Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Acid-solvent clusters-catalyzed general and regioselective Friedel-Crafts arylation of alcohols

Supplementary Information

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1.Materials and Methods

All air and moisture-insensitive reactions were carried out under an ambient atmosphere and monitored by thin-layer chromatography (TLC). High-resolution mass spectra were obtained using Q Exactive Plus from Thermo Concentration under reduced pressure was performed by rotary evaporation at 25 - 40 °C at an appropriate pressure. Purified compounds were further dried under vacuum (10^{-6} - 10^{-3} bar). Yields refer to purified and spectroscopically pure compounds, unless otherwise stated.

1.1 Solvents

All reagents were purchased from Adamas, Kermel and DAMAO, and used without further purification.

1.2 Chromatography

Thin layer chromatography (TLC) was performed using EMD TLC plates pre-coated with 250 μm thickness silica gel 60 F 254 plates and visualized by irradiation UV light or by dipping the TLC plate into a dilute, alkaline, aqueous $KMnO_4$-solution. Flash chromatography was performed using silica gel (40 - 63 μm particle size) purchased from Nuo Tai.

1.3 NMR Spectroscopy

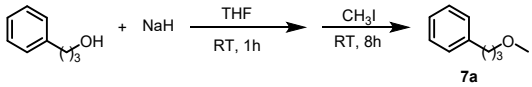
^{1}H-NMR, ^{13}C-NMR (400 MHz, 101 MHz, respectively) spectra were measured in $CDCl_3$ recorded on Bruker Avance DPX 400 MHz spectrometer. All chemical shifts (δ) were reported in ppm and coupling constants (J) in Hz. NMR Spectra recorded in $CDCl_3$ were referenced to tetramethylsilane at 0 ppm for ^{1}H or referenced to residual $CHCl_3$ at 77.16 ppm for ^{13}C. The following abbreviations are used: m (multiplet), s (singlet), d (doublet), t (triplet), q (quartet), dd (doublet of doublets), etc.

1.4 Starting materials

All substrates were used as received from commercial suppliers, unless otherwise stated. Chemicals were purchased from Energy Chemical, Bidepharm, Macklin and Aladdin.

2.Experimental procedures

The procedure for the synthesis of 7a:



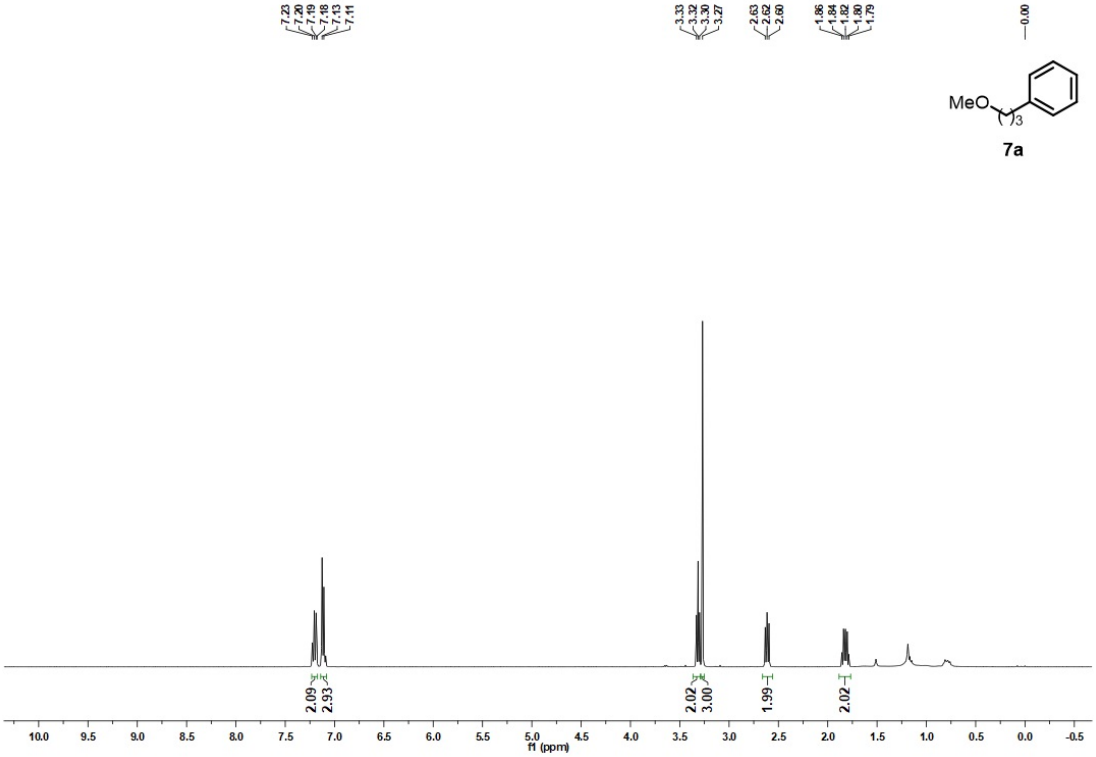
Under a nitrogen atmosphere, the solution of 3-phenylpropanol (1.3619 g, 10 mmol) and NaOH (0.48 g, 20 mmol) in THF (20 mL) was transferred into the 50 mL round-bottom equipped with a polytetrafluoroethylene-coated magnetic stir bar. The reaction system was stirred at room temperature for 1 h. Then, the solution of iodomethane (5.677 g, 40 mmol) was added to the reaction system. The reaction system was stirred at room temperature for 8 h. After the completion of reaction, CH_2Cl_2 (20 mL) was poured into the reaction mixture. The organic layers were extracted with water (3 × 20 mL). The combined organic layers were dried with anhydrous Na_2SO_4 and filtered and solvent was removed under reduced pressure. The resulting crude product was purified by column chromatography on silica gel using petroleum ether : ethyl acetate = 30 : 1 as eluent to afford the product **7a**.[1]

NMR Spectroscopy:

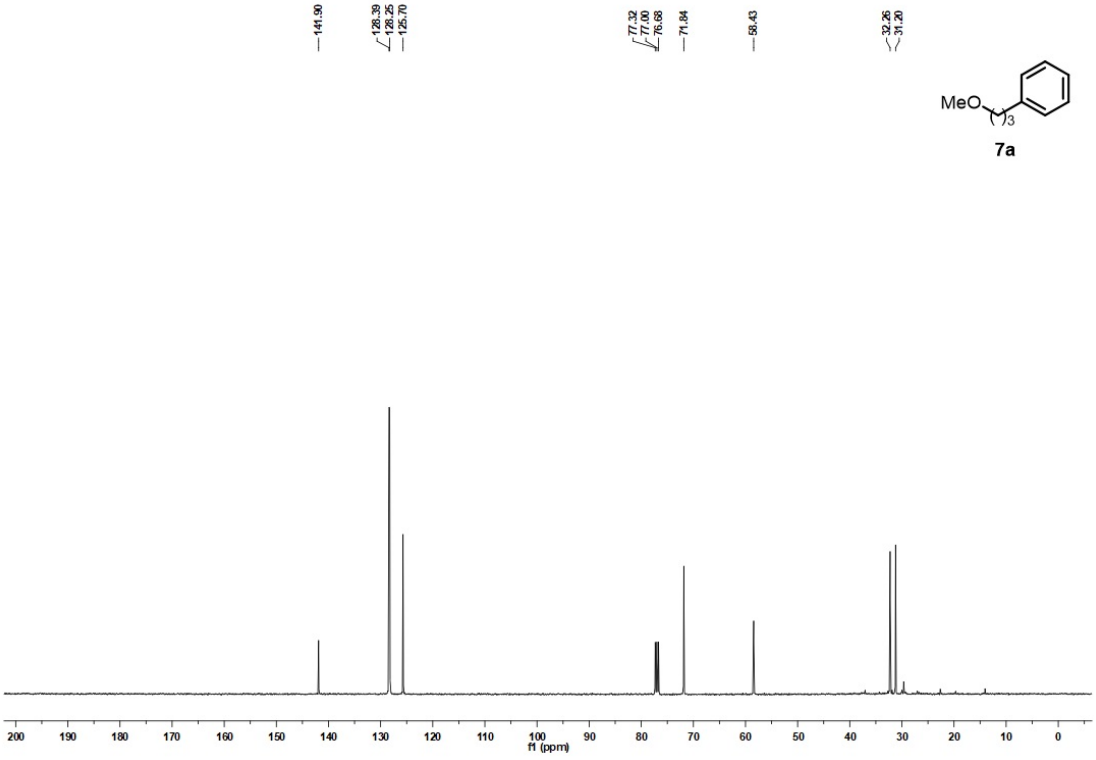
^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.20 (dd, *J* = 13.2, 6.2 Hz, 1H), 7.12 (d, *J* = 7.2 Hz, 1H), 3.32 (t, *J* = 6.4 Hz, 2H), 3.27 (s, 3H), 2.66 - 2.56 (m, 1H), 1.89 - 1.77 (m, 1H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 141.90, 128.32, 125.70, 71.84, 58.43, 32.26, 31.20; **HRMS** (ESI) m/z calculated $C_{10}H_{14}OH^+$ $[M+H]^+$ 151.1117, found 151.1124.

^{1}H-NMR of **7a**

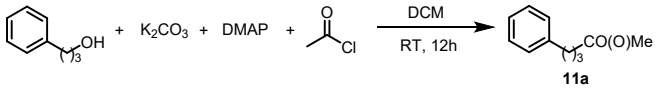
$CDCl_3$, 400 MHz, 298 K



^{13}C-NMR of **7a**
$CDCl_3$, 101 MHz, 298 K



The procedure for the synthesis of 11a:

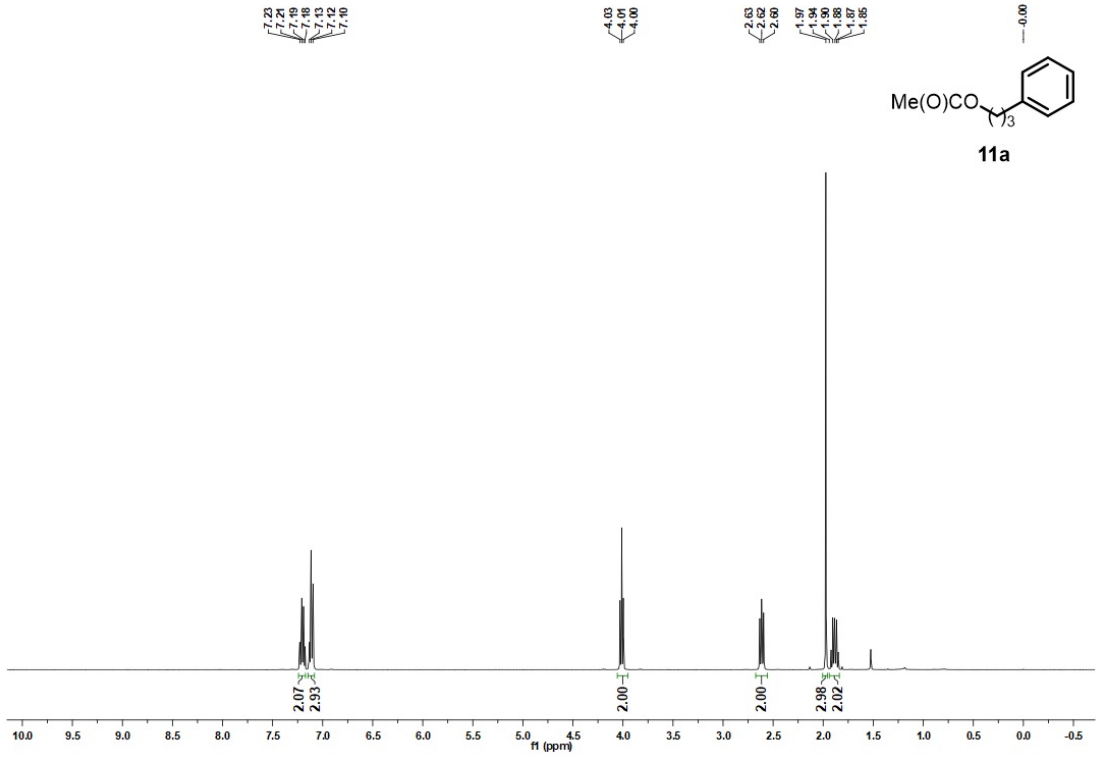


Under an ambient atmosphere, the solution of 3-phenylpropanol (1.3619 g, 10 mmol), K_2CO_3(2.7642 g, 20 mmol), DMAP (0.4887 g, 4 mmol) and acetyl chloride (1.1775g, 15 mmol) in DCM (25 mL) was transferred into the 50 mL round-bottom equipped with a polytetrafluoroethylene-coated magnetic stir bar. The reaction system was stirred at room temperature for 12 h. After the completion of reaction, water (30 mL) was poured into the reaction mixture. The combined organic layers were dried with anhydrous Na_2SO_4 and filtered and solvent was removed under reduced pressure. The resulting crude product was purified by column chromatography on silica gel using petroleum ether : ethyl acetate = 20 : 1 as eluent to afford the product **11a** in the yield of 98% as a colorless oil.[2]

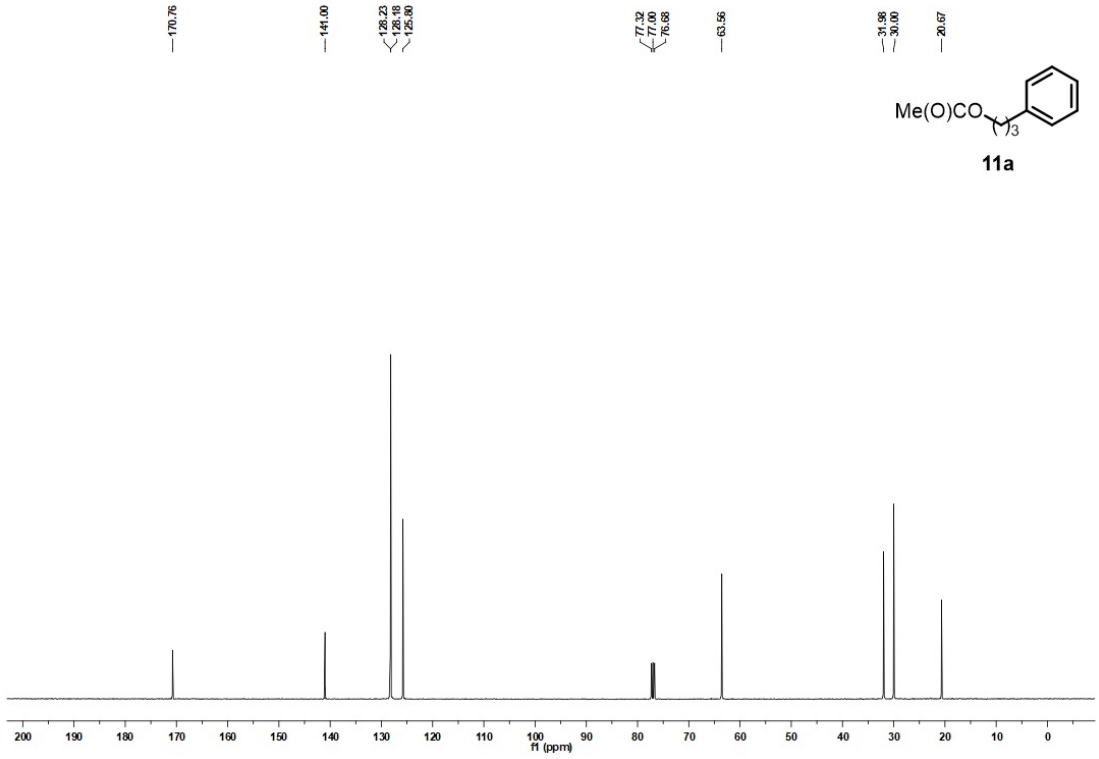
NMR Spectroscopy:

^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.24 - 7.17 (m, 1H), 7.12 (t, J = 7.2 Hz, 1H), 4.01 (t, J = 6.6 Hz, 2H), 2.67 - 2.56 (m, 1H), 1.97 (s, 1H), 1.94 - 1.84 (m, 1H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 170.76, 141.00, 128.20, 125.80, 63.56, 31.98, 30.00, 20.67; **HRMS** (ESI) m/z calculated $C_{11}H_{14}O_2H^+$ $[M+H]^+$ 179.1066, found 179.1061.

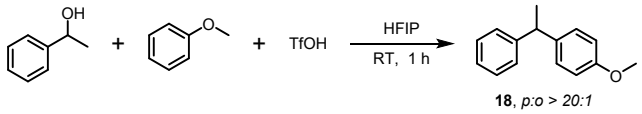
^{1}H-NMR of **11a**
$CDCl_3$, 400 MHz, 298 K



^{13}C-NMR of **11a**
$CDCl_3$, 101 MHz, 298 K



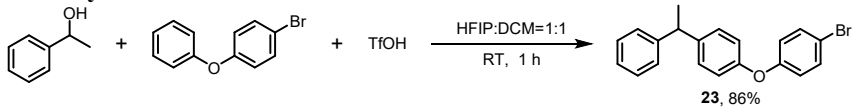
The procedure for the synthesis of 18:



18, *p:o > 20:1*

Under an ambient atmosphere, the solution of phenylethyl alcohol (0.0611 g, 0.5 mmol), anisole (0.2703 g, 2.5 mmol) and TfOH (0.0375 g, 0.25 mmol) in HFIP (2 mL) was transferred into the Schlenk tube equipped with a polytetrafluoroethylene-coated magnetic stir bar. The reaction system was stirred at room temperature for 1 h. After the completion of reaction, CH_2Cl_2 (20 mL) was poured into the reaction mixture. The organic layers were extracted with saturated $NaHCO_3$ aqueous solution (3 × 20 mL). The combined organic layers were dried with anhydrous Na_2SO_4 and filtered and solvent was removed under reduced pressure. The resulting crude product was purified by column chromatography on silica gel using petroleum ether as eluent to afford the product **18** in the yield of 98% as a colorless oil.

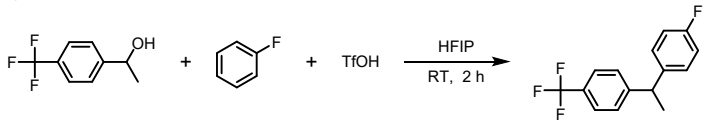
The procedure for the synthesis of 23:



23, 86%

Under an ambient atmosphere, the solution of phenylethyl alcohol (0.0611 g, 0.5 mmol), 4-bromodiphenyl ether (0.6228 g, 2.5 mmol) and TfOH (0.0375 g, 0.25 mmol) in HFIP (1 mL) and CH_2Cl_2 (1 mL) was transferred into the Schlenk tube equipped with a polytetrafluoroethylene-coated magnetic stir bar. The reaction system was stirred at room temperature for 1 h. After the completion of reaction, CH_2Cl_2 (20 mL) was poured into the reaction mixture. The organic layers were extracted with saturated $NaHCO_3$ aqueous solution (3 × 20 mL). The combined organic layers were dried with anhydrous Na_2SO_4 and filtered and solvent was removed under reduced pressure. The resulting crude product was purified by column chromatography on silica gel using petroleum ether as eluent to afford the product **23** in the yield of 86% as a colorless oil.

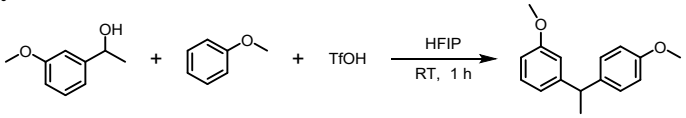
The procedure for the synthesis of 26:



26, *p:o = 16:1*

Under an ambient atmosphere, the solution of 1-(4-trifluoromethylphenyl)ethanol (0.095 g, 0.5 mmol), fluorobenzene (0.24 g, 2.5 mmol) and TfOH (0.0375 g, 0.25 mmol) in HFIP (2 mL) was transferred into the Schlenk tube equipped with a polytetrafluoroethylene-coated magnetic stir bar. The reaction system was stirred at room temperature for 2 h. After the completion of reaction, CH_2Cl_2 (20 mL) was poured into the reaction mixture. The organic layers were extracted with saturated $NaHCO_3$ aqueous solution (3 × 20 mL). The combined organic layers were dried with anhydrous Na_2SO_4 and filtered and solvent was removed under reduced pressure. The resulting crude product was purified by column chromatography on silica gel using petroleum ether as eluent to afford the product **26** in the yield of 84% as a colorless oil.

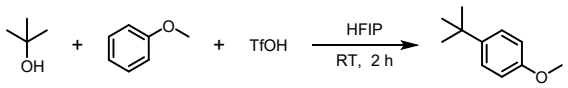
The procedure for the synthesis of 58:



58, *p:o > 20:1*

Under an ambient atmosphere, the solution of 1-(3-methoxyphenyl)ethanol (0.076 g, 0.5 mmol), anisole (0.2703 g, 2.5 mmol) and TfOH (0.0375 g, 0.25 mmol) in HFIP (2 mL) was transferred into the Schlenk tube equipped with a polytetrafluoroethylene-coated magnetic stir bar. The reaction system was stirred at room temperature for 1 h. After the completion of reaction, CH_2Cl_2 (20 mL) was poured into the reaction mixture. The organic layers were extracted with saturated $NaHCO_3$ aqueous solution (3 × 20 mL). The combined organic layers were dried with anhydrous Na_2SO_4 and filtered and solvent was removed under reduced pressure. The resulting crude product was purified by column chromatography on silica gel using petroleum ether as eluent to afford the product **58** in the yield of 94% as a colorless oil.

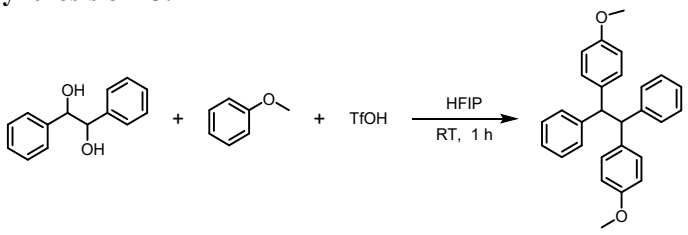
The procedure for the synthesis of 63:



63, 97%

Under an ambient atmosphere, the solution of tert-butanol (0.037 g, 0.5 mmol), anisole (0.2703 g, 2.5 mmol) and TfOH (0.0375 g, 0.25 mmol) in HFIP (2 mL) was transferred into the Schlenk tube equipped with a polytetrafluoroethylene-coated magnetic stir bar. The reaction system was stirred at room temperature for 2 h. After the completion of reaction, CH_2Cl_2 (20 mL) was poured into the reaction mixture. The organic layers were extracted with saturated $NaHCO_3$ aqueous solution (3 × 20 mL). The combined organic layers were dried with anhydrous Na_2SO_4 and filtered and solvent was removed under reduced pressure. The resulting crude product was purified by column chromatography on silica gel using petroleum ether as eluent to afford the product **63** in the yield of 97% as a colorless oil.

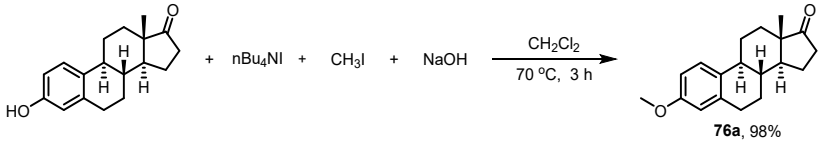
The procedure for the synthesis of 75:



75, 79%

Under an ambient atmosphere, the solution of (*1S*, *2S*)-1,2-diphenylethane-1,2-diol (0.107 g, 0.5 mmol), anisole (0.2703 g, 2.5 mmol) and TfOH (0.0375 g, 0.25 mmol) in HFIP (2 mL) was transferred into the Schlenk tube equipped with a polytetrafluoroethylene-coated magnetic stir bar. The reaction system was stirred at room temperature for 1 h. After the completion of reaction, CH_2Cl_2 (20 mL) was poured into the reaction mixture. The organic layers were extracted with saturated $NaHCO_3$ aqueous solution (3 × 20 mL). The combined organic layers were dried with anhydrous Na_2SO_4 and filtered and solvent was removed under reduced pressure. The resulting crude product was purified by column chromatography on silica gel using petroleum ether : ethyl acetate = 30 : 1 as eluent to afford the product **75** in the yield of 79% as a white solid.

The procedure for the synthesis of estrone 76a:



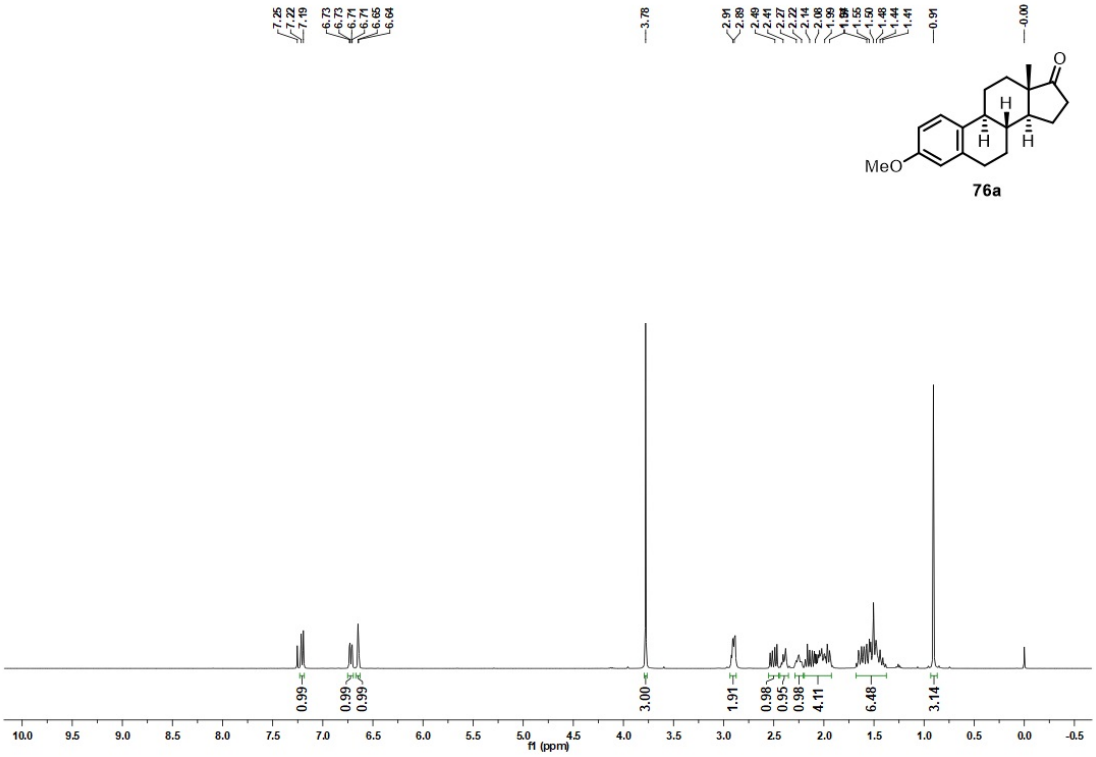
76a, 98%

Under an ambient atmosphere, the solution of estrone (0.811 g, 3 mmol), methyl iodide (1.618 g, 11.4 mmol), nBu_4NI (0.0554 g, 0.15 mmol), and NaOH aqueous solution (10 %, 20 mL) in CH_2Cl_2 (18 mL) was transferred into the 50 mL round-bottom equipped with a polytetrafluoroethylene-coated magnetic stir bar. The reaction system was stirred at 70 °C for 3 h. After the completion of reaction, CH_2Cl_2 (20 mL) was poured into the reaction mixture. The organic layers were extracted with water (3 × 20 mL). The combined organic layers were dried with anhydrous Na_2SO_4 and filtered and solvent was removed under reduced pressure to afford the product **76a** in the yield of 98% as a white solid.[3]

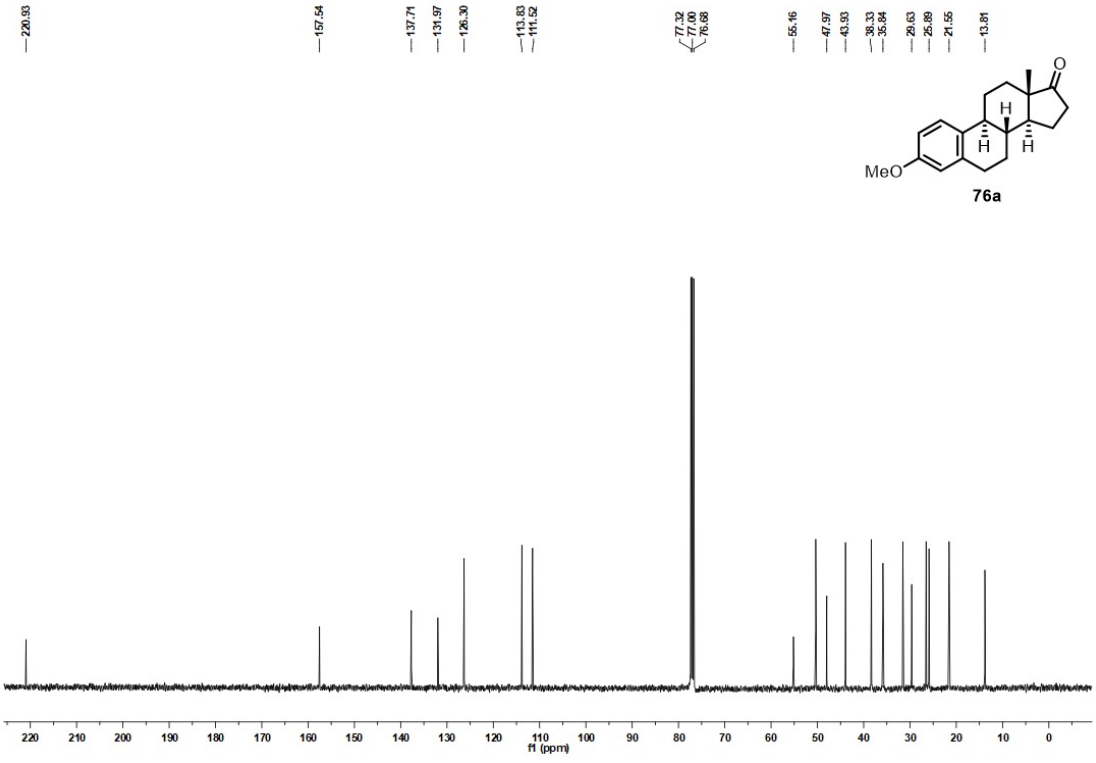
NMR Spectroscopy:

^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.20 (d, *J* = 8.6 Hz, 1H), 6.73 - 6.71 (m, 1H), 6.65 (d, *J* = 2.6 Hz, 1H), 3.78 (s, 3H), 2.90 (d, *J* = 6.4 Hz, 2H), 2.54 - 2.47 (m, 1H), 2.39 (d, *J* = 9.8 Hz, 1H), 2.25 (t, *J* = 10.4 Hz, 1H), 2.16 - 1.94 (m, 4H), 1.65 - 1.41 (m, 6H), 0.91 (s, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 220.93, 157.54, 137.71, 131.97, 126.30, 113.83, 111.52, 55.16, 50.35, 47.97, 43.93, 38.33, 35.84, 31.54, 29.63, 26.51, 25.89, 21.55, 13.81; **HRMS** (ESI) m/z calculated $C_{19}H_{24}O_2H^+$ $[M+H]^+$ 285.1849, found 285.1841.

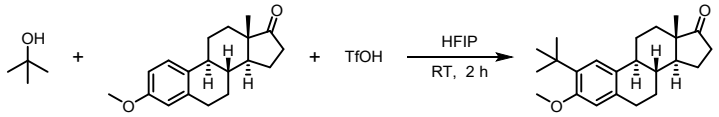
^{1}H-NMR of **76a**
$CDCl_3$, 400 MHz, 298 K



^{13}C-NMR of **76a**
$CDCl_3$, 101 MHz, 298 K



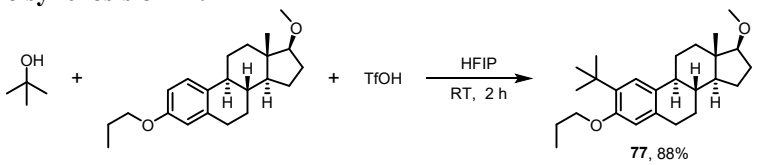
The procedure for the synthesis of 76:



76, 91%

Under an ambient atmosphere, the solution of tert-butanol (0.037 g, 0.5 mmol), **76a** (0.711 g, 2.5 mmol) and TfOH (0.0375 g, 0.25 mmol) in HFIP (2 mL) was transferred into the Schlenk tube equipped with a polytetrafluoroethylene-coated magnetic stir bar. The reaction system was stirred at room temperature for 2 h. After the completion of reaction, CH_2Cl_2 (20 mL) was poured into the reaction mixture. The organic layers were extracted with saturated $NaHCO_3$ aqueous solution (3 × 20 mL). The combined organic layers were dried with anhydrous Na_2SO_4 and filtered and solvent was removed under reduced pressure. The resulting crude product was purified by column chromatography on silica gel using petroleum ether : ethyl acetate = 30 : 1 as eluent to afford the product **76** in the yield of 91% as a yellow oil.

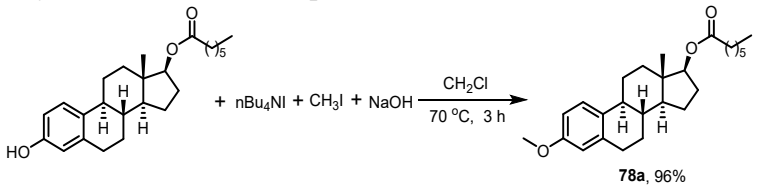
The procedure for the synthesis of 77:



77, 88%

Under an ambient atmosphere, the solution of tert-butanol (0.037 g, 0.5 mmol), promestriene (0.821 g, 2.5 mmol) and TfOH (0.0375 g, 0.25 mmol) in HFIP (2 mL) was transferred into the Schlenk tube equipped with a polytetrafluoroethylene-coated magnetic stir bar. The reaction system was stirred at room temperature for 2 h. After the completion of reaction, CH_2Cl_2 (20 mL) was poured into the reaction mixture. The organic layers were extracted with saturated $NaHCO_3$ aqueous solution (3 × 20 mL). The combined organic layers were dried with anhydrous Na_2SO_4 and filtered and solvent was removed under reduced pressure. The resulting crude product was purified by column chromatography on silica gel using petroleum ether : ethyl acetate = 60 : 1 as eluent to afford the product **77** in the yield of 88% as a white solid.

The procedure for the synthesis of estradiol heptanoate derivatives 78a:



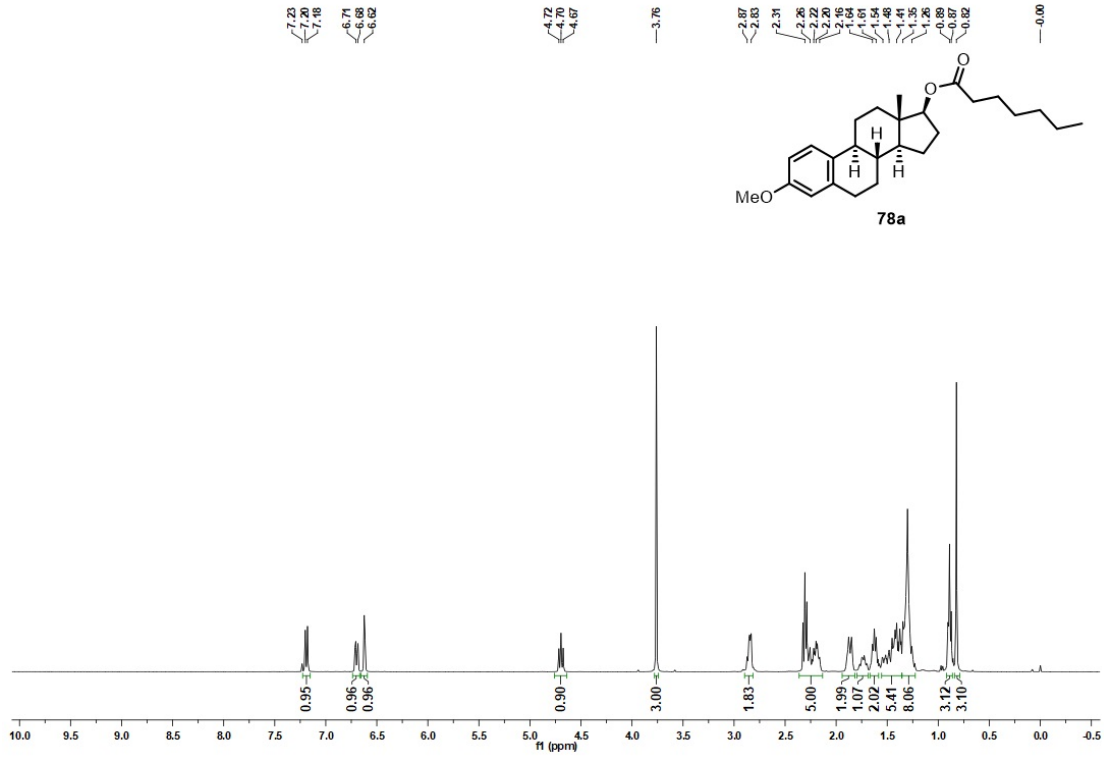
78a, 96%

Under an ambient atmosphere, the solution of estradiol heptanoate (0.9614 g, 2.5 mmol), methyl iodide (1.3484 g, 9.5 mmol), nBu_4NI (0.0462 g, 0.125 mmol), and NaOH aqueous solution (10%, 20 mL) in CH_2Cl_2 (18 mL) was transferred into the 50 mL round-bottom equipped with a polytetrafluoroethylene-coated magnetic stir bar. The reaction system was stirred at 70 °C for 3 h. After the completion of reaction, CH_2Cl_2 (20 mL) was poured into the reaction mixture. The organic layers were extracted with water (3 × 20 mL). The combined organic layers were dried with anhydrous Na_2SO_4 and filtered and solvent was removed under reduced pressure to afford the product **78a** in the yield of 96% as a white solid.[3]

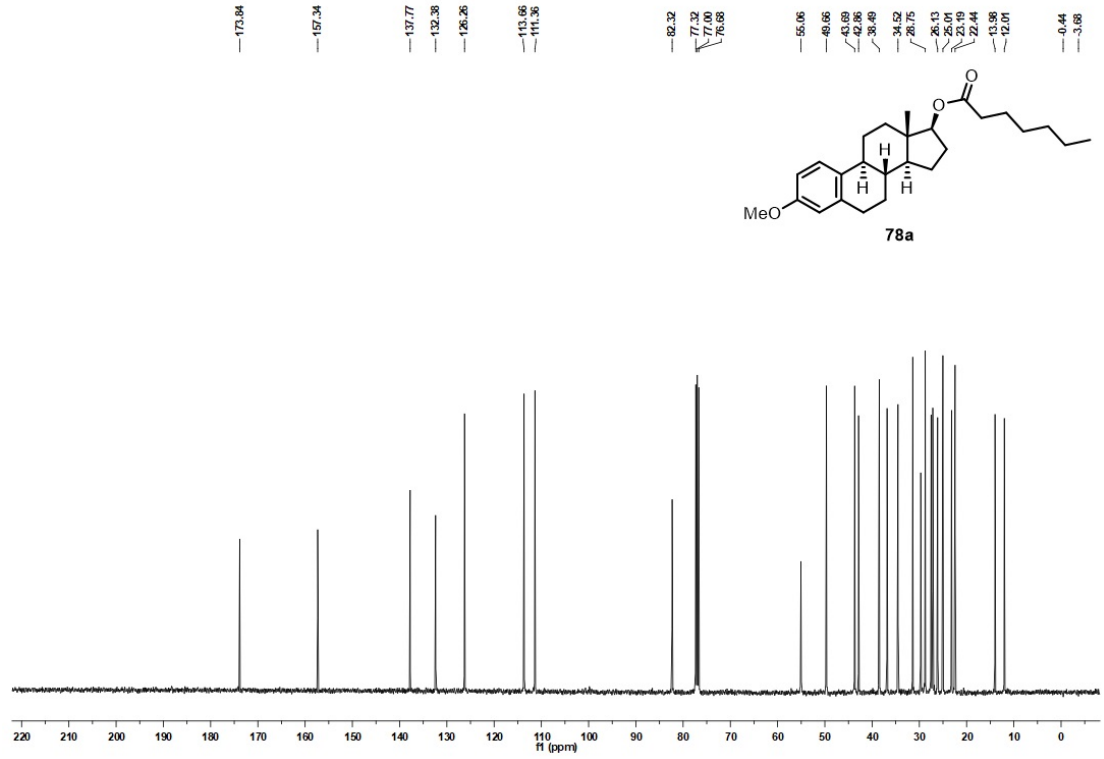
NMR Spectroscopy:

^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.19 (d, J = 8.6 Hz, 1H), 6.70 (d, J = 8.6 Hz, 1H), 6.62 (s, 1H), 4.70 (t, J = 8.4 Hz, 1H), 3.76 (s, 3H), 2.85 (d, J = 15.8 Hz, 2H), 2.33 - 2.16 (m, 5H), 1.88 - 1.85 (d, J = 11.2 Hz, 2H), 1.74 (d, J = 11.4 Hz, 1H), 1.63 - 1.59 (m, 2H), 1.54 - 1.38 (m, 5H), 1.35 - 1.26 (m, 8H), 0.88 (d, J = 6.8 Hz, 1H), 0.82 (s, 1H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 173.84, 157.34, 137.77, 132.38, 126.26, 113.66, 111.36, 82.32, 55.06, 49.66, 43.69, 42.86, 38.49, 36.83, 34.52, 31.40, 29.71, 28.75, 27.51, 27.15, 26.13, 25.01, 23.19, 22.44, 13.98, 12.01; **HRMS** (ESI) m/z calculated $C_{26}H_{38}O_3H^+$ $[M+H]^+$ 399.2894, found 399.2887.

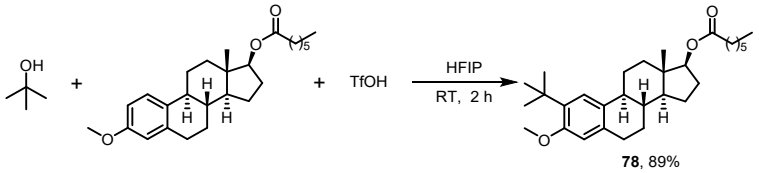
^{1}H-NMR of **78a**
$CDCl_3$, 400 MHz, 298 K



^{13}C-NMR of **78a**
$CDCl_3$, 101 MHz, 298 K



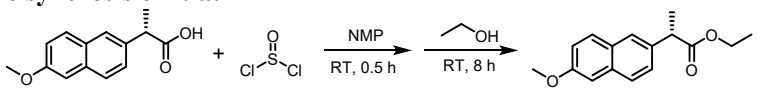
The procedure for the synthesis of 78:



78, 89%

Under an ambient atmosphere, the solution of tert-butanol (0.037 g, 0.5 mmol), **78a** (0.821 g, 2.5 mmol) and TfOH (0.0375 g, 0.25 mmol) in HFIP (2 mL) was transferred into the Schlenk tube equipped with a polytetrafluoroethylene-coated magnetic stir bar. The reaction system was stirred at room temperature for 2 h. After the completion of reaction, CH_2Cl_2 (20 mL) was poured into the reaction mixture. The organic layers were extracted with saturated $NaHCO_3$ aqueous solution (3 × 20 mL). The combined organic layers were dried with anhydrous Na_2SO_4 and filtered and solvent was removed under reduced pressure. The resulting crude product was purified by column chromatography on silica gel using petroleum ether : ethyl acetate = 40 : 1 as eluent to afford the product **78** in the yield of 89% as a yellow oil.

The procedure for the synthesis of 79a:



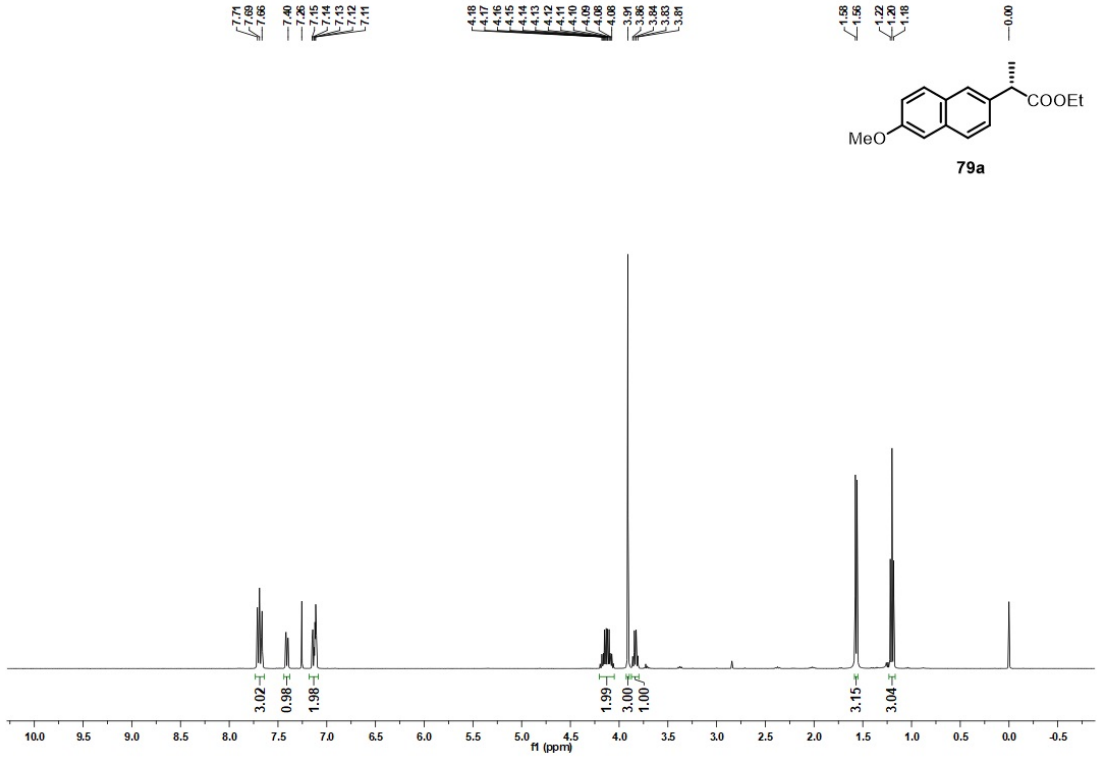
79a, 98%

Under an ambient atmosphere, the solution of naproxen (1.1513 g, 5 mmol) and thionyl chloride (0.714 g, 6 mmol) in NMP (12 mL) was transferred into the 50 mL round-bottom equipped with a polytetrafluoroethylene-coated magnetic stir bar in an ice water bath. The reaction system was stirred at room temperature for 8 h. Then, the solution of ethanol (0.323 g, 7 mmol) was added to the reaction system. The reaction system was stirred at room temperature for 8 h. After the completion of reaction, CH_2Cl_2 (20 mL) was poured into the reaction mixture. The organic layers were extracted with water (3 × 20 mL). The combined organic layers were dried with anhydrous Na_2SO_4 and filtered and solvent was removed under reduced pressure. The resulting crude product was purified by column chromatography on silica gel using petroleum ether : ethyl acetate = 10 : 1 as eluent to afford the product **79a** in the yield of 98% as a yellow solid.[4]

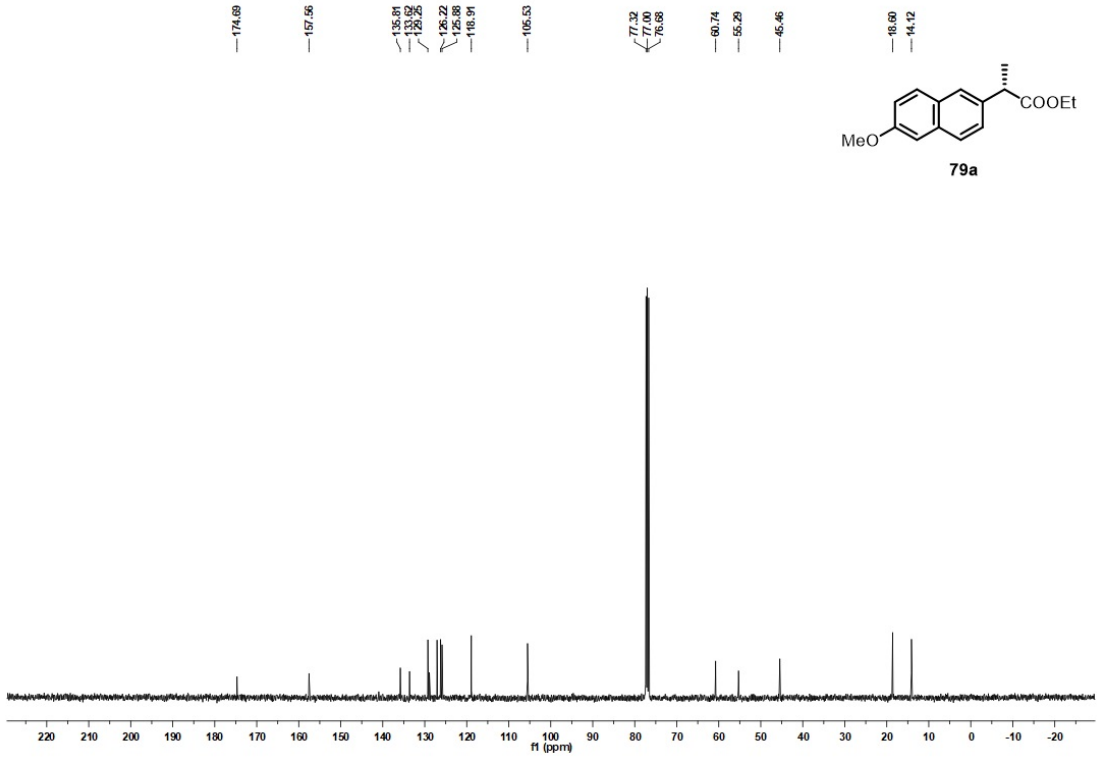
NMR Spectroscopy:

^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.69 (t, *J* = 12.0 Hz, 3H), 7.42 - 7.40 (m, 1H), 7.15 - 7.11 (m, 2H), 4.18 - 4.08 (m, 2H), 3.91 (s, 3H), 3.83 (q, *J* = 7.2 Hz, 1H), 1.57 (d, *J* = 7.2 Hz, 3H), 1.20 (t, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 174.69, 157.56, 135.81, 133.62, 129.25, 128.89, 127.07, 126.22, 125.88, 118.91, 105.53, 60.74, 55.29, 45.46, 18.60, 14.12; **HRMS** (ESI) m/z calculated $C_{16}H_{18}O_3H^+$ $[M+H]^+$ 259.1329, found 259.1321.

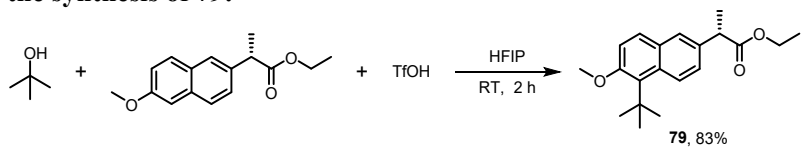
^{1}H-NMR of **79a**
$CDCl_3$, 400 MHz, 298 K



^{13}C-NMR of **79a**
$CDCl_3$, 101 MHz, 298 K

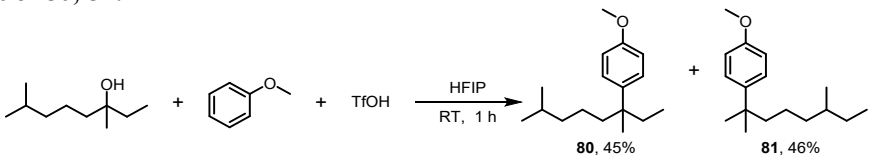


The procedure for the synthesis of 79:



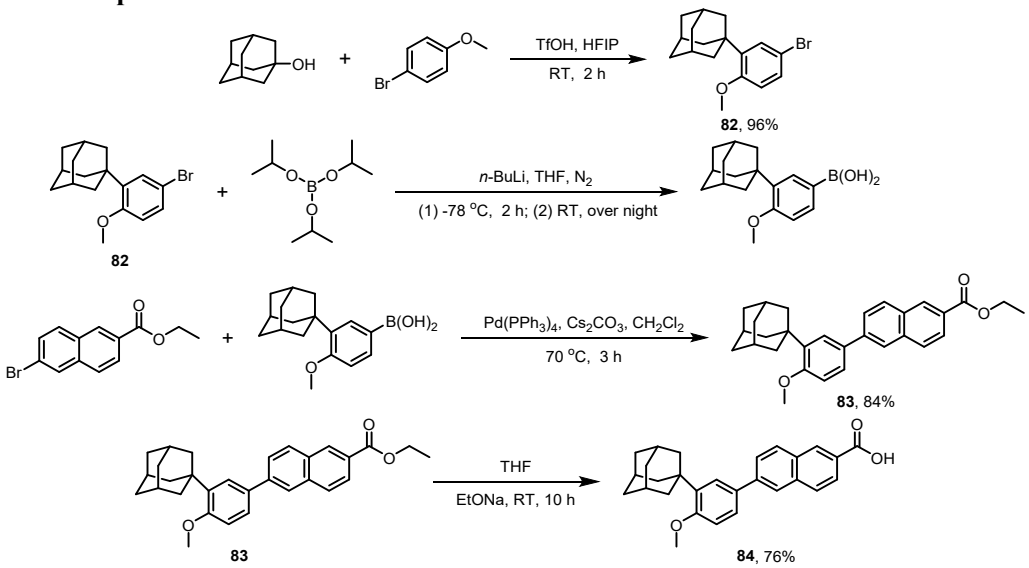
Under an ambient atmosphere, the solution of tert-butanol (0.037 g, 0.5 mmol), **79a** (0.646 g, 2.5 mmol) and TfOH (0.0375 g, 0.25 mmol) in HFIP (2 mL) was transferred into the Schlenk tube equipped with a polytetrafluoroethylene-coated magnetic stir bar. The reaction system was stirred at room temperature for 2 h. After the completion of reaction, CH_2Cl_2 (20 mL) was poured into the reaction mixture. The organic layers were extracted with saturated $NaHCO_3$ aqueous solution (3 × 20 mL). The combined organic layers were dried with anhydrous Na_2SO_4 and filtered and solvent was removed under reduced pressure. The resulting crude product was purified by column chromatography on silica gel using petroleum ether : ethyl acetate = 40 : 1 as eluent to afford the product **79** in the yield of 83% as a yellow oil.

Natural product of 80, 81:



Under an ambient atmosphere, the solution of tetrahydrolinalool (0.079 g, 0.5 mmol), anisole (0.2703 g, 2.5 mmol) and TfOH (0.0375 g, 0.25 mmol) in HFIP (2 mL) was transferred into the Schlenk tube equipped with a polytetrafluoroethylene-coated magnetic stir bar. The reaction system was stirred at room temperature for 1 h. After the completion of reaction, CH_2Cl_2 (20 mL) was poured into the reaction mixture. The organic layers were extracted with saturated $NaHCO_3$ aqueous solution (3 × 20 mL). The combined organic layers were dried with anhydrous Na_2SO_4 and filtered and solvent was removed under reduced pressure. The resulting crude product was purified by column chromatography on silica gel using petroleum ether as eluent to afford the products **80, 81** in the yield of 45%, 46% respectively.

Preparation of adapalene



Under an ambient atmosphere, the solution of 1-adamantane alcohol (0.0761 g, 0.5 mmol), 4-bromoanisole (0.4676 g, 2.5 mmol) and TfOH (0.0375 g, 0.25 mmol) in HFIP (2 mL) was transferred into the Schlenk tube equipped with a polytetrafluoroethylene-coated magnetic stir bar. The reaction system was stirred at room temperature for 2 h. After the completion of reaction, CH_2Cl_2 (20 mL) was poured into the reaction mixture. The organic layers were extracted with saturated $NaHCO_3$ aqueous solution (3 × 20 mL). The combined organic layers were dried with anhydrous Na_2SO_4 and filtered and solvent was removed under reduced pressure. The

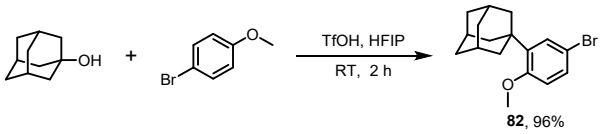
resulting crude product was purified by column chromatography on silica gel using petroleum ether as eluent to afford the product **82** in the yield of 96% as a white solid.

To a solution of the compound **82** (0.16 g, 0.5 mmol) in dried THF (2 mL), n-BuLi in n-hexane (0.3 mL, 1.6 M, 0.5 mmol) was added dropwise over 10 min at -78 °C under nitrogen atmosphere. The solution was stirred at -78 °C for 2 h. And then triisopropyl borate (0.4702 g, 2.5 mmol) dissolved in 2 mL of dry THF was added drop wise to the reaction system. After that, the reaction mixture was allowed to warm to room temperature and stirred overnight. The reaction was quenched with dilute HCl (20%, 20 mL), and the reaction mixture was stirred for 3 h at room temperature. The resulted biphasic solution was extracted with Et_2O (2 × 20 mL), washed twice with H_2O and dried over anhydrous Na_2SO_4 and concentrated by rotary evaporation. To the crude product (viscous liquid), n-hexane 20 mL was added. The white (3-(adamantan-1-yl)-4-methoxyphenyl)boronic acid)boronic acid solid precipitated in n-hexane was filtered, dried and used without further purification (84% isolated yield).[5]

Under a nitrogen atmosphere, (3-(adamantan-1-yl)-4-methoxyphenyl) boronic acid (0.0286 g, 0.1 mmol), Cs_2CO_3 (0.049 g, 0.15 mmol) and $Pd(PPh_3)_4$ (0.00023 g, 0.0002 mmol) were added to the Schlenk tube equipped with a polytetrafluoroethylene-coated magnetic stir bar to dissolve it in a dry DMF (2 mL), and ethyl 6-bromonaphthoate (0.11 g, 0.11 mmol) was added. The reaction solution was stirred at 100 °C for 8 hours. After the reaction was completed was completed, water (3 mL) was added to the reaction solution to quench the reaction. The resulting mixture was extracted with water (3 × 10 mL) and ethyl acetate. The obtained organic layer was dried with anhydrous Na_2SO_4, and the solvent was removed by vacuum filtration. The petroleum ether was used as the eluent. The product **83** was purified by silica gel column chromatography to obtain the product.[6]

To a solution of **83** (0.217 g, 0.5 mmol) in tetrahydrofuran (2 mL), a solution of NaOH (0.0367 g, 0.54 mmol) in absolute ethanol (2 mL) was added at room temperature. The solution was kept under stirring overnight at room temperature and glacial acetic acid (0.42 g, 0.08 mL, 7 mmol) was added and the solution refluxed (1 h). The insoluble residue was filtered-off on celite from the hot solution, washed with tetrahydrofuran (10 mL) then cooled to 25 °C. The solution was concentrated at reduced pressure at ambient temperature, treated with methanol (20 mL) and warmed-up at 60 °C for 15 min. After cooling at room temperature and filtration, the solid residue was suspended in methanol (20 mL) then treated with triethylamine (0.218 g, 0.1 mL, 2.2 mmol) and activated charcoal (1 h at room temperature). After filtration on celite and washing with methanol, the filtrate was poured into a flask and refluxed (65 °C). To this warm solution, a solution of glacial acetic acid (0.42 g, 0.4 mL, 0.54 mmol) in methanol (5 mL) was added dropwise and a white precipitate was formed. After cooling to room temperature, the solid was filtrated and washed with methanol to obtain pure 6-[(3-adamantyl-4-metoxyphenyl)]-2-naphthoic acid (**84**).[7]

Gram-scale experiment



Under an ambient atmosphere, the solution of 1-adamantane alcohol (1.5223 g, 10 mmol), 4-bromoanisole (9.3515 g, 50 mmol) and TfOH (0.7504 g, 5 mmol) in HFIP (30 mL) was transferred into the 50 mL round-bottom equipped with a polytetrafluoroethylene-coated magnetic stir bar. The reaction system was stirred at room temperature for 2 h. After the completion of reaction, the product **82** was obtained by suction filtration with a yield of 96%. After the filtration is completed, reaction the liquid, add 1-adamantane alcohol (1.5223 g, 10 mmol), 4-bromoanisole (1.8703 g, 10 mmol) and TfOH (0.7504 g, 5 mmol) to the reaction solution, The reaction system was stirred at room temperature for 2 h. After the completion of reaction, the product **82** was obtained by suction filtration with a yield of 94%. Repeat 4 times to obtain a total of 12.30 g of product **82** was obtained by suction filtration with a yield of 96%.

3.Optimization of reaction conditions

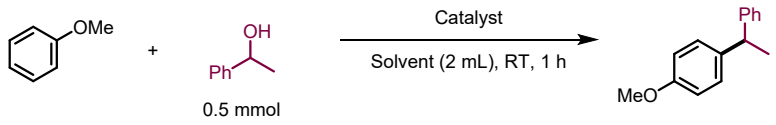


Table S1. Optimization of catalyst amount[a]

Entry	Catalyst (mol%)	Anisole (equiv.)	Solvent	Regioselectivity ratios[b]	Yield (%)[c]
1	TfOH (5%)	5	HFIP	*p*:*o* = 5:1	97
2	--	5	HFIP	--	n.r.
3	TfOH (10%)	5	HFIP	*p*:*o* = 7:1	96
4	TfOH (20%)	5	HFIP	*p*:*o* = 12:1	98
5	TfOH (30%)	5	HFIP	*p*:*o* = 18:1	96
6	TfOH (40%)	5	HFIP	*p*:*o* = 23:1	97
7	TfOH (50%)	5	HFIP	*p*:*o* = 34:1	98
8	TfOH (60%)	5	HFIP	*p*:*o* = 33:1	96

[a] Reactions were carried out on a 0.5 mmol scale. [b] Regioselectivity ratios were determined by ^{1}H-NMR spectroscopy. [c] Yields were determined by ^{1}H-NMR spectroscopy with dibromomethane as the internal standard. n.r. = no reaction.

Table S2. Optimization of anisole amount[a]

Entry	Catalyst (mol%)	Anisole (equiv.)	Solvent	Regioselectivity ratios[b]	Yield (%)[c]
1	TfOH (50%)	6	HFIP	*p*:*o* = 35:1	96
2	TfOH (50%)	5	HFIP	*p*:*o* = 34:1	98
3	TfOH (50%)	4	HFIP	*p*:*o* = 33:1	90
4	TfOH (50%)	3	HFIP	*p*:*o* = 35:1	76
5	TfOH (50%)	2	HFIP	*p*:*o* = 33:1	52
6	TfOH (50%)	1	HFIP	*p*:*o* = 33:1	33

[a] Reactions were carried out on a 0.5 mmol scale. [b] Regioselectivity ratios were determined by ^{1}H-NMR spectroscopy. [c] Yields were determined by ^{1}H-NMR spectroscopy with dibromomethane as the internal standard. n.r. = no reaction.

Table S3. Optimization of catalyst types[a]

Entry	Catalyst (mol%)	Anisole (equiv.)	Solvent	Regioselectivity ratios[b]	Yield (%)[c]
1	$Cu(TfO)_2$ (50%)	5	HFIP	*p*:*o* = 6:1	92
2	$Fe(TfO)_3$ (50%)	5	HFIP	*p*:*o* = 4:1	88
3	$Al(TfO)_3$ (50%)	5	HFIP	*p*:*o* = 8:1	91
4	$La(TfO)_3$ (50%)	5	HFIP	*p*:*o* = 5:1	66
5	$In(TfO)_3$ (50%)	5	HFIP	*p*:*o* = 9:1	87
6	$BF_3{\cdot}Et_2O$ (50%)	5	HFIP	*p*:*o* = 7:1	94
7	CF_3CO_2H (50%)	5	HFIP	*p*:*o* = 5:1	90
8	TsOH (50%)	5	HFIP	*p*:*o* = 6:1	45
9	CH_3CO_2H (50%)	5	HFIP	--	n.r.
10	$PhCO_2H$ (50%)	5	HFIP	--	n.r.

[a] Reactions were carried out on a 0.5 mmol scale. [b] Regioselectivity ratios were determined by ^{1}H-NMR spectroscopy. [c] Yields were determined by ^{1}H-NMR spectroscopy with dibromomethane as the internal standard. n.r. = no reaction.

Table S4. Optimization of Solvent[a]

Entry	Catalyst (mol%)	Anisole (equiv.)	Solvent	Regioselectivity ratios[b]	Yield (%)[c]
1	TfOH (50%)	5	DCM	*m*:*p*:*o* = 1:2:2	90
2	TfOH (50%)	5	THF	--	trace
3	TfOH (50%)	5	DMF	--	n.r.
4	TfOH (50%)	5	CF_3CH_2OH	*p*:*o* = 10:1	78
5	TfOH (50%)	5	*n*-hexane	*m*:*p*:*o* = 1:8:2	74
6	TfOH (50%)	5	ethyl acetate	*m*:*p*:*o* = 1:2:1	43

[a] Reactions were carried out on a 0.5 mmol scale. [b] Regioselectivity ratios were determined by ^{1}H-NMR spectroscopy. [c] Yields were determined by ^{1}H-NMR spectroscopy with dibromomethane as the internal

standard. n.r. = no reaction.

Table S5. Optimization of HFIP amount[a]

Entry	Catalyst (mol%)	Anisole (equiv.)	Solvent(mL)	Regioselectivity ratios[b]	Yield (%)[c]
1	TfOH (50%)	5	0.5	*p*:*o* = 33:1	95
2	TfOH (50%)	5	1	*p*:*o* = 32:1	94
3	TfOH (50%)	5	2	*p*:*o* = 34:1	97
4	TfOH (50%)	5	3	*p*:*o* = 35:1	97
5	TfOH (50%)	5	4	*p*:*o* = 34:1	96
6	TfOH (50%)	5	5	*p*:*o* = 33:1	95

[a] Reactions were carried out on a 0.5 mmol scale. [b] Regioselectivity ratios were determined by ^{1}H-NMR spectroscopy. [c] Yields were determined by ^{1}H-NMR spectroscopy with dibromomethane as the internal standard. n.r. = no reaction.

4.Determination of reaction mechanism

4.1 Influencing factors

To gain insight into the mechanism of this Friedel-Crafts alkylation, several control experiments were conducted (Figure S1-S3). First, the effect of a single variable on the regioselectivity and yield by maintaining other effect factors constant was analyzed. As shown in Figure S1-S3, the amount of trifluoromethanesulfonic acid and anisole made significant influences on reaction regioselectivity and yield, respectively, while the amount of HFIP effected neither yield nor regioselectivity of the reaction. These results suggest that the regioselectivity control of this Friedel-Crafts alkylation is dominated by the ratio of TfOH to the raw material rather than the concentration.

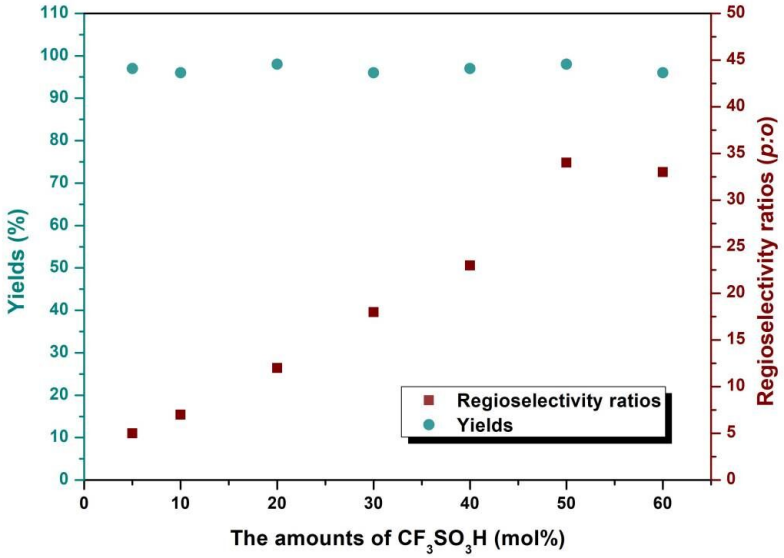


Figure S1. The amount of CF_3SO_3H (Detail data are shown in Table S1)

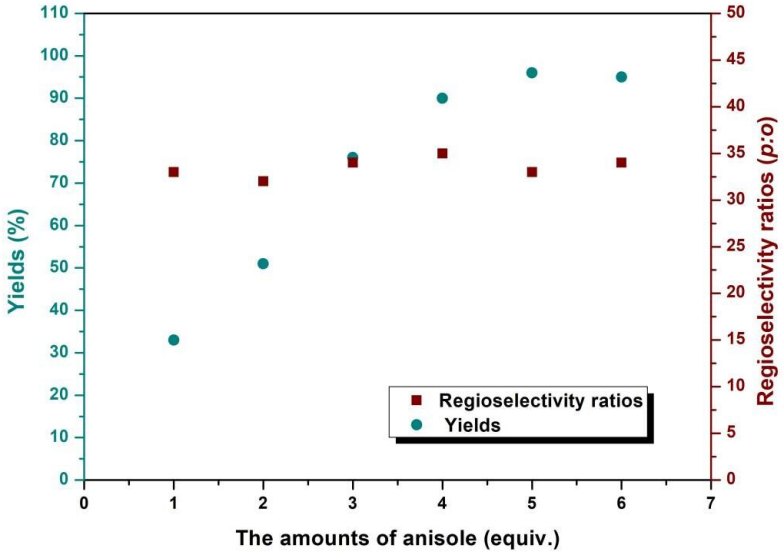


Figure S2. The amount of anisole (Detail data are shown in Table S2)

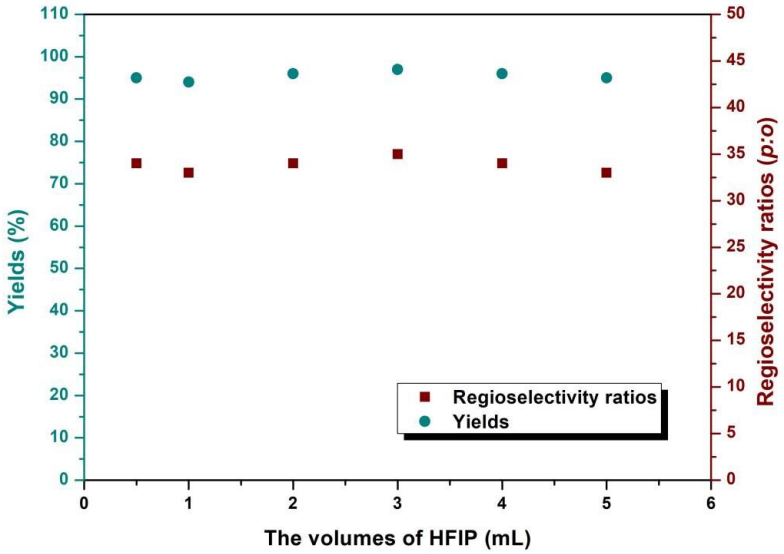
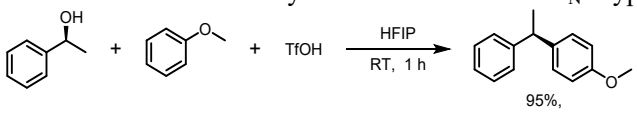


Figure S3. The volume of HFIP (Detail data are shown in Table S5)

4.2 Mechanism verification experiments

Then, the reaction of (*R*)-(+)-1-phenylethanol and anisole was performed under the standard conditions. The complete loss of stereoretention (1% *ee*) together with the above-mentioned 1,5-H shift of carbocation intermediate demonstrated that the Friedel-Crafts alkylation occurred via an S_N1-type pathway.



Under an ambient atmosphere, the solution of (*R*)-(+)-1-phenylethanol (0.060 g, 0.5 mmol), anisole (0.2703 g, 2.5 mmol) and TfOH (0.0375 g, 0.25 mmol) in HFIP (2 mL) was transferred into the Schlenk tube equipped with a polytetrafluoroethylene-coated magnetic stir bar. The reaction system was stirred at room temperature for 1 h. After the completion of reaction, CH_2Cl_2 (20 mL) was poured into the reaction mixture. The organic layers were extracted with saturated $NaHCO_3$ aqueous solution (3 × 20 mL). The combined organic layers were dried with anhydrous Na_2SO_4 and filtered and solvent was removed under reduced pressure. The resulting crude product was purified by column chromatography on silica gel using petroleum ether as eluent to afford the product in the yield of 95% as a colorless oil.

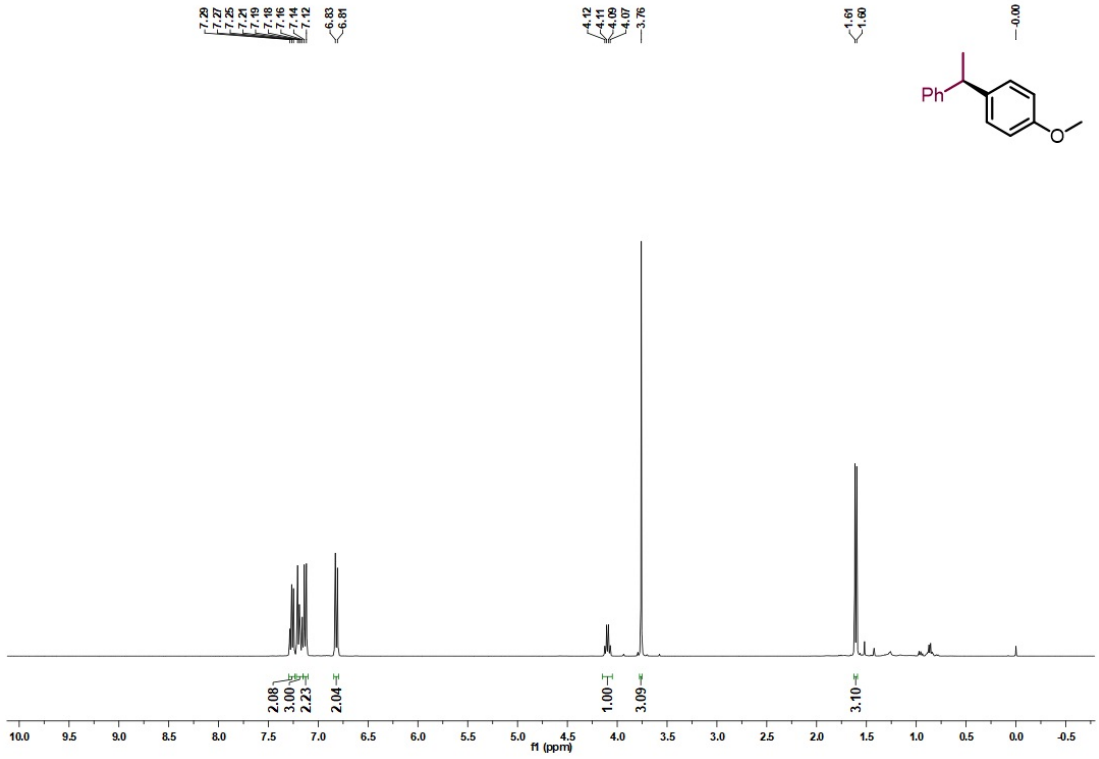
NMR Spectroscopy:

^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.27 (t, *J* = 7.4 Hz, 2H), 7.18 - 7.1 (m, 3H), 7.13 (d, *J* = 8.6 Hz, 2H), 6.82 (d, *J* = 8.6 Hz, 2H), 4.10 (q, *J* = 7.2 Hz, 1H), 3.76 (s, 3H), 1.61 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 157.77, 146.73, 138.50, 128.39, 127.49, 125.90, 113.66, 55.18, 43.88, 22.03.

HPLC: CHIRALCEL OJ-H, n-hexane/isopropanol = 98/2, flow rate = 0.8 mL/min, UV = 250 nm tR = 27,35 min (minor), 29.95 min (major), 1% ee.

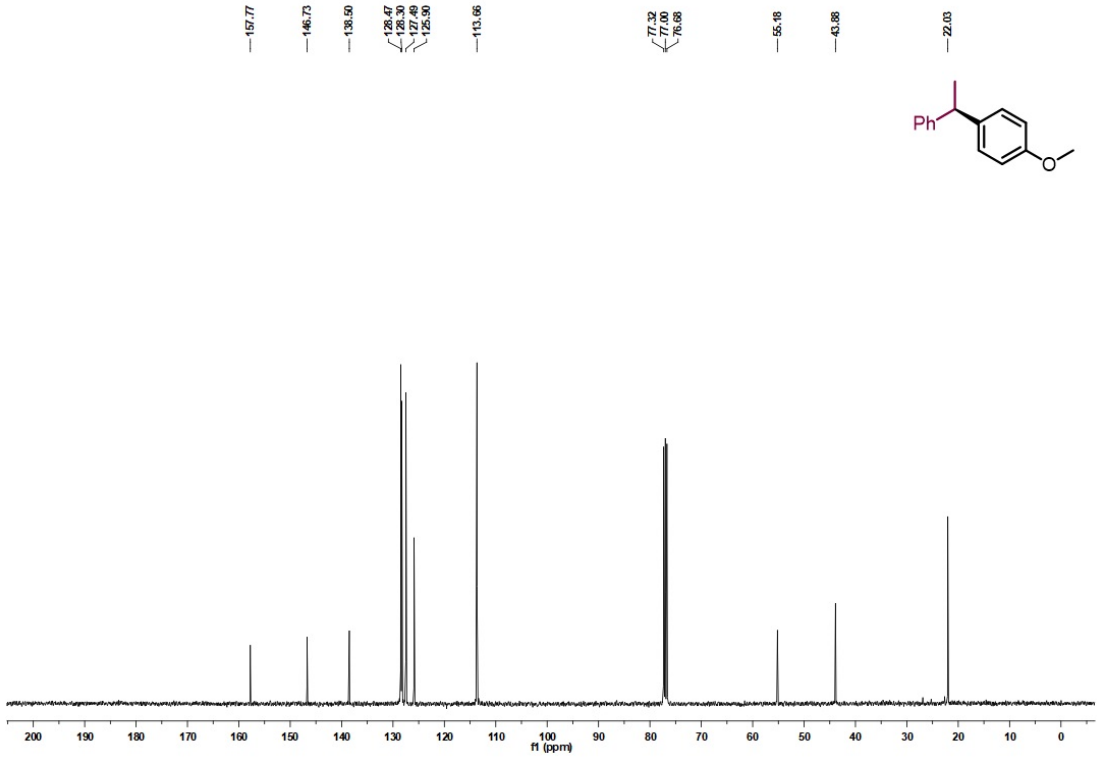
^{1}H-NMR

$CDCl_3$, 400 MHz, 298 K



^{13}C-NMR

$CDCl_3$, 101 MHz, 298 K



Report

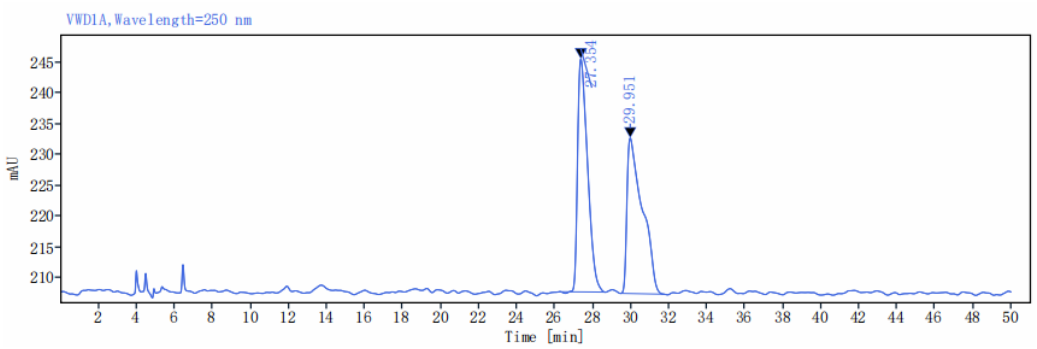
Agilent

Data File: FWT-chair-OJH-98-2-0.8+.dx

Sample Name: FWT-chair-OJH-98-2-0.8+ **Project Name:** JDY

Instrument 1260 **Injection Date:** 2022-10-18 19:35:40+08:00

Acquisition Method: OJH-98-2-0.8.AMX

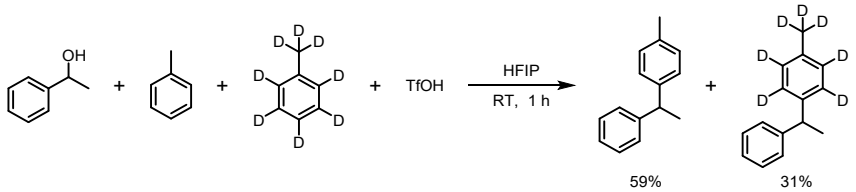


VWD1A,Wavelength=250 nm

Ret.Time [min]	Area	Height	Height%	Area%
27.354	1375.71	37.83	59.97	49.26
29.951	1417.07	25.26	40.03	50.74
Total.	2792.78	63.09	100.00	100.00

4.3 Intermolecular competition experiment

The deuterium kinetic isotope effects (KIE) associated with the deprotonation of Wheland intermediates were studied. In a competition experiment using excess toluene and deuterated toluene, the k_H/k_D value was determined to be 1.91 under standard reaction conditions.



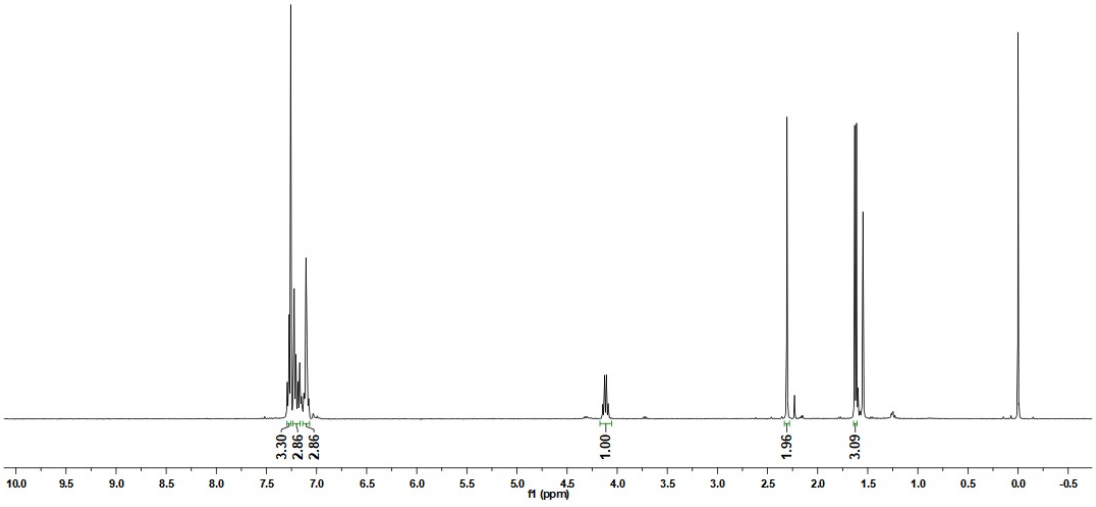
Under an ambient atmosphere, the solution of phenylethyl alcohol (0.0611 g, 0.5 mmol), toluene (0.4607 g, 5 mmol) and deuterated toluene (0.501 g, 5 mmol) and TfOH (0.0375 g, 0.25 mmol) in HFIP (2 mL) was transferred into the Schlenk tube equipped with a polytetrafluoroethylene-coated magnetic stir bar. The reaction system was stirred at room temperature for 1 h. After the completion of reaction, CH_2Cl_2 (20 mL) was poured into the reaction mixture. The organic layers were extracted with saturated $NaHCO_3$ aqueous solution (3 × 20 mL). The combined organic layers were dried with anhydrous Na_2SO_4 and filtered and solvent was removed under reduced pressure. The product was purified by silica gel column chromatography using petroleum ether as eluent.

NMR Spectroscopy:

^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.29 - 7.25 (m, 3H), 7.20 - 7.15 (m, 3H), 7.14 - 7.07 (m, 3H), 4.12 (q, *J* = 7.2 Hz, 1H), 2.31 (s, 2H), 1.62 (d, *J* = 7.2 Hz, 3H).

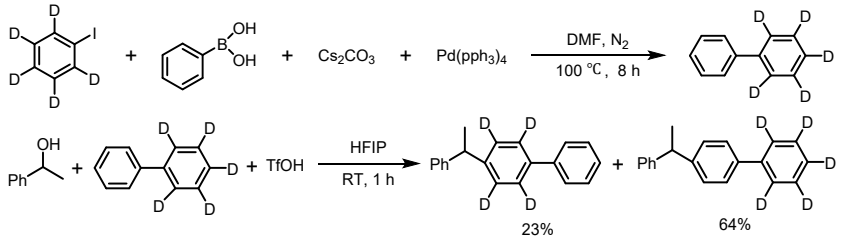
^{1}H-NMR

$CDCl_3$, 400 MHz, 298 K



4.4 Intramolecular competition experiment

Moreover, the intramolecular competition experiment of diphenyl-d_5 and 1-phenylethanol was conducted, the k_H/k_D value was determined to be 2.77. Theoretically, only KIE values from relative ratios of independently determined reaction rate constants can identify deprotonation as a rate-determining step. However, we were unable to detect this KIE value because our reaction was proceeding too quickly. As indicated by the measured KIE, deprotonation of the Wheland intermediates is expected to be at least partially controllable.



Under an nitrogen atmosphere, the solution of phenylboronic acid (0.134 g, 1.1 mmol), Cs_2CO_3 (0.488 g, 1.5 mmol), $Pd(PPh_3)_4$ (0.0024 g, 0.002 mmol) and deuterated iodobenzene (0.204 g, 1 mmol)in dry DMF (18 mL) was transferred into the 50 mL round-bottom equipped with a polytetrafluoroethylene-coated magnetic stir bar. The reaction system was stirred at 100 °C for 8 h. After the completion of reaction, CH_2Cl_2 (20 mL) was poured into the reaction mixture. The organic layers were extracted with water (3 × 20 mL). The combined organic layers were dried with anhydrous Na_2SO_4 and filtered and solvent was removed under reduced pressure to afford the product deuterated biphenyl.[6]

Under an ambient atmosphere, the solution of deuterated biphenyl (0.0977 g, 0.5 mmol), phenylethanol (0.0123 g, 0.1 mmol) and TfOH (0.0225 g, 0.15 mmol) in HFIP (2 mL) was transferred into the Schlenk tube equipped with a polytetrafluoroethylene-coated magnetic stir bar. The reaction system was stirred at room temperature for 1 h. After the completion of reaction, CH_2Cl_2 (20 mL) was poured into the reaction mixture. The organic layers were extracted with saturated $NaHCO_3$ aqueous solution (3 × 20 mL). The combined organic layers were dried with anhydrous Na_2SO_4 and filtered and solvent was removed under reduced pressure. The product was purified by silica gel column chromatography using petroleum ether as eluent.

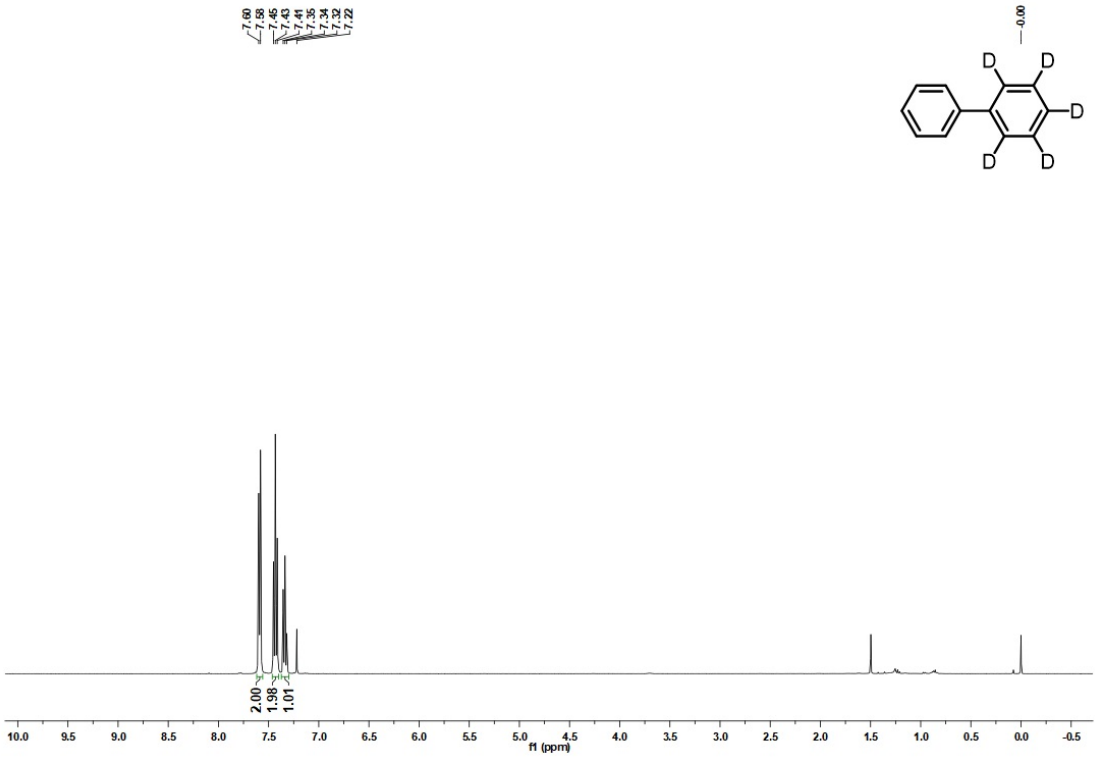
NMR Spectroscopy:

^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 7.2 Hz, 2H), 7.43 (t, *J* = 7.6 Hz, 2H), 7.34 (t, *J* = 7.2 Hz, 1H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 141.16, 141.03 128.74, 127.22, 127.13.

^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.56 (d, *J* = 7.8 Hz, 1H), 7.51 (d, *J* = 8.2 Hz, 2H), 7.41 (t, *J* = 7.6 Hz, 1H), 7.34 - 7.23 (m, 6H), 7.19 (t, *J* = 6.8 Hz, 1H), 4.20 (q, *J* = 7.2 Hz, 1H), 1.68 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 146.24, 145.46, 140.79, 138.87, 128.69, 128.40, 127.99, 127.62, 127.03, 126.08, 44.45, 21.85.

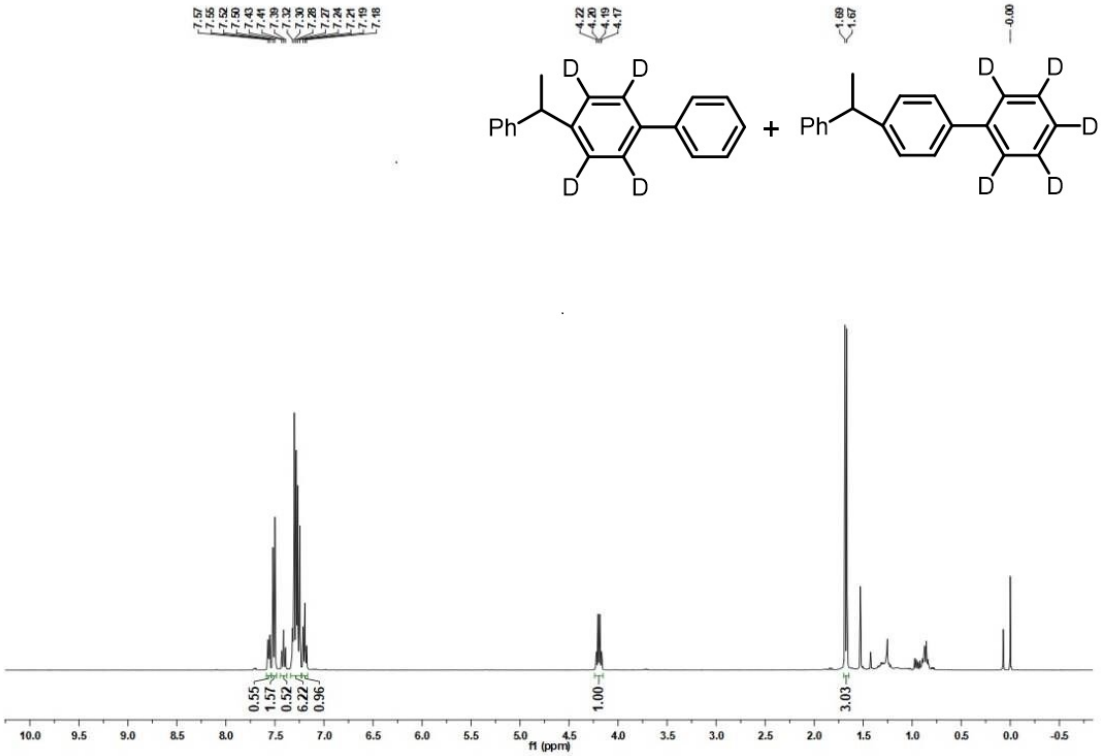
[1]H-NMR

$CDCl_3$, 400 MHz, 298 K



[1]H-NMR

$CDCl_3$, 400 MHz, 298 K



4.5 Titration experiment

To evaluate the interaction between HFIP and TfOH, HFIP was titrated with TfOH and the process was monitored by H^1 NMR (Figure S4). In addition to proton exchange between TfOH and the OH moiety of HFIP, the increasingly downfield shift of the exchanged proton was observed when increasing the concentration of TfOH. These results revealed that TfOH and HFIP can interact in any ratio to form the corresponding TfOH-HFIP clusters.

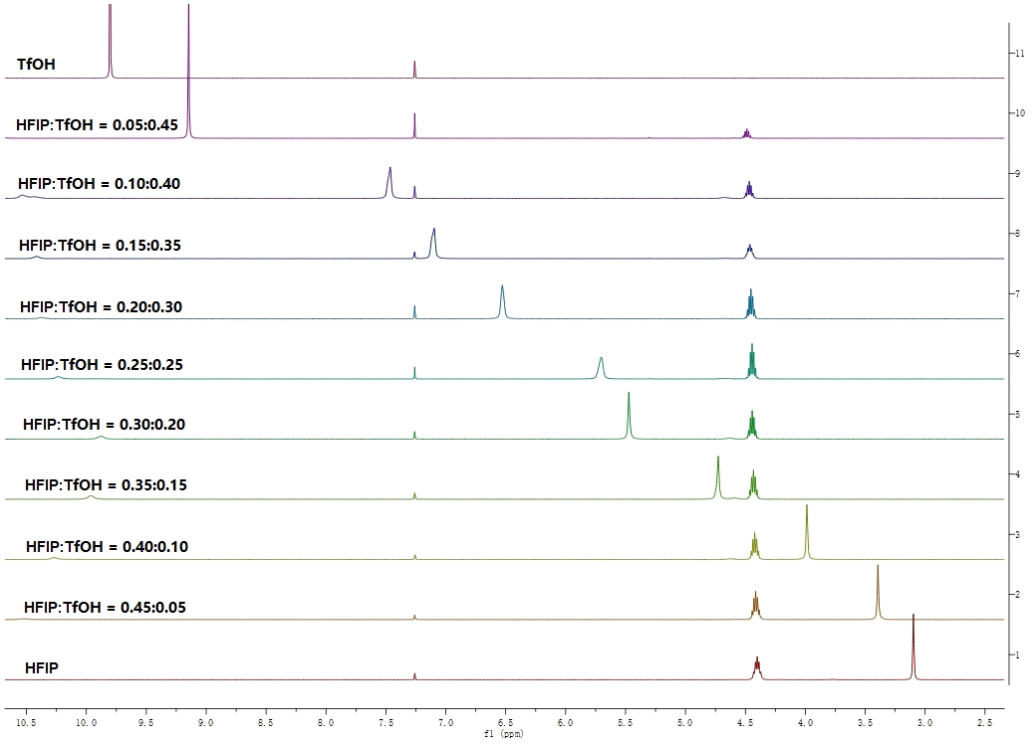
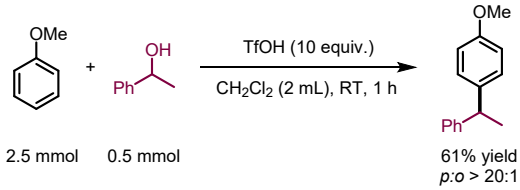


Figure S4. ^{1}H-NMR Titration of HFIP with TfOH

HFIP, TfOH and $CDCl_3$ were purchased commercially 0.10 M stock solutions of HFIP (31.6 mL, 0.300 mmol) and TfOH (41.8 mg, 0.300 mmol) were prepared in 0.60 mL of $CDCl_3$ each. The total concentration of HFIP and TfOH was kept constant. Eleven NMR samples were prepared with a constant volume of 0.60 mL, where the molar fractions of HFIP and TfOH varied from 0.0 to 1.0.

5. Computational Section



It is worth noting that when the amount of TfOH was sufficient, the alkylation reaction can yield product with excellent regioselectivity even without using HFIP as solvent, indicating that a large amount of TfOH had the same effect as the TfOH/HFIP clusters in this reaction. Moreover, the equivalent effects of TfOH/HFIP clusters and TfOH clusters in this reaction has been demonstrated by DFT (Figure S6). However, considering the complexity of acid-solvent clusters and the same effect of TfOH clusters for this reaction, the complete reaction was mainly calculated with TfOH clusters as catalyst.

All the geometries were fully optimized using the B3LYP functional[8] and the 6-31g(d) basis set with the solution model density (SMD)[9] in HFIP as well as Grimme's D3 dispersion with Becke-Johnson damping[10]. Frequency calculations at the same level of theory were performed to identify all the stationary points as minima (zero imaginary frequencies) or transition states (one imaginary frequency) and to provide the thermal correction to Gibbs free energies at 298.15 K and 1 atm. The intrinsic reaction coordinate (IRC) analysis[11] was carried out to confirm that all stationary points are smoothly connected to each other. To consider the solvent effect, the single-point energy calculations were performed for all the species at the M06-2x level[12] with a larger basis set 6-311+G(d,p) using SMD model in HFIP. A correction of 1.89 kcal/mol was applied to account for the conversion from the standard state of 1 atm in the gas phase to 1 M in solution.[13] All the DFT calculations were performed with the Gaussian 09 program.[14] The Structures were visualized with CYLView.[15]

As HFIP is not by default parametrized within the SMD model in Gaussian 09, the following parameters reported by Paton and coworkers[15] were used: eps = 16.7; epsinf = 1.625626; HBondAcidity = 1.96; hbondbasicity = 0.00; SurfaceTensionAtInterface = 23.23; ElectronegativeHalogenicity = 0.6; CarbonAromaticity = 0.00.

To understand the stable species of acid TfOH (HA) in HFIP, the acid-solvent and acid-acid interactions were calculated and found that the reaction between two HA molecules is exergic by 6.0 kcal/mol while the reaction of HA with HFIP is exergic by only 0.5 kcal/mol (Figure S5), showing more strong acid-acid interaction compared with acid-solvent interaction. Therefore, the dimer HA-HA generated from acid-acid interaction was used in the following discussion of reaction mechanism.

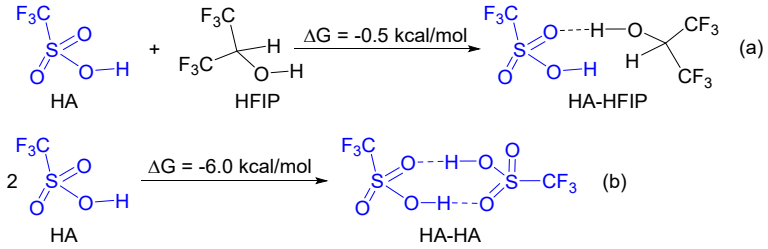


Figure S5. (a) The reaction of TfOH (HA) with HFIP; (b) The reaction of HA with HA.

The direct proton transfer from HA-HA to reactant 1-phenylethanol **R1** is exergic by 21.0 kcal/mol gives intermediate $\mathbf{1}_{02}$ having a six-membered ring (Figure S6). Addition of the second HA-HA gives intermediate $\mathbf{1}_{04}$ or $\mathbf{1'}_{04}$ bearing an eight-membered or a six-membered ring, with the former more stable by 16.5 kcal/mol. Coordination of the third HA-HA to O of H_2O in $\mathbf{1}_{04}$ generates intermediate $\mathbf{1}_{06}$. Two HFIP or HA molecules can coordinate to stabilize the species giving more stable intermediate $\mathbf{1}_{26}$ and $\mathbf{1}_{08}$. In order to form the carbocation, dissociation of H_2O molecule is needed. The energy barrier for dissociation of H_2O from $\mathbf{1}_{02}$ or $\mathbf{1}_{04}$ reaches 20 kcal/mol or even more while that from $\mathbf{1}_{06}$ is reduced to 14.8 kcal/mol. It is found that at $\mathbf{TS1}_{06}$ both dissociation of H_2O and capture of a proton from the acid occur simultaneously. The proton transfer from the acid to H_2O forming H_3O^+ lowers the energy barrier. At $\mathbf{TS1}_{26}$ and $\mathbf{TS1}_{08}$ with two HFIP and another two HA molecules

stabilizing the acid anion, the energy barriers are only 6.0 and 7.0 kcal/mol, respectively. The carbocation in intermediates $\mathbf{2}_{06}$, $\mathbf{2}_{26}$ and $\mathbf{2}_{08}$ are stabilized by the weakly coordinating anions involving one H_3O^+ cation, two acid anions and several acid or HFIP molecules.

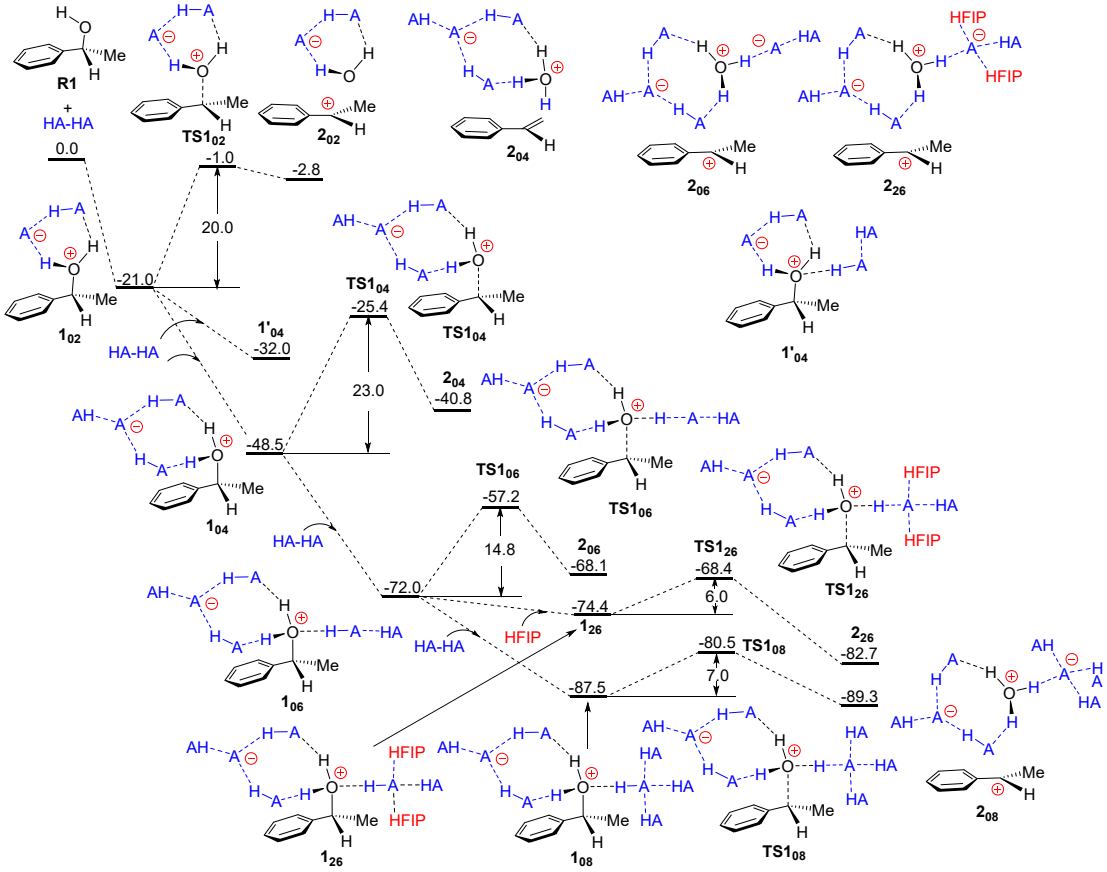


Figure S6. Gibbs free energy profiles for the reaction of reactant **R1** with acid to generate the cation species mediated by six or eight acid molecules, or six acid molecules with two HFIP molecules. The values of energies are given in kcal/mol.

For the most stable intermediate $\mathbf{2}_{08}$ mediated by eight acid molecules, the nucleophilic attack of anisole **R2** using the *para*, *ortho* and *meta* carbon of OMe to form C-C bond and the corresponding deprotonation steps have been calculated. Several possible directions of **R2** and positions of OMe have been considered. The preferred reaction pathways are shown in Figures. S7-S9. All energy barriers for C-C bond formation are very small, not more than 1 kcal/mol, indicating the nucleophilic attack of **R2** occurs quickly. The following deprotonations from carbocation have the energy barriers of 9.5, 12.1 and 12.7 kcal/mol at $\mathbf{TS3p}_{08}$, $\mathbf{TS3o}_{08}$ and $\mathbf{TS3m}_{08}$ relative to the most stable intermediate $\mathbf{5p}_{08}$, showing the *para*-selectivity consistent with observations in experiments.

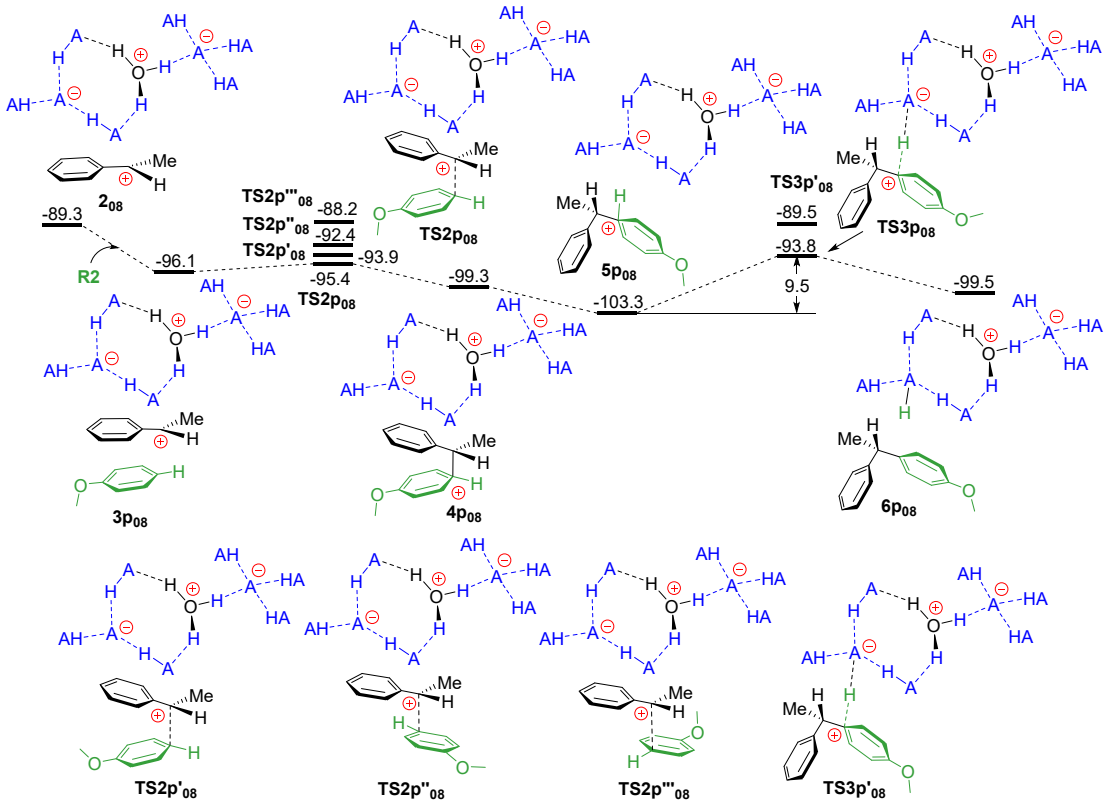


Figure S7. Gibbs free energy profile for the nucleophilic attack via the *para* carbon of OMe in anisole **R2** and the corresponding deprotonation step mediated by eight acid molecules. The values of energies are given in kcal/mol.

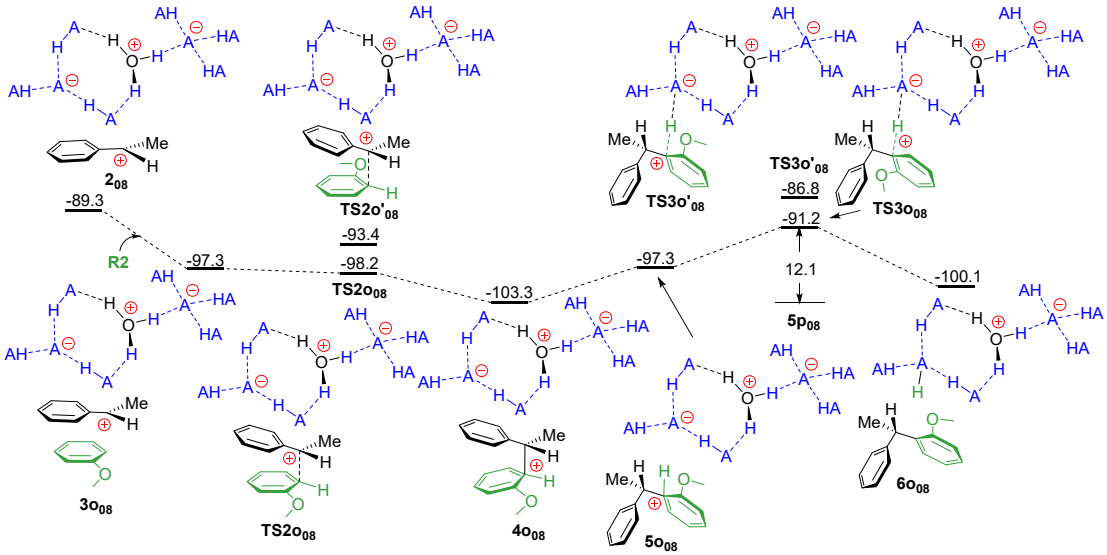


Figure S8. Gibbs free energy profile for the nucleophilic attack via the *ortho* carbon of OMe in anisole **R2** and the corresponding deprotonation step mediated by eight acid molecules. The values of energies are given in kcal/mol.

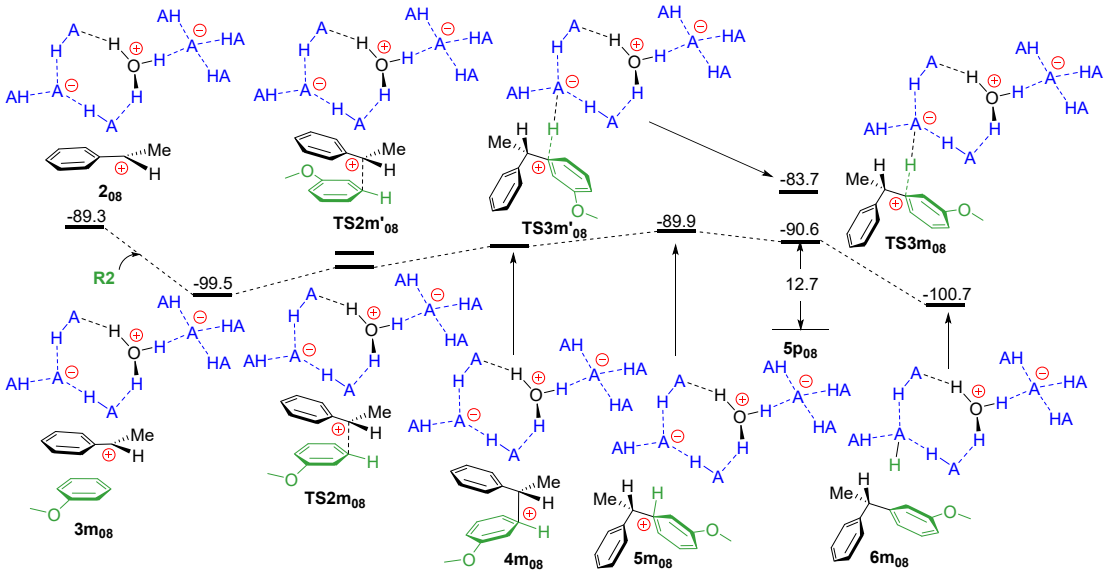


Figure S9. Gibbs free energy profile for the nucleophilic attack via the *meta* carbon of OMe in anisole **R2** and the corresponding deprotonation step mediated by eight acid molecules. The structures of transition states **TS2m$_{08}$** and **TS2m'$_{08}$**, as well as intermediate **4m$_{08}$** were not located, indicating the process is barrierless or have very small energy barrier. The values of energies are given in kcal/mol.

The difference of key transition states **TS3p$_{08}$**, **TS3o$_{08}$** and **TS3m$_{08}$** has been compared in Fig. 5 to understand the regioselectivity. The cation and anion in **TS3p$_{08}$**, **TS3o$_{08}$** and **TS3m$_{08}$** have been separated with the structures unchanged and the corresponding electronic energies have been calculated at the M06-2x/6-311+G(d,p) level with SMD model in HFIP. Transition state **TS3p$_{08}$** is lower in electronic energy than **TS3o$_{08}$** and **TS3m$_{08}$** by 4.1 and 5.8 kcal/mol at the M06-2x/6-311+G(d,p) level. The cation isomerization from the structure in **TS3o$_{08}$** to that in **TS3p$_{08}$** is endothermic by 7.2 kcal/mol, while that from the structure in **TS3m$_{08}$** to that in **TS3p$_{08}$** by 1.2 kcal/mol. Similarly, the anion isomerization from the structure in **TS3o$_{08}$** to that in **TS3p$_{08}$** is endothermic by 2.8 kcal/mol, while that from the structure in **TS3m$_{08}$** to that in **TS3p$_{08}$** by 6.9 kcal/mol. It is noted that all these changes of cation and anion are endothermic leading to relative instability of **TS3p$_{08}$** compared with **TS3o$_{08}$** and **TS3m$_{08}$**. Moreover, the interaction energies between cation and anion in **TS3p$_{08}$**, **TS3o$_{08}$** and **TS3m$_{08}$** have been calculated. The interaction energy change from **TS3o$_{08}$** to **TS3p$_{08}$** is -14.1 kcal/mol and that from **TS3m$_{08}$** to **TS3p$_{08}$** is -13.9 kcal/mol. In other words, the interaction energy between cation and anion in **TS3p$_{08}$** is stronger than that in **TS3o$_{08}$** and **TS3m$_{08}$** by 14.1 and 13.9 kcal/mol, respectively. Therefore, higher stability of **TS3p$_{08}$** than **TS3o$_{08}$** and **TS3m$_{08}$** can be understood by the strong interaction between cation and anion, consistent with the shorter O---H bond of 1.216 Å in **TS3p$_{08}$** compared with 1.264 Å in **TS3o$_{08}$** and 1.385 Å in **TS3m$_{08}$**.

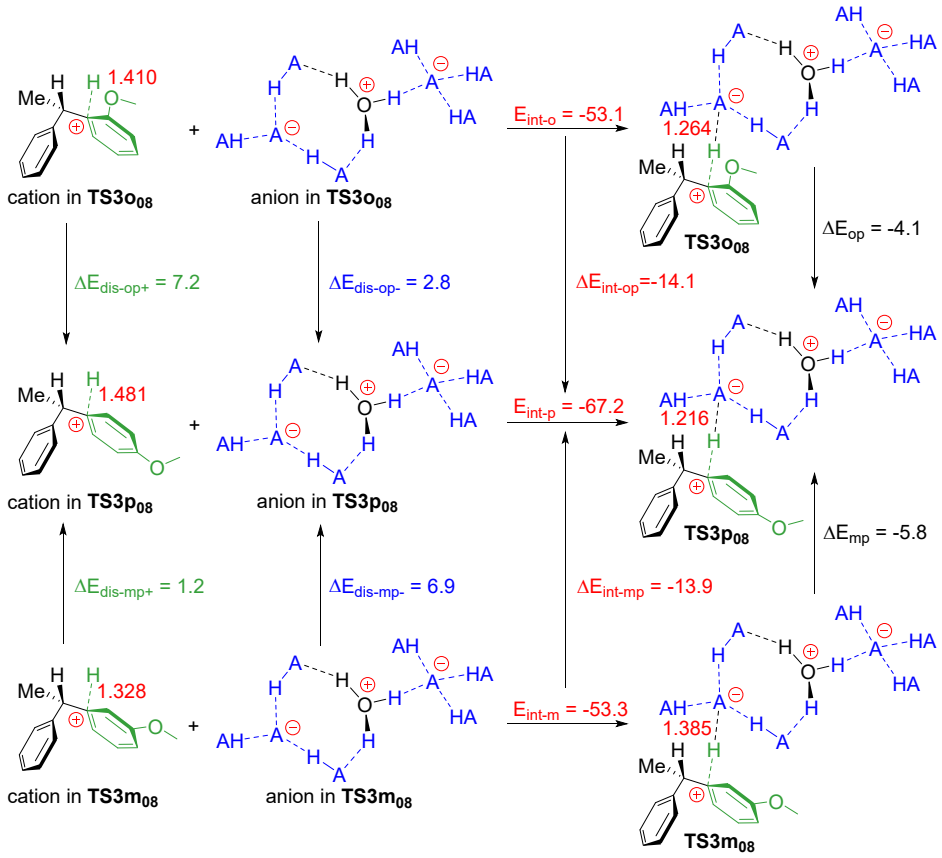


Figure S10. Comparisons of three deprotonation transition states **TS3p$_{08}$** and **TS3m$_{08}$** and **TS3o$_{08}$**. The values of electronic energy at the M06-2x/6-311+G(d,p) level and distance are given in kcal/mol and Å.

The deprotonation steps mediated by six acid molecules as well as that by six acid with two HFIP molecules have been examined and found that the energy barriers are 6.3 and 7.8 kcal/mol, respectively (Figure. S11). Considering the whole reaction, the energy barriers for the first step of carbocation formation are 14.8, 7.0 and 6.0 kcal/mol at **TS1$_{06}$**, **TS1$_{08}$** and **TS1$_{26}$**, and those for *para*-selective protonation steps are 6.3, 9.5 and 7.8 kcal/mol at **TS3$_{06}$**, **TS3$_{08}$** and **TS$_{26}$**, mediated by six acid, eight acid and six acid with two HFIP, respectively. In other words, the carbocation formation is the rate-determining step for reactions mediated by six acid, while the protonation step is the rate-determining for reactions mediated by eight acid and six acid with two HFIP.

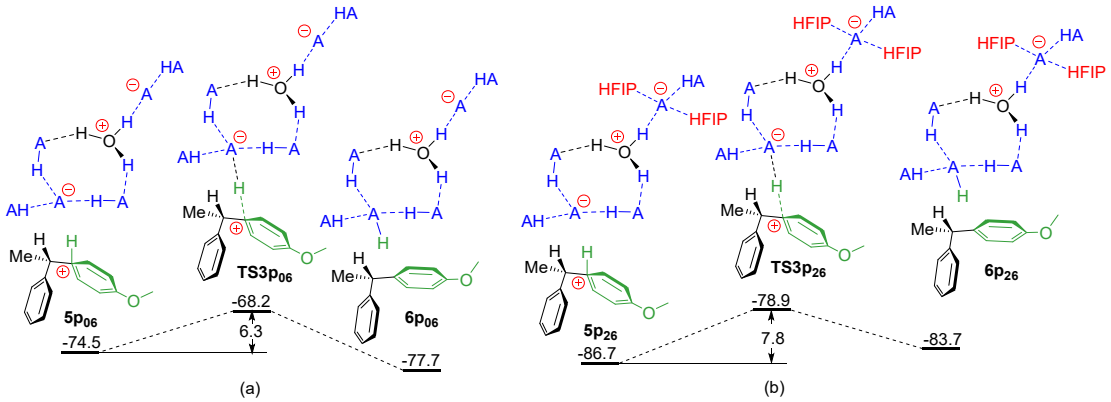


Figure S11. Gibbs free energy profiles for the deprotonation mediated by (a) six acid molecules and (b) six acid molecules with two HFIP molecules. The values of energies are given in kcal/mol.

To understand the complete reaction process, DFT analysis results were summarized in Figure S12. Direct proton transfer from TfOH to OH of **R1** mediated by six acid cluster occurs to give intermediate $\mathbf{1}_{06}$ with H_2O bonding to phenethyl (Figure S6). Dissociation of the formed H_2O and capture of a proton from the acid are found to occur simultaneously at $TS1_{06}$ for generating the carbocation. Coordination of more TfOH (at $\mathbf{TS1}_{08}$) or HFIP (at $\mathbf{TS1}_{26}$) molecules to the forming acid anion decrease the energy barrier for carbocation formation, being 7.8 kcal/mol and 8.8 kcal/mol lower than that coordinated by six TfOH molecules, respectively. For the most stable carbocation $\mathbf{2}_{08}$ coordinated by eight TfOH molecules, nucleophilic attack by anisole R2 using the *para*, *ortho* and *meta* carbon of OMe to form C-C bond and the corresponding deprotonation steps have been calculated (Figures S7-S9). Nucleophilic attack of **R2** is reversible with small energy barrier, not more than 1 kcal/mol, to give the relatively stable Wheland intermediate. The following deprotonations for *para*-, *ortho*- and *meta*- selective have been compared. $\mathbf{TS3p}_{08}$ is more stable than $\mathbf{TS3o}_{08}$ and $\mathbf{TS3m}_{08}$ by 2.6 and 3.2 kcal/mol, respectively, showing the *para*-selectivity consistent with observations in experiments. The higher stability of $\mathbf{TS3p}_{08}$ than $\mathbf{TS3o}_{08}$ and $\mathbf{TS3m}_{08}$ can be understood by the strong interaction between cation and anion supported by the shorter O---H bond of 1.216 Å in $\mathbf{TS3p}_{08}$ compared with 1.264 Å in $\mathbf{TS3o}_{08}$ and 1.385 Å in $\mathbf{TS3m}_{08}$. For the completely *para*-selective reaction, the deprotonation is the rate-determining step with relatively high energy barrier (9.5 kcal/mol) compared with that for the formation of carbocation (7.0 kcal/mol). Therefore, based on the above experimental results and DFT calculations, we speculate that the success of high site-selectivity for the Friedel-Crafts alkylation is a result of the reversible formation of Wheland intermediates and the rate-determining deprotonation.

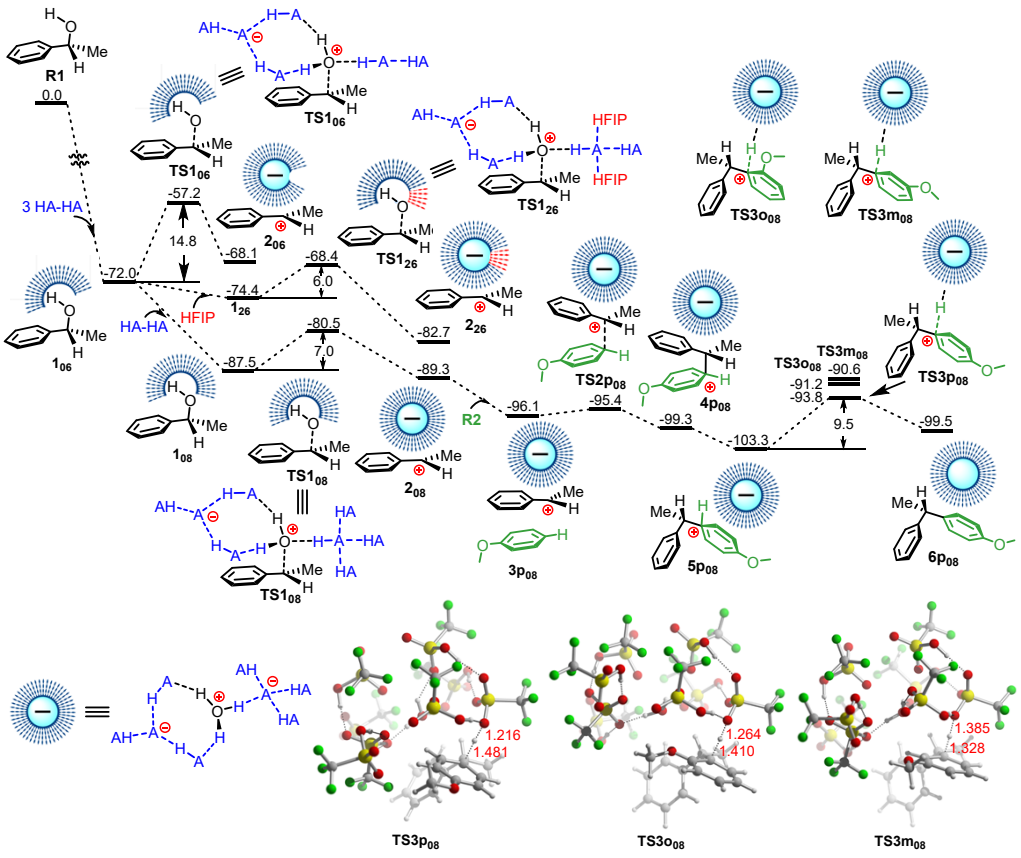


Figure S12. Summary of DFT analysis results. The values of energies and distances are given in kcal/mol and Å.

Calculated energies (in Hartree) for all stationary points

Stationary point	Thermal correction to Gibbs free energy	Single-point energy
HA	0.005507	-961.9687965
HFIP	0.027003	-789.8104586
HA-HFIP	0.050955	-1751.7955590
HA-HA	0.030553	-1923.9636859
R1	0.128999	-386.0317854
R2	0.102833	-346.7083003
1_{02}	0.180858	-2310.0442867
$TS1_{02}$	0.177200	-2310.0087125
2_{02}	0.178491	-2310.0129159
1_{04}	0.241148	-4234.0753630
$1'_{04}$	0.238798	-4234.0467299
$TS1_{04}$	0.232550	-4234.0301042
2_{04}	0.232714	-4234.0547659
1_{06}	0.298373	-6158.0972481
$TS1_{06}$	0.291999	-6158.0672387
2_{06}	0.292722	-6158.0852963
1_{26}	0.402084	-7737.7656151
$TS1_{26}$	0.397202	-7737.7512700
2_{26}	0.393574	-7737.7703316
1_{08}	0.353766	-8082.1044732
$TS1_{08}$	0.351535	-8082.0911197
2_{08}	0.352354	-8082.1059210
$3p_{08}$	0.478966	-8428.8457796
$TS2p_{08}$	0.478195	-8428.8438500
$TS2p'_{08}$	0.480164	-8428.8434477
$TS2p''_{08}$	0.481417	-8428.8422933
$TS2p'''_{08}$	0.478270	-8428.8325460
$4p_{08}$	0.478758	-8428.8506756
$5p_{08}$	0.482556	-8428.8609045
$TS3p_{08}$	0.478736	-8428.8418405
$TS3p'_{08}$	0.476320	-8428.8325966
$6p_{08}$	0.479909	-8428.8521135
$3o_{08}$	0.477384	-8428.8461033
$TS2o_{08}$	0.478700	-8428.8488242
$TS2o'_{08}$	0.480966	-8428.8434285
$4o_{08}$	0.479523	-8428.8578772
$5o_{08}$	0.479760	-8428.8485067
$TS3o_{08}$	0.476374	-8428.8353750
$TS3o'_{08}$	0.476888	-8428.8288861
$6o_{08}$	0.480710	-8428.8538718
$3m_{08}$	0.475728	-8428.8479122
$5m_{08}$	0.475132	-8428.8321018
$TS3m_{08}$	0.474604	-8428.8326247
$TS3m'_{08}$	0.476091	-8428.8231487
$6m_{08}$	0.476234	-8428.8503764
$5p_{06}$	0.419570	-6504.8249125
$TS3p_{06}$	0.415829	-6504.8110097
$6p_{06}$	0.418735	-6504.8291293

5p$_{26}$	0.522418	-8084.5079675
TS3p$_{26}$	0.520636	-8084.4938370
6p$_{26}$	0.525547	-8084.5064184

Cartesian coordinates for all the optimized structures

HA

H	-0.676959	-0.970860	1.453725
S	-2.188642	-0.853309	-0.060988
O	-1.653135	-1.019458	1.471534
O	-3.418692	-1.605917	-0.179391
O	-1.058034	-0.994737	-0.966887
C	-2.637071	0.953844	-0.007364
F	-1.550098	1.660249	0.308001
F	-3.074710	1.314128	-1.210562
F	-3.584626	1.156601	0.900450

HFIP

C	-0.000000	0.512861	-0.572925
H	0.000000	0.358237	-1.657470
O	-0.000001	1.869147	-0.202757
H	0.000000	2.415187	-1.000289
C	-1.280642	-0.136146	-0.034838
C	1.280642	-0.136144	-0.034837
F	-2.348052	0.478030	-0.580422
F	-1.338788	-1.439822	-0.367267
F	-1.372799	-0.034470	1.297102
F	1.338790	-1.439820	-0.367267
F	2.348052	0.478034	-0.580419
F	1.372797	-0.034470	1.297103

HA-HFIP

H	-1.607332	1.982410	-2.233647
S	-1.556142	2.281498	-0.106525
O	-0.283347	2.931125	-0.365327
O	-1.744798	1.304130	0.951893
O	-2.100312	1.599650	-1.480657
C	-2.842113	3.615747	0.120680
F	-2.477739	4.356388	1.161315
F	-2.868155	4.360962	-0.984067
F	-4.029951	3.074049	0.335002
O	-3.045415	-1.248792	1.131404
C	-3.178793	-1.414725	-0.248629
H	-2.363435	-0.953201	-0.818539
C	-4.479224	-0.768344	-0.748741
C	-3.121408	-2.916301	-0.536132
F	-4.543192	0.505408	-0.295816
F	-4.519372	-0.722800	-2.095070
F	-5.574702	-1.408642	-0.317342

F	-3.357751	-3.157906	-1.843345
F	-1.895510	-3.386585	-0.245427
F	-4.015543	-3.603605	0.185337
H	-2.663114	-0.367248	1.282571

HA-HA

H	0.318625	-0.459858	-1.093356
S	1.700508	0.737647	0.064513
O	0.919387	0.286459	1.228084
O	2.085575	2.122744	-0.083465
O	1.022090	0.230652	-1.282238
C	3.238864	-0.309077	0.077975
F	3.925091	-0.035345	1.182779
F	2.881809	-1.591999	0.069685
F	3.969683	-0.033325	-0.995098
H	-0.586887	-0.348054	1.559176
S	-2.065408	-1.135009	0.211276
O	-1.510947	-0.725994	1.644470
O	-3.170405	-2.049933	0.371837
O	-0.943591	-1.457469	-0.689978
C	-2.720151	0.505538	-0.378686
F	-1.711848	1.384784	-0.372549
F	-3.181435	0.360372	-1.615697
F	-3.686837	0.922122	0.426420

R1

C	0.703594	-1.246549	-0.266066
C	2.082925	-1.082860	-0.134813
C	2.615673	0.183877	0.111822
C	1.761544	1.282532	0.227512
C	0.382556	1.115127	0.100682
C	-0.158776	-0.152007	-0.145874
H	0.290875	-2.233065	-0.466538
H	2.741595	-1.941476	-0.232944
H	3.689818	0.314470	0.208924
H	2.170356	2.271499	0.416565
H	-0.288421	1.964665	0.185005
C	-1.662969	-0.337588	-0.243944
H	-1.862589	-1.237627	-0.849001
C	-2.299526	-0.526597	1.131719
H	-3.383576	-0.641440	1.031272
H	-1.890191	-1.413722	1.624940
H	-2.095649	0.346719	1.759597
O	-2.307253	0.793637	-0.828704
H	-1.856223	0.981273	-1.667236

R2

C	1.328072	1.351900	-0.000011
C	-0.039530	1.059333	-0.000004
C	-0.456584	-0.276368	-0.000003
C	0.496284	-1.305573	-0.000005
C	1.851731	-0.998415	-0.000012
C	2.278547	0.334175	-0.000016

H	1.644042	2.391607	-0.000012
H	-0.759640	1.869112	0.000004
H	0.146036	-2.332733	-0.000004
H	2.580829	-1.804048	-0.000015
H	3.337985	0.571576	-0.000021
O	-1.761341	-0.679522	0.000009
C	-2.763754	0.321023	-0.000062
H	-2.700679	0.955691	-0.894168
H	-3.718278	-0.208198	-0.000092
H	-2.700760	0.955734	0.894019

1_{02}

S	2.285236	0.108367	-0.176984
O	2.737172	1.487989	-0.275894
O	2.112712	-0.625275	-1.487917
O	1.112897	-0.158101	0.725691
C	3.621538	-0.877326	0.644909
F	4.740529	-0.820075	-0.074365
F	3.225947	-2.155896	0.744399
F	3.850495	-0.395503	1.866072
H	0.862399	-1.200237	-1.643174
C	-1.556260	-1.887968	1.449255
C	-2.732250	-1.531828	2.108723
C	-3.956948	-1.622317	1.447693
C	-4.006550	-2.081516	0.129529
C	-2.833841	-2.446532	-0.526998
C	-1.599481	-2.348208	0.129150
H	-0.597364	-1.781583	1.946475
H	-2.687426	-1.161134	3.127854
H	-4.870354	-1.324039	1.952937
H	-4.957962	-2.144338	-0.389718
H	-2.877147	-2.784745	-1.558338
C	-0.315063	-2.642149	-0.594971
H	0.531830	-2.502410	0.077600
C	-0.228808	-3.976878	-1.308485
H	-1.044398	-4.097824	-2.026295
H	0.723147	-4.068116	-1.840648
H	-0.292892	-4.781838	-0.569796
O	-0.148480	-1.584129	-1.660387
H	-0.716929	-0.789802	-1.430028
S	-1.768797	1.580417	-0.043392
O	-1.373990	0.689597	-1.150010
O	-0.885218	1.324034	1.235310
O	-3.159516	1.712315	0.336545
C	-1.127764	3.245948	-0.565285
F	0.185343	3.154580	-0.758320
F	-1.387545	4.139854	0.384066
F	-1.730803	3.601588	-1.698044
H	-0.026017	0.802385	1.011496

$TS1_{02}$

S	3.326322	-1.089533	-0.901289
O	4.232495	-0.057452	-0.407520

O	2.118122	-0.641036	-1.641310
O	3.022310	-2.200425	0.078865
C	4.237898	-2.052972	-2.194669
F	4.601597	-1.255189	-3.199606
F	3.421455	-3.013750	-2.691045
F	5.319609	-2.641699	-1.685853
H	0.568159	0.228610	-1.023116
C	0.692295	-3.814738	-0.596477
C	0.611259	-4.615492	0.529885
C	-0.627034	-4.804159	1.149302
C	-1.800407	-4.214260	0.641245
C	-1.735801	-3.422138	-0.483482
C	-0.479049	-3.194724	-1.121031
H	1.646165	-3.632196	-1.070684
H	1.507423	-5.064111	0.943431
H	-0.687411	-5.411280	2.048000
H	-2.745901	-4.371608	1.148841
H	-2.629041	-2.941518	-0.865373
C	-0.328069	-2.329293	-2.207190
H	0.695601	-2.135411	-2.523559
C	-1.379024	-1.597198	-2.918664
H	-2.385920	-1.998370	-2.791754
H	-1.329261	-0.591860	-2.450693
H	-1.133389	-1.479688	-3.978559
O	-0.382661	0.270149	-0.802841
H	-0.431771	-0.183555	0.055553
S	0.777585	-1.358342	2.614105
O	-0.047542	-1.507754	1.408499
O	2.182916	-2.036274	2.434067
O	0.242358	-1.715352	3.915494
C	1.246516	0.439607	2.644795
F	1.901376	0.733347	1.518171
F	2.018084	0.700031	3.694203
F	0.131109	1.167969	2.711807
H	2.528359	-2.019081	1.445885

2_{02}

S	1.718105	0.865876	-0.167552
O	1.659812	2.290541	-0.479770
O	1.577547	-0.067352	-1.321796
O	0.921925	0.423944	1.030765
C	3.439175	0.510777	0.423209
F	4.327841	0.896053	-0.492506
F	3.585618	-0.823283	0.616846
F	3.691301	1.131473	1.574392
H	0.644648	0.223690	-2.944427
C	0.711919	-2.436692	1.358848
C	-0.081124	-2.501118	2.492835
C	-1.446299	-2.774164	2.364340
C	-2.027688	-2.999380	1.106013
C	-1.242676	-2.951576	-0.028851
C	0.147697	-2.668184	0.074982
H	1.762723	-2.186196	1.435498

H	0.348810	-2.312138	3.470362
H	-2.073055	-2.799501	3.250782
H	-3.093862	-3.177646	1.024798
H	-1.691796	-3.099020	-1.002867
C	0.987473	-2.583255	-1.053037
H	2.027880	-2.347803	-0.855822
C	0.607182	-2.788531	-2.437453
H	-0.282682	-3.405656	-2.575849
H	0.353137	-1.769127	-2.872672
H	1.442267	-3.154899	-3.040866
O	-0.061257	-0.124706	-3.526198
H	-0.851048	-0.003316	-2.968689
S	-2.439815	0.321190	-0.060775
O	-1.670499	-0.225516	-1.184111
O	-1.582384	0.342922	1.257877
O	-3.761591	-0.197179	0.248015
C	-2.586563	2.140335	-0.409944
F	-1.362888	2.655416	-0.513967
F	-3.249769	2.741939	0.573796
F	-3.243042	2.302295	-1.559643
H	-0.556642	0.417905	1.084401

1_{04}

S	0.404902	-0.210325	2.139003
O	0.272315	-1.624116	1.719640
O	-0.485352	0.755577	1.429826
O	1.805442	0.288516	2.242941
C	-0.220896	-0.197442	3.883130
F	-1.509708	-0.546272	3.874517
F	-0.095636	1.029069	4.390094
F	0.473023	-1.060113	4.621530
H	-0.528671	1.782642	-0.979879
O	0.449458	1.841169	-1.204944
H	0.876194	0.939203	-1.070659
S	3.167356	-0.848524	-0.717355
O	1.753804	-0.425763	-0.791339
O	3.697395	-0.654197	0.757325
O	4.136090	-0.381921	-1.685812
C	3.124188	-2.709185	-0.809105
F	2.448349	-3.189843	0.231686
F	4.373771	-3.164316	-0.780911
F	2.535994	-3.061692	-1.944994
H	2.943423	-0.336048	1.371402
C	3.473211	2.579065	0.492062
C	4.851916	2.538593	0.282402
C	5.366442	2.687262	-1.004437
C	4.502167	2.878155	-2.085171
C	3.127030	2.931734	-1.877794
C	2.605891	2.781595	-0.585745
H	3.066145	2.437203	1.488381
H	5.519227	2.372566	1.122345
H	6.438543	2.640304	-1.169685
H	4.900490	2.977057	-3.090182

H	2.455773	3.071231	-2.720156
C	1.130580	2.883903	-0.331446
H	0.885314	2.595256	0.690205
C	0.517591	4.221033	-0.703236
H	0.986964	4.991129	-0.083667
H	0.713493	4.460691	-1.752137
H	-0.559037	4.231365	-0.522320
H	-2.019631	0.523624	1.056936
O	-3.011853	0.596600	0.843101
S	-3.292166	1.930021	0.040440
O	-2.060314	2.396656	-0.624516
O	-4.075792	2.873075	0.813571
C	-4.397717	1.262465	-1.304623
F	-5.331284	0.485132	-0.766452
F	-4.967172	2.308742	-1.901049
F	-3.684233	0.579639	-2.191152
H	0.059847	-2.239533	0.229048
O	-1.162317	-0.467849	-1.177996
S	-1.265921	-1.902648	-1.442717
O	-0.161930	-2.709890	-0.635130
O	-1.319537	-2.422755	-2.793497
C	-2.779534	-2.493168	-0.531018
F	-3.857588	-1.864543	-0.995721
F	-2.918335	-3.803732	-0.704697
F	-2.630436	-2.228512	0.769922

1'$_{04}$

S	3.175558	-0.055371	-1.132941
O	4.122882	0.851545	-0.523744
O	1.894397	0.728894	-1.601577
O	2.803932	-1.319395	-0.462567
C	3.832914	-0.615258	-2.779320
F	4.163614	0.436527	-3.515265
F	2.875455	-1.317678	-3.398816
F	4.895490	-1.388625	-2.580305
H	1.037225	0.167162	-1.576153
C	0.271310	-3.790948	0.228959
C	-0.226134	-4.498471	1.323451
C	-1.595852	-4.499444	1.587028
C	-2.467350	-3.801568	0.747833
C	-1.969609	-3.099492	-0.346648
C	-0.594658	-3.082017	-0.609455
H	1.339629	-3.770428	0.035073
H	0.457415	-5.029421	1.978418
H	-1.982547	-5.034231	2.449246
H	-3.533408	-3.788873	0.953184
H	-2.651066	-2.548591	-0.983355
C	-0.026882	-2.220372	-1.707728
H	1.051338	-2.378381	-1.765243
C	-0.641012	-2.391293	-3.086685
H	-1.721094	-2.219782	-3.075264
H	-0.183694	-1.691308	-3.793634
H	-0.459316	-3.410121	-3.441342

O	-0.212864	-0.798336	-1.327406
H	-0.168514	-0.741050	-0.340092
S	0.993854	-0.986160	2.466384
O	0.430852	-0.359081	1.267517
O	2.215088	-1.931881	2.058665
O	0.175032	-1.667468	3.444029
C	1.940400	0.372924	3.319088
F	2.898719	0.803342	2.499007
F	2.482105	-0.099360	4.436693
F	1.106874	1.370085	3.606957
H	2.534960	-1.677267	1.145036
H	-1.692252	-0.208532	-1.648527
S	-3.296315	0.630452	-0.472349
O	-3.634822	2.048856	-0.654595
O	-2.566207	0.190355	0.705678
O	-2.677671	0.013398	-1.798031
C	-4.944837	-0.231693	-0.538803
F	-5.694339	0.240093	0.452593
F	-5.529698	0.004749	-1.707261
F	-4.773937	-1.546692	-0.380176
H	-2.507788	3.310801	-0.509473
S	-0.380432	3.307944	-0.776988
O	-1.785577	4.001392	-0.462660
O	0.488187	4.266281	-1.426628
O	-0.616684	1.971184	-1.323066
C	0.245885	3.061151	0.956896
F	-0.633854	2.332074	1.639586
F	1.415680	2.424098	0.895306
F	0.411567	4.239512	1.550993

$TS1_{04}$

C	-0.074146	-3.612909	0.162125
C	-0.259620	-3.675592	1.529188
C	-1.518722	-3.375307	2.065552
C	-2.601193	-3.029794	1.241660
C	-2.433946	-2.974560	-0.127032
C	-1.157161	-3.254841	-0.694450
H	0.898166	-3.823842	-0.268333
H	0.569862	-3.923064	2.181940
H	-1.656893	-3.390105	3.141790
H	-3.559070	-2.778270	1.681406
H	-3.255542	-2.673838	-0.764709
C	-0.909575	-3.154804	-2.067457
H	0.125131	-3.304269	-2.369977
C	-1.832957	-2.785363	-3.128180
H	-2.890588	-2.809991	-2.871627
H	-1.534958	-1.720837	-3.305091
H	-1.617670	-3.327201	-4.055147
S	-0.708251	0.350155	1.857792
O	-0.495859	1.806827	1.712309
O	-0.158496	-0.496741	0.767154
O	-2.088318	-0.039571	2.273643
C	0.292198	-0.095412	3.356332

F	1.585377	0.114223	3.101418
F	0.117655	-1.393915	3.651007
F	-0.082981	0.640095	4.399272
H	0.355493	-0.091258	-2.402320
O	-0.575934	-0.171417	-2.662406
H	-1.050526	0.365625	-2.006473
S	-3.704863	0.380935	-0.798663
O	-2.426640	1.094140	-0.792907
O	-4.027388	-0.196793	0.638426
O	-3.991266	-0.631983	-1.807279
C	-5.041307	1.667190	-0.923022
F	-4.879386	2.565285	0.044029
F	-6.232186	1.083947	-0.805358
F	-4.942795	2.257306	-2.111695
H	-3.234794	-0.049926	1.285103
H	1.459993	-0.582268	0.451211
O	2.424075	-0.882654	0.514227
S	2.839145	-1.793250	-0.716222
O	1.831344	-1.749618	-1.777230
O	3.316225	-3.082212	-0.230604
C	4.337802	-0.855686	-1.312619
F	5.094429	-0.514998	-0.273355
F	5.019893	-1.669716	-2.119616
F	3.969475	0.227268	-1.983971
H	-0.048847	2.669053	0.414389
O	1.410941	1.208259	-1.144017
S	1.623161	2.642523	-0.959410
O	0.367900	3.306190	-0.250223
O	2.041241	3.501544	-2.047983
C	2.900189	2.767964	0.388951
F	4.034634	2.212706	-0.040145
F	3.116487	4.043112	0.697857
F	2.468421	2.112606	1.469528

2_{04}

C	-2.604081	-3.297382	0.419954
C	-3.930637	-3.035097	0.755524
C	-4.829060	-2.614317	-0.224117
C	-4.393572	-2.451579	-1.543006
C	-3.072570	-2.728109	-1.880390
C	-2.160138	-3.169389	-0.904132
H	-1.897516	-3.589869	1.191032
H	-4.254008	-3.136341	1.786913
H	-5.857427	-2.387019	0.039098
H	-5.078821	-2.088489	-2.301994
H	-2.744866	-2.589130	-2.907012
C	-0.759373	-3.486684	-1.216810
H	-0.094126	-3.540310	-0.357438
C	-0.239276	-3.710802	-2.437949
H	-0.850582	-3.713602	-3.336947
H	-0.050574	-1.655028	-2.067917
H	0.815970	-3.928289	-2.558461
S	-0.729025	-0.245462	1.777596

O	-0.431440	1.210751	1.845888
O	0.013720	-0.977916	0.711987
O	-2.172039	-0.585636	1.869626
C	-0.038167	-0.924440	3.356595
F	1.277403	-0.698482	3.383733
F	-0.262276	-2.240203	3.398919
F	-0.615841	-0.338336	4.401042
H	0.587241	-0.153633	-1.899862
O	-0.175745	-0.683462	-2.296287
H	-1.003454	-0.332006	-1.831401
S	-3.361482	1.032667	-0.916259
O	-1.936487	0.640847	-0.988140
O	-3.996003	0.434523	0.389170
O	-4.235255	0.855867	-2.056462
C	-3.303900	2.843646	-0.487799
F	-2.665819	2.993026	0.671222
F	-4.544508	3.308040	-0.384892
F	-2.653812	3.482650	-1.453513
H	-3.267271	0.021080	0.990072
H	1.660531	-0.913829	0.708837
O	2.661952	-1.023790	0.772119
S	3.184940	-1.914702	-0.438823
O	2.176842	-1.952234	-1.502986
O	3.793653	-3.139210	0.047187
C	4.577501	-0.821227	-1.029900
F	5.247375	-0.341480	0.014295
F	5.385307	-1.569860	-1.779482
F	4.100983	0.181685	-1.761731
H	-0.140879	2.133040	0.637252
O	1.461372	0.942384	-1.070992
S	1.452123	2.395492	-0.822712
O	0.137590	2.824986	-0.065335
O	1.702827	3.328919	-1.899149
C	2.740827	2.623027	0.505589
F	3.925645	2.263137	0.021757
F	2.768554	3.900600	0.869168
F	2.425618	1.860488	1.550221

1_{06}

S	3.327715	-1.577543	-0.250934
O	2.785980	-1.768423	-1.619161
O	2.305871	-1.641052	0.840264
O	4.293447	-0.457258	-0.096008
C	4.359929	-3.091925	0.024801
F	3.562345	-4.162576	-0.010212
F	4.947579	-3.015832	1.219319
F	5.287103	-3.191926	-0.924286
H	-0.138516	-0.431878	1.574714
O	0.257373	0.485912	1.613648
H	0.848631	0.616634	0.803147
S	2.307861	2.172660	-1.026204
O	1.650862	0.935977	-0.554687
O	3.870472	1.940817	-1.000803

O	1.952279	3.462284	-0.473069
C	2.000863	2.223629	-2.865018
F	2.576210	1.163442	-3.428012
F	2.535689	3.338789	-3.352975
F	0.693663	2.209286	-3.079061
H	4.065969	0.987049	-0.686767
H	-1.584625	1.411519	-0.206979
S	-1.838251	3.488569	-0.721946
O	-3.283025	3.208482	-0.662830
O	-1.279733	4.297568	-1.778777
O	-1.016406	2.137392	-0.600128
C	-1.442062	4.284019	0.915528
F	-2.253627	5.324696	1.082459
F	-1.667191	3.384997	1.885775
F	-0.180564	4.680370	0.952243
H	-4.234052	2.306415	0.395699
S	-4.008365	0.220716	0.855862
O	-4.734595	1.637626	0.947360
O	-4.536684	-0.643952	1.885773
O	-2.555796	0.417837	0.724781
C	-4.634819	-0.356605	-0.806900
F	-4.352086	0.575922	-1.709825
F	-4.047136	-1.504348	-1.124194
F	-5.949971	-0.530997	-0.728007
C	3.348105	1.386308	2.410900
C	4.304793	2.379659	2.211036
C	3.951740	3.723002	2.342521
C	2.640977	4.071186	2.672326
C	1.683530	3.080073	2.871827
C	2.031237	1.730488	2.741381
H	3.616010	0.342484	2.290643
H	5.319325	2.102370	1.942825
H	4.693913	4.498351	2.178083
H	2.360835	5.116265	2.760676
H	0.665559	3.360131	3.114010
C	1.027169	0.632543	2.927285
H	1.530641	-0.326193	3.044299
C	-0.037983	0.836558	3.984813
H	0.447691	0.975203	4.955236
H	-0.646378	1.717077	3.765269
H	-0.689916	-0.037773	4.040942
H	1.200192	-2.794106	0.759155
O	0.547027	-3.571513	0.852056
S	-0.386751	-3.351285	2.108624
O	-0.430237	-1.920229	2.460522
O	-0.137604	-4.332406	3.146255
C	-2.041521	-3.757726	1.348504
F	-1.920684	-4.803187	0.536610
F	-2.881678	-4.043382	2.337614
F	-2.492530	-2.706773	0.669634
H	1.501915	-1.112697	-2.279318
O	-0.351557	-1.166381	-0.519906
S	-0.636734	-1.100453	-1.952105

O	0.676100	-0.803020	-2.783479
O	-1.709989	-0.265139	-2.459334
C	-0.955334	-2.852764	-2.493763
F	-2.067928	-3.302563	-1.913678
F	-1.096919	-2.890723	-3.815294
F	0.079411	-3.607456	-2.126516

$TS1_{06}$

S	-1.078964	-3.435173	0.466172
O	-1.361558	-3.350992	-0.983838
O	-1.493099	-2.261908	1.281465
O	0.303019	-3.892137	0.809276
C	-2.166532	-4.815474	1.055676
F	-3.440542	-4.485382	0.844393
F	-1.967341	-5.003282	2.363111
F	-1.876351	-5.935436	0.396590
H	-0.357559	0.568227	1.592449
O	0.482360	0.091210	1.399465
H	0.333386	-0.311578	0.516192
S	2.378438	-2.235069	-1.400038
O	1.291768	-1.449307	-0.815500
O	2.315963	-3.721381	-0.822685
O	3.756096	-1.779427	-1.356125
C	1.945509	-2.551177	-3.186812
F	0.864876	-3.325957	-3.243734
F	2.969326	-3.168601	-3.771505
F	1.716711	-1.387608	-3.777076
H	1.459202	-3.851058	-0.289777
H	1.628078	1.003155	1.281815
S	2.865256	2.237485	-0.051696
O	2.816837	3.703709	0.082819
O	2.224840	1.576482	-1.175292
O	2.522247	1.553554	1.322134
C	4.688444	1.871683	-0.093151
F	5.241104	2.593104	-1.063991
F	5.243220	2.198204	1.079426
F	4.886418	0.577663	-0.327957
H	1.451307	4.600714	0.426012
S	-0.638882	4.099102	0.458293
O	0.597821	5.100745	0.591524
O	-1.796577	4.722317	1.067316
O	-0.217980	2.742317	0.803185
C	-0.873459	4.133978	-1.389823
F	0.231859	3.687816	-1.976209
F	-1.909722	3.361743	-1.713285
F	-1.118038	5.384686	-1.777900
C	3.268331	-1.845109	1.996031
C	4.605544	-1.524521	1.845203
C	5.175857	-0.561288	2.685047
C	4.420792	0.072253	3.683900
C	3.082444	-0.239120	3.837308
C	2.480417	-1.202861	2.986154
H	2.804797	-2.589129	1.361127

H	5.188452	-1.991782	1.060538
H	6.218129	-0.287190	2.552901
H	4.882036	0.823373	4.316028
H	2.487455	0.275703	4.582551
C	1.101814	-1.504726	3.020656
H	0.747255	-2.234526	2.298774
C	0.138961	-1.129370	4.065247
H	-0.064139	-2.046602	4.642787
H	0.480985	-0.350548	4.747279
H	-0.814417	-0.842736	3.612531
H	-2.766225	-1.258589	1.017301
O	-3.599586	-0.693577	1.084110
S	-3.429600	0.408288	2.217213
O	-2.004628	0.624848	2.508413
O	-4.358631	0.187552	3.310285
C	-4.024311	1.887112	1.259681
F	-5.249542	1.648621	0.797774
F	-4.041580	2.926787	2.084437
F	-3.198773	2.119600	0.245686
H	-1.171354	-2.110577	-2.013434
O	-1.280822	0.055112	-0.718128
S	-1.383859	0.039260	-2.178299
O	-1.079660	-1.418038	-2.737946
O	-0.708751	1.007780	-3.015385
C	-3.204503	0.114465	-2.562552
F	-3.687763	1.311345	-2.237526
F	-3.390353	-0.100397	-3.862828
F	-3.831146	-0.830137	-1.858018

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S	-3.159155	-1.681031	-0.176958
O	-3.026242	-1.476728	-1.632852
O	-2.537903	-0.629593	0.683497
O	-2.877898	-3.061584	0.311859
C	-4.970926	-1.473789	0.152443
F	-5.337670	-0.232582	-0.163709
F	-5.195186	-1.669761	1.466846
F	-5.682178	-2.350044	-0.546260
H	0.201837	0.685688	1.259960
O	0.515721	-0.250394	1.258599
H	0.309691	-0.649283	0.374552
S	0.361553	-3.432344	-0.830647
O	-0.141864	-2.077859	-0.574752
O	-0.849047	-4.451435	-0.627657
O	1.540320	-3.955725	-0.168166
C	0.611702	-3.543751	-2.675469
F	-0.570484	-3.400255	-3.272039
F	1.125832	-4.733244	-2.973622
F	1.435385	-2.577244	-3.043561
H	-1.685688	-3.935041	-0.389007
H	1.580467	-0.279474	1.420358
S	3.667679	-0.705097	0.386388
O	4.661477	0.364495	0.118981

O	2.792342	-1.108256	-0.716303
O	2.922363	-0.470776	1.688752
C	4.697018	-2.182778	0.832989
F	5.334232	-2.642908	-0.240199
F	5.584808	-1.851820	1.774822
F	3.900542	-3.148408	1.320978
H	4.305699	1.870598	0.574888
S	2.618608	3.248252	0.496298
O	4.127107	2.848690	0.785829
O	2.401752	4.597303	0.982714
O	1.710607	2.161151	0.857942
C	2.640534	3.296406	-1.364216
F	3.040189	2.114241	-1.819280
F	1.410496	3.568987	-1.806135
F	3.476314	4.246988	-1.777866
C	-0.481796	-2.817418	2.757829
C	0.871638	-3.067532	2.855814
C	1.678312	-2.191492	3.598113
C	1.137717	-1.066820	4.249089
C	-0.207439	-0.790985	4.136894
C	-1.054954	-1.671535	3.394730
H	-1.127183	-3.456459	2.164603
H	1.319304	-3.901065	2.329099
H	2.746296	-2.370098	3.644374
H	1.792595	-0.396957	4.794868
H	-0.622396	0.100075	4.591384
C	-2.416703	-1.447779	3.230103
H	-2.965832	-2.212368	2.687524
C	-3.223238	-0.335724	3.762694
H	-3.925471	-0.000919	2.993154
H	-3.847497	-0.728468	4.581988
H	-2.646292	0.514131	4.122403
H	-2.646871	0.990164	0.377400
O	-2.864468	1.971425	0.459734
S	-2.148539	2.575748	1.745781
O	-1.071239	1.682475	2.193180
O	-3.127949	3.035116	2.716925
C	-1.366016	4.075011	0.961579
F	-2.328198	4.902131	0.561368
F	-0.609331	4.661404	1.880417
F	-0.628900	3.703085	-0.075600
H	-1.707743	-0.955661	-2.467446
O	-0.462570	0.789075	-1.049573
S	-0.410583	0.776150	-2.511354
O	-1.012225	-0.580877	-3.086562
O	0.792950	1.078056	-3.253649
C	-1.738589	1.967067	-3.035988
F	-1.419448	3.189028	-2.615165
F	-1.858456	1.964848	-4.360149
F	-2.896099	1.589831	-2.481940

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S	-2.017958	-3.194806	1.881391

O	-1.617849	-4.062700	0.753544
O	-2.559379	-1.853473	1.529205
O	-0.994980	-3.113270	2.971253
C	-3.455841	-4.077370	2.647763
F	-4.447544	-4.115306	1.755267
F	-3.856796	-3.414221	3.732567
F	-3.102403	-5.315008	2.981925
H	-1.553535	0.428093	1.033429
O	-0.654134	0.382275	1.510454
H	-0.152405	-0.428593	1.145967
S	1.842286	-2.415869	1.147491
O	0.619888	-1.719843	0.682066
O	1.494985	-3.312062	2.402752
O	3.056998	-1.674142	1.413173
C	2.146688	-3.723980	-0.161854
F	1.200834	-4.654051	-0.035425
F	3.339770	-4.260911	0.036620
F	2.072077	-3.160340	-1.354471
H	0.481663	-3.341277	2.580076
H	0.497535	1.764574	1.064683
S	2.319697	2.236539	0.016901
O	2.269606	3.163657	-1.108739
O	2.413560	0.794808	-0.160934
O	1.117122	2.541281	1.044452
C	3.740712	2.806675	1.103761
F	4.734932	3.191512	0.320723
F	3.338405	3.818728	1.864247
F	4.119640	1.781295	1.859095
H	0.993216	3.138070	-2.443883
S	-0.340367	1.465445	-2.570992
O	0.330616	2.819936	-3.107536
O	-1.539390	1.228046	-3.338604
O	-0.334243	1.478460	-1.105075
C	0.980491	0.226611	-3.091458
F	2.177014	0.824916	-3.034742
F	0.977345	-0.798008	-2.238332
F	0.745105	-0.185485	-4.321692
H	-3.697007	-1.406997	0.414381
O	-4.491383	-0.940759	0.002029
S	-4.310876	0.631342	0.079002
O	-2.905045	0.964568	0.387181
O	-5.369786	1.241330	0.855976
C	-4.552781	1.109204	-1.719130
F	-5.857098	1.230336	-1.944318
F	-3.945842	2.275926	-1.901988
F	-4.038721	0.189632	-2.516326
H	-1.067227	-3.712118	-0.741467
O	-1.867599	-1.321482	-1.271662
S	-1.754580	-2.374836	-2.277069
O	-0.877397	-3.582433	-1.719533
O	-1.325269	-2.096737	-3.632251
C	-3.420765	-3.211393	-2.374784
F	-4.284917	-2.409505	-2.987598

F	-3.308074	-4.350135	-3.050968
F	-3.856058	-3.474297	-1.134830
H	-0.131407	4.012332	1.377604
O	-1.026831	4.266451	1.661152
C	-1.894821	4.019199	0.582627
H	-1.892839	2.973214	0.262688
C	-1.498316	4.842565	-0.649135
C	-3.308081	4.332987	1.071347
F	-0.162600	4.690211	-0.851760
F	-2.131534	4.398087	-1.747409
F	-1.736750	6.152828	-0.519448
F	-4.196455	4.140651	0.077007
F	-3.635252	3.508086	2.085242
F	-3.429992	5.591770	1.510321
H	3.299442	-0.581907	-1.303131
O	4.051598	-1.180104	-1.442925
C	5.120772	-0.670192	-0.700369
H	4.814394	-0.324671	0.292447
C	5.757707	0.527778	-1.420003
C	6.115112	-1.812280	-0.486893
F	4.778971	1.391206	-1.794577
F	6.590865	1.199489	-0.600835
F	6.433361	0.184287	-2.522212
F	7.234010	-1.350415	0.110387
F	5.579208	-2.751181	0.310678
F	6.464745	-2.397179	-1.640277
C	1.464764	-0.146634	3.967305
C	2.674923	0.307548	4.488210
C	2.855197	1.668835	4.735209
C	1.825551	2.573244	4.461508
C	0.618574	2.121811	3.933419
C	0.434173	0.755276	3.675807
H	1.317494	-1.207489	3.796918
H	3.469964	-0.400822	4.697234
H	3.797006	2.026485	5.140931
H	1.965134	3.632454	4.654300
H	-0.165853	2.834857	3.701060
C	-0.831213	0.233919	3.073256
H	-0.919326	-0.843001	3.195668
C	-2.115100	0.941810	3.434894
H	-2.203103	0.922908	4.525621
H	-2.128087	1.982407	3.107297
H	-2.977667	0.426064	3.012074

$TS1_{26}$

S	0.776873	4.218891	0.215658
O	1.802522	3.867148	1.222614
O	-0.603686	3.743567	0.479399
O	1.193924	3.957169	-1.199920
C	0.662315	6.066273	0.316709
F	0.257517	6.414434	1.536427
F	-0.217931	6.498177	-0.588136
F	1.856631	6.600605	0.068146

H	-1.034233	1.287968	-0.462636
O	-0.477082	1.116476	-1.267086
H	0.470168	1.178510	-0.992187
S	3.449595	1.380356	-1.783736
O	2.294969	0.979176	-0.961061
O	3.438435	2.961513	-1.952585
O	3.692715	0.757170	-3.073873
C	5.023155	1.183689	-0.781679
F	4.763903	1.415293	0.495965
F	5.906982	2.072332	-1.234950
F	5.490603	-0.038019	-0.962612
H	2.600906	3.370903	-1.543010
H	-0.741435	-0.289277	-1.741228
S	-0.006765	-2.304748	-1.395127
O	-0.729615	-3.571138	-1.298595
O	0.617148	-1.678215	-0.241035
O	-0.927586	-1.232786	-2.132064
C	1.278190	-2.558550	-2.725052
F	2.100934	-3.528270	-2.363656
F	0.656298	-2.883780	-3.859922
F	1.942208	-1.420010	-2.888983
H	-1.779146	-4.052393	0.019473
S	-2.447116	-2.865797	1.671041
O	-2.303011	-4.229658	0.846095
O	-3.621103	-2.951228	2.513789
O	-2.207089	-1.727413	0.784198
C	-0.955823	-3.008666	2.781394
F	0.129224	-3.247476	2.049892
F	-0.816150	-1.862979	3.448213
F	-1.143210	-4.004606	3.642991
C	0.797083	1.488915	-4.304901
C	1.249604	0.579309	-5.247859
C	0.334630	-0.283652	-5.860575
C	-1.029165	-0.236371	-5.538932
C	-1.486849	0.658913	-4.584654
C	-0.571224	1.532197	-3.949879
H	1.494945	2.162149	-3.819785
H	2.306730	0.527122	-5.480878
H	0.686561	-1.007053	-6.590197
H	-1.724329	-0.916007	-6.020729
H	-2.532320	0.661505	-4.299155
C	-0.956903	2.401250	-2.884493
H	-0.195552	3.086183	-2.520039
C	-2.350862	2.716870	-2.507444
H	-2.721743	3.420787	-3.270700
H	-3.011672	1.848863	-2.503262
H	-2.391538	3.221965	-1.542756
H	-1.327721	3.055152	1.810644
O	-2.036673	2.647081	2.397424
S	-3.172911	2.037270	1.462499
O	-2.569672	1.307513	0.336952
O	-4.240188	2.985898	1.202022
C	-3.804926	0.742044	2.643247

F	-4.441427	1.333857	3.647656
F	-4.646411	-0.028434	1.958434
F	-2.794552	0.019557	3.109917
H	2.323585	2.422228	1.759929
O	0.281790	0.984722	1.369880
S	1.294638	0.637436	2.362163
O	2.581218	1.550661	2.193836
O	1.735289	-0.730845	2.561987
C	0.661653	1.283663	3.989688
F	-0.483325	0.684283	4.295314
F	1.560832	1.054167	4.940772
F	0.462429	2.599989	3.866181
H	-2.771174	-1.078926	-2.521377
O	-3.605714	-0.578469	-2.589317
C	-4.336092	-0.839789	-1.413365
H	-3.750099	-0.652599	-0.510411
C	-4.757728	-2.313233	-1.374513
C	-5.526046	0.114247	-1.395066
F	-3.659760	-3.078031	-1.599063
F	-5.254028	-2.647010	-0.172982
F	-5.664582	-2.626681	-2.311360
F	-6.297401	-0.120928	-0.319415
F	-5.092231	1.390713	-1.321980
F	-6.284971	0.007526	-2.496060
H	2.443351	-1.406414	0.099002
O	3.376970	-1.647620	-0.023528
C	3.739905	-2.522032	1.009697
H	3.174352	-2.336997	1.927042
C	5.212634	-2.266180	1.330814
C	3.466436	-3.970788	0.590012
F	5.374672	-0.993438	1.735657
F	5.638341	-3.072320	2.322637
F	6.004317	-2.467058	0.263453
F	3.808593	-4.843203	1.555115
F	2.140231	-4.125440	0.357952
F	4.115919	-4.309100	-0.534454

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S	-0.359623	3.876505	1.095699
O	-1.582393	3.826526	0.267753
O	0.848889	3.228354	0.512099
O	-0.548270	3.502142	2.527798
C	0.073663	5.677380	1.147289
F	0.330187	6.094952	-0.093452
F	1.159331	5.845950	1.906341
F	-0.939542	6.373159	1.656212
H	1.563940	0.514400	0.298424
O	0.744373	0.338965	0.846225
H	-0.029524	0.526219	0.241127
S	-2.970553	0.899984	2.427061
O	-1.998633	0.816698	1.336768
O	-2.528601	2.070697	3.430114
O	-3.320404	-0.255595	3.231717

C	-4.546340	1.677379	1.782258
F	-4.213679	2.772284	1.092793
F	-5.289463	2.023178	2.832351
F	-5.211427	0.837096	1.017433
H	-1.856784	2.684833	2.990979
H	0.717981	-0.655974	1.135301
S	-0.191596	-2.924107	0.850485
O	0.450863	-4.101173	0.223592
O	-1.072384	-2.109885	-0.000928
O	0.771060	-2.065079	1.644484
C	-1.254926	-3.663262	2.180848
F	-2.038189	-4.604435	1.673788
F	-0.470912	-4.201113	3.128197
F	-1.999402	-2.699972	2.727157
H	1.217089	-3.972607	-1.181127
S	1.894976	-2.307649	-2.377443
O	1.714296	-3.849056	-2.056244
O	3.078244	-2.128432	-3.197357
O	1.703285	-1.504532	-1.166622
C	0.399356	-2.030706	-3.458033
F	-0.693659	-2.408017	-2.804597
F	0.321447	-0.735551	-3.767312
F	0.530831	-2.744425	-4.572651
C	0.218518	0.205971	4.172557
C	-0.259901	-0.981682	4.684937
C	0.644284	-2.024805	4.935798
C	2.019378	-1.888594	4.678905
C	2.510546	-0.711335	4.153538
C	1.609936	0.365533	3.883365
H	-0.456399	1.026714	3.963719
H	-1.321507	-1.110707	4.859561
H	0.270449	-2.967408	5.322029
H	2.688333	-2.720776	4.869023
H	3.558842	-0.621510	3.902819
C	2.002503	1.552960	3.268972
H	1.211950	2.278271	3.076778
C	3.333017	1.922791	2.786933
H	3.532941	2.978031	3.011123
H	4.147718	1.285381	3.124224
H	3.292121	1.868509	1.685038
H	1.326402	3.192519	-1.009591
O	1.899515	3.059323	-1.838314
S	3.211103	2.273491	-1.419506
O	2.888337	1.217097	-0.443197
O	4.330221	3.153360	-1.137745
C	3.521535	1.400497	-3.033303
F	3.930580	2.278007	-3.941963
F	4.470835	0.495728	-2.808427
F	2.406705	0.809116	-3.441084
H	-2.325330	2.676576	-0.633027
O	-0.492464	1.036225	-1.298779
S	-1.691367	1.254671	-2.118256
O	-2.769614	2.094678	-1.324999

O	-2.344919	0.164565	-2.809290
C	-1.128762	2.499266	-3.383446
F	-0.087140	2.003023	-4.043843
F	-2.119095	2.764594	-4.226492
F	-0.767986	3.617455	-2.745797
H	2.576301	-1.723280	1.227297
O	3.303208	-1.084986	1.381921
C	4.384739	-1.392305	0.546193
H	4.204166	-1.107467	-0.496560
C	4.665065	-2.900348	0.572244
C	5.581488	-0.581863	1.051770
F	3.504058	-3.557365	0.340684
F	5.541872	-3.258121	-0.372635
F	5.128022	-3.310807	1.767071
F	6.723450	-0.996591	0.483649
F	5.429459	0.724891	0.767722
F	5.719040	-0.684047	2.394038
H	-2.747834	-1.536743	0.159502
O	-3.693133	-1.307224	0.076545
C	-4.158309	-1.833580	-1.132489
H	-3.430510	-1.732996	-1.944411
C	-5.391487	-1.024239	-1.536648
C	-4.460605	-3.329314	-0.979435
F	-5.069338	0.269804	-1.698746
F	-5.899691	-1.474010	-2.701475
F	-6.362483	-1.091285	-0.607828
F	-4.864959	-3.876332	-2.142756
F	-3.331983	-3.970483	-0.599677
F	-5.399243	-3.575363	-0.053001

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S	2.815013	2.995353	-1.420481
O	3.756217	2.530996	-0.377739
O	1.389976	3.066343	-0.978389
O	2.956176	2.353597	-2.756960
C	3.281745	4.763140	-1.721038
F	3.094259	5.450194	-0.592928
F	2.501882	5.262190	-2.680800
F	4.556523	4.840452	-2.090739
H	-0.637982	1.570821	-0.843718
O	-0.392196	0.792662	-1.460333
H	0.491947	0.426148	-1.155068
S	2.965421	-1.059318	-2.066334
O	2.088267	-0.289802	-1.161880
O	3.301594	-0.151734	-3.329774
O	2.578614	-2.374134	-2.533130
C	4.681271	-1.137490	-1.301900
F	5.094107	0.118492	-1.122877
F	5.466046	-1.749817	-2.182221
F	4.682363	-1.785355	-0.157442
H	3.256641	0.834198	-3.080177
H	-1.702482	-0.622040	-1.253901
S	-1.538468	-2.592360	-0.402396

O	-2.576373	-3.149893	0.451384
O	-0.313159	-2.007557	0.125870
O	-2.172965	-1.480984	-1.397880
C	-1.174665	-3.911043	-1.699261
F	-1.199802	-5.092433	-1.118517
F	-2.135249	-3.842427	-2.622437
F	0.004641	-3.657668	-2.239470
H	-3.587857	-2.236718	1.702983
S	-2.931566	-0.390988	2.560523
O	-3.765494	-1.757884	2.549112
O	-3.679704	0.603904	3.300890
O	-2.381218	-0.119868	1.232562
C	-1.515121	-0.949915	3.634667
F	-0.851403	-1.917232	3.006646
F	-0.709247	0.085747	3.865659
F	-1.990439	-1.405484	4.790030
C	-0.054178	-0.913890	-4.223985
C	-0.585949	-1.987200	-4.936104
C	-1.949834	-2.021280	-5.227042
C	-2.778028	-0.975453	-4.812097
C	-2.248215	0.093328	-4.091800
C	-0.880249	0.128047	-3.783430
H	1.010484	-0.881770	-4.031141
H	0.067897	-2.790809	-5.259269
H	-2.367874	-2.856666	-5.780710
H	-3.839109	-0.993874	-5.038535
H	-2.907448	0.888660	-3.765877
C	-0.283517	1.240887	-2.979482
H	0.794391	1.302509	-3.111562
C	-0.923739	2.604605	-3.106409
H	-0.905386	2.871729	-4.167708
H	-1.960006	2.611352	-2.765494
H	-0.358286	3.349171	-2.547926
H	-3.880892	-1.347471	-2.175548
O	-4.768961	-0.982102	-2.402434
S	-5.469603	-0.426446	-1.055436
O	-5.039696	-1.221887	0.083334
O	-6.857566	-0.167575	-1.368619
C	-4.602071	1.228418	-0.930405
F	-5.134685	2.082466	-1.798140
F	-4.704857	1.696858	0.301914
F	-3.304439	1.059597	-1.246087
H	0.863001	3.593449	0.441060
O	0.283273	3.987361	1.175842
S	-1.234943	3.891623	0.736100
O	-1.458195	2.681625	-0.080097
O	-1.760417	5.154989	0.255056
C	-1.989469	3.526930	2.396421
F	-1.801480	4.568126	3.200222
F	-3.285733	3.322247	2.200941
F	-1.418761	2.446704	2.911313
H	3.475549	1.289579	0.637499
O	0.913672	0.998565	1.083694

S	1.956649	0.537958	2.001157
O	3.392500	0.551192	1.318500
O	1.824473	-0.708008	2.730108
C	2.203948	1.920655	3.225429
F	1.062147	2.177541	3.855394
F	3.136397	1.574468	4.106122
F	2.602040	3.007793	2.554808
H	1.337705	-2.326775	0.561856
O	3.534470	-4.753935	0.337792
S	2.279925	-4.229790	0.837264
O	0.984258	-4.799739	0.481522
O	2.269747	-2.650875	0.561669
C	2.365227	-4.209279	2.696271
F	3.456849	-3.564667	3.090063
F	1.279960	-3.601987	3.174500
F	2.402170	-5.469450	3.130389

$TS1_{08}$

S	2.014923	3.433684	-1.476239
O	3.041492	3.144073	-0.452483
O	0.603281	3.328280	-1.012199
O	2.216151	2.760746	-2.794248
C	2.244283	5.232603	-1.856756
F	2.020245	5.939844	-0.749139
F	1.372748	5.594997	-2.800253
F	3.484912	5.448406	-2.286842
H	-1.144413	1.167483	-0.679558
O	-0.628315	0.525905	-1.240114
H	0.281361	0.522894	-0.856878
S	3.204994	-0.503550	-2.027133
O	2.155634	0.019348	-1.142840
O	3.342913	0.475133	-3.282728
O	3.153874	-1.864011	-2.526530
C	4.881500	-0.187837	-1.242203
F	4.985562	1.128275	-1.043018
F	5.805706	-0.585116	-2.111426
F	5.017515	-0.831394	-0.102529
H	3.014682	1.405663	-3.041948
H	-1.207289	-0.889084	-1.229596
S	-0.962625	-2.889978	-0.344524
O	-2.044599	-3.604107	0.323422
O	0.092287	-2.228702	0.411613
O	-1.567998	-1.849421	-1.396572
C	-0.230219	-4.106279	-1.564186
F	0.004552	-5.247167	-0.947829
F	-1.126476	-4.295271	-2.538895
F	0.882486	-3.589421	-2.066330
H	-3.086926	-2.892157	1.644902
S	-2.863959	-0.938284	2.497885
O	-3.358445	-2.461461	2.493686
O	-3.857715	-0.119471	3.161334
O	-2.316074	-0.581609	1.188731
C	-1.427083	-1.134851	3.670096

F	-0.556724	-1.999610	3.160236
F	-0.842702	0.049916	3.846636
F	-1.878379	-1.583432	4.838766
C	0.275036	-0.905649	-4.217655
C	0.081478	-2.140192	-4.818327
C	-1.216328	-2.558545	-5.129021
C	-2.320786	-1.742759	-4.847818
C	-2.134733	-0.510881	-4.239610
C	-0.828953	-0.074803	-3.914151
H	1.277883	-0.564688	-3.995642
H	0.934414	-2.775465	-5.030535
H	-1.372934	-3.529910	-5.588556
H	-3.323764	-2.083803	-5.078856
H	-2.994638	0.098489	-3.990856
C	-0.579256	1.169700	-3.254697
H	0.461549	1.444609	-3.112120
C	-1.536432	2.296308	-3.192869
H	-1.476202	2.783919	-4.179772
H	-2.570156	1.994813	-3.025613
H	-1.227162	3.024872	-2.446045
H	-3.260448	-2.099820	-2.007630
O	-4.179758	-2.035832	-2.369364
S	-5.184100	-1.535336	-1.205486
O	-4.801866	-2.119044	0.069189
O	-6.524557	-1.606376	-1.745987
C	-4.677807	0.267176	-1.145992
F	-5.283932	0.943057	-2.121449
F	-4.976206	0.784804	0.031524
F	-3.352057	0.332448	-1.354280
H	-0.031819	3.687683	0.444074
O	-0.665626	3.947115	1.187542
S	-2.154749	3.623467	0.737512
O	-2.185294	2.415142	-0.101907
O	-2.864428	4.805969	0.283994
C	-2.832106	3.133113	2.398824
F	-2.867141	4.197169	3.194857
F	-4.059161	2.666982	2.199760
F	-2.059263	2.195546	2.932390
H	3.103558	1.918036	0.622684
O	0.687994	1.150154	1.079658
S	1.781551	0.946744	2.031743
O	3.191813	1.235374	1.357762
O	1.893061	-0.267228	2.814171
C	1.692666	2.400690	3.192336
F	0.504075	2.426184	3.786364
F	2.652478	2.305156	4.106267
F	1.863002	3.518779	2.478372
H	1.806949	-2.095331	0.550073
O	4.620759	-3.799695	0.620131
S	3.229353	-3.642116	0.992895
O	2.190635	-4.585987	0.596626
O	2.792303	-2.151403	0.592176
C	3.145961	-3.496184	2.846227

F	3.973847	-2.546100	3.262943
F	1.896325	-3.202344	3.202897
F	3.499213	-4.667829	3.377618

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S	0.872005	3.725943	-1.526112
O	2.019336	3.684776	-0.596264
O	-0.429588	3.253470	-0.966890
O	1.120824	3.164854	-2.885355
C	0.600398	5.534935	-1.824399
F	0.287506	6.119836	-0.667718
F	-0.408679	5.688320	-2.686978
F	1.702889	6.084190	-2.325184
H	-1.616925	0.736715	-0.189943
O	-0.868091	0.348627	-0.733267
H	-0.042166	0.494241	-0.182812
S	3.043988	0.288402	-2.263800
O	1.963938	0.532527	-1.304983
O	2.894714	1.328263	-3.478304
O	3.268864	-1.023283	-2.842381
C	4.654778	0.951095	-1.562113
F	4.476218	2.258584	-1.340529
F	5.596861	0.777969	-2.483149
F	4.990238	0.348654	-0.441242
H	2.333394	2.116006	-3.191585
H	-1.019742	-0.654908	-0.886157
S	-0.352285	-3.025936	-0.475408
O	-1.160285	-3.988739	0.289680
O	0.637514	-2.225332	0.263687
O	-1.190268	-2.122929	-1.375277
C	0.568387	-4.063814	-1.716584
F	1.085569	-5.128320	-1.133003
F	-0.299877	-4.453893	-2.667282
F	1.523809	-3.324138	-2.279624
H	-2.037018	-3.524185	1.677359
S	-2.264456	-1.649013	2.712996
O	-2.400680	-3.225456	2.560877
O	-3.328493	-1.156045	3.564347
O	-1.975517	-1.028839	1.418069
C	-0.689580	-1.594875	3.711499
F	0.283752	-2.205291	3.046664
F	-0.355698	-0.320461	3.932866
F	-0.892818	-2.203498	4.877227
C	-0.085204	-0.079694	-4.040983
C	0.280084	-1.347852	-4.444748
C	-0.725101	-2.284164	-4.724832
C	-2.089834	-1.966182	-4.592829
C	-2.465640	-0.712655	-4.159111
C	-1.462642	0.264386	-3.874378
H	0.664377	0.669295	-3.826577
H	1.327724	-1.614662	-4.520741
H	-0.445310	-3.285837	-5.034381
H	-2.842291	-2.720473	-4.790652

H	-3.512802	-0.482517	-4.008794
C	-1.739232	1.537173	-3.379501
H	-0.876998	2.177782	-3.203221
C	-3.034975	2.114835	-3.016041
H	-3.117833	3.123001	-3.444266
H	-3.906851	1.513105	-3.267191
H	-3.013194	2.275741	-1.924131
H	-2.665443	-2.722373	-1.792943
O	-3.585694	-2.946297	-2.139838
S	-4.694752	-2.663112	-1.019095
O	-4.193571	-2.978651	0.306671
O	-5.961442	-3.146019	-1.529104
C	-4.728657	-0.801447	-1.126747
F	-5.368297	-0.411513	-2.240315
F	-5.318151	-0.282453	-0.065238
F	-3.461073	-0.352462	-1.206274
H	-0.920841	3.515079	0.514484
O	-1.454290	3.637390	1.372231
S	-2.889739	2.990436	1.198631
O	-2.817310	1.827355	0.288402
O	-3.925321	3.977432	0.957219
C	-3.082433	2.326298	2.926896
F	-3.137656	3.346613	3.776897
F	-4.208575	1.630316	2.966781
F	-2.042044	1.554013	3.212726
H	2.574032	2.544815	0.426765
O	0.555239	1.213138	1.225114
S	1.808710	1.269616	1.993250
O	2.959326	1.938827	1.133915
O	2.337244	0.108613	2.672126
C	1.498991	2.623787	3.233713
F	0.470828	2.289983	4.006372
F	2.586251	2.800944	3.975619
F	1.218386	3.745906	2.566841
H	2.231598	-1.829856	0.186211
O	5.436143	-2.576202	-0.026925
S	4.101845	-2.862438	0.464189
O	3.372584	-4.073629	0.110983
O	3.194548	-1.573623	0.183257
C	4.157737	-2.788245	2.321878
F	4.749714	-1.665014	2.713999
F	2.914193	-2.836983	2.799218
F	4.848986	-3.838710	2.769096

$3p_{08}$

S	2.158073	-2.300238	2.327774
O	0.928725	-2.911123	2.875394
O	2.083948	-0.822158	2.112776
O	2.794237	-3.014850	1.190240
C	3.403798	-2.479730	3.687532
F	2.987980	-1.797922	4.754669
F	4.575102	-1.972397	3.272783
F	3.565281	-3.760623	4.001065

H	0.774955	1.326572	0.675394
O	0.515035	0.618648	0.017156
H	-0.217864	0.085653	0.446071
S	0.154607	-3.466306	-1.068412
O	0.006042	-2.263437	-0.249011
O	1.667199	-3.988851	-0.941245
O	-0.185303	-3.484520	-2.479323
C	-0.696329	-4.889838	-0.193862
F	-0.124643	-5.002042	1.012505
F	-0.477106	-5.996822	-0.896207
F	-1.987800	-4.677442	-0.059313
H	2.056946	-3.674726	-0.063222
H	0.198715	1.038442	-0.860992
S	-1.581242	1.168820	-2.584912
O	-2.399069	2.354441	-2.885475
O	-2.083813	0.245045	-1.550301
O	-0.117321	1.485649	-2.322815
C	-1.487598	0.225576	-4.187683
F	-2.674286	0.170303	-4.763412
F	-0.623762	0.857259	-4.999496
F	-1.028666	-1.003237	-3.940648
H	-2.784967	3.485045	-1.662201
S	-2.485951	3.537006	0.474646
O	-3.138019	4.019058	-0.891322
O	-2.462883	4.643590	1.410362
O	-1.291610	2.727537	0.223795
C	-3.826419	2.370267	1.039940
F	-4.007806	1.421120	0.129878
F	-3.463091	1.818533	2.201975
F	-4.955131	3.053395	1.213525
C	2.612435	-0.595956	-1.596138
C	2.046811	-0.843222	-2.836934
C	2.301471	0.030709	-3.895407
C	3.109529	1.168486	-3.722048
C	3.659018	1.437392	-2.486252
C	3.410263	0.567790	-1.383306
H	2.408193	-1.242642	-0.754767
H	1.393608	-1.693707	-2.987478
H	1.841940	-0.154575	-4.860624
H	3.274413	1.848153	-4.550448
H	4.253484	2.332071	-2.343828
C	3.895424	0.813281	-0.094473
H	3.574793	0.120891	0.678878
C	4.573259	2.043709	0.376103
H	5.099249	2.591526	-0.406769
H	3.792083	2.696320	0.791602
H	5.257243	1.823592	1.199339
C	4.960313	-2.449369	-1.274609
C	5.230636	-1.893596	-2.538423
C	6.045874	-0.743701	-2.644789
C	6.551946	-0.149738	-1.504281
C	6.231995	-0.664325	-0.235296
C	5.464930	-1.832006	-0.135610

H	7.177824	0.733678	-1.589882
H	6.644802	-0.208834	0.658718
H	0.597643	2.796583	-3.029669
O	1.142677	3.594399	-3.313544
S	0.771772	4.854950	-2.398885
O	-0.644478	4.864354	-2.074327
O	1.469912	6.004528	-2.938379
C	1.658547	4.359670	-0.825720
F	2.940218	4.734538	-0.874524
F	1.068530	4.903416	0.226543
F	1.627536	3.018357	-0.715875
H	1.423662	0.108479	3.215896
O	1.142118	0.829759	3.877750
S	1.511130	2.257541	3.301817
O	1.622486	2.189002	1.829547
O	2.585687	2.892125	4.040539
C	-0.082687	3.145041	3.676555
F	-0.203265	3.290178	4.991499
F	-0.026583	4.328043	3.082301
F	-1.095240	2.429633	3.202798
H	-0.620954	-2.776289	2.381984
O	-1.063857	-0.312707	1.815141
S	-2.126650	-1.227967	2.259475
O	-1.618284	-2.728284	2.242170
O	-3.458055	-1.175430	1.700628
C	-2.208772	-0.918865	4.094533
F	-2.546269	0.348254	4.311637
F	-3.108209	-1.728506	4.641978
F	-1.004224	-1.160961	4.615701
H	-2.444108	-1.342822	-1.352325
O	-3.972291	-4.149442	-2.171281
S	-3.933979	-2.700747	-2.108687
O	-3.960772	-1.858071	-3.296918
O	-2.705212	-2.288205	-1.168683
C	-5.339574	-2.145545	-1.024780
F	-5.343032	-2.838680	0.109115
F	-5.201775	-0.846120	-0.762480
F	-6.485571	-2.350163	-1.677901
H	5.228992	-2.247139	0.836758
H	4.345304	-3.334016	-1.177536
H	6.255229	-0.354951	-3.635104
O	4.763380	-2.381042	-3.702400
C	3.982418	-3.580110	-3.676596
H	3.709154	-3.772782	-4.713818
H	4.573361	-4.416809	-3.287678
H	3.080910	-3.455361	-3.070928

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S	-2.340092	-2.433627	-2.125192
O	-1.135079	-3.087706	-2.674813
O	-2.225451	-0.959733	-1.914025
O	-2.997664	-3.133482	-0.987294
C	-3.596980	-2.583316	-3.478536

F	-3.168737	-1.919513	-4.551283
F	-4.751497	-2.037123	-3.058687
F	-3.802804	-3.859138	-3.785605
H	-0.787219	1.310168	-0.646264
O	-0.473965	0.640382	0.026053
H	0.202111	0.063595	-0.435764
S	-0.367154	-3.367395	1.337166
O	-0.161398	-2.254275	0.412513
O	-1.912004	-3.808733	1.274188
O	-0.006670	-3.288328	2.740745
C	0.380191	-4.906597	0.570354
F	-0.212783	-5.072184	-0.620150
F	0.099270	-5.942386	1.355838
F	1.680218	-4.789955	0.408800
H	-2.281956	-3.589068	0.358607
H	-0.068723	1.104241	0.846373
S	1.868758	1.269684	2.413639
O	2.773643	2.419039	2.574262
O	2.260919	0.237581	1.432893
O	0.415615	1.657561	2.207486
C	1.813546	0.456666	4.088212
F	3.027301	0.370329	4.602644
F	1.037073	1.196463	4.894836
F	1.273071	-0.758111	3.960409
H	3.095060	3.452368	1.257318
S	2.643737	3.380000	-0.851914
O	3.411032	3.920824	0.429068
O	2.594722	4.424250	-1.856232
O	1.443532	2.635460	-0.466791
C	3.893945	2.125263	-1.431451
F	4.103731	1.224975	-0.478910
F	3.424495	1.522328	-2.529050
F	5.034271	2.745000	-1.727703
C	-2.580611	-0.245903	1.800185
C	-1.899408	-0.336100	3.013158
C	-2.080389	0.647048	3.984059
C	-2.926341	1.734091	3.733498
C	-3.601089	1.826865	2.523527
C	-3.437660	0.839947	1.531465
H	-2.410442	-0.987041	1.031069
H	-1.204498	-1.149930	3.186631
H	-1.531374	0.590872	4.918075
H	-3.034977	2.520510	4.472722
H	-4.234198	2.687245	2.334057
C	-4.136174	0.905719	0.242670
H	-3.644118	0.311385	-0.524903
C	-4.611357	2.241661	-0.287176
H	-5.310499	2.747040	0.383839
H	-3.737428	2.885884	-0.412930
H	-5.080516	2.130860	-1.267873
C	-4.940033	-2.113883	1.523697
C	-5.260240	-1.489468	2.757540
C	-6.062727	-0.307796	2.785609

C	-6.356955	0.327012	1.616897
C	-5.777920	-0.128975	0.374855
C	-5.247922	-1.465407	0.358088
H	-6.930462	1.248375	1.627618
H	-6.238397	0.220434	-0.545051
H	-0.219795	3.019951	2.899882
O	-0.696609	3.864792	3.167427
S	-0.342208	5.033027	2.134322
O	1.044045	4.948951	1.705814
O	-0.941782	6.253743	2.635881
C	-1.367632	4.476749	0.668811
F	-2.618288	4.933208	0.776998
F	-0.825243	4.912209	-0.458784
F	-1.417676	3.133382	0.653345
H	-1.581149	-0.067916	-3.079830
O	-1.341840	0.601482	-3.805353
S	-1.642178	2.072581	-3.296130
O	-1.693665	2.087751	-1.820752
O	-2.726877	2.693711	-4.031649
C	-0.040600	2.888276	-3.790741
F	0.005052	2.991828	-5.114676
F	-0.017973	4.088992	-3.230933
F	0.973193	2.148965	-3.358066
H	0.420018	-2.987194	-2.193708
O	0.910500	-0.493158	-1.825195
S	1.945501	-1.458293	-2.227378
O	1.419120	-2.944792	-2.069690
O	3.294843	-1.384110	-1.716414
C	1.965827	-1.299725	-4.083788
F	2.314905	-0.061265	-4.415604
F	2.831415	-2.168198	-4.595129
F	0.739195	-1.560090	-4.540706
H	2.413451	-1.387102	1.390006
O	3.832227	-4.234607	2.287703
S	3.866303	-2.791717	2.139006
O	4.040008	-1.888037	3.268160
O	2.584257	-2.365744	1.279384
C	5.206549	-2.381837	0.916099
F	5.076785	-3.135224	-0.171287
F	5.123092	-1.092672	0.590642
F	6.389274	-2.622501	1.487173
H	-4.976287	-1.916027	-0.587629
H	-4.422810	-3.063109	1.503534
H	-6.381377	0.066491	3.751571
O	-4.897247	-1.953050	3.937691
C	-4.021144	-3.097888	4.021615
H	-3.796056	-3.203007	5.081333
H	-4.533151	-3.992124	3.655353
H	-3.106927	-2.921495	3.452290

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S	-2.016515	-3.470916	0.947934
O	-1.999572	-3.956518	-0.436236

O	-2.610622	-2.160479	1.246028
O	-0.625111	-3.639635	1.617435
C	-3.020173	-4.720105	1.892728
F	-4.282878	-4.629181	1.488165
F	-2.939917	-4.446858	3.195304
F	-2.548054	-5.938365	1.658420
H	-1.846508	0.676876	0.921574
O	-0.924658	0.478288	0.586582
H	-0.998321	0.313322	-0.389827
S	1.518136	-2.806338	-1.024293
O	0.303898	-2.032349	-0.771262
O	1.553306	-4.062264	-0.016081
O	2.830296	-2.200539	-1.075895
C	1.286494	-3.734425	-2.624262
F	0.220554	-4.532811	-2.513019
F	2.366922	-4.465106	-2.866977
F	1.096724	-2.855096	-3.599503
H	0.725188	-4.047943	0.528364
H	-0.277044	1.283425	0.746423
S	2.030133	2.149183	0.213104
O	2.260802	3.244417	-0.740642
O	2.144581	0.766903	-0.306571
O	0.759616	2.297972	1.039178
C	3.336077	2.366834	1.521934
F	4.520195	2.536827	0.946347
F	3.032083	3.445945	2.248067
F	3.363771	1.293231	2.309522
H	1.183396	3.594634	-2.090483
S	-0.269599	2.289232	-3.000574
O	0.701035	3.545740	-2.964119
O	-1.271570	2.519048	-4.017200
O	-0.632461	1.893662	-1.635061
C	0.915402	0.951087	-3.605876
F	2.170924	1.347086	-3.401781
F	0.697121	-0.166797	-2.907475
F	0.716563	0.726512	-4.895324
H	0.382844	3.847388	1.535650
O	0.056781	4.760758	1.792513
S	-0.756443	5.431510	0.592314
O	-0.203031	5.057245	-0.699940
O	-1.026272	6.805166	0.965590
C	-2.358247	4.498682	0.736486
F	-2.917984	4.695779	1.930679
F	-3.185857	4.909005	-0.219264
F	-2.122444	3.184630	0.583176
H	-3.907369	-1.307492	0.442875
O	-4.760621	-0.817450	0.280308
S	-4.718137	0.596500	1.014788
O	-3.370043	0.809538	1.573644
O	-5.882718	0.771792	1.853640
C	-4.889694	1.750217	-0.444430
F	-5.943979	1.389286	-1.164492
F	-5.071762	2.972793	0.048371

F	-3.787749	1.714755	-1.181130
C	-1.147381	1.584808	3.799930
C	-0.774659	2.893371	4.099697
C	0.511172	3.163354	4.572814
C	1.406851	2.112410	4.763380
C	1.029124	0.801400	4.466204
C	-0.246950	0.523437	3.967634
H	-2.146836	1.385484	3.426929
H	-1.476087	3.704159	3.934285
H	0.811859	4.186157	4.777008
H	2.410864	2.311153	5.126738
H	1.746658	-0.001755	4.602503
C	-0.701013	-0.886958	3.597364
H	-1.319257	-0.791451	2.702298
C	-1.605622	-1.478571	4.689716
H	-1.086230	-1.541509	5.651765
H	-2.477738	-0.833977	4.827913
H	-1.967194	-2.475929	4.416614
C	2.673887	-1.868577	2.099690
C	3.070564	-2.933697	2.937342
C	2.197491	-3.414879	3.932319
C	0.958973	-2.814925	4.100367
C	0.487968	-1.791136	3.230409
C	1.424052	-1.316850	2.250184
H	3.373887	-1.498686	1.359603
H	2.489813	-4.228778	4.584007
H	0.308903	-3.178681	4.889144
H	-0.159657	-2.771256	2.352131
H	-1.771100	-3.102888	-1.917306
O	-2.320182	-0.715586	-1.347405
S	-2.430982	-1.217908	-2.720777
O	-1.805133	-2.679253	-2.818766
O	-1.998568	-0.447795	-3.864810
C	-4.230582	-1.637541	-2.937378
F	-4.952110	-0.529545	-2.801935
F	-4.428223	-2.166627	-4.137273
F	-4.573163	-2.520418	-1.992292
H	3.412499	0.340994	-1.365259
O	5.058799	-0.328909	0.362150
S	5.394610	-0.432528	-1.056956
O	4.206545	0.161972	-1.946021
O	5.903990	-1.659424	-1.639939
C	6.658531	0.883169	-1.417788
F	7.755168	0.617296	-0.704673
F	6.956691	0.874687	-2.715109
F	6.187832	2.082038	-1.076511
H	1.130346	-0.511559	1.591925
O	4.293575	-3.422541	2.706449
C	4.778591	-4.501383	3.503177
H	5.775655	-4.719440	3.121785
H	4.841156	-4.213785	4.558952
H	4.140754	-5.386235	3.395721

TS2p''$_{08}$

S	3.487508	-0.152119	1.474233
O	3.158616	-1.366963	2.248840
O	2.386816	0.837960	1.332066
O	4.238706	-0.386544	0.208883
C	4.723967	0.738024	2.530360
F	4.200154	0.980243	3.726664
F	5.047486	1.905182	1.946675
F	5.838142	0.007725	2.666240
H	-0.316575	1.607520	0.467472
O	-0.066320	0.950786	-0.245080
H	0.001127	0.066810	0.209156
S	1.909609	-2.311216	-1.614910
O	1.261173	-1.530030	-0.561489
O	3.354886	-1.668707	-1.907163
O	1.283642	-2.556132	-2.897834
C	2.492647	-3.920868	-0.850392
F	3.318748	-3.590434	0.154434
F	3.165936	-4.601153	-1.773427
F	1.493165	-4.638188	-0.386893
H	3.695587	-1.225173	-1.069733
H	-0.796572	0.925661	-0.975526
S	-2.731687	-0.229486	-2.080420
O	-4.134290	0.214540	-2.023798
O	-2.296140	-1.217951	-1.077744
O	-1.744077	0.925895	-2.162374
C	-2.546659	-1.017146	-3.755941
F	-3.549586	-1.848084	-3.983111
F	-2.546368	-0.050373	-4.685589
F	-1.382728	-1.667348	-3.801183
H	-4.774576	0.856942	-0.590010
S	-3.998647	1.166812	1.399399
O	-5.153644	1.074733	0.311502
O	-4.389572	2.106110	2.432163
O	-2.682716	1.232674	0.762981
C	-4.161462	-0.540665	2.127224
F	-3.975113	-1.454351	1.182523
F	-3.245332	-0.691006	3.089210
F	-5.375810	-0.679231	2.656504
C	1.528662	0.988367	-3.357088
C	0.611888	0.865499	-4.392192
C	-0.059020	1.998954	-4.861546
C	0.190153	3.250434	-4.291198
C	1.100829	3.372607	-3.246850
C	1.776739	2.239535	-2.759903
H	2.061601	0.115274	-3.002109
H	0.402283	-0.113347	-4.807658
H	-0.792274	1.904553	-5.655897
H	-0.351220	4.122961	-4.639144
H	1.259800	4.342976	-2.790007
C	2.707698	2.313863	-1.630044
H	2.962789	1.346760	-1.207267
C	2.537812	3.398101	-0.598225

H	2.672633	4.403777	-1.007965
H	1.515841	3.336679	-0.210954
H	3.216212	3.252337	0.242261
C	6.150500	1.636146	-0.980552
C	6.154630	0.499198	-1.824126
C	5.427714	0.503089	-3.044379
C	4.656551	1.584139	-3.366915
C	4.509184	2.692827	-2.462242
C	5.375591	2.717500	-1.320934
H	4.073162	1.576495	-4.280853
H	4.195011	3.645287	-2.879032
H	-2.349125	2.321748	-2.807714
O	-2.628747	3.218603	-3.169947
S	-3.243476	4.128191	-2.009170
O	-4.019072	3.333784	-1.071608
O	-3.747322	5.338954	-2.626484
C	-1.670844	4.582162	-1.118189
F	-0.957536	5.446856	-1.847719
F	-1.953637	5.118241	0.059889
F	-0.930837	3.472896	-0.938861
H	1.527344	1.225915	2.651835
O	1.094362	1.646662	3.462594
S	0.270076	2.934850	3.029721
O	-0.093363	2.845536	1.604884
O	0.882021	4.155422	3.519814
C	-1.271821	2.610394	4.021132
F	-0.971270	2.670755	5.316064
F	-2.156889	3.544787	3.710114
F	-1.736225	1.403859	3.722141
H	1.818265	-2.303767	2.044428
O	-0.186086	-0.694124	1.824133
S	-0.301576	-2.049457	2.377045
O	1.008625	-2.898375	2.079667
O	-1.455259	-2.882467	2.123796
C	-0.108934	-1.808470	4.215121
F	-1.105280	-1.061464	4.677675
F	-0.114641	-2.993007	4.818558
F	1.055794	-1.194397	4.439780
H	-1.405098	-2.581912	-1.029553
O	-0.820611	-5.740555	-1.801814
S	-1.739997	-4.643236	-1.564129
O	-2.652449	-4.145477	-2.584598
O	-0.896386	-3.436868	-0.935540
C	-2.781015	-5.089291	-0.088758
F	-2.006861	-5.519100	0.902521
F	-3.469256	-4.017888	0.302053
F	-3.627954	-6.058298	-0.445590
H	5.375597	3.591242	-0.678064
H	6.724449	1.643776	-0.064372
H	5.479646	-0.378295	-3.672612
O	6.807265	-0.622557	-1.561455
C	7.507811	-0.773409	-0.315231
H	7.904099	-1.787521	-0.334054

H	8.330602	-0.054462	-0.249786
H	6.817356	-0.652911	0.520861

TS2p'''$_{08}$

S	1.902216	-3.355106	0.594461
O	0.566162	-3.761697	1.059612
O	2.435468	-2.097010	1.205192
O	2.145879	-3.401507	-0.872757
C	3.007685	-4.682030	1.269119
F	2.910906	-4.707500	2.597256
F	4.280495	-4.424179	0.927099
F	2.653646	-5.861383	0.767206
H	0.869586	0.817185	0.628042
O	0.408681	0.410618	-0.160864
H	-0.370552	-0.102326	0.198125
S	-1.017185	-2.780980	-2.359060
O	-0.773073	-1.994625	-1.149939
O	0.367311	-3.433394	-2.838772
O	-1.665433	-2.220955	-3.528421
C	-1.899337	-4.356850	-1.862358
F	-1.124715	-4.977522	-0.960277
F	-2.025412	-5.124255	-2.940819
F	-3.080922	-4.106488	-1.336341
H	0.993435	-3.506980	-2.057980
H	0.074752	1.147673	-0.801683
S	-1.964804	2.135060	-1.776131
O	-2.583154	3.425901	-1.434833
O	-2.410017	0.951342	-1.015580
O	-0.443710	2.172181	-1.811450
C	-2.382879	1.860218	-3.570150
F	-3.651302	2.156118	-3.796435
F	-1.597617	2.658048	-4.309493
F	-2.135671	0.590073	-3.884203
H	-2.489709	4.066764	0.143173
S	-1.754523	3.317915	2.029507
O	-2.576969	4.317841	1.110245
O	-1.315543	4.013317	3.223805
O	-0.823239	2.520727	1.229053
C	-3.147066	2.187173	2.533259
F	-3.671594	1.620639	1.453758
F	-2.670249	1.245555	3.353942
F	-4.076977	2.892977	3.172749
C	1.902344	-0.319311	-2.648430
C	1.143118	0.035920	-3.756236
C	1.388567	1.251569	-4.402128
C	2.401769	2.098090	-3.944861
C	3.172088	1.735983	-2.842869
C	2.920498	0.527678	-2.169184
H	1.694966	-1.244164	-2.125661
H	0.346099	-0.614836	-4.098922
H	0.773845	1.548244	-5.245748
H	2.572619	3.054512	-4.427473
H	3.933863	2.416816	-2.478386

C	3.653581	0.150291	-0.948682
H	3.052503	-0.433867	-0.256807
C	4.561609	1.140339	-0.274791
H	5.440000	1.385839	-0.880959
H	4.005326	2.064677	-0.110248
H	4.889276	0.777385	0.698932
C	6.824947	-0.587331	-2.415771
C	7.476468	-0.781780	-1.170297
C	6.786876	-1.360488	-0.075493
C	5.468257	-1.706256	-0.210687
C	4.749105	-1.430760	-1.424104
C	5.504770	-0.946874	-2.539428
H	4.928703	-2.143302	0.620446
H	3.878578	-2.050459	-1.621410
H	0.352198	3.562213	-2.215792
O	0.944437	4.367079	-2.345946
S	0.942760	5.268058	-1.025461
O	-0.372387	5.299457	-0.408535
O	1.707463	6.465277	-1.314357
C	1.999147	4.190746	0.078065
F	3.296051	4.407965	-0.172251
F	1.741707	4.441527	1.352902
F	1.736192	2.901180	-0.189260
H	1.870279	-1.431390	2.538546
O	1.678788	-0.845946	3.347734
S	2.321550	0.586637	3.127386
O	2.095941	1.045437	1.744277
O	3.670946	0.685873	3.658077
C	1.156156	1.557269	4.211688
F	1.410869	1.281146	5.486319
F	1.374483	2.841042	3.963453
F	-0.092974	1.227729	3.914571
H	-1.025532	-3.287342	1.078010
O	-1.072446	-0.784964	1.586910
S	-2.144369	-1.698605	2.005876
O	-1.984640	-3.114962	1.309146
O	-3.536792	-1.315687	1.966303
C	-1.682150	-2.137058	3.756841
F	-1.608782	-1.026506	4.483783
F	-2.598110	-2.953572	4.266729
F	-0.493769	-2.746539	3.744845
H	-3.126507	-0.508420	-1.216574
O	-5.391297	-2.577117	-2.418993
S	-5.007303	-1.264561	-1.935318
O	-5.043796	-0.072195	-2.771909
O	-3.574658	-1.399985	-1.234843
C	-6.039213	-0.901230	-0.431361
F	-5.999247	-1.930093	0.409094
F	-5.570720	0.192872	0.168503
F	-7.299290	-0.691080	-0.820393
H	4.991931	-0.792183	-3.483154
H	7.358950	-0.169631	-3.259902
H	7.332994	-1.514499	0.848502

O	8.743184	-0.453331	-0.934896
C	9.535986	0.138487	-1.973483
H	10.512035	0.315875	-1.524278
H	9.635100	-0.545611	-2.822005
H	9.097996	1.087124	-2.299656

$4p_{08}$

S	-2.619404	2.188653	2.129508
O	-1.494496	2.958261	2.699241
O	-2.346280	0.743086	1.878788
O	-3.348849	2.846036	1.008564
C	-3.890182	2.162759	3.478307
F	-3.407367	1.493400	4.524038
F	-4.987297	1.531948	3.023716
F	-4.214877	3.398753	3.840456
H	-0.679391	-1.395492	0.619756
O	-0.401372	-0.701324	-0.042763
H	0.217402	-0.074437	0.432982
S	-0.756790	3.313139	-1.329683
O	-0.434295	2.228731	-0.405552
O	-2.339545	3.595954	-1.259387
O	-0.399499	3.270954	-2.736016
C	-0.172834	4.923554	-0.565996
F	-0.795916	5.037251	0.615363
F	-0.543959	5.921834	-1.362782
F	1.129881	4.936346	-0.386486
H	-2.678087	3.349425	-0.337638
H	0.053105	-1.128506	-0.857108
S	2.032165	-1.085704	-2.380420
O	3.077239	-2.113756	-2.510343
O	2.273278	-0.001807	-1.405833
O	0.634486	-1.645615	-2.197253
C	1.920291	-0.301873	-4.066133
F	3.128232	-0.081335	-4.554684
F	1.253923	-1.133956	-4.880367
F	1.242021	0.845034	-3.966797
H	3.494119	-3.108828	-1.193685
S	3.000121	-3.070760	0.904810
O	3.847312	-3.532793	-0.356342
O	3.051710	-4.104133	1.920333
O	1.731098	-2.469668	0.491534
C	4.088414	-1.676394	1.489570
F	4.206680	-0.765931	0.530865
F	3.535466	-1.122538	2.574444
F	5.288611	-2.156316	1.808299
C	-2.556961	-0.066843	-1.873750
C	-1.854087	0.090729	-3.069458
C	-1.903370	-0.908032	-4.040293
C	-2.635285	-2.073922	-3.800530
C	-3.334659	-2.228745	-2.606144
C	-3.310767	-1.226058	-1.625585
H	-2.482238	0.691801	-1.105609
H	-1.238550	0.970099	-3.224345

H	-1.338081	-0.798651	-4.959658
H	-2.639274	-2.874890	-4.532521
H	-3.880284	-3.150239	-2.430757
C	-4.097706	-1.341845	-0.351495
H	-3.591746	-0.786459	0.440822
C	-4.393055	-2.757123	0.140693
H	-5.065127	-3.307096	-0.525143
H	-3.457532	-3.313584	0.212196
H	-4.842155	-2.730172	1.137636
C	-5.088613	1.636868	-1.550561
C	-5.359541	1.036089	-2.814910
C	-6.047985	-0.220008	-2.896138
C	-6.195803	-0.960906	-1.772341
C	-5.589177	-0.535382	-0.501956
C	-5.263827	0.889469	-0.428196
H	-6.367749	-0.560371	-3.874280
H	-6.652155	-1.944227	-1.826354
H	-6.134877	-0.885583	0.376830
H	0.160016	-3.078673	-2.887217
O	-0.210023	-3.977838	-3.144561
S	0.278970	-5.080003	-2.093806
O	1.640720	-4.817826	-1.658215
O	-0.157589	-6.372662	-2.583791
C	-0.819081	-4.639362	-0.642074
F	-2.003755	-5.244467	-0.757201
F	-0.238594	-4.998888	0.494053
F	-1.028292	-3.312509	-0.638804
H	-1.631378	-0.098921	3.046206
O	-1.336643	-0.739294	3.776574
S	-1.475954	-2.233895	3.264061
O	-1.526050	-2.249318	1.789095
O	-2.486285	-2.968518	4.000530
C	0.203710	-2.875469	3.758025
F	0.252705	-2.992802	5.080766
F	0.360707	-4.058429	3.181998
F	1.133361	-2.023469	3.343801
H	0.060150	3.013768	2.213074
O	0.832555	0.584346	1.827585
S	1.745672	1.660730	2.241461
O	1.056796	3.079197	2.080517
O	3.099482	1.743893	1.743780
C	1.763997	1.504131	4.098665
F	2.227770	0.305936	4.436665
F	2.535960	2.453093	4.617041
F	0.513364	1.644382	4.543347
H	2.236607	1.626541	-1.387615
O	3.312230	4.620438	-2.288235
S	3.519132	3.192964	-2.129635
O	3.815657	2.311708	-3.250811
O	2.286977	2.619938	-1.283260
C	4.884966	2.955320	-0.889478
F	4.655101	3.696016	0.190129
F	4.952946	1.667962	-0.553890

F	6.036248	3.332000	-1.451337
H	-5.025453	1.318205	0.536834
H	-4.702343	2.645119	-1.492709
O	-5.056968	1.583057	-3.963996
C	-4.237086	2.778578	-4.013508
H	-3.307315	2.614539	-3.467582
H	-4.041418	2.936432	-5.072029
H	-4.786418	3.626862	-3.598265

$5p_{08}$

S	-2.289437	-3.401914	1.011783
O	-2.227288	-3.896740	-0.379823
O	-2.605537	-1.956981	1.186922
O	-1.147558	-3.843054	1.869452
C	-3.755550	-4.262634	1.748374
F	-4.856995	-3.845095	1.121958
F	-3.837363	-3.950368	3.045514
F	-3.630945	-5.579605	1.614132
H	-1.853151	0.809034	0.873386
O	-0.907414	0.617193	0.580056
H	-0.935079	0.376231	-0.387269
S	1.678363	-3.505560	-0.215512
O	0.764008	-2.367726	-0.307393
O	1.148844	-4.562025	0.853696
O	3.104179	-3.331097	0.011034
C	1.482463	-4.476858	-1.792746
F	0.247866	-4.983194	-1.836865
F	2.370597	-5.463940	-1.821657
F	1.673739	-3.654018	-2.814944
H	0.207577	-4.337933	1.147933
H	-0.290980	1.430442	0.721615
S	2.074053	2.099111	0.247873
O	2.413538	3.019194	-0.843728
O	2.056332	0.647708	-0.057565
O	0.820807	2.457456	1.023483
C	3.412303	2.373328	1.513731
F	4.596918	2.409595	0.915707
F	3.184093	3.537549	2.127128
F	3.397223	1.389757	2.418167
H	1.380197	3.531696	-2.240108
S	0.006382	2.140908	-3.109260
O	0.948622	3.423575	-3.130212
O	-0.937373	2.257599	-4.197871
O	-0.425692	1.866854	-1.735016
C	1.257768	0.786388	-3.522637
F	2.491430	1.241691	-3.290800
F	1.034825	-0.265025	-2.728452
F	1.140146	0.436781	-4.792115
H	0.508454	4.046897	1.386027
O	0.188770	4.984798	1.547940
S	-0.535113	5.556189	0.242970
O	0.092200	5.048564	-0.968014
O	-0.788798	6.964971	0.465544

C	-2.170161	4.677171	0.373826
F	-2.800263	5.026549	1.495655
F	-2.916295	4.994016	-0.678700
F	-1.966246	3.349800	0.389911
H	-3.780501	-1.225285	0.419348
O	-4.573458	-0.693461	0.059447
S	-4.630264	0.742019	0.714269
O	-3.356965	1.015949	1.419068
O	-5.878752	0.971477	1.408875
C	-4.617943	1.808570	-0.815704
F	-5.589968	1.423561	-1.631863
F	-4.825802	3.063705	-0.420968
F	-3.438773	1.711952	-1.417469
C	-1.269721	1.901471	3.703624
C	-0.853241	3.218502	3.879171
C	0.441939	3.490902	4.326870
C	1.305940	2.435390	4.608471
C	0.883365	1.114994	4.435758
C	-0.402948	0.830388	3.969885
H	-2.273118	1.701146	3.342006
H	-1.527627	4.032937	3.636582
H	0.774346	4.518165	4.437093
H	2.317629	2.634318	4.949039
H	1.574704	0.308839	4.659810
C	-0.899853	-0.583230	3.714479
H	-1.433072	-0.578863	2.762070
C	-1.910774	-1.055439	4.769809
H	-1.488583	-1.043782	5.780235
H	-2.773553	-0.383583	4.770932
H	-2.273669	-2.064482	4.541813
C	2.536241	-1.550908	2.484539
C	3.025349	-2.293147	3.593817
C	2.186261	-2.578260	4.721120
C	0.878474	-2.221923	4.694761
C	0.254338	-1.612970	3.501370
C	1.216530	-1.212871	2.457111
H	3.193696	-1.268791	1.673226
H	2.634409	-3.093702	5.563466
H	0.239083	-2.460818	5.537937
H	-0.276186	-2.476497	3.027708
H	-1.604158	-3.235022	-1.742394
O	-1.953907	-0.733752	-1.435419
S	-1.986863	-1.377684	-2.752353
O	-1.403707	-2.849739	-2.650915
O	-1.444444	-0.741868	-3.933001
C	-3.786947	-1.732031	-3.070501
F	-4.451243	-0.579265	-3.083225
F	-3.918653	-2.344062	-4.241134
F	-4.257209	-2.515433	-2.097529
H	2.903885	-0.296350	-1.124842
O	4.903289	-0.418168	0.380460
S	4.975438	-0.836256	-1.021397
O	3.517911	-0.883370	-1.658738

O	5.710516	-2.016018	-1.429914
C	5.675026	0.618529	-1.947978
F	6.881895	0.894848	-1.454535
F	5.772294	0.324648	-3.240273
F	4.872892	1.672239	-1.785399
H	0.831414	-0.684371	1.595384
O	4.243579	-2.760690	3.684873
C	5.176546	-2.608186	2.578134
H	6.067622	-3.144952	2.897520
H	4.750258	-3.049977	1.676632
H	5.391933	-1.552728	2.413078

TS3p$_{08}$

S	-2.153390	-3.339854	1.120441
O	-2.136710	-3.905855	-0.232654
O	-2.706324	-1.995472	1.336094
O	-0.772346	-3.509330	1.811140
C	-3.203628	-4.498094	2.128918
F	-4.463140	-4.373424	1.723439
F	-3.104078	-4.162257	3.414848
F	-2.783842	-5.744320	1.953052
H	-1.850099	0.763084	0.882963
O	-0.933379	0.507274	0.572431
H	-1.006419	0.265739	-0.388348
S	1.453071	-2.958831	-0.833986
O	0.288082	-2.097821	-0.646975
O	1.407228	-4.152393	0.245723
O	2.804132	-2.439040	-0.899732
C	1.191487	-3.966359	-2.381280
F	0.088984	-4.705579	-2.236955
F	2.239137	-4.759945	-2.566007
F	1.055533	-3.136813	-3.407310
H	0.583776	-4.053883	0.789765
H	-0.262350	1.299958	0.676117
S	2.090756	2.073430	0.162536
O	2.383565	3.084362	-0.863963
O	2.191147	0.652496	-0.248717
O	0.797725	2.308219	0.927717
C	3.354630	2.366588	1.498697
F	4.560144	2.487268	0.954796
F	3.038624	3.496654	2.136687
F	3.340630	1.350269	2.358845
H	1.338880	3.408098	-2.245229
S	-0.121899	2.084262	-3.112443
O	0.874013	3.321536	-3.125100
O	-1.097141	2.277643	-4.161987
O	-0.519890	1.770313	-1.736170
C	1.047474	0.691973	-3.616821
F	2.306716	1.065664	-3.387677
F	0.779909	-0.387862	-2.877025
F	0.886477	0.413743	-4.901079
H	0.463511	3.895161	1.359043
O	0.166412	4.832711	1.552020

S	-0.583141	5.458807	0.287019
O	-0.003377	4.986023	-0.960699
O	-0.810680	6.861486	0.568610
C	-2.222829	4.594489	0.432937
F	-2.806539	4.875787	1.598162
F	-3.007495	4.983481	-0.566902
F	-2.032444	3.266569	0.355365
H	-3.969204	-1.161882	0.473903
O	-4.794121	-0.650237	0.244611
S	-4.722524	0.805277	0.891635
O	-3.382468	1.008758	1.473194
O	-5.901061	1.073240	1.685091
C	-4.815887	1.863604	-0.644355
F	-5.868316	1.496264	-1.363720
F	-4.957995	3.123236	-0.240233
F	-3.700351	1.733150	-1.349569
C	-1.193558	1.802486	3.733812
C	-0.784659	3.119595	3.934064
C	0.498755	3.387269	4.414461
C	1.355867	2.328008	4.710902
C	0.942112	1.009410	4.512672
C	-0.332151	0.731645	4.008373
H	-2.191135	1.603046	3.355445
H	-1.455489	3.935403	3.686661
H	0.828515	4.413514	4.542130
H	2.357446	2.525279	5.081745
H	1.629128	0.196790	4.729120
C	-0.822220	-0.690200	3.744805
H	-1.467103	-0.636019	2.863507
C	-1.705222	-1.191249	4.898254
H	-1.151524	-1.222355	5.842490
H	-2.549814	-0.510009	5.032584
H	-2.107902	-2.189128	4.691311
C	2.496860	-1.860043	2.233765
C	2.840362	-2.947931	3.063707
C	1.965455	-3.342173	4.100093
C	0.772608	-2.676616	4.292719
C	0.337629	-1.642614	3.405636
C	1.281865	-1.231632	2.415172
H	3.170223	-1.505049	1.466290
H	2.262454	-4.167945	4.737383
H	0.120418	-2.991980	5.099969
H	-0.318436	-2.624854	2.511814
H	-1.852904	-3.175334	-1.764491
O	-2.301618	-0.742802	-1.341645
S	-2.401765	-1.312890	-2.689290
O	-1.839261	-2.803246	-2.688849
O	-1.906114	-0.627991	-3.861306
C	-4.212729	-1.665959	-2.929559
F	-4.887542	-0.522451	-2.876770
F	-4.403461	-2.254597	-4.102415
F	-4.615477	-2.477309	-1.945402
H	3.443824	0.143200	-1.250257

O	5.020937	-0.339311	0.598488
S	5.400057	-0.615058	-0.788032
O	4.256479	-0.115547	-1.779365
O	5.898046	-1.921473	-1.181349
C	6.706368	0.623461	-1.254447
F	7.773863	0.410928	-0.482779
F	7.037986	0.465695	-2.532964
F	6.251941	1.859294	-1.056653
H	1.027240	-0.409973	1.761309
O	3.957124	-3.665302	2.939903
C	4.866854	-3.357262	1.865653
H	5.658458	-4.101753	1.941076
H	4.363608	-3.436576	0.899309
H	5.277008	-2.352122	1.981553

TS3p'$_{08}$

S	-2.016515	-3.470916	0.947934
O	-1.999572	-3.956518	-0.436236
O	-2.610622	-2.160479	1.246028
O	-0.625111	-3.639635	1.617435
C	-3.020173	-4.720105	1.892728
F	-4.282878	-4.629181	1.488165
F	-2.939917	-4.446858	3.195304
F	-2.548054	-5.938365	1.658420
H	-1.846508	0.676876	0.921574
O	-0.924658	0.478288	0.586582
H	-0.998321	0.313322	-0.389827
S	1.518136	-2.806338	-1.024293
O	0.303898	-2.032349	-0.771262
O	1.553306	-4.062264	-0.016081
O	2.830296	-2.200539	-1.075895
C	1.286494	-3.734425	-2.624262
F	0.220554	-4.532811	-2.513019
F	2.366922	-4.465106	-2.866977
F	1.096724	-2.855096	-3.599503
H	0.725188	-4.047943	0.528364
H	-0.277044	1.283425	0.746423
S	2.030133	2.149183	0.213104
O	2.260802	3.244417	-0.740642
O	2.144581	0.766903	-0.306571
O	0.759616	2.297972	1.039178
C	3.336077	2.366834	1.521934
F	4.520195	2.536827	0.946347
F	3.032083	3.445945	2.248067
F	3.363771	1.293231	2.309522
H	1.183396	3.594634	-2.090483
S	-0.269599	2.289232	-3.000574
O	0.701035	3.545740	-2.964119
O	-1.271570	2.519048	-4.017200
O	-0.632461	1.893662	-1.635061
C	0.915402	0.951087	-3.605876
F	2.170924	1.347086	-3.401781
F	0.697121	-0.166797	-2.907475

F	0.716563	0.726512	-4.895324
H	0.382844	3.847388	1.535650
O	0.056781	4.760758	1.792513
S	-0.756443	5.431510	0.592314
O	-0.203031	5.057245	-0.699940
O	-1.026272	6.805166	0.965590
C	-2.358247	4.498682	0.736486
F	-2.917984	4.695779	1.930679
F	-3.185857	4.909005	-0.219264
F	-2.122444	3.184630	0.583176
H	-3.907369	-1.307492	0.442875
O	-4.760621	-0.817450	0.280308
S	-4.718137	0.596500	1.014788
O	-3.370043	0.809538	1.573644
O	-5.882718	0.771792	1.853640
C	-4.889694	1.750217	-0.444430
F	-5.943979	1.389286	-1.164492
F	-5.071762	2.972793	0.048371
F	-3.787749	1.714755	-1.181130
C	-1.147381	1.584808	3.799930
C	-0.774659	2.893371	4.099697
C	0.511172	3.163354	4.572814
C	1.406851	2.112410	4.763380
C	1.029124	0.801400	4.466204
C	-0.246950	0.523437	3.967634
H	-2.146836	1.385484	3.426929
H	-1.476087	3.704159	3.934285
H	0.811859	4.186157	4.777008
H	2.410864	2.311153	5.126738
H	1.746658	-0.001755	4.602503
C	-0.701013	-0.886958	3.597364
H	-1.319257	-0.791451	2.702298
C	-1.605622	-1.478571	4.689716
H	-1.086230	-1.541509	5.651765
H	-2.477738	-0.833977	4.827913
H	-1.967194	-2.475929	4.416614
C	2.673887	-1.868577	2.099690
C	3.070564	-2.933697	2.937342
C	2.197491	-3.414879	3.932319
C	0.958973	-2.814925	4.100367
C	0.487968	-1.791136	3.230409
C	1.424052	-1.316850	2.250184
H	3.373887	-1.498686	1.359603
H	2.489813	-4.228778	4.584007
H	0.308903	-3.178681	4.889144
H	-0.159657	-2.771256	2.352131
H	-1.771100	-3.102888	-1.917306
O	-2.320182	-0.715586	-1.347405
S	-2.430982	-1.217908	-2.720777
O	-1.805133	-2.679253	-2.818766
O	-1.998568	-0.447795	-3.864810
C	-4.230582	-1.637541	-2.937378
F	-4.952110	-0.529545	-2.801935

F	-4.428223	-2.166627	-4.137273
F	-4.573163	-2.520418	-1.992292
H	3.412499	0.340994	-1.365259
O	5.058799	-0.328909	0.362150
S	5.394610	-0.432528	-1.056956
O	4.206545	0.161972	-1.946021
O	5.903990	-1.659424	-1.639939
C	6.658531	0.883169	-1.417788
F	7.755168	0.617296	-0.704673
F	6.956691	0.874687	-2.715109
F	6.187832	2.082038	-1.076511
H	1.130346	-0.511559	1.591925
O	4.293575	-3.422541	2.706449
C	4.778591	-4.501383	3.503177
H	5.775655	-4.719440	3.121785
H	4.841156	-4.213785	4.558952
H	4.140754	-5.386235	3.395721

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S	-1.961154	-3.423792	1.128974
O	-2.345763	-3.958527	-0.177535
O	-2.474619	-2.160830	1.627563
O	-0.362316	-3.493882	1.182490
C	-2.385217	-4.750760	2.372201
F	-3.705691	-4.843820	2.440724
F	-1.886229	-4.393422	3.554644
F	-1.856152	-5.900662	1.982421
H	-1.647596	0.273129	0.990882
O	-0.701910	-0.016351	0.838569
H	-0.597587	-0.243279	-0.121636
S	1.052834	-2.395469	-1.829134
O	-0.155679	-1.784556	-1.265208
O	1.498617	-3.618768	-0.886655
O	2.221509	-1.625857	-2.190747
C	0.520480	-3.381834	-3.322231
F	-0.354597	-4.308388	-2.927030
F	1.587780	-3.966748	-3.850155
F	-0.042670	-2.567864	-4.202946
H	0.838419	-3.722676	-0.159270
H	-0.089268	0.813187	1.023098
S	2.085102	1.874601	0.432382
O	2.254630	2.969690	-0.535923
O	2.277975	0.496886	-0.076233
O	0.805615	1.966940	1.250773
C	3.375772	2.159170	1.744427
F	4.548499	2.408928	1.174692
F	3.005570	3.206426	2.486167
F	3.461156	1.076295	2.514453
H	0.969104	3.435326	-1.608047
S	-0.411544	2.125071	-2.647340
O	0.294579	3.514525	-2.344770
O	-1.645854	2.391513	-3.354761
O	-0.376926	1.265532	-1.462988

C	0.824091	1.376918	-3.826806
F	2.034407	1.442167	-3.272118
F	0.504930	0.102981	-4.051661
F	0.815525	2.049170	-4.972544
H	0.417381	3.501086	1.884372
O	0.089026	4.371342	2.253009
S	-0.445238	5.345593	1.102097
O	0.400909	5.280193	-0.079045
O	-0.813465	6.594230	1.737781
C	-2.019406	4.456548	0.665027
F	-2.772361	4.281739	1.753825
F	-2.690856	5.164095	-0.236477
F	-1.715574	3.254428	0.152482
H	-4.115415	-0.766630	0.056893
O	-4.876341	-0.413394	0.594499
S	-4.486960	1.020835	1.177466
O	-3.043692	1.071750	1.452212
O	-5.448149	1.380123	2.193611
C	-4.780147	2.106603	-0.319815
F	-5.956269	1.792113	-0.853084
F	-4.787693	3.373914	0.078297
F	-3.810587	1.911630	-1.207270
C	-1.035955	0.638296	4.029393
C	-0.915929	2.026750	4.115694
C	0.254235	2.593506	4.622450
C	1.306434	1.767256	5.022838
C	1.183130	0.382518	4.932803
C	0.007087	-0.197298	4.439637
H	-1.950565	0.200715	3.639654
H	-1.725248	2.662402	3.770279
H	0.352105	3.671647	4.682633
H	2.226740	2.203832	5.400002
H	2.010981	-0.255121	5.231239
C	-0.155342	-1.706151	4.380988
H	-1.118377	-1.893752	3.887503
C	-0.275183	-2.278737	5.807338
H	0.676365	-2.199041	6.342992
H	-1.028635	-1.715402	6.365302
H	-0.580903	-3.329840	5.803314
C	2.659556	-2.280879	1.796315
C	2.982905	-3.628327	2.008565
C	2.290918	-4.348111	3.000530
C	1.306909	-3.736642	3.762468
C	0.946617	-2.385922	3.558148
C	1.652457	-1.686000	2.560804
H	3.182071	-1.679898	1.063812
H	2.554919	-5.388774	3.158088
H	0.802616	-4.322278	4.522635
H	0.055125	-2.926123	1.916485
H	-2.558358	-3.205910	-1.680924
O	-2.835112	-0.834961	-1.071444
S	-2.926690	-1.241582	-2.488108
O	-2.731350	-2.819363	-2.583839

O	-2.168219	-0.577699	-3.519512
C	-4.735356	-1.141982	-2.927917
F	-5.099593	0.135105	-2.934917
F	-4.933389	-1.684955	-4.119801
F	-5.429019	-1.804427	-1.998901
H	3.441013	0.350282	-1.313071
O	5.191677	-0.321047	0.330216
S	5.476100	-0.302947	-1.103884
O	4.252652	0.338519	-1.901641
O	5.966950	-1.491859	-1.781969
C	6.713784	1.049546	-1.414799
F	7.855119	0.709705	-0.814335
F	6.916394	1.180929	-2.723009
F	6.268379	2.197569	-0.910031
H	1.427299	-0.642938	2.387178
O	3.914312	-4.319207	1.320031
C	4.695915	-3.614798	0.348687
H	5.396651	-4.346991	-0.052102
H	4.067510	-3.231399	-0.459721
H	5.241775	-2.788228	0.810012

$3o_{08}$

S	2.590007	-2.042900	1.975811
O	1.683532	-2.674053	2.957875
O	2.515868	-0.561771	1.883361
O	2.618428	-2.691135	0.630607
C	4.302988	-2.356013	2.615365
F	4.391845	-1.934044	3.874540
F	5.175376	-1.676575	1.859448
F	4.586562	-3.658078	2.559728
H	0.629287	1.156331	0.479599
O	0.570963	0.468004	-0.240239
H	0.062427	-0.321519	0.096947
S	-0.621798	-3.197585	-0.528580
O	-0.437985	-1.966788	0.255110
O	0.804879	-3.890067	-0.739590
O	-1.308946	-3.187904	-1.803211
C	-1.384328	-4.443161	0.652689
F	-0.456848	-4.708775	1.580181
F	-1.669445	-5.544011	-0.028075
F	-2.459539	-3.945312	1.222561
H	1.464956	-3.510075	-0.069639
H	0.103343	0.851703	-1.070485
S	-1.981470	0.994365	-2.437200
O	-2.775736	2.222349	-2.610137
O	-2.314441	0.107271	-1.312567
O	-0.477669	1.230821	-2.464803
C	-2.252777	0.057411	-4.021708
F	-3.541929	0.008203	-4.309357
F	-1.600171	0.705302	-5.003140
F	-1.751804	-1.171491	-3.910356
H	-2.884875	3.398630	-1.402473
S	-2.143546	3.556357	0.615970

O	-3.060217	3.985138	-0.608883
O	-1.845562	4.721569	1.424041
O	-1.091347	2.638474	0.176248
C	-3.382070	2.532156	1.558403
F	-3.706320	1.459283	0.842265
F	-2.840559	2.157948	2.719458
F	-4.470275	3.260257	1.796917
C	2.146016	-1.329147	-2.471103
C	1.333795	-1.464118	-3.582792
C	1.333016	-0.454465	-4.552071
C	2.137267	0.687661	-4.413007
C	2.922043	0.846953	-3.286070
C	2.929170	-0.156767	-2.279284
H	2.160401	-2.090401	-1.704155
H	0.691315	-2.331022	-3.686227
H	0.684285	-0.545201	-5.416839
H	2.109128	1.465398	-5.167313
H	3.506653	1.749727	-3.158820
C	3.621911	-0.036706	-1.064145
H	3.534586	-0.878198	-0.388211
C	4.224239	1.180853	-0.498645
H	4.511730	1.934754	-1.231869
H	3.446076	1.618985	0.149793
H	5.060400	0.937524	0.161021
C	4.820560	-3.000999	-2.930499
C	4.952370	-2.134521	-4.019821
C	5.628078	-0.916328	-3.905256
C	6.153949	-0.550032	-2.667844
C	5.990340	-1.380088	-1.556265
C	5.352657	-2.631166	-1.690866
H	4.305077	-3.945083	-3.056486
H	5.737072	-0.266992	-4.767125
H	6.677013	0.394505	-2.550633
H	6.406122	-1.124188	-0.587693
H	0.098130	2.508871	-3.327431
O	0.598897	3.259449	-3.776540
S	0.566512	4.569736	-2.855744
O	-0.705211	4.686434	-2.162847
O	1.158514	5.651831	-3.616173
C	1.814122	4.049264	-1.567776
F	3.059024	4.175288	-2.047466
F	1.677247	4.779801	-0.473957
F	1.616236	2.752473	-1.276610
H	2.010453	0.465015	3.077046
O	1.938626	1.275383	3.671966
S	2.087965	2.575348	2.767903
O	1.673763	2.278730	1.387608
O	3.358098	3.244216	2.984982
C	0.744258	3.603989	3.540280
F	1.022813	3.787388	4.828211
F	0.715982	4.767591	2.906208
F	-0.416732	2.974763	3.413729
H	4.522095	-2.424758	-4.973668

O	5.298415	-3.381426	-0.569457
C	4.665206	-4.656377	-0.633204
H	4.702436	-5.049373	0.381284
H	3.620071	-4.565754	-0.945520
H	5.201822	-5.324211	-1.317302
H	0.061337	-2.376514	3.058769
O	-0.416761	0.014353	2.285826
S	-1.411804	-0.776210	3.013513
O	-0.932403	-2.287410	3.170338
O	-2.811554	-0.777021	2.646845
C	-1.256425	-0.241153	4.789002
F	-1.574523	1.045600	4.899414
F	-2.066362	-0.970996	5.549643
F	0.009845	-0.425347	5.174516
H	-3.257715	-1.078870	-0.632164
O	-4.306151	-4.131329	-1.078265
S	-4.477601	-2.712009	-1.332513
O	-4.295317	-2.118476	-2.650263
O	-3.648009	-1.900933	-0.228484
C	-6.190395	-2.259906	-0.771128
F	-6.394139	-2.694049	0.469723
F	-6.329371	-0.933726	-0.811732
F	-7.073933	-2.826231	-1.594654

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S	-2.226124	2.928071	1.323367
O	-1.250253	3.600493	2.207211
O	-2.284573	1.448418	1.446867
O	-2.234577	3.399631	-0.092321
C	-3.887311	3.490335	1.931526
F	-3.959313	3.339946	3.250451
F	-4.843536	2.744086	1.353482
F	-4.085984	4.770658	1.611240
H	-0.694337	-0.891615	0.751958
O	-0.625745	-0.431099	-0.127297
H	-0.049004	0.377444	-0.035213
S	0.986470	2.852430	-1.351190
O	0.615608	1.947913	-0.251584
O	-0.316253	3.659593	-1.806874
O	1.657819	2.371171	-2.539490
C	1.944056	4.251191	-0.546834
F	1.086354	4.887846	0.261080
F	2.362219	5.075918	-1.496471
F	2.953857	3.778354	0.150305
H	-0.996707	3.640012	-1.056659
H	-0.225980	-1.064979	-0.829667
S	1.826004	-1.786116	-2.060896
O	2.515705	-3.072655	-1.862640
O	2.252273	-0.639713	-1.240753
O	0.310034	-1.887452	-2.028539
C	2.140721	-1.374485	-3.849046
F	3.418765	-1.550892	-4.142468
F	1.392775	-2.200131	-4.600603

F	1.775652	-0.118059	-4.094663
H	2.419918	-3.960449	-0.418122
S	1.721573	-3.461373	1.555676
O	2.503596	-4.354886	0.499770
O	1.289909	-4.293119	2.661158
O	0.800823	-2.550972	0.875658
C	3.139922	-2.420111	2.165339
F	3.583921	-1.652680	1.173778
F	2.715515	-1.658460	3.175480
F	4.120299	-3.211437	2.595865
C	-2.183149	0.903169	-2.504839
C	-1.312835	0.687892	-3.563951
C	-1.421466	-0.485061	-4.320936
C	-2.388429	-1.437342	-4.002256
C	-3.248980	-1.229113	-2.924512
C	-3.156677	-0.054838	-2.159259
H	-2.093782	1.796588	-1.899266
H	-0.536185	1.412126	-3.784207
H	-0.730896	-0.667280	-5.136951
H	-2.452102	-2.360944	-4.567042
H	-3.970485	-1.995287	-2.666172
C	-4.017530	0.220457	-0.999907
H	-3.685669	1.091664	-0.442870
C	-4.427720	-0.899754	-0.079039
H	-4.790312	-1.788226	-0.598367
H	-3.534217	-1.186137	0.484544
H	-5.176719	-0.570809	0.646763
C	-5.037143	2.099005	-3.684846
C	-5.492225	0.960780	-4.335755
C	-6.167601	-0.086711	-3.661940
C	-6.309509	-0.017174	-2.301539
C	-5.671195	1.036158	-1.559768
C	-5.189195	2.181410	-2.295254
H	-4.567161	2.896052	-4.246172
H	-6.561376	-0.924004	-4.226825
H	-6.809927	-0.806130	-1.750405
H	-6.031980	1.255083	-0.559002
H	-0.448091	-3.210449	-2.616746
O	-1.041583	-3.981851	-2.882231
S	-1.156624	-5.020499	-1.672117
O	0.094141	-5.104298	-0.936183
O	-1.867248	-6.186037	-2.160495
C	-2.334232	-4.073933	-0.580826
F	-3.572859	-4.109393	-1.095578
F	-2.344830	-4.592368	0.637722
F	-1.941133	-2.794023	-0.524954
H	-1.973605	0.690464	2.902042
O	-2.061676	0.143591	3.742451
S	-2.274837	-1.382835	3.344032
O	-1.839754	-1.604271	1.958885
O	-3.581222	-1.856630	3.764422
C	-0.998324	-2.159554	4.452644
F	-1.236736	-1.801238	5.712420

F	-1.099964	-3.475203	4.323832
F	0.211084	-1.751552	4.088442
H	-5.347517	0.885761	-5.409654
O	-4.831201	3.208479	-1.546321
C	-4.172308	4.344025	-2.137673
H	-3.938122	4.995302	-1.299724
H	-3.249282	4.032050	-2.631941
H	-4.844956	4.839861	-2.843690
H	0.319712	3.117864	2.344764
O	0.491979	0.567948	2.238697
S	1.611664	1.396976	2.687723
O	1.301629	2.943261	2.459654
O	2.974847	1.139161	2.274956
C	1.543226	1.370517	4.548363
F	1.860149	0.158698	4.996587
F	2.397896	2.264410	5.038506
F	0.301268	1.679220	4.930504
H	3.413854	0.489078	-0.914884
O	4.738309	3.186925	-2.150087
S	4.765876	1.738770	-2.038614
O	4.451011	0.857987	-3.155391
O	3.946933	1.312455	-0.732187
C	6.467506	1.278189	-1.452437
F	6.776808	1.965823	-0.355712
F	6.506947	-0.028533	-1.188062
F	7.341847	1.563178	-2.419668

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S	-1.312074	3.512013	1.384682
O	0.067825	3.854030	1.782860
O	-1.683829	2.073059	1.544035
O	-1.785626	4.089958	0.098475
C	-2.366148	4.369141	2.644802
F	-2.103359	3.866549	3.850543
F	-3.661275	4.147940	2.355123
F	-2.135635	5.677317	2.637600
H	-1.022171	-0.733262	0.848375
O	-0.587449	-0.354025	0.032327
H	0.265143	0.073526	0.333856
S	0.719120	2.938415	-2.106991
O	0.623094	2.092104	-0.918314
O	-0.633488	3.793899	-2.235800
O	1.019253	2.400326	-3.419957
C	1.896804	4.342115	-1.716264
F	1.421442	4.958231	-0.624681
F	1.895841	5.189929	-2.740937
F	3.115436	3.901886	-1.483992
H	-1.019619	3.937790	-1.315297
H	-0.404401	-1.090884	-0.658277
S	1.306457	-2.207545	-2.080121
O	1.809568	-3.584572	-1.947938
O	2.032531	-1.151243	-1.349269
O	-0.186851	-2.077447	-1.830854

C	1.431380	-1.820858	-3.896987
F	2.599281	-2.215927	-4.373346
F	0.445277	-2.469167	-4.536666
F	1.275128	-0.508019	-4.072025
H	1.893430	-4.347570	-0.422437
S	1.587481	-3.661196	1.601284
O	2.100404	-4.683892	0.498791
O	1.274680	-4.386192	2.817276
O	0.647220	-2.698186	1.025040
C	3.183743	-2.748675	1.904385
F	3.586985	-2.169642	0.780531
F	2.984602	-1.821221	2.846427
F	4.107550	-3.608975	2.327597
C	-2.398929	0.748461	-2.046187
C	-1.820373	0.354518	-3.253520
C	-2.298605	-0.776624	-3.910884
C	-3.338756	-1.529411	-3.350016
C	-3.912585	-1.140174	-2.145391
C	-3.455864	0.012681	-1.481502
H	-2.010649	1.605461	-1.513823
H	-0.983905	0.912511	-3.659648
H	-1.832637	-1.101839	-4.835132
H	-3.667349	-2.444314	-3.831995
H	-4.684268	-1.756486	-1.696448
C	-4.079922	0.490565	-0.234765
H	-3.403683	1.107963	0.352891
C	-4.865914	-0.478501	0.618561
H	-5.749947	-0.868022	0.109352
H	-4.210166	-1.317142	0.863717
H	-5.172120	-0.012041	1.558058
C	-4.111067	3.407405	-2.032336
C	-4.573016	2.727334	-3.182180
C	-5.534077	1.721564	-3.125809
C	-5.991620	1.303996	-1.876602
C	-5.379626	1.827284	-0.672480
C	-4.558524	3.005873	-0.802194
H	-3.401546	4.219054	-2.130239
H	-5.890183	1.264440	-4.039228
H	-5.980684	1.740871	0.228022
H	-1.199567	-3.335550	-2.158841
O	-1.913403	-4.043494	-2.233280
S	-1.877234	-4.994780	-0.949052
O	-0.511519	-5.245900	-0.521133
O	-2.844684	-6.052787	-1.165455
C	-2.609361	-3.829690	0.320797
F	-3.944990	-3.878536	0.279273
F	-2.185010	-4.147491	1.534387
F	-2.233482	-2.573535	0.027481
H	-1.280954	1.325350	2.893835
O	-1.208238	0.792045	3.757081
S	-1.950809	-0.597431	3.587198
O	-2.053752	-0.934864	2.154308
O	-3.146998	-0.682876	4.403530

C	-0.650407	-1.715795	4.313693
F	-0.563216	-1.492764	5.620963
F	-1.025750	-2.965504	4.081319
F	0.513570	-1.459255	3.730953
H	-4.187861	3.020677	-4.154384
H	1.497398	3.163132	1.384749
O	1.225054	0.616612	1.609098
S	2.501723	1.307309	1.844381
O	2.437361	2.806419	1.334394
O	3.765137	0.733023	1.441998
C	2.506407	1.577584	3.687656
F	2.480252	0.401082	4.306107
F	3.599958	2.247755	4.035301
F	1.421038	2.281991	4.015638
H	2.747422	0.299530	-1.609868
O	4.945916	2.273950	-3.079251
S	4.527026	0.962603	-2.621306
O	4.317231	-0.158734	-3.527336
O	3.245521	1.161815	-1.682672
C	5.753398	0.396260	-1.343077
F	5.952464	1.355356	-0.444849
F	5.287951	-0.699002	-0.743833
F	6.905293	0.113503	-1.956861
H	-4.211348	3.496039	0.098188
O	-6.897856	0.352725	-1.678307
C	-7.419689	-0.366999	-2.809817
H	-6.605760	-0.853564	-3.354077
H	-8.093031	-1.112556	-2.389974
H	-7.973035	0.309795	-3.467519

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S	2.064192	-3.217786	0.999203
O	1.066542	-3.898238	1.852824
O	2.165877	-1.747806	1.197013
O	2.060733	-3.627498	-0.435937
C	3.702569	-3.854351	1.585903
F	3.847509	-3.585120	2.880466
F	4.682961	-3.239449	0.898779
F	3.793694	-5.167195	1.382643
H	0.737059	0.790775	0.871140
O	0.660864	0.421349	-0.048910
H	0.059987	-0.372653	-0.038872
S	-1.076328	-2.628372	-1.678093
O	-0.682366	-1.879371	-0.475682
O	0.199788	-3.425650	-2.220646
O	-1.713185	-1.982730	-2.805684
C	-2.096284	-4.075596	-1.057168
F	-1.272853	-4.836858	-0.324029
F	-2.531166	-4.765111	-2.102419
F	-3.098004	-3.653363	-0.317291
H	0.853347	-3.563903	-1.458125
H	0.287002	1.135480	-0.688464
S	-1.724324	2.096982	-1.824950

O	-2.342160	3.387624	-1.473473
O	-2.228161	0.886417	-1.155826
O	-0.205559	2.105938	-1.773548
C	-2.036699	1.925988	-3.652050
F	-3.300683	2.205945	-3.928861
F	-1.237163	2.795054	-4.292330
F	-1.737414	0.690941	-4.048001
H	-2.212510	4.086137	0.066389
S	-1.568465	3.311906	1.967271
O	-2.285007	4.371581	1.025429
O	-1.100382	3.973624	3.168829
O	-0.695088	2.440238	1.182760
C	-3.051378	2.288622	2.439263
F	-3.524970	1.670148	1.361347
F	-2.684511	1.389415	3.354695
F	-3.991183	3.078992	2.954336
C	2.148782	-0.648313	-2.490823
C	1.312505	-0.303460	-3.547454
C	1.509781	0.905839	-4.222933
C	2.529290	1.765056	-3.821223
C	3.364617	1.417188	-2.754902
C	3.188918	0.202886	-2.082903
H	1.979635	-1.567225	-1.942218
H	0.490252	-0.954875	-3.823516
H	0.843492	1.190593	-5.030021
H	2.660268	2.724338	-4.310654
H	4.134495	2.112085	-2.439486
C	4.100412	-0.266776	-0.985125
H	3.643927	-1.118945	-0.482857
C	4.513654	0.756575	0.063251
H	4.911758	1.679108	-0.364770
H	3.629178	1.016793	0.647321
H	5.253861	0.337855	0.753520
C	4.988536	-1.666376	-3.974710
C	5.631228	-0.514659	-4.389035
C	6.356482	0.333908	-3.501391
C	6.341322	0.063500	-2.169421
C	5.493479	-1.000643	-1.624671
C	4.988891	-1.973750	-2.605673
H	4.489846	-2.303512	-4.692855
H	6.905239	1.178948	-3.901600
H	6.869483	0.696484	-1.464544
H	5.904294	-1.493047	-0.741402
H	0.625404	3.434453	-2.240649
O	1.243159	4.209938	-2.426666
S	1.384892	5.117558	-1.118612
O	0.135326	5.167272	-0.377051
O	2.132235	6.304141	-1.487716
C	2.527293	4.032025	-0.125738
F	3.760009	4.051455	-0.655213
F	2.578689	4.451276	1.130210
F	2.071413	2.773697	-0.163977
H	1.909073	-1.133235	2.738275

O	2.031111	-0.728931	3.651593
S	2.305964	0.832137	3.502157
O	1.902741	1.285169	2.165149
O	3.620912	1.178746	4.010271
C	1.043386	1.478491	4.707440
F	1.222500	0.886406	5.886459
F	1.225663	2.787284	4.820550
F	-0.177384	1.221908	4.254448
H	5.609213	-0.263211	-5.445775
O	4.468699	-3.048871	-2.076412
C	3.739227	-3.997007	-2.890868
H	3.394479	-4.750999	-2.189370
H	2.886273	-3.498321	-3.356372
H	4.406575	-4.428574	-3.641063
H	-0.482976	-3.365736	1.999333
O	-0.544497	-0.810380	2.162228
S	-1.706846	-1.633637	2.498388
O	-1.460138	-3.156409	2.099253
O	-3.049415	-1.268960	2.098446
C	-1.674529	-1.823710	4.351060
F	-1.966766	-0.663840	4.933227
F	-2.564104	-2.742316	4.718643
F	-0.449827	-2.212330	4.715311
H	-3.422543	-0.244028	-0.984803
O	-4.804387	-2.713795	-2.579895
S	-4.796676	-1.293353	-2.274993
O	-4.449344	-0.279002	-3.260991
O	-3.981225	-1.067994	-0.917528
C	-6.492090	-0.871363	-1.643234
F	-6.845388	-1.717427	-0.678414
F	-6.491991	0.375197	-1.169027
F	-7.357652	-0.962201	-2.655183

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S	-3.559402	-2.475707	0.189235
O	-3.113387	-3.296612	-0.952867
O	-3.407410	-1.005033	0.069573
O	-3.088381	-2.979513	1.523118
C	-5.392204	-2.731774	0.275399
F	-5.954000	-2.233345	-0.823839
F	-5.867634	-2.080110	1.349428
F	-5.678048	-4.024900	0.385438
H	-0.936278	1.004022	-0.199097
O	-0.324498	0.602289	0.478758
H	-0.138761	-0.353586	0.241372
S	0.387360	-3.099226	1.018905
O	-0.269041	-2.016201	0.265476
O	-0.684283	-3.809923	1.947661
O	1.581711	-2.858356	1.803583
C	0.731381	-4.414677	-0.264121
F	-0.440100	-4.932498	-0.641000
F	1.497917	-5.354224	0.266854
F	1.327796	-3.844566	-1.296363

H	-1.636169	-3.558585	1.680310
H	0.536155	1.136754	0.574714
S	3.060002	1.108953	0.717143
O	3.871565	1.768285	-0.311624
O	2.633992	-0.289866	0.496832
O	1.841431	1.892189	1.184967
C	4.173283	1.141747	2.212305
F	5.381552	0.713568	1.878694
F	4.243305	2.403405	2.647162
F	3.675369	0.372491	3.185171
H	3.410782	2.310705	-1.927272
S	1.840643	1.286448	-2.955720
O	3.121507	2.233460	-2.877242
O	1.214780	1.497262	-4.242272
O	1.086542	1.363562	-1.704605
C	2.658258	-0.417303	-2.937834
F	3.862781	-0.327975	-2.366364
F	1.907024	-1.251489	-2.212461
F	2.784714	-0.869791	-4.174186
H	1.860154	3.513655	1.337930
O	1.705401	4.501991	1.445621
S	1.707349	5.222194	0.015900
O	2.528846	4.483812	-0.931845
O	1.845947	6.647081	0.240614
C	-0.058392	4.915968	-0.477888
F	-0.891273	5.365604	0.463866
F	-0.306986	5.532676	-1.628000
F	-0.246936	3.598234	-0.627091
H	-3.700296	-0.001362	-1.226630
O	-4.037710	0.735655	-1.824733
S	-3.472052	2.134758	-1.330901
O	-2.407077	1.914632	-0.339151
O	-4.552509	3.049055	-1.016957
C	-2.651876	2.750604	-2.892709
F	-3.507310	2.645270	-3.903977
F	-2.345659	4.030777	-2.686552
F	-1.552731	2.058356	-3.141623
C	-1.586431	2.892403	2.870134
C	-0.946619	3.909992	3.579011
C	-1.029115	3.949562	4.971994
C	-1.763776	2.974811	5.650165
C	-2.405590	1.960994	4.937051
C	-2.319214	1.905801	3.541878
H	-1.523736	2.869201	1.787630
H	-0.374056	4.657026	3.039840
H	-0.523193	4.734766	5.525937
H	-1.837616	3.002835	6.733831
H	-2.977890	1.208586	5.476990
C	-2.992329	0.805956	2.741190
H	-2.472374	0.719253	1.790510
C	-4.458997	1.126776	2.427386
H	-5.032361	1.343060	3.335290
H	-4.497361	2.016147	1.792589

H	-4.939153	0.307358	1.883295
C	-1.219209	-1.640863	5.075046
C	-2.299562	-2.084190	5.810499
C	-3.648307	-1.781659	5.466148
C	-3.900441	-1.051889	4.346504
C	-2.829501	-0.600140	3.434916
C	-1.453992	-0.859067	3.928946
H	-0.209309	-1.888782	5.375580
H	-4.454702	-2.151349	6.089720
H	-4.919595	-0.854755	4.033982
H	-2.940858	-1.330119	2.594739
H	-2.110541	-2.690879	6.692252
O	-0.519896	-0.321749	3.206216
C	0.867302	-0.270171	3.633565
H	1.276860	0.563423	3.074562
H	0.915296	-0.067390	4.704836
H	1.367584	-1.199471	3.360946
H	-1.860339	-3.065763	-1.994068
O	-1.397957	-0.536517	-2.011332
S	-1.208726	-1.391119	-3.181354
O	-1.221122	-2.926839	-2.754396
O	-0.124005	-1.198522	-4.119182
C	-2.799973	-1.291110	-4.144458
F	-2.975977	-0.038051	-4.556276
F	-2.747433	-2.107849	-5.190083
F	-3.817178	-1.649316	-3.350429
H	3.288571	-1.683714	-0.073308
O	4.680763	-2.149483	1.968972
S	4.866118	-2.886402	0.725865
O	3.684112	-2.571960	-0.307047
O	5.120313	-4.313827	0.690641
C	6.250659	-2.035026	-0.179859
F	7.349815	-2.067659	0.573088
F	6.483085	-2.642708	-1.339772
F	5.904494	-0.762440	-0.406518

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S	-3.872028	-2.034320	0.005073
O	-3.376965	-2.903954	-1.067942
O	-3.925471	-0.584671	-0.175081
O	-3.185782	-2.418191	1.344044
C	-5.621848	-2.564113	0.338067
F	-6.374829	-2.243815	-0.706283
F	-6.052276	-1.915867	1.426093
F	-5.662749	-3.873694	0.551710
H	-0.614894	1.034945	-0.247474
O	-0.272819	0.576361	0.560544
H	-0.114603	-0.387522	0.339511
S	0.172049	-3.247822	0.646185
O	-0.360000	-2.009011	0.052002
O	-1.000412	-3.964130	1.463637
O	1.370307	-3.261742	1.455782
C	0.372233	-4.418062	-0.800864

F	-0.848205	-4.742381	-1.237344
F	1.015358	-5.501310	-0.397716
F	1.041396	-3.793353	-1.752679
H	-1.861850	-3.479411	1.320382
H	0.601309	1.017700	0.875026
S	3.074801	0.732243	0.899049
O	3.924022	1.407911	-0.086310
O	2.518113	-0.594663	0.548913
O	1.937553	1.576336	1.461631
C	4.205765	0.521747	2.366478
F	5.369058	0.034388	1.960528
F	4.386357	1.724028	2.919480
F	3.659918	-0.298754	3.265379
H	3.493128	2.250417	-1.602030
S	1.882020	1.480907	-2.790057
O	3.232783	2.292023	-2.562159
O	1.350871	1.867830	-4.078238
O	1.067318	1.513983	-1.572766
C	2.534035	-0.292398	-2.909796
F	3.751251	-0.363054	-2.369467
F	1.715175	-1.098694	-2.225002
F	2.586341	-0.664468	-4.177914
H	2.157104	3.173443	1.797154
O	2.177413	4.157492	1.997765
S	2.317173	5.003423	0.646782
O	3.027623	4.242684	-0.371252
O	2.678816	6.358222	1.010737
C	0.536480	5.026861	0.116712
F	-0.222722	5.597358	1.052653
F	0.428613	5.703127	-1.022411
F	0.121673	3.766191	-0.069513
H	-3.745757	0.722311	-1.406780
O	-3.988771	1.571249	-1.855949
S	-3.138089	2.770455	-1.217742
O	-2.161309	2.218409	-0.276173
O	-4.022535	3.846929	-0.820050
C	-2.213904	3.339991	-2.735820
F	-3.090873	3.607912	-3.698225
F	-1.547309	4.442719	-2.404707
F	-1.367415	2.403195	-3.138429
C	-1.367776	2.694861	3.043448
C	-0.656960	3.602271	3.829637
C	-0.707024	3.512731	5.221899
C	-1.481767	2.519202	5.822138
C	-2.194105	1.615059	5.033031
C	-2.138780	1.688310	3.637151
H	-1.332197	2.774234	1.962445
H	-0.059541	4.371505	3.353275
H	-0.146737	4.213750	5.833634
H	-1.531946	2.445494	6.905115
H	-2.789866	0.841548	5.512485
C	-2.924058	0.718147	2.758447
H	-2.416136	0.673007	1.794031

C	-4.342920	1.251083	2.504965
H	-4.873153	1.441739	3.444299
H	-4.273991	2.200591	1.967229
H	-4.935513	0.563381	1.893594
C	-1.531281	-2.429597	4.471502
C	-2.685582	-2.974649	5.023018
C	-3.945087	-2.393471	4.812760
C	-4.040096	-1.256591	4.030924
C	-2.904546	-0.698154	3.364158
C	-1.622134	-1.272263	3.686854
H	-0.568479	-2.893843	4.646604
H	-4.831331	-2.827738	5.262247
H	-5.008589	-0.807424	3.843929
H	-3.124808	-1.558820	2.269236
H	-2.603595	-3.874909	5.625200
O	-0.572468	-0.659652	3.147559
C	0.746864	-0.864248	3.690321
H	1.303214	0.015890	3.383971
H	0.698577	-0.910587	4.781504
H	1.204939	-1.762722	3.273192
H	-2.110093	-2.677182	-2.197829
O	-1.595930	-0.207889	-1.930596
S	-1.418226	-0.909783	-3.201833
O	-1.506106	-2.488668	-2.966202
O	-0.311325	-0.649963	-4.094212
C	-2.990106	-0.629111	-4.163365
F	-3.057616	0.646792	-4.524348
F	-3.007196	-1.408457	-5.236905
F	-4.033367	-0.930259	-3.375689
H	3.114411	-1.910373	-0.227509
O	4.512662	-2.755863	1.677418
S	4.621865	-3.320631	0.339227
O	3.449708	-2.774137	-0.606212
O	4.763609	-4.743218	0.094550
C	6.051006	-2.452710	-0.477001
F	7.153822	-2.654252	0.242788
F	6.227999	-2.919615	-1.709875
F	5.787561	-1.142152	-0.530891

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S	-2.648258	-3.044426	0.559928
O	-2.613475	-3.465658	-0.844929
O	-2.990869	-1.653745	0.886631
O	-1.377006	-3.516302	1.320420
C	-3.951014	-4.110381	1.352587
F	-5.129412	-3.776955	0.836042
F	-3.953902	-3.897524	2.667697
F	-3.684548	-5.387373	1.104146
H	-1.639437	1.004151	0.747753
O	-0.757244	0.641724	0.444399
H	-0.798491	0.547238	-0.543104
S	1.057795	-3.032048	-1.165313
O	0.012284	-2.035942	-0.937591

O	0.772564	-4.310012	-0.228393
O	2.466218	-2.706693	-1.110238
C	0.753947	-3.822393	-2.826191
F	-0.458171	-4.383421	-2.826728
F	1.675213	-4.752292	-3.042568
F	0.821468	-2.881940	-3.760079
H	-0.057782	-4.142923	0.286116
H	0.032450	1.279230	0.696677
S	2.511253	1.622102	0.405907
O	3.056017	2.687356	-0.449166
O	2.368949	0.278464	-0.200299
O	1.235567	2.008723	1.142431
C	3.708039	1.475704	1.824058
F	4.946654	1.383564	1.354568
F	3.597999	2.566652	2.585954
F	3.414327	0.395911	2.546451
H	2.193625	3.307658	-1.863915
S	0.564808	2.405339	-2.952642
O	1.793874	3.395721	-2.775305
O	-0.270819	2.901767	-4.022980
O	0.009703	2.052016	-1.641415
C	1.450795	0.849390	-3.550111
F	2.746266	0.933253	-3.251529
F	0.930794	-0.208667	-2.920946
F	1.295272	0.719803	-4.858244
H	1.180010	3.582894	1.697008
O	1.055150	4.537071	1.980558
S	0.456963	5.405628	0.781134
O	0.961845	4.954170	-0.506424
O	0.482270	6.794104	1.193846
C	-1.315375	4.846927	0.846935
F	-1.861272	5.138278	2.027879
F	-1.997580	5.447729	-0.122692
F	-1.369706	3.515533	0.665471
H	-4.030430	-0.518265	0.077504
O	-4.741129	0.156399	-0.110526
S	-4.456398	1.485201	0.722069
O	-3.134618	1.376122	1.368066
O	-5.613375	1.858641	1.504601
C	-4.277031	2.726727	-0.662141
F	-5.317606	2.628194	-1.478988
F	-4.251645	3.932158	-0.099764
F	-3.146036	2.505834	-1.319131
C	-0.926619	1.668747	3.754917
C	-0.282573	2.825230	4.188643
C	0.970206	2.742311	4.800105
C	1.557490	1.492878	4.990600
C	0.907177	0.334724	4.558339
C	-0.335722	0.407742	3.923500
H	-1.894764	1.748170	3.271605
H	-0.744720	3.792148	4.021035
H	1.484650	3.645716	5.112591
H	2.533036	1.414849	5.461842

H	1.392209	-0.626833	4.696535
C	-1.068416	-0.820647	3.380786
H	-1.430229	-0.546557	2.389007
C	-2.329046	-1.125568	4.209273
H	-2.095611	-1.272759	5.264300
H	-3.012695	-0.275864	4.122748
H	-2.846533	-2.014149	3.840692
C	2.112690	-2.458947	2.090192
C	2.247504	-3.573084	2.927457
C	1.275209	-3.897186	3.868734
C	0.140812	-3.084448	4.019720
C	-0.087123	-1.983974	3.121350
C	0.975090	-1.685656	2.205431
H	2.890772	-2.197925	1.384395
H	1.419833	-4.758133	4.508840
H	-0.813377	-2.778562	2.122419
H	-2.141158	-2.583719	-2.259117
O	-2.225964	-0.155168	-1.609377
S	-2.340985	-0.574334	-3.009828
O	-2.028496	-2.130798	-3.139724
O	-1.676012	0.128195	-4.083806
C	-4.169307	-0.593294	-3.355348
F	-4.649190	0.636524	-3.199821
F	-4.391365	-1.016868	-4.592089
F	-4.753132	-1.421731	-2.481941
H	3.608108	-0.367715	-1.185736
O	4.908827	-1.479288	0.613605
S	5.346895	-1.567412	-0.778857
O	4.398611	-0.681676	-1.711485
O	5.640272	-2.839862	-1.411006
C	6.887648	-0.535599	-0.931220
F	7.811539	-1.044665	-0.113410
F	7.331570	-0.573516	-2.185381
F	6.635723	0.726108	-0.585238
H	0.850242	-0.828618	1.558719
H	3.130256	-4.200183	2.843728
O	-0.801514	-3.316549	4.947678
C	-0.690817	-4.459168	5.794548
H	0.211917	-4.405046	6.412692
H	-1.573883	-4.432540	6.432756
H	-0.684920	-5.384822	5.208090

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S	-3.374920	-2.572231	0.400273
O	-2.897602	-3.392286	-0.711276
O	-3.047517	-1.168869	0.543434
O	-2.984438	-3.412882	1.723165
C	-5.236135	-2.709752	0.429750
F	-5.705420	-2.001634	-0.584668
F	-5.663720	-2.208166	1.588921
F	-5.592961	-3.980379	0.322291
H	-0.100585	0.706037	-0.542121
O	-0.286413	0.578176	0.433657

H	-0.208873	-0.390099	0.655640
S	0.595013	-3.249365	0.903837
O	-0.274957	-2.160518	0.423710
O	-0.301131	-4.304343	1.717177
O	1.802353	-2.987405	1.653645
C	0.982286	-4.291213	-0.607062
F	-0.153166	-4.890093	-0.983371
F	1.893943	-5.192705	-0.291281
F	1.407179	-3.499989	-1.575674
H	-1.257742	-4.058117	1.673438
H	0.443523	1.098767	0.924135
S	2.975929	1.217731	0.685111
O	3.629970	1.954189	-0.403447
O	2.589311	-0.190187	0.427290
O	1.785287	1.922393	1.315506
C	4.265859	1.236278	2.032966
F	5.440345	0.902195	1.514985
F	4.322303	2.477416	2.522373
F	3.945729	0.390352	3.008712
H	3.050402	2.614739	-1.940707
S	1.546153	1.529517	-3.004268
O	2.766504	2.532425	-2.895020
O	0.875271	1.753612	-4.263466
O	0.805829	1.527054	-1.733748
C	2.432235	-0.138365	-3.058496
F	3.658202	-0.016327	-2.555429
F	1.739872	-0.999891	-2.304575
F	2.495900	-0.570209	-4.306272
H	1.782079	3.563628	1.443438
O	1.665342	4.558168	1.530442
S	1.471545	5.240192	0.098364
O	2.214703	4.521443	-0.927651
O	1.574182	6.673894	0.278175
C	-0.318656	4.840039	-0.203237
F	-1.081506	5.362602	0.755309
F	-0.676645	5.333463	-1.385217
F	-0.474245	3.509602	-0.209548
H	-3.179425	0.178142	-1.215030
O	-4.035488	0.630277	-1.408972
S	-3.944653	2.172276	-0.949306
O	-3.005770	2.304218	0.156303
O	-5.298884	2.682873	-0.899654
C	-3.104404	2.902679	-2.444117
F	-3.838212	2.679430	-3.530303
F	-2.972652	4.211660	-2.246696
F	-1.903989	2.341877	-2.587956
C	-1.362627	2.774228	3.113433
C	-0.651212	3.764041	3.791858
C	-0.481025	3.679914	5.175350
C	-1.039199	2.609159	5.875051
C	-1.755815	1.623668	5.193938
C	-1.916535	1.691461	3.805988
H	-1.501727	2.843740	2.040148

H	-0.224748	4.592960	3.237868
H	0.079686	4.445898	5.703355
H	-0.917582	2.539092	6.952751
H	-2.181223	0.789104	5.745453
C	-2.698369	0.628349	3.039106
H	-2.338754	0.656840	2.008408
C	-4.193236	0.977892	2.997518
H	-4.627910	1.016783	4.002760
H	-4.317207	1.960917	2.538385
H	-4.756466	0.254552	2.397094
C	-0.740017	-2.448609	4.195751
C	-1.739435	-3.264396	4.729245
C	-3.071025	-2.851100	4.681440
C	-3.391465	-1.605786	4.110094
C	-2.406327	-0.759017	3.584501
C	-1.071572	-1.221268	3.614617
H	0.293229	-2.776495	4.204899
H	-3.858903	-3.476182	5.090132
H	-4.424826	-1.277417	4.108510
H	-3.128390	-2.879969	2.568067
H	-1.474815	-4.220894	5.168828
O	-0.137175	-0.413734	3.045673
C	1.148732	-0.325095	3.683115
H	1.503523	0.681844	3.477391
H	1.042911	-0.460599	4.763133
H	1.837163	-1.062381	3.265004
H	-1.748369	-3.046641	-1.945641
O	-1.540976	-0.516625	-1.864106
S	-1.401533	-1.274949	-3.115147
O	-1.257578	-2.829685	-2.782635
O	-0.418137	-0.933155	-4.115356
C	-3.085059	-1.242897	-3.915719
F	-3.379555	0.011365	-4.230375
F	-3.077459	-2.002379	-5.001417
F	-3.979139	-1.716618	-3.038095
H	3.313565	-1.475535	-0.250016
O	4.900087	-2.019829	1.609848
S	4.987840	-2.686724	0.318347
O	3.717561	-2.327679	-0.589531
O	5.246982	-4.106963	0.179496
C	6.279545	-1.770346	-0.658428
F	7.433310	-1.802412	0.005757
F	6.433789	-2.332110	-1.854628
F	5.887839	-0.500112	-0.811945

$3m_{08}$

S	2.482999	-2.150085	1.970074
O	1.364003	-2.872570	2.610626
O	2.284149	-0.669318	1.855197
O	3.044502	-2.751077	0.737008
C	3.870698	-2.298243	3.189244
F	3.520893	-1.702487	4.328970
F	4.957212	-1.684161	2.690999

F	4.155200	-3.576387	3.413717
H	0.633106	1.393099	0.653441
O	0.472041	0.684088	-0.035638
H	-0.157020	0.028276	0.385152
S	0.311371	-3.326541	-1.315918
O	0.154023	-2.193112	-0.403268
O	1.868194	-3.692294	-1.427731
O	-0.211185	-3.303593	-2.669146
C	-0.274206	-4.875841	-0.439332
F	0.427150	-4.969481	0.698330
F	-0.001429	-5.919204	-1.217352
F	-1.561739	-4.827981	-0.170206
H	2.347013	-3.410284	-0.589920
H	0.055815	1.092943	-0.879174
S	-1.845449	1.134195	-2.458100
O	-2.789663	2.247950	-2.638599
O	-2.178005	0.115238	-1.447861
O	-0.402023	1.586306	-2.273130
C	-1.760777	0.290036	-4.115151
F	-2.970973	0.118934	-4.613852
F	-1.038463	1.064004	-4.943641
F	-1.141198	-0.881920	-3.971310
H	-3.190861	3.279832	-1.325013
S	-2.751940	3.254239	0.787055
O	-3.535724	3.742708	-0.506969
O	-2.758324	4.311189	1.778822
O	-1.513356	2.569307	0.413598
C	-3.947860	1.946428	1.367710
F	-4.090590	1.022828	0.424844
F	-3.474581	1.384396	2.483691
F	-5.123156	2.513914	1.627858
C	2.673508	-0.336057	-1.807374
C	2.044319	-0.615015	-3.012402
C	2.001022	0.364832	-4.005409
C	2.603979	1.623546	-3.818430
C	3.219435	1.917981	-2.621615
C	3.247047	0.949246	-1.574157
H	2.686204	-1.064558	-1.008197
H	1.562698	-1.571355	-3.174006
H	1.472299	0.161169	-4.930902
H	2.544146	2.374120	-4.598233
H	3.642790	2.901468	-2.460758
C	3.763907	1.215447	-0.303240
H	3.655105	0.423448	0.432061
C	4.245565	2.508828	0.218449
H	4.492393	3.247235	-0.543674
H	3.434721	2.906702	0.848716
H	5.096766	2.357472	0.888676
C	5.324622	-1.895953	-1.849867
C	5.617839	-0.982543	-2.880391
C	6.225466	0.236282	-2.573517
C	6.515239	0.573620	-1.253848
C	6.218638	-0.344598	-0.230387

C	5.646915	-1.575825	-0.524236
H	6.983004	1.524195	-1.018349
H	6.453803	-0.105635	0.803062
H	0.066468	2.987033	-2.966812
O	0.489825	3.841624	-3.297151
S	0.132445	5.045788	-2.306907
O	-1.201384	4.889522	-1.753065
O	0.600381	6.272312	-2.919900
C	1.312107	4.640491	-0.920475
F	2.562811	4.984660	-1.258323
F	0.959707	5.272360	0.187142
F	1.293588	3.312569	-0.704293
H	1.596369	0.102874	3.038886
O	1.262494	0.735802	3.768070
S	1.439433	2.235825	3.301652
O	1.396878	2.313427	1.825775
O	2.529233	2.909786	3.982811
C	-0.174918	2.914780	3.933151
F	-0.181699	2.849931	5.260620
F	-0.266223	4.173854	3.530674
F	-1.170638	2.192117	3.437613
H	-0.218355	-2.902508	2.221816
O	-0.934575	-0.470972	1.802894
S	-1.867217	-1.505399	2.276662
O	-1.222947	-2.946911	2.145704
O	-3.237514	-1.557648	1.820117
C	-1.843774	-1.302431	4.128434
F	-2.286719	-0.089972	4.446379
F	-2.619339	-2.227277	4.683841
F	-0.587905	-1.450582	4.553760
H	-2.434081	-1.498349	-1.242440
O	-3.764570	-4.386485	-2.099150
S	-3.842771	-2.942866	-1.983097
O	-3.978257	-2.063126	-3.136899
O	-2.623696	-2.460139	-1.064854
C	-5.249613	-2.547987	-0.832579
F	-5.145759	-3.270610	0.277746
F	-5.218873	-1.249361	-0.533256
F	-6.398009	-2.836611	-1.449111
H	5.408255	-2.288616	0.252662
H	5.377532	-1.217333	-3.910033
H	6.452367	0.930288	-3.377165
O	4.725587	-3.095659	-2.034482
C	4.398866	-3.504136	-3.359247
H	3.903766	-4.468429	-3.255028
H	3.708831	-2.797992	-3.833395
H	5.302672	-3.607530	-3.971860

$5m_{08}$

S	-3.728413	-2.111860	0.768205
O	-3.644032	-3.215261	-0.208292
O	-4.484923	-0.904690	0.384329
O	-2.403302	-1.790394	1.416302

C	-4.700273	-2.824628	2.177400
F	-5.850158	-3.323227	1.745602
F	-4.942189	-1.859249	3.077808
F	-3.977558	-3.784990	2.761543
H	-1.258436	0.426891	-0.304996
O	-0.543109	0.161736	0.336261
H	-0.130154	-0.695099	0.018870
S	0.580014	-3.429121	0.720467
O	0.281714	-2.329478	-0.207616
O	-0.474332	-3.428422	1.918879
O	1.894715	-3.633595	1.287065
C	0.080499	-4.984855	-0.184115
F	-1.251834	-5.028552	-0.259482
F	0.521345	-6.035595	0.497818
F	0.609807	-4.961573	-1.395405
H	-1.292903	-2.882637	1.674038
H	0.172291	0.893255	0.370104
S	2.614641	1.142488	0.624435
O	3.414432	1.646571	-0.496963
O	2.350950	-0.310874	0.701312
O	1.301728	1.884849	0.858092
C	3.588690	1.586665	2.140703
F	4.751976	0.948647	2.126056
F	3.788480	2.906246	2.141332
F	2.900026	1.248271	3.233343
H	2.756005	2.219575	-2.051700
S	1.466925	0.892525	-3.155042
O	2.383056	2.187496	-2.975292
O	0.662521	1.084217	-4.342781
O	0.875002	0.516871	-1.870057
C	2.762039	-0.411757	-3.505742
F	3.805757	-0.212027	-2.697061
F	2.239929	-1.608988	-3.275433
F	3.154641	-0.317148	-4.772065
H	1.282916	3.530206	1.008110
O	1.109035	4.518022	1.020238
S	1.369574	5.139790	-0.431575
O	2.487264	4.473772	-1.084156
O	1.272317	6.579968	-0.305546
C	-0.168646	4.553970	-1.302131
F	-1.254172	4.900028	-0.604379
F	-0.214178	5.101224	-2.510062
F	-0.137094	3.218518	-1.411587
H	-4.355657	0.108156	-0.914776
O	-4.457498	0.826566	-1.610025
S	-3.621620	2.121380	-1.219093
O	-2.495003	1.752613	-0.345637
O	-4.481762	3.222381	-0.831071
C	-2.932794	2.495954	-2.916140
F	-3.885253	2.327247	-3.825668
F	-2.534157	3.766713	-2.918094
F	-1.905311	1.697292	-3.166757
C	-1.161791	3.839612	3.085356

C	-0.540526	4.882571	3.773885
C	-0.380414	4.807185	5.157776
C	-0.841144	3.684843	5.850316
C	-1.457580	2.642514	5.158883
C	-1.623025	2.711849	3.771195
H	-1.279115	3.900999	2.007451
H	-0.167902	5.738511	3.221008
H	0.108590	5.614659	5.694691
H	-0.715124	3.618848	6.927352
H	-1.804895	1.767190	5.705253
C	-2.285976	1.591909	2.990588
H	-1.992990	1.703174	1.944961
C	-3.818698	1.664104	3.029849
H	-4.198393	1.676473	4.057243
H	-4.142589	2.590002	2.546839
H	-4.275410	0.828678	2.487804
C	0.340503	-1.064262	3.882166
C	-0.389093	-1.874326	4.777459
C	-1.742750	-1.629062	5.054487
C	-2.411385	-0.589307	4.442026
C	-1.734693	0.216214	3.438227
C	-0.307799	0.022764	3.301754
H	-2.262938	-2.278709	5.750707
H	-3.474263	-0.449208	4.590317
H	-2.046417	-0.498883	2.573143
H	0.100110	-2.716509	5.253258
H	-2.612370	-3.303015	-1.506146
O	-2.040768	-0.877719	-1.643650
S	-1.816352	-1.773289	-2.783788
O	-2.015119	-3.282299	-2.311874
O	-0.639099	-1.698427	-3.617819
C	-3.324545	-1.572229	-3.857972
F	-3.341834	-0.344851	-4.366321
F	-3.297563	-2.468153	-4.837874
F	-4.408331	-1.764044	-3.100258
H	3.089512	-1.485280	-0.181685
O	4.698306	-2.144417	1.641230
S	4.869332	-2.597936	0.264581
O	3.600711	-2.221999	-0.628922
O	5.272956	-3.951086	-0.065448
C	6.108470	-1.442024	-0.500546
F	7.284685	-1.605922	0.106190
F	6.234847	-1.700168	-1.799864
F	5.695690	-0.182079	-0.336105
H	0.259628	0.686699	2.661809
O	1.620395	-1.238855	3.544571
C	2.365820	-2.341103	4.078284
H	3.319018	-2.312313	3.553847
H	2.504950	-2.217155	5.159038
H	1.864397	-3.286687	3.855685

TS3m$_{08}$

S	-3.409650	-2.479428	0.681427

O	-3.077186	-3.419607	-0.397464
O	-4.135933	-1.241630	0.375743
O	-2.185887	-2.226137	1.576860
C	-4.529504	-3.452286	1.800736
F	-5.612128	-3.817613	1.128641
F	-4.882688	-2.693299	2.845563
F	-3.875714	-4.525456	2.240057
H	-1.217190	0.502233	-0.261150
O	-0.558647	0.145802	0.393065
H	-0.124692	-0.664252	-0.003372
S	0.924974	-3.372198	0.352599
O	0.336658	-2.245297	-0.384334
O	-0.017661	-3.749901	1.590167
O	2.296753	-3.383101	0.803880
C	0.657287	-4.856621	-0.745331
F	-0.653778	-5.086693	-0.849869
F	1.252361	-5.909910	-0.199796
F	1.173237	-4.593879	-1.935068
H	-0.885095	-3.252569	1.531034
H	0.171996	0.864439	0.565750
S	2.610923	1.226029	0.669761
O	3.298434	1.997126	-0.372876
O	2.488022	-0.235397	0.483100
O	1.248609	1.789666	1.074535
C	3.617324	1.540198	2.202781
F	4.887176	1.226367	1.979528
F	3.516700	2.840436	2.492896
F	3.144129	0.824115	3.219799
H	2.635739	2.599607	-1.899009
S	1.326301	1.334786	-3.044900
O	2.296878	2.581830	-2.836817
O	0.609095	1.541887	-4.284407
O	0.635729	1.022960	-1.793087
C	2.560810	-0.068912	-3.276293
F	3.708815	0.250136	-2.675805
F	2.065694	-1.170422	-2.715645
F	2.770533	-0.269128	-4.570314
H	1.084694	3.419284	1.303769
O	0.854899	4.384465	1.451908
S	1.004157	5.233045	0.107303
O	2.084775	4.718489	-0.720985
O	0.880542	6.631768	0.466672
C	-0.570863	4.742635	-0.750592
F	-1.630739	4.995744	0.023822
F	-0.678291	5.419576	-1.888340
F	-0.529306	3.429458	-1.010458
H	-4.199143	-0.123384	-0.961366
O	-4.482623	0.629490	-1.548120
S	-3.766654	1.981366	-1.087182
O	-2.617517	1.658335	-0.228392
O	-4.737798	2.962643	-0.648691
C	-3.112067	2.535111	-2.748747
F	-4.069081	2.394846	-3.659371

F	-2.780134	3.819369	-2.639603
F	-2.049949	1.816432	-3.079347
C	-1.987753	3.204853	2.904509
C	-1.515399	4.395752	3.459844
C	-1.291598	4.485739	4.833131
C	-1.542738	3.381430	5.651615
C	-2.019929	2.195302	5.096599
C	-2.249663	2.098702	3.718804
H	-2.155715	3.137312	1.834273
H	-1.309008	5.241583	2.814044
H	-0.915895	5.409146	5.263770
H	-1.364805	3.444074	6.721581
H	-2.210053	1.337361	5.738352
C	-2.808246	0.823211	3.107396
H	-2.671155	0.895114	2.025097
C	-4.316829	0.697324	3.362379
H	-4.544634	0.687360	4.433787
H	-4.822170	1.563302	2.926292
H	-4.734698	-0.202055	2.900266
C	0.232934	-1.424371	3.781024
C	-0.310309	-2.408346	4.627155
C	-1.664593	-2.372426	4.973865
C	-2.506404	-1.383496	4.482470
C	-1.997554	-0.401103	3.571672
C	-0.591654	-0.385386	3.343735
H	-2.062149	-3.141198	5.628805
H	-3.566835	-1.408542	4.696674
H	-2.151989	-1.279636	2.587959
H	0.315680	-3.211033	4.998615
H	-2.113140	-3.290297	-1.788700
O	-1.936895	-0.822224	-1.739523
S	-1.665620	-1.567556	-2.972205
O	-1.623882	-3.129259	-2.642081
O	-0.569548	-1.250766	-3.858447
C	-3.253063	-1.491755	-3.943362
F	-3.466411	-0.241535	-4.338319
F	-3.174243	-2.294820	-4.997078
F	-4.249580	-1.890121	-3.144727
H	3.495755	-1.258508	-0.370250
O	4.983881	-1.693850	1.591919
S	5.371900	-2.089883	0.241529
O	4.165773	-1.876464	-0.783191
O	5.998668	-3.366176	-0.042782
C	6.506408	-0.753775	-0.384786
F	7.521967	-0.612549	0.467164
F	6.971935	-1.079937	-1.587569
F	5.829754	0.395004	-0.466321
H	-0.150263	0.402590	2.749022
O	1.496467	-1.381566	3.337716
C	2.445957	-2.358429	3.780844
H	3.360651	-2.133707	3.235525
H	2.603139	-2.270019	4.862450
H	2.109199	-3.366635	3.523271

TS3m'$_{08}$

S	-1.993696	-3.478493	0.672683
O	-2.013107	-3.863568	-0.745146
O	-2.585376	-2.188762	1.065227
O	-0.602149	-3.692523	1.302061
C	-2.996400	-4.782395	1.538971
F	-4.262277	-4.662906	1.149912
F	-2.909095	-4.595506	2.856899
F	-2.530750	-5.985356	1.224226
H	-1.819885	0.641468	0.949629
O	-0.904649	0.466263	0.581525
H	-0.997192	0.371771	-0.403332
S	1.479754	-2.698870	-1.321629
O	0.282495	-1.926193	-0.997062
O	1.516800	-4.016075	-0.398900
O	2.799873	-2.105709	-1.351777
C	1.214853	-3.514704	-2.977380
F	0.147579	-4.313483	-2.902599
F	2.288319	-4.231669	-3.285520
F	1.015736	-2.570480	-3.888102
H	0.698637	-4.028861	0.164587
H	-0.248239	1.249359	0.789571
S	2.088947	2.111449	0.330280
O	2.331721	3.273877	-0.536655
O	2.190469	0.771617	-0.294431
O	0.823440	2.210369	1.169399
C	3.401714	2.210719	1.645139
F	4.587816	2.393627	1.076727
F	3.124096	3.241417	2.446997
F	3.410375	1.083328	2.355996
H	1.266293	3.739350	-1.859853
S	-0.215374	2.532791	-2.853885
O	0.781395	3.763672	-2.732926
O	-1.219624	2.855303	-3.842590
O	-0.576996	2.045149	-1.518080
C	0.939793	1.222095	-3.566567
F	2.204347	1.571081	-3.331889
F	0.695239	0.057319	-2.960875
F	0.737488	1.107269	-4.869822
H	0.455503	3.727621	1.768078
O	0.138177	4.621710	2.093434
S	-0.673082	5.387701	0.949682
O	-0.130024	5.101383	-0.369150
O	-0.924280	6.733723	1.422999
C	-2.284827	4.464635	1.038494
F	-2.841392	4.597139	2.242900
F	-3.108866	4.937353	0.109195
F	-2.061933	3.159337	0.808575
H	-3.885730	-1.296487	0.350039
O	-4.733559	-0.781525	0.228178
S	-4.678375	0.561977	1.080941
O	-3.321672	0.729293	1.636356

O	-5.828609	0.667564	1.950851
C	-4.867371	1.838360	-0.269427
F	-5.935195	1.546961	-1.000607
F	-5.033600	3.014421	0.331516
F	-3.777454	1.863286	-1.024380
C	-1.095795	1.330745	3.892615
C	-0.710840	2.612526	4.280762
C	0.581374	2.840736	4.758054
C	1.473355	1.774321	4.861683
C	1.084531	0.490738	4.474156
C	-0.198905	0.256751	3.972663
H	-2.100018	1.164077	3.516938
H	-1.408772	3.436913	4.180296
H	0.890326	3.844440	5.032358
H	2.482143	1.940977	5.227683
H	1.798577	-0.324641	4.545970
C	-0.664904	-1.121765	3.511249
H	-1.297883	-0.967980	2.635171
C	-1.541436	-1.797962	4.575783
H	-1.002711	-1.921019	5.520953
H	-2.415676	-1.172203	4.774174
H	-1.899917	-2.776809	4.240436
C	2.662956	-1.994044	1.857364
C	3.086010	-3.092359	2.611209
C	2.252042	-3.647743	3.595031
C	1.010590	-3.060319	3.849397
C	0.527023	-1.983008	3.054024
C	1.410736	-1.441128	2.068443
H	3.327423	-1.568300	1.115261
H	-0.060245	-2.832193	2.140542
H	-1.836980	-2.902051	-2.144185
O	-2.328200	-0.540932	-1.425266
S	-2.450572	-0.952956	-2.827727
O	-1.865377	-2.420423	-3.018465
O	-1.997461	-0.121419	-3.919876
C	-4.260821	-1.309111	-3.066674
F	-4.953522	-0.198012	-2.836159
F	-4.476671	-1.732278	-4.304920
F	-4.621309	-2.257487	-2.195248
H	3.462926	0.418997	-1.371461
O	5.099160	-0.463391	0.285804
S	5.426068	-0.436449	-1.140361
O	4.263858	0.293144	-1.957818
O	5.883724	-1.622351	-1.839899
C	6.743253	0.854810	-1.377624
F	7.837587	0.459198	-0.723831
F	7.017834	0.981083	-2.673601
F	6.335129	2.025656	-0.891286
H	1.079580	-0.613271	1.460764
H	4.065037	-3.512431	2.413593
H	0.394319	-3.487037	4.631601
O	2.566884	-4.719254	4.361866
C	3.841271	-5.328646	4.176490

H	4.653789	-4.623381	4.389220
H	3.879426	-6.153708	4.887946
H	3.950723	-5.717744	3.156966

$6m_{08}$

S	-3.099529	-2.822316	0.592308
O	-2.560041	-3.823862	-0.322010
O	-3.864891	-1.669244	0.138775
O	-1.885456	-2.372469	1.527392
C	-4.170113	-3.783539	1.792211
F	-4.981858	-4.546460	1.074633
F	-4.870430	-2.939237	2.536159
F	-3.382006	-4.529924	2.555497
H	-0.884612	0.084095	-0.541597
O	-0.421484	-0.068760	0.320597
H	0.250346	-0.793831	0.173286
S	1.443953	-3.386671	0.768347
O	0.819198	-2.378227	-0.099626
O	0.429225	-3.762611	1.957700
O	2.764850	-3.235639	1.327508
C	1.380243	-4.968014	-0.218492
F	0.097514	-5.285581	-0.428138
F	1.972831	-5.934288	0.467795
F	1.994196	-4.767887	-1.372670
H	-0.445412	-3.325966	1.808147
H	0.097221	0.801444	0.574000
S	2.390513	1.547961	0.847232
O	3.110809	2.317158	-0.175377
O	2.476129	0.071286	0.772974
O	0.929346	1.948016	1.024479
C	3.145414	2.103302	2.454503
F	4.456734	1.906561	2.424899
F	2.882089	3.404362	2.593572
F	2.608289	1.433345	3.471229
H	2.530664	2.717249	-1.767086
S	1.563425	1.240971	-3.004929
O	2.289885	2.631815	-2.733513
O	1.007936	1.288966	-4.340398
O	0.756955	0.859759	-1.844157
C	3.010448	0.035423	-2.995083
F	4.010800	0.547367	-2.277599
F	2.604468	-1.103253	-2.435891
F	3.414524	-0.185320	-4.238640
H	0.470572	3.535240	1.162960
O	0.062940	4.448682	1.212344
S	0.372155	5.284923	-0.112535
O	1.669766	4.925038	-0.666926
O	-0.030066	6.654632	0.139323
C	-0.888681	4.541194	-1.257749
F	-2.117237	4.636497	-0.739778
F	-0.848869	5.173496	-2.425598
F	-0.592759	3.247681	-1.436951
H	-3.824810	-0.641980	-1.412590

O	-4.209150	0.036338	-2.017197
S	-3.596020	1.475816	-1.638368
O	-2.505866	1.286692	-0.677722
O	-4.662503	2.420211	-1.379351
C	-2.860446	1.899735	-3.305549
F	-3.743324	1.600517	-4.253133
F	-2.605094	3.204383	-3.327012
F	-1.741862	1.211386	-3.487720
C	-3.050831	3.268986	2.227339
C	-2.764978	4.579457	2.617102
C	-2.814935	4.933772	3.964376
C	-3.149418	3.972950	4.922587
C	-3.434915	2.666323	4.531846
C	-3.393575	2.304186	3.179396
H	-3.006328	2.997010	1.177981
H	-2.492604	5.314876	1.868266
H	-2.586746	5.951168	4.268298
H	-3.182460	4.241391	5.975000
H	-3.681668	1.918470	5.281845
C	-3.726807	0.880136	2.751475
H	-3.510519	0.814816	1.678608
C	-5.219212	0.573452	2.935119
H	-5.522559	0.656424	3.984164
H	-5.809285	1.294415	2.362636
H	-5.467954	-0.431555	2.578392
C	-0.479312	-0.897260	3.717035
C	-0.914996	-1.881846	4.615452
C	-2.277524	-1.967938	4.910771
C	-3.215483	-1.110060	4.331358
C	-2.793342	-0.112759	3.439689
C	-1.422769	-0.019521	3.149522
H	-2.614108	-2.732646	5.605291
H	-4.264771	-1.215108	4.578257
H	-1.963703	-1.461762	1.985110
H	-0.214408	-2.570661	5.070922
H	-1.414360	-3.741333	-1.672160
O	-1.564728	-1.279220	-1.803278
S	-1.075167	-2.057903	-2.948103
O	-0.879175	-3.579757	-2.490070
O	0.062672	-1.662927	-3.743009
C	-2.556826	-2.246243	-4.063718
F	-2.849204	-1.071444	-4.605231
F	-2.293445	-3.135656	-5.010941
F	-3.582962	-2.668826	-3.315431
H	3.676120	-0.856985	0.079052
O	4.961517	-1.021685	2.213503
S	5.543571	-1.441385	0.943352
O	4.441858	-1.427508	-0.216707
O	6.336503	-2.647516	0.807453
C	6.583390	-0.017327	0.348297
F	7.509768	0.258269	1.265969
F	7.171963	-0.334340	-0.802111
F	5.802923	1.052280	0.167512

H	-1.059930	0.787219	2.527132
O	0.791498	-0.742483	3.282515
C	1.847585	-1.457930	3.937789
H	2.758071	-1.190978	3.405111
H	1.912424	-1.153765	4.988353
H	1.691642	-2.537278	3.866514

$5p_{06}$

S	1.810236	-2.182117	1.823377
O	2.924593	-1.272849	2.163721
O	1.339509	-2.110182	0.405007
O	0.684989	-2.214476	2.795764
C	2.534065	-3.883191	1.939681
F	3.496469	-4.004475	1.024470
F	1.571294	-4.780008	1.689590
F	3.033628	-4.096260	3.153161
H	0.224423	-0.676784	-1.820959
O	-0.196328	0.019663	-1.237024
H	0.504286	0.666882	-0.961516
S	-0.297570	1.165987	2.900454
O	0.271114	0.827480	1.600053
O	-0.635563	-0.167436	3.713266
O	-1.430584	2.062916	3.050787
C	1.085187	1.818829	3.967246
F	2.047123	0.894107	4.021793
F	0.617117	2.046831	5.192409
F	1.562961	2.941687	3.450772
H	-0.067732	-0.938038	3.378832
H	-1.007089	0.495778	-1.718728
S	-3.041188	2.000840	-1.687688
O	-2.901398	3.238330	-2.493260
O	-2.885308	2.138662	-0.233805
O	-2.301418	0.816809	-2.271207
C	-4.806976	1.484033	-1.947949
F	-5.614529	2.533118	-1.798755
F	-4.981061	0.958513	-3.163256
F	-5.123186	0.559116	-1.026911
H	-1.658297	4.209663	-2.186064
S	0.407688	4.064477	-1.519670
O	-0.877855	4.840481	-2.032292
O	1.594038	4.735447	-2.005532
O	0.217071	2.619397	-1.681028
C	0.275215	4.387588	0.307547
F	-0.923753	4.010360	0.742861
F	1.216278	3.679290	0.936814
F	0.457380	5.683008	0.552126
H	2.369201	-2.136546	-0.798270
O	2.961058	-2.293250	-1.613275
S	2.090064	-2.437870	-2.924256
O	0.703166	-1.997561	-2.658290
O	2.313079	-3.710497	-3.577561
C	2.871156	-1.108133	-3.971089
F	4.186422	-1.286721	-4.003438

F	2.365443	-1.213398	-5.197212
F	2.579606	0.085024	-3.464393
C	-4.087870	-2.286243	-1.955123
C	-5.457087	-2.338949	-2.218325
C	-6.263532	-3.255121	-1.543681
C	-5.694140	-4.114096	-0.600862
C	-4.326496	-4.054329	-0.334812
C	-3.507376	-3.141636	-1.010999
H	-3.469985	-1.559271	-2.474950
H	-5.887250	-1.654092	-2.942312
H	-7.329371	-3.300114	-1.748171
H	-6.315718	-4.830965	-0.071553
H	-3.898119	-4.724382	0.405804
C	-2.030333	-3.005519	-0.687549
H	-1.579892	-2.367787	-1.452583
C	-1.250394	-4.323722	-0.682529
H	-1.696303	-5.072474	-0.020150
H	-1.241512	-4.743311	-1.692504
H	-0.214654	-4.161543	-0.369525
C	-3.210670	-0.354519	1.637336
C	-3.331104	-1.109122	2.835206
C	-2.803384	-2.437958	2.933939
C	-2.096337	-2.958182	1.902334
C	-1.848724	-2.203964	0.656098
C	-2.524228	-0.897231	0.599586
H	-3.620248	0.641450	1.540303
H	-2.945550	-2.965490	3.870461
H	-1.633384	-3.933694	2.003039
H	-0.764505	-1.965404	0.667023
H	3.113235	0.303581	1.744146
O	2.312767	0.530554	-0.685047
S	3.389250	1.350509	-0.121384
O	3.406512	1.224634	1.463111
O	3.567080	2.740126	-0.477095
C	4.943172	0.424437	-0.564397
F	5.015220	0.325875	-1.890868
F	6.003314	1.077619	-0.101678
F	4.895463	-0.795634	-0.025297
H	-2.440806	-0.333993	-0.316036
O	-3.917821	-0.663033	3.917446
C	-4.387031	0.707381	3.975725
H	-4.748085	0.832409	4.994870
H	-3.559119	1.387923	3.767450
H	-5.204196	0.850643	3.264146

TS3p$_{06}$

S	0.885733	-2.939962	0.844173
O	1.987246	-2.487346	1.699106
O	0.994678	-2.852160	-0.616151
O	-0.456217	-2.365902	1.357341
C	0.683080	-4.747536	1.232092
F	1.714675	-5.416719	0.732941
F	-0.452721	-5.183960	0.676043

F	0.622016	-4.911004	2.548758
H	0.171504	-0.251338	-1.639820
O	-0.311903	0.091260	-0.841337
H	0.361108	0.507271	-0.252605
S	-0.067079	0.687142	3.153733
O	0.497868	0.648411	1.808366
O	-0.773357	-0.721012	3.475792
O	-0.931051	1.746537	3.629289
C	1.368052	0.553212	4.337980
F	1.975312	-0.623970	4.152873
F	0.912429	0.622754	5.585326
F	2.219471	1.542383	4.107142
H	-0.585199	-1.358990	2.736055
H	-1.010480	0.888232	-1.182769
S	-2.517214	2.677962	-0.628878
O	-2.149929	4.093363	-0.868521
O	-2.417210	2.177948	0.747050
O	-1.909341	1.736430	-1.654005
C	-4.312009	2.588580	-1.091606
F	-5.004700	3.470344	-0.367681
F	-4.474859	2.851265	-2.386905
F	-4.766500	1.356890	-0.828304
H	-0.609851	4.555782	-0.965608
S	1.405475	3.854508	-0.519414
O	0.334580	4.922755	-1.001569
O	2.716050	4.308577	-0.933409
O	0.934079	2.496770	-0.798340
C	1.260962	4.065822	1.323978
F	-0.007342	3.860582	1.681544
F	2.043996	3.179414	1.940369
F	1.631268	5.297273	1.667450
H	2.209996	-2.170710	-1.725241
O	2.743900	-2.057271	-2.557173
S	1.865476	-1.349406	-3.686687
O	0.558693	-0.965960	-3.123206
O	1.934507	-2.103154	-4.919400
C	2.830859	0.230635	-3.939309
F	4.105760	-0.069687	-4.159930
F	2.313158	0.836712	-5.003497
F	2.715989	1.010636	-2.873452
C	-3.023125	-0.844431	-3.263428
C	-3.917143	-0.047417	-3.981332
C	-5.289178	-0.171244	-3.770609
C	-5.765263	-1.098598	-2.839800
C	-4.870732	-1.884919	-2.117684
C	-3.489805	-1.763482	-2.320336
H	-1.954868	-0.737597	-3.426790
H	-3.535777	0.680897	-4.690486
H	-5.984886	0.456411	-4.319829
H	-6.833359	-1.198434	-2.667524
H	-5.245940	-2.583151	-1.372875
C	-2.508021	-2.578809	-1.488042
H	-1.506639	-2.193611	-1.706093

C	-2.514865	-4.060765	-1.884873
H	-3.499219	-4.515278	-1.728470
H	-2.272807	-4.151846	-2.947350
H	-1.771198	-4.632082	-1.320222
C	-3.393142	-0.651160	1.700527
C	-3.735366	-1.679565	2.599176
C	-3.677653	-3.028448	2.182482
C	-3.248415	-3.345037	0.909440
C	-2.779405	-2.334802	0.010753
C	-2.966406	-0.984624	0.432801
H	-3.442232	0.394593	1.972423
H	-3.970502	-3.797608	2.888808
H	-3.184443	-4.387154	0.616277
H	-1.482478	-2.369006	0.642680
H	2.894722	-1.025399	1.888764
O	2.324536	-0.195872	-0.362696
S	3.518057	0.292849	0.331183
O	3.502521	-0.240120	1.838317
O	3.922183	1.679297	0.327783
C	4.917333	-0.724504	-0.354405
F	5.108287	-0.391191	-1.627591
F	6.025594	-0.505045	0.342667
F	4.580989	-2.016889	-0.271061
H	-2.721283	-0.193756	-0.257675
O	-4.114766	-1.472324	3.864271
C	-4.145087	-0.125486	4.360055
H	-4.427409	-0.212491	5.408905
H	-3.162274	0.344925	4.271437
H	-4.893609	0.466373	3.822786

$6p_{06}$

S	0.332738	-3.132974	0.447356
O	-0.708519	-3.556295	-0.489863
O	0.035098	-2.485011	1.710431
O	1.385110	-2.303365	-0.431220
C	1.323783	-4.675805	0.807667
F	0.497648	-5.577815	1.321986
F	2.279727	-4.379665	1.685161
F	1.860879	-5.126769	-0.317343
H	-0.200059	0.238386	1.545876
O	0.416412	0.292028	0.769186
H	-0.150735	0.358711	-0.037317
S	0.112257	-0.464739	-3.146922
O	-0.474275	-0.367825	-1.809320
O	1.333247	-1.513758	-3.104035
O	0.512452	0.681555	-3.929499
C	-1.090131	-1.463849	-4.164392
F	-1.173112	-2.694854	-3.652433
F	-0.652656	-1.532429	-5.416967
F	-2.276283	-0.871738	-4.124462
H	1.387144	-1.911413	-2.201900
H	0.940662	1.289689	0.863709
S	1.795892	3.144947	-0.333526

O	1.014738	4.394722	-0.491561
O	1.838928	2.221442	-1.473082
O	1.522357	2.446811	0.988051
C	3.527802	3.753253	-0.065213
F	3.901971	4.504212	-1.101817
F	3.599046	4.472154	1.054545
F	4.355700	2.704296	0.033301
H	-0.593236	4.444155	-0.469777
S	-2.231098	3.064442	-0.804254
O	-1.605837	4.495095	-0.518132
O	-3.655621	3.125986	-0.548769
O	-1.393263	2.021746	-0.210907
C	-1.967103	2.961629	-2.647128
F	-0.683625	3.189377	-2.910484
F	-2.306931	1.747077	-3.082977
F	-2.722793	3.874324	-3.254039
H	-2.464759	-1.396251	2.099021
O	-2.769354	-1.360161	3.046732
S	-2.289635	0.023678	3.687362
O	-1.065749	0.478753	3.019403
O	-2.359416	-0.089212	5.126988
C	-3.639044	1.184304	3.124102
F	-4.816046	0.719277	3.532306
F	-3.404209	2.375131	3.662236
F	-3.621105	1.271709	1.797855
C	2.111303	0.117019	3.640065
C	1.759202	1.368615	4.151181
C	2.658176	2.430301	4.075048
C	3.910675	2.235042	3.489352
C	4.261967	0.982462	2.991693
C	3.365109	-0.093474	3.060409
H	1.399853	-0.703241	3.689742
H	0.777573	1.508919	4.590312
H	2.380807	3.408826	4.455475
H	4.608676	3.062936	3.407176
H	5.232470	0.844226	2.522823
C	3.741153	-1.461538	2.516017
H	2.906369	-2.136884	2.749220
C	4.980695	-2.014953	3.249432
H	5.869223	-1.417800	3.021807
H	4.816171	-1.983837	4.330691
H	5.191080	-3.051952	2.969543
C	3.751510	-0.353418	-1.188452
C	4.289569	-1.474320	-1.824668
C	4.632145	-2.599913	-1.051766
C	4.459576	-2.589884	0.324302
C	3.929806	-1.465807	0.994632
C	3.575947	-0.363936	0.201755
H	3.452457	0.529942	-1.736792
H	5.040879	-3.468115	-1.558893
H	4.738558	-3.473540	0.888336
H	2.012431	-1.717358	0.098076
H	-2.077261	-2.762956	-1.156005

O	-2.238729	-0.956925	0.459933
S	-3.281275	-1.088271	-0.575276
O	-2.898404	-2.322177	-1.508929
O	-3.725544	0.027724	-1.373406
C	-4.765218	-1.809563	0.294075
F	-5.252893	-0.899324	1.131046
F	-5.682617	-2.151724	-0.598889
F	-4.368341	-2.883954	0.980598
H	3.176529	0.521947	0.673047
O	4.501535	-1.575799	-3.158908
C	4.292247	-0.409491	-3.954911
H	4.563399	-0.696639	-4.971531
H	3.246999	-0.089005	-3.929930
H	4.937150	0.411633	-3.619065

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S	1.027526	3.972673	0.292823
O	-0.156686	4.557819	-0.372107
O	2.274847	3.869465	-0.498110
O	0.735687	2.728094	1.074605
C	1.442289	5.215537	1.605927
F	1.538446	6.432371	1.085216
F	2.606982	4.888950	2.185387
F	0.480657	5.194780	2.535791
H	0.879530	0.276237	-0.621761
O	0.238853	0.070450	0.110678
H	-0.657569	0.496450	-0.067836
S	-2.550183	1.682049	1.421356
O	-2.003497	1.376073	0.087343
O	-1.442430	2.388717	2.309124
O	-3.185775	0.669084	2.245345
C	-3.729355	3.094184	1.107383
F	-3.009435	4.128360	0.668546
F	-4.332920	3.412960	2.247055
F	-4.610474	2.732763	0.195010
H	-0.596373	2.611834	1.760018
H	0.140824	-0.929065	0.263345
S	-1.457760	-2.744171	0.689215
O	-1.601077	-3.917876	-0.190968
O	-2.239601	-1.542114	0.361755
O	-0.028157	-2.359125	1.000755
C	-2.097830	-3.308629	2.335170
F	-3.412783	-3.506469	2.268756
F	-1.488571	-4.426979	2.715611
F	-1.853813	-2.347188	3.249423
H	-1.116004	-3.941711	-1.822312
S	-0.504820	-2.294136	-3.063455
O	-0.902370	-3.810168	-2.793937
O	0.015061	-2.190273	-4.409798
O	0.245156	-1.766877	-1.916317
C	-2.200761	-1.452933	-3.003166
F	-3.096549	-2.293582	-2.490030
F	-2.113393	-0.379069	-2.217801

F	-2.553413	-1.102175	-4.227465
H	2.659615	2.899315	-1.706228
O	3.090045	2.367012	-2.455754
S	3.508671	0.917708	-1.982900
O	2.614072	0.442320	-0.908381
O	4.941844	0.808773	-1.786375
C	3.041203	-0.015330	-3.531577
F	3.786647	0.419163	-4.539607
F	3.285226	-1.306426	-3.306838
F	1.756336	0.162384	-3.799225
C	4.767704	-2.026513	3.321719
C	4.991326	-2.796536	4.464458
C	5.207000	-2.179345	5.696691
C	5.202145	-0.785336	5.780918
C	4.979289	-0.017233	4.638651
C	4.758029	-0.628000	3.397755
H	4.596388	-2.516639	2.368238
H	4.997228	-3.879945	4.387376
H	5.382007	-2.778479	6.585646
H	5.375676	-0.295981	6.735304
H	4.984464	1.066845	4.718603
C	4.463455	0.188495	2.152161
H	4.415234	-0.496896	1.304438
C	5.523356	1.245431	1.828694
H	5.666809	1.963595	2.642557
H	6.483285	0.749542	1.658515
H	5.265801	1.794010	0.916859
C	0.955065	-0.175216	3.258000
C	0.835353	0.983840	4.076284
C	1.811330	2.030239	4.030891
C	2.847473	1.943042	3.163652
C	3.015654	0.802544	2.241078
C	2.008500	-0.261704	2.403008
H	1.658087	2.888422	4.675489
H	3.556931	2.759095	3.091359
H	2.826483	1.210687	1.227500
H	-1.123302	3.898496	-1.542749
O	0.206175	1.828478	-2.028971
S	-0.652830	2.446248	-3.043789
O	-1.588112	3.533635	-2.356239
O	-1.438621	1.658823	-3.968872
C	0.454511	3.539323	-4.067896
F	1.293488	2.773553	-4.759877
F	-0.286702	4.262738	-4.900226
F	1.142463	4.350983	-3.260544
H	1.579510	-3.130914	0.837674
O	2.555373	-3.151122	0.734914
C	2.833869	-3.213363	-0.638461
H	2.356394	-2.408259	-1.204253
C	2.327864	-4.530493	-1.246870
C	4.345265	-3.062186	-0.797876
F	1.075701	-4.769030	-0.800834
F	2.282411	-4.448114	-2.588070

F	3.087230	-5.586098	-0.912604
F	4.728805	-3.337186	-2.055101
F	4.714948	-1.788201	-0.528836
F	5.023794	-3.859434	0.041334
H	-3.739320	-0.666870	-0.372052
O	-4.644970	-0.310984	-0.325795
C	-5.303381	-1.020470	0.682675
H	-4.666708	-1.196258	1.555459
C	-5.754619	-2.399135	0.177921
C	-6.476567	-0.158887	1.151150
F	-4.702367	-3.043525	-0.369840
F	-6.213316	-3.160957	1.192062
F	-6.716127	-2.319180	-0.754182
F	-7.229313	-0.825867	2.049828
F	-6.023439	0.959644	1.755416
F	-7.267418	0.216311	0.137439
H	2.136907	-1.145696	1.785536
H	0.216248	-0.964591	3.297323
O	-0.147538	1.183671	4.916899
C	-1.248147	0.245806	5.005357
H	-1.908707	0.667974	5.760123
H	-1.762504	0.181704	4.045582
H	-0.880834	-0.731968	5.325514

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S	0.408156	4.019571	-0.383295
O	-0.450090	4.023205	-1.572163
O	1.762408	3.466570	-0.428972
O	-0.394173	3.467821	0.825570
C	0.589702	5.812192	0.079637
F	1.351106	6.416086	-0.822852
F	1.160194	5.895648	1.285821
F	-0.613469	6.374874	0.119686
H	1.267946	0.387985	-0.260541
O	0.524643	0.380847	0.402160
H	-0.352693	0.446532	-0.068082
S	-3.118857	1.500320	0.038613
O	-1.844018	1.146360	-0.601873
O	-2.994226	2.954331	0.701604
O	-3.774950	0.626379	0.991785
C	-4.265089	1.952285	-1.371474
F	-3.681682	2.952972	-2.038818
F	-5.421522	2.360996	-0.864982
F	-4.436333	0.919109	-2.167998
H	-2.039974	3.248217	0.672602
H	0.564982	-0.522989	0.924454
S	-0.743961	-2.493022	1.312730
O	-0.495442	-3.830870	0.757212
O	-1.619158	-1.574830	0.556924
O	0.508366	-1.755697	1.760605
C	-1.630734	-2.780401	2.915907
F	-2.841617	-3.283979	2.676034
F	-0.937742	-3.610449	3.685938

F	-1.770141	-1.602772	3.548426
H	0.279215	-4.195237	-0.769759
S	0.739825	-2.761730	-2.301424
O	0.599326	-4.235516	-1.714967
O	1.507516	-2.831839	-3.525098
O	1.089688	-1.831827	-1.221819
C	-1.060246	-2.394094	-2.743234
F	-1.847484	-3.267525	-2.117601
F	-1.362581	-1.160685	-2.327771
F	-1.225730	-2.489657	-4.051195
H	2.795847	2.489902	-1.573124
O	3.636053	2.141668	-1.967395
S	4.096790	0.818117	-1.188515
O	3.039670	0.428904	-0.242602
O	5.468104	0.953068	-0.751037
C	4.068996	-0.419350	-2.594431
F	5.098920	-0.172322	-3.394985
F	4.179757	-1.631298	-2.061811
F	2.934913	-0.321678	-3.273223
C	3.166137	0.073413	3.636162
C	3.600526	-0.853040	4.586661
C	3.385177	-0.608852	5.942528
C	2.733166	0.560931	6.344016
C	2.300192	1.481757	5.391837
C	2.518587	1.246611	4.028451
H	3.342188	-0.117907	2.583830
H	4.087189	-1.761980	4.251297
H	3.717650	-1.328066	6.685648
H	2.558636	0.752884	7.399252
H	1.781621	2.383781	5.709846
C	2.067570	2.250694	2.977551
H	2.176298	1.767622	2.000903
C	2.971381	3.491603	2.971288
H	2.972871	3.993160	3.945030
H	3.998913	3.183313	2.760373
H	2.671840	4.211474	2.204014
C	-1.678301	1.631430	3.492097
C	-2.139599	2.893860	3.924790
C	-1.232732	3.966506	4.054382
C	0.094866	3.796125	3.716213
C	0.573506	2.568962	3.158421
C	-0.347249	1.475133	3.166168
H	-1.608766	4.917529	4.415066
H	0.771550	4.640911	3.783109
H	0.154536	3.048850	1.874471
H	-1.052210	2.800592	-2.684916
O	0.830049	1.260761	-2.167994
S	0.263813	1.346204	-3.515806
O	-1.099278	2.179921	-3.459159
O	0.065284	0.183800	-4.351542
C	1.355743	2.533770	-4.456605
F	2.484681	1.917501	-4.781775
F	0.726321	2.941059	-5.552130

F	1.626376	3.586596	-3.676023
H	2.089368	-2.602591	2.171615
O	3.017598	-2.898829	2.240291
C	3.566422	-2.910583	0.955412
H	3.067469	-2.217308	0.271724
C	3.450148	-4.307151	0.325435
C	5.025760	-2.466892	1.082001
F	2.211214	-4.793056	0.538951
F	3.649756	-4.245792	-1.007604
F	4.326372	-5.186221	0.838338
F	5.701588	-2.668325	-0.066086
F	5.085880	-1.146887	1.362068
F	5.661037	-3.117590	2.067327
H	-2.999490	-1.641524	-0.619042
O	-3.891257	-1.584823	-1.012998
C	-4.778872	-2.115649	-0.075988
H	-4.546956	-1.800520	0.947908
C	-4.726492	-3.651118	-0.090665
C	-6.170490	-1.577849	-0.411056
F	-3.442825	-4.052010	0.033993
F	-5.418846	-4.171065	0.942139
F	-5.210196	-4.173873	-1.226727
F	-7.100427	-2.123699	0.397836
F	-6.211631	-0.240235	-0.230681
F	-6.516921	-1.826689	-1.680588
H	0.010870	0.492982	2.881952
H	-2.348411	0.786489	3.414119
O	-3.410769	3.164634	4.231489
C	-4.397811	2.133443	4.082969
H	-5.346171	2.605717	4.337110
H	-4.421917	1.764554	3.054458
H	-4.199703	1.308192	4.775485

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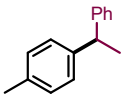
S	0.462196	4.203209	0.069071
O	-0.207728	4.300312	-1.226725
O	1.441921	3.182204	0.383042
O	-0.718762	4.258068	1.164740
C	1.252561	5.863841	0.382508
F	2.330643	5.955810	-0.382807
F	1.591081	5.923183	1.670678
F	0.391443	6.827364	0.092568
H	1.457432	0.261454	0.065362
O	0.664046	0.294989	0.664776
H	-0.144974	0.582946	0.165341
S	-2.891471	1.721978	-0.014230
O	-1.450618	1.635115	-0.314823
O	-3.189111	3.152735	0.646759
O	-3.582184	0.710585	0.751361
C	-3.714012	1.996147	-1.677999
F	-3.292430	3.186266	-2.125456
F	-5.026573	2.008337	-1.527509
F	-3.334289	1.049559	-2.513316

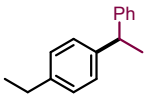
H	-2.342351	3.654888	0.755483
H	0.518185	-0.669209	1.059453
S	-0.960768	-2.560872	1.015370
O	-0.755546	-3.850119	0.336987
O	-1.704818	-1.511570	0.290758
O	0.299644	-1.982517	1.638000
C	-1.977810	-2.942276	2.519080
F	-3.177700	-3.400600	2.156160
F	-1.358642	-3.845033	3.270081
F	-2.141877	-1.812136	3.222319
H	0.067298	-4.033583	-1.174980
S	0.697038	-2.466160	-2.511745
O	0.449788	-3.981704	-2.098644
O	1.519919	-2.450310	-3.701387
O	1.040223	-1.671118	-1.328344
C	-1.055960	-1.947829	-2.990588
F	-1.923665	-2.834245	-2.507591
F	-1.315503	-0.749148	-2.452624
F	-1.159398	-1.883920	-4.307658
H	2.852048	1.976363	-1.567539
O	3.839674	1.963391	-1.465624
S	4.266281	0.542732	-0.854641
O	3.162747	0.035729	-0.028131
O	5.609780	0.651195	-0.338597
C	4.291271	-0.525224	-2.398919
F	5.450235	-0.351161	-3.020252
F	4.143636	-1.790137	-2.038300
F	3.291550	-0.156623	-3.198391
C	2.795934	-0.438304	3.808035
C	3.133030	-1.514441	4.632628
C	2.858136	-1.454797	5.998328
C	2.247460	-0.318120	6.535797
C	1.914200	0.752829	5.709222
C	2.189963	0.703948	4.336365
H	3.021075	-0.485889	2.747779
H	3.591314	-2.393538	4.194556
H	3.114219	-2.291213	6.642585
H	2.027156	-0.268713	7.598845
H	1.426314	1.629557	6.128402
C	1.850292	1.881809	3.433473
H	2.000441	1.549897	2.400712
C	2.815258	3.052454	3.672284
H	2.738239	3.436037	4.695712
H	3.843304	2.710923	3.523353
H	2.630319	3.876750	2.974848
C	-1.960371	1.528552	3.491403
C	-2.396482	2.824394	3.815398
C	-1.440447	3.823272	4.036690
C	-0.072253	3.537341	3.905336
C	0.378581	2.248415	3.570969
C	-0.599839	1.259210	3.382212
H	-1.779879	4.818548	4.305199
H	0.643965	4.328351	4.106175

H	-0.439337	3.924299	2.082895
H	-0.682400	3.095031	-2.406890
O	1.204576	1.521416	-1.970803
S	0.639351	1.684563	-3.321517
O	-0.717464	2.512165	-3.212322
O	0.443549	0.568660	-4.215193
C	1.744895	2.927176	-4.167493
F	2.934098	2.368566	-4.361481
F	1.209353	3.290264	-5.322510
F	1.874647	3.990745	-3.367020
H	1.765097	-3.023968	2.077903
O	2.653868	-3.424121	2.136543
C	3.277700	-3.272878	0.895408
H	2.844260	-2.467649	0.295005
C	3.146425	-4.560245	0.065943
C	4.741591	-2.911605	1.160277
F	1.876841	-5.005922	0.128406
F	3.440402	-4.324932	-1.230835
F	3.947733	-5.546109	0.500820
F	5.462285	-2.918257	0.018802
F	4.826925	-1.670278	1.683332
F	5.317369	-3.755158	2.027484
H	-3.126186	-1.436750	-0.888979
O	-4.025775	-1.332906	-1.253497
C	-4.890807	-1.931616	-0.334865
H	-4.586494	-1.757213	0.702995
C	-4.917018	-3.453568	-0.542815
C	-6.267708	-1.292405	-0.511242
F	-3.649279	-3.918264	-0.563836
F	-5.563975	-4.073261	0.463421
F	-5.501751	-3.804706	-1.697964
F	-7.184827	-1.916428	0.255335
F	-6.231654	0.000986	-0.131679
F	-6.684439	-1.334118	-1.784189
H	-0.288621	0.242432	3.169786
H	-2.668846	0.729602	3.316966
O	-3.693036	3.198887	3.933819
C	-4.699601	2.205978	3.746993
H	-5.649585	2.720422	3.895402
H	-4.660820	1.784358	2.738057
H	-4.600791	1.401797	4.486645

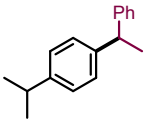
6.Characterization data of the products



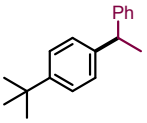
1-methyl-4-(1-phenylethyl)benzene (1)[16]**, colorless oil; ^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.30 - 7.16 (m, 5H), 7.13 - 7.06 (m, 4H), 4.11 (q, *J* = 7.4 Hz, 1H), 2.30 (s, 3H), 1.62 (d, *J* = 7.2 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 146.56, 143.38, 135.46, 129.02, 128.31, 127.54, 127.45, 125.91, 44.32, 21.90, 20.96; **HRMS** (ESI) m/z calculated $C_{15}H_{16}H^+$ $[M+H]^+$ 197.1325, found 197.1323.



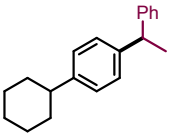
1-ethyl-4-(1-phenylethyl)benzene (2), colorless oil; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.30 - 7.20 (m, 4H), 7.20 - 7.13 (m, 2H), 7.13 - 7.09 (m, 3H), 4.12 (q, *J* = 7.2 Hz, 1H), 2.60 (q, *J* = 7.6 Hz, 2H), 1.62 (d, *J* = 7.2 Hz, 3H), 1.21 (t, *J* = 7.6 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 148.65, 146.57, 143.21, 128.30, 127.60, 127.14, 125.96, 125.19, 44.30, 34.31, 31.38, 21.89; **HRMS** (ESI) m/z calculated $C_{16}H_{18}H^+$ $[M+H]^+$ 211.1481, found 211.1489.



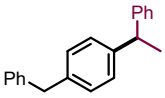
1-isopropyl-4-(1-phenylethyl)benzene (3), colorless oil; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.30 - 7.16 (m, 5H), 7.14 (s, 4H), 4.12 (q, *J* = 7.2 Hz, 1H), 2.91 - 2.81 (m, 1H), 1.63 (d, *J* = 7.2 Hz, 3H), 1.22 (d, *J* = 6.8 Hz, 6H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 148.65, 146.57, 143.21, 128.30, 127.60, 127.14, 125.96, 125.19, 44.30, 34.31, 31.38, 21.89; **HRMS** (ESI) m/z calculated $C_{17}H_{20}H^+$ $[M+H]^+$ 225.1638, found 225.1635.



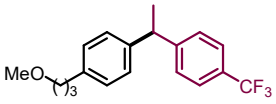
1-(tert-butyl)-4-(1-phenylethyl)benzene (4), colorless oil; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.31 - 7.24 (m, 4H), 7.24 - 7.21 (m, 2H), 7.19 - 7.12 (m, 3H), 4.11 (q, *J* = 7.2 Hz, 1H), 1.62 (d, *J* = 7.2 Hz, 3H), 1.29 (s, 9H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 148.65, 146.57, 143.21, 128.30, 127.60, 127.14, 125.96, 125.19, 44.30, 34.31, 31.38, 21.89; **HRMS** (ESI) m/z calculated $C_{21}H_{20}Na^+$ $[M+Na]^+$ 295.1457, found 295.1452.



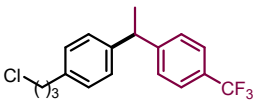
1-cyclohexyl-4-(1-phenylethyl)benzene (5), colorless oil; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.29 - 7.24 (m, 2H), 7.24 - 7.20 (m, 2H), 7.19 - 7.13 (m, 2H), 7.12 (d, *J* = 3.6 Hz, 3H), 4.11 (q, *J* = 7.2 Hz, 1H), 2.49 - 2.41 (m, 1H), 1.89 - 1.78 (m, 5H), 1.76 - 1.68 (m, 1H), 1.62 (d, *J* = 7.2 Hz, 3H), 1.42 - 1.33 (m, 4H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 146.61, 145.68, 143.60, 128.29, 127.59, 126.71, 125.90, 44.40, 44.05, 34.45, 26.91, 26.15, 21.91; **HRMS** (ESI) m/z calculated $C_{20}H_{24}H^+$ $[M+H]^+$ 265.1951, found 265.1945.



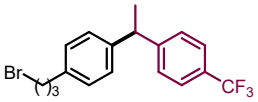
1-benzyl-4-(1-phenylethyl)benzene (6), colorless oil; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.30 - 7.22 (m, 4H), 7.21 (d, *J* = 1.8 Hz, 1H), 7.19 - 7.14 (m, 5H), 7.13 (d, *J* = 2.0 Hz, 1H), 7.11 (s, 1H), 7.09 (s, 1H), 7.08 - 7.02 (m, 1H), 4.10 (q, *J* = 7.2 Hz, 1H), 3.92 (s, 2H), 1.60 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 146.43, 144.07, 141.15, 138.72, 128.89, 128.82, 128.40, 128.31, 127.64, 127.56, 125.99, 125.95, 44.39, 41.50, 21.88; **HRMS** (ESI) m/z calculated $C_{21}H_{20}Na^+$ $[M+Na]^+$ 295.1457, found 295.1452.



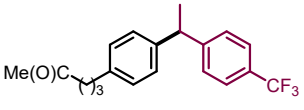
1-(3-methoxypropyl)-4-(1-(4-(trifluoromethyl)phenyl)ethyl)benzene (7), colorless oil; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.44 (d, *J* = 8.2 Hz, 2H), 7.23 (d, *J* = 8.2 Hz, 2H), 7.03 (s, 4H), 4.09 (q, *J* = 7.2 Hz, 1H), 3.30 (t, *J* = 6.4 Hz, 2H), 3.25 (s, 3H), 2.60 - 2.53 (m, 2H), 1.78 (dd, *J* = 14.8, 7.2 Hz, 2H), 1.55 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 150.65, 142.66, 140.08, 128.60, 127.89, 127.47, 125.26, 71.96, 58.52, 44.30, 31.86, 31.21, 21.65; **HRMS** (ESI) m/z calculated $C_{19}H_{21}F_3OH^+$ $[M+H]^+$ 323.1617, found 323.1621.



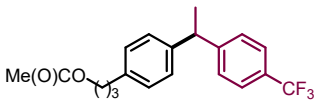
1-(3-chloropropyl)-4-(1-(4-(trifluoromethyl)phenyl)ethyl)benzene (8), colorless oil; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.43 (d, *J* = 8.2 Hz, 2H), 7.22 (d, *J* = 8.2 Hz, 2H), 7.03 (s, 4H), 4.07 (q, *J* = 7.2 Hz, 1H), 3.40 (t, *J* = 6.6 Hz, 2H), 2.67 - 2.61 (m, 2H), 1.98 - 1.93 (m, 2H), 1.54(d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 150.55, 143.08, 138.76, 128.68, 128.46, 127.88, 127.63, 125.27, 44.23, 33.94, 32.28, 21.59; **HRMS** (ESI) m/z calculated $C_{18}H_{18}ClF_3Na^+$ $[M+Na]^+$ 349.0941, found 349.0939.



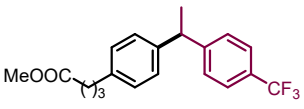
1-(3-bromopropyl)-4-(1-(4-(trifluoromethyl)phenyl)ethyl)benzene (9), colorless oil; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.42 (d, *J* = 8.2 Hz, 2H), 7.22 (d, *J* = 7.8 Hz, 2H), 7.03 (s, 4H), 4.07 (q, *J* = 7.2 Hz, 1H), 3.27 (t, *J* = 5.6 Hz, 2H), 2.66 - 2.61 (m, 2H), 2.07 - 2.01 (m, 2H), 1.53 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 150.51, 143.09, 138.59, 128.68, 128.46, 127.86, 127.62, 126.12, 125.29, 44.29, 34.05, 33.48, 33.02, 21.59; **HRMS** (ESI) m/z calculated $C_{18}H_{18}BrF_3Na^+$ $[M+Na]^+$ 393.0436, found 393.0430.



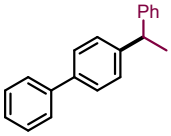
4-(4-(1-(4-(trifluoromethyl)phenyl)ethyl)phenyl)butan-2-one (10), colorless oil; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.44 (d, *J* = 8.0 Hz, 2H), 7.23 (d, *J* = 8.0 Hz, 2H), 7.03 (s, 4H), 4.08 (q, *J* = 7.2 Hz, 1H), 2.78 (t, *J* = 7.6 Hz, 2H), 2.65 (t, *J* = 7.6 Hz, 2H), 2.05 (s, 3H), 1.55 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 207.82, 150.51, 143.04, 139.06, 128.44, 127.86, 127.62, 125.29, 45.05, 44.27, 29.97, 29.20, 21.59; **HRMS** (ESI) m/z calculated $C_{19}H_{19}F_3OH^+$ $[M+H]^+$ 321.1461, found 321.1457.



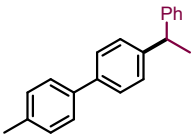
3-(4-(1-(4-(trifluoromethyl)phenyl)ethyl)phenyl)propyl acetate (11), colorless oil; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.44 (d, *J* = 8.2 Hz, 2H), 7.23 (d, *J* = 8.2 Hz, 2H), 7.03 (s, 4H), 4.08 (q, *J* = 7.2 Hz, 1H), 3.99 (t, *J* = 6.6 Hz, 2H), 2.61 - 2.52 (m, 2H), 1.94 (s, 3H), 1.90 - 1.80 (m, 2H), 1.55 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 162.38, 159.96, 158.42, 142.59, 138.36, 128.82, 127.00, 123.97, 115.08, 114.87, 108.90, 71.16, 43.46, 29.78, 22.33; **HRMS** (ESI) m/z calculated $C_{20}H_{21}F_3O_2H^+$ $[M+H]^+$ 351.1566, found 351.1561.



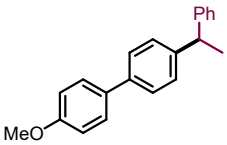
methyl 3-(4-(1-(4-(trifluoromethyl)phenyl)ethyl)phenyl)propanoate (12), colorless oil; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.45 (d, *J* = 8.2 Hz, 2H), 7.24 (d, *J* = 8.2 Hz, 2H), 7.05 (s, 4H), 4.09 (q, *J* = 7.2 Hz, 1H), 3.59 (s, 3H), 2.84 (t, *J* = 7.8 Hz, 2H), 2.53 (t, *J* = 7.8 Hz, 2H), 1.56 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 173.30, 150.49, 143.21, 138.60, 128.42, 127.88, 127.66, 125.32, 51.58, 44.29, 35.59, 30.45, 21.61; **HRMS** (ESI) m/z calculated $C_{19}H_{19}F_3O_2H^+$ $[M+H]^+$ 337.1410, found 337.1417.



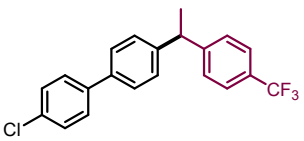
4-(1-phenylethyl)-1,1'-biphenyl (13), colorless oil; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.58 - 7.54 (m, 2H), 7.53 - 7.49 (m, 2H), 7.44 - 7.38 (m, 2H), 7.34 - 7.29 (m, 3H), 7.27 (m, 3H), 7.25 - 7.22 (m, 1H), 7.22 - 7.17 (m, 1H), 4.19 (q, *J* = 7.2 Hz, 1H), 1.67 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 146.23, 145.47, 140.96, 138.92, 128.68, 128.40, 127.99, 127.61, 127.09, 127.03, 127.00, , 126.08, 44.45, 21.85; **HRMS** (ESI) m/z calculated $C_{20}H_{18}H^+$ $[M+H]^+$ 259.1481, found 259.1487.



4-methyl-4'-(1-phenylethyl)-1,1'-biphenyl (14), colorless oil; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 1.8 Hz, 1H), 7.49 - 7.46 (m, 2H), 7.45 (d, *J* = 2.0 Hz, 1H), 7.30 (d, *J* = 7.8 Hz, 1H), 7.28 - 7.24 (m, 5H), 7.22 - 7.18 (m, 3H), 4.18 (q, *J* = 7.2 Hz, 1H), 2.37 (s, 3H), 1.66 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 146.27, 145.15, 138.83, 138.07, 136.76, 129.41, 128.39, 127.94, 127.6, 126.88, 126.82, 126.05, 44.43, 21.86, 21.08; **HRMS** (ESI) m/z calculated $C_{21}H_{20}Na^+$ $[M+Na]^+$ 295.1457, found 295.1456.

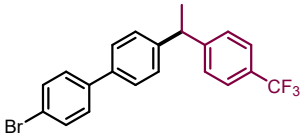


4-methoxy-4'-(1-phenylethyl)-1,1'-biphenyl (15), white solid; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 2.0 Hz, 1H), 7.48 (t, *J* = 2.6 Hz, 2H), 7.45 (d, *J* = 2.0 Hz, 1H), 7.30 (d, *J* = 7.8 Hz, 1H), 7.27 - 7.24 (m, 5H), 7.21 - 7.16 (m, 1H), 6.96 - 6.92 (m, 2H), 4.17 (q, *J* = 7.2 Hz, 1H), 3.81 (s, 3H), 1.66 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 158.92, 146.29, 144.81, 138.50, 133.49, 128.37, 127.96, 127.93, 127.59, 126.63, 126.03, 114.10, 55.26, 44.39, 21.84; **HRMS** (ESI) m/z calculated $C_{21}H_{20}OH^+$ $[M+H]^+$ 289.1587, found 289.1592.

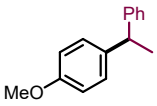


4-chloro-4'-(1-phenylethyl)-1,1'-biphenyl (16), white solid; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.58 - 7.49 (m, 2H), 7.47 (s, 4H), 7.39 -7.34 (m, 4H), 7.27 (d, *J* =

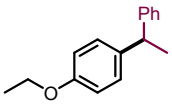
8.0 Hz, 2H), 4.24 (q, *J* = 7.2 Hz, 1H), 1.68 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 150.17, 144.75, 139.20, 138.11, 133.29, 128.90, 128.21, 128.09, 127.92, 127.10, 125.43, 125.36, 44.34, 21.58; **HRMS** (ESI) m/z calculated $C_{20}H_{17}ClNa^+$ $[M+Na]^+$ 315.0911, found 315.0929.



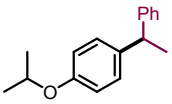
4-bromo-4'-(1-phenylethyl)-1,1'-biphenyl (17), white solid; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.58 - 7.49 (m, 4H), 7.50 - 7.45 (m, 2H), 7.42 (d, *J* = 2.2 Hz, 1H), 7.41 (d, *J* = 1.8 Hz, 1H), 7.35 (d, *J* = 8.2 Hz, 2H), 7.30 - 7.23 (m, 2H), 4.24 (q, *J* = 7.2 Hz, 1H), 1.68 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 150.15, 144.82, 139.67, 138.12, 131.85, 128.57, 128.11, 127.92, 127.06, 125.43, 125.36, 121.44, 44.35, 21.58; **HRMS** (ESI) m/z calculated $C_{20}H_{17}BrH^+$ $[M+H]^+$ 337.0586, found 337.0572.



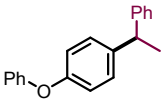
1-Isopropyl-4-(1-phenylethyl)benzene (18)[17]**, colorless oil; ^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.38 - 7.25 (m, 2H), 7.21 - 7.12 (m, 5H), 6.83 - 6.81 (m, 2H), 4.09 (q, *J* = 7.2 Hz, 1H), 3.75 (s, 3H), 1.60 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 157.74, 146.71, 138.48, 128.46, 128.30, 127.48, 125.89, 113.64, 55.16, 43.86, 22.02; **HRMS** (ESI) m/z calculated $C_{15}H_{16}OH^+$ $[M+H]^+$ 213.1274, found 213.1270.



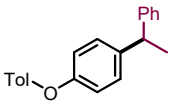
1-ethoxy-4-(1-phenylethyl)benzene (19), yellow oil; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.41 - 7.34 (m, 2H), 7.34 - 7.26 (m, 3H), 7.26 - 7.21 (m, 2H), 6.95 - 6.89 (m, 2H), 4.21 (q, *J* = 7.2 Hz, 1H), 4.09 (q, *J* = 7.0 Hz, 2H), 1.72 (d, *J* = 7.2 Hz, 3H), 1.49 (t, *J* = 7.0 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 157.14, 146.77, 138.31, 128.44, 128.27, 127.48, 125.86, 114.21, 63.27, 43.87, 22.03, 14.85; **HRMS** (ESI) m/z calculated $C_{16}H_{18}ONa^+$ $[M+Na]^+$ 249.1249, found 249.1249.



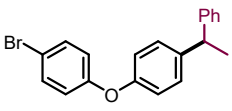
1-isopropoxy-4-(1-phenylethyl)benzene (20), yellow oil; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.26 (d, *J* = 7.4 Hz, 2H), 7.23 - 7.14 (m, 3H), 7.13 - 7.08 (m, 2H), 6.82 - 6.77 (m, 2H), 4.51 - 4.44 (m, 1H), 4.09 (q, *J* = 7.2 Hz, 1H), 1.60 (d, *J* = 7.2 Hz, 3H), 1.30 (d, *J* = 6.2 Hz, 6H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 156.04, 146.78, 138.23, 128.47, 128.28, 127.51, 125.87, 115.54, 69.69, 43.89, 22.72, 22.06; **HRMS** (ESI) m/z calculated $C_{17}H_{20}OH^+$ $[M+H]^+$ 241.1587, found 241.1574.



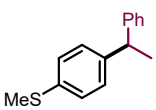
1-phenoxy-4-(1-phenylethyl)benzene (21), white solid; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.33 - 7.25 (m, 4H), 7.24 - 7.20 (m, 3H), 7.18 - 7.15 (m, 2H), 7.09 - 7.04 (m, 1H), 7.00 - 6.95 (m, 2H), 6.94 - 6.90 (m, 2H), 4.13 (q, *J* = 7.2 Hz, 1H), 1.63 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 157.40, 155.24, 146.38, 141.28, 129.64, 128.77, 128.37, 127.53, 126.04, 122.99, 118.78, 118.65, 44.10, 22.01; **HRMS** (ESI) m/z calculated $C_{20}H_{18}OH$ $[M+H]^+$ 275.1430, found 275.1438.



1-methyl-4-(4-(1-phenylethyl)phenoxy)benzene (22), colorless oil; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.32 - 7.26 (m, 2H), 7.25 - 7.19 (m, 3H), 7.17 (d, *J* = 8.0 Hz, 1H), 7.15 - 7.08 (m, 3H), 6.92 - 6.86 (m, 4H), 4.12 (q, *J* = 7.2 Hz, 1H), 2.32 (s, 3H), 1.62 (d, *J* = 7.2 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 155.82, 154.85, 146.44, 140.82, 132.67, 130.14, 128.68, 128.35, 127.53, 126.02, 118.90, 118.22, 44.06, 22.01, 20.68; **HRMS** (ESI) m/z calculated $C_{21}H_{20}ONa^+$ $[M+Na]^+$ 311.1406, found 311.1407.

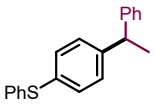


1-bromo-4-(4-(1-phenylethyl)phenoxy)benzene (23), colorless oil; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.42 - 7.35 (m, 2H), 7.32 - 7.25 (m, 2H), 7.23 - 7.17 (m, 5H), 6.95 - 6.88 (m, 2H), 6.88 - 6.82 (m, 2H), 4.13 (q, *J* = 7.2 Hz, 1H), 1.63 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 156.71, 154.68, 146.22, 141.84, 132.55, 128.90, 128.40, 127.51, 126.10, 120.17, 118.93, 115.32, 44.10, 21.97; **HRMS** (ESI) m/z calculated $C_{20}H_{17}BrONa^+$ $[M+Na]^+$ 375.0355, found 375.0352.

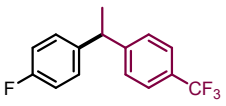


methyl(4-(1-phenylethyl)phenyl)sulfane (24), colorless oil; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.30 - 7.25 (m, 2H), 7.22 - 7.17 (m, 5H), 7.14 (d, *J* = 8.6 Hz, 2H), 4.11 (q, *J* = 7.2 Hz, 1H), 2.45 (s, 3H), 1.62 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 146.17, 143.47, 135.56, 128.36,

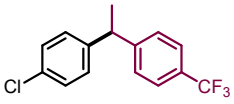
128.12, 127.53, 126.93, 126.06, 44.21, 21.78, 16.13; **HRMS** (ESI) m/z calculated $C_{15}H_{16}SH^+$ $[M+H]^+$ 229.1045, found 229.1036.



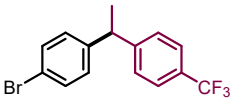
phenyl(4-(1-phenylethyl)phenyl)sulfane (25), yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 - 7.28 (m, 4H), 7.27 - 7.23 (m, 4H), 7.21 - 7.18 (m, 4H), 7.17 - 7.14 (m, 2H), 4.12 (q, *J* = 7.2 Hz, 1H), 1.62 (d, *J* = 7.2 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 145.90, 145.66, 136.24, 132.58, 131.47, 130.52, 129.08, 128.50, 128.41, 127.56, 126.73, 126.16, 44.40, 21.76; **HRMS** (ESI) m/z calculated $C_{20}H_{18}SH$ $[M+H]^+$ 291.1201, found 291.1199.



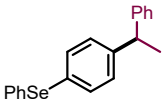
1-fluoro-4-(1-(4-(trifluoromethyl)phenyl)ethyl)benzene (26)[18]**, colorless oil; ^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 7.17 - 7.12 (m, 2H), 7.00 - 6.94 (m, 2H), 4.18 (q, *J* = 7.2 Hz, 1H), 1.62 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 162.68, 160.25, 150.24, 140.96, 129.02, 128.95, 125.39, 115.31, 43.92, 21.75; **HRMS** (ESI) m/z calculated $C_{15}H_{12}F_4H^+$ $[M+H]^+$ 269.0948, found 269.0949.



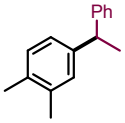
1-chloro-4-(1-(4-(trifluoromethyl)phenyl)ethyl)benzene (27), colorless oil; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.54 - 7.52 (m, 2H), 7.30 (s, 1H), 7.27 (d, *J* = 3.2 Hz, 1H), 7.25 - 7.22 (m, 2H), 7.14 - 7.10 (m, 2H), 4.17 (q, *J* = 7.2 Hz, 1H), 1.63 (d, *J* = 7.2 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 149.85, 143.72, 132.20, 128.92, 128.66, 128.04, 127.81, 125.43, 125.42, 44.05, 21.56; **HRMS** (ESI) m/z calculated $C_{15}H_{12}ClF_3H^+$ $[M+H]^+$ 285.0652, found 285.0658.



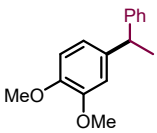
1-bromo-4-(1-(4-(trifluoromethyl)phenyl)ethyl)benzene (28), colorless oil; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.2 Hz, 2H), 7.44 - 7.37 (m, 2H), 7.29 (d, *J* = 8.2 Hz, 2H), 7.09 - 7.03 (m, 2H), 4.15 (q, *J* = 7.2 Hz, 1H), 1.62 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 149.73, 144.25, 131.61, 129.32, 128.08, 127.86, 125.43, 125.37, 120.25, 44.10, 21.48; **HRMS** (ESI) m/z calculated $C_{15}H_{12}BrF_3H^+$ $[M+H]^+$ 329.0147, found 329.0156.



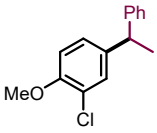
phenyl(4-(1-phenylethyl)phenyl)selane (29), white solid; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.45 - 7.43(m, 2H), 7.38 (d, *J* = 7.8 Hz, 2H), 7.30 - 7.23 (m, 5H), 7.21 - 7.18(m, 3H), 7.13 (d, *J* = 8.0 Hz, 2H), 4.11 (q, *J* = 7.2 Hz, 1H), 1.62 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 145.89, 145.84, 133.21, 132.66, 131.33, 129.24, 128.65, 128.40, 128.00, 127.56, 127.13, 126.14, 44.40, 21.75; **HRMS** (ESI) m/z calculated $C_{20}H_{18}SeH^+$ $[M+H]^+$ 333.0706, found 333.0713.



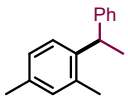
1,2-dimethyl-4-(1-phenylethyl)benzene (30)[19]**, colorless oil; ^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.29 - 7.20 (m, 4H), 7.18 - 7.13 (m, 1H), 7.04 (d, *J* = 7.2 Hz, 1H), 7.00 - 6.93 (m, 2H), 4.08 (q, *J* = 7.2 Hz, 1H), 2.21 (t, *J* = 1.4 Hz, 6H), 1.61 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 146.62, 143.85, 136.40, 134.15, 129.57, 128.94, 128.29, 127.51, 125.86, 124.83, 44.33, 21.93, 19.87, 19.31; **HRMS** (ESI) m/z calculated $C_{16}H_{18}H^+$ $[M+H]^+$ 211.1481, found 211.1489.



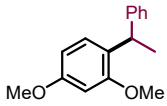
1,2-dimethoxy-4-(1-phenylethyl)benzene (31), colorless oil; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.28 (t, *J* = 7.6 Hz, 2H), 7.24 - 7.14 (m, 3H), 6.78 (t, *J* = 8.4 Hz, 2H), 6.72 (d, *J* = 1.6 Hz, 1H), 4.10 (q, *J* = 7.2 Hz, 1H), 3.83 (d, *J* = 11.2 Hz, 6H), 1.62 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 148.67, 147.19, 146.54, 138.90, 128.29, 127.42, 125.93, 119.22, 111.07, 110.88, 55.76, 44.26, 22.02; **HRMS** (ESI) m/z calculated $C_{16}H_{18}O_2Na^+$ $[M+Na]^+$ 265.1199, found 265.1198.



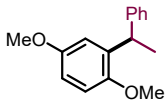
2-chloro-1-methoxy-4-(1-phenylethyl)benzene (32), colorless oil; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.27 (t, *J* = 7.4 Hz, 2H), 7.22 (d, *J* = 2.2 Hz, 1H), 7.18 (d, *J* = 7.2 Hz, 3H), 7.05 - 7.03 (m, 1H), 6.81 (d, *J* = 8.4 Hz, 1H), 4.05 (q, *J* = 7.2 Hz, 1H), 3.82 (d, *J* = 1.2 Hz, 3H), 1.58 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 153.16, 145.92, 139.61, 129.28, 128.40, 127.41, 126.68, 126.13, 122.12, 111.93, 56.06, 43.69, 21.82; **HRMS** (ESI) m/z calculated $C_{15}H_{15}ClONa^+$ $[M+Na]^+$ 269.0703, found 269.0702.



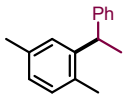
2,4-dimethyl-1-(1-phenylethyl)benzene (33)[20]**, colorless oil;** **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.27 - 7.22 (m, 2H), 7.16 - 7.14 (m, 4H), 7.01 - 6.99 (m, 1H), 6.95(s, 1H), 4.36 (q, *J* = 7.2 Hz, 1H), 2.38 (s, 3H), 2.28 (s, 3H), 1.68 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 146.42, 140.93, 135.87, 135.45, 131.21, 128.26, 127.59, 126.59, 125.71, 40.63, 22.16, 20.87, 19.65; **HRMS** (ESI) m/z calculated $C_{16}H_{18}H^+$ $[M+H]^+$ 211.1481, found 211.1489.



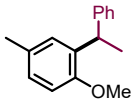
1-cyclohexyl-4-(1-phenylethyl)benzene (34), colorless oil; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.28 - 7.21 (m, 4H), 7.14 (t, *J* = 6.8, 1H), 7.03 (d, *J* = 9.2, 1H), 6.45 - 6.43 (m, 2H), 4.47 (q, *J* = 7.2, 1H), 3.78 (s, 3H), 3.74 (s, 3H), 1.55 (d, *J* = 7.2, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 159.00, 157.69, 146.70, 127.97, 127.50, 125.55, 103.81, 98.56, 55.33, 36.91, 21.04; **HRMS** (ESI) m/z calculated $C_{16}H_{18}O_2Na^+$ $[M+Na]^+$ 265.1199, found 265.1198.



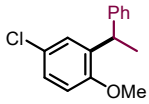
1,4-dimethoxy-2-(1-phenylethyl)benzene (35), colorless oil; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.24 (d, *J* = 2.6 Hz, 4H), 7.17 - 7.13 (m, 1H), 6.79 - 6.73 (m, 2H), 6.70 - 6.67 (m, 1H), 4.54 (q, *J* = 7.2 Hz, 1H), 3.72 (d, *J* = 7.2 Hz, 6H), 1.57 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 153.60, 151.23, 146.08, 136.35, 128.11, 127.65, 125.73, 114.73, 111.64, 110.47, 56.17, 55.59, 37.54, 20.85; **HRMS** (ESI) m/z calculated $C_{16}H_{18}O_2Na^+$ $[M+Na]^+$ 265.1199, found 265.1198.



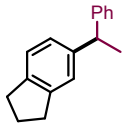
1,4-dimethyl-2-(1-phenylethyl)benzene (36)[21]**, colorless oil;** **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.26 - 7.22 (m, 2H), 7.16 - 7.12 (m, 3H), 7.07 (d, *J* = 1.8 Hz, 1H), 7.01 (d, *J* = 7.6 Hz, 1H), 6.94 - 6.92 (m, 1H), 4.28 (q, *J* = 7.2 Hz, 1H), 2.31 (s, 3H), 2.15 (s, 3H), 1.59 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 146.28, 143.65, 135.26, 132.88, 130.26, 128.25, 127.60, 127.40, 126.70, 125.72, 40.88, 22.08, 21.24, 19.28; **HRMS** (ESI) m/z calculated $C_{16}H_{18}H^+$ $[M+H]^+$ 211.1481, found 211.1489.



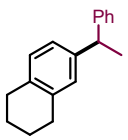
1-methoxy-4-methyl-2-(1-phenylethyl)benzene (37)[22]**, colorless oil;** **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.26 - 7.23 (m, 4H), 7.17 - 7.14 (m, 1H), 6.96 (d, *J* = 8.8 Hz, 2H), 6.74 (d, *J* = 8.0 Hz, 1H), 4.54 (q, *J* = 7.2 Hz, 1H), 3.73 (s, 3H), 2.25 (s, 3H), 1.56 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 154.68, 146.41, 134.58, 129.55, 128.33, 128.04, 127.66, 127.24, 125.59, 110.58, 55.60, 37.20, 20.80; **HRMS** (ESI) m/z calculated $C_{17}H_{20}H^+$ $[M+H]^+$ 225.1638, found 225.1645.



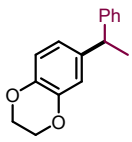
4-chloro-4'-(1-phenylethyl)-1,1'-biphenyl (38), colorless oil; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.29 - 7.24 (m, 3H), 7.23 - 7.19 (m, 2H), 7.19 - 7.14 (m, 1H), 7.13 - 7.05 (m, 2H), 6.74 (d, *J* = 8.2 Hz, 1H), 4.51 (q, *J* = 7.2 Hz, 1H), 3.74 (s, 3H), 1.54 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** δ (101 MHz, $CDCl_3$) δ 155.44, 145.49, 136.79, 128.21, 127.69, 127.61, 126.69, 125.95, 125.50, 111.78, 55.72, 37.43, 20.74; **HRMS** (ESI) m/z calculated $C_{15}H_{15}ClONa^+$ $[M+Na]^+$ 269.0703, found 269.0702.



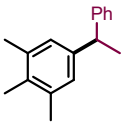
5-(1-phenylethyl)-2,3-dihydro-1H-indene (39), yellow oil; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.46 - 7.38 (m, 4H), 7.35 - 7.28 (m, 2H), 7.25 (d, *J* = 1.8 Hz, 1H), 7.07 (s, 1H), 4.29 (q, *J* = 7.2 Hz, 1H), 3.02 (t, *J* = 7.4 Hz, 4H), 2.06 - 1.98 (m, 2H), 1.80 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 146.70, 144.37, 144.34, 141.83, 128.28, 127.54, 125.80, 125.43, 124.12, 123.53, 44.64, 32.83, 32.42, 25.46, 22.07; **HRMS** (ESI) m/z calculated $C_{17}H_{18}H^+$ $[M+H]^+$ 223.1481, found 223.1473.



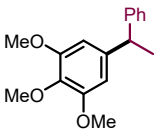
6-(1-phenylethyl)-1,2,3,4-tetrahydronaphthalene (40), yellow oil; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.30 - 7.20 (m, 4H), 7.18 - 7.14 (m, 1H), 6.99 - 6.90 (m, 3H), 4.07 (q, *J* = 7.2 Hz, 1H), 2.71 (s, 4H), 1.76 (s, 4H), 1.61 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 146.60, 143.43, 136.94, 134.76, 129.08, 128.29, 128.18, 127.54, 125.86, 124.71, 44.42, 29.46, 28.97, 23.24, 21.94; **HRMS** (ESI) m/z calculated $C_{18}H_{20}H^+$ $[M+H]^+$ 237.1638, found 237.1642.



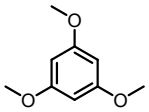
6-(1-phenylethyl)-2,3-dihydrobenzo[b][1,4]dioxine (41), colorless oil; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.28 (d, *J* = 7.8 Hz, 1H), 7.25 (s, 1H), 7.23 - 7.14 (m, 3H), 6.77 (d, *J* = 8.4 Hz, 1H), 6.74 - 6.66 (m, 2H), 4.22 (s, 4H), 4.04 (q, *J* = 7.2 Hz, 1H), 1.59 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 146.46, 143.20, 141.69, 139.86, 128.33, 127.48, 125.96, 120.56, 116.97, 116.23, 64.35, 44.07, 21.91; **HRMS** (ESI) m/z calculated $C_{16}H_{16}O_2H^+$ $[M+H]^+$ 241.1223, found 241.1218.



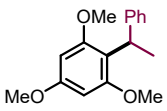
1,2,3-trimethyl-5-(1-phenylethyl)benzene (42), colorless oil; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.27 (d, *J* = 8.0 Hz, 1H), 7.25 - 7.20 (m, 3H), 7.17 - 7.13 (m, 1H), 6.86 (s, 2H), 4.04 (q, *J* = 7.2 Hz, 1H), 2.23 (s, 6H), 2.11 (s, 3H), 1.60 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 146.66, 143.16, 136.29, 132.67, 128.28, 127.50, 126.78, 125.82, 44.33, 21.94, 20.67, 15.03; **HRMS** (ESI) m/z calculated $C_{17}H_{20}Na^+$ $[M+Na]^+$ 273.1485, found 247.1476.



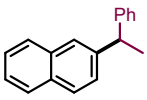
1,2,3-trimethoxy-4-(1-phenylethyl)benzene (43)[23]**, colorless oil;** **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.25 (d, *J* = 7.2 Hz, 2H), 7.24 - 7.19 (m, 2H), 7.18 - 7.12 (m, 1H), 6.89 (d, *J* = 8.6 Hz, 1H), 6.64 (d, *J* = 8.6 Hz, 1H), 4.44 (q, *J* = 7.2 Hz, 1H), 3.84 (d, *J* = 3.8 Hz, 6H), 3.61 (s, 3H), 1.57 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 152.01, 151.49, 146.93, 142.21, 132.47, 128.16, 127.52, 125.70, 121.78, 106.87, 60.63, 55.89, 37.83, 21.64; **HRMS** (ESI) m/z calculated $C_{17}H_{20}O_3H^+$ $[M+H]^+$ 273.1485, found 273.1479.



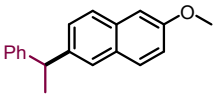
1,3,5-trimethoxybenzene (44a), white solid; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 6.10 (s, 9H), 3.77 (s, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 161.52, 92.89, 55.25; **HRMS** (ESI) m/z calculated $C_9H_{12}O_3H^+$ $[M+H]^+$ 169.0859, found 169.0861.



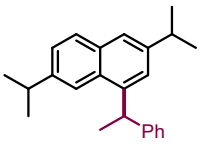
1,3,5-trimethoxy-2-(1-phenylethyl)benzene (44), white solid; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.29 - 7.25 (s, 4H), 7.10 (q, *J* = 7.2 Hz, 1H), 6.12 (s, 2H), 4.79 - 4.70 (m, 1H), 3.79 (s, 3H), 3.68 (s, 6H), 1.63 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 159.37, 158.91, 146.54, 127.39, 127.16, 124.74, 91.32, 55.59, 55.56, 32.87, 17.67;**HRMS** (ESI) m/z calculated $C_{17}H_{20}O_3H^+$ $[M+H]^+$ 273.1485, found 273.1486.



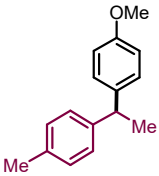
1-(1-phenylethyl)naphthalene (45)[24]**, colorless oil;** **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.77 - 7.14 (m, 2H), 7.72 - 7.66 (m, 2H), 7.45 - 7.37 (m, 2H), 7.30 - 7.25 (m, 2H), 7.25 - 7.21 (m, 3H), 7.19 - 7.13 (m, 1H), 4.28 (q, *J* = 7.2 Hz, 1H), 1.71 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 146.18, 143.73, 133.46, 132.07, 128.37, 127.92, 127.72, 127.69, 127.54, 126.81, 126.07, 125.90, 125.33, 44.81, 21.74; **HRMS** (ESI) m/z calculated $C_{18}H_{16}H^+$ $[M+H]^+$ 233.1325, found 233.1321.



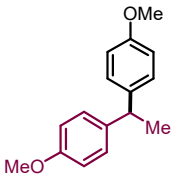
2-methoxy-6-(1-phenylethyl)naphthalene (46), yellow solid; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.8 Hz, 1H), 7.65 - 7.60 (m, 2H), 7.28 - 7.24 (m, 5H), 7.21 - 7.15 (m, 1H), 7.14 - 7.07 (m, 2H), 4.27 (q, *J* = 7.2 Hz, 1H), 3.89 (s, 3H), 1.71 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 157.33, 146.45, 141.48, 133.08, 129.18, 128.94, 128.35, 127.71, 127.29, 126.81, 126.01, 125.20, 118.64, 105.63, 55.29, 44.64, 21.82; **HRMS** (ESI) m/z calculated $C_{19}H_{18}OH^+$ $[M+H]^+$ 263.1430, found 263.1431.



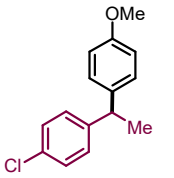
3,7-diisopropyl-1-(1-phenylethyl)naphthalene (47), colorless oil; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.77 (s, 1H), 7.71 - 7.69 (m, 1H), 7.50 (d, *J* = 1.8 Hz, 1H), 7.31 - 7.27 (m, 2H), 7.24 (d, *J* = 1.8 Hz, 4H), 7.15 - 7.12 (m, 1H), 4.88 (q, *J* = 7.2 Hz, 1H), 3.07 - 3.00 (m, 1H), 2.99 - 2.92 (m, 1H), 1.77 (d, *J* = 7.2 Hz, 3H), 1.32 (d, *J* = 7.2 Hz, 8H), 1.24 (s, 1H), 1.22 (d, *J* = 4.0 Hz, 2H), 1.19 (s, 1H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 146.89, 145.24, 144.83, 140.95, 132.78, 130.35, 128.31, 127.57, 125.79, 125.10, 124.39, 122.56, 120.34, 40.80, 34.36, 34.20, 24.23, 23.71, 22.49; **HRMS** (ESI) m/z calculated $C_{24}H_{28}Na^+$ $[M+Na]^+$ 339.2083, found 339.2083.



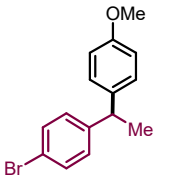
1-methoxy-4-(1-(p-tolyl)ethyl)benzene (48)[25]**, colorless oil;** **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.15 - 7.10 (m, 2H), 7.09 (s, 4H), 6.84 - 6.79 (m, 2H), 4.06 (q, *J* = 7.2 Hz, 1H), 3.76 (s, 3H), 2.30 (s, 3H), 1.59 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 157.70, 143.77, 138.74, 135.35, 128.99, 128.41, 127.35, 113.64, 55.18, 43.47, 22.10, 20.95; **HRMS** (ESI) m/z calculated $C_{16}H_{18}ONa^+$ $[M+Na]^+$ 249.1249, found 249.1249.



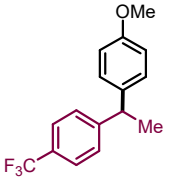
1-methoxy-4-(1-(p-tolyl)ethyl)benzene (49), white solid; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.15 - 7.09 (m, 4H), 6.85 - 6.79 (m, 4H), 4.06 (q, *J* = 7.2 Hz, 1H), 3.77 (s, 6H), 1.58 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 157.70, 138.92, 128.38, 113.65, 55.21, 43.04, 22.23; **HRMS** (ESI) m/z calculated $C_{16}H_{18}O_2Na^+$ $[M+Na]^+$ 265.1199, found 265.1198.



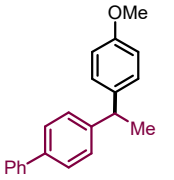
1-chloro-4-(1-(4-methoxyphenyl)ethyl)benzene (50)[26]**, colorless oil;** **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.23 (d, *J* = 2.0 Hz, 1H), 7.22 (d, *J* = 2.2 Hz, 1H), 7.14 - 7.06 (m, 4H), 6.85 - 6.80 (m, 2H), 4.06 (q, *J* = 7.2 Hz, 1H), 3.76 (s, 3H), 1.58 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 157.90, 145.24, 137.90, 131.56, 128.85, 128.39, 128.37, 113.76, 55.19, 43.28, 21.95; **HRMS** (ESI) m/z calculated $C_{15}H_{15}ClOH^+$ $[M+H]^+$ 247.0884, found 247.0892.



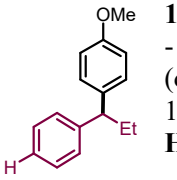
1-bromo-4-(1-(4-methoxyphenyl)ethyl)benzene (51), colorless oil; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.40 - 7.35 (m, 2H), 7.12 - 7.04 (m, 4H), 6.85 - 6.80 (m, 2H), 4.05 (q, *J* = 7.2 Hz, 1H), 3.76 (s, 3H), 1.57 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 157.91, 145.77, 137.79, 131.33, 129.27, 128.39, 119.65, 113.76, 55.19, 43.34, 21.89; **HRMS** (ESI) m/z calculated $C_{15}H_{15}BrOH^+$ $[M+H]^+$ 291.0379, found 291.0371.



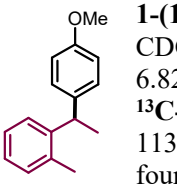
1-methoxy-4-(1-(4-(trifluoromethyl)phenyl)ethyl)benzene (52)[27]**, colorless oil;** **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 8.2 Hz, 2H), 7.31 (d, *J* = 8.2 Hz, 2H), 7.15 - 7.09 (m, 2H), 6.87 - 6.82 (m, 2H), 4.16 (q, *J* = 7.2 Hz, 1H), 3.78 (d, *J* = 0.8 Hz, 3H), 1.63 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 158.06, 150.85, 137.36, 128.47, 127.81, 125.25, 113.86, 55.18, 43.80, 21.77; **HRMS** (ESI) m/z calculated $C_{16}H_{15}F_3OH^+$ $[M+H]^+$ 281.1148, found 281.1140.



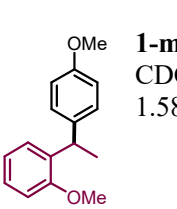
4-(1-(2-methoxyphenyl)ethyl)-1,1'-biphenyl (53)[28]**, white solid;** **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.60 - 7.53 (m, 2H), 7.51 - 7.47 (m, 2H), 7.43 - 7.39 (m, 2H), 7.34 - 7.27 (m, 3H), 7.21 - 7.17 (m, 2H), 6.95 - 6.91 (m, 1H), 6.89 - 6.84 (m, 1H), 4.62 (q, *J* = 7.2 Hz, 1H), 3.80 (s, 3H), 1.61 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 156.77, 145.51, 141.11, 138.52, 134.71, 128.64, 128.08, 127.60, 127.10, 126.97, 126.90, 126.82, 120.51, 110.55, 55.43, 37.00, 20.88; **HRMS** (ESI) m/z calculated $C_{21}H_{20}ONa^+$ $[M+Na]^+$ 311.1406, found 311.1407.



1-methoxy-4-(1-phenylpropyl)benzene (54), colorless oil; **^{1}H-NMR** (400 MHz, CDCl3) δ 7.28 - 7.24 (m, 2H), 7.23 - 7.18 (m, 2H), 7.16 - 7.13 (m, 3H), 6.84 - 6.79 (m, 2H), 3.75 (s, 3H), 3.72 (d, *J* = 7.8 Hz, 1H), 2.07 - 1.99 (m, 2H), 0.88 (t, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 157.73, 145.53, 137.28, 128.74, 128.30, 127.77, 125.88, 113.66, 55.15, 52.31, 28.70, 12.78; **HRMS** (ESI) m/z calculated $C_{16}H_{18}ONa^+$ $[M+Na]^+$ 249.1249, found 249.1247.

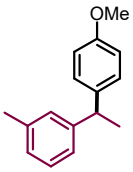


1-(1-(4-methoxyphenyl)ethyl)-2-methylbenzene (55)[17]**, colorless oil;** **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.25 (d, *J* = 7.6 Hz, 1H), 7.21 - 7.14 (m, 1H), 7.11 (t, *J* = 2.4 Hz, 2H), 7.09 - 7.03 (m, 2H), 6.82 - 6.75 (m, 2H), 4.26 (q, *J* = 7.2 Hz, 1H), 3.74 (s, 3H), 2.22 (s, 3H), 1.57 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 157.59, 144.20, 138.30, 135.96, 130.34, 128.51, 126.48, 125.95, 113.61, 55.13, 40.07, 22.20, 19.68; **HRMS** (ESI) m/z calculated $C_{16}H_{18}OH^+$ $[M+H]^+$ 227.1430, found 227.1438.

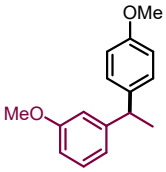


1-methoxy-2-(1-(4-methoxyphenyl)ethyl)benzene (56), colorless oil; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.12 (d, *J* = 8.6 Hz, 4H), 6.82 (d, *J* = 8.8 Hz, 4H), 4.05 (q, *J* = 7.2 Hz, 1H), 3.76 (s, 6H), 1.58 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 157.70, 138.90, 128.56, 128.36, 120.44,

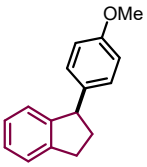
113.63, 113.41, 55.18, 43.03, 22.22; **HRMS** (ESI) m/z calculated $C_{16}H_{18}O_2H^+$ $[M+H]^+$ 243.1379, found 243.1374.



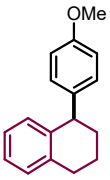
1-(1-(4-methoxyphenyl)ethyl)-3-methylbenzene (57), colorless oil; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.17 - 7.09 (m, 3H), 7.02 - 6.94 (m, 3H), 6.83 - 6.77 (m, 2H), 4.04 (q, *J* = 7.2 Hz, 1H), 3.72 (s, 3H), 2.28 (s, 3H), 1.58 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 157.71, 146.64, 138.56, 137.75, 128.41, 128.27, 128.17, 126.65, 124.46, 113.61, 55.09, 43.82, 22.03, 21.45; **HRMS** (ESI) m/z calculated $C_{16}H_{18}ONa^+$ $[M+Na]^+$ 249.1249, found 249.1249.



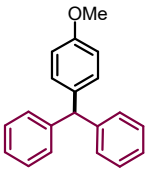
1-methoxy-3-(1-(4-methoxyphenyl)ethyl)benzene of (58), colorless oil; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.21 - 7.10 (m, 3H), 6.84 - 6.78 (m, 3H), 6.75 (t, *J* = 2.2 Hz, 1H), 6.72 - 6.70 (m, 1H), 4.06 (q, *J* = 7.2 Hz, 1H), 3.75 (d, *J* = 2.0 Hz, 6H), 1.59 (d, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 159.51, 157.77, 148.41, 138.28, 129.22, 128.40, 119.96, 113.64, 113.60, 110.75, 55.12, 55.03, 43.88, 21.94; **HRMS** (ESI) m/z calculated $C_{16}H_{18}O_2Na^+$ $[M+Na]^+$ 265.1199, found 265.1199.



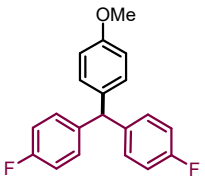
1-(4-methoxyphenyl)-2,3-dihydro-1H-indene (59), yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (d, *J* = 7.4 Hz, 1H), 7.20 - 7.07 (m, 4H), 6.94 (d, *J* = 7.4 Hz, 1H), 6.88 - 6.81 (m, 2H), 4.28 (t, *J* = 8.4 Hz, 1H), 3.78 (s, 3H), 3.07 - 2.87 (m, 2H), 2.57 - 2.50 (m, 1H), 2.06 - 1.96 (m, 1H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 158.04, 147.13, 144.20, 137.42, 129.00, 126.41, 126.27, 124.80, 124.28, 113.78, 55.21, 50.79, 36.71, 31.72; **HRMS** (ESI) m/z calculated $C_{16}H_{16}O_2H^+$ $[M+H]^+$ 241.1223, found 241.1221.



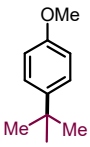
1-(4-methoxyphenyl)-1,2,3,4-tetrahydronaphthalene (60), colorless oil; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.14 - 7.07 (m, 2H), 7.05 - 6.98 (m, 3H), 6.86 - 6.79 (m, 3H), 4.06 (t, *J* = 6.8 Hz, 1H), 3.77 (s, 3H), 2.95 - 2.76 (m, 2H), 2.18 - 2.07 (m, 1H), 1.93 - 1.67 (m, 3H); **^{13}C-NMR** (101 MHz, CDCl3) δ 157.73, 139.68, 139.61, 137.47, 130.08, 129.65, 128.89, 125.78, 125.56, 113.53, 55.16, 44.69, 33.29, 29.73, 20.91; **HRMS** (ESI) m/z calculated $C_{17}H_{18}OH^+$ $[M+H]^+$ 239.1430, found 239.1431.



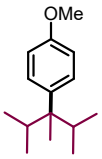
((4-methoxyphenyl)methylene)dibenzene (61), white solid; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.30 - 7.23 (m, 5H), 7.21 - 7.19 (m, 2H), 7.01 - 7.08 (m, 4H), 6.90 - 6.83 (m, 3H), 5.93 (s, 1H), 3.71 (s, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 157.02, 143.86, 132.54, 130.32, 129.42, 128.07, 127.49, 125.98, 120.21, 110.59, 55.55, 49.49; **HRMS** (ESI) m/z calculated $C_{20}H_{18}ONa^+$ $[M+Na]^+$ 297.1250, found 297.1250.



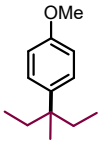
4,4'-((4-methoxyphenyl)methylene)bis(fluorobenzene) (62)[29], colorless oil; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.26 - 7.20 (m, 1H), 7.04 - 7.00 (m, 4H), 6.97 (d, *J* = 2.4 Hz, 1H), 6.95 (d, *J* = 2.4 Hz, 2H), 6.93 (d, *J* = 2.2 Hz, 1H), 6.91 - 6.84 (m, 2H), 6.79 (dd, *J* = 7.8, 1.8 Hz, 1H), 5.86 (s, 1H), 3.72 (s, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 162.51, 160.08, 156.88, 139.34, 132.19, 130.70, 130.62, 129.97, 127.80, 120.30, 115.04, 114.83, 110.63, 55.50, 48.09; **HRMS** (ESI) m/z calculated $C_{20}H_{16}F_2OH^+$ $[M+H]^+$ 311.1242, found 311.1266.



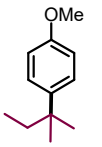
1-(tert-butyl)-4-methoxybenzene (63)[30], colorless oil; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.33 - 7.28 (m, 2H), 6.87 - 6.82 (m, 2H), 3.79 (s, 3H), 1.30 (s, 9H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 157.23, 143.28, 126.19, 113.28, 55.19, 34.02, 31.50; **HRMS** (ESI) m/z calculated $C_{11}H_{16}OH^+$ $[M+H]^+$ 165.1273, found 165.1270.



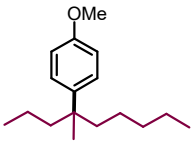
1-methoxy-4-(1-methylcyclopentyl)benzene (64), colorless oil; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.23 - 7.16 (m, 2H), 6.87 - 6.81 (m, 2H), 3.79 (s, 3H), 1.63 (q, *J* = 7.4 Hz, 6H), 0.64 (t, *J* = 7.4 Hz, 9H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 156.96, 139.27, 127.75, 113.03, 55.07, 42.98, 28.70, 7.94; **HRMS** (ESI) m/z calculated $C_{15}H_{24}ONa^+$ $[M+Na]^+$ 243.1719, found 243.1723.



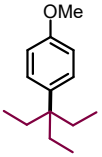
1-methoxy-4-(3-methylpentan-3-yl)benzene (65), colorless oil; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.21 - 7.16 (m, 2H), 6.87 - 6.80 (m, 2H), 3.79 (s, 3H), 1.74 - 1.65 (m, 2H), 1.58 - 1.47 (m, 2H), 1.21 (s, 3H), 0.66 (t, *J* = 7.4 Hz, 6H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 157.04, 139.64, 127.51, 113.12, 55.12, 40.57, 35.23, 22.97, 8.66; **HRMS** (ESI) m/z calculated $C_{13}H_{20}OK^+$ $[M+K]^+$ 231.1146, found 231.1164.



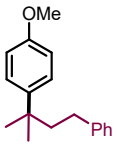
1-methoxy-4-(1-methylcyclopentyl)benzene (66), colorless oil; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.23 - 7.16 (m, 2H), 6.87 - 6.81 (m, 2H), 3.79 (s, 3H),1.62 (q, *J* = 7.2 Hz, 2H), 1.26 (q, *J* = 7.4 Hz, 6H), 0.67 (t, *J* = 7.4 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 157.14, 141.51, 126.86, 113.19, 55.13, 37.22, 36.92, 28.59, 9.12; **HRMS** (ESI) m/z calculated $C_{12}H_{18}OK^+$ $[M+K]^+$ 217.0989, found 217.1002.



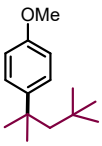
1-methoxy-4-(4-methylnonan-4-yl)benzene (67), colorless oil; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.28 - 7.22 (m, 2H), 6.86 - 6.80 (d, *J* = 8.8 Hz, 2H), 3.79 (s, 3H), 1.67 - 1.57 (m, 2H), 1.50 - 1.44 (m, 2H), 1.08 - 1.28 (m, 9H), 0.99 - 0.91 (m, 2H), 0.77 - 0.85 (m, 6H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 157.06, 142.65, 127.06, 113.01, 55.14, 48.31, 40.99, 27.70, 27.10, 24.82, 24.66, 17.81, 8.83; **HRMS** (ESI) m/z calculated $C_{17}H_{28}OK^+$ $[M+K]^+$ 287.1771, found 287.1773.



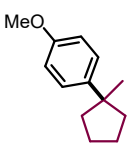
1-methoxy-4-(4-methylnonan-4-yl)benzene (68), colorless oil; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.21 - 7.16 (m, 2H), 6.86 - 6.80 (m, 2H), 3.78 (s, 3H), 1.67 - 1.56 (m, 2H), 1.50 - 1.44 (m, 2H), 1.24 (s, 3H), 1.22 - 1.09 (m, 5H), 1.02 - 0.90 (m, 2H), 0.84 - 0.79 (m, 6H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 156.96, 140.41, 127.23, 113.08, 55.05, 45.99, 43.37, 40.14, 32.66, 24.18, 23.82, 22.59, 17.41, 14.84, 14.10; **HRMS** (ESI) m/z calculated $C_{12}H_{18}OK^+$ $[M+K]^+$ 217.0989, found 217.1001.



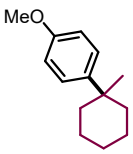
1-methoxy-4-(2-methyl-4-phenylbutan-2-yl)benzene (69), colorless oil; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.31 - 7.26 (m, 2H), 7.22 (t, *J* = 7.4 Hz, 2H), 7.15 - 7.09 (m, 1H), 7.09 - 7.05 (m, 2H), 6.89 - 6.83 (m, 2H), 3.77 (s, 3H), 2.38 - 2.30 (m, 2H), 1.93 - 1.85 (m, 2H), 1.34 (s, 6H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 157.28, 143.09, 141.02, 128.21, 128.18, 126.75, 125.46, 113.36, 55.09, 46.81, 37.20, 31.31, 29.09; **HRMS** (ESI) m/z calculated $C_{18}H_{22}OH^+$ $[M+H]^+$ 315.1954, found 315.1954.



1-methoxy-4-(2,4,4-trimethylpentan-2-yl)benzene (70), colorless oil; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.27 (d, *J* = 8.8 Hz, 2H), 6.82 (d, *J* = 8.8 Hz, 1H), 3.78 (s, 2H), 1.70 (s, 1H), 1.34 (s, 3H), 0.71 (s, 5H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 157.13, 142.13, 127.01, 112.98, 56.95, 55.11, 37.89, 32.30, 31.71; **HRMS** (ESI) m/z calculated $C_{15}H_{24}OH^+$ $[M+H]^+$ 221.1900, found 221.1905.

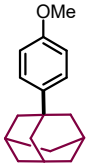


1-methoxy-4-(1-methylcyclopentyl)benzene (71), colorless oil; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.24 (d, *J* = 2.2 Hz, 2H), 6.87 - 6.80 (m, 2H), 3.79 (s, 3H), 1.94 - 1.60 (m, 8H), 1.22 (s, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 157.18, 143.59, 126.92, 113.31, 55.21, 46.44, 39.80, 29.53, 23.68; **HRMS** (ESI) m/z calculated $C_{13}H_{18}OH^+$ $[M+H]^+$ 191.1430, found 191.1428.

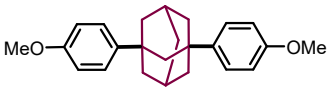


1-methoxy-4-(1-methylcyclohexyl)benzene (72), colorless oil; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.26 - 7.24 (m, 2H), 6.85 - 6.83 (m, 2H), 3.79 (s, 3H), 1.89 - 1.86 (m, 2H), 1.78 - 1,70 (d, *J* = 5.2

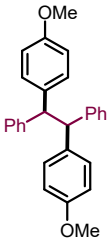
Hz, 4H), 1.57 (s, 3H), 1.27 - 1.23 (m, 1H), 1.22 (s, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 157.05,142.08, 126.83, 113.45, 55.16, 38.02, 37.24, 30.65, 26.40, 22.64; **HRMS** (ESI) m/z calculated $C_{16}H_{20}OH^+$ $[M+H]^+$ 205.1587, found 205.1592.



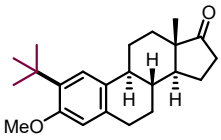
(*3r*,*5r*,*7r*)-1-(4-methoxyphenyl)adamantane (73)[31]**, white solid; ^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.31 - 7.24 (m, 2H), 6.89 - 6.82 (m, 2H), 3.79 (s, 3H), 2.08 (q, *J* = 3.2 Hz, 3H), 1.89 (d, *J* = 2.8 Hz, 6H), 1.82 - 1.70 (m, 6H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 157.27, 143.68, 125.76, 113.34, 55.18, 43.34, 36.76, 35.50, 28.95; **HRMS** (ESI) m/z calculated $C_{17}H_{22}OH^+$ $[M+H]^+$ 243.1743, found 243.1738.



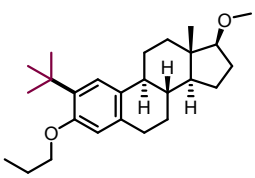
1,3-bis(4-methoxyphenyl)adamantane (74), white solid; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.34 - 7.28 (m, 4H), 6.90 - 6.82 (m, 4H), 3.79 (s, 6H), 2.29 (s, 2H), 1.98 (s, 2H), 1.91 (d, *J* = 3.2 Hz, 8H), 1.77 (t, *J* = 3.2 Hz, 2H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 157.42, 142.98, 125.83, 113.42, 55.20, 49.34, 42.45, 36.62, 35.85, 29.58; **HRMS** (ESI) m/z calculated $C_{24}H_{28}O_2H^+$ $[M+H]^+$ 349.2162, found 349.2168.



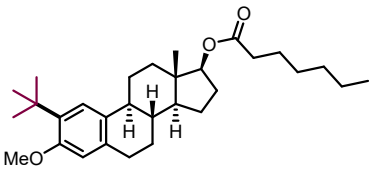
4,4'-((4-methoxyphenyl)methylene)bis(fluorobenzene) (75), white solid; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.16 - 7.14 (m, 4H), 7.09 - 7.02 (m, 8H), 6.99 - 6.96 (m, 2H), 6.62 - 6.60 (m, 4H), 4.71 - 4.64 (m, 2H), 3.59 (s, 6H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 157.34, 143.63, 135.98, 129.18, 128.45, 128.06, 125.69, 113.43, 56.64, 54.90, 54.44; **HRMS** (ESI) m/z calculated $C_{28}H_{26}O_2H^+$ $[M+H]^+$ 395.2006, found 395.2011.



(*8R*,*9S*,*13S*,*14S*)-2-(tert-butyl)-3-methoxy-13-methyl-6,7,8,9,11,12,13,14,15,16-decahydro-17H-cyclopenta[a]phenanthren-17-one (76), yellow solid; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.21 (s, 1H), 6.62 (s, 1H), 3.81 (s, 3H), 2.92 - 2.87 (m, 2H), 2.54 - 2.43 (m, 2H), 2.27 - 1.95 (m, 6H), 1.68 - 1.60 (m, 2H), 1.45 - 1.41 (m, 1H), 1.36 (s, 9H), 1.25 (s, 2H), 0.91 (s, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 220.99, 156.39, 135.54, 134.85, 130.72, 123.61, 111.83, 54.93, 50.28, 47.97, 44.19, 38.43, 35.81, 34.69, 31.57, 29.77, 29.25, 26.53, 25.90, 21.50, 13.80; **HRMS** (ESI) m/z calculated $C_{23}H_{32}O_2Na^+$ $[M+Na]^+$ 363.2294, found 363.2295.

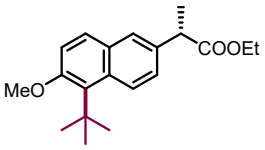


(*8R*,*9S*,*13S*,*14S*,*17S*)-2-(tert-butyl)-17-methoxy-13-methyl-3-propoxy-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthrene (77), white solid; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.21 - 7.17 (m, 1H), 6.71 - 6.63 (m, 1H), 3.93 - 3.87 (m, 2H), 3.38 (s, 3H), 3.31 (t, *J* = 8.4 Hz, 1H), 2.86 - 2.79 (m, 2H), 2.05 (d, *J* = 11.8 Hz, 2H), 1.87 - 1.65 (m, 5H), 1.55 - 1.44 (m, 4H), 1.38 (s, 9H), 1.34 - 1.22 (m, 3H), 1.09 - 1.00 (m, 4H), 0.79 (s, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 155.65, 137.85, 135.01, 131.05, 126.25, 123.70, 114.40, 112.00, 90.78, 69.27, 57.86, 50.23, 44.19, 43.22, 38.02, 34.77, 29.90, 26.47, 23.02, 22.62, 11.54, 11.15, 10.54; **HRMS** (ESI) m/z calculated $C_{26}H_{40}O_2H^+$ $[M+H]^+$ 385.3101, found 385.3119.

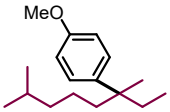


(*8R*,*9S*,*13S*,*14S*,*17S*)–2-(tert-butyl)–3–methoxy–13–methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-ylheptanoate (78), yellow oil; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.20 (s, 1H), 6.59 (s, 1H), 4.74 - 4.65 (t, *J* = 12.0 Hz, 1H), 3.80 (s, 3H), 2.83 (t, *J* = 15.2 Hz, 2H), 2.34 - 2.28 (m, 3H), 2.21 (t, *J* = 11.2 Hz, 2H), 1.87 (d, *J* = 12.4 Hz, 2H), 1.73 (d, *J* = 9.4 Hz, 1H), 1.67 - 1.58 (m, 3H), 1.49 - 1.41 (m, 4H), 1.36 (s, 9H), 1.30 (s, 7H), 0.89 (t, *J* = 6.8 Hz, 4H), 0.82 (s, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 173.94, 156.30, 135.42, 135.05, 131.26, 123.68, 111.87, 82.43, 54.96, 49.71 44.07, 42.93, 38.69, 36.94, 34.66, 31.45, 29.82,

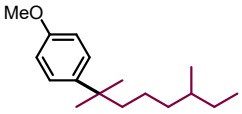
29.41, 28.79, 27.61, 27.26, 26.22, 25.07, 23.26, 22.48, 14.03, 12.10; **HRMS** (ESI) m/z calculated $C_{30}H_{46}O_3Na^+$ $[M+Na]^+$ 477.3339, found 477.3341.



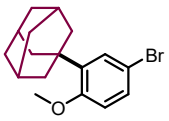
ethyl (S)-2-(5-(tert-butyl)-6-methoxynaphthalen-2-yl)propanoate (79), yellow oil; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 9.0 Hz, 3H), 7.35 (d, *J* = 8.4 Hz, 1H), 7.10 (s, 1H), 4.19 - 4.04 (m, 2H), 3.93 (s, 3H), 3.82 (q, *J* = 7.2 Hz, 1H), 1.56 (d, *J* = 7.2 Hz, 3H), 1.45 (s, 9H), 1.19 (t, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 174.79, 157.63, 140.06, 135.70, 132.13, 128.51, 126.12, 125.79, 125.54, 125.31, 105.74, 60.68, 54.88, 45.50, 35.24, 29.82, 18.64, 14.12; **HRMS** (ESI) m/z calculated $C_{20}H_{26}O_3H^+$ $[M+H]^+$ 315.1954, found 315.1954.



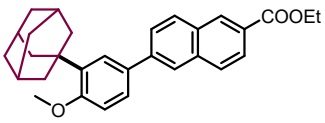
1-(3,7-dimethyloctan-3-yl)-4-methoxybenzene (80), colorless oil; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.24 (d, *J* = 6.8 Hz, 2H), 6.83 (d, *J* = 8.6 Hz, 2H), 3.78 (s, 3H), 1.56 - 1.52 (m, 2H), 1.49 - 1.40 (m, 1H), 1.26 (s, 6H), 1.10 - 1.00 (m, 4H), 0.83 - 0.76 (m, 7H), 0.65 (t, *J* = 6.8 Hz, 1H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 157.05, 140.07, 127.37, 113.16, 55.12, 43.15, 40.35, 39.75, 35.65, 27.73, 22.63, 22.12, 21.89, 8.64; **HRMS** (ESI) m/z calculated $C_{16}H_{26}ONa^+$ $[M+Na]^+$ 271.2032, found 271.2035.



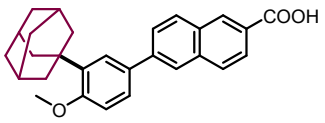
1-(2,6-dimethyloctan-2-yl)-4-methoxybenzene (81), colorless oil; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.24 (d, *J* = 6.8 Hz, 2H), 6.84 (d, *J* = 7.0 Hz, 2H), 3.78 (s, 3H), 1.66 (dd, *J* = 20.8 Hz, 13.2 Hz, 1H), 1.54 (dd, *J* = 10.6 Hz, 5.2 Hz, 2H), 1.49 - 1.40 (m, 1H), 1.26 (s, 6H), 1.11 - 1.00 (m, 4H), 0.83 - 0.76 (m, 7H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 157.05, 141.95, 126.72, 113.16, 55.12, 44.92, 37.31, 34.17, 29.48, 29.14, 22.12, 19.14, 11.37; **HRMS** (ESI) m/z calculated $C_{16}H_{26}ONa^+$ $[M+Na]^+$ 271.2032, found 271.2035.



1-(5-bromo-2-methoxyphenyl)adamantane (82)[32], white solid; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.29 - 7.26 (m, 1H), 7.25 (d, *J* = 2.6 Hz, 1H), 6.73 (d, *J* = 8.6 Hz, 1H), 3.80 (s, 3H), 2.05 (s, 9H), 1.75 (s, 6H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 157.84, 140.72, 129.70, 129.23, 113.19, 55.15, 40.25, 37.03, 28.92; **HRMS** (ESI) m/z calculated $C_{17}H_{21}BrOH^+$ $[M+H]^+$ 321.0849, found 321.0848.



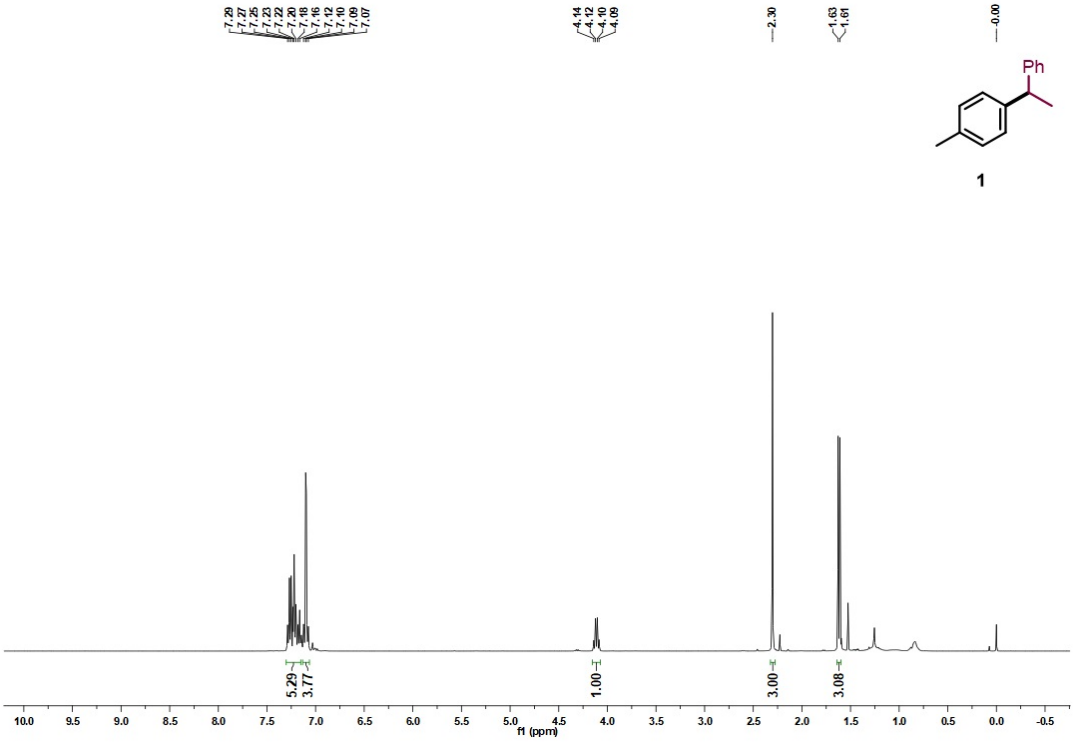
ethyl6-(3-(adamantan-1-yl)-4-methoxyphenyl)-2-naphthoate(83), white solid; ^{1}H-NMR (400 MHz, $CDCl_3$) δ = 8.61 (s, 1H), 8.08 (d, *J* = 8.6 Hz, 1H), 8.00 (d, *J* = 12.2 Hz, 2H), 7.92 (d, *J* = 8.6 Hz, 1H), 7.80 (d, *J* = 8.6 Hz, 1H), 7.60 (s, 1H), 7.55 (d, *J* = 8.4 Hz, 1H), 7.00 (d, *J* = 8.4 Hz, 1H), 4.45 (q, *J* = 7.2 Hz, 2H), 3.91 (s, 3H), 2.18 (s, 6H), 2.10 (s, 3H), 1.80 (s, 6H), 1.46 (t, *J* = 7.2 Hz, 3H); **^{13}C-NMR** (101 MHz, $CDCl_3$) δ 166.85, 158.85, 141.26, 138.93, 135.87, 132.52, 131.20, 130.70, 129.67, 128.14, 127.20, 126.41, 125.96, 125.70, 125.57, 124.71, 112.02, 61.06, 55.14, 40.54, 37.12, 29.05, 14.41; **HRMS** (ESI) m/z calculated $C_{30}H_{32}O_3H^+$ $[M+H]^+$ 441.2424, found 441.2429.



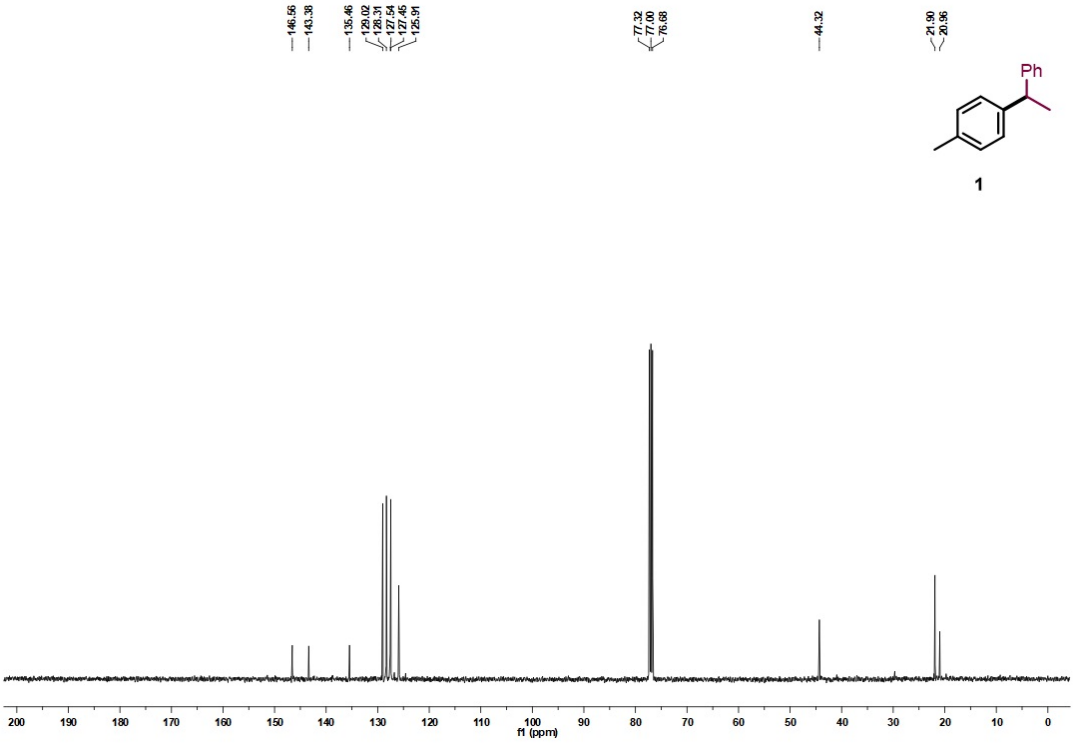
adapalene (84), white solid; ^{1}H-NMR (400 MHz, DMSO) δ 13.08 (s, 1H), 8.61 (s, 1H), 8.23 (s, 1H), 8.16 (d, *J* = 8.8 Hz, 1H), 8.08 (d, *J* = 8.8 Hz, 1H), 7.98 (d, *J* = 8.6 Hz, 1H), 7.90 (d, *J* = 8.8 Hz, 1H), 7.67 (d, *J* = 10.6 Hz, 1H), 7.59 (s, 1H), 7.13 (d, *J* = 8.6 Hz, 1H), 3.87 (s, 3H), 2.11 (m, 9H), 1.76 (s, 6H); **^{13}C-NMR** (101 MHz, DMSO) δ 167.90, 159.07 , 140.68 , 138.52, 135.93, 131.99, 131.37, 130.70, 130.28, 128.79, 128.10, 126.40, 126.20, 125.94, 125.54, 124.54, 113.19, 55.81, 37.08, 37.02, 28.86; **HRMS** (ESI) m/z calculated $C_{28}H_{28}O_3H^+$ $[M+H]^+$ 413.2111, found 413.2118.

7. Copies of NMR spectra

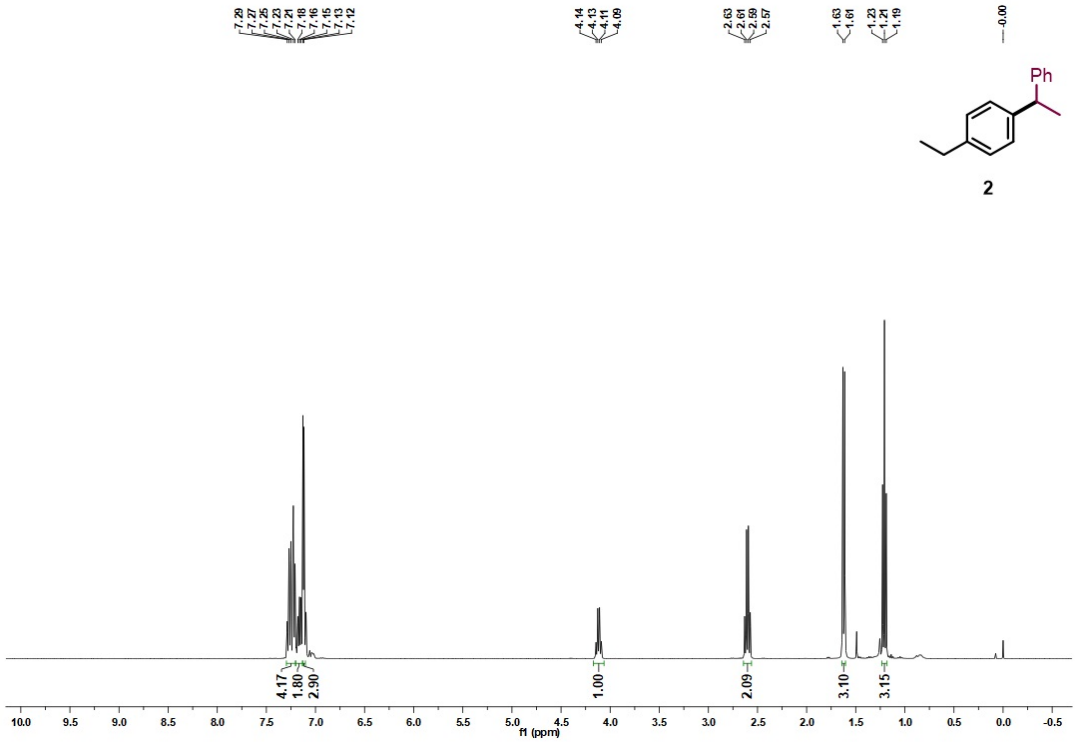
^{1}H-NMR of **1**
$CDCl_3$, 400 MHz, 298 K



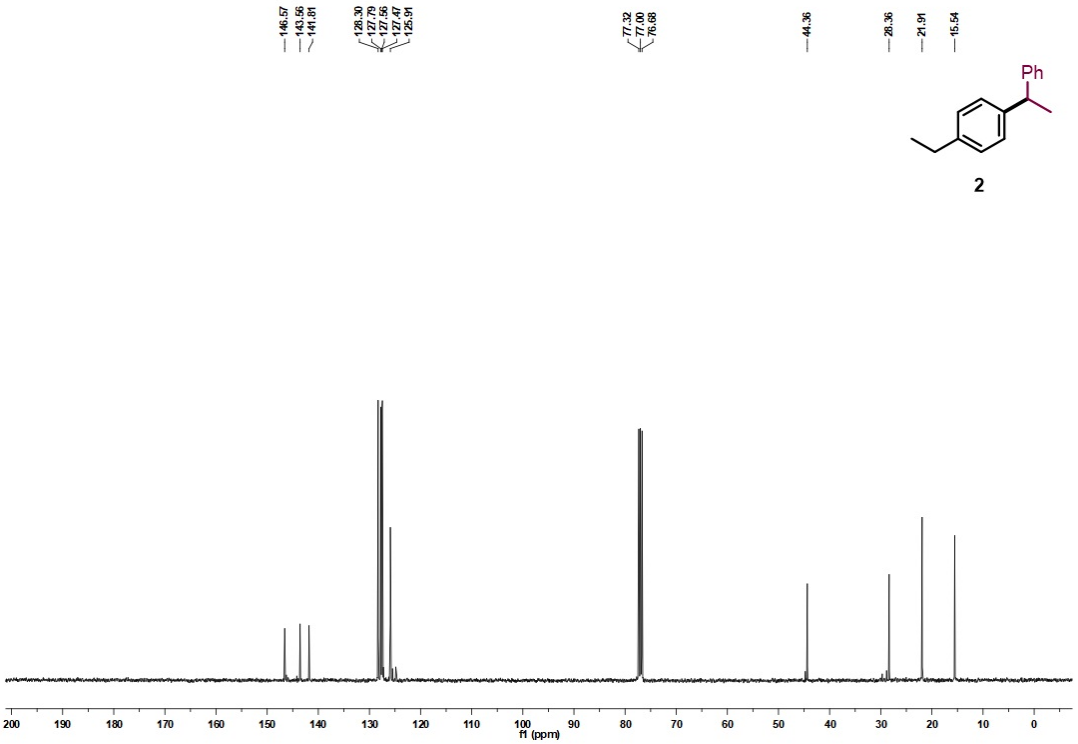
^{13}C-NMR of **1**
$CDCl_3$, 101 MHz, 298 K



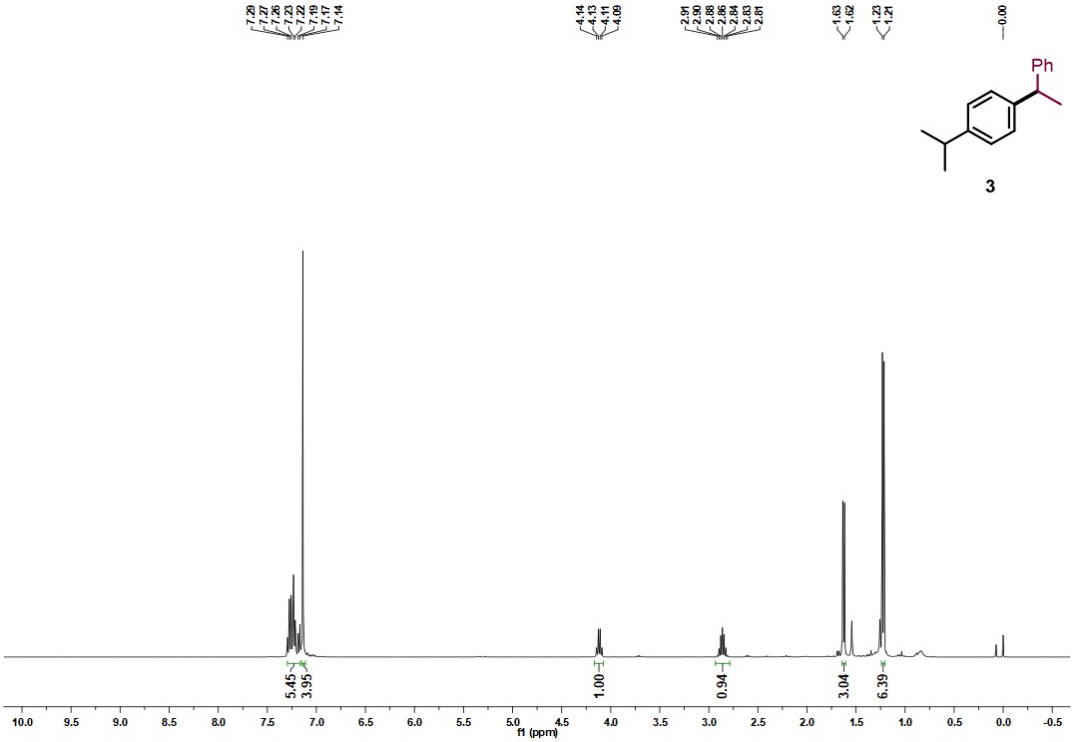
^{1}H-NMR of **2**
$CDCl_3$, 400 MHz, 298 K



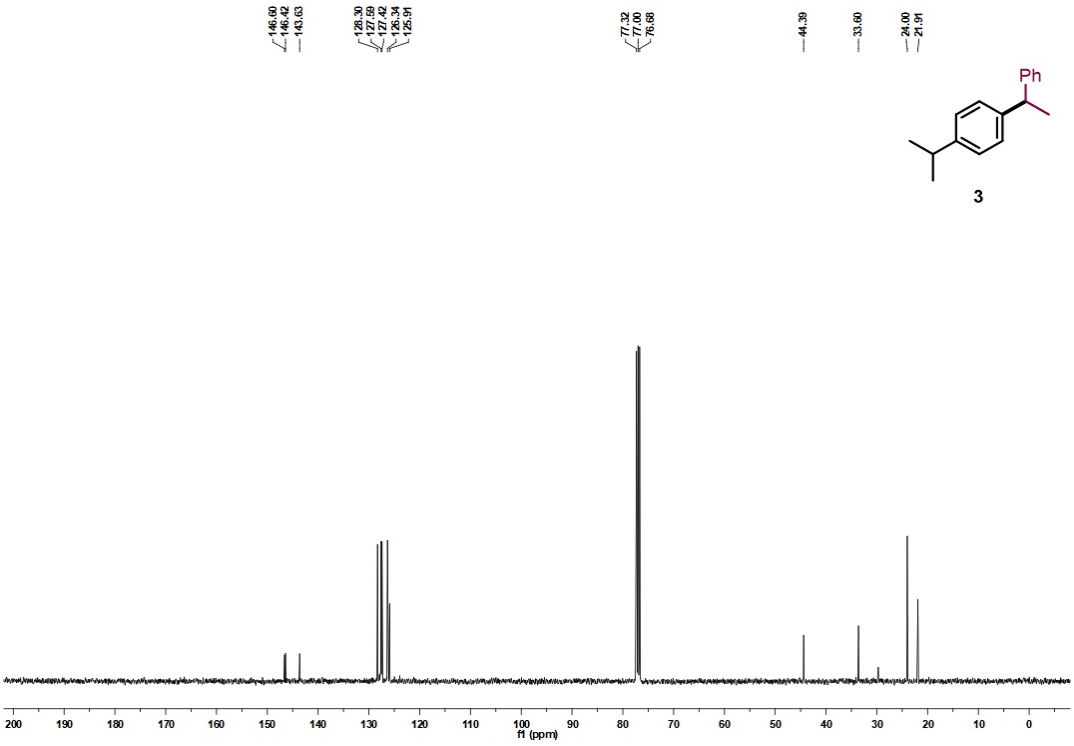
^{13}C-NMR of **2**
$CDCl_3$, 101 MHz, 298 K



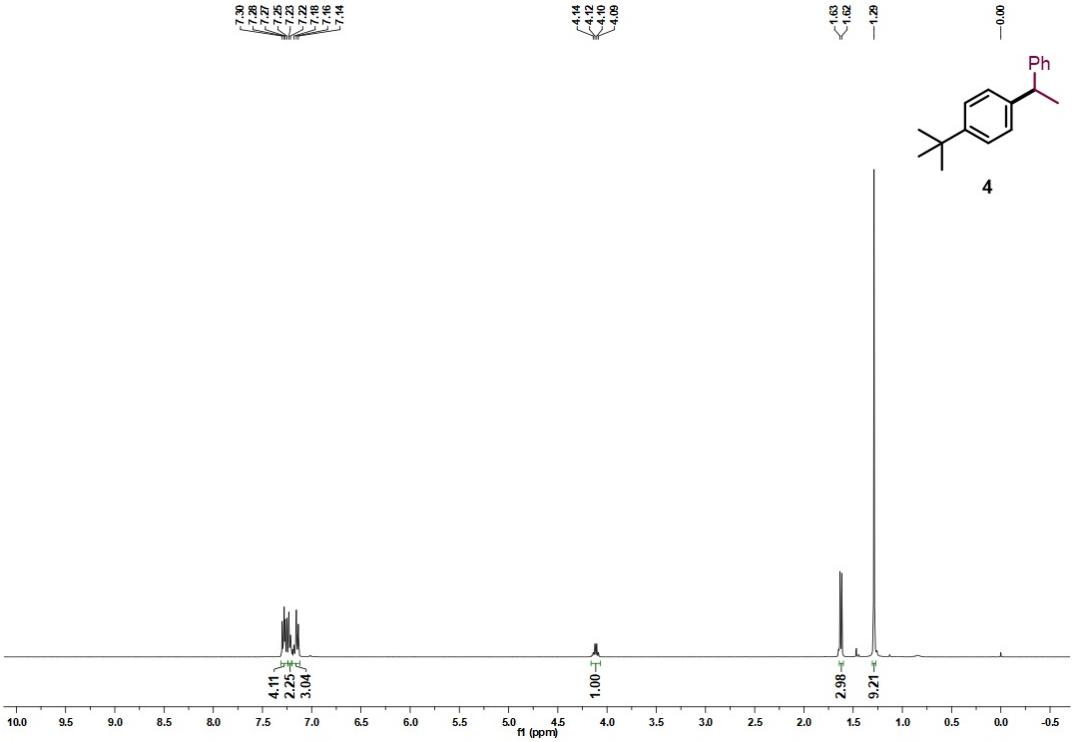
^{1}H-NMR of **3**
$CDCl_3$, 400 MHz, 298 K



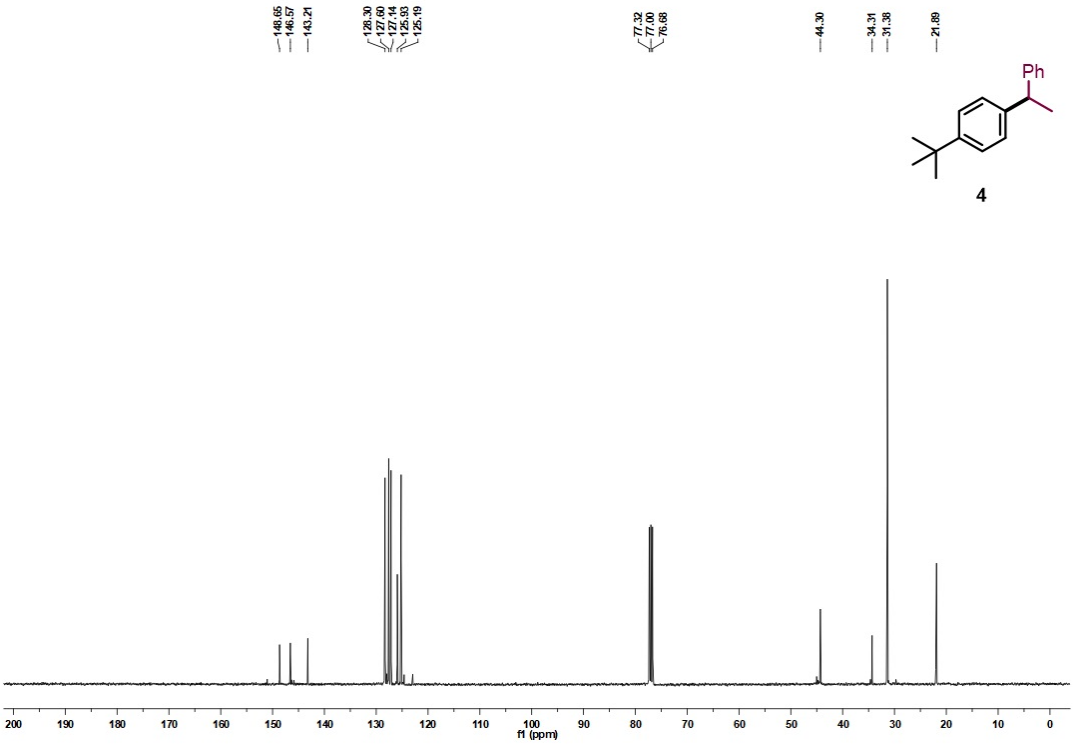
^{13}C-NMR of **3**
$CDCl_3$, 101 MHz, 298 K



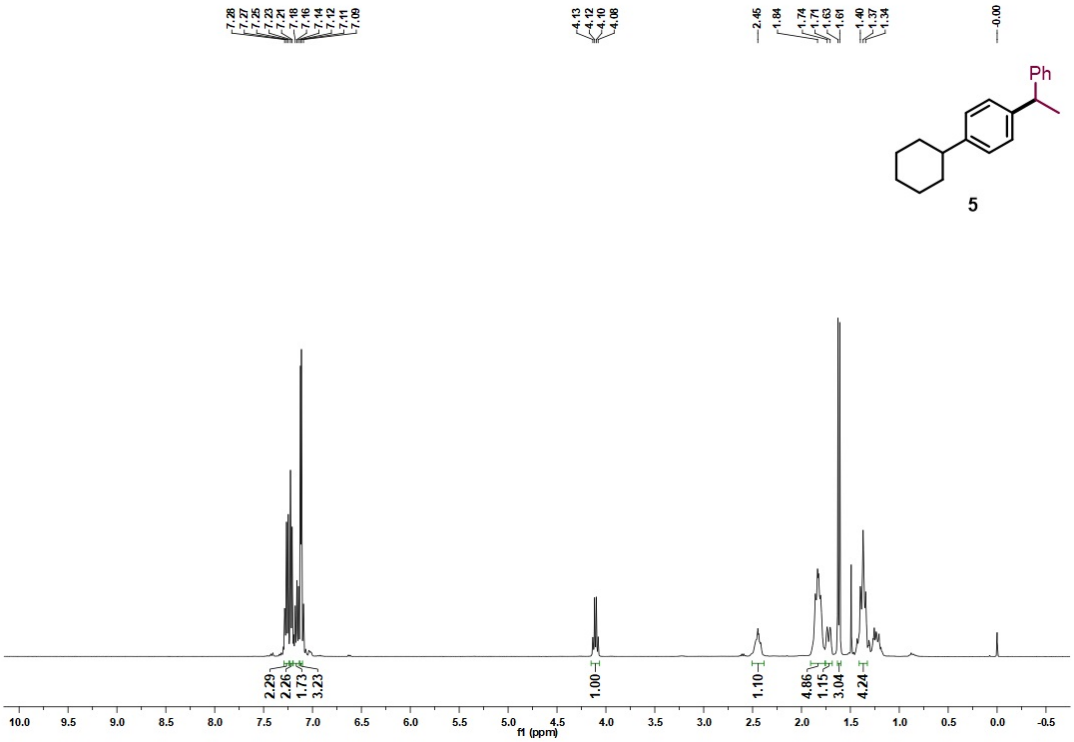
^{1}H-NMR of **4**
$CDCl_3$, 400 MHz, 298 K



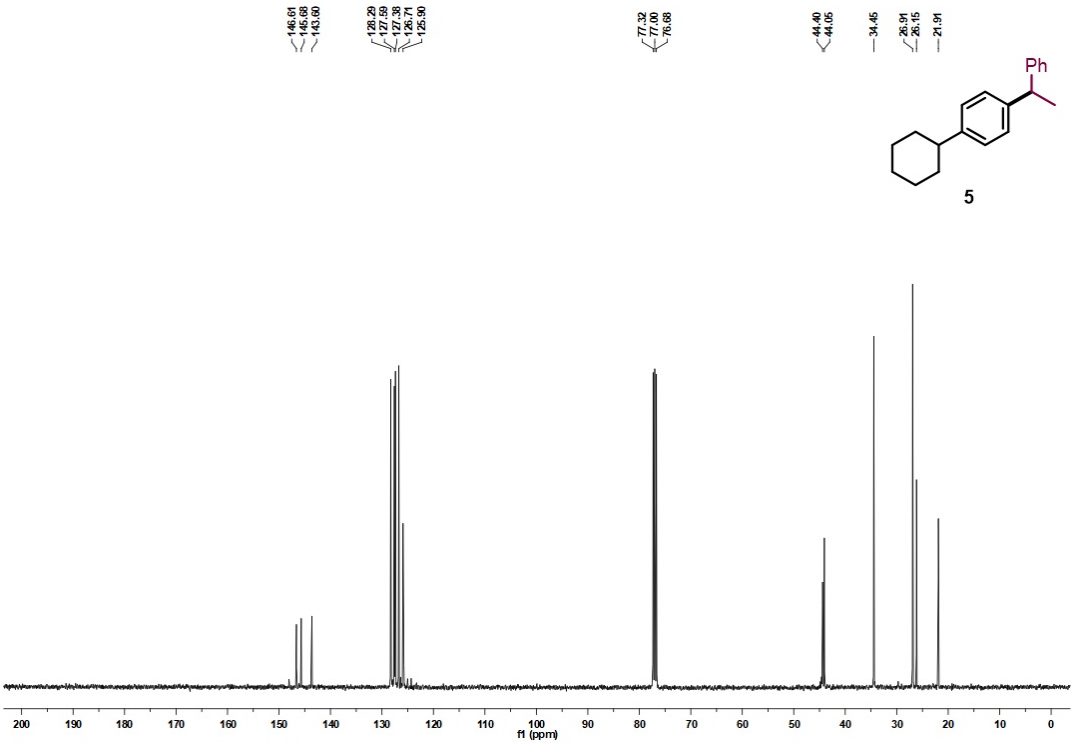
^{13}C-NMR of **4**
$CDCl_3$, 101 MHz, 298 K



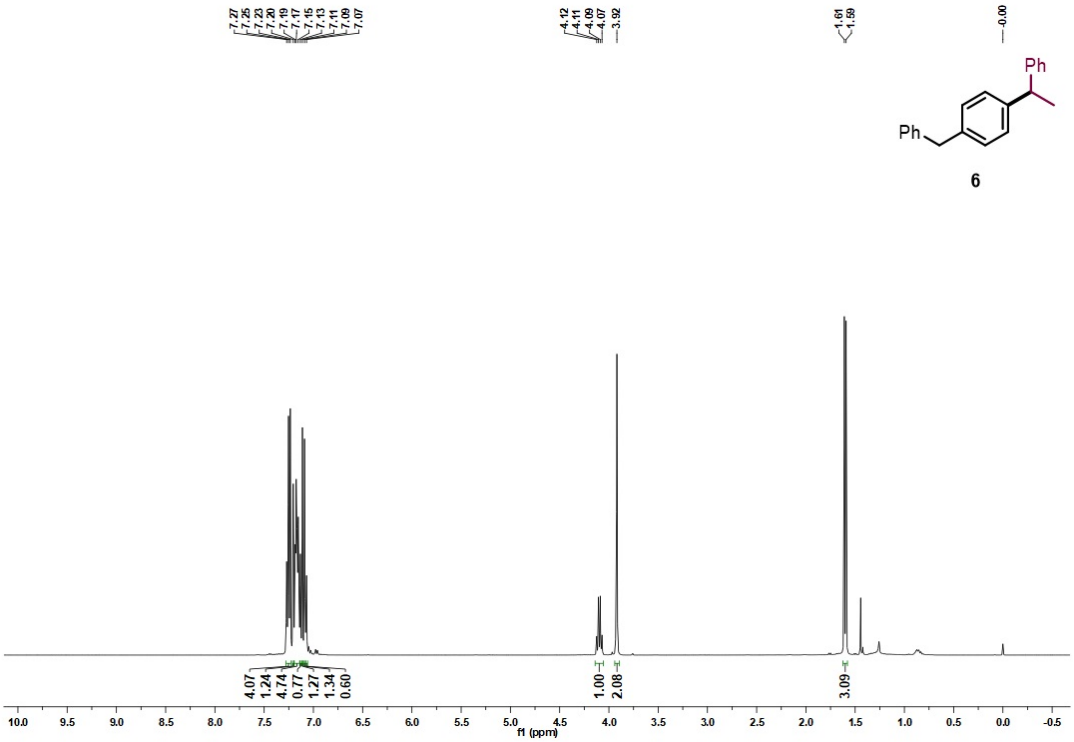
^{1}H-NMR of **5**
$CDCl_3$, 400 MHz, 298 K



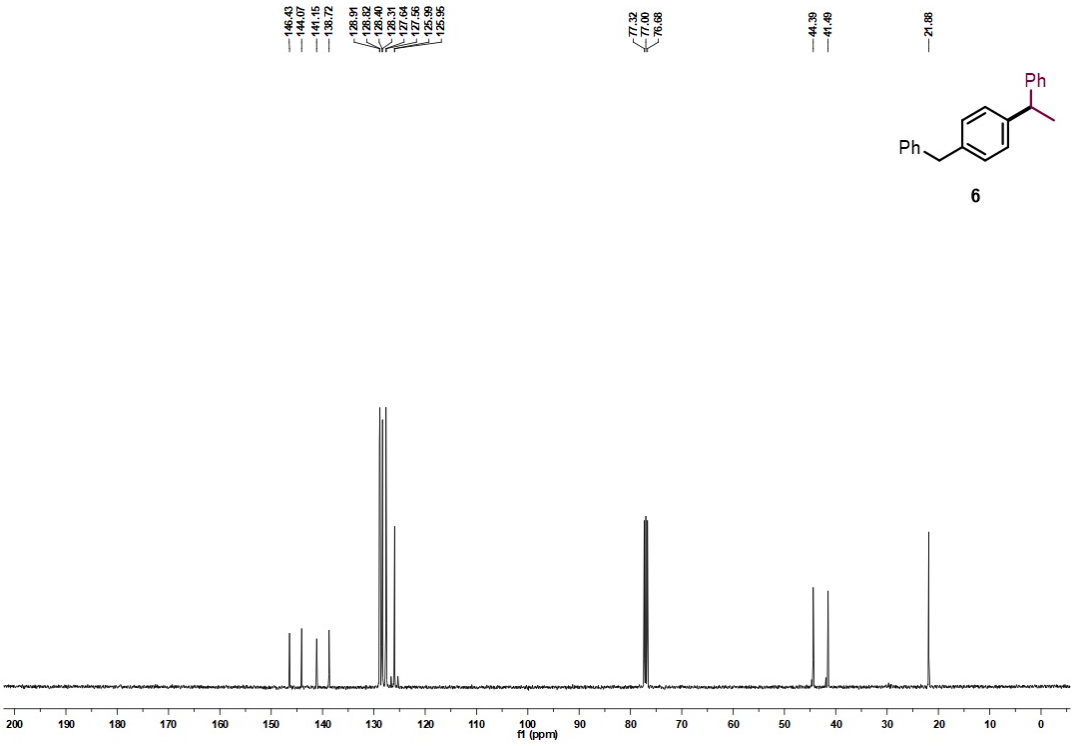
^{13}C-NMR of **5**
$CDCl_3$, 101 MHz, 298 K



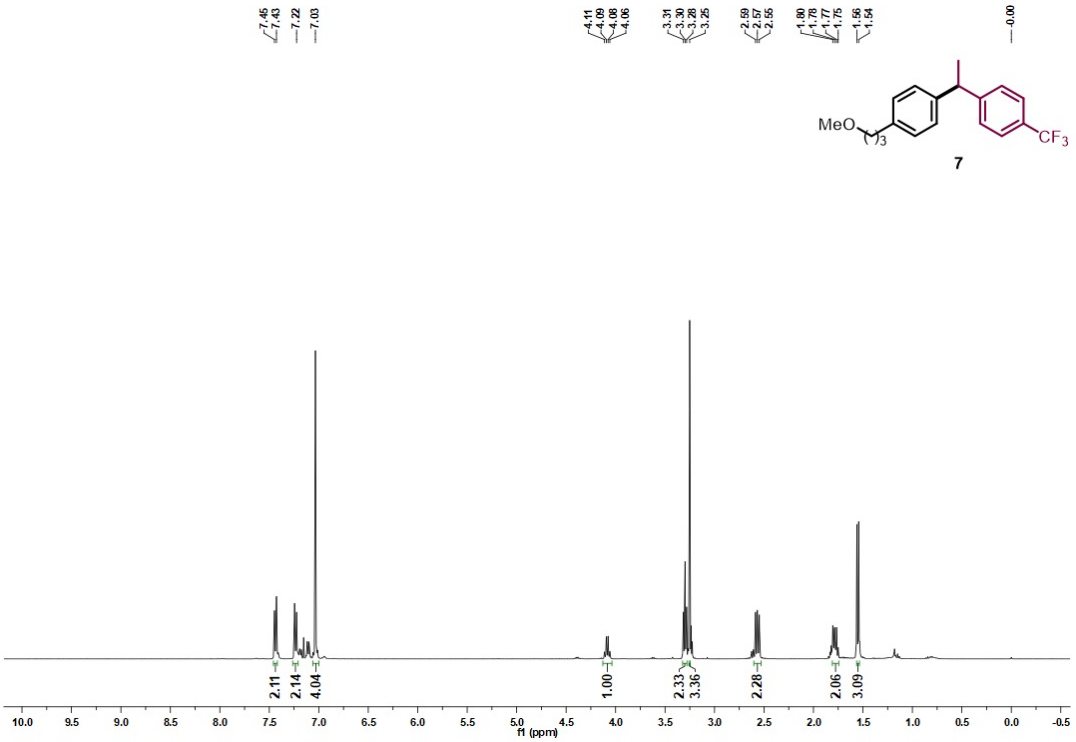
^{1}H-NMR of **6**
$CDCl_3$, 400 MHz, 298 K



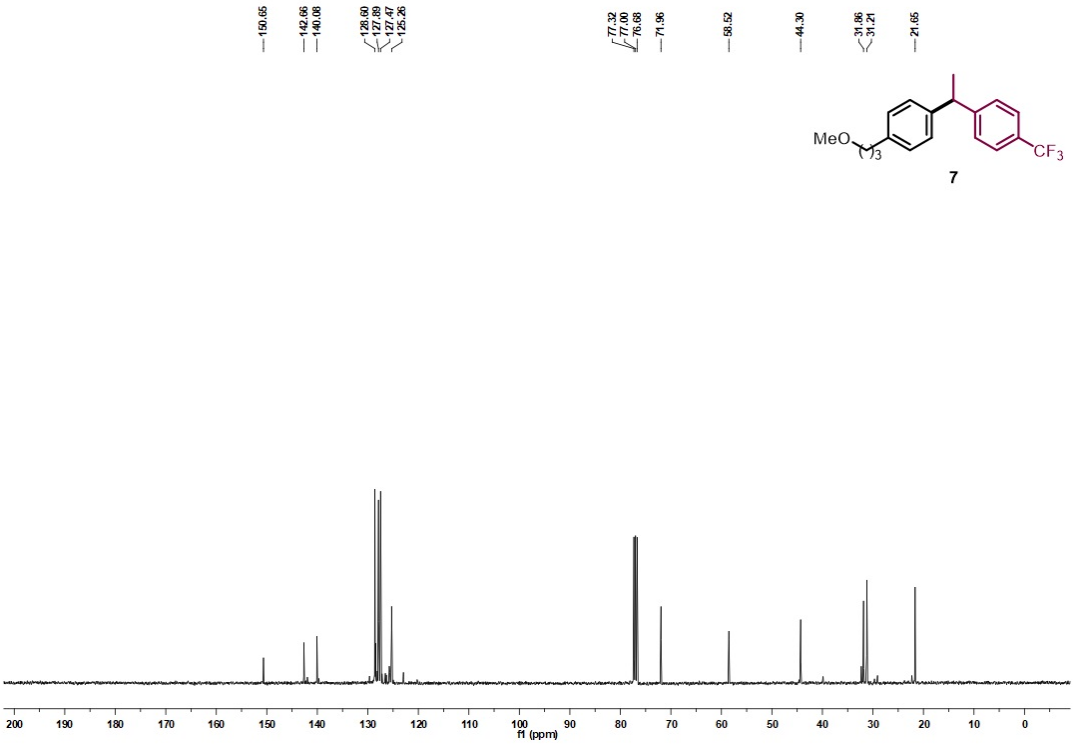
^{13}C-NMR of **6**
$CDCl_3$, 101 MHz, 298 K



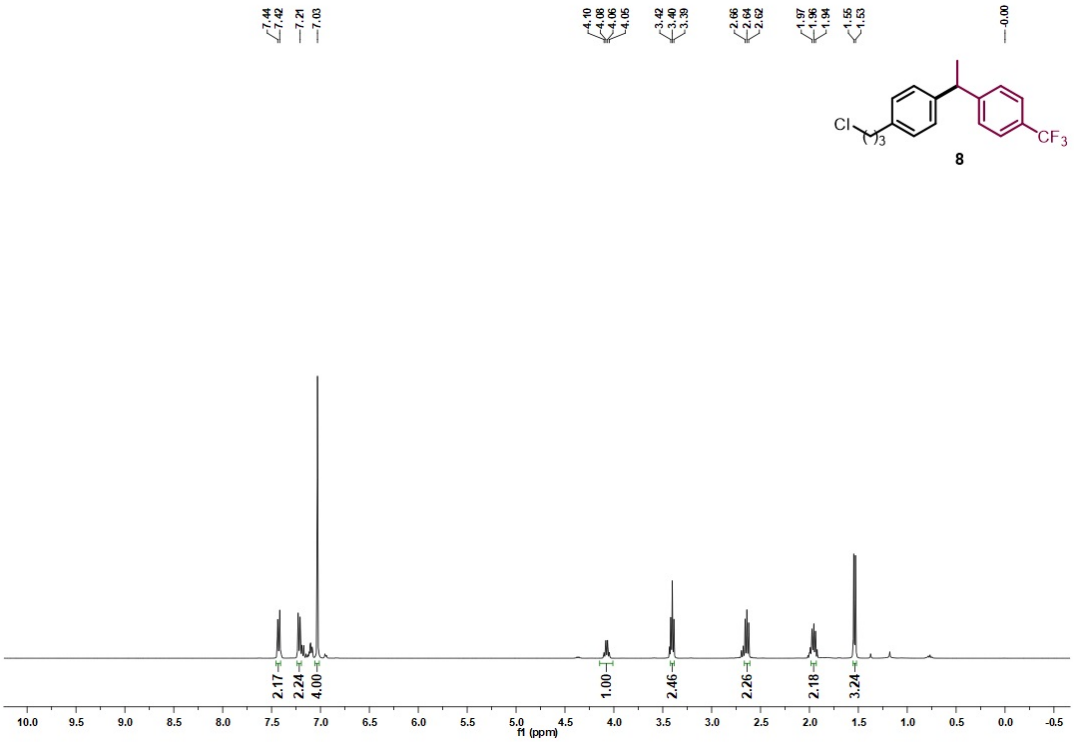
^{1}H-NMR of **7**
$CDCl_3$, 400 MHz, 298 K



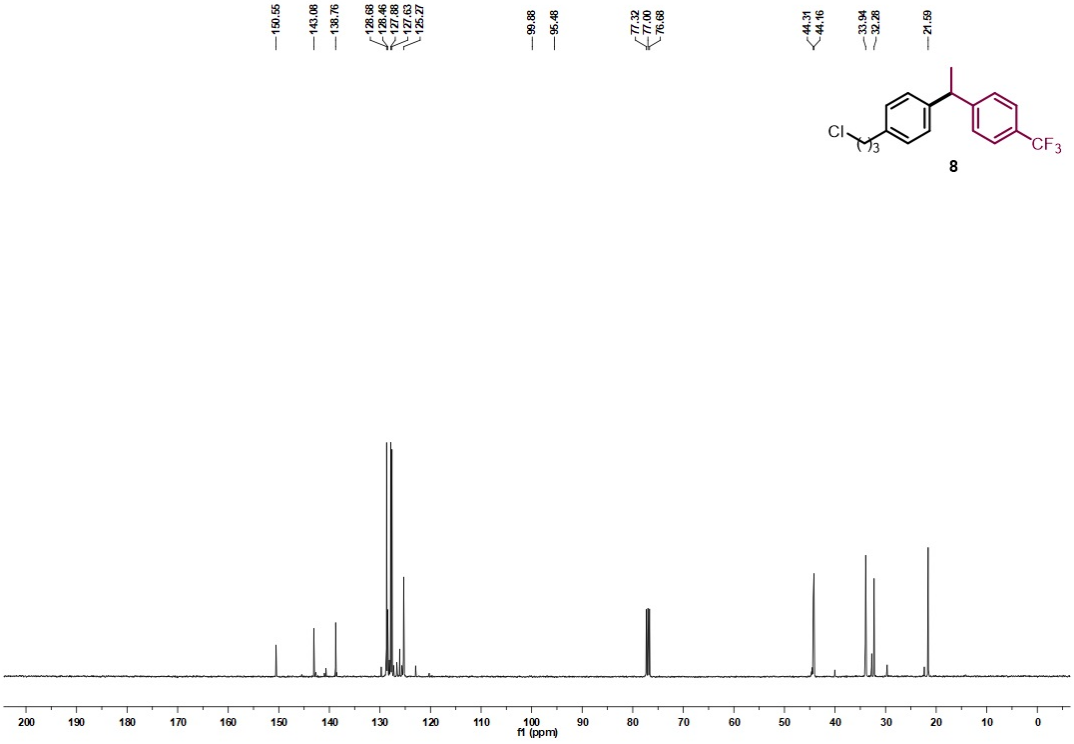
^{13}C-NMR of **7**
$CDCl_3$, 101 MHz, 298 K



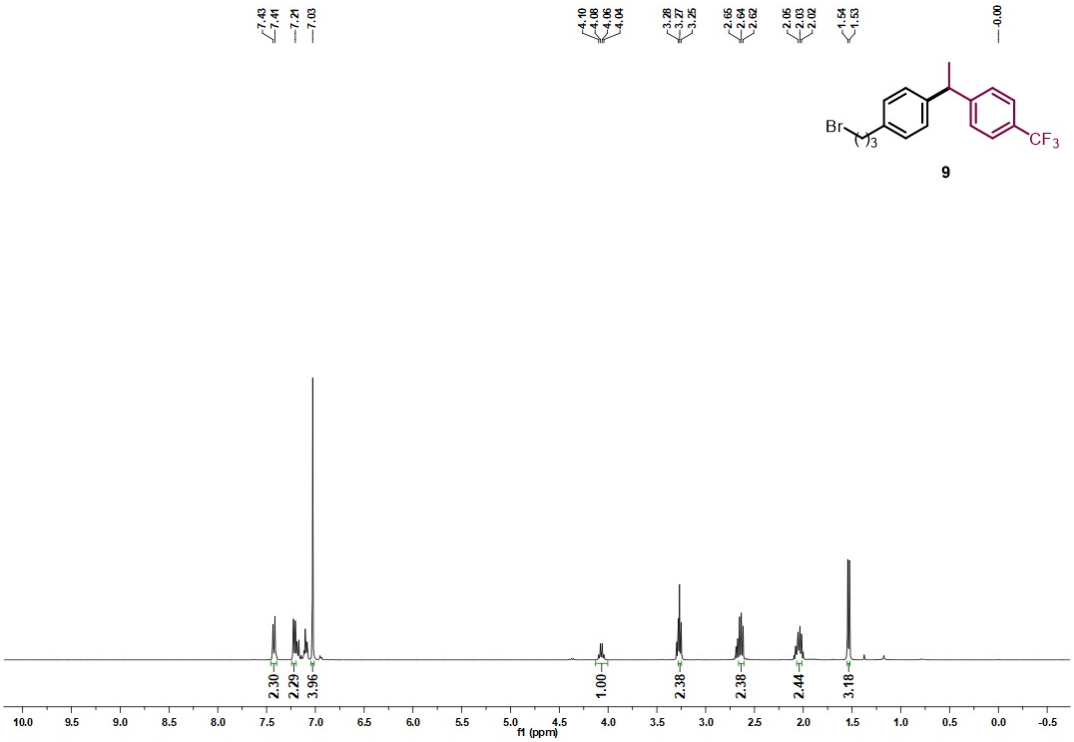
^{1}H-NMR of **8**
$CDCl_3$, 400 MHz, 298 K



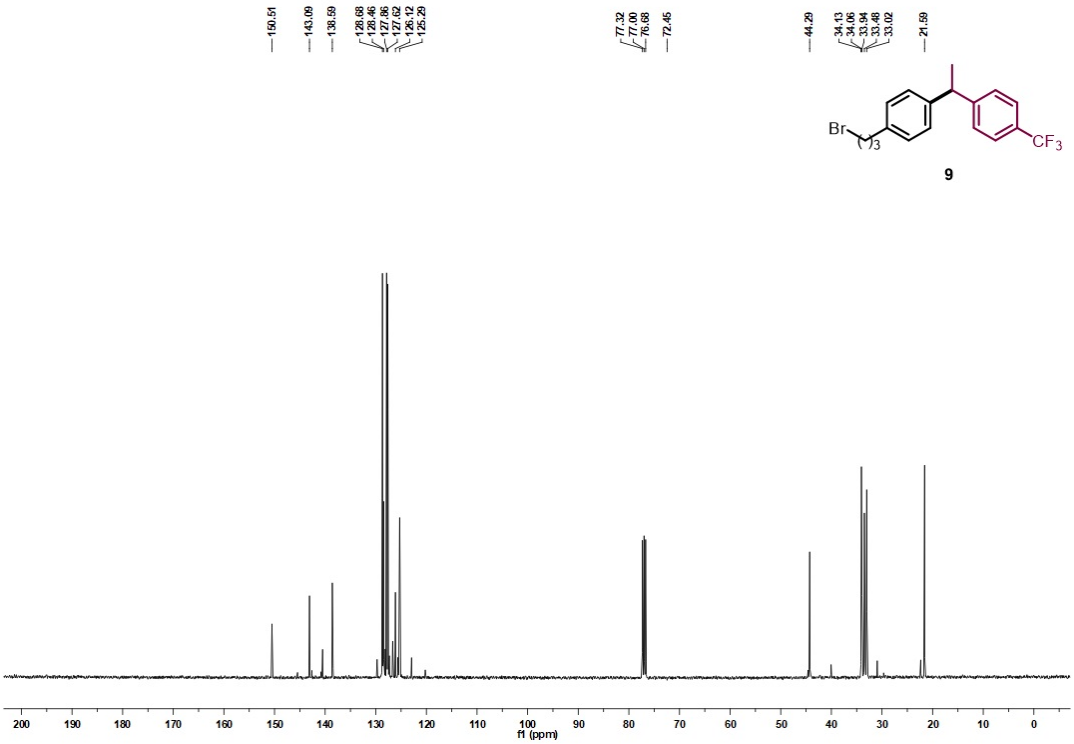
^{13}C-NMR of **8**
$CDCl_3$, 101 MHz, 298 K



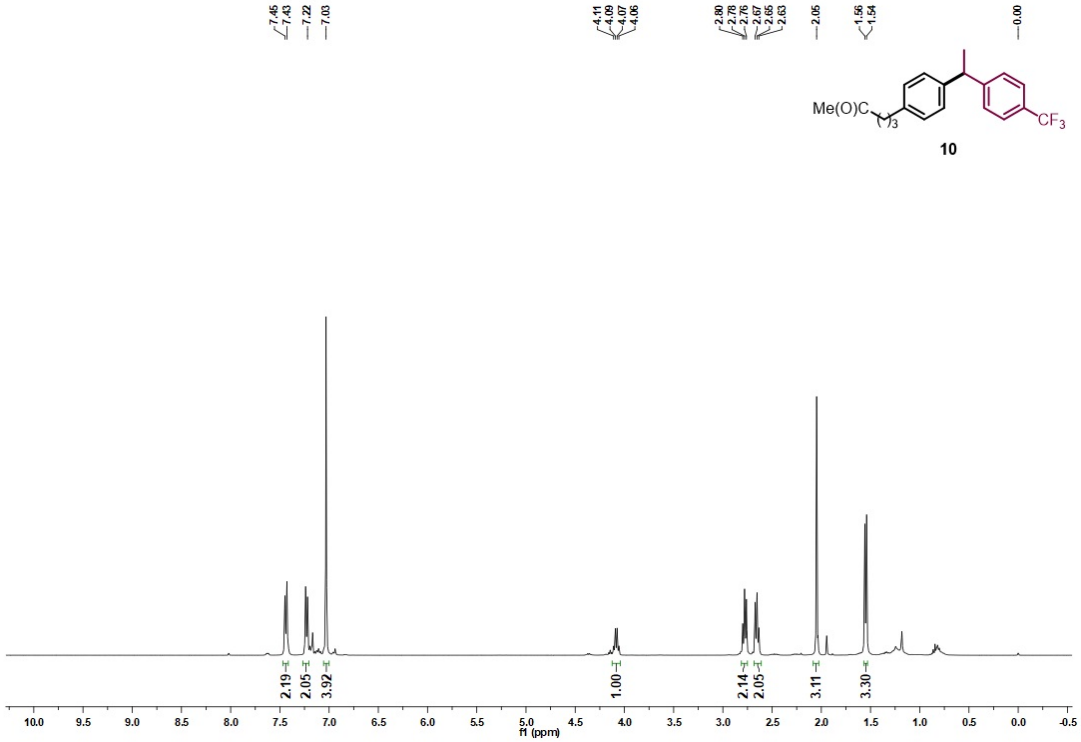
^{1}H-NMR of **9**
$CDCl_3$, 400 MHz, 298 K



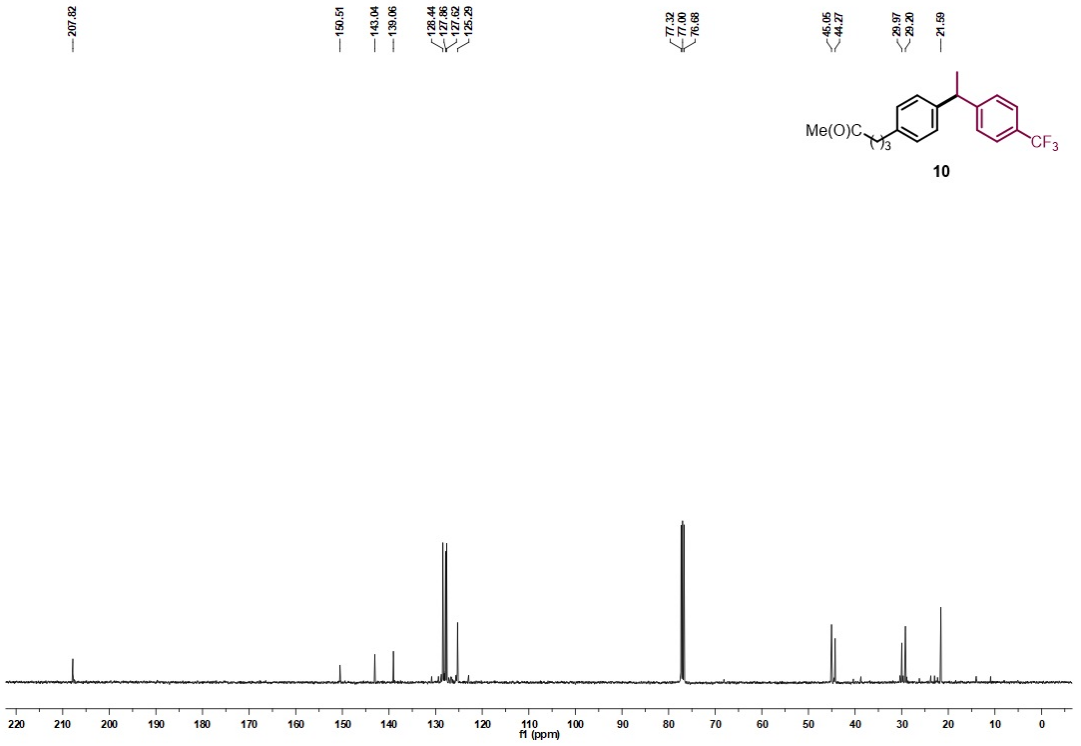
^{13}C-NMR of **9**
$CDCl_3$, 101 MHz, 298 K



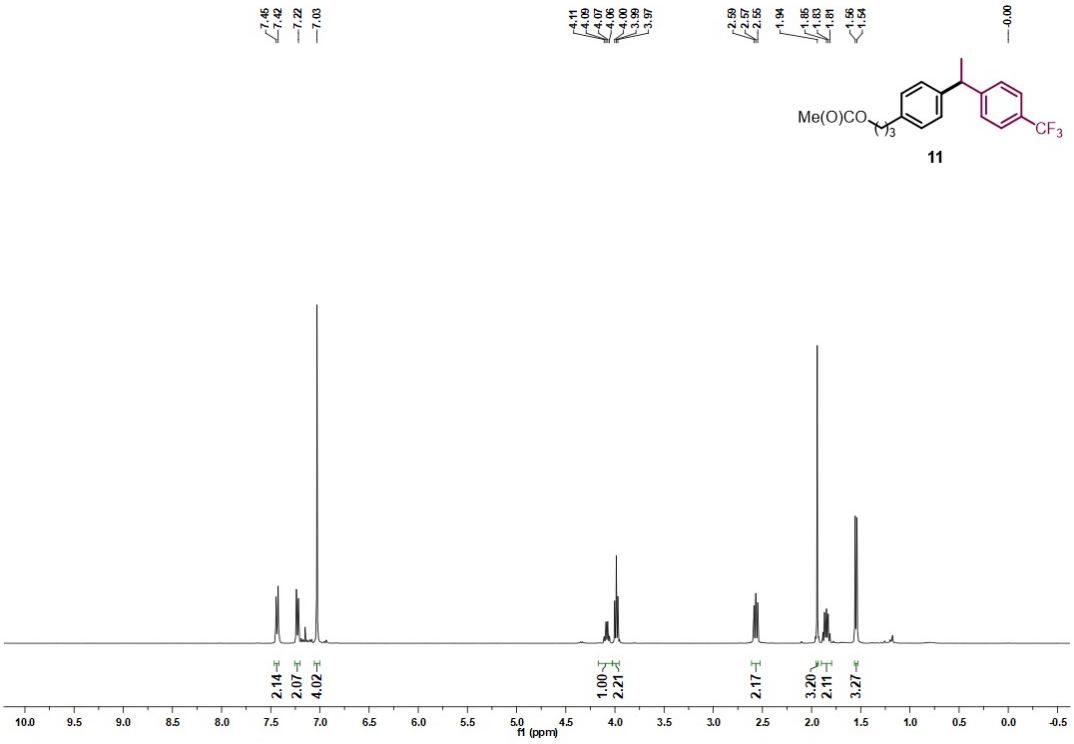
^{1}H-NMR of **10**
$CDCl_3$, 400 MHz, 298 K



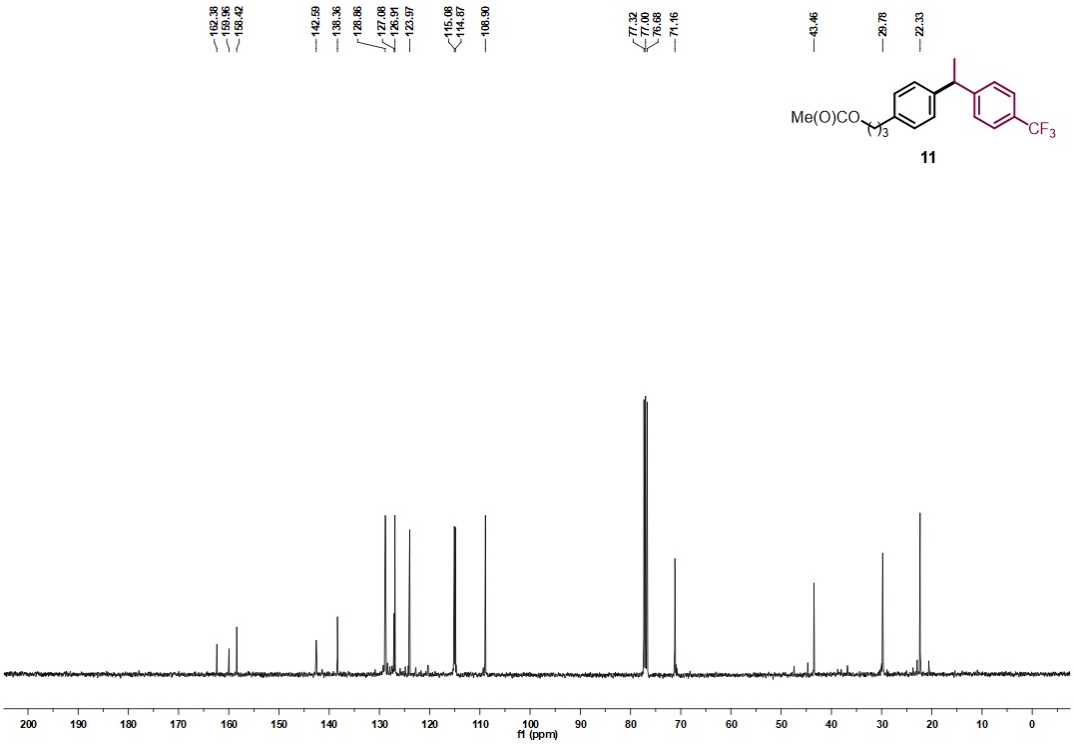
^{13}C-NMR of **10**
$CDCl_3$, 101 MHz, 298 K



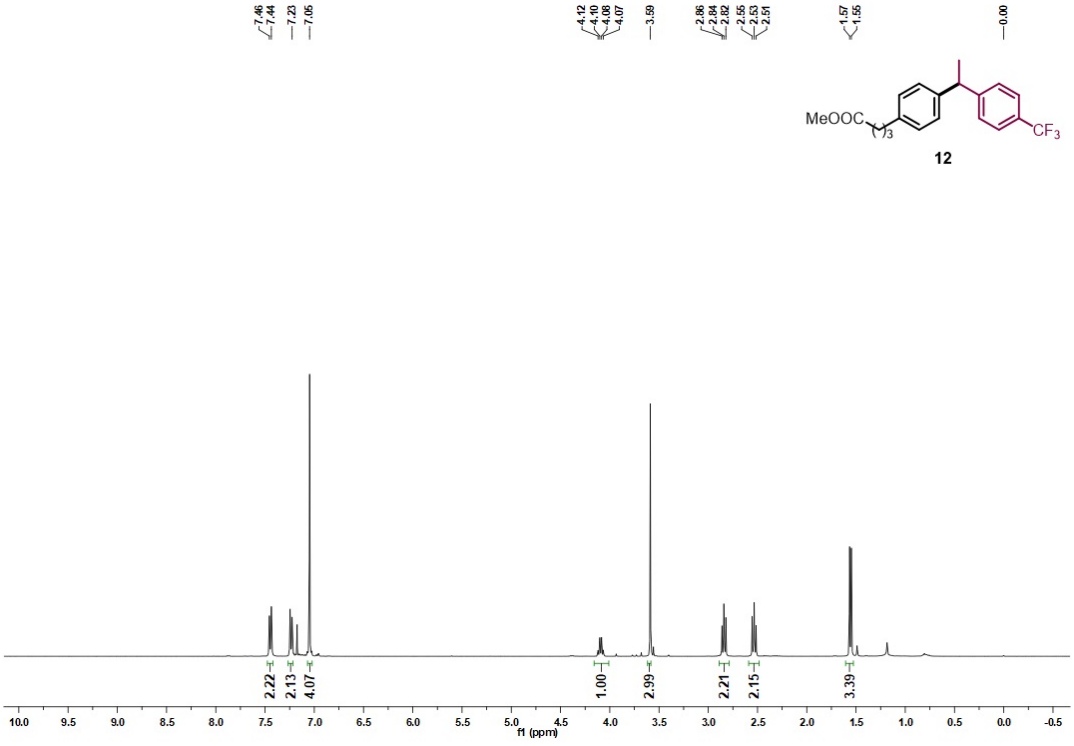
^{1}H-NMR of **11**
$CDCl_3$, 400 MHz, 298 K



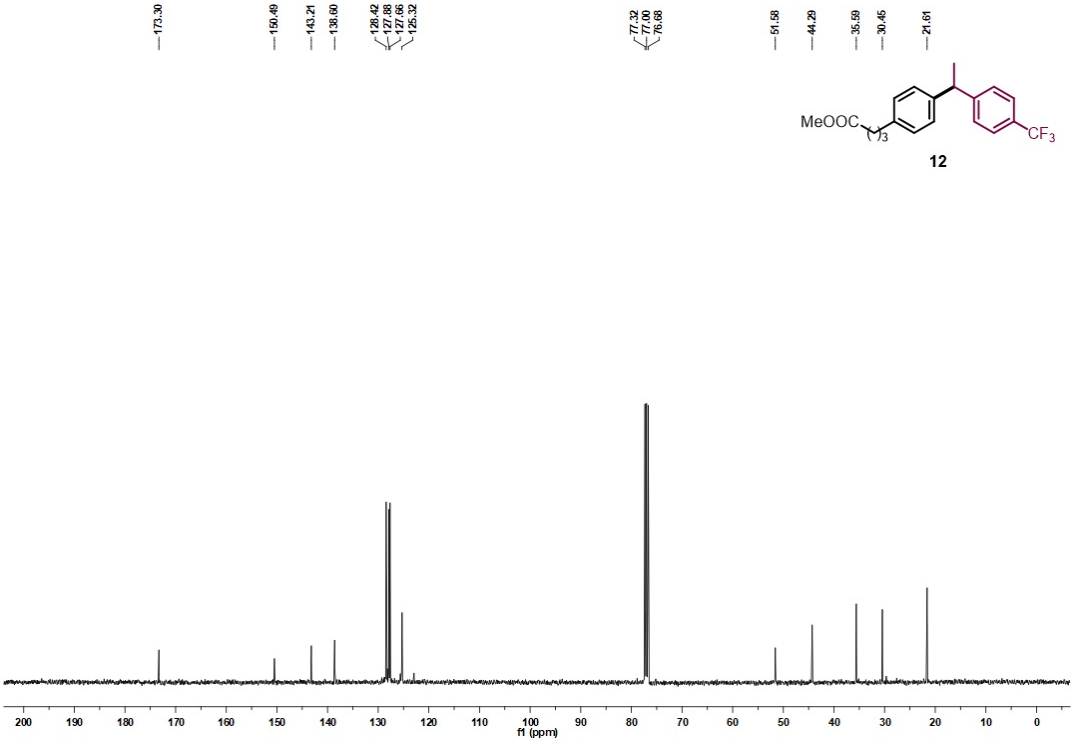
^{13}C-NMR of **11**
$CDCl_3$, 101 MHz, 298 K



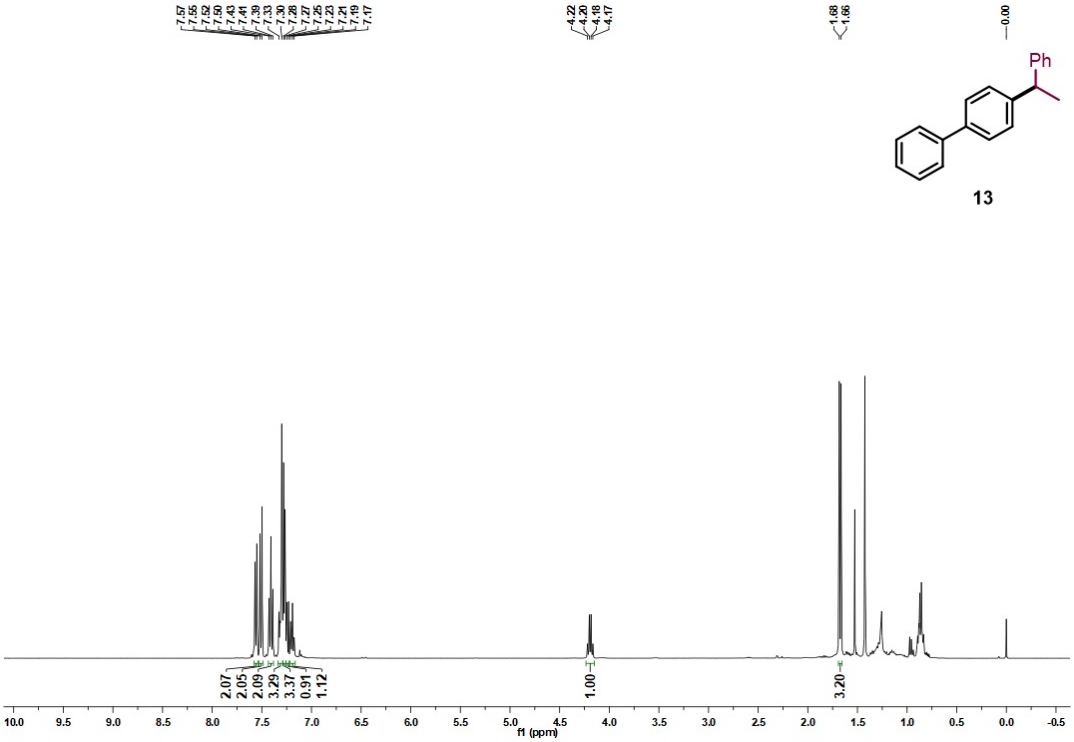
^{1}H-NMR of **12**
$CDCl_3$, 400 MHz, 298 K



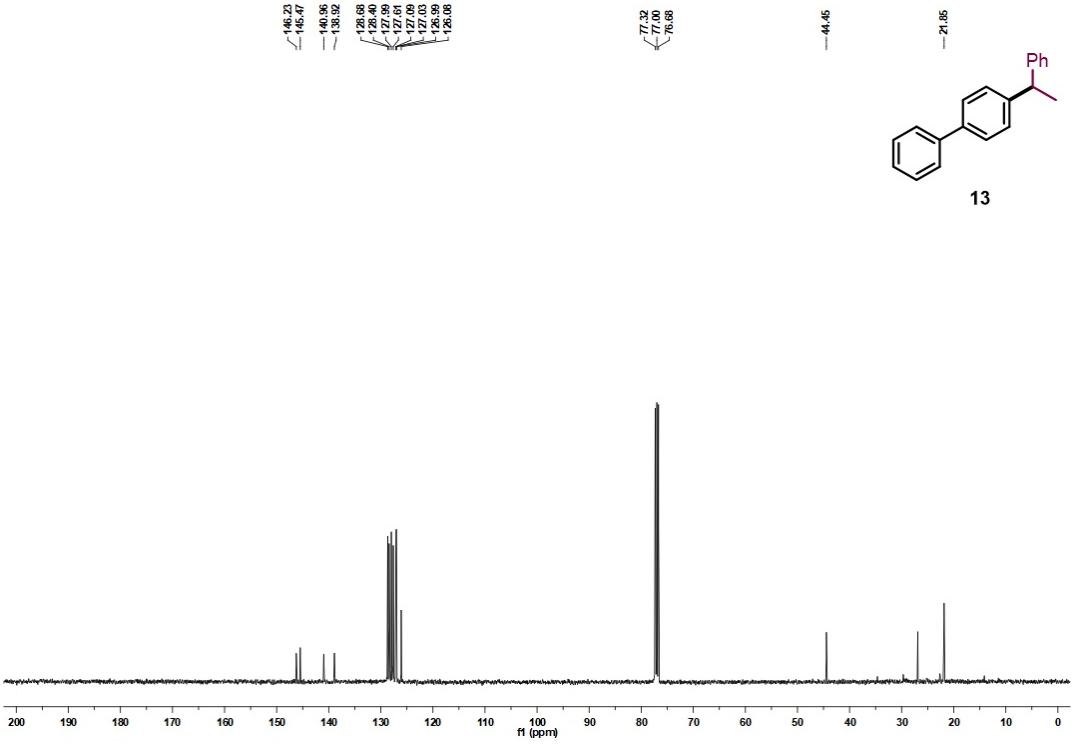
^{13}C-NMR of **12**
$CDCl_3$, 101 MHz, 298 K



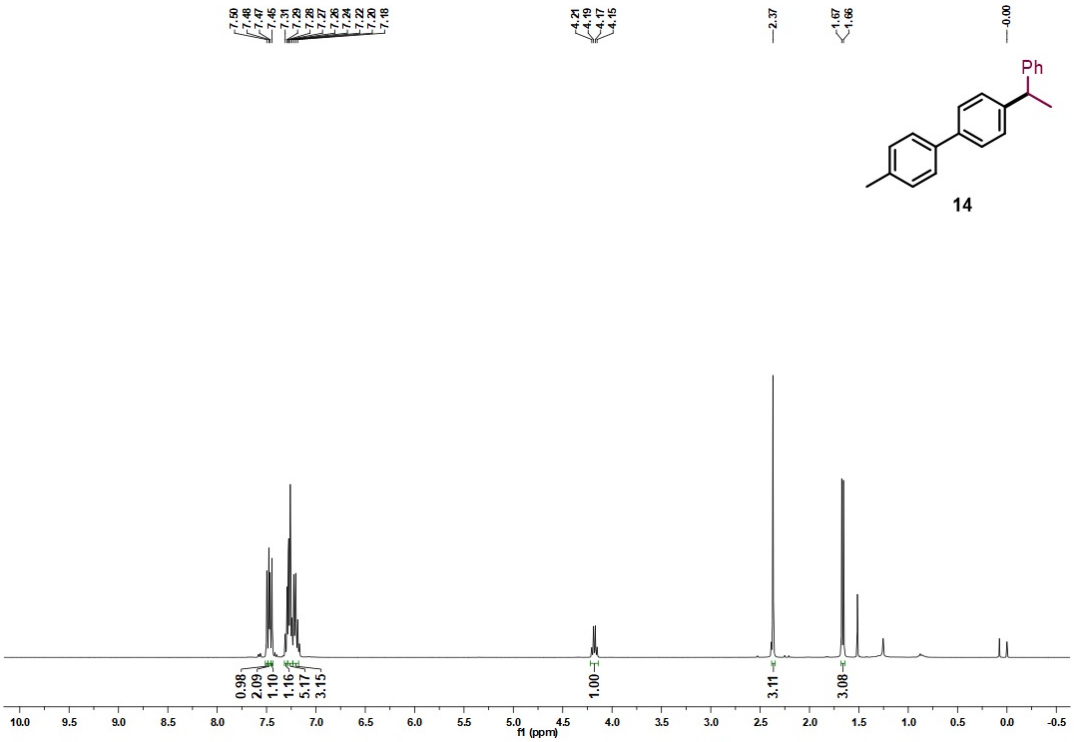
^{1}H-NMR of **13**
$CDCl_3$, 400 MHz, 298 K



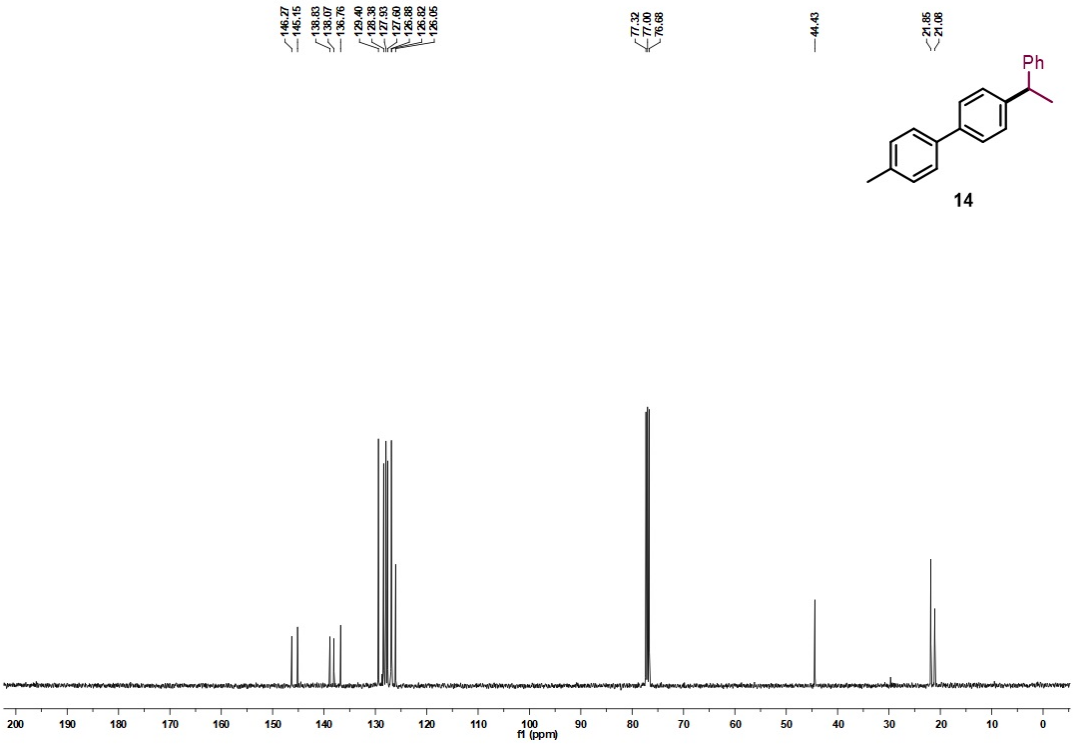
^{13}C-NMR of **13**
$CDCl_3$, 101 MHz, 298 K



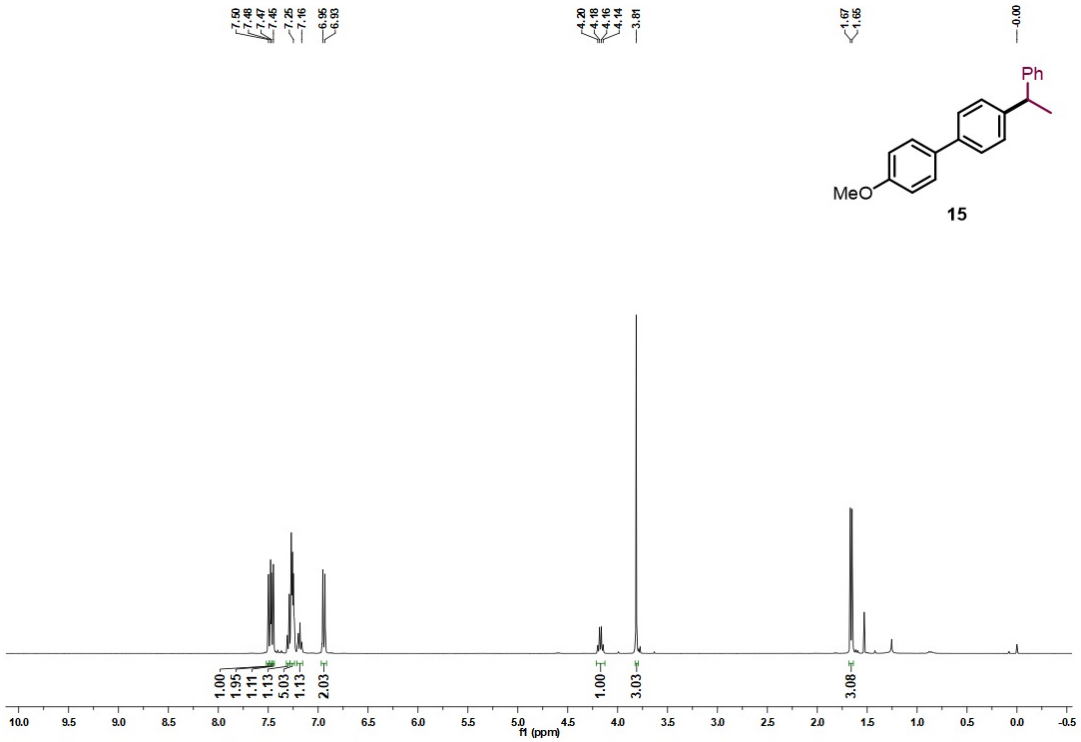
^{1}H-NMR of **14**
$CDCl_3$, 400 MHz, 298 K



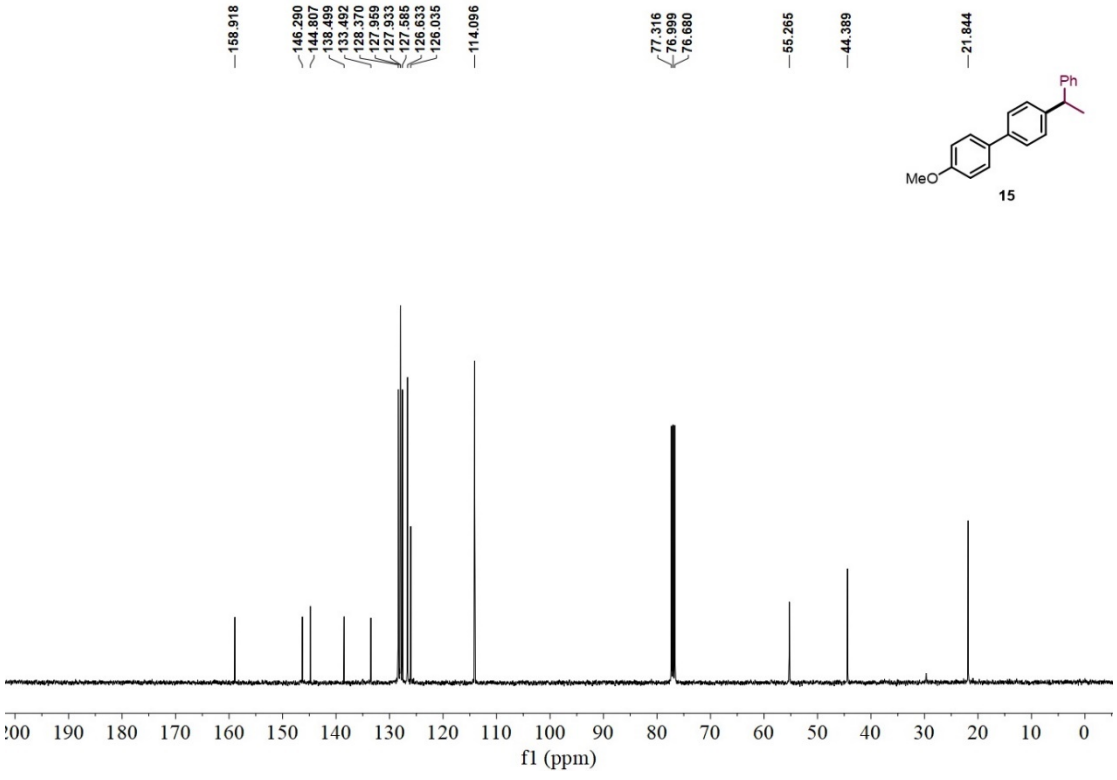
^{13}C-NMR of **14**
$CDCl_3$, 101 MHz, 298 K



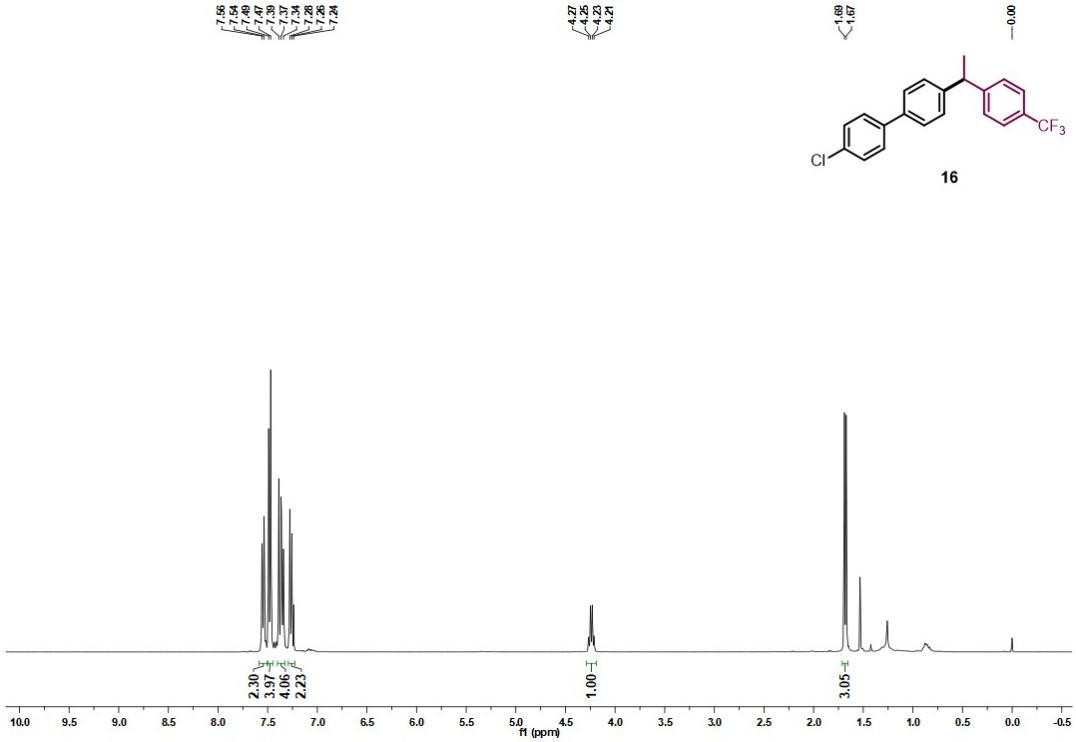
^{1}H-NMR of **15**
$CDCl_3$, 400 MHz, 298 K



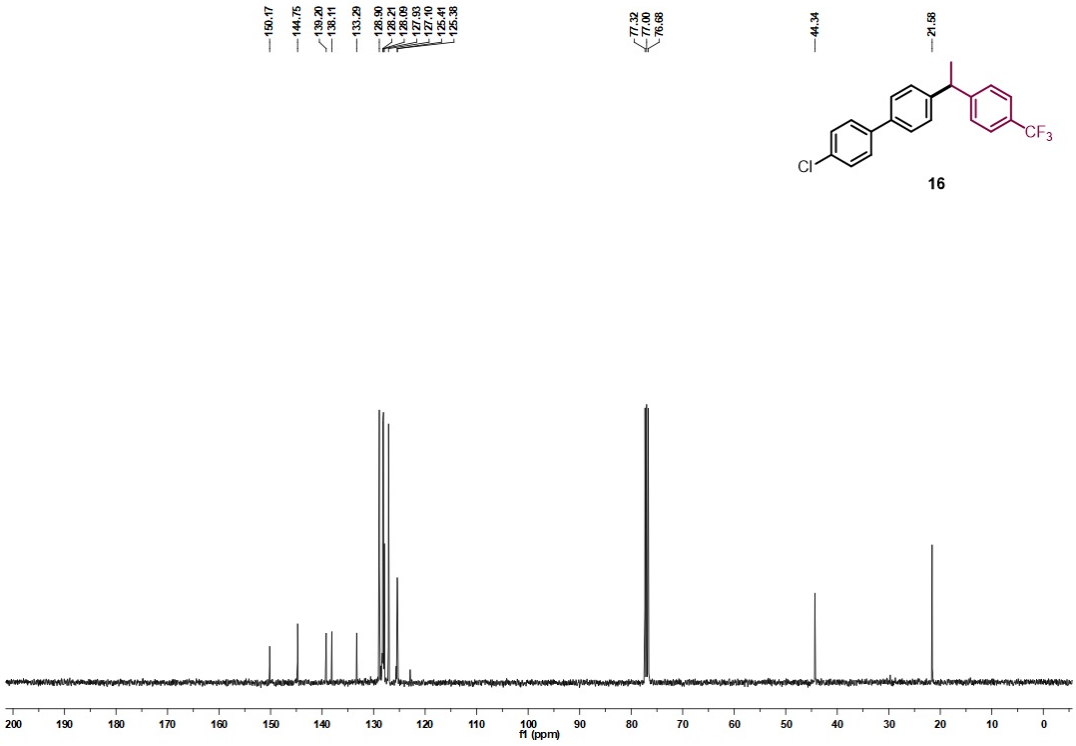
^{13}C-NMR of **15**
$CDCl_3$, 101 MHz, 298 K



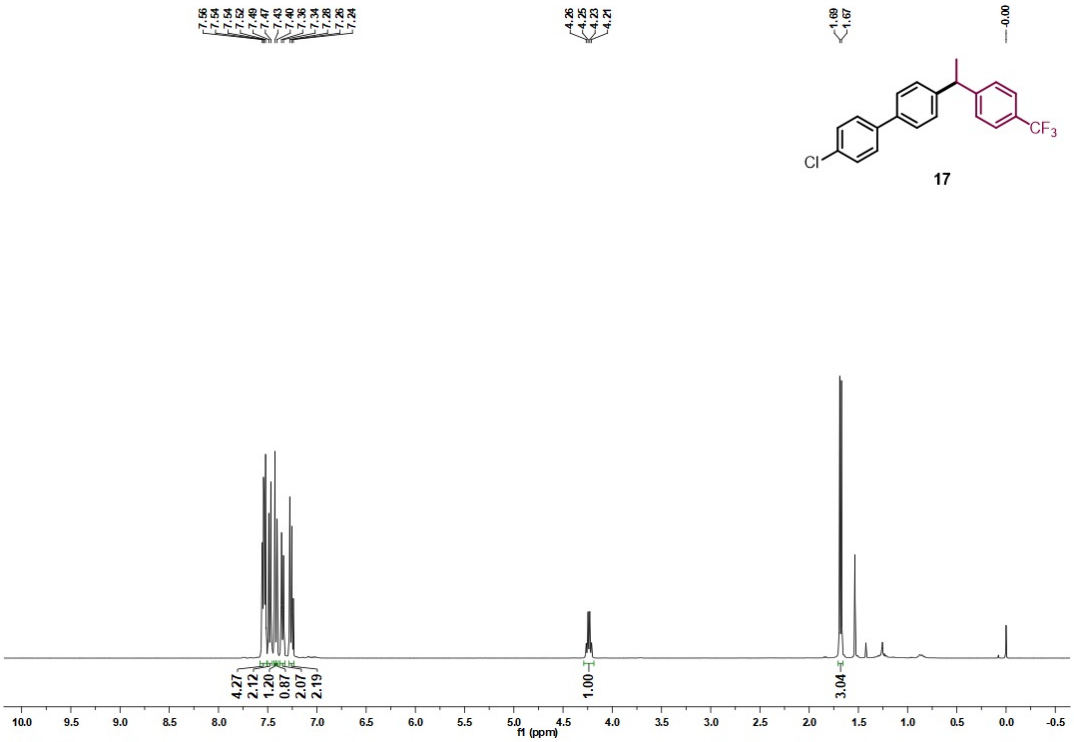
^{1}H-NMR of **16**
$CDCl_3$, 400 MHz, 298 K



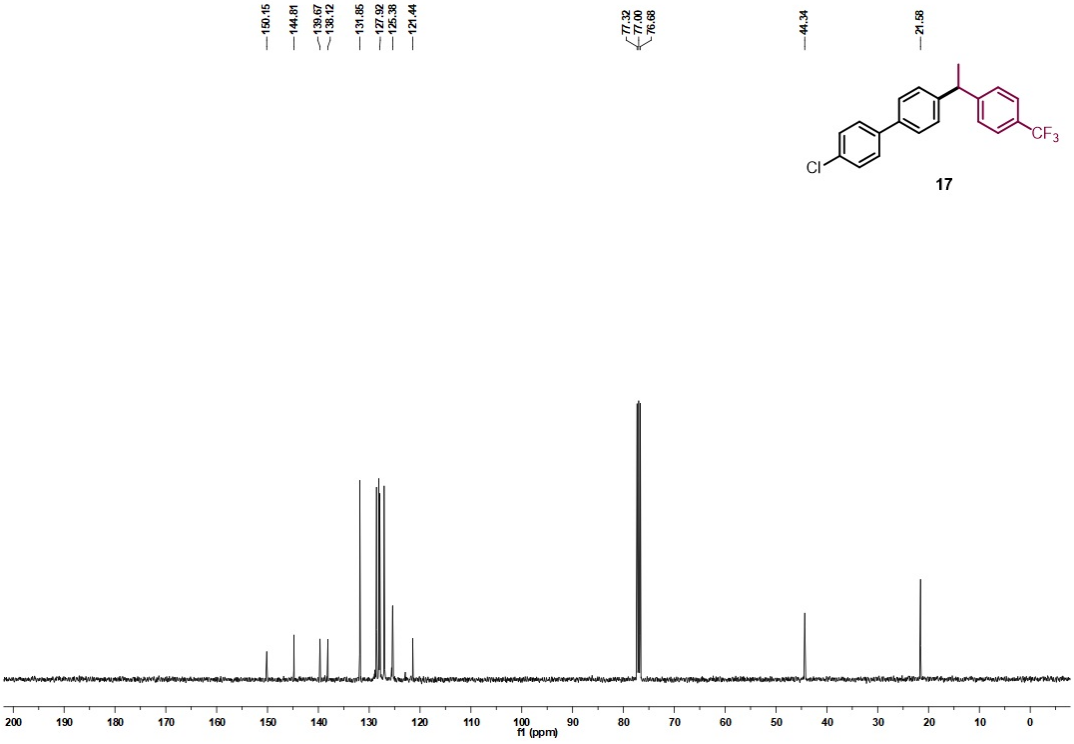
^{13}C-NMR of **16**
$CDCl_3$, 101 MHz, 298 K



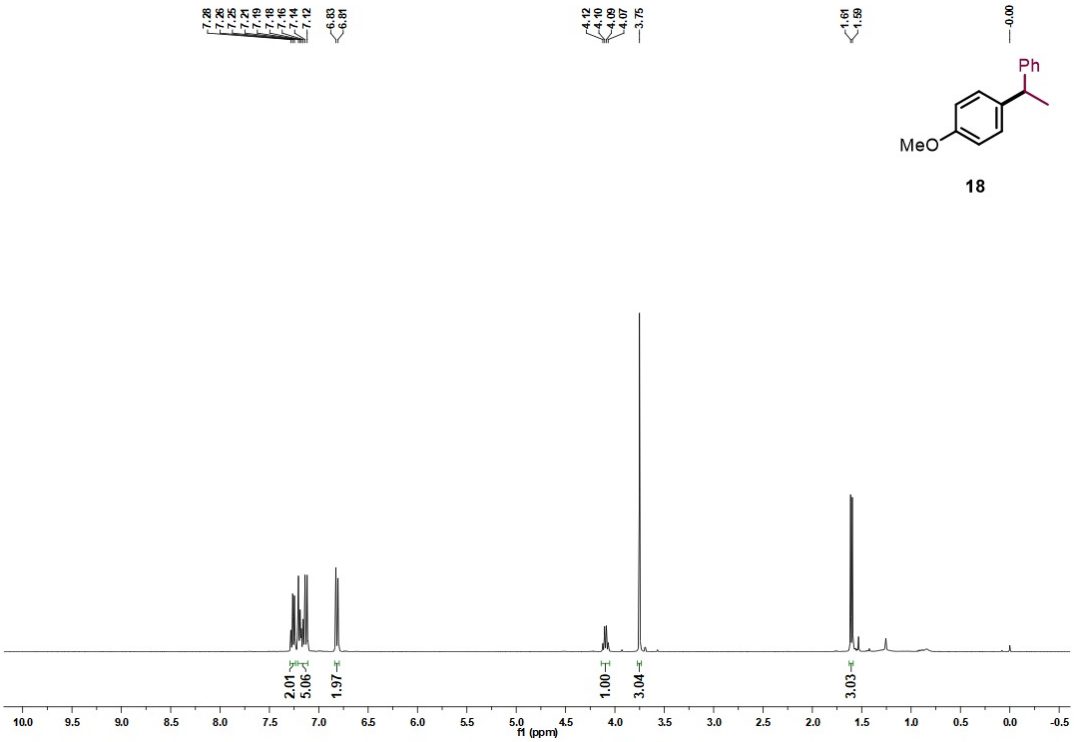
^{1}H-NMR of **17**
$CDCl_3$, 400 MHz, 298 K



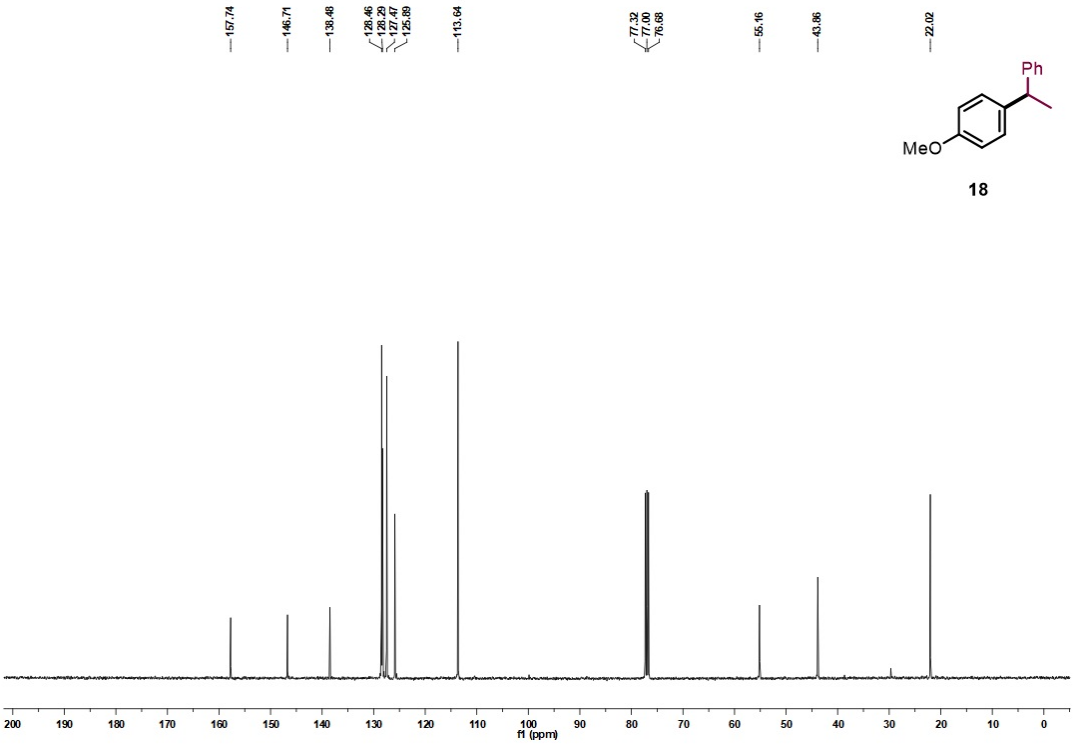
^{13}C-NMR of **17**
$CDCl_3$, 101 MHz, 298 K



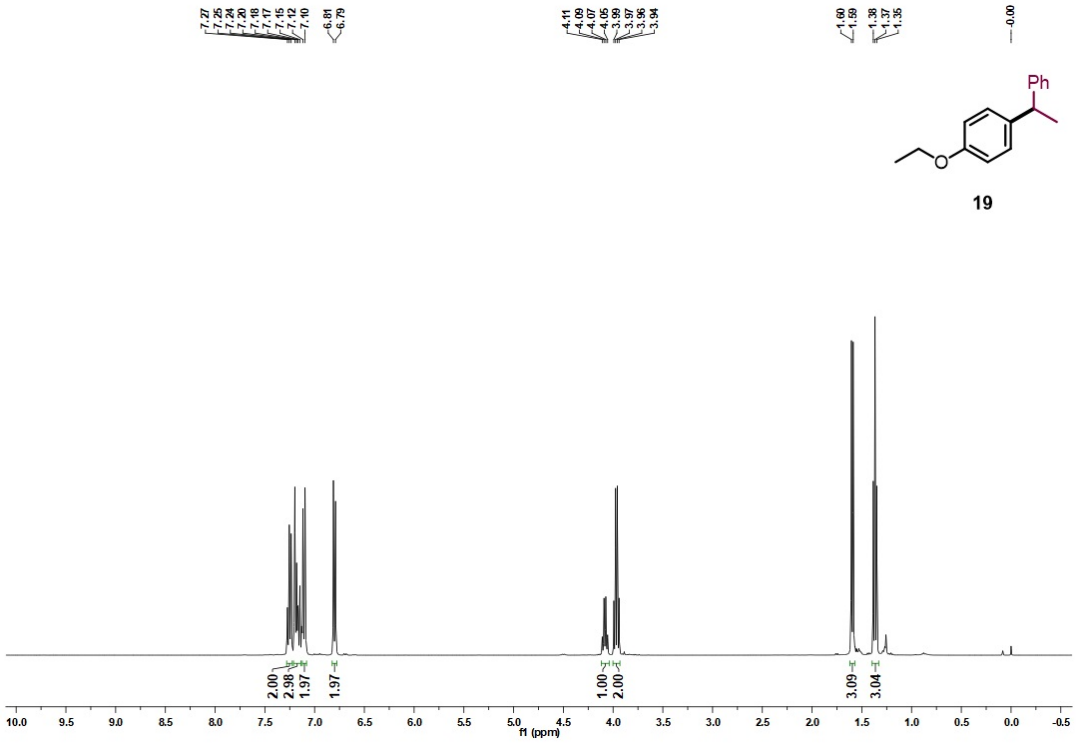
^{1}H-NMR of **18**
$CDCl_3$, 400 MHz, 298 K



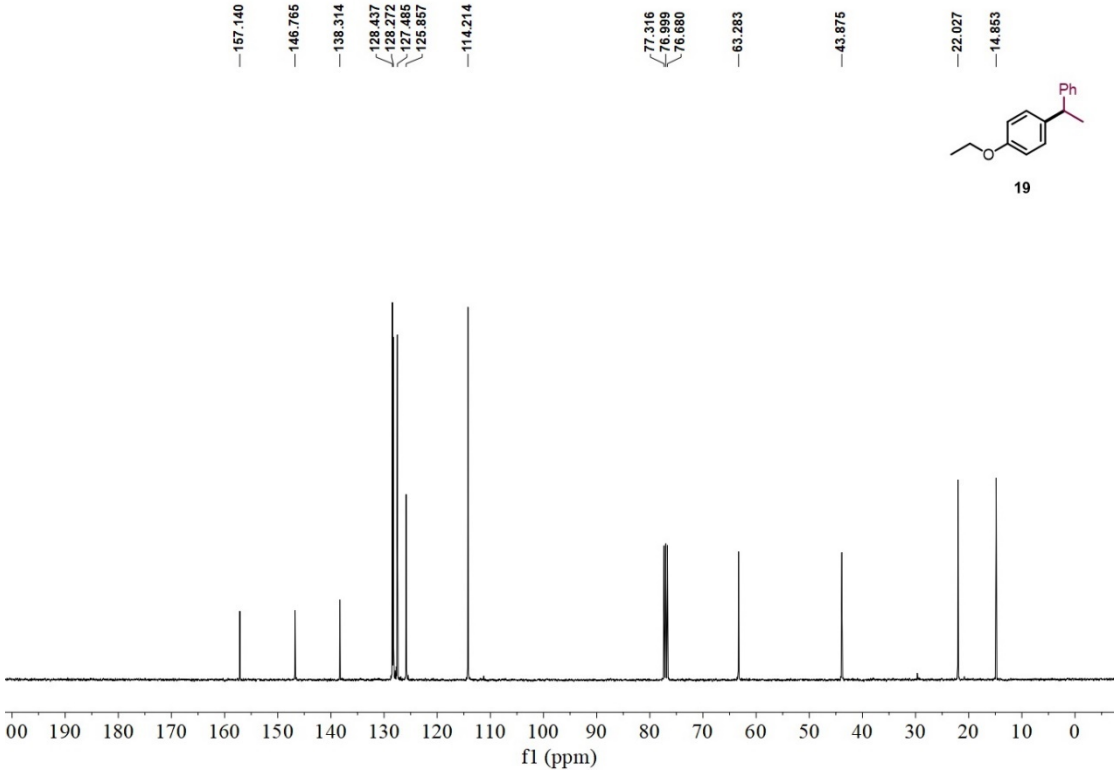
^{13}C-NMR of **18**
$CDCl_3$, 101 MHz, 298 K



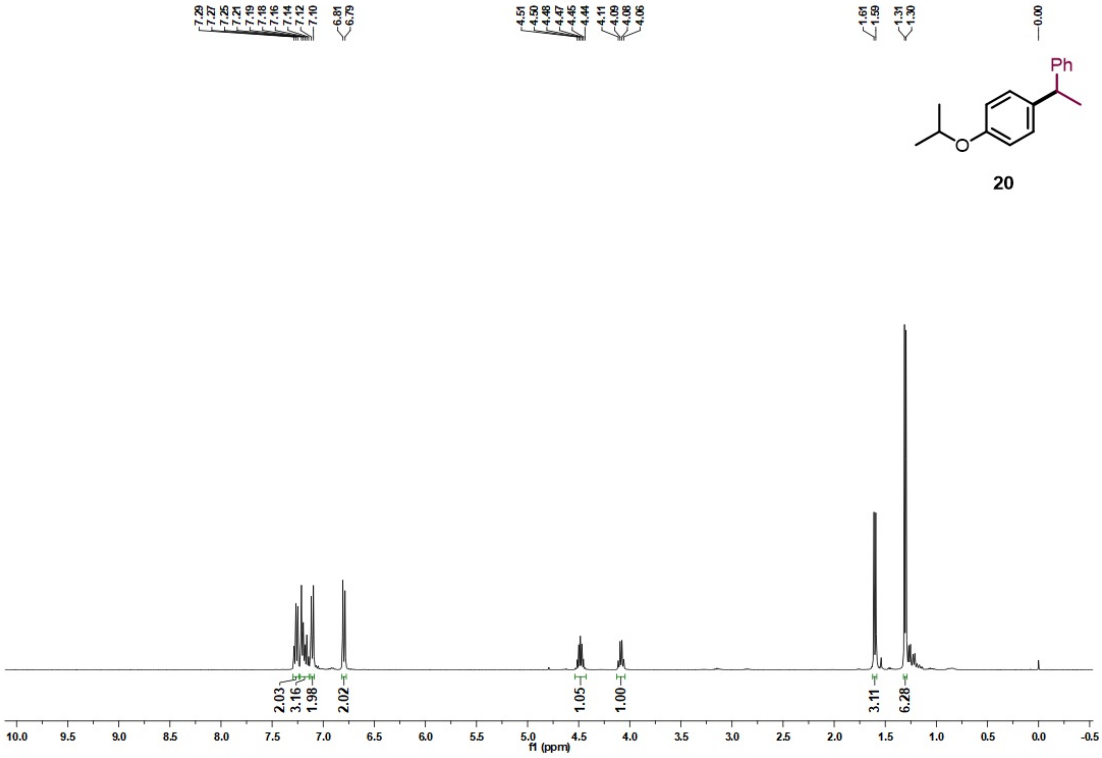
^{1}H-NMR of **19**
$CDCl_3$, 400 MHz, 298 K



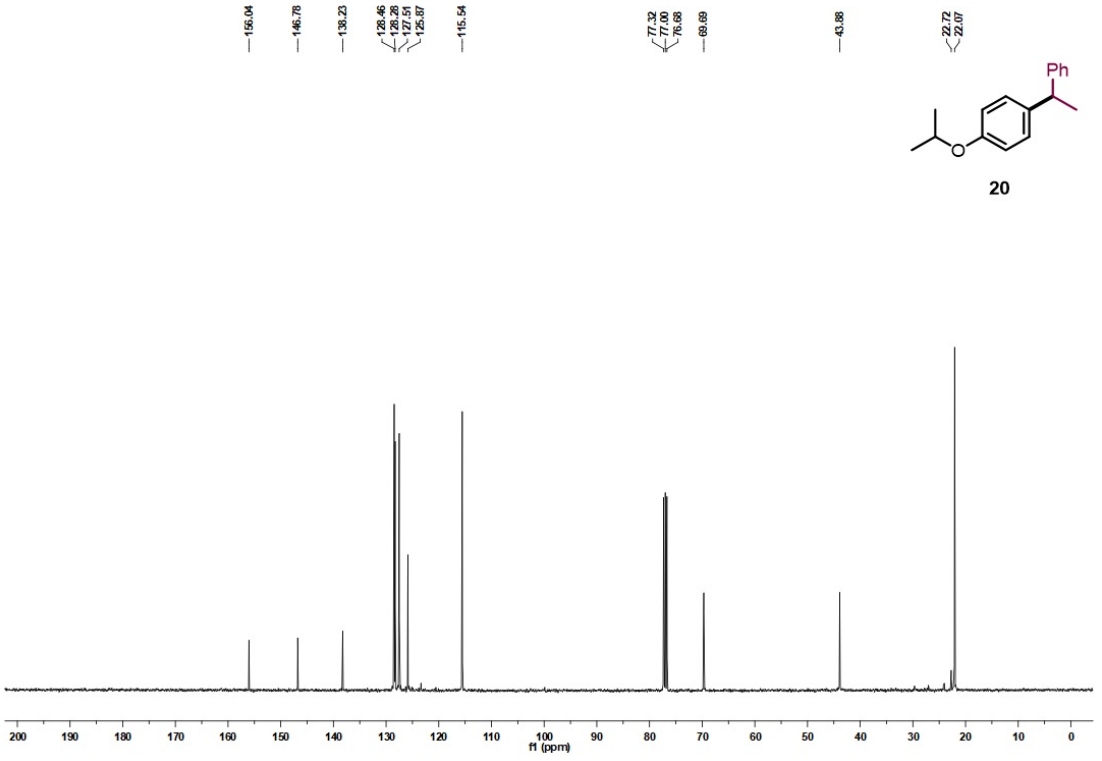
^{13}C-NMR of **19**
$CDCl_3$, 101 MHz, 298 K



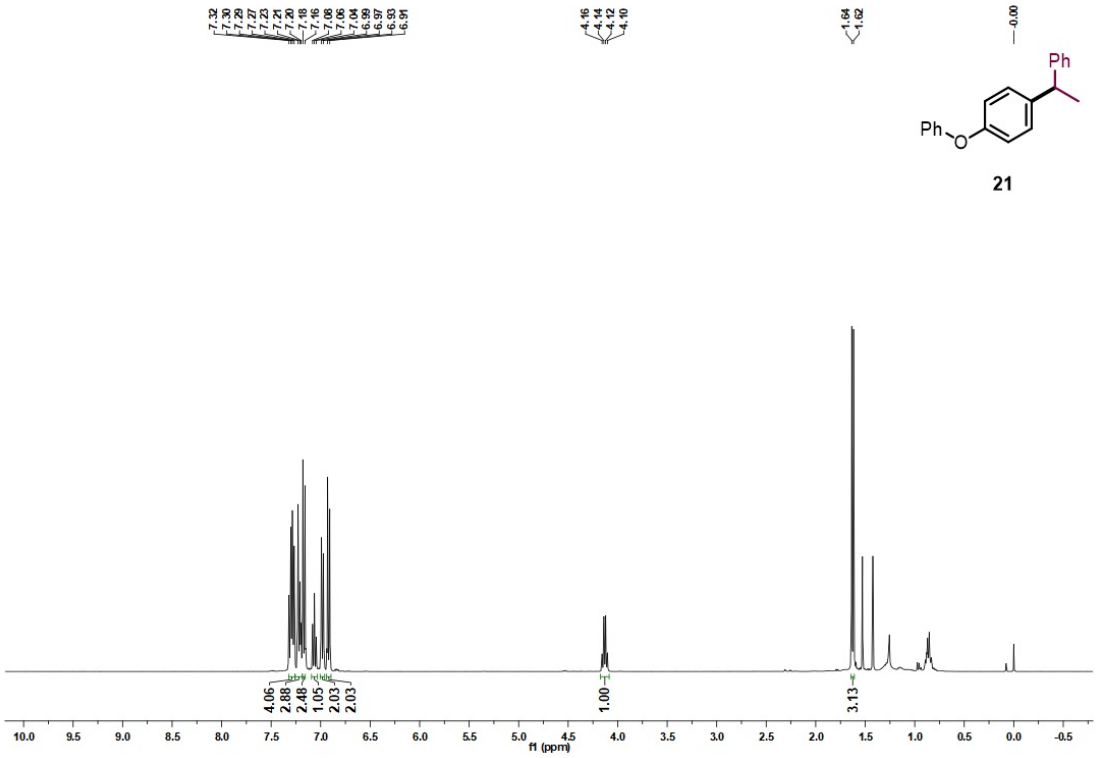
^{1}H-NMR of **20**
$CDCl_3$, 400 MHz, 298 K



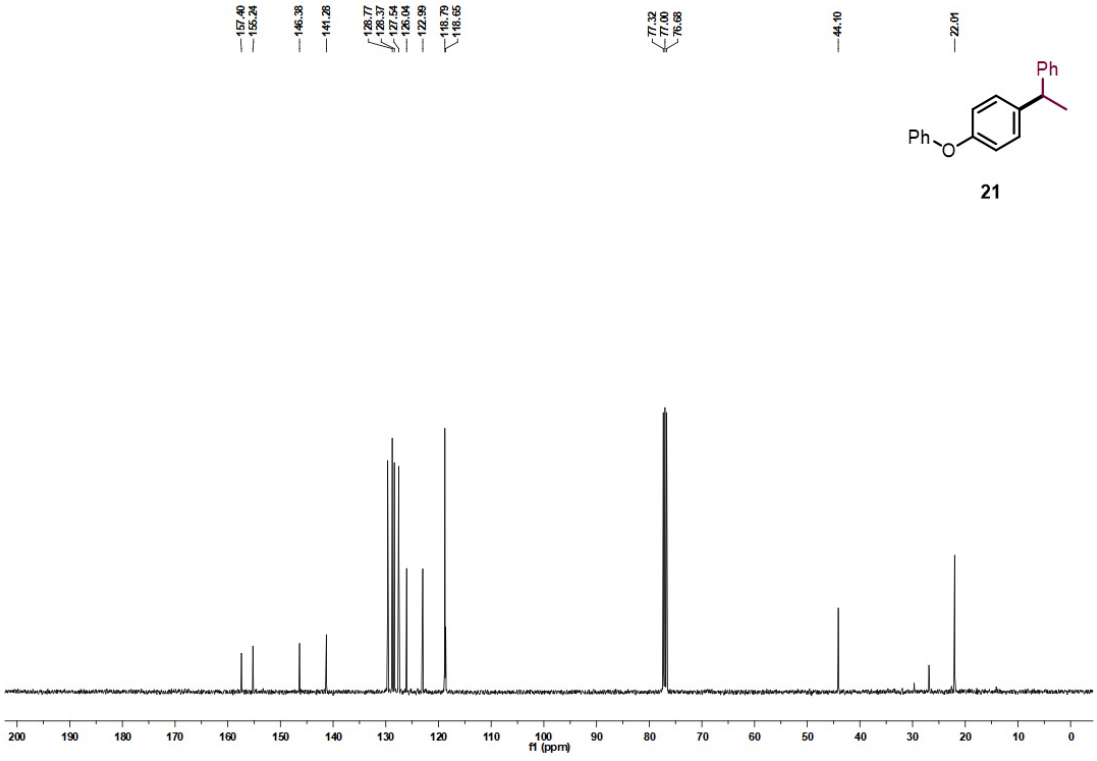
^{13}C-NMR of **20**
$CDCl_3$, 101 MHz, 298 K



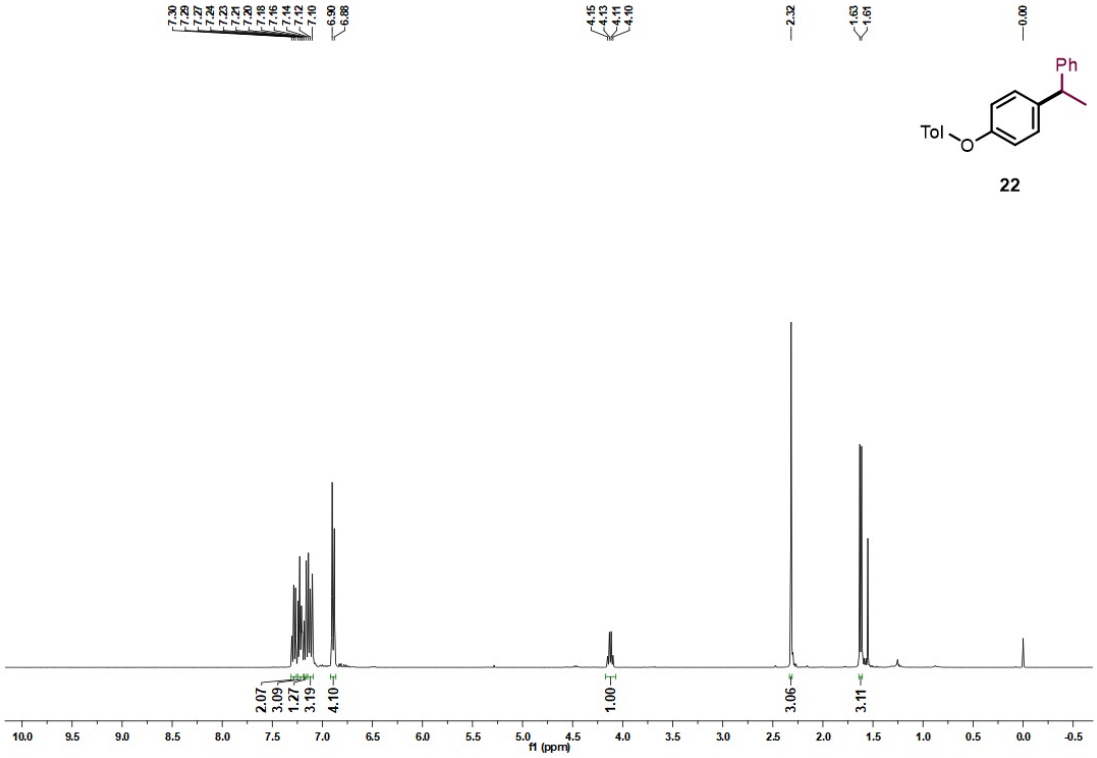
^{1}H-NMR of **21**
$CDCl_3$, 400 MHz, 298 K



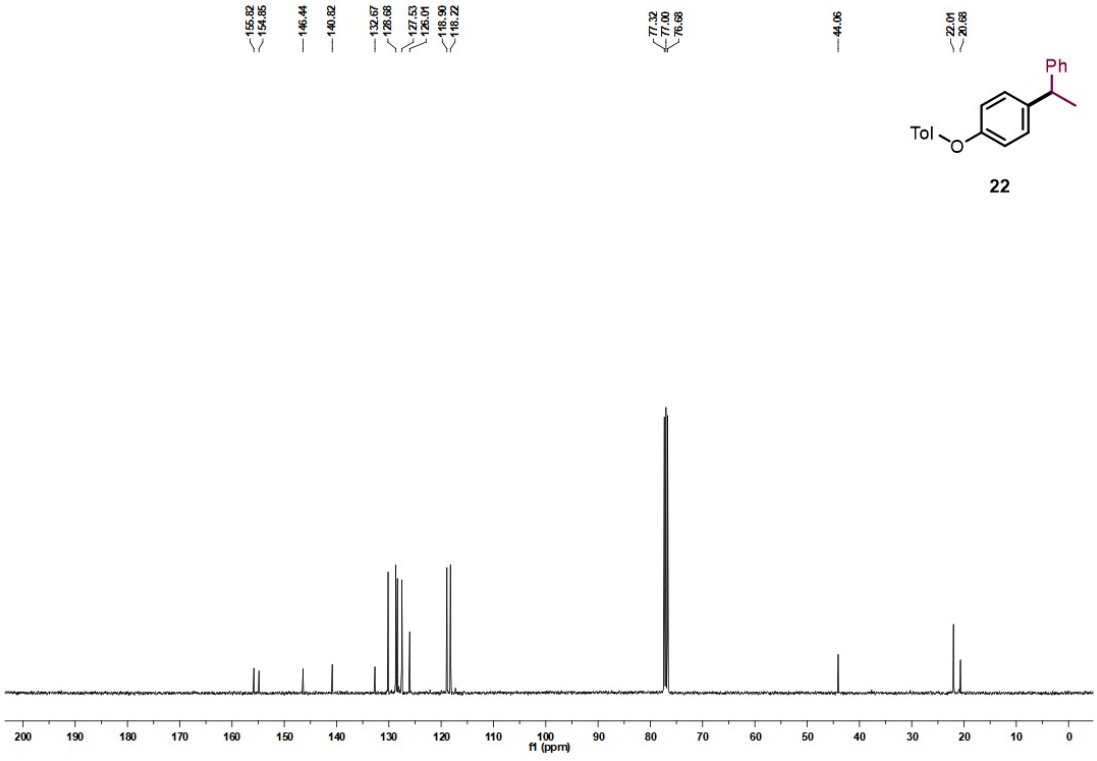
^{13}C-NMR of **21**
$CDCl_3$, 101 MHz, 298 K



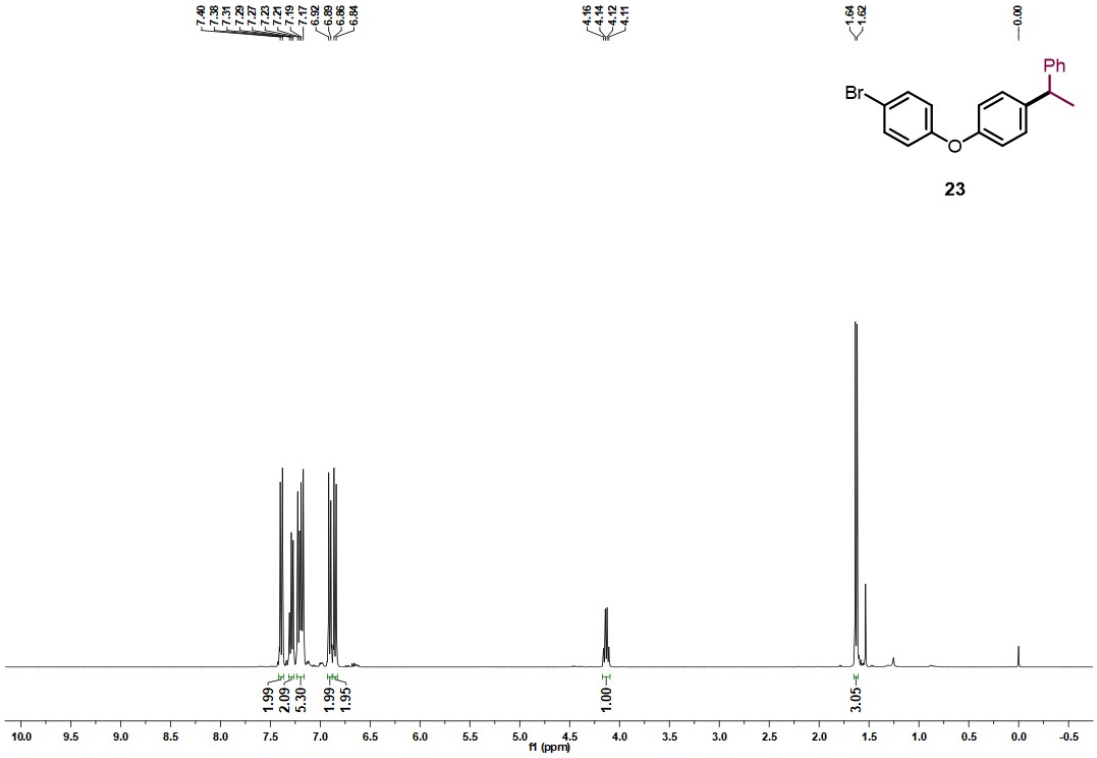
^{1}H-NMR of **22**
$CDCl_3$, 400 MHz, 298 K



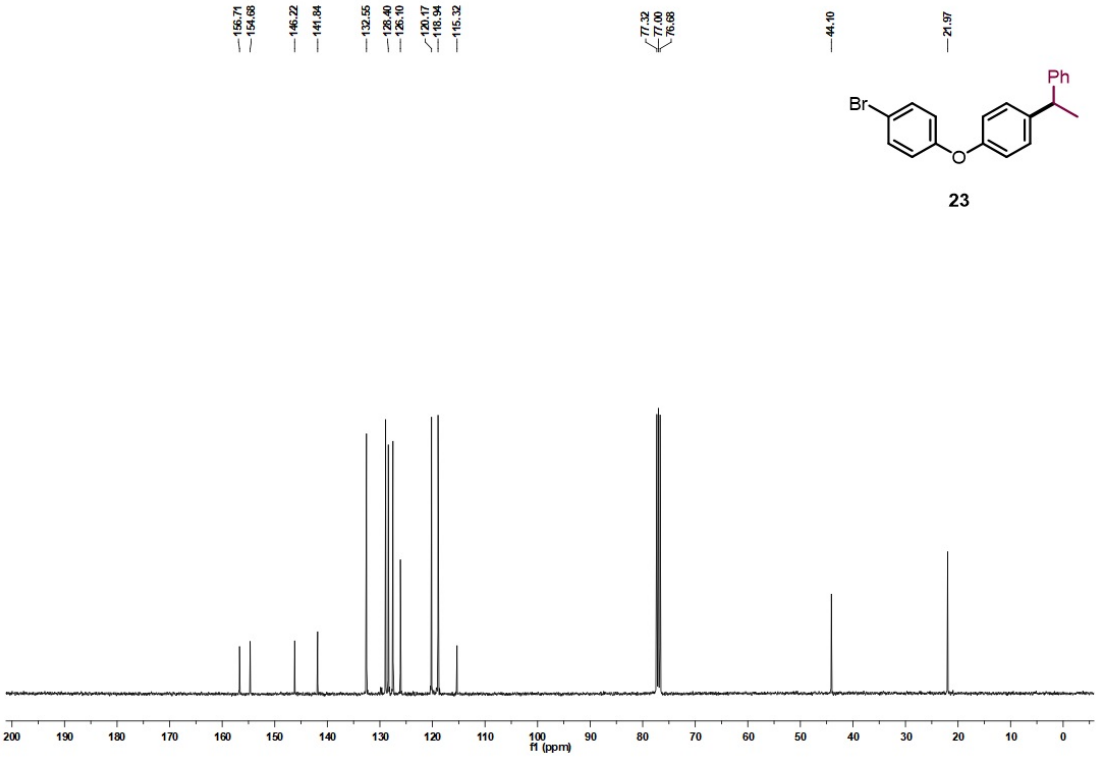
^{13}C-NMR of **22**
$CDCl_3$, 101 MHz, 298 K



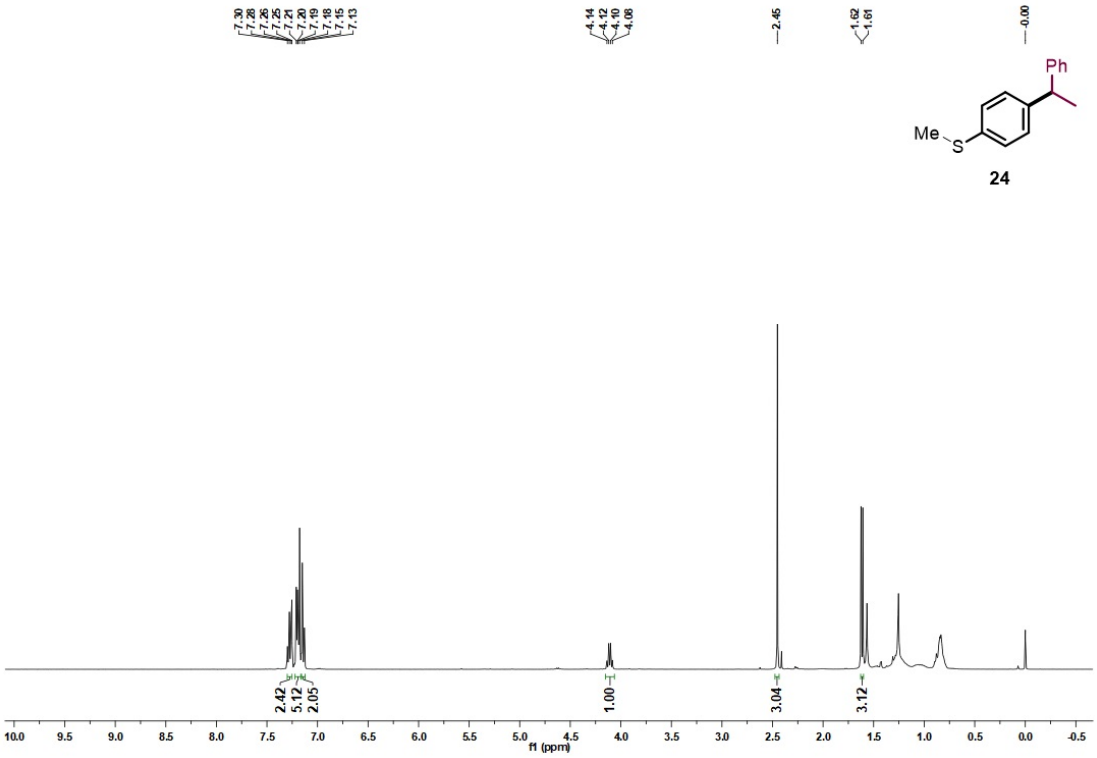
^{1}H-NMR of **23**
$CDCl_3$, 400 MHz, 298 K



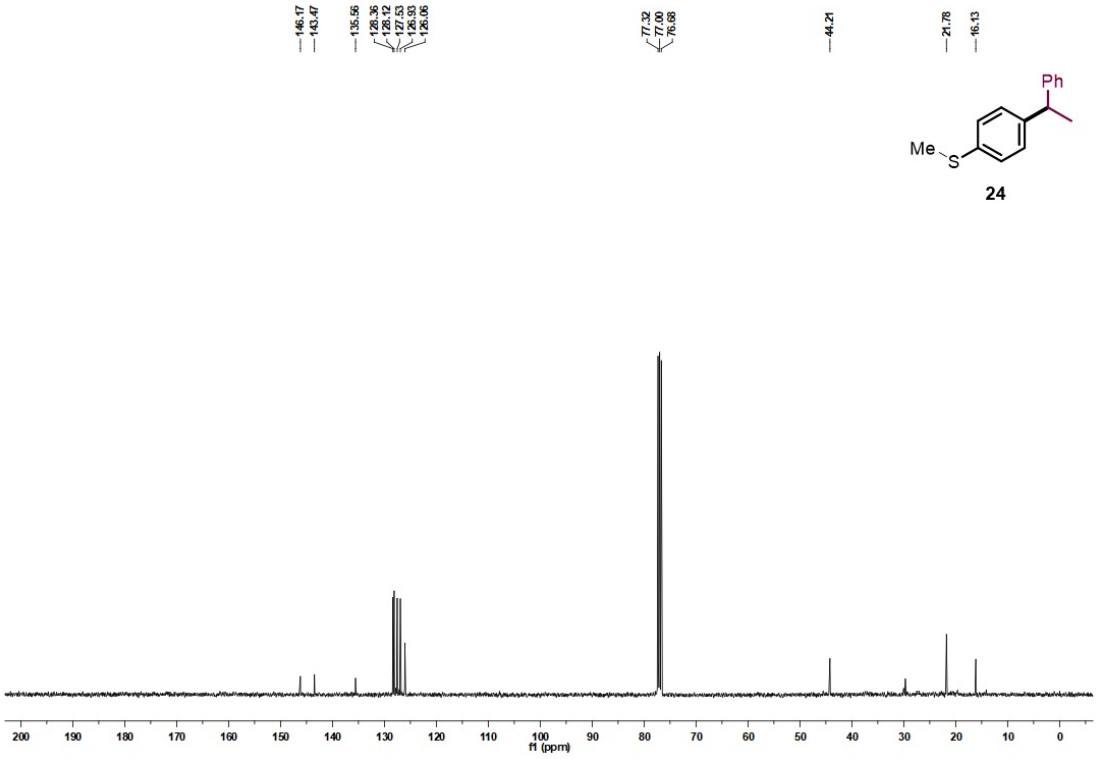
^{13}C-NMR of **23**
$CDCl_3$, 101 MHz, 298 K



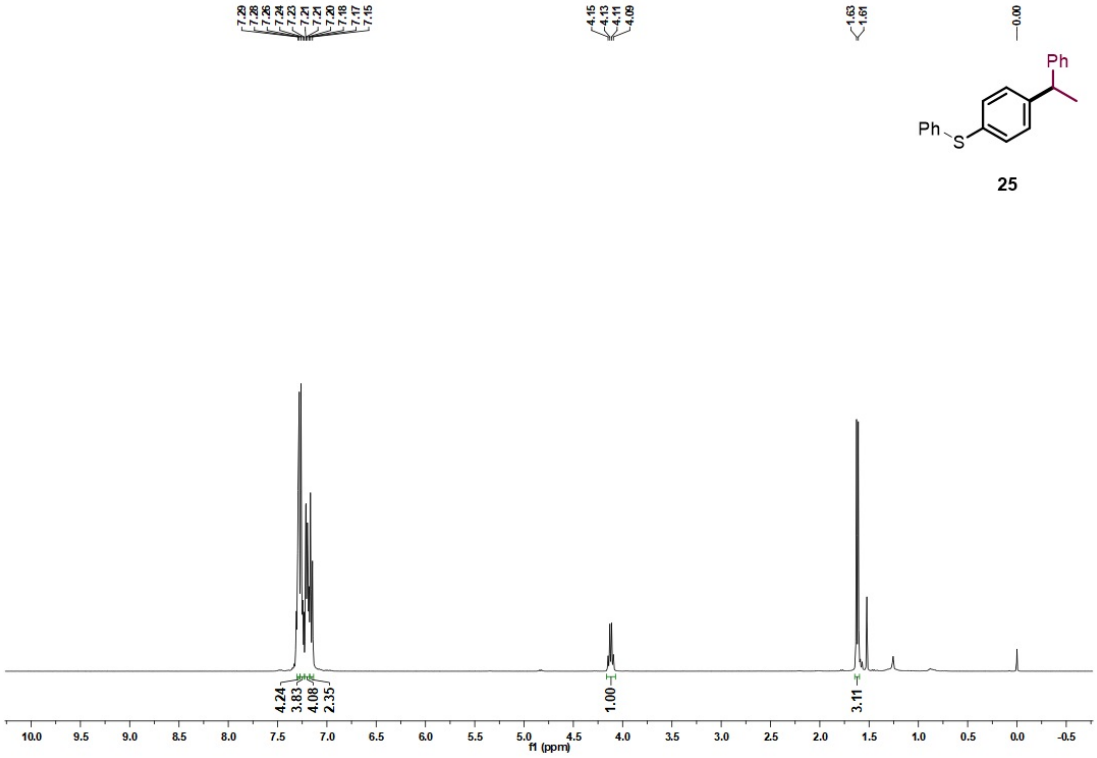
^{1}H-NMR of **24**
$CDCl_3$, 400 MHz, 298 K



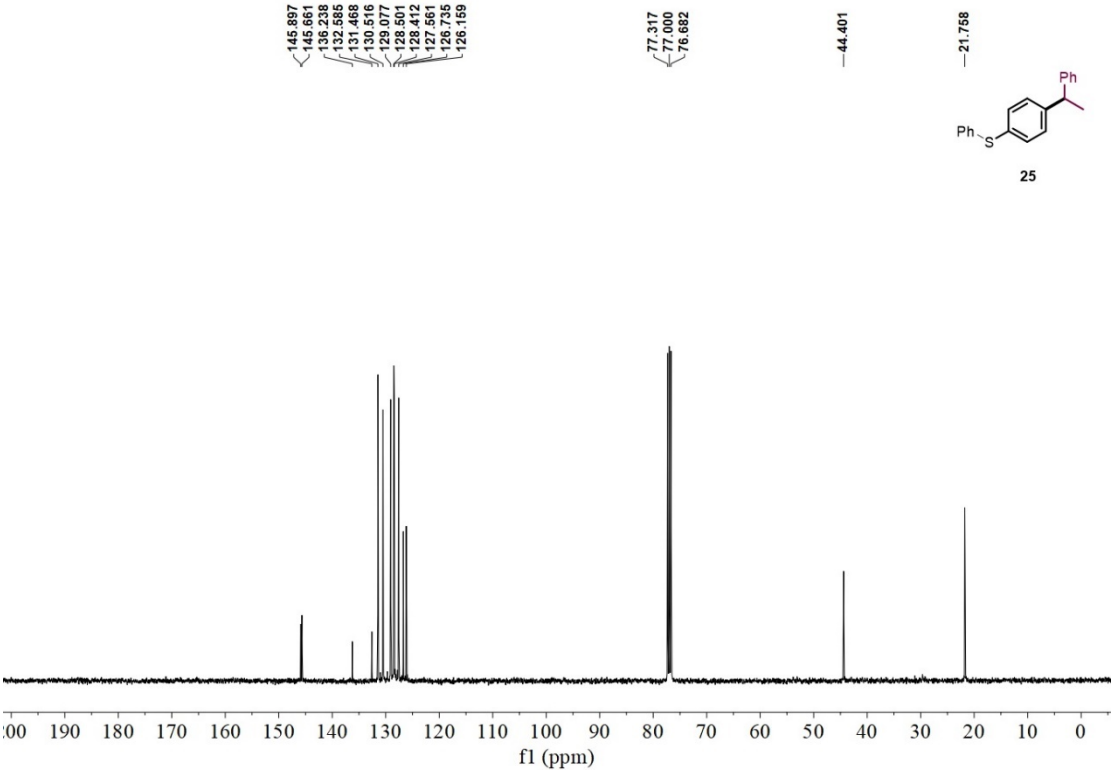
^{13}C-NMR of **24**
$CDCl_3$, 101 MHz, 298 K



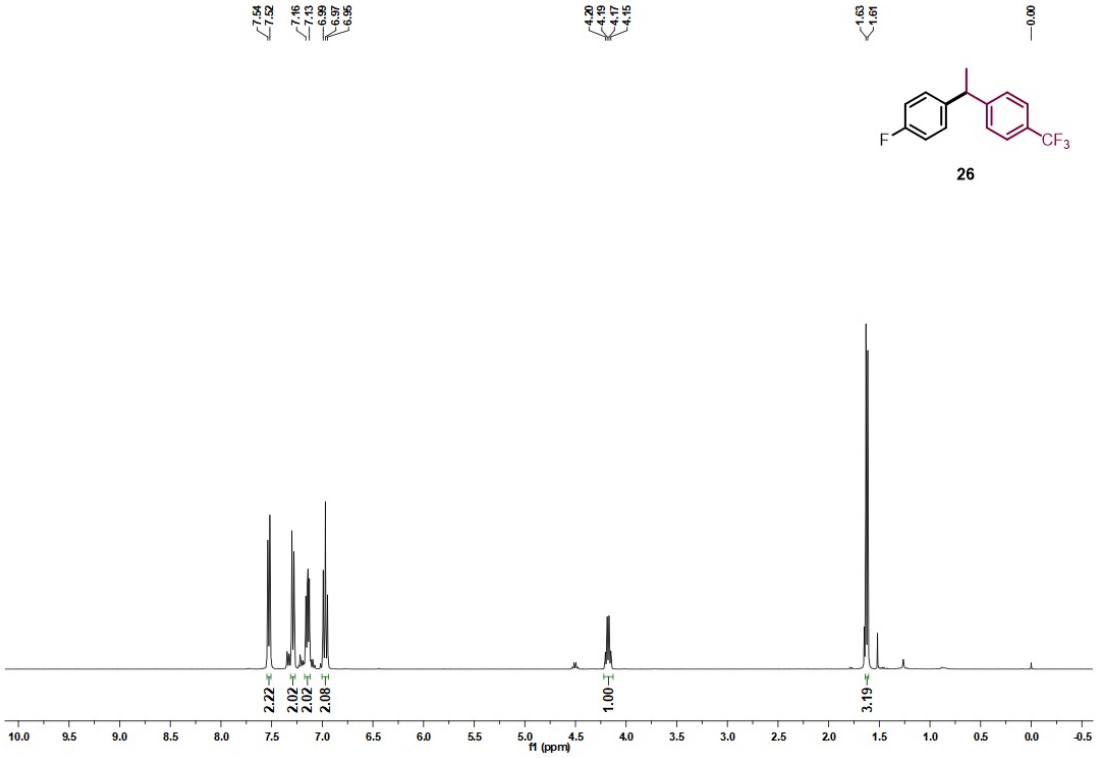
^{1}H-NMR of **25**
$CDCl_3$, 400 MHz, 298 K



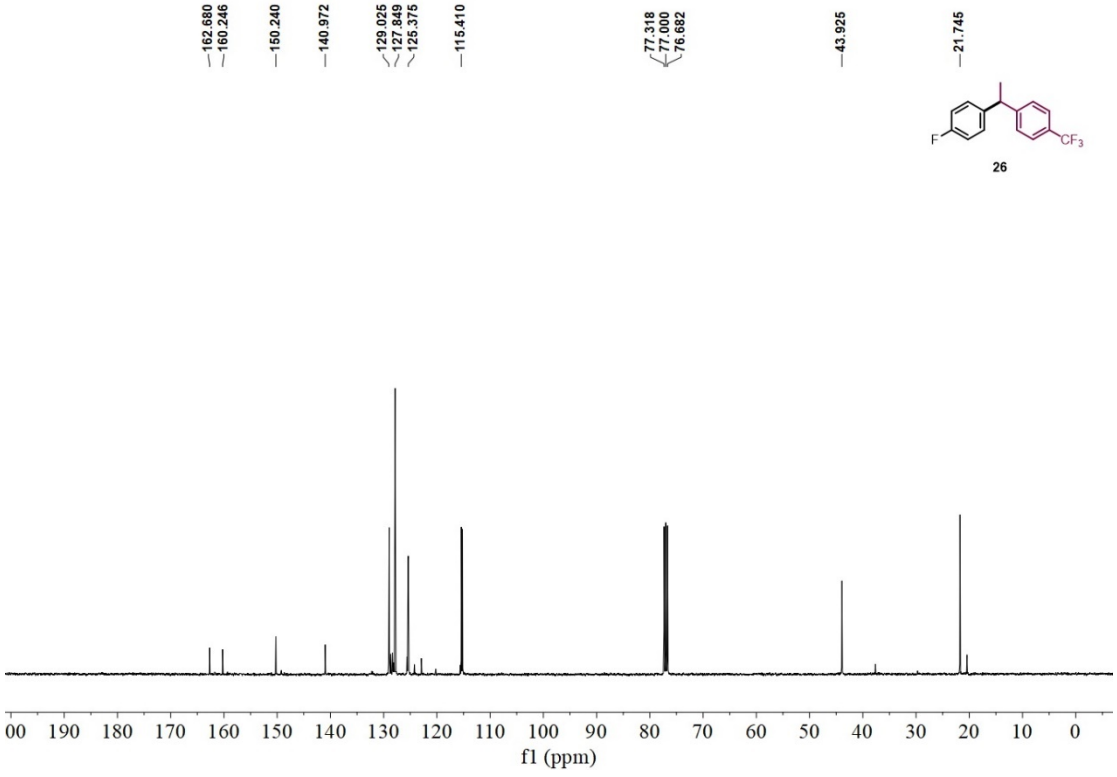
^{13}C-NMR of **25**
$CDCl_3$, 101 MHz, 298 K



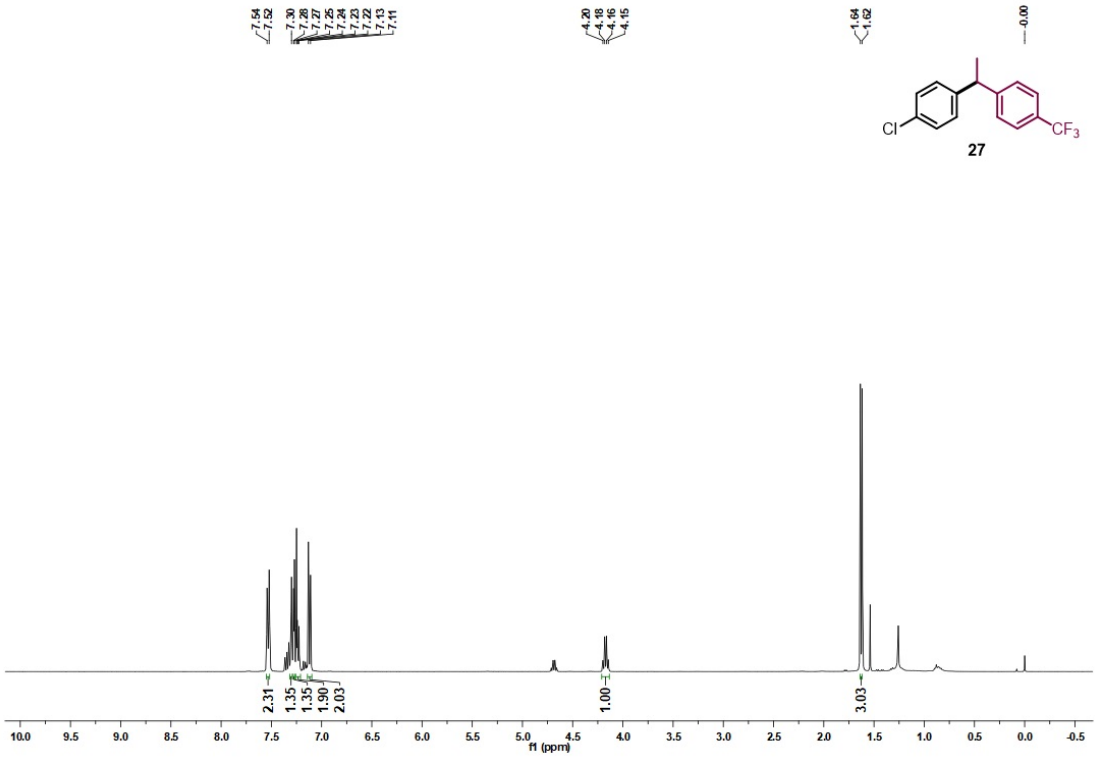
^{1}H-NMR of **26**
$CDCl_3$, 400 MHz, 298 K



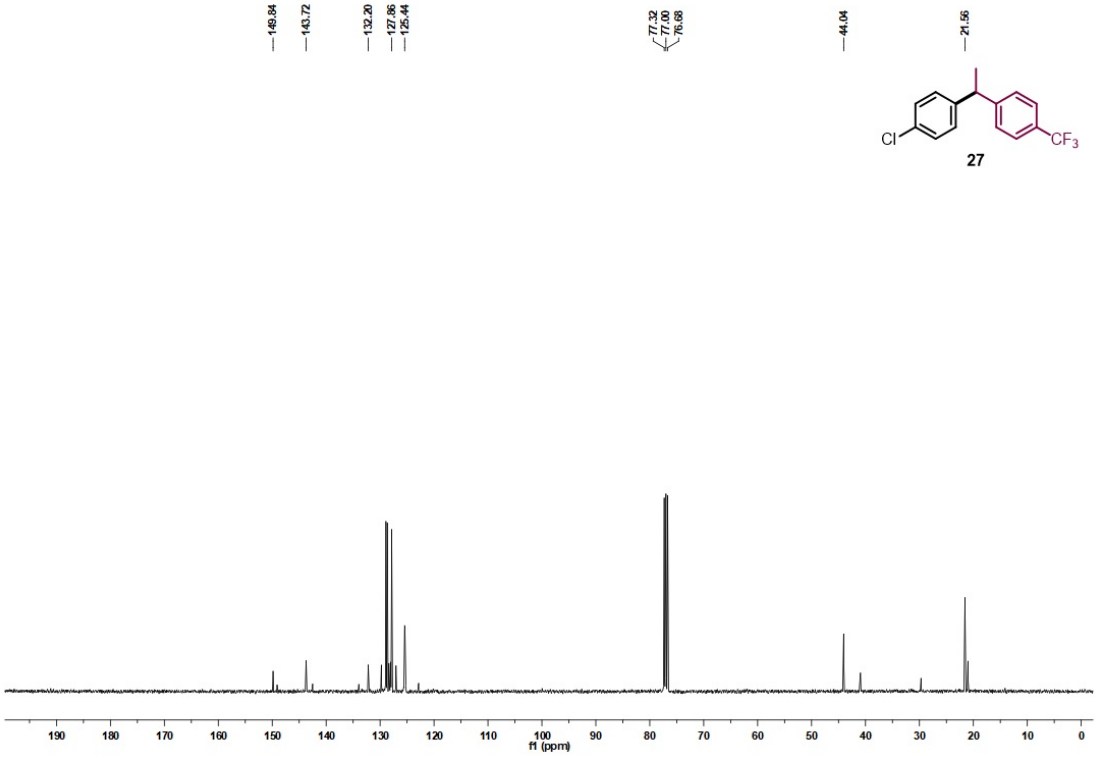
^{13}C-NMR of **26**
$CDCl_3$, 101 MHz, 298 K



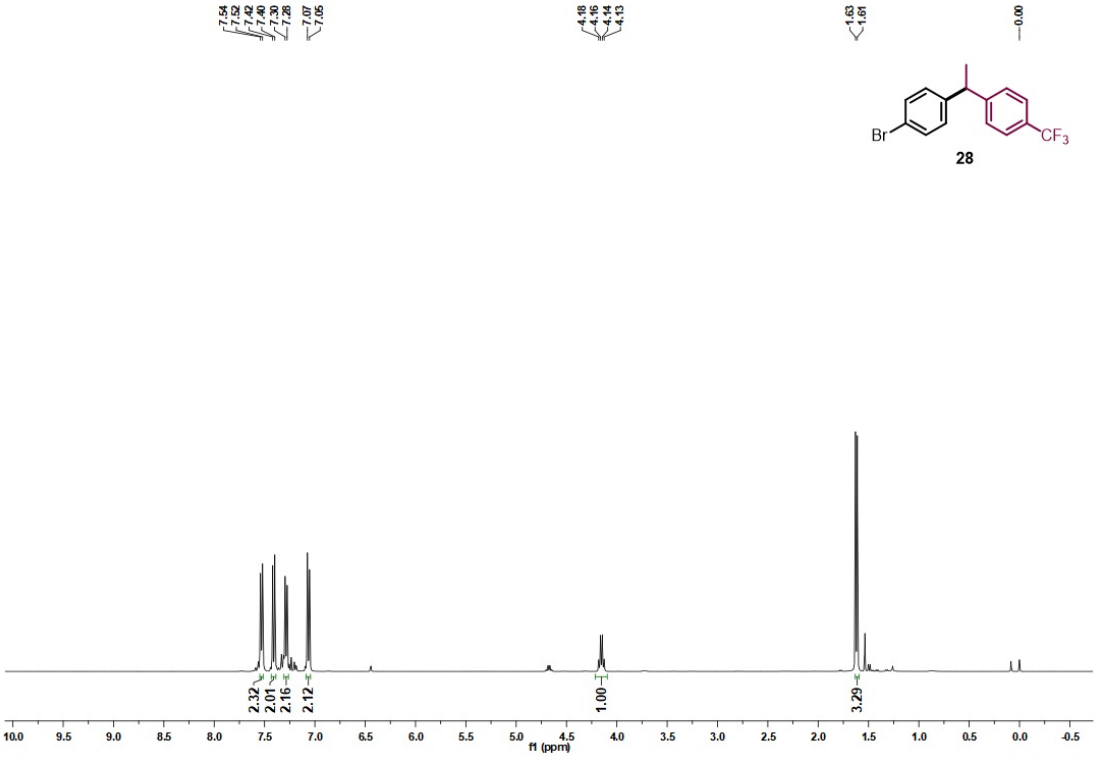
^{1}H-NMR of **27**
$CDCl_3$, 400 MHz, 298 K



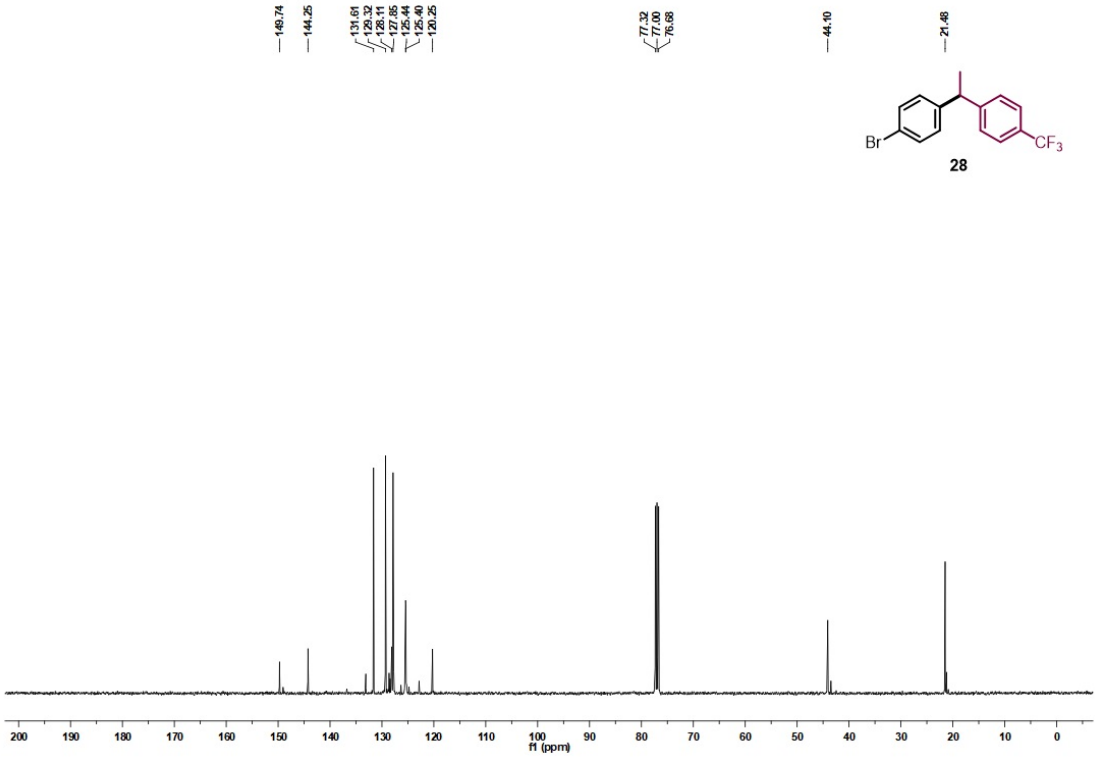
^{13}C-NMR of **27**
$CDCl_3$, 101 MHz, 298 K



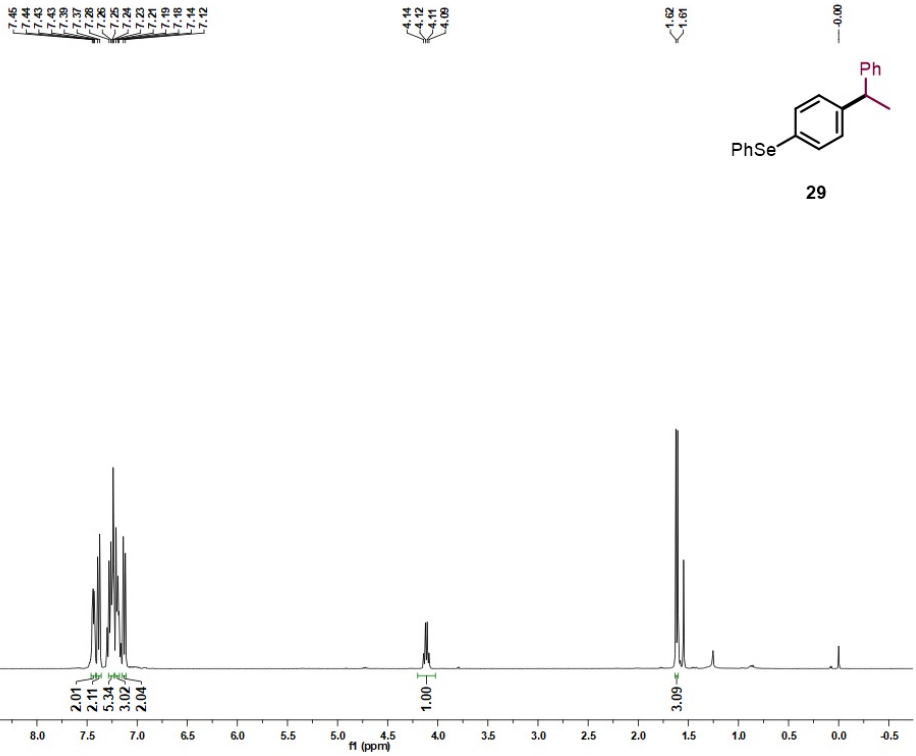
^{1}H-NMR of **28**
$CDCl_3$, 400 MHz, 298 K



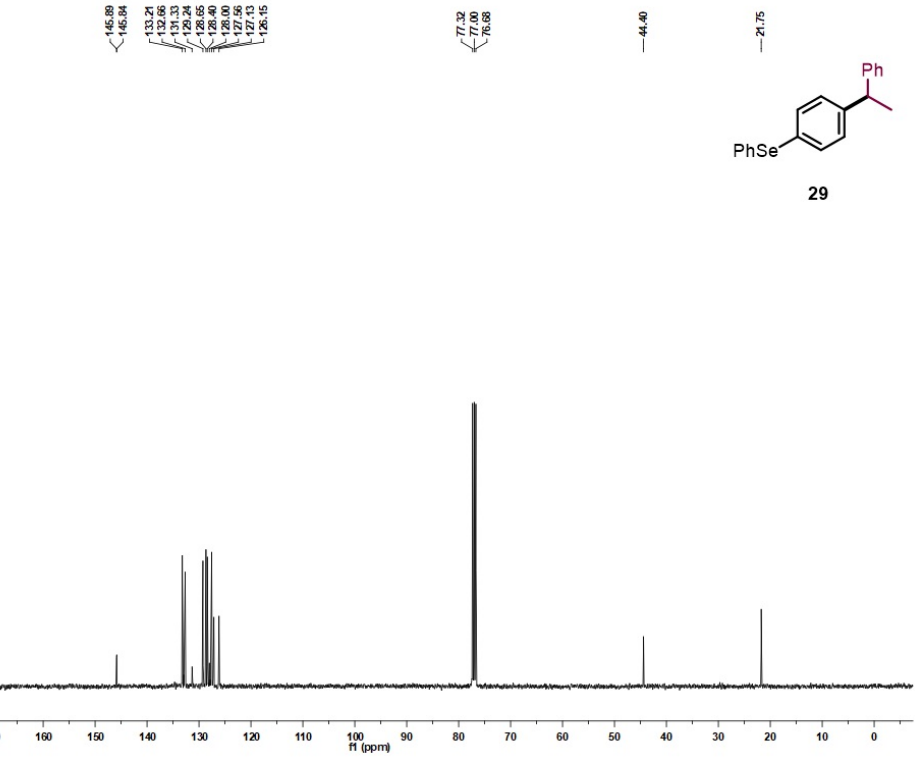
^{13}C-NMR of **28**
$CDCl_3$, 101 MHz, 298 K



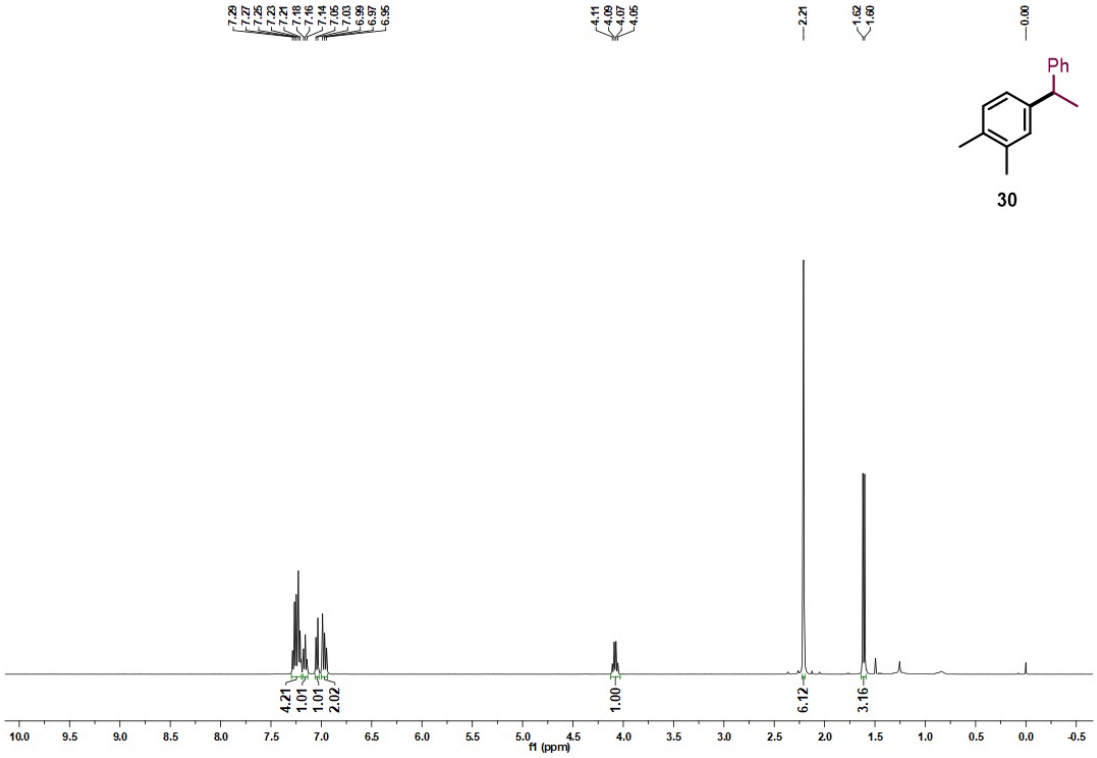
^{1}H-NMR of **29**
$CDCl_3$, 400 MHz, 298 K



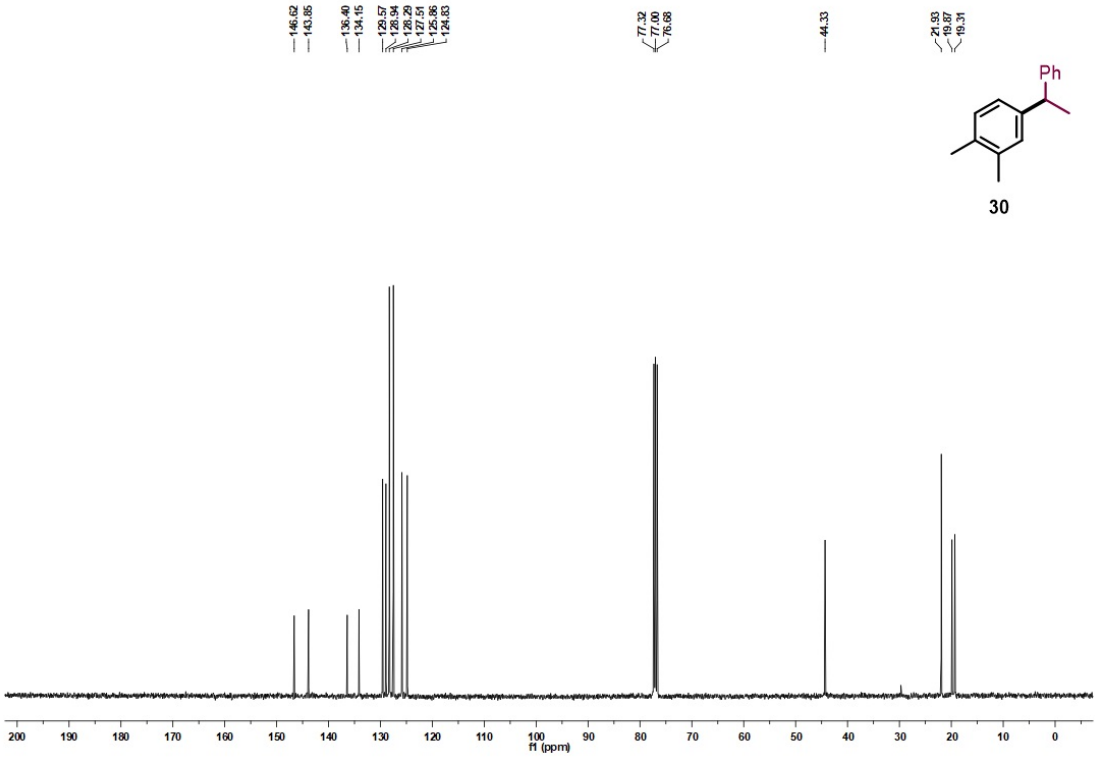
^{13}C-NMR of **29**
$CDCl_3$, 101 MHz, 298 K



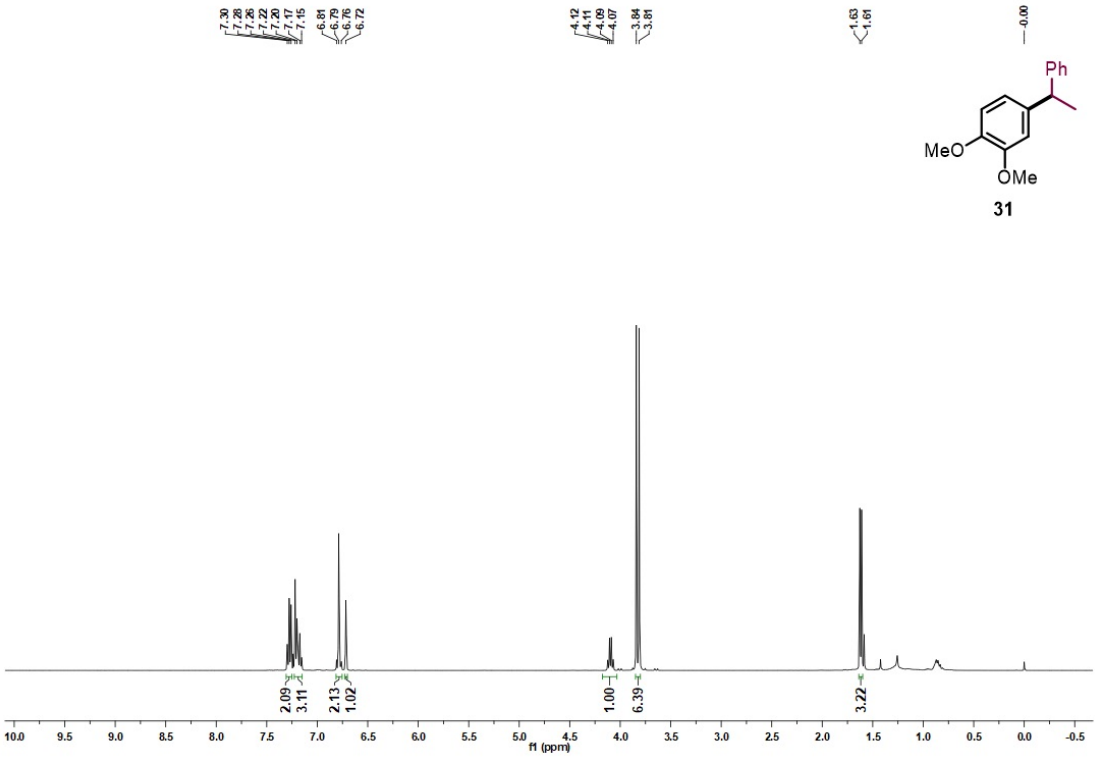
^{1}H-NMR of **30**
$CDCl_3$, 400 MHz, 298 K



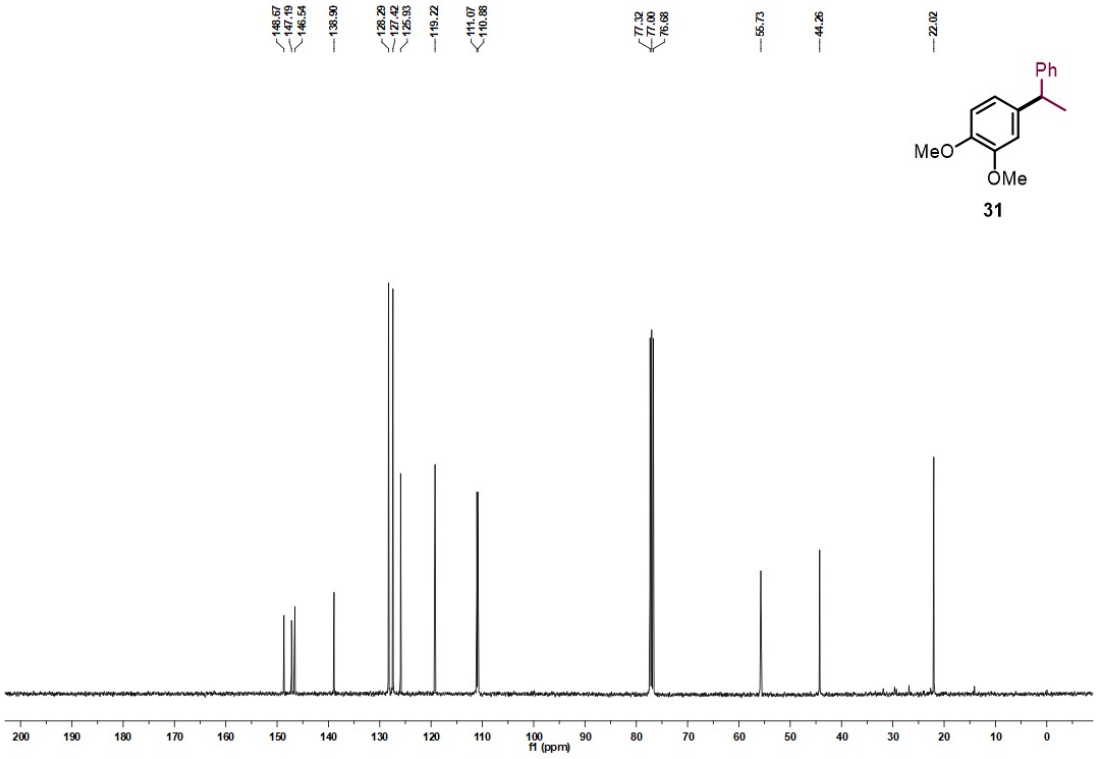
^{13}C-NMR of **30**
$CDCl_3$, 101 MHz, 298 K



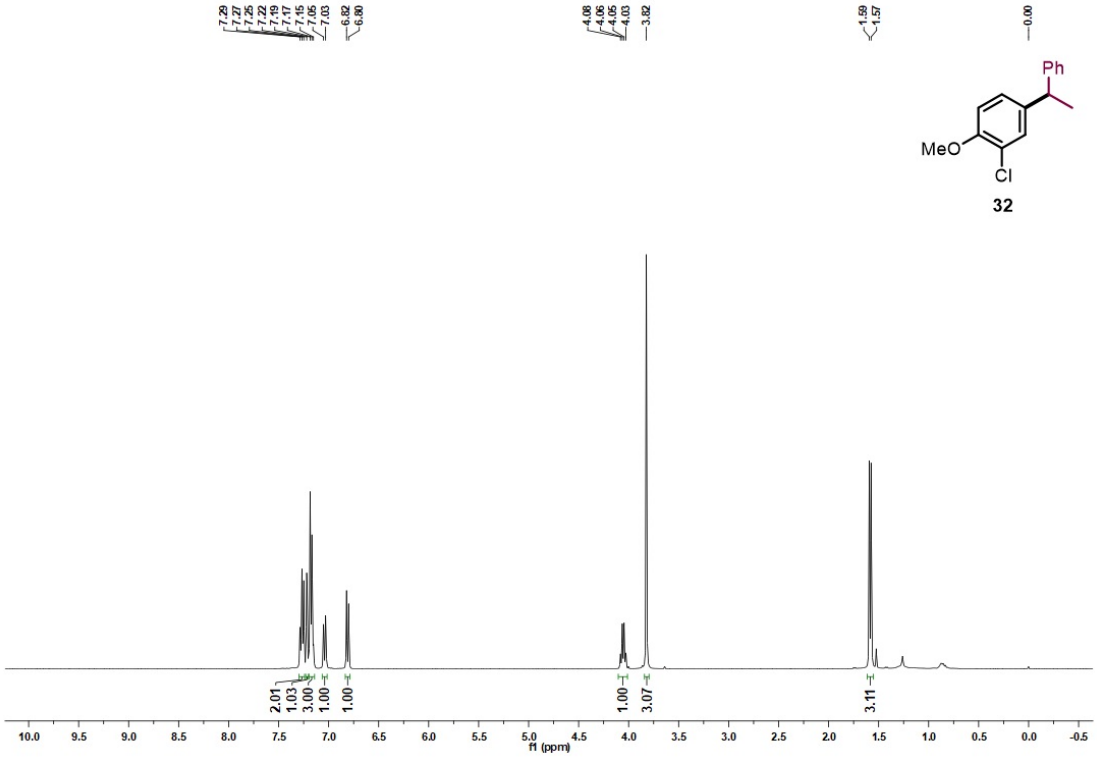
^{1}H-NMR of **31**
$CDCl_3$, 400 MHz, 298 K



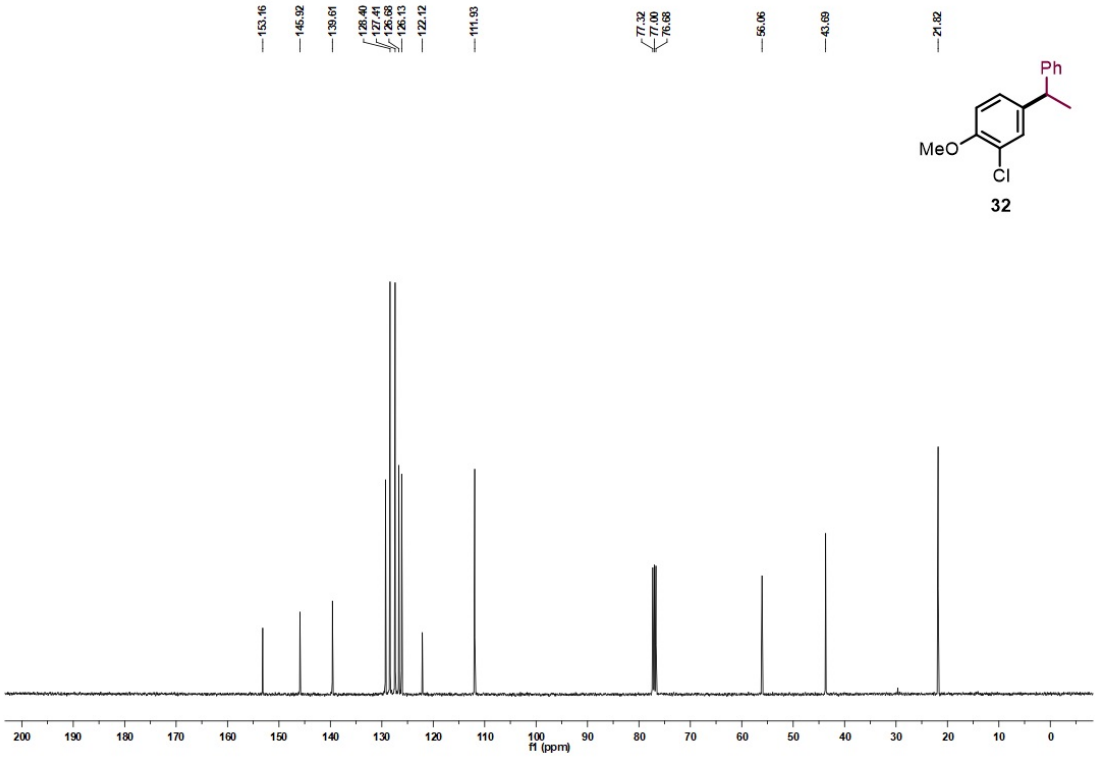
^{13}C-NMR of **31**
$CDCl_3$, 101 MHz, 298 K



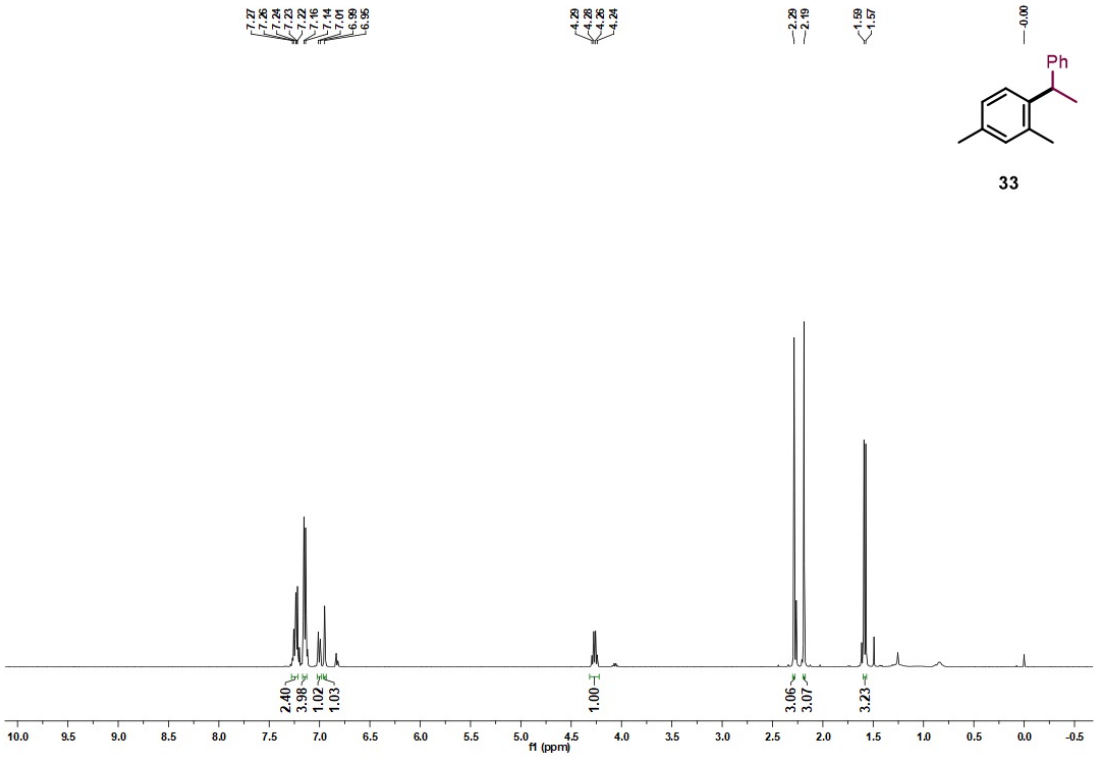
^{1}H-NMR of **32**
$CDCl_3$, 400 MHz, 298 K



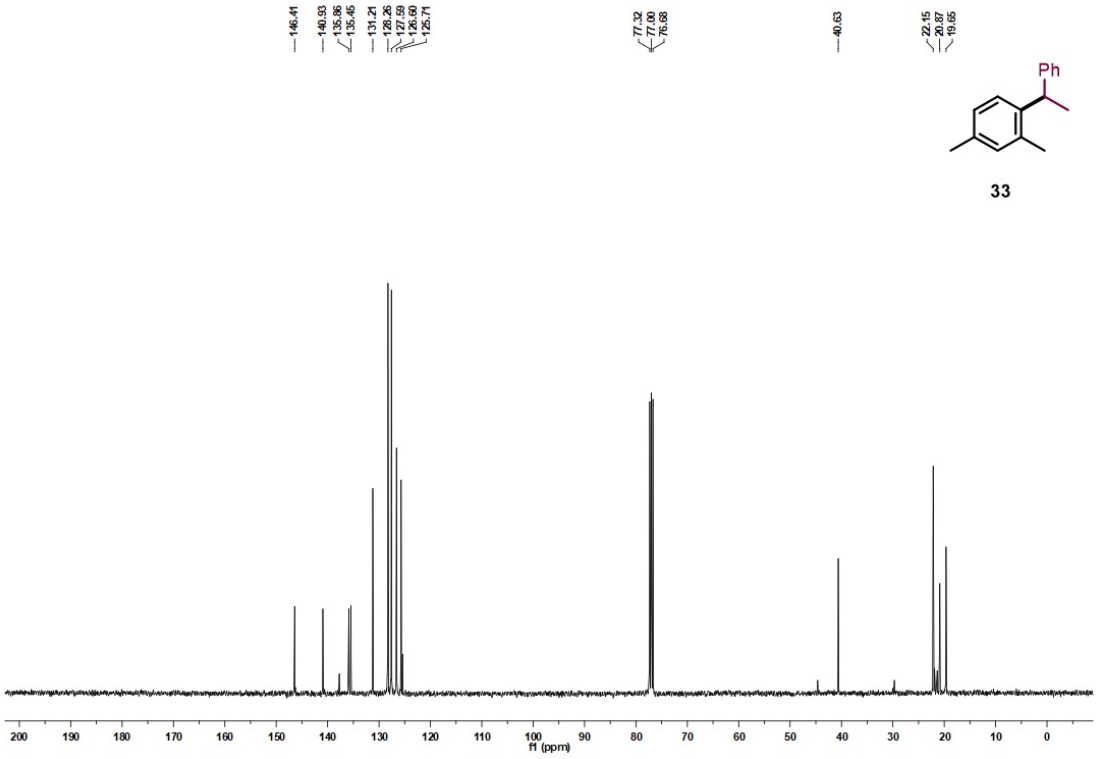
^{13}C-NMR of **32**
$CDCl_3$, 101 MHz, 298 K



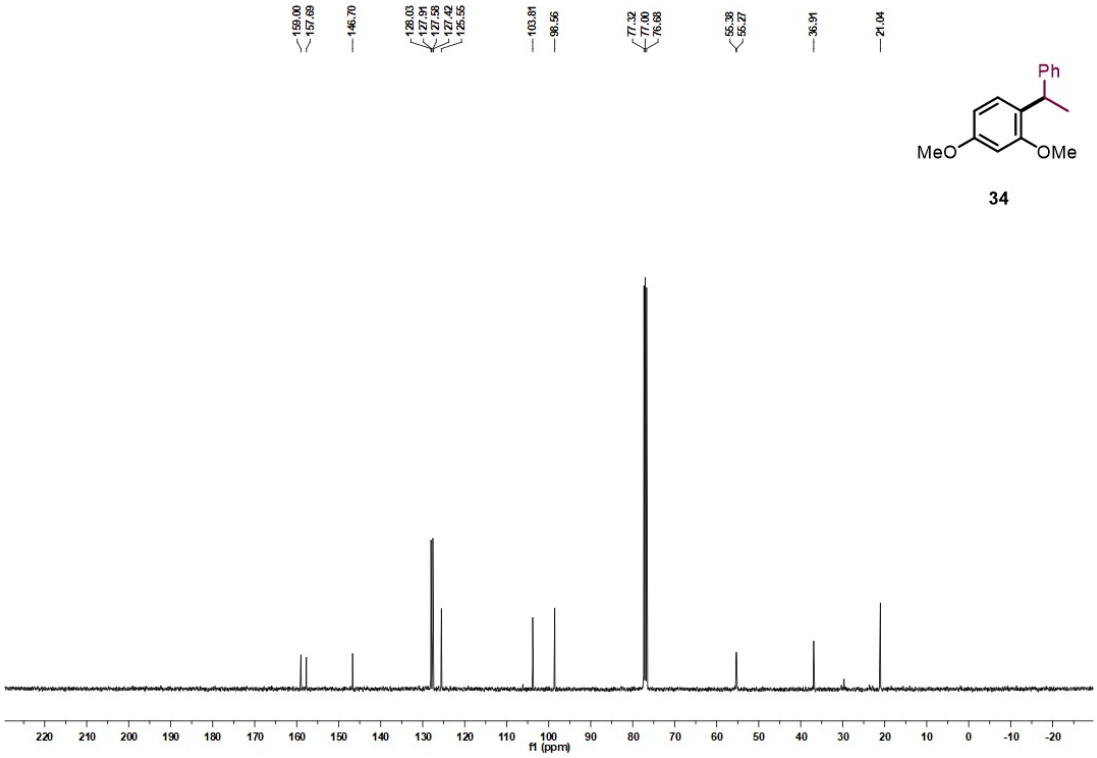
^{1}H-NMR of **33**
$CDCl_3$, 400 MHz, 298 K



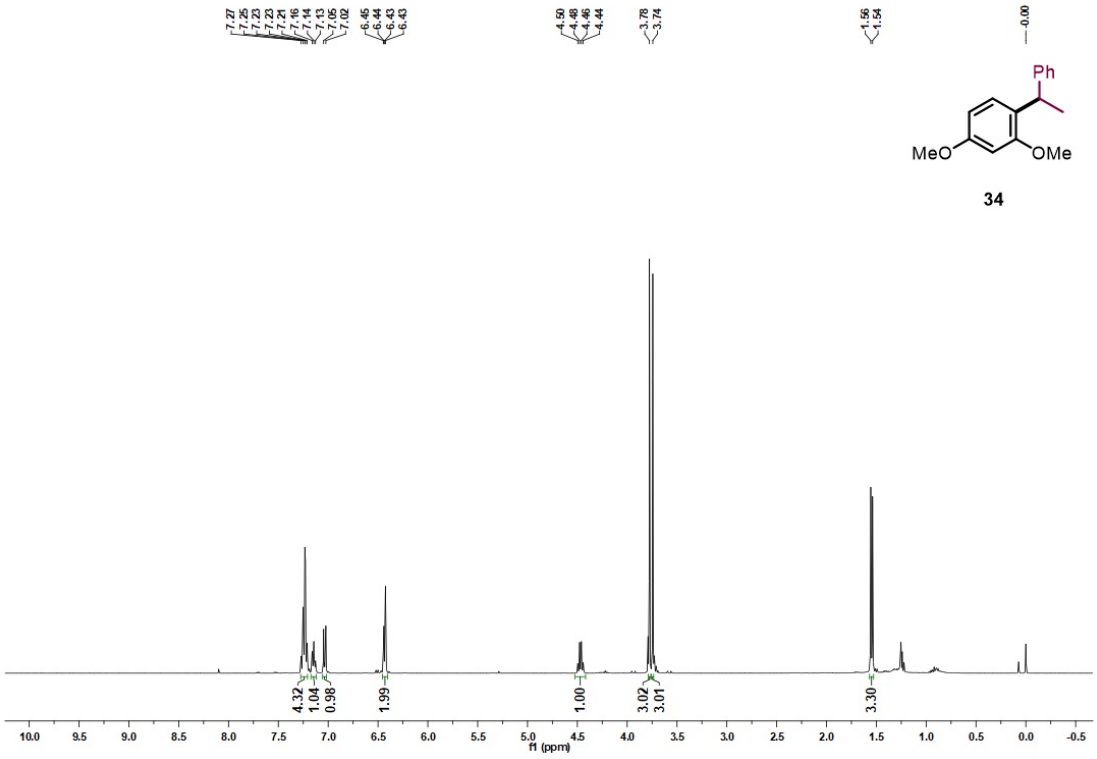
^{13}C-NMR of **33**
$CDCl_3$, 101 MHz, 298 K



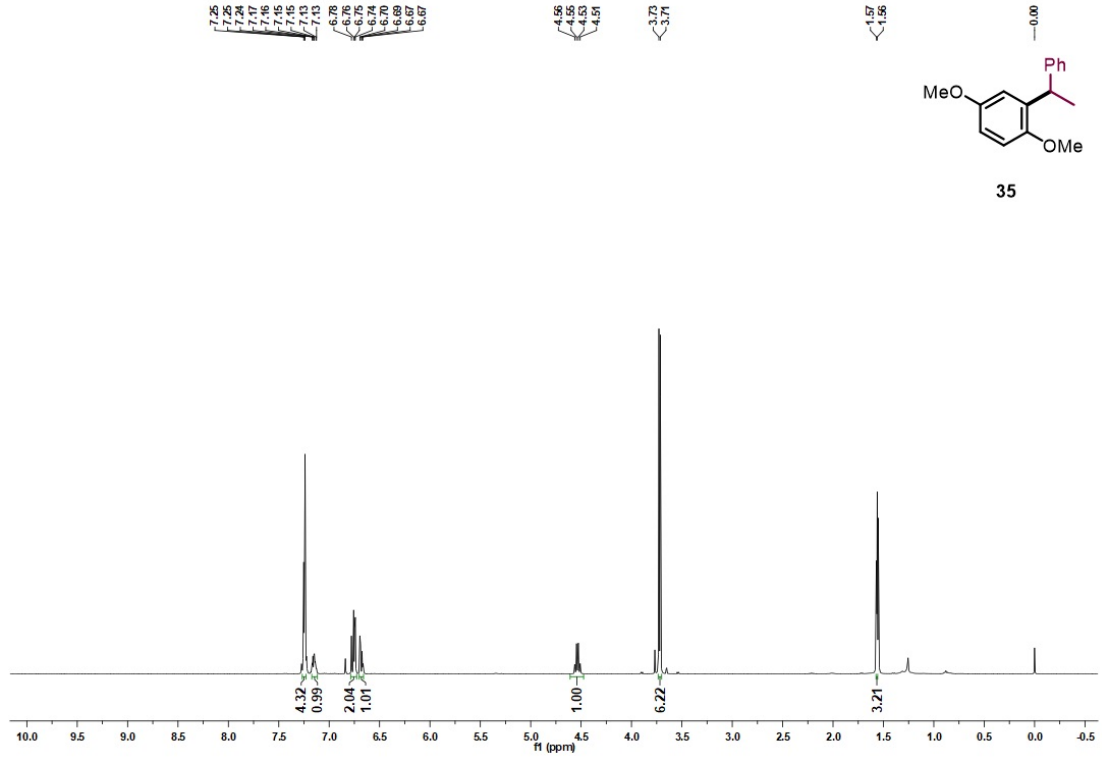
^{1}H-NMR of **34**
$CDCl_3$, 400 MHz, 298 K



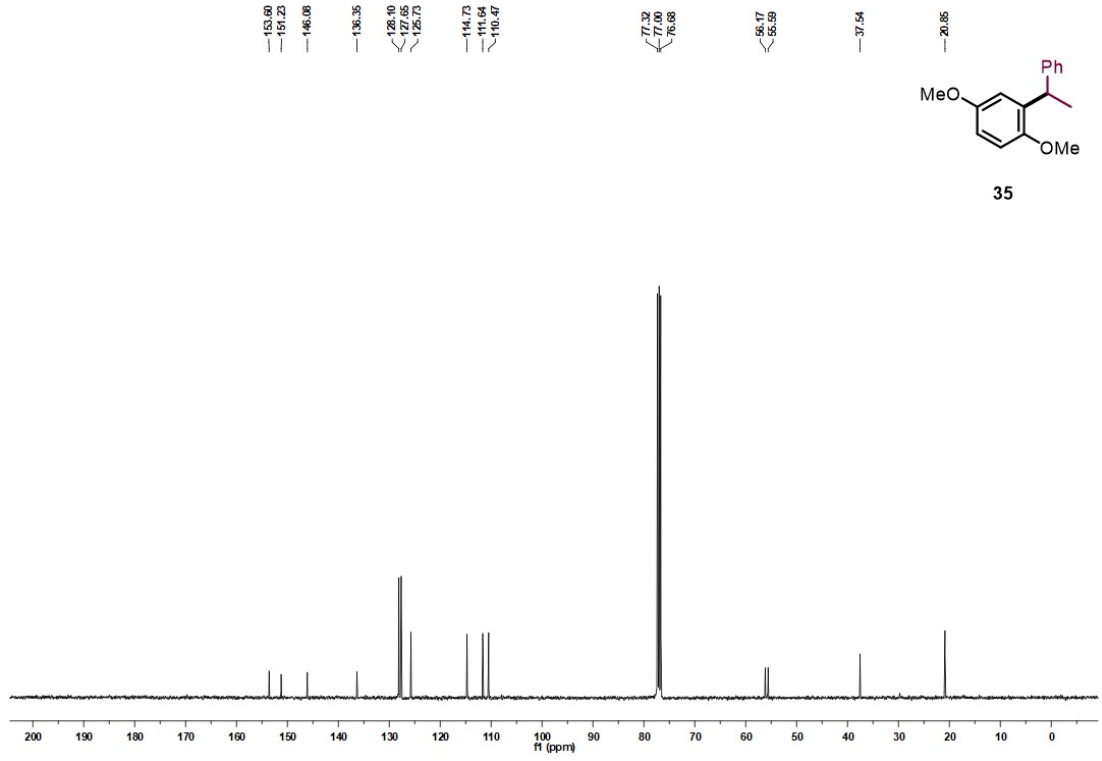
^{13}C-NMR of **34**
$CDCl_3$, 101 MHz, 298 K



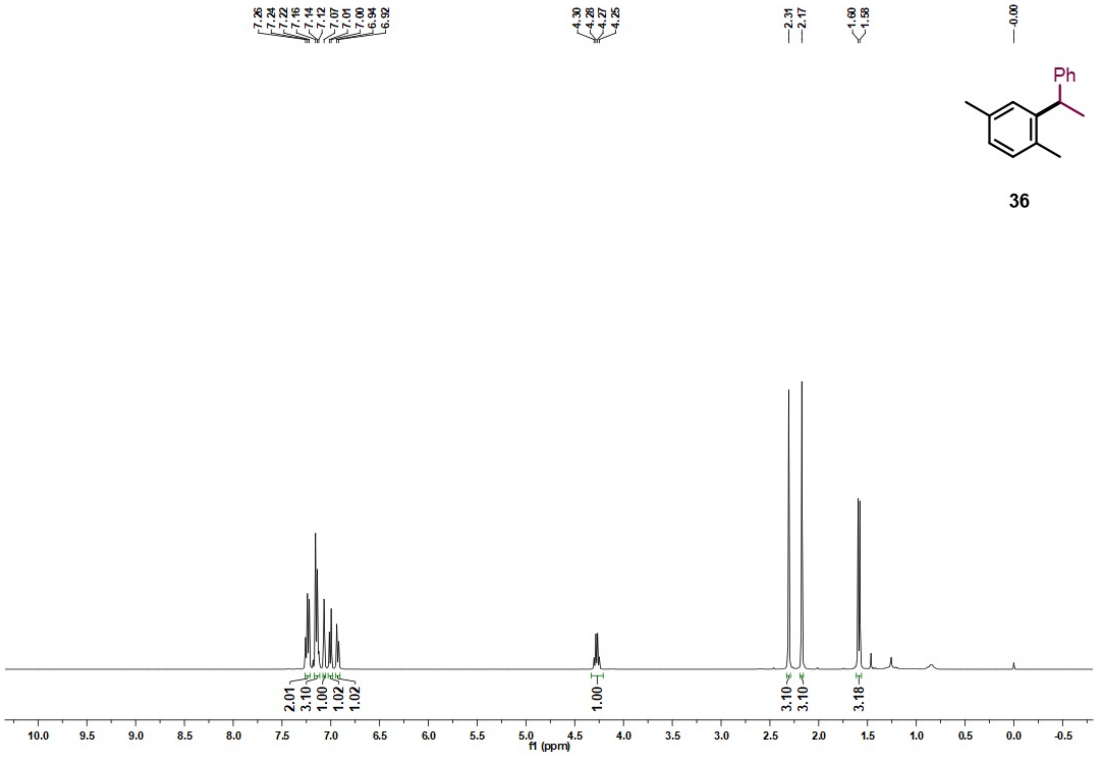
^{1}H-NMR of **35**
$CDCl_3$, 400 MHz, 298 K



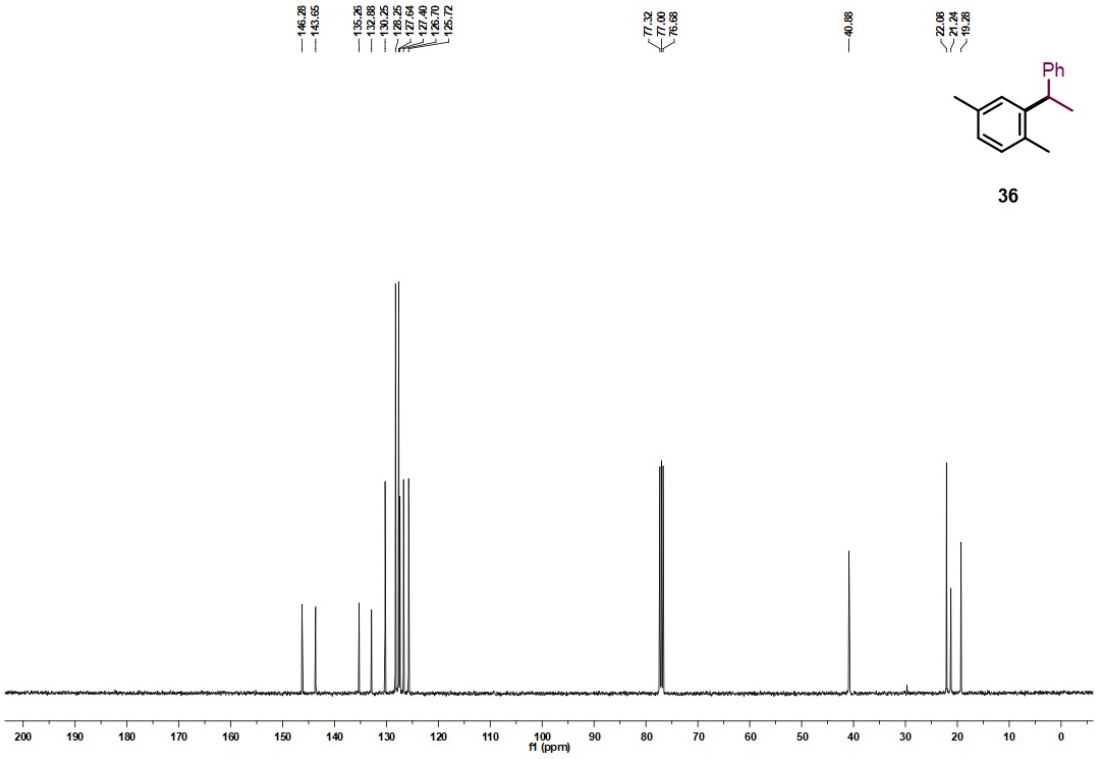
^{13}C-NMR of **35**
$CDCl_3$, 101 MHz, 298 K



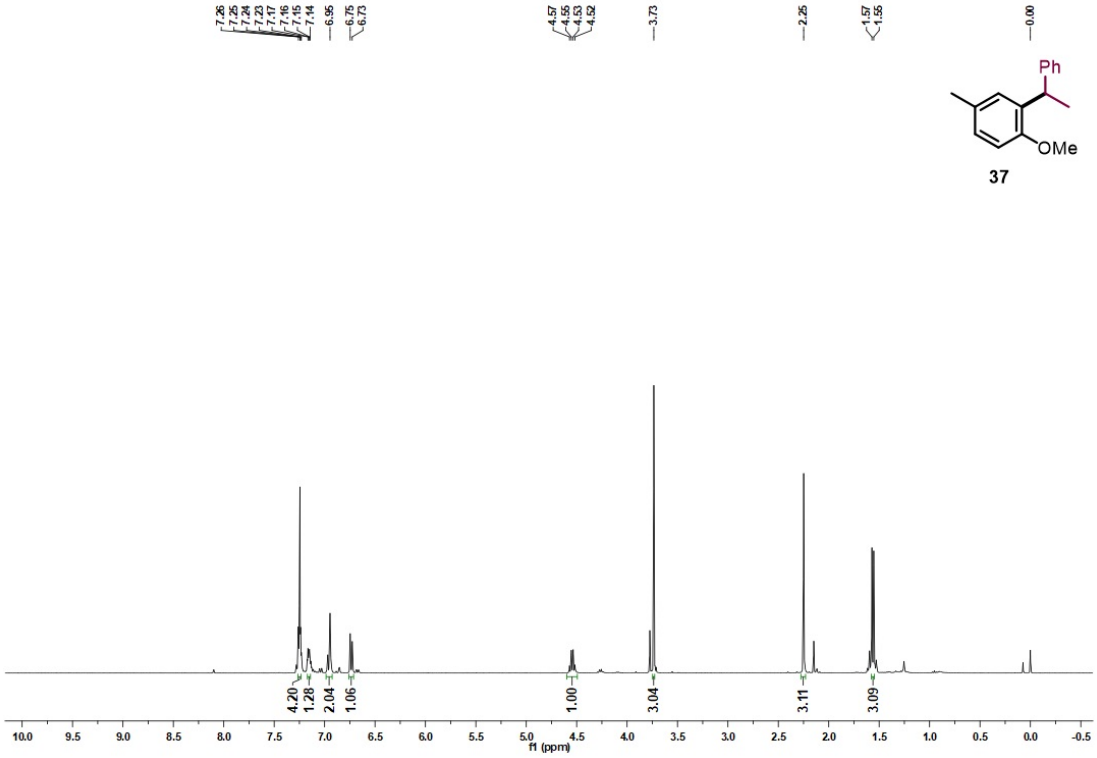
^{1}H-NMR of **36**
$CDCl_3$, 400 MHz, 298 K



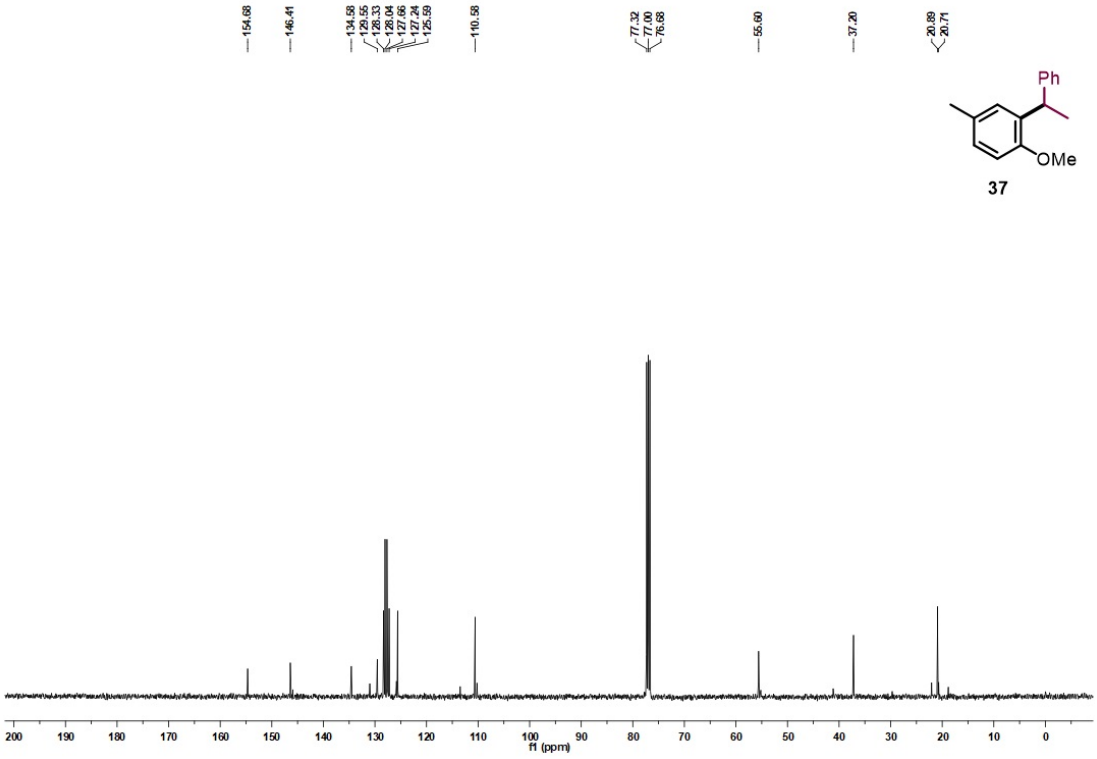
^{13}C-NMR of **36**
$CDCl_3$, 101 MHz, 298 K



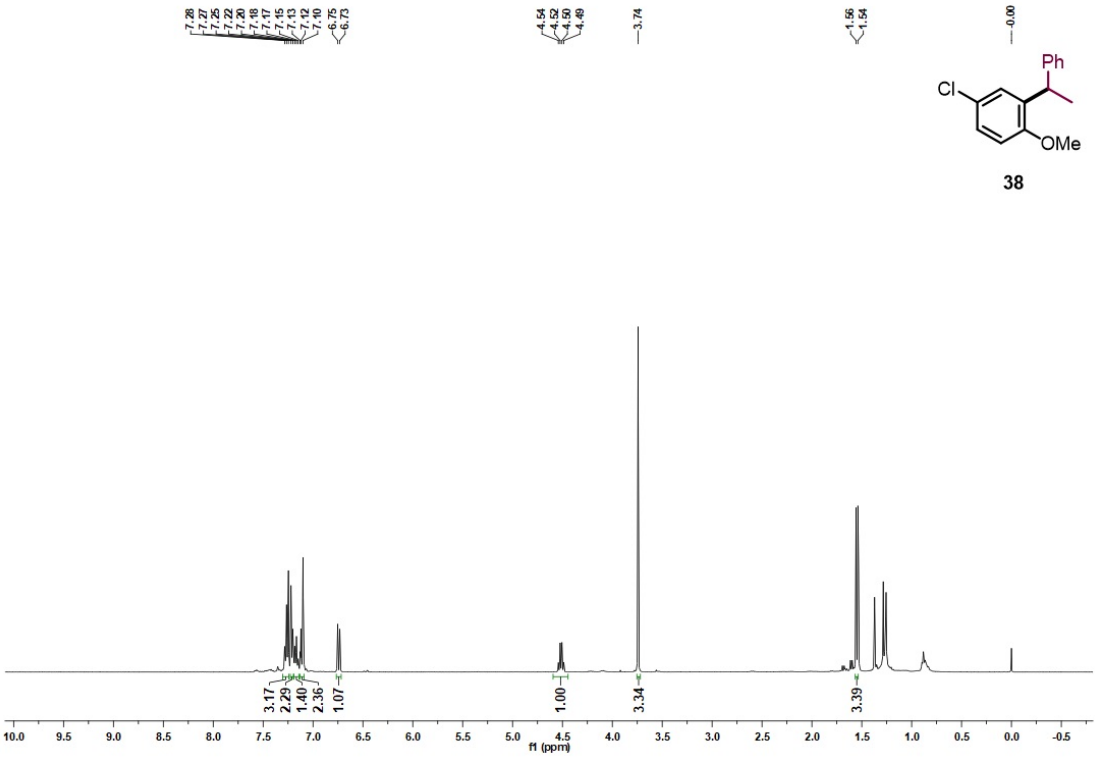
^{1}H-NMR of **37**
$CDCl_3$, 400 MHz, 298 K



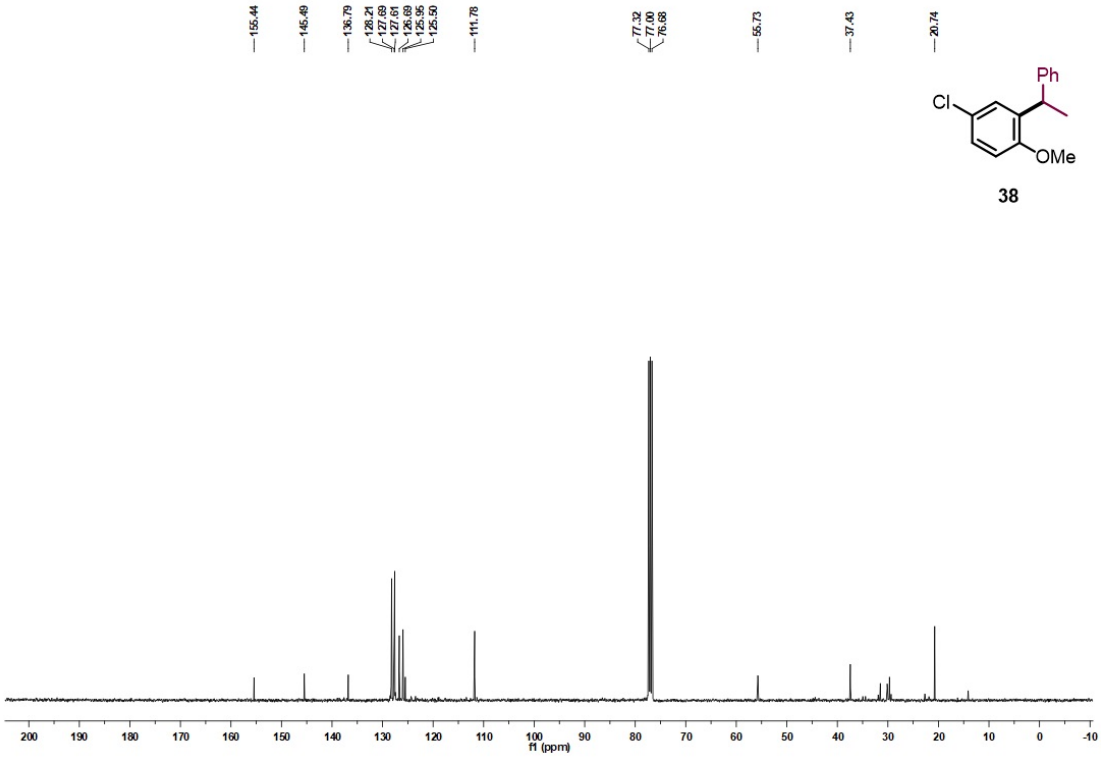
^{13}C-NMR of **37**
$CDCl_3$, 101 MHz, 298 K



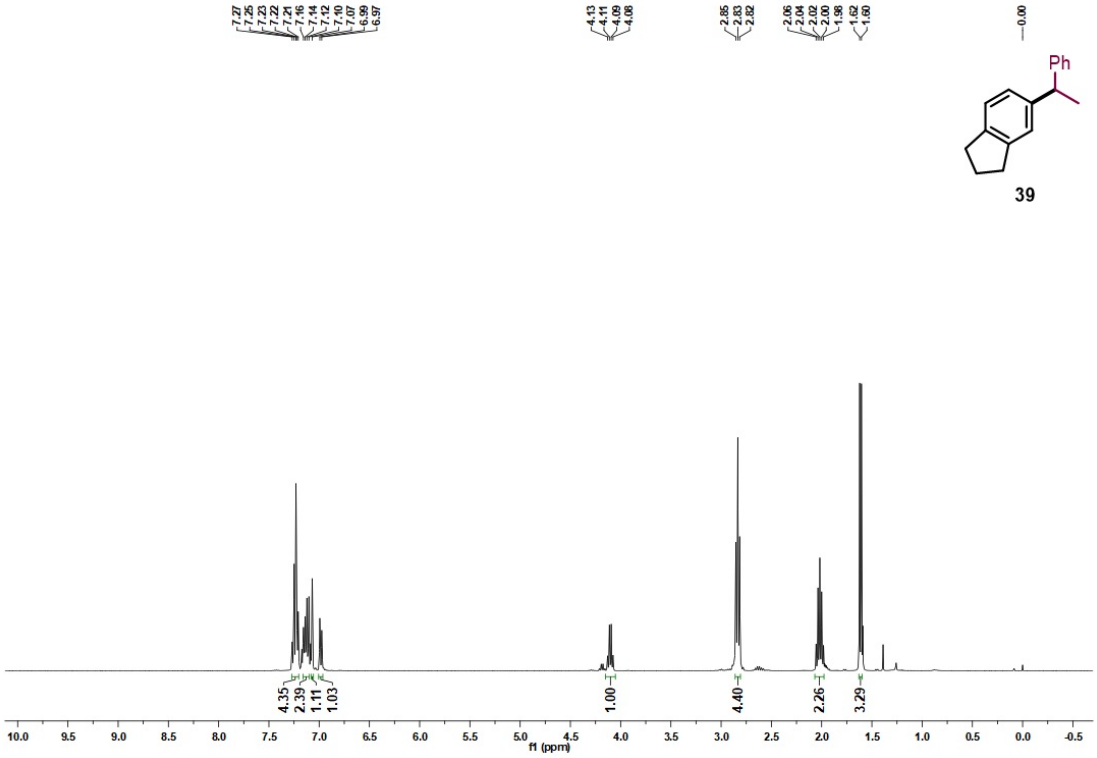
^{1}H-NMR of **38**
$CDCl_3$, 400 MHz, 298 K



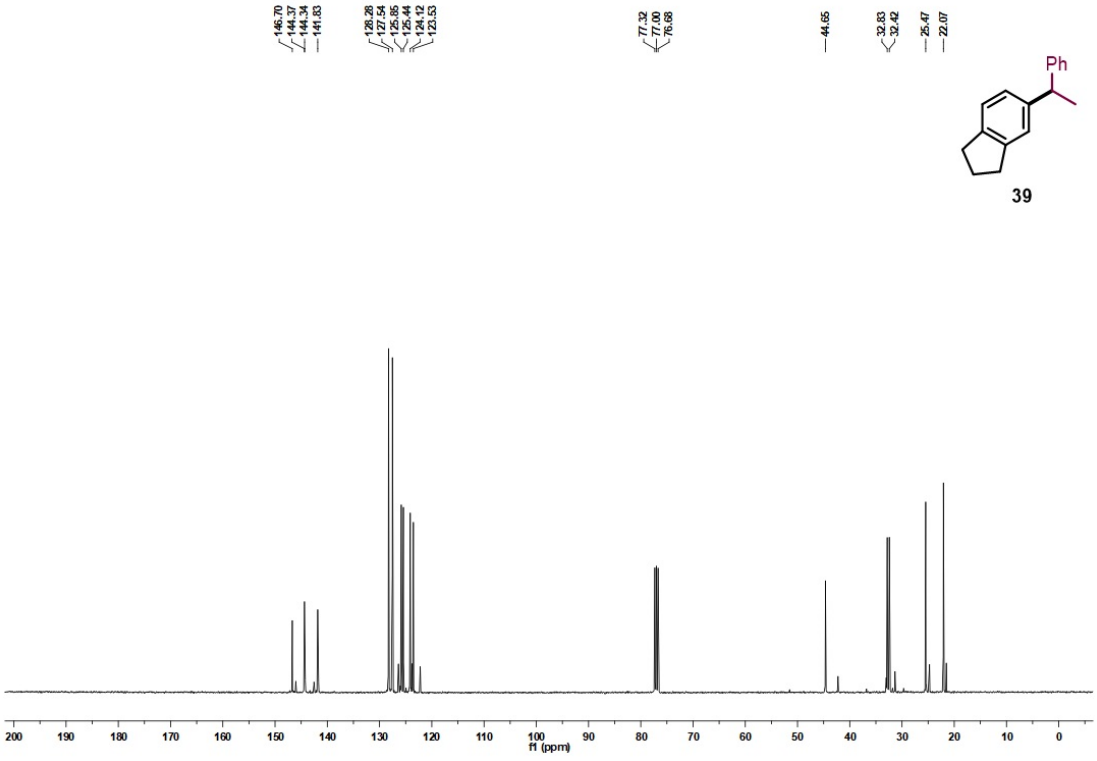
^{13}C-NMR of **38**
$CDCl_3$, 101 MHz, 298 K



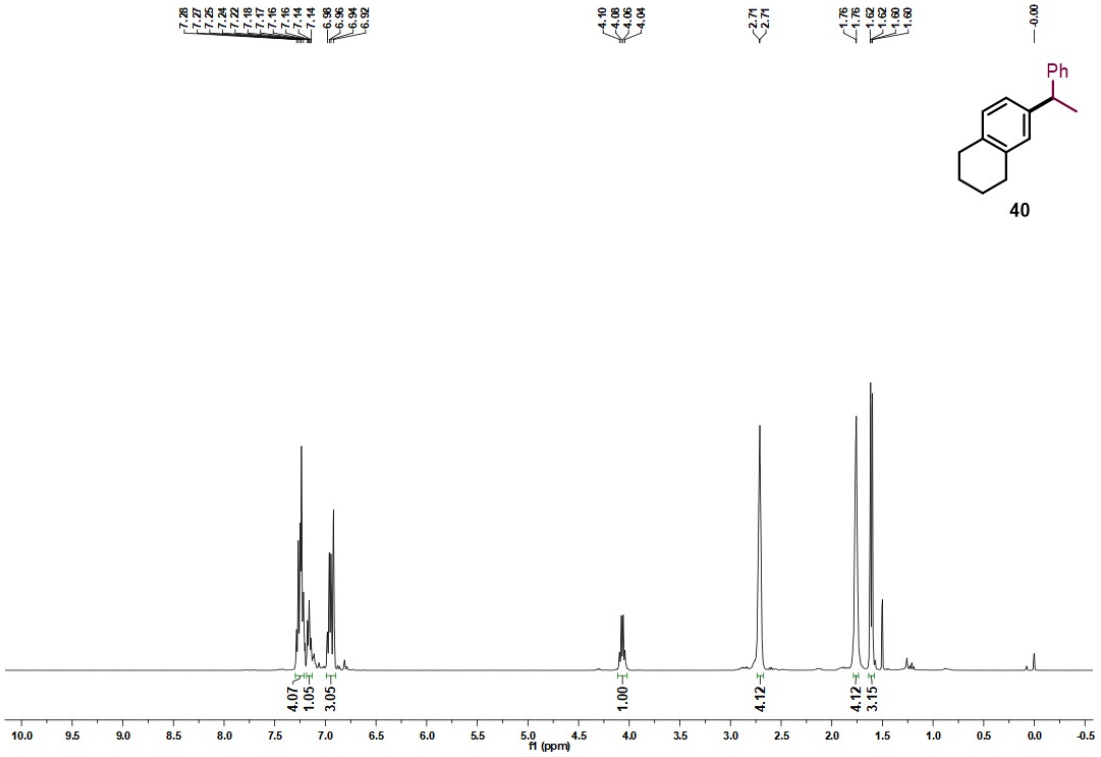
^{1}H-NMR of **39**
$CDCl_3$, 400 MHz, 298 K



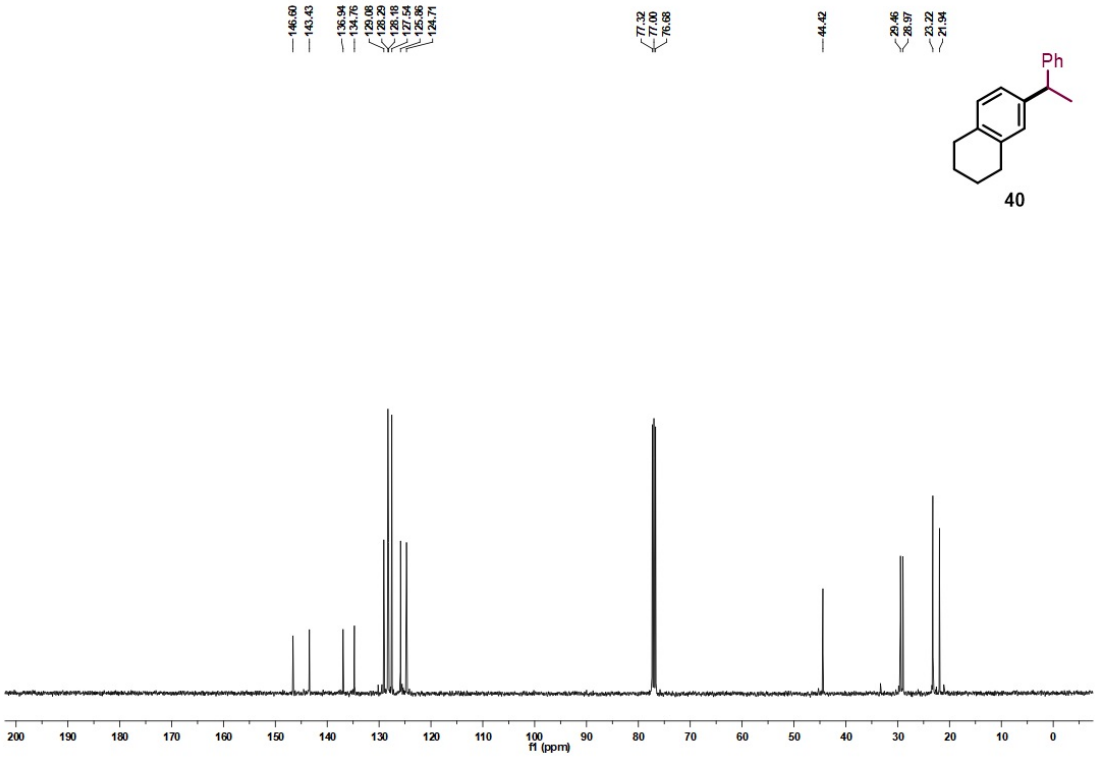
^{13}C-NMR of **39**
$CDCl_3$, 101 MHz, 298 K



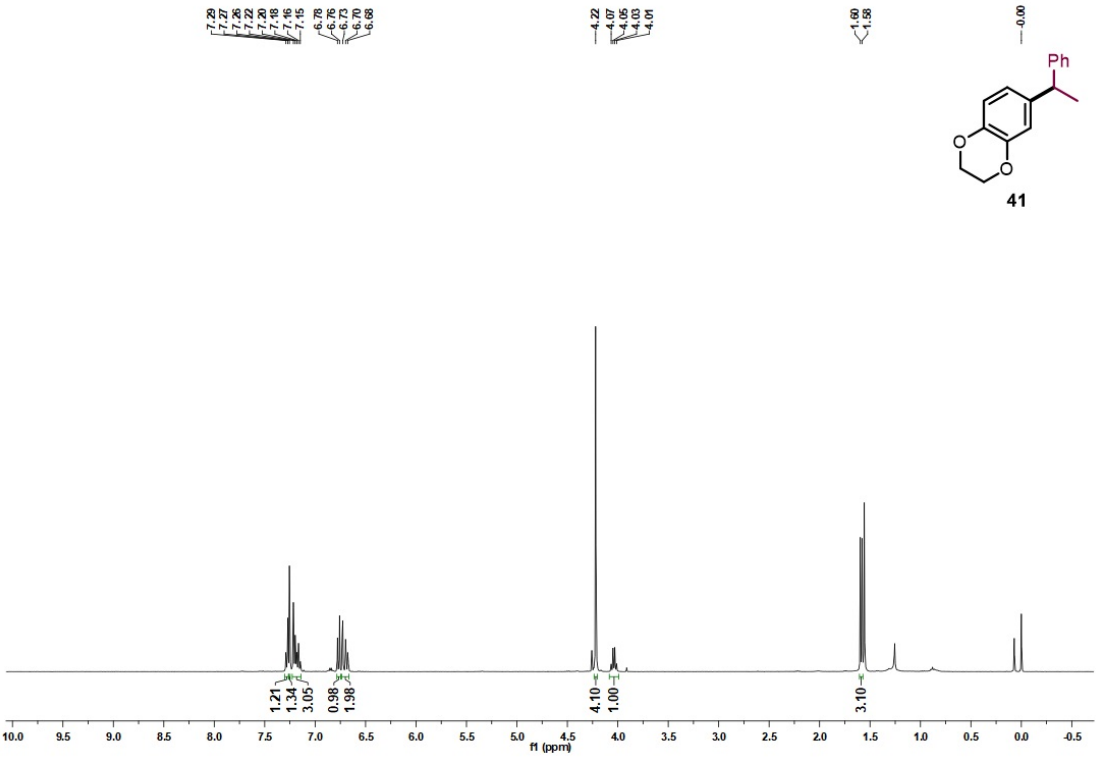
^{1}H-NMR of **40**
$CDCl_3$, 400 MHz, 298 K



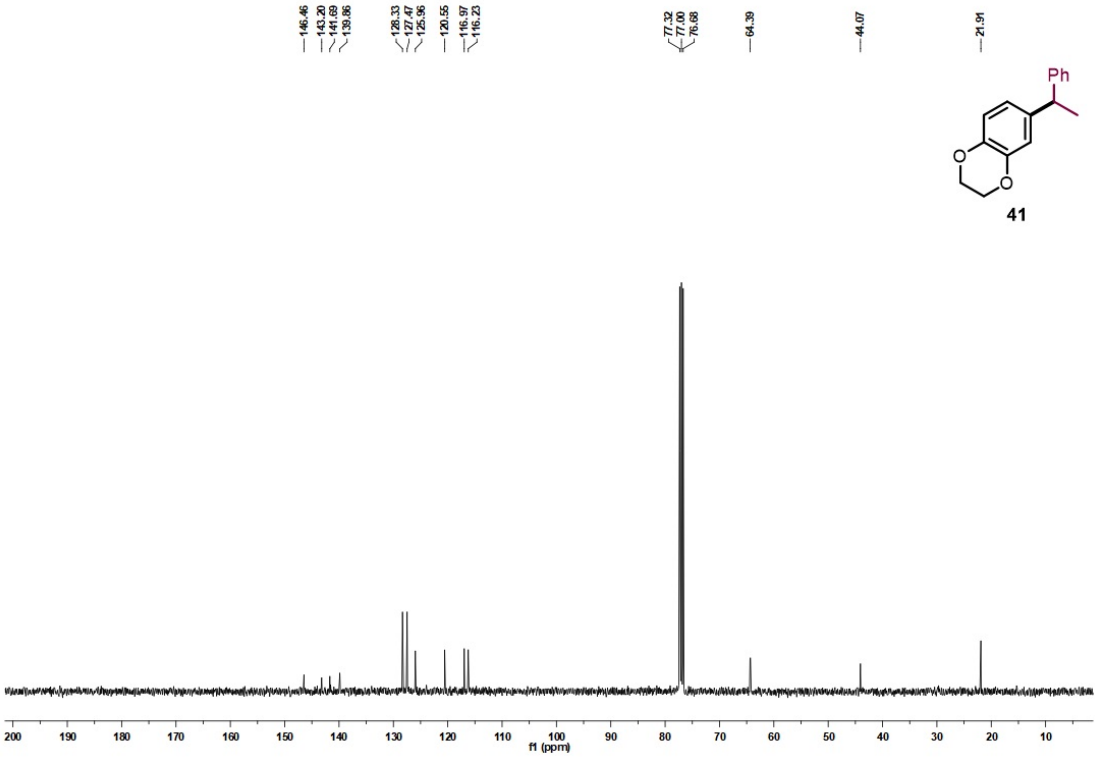
^{13}C-NMR of **40**
$CDCl_3$, 101 MHz, 298 K



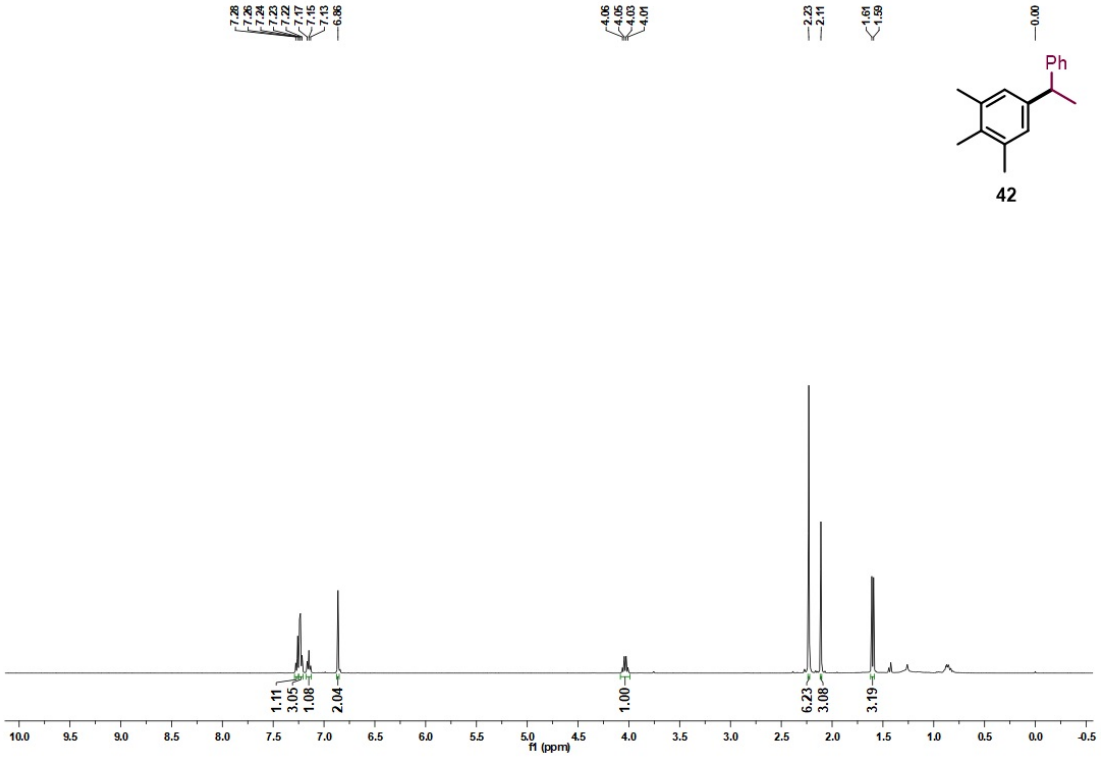
^{1}H-NMR of **41**
$CDCl_3$, 400 MHz, 298 K



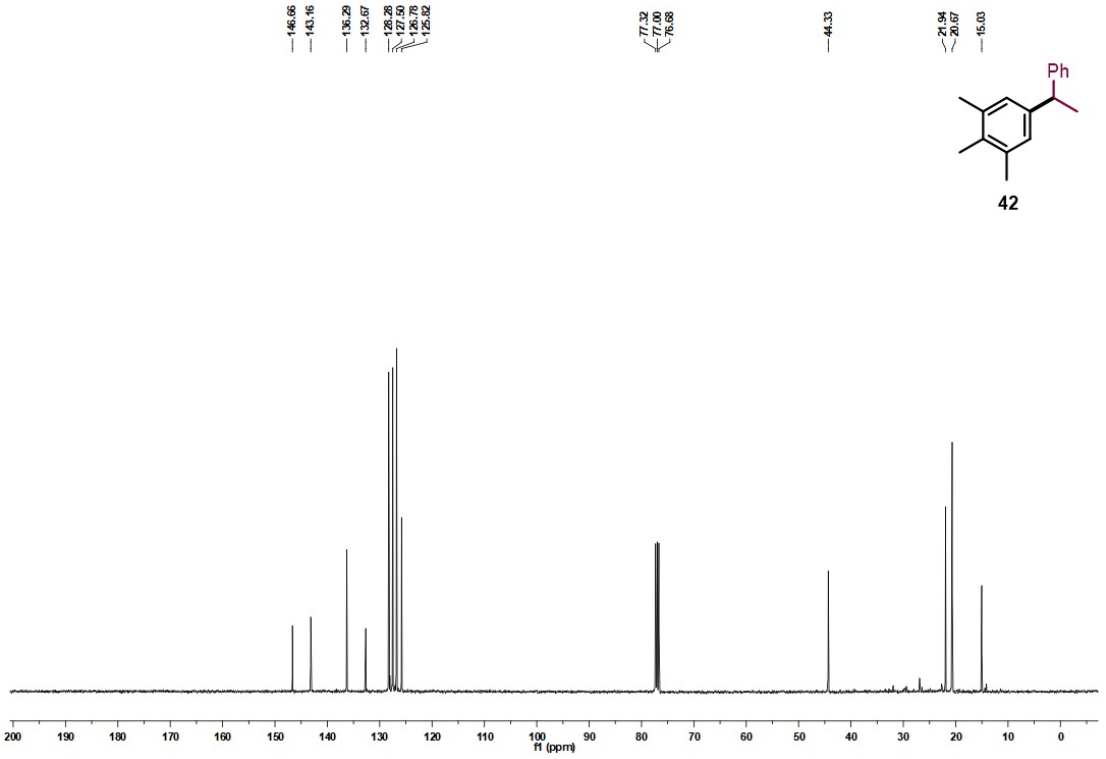
^{13}C-NMR of **41**
$CDCl_3$, 101 MHz, 298 K



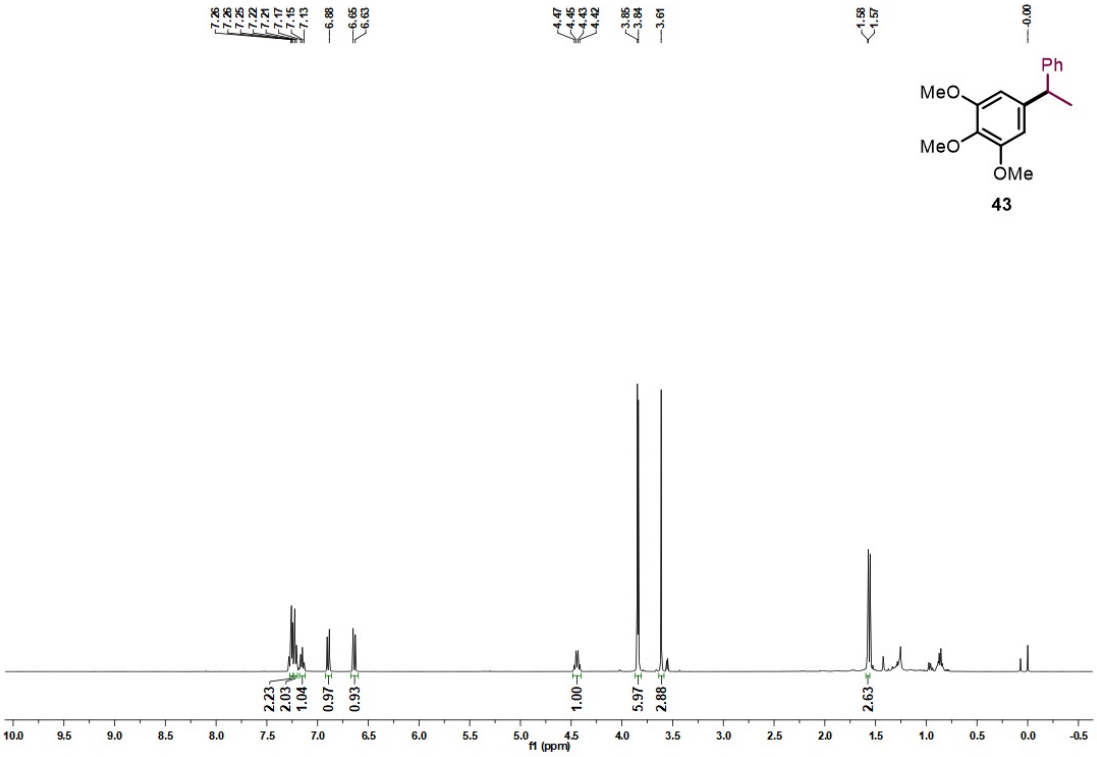
^{1}H-NMR of **42**
$CDCl_3$, 400 MHz, 298 K



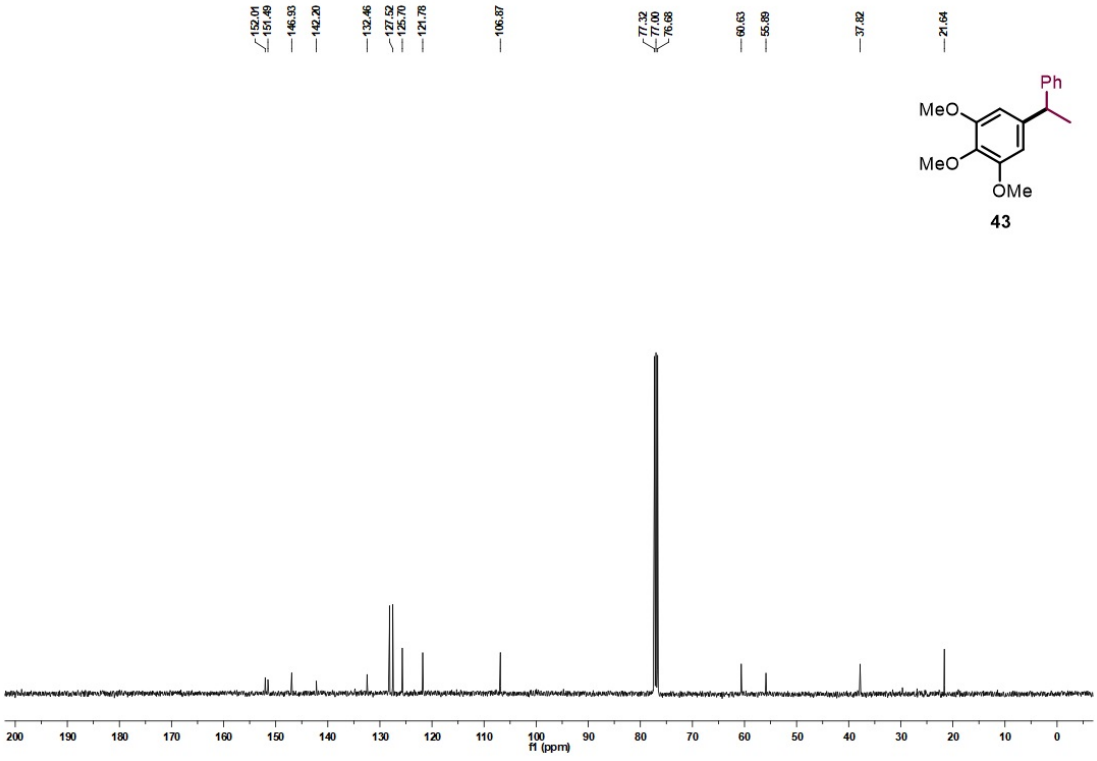
^{13}C-NMR of **42**
$CDCl_3$, 101 MHz, 298 K



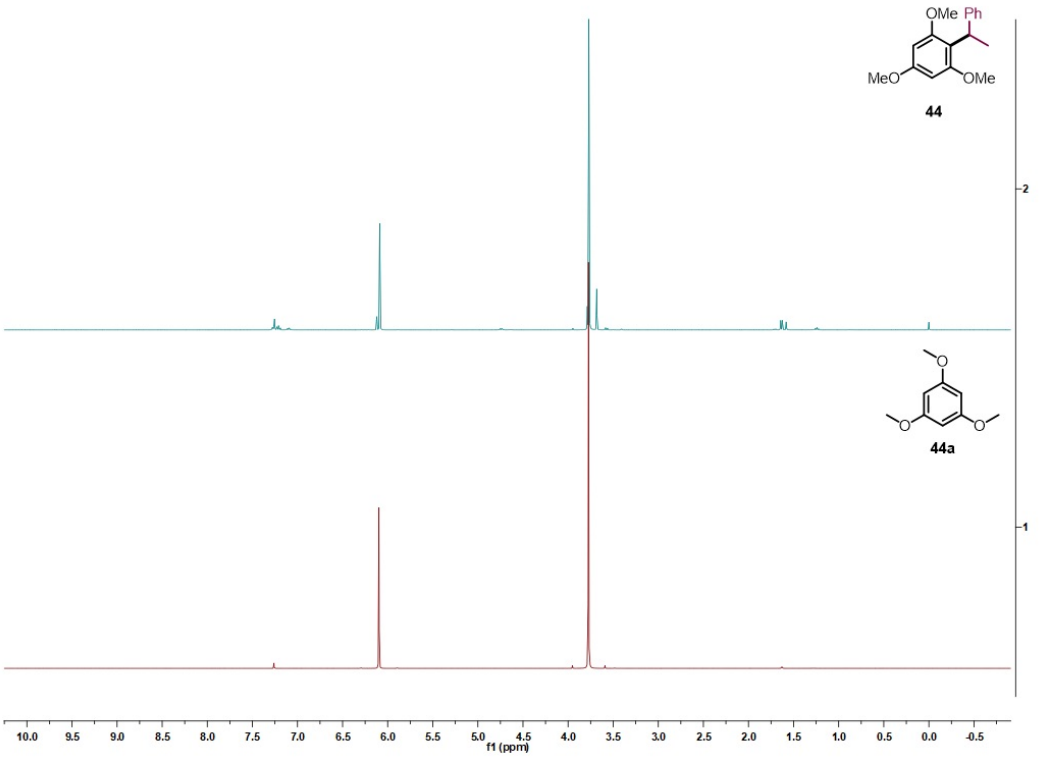
^{1}H-NMR of **43**
$CDCl_3$, 400 MHz, 298 K



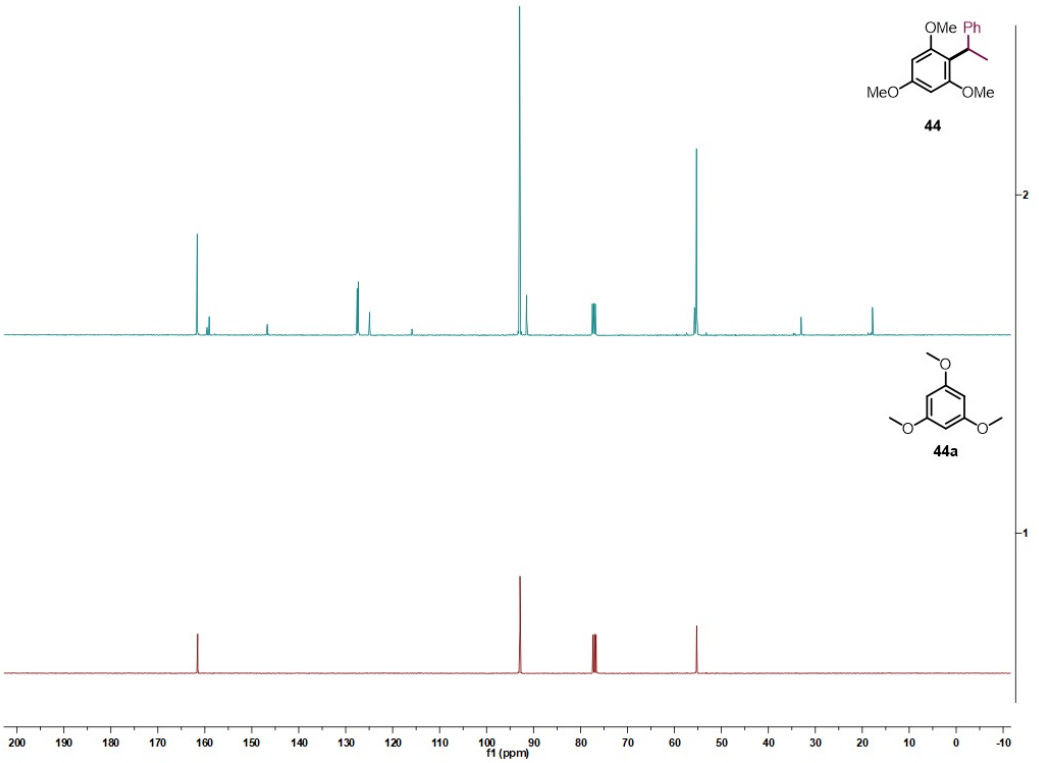
^{13}C-NMR of **43**
$CDCl_3$, 101 MHz, 298 K



^{1}H-NMR of **44**
$CDCl_3$, 400 MHz, 298 K

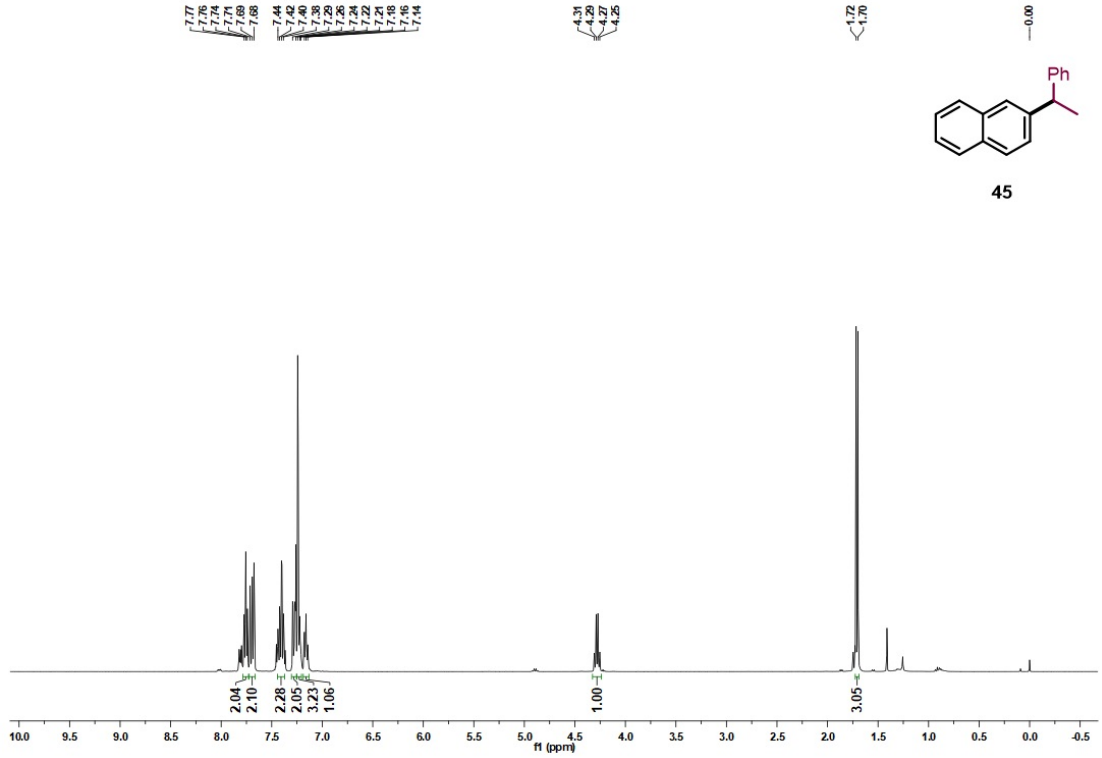


^{13}C-NMR of **44**
$CDCl_3$, 101 MHz, 298 K

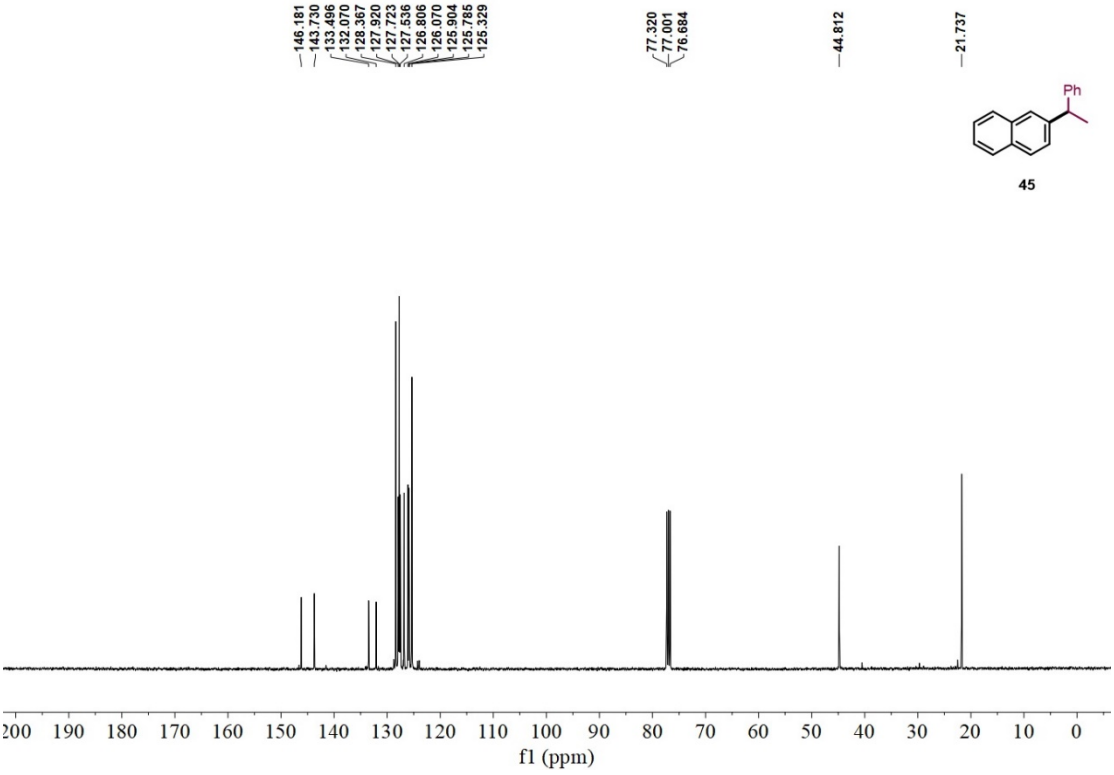


The polarity of product **44** is consistent with that of raw material **44a**, and this spectrum is a mixed spectrum.

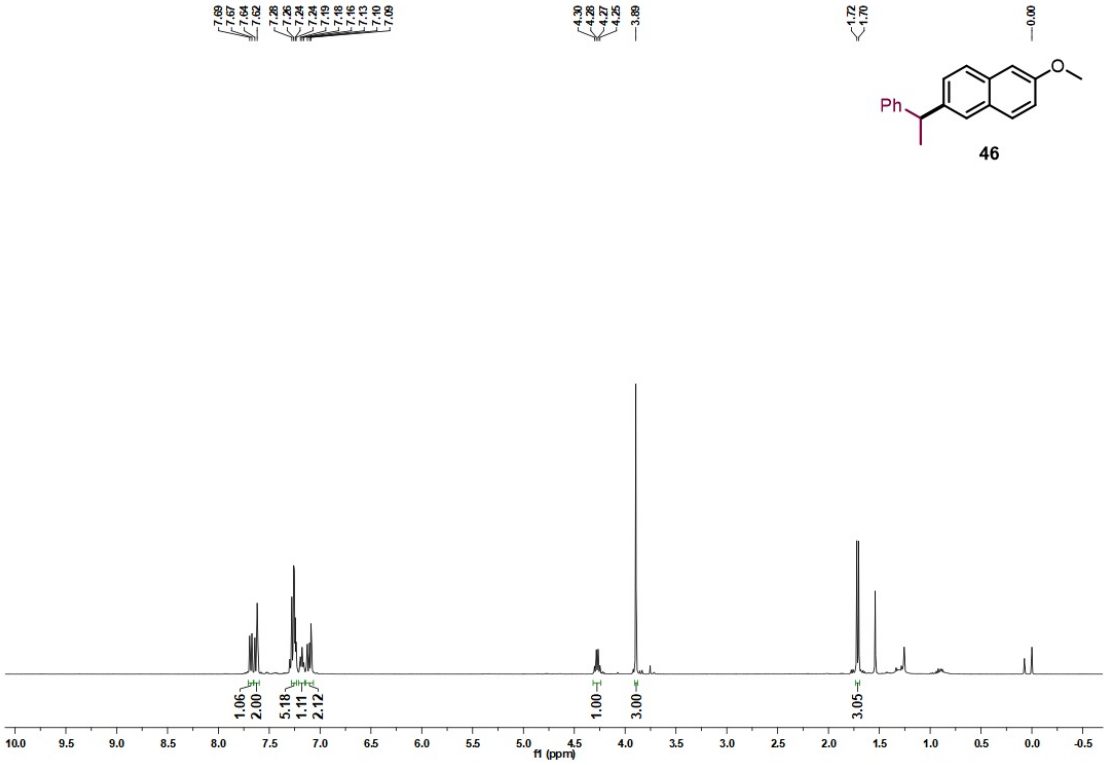
^{1}H-NMR of **45**
$CDCl_3$, 400 MHz, 298 K



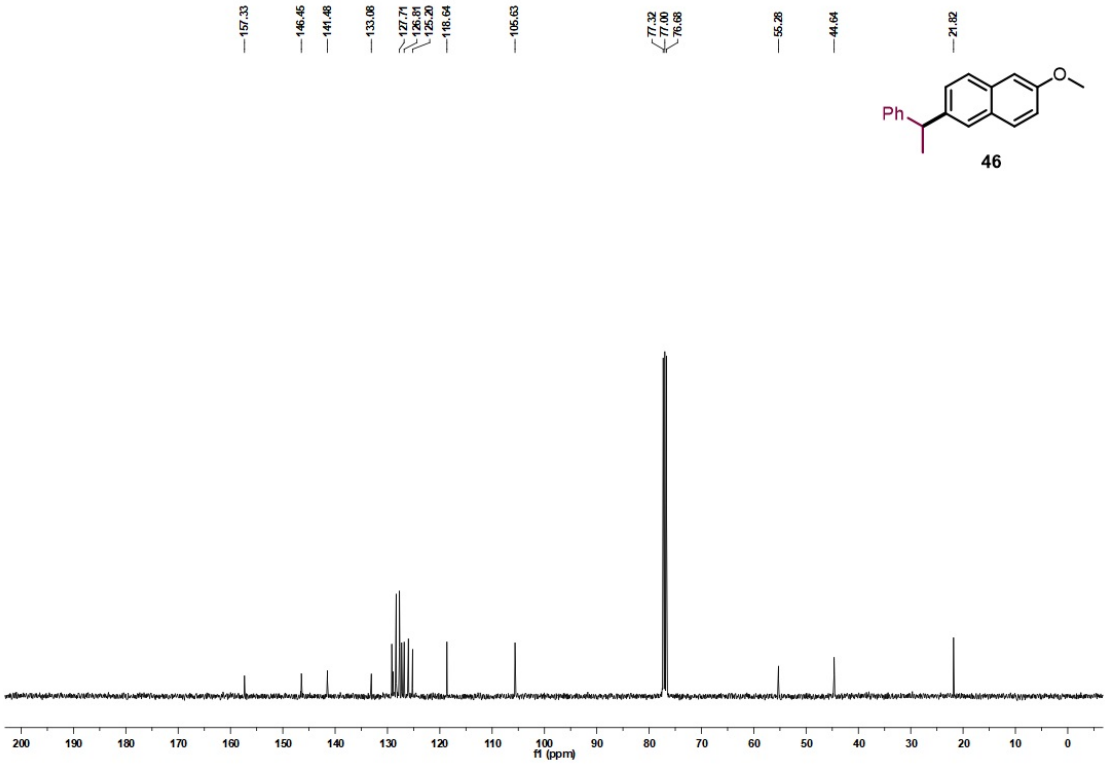
^{13}C-NMR of **45**
$CDCl_3$, 101 MHz, 298 K



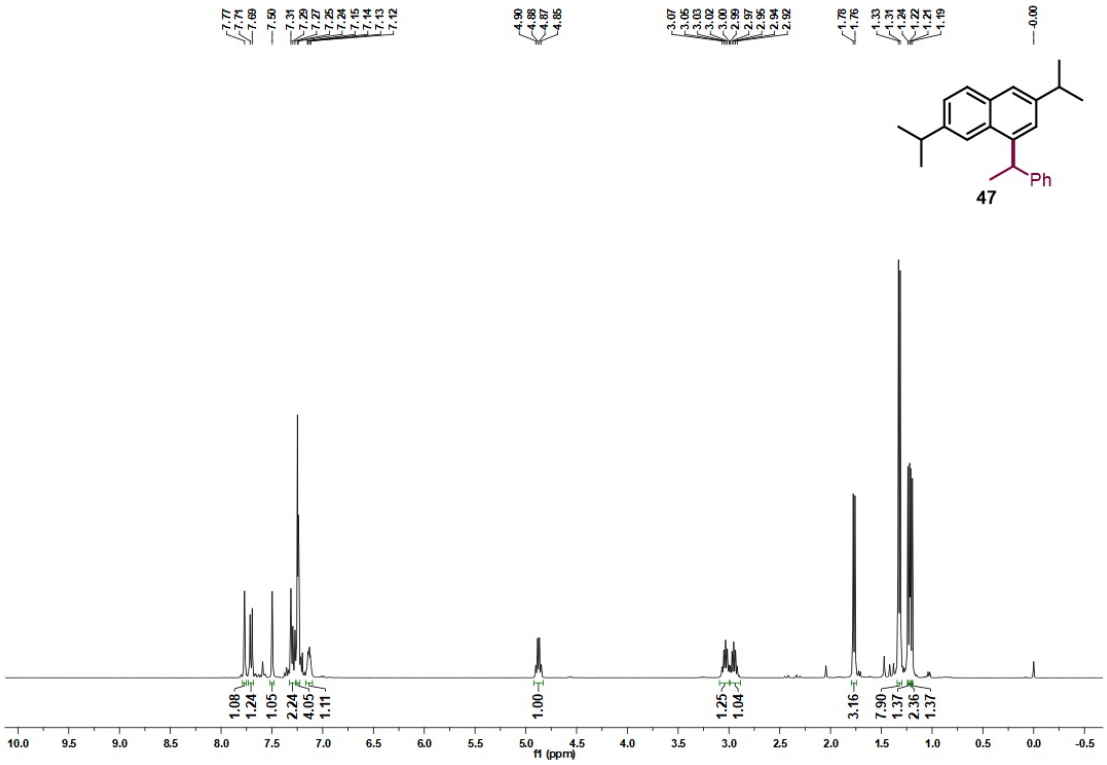
^{1}H-NMR of **46**
$CDCl_3$, 400 MHz, 298 K



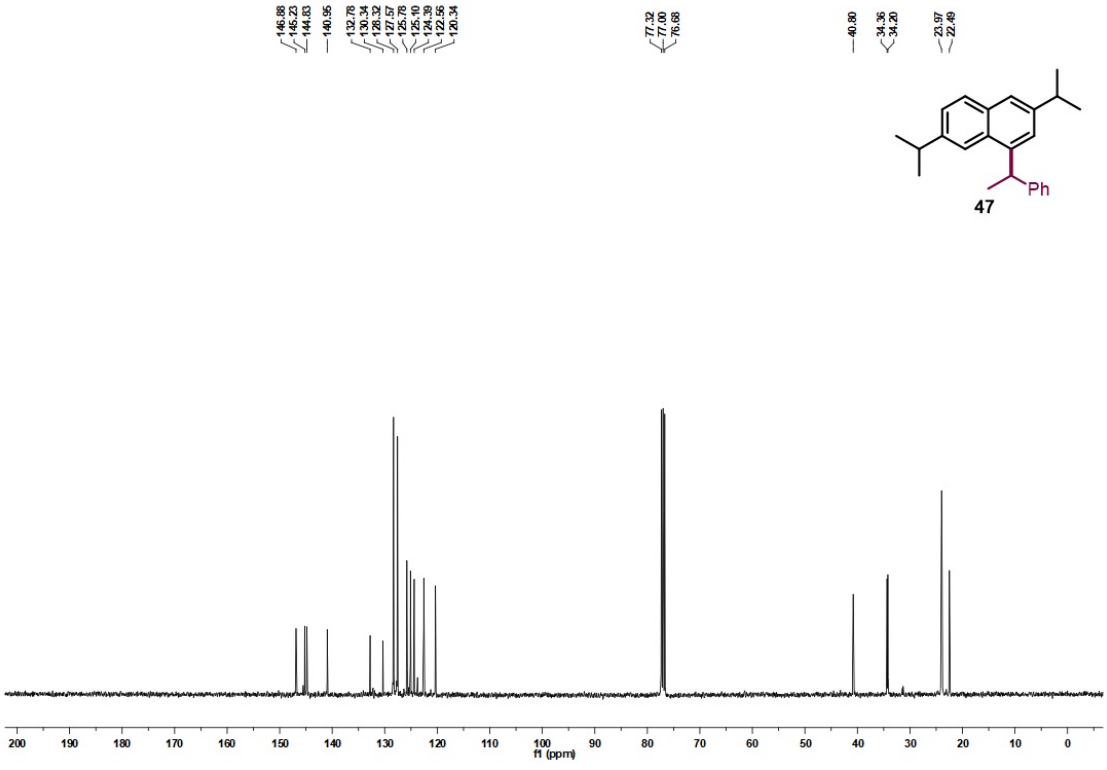
^{13}C-NMR of **46**
$CDCl_3$, 101 MHz, 298 K



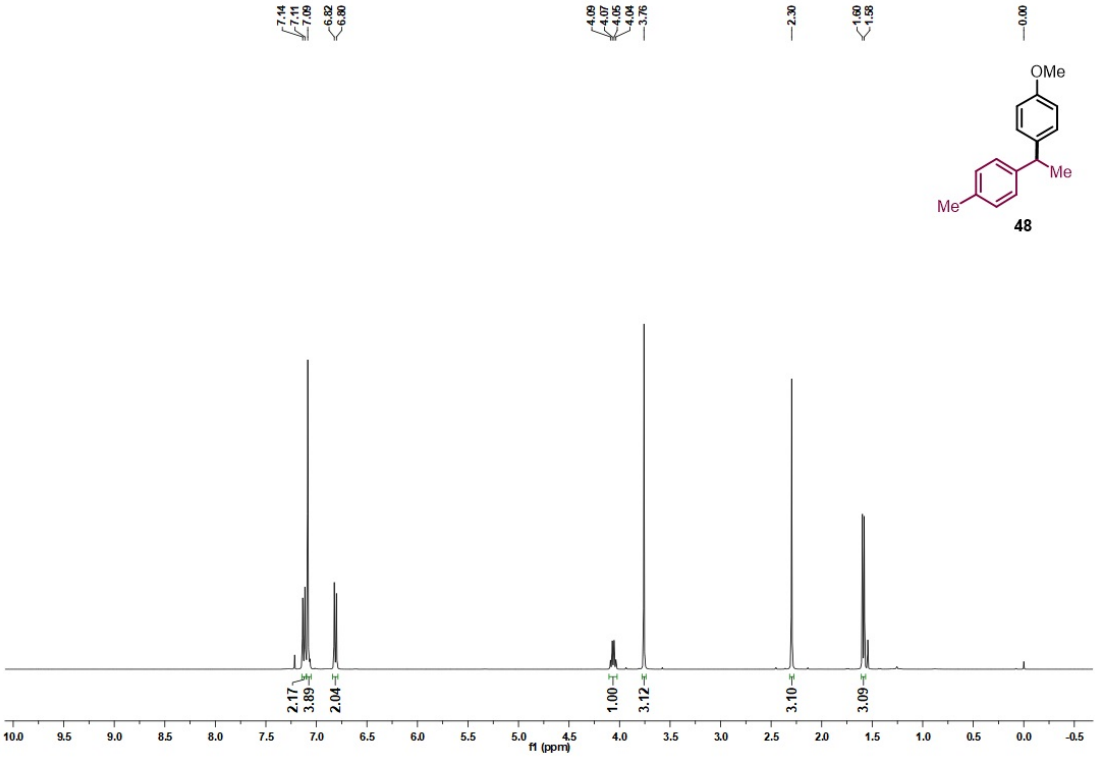
^{1}H-NMR of **47**
$CDCl_3$, 400 MHz, 298 K



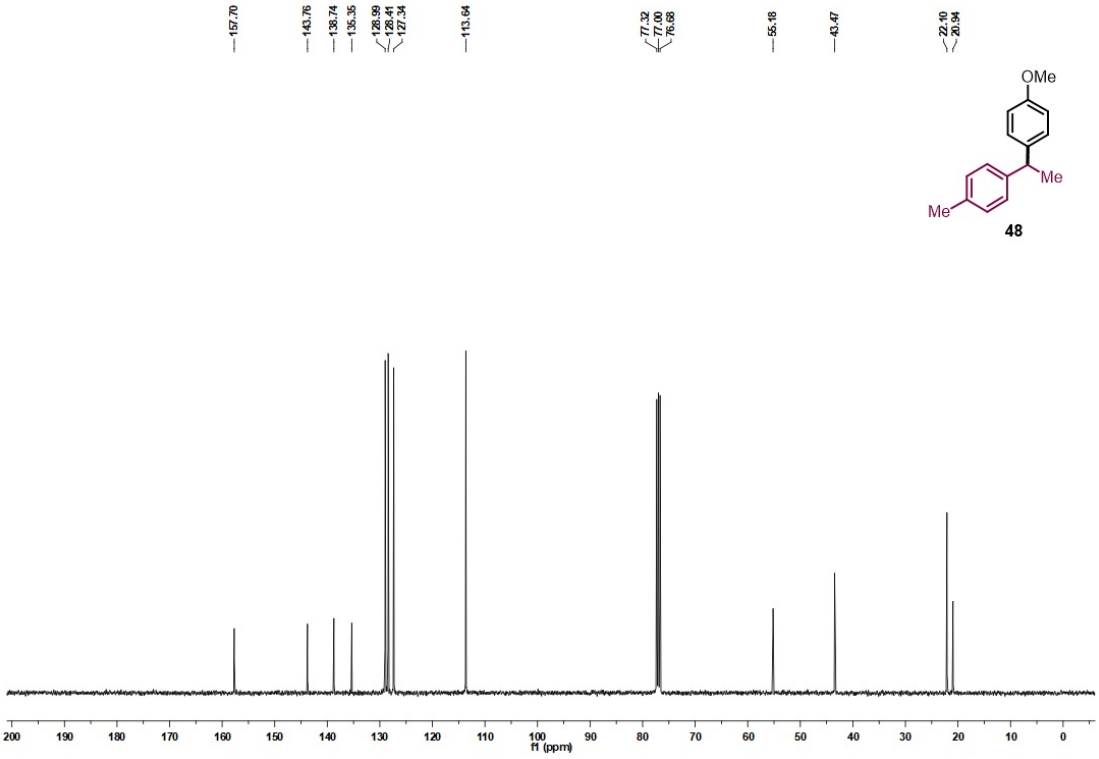
^{13}C-NMR of **47**
$CDCl_3$, 101 MHz, 298 K



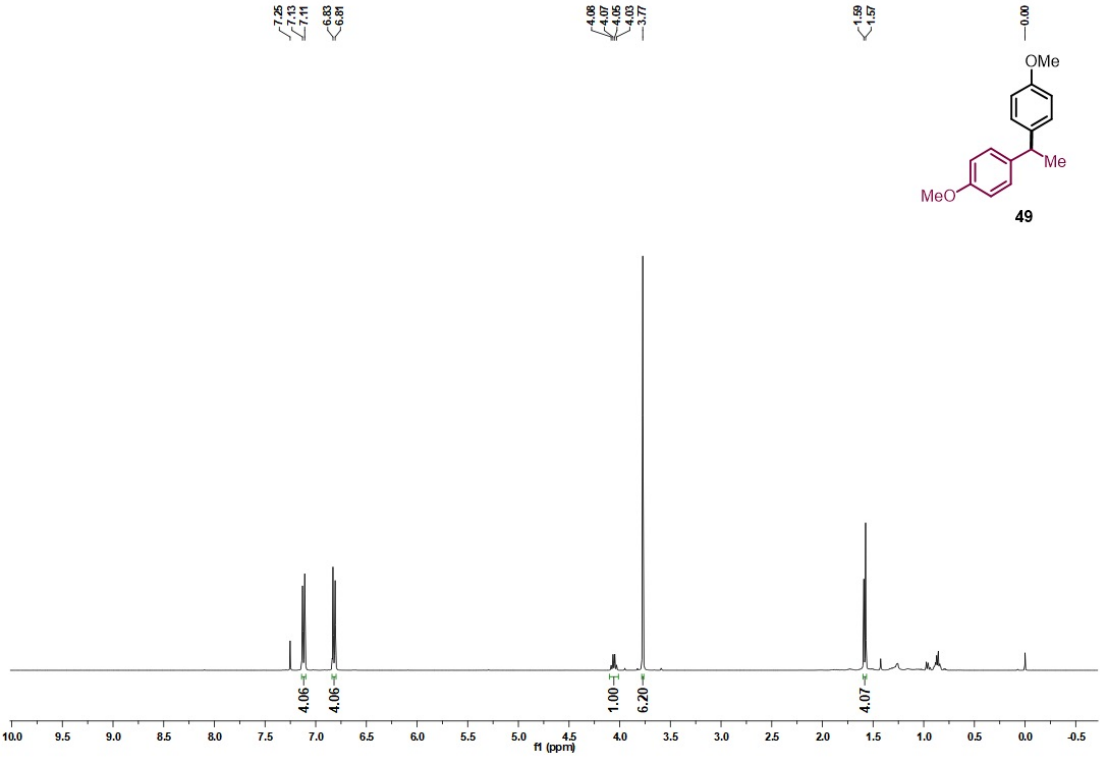
^{1}H-NMR of **48**
$CDCl_3$, 400 MHz, 298 K



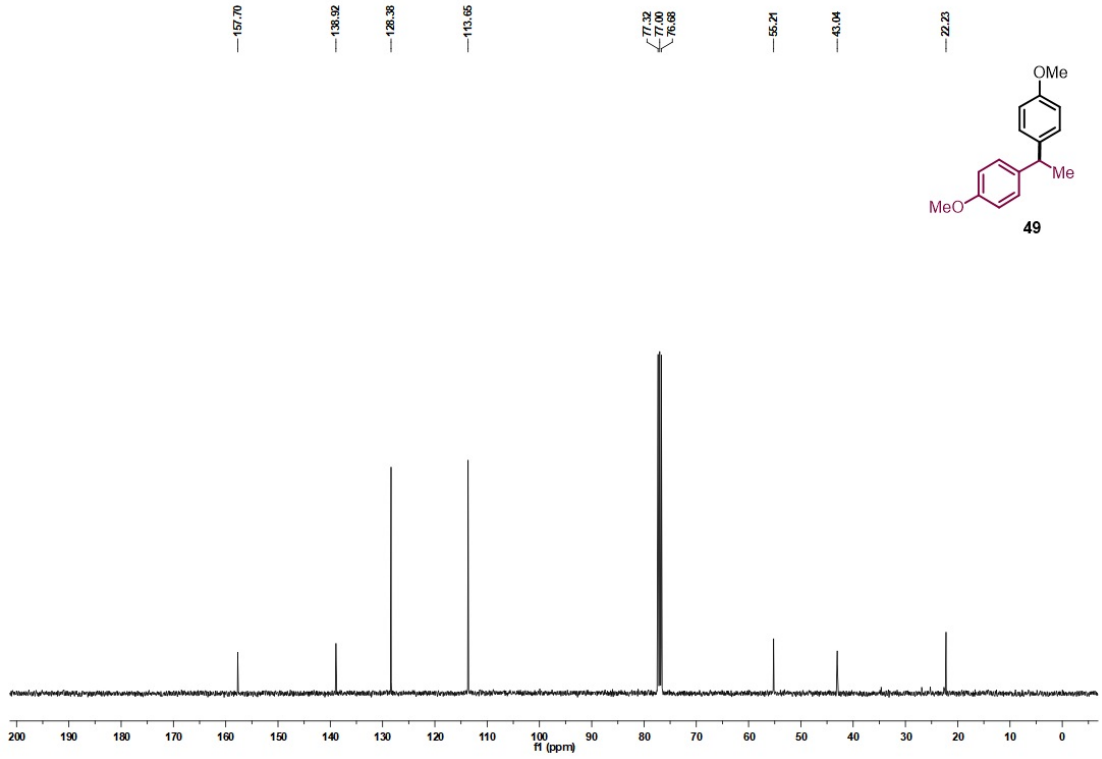
^{13}C-NMR of **48**
$CDCl_3$, 101 MHz, 298 K



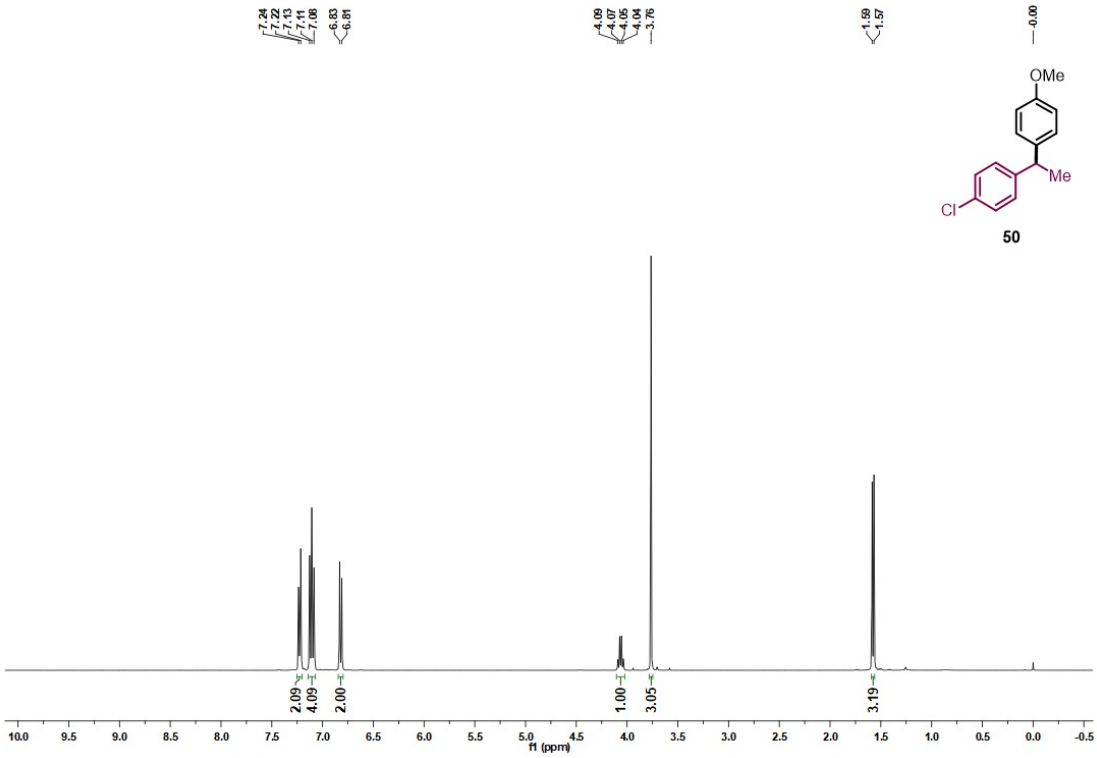
^{1}H-NMR of **49**
$CDCl_3$, 400 MHz, 298 K



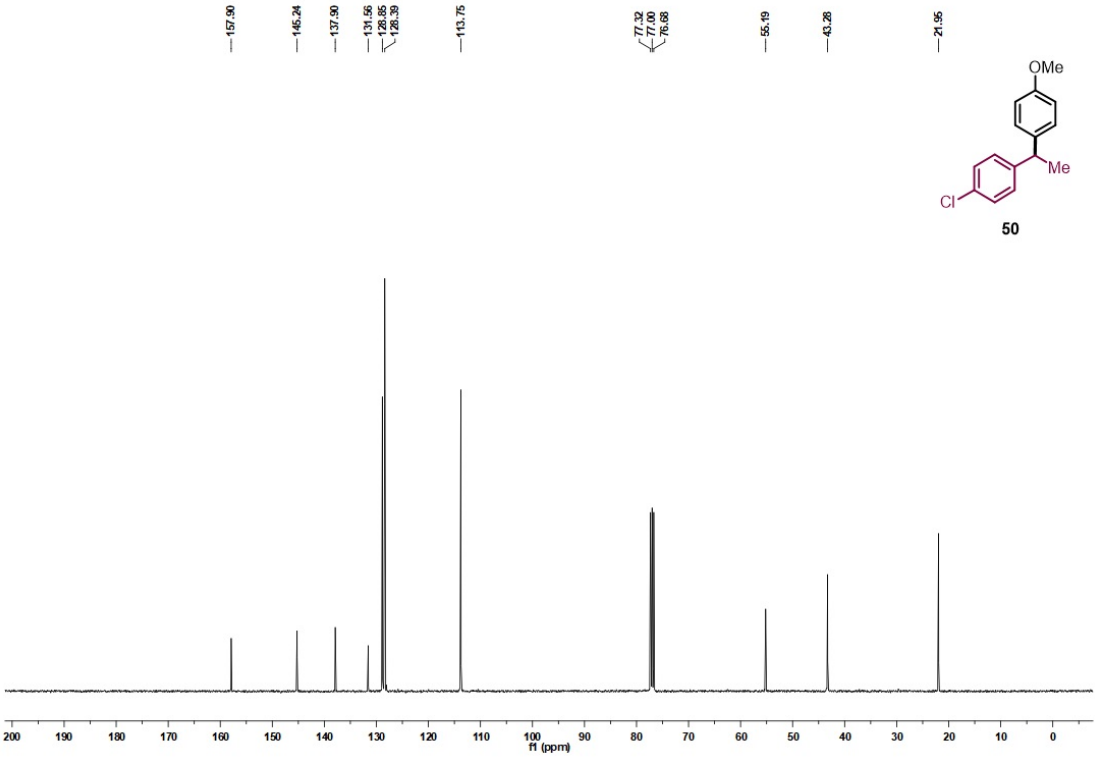
^{13}C-NMR of **49**
$CDCl_3$, 101 MHz, 298 K



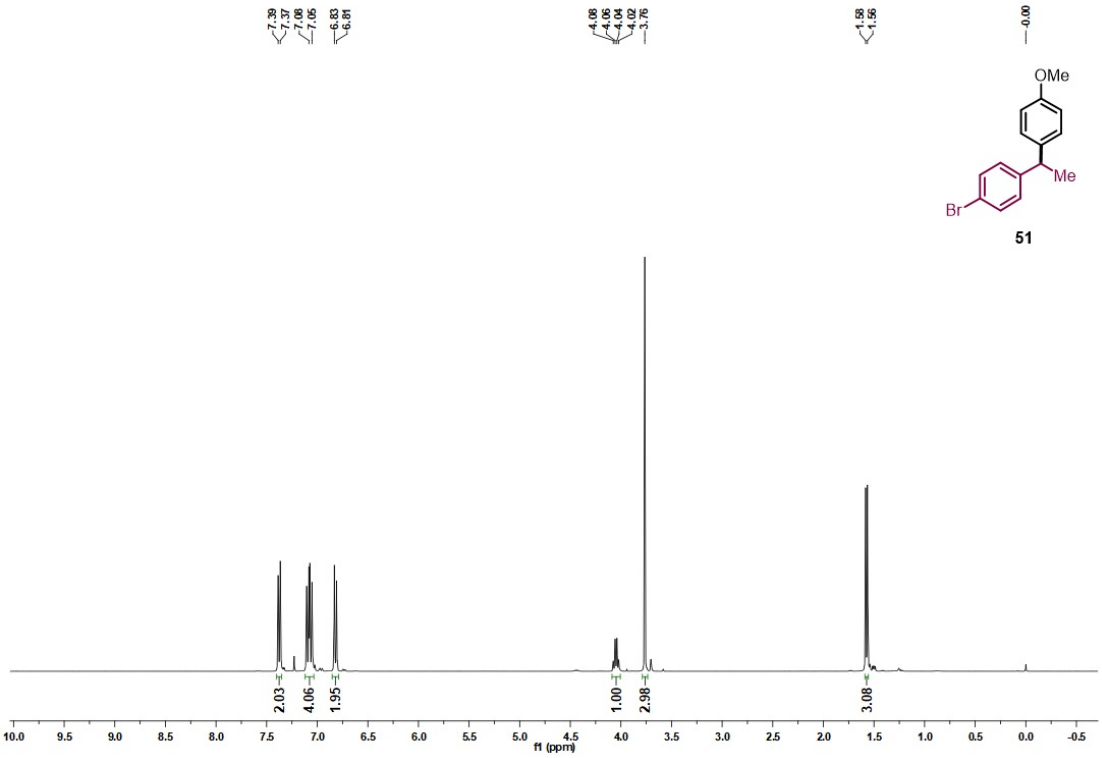
^{1}H-NMR of **50**
$CDCl_3$, 400 MHz, 298 K



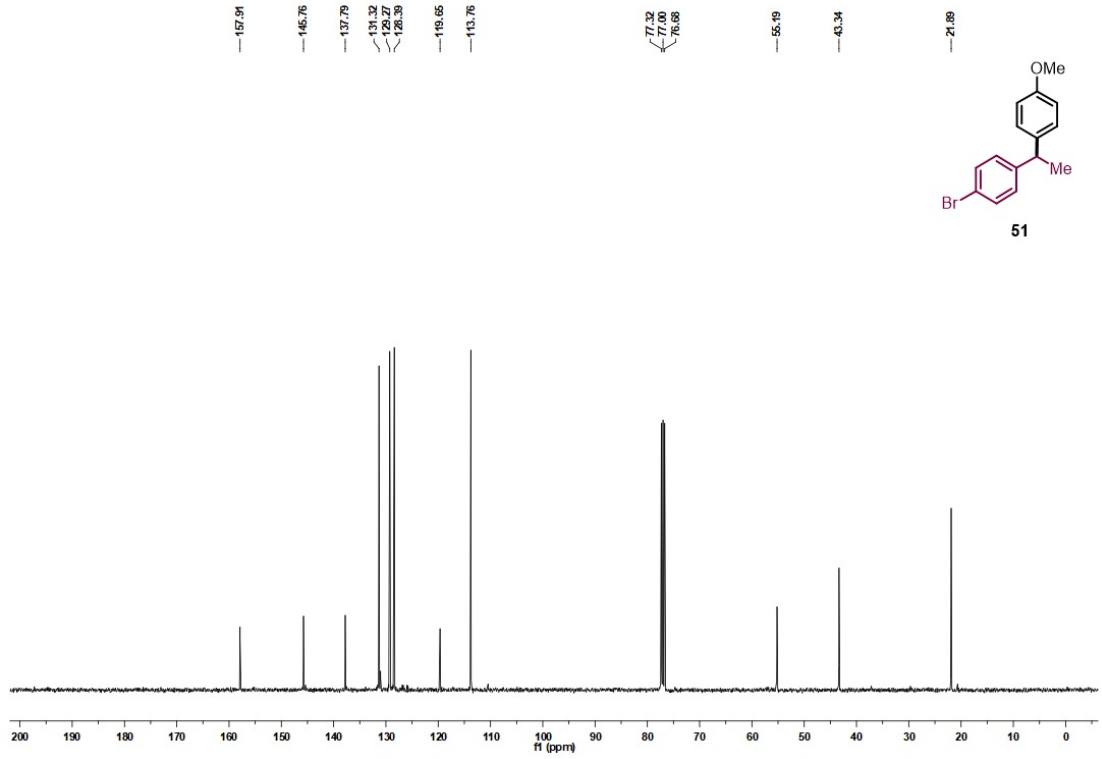
^{13}C-NMR of **50**
$CDCl_3$, 101 MHz, 298 K



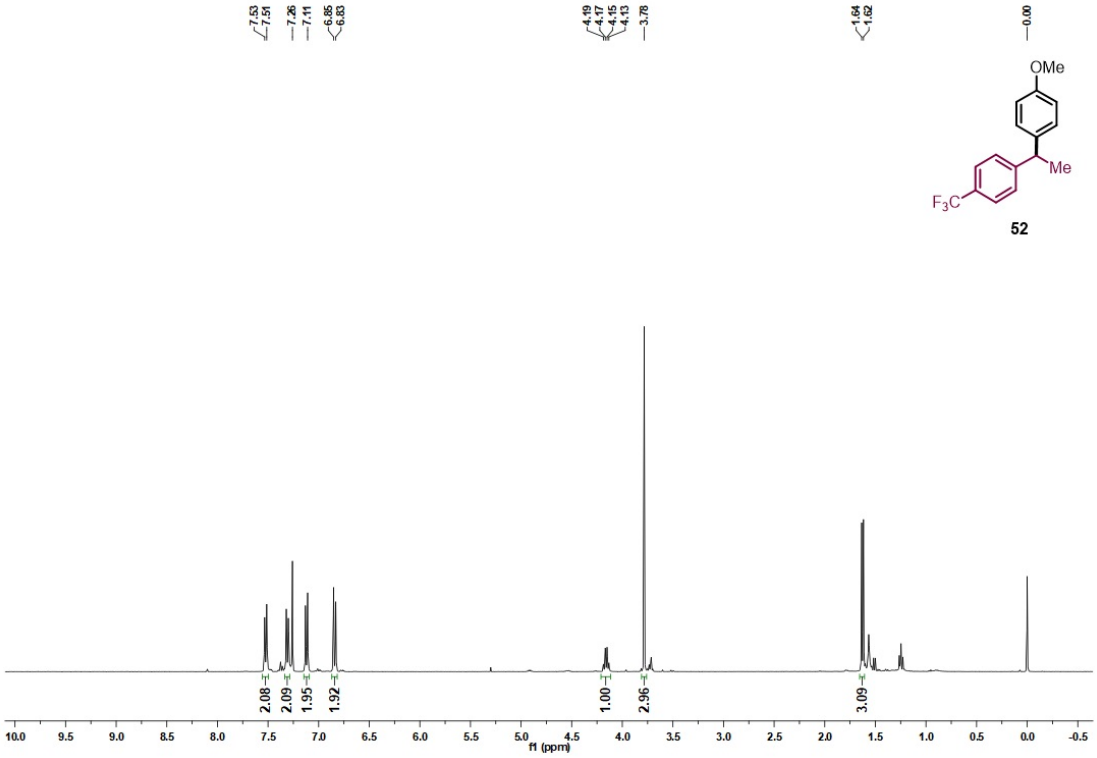
^{1}H-NMR of **51**
$CDCl_3$, 400 MHz, 298 K



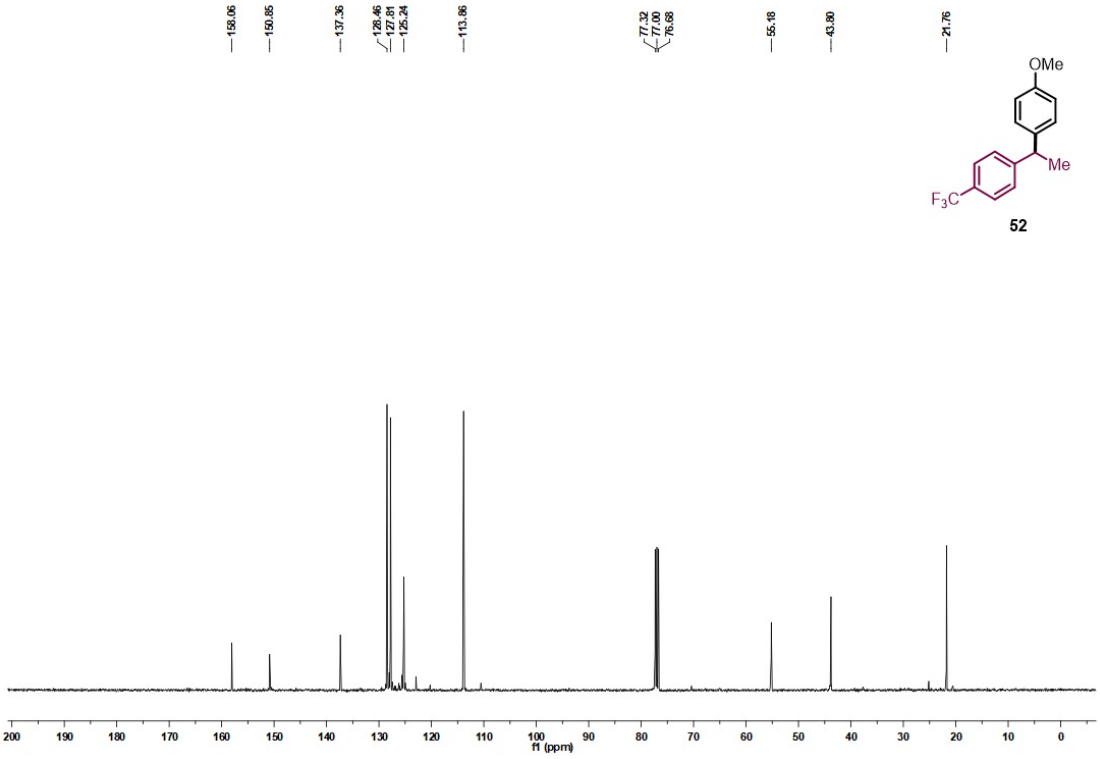
^{13}C-NMR of **51**
$CDCl_3$, 101 MHz, 298 K



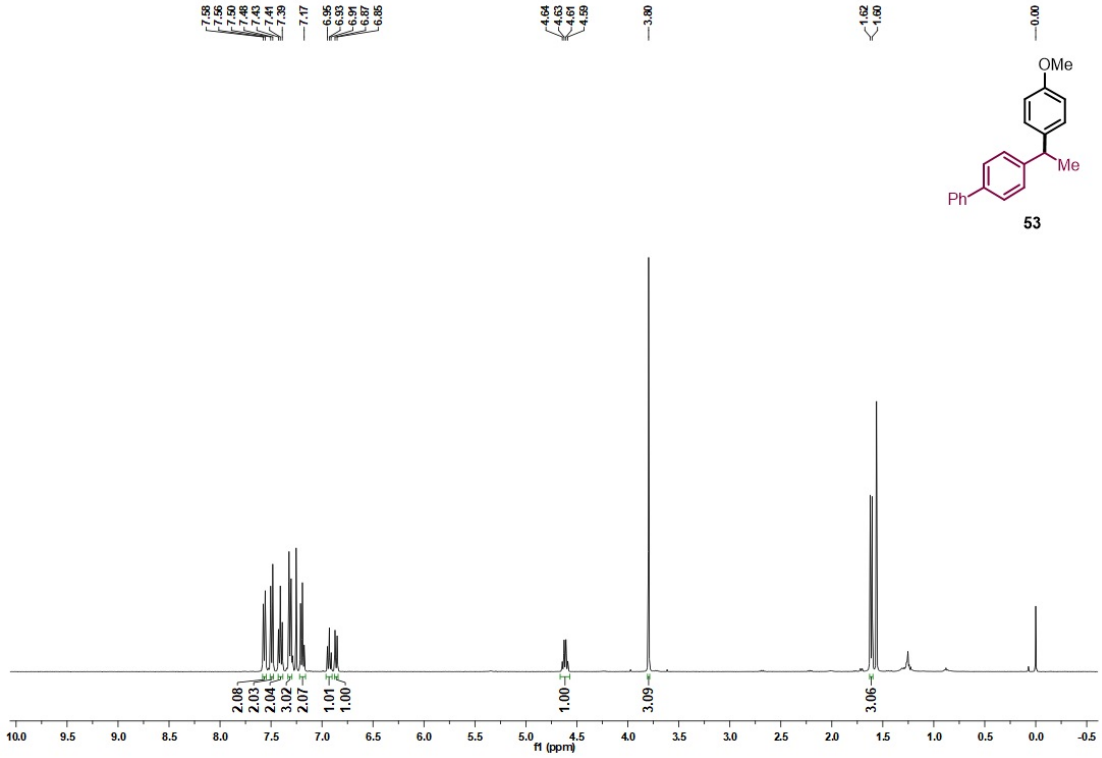
^{1}H-NMR of **52**
$CDCl_3$, 400 MHz, 298 K



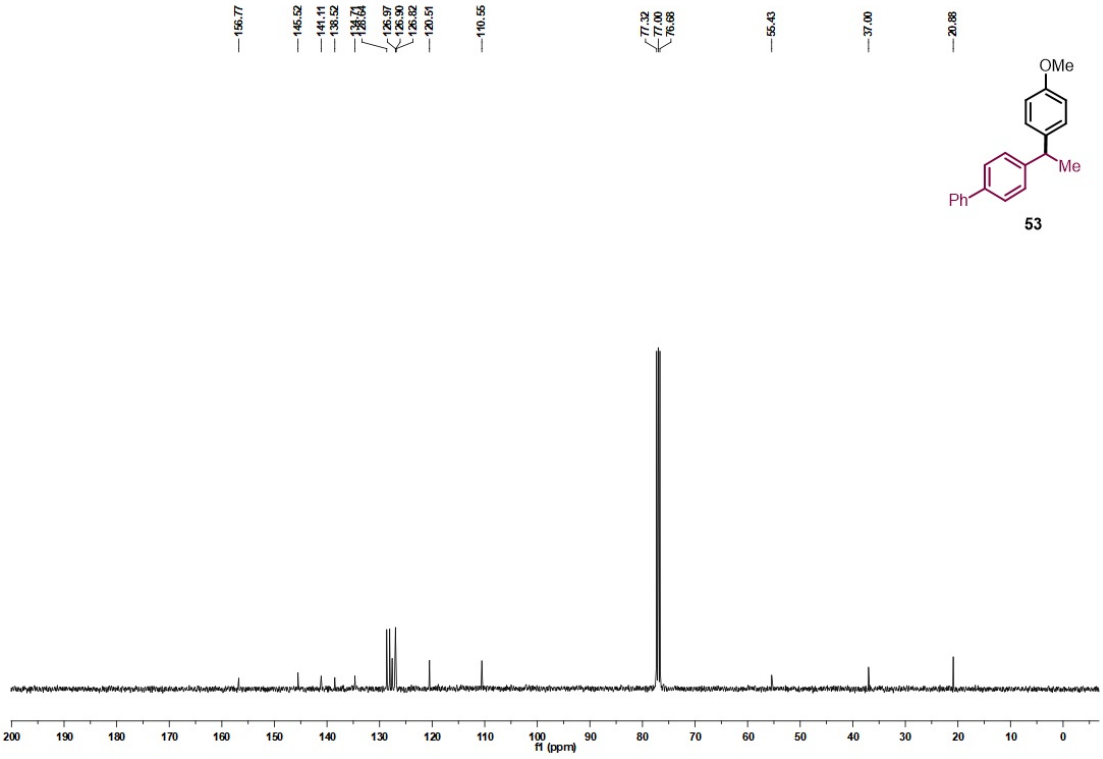
^{13}C-NMR of **52**
$CDCl_3$, 101 MHz, 298 K



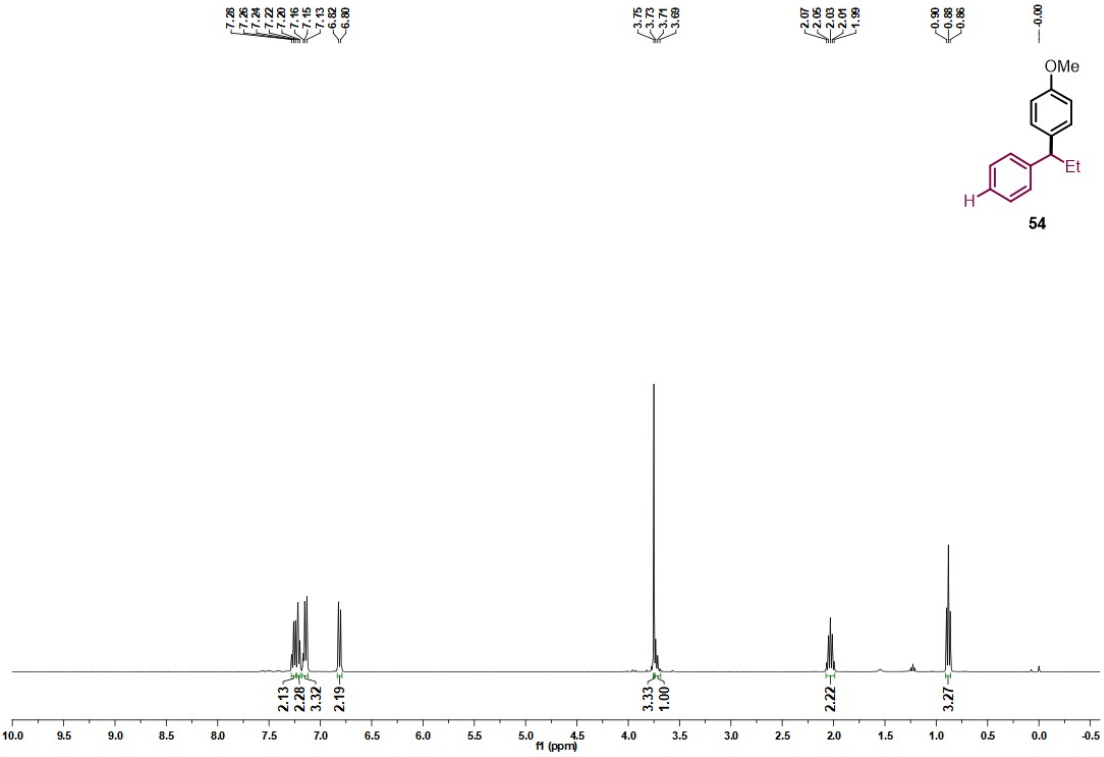
^{1}H-NMR of **53**
$CDCl_3$, 400 MHz, 298 K



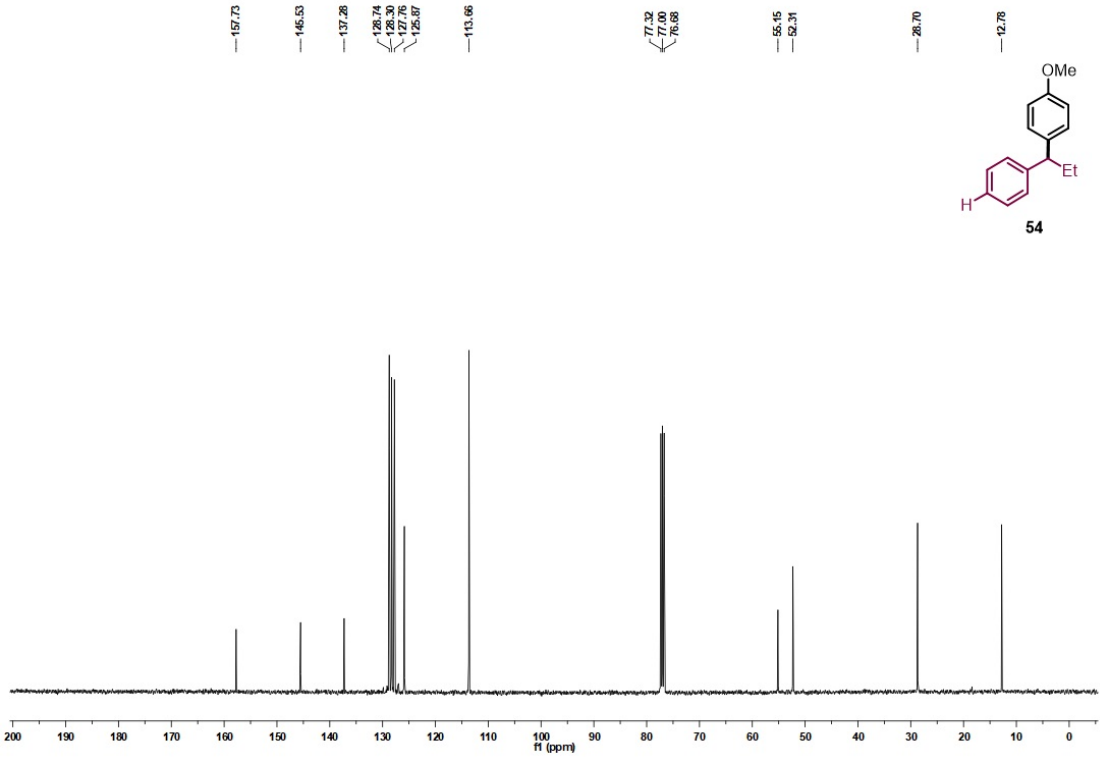
^{13}C-NMR of **53**
$CDCl_3$, 101 MHz, 298 K



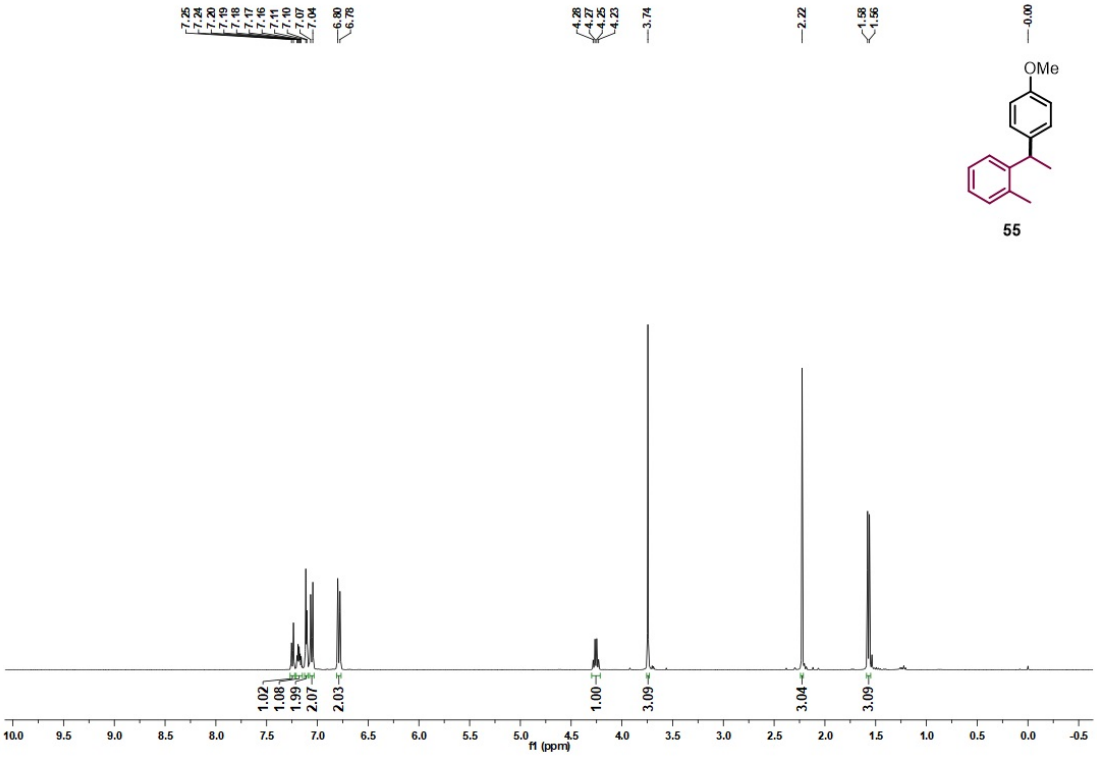
^{1}H-NMR of **54**
$CDCl_3$, 400 MHz, 298 K



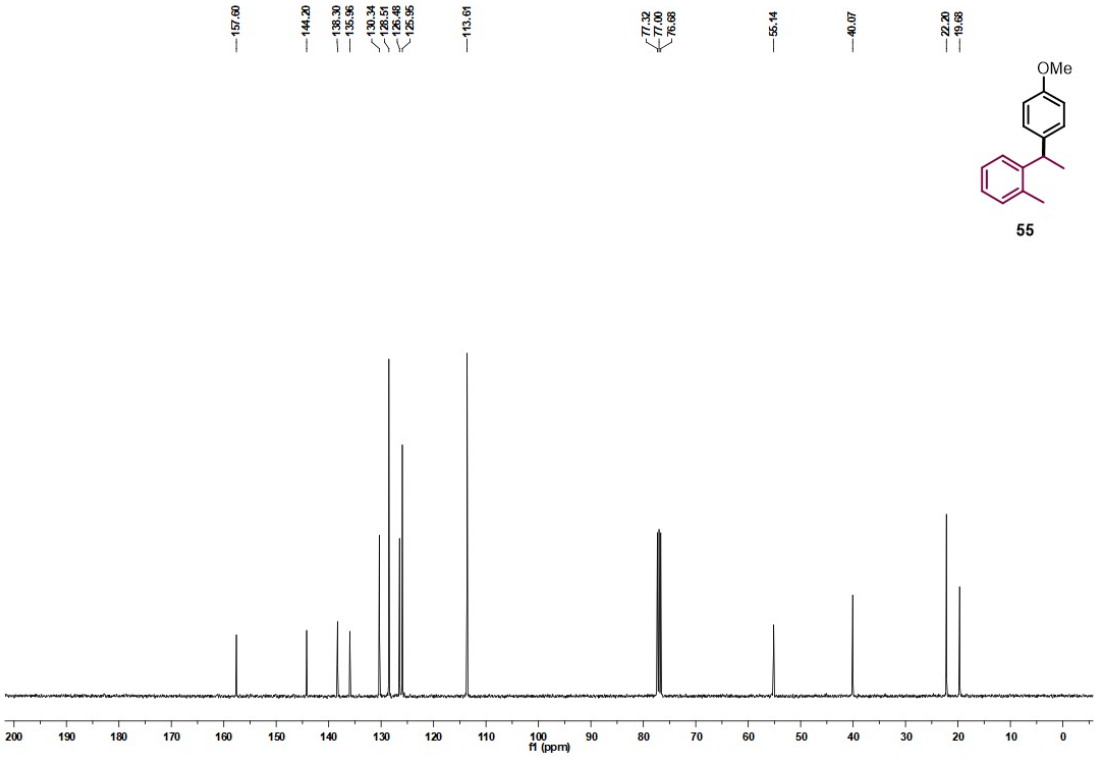
^{13}C-NMR of **54**
$CDCl_3$, 101 MHz, 298 K



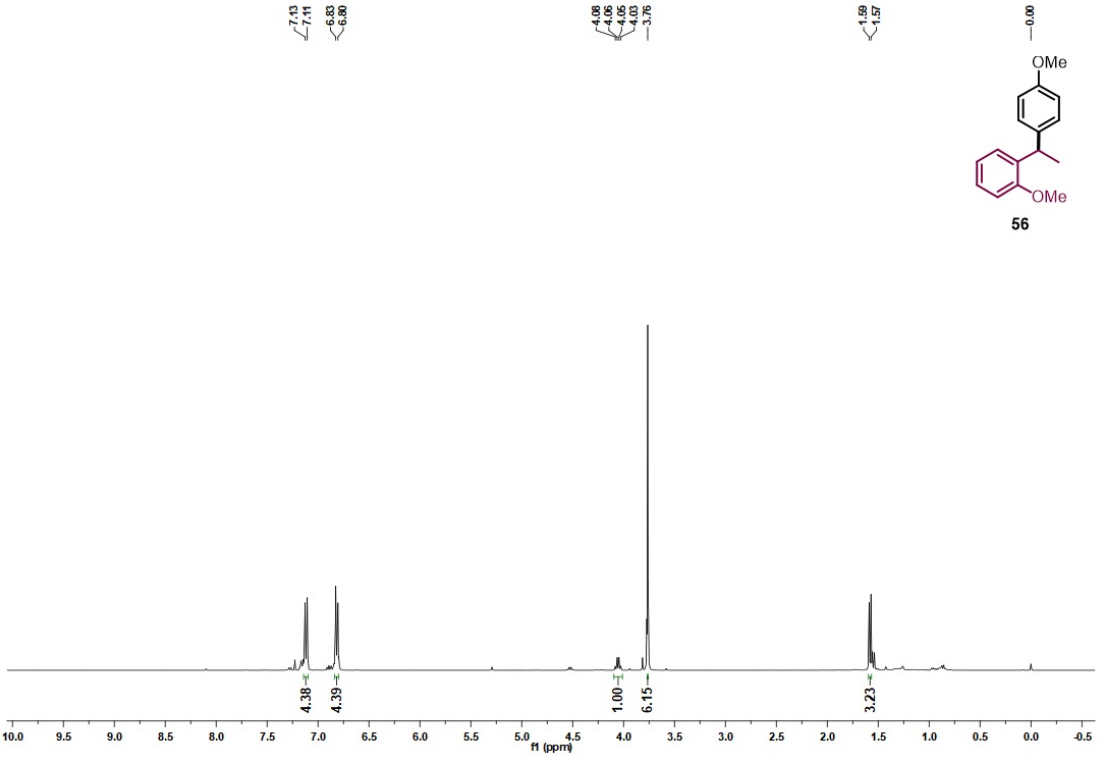
^{1}H-NMR of **55**
$CDCl_3$, 400 MHz, 298 K



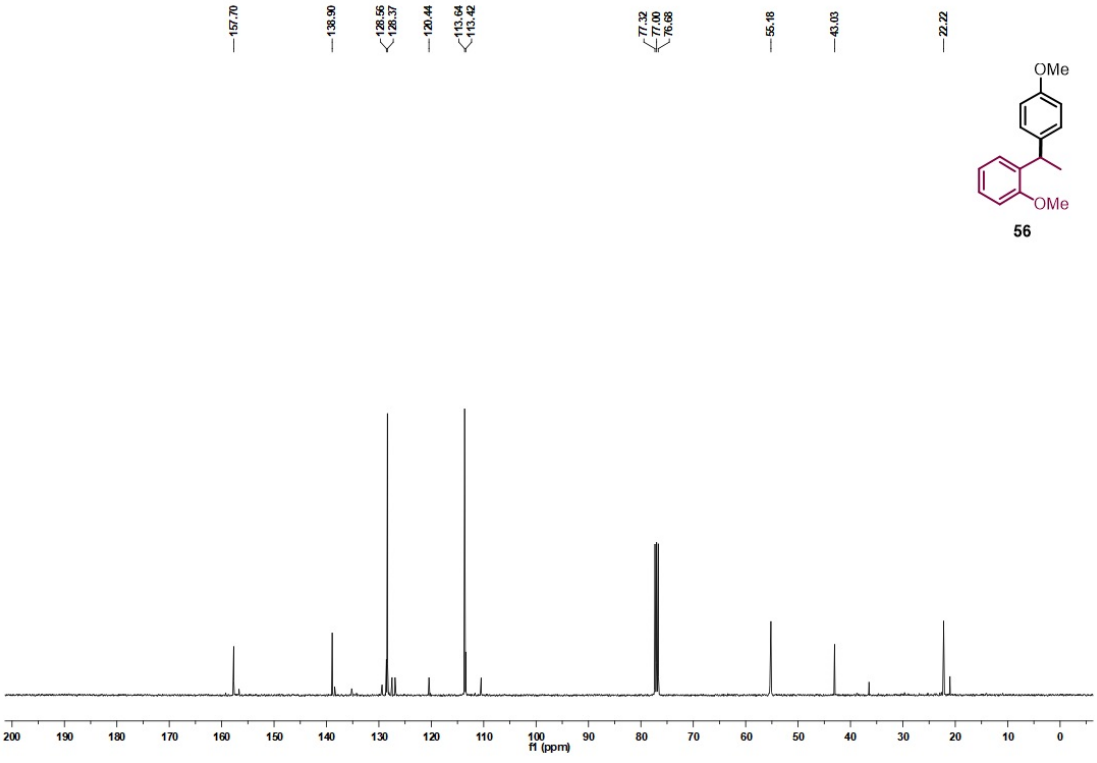
^{13}C-NMR of **55**
$CDCl_3$, 101 MHz, 298 K



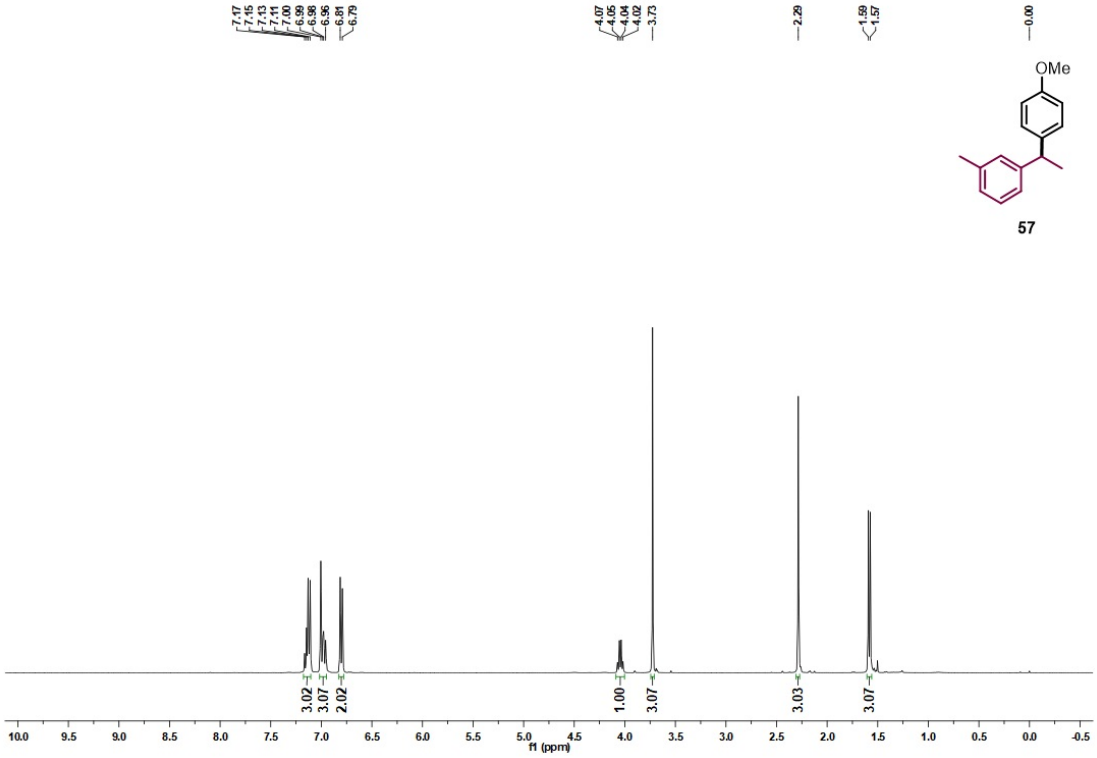
^{1}H-NMR of **56**
$CDCl_3$, 400 MHz, 298 K



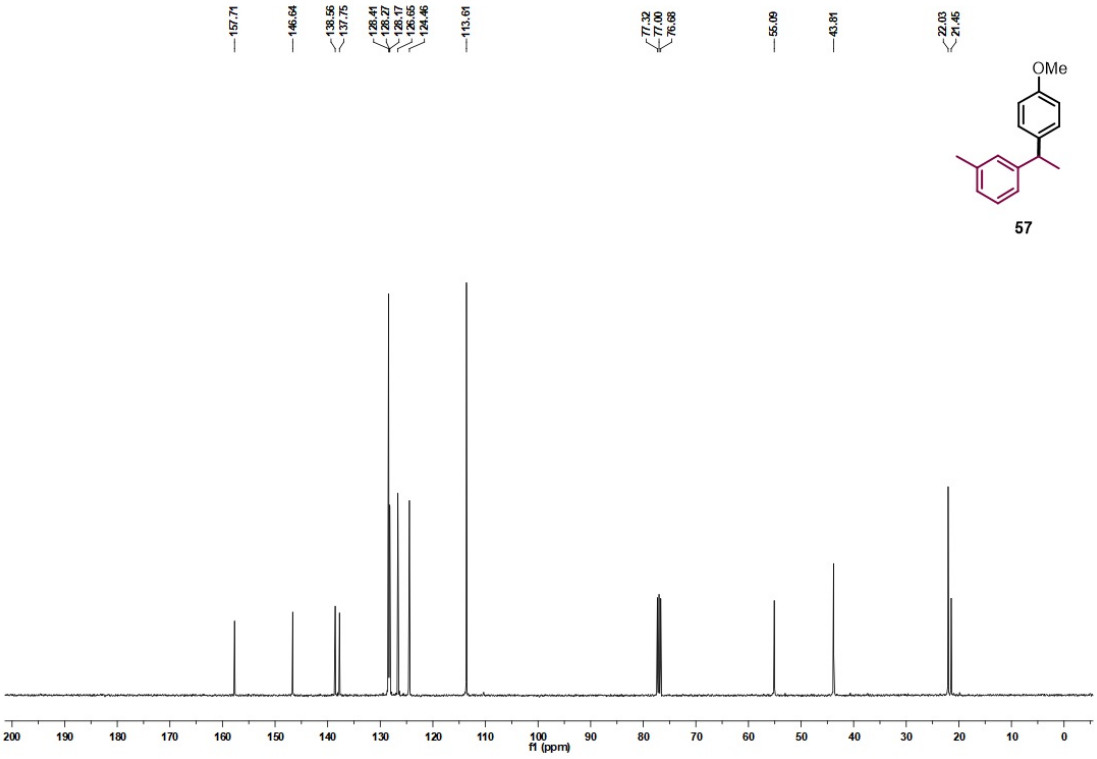
^{13}C-NMR of **56**
$CDCl_3$, 101 MHz, 298 K



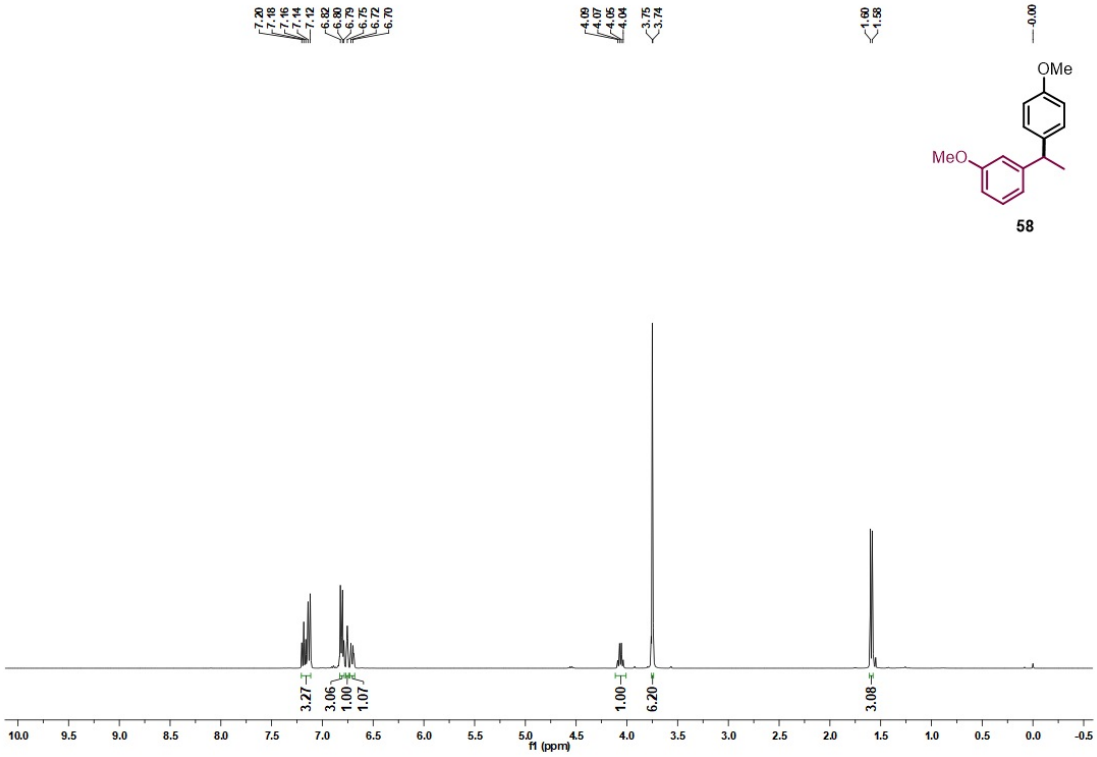
^{1}H-NMR of **57**
$CDCl_3$, 400 MHz, 298 K



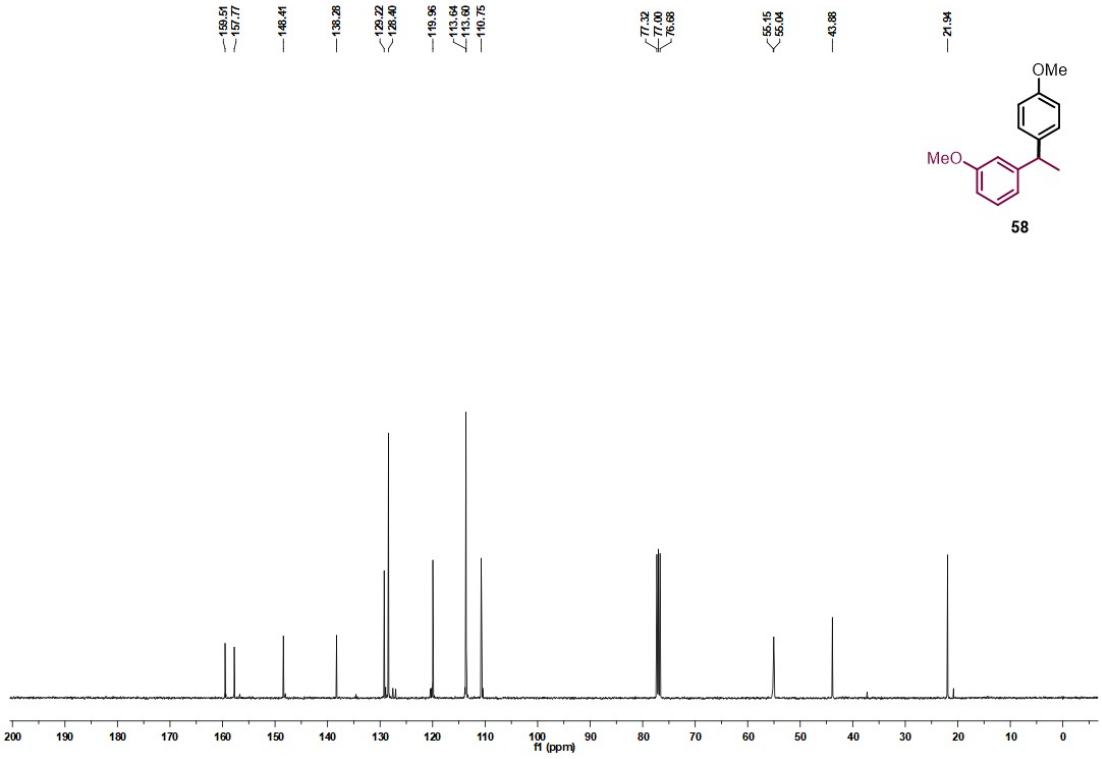
^{13}C-NMR of **57**
$CDCl_3$, 101 MHz, 298 K



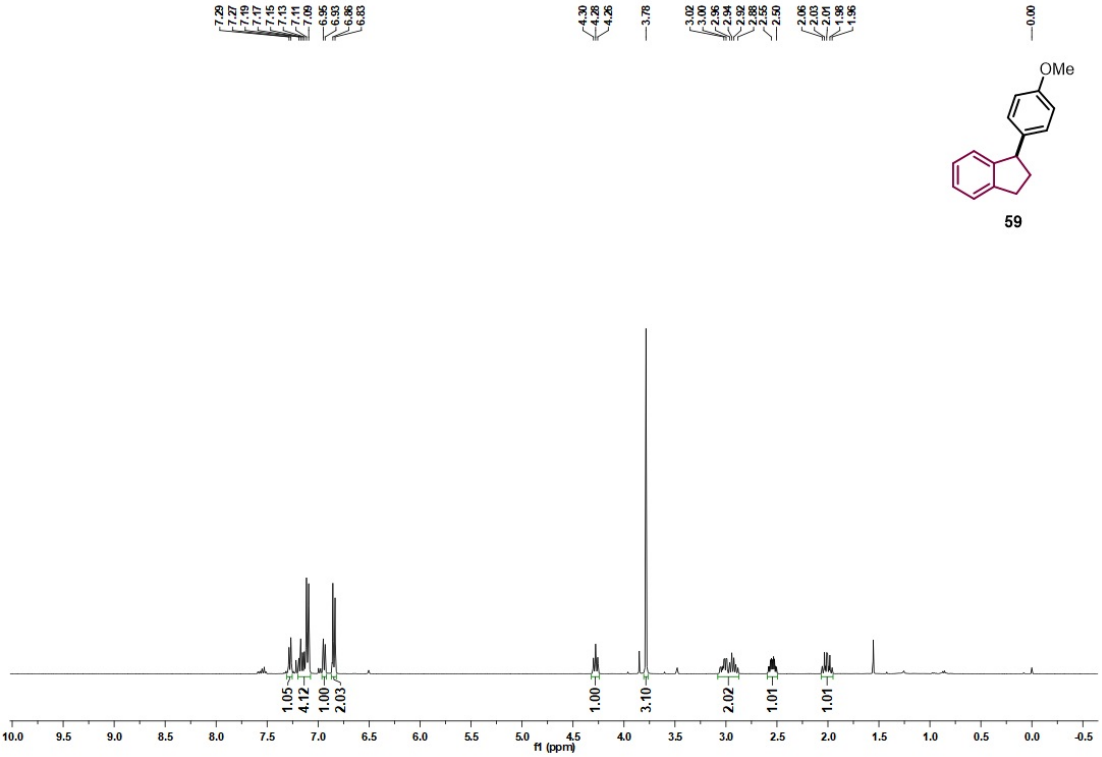
^{1}H-NMR of **58**
$CDCl_3$, 400 MHz, 298 K



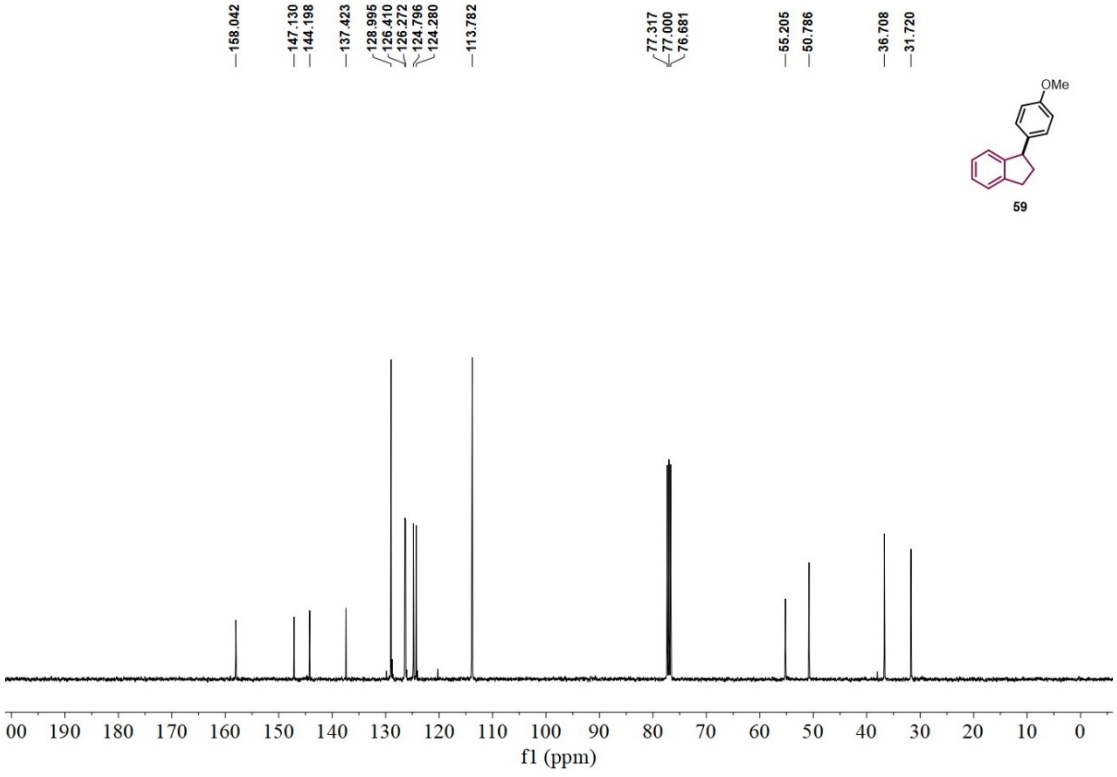
^{13}C-NMR of **58**
$CDCl_3$, 101 MHz, 298 K



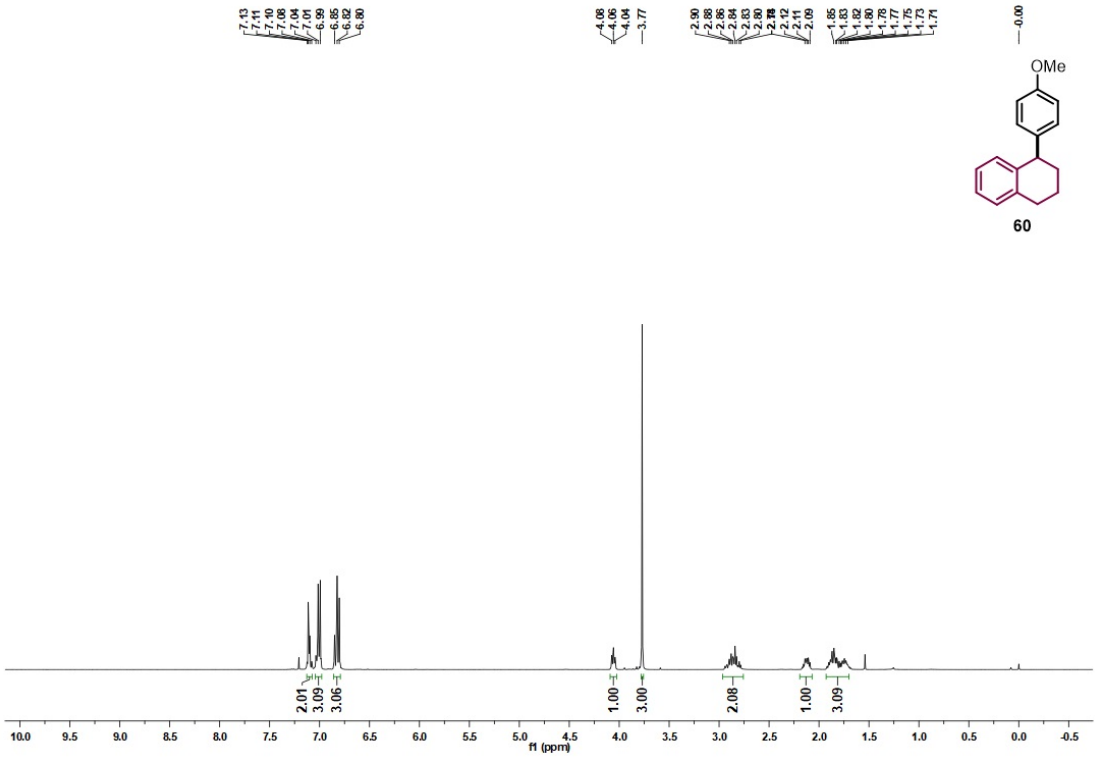
^{1}H-NMR of **59**
$CDCl_3$, 400 MHz, 298 K



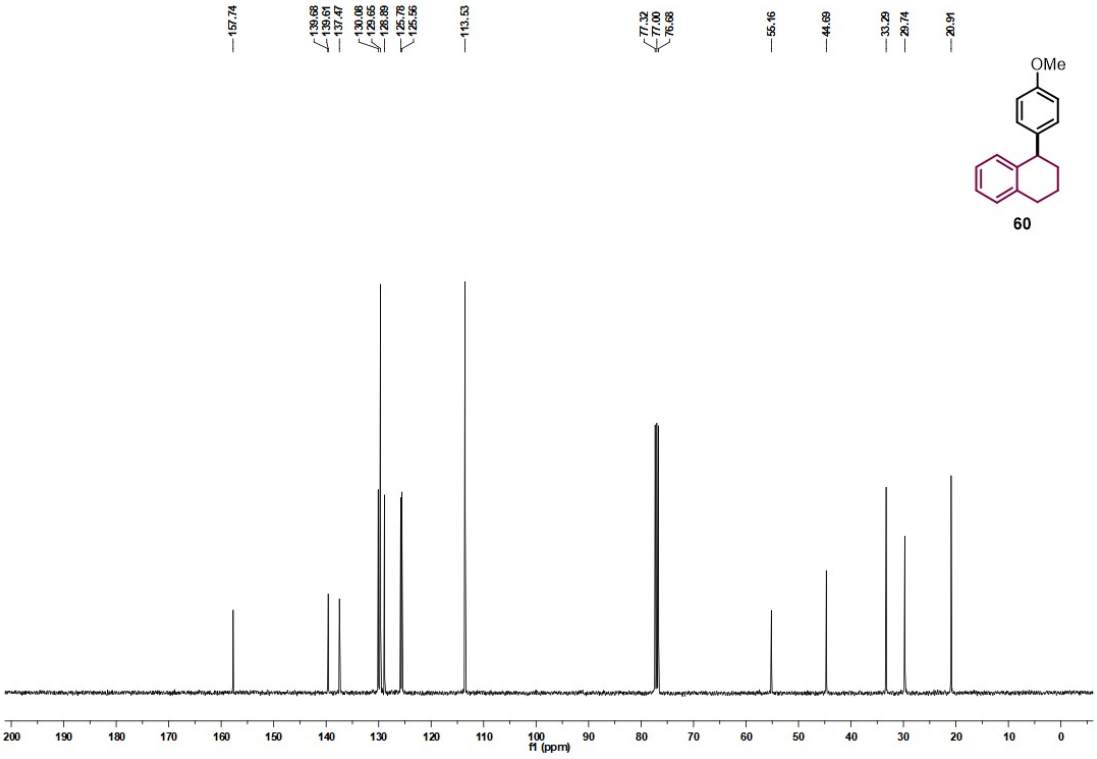
^{13}C-NMR of **59**
$CDCl_3$, 101 MHz, 298 K



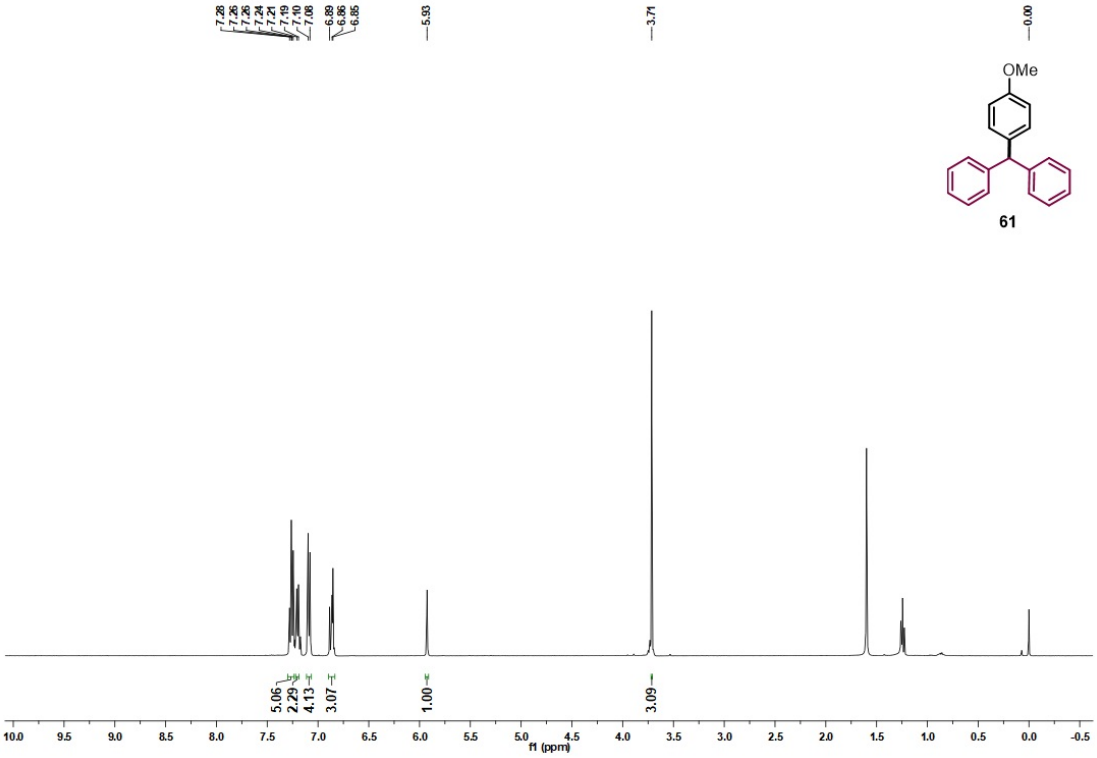
^{1}H-NMR of **60**
$CDCl_3$, 400 MHz, 298 K



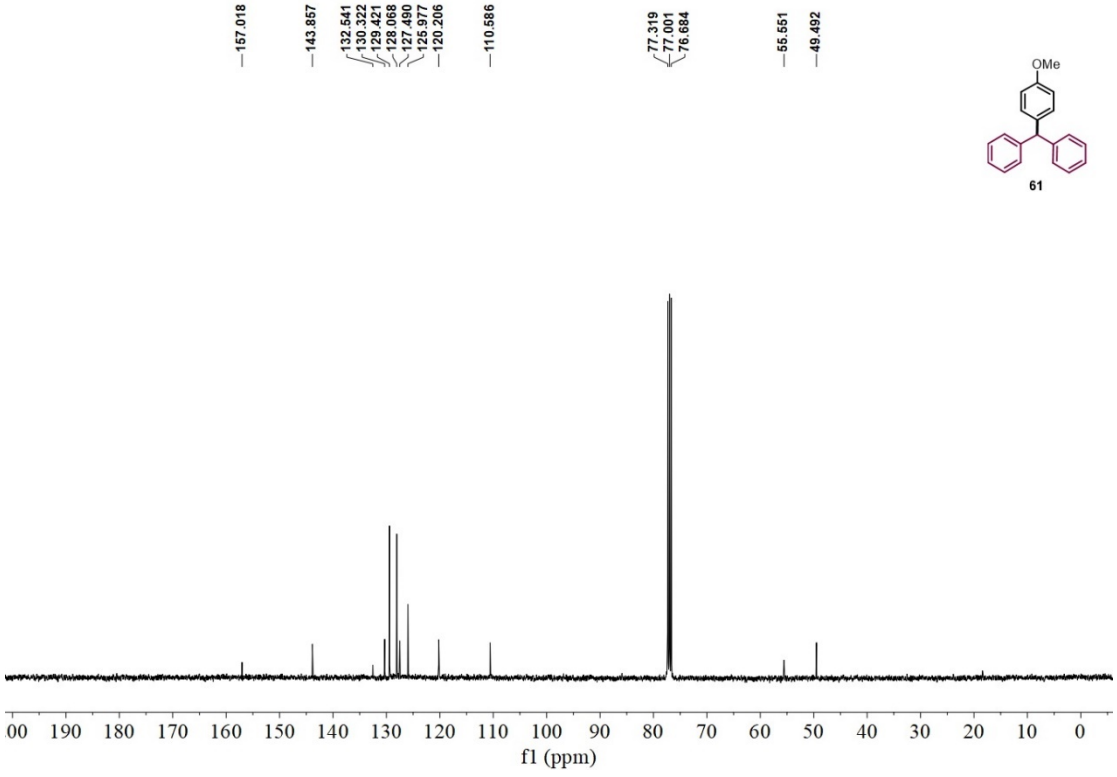
^{13}C-NMR of **60**
$CDCl_3$, 101 MHz, 298 K



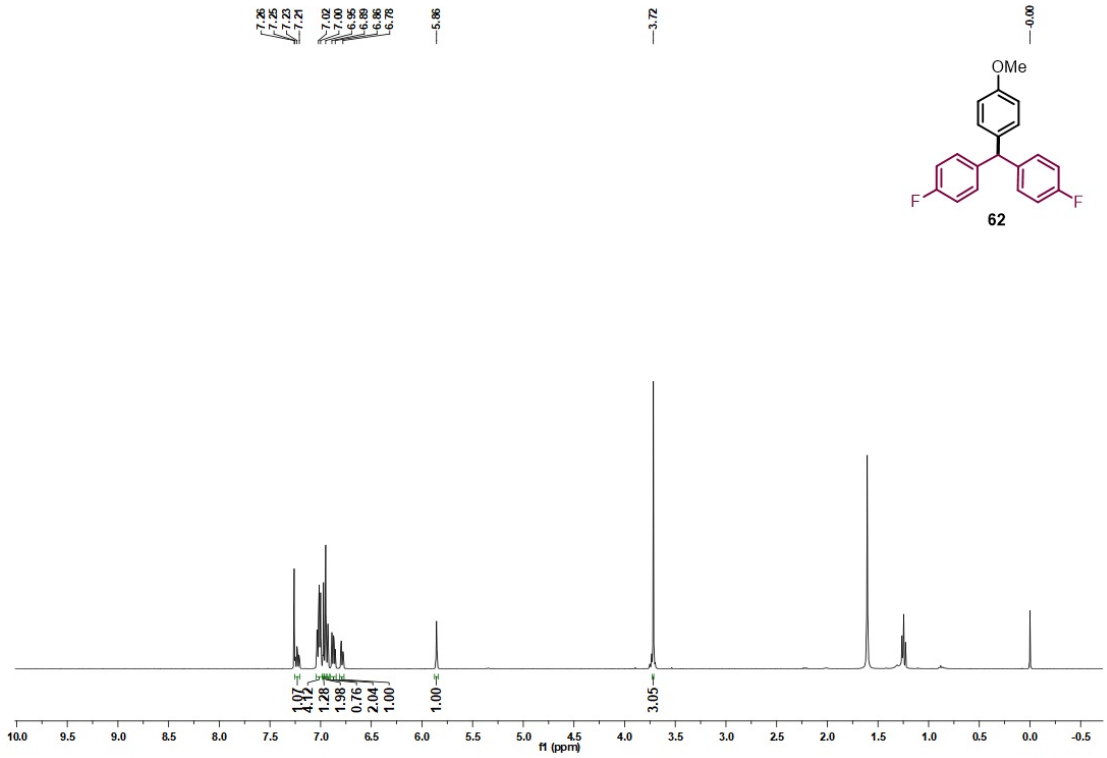
^{1}H-NMR of **61**
$CDCl_3$, 400 MHz, 298 K



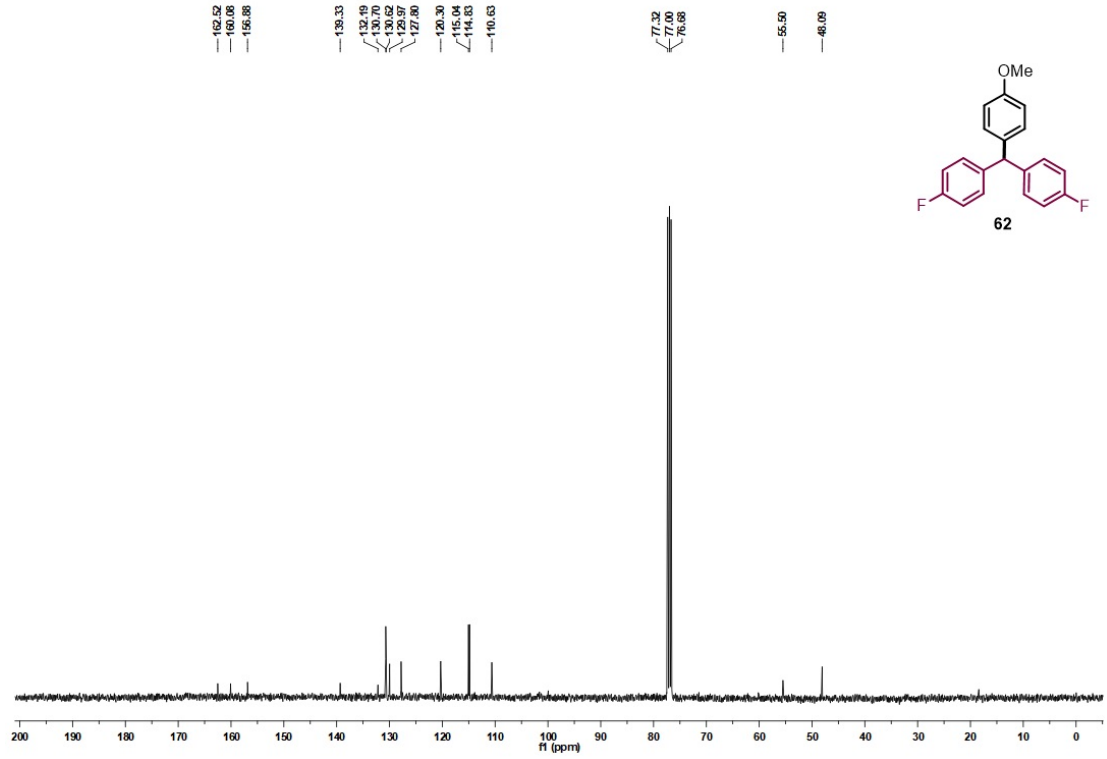
^{13}C-NMR of **61**
$CDCl_3$, 101 MHz, 298 K



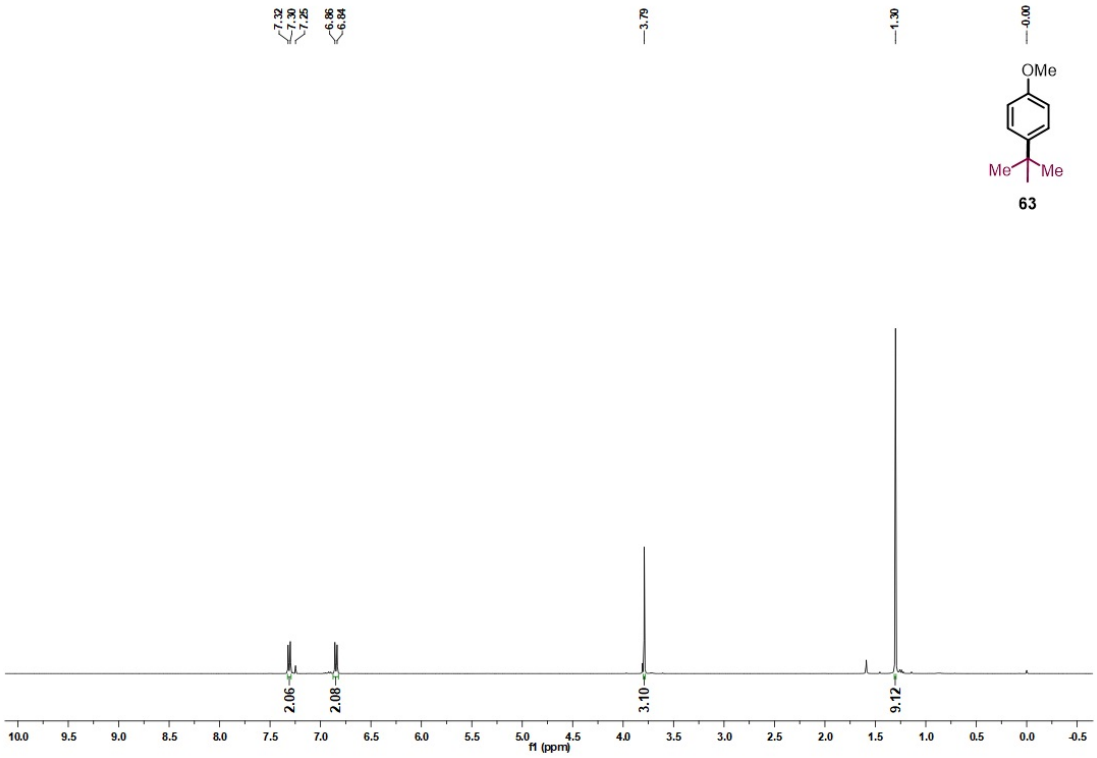
^{1}H-NMR of **62**
$CDCl_3$, 400 MHz, 298 K



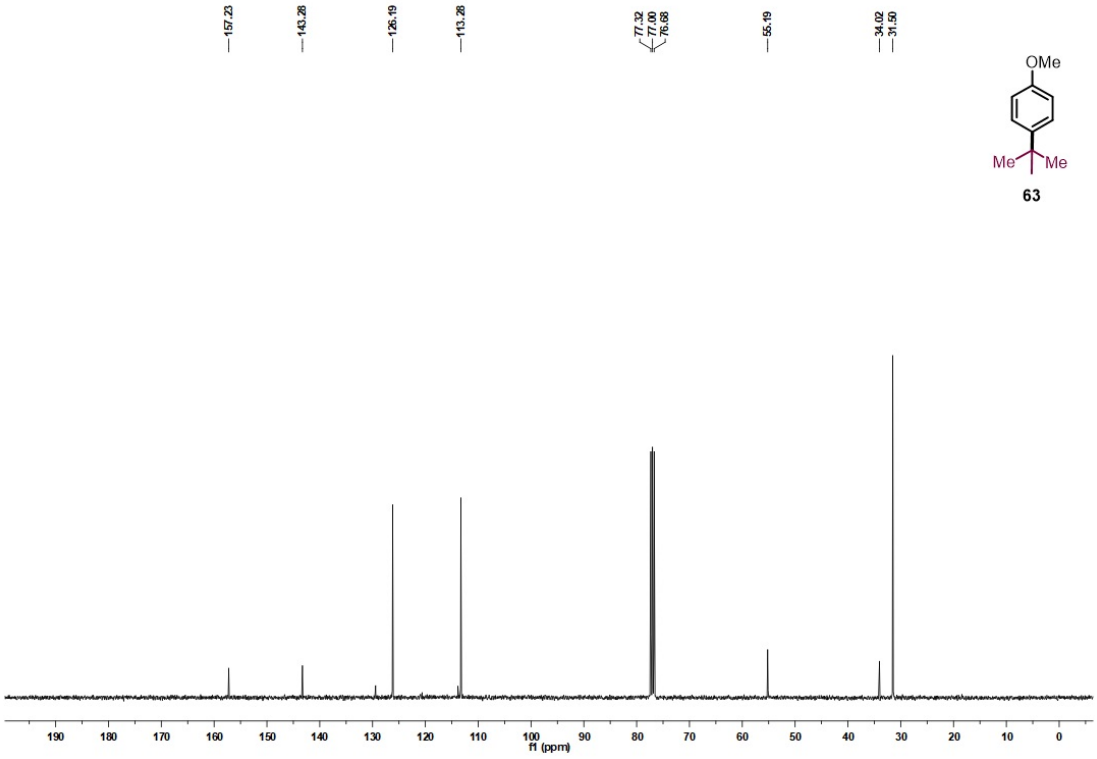
^{13}C-NMR of **62**
$CDCl_3$, 101 MHz, 298 K



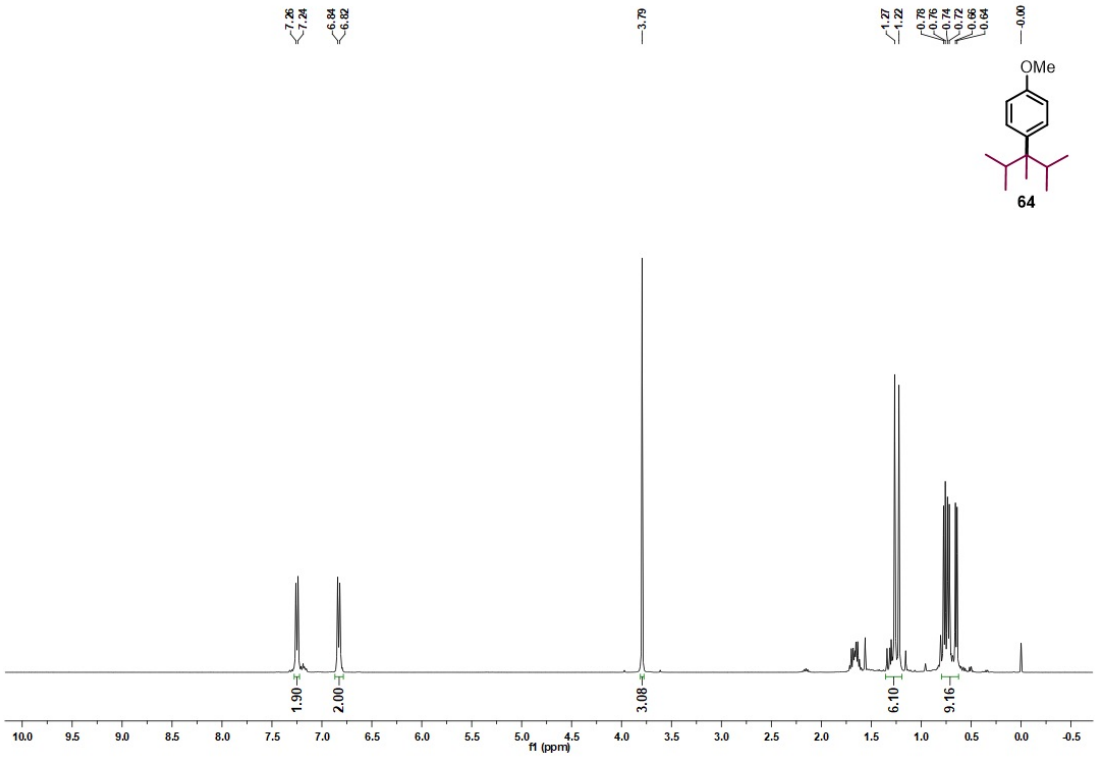
^{1}H-NMR of **63**
$CDCl_3$, 400 MHz, 298 K



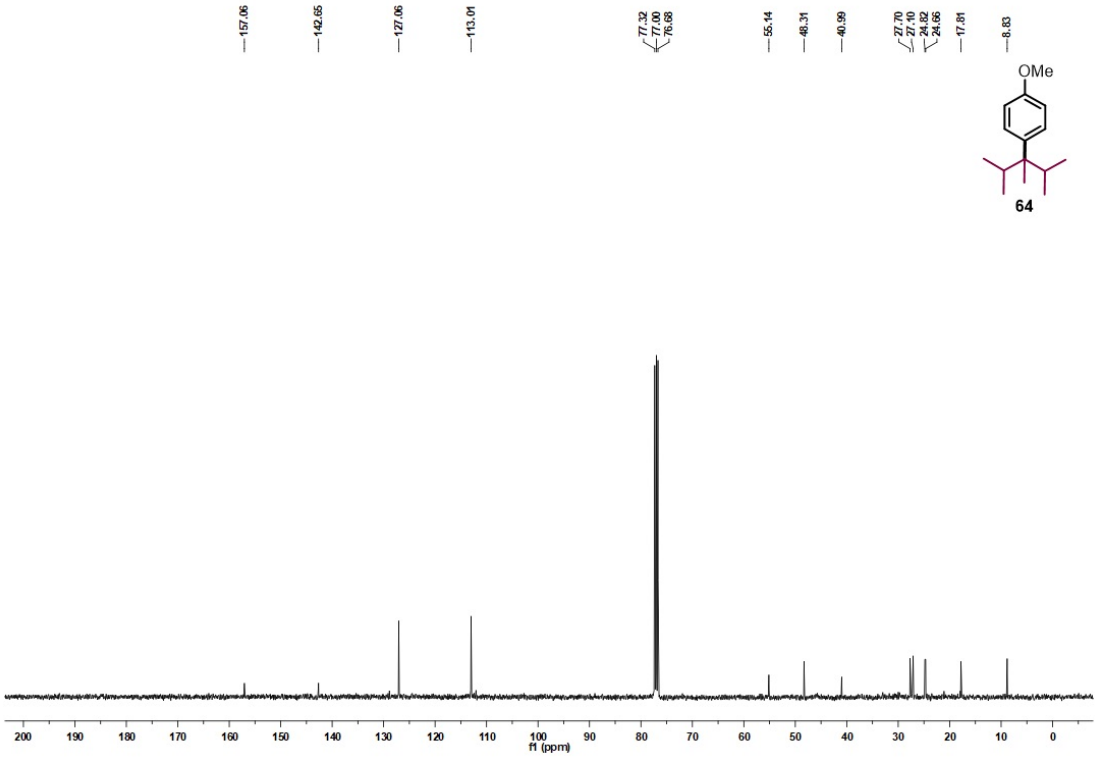
^{13}C-NMR of **63**
$CDCl_3$, 101 MHz, 298 K



^{1}H-NMR of **64**
$CDCl_3$, 400 MHz, 298 K

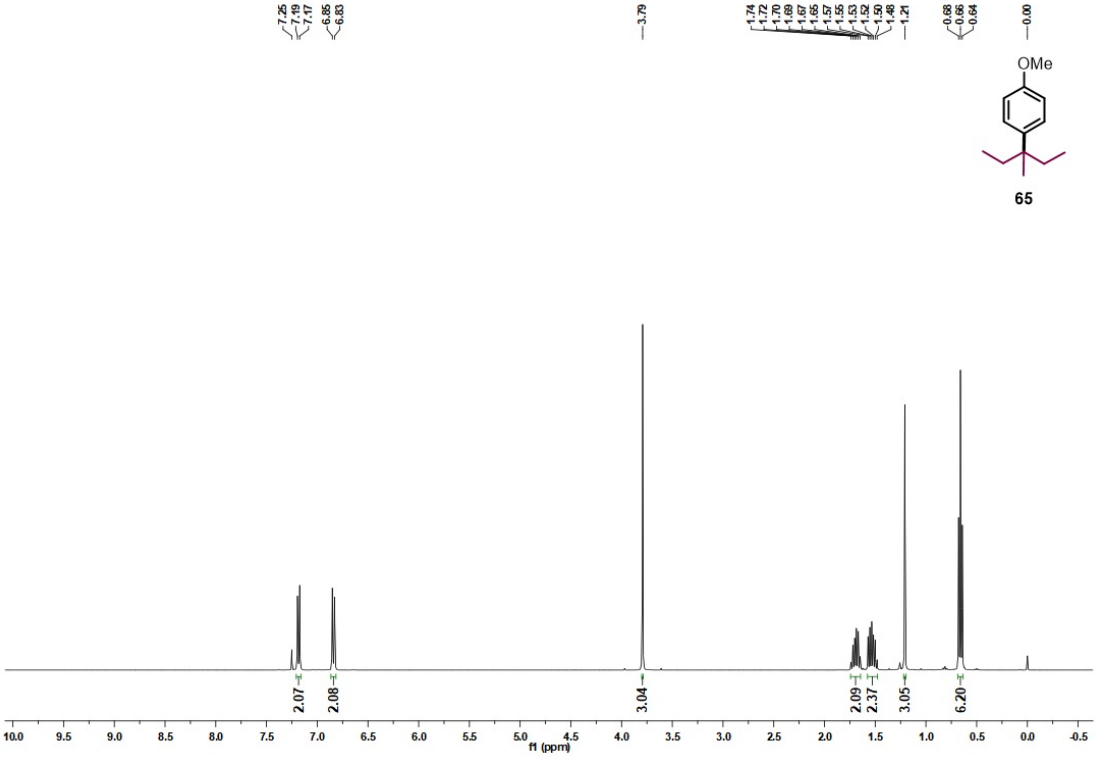


^{13}C-NMR of **64**
$CDCl_3$, 101 MHz, 298 K



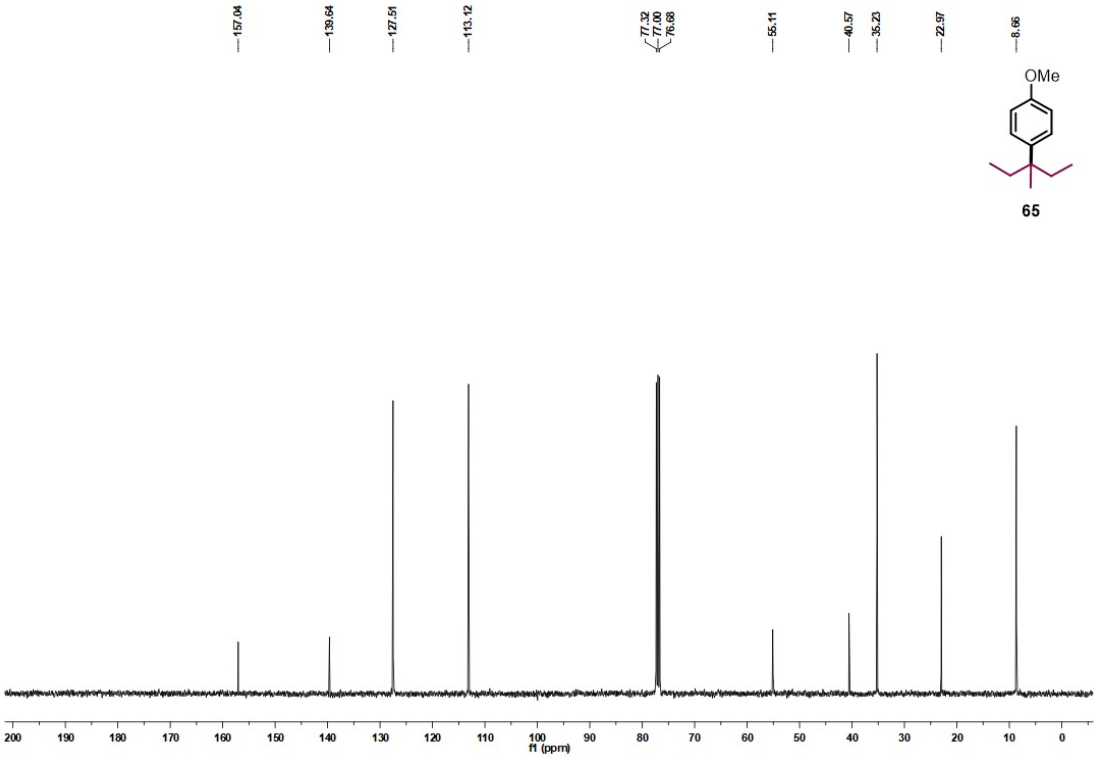
^{1}H-NMR of **65**

$CDCl_3$, 400 MHz, 298 K

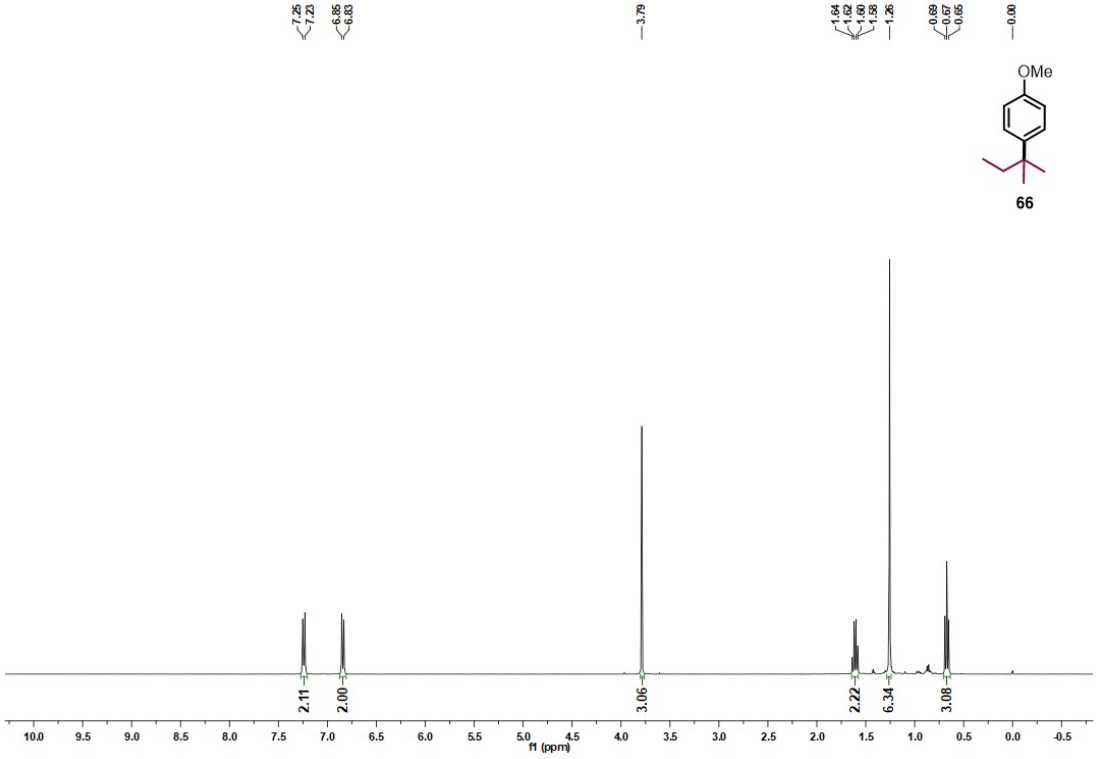


^{13}C-NMR of **65**

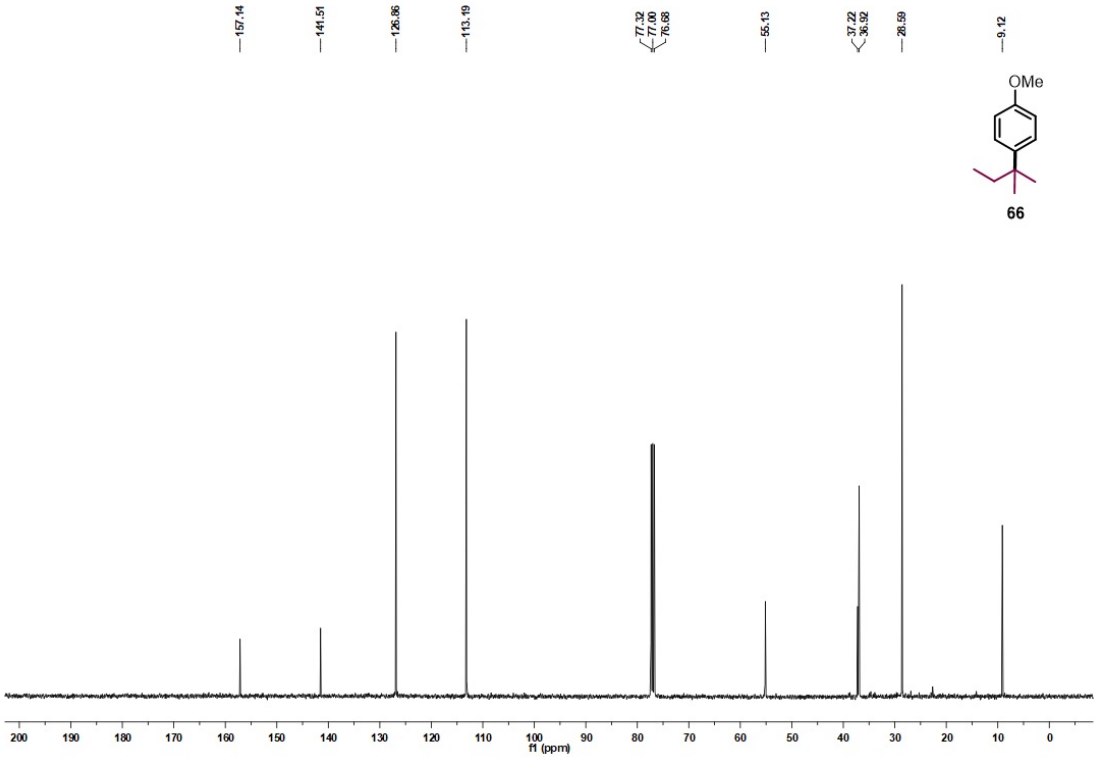
$CDCl_3$, 101 MHz, 298 K



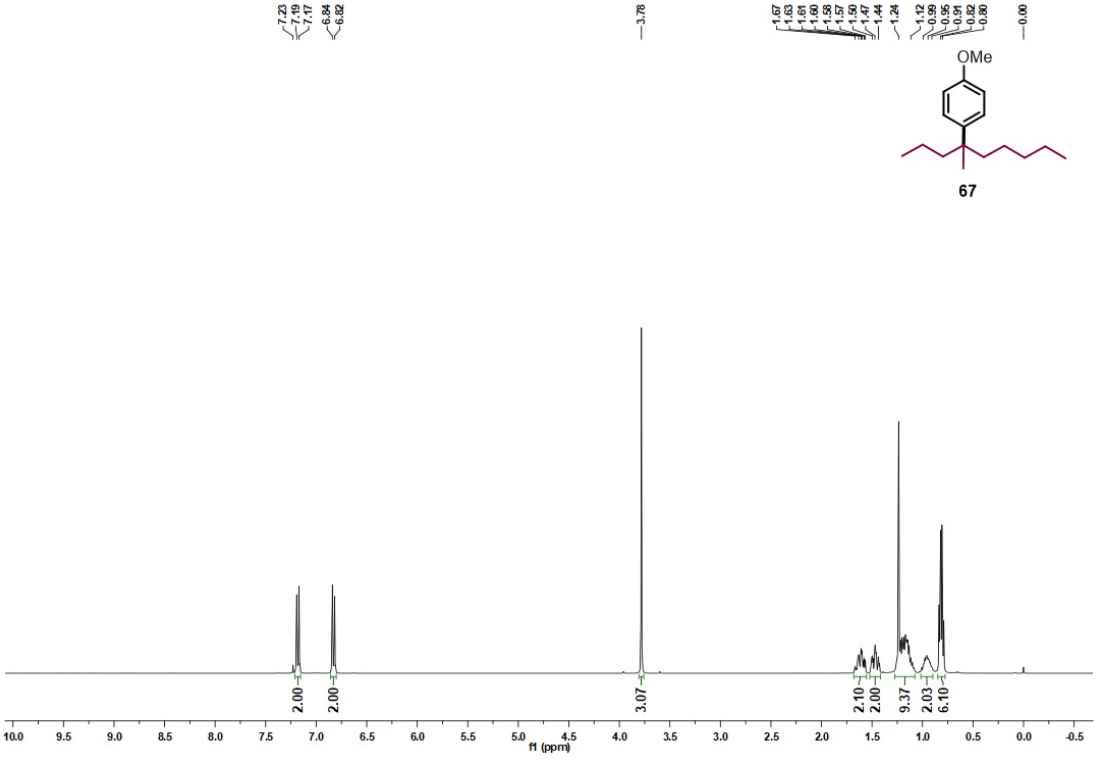
^{1}H-NMR of **66**
$CDCl_3$, 400 MHz, 298 K



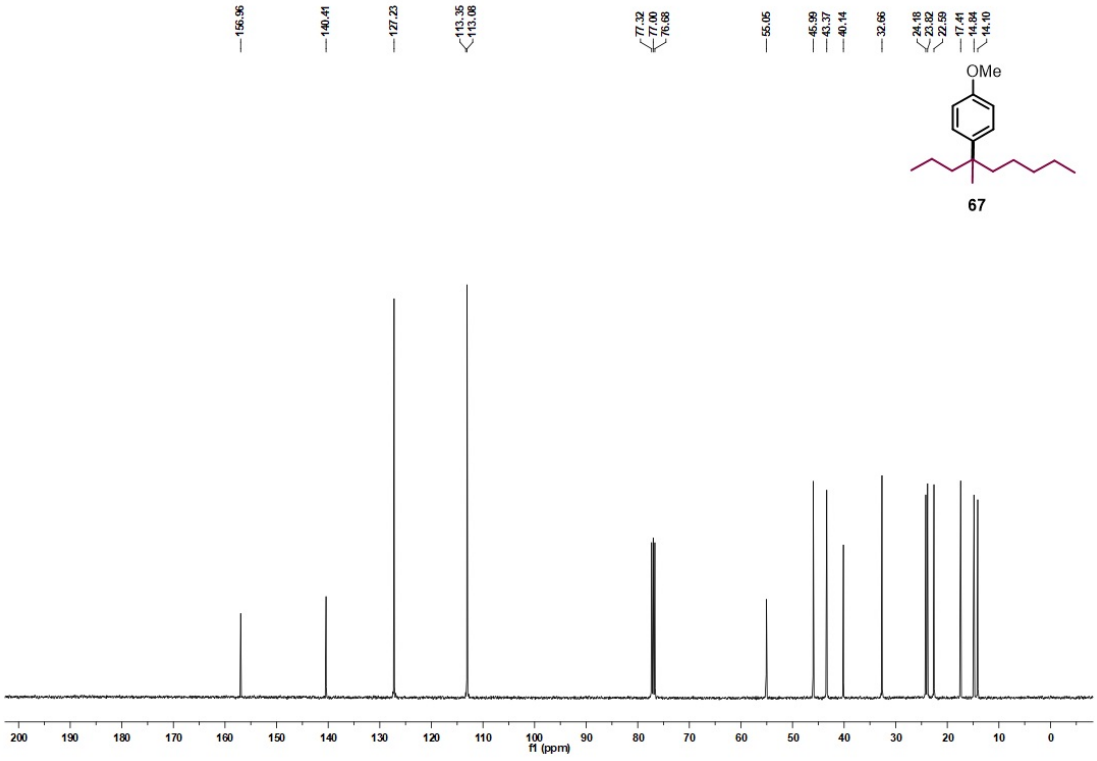
^{13}C-NMR of **66**
$CDCl_3$, 101 MHz, 298 K



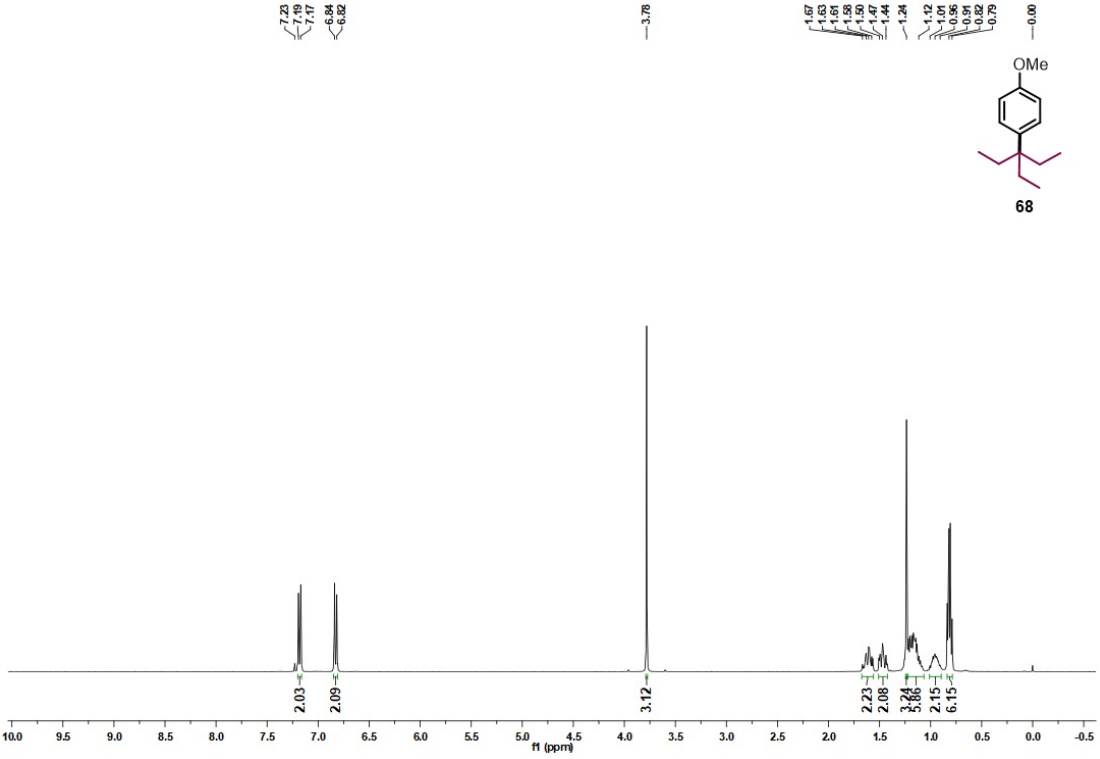
^{1}H-NMR of **67**
$CDCl_3$, 400 MHz, 298 K



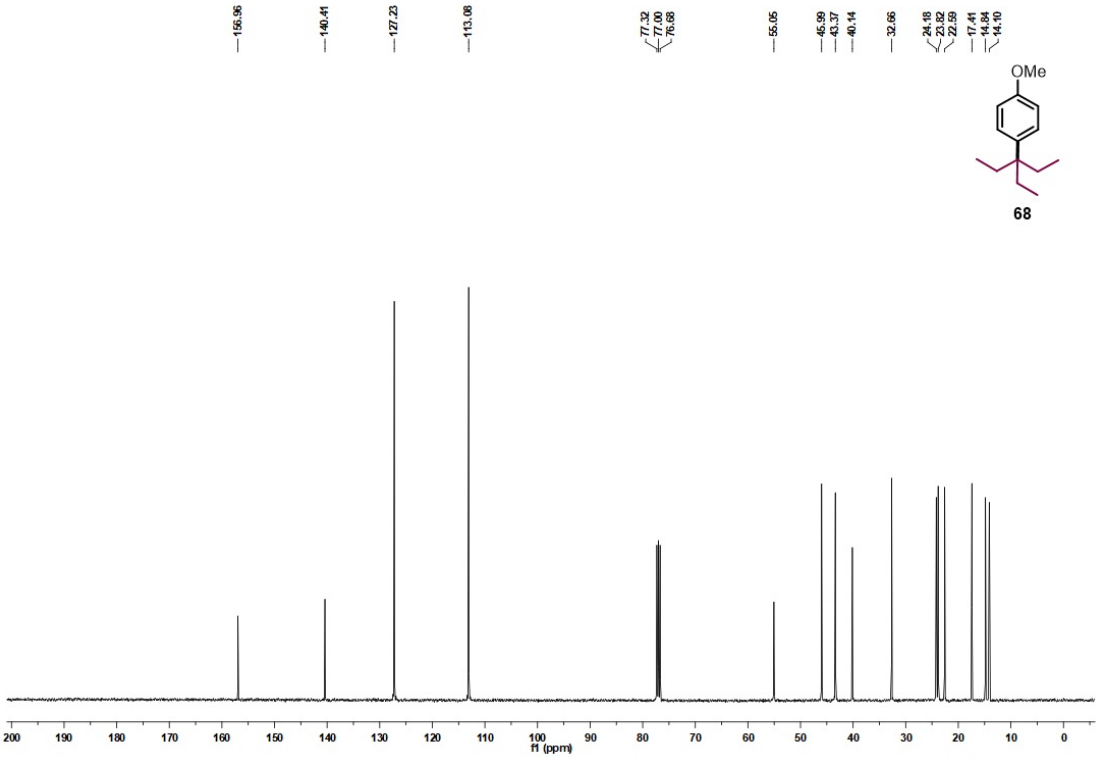
^{13}C-NMR of **67**
$CDCl_3$, 101 MHz, 298 K



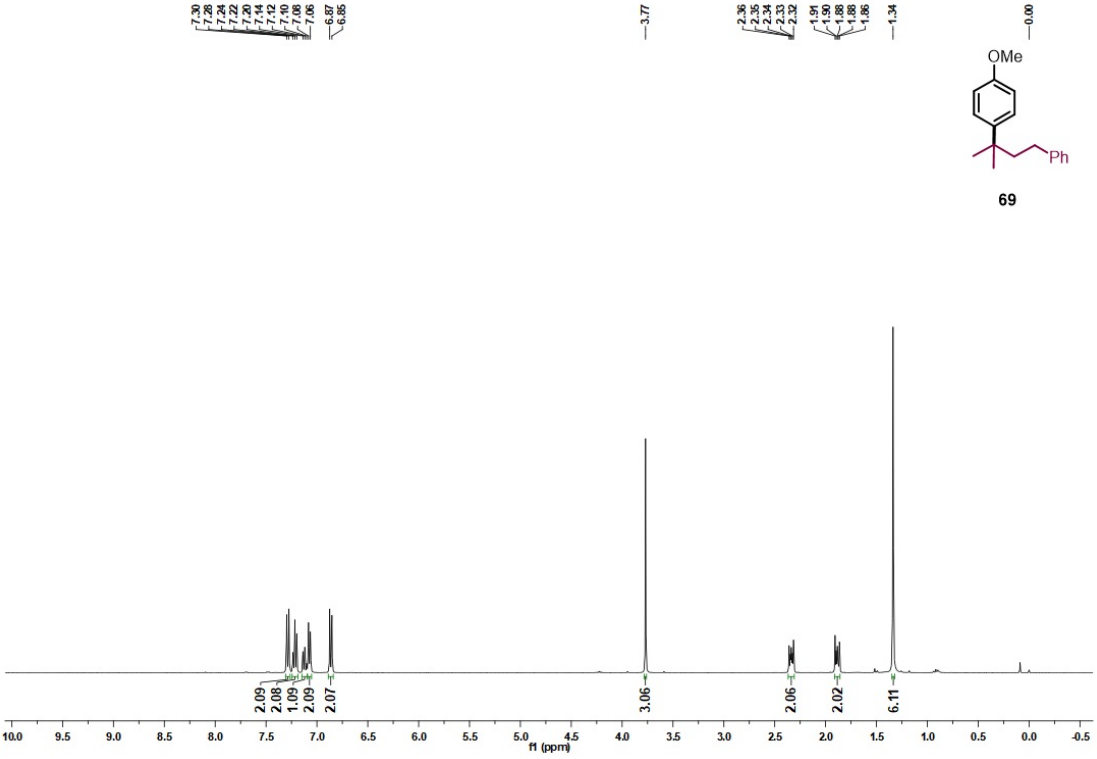
^{1}H-NMR of **68**
$CDCl_3$, 400 MHz, 298 K



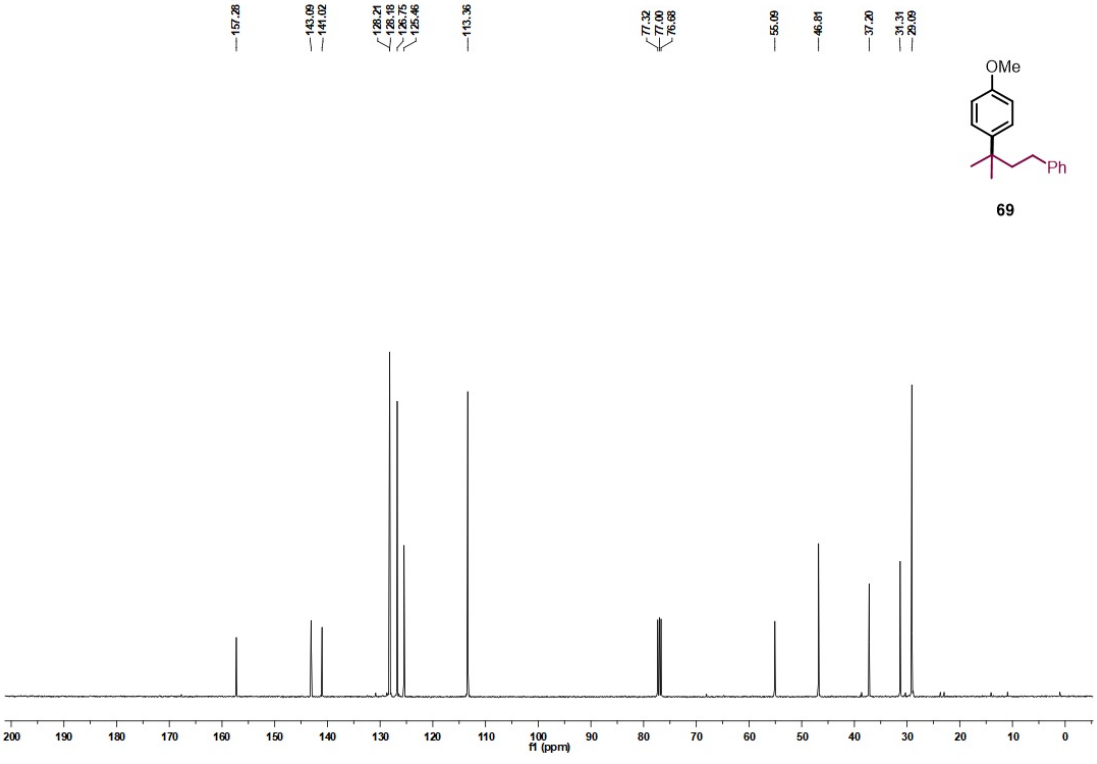
^{13}C-NMR of **68**
$CDCl_3$, 101 MHz, 298 K



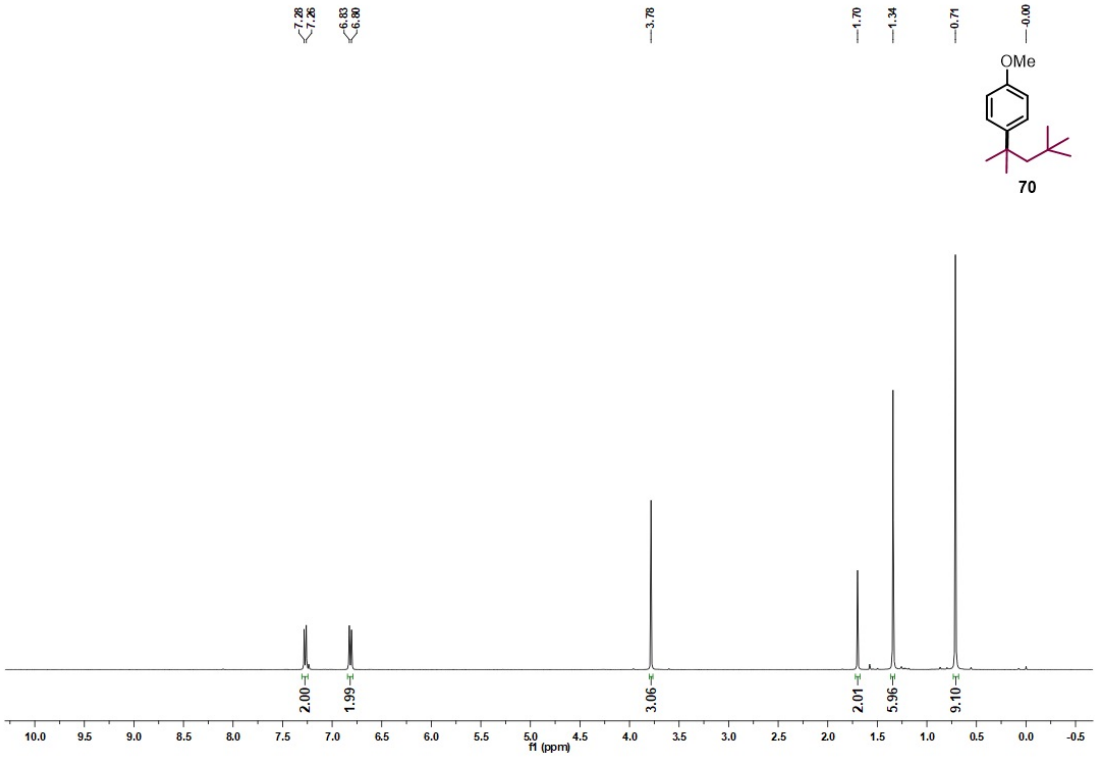
^{1}H-NMR of **69**
$CDCl_3$, 400 MHz, 298 K



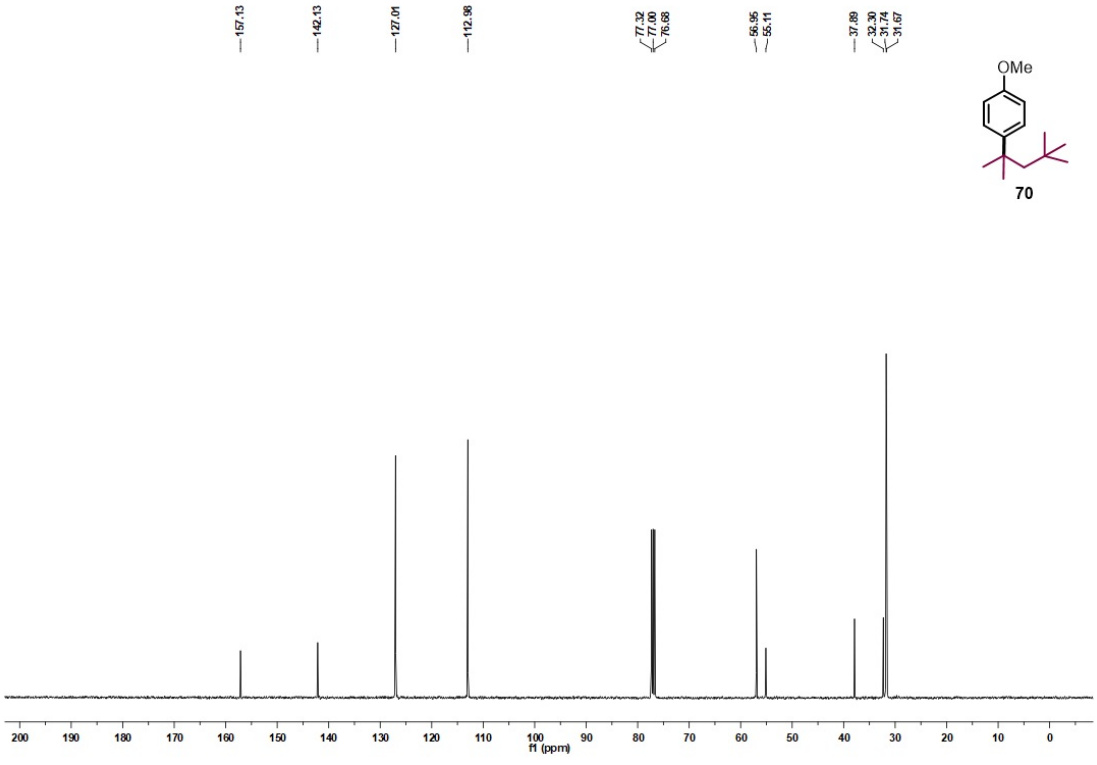
^{13}C-NMR of **69**
$CDCl_3$, 101 MHz, 298 K



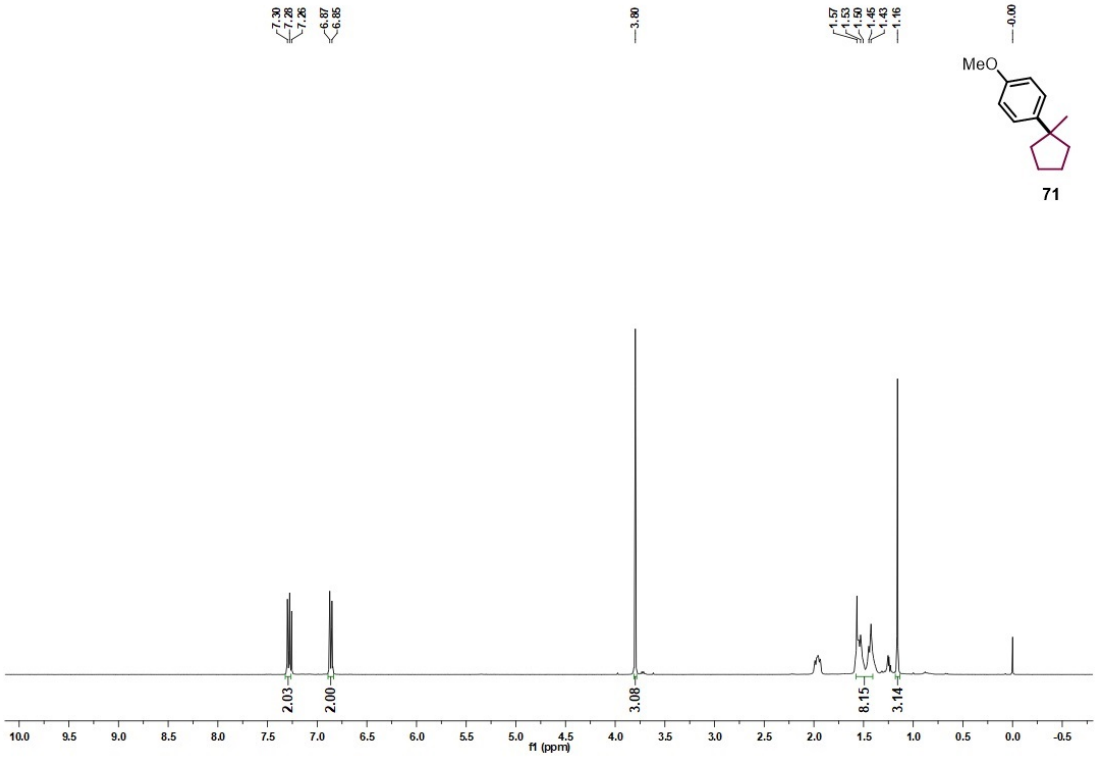
^{1}H-NMR of **70**
$CDCl_3$, 400 MHz, 298 K



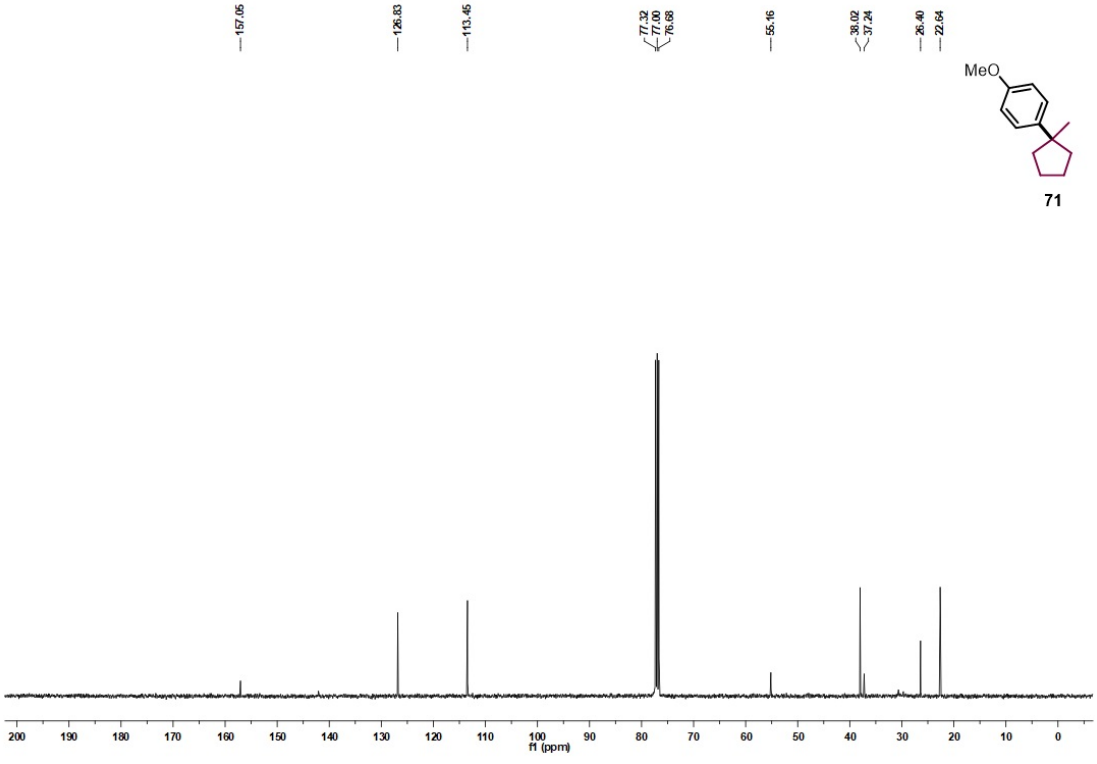
^{13}C-NMR of **70**
$CDCl_3$, 101 MHz, 298 K



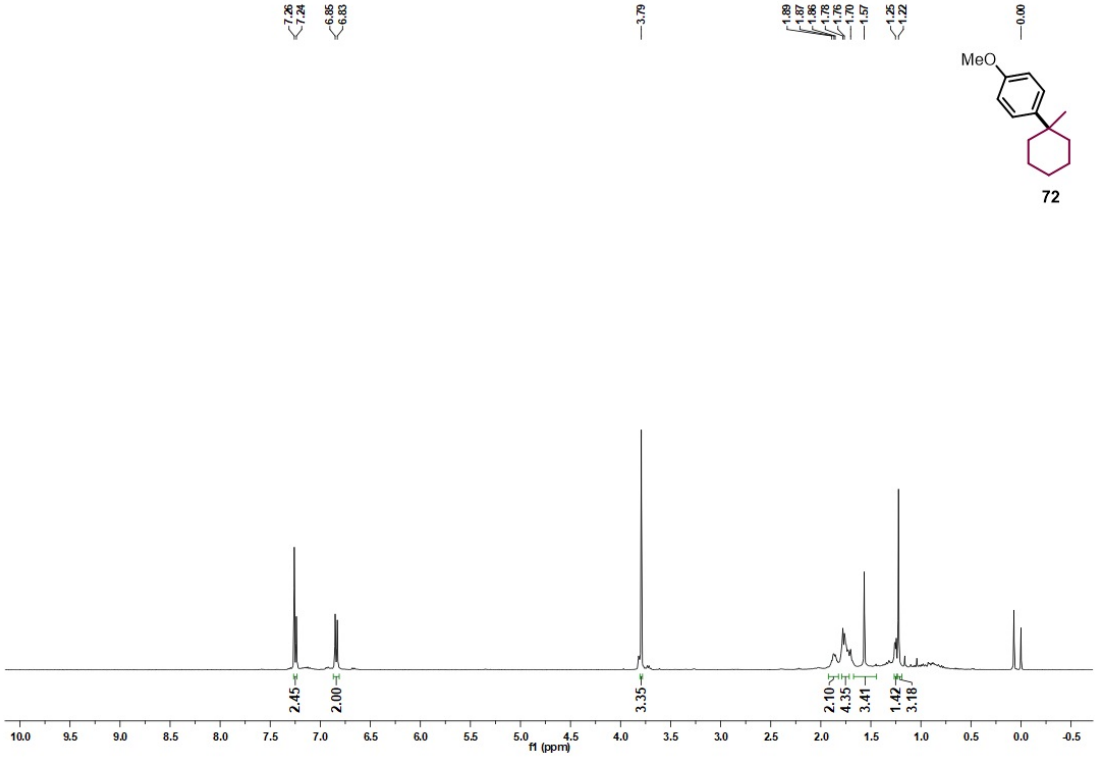
^{1}H-NMR of **71**
$CDCl_3$, 400 MHz, 298 K



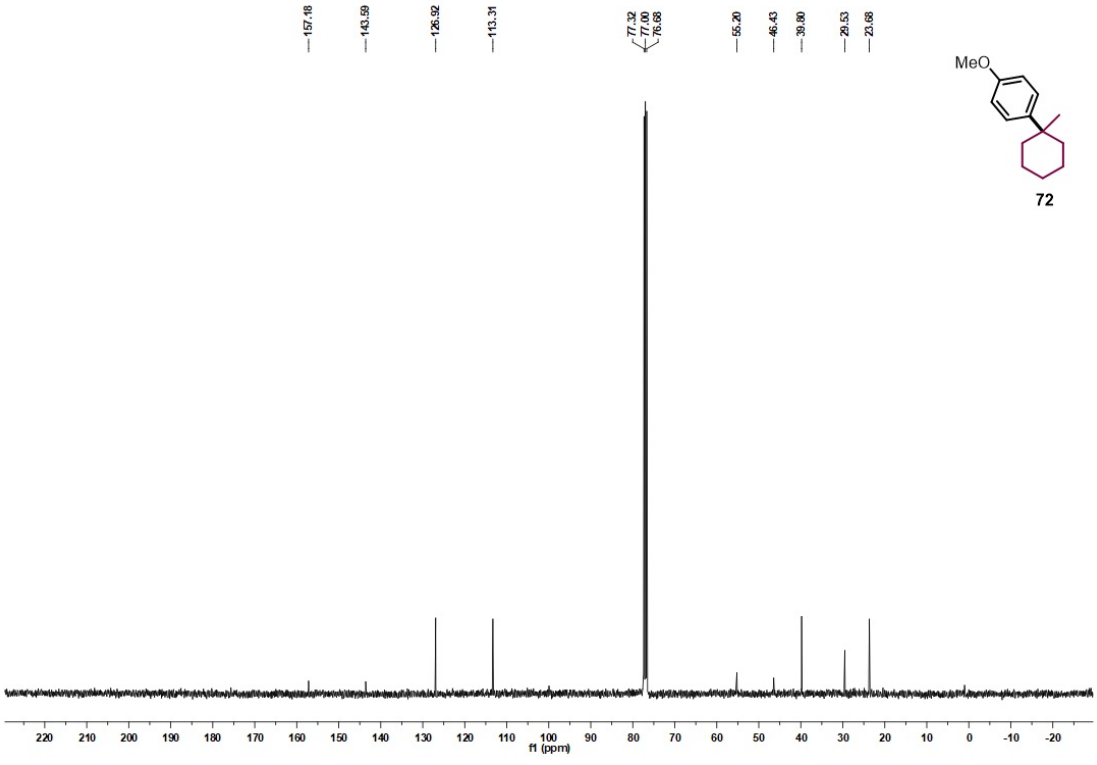
^{13}C-NMR of **71**
$CDCl_3$, 101 MHz, 298 K



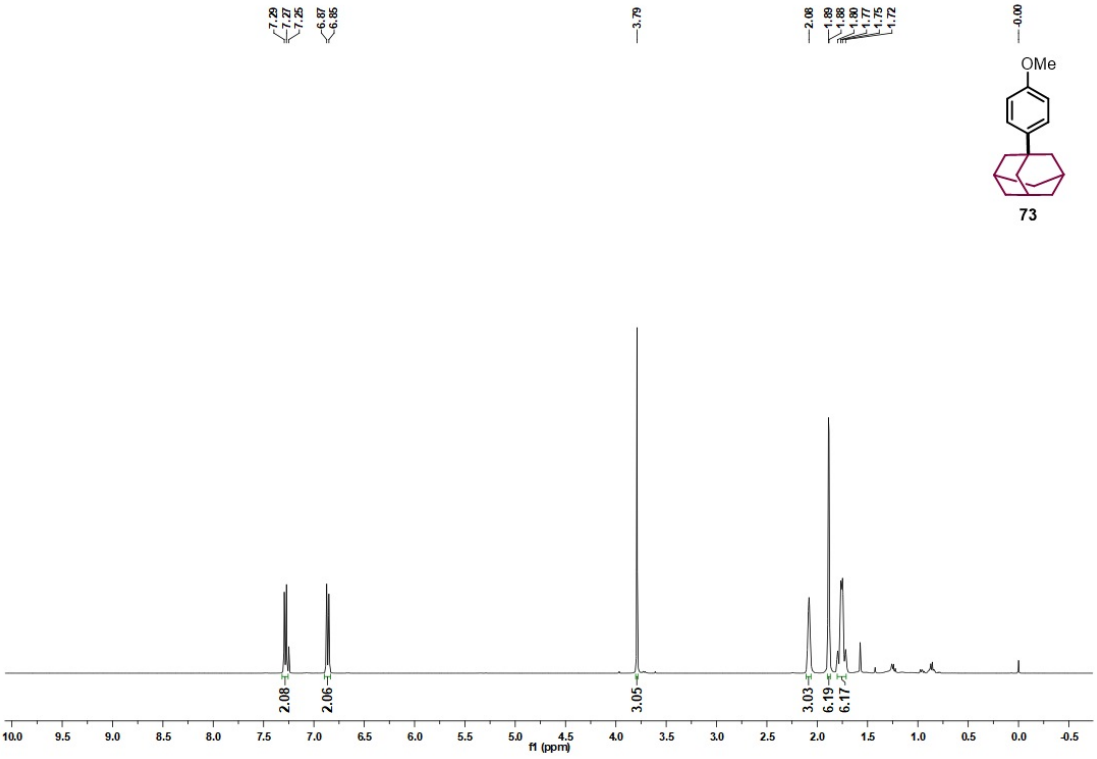
^{1}H-NMR of **72**
$CDCl_3$, 400 MHz, 298 K



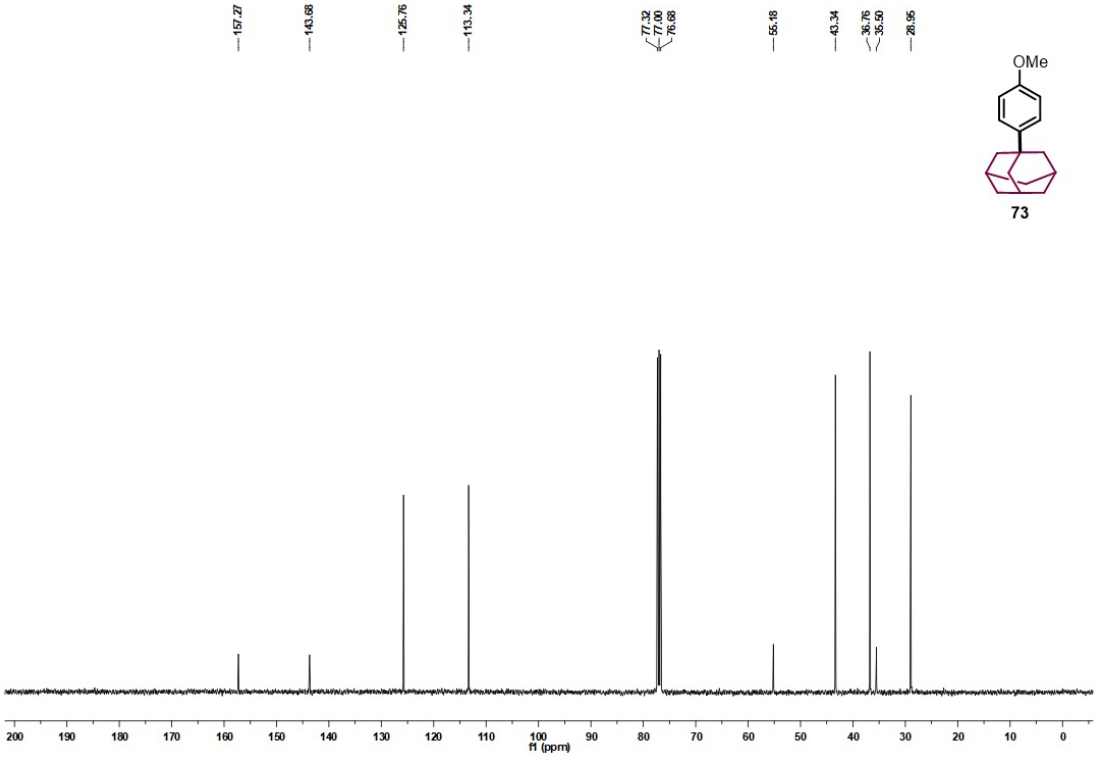
^{13}C-NMR of **72**
$CDCl_3$, 101 MHz, 298 K



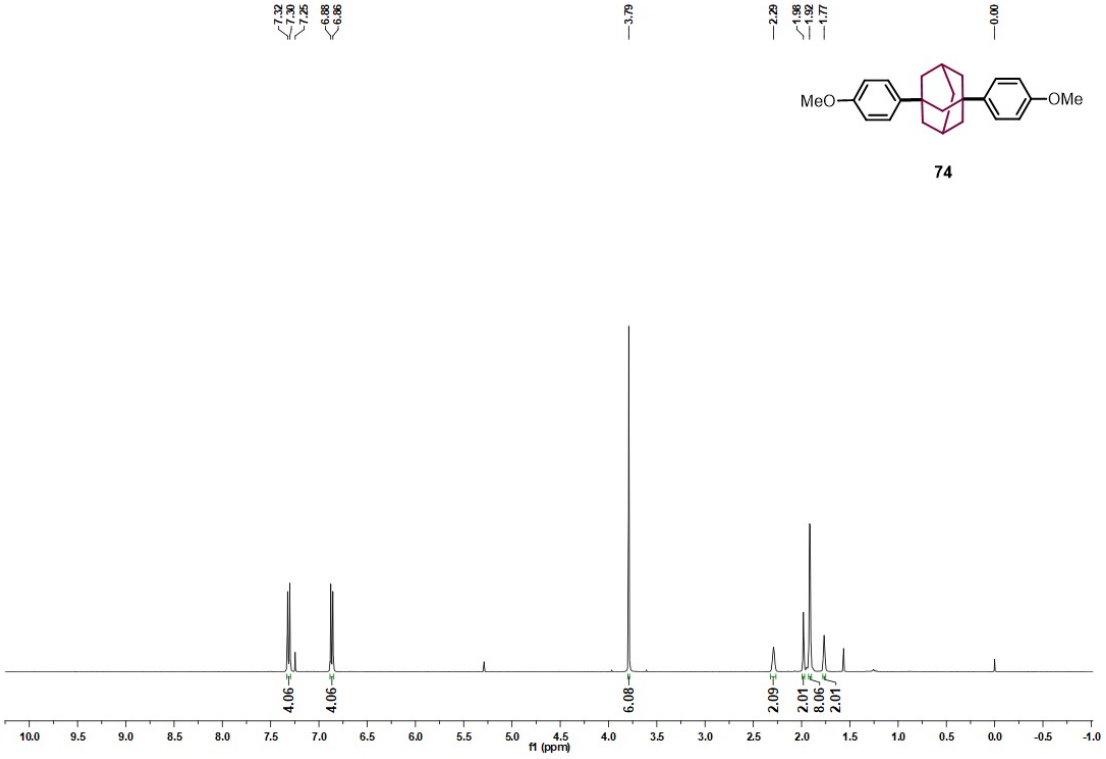
^{1}H-NMR of **73**
$CDCl_3$, 400 MHz, 298 K



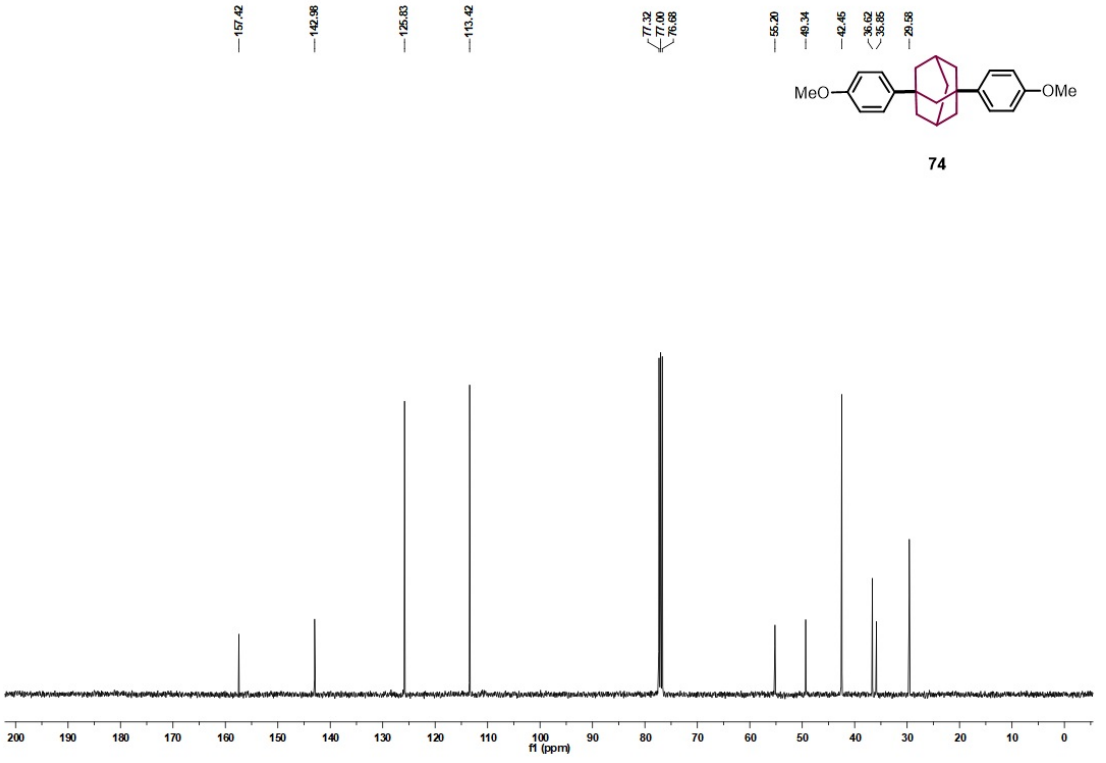
^{13}C-NMR of **73**
$CDCl_3$, 101 MHz, 298 K



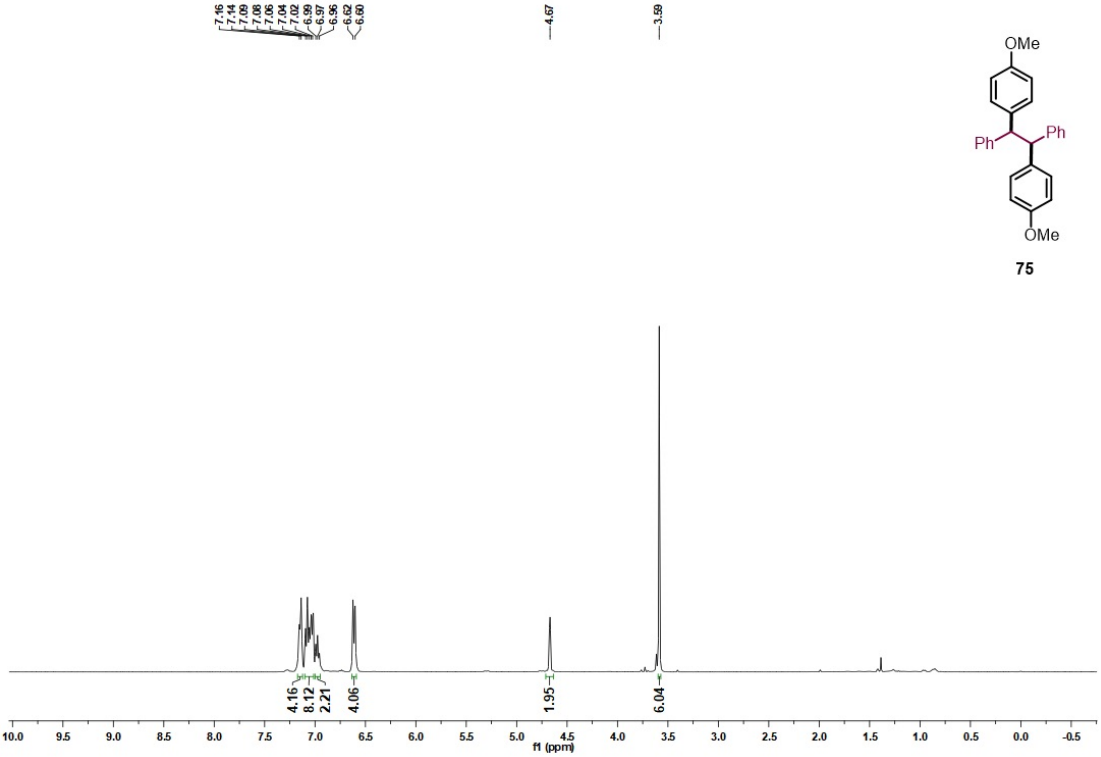
^{1}H-NMR of **74**
$CDCl_3$, 400 MHz, 298 K



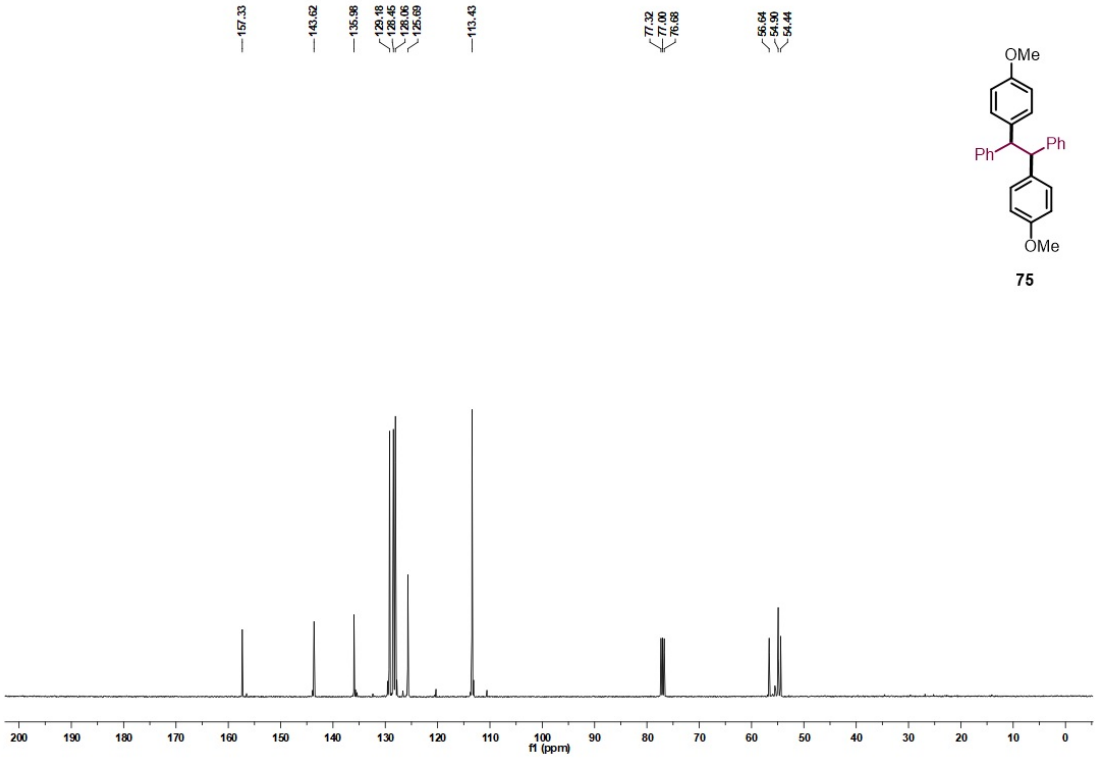
^{13}C-NMR of **74**
$CDCl_3$, 101 MHz, 298 K



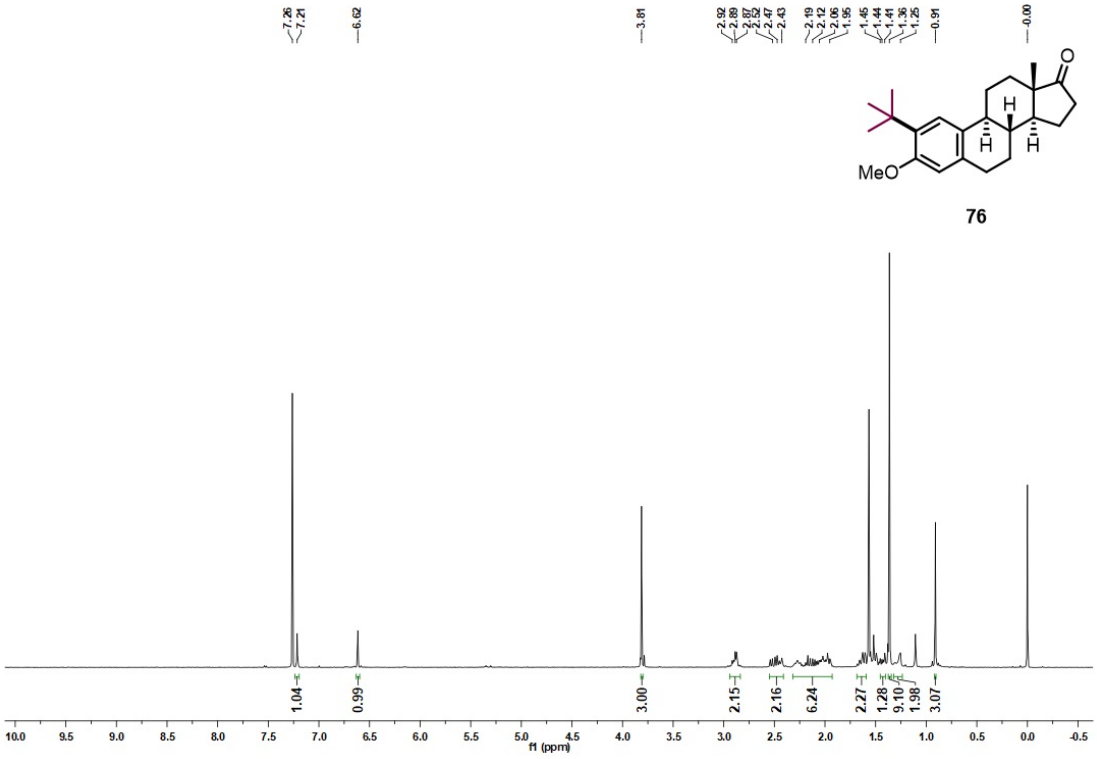
^{1}H-NMR of **75**
$CDCl_3$, 400 MHz, 298 K



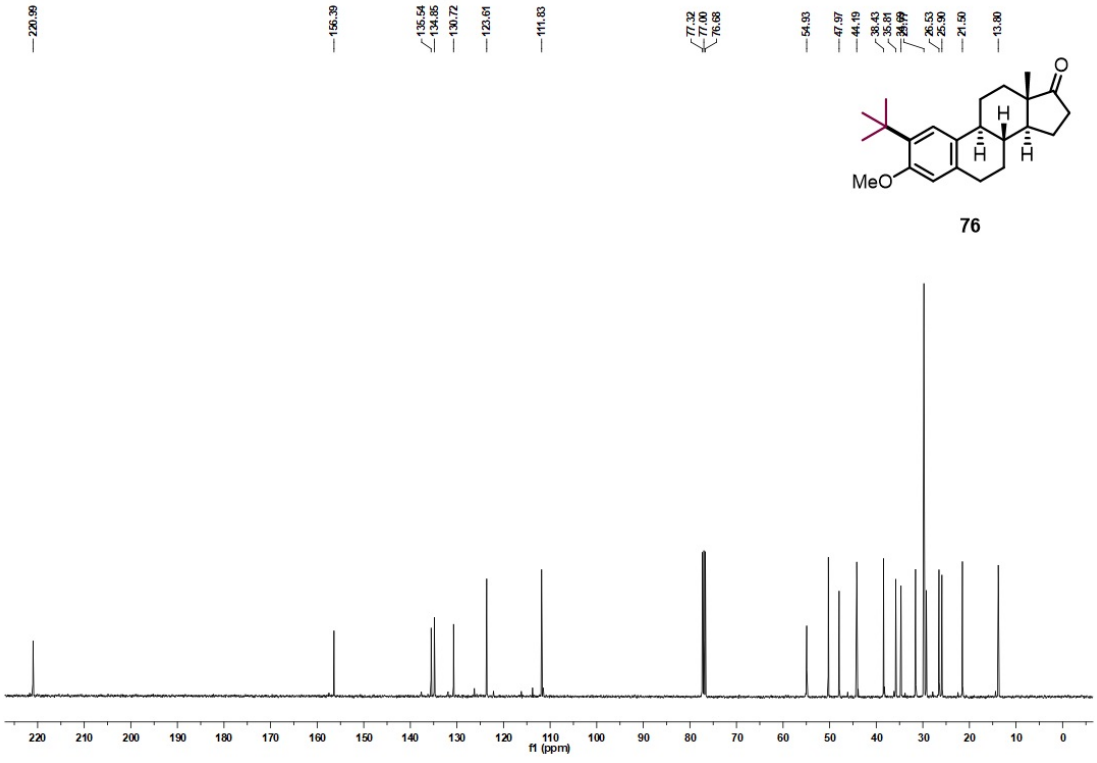
^{13}C-NMR of **75**
$CDCl_3$, 101 MHz, 298 K



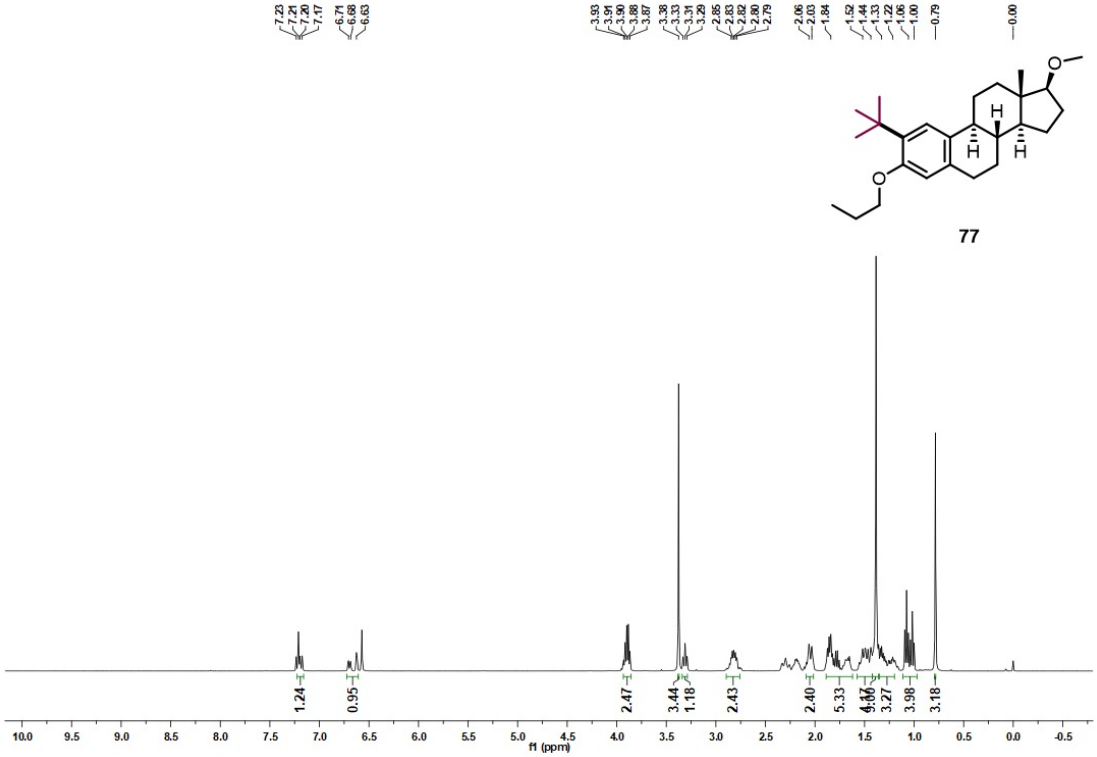
^{1}H-NMR of **76**
$CDCl_3$, 400 MHz, 298 K



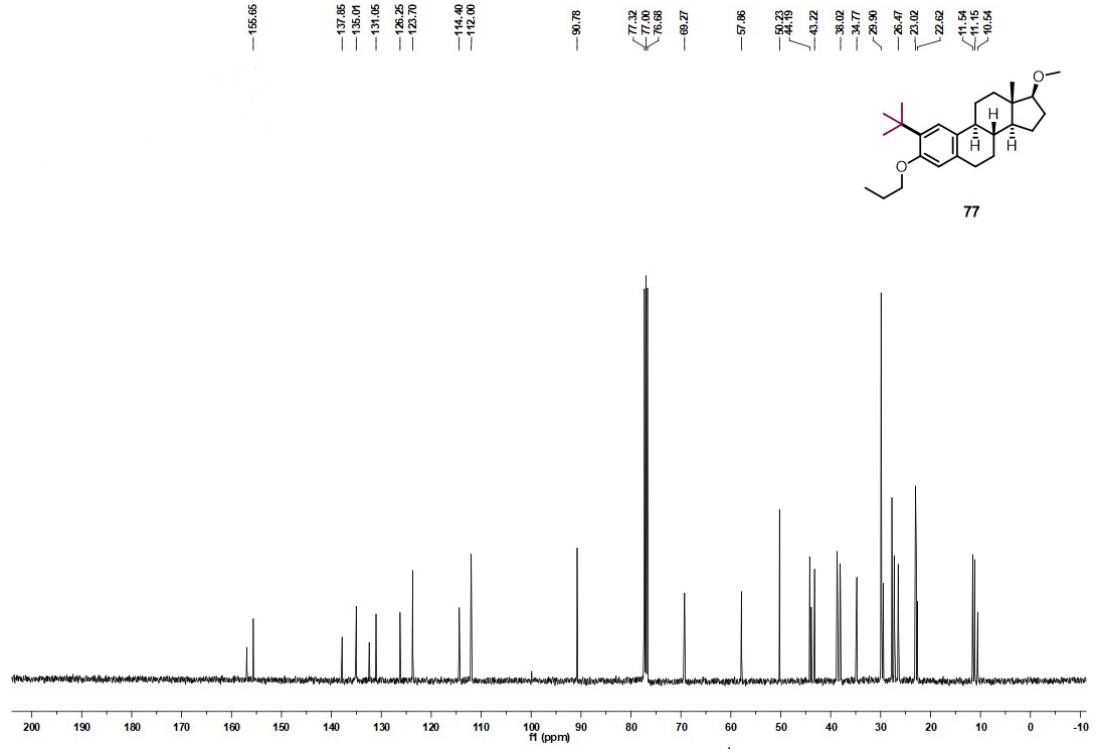
^{13}C-NMR of **76**
$CDCl_3$, 101 MHz, 298 K



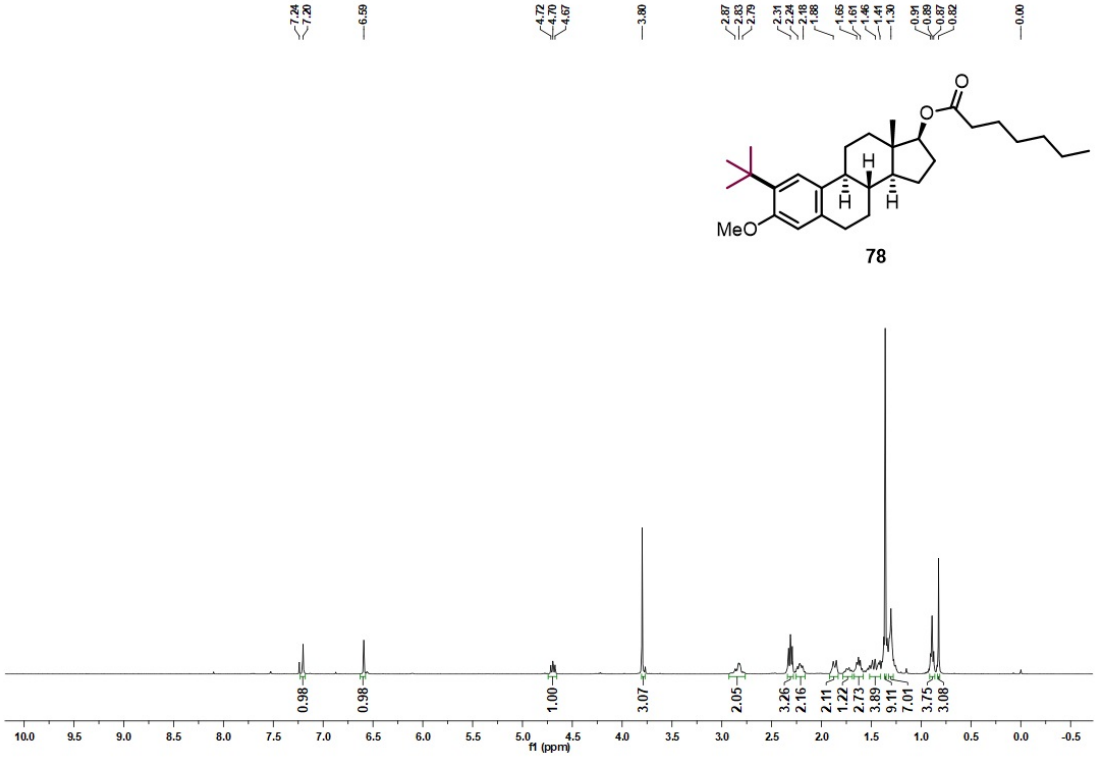
^{1}H-NMR of **77**
$CDCl_3$, 400 MHz, 298 K



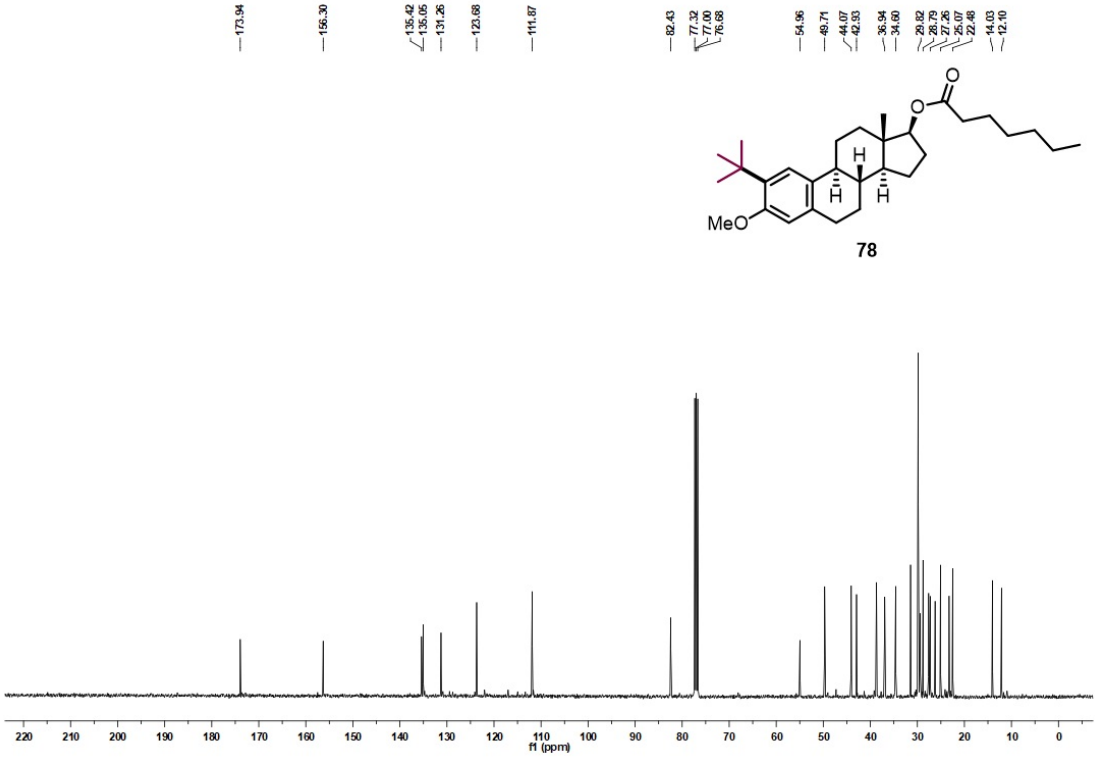
^{13}C-NMR of 77
$CDCl_3$, 101 MHz, 298 K



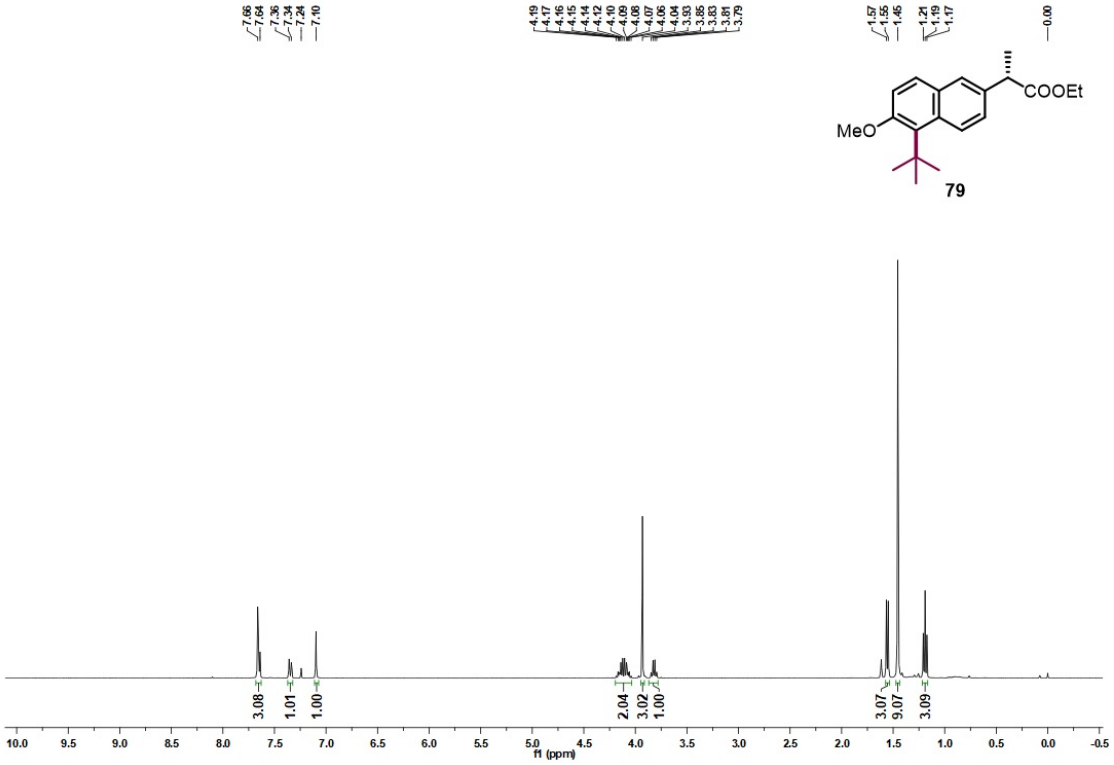
^{1}H-NMR of **78**
$CDCl_3$, 400 MHz, 298 K



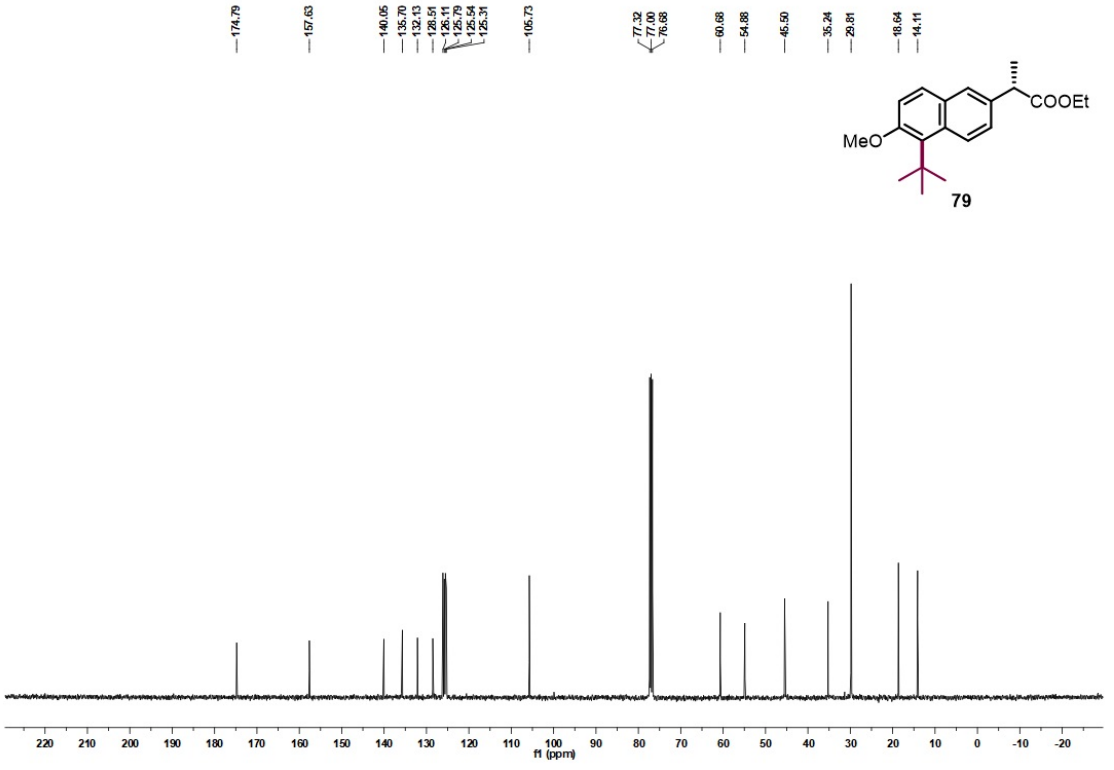
^{13}C-NMR of **78**
$CDCl_3$, 101 MHz, 298 K



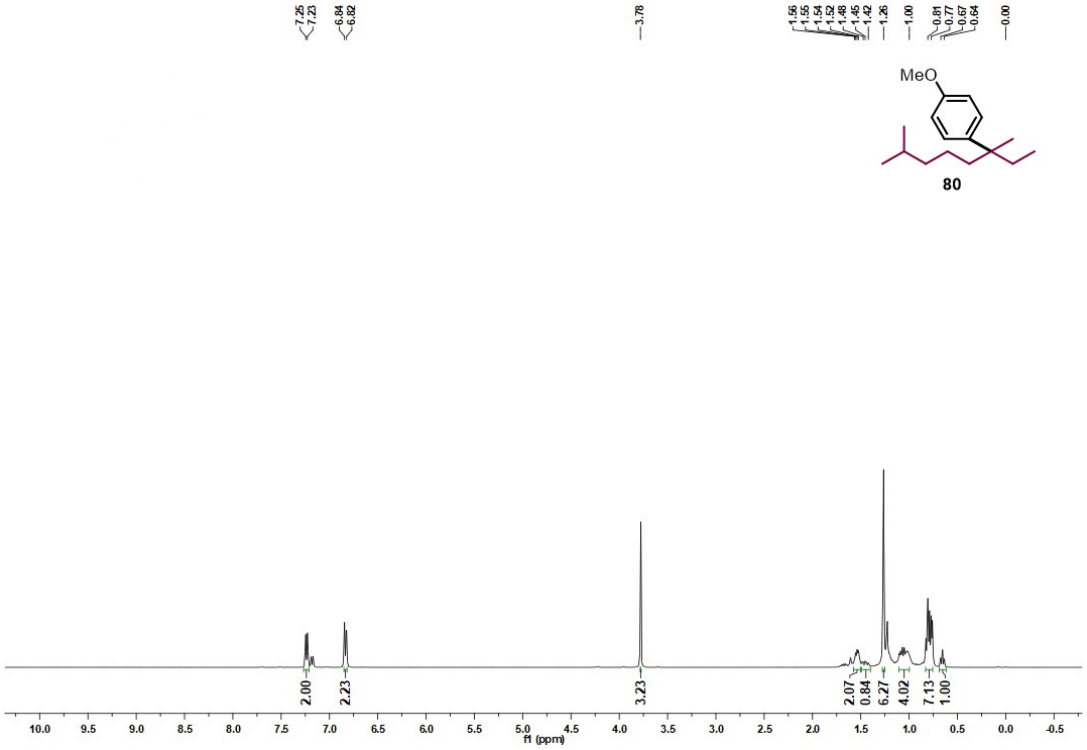
^{1}H-NMR of **79**
$CDCl_3$, 400 MHz, 298 K



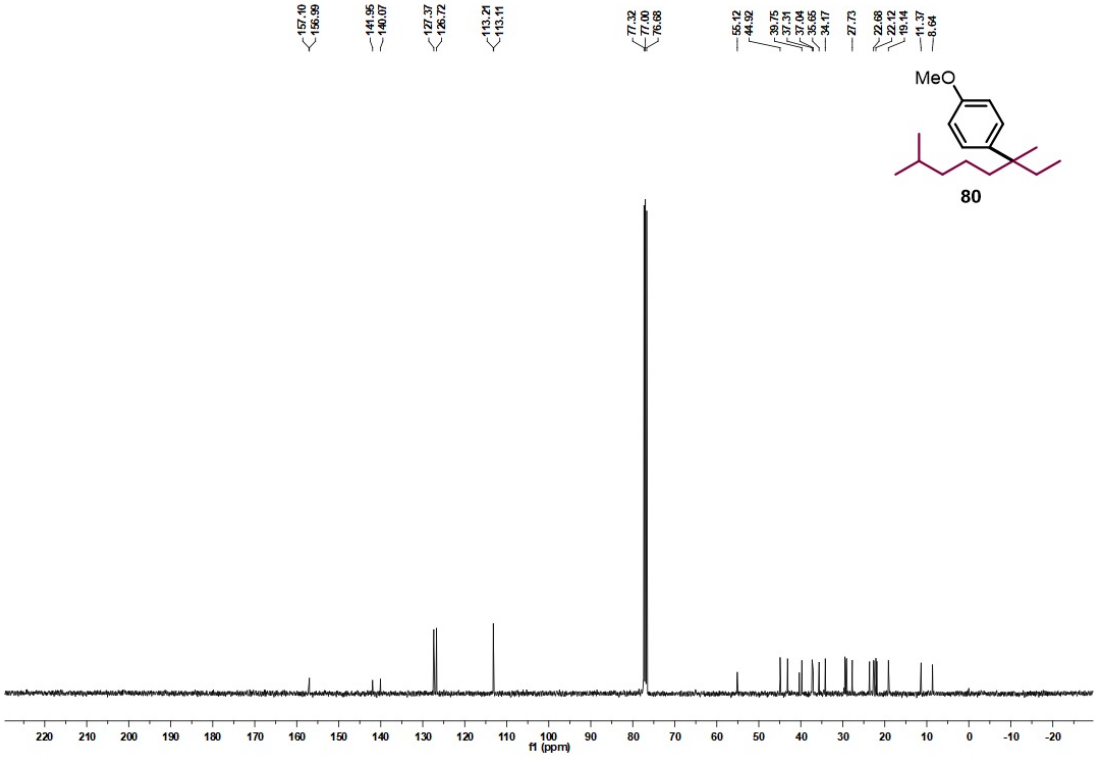
^{13}C-NMR of **79**
$CDCl_3$, 101 MHz, 298 K



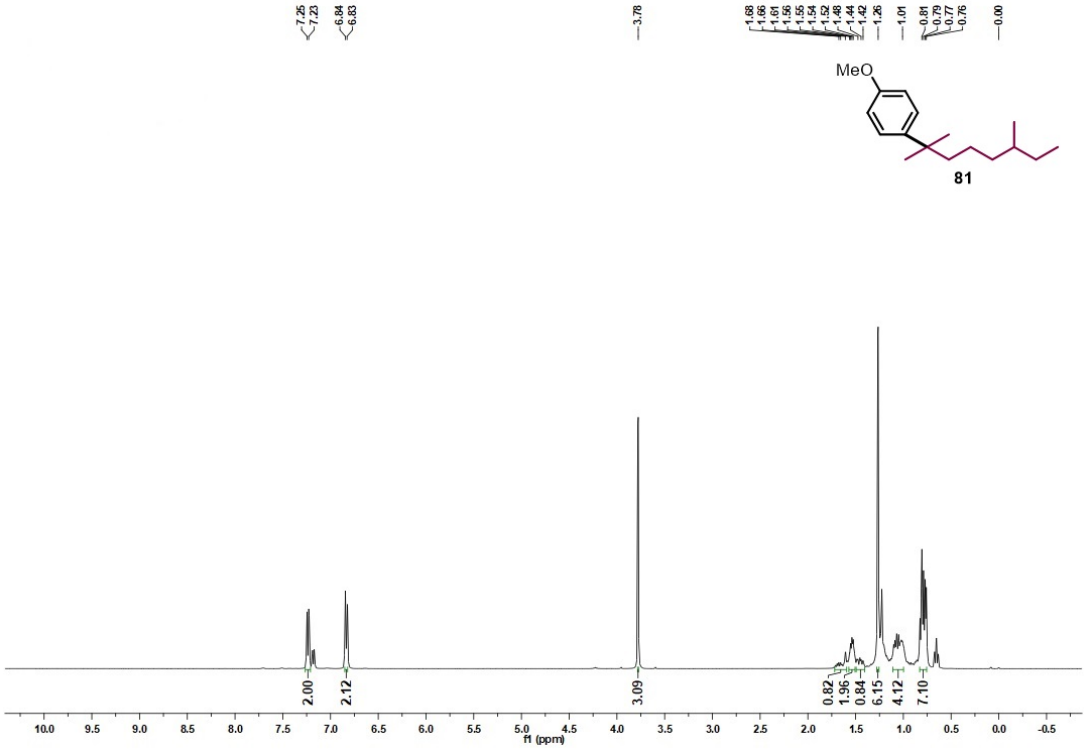
^{1}H-NMR of **80**
$CDCl_3$, 400 MHz, 298 K



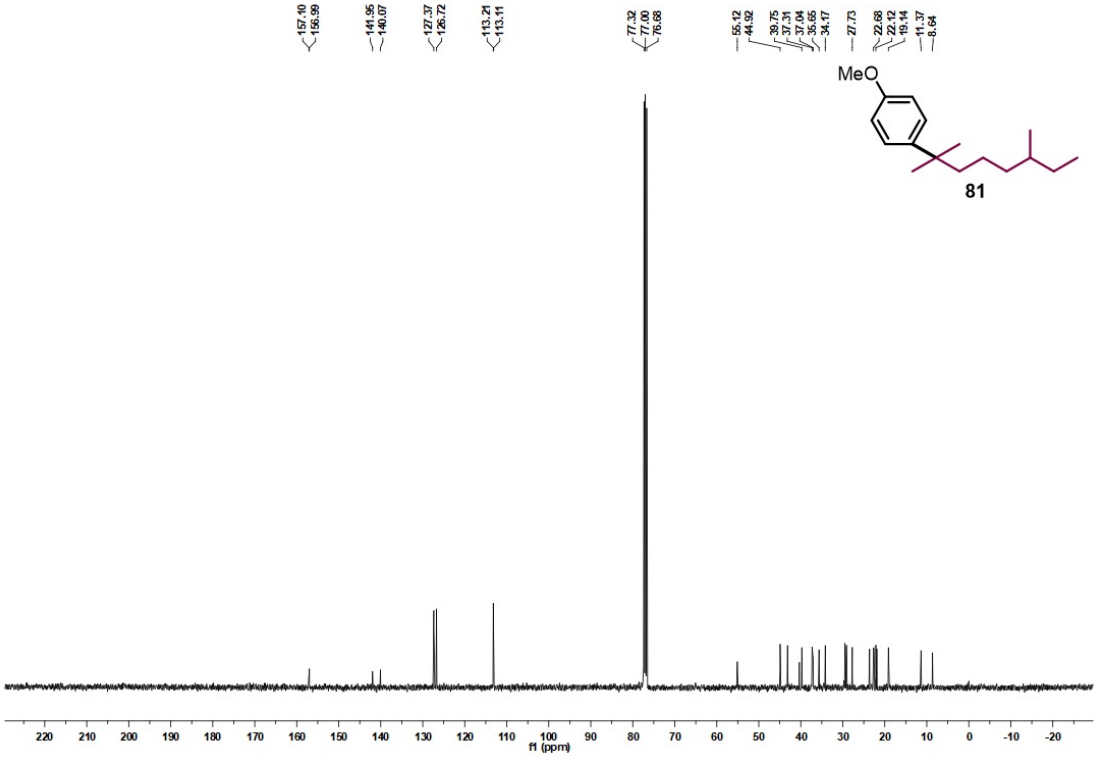
^{13}C-NMR of **80**
$CDCl_3$, 101 MHz, 298 K



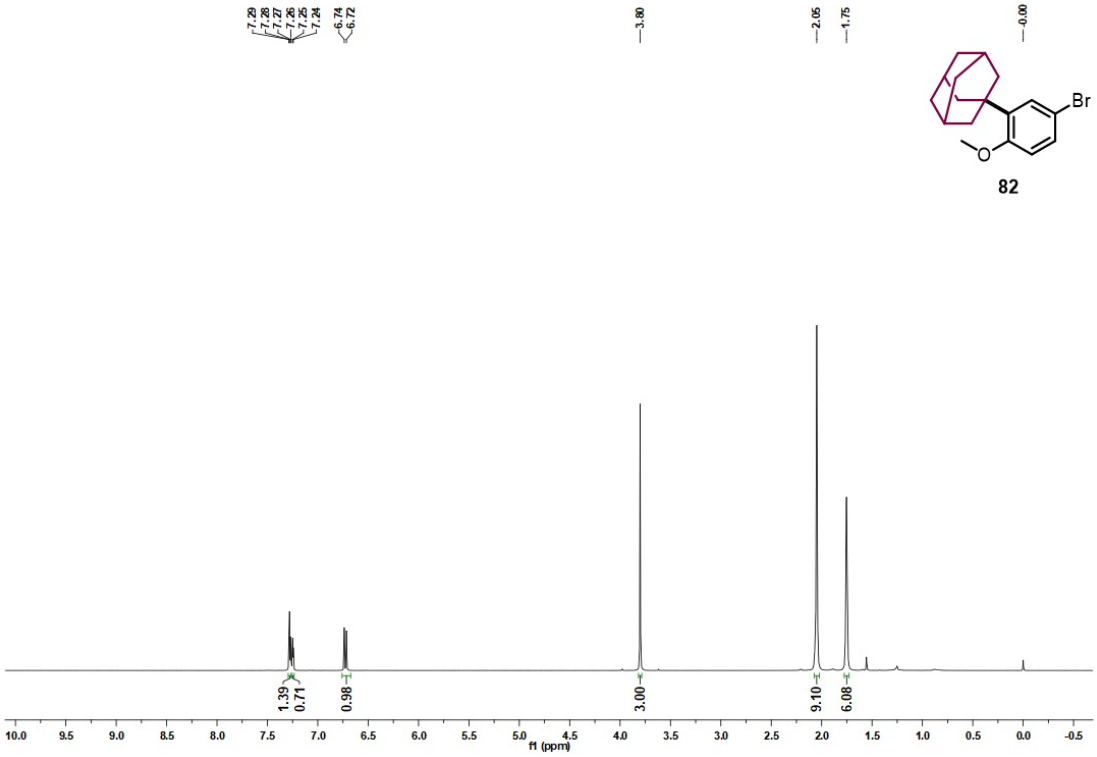
^{1}H-NMR of **81**
$CDCl_3$, 400 MHz, 298 K



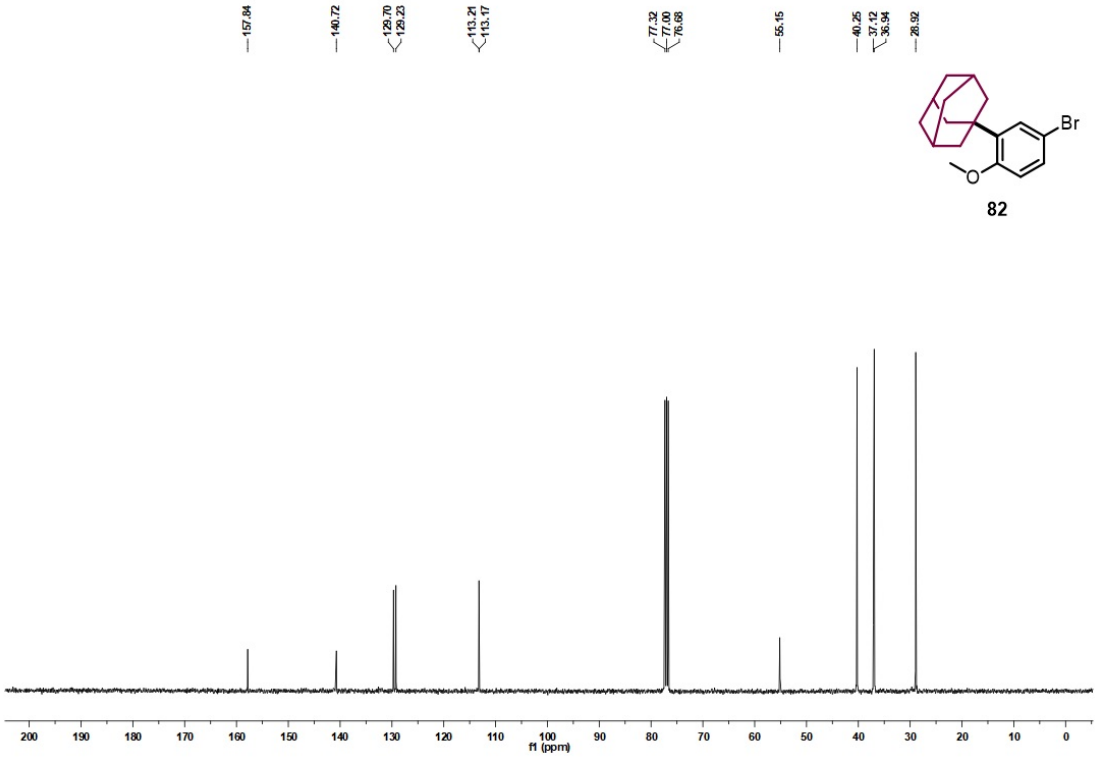
^{13}C-NMR of **81**
$CDCl_3$, 101 MHz, 298 K



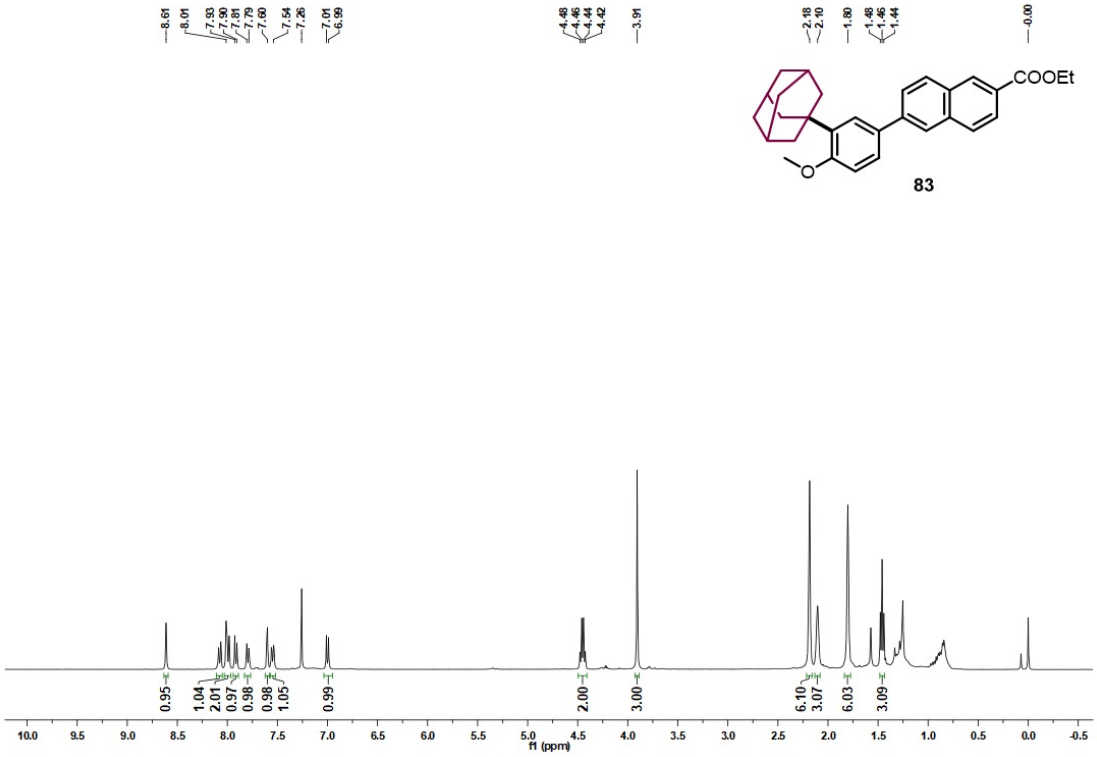
^{1}H-NMR of **82**
$CDCl_3$, 400 MHz, 298 K



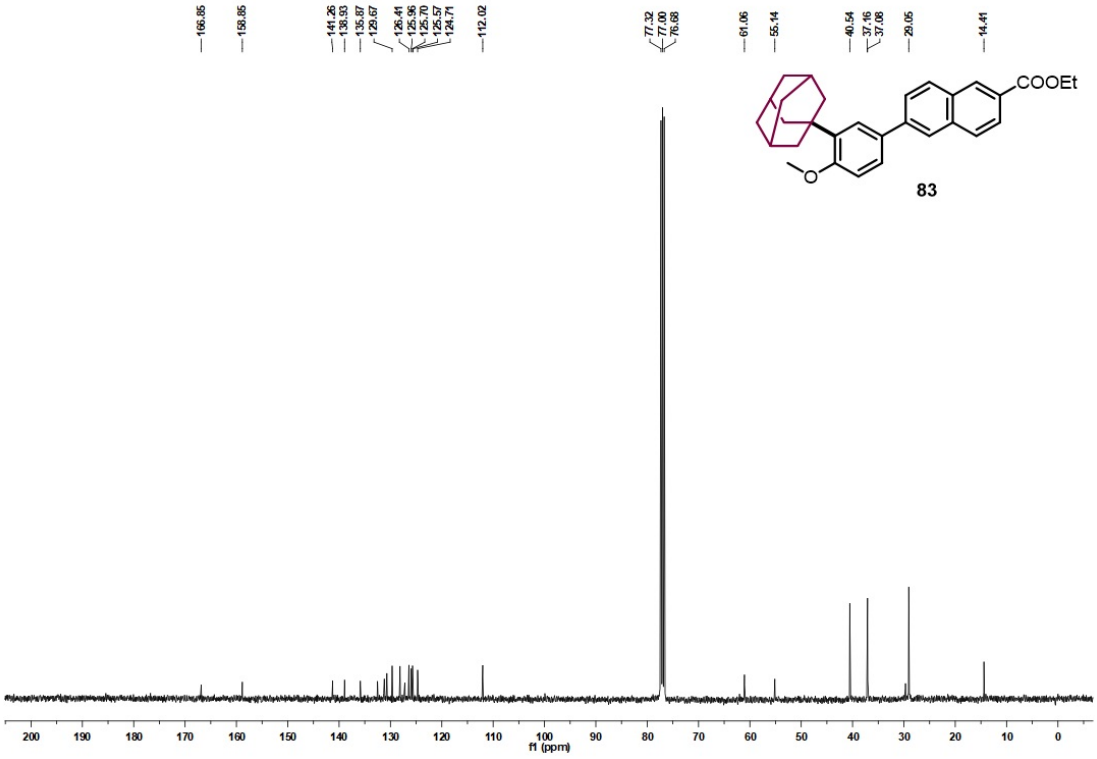
^{13}C-NMR of **82**
$CDCl_3$, 101 MHz, 298 K



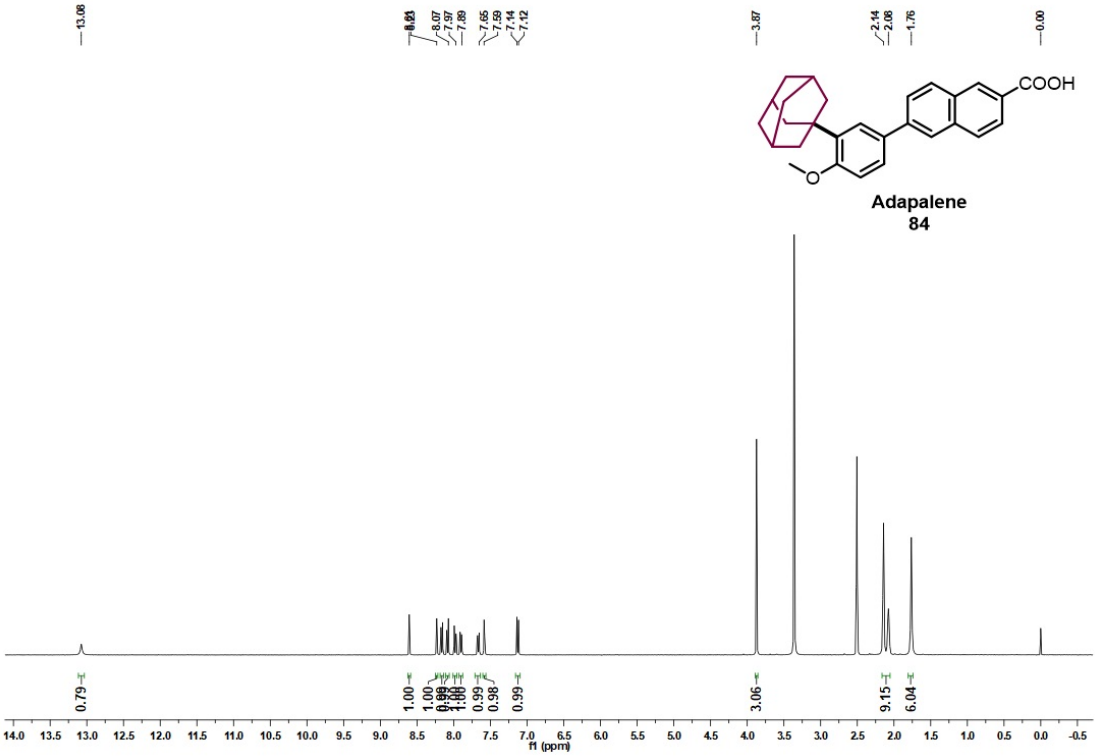
^{1}H-NMR of **83**
$CDCl_3$, 400 MHz, 298 K



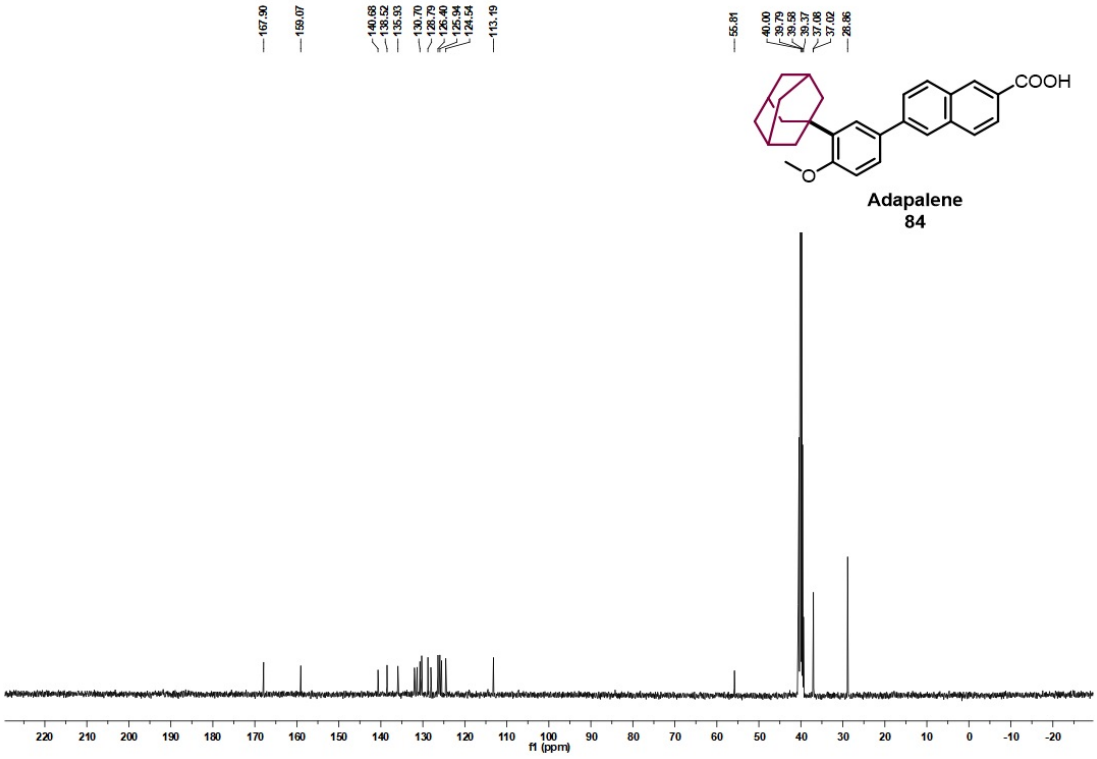
^{13}C-NMR of **83**
$CDCl_3$, 101 MHz, 298 K



^{1}H-NMR of **84**
DMSO, 400 MHz, 298 K



^{13}C-NMR of **84**
DMSO, 101 MHz, 298 K



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