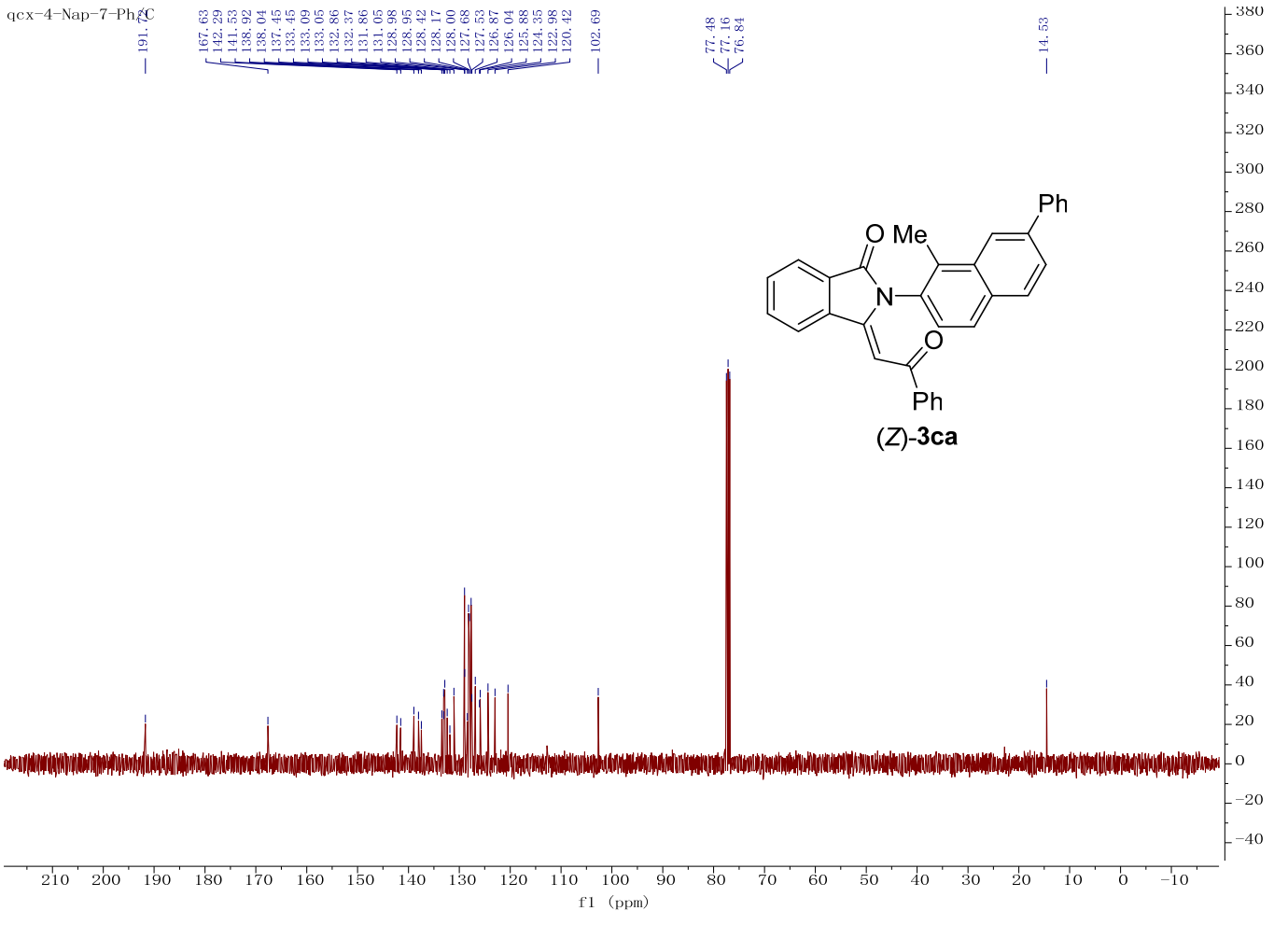
(*Z*)-**3ba**



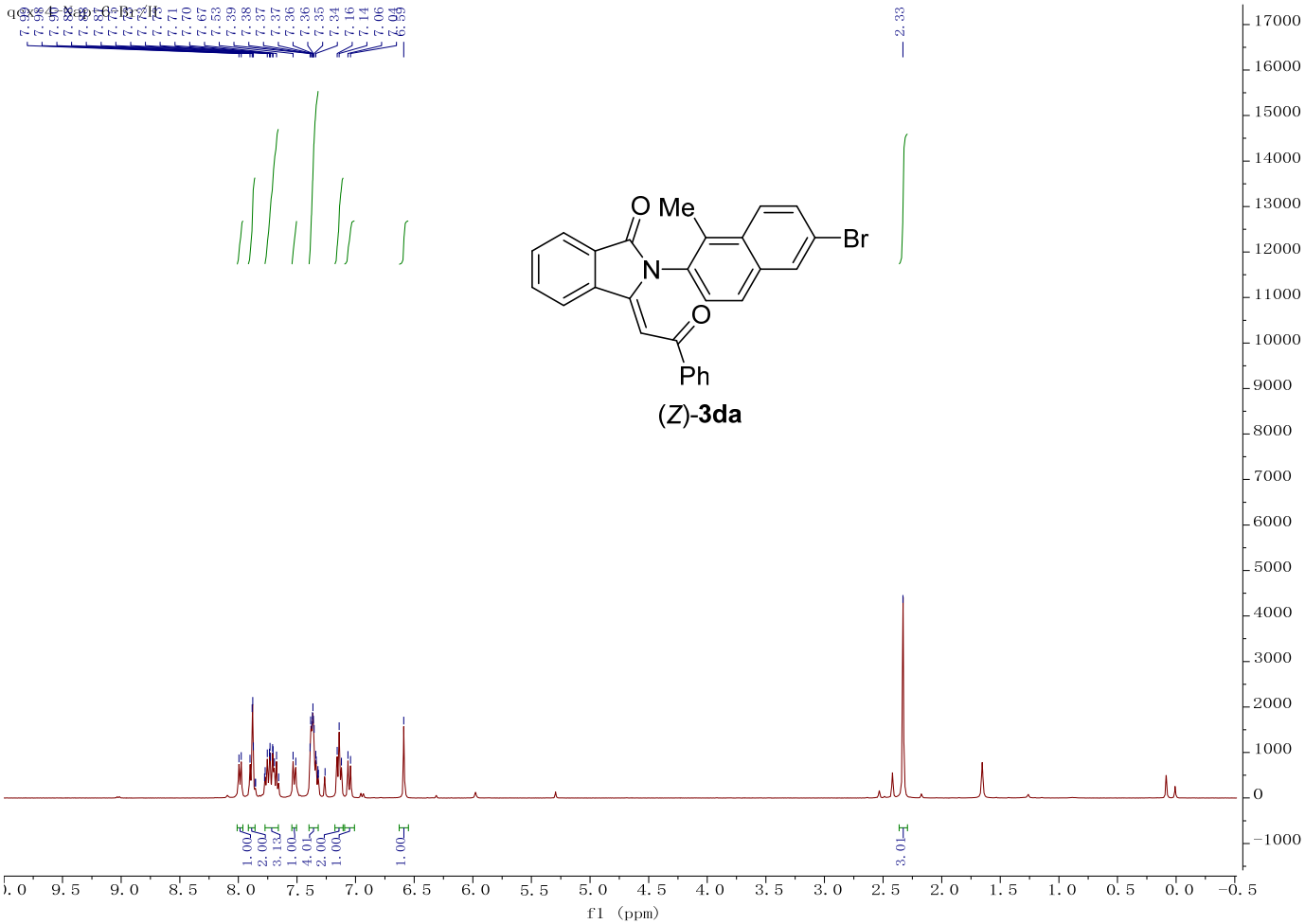
(*Z*)-**3ba**

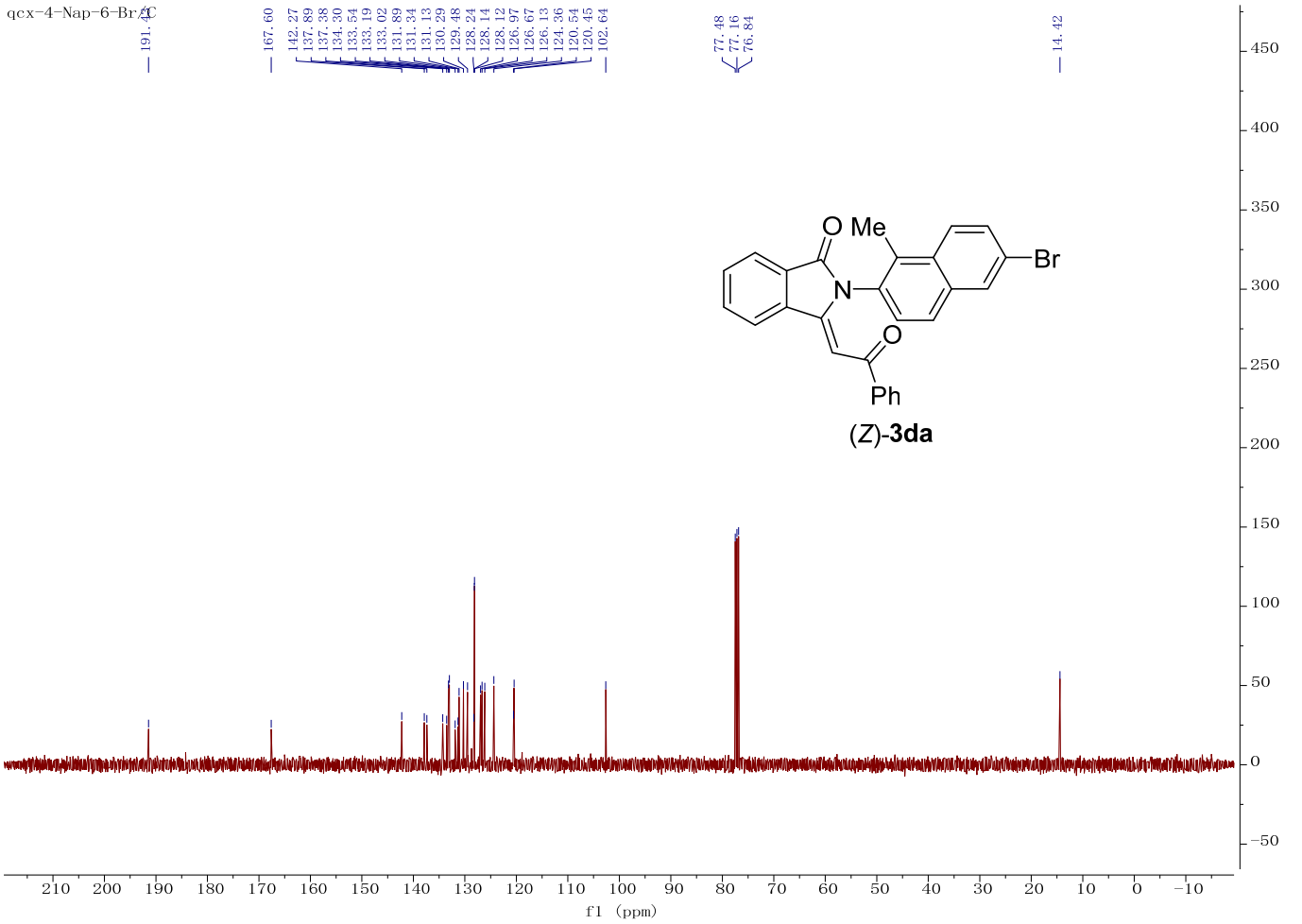


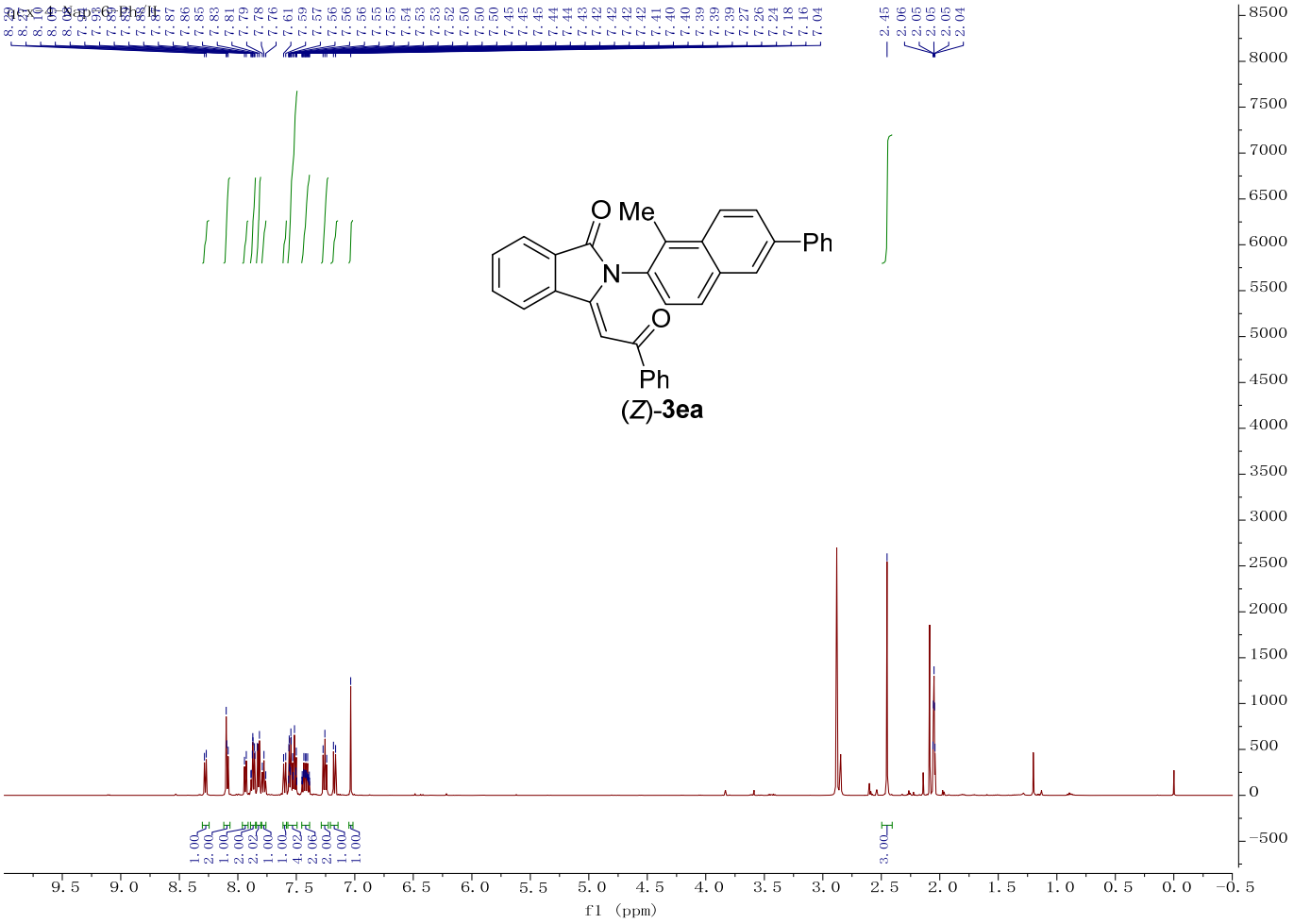
(*Z*)-**3ca**

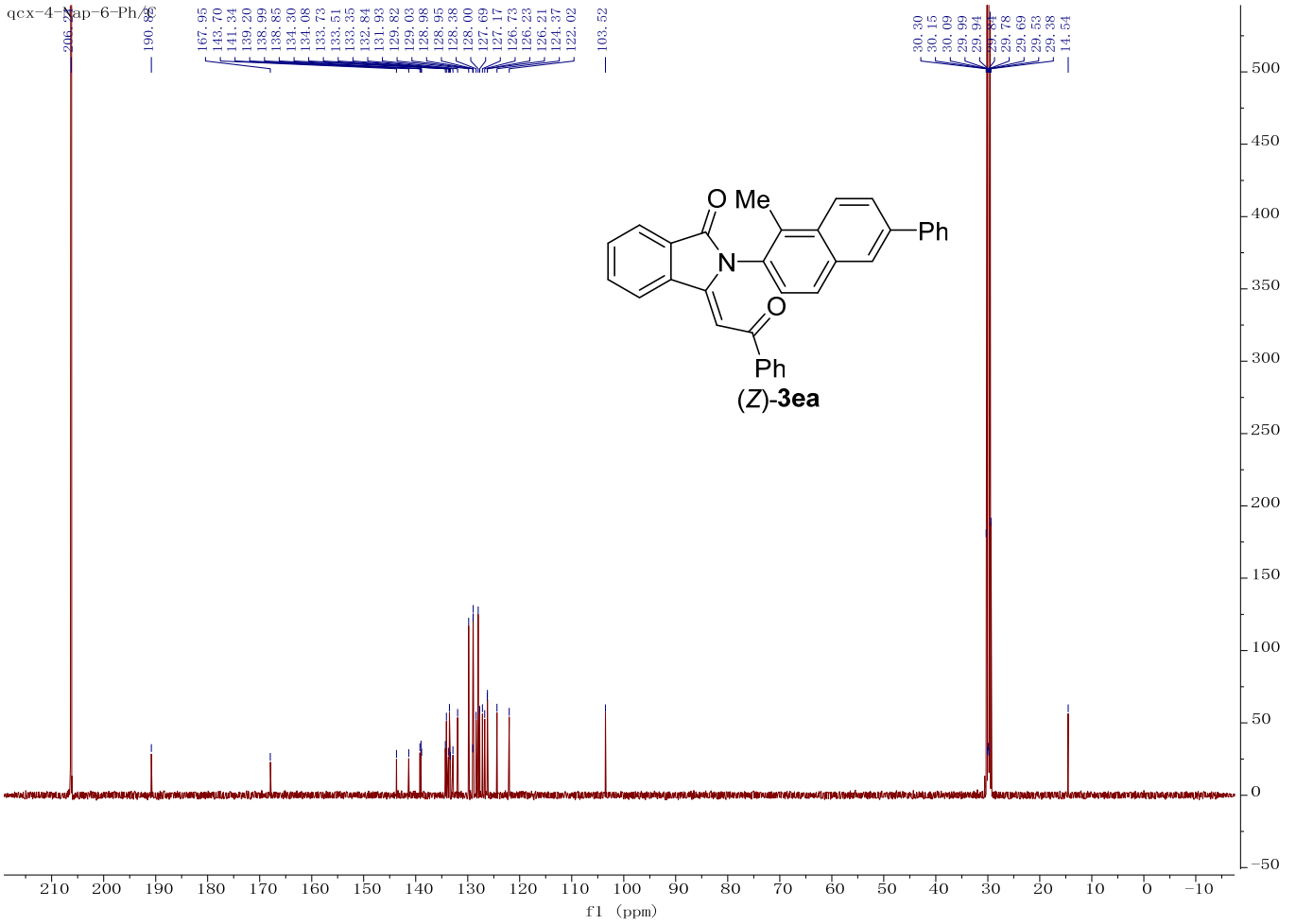


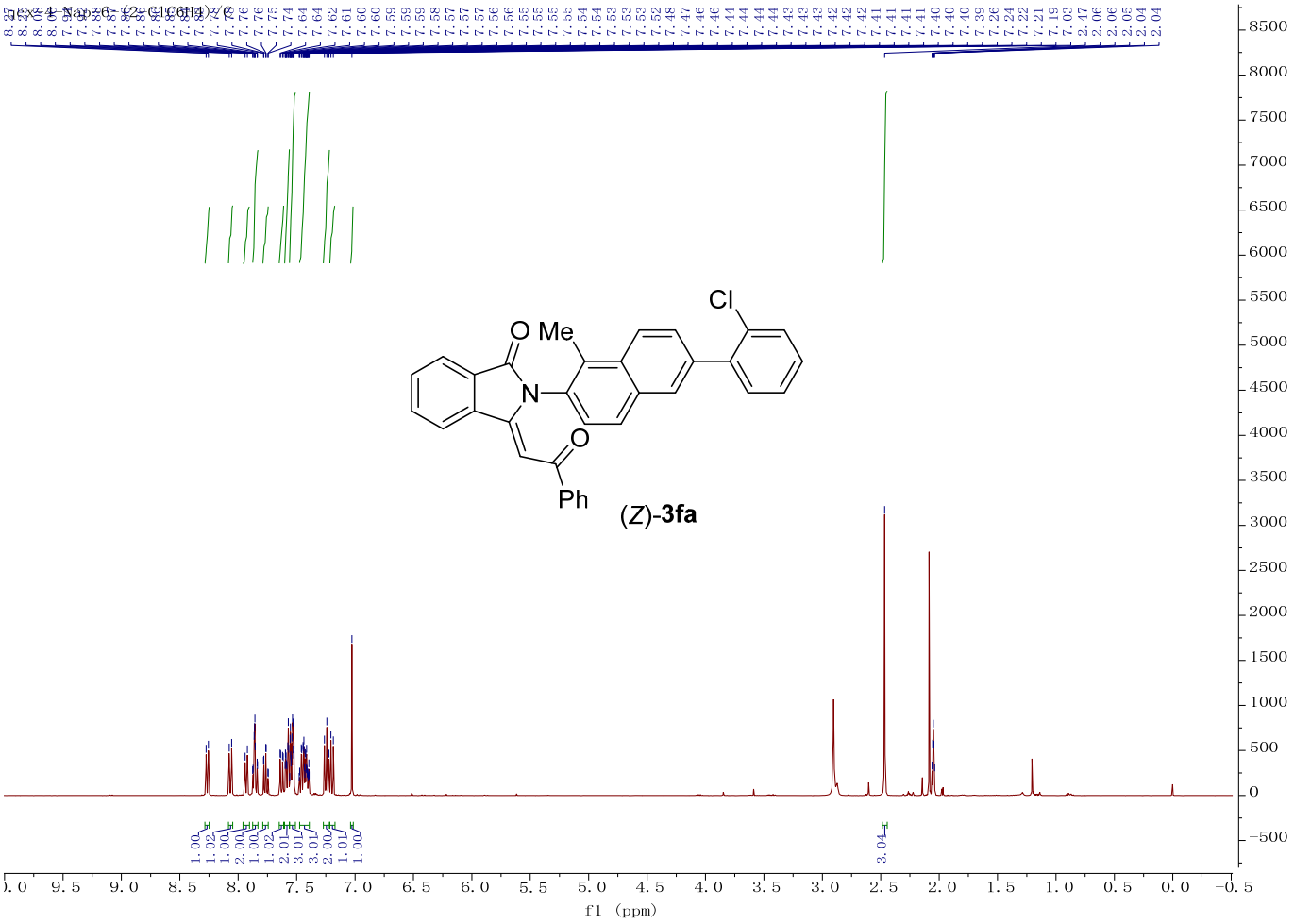
(*Z*)-**3ca**

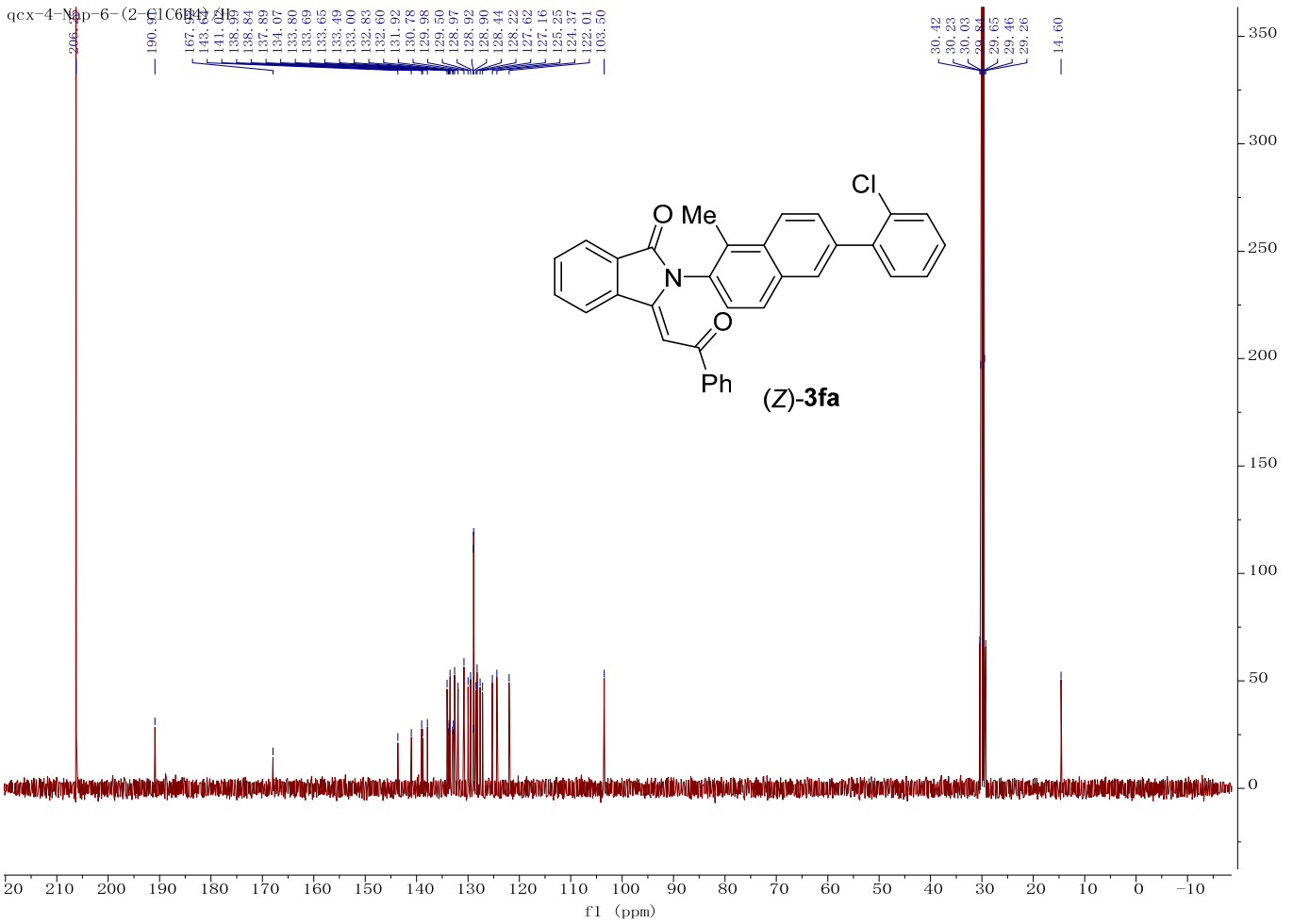

O Me
Br
N
O
Ph
(Z)-3da
f1 (ppm)

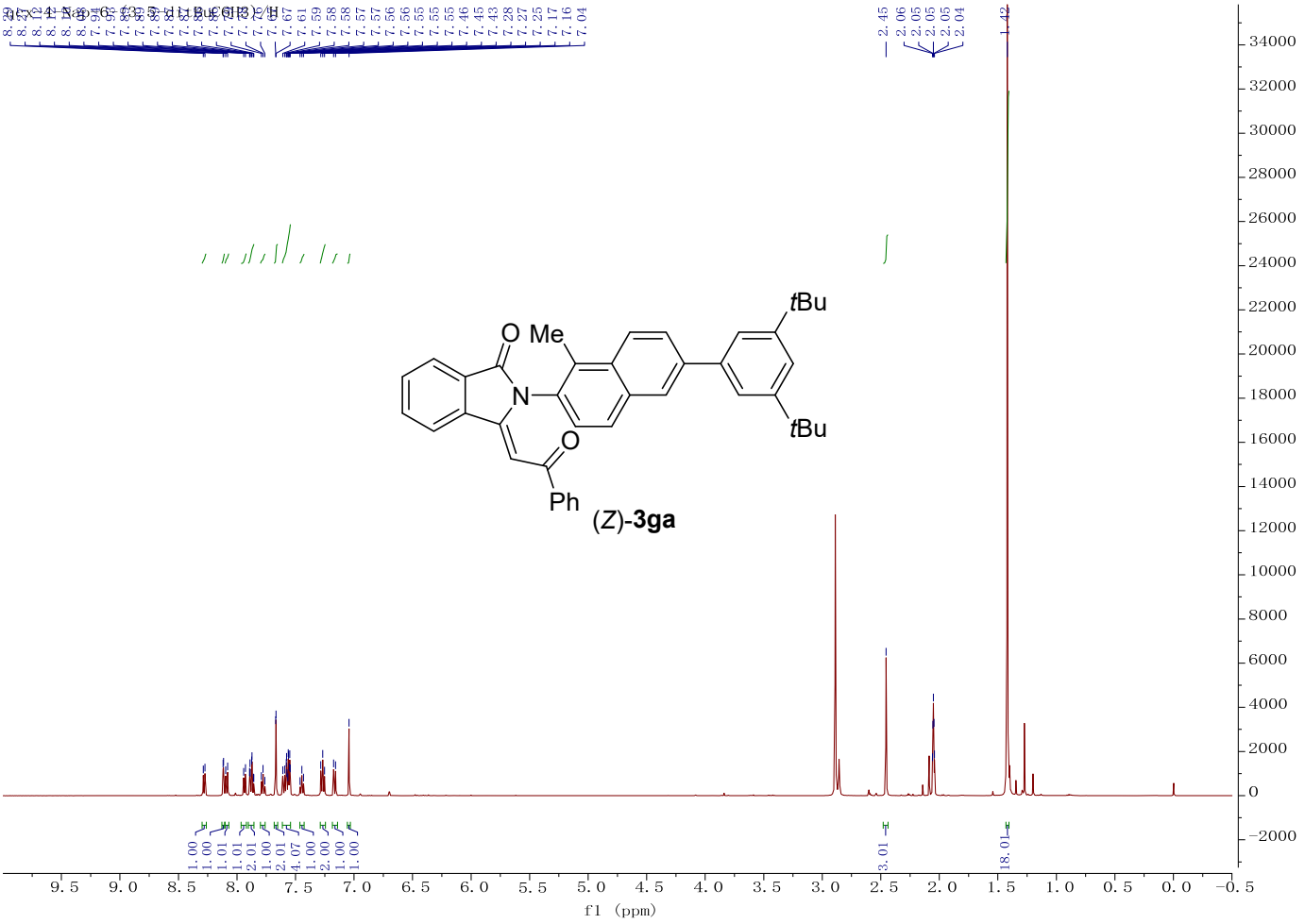

O Me
Br
N
O
Ph
(Z)-3da
f1 (ppm)

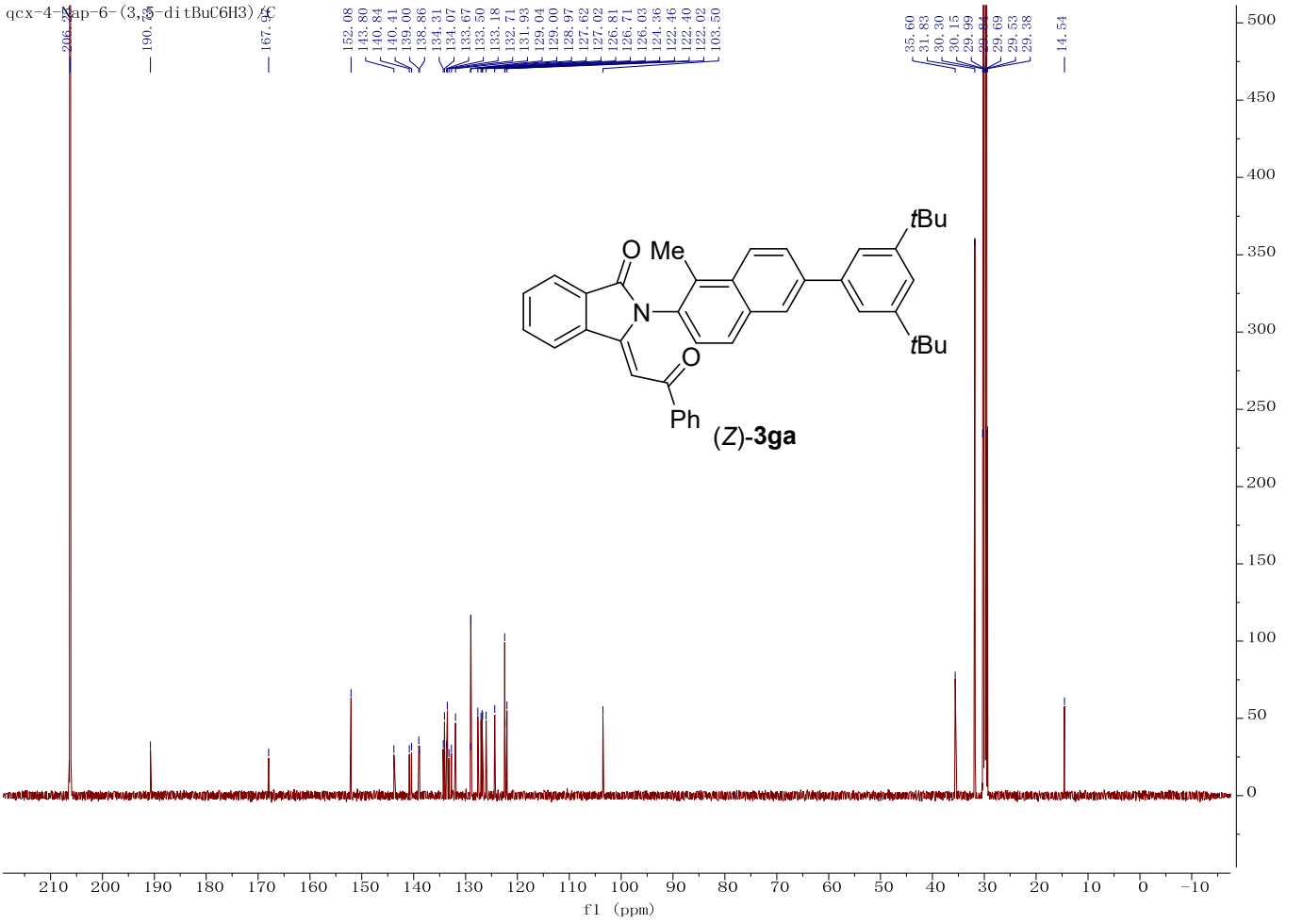

O Me
Ph
N
O
Ph
(Z)-3ea
f1 (ppm)

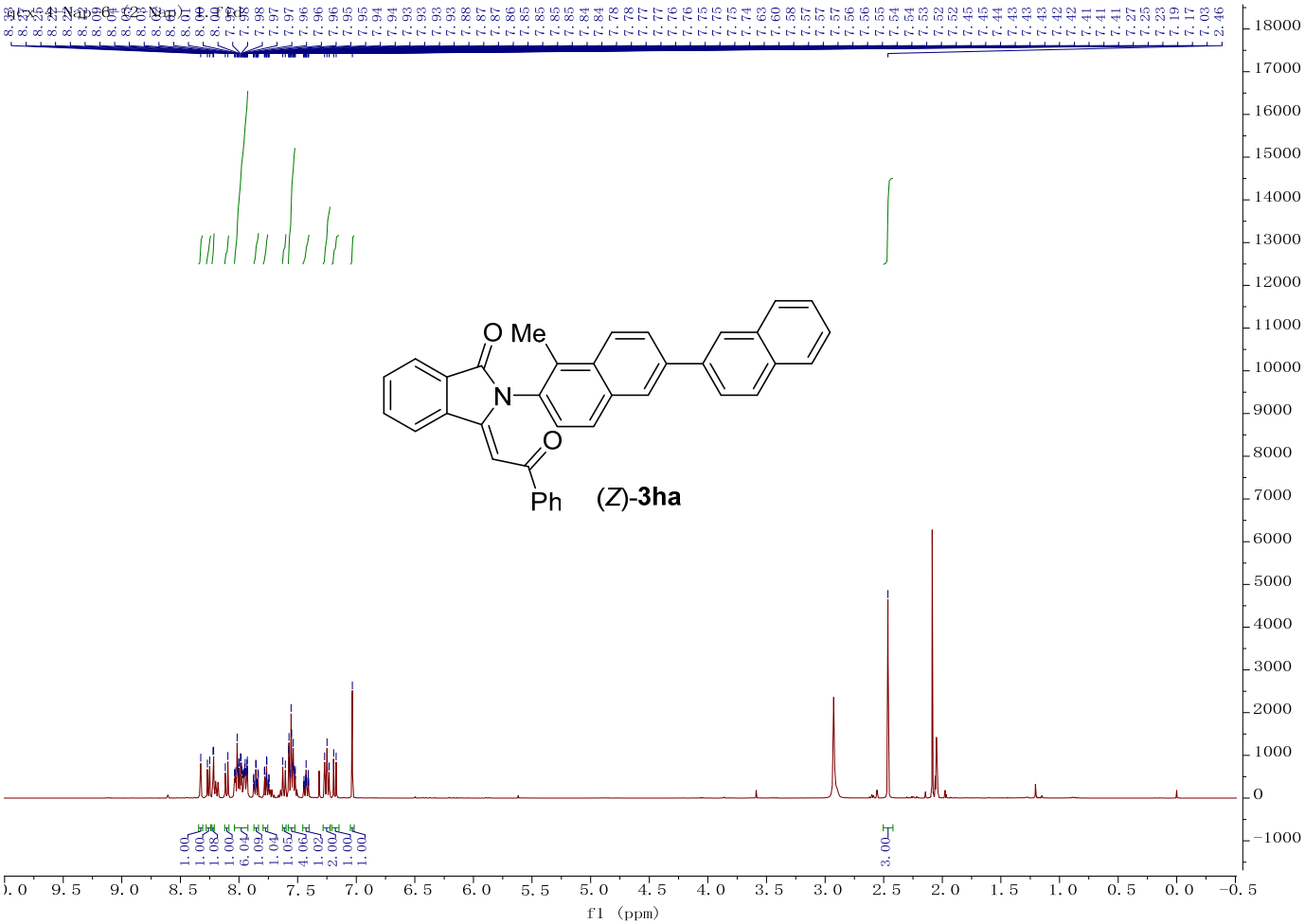

O Me
Ph
N
O
Ph
(Z)-3ea
f1 (ppm)

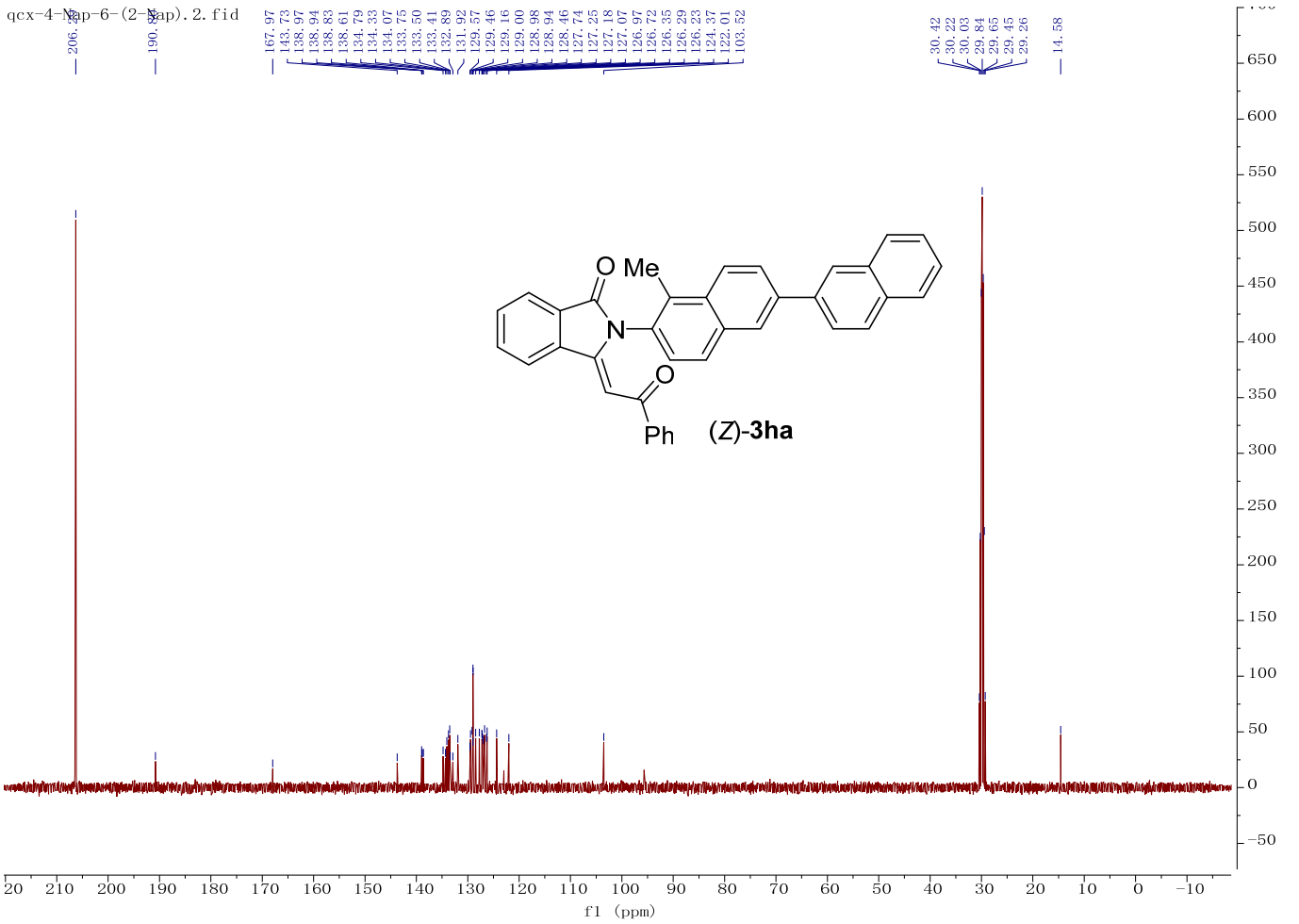

Cl
O Me
N
O
Ph
(Z)-3fa
f1 (ppm)

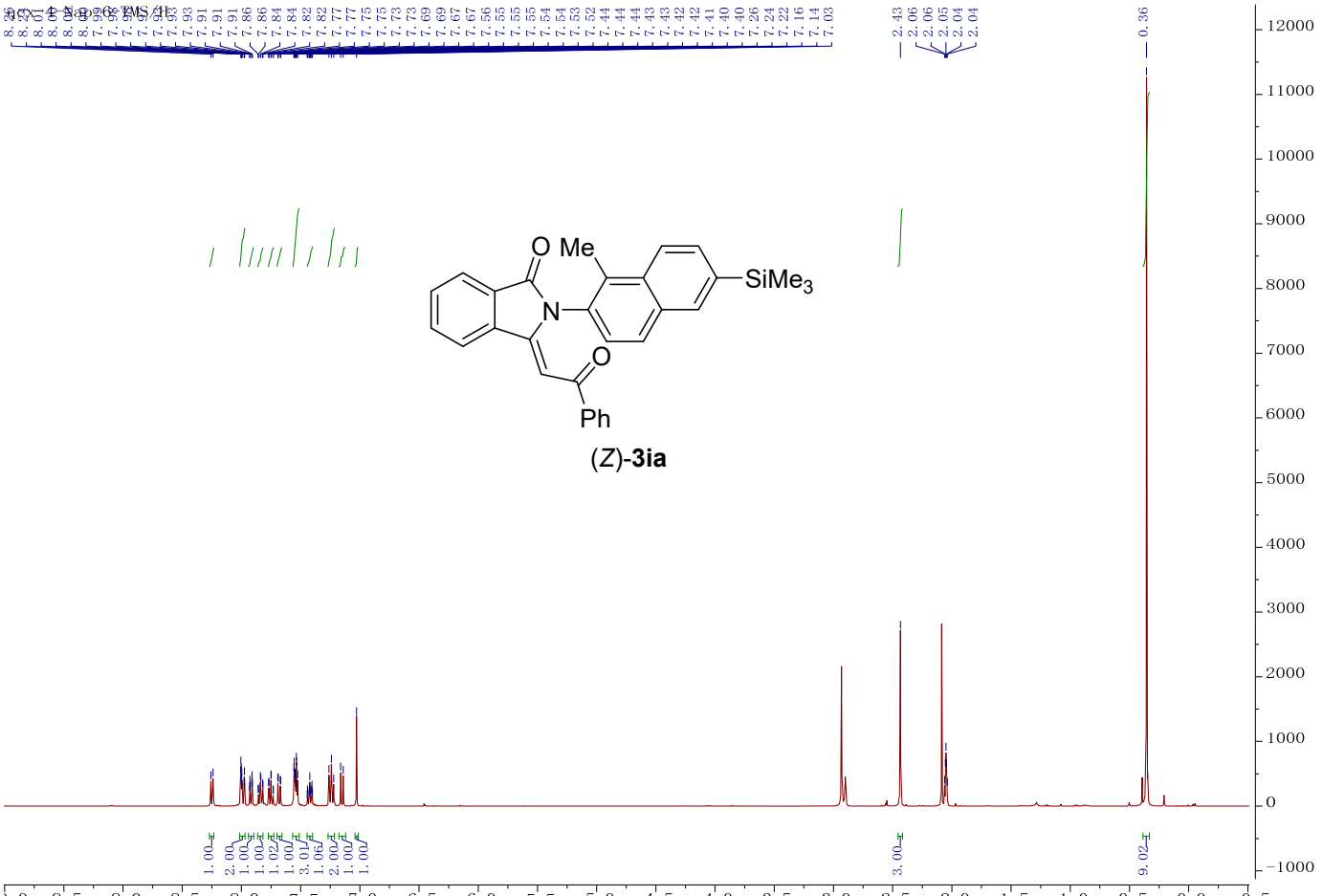

Cl
O Me
N
O
Ph
(Z)-3fa
f1 (ppm)


tBu
O Me
N
O
tBu
Ph
(Z)-3ga
f1 (ppm)


tBu
O Me
N
O
tBu
Ph
(Z)-3ga
f1 (ppm)

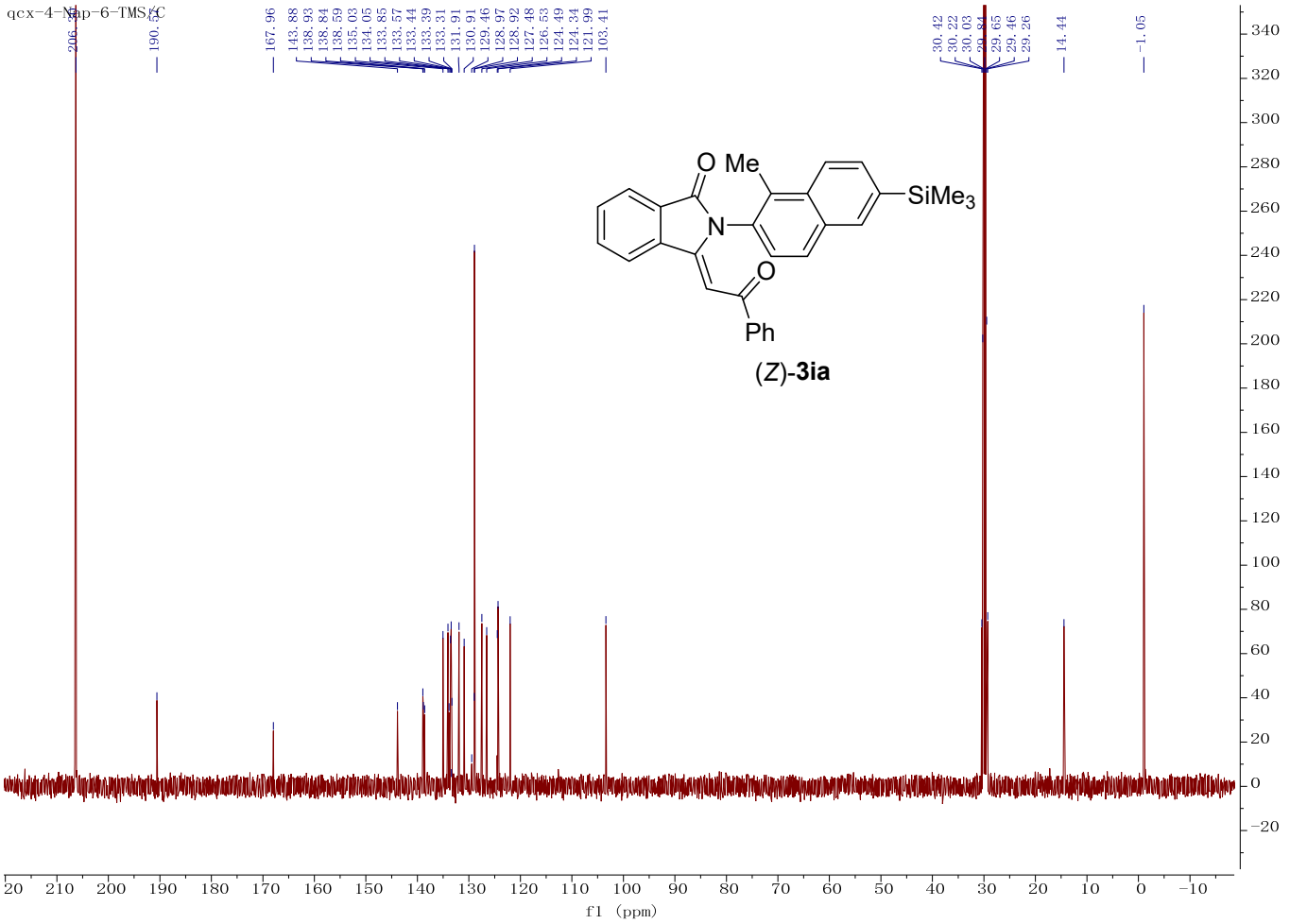

O Me
N
O
Ph
(Z)-3ha
f1 (ppm)


O Me
N
O
Ph
(Z)-3ha
f1 (ppm)



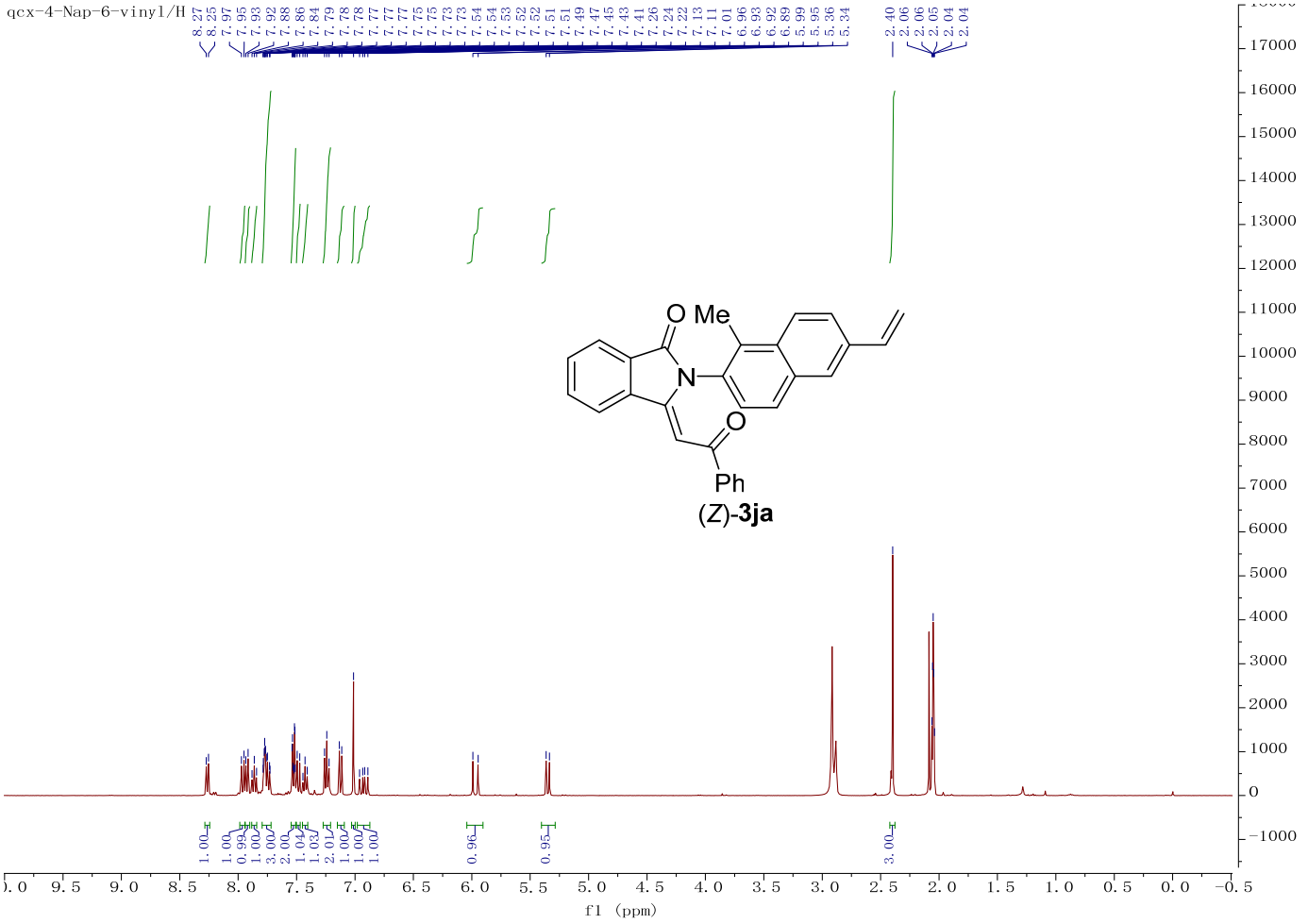
(*Z*)-**3ia**

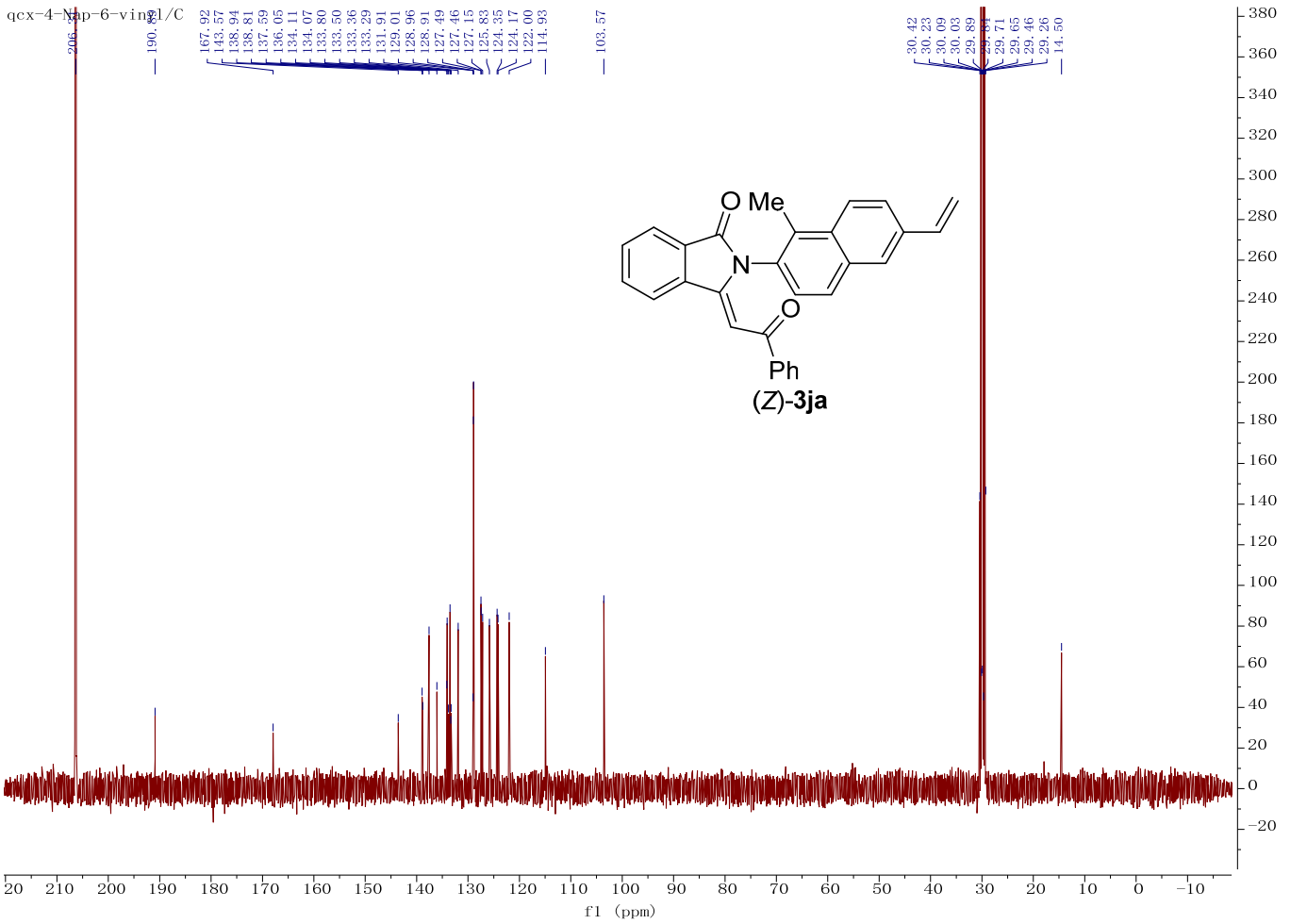
f1 (ppm)

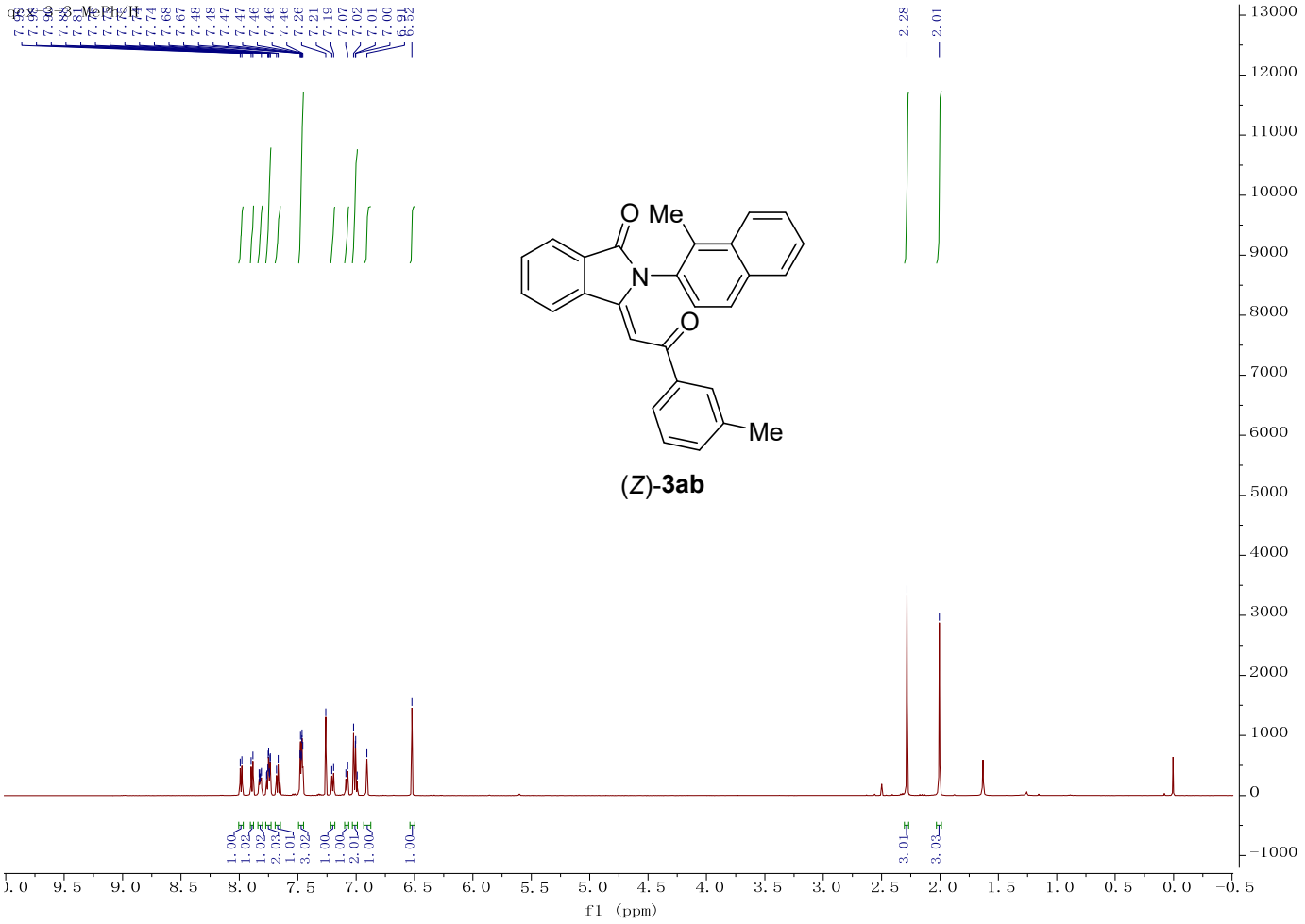


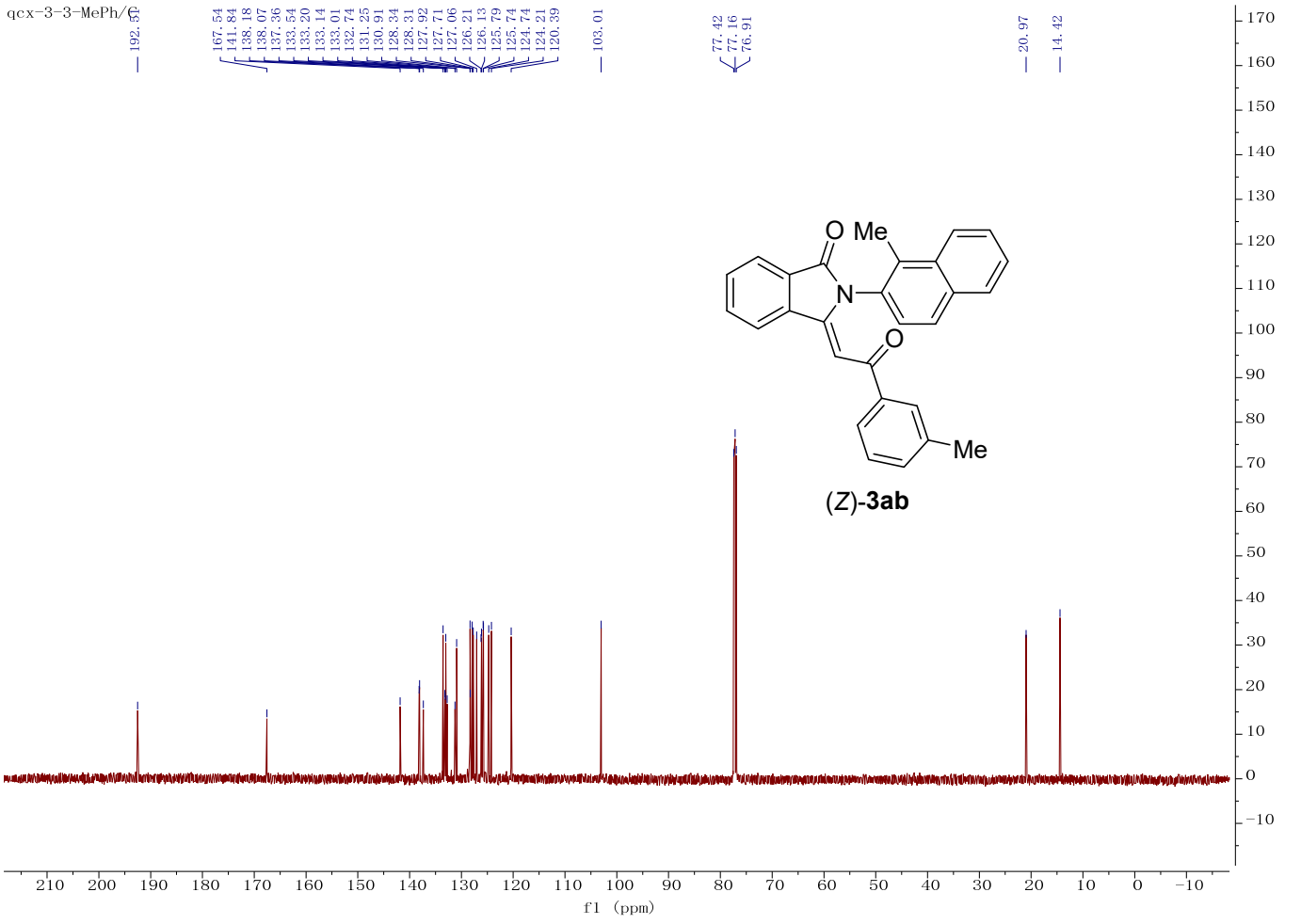
(*Z*)-**3ia**

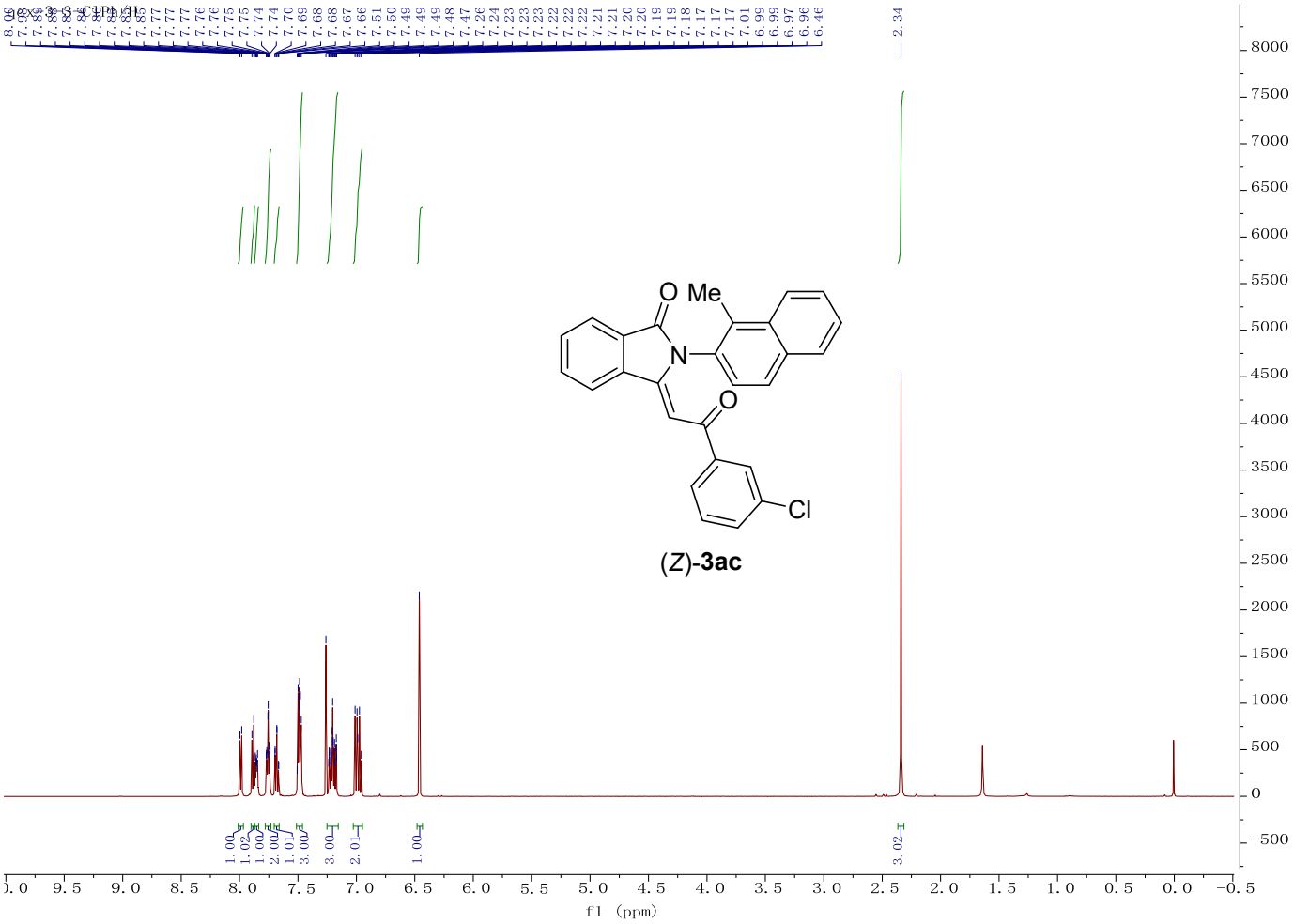
f1 (ppm)

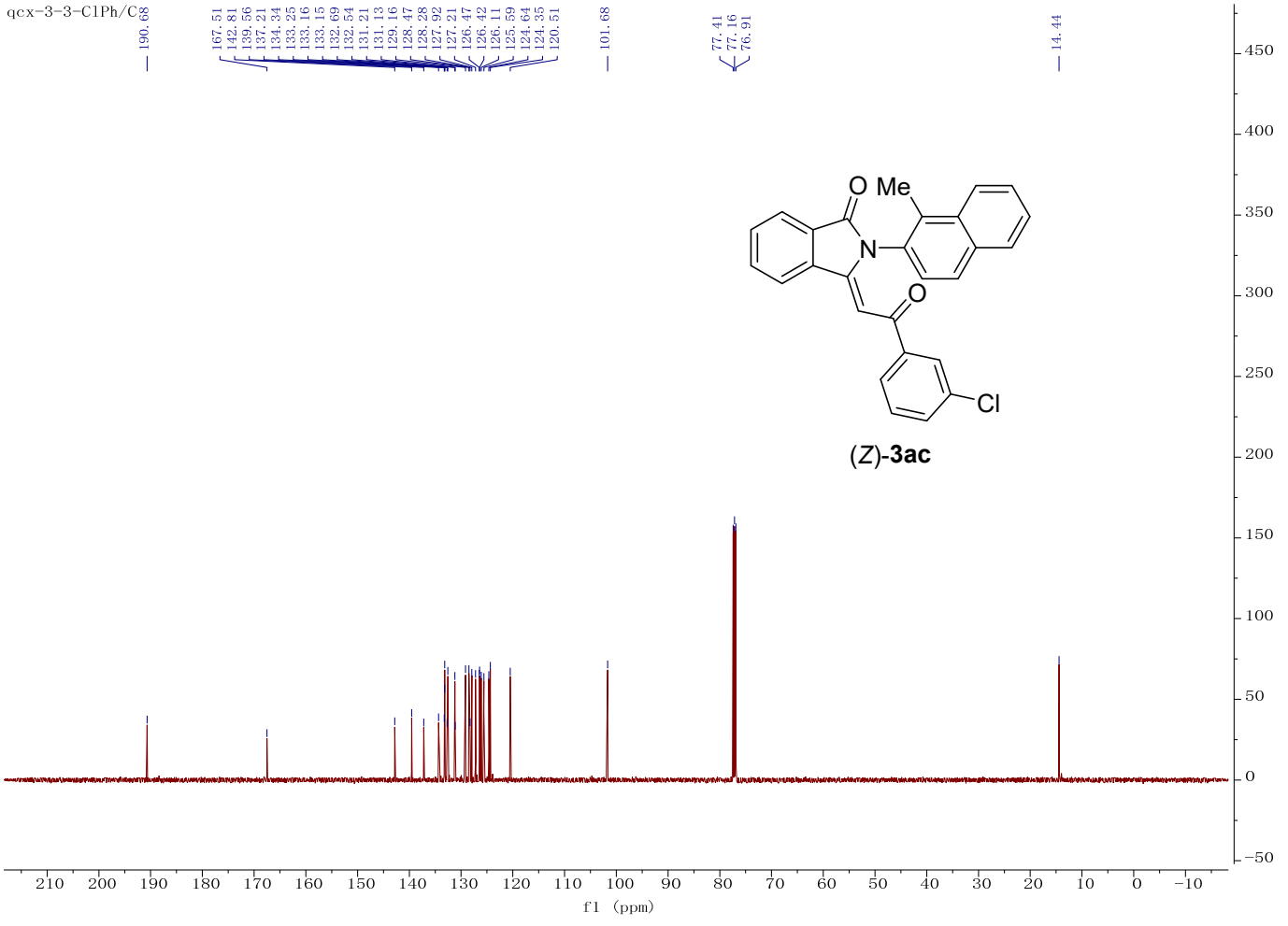

qcx-4-Nap-6-vinyl/H
O Me
N
O
Ph
(Z)-3ja
f1 (ppm)

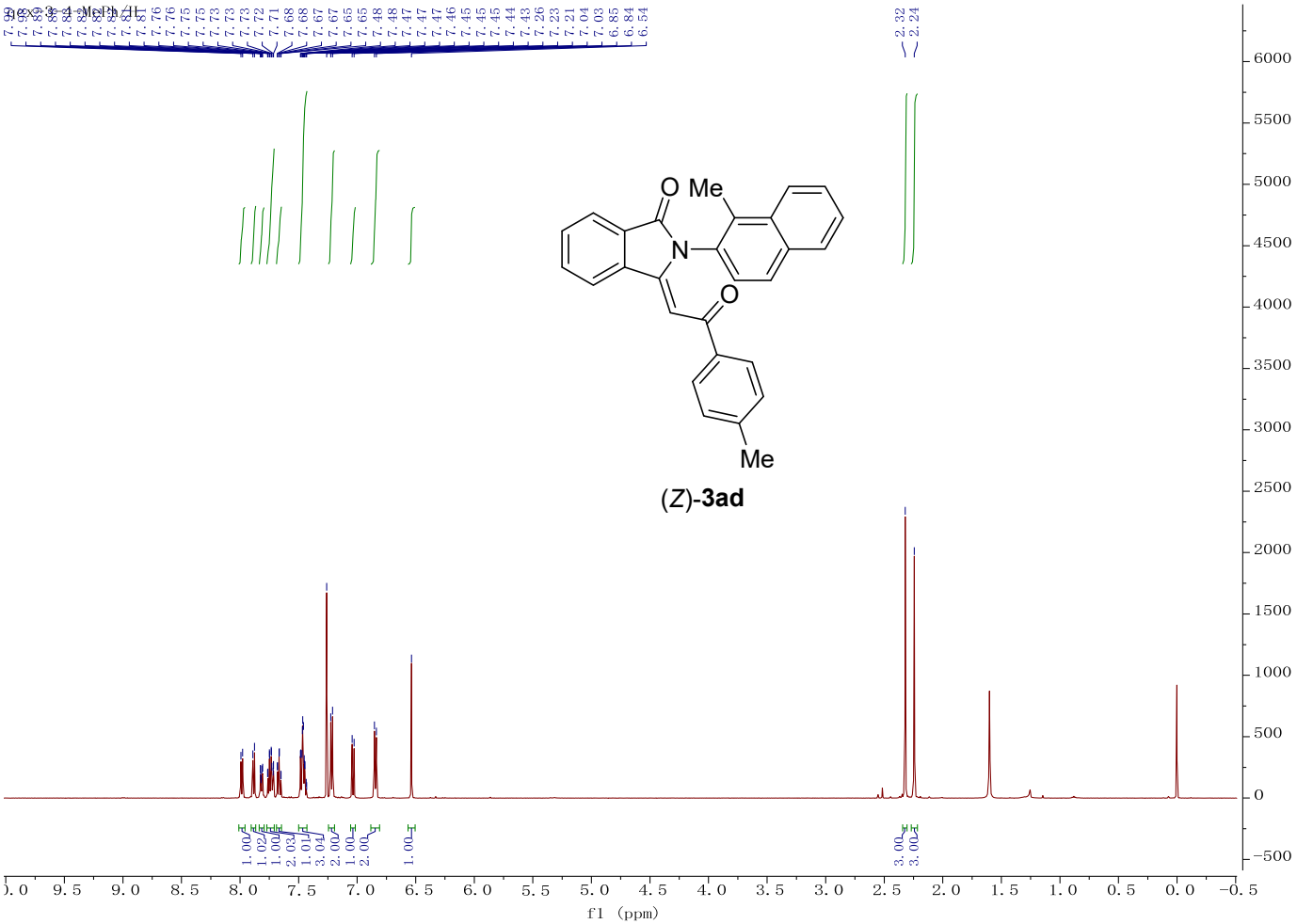

qcx-4-Nap-6-vinyl/C
O Me
N
O
Ph
(Z)-3ja
f1 (ppm)

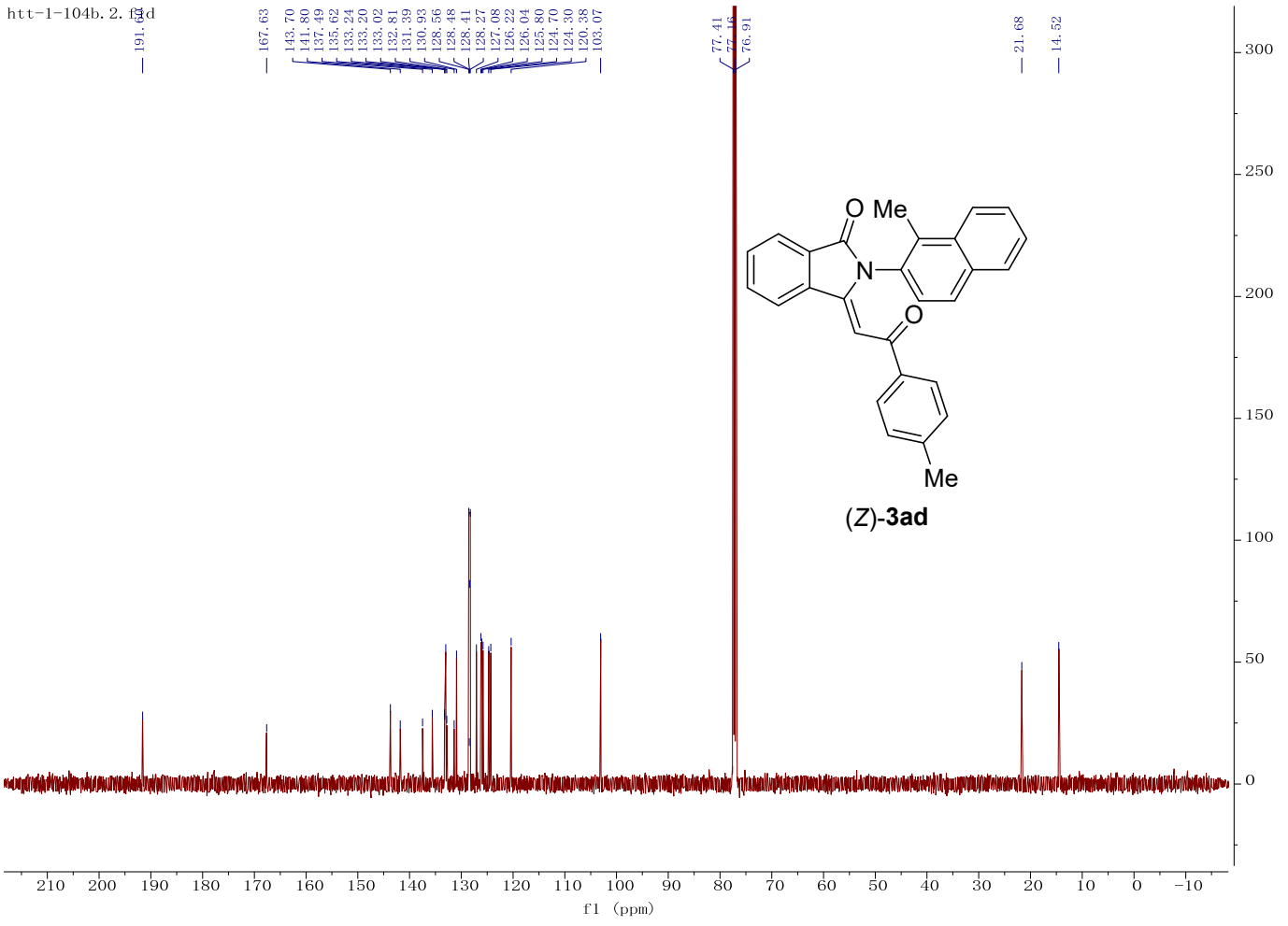

O Me
N
O
Me
(Z)-3ab
f1 (ppm)

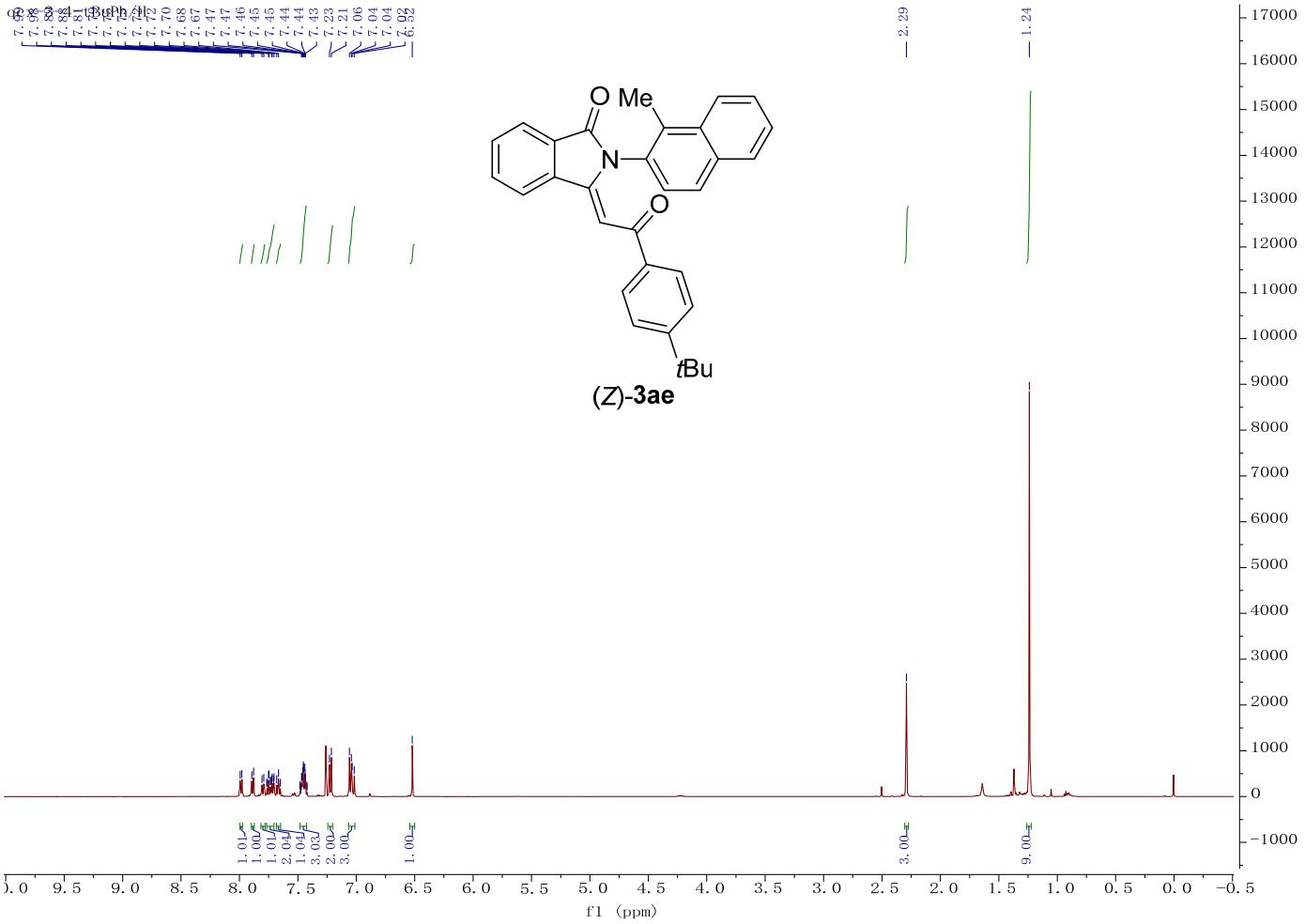

O Me
N
O
Me
(Z)-3ab
f1 (ppm)

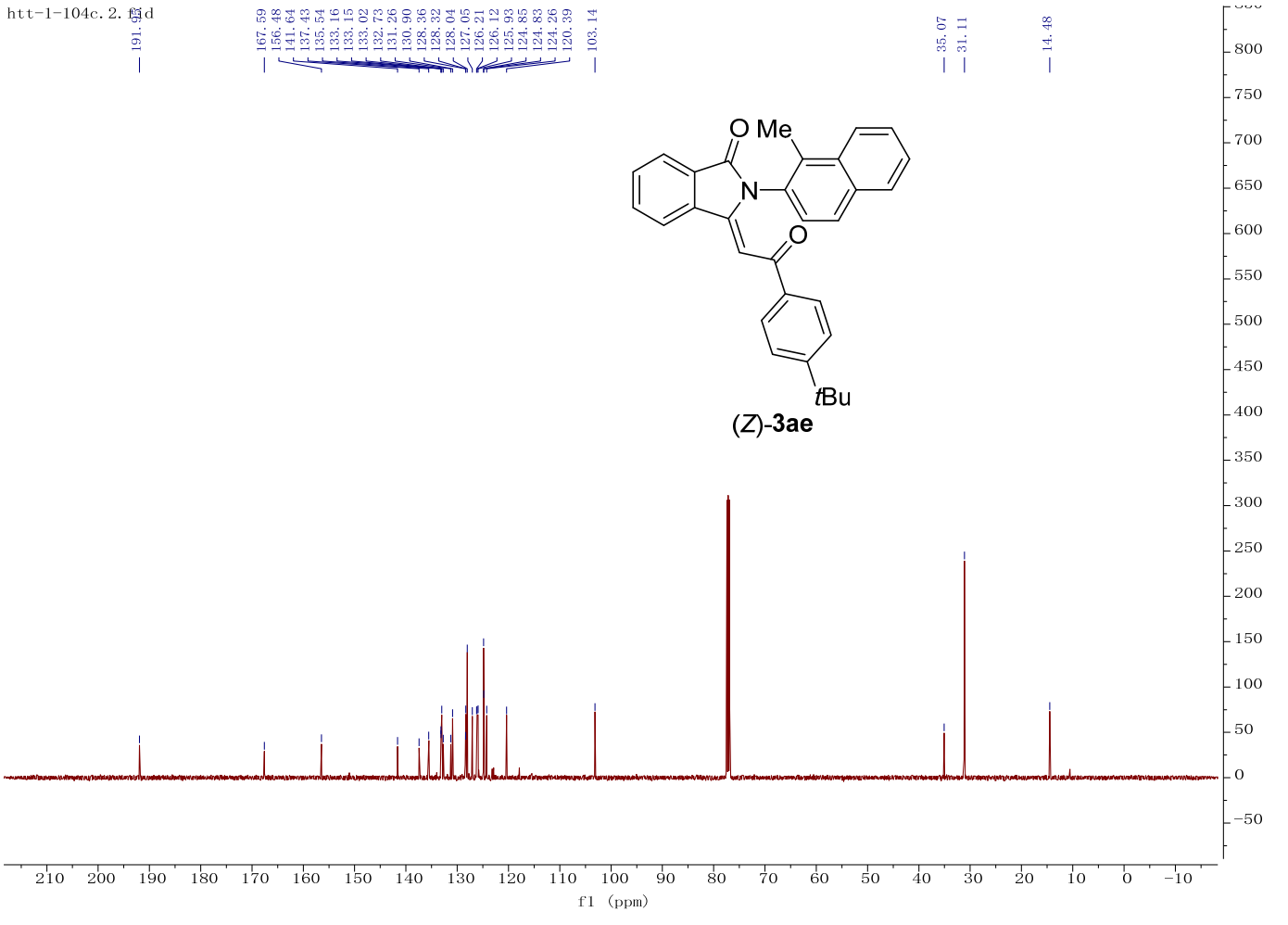

O Me
N
O
Cl
(Z)-3ac
f1 (ppm)

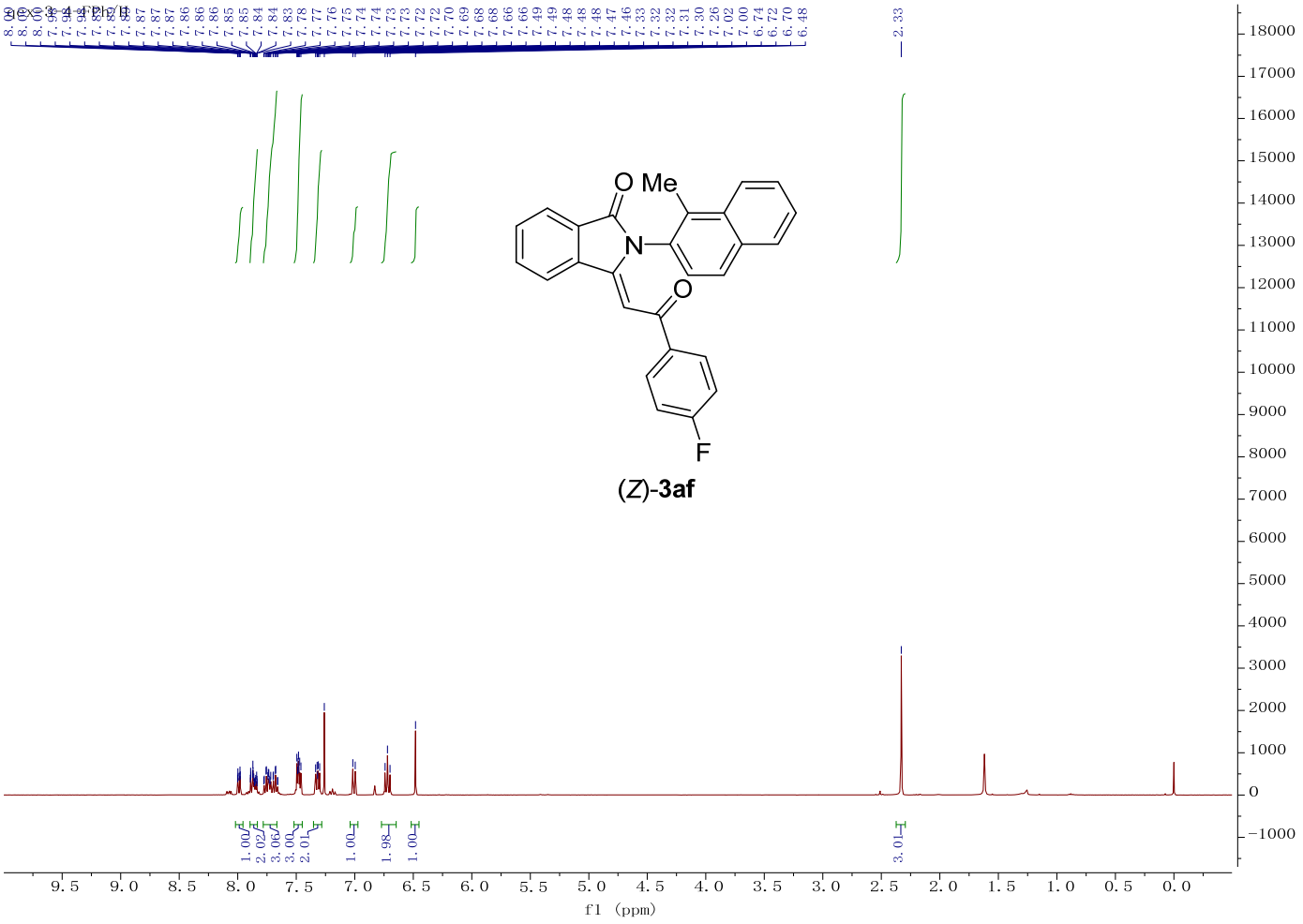

qcx-3-3-ClPh/C
O Me
N
O
Cl
(Z)-3ac
f1 (ppm)

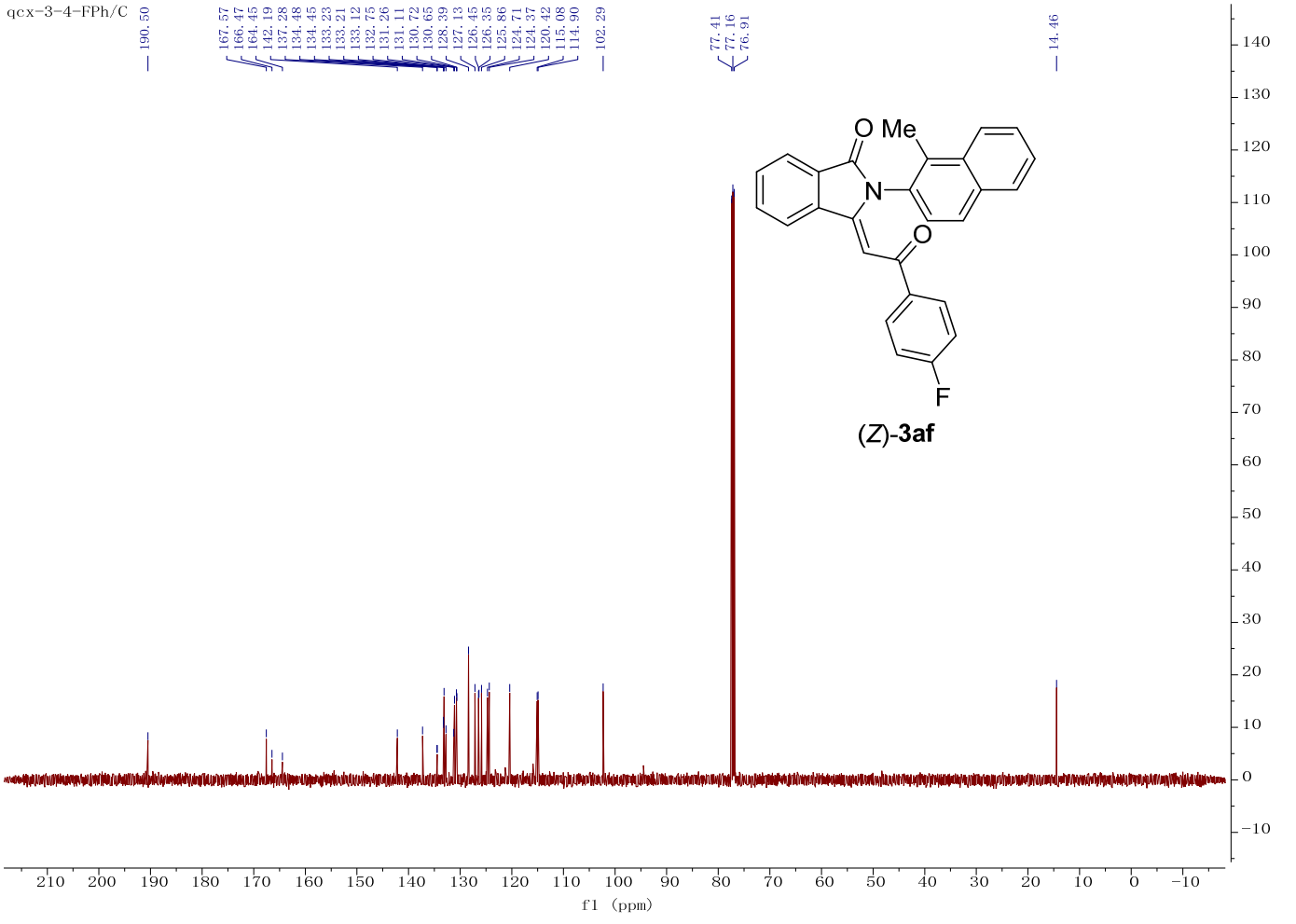

O Me
N
O
Me
(Z)-3ad
f1 (ppm)


O Me
N
O
Me
(Z)-3ad
f1 (ppm)

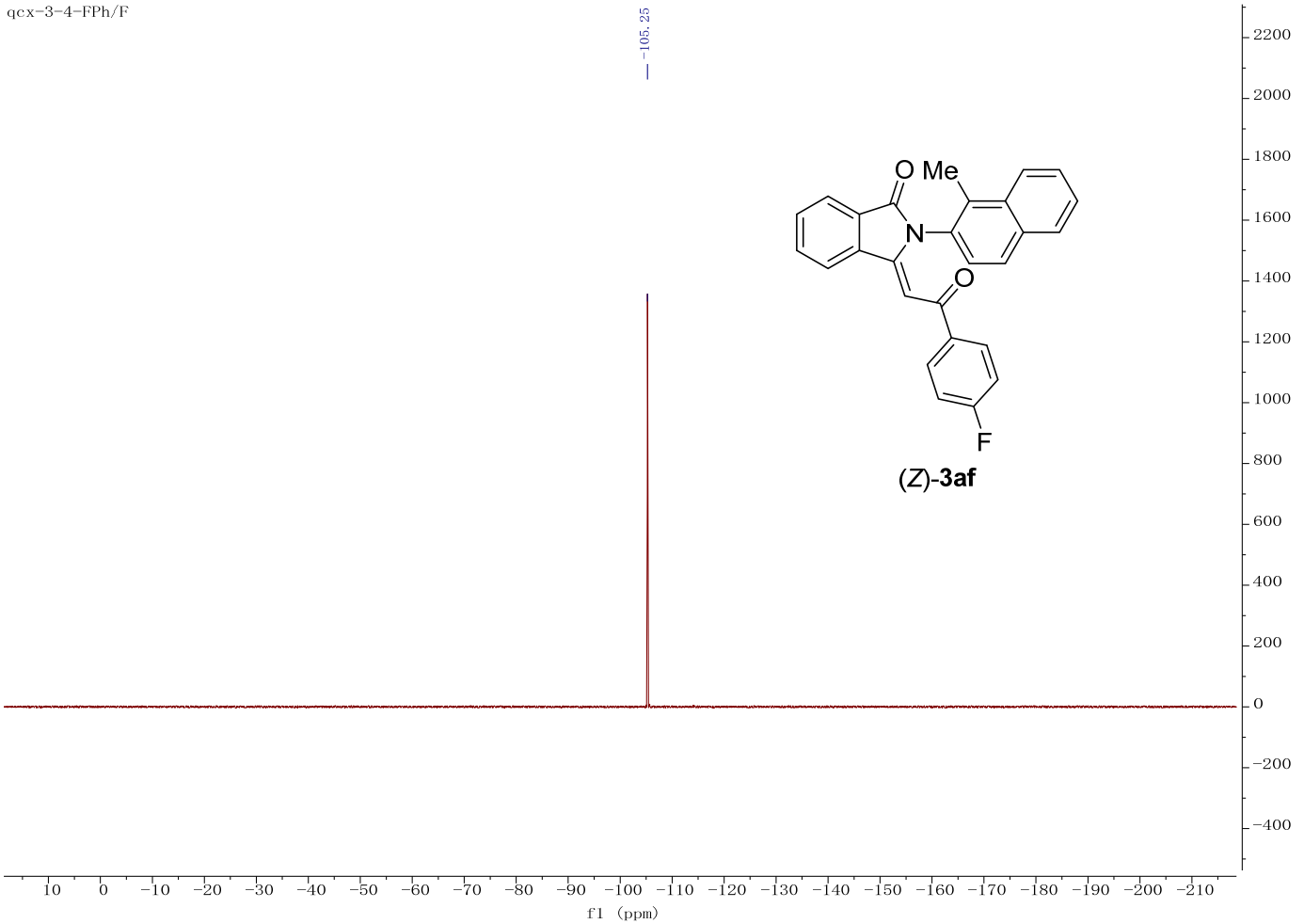

O Me
N
O
tBu
(Z)-3ae
2.29
1.24
f1 (ppm)


htt-1-104c.2.fid
O Me
N
O
tBu
(Z)-3ae
f1 (ppm)

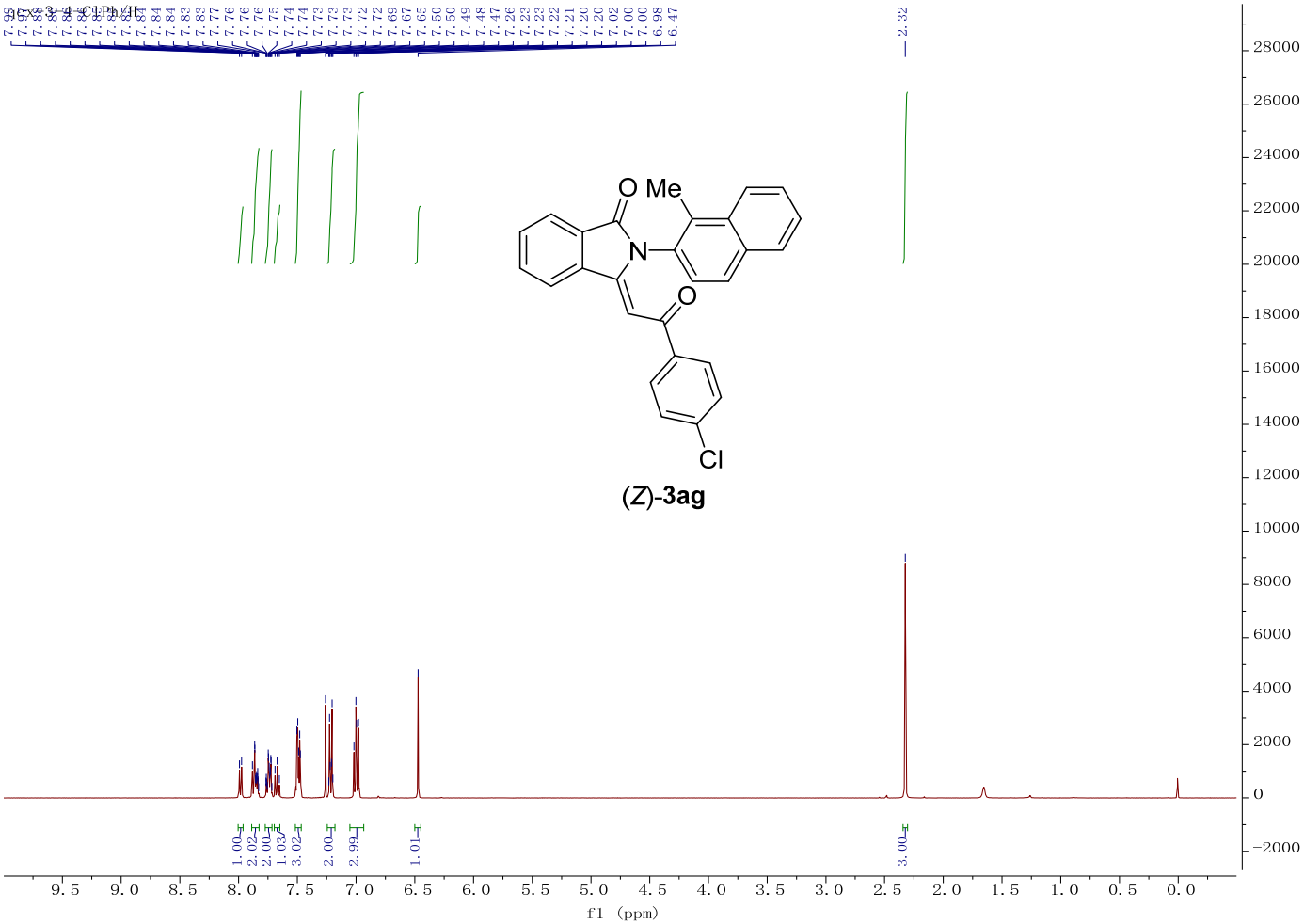

O Me
N
O
F
(Z)-3af
f1 (ppm)


qcx-3-4-FPh/C
O Me
N
O
F
(Z)-3af
f1 (ppm)

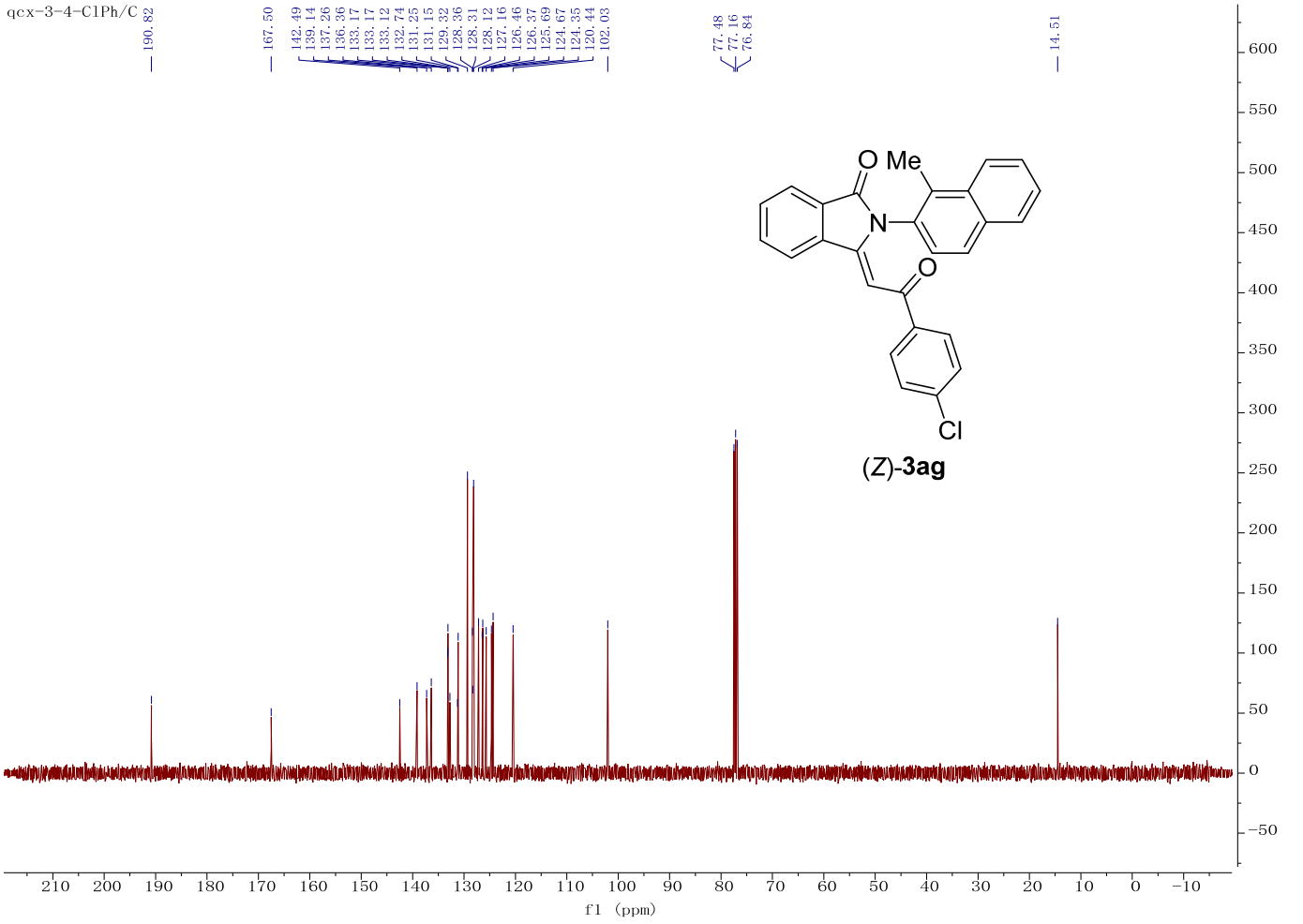
qcx-3-4-FPh/F



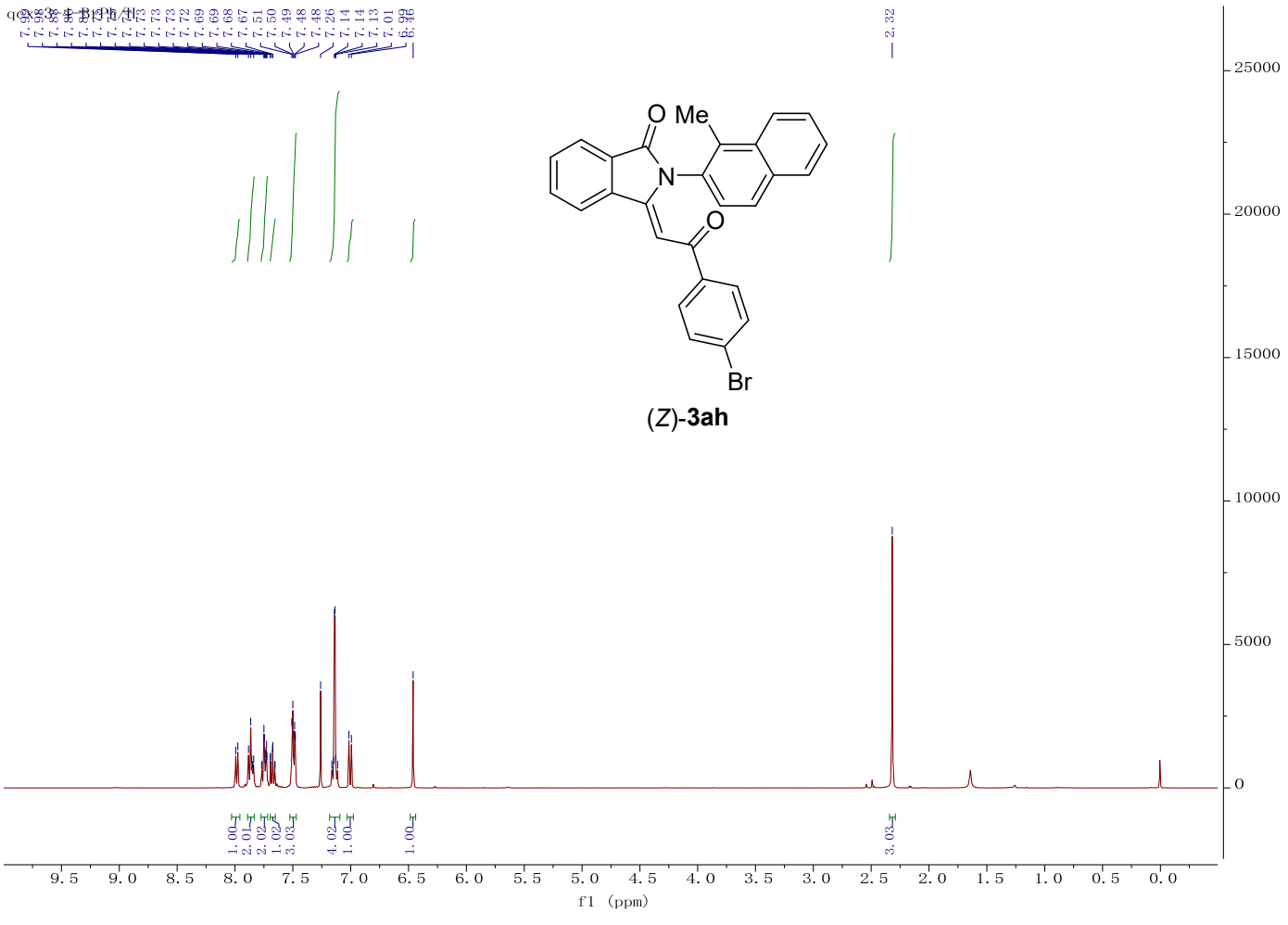
(*Z*)-**3af**



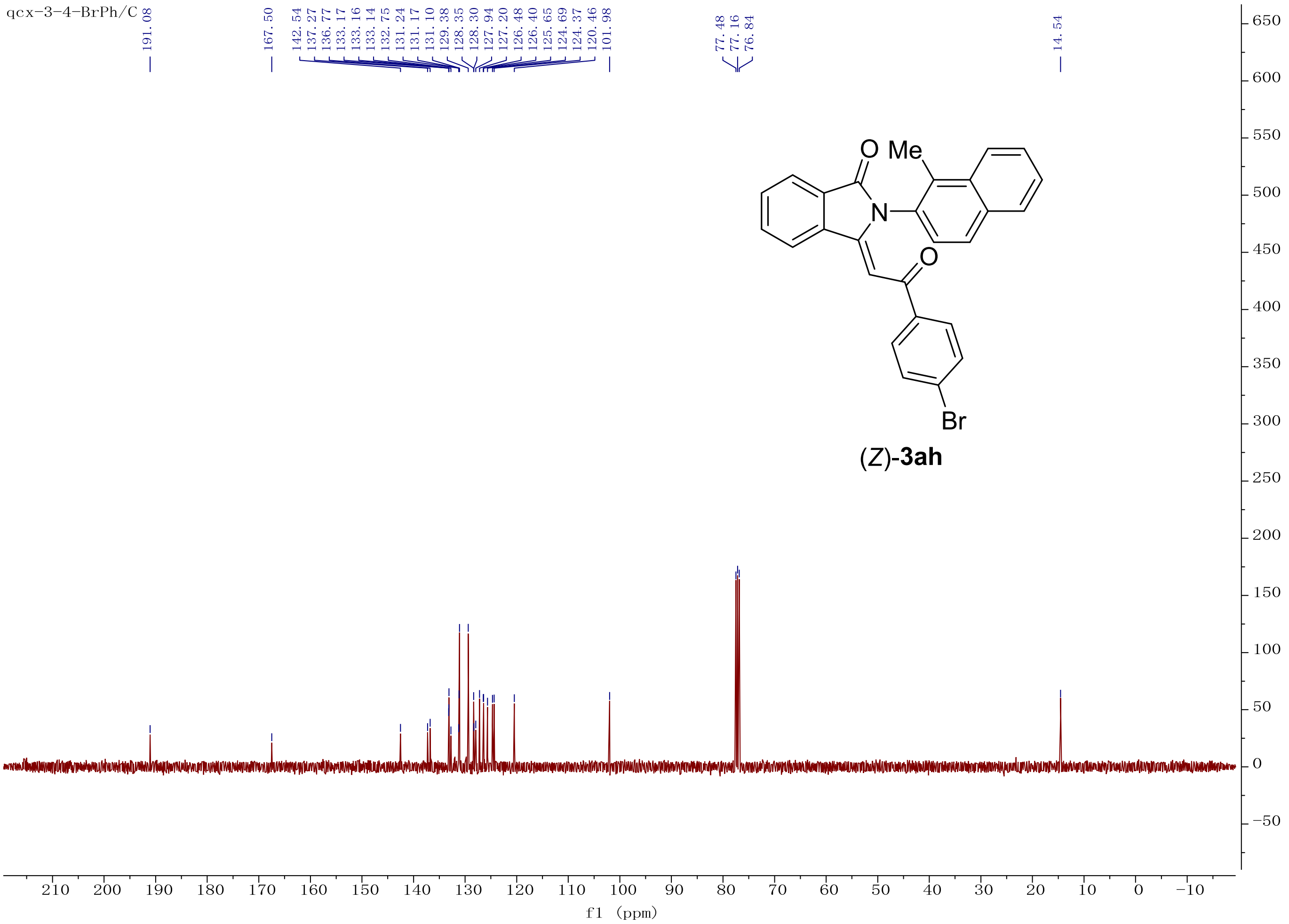
(*Z*)-**3ag**

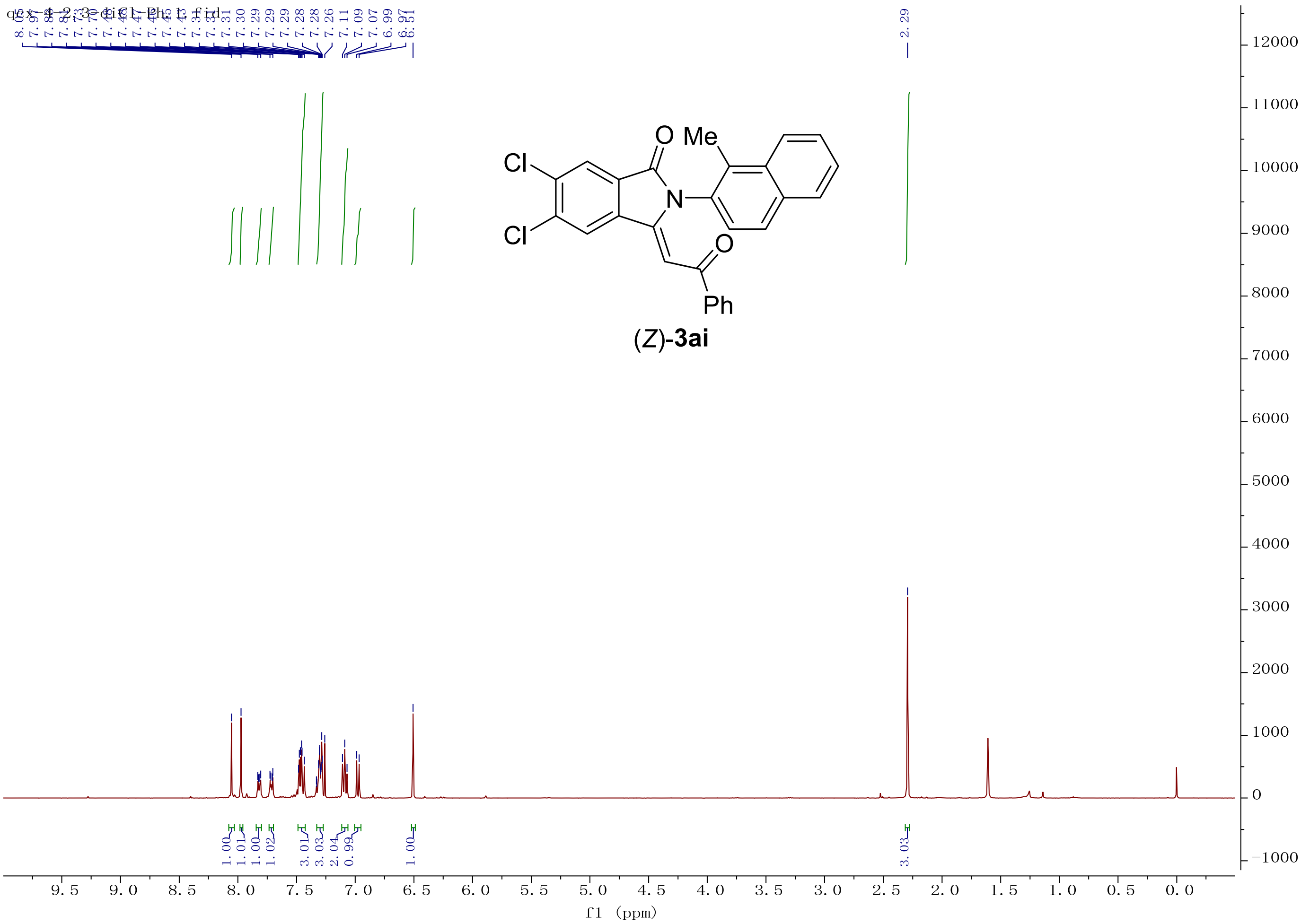

qcx-3-4-ClPh/C
190.82
167.50
142.49
139.14
137.26
136.36
133.17
133.12
132.74
131.25
131.15
129.32
128.36
128.31
128.12
127.16
126.46
126.37
125.69
124.67
124.35
120.44
102.03
77.48
77.16
76.84
14.51
O Me
N
O
Cl
f1 (ppm)

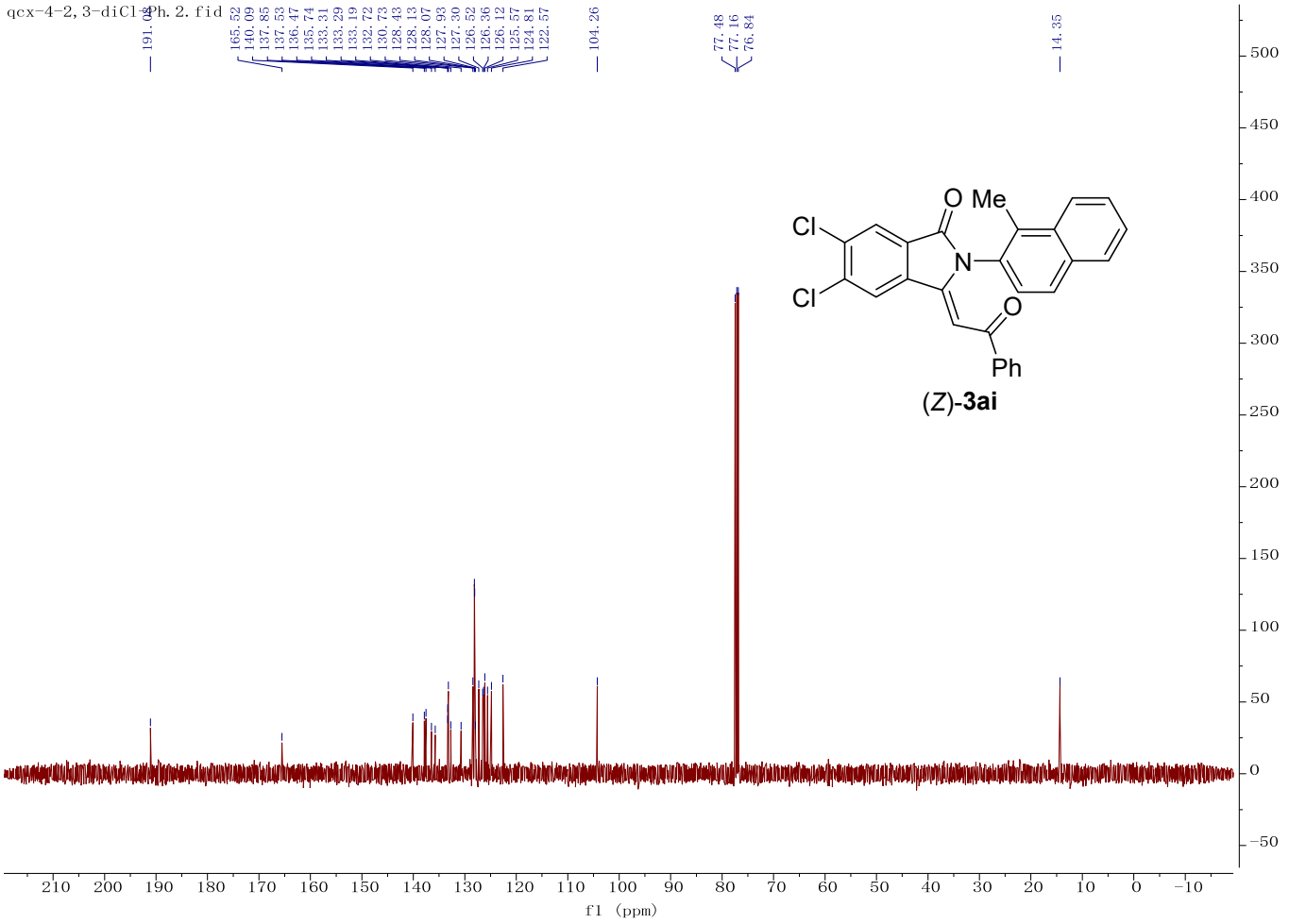
(*Z*)-**3ag**


2.32
O Me
N
O
Br
1.00
2.01
2.02
1.02
3.02
4.02
1.00
1.00
3.03
f1 (ppm)

(*Z*)-**3ah**


qcx-3-4-BrPh/C
191.08
167.50
142.54
137.27
136.77
133.17
133.16
133.14
132.75
131.24
131.17
131.10
129.38
128.35
128.30
127.94
127.20
126.48
126.40
125.65
124.69
124.37
120.46
101.98
77.48
77.16
76.84
14.54
O
Me
N
O
Br
(Z)-3ah
f1 (ppm)


7.11
7.09
7.07
6.99
6.97
6.51
2.29
Cl
Cl
O
Me
N
O
Ph
(Z)-3ai
1.00
1.01
1.00
1.02
3.01
3.03
2.04
0.99
1.00
3.03
f1 (ppm)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140.09
137.85
137.53
136.47
135.74
133.31
133.29
133.19
132.72
130.73
128.43
128.13
128.07
127.93
127.30
126.52
126.36
126.12
125.57
124.81
122.57
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77.16
76.84
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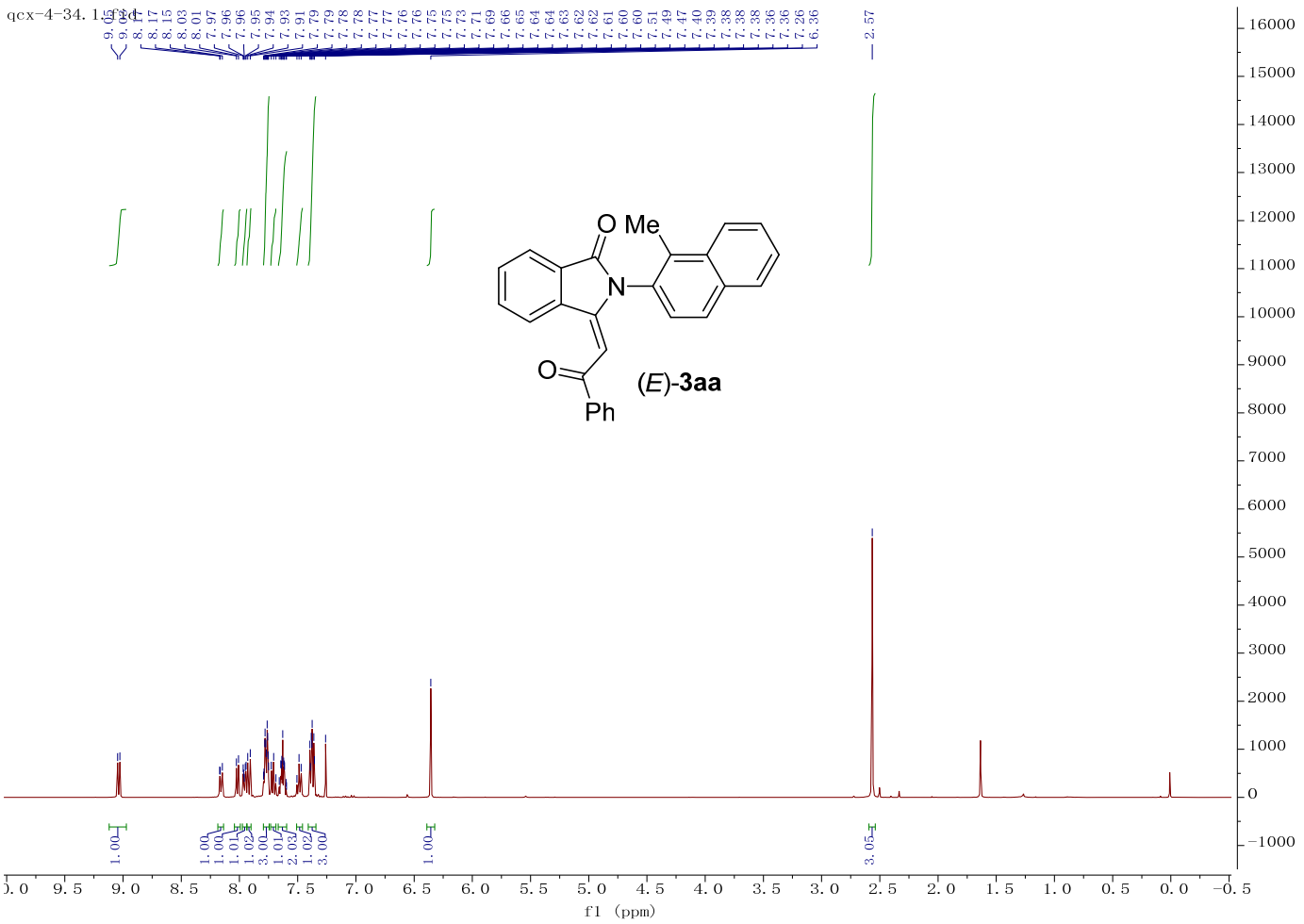
O
Me
Cl
Cl
N
O
Ph
(Z)-3ai
f1 (ppm)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7.63
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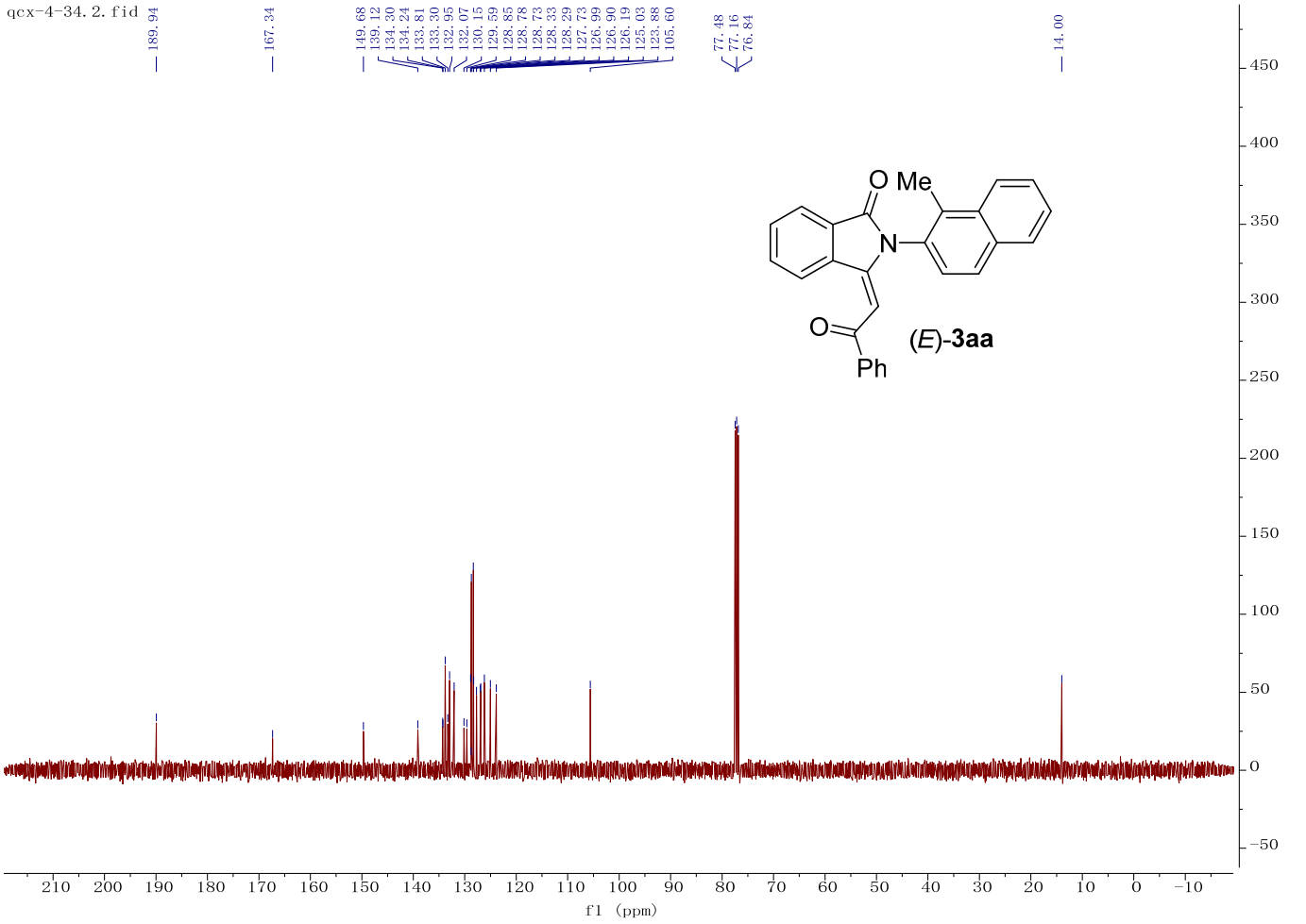
7.62
7.61
7.60
7.60
7.51
7.49
7.47
7.40
7.39
7.38
7.38
7.36
7.36
7.26
6.36
2.57
O
Me
N
O
Ph
(E)-3aa
1.00
1.00
1.00
1.01
1.02
3.00
1.01
2.03
1.02
3.00
1.00
3.05
f1 (ppm)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128.73
128.33
128.29
127.73
126.99
126.90
126.19
125.03
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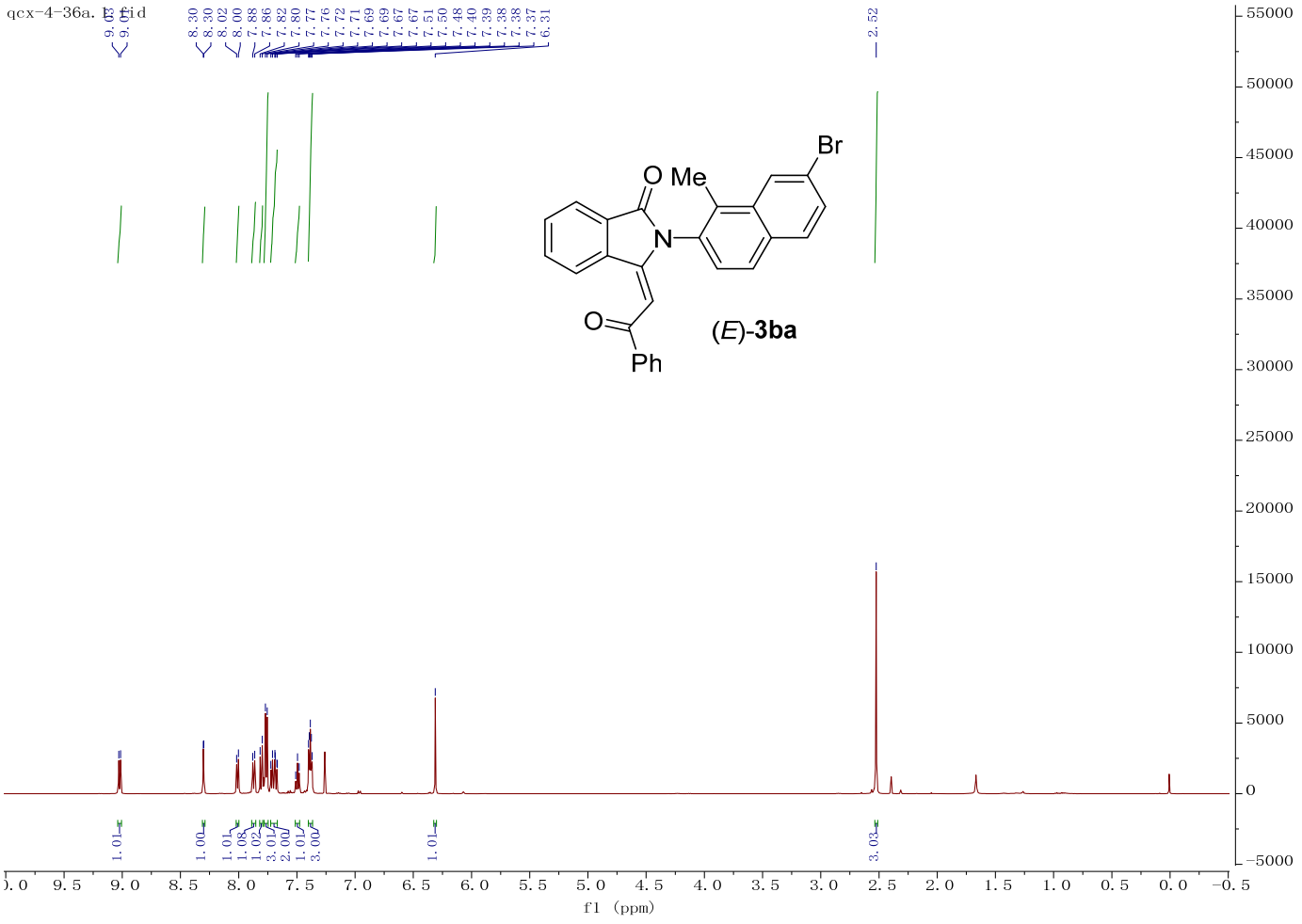
Ph
(E)-3aa
f1 (ppm)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8.30
8.02
8.00
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7.86
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7.80
7.77
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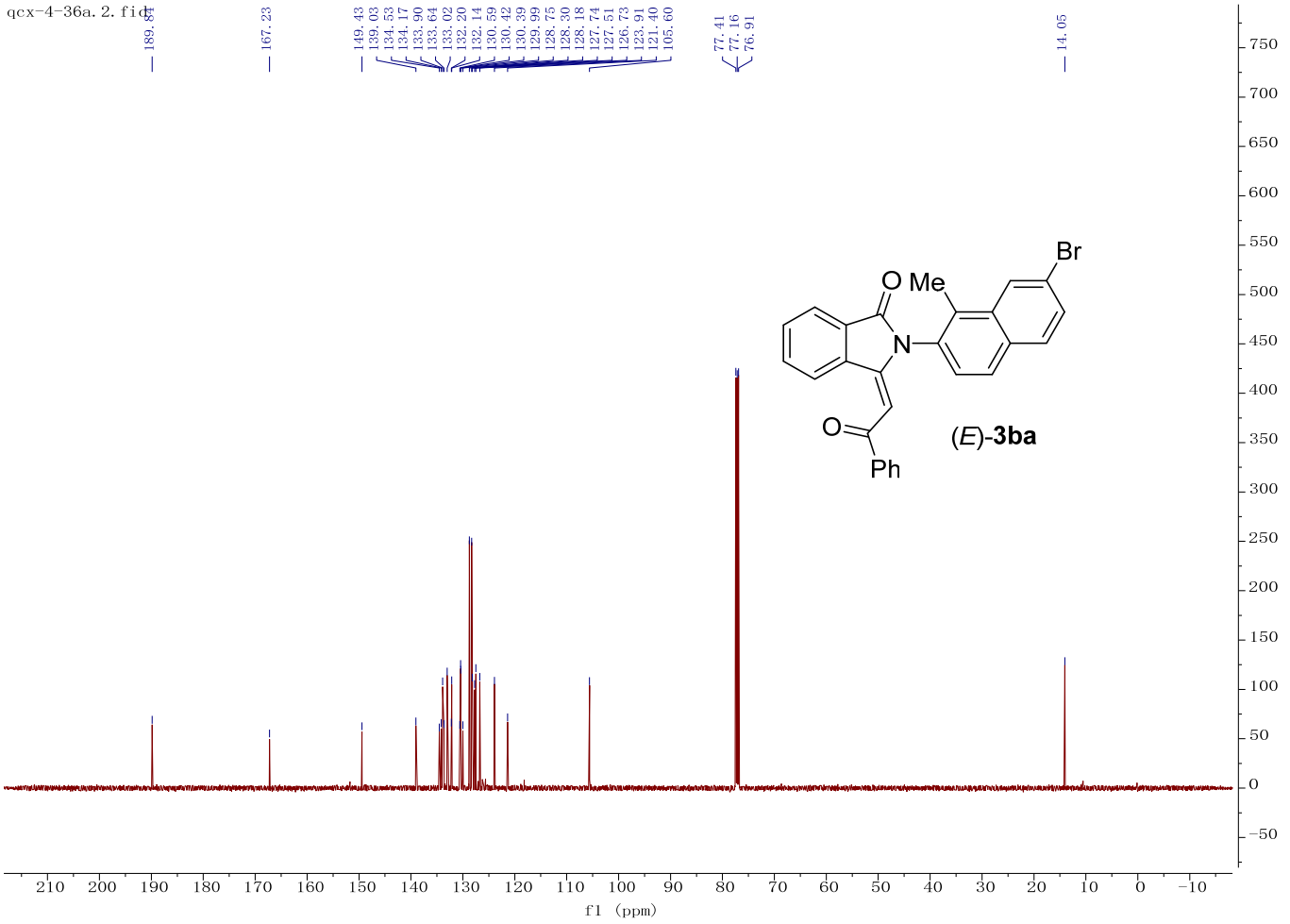
7.67
7.51
7.50
7.48
7.40
7.39
7.38
7.38
7.37
6.31
2.52
Br
O
Me
N
O
Ph
(E)-3ba
1.01
1.00
1.01
1.08
1.02
3.01
2.00
1.01
3.00
1.01
3.03
f1 (ppm)

qcx-4-36a.2.fid



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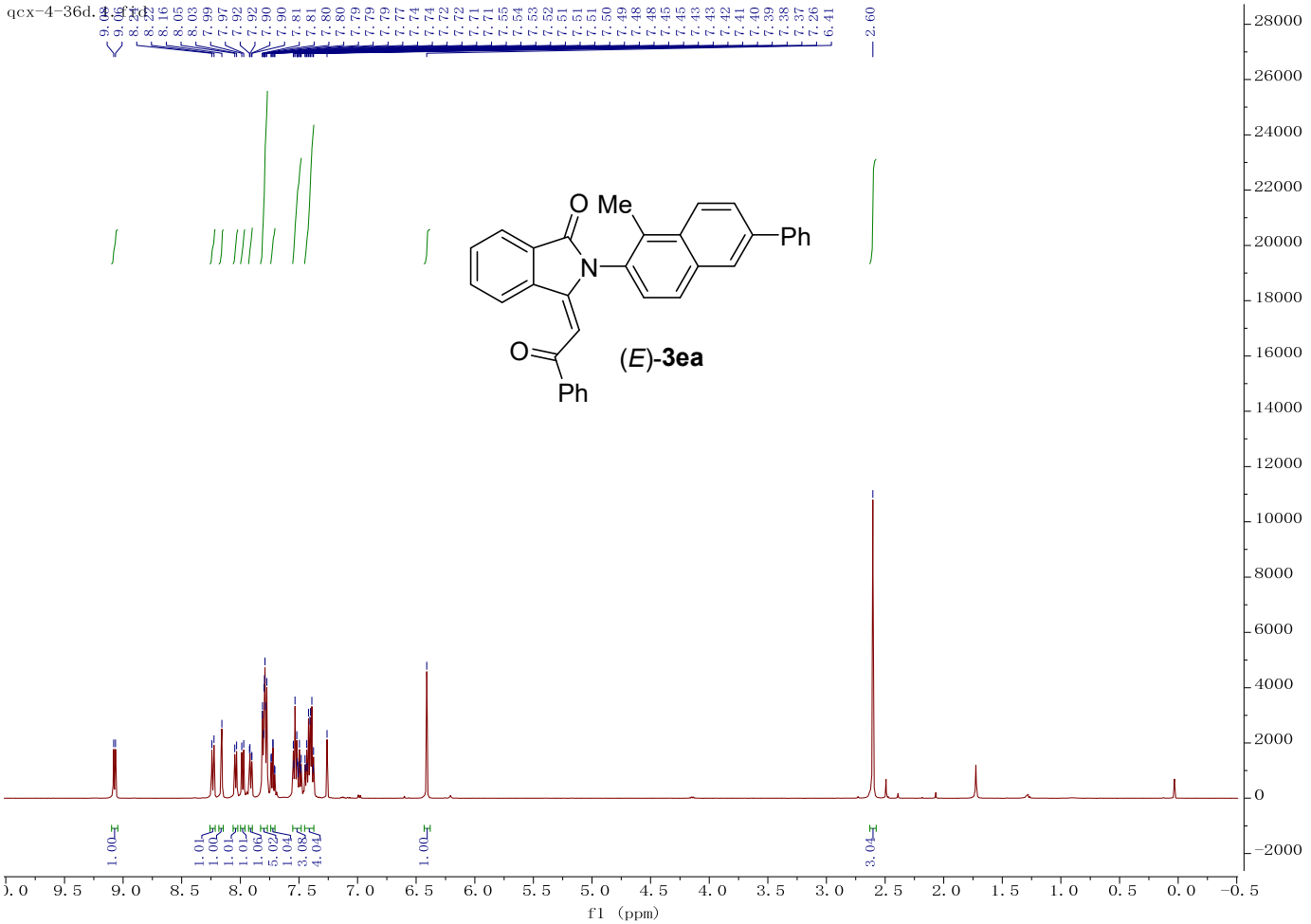

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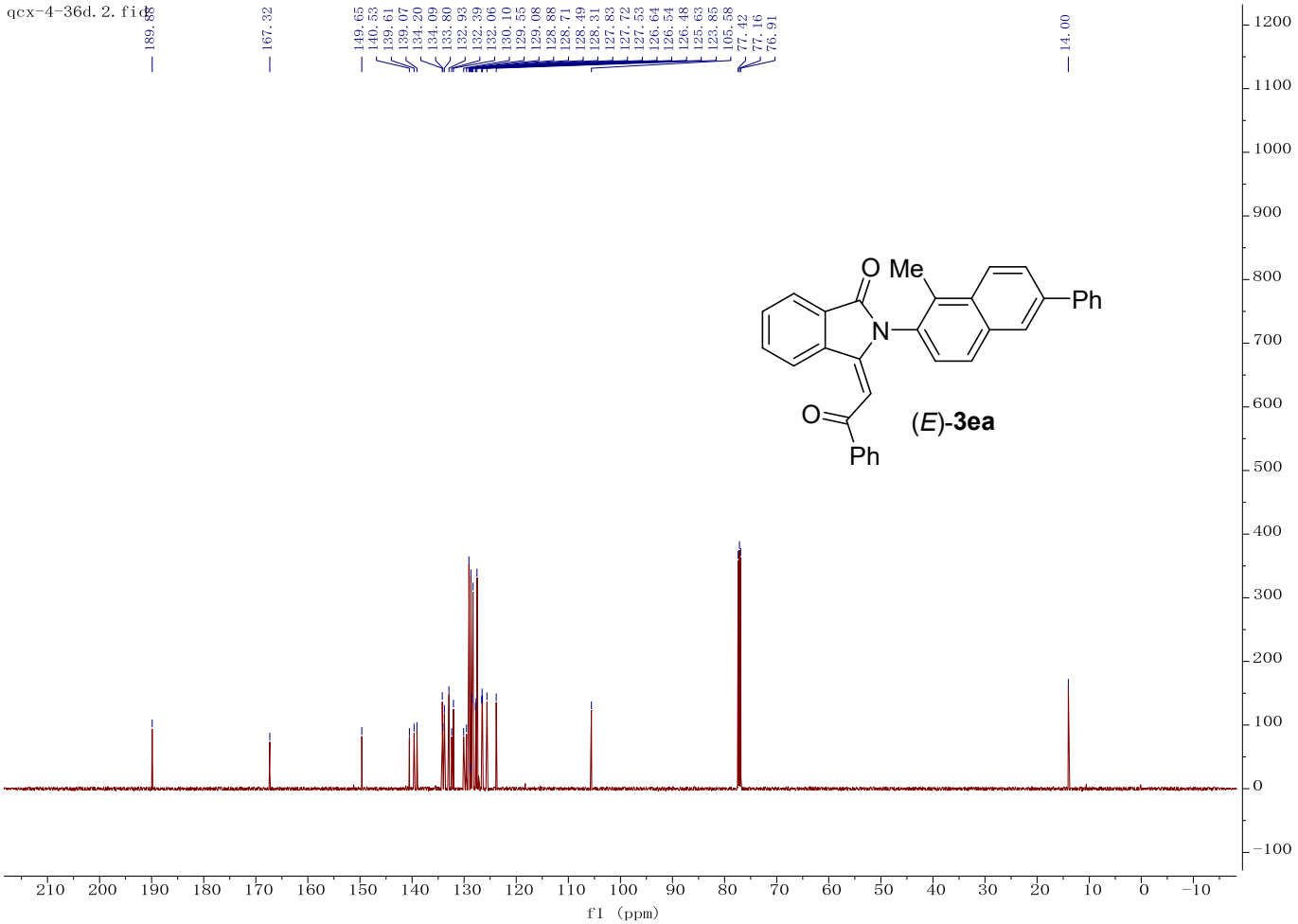

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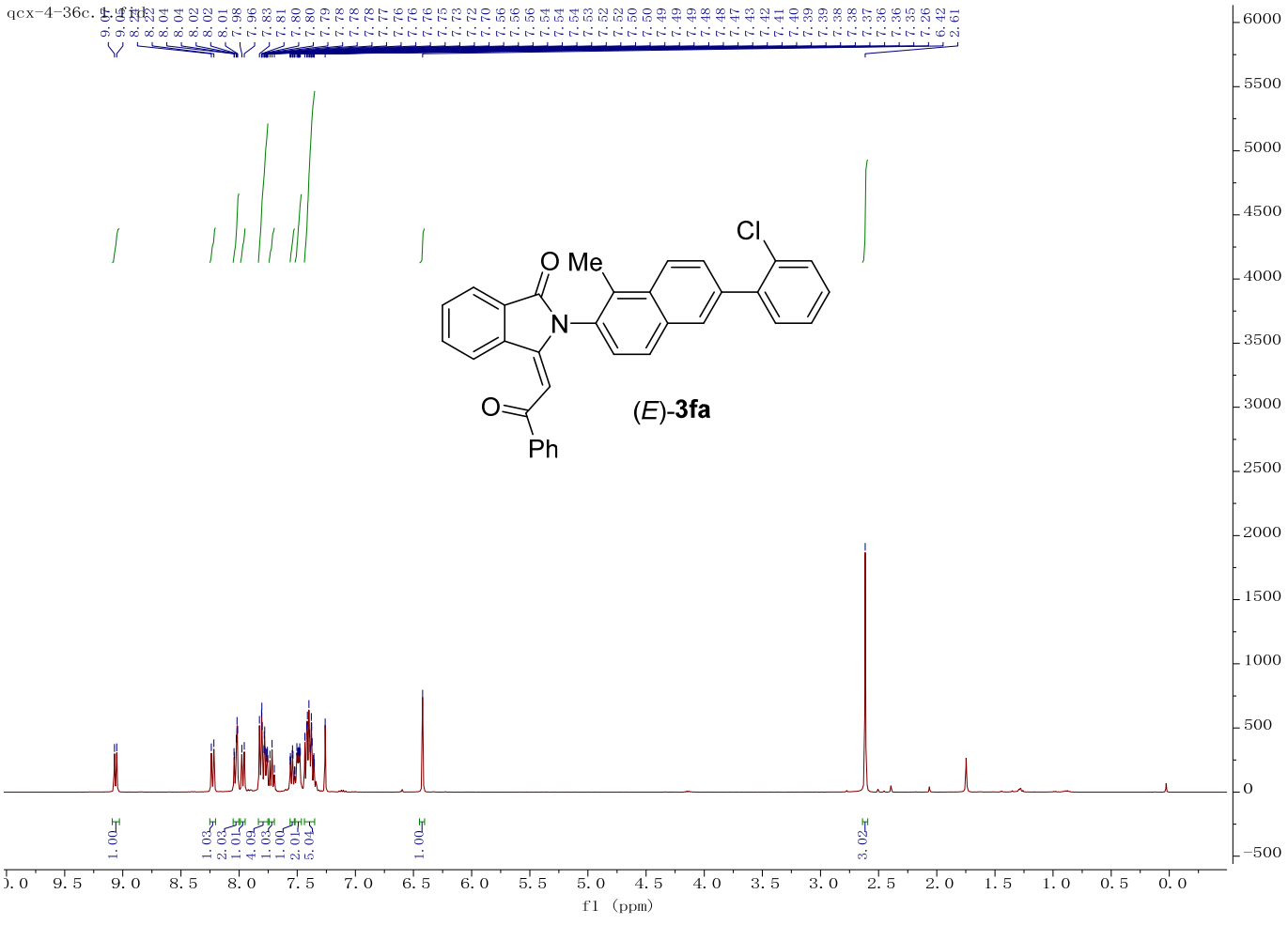

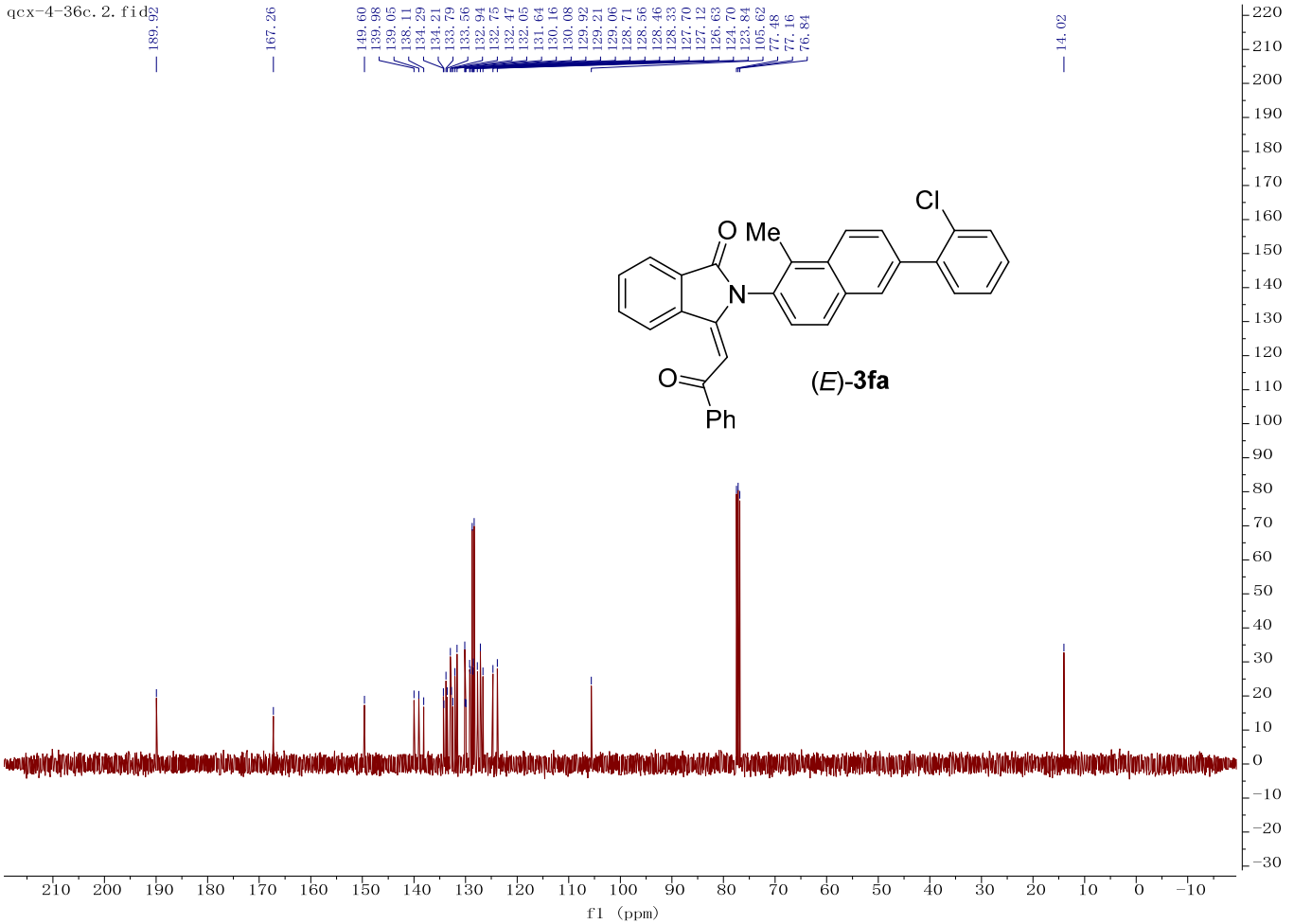
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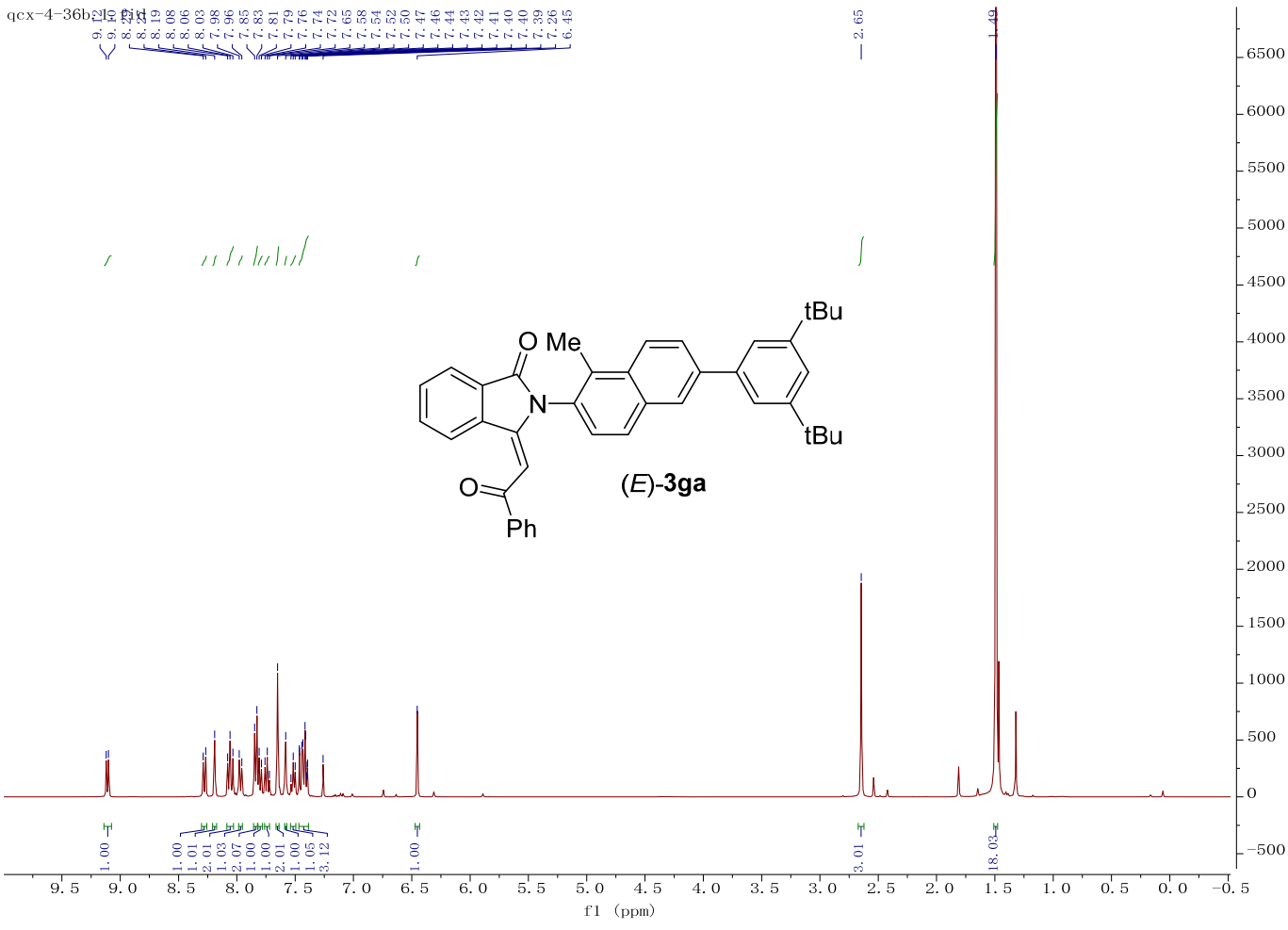
138.11
134.29
134.21
133.79
133.56
132.94
132.75
132.47
132.05
131.64
130.16
130.08
129.92
129.21
129.06
128.71
128.56
128.46
128.33
127.70
127.12
126.63
124.70
123.84
105.62
77.48
77.16
76.84
14.02
Cl
O
Me
N
O
Ph
(E)-3fa
f1 (ppm)


qcx-4-36b.2.fid
2.65
1.49
tBu
tBu
O
Me
N
O
Ph
(E)-3ga
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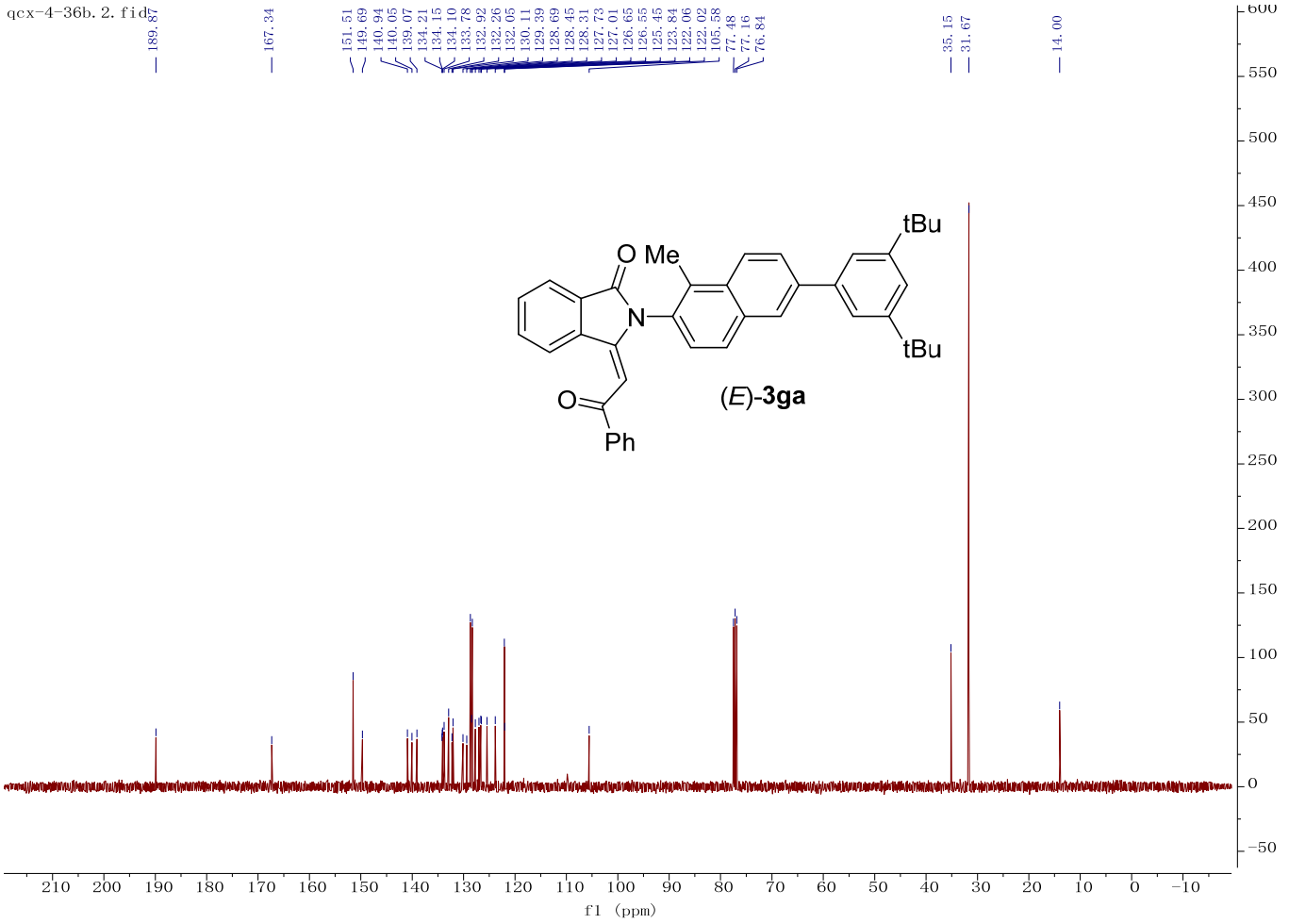
1.00
1.01
2.01
1.03
2.07
1.00
1.00
2.01
1.00
1.05
3.12
1.00
3.01
18.03
f1 (ppm)

qcx-4-36b.2.fid



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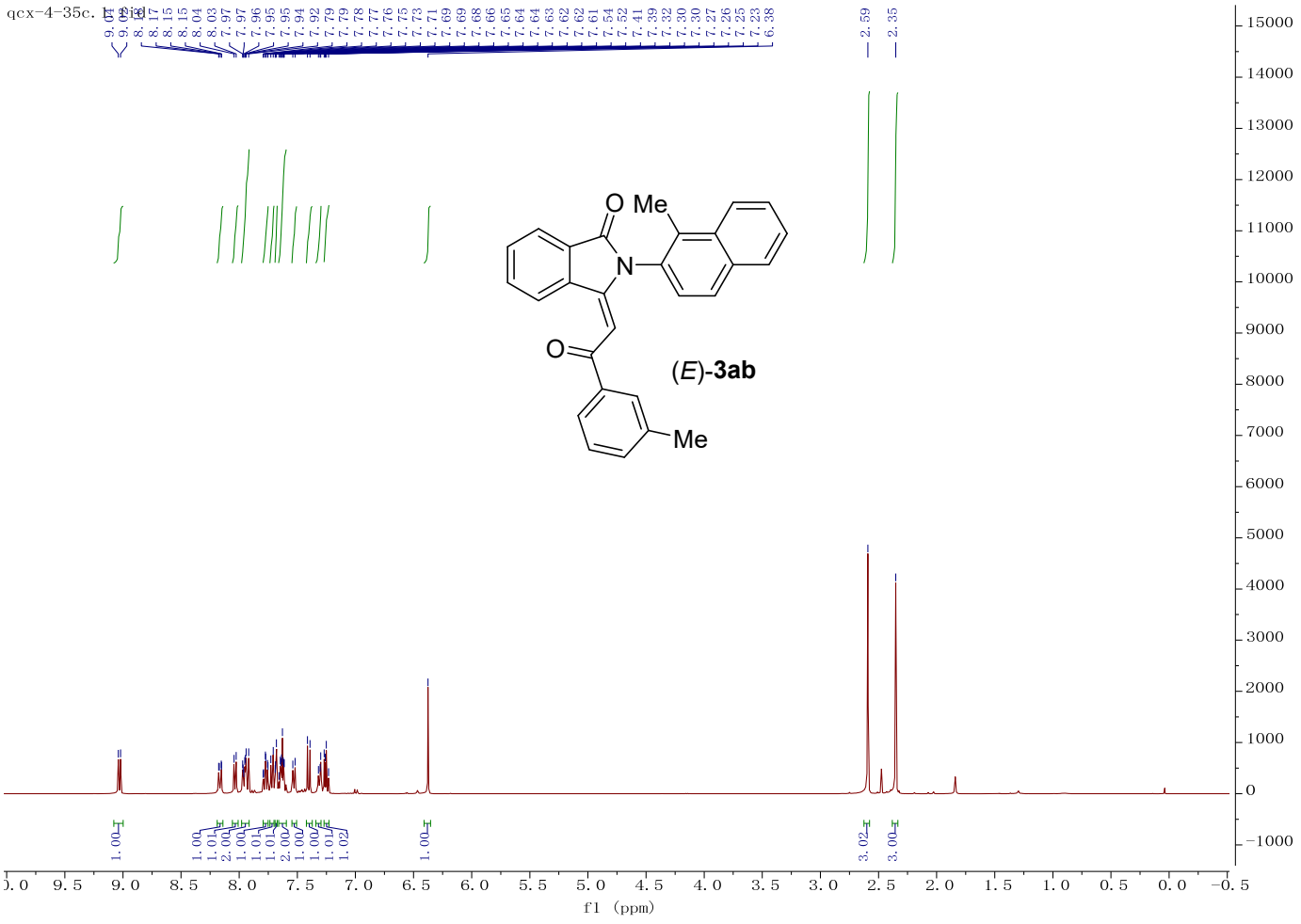

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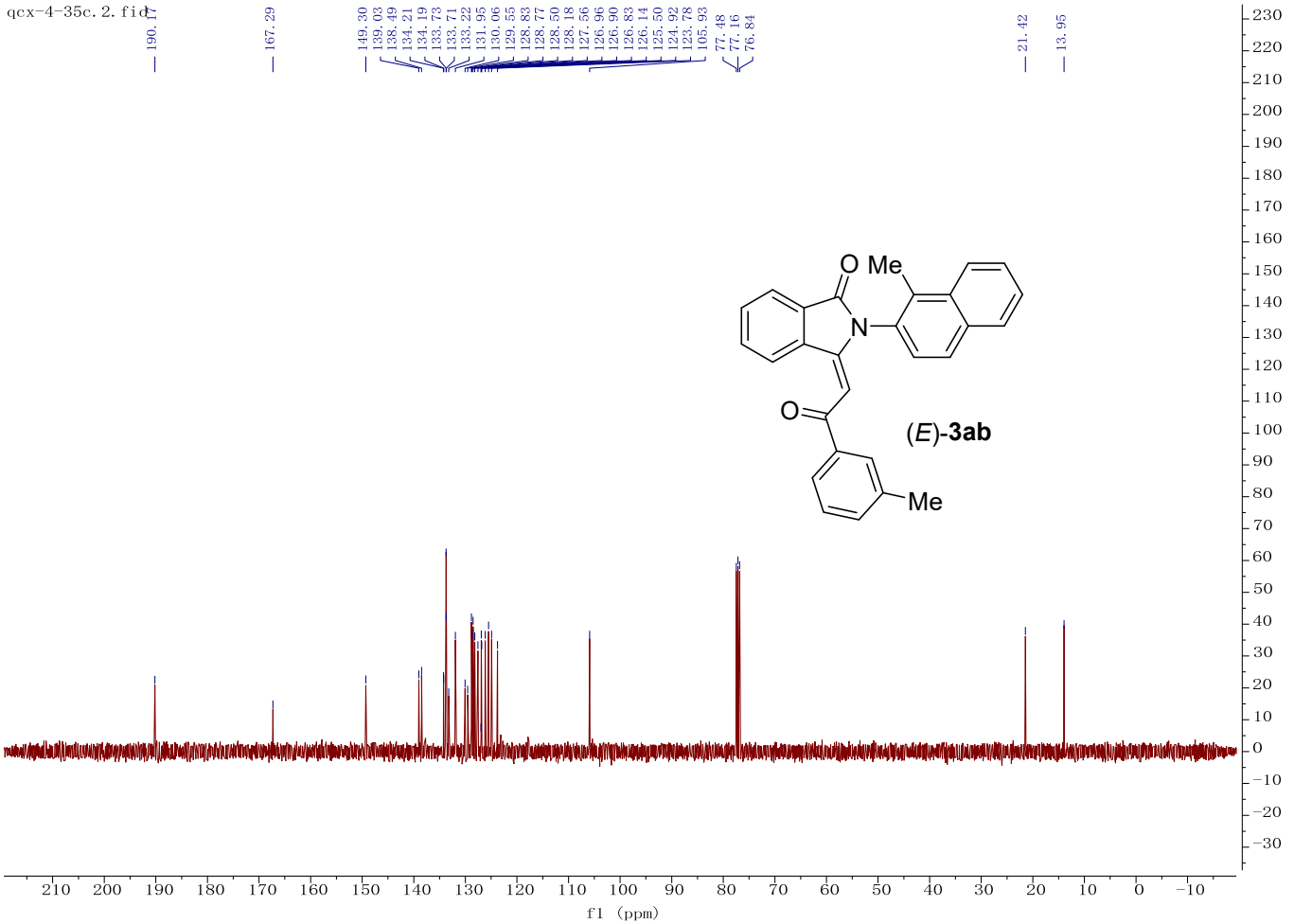
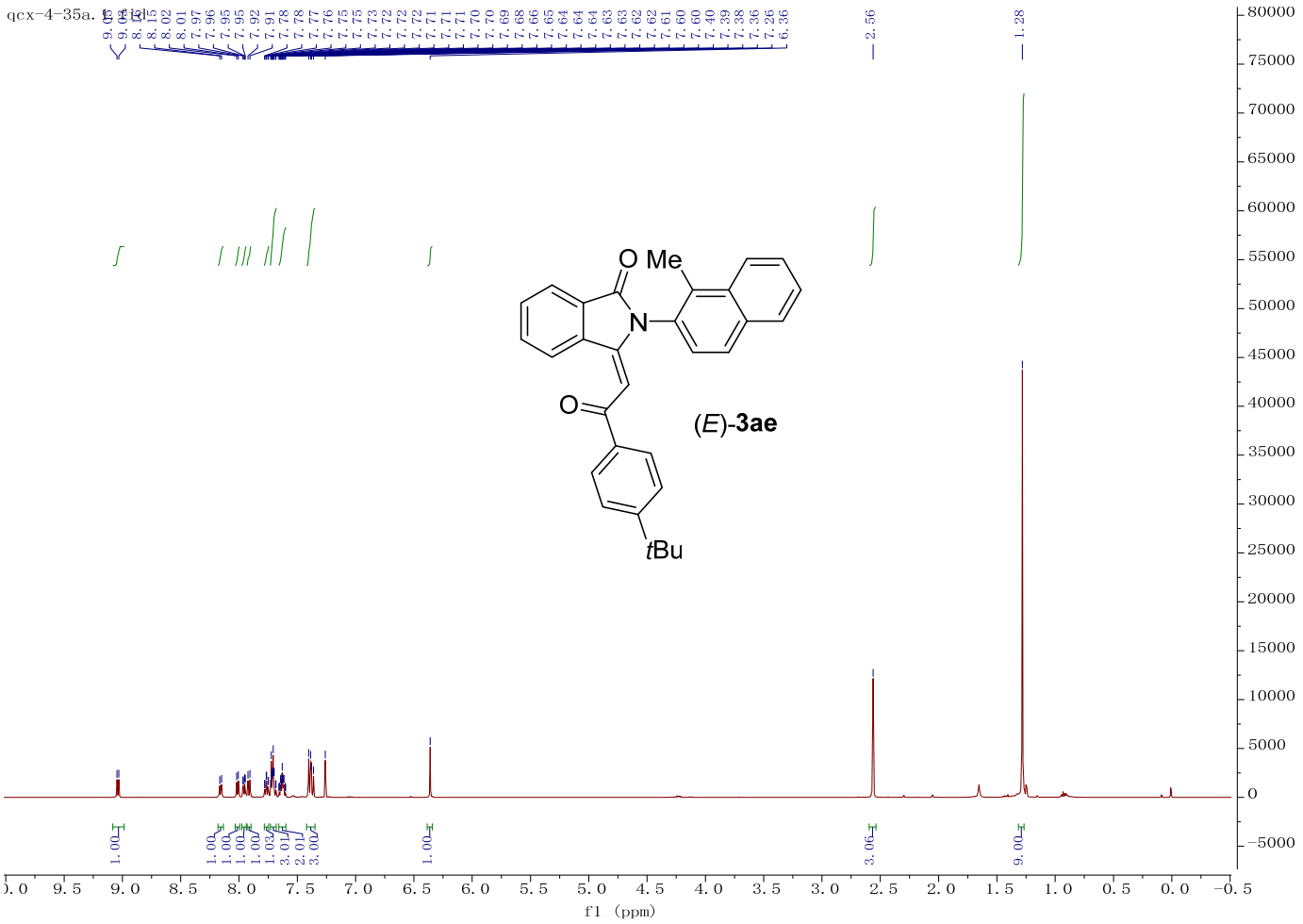
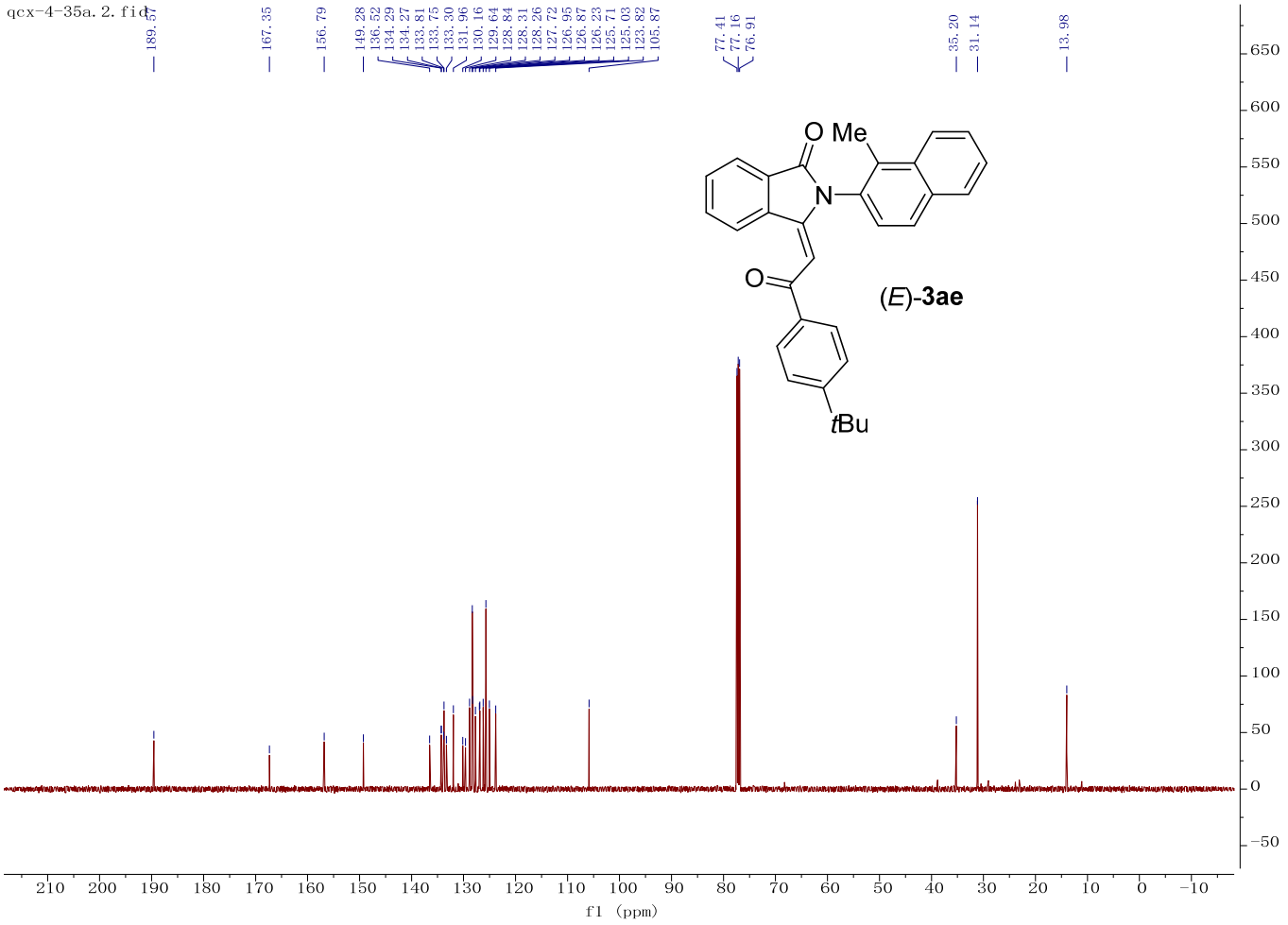


qcx-4-35a.




qcx-4-35a.2.fid
189.57
167.35
156.79
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136.52
134.29
134.27
133.81
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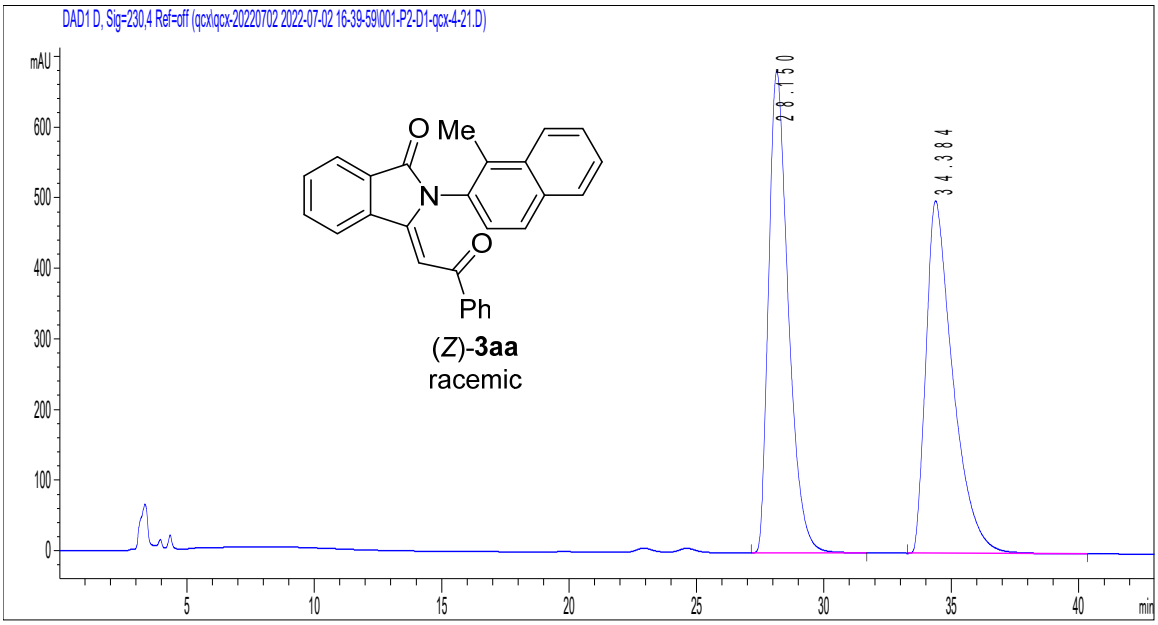
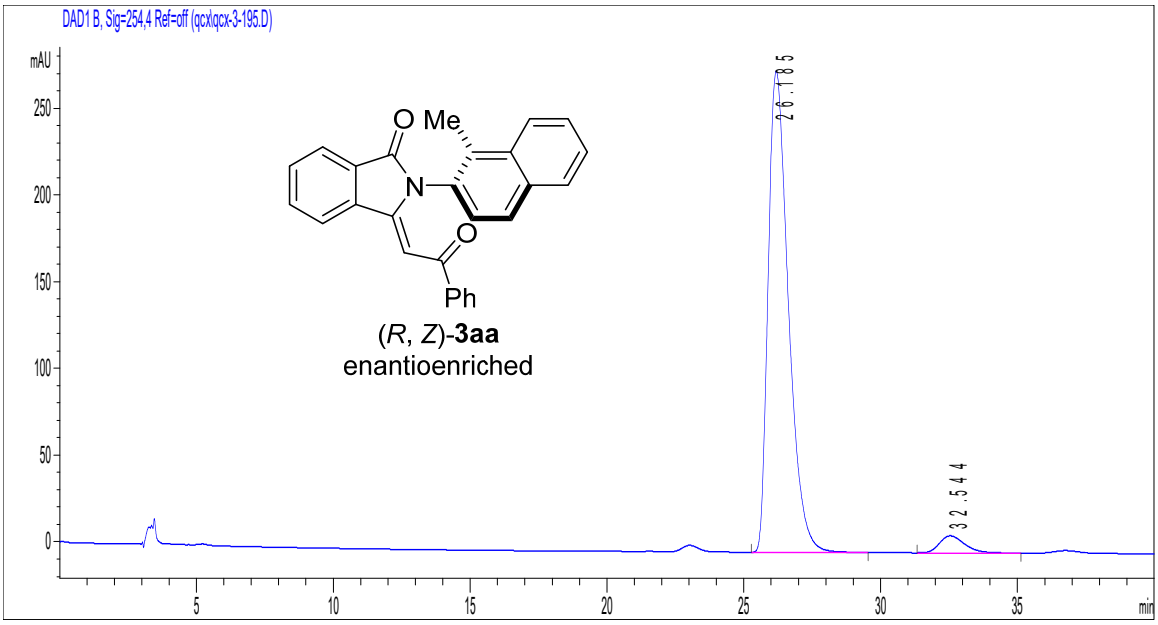
133.30
131.96
130.16
129.64
128.84
128.31
128.26
127.72
126.95
126.87
126.23
125.71
125.03
123.82
105.87
77.41
77.16
76.91
35.20
31.14
13.98
O
Me
N
O
(E)-3ae
tBu
650
600
550
500
450
400
350
300
250
200
150
100
50
0
−50
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

3aa

Daicel CHIRALPAK IE-3 column; 30% *i*-PrOH in hexanes; 1.0 mL/min.



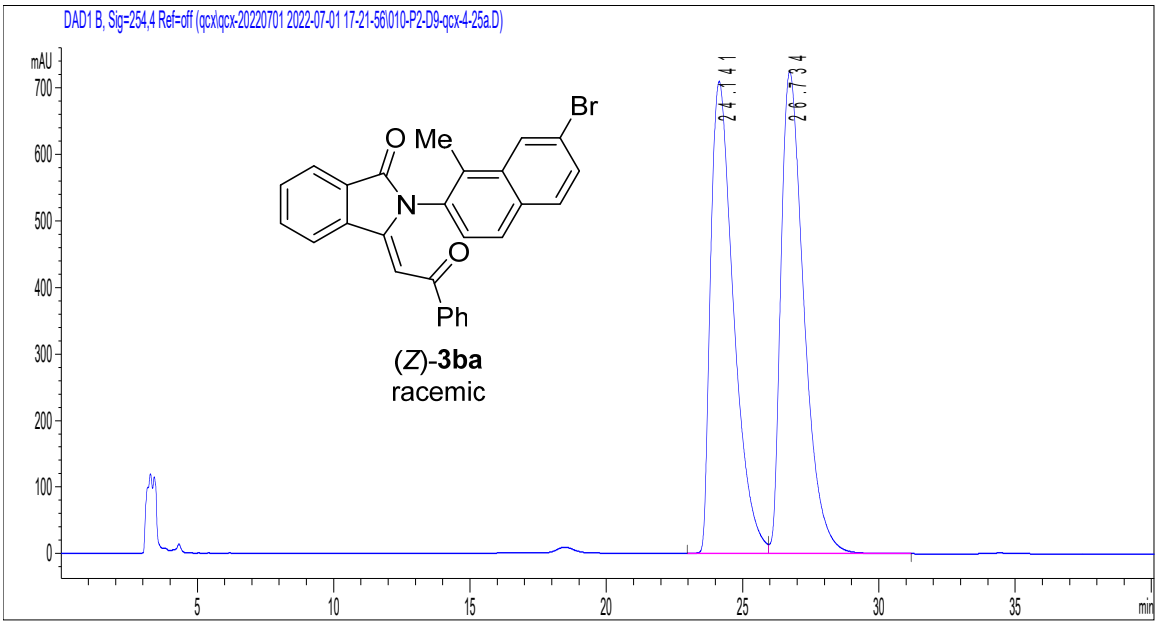
#	Time	Type	Area	Height	Width	Area%	Symmetry
1	28.15	BB	36636.6	681.7	0.815	49.963	0.65
2	34.384	BB	36690.1	499.2	1.0674	50.037	0.515



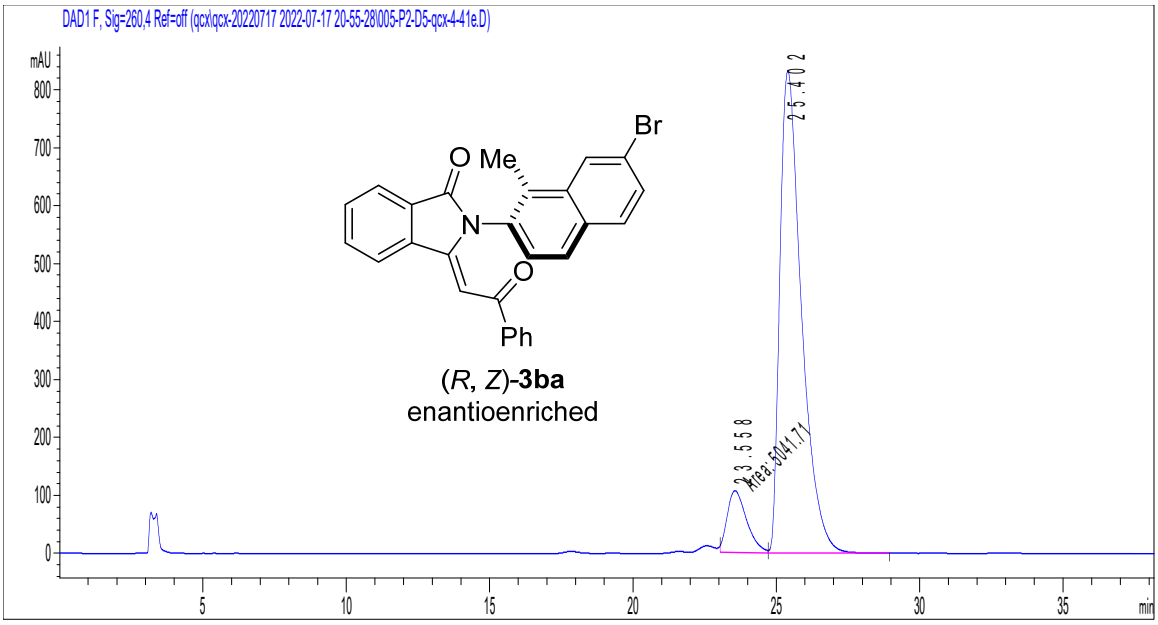
#	Time	Type	Area	Height	Width	Area%	Symmetry
1	26.185	BB	14261.6	277.6	0.7895	95.726	0.609
2	32.544	BB	636.7	9.9	0.9094	4.274	0.704

3ba

Daicel CHIRALPAK IE-3 column; 30% *i*-PrOH in hexanes; 1.0 mL/min.



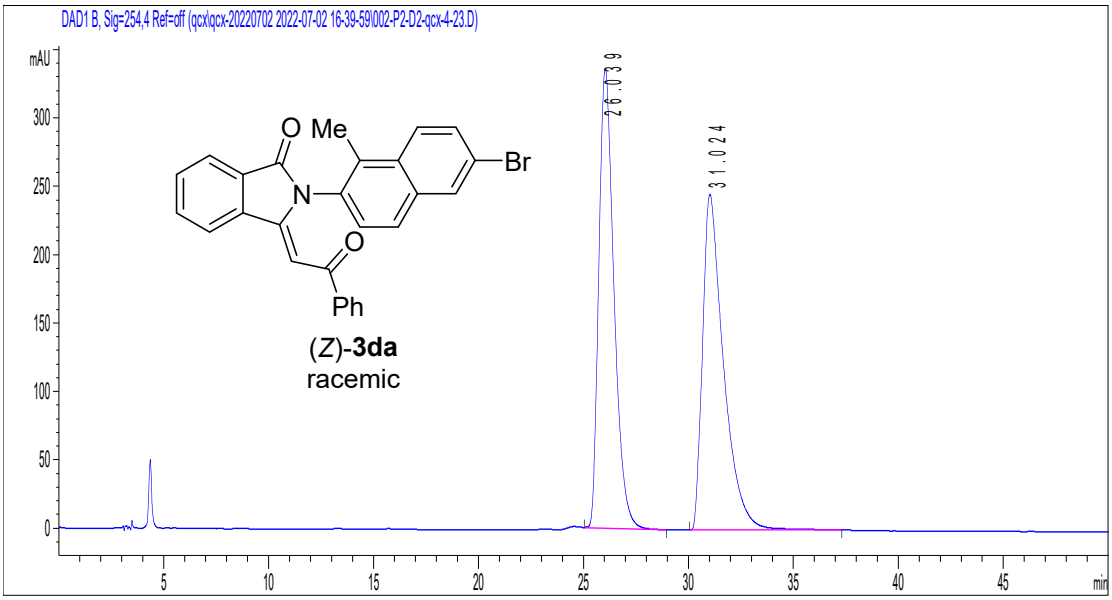
#	Time	Type	Area	Height	Width	Area%	Symmetry
1	24.141	BV	41718.3	709.4	0.9061	49.412	0.535
2	26.734	VB	42711.2	724.1	0.9101	50.588	0.576



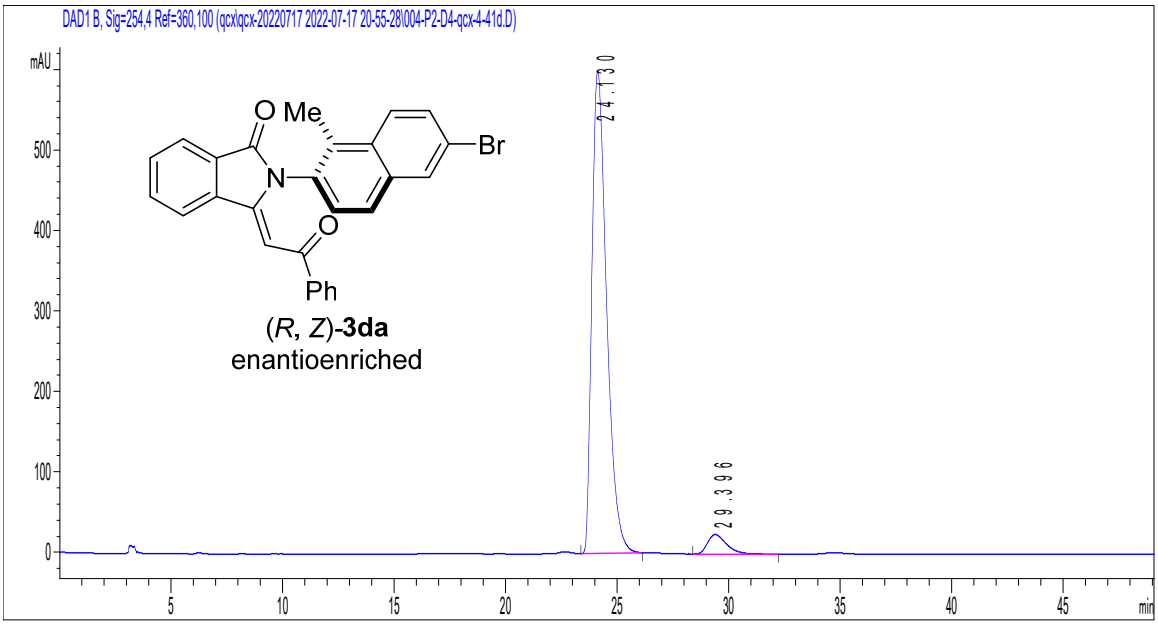
#	Time	Type	Area	Height	Width	Area%	Symmetry
1	23.558	FM	5041.7	106.7	0.7873	10.370	0.651
2	25.402	VB	43576.7	832.1	0.789	89.630	0.533

3da

Daicel CHIRALPAK IE-3 column; 30% *i*-PrOH in hexanes; 1.0 mL/min.



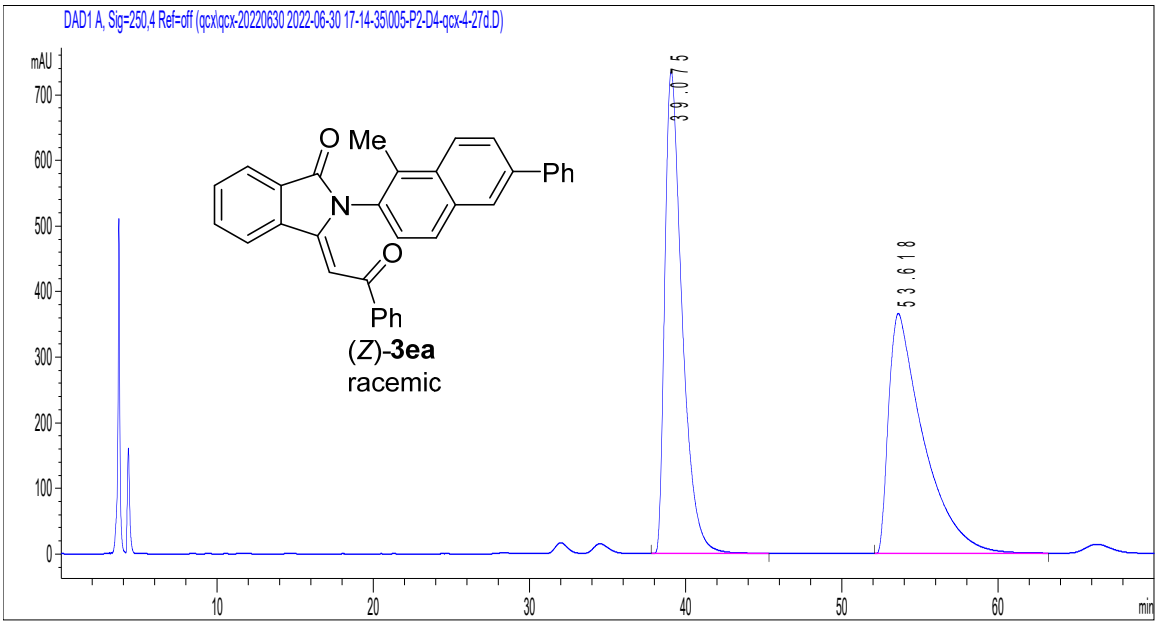
#	Time	Type	Area	Height	Width	Area%	Symmetry
1	26.039	BB	16856	335.7	0.7678	49.673	0.681
2	31.024	BB	17077.7	245.5	0.9994	50.327	0.489



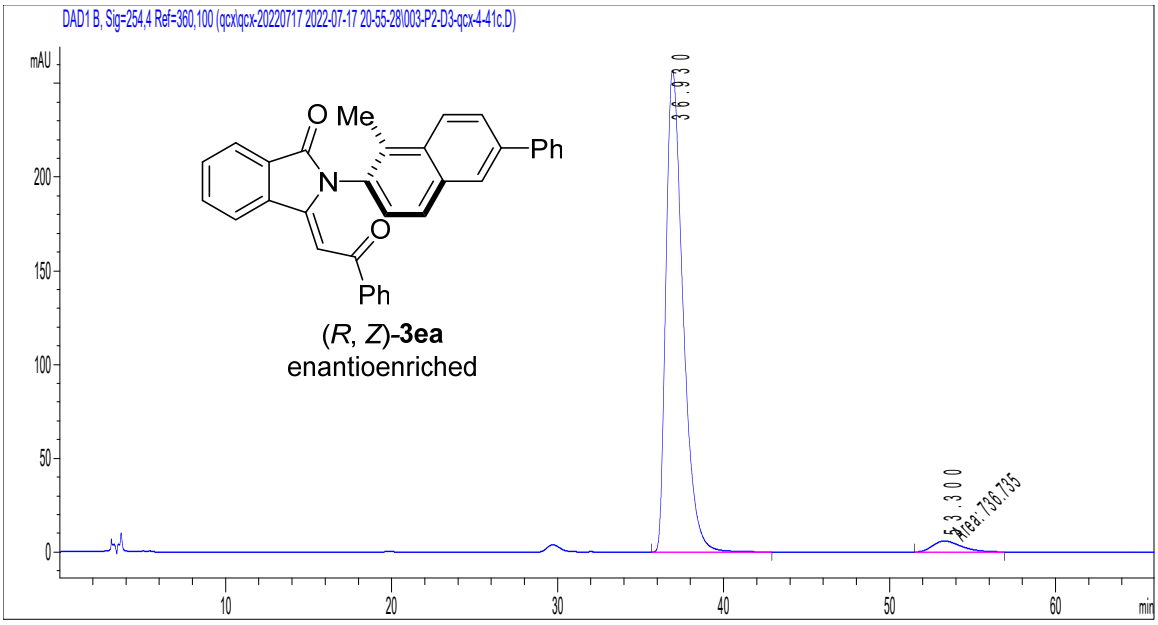
#	Time	Type	Area	Height	Width	Area%	Symmetry
1	24.13	BB	27354.5	599	0.7048	95.080	0.609
2	29.396	BB	1415.5	24	0.8813	4.920	0.632

3ea

Daicel CHIRALPAK IE-3 column; 30% *i*-PrOH in hexanes; 1.0 mL/min.



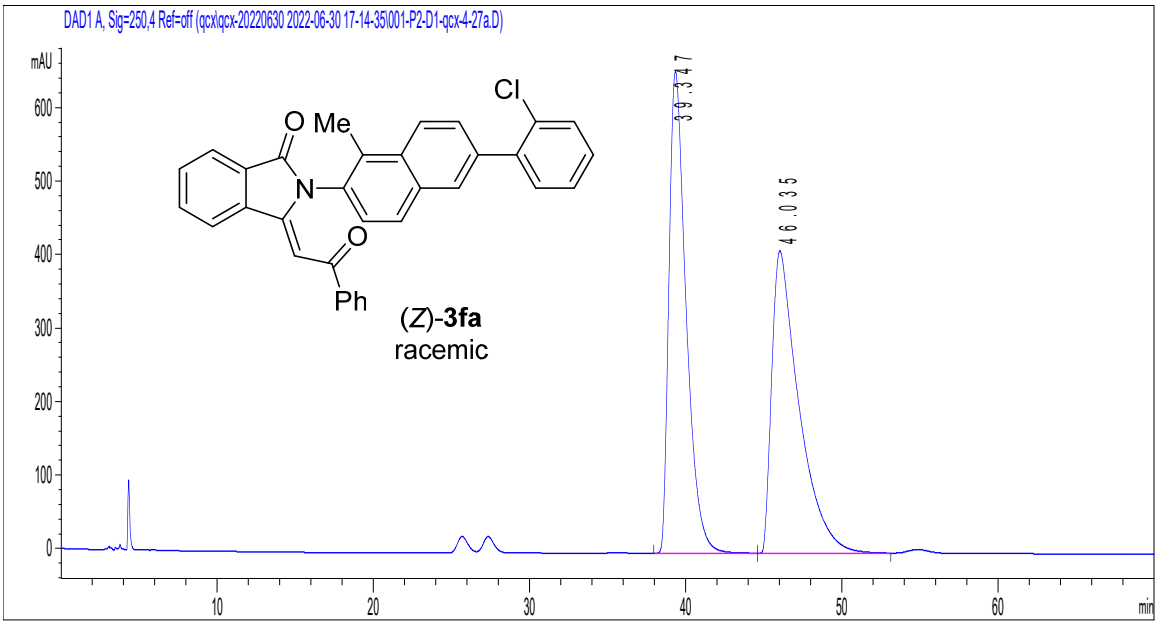
#	Time	Type	Area	Height	Width	Area%	Symmetry
1	39.075	BB	56741.8	734.9	1.1628	50.067	0.535
2	53.618	BB	56589.3	366.3	2.1924	49.933	0.352



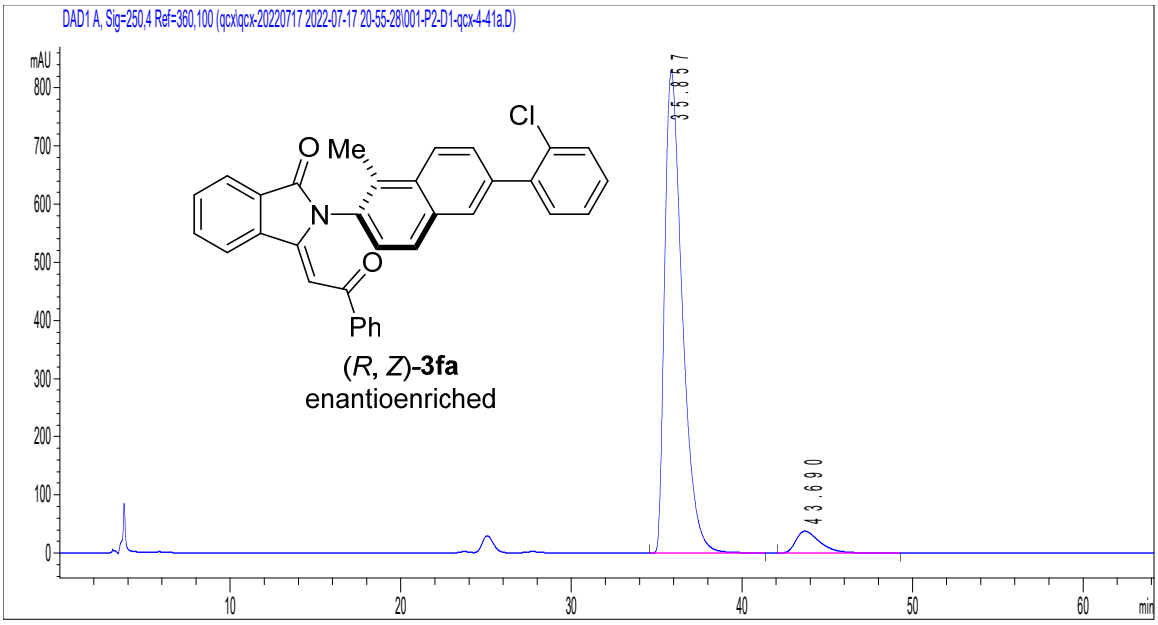
#	Time	Type	Area	Height	Width	Area%	Symmetry
1	36.93	BB	18349.7	256.9	1.0895	96.140	0.598
2	53.3	MM	736.7	6	2.0566	3.860	0.665

3fa

Daicel CHIRALPAK IE-3 column; 30% *i*-PrOH in hexanes; 1.0 mL/min.



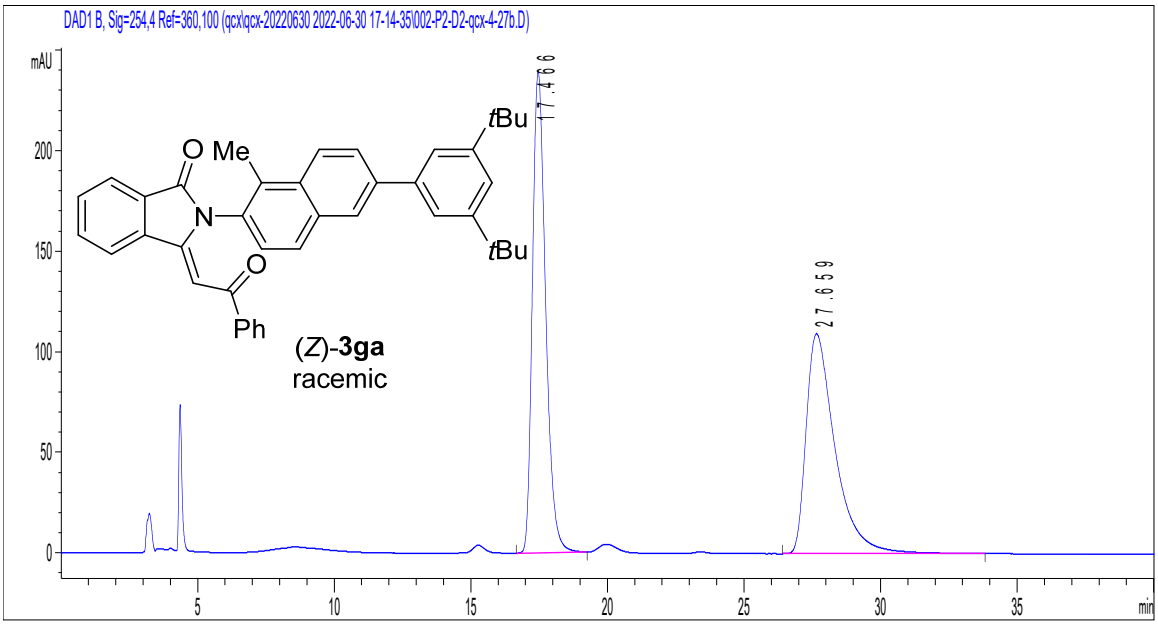
#	Time	Type	Area	Height	Width	Area%	Symmetry
1	39.347	BB	50089.3	655.3	1.1558	50.127	0.561
2	46.035	BB	49835.1	411.5	1.7291	49.873	0.394



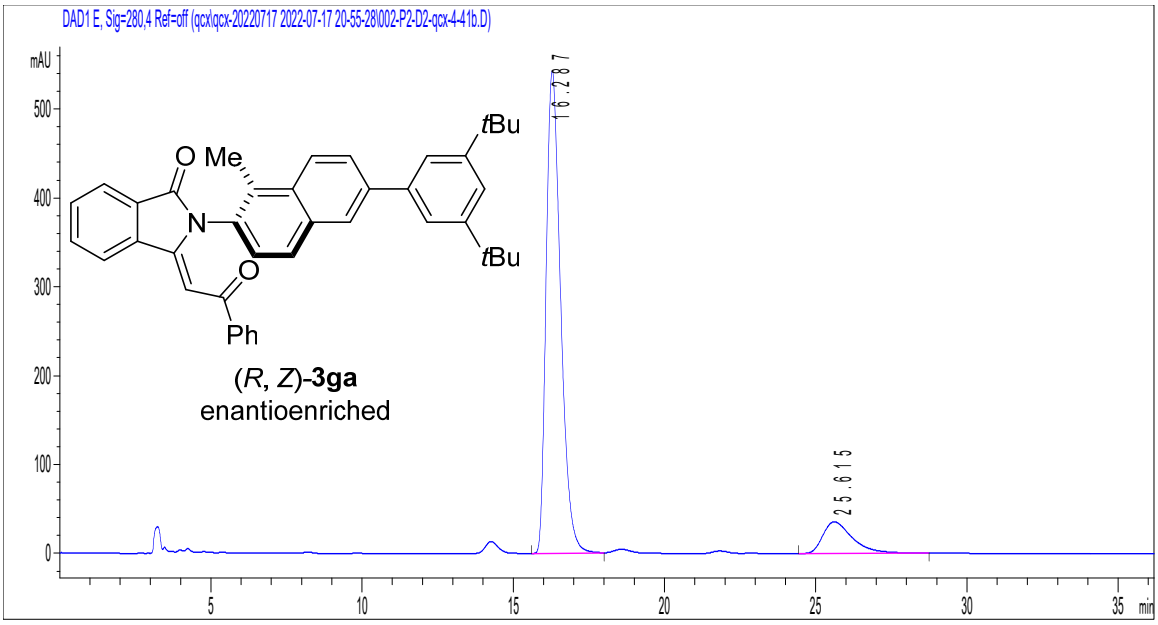
#	Time	Type	Area	Height	Width	Area%	Symmetry
1	35.857	BB	59572.1	829.5	1.0919	94.215	0.551
2	43.69	BB	3658.2	37.5	1.4272	5.785	0.552

3ga

Daicel CHIRALPAK IE-3 column; 30% *i*-PrOH in hexanes; 1.0 mL/min.



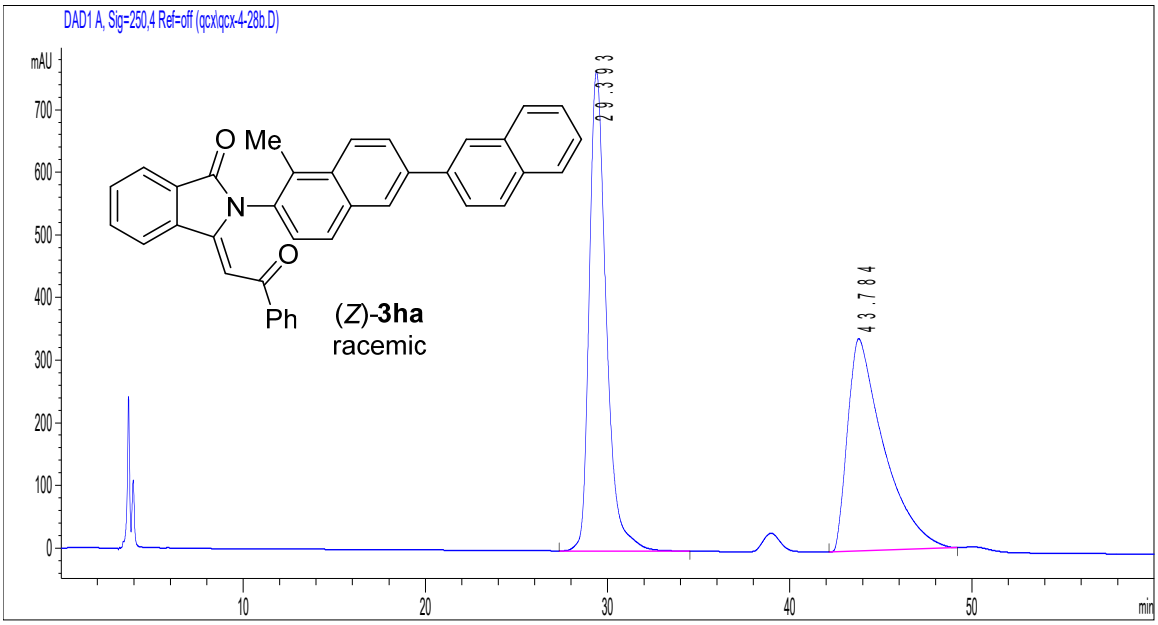
#	Time	Type	Area	Height	Width	Area%	Symmetry
1	17.466	BB	8071.7	239.3	0.5215	50.052	0.714
2	27.659	BB	8054.9	109.4	1.091	49.948	0.518



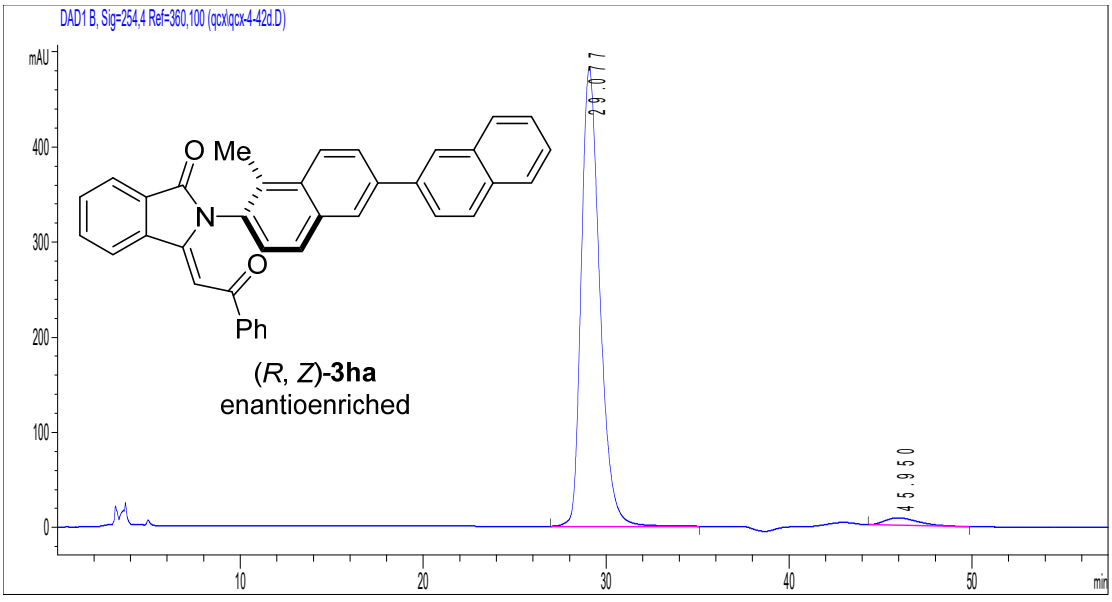
#	Time	Type	Area	Height	Width	Area%	Symmetry
1	16.287	BB	18092.9	543	0.5167	88.189	0.673
2	25.615	BB	2423.3	35.6	1.0017	11.811	0.586

3ha

Daicel CHIRALPAK IE-3 column; 50% *i*-PrOH in hexanes; 1.0 mL/min.



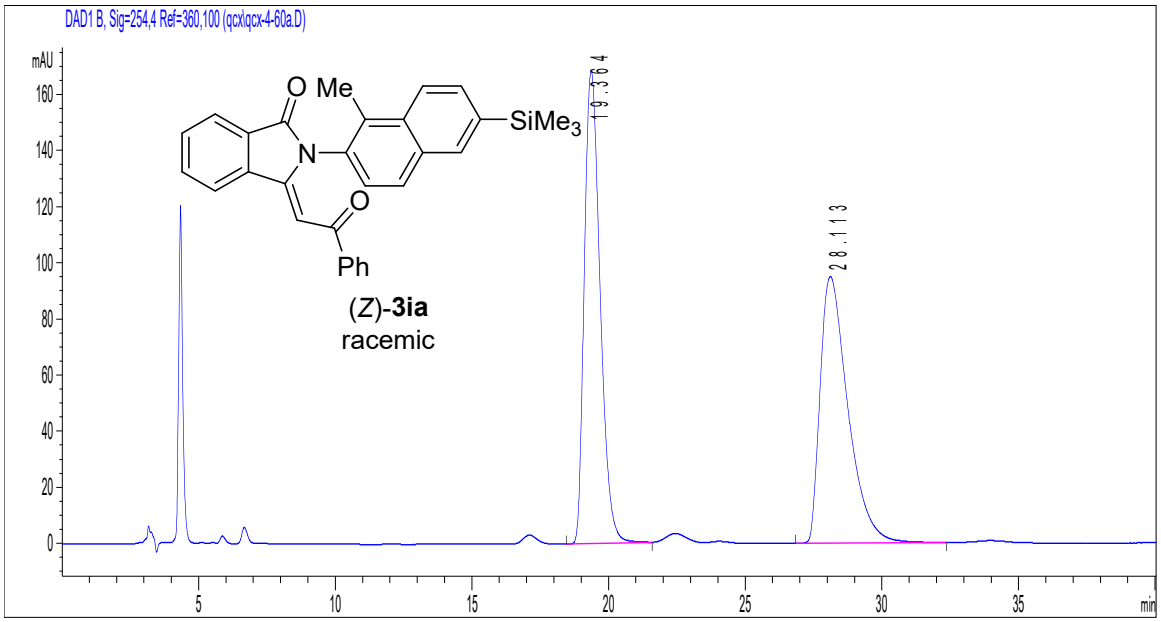
#	Time	Type	Area	Height	Width	Area%	Symmetry
1	29.393	BB	49730	765.6	0.9898	51.536	0.69
2	43.784	BB	46765.5	339.1	1.9751	48.464	0.412



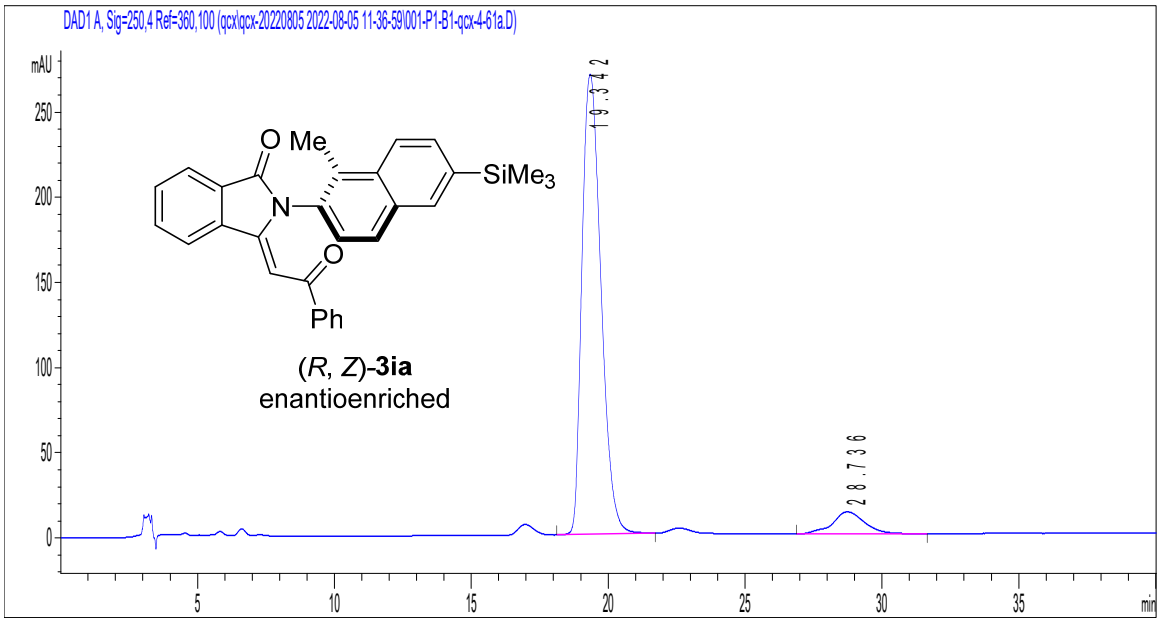
#	Time	Type	Area	Height	Width	Area%	Symmetry
1	29.077	BB	34014.7	481.7	1.0839	97.173	0.709
2	45.95	BB	989.5	7.9	1.4782	2.827	0.61

3ia

Daicel CHIRALPAK IE-3 column; 30% *i*-PrOH in hexanes; 1.0 mL/min.



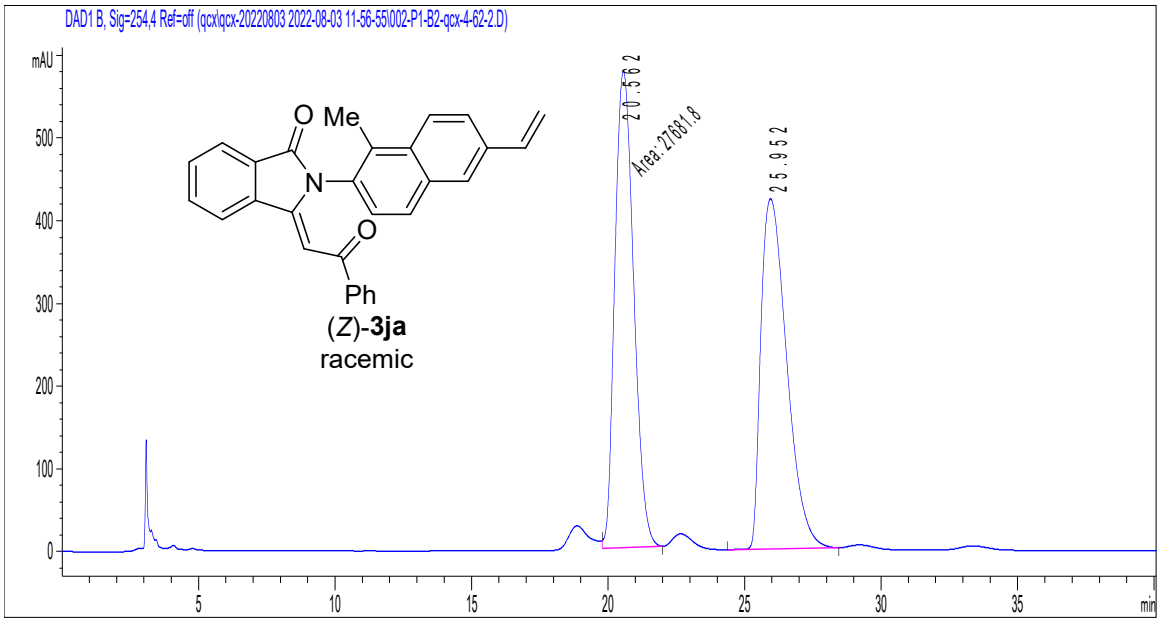
#	Time	Type	Area	Height	Width	Area%	Symmetry
1	19.364	BB	6752.1	168.4	0.6279	50.172	0.707
2	28.113	BB	6705.7	95.1	1.0468	49.828	0.529



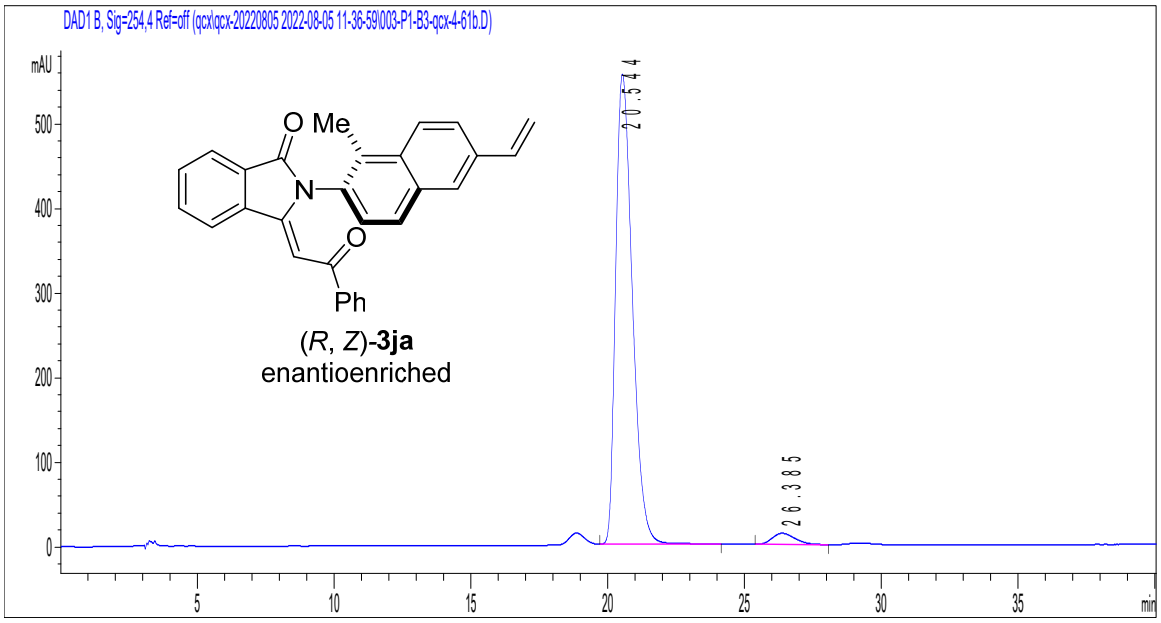
#	Time	Type	Area	Height	Width	Area%	Symmetry
1	19.342	BB	13042	270.2	0.7671	92.496	0.708
2	28.736	BB	1058.1	12.9	1.1443	7.504	0.873

3ja

Daicel CHIRALPAK IE-3 column; 40% *i*-PrOH in hexanes; 1.0 mL/min.



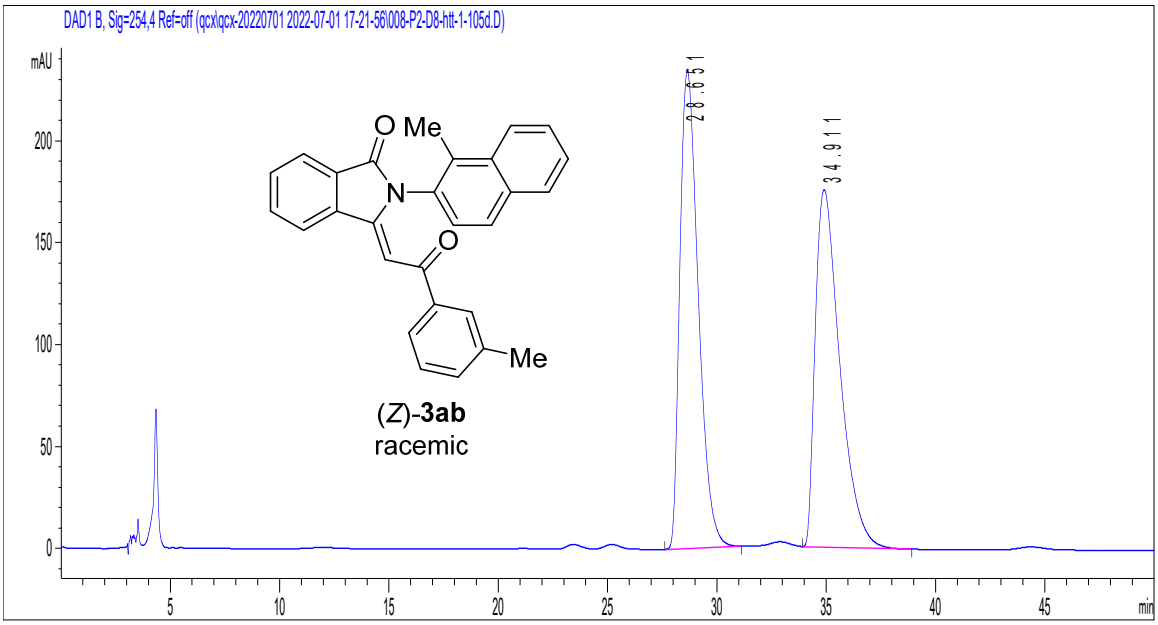
#	Time	Type	Area	Height	Width	Area%	Symmetry
1	20.562	MM	28253	585	0.8049	49.977	0.782
2	25.952	BB	28278.9	430	1.0392	50.023	0.558



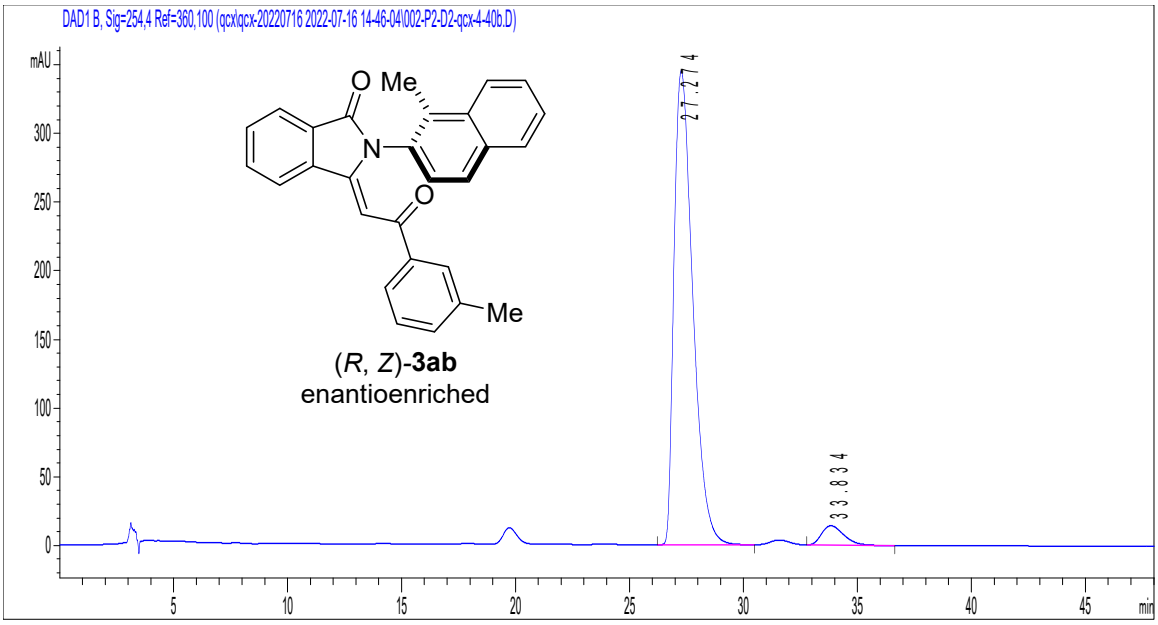
#	Time	Type	Area	Height	Width	Area%	Symmetry
1	20.544	BB	23618.6	555.9	0.6637	96.868	0.641
2	26.385	BB	763.7	13.3	0.8357	3.132	0.74

3ab

Daicel CHIRALPAK IE-3 column; 30% *i*-PrOH in hexanes; 1.0 mL/min.



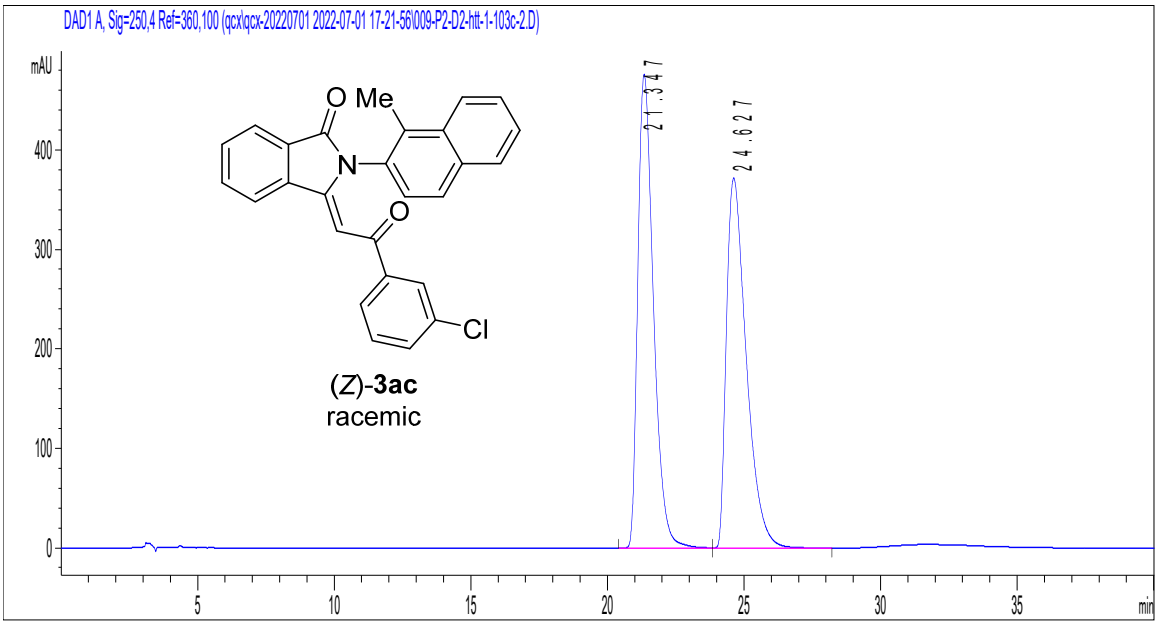
#	Time	Type	Area	Height	Width	Area%	Symmetry
1	28.651	BB	13713.5	234	0.9117	50.024	0.631
2	34.911	BB	13700.5	175.4	1.1995	49.976	0.521



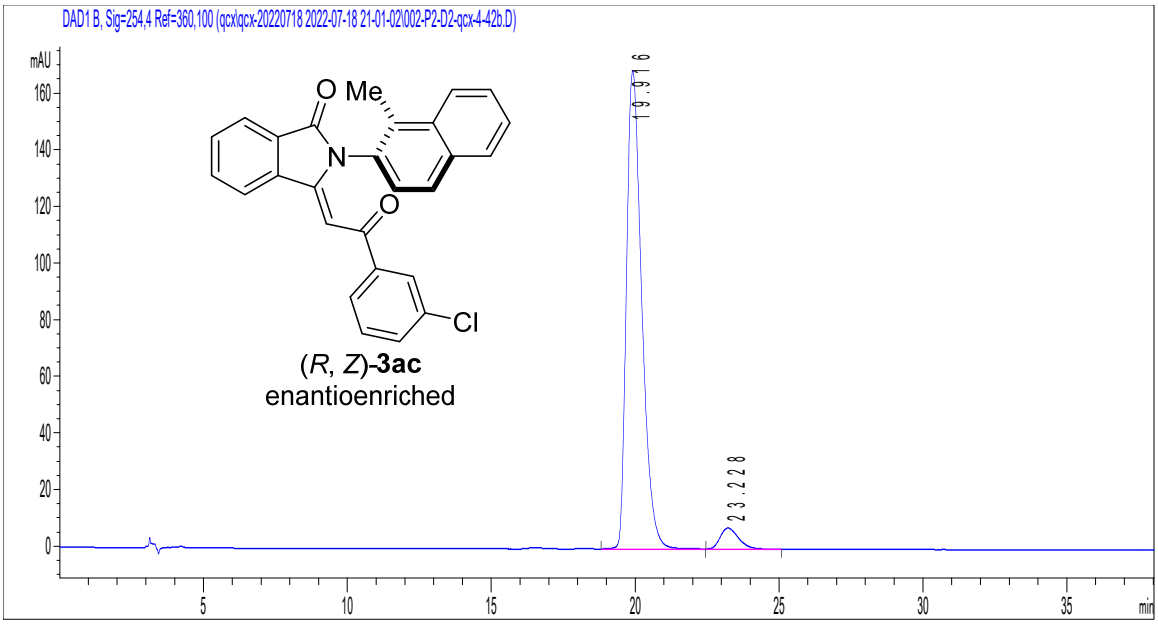
#	Time	Type	Area	Height	Width	Area%	Symmetry
1	27.274	BB	19720.5	345.1	0.8866	95.397	0.586
2	33.834	BB	951.5	14.1	0.9847	4.603	0.681

3ac

Daicel CHIRALPAK IE-3 column; 30% *i*-PrOH in hexanes; 1.0 mL/min.



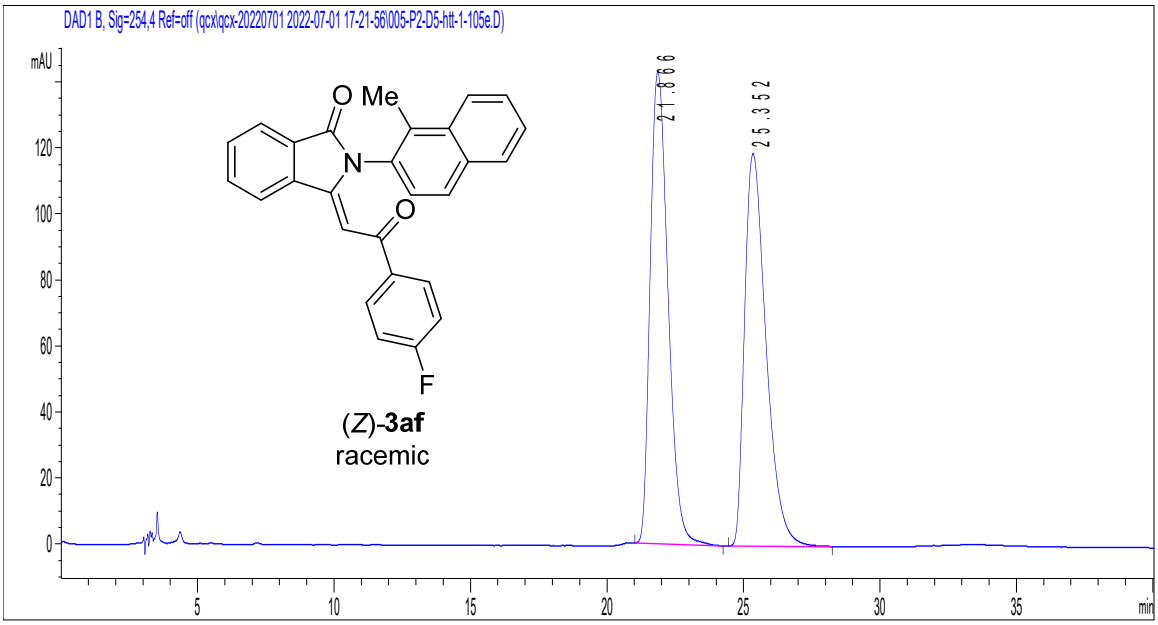
#	Time	Type	Area	Height	Width	Area%	Symmetry
1	21.346	BB	20146.4	503.3	0.619	50.417	0.628
2	24.627	BB	19813.3	391.9	0.7719	49.583	0.538



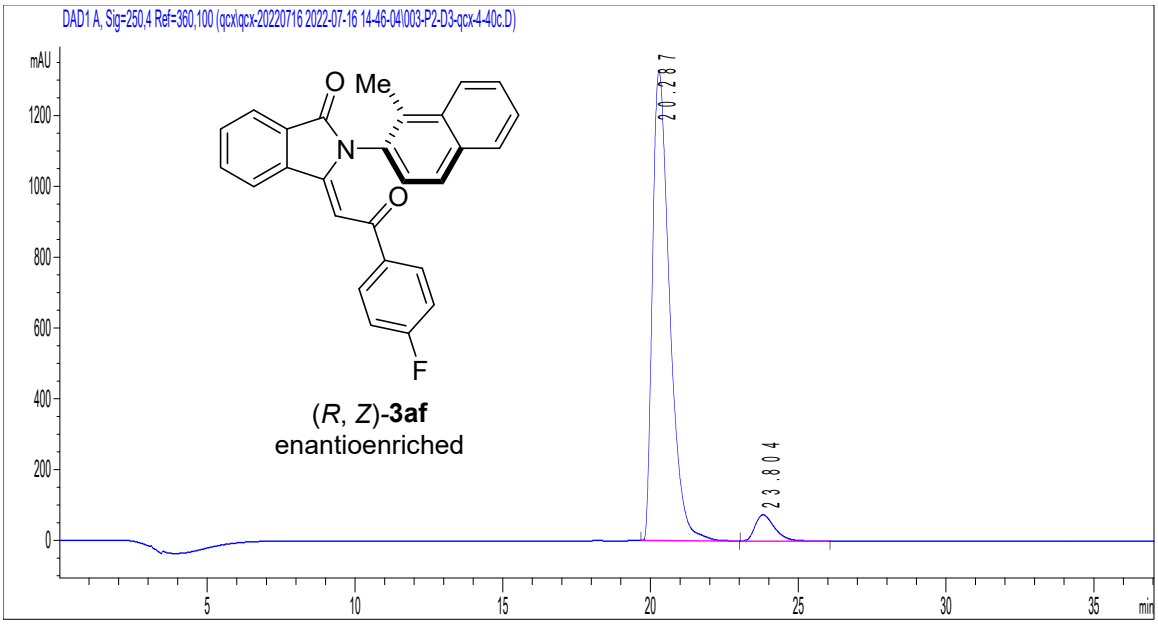
#	Time	Type	Area	Height	Width	Area%	Symmetry
1	19.916	BB	6213.3	168.9	0.5692	95.014	0.645
2	23.228	BB	326.1	7.4	0.6425	4.986	0.708

3af

Daicel CHIRALPAK IE-3 column; 30% *i*-PrOH in hexanes; 1.0 mL/min.



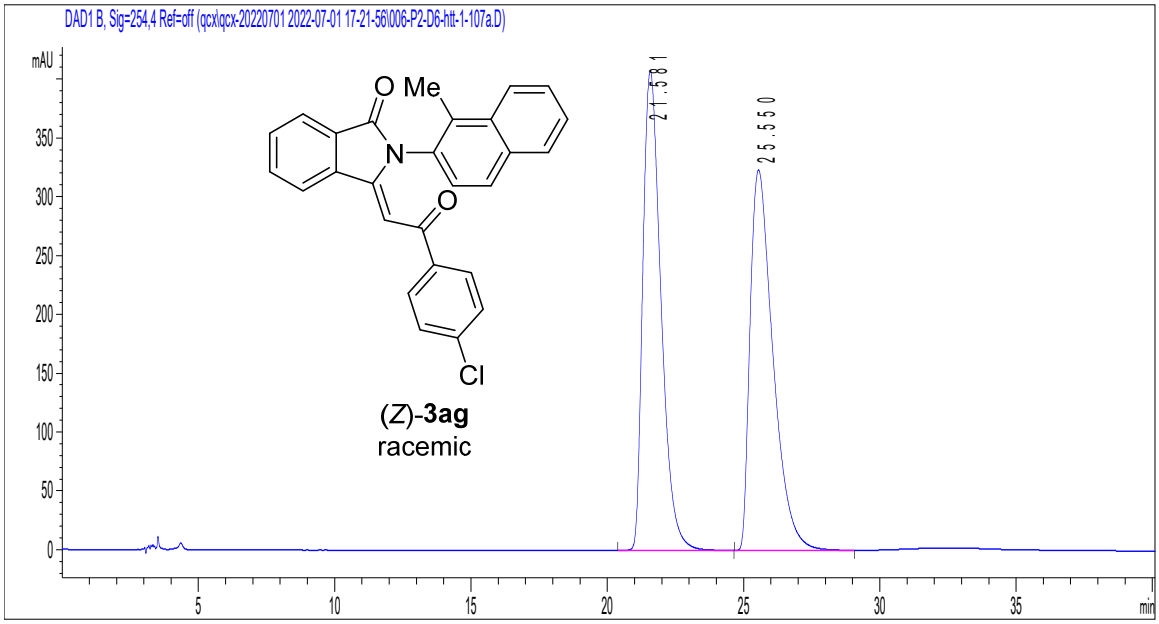
#	Time	Type	Area	Height	Width	Area%	Symmetry
1	21.866	BB	6474.2	143	0.7121	49.874	0.702
2	25.352	BB	6507.1	118.9	0.8423	50.126	0.601



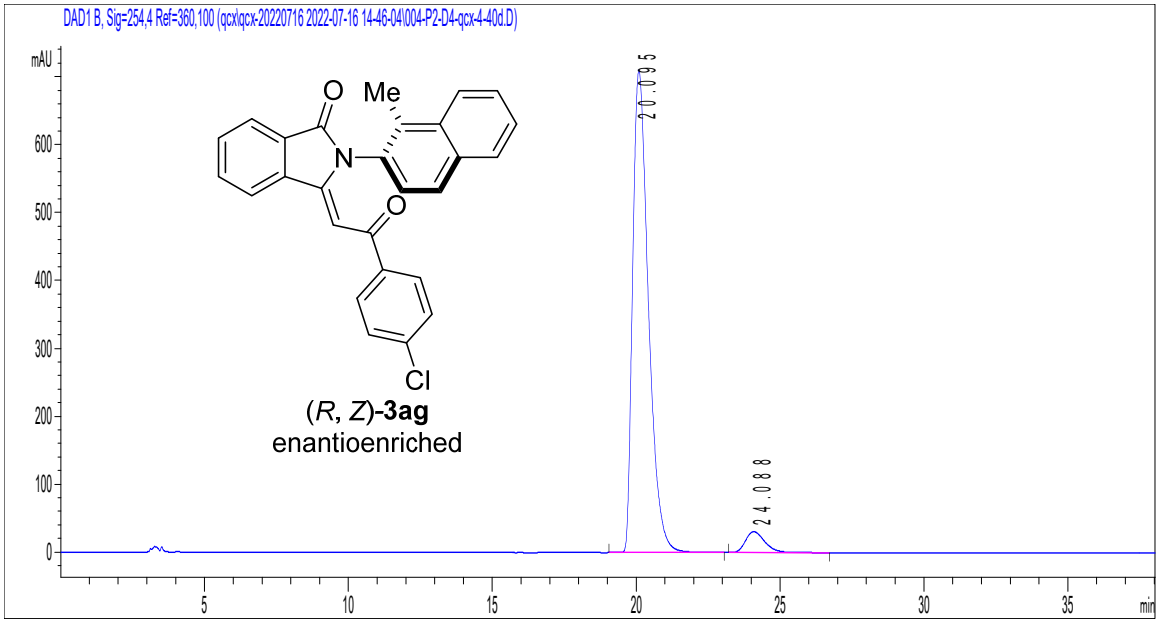
#	Time	Type	Area	Height	Width	Area%	Symmetry
1	20.287	BB	53427.3	1327.1	0.6137	94.085	0.563
2	23.804	BB	3358.8	73.9	0.6982	5.915	0.636

3ag

Daicel CHIRALPAK IE-3 column; 30% *i*-PrOH in hexanes; 1.0 mL/min.



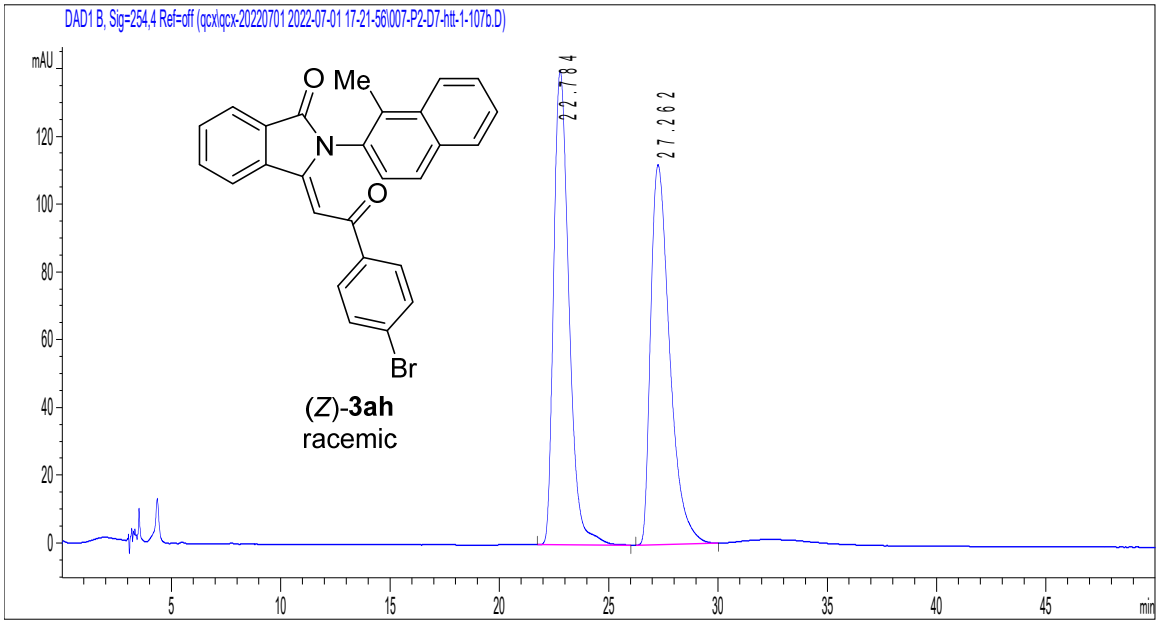
#	Time	Type	Area	Height	Width	Area%	Symmetry
1	21.581	BB	18926	407.6	0.7236	50.064	0.65
2	25.55	BB	18877.7	323.5	0.8968	49.936	0.538



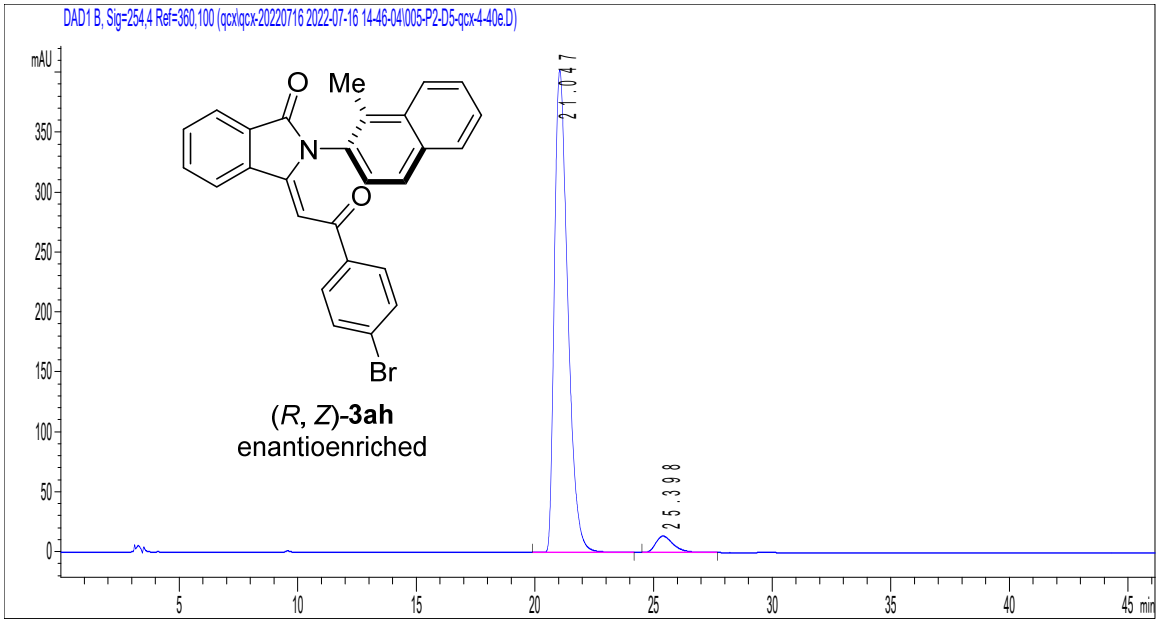
#	Time	Type	Area	Height	Width	Area%	Symmetry
1	20.095	BB	27026.6	710.7	0.5837	94.977	0.6
2	24.088	BB	1429.2	30.8	0.7162	5.023	0.705

3ah

Daicel CHIRALPAK IE-3 column; 30% *i*-PrOH in hexanes; 1.0 mL/min.



#	Time	Type	Area	Height	Width	Area%	Symmetry
1	22.784	BB	6823.1	139.9	0.759	50.169	0.681
2	27.262	BB	6777.2	112.2	0.9249	49.831	0.59



#	Time	Type	Area	Height	Width	Area%	Symmetry
1	21.047	BB	15758.3	402.5	0.6028	95.718	0.624
2	25.398	BB	705	13.7	0.76	4.282	0.655