SUPPORTING INFORMATION

Iron Catalyzed Tandem Ring Opening/1,6-Conjugate Addition of Cyclopropanols with *p*-Quinone Methides: New Access to γ, γ -Diaryl Ketones

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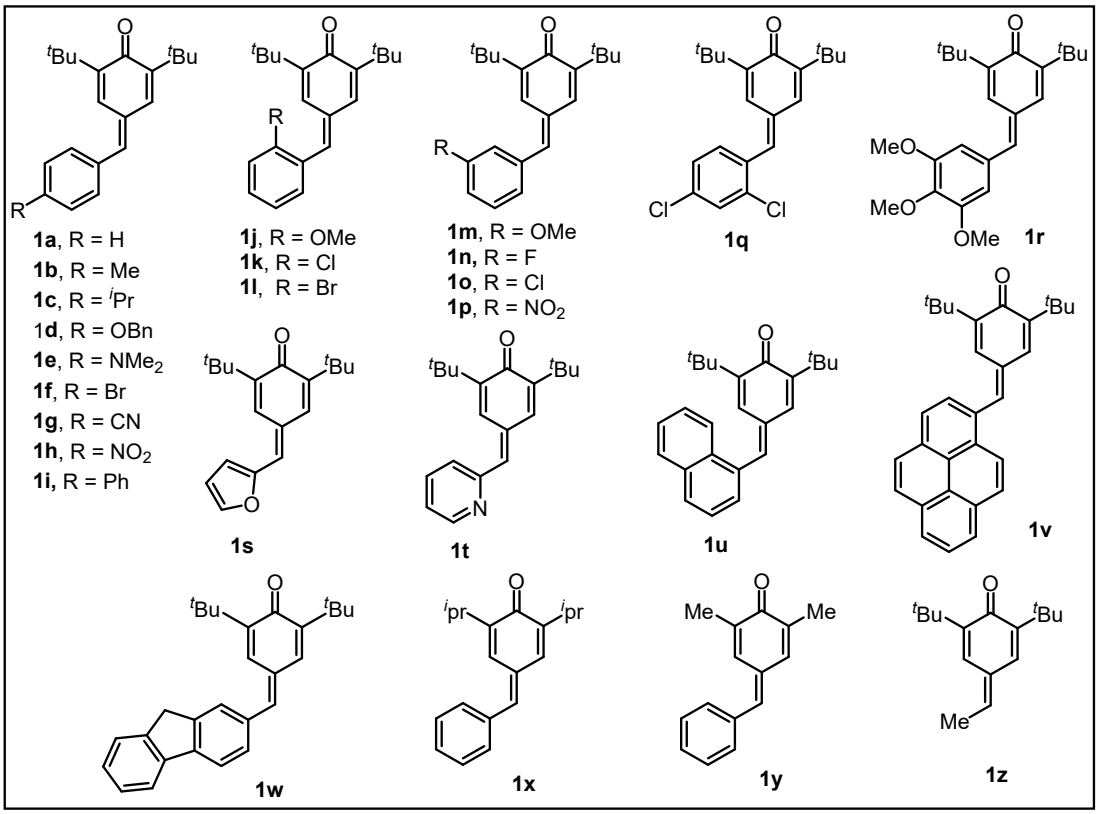
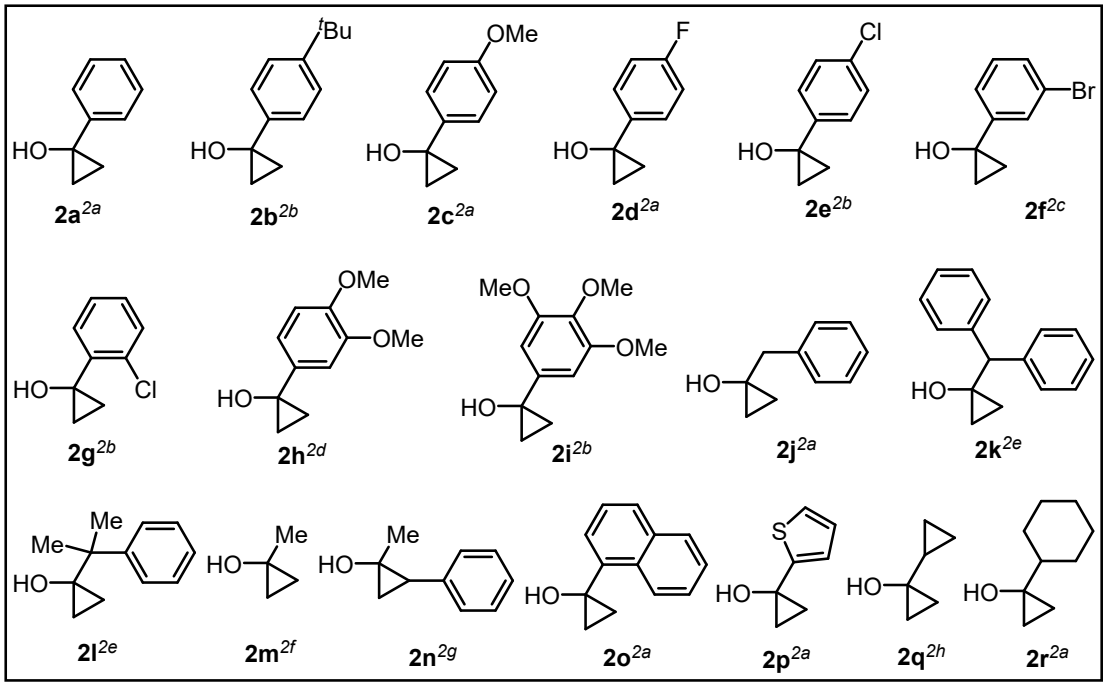
1. General information

Most of the reagents and starting materials used were purchased from commercial sources and used as such. Commercially available dry CH_3CN was used without further distillation. Melting points are uncorrected and recorded using digital Buchi Melting Point Apparatus B-540. ^{1}H, ^{13}C, DEPT and ^{19}F NMR spectra were recorded on Bruker AV 400/500, AV 100/125 & AV 376 MHz spectrometers, respectively in $CDCl_3$ using TMS as internal standard and the chemical shifts are shown in δ scale. Multiplicities of ^{1}H NMR signals are designated as s (singlet), d (doublet), dd (doublet of doublet), t (triplet), quin (quintet), spt (septet) br.s. (broad signal), m (multiplet) etc. Thin-layer chromatography was performed on Merck silica gel 60 F254 TLC plates using ethyl acetate in petroleum ether as eluent. Column chromatography was carried out through silica gel (100-200 mesh) using ethyl acetate/pet ether as eluent. High-resolution mass spectra (HRMS) data were recorded on Q Exactive Hybrid™ Quadrupole-Orbitrap™ mass spectrometer (Thermo Scientific,™ Accela 1250 pump), where the mass analyzer used for analysis is orbitrap.

2. Experimental section:

2.1 Starting materials used in this study:

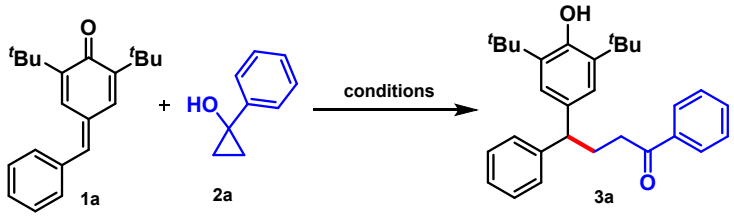




The *p*-quinone methides **1a-1z**[1] and all cyclopropanols **2a -2r**[2] were prepared according to reported literature procedures.

2.2 Optimization studies:

Table S1. Optimization of the reaction conditions[a]



entry	catalyst (mol %)	solvent (mL)	temp (°C)	time (h)	yield[b] (%)
1	$Mn(acac)_2$	CH_3CN	80	16 h	60
2	$Cu(acac)_2$	CH_3CN	80	16 h	65
3	$Pd(OAc)_2$	CH_3CN	80	16 h	NR
4	$InCl_3$	CH_3CN	80	16 h	20
5	$Fe(OAc)_2$	CH_3CN	80	16 h	69
6	$Fe(OTf)_3$	CH_3CN	80	5 h	79
7	$FeCl_3$	CH_3CN	80	5 h	94
8	$Fe(NO_3)_3.9H_2O$	CH_3CN	80	5 h	54
9	**$Fe(acac)_3$**	**CH_3CN**	**80**	**5 h**	**97**
10	$Fe(acac)_3$	DCE	80	5 h	86
11	$Fe(acac)_3$	Toluene	80	5 h	81
12	$Fe(acac)_3$	THF	80	5 h	76
13	$Fe(acac)_3$	DMF	80	5 h	80
14	$Fe(acac)_3$	1,4-dioxane	80	5 h	18
15	$Fe(acac)_3$	CH_3CN	80	5 h	68[c]
16	$Fe(acac)_3$	CH_3CN	60	5 h	65
17	$Fe(acac)_3$	CH_3CN	RT	24 h	NR
18	--	CH_3CN	80	5 h	NR

[a]Unless otherwise noted, all reactions were performed with **1a** (0.17 mmol), **2a** (0.25 mmol), 10 mol % of catalyst in a solvent (2 mL). [b]Isolated yield. [c]5 mol % of catalyst was used. NR = No reaction.

2.3 Experimental procedures:

I) General procedure for the preparation of cyclopropanols:

Cyclopropanols **2a-2m**, **2q** and **2r** were prepared according to procedure A and cyclopropanols **2o** and **2p** were prepared by following procedure B.

a) Procedure A: Kulinkovich reaction: Ethylmagnesium bromide (2.8 equiv, 2M in THF) in THF was added dropwise over 30 min at 0 °C to a solution of ester (1.0 equiv) and titanium isopropoxide (1.4 equiv) in THF under argon. The mixture was warmed to room temperature and stirred overnight. The reaction was quenched with water and the precipitated solid was removed by filtration. The filtrate was extracted with ethyl acetate (3 × 30 mL), washed with water, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash column chromatography to afford the cyclopropanols **2a-2m**, **2q** and **2r**.

b) Procedure B: Simmons–Smith reaction:

Step 1: An oven-dried round-bottom flask equipped with a stir bar was added sodium iodide (1.4 equiv) and the flask was flame-dried and cooled under vacuum. The flask was backfilled with argon and MeCN (20 mL) was added, followed by the desired ketone (1.0 equiv). The solution was cooled to 0 ºC, and TMSCl (1.3 equiv) was added, followed by triethylamine (1.5 equiv). The reaction was stirred at 0 ºC for 1 h under argon. The reaction mixture was extracted with hexane (3 × 30 mL). The combined organic layers were washed washed with water, brine, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure to yield the crude silyl enol ether.

Step 2: An oven-dried round-bottom flask equipped with a stir bar was transferred the crude silyl enol ether (1.0 equiv) under the argon. The flask was charged with anhydrous DCM (20 mL) and diiodomethane (1.2 equiv). The resulting solution was cooled to 0 ºC using an ice bath. Diethylzinc (1.2 equiv, 1.0 M in heptane) was added dropwise over 10 min. The reaction was stirred at 0 ºC for 1 h, then at room temperature until the complete conversion of the silyl enol ether was achieved as determined by TLC. The reaction was quenched with sat. $NaHCO_3$ and extracted with DCM (3 × 30 mL). The combined organic layers were washed washed with water, brine, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure to yield the crude trimethylsilyl cyclopropanol.

Step 3: An oven-dried round-bottom flask equipped with a stir bar was transferred the crude trimethylsilyl cyclopropanol, and MeOH (20 mL) was added. The solution was cooled to 0 ºC and TMSCl (1 drop from a 1-mL syringe) was added. The reaction was stirred at 0 ºC for 5 min. After completion, the resulting mixture was evaporated under vacuum. The residue was purified by

column chromatography on silica gel using petroleum ether/ethyl acetate to yield the desired cyclopropanols **2o** and **2p.**

Procedure for the synthesis of 2n: Titanium isopropoxide (1.36 g, 1.45 mL, 4.8 mmol, 1.0 equiv) was added to a flame dried flask at room temperature under argon. Anhydrous THF (20 mL) was added to the flask, followed by the styrene (0.5 g, 4.8 mmol, 1.0 equiv) and EtOAc (0.69 mL, 7.2 mmol, 1.5 eq). Then freshly prepared cyclohexyl magnesium bromide (19 mL, 19.2 mmol, 4 equiv, ~1M in THF) was added dropwise over the period of 1 h at 25 ºC. The reaction was stirred overnight at room temperature, diluted with EtOAc (50 mL) and poured into NH_4Cl (50 mL). The mixture was stirred vigorously for 0.5 h to break up the emulsion and then filtered through celite. The layers were separated and the aqueous layer was extracted twice with EtOAc (3 × 50 mL). The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4, and concentrated under reduced pressure. The residue was purified by flash column chromatography to yield the desired cyclopropanols **2n**.

II) General procedure for the synthesis of γ, γ -Diaryl Ketones (3/4):

To a 5 mL oven dried screw-capped vial equipped with a magnetic stir bar were added *p*-Quinone methide **1** (0.34 mmol), cyclopropanol derivative **2** (0.51 mmol), $Fe(acac)_3$ (10 mol%) and anhydrous CH_3CN (2.0 mL) under argon atmosphere at room temperature. The resultant reaction mixture was kept stirring at 80 °C for 8 h. After completion, the resulting mixture was evaporated under vacuum. The residue was purified by column chromatography on silica gel using petroleum ether/ethyl acetate to give the products **3/4**.

III) Procedure for Product Transformations:

a) Procedure for the synthesis of 5: To a solution of **3a** (0.100 g, 0.233 mmol) in benzene (3 mL) was added $AlCl_3$ (0.155 g, 1.166 mmol) under an argon atmosphere, and the resulting mixture was stirred at room temperature for 16 h. The reaction mixture was then quenched with 10 mL of ice-cold water and extracted with ethyl acetate (3 × 10 mL). The combined organic layers were dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was subjected to column chromatography on silica gel using a petroleum ether/ethyl acetate = 20:1 mixture as an eluent to afford **5** as a yellow solid (0.066 g, 89%).

b) Procedure for the synthesis of 6: To an oven-dried 25 mL round-bottom flask equipped with a stir bar was added **3a** (0.100 g, 0.233 mmol) and 10% palladium on carbon (33.9 mg, 0.32 mmol), then MeOH (8 mL) and EtOAc (1 mL) was added under an atmosphere of H_2. The reaction was stirred at room temperature for 5 h. The solvent was removed under vacuum and the residue was

subjected to column chromatography on silica gel using petroleum ether/ethyl acetate = 20:1 as an eluent to give **6** as a white solid (0.092 g, 95% yield).

c) Procedure for the synthesis of 7: 0.1 mL of *n*-BuLi (2.5 M, 0.268 mmol) was added dropwise to a solution of methyltriphenylphosphonium bromide (0.096 g, 0.268 mmol) in 6.0 mL of THF at 0 ºC. The reaction was stirred for about 15 min, and then **3a** (0.100 g, 0.233 mmol) in 2.0 mL of THF was added. After an additional 15 min, the ice bath was removed, and the reaction was allowed to stir at room temperature for 12 h. The reaction mixture was diluted with water (10 mL) and extracted with EtOAc (3 × 10 mL). The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4, and concentrated under reduced pressure. The crude product was purified as a pale yellow solid by a silica gel column chromatography (petroleum ether/ethyl acetate = 100:1) to afford 7 (0.062 g, 63% yield).

d) Procedure for the synthesis of 8: To an oven-dried 25 mL round-bottom flask equipped with a stir bar was added **3a** (0.100g, 0.233 mmol) and MeOH (4 mL), then the mixture was cooled to 0 °C, and sodium borohydride (28.4 mg, 0.75 mmol) was added. The reaction was stirred at room temperature for 1.5 h. The reaction was then quenched with saturated ammonium chloride (10 mL) and vigorously stirred and filtered through Celite. The aqueous layer was extracted with EtOAc (2 x 15 mL), and the organic layers were combined and washed with brine (10 mL) then dried with anhydrous Na_2SO_4. The solvent was removed under a vacuum. The residue was subjected to flash chromatography on silica gel using petroleum ether/ethyl acetate (20:1) as an eluent to give **8** as a sticky solid (0.087 g, 87% yield).

e) Procedure for the synthesis of 9: To a solution of **8** (0.100 g, 0.232 mmol) in CH_2Cl_2 (3 mL) was added $BF_3{\cdot}OEt_2$ (0.029 mL, 0.232 mmol) under an argon atmosphere, and the resulting mixture was stirred at room temperature for 1 h. The colour of the solution changed from yellow to orange during the reaction. After completing the reaction, the solvent was removed under a vacuum. The residue was subjected to flash chromatography on silica gel using petroleum ether/ethyl acetate (100:1) as an eluent to give **9** as a white solid (0.090 g, 94% yield).

f) Procedure for the synthesis of 10: A mixture of **4b** (0.100 g, 0.218 mmol), *meta*-chloroperoxybenzoic acid (*m*CPBA, 0.150 g, 0.872 mmol), TFA (0.033 mL, 0.436 mmol) in CH_2Cl_2 (10 mL) was stirred at room temperature. Upon completion of the reaction (monitored by TLC), the mixture was diluted with CH_2Cl_2 (20 mL), washed with saturated aqueous Na_2SO_3 (1 × 30 mL) and saturated aqueous $NaHCO_3$ (1 × 30 mL). After extraction, the resulting organic layer was dried over anhydrous Na_2SO_4 and concentrated under a vacuum. The residue was purified by

flash chromatography on silica gel eluting with petroleum ether/ethyl acetate (20:1) to give **10** as a white solid. (0.076 g, 74%)

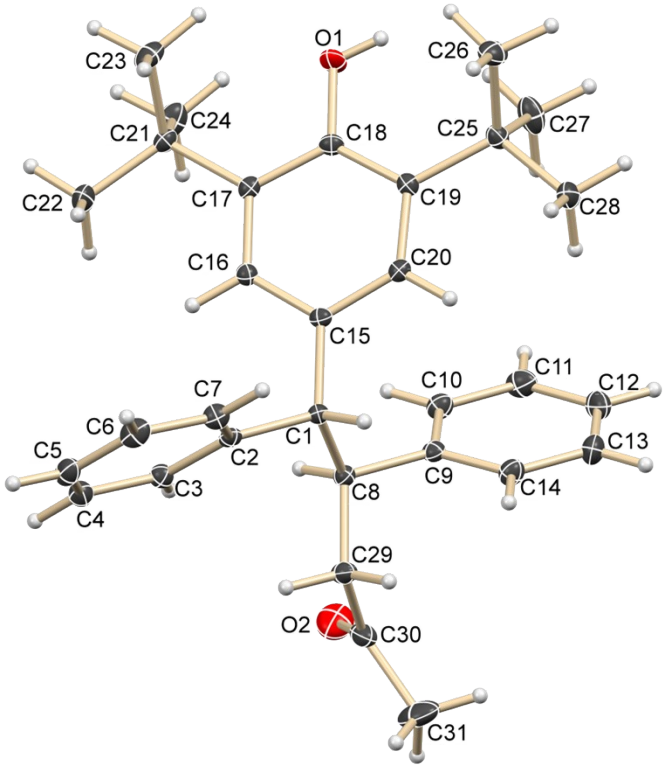
g) Procedure for the synthesis of 11: Lithium hydroxide (0.005 g, 0.211 mmol) was added to the solution of ester **10** (0.050 g, 0.105 mmol) in 10 mL of ethanol/water (4:1) mixture. The resulting solution was stirred at room temperature for 2 h, then acidified with 2 N HCl to pH 1, diluted with water (10 mL) and extracted with ethyl acetate (3 × 10 mL). The combined organic layers were dried over anhydrous Na_2SO_4 and concentrated under a vacuum. The residue was purified by flash chromatography on silica gel eluting with petroleum ether/ethyl acetate (9:1) to give **11** as a white solid. (0.020 g, 51%).

IV) Procedure for the Control Reaction:

To 5 mL screw-cap reaction vial was added *p*-Quinone methide **1a** (0.100 g, 0.340 mmol), 1-phenyl cyclopropanols **2a** (0.068 g, 0.509 mmol), $Fe(acac)_3$ (0.012 g, 0.034 mmol), and 2,2,6,6-tetramethylpiperidinooxy (TEMPO) (3 equiv) or butylated hydroxytoluene (BHT) (3 equiv) or 1,4-benzoquinone (3 equiv). Then 2.0 mL anhydrous CH_3CN was added under nitrogen. The reaction mixture was stirred at 80 °C for 5 h, and the reaction was monitored by TLC.

2.4 X-ray crystallography:

Compound 4m:



ORTEP view of compound **4m** showing the atom-numbering scheme. The displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres with arbitrary radii**.** X-ray intensity data measurements of compound **4m** was carried out on a Bruker D8 VENTURE Kappa Duo PHOTON II CPAD diffractometer equipped with Incoatec multilayer mirrors optics. The intensity measurements were carried out with Mo micro-focus sealed tube diffraction source (MoK_α= 0.71073 Å) at 100(2) K temperature. The X-ray generator was operated at 50 kV and 1.4 mA. A preliminary set of cell constants and an orientation matrix were calculated from three sets of 36 frames. Data were collected with ω scan width of 0.5° at different settings of φ and 2θ with a frame time of 15 secs keeping the sample-to-detector distance fixed at 5.00 cm. The X-ray data collection was monitored by APEX3 program (Bruker, 2016).[3] All the data were corrected for Lorentzian, polarization and absorption effects using SAINT[4] and SADABS programs (Bruker, 2016). Using APEX3 (Bruker) program suite, the structure was solved with the ShelXS-97[5] (Sheldrick, 2008) structure solution program, using direct methods. The model was refined with version of ShelXL-2014[6] (Sheldrick, 2014) using Least Squares minimisation. All the hydrogen atoms were placed in a geomerically idalized positions and constrained to ride on its parent atoms except H-atom attached to the hydroxy group. The H-atom bound to the –OH group has been located in the difference Fourier and refined isotropically. An *ORTEP* III[7] view of compound was drawn with 50% probability displacement ellipsoids and H atoms are shown as small spheres of arbitrary radii.

Compound **4m** having molecular formula $C_{31}H_{38}O_2$, approximate dimensions 0.090 mm × 0.110 mm × 0.150 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured (λ = 0.71073 Å). The integration of the data using a triclinic unit cell yielded a total of 36099 reflections to a maximum θ angle of 28.70° (0.74 Å resolution), of which 6574 were independent (average redundancy5.491, completeness = 99.7%, R_{int} = 5.00%, R_{sig} = 3.65%) and 6151 (93.57%) were greater than $2\sigma(F^2)$. The final cell constants

of a = 5.8692(3) Å, b = 11.1234(7) Å, c = 20.1269(13) Å, α = 97.223(2)°, β = 90.009(2)°, γ = 101.093(2)°, volume = 1278.81(13) Å^3, are based upon the refinement of the XYZ-centroids of reflections above 20 $\sigma(I)$. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.9900 and 0.9940. The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P-1, with Z = 2 for the formula unit, $C_{31}H_{38}O_2$. The final anisotropic full-matrix least-squares refinement on F^2 with 309 variables converged at $R1$ = 4.78%, for the observed data and $wR2$ = 12.65% for all data. The goodness-of-fit (S) was 1.056. The largest peak in the final difference electron density synthesis was 0.392 e$^-$/Å^3 and the largest hole was -0.254 e$^-$/Å^3 with an RMS deviation of 0.053 e$^-$/Å^3. On the basis of the final model, the calculated density was 1.149 g/cm^3 and F(000), 480 e$^-$.

Table S2. Sample and crystal data for 4m.

Identification code	**4m**	
Chemical formula	$C_{31}H_{38}O_2$	
Formula weight	442.61 g/mol	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal size	0.090 x 0.110 x 0.150 mm	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	a = 5.8692(3) Å	α = 97.223(2)°
	b = 11.1234(7) Å	β = 90.009(2)°
	c = 20.1269(13) Å	γ = 101.093(2)°
Volume	1278.81(13) Å^3	

Z	2
Density (calculated)	1.149 g/cm^3
Absorption coefficient	0.070 mm^{-1}
F(000)	480

Table S3. Data collection and structure refinement for 4m.

Theta range for data collection	1.88 to 28.70°	
Index ranges	-6<=h<=7, -15<=k<=14, -27<=l<=27	
Reflections collected	36099	
Independent reflections	6574 [R_{int} = 0.0500]	
Max. and min. transmission	0.9940 and 0.9900	
Structure solution technique	direct methods	
Structure solution program	SHELXT 2014/5 (Sheldrick, 2014)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2018/3 (Sheldrick, 2018)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	6574 / 0 / 309	
Goodness-of-fit on F^2	1.056	
Δ/σ_{max}	0.001	
Final R indices	6151 data; I>2σ(I)	R1 = 0.0478, wR2 = 0.1242
	all data	R1 = 0.0505, wR2 =

		0.1265
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0575P)^2+0.6244P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.392 and -0.254 eÅ^{-3}	
R.M.S. deviation from mean	0.053 eÅ^{-3}	

Table S4. Bond lengths (Å) for 4m.

O1-C18	1.3780(12)	O1-H1A	0.82(2)
O2-C30	1.2074(16)	C1-C2	1.5201(14)
C1-C15	1.5305(13)	C1-C8	1.5572(14)
C1-H1	1.0	C2-C7	1.3949(15)
C2-C3	1.3970(15)	C3-C4	1.3953(15)
C3-H3	0.95	C4-C5	1.3881(16)
C4-H4	0.95	C5-C6	1.3881(17)
C5-H5	0.95	C6-C7	1.3927(15)
C6-H6	0.95	C7-H7	0.95
C8-C9	1.5191(14)	C8-C29	1.5379(14)
C8-H8	1.0	C9-C10	1.3932(15)
C9-C14	1.3967(15)	C10-C11	1.3944(15)
C10-H10	0.95	C11-C12	1.3853(17)
C11-H11	0.95	C12-C13	1.3898(17)
C12-H12	0.95	C13-C14	1.3908(16)
C13-H13	0.95	C14-H14	0.95
C15-C16	1.3926(14)	C15-C20	1.3934(14)
C16-C17	1.3973(14)	C16-H16	0.95

C17-C18	1.4095(14)	C17-C21	1.5413(14)
C18-C19	1.4105(14)	C19-C20	1.3965(14)
C19-C25	1.5423(14)	C20-H20	0.95
C21-C22	1.5356(16)	C21-C24	1.5368(15)
C21-C23	1.5408(15)	C22-H22A	0.98
C22-H22B	0.98	C22-H22C	0.98
C23-H23A	0.98	C23-H23B	0.98
C23-H23C	0.98	C24-H24A	0.98
C24-H24B	0.98	C24-H24C	0.98
C25-C28	1.5354(15)	C25-C26	1.5424(15)
C25-C27	1.5447(15)	C26-H26A	0.98
C26-H26B	0.98	C26-H26C	0.98
C27-H27A	0.98	C27-H27B	0.98
C27-H27C	0.98	C28-H28A	0.98
C28-H28B	0.98	C28-H28C	0.98
C29-C30	1.5168(16)	C29-H29A	0.99
C29-H29B	0.99	C30-C31	1.5034(18)
C31-H31A	0.98	C31-H31B	0.98

Table S5. Bond angles (°) for 4m.

C18-O1-H1A	108.8(14)	C2-C1-C15	111.33(8)
C2-C1-C8	113.31(8)	C15-C1-C8	111.21(8)
C2-C1-H1	106.9	C15-C1-H1	106.9
C8-C1-H1	106.9	C7-C2-C3	118.12(10)
C7-C2-C1	118.78(9)	C3-C2-C1	123.04(9)

C4-C3-C2	120.82(10)	C4-C3-H3	119.6
C2-C3-H3	119.6	C5-C4-C3	120.28(10)
C5-C4-H4	119.9	C3-C4-H4	119.9
C4-C5-C6	119.49(10)	C4-C5-H5	120.3
C6-C5-H5	120.3	C5-C6-C7	120.08(10)
C5-C6-H6	120.0	C7-C6-H6	120.0
C6-C7-C2	121.19(10)	C6-C7-H7	119.4
C2-C7-H7	119.4	C9-C8-C29	109.92(8)
C9-C8-C1	111.17(8)	C29-C8-C1	111.41(8)
C9-C8-H8	108.1	C29-C8-H8	108.1
C1-C8-H8	108.1	C10-C9-C14	118.31(10)
C10-C9-C8	120.16(9)	C14-C9-C8	121.52(9)
C9-C10-C11	120.91(10)	C9-C10-H10	119.5
C11-C10-H10	119.5	C12-C11-C10	120.23(10)
C12-C11-H11	119.9	C10-C11-H11	119.9
C11-C12-C13	119.43(10)	C11-C12-H12	120.3
C13-C12-H12	120.3	C12-C13-C14	120.29(11)
C12-C13-H13	119.9	C14-C13-H13	119.9
C13-C14-C9	120.82(10)	C13-C14-H14	119.6
C9-C14-H14	119.6	C16-C15-C20	118.19(9)
C16-C15-C1	121.94(9)	C20-C15-C1	119.85(9)
C15-C16-	122.48(9)	C15-C16-	118.8

C17		H16	
C17-C16-H16	118.8	C16-C17-C18	117.08(9)
C16-C17-C21	121.05(9)	C18-C17-C21	121.87(9)
O1-C18-C17	115.92(9)	O1-C18-C19	121.51(9)
C17-C18-C19	122.57(9)	C20-C19-C18	116.89(9)
C20-C19-C25	120.51(9)	C18-C19-C25	122.60(9)
C15-C20-C19	122.67(9)	C15-C20-H20	118.7
C19-C20-H20	118.7	C22-C21-C24	107.59(10)
C22-C21-C23	106.75(9)	C24-C21-C23	109.84(9)
C22-C21-C17	111.47(9)	C24-C21-C17	110.31(9)
C23-C21-C17	110.76(9)	C21-C22-H22A	109.5
C21-C22-H22B	109.5	H22A-C22-H22B	109.5
C21-C22-H22C	109.5	H22A-C22-H22C	109.5
H22B-C22-H22C	109.5	C21-C23-H23A	109.5
C21-C23-H23B	109.5	H23A-C23-H23B	109.5
C21-C23-H23C	109.5	H23A-C23-H23C	109.5
H23B-C23-H23C	109.5	C21-C24-H24A	109.5

C21-C24-H24B	109.5	H24A-C24-H24B	109.5
C21-C24-H24C	109.5	H24A-C24-H24C	109.5
H24B-C24-H24C	109.5	C28-C25-C19	111.36(9)
C28-C25-C26	105.98(9)	C19-C25-C26	111.65(9)
C28-C25-C27	105.81(9)	C19-C25-C27	111.00(9)
C26-C25-C27	110.77(9)	C25-C26-H26A	109.5
C25-C26-H26B	109.5	H26A-C26-H26B	109.5
C25-C26-H26C	109.5	H26A-C26-H26C	109.5
H26B-C26-H26C	109.5	C25-C27-H27A	109.5
C25-C27-H27B	109.5	H27A-C27-H27B	109.5
C25-C27-H27C	109.5	H27A-C27-H27C	109.5
H27B-C27-H27C	109.5	C25-C28-H28A	109.5
C25-C28-H28B	109.5	H28A-C28-H28B	109.5
C25-C28-H28C	109.5	H28A-C28-H28C	109.5
H28B-C28-H28C	109.5	C30-C29-C8	112.52(9)
C30-C29-H29A	109.1	C8-C29-H29A	109.1

C30-C29-H29B	109.1	C8-C29-H29B	109.1
H29A-C29-H29B	107.8	O2-C30-C31	122.24(12)
O2-C30-C29	121.52(11)	C31-C30-C29	116.24(11)
C30-C31-H31A	109.5	C30-C31-H31B	109.5
H31A-C31-H31B	109.5	C30-C31-H31C	109.5
H31A-C31-H31C	109.5	H31B-C31-H31C	109.5

Table S6. Torsion angles (°) for 4m.

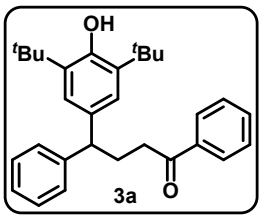
C15-C1-C2-C7	-81.21(11)	C8-C1-C2-C7	152.55(9)
C15-C1-C2-C3	95.85(11)	C8-C1-C2-C3	-30.39(13)
C7-C2-C3-C4	-0.91(15)	C1-C2-C3-C4	-177.98(9)
C2-C3-C4-C5	1.15(16)	C3-C4-C5-C6	-0.43(17)
C4-C5-C6-C7	-0.51(17)	C5-C6-C7-C2	0.75(17)
C3-C2-C7-C6	-0.04(16)	C1-C2-C7-C6	177.16(10)
C2-C1-C8-C9	-178.16(8)	C15-C1-C8-C9	55.54(11)
C2-C1-C8-C29	-55.19(11)	C15-C1-C8-C29	178.52(8)
C29-C8-C9-C10	132.11(10)	C1-C8-C9-C10	-104.07(11)

C29-C8-C9-C14	-48.45(13)	C1-C8-C9-C14	75.38(12)
C14-C9-C10-C11	0.62(16)	C8-C9-C10-C11	-179.91(10)
C9-C10-C11-C12	-0.25(18)	C10-C11-C12-C13	-0.02(18)
C11-C12-C13-C14	-0.10(18)	C12-C13-C14-C9	0.49(18)
C10-C9-C14-C13	-0.75(16)	C8-C9-C14-C13	179.80(10)
C2-C1-C15-C16	-35.25(13)	C8-C1-C15-C16	92.14(11)
C2-C1-C15-C20	146.52(9)	C8-C1-C15-C20	-86.09(11)
C20-C15-C16-C17	1.56(15)	C1-C15-C16-C17	-176.70(9)
C15-C16-C17-C18	1.67(15)	C15-C16-C17-C21	-177.65(9)
C16-C17-C18-O1	176.42(9)	C21-C17-C18-O1	-4.26(14)
C16-C17-C18-C19	-3.47(15)	C21-C17-C18-C19	175.84(9)
O1-C18-C19-C20	-177.96(9)	C17-C18-C19-C20	1.93(15)
O1-C18-C19-C25	1.76(15)	C17-C18-C19-C25	-178.34(9)
C16-C15-C20-C19	-3.24(15)	C1-C15-C20-C19	175.05(9)
C18-C19-C20-C15	1.53(15)	C25-C19-C20-C15	-178.19(9)
C16-C17-C21-C22	4.55(14)	C18-C17-C21-C22	-174.74(10)

C16-C17-C21-C24	-114.92(11)	C18-C17-C21-C24	65.79(13)
C16-C17-C21-C23	123.25(11)	C18-C17-C21-C23	-56.03(13)
C20-C19-C25-C28	-1.22(14)	C18-C19-C25-C28	179.06(9)
C20-C19-C25-C26	-119.48(10)	C18-C19-C25-C26	60.81(13)
C20-C19-C25-C27	116.39(11)	C18-C19-C25-C27	-63.32(13)
C9-C8-C29-C30	-60.05(12)	C1-C8-C29-C30	176.26(9)
C8-C29-C30-O2	-38.04(15)	C8-C29-C30-C31	142.65(11)

2.5 Characterization of 3a-3z, 4a-4q and 5-12:

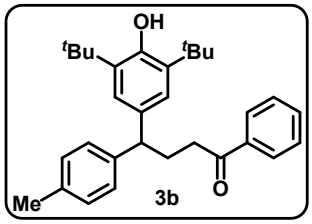
4-(3,5-di-tert-butyl-4-hydroxyphenyl)-1,4-diphenylbutan-1-one (3a):



The product **3a** was obtained in 97% yield (141 mg, White solid); **mp** = 96-97 °C; R_f = 0.59 (10% EtOAc in petroleum ether);

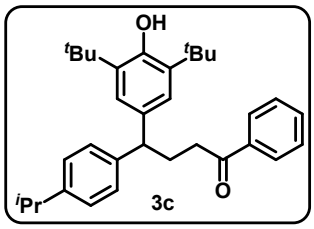
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.84 – 7.82 (m, 2H), 7.51 – 7.47 (m, 1H), 7.37 (dd, *J* = 10.6, 4.6 Hz, 2H), 7.30 – 7.28 (m, 4H), 7.20 – 7.14 (m, 1H), 7.05 (s, 2H), 5.05 (s, 1H), 3.91 (t, *J* = 8.0 Hz, 1H), 2.97 – 2.84 (m, 2H), 2.50 – 2.41 (m, 2H), 1.39 (s, 18H); **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 200.3, 152.1, 144.8, 136.9, 135.6, 134.9, 132.8, 128.4, 128.4, 128.0, 127.8, 126.1, 124.2, 50.7, 37.1, 34.3, 30.7, 30.3; **HRMS (ESI-TOF)** *m/z*: [M – H]$^-$ calcd for $C_{30}H_{35}O_2$ 427.2632; found 427.2641.

4-(3,5-di-tert-butyl-4-hydroxyphenyl)-1-phenyl-4-(p-tolyl)butan-1-one (3b):



The product **3b** was obtained in 89% yield (128 mg, White solid); **mp** = 116-117 °C; R_f = 0.47 (10% EtOAc in petroleum ether);**^{1}H NMR (400 MHz, $CDCl_3$) δ** = 7.86 – 7.84 (m, 2H), 7.53 (t, *J* = 7.2 Hz, 1H), 7.41 (t, *J* = 7.6 Hz, 2H), 7.19 (d, *J* = 7.8 Hz, 2H), 7.11 (d, *J* = 7.7 Hz, 2H), 7.05 (s, 2H), 5.04 (s, 1H), 3.87 (t, *J* = 7.8 Hz, 1H), 2.91 (t, *J* = 7.3 Hz, 2H), 2.47 – 2.39 (m, 2H), 2.32 (s, 3H), 1.41 (s, 18H); **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 200.4, 152.0, 141.9, 137.0, 135.6, 135.5, 135.2, 132.9, 129.1, 128.5, 128.0, 127.7, 124.2, 50.4, 37.2, 34.3, 30.8, 30.3, 21.0; **HRMS (ESI-TOF)** *m/z*: [M – H]$^-$ calcd for $C_{31}H_{37}O_2$ 441.2788; found 441.2809.

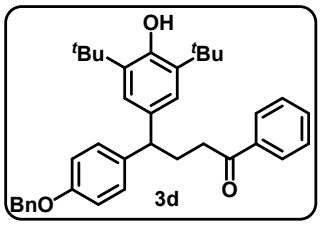
4-(3,5-di-tert-butyl-4-hydroxyphenyl)-4-(4-isopropylphenyl)-1-phenylbutan-1-one (3c):



The product **3c** was obtained in 85% yield (119 mg, sticky solid); R_f = 0.62 (10% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.83 (d, *J* = 7.7 Hz, 2H), 7.50 (t, *J* = 7.6 Hz, 1H), 7.39 (t, *J* = 7.6 Hz, 2H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.13 (d, *J* = 8.1 Hz, 2H), 7.05 (s, 2H), 5.03 (s, 1H), 3.86 (t, *J* = 7.9 Hz, 1H), 2.92 – 2.81 (m, 3H), 2.49 – 2.37 (m, 2H), 1.39 (s, 18H), 1.21 (d, *J* = 6.9 Hz, 6H); **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 200.5, 152.1, 146.5, 142.2, 137.0, 135.6, 135.1, 132.8, 128.4, 128.0, 127.6, 126.4, 124.2, 50.5, 37.3, 34.3, 33.6, 31.0, 30.3, 24.0; **HRMS (ESI-TOF)** *m/z*: [M – H]$^-$ calcd for $C_{33}H_{41}O_2$ 469.3101; found 469.3115.

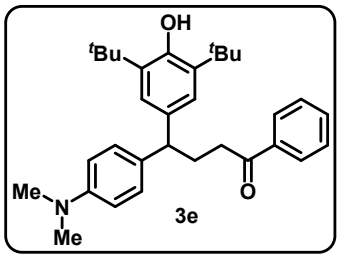
4-(4-(benzyloxy)phenyl)-4-(3,5-di-tert-butyl-4-hydroxyphenyl)-1-phenylbutan-1-one (3d):



The product **3d** was obtained in 97% yield (129 mg, White solid); **mp** = 108-109 °C; R_f = 0.50 (10% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.86 (d, *J* = 7.7 Hz, 2H), 7.53 (t, *J* = 7.5 Hz, 1H), 7.48 – 7.36 (m, 6H), 7.36 – 7.28 (m, 1H), 7.22 (d, *J* = 8.6 Hz, 2H), 7.05 (s, 2H), 6.93 (d, *J* = 8.5 Hz, 2H), 5.05 (s, 3H), 3.88 (t, *J* = 7.9 Hz, 1H), 2.95 – 2.87 (m, 2H), 2.42 (dd, *J* = 12.6, 5.0 Hz, 2H), 1.42 (s, 18H); **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 200.4, 157.1, 152.0, 137.3, 137.1, 137.0, 135.6, 135.3, 132.9, 128.8, 128.5, 128.5, 128.0, 127.9, 127.5, 124.2, 114.8, 70.0, 49.9, 37.2, 34.3, 30.9, 30.3; **HRMS (ESI-TOF)** *m/z*: [M – H]$^-$ calcd for $C_{37}H_{41}O_3$ 533.3050; found 533.3069.

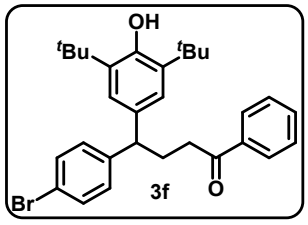
4-(3,5-di-tert-butyl-4-hydroxyphenyl)-4-(4-(dimethylamino)phenyl)-1-phenylbutan-1-one (3e):



The product **3e** was obtained in 92% yield (129 mg, White solid); **mp** = 128-129 °C; R_f = 0.51 (10% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.87 (d, *J* = 7.7 Hz, 2H), 7.53 (t, *J* = 7.3 Hz, 1H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.19 (d, *J* = 8.7 Hz, 2H), 7.08 (s, 2H), 6.73 (t, *J* = 5.7 Hz, 2H), 5.04 (s, 1H), 3.84 (t, *J* = 7.9 Hz, 1H), 2.93 (s, 6H), 2.93 (t, 2H), 2.49 – 2.39 (m, 2H), 1.43 (s, 18H); **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 200.6, 151.9, 149.1, 137.0, 135.7, 135.5, 133.0, 132.8, 128.4, 128.4, 128.0, 124.1, 112.9, 49.9, 40.7, 37.4, 34.3, 31.0, 30.3; **HRMS (ESI-TOF)** *m/z*: [M – H]$^-$ calcd for $C_{32}H_{40}NO_2$ 470.3054; found 470.3069.

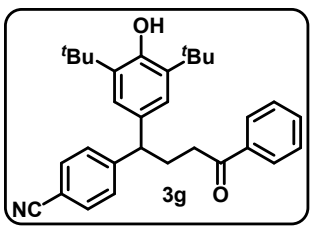
4-(4-bromophenyl)-4-(3,5-di-tert-butyl-4-hydroxyphenyl)-1-phenylbutan-1-one (3f):



The product **3f** was obtained in 84% yield (114 mg, White solid); **mp** = 126-127 °C; R_f = 0.45 (10% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.85 (d, *J* = 7.3 Hz, 2H), 7.54 (t, *J* = 7.3 Hz, 1H), 7.42 (t, *J* = 7.8 Hz, 4H), 7.16 (d, *J* = 8.2 Hz, 2H), 7.00 (s, 2H), 5.07 (s, 1H), 3.88 (t, *J* = 7.8 Hz, 1H), 2.90 (t, *J* = 7.2 Hz, 2H), 2.43 (q, *J* = 7.5 Hz, 2H), 1.40 (s, 18H) ; **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 200.0, 152.3, 144.0, 136.9, 135.8, 134.3, 133.0, 131.5, 129.6, 128.5, 128.0, 124.1, 119.8, 50.1, 36.9, 34.3, 30.4, 30.3 ; **HRMS (ESI-TOF)** *m/z*: [M – H]$^-$ calcd for $C_{30}H_{34}O_2Br$ 505.1737; found 505.1758.

4-(1-(3,5-di-tert-butyl-4-hydroxyphenyl)-4-oxo-4-phenylbutyl)benzonitrile (3g):

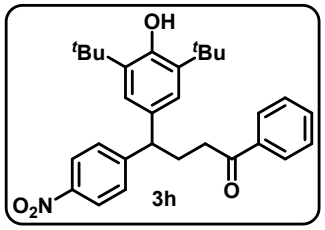


The product **3g** was obtained in 83% yield (118 mg, White solid); **mp** = 106-107 °C; R_f = 0.26 (10% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.85 (d, *J* = 7.3 Hz, 2H), 7.59 – 7.52 (m, 3H), 7.42 (dd, *J* = 13.9, 8.0 Hz, 4H), 6.99 (s, 2H), 5.13 (s, 1H), 4.00 (t, *J* = 7.9 Hz, 1H), 2.94 – 2.90 (m, 2H), 2.47 (dd, *J* = 14.7, 7.2 Hz, 2H), 1.40 (s, 18H) ; **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 199.7, 152.5, 150.7, 136.8, 136.1, 133.2,

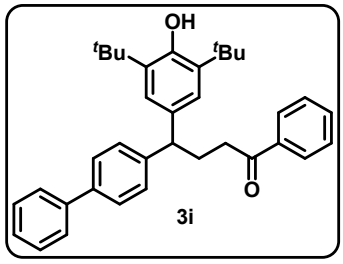
133.1, 132.3, 128.6, 128.5, 127.9, 124.2, 119.0, 109.9, 50.5, 36.5, 34.3, 30.2, 29.9 ; **HRMS (ESI-TOF)** *m/z*: [M – H]$^-$ calcd for $C_{31}H_{34}NO_2$ 452.2584; found 452.2602.

4-(3,5-di-tert-butyl-4-hydroxyphenyl)-4-(4-nitrophenyl)-1-phenylbutan-1-one (3h):



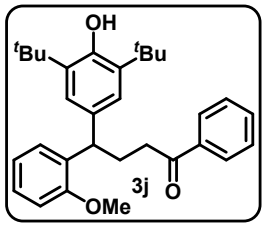
The product **3h** was obtained in 79% yield (110 mg, White solid); **mp** = 113-114 °C; $\boldsymbol{R_f}$ = 0.27 (10% EtOAc in petroleum ether); **^{1}H NMR (400 MHz, $CDCl_3$) δ** = 8.27 – 8.14 (m, 2H), 7.85 (d, *J* = 7.3 Hz, 2H), 7.57 – 7.52 (m, 1H), 7.46 – 7.41 (m, 4H), 7.00 (s, 2H), 5.12 (d, *J* = 1.0 Hz, 1H), 4.05 (t, *J* = 7.9 Hz, 1H), 2.93 (t, *J* = 7.2 Hz, 2H), 2.49 (q, *J* = 7.3 Hz, 2H), 1.40 (s, 18H) ; **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 199.7, 152.9, 152.6, 146.4, 136.8, 136.2, 133.1, 133.0, 128.6, 128.6, 127.9, 124.2, 123.8, 50.4, 36.5, 34.4, 30.2, 30.0 ; **HRMS (ESI-TOF)** *m/z*: [M – H]$^-$ calcd for $C_{30}H_{34}NO_4$ 472.2482; found 472.2501.

4-([1,1'-biphenyl]-4-yl)-4-(3,5-di-tert-butyl-4-hydroxyphenyl)-1-phenylbutan-1-one (3i) :



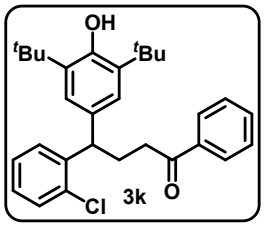
The product **3i** was obtained in 98% yield (133 mg, White solid); **mp** = 99-100 °C; $\boldsymbol{R_f}$ = 0.39 (10% EtOAc in petroleum ether); **^{1}H NMR (400 MHz, $CDCl_3$) δ** =7.83 (d, *J* = 7.3 Hz, 2H), 7.56 – 7.46 (m, 5H), 7.37 (dd, *J* = 14.8, 7.8 Hz, 6H), 7.29 (dd, *J* = 14.7, 7.3 Hz, 1H), 7.08 (s, 2H), 5.05 (s, 1H), 3.95 (t, *J* = 7.9 Hz, 1H), 2.93 (t, *J* = 7.4 Hz, 2H), 2.55 – 2.42 (m, 2H), 1.40 (s, 18H); **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 200.3, 152.2, 144.0, 140.9, 138.9, 136.9, 135.7, 134.8, 132.9, 128.7, 128.5, 128.2, 128.0, 127.1, 127.0, 126.9, 124.2, 50.4, 37.1, 34.3, 30.7, 30.3 ; **HRMS (ESI-TOF)** *m/z*: [M – H]$^-$ calcd for $C_{36}H_{39}O_2$ 503.2945; found 503.2962.

4-(3,5-di-tert-butyl-4-hydroxyphenyl)-4-(2-methoxyphenyl)-1-phenylbutan-1-one (3j) :



The product **3j** was obtained in 78% yield (110 mg, White solid); **mp** = 161-162 °C; $\boldsymbol{R_f}$ = 0.56 (10% EtOAc in petroleum ether); **^{1}H NMR (400 MHz, $CDCl_3$) δ** = 7.85 (d, *J* = 7.6 Hz, 2H), 7.51 (t, *J* = 7.3 Hz, 1H), 7.40 (t, *J* = 7.6 Hz, 2H), 7.25 (d, *J* = 7.2 Hz, 1H), 7.17 – 7.13 (m, 1H), 7.12 (s, 2H), 6.92 (t, *J* = 7.4 Hz, 1H), 6.83 (d, *J* = 8.1 Hz, 1H), 5.02 (s, 1H), 4.40 (t, *J* = 7.9 Hz, 1H), 3.76 (s, 3H), 2.99 – 2.84 (m, 2H), 2.44 (dd, *J* = 15.2, 7.6 Hz, 2H), 1.41 (s, 18H); **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 200.6, 157.0, 151.9, 137.0, 135.3, 134.6, 133.4, 132.7, 128.4, 128.0, 127.6, 126.9, 124.6, 120.6, 110.6, 55.3, 42.7, 37.4, 34.3, 30.4, 29.9; **HRMS (ESI-TOF)** *m/z*: [M – H]$^-$ calcd for $C_{31}H_{37}O_3$ 457.2737; found 457.2760.

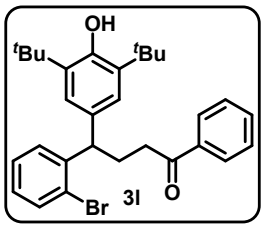
4-(2-chlorophenyl)-4-(3,5-di-tert-butyl-4-hydroxyphenyl)-1-phenylbutan-1-one (3k):



The product **3k** was obtained in 79% yield (111 mg, White solid); **mp** = 131-132 °C; R_f = 0.46 (10% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.85 (d, *J* = 7.6 Hz, 2H), 7.51 (t, *J* = 7.3 Hz, 1H), 7.42 – 7.32 (m, 4H), 7.22 (dd, *J* = 11.0, 4.3 Hz, 1H), 7.12 – 7.08 (m, 3H), 5.06 (s, 1H), 4.49 (t, *J* = 7.9 Hz, 1H), 3.02 – 2.85 (m, 2H), 2.52 – 2.37 (m, 2H), 1.40 (s, 18H); **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 200.0, 152.2, 142.4, 136.9, 135.6, 134.1, 133.4, 132.9, 129.6, 128.5, 128.2, 128.0, 127.2, 127.0, 124.5, 45.9, 37.0, 34.3, 30.3, 30.0 ; **HRMS (ESI-TOF)** *m/z*: [M – H]$^-$ calcd for $C_{30}H_{34}O_2Cl$ 461.2242; found 461.2269.

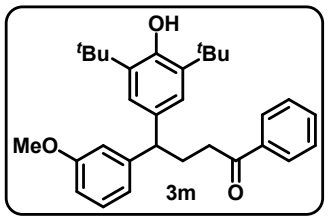
4-(2-bromophenyl)-4-(3,5-di-tert-butyl-4-hydroxyphenyl)-1-phenylbutan-1-one (3l):



The product **3l** was obtained in 92% yield (125 mg, White solid); **mp** = 104-105 °C; R_f = 0.50 (10% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.87 – 7.85 (m, 2H), 7.54 – 7.50 (m, 2H), 7.41 (t, *J* = 7.6 Hz, 2H), 7.35 (dd, *J* = 7.7, 1.4 Hz, 1H), 7.26 (dd, *J* = 10.7, 3.9 Hz, 1H), 7.13 (s, 2H), 7.04 – 7.00 (m, 1H), 5.07 (s, 1H), 4.49 (t, *J* = 7.9 Hz, 1H), 3.04 – 2.85 (m, 2H), 2.53 – 2.38 (m, 2H), 1.41 (s, 18H) ; **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 200.1, 152.2, 144.1, 136.9, 135.6, 133.4, 132.9, 132.9, 128.5, 128.4, 128.0, 127.7, 127.6, 125.2, 124.5, 48.5, 37.0, 34.3, 30.3, 30.2 ; **HRMS (ESI-TOF)** *m/z*: [M – H]$^-$ calcd for $C_{30}H_{34}O_2Br$ 505.1737; found 505.1761.

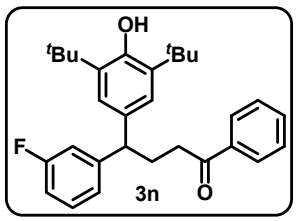
4-(3,5-di-tert-butyl-4-hydroxyphenyl)-4-(3-methoxyphenyl)-1-phenylbutan-1-one (3m) :



The product **3m** was obtained in 91% yield (128 mg, sticky solid); R_f = 0.50 (10% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.90 – 7.88 (m, 2H), 7.56 – 7.52 (m, 1H), 7.45 – 7.37 (m, 2H), 7.26 (dd, *J* = 9.0, 6.7 Hz, 1H), 7.12 (s, 2H), 6.95 (d, *J* = 7.6 Hz, 1H), 6.89 (d, *J* = 1.7 Hz, 1H), 6.77 (dd, *J* = 8.2, 2.3 Hz, 1H), 5.11 (s, 1H), 3.93 (t, *J* = 7.9 Hz, 1H), 3.80 (s, 3H), 2.98 – 2.94 (m, 2H), 2.53 – 2.47 (m, 2H), 1.45 (s, 18H) ; **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 200.3, 159.6, 152.1, 146.5, 136.9, 135.6, 134.7, 132.8, 129.3, 128.4, 128.0, 124.1, 120.2, 113.8, 111.2, 55.0, 50.8, 37.1, 34.3, 30.7, 30.3 ; **HRMS (ESI-TOF)** *m/z*: [M – H]$^-$calcd for $C_{31}H_{37}O_3$ 457.5737; found 457.2750.

4-(3,5-di-tert-butyl-4-hydroxyphenyl)-4-(3-fluorophenyl)-1-phenylbutan-1-one (3n):

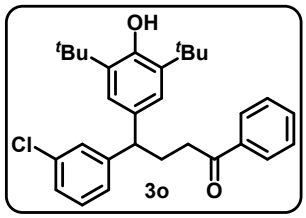


The product **3n** was obtained in 90% yield (129 mg, White solid); **mp** = 80-81 °C; R_f = 0.60 (10% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.84 (d, *J* = 7.3 Hz, 2H), 7.50 (t, *J* = 7.4 Hz, 1H), 7.39 (t, *J* = 7.6 Hz, 2H), 7.26 – 7.21 (m, 1H), 7.07 (d, *J* =

7.7 Hz, 1H), 7.02 (s, 2H), 6.98 (d, J = 10.3 Hz, 1H), 6.86 (td, J = 8.4, 1.9 Hz, 1H), 5.08 (s, 1H), 3.91 (t, J = 7.9 Hz, 1H), 2.90 (t, J = 7.1 Hz, 2H), 2.44 (q, J = 7.3 Hz, 2H), 1.39 (s, 18H) ; **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 200.0, 163.0 (d, J_{C-F} = 245.67 Hz), 152.3, 147.7 (d, J_{C-F} = 6.87 Hz), 136.9, 135.8, 134.2, 132.9, 129.9 (d, J_{C-F} = 7.63 Hz), 128.5, 128.0, 124.2, 123.5(d, J_{C-F} = 3.05 Hz), 14.7 (d, J_{C-F} = 21.36 Hz), 113.0 (d, J_{C-F} = 20.60 Hz), 50.4, 36.9, 34.3, 30.4, 30.3 ; **^{19}F NMR (376 MHz, $CDCl_3$) δ =** -113.2; **HRMS (ESI-TOF)** *m/z*: $[M - H]^-$ calcd for $C_{30}H_{34}FO_2$ 445.2537; found 445.2560.

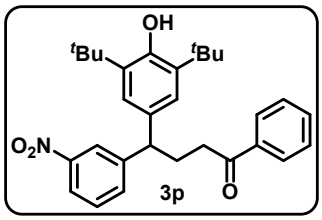
4-(3-chlorophenyl)-4-(3,5-di-tert-butyl-4-hydroxyphenyl)-1-phenylbutan-1-one (3o) :



The product **3o** was obtained in 89% yield (126 mg, White solid); **mp** = 72-73 °C; R_f = 0.60 (10% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.84 (d, J = 7.6 Hz, 2H), 7.52 (t, J = 7.5 Hz, 1H), 7.41 (t, J = 7.7 Hz, 2H), 7.26– 7.14 (m, 4H), 7.00 (s, 2H), 5.07 (s, 1H), 3.88 (t, J = 7.9 Hz, 1H), 2.91 – 2.87 (m, 2H), 2.42 (dt, J = 13.2, 6.6 Hz, 2H), 1.39 (s, 18H); **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 200.0, 152.3, 147.0, 136.9, 135.9, 134.2, 134.0, 133.0, 129.7, 128.5, 128.1, 128.0, 126.3, 126.0, 124.2, 50.4, 36.9, 34.4, 30.4, 30.3; **HRMS (ESI-TOF)** *m/z*: $[M - H]^-$ calcd for $C_{30}H_{34}ClO_2$ 461.2242; found 461.2260.

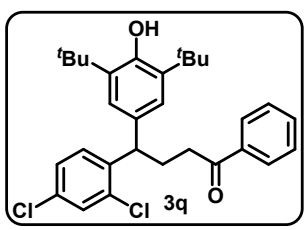
4-(3,5-di-tert-butyl-4-hydroxyphenyl)-4-(3-nitrophenyl)-1-phenylbutan-1-one (3p) :



The product **3p** was obtained in 76% yield (106 mg, White solid); **mp** = 79-80 °C; R_f = 0.26 (10% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.20 – 8.19 (m, 1H), 8.06 (dd, J = 8.5, 1.9 Hz, 1H), 7.86 (d, J = 7.7 Hz, 2H), 7.65 (d, J = 7.7 Hz, 1H), 7.54 (dd, J = 10.5, 4.2 Hz, 1H), 7.49-7.34 (m, 3H), 7.04 (s, 2H), 5.15 (s, 1H), 4.07 (t, J = 7.9 Hz, 1H), 2.95 (t, J = 7.2 Hz, 2H), 2.59 – 2.45 (m, 2H), 1.42 (s, 18H) ; **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 199.7, 152.5, 148.3, 147.3, 136.8, 136.1, 134.0, 133.2, 133.1, 129.3, 128.5, 127.9, 124.2, 122.7, 121.3, 50.2, 36.5, 34.3, 31.8, 30.2; **HRMS (ESI-TOF)** *m/z*: $[M - H]^-$ calcd for $C_{30}H_{24}NO_4$ 472.2482; found 472.2501.

4-(3,5-di-tert-butyl-4-hydroxyphenyl)-4-(2,4-dichlorophenyl)-1-phenylbutan-1-one (3q) :

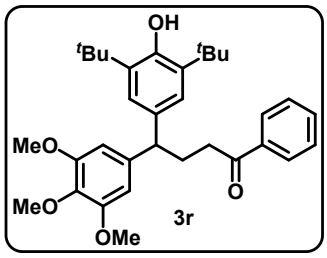


The product **3q** was obtained in 98% yield (134 mg, White solid); **mp** = 144-145 °C; R_f = 0.47 (10% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, $CDCl_3$) δ =7.85 (d, J = 7.7 Hz, 2H), 7.52 (t, J = 7.3 Hz, 1H), 7.41 (t, J = 7.6 Hz, 2H), 7.35 (d, J = 1.4 Hz, 1H), 7.26 (t, J = 6.6 Hz, 1H), 7.19 (dd, J = 8.4, 1.8 Hz, 1H), 7.05 (s, 2H), 5.07 (s, 1H), 4.43 (t, J = 7.8 Hz, 1H), 3.01 – 2.84 (m, 2H), 2.50 – 2.33 (m, 2H), 1.39 (s, 18H); **^{13}C{^{1}H} NMR**

(100 MHz,$CDCl_3$) δ = 199.8, 152.4, 141.2, 136.8, 135.8, 134.7, 133.0, 132.8, 132.1, 129.4, 129.1, 128.5, 128.0, 127.3, 124.4, 45.5, 36.8, 34.3, 30.3, 29.8; **HRMS (ESI-TOF)** *m/z*: $[M - H]^-$ calcd for $C_{30}H_{33}O_2Cl_2$ 495.1852; found 495.1873.

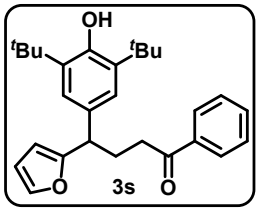
4-(3,5-di-tert-butyl-4-hydroxyphenyl)-1-phenyl-4-(3,4,5-trimethoxyphenyl)butan-1-one (3r):



The product **3r** was obtained in 87% yield (117 mg, White solid); **mp** = 109-110 °C; R_f = 0.42 (20% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.85 (dd, *J* = 5.2, 3.3 Hz, 2H), 7.55 – 7.51 (m, 1H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.09 (s, 2H), 6.52 (s, 2H), 5.08 (s, 1H), 3.86 (t, *J* = 8.0 Hz, 1H), 3.83 (s, 6H), 3.82 (s, 3H), 2.95 – 2.91 (m, 2H), 2.42 (dt, *J* = 11.6, 5.9 Hz, 2H), 1.42 (s, 18H) ; **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 200.4, 153.0, 152.2, 140.5, 136.9, 136.3, 135.7, 134.6, 132.9, 128.5, 128.0, 124.1, 104.8, 60.8, 56.0, 51.0, 37.0, 34.3, 31.2, 30.3 ; **HRMS (ESI-TOF)** *m/z*: $[M - H]^-$ calcd for $C_{33}H_{41}O_5$ 517.2949; found 517.2958.

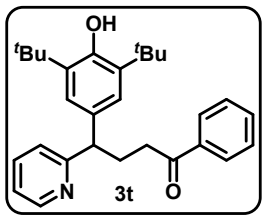
4-(3,5-di-tert-butyl-4-hydroxyphenyl)-4-(furan-2-yl)-1-phenylbutan-1-one (3s) :



The product **3s** was obtained in 75% yield (110 mg, sticky solid); R_f = 0.44 (10% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.88 – 7.86 (m, 2H), 7.56 – 7.52 (m, 1H), 7.43 (t, *J* = 7.7 Hz, 2H), 7.34 (s, 1H), 7.04 (s, 2H), 6.31 – 6.30 (m, 1H), 6.10 (d, *J* = 3.1 Hz, 1H), 5.09 (s, 1H), 3.98 (t, *J* = 7.9 Hz, 1H), 2.94 (dt, *J* = 8.2, 6.1 Hz, 2H), 2.55 – 2.46 (m, 1H), 2.33 – 2.24 (m, 1H), 1.41 (s, 18H) ; **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 200.1, 157.8, 152.4, 141.2, 136.9, 135.7, 132.9, 132.7, 128.5, 128.0, 124.3, 110.0, 105.5, 44.4, 36.6, 34.3, 30.3, 29.9; **HRMS (ESI-TOF)** *m/z*: $[M - H]^-$ calcd for $C_{28}H_{33}O_3$ 417.2424; found 417.2440.

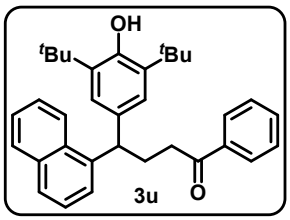
4-(3,5-di-tert-butyl-4-hydroxyphenyl)-1-phenyl-4-(pyridin-2-yl)butan-1-one (3t) :



The product **3t** was obtained in 79% yield (115 mg, sticky solid); R_f = 0.41 (20% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.58 (ddd, *J* = 4.9, 1.8, 0.8 Hz, 1H), 7.89 – 7.86 (m, 2H), 7.56 (td, *J* = 7.7, 1.9 Hz, 1H), 7.53 – 7.49 (m, 1H), 7.43 – 7.39 (m, 2H), 7.21 (d, *J* = 7.9 Hz, 1H), 7.15 (s, 2H), 7.09 (ddd, *J* = 7.5, 4.9, 1.1 Hz, 1H), 5.10 (s, 1H), 4.11 (t, *J* = 7.8 Hz, 1H), 2.95 (dd, *J* = 11.1, 4.3 Hz, 2H), 2.72 – 2.63 (m, 1H), 2.53 – 2.44 (m, 1H), 1.41 (s, 18H) ; **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 200.3, 163.7, 152.3, 149.0, 136.9, 136.4, 135.7, 133.8, 132.8, 128.4, 128.0, 124.5, 122.9, 121.2, 52.7, 37.0, 34.3, 30.3, 30.2; **HRMS (ESI-TOF)** *m/z*: $[M - H]^-$ calcd for $C_{29}H_{34}NO_2$ 428.2584; found 428.2599.

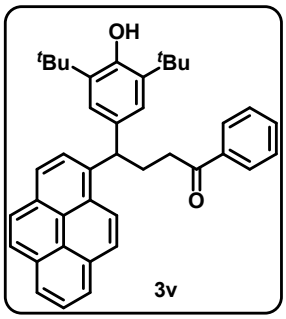
4-(3,5-di-tert-butyl-4-hydroxyphenyl)-4-(naphthalen-1-yl)-1-phenylbutan-1-one (3u):



The product **3u** was obtained in 86% yield (119 mg, White solid); **mp** = 124-125 °C; R_f = 0.57 (10% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.30 (d, *J* = 8.4 Hz, 1H), 7.88 – 7.85 (m, 3H), 7.76 (d, *J* = 7.9 Hz, 1H), 7.56 – 7.46 (m, 5H), 7.40 (dd, *J* = 10.7, 4.6 Hz, 2H), 7.17 (s, 2H), 5.07 (s, 1H), 4.83 (t, *J* = 7.7 Hz, 1H), 3.05 (t, *J* = 7.5 Hz, 2H), 2.73 – 2.54 (m, 2H), 1.42 (s, 18H); **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 200.4, 152.1, 140.6, 136.9, 135.6, 134.4, 134.1, 132.9, 132.0, 128.8, 128.4, 128.0, 126.8, 125.8, 125.4, 125.3, 124.5, 124.0, 123.8, 45.3, 37.2, 34.3, 31.0, 30.3; **HRMS (ESI-TOF)** *m/z*: $[M - H]^-$ calcd for $C_{34}H_{37}O_2$ 477.2788; found 477.2798.

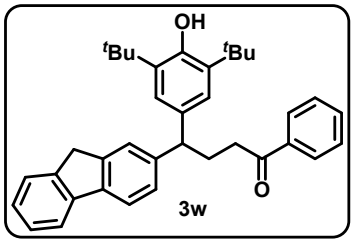
4-(3,5-di-tert-butyl-4-hydroxyphenyl)-1-phenyl-4-(pyren-1-yl)butan-1-one (3v):



The product **3v** was obtained in 81% yield (107 mg, White solid); **mp** = 183-184 °C; R_f = 0.34 (10% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.51 (d, *J* = 9.5 Hz, 1H), 8.15 – 8.02 (m, 5H), 8.00 – 7.95 (m, 2H), 7.94 – 7.90 (m, 1H), 7.76 – 7.74 (m, 2H), 7.40 (t, *J* = 7.5 Hz, 1H), 7.29 (t, *J* = 5.5 Hz, 2H), 7.19 (s, 2H), 5.12 (t, *J* = 7.8 Hz, 1H), 5.01 (s, 1H), 3.05 – 2.92 (m, 2H), 2.78 – 2.69 (m, 2H), 1.35 (s, 18H) ; **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 200.3, 152.1, 138.7, 136.9, 135.7, 134.9, 132.8, 131.4, 130.7, 129.6, 128.9, 128.4, 128.3, 127.9, 127.4, 127.4, 126.8, 125.9, 125.8, 125.1, 124.9, 124.9, 124.7, 124.6, 124.5, 123.2, 45.2, 37.1, 34.3, 31.1, 30.3 ; **HRMS (ESI-TOF)** *m/z*: $[M - H]^-$ calcd for $C_{40}H_{39}O_2$ 551.2945; found 551.2971.

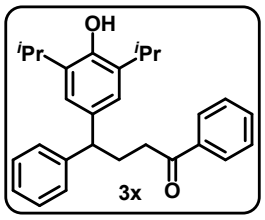
4-(3,5-di-tert-butyl-4-chlorophenyl)-4-(9H-fluoren-2-yl)-1-phenylbutan-1-one (3w) :



The product **3w** was obtained in 76% yield (103 mg, White solid); **mp** = 114-115 °C; R_f = 0.41 (10% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.84 (d, *J* = 7.7 Hz, 2H), 7.72 (dd, *J* = 11.9, 7.7 Hz, 2H), 7.50 (t, *J* = 6.4 Hz, 2H), 7.46 (s, 1H), 7.38 (dd, *J* = 13.2, 5.6 Hz, 2H), 7.32 (t, *J* = 7.9 Hz, 2H), 7.28 – 7.24 (m, 1H), 7.09 (s, 2H), 5.05 (d, *J* = 1.6 Hz, 1H), 3.99 (t, *J* = 7.6 Hz, 1H), 3.85 (s, 2H), 2.94 (t, *J* = 7.2 Hz, 2H), 2.50 (dd, *J* = 14.3, 7.1 Hz, 2H), 1.40 (s, 18H); **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 200.4, 152.1, 143.6, 143.2, 141.6, 139.8, 137.0, 135.7, 135.2, 132.9, 128.5, 128.0, 126.6, 126.5, 126.3, 125.0, 124.6, 124.2, 119.8, 119.6, 50.8, 37.2, 36.9, 34.4, 30.9, 30.3; **HRMS (ESI-TOF)** *m/z*: $[M - H]^-$ calcd for $C_{37}H_{39}O_2$ 515.2945; found 515.2963.

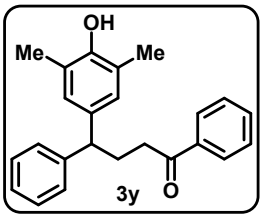
4-(4-hydroxy-3,5-diisopropylphenyl)-1,4-diphenylbutan-1-one (3x) :



The product **3x** was obtained in 92% yield (138 mg, White solid); **mp** = 118-119 °C; $\boldsymbol{R_f}$ = 0.35 (10% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.84 – 7.82 (m, 2H), 7.51 – 7.47 (m, 1H), 7.38 (t, *J* = 7.6 Hz, 2H), 7.27 (d, *J* = 4.4 Hz, 4H), 7.16 (dq, *J* = 8.5, 4.3 Hz, 1H), 6.93 (s, 2H), 4.79 (s, 1H), 3.93 (t, *J* = 7.9 Hz, 1H), 3.16 – 3.06 (m, 2H), 2.97 – 2.84 (m, 2H), 2.53 – 2.39 (m, 2H), 1.22 (d, *J* = 2.7 Hz, 6H), 1.20 (d, *J* = 2.7 Hz, 6H) ; **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 200.4, 148.4, 145.0, 136.9, 136.1, 133.6, 132.9, 128.4, 128.4, 128.0, 127.7, 126.0, 122.8, 50.5, 37.1, 30.5, 27.3, 22.7; **HRMS (ESI-TOF)** *m/z*: [M – H]$^-$ calcd for $C_{28}H_{31}O_2$ 399.2319; found 399.2338.

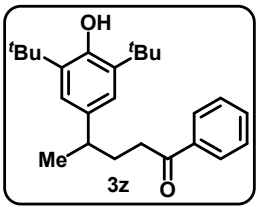
4-(4-hydroxy-3,5-dimethylphenyl)-1,4-diphenylbutan-1-one (3y) :



The product **3y** was obtained in 63% yield (104 mg, sticky solid); $\boldsymbol{R_f}$ = 0.26 (10% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.85 – 7.83 (m, 2H), 7.52 – 7.48 (m, 1H), 7.38 (dd, *J* = 10.6, 4.7 Hz, 2H), 7.28 – 7.26 (m, 4H), 7.16 (ddd, *J* = 8.6, 6.1, 2.8 Hz, 1H), 6.86 (s, 2H), 4.69 (s, 1H), 3.86 (t, *J* = 8.0 Hz, 1H), 2.93 – 2.89 (m, 2H), 2.44 (dd, *J* = 15.2, 7.7 Hz, 2H), 2.18 (s, 6H); **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 200.3, 150.6, 145.0, 136.9, 135.9, 132.9, 128.5, 128.4, 128.0, 127.9, 127.7, 126.1, 123.0, 49.8, 37.0, 30.0, 16.0; **HRMS (ESI-TOF)** *m/z*: [M – H]$^-$calcd for $C_{24}H_{23}O_2$ 343.1693; found 343.1710.

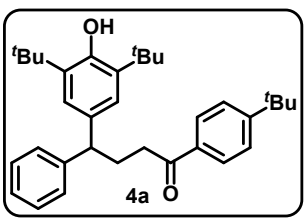
4-(3,5-di-tert-butyl-4-hydroxyphenyl)-1-phenylpentan-1-one (3z) :



The product **3z** was obtained in 89% yield (140 mg, White solid); **mp** = 93-94 °C; $\boldsymbol{R_f}$ = 0.59 (10% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.87 – 7.84 (m, 2H), 7.55 – 7.51 (m, 1H), 7.44 – 7.40 (m, 2H), 6.98 (s, 2H), 5.05 (s, 1H), 2.92 – 2.77 (m, 2H), 2.78 – 2.67 (m, 1H), 2.07 – 1.89 (m, 2H), 1.43 (s, 18H), 1.29 (d, *J* = 7.0 Hz, 3H) ; **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 200.8, 151.9, 137.1, 137.0, 135.7, 132.8, 128.5, 128.0, 123.4, 39.3, 36.9, 34.4, 33.2, 30.4, 22.4 ; **HRMS (ESI-TOF)** *m/z*: [M – H]$^-$calcd for $C_{25}H_{33}O_2$ 365.2475; found 365.2493.

1-(4-(tert-butyl)phenyl)-4-(3,5-di-tert-butyl-4-hydroxyphenyl)-4-phenylbutan-1-one (4a) :

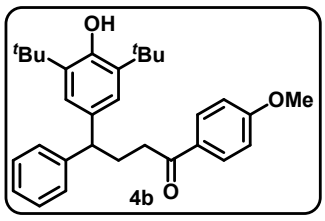


The product **4a** was obtained in 71% yield (117 mg, White solid); **mp** = 99-100 °C; $\boldsymbol{R_f}$ = 0.62 (10% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.81 (d, *J* = 8.3 Hz, 2H), 7.45 (d, *J* = 8.4 Hz, 2H), 7.32 (d, *J* = 4.4 Hz, 4H), 7.23 – 7.18 (m, 1H), 7.07 (s, 2H), 5.07 (s, 1H), 3.94 (t, *J* = 7.9 Hz, 1H), 2.93 – 2.90 (m, 2H), 2.48 (dd, *J* = 14.8, 7.0 Hz, 2H), 1.43 (s, 18H), 1.35 (s, 9H); **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 200.0, 156.5, 152.1, 144.9, 135.6, 135.0,

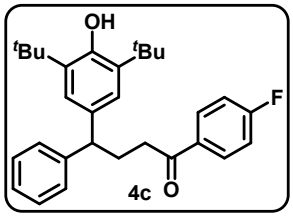
134.4, 128.4, 128.0, 127.9, 126.1, 125.4, 124.3, 50.7, 37.0, 35.0, 34.3, 31.0, 30.8, 30.3; **HRMS (ESI-TOF)** *m/z*: [M – H]$^-$ calcd for $C_{34}H_{43}O_2$ 483.3258; found 483.3274.

4-(3,5-di-tert-butyl-4-hydroxyphenyl)-1-(4-methoxyphenyl)-4-phenylbutan-1-one (4b) :



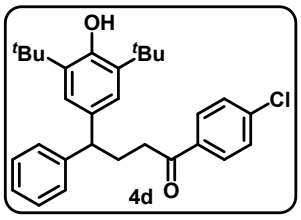
The product **4b** was obtained in 86% yield (134 mg, White solid); **mp** = 103-104 °C; $\boldsymbol{R_f}$ = 0.35 (10% EtOAc in petroleum ether); **^{1}H NMR (400 MHz, $CDCl_3$) δ** = 7.84 (d, *J* = 8.7 Hz, 2H), 7.30 (d, *J* = 4.3 Hz, 4H), 7.22 – 7.17 (m, 1H), 7.06 (s, 2H), 6.89 (d, *J* = 8.7 Hz, 2H), 5.06 (s, 1H), 3.92 (t, *J* = 7.9 Hz, 1H), 3.85 (s, 3H), 2.87 (td, *J* = 6.8, 2.1 Hz, 2H), 2.46 (dd, *J* = 15.0, 7.4 Hz, 2H), 1.41 (s, 18H); **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 198.9, 163.3, 152.1, 144.9, 135.6, 135.0, 130.3, 130.1, 128.4, 127.9, 126.1, 124.2, 113.6, 55.4, 50.8, 36.8, 34.3, 30.9, 30.3; **HRMS (ESI-TOF)** *m/z*: [M – H]$^-$ calcd for $C_{31}H_{37}O_3$ 457.2737; found 457.2750.

4-(3,5-di-tert-butyl-4-hydroxyphenyl)-1-(4-fluorophenyl)-4-phenylbutan-1-one (4c):



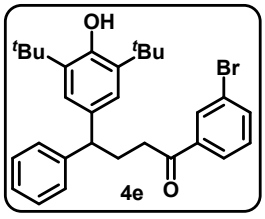
The product **4c** was obtained in 86% yield (134 mg, White solid); **mp** = 82-83 °C; $\boldsymbol{R_f}$ = 0.69 (10% EtOAc in petroleum ether); **^{1}H NMR (400 MHz, $CDCl_3$) δ** = 7.89 – 7.85 (m, 2H), 7.33 – 7.30 (m, 4H), 7.23 – 7.18 (m, 1H), 7.11 – 7.08 (m, 2H), 7.06 (s, 2H), 5.07 (s, 1H), 3.92 (t, *J* = 7.9 Hz, 1H), 2.89 (td, *J* = 7.0, 2.7 Hz, 2H), 2.46 (q, *J* = 7.3 Hz, 2H), 1.41 (s, 18H); **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 198.7, 165.6 (d, $J_{C\text{-}F}$ = 153.99 Hz), 152.1, 144.7, 135.6, 134.8, 133.4, 133.3, 130.6 (d, $J_{C\text{-}F}$ = 8.63 Hz), 128.1 (d, $J_{C\text{-}F}$ = 62.30 Hz), 126.1, 124.2, 115.5 (d, $J_{C\text{-}F}$ = 22.04 Hz), 50.7, 37.0, 34.3, 30.7, 30.3; **^{19}F NMR (376 MHz, $CDCl_3$) δ =** -105.56; **HRMS (ESI-TOF)** *m/z*: [M – H]$^-$ calcd for $C_{30}H_{34}FO_2$ 445.2537; found 445.2560.

1-(4-chlorophenyl)-4-(3,5-di-tert-butyl-4-hydroxyphenyl)-4-phenylbutan-1-one (4d) :



The product **4d** was obtained in 83% yield (131 mg, White solid); **mp** = 84-85 °C; $\boldsymbol{R_f}$ = 0.53 (10% EtOAc in petroleum ether); **^{1}H NMR (500 MHz, $CDCl_3$) δ** = 7.81 (d, *J* = 8.3 Hz, 2H), 7.40 (d, *J* = 8.5 Hz, 2H), 7.33 (d, *J* = 3.9 Hz, 4H), 7.22 (dt, *J* = 8.5, 4.1 Hz, 1H), 7.09 (s, 2H), 5.11 (s, 1H), 3.95 (t, *J* = 7.6 Hz, 1H), 2.94 – 2.91 (m, 2H), 2.50 (dd, *J* = 14.3, 7.1 Hz, 2H), 1.45 (s, 18H); **^{13}C{^{1}H} NMR (125 MHz,$CDCl_3$) δ** = 199.0, 152.1, 144.7, 139.2, 135.7, 135.2, 134.8, 129.4, 128.7, 128.4, 127.8, 126.1, 124.2, 50.7, 37.0, 34.3, 30.6, 30.3; **HRMS (ESI-TOF)** *m/z*: [M – H]$^-$ calcd for $C_{30}H_{34}ClO_2$ 461.2242; found 461.2258.

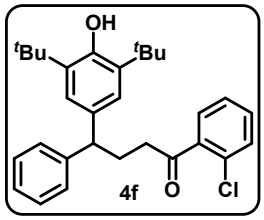
1-(3-bromophenyl)-4-(3,5-di-tert-butyl-4-hydroxyphenyl)-4-phenylbutan-1-one (4e):



The product **4e** was obtained in 90% yield (155 mg, sticky solid); $\boldsymbol{R_f}$ = 0.73 (10% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.88 (t, *J* = 1.8 Hz, 1H), 7.66 – 7.63 (m, 1H), 7.55 (ddd, *J* = 8.0, 2.0, 1.0 Hz, 1H), 7.24 – 7.16 (m, 5H), 7.13 – 7.08 (m, 1H), 6.95 (s, 2H), 4.97 (s, 1H), 3.82 (t, *J* = 8.0 Hz, 1H), 2.80 (dd, *J* = 10.4, 4.9 Hz, 2H), 2.40 – 2.34 (m, 2H), 1.31 (s, 18H); **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 198.8, 152.1, 144.6, 138.6, 135.7, 135.6, 134.7, 131.0, 130.0, 128.5, 127.8, 126.5, 126.2, 124.2, 122.8, 50.6, 37.1, 34.3, 30.5, 30.3; **HRMS (ESI-TOF)** *m/z*: $[M - H]^-$ calcd for $C_{30}H_{34}BrO_2$ 505.1737; found 505.1761.

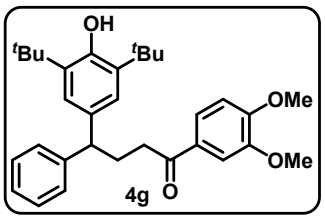
1-(2-chlorophenyl)-4-(3,5-di-tert-butyl-4-hydroxyphenyl)-4-phenylbutan-1-one (4f):



The product **4f** was obtained in 77% yield (121 mg, sticky solid); R_f = 0.44 (10% EtOAc in petroleum ether);

^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.37 – 7.30 (m, 2H), 7.28 – 7.23 (m, 6H), 7.17 (td, *J* = 5.9, 2.9 Hz, 1H), 7.03 (s, 2H), 5.04 (s, 1H), 3.88 (t, *J* = 8.0 Hz, 1H), 2.92 – 2.81 (m, 2H), 2.46 – 2.41 (m, 2H), 1.39 (s, 18H) ; **^{13}C{^{1}H} NMR (125 MHz,$CDCl_3$) δ** = 203.5, 152.1, 144.7, 139.7, 135.7, 134.6, 131.4, 130.7, 130.4, 128.6, 128.4, 127.8, 126.8, 126.1, 124.3, 50.6, 41.6, 34.3, 30.4, 30.3; **HRMS (ESI-TOF)** *m/z*: $[M - H]^-$ calcd for $C_{30}H_{34}ClO_2$ 461.2243; found 461.2259.

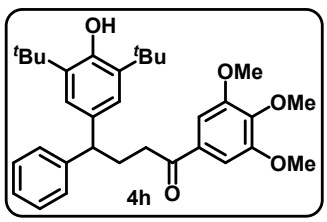
4-(3,5-di-tert-butyl-4-hydroxyphenyl)-1-(3,4-dimethoxyphenyl)-4-phenylbutan-1-one (4g) :



The product **4g** was obtained in 85% yield (141 mg, White solid); **mp** = 151-152 °C; R_f = 0.55 (20% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.47 (d, *J* = 1.9 Hz, 1H), 7.40 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.28 (t, *J* = 6.5 Hz, 4H), 7.18 (dq, *J* = 8.6, 4.2 Hz, 1H), 7.04 (s, 2H), 6.80 (d, *J* = 8.4 Hz, 1H), 5.04 (s, 1H), 3.93 (s, 1H), 3.90 (s, 3H), 3.89 (s, 3H), 2.88 – 2.85 (m, 2H), 2.44 (q, *J* = 7.3 Hz, 2H), 1.39 (s, 18H); **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 199.0, 153.0, 152.0, 148.9, 144.8, 135.6, 135.0, 130.2, 128.4, 127.8, 126.0, 124.2, 122.6, 110.0, 109.8, 55.9, 55.9, 50.7, 36.5, 34.3, 31.0, 30.3; **HRMS (ESI-TOF)** *m/z*: $[M - H]^-$ calcd for $C_{32}H_{39}O_4$ 487.2843; found 487.2857.

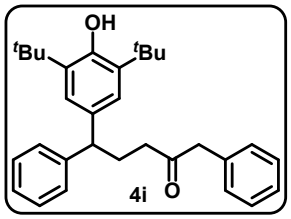
4-(3,5-di-tert-butyl-4-hydroxyphenyl)-4-phenyl-1-(3,4,5-trimethoxyphenyl)butan-1-one (4h):



The product **4h** was obtained in 89% yield (157 mg, sticky solid); R_f = 0.54 (20% EtOAc in petroleum ether); **^{1}H NMR (400 MHz, $CDCl_3$) δ** = 7.31 – 7.28 (m, 4H), 7.26 (s, 1H), 7.08 (s, 2H), 7.02 (s, 2H), 5.04 (s, 1H), 3.90 (s, 1H), 3.89 (s, 3H), 3.85 (s, 6H), 2.87 (td, *J* = 7.3, 3.0 Hz, 2H), 2.44 (tdd, *J* = 10.1, 5.7, 2.8 Hz, 2H), 1.38 (s, 18H) ; **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 199.2, 153.0, 152.1, 144.8, 135.6, 135.0, 132.3, 130.1, 128.5, 128.0, 126.1, 124.3, 105.6, 60.9,

56.2, 50.6, 36.7, 34.3, 31.0, 30.3, 29.4 ; **HRMS (ESI-TOF)** *m/z*: [M – H]$^-$ calcd for $C_{33}H_{41}O_5$ 517.2949; found 517.2960.

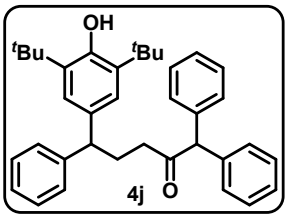
5-(3,5-di-tert-butyl-4-hydroxyphenyl)-1,5-diphenylpentan-2-one (4i):



The product **4i** was obtained in 87% yield (131 mg, sticky solid); $\boldsymbol{R_f}$ = 0.60 (10% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.30 – 7.22 (m, 5H), 7.21 – 7.14 (m, 3H), 7.14 – 7.09 (m, 2H), 6.98 (s, 2H), 5.04 (s, 1H), 3.76 (t, *J* = 7.9 Hz, 1H), 3.56 (s, 2H), 2.42 – 2.38 (m, 2H), 2.29 – 2.23 (m, 2H), 1.39 (s, 18H) ; **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 208.2, 152.0, 144.7, 135.6, 134.8, 134.2, 129.3, 128.6, 128.4, 127.8, 126.9, 126.0, 124.2, 50.4, 50.1, 40.5, 34.3, 30.3, 30.0; **HRMS (ESI-TOF)** *m/z*: [M – H]$^-$ calcd for $C_{31}H_{37}O_2$ 441.2788; found 441.2798.

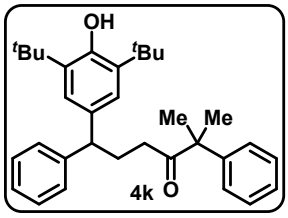
5-(3,5-di-tert-butyl-4-hydroxyphenyl)-1,1,5-triphenylpentan-2-one (4j):



The product **4j** was obtained in 94% yield (165 mg, sticky solid); $\boldsymbol{R_f}$ = 0.56 (10% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.30 – 7.22 (m, 8H), 7.15 (dd, *J* = 8.0, 7.0 Hz, 7H), 6.97 (s, 2H), 5.03 (s, 1H), 5.00 (s, 1H), 3.77 (t, *J* = 7.9 Hz, 1H), 2.88 – 2.74 (m, 1H), 2.53 – 2.49 (m, 2H), 2.29 (dd, *J* = 14.9, 7.5 Hz, 2H), 1.37 (s, 18H) ; **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 208.5, 152.0, 144.6, 138.4, 138.3, 135.5, 134.7, 129.3, 128.9, 128.8, 128.6, 128.4, 127.8, 127.1, 127.0, 126.0, 124.1, 64.1, 50.3, 43.4, 41.4, 34.3, 30.3 ; **HRMS (ESI-TOF)** *m/z*: [M – H]$^-$ calcd for $C_{37}H_{41}O_2$ 517.3101; found 517.3125.

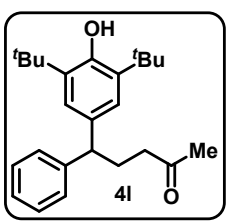
6-(3,5-di-tert-butyl-4-hydroxyphenyl)-2-methyl-2,6-diphenylhexan-3-one (4k):



The product **4k** was obtained in 75% yield (120 mg, Semi-solid); $\boldsymbol{R_f}$ = 0.62 (10% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.30 – 7.25 (m, 2H), 7.23 – 7.14 (m, 5H), 7.12 – 7.07 (m, 3H), 6.90 (s, 2H), 4.99 (s, 1H), 3.64 (t, *J* = 7.3 Hz, 1H), 2.14 (d, *J* = 3.8 Hz, 4H), 1.38 (s, 3H), 1.37 (s, 3H), 1.36 (s, 18H) ; **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 213.1, 152.0, 144.7, 144.0, 135.5, 135.0, 128.6, 128.3, 127.8, 126.7, 126.0, 125.9, 124.2, 52.2, 50.4, 36.1, 34.3, 30.9, 30.3, 25.2, 25.1; **HRMS (ESI-TOF)** *m/z*: [M – H]$^-$ calcd for $C_{33}H_{41}O_2$ 469.3101; found 469.3123.

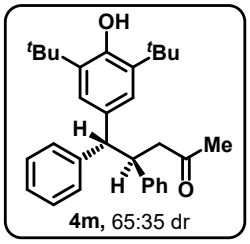
5-(3,5-di-tert-butyl-4-hydroxyphenyl)-5-phenylpentan-2-one (4l):



The product **4l** was obtained in 93% yield (115 mg, White solid); **mp** = 89-90 °C; $\boldsymbol{R_f}$ = 0.62 (10% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.31 – 7.21 (m, 4H), 7.20 – 7.13 (m, 1H), 7.01 (s, 2H), 5.04 (s, 1H), 3.78 (t, *J* = 7.9 Hz, 1H), 2.38 (dd, *J* = 10.9, 5.1 Hz, 2H), 2.32 – 2.24 (m, 2H), 2.04 (s, 3H), 1.40 (s, 18H) ; **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = ^{13}C NMR (101 MHz, $CDCl_3$) δ 208.8, 152.1, 144.7, 135.6, 134.9, 128.4, 127.8, 126.1, 124.1, 50.6, 42.2, 34.3, 30.3, 30.0, 30.0 ; **HRMS (ESI-TOF)** *m/z*: $[M - H]^-$ calcd for $C_{25}H_{33}O_2$ 365.2475; found 365.2479.

5-(3,5-di-tert-butyl-4-hydroxyphenyl)-4,5-diphenylpentan-2-one (4m):

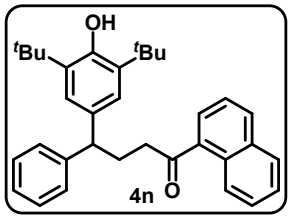


4m, 65:35 dr

The product **4m** was obtained in 73% yield (109 mg, White solid); dr = 65:35; **mp** = 84-85 °C; R_f = 0.44 (10% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.38 (dd, *J* = 8.1, 1.0 Hz, 1.09$H_{major\ \&\ minor}$), 7.28 (dd, *J* = 10.6, 4.9 Hz, 1.20$H_{major\ \&\ minor}$), 7.18 – 7.13 (m, 1.01$H_{major\ \&\ minor}$), 7.13 – 7.06 (m, 6.93$H_{major\ \&\ minor}$), 7.06 – 6.94 (m, 7.18$H_{major\ \&\ minor}$), 6.93 – 6.88 (m, 1.13$H_{major\ \&\ minor}$), 6.70 (s, 1.06$H_{major\ \&\ minor}$), 5.03 (s, 1H_{major}), 4.80 (s, 0.51H_{minor}), 4.06 – 3.83 (m, 3.14$H_{major\ \&\ minor}$), 2.82 – 2.59 (m, 3.12$H_{major\ \&\ minor}$), 1.77 (s, 1.58H_{minor}), 1.69 (s, 3.01H_{major}), 1.39 (s, 18H_{major}), 1.21 (s, 9.79H_{minor}) ; **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = major diastereomer: 207.7, 152.3, 143.6, 143.4, 135.8, 133.4, 128.2, 128.0, 128.0, 127.9, 126.0, 125.6, 124.9, 58.4, 49.5, 45.9, 34.3, 30.6, 30.3 ; minor diastereomer: 207.9, 151.5, 143.4, 142.9, 134.9, 133.0, 128.7, 128.3, 128.3, 127.8, 126.4, 126.0, 124.8, 58.2, 48.8, 46.6, 34.1, 30.8, 30.1 ; **HRMS (ESI-TOF)** *m/z*: $[M - H]^-$ calcd for $C_{31}H_{37}O_2$ 441.2788; found 441.2809.

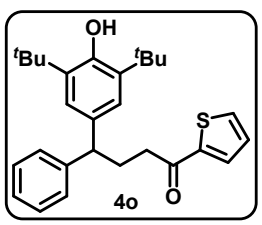
4-(3,5-di-tert-butyl-4-hydroxyphenyl)-1-(naphthalen-1-yl)-4-phenylbutan-1-one (4n):



The product **4n** was obtained in 92% yield (149 mg, White solid); **mp** = 100-101 °C; R_f = 0.44 (10% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.50 – 8.48 (m, 1H), 7.91 (d, *J* = 8.2 Hz, 1H), 7.83 (dd, *J* = 8.3, 1.0 Hz, 1H), 7.59 (dd, *J* = 7.2, 1.1 Hz, 1H), 7.54 (ddd, *J* = 8.5, 6.9, 1.6 Hz, 1H), 7.49 (ddd, *J* = 8.0, 6.9, 1.3 Hz, 1H), 7.38 (dd, *J* = 8.1, 7.3 Hz, 1H), 7.28 (dd, *J* = 8.3, 5.6 Hz, 4H), 7.17 (ddd, *J* = 8.6, 5.7, 2.8 Hz, 1H), 7.05 (s, 2H), 5.04 (s, 1H), 3.95 (t, *J* = 8.0 Hz, 1H), 3.01 – 2.97 (m, 2H), 2.55 – 2.49 (m, 2H), 1.38 (s, 18H) ; **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 204.7, 152.1, 144.8, 136.3, 135.7, 134.8, 133.9, 132.2, 130.0, 128.5, 128.3, 127.9, 127.7, 127.1, 126.3, 126.1, 125.7, 124.3, 50.7, 40.8, 34.3, 31.0, 30.3 ; **HRMS (ESI-TOF)** *m/z*: $[M - H]^-$ calcd for $C_{34}H_{37}O_2$ 477.2788; found 477.2814.

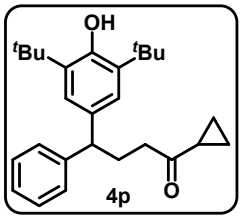
4-(3,5-di-tert-butyl-4-hydroxyphenyl)-4-phenyl-1-(thiophen-2-yl)butan-1-one (4o):



The product **4o** was obtained in 89% yield (81 mg, White solid); **mp** = 97-98 °C; R_f = 0.41 (10% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.57 (dd, *J* = 4.9, 1.1 Hz, 1H), 7.50 (dd, *J* = 3.8, 1.1 Hz, 1H), 7.29 (s, 2H), 7.28 (s, 2H), 7.21 – 7.16 (m, 1H), 7.06 – 7.04 (m, 1H), 7.04 (s, 2H), 5.05 (s, 1H), 3.90 (t, *J* = 8.0 Hz, 1H), 2.84 (dd, *J* = 8.6, 6.7 Hz, 2H), 2.49 – 2.43 (m, 2H), 1.39 (s, 18H); **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 193.2, 152.1, 144.7, 144.4, 135.6, 134.7, 133.4, 131.7, 128.4, 127.9, 127.9, 126.1, 124.3, 50.6, 37.8, 34.3, 31.0, 30.3; **HRMS (ESI-TOF)** *m/z*: $[M - H]^-$ calcd for $C_{28}H_{33}O_2S$ 433.2196; found 433.2217.

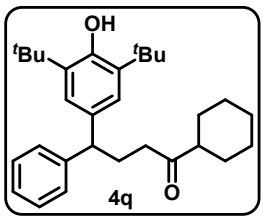
1-cyclopropyl-4-(3,5-di-tert-butyl-4-hydroxyphenyl)-4-phenylbutan-1-one (4p):



The product **4p** was obtained in 71% yield (94 mg, White solid); **mp** = 114-115 °C; R_f = 0.47 (10% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.31 – 7.24 (m, 4H), 7.19 – 7.15 (m, 1H), 7.01 (s, 2H), 5.03 (s, 1H), 3.80 (t, *J* = 7.9 Hz, 1H), 2.50 (dd, *J* = 8.3, 6.5 Hz, 2H), 2.31 (q, *J* = 7.1 Hz, 2H), 1.85 – 1.79 (m, 1H), 1.40 (s, 18H), 0.99 – 0.95 (m, 2H), 0.82 – 0.78 (m, 2H); **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 210.8, 152.0, 144.8, 135.6, 135.0, 128.4, 127.9, 126.0, 124.2, 50.7, 41.9, 34.3, 30.3, 30.2, 20.5, 10.6; **HRMS (ESI-TOF)** *m/z*: $[M - H]^-$ calcd for $C_{27}H_{35}O_2$ 391.2632; found 391.2649.

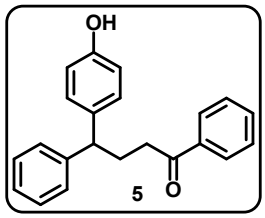
1-cyclohexyl-4-(3,5-di-tert-butyl-4-hydroxyphenyl)-4-phenylbutan-1-one (4q):



The product **4q** was obtained in 82% yield (121 mg, Semi-solid); R_f = 0.78 (10% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.32 – 7.26 (m, 4H), 7.21 – 7.16 (m, 1H), 7.04 (s, 2H), 5.07 (s, 1H), 3.82 (t, *J* = 7.8 Hz, 1H), 2.43 – 2.36 (m, 2H), 2.34 – 2.22 (m, 3H), 1.75 – 1.73 (m, 5H), 1.43 (s, 18H), 1.29 – 1.19 (m, 5H); **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 214.0, 152.0, 144.9, 135.5, 134.9, 128.3, 127.8, 126.0., 124.2, 50.8, 50.6, 39.0, 34.3, 30.3, 29.9, 28.4, 25.8, 25.6, 12.6, 7.5; **HRMS (ESI-TOF)** *m/z*: $[M - H]^-$ calcd for $C_{30}H_{41}O_2$ 433.3101; found 433.3111.

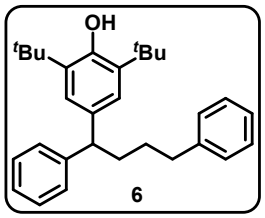
4-(4-hydroxyphenyl)-1,4-diphenylbutan-1-one (5):



The product **5** was obtained in 89% yield (66 mg, Yellow solid); **mp** = 77-78 °C; R_f = 0.56 (10% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.84 – 7.82 (m, 2H), 7.51 – 7.47 (m, 1H), 7.40 – 7.36 (m, 2H), 7.27 (d, *J* = 1.3 Hz, 3H), 7.26 (s, 4H), 7.20 – 7.14 (m, 2H), 4.01 (t, *J* = 7.9 Hz, 1H), 2.93 – 2.89 (m, 2H), 2.49 (dd, *J* = 15.0, 7.8 Hz, 2H) ; **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 199.9, 144.4, 136.9, 132.9, 128.5, 128.5, 127.9, 127.8, 126.3, 50.5, 36.9, 29.8.

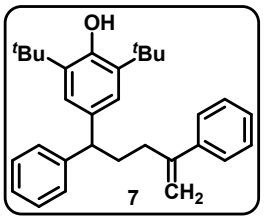
2,6-di-tert-butyl-4-(1,4-diphenylbutyl)phenol (6):



The product **6** was obtained in 95% yield (92 mg, sticky solid); R_f = 0.74 (10% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.35 – 7.29 (m, 6H), 7.24 – 7.18 (m, 4H), 7.08 (s, 2H), 5.08 (s, 1H), 3.89 (t, *J* = 7.8 Hz, 1H), 2.70 (t, *J* = 7.6 Hz, 2H), 2.16 – 2.07 (m, 2H), 1.70 – 1.62 (m, 2H), 1.47 (s, 18H) ; **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 151.9, 145.6, 142.5, 135.6, 135.4, 128.4, 128.3, 128.2, 127.8, 125.8, 125.6, 124.2, 51.3, 35.9, 35.8, 34.3, 30.3, 29.9 ; **HRMS (ESI-TOF)** *m/z*: $[M - H]^-$ calcd for $C_{30}H_{37}O$ 413.2839; found 413.2859.

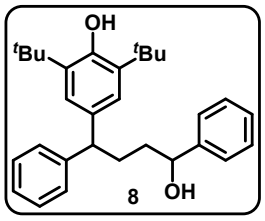
2,6-di-tert-butyl-4-(1,4-diphenylpent-4-en-1-yl)phenol (7):



The product **7** was obtained in 63% yield (62 mg, sticky solid); R_f = 0.78 (10% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.35 – 7.19 (m, 10H), 6.98 (s, 2H), 5.26 (s, 1H), 5.01 (s, 2H), 3.84 (t, *J* = 7.8 Hz, 1H), 2.46 – 2.42 (m, 2H), 2.13 (dd, *J* = 15.5, 7.8 Hz, 2H), 1.38 (s, 18H); **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 151.9, 148.4, 145.3, 141.1, 135.5, 135.3, 128.3, 128.2, 127.9, 127.3, 126.1, 125.9, 124.3, 112.5, 51.0, 35.1, 34.3, 33.9, 30.3; **HRMS (ESI-TOF)** *m/z*: $[M - H]^-$ calcd for $C_{31}H_{37}O$ 425.2839; found 425.2843.

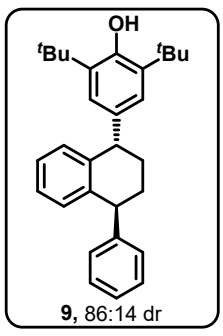
2,6-di-tert-butyl-4-(4-hydroxy-1,4-diphenylbutyl)phenol (8):



The product **8** was obtained in 87% yield (87 mg, sticky solid); R_f = 0.40 (10% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.31 – 7.17 (m, 9H), 7.14 – 7.10 (m, 1H), 6.96 (d, *J* = 3.3 Hz, 2H), 5.00 (s, 1H), 4.66 – 4.62 (m, 1H), 3.78 – 3.74 (m, 1H), 2.17 – 2.06 (m, 1H), 2.01 – 1.83 (m, 2H), 1.81 – 1.70 (m, 1H), 1.70 – 1.60 (m, 1H), 1.37 (s, 18H) ; **^{13}C{^{1}H} NMR (100 MHz,$CDCl_3$) δ** = 151.9, 145.4, 145.2, 144.5, 135.5, 135.4, 135.2, 128.4, 128.4, 128.3, 127.8, 127.7, 127.5, 127.5, 125.9, 125.9, 124.1, 124.1, 74.6, 74.4, 51.3, 51.2, 37.5, 37.4, 34.3, 32.4, 32.2, 30.3; **HRMS (ESI-TOF)** *m/z*: $[M - H]^-$ calcd for $C_{30}H_{37}O_2$ 429.2788; found 429.2798.

2,6-di-tert-butyl-4-(4-phenyl-1,2,3,4-tetrahydronaphthalen-1-yl)phenol (9):

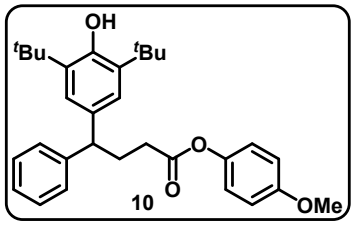


The product **9** was obtained in 94% yield (90 mg, White solid); dr = 86:14, **mp** = 151-152 °C; R_f = 0.78 (10% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.32 – 7.27 (m, 2.21$H_{major\ \&\ minor}$), 7.23 – 7.17 (m, 1.66$H_{major\ \&\ minor}$), 7.15 (dd, *J* = 5.2, 3.2 Hz, 2.14$H_{major\ \&\ minor}$), 7.07 (ddd, *J* = 13.4, 7.2, 3.1 Hz, 0.56$H_{major\ \&\ minor}$), 7.03 – 6.98 (m, 2.18$H_{major\ \&\ minor}$), 6.95 – 6.88 (m, 3.47$H_{major\ \&\ minor}$), 6.85 – 6.83 (m, 1$H_{major\ \&\ minor}$), 5.06 (s, 1H_{major}), 5.03

(s, 0.16H$_{minor}$), 4.26 – 4.19 (m, 1.16H$_{major\ \&\ minor}$), 4.13 (dd, *J* = 11.0, 7.7 Hz, 1.16H$_{major\ \&\ minor}$), 2.28 – 2.17 (m, 2.15H$_{major\ \&\ minor}$), 1.95 – 1.84 (m, 2.32H$_{major\ \&\ minor}$), 1.41 (s, 20.88H$_{major\ \&\ minor}$) ; **^{13}C{^{1}H} NMR (100 MHz,CDCl$_3$) δ** = major diastereomer: 151.9, 147.7, 140.8, 139.8, 137.7, 135.5, 135.4, 129.8, 129.7, 128.8, 128.3, 126.0, 125.8, 125.7, 125.3, 46.3, 46.2, 34.3, 32.1, 31.7, 30.4 ; minor diastereomer: 151.8, 147.5, 140.5, 139.4, 138.0, 135.4, 130.5, 130.0, 128.9, 128.1, 126.1, 126.0, 125.9, 125.4, 45.6, 45.3, 34.4, 30.4, 30.1, 30.0 ; **HRMS (ESI-TOF)** *m/z*: [M – H]$^-$ calcd for $C_{30}H_{35}O$ 411.2682; found 411.2694.

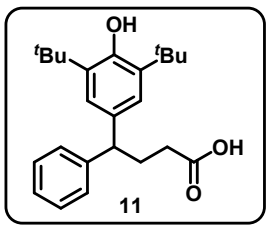
4-methoxyphenyl 4-(3,5-di-tert-butyl-4-hydroxyphenyl)-4-phenylbutanoate (10):



The product **10** was obtained in 74% yield (76 mg, White solid); **mp** = 82-83 °C; ***R$_f$*** = 0.44 (10% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, CDCl$_3$) δ = 7.34 (d, *J* = 4.3 Hz, 4H), 7.26 – 7.21 (m, 1H), 7.10 (s, 2H), 6.99 – 6.97 (m, 2H), 6.91 – 6.89 (m, 2H), 5.11 (s, 1H), 3.95 (t, *J* = 7.4 Hz, 1H), 3.81 (s, 3H), 2.57 – 2.46 (m, 4H), 1.45 (s, 18H) ; **^{13}C{^{1}H} NMR (100 MHz,CDCl$_3$) δ** = 172.4, 157.1, 152.1, 144.4, 144.1, 135.6, 134.5, 128.5, 127.8, 126.2, 124.2, 122.2, 114.3, 55.5, 50.7, 34.3, 33.0, 31.2, 30.3 ; **HRMS (ESI-TOF)** *m/z*: [M – H]$^-$ calcd for $C_{31}H_{37}O_4$ 473.2686; found 473.2710.

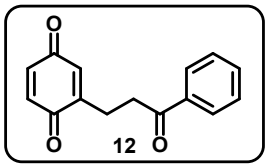
4-(3,5-di-tert-butyl-4-hydroxyphenyl)-4-phenylbutanoic acid (11):



The product **11** was obtained in 51% yield (20 mg, White solid); mp = 119-120 °C; ***R$_f$*** = 0.59 (20% EtOAc in petroleum ether);

^{1}H NMR (500 MHz, CDCl$_3$) δ = 7.30 – 7.24 (m, 5H), 7.20 – 7.16 (m, 1H), 7.01 (s, 2H), 5.05 (s, 1H), 3.83 (t, *J* = 7.5 Hz, 1H), 2.38 – 2.29 (m, 4H), 1.40 (s, 18H) ; **^{13}C{^{1}H} NMR (125 MHz,CDCl$_3$) δ** = 178.9, 152.2, 144.5, 135.7, 134.5, 128.5, 127.8, 126.2, 124.2, 50.6, 34.3, 32.5, 31.0, 30.3 ; **HRMS (ESI-TOF)** *m/z*: [M – H]$^-$ calcd for $C_{24}H_{31}O_3$ 367.2268; found 367.2279.

2-(3-oxo-3-phenylpropyl)cyclohexa-2,5-diene-1,4-dione (12):



The product **12** was obtained in 20% yield (36 mg, Yellow solid); ***R$_f$*** = 0.59 (20% EtOAc in petroleum ether);

^{1}H NMR (400 MHz, CDCl$_3$) δ = 7.95 (d, *J* = 7.6 Hz, 2H), 7.58 (t, *J* = 7.5 Hz, 1H), 7.47 (t, *J* = 7.7 Hz, 2H), 6.79 – 6.71 (m, 2H), 6.65 (d, *J* = 1.7 Hz, 1H), 3.26 (t, *J* = 7.1 Hz, 2H), 2.88 (t, *J* = 7.0 Hz, 2H) ; **^{13}C{^{1}H} NMR (100 MHz,CDCl$_3$) δ** = 197.9, 187.5, 187.4, 148.2, 136.8, 136.4, 136.3, 133.4, 133.3, 128.7, 128.0, 36.4, 24.0 ; **HRMS (ESI-TOF)** *m/z*: [M + H]$^+$ calcd for $C_{15}H_{13}O_3$ 241.0859; found 241.0855.

3. References:

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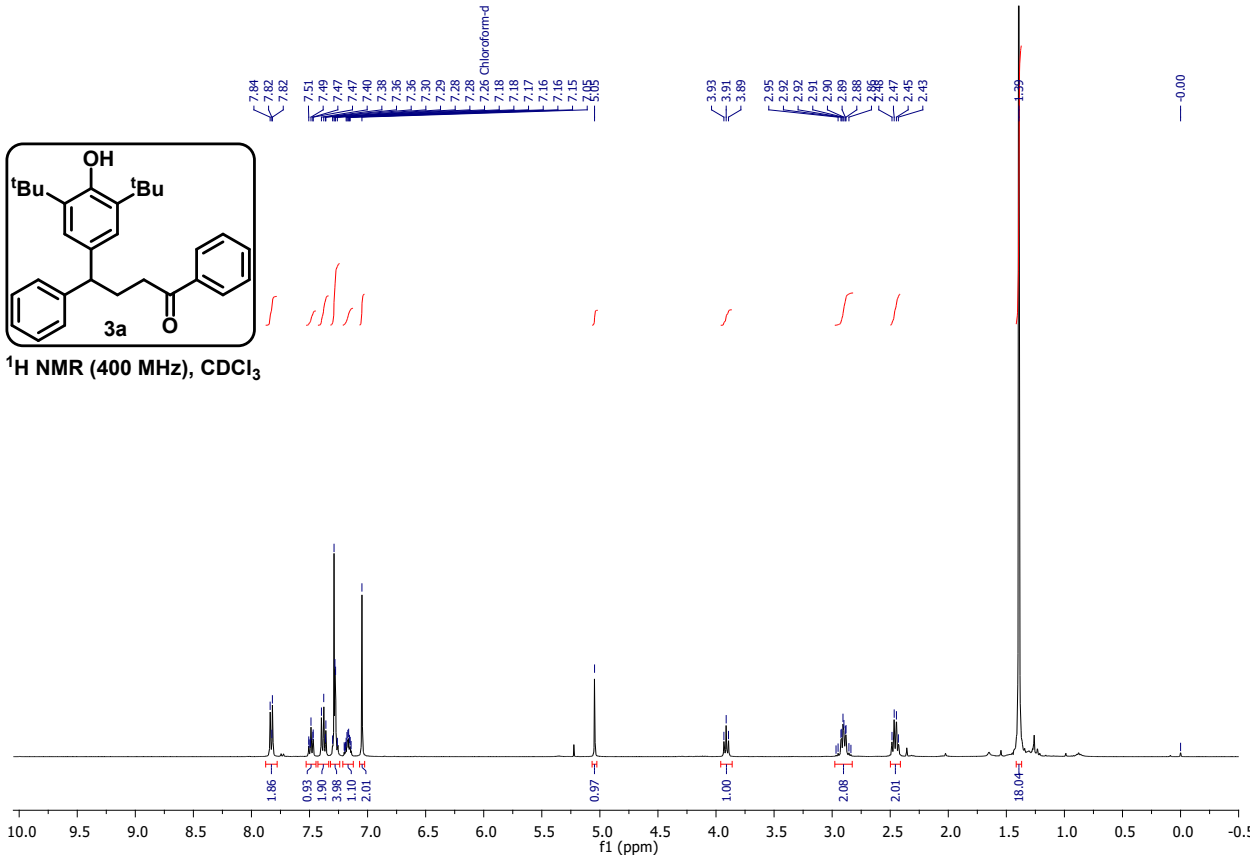
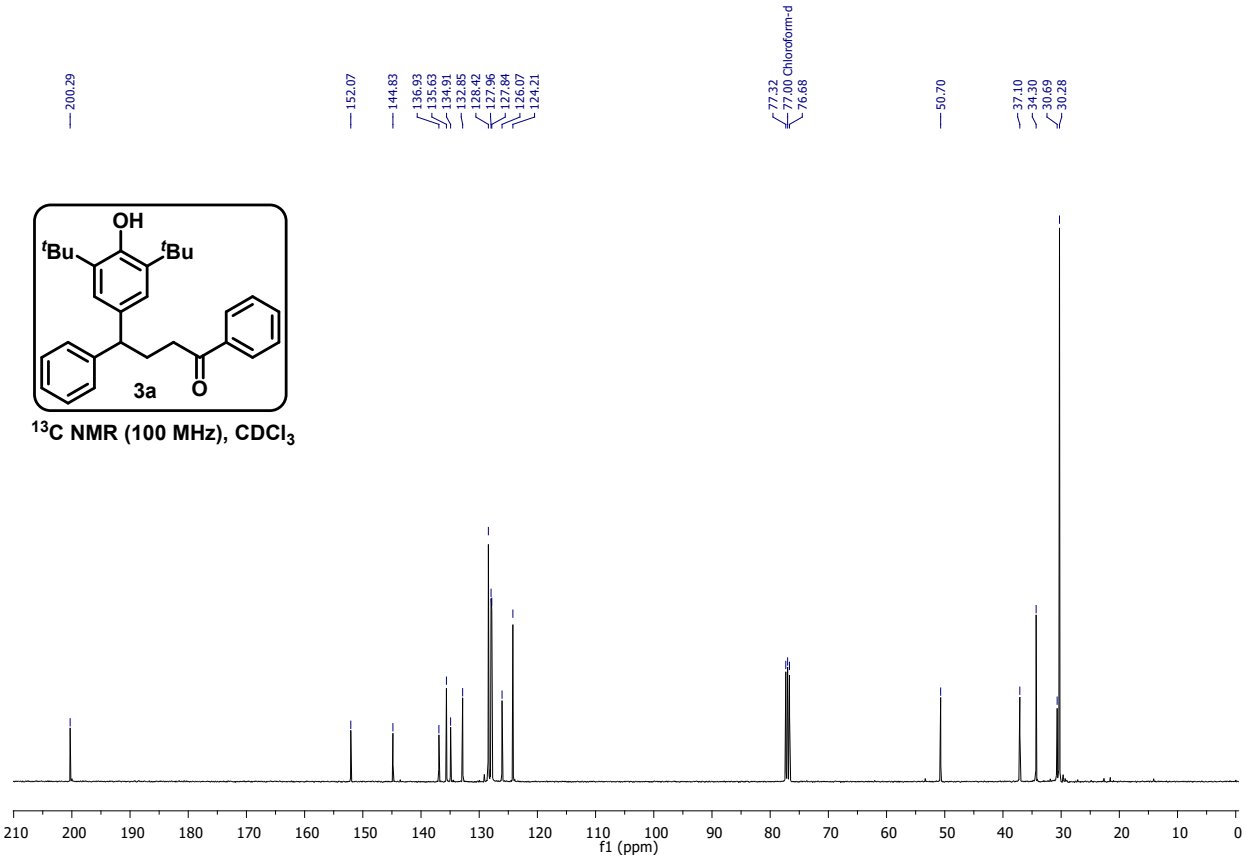
7. L. J. Farrugia, *J. Appl. Cryst*., 1997, **30,** 565–565.

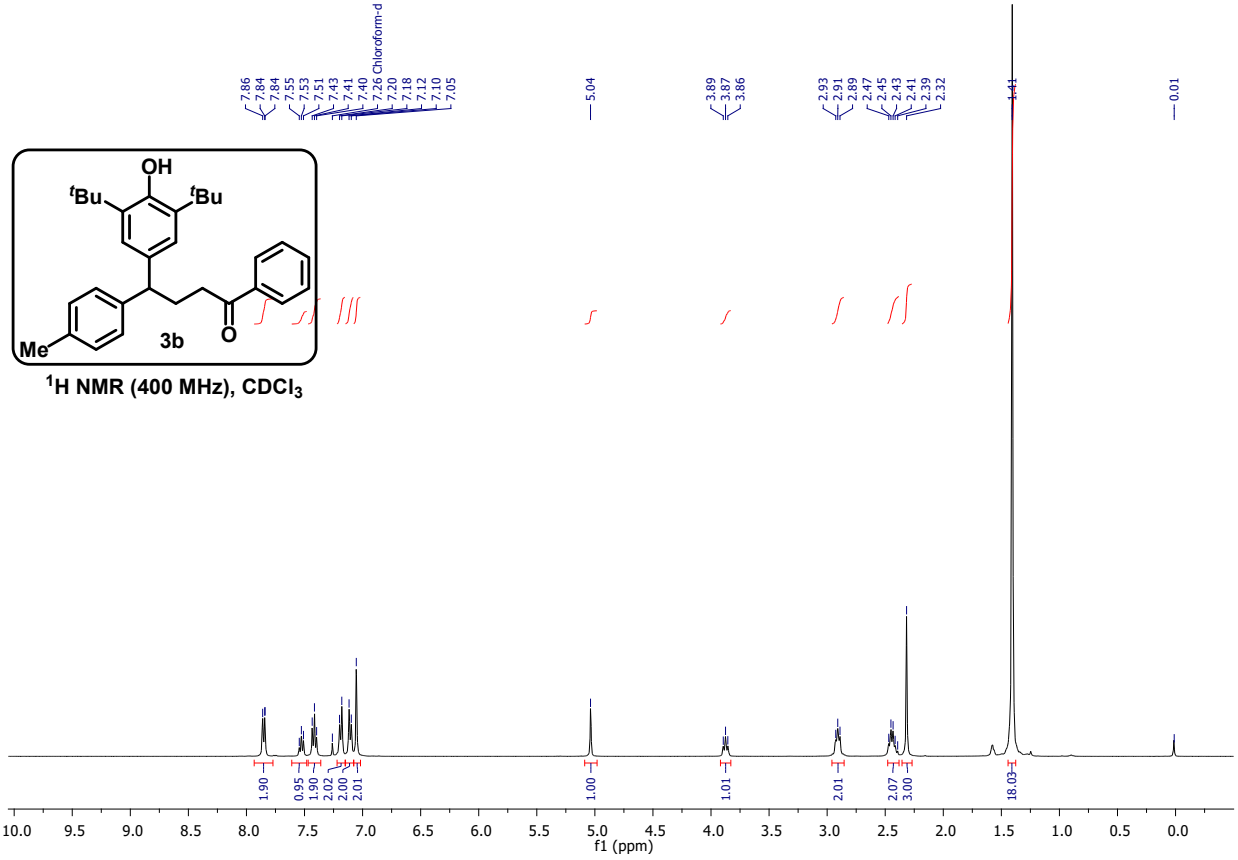
4. Spectral Data



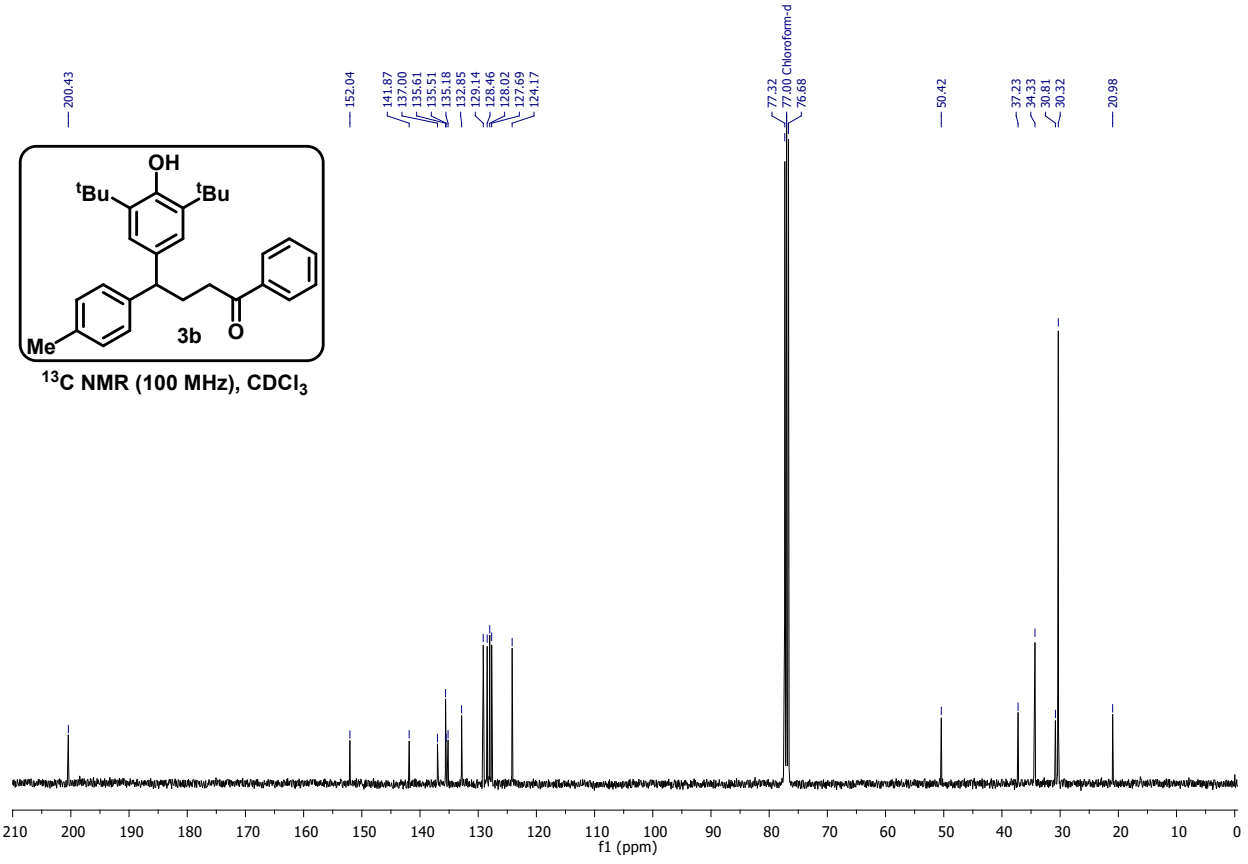
^{1}H NMR (400 MHz), $CDCl_3$



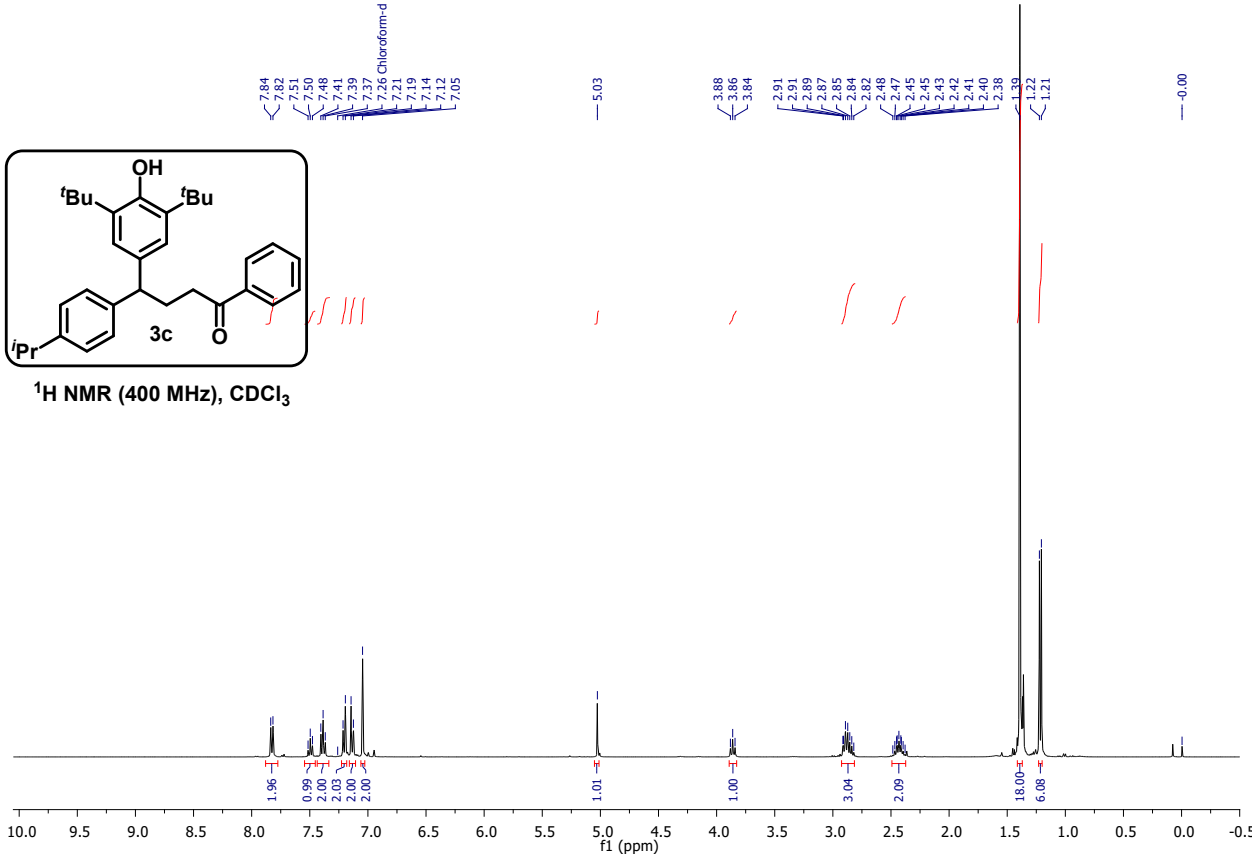
^{13}C NMR (100 MHz), $CDCl_3$



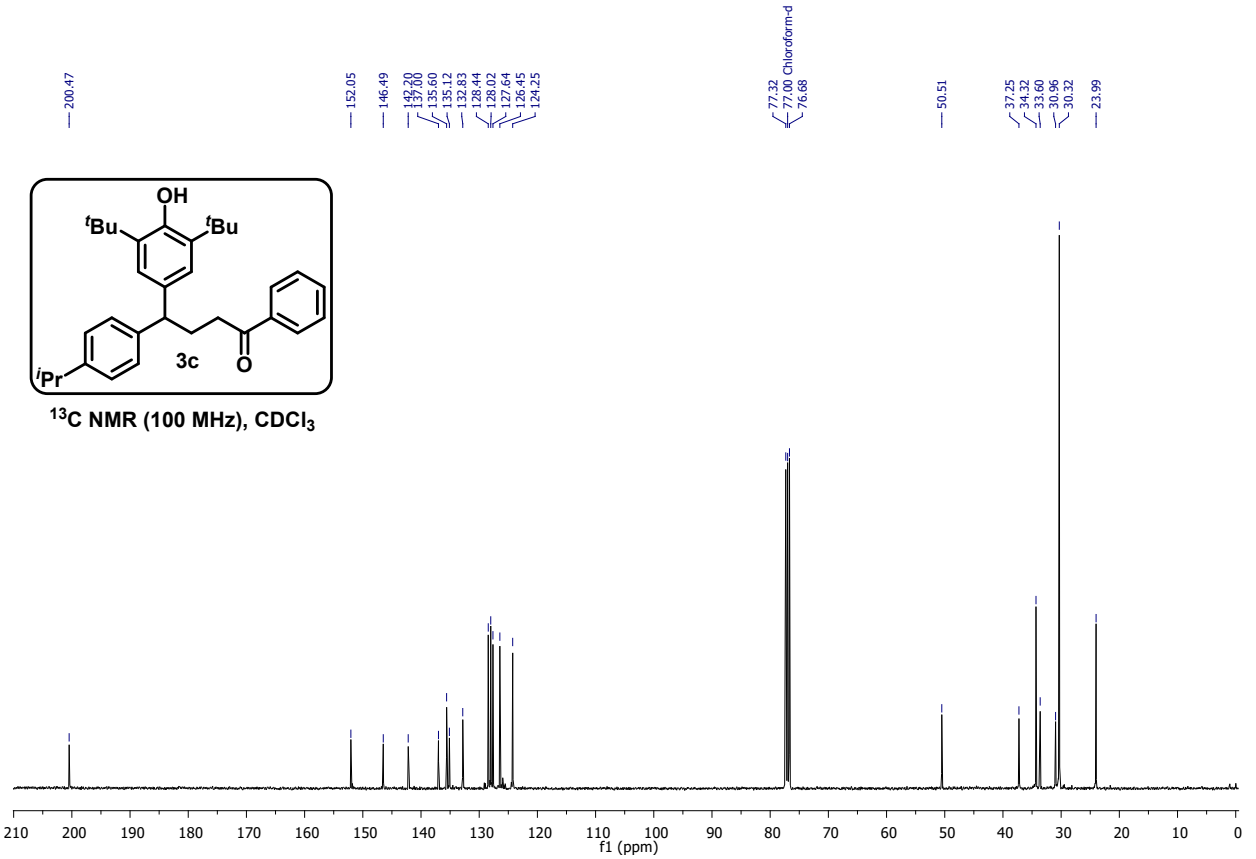
^{1}H NMR (400 MHz), $CDCl_3$



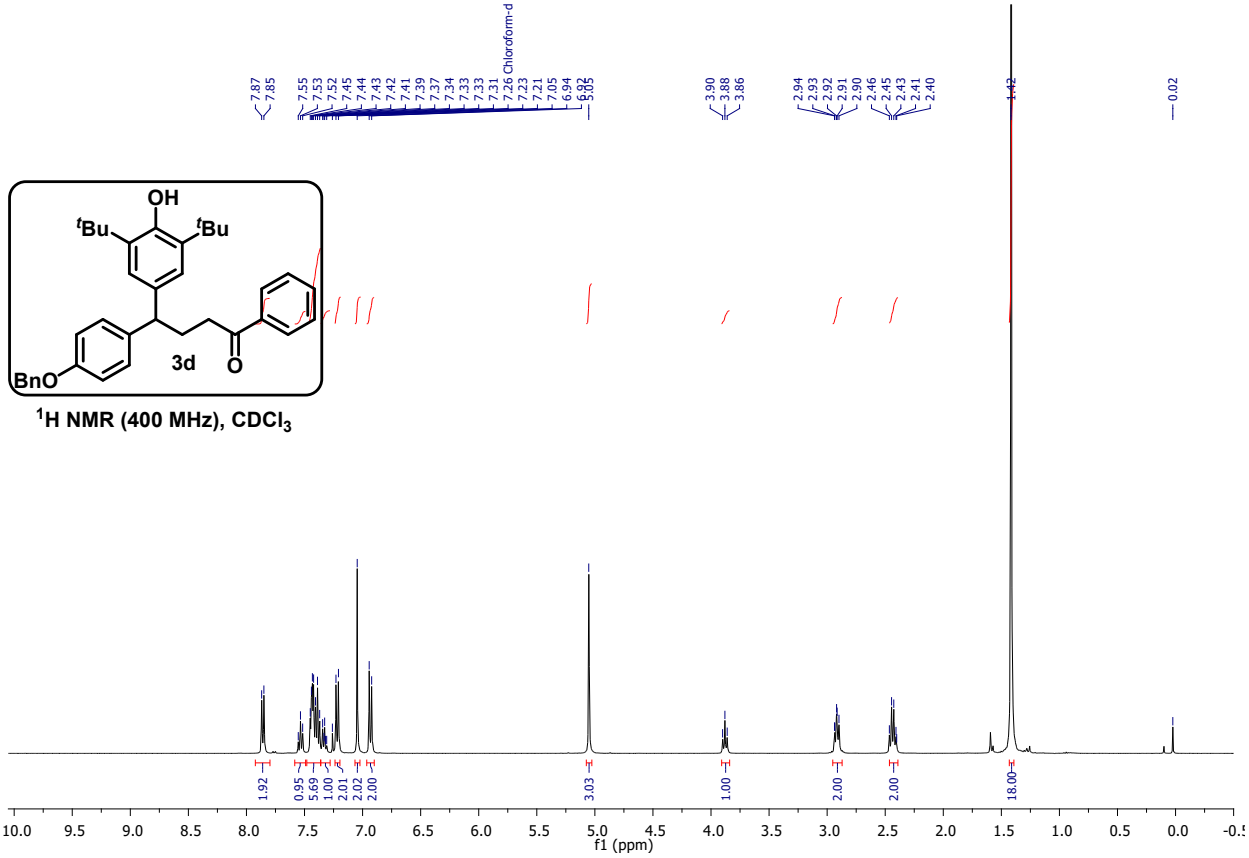
^{13}C NMR (100 MHz), $CDCl_3$



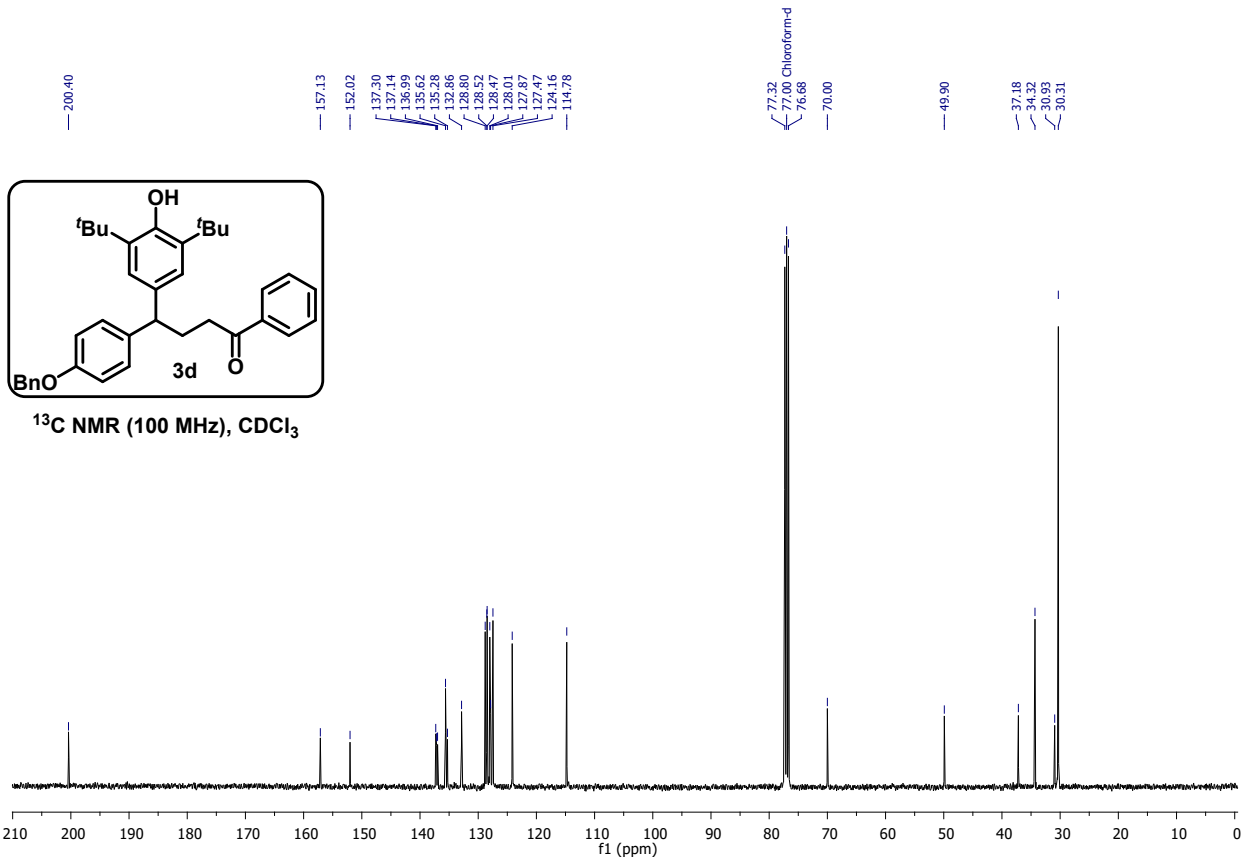
^{1}H NMR (400 MHz), $CDCl_3$



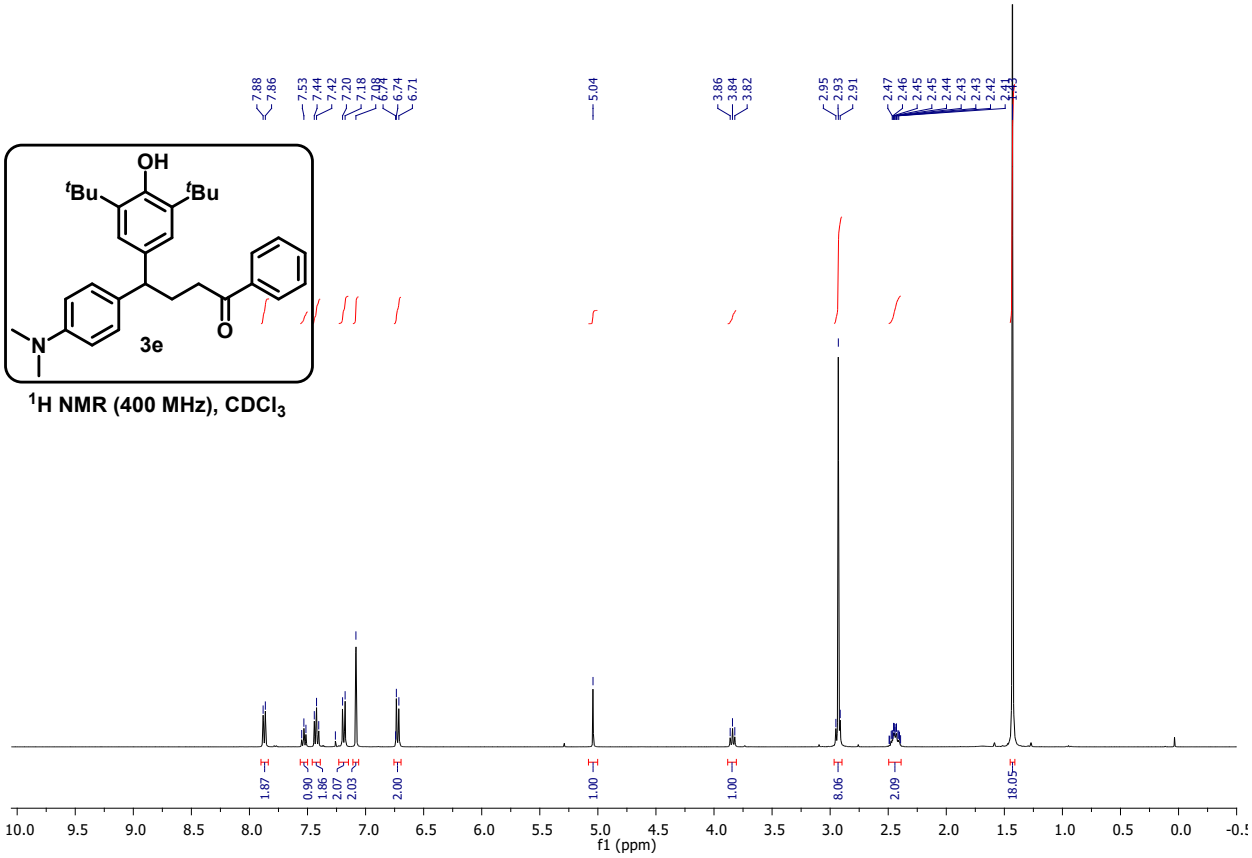
^{13}C NMR (100 MHz), $CDCl_3$



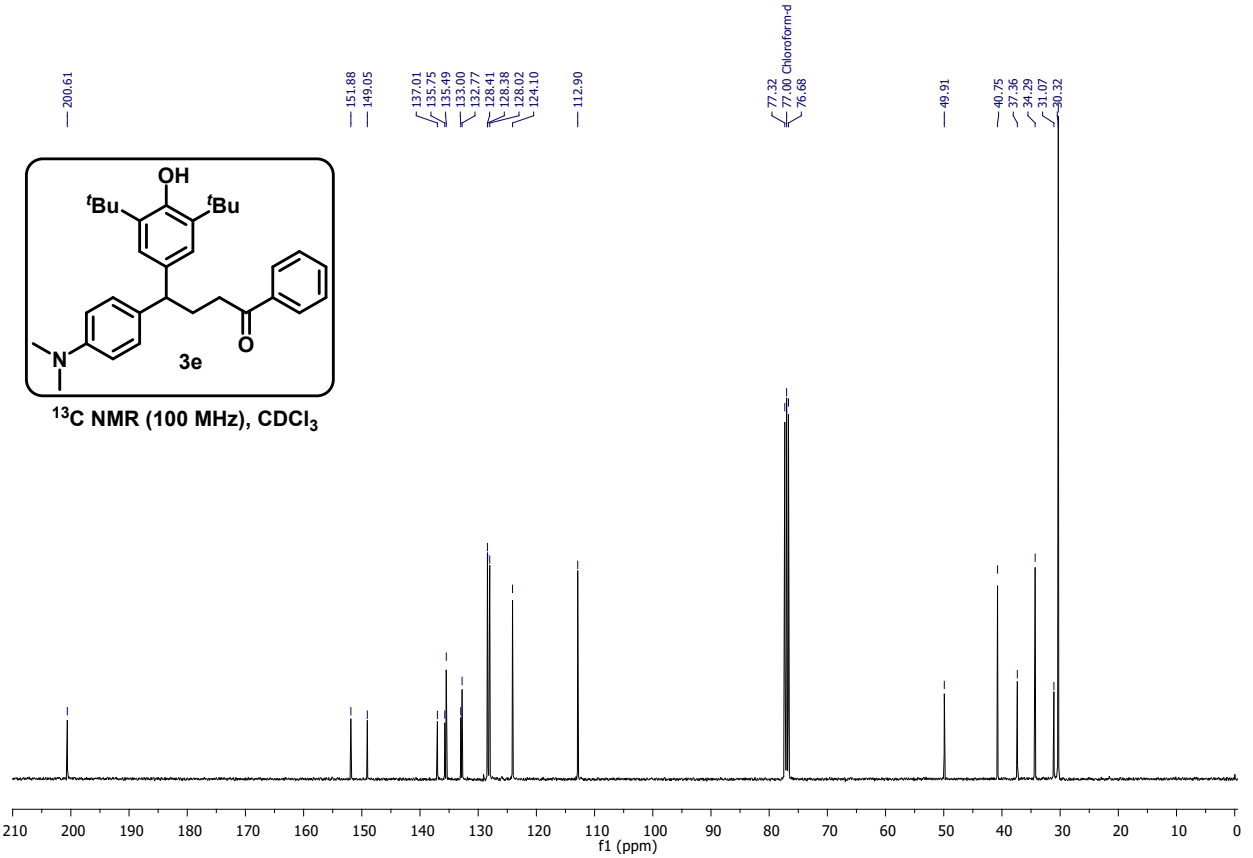
^{1}H NMR (400 MHz), $CDCl_3$



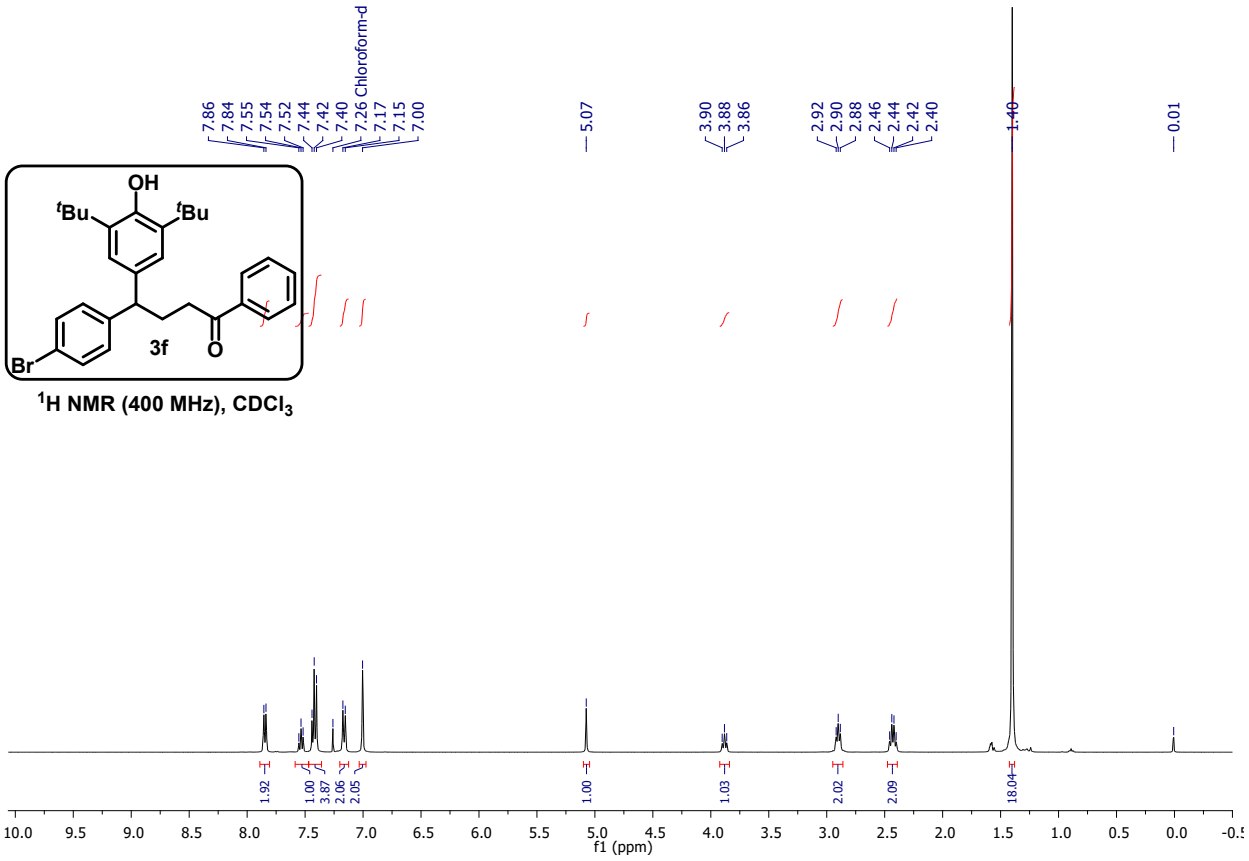
^{13}C NMR (100 MHz), $CDCl_3$



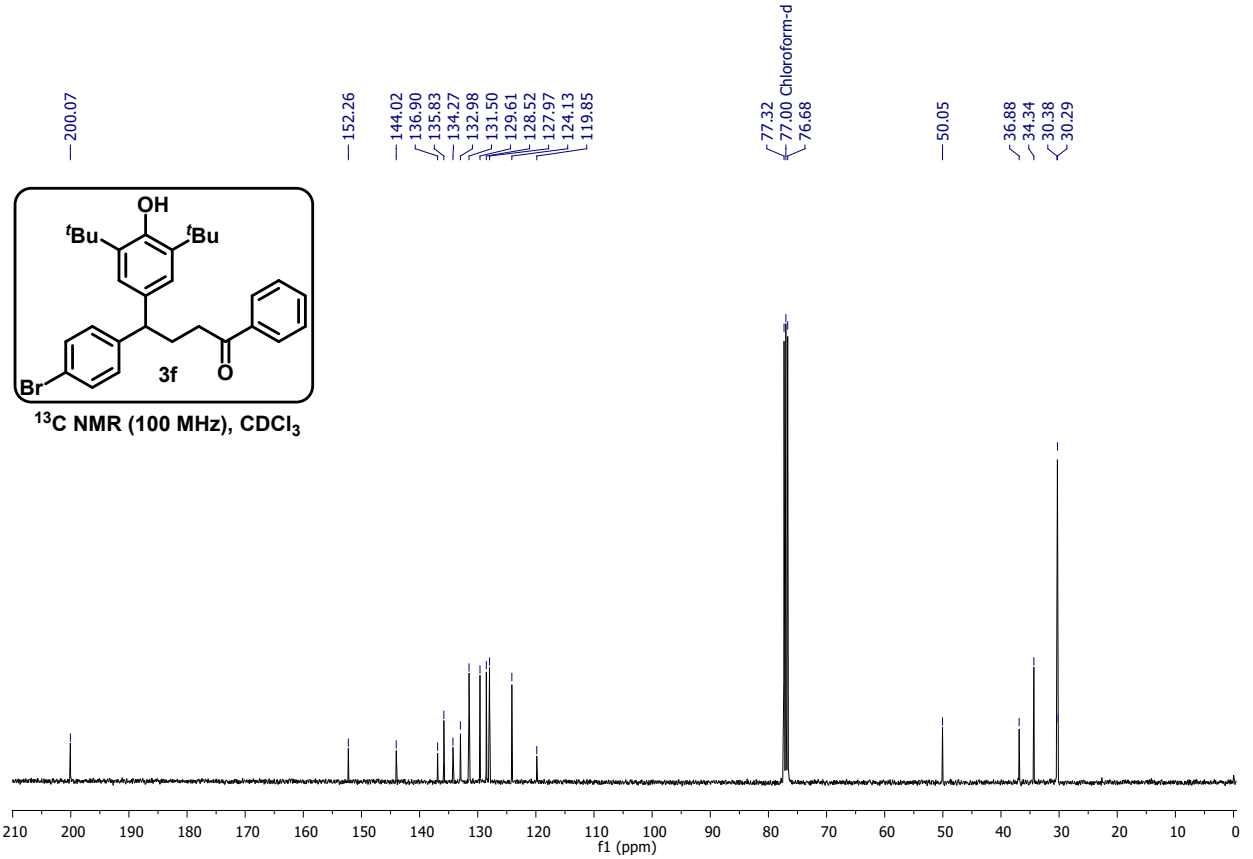
^{1}H NMR (400 MHz), $CDCl_3$



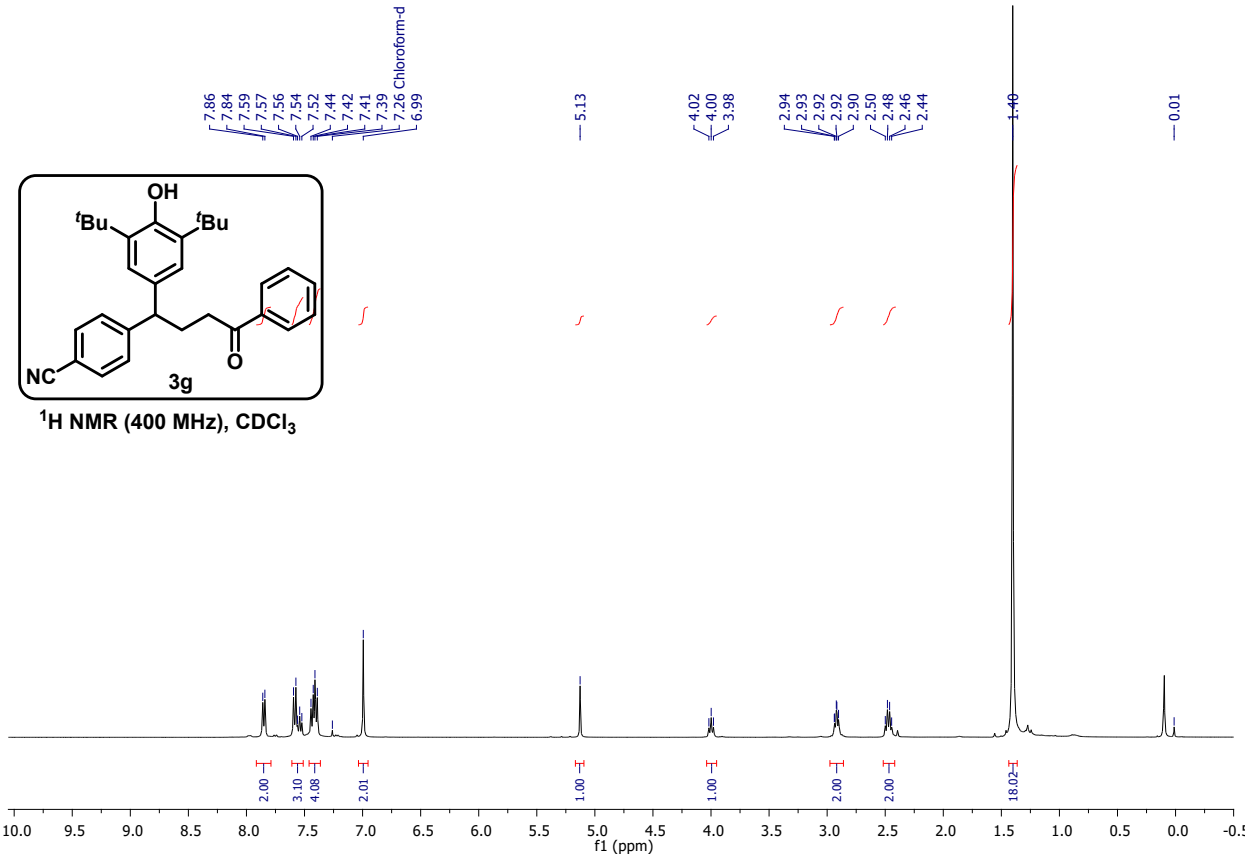
^{13}C NMR (100 MHz), $CDCl_3$



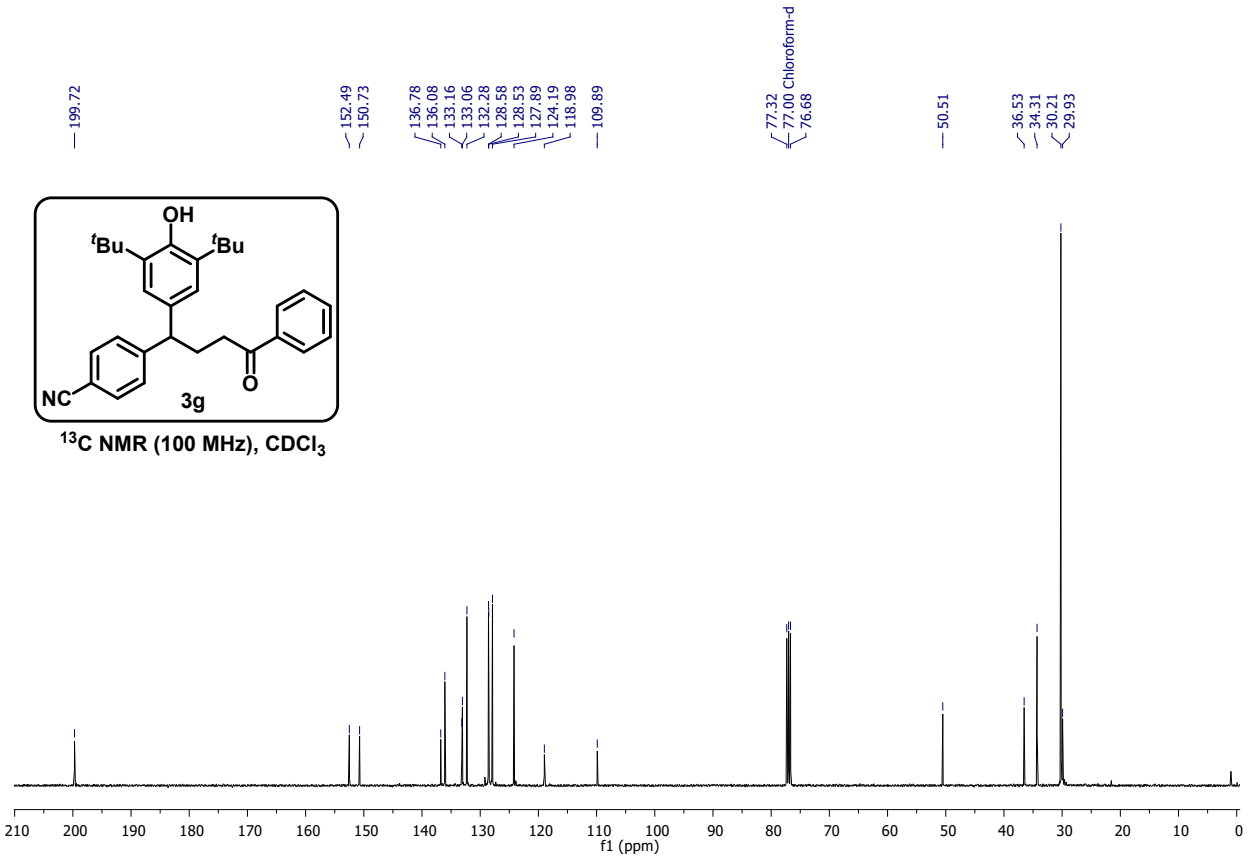
^{1}H NMR (400 MHz), $CDCl_3$



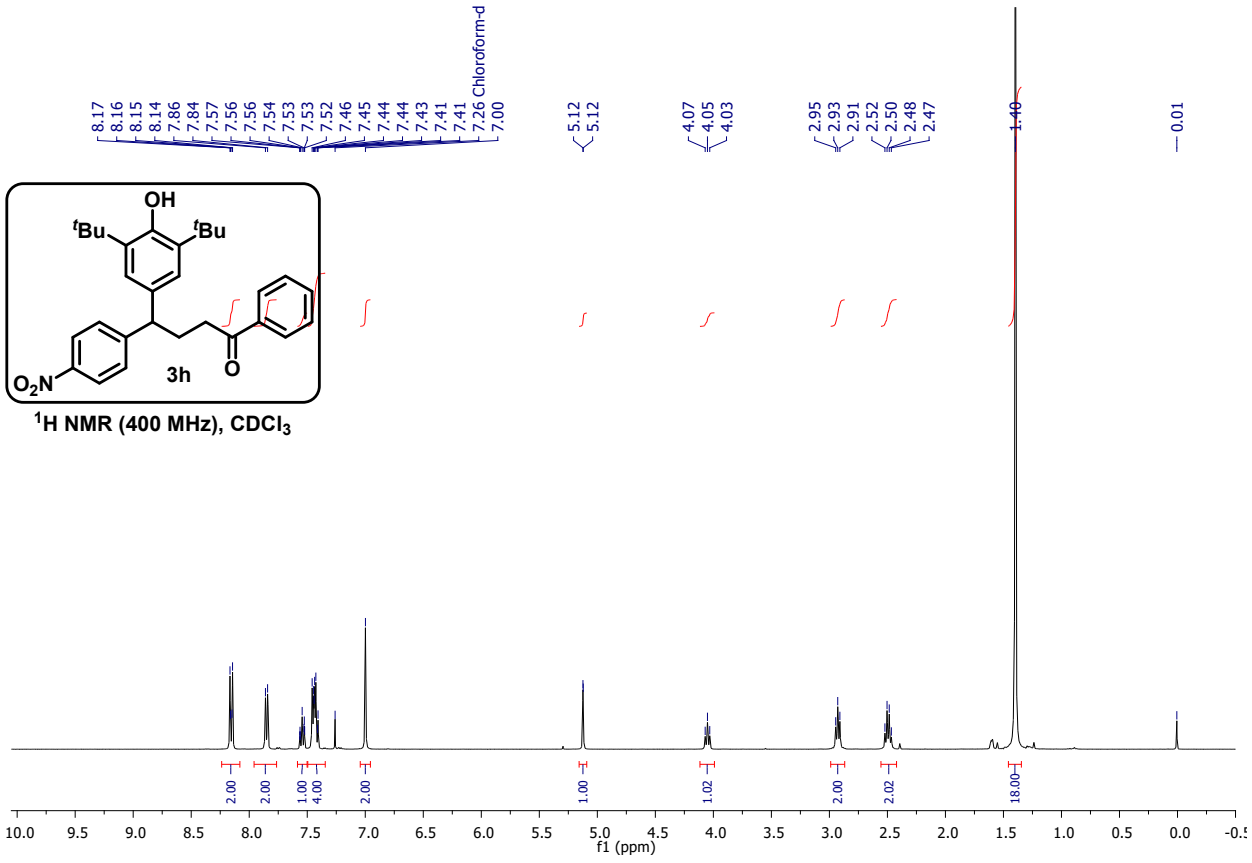
^{13}C NMR (100 MHz), $CDCl_3$



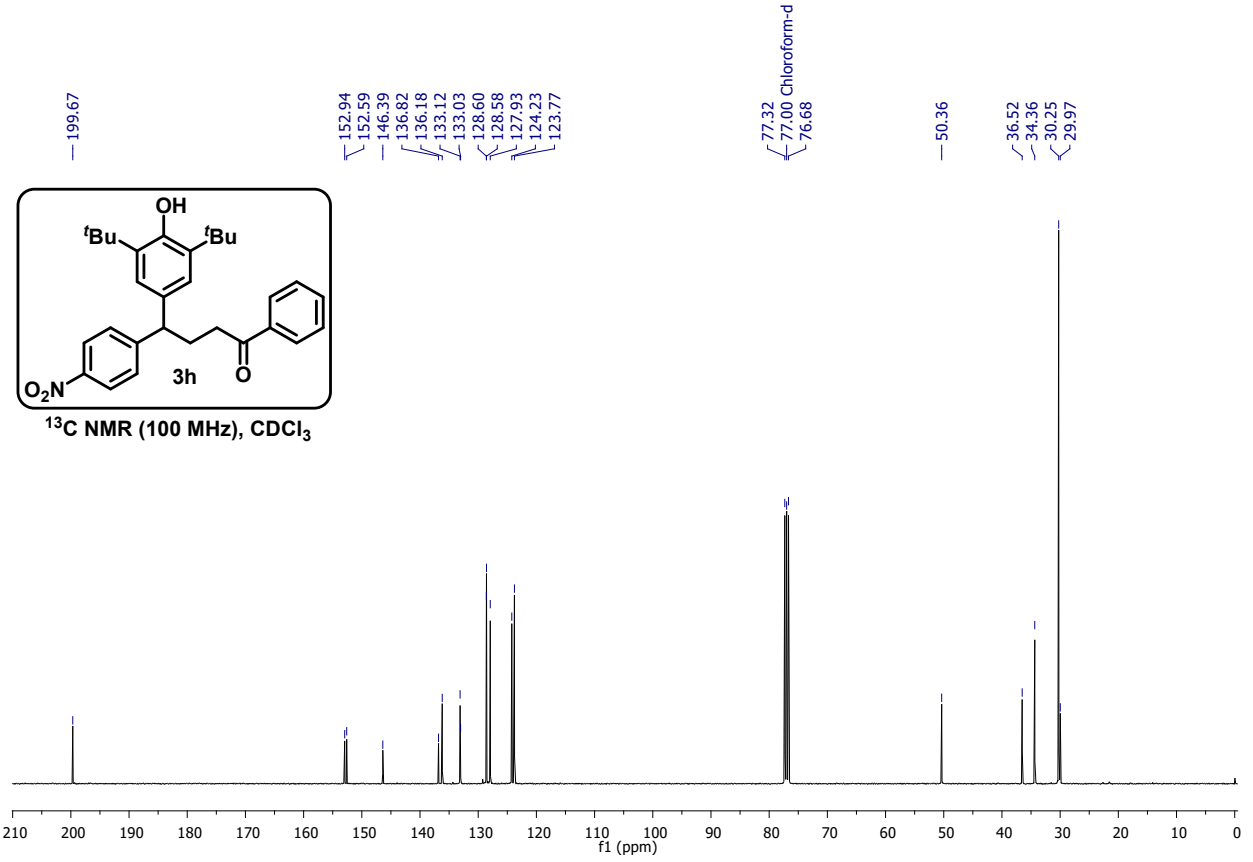
^{1}H NMR (400 MHz), $CDCl_3$



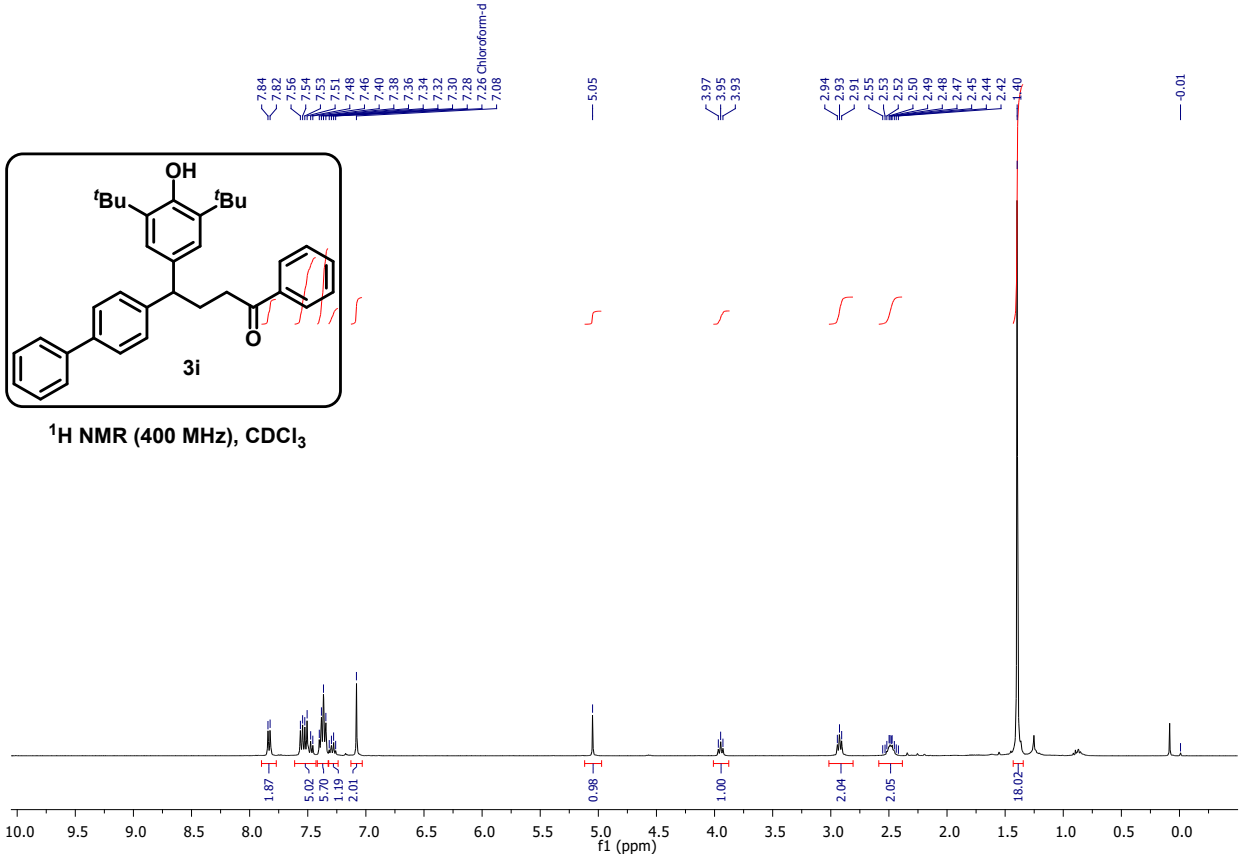
^{13}C NMR (100 MHz), $CDCl_3$



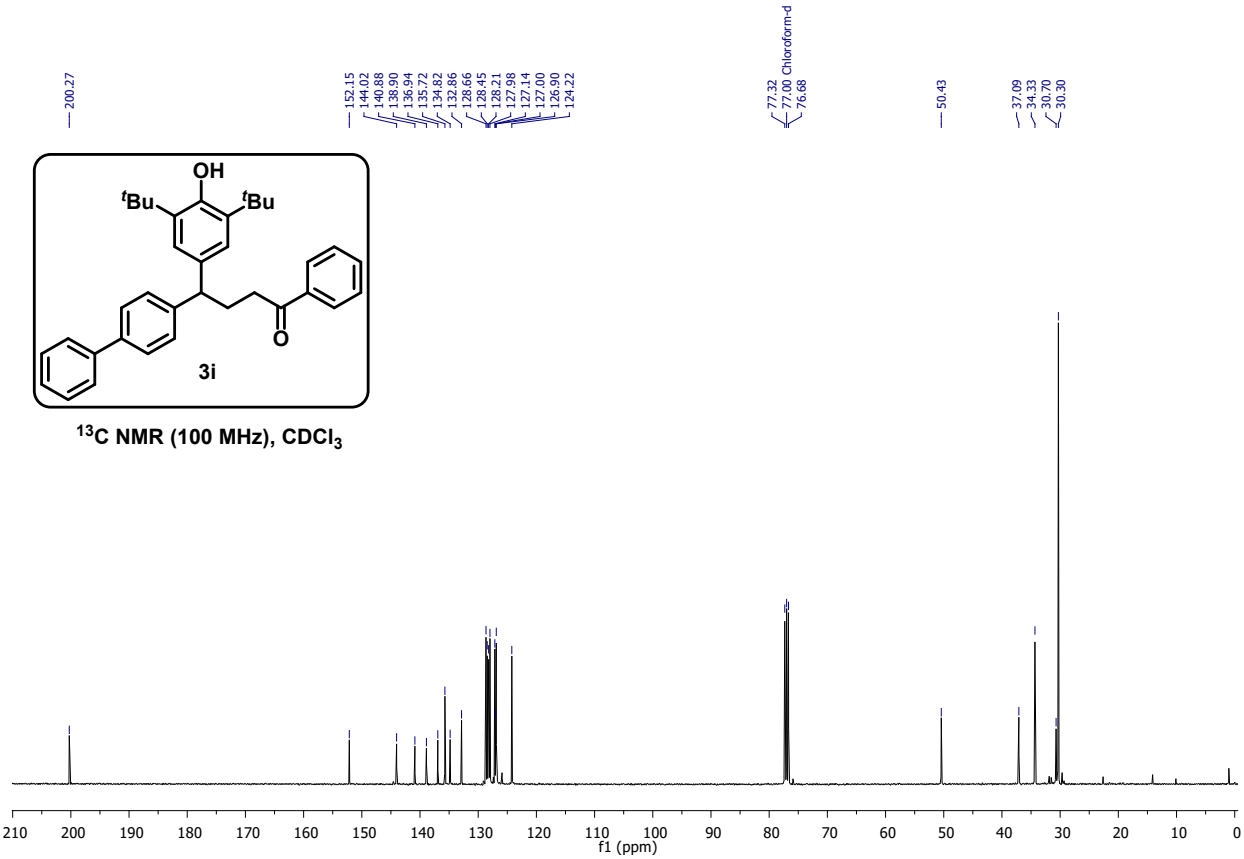
^{1}H NMR (400 MHz), $CDCl_3$



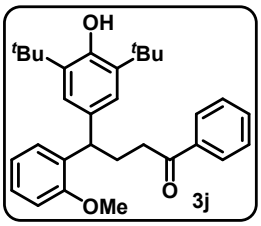
^{13}C NMR (100 MHz), $CDCl_3$



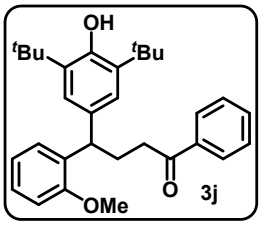
^{1}H NMR (400 MHz), $CDCl_3$



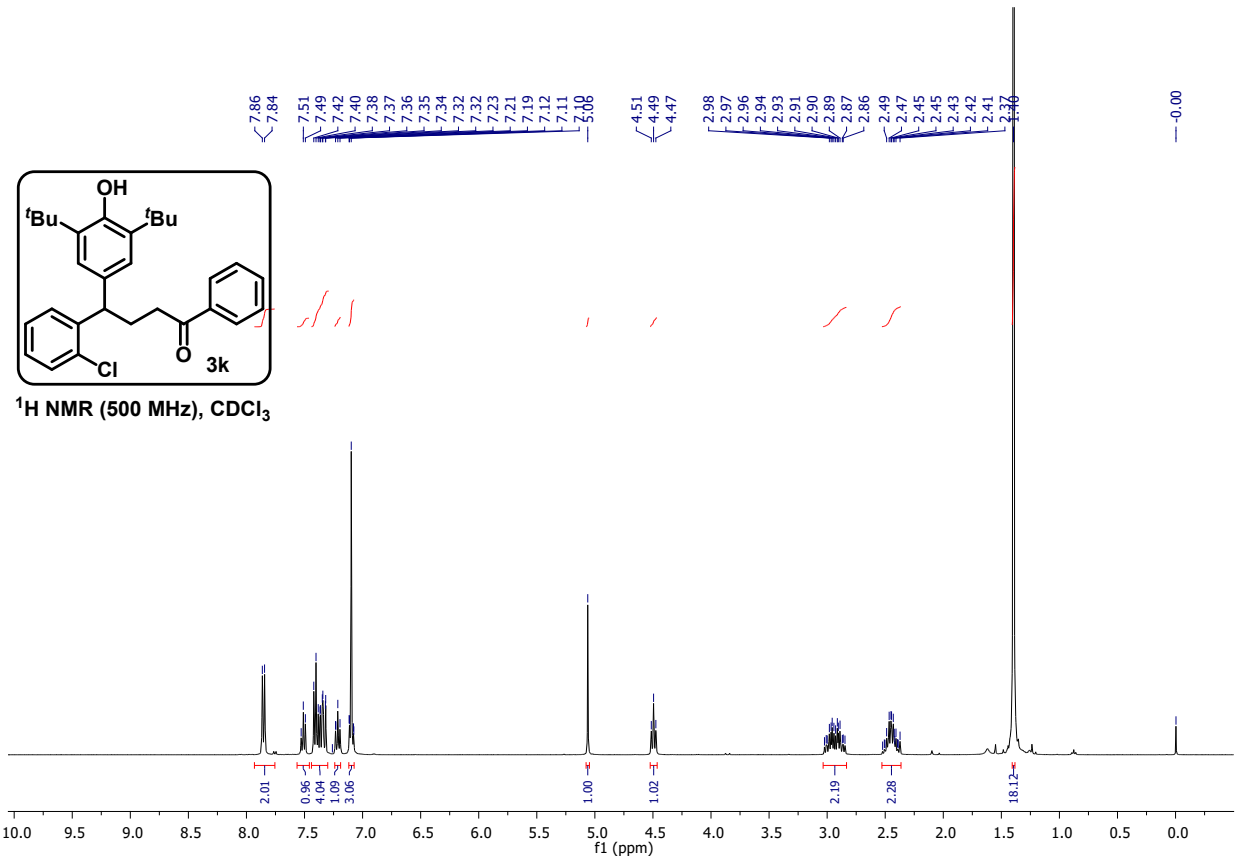
^{13}C NMR (100 MHz), $CDCl_3$



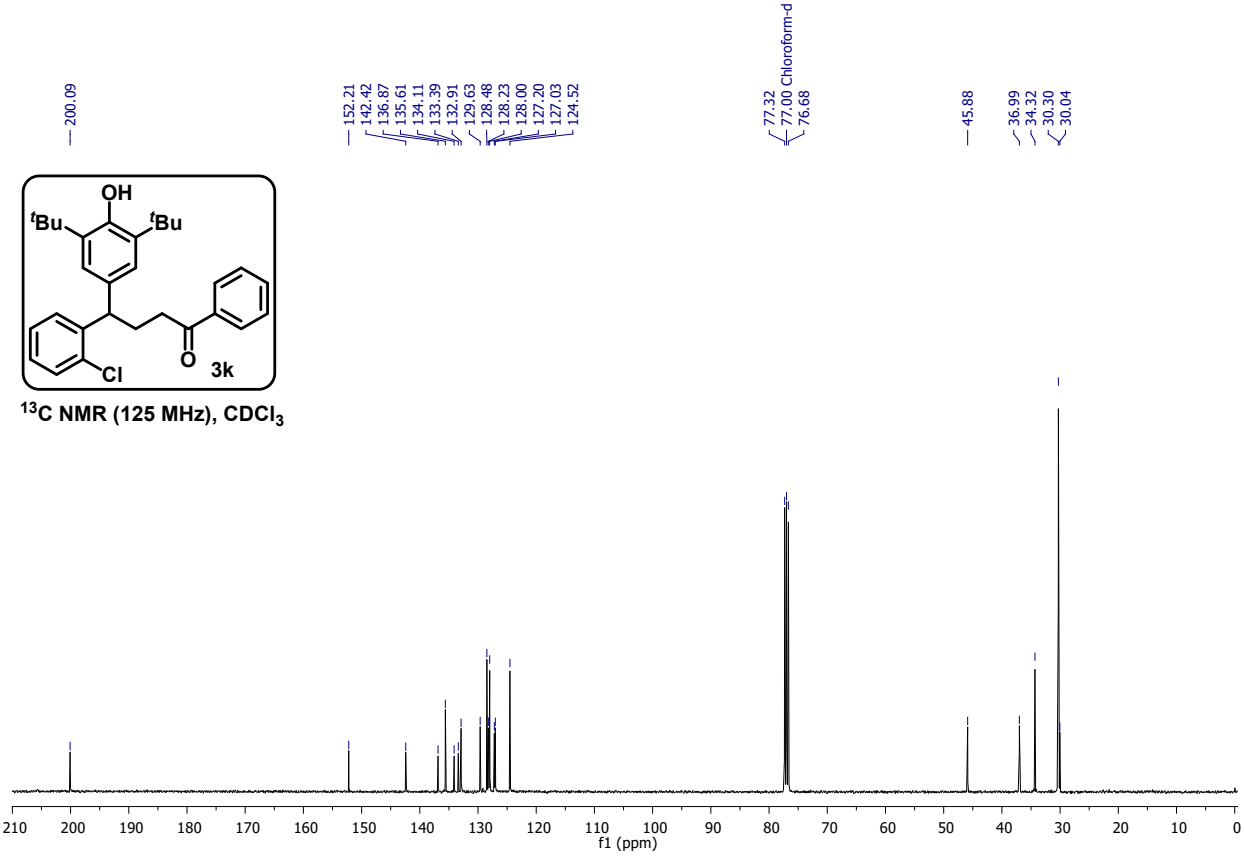
^{1}H NMR (400 MHz), $CDCl_3$



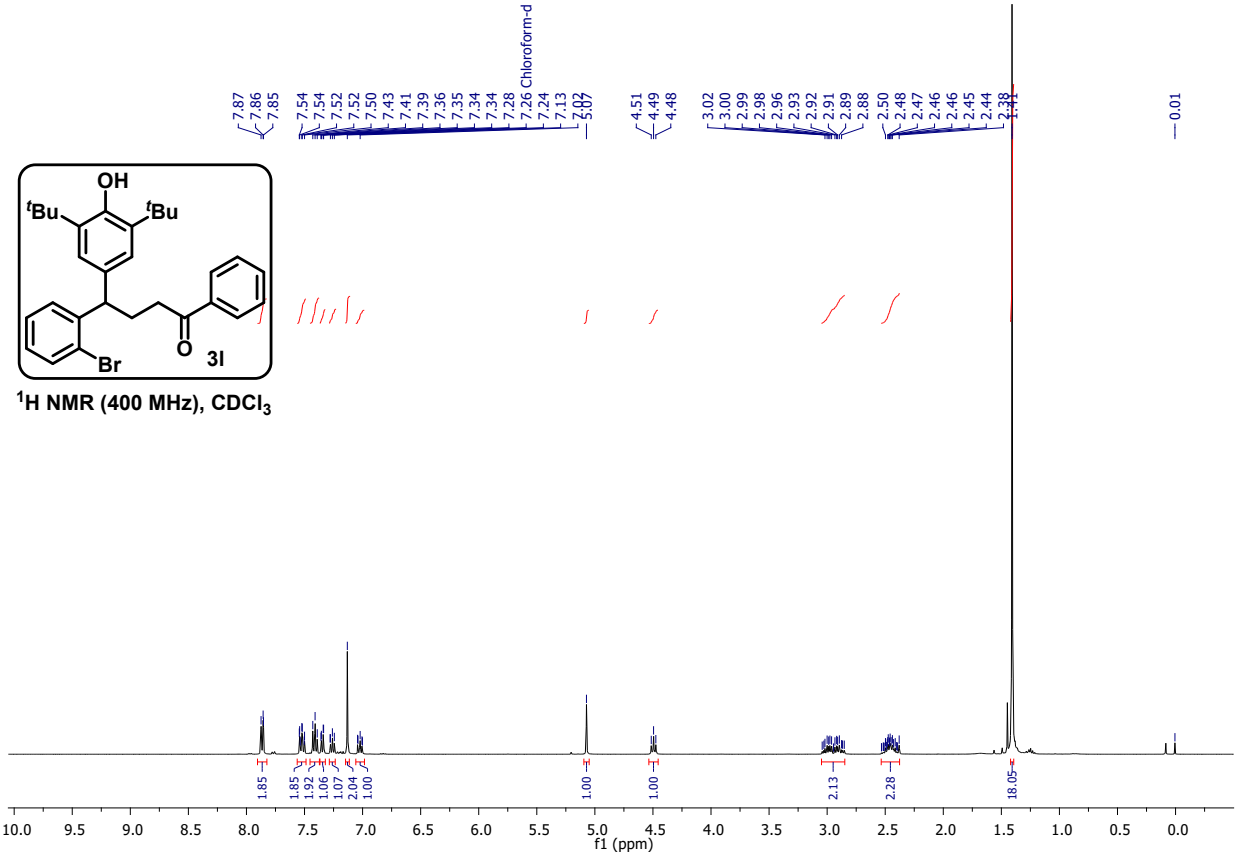
^{13}C NMR (100 MHz), $CDCl_3$

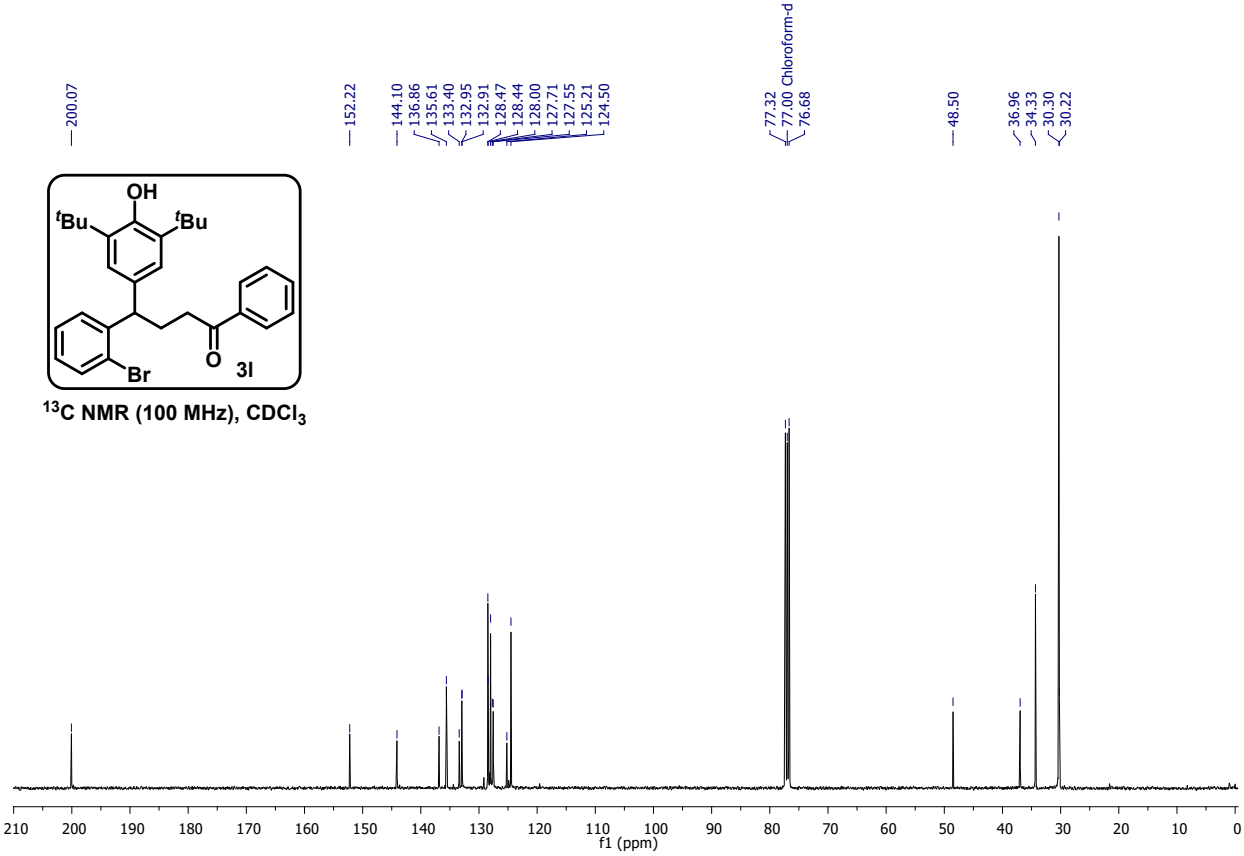


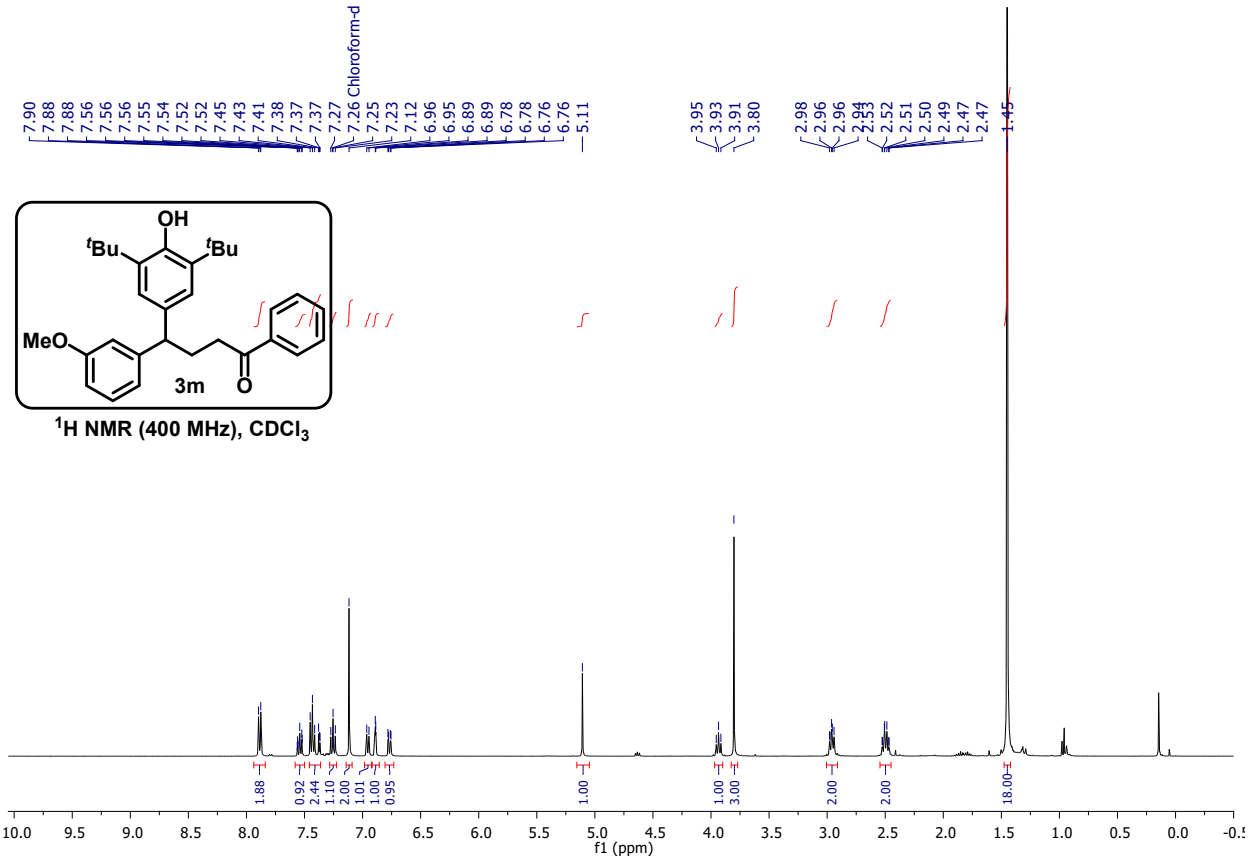
^{1}H NMR (500 MHz), $CDCl_3$



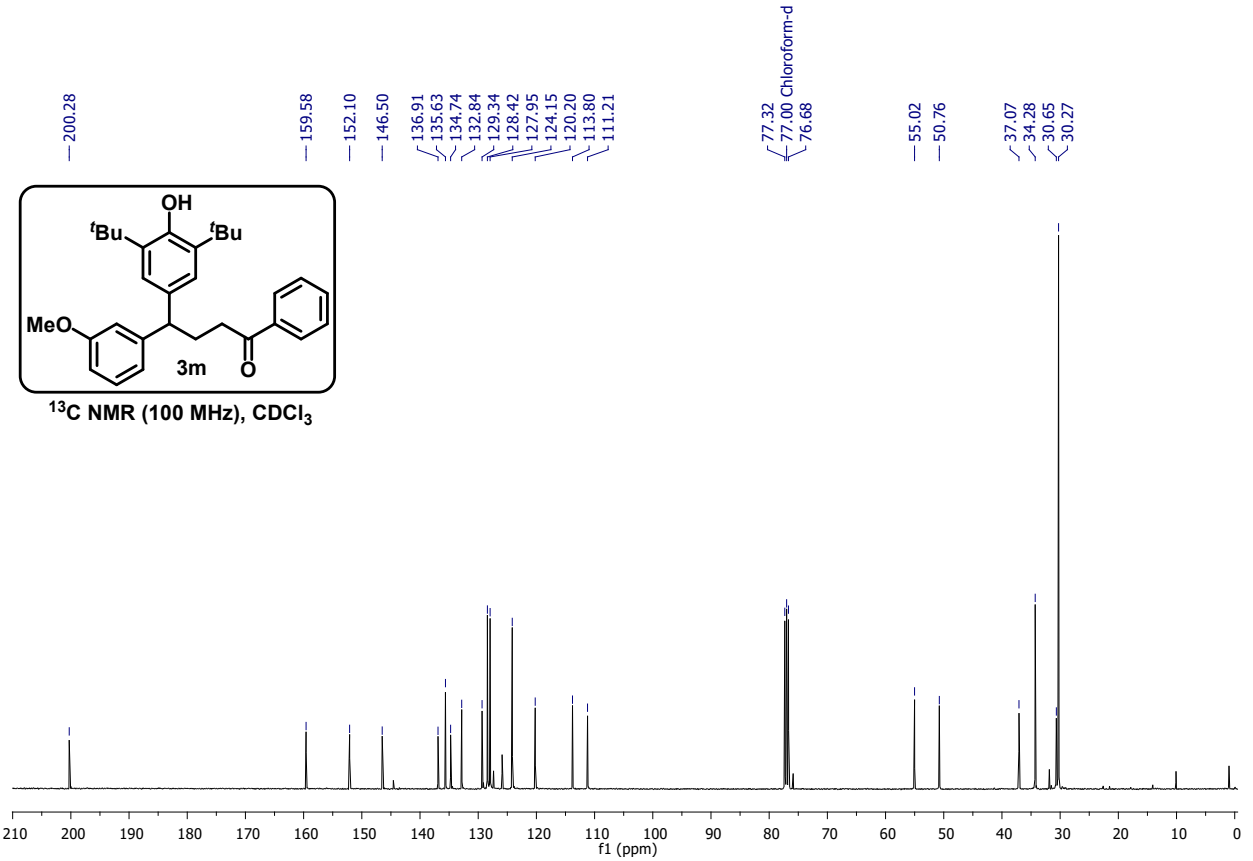
^{13}C NMR (125 MHz), $CDCl_3$


OH
tBu
tBu
Br
O
3l
1H NMR (400 MHz), CDCl3
Chloroform-d
f1 (ppm)

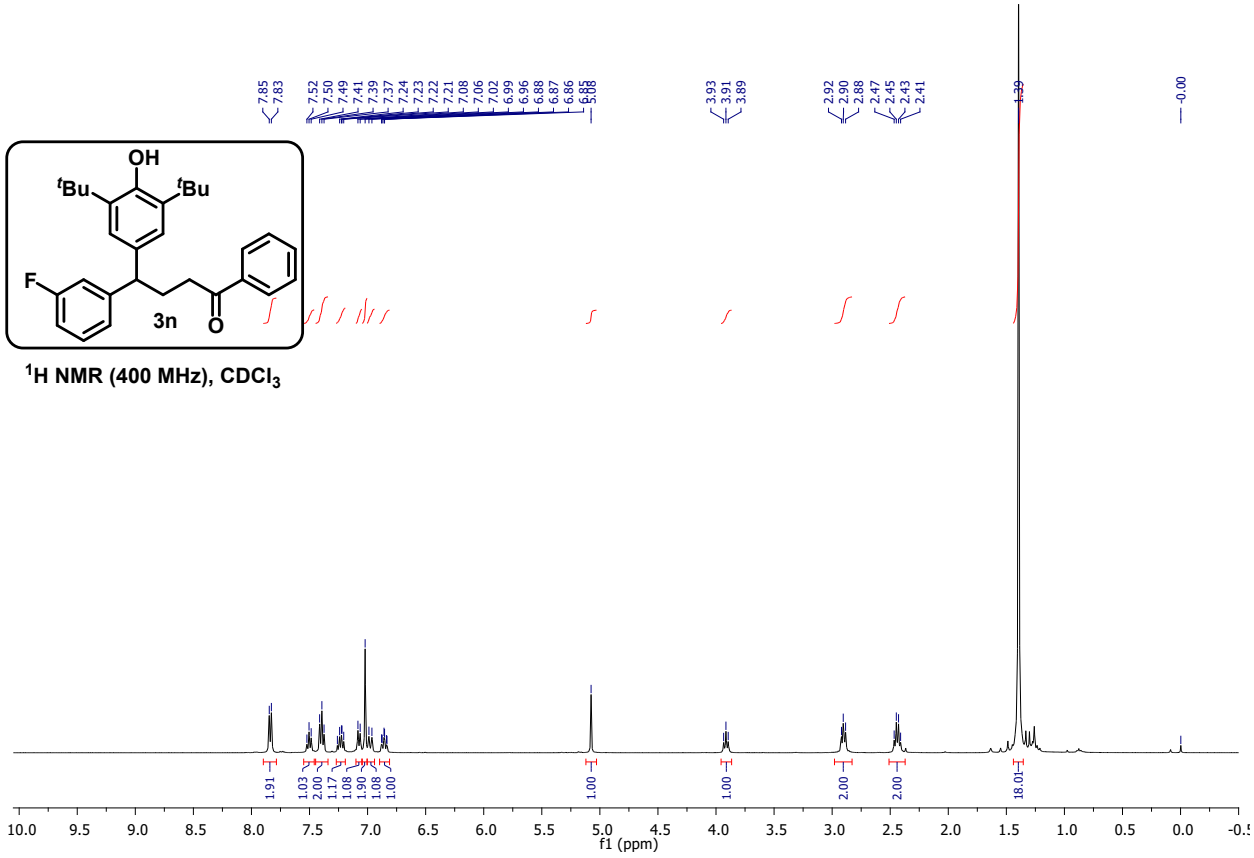

OH
tBu
tBu
Br
O
3l
13C NMR (100 MHz), CDCl3
Chloroform-d
f1 (ppm)



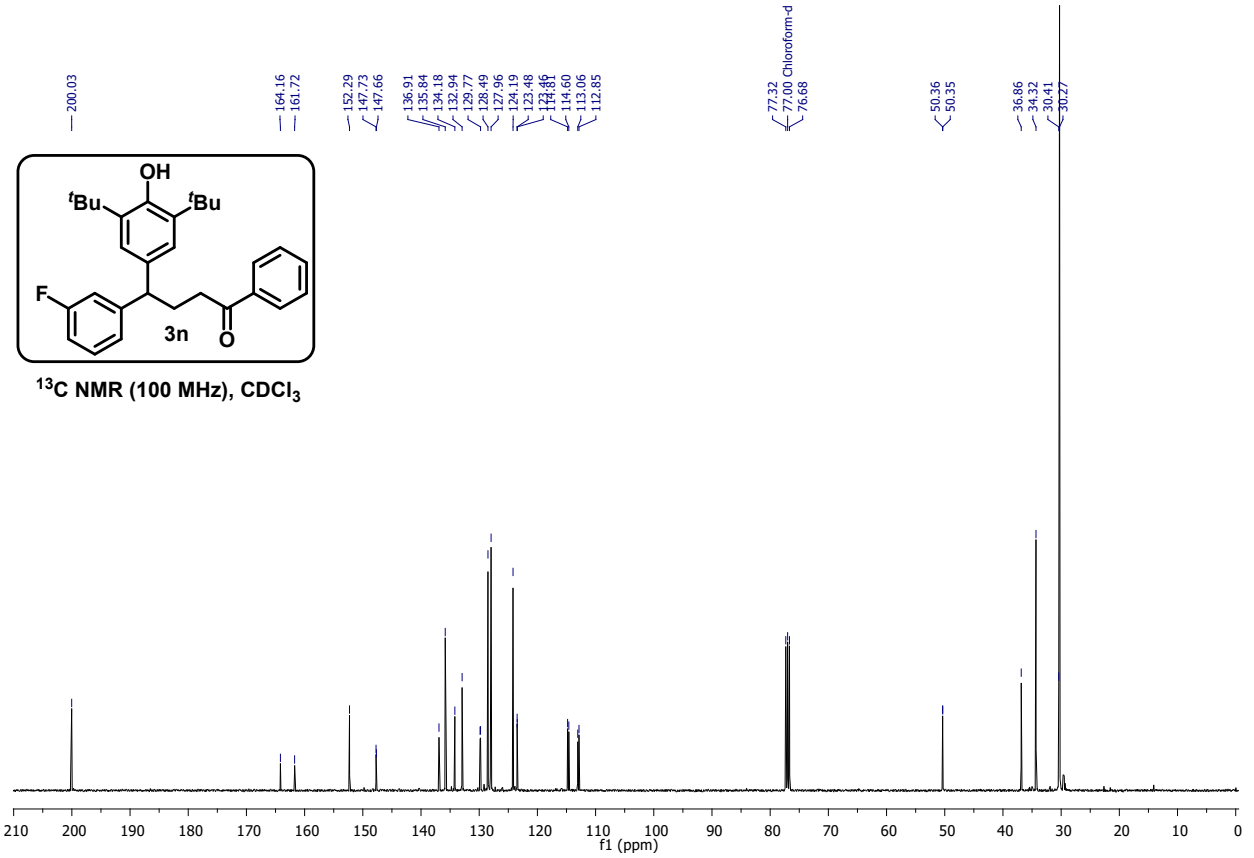
^{1}H NMR (400 MHz), $CDCl_3$



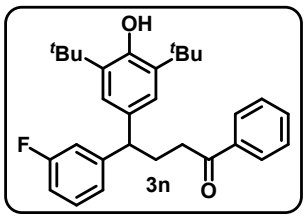
^{13}C NMR (100 MHz), $CDCl_3$



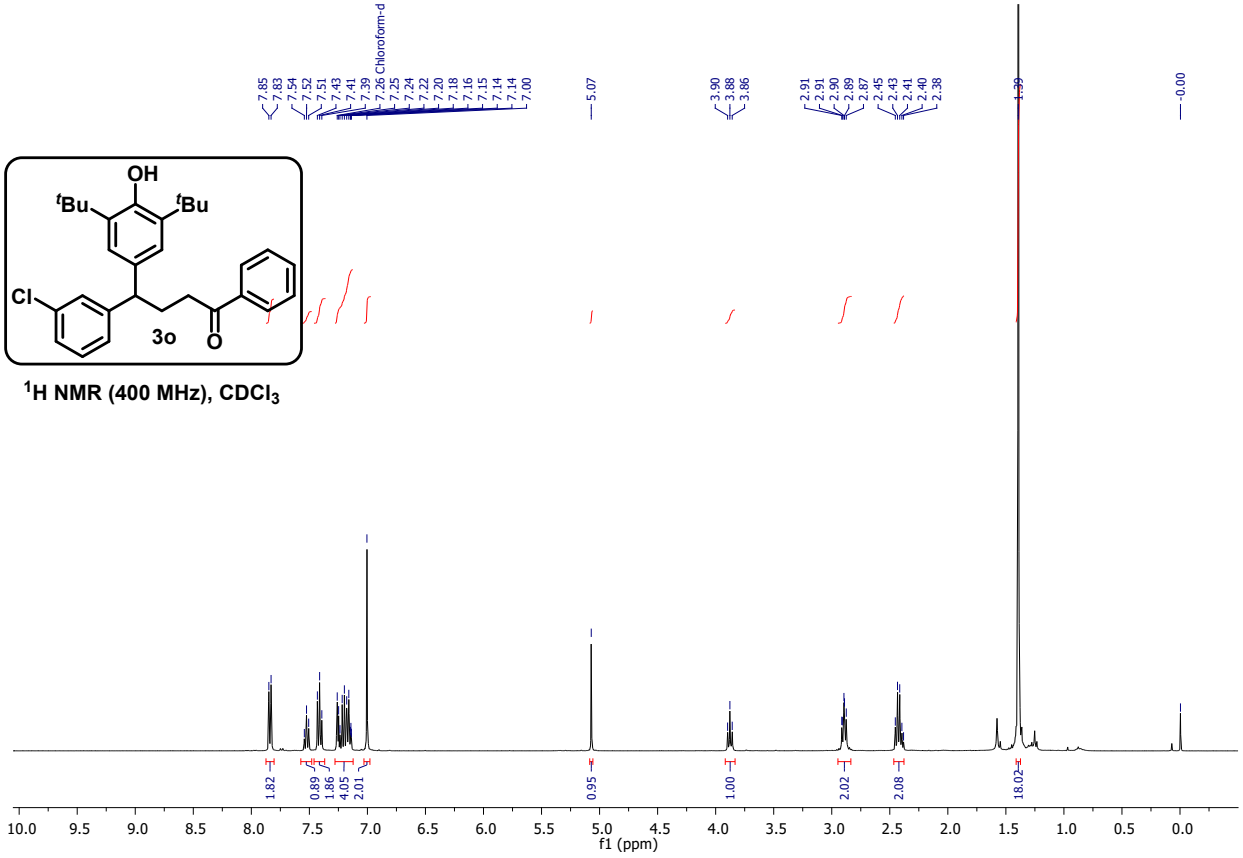
^{1}H NMR (400 MHz), $CDCl_3$



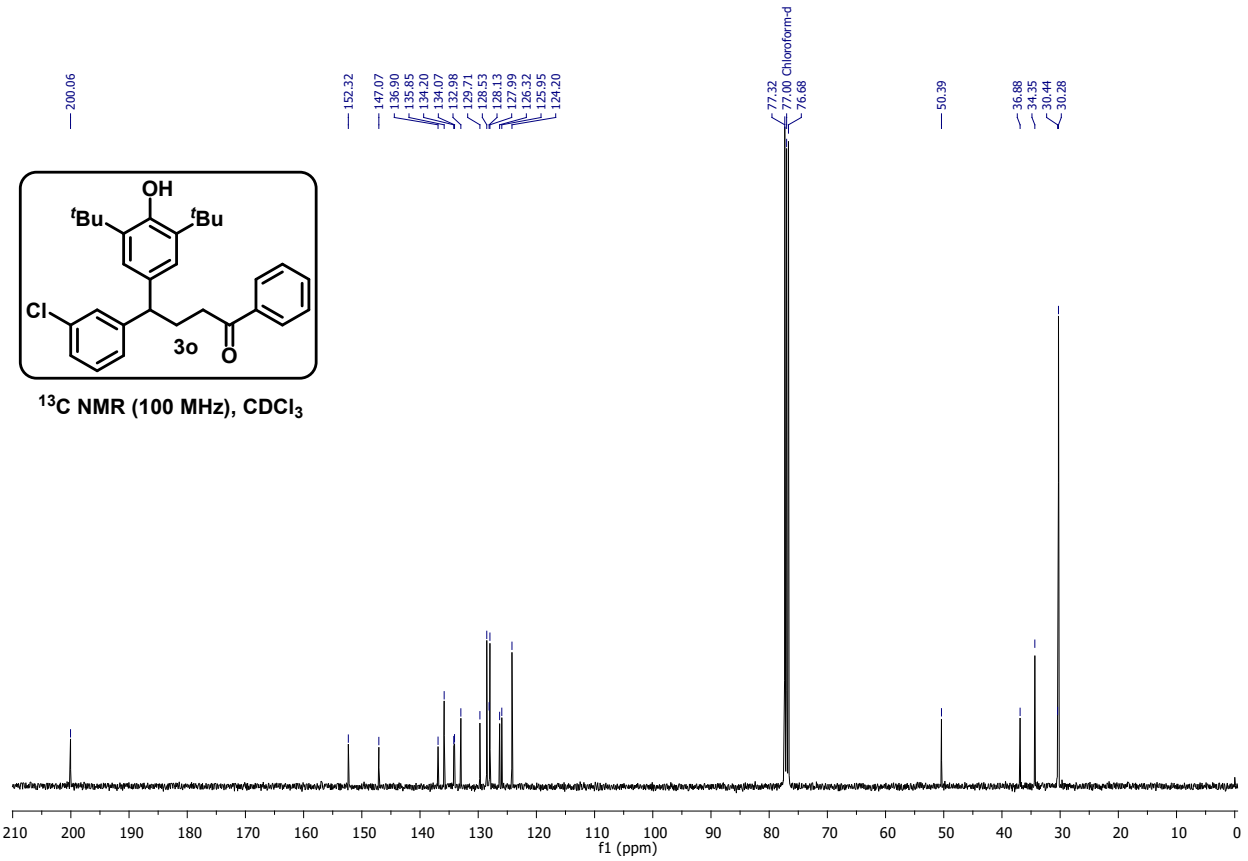
^{13}C NMR (100 MHz), $CDCl_3$



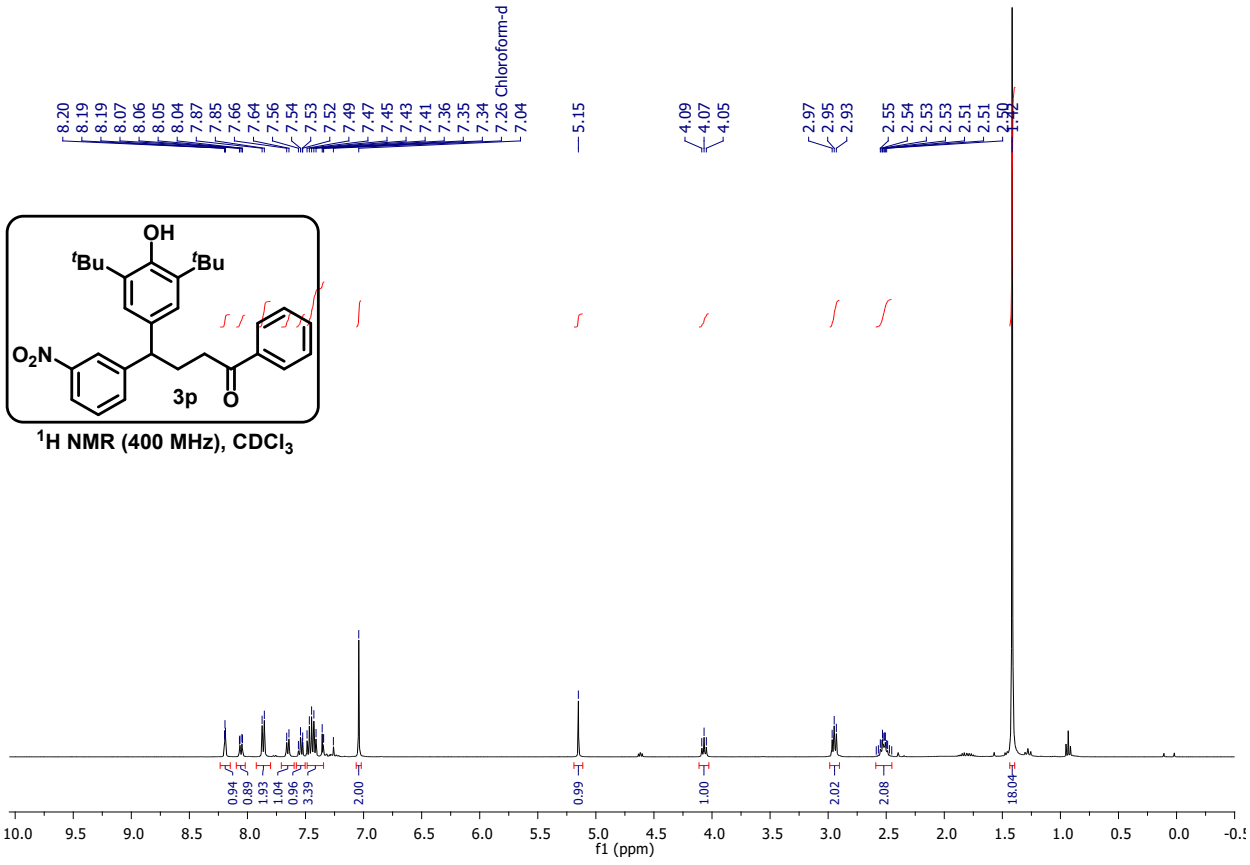
^{19}F NMR (376 MHz), $CDCl_3$



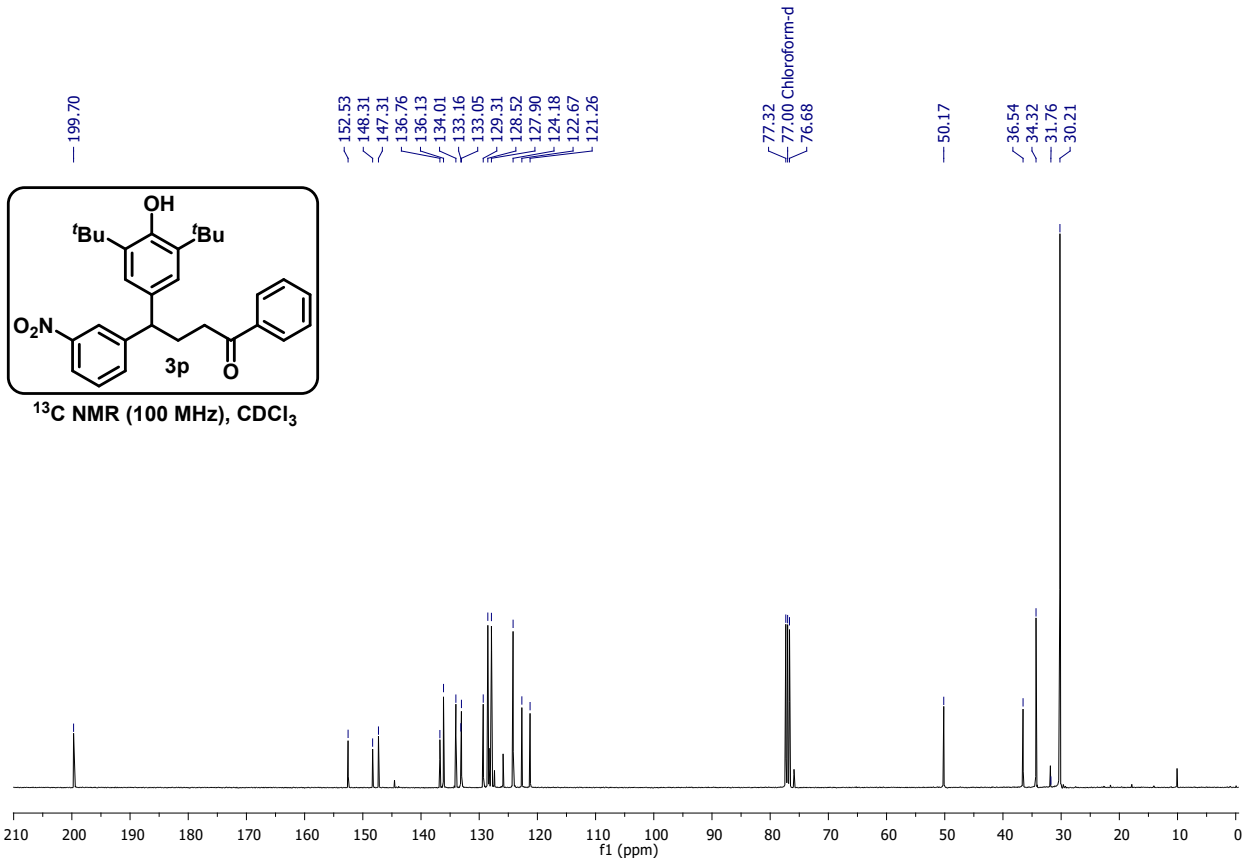
^{1}H NMR (400 MHz), $CDCl_3$

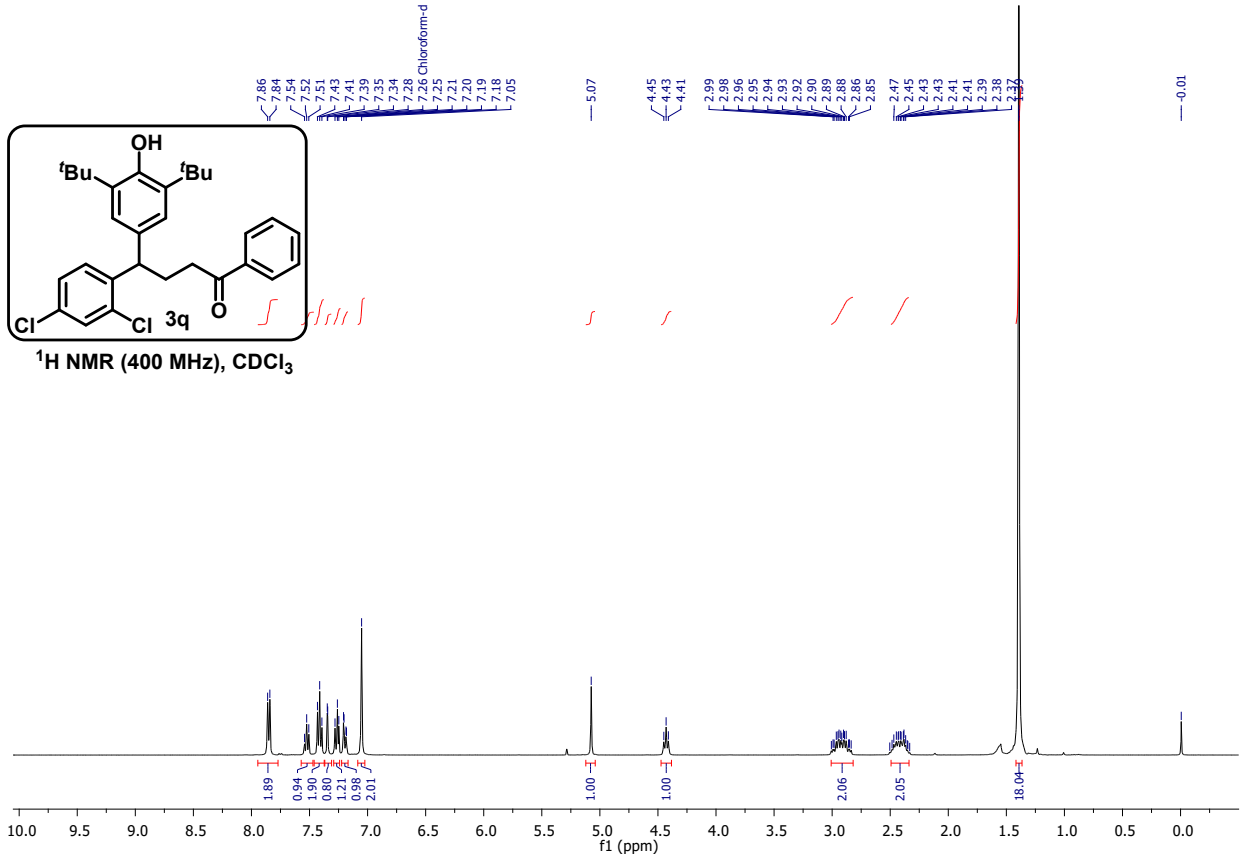


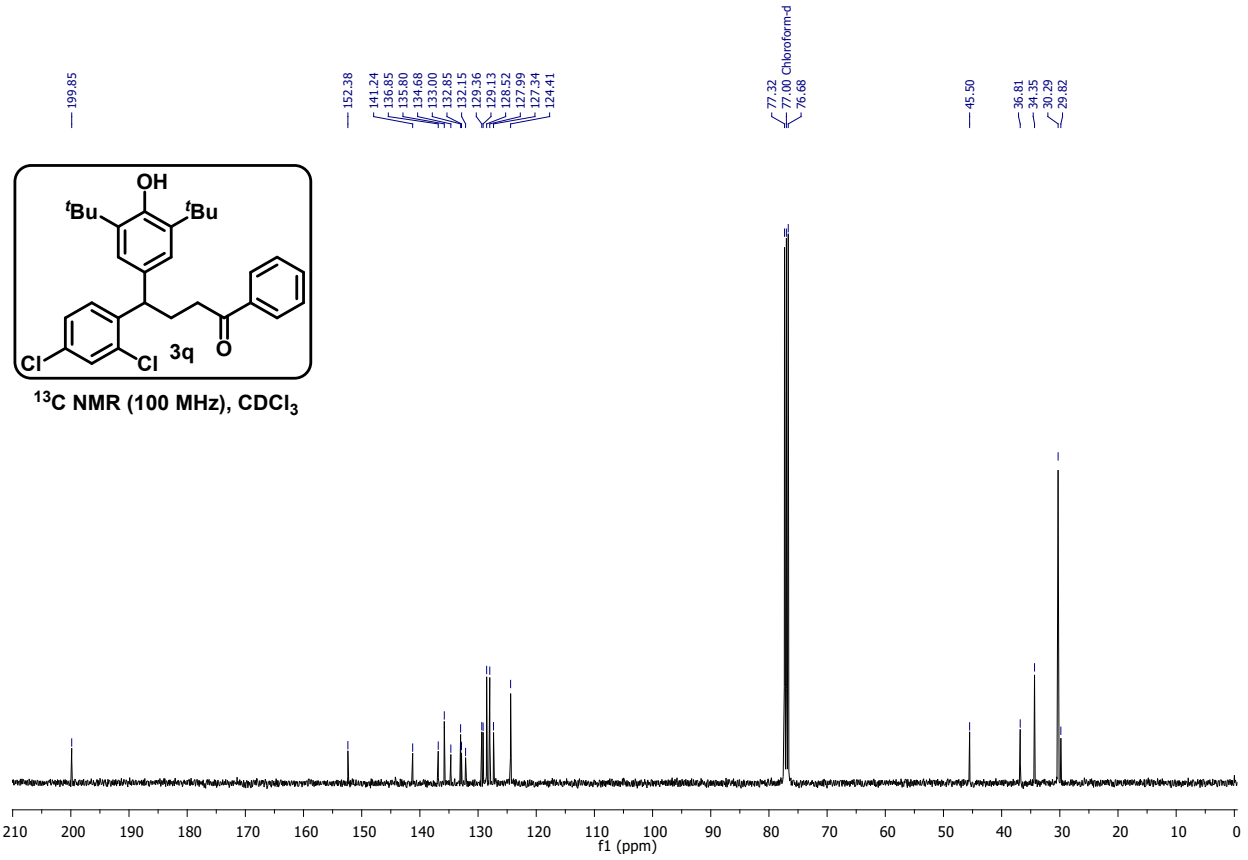
^{13}C NMR (100 MHz), $CDCl_3$



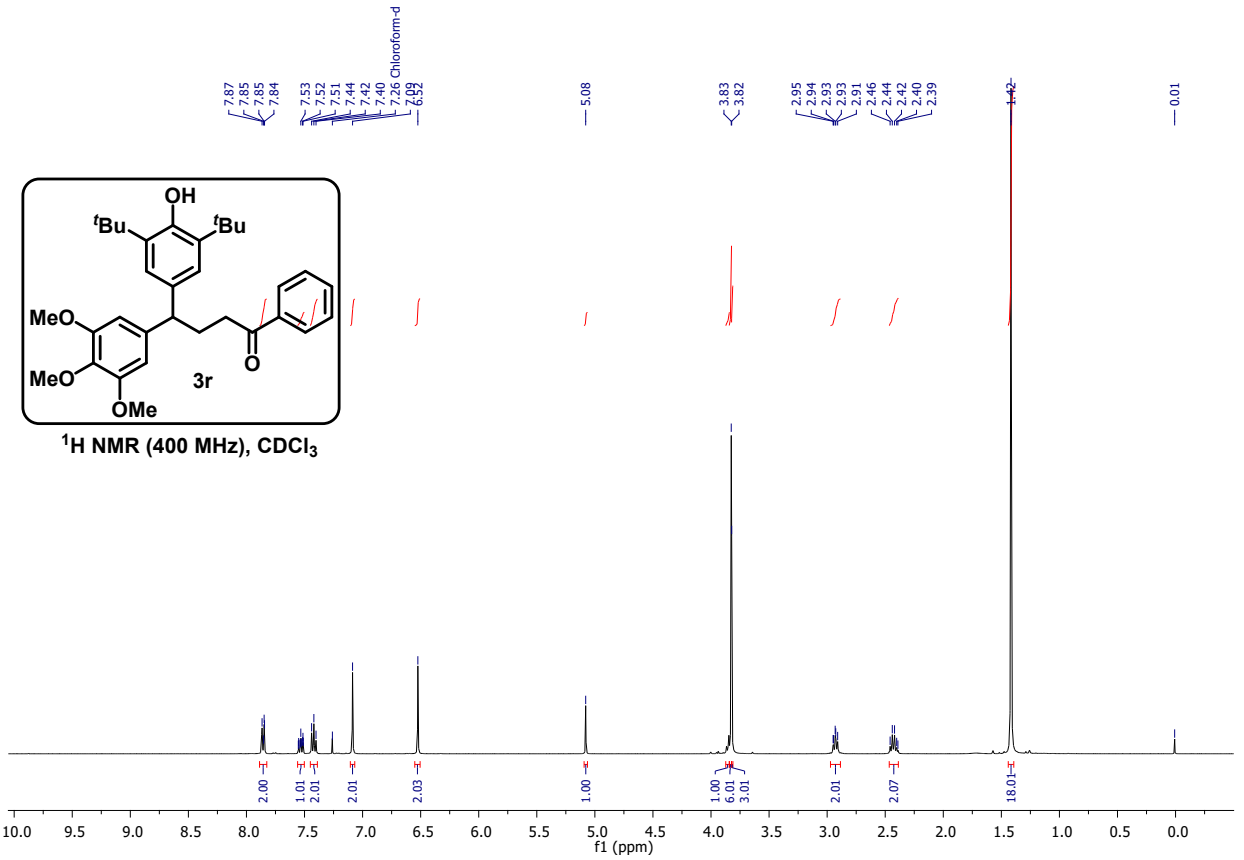
^{1}H NMR (400 MHz), $CDCl_3$


199.70
152.53
148.31
147.31
136.76
136.13
134.01
133.16
133.05
129.31
128.52
127.90
124.18
122.67
121.26
77.32
77.00 Chloroform-d
76.68
50.17
36.54
34.32
31.76
30.21
OH
tBu
tBu
O2N
3p
O
13C NMR (100 MHz), CDCl3
f1 (ppm)

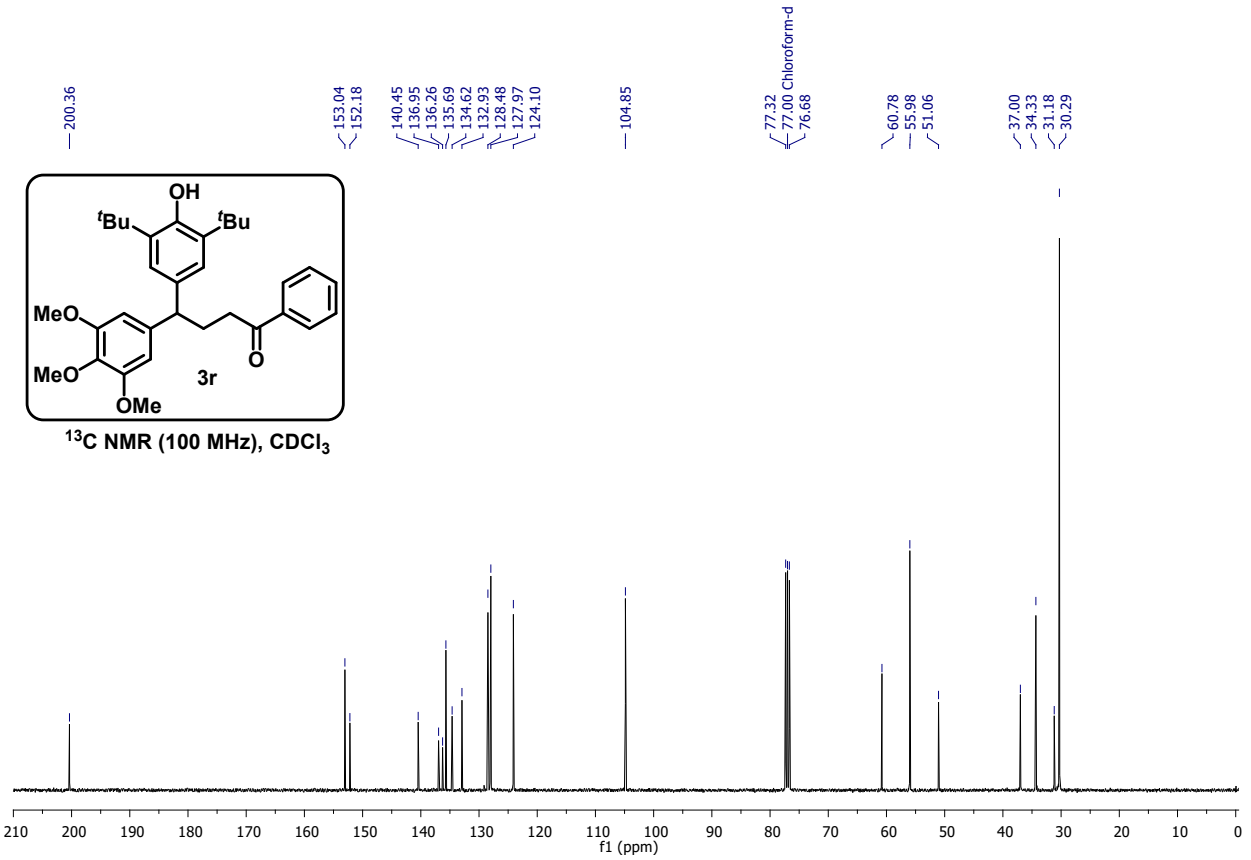

7.86
7.84
7.54
7.52
7.51
7.43
7.41
7.39
7.35
7.34
7.28
Chloroform-d
7.26
7.25
7.21
7.20
7.19
7.18
7.05
5.07
4.45
4.43
4.41
2.99
2.98
2.96
2.95
2.94
2.93
2.92
2.90
2.89
2.88
2.86
2.85
2.47
2.45
2.43
2.43
2.41
2.41
2.39
2.38
2.37
1.33
-0.01
OH
tBu
tBu
Cl
Cl
3q
O
1H NMR (400 MHz), CDCl3
1.89
0.94
1.90
0.80
1.21
0.98
2.01
1.00
1.00
2.06
2.05
18.04
f1 (ppm)

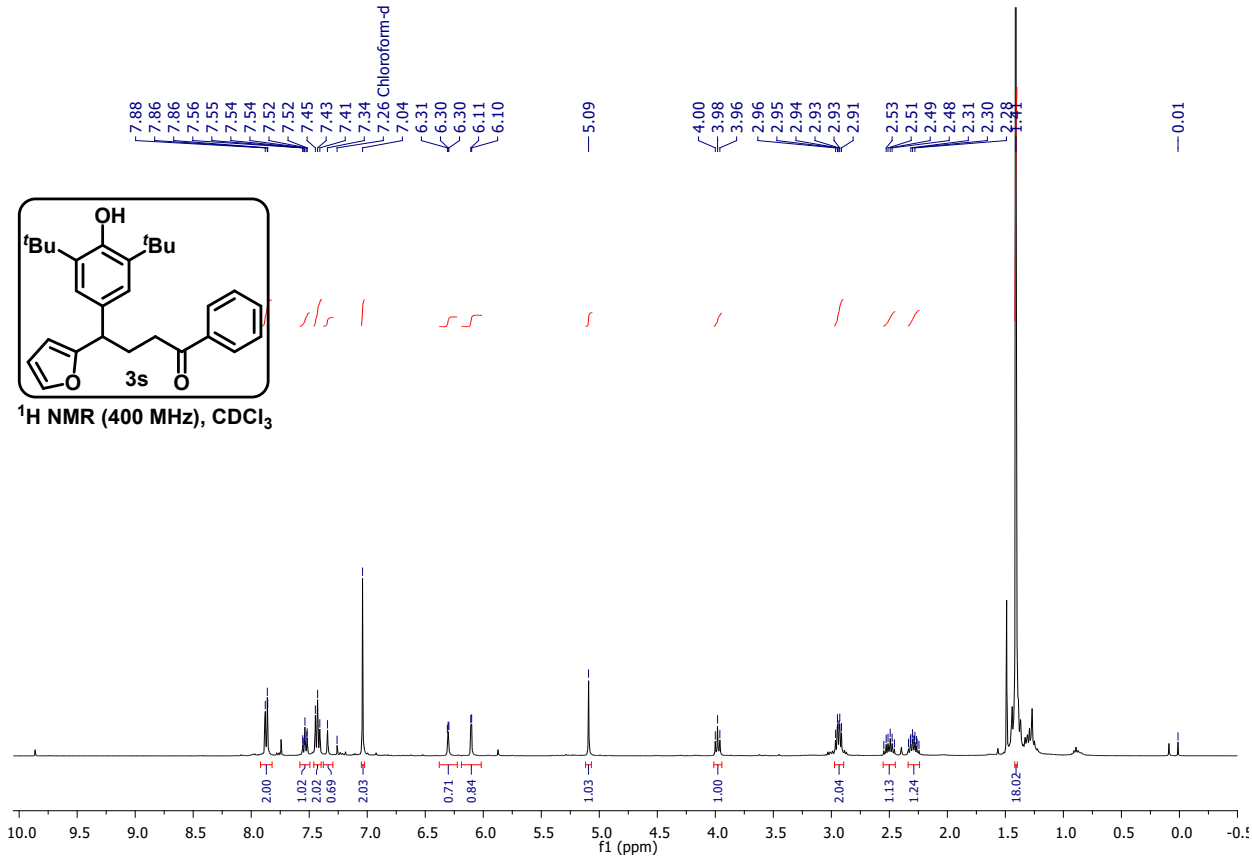


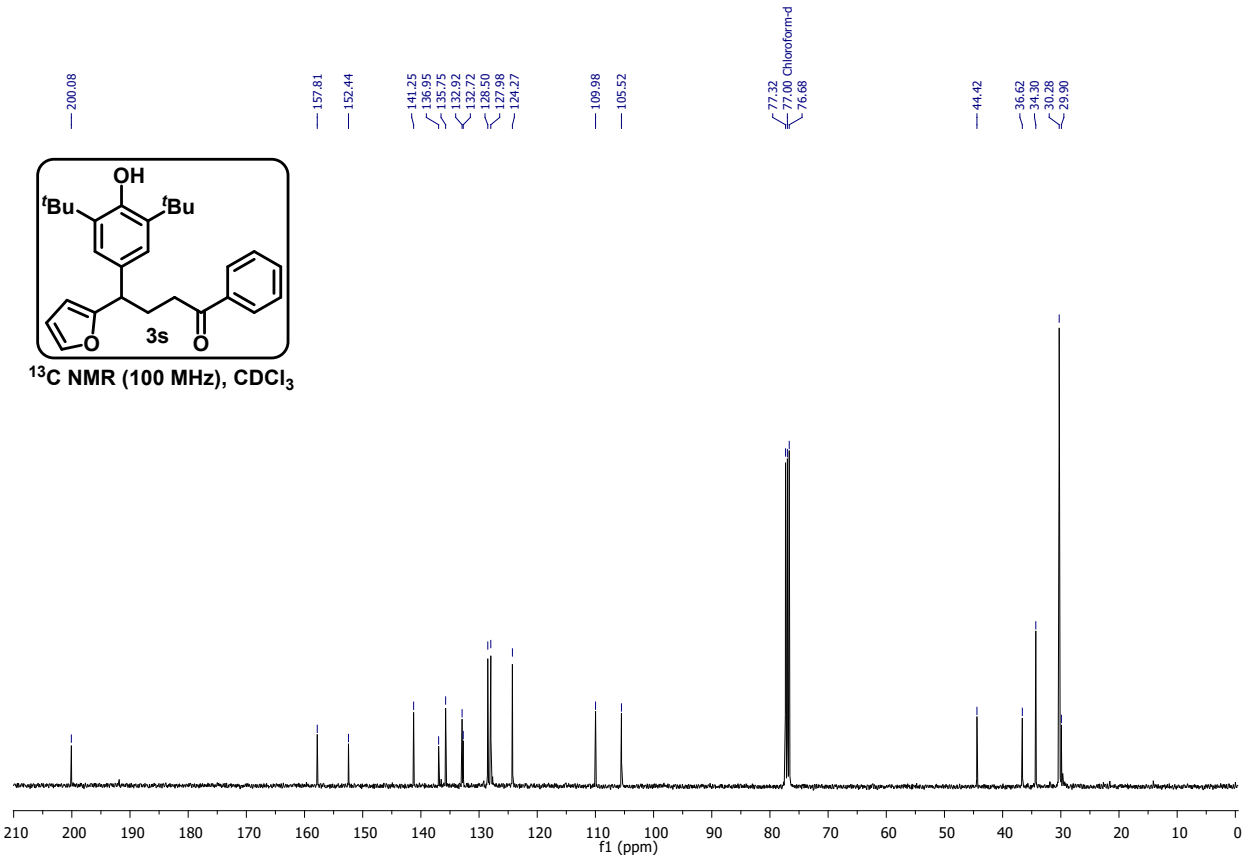
^{13}C NMR (100 MHz), $CDCl_3$

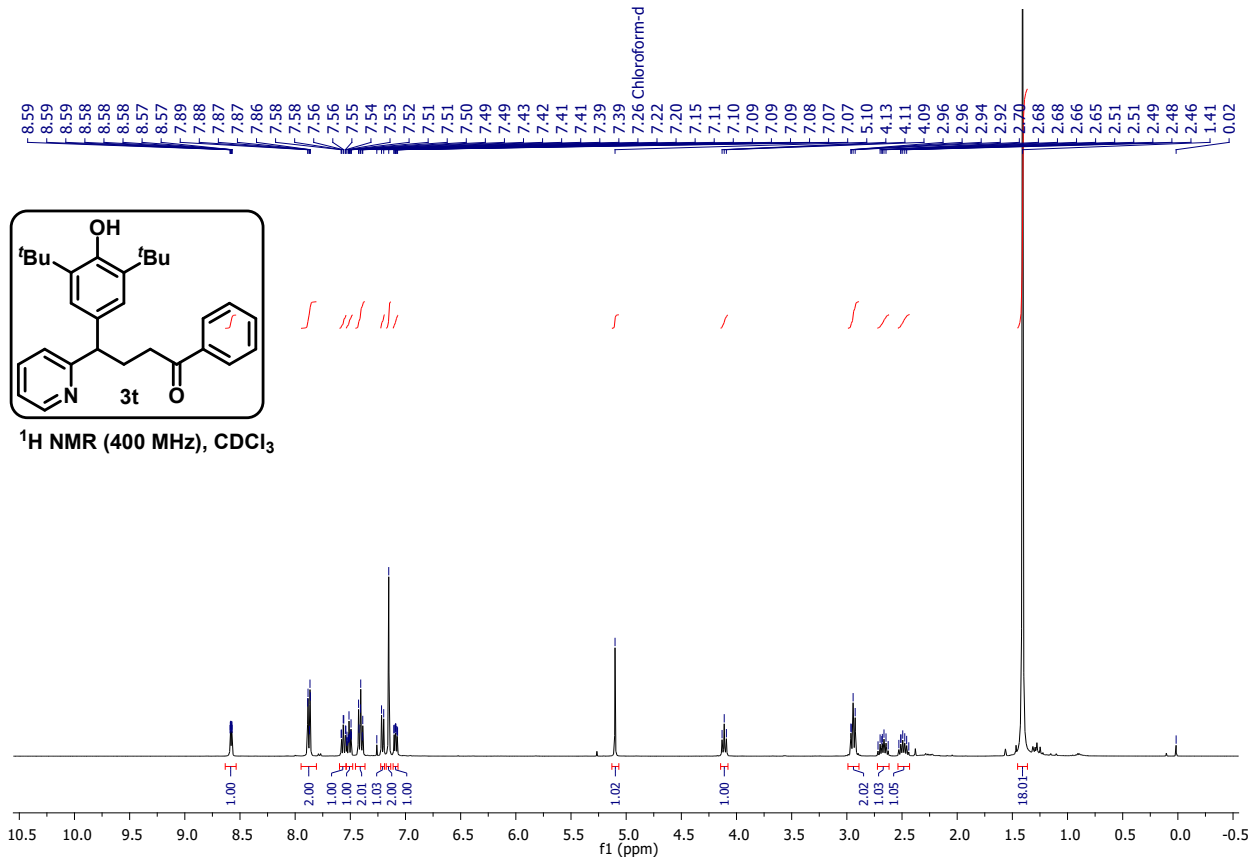


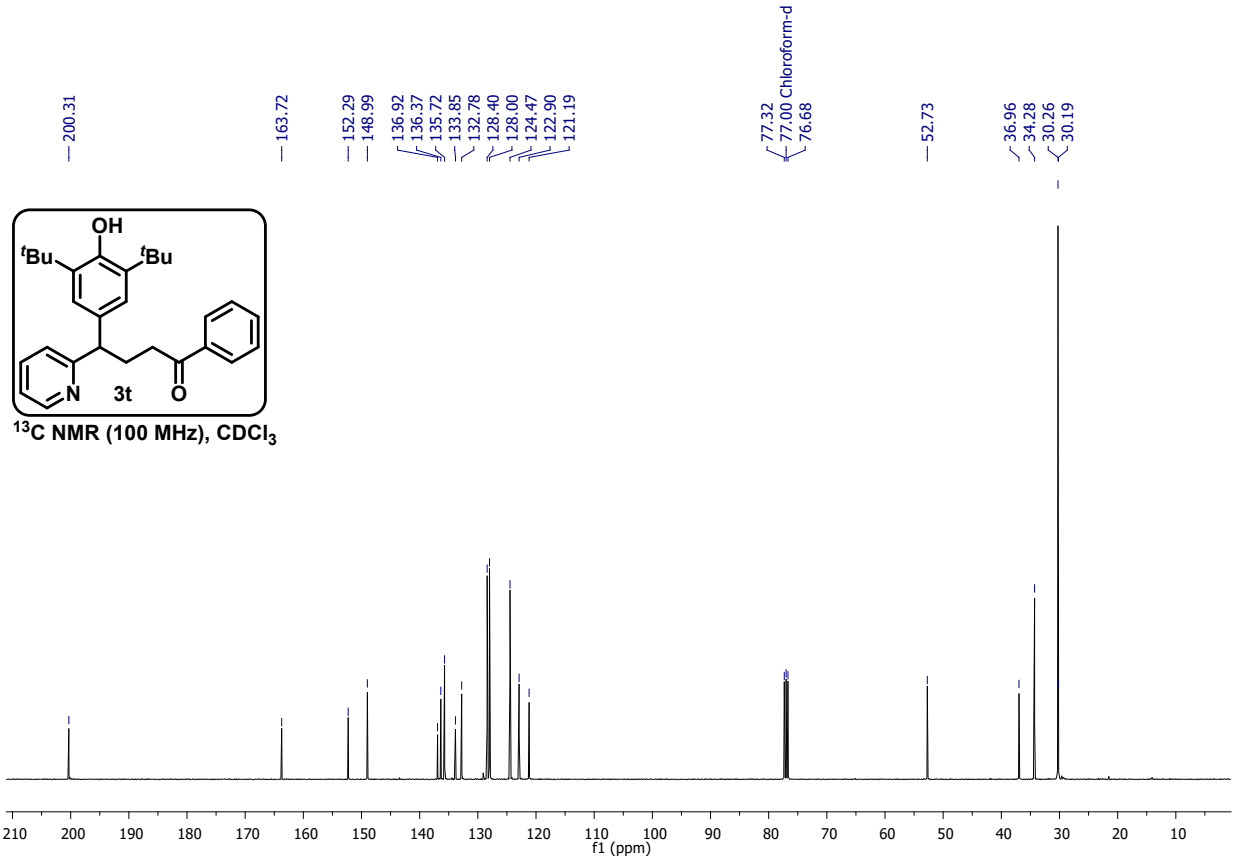
^{1}H NMR (400 MHz), $CDCl_3$


200.36
153.04
152.18
140.45
136.95
136.26
135.69
134.62
132.93
128.48
127.97
124.10
104.85
77.32
77.00 Chloroform-d
76.68
60.78
55.98
51.06
37.00
34.33
31.18
30.29
OH
tBu
tBu
MeO
MeO
OMe
O
3r
13C NMR (100 MHz), CDCl3
f1 (ppm)

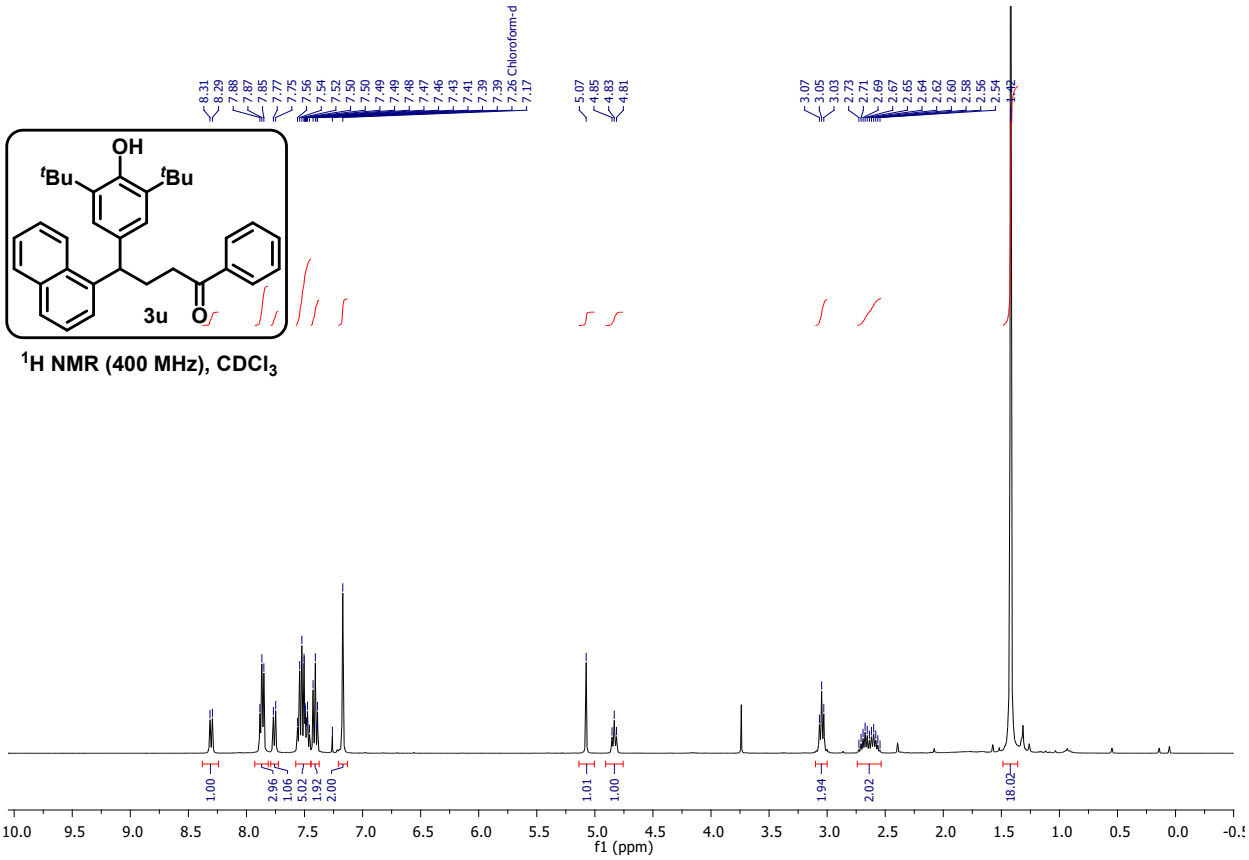

7.88
7.86
7.86
7.56
7.55
7.54
7.54
7.52
7.52
7.45
7.43
7.41
7.34
7.26 Chloroform-d
7.04
6.31
6.30
6.30
6.11
6.10
5.09
4.00
3.98
3.96
2.96
2.95
2.94
2.93
2.93
2.91
2.53
2.51
2.49
2.48
2.31
2.30
2.28
1.41
0.01
OH
tBu
tBu
O
3s
O
2.00
1.02
2.02
0.69
2.03
0.71
0.84
1.03
1.00
2.04
1.13
1.24
18.02
1H NMR (400 MHz), CDCl3
f1 (ppm)


200.08
157.81
152.44
141.25
136.95
135.75
132.92
132.72
128.50
127.98
124.27
109.98
105.52
77.32
77.00 Chloroform-d
76.68
44.42
36.62
34.30
30.28
29.90
OH
tBu
tBu
3s
O
O
13C NMR (100 MHz), CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

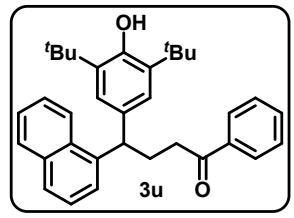

8.59 8.59 8.59 8.58 8.58 8.58 8.57 8.57 7.89 7.88 7.87 7.87 7.86 7.58 7.58 7.56 7.56 7.55 7.54 7.53 7.52 7.51 7.51 7.50 7.49 7.49 7.43 7.42 7.41 7.41 7.39 7.39 7.26 Chloroform-d 7.22 7.20 7.15 7.11 7.10 7.09 7.09 7.09 7.08 7.07 7.07 5.10 4.13 4.11 4.09 2.96 2.94 2.92 2.70 2.68 2.68 2.66 2.65 2.51 2.51 2.49 2.48 2.46 1.41 0.02
OH
tBu
tBu
N
3t
O
1H NMR (400 MHz), CDCl3
1.00 2.00 1.00 1.00 2.01 1.03 2.00 1.00 1.02 1.00 2.02 1.03 1.05 18.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)



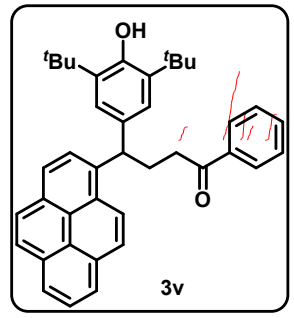
^{13}C NMR (100 MHz), $CDCl_3$



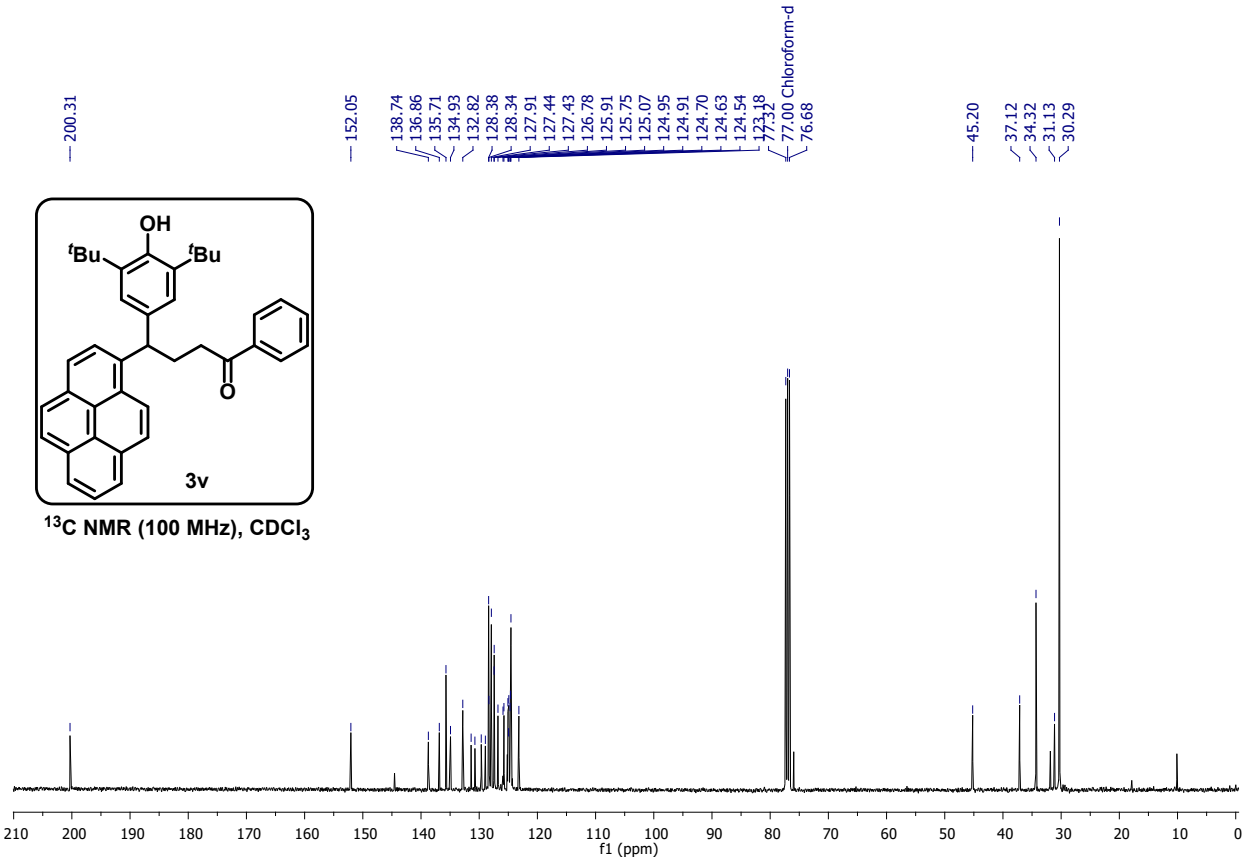
^{1}H NMR (400 MHz), $CDCl_3$

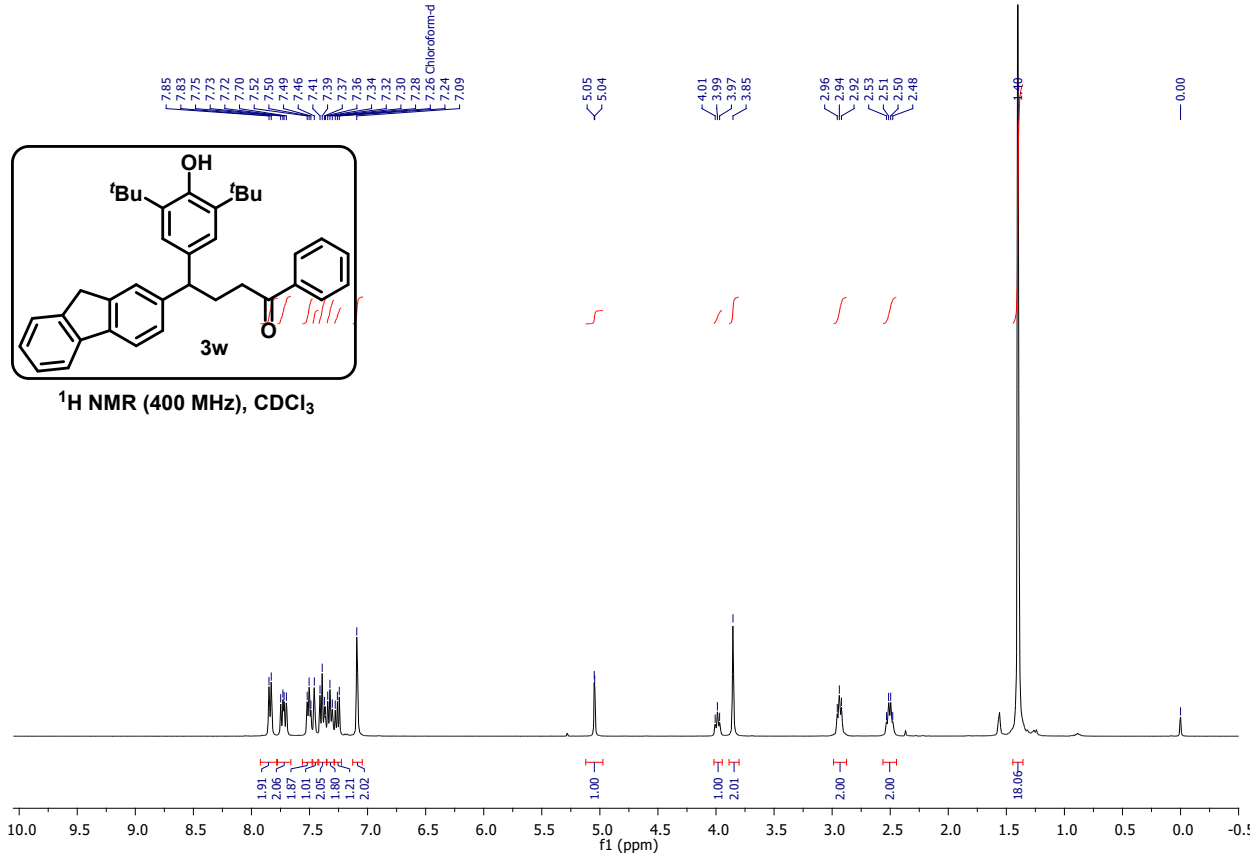


^{13}C NMR (100 MHz), $CDCl_3$



^{1}H NMR (400 MHz), $CDCl_3$


200.31
152.05
138.74
136.86
135.71
134.93
132.82
128.38
128.34
127.91
127.44
127.43
126.78
125.91
125.75
125.07
124.95
124.91
124.70
124.63
124.54
123.18
77.32
77.00 Chloroform-d
76.68
45.20
37.12
34.32
31.13
30.29
OH
tBu
tBu
O
3v
13C NMR (100 MHz), CDCl3
f1 (ppm)


7.85
7.83
7.75
7.73
7.72
7.70
7.52
7.50
7.49
7.46
7.41
7.39
7.37
7.36
7.34
7.32
7.30
7.28
7.26 Chloroform-d
7.24
7.09
5.05
5.04
4.01
3.99
3.97
3.85
2.96
2.94
2.92
2.53
2.51
2.50
2.48
1.48
0.00
OH
tBu
tBu
O
3w
1H NMR (400 MHz), CDCl3
1.91
2.06
1.87
1.01
2.05
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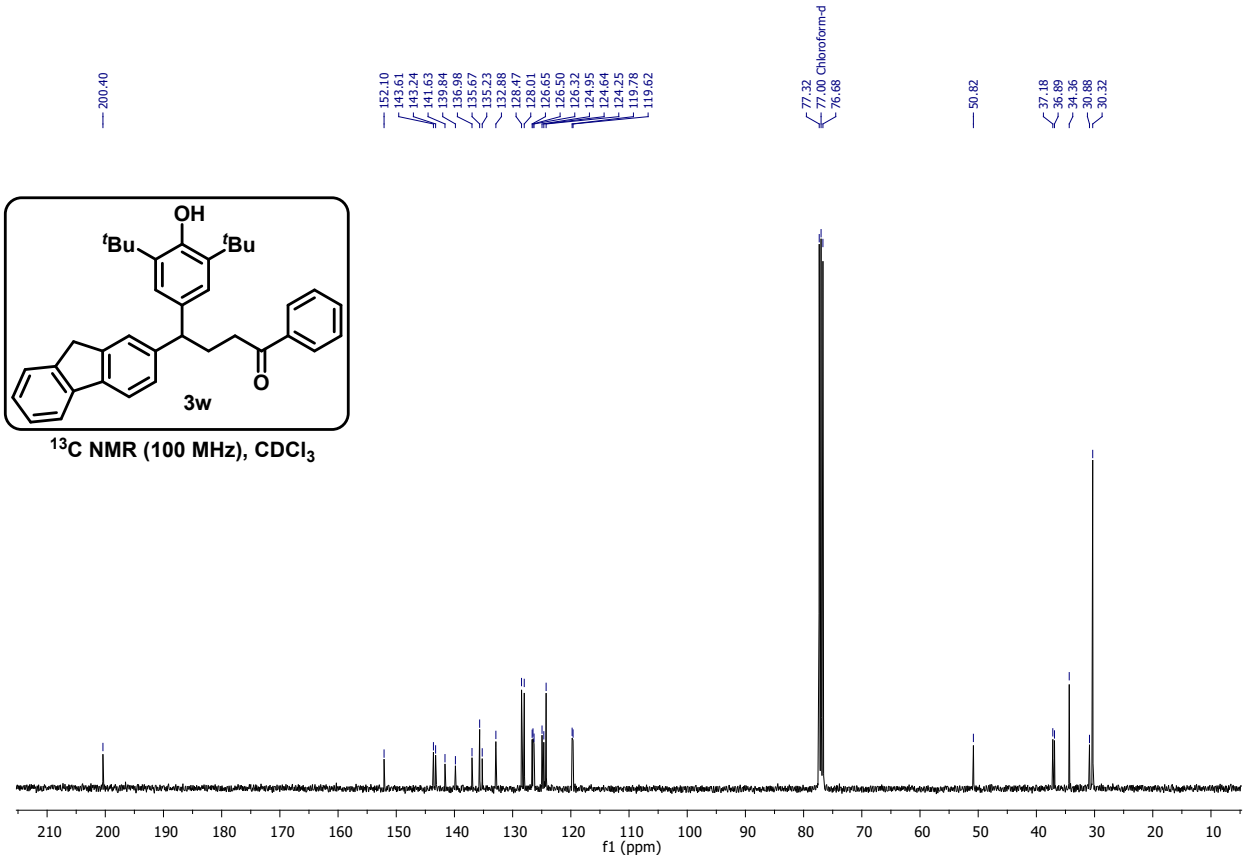
2.02
1.00
1.00
2.01
2.00
2.00
18.06
f1 (ppm)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126.50
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124.95
124.64
124.25
119.78
119.62
77.32
77.00 Chloroform-d
76.68
50.82
37.18
36.89
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30.32
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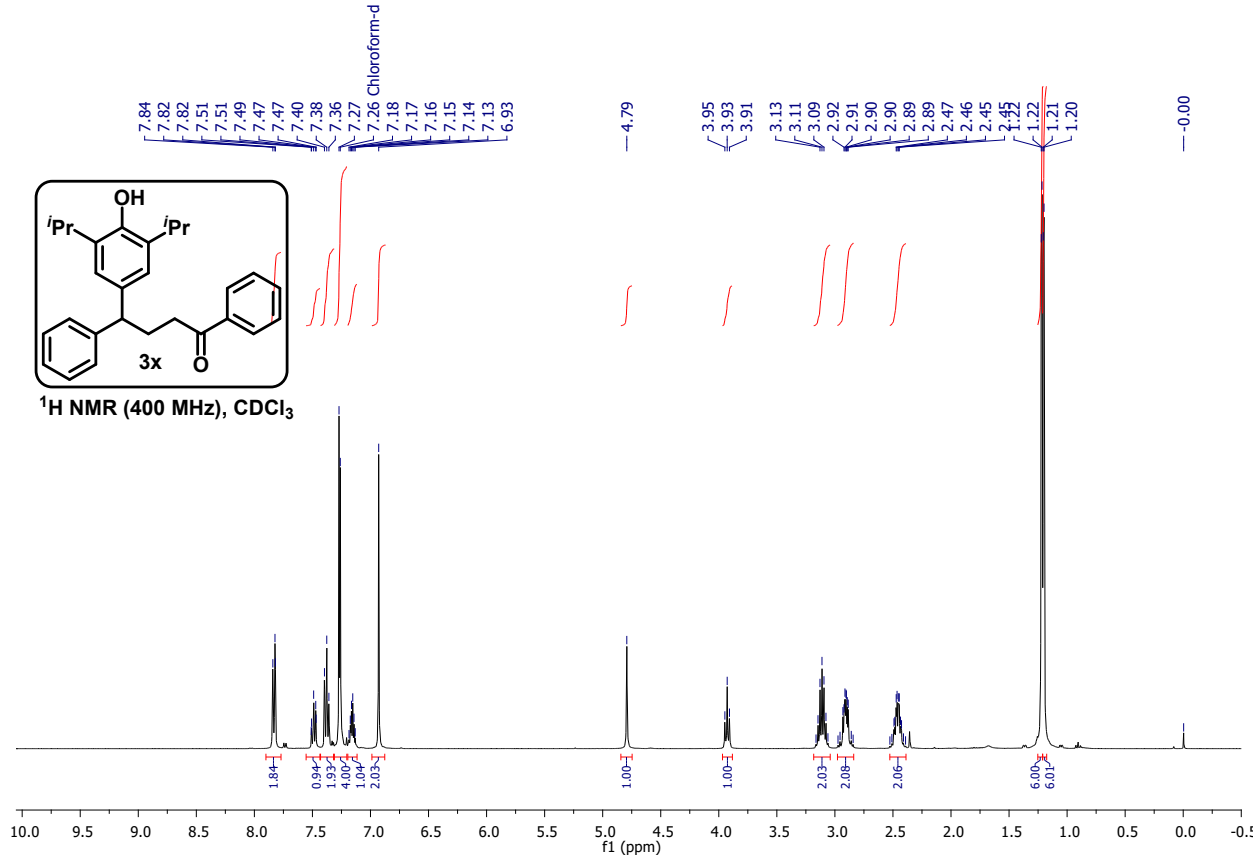
13C NMR (100 MHz), CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)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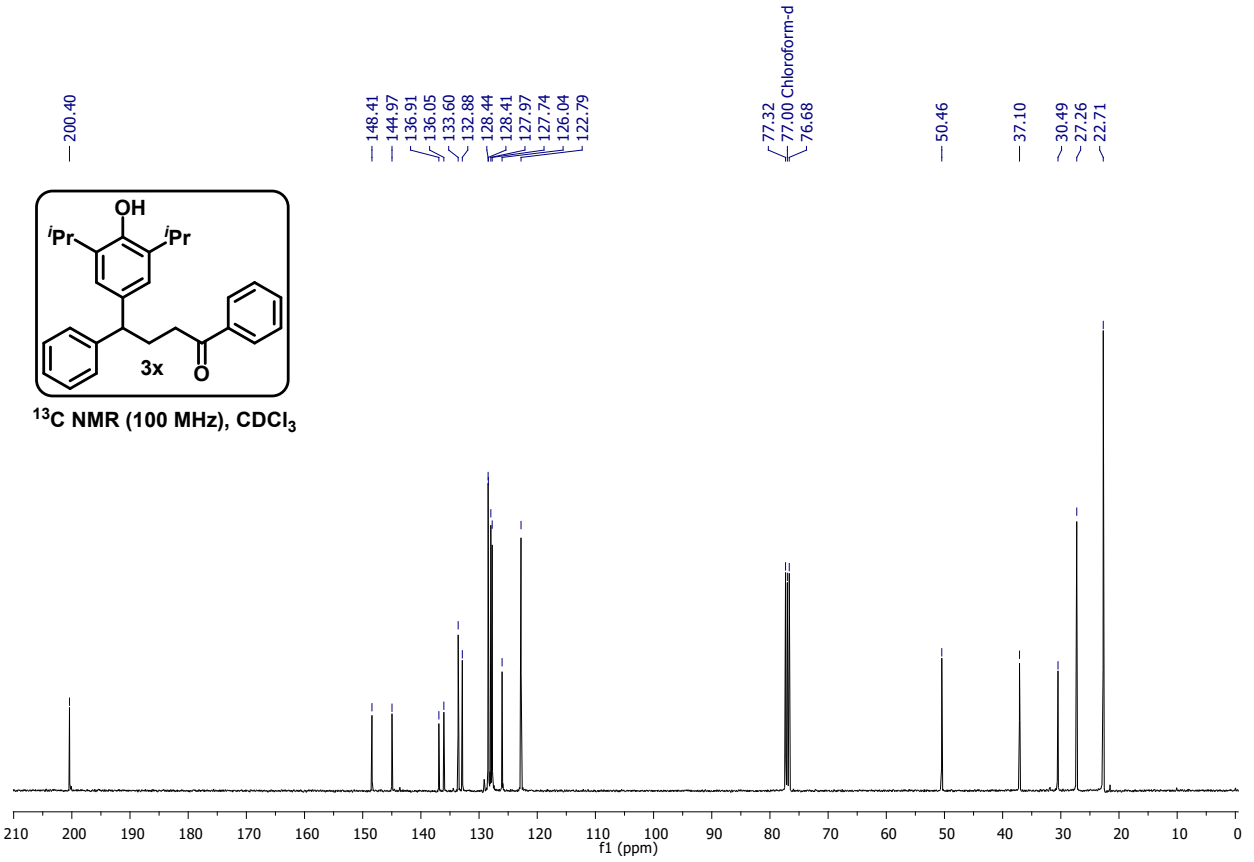
7.16
7.15
7.14
7.13
6.93
4.79
3.95
3.93
3.91
3.13
3.11
3.09
2.92
2.91
2.90
2.90
2.89
2.89
2.47
2.46
2.45
1.22
1.21
1.20
-0.00
OH
iPr
iPr
O
3x
1H NMR (400 MHz), CDCl3
1.84
0.94
1.93
4.00
1.04
2.03
1.00
1.00
2.03
2.08
2.06
6.00
6.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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77.32
77.00 Chloroform-d
76.68
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27.26
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OH
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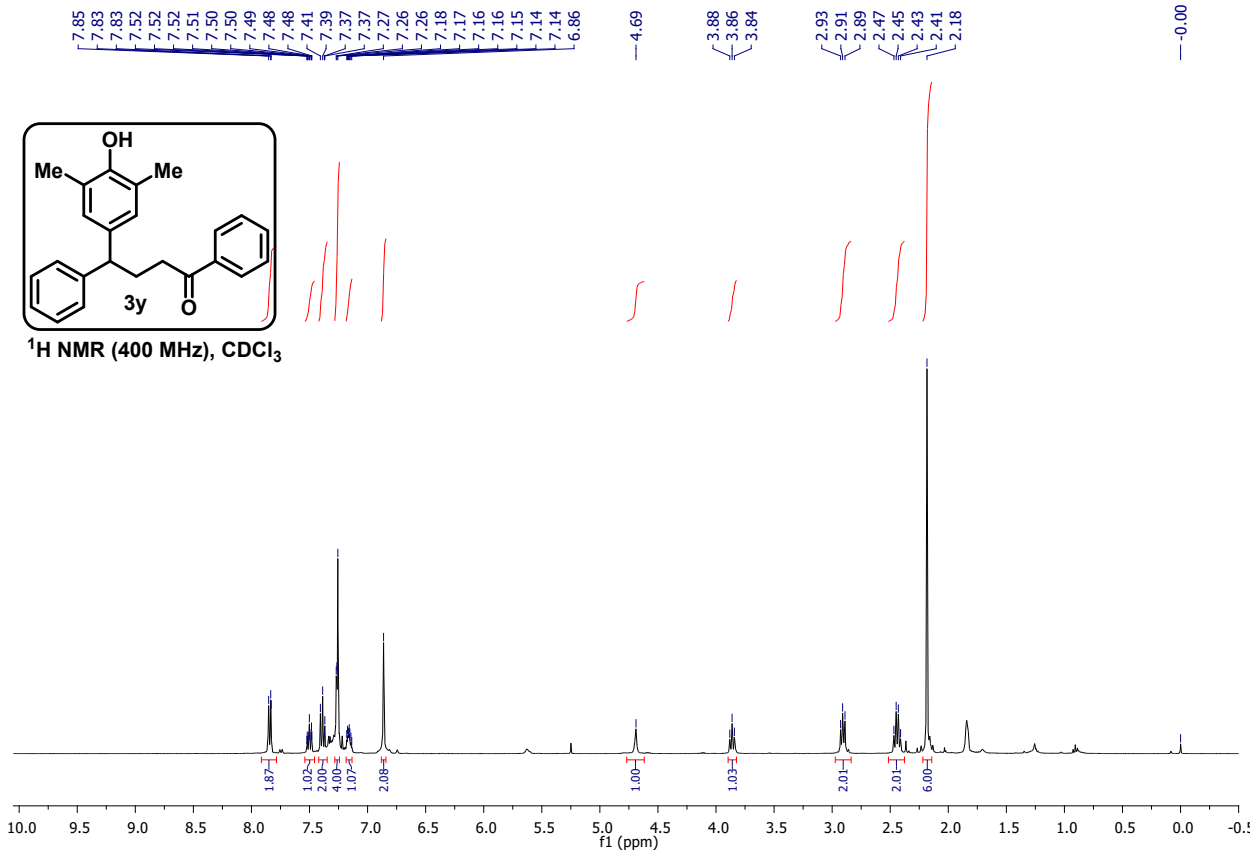
iPr
3x
O
13C NMR (100 MHz), CDCl3
f1 (ppm)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7.14
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2.93
2.91
2.89
2.47
2.45
2.43
2.41
2.18
-0.00
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Me
Me
3y
O
1H NMR (400 MHz), CDCl3
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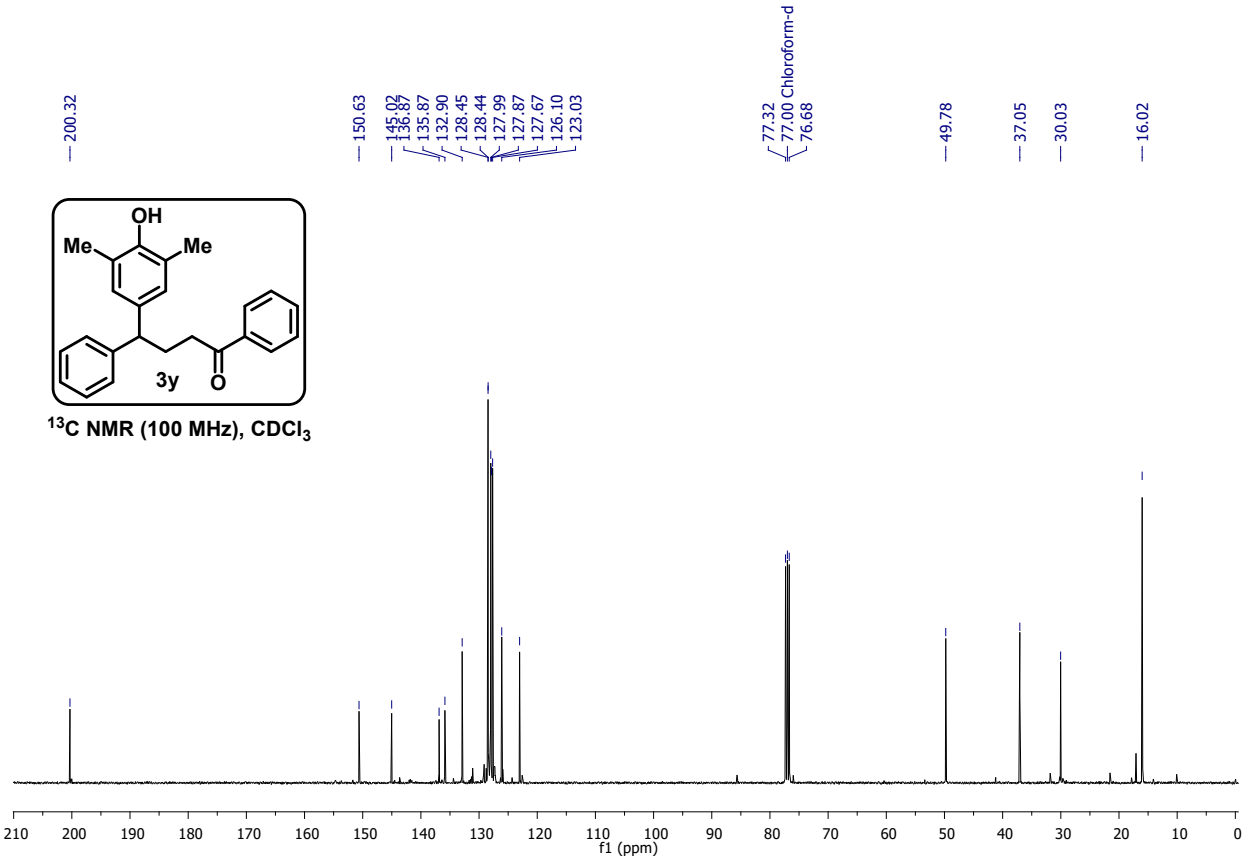
1.07
2.08
1.00
1.03
2.01
2.01
6.00
f1 (ppm)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128.44
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123.03
77.32
77.00 Chloroform-d
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37.05
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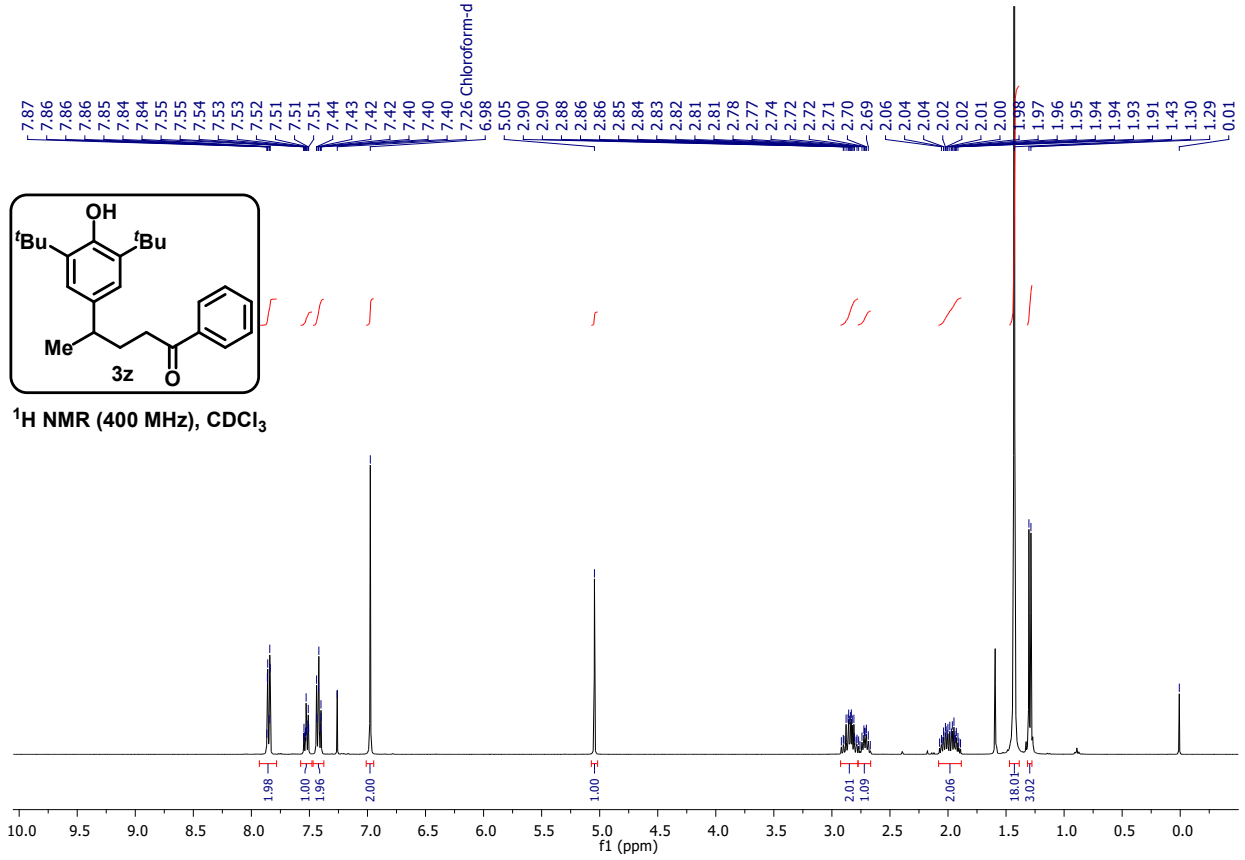
Me
Me
3y
O
13C NMR (100 MHz), CDCl3
f1 (ppm)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1.96
1.95
1.94
1.94
1.93
1.91
1.43
1.30
1.29
0.01
OH
tBu
tBu
Me
3z
O
1H NMR (400 MHz), CDCl3
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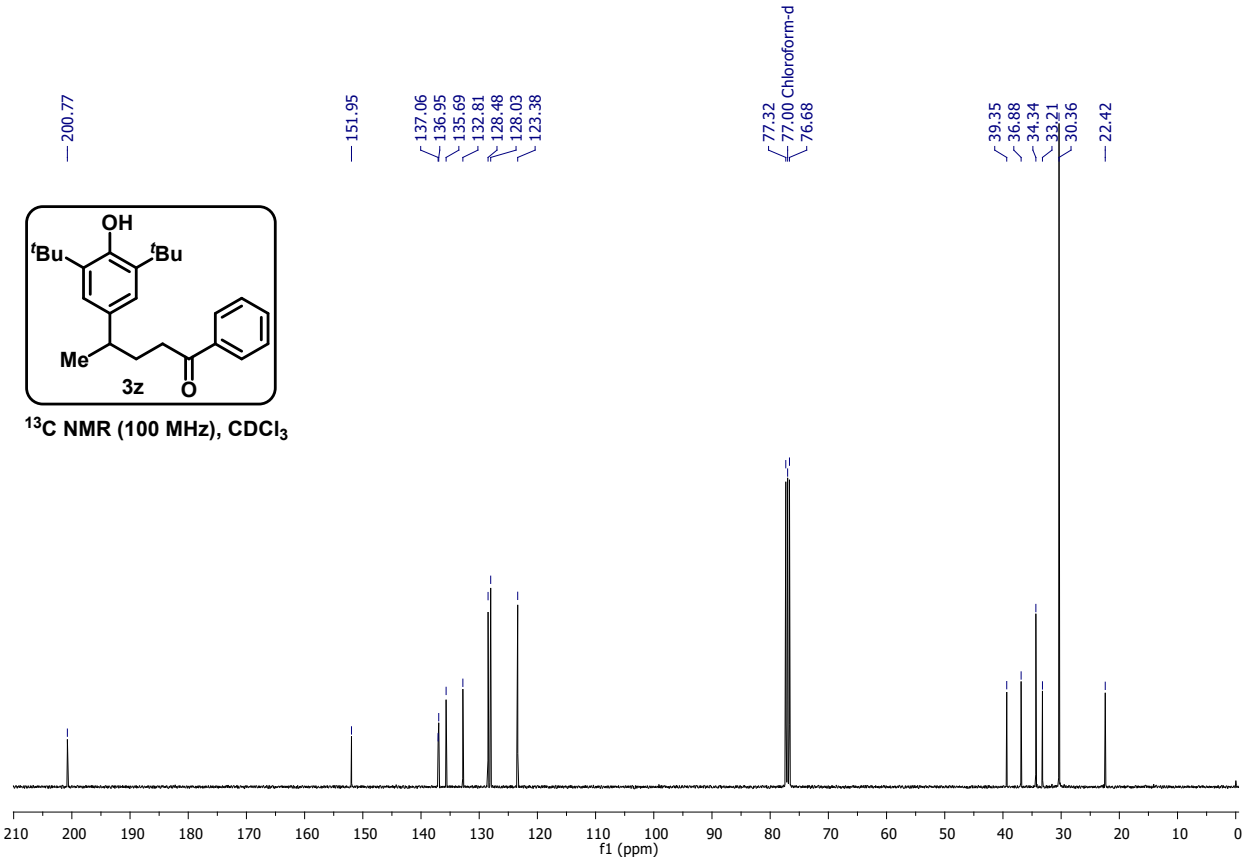
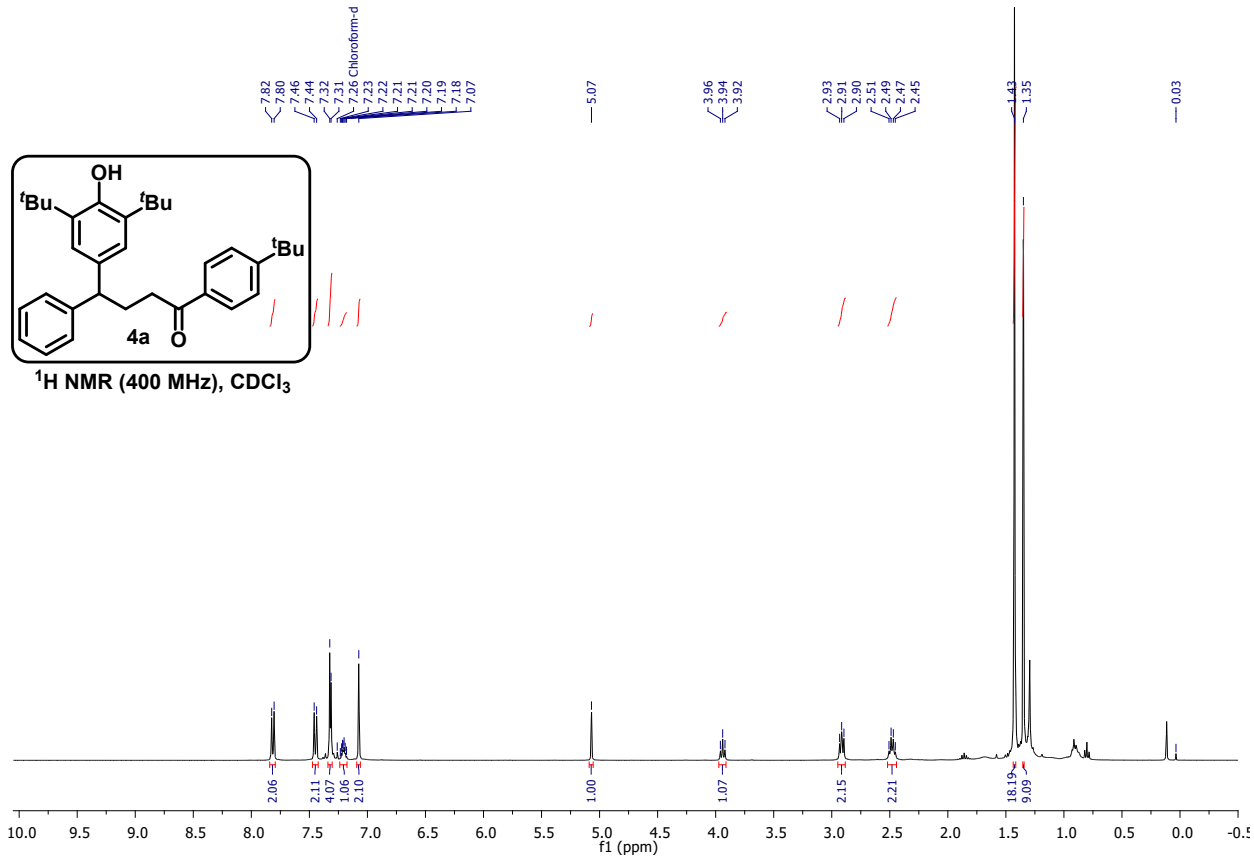
1.96
2.00
1.00
2.01
1.09
2.06
18.01
3.02
f1 (ppm)



^{13}C NMR (100 MHz), $CDCl_3$



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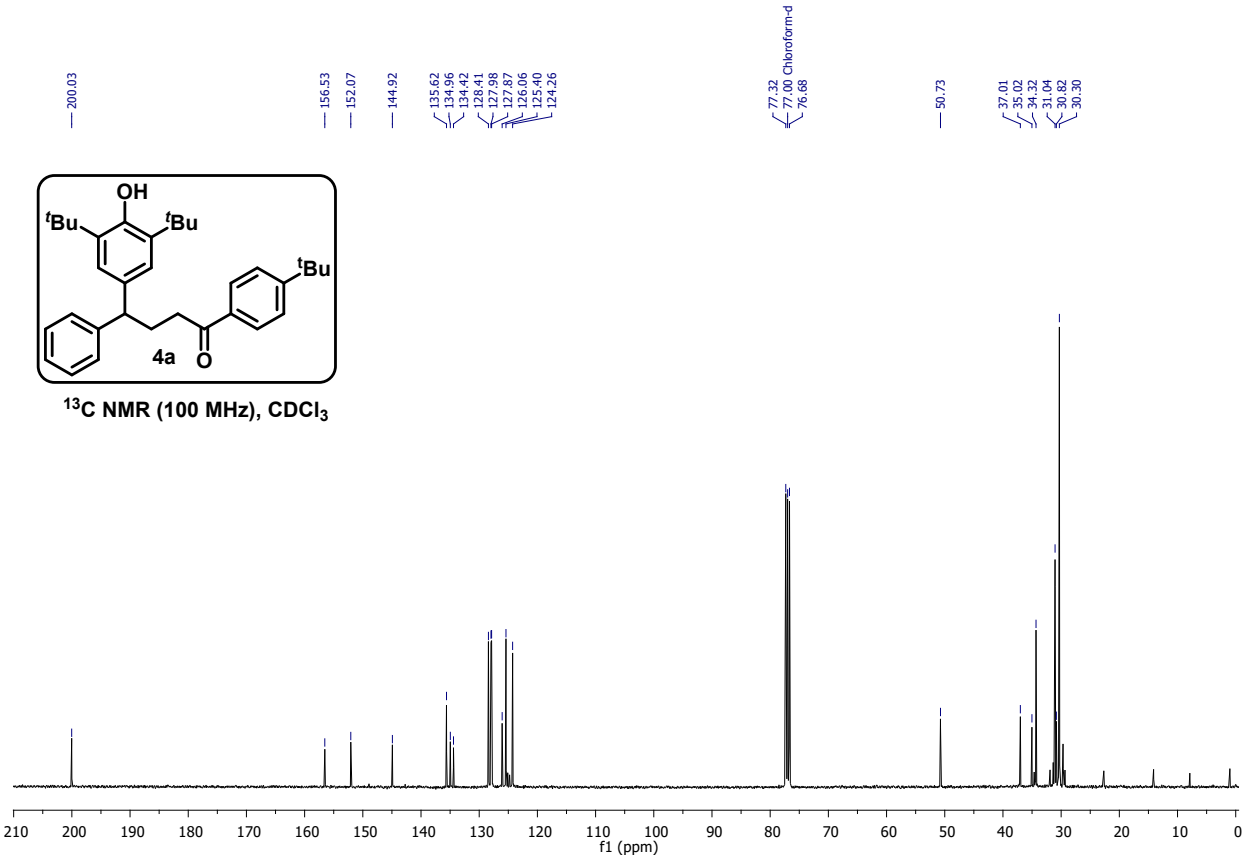
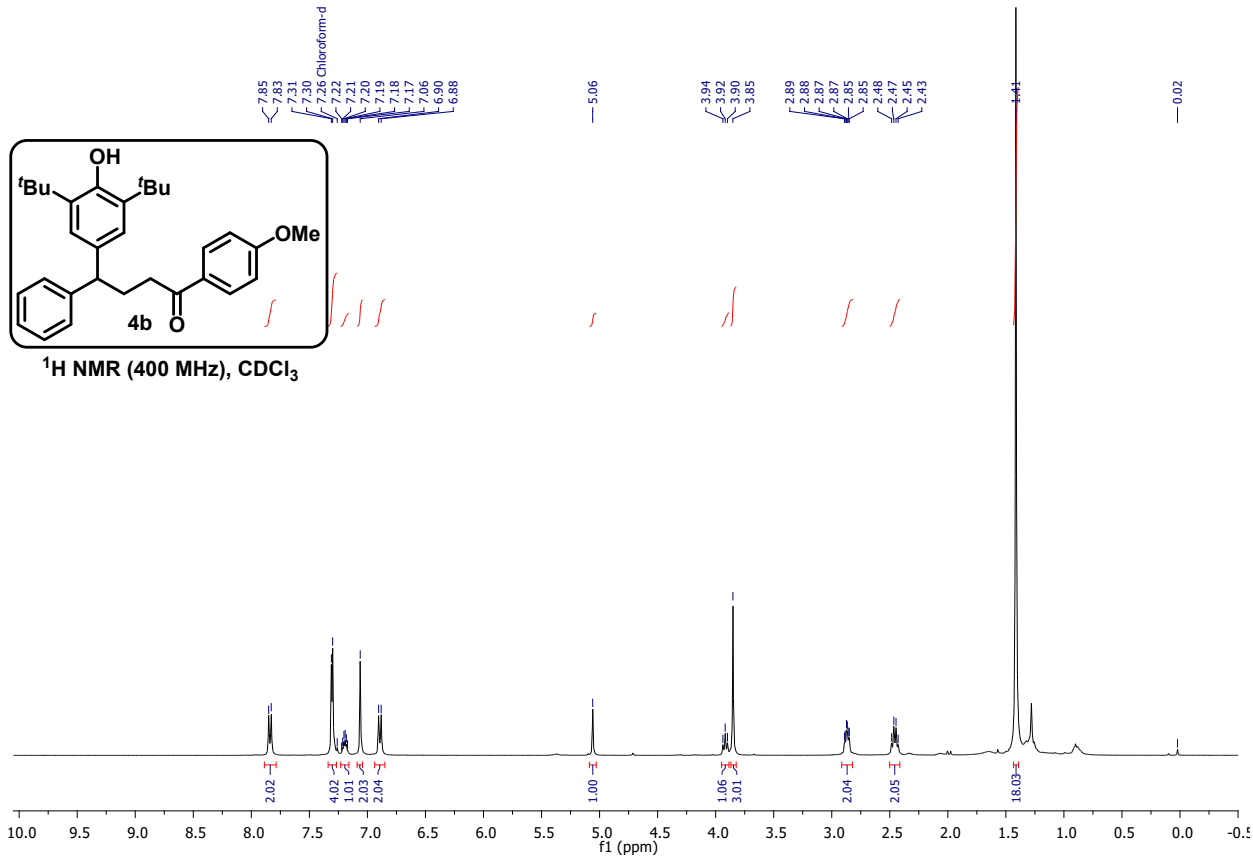
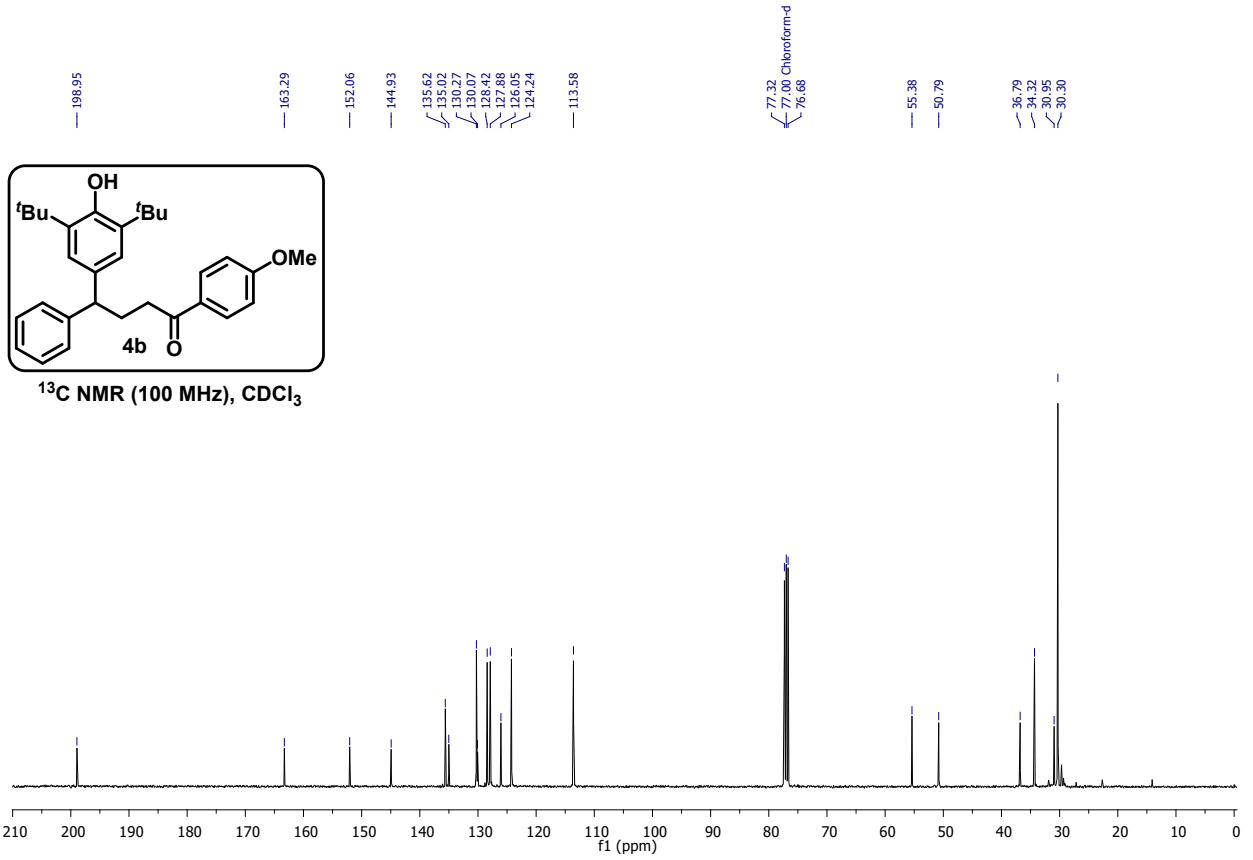


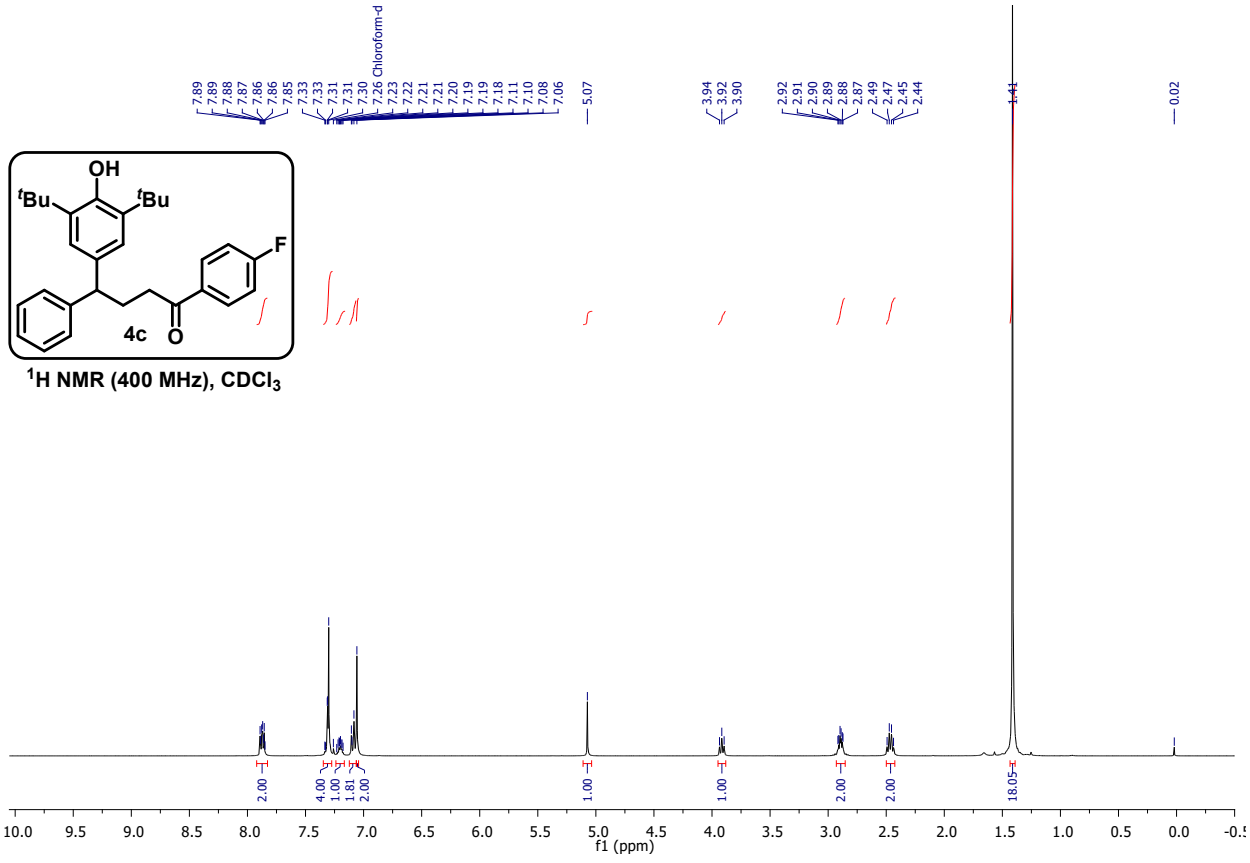
^{13}C NMR (100 MHz), $CDCl_3$



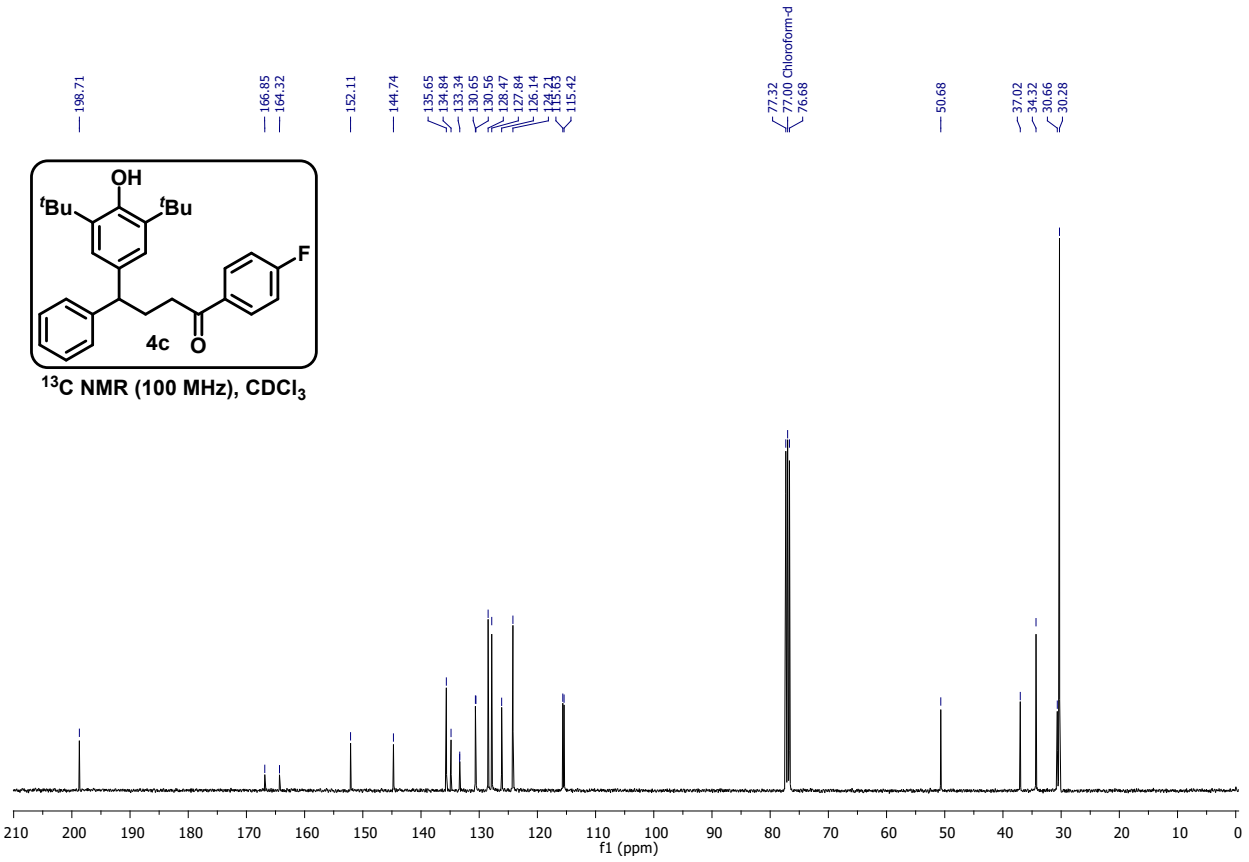
^{1}H NMR (400 MHz), $CDCl_3$



^{13}C NMR (100 MHz), $CDCl_3$



^{1}H NMR (400 MHz), $CDCl_3$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152.11
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135.65
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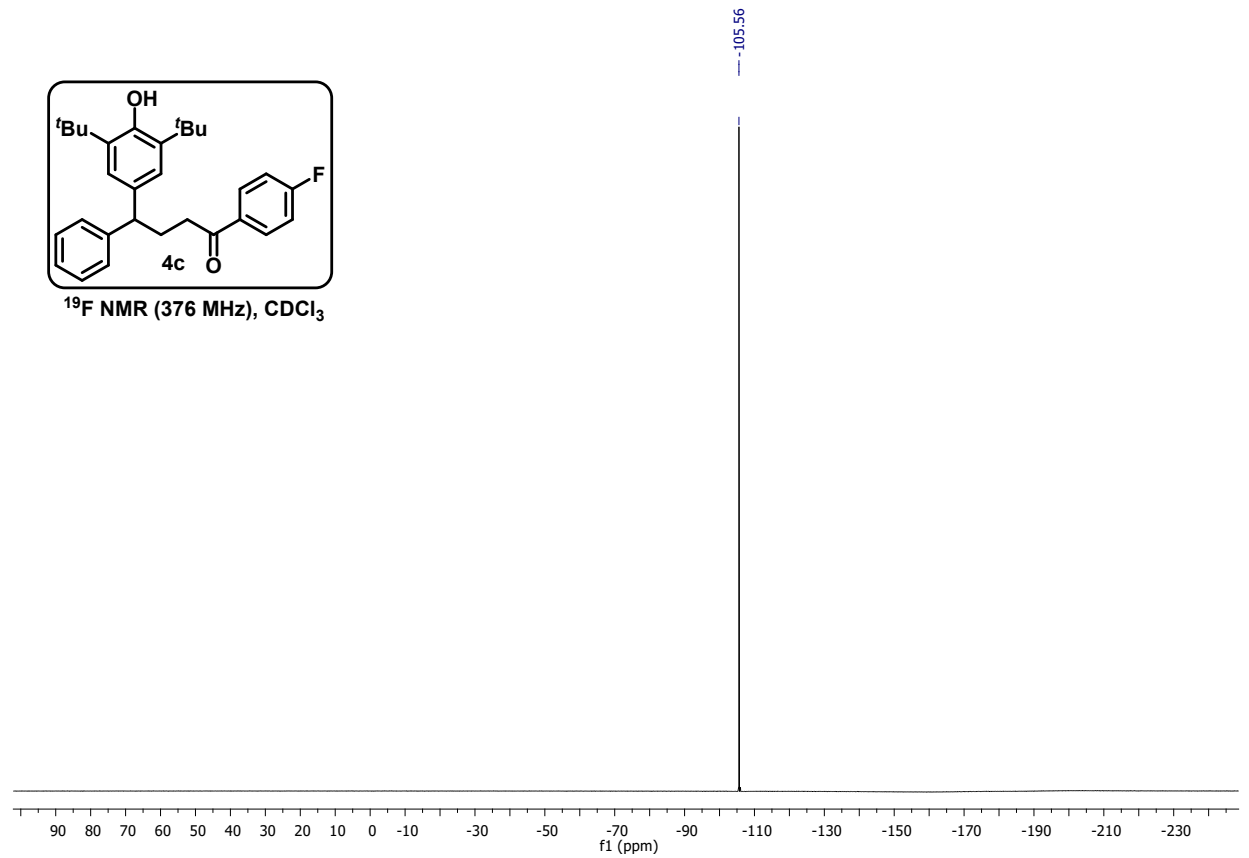
126.14
124.21
115.63
115.42
77.32
77.00 Chloroform-d
76.68
50.68
37.02
34.32
30.66
30.28
OH
tBu
tBu
F
4c
O
13C NMR (100 MHz), CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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tBu
tBu
F
4c
O
19F NMR (376 MHz), CDCl3
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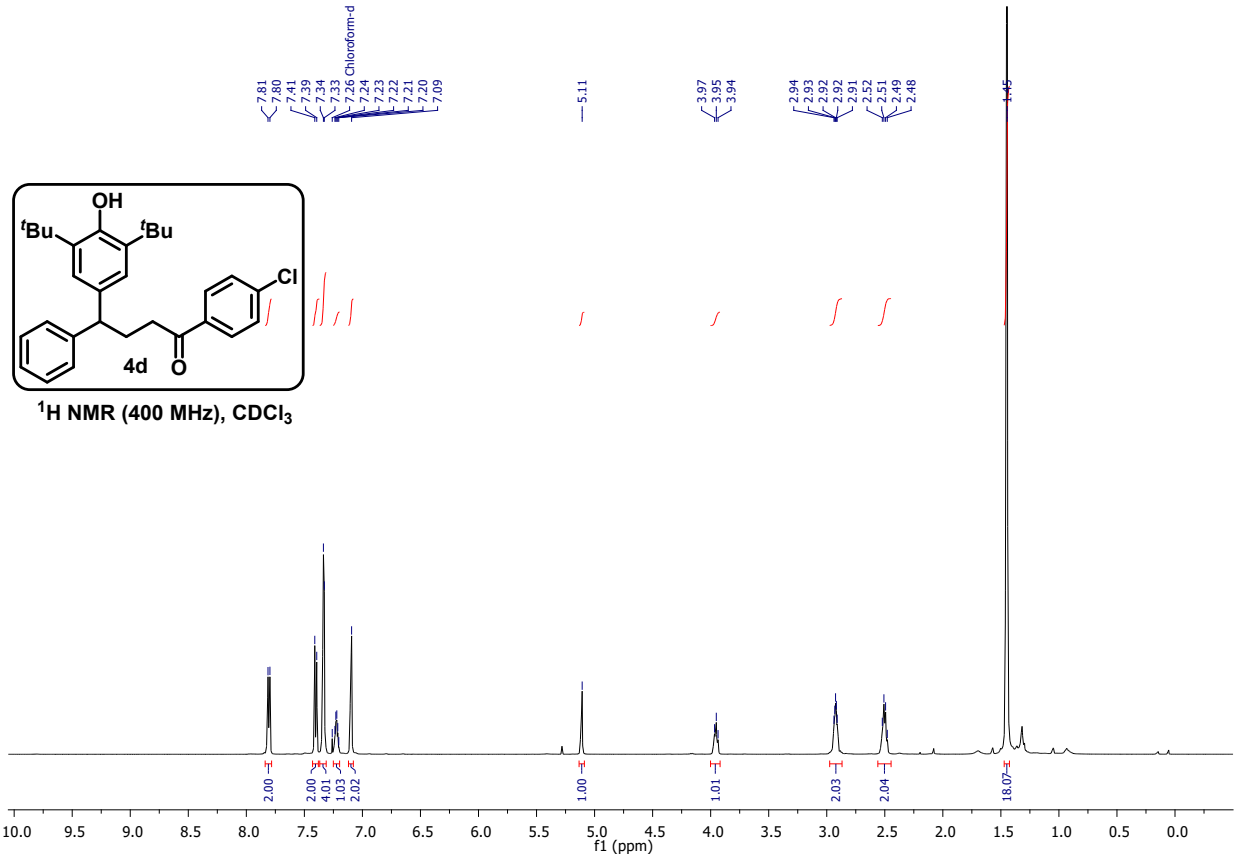
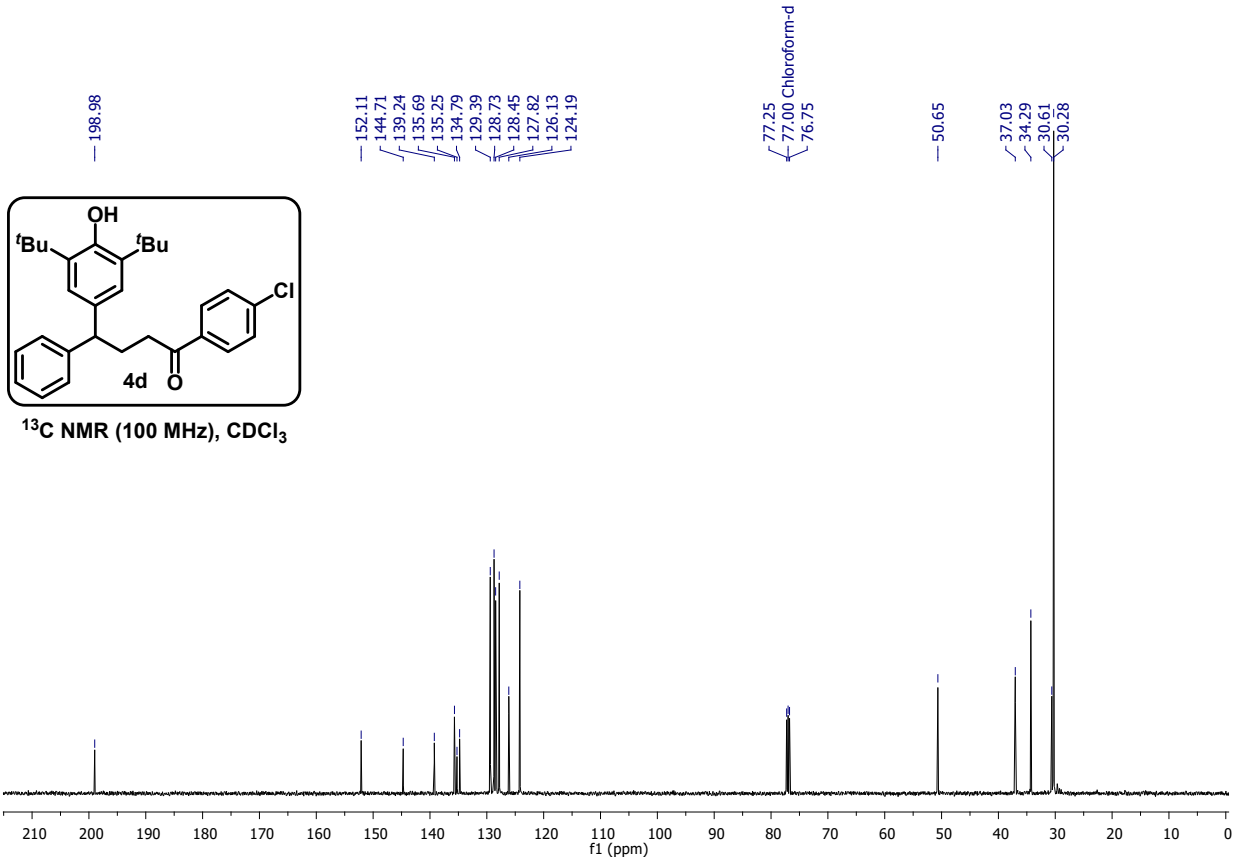
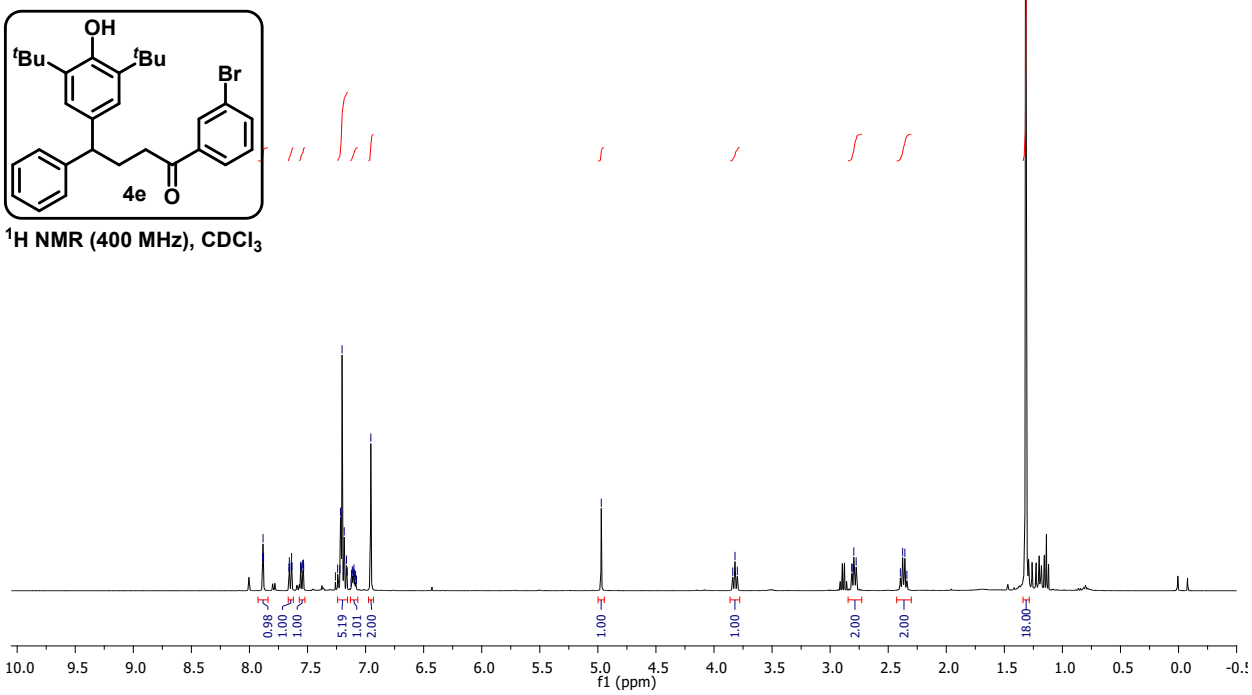
f1 (ppm)



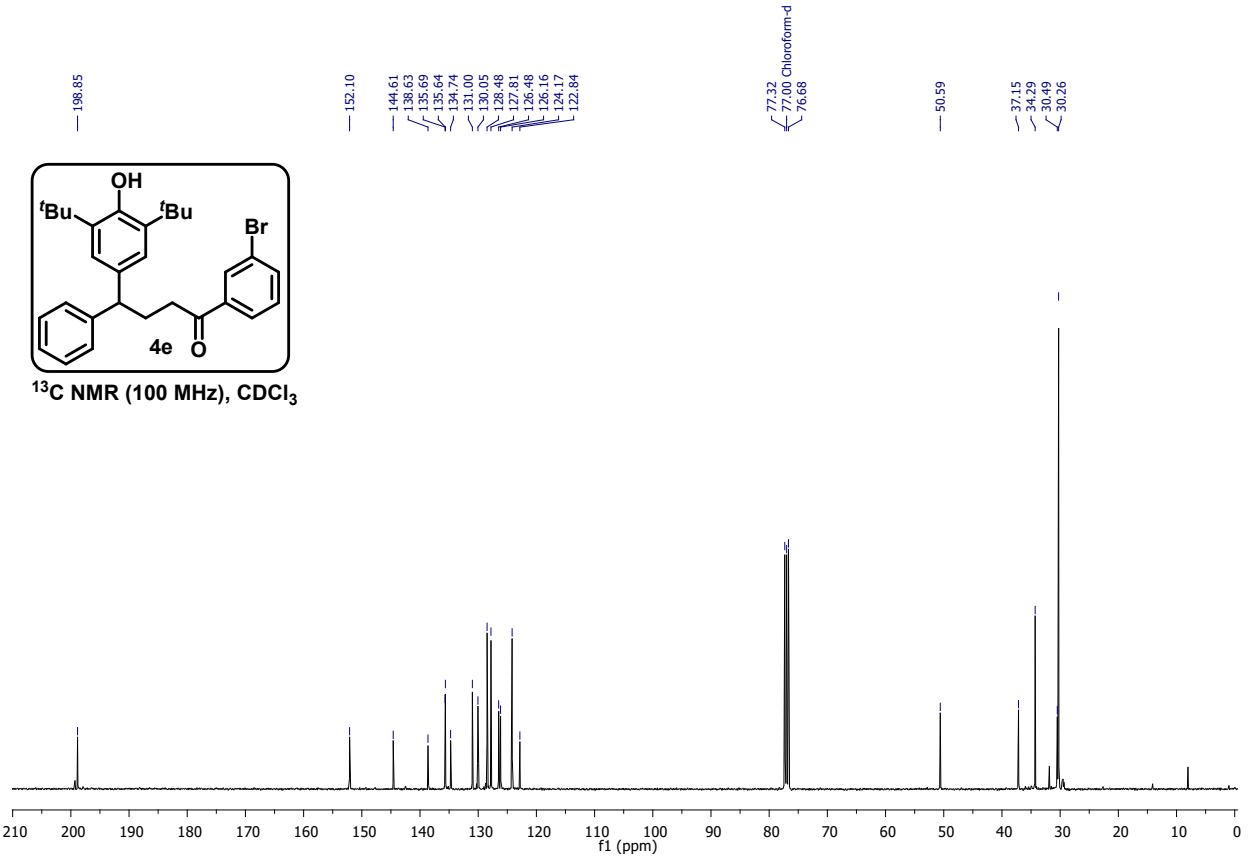
^{1}H NMR (400 MHz), $CDCl_3$



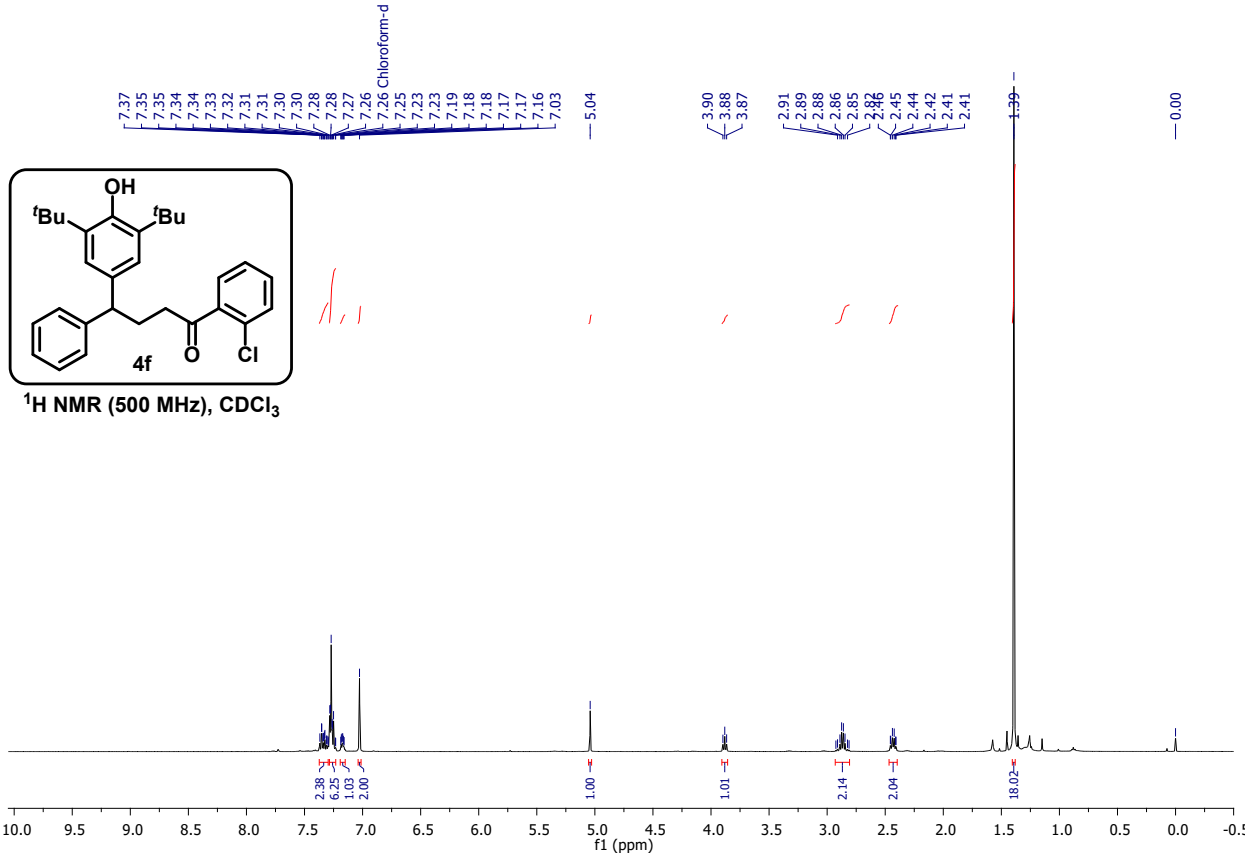
^{13}C NMR (100 MHz), $CDCl_3$



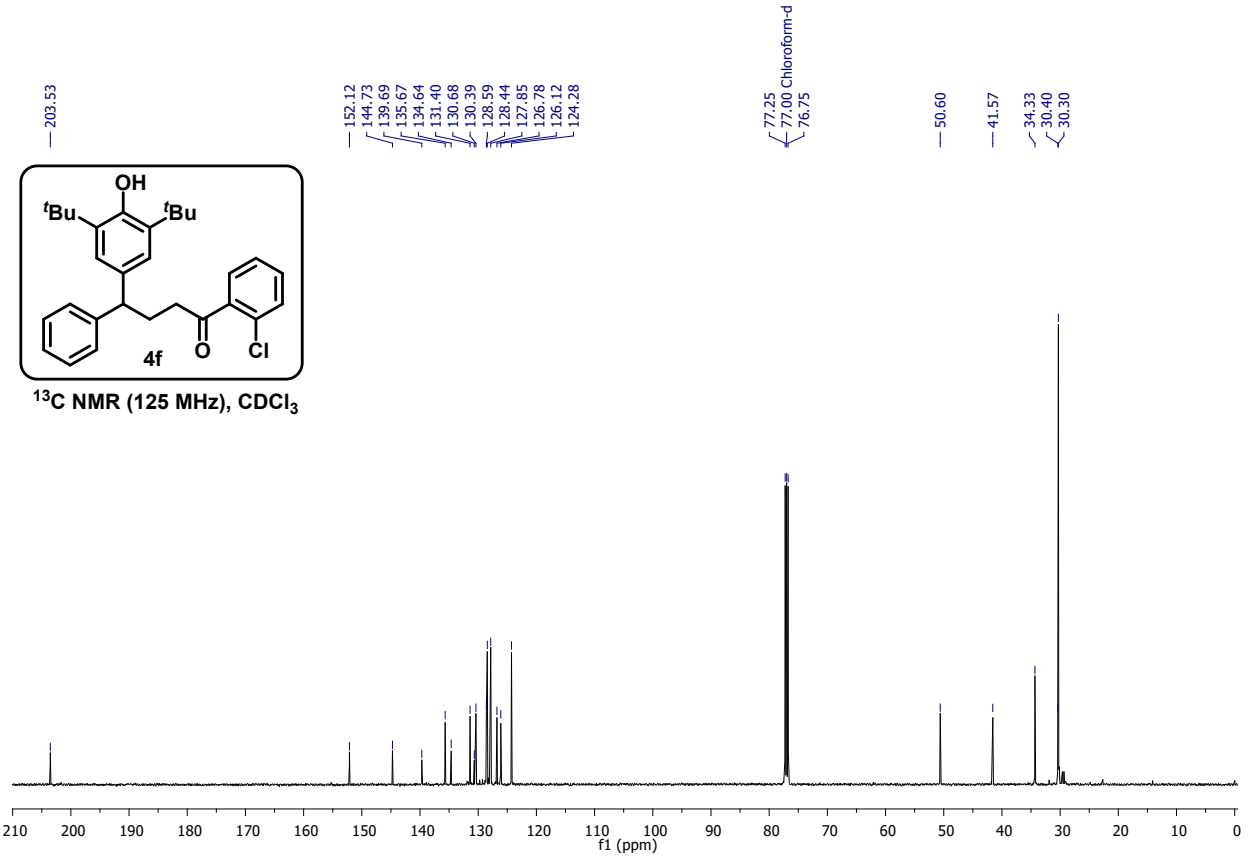
^{1}H NMR (400 MHz), $CDCl_3$



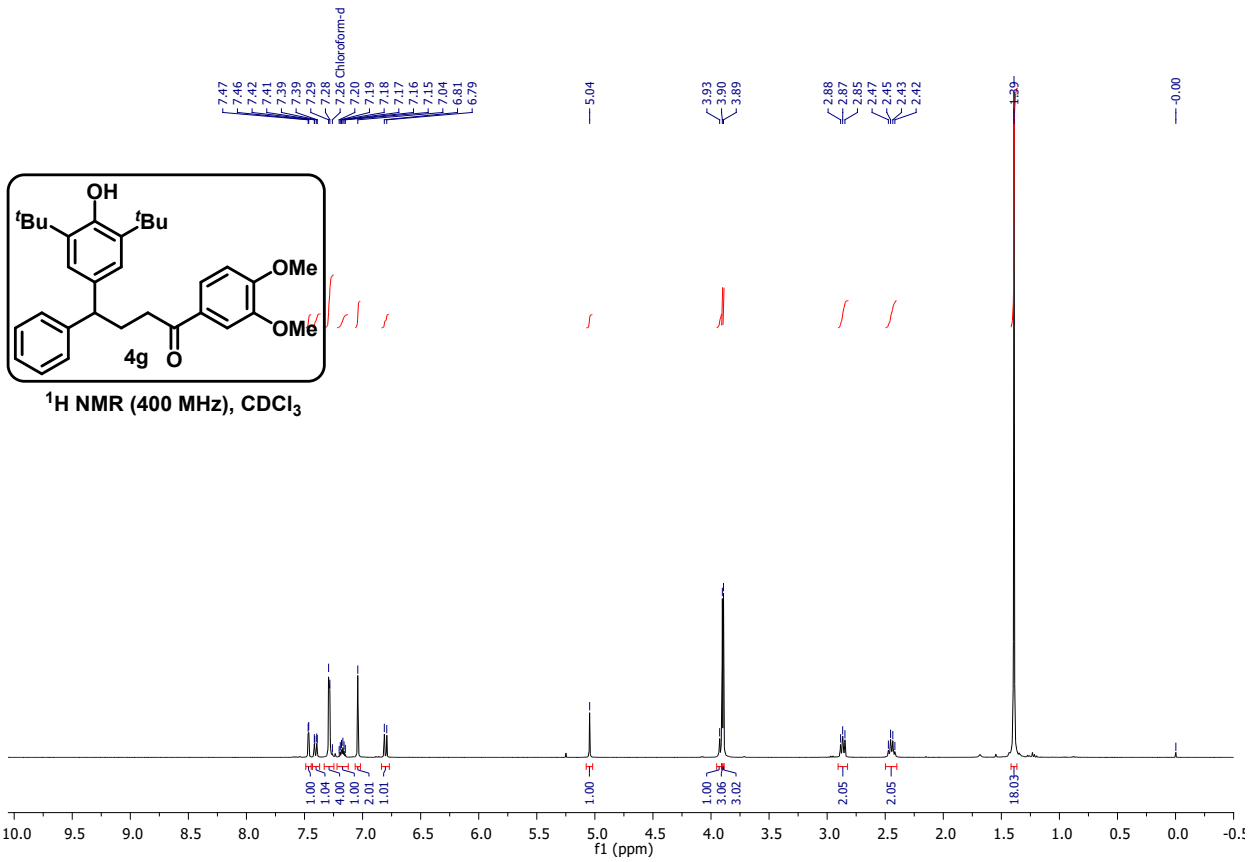
^{13}C NMR (100 MHz), $CDCl_3$



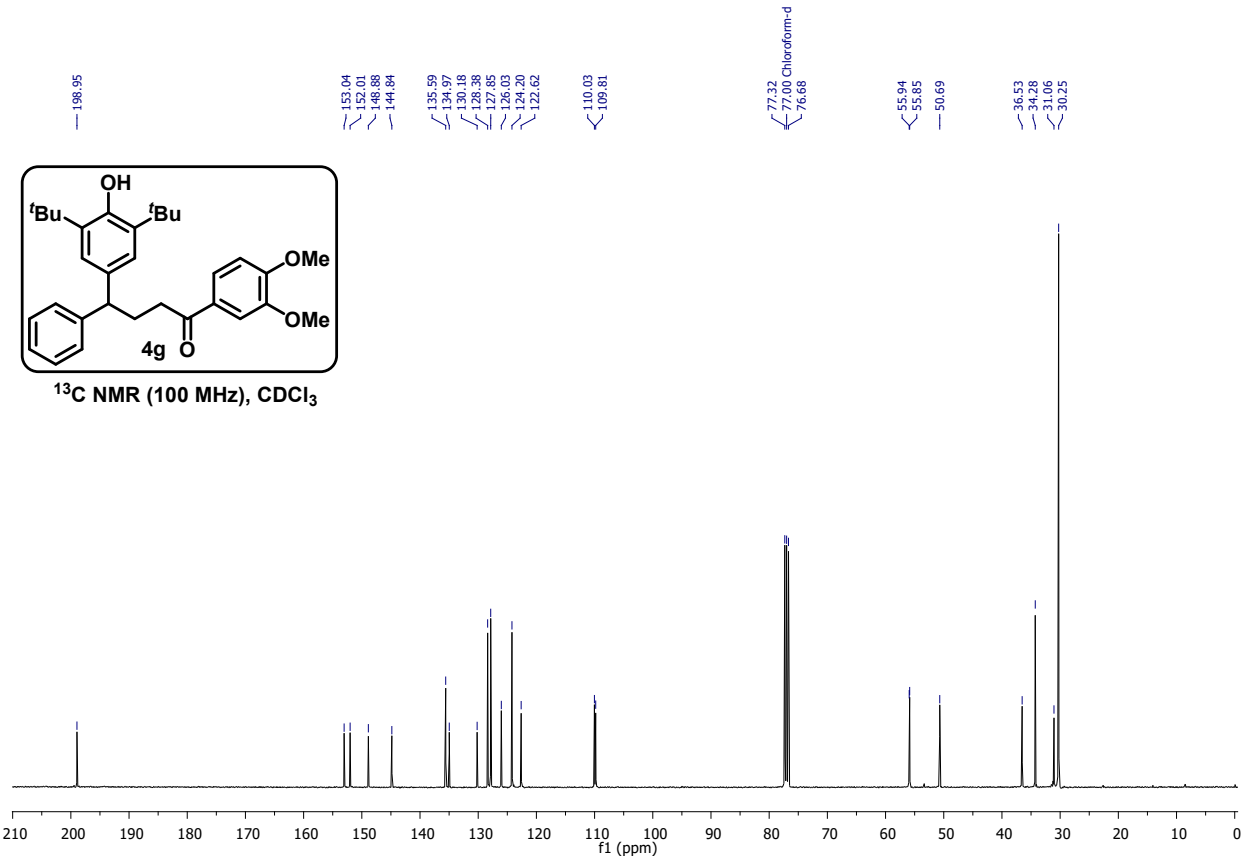
^{1}H NMR (500 MHz), $CDCl_3$



^{13}C NMR (125 MHz), $CDCl_3$



^{1}H NMR (400 MHz), $CDCl_3$



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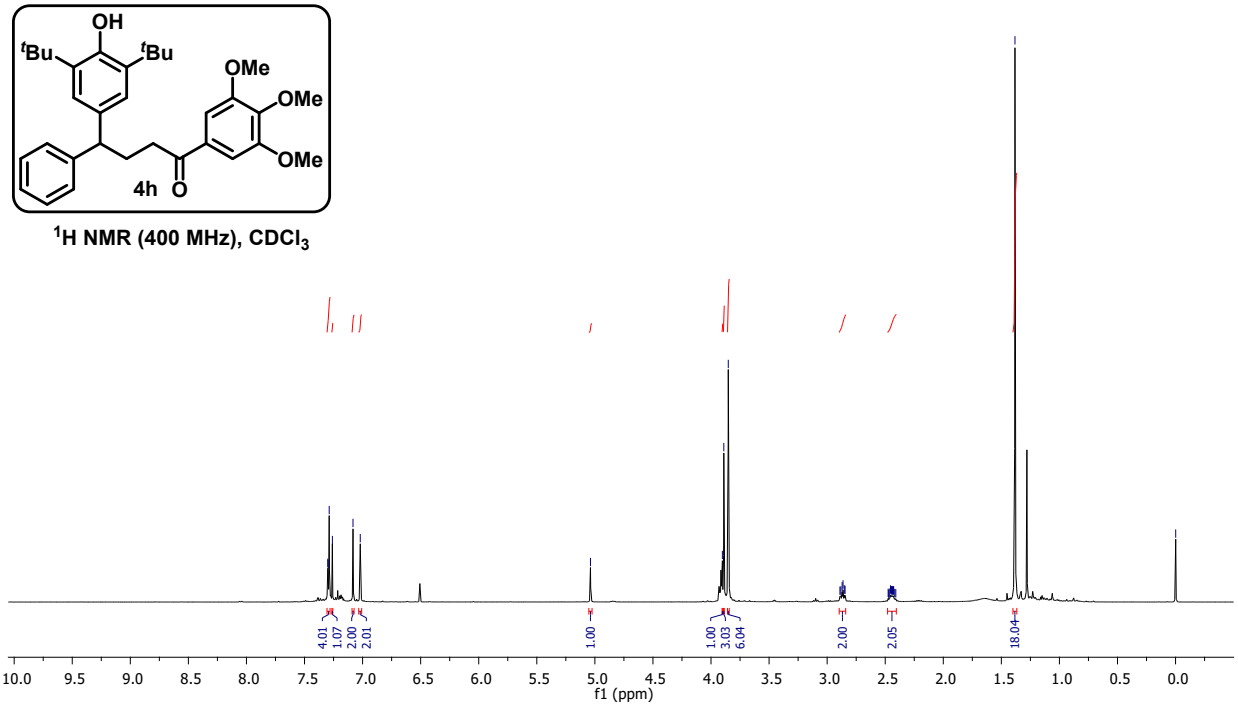

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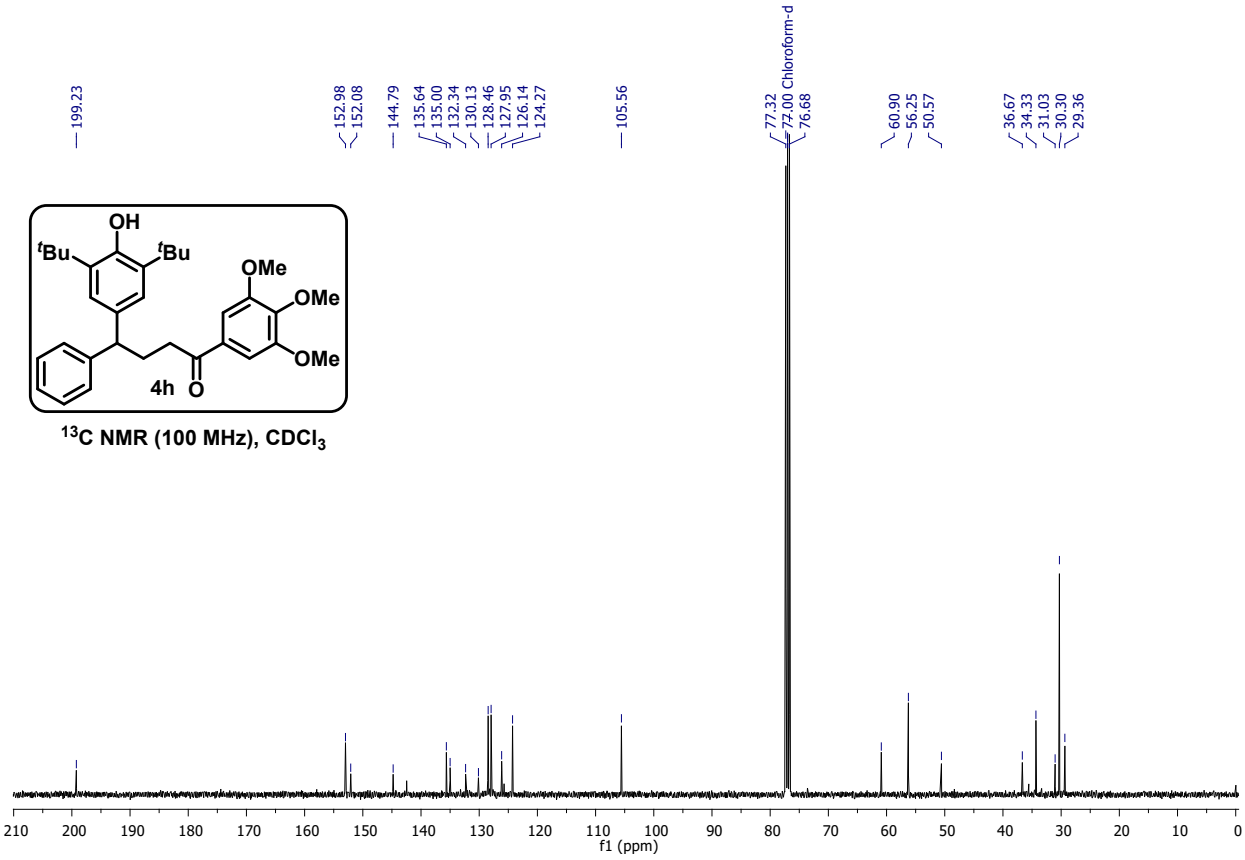

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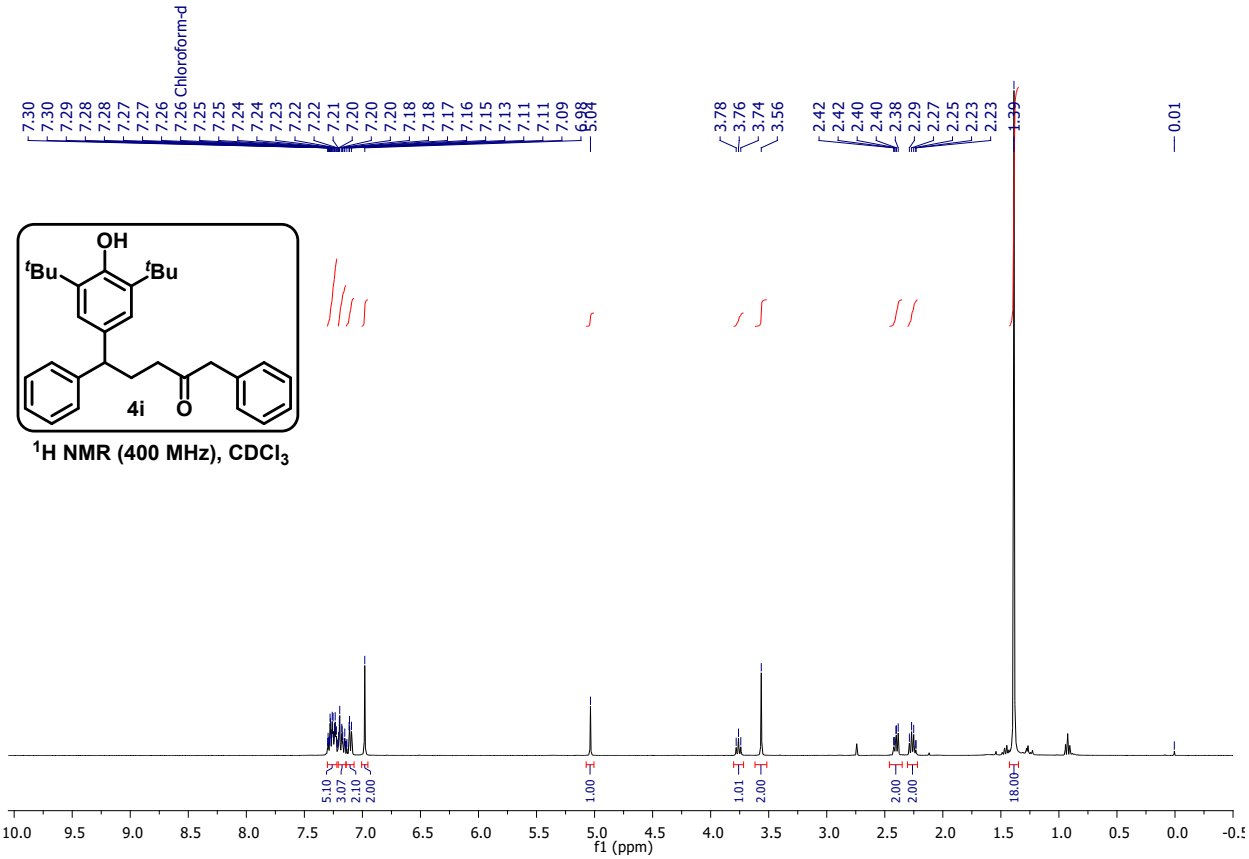

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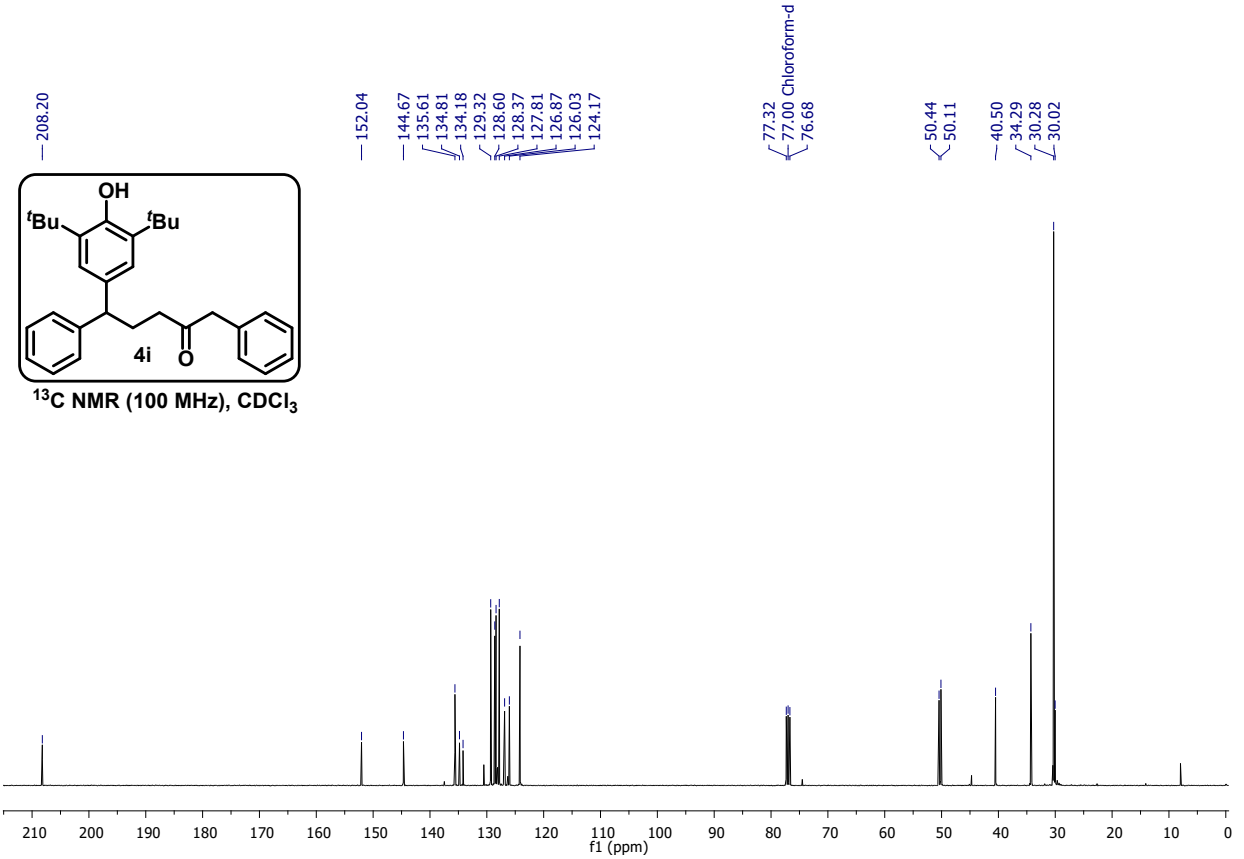

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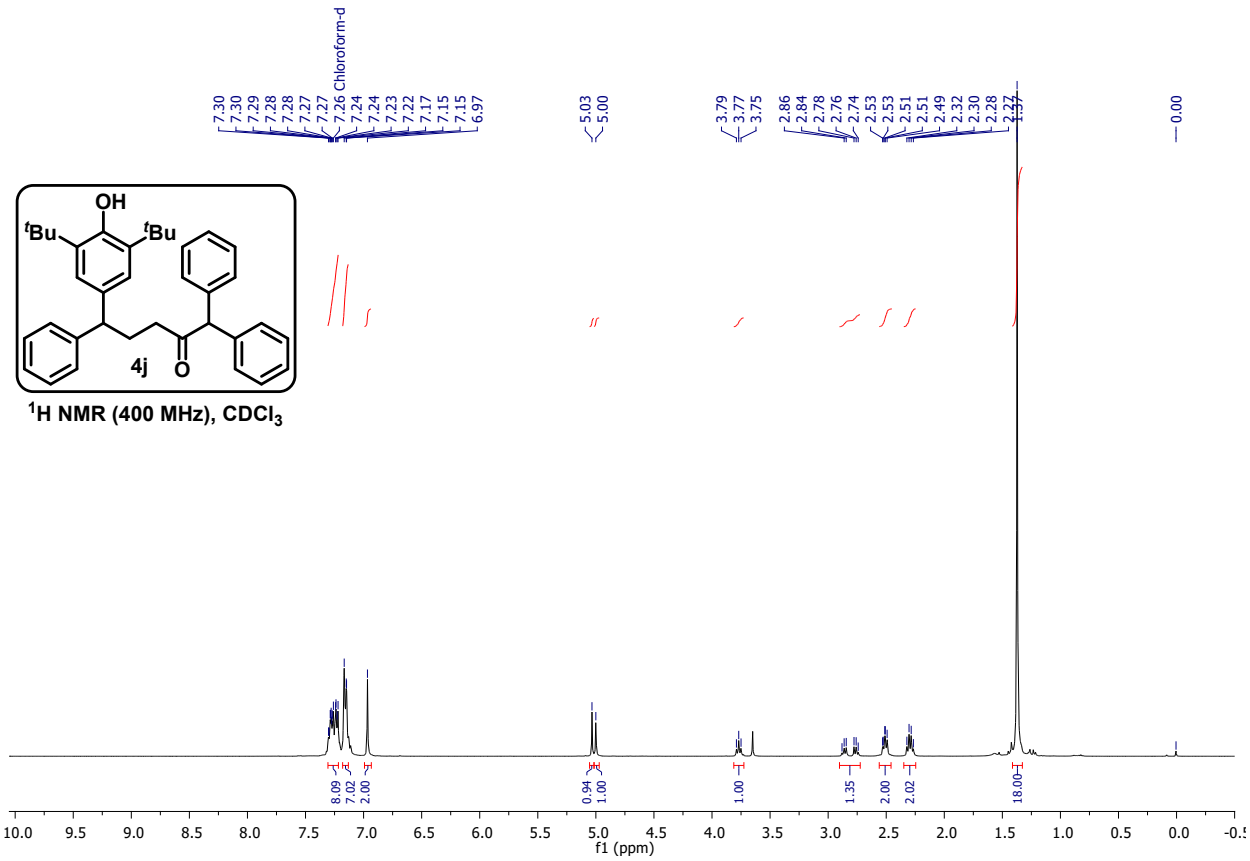

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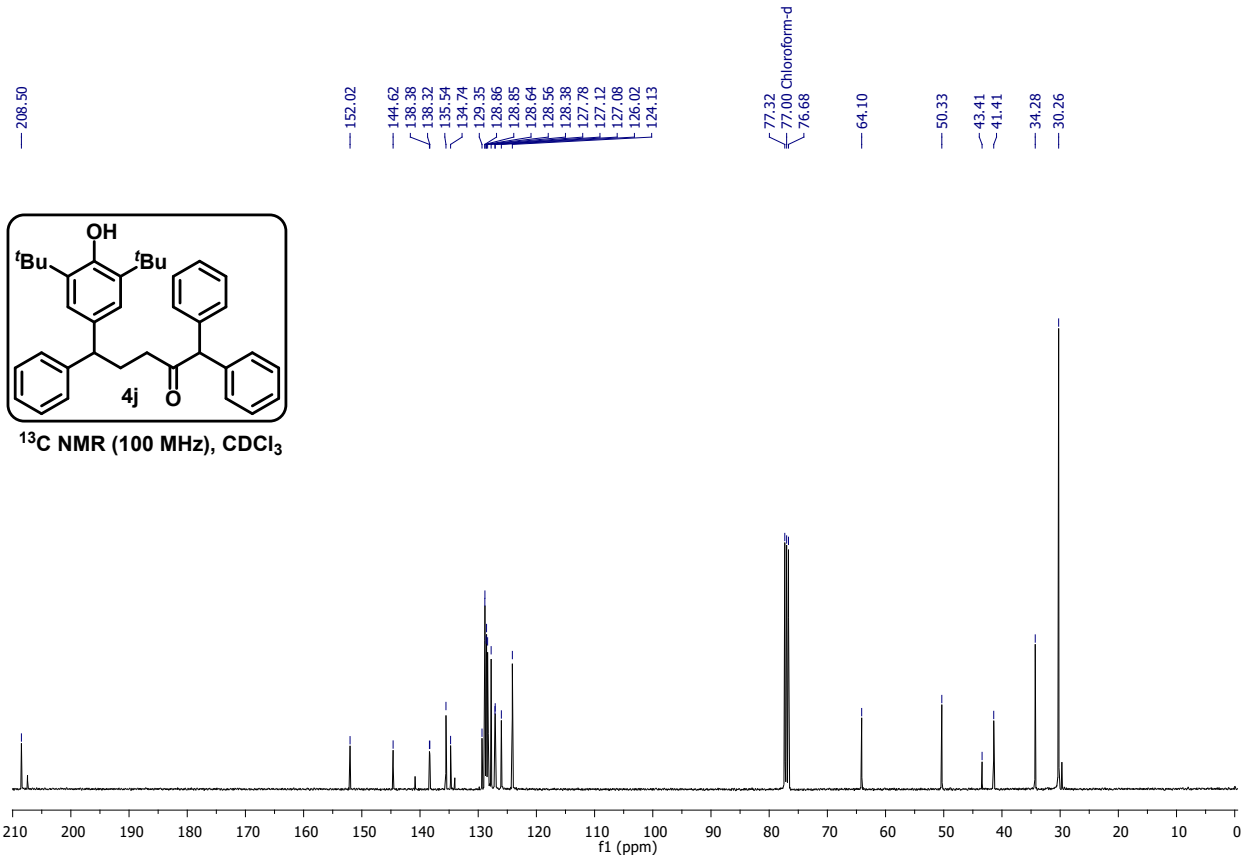

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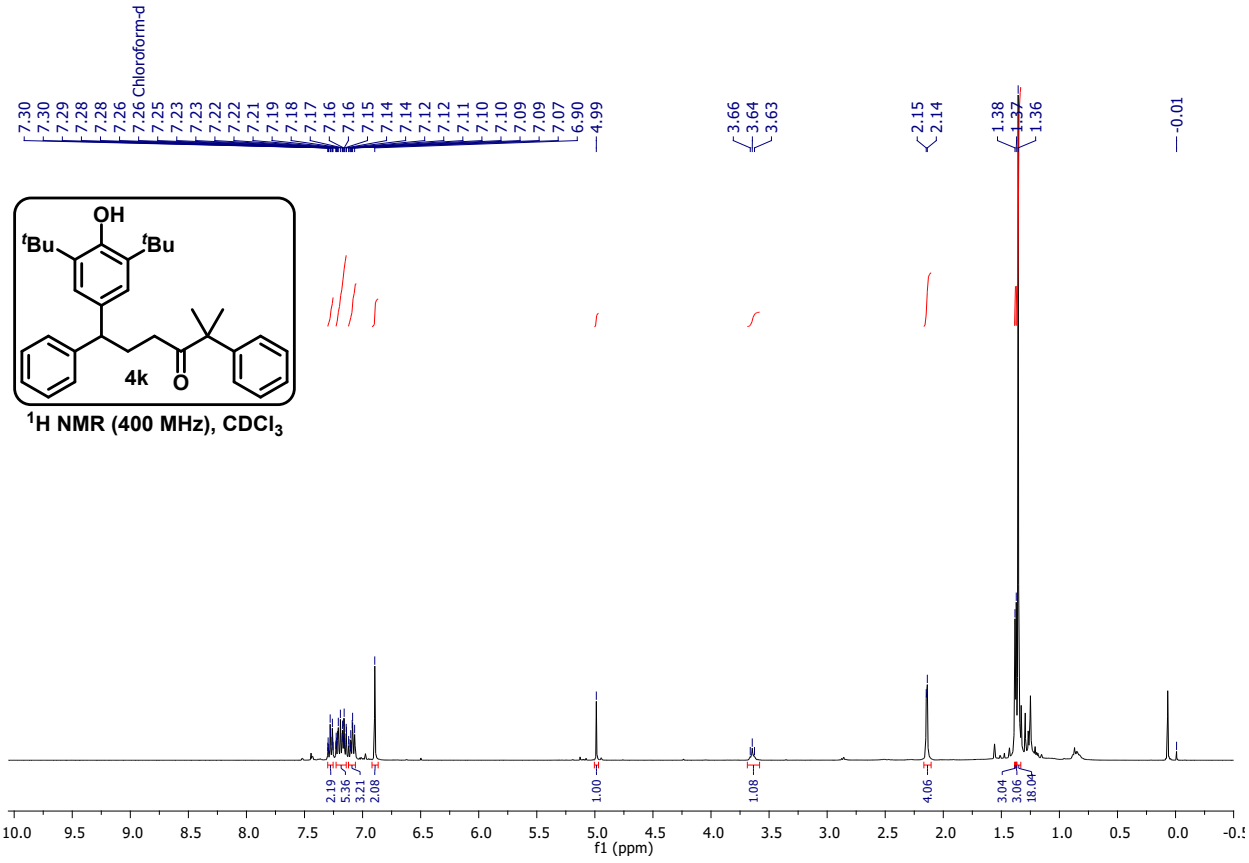

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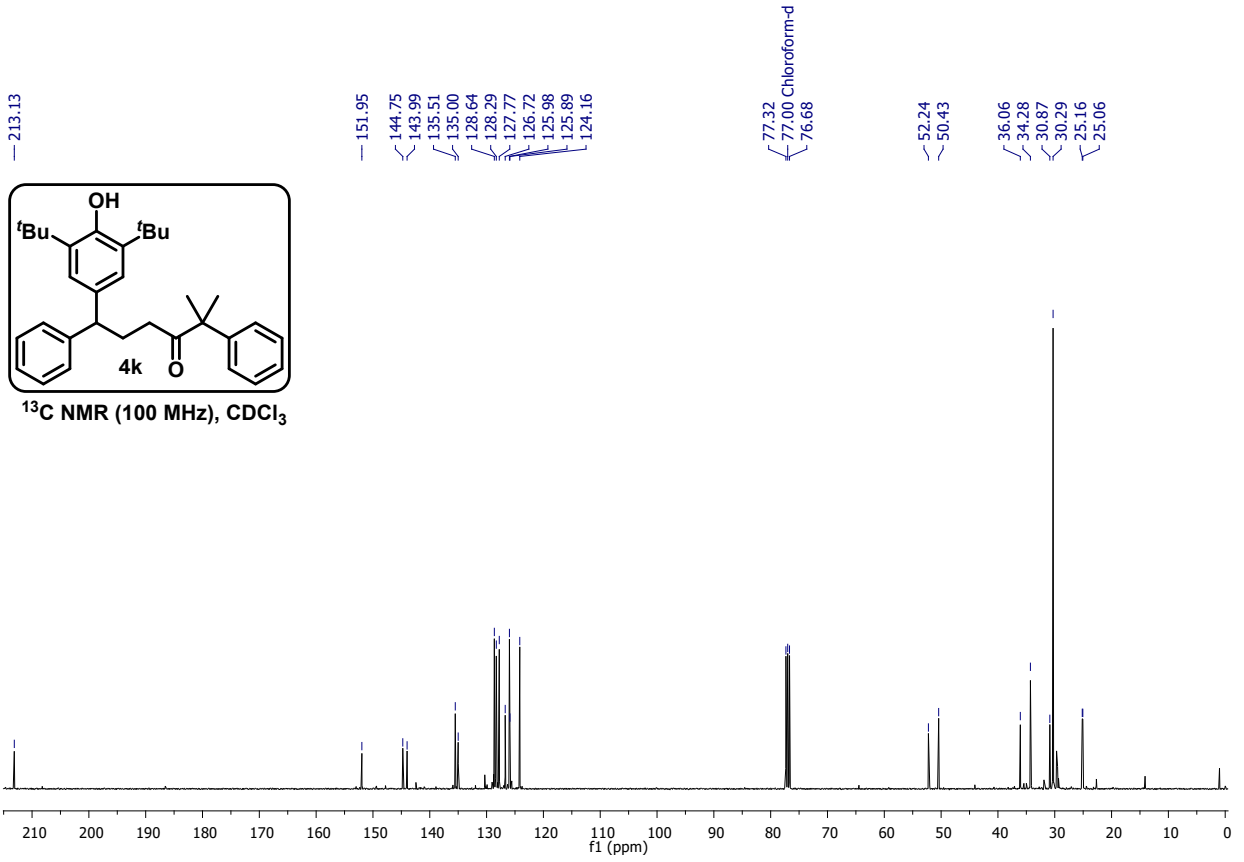

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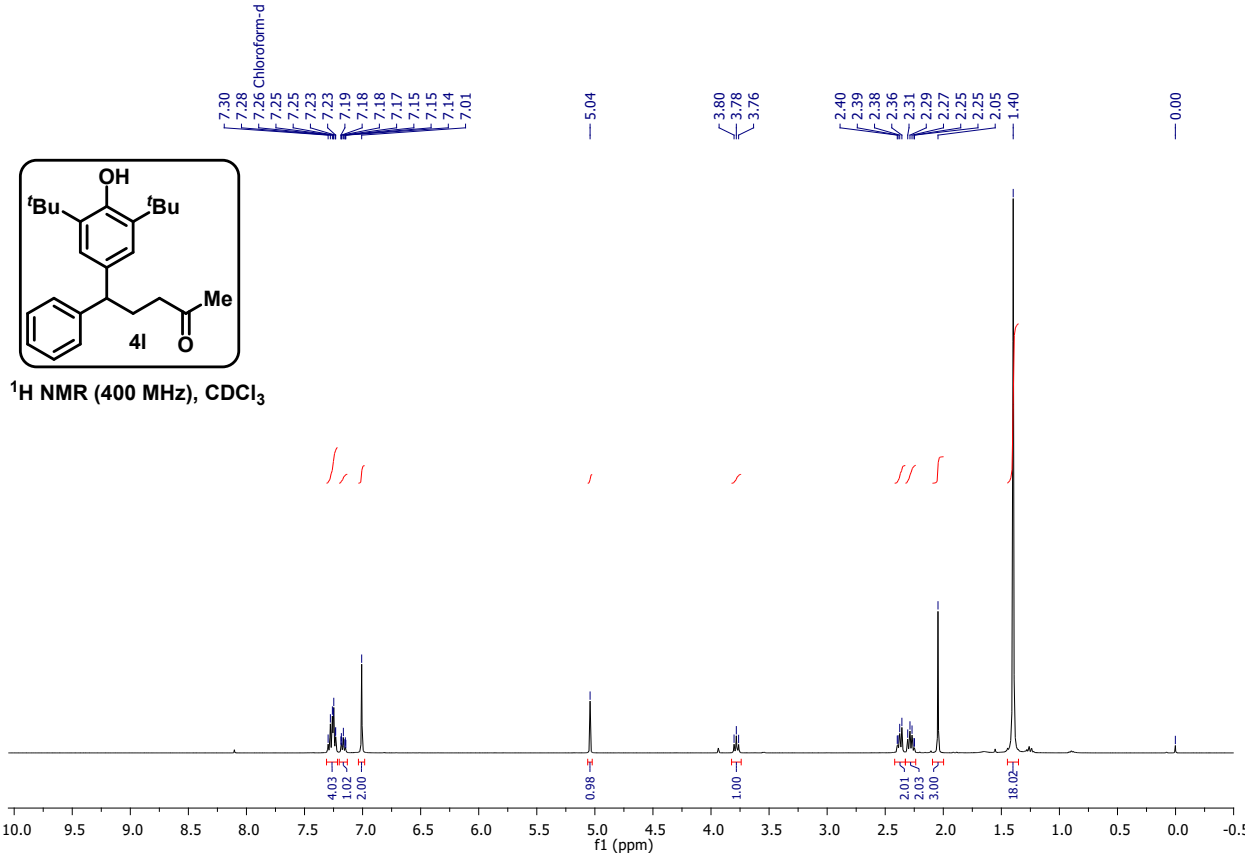

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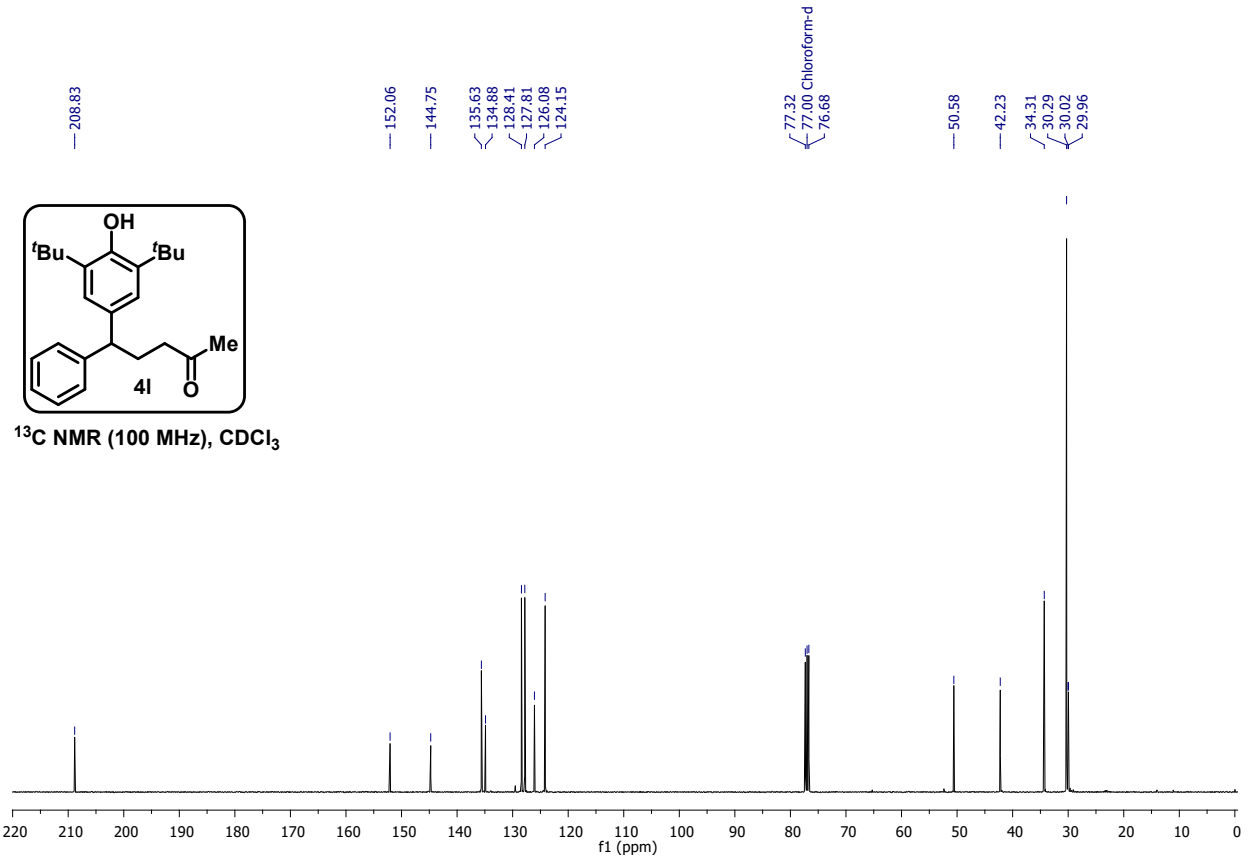

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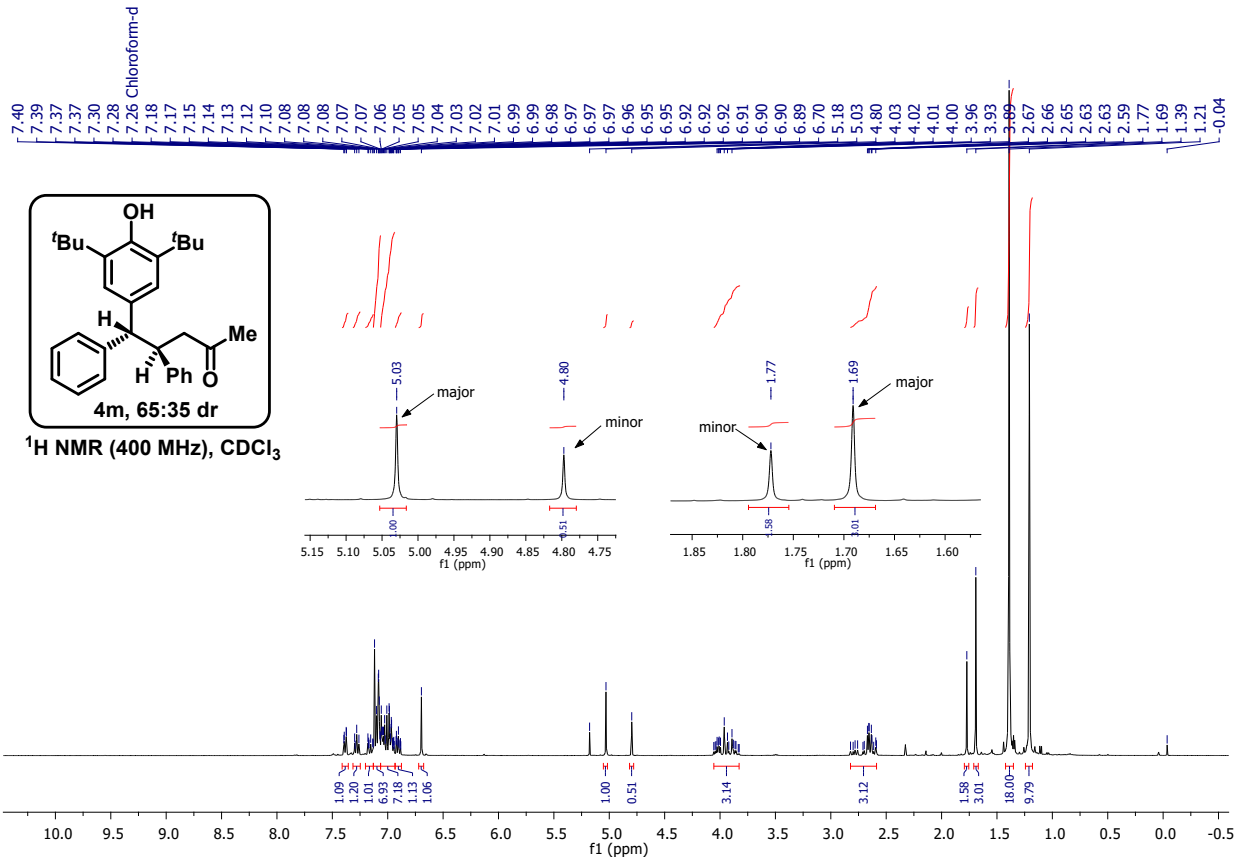

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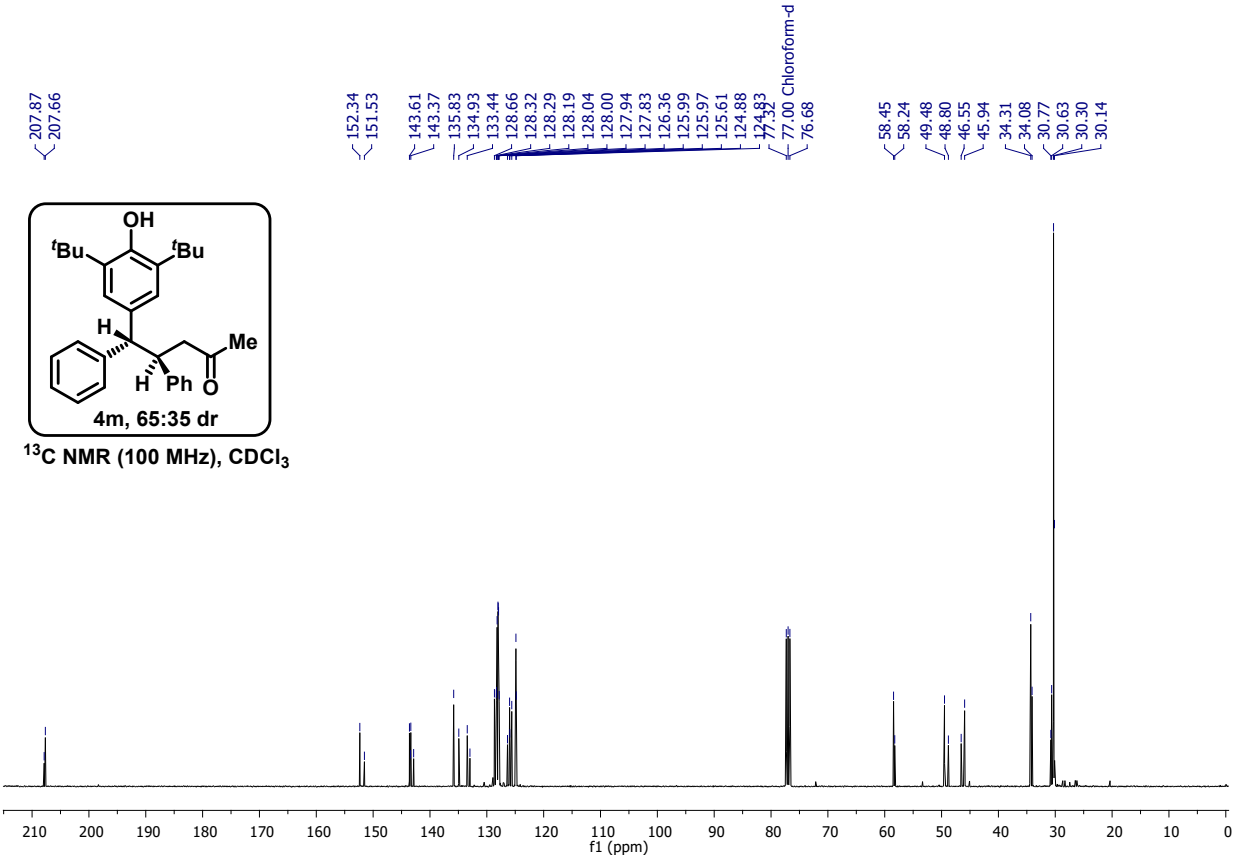

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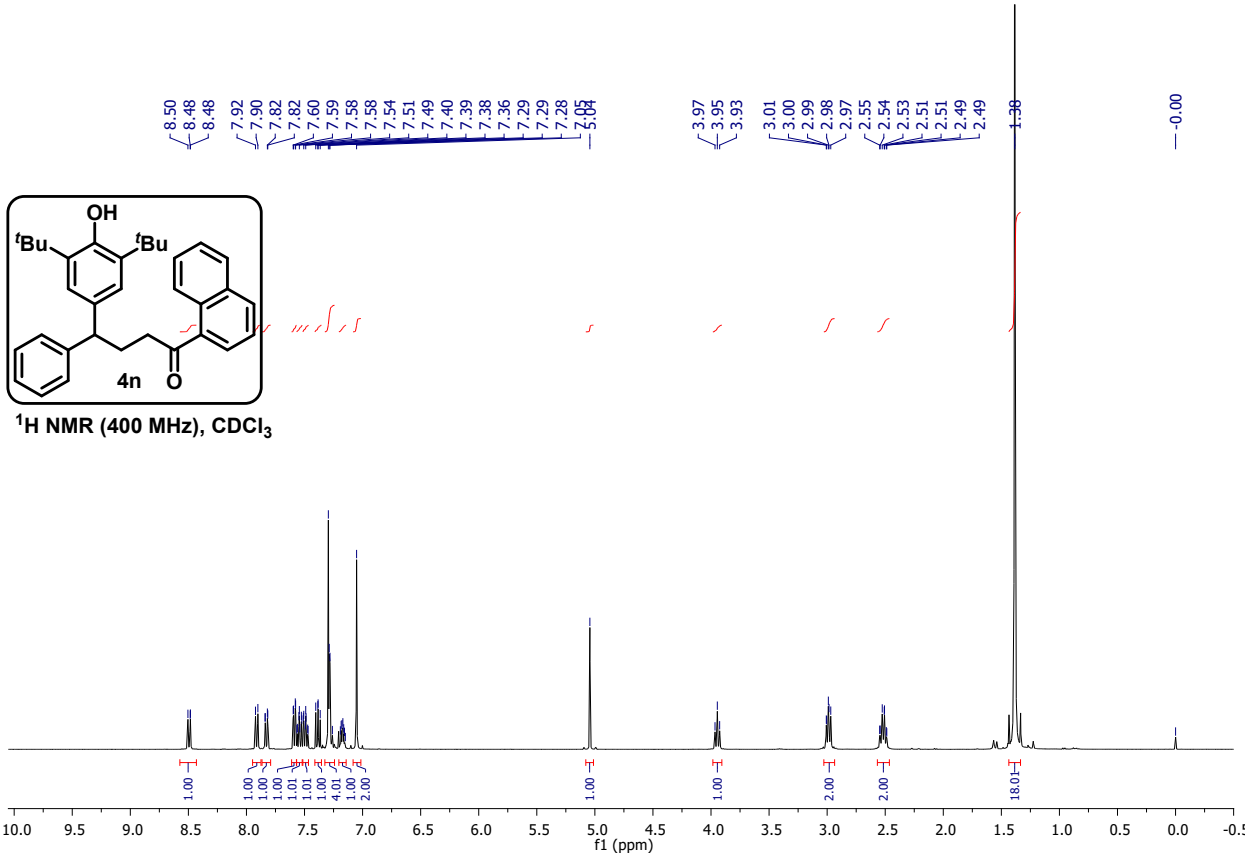
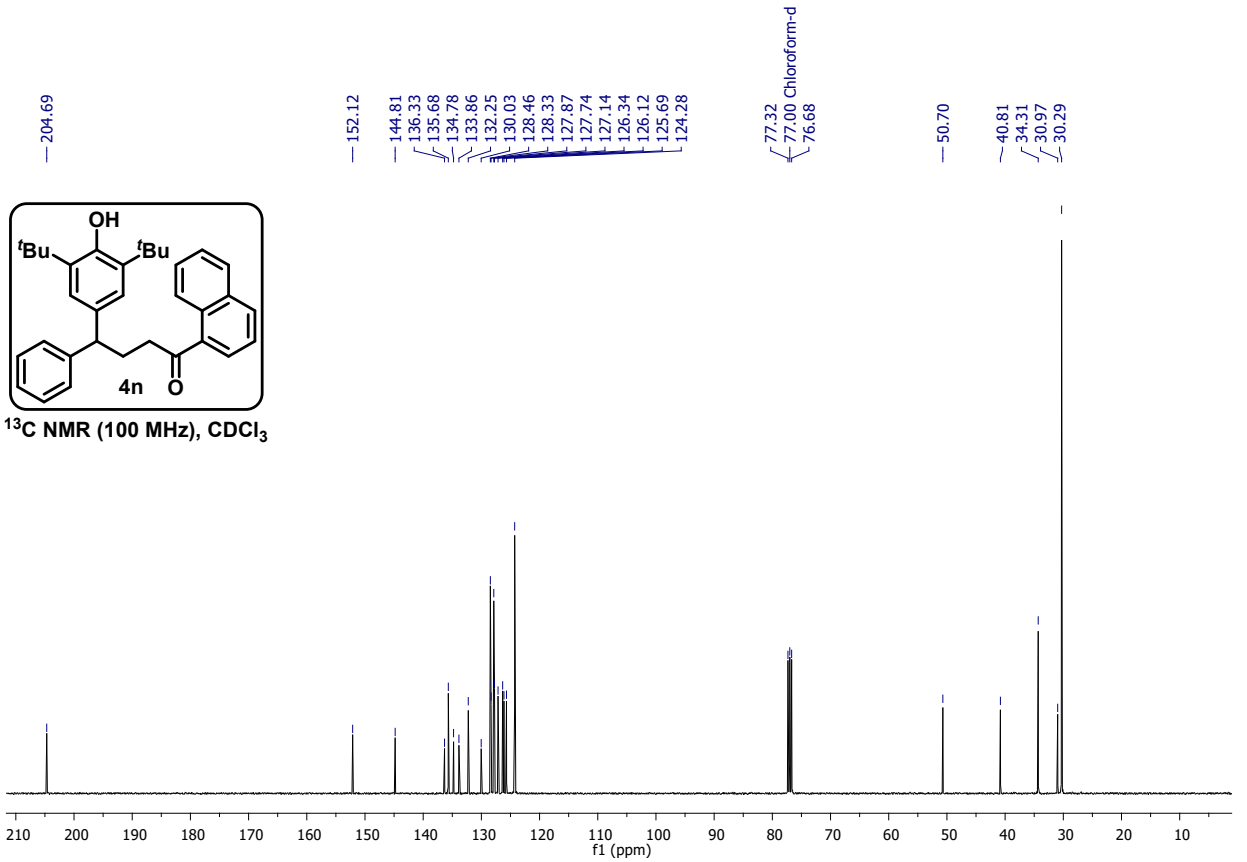


^{1}H NMR (400 MHz), $CDCl_3$



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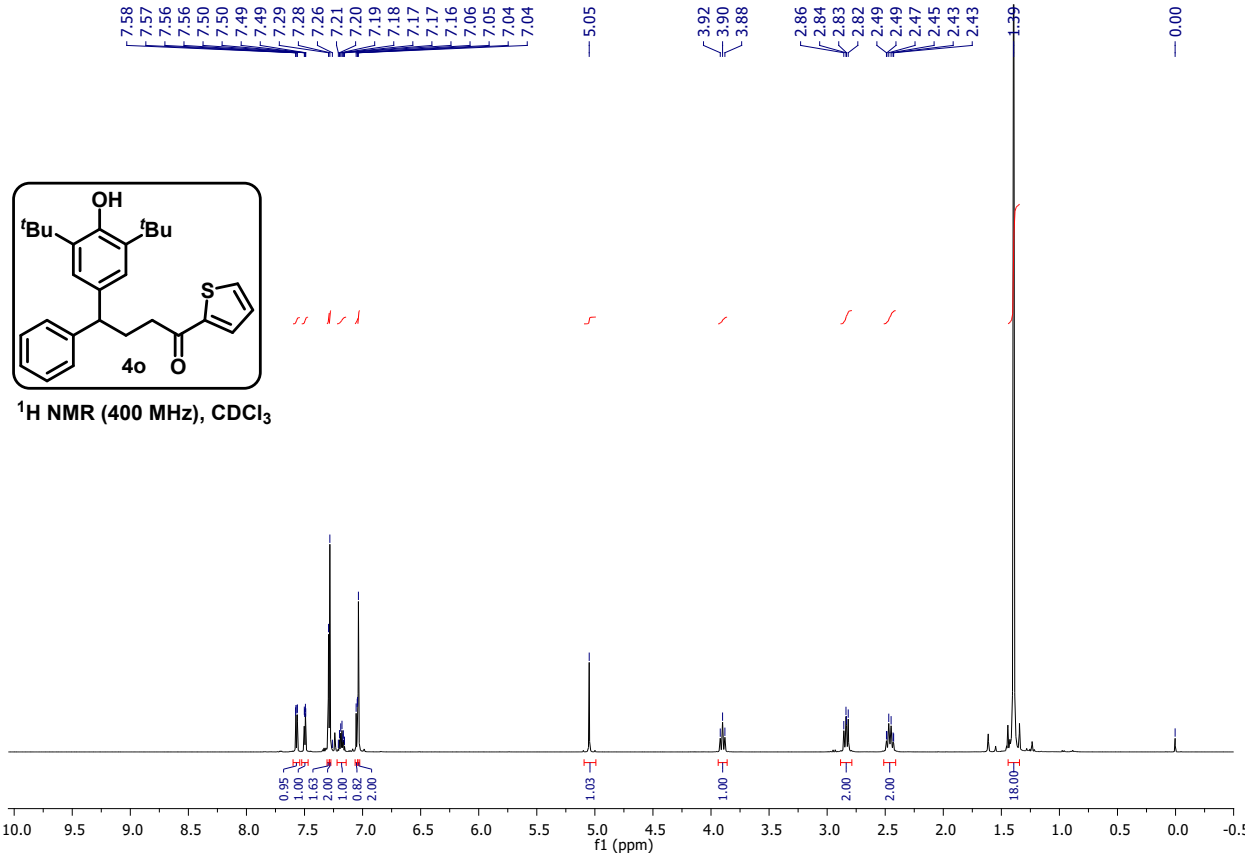

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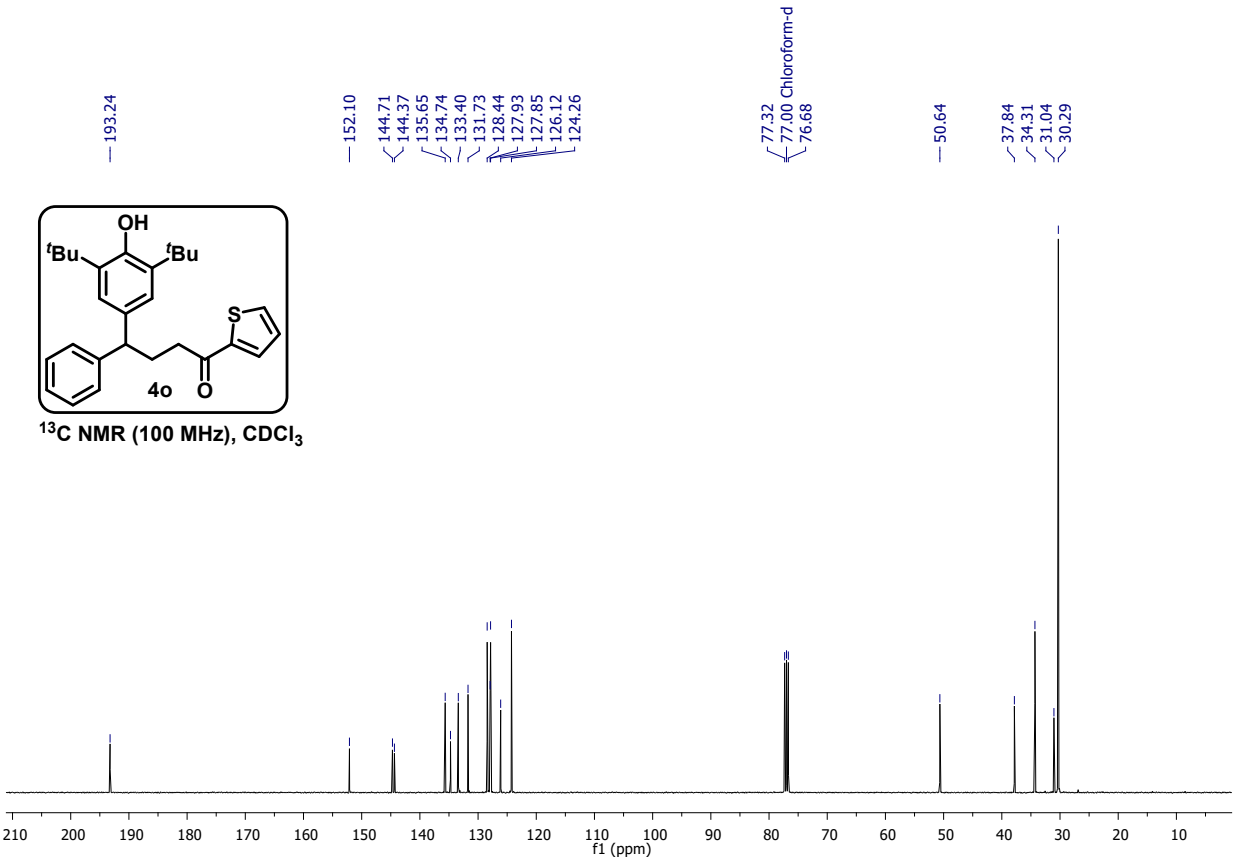

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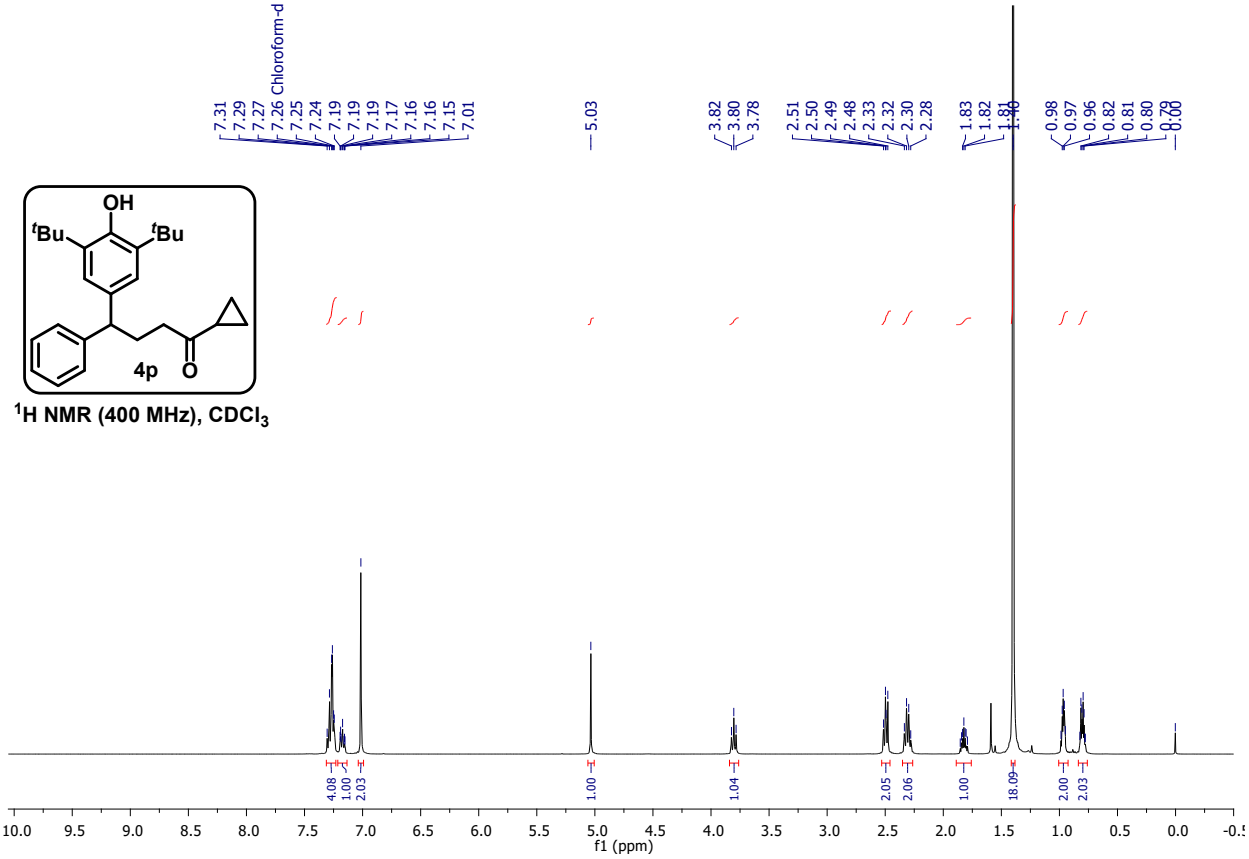

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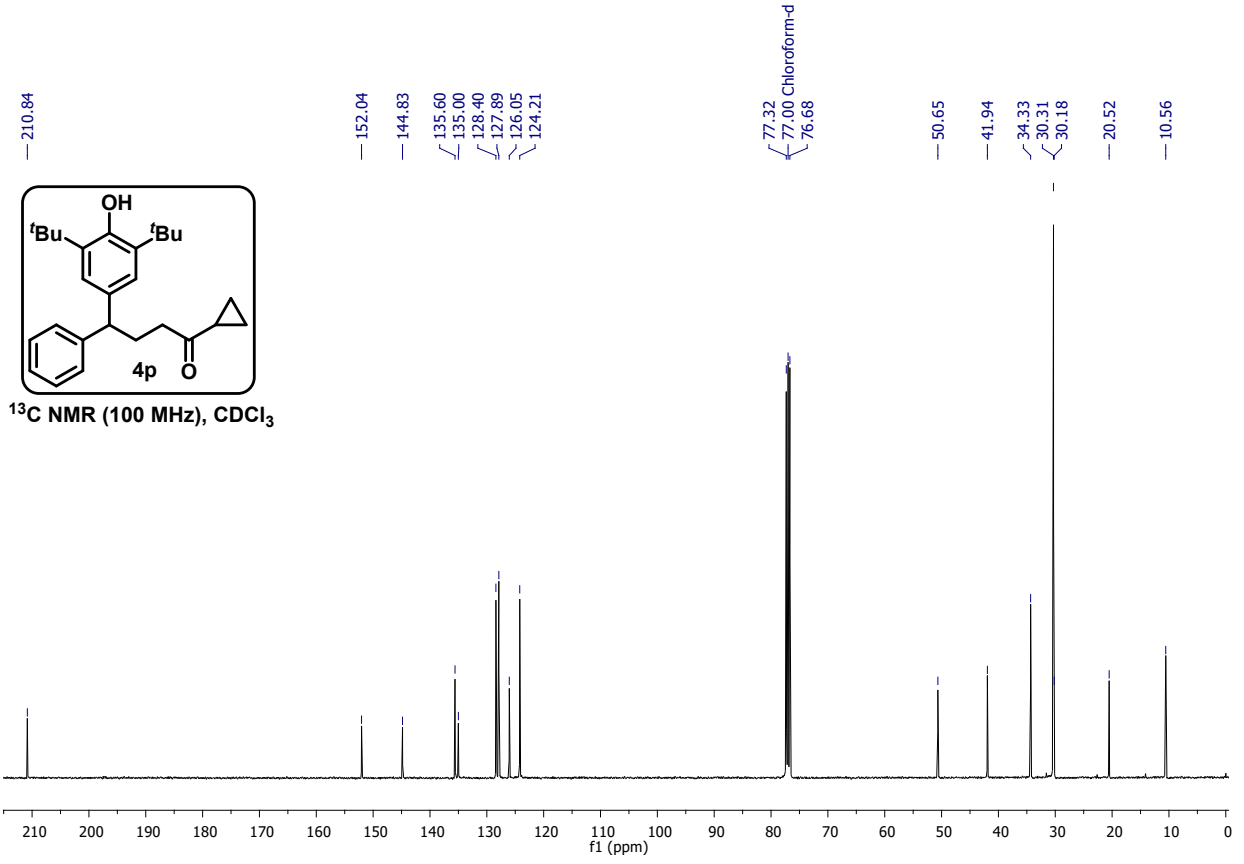

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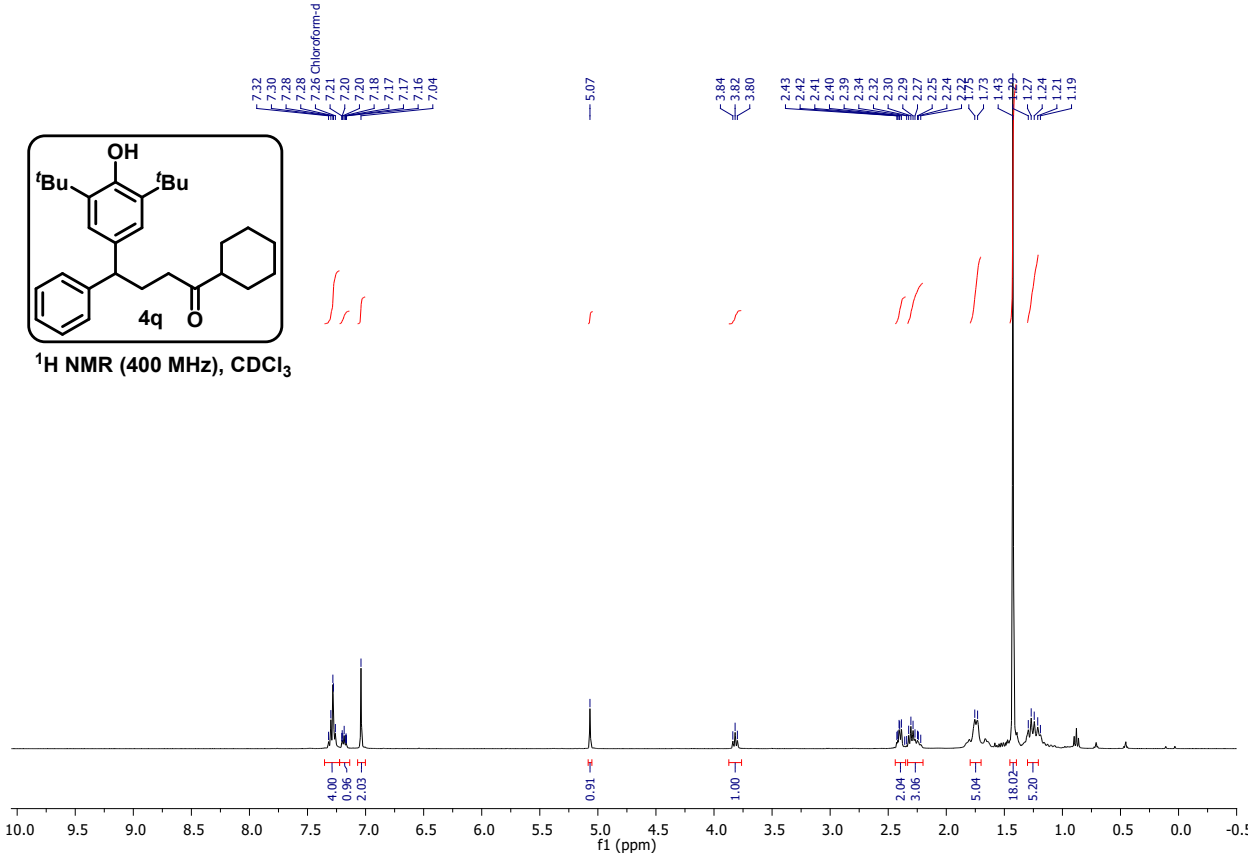
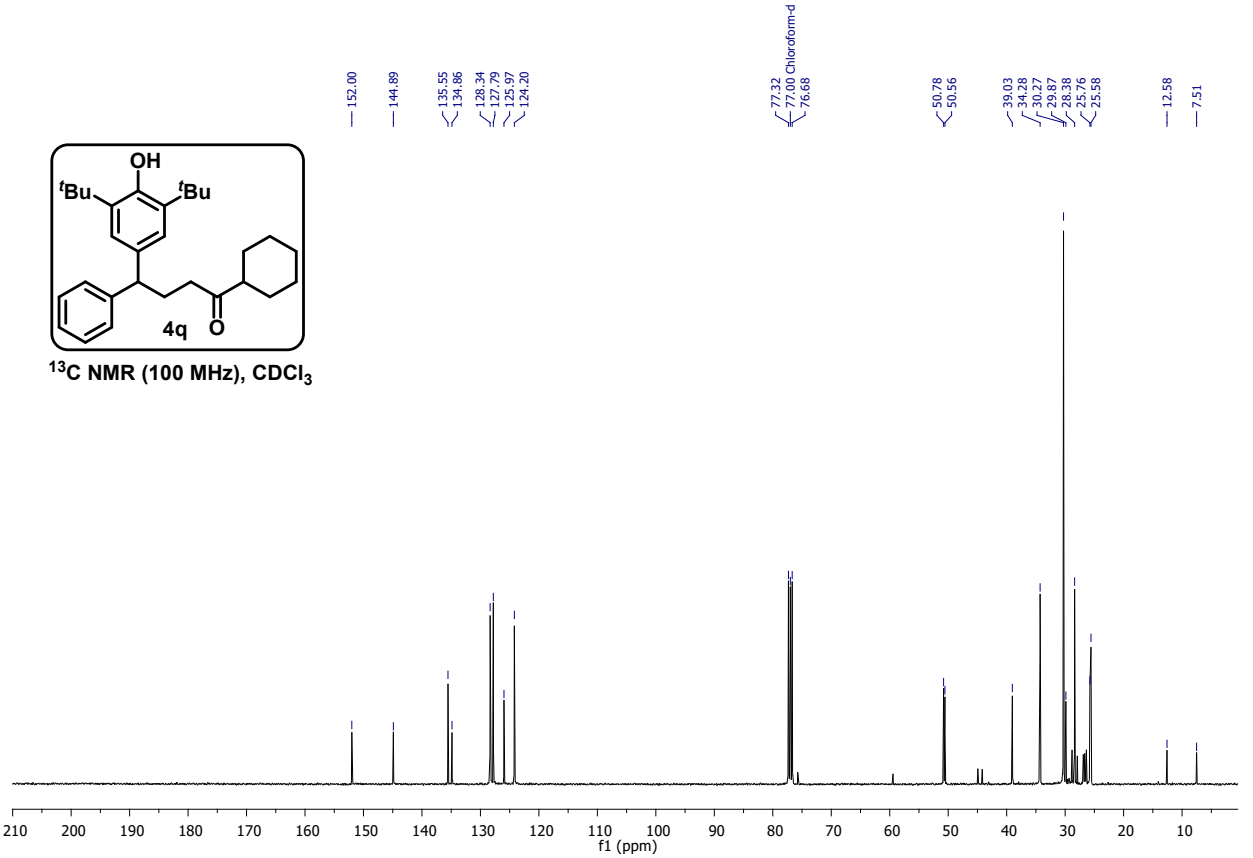
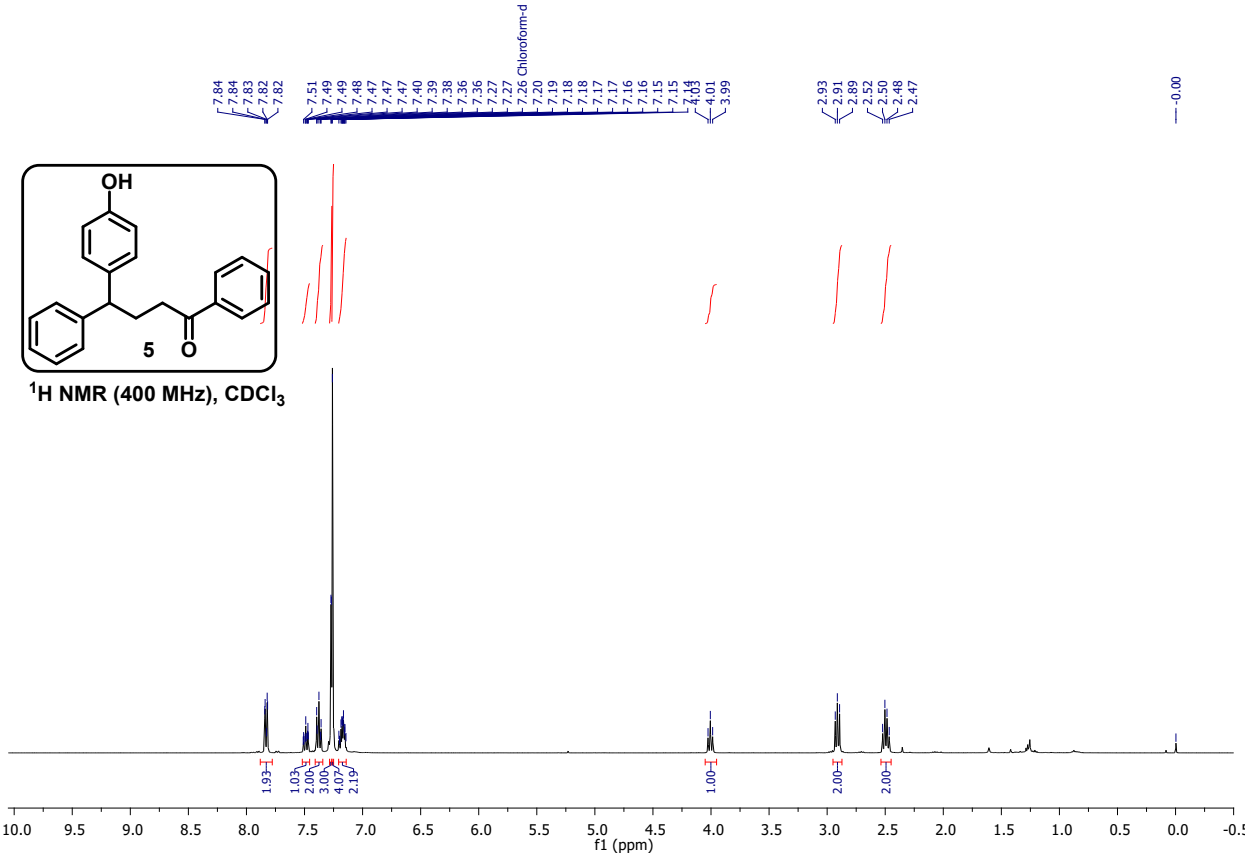
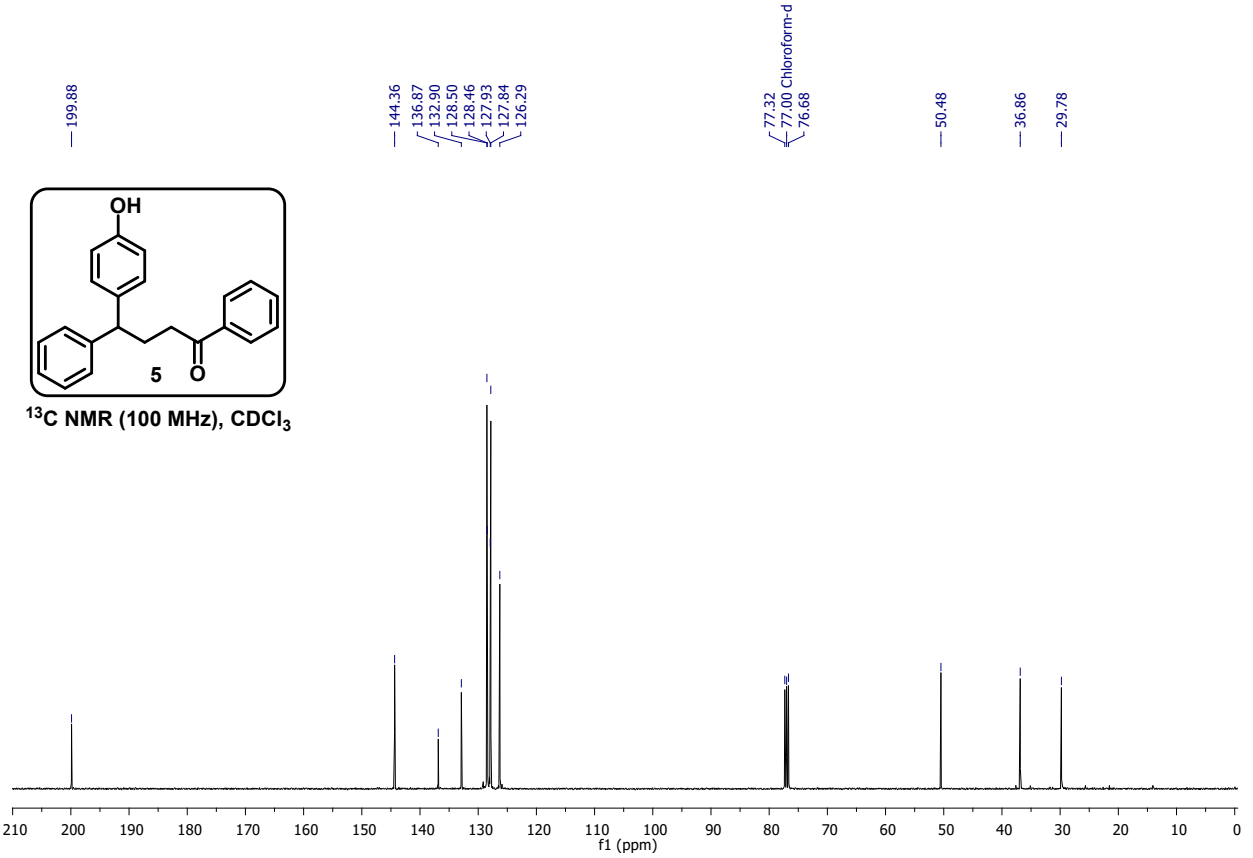


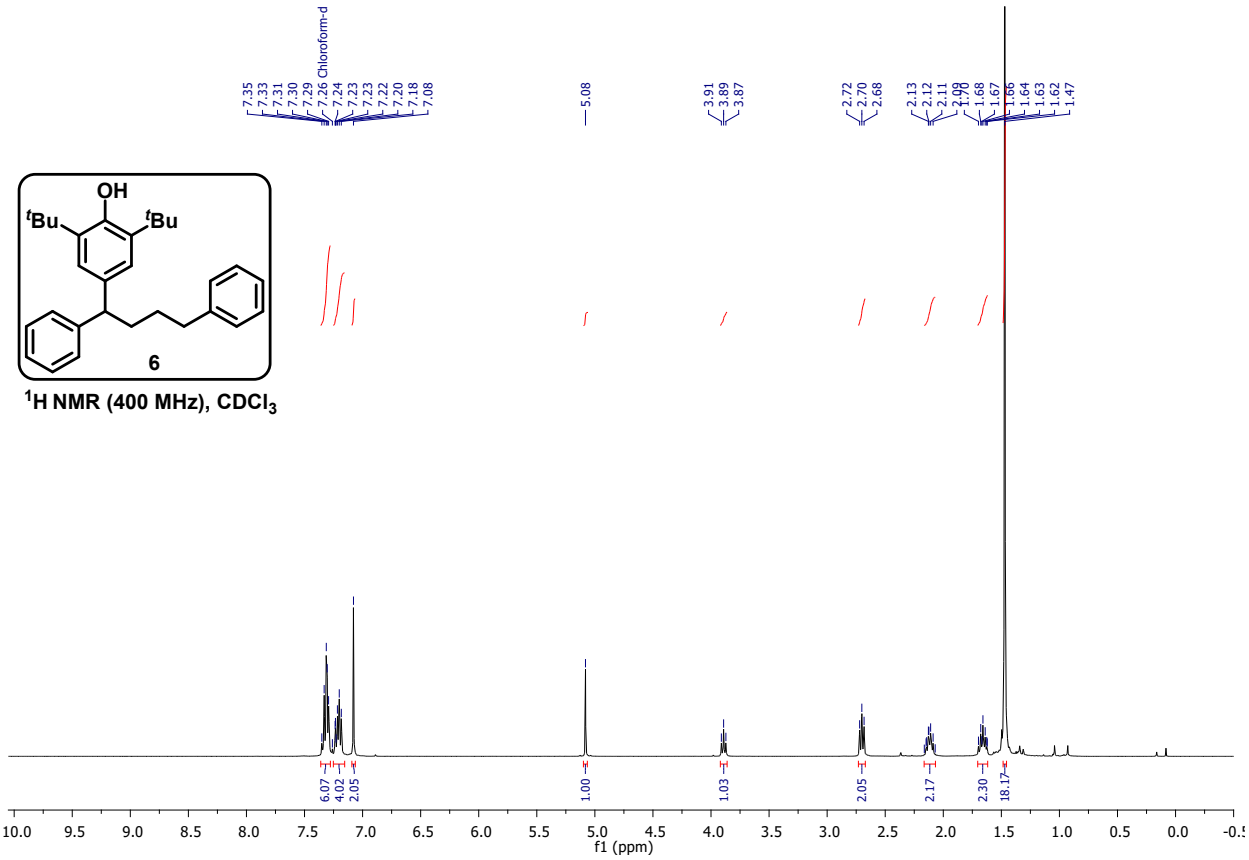
^{1}H NMR (400 MHz), $CDCl_3$



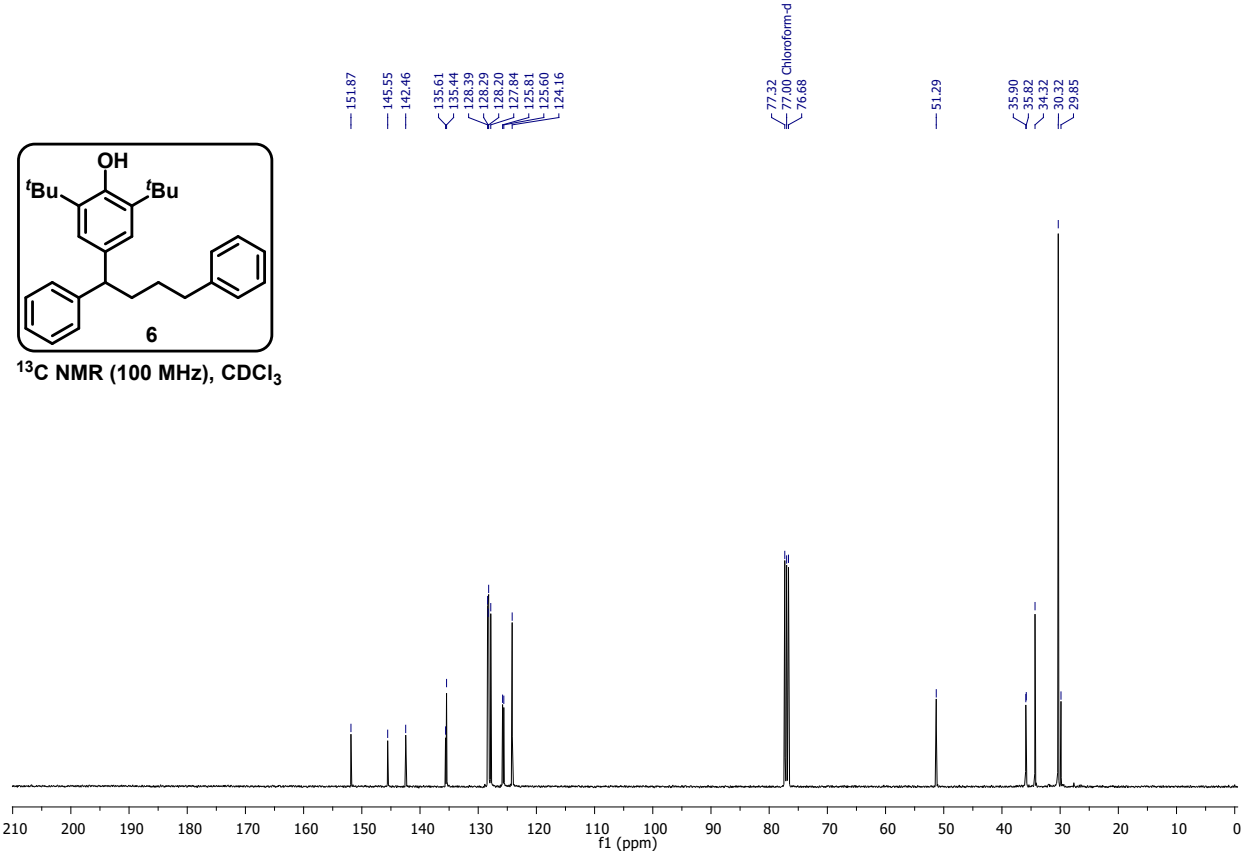
^{13}C NMR (100 MHz), $CDCl_3$


OH
5
O
^{1}H NMR (400 MHz), CDCl$_3$
f1 (ppm)

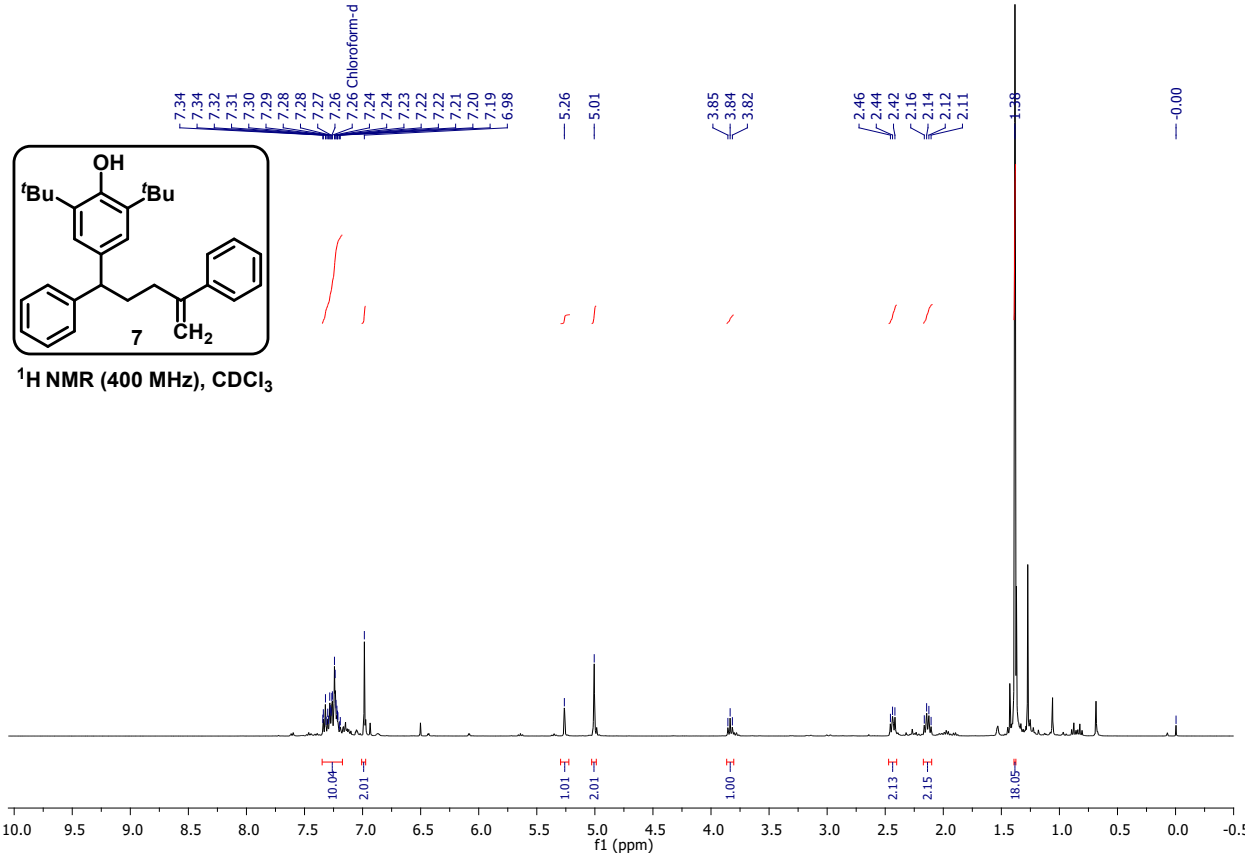

OH
5
O
^{13}C NMR (100 MHz), CDCl$_3$
f1 (ppm)



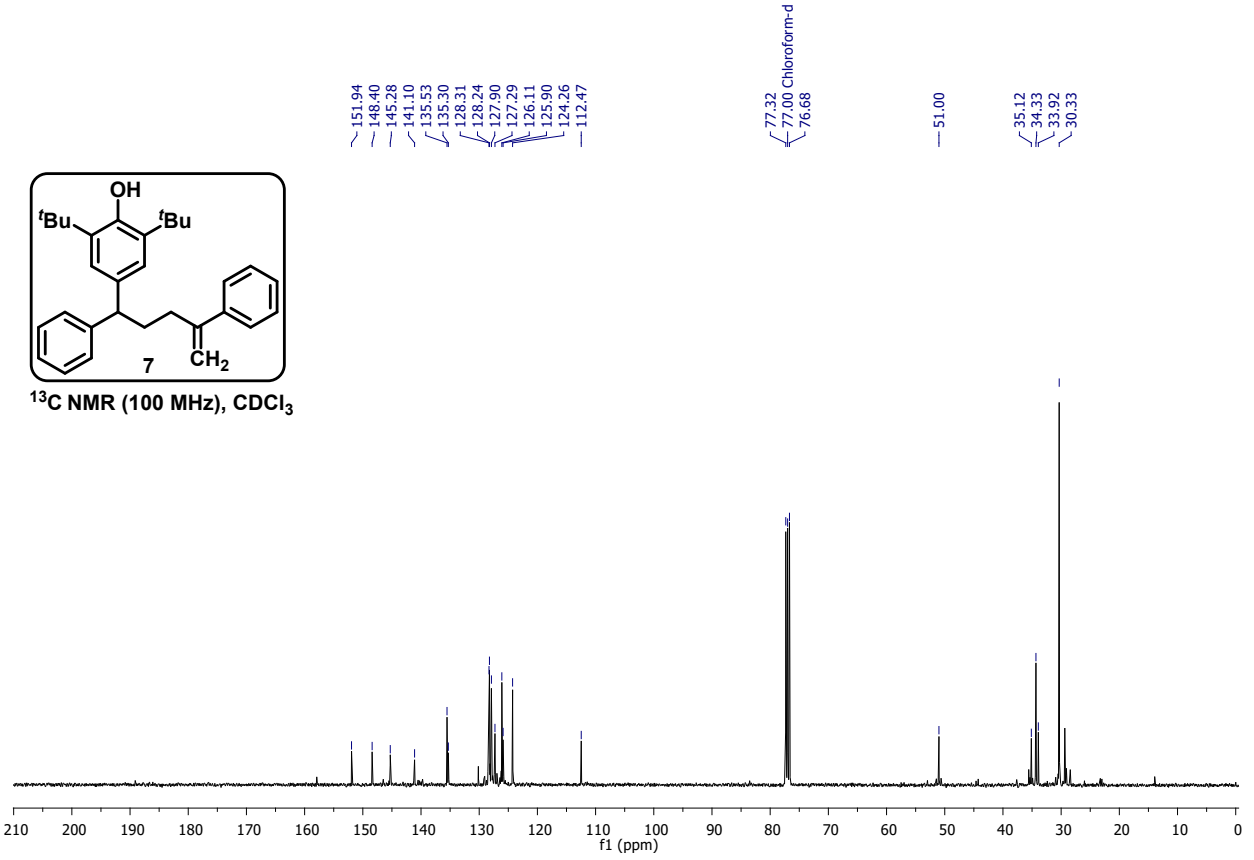
^{1}H NMR (400 MHz), $CDCl_3$



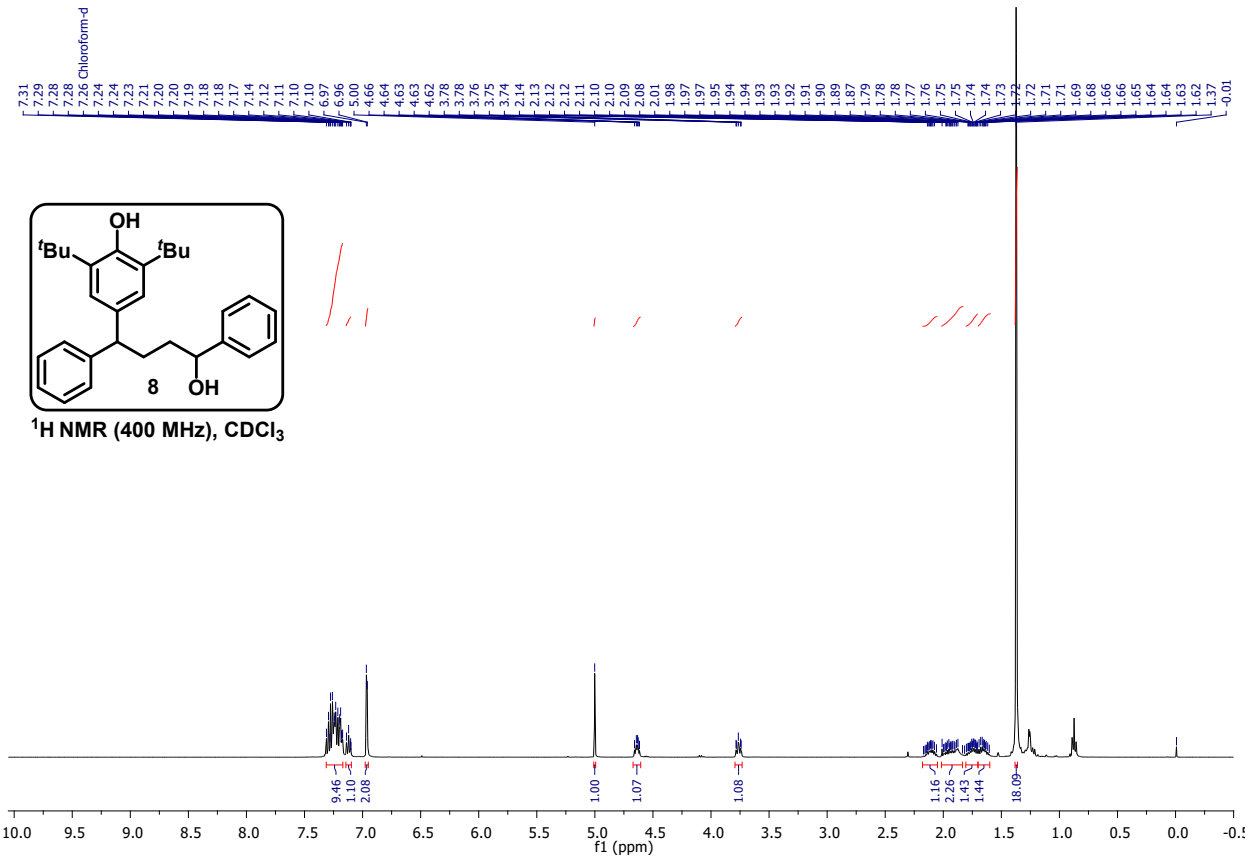
^{13}C NMR (100 MHz), $CDCl_3$



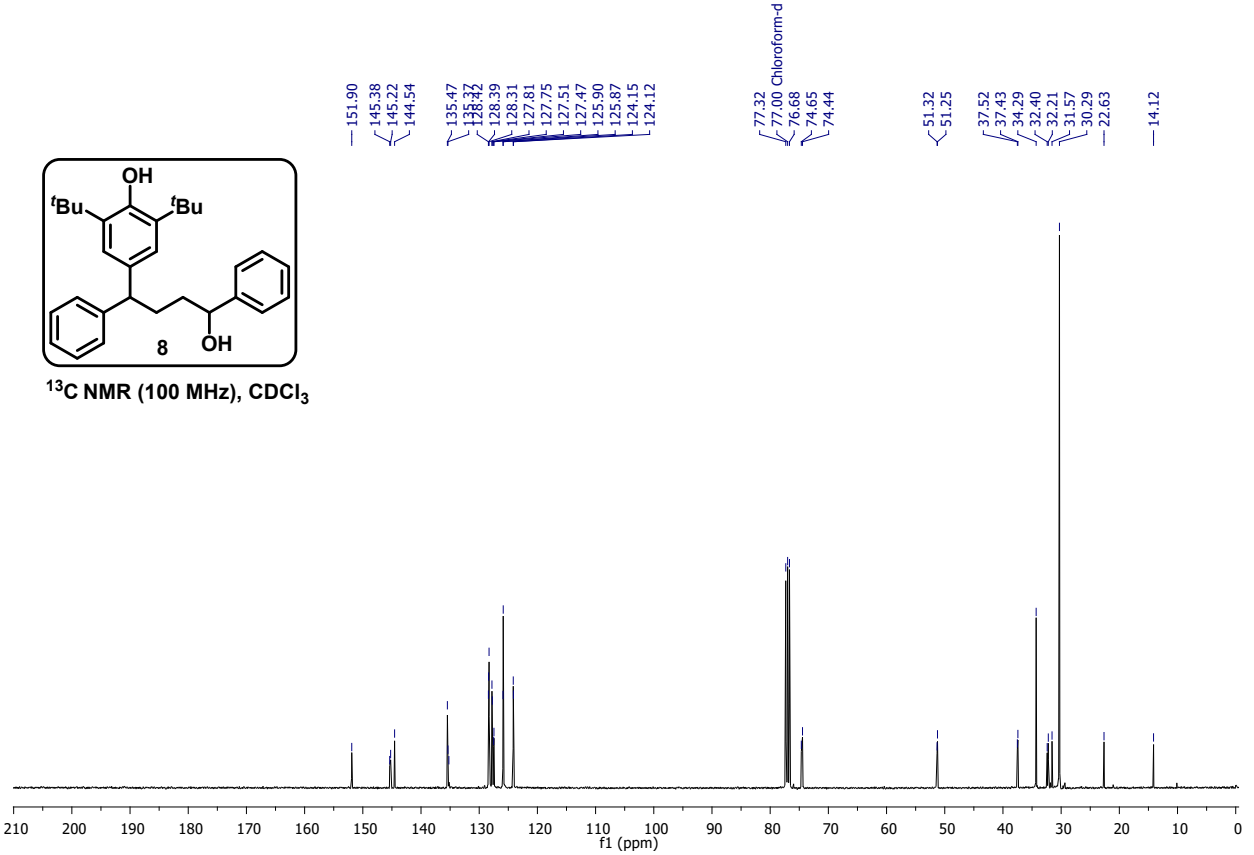
^{1}H NMR (400 MHz), $CDCl_3$



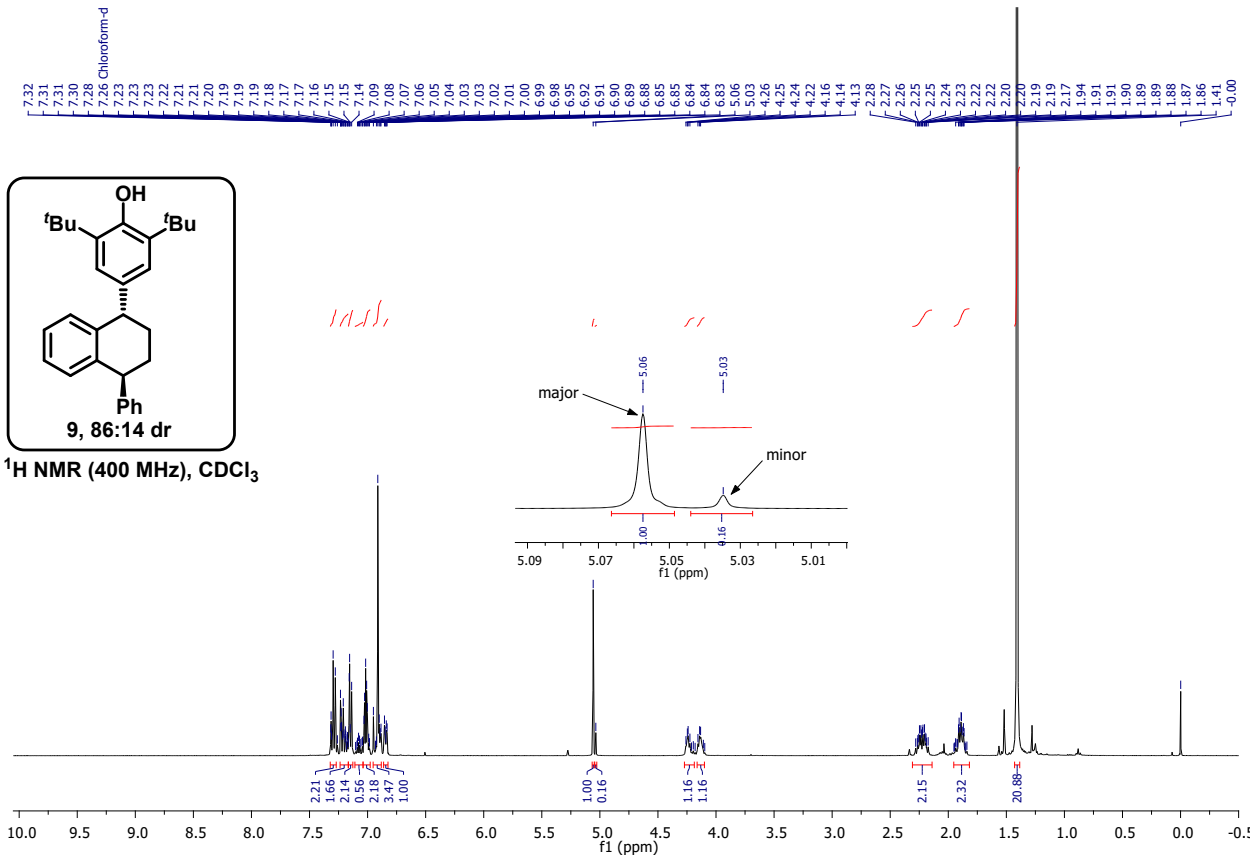
^{13}C NMR (100 MHz), $CDCl_3$



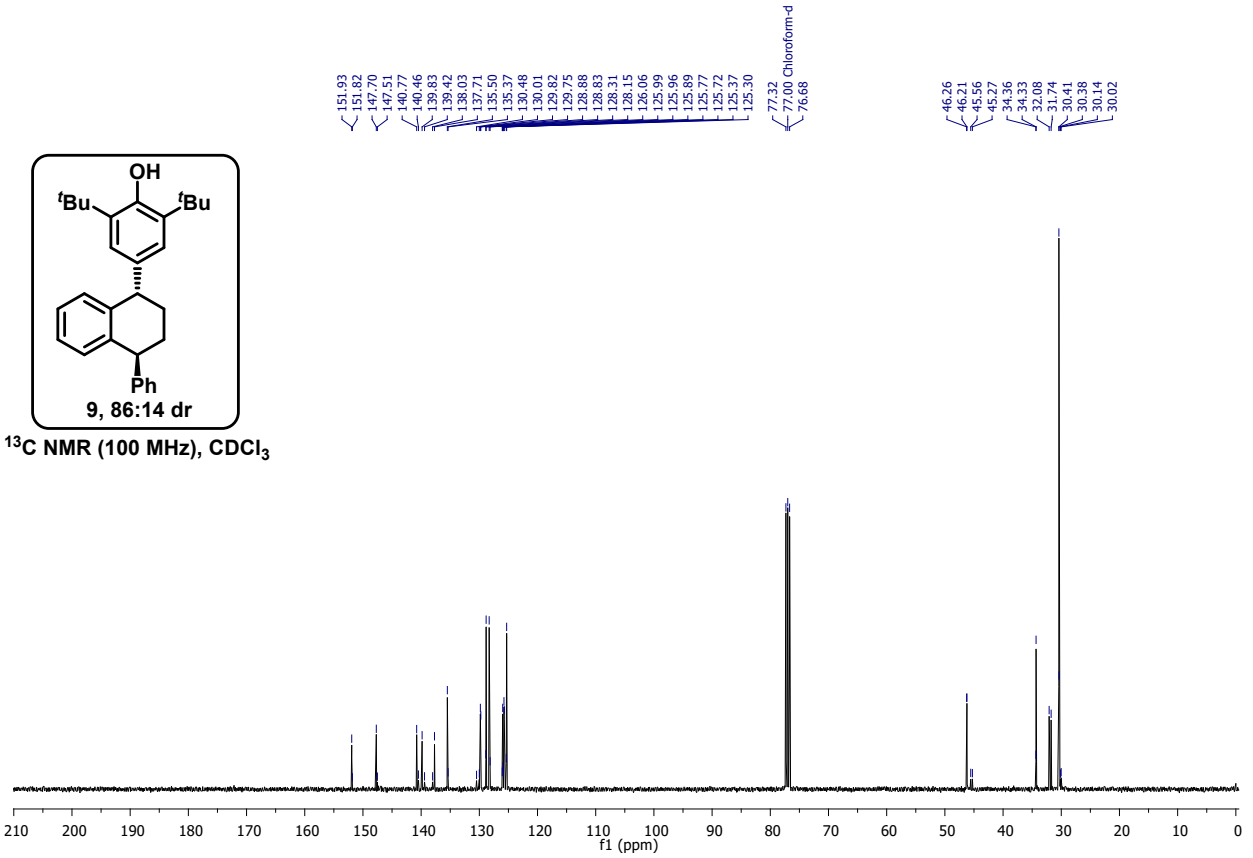
^{1}H NMR (400 MHz), $CDCl_3$



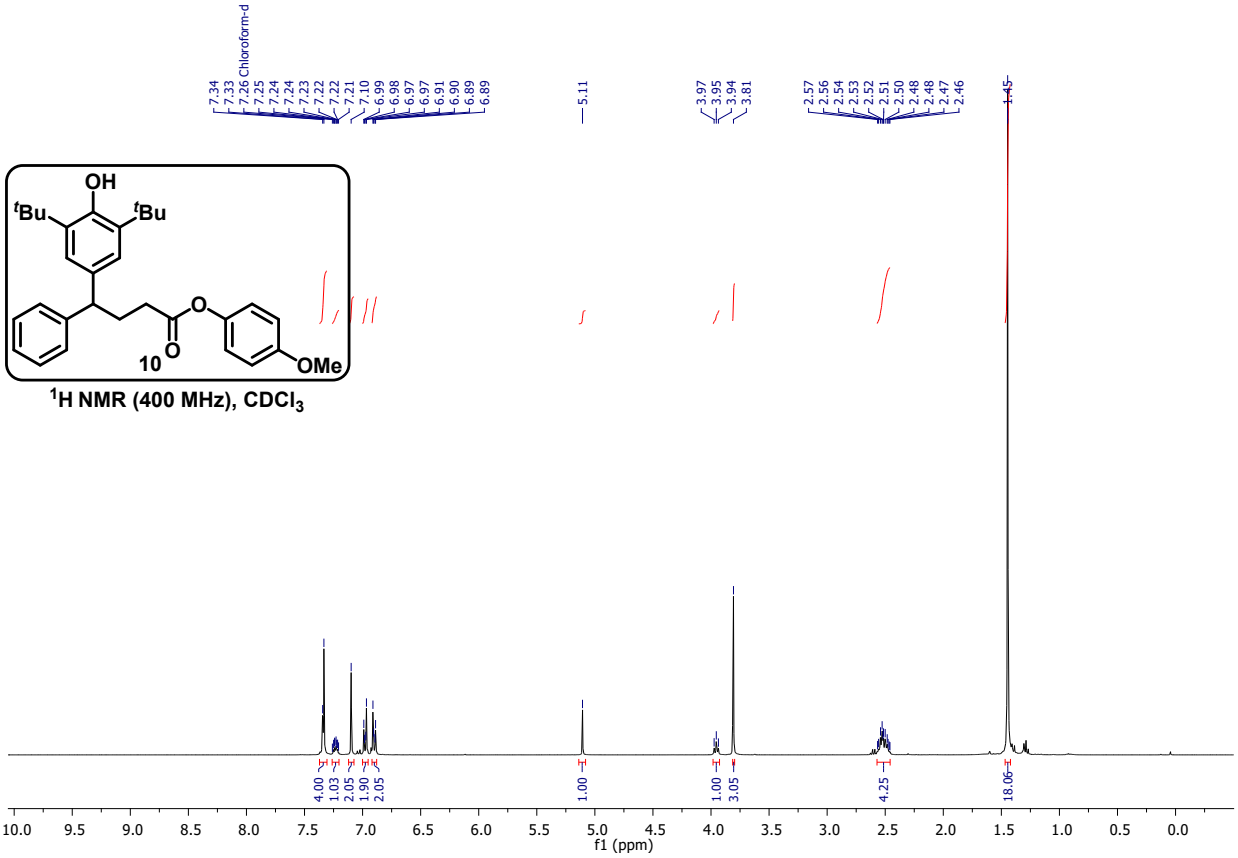
^{13}C NMR (100 MHz), $CDCl_3$



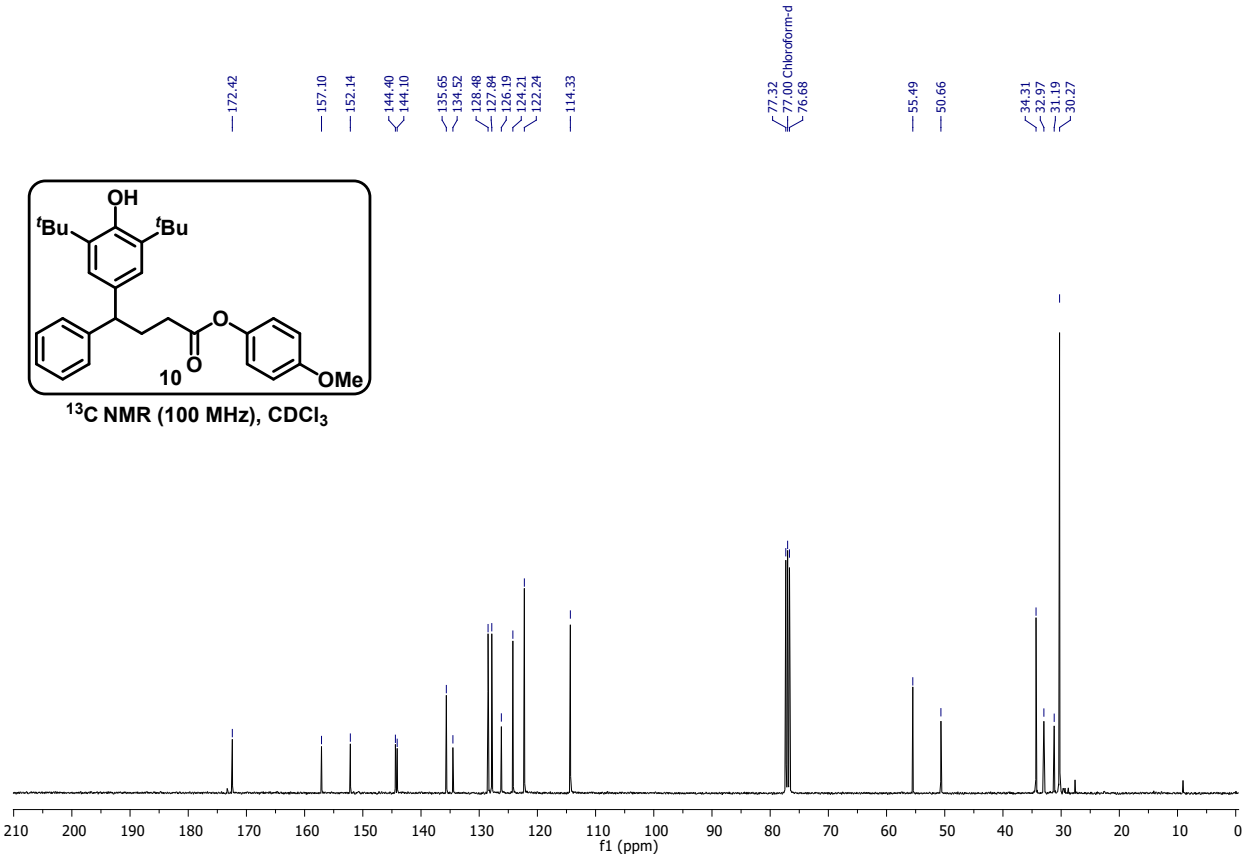
^{1}H NMR (400 MHz), $CDCl_3$



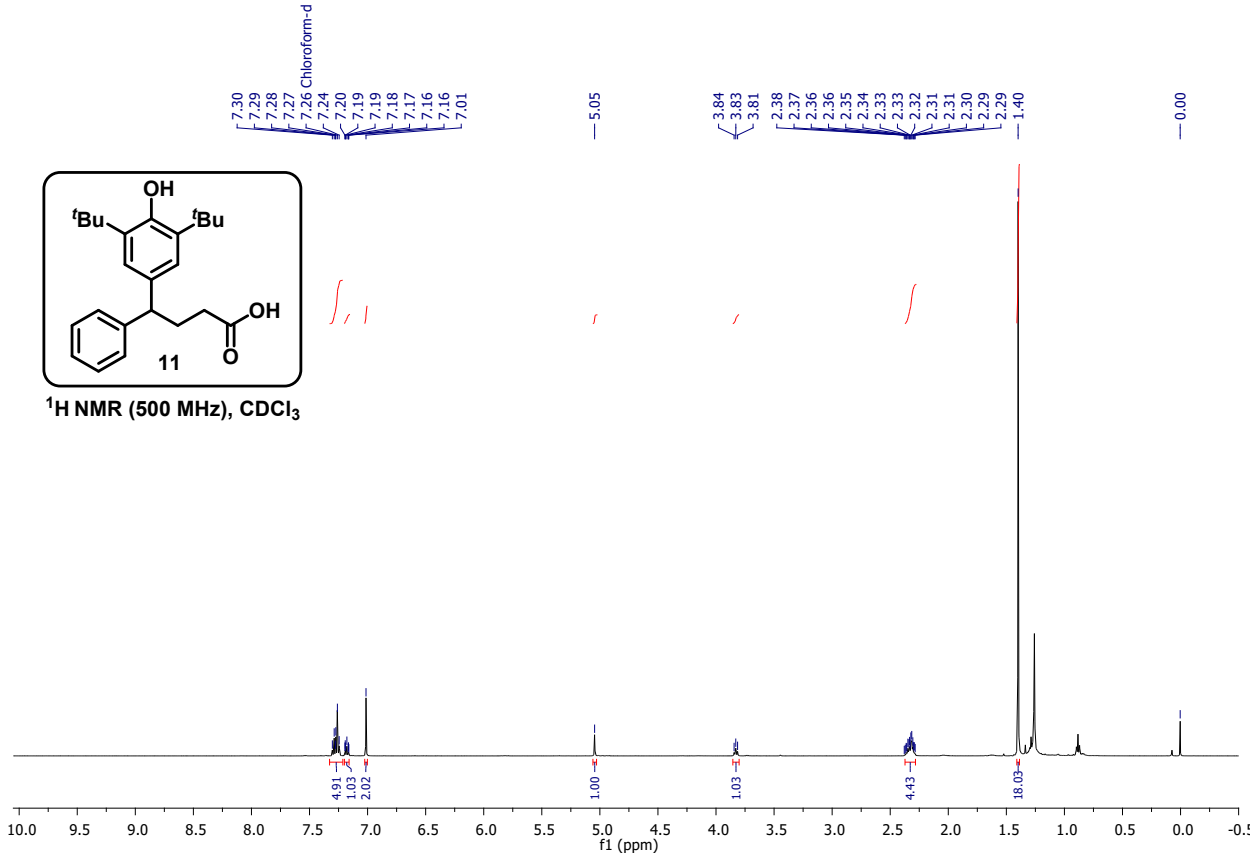
^{13}C NMR (100 MHz), $CDCl_3$



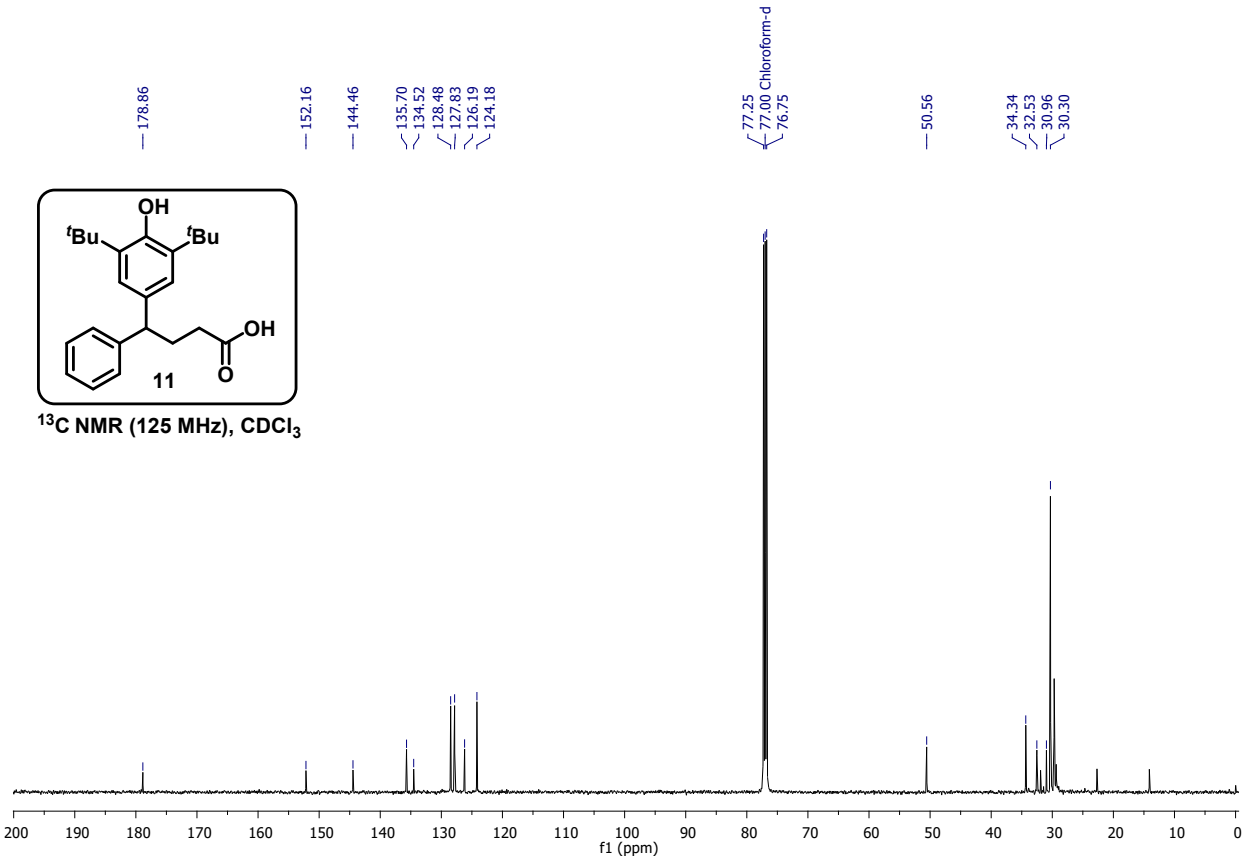
^{1}H NMR (400 MHz), $CDCl_3$



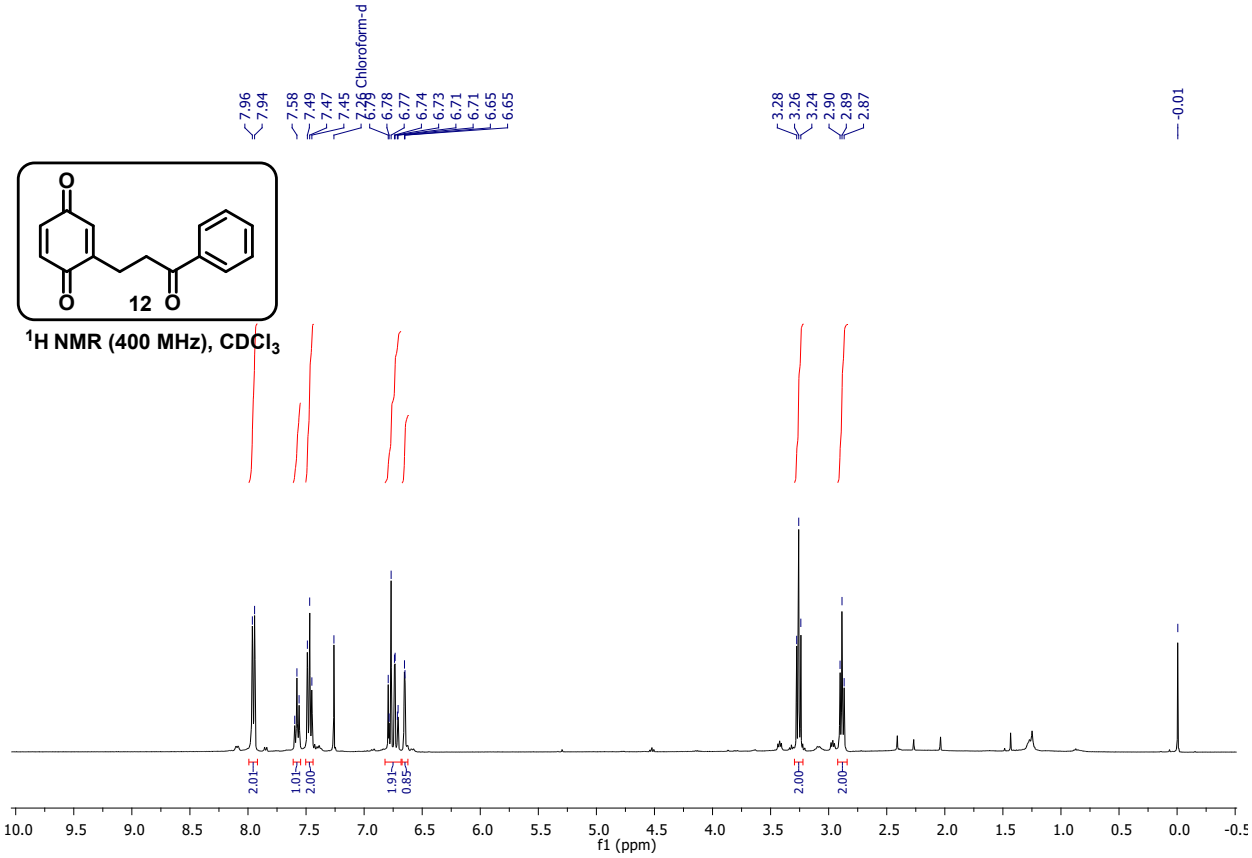
^{13}C NMR (100 MHz), $CDCl_3$



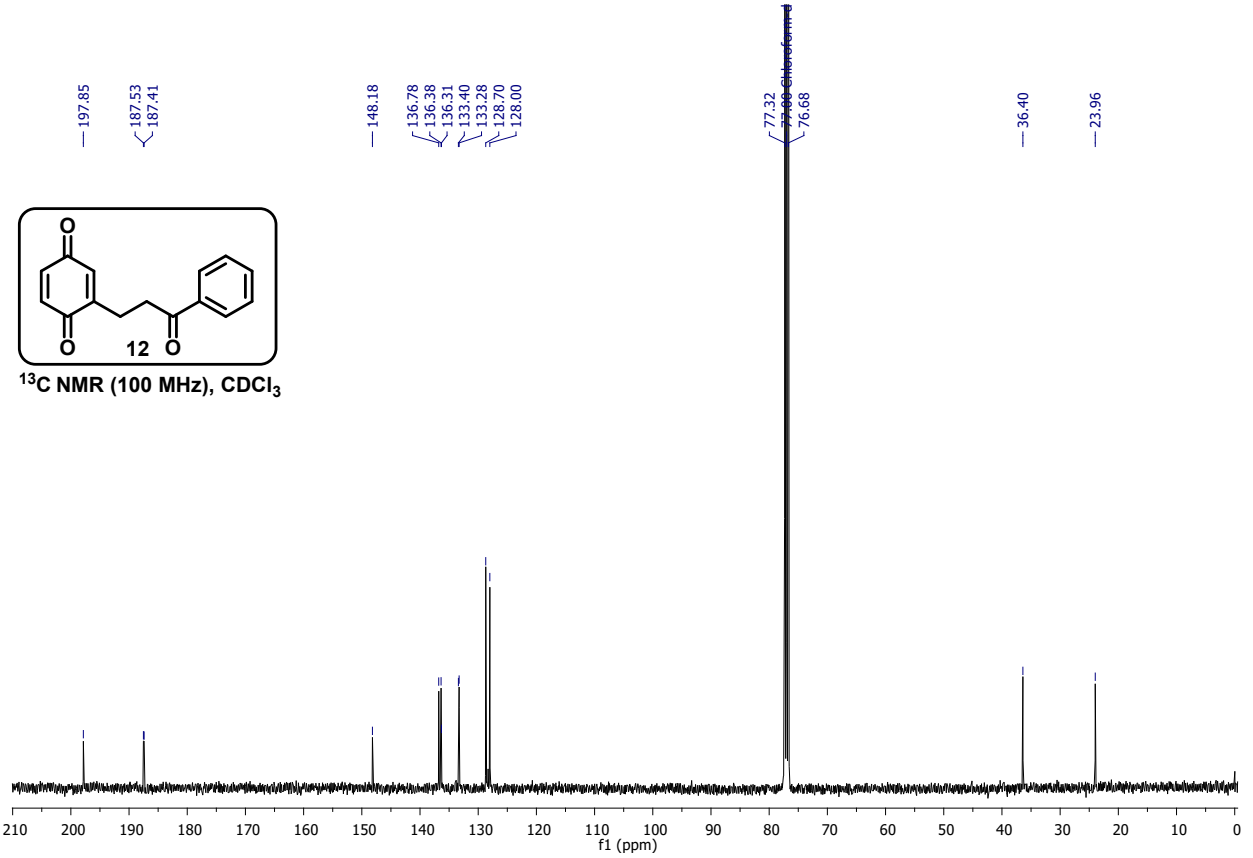
^{1}H NMR (500 MHz), $CDCl_3$



^{13}C NMR (125 MHz), $CDCl_3$



^{1}H NMR (400 MHz), $CDCl_3$



^{13}C NMR (100 MHz), $CDCl_3$