Supporting Information

X-ray Absorption and Electron Paramagnetic Resonance Guided Discovery of the Cu-Catalyzed Synthesis of Multiaryl-Substituted Furans from Aryl Styrene and Ketones Using DMSO as the Oxidant

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1. EPR Data Collection and Analysis

1.1 General Information

EPR spectra were recorded on a Bruker X-band A200 spectrometer. The samples were taken out into a small tube, and then recorded by EPR spectrometer at indicated temperature and parameters. DMSO was degassed the air by the method of freeze-pump-thaw cycle for 5 times.

1.2 Experimental Details

1.2.1 The interaction between DMSO and CuBr

To an oven-dried Schlenk tube equipped with a stir bar was loaded with *CuBr* (72 mg, 0.5 mmol) in glovebox, subsequently, *DMSO* (5 mL) was injected into the tube, the solution sample was taken out into a small tube, then analyzed by EPR at 5 mins, 30 mins, 60 mins and 120 mins. EPR spectrum was recorded at 298 K on EPR spectrometer operated at 9.4158 GHz. Typical spectrometer parameters are shown as follows: Scan range: 100 G; center field set: 3359.8 G; time constant: 163.84 ms; scan time: 30.72 s; modulation amplitude: 1.0 G; modulation frequency: 100 kHz; receiver gain: 1.00×10^5; microwave power: 19.05 mW.

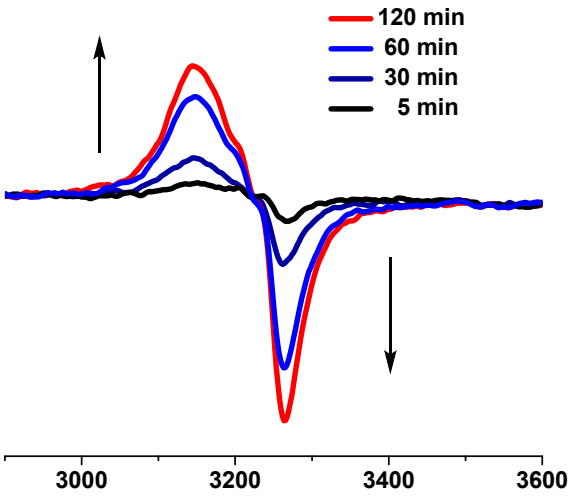


Fig S1. CuBr (0.5 mmol) in DMSO (5.0 mL) at rt under N_2.

1.2.2 The interaction between deoxybenzoin and $CuBr_2$

A dried Schlenk tube equipped with a stir bar was loaded with *$CuBr_2$* (0.5 mmol, 112 mg), deoxybenzoin (1.0 mmol, 196 mg) and *DMF* (5 mL) under the atmosphere of nitrogen at 100 ℃. The solution sample was taken out into a small tube, then analyzed by EPR at 5 mins, 30 mins, 60

mins and 120 mins. EPR spectrum was recorded at 298 K on EPR spectrometer operated at 9.4158 GHz. Typical spectrometer parameters are shown as follows: Scan range: 100 G; center field set: 3359.8 G; time constant: 163.84 ms; scan time: 30.72 s; modulation amplitude: 1.0 G; modulation frequency: 100 kHz; receiver gain: 1.00×10^5; microwave power: 19.05 mW.

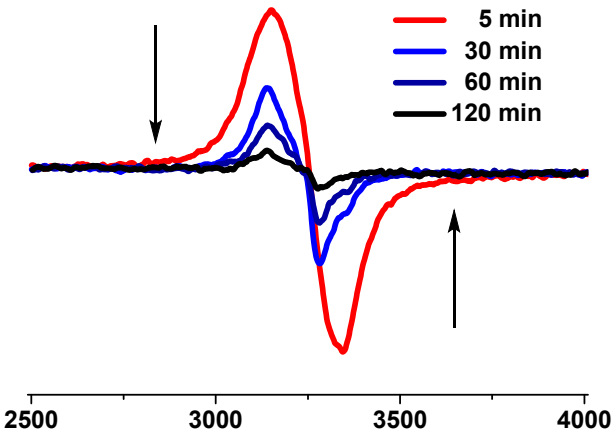


Fig S2. $CuBr_2$ (0.5 mmol) in DMF (5.0 mL), deoxybenzoin (1.0 mmol) at 100 ℃ under N_2.

2. XANES and EXAFS Data Collection and Analysis

2.1 General Information

X-ray absorption measurements were acquired on the insertion device beam line of the Materials Research Collaborative Access Team (MRCAT) at the Advanced Photon Source, Argonne National Laboratory and the beamline 17C1 of National Synchrotron Radiation Research Center (NSSRC) in Taiwan. The data were collected in transmission quick scan mode. Insertion device experiments utilized a cryogenically cooled double-crystal Si (111) monochromator. The monochromator was scanned continuously during the measurements with data points integrated over 0.5 eV for 0.03 s per data point. The ionization chambers were optimized for the maximum current with linear response (~10^{10} photons detected/sec) with 10% absorption (N_2) in the incident ion chamber and 70% absorption (60% N_2 and 40% Ar) in the transmission detector. A Cu foil spectrum (edge energy 8979 eV) was acquired simultaneously with each measurement for energy calibration. Multiple scans were taken to reduce the noise.

All solution samples were placed in a sample holder (the XAS solution cell) made of PEEK (polyether ether ketone) equipped with a screw top and O-ring fitting to prevent exposure to air and water.[1] For solution samples, the Cu concentration was adjusted to be 0.05 - 0.1 M with a path length of 3.5 mm. The sample holder was placed in a quartz tube (1–in. OD, 10–in. length) sealed with Kapton windows by two Ultra-Torr fittings and then used for transmission mode measurement.

The edge energy of the X-Ray absorption near edge structure (XANES) spectrum was determined from the inflection point in the edge, i.e., the maximum in the first derivative of the XANES spectrum. The pre-edge energy was determined from the maximum of the pre-edge peak.

Background removal and normalization procedures were carried out using the Athena software package using standard methods.[2] Standard procedures based on Artemis software (Demeter 0.9.20) were used to extract the extended X-ray absorption fine structure (EXAFS) data. The coordination parameters were obtained by a least square fit in R-space of the nearest neighbor, k^2 weighted Fourier transform data.

2.2 Experimental Details

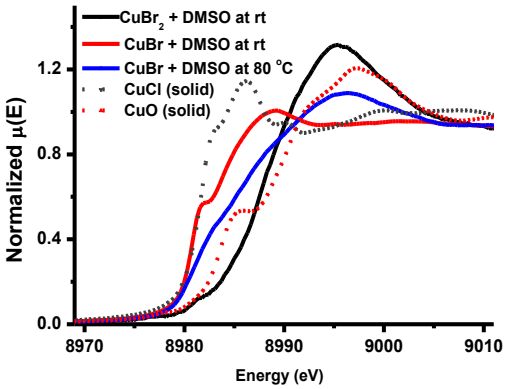
$CuBr_2$ / DMSO solution: $CuBr_2$ (0.1 mmol, 11.2 mg) was added to the XAS solution cell in a glovebox beforehand. Then, 5.0 mL of DMSO was injected into the cell and the solution was stirred under N_2 at room temperature for 5 minutes. XANES spectrum was measured at room temperature.

CuBr / DMSO solution: CuBr (0.1 mmol, 7.2 mg) was added to the XAS solution cell in a glovebox beforehand. Then, 5.0 mL of DMSO was injected into the cell and the solution was stirred under N_2 at room temperature for 5 minutes. XANES spectrum was measured at room temperature.

CuBr / DMSO solution at 80 ℃ : CuBr (0.1 mmol, 7.2 mg) was added to the XAS solution cell in a glovebox beforehand. Then, 5.0 mL of DMSO was injected into the cell and the solution was stirred under N_2 at 80 ℃ for 120 minutes. XANES spectrum was measured at room temperature.

CuCl solid sample: CuCl was mixed with boron nitride to a weight ratio of about 2% (Cu) in the glove box. The mixture was grinded well with mortar and pestle, and then 25 mg of the mixture was pressed into a cylindrical sample holder consisting of six wells with a radius of 2.0 mm, forming a self-supporting wafer. The sample holder was placed in a quartz tube (1–in. OD, 10–in. length) sealed with Kapton windows by two Ultra-Torr fittings and then used for transmission mode measurement.

CuO solid sample: CuO was mixed with boron nitride to a weight ratio of about 2% (Cu) in air. The mixture was grinded well with mortar and pestle, and then 25 mg of the mixture was pressed into a cylindrical sample holder consisting of six wells with a radius of 2.0 mm, forming a self-supporting wafer. The sample holder was placed in a quartz tube (1–in. OD, 10–in. length) and then used for transmission mode measurement.



XANES spectra of the oxidation process: CuBr (0.1 mmol, 7.2 mg) was added to the XAS solution cell in a glovebox beforehand. Then, 5.0 mL of DMSO was injected into the cell and the solution was stirred under N_2 at room temperature for 5 minutes. XANES spectrum was measured at intervals (2 minutes) at room temperature.

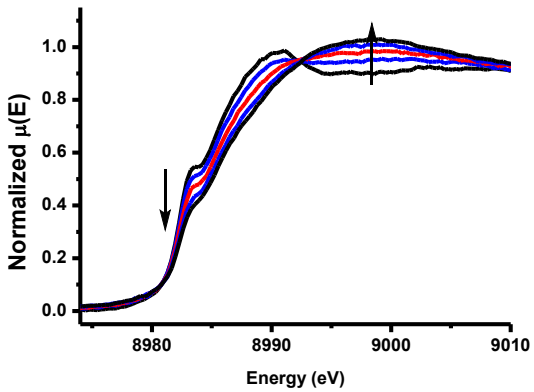


Table S1 Edge Energy and Oxidation States

sample	Pre-edge Energy (eV)	Edge Energy (eV)	Oxidation State
Cu foil	N.A.	8979.0	0
CuCl (Solid)	N.A.	8982.0	+1
CuO (solid)	8978.3	8983.3	+2

3. Detail of the reaction

3.1 General considerations

Unless otherwise noted, all reagents were purchased from commercial suppliers and used without purification. All the solvents were purified according to the solvents handbook. All reactions were performed in resealable screw-capped Schlenk tube (approx. 20 mL volume) in the presence of Teflon-coated magnetic stirrer bar (4 mm × 10 mm). General procedures for coupling reactions. Thin layer chromatography was performed on Merck precoated silica gel 60 F_{254} plates. Silica gel (Merck, 70-230 and 230-400 mesh) was used for column chromatography. High resolution mass spectra (HRMS) were measured with a Waters Micromass GCT instrument. ^{1}H NMR spectra were recorded with ADVANCE III (400 MHz). Spectra were referenced internally to the residual proton resonance in $CDCl_3$ (δ 7.27 ppm), or with tetramethylsilane (TMS, δ 0.00 ppm) as the internal standard. Chemical shifts (δ) were reported as part per million (ppm) in δ scale downfield from TMS. ^{13}C NMR spectra were referenced to $CDCl_3$ (δ 77.0 ppm, the middle peak). Coupling constants (*J*) were reported in Hertz (Hz).

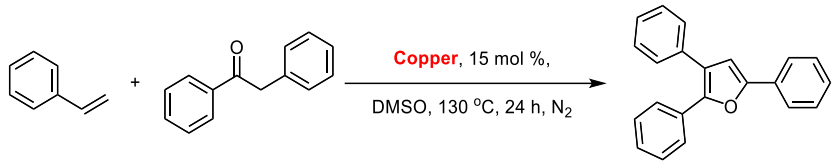
3.2 Experimental details

3.2.1 General Procedure for synthesis of Multiaryl-Substituted Furan:

To an oven-dried Schlenk tube equipped with a stir bar was added *$CuCl_2$* (0.037 mmol, 5 mg), *deoxybenzoin* (0.4 mmol, 78.4 mg), Then, *styrenes* (0.25 mmol, 28.6 μL) and *DMSO* (1 mL) were successively injected in the reaction tube with magnetic stirring. The reaction mixture was allowed to stir vigorously at 120 ℃ for 40 h. Thereafter, the reaction mixture was cooled to room temperature and extracted thrice with ethyl acetate (3 * 5 mL). The organic layer was collected and dried over anhydrous Na_2SO_4. After filtration and evaporation of the solvent, the resulting crude product was separated on a silica gel column with hexane and dichloromethane as eluent to afford the desired product.

3.2.2 Impact of reaction parameters

Table S1: Impact of varying copper catalyst [a]

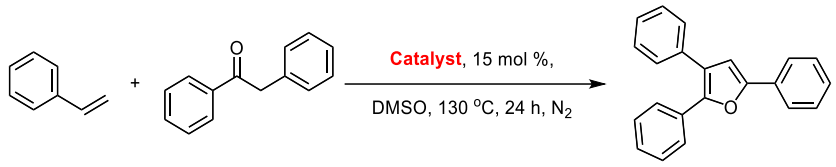


1a **2a** **4a**

entry	Copper	**4a** yield (%)[b]
1	none	n.d.
2	$CuBr_2$	26
3	CuBr	13
4	$CuCl_2$	67
5	CuCl	9
6	CuI	15
7	$Cu(OAc)_2$	Trace
8	$Cu(acac)_2$	n.d.
9	$CuSO_4•5H_2O$	n.d.
10	$Cu(OTf)_2$	15
11	CuF_2	n.d.
12	CuCN	n.d.
13[d]	$CuCl_2$	20

[a] Conditons: styrene (0.25 mmol), ketone (0.4 mmol), catalyst (15 mol %), DMSO (1 mL), 130 ℃ for 24 h under N_2. [b] calibrated GC yields were reported using dodecane as the internal standard. [c]120 °C for 40 h. [d] DMF was used as solvent, under air atmosphere.

Table S2: Impact of varying different catalyst [a]

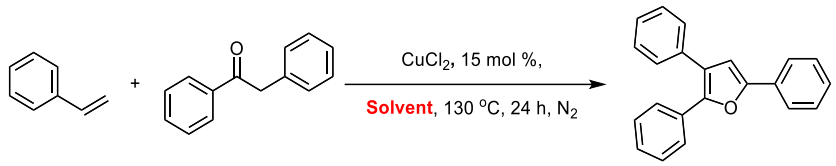


1a **2a** **4a**

entry	Catalyst	**4a** yield (%)[b]
1	$CuCl_2$	67
2	$CuCl_2•2H_2O$	64
3	$NiBr_2$	n.d.
4	$NiCl_2$	n.d.
5	$CoCl_2$	n.d.
6	$MnCl_2$	n.d.
7	AgI	n.d.
8	$PdCl_2$	trace.
9	I_2	trace.
10	Bu_4NI	n.d..
11	NBS	trace.
12	Bu_4NCl	n.d.
13	$ZnCl_2$	n.d.
14	$AlCl_3$	n.d.

[a] Conditons: styrene (0.25 mmol), ketone (0.4 mmol), catalyst (15 mol %), DMSO (1 mL), 130 ℃ for 24 h under N_2. [b] calibrated GC yields were reported using dodecane as the internal standard.

Table S3: Impact of different solvent [a]

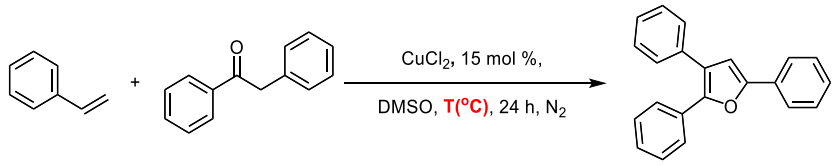


1a **2a** **4a**

entry	solvent	**4a** yield (%)[b]
1	DMF	n.d.
2	NMP	n.d.
3	toluene	n.d.
4	dioxane	n.d.
5	MeCN	n.d.
6	t-BuOH	n.d.

[a] Conditons: styrene (0.25 mmol), ketone (0.4 mmol), $CuCl_2$ (15 mol %), Solvent (1 mL), 130 ℃ for 24 h under N_2. [b] calibrated GC yields were reported using dodecane as the internal standard.

Table S4: Optimization of reaction Temperature [a]

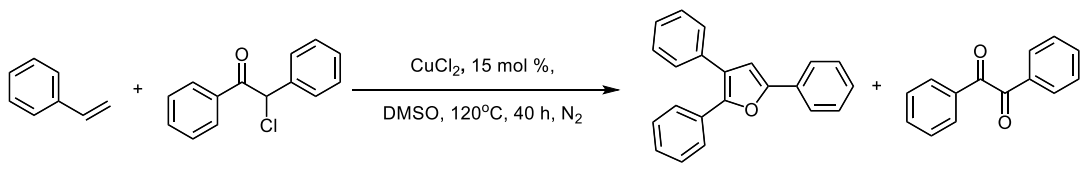


1a **2a** **4a**

entry	temperature (℃)	**4a** yield (%)[b]
1	140	20
2	130	67
3	120	52
4	110	13
5	100	trace
6[c]	120	82

[a] Conditons: styrene (0.25 mmol), ketone (0.4 mmol), $CuCl_2$ (15 mol %), DMSO (1 mL), T ℃ for 24 h under N_2. [b] calibrated GC yields were reported using dodecane as the internal standard. [c] 40 h.

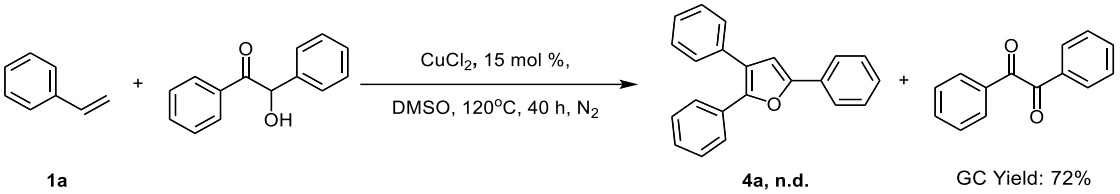
3.2.3 **Intermediate experiments**



1a **4a, n.d.** GC Yield: 90%

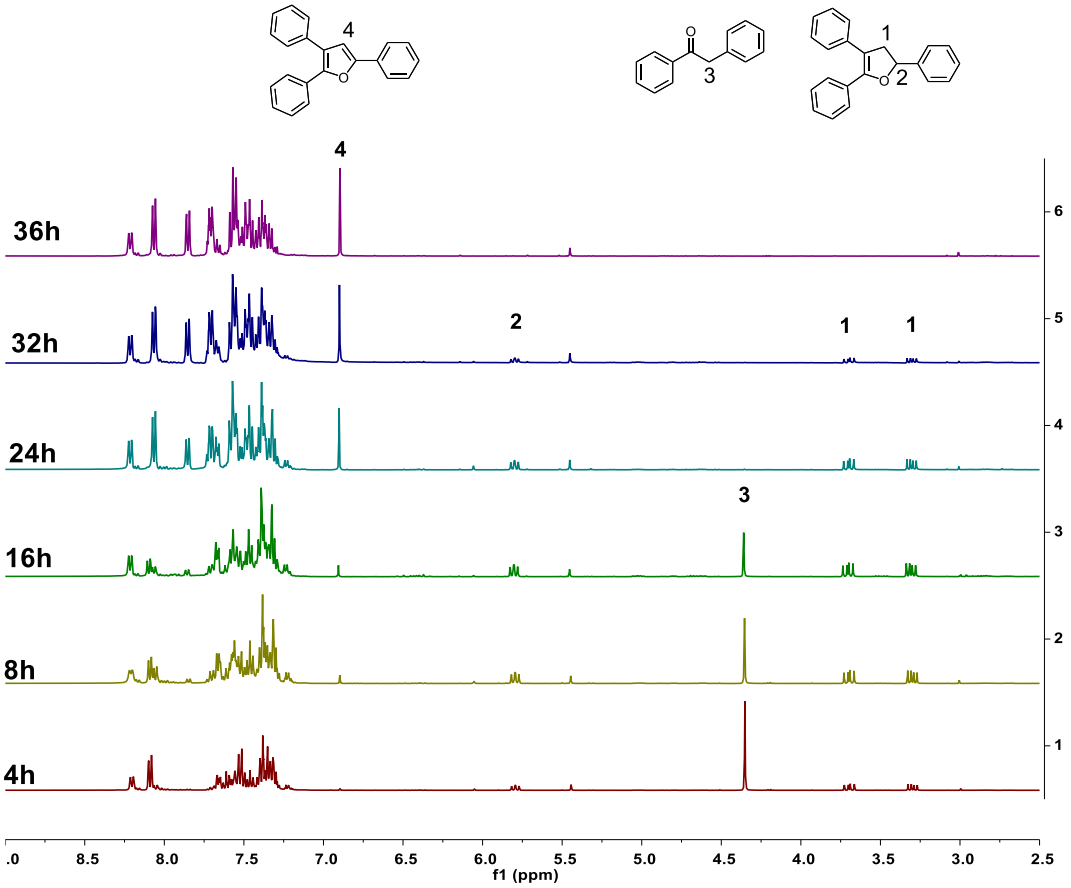
To an oven-dried Schlenk tube equipped with a stir bar was added *$CuCl_2$* (0.037 mmol, 5 mg), *desyl chloride* (0.4 mmol, 92 mg), Then, *styrenes* (0.25 mmol, 28.6 μL) and *DMSO* (1 mL) were successively injected in the reaction tube with magnetic stirring. The reaction mixture was allowed

to stir vigorously at 120 ℃ for 40 h. Thereafter, ethyl acetate (~3 mL), dodecane (57 mg, internal standard) and water (~2 mL) were added. The organic layer was subjected to GC analysis. The GC yield was previously calibrated by authentic sample/dodecane calibration curve.



To an oven-dried Schlenk tube equipped with a stir bar was added *$CuCl_2$* (0.037 mmol, 5 mg), *2-hydroxy-2-phenylacetophenone* (0.4 mmol, 84.8 mg), Then, *styrenes* (0.25 mmol, 28.6 μL) and *DMSO* (1 mL) were successively injected in the reaction tube with magnetic stirring. The reaction mixture was allowed to stir vigorously at 120 ℃ for 40 h. Thereafter, ethyl acetate (~3 mL), dodecane (57 mg, internal standard) and water (~2 mL) were added. The organic layer was subjected to GC analysis. The GC yield was previously calibrated by authentic sample/dodecane calibration curve.

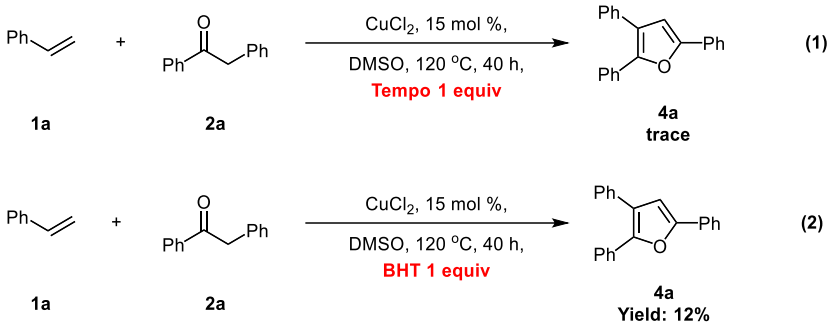
3.2.4 ^{1}H NMR experiment



The reaction between **1a** and **2a** in DMSO monitored by ^{1}H NMR: To an oven-dried Schlenk tube equipped with a stir bar was added *$CuCl_2$* (0.037 mmol, 5 mg), ***2a*** (0.4 mmol, 78.4 mg), Then, *styrenes* (0.25 mmol, 28.6 μL) and *DMSO* (1 mL) were successively injected in the reaction tube with magnetic stirring. The reaction mixture was allowed to stir vigorously at 120 ℃ for 4 h, 8 h,

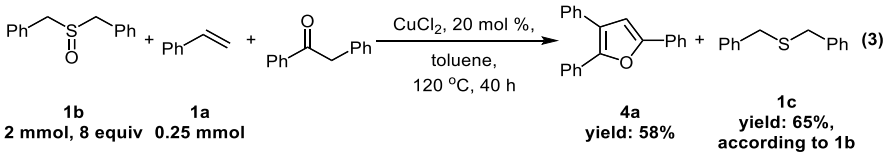
16 h, 24 h, 32 h and 36 h, respectively. Then, ethyl acetate (~3 mL) and water (~5 mL) were added. The organic layer was collected and concentrated. Thereafter, 0.5 mL of $CDCl_3$ was added, the mixture was detected by ^1H NMR.

3.2.5 Radical-trapping/inhibiting experiments



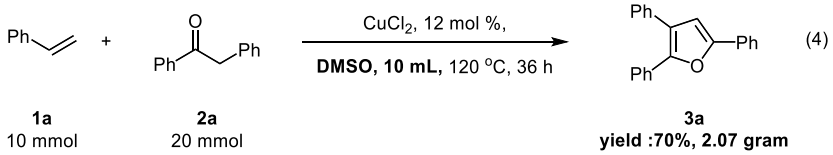
To an oven-dried Schlenk tube equipped with a stir bar was added *CuCl₂* (0.037 mmol, 5 mg), ***2a*** (0.4 mmol, 78.4 mg), Then, *styrenes* (0.25 mmol, 28.6 μL), Tempo (0.25 mmol, 39 mg) or BHT (0.25 mmol, 55 mg) and *DMSO* (1 mL) were successively injected in the reaction tube with magnetic stirring. The reaction mixture was allowed to stir vigorously at 120 ℃ for 40 h. Thereafter, ethyl acetate (~3 mL), dodecane (57 mg, internal standard) and water (~2 mL) were added. The organic layer was subjected to GC analysis. The GC yield was previously calibrated by authentic sample/dodecane calibration curve.

3.2.6 Reaction with dibenzyl sulfoxide instead of DMSO



To an oven-dried Schlenk tube equipped with a stir bar was added *CuCl₂* (0.05 mmol, 6.7 mg), ***2a*** (0.4 mmol, 78.4 mg), Then, *styrenes* (0.25 mmol, 28.6 μL), ***1b*** (2 mmol, 460 mg) and toluene (1 mL) were successively injected in the reaction tube with magnetic stirring. The reaction mixture was allowed to stir vigorously at 120 ℃ for 40 h. Thereafter, ethyl acetate (~3 mL), dodecane (57 mg, internal standard) and water (~2 mL) were added. The organic layer was subjected to GC analysis. The GC yield was previously calibrated by authentic sample/dodecane calibration curve.

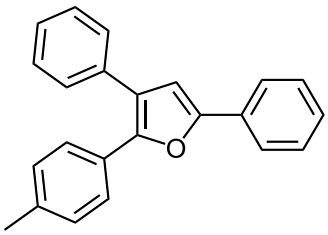
3.2.7 Gram-scale reaction



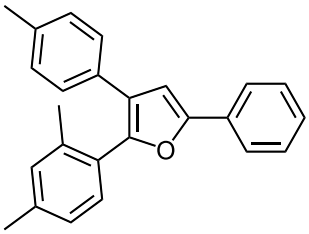
To an oven-dried Schlenk tube equipped with a stir bar was added *CuCl₂* (1.2 mmol, 160.8 mg), ***2a*** (20 mmol, 3920 mg), Then, *styrenes* (10 mmol, 1040 mg) and DMSO (10 mL) were successively

injected in the reaction tube with magnetic stirring. The reaction mixture was allowed to stir vigorously at 120 ℃ for 36 h. Thereafter, ethyl acetate (~30 mL) and water (~30 mL) were added. The organic layer was collected and dried over anhydrous Na_2SO_4. After filtration and evaporation of the solvent, the resulting crude product was separated on a silica gel column with hexane and dichloromethane as eluent to afford the desired product.

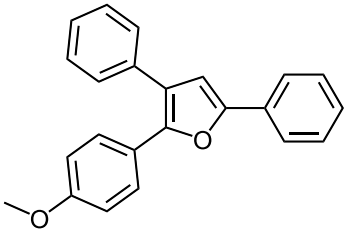
3.3 Characterization of Products



3,5-Diphenyl-2-(p-tolyl)furan (3a)[3]: Eluent: petroleum ether; colorless liquid; isolated yield: 77% (59.7 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 – 7.76 (m, 2H), 7.56 – 7.47 (m, 4H), 7.42 (m, 4H), 7.37 – 7.28 (m, 2H), 7.15 (d, *J* = 8.0 Hz, 2H), 6.84 (s, 1H), 2.38 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.2, 148.2, 137.4, 134.4, 130.6, 129.1, 128.69, 128.65, 128.6, 128.3, 127.4, 127.2, 126.1, 123.8, 123.7, 109.3, 21.3.

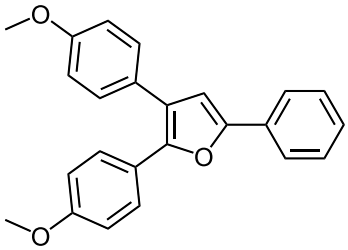


2-(2,4-Dimethylphenyl)-5-phenyl-3-(p-tolyl)furan (3b): Eluent: petroleum ether; colorless liquid; isolated yield: 66% (55.8 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 – 7.80 (m, 2H), 7.49 – 7.40 (m, 4H), 7.35 – 7.30 (m, 1H), 7.24 (d, *J* = 7.7 Hz, 1H), 7.20 – 7.15 (m, 2H), 7.12 (d, *J* = 8.0 Hz, 2H), 6.73 (s, 1H), 2.39 (s, 6H), 2.19 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.6, 147.9, 136.8, 135.5, 134.0, 133.6, 130.6, 130.1, 129.1, 128.7, 128.6, 128.5, 127.3, 124.5, 123.6, 123.1, 110.3, 21.2, 20.9, 19.6. HRMS (ESI): calcd. for $C_{25}H_{23}O^+$: 339.1743, found: 339.1742.

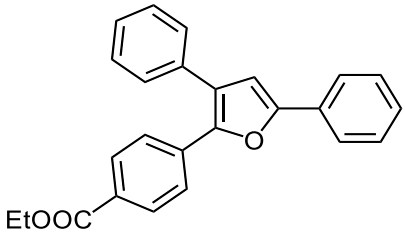


2-(4-Methoxyphenyl)-3,5-diphenylfuran (3c)[4]: Eluent: petroleum ether/ethyl acetate (95:5 v/v); white solid; isolated yield: 71% (57.9 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, *J* = 7.6 Hz, 2H), 7.66 – 7.60 (m, 2H), 7.54 (d, *J* = 7.2 Hz, 2H), 7.50 – 7.42 (m, 4H), 7.36 (m, 2H), 6.93 (d, *J* = 8.8

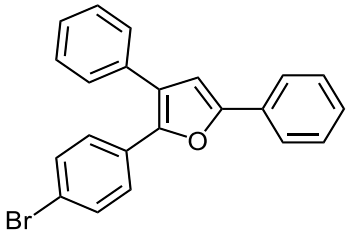
Hz, 2H), 6.88 (s, 1H), 3.86 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.1, 152.0, 148.0, 134.4, 130.6, 128.64, 128.58, 128.56, 127.6, 127.2, 127.0, 123.9, 123.6, 123.0, 113.8, 109.2, 55.2.



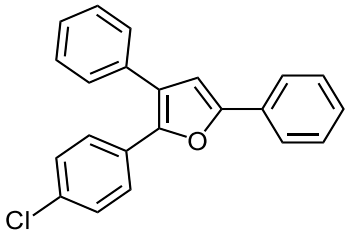
2,3-Bis(4-methoxyphenyl)-5-phenylfuran (3d)[5]: Eluent: petroleum ether/ethyl acetate (90:10 v/v); white solid; isolated yield: 52% (46.3 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (dd, *J* = 7.7, 1.2 Hz, 2H), 7.60 – 7.56 (m, 2H), 7.46 – 7.39 (m, 4H), 7.32 – 7.28 (m, 1H), 6.98 – 6.93 (m, 2H), 6.91 – 6.87 (m, 2H), 6.80 (s, 1H), 3.87 (d, *J* = 0.6 Hz, 3H), 3.84 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.9, 158.7, 151.8, 147.6, 130.6, 129.7, 128.6, 127.5, 127.2, 126.7, 124.0, 123.6, 122.7, 114.0, 113.8, 109.3, 55.21, 55.20.



Ethyl 4-(3,5-diphenylfuran-2-yl)benzoate (3e): Eluent: petroleum ether/ethyl acetate (95:5 v/v); colorless liquid; isolated yield: 53% (58.8 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 – 8.01 (m, 2H), 7.82 – 7.75 (m, 2H), 7.63 – 7.53 (m, 4H), 7.44 (m, 2H), 7.38 – 7.29 (m, 4H), 6.86 (s, 1H), 4.42 (q, *J* = 7.1 Hz, 2H), 1.43 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.4, 152.9, 148.6, 138.9, 130.7, 130.2, 129.9, 129.1, 128.7, 128.5, 128.4, 127.9, 127.7, 126.4, 123.8, 123.5, 108.8, 61.0, 31.6, 22.6, 14.3, 14.1. HRMS (ESI): calcd. for $C_{25}H_{21}O_3^+$: 369.1485, found: 369.1480.

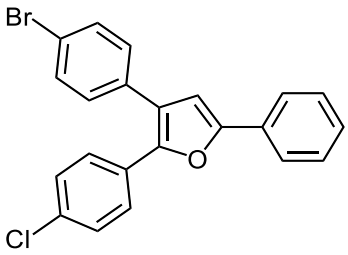


2-(4-Bromophenyl)-3,5-diphenylfuran (3f)[3]: Eluent: petroleum ether; colorless liquid; isolated yield: 68% (63.6 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 – 7.73 (m, 2H), 7.58 – 7.37 (m, 11H), 7.36 – 7.31 (m, 1H), 6.83 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.8, 146.7, 133.9, 131.5, 130.2, 129.9, 128.8, 128.7, 128.6, 127.7, 127.5, 127.4, 125.1, 123.8, 121.3, 109.6.

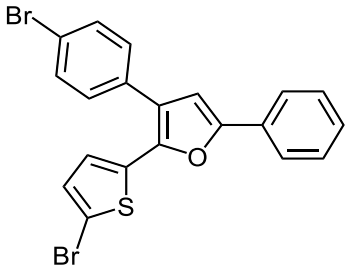


2-(4-Chlorophenyl)-3,5-diphenylfuran (3g): Eluent: petroleum ether; colorless liquid; isolated yield: 72% (59.4 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 – 7.75 (m, 2H), 7.60 – 7.54 (m, 2H), 7.50

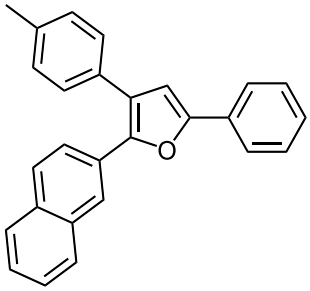
– 7.29 (m, 10H), 6.84 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.7, 146.7, 133.9, 133.1, 130.2, 129.5, 128.7, 128.7, 128.6, 127.7, 127.5, 127.2, 125.0, 123.8, 109.5. HRMS (ESI): calcd. for $C_{22}H_{16}ClO^+$: 331.0884, found: 331.0879.



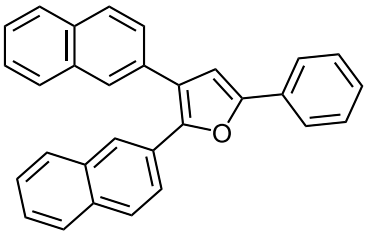
3-(4-Bromophenyl)-2-(4-chlorophenyl)-5-phenylfuran (**3h**): Eluent: petroleum ether; white solid; isolated yield: 74% (75.3 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 – 7.73 (m, 2H), 7.55 – 7.50 (m, 4H), 7.44 (m, 2H), 7.32 (m, 5H), 6.78 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.0, 146.8, 133.4, 132.9, 131.9, 130.2, 130.0, 129.2, 128.8, 128.7, 127.8, 127.3, 123.8, 123.7, 121.5, 109.0. HRMS (ESI): calcd. for $C_{22}H_{15}BrClO^+$: 408.9989, found: 408.9980.



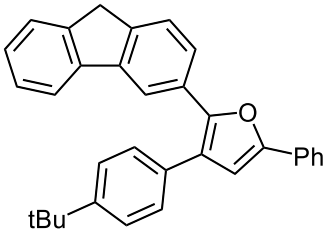
3-(4-bromophenyl)-2-(5-bromothiophen-2-yl)-5-phenylfuran (**3i**): Eluent: petroleum ether; light yellow solid; isolated yield: 74% (85.1 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 – 7.72 (m, 2H), 7.64 – 7.56 (m, 2H), 7.49 – 7.34 (m, 5H), 7.05 – 6.95 (m, 2H), 6.75 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.8, 142.7, 134.1, 131.9, 131.9, 130.2, 130.1, 129.7, 128.7, 127.9, 124.1, 123.7, 123.3, 121.8, 111.9, 108.7. HRMS (ESI): calcd. for $C_{20}H_{13}Br_2OS^+$: 458.9048, found: 458.9031.



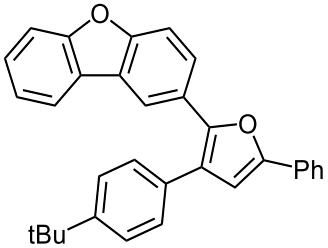
2-(Naphthalen-2-yl)-5-phenyl-3-(p-tolyl)furan (**3j**): Eluent: petroleum ether/ethyl acetate (99:1 v/v); white solid; isolated yield: 61% (54.9 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 1.7 Hz, 1H), 7.92 – 7.81 (m, 5H), 7.62 – 7.51 (m, 5H), 7.46 (t, *J* = 7.7 Hz, 2H), 7.38 – 7.29 (m, 1H), 7.14 (d, *J* = 8.0 Hz, 2H), 6.94 (s, 1H), 2.38 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.4, 148.5, 137.5, 133.6, 132.6, 131.9, 130.6, 129.1, 128.7, 128.3, 128.1, 127.9, 127.7, 127.4, 127.2, 127.1, 126.2, 125.9, 123.8, 123.8, 109.4, 21.3. HRMS (ESI): calcd. for $C_{27}H_{21}O^+$: 361.1587, found: 361.1592.



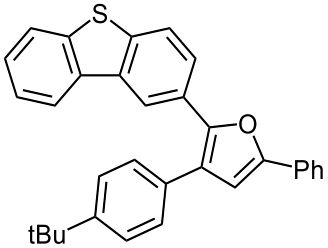
2,3-Di(naphthalen-2-yl)-5-phenylfuran (**3k**)[5]: Eluent: petroleum ether/dichloromethane (95:5 v/v); white solid; isolated yield: 69% (68.3 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (s, 1H), 8.11 (d, *J* = 1.6 Hz, 1H), 7.99 – 7.85 (m, 7H), 7.80 (d, *J* = 1.6 Hz, 2H), 7.69 (dd, *J* = 8.4, 1.8 Hz, 1H), 7.64 – 7.53 (m, 6H), 7.44 (m, 1H), 7.05 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.9, 148.2, 133.6, 133.3, 132.62, 132.58, 131.7, 130.4, 128.7, 128.4, 128.2, 128.1, 127.95, 127.91, 127.86, 127.7, 127.60, 127.56, 127.2, 127.0, 126.2, 126.1, 126.0, 124.95, 124.88, 124.2, 123.8, 109.7.



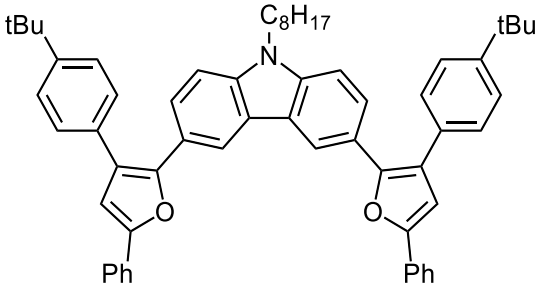
3-(4-(tert-butyl)phenyl)-2-(9H-fluoren-3-yl)-5-phenylfuran (**3l**): Eluent: petroleum ether/dichloromethane (95:5 v/v); white solid; isolated yield: 75% (82.5 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 – 7.96 (m, 1H), 7.94 – 7.90 (m, 2H), 7.87 – 7.84 (m, 1H), 7.81 – 7.75 (m, 2H), 7.65 – 7.61 (m, 1H), 7.59 – 7.52 (m, 6H), 7.48 (m, 1H), 7.40 (m, 2H), 6.95 (s, 1H), 3.97 (s, 2H), 1.52 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.2, 150.1, 148.2, 143.5, 143.3, 141.3, 140.9, 131.3, 130.5, 129.6, 128.6, 128.2, 127.3, 126.72, 126.66, 125.5, 125.0, 124.9, 124.1, 123.7, 122.6, 119.8, 119.7, 109.6, 36.9, 34.5, 31.3. HRMS (ESI): calcd. for $C_{33}H_{29}O^+$: 441.2213, found: 441.2190.



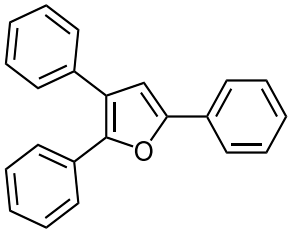
2-(3-(4-(Tert-butyl)phenyl)-5-phenylfuran-2-yl)dibenzo[b,d]furan (**3m**): Eluent: petroleum ether/dichloromethane (95:5 v/v); white solid; isolated yield: 65% (71.8 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, *J* = 1.7 Hz, 1H), 7.95 – 7.91 (m, 1H), 7.89 – 7.85 (m, 2H), 7.78 (m, 1H), 7.63 (d, *J* = 8.2 Hz, 1H), 7.55 (d, *J* = 8.8 Hz, 1H), 7.52 – 7.47 (m, 7H), 7.41 – 7.35 (m, 2H), 6.93 (s, 1H). 1.45 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.5, 155.5, 152.3, 150.3, 147.9, 131.2, 130.6, 128.7, 128.2, 127.4, 127.3, 126.3, 126.0, 125.6, 124.4, 124.1, 123.7, 122.8, 120.7, 118.5, 111.7, 111.5, 109.4, 34.6, 31.4. HRMS (ESI): calcd. for $C_{27}H_{21}O^+$: 443.2006, found: 443.2013.



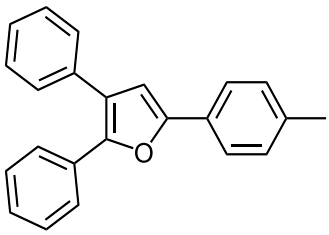
3-(4-(tert-butyl)phenyl)-2-(dibenzo[b,d]thiophen-2-yl)-5-phenylfuran (**3n**): Eluent: petroleum ether/dichloromethane (95:5 v/v); white solid; isolated yield: 63% (72.1 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 – 8.34 (m, 1H), 8.00 – 7.95 (m, 1H), 7.86 (m, 3H), 7.82 – 7.76 (m, 2H), 7.49 – 7.42 (m, 8H), 7.37 – 7.32 (m, 1H), 6.91 (s, 1H), 1.44 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.4, 150.5, 147.8, 139.7, 138.3, 135.6, 135.4, 131.3, 130.5, 128.7, 128.4, 127.7, 127.5, 126.8, 125.6, 124.8, 124.4, 124.3, 123.8, 122.8, 122.6, 121.6, 118.9, 109.5, 34.6, 31.4. HRMS (ESI): calcd. for $C_{32}H_{27}OS^+$: 459.1777, found: 459.1752.



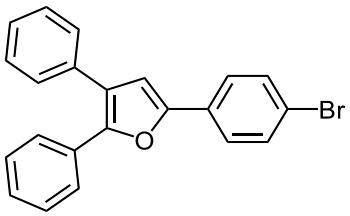
3,6-Bis(3-(4-(tert-butyl)phenyl)-5-phenylfuran-2-yl)-9-octyl-9H-carbazole (**3o**): Eluent: petroleum ether/ethyl acetate (95:5 v/v); white solid; isolated yield: 44% (91.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (d, *J* = 1.7 Hz, 2H), 7.86 – 7.81 (m, 4H), 7.71 (m, 2H), 7.50 – 7.39 (m, 12H), 7.36 – 7.28 (m, 4H), 6.91 (s, 2H), 4.29 (t, *J* = 7.2 Hz, 2H), 1.90 (p, *J* = 7.3 Hz, 2H), 1.36 (s, 22H), 1.28 (m, 6H), 0.92 – 0.86 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.0, 149.9, 149.2, 140.2, 131.4, 130.8, 128.7, 128.1, 127.1, 125.5, 125.2, 123.7, 123.0, 122.7, 118.9, 109.2, 108.7, 99.9, 43.3, 34.6, 31.8, 31.4, 29.3, 29.2, 29.0, 27.3, 22.6, 14.1. HRMS (ESI): calcd. for $C_{60}H_{62}NO_2^+$: 828.4775, found: 828.4778.



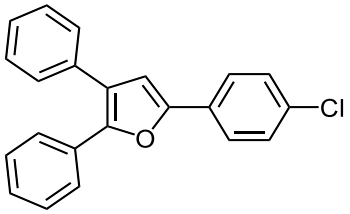
2,3,5-Triphenylfuran (**4a**)[3]: Eluent: petroleum ether; colorless liquid; isolated yield: 82% (60.7 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 7.7 Hz, 2H), 7.71 (d, *J* = 7.4 Hz, 2H), 7.56 (d, *J* = 7.1 Hz, 2H), 7.52 – 7.44 (m, 4H), 7.44 – 7.35 (m, 4H), 7.35 – 7.32 (m, 1H), 6.89 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.5, 147.9, 134.3, 131.1, 130.5, 128.7, 128.7, 128.6, 128.4, 127.49, 127.46, 127.3, 126.1, 124.5, 123.8, 109.4.



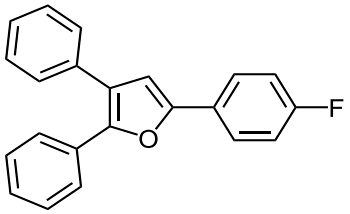
2,3-Diphenyl-5-(p-tolyl)furan (**4b**)[3]: Eluent: petroleum ether; colorless liquid; isolated yield: 74% (57.3 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.1 Hz, 2H), 7.66 (d, *J* = 7.5 Hz, 2H), 7.52 (d, *J* = 7.1 Hz, 2H), 7.43 (t, *J* = 7.3 Hz, 2H), 7.40 – 7.32 (m, 3H), 7.28 (t, *J* = 8.6 Hz, 3H), 6.81 (s, 1H), 2.43 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.8, 147.5, 137.4, 134.4, 131.2, 129.4, 128.7, 128.6, 128.4, 127.8, 127.3, 127.2, 126.1, 124.5, 123.8, 108.8, 21.3.



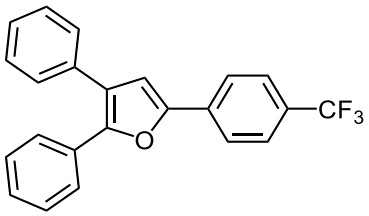
5-(4-Bromophenyl)-2,3-diphenylfuran (**4c**)[3]: Eluent: petroleum ether; colorless liquid; isolated yield: 67% (62.6 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 – 7.62 (m, 4H), 7.57 (d, *J* = 8.6 Hz, 2H), 7.54 – 7.49 (m, 2H), 7.47 – 7.30 (m, 6H), 6.84 (s, 1H).^{13}C NMR (101 MHz, $CDCl_3$) δ 152.8, 146.7, 133.9, 131.5, 130.2, 129.9, 128.8, 128.7, 128.6, 127.7, 127.5, 127.4, 125.1, 123.8, 121.3, 109.6.



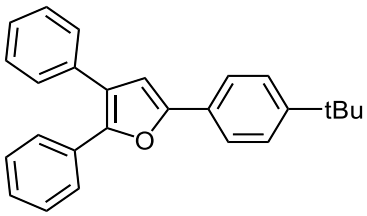
5-(4-Chlorophenyl)-2,3-diphenylfuran (**4d**)[5]: Eluent: petroleum ether; colorless liquid; isolated yield: 71% (58.6 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 – 7.69 (m, 2H), 7.63 (d, *J* = 7.3 Hz, 2H), 7.49 (d, *J* = 7.1 Hz, 2H), 7.37 (m, 8H), 6.83 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.5, 148.2, 134.1, 133.1, 130.9, 129.0, 128.9, 128.7, 128.6, 128.4, 127.7, 127.4, 126.1, 125.0, 124.6, 109.9.



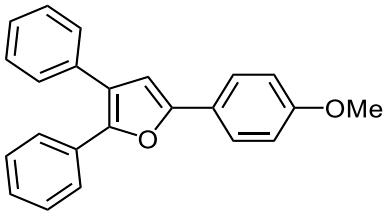
5-(4-Fluorophenyl)-2,3-diphenylfuran (**4e**)[3]: Eluent: petroleum ether; colorless liquid; isolated yield: 72% (56.5 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 – 7.59 (m, 2H), 7.51 (m, 2H), 7.37 (d, *J* = 7.0 Hz, 2H), 7.31 – 7.14 (m, 6H), 7.05 – 6.96 (m, 2H), 6.65 (s, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -113.9. ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.3 (d, *J* = 248.0 Hz), 151.7, 147.9, 134.2, 131.0, 128.68, 128.66, 128.4, 127.4 (d, *J* = 20.0 Hz), 126.92, 126.89, 126.1, 125.5 (d, *J* = 8.2 Hz), 124.5, 115.8 (d, *J* = 22.1 Hz), 109.1. ^{19}F NMR (376 MHz, $CDCl_3$) δ -113.9.



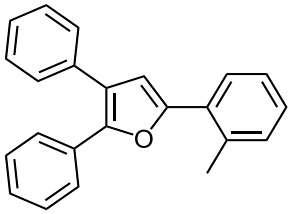
2,3-Diphenyl-5-(4-(trifluoromethyl)phenyl)furan (**4f**): Eluent: petroleum ether; colorless liquid; isolated yield: 62% (56.4 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.1 Hz, 2H), 7.72 – 7.61 (m, 4H), 7.52 – 7.45 (m, 2H), 7.45 – 7.28 (m, 6H), 6.94 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.0, 149.0, 133.8, 133.6, 130.7, 128.7, 128.6, 128.5, 127.9, 127.5, 126.3, 125.8 (q, *J* = 3.8 Hz), 124.7, 123.7, 111.3. ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.4. HRMS (ESI): calcd. for $C_{23}H_{16}F_3O^+$: 365.1148, found: 365.1141.



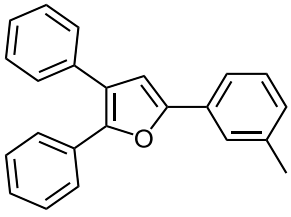
5-(4-(Tert-butyl)phenyl)-2,3-diphenylfuran (**4g**)[3]: Eluent: petroleum ether; colorless liquid; isolated yield: 80% (70.4 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 – 7.74 (m, 2H), 7.72 – 7.66 (m, 2H), 7.56 – 7.50 (m, 4H), 7.47 – 7.42 (m, 2H), 7.41 – 7.35 (m, 3H), 7.33 – 7.28 (m, 1H), 6.84 (s, 1H), 1.43 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.8, 150.6, 147.5, 134.4, 131.2, 128.7, 128.6, 128.3, 127.8, 127.3, 127.2, 126.0, 125.6, 124.5, 123.7, 108.9, 34.6, 31.3.



5-(4-Methoxyphenyl)-2,3-diphenylfuran (**4h**)[4]: petroleum ether/ethyl acetate (95:5 v/v); white solid; isolated yield: 72% (58.4 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 – 7.75 (m, 2H), 7.71 (d, *J* = 7.5 Hz, 2H), 7.57 (d, *J* = 7.1 Hz, 2H), 7.47 (t, *J* = 7.3 Hz, 2H), 7.40 (q, *J* = 7.5 Hz, 3H), 7.35 – 7.29 (m, 1H), 7.03 (d, *J* = 8.9 Hz, 2H), 6.76 (s, 1H), 3.89 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.2, 152.6, 147.1, 134.4, 131.2, 128.6, 128.6, 128.3, 127.20, 127.15, 125.9, 125.2, 124.4, 123.5, 114.1, 107.9, 55.2.

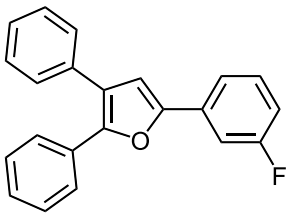


2,3-Diphenyl-5-(o-tolyl)furan (**4i**): Eluent: petroleum ether; colorless liquid; isolated yield: 65% (50.4 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (m, 1H), 7.70 – 7.65 (m, 2H), 7.58 – 7.52 (m, 2H), 7.48 – 7.43 (m, 2H), 7.41 – 7.29 (m, 7H), 6.78 (s, 1H), 2.66 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.2, 147.4, 134.5, 134.4, 131.3, 131.1, 129.7, 128.7, 128.6, 128.4, 127.5, 127.4, 127.2, 126.8, 126.04, 126.01, 124.1, 112.9, 22.1. HRMS (ESI): calcd. for $C_{23}H_{19}O^+$: 311.1430, found: 311.1427.

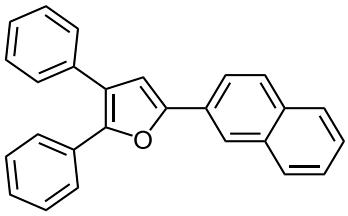


2,3-Diphenyl-5-(m-tolyl)furan (**4j**): Eluent: petroleum ether; colorless liquid; isolated yield: 74% (57.4 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 – 7.71 (m, 2H), 7.71 – 7.65 (m, 2H), 7.60 – 7.55 (m, 2H), 7.51 – 7.45 (m, 2H), 7.45 – 7.37 (m, 4H), 7.37 – 7.31 (m, 1H), 7.20 (dq, *J* = 7.5, 0.9 Hz, 1H), 6.89 (s, 1H), 2.51 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.6, 147.7, 138.2, 134.3, 131.1, 130.4,

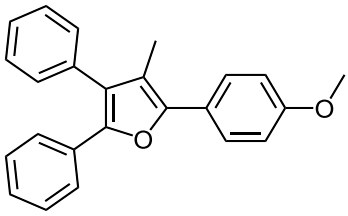
128.62, 128.60, 128.59, 128.33, 128.32, 127.4, 127.2, 126.1, 124.4, 124.3, 121.0, 109.3, 21.5. HRMS (ESI): calcd. for $C_{23}H_{19}O^+$: 311.1430, found: 311.1431.



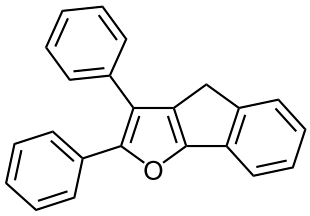
5-(3-Fluorophenyl)-2,3-diphenylfuran (**4k**): Eluent: petroleum ether; colorless liquid; isolated yield: 72% (56.5 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 – 7.61 (m, 2H), 7.55 (m, 1H), 7.49 (m, 3H), 7.46 – 7.30 (m, 7H), 7.01 (m, 2.6, 1.0 Hz, 1H), 6.86 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.2 (d, *J* = 246.0 Hz), 151.3, 151.2, 148.4, 134.0, 132.5 (d, *J* = 8.6 Hz), 130.8, 130.3 (d, *J* = 8.6 Hz), 128.7, 128.6, 128.4, 127.6 (d, *J* = 31.4 Hz), 126.2, 124.6, 119.4 (d, *J* = 2.8 Hz), 114.2 (d, *J* = 21.5 Hz), 110.6 (d, *J* = 23.6 Hz), 110.4. HRMS (ESI): calcd. for $C_{22}H_{16}FO^+$: 315.1180, found: 315.1189.



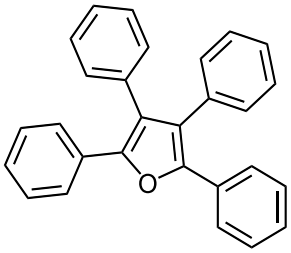
5-(Naphthalen-2-yl)-2,3-diphenylfuran (**4l**)[5]: Eluent: petroleum ether; white solid; isolated yield: 69% (59.7 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, *J* = 1.5 Hz, 1H), 8.01 – 7.84 (m, 4H), 7.79 – 7.70 (m, 2H), 7.61 – 7.32 (m, 10H), 6.99 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.5, 148.1, 134.2, 133.5, 132.7, 131.0, 128.6, 128.4, 128.1, 127.7, 127.5, 127.3, 126.5, 126.1, 125.9, 124.6, 122.2, 122.1, 110.1.



2-(4-Methoxyphenyl)-3-methyl-4,5-diphenylfuran (**4m**): Eluent: petroleum ether; white solid; isolated yield: 57% (48.4 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 – 7.67 (m, 2H), 7.49 – 7.40 (m, 4H), 7.40 – 7.32 (m, 3H), 7.25 – 7.19 (m, 2H), 7.18 – 7.13 (m, 1H), 7.02 – 6.96 (m, 2H), 3.85 (s, 3H), 2.10 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.6, 147.8, 146.5, 134.0, 131.1, 130.2, 128.7, 128.2, 127.3, 127.0, 126.7, 125.9, 125.3, 124.6, 117.3, 114.0, 55.3, 10.3. HRMS (ESI): calcd. for $C_{24}H_{21}O_2^+$: 341.1536, found: 341.1532.

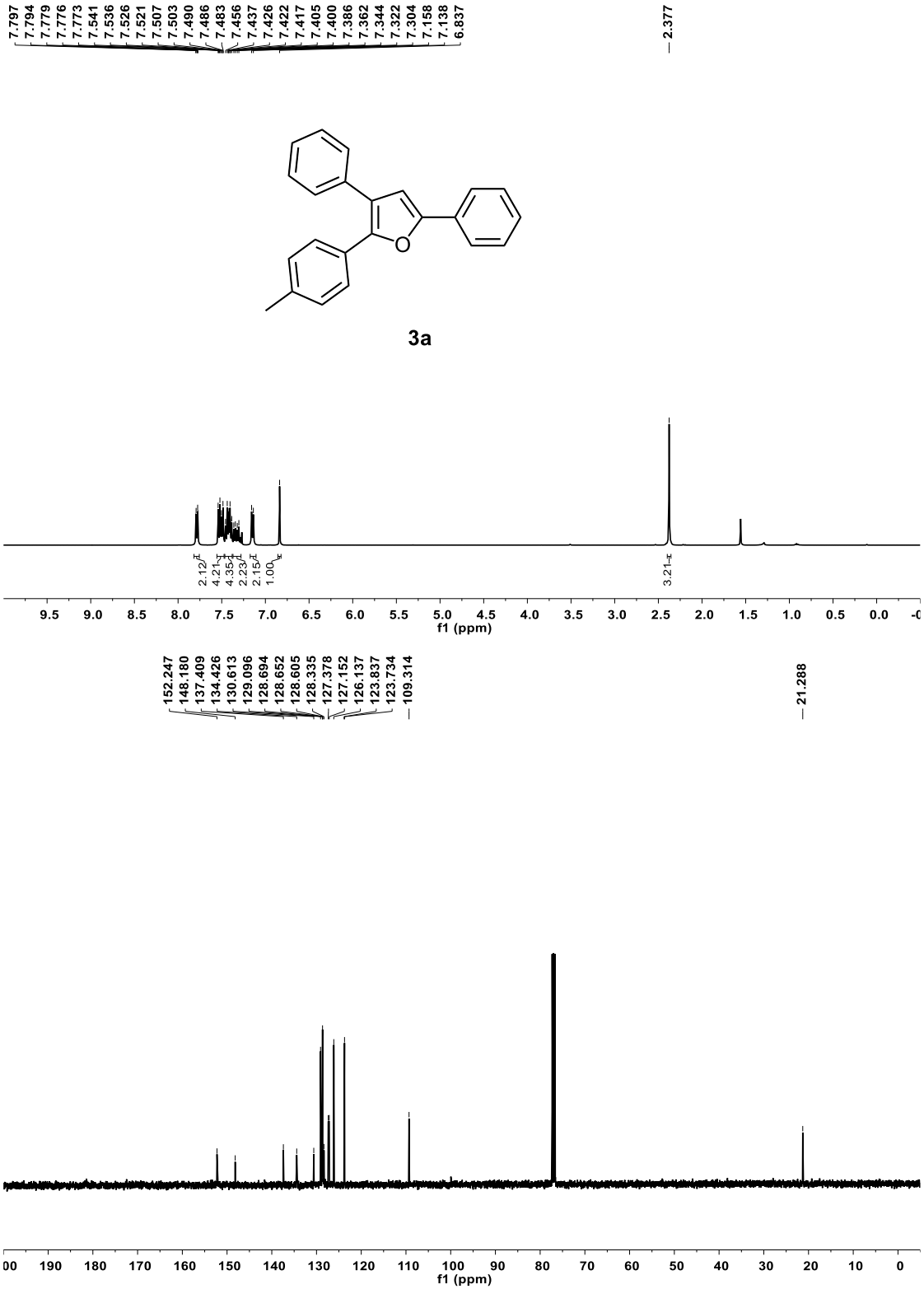


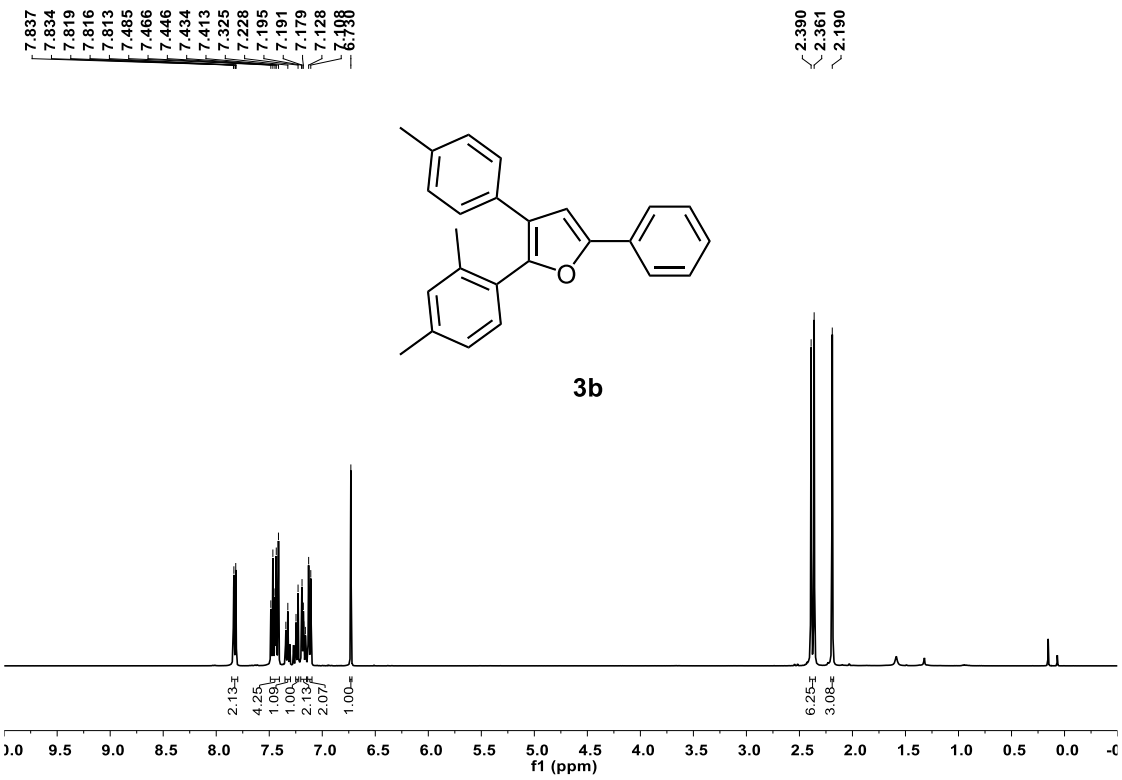
2,3-Diphenyl-4H-indeno[1,2-b]furan (**4n**): Eluent: petroleum ether; white solid; isolated yield: 40% (30.8mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 7.7 Hz, 2H), 7.44 (m, 3H), 7.37 (d, *J* = 7.5 Hz, 1H), 7.31 (t, *J* = 7.4 Hz, 2H), 7.28 – 7.19 (m, 4H), 7.15 (m, 1H), 7.09 (t, *J* = 7.5 Hz, 1H), 3.46 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.3, 152.0, 146.0, 133.8, 133.3, 131.8, 130.8, 128.7, 128.6, 128.4, 127.4, 127.3, 126.9, 126.3, 125.4, 124.5, 121.4, 116.6, 29.6. HRMS (ESI): calcd. for $C_{23}H_{17}O^{+}$: 309.1274, found: 309.1283.



2,3,4,5-Tetraphenylfuran (**4o**)[6]: Eluent: petroleum ether; white solid; isolated yield: 24% (22.3 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 – 7.52 (m, 4H), 7.29 (m, 12H), 7.21 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.6, 133.1, 130.8, 130.4, 128.35, 128.32, 127.3, 127.1, 125.8, 125.1.

3.4 NMR Spectra of Products

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7.813
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7.434
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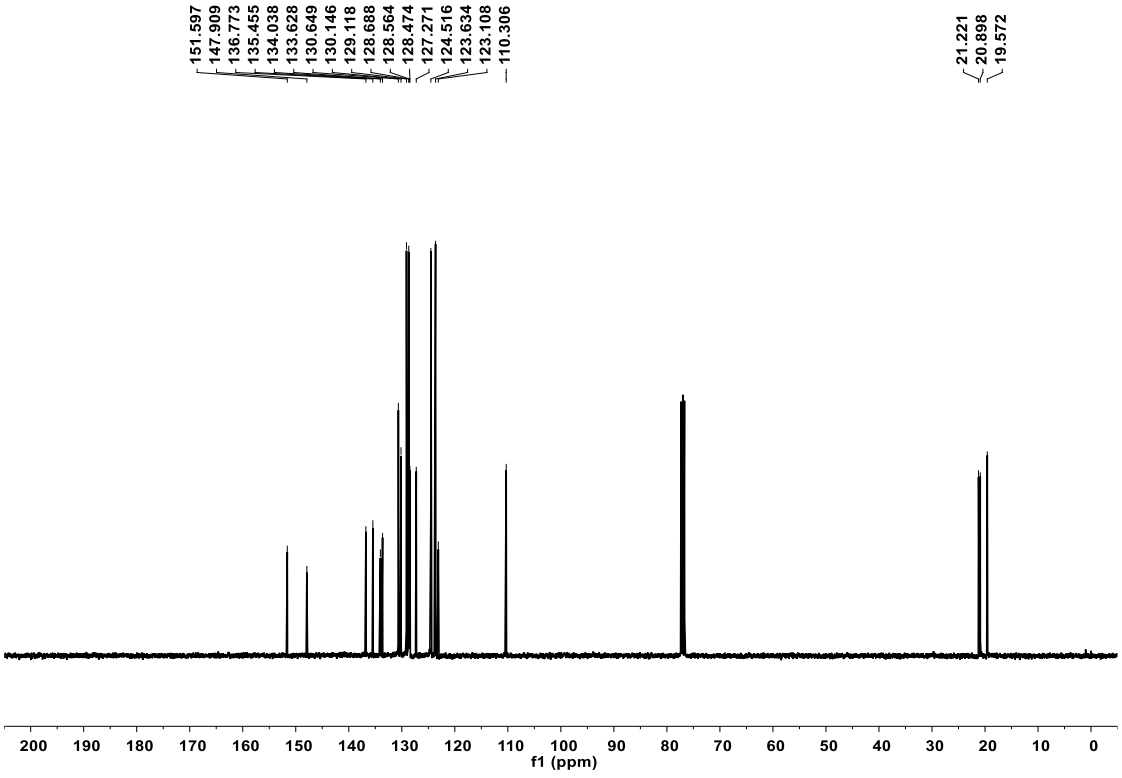
7.325
7.228
7.195
7.191
7.179
7.128
2.390
2.361
2.190
O
2.13
4.25
1.09
1.00
2.13
2.07
1.00
6.25
3.08
f1 (ppm)

3b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136.773
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133.628
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130.146
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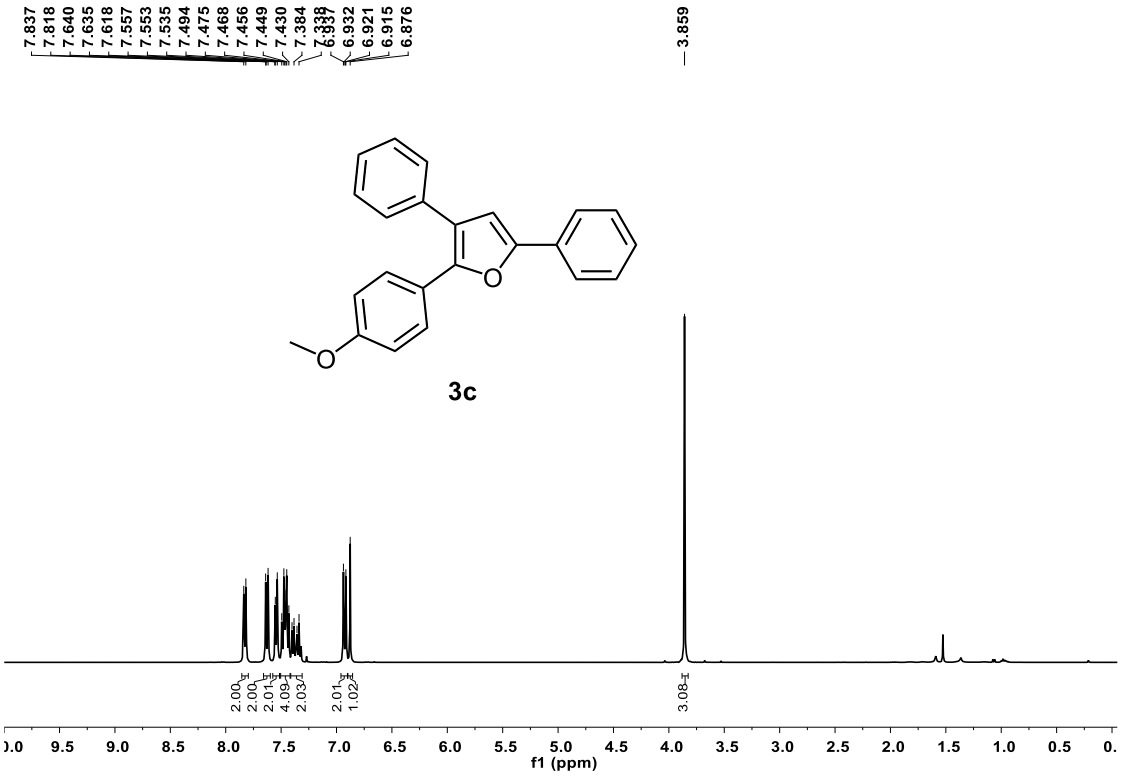
127.271
124.516
123.634
123.108
110.306
21.221
20.898
19.572
f1 (ppm)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7.618
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7.553
7.535
7.494
7.475
7.468
7.456
7.449
7.430
7.384
6.932
6.921
6.915
6.876
3.859
O
O
3c
2.00
2.00
2.01
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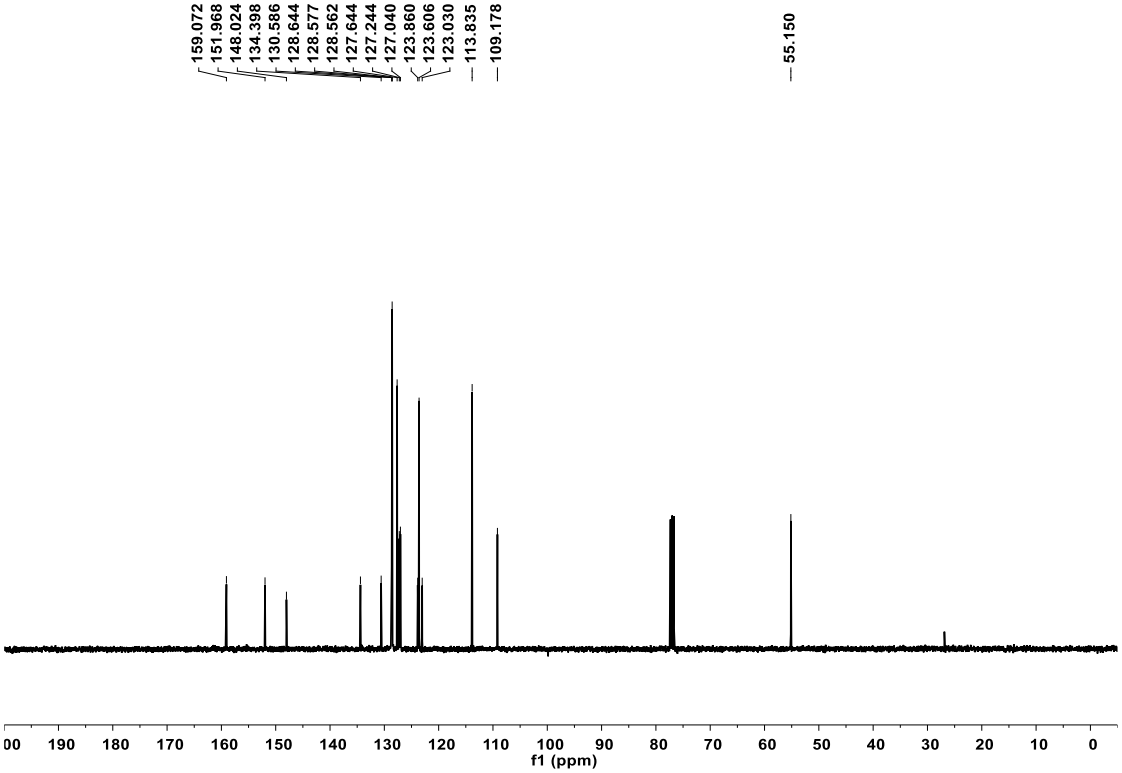
2.03
2.01
1.02
3.08
f1 (ppm)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123.030
113.835
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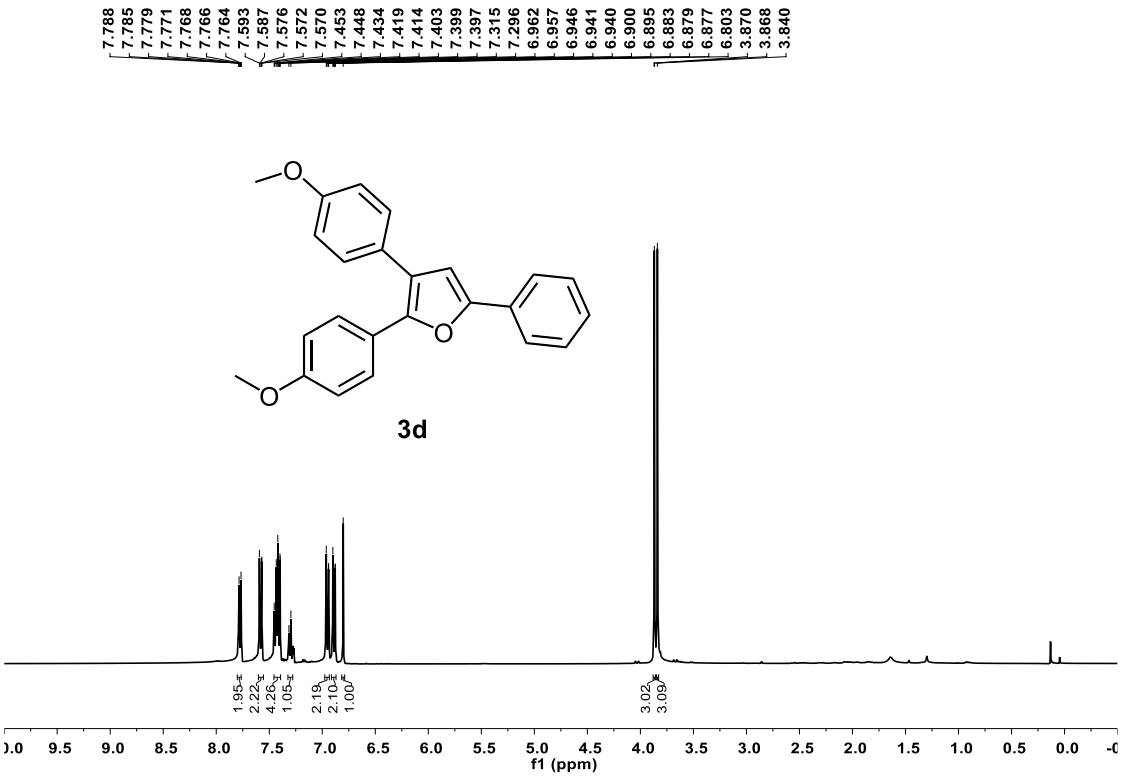
55.150
f1 (ppm)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7.766
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7.593
7.587
7.576
7.572
7.570
7.453
7.448
7.434
7.419
7.414
7.403
7.399
7.397
7.315
7.296
6.962
6.957
6.946
6.941
6.940
6.900
6.895
6.883
6.879
6.877
6.803
3.870
3.868
3.840
O
O
O
3d
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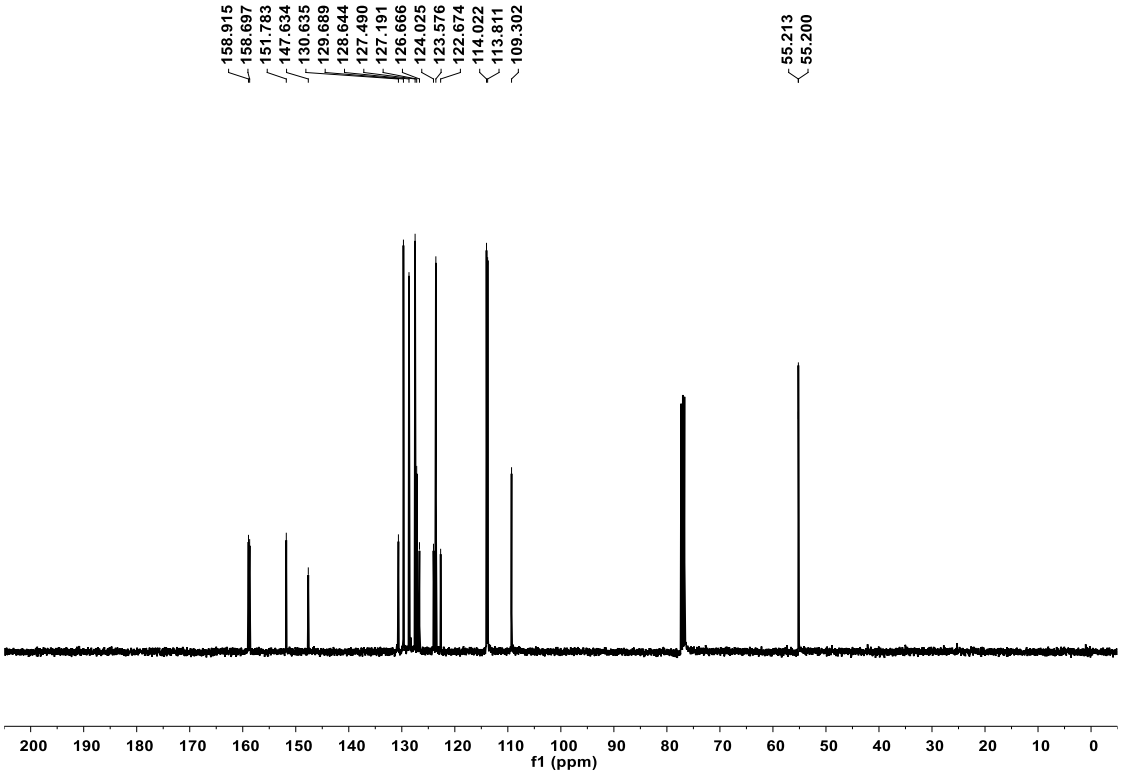
2.22
4.26
1.05
2.19
2.10
1.00
3.02
3.09
f1 (ppm)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158.697
151.783
147.634
130.635
129.689
128.644
127.490
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124.025
123.576
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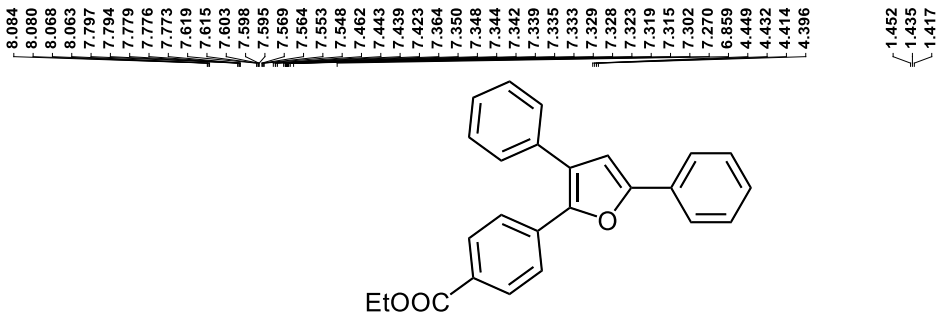
113.811
109.302
55.213
55.200
f1 (ppm)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8.080
8.068
8.063
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7.794
7.779
7.776
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7.603
7.598
7.595
7.569
7.564
7.553
7.548
7.462
7.443
7.439
7.423
7.364
7.350
7.348
7.344
7.342
7.339
7.335
7.333
7.329
7.328
7.323
7.319
7.315
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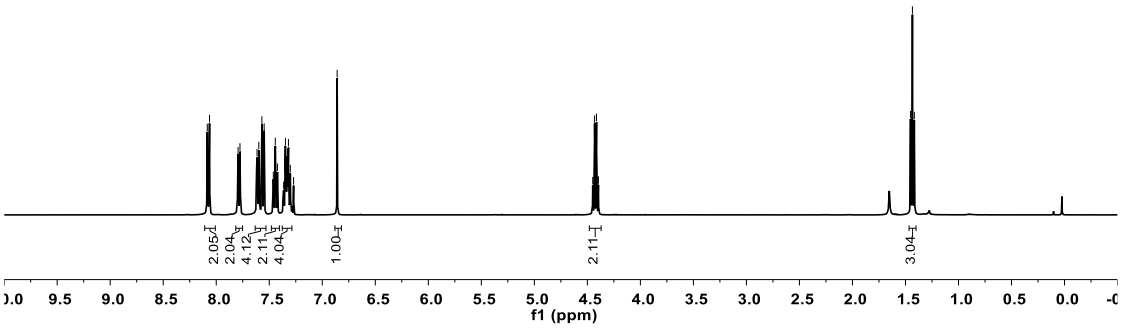
1.435
1.417
O
EtOOC

3e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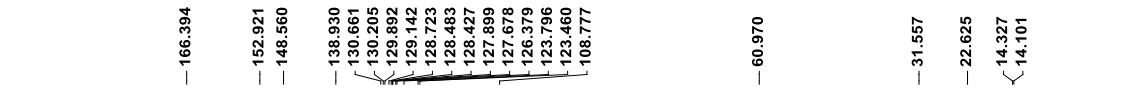
4.04
1.00
2.11
3.04
f1 (ppm)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130.661
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127.899
127.678
126.379
123.796
123.460
108.777
60.970
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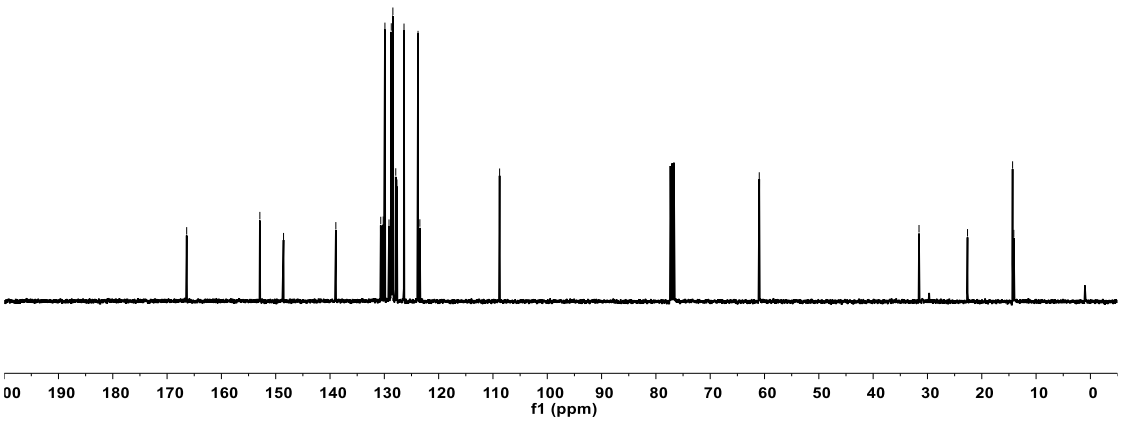
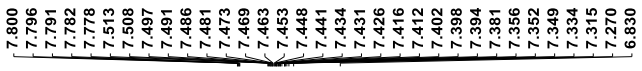
22.625
14.327
14.101


f1 (ppm)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7.497
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7.469
7.463
7.453
7.448
7.441
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7.426
7.416
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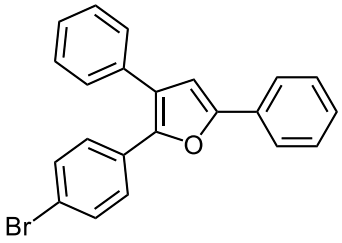
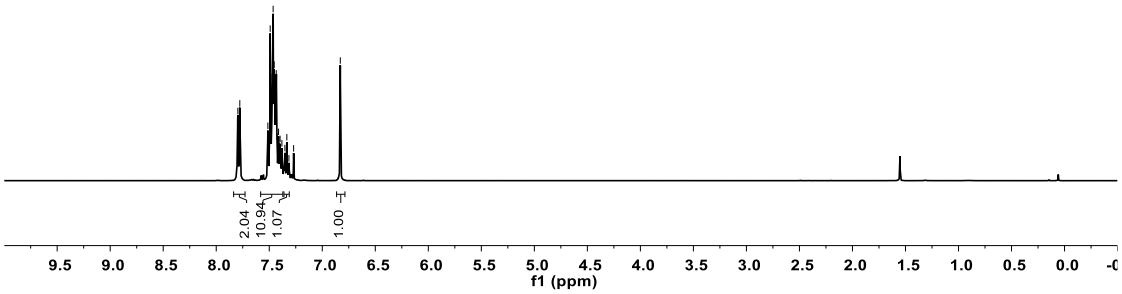
7.270
6.830


O
Br

3f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1.07
1.00
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)


152.799
146.693
133.929
131.535
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128.744
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127.435
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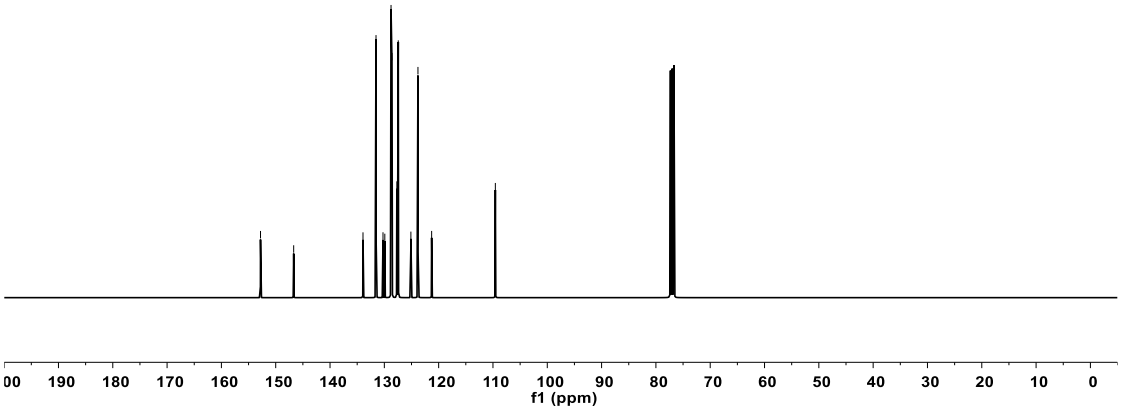
109.562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f1 (ppm)


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7.568
7.563
7.500
7.495
7.483
7.479
7.475
7.462
7.457
7.445
7.442
7.439
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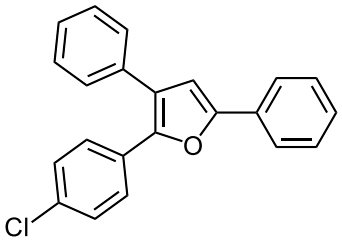
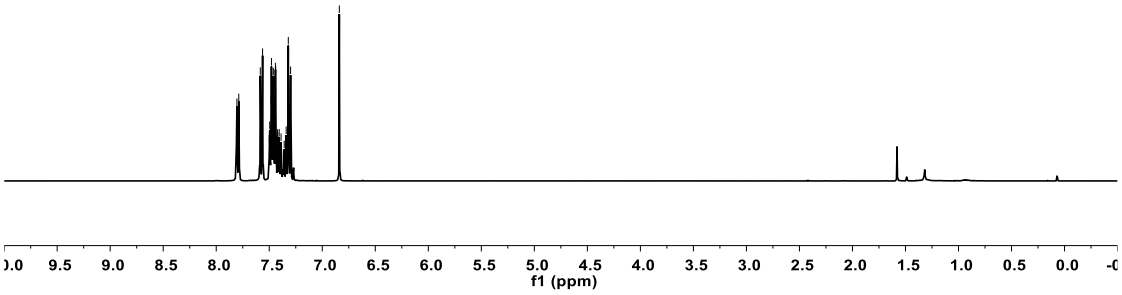
6.839


O
Cl

3g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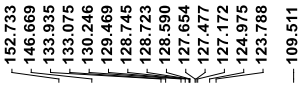
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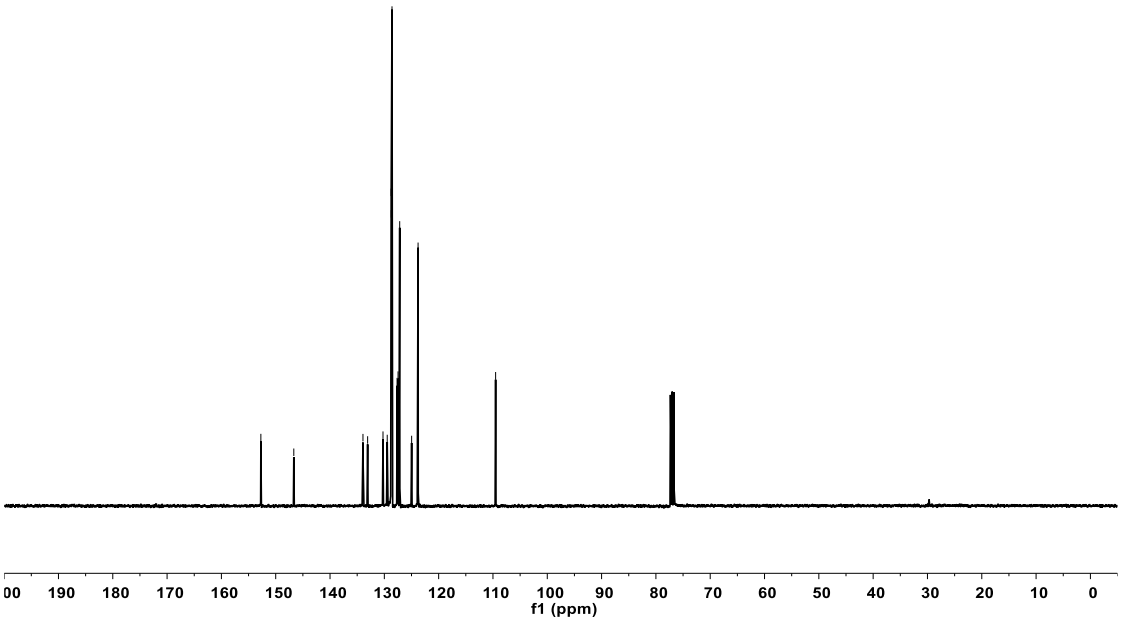
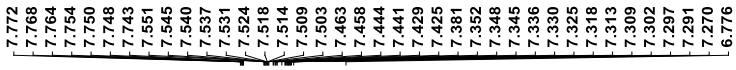
109.511


f1 (ppm)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7.503
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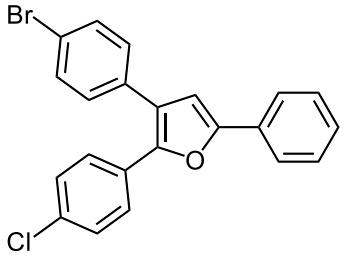
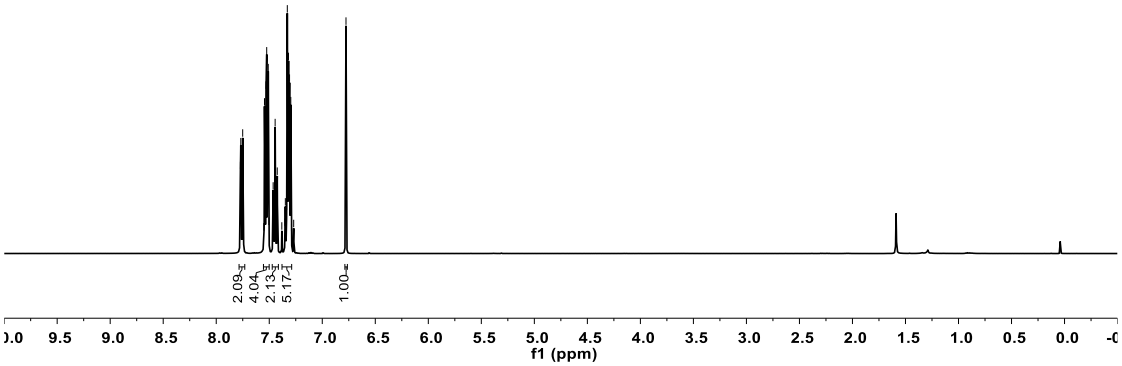

Br
O
Cl

3h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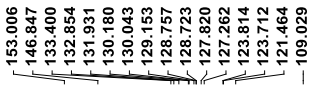
4.04
2.13
5.17
1.00
f1 (ppm)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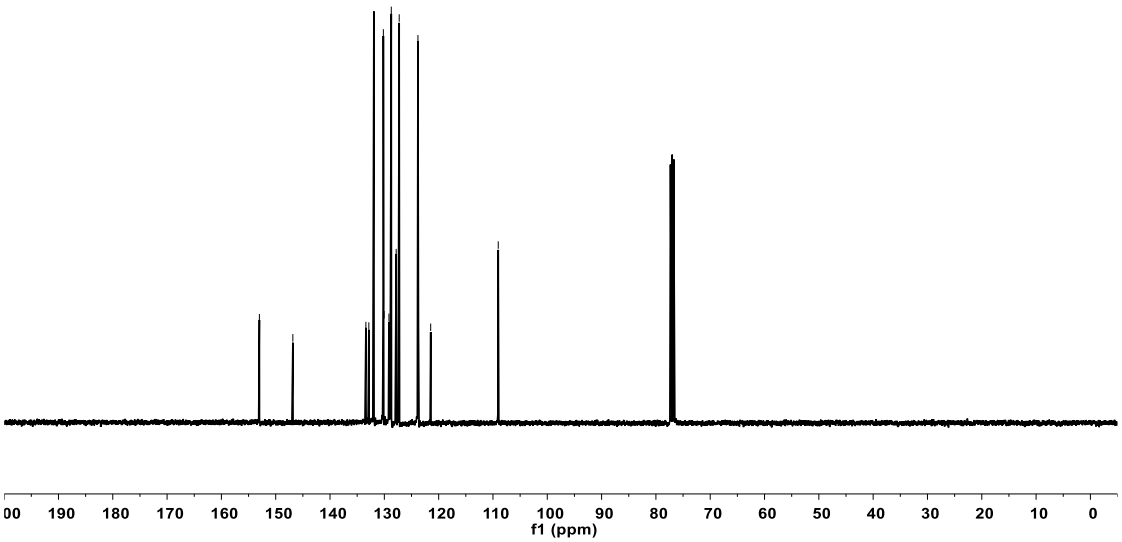
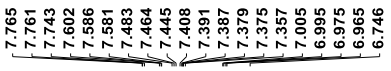
133.400
132.854
131.931
130.180
130.043
129.153
128.757
128.723
127.820
127.262
123.814
123.712
121.464
109.029


f1 (ppm)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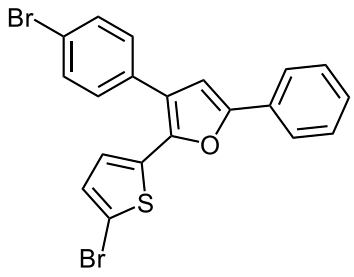
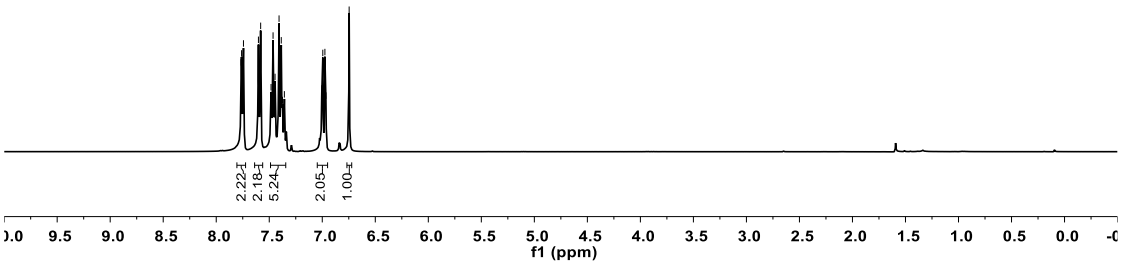
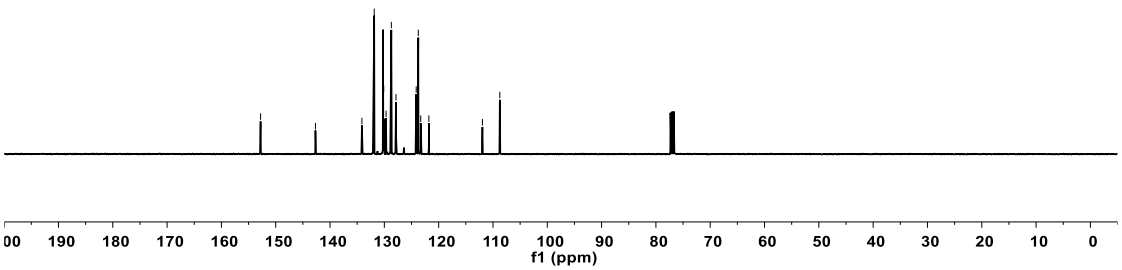
7.761
7.743
7.602
7.586
7.581
7.483
7.464
7.445
7.408
7.391
7.387
7.379
7.375
7.357
7.005
6.995
6.975
6.965
6.746


Br
O
S
Br

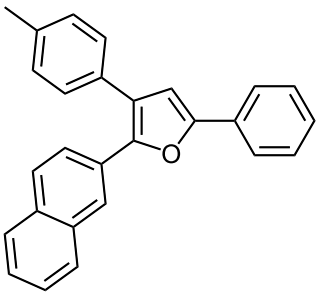
3i


2.22
2.18
5.24
2.05
1.00
f1 (ppm)


152.786
142.683
134.131
131.897
131.864
130.246
130.115
129.681
128.712
127.859
124.134
123.747
123.304
121.805
111.940
108.740


f1 (ppm)


7.997
7.993
7.903
7.898
7.892
7.888
7.880
7.873
7.868
7.860
7.852
7.844
7.838
7.834
7.829
7.817
7.814
7.603
7.599
7.582
7.578
7.563
7.558
7.548
7.545
7.537
7.531
7.528
7.523
7.520
7.514
7.480
7.475
7.461
7.441
7.348
7.345
7.341
7.331
7.326
7.307
7.270
7.153
7.133
6.944
2.382



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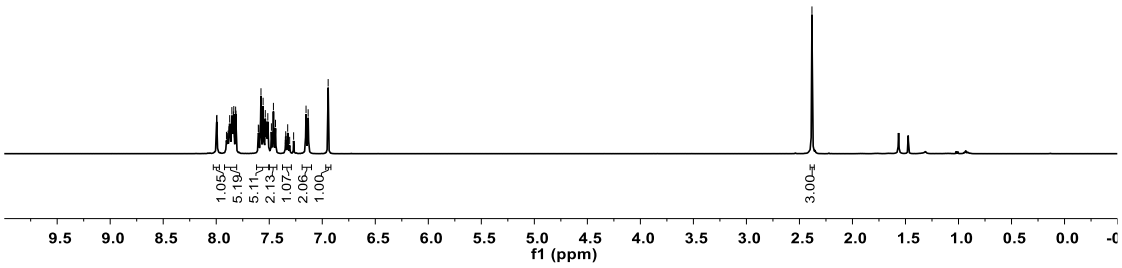
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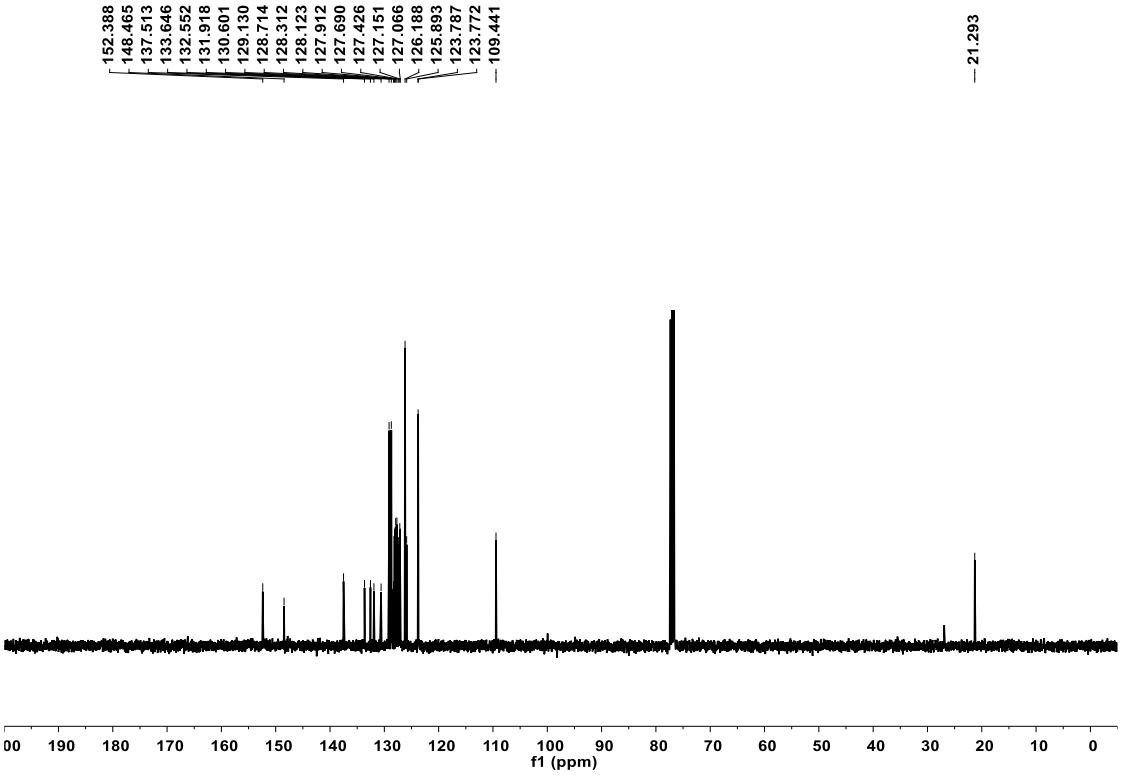
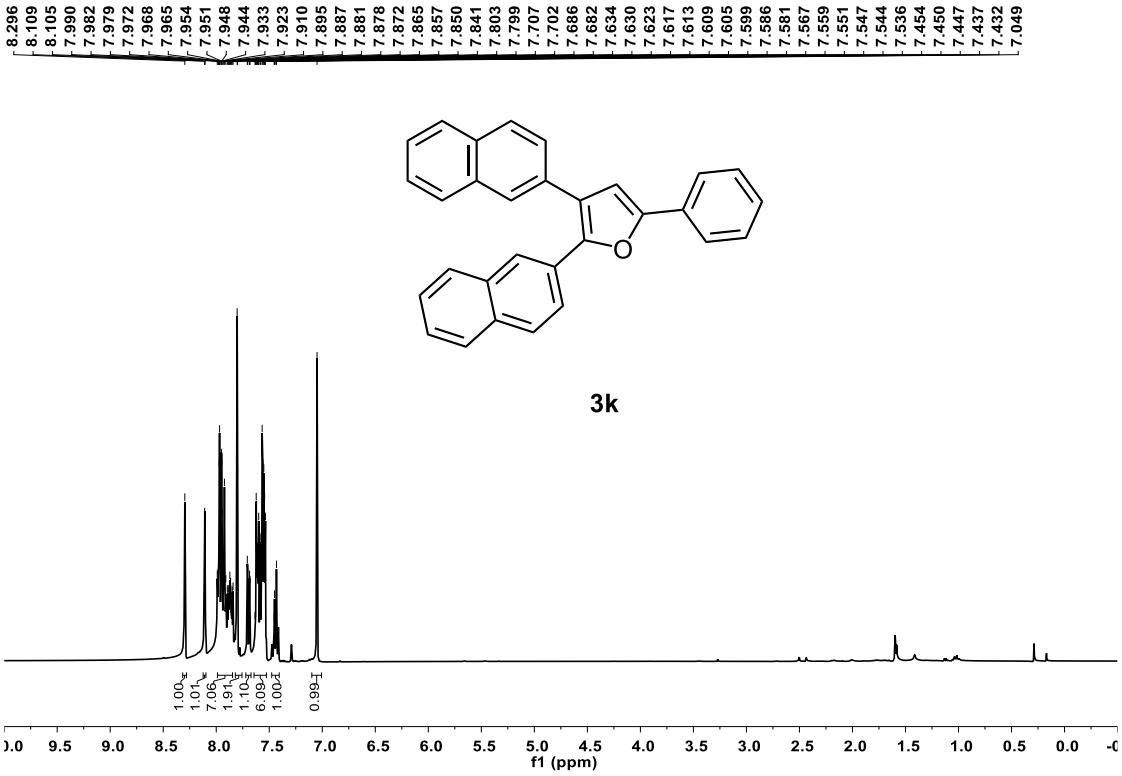
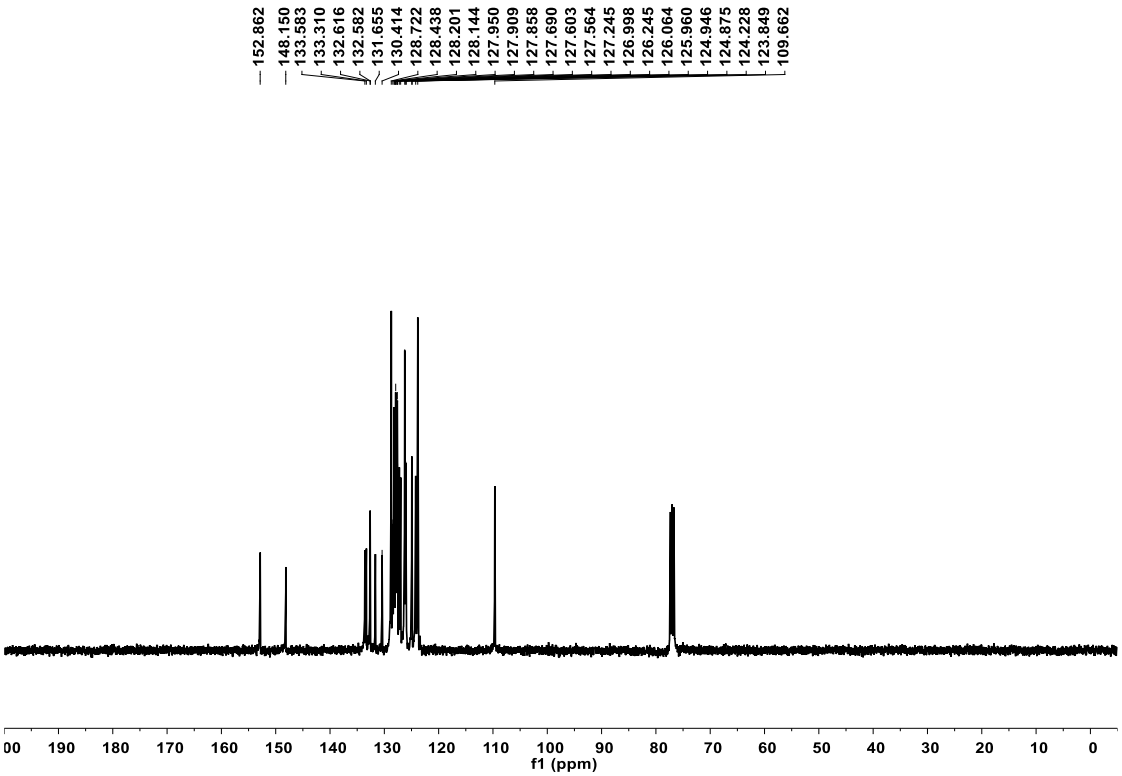
5.19
5.11
2.13
1.07
2.06
1.00
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


152.388
148.465
137.513
133.646
132.552
131.918
130.601
129.130
128.714
128.312
128.123
127.912
127.690
127.426
127.151
127.066
126.188
125.893
123.787
123.772
109.441
21.293
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.296
8.109
8.105
7.990
7.982
7.979
7.972
7.968
7.965
7.954
7.951
7.948
7.944
7.933
7.923
7.910
7.895
7.887
7.881
7.878
7.872
7.865
7.857
7.850
7.841
7.803
7.799
7.707
7.702
7.686
7.682
7.634
7.630
7.623
7.617
7.613
7.609
7.605
7.599
7.586
7.581
7.567
7.559
7.551
7.547
7.544
7.536
7.454
7.450
7.447
7.437
7.432
7.049
3k
1.00
1.01
7.06
1.91
1.10
6.09
1.00
0.99
f1 (ppm)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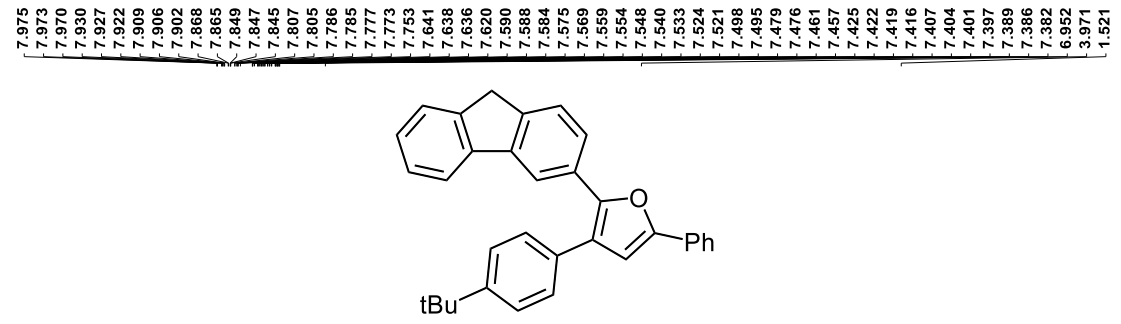
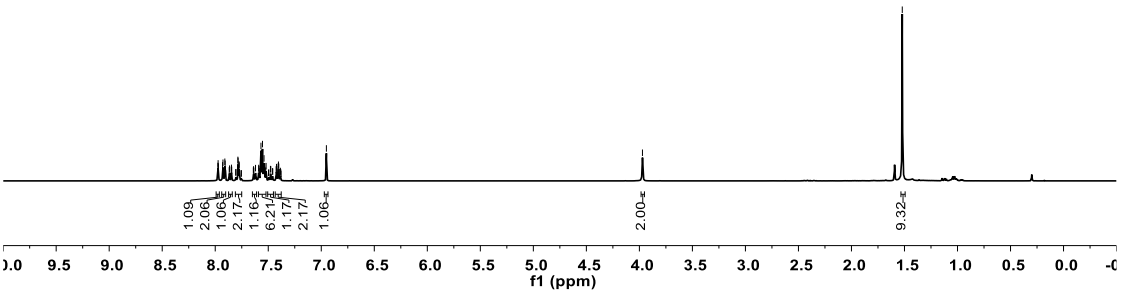
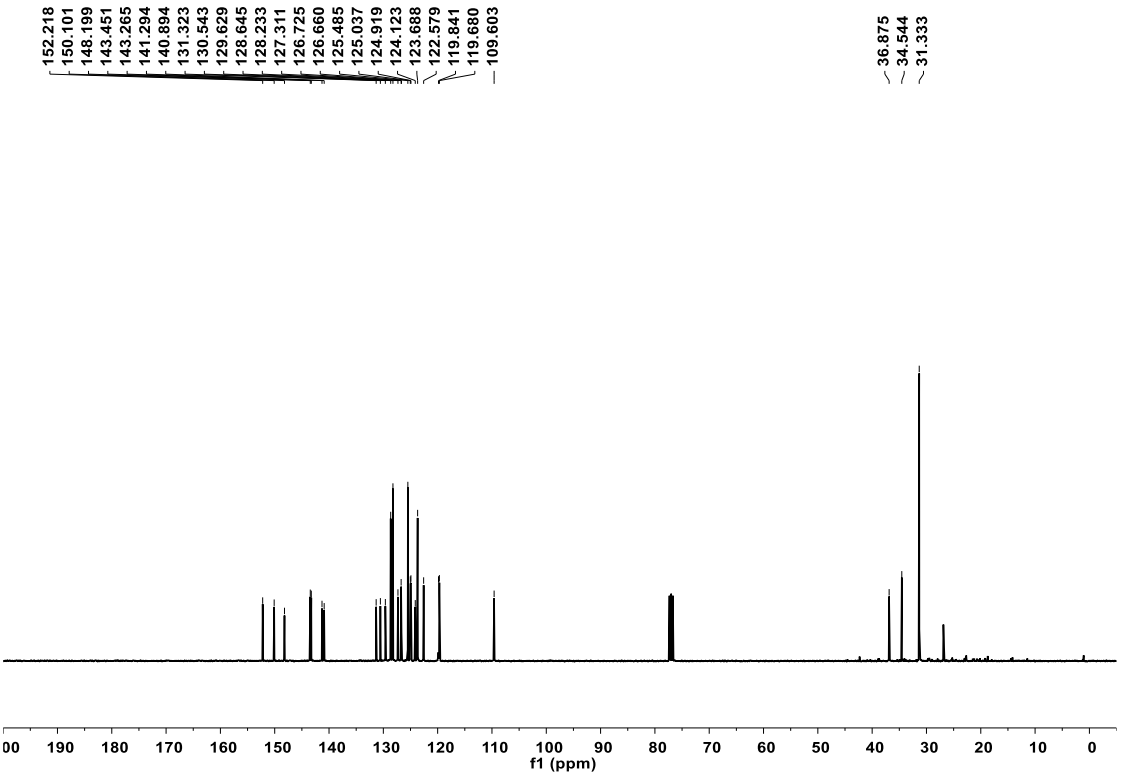
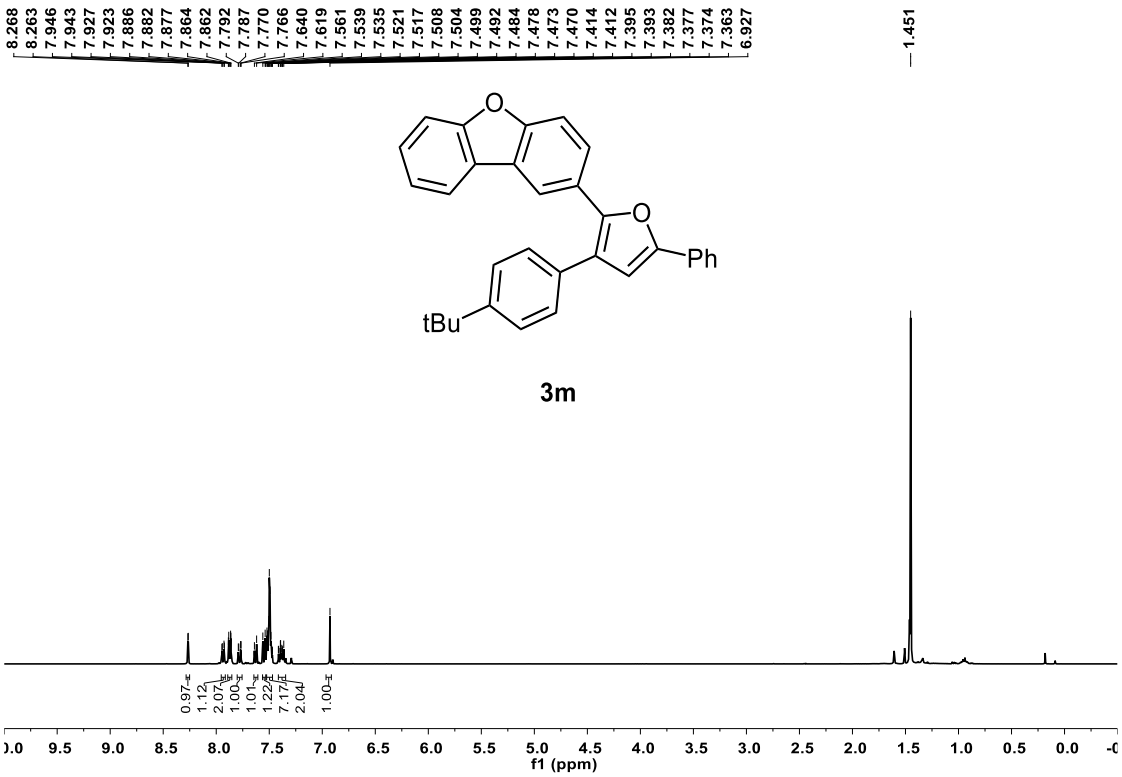
148.150
133.583
133.310
132.616
132.582
131.655
130.414
128.722
128.438
128.201
128.144
127.950
127.909
127.858
127.690
127.603
127.564
127.245
126.998
126.245
126.064
125.960
124.946
124.875
124.228
123.849
109.662
f1 (ppm)


7.975
7.973
7.970
7.930
7.927
7.922
7.909
7.906
7.902
7.868
7.865
7.849
7.847
7.845
7.807
7.805
7.786
7.785
7.777
7.773
7.753
7.641
7.638
7.636
7.620
7.590
7.588
7.584
7.575
7.569
7.559
7.554
7.548
7.540
7.533
7.524
7.521
7.498
7.495
7.479
7.476
7.461
7.457
7.425
7.422
7.419
7.416
7.407
7.404
7.401
7.397
7.389
7.386
7.382
6.952
3.971
1.521
O
Ph
tBu

3l


1.09
2.06
1.06
2.17
1.16
6.21
1.17
2.17
1.06
2.00
9.32
f1 (ppm)


152.218
150.101
148.199
143.451
143.265
141.294
140.894
131.323
130.543
129.629
128.645
128.233
127.311
126.725
126.660
125.485
125.037
124.919
124.123
123.688
122.579
119.841
119.680
109.603
36.875
34.544
31.333
f1 (ppm)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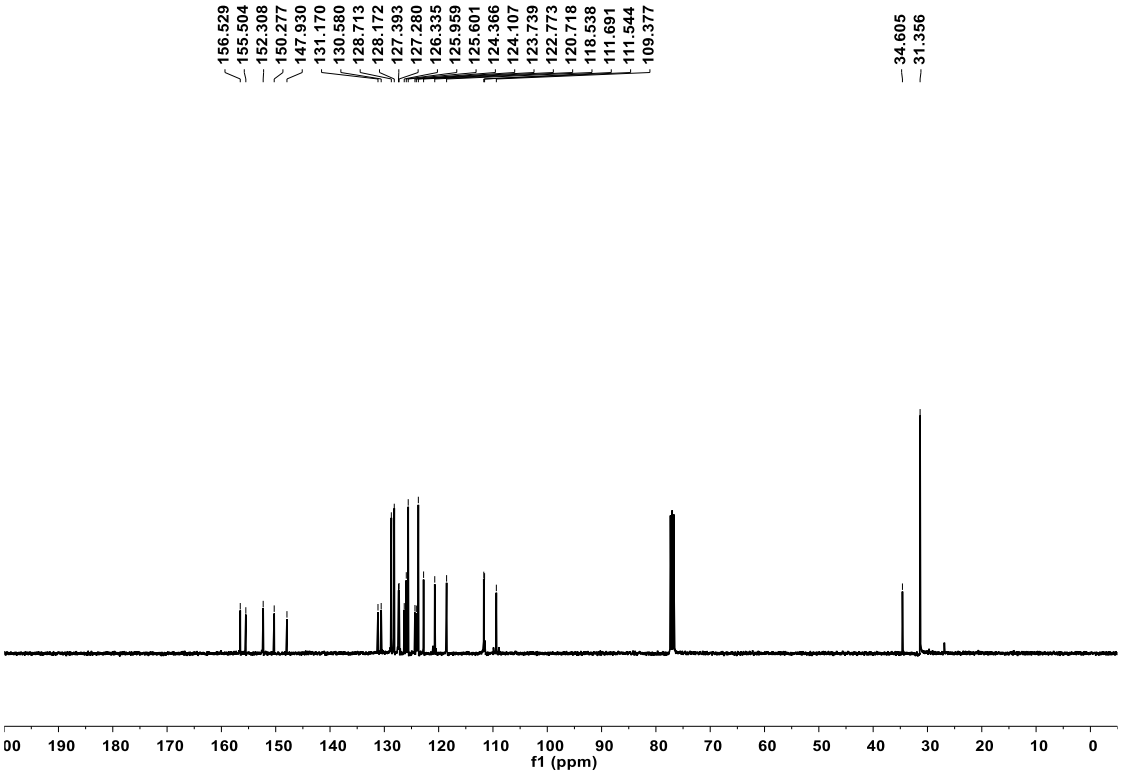
8.263
7.946
7.943
7.927
7.923
7.886
7.882
7.877
7.864
7.862
7.792
7.787
7.770
7.766
7.640
7.619
7.561
7.539
7.535
7.521
7.517
7.508
7.504
7.499
7.492
7.484
7.478
7.473
7.470
7.414
7.412
7.395
7.393
7.382
7.377
7.374
7.363
6.927
1.451
O
O
Ph
tBu
0.97
1.12
2.07
1.00
1.01
1.22
7.17
2.04
1.00
f1 (ppm)

3m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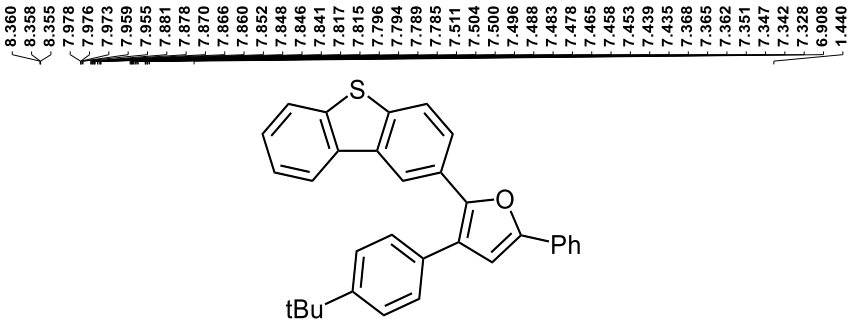
155.504
152.308
150.277
147.930
131.170
130.580
128.713
128.172
127.393
127.280
126.335
125.959
125.601
124.366
124.107
123.739
122.773
120.718
118.538
111.691
111.544
109.377
34.605
31.356
f1 (ppm)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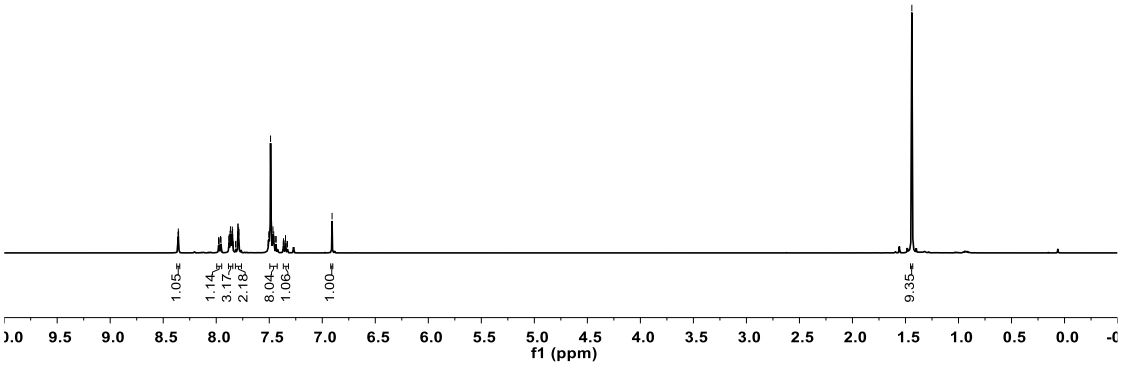
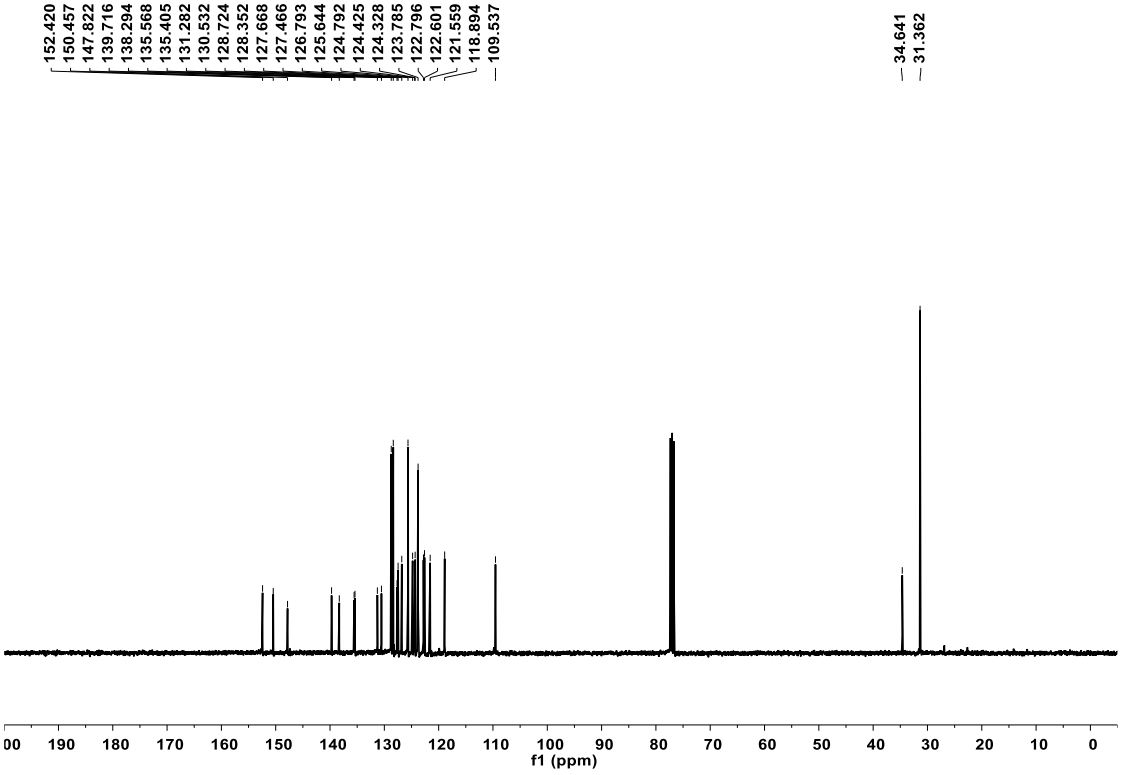
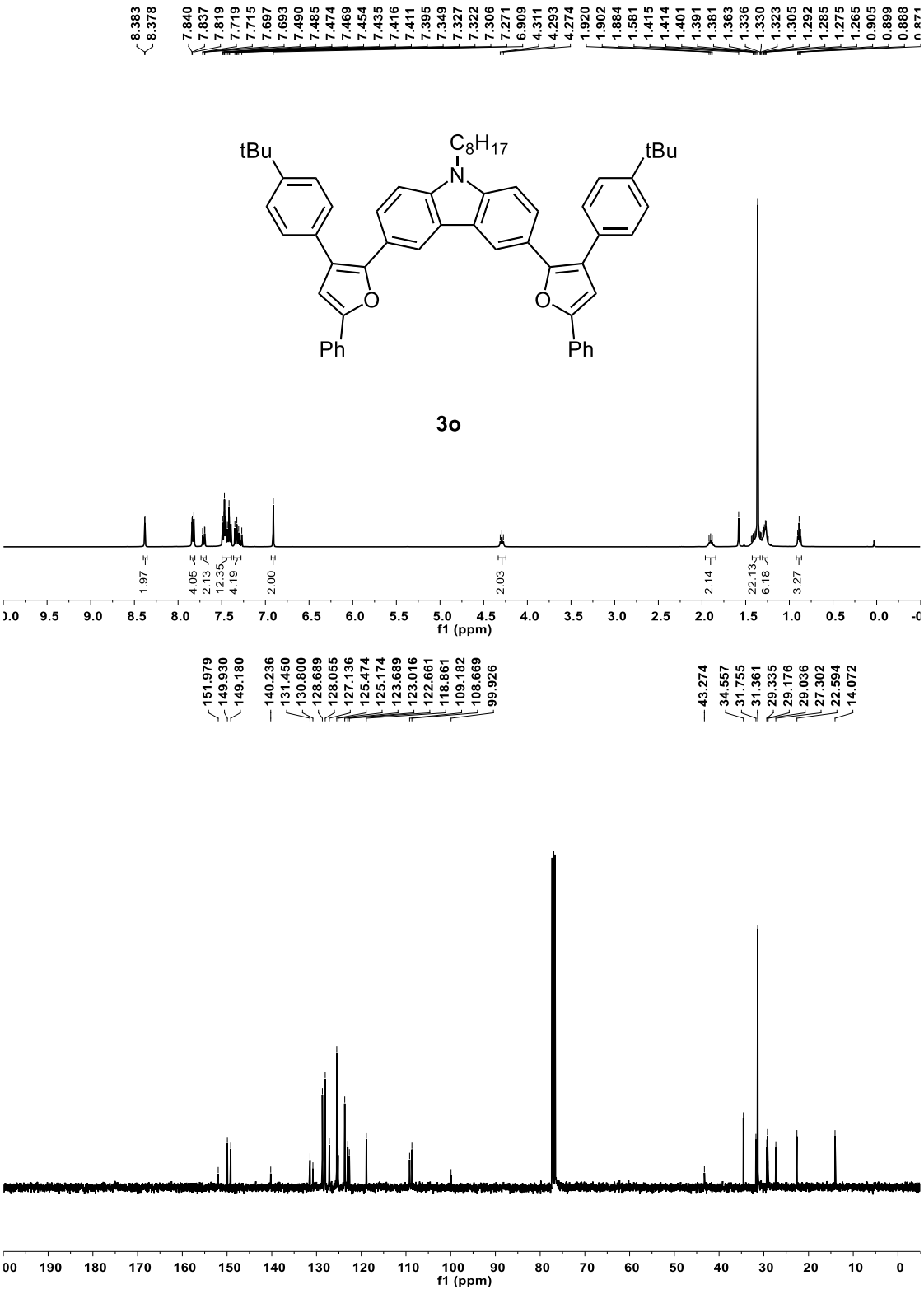
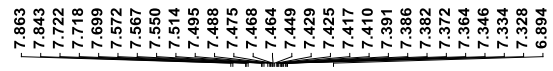
8.358
8.355
7.978
7.976
7.973
7.959
7.955
7.881
7.878
7.870
7.866
7.860
7.852
7.848
7.846
7.841
7.817
7.815
7.796
7.794
7.789
7.785
7.511
7.504
7.500
7.496
7.488
7.483
7.478
7.465
7.458
7.453
7.439
7.435
7.368
7.365
7.362
7.351
7.347
7.342
7.328
6.908
1.440
S
O
Ph
tBu

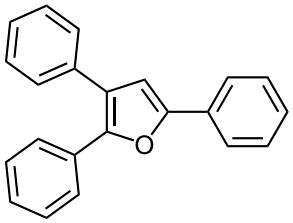
3n


1.05
1.14
3.17
2.18
8.04
1.06
1.00
9.35
f1 (ppm)

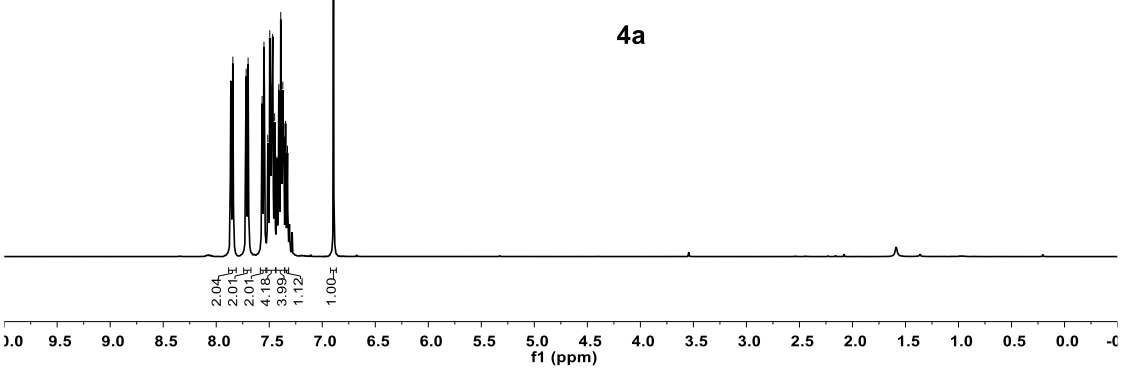

152.420
150.457
147.822
139.716
138.294
135.568
135.405
131.282
130.532
128.724
128.352
127.668
127.466
126.793
125.644
124.792
124.425
124.328
123.785
122.796
122.601
121.559
118.894
109.537
34.641
31.362
f1 (ppm)


8.383
8.378
7.840
7.837
7.819
7.719
7.715
7.697
7.693
7.490
7.485
7.474
7.469
7.454
7.435
7.416
7.411
7.395
7.349
7.327
7.322
7.306
7.271
6.909
4.311
4.293
4.274
1.920
1.902
1.884
1.581
1.415
1.414
1.401
1.391
1.381
1.363
1.336
1.330
1.323
1.305
1.292
1.285
1.275
1.265
0.905
0.899
0.888
tBu
C8H17
N
tBu
O
O
Ph
Ph
3o
1.97
4.05
2.13
12.35
4.19
2.00
2.03
2.14
22.13
6.18
3.27
f1 (ppm)
151.979
149.930
149.180
140.236
131.450
130.800
128.689
128.055
127.136
125.474
125.174
123.689
123.016
122.661
118.861
109.182
108.669
99.926
43.274
34.557
31.755
31.361
29.335
29.176
29.036
27.302
22.594
14.072
f1 (ppm)

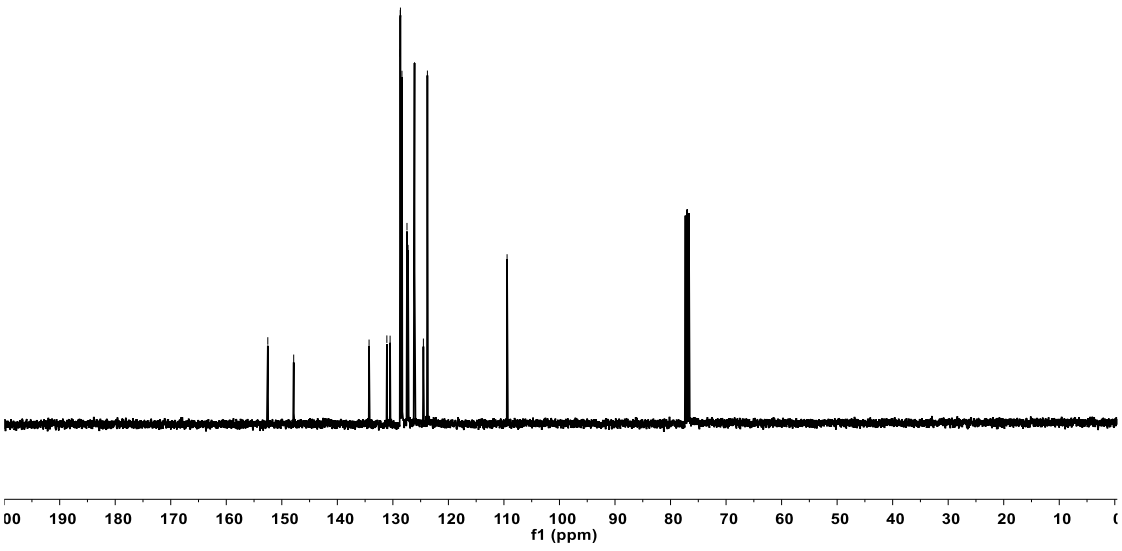

7.863
7.843
7.722
7.718
7.699
7.572
7.567
7.550
7.514
7.495
7.488
7.475
7.468
7.464
7.449
7.429
7.425
7.417
7.410
7.391
7.386
7.382
7.372
7.364
7.346
7.334
7.328
6.894

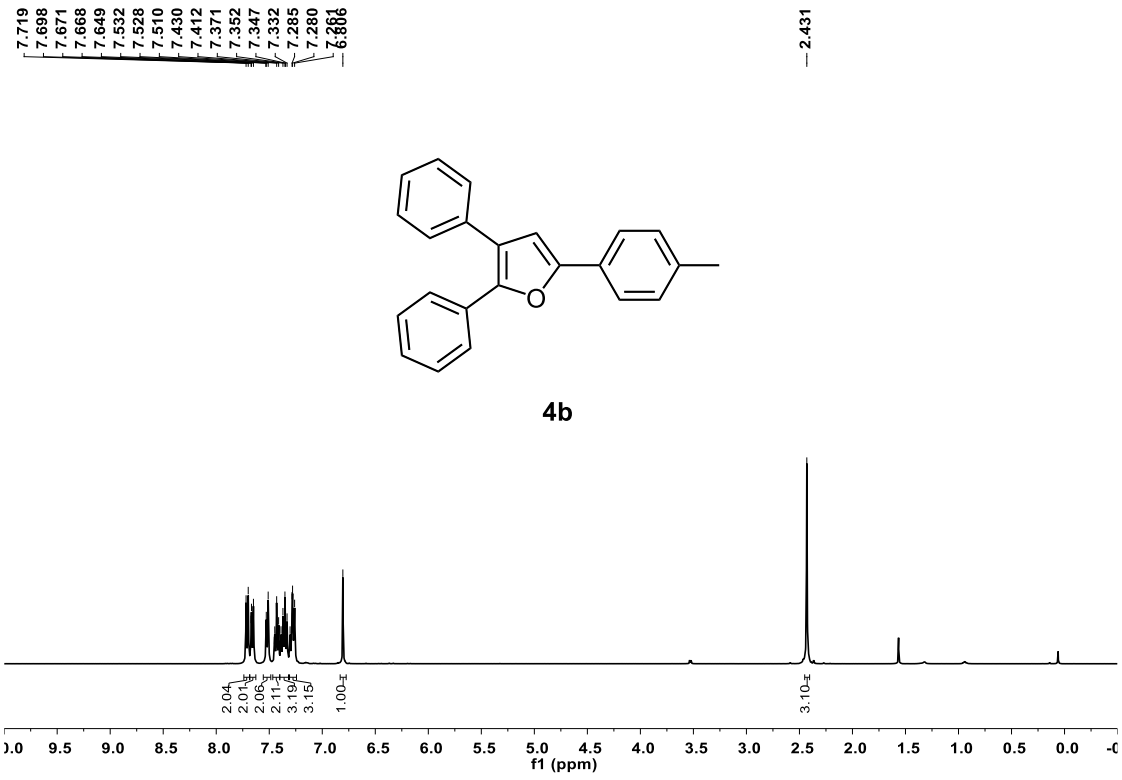


4a

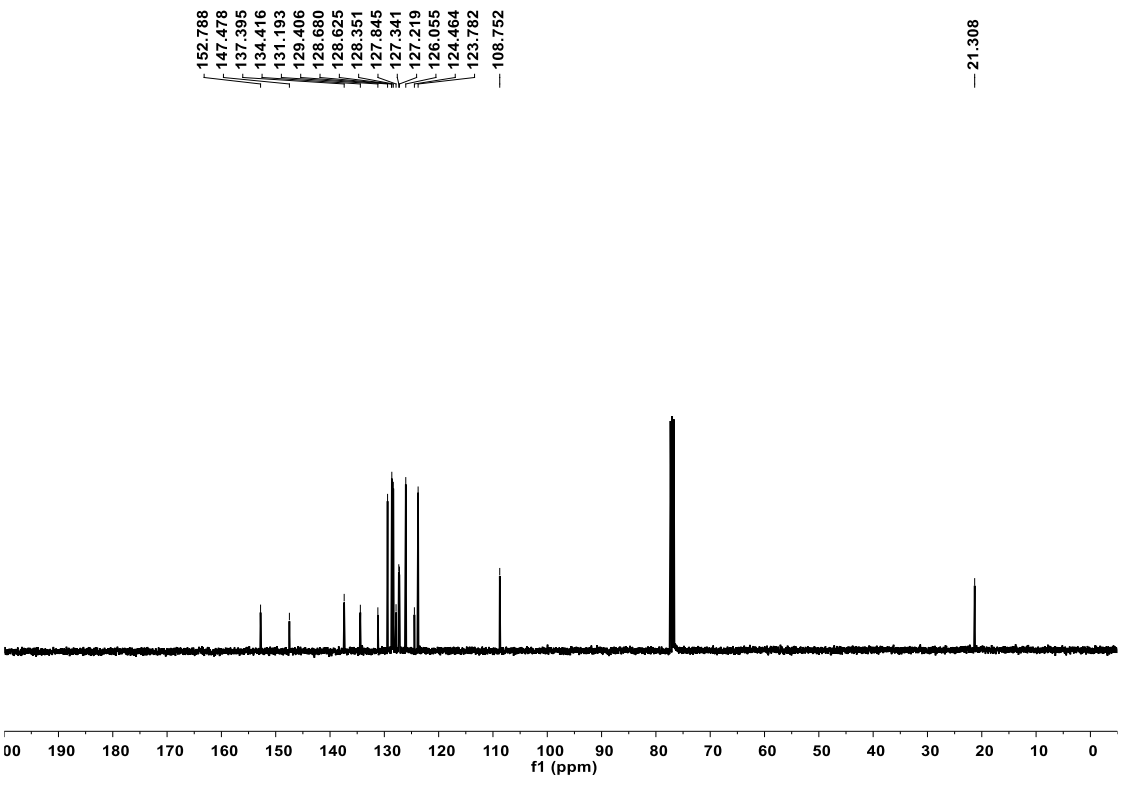

2.04
2.01
2.01
4.18
3.99
1.12
1.00
f1 (ppm)


152.521
147.859
134.287
131.083
130.497
128.699
128.669
128.637
128.364
127.486
127.459
127.265
126.099
124.503
123.781
109.434


f1 (ppm)


7.719
7.698
7.671
7.668
7.649
7.532
7.528
7.510
7.430
7.412
7.371
7.352
7.347
7.332
7.285
7.280
6.806
2.431
O
2.04
2.01
2.06
2.11
3.19
3.15
1.00
3.10
f1 (ppm)

4b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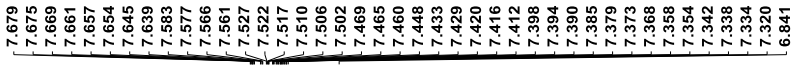
137.395
134.416
131.193
129.406
128.680
128.625
128.351
127.845
127.341
127.219
126.055
124.464
123.782
108.752
21.308
f1 (ppm)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7.675
7.669
7.661
7.657
7.654
7.645
7.639
7.583
7.577
7.566
7.561
7.527
7.522
7.517
7.510
7.506
7.502
7.469
7.465
7.460
7.448
7.433
7.429
7.420
7.416
7.412
7.398
7.394
7.390
7.385
7.379
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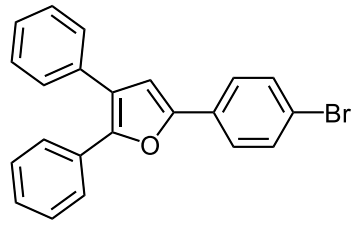
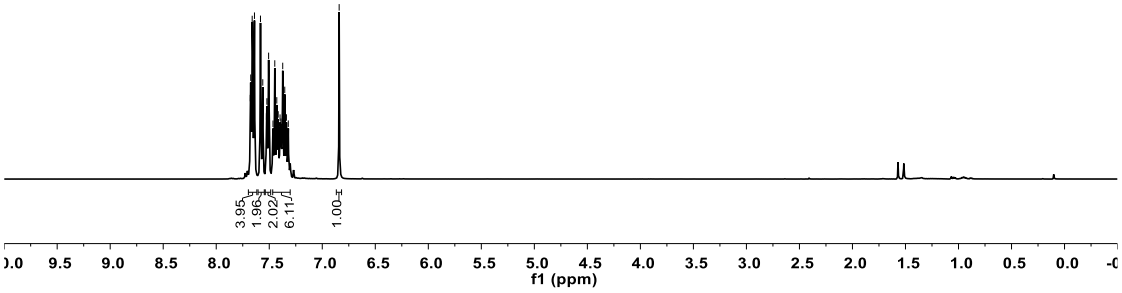
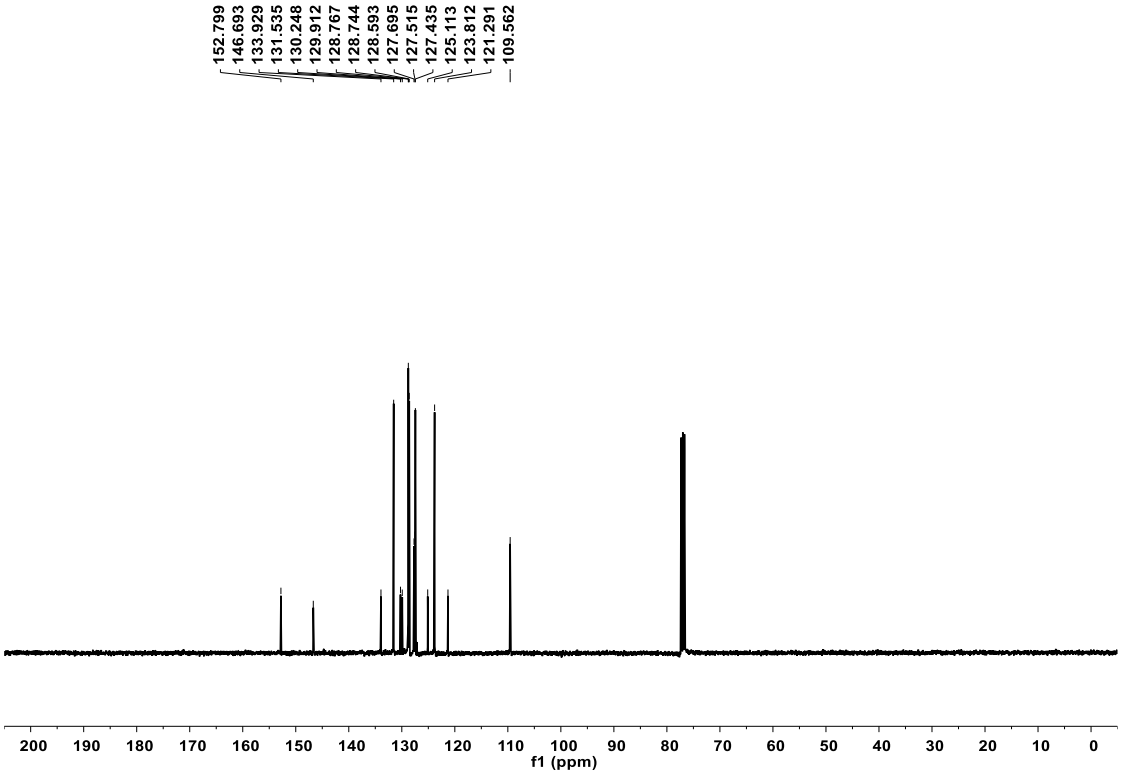
7.354
7.342
7.338
7.334
7.320
6.841


Br
O

4c


3.95
1.96
2.02
6.11
1.00
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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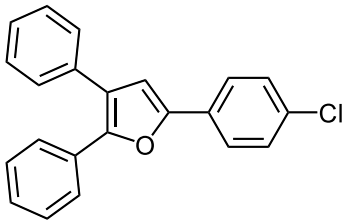
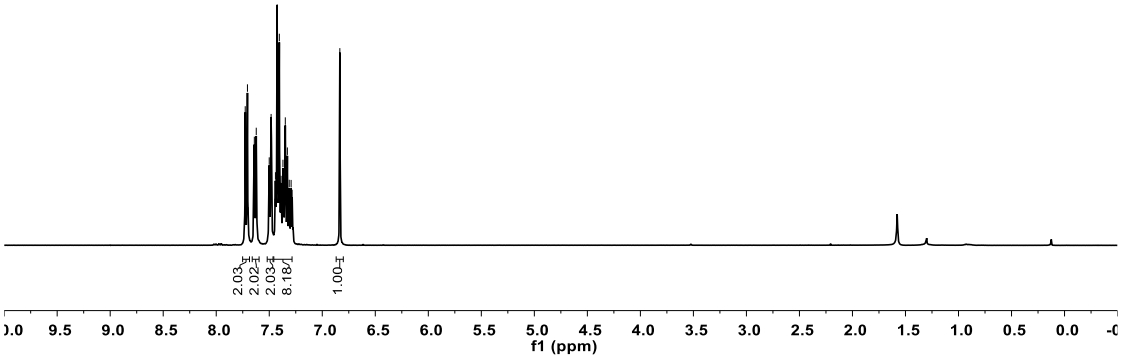
131.535
130.248
129.912
128.767
128.744
128.593
127.695
127.515
127.435
125.113
123.812
121.291
109.562
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.727
7.710
7.706
7.646
7.641
7.623
7.500
7.482
7.442
7.425
7.405
7.389
7.371
7.349
7.343
6.834


Cl
O

4d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2.02
2.03
8.18
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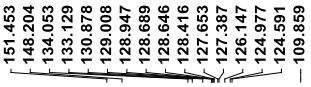
f1 (ppm)


151.453
148.204
134.053
133.129
130.878
129.008
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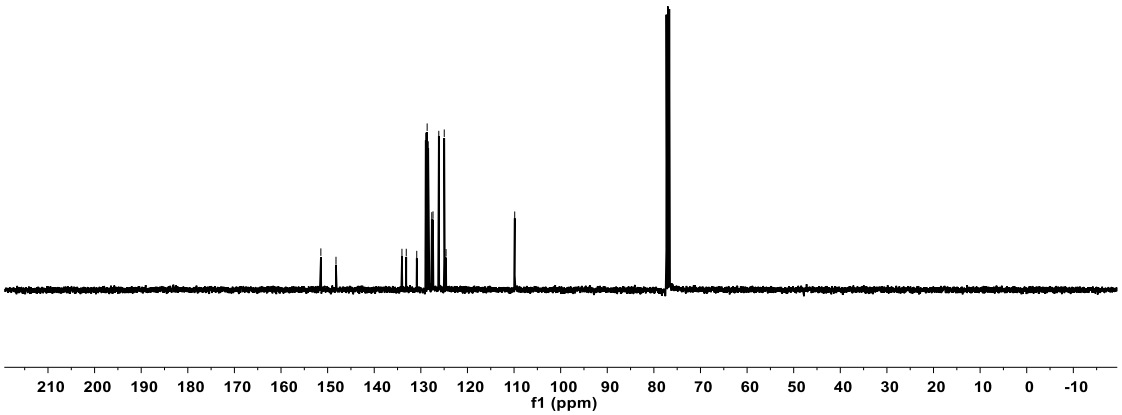
128.689
128.646
128.416
127.653
127.387
126.147
124.977
124.591
109.859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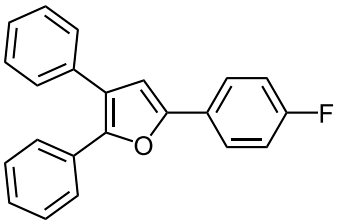
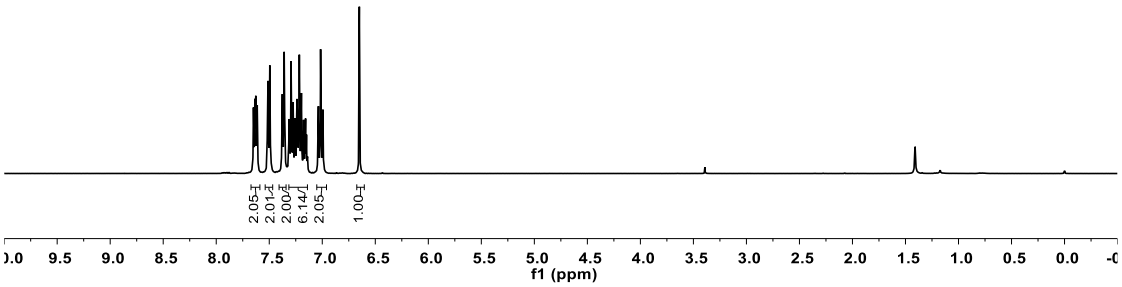

F
O

4e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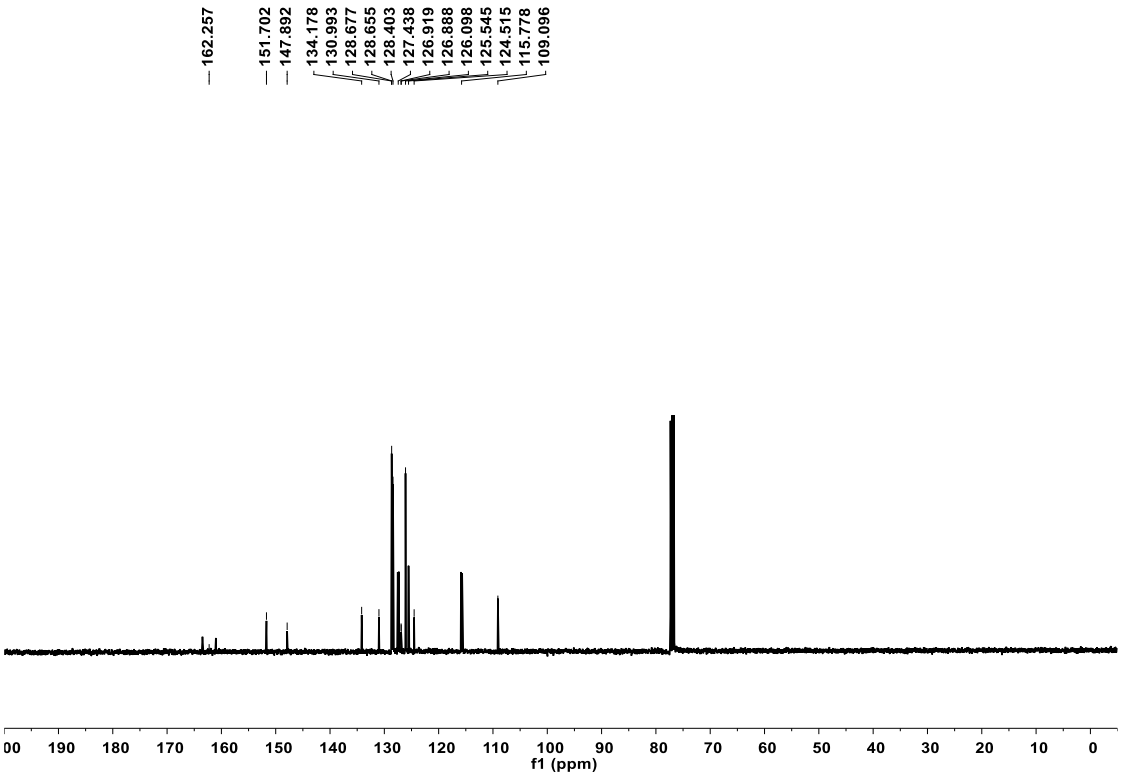
2.01
2.00
6.14
2.05
1.00
f1 (ppm)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151.702
147.892
134.178
130.993
128.677
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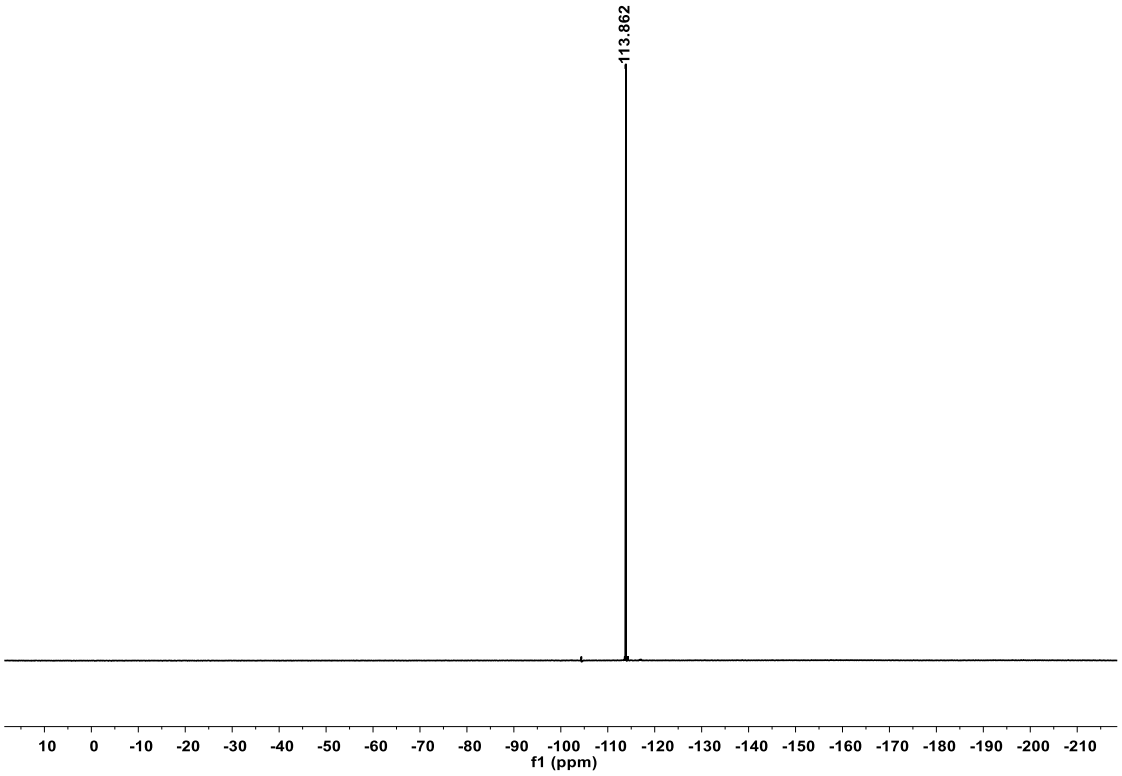
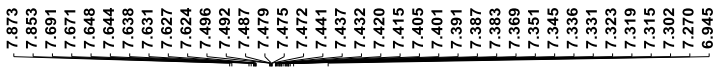
127.438
126.919
126.888
126.098
125.545
124.515
115.778
109.096
f1 (ppm)


-113.862
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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7.691
7.671
7.648
7.644
7.638
7.631
7.627
7.624
7.496
7.492
7.487
7.479
7.475
7.472
7.441
7.437
7.432
7.420
7.415
7.405
7.401
7.391
7.387
7.383
7.369
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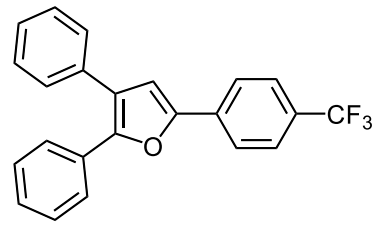
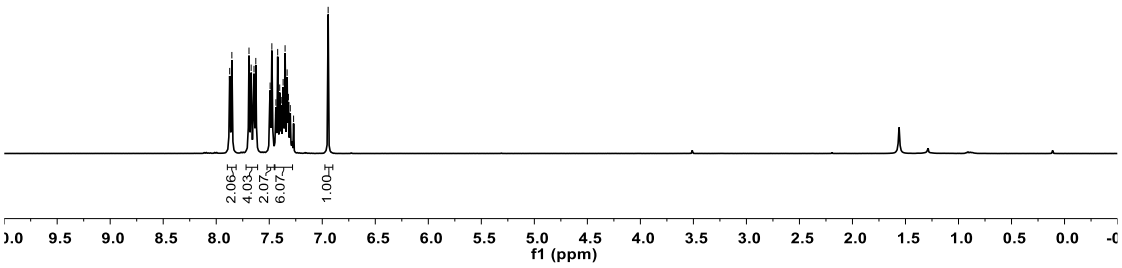
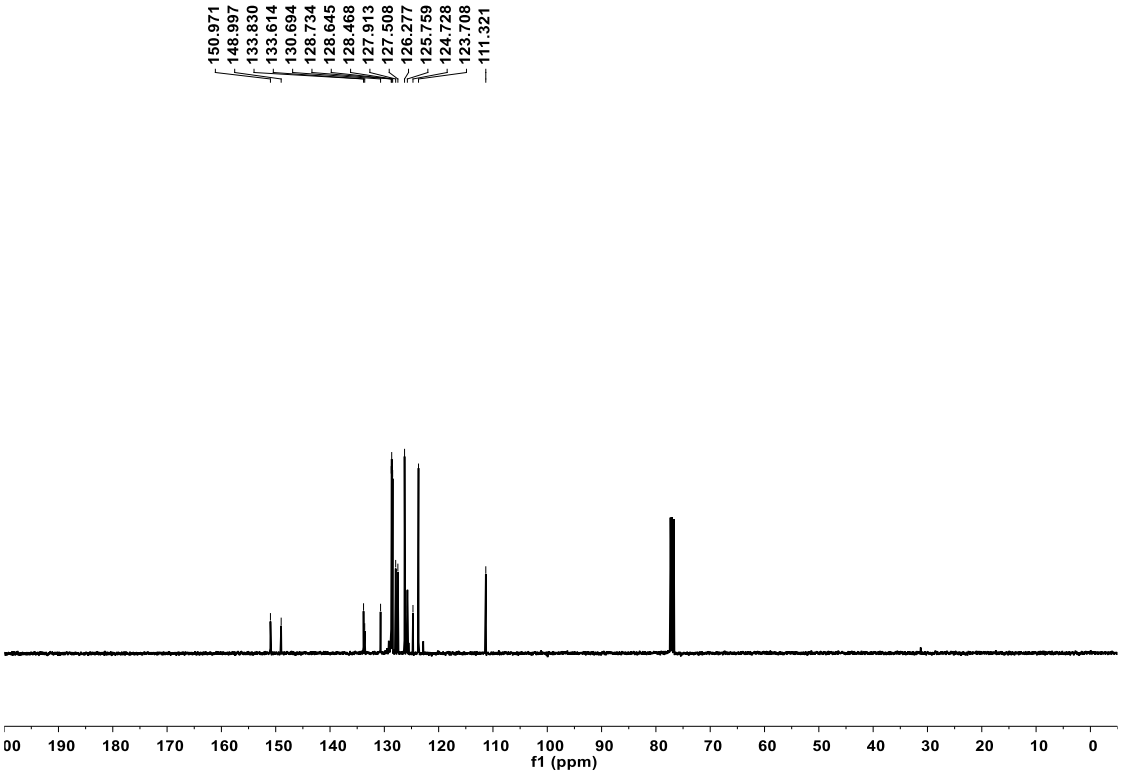
7.323
7.319
7.315
7.302
7.270
6.945


CF3
O

4f


2.06
4.03
2.07
6.07
1.00
f1 (ppm)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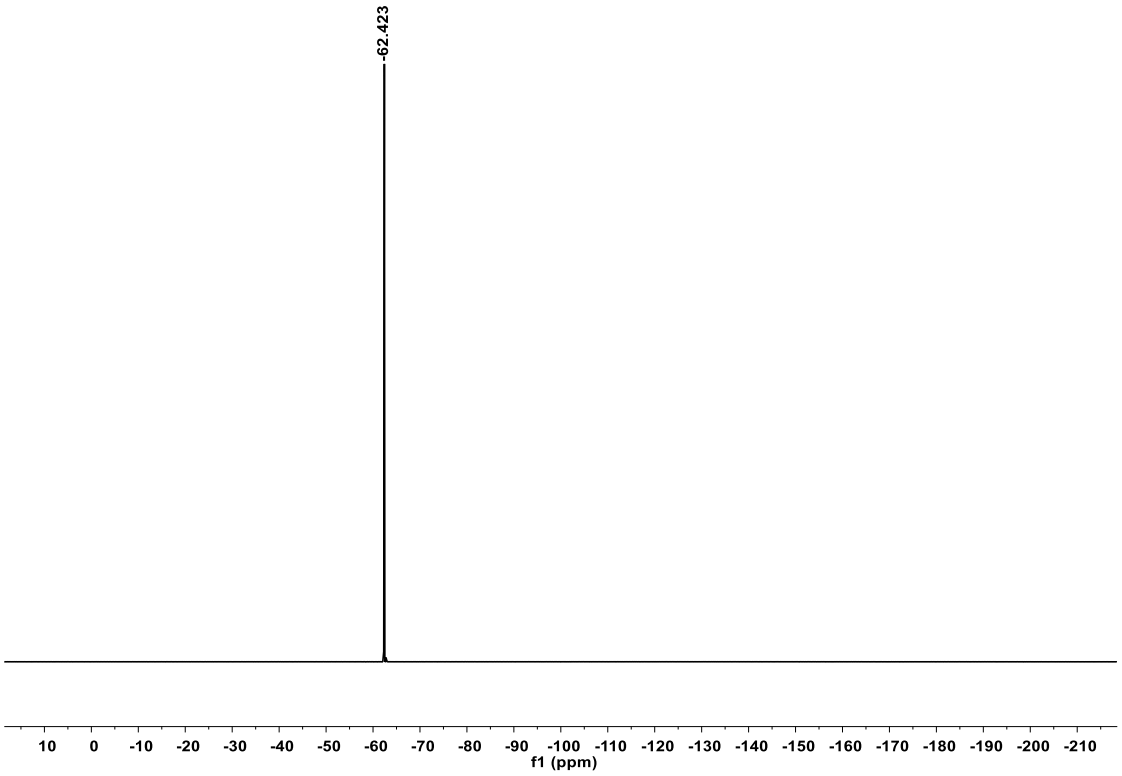
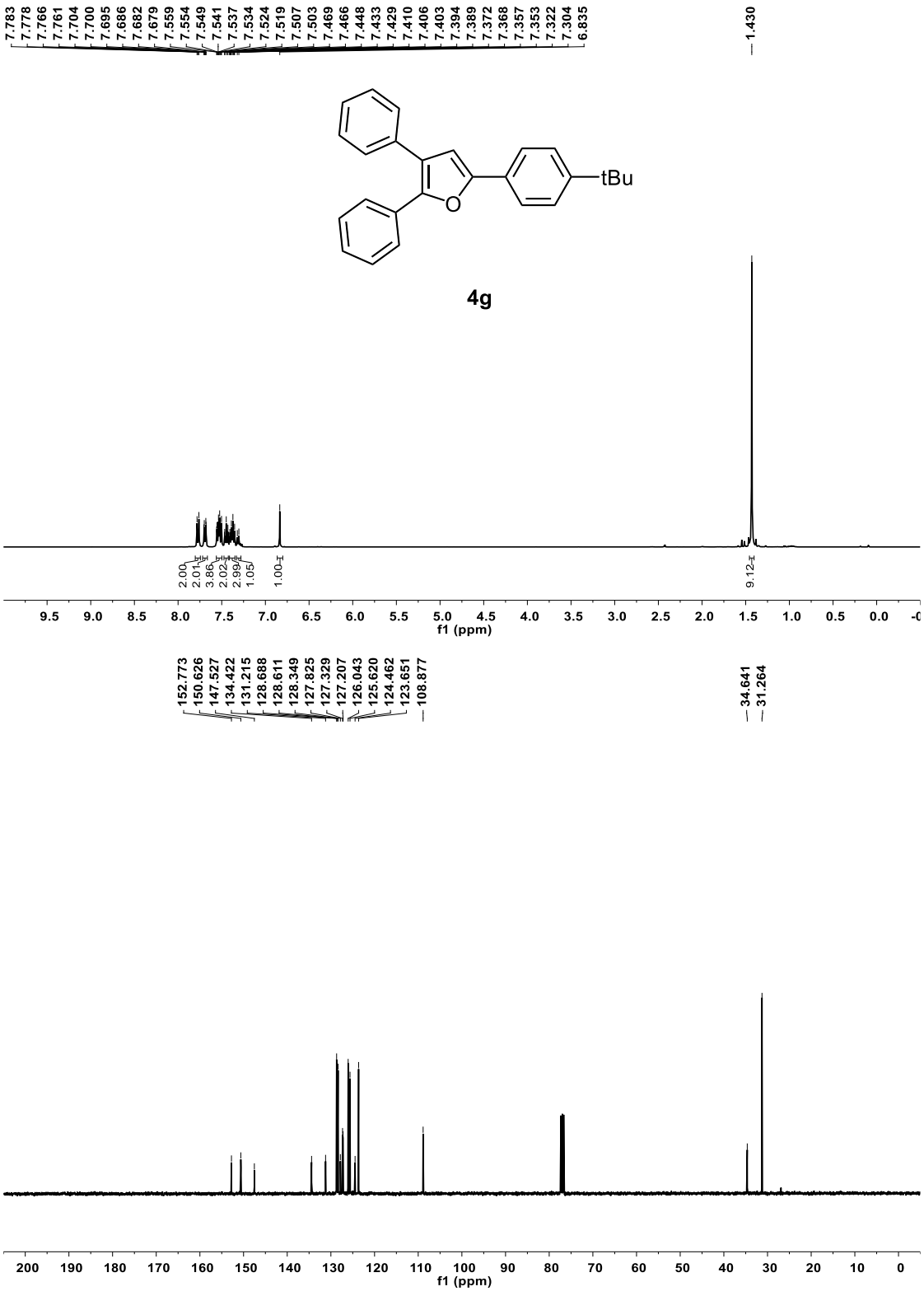
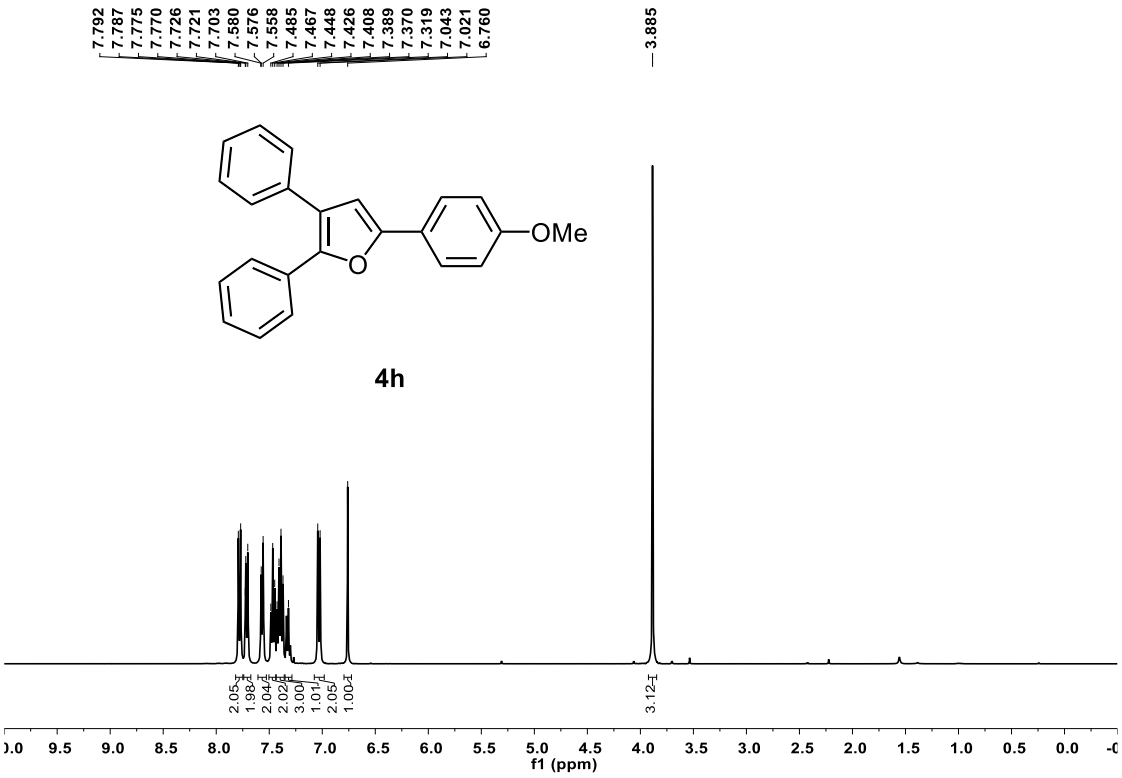
148.997
133.830
133.614
130.694
128.734
128.645
128.468
127.913
127.508
126.277
125.759
124.728
123.708
111.321
f1 (ppm)


-62.423
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


7.783
7.778
7.766
7.761
7.704
7.700
7.695
7.686
7.682
7.679
7.559
7.554
7.549
7.541
7.537
7.534
7.524
7.519
7.507
7.503
7.469
7.466
7.448
7.433
7.429
7.410
7.406
7.403
7.394
7.389
7.372
7.368
7.357
7.353
7.322
7.304
6.835
1.430
tBu
O
4g
2.00
2.01
3.86
2.02
2.99
1.05
1.00
9.12
f1 (ppm)
152.773
150.626
147.527
134.422
131.215
128.688
128.611
128.349
127.825
127.329
127.207
126.043
125.620
124.462
123.651
108.877
34.641
31.264
f1 (ppm)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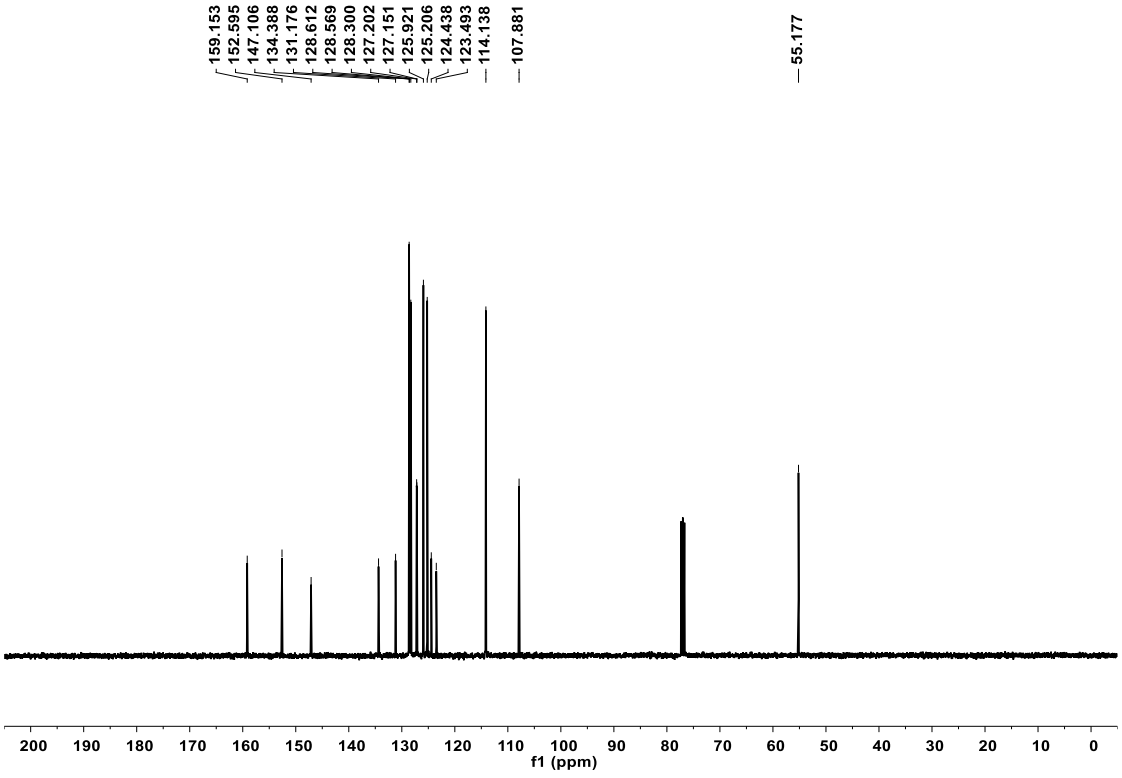
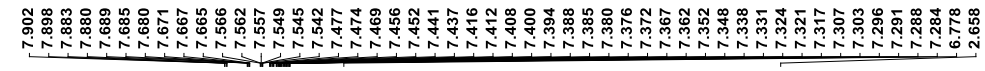
7.787
7.775
7.770
7.726
7.721
7.703
7.580
7.576
7.558
7.485
7.467
7.448
7.426
7.408
7.389
7.370
7.319
7.043
7.021
6.760
3.885
OMe
O
4h
2.05
1.98
2.04
2.02
3.00
1.01
2.05
1.00
3.12
f1 (ppm)


159.153
152.595
147.106
134.388
131.176
128.612
128.569
128.300
127.202
127.151
125.921
125.206
124.438
123.493
114.138
107.881
55.177
f1 (ppm)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7.898
7.883
7.880
7.689
7.685
7.680
7.671
7.667
7.665
7.566
7.562
7.557
7.549
7.545
7.542
7.477
7.474
7.469
7.456
7.452
7.441
7.437
7.416
7.412
7.408
7.400
7.394
7.388
7.385
7.380
7.376
7.372
7.367
7.362
7.352
7.348
7.338
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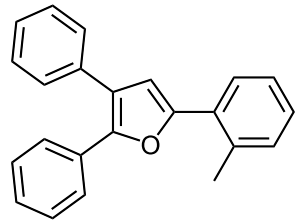
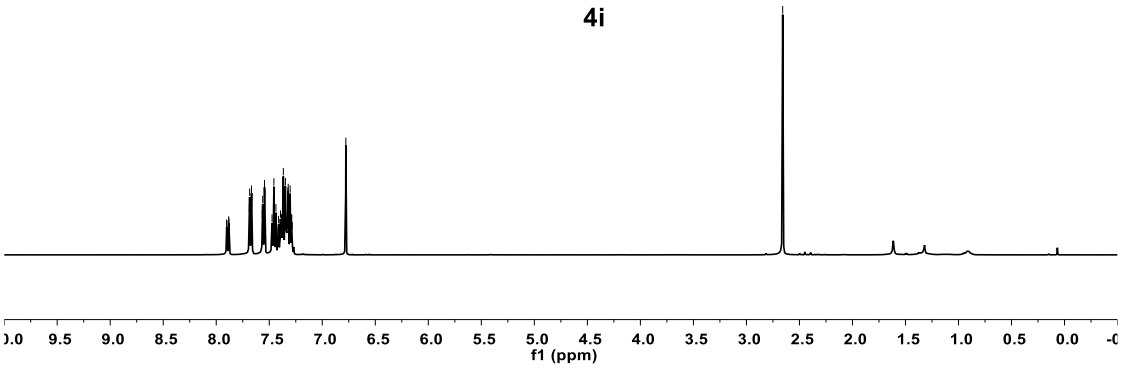
7.296
7.291
7.288
7.284
6.778
2.658


O

4i


f1 (ppm)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134.378
131.267
131.053
129.716
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128.648
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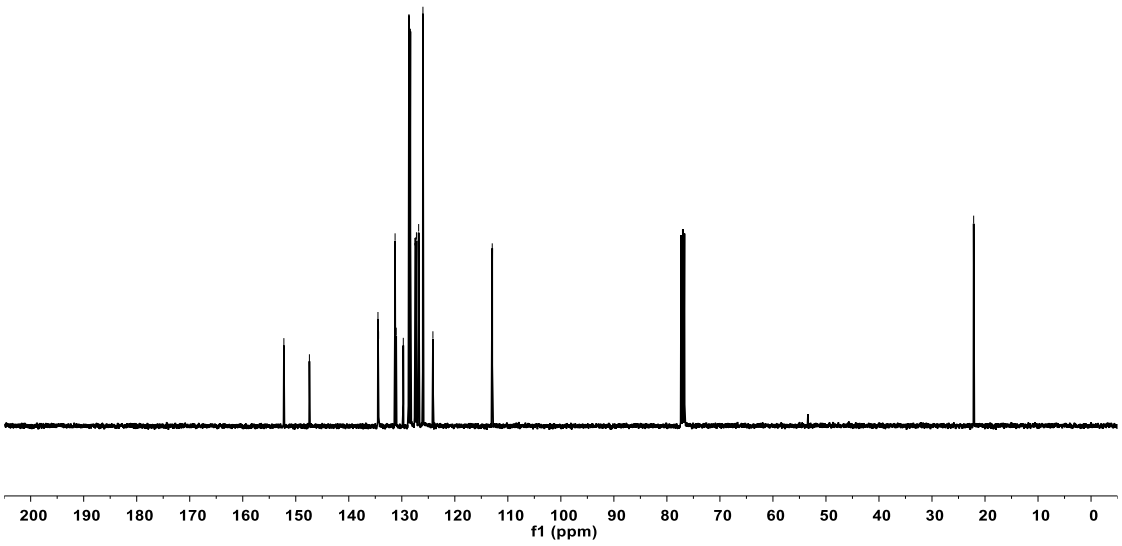
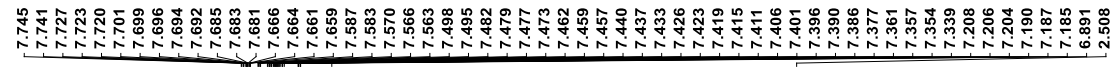
127.540
127.414
127.238
126.822
126.043
126.013
124.133
112.942
22.141


f1 (ppm)


7.745
7.741
7.727
7.723
7.720
7.701
7.699
7.696
7.694
7.692
7.685
7.683
7.681
7.666
7.664
7.661
7.659
7.587
7.583
7.570
7.566
7.563
7.498
7.495
7.482
7.479
7.477
7.473
7.462
7.459
7.457
7.440
7.437
7.433
7.426
7.423
7.419
7.415
7.411
7.406
7.401
7.396
7.390
7.386
7.377
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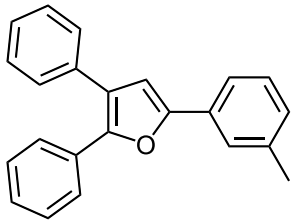
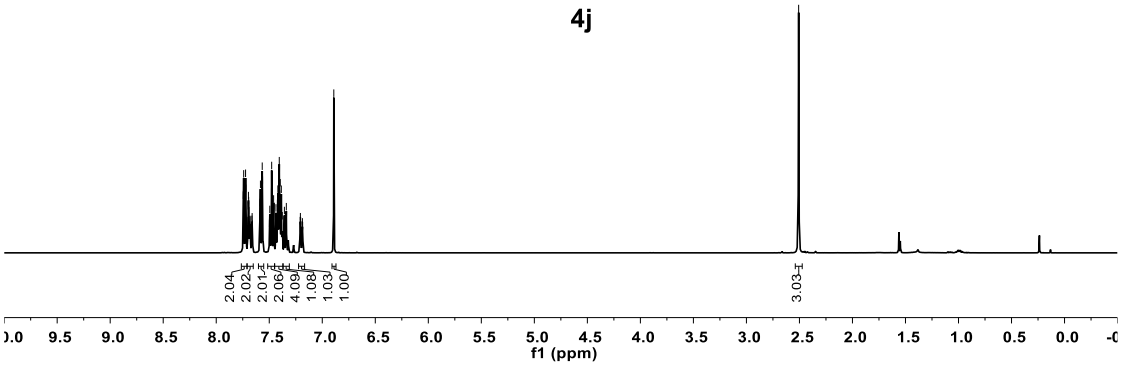
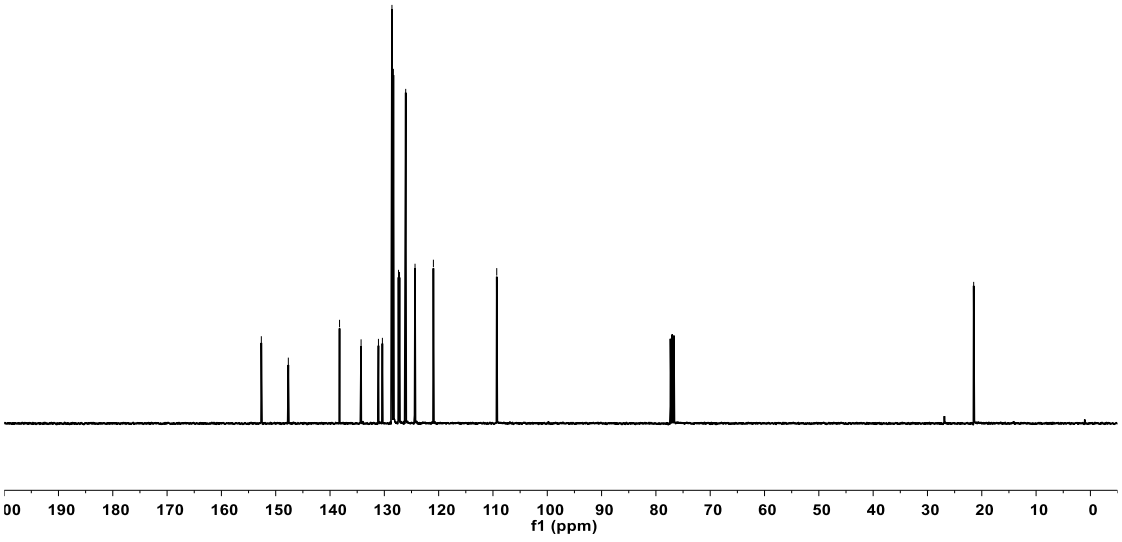
7.204
7.190
7.187
7.185
6.891
2.508

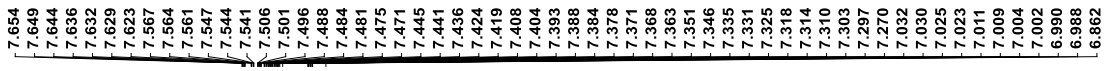


4j


2.04
2.02
2.01
2.06
4.09
1.08
1.03
1.00
3.03
f1 (ppm)


152.649
147.679
138.249
134.281
131.084
130.358
128.624
128.599
128.587
128.333
128.318
127.393
127.206
126.066
124.425
124.348
120.968
109.306
21.490


f1 (ppm)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7.644
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7.632
7.629
7.623
7.567
7.564
7.561
7.547
7.544
7.541
7.506
7.501
7.496
7.488
7.484
7.481
7.475
7.471
7.445
7.441
7.436
7.424
7.419
7.408
7.404
7.393
7.388
7.384
7.378
7.371
7.368
7.363
7.351
7.346
7.335
7.331
7.325
7.318
7.314
7.310
7.303
7.297
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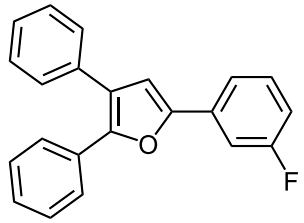
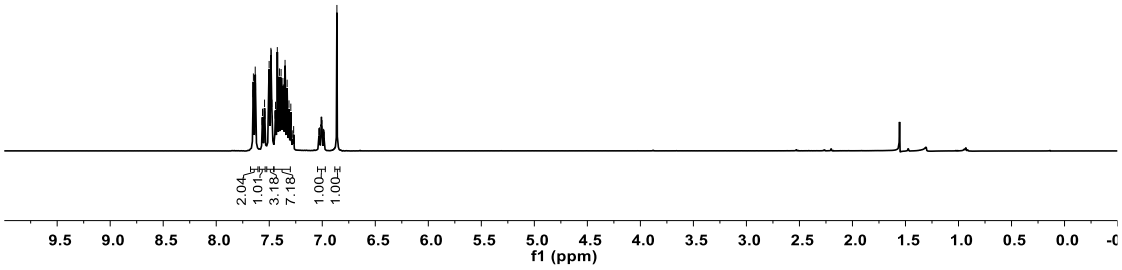
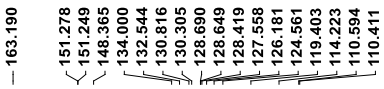
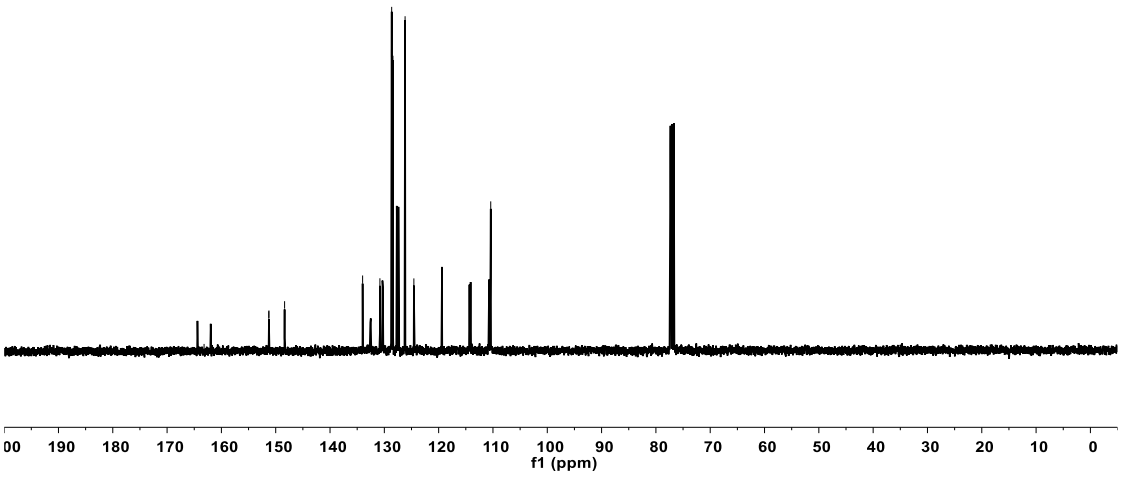
7.032
7.030
7.025
7.023
7.011
7.009
7.004
7.002
6.990
6.988
6.862

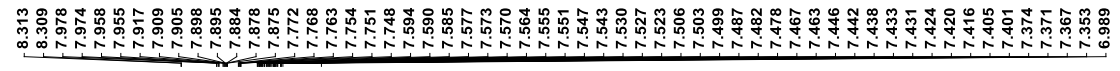

O
F

4k


2.04
1.01
3.18
7.18
1.00
1.00
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)


163.190
151.278
151.249
148.365
134.000
132.544
130.816
130.305
128.690
128.649
128.419
127.558
126.181
124.561
119.403
114.223
110.594
110.411


00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.309
7.978
7.974
7.958
7.955
7.917
7.909
7.905
7.898
7.895
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7.878
7.875
7.772
7.768
7.763
7.754
7.751
7.748
7.594
7.590
7.585
7.577
7.573
7.570
7.564
7.555
7.551
7.547
7.543
7.530
7.527
7.523
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7.503
7.499
7.487
7.482
7.478
7.467
7.463
7.446
7.442
7.438
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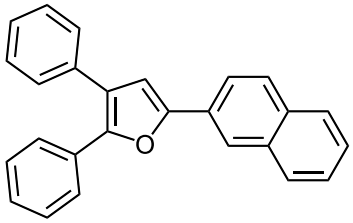
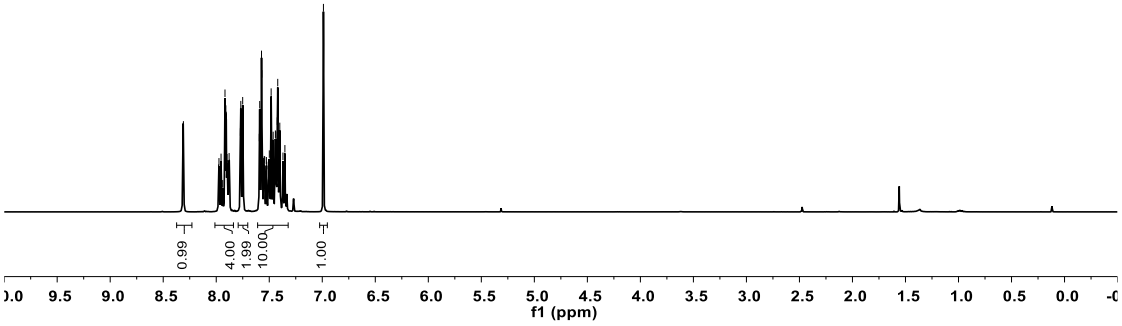
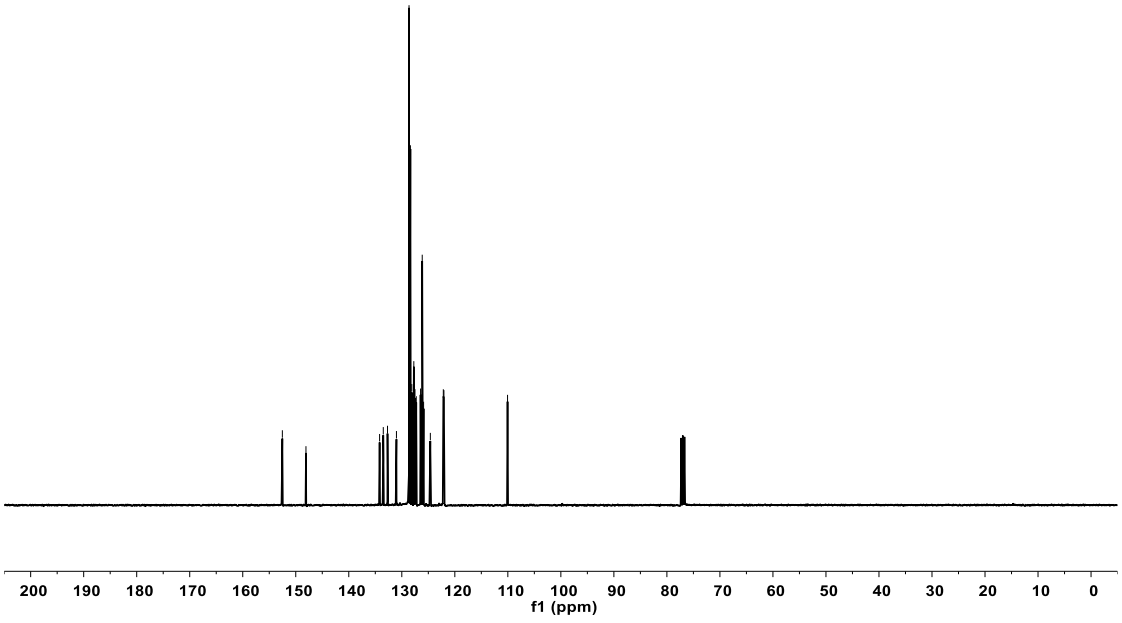
7.401
7.374
7.371
7.367
7.353
6.989

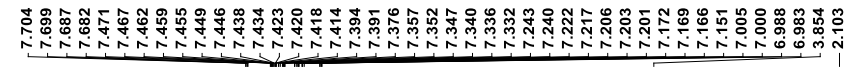


4l


0.99
4.00
1.99
10.00
1.00
f1 (ppm)


152.529
148.077
134.187
133.491
132.693
131.009
128.636
128.379
128.116
127.732
127.515
127.272
126.462
126.148
125.890
124.617
122.168
122.059
110.054


f1 (ppm)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7.467
7.462
7.459
7.455
7.449
7.446
7.438
7.434
7.423
7.420
7.418
7.414
7.394
7.391
7.376
7.357
7.352
7.347
7.340
7.336
7.332
7.243
7.240
7.222
7.217
7.206
7.203
7.201
7.172
7.169
7.166
7.151
7.005
7.000
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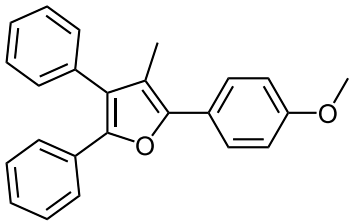
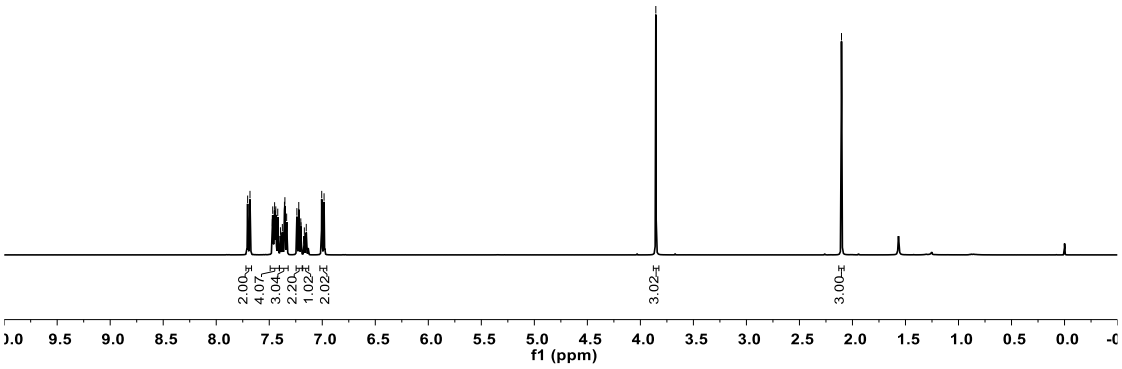
6.983
3.854
2.103


O
O

4m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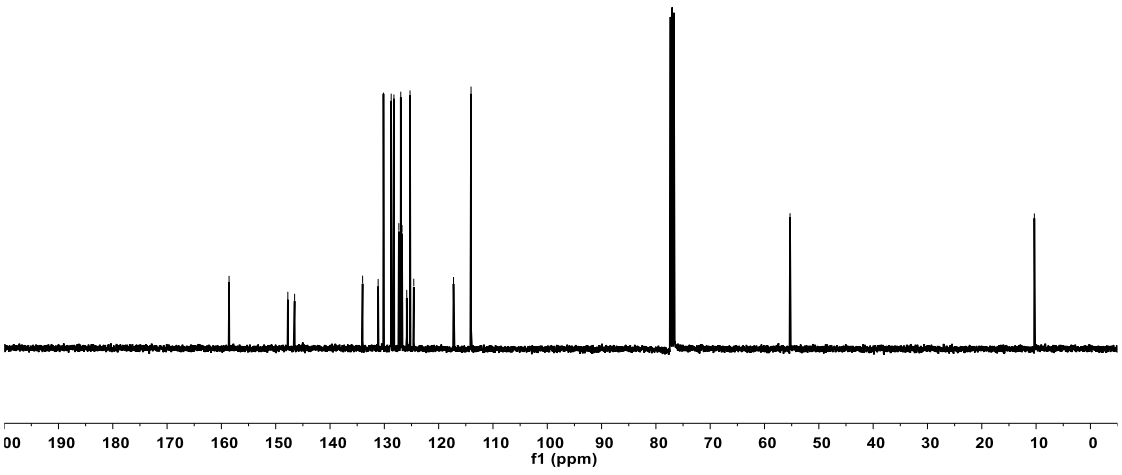
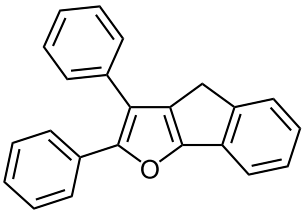
4.07
3.04
2.20
1.02
2.02
3.02
3.00
f1 (ppm)

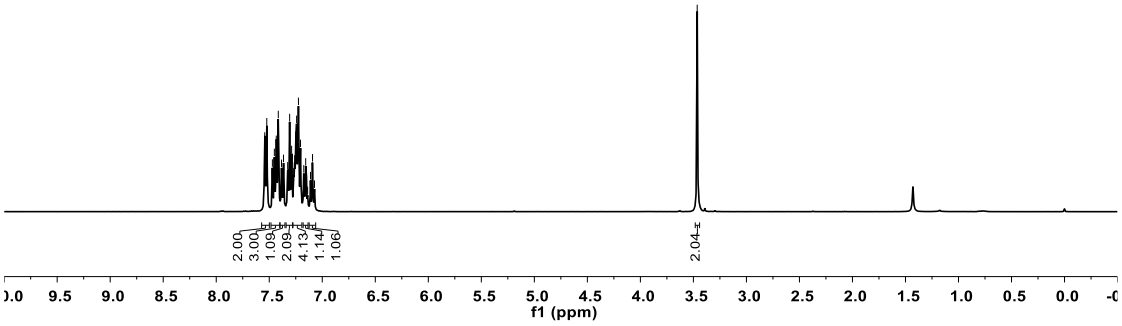

158.589
147.768
146.523
134.003
131.140
130.159
128.736
128.234
127.334
126.975
126.743
125.875
125.268
124.582
117.261
114.035
55.302
10.316

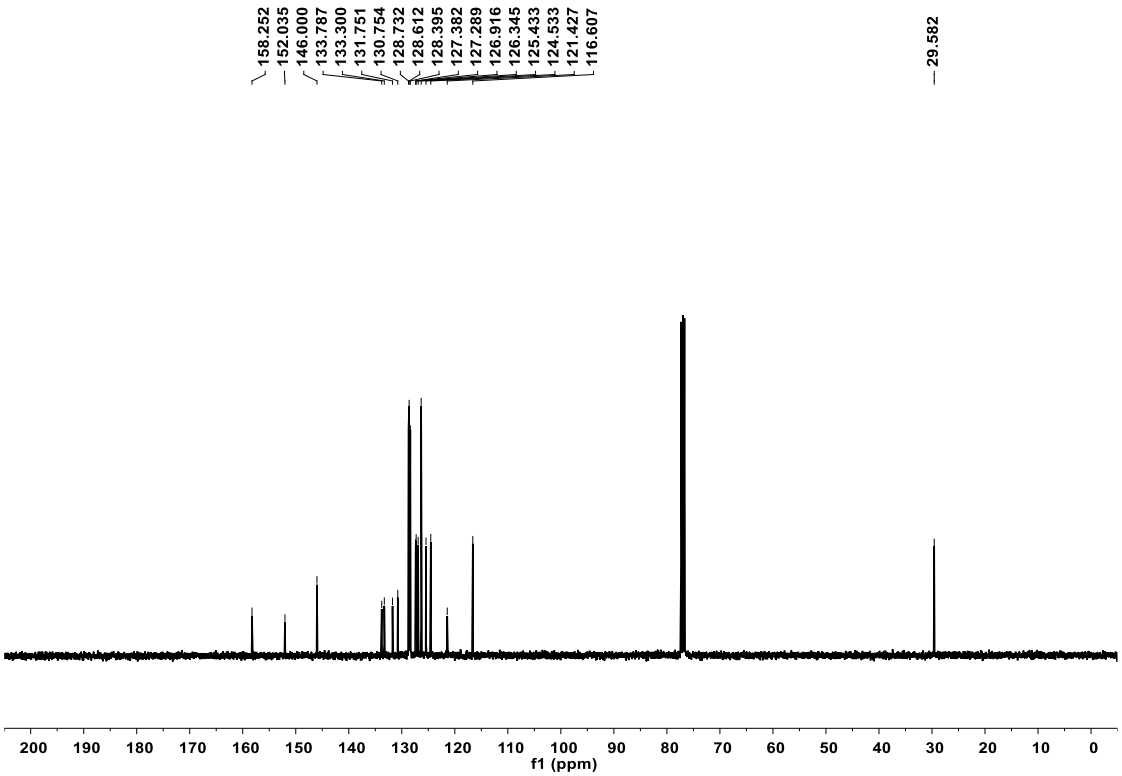

f1 (ppm)

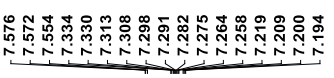

7.543
7.523
7.470
7.452
7.434
7.415
7.384
7.365
7.326
7.308
7.289
7.270
7.261
7.250
7.242
7.225
7.205
7.174
7.156
7.149
7.138
7.111
7.092
7.073
3.464

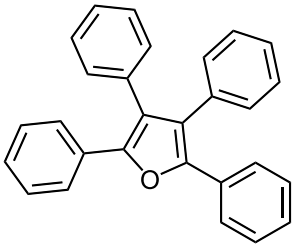


4n

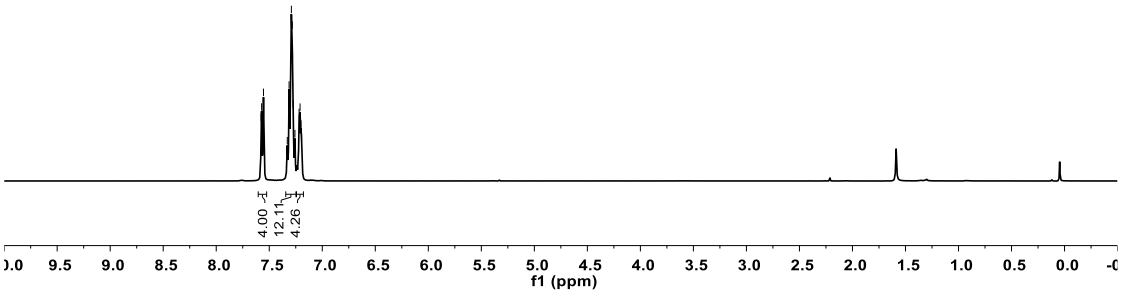

2.00
3.00
1.09
2.09
4.13
1.14
1.06
2.04
f1 (ppm)

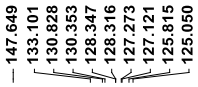

158.252
152.035
146.000
133.787
133.300
131.751
130.754
128.732
128.612
128.395
127.382
127.289
126.916
126.345
125.433
124.533
121.427
116.607
29.582
f1 (ppm)

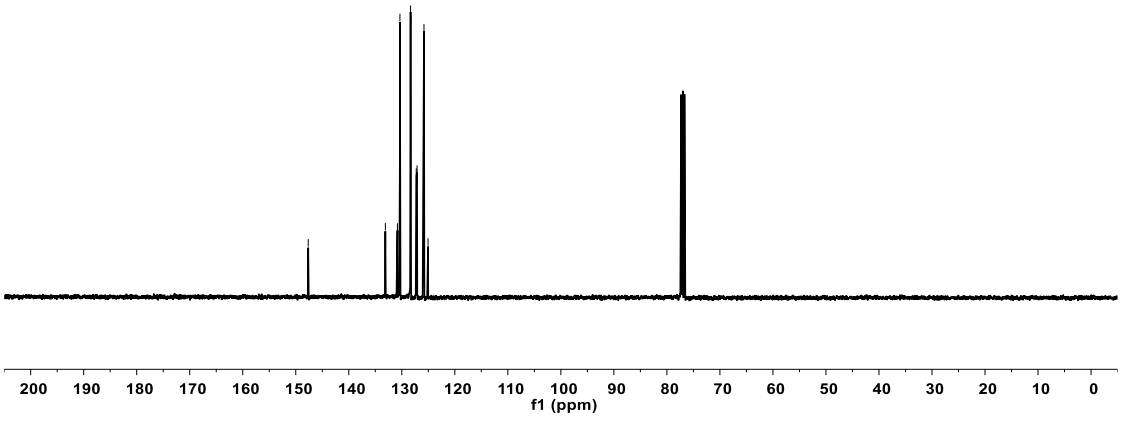

7.576
7.572
7.554
7.334
7.330
7.313
7.308
7.298
7.291
7.282
7.275
7.264
7.258
7.219
7.209
7.200
7.194



4o


4.00
12.11
4.26
f1 (ppm)


147.649
133.101
130.828
130.353
128.347
128.316
127.273
127.121
125.815
125.050


f1 (ppm)

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