

Supporting Information

**A Biocatalytic Green Alternative to Existing Hazardous Reaction Medium: Synthesis of
Chalcone and Flavone Derivatives *via* Claisen-Schmidt Reaction at Room Temperature**

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1. Materials and Methods

All chemicals were purchased from commercially available sources and were used without further purification. Reactions were carried out with Carousel six plus reaction station (Radleys). ^1H NMR spectra were recorded at 500 MHz and ^{13}C NMR spectra were recorded at 125 MHz in CDCl_3 and/or DMSO-d_6 . Tetramethylsilane (TMS) using as an internal standard. All chemical shifts (δ) are reported in ppm and coupling constant (J) in Hz. Mass spectra data were recorded on Trace DSQ GC-MS instrument. Melting points were determined in open capillary tubes with a Buchi-540 micro melting point apparatus. TLC experiments were performed using pre-coated Silica gel 60 F₂₅₄ sheets (Merck).

IR Affinity, Shimadzu, Japan FT-IR spectrophotometer equipped with a Shimadzu DRS-8000 DRIFT accessory and IR solution software were used to record the Fourier transform infrared (FT-IR) spectra with 4 cm^{-1} spectral resolutions.

X-ray diffraction (XRD) analysis was carried out to determine the crystal structure of the prepared sample using a Rigaku X – ray diffractometer (model: ULTIMA IV, Rigaku, Japan). XRD instrument was operated with a scanning rate of 3° min^{-1} in the 2θ value ranging from $5-100^\circ$ with a $\text{CuK}\alpha$ X – ray radiation ($\lambda = 1.54056\text{ \AA}$).

FESEM images and EDS spectra were recorded using a scanning electron microscope (FESEM, Zeiss Gemini, Germany) at an accelerating voltage of 9-7 kV. The FESEM is equipped with Oxford EDS operated at 10 and 3 kV to investigate the surface morphology and the elemental composition of the samples.

The morphology of the prepared samples was determined using High-resolution transmission electron microscopy (HRTEM) using JEOL -JEM 2100, Japan operated at an accelerating voltage of 200 kV.

X-ray photoelectron spectroscopy (XPS) measurements were carried out using a Thermo-Scientific ESCALAB Xi+ spectrometer having a monochromatic $\text{Al K}\alpha$ X-ray source (1486.6 eV) and a spherical energy analyzer that operates in the CAE (constant analyzer energy) mode using the electromagnetic lens mode. The CAE for survey spectra is 100 eV and that for high-resolution spectra is 50 eV. Ultraviolet photoelectron spectroscopy (UPS) measurement was carried out in a

UPS lens mode. The CAE for UPS spectrum was 50 eV. The He I (21.22 eV) excitation line was used for UPS measurement.

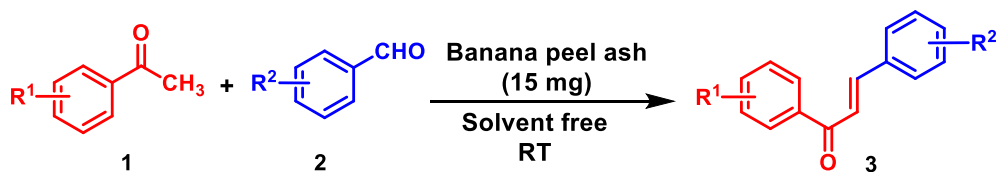
The BET isotherm, specific surface area and porosity measurements were obtained from Autosorb-iQ (Quantachrome, USA) analyser using Brunauer-Emette-Teller (BET) method under N₂ adsorption desorption methods.

TGA of the nanocomposite was carried out using a Thermal Analyzer (Model: Netzsch STA 449F3, Germany) and heated from 20 to 1000°C at a heating rate of 10°C min⁻¹ in a nitrogen environment.

The Micro-Raman spectroscopy measurements were carried out on a Thermo- Scientific DXR2 Smart Raman having excitation wavelength 785 nm.

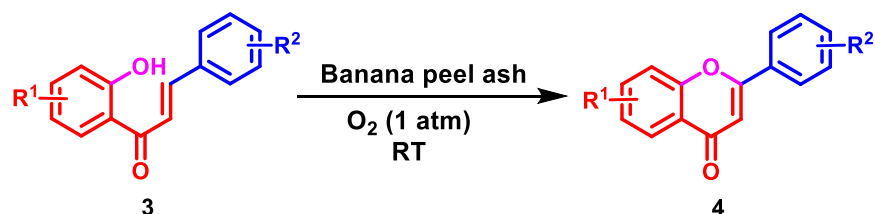
2. General experimental Procedures

2.1 Experimental procedure for Chalcone derivatives



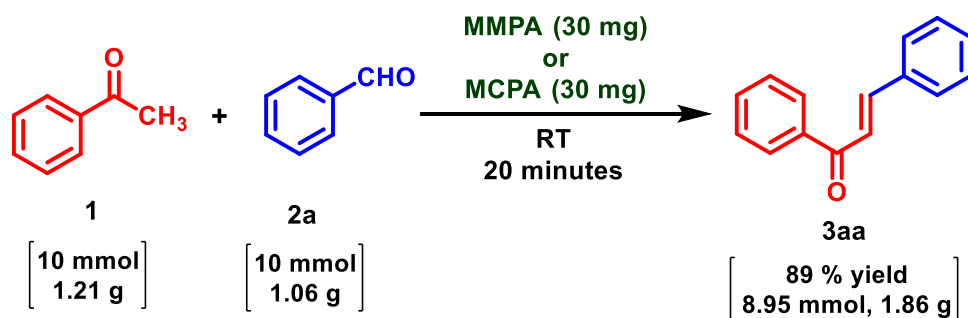
A mixture of substituted acetophenones (1 mmol) and substituted aldehydes (1 mmol) were taken in a oven dried 50 ml round bottom flask containing prepared banana peel ash catalysts (MMPA or MCPA) of 15 mg and stirred for 10-24 minutes at room temperature in a Carousel six plus reaction station. The progress of the reaction was checked by TLC. After completion of the reaction, the reaction mixture was subjected to the Büchner funnel for filtration. In the filtration process, the resulted solid was washed with distilled water (10 mL X 3). Then the products were collected and allowed to dry in an oven at 50°C. Further, the catalyst was washed with ethanol followed by hexane to eliminate impurities. Then, the washed catalyst was dried in an oven at 100°C for 4 h and used for successive cycles.

2.2 Experimental procedure for Flavone derivatives



To a mixture of 2-hydroxychalcones (1 mmol), prepared banana peel ash catalysts (MMPA or MCPA) of 15 mg with oxygen balloon (1 atm) were taken in a round bottom flask and the mixture was stirred in a Carousel six plus reaction station at room temperature for 35-60 minutes, until complete disappearance of the starting materials as monitored by TLC. After that, the reaction mixture was subjected to the Büchner funnel for filtration. In the filtration process, the resulted solid was washed with distilled water (10 mL X 3). Then the products were collected and allowed to dry in an oven at 50°C to afford flavone derivatives.

2.3 Experimental procedure for gram-scale production of Chalcone



In a 250 ml round bottom flask containing magnetic stirrer, acetophenone (1.21 g, 10 mmol), benzaldehyde (1.06 g, 10 mmol) along with prepared banana peel ash catalysts (MMPA or MCPA) of 30 mg was stirred for 20 minutes at room temperature. The progress of the reaction was checked by TLC. After completion of the reaction, the reaction mixture was subjected to the Büchner funnel for filtration. In the filtration process, the resulted solid was washed with distilled water (10 mL X 5). Then the product was collected and allowed to dry in an oven at 50°C to obtain chalcone as 1.86 g with 89% of yield.

3. Composition of fresh MMPA and MCPA

3.1 Moisture content of the peels

Moisture content (%) of the fresh banana peels were determined by measuring the weight difference before and after drying for 24 h at 110°C using a hot air oven (IKON instruments, New

Delhi-95, India). By comparison of the two weights the % of moisture present in the samples were calculated. The moisture contents of samples were not determined on the assumption that these are already in the dried state.

Table S1: Moisture content of banana peel ash

Sl. No.	Samples name	Weight before drying (g)	Weight after drying (g)	% loss
1	MMPA	10	1.78	82.20
2	MCPA	10	1.55	84.50

3.2 Element detection by atomic absorption spectroscopy (AAS)

Atomic absorption spectroscopy (AAS) analysis was carried out with using PerkinElmer (Model-Analyst-700) spectrometer to determine the metal and element contents of two banana peel ash.

Table S2: Elements present in both the banana peel ash

Sl No.	Elements	Contents (%)	
		MMPA	MCPA
1	Sodium	0.58	0.42
2	Potassium	1.60	1.48
3	Iron	BDL	BDL
4	Manganese	0.048	0.028
5	Calcium	0.42	0.38
6	Magnesium	0.36	0.32
*BDL= Below Detection Limit.			

3.3 Element detection by Ion Chromatography (IC)

Ion Chromatography (IC) analysis was carried out with using Metrohm Compact IC Pro882, Setzerland, to determine the cations and anions present in two banana peel ash (figure S1).

Table S3: Details of chemical composition of banana peel ash

Sl. No.	Ions (Cations and Anions)	Amounts in ppm	
		MMPA	MCPA
1	Ammonium	1.401	1.238
2	Magnesium	0.125	0.060
3	Chloride	3.620	4.304
4	Bromide	0.016	--
5	Phosphate	0.704	0.993
6	Sulfate	0.063	0.351

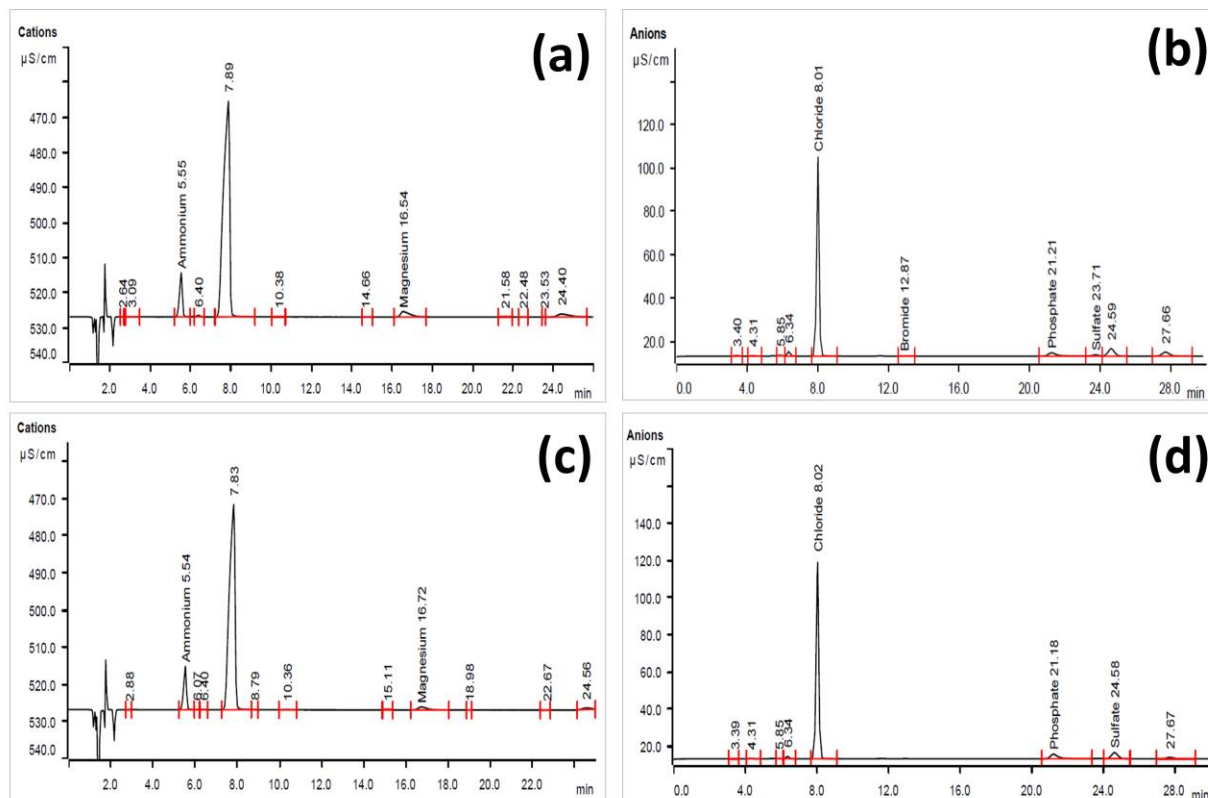


Figure S1: Ion chromatogram; (a) cations present in MMPA; (b) anions present in MCPA; (c) cations present in MMPA; (d) anions present in MCPA

4. Characterization of recovered catalysts (MMPA and MCPA)

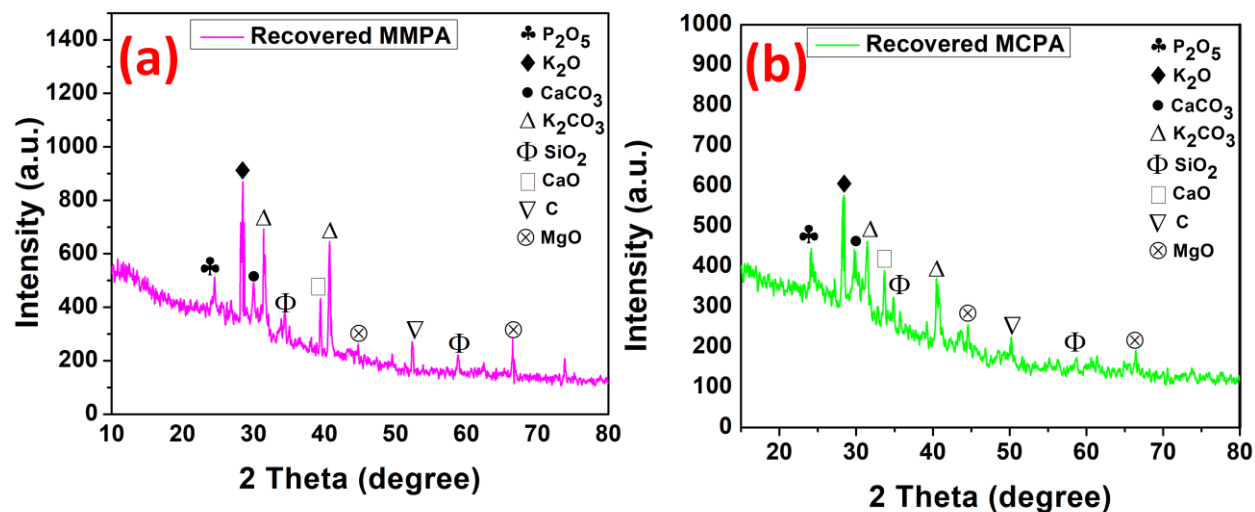


Figure S2: XRD spectra of recovered (a) MMPA and (b) MCPA after 5th cycle

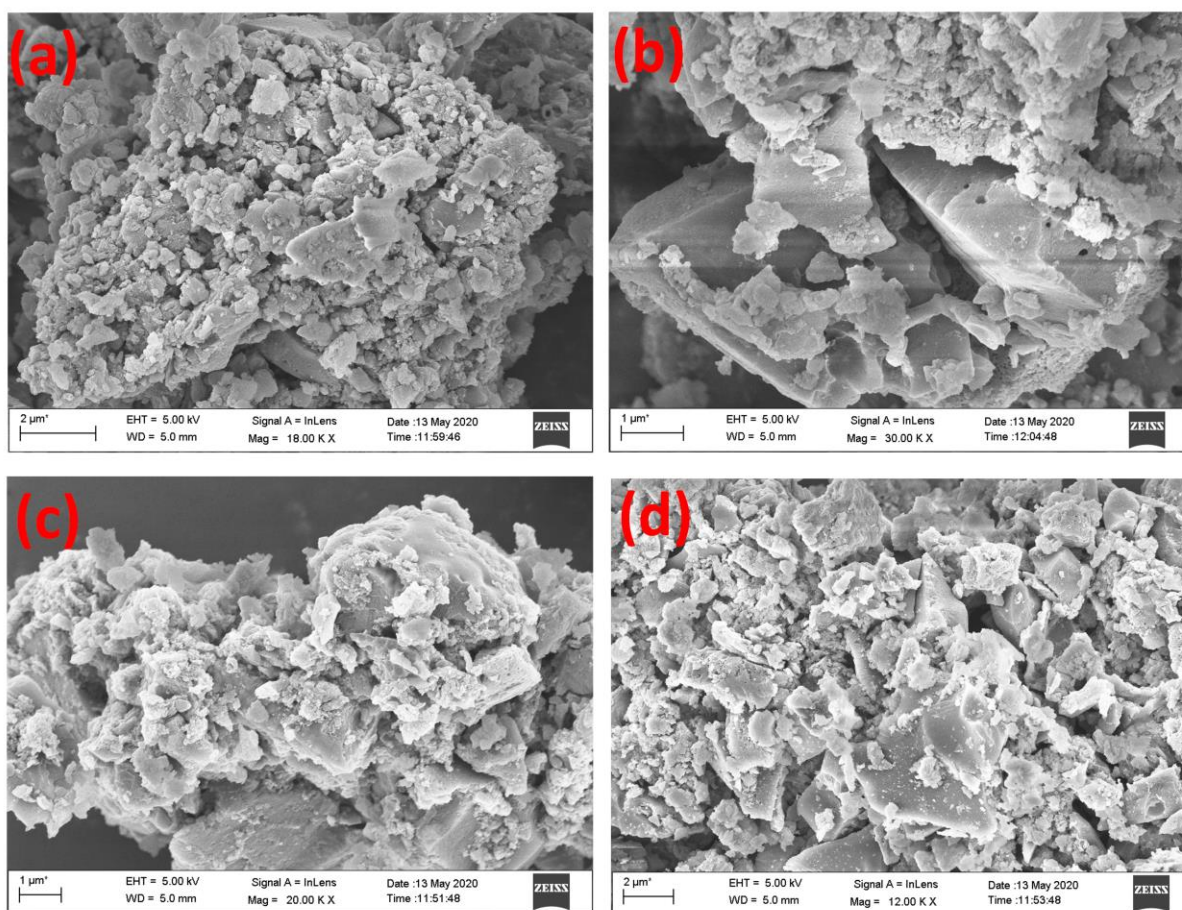


Figure S3: (a-b) SEM images of recovered catalyst (MMPA) after 5th cycle; (c-d) SEM images of recovered catalyst (MCPA) after 5th cycle

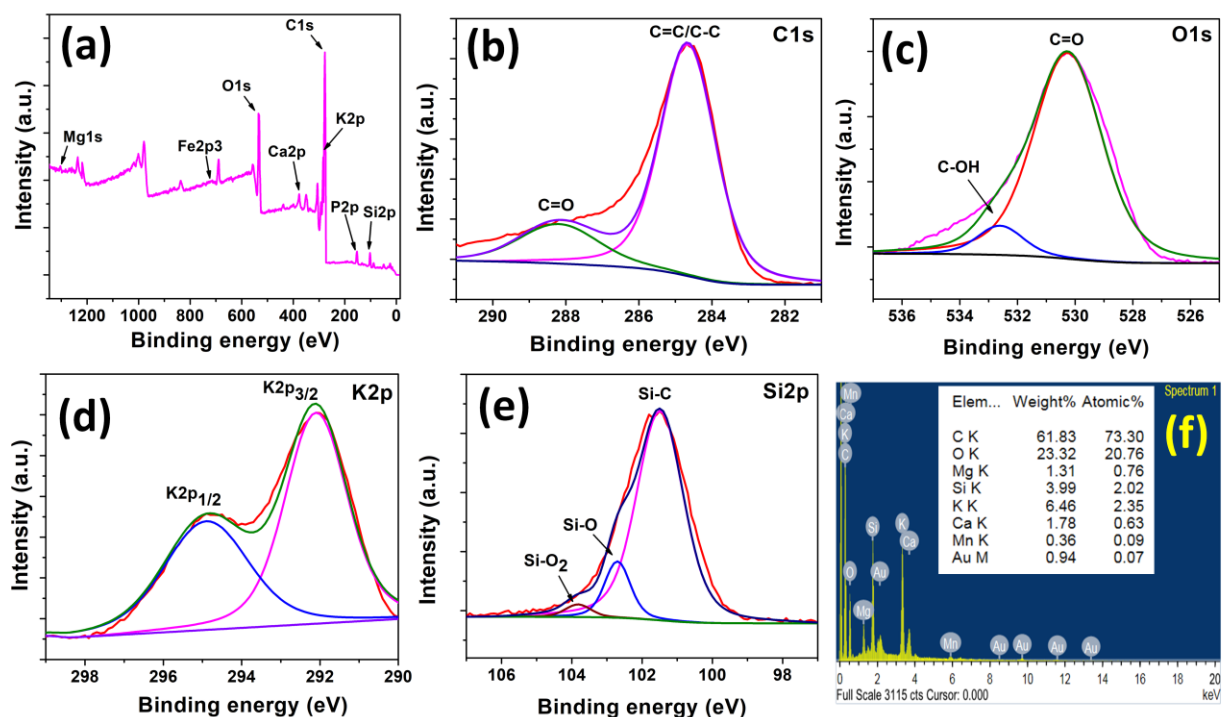


Fig. S4: (a) XPS survey spectrum of recovered MMPA and high-resolution spectra of (b) C 1s; (c) O 1s; (d) K 2p; (e) Si 2p; (f) EDX of fresh MMPA after 5th cycles

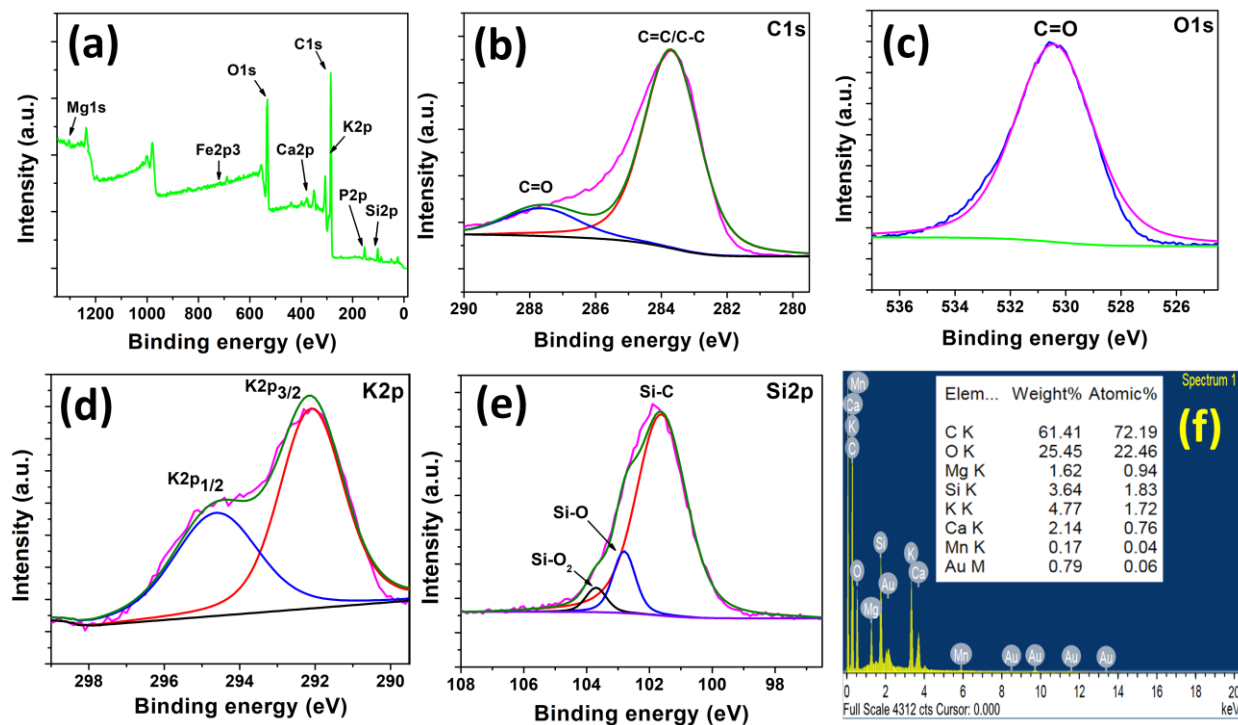
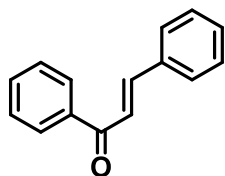


Fig. S5: (a) XPS survey spectrum of recovered MCPA and high-resolution spectra of (b) C 1s; (c) O 1s; (d) K 2p; (e) Si 2p; (f) EDX of fresh MCPA after 5th cycles

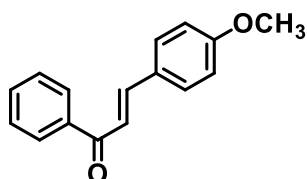
5. Characterization data of all products

5.1 Characterization data of Chalcone derivatives (Table 2 of the manuscript)



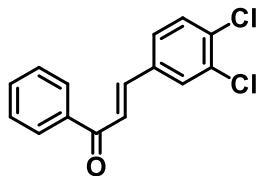
Chalcone (1,3-Diphenyl-2-propen-1-one) (Table 2, 3aa)^{1a}:

198 mg, 95% yield, M.P 56°C [Lit: 57°C], light yellow solid, ¹H NMR (CDCl₃, 500MHz): δ 7.28-7.52 (m, 7H), 7.70 (d, 1H, *J*= 20 Hz), 7.91 (d, 1H, *J*=10 Hz); ¹³C NMR (CDCl₃, 125MHz):121.95, 128.38, 128.72, 128.55, 128.87, 130.48, 132.72, 134.76, 138.09, 144.75, 190.42; FT-IR (KBR, cm⁻¹): 2929, 1659, 1444, 1335, 1210, 1080, 990, 748; HRMS (+ESI) *m/z* calculated for C₁₅H₁₂O [M+H]⁺: 209.0785; found: 209.0554.



(*E*)-3-(4-methoxyphenyl)-1-phenylprop-2-en-1-one (Table 2, 3ab)^{1b}:

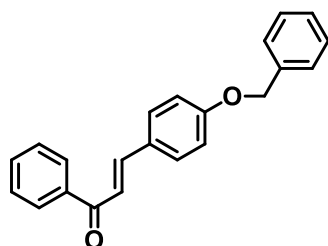
220 mg, 92% yield, M.P 91°C [Lit: 91°C], yellow solid, ¹H NMR (CDCl₃, 500MHz): δ 3.74 (s, 3H), 7.31-7.51 (m, 7H), 7.69 (d, 1H, *J*= 15 Hz), 7.92 (d, 1H, *J*=10 Hz); ¹³C NMR (CDCl₃, 125MHz): 55.30, 114.32, 119.62, 127.48, 128.31, 128.47, 130.15, 132.48, 144.62, 161.57, 190.48; FT-IR (KBR, cm⁻¹): 2941, 2815, 1622, 1519, 1474, 1329, 1250, 1109, 965, 751; HRMS (+ESI) *m/z* calculated for C₁₆H₁₄O₂ [M+H]⁺: 239.2410; found: 239.1125.



(*E*)-3-(3,4-dichlorophenyl)-1-phenylprop-2-en-1-one (Table 2, 3ac)^{1c}:

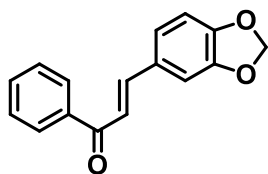
238mg, 86% yield, M.P 117°C [Lit: 116°C], yellow solid, ¹H NMR (CDCl₃, 500MHz): δ 6.96 (d, 1H, *J*= 15 Hz), 7.23-7.25 (m, 3H), 7.41 (s, 1H), 7.59 (d, 1H, *J*=10 Hz), 7.99 (d, 1H, *J*= 15 Hz); ¹³C NMR (CDCl₃, 125MHz): 126.78, 127.49, 127.54, 128.84, 129.16, 129.98, 130.04, 131.87, 135.91,

136.23, 136.57, 138.24, 138.71, 188.10; FT-IR (KBR, cm^{-1}): 3090, 1697, 1566, 1496, 1345, 1139, 965, 742; HRMS (+ESI) m/z calculated for $\text{C}_{15}\text{H}_{10}\text{Cl}_2\text{O}$ $[\text{M}+\text{H}]^+$: 277.4204; found: 277.3124.



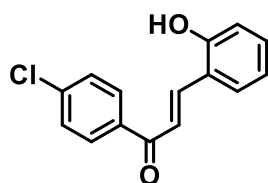
(E)-3-(4-(benzyloxy)phenyl)-1-phenylprop-2-en-1-one (Table 2, 3ad):

220 mg, 82% yield, M.P 220°C, light brown solid, ^1H NMR (CDCl_3 , 500MHz): δ 5.13 (s, 2H), 7.02 (d, 1H, J = 10 Hz), 7.26-7.48 (m, 8H), 7.61 (d, 1H, J = 10 Hz), 7.80 (d, 1H, J =15 Hz), 7.96 (d, 1H, J =10 Hz); ^{13}C NMR (CDCl_3 , 125MHz): 70.02, 115.22, 119.13, 127.38, 129.11, 128.77, 129.72, 130.24, 136.20, 136.65, 145.06, 180.87, 189.11; FT-IR (KBR, cm^{-1}): 3300, 3129, 2784, 1709, 1544, 1411, 1197, 945, 749; HRMS (+ESI) m/z calculated for $\text{C}_{22}\text{H}_{18}\text{O}_2$ $[\text{M}+\text{H}]^+$: 315.1430; found: 315.0885.



(E)-3-(benzo[d][1,3]dioxol-5-yl)-1-phenylprop-2-en-1-one (Table 2, 3ae)^{1d}:

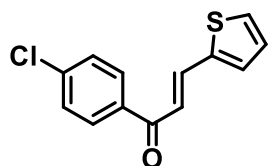
212 mg, 84% yield, M.P 122°C [Lit: 120°C], yellow solid, ^1H NMR (CDCl_3 , 500MHz): δ 5.94 (s, 2H), 6.77 (d, 1H, J = 5 Hz), 7.07 (dd, 1H, J = 5 Hz; 1 Hz), 7.09 (d, 1H, J =15 Hz), 7.28 (d, 1H, J =15 Hz), 7.49(d, 2H, J =15 Hz) 7.65 (d, 1H, J =15 Hz), 7.93 (d, 1H, J =5 Hz); ^{13}C NMR (CDCl_3 , 125MHz): 101.54, 106.52, 108.56, 119.93, 125.17, 128.30, 128.48, 129.21, 132.56, 138.25, 144.59, 148.29, 149.82, 190.30; FT-IR (KBR, cm^{-1}): 3044, 2912, 1601, 1589, 1482, 1421, 1228, 1090, 977, 960, 783; HRMS (+ESI) m/z calculated for $\text{C}_{16}\text{H}_{12}\text{O}_3$ $[\text{M}+\text{H}]^+$: 253.0821; found: 253.0745.



(E)-1-(4-chlorophenyl)-3-(2-hydroxyphenyl)prop-2-en-1-one (Table 2, 3af)^{2a}:

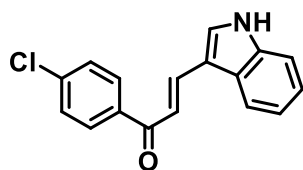
211 mg, 82% yield, M.P 148°C [Lit: 151°C], yellow solid, ^1H NMR (CDCl_3 , 500MHz): δ 6.06 (brd, 1H), 6.80 (d, 1H, J =5 Hz), 6.91 (d, 1H, J =5 Hz) 7.40-7.92 (m, 7H), 8.03 (d, 1H, J =15 Hz); ^{13}C NMR

(CDCl₃, 125MHz): 116.43, 120.92, 122.12, 128.82, 129.73, 129.396, 131.88, 136.45, 139.03, 141.13, 155.60, 190.20; FT-IR (KBR, cm⁻¹): 2927, 1655, 1447, 1330, 1209, 1092, 989, 744; HRMS (+ESI) m/z calculated for C₁₅H₁₁ClO₂ [M+H]⁺: 259.5001.; found: 259.4710.



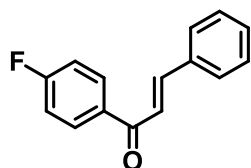
(E)-1-(4-chlorophenyl)-3-(thiophen-2-yl)prop-2-en-1-one (Table 2, 3ag)^{2b}:

225 mg, 90% yield, M.P 119°C [Lit: 122°C], yellow solid, ¹H NMR (CDCl₃, 500MHz): δ 7.03 (d, 1H, J= 5 Hz), 7.17-7.30 (m, 7H), 7.36-7.41 (m, 5H), 7.89 (d, 1H, J= 10 Hz). ¹³C NMR (CDCl₃, 125MHz): 120.01, 128.33, 128.82, 129.70, 132.30, 136.29, 137.58, 139.07, 140.09, 188.38; FT-IR (KBR, cm⁻¹): 3081, 1655, 1590, 1447, 1221, 972, 678; HRMS (+ESI) m/z calculated for C₁₃H₉ClOS [M+H]⁺: 249.1244; found: 249.0995.



(E)-1-(4-chlorophenyl)-3-(1H-indol-3-yl)prop-2-en-1-one (Table 2, 3ah)^{2a}:

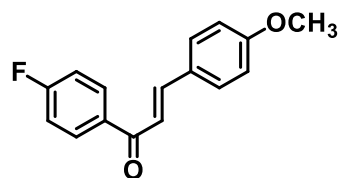
250 mg, 88% yield, M.P 121°C [Lit: 119°C], yellow solid, ¹H NMR (CDCl₃, 500MHz): δ 7.34-7.36 (m, 2H), 7.49-7.751 (m, 2H), 7.56 (d, 2H, J= 10 Hz), 7.66 (d, 2H, J= 10 Hz), 8.01 (d, 2H, J= 10 Hz), 8.15 (d, 1H, J= 15 Hz), 8.76 (br, s, 1H). ¹³C NMR (CDCl₃, 125MHz): 111.98, 114.29, 116.92, 120.66, 121.82, 123.59, 125.09, 128.76, 129.70, 130.81, 138.51, 139.48, 189.51; FT-IR (KBR, cm⁻¹): 3028, 2998, 1755, 1592, 1454, 1278, 977, 712; HRMS (+ESI) m/z calculated for C₁₇H₁₂ClNO [M+H]⁺: 281.2883; found: 281.2347.



(E)-1-(4-fluorophenyl)-3-phenylprop-2-en-1-one (Table 2, 3ai)^{2b}:

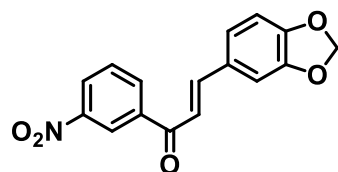
200 mg, 88% yield, M.P 101°C [Lit: 100°C], pale yellow solid, ¹H NMR (CDCl₃, 500MHz): δ 6.92 (d, 1H, J= 15 Hz), 7.03-7.56 (m, 8H), 7.63 (d, 1H, J= 15 Hz); ¹³C NMR (CDCl₃, 125MHz): 115.98, 116.15, 124.95, 130.15, 130.22, 130.87, 142.02, 162.95, 164.95, 188.39; FT-IR (KBR, cm⁻¹): 2927,

1655, 1447, 1350, 1209, 1092, 989, 744; HRMS (+ESI) m/z calculated for $C_{15}H_{11}FO$ $[M+H]^+$: 227.3109; found: 227.2998.



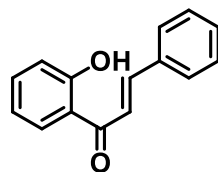
(E)-1-(4-fluorophenyl)-3-(4-methoxyphenyl)prop-2-en-1-one (Table 2, 3aj)^{3a}:

210 mg, 82% yield, M.P 115°C [Lit: 114 °C], yellow solid, 1H NMR ($CDCl_3$, 500MHz): δ 3.07 (s, 3H), 7.04 (d, 1H, J = 10 Hz), 7.65-7.97 (m, 8H), 8.15 (d, 1H, J = 15 Hz); ^{13}C NMR ($CDCl_3$, 125MHz): 55.80, 114.98, 116.17, 121.35, 127.60, 130.05, 131.27, 133.11, 143.51, 159.45, 167.83, 189.72; FT-IR (KBR, cm^{-1}): 3028, 2890, 1659, 1560, 1350, 1330, 958; HRMS (+ESI) m/z calculated for $C_{16}H_{13}FO_2$ $[M+H]^+$: 257.0933; found: 257.0907.



(E)-3-(benzo[d][1,3]dioxol-5-yl)-1-(3-nitrophenyl)prop-2-en-1-one (Table 2, 3ak)^{2c}:

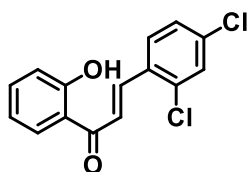
250 mg, 84% yield, M.P 191°C [Lit: 189°C], light yellow solid, 1H NMR ($CDCl_3$, 500MHz): δ 5.99 (s, 2H), 6.80 (d, 1H, J = 15 Hz), 7.09 (dd, 1H, J = 5 Hz; 1 Hz), 7.12 (d, 1H, J = 10 Hz), 7.30 (d, 1H, J =15 Hz), 7.64 (d, 2H, J = 10 Hz), 7.75 (d, 1H, J = 15 Hz), 8.37 (d, 2H, J = 10 Hz); ^{13}C NMR ($CDCl_3$, 125MHz): 101.71, 106.65, 108.68, 118.43, 123.07, 125.85, 126.82, 128.67, 129.76, 133.93, 139.59, 146.51, 148.44, 150.42, 187.70; FT-IR (KBR, cm^{-1}): 3056, 2924, 1619, 1594, 1497, 1429, 1244, 1103, 991, 984, 798; HRMS (+ESI) m/z calculated for $C_{16}H_{11}NO_5$ $[M+H]^+$: 298.1556; found: 298.1207.



(E)-1-(2-hydroxyphenyl)-3-phenylprop-2-en-1-one (Table 2, 3al)^{3b}:

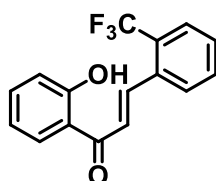
200 mg, 89% yield, M.P 72°C [Lit: 72°C], pale yellow solid, 1H NMR ($CDCl_3$, 500MHz): δ 7.03-7.05 (m, 2H), 7.26-7.46 (m, 7H), 7.68 (dd, 1H, J = 15 Hz), 7.94 (d, 1H, J = 10 Hz, 5 Hz), 12.83 (s, 1H); ^{13}C NMR ($CDCl_3$, 125MHz): 118.54, 118.77, 119.88, 119.96, 128.56, 128.58, 128.95, 129.55, 130.85,

134.45, 136.34, 145.39, 163.47, 193.63; FT-IR (KBR, cm^{-1}): 3045, 1639, 1579, 751; HRMS (+ESI) m/z calculated for $\text{C}_{15}\text{H}_{12}\text{O}_2$ $[\text{M}+\text{H}]^+$: 225.2275; found: 225.1835.



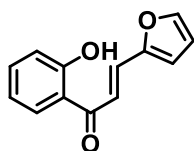
(E)-3-(2,4-dichlorophenyl)-1-(2-hydroxyphenyl)prop-2-en-1-one (Table 2, 3am)^{3b}:

235mg, 80% yield, M.P 159°C [Lit: 158°C], yellow solid, ^1H NMR (CDCl_3 , 500MHz): δ 6.96-7.06 (m, 2H), 7.34-7.53 (m, 3H), 7.62-7.72 (m, 3H), 7.89 (t, 2H, $J = 5$ Hz, 5 Hz), 8.23 (d, 2H, $J = 10$ Hz, 15 Hz), 12.68 (s, 1H); ^{13}C NMR (CDCl_3 , 125MHz): 118.65, 118.87, 122.91, 127.52, 128.52, 128.56, 129.56, 130.17, 131.40, 136.21, 136.65, 139.80, 163.55, 193.12; FT-IR (KBR, cm^{-1}): 3017, 1645, 1589, 750; HRMS (+ESI) m/z calculated for $\text{C}_{15}\text{H}_{10}\text{Cl}_2\text{O}_2$ $[\text{M}+\text{H}]^+$: 294.8007; found: 294.7123.



(E)-1-(2-hydroxyphenyl)-3-(2-(trifluoromethyl)phenyl)prop-2-en-1-one (Table 2, 3an):

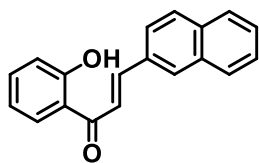
237 mg, 81% yield, M.P 122°C, yellow solid, ^1H NMR (CDCl_3 , 500MHz): δ 6.97 (t, 2H, $J = 5$ Hz, 10 Hz), 7.00 (d, 2H, $J = 15$ Hz), 7.53 (t, 2H, $J = 5$ Hz), 7.71-7.78 (m, 2H), 7.93 (d, 2H, $J = 15$ Hz), 12.69 (s, 1H); ^{13}C NMR (CDCl_3 , 125MHz): 118.65, 118.91, 119.70, 122.32, 125.90, 125.93, 128.60, 129.57, 136.71, 137.79, 143.24, 163.54, 193.21; FT-IR (KBR, cm^{-1}): 3104, 1671, 1224, 760; HRMS (+ESI) m/z calculated for $\text{C}_{16}\text{H}_{11}\text{F}_3\text{O}_2$ $[\text{M}+\text{H}]^+$: 293.0745; found: 293.0657.



(E)-3-(furan-2-yl)-1-(2-hydroxyphenyl)prop-2-en-1-one (Table 2, 3ao)^{2b}:

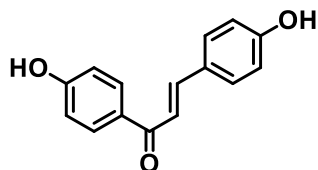
180 mg, 84% yield, M.P 139°C [Lit: 140°C], yellow solid, ^1H NMR (CDCl_3 , 500MHz): δ 6.96 (t, 2H, $J = 5$ Hz, 10 Hz), 7.08 (dd, 2H, $J = 10$ Hz, 15 Hz), 7.41-7.51 (m, 2H), 7.89 (d, 1H, $J = 5$ Hz), 8.04 (s, 2H), 8.07 (s, 2H), 12.86 (s, 1H); ^{13}C NMR (CDCl_3 , 125MHz): 118.49, 118.66, 118.76, 119.80, 128.43, 129.41, 129.46, 132.71, 136.26, 137.78, 140.03, 163.41, 193.02; FT-IR (KBR, cm^{-1}): 3124,

3081, 1680, 1549, 1412, 1211, 965; HRMS (+ESI) m/z calculated for $C_{13}H_{10}O_3$ $[M+H]^+$: 215.0748; found: 215.0667 $[M]^+$.



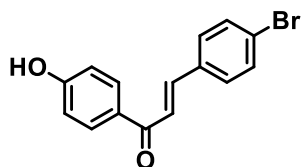
(E)-1-(2-hydroxyphenyl)-3-(naphthalen-2-yl)prop-2-en-1-one (Table 2, 3ap)^{2c}:

219 mg, 80% yield, M.P 151°C [Lit: 155°C], yellow solid, 1H NMR ($CDCl_3$, 500MHz): δ 6.97-6.99 (t, 2H, $J=5$ Hz, 10 Hz), 7.00-7.27 (m, 6H), 7.55 (m, 4H), 7.78-7.93 (m, 4H), 8.00 (dd, 1H, $J=5$ Hz), 8.09 (s, 2H), 8.12 (s, 2H), 12.89 (s, 1H); ^{13}C NMR ($CDCl_3$, 125MHz): 118.56, 118.78, 119.95, 120.03, 123.52, 126.79, 127.54, 127.73, 128.65, 128.75, 129.57, 131.09, 131.95, 133.21, 134.43, 136.33, 145.48, 163.50, 193.46; FT-IR (KBR, cm^{-1}): 3177, 3063, 1681, 1547, 1490, 1214, 960, 762; HRMS (+ESI) m/z calculated for $C_{19}H_{14}O_2$ $[M+H]^+$: 275.3231; found: 275.3221.



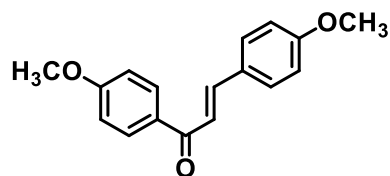
(E)-1,3-bis(4-hydroxyphenyl)prop-2-en-1-one (Table 2, 3aq)^{2c}:

212 mg, 88% yield, M.P 197°C [Lit: 194°C], yellow solid, 1H NMR ($CDCl_3$ and DMSO, 500MHz): δ 6.87-6.93 (m, 4H), 7.44 (d, 1H, $J=15$ Hz), 7.61 (m, 4H), 7.94 (d, 1H, $J=10$ Hz), 9.76 (s, 1H), 10.05 (s, 1H); ^{13}C NMR ($CDCl_3$ and DMSO, 125MHz): 120.16, 120.76, 123.12, 130.85, 134.52, 134.96, 135.50, 164.62, 166.67, 193.05; FT-IR (KBR, cm^{-1}): 3388, 3044, 1692, 1590, 1485, 1433, 1222, 748; HRMS (+ESI) m/z calculated for $C_{15}H_{12}O_3$ $[M+H]^+$: 241.2258; found: 241.1993.



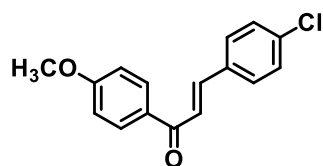
(E)-3-(4-bromophenyl)-1-(4-hydroxyphenyl)prop-2-en-1-one (Table 2, 3ar)^{2c}:

250 mg, 82% yield, M.P 181°C [Lit: 183°C], yellow solid, 1H NMR ($CDCl_3$ and DMSO, 500MHz): δ 6.89 (dd, 2H, $J=5$ Hz), 7.49 (d, 2H, $J=15$ Hz), 7.61-7.83 (m, 5H), 8.02 (s, 1H); ^{13}C NMR ($CDCl_3$ and DMSO, 125MHz): 115.63, 121.55, 122.31, 128.59, 130.06, 131.29, 134.12, 145.59, 164.35, 189.70; FT-IR (KBR, cm^{-1}): 3330, 3020, 2910, 1659, 1590, 1380, 847, 545; HRMS (+ESI) m/z calculated for $C_{15}H_{11}BrO_2$ $[M+H]^+$: 303.9921; found: 303.8523.



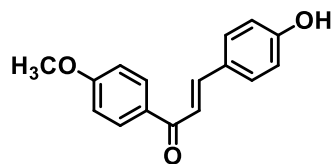
(E)-1,3-bis(4-methoxyphenyl)prop-2-en-1-one (Table 2, 3as)^{2b}:

242 mg, 90% yield, M.P 94°C [Lit: 99°C], light yellow solid, ¹H NMR (CDCl₃, 500MHz): δ 3.79 (s, 3H), 3.83 (s, 3H), 6.86-6.92 (m, 7H), 7.54 (d, 1H, *J*= 10 Hz), 7.73 (d, 1H, *J*=15 Hz), 7.97 (d, 1H, *J*=10 Hz); ¹³C NMR (CDCl₃, 125MHz): 55.31, 55.39, 113.66, 114.26, 119.41, 127.67, 130.00, 130.60, 131.21, 143.73, 161.37, 163.14, 188.70; FT-IR (KBR, cm⁻¹): 2949, 2811, 1620, 1514, 1466, 1312, 1241, 1090, 955, 743; HRMS (+ESI) *m/z* calculated for C₁₇H₁₆O₃ [M+H]⁺: 269.4307; found: 269.4027.



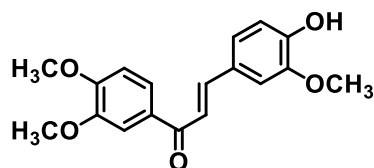
(E)-3-(4-chlorophenyl)-1-(4-methoxyphenyl)prop-2-en-1-one (Table 2, 3at)⁴:

242 mg, 89% yield, M.P 131°C [Lit: 133°C], light yellow solid, ¹H NMR (CDCl₃, 500MHz): δ 3.84 (s, 3H), 6.93 (d, 1H, *J*=10 Hz), 7.32-7.53 (m, 7H), 7.70 (d, 1H, *J*=15 Hz), 7.98 (d, 1H, *J*=10 Hz); ¹³C NMR (CDCl₃, 125MHz): 55.49, 113.78, 121.96, 129.12, 129.47, 130.69, 130.79, 133.36, 136.09, 142.48, 163.41, 188.36; FT-IR (KBR, cm⁻¹): 2977, 2831, 1669, 1598 1443, 1337, 1191, 991, 709; HRMS (+ESI) *m/z* calculated for C₁₆H₁₃ClO₂ [M+H]⁺: 273.2531; found: 273.1198.



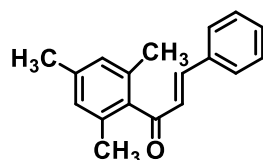
(E)-3-(4-hydroxyphenyl)-1-(4-methoxyphenyl)prop-2-en-1-one (Table 2, 3au)⁴:

222 mg, 87% yield, M.P 127°C [Lit: 130°C], light brown solid, ¹H NMR (CDCl₃, 500MHz): δ 3.81 (s, 3H), 6.89 (d, 2H, *J*=10 Hz), 7.18 (d, 2H, *J*=10 Hz), 7.58-7.73 (m, 7H), 7.79 (d, 1H, *J*=15 Hz), 8.01 (s, 1H); ¹³C NMR (CDCl₃, 125MHz): 55.85, 115.36, 116.44, 121.03, 126.11, 126.37, 127.42, 130.88, 131.13, 131.36 145.3, 156.29, 168.14, 195.58; FT-IR (KBR, cm⁻¹): 3339, 3029, 2907, 1662, 1530, 1403, 1156, 853; HRMS (+ESI) *m/z* calculated for C₁₆H₁₄O₃ [M+H]⁺: 255.3452; found: 255.3051.



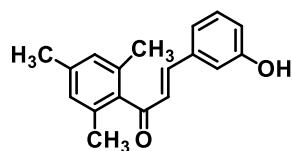
(E)-1-(3,4-dimethoxyphenyl)-3-(4-hydroxy-3-methoxyphenyl)prop-2-en-1-one (Table 2, 3av)^{2b}:

270 mg, 85% yield, M.P 198°C [Lit: 200°C], yellow solid, ¹H NMR (CDCl₃ and DMSO, 500MHz): δ 3.76 (s, 3H), 3.79 (s, 3H), 3.80 (s, 3H), 6.40-6.47 (m, 7H), 6.84 (d, 1H, *J* = 5 Hz), 6.98 (d, 1H, *J* = 5 Hz), 7.05-7.64 (m, 7H), 9.71 (s, 1H); ¹³C NMR (CDCl₃ and DMSO, 125MHz): 55.42, 55.61, 55.78, 98.55, 104.96, 110.96, 113.97, 114.78, 114.80, 122.89, 122.71, 124.72, 127.74, 132.57, 139.16, 142.76, 146.70, 147.83, 147.87, 160.10, 163.85, 190.80; FT-IR (KBR, cm⁻¹): 3031, 2959, 2841, 1650, 1544, 1479, 1347, 1209, 1110, 983, 803; HRMS (+ESI) *m/z* calculated for C₁₈H₁₈O₅ [M+H]⁺: 315.2544; found: 315.1856.



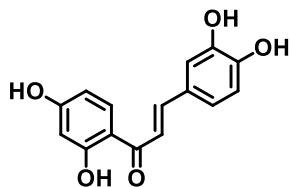
(E)-1-mesityl-3-phenylprop-2-en-1-one (Table 2, 3aw)^{5a}:

235 mg, 94% yield, M.P 118°C [Lit: 119°C], yellow solid, ¹H NMR (CDCl₃, 500MHz): δ 2.18 (s, 3H), 2.32 (s, 3H), 6.84-6.90 (m, 7H), 7.18 (d, 1H, *J* = 5 Hz), 7.28 (t, 1H, *J* = 5 Hz), 7.45 (s, 1H); ¹³C NMR (CDCl₃, 125MHz): 19.80, 21.23, 129.01, 129.18, 130.10, 135.89, 136.39, 138.65, 139.81, 146.27, 200.28; FT-IR (KBR, cm⁻¹): 3103, 2945, 1696, 1518, 1498, 1350, 1248, 1123, 972, 753; HRMS (+ESI) *m/z* calculated for C₁₈H₁₈O₂ [M+H]⁺: 251.3586; found: 251.3453.



(E)-3-(3-hydroxyphenyl)-1-mesitylprop-2-en-1-one (Table 2, 3ax)^{2a}:

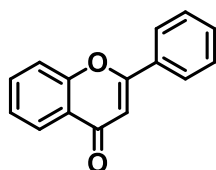
237 mg, 89% yield, M.P 142°C [Lit: 144°C], pale yellow solid, ¹H NMR (CDCl₃, 500MHz): δ 2.09 (s, 3H), 2.24 (s, 3H), 6.80-6.87 (m, 7H), 6.94 (d, 1H, *J* = 5 Hz), 7.14 (t, 1H, *J* = 5 Hz), 7.19 (s, 1H); ¹³C NMR (CDCl₃, 125MHz): 19.28, 21.13, 114.60, 118.51, 121.22, 128.06, 128.38, 130.04, 133.97, 135.42, 136.35, 138.60, 148.19, 156.48, 203.11; FT-IR (KBR, cm⁻¹): 2892, 1647, 1544, 1412, 1339, 1211, 1103, 978, 787; HRMS (+ESI) *m/z* calculated for C₁₈H₁₈O₂ [M+H]⁺: 267.3286; found: 267.3119.



(*E*)-1-(2,4-dihydroxyphenyl)-3-(3,4-dihydroxyphenyl)prop-2-en-1-one (Table 2, 3ay)^{5b}:

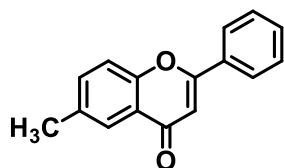
219 mg, 80% yield, M.P 216°C [Lit: 216°C], yellow solid, ¹H NMR (DMSO, 500MHz): δ 6.27 (d, 1H, *J* = 2.5 Hz), 6.40 (d, 1H, *J* = 3.5 Hz), 6.81 (d, 1H, *J* = 8.5 Hz), 7.27 (d, 1H, *J* = 8.5 Hz), 7.66 (d, 1H, *J* = 10.5 Hz), 8.15 (d, 1H, *J* = 8.5 Hz), 9.12 (s, 1H), 9.79 (s, 1H), 10.67 (s, 1H), 13.60 (s, 1H); ¹³C NMR (DMSO 125MHz): 102.90, 108.42, 113.35, 116.06, 116.18, 117.65, 122.73, 126.58, 133.16, 145.08, 145.95, 149.22, 165.22, 166.07, 191.79; FT-IR (KBR, cm⁻¹): 3321, 3025, 2891, 2741, 1688, 1539, 1436, 1322, 1207, 1101, 853, 659; HRMS (+ESI) *m/z* calculated for C₁₅H₁₂O₅ [M+H]⁺: 273.1586; found: 273.1249.

5.2 Characterization data of Flavone derivatives (Table 3 of the manuscript)



Flavone, (2-Phenyl-4*H*-chromen-4-one) (Table 3, 4aa)^{6a}:

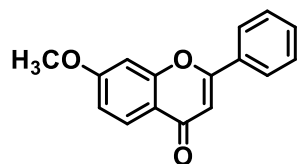
198 mg, 89% yield, M.P 96°C [Lit: 98°C], white solid, ¹H NMR (CDCl₃, 500MHz): δ 6.77 (s, 1H), 7.35 (td, 1H, *J* = 5 Hz, 1 Hz), 7.41-7.65 (m, 4H), 7.87 (td, 1H, *J* = 5 Hz, 10 Hz), 8.15 (dd, 1H, *J* = 5 Hz, 10 Hz), 8.17 (dd, 2H, *J* = 5 Hz, 10 Hz); ¹³C NMR (CDCl₃, 125MHz): 107.46, 117.98, 123.82, 125.13, 125.58, 126.19, 128.94, 131.51, 131.64, 133.69, 156.14, 163.33, 178.38; FT-IR (KBR, cm⁻¹): 2892, 1647, 1544, 1412, 1339, 1211, 1103, 978, 787; HRMS (+ESI) *m/z* calculated for C₁₅H₁₀O₂ [M+H]⁺: 223.2589; found: 223.2269 [M⁺].



6-methyl-2-phenyl-4*H*-chromen-4-one (Table 3, 4ab)^{6a}:

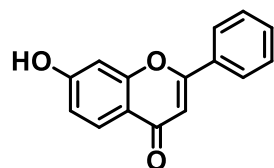
196 mg, 83% yield, M.P 110°C [Lit: 112°C], white solid, ¹H NMR (CDCl₃, 500MHz): δ 2.48 (s, 3H), 6.83 (s, 1H), 7.27 (s, 1H), 7.49-7.54 (m, 7H), 7.94 (dd, *J* = 5 Hz, 10 Hz, 1H), 8.02 (dd, 1H *J* = 5 Hz, 5

Hz), 8.03 (s, 2H); ^{13}C NMR (CDCl_3 , 125MHz): 20.88, 107.33, 11775, 123.47, 124.93, 126.17, 128.92, 131.42, 131.78, 134.92, 135.12, 154.43, 163.16, 178.53; FT-IR (KBR, cm^{-1}): 2953, 1686, 1578, 1375, 1211; HRMS (+ESI) m/z calculated for $\text{C}_{16}\text{H}_{12}\text{O}_2$ $[\text{M}+\text{H}]^+$: 237.2685; found: 237.1985.



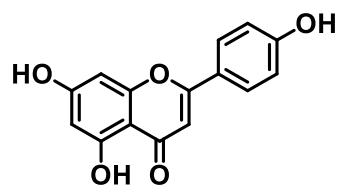
7-methoxy-2-phenyl-4H-chromen-4-one (Table 3, 4ac)^{6b}:

202 mg, 80% yield, M.P 131°C [Lit: 133°C], white solid, ^1H NMR (CDCl_3 , 500MHz): δ 3.94 (s, 3H), 6.77 (s, 1H), 6.99 (dd, 1H J = 5 Hz, 10 Hz), 7.27 (s, 1H), 7.53 (dd, 2H, J = 5 Hz, 5 Hz), 7.91 (dd, 1H, J = 5 Hz, 5 Hz), 8.13 (s, 2H), 8.15 (s, 2H); ^{13}C NMR (CDCl_3 , 125MHz): 55.75, 100.29, 107.43, 114.35, 117.72, 126.06, 128.91, 131.33, 131.74, 157.91, 162.92, 164.08, 177.82; FT-IR (KBR, cm^{-1}): 3582, 3419, 2922, 1647, 1607, 1268; HRMS (+ESI) m/z calculated for $\text{C}_{16}\text{H}_{12}\text{O}_3$ $[\text{M}+\text{H}]^+$: 253.1685; found: 253.1543.



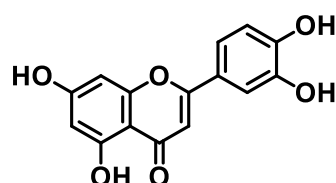
7-hydroxy-2-phenyl-4H-chromen-4-one (Table 3, 4ad)^{6a}:

186 mg, 78% yield, M.P 172°C [Lit: 133°C], white solid, ^1H NMR (CDCl_3 and DMSO, 500MHz): δ 6.72 (s, 1H), 6.94 (dd, J = 5 Hz, 10 Hz 2H), 7.47 (s, 1H), 7.51-7.91 (m, 7H), 8.02 (d, J = 5 Hz, 2H), 8.03 (d, J = 5 Hz, 2H), 10.22 (s, 1H); ^{13}C NMR (CDCl_3 and DMSO, 125MHz): 107.38, 111.67, 119.82, 121.33, 130.64, 130.77, 131.55, 133.59, 135.95, 136.47, 162.65, 167.57, 182.50; FT-IR (KBR, cm^{-1}): 3313, 3041, 1723, 1609, 1347; HRMS (+ESI) m/z calculated for $\text{C}_{15}\text{H}_{10}\text{O}_3$ $[\text{M}+\text{H}]^+$: 239.0668; found: 239.0665.



5,7-dihydroxy-2-(4-hydroxyphenyl)-4H-chromen-4-one (Table 3, 4ae):

210 mg, 77% yield, M.P 228°C [Lit: 230°C], white solid, ^1H NMR (DMSO, 500MHz): δ 6.20 (d, J = 5 Hz, 2H), 6.49 (d, J = 5 Hz, 2H), 6.80 (s, 1H), 6.90 (d, J = 5 Hz, 2H), 7.94 (d, J = 10 Hz, 4H), 10.39 (s, 1H), 10.87 (s, 1H), 12.98 (s, 1H); ^{13}C NMR (DMSO, 125MHz): 94.30, 99.16, 103.16, 104.01, 116.28, 121.48, 128.83, 157.62, 161.50, 161.76, 164.05, 164.45, 182.09; FT-IR (KBR, cm^{-1}): 3401, 3353, 2987, 1670, 1612, 1561; HRMS (+ESI) m/z calculated for $\text{C}_{15}\text{H}_{10}\text{O}_5$ $[\text{M}+\text{H}]^+$: 271.0586; found: 271.0569.



2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-4H-chromen-4-one (Table 3, 4af)^{5c}:

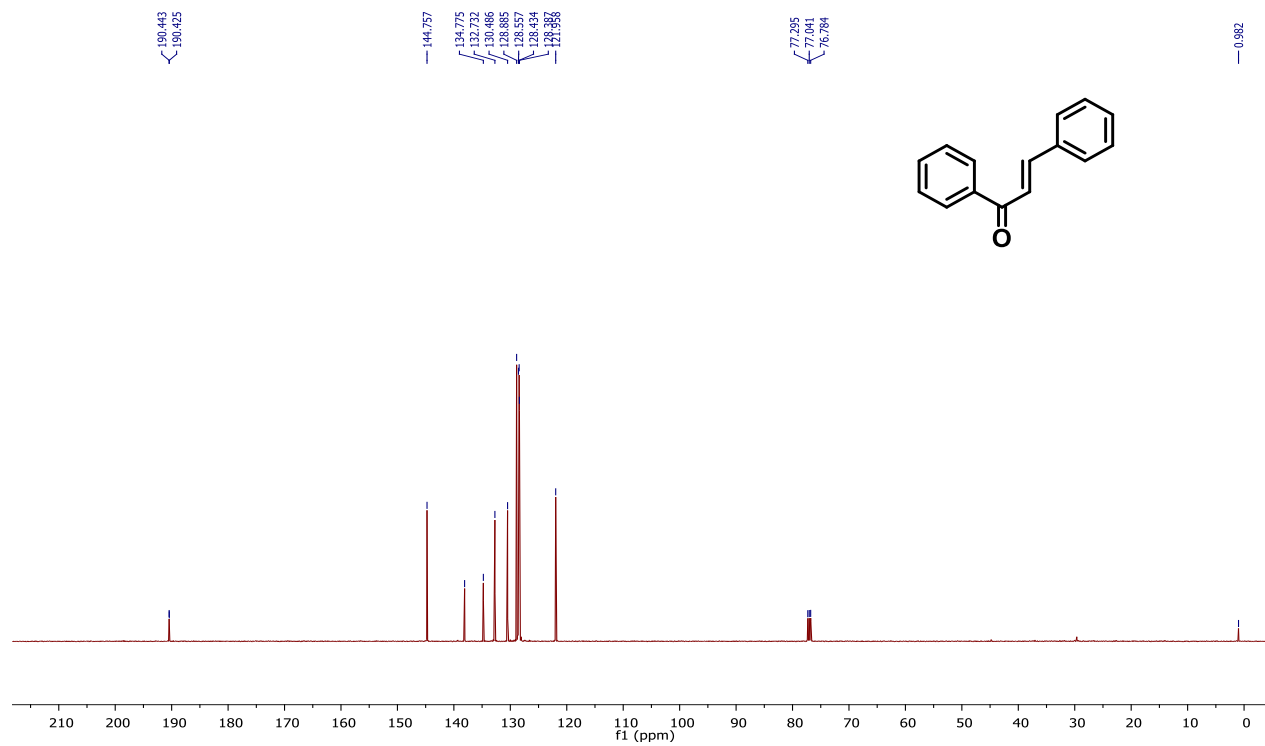
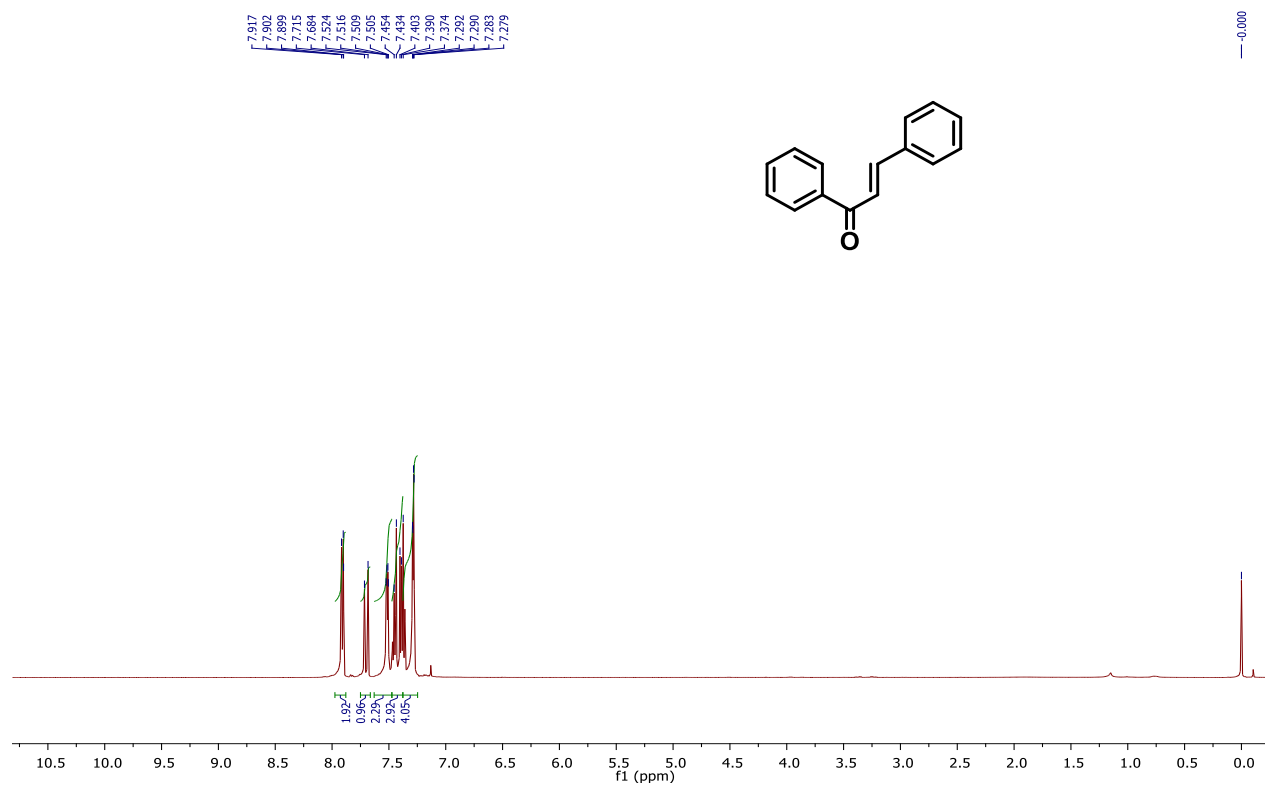
208 mg, 72% yield, M.P >300 °C [Lit: 333°C], white solid, ^1H NMR (DMSO, 500MHz): δ 6.18-6.19 (d, J = 8.5 Hz, 2H), 6.45 (d, J = 5 Hz, 2H), 6.68 (s, 1H), 6.88-6.89 (d, J = 8 Hz, 2H), 7.39-7.42 (m, 2H), 9.51 (s, 1H), 9.99 (s, 1H), 10.92 (s, 1H), 12.97 (s, 1H); ^{13}C NMR (DMSO, 125MHz): 94.19, 99.15, 103.16, 104.00, 113.62, 116.33, 119.32, 121.79, 146.04, 150.02, 157.61, 163.77, 164.21, 164.43, 182.00; FT-IR (KBR, cm^{-1}): 3440, 3358, 2992, 2885, 1662, 1607, 1538; HRMS (+ESI) m/z calculated for $\text{C}_{15}\text{H}_{10}\text{O}_6$ $[\text{M}+\text{H}]^+$: 287.6653; found: 287.6512.

7. References

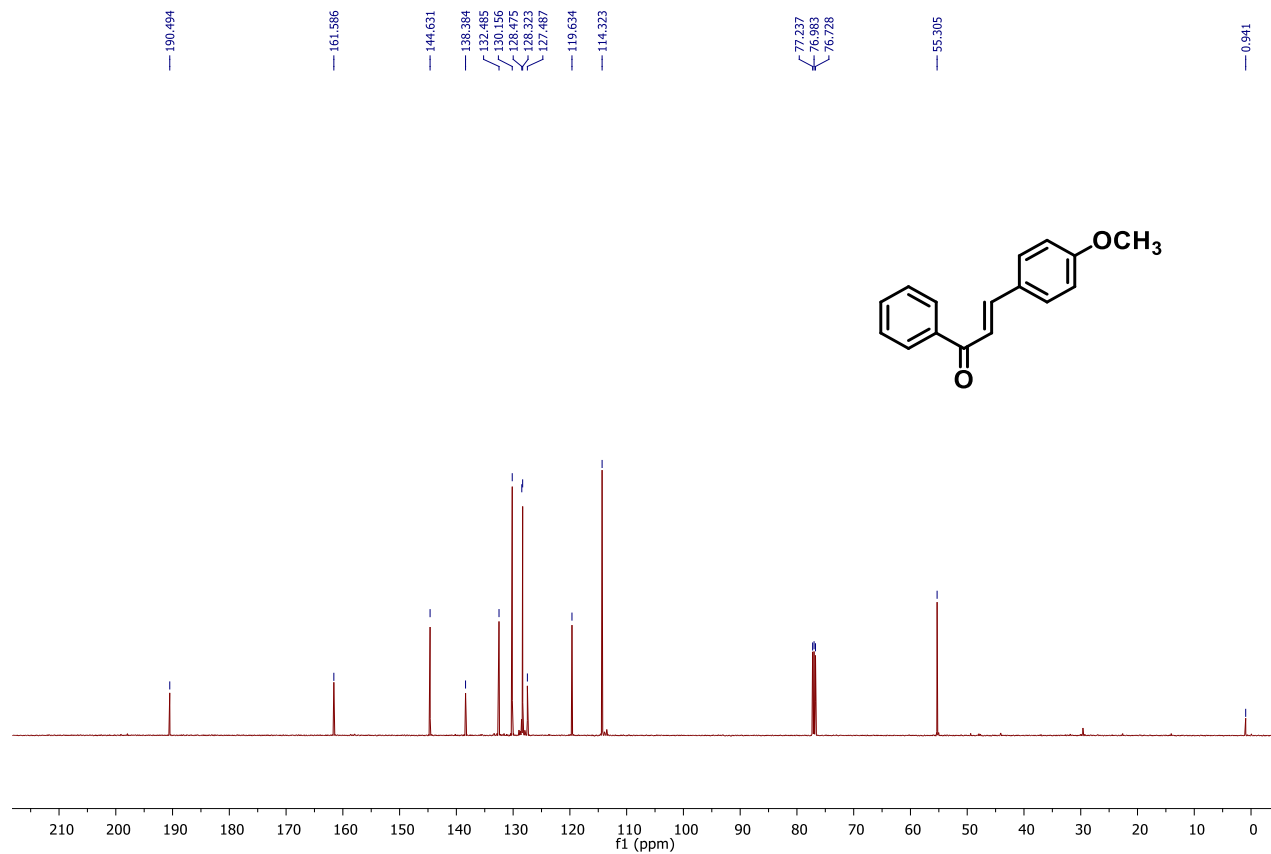
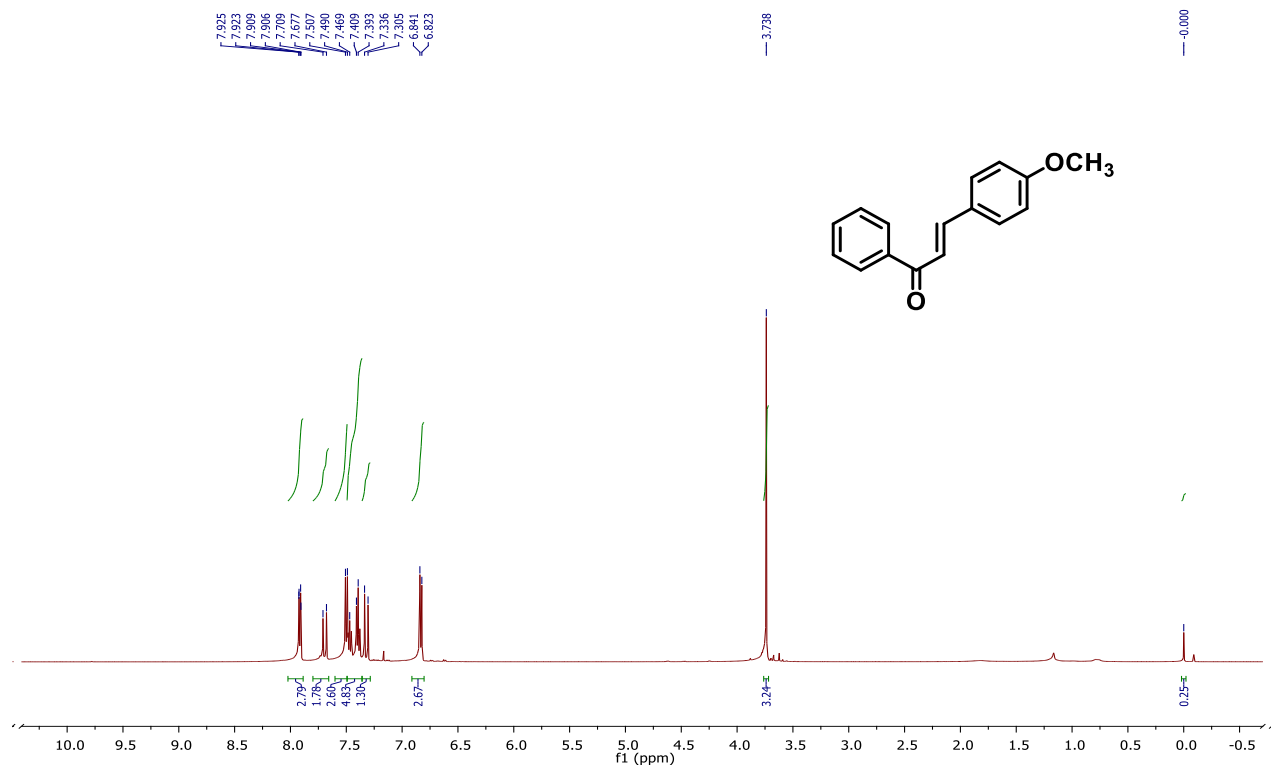
- (a) M. Vellakkaran, M. M. S. Andappan and K. Nagaiah, *RSC Adv.*, 2014, **4**, 45490-45494; (b) P. C. Lv, J. Sun, Y. Luo, Y. Yang and H.L. Zhu, *Bioorg. Med. Chem. Lett.*, 2010, **20**, 4657; (c) H. N. Pati, U. Das, Erik De Clercq, J. Balzarini and J. R. Dimmock, *J. Enzyme Inhib. Med. Chem.* 2007, **22**, 37-42; (d) R. K. Saini, N. Kumari, Y. C. Joshi, Yogesh P. Joshi and S. S. Shekhawa, *Asian J. Chem.*, 2007, **19**, 4483-4486.
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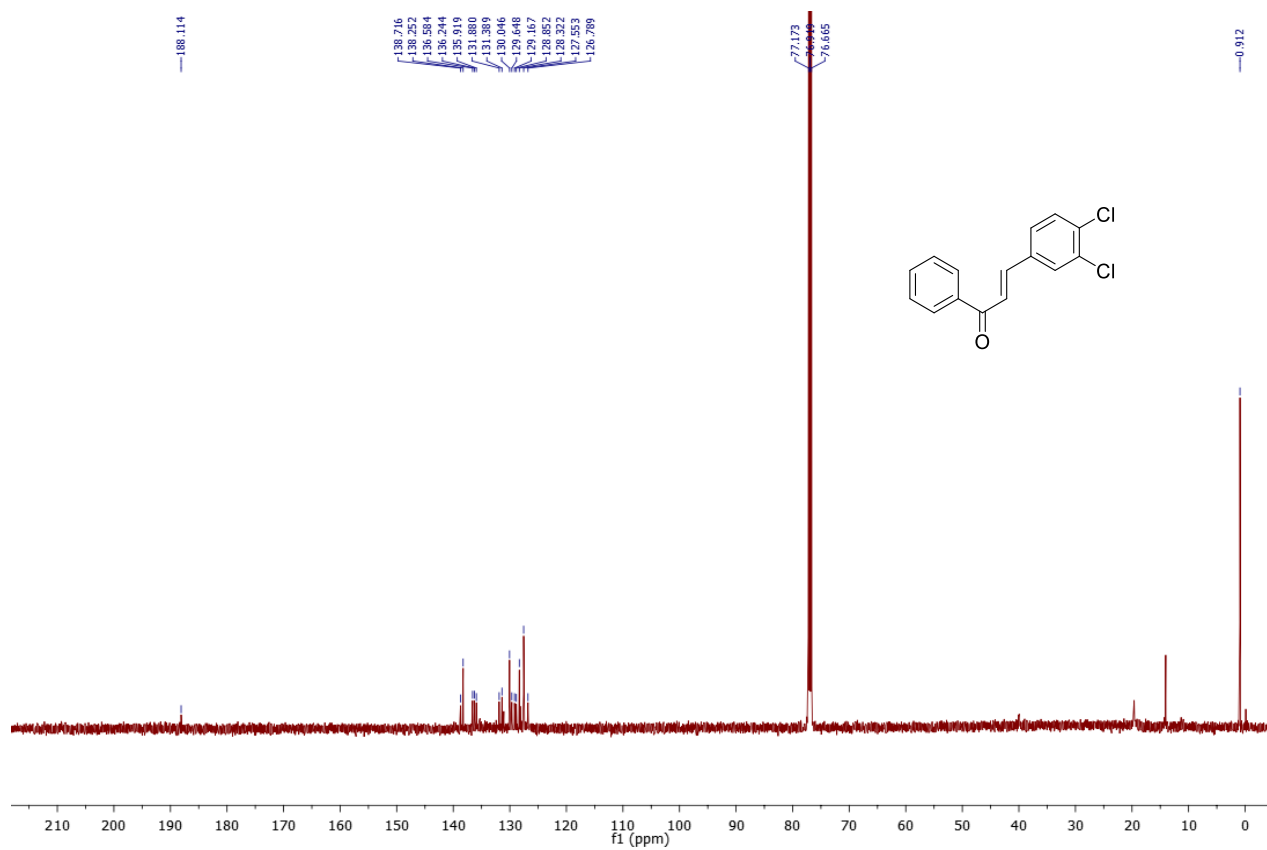
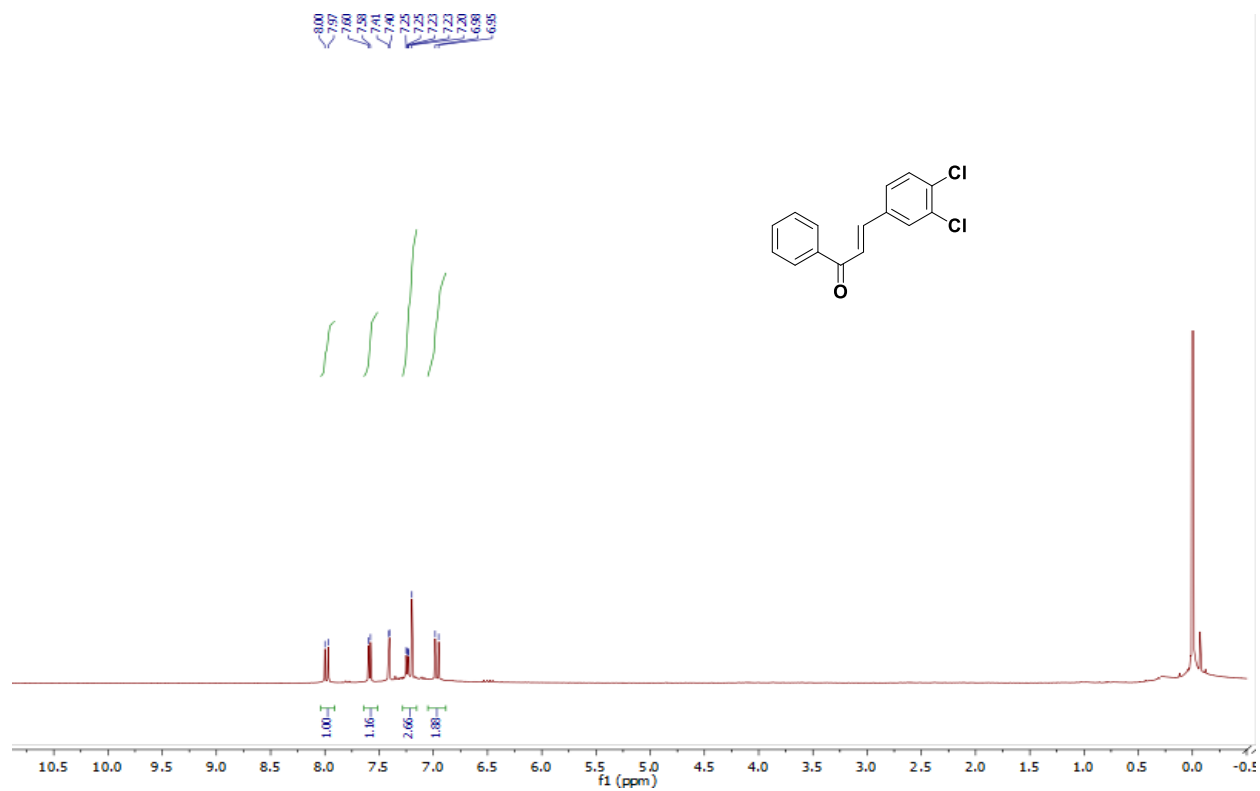
7. NMR Spectra of the products



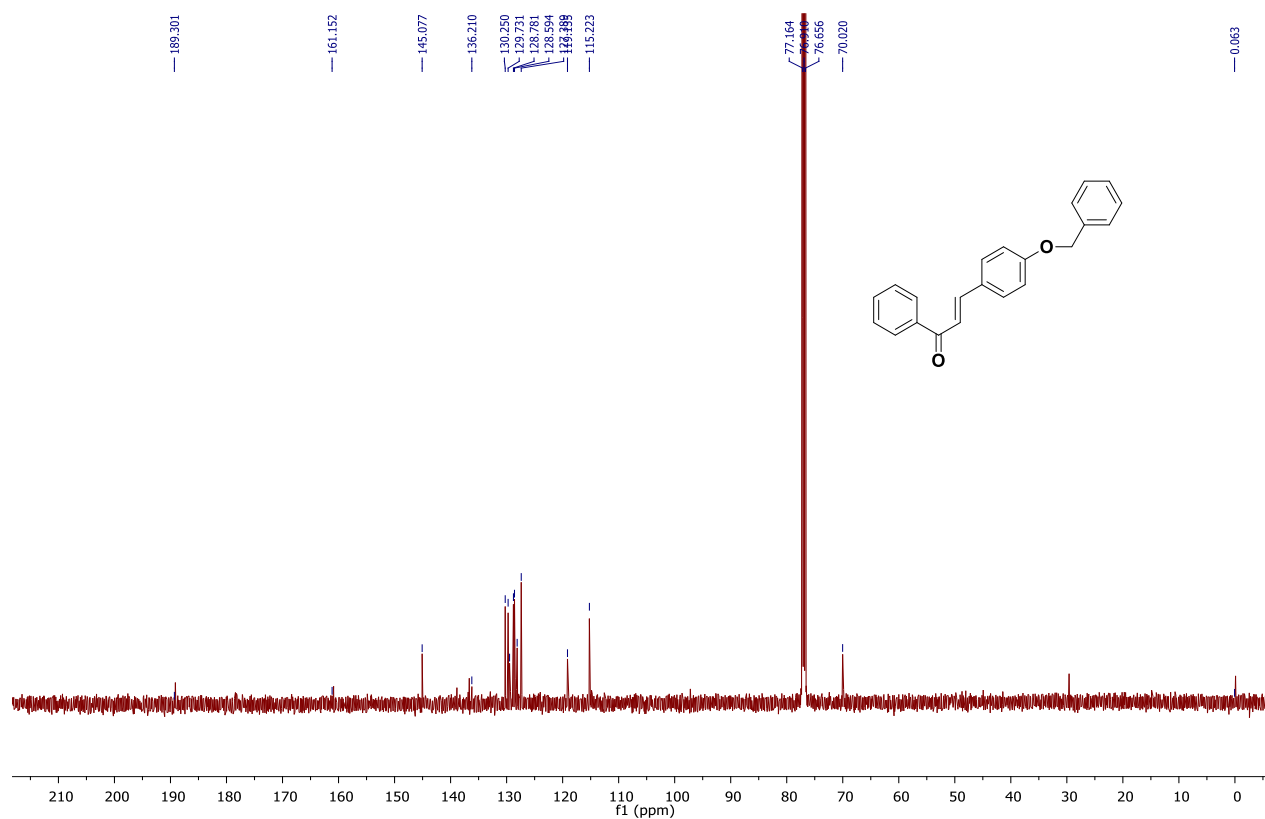
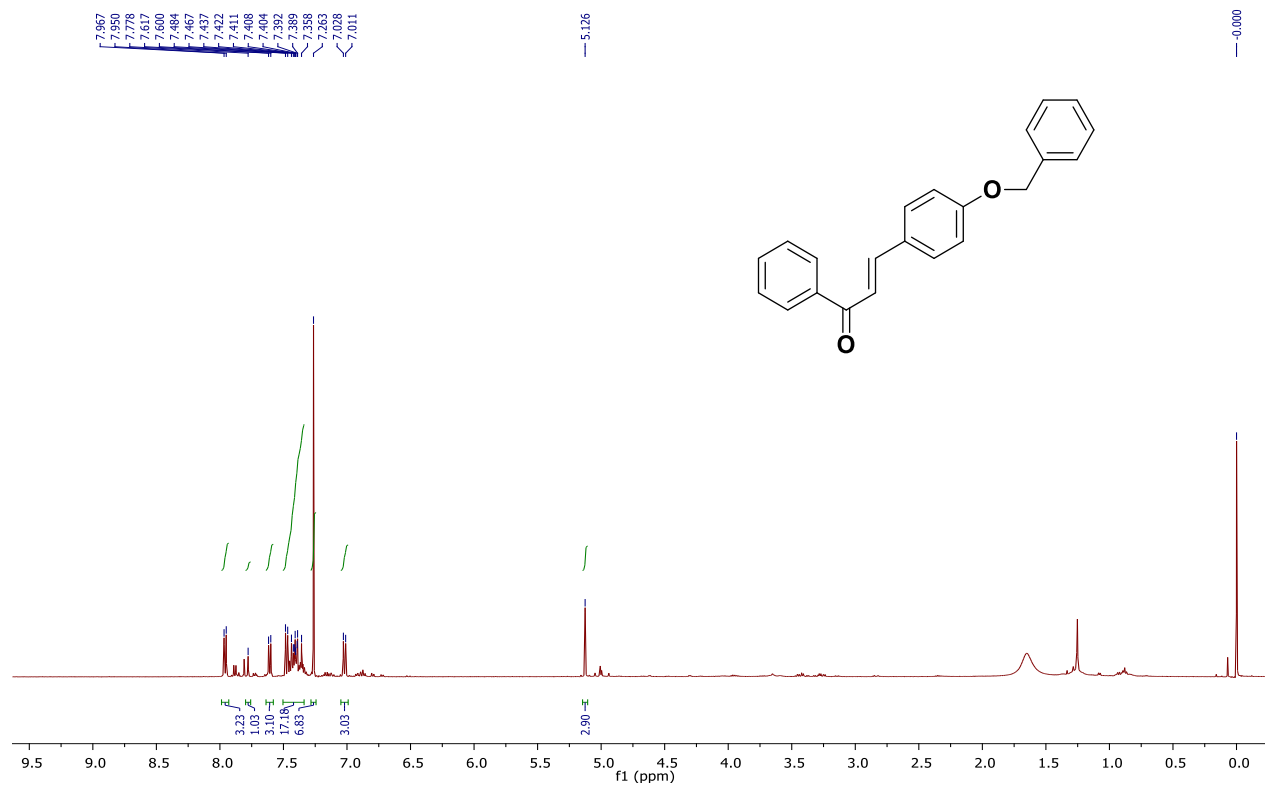
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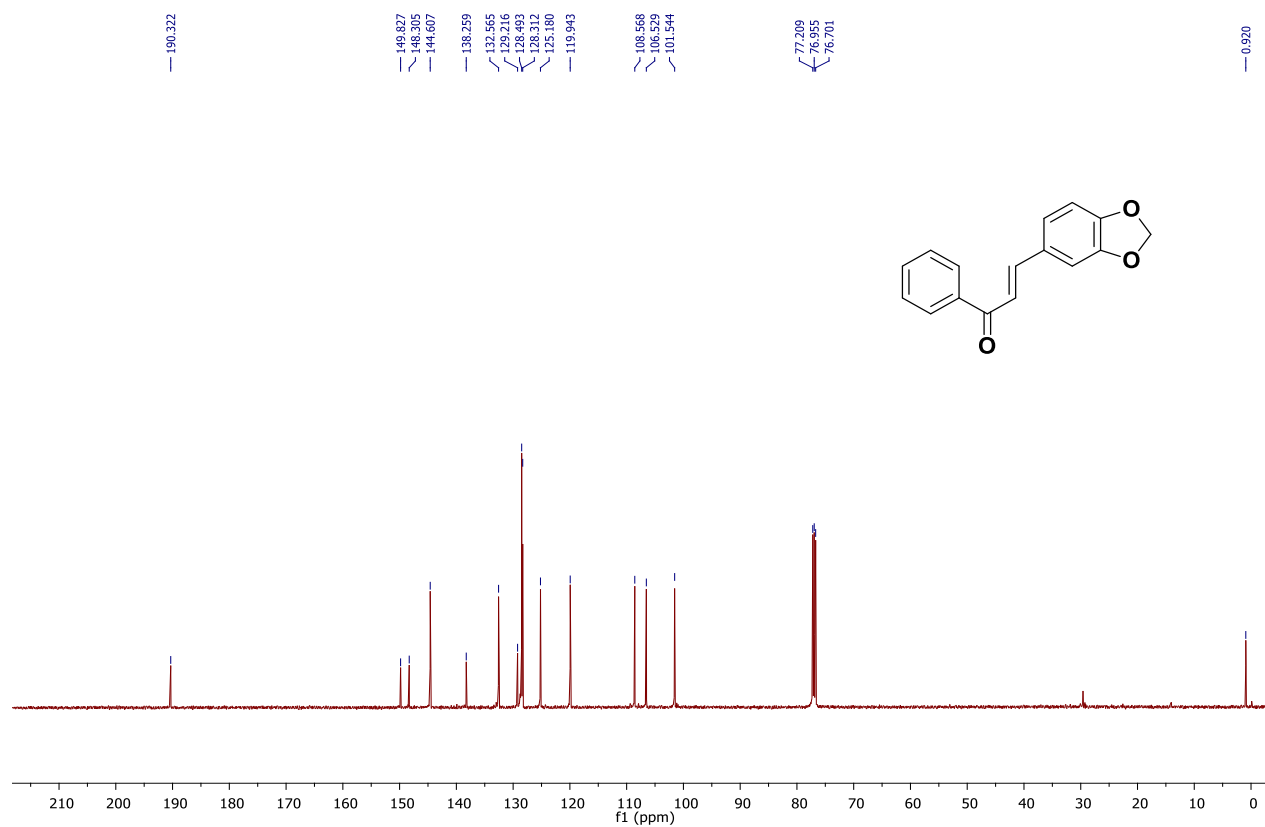
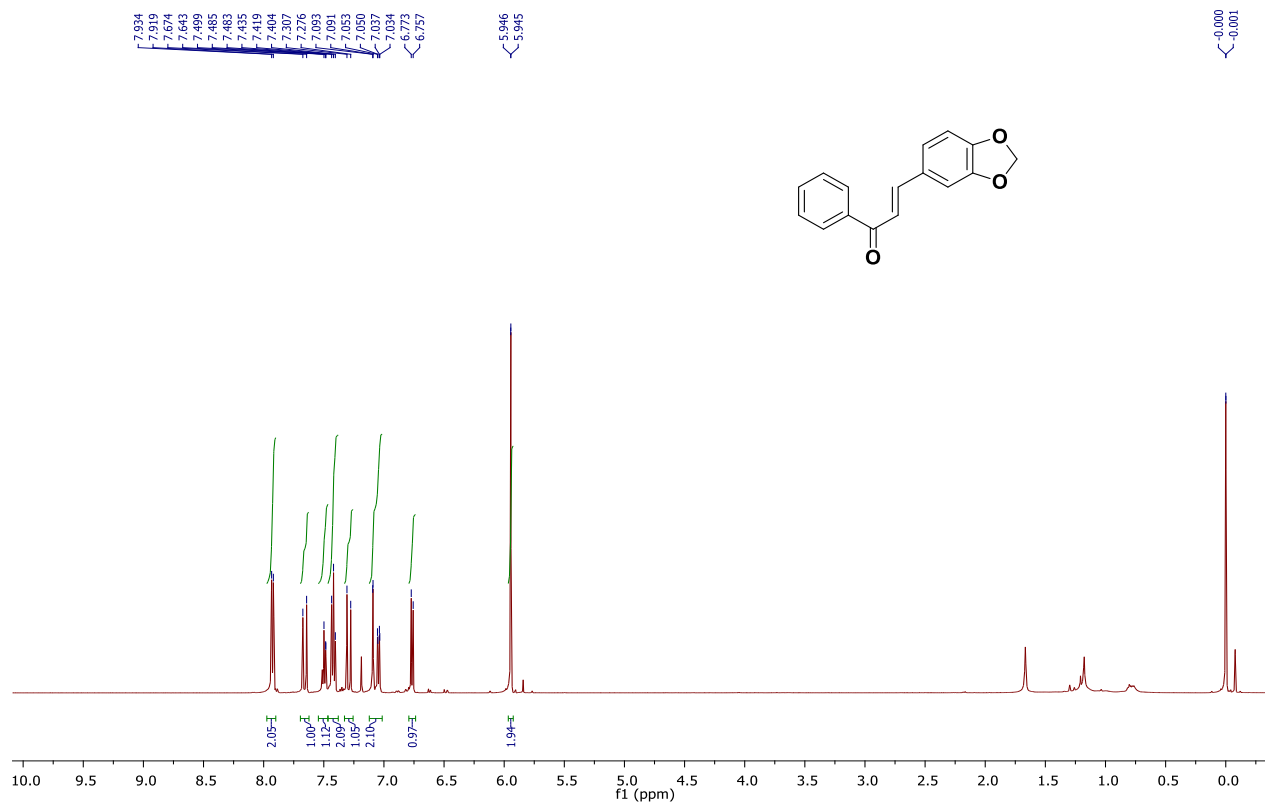
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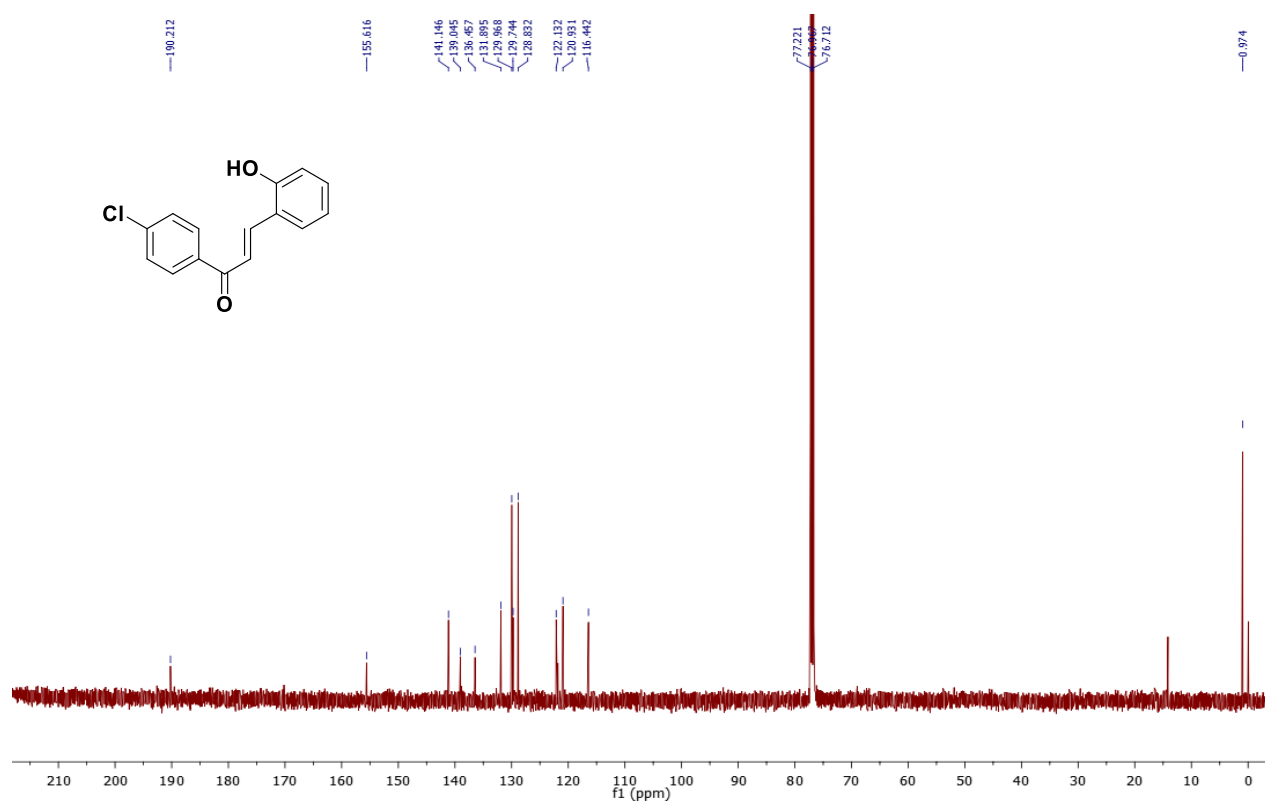
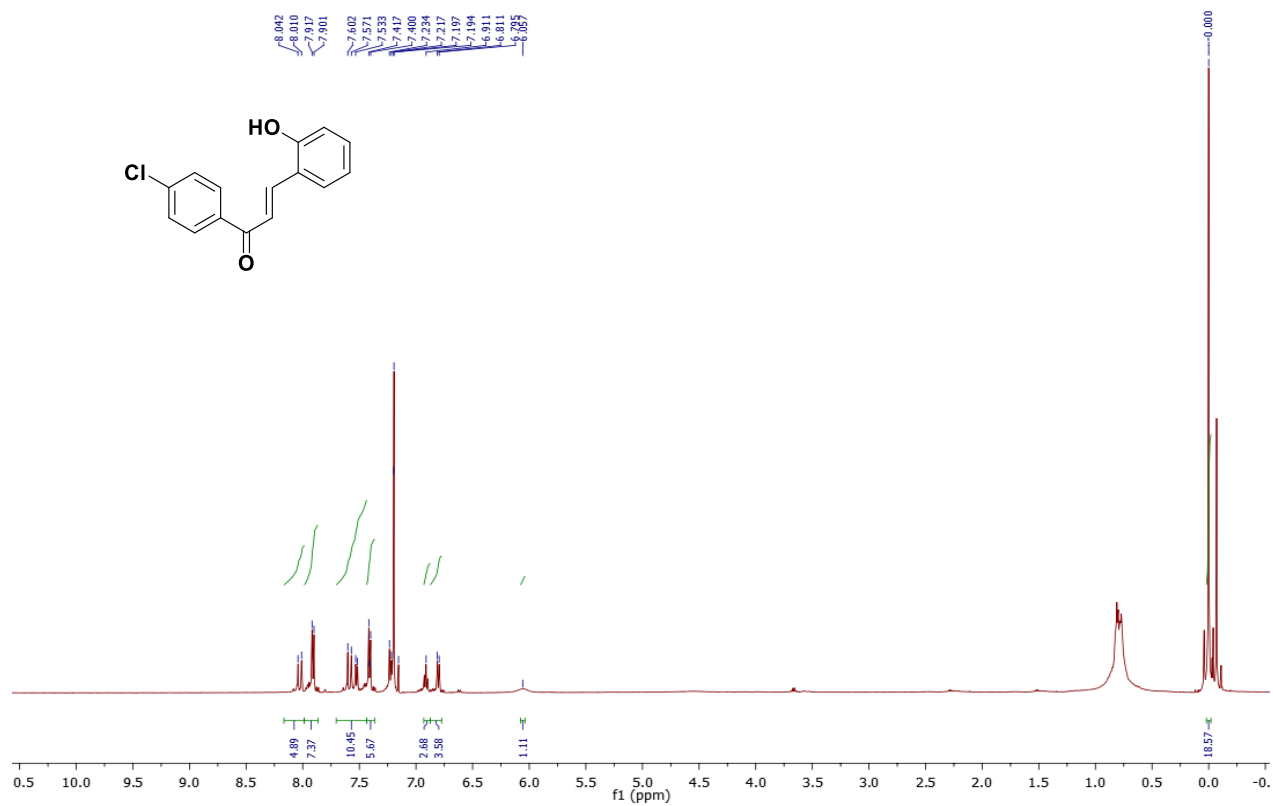
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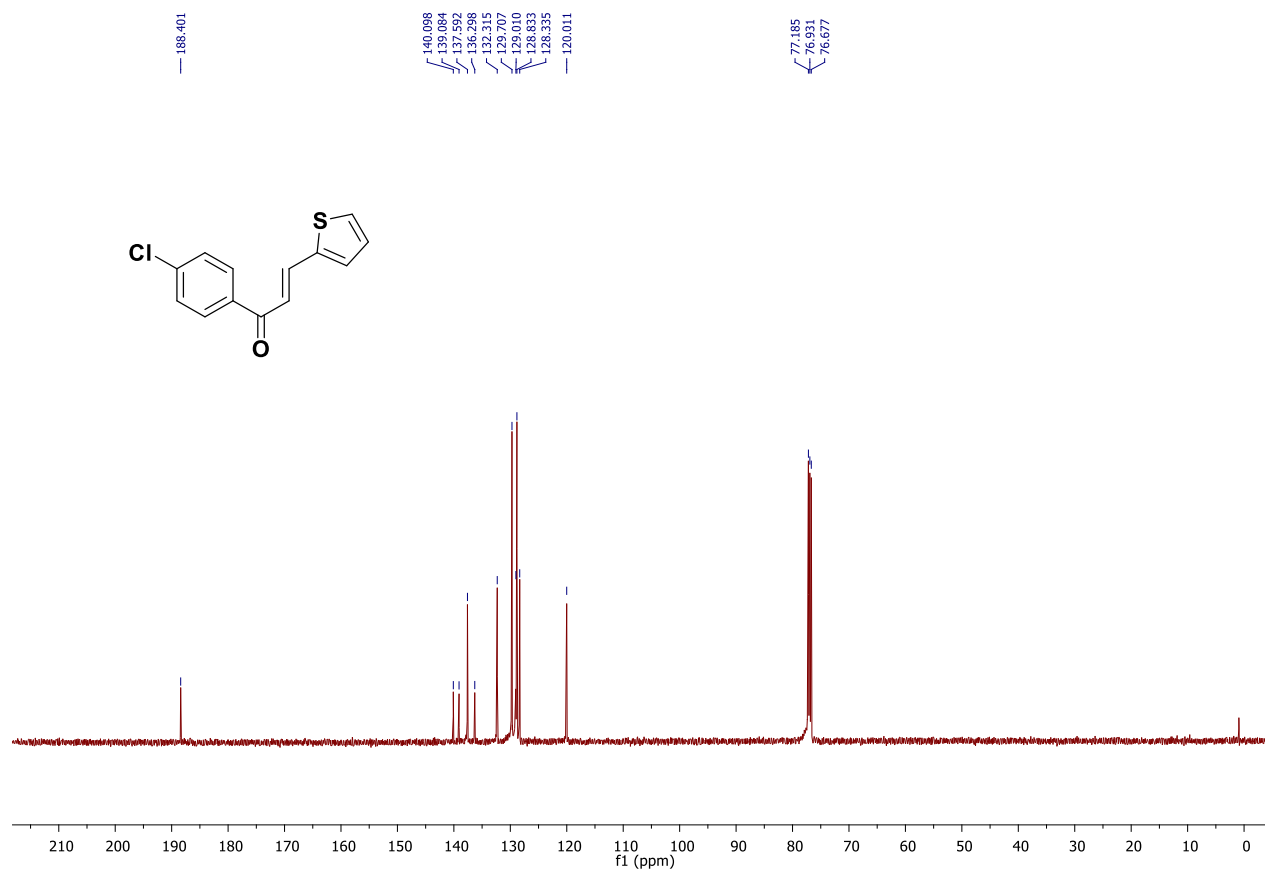
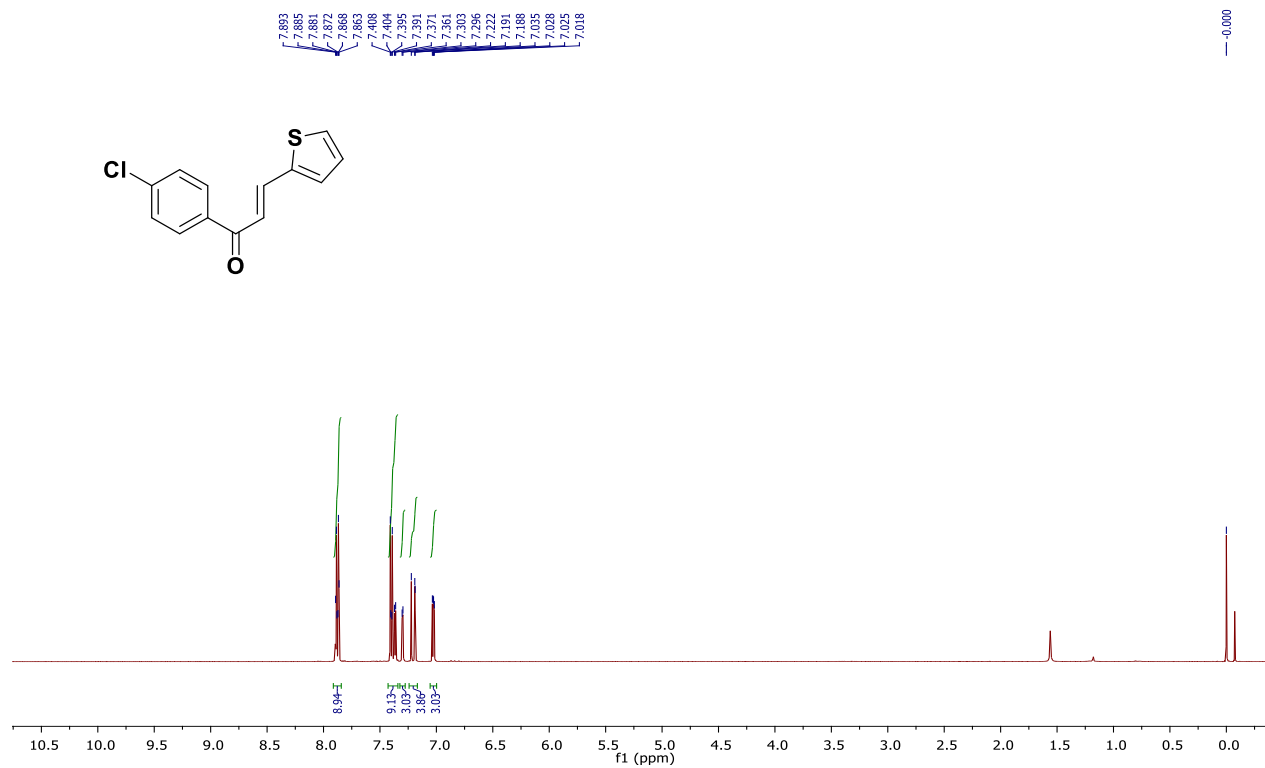
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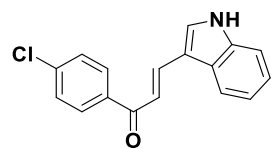
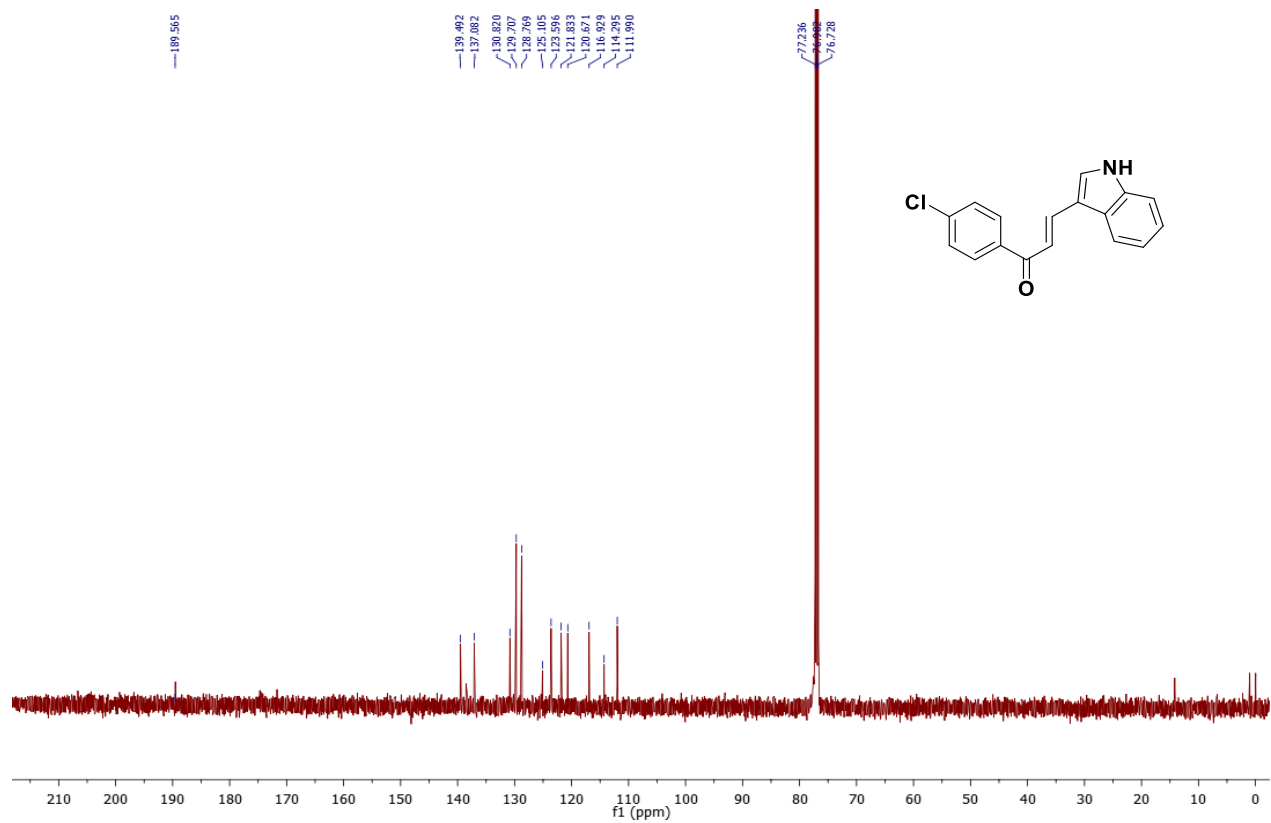
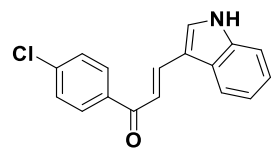
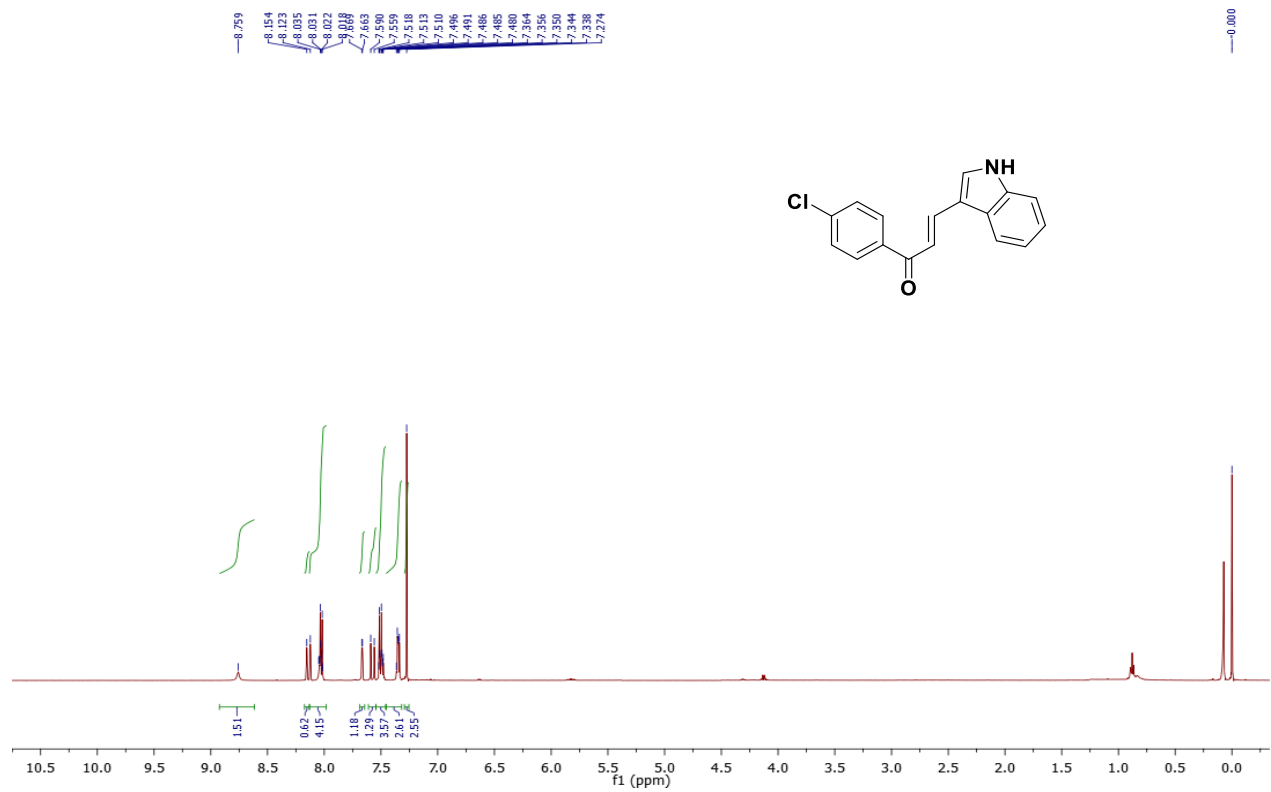
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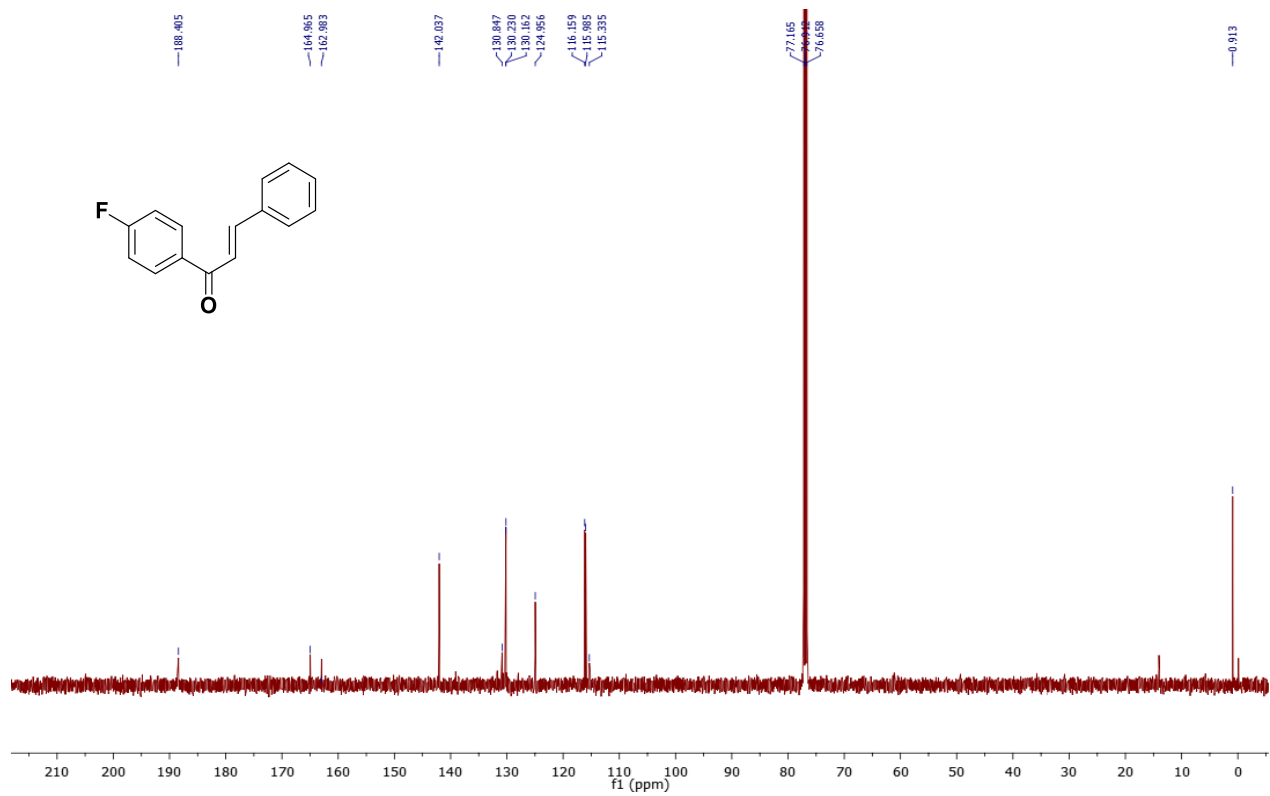
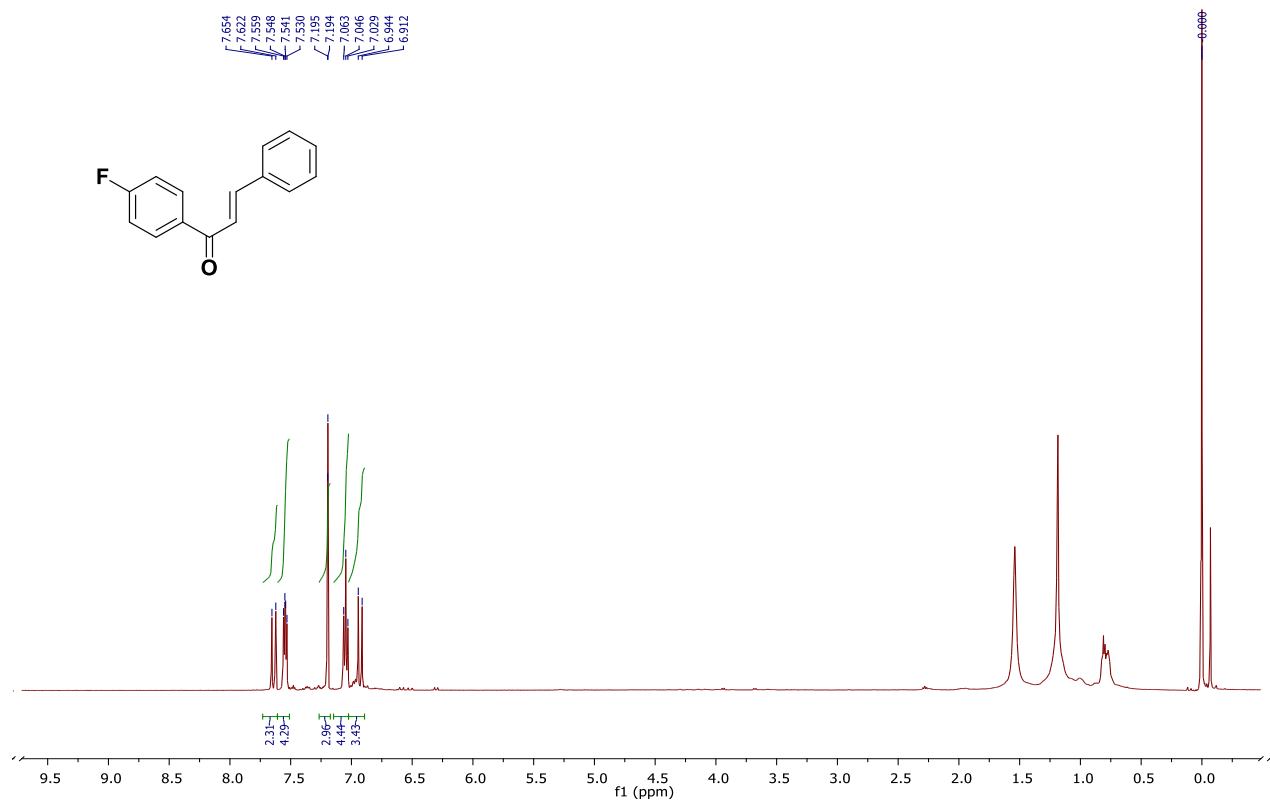
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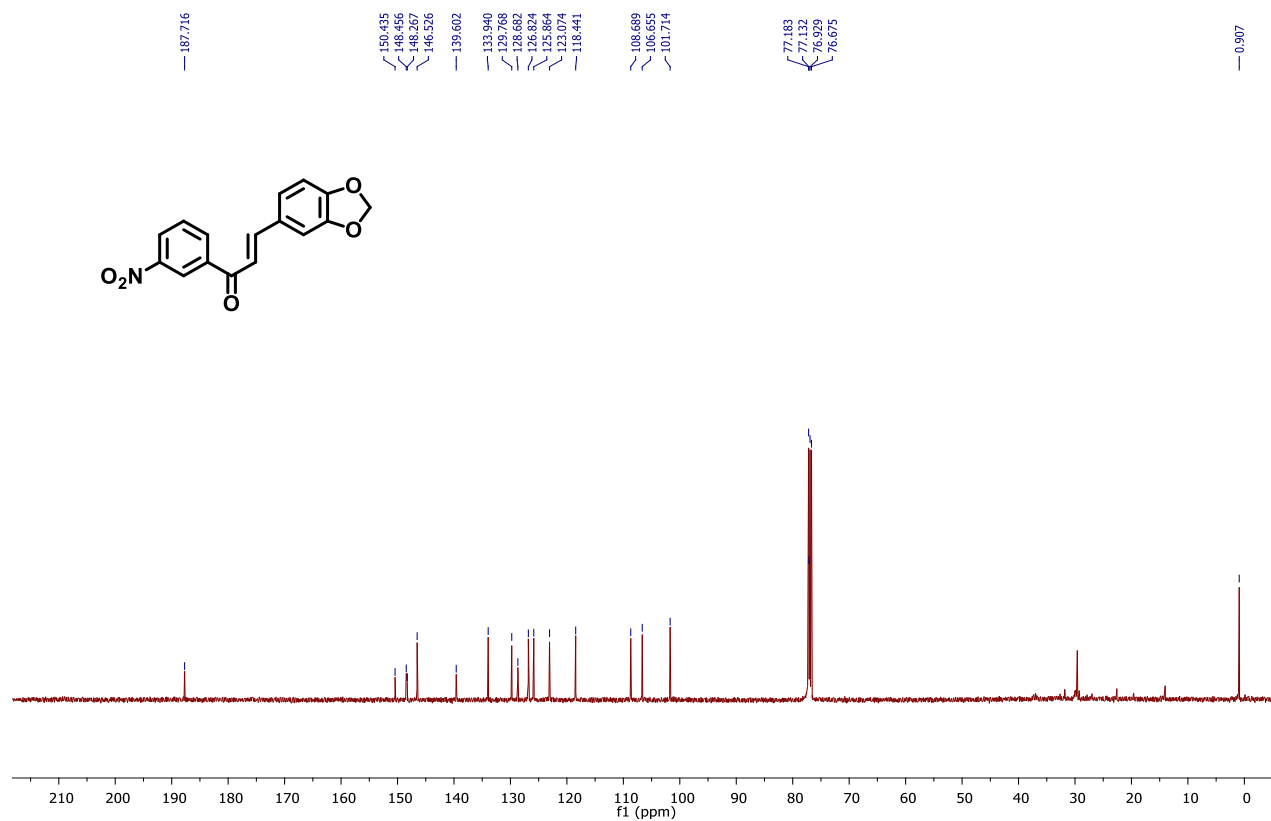
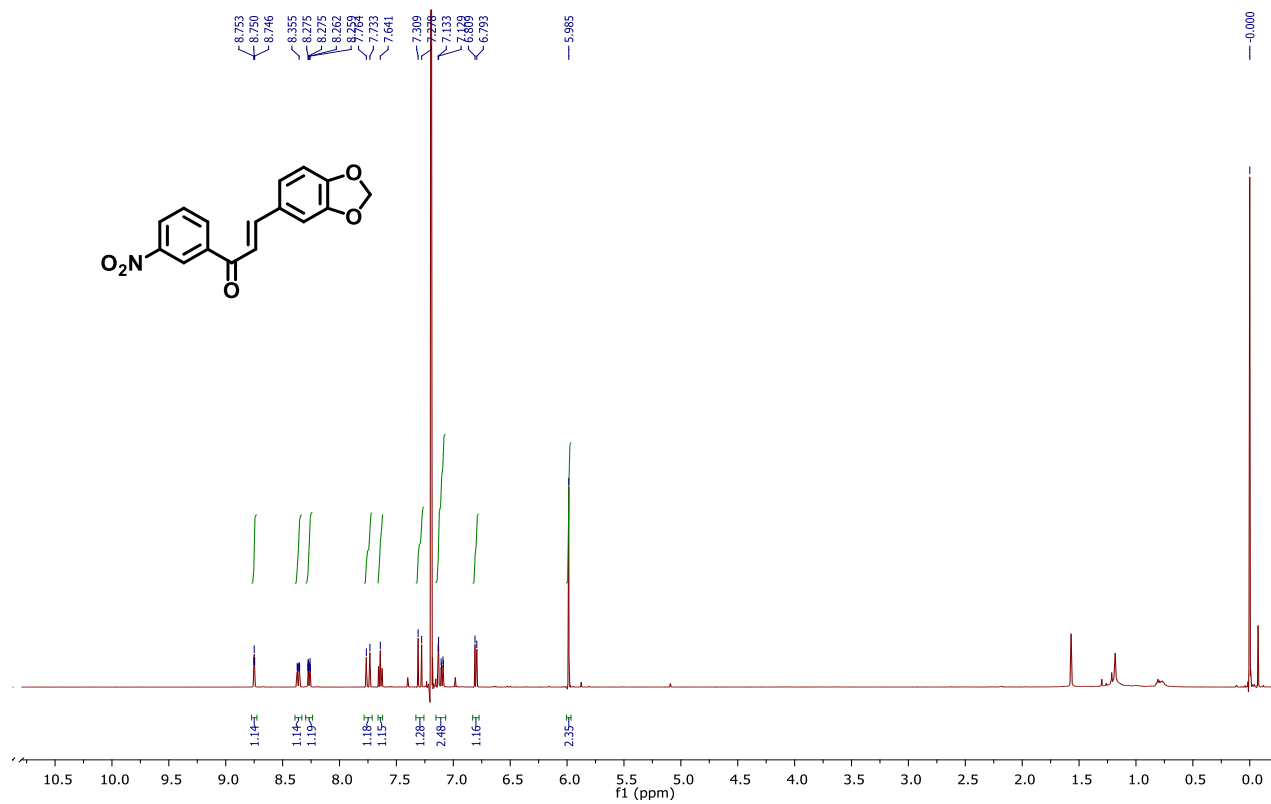
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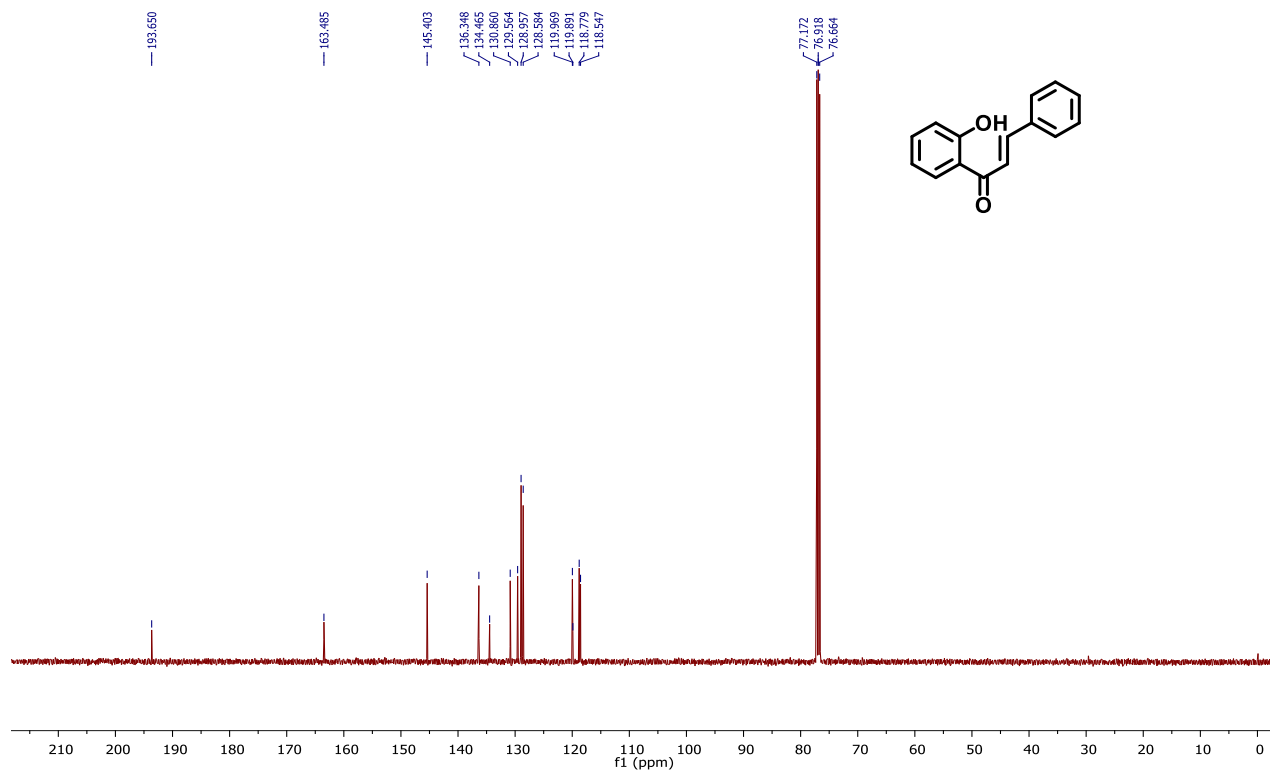
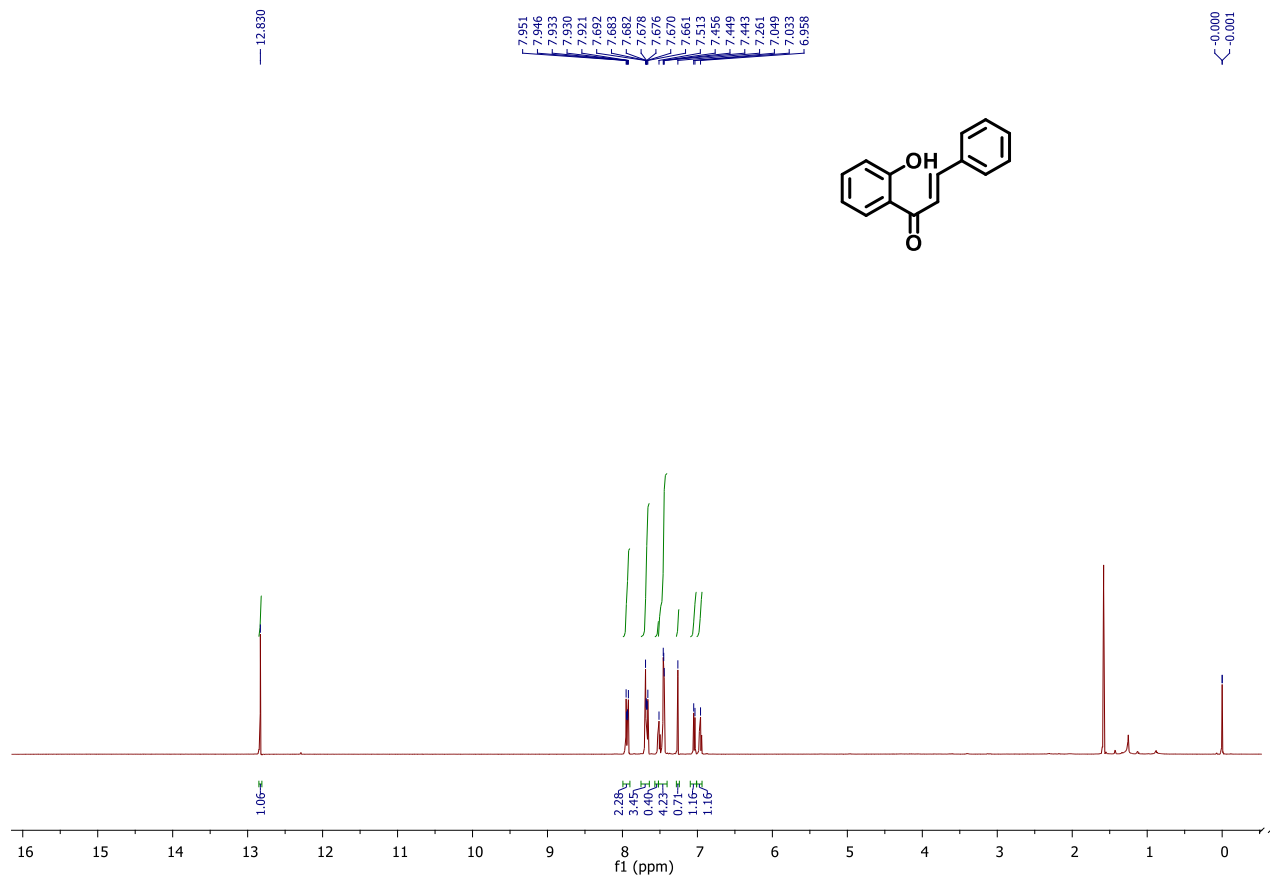
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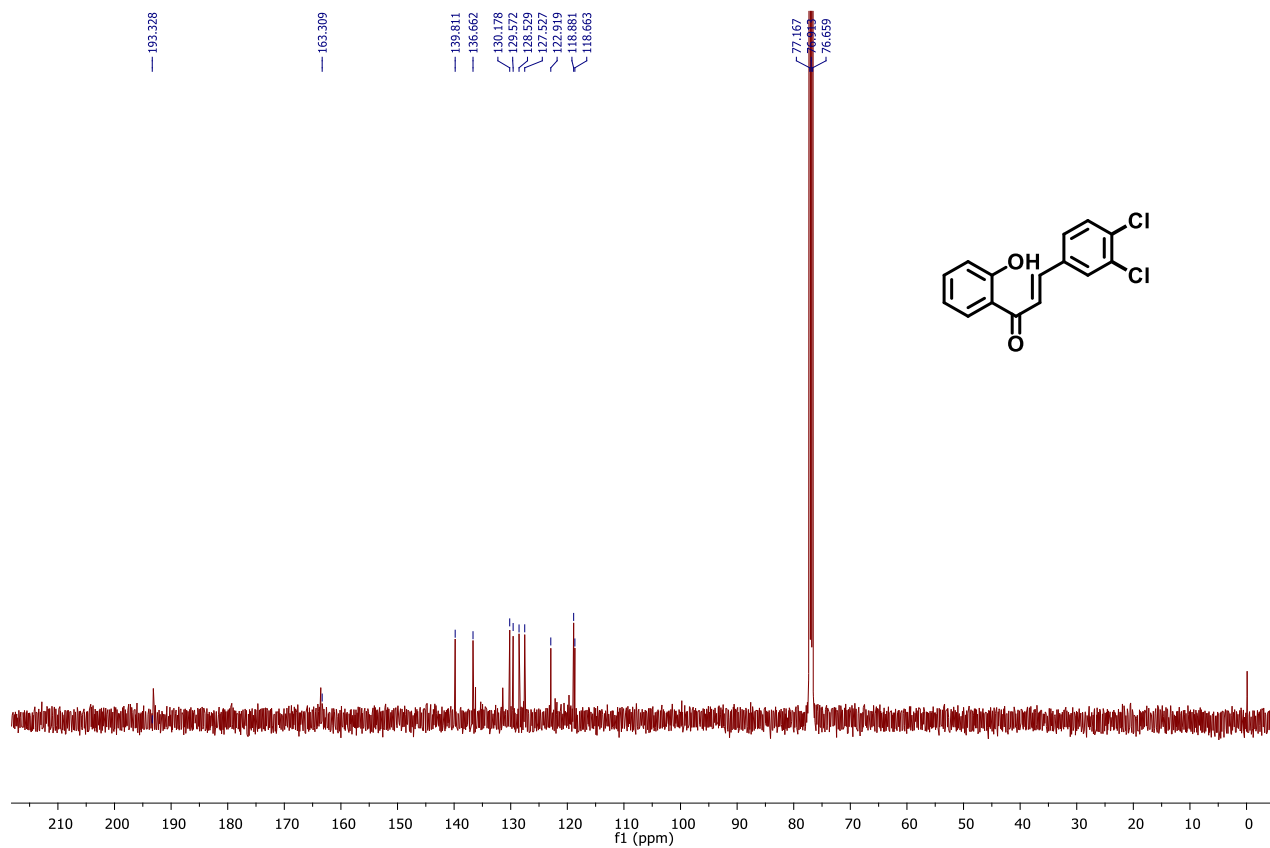
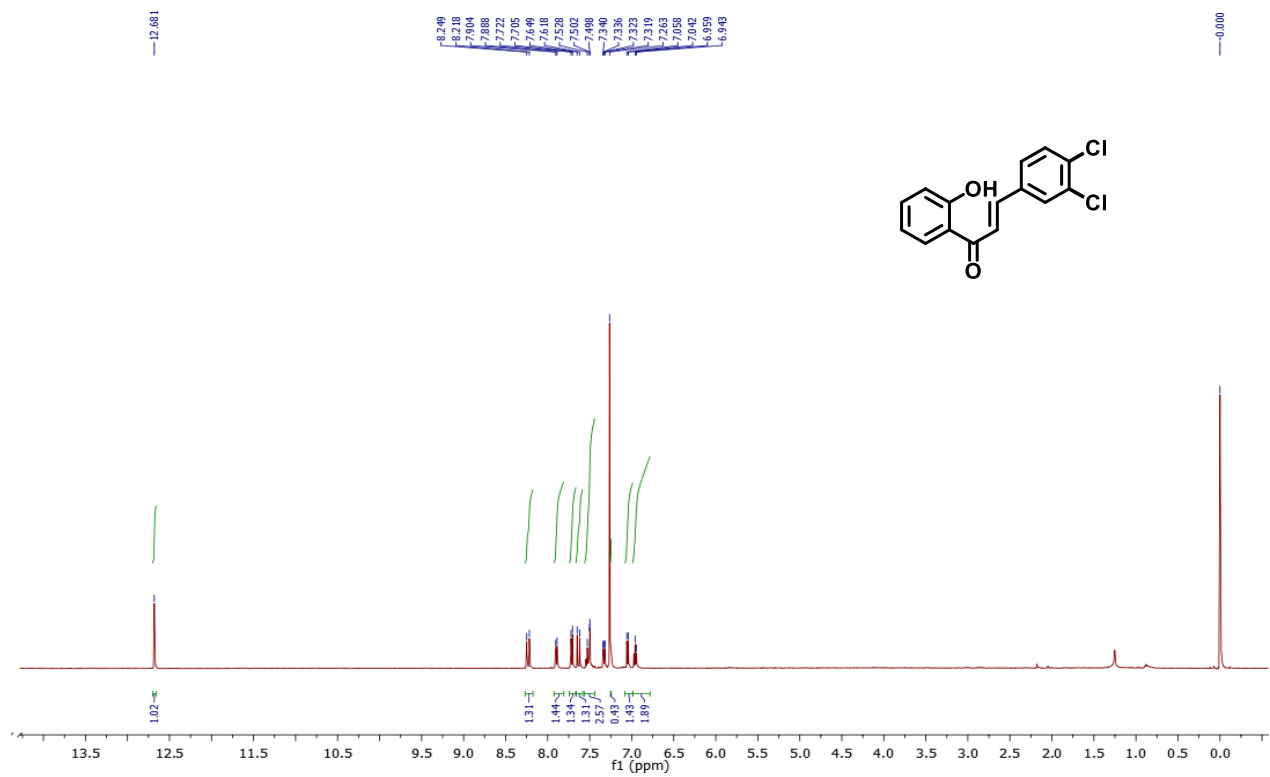
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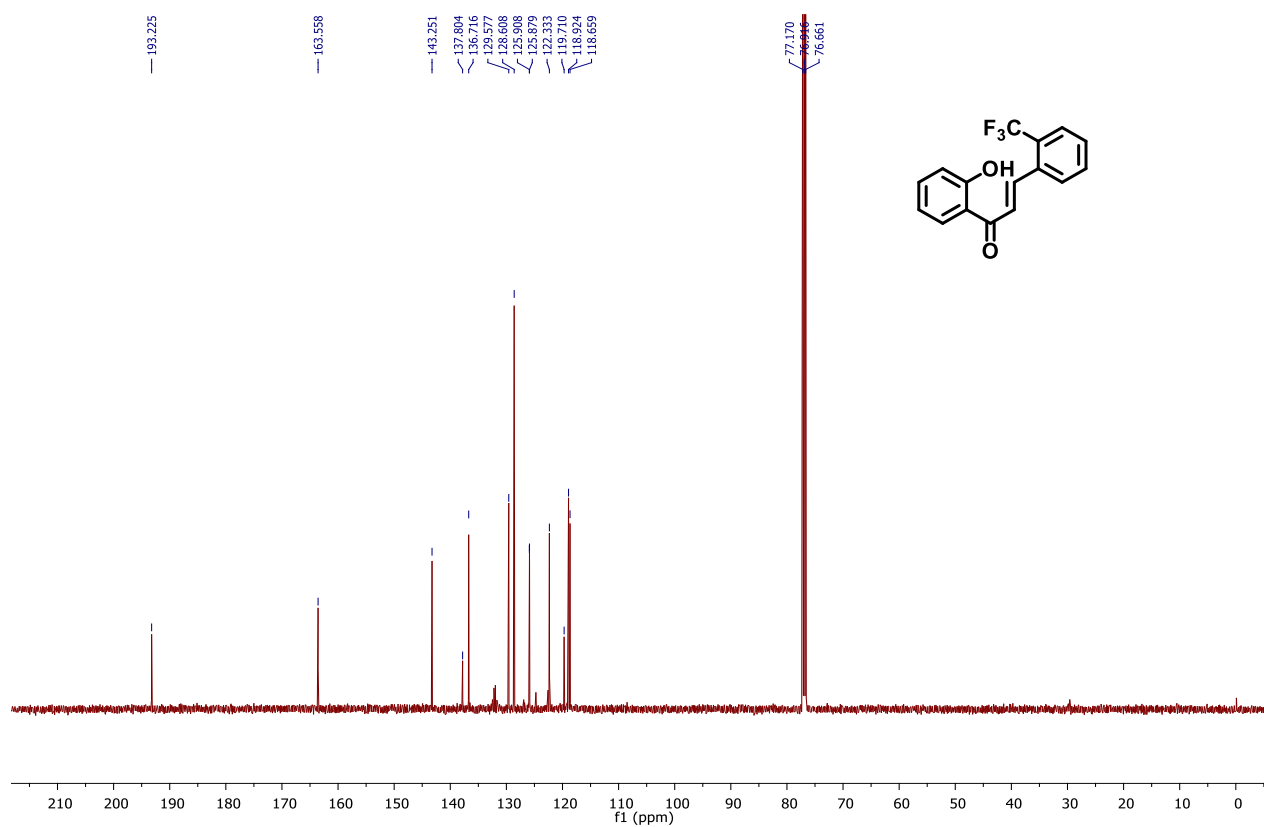
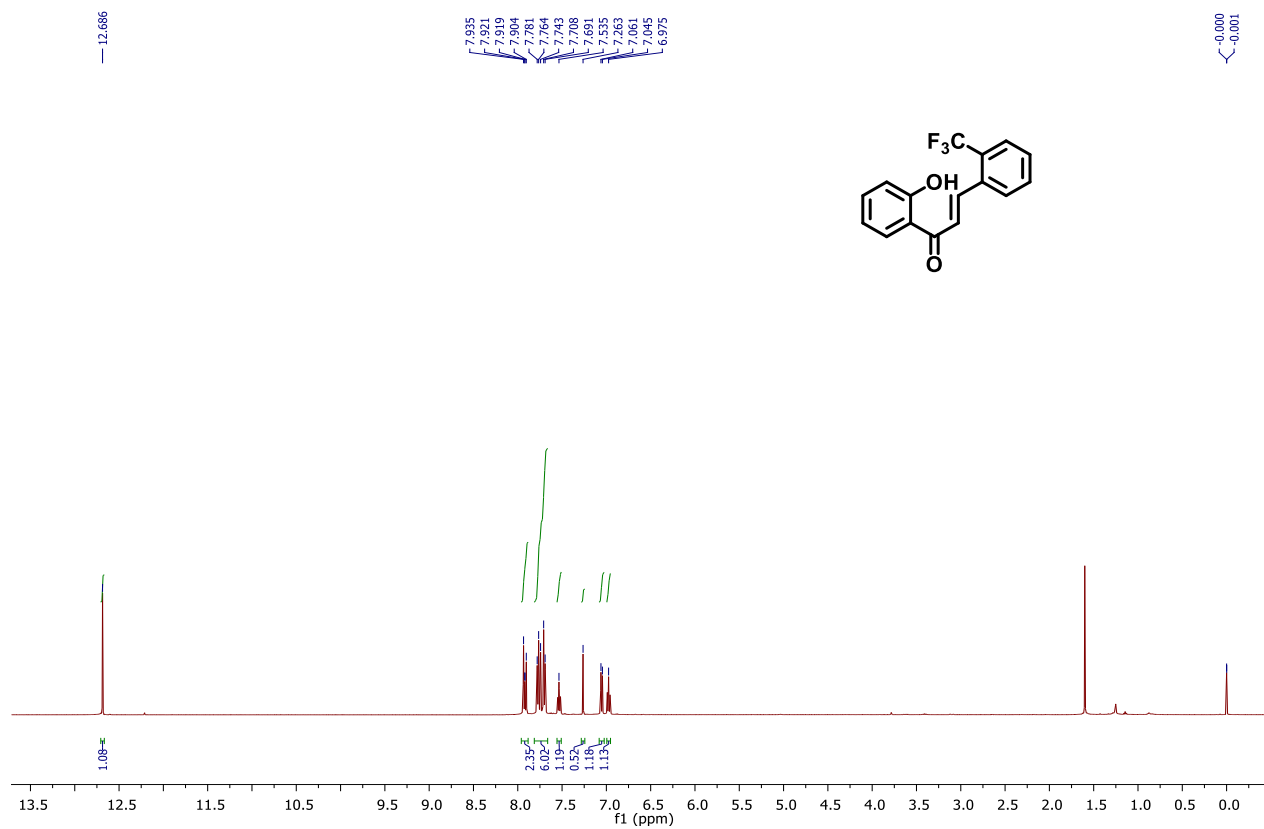
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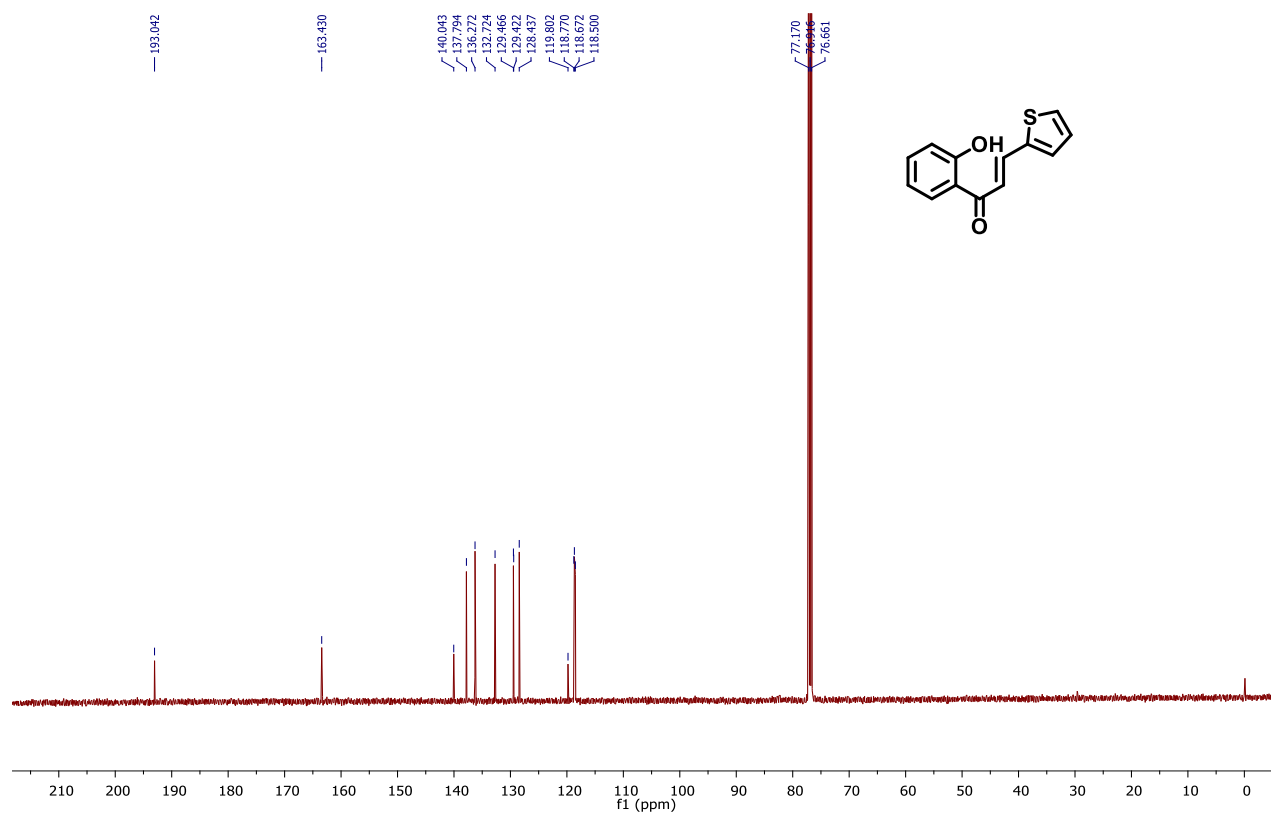
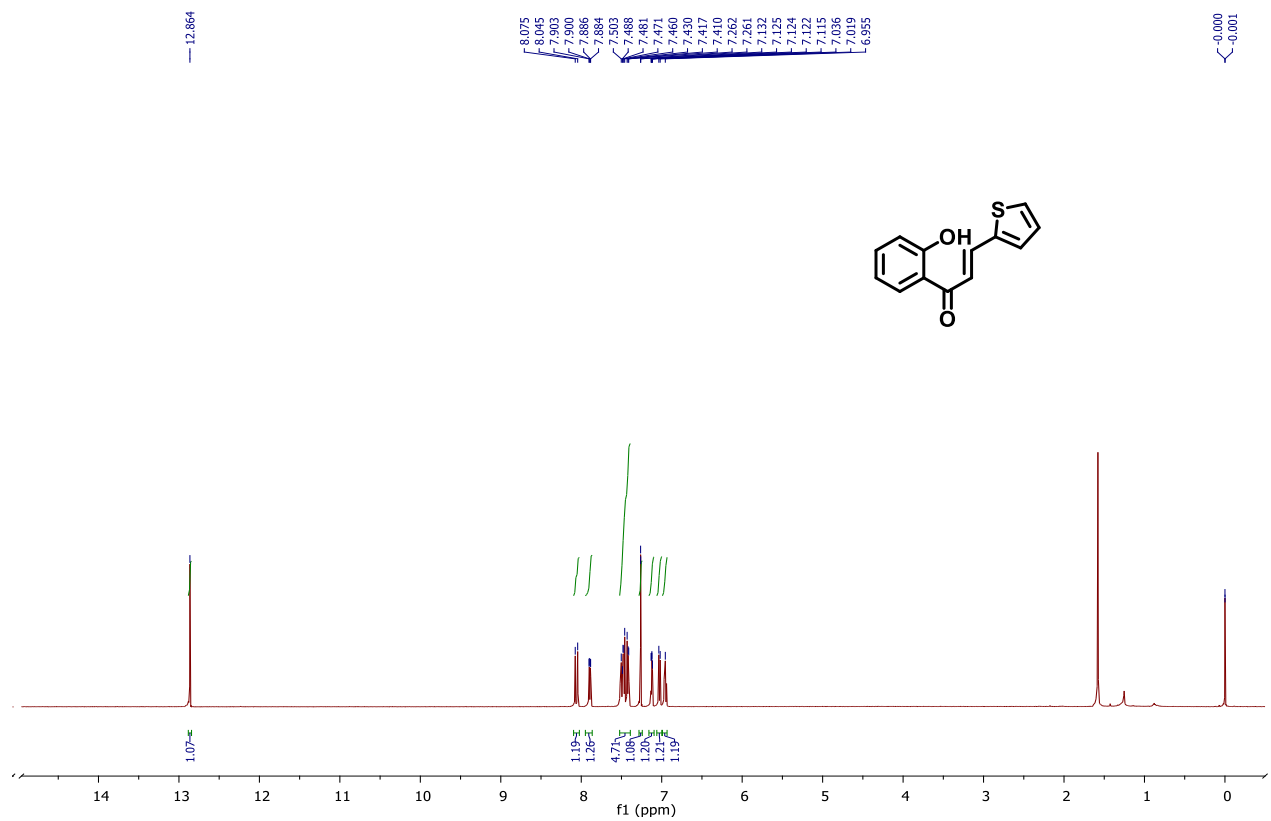
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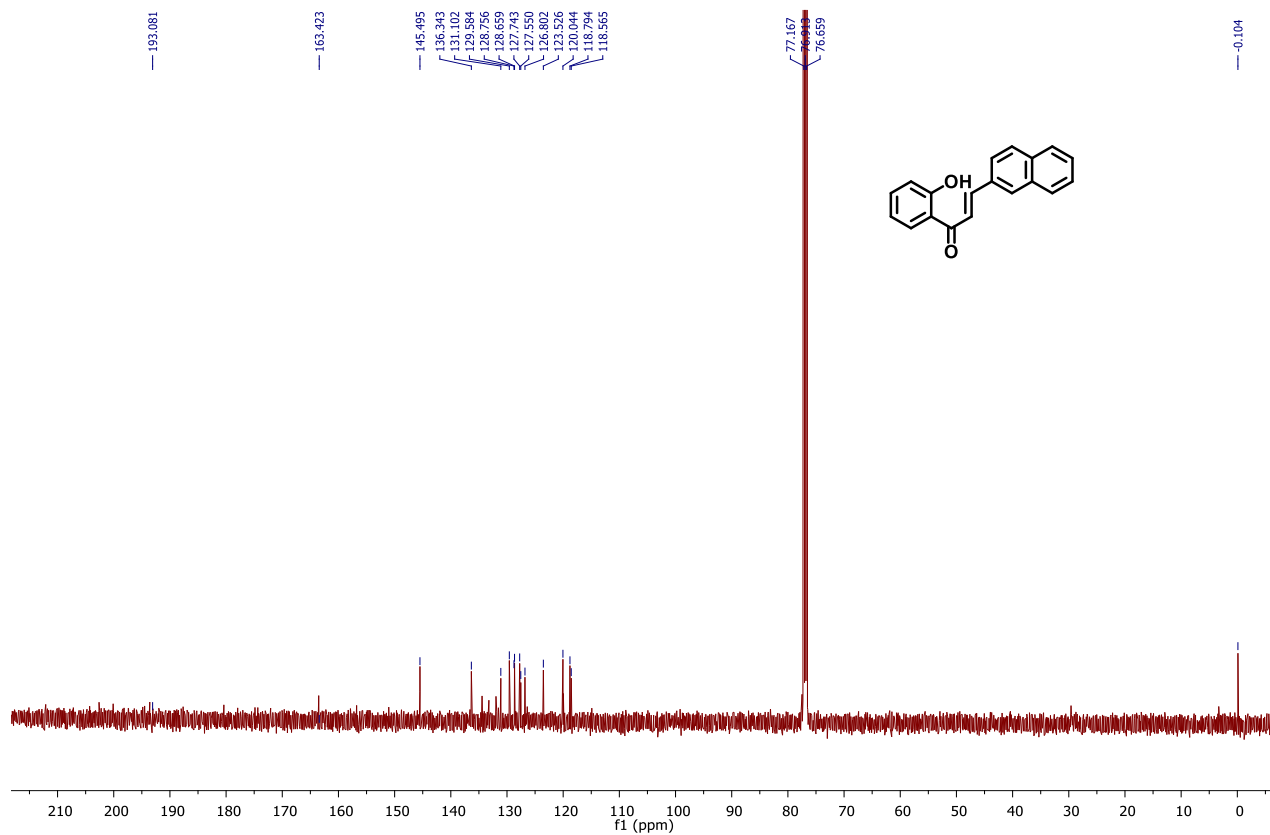
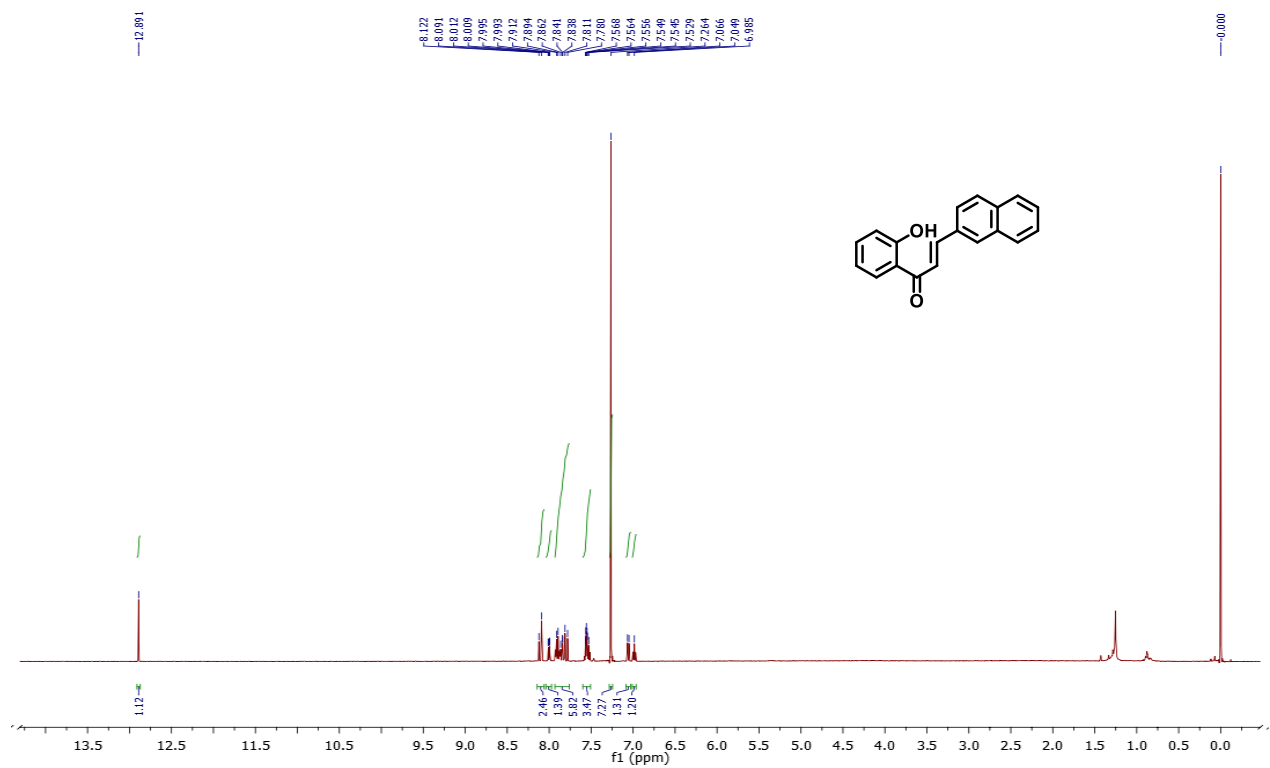
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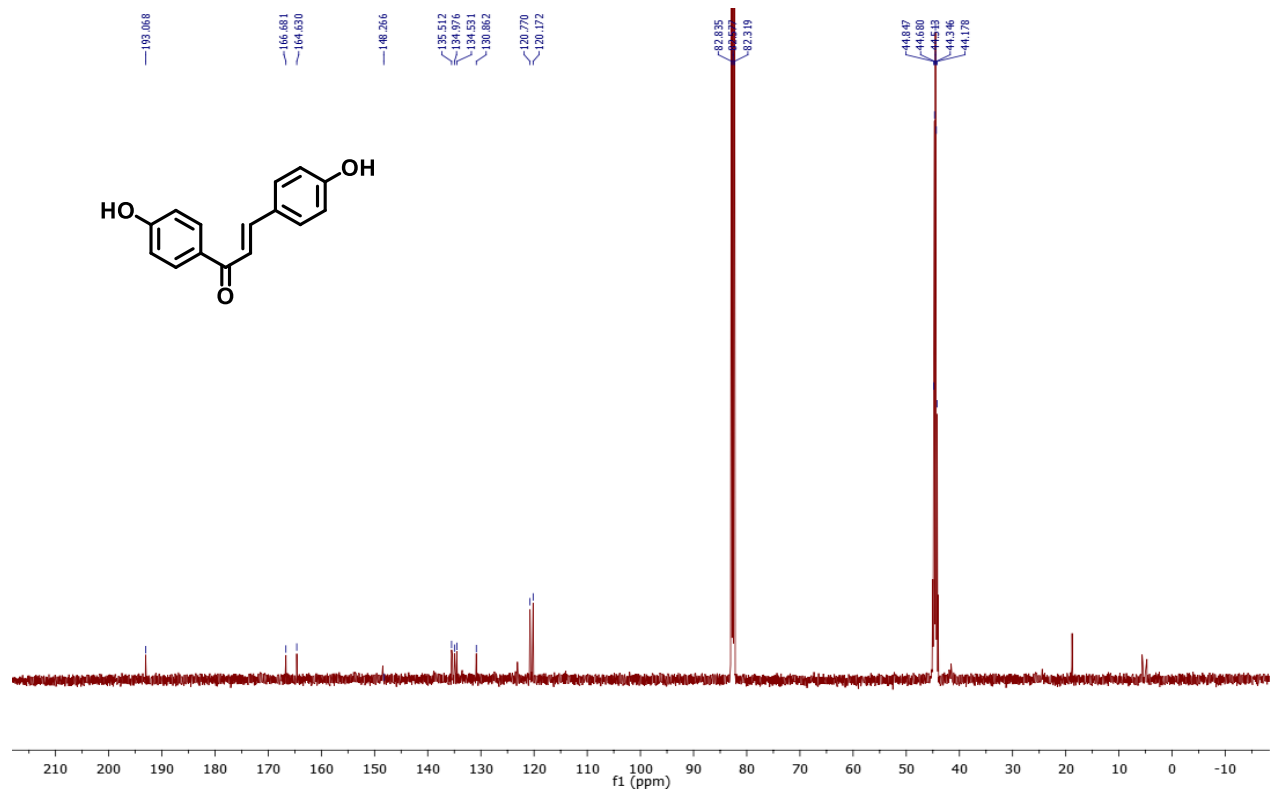
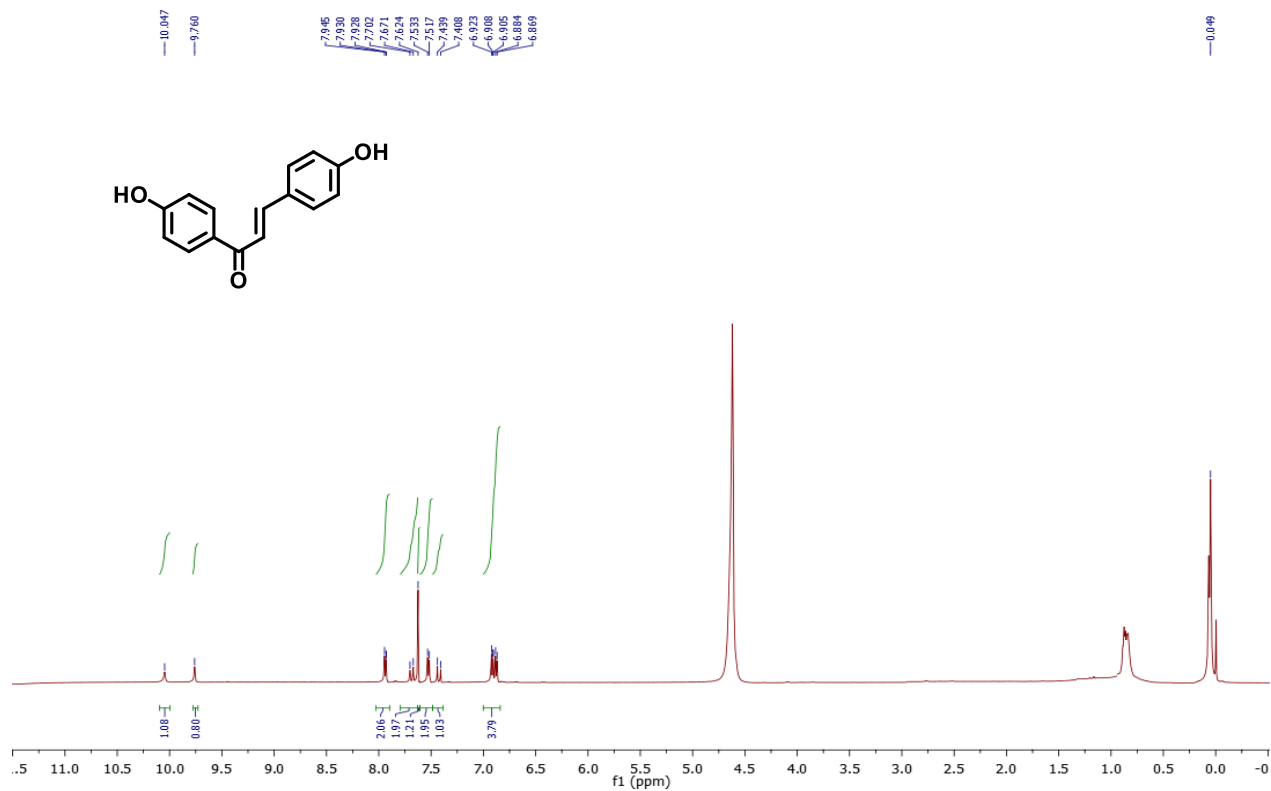
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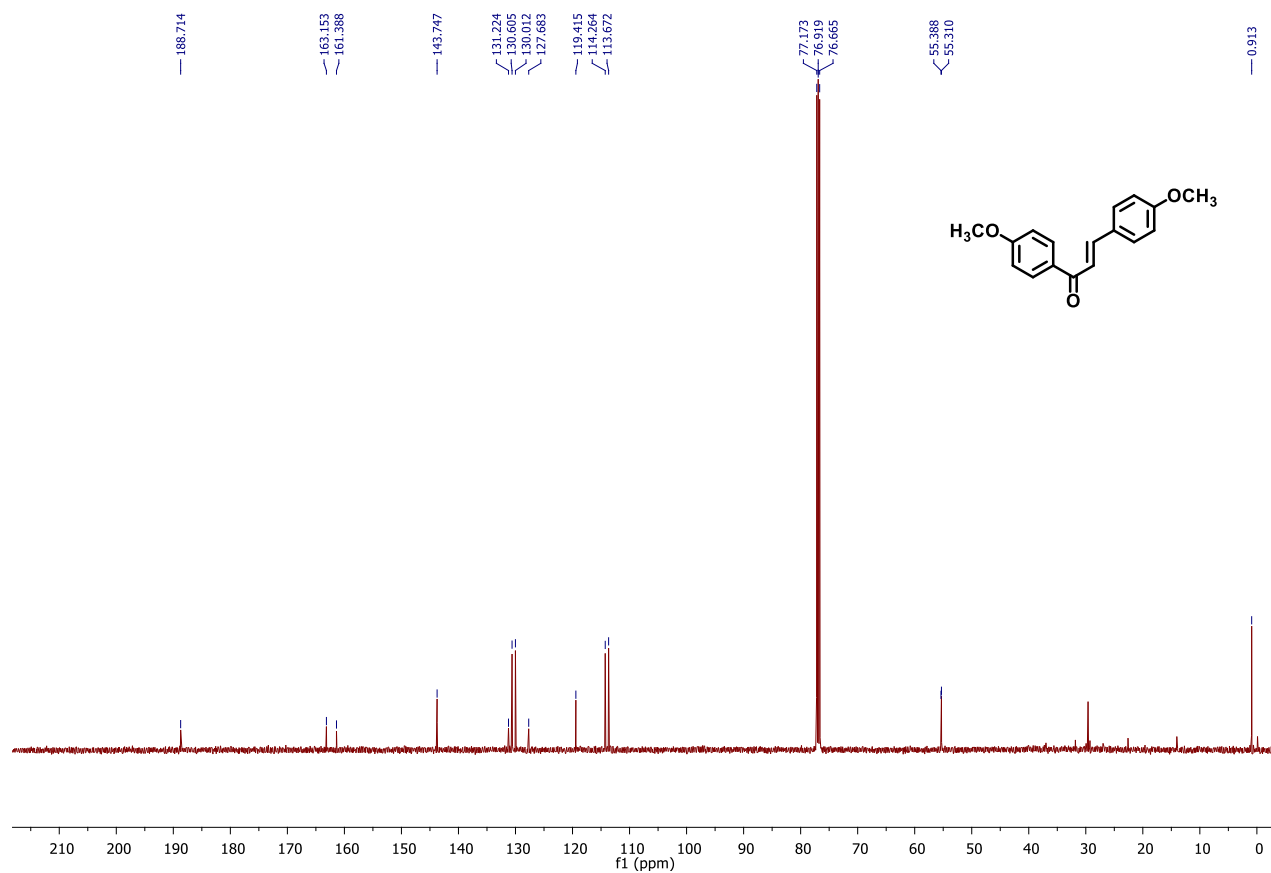
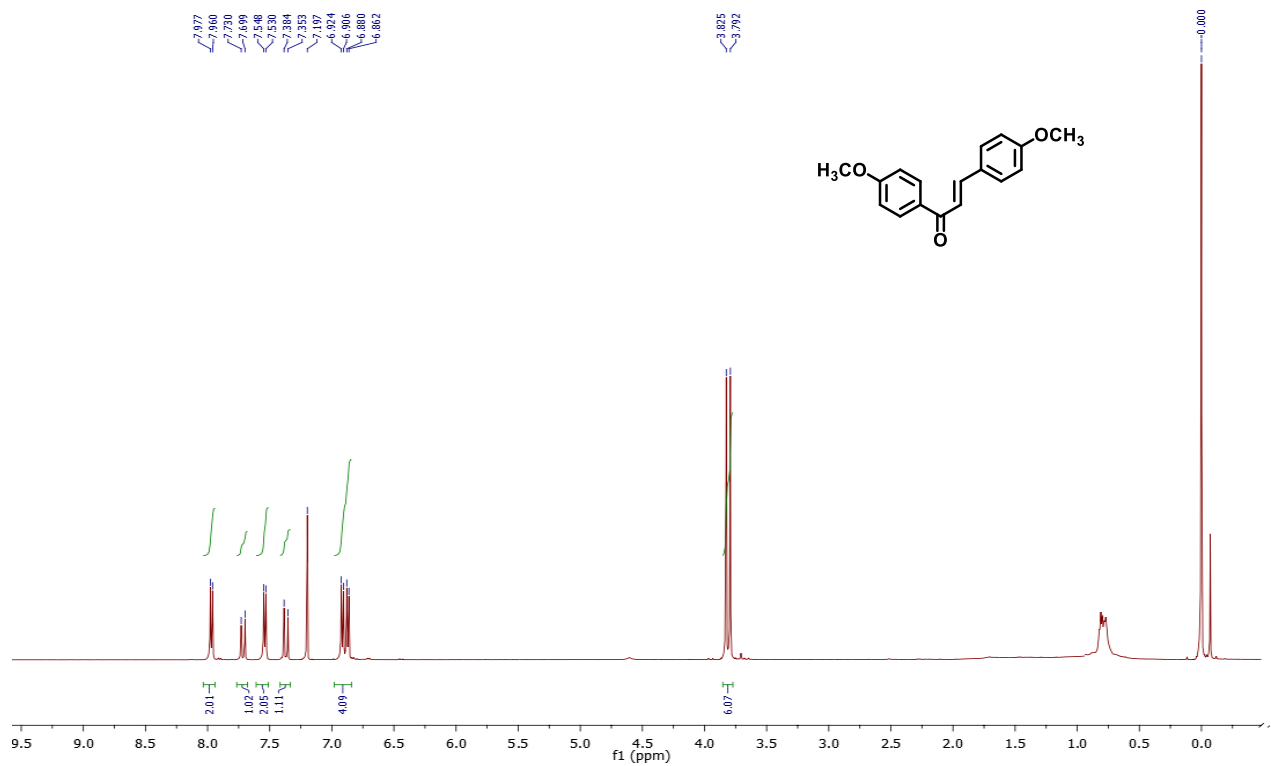
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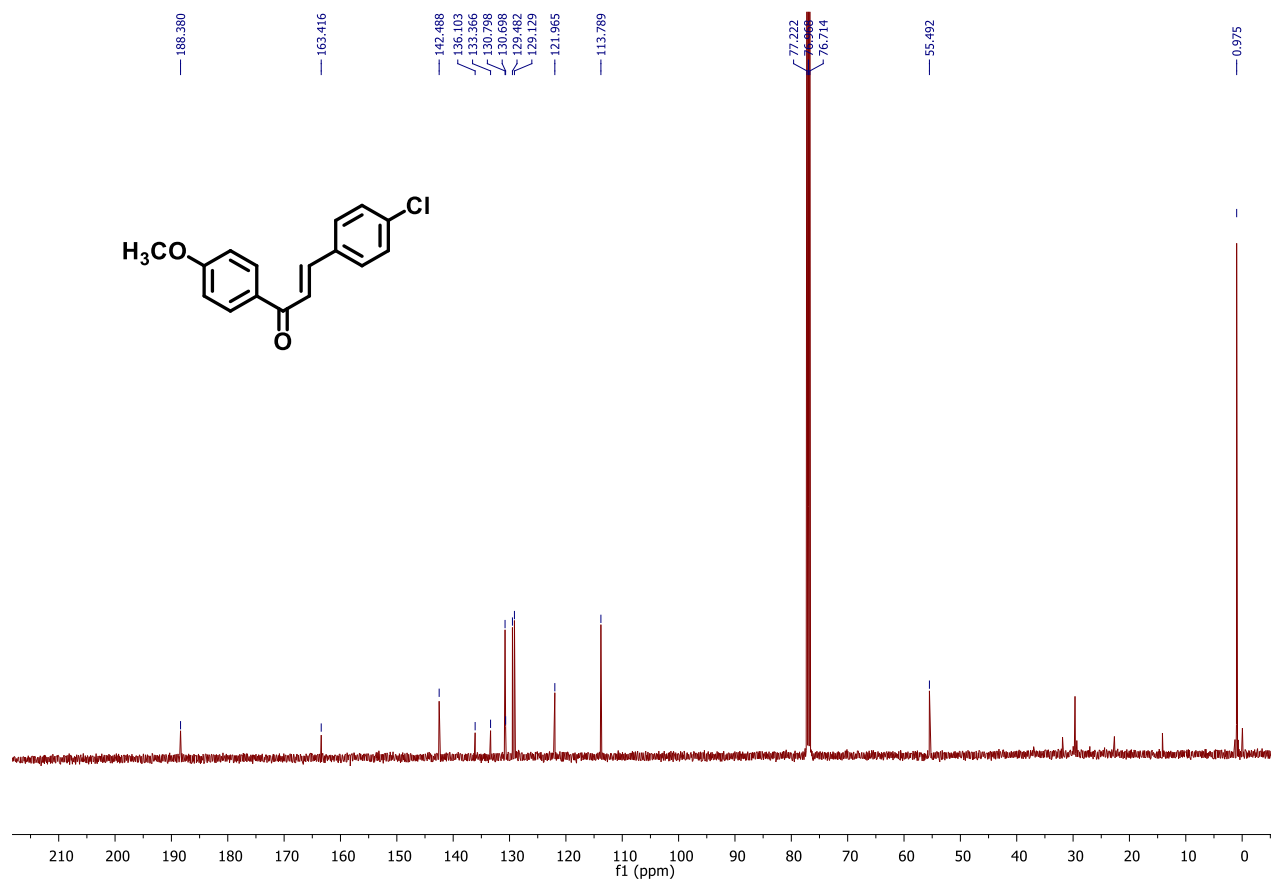
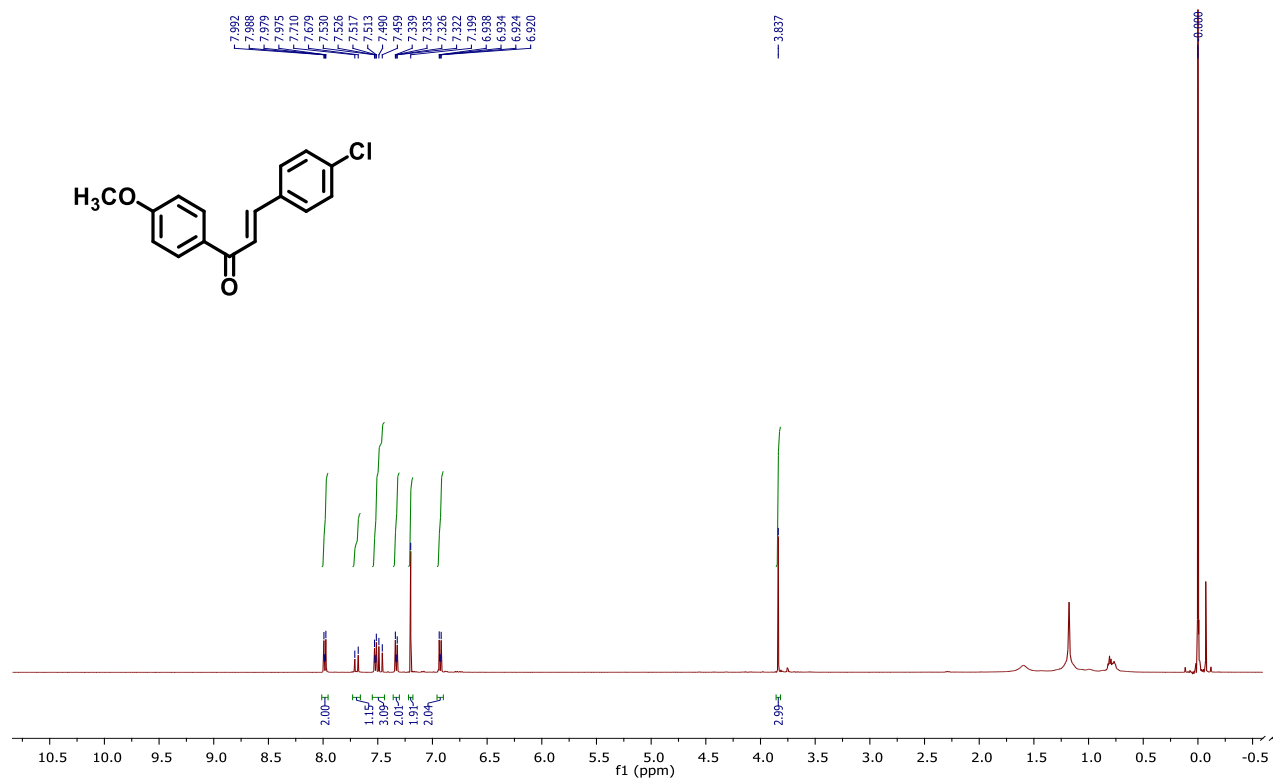
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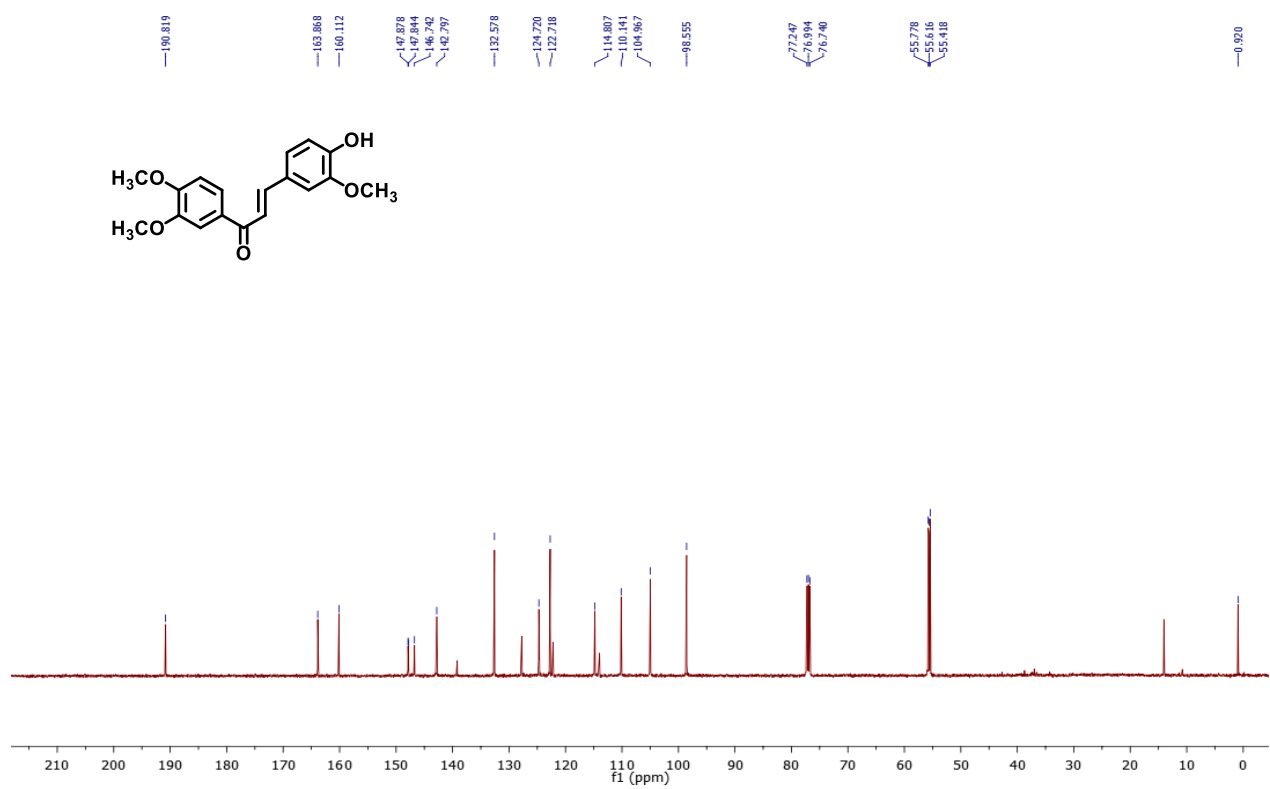
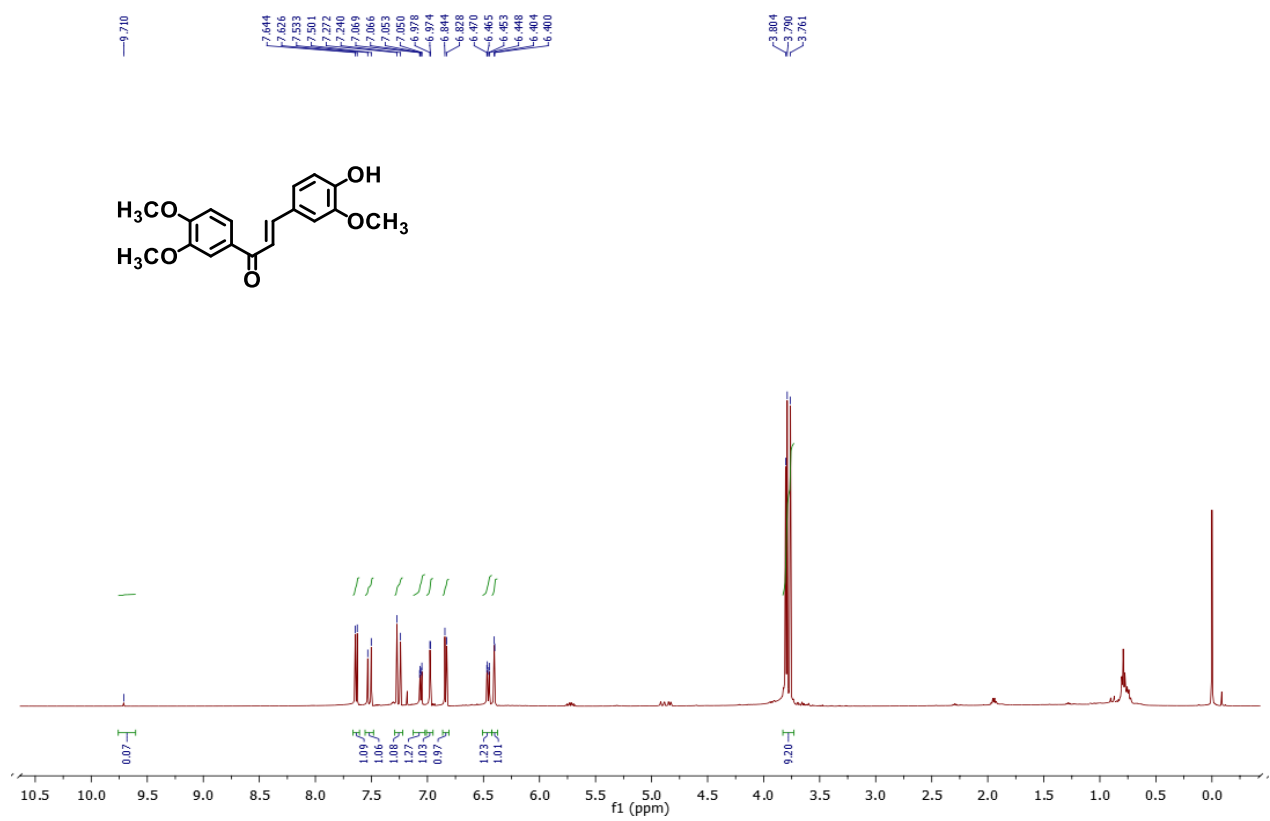
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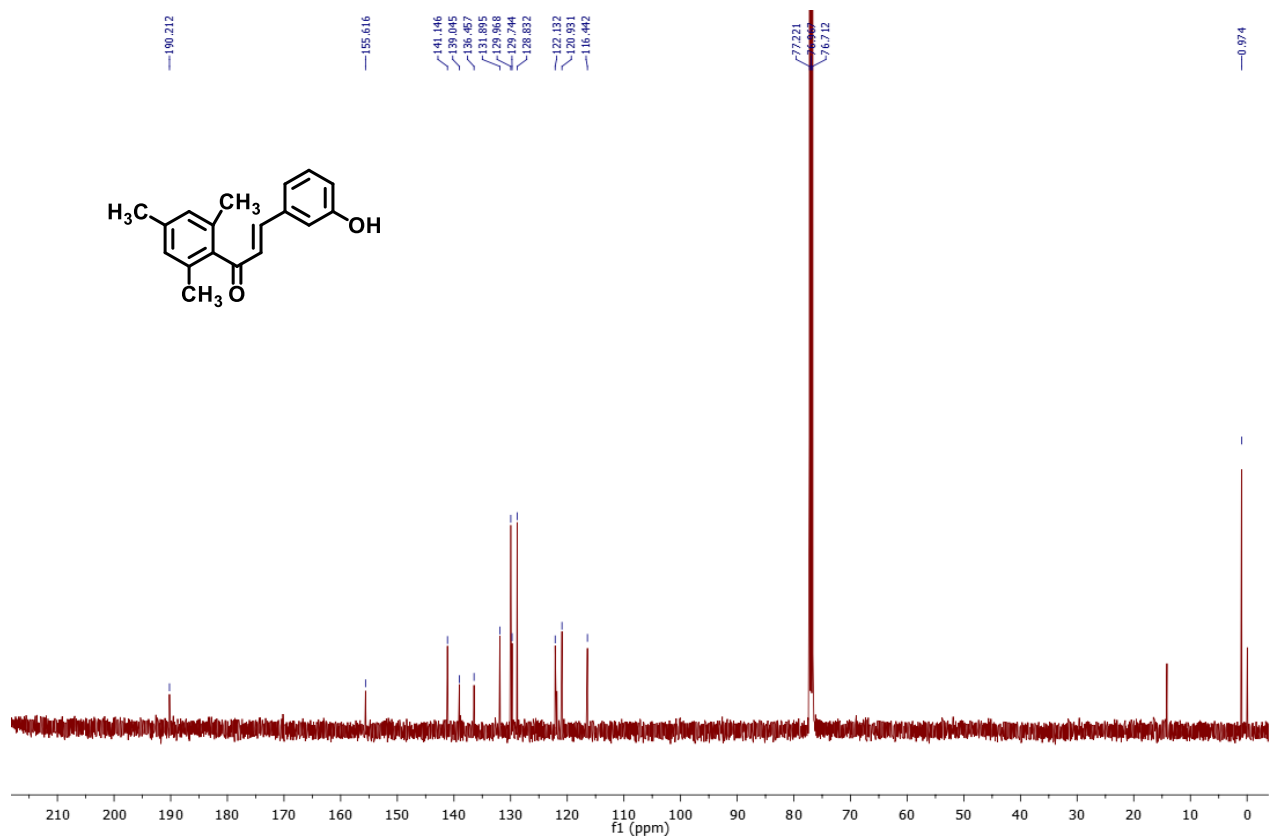
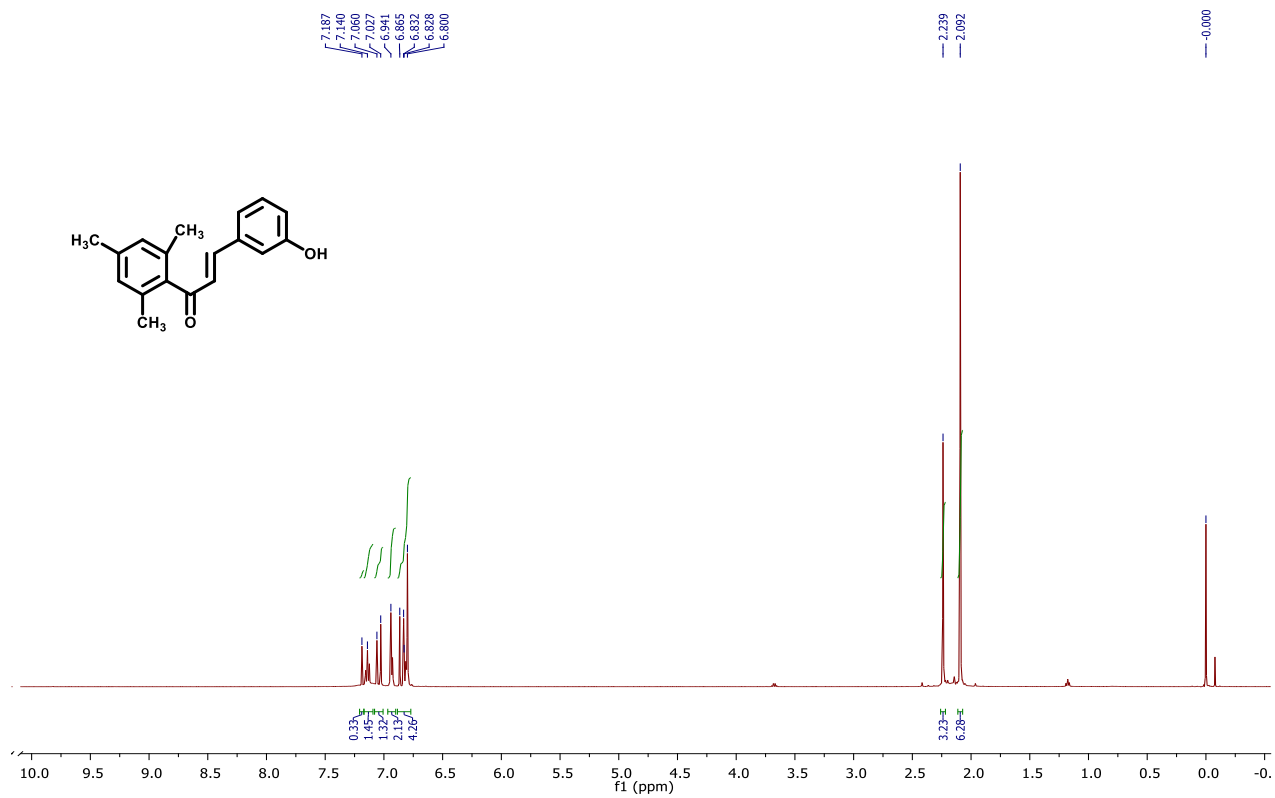
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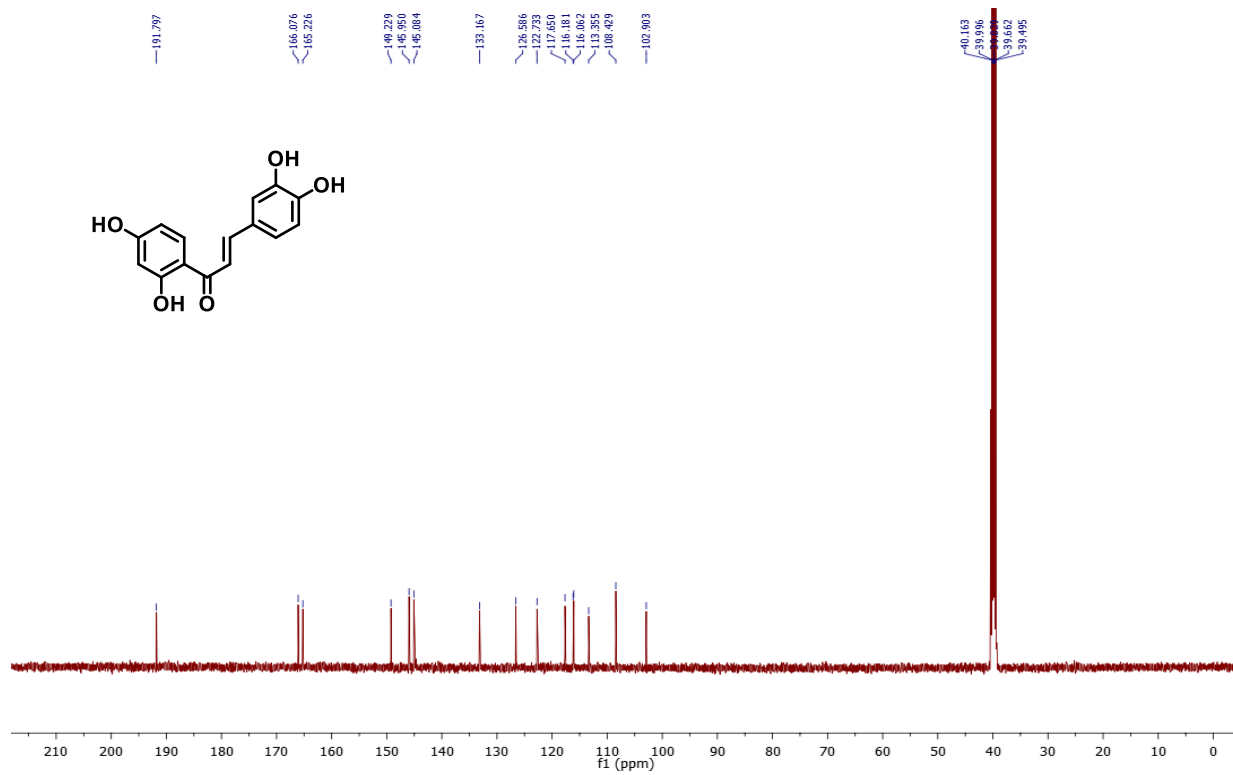
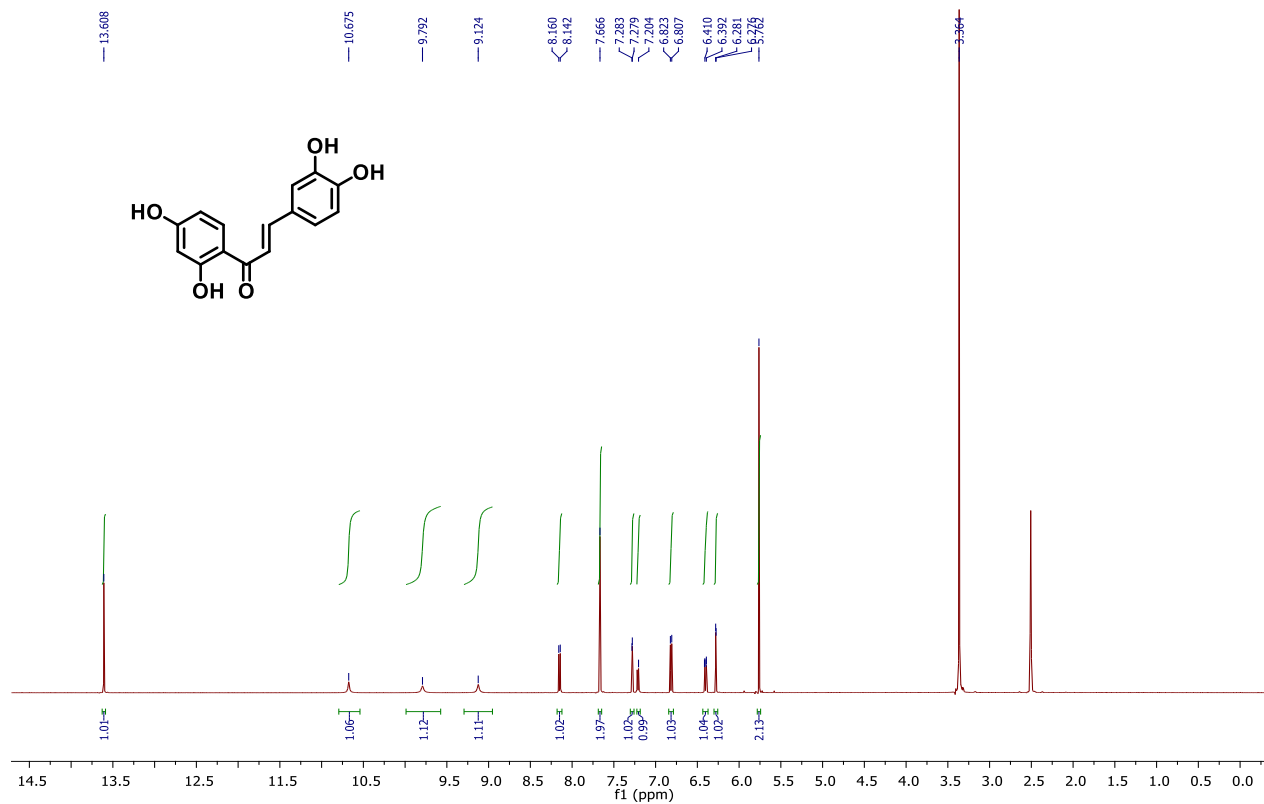
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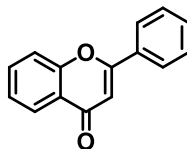
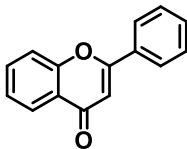
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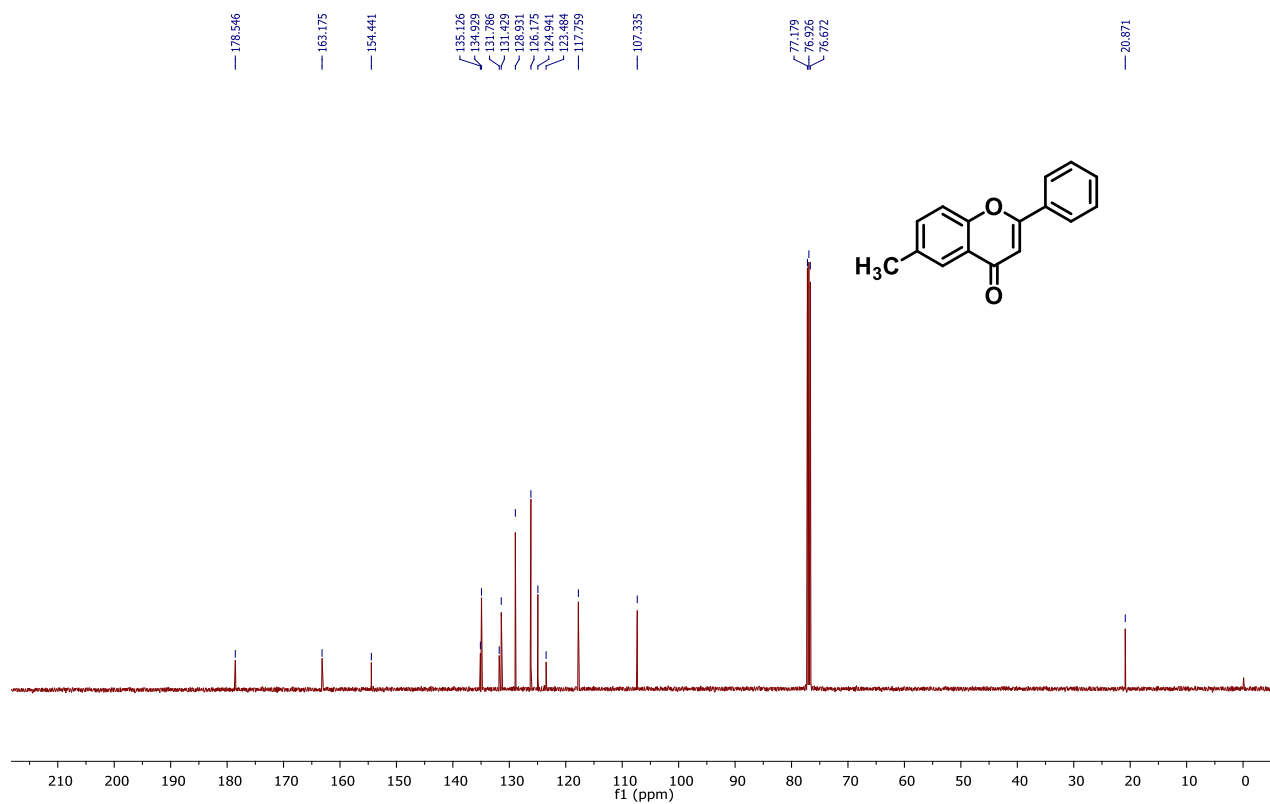
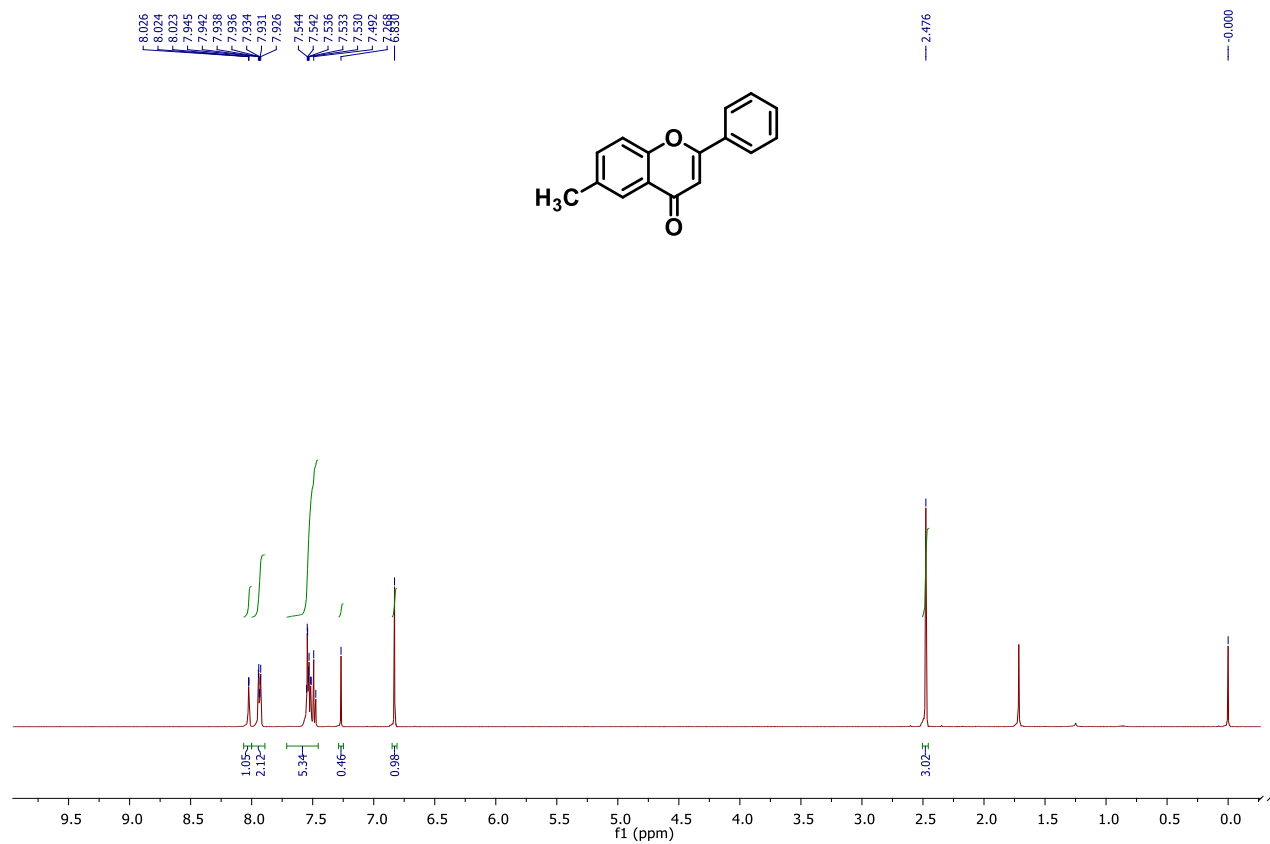


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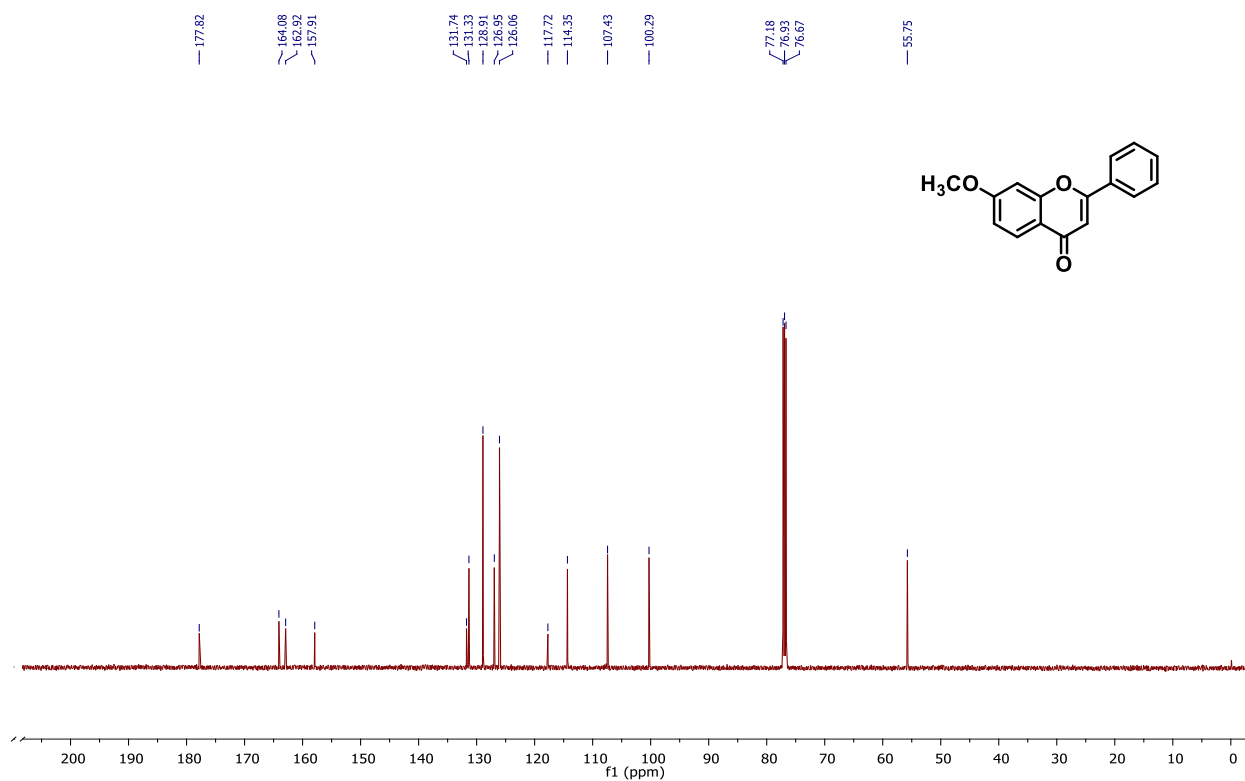
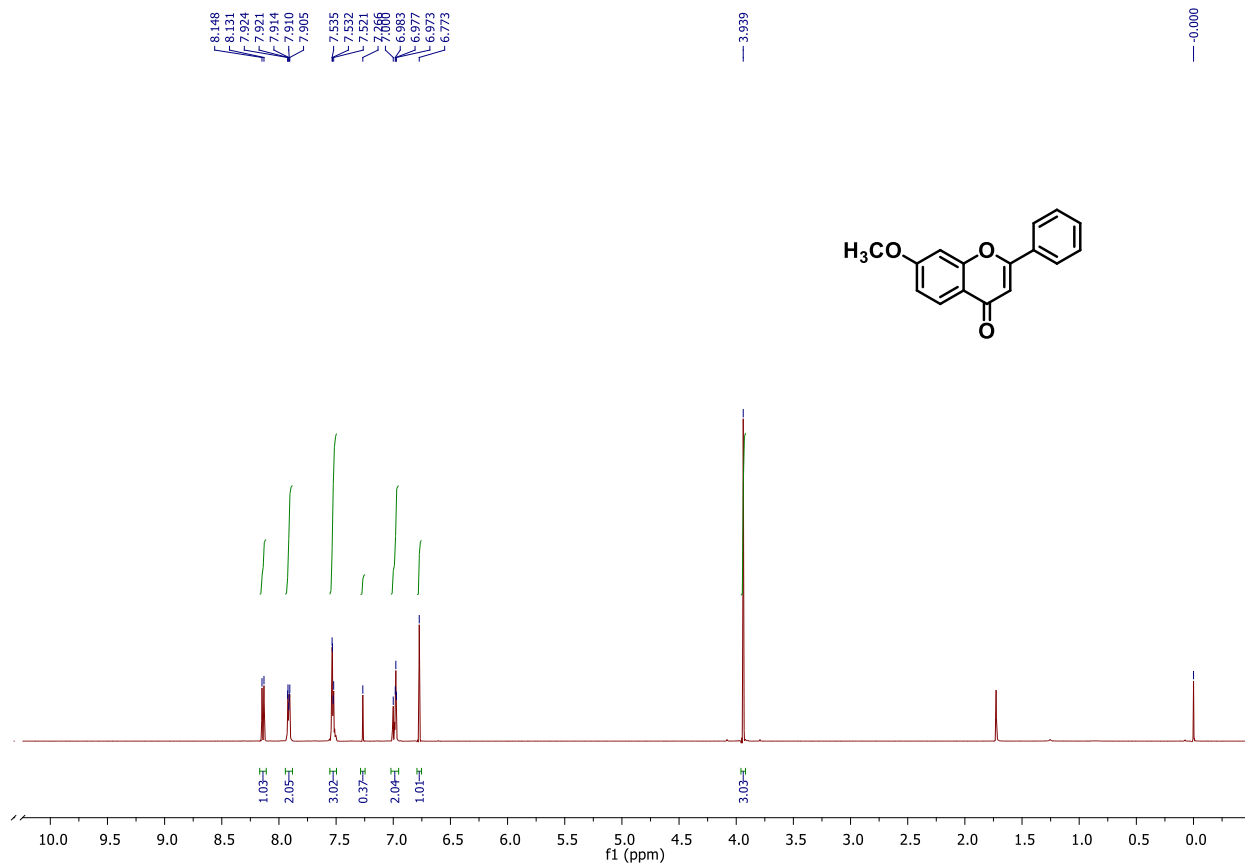


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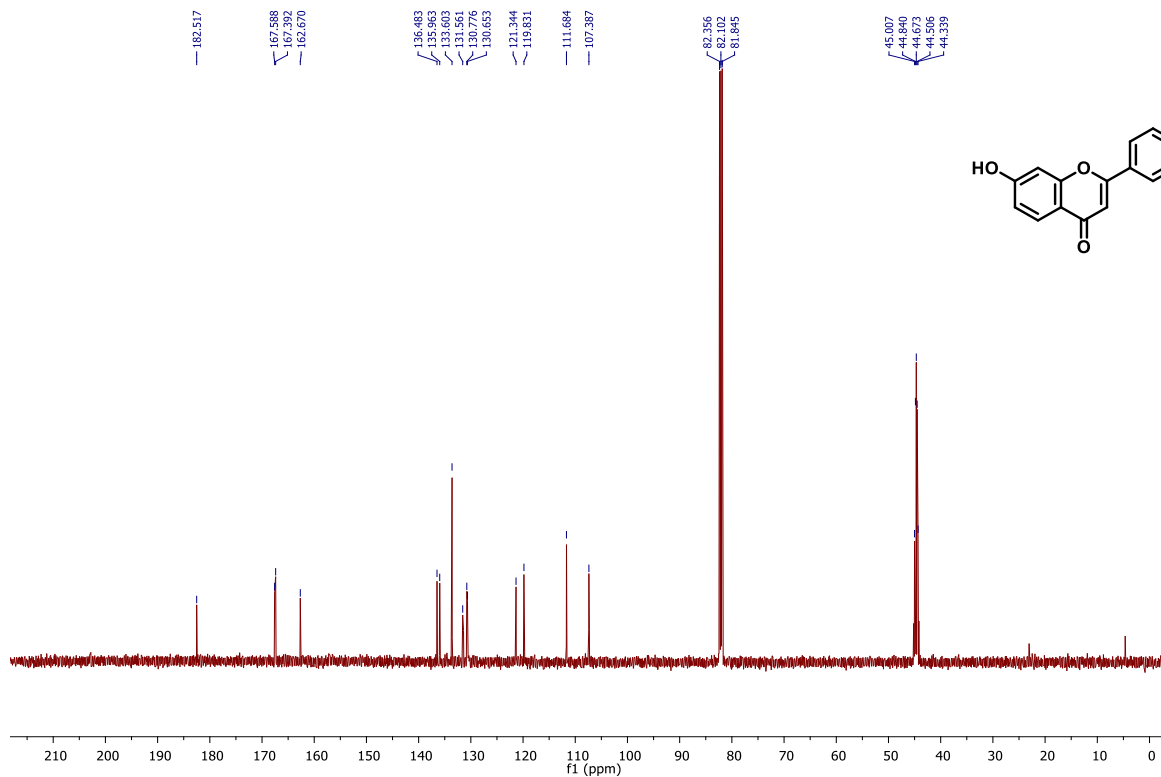
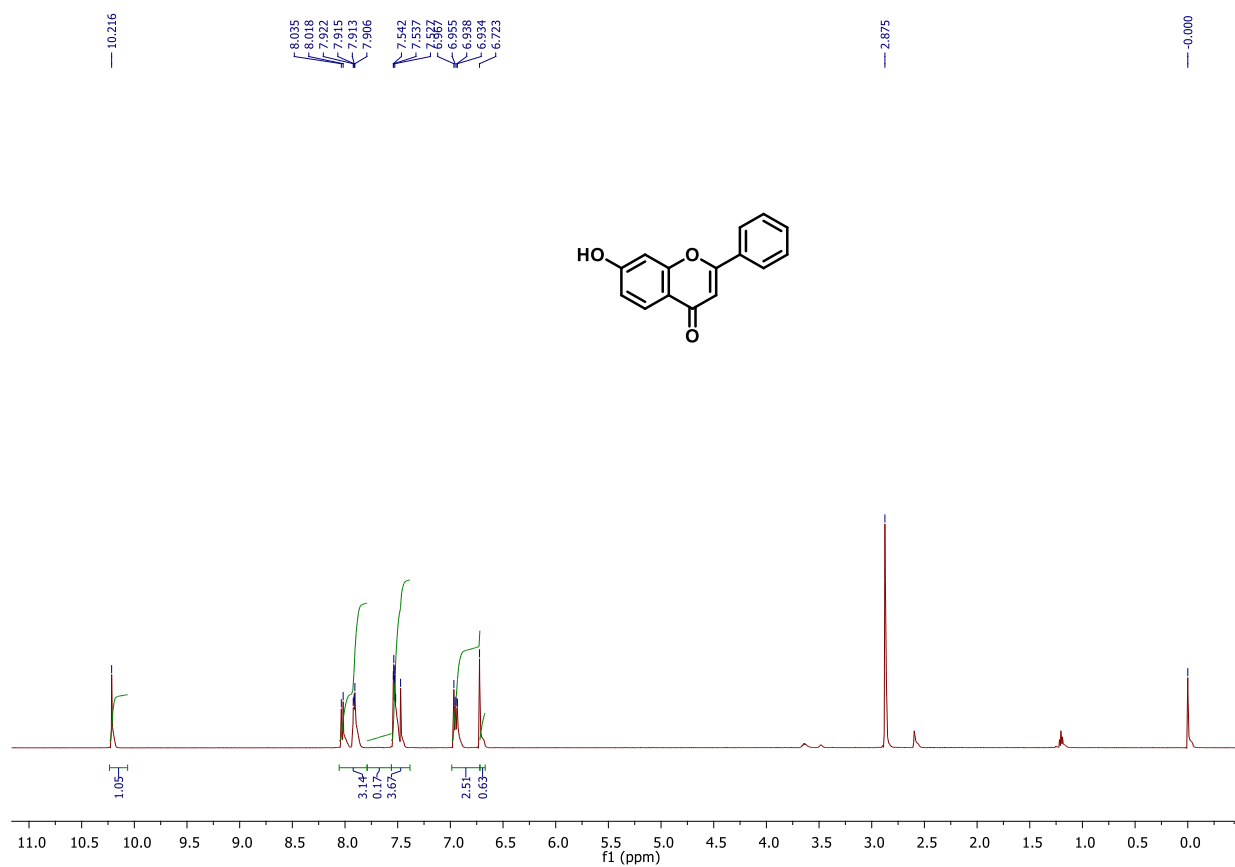




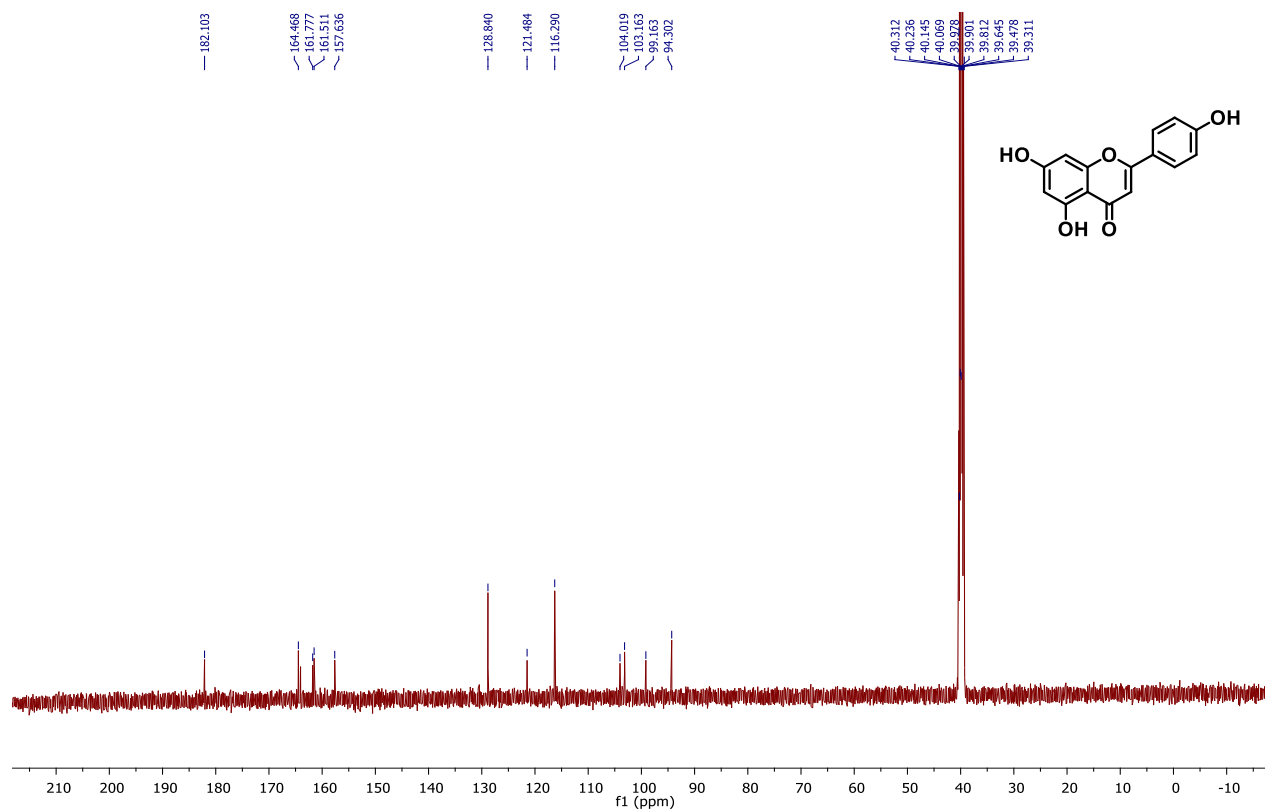
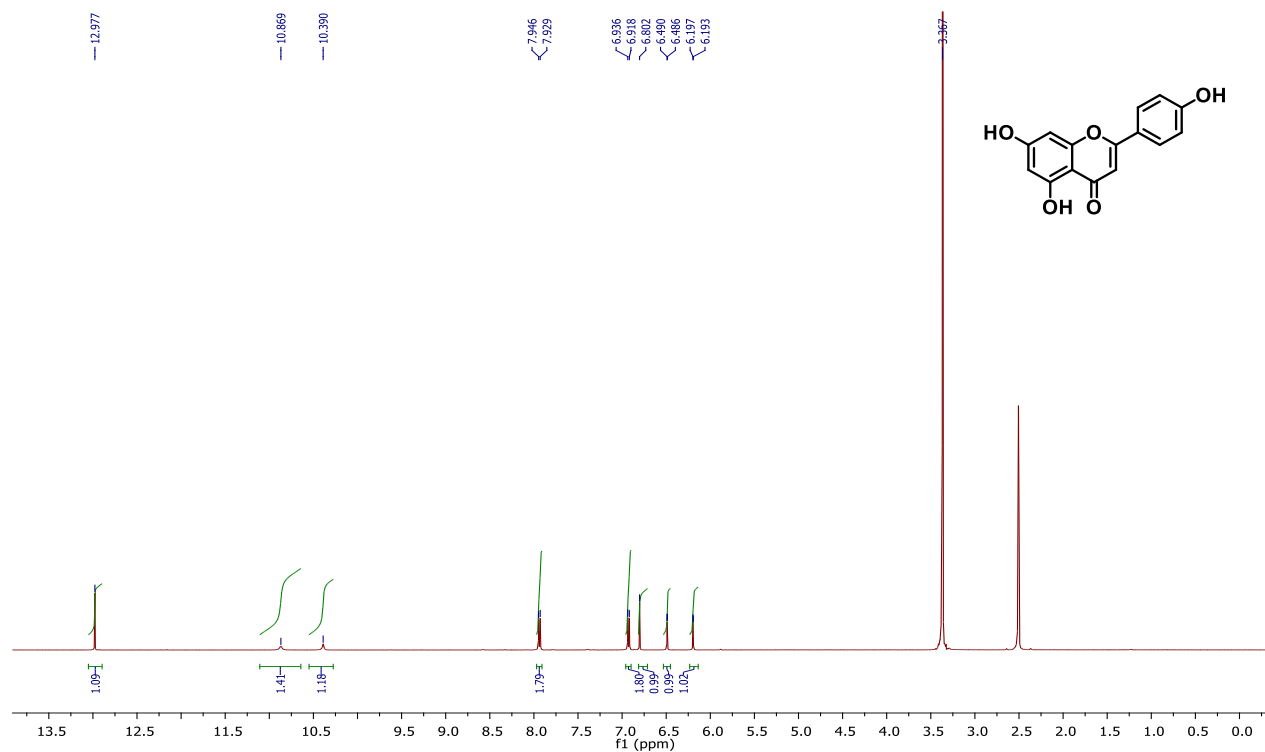
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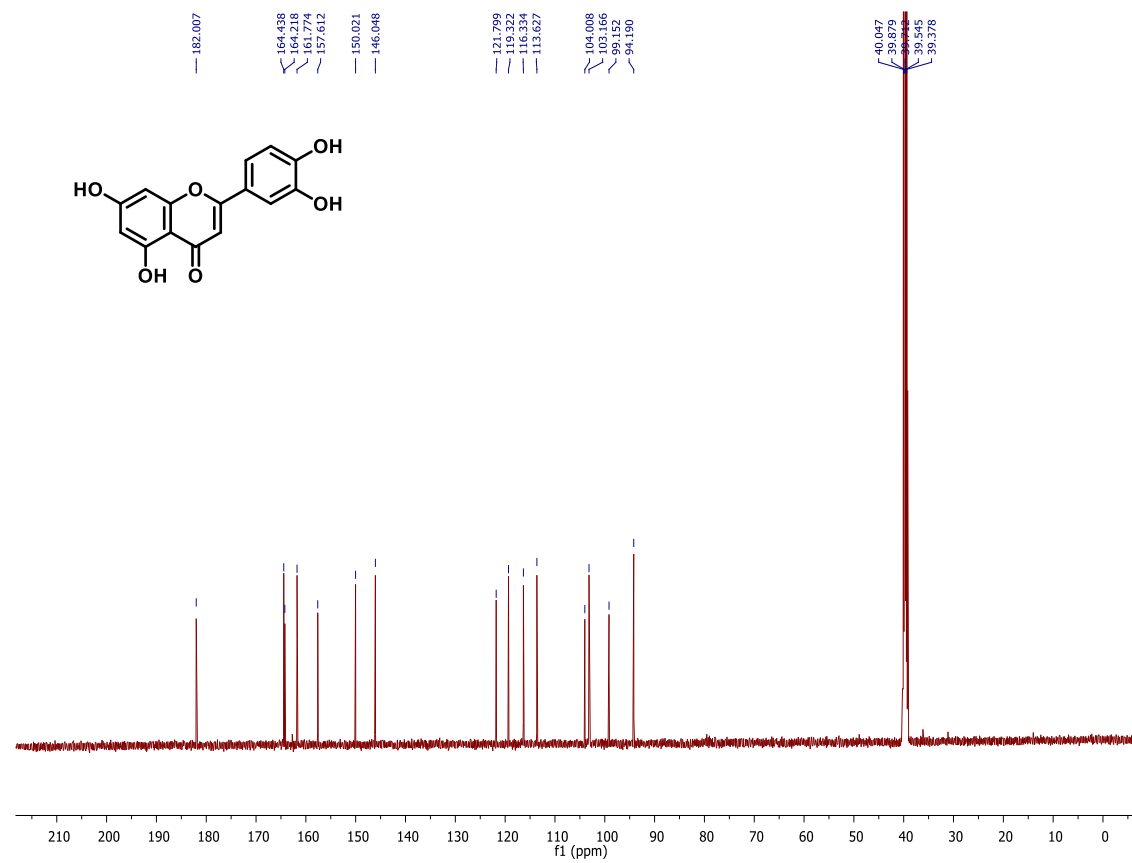
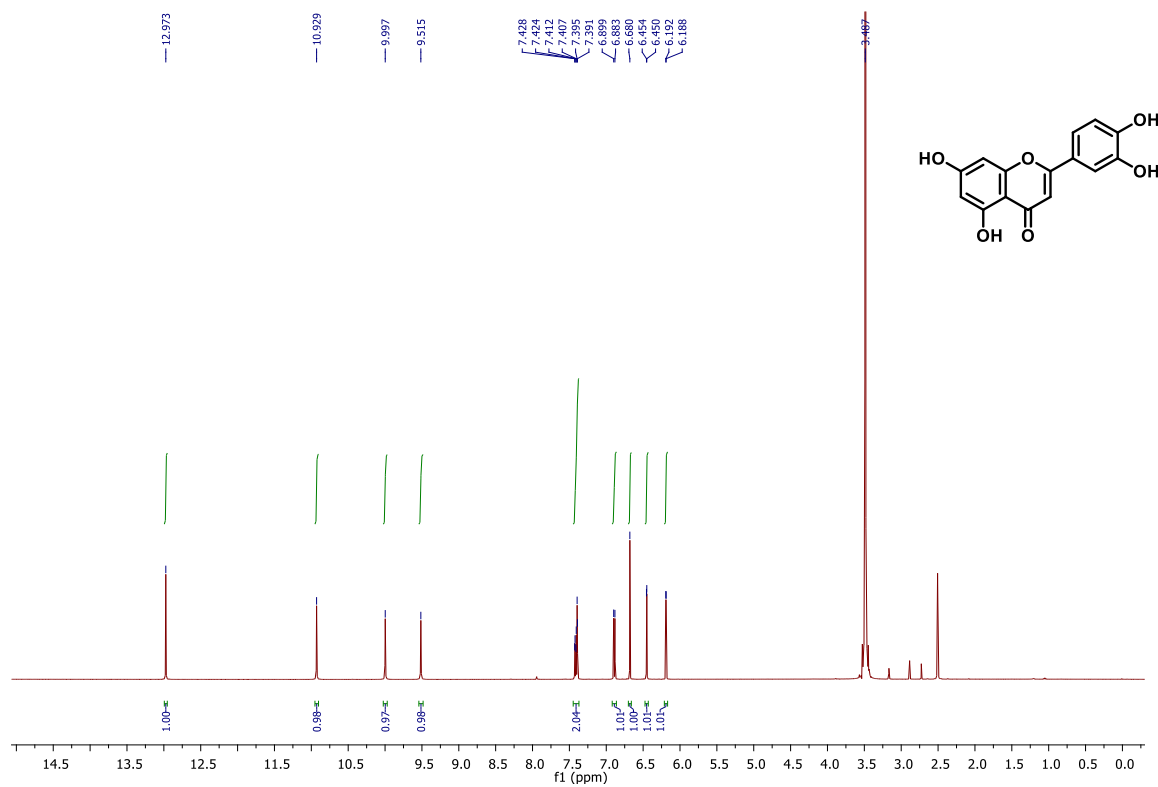
¹H and ¹³C NMR of product 4ac



¹H and ¹³C NMR of product 4ad



¹H and ¹³C NMR of product 4ae



¹H and ¹³C NMR of product 4af