

Electronic Supporting Information

Fe(OTf)₃ Catalyzed Friedel-Crafts Reaction of Benzenoid Arenes with α , β -Unsaturated Carbonyl Compounds: Easy Access to 1,1-Diarylalkanes

Aditya Bhattacharya, Pushpendra mani Shukla and Biswajit Maji*

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Department of Chemistry
Indira Gandhi National Tribal University
Amarkantak, Madhya Pradesh-484887
India
Email: biswajit.maji@igntu.ac.in

General Information

All reactions were conducted using oven-dried glassware under an atmosphere of Argon (Ar). Commercial grade reagents were used without further purification. Solvents were dried and distilled following usual protocols. 1,2-Dichloroethylene was used in substrates scope (Bottle solvent) directly as such received from Himedia, India. Flash chromatography was carried out using Spectrochem Silica gel (230-400 mesh) purchased from Spectrochem, India. TLC was performed on aluminum-backed plates coated with Silica gel 60 with F₂₅₄ indicator (Merck).

The ¹H NMR spectra were measured with Bruker-400 (200 MHz) and ¹³C NMR spectra were measured with Bruker-200 (50 MHz) using CDCl₃. ¹H NMR chemical shifts are expressed in parts per million (δ) downfield to CHCl₃ (δ = 7.26), ¹³C NMR chemical shifts are expressed in parts per million (δ) relative to the central CDCl₃ resonance (δ = 77.0. Coupling constants in ¹H NMR are in Hz. The following abbreviations classify the multiplicity: s = singlet, d = doublet, t = triplet, m = multiplet or unresolved, dd = doublet of doublet. HR-MS (ESI) spectra were recorded on a Waters Q-Tof premierTM mass spectrometer.

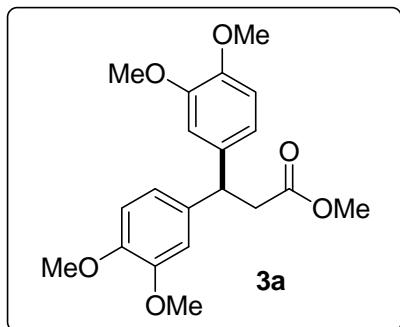
General Procedure for the Friedel-Crafts alkylation reaction with cinnamate esters and chalcones:

To a well stirred solution of cinnamate esters or chalcones **1** (1.0 equiv, 0.4 mmol) and arene **2** or **4** (1.2 equiv) in dichloroethane (2.0 mL) was added iron (III) triflate Lewis acid (10 mol %) under argon atmosphere. Next the reaction mixture is allowed to heat at 85 °C for 24 h. Progress of the reaction was monitored by TLC. On completion of the reaction, the reaction mixture was concentrated under reduced pressure and subjected to put directly in the column chromatography for the purification by using ethyl acetate and petroleum ether (60-80 °C) as eluent.

Representative procedure for the preparation of Friedel-Crafts alkylated product **3a:**
Under an argon atmosphere, iron (III) triflate (0.1 equiv, 22.6 mg, 0.045 mmol) was added to a solution of 3-(3,4-dimethoxy-phenyl)-acrylic acid methyl ester (1.0 equiv, 100 mg, 0.450 mmol) and 1,2-dimethoxybenzene (1.2 equiv, 75 mg, 0.540 mmol) in dichloroethane (2.5 ml). After stirring at room temperature for 5 minutes, the reaction mixture was slowly heated to 85 °C and continued for 24 hours. After 24 hours, the mixture was concentrated under reduced pressure and

purified under flash chromatography eluted with EtOAc: Petroleum ether (60-80 °C) = 4:1 to afford white solid **3a** (126 mg) in 78%.

Spectral Data of all the Friedel-Crafts Alkylated Products 3a-3m

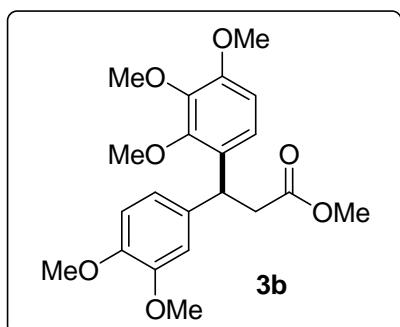


3,3-Bis-(3,4-dimethoxy-phenyl)-propionic acid methyl ester. Yield = 78%, Column purified with EtOAc: Pet Ether = 1:4, White amorphous solid, mp 122-123 °C.

¹H NMR (CDCl₃, 400 MHz): δ 6.98 (d, *J* = 8.0 Hz, 1H), 6.80-6.77 (m, 3H), 6.44-6.39 (m, 2H), 4.79 (t, *J* = 8.8 Hz, 1H), 3.828 (s, 3H), 3.823 (s, 3H), 3.77 (s, 3H), 3.76 (s, 3H), 3.58 (s, 3H), 2.99 (dd, *J* = 16.0, 7.2 Hz, 2H).

¹³C-NMR (CDCl₃, 100 MHz): δ 172.7, 159.4, 157.7, 148.6, 147.3, 136.1, 128.1, 124.7, 119.4, 111.6, 110.9, 104.0, 98.8, 55.8, 55.78, 55.4, 55.2, 51.5, 39.8, 39.6.

HRMS (EI) calcd for C₂₀H₂₄O₆, 361.1651 *m/z* (M+H)⁺; Found, 361.1654 *m/z*.

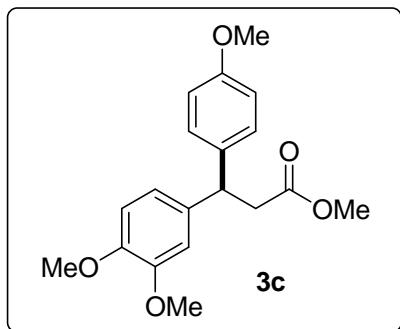


3-(3,4-Dimethoxy-phenyl)-3-(2,3,4-trimethoxy-phenyl)-propionic acid methyl ester. Yield = 73%, Column purified with EtOAc: Pet Ether = 1:4, White amorphous solid, mp 131-132 °C.

¹H NMR (CDCl₃, 400 MHz): δ 6.85 (d, *J* = 8.4 Hz, 1H), 6.77-6.75 (m, 3H), 6.60 (d, *J* = 8.4 Hz, 1H), 4.76 (t, *J* = 8.0 Hz, 1H), 3.82 (s, 6H), 3.81 (s, 6H), 3.68 (s, 3H), 3.57 (s, 3H), 2.98 (d, *J* = 8.0 Hz, 2H).

¹³C-NMR (CDCl₃, 100 MHz): δ 172.4, 152.4, 151.5, 148.7, 147.4, 142.4, 136.5, 129.7, 121.6, 119.3, 111.4, 111.0, 106.9, 60.7, 60.6, 55.8 (3C), 51.6, 40.2, 40.1.

HRMS (EI) calcd for C₂₀H₂₆O₇, 391.1757 *m/z* (M+H)⁺; Found, 391.1759 *m/z*.

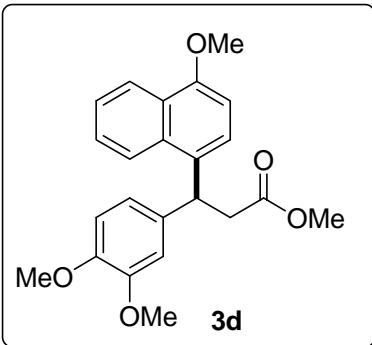


3-(3,4-Dimethoxy-phenyl)-3-(4-methoxy-phenyl)-propionic acid methyl ester. Yield = 68%, Column purified with EtOAc: Pet Ether = 1:5, Gummy liquid.

¹H NMR (CDCl₃, 400 MHz): δ 7.13 (d, *J* = 8.4 Hz, 2H), 6.81 (d, *J* = 8.4 Hz, 2H), 6.80-6.78 (m, 2H), 6.71 (s, 1H), 4.45 (t, *J* = 7.6 Hz, 1H), 3.83 (s, 3H), 3.81 (s, 3H), 3.76 (s, 3H), 3.58 (s, 3H), 2.99 (d, *J* = 8.0 Hz, 2H).

¹³C-NMR (CDCl₃, 100 MHz): δ 172.5, 158.2, 148.9, 147.7, 136.5, 135.9, 128.6 (2C), 119.3, 114.0 (2C), 111.3, 111.2, 55.94, 55.92, 55.3, 51.8, 45.9, 41.1.

HRMS (EI) calcd for C₁₉H₂₂O₅, 331.1546 *m/z* (M+H)⁺; Found, 331.1551 *m/z*.

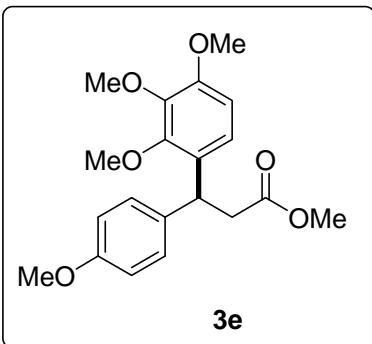


3-(3,4-Dimethoxy-phenyl)-3-(4-methoxy-naphthalen-1-yl)-propionic acid methyl ester. Yield = 83%, Column purified with EtOAc: Pet Ether = 1:4, White amorphous solid, mp 134-136 °C.

¹H NMR (CDCl₃, 400 MHz): δ 8.30 (d, *J* = 8.0 Hz, 1H), 8.07 (d, *J* = 8.0 Hz, 1H), 7.50-7.44 (m, 2H), 7.25 (d, *J* = 8.0 Hz, 1H), 6.84-6.74 (m, 4H), 5.24 (t, *J* = 8.0 Hz, 1H), 3.98 (s, 3H), 3.84 (s, 3H), 3.80 (s, 3H), 3.61 (s, 3H), 3.12 (dd, *J* = 16.0, 7.2 Hz, 2H).

¹³C-NMR (CDCl₃, 100 MHz): δ 172.5, 154.6, 148.9, 147.6, 136.8, 132.3, 131.0, 126.7, 126.4, 125.5, 124.0, 123.5, 122.6, 119.6, 111.4, 111.1, 103.0, 55.83, 55.80, 55.43, 51.7, 41.9, 41.3.

HRMS (EI) calcd for C₂₃H₂₄O₅, 381.1702 *m/z* (M+H)⁺; Found, 381.1705 *m/z*.

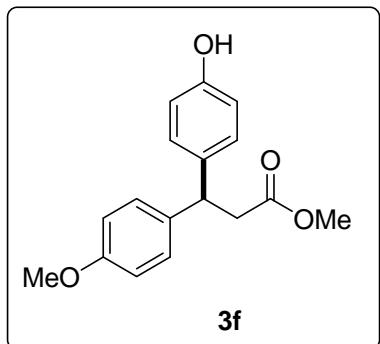


3-(4-Methoxy-phenyl)-3-(2,3,4-trimethoxy-phenyl)-propionic acid methyl ester. Yield = 71%, Column purified with EtOAc: Pet Ether = 1:6, Colorless crystalline solid (Recrystallised from EA-Petroleum ether mixture), mp 127°C.

¹H NMR (CDCl₃, 400 MHz): δ 7.14 (d, *J* = 8.8 Hz, 2H), 6.87 (d, *J* = 8.8 Hz, 1H), 6.80 (d, *J* = 8.8 Hz, 2H), 6.61 (d, *J* = 8.8 Hz, 1H), 4.77 (t, *J* = 8.0 Hz, 1H), 3.84 (s, 3H), 3.83 (s, 3H), 3.75 (s, 3H), 3.67 (s, 3H), 3.58 (s, 3H), 2.98 (d, *J* = 7.6 Hz, 2H).

¹³C-NMR (CDCl₃, 100 MHz): δ 172.7, 158.1, 152.6, 151.7, 142.6, 136.1, 130.6, 128.8 (2C), 121.7, 113.9 (2C), 107.0, 60.83, 60.79, 56.0, 55.3, 51.8, 40.4, 39.9.

HRMS (EI) calcd for C₂₀H₂₄O₆, 361.1651 *m/z* (M+H)⁺; Found, 361.1653 *m/z*.

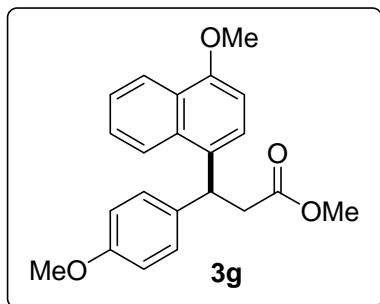


3-(4-Hydroxy-phenyl)-3-(4-methoxy-phenyl)-propionic acid methyl ester. Yield = 66%, Column purified with EtOAc: Pet Ether = 1:6, Colorless cubic crystal (Recrystallised from MeOH), mp 130 °C.

¹H NMR (CDCl₃, 400 MHz): δ 7.12 (d, *J* = 8.2 Hz, 2H), 7.05 (d, *J* = 8.2 Hz, 2H), 6.81 (d, *J* = 8.4 Hz, 2H), 6.76 (d, *J* = 8.2 Hz, 2H), 6.02 (s, 1H), 4.44 (t, *J* = 8.0 Hz, 1H), 3.73 (s, 3H), 3.59 (s, 3H), 3.01 (d, *J* = 8.4 Hz, 2H).

¹³C-NMR (CDCl₃, 100 MHz): δ 172.9, 157.9, 154.3, 135.9, 135.5, 128.56 (2C), 128.4 (2C), 115.35 (2C), 113.8 (2C), 55.16, 51.8, 45.3, 41.0.

HRMS (EI) calcd for C₁₇H₁₈O₄, 287.1283 *m/z* (M+H)⁺; Found, 287.1283 *m/z*.

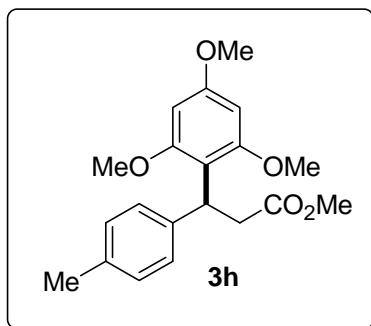


3-(4-Methoxy-naphthalen-1-yl)-3-(4-methoxy-phenyl)-propionic acid methyl ester. Yield = 77%, Column purified with EtOAc: Pet Ether = 1:5, Gummy liquid.

¹H NMR (CDCl₃, 400 MHz): δ 8.27 (d, *J* = 8.4 Hz, 1H), 8.03 (d, *J* = 8.0 Hz, 1H), 7.50-7.38 (m, 2H), 7.25 (d, *J* = 8.0 Hz, 1H), 7.16 (d, *J* = 8.8 Hz, 2H), 6.77 (d, *J* = 8.8 Hz, 2H), 6.74 (d, *J* = 8.8 Hz, 1H), 5.22 (t, *J* = 8.0 Hz, 1H), 3.94 (s, 3H), 3.70 (s, 3H), 3.57 (s, 3H), 3.17-3.03 (m, 2H).

¹³C-NMR (CDCl₃, 100 MHz): δ 172.7, 158.2, 154.7, 136.0, 132.5, 131.26, 128.9 (2C), 126.8, 126.3, 125.0, 124.1, 123.7, 122.7, 114.1 (2C), 103.2, 55.6, 55.3, 51.8, 41.67, 41.57.

HRMS (EI) calcd for C₂₂H₂₂O₄, 351.1596 *m/z* (M+H)⁺; Found, 351.1597 *m/z*.

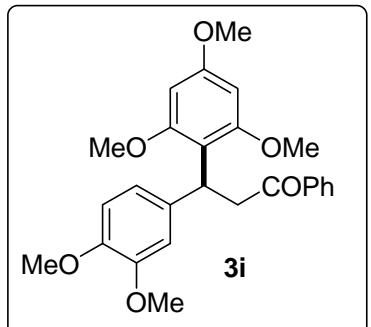


3-*p*-Tolyl-3-(2,4,6-trimethoxy-phenyl)-propionic acid methyl ester. Yield = 65%, Column purified with EtOAc: Pet Ether = 1:7, Gummy liquid.

¹H NMR (CDCl₃, 400 MHz): δ 7.20 (d, *J* = 8.0 Hz, 2H), 7.02 (d, *J* = 8.0 Hz, 2H), 6.10 (s, 2H), 5.13 (t, *J* = 8.0 Hz, 1H), 3.77 (s, 3H), 3.76 (s, 6H), 3.58 (s, 3H), 3.30 (dd, *J* = 15.6, 7.6 Hz, 1H), 3.15 (dd, *J* = 15.6, 7.6 Hz, 1H), 2.27 (s, 3H).

¹³C-NMR (CDCl₃, 100 MHz): δ 173.7, 159.7, 159.0 (2C), 141.0, 134.9, 128.5 (2C), 127.4 (2C), 112.8, 91.2 (2C), 55.76 (2C), 55.2, 51.4, 37.7, 35.4, 21.0.

HRMS (EI) calcd for C₂₀H₂₄O₅, 345.1702 *m/z* (M+H)⁺; Found, 345.1705 *m/z*.

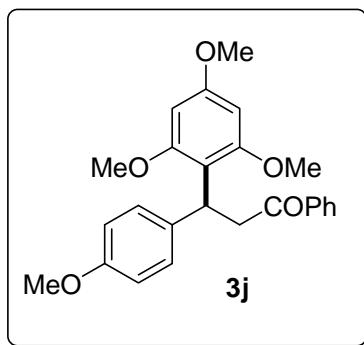


3-(3,4-Dimethoxy-phenyl)-1-phenyl-3-(2,4,6-trimethoxy-phenyl)-propan-1-one. Yield = 86%, Column purified with EtOAc: Pet Ether = 1:4, White amorphous solid, mp 145-146 °C.

¹H NMR (CDCl₃, 400 MHz): δ 7.93 (d, *J* = 8.0 Hz, 2H), 7.55-7.48 (m, 1H), 7.47-7.42 (m, 2H), 6.92 (s, 1H), 6.85 (d, *J* = 8.0 Hz, 1H), 6.71 (d, *J* = 8.0 Hz, 1H), 6.10 (s, 2H), 5.30 (t, *J* = 8.0 Hz, 1H), 3.85 (dd, *J* = 8.8, 2.8 Hz, 2H), 3.80 (s, 3H), 3.79 (s, 3H), 3.77 (s, 3H), 3.73 (s, 6H).

¹³C-NMR (CDCl₃, 100 MHz): δ 199.9, 159.6, 158.9 (2C), 148.3, 146.9, 137.5, 132.6, 128.0 (2C), 127.9, 127.8 (2C), 119.5, 113.1, 111.6, 110.7, 91.3 (2C), 55.81 (2C), 55.74, 55.72, 55.2, 42.68, 34.9.

HRMS (EI) calcd for C₂₆H₂₈O₆, 437.1964 *m/z* (M+H)⁺; Found, 437.1969 *m/z*.

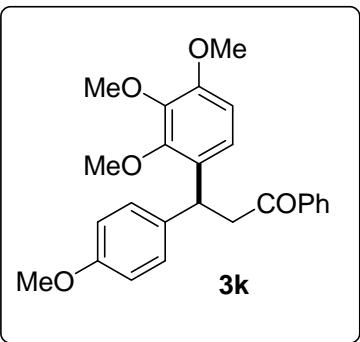


3-(4-Methoxy-phenyl)-1-phenyl-3-(2,4,6-trimethoxy-phenyl)-propan-1-one. Yield = 75%, Column purified with EtOAc: Pet Ether = 1:5, White crystalline needles (Recrystallised from EA-Petroleum ether mixture), mp 141-142 °C.

¹H NMR (CDCl₃, 200 MHz): δ 7.98 (d, *J* = 8.0 Hz, 2H), 7.57-7.53 (m, 1H), 7.47-7.43 (m, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 6.81 (d, *J* = 8.0 Hz, 2H), 6.13 (s, 2H), 5.37 (t, *J* = 7.6 Hz, 1H), 3.91 (dd, *J* = 7.4, 1.9 Hz, 2H), 3.79 (s, 3H), 3.77 (s, 3H), 3.75 (s, 6H).

¹³C-NMR (CDCl₃, 100 MHz): δ 199.7, 159.5, 158.7 (2C), 157.2, 137.3, 136.7, 132.4, 128.4 (2C), 128.2 (2C), 127.9 (2C), 113.1 (3C), 91.1 (2C), 55.6 (3C), 55.0, 42.4, 34.3.

HRMS (EI) calcd for C₂₅H₂₆O₅, 407.1859 *m/z* (M+H)⁺; Found, 407.1865 *m/z*.

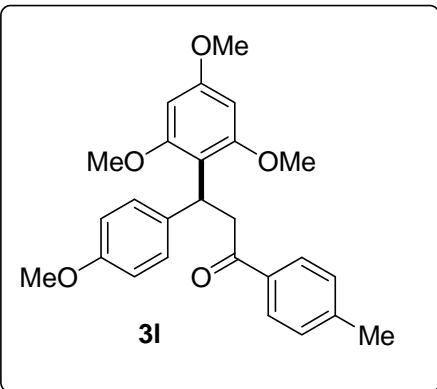


3-(4-Methoxy-phenyl)-1-phenyl-3-(2,3,4-trimethoxy-phenyl)-propan-1-one. Yield = 74%, Column purified with EtOAc: Pet Ether = 1:5, White amorphous solid, mp 138-140 °C.

¹H NMR (CDCl₃, 200 MHz): δ 7.96 (d, *J* = 7.6 Hz, 2H), 7.55-7.41 (m, 3H), 7.18 (d, *J* = 8.0 Hz, 2H), 6.78 (m, 3H), 6.60 (d, *J* = 8.0 Hz, 1H), 5.00 (t, *J* = 8.0 Hz, 1H), 3.84 (s, 3H), 3.82 (s, 3H), 3.78 (s, 3H), 3.68 (s, 3H), 3.66 (m, 2H).

¹³C-NMR (CDCl₃, 100 MHz): δ 198.6, 158.0, 152.3, 151.6, 142.5, 136.44, 136.0, 133.0, 131.2, 130.3, 128.9, 128.6, 128.2, 124.2, 122.0, 113.8, 113.6, 107.0, 106.5, 60.8, 60.5, 56.0, 55.3, 44.4, 39.4.

HRMS (EI) calcd for C₂₅H₂₆O₅, 407.1859 *m/z* (M+H)⁺; Found, 407.1863 *m/z*.

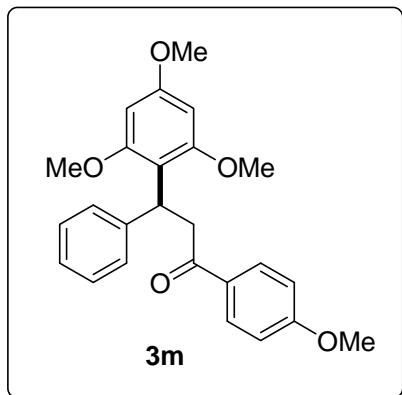


3-(4-Methoxy-phenyl)-1-p-tolyl-3-(2,4,6-trimethoxy-phenyl)-propan-1-one. Yield = 86%, Column purified with EtOAc: Pet Ether = 1:5, White solid, mp 151-153 °C.

¹H NMR (CDCl₃, 200 MHz): δ 7.88 (d, *J* = 8.0 Hz, 2H), 7.27 (d, *J* = 8.6 Hz, 2H), 7.25 (d, *J* = 8.0 Hz, 2H), 6.78 (d, *J* = 8.0 Hz, 2H), 6.12 (s, 2H), 5.34 (t, *J* = 8.0 Hz, 1H), 3.86 (d, *J* = 7.6 Hz, 2H), 3.79 (s, 3H), 3.77 (s, 3H), 3.75 (s, 6H), 2.42 (s, 3H).

¹³C-NMR (CDCl₃, 100 MHz): δ 199.5, 159.7, 159.0, 157.4, 143.3, 137.1, 135.1, 129.1 (2C), 128.7 (2C), 128.3 (2C), 128.6, 113.6, 113.3 (2C), 91.37 (2C), 55.85 (3C), 55.31, 42.5, 34.5, 21.7.

HRMS (EI) calcd for C₂₆H₂₈O₅, 421.2015 *m/z* (M+H)⁺; Found, 421.2019 *m/z*.



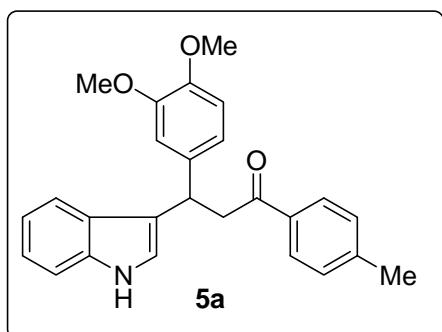
1-(4-Methoxy-phenyl)-3-phenyl-3-(2,4,6-trimethoxy-phenyl)-propan-1-one. Yield = 71%, Column purified with EtOAc: Pet Ether = 1:4, Colorless crystalline needles solid (Recrystallised from EA-Petroleum ether mixture), 134-135 °C.

¹H NMR (CDCl₃, 200 MHz): δ 7.98 (d, *J* = 8.4 Hz, 2H), 7.37-7.34 (m, 2H), 7.25-7.22 (m, 2H), 7.16-7.11 (m, 1H), 6.92 (d, *J* = 8.4 Hz, 2H), 6.12 (s, 2H), 5.41 (t, *J* = 8.0 Hz, 1H), 3.88 (d, *J* = 8.0 Hz, 2H), 3.86 (s, 3H), 3.79 (s, 3H), 3.73 (s, 6H).

¹³C-NMR (CDCl₃, 100 MHz): δ 198.3, 163.1, 159.7, 159.0 (2C), 144.9, 130.6, 130.4 (2C), 127.8 (2C), 127.7 (2C), 125.4, 113.5 (2C), 113.3, 91.3 (2C), 55.78 (2C), 55.44, 55.23, 41.9, 35.2.

HRMS (EI) calcd for C₂₅H₂₆O₅, 407.1859 *m/z* (M+H)⁺; Found, 407.1864 *m/z*.

Spectral Data of all the Friedel-Crafts Alkylated Products 5a-5d

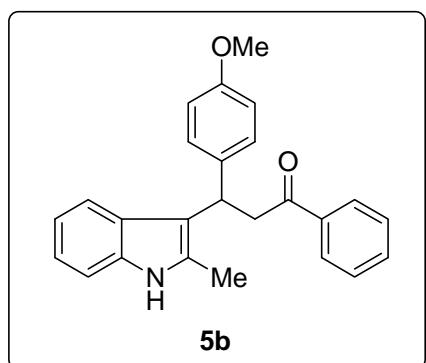


3-(3,4-Dimethoxy-phenyl)-3-(1*H*-indol-3-yl)-1-*p*-tolyl-propan-1-one. Yellow amorphous solid (Recrystallised from MeOH), Yield = 87%, Column purified with EtOAc: Pet Ether = 1:6, mp 152 °C.

¹H NMR (CDCl₃, 400 MHz): δ 8.10 (bs, 1H), 7.87 (d, *J* = 8.0 Hz, 2H), 7.48 (d, *J* = 8.0 Hz, 1H), 7.34 (d, *J* = 8.0 Hz, 1H), 7.27 (d, *J* = 8.0 Hz, 2H), 7.19-7.15 (m, 1H), 7.05 (t, *J* = 7.6 Hz, 1H), 6.97 (s, 1H), 6.96-6.88 (m, 2H), 6.76 (d, *J* = 8.0 Hz, 1H), 5.04 (t, *J* = 6.8 Hz, 1H), 4.06 (d, *J* = 16.0 Hz, 1H), 3.90 (d, *J* = 16.0 Hz, 1H), 3.87 (s, 3H), 3.83 (s, 3H), 2.38 (s, 3H).

¹³C-NMR (CDCl₃, 100 MHz): δ 198.5, 148.7, 147.3, 143.8, 136.9, 136.7, 134.7, 129.3 (2C), 128.2 (2C), 126.6, 122.1, 121.4, 119.57, 119.54, 119.5, 119.3, 111.5, 111.2, 111.1, 55.8 (2C), 45.2, 38.0, 22.0.

HRMS (EI) calcd for C₂₆H₂₅NO₃, 400.1913 *m/z* (M+H)⁺; Found, 400.1911 *m/z*.

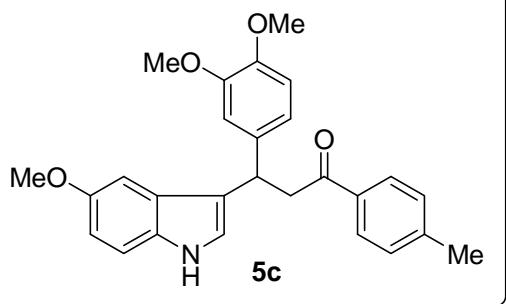


3-(4-Methoxy-phenyl)-3-(2-methyl-1*H*-indol-3-yl)-1-phenyl-propan-1-one. Yellow amorphous solid (Recrystallised from MeOH), Yield = 93%, Column purified with EtOAc: Pet Ether = 1:5, mp 143 °C.

¹H NMR (CDCl₃, 400 MHz): δ 7.91 (d, *J* = 8.0 Hz, 2H), 7.53-7.48 (m, 2H), 7.39 (t, *J* = 7.8 Hz, 2H), 7.33-7.28 (m, 2H), 7.24-7.17 (m, 1H), 7.11-6.99 (m, 2H), 6.82 (d, *J* = 8.0 Hz, 2H), 5.07 (t, *J* = 7.2 Hz, 1H), 3.93 (dd, *J* = 7.2, 4.0 Hz, 2H), 3.76 (s, 3H), 2.37 (s, 3H).

¹³C-NMR (CDCl₃, 100 MHz): δ 199.4, 157.7, 137.2, 136.4, 135.6, 133.0, 131.7, 128.5 (3C), 128.1 (3C), 127.5, 120.7, 119.1, 113.8 (2C), 113.7 (2C), 110.5, 55.26, 43.9, 36.1, 12.1.

HRMS (EI) calcd for C₂₅H₂₃NO₂, 370.1807 *m/z* (M+H)⁺; Found, 370.1816 *m/z*.

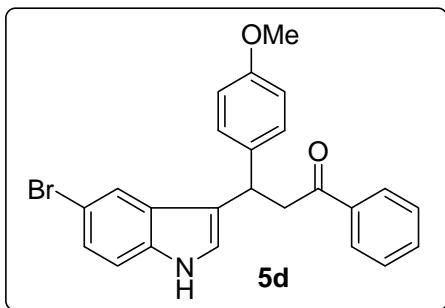


3-(3,4-Dimethoxy-phenyl)-3-(5-methoxy-1*H*-indol-3-yl)-1-*p*-tolyl-propan-1-one. Yield = 91%, Column purified with EtOAc: Pet Ether = 1:4, Brown needles solid (Recrystallised from MeOH), mp 154 °C.

¹H NMR (CDCl₃, 400 MHz): δ 8.04 (s, 1H), 7.94-7.78 (m, 2H), 7.34-7.11 (m, 3H), 7.00-6.71 (m, 6H), 4.97 (t, *J* = 7.2 Hz, 1H), 3.82 (s, 3H), 3.77 (s, 3H), 3.75 (s, 3H), 3.74-3.67 (m, 2H), 2.39 (s, 3H).

¹³C-NMR (CDCl₃, 100 MHz): δ 198.7, 153.8, 148.9, 147.5, 143.9, 137.0, 134.8, 131.9, 129.4 (2C), 128.3 (2C), 127.1, 122.3, 119.6, 119.3, 112.2, 111.9, 111.7, 111.2, 101.7, 56.0, 55.9, 55.9, 48.2, 38.1, 21.7.

HRMS (EI) calcd for C₂₇H₂₇NO₄, 430.2018 *m/z* (M+H)⁺; Found, 430.2021 *m/z*.



3-(5-Bromo-1*H*-indol-3-yl)-3-(4-methoxy-phenyl)-1-phenyl-propan-1-one.¹ Yield = 86%, Column purified with EtOAc: Pet Ether = 1:4, Brown crystalline solid (Recrystallised from MeOH), mp 153 °C.

¹H NMR (CDCl₃, 400 MHz): δ 8.13 (bs, 1H), 7.92 (d, *J* = 8.2 Hz, 2H), 7.58-7.50 (m, 2H), 7.50-7.39 (m, 2H), 7.24-7.12 (m, 4H), 6.93 (s, 1H), 6.82 (d, *J* = 8.6 Hz, 2H), 4.95 (t, *J* = 7.2 Hz, 1H), 3.74 (s, 3H), 3.74-3.67 (m, 2H).

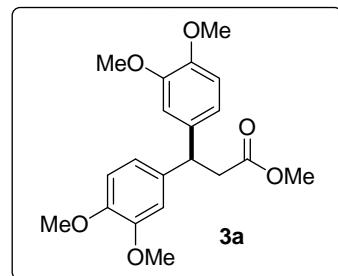
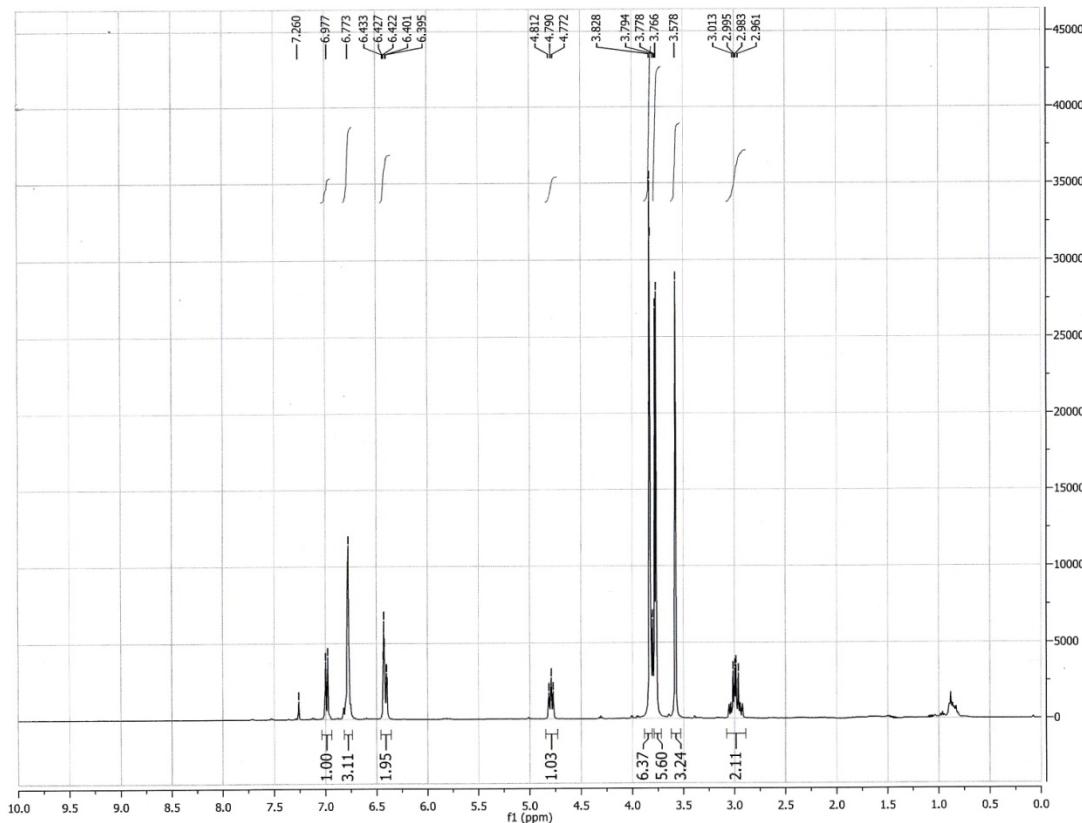
¹³C-NMR (CDCl₃, 100 MHz): δ 198.8, 158.2, 137.1, 136.0, 135.4, 133.2, 129.5, 128.7 (2C), 128.5, 128.2 (2C), 125.1, 124.9, 122.6, 122.3, 122.1, 119.4, 114.1, 113.9, 112.8, 55.4, 45.5, 37.4.

HRMS (EI) calcd for C₂₄H₂₀BrNO₂, 434.0756 *m/z* (M+H)⁺; Found, 434.0757 *m/z*.

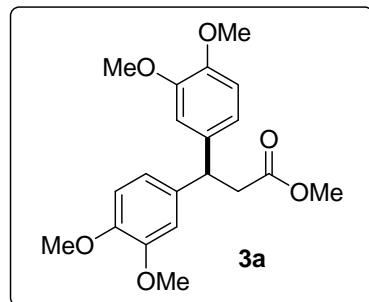
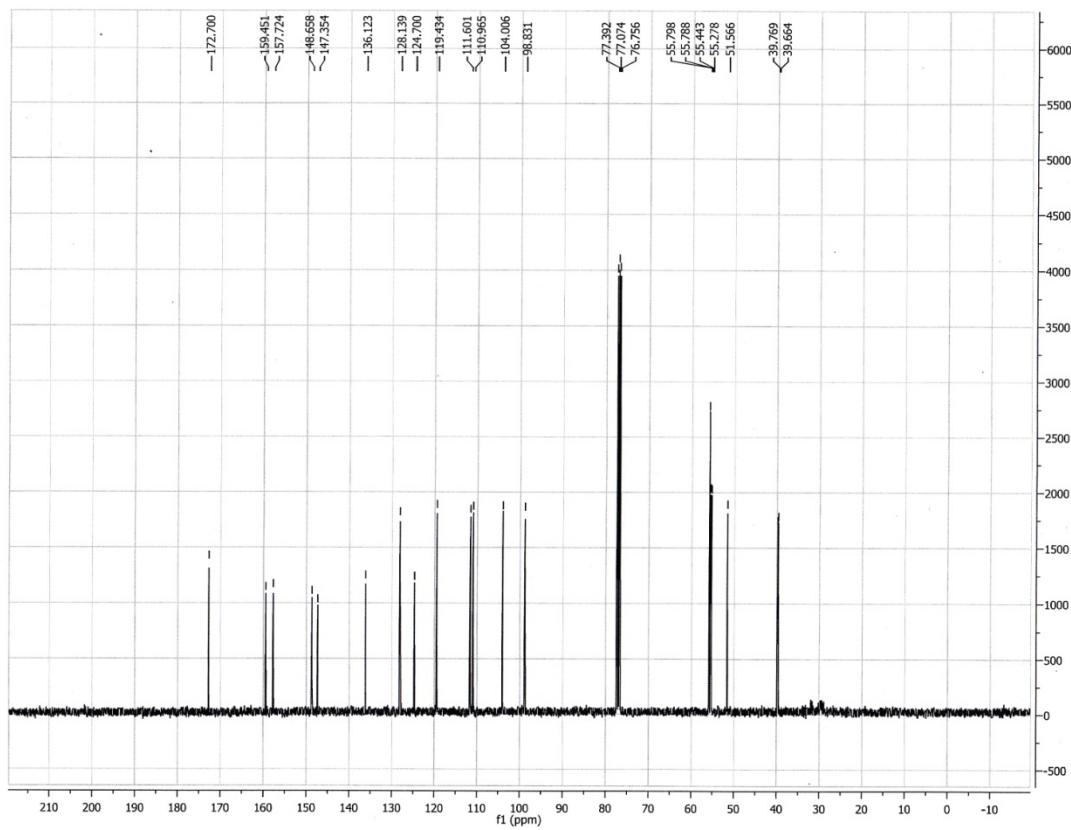
Reference 1: *Indian Journal of Chemistry*, Volume 54B, **2015**, 240-244

Copy of ¹H NMR and ¹³C Spectra of Friedel-Crafts Alkylated Products 3a-3m

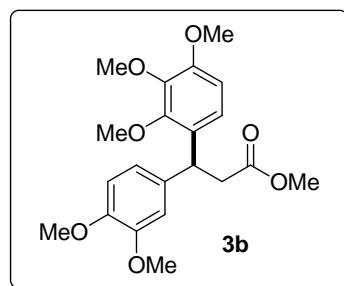
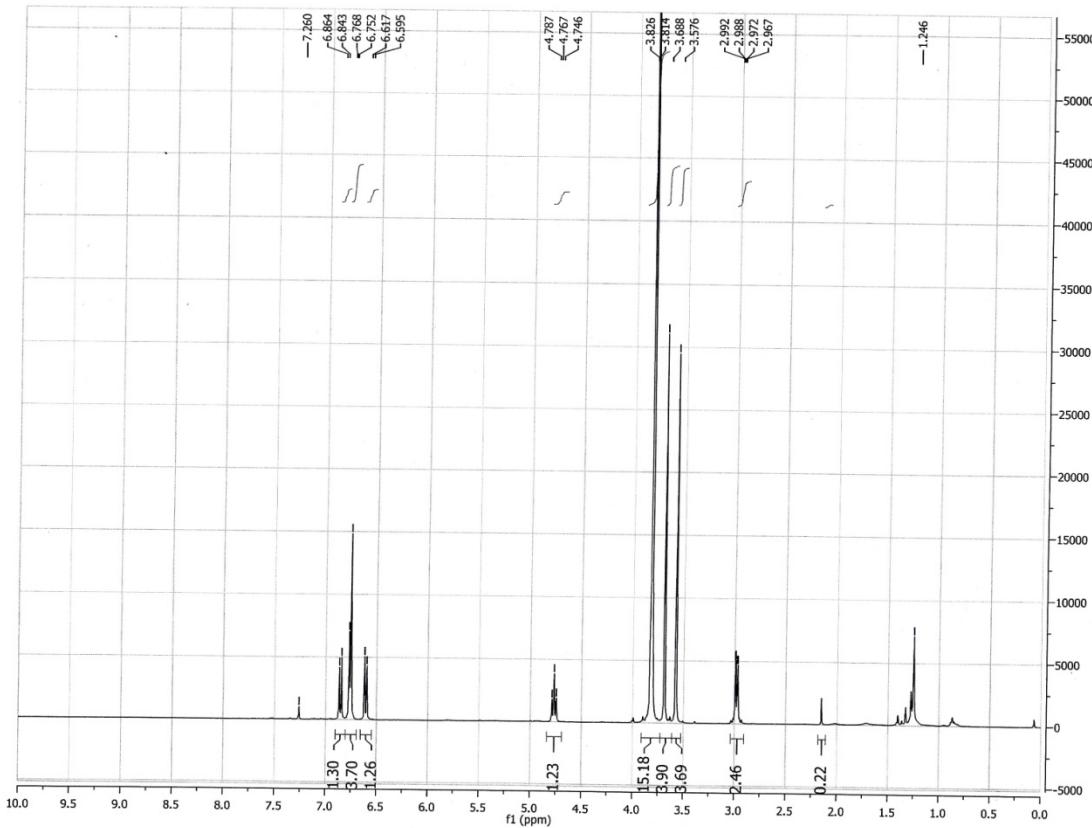
¹H-NMR of compound 3a



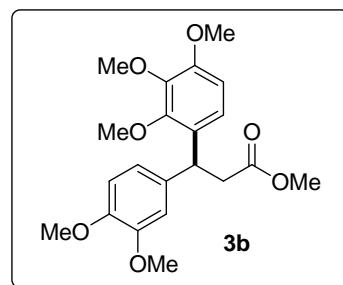
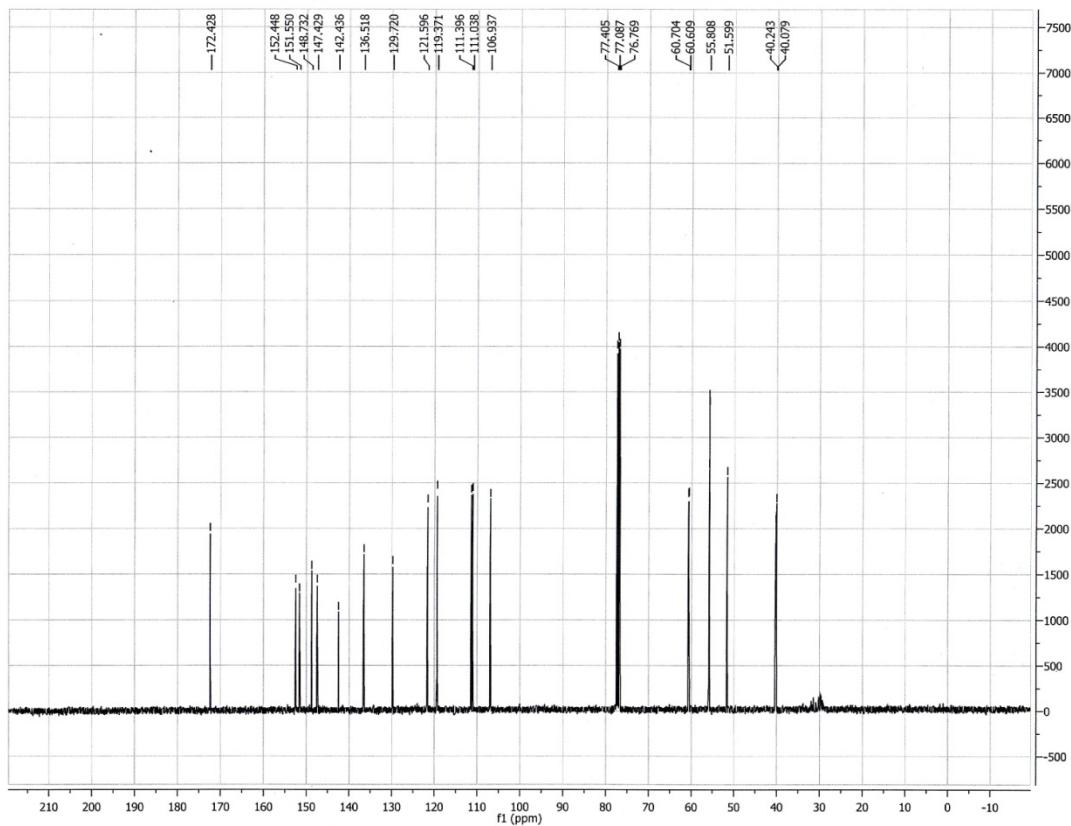
¹³C-NMR of compound 3a



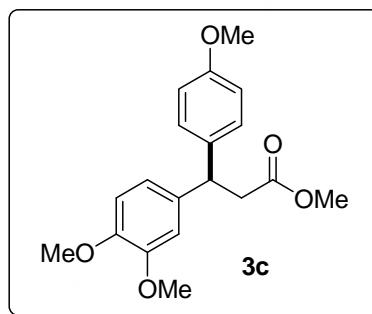
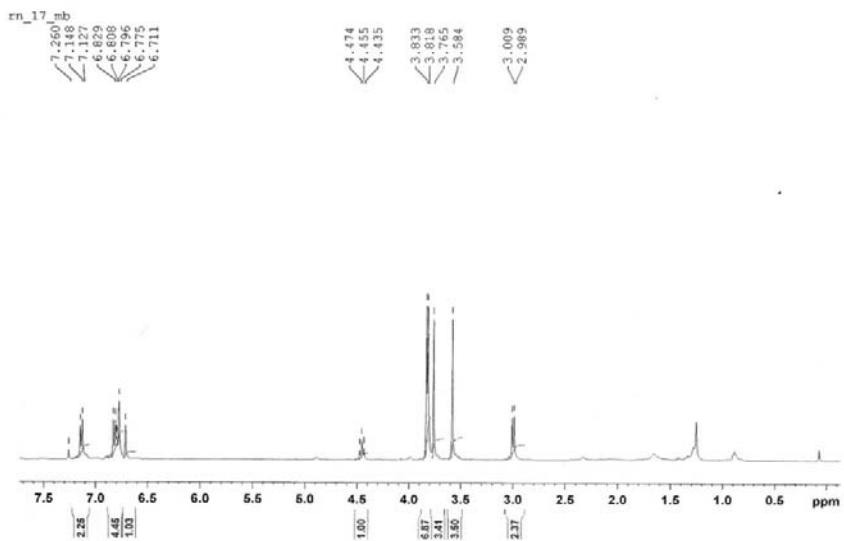
¹H-NMR of compound **3b**



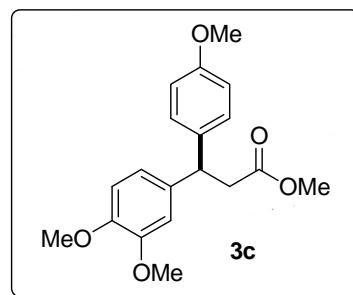
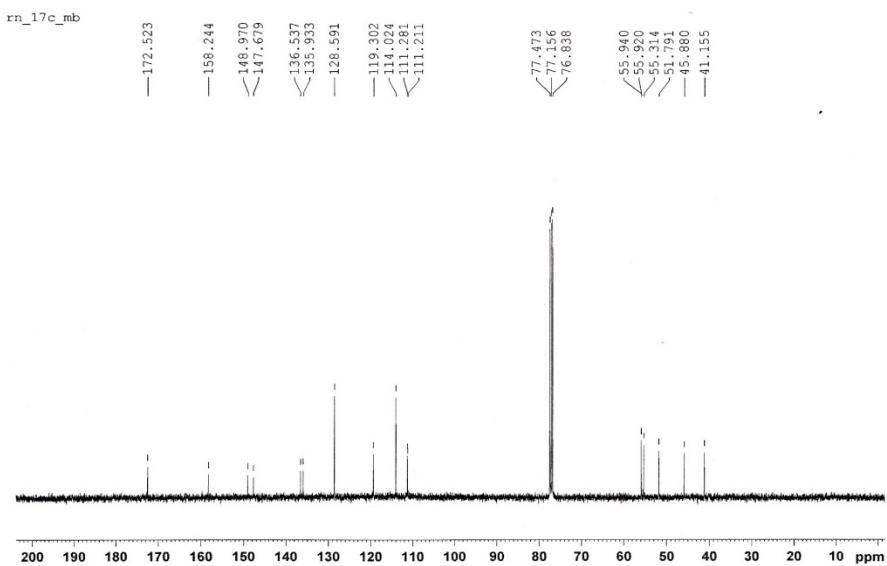
¹³C-NMR of compound **3b**



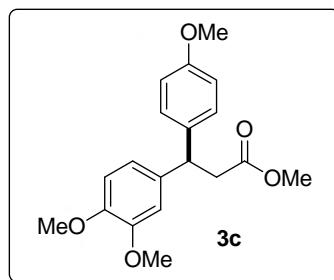
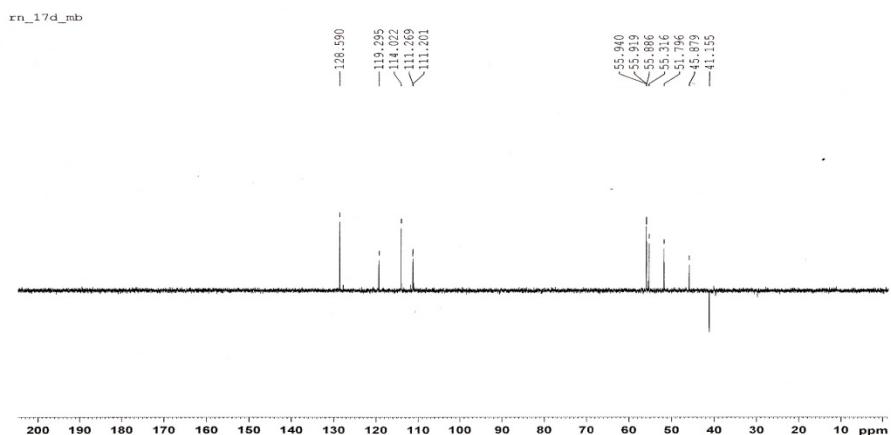
¹H-NMR of compound 3c



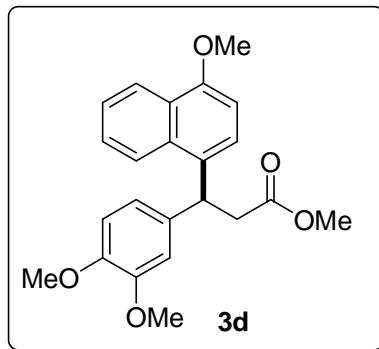
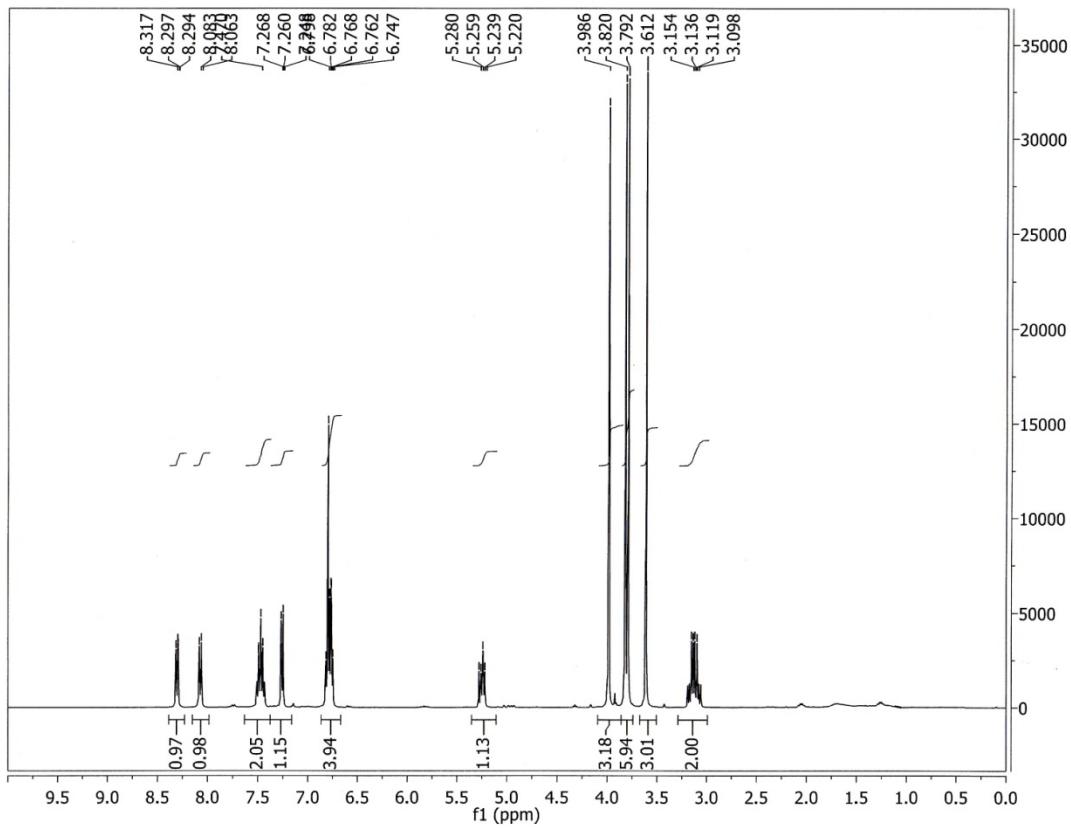
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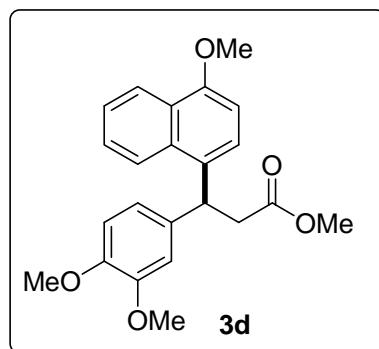
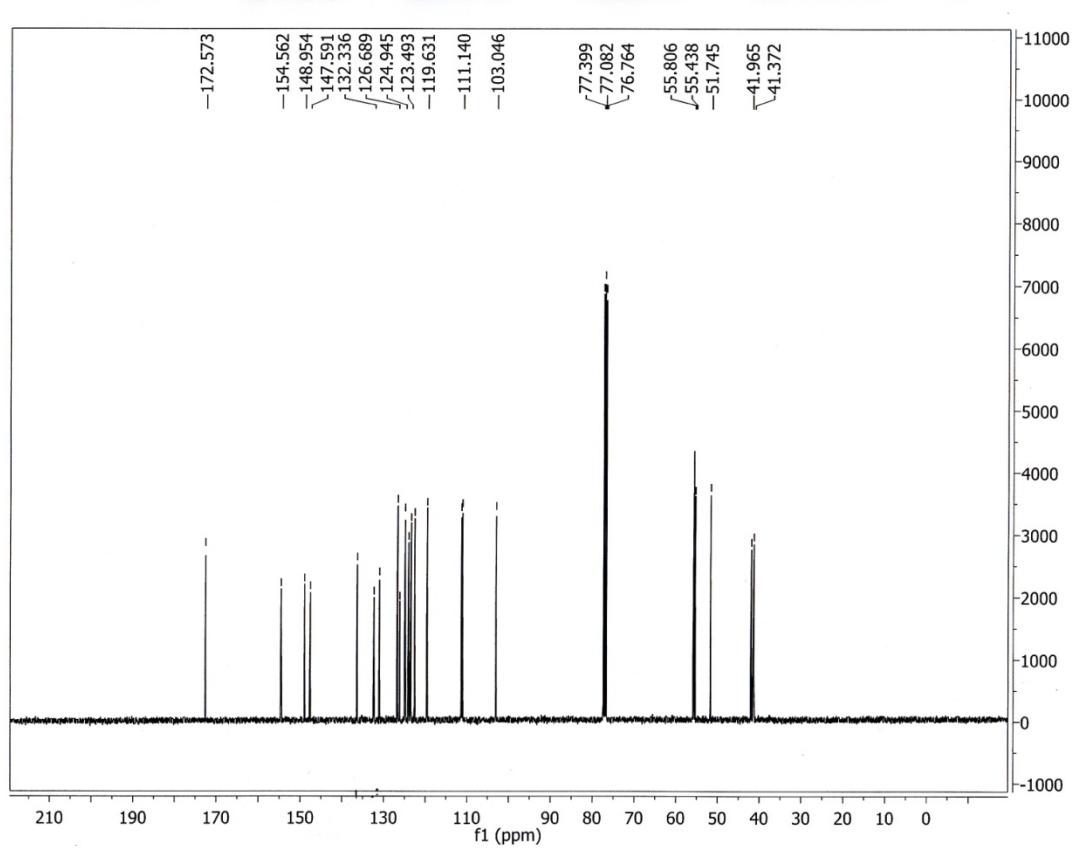
DEPT-135 of compound **3c**



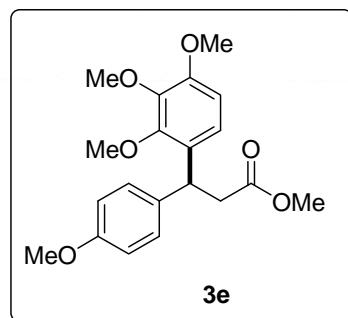
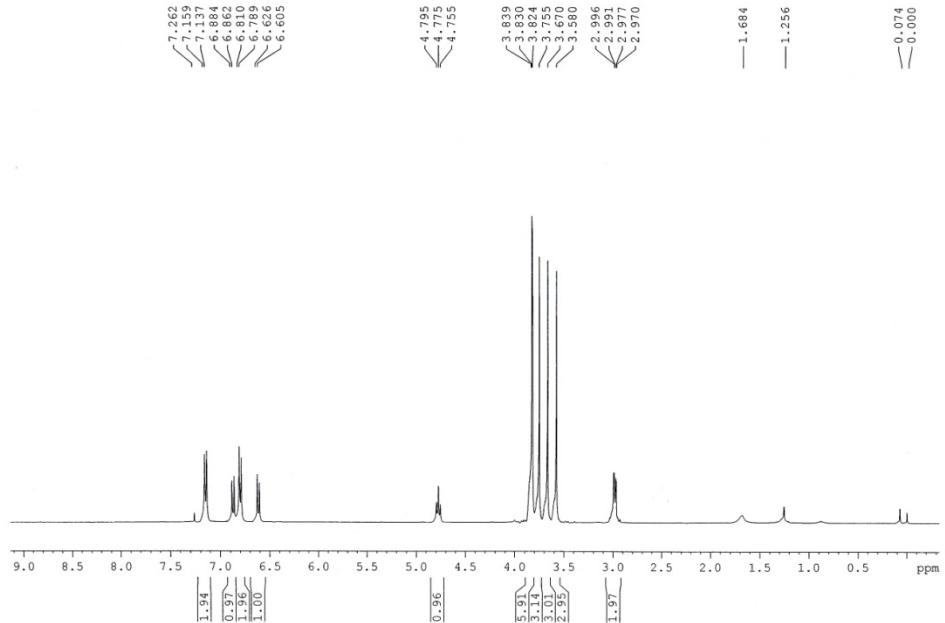
¹H-NMR of compound 3d



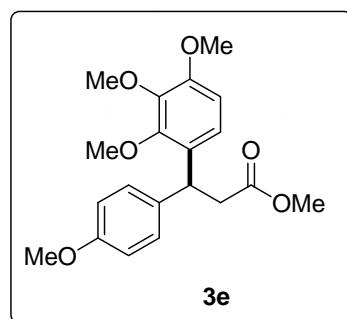
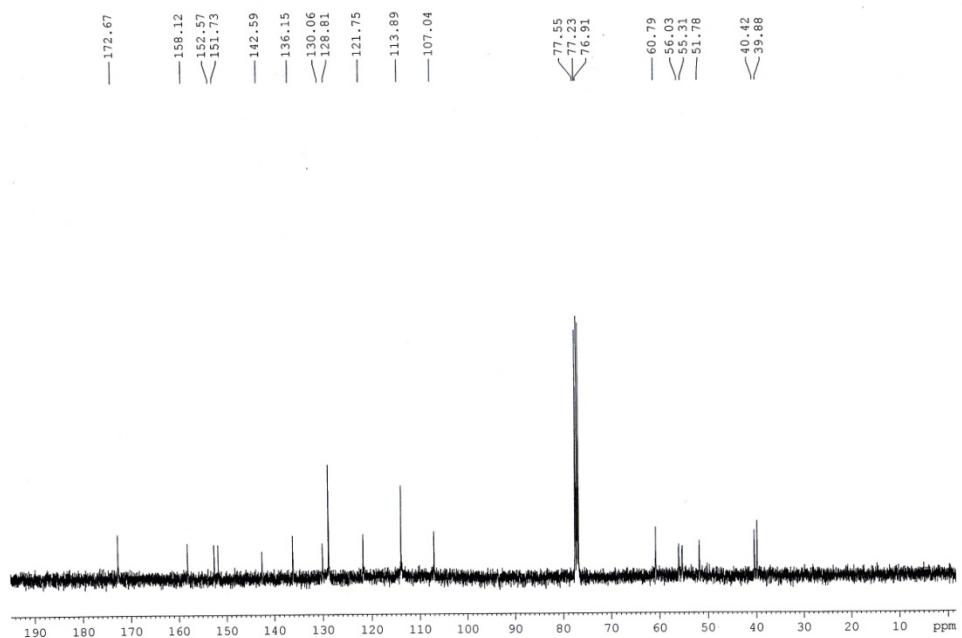
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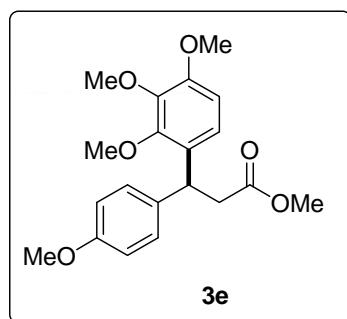
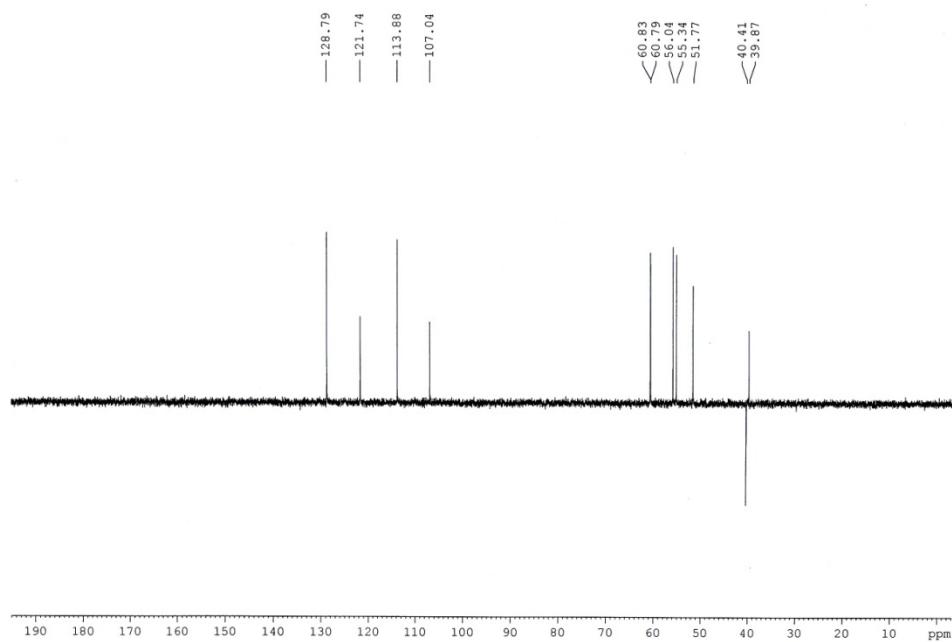
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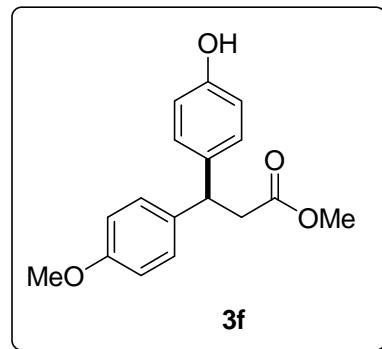
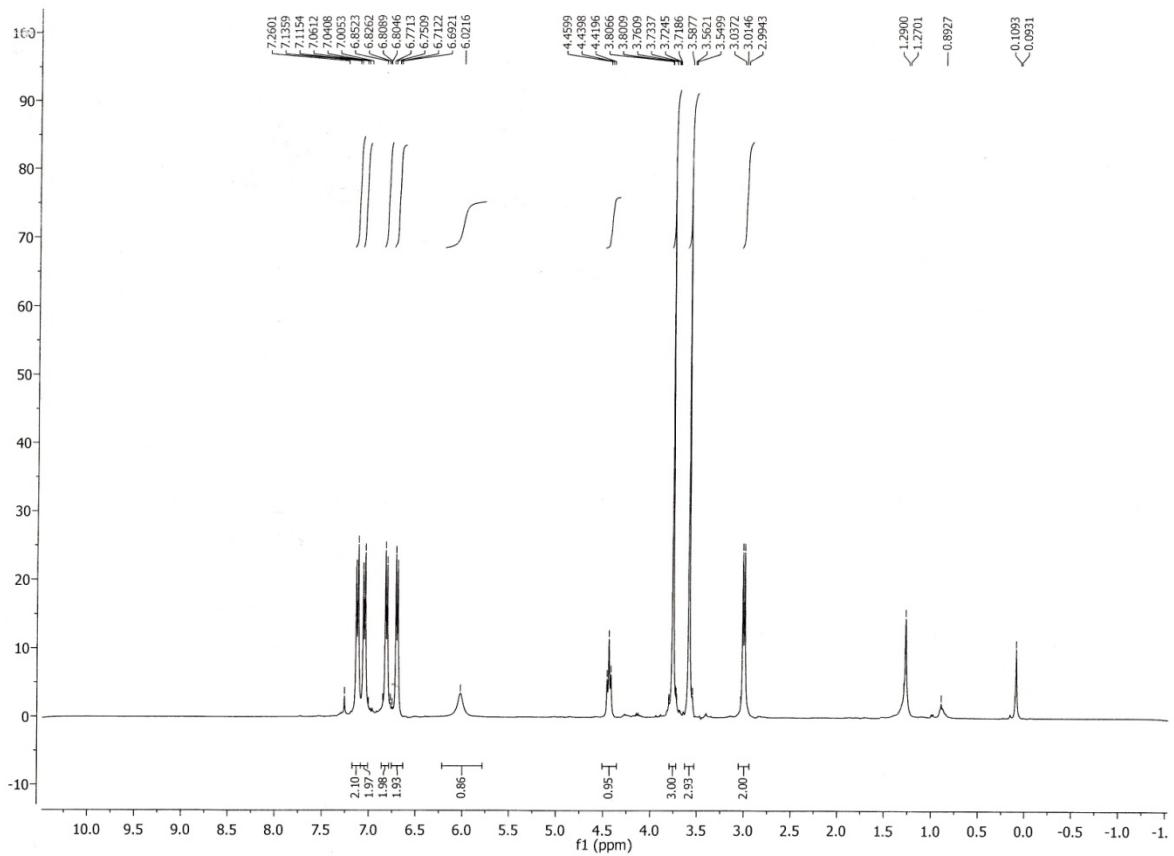
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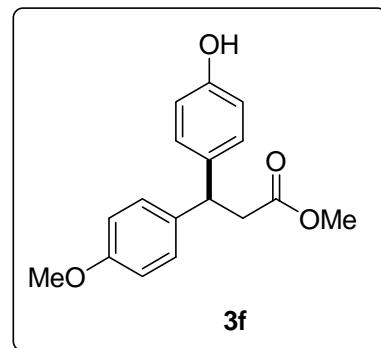
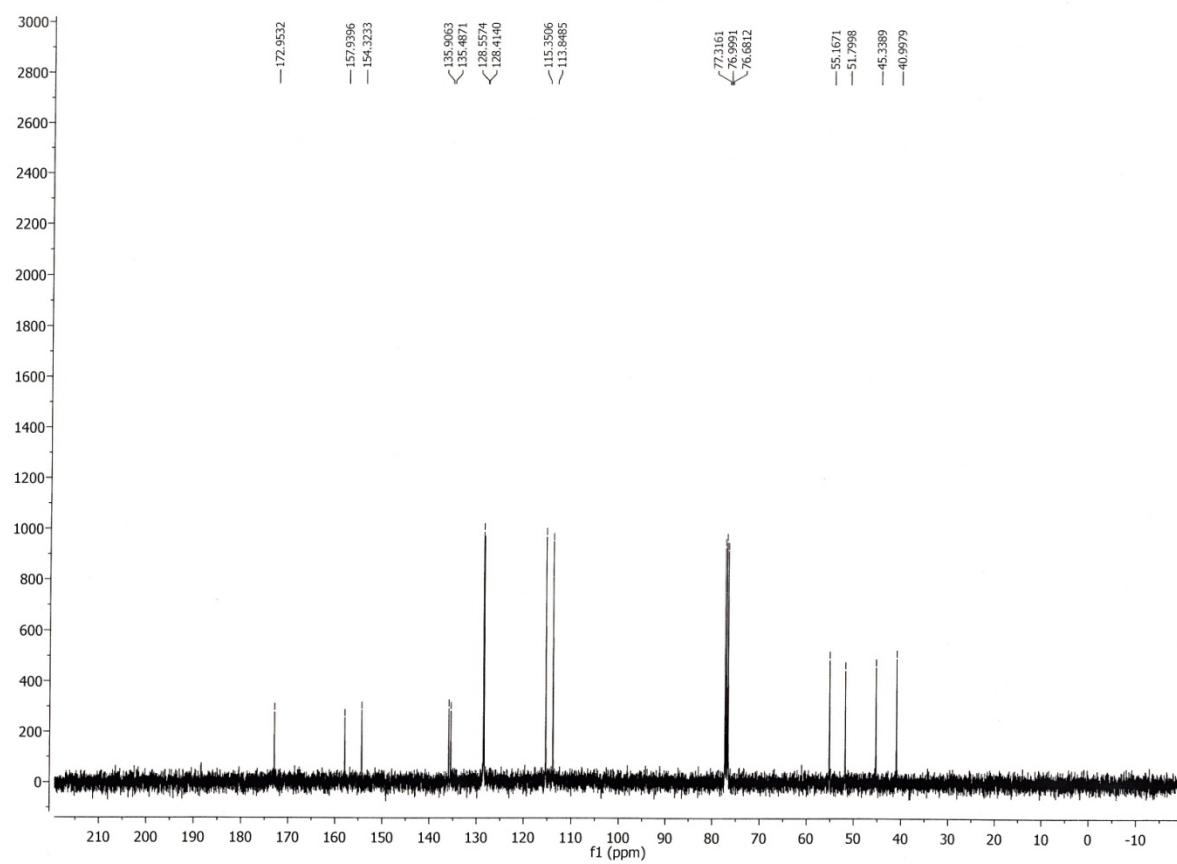
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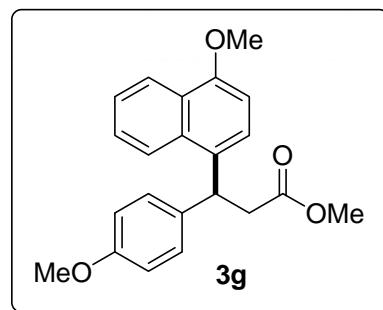
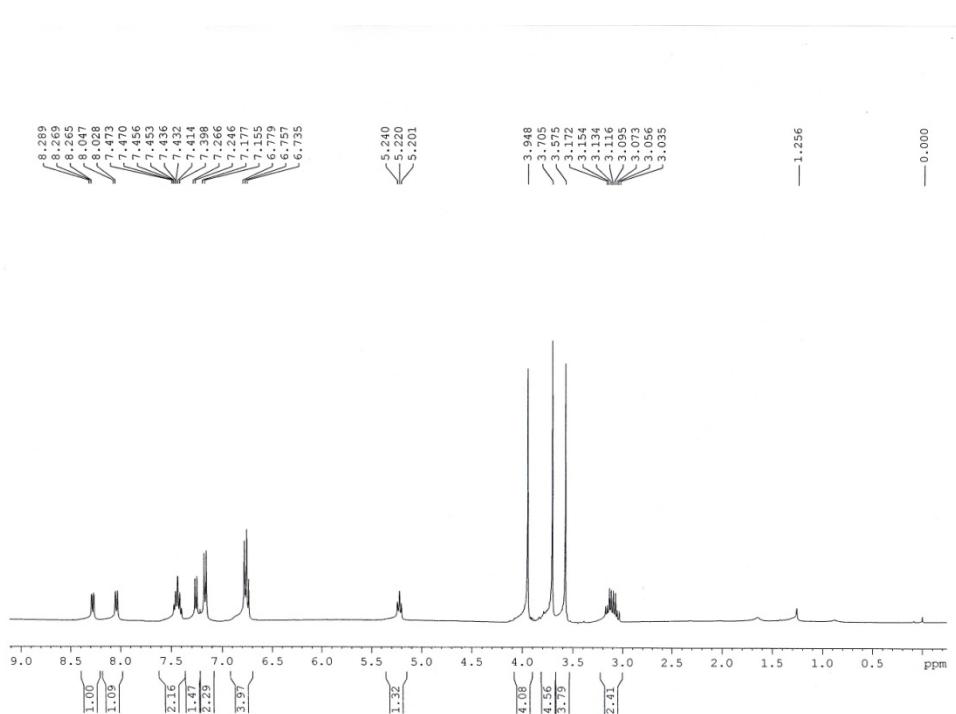
¹H-NMR of compound 3f



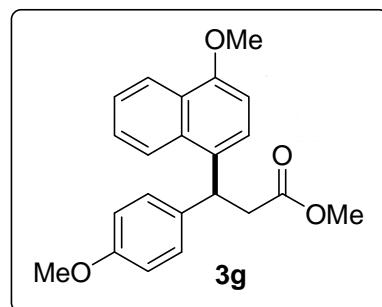
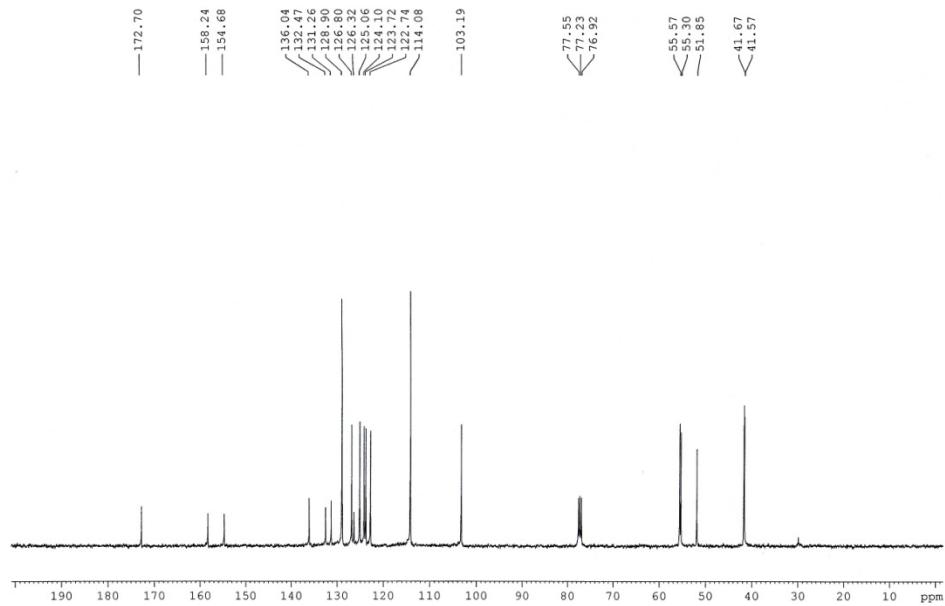
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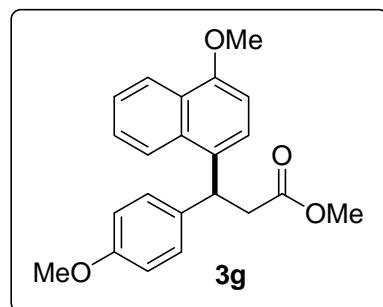
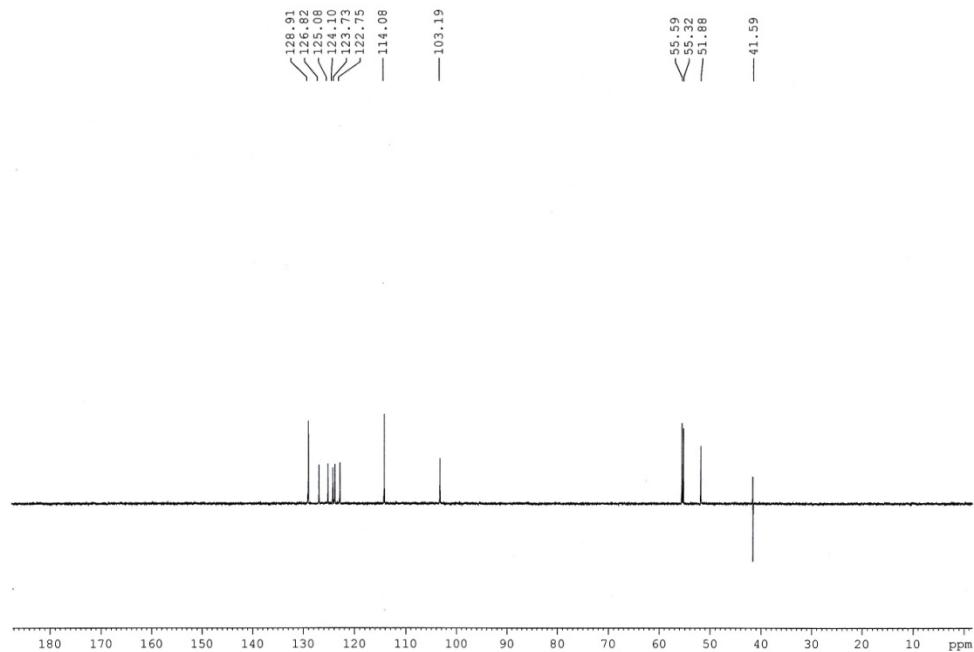
¹H-NMR of compound 3g



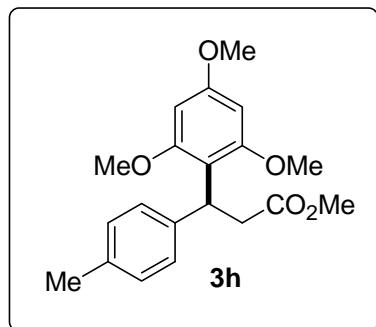
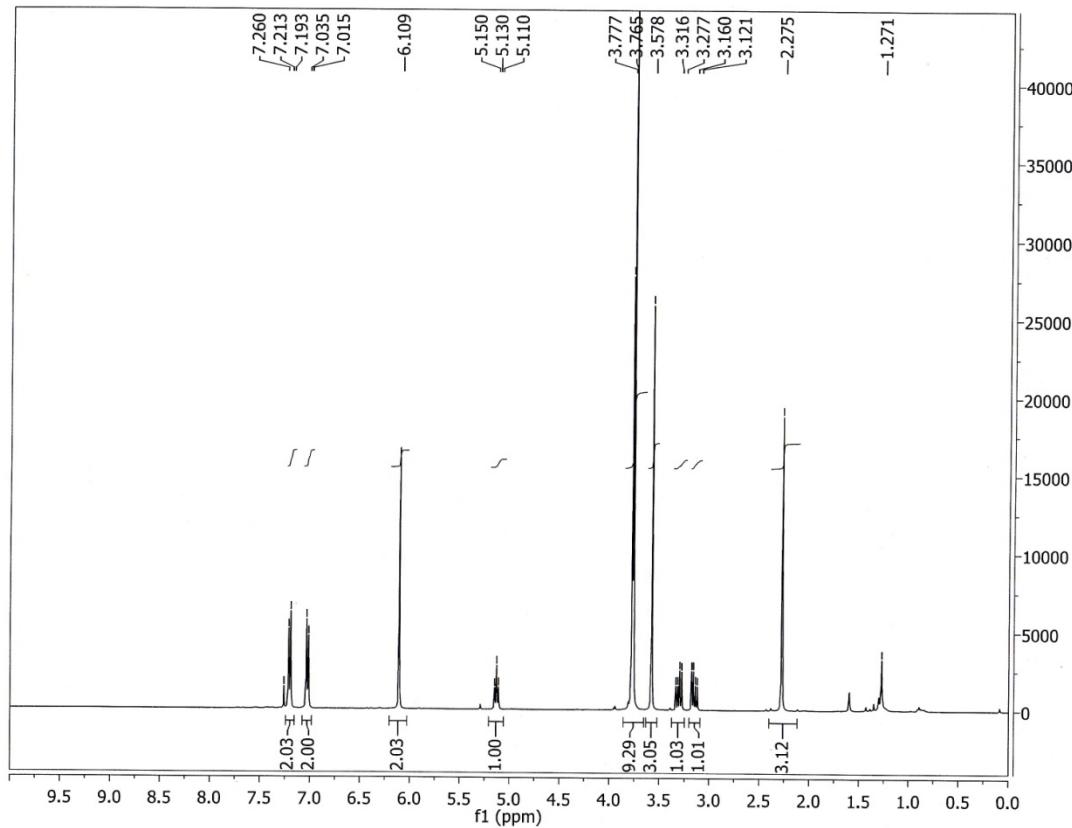
¹³C-NMR of compound 3g



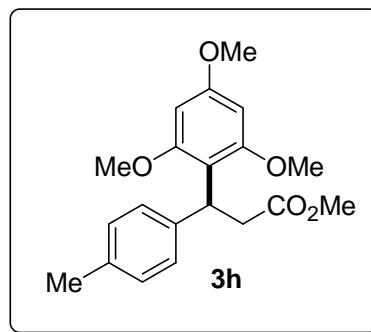
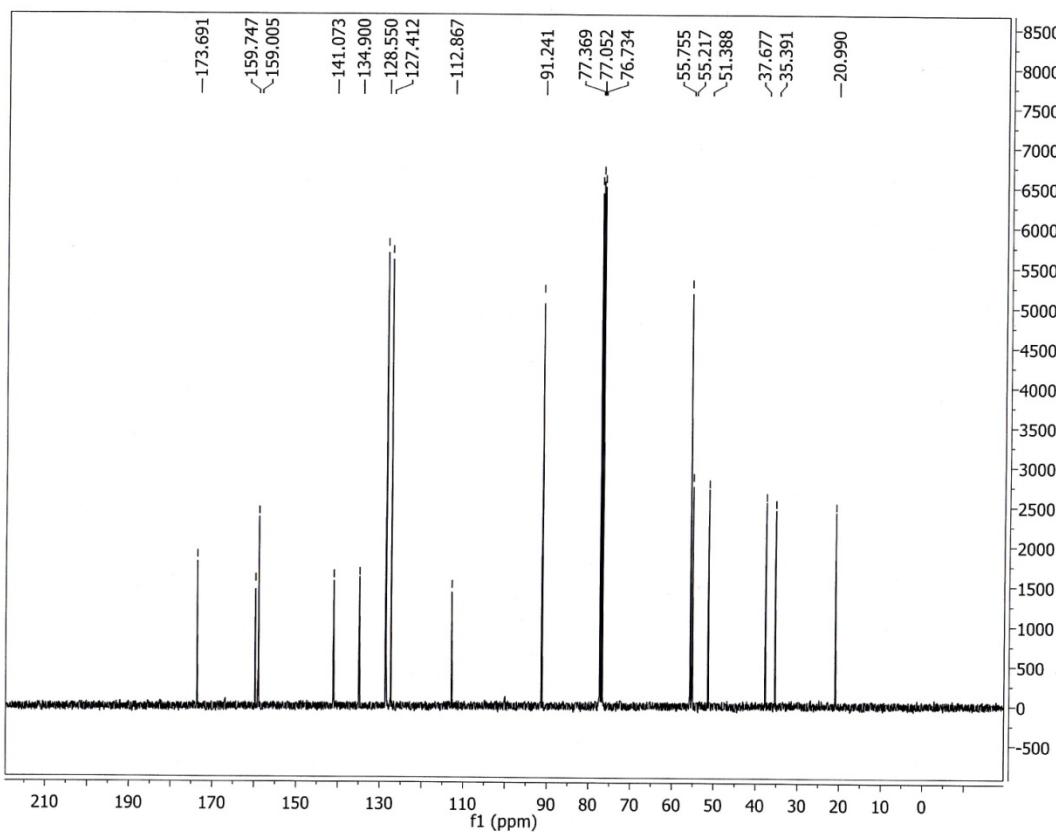
DEPT-135 of compound **3g**



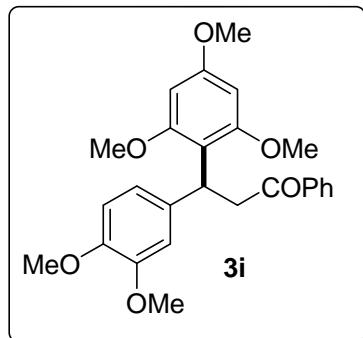
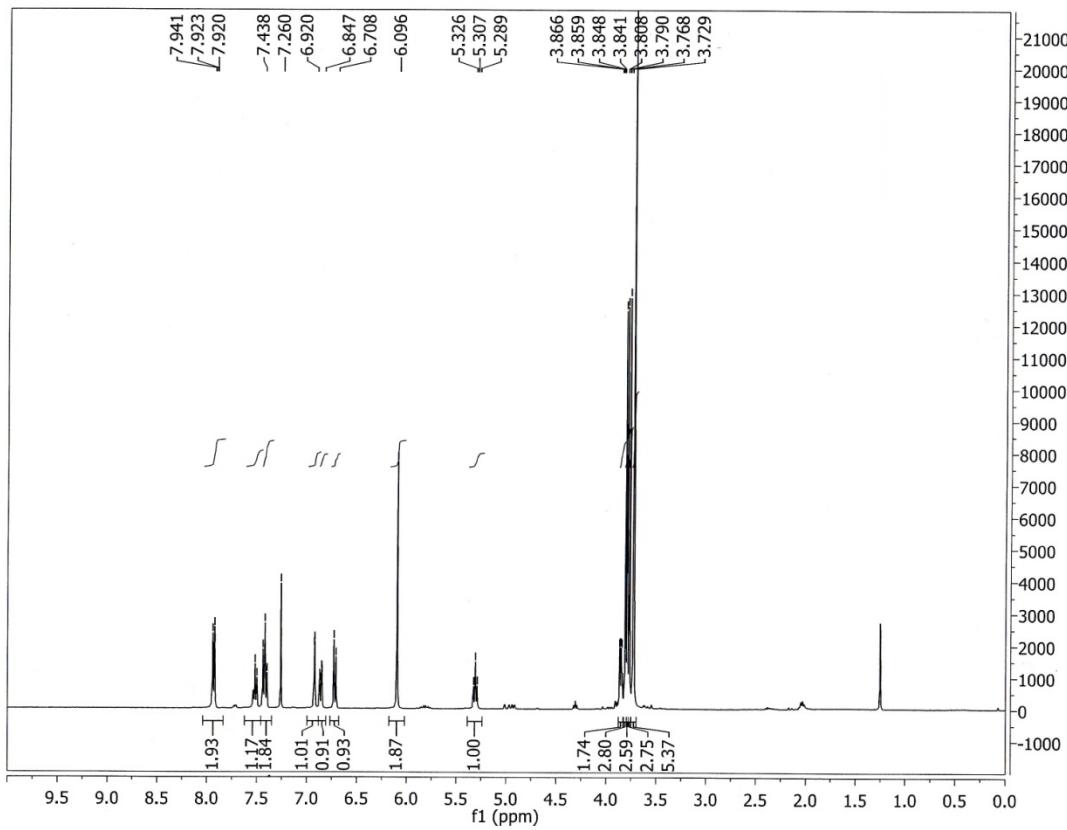
¹H-NMR of compound 3h



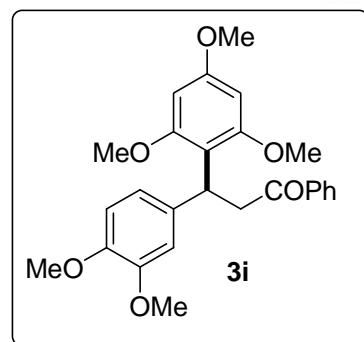
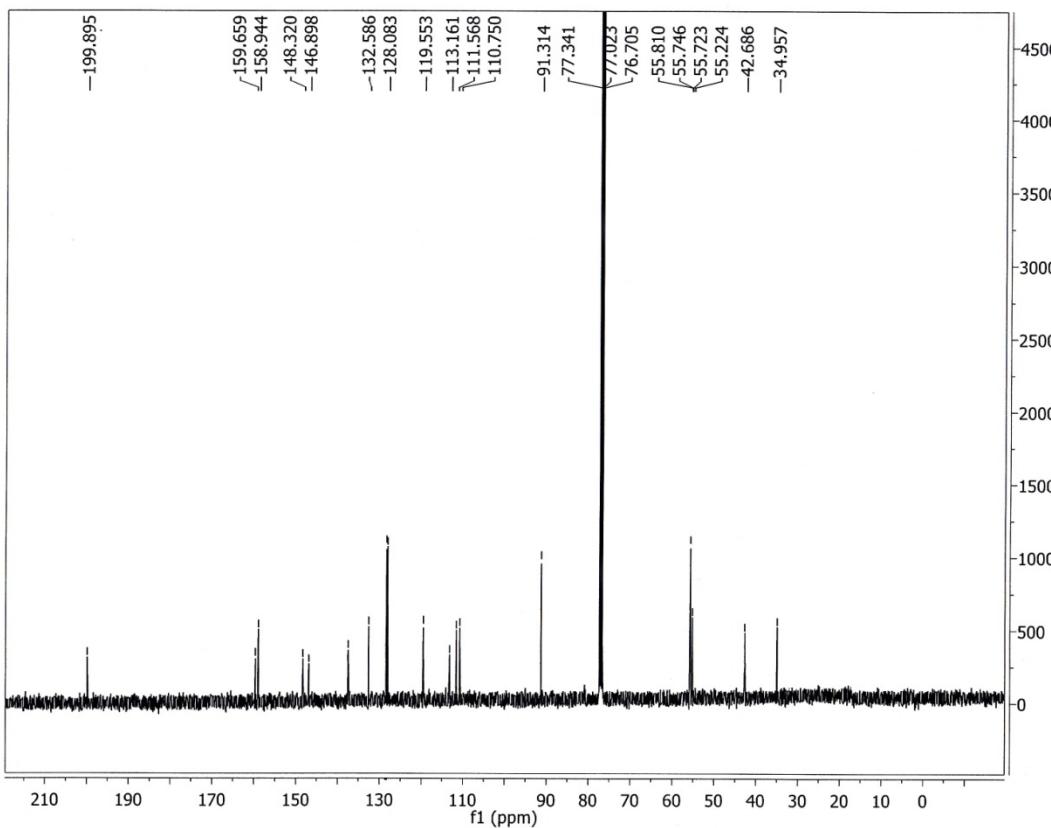
¹³C-NMR of compound **3h**



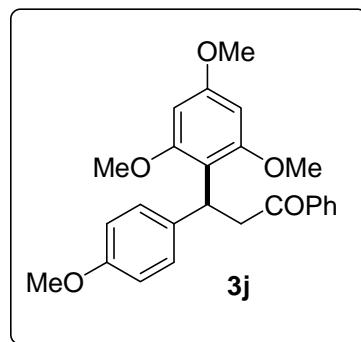
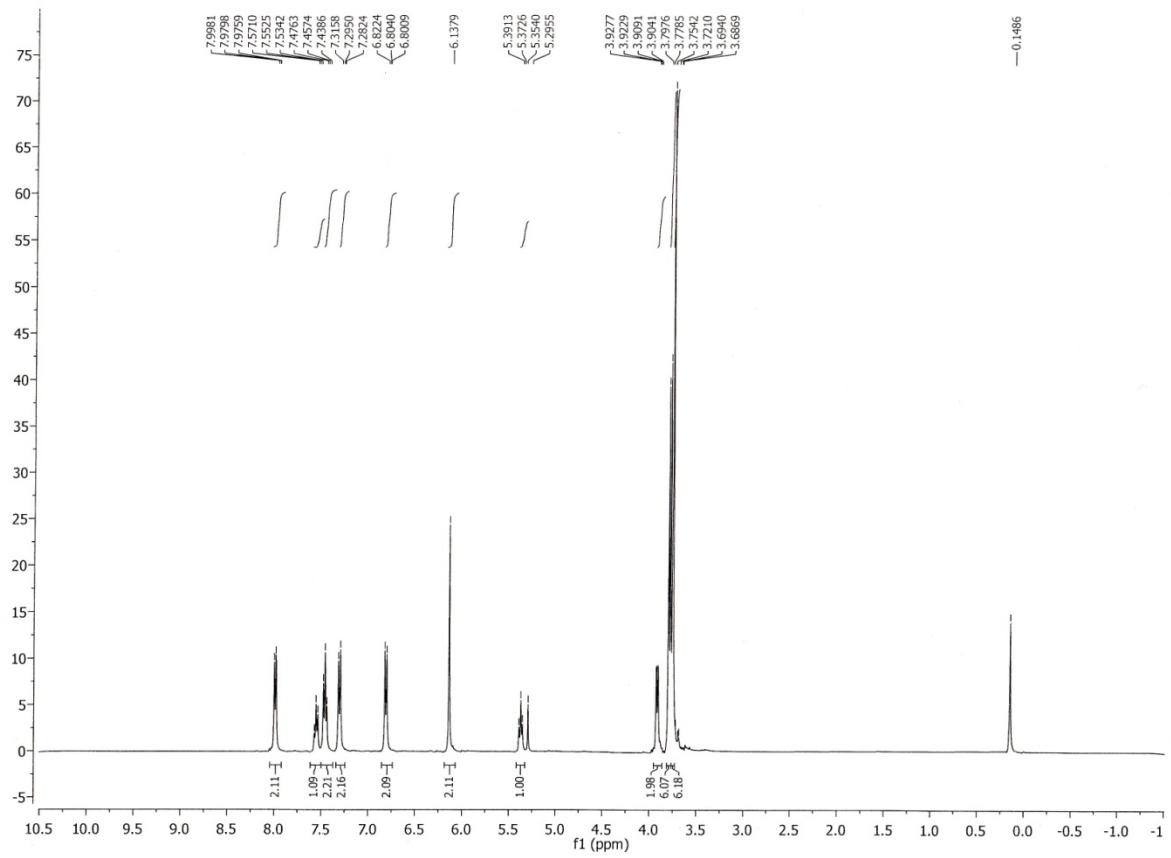
¹H-NMR of compound **3i**



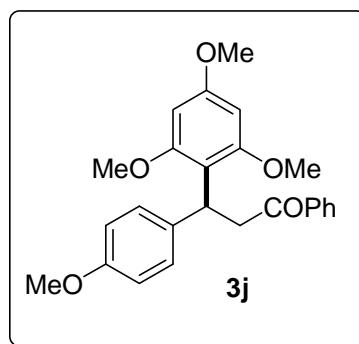
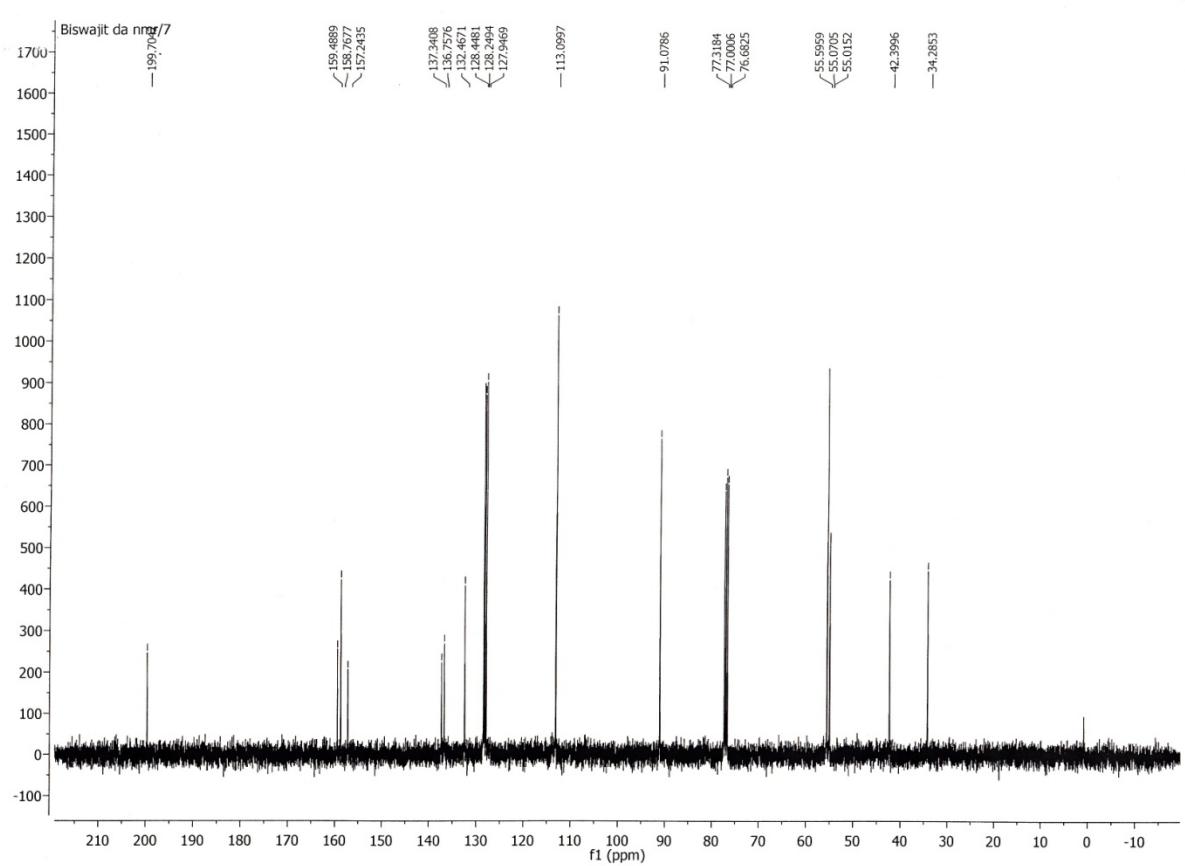
¹³C-NMR of compound **3i**



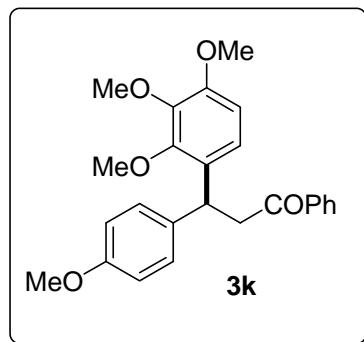
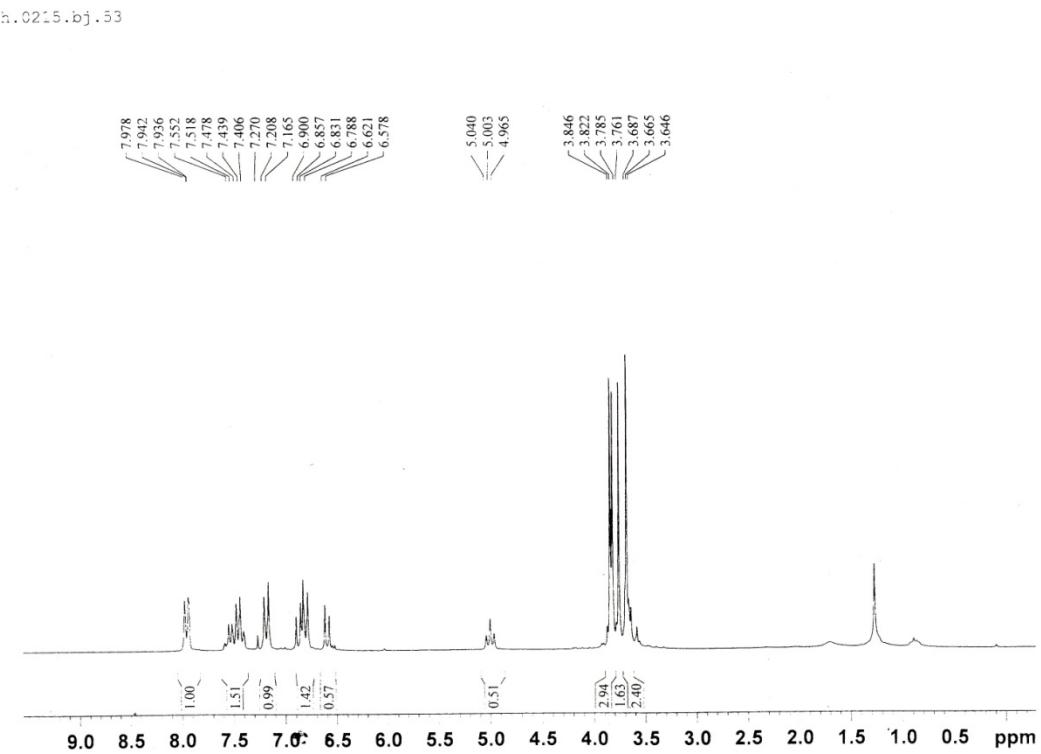
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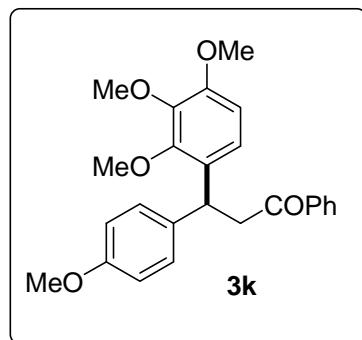
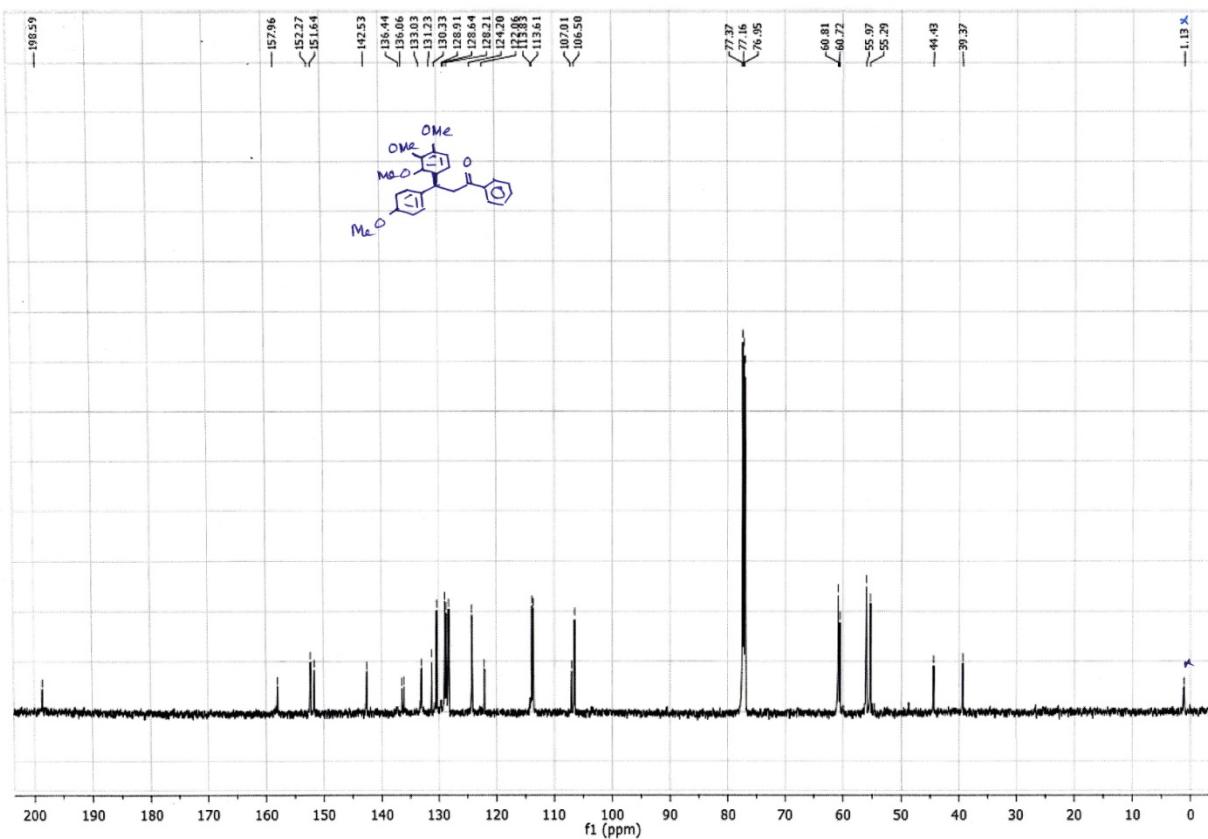
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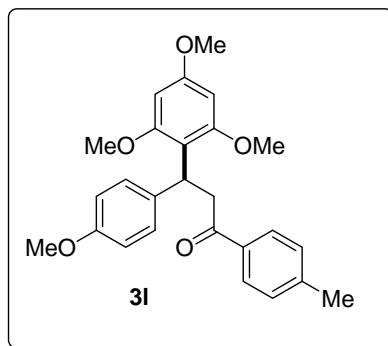
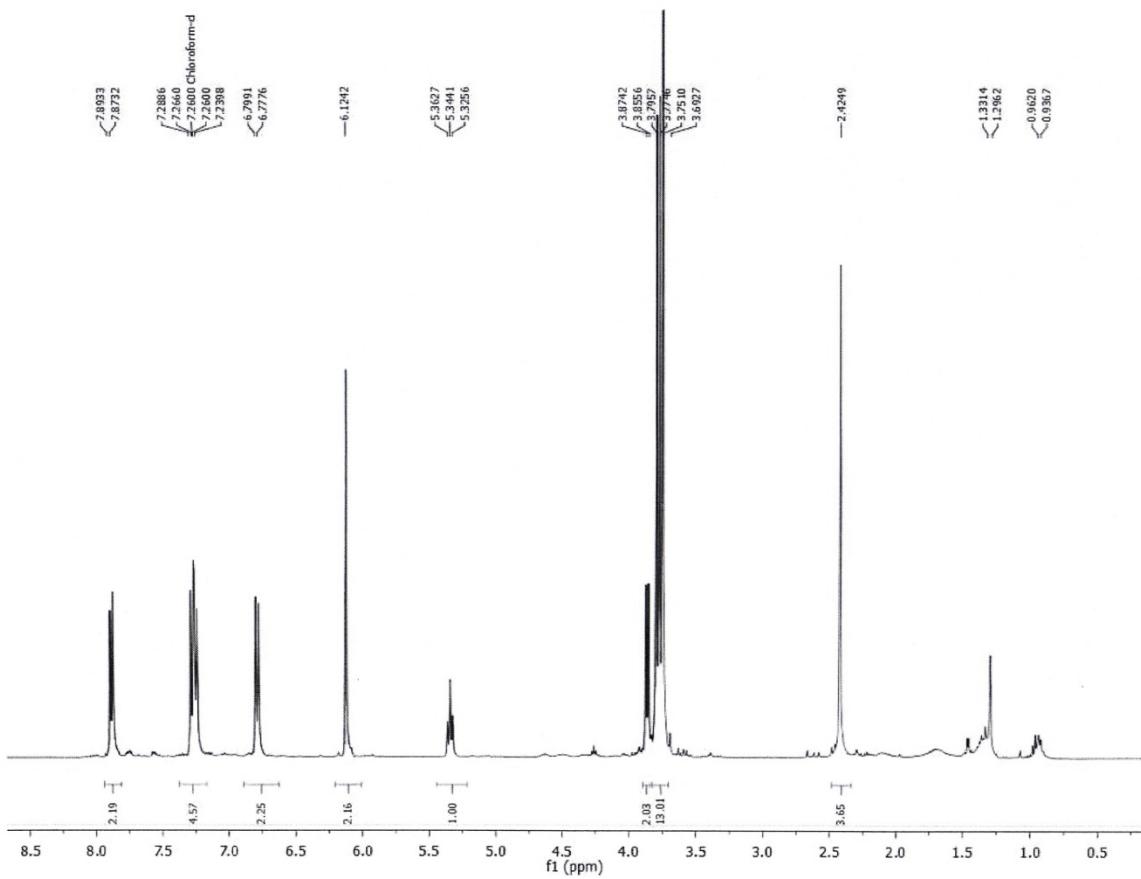
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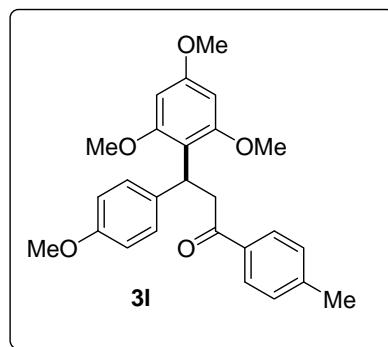
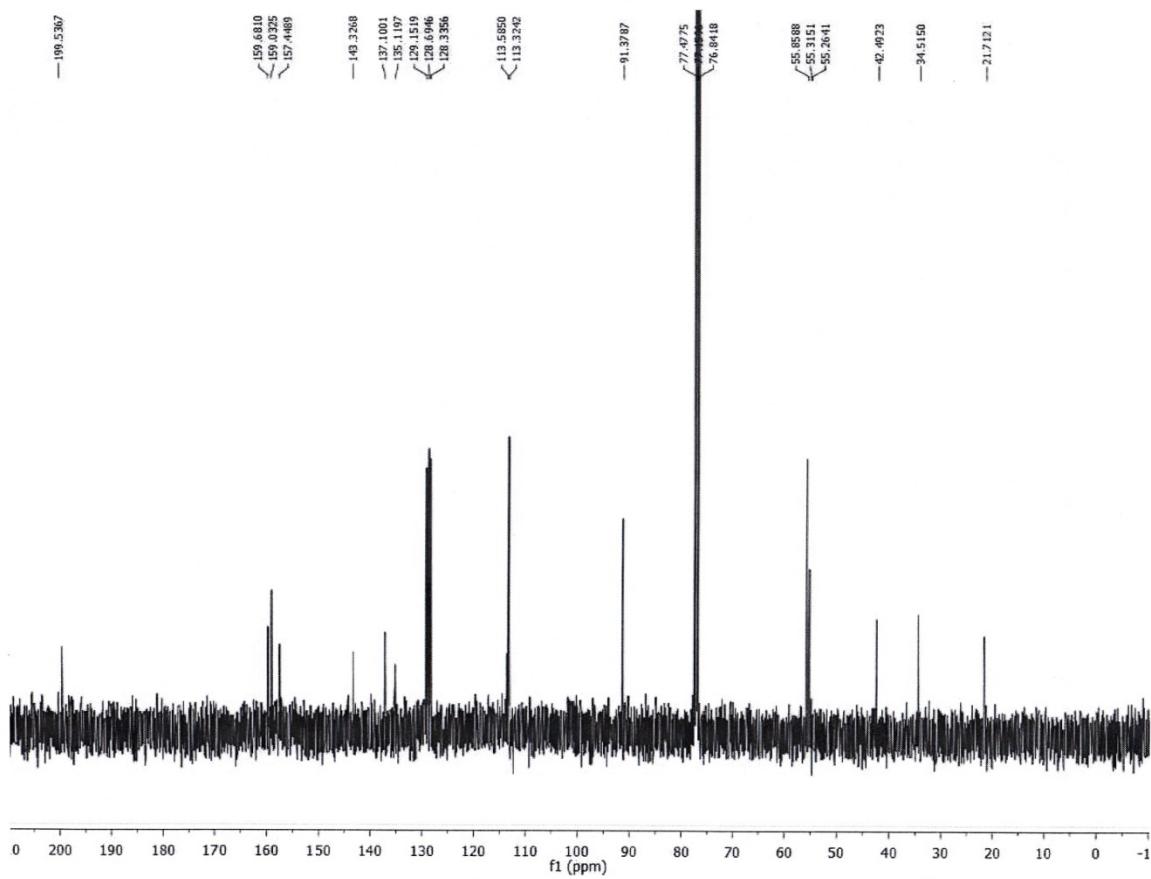
¹³C-NMR of compound 3k



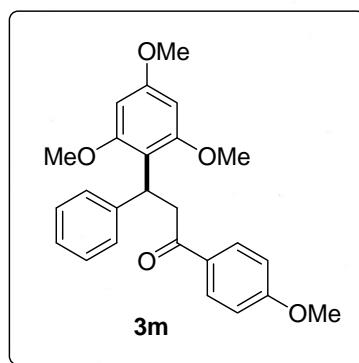
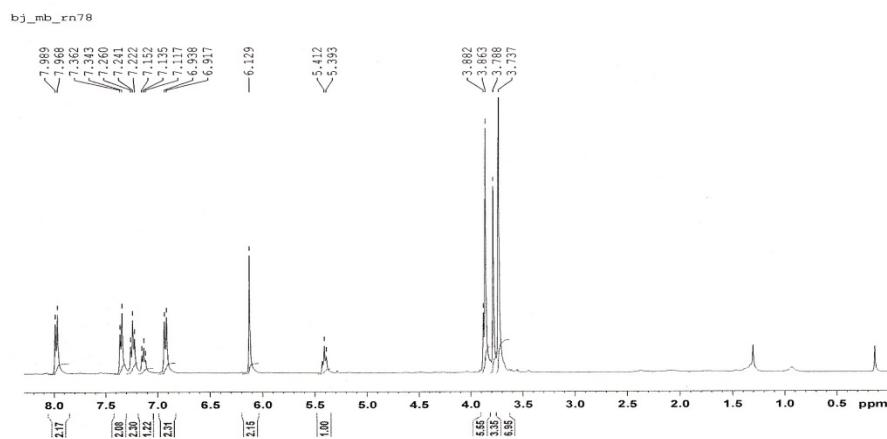
¹H-NMR of compound **3I**



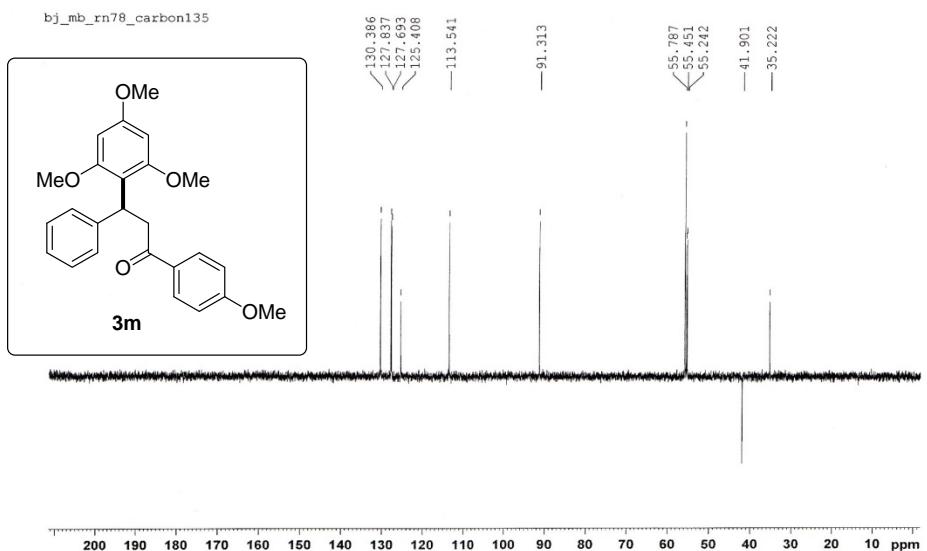
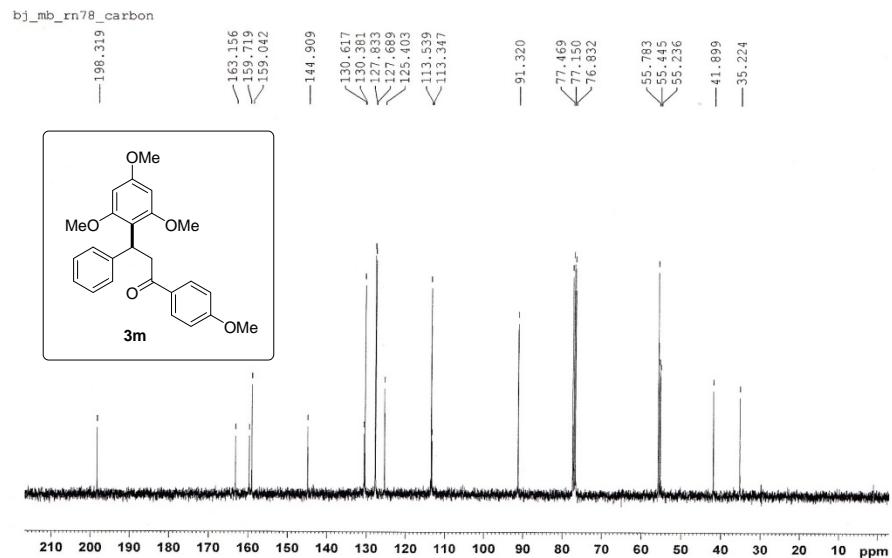
¹³C-NMR of compound **3I**



¹H-NMR of compound 3m

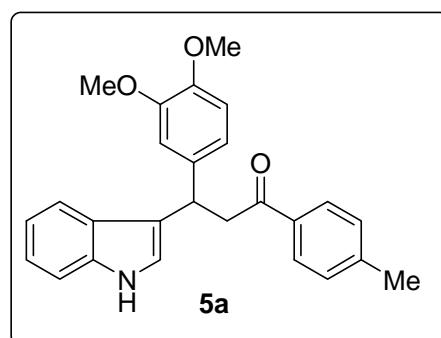
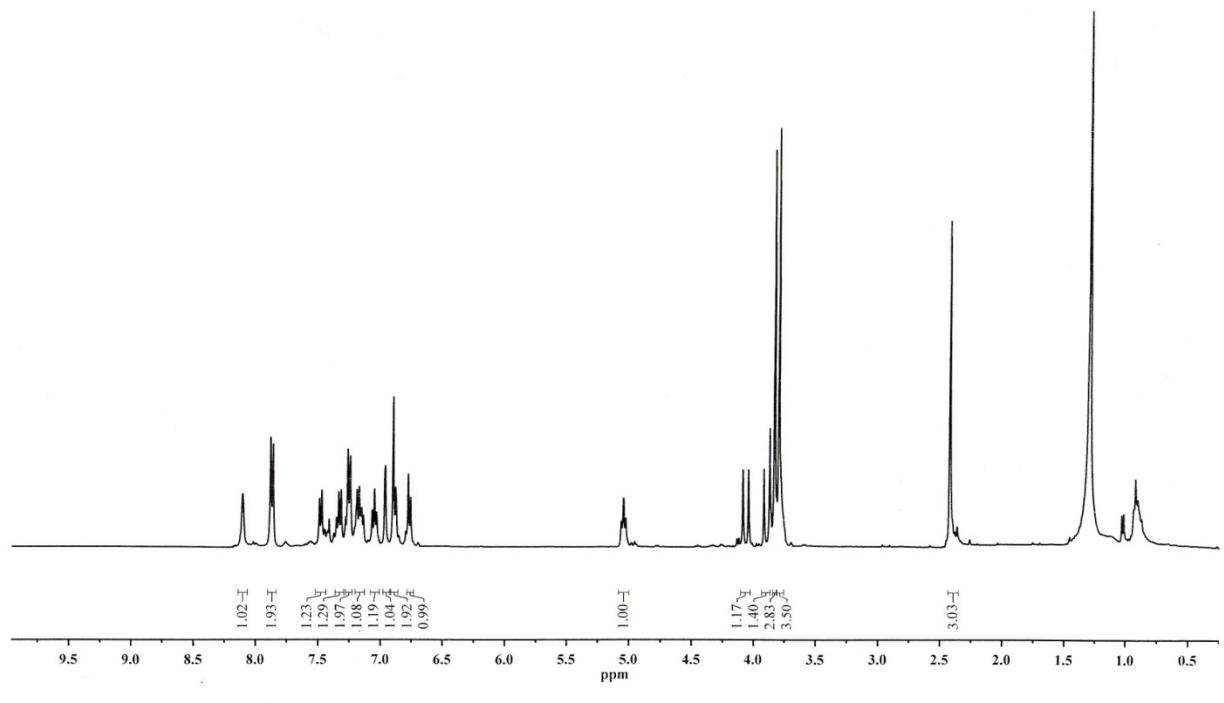


¹³C-NMR of compound 3m

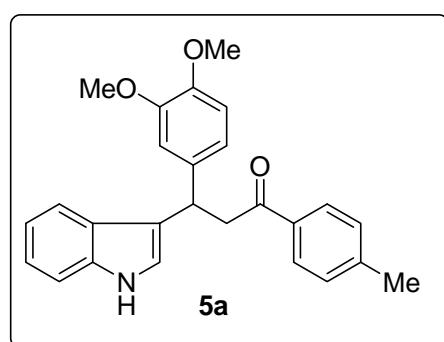
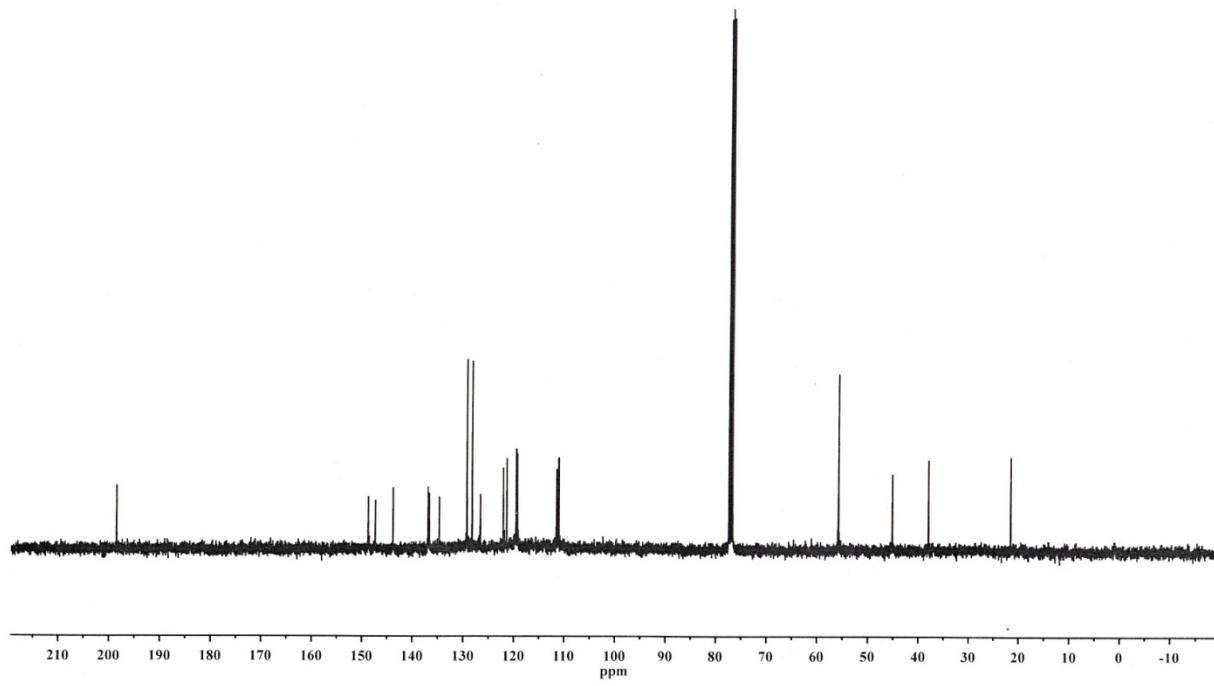


Copy of ^1H NMR and ^{13}C Spectra of Friedel-Crafts Alkylated Products 5a-5d

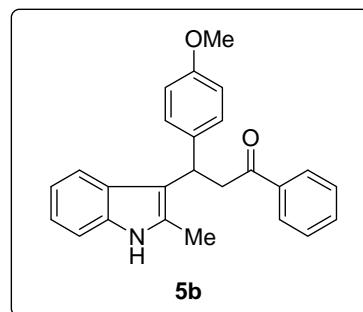
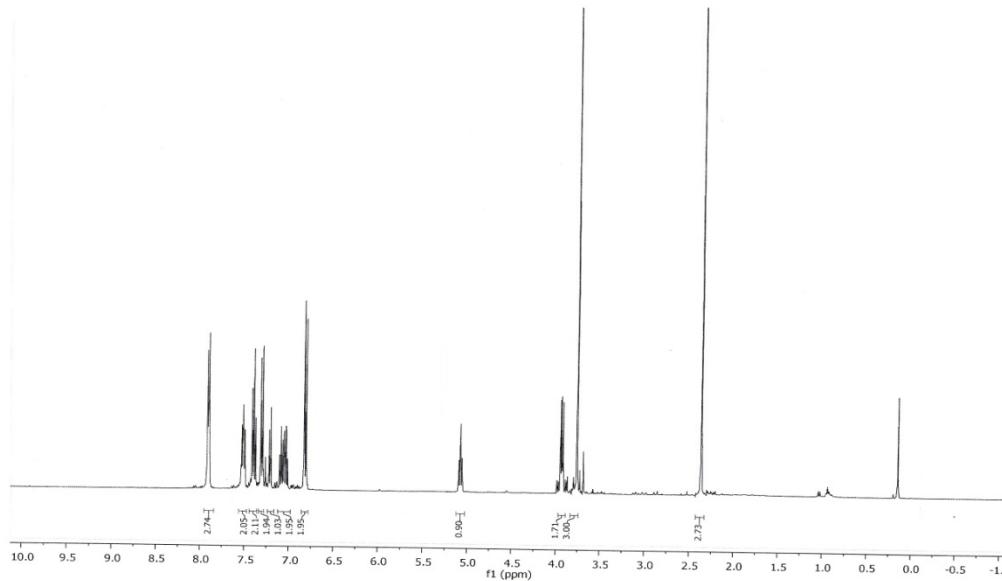
¹H-NMR of compound **5a**



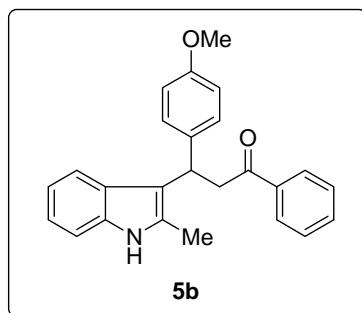
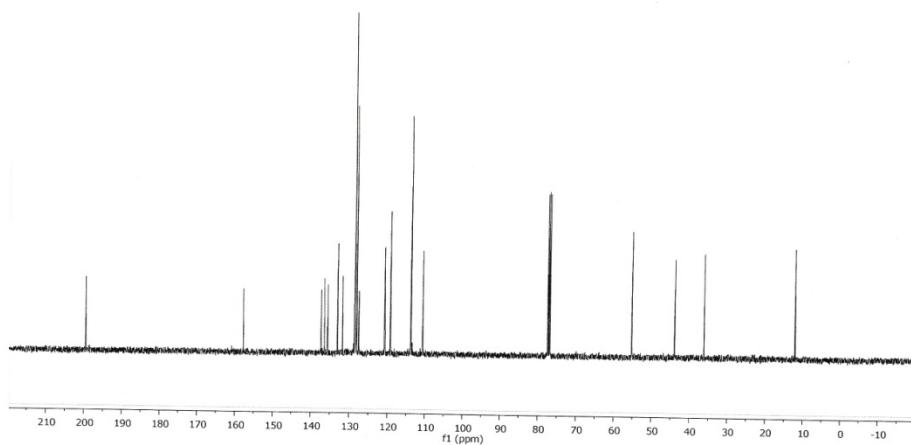
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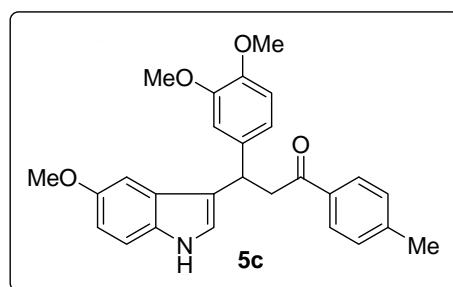
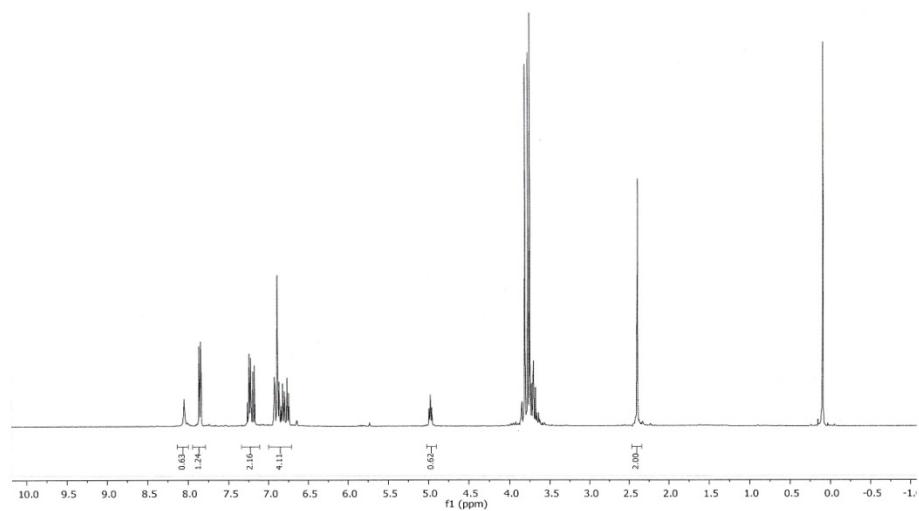
¹H-NMR of compound **5b**



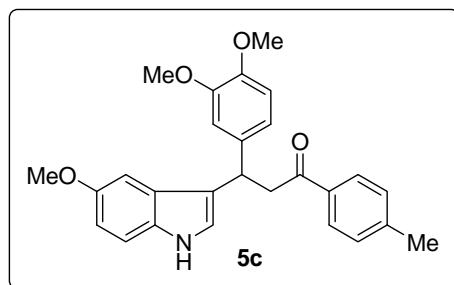
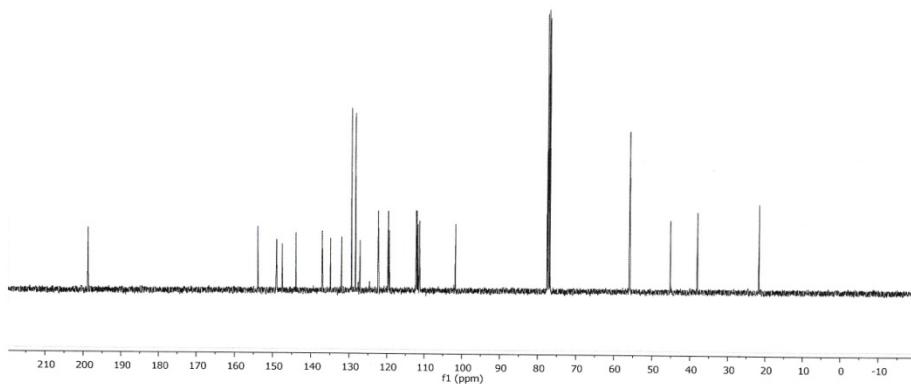
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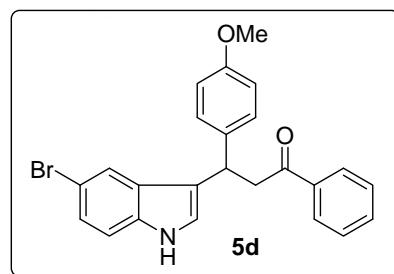
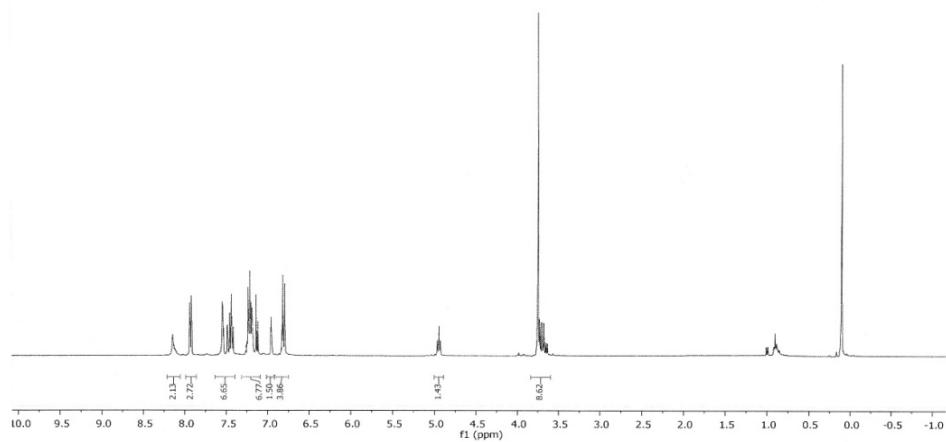
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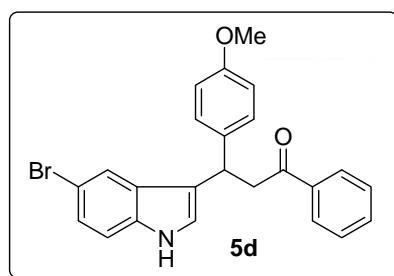
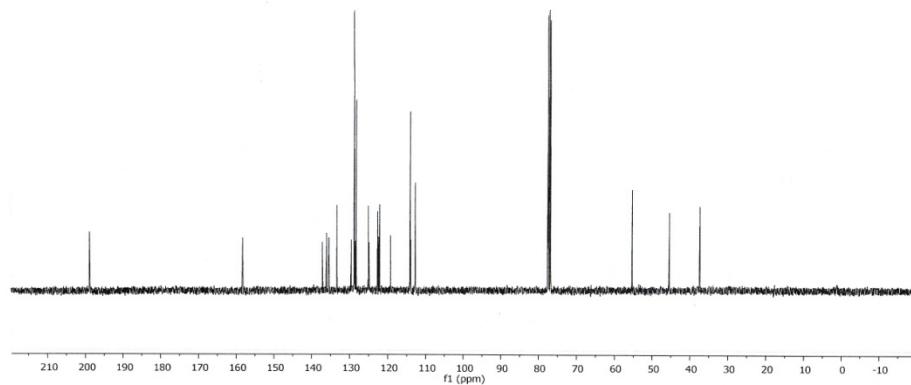
¹³C-NMR of compound **5c**



¹H-NMR of compound **5d**

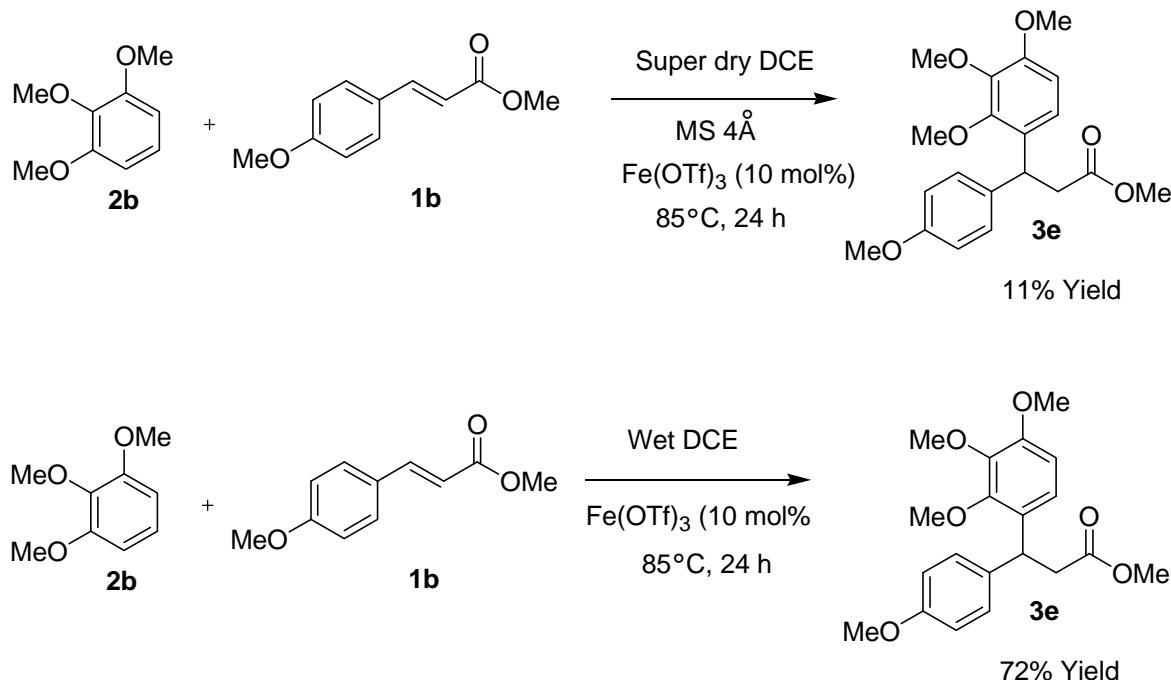


¹³C-NMR of compound **5d**

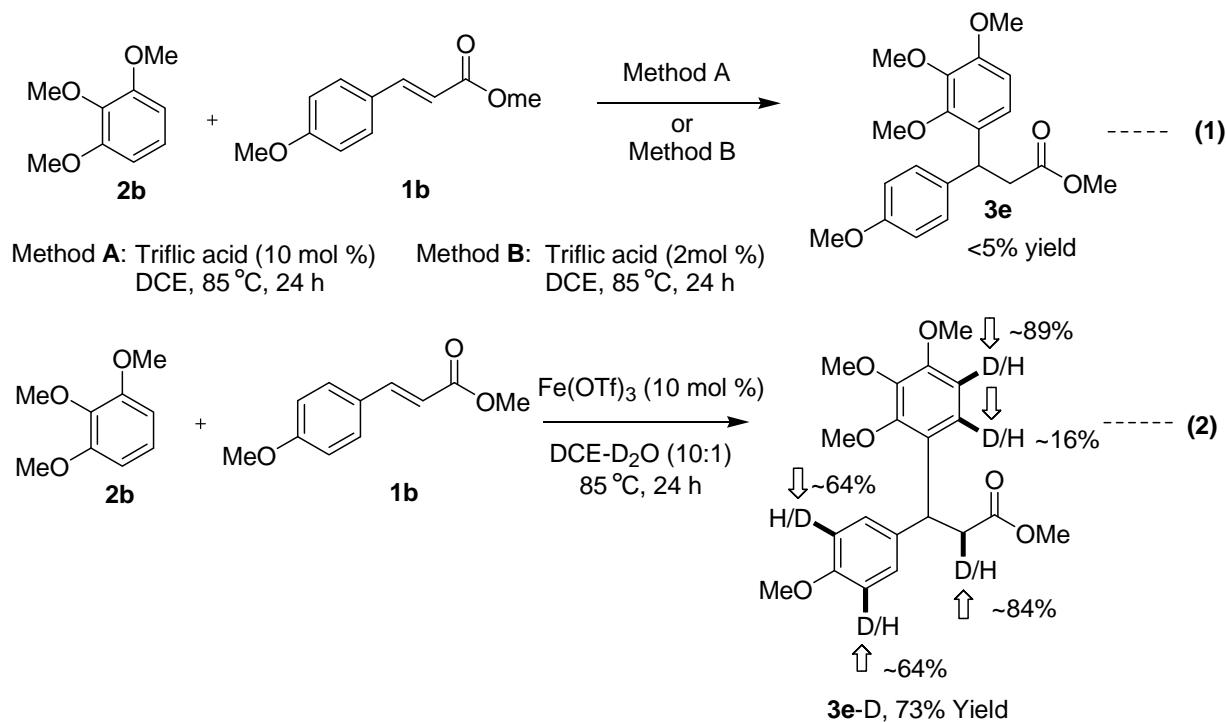


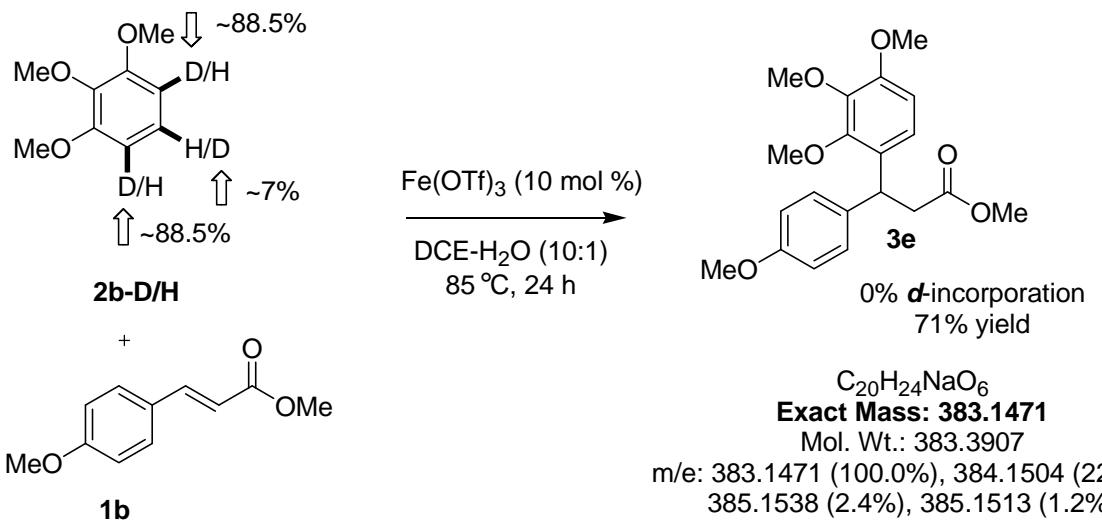
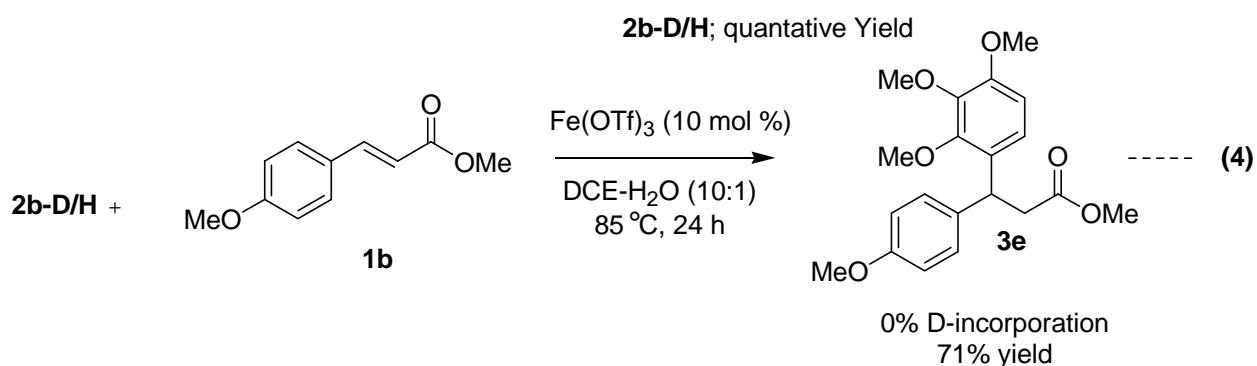
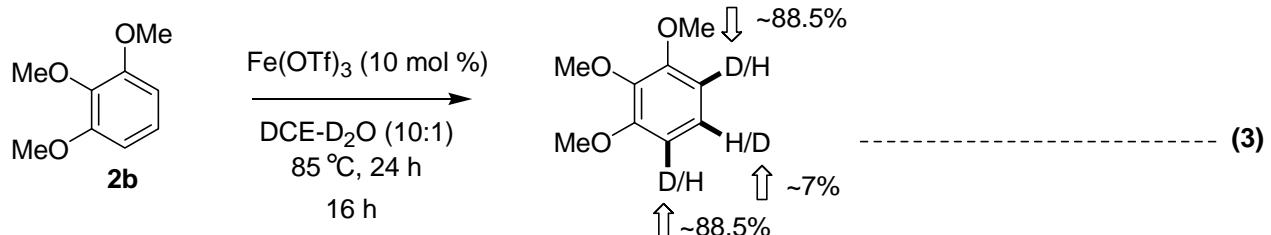
Mechanism Investigation

Scheme 1

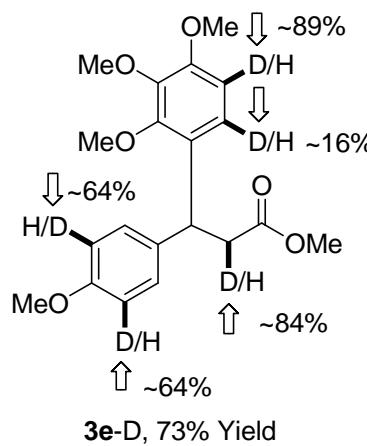


Scheme 2



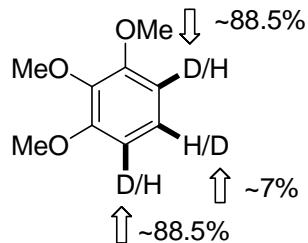


Spectral data of 3e-D and 2b-D/H



¹H NMR (CDCl₃, 400 MHz): δ 7.15 (s, 2H), 6.87 (s, 0.84H), 6.80 (d, *J* = 8.0 Hz, 0.71H), 6.62 (d, *J* = 8.0 Hz, 0.11H), 4.77 (d, *J* = 8.0 Hz, 2H), 3.83 (s, 3H), 3.82 (s, 3H), 3.75 (s, 3H), 3.67 (s, 3H), 3.58 (s, 3H), 2.97 (m, 0.84H).

HRMS (EI) calcd for C₂₀H₂₁D₃O₆, 386.1656 *m/z* (M+Na)⁺; Found, 386.1639 *m/z*.

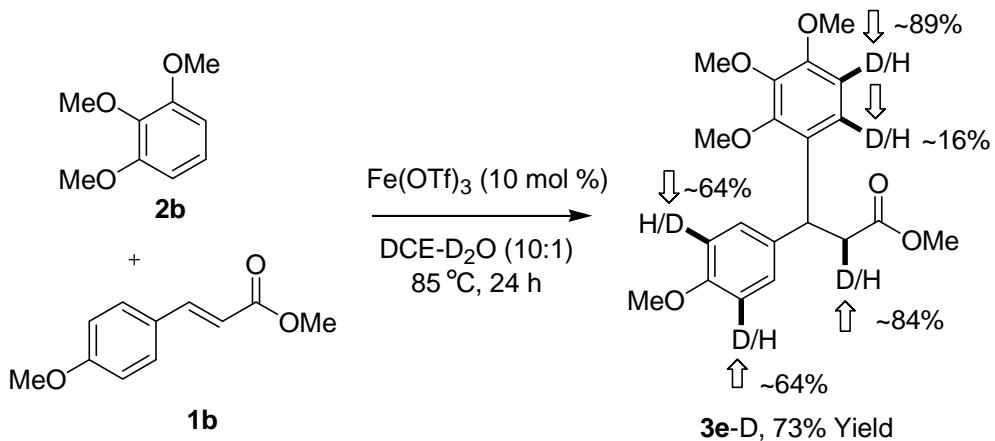
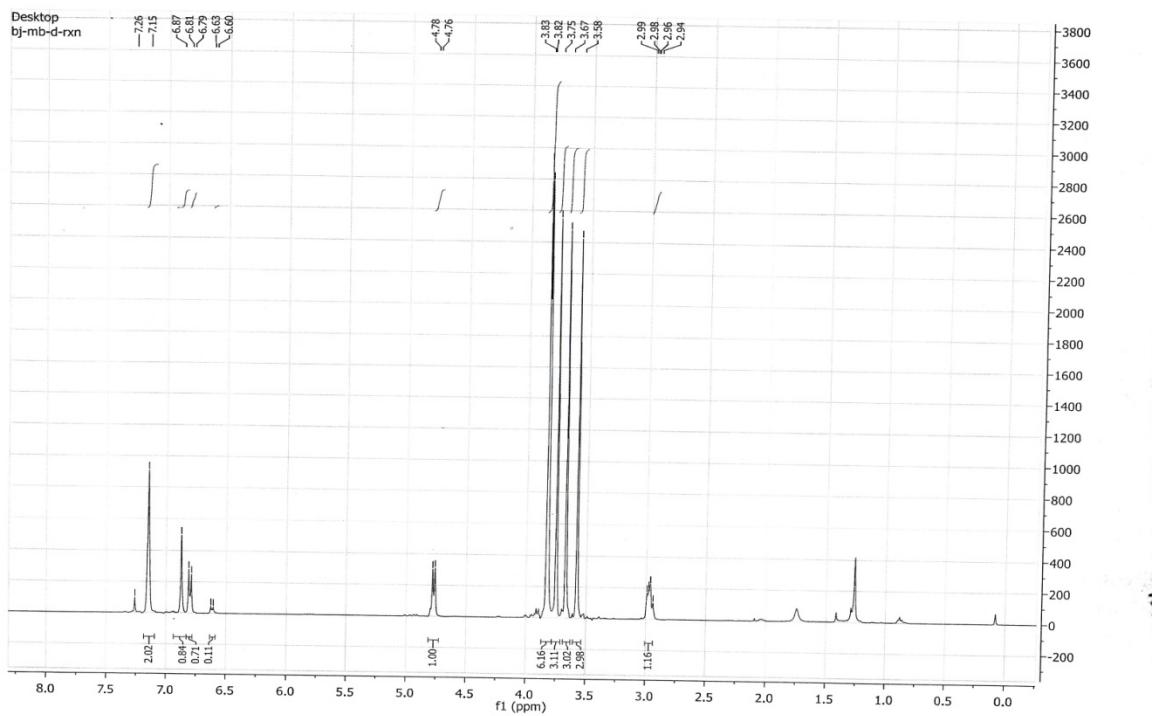


2b-D/H

¹H NMR (CDCl₃, 400 MHz): δ 6.99 (s, 0.93H), 6.58 (d, *J* = 8.0 Hz, 0.23H), 3.86 (s, 6H), 3.85 (s, 3H).

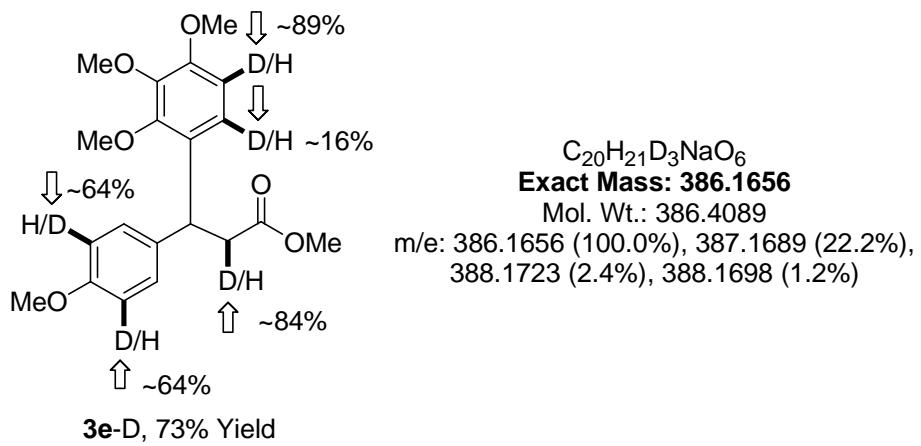
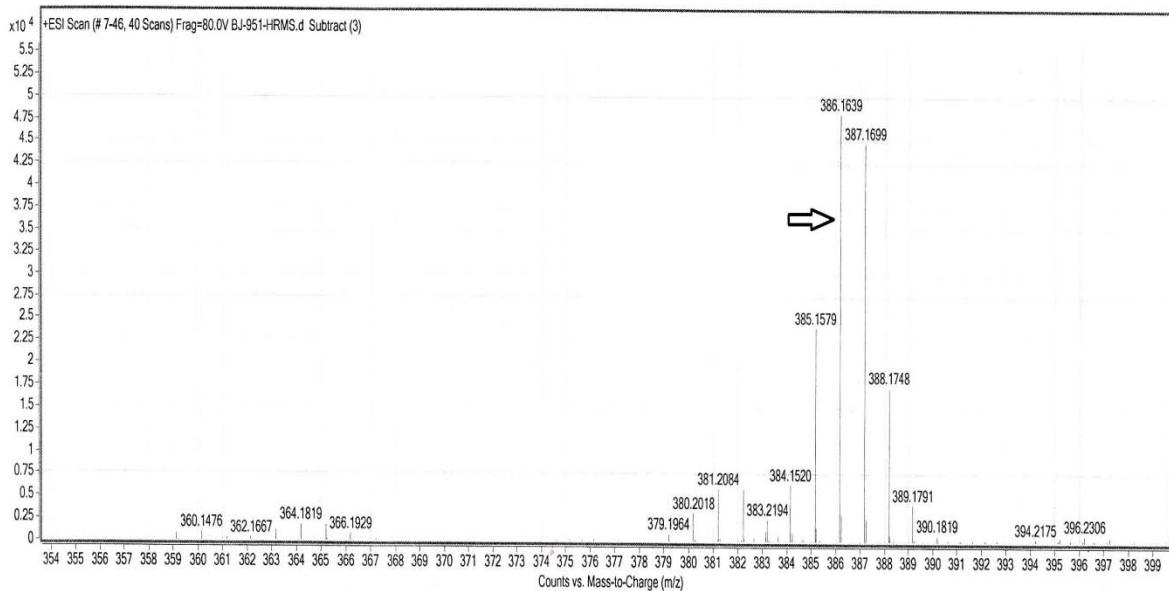
Copy of ^1H NMR and HRMS Spectra with *d*-incorporation in Friedel-Crafts Alkylated Products 3e-D & 2b-D/H

^1H -NMR of compound 3e-D (400 MHz)

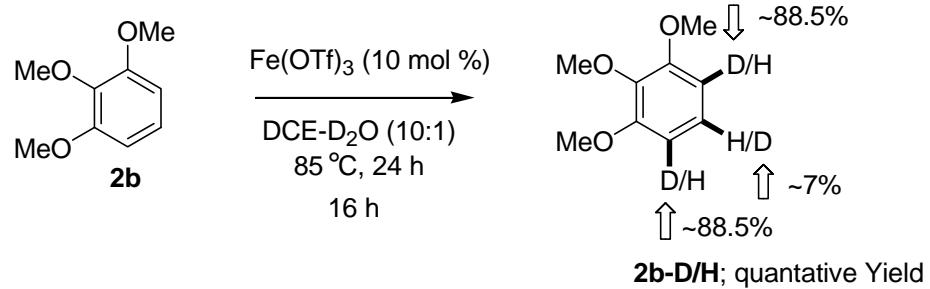
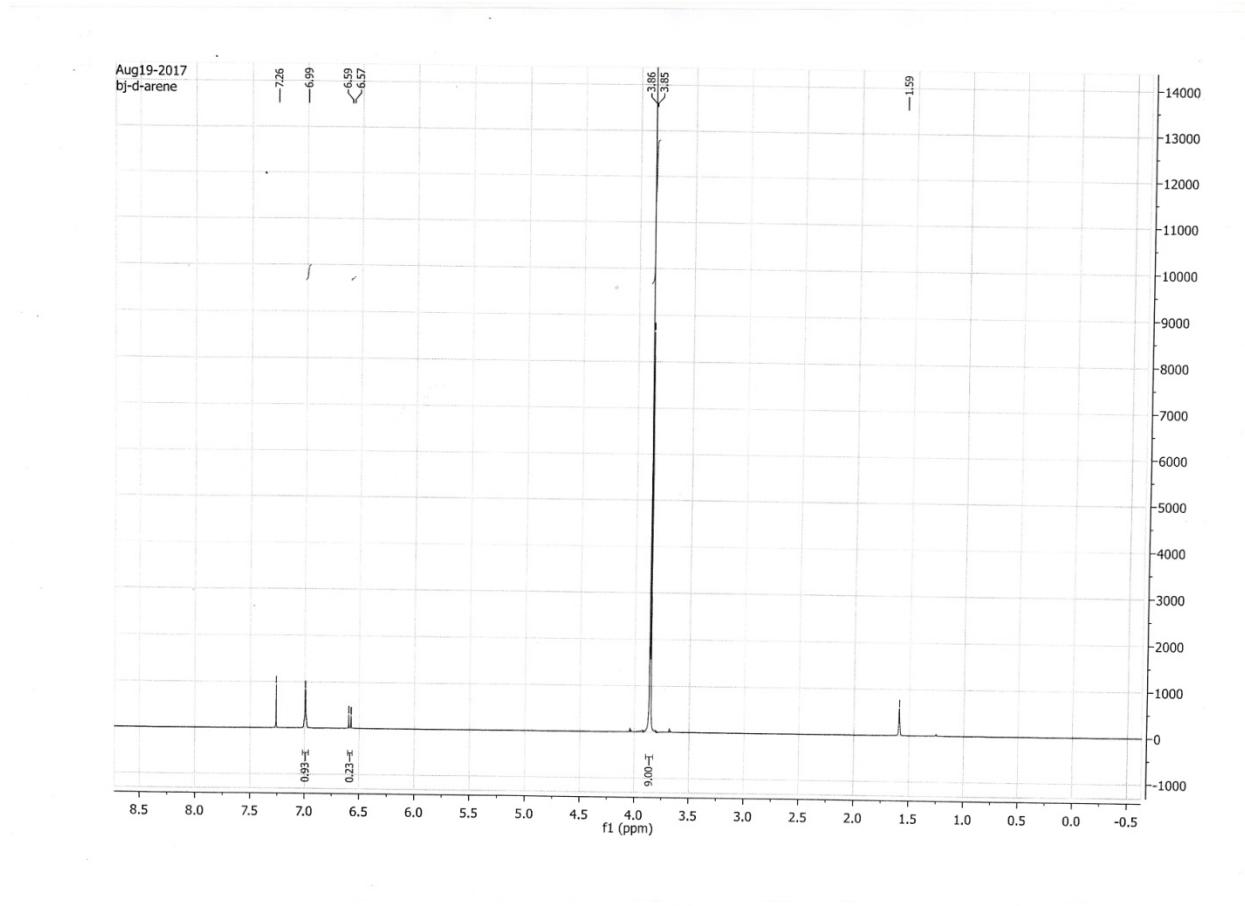


$\text{C}_{20}\text{H}_{21}\text{D}_3\text{NaO}_6$
Exact Mass: 386.1656
 Mol. Wt.: 386.4089
 m/e: 386.1656 (100.0%), 387.1689 (22.2%),
 388.1723 (2.4%), 388.1698 (1.2%)

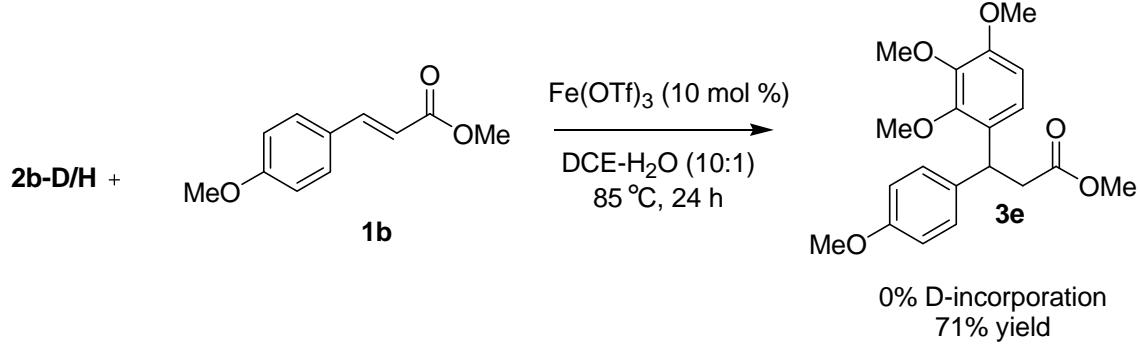
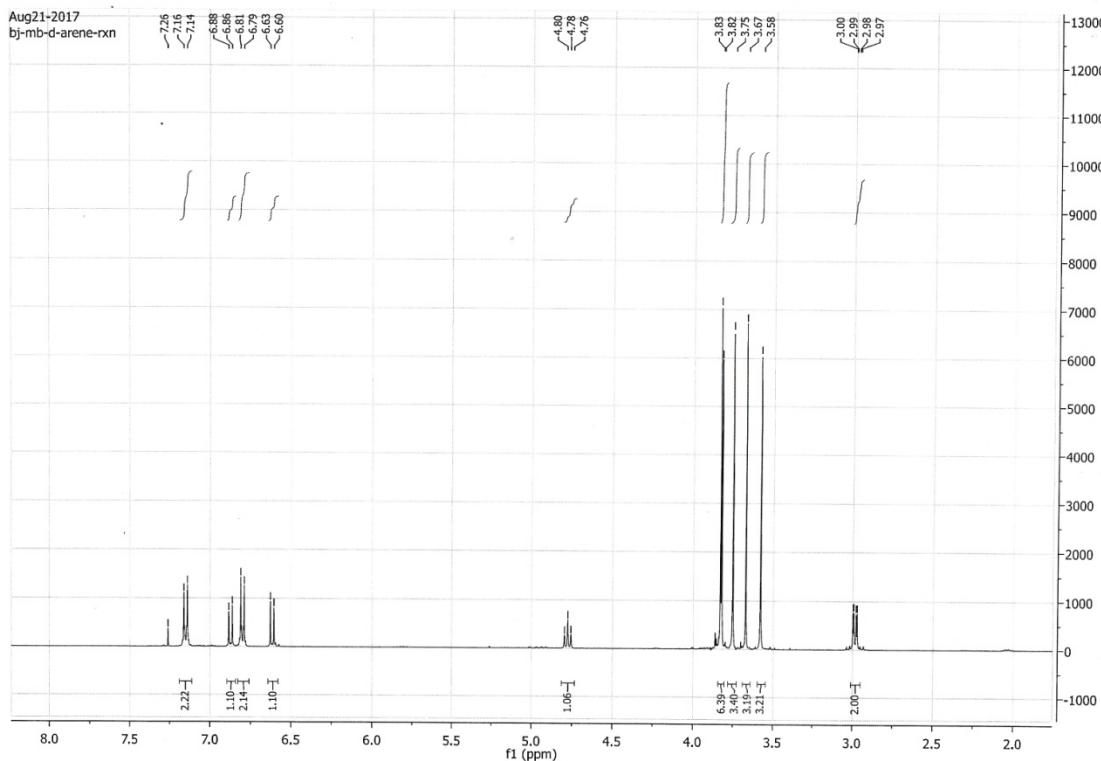
HRMS Spectrum of **3e-D**



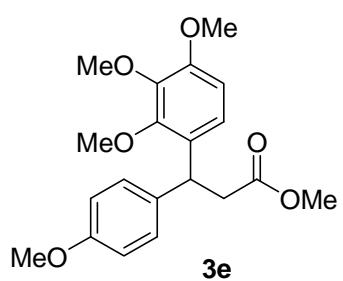
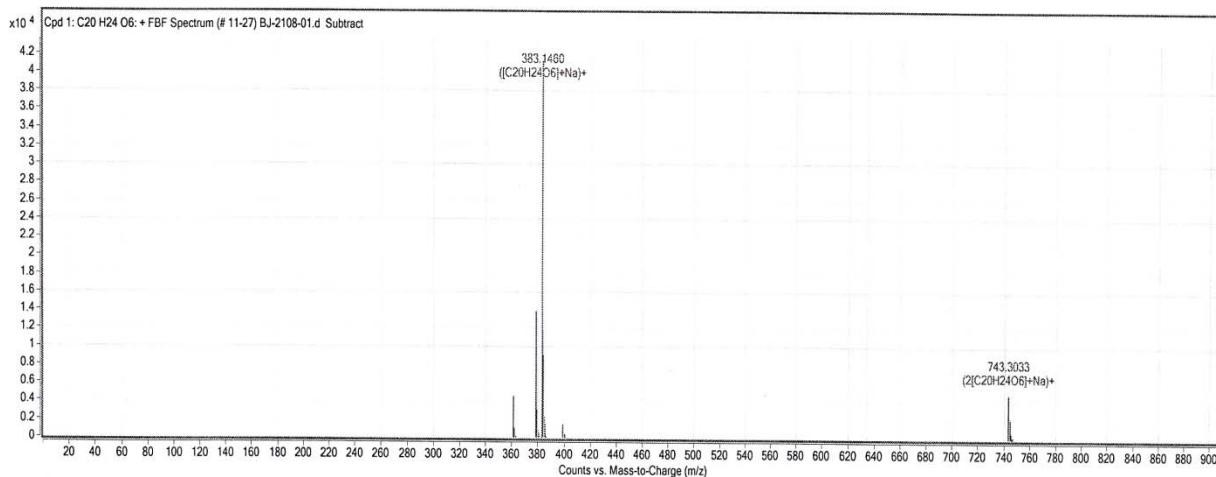
¹H-NMR of compound **2b**-D/H (400 MHz)



¹H-NMR of compound **3e** after reaction between **2b**-D/H and alkene **1b** in the presence of DCE-H₂O (10:1) (400 MHz)



HRMS Spectrum of **3e** after reaction between **2b**-D/H and alkene **1b** in the presence of DCE-H₂O (10:1)



C₂₀H₂₄NaO₆
Exact Mass: 383.1471
 Mol. Wt.: 383.3907
 m/e: 383.1471 (100.0%), 384.1504 (22.2%),
 385.1538 (2.4%),
 385.1513 (1.2%)