Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Palladium-Catalyzed Ring-Contraction Reaction of Naphthalquinones Upon Reaction with Alkynes

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Supporting Information

Contents:

1. General Information

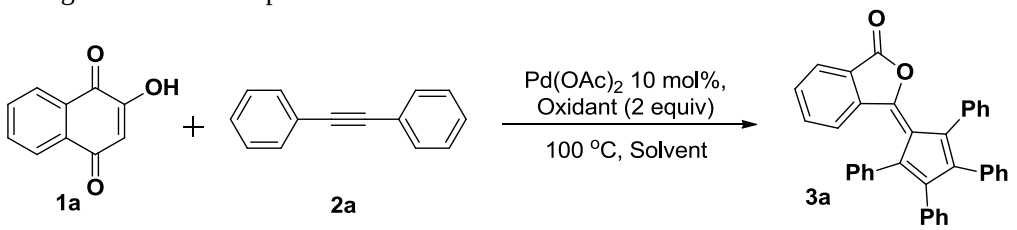
Chemicals and solvents were purchased from commercial suppliers and used as received. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker ACF300 (300 MHz) or a AMX500 (500 MHz) spectrometer. Chemical shifts were reported in parts per million (ppm), and the residual solvent peak was used as an internal reference: proton (chloroform δ 7.26), carbon (chloroform δ 77.0) or tetramethylsilane (TMS δ 0.00) was used as a reference. Multiplicity was indicated as follows: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), dd (doublet of doublet), bs (broad singlet). Coupling constants were reported in Hertz (Hz). Low resolution mass spectra were obtained on a Finnigan/MAT LCQ spectrometer in ESI mode. All high resolution mass spectra were obtained on a Finnigan/MAT 95XL-T spectrometer. For thin layer chromatography (TLC), Merck pre-coated TLC plates (Merck 60 F254) were used, and compounds were visualized with a UV light at 254 nm. Further visualization was achieved by staining with iodine. Flash chromatography separations were performed on Merck 60 (0.040-0.063 mm) mesh silica gel.

2. Starting materials

Compounds 1a, 2k, 2n, 2o, 2p were commercially available. Compounds **1b-j**[1], **2b-k**[2] were prepared according to literature, respectively.

3. Optimization of reaction conditions

Table a. Investigation of reaction parameters.[a]

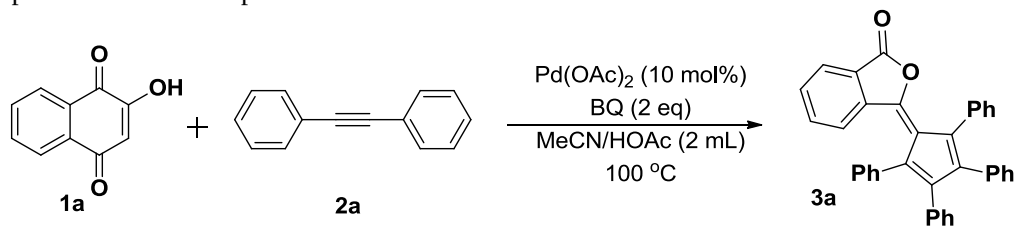


Entry	Solvent	Catalyst	Oxidant	Temp/ ℃	Yield/%[b]
1	MeCN	$Pd(OAc)_2$	AgOAc	100	47%
2	MeCN	$Pd(OAc)_2$	AgI	100	No reaction
3	MeCN	$Pd(OAc)_2$	$AgOOCCF_3$	100	55%
4	MeCN	$Pd(OAc)_2$	$AgSbF_6$	100	<10%
5	MeCN	$Pd(OAc)_2$	$Fe(OAc)_2$	100	49%
6	MeCN	$Pd(OAc)_2$	$FeCl_3$	100	<10%
7	MeCN	$Pd(OAc)_2$	$Fe(CH_3COCH_2CCOCH_3)_3$	100	No reaction
8	MeCN	$Pd(OAc)_2$	$Fe(OAc)_2$	100	49%
9	MeCN	$Pd(OAc)_2$	$FeCl_2$	100	<10%
10	MeCN	$Pd(OAc)_2$	CuCl	100	<10%
11	MeCN	$Pd(OAc)_2$	$CuBr_2$	100	No reaction
12	MeCN	$Pd(OAc)_2$	$Cu(CH_3ClO_4)_2$	100	No reaction
13	MeCN	$Pd(OAc)_2$	CuOAc	100	16%
14	MeCN	$Pd(OAc)_2$	$Cu(OAc)_2$	100	21%
15	MeCN	$Pd(OAc)_2$	$CuCl_2$	100	Compound 10
16	MeCN	$Pd(OAc)_2$	CuI	100	No reaction
17	MeCN	$Pd(OAc)_2$	$PhI(OAc)_2$	100	No reaction
18	MeCN	$Pd(OAc)_2$	BQ	100	65%
19	MeCN	$Pd(OAc)_2$	Oxones	100	Compound 9
20	MeCN	$Pd(OAc)_2$	$K_2S_2O_8$	100	No reaction
21	MeCN	$Pd(OAc)_2$	$(NH_4)_2S_2O_8$	100	No reaction

22	MeCN/HOAc (1:1 v/v)	$Pd(OAc)_2$	$AgOAc/Fe(OAc)_2$	100	55%
23	MeCN/HOAc (1:1 v/v)	$Pd(OAc)_2$	$AgOAc/Fe(OAc)_2$	120	64%
24	MeCN/HOAc (1:1 v/v)	$Pd(OAc)_2$	BQ	100	60%
25	MeCN/HOAc (2:1 v/v)	$Pd(OAc)_2$	BQ	100	69%
26	MeCN/HOAc (3:1 v/v)	$Pd(OAc)_2$	BQ	100	81%
27	MeCN/HOAc (3:1 v/v)	$Pd(OAc)_2$	BQ	120	79%
28	MeCN/HOAc (3:1 v/v)	$Pd(OAc)_2$	BQ	80	53%
29	MeCN/HOAc (1:4 v/v)	$Pd(OAc)_2$	BQ	100	50%
30	MeCN/HOAc (3:1 v/v)	$Pd(OAc)_2$	BQ/N_2	100	75%
31	MeCN/HOAc (3:1 v/v)	$Pd(OAc)_2$	BQ/O_2	100	47%

Reaction conditions: MeCN (2 mL), **1a** (0.2 mmol, 1.0 equiv.), **2a** (1.0 mmol, 5.0 equiv.), 10 mol% catalyst, oxidant (0.4 mmol, 2.0 equiv.) at 100 ^{o}C, 24 h.

Table b. Optimization of other parameters.[a]



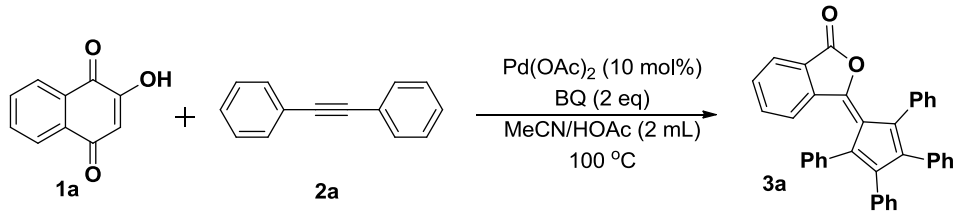
Entry	Solvent	Catalyst	Oxidant	Temp/℃	Yield/%[b]
1	MeCN/HOAc (3:1 v/v)	$Pd(OAc)_2$	BQ	100	81%
2	MeOH	$Pd(OAc)_2$	BQ	100	No reaction
3	IPA	$Pd(OAc)_2$	BQ	100	No reaction
4	THF	$Pd(OAc)_2$	BQ	80	20%
4	MeCN	$Pd(OAc)_2$	BQ	100	65%
5	Diglyme	$Pd(OAc)_2$	BQ	100	No reaction
6	$CHCl_3$	$Pd(OAc)_2$	BQ	80	No reaction
7	Toluene	$Pd(OAc)_2$	BQ	100	No reaction
8	1,4-Dioxane	$Pd(OAc)_2$	BQ	100	30%
9	DCE	$Pd(OAc)_2$	BQ	100	No reaction

10	DMA	$Pd(OAc)_2$	BQ	100	56%
11	DMSO	$Pd(OAc)_2$	BQ	100	62%
12	DMF	$Pd(OAc)_2$	BQ	100	32%

Reaction condition: solvent (2 mL), 2-hydroxynaphthalene-1,4-dione **1a** (0.2 mmol, 1 equiv), diphenylaceteyne **2a** (1 mmol, 5 equiv), 10 mol% catalyst, additives (0.4 mmol, 2 equiv), 80 or 100^{o}C, 24 h.

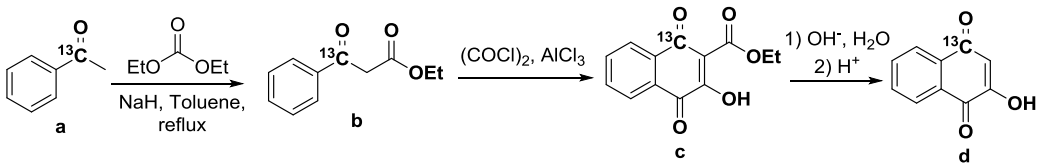
4. Representative Procedure for Palladium-catalyzed Reaction.

a) Procedure for **3a** synthesis:



To a solution of diphenylacetylene **2a** (178.0 mg, 1.0 mmol) and 2-hydroxy-1,4-naphthoquinone **1a** (34.8 mg, 0.2 mmol) in 2.0 ml of MeCN/HOAc (v/v = 3:1), $Pd(OAc)_2$ (4.5 mg, 0.02 mmol) as catalyst and 1,4-benzoquinone (BQ) (43.2 mg, 0.4 mmol) as oxidant were added. The reaction was refluxed at 100 ^{o}C for 24 h. The reaction mixture was cooled to room temperature, poured into H_2O and extracted with DCM for 3 times, combined organic layers were then dried over anhydrous $MgSO_4$, filtered, and the solvent removed in-vacuum. The crude product was purified by column chromatography on silica gel, eluted by hexane/EtOAc=25:1 then 10:1 to afford 81.3 mg (81 % yield) of the desired product **3a** as dark green powder.

b) ^{13}C-labeled experiment:



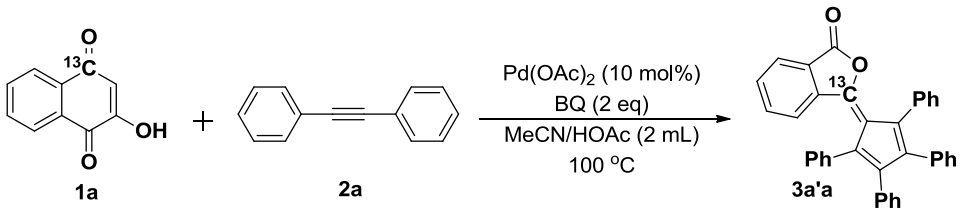
1) Procedure for preparing compound **d** (^{13}C-labeled-2-hydroxy-1,4-naphthoquinone) [1,3]**.** To a dried two-necked flask equipped with a magnetic stirred, and condenser was added NaH (7.0 mmol), diethyl carbonate (5.0 mmol), and toluene (2.5 ml). The mixture was heated to reflux. A solution of ketone **a** (2.5 mmol) in toluene (1.5 ml) was added dropwise with syringe over 10-20 min. After the addition, the mixture was heated

to reflux until the evolution of hydrogen ceased (3.0 – 5.0 min.). When the reaction was cooled to room temperature, glacial acetic acid (5.0 mL) was added dropwise and a heavy, pasty solid appeared. Ice-water was added until the solid was dissolved completely. The toluene layer was separated, and the water layer was extracted with EtOAc three times. The combined organic solution was washed with water and brine, then dried over $MgSO_4$. After evaporation of the solvent, the mixture was distilled under reduced pressure and subjected chromatography to give the desired β–keto esters **b** in 95% yield.

To a solution of β–keto esters **b** (2.0 mmol) in dry nitromethane (5.0 mL) under nitrogen was added $AlC1_3$ (6.0 mmol). After stirring for 15 min, oxalyl chloride (2.0 mmol) in dry nitromethane (2.0 mL) was added dropwise. After 15 min the solution was heated to 80 ^oC for 3 h. A solution of 10% aqueous oxalic acid was added under stirring at r.t. The resulting mixture was extracted with EtOAc (3 x 10 mL). The combined organic solution was washed with water and brine, dried over $MgSO_4$. After evaporation of the solvent, the mixture was distilled under reduced pressure and subjected chromatography (DCM/EtOAc = 50:1 then 10:1) to give the desired β–Keto Ester Oxaloylation product **c** in 90% yield.

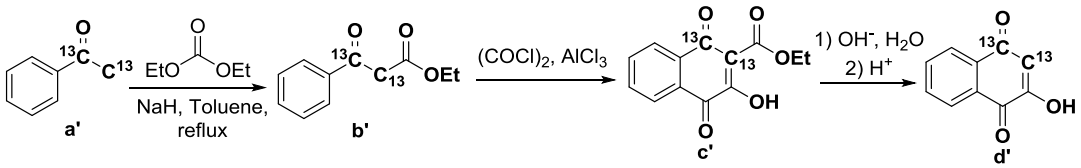
A solution of the compound **c** (1.5 mmol) in 5% aqueous NaOH (20 mL) was stirred at 60 ^oC for 8 h. A solution of 10% aqueous HCl (20 mL) was added, and heating was continued for 30 min. After cooling to r.t., the mixture was extracted with EtOAc (3 X 20 mL). The combined organic solution was washed with water and brine, dried over $MgSO_4$. After evaporation of the solvent, the mixture was distilled under reduced pressure and subjected chromatography (DCM/EtOAc = 50:1 then 4:1) to give the desired ^{13}C-labeled-2-hydroxy-1, 4-naphthoquinone product **d** in 82% yield.

2) Procedure for **3a'a** synthesis:



To a solution of diphenylacetylene **2a** (178.0 mg, 1.0 mmol) and 2-hydroxy-1,4-naphthoquinone **1a'** (35.0 mg, 0.2 mmol) in 2.0 ml MeCN/HOAc (v/v = 3:1), palladium acetate (4.5 mg, 0.02 mmol) as catalyst and 1,4-

Benzoquinone (43.2 mg, 0.4 mmol) as an oxidant were added. The reaction was refluxed at 100 ^{o}C for 24 h. The reaction mixture was cooled to room temperature, poured into H_2O and extracted with DCM for 3 times, combined organic layers were then dried over anhydrous $MgSO_4$, filtered, and the solvent removed in-vacuum. The crude product was purified by column chromatography on silica gel, eluted by hexane/EtOAc=25:1 then 10:1 to afford 78.3 mg (78 % yield) of the desired product **3a'a** as dark green powder.



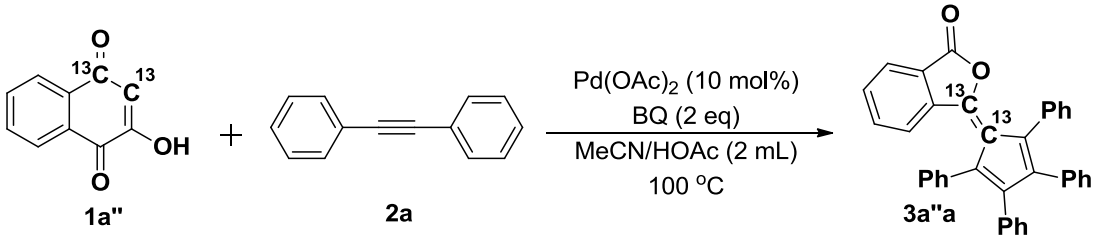
3) Procedure for **d'** synthesis[1,3]**.** To a dried two-necked flask equipped with a magnetic stirred, and condenser was added NaH (7.0 mmol), diethyl carbonate (5.0 mmol), and toluene (2.5 ml). The mixture was heated to reflux. A solution of ketone **a'** (2.5 mmol) in toluene (1.5 ml) was added dropwise with syringe over 10-20 min. After the addition, the mixture was heated to reflux until the evolution of hydrogen ceased (3.0 – 5.0 min.). When the reaction was cooled to room temperature, glacial acetic acid (5.0 mL) was added dropwise and a heavy, pasty solid appeared. Ice-water was added until the solid was dissolved completely. The toluene layer was separated, and the water layer was extracted with EtOAc three times. The combined organic solution was washed with water and brine, then dried over $MgSO_4$. After evaporation of the solvent, the mixture was distilled under reduced pressure and subjected chromatography to give the desired β–keto esters **b'** in 92% yield.

To a solution of β–keto esters **b'** (2.0 mmol) in dry nitromethane (5.0 mL) under nitrogen was added $AlC1_3$ (6.0 mmol). After stirring for 15 min, oxalyl chloride (2.0 mmol) in dry nitromethane (2.0 mL) was added dropwise. After 15 min the solution was heated to 80 ^{o}C for 3 h. A solution of 10% aqueous oxalic acid was added under stirring at r.t. The resulting mixture was extracted with EtOAc (3 x 10 mL). The combined organic solution was washed with water and brine, dried over $MgSO_4$. After evaporation of the solvent, the mixture was distilled under reduced pressure and subjected chromatography (DCM/EtOAc = 50:1 then 10:1) to give the desired β–Keto Ester Oxaloylation product **c'** in 87% yield.

A solution of the compound **c'** (1.5 mmol) in 5% aqueous NaOH (20 mL) was stirred at 60 ^{o}C for 8 h. A

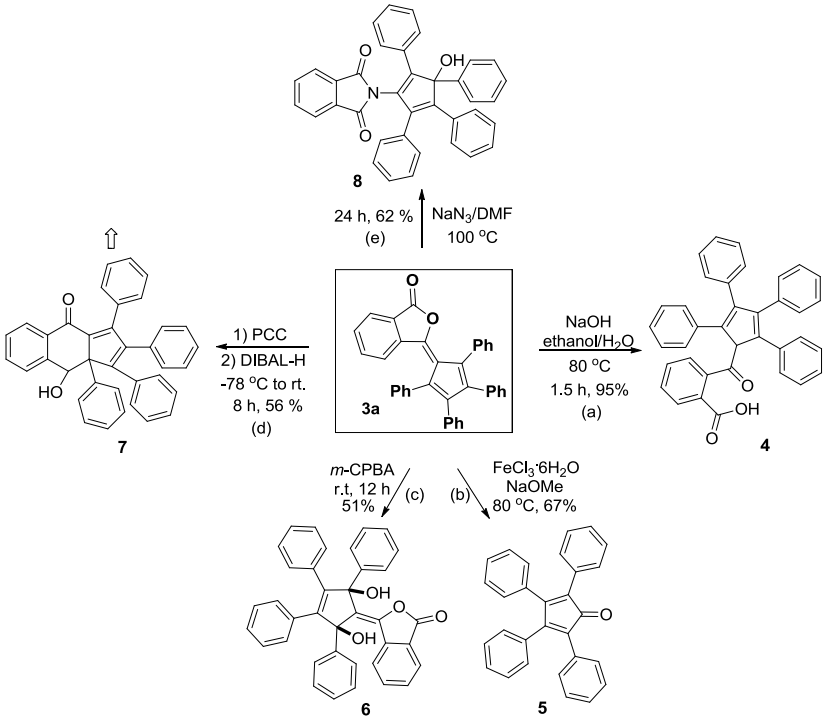
solution of 10% aqueous HCl (20 mL) was added, and heating was continued for 30 min. After cooling to r.t., the mixture was extracted with EtOAc (3 X 20 mL). The combined organic solution was washed with water and brine, dried over $MgSO_4$. After evaporation of the solvent, the mixture was distilled under reduced pressure and subjected chromatography (DCM/EtOAc = 50:1 then 4:1) to give the desired ^{13}C-labelled-2-hydroxy-1,4-naphthoquinone product **d'** in 75% yield.

4) Procedure for **3a"a** synthesis:



To a solution of diphenylacetylene **2a** (178.0 mg, 1.0 mmol) and 2-hydroxy-1,4-naphthoquinone **1a"** (35.2 mg, 0.2 mmol) in 2.0 ml MeCN/HOAc (v/v = 3:1), palladium acetate (4.5 mg, 0.02 mmol) as catalyst and 1,4-Benzoquinone (43.2 mg, 0.4 mmol) as an oxidant were added. The reaction was refluxed at 100 ^{o}C for 24 h. The reaction mixture was cooled to room temperature, poured into H_2O and extracted with DCM for 3 times, combined organic layers were then dried over anhydrous $MgSO_4$, filtered, and the solvent removed in-vacuum. The crude product was purified by column chromatography on silica gel, eluted by hexane/EtOAc=25:1 then 10:1 to afford 65.4 mg (64 % yield) of the desired product **3a"a** as dark green powder.

5. Synthetic transformations of **3a**.



Product 4[4]

To a stirred solution of **3a** (100 mg, 0.2 mmol) in ethanol/H_2O (2.0 mL, v/v = 1:1) was added aqueous NaOH (10 mol/L, 0.4 mL). The resulting mixture was stirred at 80 °C for 1.0 h. After complete conversion as indicated by TLC, aqueous HCl (4 mol/L, 0.6 mL) was dropped into the reaction system, the resulting mixture was stirred at r.t. for 0.5 h, the mixture was poured into H_2O and extracted with DCM three times. The combined organic phases were dried over anhydrous $MgSO_4$, filtered, and concentrated under reduced pressure. The crude product was purified by silica gel flash chromatography and eluted by hexane/EtOAc=10:1 then 1:1 to afford the product **4** (98.4 mg, 95 %) as pale yellow oil.

Product 5

To a stirred solution of **3a** (50.1 mg, 0.1 mmol) in EtOH (2.0 mL) was added $FeCl_3$ $6H_2O$ (54.6 mg, 0.2 mmol), NaOMe (10.8 mg, 0.2 mmol). The resulting mixture was stirred at 80 °C for 24 h. After complete conversion as indicated by TLC, the solvent was removed by evaporation and the residue was directly purified by silica gel flash chromatography and eluted by hexane/EtOAc=100:1 to 20:1 afford the product **5** (26.2 mg, 68 %) as red-dark powder.

Product 6

To a stirred solution of **3a** (50.1 mg, 0.1 mmol) in DCM (2.0 mL) was added *m*-CPBA (34.6 mg, 0.2 mmol). The resulting mixture was stirred at r.t. for 0.5 h. After complete conversion as indicated by TLC, the solvent was removed by evaporation and the residue was directly purified by silica gel flash chromatography and eluted by hexane/EtOAc=20:1 to 4:1 afford the product **6** (27.2 mg, 51 % yield) as white solid.

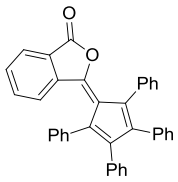
Product 7[5]

A solution of DIBAL-H (0.2 mmol, 1.0 M in CH_2Cl_2) was injected via a syringe into a stirred solution of **3a** (50.1 mg, 0.1 mmol) in anhydrous DCM (4 mL) at -78 ^oC under an Ar atmosphere. After stirring at -78 ^oC for 6 h, a catalytic amount of NaOMe (3.3 mg, 0.06 mmol) was added to the mixture and the solution owas allowed to warm to r.t. for 12 h. The mixture was poured into sat. NH_4Cl solution and extracted with DCM three times. The combined organic phases were dried over anhydrous $MgSO_4$, filtered, and concentrated under reduced pressure to give an intermediate which without isolation was used in the next step. To a solution of the intermediate in DCM (2 mL) was added PCC (86 mg, 0.4 mmol) and the mixture was stirred for 12 h. Then, the mixture was poured into H_2O and extracted with DCM three times. The combined organic phases were dried over anhydrous $MgSO_4$, filtered, and concentrated under reduced pressure. The crude product was purified by silica gel flash chromatography and eluted by hexane/EtOAc = 20:1 then 4:1 to afford the product **6** (21.2 mg, 56 % yield) as white solid.

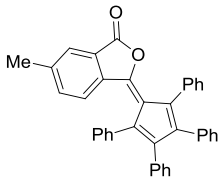
Product 8 [6]

To a stirred solution of **3a** (50.1 mg, 0.1 mmol) in DMF (2.0 mL) were added NaN_3 (32.5 mg, 0.5 mmol). The resulting mixture was stirred at 100 ^oC for 24 h. After complete conversion as indicated by TLC, the solvent was removed by evaporation and the residue was diluted with water and extracted with ethyl acetate (3 x 10.0 mL). The combined organic layers were dried over anhydrous $MgSO_4$ and concentrated *in vacuo*. The resulting product was purified by column chromatography on silica gel using hexane/ ethyl acetate (20:1 to 2:1) as eluent to afford the product **8 (**32.9 mg, 62 %) as white solid.

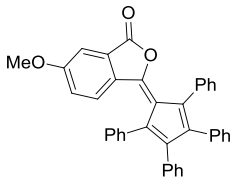
6. Analytical Data.



3-(2,3,4,5-Tetraphenylcyclopenta-2,4-dienylidene)isobenzofuran-1(3*H*)-one (3a). 81% yield; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.83 (d, *J* = 7.6 Hz, 1H), 7.42 (t, *J* = 7.5 Hz, 1H), 7.29 – 7.25(m, 10H), 7.14 – 6.99 (m, 7H), 6.91 – 6.82 (m, 4H), 6.09 (d, *J* = 8.2 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 165.42, 151.65, 147.02, 145.31, 138.01, 137.64, 135.75, 135.41, 134.57, 133.85, 131.49, 130.95, 130.76, 129.97, 129.32, 128.43, 127.94, 127.76, 127.61, 127.50, 127.07, 126.93, 126.88, 126.82, 125.70; HRMS (ESI) calcd for $C_{37}H_{24}NaO_2$ $[M+Na]^+$ 523.1669, found 523.1679.

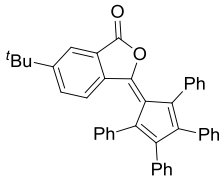


5-Methyl-3-(2,3,4,5-tetraphenylcyclopenta-2,4-dienylidene)isobenzofuran-1(3*H*)-one (3b). 82% yield; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.62 (s, 1H), 7.29 – 7.26 (m, 10H), 7.11 – 6.95 (m, 6H), 6.93 (dd, *J* = 8.4, 1.6 Hz, 1H), 6.88 – 6.86 (m, 2H), 6.83 – 6.82 (m, 2H), 5.93 (d, *J* = 8.4 Hz, 1H), 2.38 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 165.57, 151.97, 146.66, 144.93, 142.74, 138.15, 137.75, 135.85, 135.52, 135.10, 134.51, 131.56, 131.50, 130.97, 130.79, 130.77, 129.27, 129.10, 128.18, 127.89, 127.73, 127.58, 127.42, 127.17, 126.98, 126.84, 126.81, 125.81, 21.88; HRMS (ESI) calcd for $C_{38}H_{27}O_2$ $[M+H]^+$ 515.2006, found 515.2015.

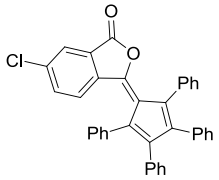


5-Methoxy-3-(2,3,4,5-tetraphenylcyclopenta-2,4-dienylidene)isobenzofuran-1(3*H*)-one (3c). 86% yield; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.25 – 7.23 (m, 11H), 7.11 – 6.99 (m, 6H), 6.87 – 6.81 (m, 4H), 6.65 (dd, *J* = 9.0, 2.5 Hz, 0H), 5.94 (d, *J* = 9.0 Hz, 0H), 3.84 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 165.52, 162.63, 151.94, 146.35, 144.62, 138.22, 137.76, 135.92, 135.61, 134.43, 131.52, 131.01, 130.81, 130.62, 129.72, 129.30,

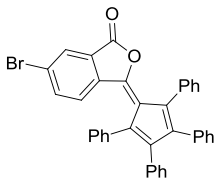
129.11, 128.29, 127.87, 127.72, 127.58, 127.42, 126.94, 126.79, 122.42, 107.80, 56.38; HRMS (ESI) calcd for $C_{38}H_{27}O_3$ $[M+H]^+$ 531.1995, found 531.1963.



5-*Tert*-butyl-3-(2,3,4,5-tetraphenylcyclopenta-2,4-dienylidene)isobenzofuran-1(3*H*)-one (3d). 72% yield; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.81 (d, *J* = 1.9 Hz, 1H), 7.30 – 7.23 (m, 10H), 7.15 – 7.00 (m, 7H), 6.88 – 6.86 (m, 2H), 6.83 – 6.81 (m, 2H), 5.91 (d, *J* = 8.5 Hz, 1H), 1.27 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 165.89, 156.05, 151.91, 146.61, 144.92, 138.20, 137.77, 135.87, 135.56, 135.45, 134.50, 131.64, 131.60, 131.54, 130.97, 130.80, 130.79, 129.30, 129.20, 128.15, 127.89, 127.72, 127.58, 127.49, 127.00, 126.97, 126.84, 126.80, 122.39, 35.73, 31.45.; HRMS (ESI) calcd for $C_{41}H_{33}O_2$ $[M+H]^+$ 557.2475, found 557.2481.

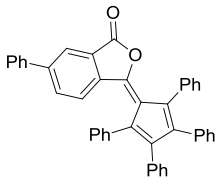


6-Chloro-3-(2,3,4,5-tetraphenylcyclopenta-2,4-dienylidene)isobenzofuran-1(3*H*)-one (3e). 74% yield; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.78 (d, *J* = 2.0 Hz, 1H), 7.28 – 7.22 (m, 10H), 7.14 – 6.98 (m, 7H), 6.89 – 6.85 (m, 2H), 6.82 (dd, *J* = 8.2, 1.4 Hz, 2H), 5.92 (d, *J* = 8.7 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 164.21, 150.46, 147.45, 145.72, 138.10, 137.84, 137.49, 136.25, 135.57, 135.26, 134.52, 134.11, 131.44, 131.32, 130.92, 130.71, 129.50, 129.34, 128.42, 127.99, 127.81, 127.73, 127.65, 127.22, 127.06, 127.01, 125.57; HRMS (ESI) calcd for $C_{37}H_{24}ClO_2$ $[M+H]^+$ 535.1412, found 535.1422.

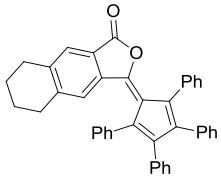


6-Bromo-3-(2,3,4,5-tetraphenylcyclopenta-2,4-dienylidene)isobenzofuran-1(3H)-one (3f). 79% yield; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.95 (d, *J* = 1.5 Hz, 1H), 7.30 – 7.22 (m, 10H), 7.15 – 7.00 (m, 7H), 6.99 – 6.86

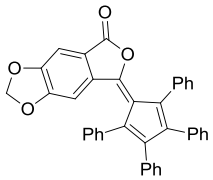
(m, 2H), 6.83 – 6.79 (m, 2H), 5.84 (d, *J* = 8.7 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 164.08, 150.54, 147.49, 145.76, 137.83, 137.47, 136.92, 136.67, 135.57, 135.26, 134.53, 131.43, 131.34, 130.92, 130.69, 129.51, 129.45, 128.65, 128.49, 127.99, 127.81, 127.75, 127.65, 127.22, 127.07, 127.01, 126.26.; HRMS(ESI) calcd for $C_{37}H_{24}BrO_2$ $[M+H]^+$ 579.0954, found 579.0962.



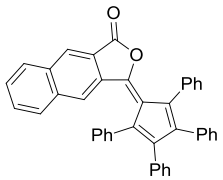
6-Phenyl-3-(2,3,4,5-tetraphenylcyclopenta-2,4-dienylidene)isobenzofuran-1(3*H*)-one (3g). 83% yield; ^{1}H NMR (500 MHz, $CDCl_3$): δ =8.05 (d, *J* = 1.4 Hz, 1H), 7.57 (dd, *J* = 8.2, 1.0 Hz, 2H), 7.47 (t, *J* = 7.4 Hz, 2H), 7.42 (m, 1H), 7.37 (dd, *J* = 8.5, 1.6 Hz, 1H), 7.33 – 7.23 (m, 10H), 7.16 – 6.99 (m, 6H), 6.92 – 6.87 (m, 2H), 6.85 – 6.82 (m, 2H), 6.08 (d, *J* = 8.5 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 165.50, 151.60, 150.47, 146.98, 145.28, 144.68, 138.94, 138.11, 137.75, 136.57, 135.82, 135.50, 134.56, 132.59, 131.57, 131.00, 130.80, 129.97, 129.61, 129.39, 129.26, 128.78, 127.95, 127.77, 127.62, 127.57, 127.08, 126.94, 126.90, 123.74; HRMS(ESI) calcd for $C_{43}H_{29}O_2$ $[M+H]^+$ 577.2162, found 577.2181.



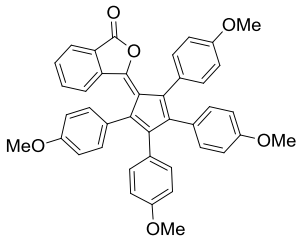
3-(2,3,4,5-Tetraphenylcyclopenta-2,4-dienylidene)-5,6,7,8-tetrahydronaphtho[2,3-c]furan-1(3*H*)-one (3h). 62% yield; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.29 – 7.24 (m, 10H), 7.10 – 7.00 (m, 6H), 6.87–6.79 (m, 5H), 5.86 (d, *J* = 8.5 Hz, 1H), 3.11 (d, *J* = 5.5 Hz, 2H), 2.73 (d, *J* = 5.0 Hz, 2H), 1.79 (d, *J* = 2.4 Hz, 4H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 165.52, 152.30, 146.41, 144.55, 142.47, 138.95, 138.32, 137.93, 136.26, 136.05, 135.70, 134.83, 134.59, 131.57, 131.53, 131.01, 130.87, 130.84, 129.19, 128.45, 127.87, 127.71, 127.57, 127.28, 126.90, 126.76, 126.71, 125.46, 124.02, 30.01, 25.48, 22.72, 22.42; HRMS(ESI) calcd for $C_{41}H_{31}O_2$ $[M+H]^+$ 555.2319, found 555.2320.



7-(2,3,4,5-Tetraphenylcyclopenta-2,4-dienylidene)isobenzofuro[5,6-d][1,3]dioxol-5(7*H*)-one (3i). 73% yield; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.27 – 7.20 (m, 11H), 7.09 – 6.97 (m, 7H), 6.85 – 6.83 (m, 2H), 6.80 – 6.78 (m, 2H), 5.99 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 164.83, 153.26, 151.62, 151.24, 146.79, 144.88, 138.17, 137.80, 135.81, 135.51, 134.59, 134.20, 131.49, 131.28, 130.96, 130.78, 129.36, 129.05, 127.87, 127.74, 127.59, 127.02, 126.85, 126.81, 122.51, 107.56, 104.33, 103.37; HRMS(ESI) calcd for $C_{38}H_{25}O_4$ $[M+H]^+$ 545.1747, found 547.1742.

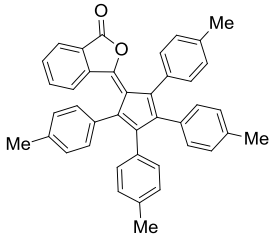


3-(2,3,4,5-Tetraphenylcyclopenta-2,4-dienylidene)naphtho[2,3-c]furan-1(3*H*)-one (3j). 69% yield; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 8.88 (d, *J* =8.5 Hz, 1H), 7.79 (d, *J* = 8.1 Hz, 1H), 7.69 (t, *J* = 7.6 Hz, 1H), 7.62 (t, *J* = 7.5 Hz, 1H), 7.51 (d, *J* = 8.5 Hz, 1H), 7.35 – 7.20 (m, 10H), 7.17 – 6.98 (m, 6H), 6.89 (d, *J* = 7.0 Hz, 2H), 6.83 (d, *J* = 7.3 Hz, 2H), 6.24 (d, *J* = 8.9 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 165.61, 151.81, 147.21, 145.65, 138.82, 137.97, 137.69, 135.82, 135.43, 134.55, 134.65, 134.13, 131.64, 131.60, 131.54, 131.02, 130.97, 130.80, 129.71, 129.29, 129.24, 128.49, 127.98, 127.81, 127.68, 127.64, 127.47, 127.14, 126.99, 126.91, 124.80, 123.33, 122.07; HRMS (ESI) calcd for $C_{41}H_{27}O_2$ $[M+H]^+$ 551.2006, found 551.2009.

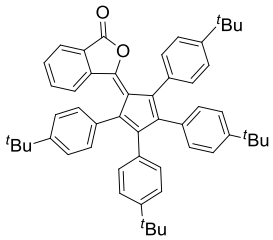


(*Z*)-3-(3-(3-methoxyphenyl)-2,4,5-tris(4-methoxyphenyl)cyclopenta-2,4-dienylidene)isobenzofuran-

1(3*H*)-one (3k). 81% yield; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.79 (d, *J* = 7.5 Hz, 1H), 7.38 (t, *J* = 7.5 Hz, 1H), 7.16 – 7.11 (m, 5H), 6.81 – 6.75 (m, 6H), 6.70 (d, *J* = 8.7 Hz, 2H), 6.62 (d, *J* = 8.7 Hz, 2H), 6.55 (d, *J* = 8.7 Hz, 2H), 6.17 (d, *J* = 8.2 Hz, 1H), 3.81 (s, 3H), 3.80 (s, 3H), 3.73 (s, 3H), 3.70 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 165.77, 159.28, 158.59, 158.52, 158.45, 150.64, 146.46, 145.18, 138.27, 133.79, 133.25, 132.53, 132.11, 132.08, 131.14, 130.71, 130.59, 130.22, 128.43, 128.39, 128.08, 126.74, 125.59, 114.81, 113.49, 113.27, 113.14, 55.81, 55.59, 55.50, 55.45; HRMS(ESI) calcd for $C_{41}H_{33}O_6$ $[M+H]^+$ 621.2272, found 621.2285.

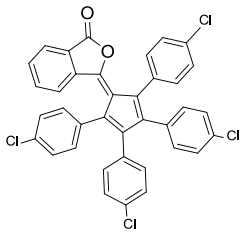


3-(2,3,4,5-Tetrap-tolylcyclopenta-2,4-dienylidene)isobenzofuran-1(3*H*)-one (3l). 79% yield; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.78 (d, *J* = 7.6, 1H), 7.37 (t, *J* = 7.4 Hz, 1H), 7.12 – 7.02 (m, 9H), 6.86 (d, *J* = 8.0 Hz, 2H), 6.80 (d, *J* = 8.0 Hz, 2H), 6.73 (d, *J* = 8.1 Hz, 2H), 6.68 (d, *J* = 8.1 Hz, 2H), 6.08 (d, *J* = 8.2 Hz, 1H), 2.34 (s, 6H), 2.24 (s, 3H), 2.20 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 165.74, 150.99, 146.92, 145.43, 138.26, 137.01, 136.48, 136.31, 136.03, 135.13, 134.81, 134.05, 133.62, 132.98, 132.65, 131.36, 131.21, 131.17, 130.85, 130.70, 129.95, 128.66, 128.56, 128.46, 128.34, 126.75, 125.52, 21.86, 21.75, 21.72; HRMS(ESI) calcd for $C_{41}H_{33}O_2$ $[M+H]^+$ 557.2475, found 557.2483.

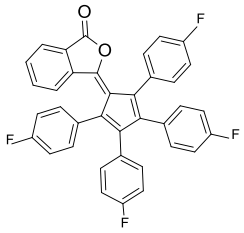


3-(2,3,4,5-Tetrakis(4-*tert*-butylphenyl)cyclopenta-2,4-dienylidene)isobenzofuran-1(3*H*)-one (3m). 61% yield; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.78 (d, *J* = 7.6 Hz, 1H), 7.37 (dd, *J* = 7.5, 2.5 Hz, 1H), 7.32 – 7.24 (m, 4H), 7.24 – 7.15 (m, 4H), 7.10 – 6.95 (m, 5H), 6.88 – 6.80 (m, 2H), 6.75 – 6.69 (m, 2H), 5.91 (d, *J* = 8.2 Hz, 1H), 1.35 (s, 9H), 1.35 (s, 9H), 1.25 (s, 9H), 1.22 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 165.71, 150.87,

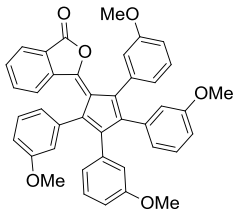
150.64, 149.70, 149.43, 149.39, 146.99, 145.80, 138.30, 135.33, 134.84, 133.99, 133.49, 132.98, 132.68, 131.16, 131.05, 130.99, 130.75, 130.51, 130.49, 128.45, 126.77, 126.09, 125.40, 124.59, 124.38, 124.16, 35.04, 34.93, 34.88, 34.80, 31.95, 31.91, 31.75, 31.70; HRMS(ESI) calcd for $C_{53}H_{57}O_2$ $[M+H]^+$ 725.4353, found 725.4363.



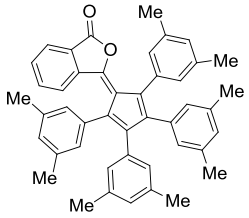
3-(2,3,4,5-Tetrakis(4-chlorophenyl)cyclopenta-2,4-dienylidene)isobenzofuran-1(3*H*)-one (3n). 73% yield; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.87 (d, *J* = 7.6 Hz, 1H), 7.50 (t, *J* = 7.4 Hz, 1H), 7.29 – 7.24 (m, 6H), 7.13 – 7.10 (m, 5H), 7.05 (d, *J* = 8.5 Hz, 2H), 6.76 (d, *J* = 8.5 Hz, 2H), 6.70 (d, *J* = 8.5 Hz, 2H), 6.22 (d, *J* = 8.1 Hz, 1H).; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 164.91, 152.59, 145.69, 143.99, 137.53, 135.89, 135.55, 134.13, 134.05, 133.62, 133.58, 133.43, 133.24, 133.15, 132.61, 132.41, 132.28, 132.12, 131.91, 130.98, 130.70, 130.63, 129.77, 129.72, 128.64, 128.52, 128.49, 128.37, 128.31, 128.11, 126.94, 126.19; HRMS(ESI) calcd for $C_{37}H_{20}Cl_4NaO_2$ $[M+Na]^+$ 659.0110, found 659.0121.



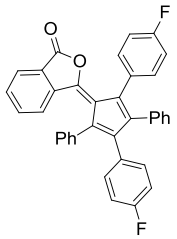
3-(2,3,4,5-Tetrakis(4-fluorophenyl)cyclopenta-2,4-dienylidene)isobenzofuran-1(3*H*)-one (3o). 77% yield; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.84 (d, *J* = 7.6 Hz, 1H), 7.46 (t, *J* = 7.5 Hz, 1H), 7.25 – 7.09 (m, 5H), 6.98 – 6.94 (m, 4H), 6.81 – 6.72 (m, 8H), 6.15 (d, *J* = 8.2 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 165.13, 163.23, 163.17, 163.04, 161.71, 161.28, 161.19, 161.08, 152.01, 146.03, 144.35, 137.72, 134.09, 133.75, 132.95, 133.56, 133.30, 132.89, 132.41, 132.35, 132.28, 132.00, 131.33, 131.00, 130.70, 129.20, 128.18, 126.92, 126.09, 116.63, 116.46, 115.28, 115.12, 114.95; HRMS(ESI) calcd for $C_{37}H_{20}F_4O_2$ $[M+H]^+$ 573.1472, found 573.1489.



3-(2,3,4,5-Tetrakis(3-methoxyphenyl)cyclopenta-2,4-dienylidene)isobenzofuran-1(3H)-one (3p). 74% yield; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.81 (d, *J* = 7.6 Hz, 1H), 7.41 (t, *J* = 7.5 Hz, 1H), 7.20 – 7.13 (m, 3H), 6.99 (t, *J* = 7.9 Hz, 1H), 6.92 (t, *J* = 7.9 Hz, 1H), 6.87 – 6.76 (m, 6H), 6.66 (dd, *J* = 8.2, 2.5 Hz, 1H), 6.60 (dd, *J* = 8.2, 2.5 Hz, 1H), 6.49 (d, *J* = 7.6 Hz, 1H), 6.43 – 6.39 (m, 3H), 6.21 (d, *J* = 8.2 Hz, 1H), 3.69 (s, 3H), 3.57 (s, 3H), 3.47 (s, 3H), 3.42 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 165.38, 160.48, 159.47, 159.09, 158.94, 151.89, 146.72, 145.01, 139.34, 138.80, 138.05, 137.03, 136.58, 134.33, 133.90, 131.64, 131.42, 130.36, 129.57, 128.91, 128.80, 128.62, 128.57, 126.81, 125.71, 124.04, 123.68, 123.35, 123.31, 116.60, 116.47, 115.56, 115.32, 114.02, 113.99, 113.88, 112.84, 55.73, 55.71, 55.45, 55.40; HRMS(ESI) calcd for $C_{41}H_{33}O_6$ $[M+H]^+$ 621.2272, found 621.2286.

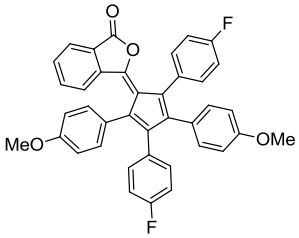


3-(2,3,4,5-Tetrakis(3,5-dimethylphenyl)cyclopenta-2,4-dienylidene)isobenzofuran-1(3*H*)-one (3q). 64% yield; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.77 (d, *J* = 7.6 Hz, 1H), 7.36 (t, *J* = 7.4 Hz, 1H), 7.09 (t, *J* = 7.8 Hz, 1H), 6.85 – 6.83 (m, 6H), 6.69 (s, 1H), 6.63 (s, 1H), 6.49 (s, 2H), 6.43 (s, 2H), 6.07 (d, *J* = 8.2 Hz, 1H), 2.23 (s, 6H), 2.13 (s, 6H), 2.06 (s, 6H), 2.01 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 165.78, 150.72, 147.28, 145.57, 138.47, 138.41, 138.03, 137.61, 136.66, 136.42, 136.22, 135.79, 135.38, 134.27, 133.50, 131.21, 130.98, 130.94, 129.36, 128.84, 128.82, 128.72, 128.68, 128.43, 128.29, 126.78, 125.34, 21.85, 21.68, 21.65, 21.62; HRMS(ESI) calcd for $C_{45}H_{41}O_2$ $[M+H]^+$ 613.3101, found 613.3115.



3-(2,4-Bis(4-fluorophenyl)-3,5-diphenylcyclopenta-2,4-dienylidene)isobenzofuran-1(3*H*)-one (3r) 81% yield, regioisomer ratio = 5:3; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.87 – 7.83 (m, 4H), 7.49 – 7.42 (m, 5H), 7.31 – 7.18 (m, 31H), 7.13 – 7.02 (m, 27H), 6.99 – 6.95 (m, 15H), 6.86 – 6.76 (m, 20H), 6.71 (t, *J* = 8.8 Hz, 2H), 6.20 (d, *J* = 8.2 Hz, 3H), 6.07 (d, *J* = 8.2 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 164.76, 163.09, 162.66, 161.12, 151.14, 146.97, 145.26, 137.34, 135.00, 134.64, 133.49, 133.06, 133.04, 133.01, 132.50, 132.43, 131.98, 131.92, 131.90, 131.81, 131.29, 130.92, 130.36, 130.16, 129.90, 129.18, 128.97, 127.93, 127.68, 127.59, 127.51, 127.41, 127.34, 127.25, 126.78, 126.62, 126.38, 125.49, 125.31, 115.94, 115.77, 114.60, 114.43, 104.97; HRMS(ESI) calcd for $C_{37}H_{23}F_2O_4$ $[M+H]^+$ 537.1661, found 537.1672.

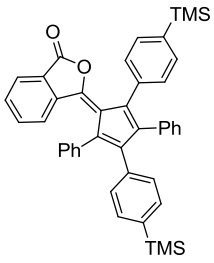
^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.84 – 7.82 (m, 3H), 7.48 – 7.42 (m, 3H), 7.33 – 7.19 (m, 31H), 7.15 – 7.03 (m, 10H), 6.99 – 6.84 (m, 5H), 6.82 – 6.69 (m, 24H), 6.20 (d, *J* = 8.0 Hz, 1H), 6.07 (d, *J* = 8.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 165.32, 165.28, 165.22, 163.16, 163.08, 162.96, 161.62, 161.21, 161.12, 161.01, 152.01, 151.87, 151.79, 147.29, 145.83, 145.63, 145.56, 144.15, 143.92, 137.91, 137.82, 137.45, 135.51, 134.82, 133.97, 133.93, 133.53, 132.99, 132.94, 132.48, 132.41, 132.39, 132.36, 132.35, 131.81, 131.78, 131.69, 131.67, 131.43, 130.88, 130.86, 130.69, 129.48, 128.43, 128.18, 128.08, 128.02, 127.85, 127.72, 127.35, 127.18, 127.09, 127.07, 126.89, 125.97, 125.79, 116.45, 116.28, 115.09, 114.99, 114.93, 114,84, 114.83, 114.77, 114.68; HRMS(ESI) calcd for $C_{37}H_{23}F_2O_4$ $[M+H]^+$ 537.1661, found 537.1672.



3-(2,4-bis(4-fluorophenyl)-3,5-bis(4-methoxyphenyl)cyclopenta-2,4-dienylidene)isobenzofuran-1(3*H*)-one

(3s). 70% yield, regioselectivity ratio = 3:2; ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.84 (t, *J* = 7.0 Hz, 6.4, 1H), 7.46 – 7.42 (m, 1H), 7.23 – 7.12 (m, 7H), 7.00 – 6.96 (m, 3H), 6.85 – 6.58 (m, 15H), 6.22 – 6.17 (m, 1H), 3.83 (s, 3H), 3.75 (s, 2H), 3.72 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 165.45, 165.44, 165.38, 163.50, 163.06, 162.97, 162.85, 161.50, 161.12, 161.01, 160.89, 159.50, 158.84, 158.81, 158.70, 158.67, 151.27, 151.26, 150.77, 147.17, 146.99, 145.49, 145.24, 144.27, 137.98, 137.94, 137.88, 134.17, 133.98, 133.88, 133.80, 133.03, 132.97, 132.77, 132.56, 132.53, 132.47, 132.41, 132.39, 132.01, 131.97, 131.94, 131.90, 131.72, 131.61, 131.54, 131.49, 129.95, 129.91, 129.63, 128.43, 128.13, 128.03, 127.80, 127.70, 127.48, 127.44, 126.84, 126.76, 126.73, 125.89, 125.87, 125.75, 116.41, 116.24, 115.07, 114.99, 114.84, 114.81, 114.67, 113.56, 113.44, 113.39, 113.29, 113.24, 55.79, 55.55, 55.49, 55.44. HRMS (ESI) calcd for $C_{39}H_{27}F_2O_4$ $[M+H]^+$ 597.1872, found 597.1902.

^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.81 (d, *J* = 7.6 Hz, 1H), 7.43 – 7.39 (m, 1H), 7.18 – 7.15 (m, 1H), 7.11 – 7.08 (m, 4H), 6.80 – 6.71 (m, 12H), 6.18 (d, *J* = 8.2 Hz, 1H), 3.81 (s, 3H), 3.80 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 165.53, 159.50, 158.73, 151.79, 145.31, 144.07, 138.08, 134.21, 133.97, 132.42, 132.37, 131.98, 131.57, 129.97, 129.66, 128.55, 126.85, 125.75, 115.08, 114.93, 114.91, 114.76, 113.58, 55.82, 55.59; HRMS(ESI) calcd for $C_{39}H_{27}F_2O_4$ $[M+H]^+$ 597.1872, found 597.1902.

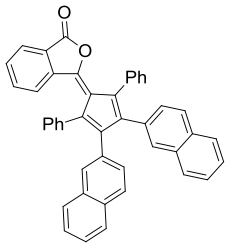


3-(2,4-diphenyl-3,5-bis(4-(trimethylsilyl)phenyl)cyclopenta-2,4-dienylidene)isobenzofuran-1(3*H*)-one (3t)

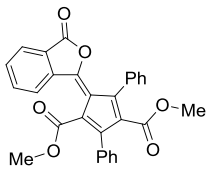
87% yield, regioisomer ratio = 2:1; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.80 (d, *J* = 7.6 Hz, 1H), 7.40 (t, *J* = 7.9 Hz, 5H), 7.29 – 7.21 (m, 4H), 7.12 – 7.00 (m, 7H), 6.91 – 6.90 (m, 2H), 6.82 (d, *J* = 7.1 Hz, 2H), 5.91 (d, *J* = 8.2 Hz, 1H), 0.29 (s, 18H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 165.41, 151.71, 146.81, 145.40, 139.62, 138.41, 138.32, 138.08, 137.96, 135.82, 135.50, 134.61, 134.22, 133.57, 132.86, 131.67, 131.43, 130.83, 130.26, 128.52, 127.78, 127.59, 127.06, 126.88, 125.58, -0.51, -0.55; HRMS(ESI) calcd for $C_{43}H_{41}O_2Si_2$ $[M+H]^+$

645.2640, found 645.2656.

^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.82 (d, *J* = 7.6 Hz, 1H), 7.41 (t, *J* = 7.5 Hz, 1H), 7.27 – 7.20 (m, 10H), 7.21 (d, *J* = 7.9 Hz, 2H), 7.13 (d, *J* = 7.8 Hz, 3H), 6.84 (d, *J* = 7.8 Hz, 2H), 6.78 (d, *J* = 7.8 Hz, 2H), 6.07 (d, *J* = 8.2 Hz, 1H), 0.22 (s, 9H), 0.19 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 165.46, 151.52, 147.19, 145.40, 138.93, 138.71, 138.14, 138.09, 137.73, 136.09, 135.72, 134.52, 133.82, 132.59, 132.46, 131.55, 131.47, 131.41, 131.02, 130.30, 129.98, 129.94, 129.30, 128.41, 127.93, 127.47, 126.86, 126.81, 125.68, -0.66, -0.68; HRMS(ESI) calcd for $C_{43}H_{41}O_2Si_2$ $[M+H]^+$ 645.2640, found 645.2656.

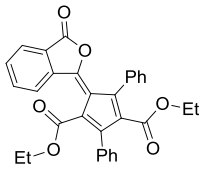


3-(3,4-Di(naphthalen-2-yl)-2,5-diphenylcyclopenta-2,4-dienylidene)isobenzofuran-1(3*H*)-one (3u). 76% yield, regioselectivity ratio > 19:1; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.85 (d, *J* = 1.5 Hz, 1H), 7.70 (d, *J* = 8.1 Hz, 1H), 7.65 (d, *J* = 8.2 Hz, 1H), 7.51 – 7.21 (m, 21H), 7.14 (t, *J* = 7.5, 1H), 7.01 (dd, *J* = 8.5, 1.5 Hz, 1H), 6.97 – 6.95 (m, 1H), 6.11 (d, *J* = 8.2 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 165.43, 151.87, 146.70, 144.98, 138.06, 138.04, 137.65, 135.20, 133.90, 133.39, 133.21, 133.17, 133.03, 132.54, 132.45, 132.16, 131.56, 131.00, 130.22, 130.15, 130.11, 129.44, 128.76, 128.74, 128.52, 128.08, 127.95, 127.87, 127.61, 127.18, 126.99, 126.97, 126.87, 126.24, 126.13, 126.10, 125.96, 125.76; HRMS(ESI) calcd for $C_{45}H_{29}O_2$ $[M+H]^+$ 601.2162, found 601.2175.



Diethyl 4-(3-oxoisobenzofuran-1(3*H*)-ylidene)-3,5-diphenylcyclopenta-2,5-diene-1,2-dicarboxylate (3v). 69% yield, regioisomer ratio > 19:1; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.97 (dd, *J* = 5.6, 3.1 Hz, 2H), 7.79 (dd, *J*

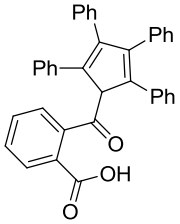
= 5.7, 3.1 Hz, 2H), 7.45 – 7.39 (m, 5H), 7.15 – 7.10 (m, 3H), 7.05 (dd, *J* = 8.1, 1.4 Hz, 2H), 3.40 (s, 3H), 3.34 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 195.04, 164.45, 163.26, 160.01, 153.57, 143.92, 141.19, 136.25, 133.95, 132.70, 132.31, 129.43, 129.11, 128.87, 128.71, 128.31, 128.04, 124.52, 52.21, 52.01; HRMS(ESI) calcd for $C_{29}H_{21}O_6$ $[M+H]^+$ 465.1333, found 465.1339.



Diethyl 4-(3-oxoisobenzofuran-1(3*H*)-ylidene)-3,5-diphenylcyclopenta-2,5-diene-1,2-dicarboxylate (3w). 73% yield, regioisomer ratio > 19:1; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.97 (d, *J* = 5.7, 3.1 Hz, 2H), 7.78 (dd, *J* = 5.7, 3.0 Hz, 2H), 7.47 – 7.45 (m, 2H), 7.40 – 7.32 (m, 3H), 7.15 – 7.10 (m, 3H), 7.08 – 7.06 (m, 2H), 3.88 (q, *J* = 7.1 Hz, 2H), 3.80 (q, *J* = 7.1 Hz, 2H), 0.77 (t, *J* = 7.1 Hz, 3H), 0.66 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 195.16, 163.77, 162.42, 160.33, 153.56, 144.00, 141.34, 136.19, 134.21, 132.89, 132.45, 130.82, 129.70, 129.32, 129.29, 128.92, 128.89, 128.59, 128.39, 127.91, 127.87, 124.45, 61.26, 60.97, 13.82, 13.51; HRMS(ESI) calcd for $C_{31}H_{25}O_6$ $[M+H]^+$ 493.1646, found 493.1650.

Synthetic transformations of 3a

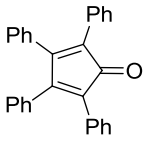
Compound 4



2-(2,3,4,5-Tetraphenylcyclopenta-2,4-dienecarbonyl)benzoic acid (4). 95% yield; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 10.72 (broad s, 1H), 7.70 (d, *J* = 7.4 Hz, 1H), 7.43 (d, *J* = 7.7 Hz, 2H), 7.32 – 7.29 (m, 2H), 7.19 – 7.04 (m, 13H), 6.96 – 6.91 (m, 6H), 5.55 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 191.93, 171.95, 158.80, 154.09, 145.41, 144.53, 144.14, 137.53, 135.32, 134.94, 134.57, 132.33, 130.70, 130.45, 129.68, 129.57, 128.91,

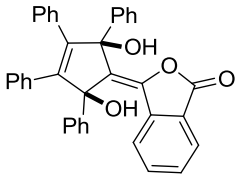
128.83, 128.62, 128.42, 128.28, 128.11, 128.05, 128.00, 127.94, 127.60, 127.55, 127.48, 127.04, 60.74; HRMS(ESI) calcd for $C_{37}H_{27}O_3$ $[M+H]^+$ 519.1926, found 519.1941.

Compound 5



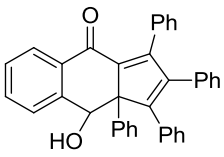
2,3,4,5-Tetraphenylcyclopenta-2,4-dienone (5). 67% yield; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.26 – 7.22 (m, 11H), 7.18 (t, *J* = 7.6 Hz, 4H), 6.93 (d, *J* = 7.6 Hz, 4H), 6.85 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 200.82, 154.97, 133.57, 131.90, 131.24, 130.88, 130.63, 129.81, 128.97, 128.85, 128.82, 128.50, 128.46, 127.93, 127.05, 126.34, 125.81; HRMS(ESI) calcd for $C_{29}H_{21}O$ $[M+H]^+$ 385.1587, found 385.1592.

Compound 6



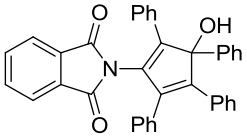
(*Z*)-3-((2*R*,5*S*)-2,5-dihydroxy-2,3,4,5-tetraphenylcyclopent-3-enylidene)isobenzofuran-1(3*H*)-one (6). 51% yield; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.83 (d, *J* = 7.6 Hz, 1H), 7.79 (d, *J* = 7.7 Hz, 1H), 7.67 (t, *J* = 7.5 Hz, 1H), 7.58 – 7.55(m, 3H),7.29 – 7.20 (m, 4H), 7.17 – 7.12 (m, 4H), 7.08 – 7.04 (m, 3H), 6.99 – 6.97 (m, 2H), 6.88 (s, 5H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 165.81, 148.09, 145.49, 142.58, 142.41, 140.32, 137.05, 134.53, 134.42, 134.05, 133.42, 130.69, 130.53, 130.04, 128.30, 128.06, 127.86, 127.73, 127.69, 127.64, 127.54, 127.01, 126.98, 125.14, 124.68, 87.32, 86.21; HRMS(ESI) calcd for $C_{37}H_{27}O_4$ $[M+H]^-$ 535.1904, found 535.1912.

Compound 7



4-Hydroxy-1,2,3,3a-tetraphenyl-3a*H*-cyclopenta[*b*]naphthalen-9(4*H*)-one (7). 56% yield; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.83 (d, *J* = 7.6 Hz, 1H), 7.79 (d, *J* = 7.7 Hz, 1H), 7.67 (t, *J* = 7.5 Hz, 1H), 7.58 – 7.55(m, 3H),7.29 – 7.20 (m, 4H), 7.17 – 7.12 (m, 4H), 7.08 – 7.04 (m, 3H), 6.99 – 6.97 (m, 2H), 6.88 (s, 5H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 165.81, 148.09, 145.49, 142.58, 142.41, 140.32, 137.05, 134.53, 134.42, 134.05, 133.42, 130.69, 130.53, 130.04, 128.30, 128.06, 127.86, 127.73, 127.69, 127.64, 127.54, 127.01, 126.98, 125.14, 124.68, 87.32, 86.21; HRMS(ESI) calcd for $C_{37}H_{27}O_2$ $[M+H]^+$ 503.2006, found 503.2002.

Compound 8



2-(3-Hydroxy-2,3,4,5-tetraphenylcyclopenta-1,4-dienyl)isoindoline-1,3-dione (8). 62% yield; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.79 – 7.73 (m, 4H), 7.68 – 7.62 (m, 2H), 7.35 – 7.32 (m, 2H), 7.22 – 7.16 (m, 8H), 7.12 – 7.03 (m, 7H), 3.16 (s, 1H), 3.16 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 168.07, 167.51, 152.10, 148.18, 139.67, 138.68, 134.74, 134.71, 134.13, 133.46, 132.23, 132.15, 132.03, 131.19, 129.60, 129.16, 129.12, 129.07, 128.70, 128.67, 128.33, 128.24, 127.80, 127.73, 125.80, 124.26, 124.17, 89.35; HRMS(ESI) calcd for $C_{37}H_{25}NNaO_3$ $[M+Na]^+$ 554.1727, found 554.1726.

8. Reference

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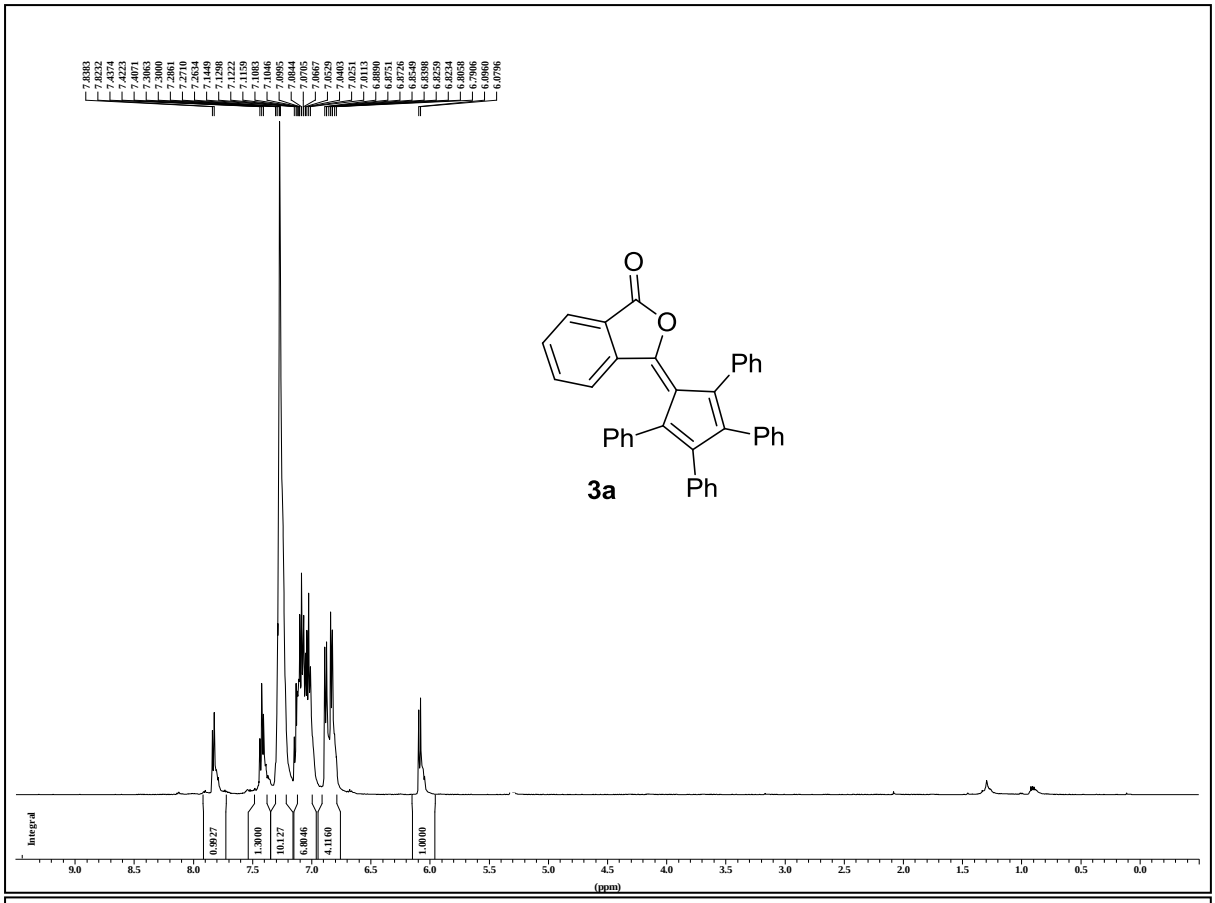
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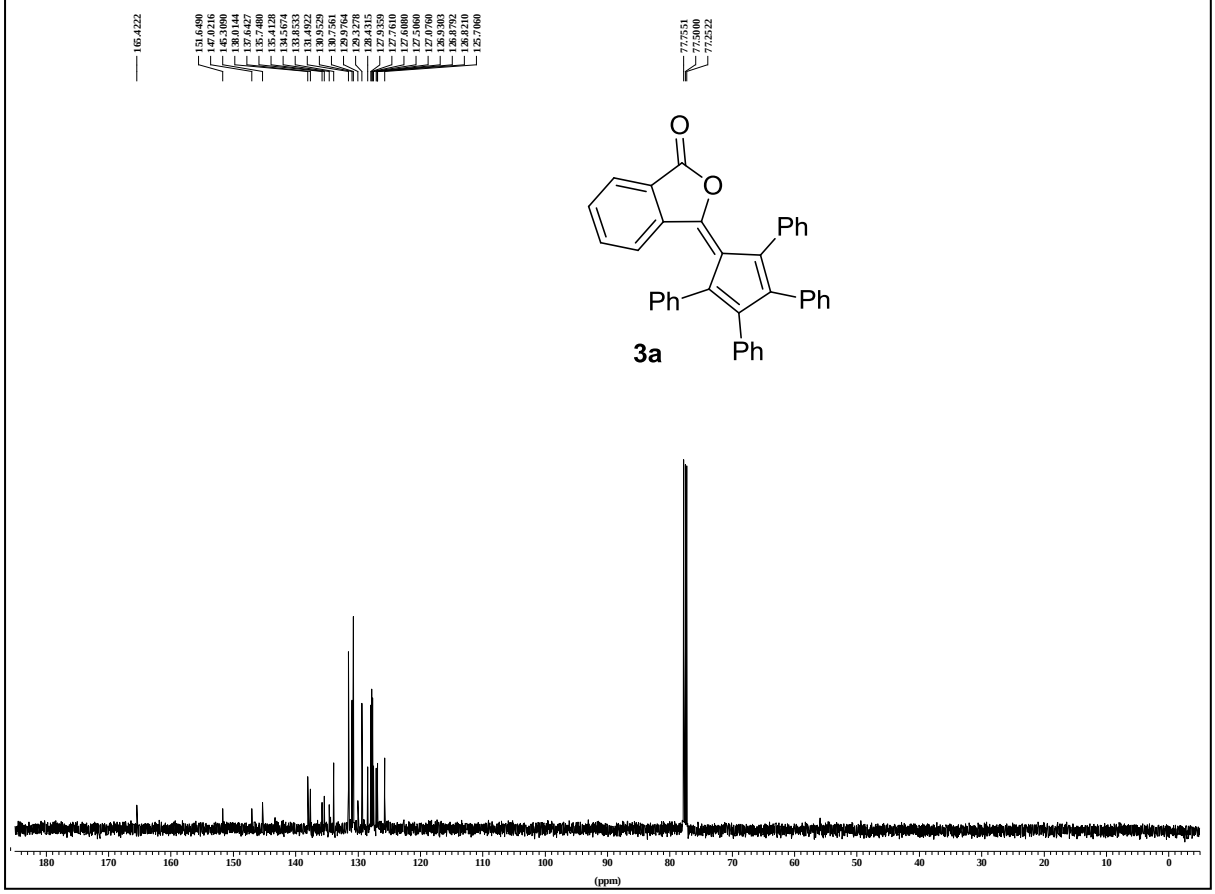
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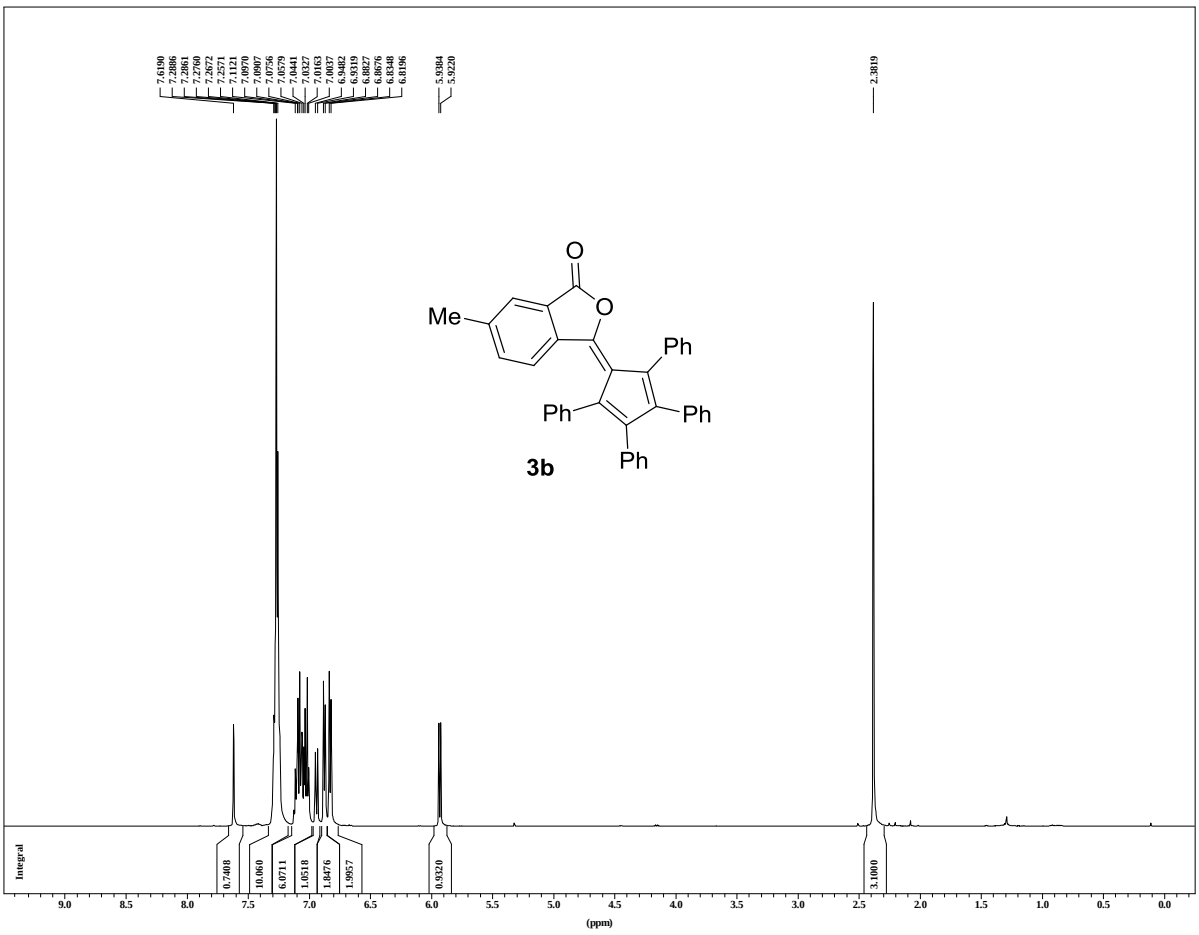
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Ph
Ph
Ph
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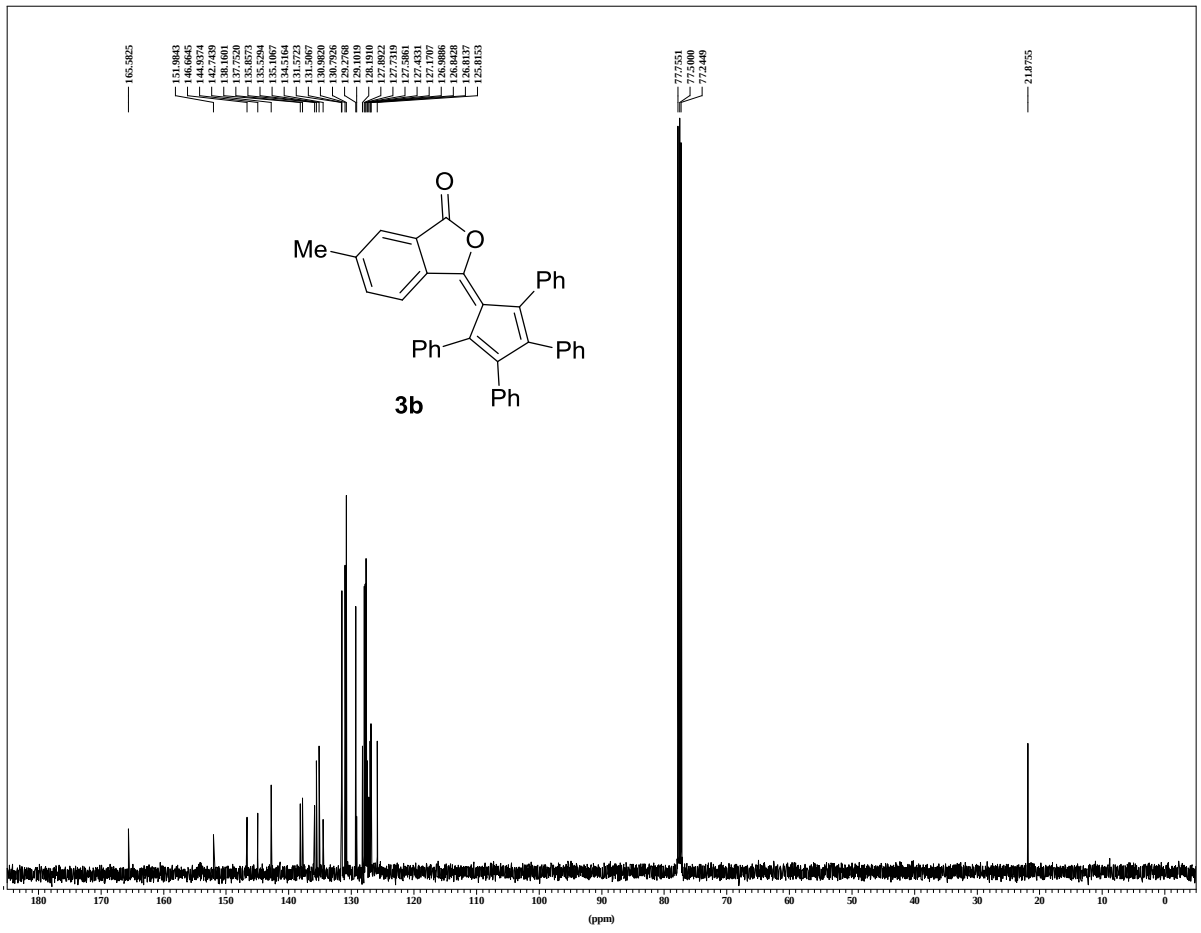
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Ph
Ph
Ph
Ph
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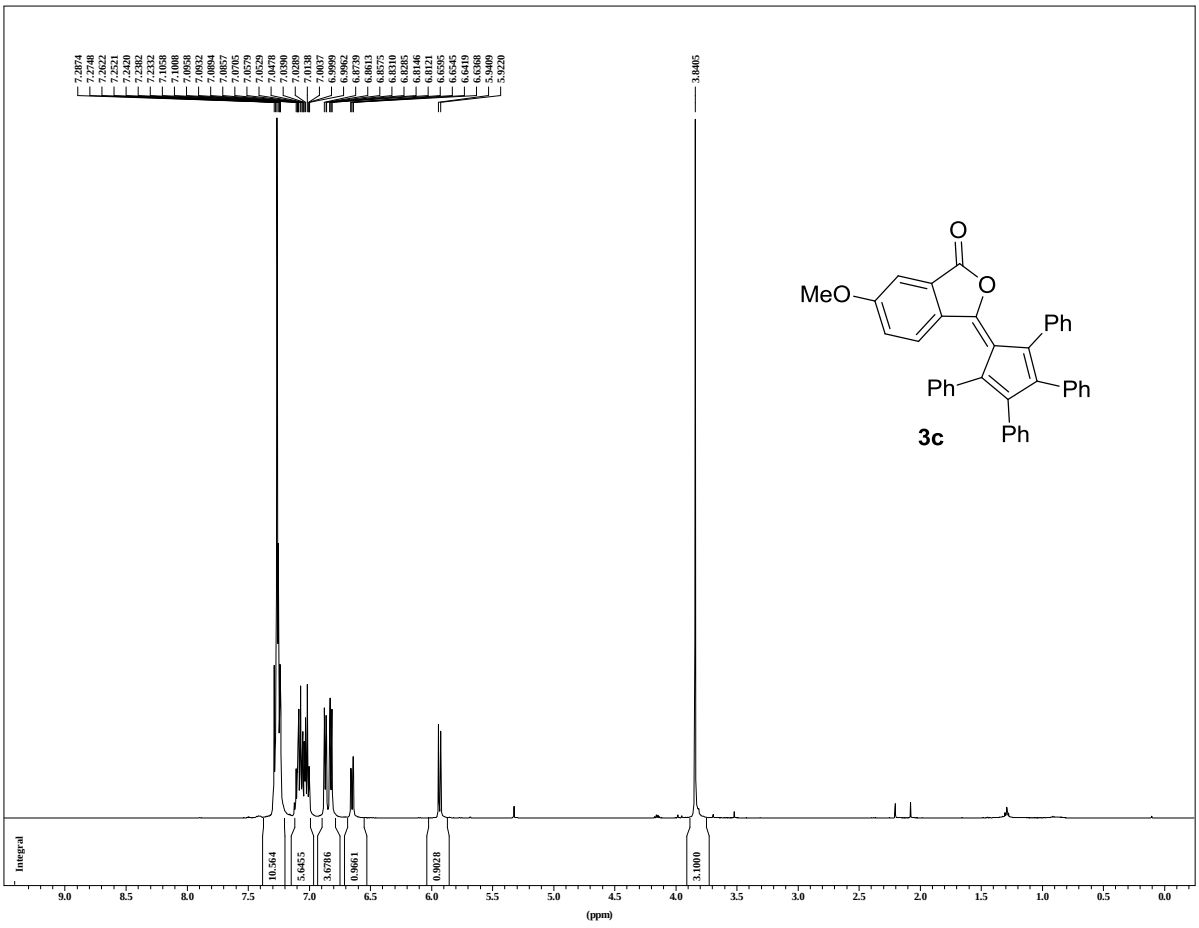
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7.0857
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7.0579
7.0529
7.0478
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7.0087
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6.8575
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5.3220
3.8405
MeO
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O
Ph
Ph
Ph
Ph
3c
Integral
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8.0
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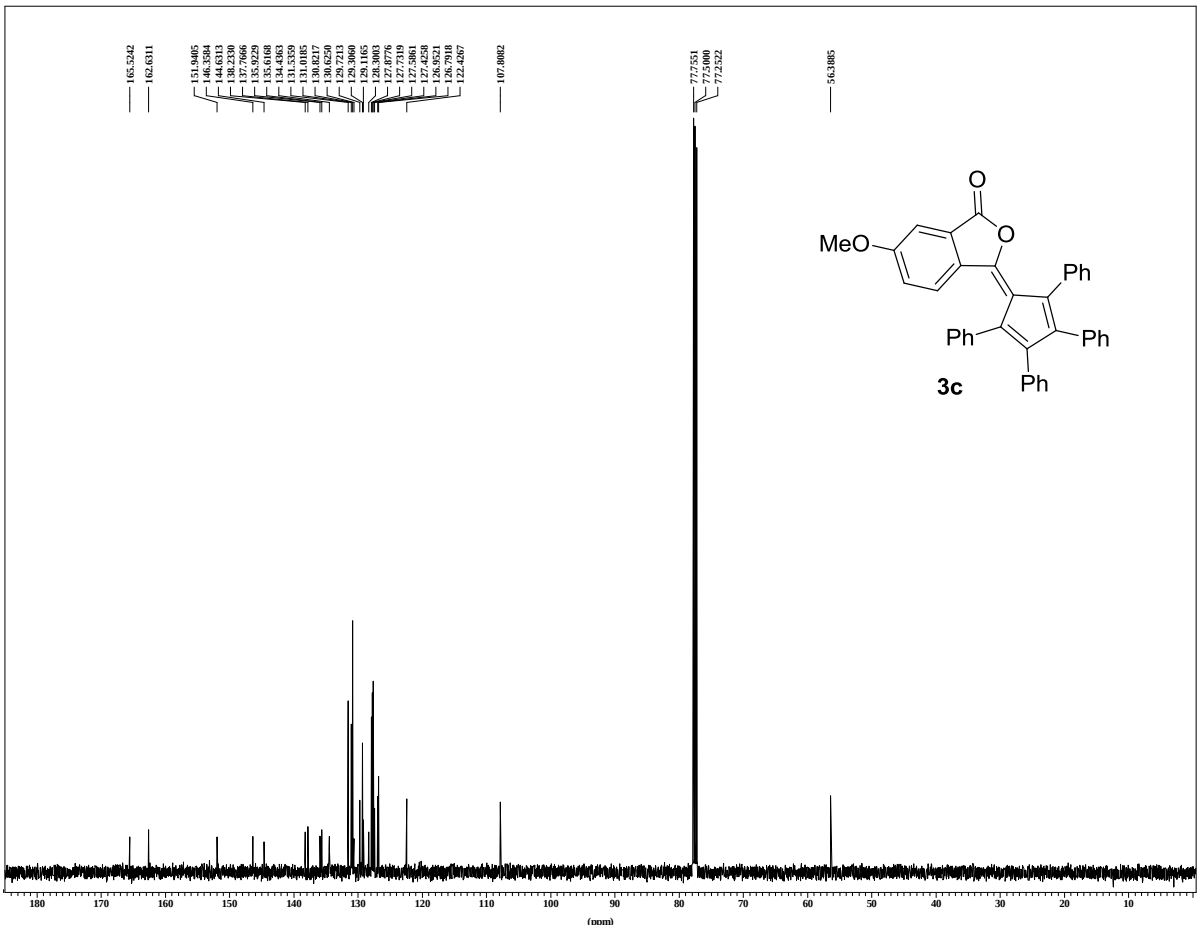
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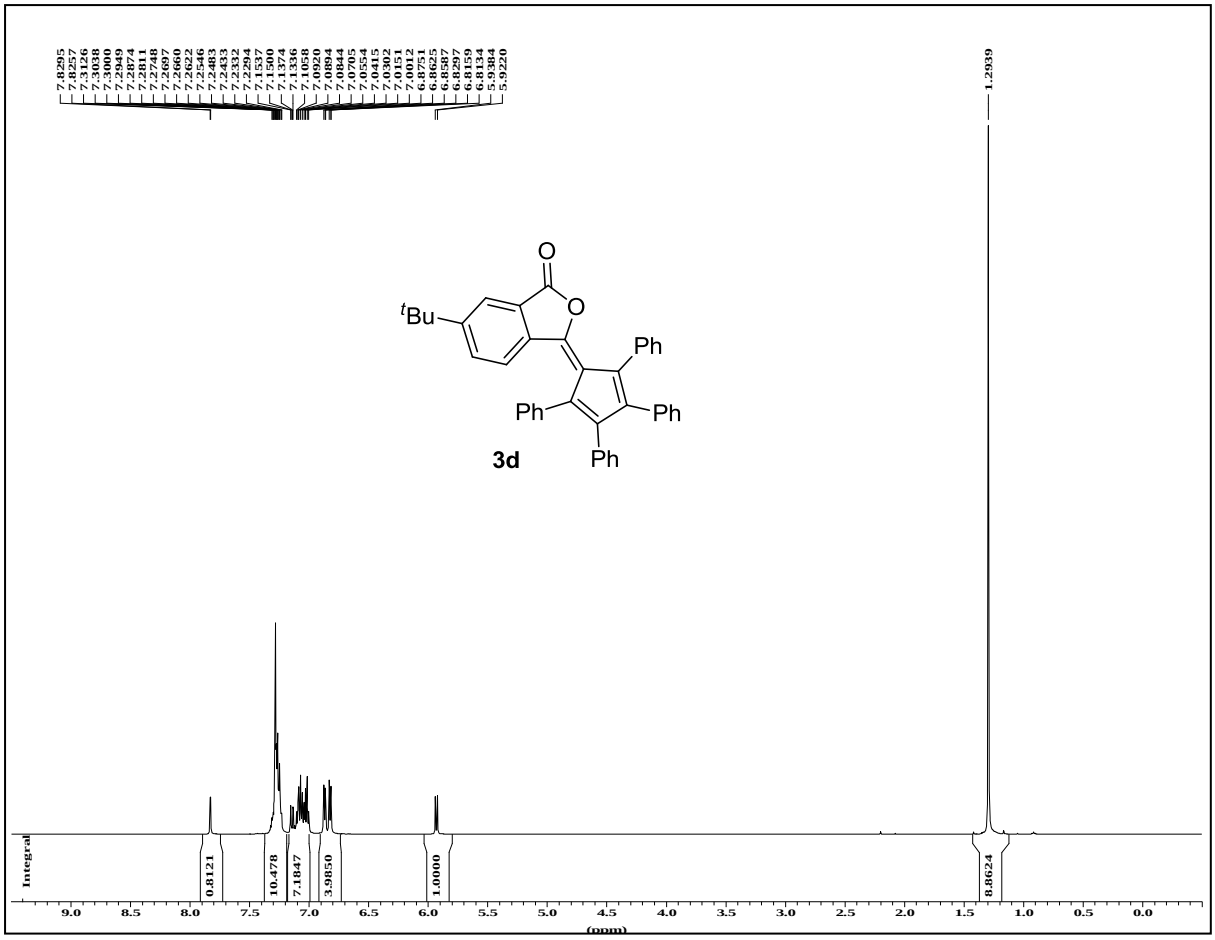
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O
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Ph
Ph
Ph
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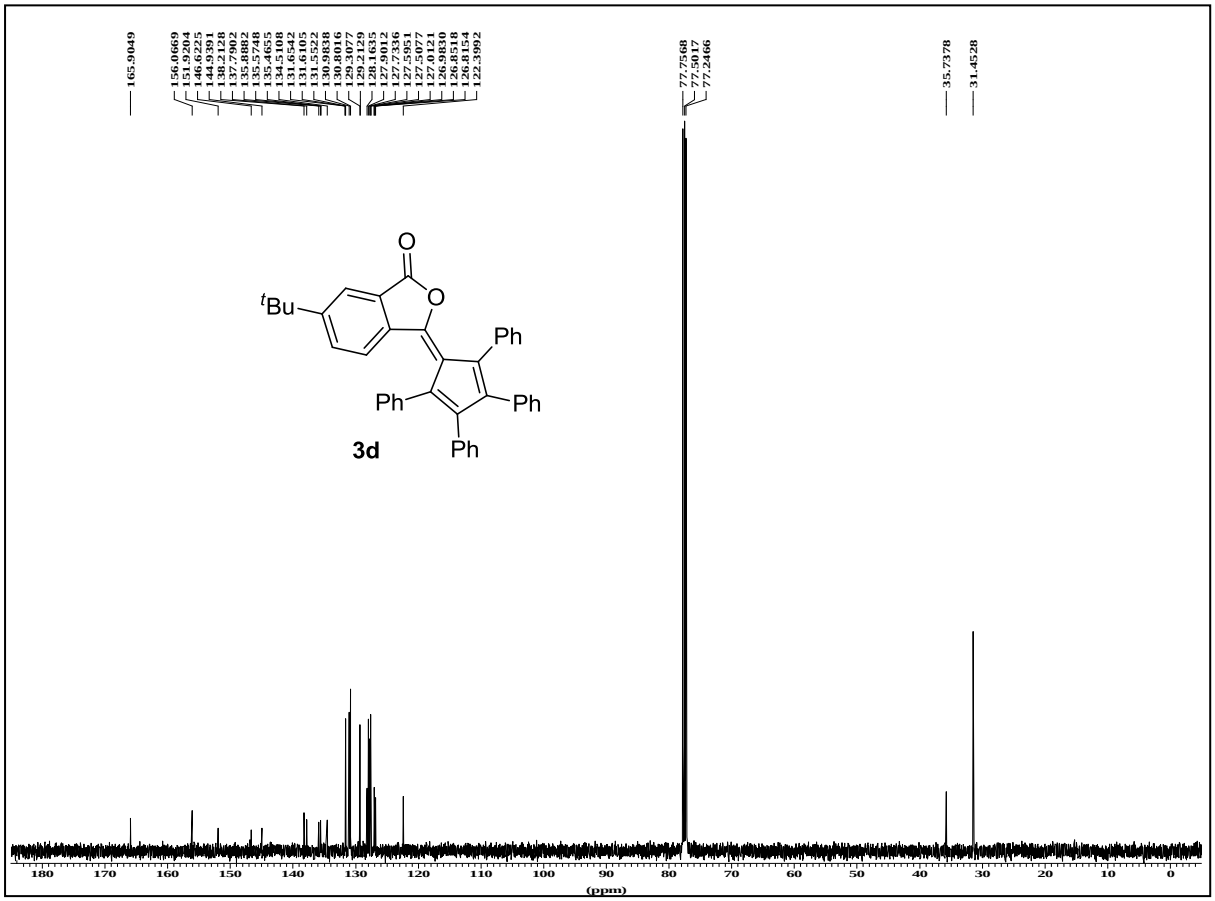
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O
O
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Ph
Ph
Ph
Ph
3d
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100
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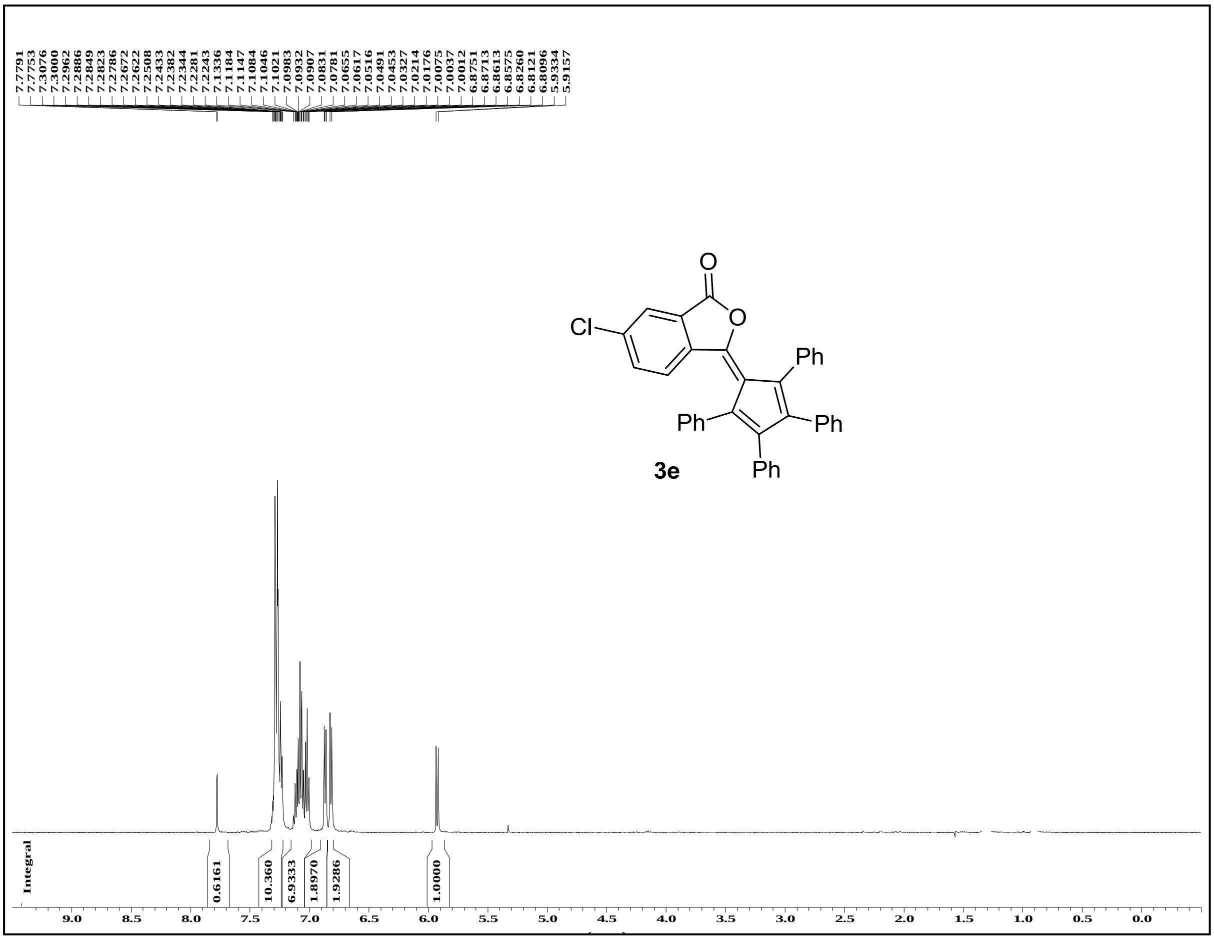
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7.0781
7.0655
7.0617
7.0516
7.0491
7.0453
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5.9157
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O
Cl
Ph
Ph
Ph
Ph
3e
Integral
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1.0000
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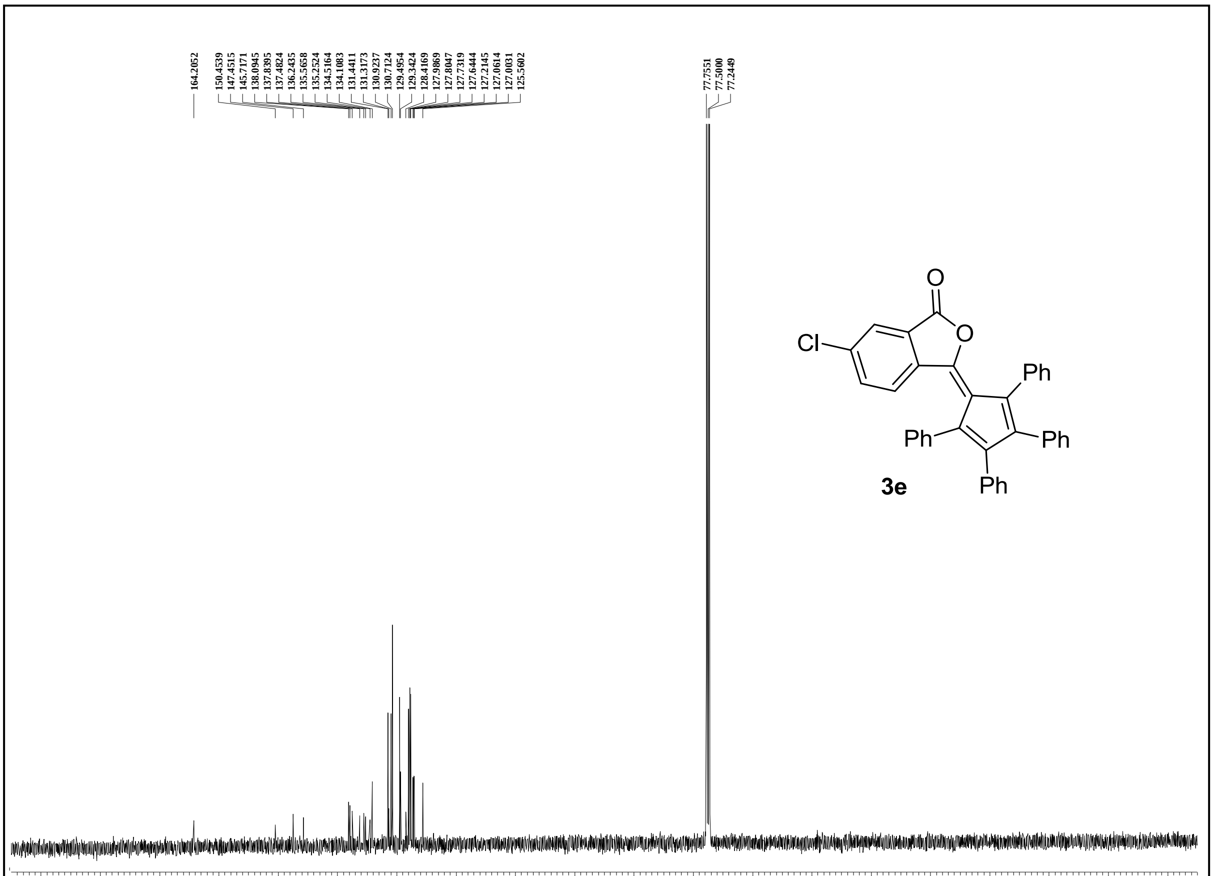
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Cl
Ph
Ph
Ph
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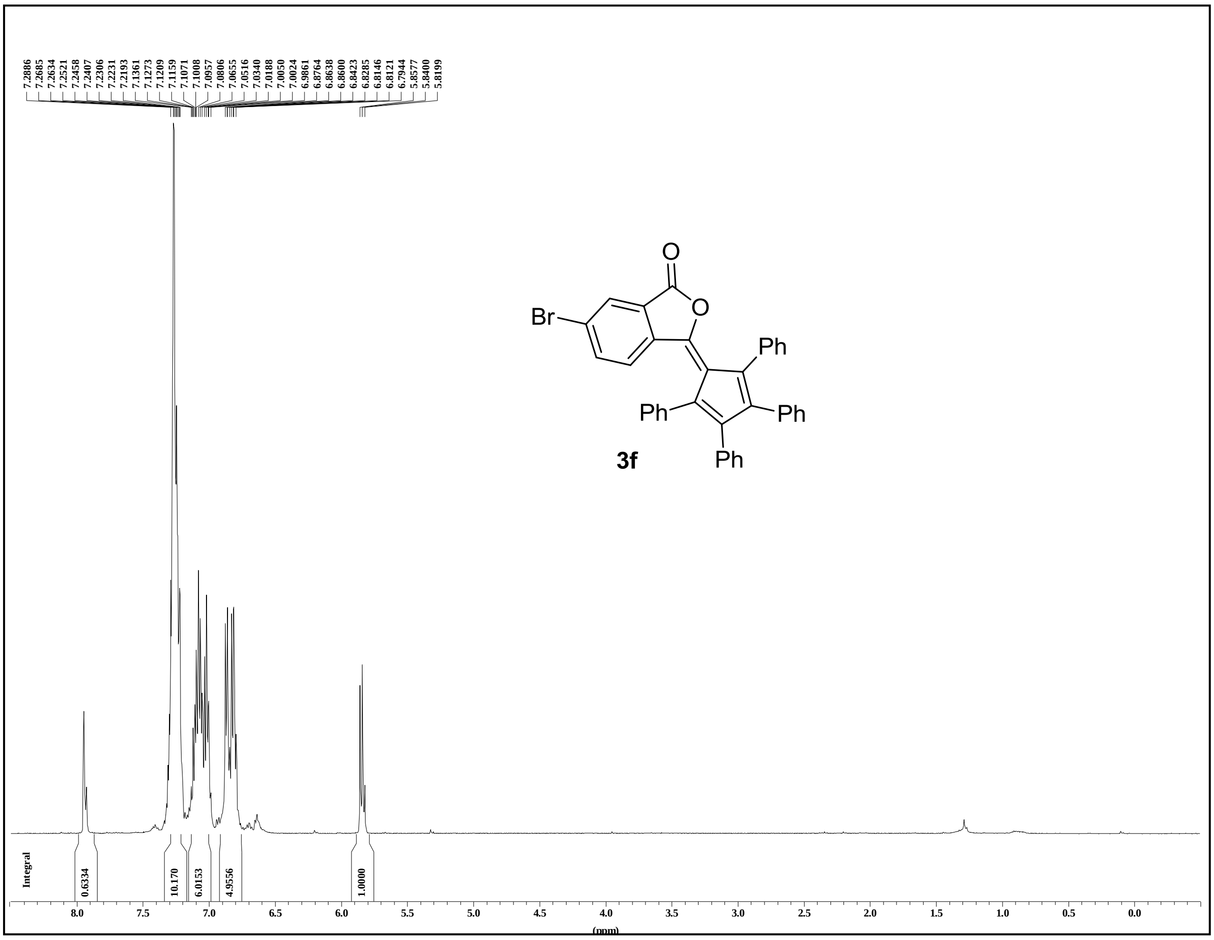
(ppm)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Br
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Ph
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Ph
Ph
3f
Integral
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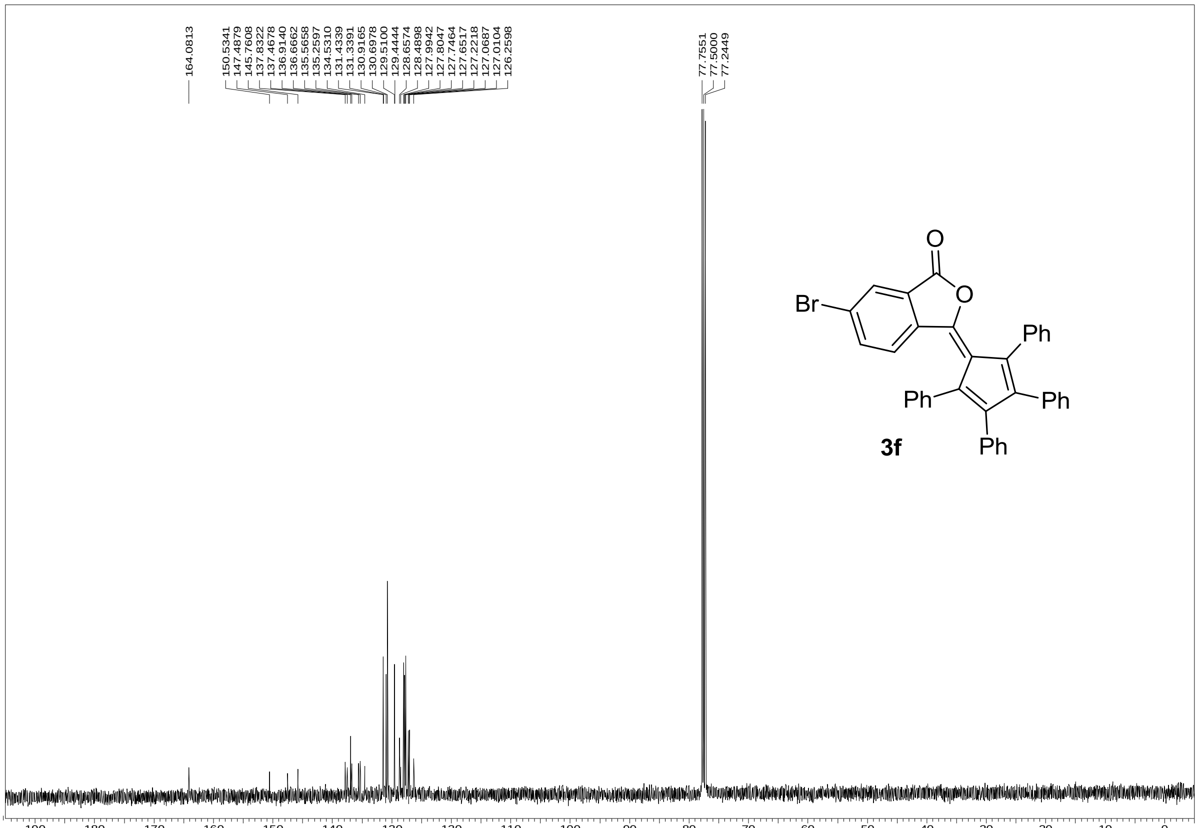
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77.7551 77.5000 77.2449
Br
O
O
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Ph
Ph
Ph
3f
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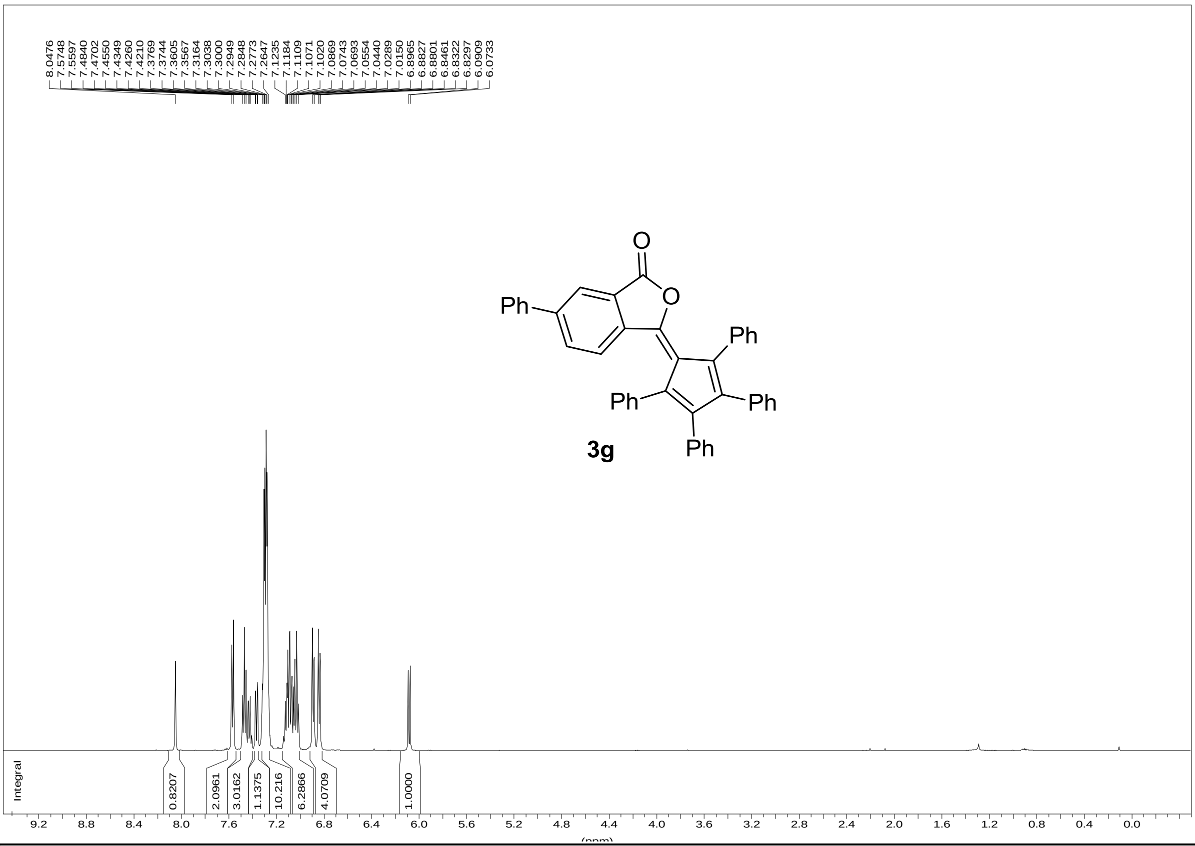

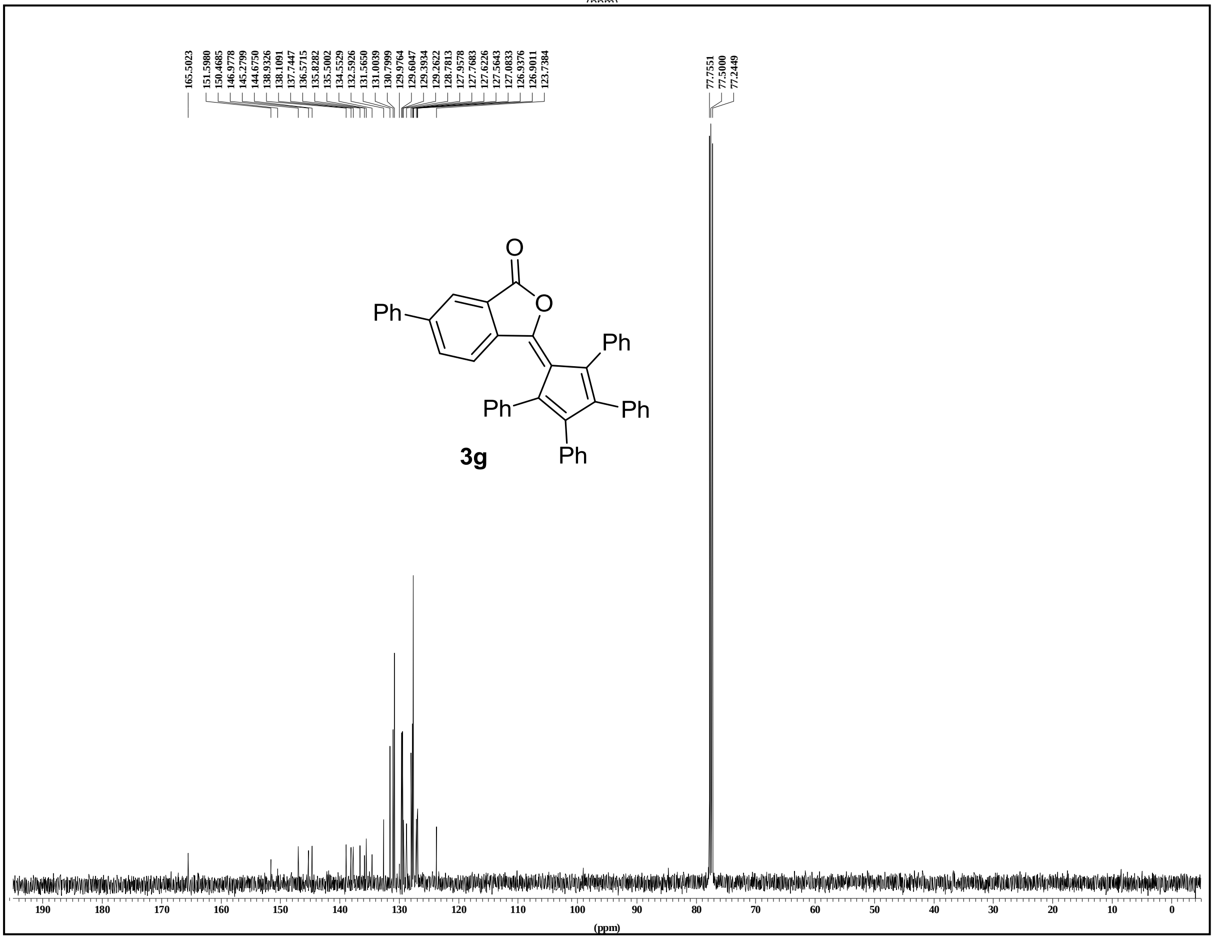

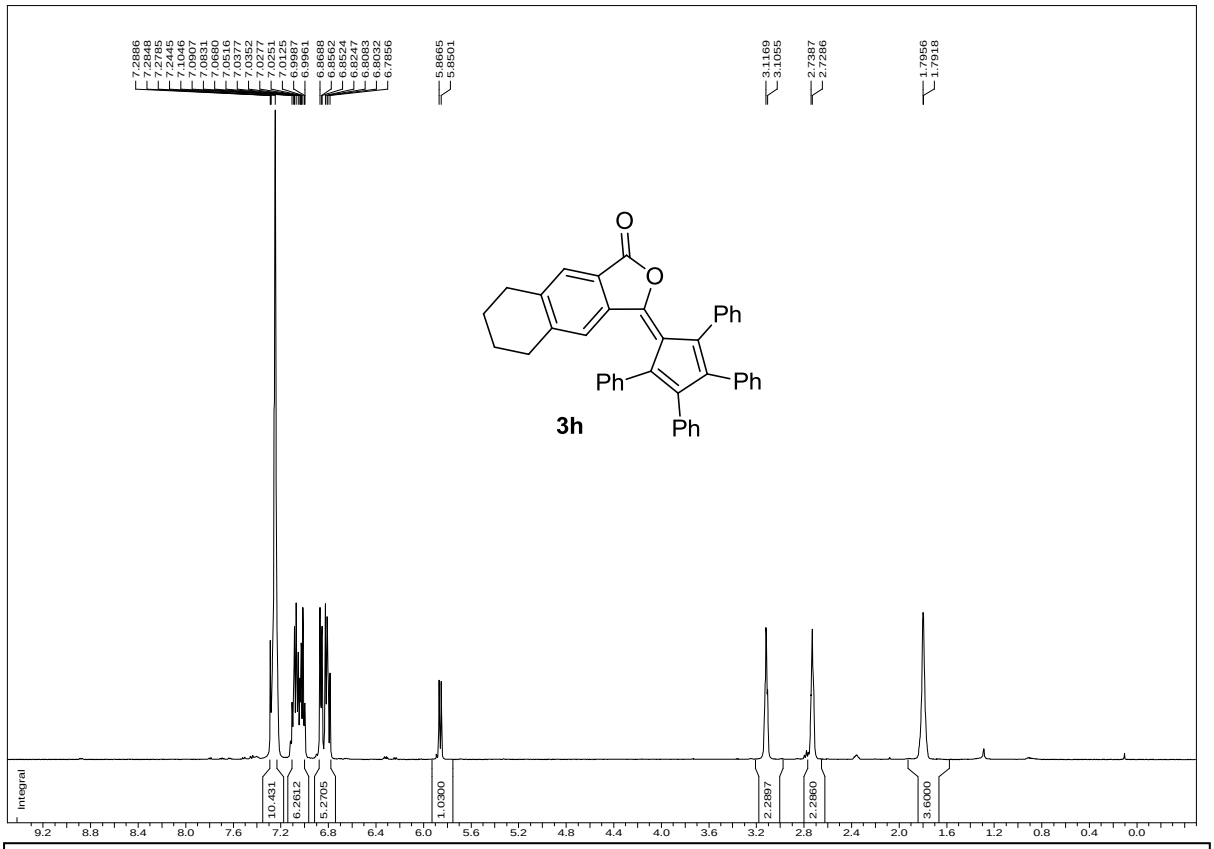
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Ph
Ph
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6.4
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5.6
5.2
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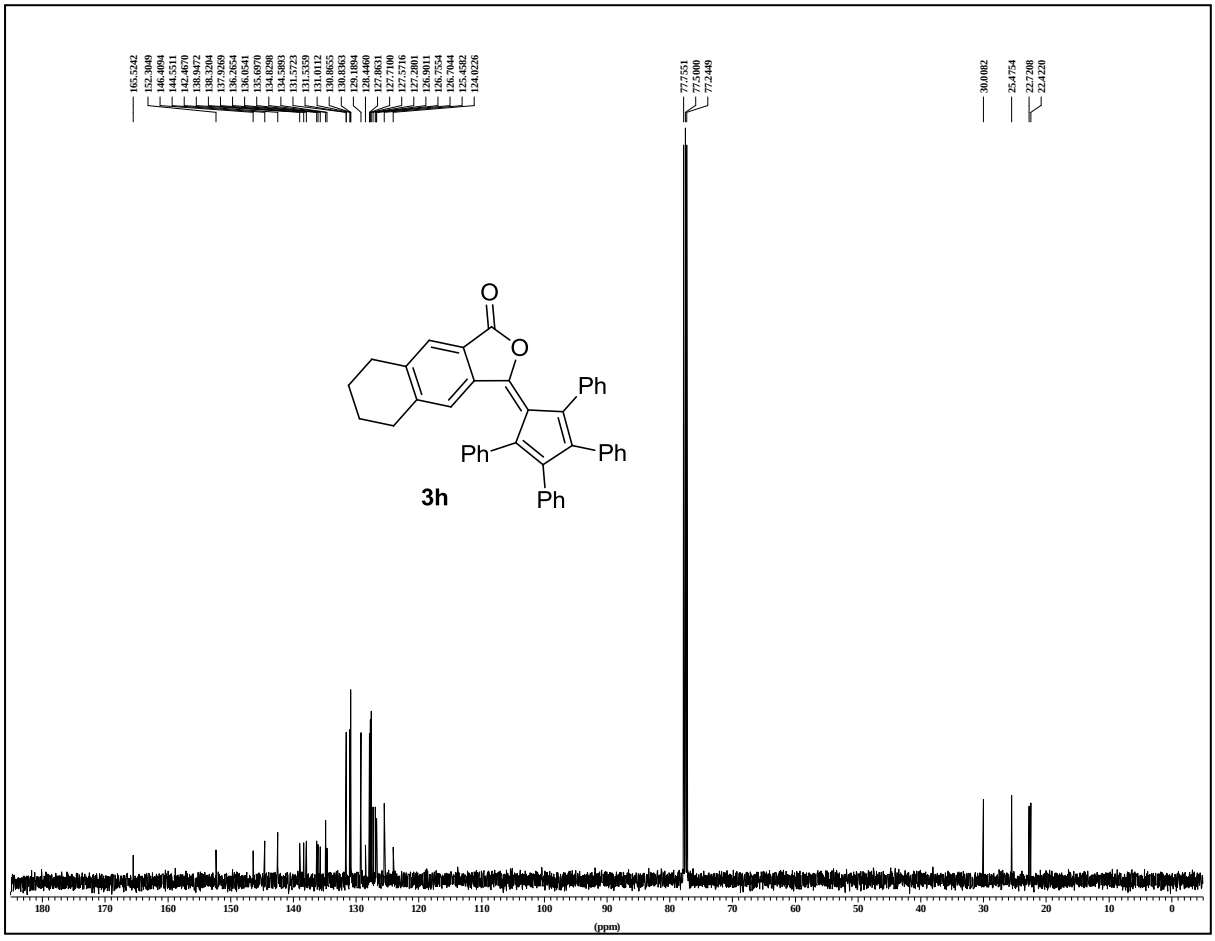
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O
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Ph
Ph
Ph
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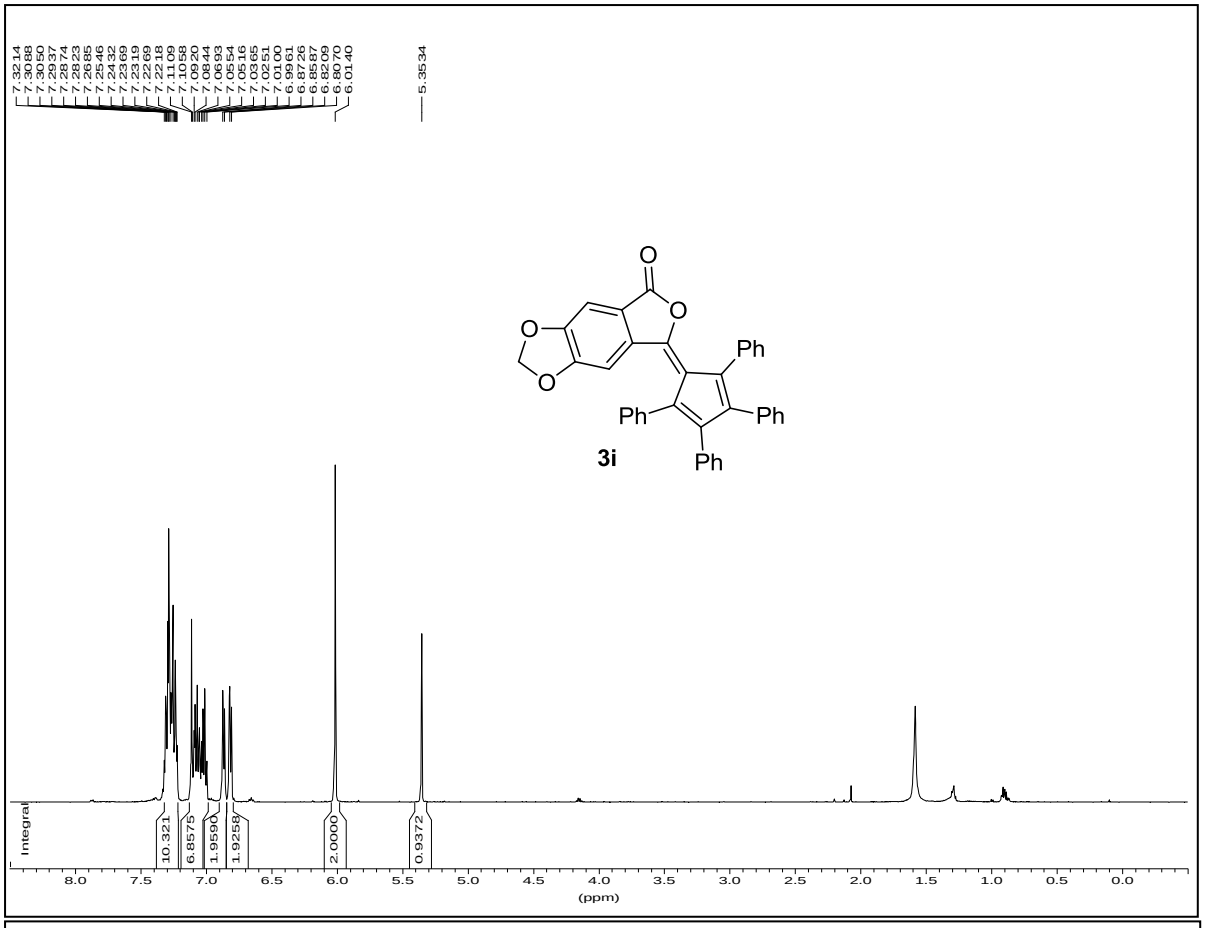
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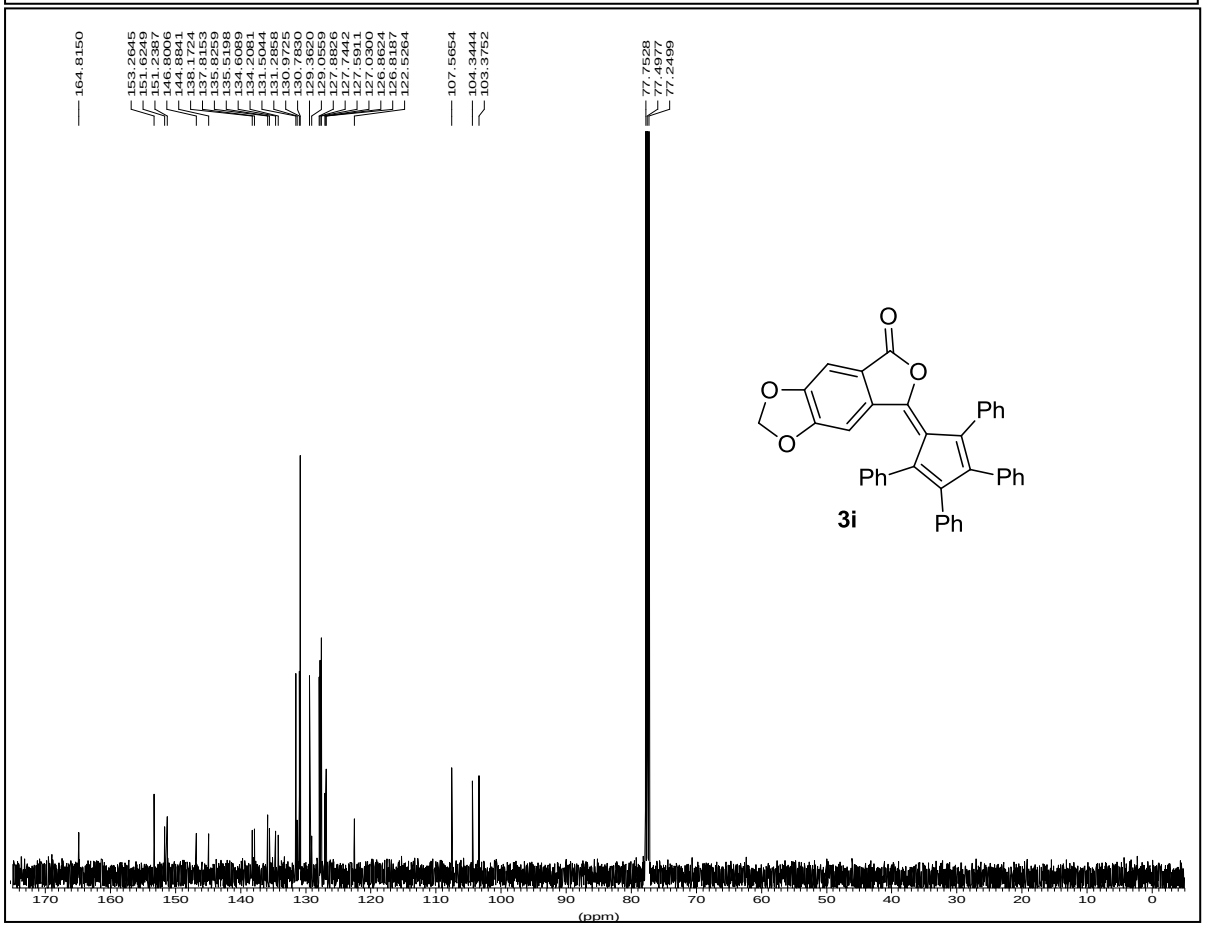
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O
O
Ph
Ph
Ph
Ph
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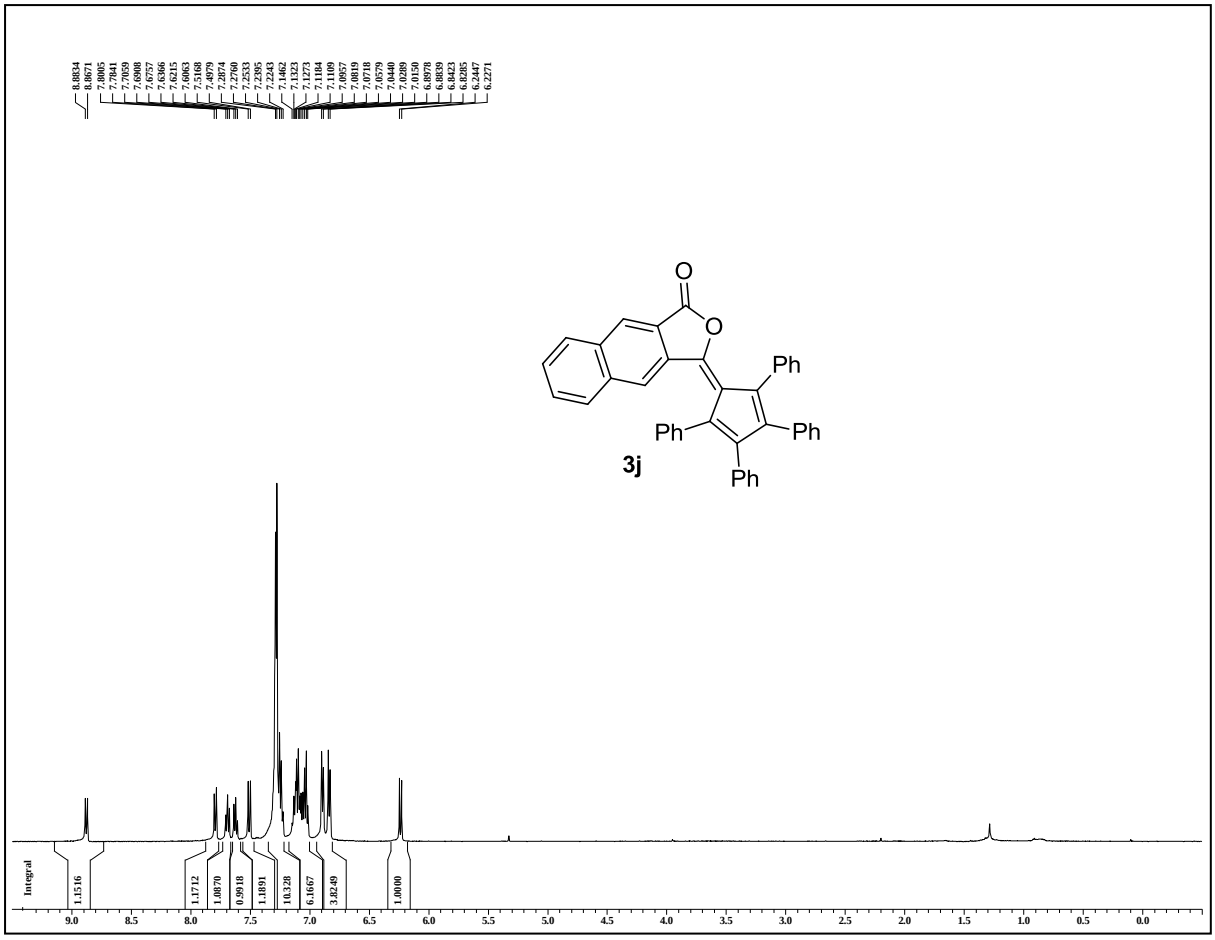
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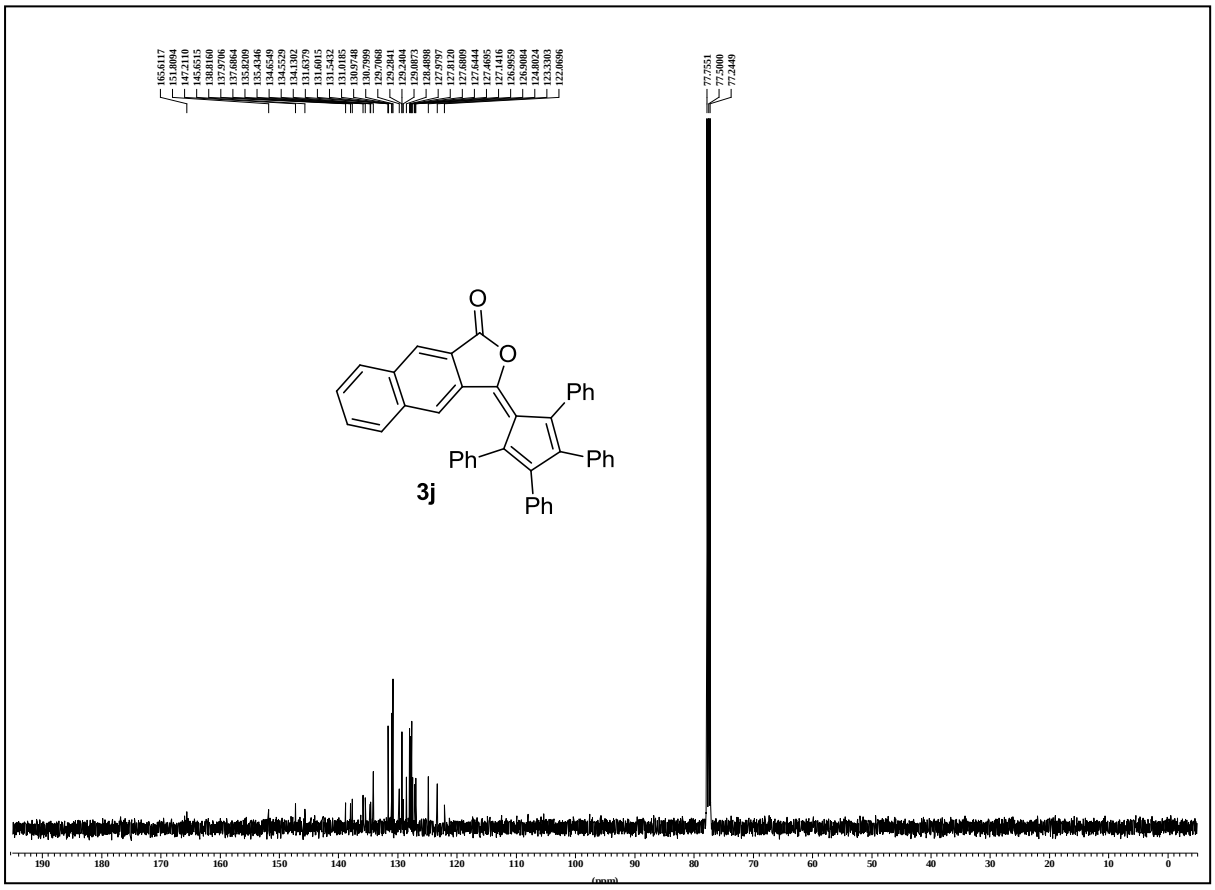
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3j
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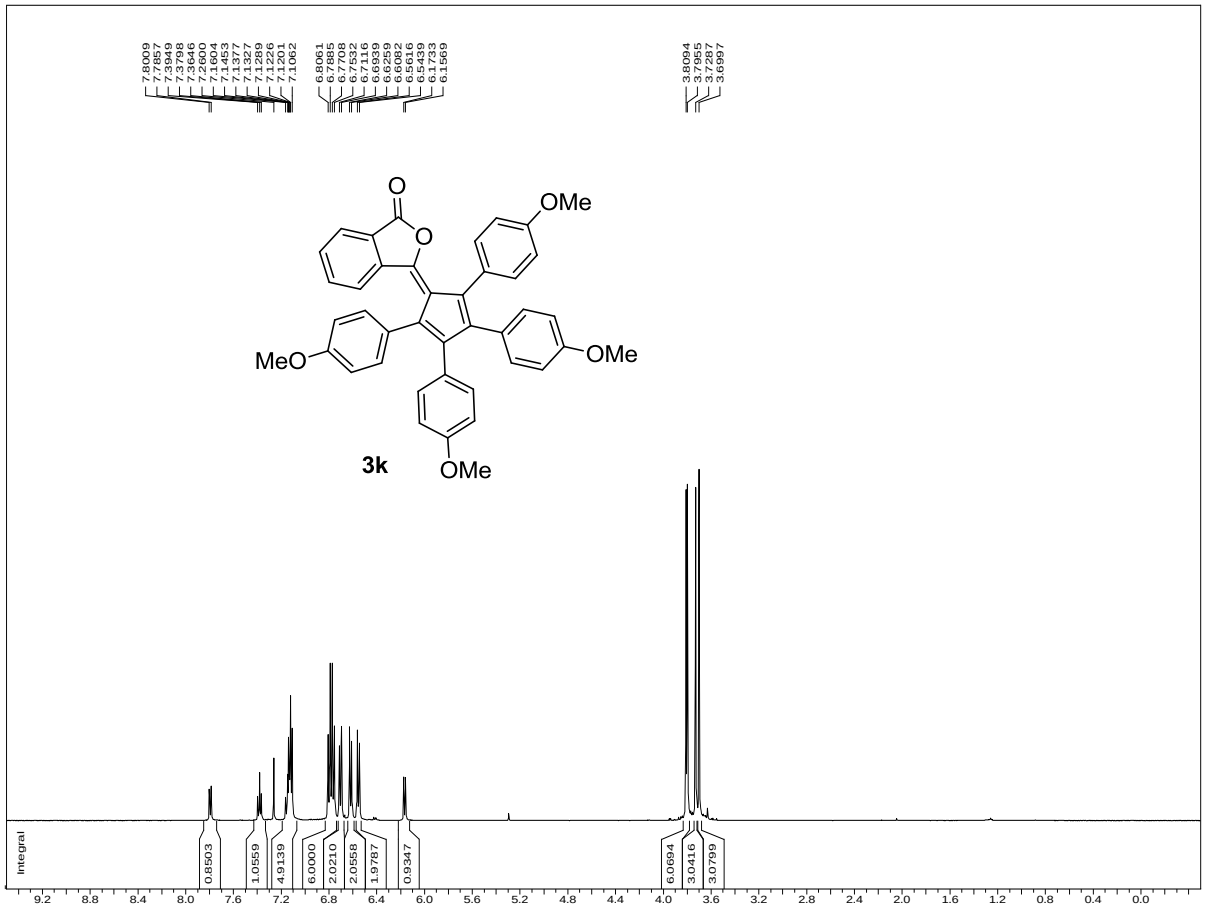
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MeO
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OMe
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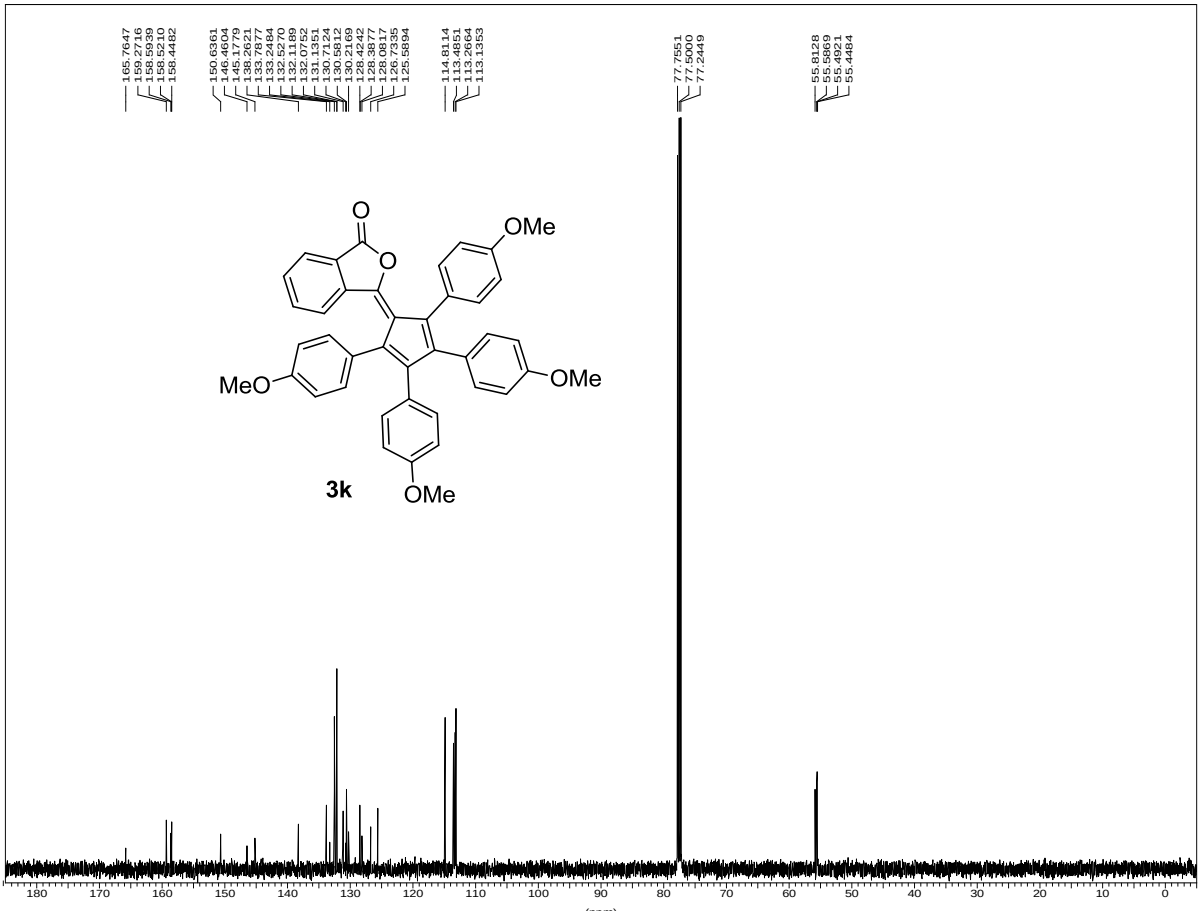
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OMe
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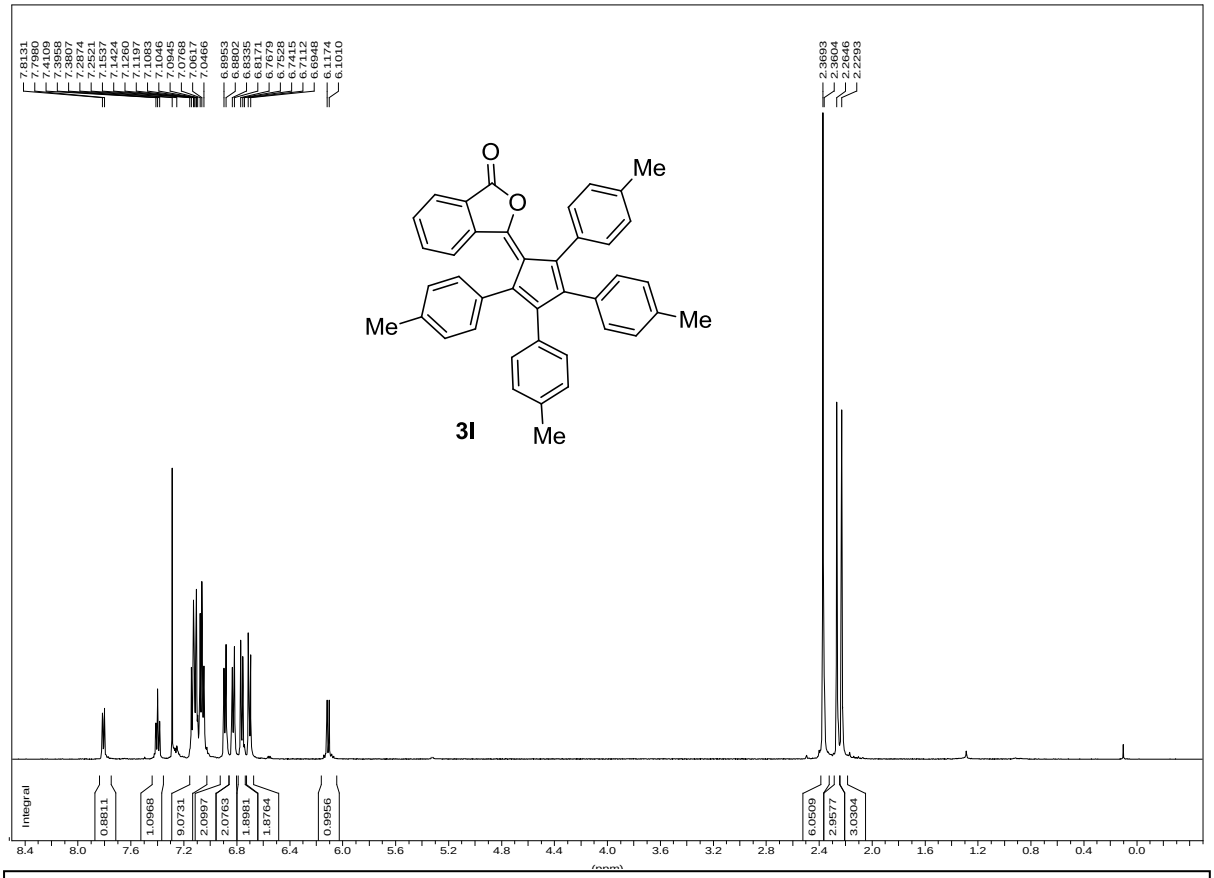
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2.3604
2.2946
2.2293
O
O
Me
Me
Me
Me
3l
Integral
0.8811
1.0968
9.0731
2.0997
2.0763
1.8981
1.8764
0.9956
6.0509
2.9577
3.0304
8.4
8.0
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7.2
6.8
6.4
6.0
5.6
5.2
4.8
4.4
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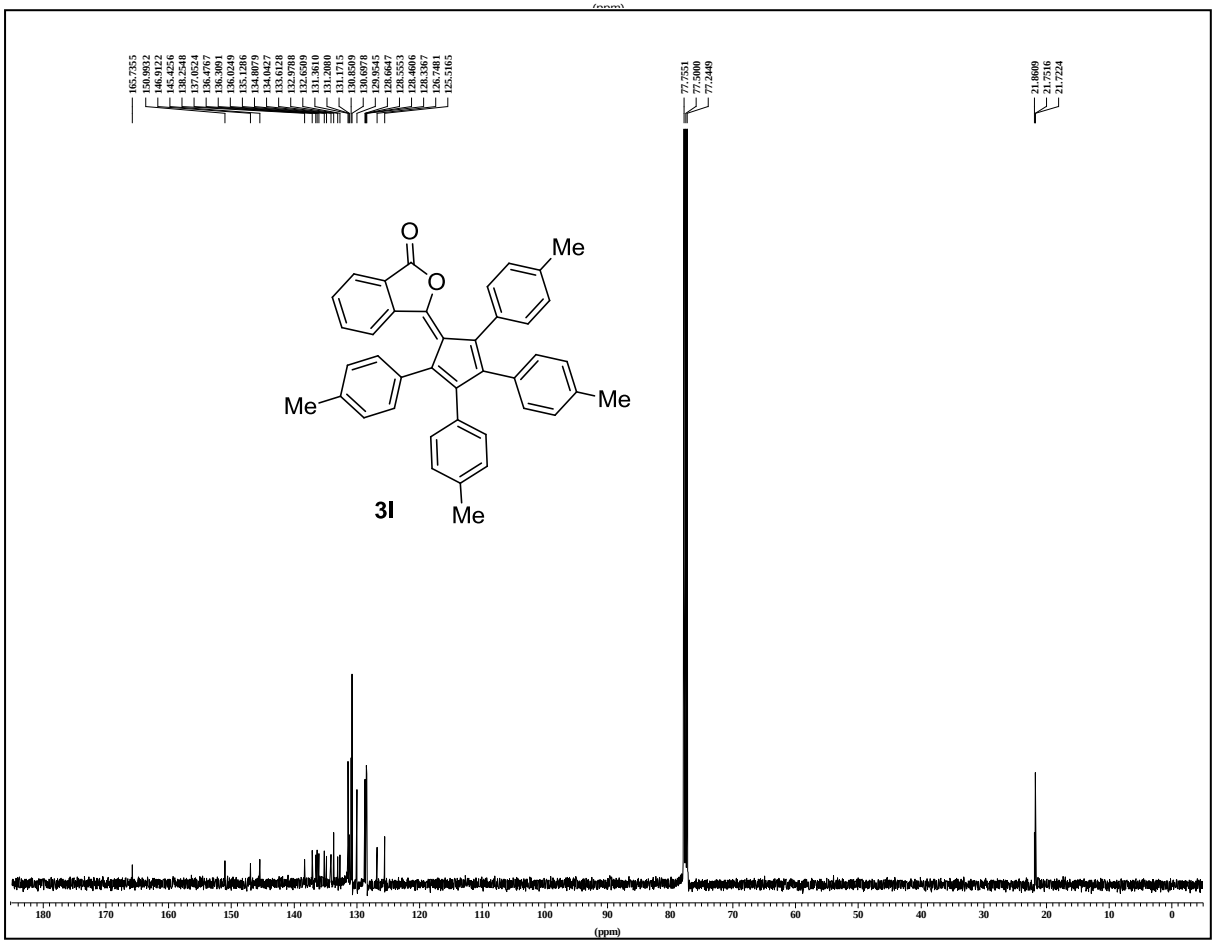
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130.8509
130.6978
129.9545
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128.5553
128.4466
128.3367
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125.5165
77.7551
77.5000
77.2449
21.8609
21.7516
21.7224
O
O
Me
Me
Me
Me
3l
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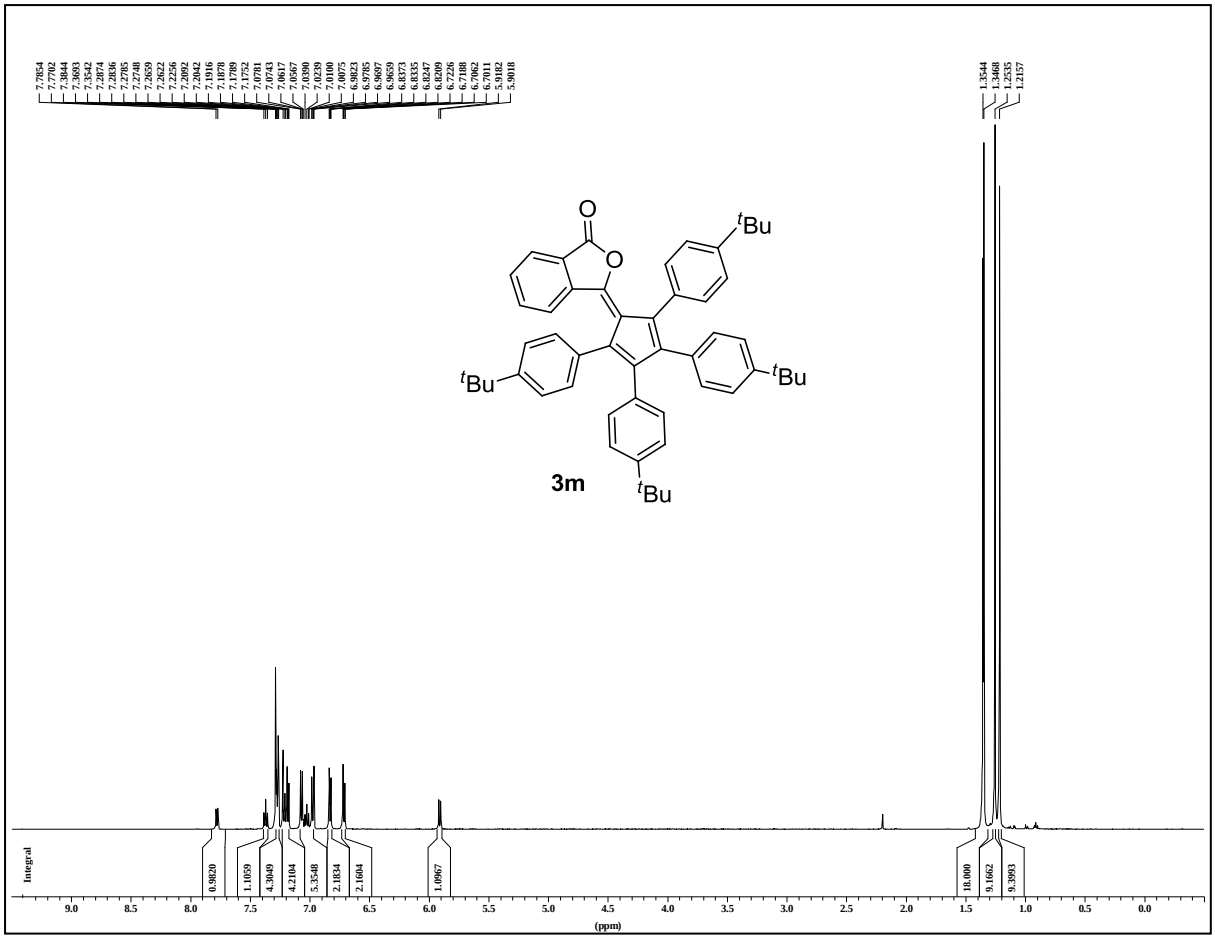
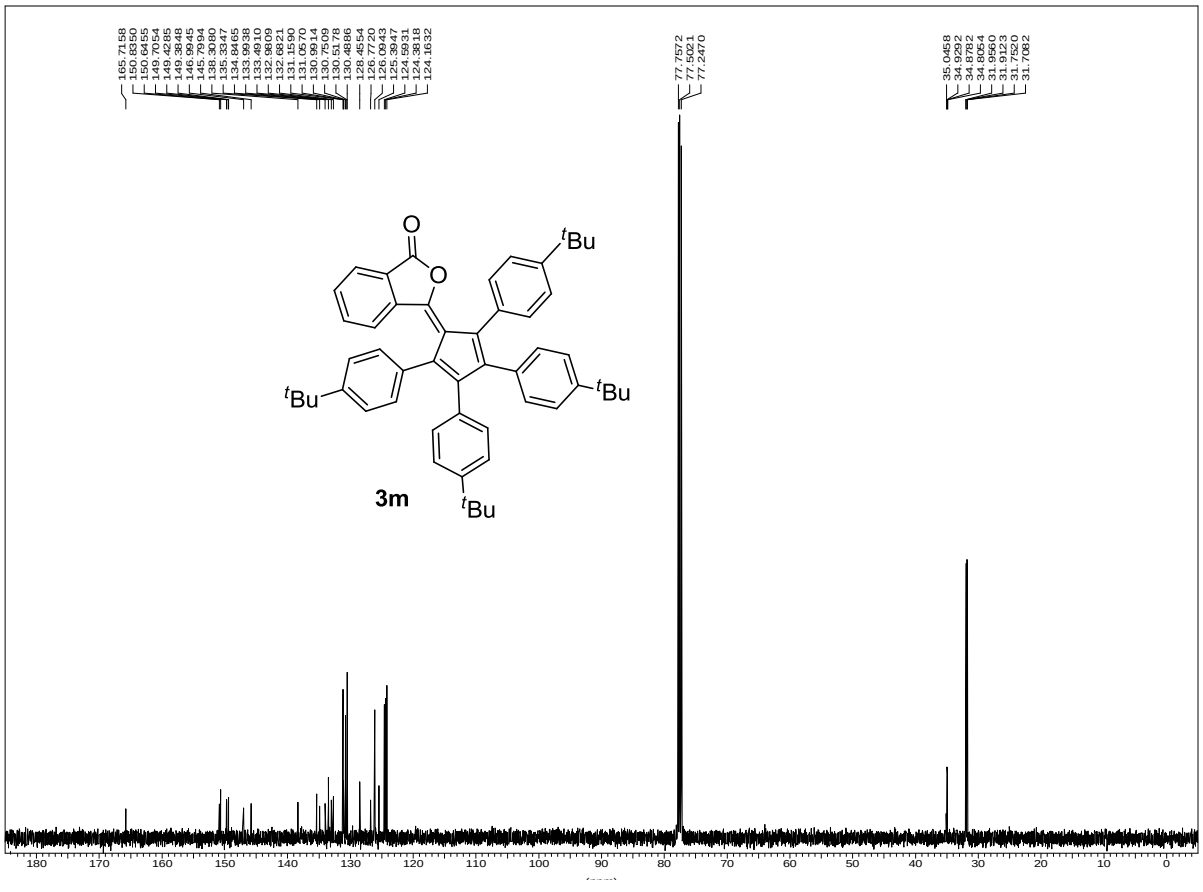
(ppm)


3m
Integral
(ppm)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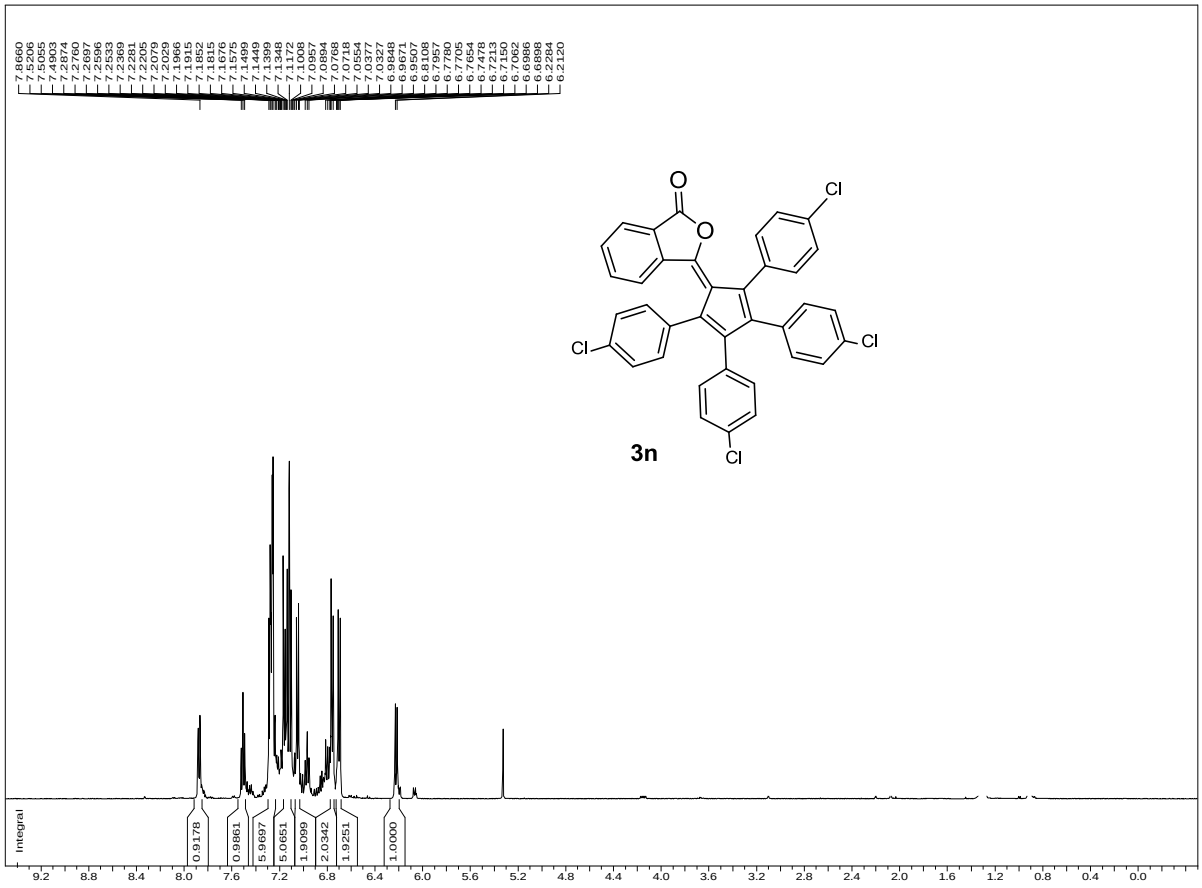
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7.2079
7.2029
7.1966
7.1915
7.1882
7.1845
7.1676
7.1575
7.1499
7.1449
7.1399
7.1348
7.1172
7.1008
7.0957
7.0894
7.0788
7.0718
7.0554
7.0377
7.0327
7.0244
6.9671
6.9507
6.8108
6.7957
6.7769
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6.7478
6.7213
6.7159
6.7062
6.6986
6.6898
6.2284
6.2120
O
O
Cl
Cl
Cl
Cl
3n
Integral
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5.9697
5.0651
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2.0342
1.9251
1.0000
9.2
8.8
8.4
8.0
7.6
7.2
6.8
6.4
6.0
5.6
5.2
4.8
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2.4
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1.6
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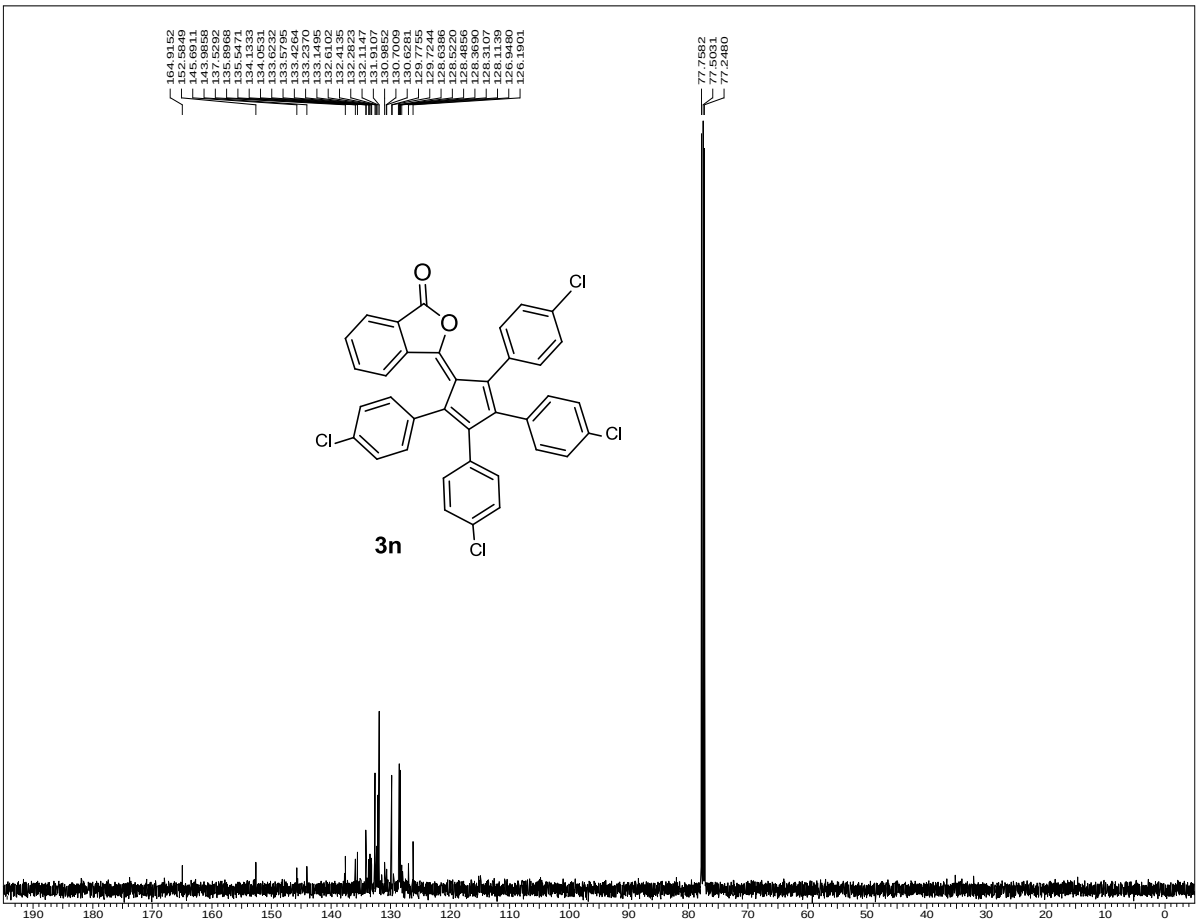
0.4
0.0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77.5031
77.2480
O
O
Cl
Cl
Cl
Cl
3n
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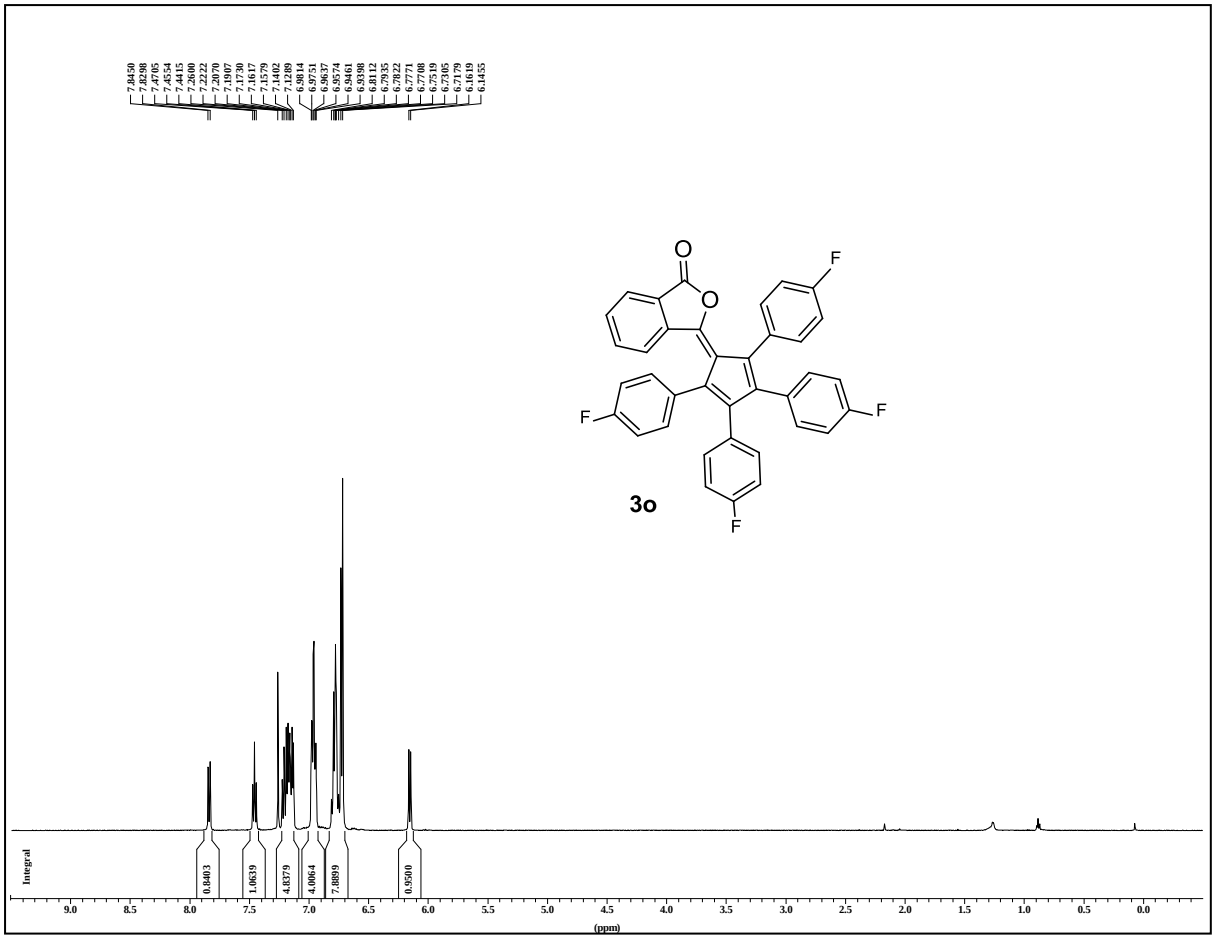
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7.4415
7.2600
7.2222
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7.1730
7.1617
7.1579
7.1402
7.1189
6.9914
6.9751
6.9637
6.9574
6.9461
6.9398
6.8112
6.7935
6.7822
6.7771
6.7708
6.7519
6.7305
6.7179
6.1619
6.1455
O
O
F
F
F
F
3o
Integral
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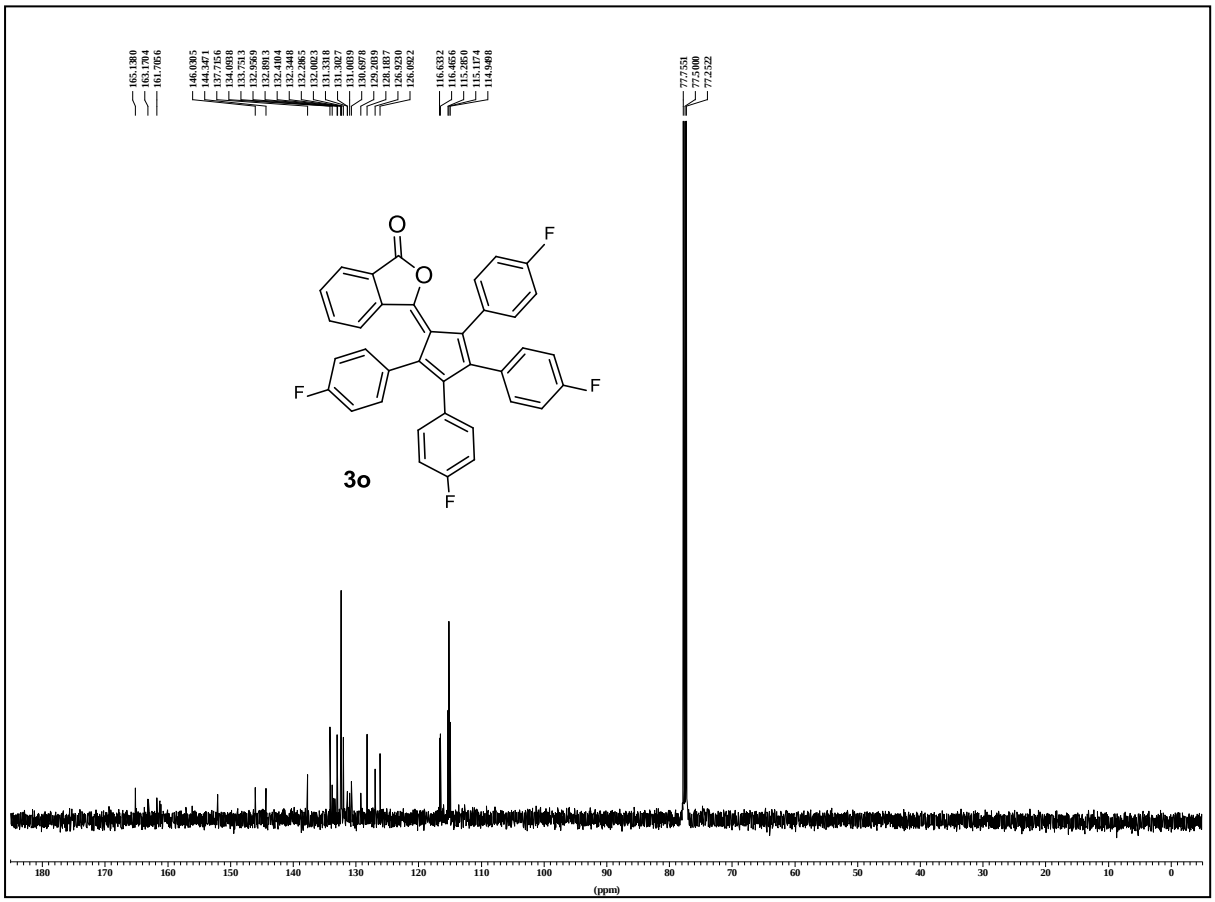
1.0639
4.8379
4.0064
7.8899
0.9500
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
(ppm)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132.4104
132.3448
132.2865
132.0003
131.3318
131.3027
131.0039
130.6978
129.2039
128.1837
126.7970
126.6822
116.6232
116.4656
115.2850
115.1174
114.9498
77.7551
77.5000
77.2522
O
O
F
F
F
F
3o
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140
130
120
110
100
90
80
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60
50
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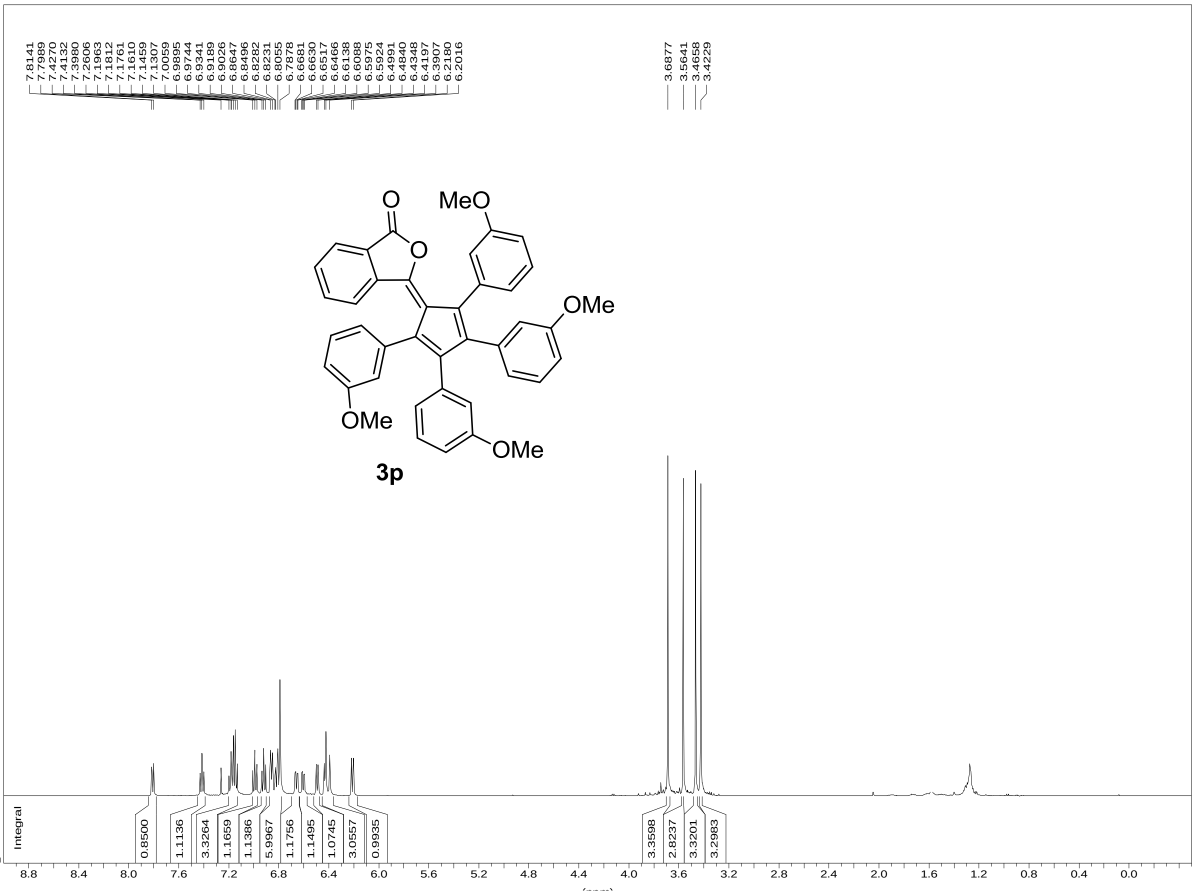
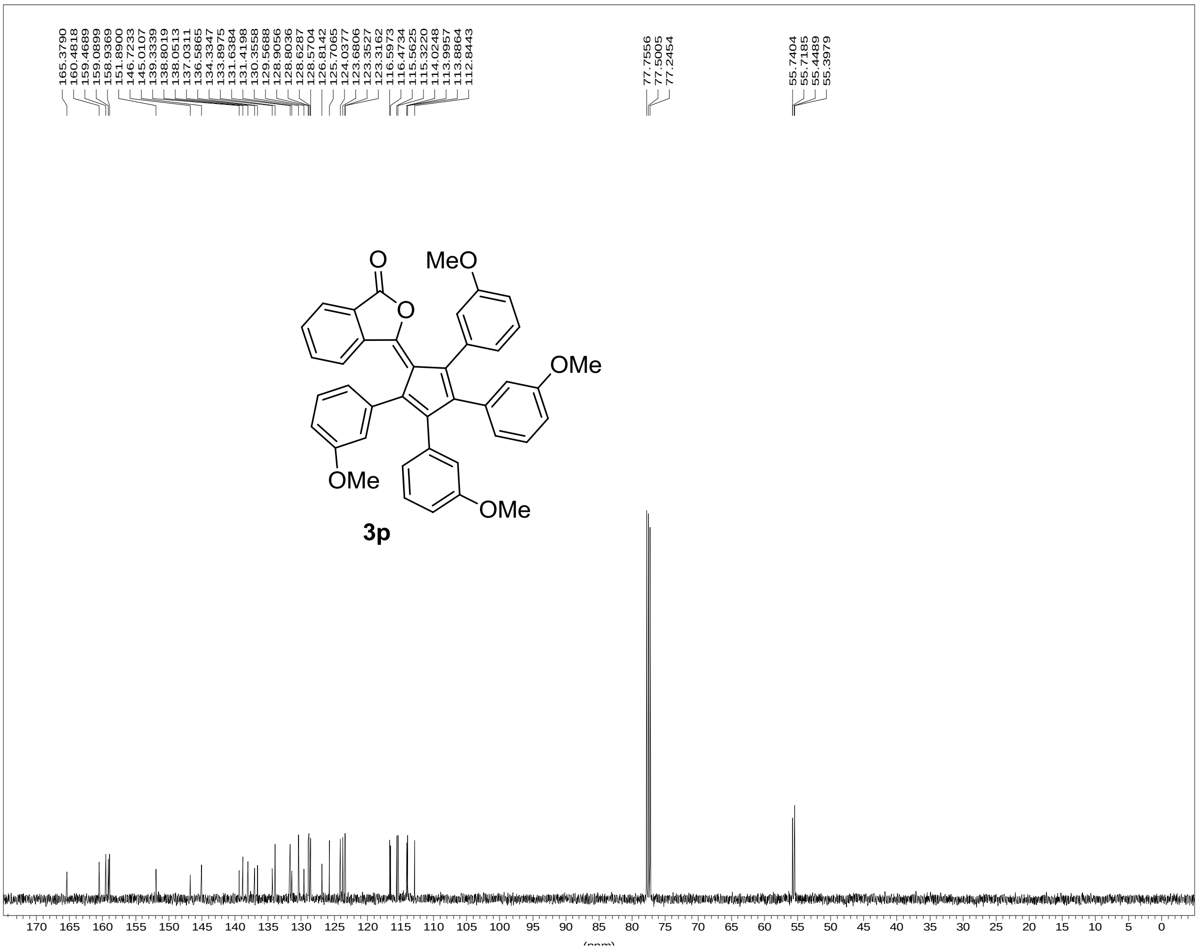
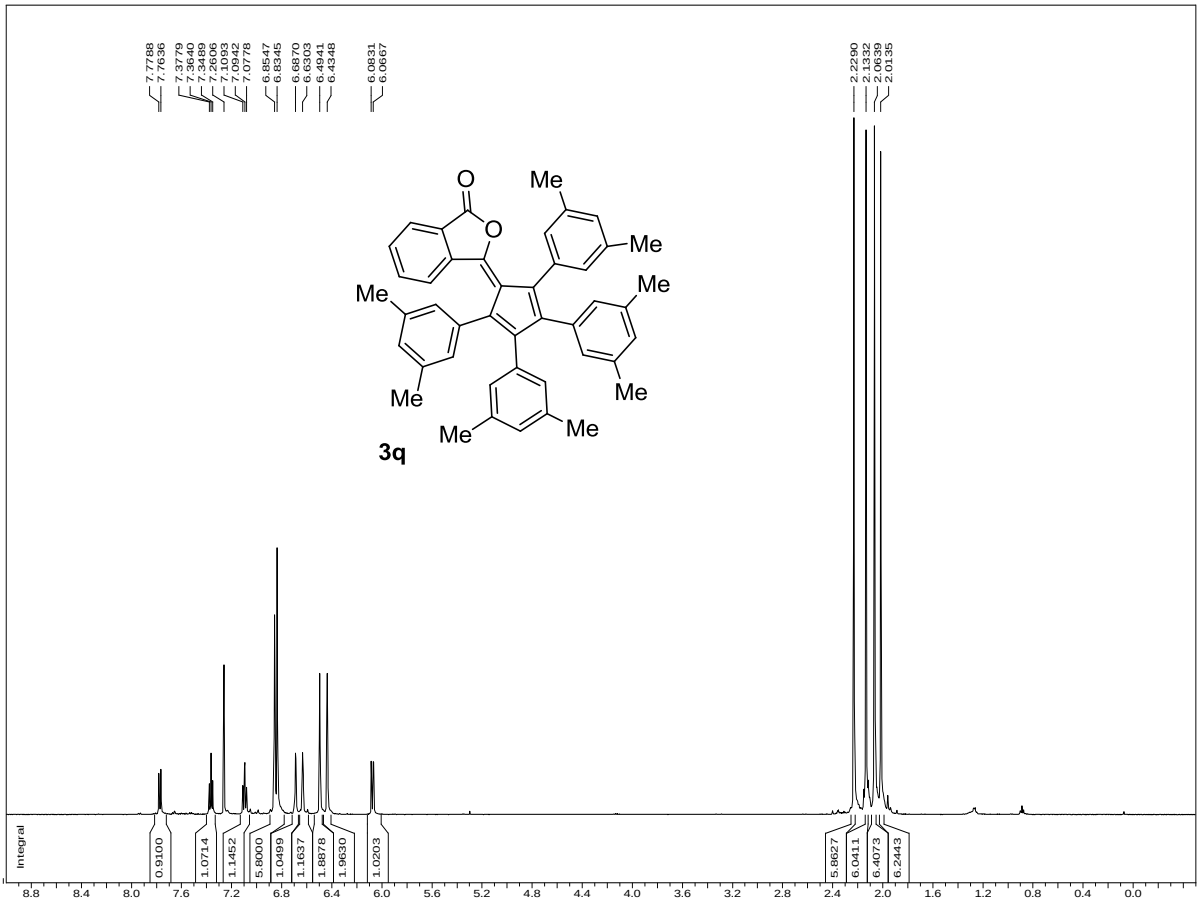
30
20
10
0
(ppm)


MeO
OMe
OMe
OMe
3p
Integral
(ppm)


MeO
OMe
OMe
OMe
3p
(ppm)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7.3489
7.2966
7.1093
7.0942
7.0778
6.8547
6.8345
6.6870
6.6303
6.4941
6.4348
6.0831
6.0667
2.2290
2.1332
2.0639
2.0135
O
O
Me
Me
Me
Me
Me
Me
Me
Me
3q
Integral
0.9100
1.0714
1.1452
5.8000
1.0499
1.1637
1.8878
1.9630
1.0203
5.8627
6.0411
6.4073
6.2443
8.8
8.4
8.0
7.6
7.2
6.8
6.4
6.0
5.6
5.2
4.8
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3.2
2.8
2.4
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1.6
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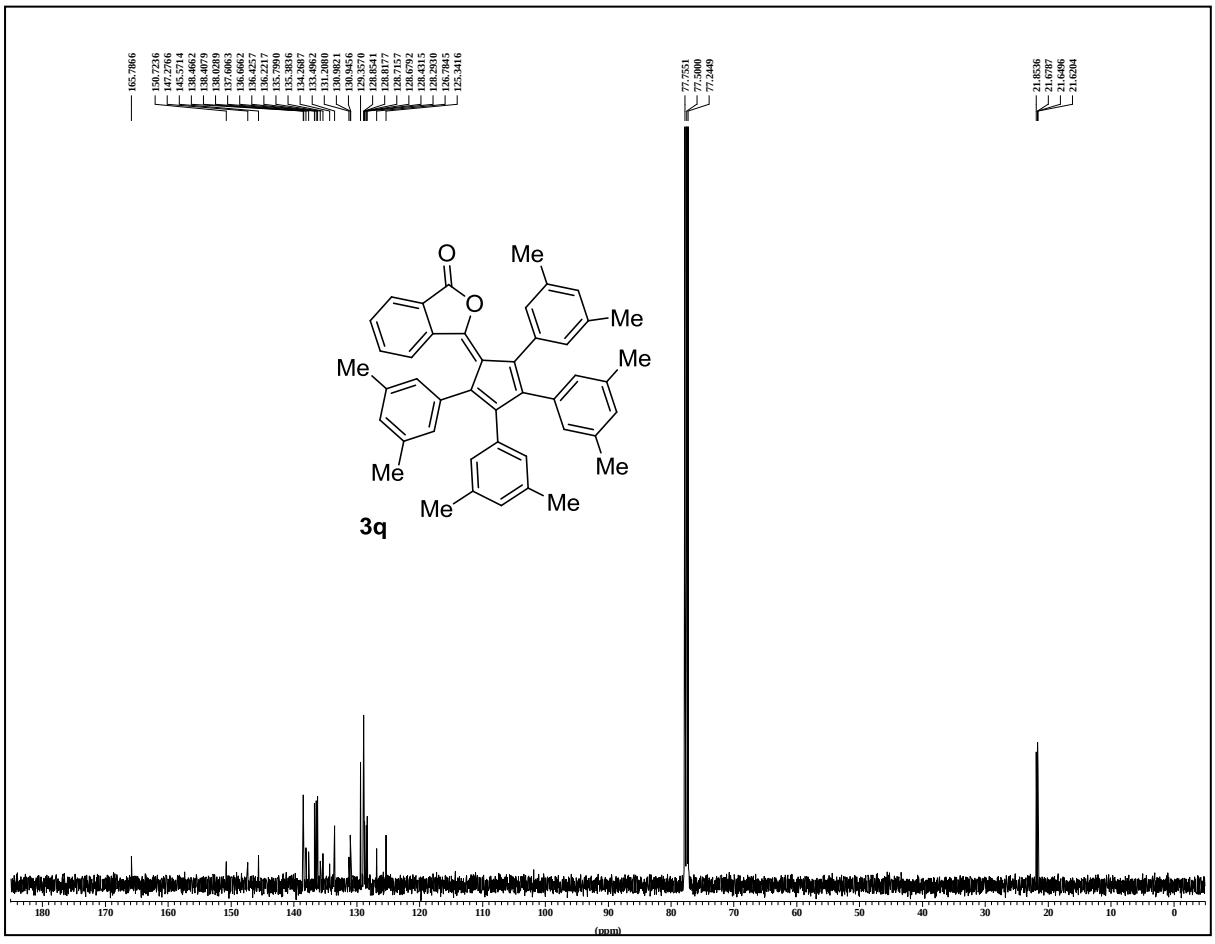
0.4
0.0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134.2687
133.4662
131.2080
130.9821
130.9456
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128.8541
128.6177
128.5757
128.6792
128.4315
128.2930
126.7845
125.3416
77.7551
77.5000
77.2449
21.8536
21.6787
21.6496
21.6204
O
O
Me
Me
Me
Me
Me
Me
Me
Me
3q
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160
150
140
130
120
110
100
90
80
70
60
50
40
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20
10
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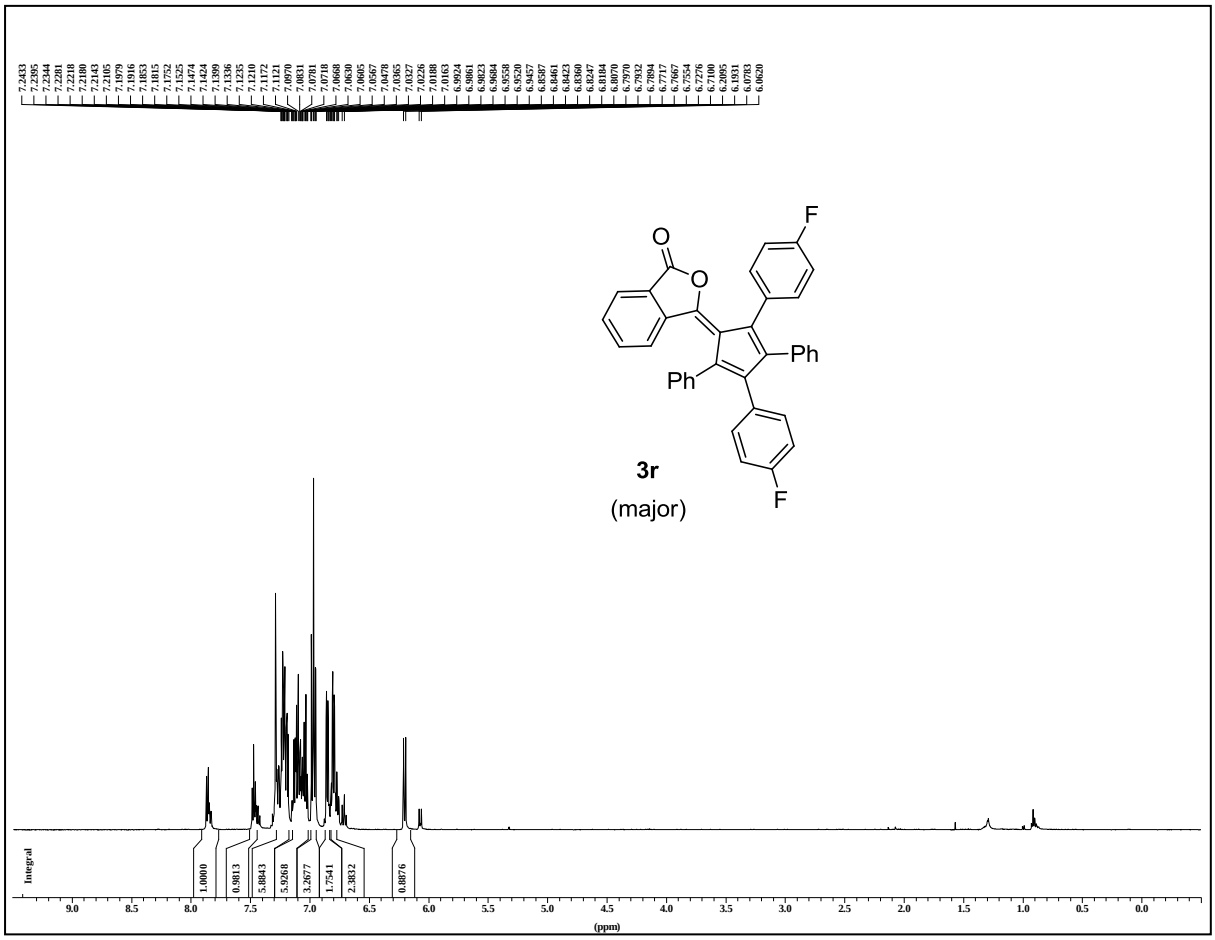
(ppm)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O
O
Ph
Ph
F
3r
(major)
Integral
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1.7541
2.3832
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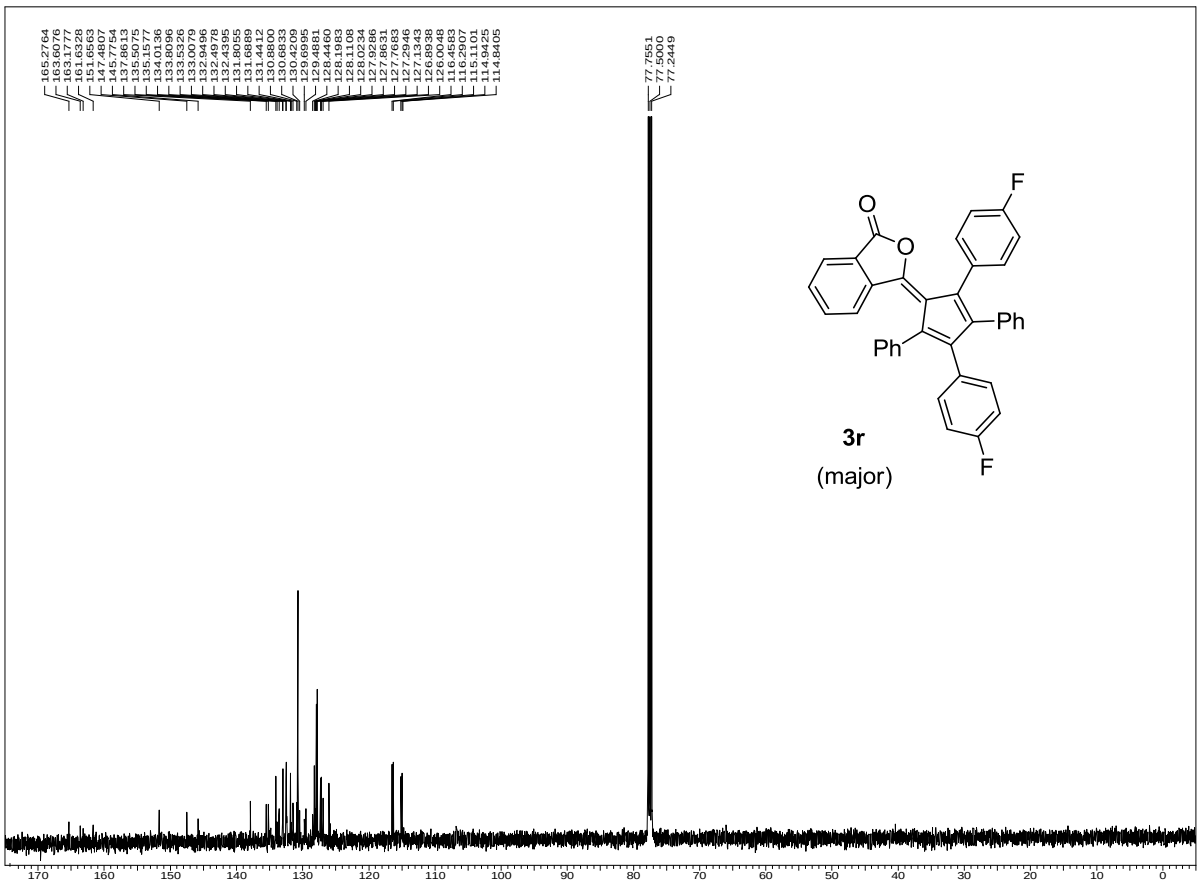
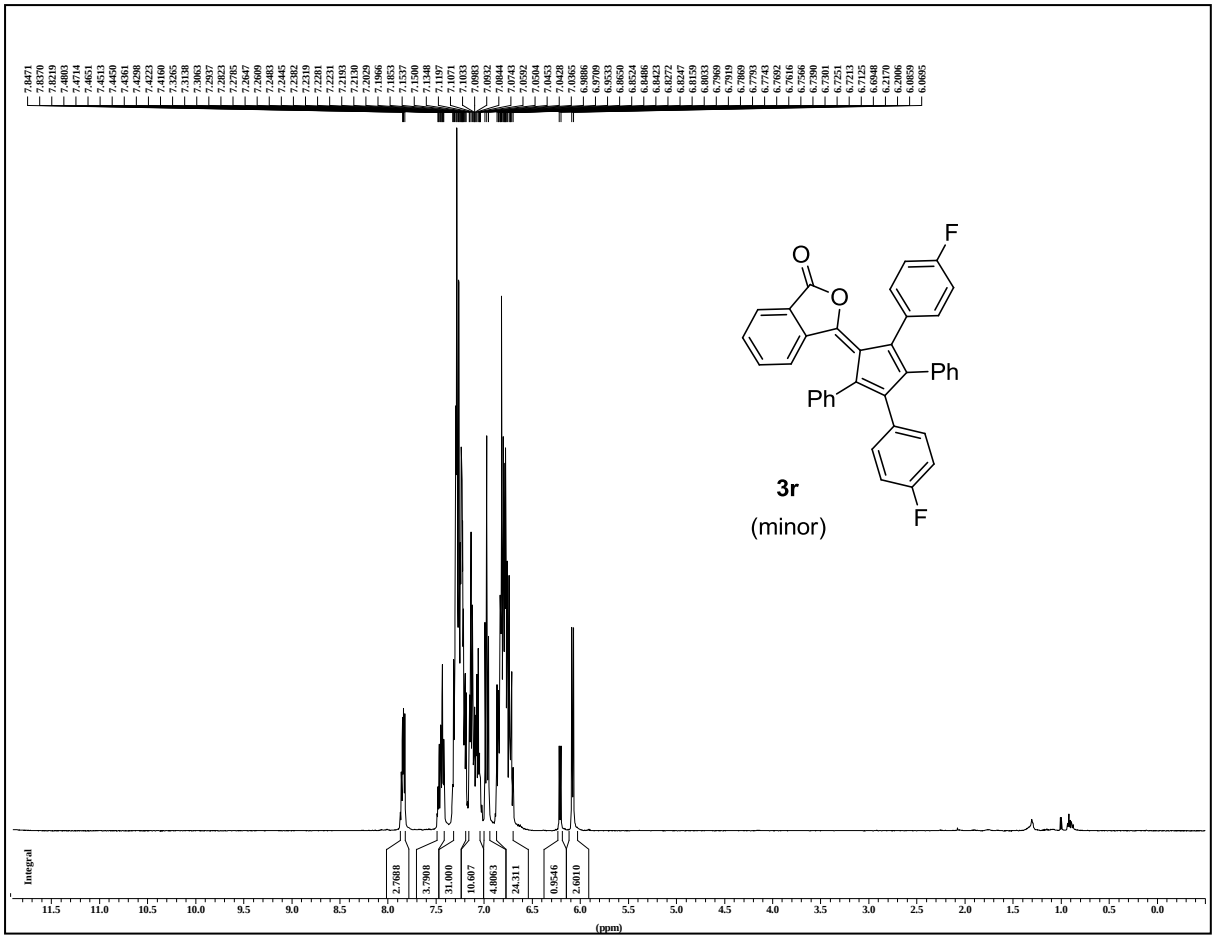
(ppm)


F
O
O
Ph
Ph
F
3r
(major)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(minor)
Integral
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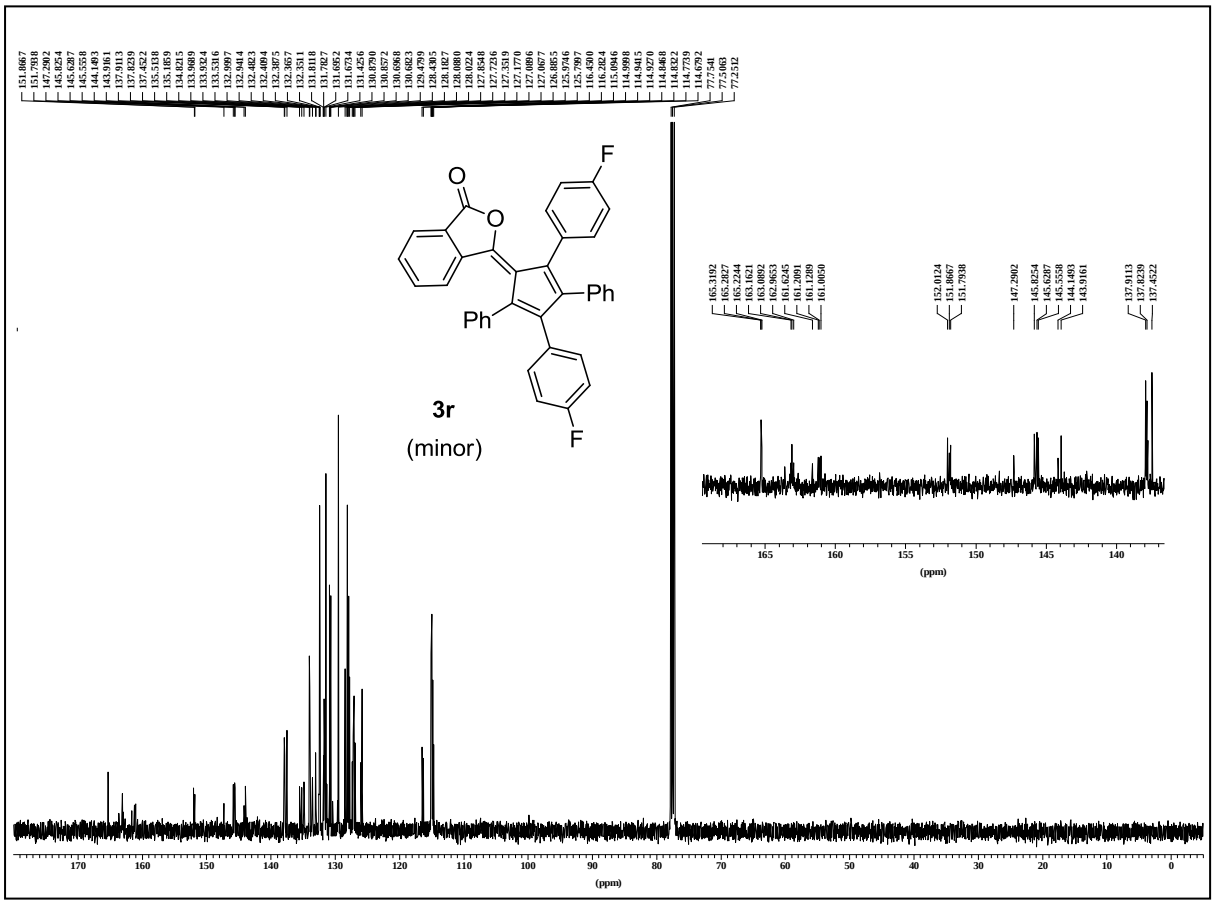
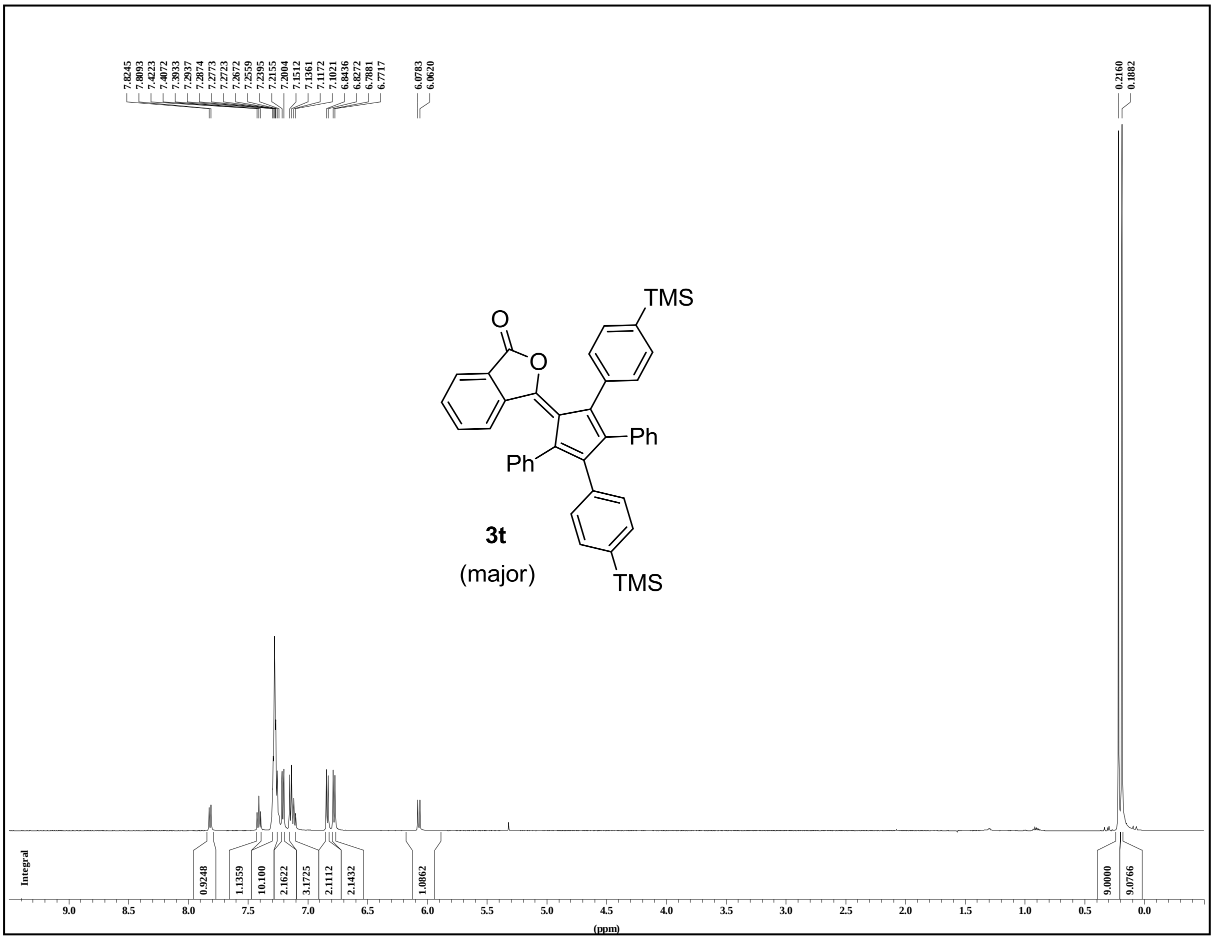
2.6010
(ppm)


3r
(minor)
(ppm)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7.2874
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7.2723
7.2672
7.2559
7.2395
7.2155
7.2004
7.1512
7.1361
7.1172
7.1021
6.8436
6.8272
6.7881
6.7717
6.0783
6.0620
0.2160
0.1882
O
O
TMS
Ph
Ph
TMS
3t
(major)
Integral
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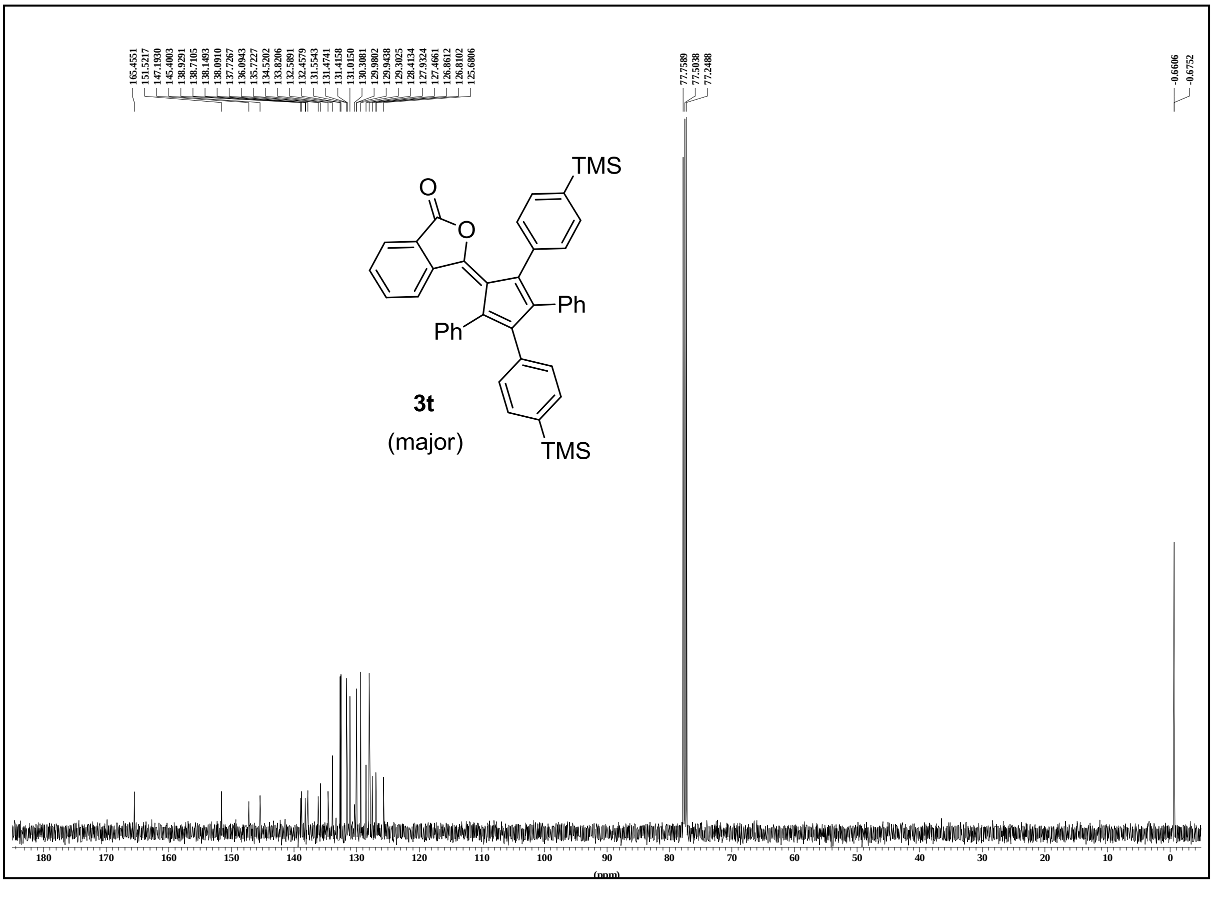
10.100
2.1622
3.1725
2.1112
2.1432
1.0862
9.0000
9.0766
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)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129.9802
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129.3025
128.4134
127.9324
127.4661
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126.8102
125.6806
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77.2488
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TMS
Ph
Ph
TMS
3t
(major)
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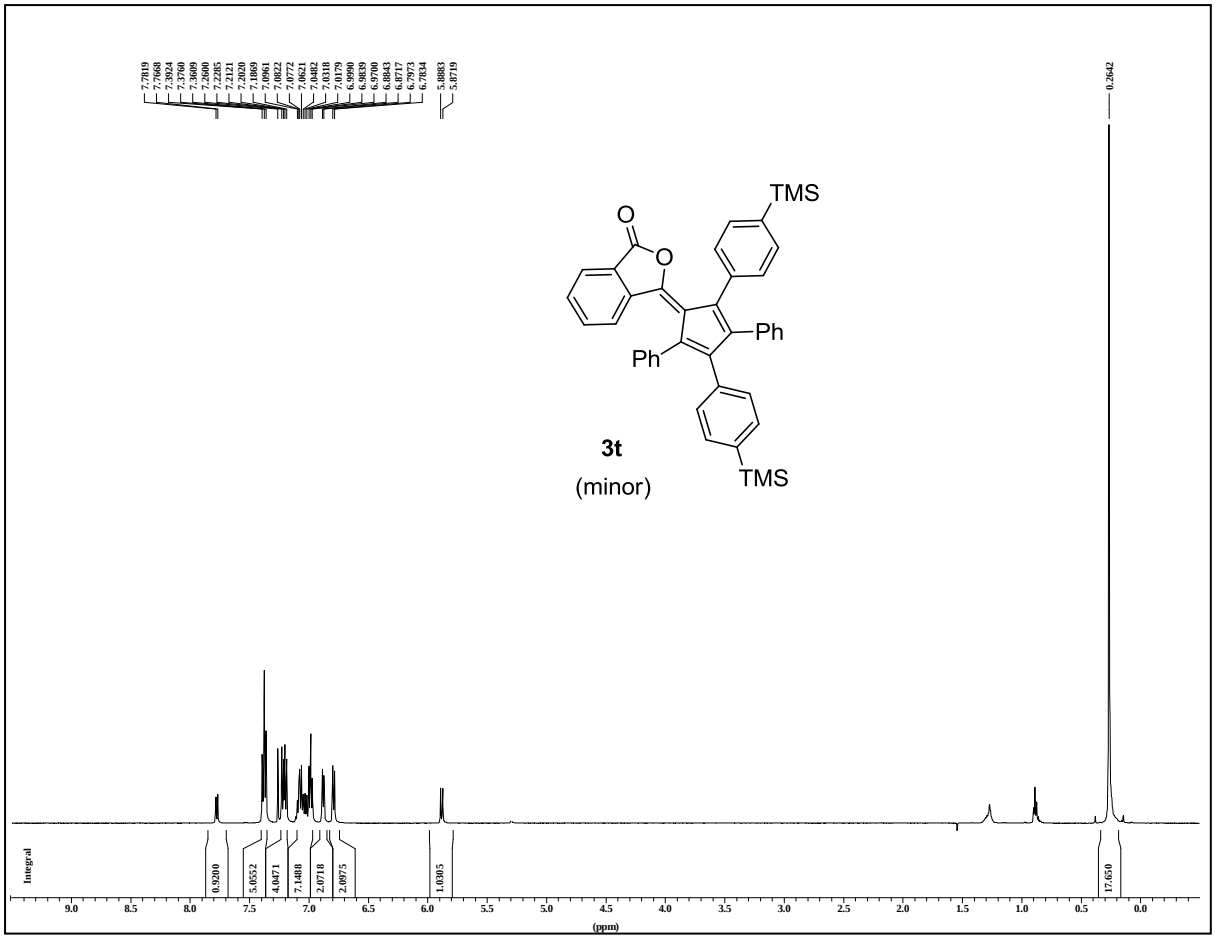
(ppm)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7.2020
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7.0822
7.0772
7.0621
7.0468
7.0318
7.0179
6.9990
6.9839
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6.8843
6.8777
6.8575
6.7834
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5.8719
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TMS
O
O
Ph
Ph
TMS
3t
(minor)
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6.5
6.0
5.5
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1.5
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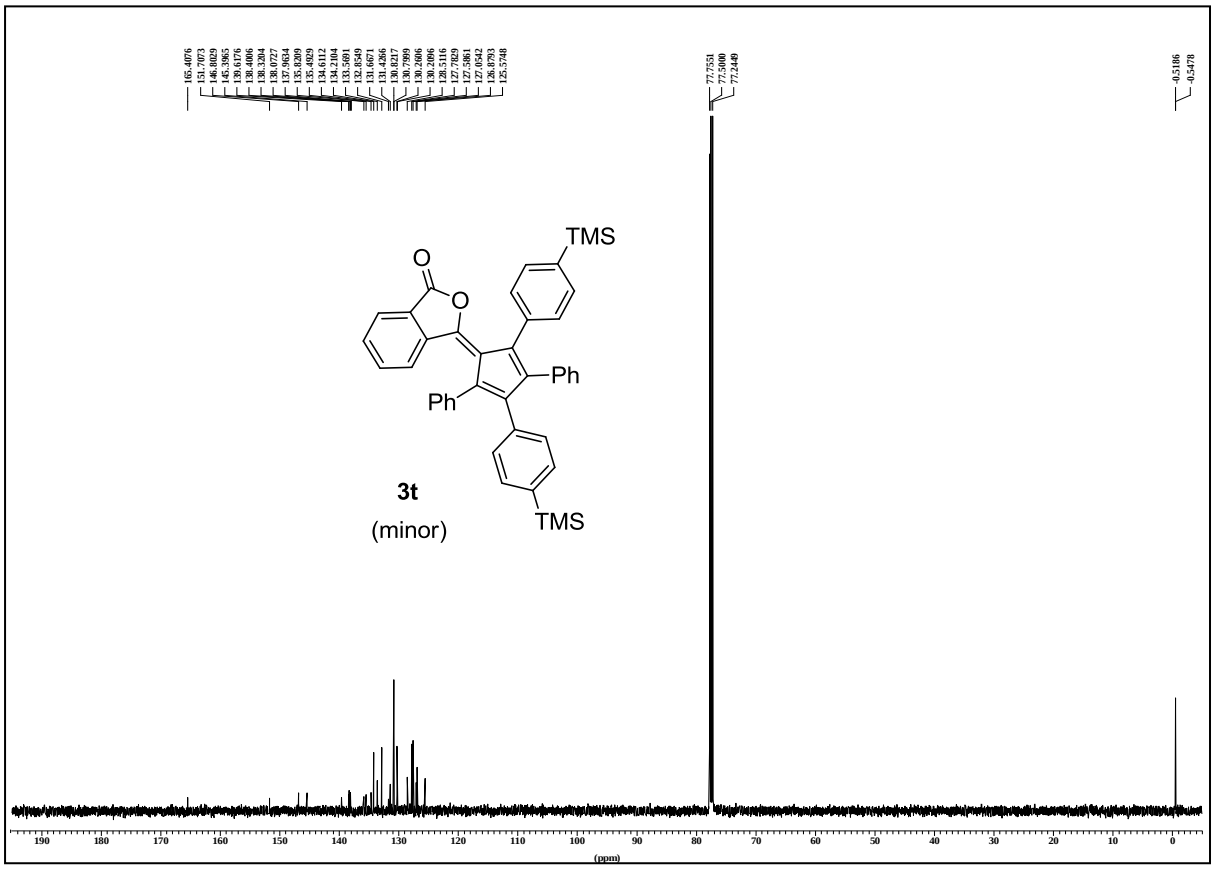
(ppm)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127.0342
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125.5748
77.7551
77.5000
77.2449
-0.5186
-0.5478
TMS
O
O
Ph
Ph
TMS
3t
(minor)
190
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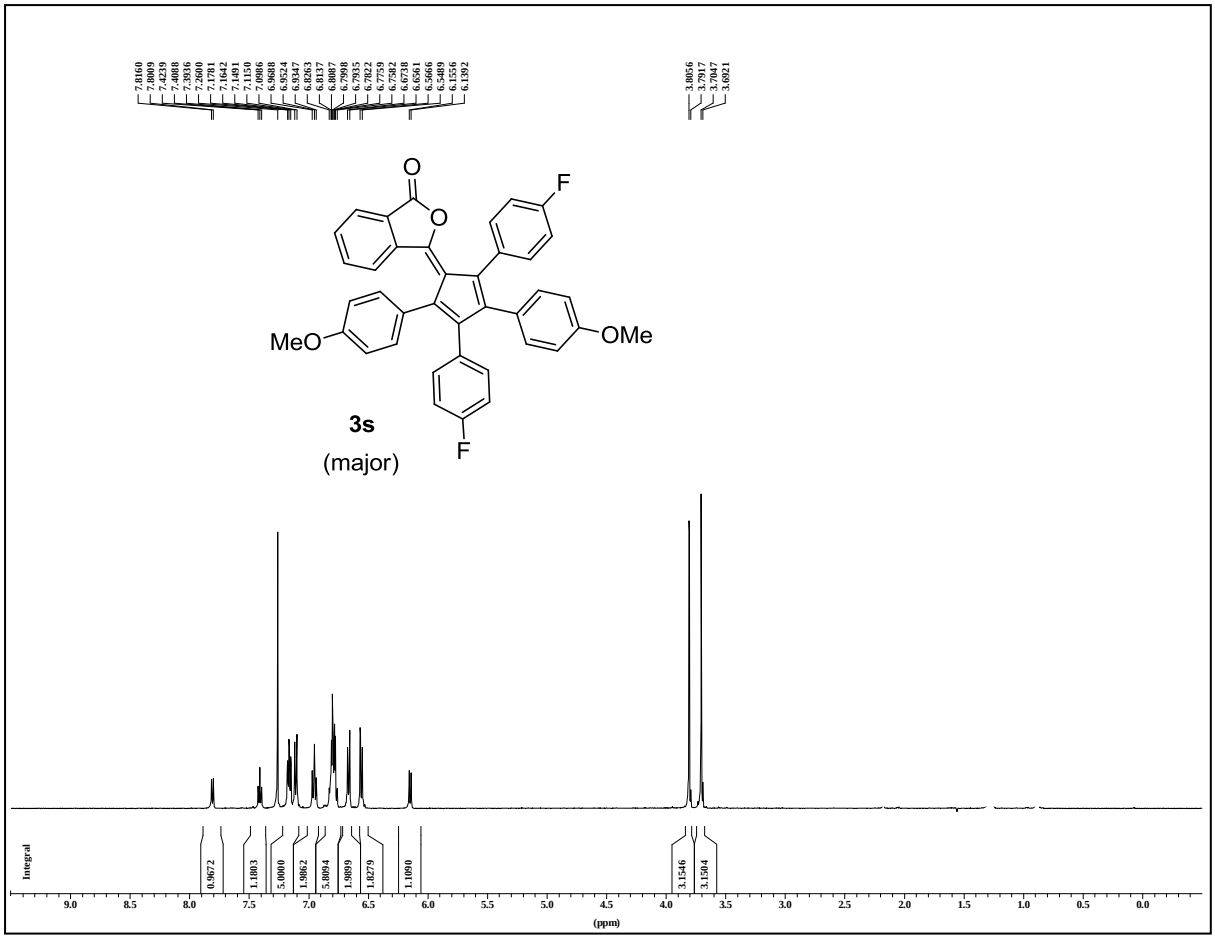
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)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7.1781
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7.1150
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6.9524
6.9347
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6.8137
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6.7898
6.7855
6.7822
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6.7582
6.6738
6.6561
6.5666
6.5469
6.1555
6.1392
3.8056
3.7917
3.7047
3.6921
O
O
F
MeO
OMe
F
3s
(major)
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3.1504
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8.0
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7.0
6.5
6.0
5.5
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3.5
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1.5
1.0
0.5
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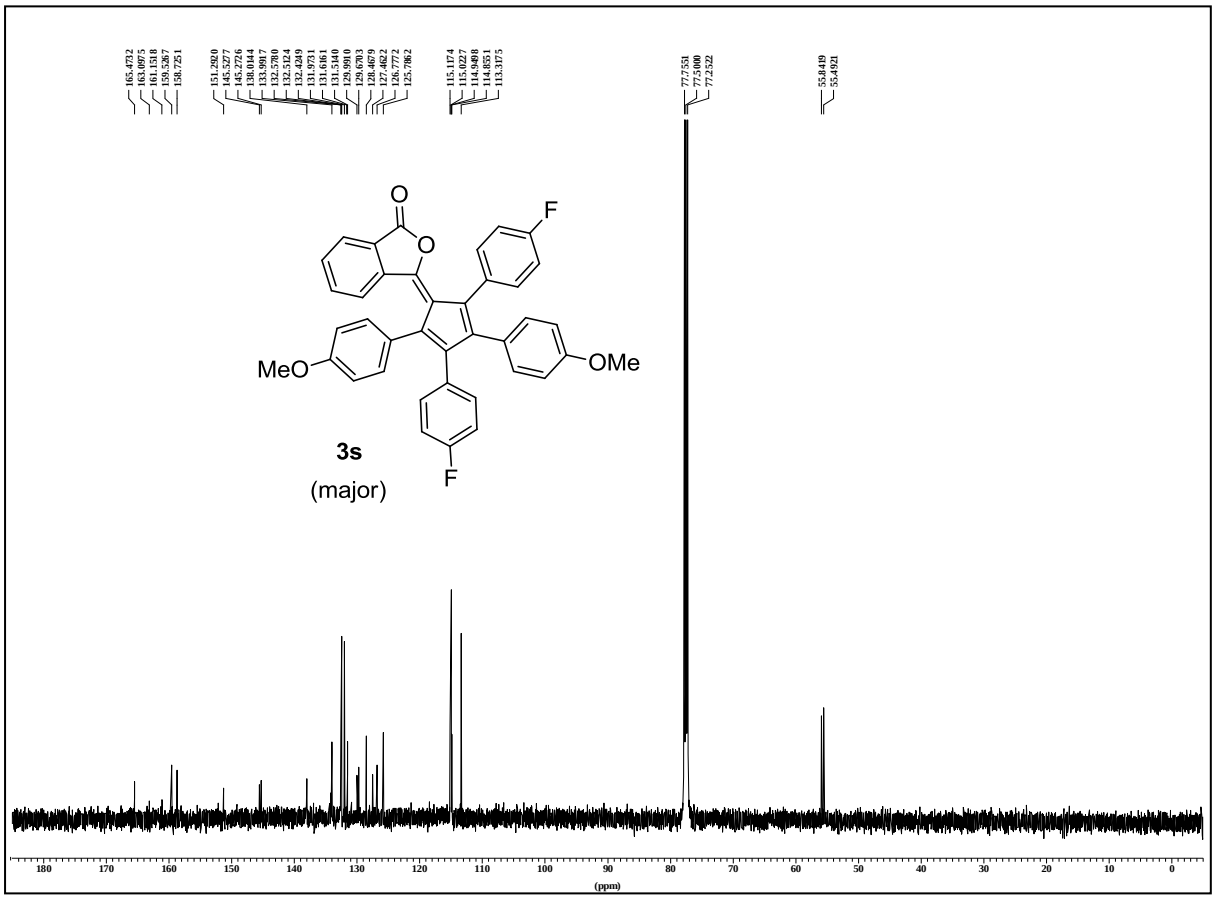
(ppm)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129.9910
129.6703
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127.4952
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125.7862
115.1174
115.0227
114.9498
114.8551
113.3175
77.7551
77.5000
77.2522
55.8449
55.4921
O
O
F
MeO
OMe
F
3s
(major)
180
170
160
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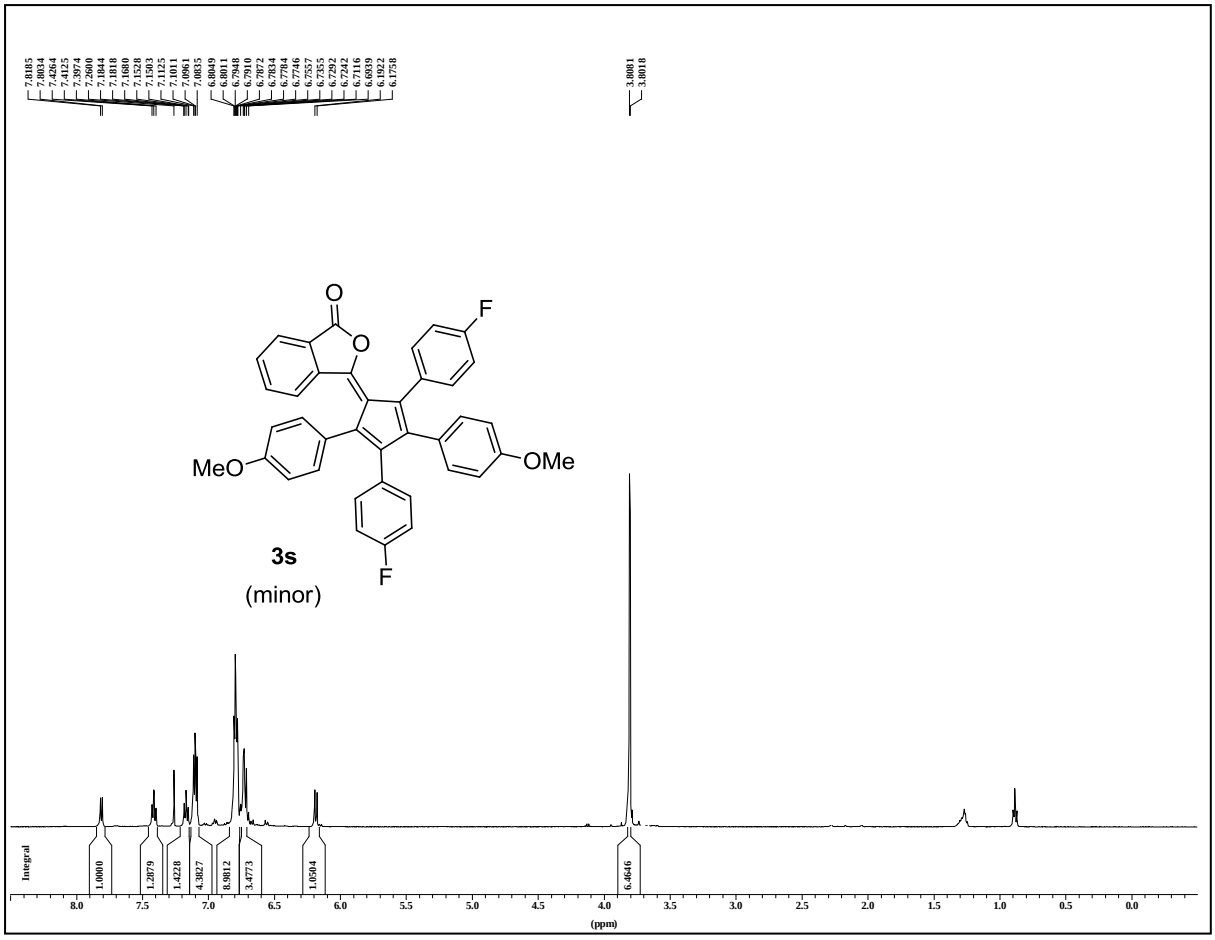
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)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7.1125
7.1011
7.1061
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6.8011
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6.7910
6.7872
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6.7746
6.7557
6.7355
6.7292
6.7242
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6.1758
3.8081
3.8018
O
O
F
MeO
OMe
F
3s
(minor)
Integral
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7.0
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6.0
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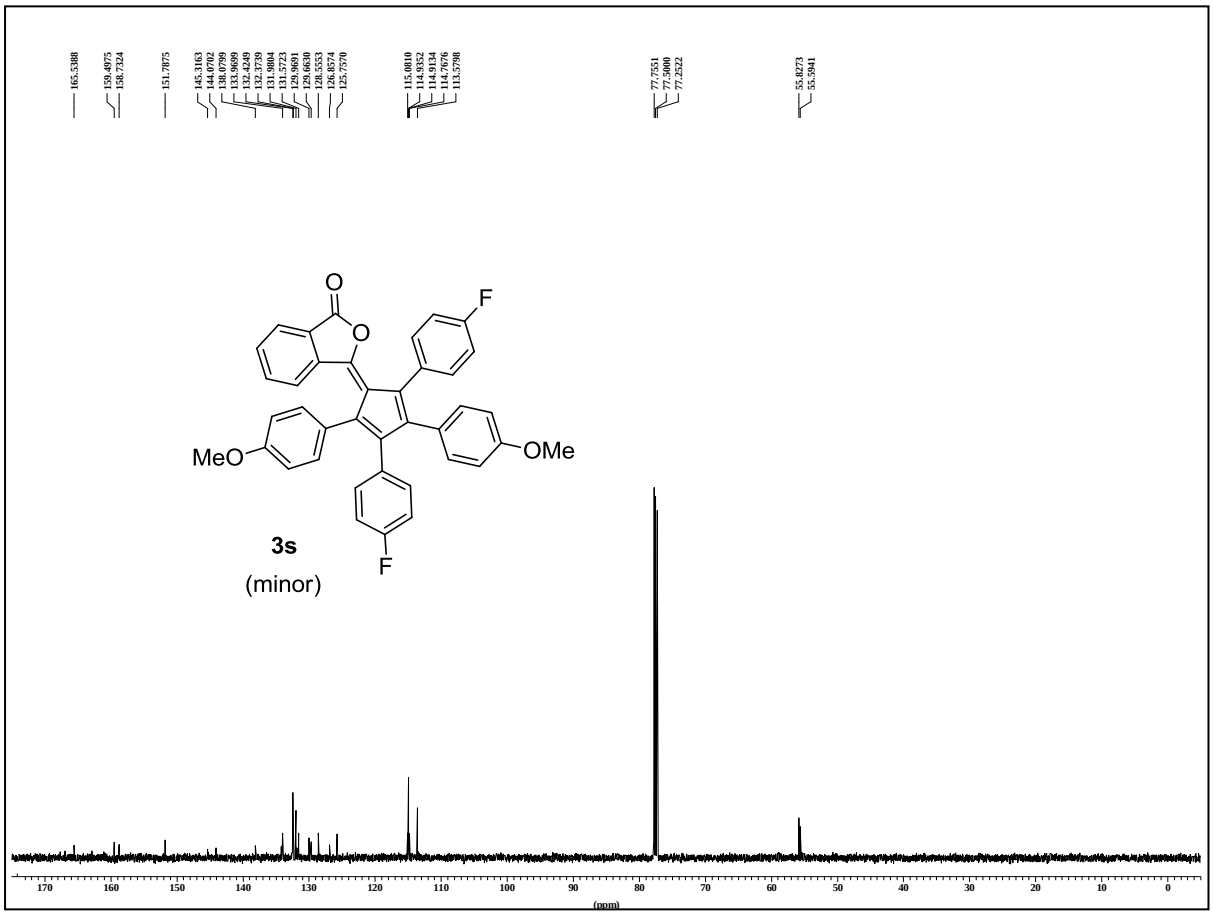
(ppm)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114.9134
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113.5798
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77.5000
77.2522
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55.5941
O
O
F
MeO
OMe
F
3s
(minor)
170
160
150
140
130
120
110
100
90
80
70
60
50
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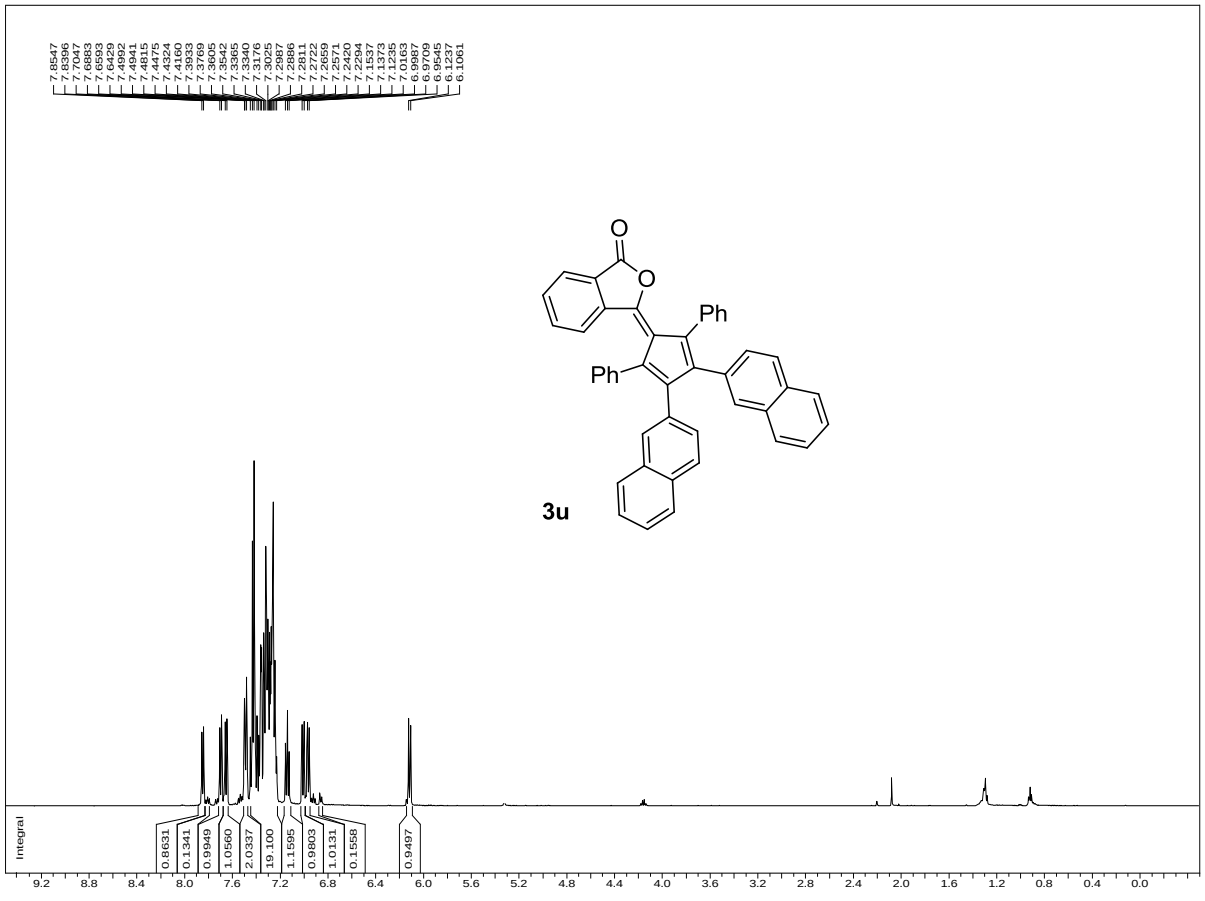
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7.4160
7.3933
7.3769
7.3605
7.3542
7.3365
7.3340
7.3176
7.3025
7.2987
7.2886
7.2811
7.2722
7.2659
7.2571
7.2420
7.2294
7.1537
7.1373
7.1235
7.0163
6.9987
6.9709
6.9545
6.9357
6.1061
O
O
Ph
Ph
3u
Integral
0.8631
0.1341
0.9949
1.0560
2.0337
19.100
1.1595
0.9803
1.0131
0.1558
0.9497
9.2
8.8
8.4
8.0
7.6
7.2
6.8
6.4
6.0
5.6
5.2
4.8
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2.4
2.0
1.6
1.2
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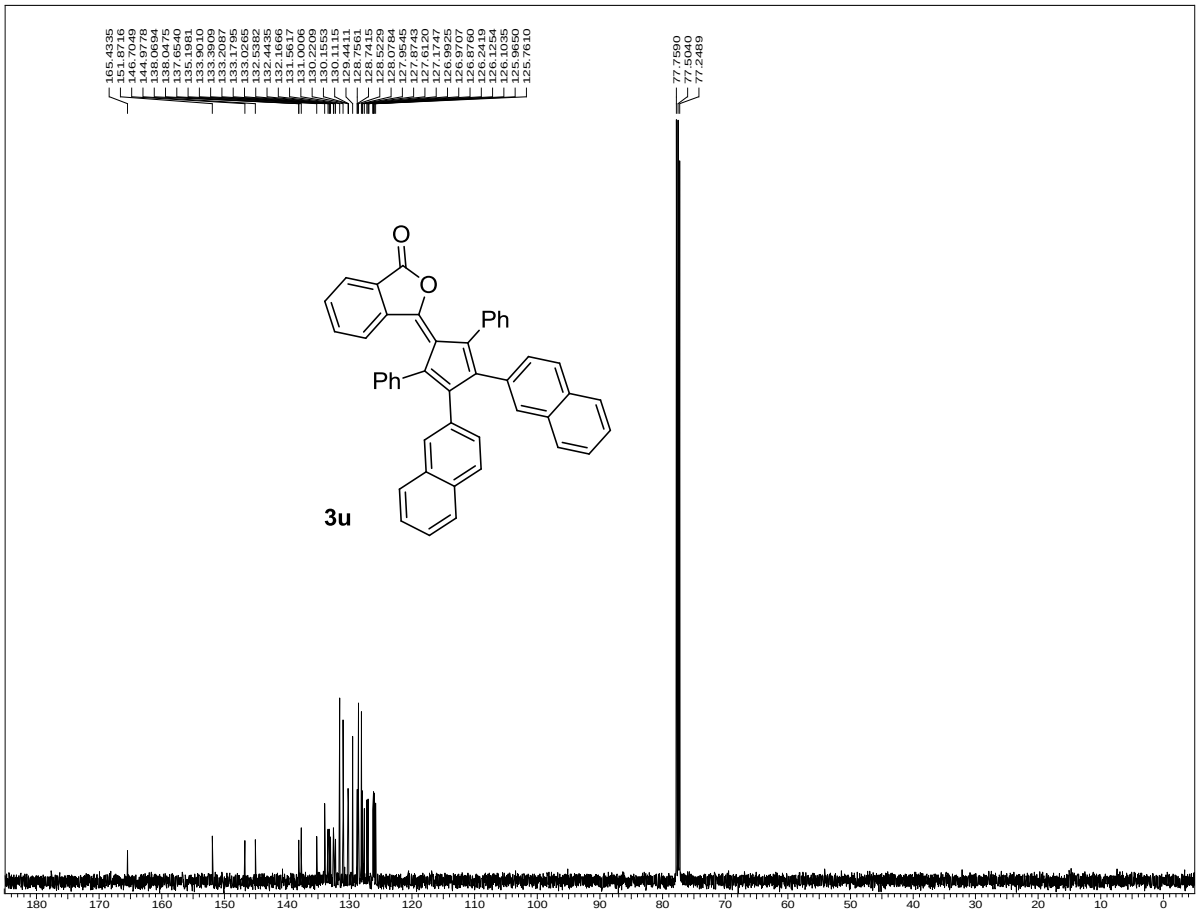
0.4
0.0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131.5617
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130.1553
130.1115
129.4411
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128.7415
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127.9545
127.8743
127.6120
127.1747
126.9835
126.9707
126.8760
126.2419
126.1254
126.1035
125.9650
125.7610
77.7590
77.5040
77.2489
O
O
Ph
Ph
3u
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150
140
130
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110
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70
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30
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10
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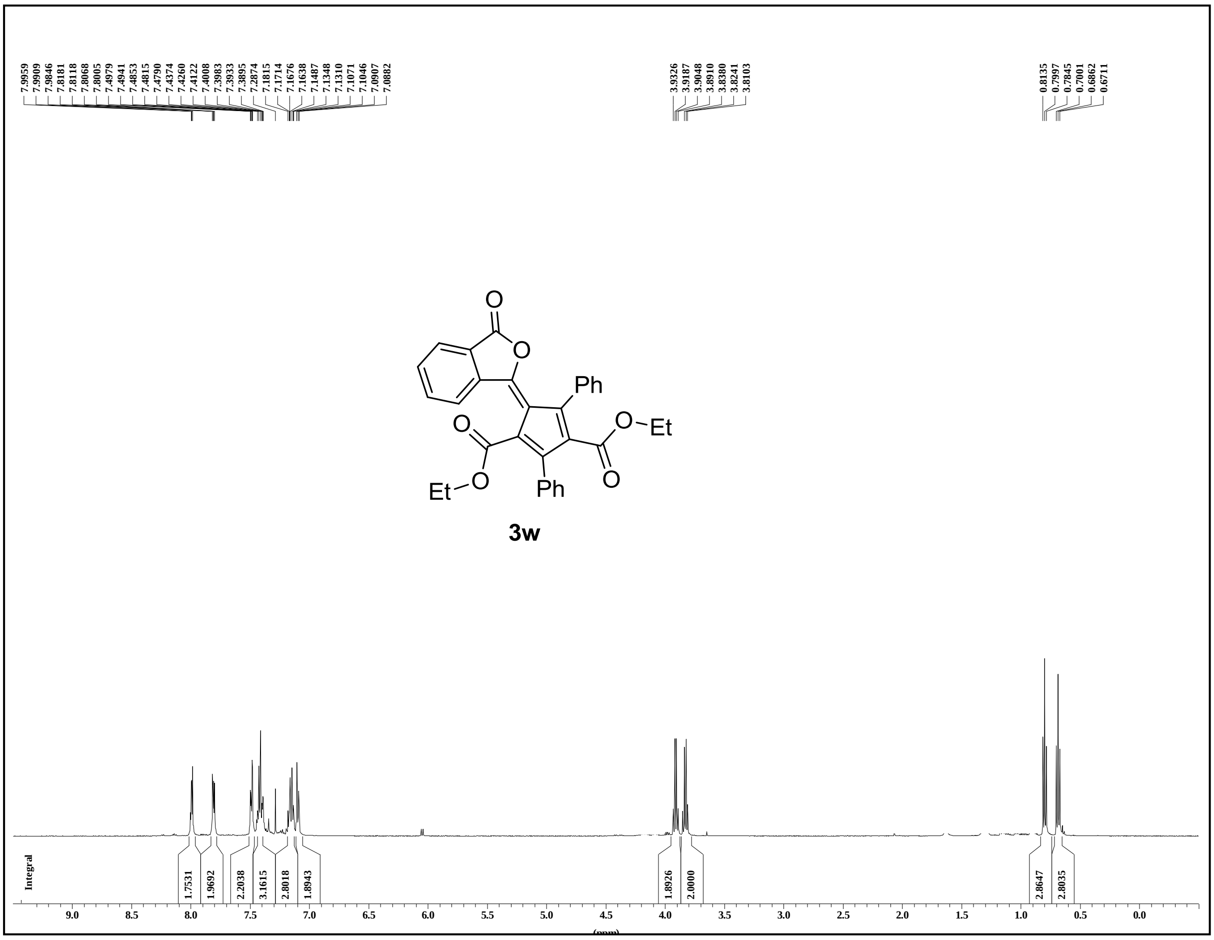
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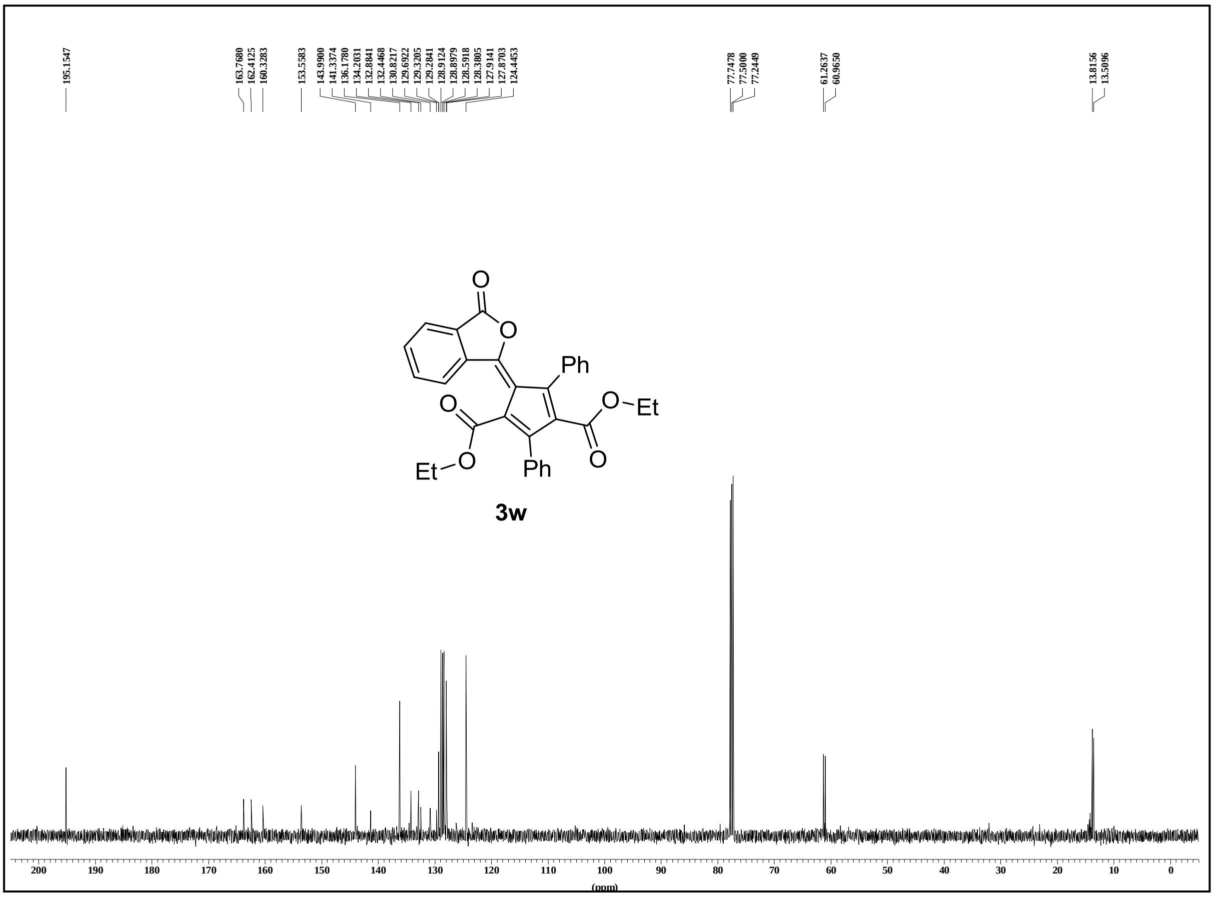
3.9326 3.9187 3.9048 3.8910 3.8380 3.8241 3.8103
0.8135 0.7997 0.7845 0.7001 0.6862 0.6711
O
O
Ph
O
O–Et
Et–O
Ph
O
3w
Integral
1.7531 1.9692 2.2038 3.1615 2.8018 1.8943 1.8926 2.0000 2.8647 2.8035
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)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163.7680 162.4125 160.3283
153.5583
143.9900 141.3374 136.1780 134.2031 132.8841 132.4468 130.8217 129.6922 129.3205 129.2841 128.9124 128.8979 128.5918 128.3805 127.9141 127.8703 124.4453
77.7478 77.5000 77.2449
61.2637 60.9650
13.8156 13.5096
O
O
Ph
O
O–Et
Et–O
Ph
O
3w
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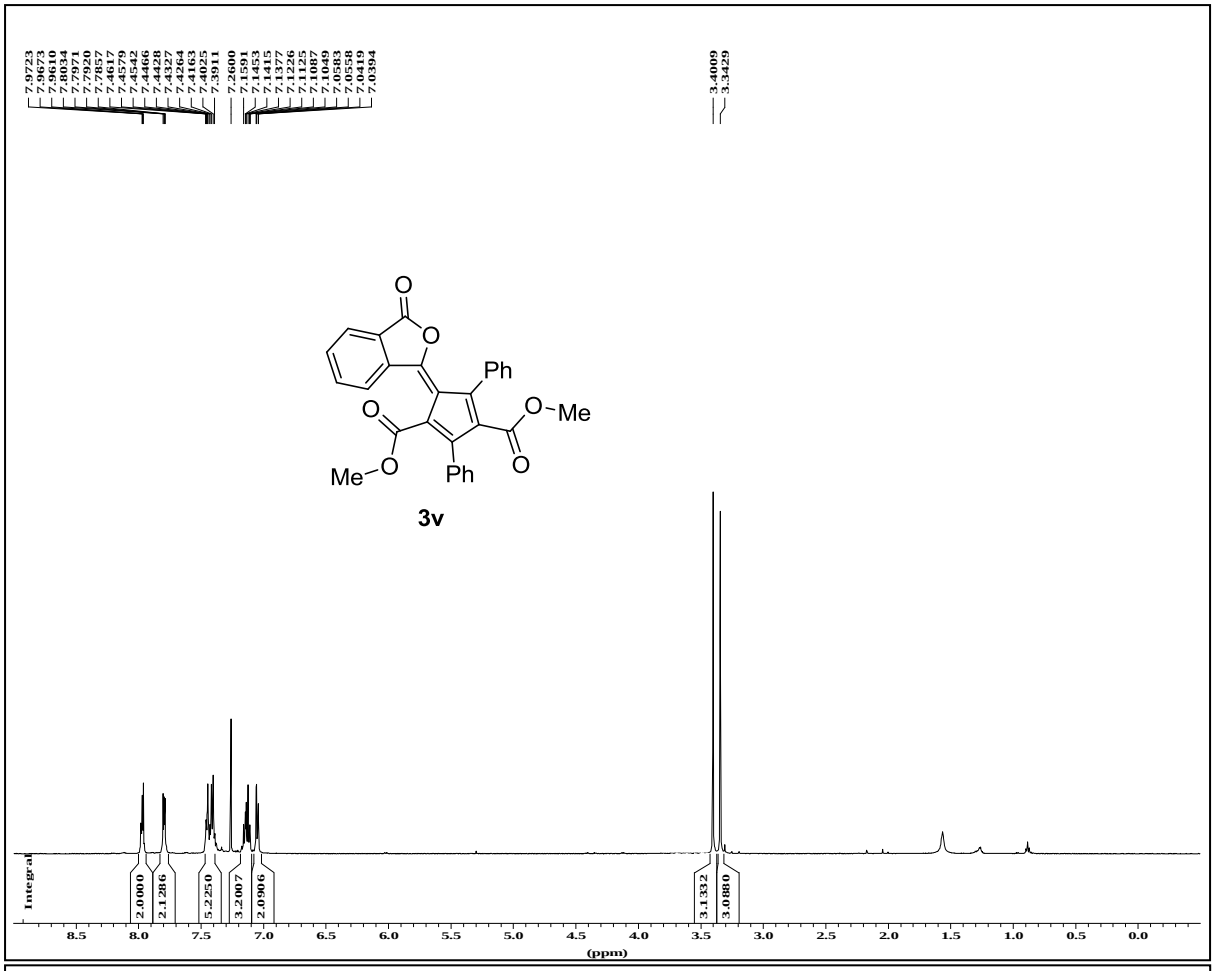
(ppm)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7.7920
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7.4542
7.4466
7.4428
7.4327
7.4264
7.4163
7.4025
7.3911
7.2600
7.1551
7.1453
7.1415
7.1377
7.1226
7.1125
7.1097
7.1049
7.0583
7.0558
7.0419
7.0394
3.4009
3.3429
O
O
Ph
O
O-Me
Me-O
Ph
O
3v
Integral
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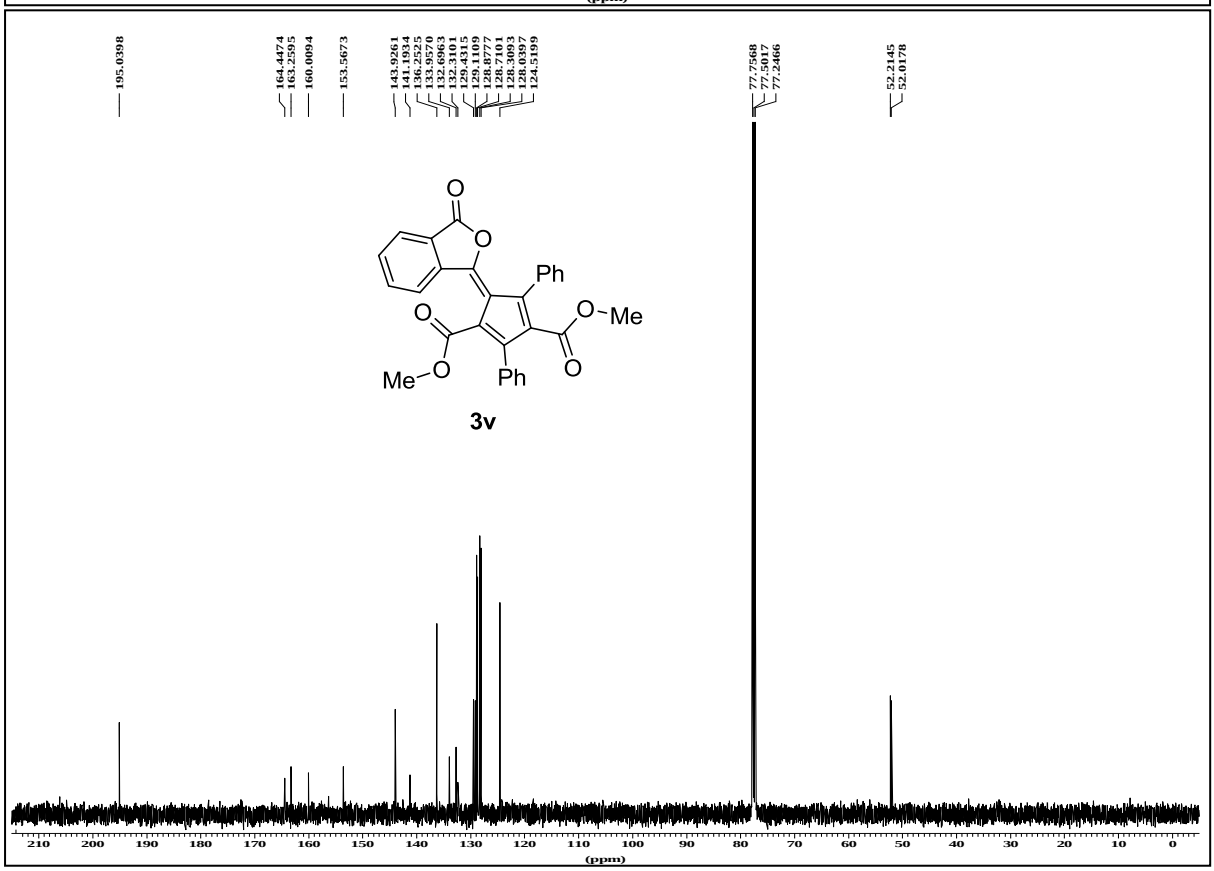
5.2250
3.2007
2.0906
3.1332
3.0880
(ppm)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163.2595
160.0094
153.5673
143.9261
141.1934
136.2525
133.9570
132.6963
132.3101
129.4315
129.1109
128.8777
128.7101
128.3993
128.1997
124.5199
77.7568
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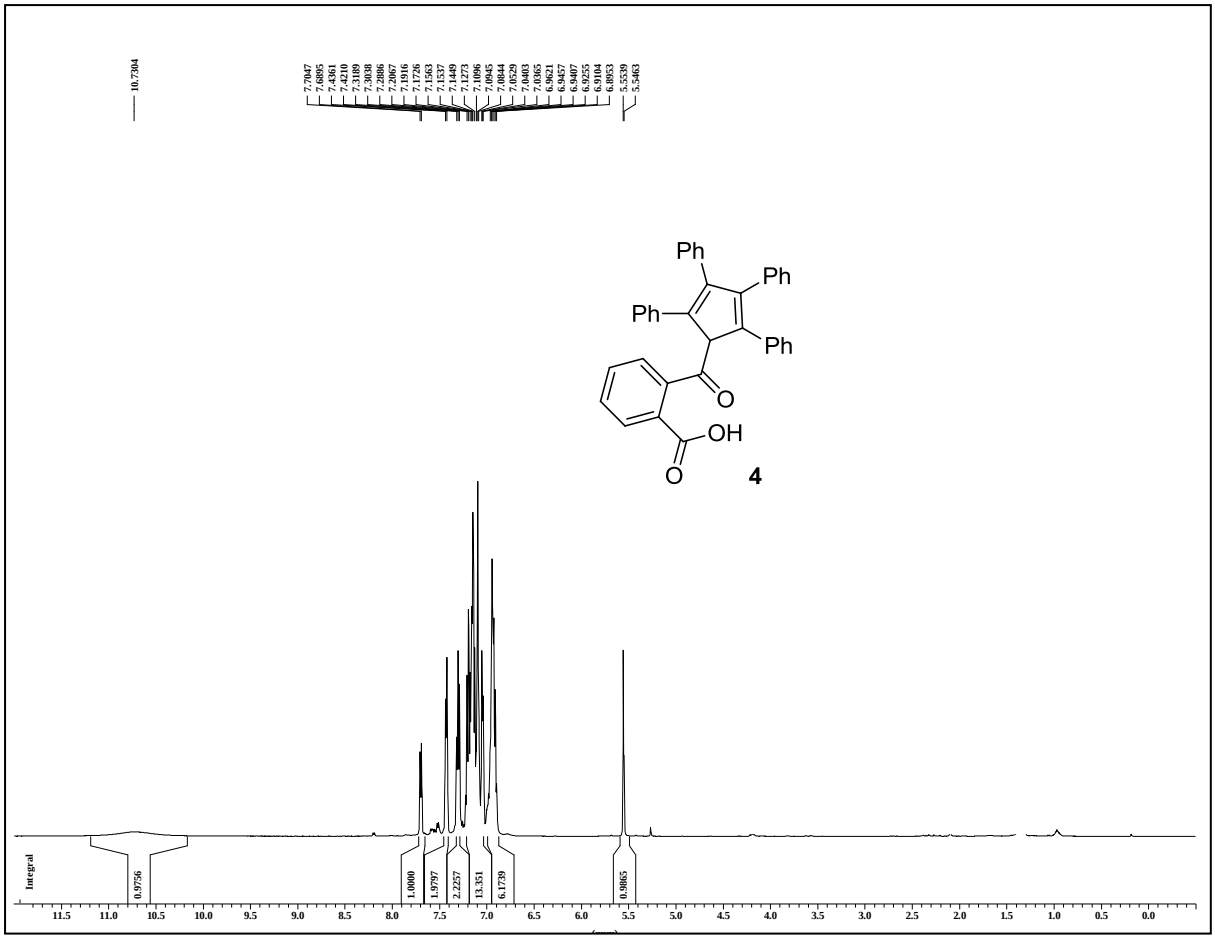
77.2466
52.2145
52.0178
O
O
Ph
O
O-Me
Me-O
Ph
O
3v
(ppm)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7.4210
7.3589
7.3038
7.2886
7.2067
7.1916
7.1726
7.1563
7.1537
7.1449
7.1273
7.1096
7.0945
7.0844
7.0529
7.0403
7.0256
6.9621
6.9457
6.9407
6.9255
6.9104
6.8953
5.5539
5.5465
Ph
Ph
Ph
Ph
O
OH
O
4
Integral
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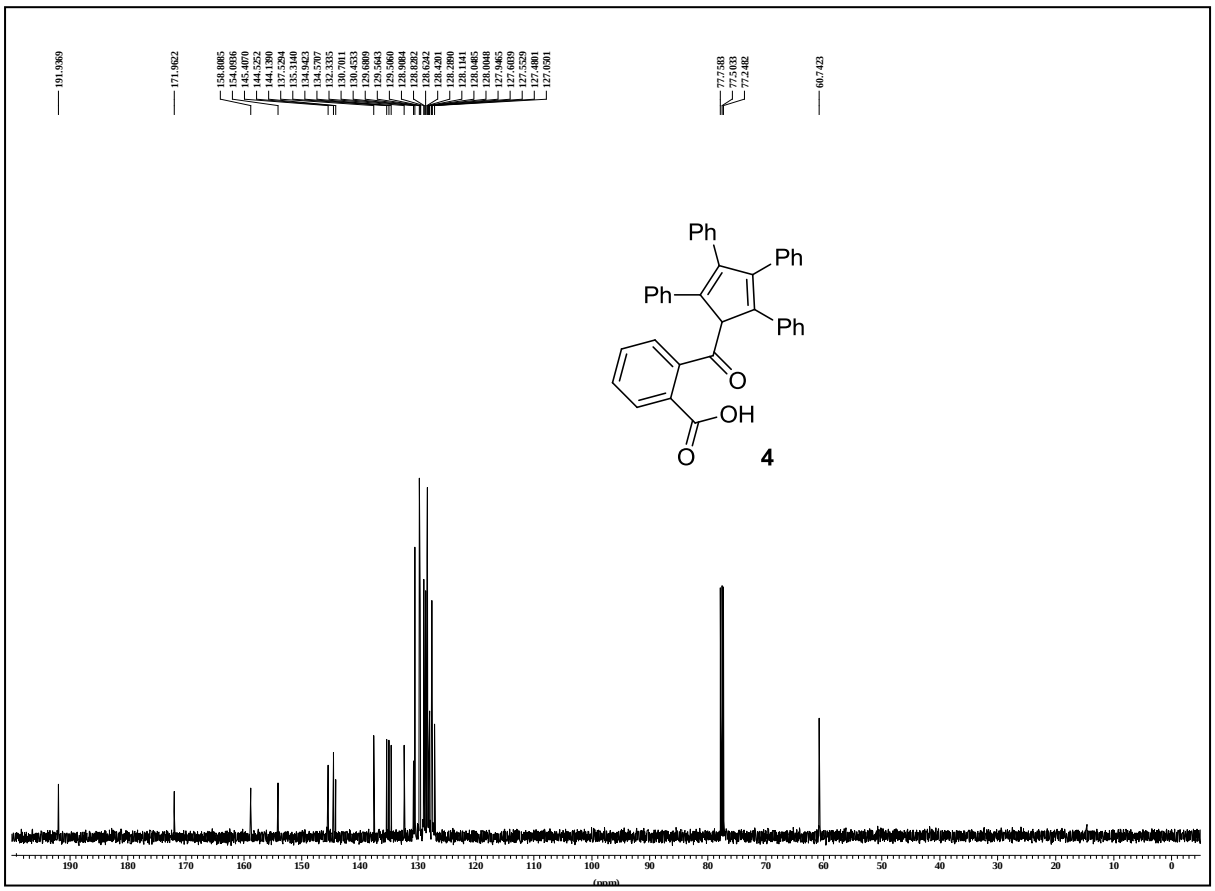
2.2257
13.351
6.1739
0.9865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145.4070
144.5253
144.1390
137.5294
135.3140
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134.5707
132.3335
130.7011
130.4533
129.6809
129.5643
129.5060
128.9884
128.8282
128.6543
128.4201
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127.5529
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77.5103
77.2482
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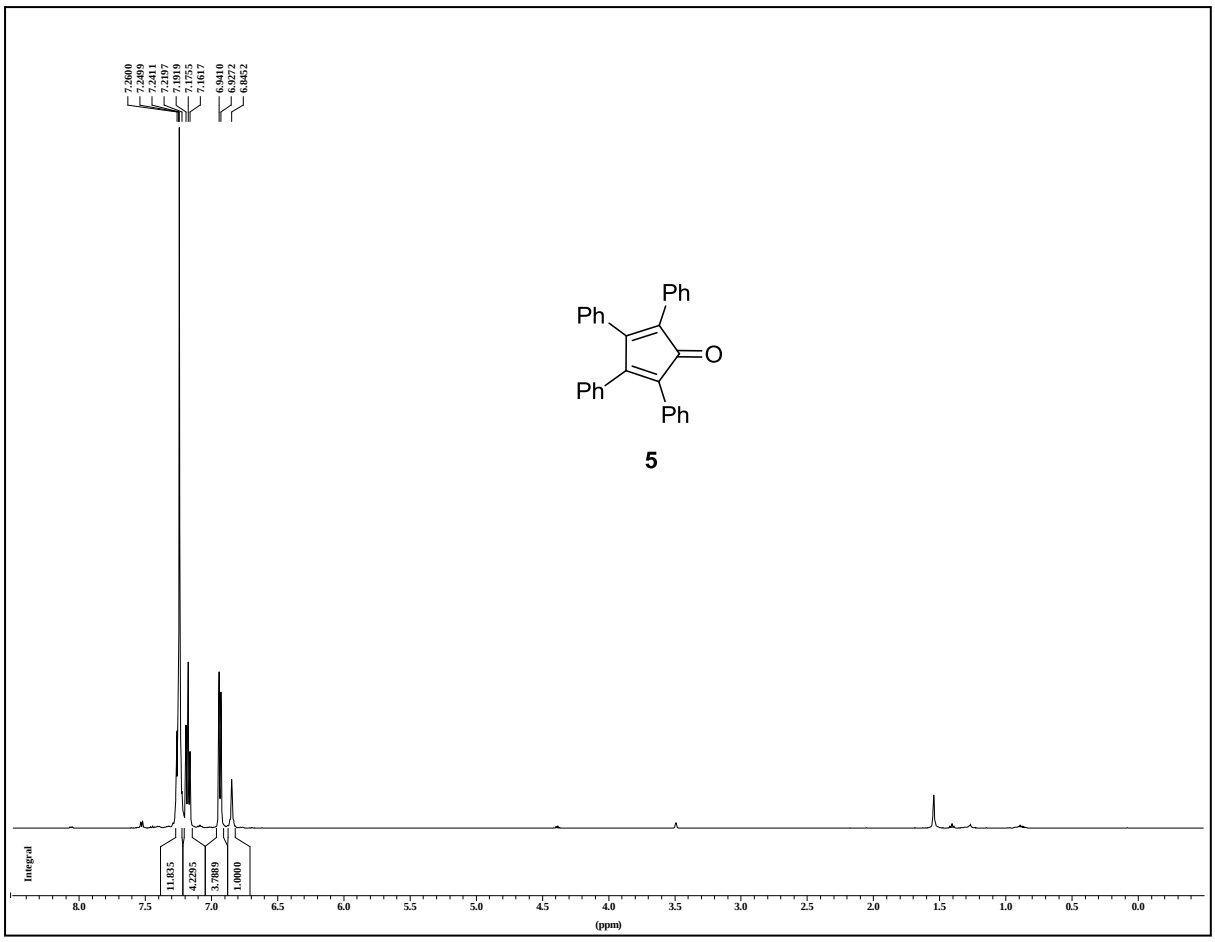
Ph
Ph
Ph
O
OH
O
4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7.2499
7.2411
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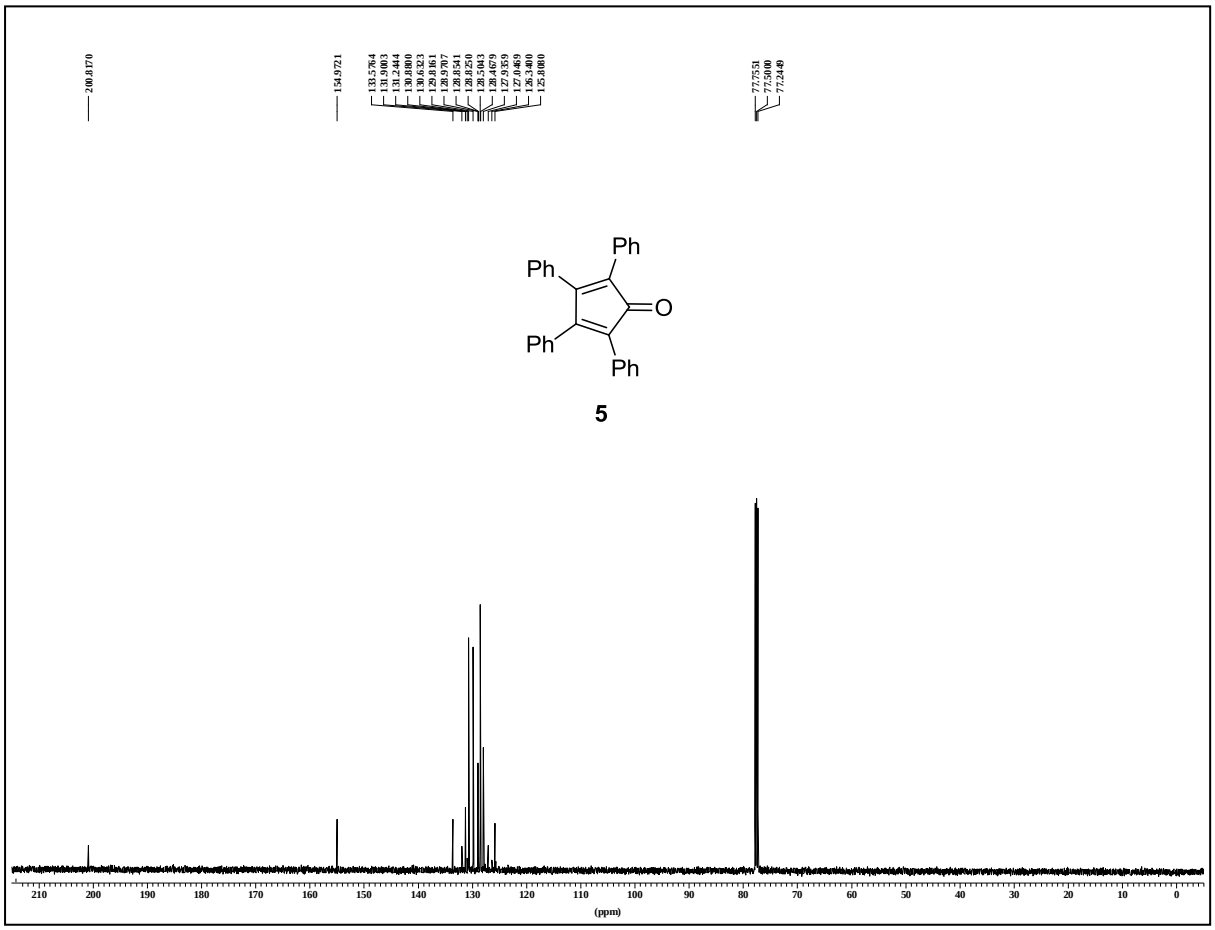
7.1919
7.1755
7.1617
6.9410
6.9272
6.8432
Ph
Ph
Ph
Ph
O
Integral
11.1835
4.2295
3.7889
1.0000
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
(ppm)

5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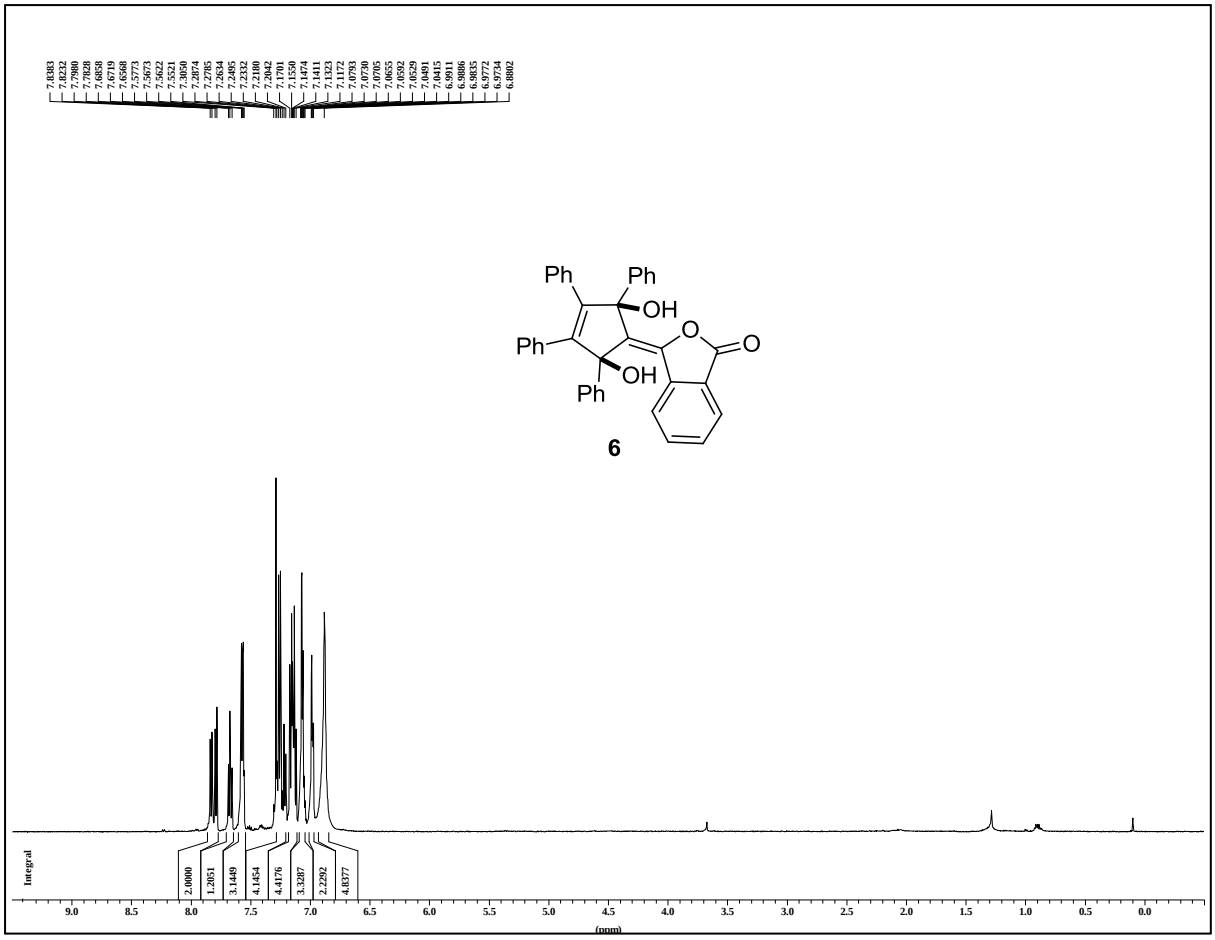
128.7455
128.4679
127.9359
127.0469
126.3400
125.8080
77.7551
77.5000
77.2449
Ph
Ph
Ph
Ph
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)

5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7.5673
7.5522
7.3521
7.3050
7.2874
7.2785
7.2634
7.2495
7.2332
7.2180
7.2042
7.1701
7.1550
7.1474
7.1411
7.1333
7.1177
7.0793
7.0730
7.0705
7.0655
7.0592
7.0529
7.0461
7.0415
6.9911
6.9886
6.9835
6.9772
6.9734
6.8862
Ph
Ph
OH
O
O
Ph
OH
Ph
6
Integral
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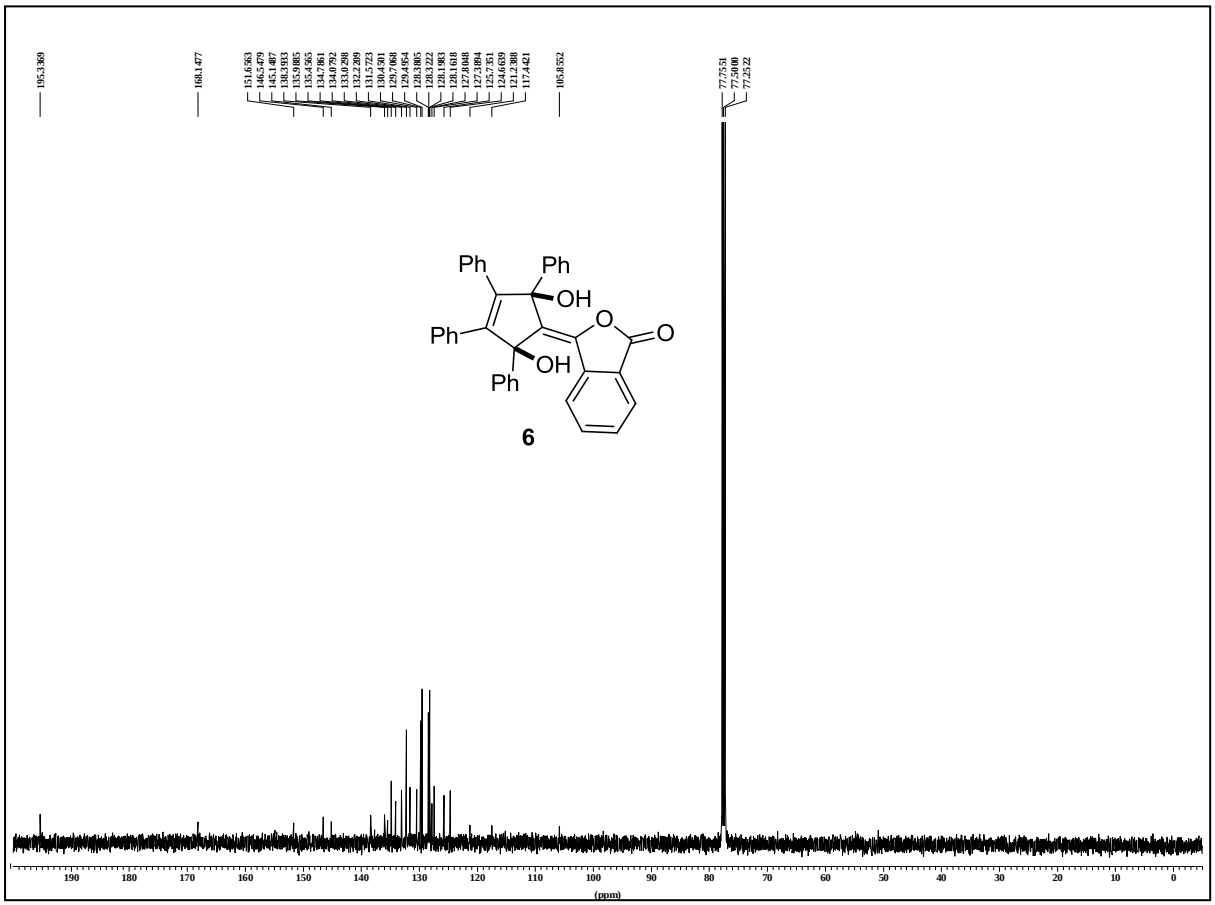
3.1449
4.1454
4.4176
3.3287
2.2292
4.8377
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
(ppm)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133.0298
132.2289
131.5723
130.4501
129.7068
129.4954
128.3805
128.3222
128.1983
127.9148
127.8048
127.3894
125.7351
124.6639
121.2388
117.4421
105.8552
77.7551
77.5000
77.2522
Ph
Ph
OH
O
O
Ph
OH
Ph
6
190
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120
110
100
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50
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20
10
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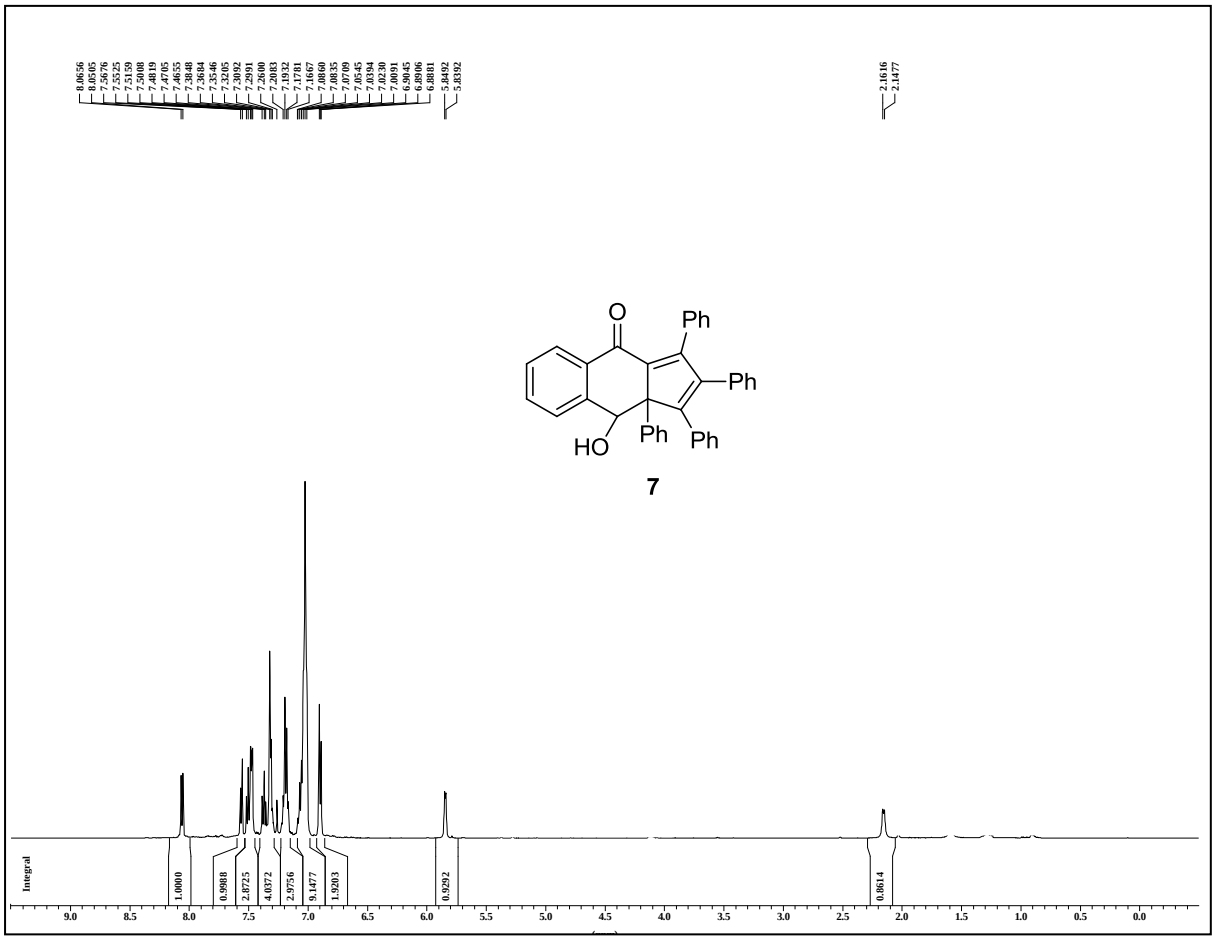
(ppm)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7.3546
7.3205
7.3092
7.2991
7.2690
7.2083
7.1933
7.1781
7.1667
7.0860
7.0835
7.0709
7.0545
7.0394
7.0230
7.0091
6.9045
6.8906
6.8881
5.8492
5.8392
2.1616
2.1477
O
Ph
Ph
Ph
Ph
HO
7
Integral
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2.8725
4.0372
2.9756
9.1477
1.9203
0.9292
0.8614
9.0
8.5
8.0
7.5
7.0
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6.0
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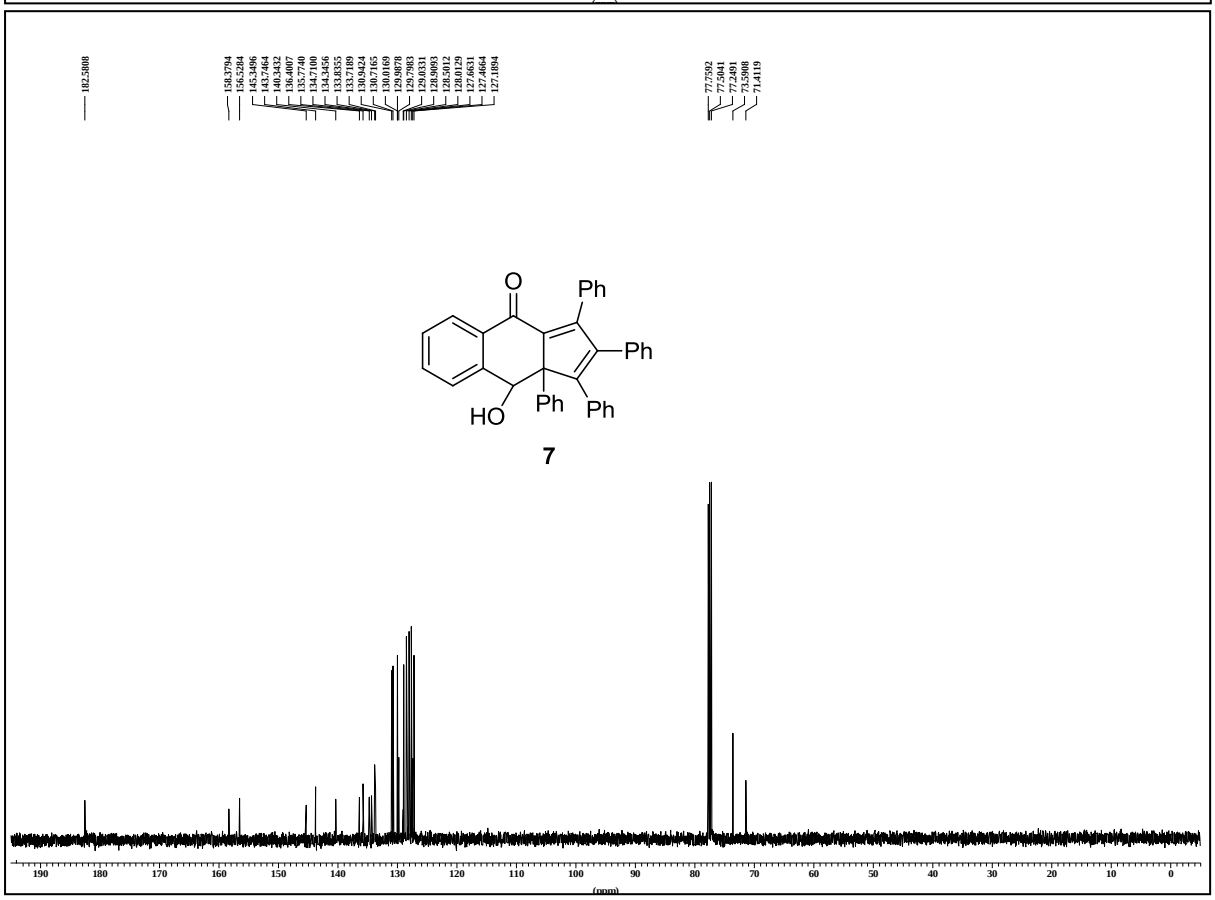
0.0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129.0331
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128.0129
127.6631
127.4464
127.1894
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77.5041
77.2491
73.5908
71.4119
O
Ph
Ph
Ph
Ph
HO
7
190
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160
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140
130
120
110
100
90
80
70
60
50
40
30
20
10
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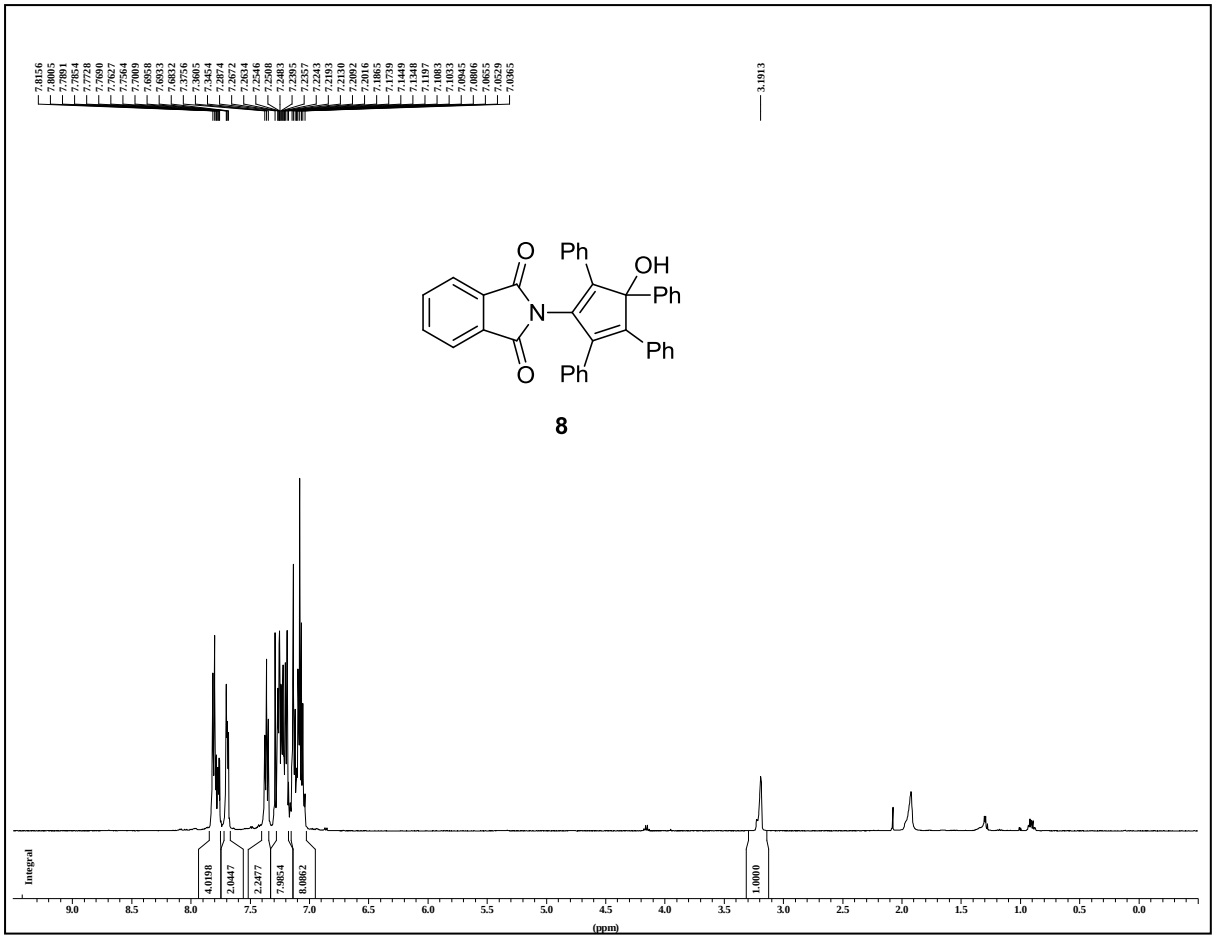
(ppm)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7.6833
7.6832
7.3756
7.3605
7.3454
7.2874
7.2672
7.2634
7.2546
7.2508
7.2483
7.2395
7.2357
7.2243
7.2193
7.2110
7.2092
7.2016
7.1865
7.1739
7.1449
7.1340
7.1197
7.1083
7.1033
7.0945
7.0806
7.0655
7.0529
7.0365
3.1913
O
Ph
OH
Ph
N
Ph
O
Ph
Integral
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2.0447
2.2477
7.9854
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1.0000
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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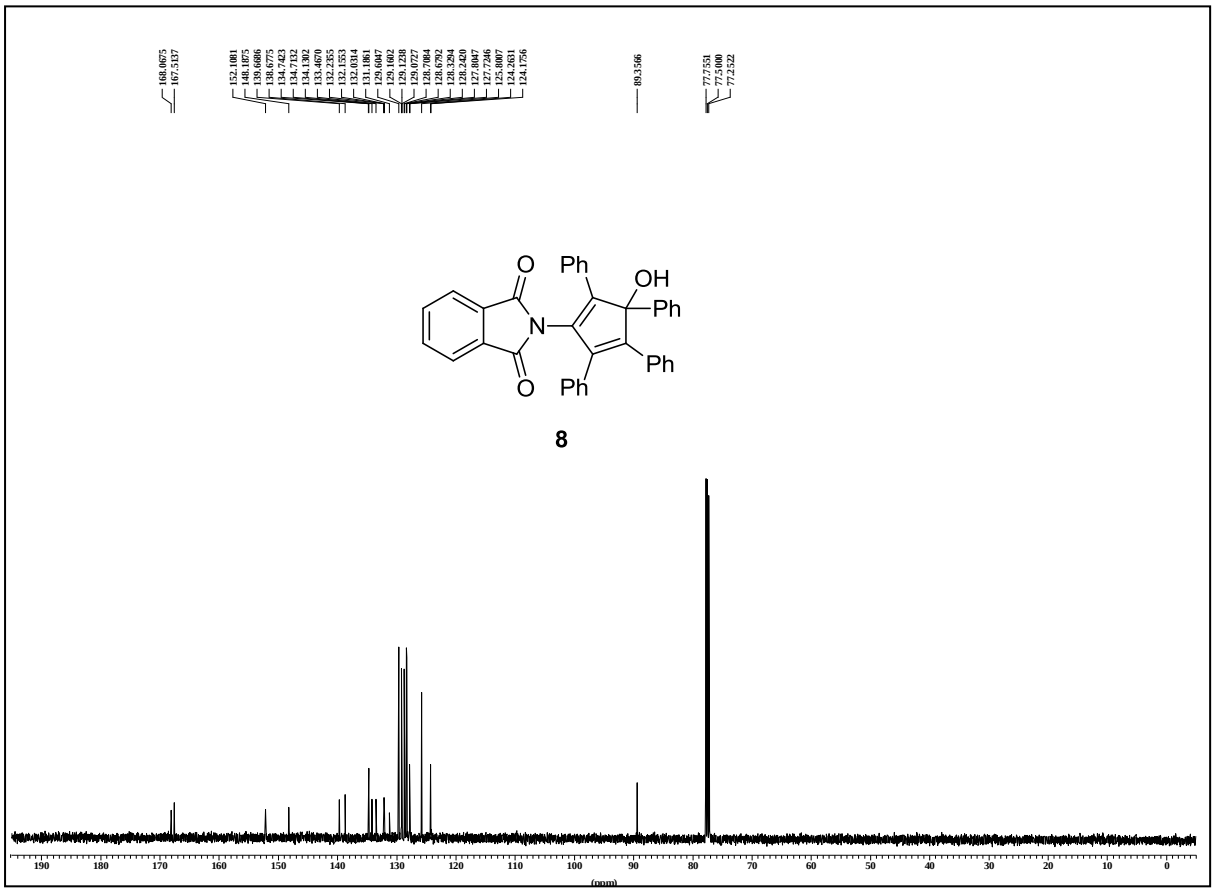
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
(ppm)

8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131.1861
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129.1602
129.1238
129.0727
128.7994
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128.3294
128.2420
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127.7246
125.1007
124.2631
124.1756
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77.5400
77.2522
O
Ph
OH
Ph
N
Ph
O
Ph
190
180
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120
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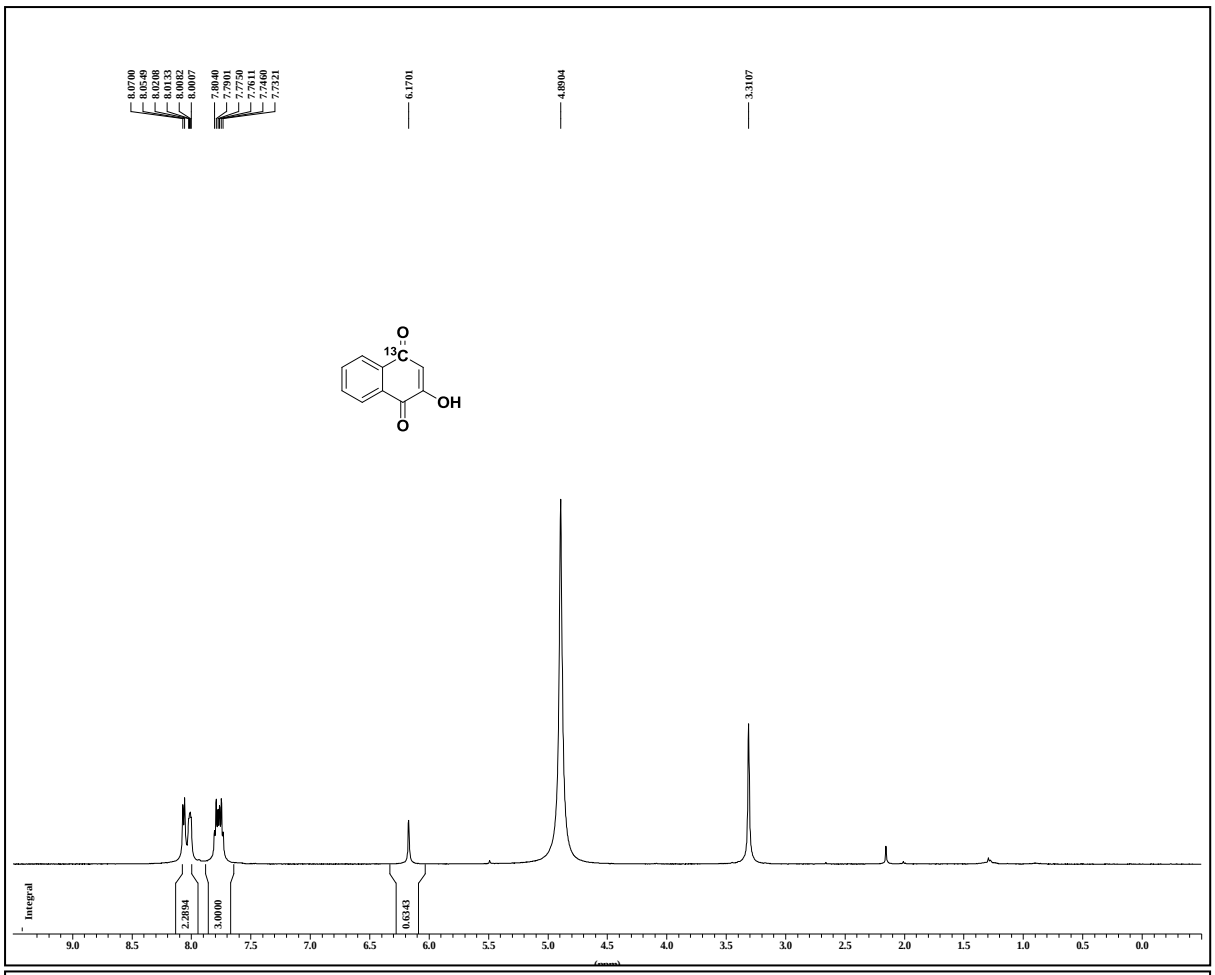
0
(ppm)

8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7.7750
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7.7460
7.7321
6.1701
4.8904
3.3107
O
13C
OH
O
Integral
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9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.5
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1.5
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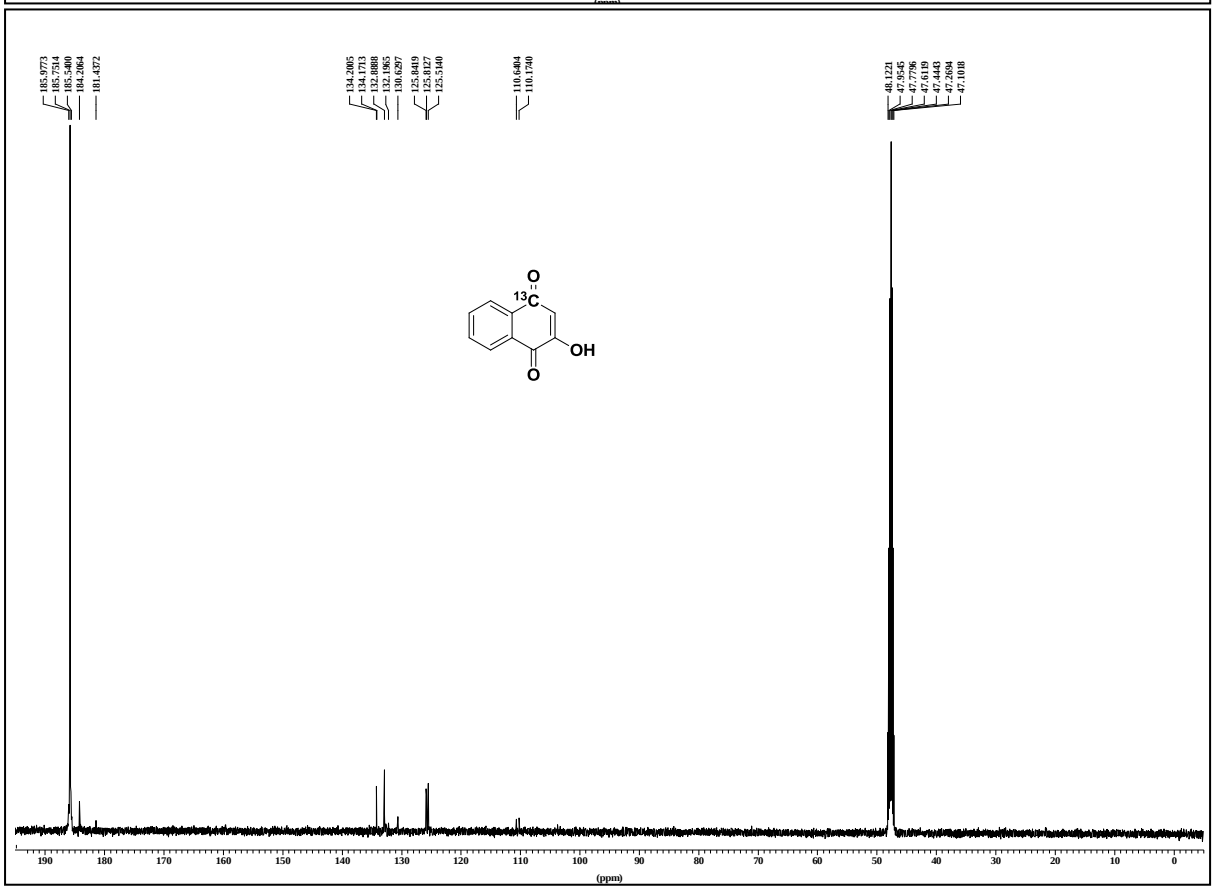
0.0
(ppm)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125.8127
125.5340
110.6404
110.1740
48.1221
47.9545
47.7796
47.6119
47.4443
47.2694
47.1018
O
13C
OH
O
190
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120
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100
90
80
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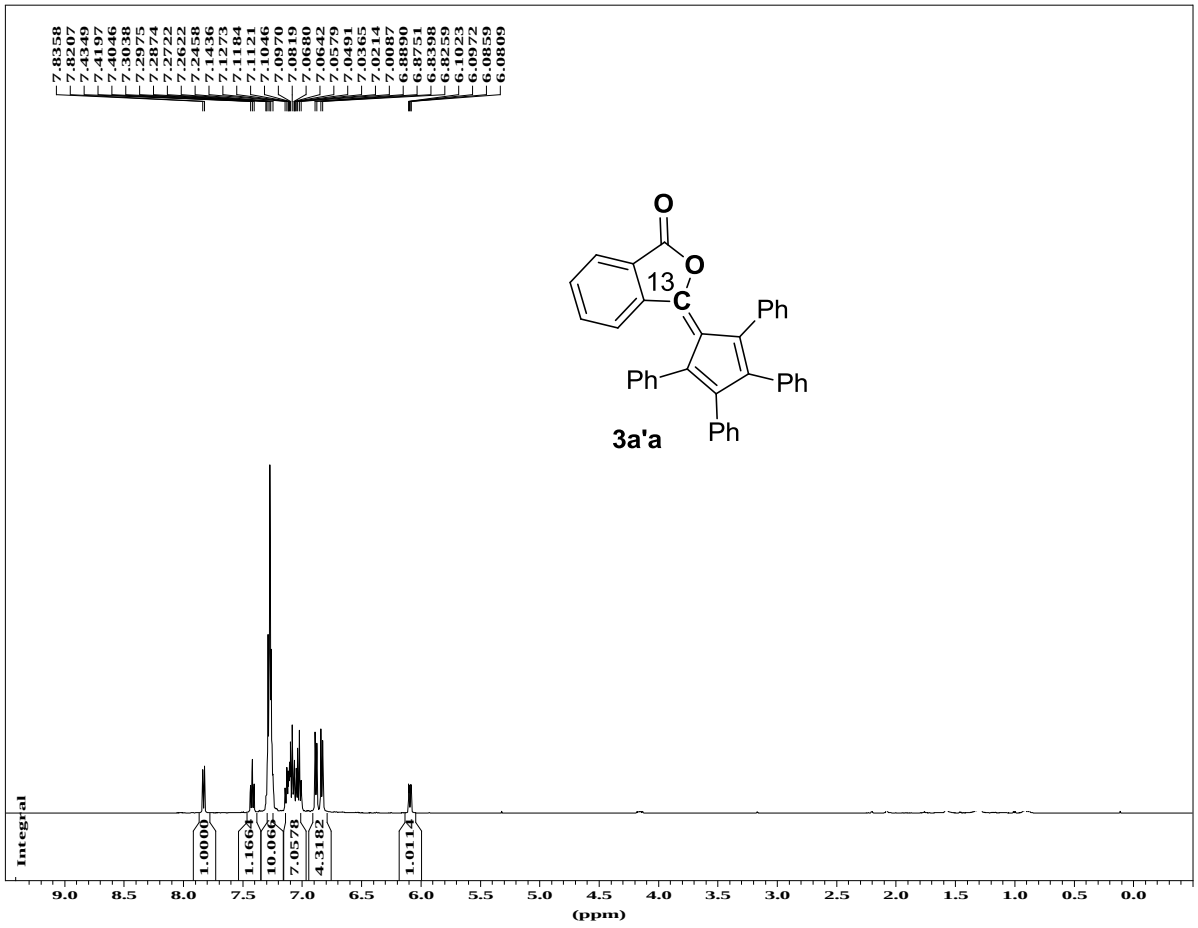
60
50
40
30
20
10
0
(ppm)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7.0579
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7.0365
7.0214
7.0087
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6.8751
6.8398
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6.0972
6.0859
6.0809
O
O
13
C
Ph
Ph
Ph
Ph
3a'a
Integral
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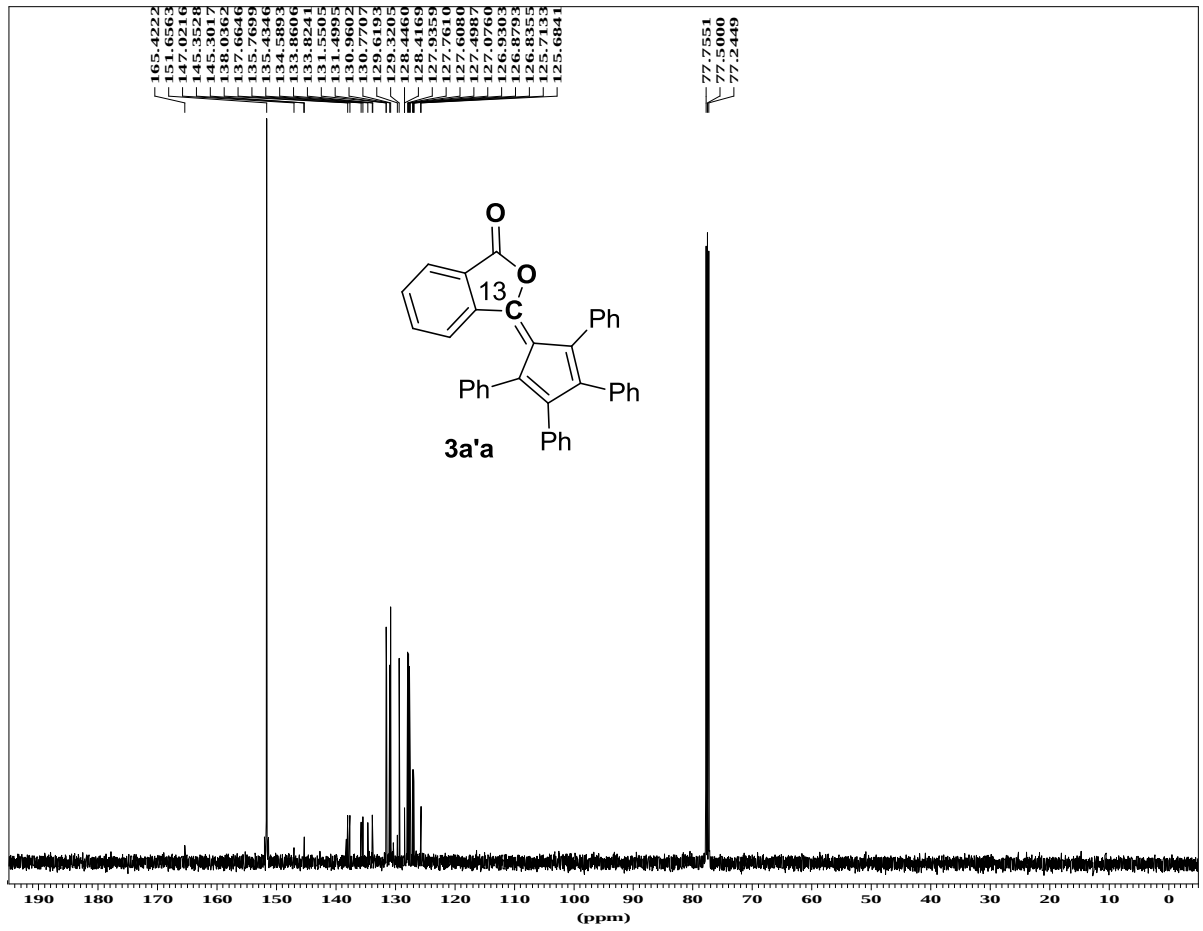
10.066
7.0578
4.3182
1.0114
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)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128.4460
128.4169
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127.7610
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126.8355
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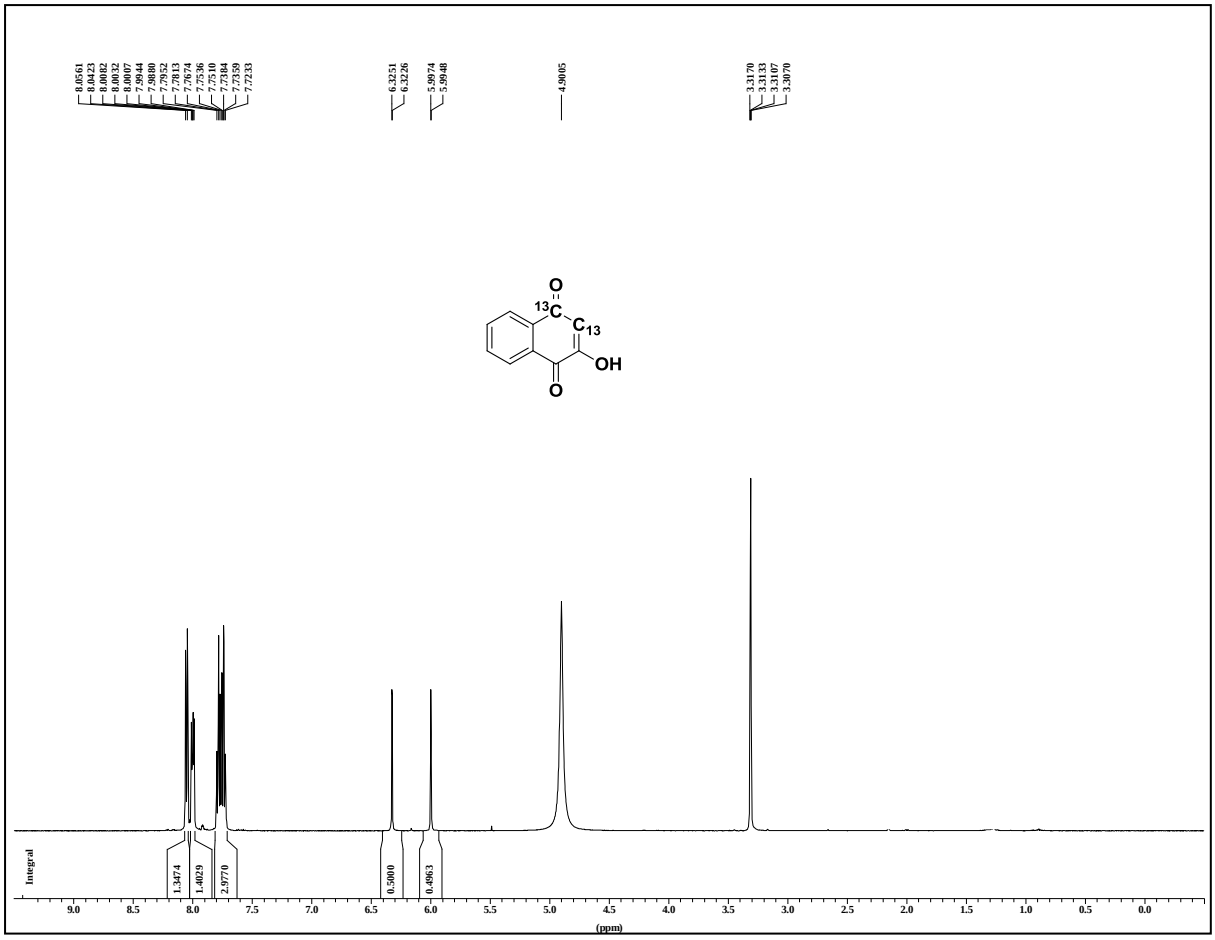
77.7551
77.5000
77.2449
O
O
13
C
Ph
Ph
Ph
Ph
3a'a
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)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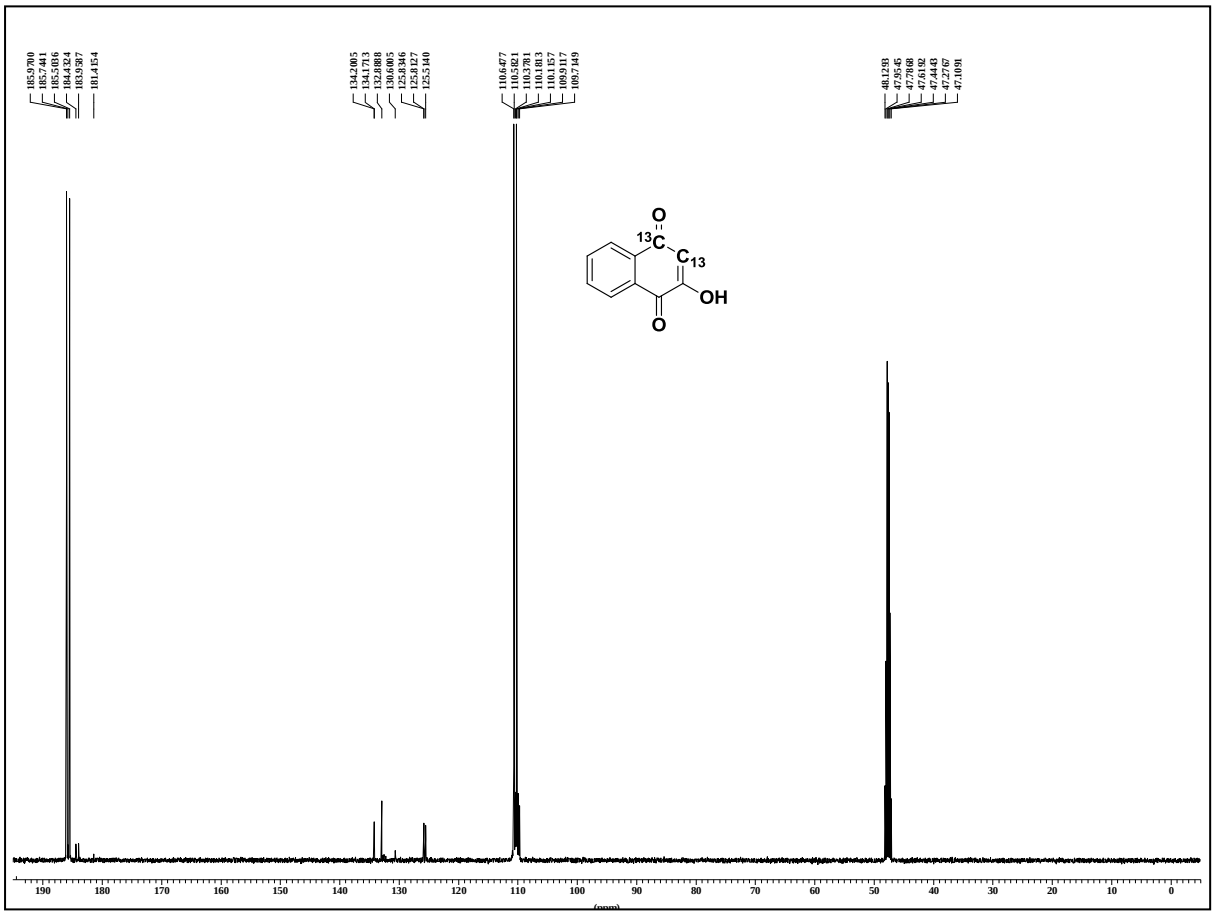
7.7384
7.7359
7.7233
6.3251
6.3226
5.9974
5.9948
4.9005
3.3170
3.3133
3.3107
3.3070
O
13C
C13
OH
O
Integral
1.3474
1.4029
2.9770
0.5000
0.4963
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)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109.9117
109.7149
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47.9545
47.7868
47.6192
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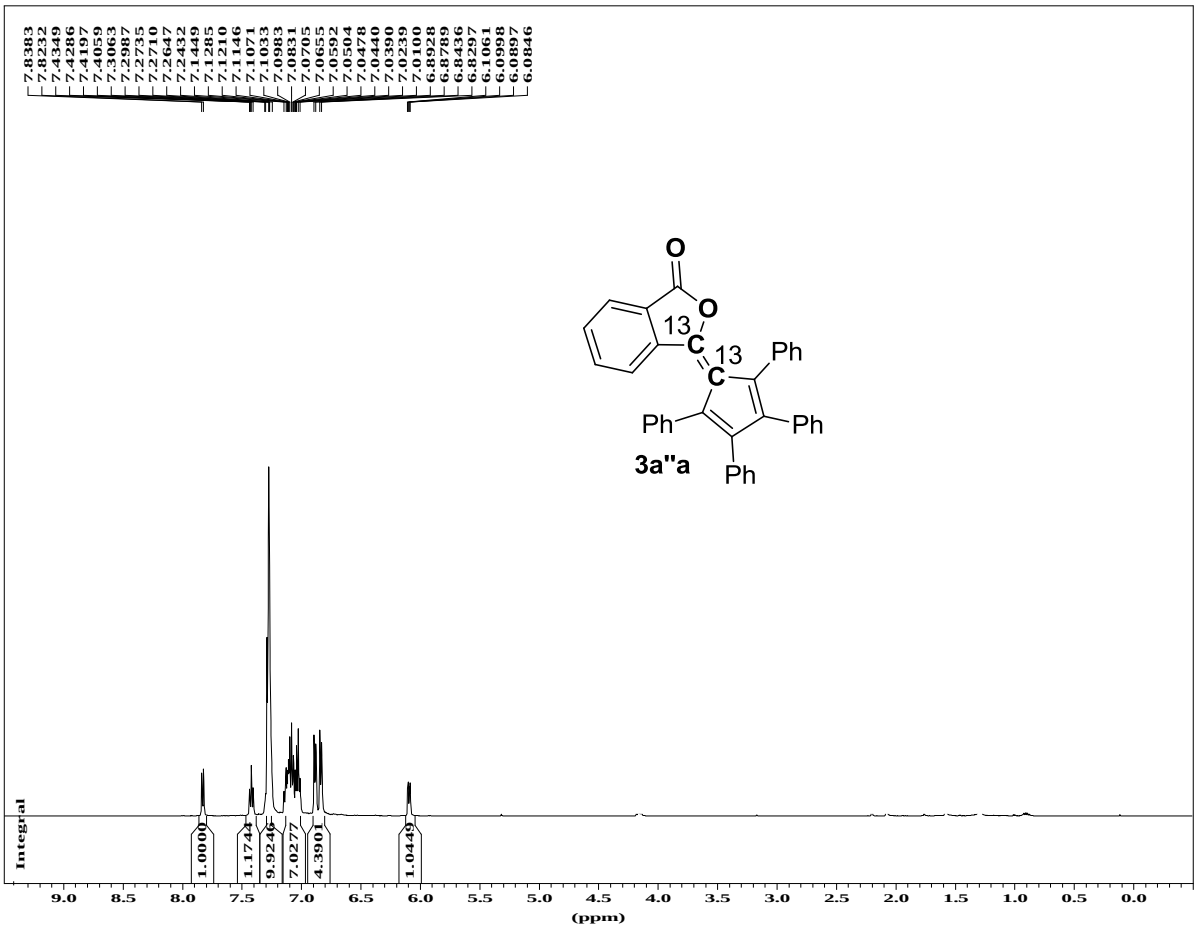
O
13C
C13
OH
O
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)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7.8232
7.4346
7.4286
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7.2735
7.2710
7.2647
7.2432
7.1449
7.1285
7.1210
7.1146
7.1071
7.1033
7.0983
7.0831
7.0705
7.0655
7.0592
7.0504
7.0478
7.0440
7.0390
7.0239
7.0100
6.8928
6.8789
6.8436
6.8297
6.1061
6.0998
6.0897
6.0846
O
O
13
C
13
C
Ph
Ph
Ph
Ph
3a''a
Integral
1.0000
1.1744
9.9246
7.0027
4.3901
1.0449
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
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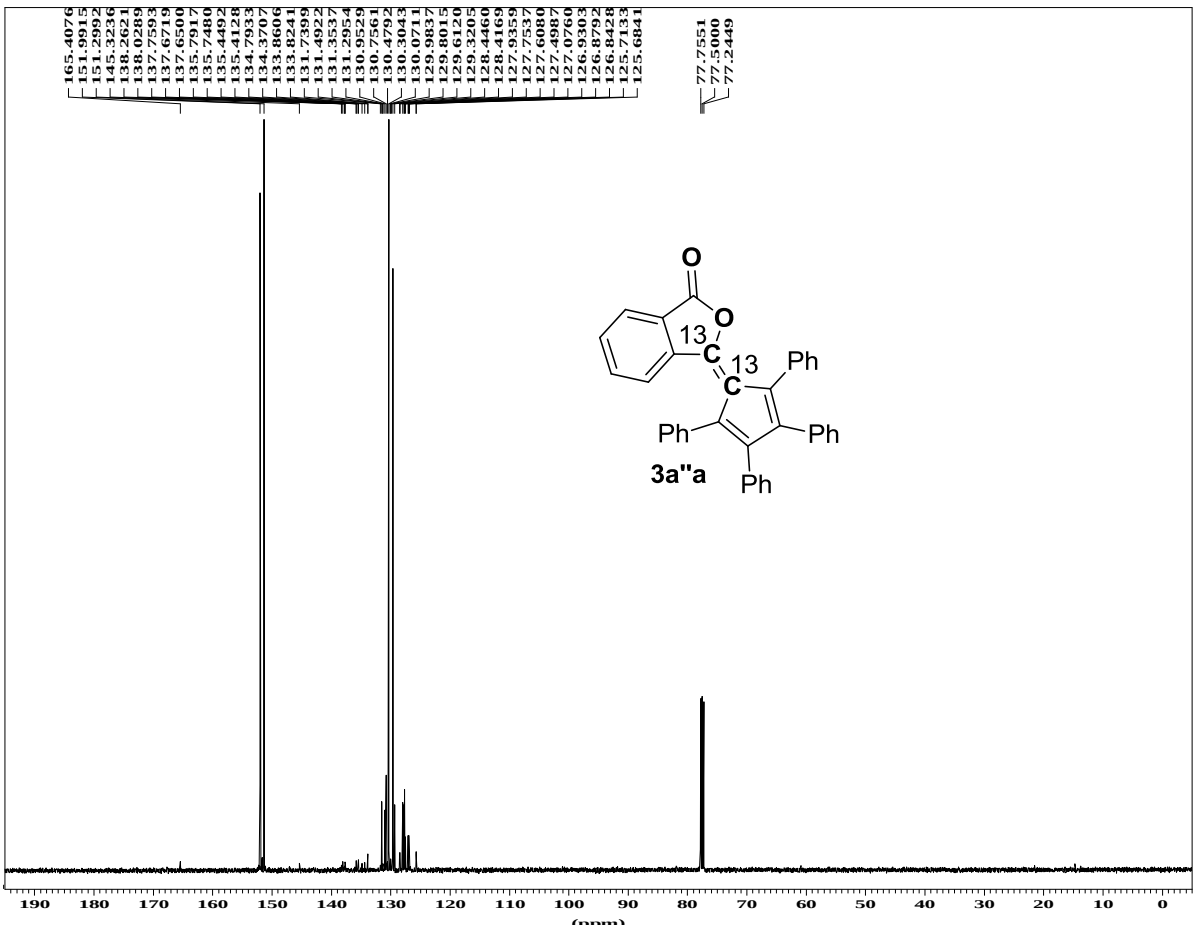
0.0
(ppm)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135.4492
135.4128
134.7933
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133.8606
133.8241
131.7399
131.4922
131.3537
131.2954
130.9529
130.7561
130.4792
130.3043
130.0711
129.9837
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128.4460
128.4169
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127.4987
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77.7551
77.5000
77.2449
O
O
13
C
13
C
Ph
Ph
Ph
Ph
3a''a
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)