Electronic Supplementary Material (ESI) for ChemComm.

Para-Selective Arylation and Alkenylation of Monosubstituted Arenes Using Thianthrene *S*-Oxide as a Transient Mediator

Xiao-Yue Chen[†], Xiao-Xue Nie[†], Yichen Wu[†], and Peng Wang*[,†,‡]

[†]State Key Laboratory of Organometallic Chemistry, Center for Excellence in Molecular Synthesis, Shanghai Institute of Organic Chemistry, CAS 345 Lingling Road, Shanghai 200032, P.R. China

[‡]CAS Key Laboratory of Energy Regulation Materials, Shanghai Institute of Organic Chemistry, CAS 345 Lingling Road, Shanghai 200032, P.R. China

Table of Contents

1. General Information S2
2. Experimental Section S3
2.1 Preparation of Substrates S3
2.2 Experimental Optimization S5
2.2.1 Screening of Palladium Sources S5
2.2.2 Base Effects S5
2.2.3 Solvent Effects S6
2.2.4 Ni-Catalyzed thio-Suzuki Coupling S6
2.2.4 Control Experiments S6
2.3 General Procedure for *para*-Selective Arylation of Toluene S8
2.4 General Procedure for *para*-Selective Alkenylation of Toluene S18
2.5 General Procedure for *para*-Selective Arylation of Monosubstituted Arenes S22
2.6 Applications of *para*-Functionalization of Arenes S33
3. References S37
4. NMR Spectra S39

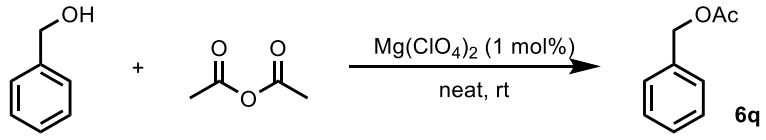
1. General Information

Thianthrene S-oxide was synthesized following the known procedure.[1] Trifluoromethanesulfonic anhydride (Tf_2O) was purchased from Energy Chemical. Other reagents were purchased from TCI, Sigma-Aldrich, Acros, Adamas-beta, J&K, 9-Ding, Bidepharm and Energy Chemical of the highest purity grade and used without further purification, unless otherwise indicated. Dichloromethane (CH_2Cl_2) and *N*,*N*-dimethylformamide (DMF) were dried using the solvent purification system. Acetone was distilled following the general purification methods. Other anhydrous solvents were purchased from J&K. The extent of reaction was monitored by thin–layer chromatography (TLC), performed on 0.25 mm silica gel HSGF254. The TLC plates were visualized by ultraviolet light (254 nm) or treatment with potassium permanganate stain followed by gentle heating if needed.

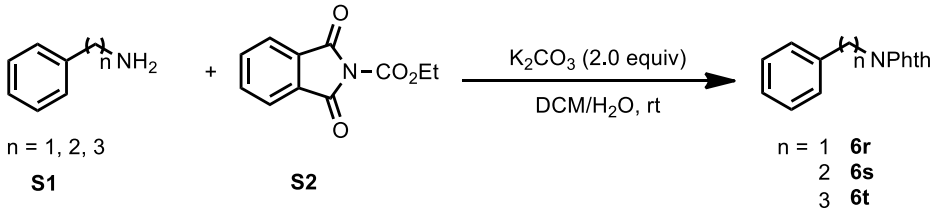
NMR spectra were recorded on Varian 400, Bruker 400 and Agilent 400 (400 Hz for ^1H; 375 Hz for ^{19}F; 100 Hz for ^{13}C) spectrometer.The chemical shifts (δ) were quoted in parts per million (ppm) referenced to TMS (0.0 ppm for ^1H NMR), $CDCl_3$ (77.0 ppm for ^{13}C NMR) and $(CD_3)_2SO$ (39.52 ppm for ^{13}C NMR). The following abbreviations were used to explain multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, p = pentet, h = heptet, m = multiplet, and br = broad. Coupling constants, *J*, were reported in Hertz unit (Hz). ^{13}C NMR spectra were fully decoupled by broad band proton decoupling. ^{19}F NMR spectra were recorded on Agilent 400 MR DD2 instrument (375 MHz), and were fully decoupled by broad band proton decoupling. Chemical shifts were quoted in parts per million (ppm) referenced to 0.0 ppm for $CFCl_3$. High-resolution mass spectra (HRMS) were recorded on an Agilent Mass spectrometer using ESI–TOF or CI/EI or on a Thermo Mass spectrometer using ESI–TOF.

2. Experimental Section

2.1 Preparation of Substrates



Benzyl alcohol (0.51 mL, 5.0 mmol) was treated with Ac_2O (0.47 mL, 5.0 mmol) in the absence of solvent at room temperature for 6 h under magnetic stirring in the presence of $Mg(ClO_4)_2$ (11.2 mg, 0.05 mmol, 1 mol%). After the reaction completed, H_2O (10 mL) was added. The mixture was extracted with DCM (3 × 10 mL). The combined organic layers were then washed with brine, dried over anhydrous Na_2SO_4, filtered and concentrated under vacuum. The resulting mixture was purified by silica gel chromatography (EtOAc/hexane = 1/20) to afford **6q** as a colorless liquid (678 mg, 90% yield).[2] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40–7.30 (m, 5H), 5.11 (s, 2H), 2.10 (s, 3H).

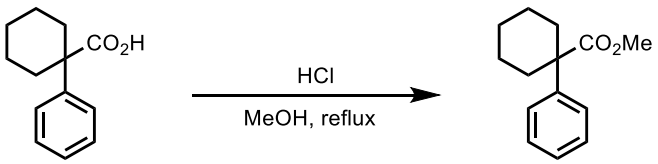


To a suspension of **S1** (6.0 mmol) and K_2CO_3 (1.27 g, 12.0 mmol.) in water (14.0 mL) and DCM (6.0 mL) was added **S2** (1.75 g, 8.0 mmol). The mixture was stirred at room temperature overnight. H_2O (10 mL) was added. The mixture was extracted with DCM (3 × 10 mL). The combined organic layers were then washed with brine**,** dried over anhydrous Na_2SO_4, filtered and concentrated under vacuum. The product was purified by flash column chromatography (EtOAc/hexane = 1/10).

6r: 1.22 g (86%). White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87–7.82 (m, 2H), 7.75–7.67 (m, 2H), 7.44 (d, J = 7.6 Hz 2H), 7.35–7.27 (m, 3H), 4.85 (s, 2H).

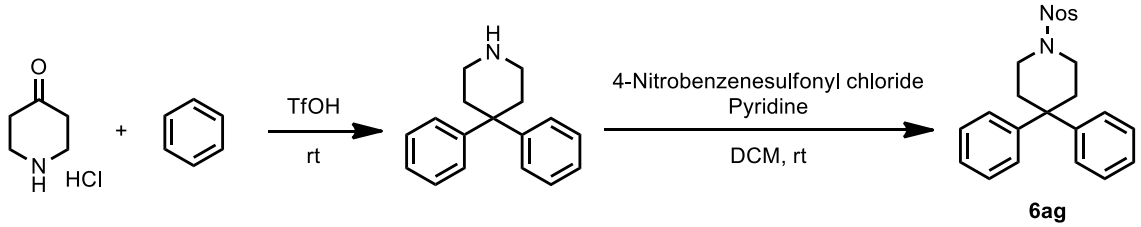
6s: 1.11 g (74%). White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85–7.81 (m, 2H), 7.73–7.67 (m, 2H), 7.32 – 7.19 (m, 5H), 3.96–3.90 (m, 2H), 3.02–2.97 (m, 2H).

6t: 1.49 g (94%). White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86–7.76 (m, 2H), 7.75–7.65 (m, 2H), 7.30–7.11 (m, 5H), 3.75 (t, J = 7.2 Hz, 2H), 2.69 (t, J = 7.5 Hz, 2H), 2.10–1.96 (m, 2H).



A solution of **S3** (5.0 mmol) in MeOH (10 mL) was added hydrochloric acid aqueous solution (7.5 mL, w/w, 38%). The mixture was stirred at reflux for 12 h. The reaction mixture was allowed to cool to room temperature and neutralized by saturated aqueous solution of sodium bicarbonate (10 mL). After removal of MeOH under vacuum, the mixture was extracted with DCM (3 × 10 mL). The combined organic layers were then washed with brine**,** dried over anhydrous Na_2SO_4, filtered and concentrated under vacuum. **6ab** was purified by flash column chromatography (EtOAc/hexane = 1/10) as a colorless liquid (1.01 g, 93% yield).

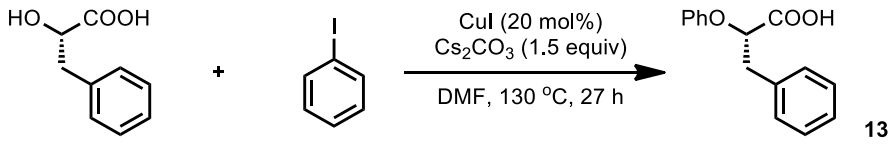
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41–7.37 (m, 2H), 7.32 (t, *J* = 7.6 Hz, 2H), 7.23 (t, *J* = 7.6 Hz, 1H), 3.64 (s, 3H), 2.52–2.45 (m, 2H), 1.76–1.59 (m, 5H), 1.53–1.41 (m, 2H), 1.32–1.24 (m, 1H).



6ag

The piperidone hydrochloride (2.78 g, 18.1 mmol) was dissolved in 20 mL of dry C_6H_6, and 10 mL of triflic acid was added. The solution was stirred at room temperature for 24 h. The reaction was quenched by addition of cold water (30 mL), the aqueous layer was extracted with DCM (3 × 20 mL). The combined organic portions were washed with brine, dried over anhydrous Na_2SO_4, filtered and concentrated in vacuo to afford the diphenyl piperidine as a white solid.[3]

To a solution of the diphenyl piperidine (1.19 g, 5.0 mmol) and 4-nitrobenzenesulfonyl chloride (1.33 g, 6.0 mmol) in DCM (20.0 mL) was added pyridine (0.49 mL, 6.0 mmol) in an ice-water bath. The mixture was then stirred at the room temperature for 24 hours. Then the reaction mixture was quenched by addition of cold saturated sodium bicarbonate aqueous solution, and the aqueous layer was extracted with DCM (3 × 10 mL). The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4, filtered and concentrated in vacuo. The crude product was purified by column chromatography on silica gel (DCM/hexane = 2/1) to afford **6ag** as a white solid (1.81 g, 86% yield based on diphenyl piperidine). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, *J* = 8.4 Hz, 2H), 7.88 (d, *J* = 8.4 Hz, 2H), 7.23 (d, *J* = 7.6 Hz, 4H), 7.16–7.11 (m, 6H), 3.25–3.19 (m, 4H), 2.57–2.49 (m, 4H).

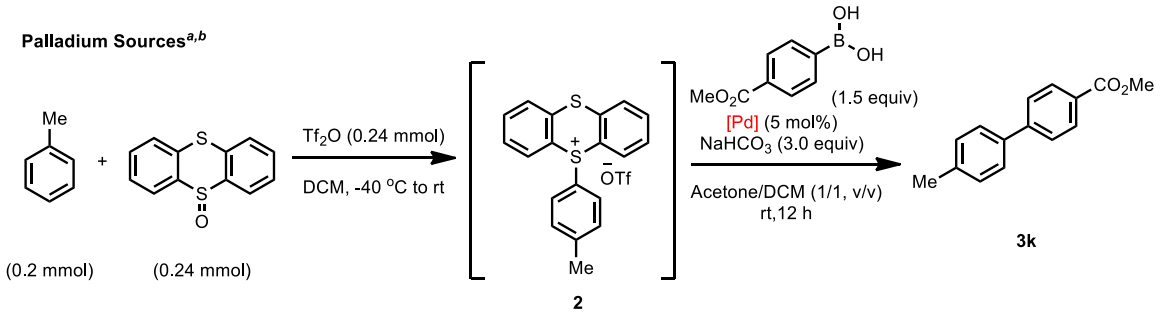


13

An oven dried Schlenk tube was charged with *L*-(-)-3-phenyllactic acid (332.0 mg, 2 mmol), CuI (76.2 mg, 20 mol%), Cs_2CO_3 (977.5 mg, 3.0 mmol) under nitrogen atmosphere, followed by the addition of dry DMF (10 mL) and PhI (0.44 mL, 4.0 mmol). The resulted reaction mixture was stirred at 130 °C in dark for 27 h. The reaction was monitored by TLC until the starting material was consumed. The reaction was then acidified by addition of HCl aqueous solution (1.0 M), and extracted with ethyl acetate (3 times). The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4, and concentrated under reduced pressure. Purification of the residue on a silica gel column chromatography using PE/EA/DCM(1/1/1) as eluent furnished the (*S*)-2-phenoxy-3-phenylpropanoic acid (368.0 mg, 76%) as a yellow solid. ^{1}H NMR (400 MHz, $(CD_3)_2CO$) δ 7.38 (d, *J* = 7.6 Hz, 2H), 7.32–7.19 (m, 5H), 6.95–6.86 (m, 3H), 4.94 (dd, *J* = 8.4, 4.8 Hz, 1H), 3.34–3.18 (m, 2H).

2.2 Experimental optimization

2.2.1 Screening of Palladium Sources

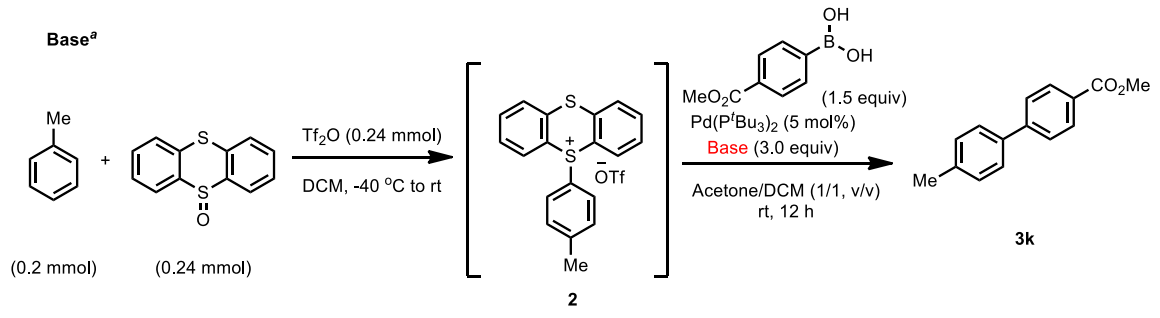


(0.2 mmol) (0.24 mmol) **2** **3k**

Entry	[Pd]	**2** (%)	**3** (%)	Entry	[Pd]	**2** (%)	**3** (%)
1	$Pd(P^tBu_3)_2$	0	**99**	10	$Pd(OAc)_2$/SPhos	91	2
2	$Pd(PPh_3)_4$	19	54	11	$Pd(OAc)_2$/BrettPhos	47	49
3	$PdCl_2(PPh_3)_2$	81	10	12	$Pd(OAc)_2/P(Cy)_3$	36	43
4	$PdCl_2$(dppf)	85	9	13	$Pd(OAc)_2/P(^tBu)_3$	77	14
5	$PdCl_2(MeCN)_2$	62	17	14	$Pd_2(dba)_3$	47	26
6	$Pd(OAc)_2$	42	57	15	$Pd_2(dba)_3/PPh_3$	43	40
7	$Pd(OAc)_2/PPh_3$	38	46	16	$Pd_2(dba)_3$/XPhos	71	10
8	$Pd(OAc)_2$/BINAP	91	4	17	$Pd_2(dba)_3$/BrettPhos	38	47
9	$Pd(OAc)_2$/XPhos	97	2				

[a]10 mol% ligand was used. [b]The yield was determined by ^{1}H NMR using CH_2Br_2 as the internal standard.

2.2.2 Base Effects

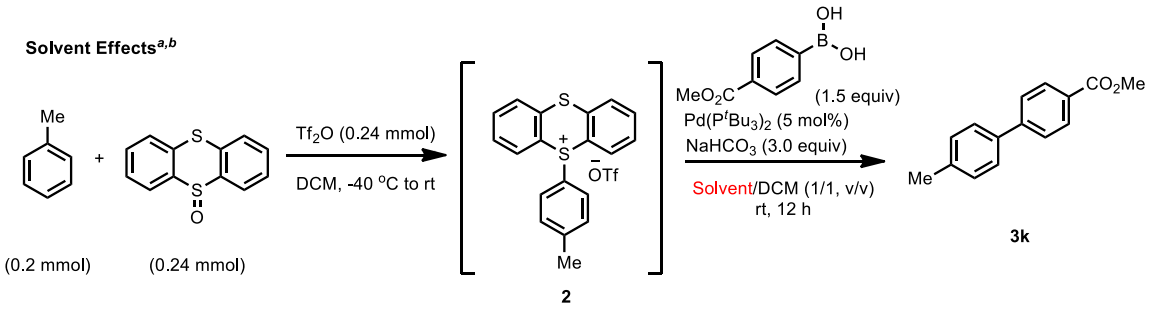


(0.2 mmol) (0.24 mmol) **2** **3k**

Entry	Base	**2** (%)	**3** (%)	Entry	Base	**2** (%)	**3** (%)
1	K_3PO_4	0	86	8	Li_2CO_3	24	65
2	K_2HPO_4	9	82	9	Na_2CO_3	39	52
3	KH_2PO_4	92	0	10	K_2CO_3	0	91
4	LiOAc	83	10	11	Cs_2CO_3	0	89
5	NaOAc	6	87	12	$NaHCO_3$	0	**99**
6	KOAc	58	34	13	$KHCO_3$	0	85
7	CsOAc	51	29				

[a]The yield was determined by ^{1}H NMR using CH_2Br_2 as the internal standard.

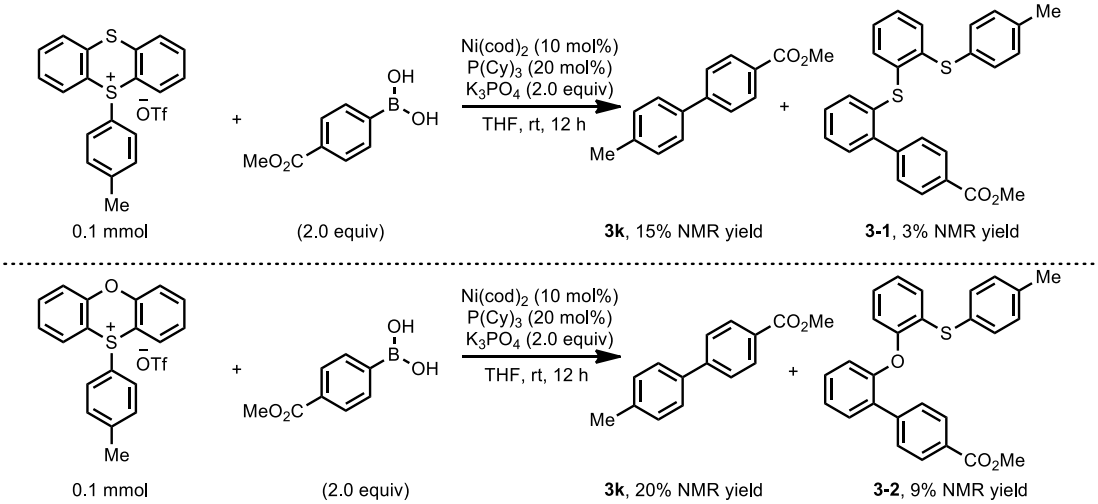
2.2.3 Solvent Effects



Entry	Solvent	**2** (%)	**3** (%)	Entry	Solvent	**2** (%)	**3** (%)
1	DCE	72	21	9	PhMe	88	0
2	DCM	55	43	10	THF	99	0
3	MeOH	0	**99**	11	CH_3CN	85	15
4[b]	MeOH	0	**99**	12	DMF	0	**99**
5	*t*-AmylOH	20	72	13[b]	DMF	14	85
6	HFIP	89	5	14	DMA	0	**99**
7	Acetone	0	**99**	15[b]	DMA	0	**98**
8[b]	Acetone	0	**99**				

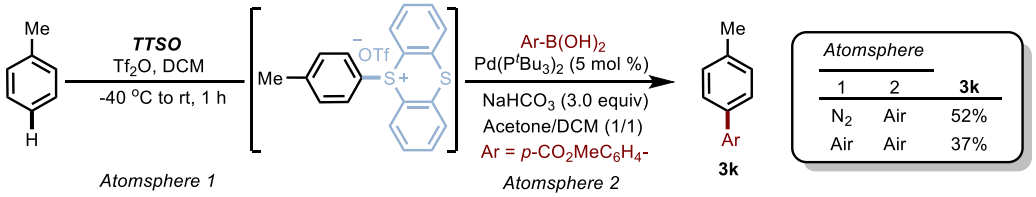
[a]The yield was determined by ^{1}H NMR using CH_2Br_2 as the internal standard. [b]2.5 mol% $Pd(P^tBu_3)_2$ was used.

2.2.4 Ni-Catalyzed thio-Suzuki Coupling



2.2.5 Control Experiments

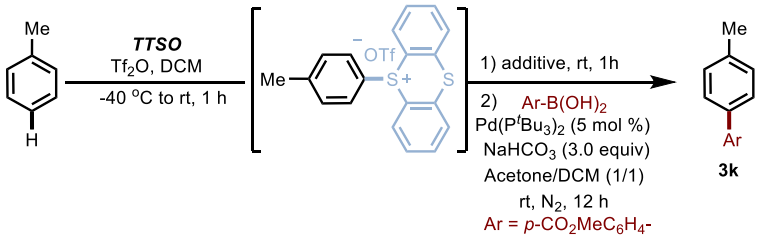
2.2.5.1 Atmosphere Effect



Atomsphere		
1	2	**3k**
N_2	Air	52%
Air	Air	37%

Those experimental results indicated that this reaction must be carried out with Schlenk technology.

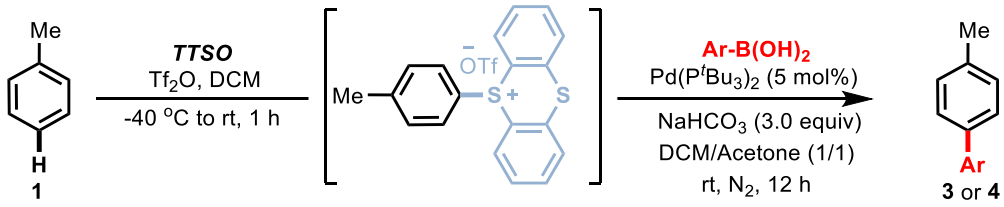
2.2.5.2 Counteranion Effect



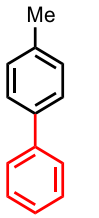
additive	3k
---	98%
KPF_6	79%
$NaBF_4$	78%

The results above indicated the counteranion might affect the reaction outputs.

2.3 General Procedure for *para*-Selective Arylation of Toluene



General Procedure for *para*-Arylation: A 25 mL Schlenk tube was charged with thianthrene *S*-oxide (55.7 mg, 0.24 mmol, 1.2 equiv), CH_2Cl_2 (1.0 mL) and toluene (21.2 μL, 0.2 mmol, 1.0 equiv) under nitrogen atmosphere. The reaction mixture was then cooled to -40 °C, followed by the dropwise of Tf_2O (44 μL, 0.24 mmol, 1.2 equiv). The reaction mixture was stirred at the same temperature for 30 min, and then allowed to stir at room temperature for another 1 hour. Then arylboronic acid (0.3 mmol, 1.5 equiv), $Pd(P^tBu_3)_2$ (5.1 mg, 5.0 mol%), $NaHCO_3$ (50.4 mg, 0.6 mmol, 3.0 equiv) were added under nitrogen atmosphere, subsequently the acetone (1.0 mL) was added to wash the Schlenk tube. The reaction mixture was stirred at room temperature for 12 hours. Upon completion, the reaction mixture was diluted with DCM, and passed through a pad of Celite with DCM as the eluent to remove the insoluble precipitate. The resulting solution was concentrated and purified by preparative thin-layer chromatography to afford the desired product **3** or **4**.

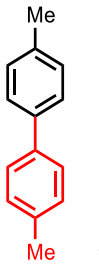


3a

4-Methyl-1,1'-biphenyl[4]

3a was synthesized following the general procedure. After purification by preparative thin-layer chromatography using hexane/EtOAc/DCM(50/1/1) as the eluent, **3a** was obtained in 91% yield.

30.5 mg, colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, J = 7.6 Hz, 2H), 7.49 (d, J = 8.0 Hz, 2H), 7.42 (t, J = 7.6 Hz, 2H), 7.32 (t, J = 7.2 Hz, 1H), 7.26–7.23 (m, 2H), 2.40 (s, 3H).

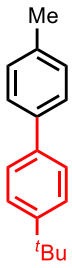


3b

4,4'-Dimethyl-1,1'-biphenyl[3]

3b was synthesized following the general procedure. After purification by preparative thin-layer chromatography using hexane as the eluent, **3b** was obtained in 85% yield.

31.0 mg, colorless crystal. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (d, J = 8.0 Hz, 4H), 7.23 (d, J = 8.4 Hz, 4H), 2.39 (s, 6H).

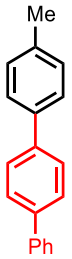


3c

4-(*tert*-Butyl)-4'-methyl-1,1'-biphenyl[5]

3c was synthesized following the general procedure. After purification by preparative thin-layer chromatography using hexane/EtOAc (50/1) as the eluent, **3c** was obtained in 98% yield.

43.9 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54–7.43 (m, 6H), 7.25–7.22 (m, 2H), 2.38 (s, 3H), 1.36 (s, 9H).

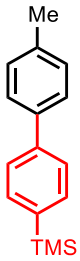


3d

4-Methyl-1,1':4',1''-terphenyl[6]

3d was synthesized following the general procedure. After purification by preparative thin-layer chromatography using hexane/DCM (9/1) as the eluent, **3d** was obtained in 97% yield.

47.7 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66–7.61 (m, 6H), 7.54 (d, J = 8.0 Hz, 2H), 7.45 (t, J = 7.4 Hz, 2H), 7.35 (t, J= 7.4 Hz, 1H), 7.27–7.23 (m, 2H), 2.40 (s, 3H).

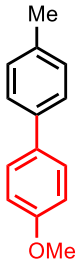


3e

Trimethyl(4'-methyl-[1,1'-biphenyl]-4-yl)silane[7]

3e was synthesized following the general procedure. After purification by preparative thin-layer chromatography using hexane as the eluent, **3e** was obtained in 96% yield.

46.0 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60–7.55 (m, 4H), 7.50 (d, J = 8.0 Hz, 2H), 7.24 (d, J = 7.6 Hz, 2H), 2.39 (s, 3H), 0.30 (s, 9H).

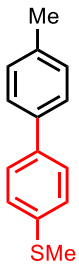


3f

4-Methoxy-4'-methyl-1,1'-biphenyl[5]

3f was synthesized following the general procedure. After purification by preparative thin-layer chromatography using hexane/EtOAc/DCM (50/1/1) as the eluent, **3f** was obtained in 83% yield.

33.0 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, J = 8.8 Hz, 2H), 7.45 (d, J = 8.0 Hz, 2H), 7.24–7.20 (m, 2H), 6.96 (d, J = 8.8 Hz, 2H), 3.84 (s, 3H), 2.38 (s, 3H).

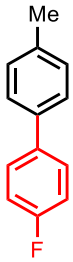


3g

Methyl(4'-methyl-[1,1'-biphenyl]-4-yl)sulfane[8]

3g was synthesized following the general procedure. After purification by preparative thin-layer chromatography using hexane/EtOAc/DCM (50/1/1) as the eluent, **3g** was obtained in 93% yield.

40.0 mg, light yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ7.56–7.48 (m, 4H), 7.37–7.33 (m, 2H), 7.29–7.25 (m, 2H), 2.52 (s, 3H), 2.39 (s, 3H).

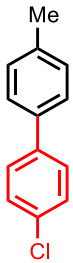


3h

4-Fluoro-4'-methyl-1,1'-biphenyl[5]

3h was synthesized following the general procedure. After purification by preparative thin-layer chromatography using hexane as the eluent, **3h** was obtained in 91% yield.

42.0 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55–7.50 (m, 2H), 7.44 (d, J = 8.4 Hz, 2H), 7.24 (d, J = 8.0 Hz, 2H), 7.14–7.08 (m, 2H), 2.39 (s, 3H).

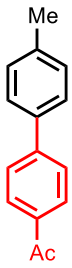


3i

4-Fluoro-4'-methyl-1,1'-biphenyl[3]

3i was synthesized following the general procedure. After purification by preparative thin-layer chromatography using hexane/EtOAc/DCM (100/1/1) as the eluent, **3i** was obtained in 93% yield.

37.5 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, J = 8.4 Hz, 2H), 7.45 (d, J = 8.0 Hz, 2H), 7.39 (d, J = 8.4 Hz, 2H), 7.26–7.24 (m, 2H), 2.40 (s, 3H).

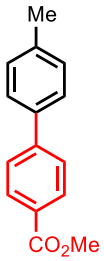


3j

1-(4'-Methyl-[1,1'-biphenyl]-4-yl)ethanone[9]

3j was synthesized following the general procedure. After purification by preparative thin-layer chromatography using hexane/EtOAc (50/1) as the eluent, **3j** was obtained in 91% yield.

38.4 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, J = 8.8 Hz, 2H), 7.66 (d, J = 8.4 Hz, 2H), 7.53 (d, J = 8.4 Hz, 2H), 7.30–7.26 (m, 2H)., 2.62 (s, 3H), 2.41 (s, 3H).

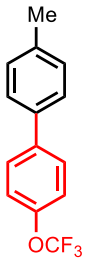


3k

Methyl 4'-methyl-[1,1'-biphenyl]-4-carboxylate[10]

3k was synthesized following the general procedure. After purification by preparative thin-layer chromatography using hexane/EtOAc (20/1) as the eluent, **3k** was obtained in 99% yield.

45.0 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, J = 8.4 Hz, 2H), 7.65 (d, J = 7.2 Hz, 2H), 7.53 (d, J = 7.6 Hz, 2H), 7.30–7.26 (m, 2H), 3.94 (s, 3H), 2.41 (s, 3H).

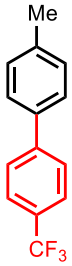


3l

4-Methyl-4'-(trifluoromethoxy)-1,1'-biphenyl[11]

3l was synthesized following the general procedure. After purification by preparative thin-layer chromatography using hexane as the eluent, **3l** was obtained in 97% yield.

49.0 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59–7.55 (m, 2H), 7.47–7.43 (m, 2H), 7.28–7.23 (m, 4H), 2.40 (s, 3H).

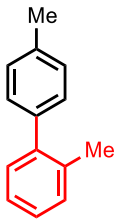


3m

4-Methyl-4'-(trifluoromethyl)-1,1'-biphenyl[8]

3m was synthesized following the general procedure. After purification by preparative thin-layer chromatography using hexane/EtOAc (20/1) as the eluent, **3m** was obtained in 90% yield.

42.5 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (s, 4H), 7.50 (d, J = 8.4 Hz, 2H), 7.28 (d, J = 7.6 Hz, 2H), 2.42 (s, 3H).

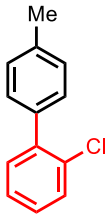


3n

2,4'-Dimethyl-1,1'-biphenyl[3]

3n was synthesized following the general procedure using Pd(P^{t}Bu$_3$)$_2$ (10 mol%). After purification by preparative thin-layer chromatography using hexane/EtOAc/DCM (100/1/1) as the eluent, **3n** was obtained in 96% yield.

35.2 mg, colorless crystal. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26–7.21 (m, 8H), 2.40 (s, 3H), 2.28 (s, 3H).

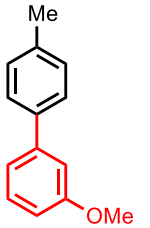


3o

2-Chloro-4'-methyl-1,1'-biphenyl[12]

3o was synthesized following the general procedure. After purification by preparative thin-layer chromatography using hexane as the eluent, **30** was obtained in 82% yield.

33.0 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, J = 8.0 Hz, 1H), 7.35–7.20 (m, 7H), 2.40 (s, 3H).

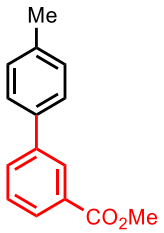


3p

3-Methoxy-4'-methyl-1,1'-biphenyl[3]

3p was synthesized following the general procedure. After purification by preparative thin-layer chromatography using hexane/EtOAc/DCM (50/1/1) as the eluent, **3p** was obtained in 89% yield.

35.2 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, J = 8.4 Hz, 2H), 7.34 (t, J = 8.0 Hz, 1H), 7.26–7.23 (m, 2H), 7.18–7.14 (m, 1H), 7.12–7.09 (m, 1H), 6.89–6.84 (m, 1H), 3.86 (s, 3H), 2.39 (s, 3H).

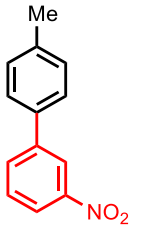


3q

Methyl 4'-methyl-[1,1'-biphenyl]-3-carboxylate[13]

3q was synthesized following the general procedure. After purification by preparative thin-layer chromatography using hexane/EtOAc (20/1) as the eluent, **3q** was obtained in 97% yield.

44.0 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (s, 1H), 7.99 (d, J = 7.6 Hz, 1H), 7.77 (d, J = 7.6 Hz, 1H), 7.55–7.46 (m, 3H), 7.29–7.26 (m, 2H), 3.94 (s, 3H), 2.41 (s, 3H).

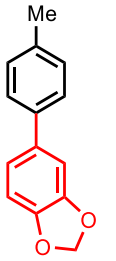


3r

4'-Methyl-3-nitro-1,1'-biphenyl[14]

3r was synthesized following the general procedure. After purification by preparative thin-layer chromatography using hexane/EtOAc (50/1) as the eluent, **3r** was obtained in 83% yield.

35.6 mg, light yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (t, J = 1.8 Hz, 1H), 8.18–8.14 (m, 1H), 7.91–7.87 (m, 1H), 7.58 (t, J = 8.0 Hz, 1H), 7.52 (d, J = 8.0 Hz, 2H), 7.30 (d, J = 8.0 Hz, 2H), 2.42 (s, 3H).

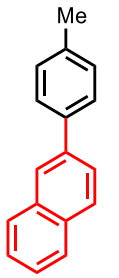


3s

5-(*p*-Tolyl)benzo[d][1,3]dioxole[15]

3s was synthesized following the general procedure. After purification by preparative thin-layer chromatography using hexane as the eluent, **3s** was obtained in 74% yield.

32.0 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (d, J = 8.0 Hz, 2H), 7.21 (d, J = 7.6 Hz, 2H), 7.06–7.01 (m, 2H), 6.86 (d, J = 8.4 Hz, 1H), 5.98 (s, 2H), 2.38 (s, 3H).

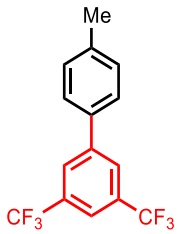


3t

2-(*p*-Tolyl)naphthalene[5]

3t was synthesized following the general procedure. After purification by preparative thin-layer chromatography using hexane as the eluent, **3t** was obtained in 87% yield.

38.0 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (s, 1H), 7.92–7.83 (m, 3H), 7.76–7.72 (m, 1H), 7.63 (d, J = 8.0 Hz, 2H), 7.52–7.44 (m, 2H), 7.30 (d, J = 8.0 Hz, 2H), 2.42 (s, 3H).

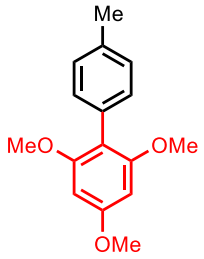


3u

4'-Methyl-3,5-bis(trifluoromethyl)-1,1'-biphenyl[16]

3u was synthesized following the general procedure. After purification by preparative thin-layer chromatography using hexane/EtOAc/DCM (100/1/1) as the eluent, **3u** was obtained in 91% yield.

55.0 mg, colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (s, 2H), 7.82 (s, 1H), 7.51 (d, J = 8.0 Hz, 2H), 7.31 (d, J = 8.0 Hz, 2H), 2.42 (s, 3H).

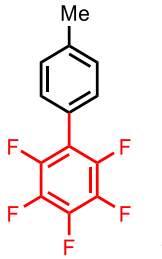


3v

2,4,6-Trimethoxy-4'-methyl-1,1'-biphenyl[17]

3v was synthesized following the general procedure. After purification by preparative thin-layer chromatography using hexane/EtOAc/DCM (25/1/1) as the eluent, **3v** was obtained in 97% yield.

50.0 mg, light yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, J = 8.0 Hz, 2H), 7.24 (d, J = 8.0 Hz, 2H), 6.76 (s, 2H), 3.92 (s, 6H), 3.89 (s, 3H), 2.40 (s, 3H).

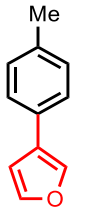


3w

2,3,4,5,6-Pentafluoro-4'-methyl-1,1'-biphenyl[18]

3w was synthesized following the general procedure. After purification by preparative thin-layer chromatography using hexane as the eluent, **3w** was obtained in 85% yield.

44.0 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33–7.28 (m, 4H), 2.42 (s, 3H).

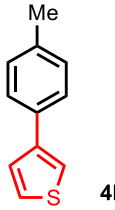


4a

3-(*p*-Tolyl)furan[19]

4a was synthesized following the general procedure. After purification by preparative thin-layer chromatography using hexane as the eluent, **4a** was obtained in 85% yield.

26.9 mg, yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (s, 1H), 7.46 (t, J = 1.6 Hz, 1H), 7.38 (d, J = 8.0 Hz, 2H), 7.18 (d, J = 7.6 Hz, 2H), 6.70–6.68 (m, 1H), 2.36 (s, 3H).

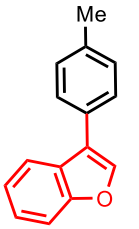


4b

3-(*p*-Tolyl)thiophene[20]

4b was synthesized following the general procedure. After purification by preparative thin-layer chromatography using hexane/EtOAc (50/1) as the eluent, **4b** was obtained in 99% yield.

34.5 mg, light yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, J = 8.0 Hz, 2H), 7.41 (t, J = 2.2 Hz, 1H), 7.37 (d, J = 2.0 Hz, 2H), 7.21 (d, J = 8.0 Hz, 2H), 2.37 (s, 3H).

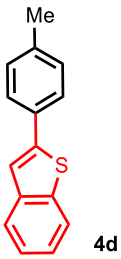


4c

3-(*p*-Tolyl)benzofuran[21]

4c was synthesized following the general procedure. After purification by preparative thin-layer chromatography using hexane as the eluent, **4c** was obtained in 84% yield.

34.5 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, J = 8.0 Hz, 1H), 7.77 (s, 1H), 7.54 (d, J = 8.0 Hz, 3H), 7.36–7.28 (m, 4H), 2.42 (s, 3H).

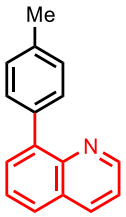


4d

2-(*p*-Tolyl)benzo[b]thiophene[15]

4d was synthesized following the general procedure. After purification by preparative thin-layer chromatography using hexane as the eluent, **4d** was obtained in 94% yield.

42.0 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, J = 8.0 Hz, 1H), 7.75 (d, J = 8.0 Hz, 1H), 7.61 (d, J = 8.0 Hz, 2H), 7.50 (s, 1H), 7.36–7.27 (m, 2H), 7.23 (d, J = 8.0 Hz, 2H), 2.39 (s, 3H).

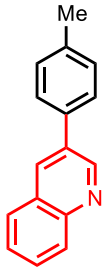


4e

8-(*p*-Tolyl)quinoline[22]

4e was synthesized following the general procedure using Pd(^{t}Bu$_3$P)$_2$ (10 mol%) at 50 °C. After purification by preparative thin-layer chromatography using hexane/DCM (1/1) as the eluent, **4e** was obtained in 89% yield.

36.0 mg, colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.95 (dd, J = 4.0, 1.6 Hz, 1H), 8.19 (dd, J = 8.4, 1.6 Hz, 1H), 7.80 (dd, J = 8.4, 1.6 Hz, 1H), 7.72 (dd, J = 7.2, 1.6 Hz, 1H), 7.61–7.56 (m, 3H), 7.40 (dd, J = 8.4, 4.0 Hz, 1H), 7.31 (d, J = 7.6 Hz, 2H), 2.43 (s, 3H).

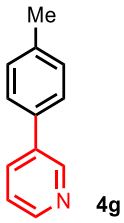


4f

3-(*p*-Tolyl)quinoline[23]

4f was synthesized following the general procedure using Pd(^{t}Bu$_3$P)$_2$ (10 mol%) at 50 °C. After purification by preparative thin-layer chromatography using hexane/DCM (1/1) as the eluent, **4f** was obtained in 73% yield.

32.0 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.18 (d, J = 2.4 Hz, 1H), 8.29 (d, J = 2.0 Hz, 1H), 8.13 (d, J = 8.4 Hz, 1H), 7.88 (d, J = 8.0 Hz, 1H), 7.73–7.68 (m, 1H), 7.63 (d, J = 8.4 Hz, 2H), 7.58 (t, J = 7.4 Hz, 1H), 7.34 (d, J = 8.0 Hz, 2H), 2.44 (s, 3H).



4g

3-(*p*-Tolyl)pyridine[19]

4g was synthesized following the general procedure using Pd(^{t}Bu$_3$P)$_2$ (10 mol%) at 50 °C. After purification by preparative thin-layer chromatography using hexane/DCM (1/5) as the eluent, **4g** was obtained in 75% yield.

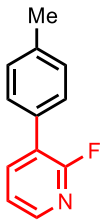
25.0 mg, colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.84 (s, 1H), 8.57 (d, J = 4.8 Hz, 1H), 7.87–7.84 (m, 1H), 7.49 (d, J = 8.0 Hz, 2H), 7.35 (dd, J = 7.6, 4.8 Hz, 1H), 7.29 (d, J = 8.0 Hz, 2H), 2.41 (s, 3H).

4h

2-Chloro-3-(*p*-tolyl)pyridine

4h was synthesized following the general procedure using Pd(^{t}Bu$_3$P)$_2$ (10 mol%) at 50 °C. After purification by preparative thin-layer chromatography using hexane/DCM (1/1) as the eluent, **4h** was obtained in 92% yield.

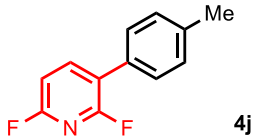
37.4 mg, light yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (dd, J = 4.8, 2.0 Hz, 1H), 7.66 (dd, J = 7.6, 2.0 Hz, 1H), 7.35 (d, J = 8.0 Hz, 2H), 7.31–7.28 (m, 3H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.77, 148.13, 139.61, 138.24, 136.97, 134.56, 129.13, 129.04, 122.49, 21.25; HRMS (ESI-TOF) *m/z* Calcd for $C_{12}H_{11}ClN$ $[M+H]^+$: 204.0575, found: 204.0575.



4i

2-Fluoro-3-(*p*-tolyl)pyridine

4i was synthesized following the general procedure using Pd(^{t}Bu$_3$P)$_2$ (10 mol%) at 50 °C. After purification by preparative thin-layer chromatography using hexane/DCM (1/1) as the eluent, **4i** was obtained in 93% yield.
35.0 mg, light yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18–8.16 (m, 1H), 7.88–7.83 (m, 1H), 7.47 (dd, *J* = 8.0, 1.4 Hz, 2H), 7.29–7.24 (m, 3H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.44 (d, *J* = 239.0 Hz), 145.94 (d, *J* = 14.0 Hz), 140.45 (d, *J* = 5.0 Hz), 138.42, 130.93 (d, *J* = 5.0 Hz), 129.42, 128.63 (d, *J* = 3.0 Hz), 123.88 (d, *J* = 28.0 Hz), 121.75 (d, *J* = 4.0 Hz), 21.20; ^{19}F NMR (375 MHz, $CDCl_3$) δ -72.51; HRMS (ESI-TOF) m/z Calcd for $C_{12}H_{11}FN$ $[M+H]^+$ 188.0870, found: 188.0869.

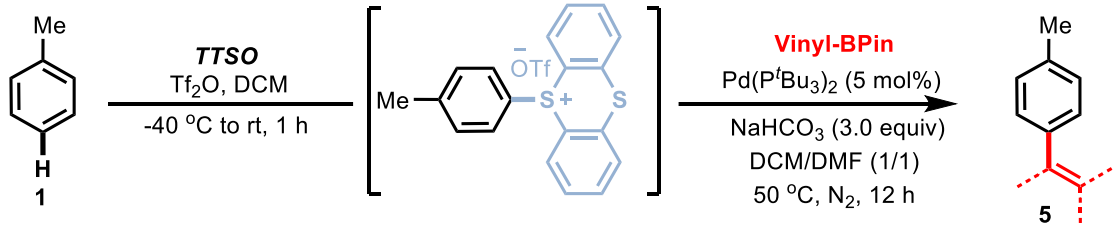


4j

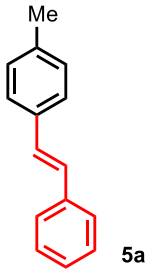
2,6-Difluoro-3-(*p*-tolyl)pyridine

4j was synthesized following the general procedure using Pd(^{t}Bu$_3$P)$_2$ (10 mol%) at 50 °C. After purification by preparative thin-layer chromatography using hexane/DCM (9/1) as the eluent, **4j** was obtained in 95% yield.
39.0 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (dd, *J* = 17.2, 8.0 Hz, 1H), 7.42 (d, *J* = 7.6 Hz, 2H), 7.28 (d, *J* = 8.0 Hz, 2H), 6.90 (dd, *J* = 8.0, 2.8 Hz, 1H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.33 (dd, *J* = 231.3, 13.1 Hz), 157.74 (dd, *J* = 234.5, 13.7 Hz), 144.73 (dd, *J* = 7.0, 5.0 Hz), 138.50, 129.92 (d, *J* = 4.8 Hz), 129.51, 128.49 (d, *J* = 2.9 Hz), 120.61 (dd, *J* = 25.6, 5.9 Hz), 106.39 (ddd, *J* = 34.5, 5.7, 1.5 Hz), 21.20 (d, *J* = 2.2 Hz); ^{19}F NMR (375 MHz, $CDCl_3$) δ -71.19, -71.71; HRMS (EI) m/z Calcd for $C_{12}H_9F_2N$ (M^+) 205.0698, found: 205.0696.

2.4 General Procedure for *para*-Selective Alkenylation of Toluene



General Procedure for *para*-Alkenylation: A 25 mL Schlenk tube was charged with thianthrene *S*-oxide (55.7 mg, 0.24 mmol, 1.2 equiv), CH_2Cl_2 (1.0 mL) and toluene (21.2 μL, 0.2 mmol, 1.0 equiv) under nitrogen atmosphere. The reaction mixture was then cooled to -40 °C, followed by the dropwise of Tf_2O (44 μL, 0.24 mmol, 1.2 equiv). The reaction mixture was stirred at the same temperature for 30 min, and then allowed to stir at room temperature for another 1 hour. Then alkenylboronic acid pinacol ester (0.3 mmol, 1.5 equiv), $Pd(P^tBu_3)_2$ (5.1 mg, 5.0 mol%), $NaHCO_3$ (50.4 mg, 0.6 mmol, 3.0 equiv) were added under nitrogen atmosphere, subsequently the DMF (1.0 mL) was added to wash the Schlenk tube. The reaction mixture was stirred at 50 °C for 12 hours. Upon completion, the reaction mixture was allowed to cool to room temperature, and diluted with DCM. Then water was added, and the organic phase was separated. The aqueous phase was extracted with DCM (3 times). The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4. The resulting solution was concentrated and purified by preparative thin-layer chromatography to afford the desired product **5**.

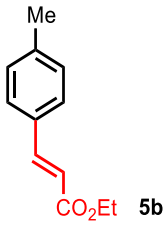


5a

(*E*)-1-Methyl-4-styrylbenzene[24]

5a was synthesized following the general procedure. After purification by preparative thin-layer chromatography using hexane as the eluent, **5a** was obtained in 72% yield.

28.0 mg, colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36–7.29 (m, 5H), 7.24 (d, *J* = 8.0 Hz, 2H), 7.14 (d, *J* = 8.0 Hz, 2H), 5.43 (d, *J* = 1.2 Hz, 1H), 5.40 (d, *J* = 1.2 Hz, 1H), 2.37 (s, 3H).

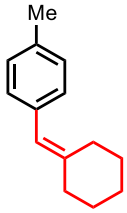


5b

Ethyl (*E*)-3-(*p*-tolyl)acrylate[25]

5b was synthesized following the general procedure. After purification by preparative thin-layer chromatography using hexane as the eluent, **5b** was obtained in 79% yield.

30.0 mg, colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 16.0 Hz, 1H), 7.42 (d, *J* = 8.0 Hz, 2H), 7.19 (d, *J* = 8.0 Hz, 2H), 6.39 (d, *J* = 16.0 Hz, 1H), 4.26 (q, *J* = 6.8 Hz, 2H), 2.37 (s, 3H) , 1.33 (t, *J* = 7.2 Hz, 3H).

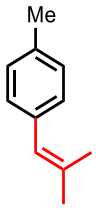


5c

1-(Cyclohexylidenemethyl)-4-methylbenzene[26]

5c was synthesized following the general procedure. After purification by preparative thin-layer chromatography using hexane as the eluent, **5c** was obtained in 83% yield.

22.0 mg, colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.14–7.04 (m, 4H), 6.19 (s, 1H), 2.40–2.35 (m, 2H), 2.33 (s, 3H), 2.27–2.22 (m, 2H), 1.66–1.58 (m, 4H), 1.55–1.50 (m, 2H).

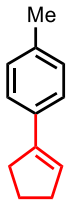


5d

1-Methyl-4-(2-methylprop-1-en-1-yl)benzene[27]

5d was synthesized following the general procedure. After purification by preparative thin-layer chromatography using hexane as the eluent, **5d** was obtained in 76% yield.

22.0 mg, colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.12 (s, 4H), 6.23 (s, 1H), 2.33 (s, 3H), 1.89 (s, 3H), 1.85 (s, 3H).

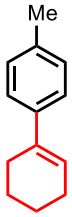


5e

1-(Cyclopent-1-en-1-yl)-4-methylbenzene[26]

5e was synthesized following the general procedure. After purification by preparative thin-layer chromatography using hexane as the eluent, **5e** was obtained in 57% yield.

18.0 mg, colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (d, J = 8.4 Hz, 2H), 7.11 (d, J = 8.0 Hz, 2H), 6.13–6.11 (m, 1H), 2.71–2.67 (m, 2H), 2.54–2.49 (m, 2H), 2.33 (s, 3H), 2.04–1.97 (m, 2H).

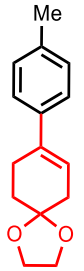


5f

4'-Methyl-2,3,4,5-tetrahydro-1,1'-biphenyl[28]

5f was synthesized following the general procedure. After purification by preparative thin-layer chromatography using hexane as the eluent, **5f** was obtained in 90% yield.

31.0 mg, colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27 (d, J = 8.0 Hz, 2H), 7.11 (d, J = 8.0 Hz, 2H), 6.10–6.05 (m, 1H), 2.42–2.36 (m, 2H), 2.32 (s, 3H), 2.22–2.16 (m, 2H), 1.81–1.73 (m, 2H), 1.68–1.62 (m, 2H).

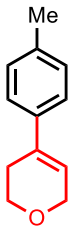


5g

8-(*p*-Tolyl)-1,4-dioxaspiro[4.5]dec-7-ene[29]

5g was synthesized following the general procedure. After purification by preparative thin-layer chromatography using hexane/EtOAc (5/1) as the eluent, **5g** was obtained in 63% yield.

29.0 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 (d, J = 8.0 Hz, 2H), 7.11 (d, J = 8.0 Hz, 2H), 5.96–5.93 (m, 1H), 4.02 (s, 4H), 2.67–2.63 (m, 2H), 2.48–2.44 (m, 2H), 2.33 (s, 3H), 1.92 (t, J = 6.4 Hz, 2H).

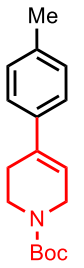


5h

4-(*p*-Tolyl)-3,6-dihydro-2*H*-pyran[30]

5h was synthesized following the general procedure. After purification by preparative thin-layer chromatography using hexane as the eluent, **5h** was obtained in 57% yield.

20.0 mg, colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 (d, J = 8.0 Hz, 2H), 7.15 (d, J = 8.0 Hz, 2H), 6.10–6.07 (m, 1H), 4.32 (q, J = 2.8 Hz, 2H), 3.93 (t, J = 5.2 Hz, 2H), 2.53–2.49 (m, 2H), 2.35 (s, 3H).

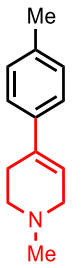


5i

***tert*-Butyl 4-(*p*-tolyl)-3,6-dihydropyridine-1(2*H*)-carboxylate**[31]

5i was synthesized following the general procedure. After purification by preparative thin-layer chromatography using hexane/EtOAc (10/1) as the eluent, **5i** was obtained in 50% yield.

27.0 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27 (d, J = 8.4 Hz, 2H), 7.14 (d, J = 8.0 Hz, 2H), 5.99 (s, 1H), 4.06 (s, 2H), 3.63 (t, J = 5.6 Hz, 2H), 2.51 (s, 2H), 2.34 (s, 3H), 1.49 (s, 9H).



5j

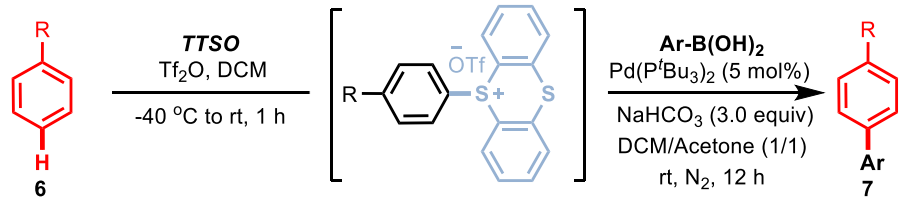
1-Methyl-4-(*p*-tolyl)-1,2,3,6-tetrahydropyridine

5j was synthesized following the general procedure. After purification by preparative thin-layer chromatography

using DCM/MeOH (20/1) as the eluent, **5j** was obtained in 53% yield.

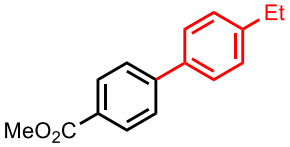
20.0 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (d, J = 8.0 Hz, 2H), 7.13 (d, J = 8.0 Hz, 2H), 6.02–6.00 (m, 1H), 3.13 (d, J = 3.2 Hz, 2H), 2.69 (t, J = 5.6 Hz, 2H), 2.62–2.58 (m, 2H), 2.43 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.01, 136.72, 134.57, 128.97, 124.82, 120.67, 54.91, 52.28, 45.62, 28.03, 21.04; HRMS (EI) m/z Calcd for $C_{13}H_{17}N$ (M^+) 187.1355, found: 187.1356.

2.5 General Procedure for *para*-Selective Arylation of Monosubstituted Arenes



General Procedure A for *para*-Arylation of Monosubstituted Arenes: A 25 mL Schlenk tube was charged with thianthrene *S*-oxide (55.7 mg, 0.24 mmol, 1.2 equiv), CH_2Cl_2 (1.0 mL) and **6** (0.2 mmol, 1.0 equiv) under nitrogen atmosphere. The reaction mixture was then cooled to -40 °C, followed by the dropwise of Tf_2O (44 μL, 0.24 mmol, 1.2 equiv). The reaction mixture was stirred at the same temperature for 30 min, and then allowed to stir at room temperature for another 1 hour. Then 4-(methoxycarbonyl)benzeneboronic acid (54 mg, 0.3 mmol, 1.5 equiv), $Pd(P^tBu_3)_2$ (5.1 mg, 5.0 mol%), $NaHCO_3$ (50.4 mg, 0.6 mmol, 3.0 equiv) were added under nitrogen atmosphere, subsequently the acetone (1.0 mL) was added to wash the Schlenk tube. The reaction mixture was stirred at room temperature for 12 hours. Upon completion, the reaction mixture was diluted with DCM, and passed through a pad of Celite with DCM as the eluent to remove the insoluble precipitate. The resulting solution was concentrated and purified by preparative thin-layer chromatography to afford the desired product **7**.

General Procedure B for *para*-Arylation of Monosubstituted Arenes: A 25 mL Schlenk tube was charged with thianthrene *S*-oxide (55.7 mg, 0.24 mmol, 1.2 equiv), CH_2Cl_2 (0.2 mL) and **6** (0.2 mmol, 1.0 equiv) under nitrogen atmosphere. The reaction mixture was then cooled to -40 °C, followed by the dropwise of Tf_2O (44 μL, 0.24 mmol, 1.2 equiv). The reaction mixture was stirred at the same temperature for 30 min, and then allowed to stir at room temperature for another 1 hour. Then 4-(methoxycarbonyl)benzeneboronic acid (54 mg, 0.3 mmol, 1.5 equiv), $Pd(P^tBu_3)_2$ (5.1 mg, 5.0 mol%), $NaHCO_3$ (50.4 mg, 0.6 mmol, 3.0 equiv) were added under nitrogen atmosphere, subsequently the DMF (1.0 mL) was added to wash the Schlenk tube. The reaction mixture was stirred at 50 °C for 12 hours. Upon completion, the reaction mixture was diluted with DCM, and passed through a pad of Celite with DCM as the eluent to remove the insoluble precipitate. The resulting solution was concentrated and purified by preparative thin-layer chromatography to afford the desired product **7**.

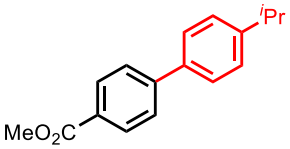


7a

Methyl 4'-ethyl-[1,1'-biphenyl]-4-carboxylate

7a was synthesized following the general procedure **A**. After purification by preparative thin-layer chromatography using hexane/EtOAc (10/1) as the eluent, **7a** was obtained in 92% yield.

44.0 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, *J* = 8.4 Hz, 2H), 7.65 (d, *J* = 8.0 Hz, 2H), 7.56 (d, *J* = 8.0 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 3.94 (s, 3H), 2.71 (q, *J* = 7.6 Hz, 2H), 1.28 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.05, 145.58, 144.44, 137.31, 130.05, 128.56, 128.45, 127.18, 126.80, 52.07, 28.54, 15.52; HRMS (EI) m/z Calcd for $C_{16}H_{16}O_2$ (M^+) 240.1145, found: 240.1142.



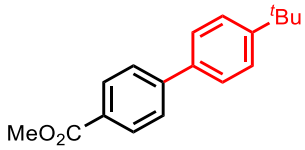
7b

Methyl 4'-isopropyl-[1,1'-biphenyl]-4-carboxylate

7b was synthesized following the general procedure **A**. After purification by preparative thin-layer chromatography

using hexane/EtOAc (20/1) as the eluent, **7b** was obtained in 93% yield.

47.3 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, *J*= 8.4 Hz, 2H), 7.65 (d, *J* = 8.8 Hz, 2H), 7.56 (d, *J* = 8.0 Hz, 2H), 7.33 (d, *J* = 8.4 Hz, 2H), 3.93 (s, 3H), 3.00–2.93 (m, 1H), 1.29 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.04, 149.04, 145.55, 137.43, 130.04, 128.54, 127.17, 127.00, 126.80, 52.07, 33.83, 23.93; HRMS (EI) m/z Calcd for $C_{17}H_{18}O_2$ (M^+) 254.1301, found: 254.1298.

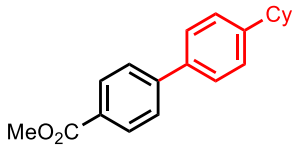


7c

Methyl 4'-(*tert*-butyl)-[1,1'-biphenyl]-4-carboxylate

7c was synthesized following the general procedure **A**. After purification by preparative thin-layer chromatography using hexane/EtOAc (20/1) as the eluent, **7c** was obtained in 99% yield.

53.0 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, *J* = 8.4 Hz, 2H), 7.65 (d, *J* = 8.4 Hz, 2H), 7.57 (d, *J* = 8.4 Hz, 2H), 7.49 (d, *J* = 8.4 Hz, 2H), 3.93 (s, 3H), 1.36 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.03, 151.31, 145.44, 137.01, 130.05, 128.58, 126.89, 126.80, 125.87, 52.06, 34.60, 31.29; HRMS (EI) m/z Calcd for $C_{18}H_{20}O_2$ (M^+) 268.1458, found: 268.1460.

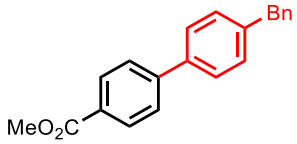


7d

Methyl 4'-cyclohexyl-[1,1'-biphenyl]-4-carboxylate

7d was synthesized following the general procedure **A**. After purification by preparative thin-layer chromatography using hexane/EtOAc (20/1) as the eluent, **7d** was obtained in 98% yield.

57.6 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, *J* = 8.4 Hz, 2H), 7.64 (d, *J* = 8.4 Hz, 2H), 7.55 (d, *J* = 8.4 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 3.93 (s, 3H), 2.58–2.52 (m, 1H), 1.93–1.83 (m, 4H), 1.77 (d, *J* = 12.8 Hz, 1H), 1.51–1.36 (m, 4H), 1.32–1.25 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.05, 148.28, 145.58, 137.43, 130.04, 128.55, 127.41, 127.15, 126.80, 52.07, 44.28, 34.40, 26.85, 26.12; HRMS (ESI-TOF) m/z Calcd for $C_{20}H_{22}NaO_2$ $[M+Na]^+$ 317.1512, found: 317.1517.

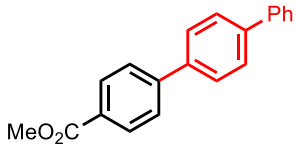


7e

Methyl 4'-benzyl-[1,1'-biphenyl]-4-carboxylate[32]

7e was synthesized following the general procedure **A**. After purification by preparative thin-layer chromatography using hexane/EtOAc (20/1) as the eluent, **7e** was obtained in 84% yield.

51.0 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, *J* = 8.4 Hz, 2H), 7.64 (d, *J* = 8.4 Hz, 2H), 7.55 (d, *J* = 8.0 Hz, 2H), 7.33–7.27 (m, 4H), 7.23–7.18 (m, 3H), 4.03 (s, 2H), 3.93 (s, 3H).

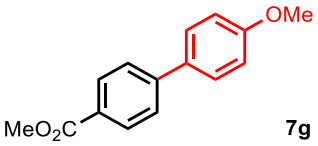


7f

Methyl [1,1':4',1''-terphenyl]-4-carboxylate[33]

7f was synthesized following the general procedure **A** using $Pd(P^tBu_3)_2$ (10 mol%) at 50 °C. After purification by preparative thin-layer chromatography using hexane/EtOAc (20/1) as the eluent, **7f** was obtained in 80% yield.

46.0 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, J = 8.0 Hz, 2H), 7.74–7.67 (m, 6H), 7.65 (d, J = 7.2 Hz, 2H), 7.47 (t, J = 7.6 Hz, 2H), 7.38 (t, J = 7.6 Hz, 1H), 3.95 (s, 3H).

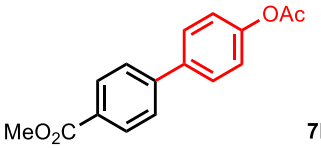


7g

Methyl 4'-methoxy-[1,1'-biphenyl]-4-carboxylate[34]

7g was synthesized following the general procedure **A**. After purification by preparative thin-layer chromatography using hexane/DCM (1/1) as the eluent, **7g** was obtained in 81% yield.

39.8 mg, colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, J = 8.0 Hz, 2H), 7.61 (d, J = 8.4 Hz, 2H), 7.57 (d, J = 8.8 Hz, 2H), 6.99 (d, J = 8.4 Hz, 2H), 3.93 (s, 3H), 3.86 (s, 3H).

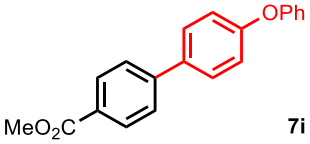


7h

Methyl 4'-acetoxy-[1,1'-biphenyl]-4-carboxylate

7h was synthesized following the general procedure **A** using $Pd(P^tBu_3)_2$ (10 mol%) at 50 °C. After purification by preparative thin-layer chromatography using hexane/EtOAc (20/1) as the eluent, **7h** was obtained in 80% yield.

43.0 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, J = 8.8 Hz, 2H), 7.63 (dd, J = 8.8, 1.6 Hz, 4H), 7.19 (d, J = 8.8 Hz, 2H), 3.94 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.45, 166.93, 150.72, 144.71, 137.73, 130.13, 128.98, 128.34, 126.99, 122.07, 52.14, 21.14; HRMS (ESI-TOF) m/z Calcd for $C_{16}H_{15}O_4$ $[M+H]^+$ 271.0965, found: 271.0969.

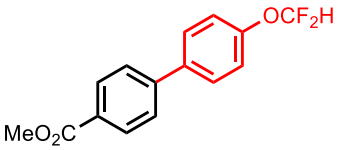


7i

Methyl 4'-phenoxy-[1,1'-biphenyl]-4-carboxylate

7i was synthesized following the general procedure **A** using $Pd(P^tBu_3)_2$ (10 mol%) at 50 °C. After purification by preparative thin-layer chromatography using hexane/DCM (3/1) as the eluent, **7i** was obtained in 82% yield.

50.0 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, J = 8.4 Hz, 2H), 7.63 (d, J = 8.4 Hz, 2H), 7.59 (d, J = 8.8 Hz, 2H), 7.37 (t, J = 8.4 Hz, 2H), 7.14 (t, J = 7.6 Hz, 1H), 7.08 (t, J = 8.4 Hz, 4H), 3.94 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.97, 157.68, 156.78, 144.90, 134.80, 130.12, 129.84, 128.60, 126.68, 123.63, 119.21, 118.95, 52.09; HRMS (ESI-TOF) m/z Calcd for $C_{20}H_{16}NaO_3$ $[M+Na]^+$ 327.0992, found: 327.0999.

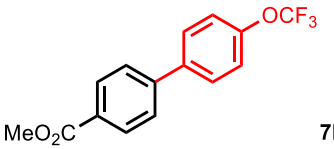


7j

Methyl 4'-(difluoromethoxy)-[1,1'-biphenyl]-4-carboxylate

7j was synthesized following the general procedure **A** using $Pd(P^tBu_3)_2$ (10 mol%) at 50 °C. After purification by preparative thin-layer chromatography using hexane/EtOAc (10/1) as the eluent, **7j** was obtained in 62% yield.

34.7 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (d, J = 8.4 Hz, 2H), 7.62 (dd, J = 8.4, 2.4 Hz, 4H), 7.22 (d, J = 8.8 Hz, 2H), 6.56 (t, J = 73.8 Hz, 1H), 3.94 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.88, 151.16 (d, J = 2.8 Hz), 144.39, 137.29, 130.18, 129.08, 128.69, 126.90, 119.95, 115.78 (t, J = 258.8 Hz), 52.16; ^{19}F NMR (375 MHz, $CDCl_3$) δ -81.34, -81.54; HRMS (EI) m/z Calcd for $C_{15}H_{12}F_2O_3$ (M^+) 278.0749, found: 278.0751.

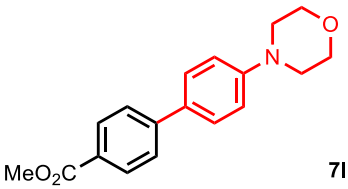


7k

Methyl 4'-(trifluoromethoxy)-[1,1'-biphenyl]-4-carboxylate

7k was synthesized following the general procedure **B** using TTSO (2.0 equiv), Tf_2O (2.0 equiv) for thianthrenation, and using $NaHCO_3$ (4.0 equiv) and $Pd(P^tBu_3)_2$ (10 mol%) for thio-Suzuki coupling. After purification by preparative thin-layer chromatography using hexane/EtOAc (20/1) as the eluent, **7k** was obtained in 50% yield.

29.7 mg, white solid. ^1H NMR (400 MHz, $CDCl_3$) δ 8.11 (d, J = 8.8 Hz, 2H), 7.66–7.61 (m, 4H), 7.31 (d, J = 8.0 Hz, 2H), 3.95 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.82, 149.21 (d, J = 1.6 Hz), 144.13, 138.68, 130.19, 129.26, 128.65, 127.00, 121.33, 120.44 (q, J = 255.8 Hz), 52.20; ^{19}F NMR (375 MHz, $CDCl_3$) δ -58.31; HRMS (EI) m/z Calcd for $C_{15}H_{11}F_3O_3$ (M^+) 296.0655, found: 296.0658.

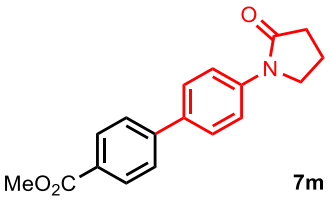


7l

Methyl 4'-morpholino-[1,1'-biphenyl]-4-carboxylate

7l was synthesized following the general procedure **A**. After purification by preparative thin-layer chromatography using hexane/DCM (1/1) as the eluent, **7l** was obtained in 47% yield.

28.0 mg, white solid. ^1H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, J = 8.0 Hz, 2H), 7.62 (d, J = 8.0 Hz, 2H), 7.57 (d, J = 8.8 Hz, 2H), 6.99 (d, J = 8.4 Hz, 2H), 3.93 (s, 3H), 3.89 (t, J = 4.0 Hz, 4H), 3.23 (t, J = 4.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.10, 151.16, 145.16, 131.00, 130.08, 127.98, 126.15, 115.57, 66.80, 52.04, 48.84; HRMS (EI) m/z Calcd for $C_{18}H_{19}NO_3$ (M^+) 297.1361, found: 297.1359.

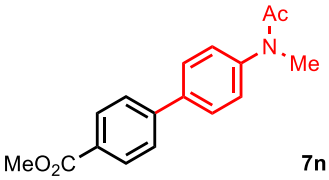


7m

Methyl 4'-(2-oxopyrrolidin-1-yl)-[1,1'-biphenyl]-4-carboxylate

7m was synthesized following the general procedure **A**. After purification by preparative thin-layer chromatography using DCM as the eluent, **7m** was obtained in 73% yield.

43.0 mg, white solid. ^1H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, J = 8.0 Hz, 2H), 7.73 (d, J = 8.8 Hz, 2H), 7.67–7.62 (m, 4H), 3.95–3.88 (m, 5H), 2.65 (t, J = 7.6 Hz, 2H), 2.24–2.16 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.36, 166.97, 144.82, 139.44, 135.77, 130.11, 128.69, 127.57, 126.67, 120.07, 52.10, 48.66, 32.75, 17.96; HRMS (ESI-TOF) m/z Calcd for $C_{18}H_{18}NO_3$ $[M+H]^+$ 296.1281, found: 296.1285.



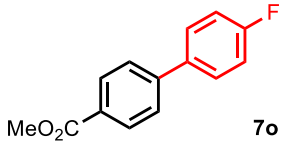
7n

Methyl 4'-(*N*-methylacetamido)-[1,1'-biphenyl]-4-carboxylate

7n was synthesized following the general procedure **A**. After purification by preparative thin-layer chromatography

using DCM as the eluent, **7n** was obtained in 64% yield.

36.2 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, J = 8.4 Hz, 2H), 7.67 (dd, J = 8.0, 2.0 Hz, 4H), 7.30 (d, J = 8.4 Hz, 2H), 3.95 (s, 3H), 3.31 (s, 3H), 1.94 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.50, 166.82, 144.45, 144.27, 139.41, 130.20, 129.31, 128.53, 127.51, 126.97, 52.18, 37.16, 22.48; HRMS (ESI-TOF) m/z Calcd for $C_{17}H_{18}NO_3$ $[M+H]^+$ 284.1281, found: 284.1288.

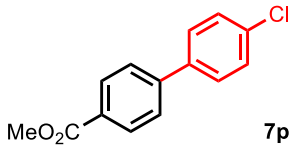


7o

Methyl 4'-fluoro-[1,1'-biphenyl]-4-carboxylate

7o was synthesized following the general procedure **B**. After purification by preparative thin-layer chromatography using hexane/EtOAc (20/1) as the eluent, **7o** was obtained in 65% yield.

30.0 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, J = 8.4 Hz, 2H), 7.63–7.56 (m, 4H), 7.15 (t, J = 8.8 Hz, 2H), 3.94 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.91, 164.16, 161.70, 144.58, 136.11 (d, J = 4.0 Hz), 130.15, 128.91 (d, J = 8.0 Hz), 126.87, 115.86 (d, J = 21.0 Hz), 52.14; ^{19}F NMR (375 MHz, $CDCl_3$) δ -114.75; HRMS (EI) m/z Calcd for $C_{14}H_{11}FO_2$ (M^+) 230.0738, found: 230.0737.

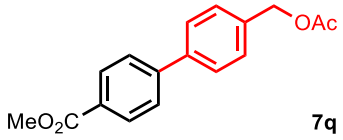


7p

Methyl 4'-chloro-[1,1'-biphenyl]-4-carboxylate[35]

7p was synthesized following the general procedure **B**. After purification by preparative thin-layer chromatography using hexane/EtOAc (20/1) as the eluent, **7p** was obtained in 33% yield.

16.0 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, J = 8.0 Hz, 2H), 7.62 (d, J = 8.4 Hz, 2H), 7.55 (d, J = 8.4 Hz, 2H), 7.43 (d, J = 8.4 Hz, 2H), 3.94 (s, 3H).

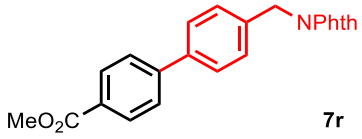


7q

Methyl 4'-(acetoxymethyl)-[1,1'-biphenyl]-4-carboxylate

7q was synthesized following the general procedure **B**. After purification by preparative thin-layer chromatography using hexane/EtOAc (10/1) as the eluent, **7q** was obtained in 54% yield.

30.7 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (d, J = 8.4 Hz, 2H), 7.65 (d, J = 8.4 Hz, 2H), 7.62 (d, J = 8.0 Hz, 2H), 7.46 (d, J = 8.0 Hz, 2H), 5.16 (s, 2H), 3.94 (s, 3H), 2.13 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.86, 166.92, 145.02, 139.96, 135.89, 130.12, 129.06, 128.82, 127.45, 127.00, 65.88, 52.13, 21.00; HRMS (EI) m/z Calcd for $C_{17}H_{16}O_4$ (M^+) 284.1043, found: 284.1046.



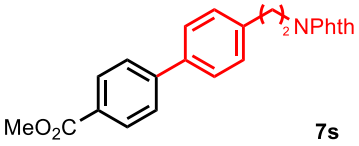
7r

Methyl 4'-((1,3-dioxoisoindolin-2-yl)methyl)-[1,1'-biphenyl]-4-carboxylate

7r was synthesized following the general procedure **B**. After purification by preparative thin-layer chromatography using hexane/DCM (3/2) as the eluent, **7r** was obtained in 51% yield.

37.0 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, J = 8.4 Hz, 2H), 7.88–7.84 (m, 2H), 7.74–7.69 (m, 2H),

7.62-7.52 (m, 6H), 4.90 (s, 2H), 3.93 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.02, 166.93, 145.05, 139.55, 136.29, 134.04, 132.07, 130.07, 129.18, 128.94, 127.56, 126.96, 123.39, 52.11, 41.24; HRMS (EI) m/z Calcd for $C_{23}H_{17}NO_4$ (M^+) 371.1156, found: 371.1152.

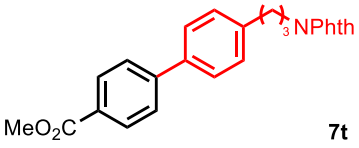


7s

Methyl 4'-(2-(1,3-dioxoisoindolin-2-yl)ethyl)-[1,1'-biphenyl]-4-carboxylate

7s was synthesized following the general procedure **B**. After purification by preparative thin-layer chromatography using DCM as the eluent, **7s** was obtained in 66% yield.

51.0 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, J = 8.4 Hz, 2H), 7.85–7.80 (m, 2H), 7.73–7.68 (m, 2H), 7.63 (d, J = 8.4 Hz, 2H), 7.55 (d, J = 8.0 Hz, 2H), 7.35 (d, J = 8.0 Hz, 2H), 3.99–3.91 (m, 5H), 3.05 (t, J = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.14, 166.97, 145.21, 138.26, 138.10, 133.93, 132.02, 130.04, 129.42, 128.74, 127.37, 126.83, 123.23, 52.08, 39.07, 34.22; HRMS (EI) m/z Calcd for $C_{24}H_{20}NO_4$ $[M+H]^+$ 386.1387, found: 386.1389.

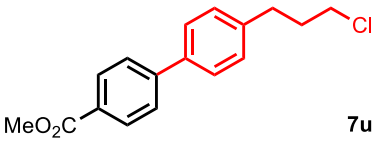


7t

Methyl 4'-(3-(1,3-dioxoisoindolin-2-yl)propyl)-[1,1'-biphenyl]-4-carboxylate

7t was synthesized following the general procedure **B**. After purification by preparative thin-layer chromatography using hexane/DCM (1/1) as the eluent, **7t** was obtained in 97% yield.

78.0 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, J = 8.4 Hz, 2H), 7.84–7.78 (m, 2H), 7.70–7.65 (m, 2H), 7.59 (d, J = 8.0 Hz, 2H), 7.49 (d, J = 8.4 Hz, 2H), 7.28 (d, J = 8.0 Hz, 2H), 3.93 (s, 3H), 3.77 (t, J = 7.2 Hz, 2H), 2.74 (t, J = 7.8 Hz, 2H), 2.12–2.03 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.36, 166.97, 145.32, 141.16, 137.56, 133.83, 132.04, 129.98, 128.84, 128.58, 127.17, 126.75, 123.09, 52.04, 37.72, 32.80, 29.54; HRMS (EI) m/z Calcd for $C_{25}H_{21}NO_4$ (M^+) 399.1471, found: 399.1465.

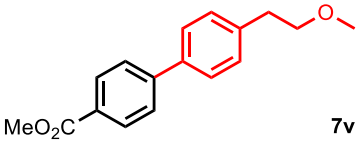


7u

Methyl 4'-(3-chloropropyl)-[1,1'-biphenyl]-4-carboxylate

7u was synthesized following the general procedure **A**. After purification by preparative thin-layer chromatography using hexane/EtOAc (20/1) as the eluent, **7u** was obtained in 68% yield.

39.0 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, J = 8.4 Hz, 2H), 7.65 (d, J = 8.4 Hz, 2H), 7.57 (d, J = 8.0 Hz, 2H), 7.30 (d, J = 8.0 Hz, 2H), 3.94 (s, 3H), 3.56 (t, J = 6.4 Hz, 2H), 2.84 (t, J = 7.4 Hz, 2H), 2.16–2.09 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.98, 145.32, 140.83, 137.85, 130.08, 129.12, 128.72, 127.33, 126.81, 52.08, 44.13, 33.88, 32.38; HRMS (EI) m/z Calcd for $C_{17}H_{17}ClO_2$ (M^+) 288.0912, found: 288.0914.



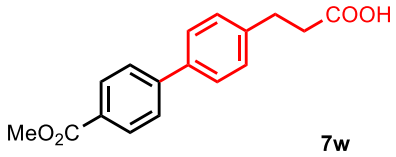
7v

Methyl 4'-(2-methoxyethyl)-[1,1'-biphenyl]-4-carboxylate

7v was synthesized following the general procedure **A** at 50 °C. After purification by preparative thin-layer

chromatography using hexane/EtOAc (10/1) as the eluent, **7v** was obtained in 87% yield.

47.0 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, J = 8.4 Hz, 2H), 7.65 (d, J = 8.4 Hz, 2H), 7.56 (d, J = 8.4 Hz, 2H), 7.32 (d, J = 8.4 Hz, 2H), 3.94 (s, 3H), 3.65 (t, J = 7.2 Hz, 2H), 3.38 (s, 3H), 2.94 (t, J = 7.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.00, 145.44, 139.20, 137.90, 130.05, 129.41, 128.67, 127.23, 126.83, 73.38, 58.71, 52.09, 35.84; HRMS (ESI-TOF) m/z Calcd for $C_{17}H_{19}O_3$ $[M+H]^+$ 271.1329, found: 271.1335.

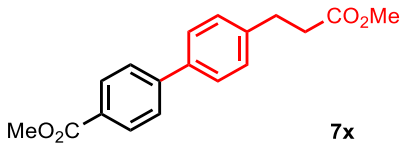


7w

3-(4'-(Methoxycarbonyl)-[1,1'-biphenyl]-4-yl)propanoic acid

7w was synthesized following the general procedure **B** using $NaHCO_3$ (67.2 mg, 0.8 mmol, 4.0 equiv). The reaction mixture was quenched by adding 1 M HCl (5.0 mL). The organic phase was separated, and the aqueous layer was extracted with DCM (3 × 10 mL). The combined organic layers were dried over anhydrous Na_2SO_4, filtered and concentrated under vacuum. After purification by preparative thin-layer chromatography using DCM/MeOH (20/1) as the eluent, **7w** was obtained in 85% yield.

46.0 mg, white solid. ^{1}H NMR (400 MHz, $(CD_3)_2SO$) δ 8.02 (d, J = 8.4 Hz, 2H), 7.81 (d, J = 8.4 Hz, 2H), 7.66 (d, J = 8.4 Hz, 2H), 7.36 (d, J = 8.0 Hz, 2H), 3.87 (s, 3H), 2.87 (t, J = 7.2 Hz, 2H), 2.58–2.53 (m, 2H). ^{13}C NMR (100 MHz, $(CD_3)_2SO$) δ 173.91, 166.11, 144.59, 141.55, 136.50, 129.82, 129.07, 128.20, 126.91, 126.75, 52.19, 35.35, 30.74; HRMS (ESI-TOF) m/z Calcd for $C_{17}H_{15}O_4$ $[M-H]^-$ 283.0976, found: 283.0981.

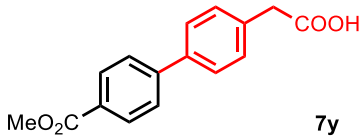


7x

Methyl 4'-(3-methoxy-3-oxopropyl)-[1,1'-biphenyl]-4-carboxylate

7x was synthesized following the general procedure **A**. After purification by preparative thin-layer chromatography using hexane/EtOAc (10/1) as the eluent, **7x** was obtained in 68% yield.

40.0 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, J = 8.0 Hz, 2H), 7.64 (d, J = 8.0 Hz, 2H), 7.56 (d, J = 8.0 Hz, 2H), 7.30 (d, J = 8.0 Hz, 2H), 3.94 (s, 3H), 3.69 (s, 3H), 3.01 (t, J = 7.8 Hz, 2H), 2.68 (t, J = 7.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.21, 167.00, 145.32, 140.65, 138.00, 130.08, 128.88, 128.74, 127.37, 126.84, 52.10, 51.68, 35.52, 30.55; HRMS (EI) m/z Calcd for $C_{18}H_{18}O_4$ (M^+) 298.1203, found: 298.1200.

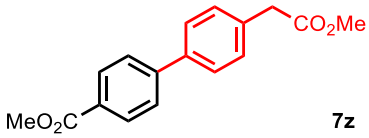


7y

2-(4'-(Methoxycarbonyl)-[1,1'-biphenyl]-4-yl)acetic acid

7y was synthesized following the general procedure **B** using $NaHCO_3$ (67.2 mg, 0.8 mmol, 4.0 equiv). The reaction mixture was quenched by adding 1 M HCl (5.0 mL). The organic phase was separated and the aqueous layer was extracted with DCM (3 × 10 mL). The combined organic layers were dried over anhydrous Na_2SO_4, filtered and concentrated under vacuum. After purification by preparative thin-layer chromatography using DCM/MeOH (20/1) as the eluent, **7y** was obtained in 80% yield.

43.0 mg, white solid. ^{1}H NMR (400 MHz, $(CD_3)_2SO$) δ 8.04 (d, J = 8.0 Hz, 2H), 7.83 (d, J = 8.4 Hz, 2H), 7.70 (d, J = 8.4 Hz, 2H), 7.39 (d, J = 8.0 Hz, 2H), 3.88 (s, 3H), 3.64 (s, 2H); ^{13}C NMR (100 MHz, $(CD_3)_2SO$) δ 172.58, 166.08, 144.47, 137.12, 135.43, 130.19, 129.82, 128.33, 126.86, 126.83, 52.18, 40.28; HRMS (ESI-TOF) m/z Calcd for $C_{16}H_{13}O_4$ $[M-H]^-$ 269.0819, found: 269.0824.

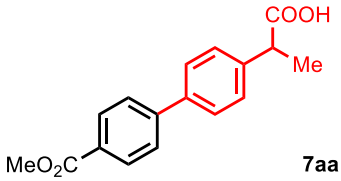


7z

Methyl 4'-(2-methoxy-2-oxoethyl)-[1,1'-biphenyl]-4-carboxylate

7z was synthesized following the general procedure **B**. After purification by preparative thin-layer chromatography using hexane/EtOAc (10/1) as the eluent, **7z** was obtained in 79% yield.

45.0 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, J = 8.8 Hz, 2H), 7.65 (d, J = 8.4 Hz, 2H), 7.59 (d, J = 8.4 Hz, 2H), 7.38 (d, J = 8.4 Hz, 2H), 3.94 (s, 3H), 3.72 (s, 3H), 3.69 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.86, 166.99, 145.17, 138.87, 133.98, 130.10, 129.86, 128.90, 127.46, 126.94, 52.15, 52.12, 40.81; HRMS (EI) m/z Calcd for $C_{17}H_{16}O_4$ (M^+) 284.1043, found: 284.1043.

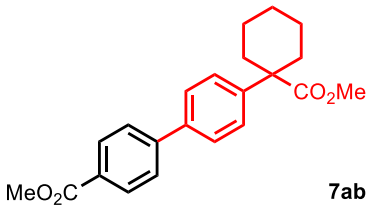


7aa

2-(4'-(Methoxycarbonyl)-[1,1'-biphenyl]-4-yl)propanoic acid

7aa was synthesized following the general procedure **B** using $NaHCO_3$ (67.2 mg, 0.8 mmol, 4.0 equiv). The reaction mixture was quenched by adding 1 M HCl (5.0 mL). The organic phase was separated and the aqueous layer was extracted with DCM (3 × 10 mL). The combined organic layers were dried over anhydrous Na_2SO_4, filtered and concentrated under vacuum. After purification by preparative thin-layer chromatography using DCM/MeOH (20/1) as the eluent, **7aa** was obtained in 79% yield.

45.0 mg, white solid. ^{1}H NMR (400 MHz, $(CD_3)_2SO$) δ 8.02 (d, J = 8.8 Hz, 2H), 7.80 (d, J = 8.4 Hz, 2H), 7.66 (d, J = 8.4 Hz, 2H), 7.40 (d, J = 8.4 Hz, 2H), 3.88 (s, 3H), 3.65 (dd, J = 14.0, 7.0 Hz, 1H), 1.36 (d, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $(CD_3)_2SO$) δ 175.69, 166.07, 144.59, 143.04, 136.77, 129.78, 128.22, 128.20, 126.78, 127.74, 52.14, 45.53, 18.90; HRMS (EI) m/z Calcd for $C_{17}H_{16}O_4$ (M^+) 284.1045, found: 284.1043.

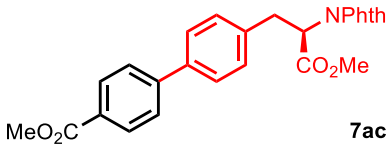


7ab

Methyl 4'-(1-(methoxycarbonyl)cyclohexyl)-[1,1'-biphenyl]-4-carboxylate

7ab was synthesized following the general procedure **A** at 50 °C. After purification by preparative thin-layer chromatography using hexane/EtOAc (10/1) as the eluent, **7ab** was obtained in 63% yield.

44.0 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, J = 8.0 Hz, 2H), 7.65 (d, J = 8.4 Hz, 2H), 7.59 (d, J = 8.4 Hz, 2H), 7.49 (d, J = 8.4 Hz, 2H), 3.94 (s, 3H), 3.67 (s, 3H), 2.55–2.48 (m, 2H), 1.79–1.65 (m, 5H), 1.55–1.45 (m, 2H), 1.32–1.28 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.56, 167.00, 145.06, 143.91, 138.31, 130.08, 128.85, 127.28, 126.88, 126.54, 52.11, 50.80, 34.68, 25.53, 23.64; HRMS (EI) m/z Calcd for $C_{22}H_{24}O_4$ (M^+) 352.1669, found: 352.1672.

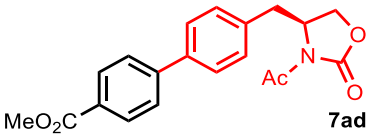


7ac

Methyl (*R*)-4'-(2-(1,3-dioxoisoindolin-2-yl)-3-methoxy-3-oxopropyl)-[1,1'-biphenyl]-4-carboxylate

7ac was synthesized following the general procedure **B**. After purification by preparative thin-layer chromatography using hexane/EtOAc (5/1) as the eluent, **7ac** was obtained in 61% yield.

54.6 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, J = 8.8 Hz, 2H), 7.82–7.78 (m, 2H), 7.72–7.67 (m, 2H), 7.57 (d, J = 8.8 Hz, 2H), 7.47 (d, J = 8.0 Hz, 2H), 7.26 (d, J = 8.0 Hz, 2H), 5.21 (dd, J = 10.8, 6.0 Hz, 1H), 3.92 (s, 3H), 3.80 (s, 3H), 3.69–3.58 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.24, 167.46, 166.93, 144.99, 138.36, 136.82, 134.15, 131.54, 129.99, 129.40, 128.75, 127.36, 126.76, 123.52, 53.06, 52.94, 52.07, 34.30; HRMS (EI) m/z Calcd for $C_{26}H_{22}NO_6$ $[M+H]^+$ 444.1442, found: 444.1443.

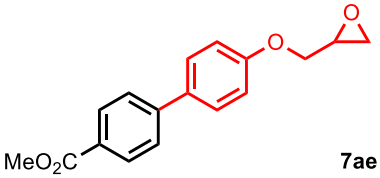


7ad

Methyl (*S*)-4'-((3-acetyl-2-oxooxazolidin-4-yl)methyl)-[1,1'-biphenyl]-4-carboxylate

7ad was synthesized following the general procedure **A**. After purification by preparative thin-layer chromatography using hexane/EtOAc (2/1) as the eluent, **7ad** was obtained in 57% yield.

40.0 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, J = 8.4 Hz, 2H), 7.64 (d, J = 8.0 Hz, 2H), 7.60 (d, J = 8.0 Hz, 2H), 7.31 (d, J = 8.0 Hz, 2H), 4.75–4.69 (m, 1H), 4.28–4.19 (m, 2H), 3.94 (s, 3H), 3.36 (dd, J = 13.2, 3.2 Hz, 1H), 2.85 (dd, J = 13.6, 9.6 Hz, 1H), 2.58 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.59, 167.13, 153.65, 144.91, 139.14, 135.18, 130.17, 130.01, 128.98, 127.83, 126.94, 66.18, 54.96, 52.24, 37.50, 23.82; HRMS (ESI-TOF) m/z Calcd for $C_{20}H_{19}NNaO_5$ $[M+Na]^+$ 376.1155, found: 376.1161.

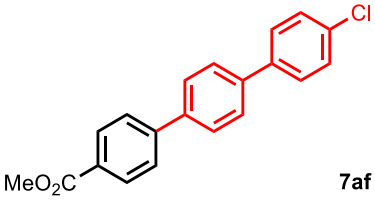


7ae

Methyl 4'-(oxiran-2-ylmethoxy)-[1,1'-biphenyl]-4-carboxylate

7ae was synthesized following the general procedure **A** at 50 °C. After purification by preparative thin-layer chromatography using hexane/EtOAc (10/1) as the eluent, **7ae** was obtained in 82% yield.

47.0 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, J = 8.8 Hz, 2H), 7.61 (d, J = 8.8 Hz, 2H), 7.57 (d, J = 8.8 Hz, 2H), 7.01 (d, J = 8.8 Hz, 2H), 4.29 (dd, J = 10.8, 3.2 Hz, 1H), 4.01 (dd, J = 10.8, 5.6 Hz, 1H), 3.93 (s, 3H), 3.41–3.36 (m, 1H), 2.93 (t, J = 4.4 Hz, 1H), 2.79 (dd, J = 4.8, 2.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.03, 158.70, 145.05, 132.97, 130.10, 128.40, 128.34, 126.49, 115.06, 68.84, 52.07, 50.10, 44.69; HRMS (ESI-TOF) m/z Calcd for $C_{17}H_{17}O_4$ $[M+H]^+$ 285.1121, found: 285.1126.

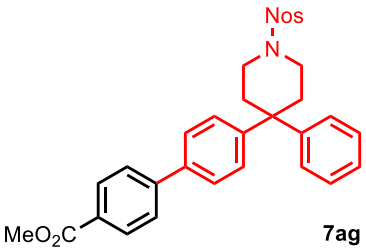


7af

Methyl 4''-chloro-[1,1':4',1''-terphenyl]-4-carboxylate

7af was synthesized following the general procedure **A** at 50 °C. After purification by preparative thin-layer chromatography using hexane/EtOAc (2/1) as the eluent, **7af** was obtained in 62% yield.

40.0 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, J = 8.4 Hz, 2H), 7.73–7.68 (m, 4H), 7.66 (d, J = 8.0 Hz, 2H), 7.57 (d, J = 8.4 Hz, 2H), 7.43 (d, J = 8.4 Hz, 2H), 3.95 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.95, 144.89, 139.73, 139.17, 138.85, 133.68, 130.17, 129.02, 128.27, 127.74, 127.46, 126.89, 52.15; HRMS (EI) m/z Calcd for $C_{20}H_{15}ClO_2$ (M^+) 322.0755, found: 322.0756.

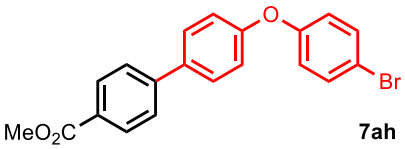


7ag

Methyl 4'-(1-((4-nitrophenyl)sulfonyl)-4-phenylpiperidin-4-yl)-[1,1'-biphenyl]-4-carboxylate

7ag was synthesized following the general procedure **B**. After purification by preparative thin-layer chromatography using hexane/DCM (1/1) as the eluent, **7ag** was obtained in 97% yield.

108.0 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, J = 8.8 Hz, 2H), 8.07 (d, J = 8.4 Hz, 2H), 7.89 (d, J = 8.8 Hz, 2H), 7.58 (d, J = 8.4 Hz, 2H), 7.51 (d, J = 8.4 Hz, 2H), 7.29–7.26 (m, 2H), 7.25–7.21 (m, 2H), 7.19–7.13 (m, 3H), 3.92 (s, 3H), 3.34–3.28 (m, 2H), 3.23–3.18 (m, 2H), 2.62–2.51 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.88, 150.02, 145.94, 145.04, 144.60, 143.12, 137.84, 130.11, 128.97, 128.82, 128.51, 127.46, 127.29, 126.78, 126.73, 126.51, 124.32, 52.13, 44.17, 43.16, 35.53; HRMS (ESI-TOF) m/z Calcd for $C_{31}H_{28}O_6N_2SNa$ $[M+Na]^+$ 579.1560, found: 579.1565.

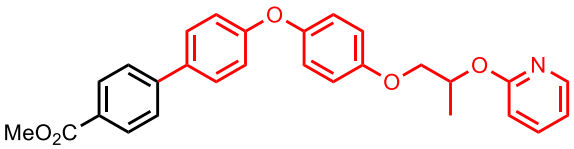


7ah

Methyl 4'-(4-bromophenoxy)-[1,1'-biphenyl]-4-carboxylate

7ah was synthesized following the general procedure **A**. After purification by preparative thin-layer chromatography using hexane/EtOAc (10/1) as the eluent, **7ah** was obtained in 91% yield.

70.0 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, J = 8.8 Hz, 2H), 7.63 (d, J = 8.4 Hz, 2H), 7.60 (d, J = 8.8 Hz, 2H), 7.46 (d, J = 9.2 Hz, 2H), 7.08 (d, J = 8.8 Hz, 2H), 6.94 (d, J = 9.2 Hz, 2H), 3.95 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.12, 156.12, 144.80, 135.36, 132.81, 130.18, 128.76, 128.67, 126.75, 120.76, 119.16, 116.09, 52.20; HRMS (ESI-TOF) m/z Calcd for $C_{20}H_{15}BrNaO_3$ $[M+Na]^+$ 405.0097, found: 405.0102.

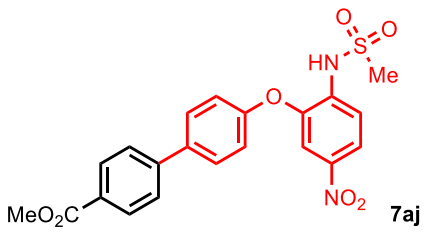


7ai

Methyl 4'-(4-(2-(pyridin-2-yloxy)propoxy)phenoxy)-[1,1'-biphenyl]-4-carboxylate

7ai was synthesized following the general procedure **A** at 50 °C. After purification by preparative thin-layer chromatography using hexane/EtOAc (20/1) as the eluent, **7ai** was obtained in 70% yield.

64.0 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (dd, J = 5.2, 1.2 Hz, 1H), 8.08 (d, J = 8.4 Hz, 2H), 7.62 (d, J = 8.4 Hz, 2H), 7.59–7.53 (m, 3H), 7.03–6.98 (m, 4H), 6.97–6.93 (m, 2H), 6.89–6.84 (m, 1H), 6.75 (d, J = 8.4 Hz, 1H), 5.63–5.56 (m, 1H), 4.23–4.18 (m, 1H), 4.11–4.06 (m, 1H), 3.93 (s, 3H), 1.49 (d, J = 6.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.02, 163.13, 158.90, 155.49, 149.81, 146.76, 144.99, 138.70, 134.07, 130.11, 128.49, 126.62, 121.00, 117.75, 116.77, 115.87, 111.67, 109.97, 71.05, 69.23, 52.09, 16.99; HRMS (ESI-TOF) m/z Calcd for $C_{28}H_{26}NO_5$ $[M+H]^+$ 456.1805, found: 456.1818.

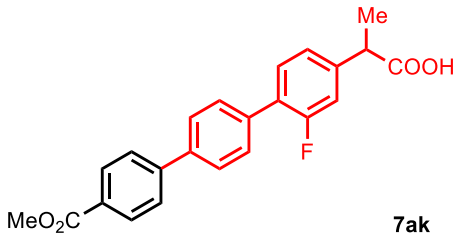


7aj

Methyl 4'-(2-(methylsulfonamido)-5-nitrophenoxy)-[1,1'-biphenyl]-4-carboxylate

7aj was synthesized following the general procedure **A**. After purification by preparative thin-layer chromatography using DCM as the eluent, **7aj** was obtained in 99% yield.

87.0 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, J = 8.4 Hz, 2H), 8.04 (dd, J = 8.8, 2.4 Hz, 1H), 7.80 (d, J = 9.2 Hz, 1H), 7.74 (d, J = 2.4 Hz, 1H), 7.70 (d, J = 8.8 Hz, 2H), 7.67 (d, J = 8.4 Hz, 2H), 7.41 (s, 1H), 7.17 (d, J = 8.4 Hz, 2H), 3.96 (s, 3H), 3.20 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.84, 154.23, 146.01, 144.10, 143.69, 137.84, 134.06, 130.25, 129.52, 129.28, 126.98, 120.05, 119.67, 117.37, 112.10, 52.20, 40.65; HRMS (ESI-TOF) m/z Calcd for $C_{21}H_{17}O_7N_2S$ $[M-H]^-$ 441.0762, found: 441.0768.



7ak

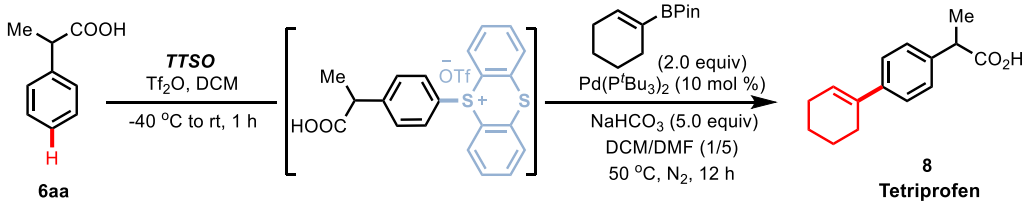
2-(2-Fluoro-4''-(methoxycarbonyl)-[1,1':4',1''-terphenyl]-4-yl)propanoic acid

7ak was synthesized following the general procedure **B** using $NaHCO_3$ (67.2 mg, 0.8 mmol, 4.0 equiv). The reaction mixture was quenched by adding 1 M HCl (5.0 mL). The organic phase was separated, and the aqueous layer was extracted with DCM (3 × 10 mL). The combined organic layers were dried over anhydrous Na_2SO_4, filtered and concentrated under vacuum. After purification by preparative thin-layer chromatography using hexane/EtOAc (2/1) as the eluent, **7ak** was obtained in 76% yield.

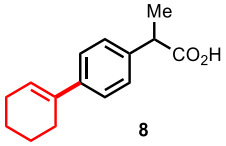
57.0 mg, white solid. ^{1}H NMR (400 MHz, $(CD_3)_2SO$) δ 12.51 (s, 1H), 8.07 (d, J = 8.4 Hz, 2H), 7.90 (d, J = 8.4 Hz, 2H), 7.87 (d, J = 8.0 Hz, 2H), 7.69 (d, J = 7.6 Hz, 2H), 7.57 (t, J = 8.2 Hz, 1H), 7.30–7.23 (m, 2H), 3.89 (s, 3H), 3.80 (q, J = 7.0 Hz, 1H), 1.42 (d, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $(CD_3)_2SO$) δ 174.85, 166.03, 160.20, 157.75, 144.04, 143.42 (d, J = 8.0 Hz), 138.11, 134.90, 130.58 (d, J = 4.0 Hz), 129.85, 129.39 (d, J = 3.0 Hz), 128.59, 127.08 (d, J = 27.0 Hz), 125.92 (d, J = 13.0 Hz), 124.14 (d, J = 3.0 Hz), 115.27 (d, J = 23.0 Hz), 52.18, 44.12, 18.27; ^{19}F NMR (375 MHz, $(CD_3)_2SO$) δ -117.89; HRMS (ESI-TOF) m/z Calcd for $C_{23}H_{20}FO_4$ $[M+H]^+$ 379.1340, found: 379.1339.

2.6 Applications of *para*-Functionalization of Arenes

2.6.1 Synthesis of Tetriprofen

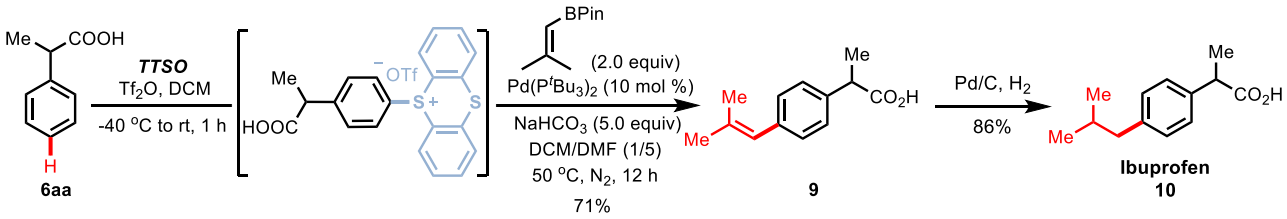


A 25 mL Schlenk tube was charged with thianthrene *S*-oxide (55.7 mg, 0.24 mmol, 1.2 equiv), CH_2Cl_2 (0.2 mL) and **6aa** (0.2 mmol, 1.0 equiv) under nitrogen atmosphere. The reaction mixture was then cooled to -40 °C, followed by the dropwise of Tf_2O (44 μL, 0.24 mmol, 1.2 equiv). The reaction mixture was stirred at the same temperature for 30 min, and then allowed to stir at room temperature for another 1 hour. Then alkenylboric acid pinacol ester (0.4 mmol, 2.0 equiv), $Pd(P^tBu_3)_2$ (10.2 mg, 10 mol%), $NaHCO_3$ (84.0 mg, 1.0 mmol, 5.0 equiv) were added under nitrogen atmosphere, subsequently the DMF (1.0 mL) was added to wash the Schlenk tube. The reaction mixture was stirred at 50 °C for 12 hours. Upon completion, 0.25 M HCl (5.0 mL) was added to the mixture. The organic phase was separated, and the aqueous phase was extracted with DCM (3 × 10 mL). The combined organic layers were dried over anhydrous Na_2SO_4, filtered and concentrated under vacuum. The resulting mixture was purified by silica gel chromatography (DCM/MeOH = 25/1) to afford **Tetriprofen** in 52% yield.



24.0 mg, colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 (d, *J* = 8.4 Hz, 2H), 7.26–7.23 (m, 2H), 6.12–6.07 (m, 1H), 3.72 (q, *J* = 7.2 Hz, 1H), 2.41–2.35 (m, 2H), 2.23–2.17 (m, 2H), 1.80–1.74 (m, 2H), 1.69–1.62 (m, 2H), 1.50 (d, *J* = 7.2 Hz, 3H).

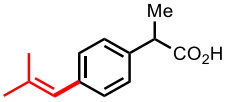
2.6.2 Synthesis of Ibuprofen



A 25 mL Schlenk tube was charged with thianthrene *S*-oxide (55.7 mg, 0.24 mmol, 1.2 equiv), CH_2Cl_2 (0.2 mL) and **6aa** (0.2 mmol, 1.0 equiv) under nitrogen atmosphere. The reaction mixture was then cooled to -40 °C, followed by the dropwise of Tf_2O (44 μL, 0.24 mmol, 1.2 equiv). The reaction mixture was stirred at the same temperature for 30 min, and then allowed to stir at room temperature for another 1 hour. Then alkenylboric acid pinacol ester (0.4 mmol, 2.0 equiv), $Pd(P^tBu_3)_2$ (10.2 mg, 10 mol%), $NaHCO_3$ (84.0 mg, 1.0 mmol, 5.0 equiv) were added under nitrogen atmosphere, subsequently the DMF (1.0 mL) was added to wash the Schlenk tube. The reaction mixture was stirred at 50 °C for 12 hours. Upon completion, 0.25 M HCl (5.0 mL) was added to the mixture. The organic phase was separated, and the aqueous phase was extracted with DCM (3 × 10 mL). The combined organic layers were dried over anhydrous Na_2SO_4, filtered and concentrated under vacuum. The resulting mixture was purified by silica gel chromatography (DCM/MeOH = 25/1) to afford **9** in 71% yield.

To a solution alkenylated 2-phenylpropanoic acid **9** (42 mg, 0.2 mmol) in ethanol (5.0 mL) was added palladium on activated carbon (4.2 mg, 10 wt%). Then the flask was back-filled with hydrogen gas five times. A hydrogen balloon

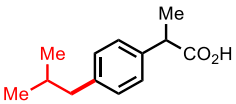
was left on the flask and the reaction mixture was stirred for 4 hours at 50 °C. Upon completion, the reaction mixture was filtered through a pad of Celite, and the pad was washed with EtOH. The resulting solution was concentrated. The crude product was purified by silica gel chromatography using DCM/MeOH (20/1) as the eluent to afford **Ibuprofen** in 86% yield.



9

2-(4-(2-Methylprop-1-en-1-yl)phenyl)propanoic acid[36]

29.0 mg, colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28–7.25 (m, 2H), 7.18 (d, *J* = 8.4 Hz, 2H), 6.23 (s, 1H), 3.72 (q, *J* = 7.2 Hz, 1H), 1.89 (s, 3H), 1.85 (s, 3H), 1.51 (d, *J* = 7.2 Hz, 3H).

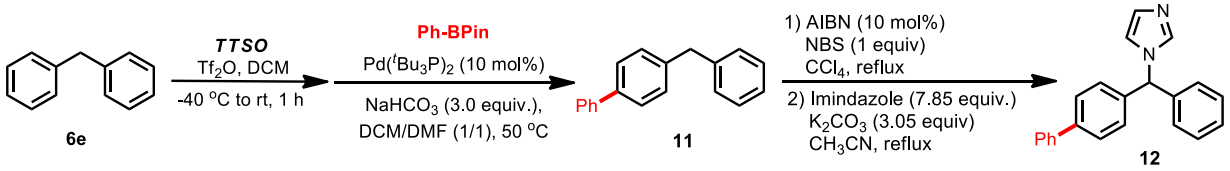


10

Ibuprofen[37]

36.0 mg, colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22 (d, *J* = 8.0 Hz, 2H), 7.10 (d, *J* = 8.0 Hz, 2H), 3.70 (q, *J* = 7.2 Hz, 1H), 2.44 (d, *J* = 7.2 Hz, 2H), 1.89–1.79 (m, 1H), 1.49 (d, *J* = 7.2 Hz, 3H), 0.89 (d, *J* = 6.8 Hz, 6H).

2.6.3 Synthesis of Bifonazole



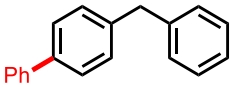
6e **11** **12**

An oven-dried 100 mL Schlenk tube was charged with thianthrene *S*-oxide (1.67 g, 7.2 mmol, 1.2 equiv), CH_2Cl_2 (30 mL) and diphenylmethane (1.00 g, 6 mmol, 1.0 equiv) under nitrogen atmosphere. The reaction mixture was then cooled to -40 °C, followed by the dropwise of Tf_2O (1.2 mL, 7.2 mmol, 1.2 equiv). The reaction mixture was stirred at the same temperature for 30 min, and then allowed to stir at room temperature for another 1 hour. Then PhBPin (1.10 g, 9.0 mmol, 1.5 equiv), $Pd(P^tBu_3)_2$ (153.0 mg, 5.0 mol%), $NaHCO_3$ (1.51 g, 18 mmol, 3.0 equiv) were added under nitrogen atmosphere, subsequently DMF (30 mL) was added to wash the Schlenk tube. The reaction mixture was stirred with a condenser (cold finger) at 50 °C for 12 hours. Upon completion, the reaction mixture was diluted with DCM, and passed through a pad of Celite with DCM as the eluent to remove the insoluble precipitate. The filtrate was concentrated, and the resulting residue was purified via silica gel chromatography (toluene/hexane = 1/40) to afford the desired product **11** (1.24 g, 84% yield) as a white solid. Meanwhile, thianthrene was isolated in 92% yield (1.42 g).

Notably, TTSO could be readily recovered in 89% total yield (1.492 g) after oxidation of thianthrene using the known procedure[1]

A suspension of **11** (48.9 mg, 0.2 mmol, 1.0 equiv), NBS (35.6 mg, 0.2 mmol, 1.0 equiv), AIBN (3.3 mg, 0.02 mmol, 10 mol%) in CCl_4 (2.5 mL) was refluxed for 50 min under nitrogen atmosphere. After cooling to room temperature, the reaction mixture was filtered and the solid was washed with hexane (2 × 2 mL). The filtrate was concentrated, followed by addition of imidazole (106.5 mg, 1.57 mmol, 7.85 equiv), K_2CO_3 (84.7 mg, 0.61 mmol, 3.05 equiv) and MeCN (4.3 mL). The mixture was then allowed to reflux for 1 h. After cooling to room temperature, the mixture was passed through a pad of Celite with DCM as the eluent to remove the insoluble precipitate. The resulting solution

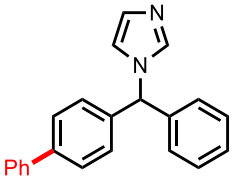
was concentrated and purified by preparative thin-layer chromatography (hexane/EtOAc = 5/3) to afford the desired **12** (47.9 mg, 77% yield) as a white solid.



11

4-benzyl-1,1'-biphenyl[38]

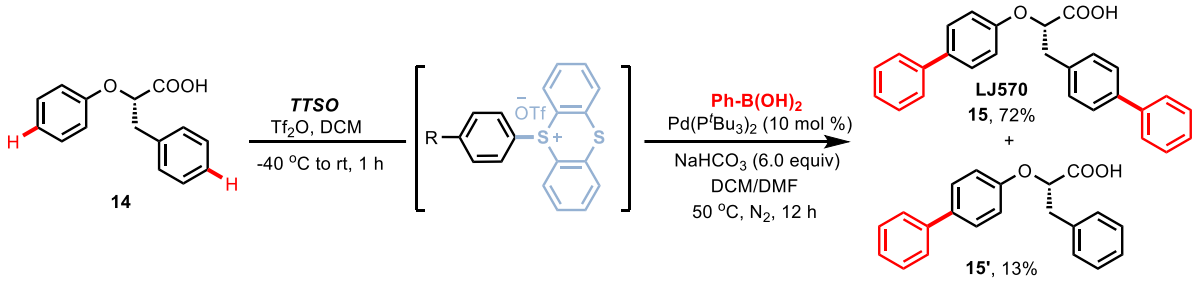
1.24 g, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59–7.54 (m, 2H), 7.54–7.50 (m, 2H), 7.45–7.39 (m, 2H), 7.35–7.19 (m, 8H), 4.03 (s, 2H).



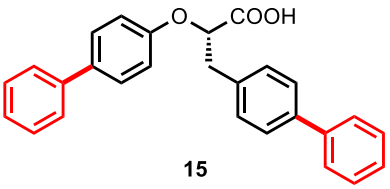
Bifonazole[39]

47.9 mg, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, J = 8.1Hz, 4H), 7.49–7.42 (m, 3H), 7.41–7.33 (m, 4H), 7.22–7.10 (m, 5H), 6.90 (s, 1H), 6.57 (s, 1H).

2.6.4 Synthesis of LJ570



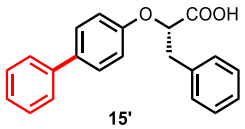
A 25 mL Schlenk tube was charged with thianthrene *S*-oxide (139.2 mg, 0.6 mmol, 3.0 equiv), CH_2Cl_2 (0.3 mL) and **14** (0.2 mmol, 1.0 equiv) under nitrogen atmosphere. The reaction mixture was then cooled to -40 °C, followed by the dropwise of Tf_2O (110 μL, 0.6 mmol, 3.0 equiv). The reaction mixture was stirred at -40 °C for 30 min, and then allowed to stir at room temperature for 1 hour. Then benzeneboronic acid (73.2 mg, 0.6 mmol, 3.0 equiv), $Pd(P^tBu_3)_2$ (10.2 mg, 10 mol%), $NaHCO_3$ (100.8 mg, 1.2 mmol, 6.0 equiv) were added under nitrogen atmosphere, subsequently the DMF (1.0 mL) was added to wash the Schlenk tube. The reaction mixture was stirred at 50 °C for 12 hours. Upon completion, 0.25 M HCl (10.0 mL) was added to the mixture. The organic phase was separated, and the aqueous phase was extracted with DCM (3 × 10 mL). The combined organic layers were dried over anhydrous Na_2SO_4, filtered and concentrated under vacuum. The resulting mixture was purified by silica gel chromatography (PhMe/isopropanol/AcOH = 100/10/1) to afford **15** (**LJ570**) and mono-arylated **15'**.



15

(*S*)-3-([1,1'-Biphenyl]-4-yl)-2-([1,1'-biphenyl]-4-yloxy)propanoic acid[40]

57.0 mg (72%), white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59–7.27 (m, 16H), 6.95 (d, J = 8.8 Hz, 2H), 4.96–4.91 (m, 1H), 3.40–3.33 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.34, 156.88, 140.75, 140.45, 140.04, 135.32, 135.01, 129.92, 128.74, 128.73, 128.36, 127.24, 127.03, 126.90, 126.80, 115.65, 77.42, 38.42; HRMS (ESI-TOF) m/z Calcd for $C_{27}H_{21}O_3$ $[M-H]^-$ 393.1496, found: 393.1504.



15'

(*S*)-2-([1,1'-Biphenyl]-4-yloxy)-3-phenylpropanoic acid[41]

8.0 mg (13%), white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53–7.25 (m, 12H), 6.91 (d, J = 8.8 Hz, 2H), 4.89 (t, J = 6.4 Hz, 1H), 3.35–3.26 (m, 2H).

3. References

[1] a) Amani, K.; Zolfigol, M. A.; Ghorbani-Choghamarani, A.; Hajjami, M. *Monatsh Chem.* **2009**, *140*, 65. b) Berger, F.; Plutschack, M.B.; Riegger, J.; Yu, W.; Speicher, S.; Ho, M.; Frank, N,; Ritter, T. *Nature* **2019,** *567,* 223.

[2] Chakraborti, A. K.; Sharma, L.; Gulhane, R.; Shivani. *Tetrahedron.* **2003**, 59, 7661.

[3] Klumpp, D. A.; Garza, M.; Jones, A.; Mendoza, S. *J. Org. Chem.* **1999**, *64*, 6702.

[4] Grasa, G. A.; Hillier, A. C.; Nolan, S. P. *Org. Lett.* **2001**, *3*, 1077.

[5] Guan, Z.-H.; Hu, J.-L.; Gu, Y.-L.; Zhang, H.-J.; Li, G.-X.; Li, T. *Green Chem*. **2012**, *14*, 1964.

[6] Kuriyama, M.; Shimazawa, R.; Shirai, R. Tetrahedron **2007**, *63*, 9393.

[7] Song, H.-J,; Jiang, W.-T.; Zhou, Q.-L.; Xu, M.-Y.; Xiao, B. *ACS Catal.* **2018**, *8*, 9287.

[8] Hatakeyama, T.; Nakamura, M. *J. Am. Chem. Soc.* **2007**, *129*, 9844.

[9] Iwai, T.; Tanaka, R.; Harada, T.; Sawamura, M. *Chem. Eur. J.* **2014**, *20*, 1057.

[10] So, C. M.; Lau, C. P.; Kwong, F. Y. *Org. Lett*. **2007**, *9*, 2795.

[11] Tang, J.; Biafora, A,; Goossen, L. J. *Angew. Chem. Int. Ed.* **2015**, *54*, 13130.

[12] Jin, M.-J.; Taher, A.; Kang, H.-J.; Choi, M.; Ryoo, R. *Green Chem.* **2009**, *11*, 309.

[13] Xu, C.-F.; Yin, L.; Huang, B.; Liu, H.-Y.; Cai, M.-Z. *Tetrahedron* **2016**, *72*, 2065.

[14] Wang, J.-Y.; Song, G.-H.; Peng, Y.-Q. *Tetrahedron Lett.* **2011**, *52*, 1477.

[15] Savarin, C.; Liebeskind, L. S. *Org. Lett.* **2001**, *3*, 2149.

[16] Uozumi, Y.; Nakai, Y. *Org. Lett.* **2002**, *4*, 2997.

[17] Dai, J.-J.; Liu, J.-H.; Luo, D.-F.; Liu, L. *Chem. Commun.* **2011**, *47*, 677.

[18] Do, H.-Q.; Daugulis, O. *J. Am. Chem. Soc.* **2008**, *130*, 1128.

[19] Nanayakkara, P.; Alper, H. *Adv. Synth. Catal*. **2006**, *348*, 545.

[20] Chen, X.; Zhou, L.-M.; Li, Y.-M.; Xie, T.; Zhou, S.-L. *J. Org. Chem.* **2014**, *79*, 230.

[21] Yang, D.-J.; Zhu, Y.-F.; Yang, N.; Jiang, Q.-Q.; Liu, R.-H. *Adv. Synth. Catal*. **2016**, *358*, 1731.

[22] Pschierer, J.; Plenio, H. *Eur. J. Org. Chem*. **2010**, 2934

[23] Nishimura, M.; Ueda, M.; Miyaura, N. *Tetrahedron* **2002**, *58*, 5779.

[24] McLaughlin, M. G.; McAdam, C. A.; Cook, M. J. *Org. Lett.* **2015**, *17*, 10.

[25] Huang, Z.-Z.; Tang, Y. *J. Org. Chem*. **2002**, *67*, 5320.

[26] Barluenga, J.; Moriel, P.; Valdes, C.; Aznar, F. *Angew. Chem. Int. Ed.*, **2007**, *46*, 5587.

[27] Liu, N.; Wang, Z.-X. *J. Org. Chem*., **2011**, *76*, 10031.

[28] Shirakawa, E.; Watabe, R.; Murakami, T.; Hayashi, T. *Chem. Commun.* **2013**, *49*, 5219.

[29] Vilums, M.; Zweemer, A. J. M.; Dekkers, S.; Askar, Y.; de Vries, H.; Saunders, J.; Stamos, D.; Brussee, J.; Heitman, L. H.; Ijzerman, A. P. *Bioorg. Med. Chem. Lett.* **2014**, *24*, 5377.

[30] Zhao, R.; Feng, G.-D.; Xin, X.-D.; Guan, H.-H.; Hua, J.; Wan, R.-Z.; Li, W.; Liu, L. *Chin. Chem. Lett.* **2019**, *30*, 1432.

[31] Larsen, U. S.; Martiny, L.; Begtrup, M. *Tetrahedron Lett.* **2005,** *46***,** 4261.

[32] Zhao, G.-K.; Yuan, L.-Z.; Alami, M.; Provot, O. *Adv. Synth. Catal*. **2018**, *360*, 2522.

[33] Qiu, D.; Meng, H.; Jin, L.; Wang, S.; Tang, S.; Wang, X.; Mo, F.; Zhang, Y.; Wang, J. *Angew. Chem., Int. Ed.* **2013**, *52*, 11581.

[34] Keaveney, S. T.; Kundu, G.; Schoenebeck, F. *Angew. Chem., Int. Ed*. **2018**, *57*, 12573.

[35] Wang, J.-K.; Zong, Y.-X.; Wang, X.-C.; Hu, Y.-L.; Yue, G.-R.; Pan, Y. *Green Chem*. **2016**, *18*, 967.

[36] Moriconi, A.; Cesta, M. C.; Cervellera, M. N.; Aramini, A.; Coniglio, S.; Colagioia, S.; Beccari, A. R.; Bizzarri, C.; Cavicchia, M. R.; Locati, M.; Galliera, E.; Di Benedetto, P.; Vigilante, P.; Bertini, R.; Allegretti,

M. *J. Med. Chem*. **2007**, *50*, 3984.

[37] He, Z.-T.; Hartwig, J. F. *J. Am. Chem. Soc.* **2019**, *141*, 11749.

[38] He, Z.; Song, F.; Sun, H.; Huang, Y., *J. Am. Chem. Soc.* **2018**, *140*, 2693.

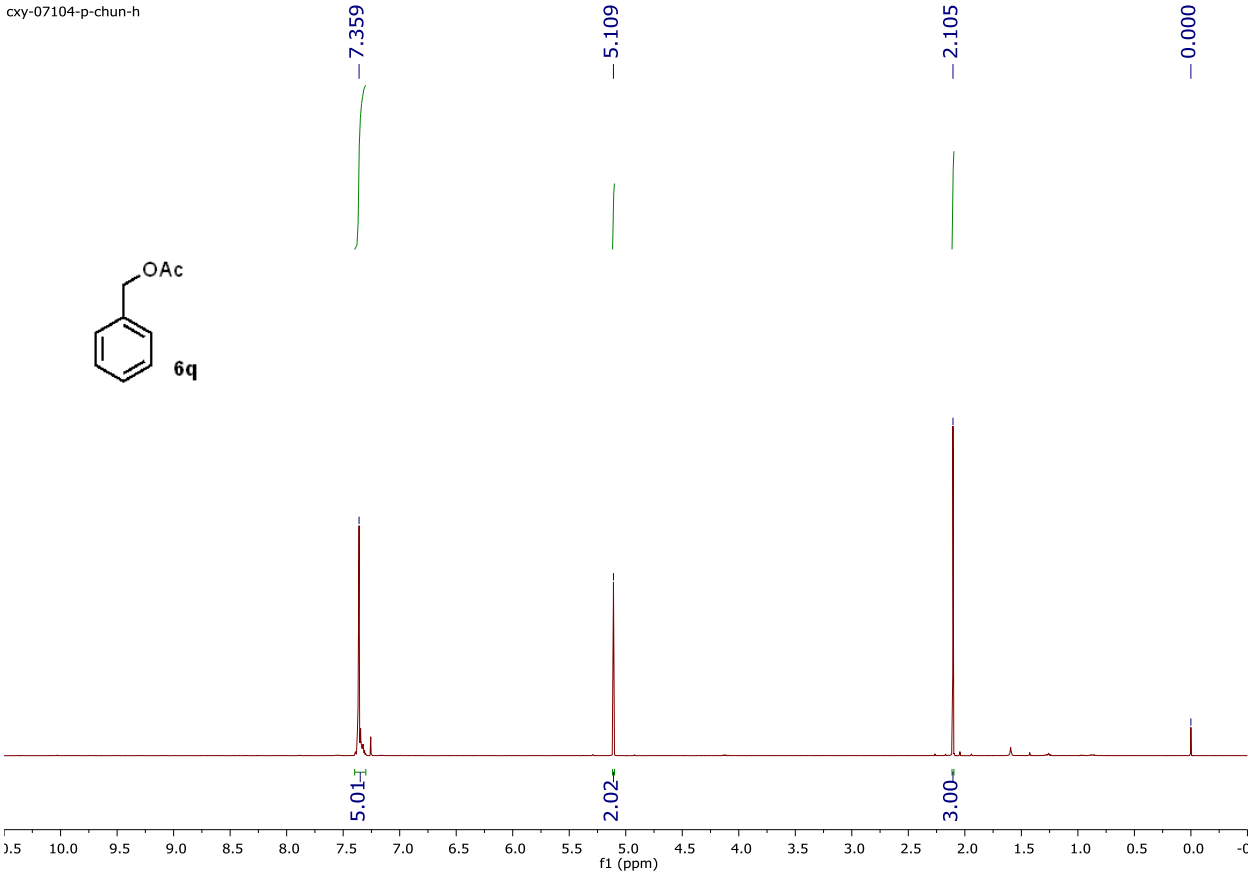
[39] Cuevas-Yañez, E.; Serrano, J. M.; Huerta, G.; Muchowski, J. M.; Cruz-Almanza, R., *Tetrahedron* **2004**, *60*, 9391.

[40] Laghezza, A.; Piemontese, L.; Cerchia, C.; Montanari, R.; Capelli, D.; Giudici, M.; Crestani, M.; Tortorella, P.; Peiretti, F.; Pochetti, G.; Lavecchia, A.; Loiodice, F. *J. Med. Chem*. **2018**, *61*, 8282.

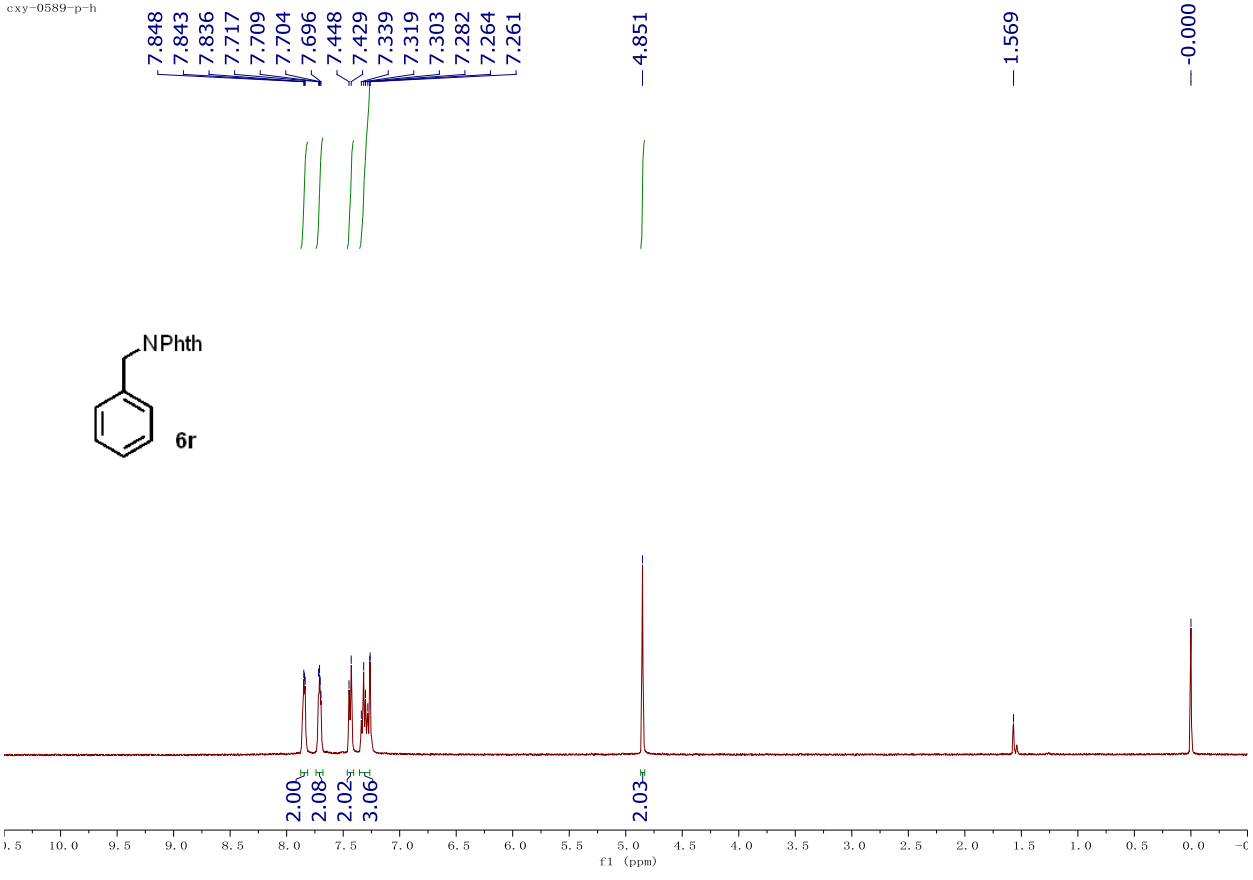
[41] Montanari, R.; Saccoccia, F.; Scotti, E.; Crestani, M.; Godio, C.; Gilardi, F.; Loiodice, F.; Fracchiolla, G.; Laghezza, A.; Tortorella, P.; Lavecchia, A.; Novellino, E.; Mazza, F.; Aschi, M.; Pochetti, G. *J. Med. Chem*. **2008**, *51*, 7768.

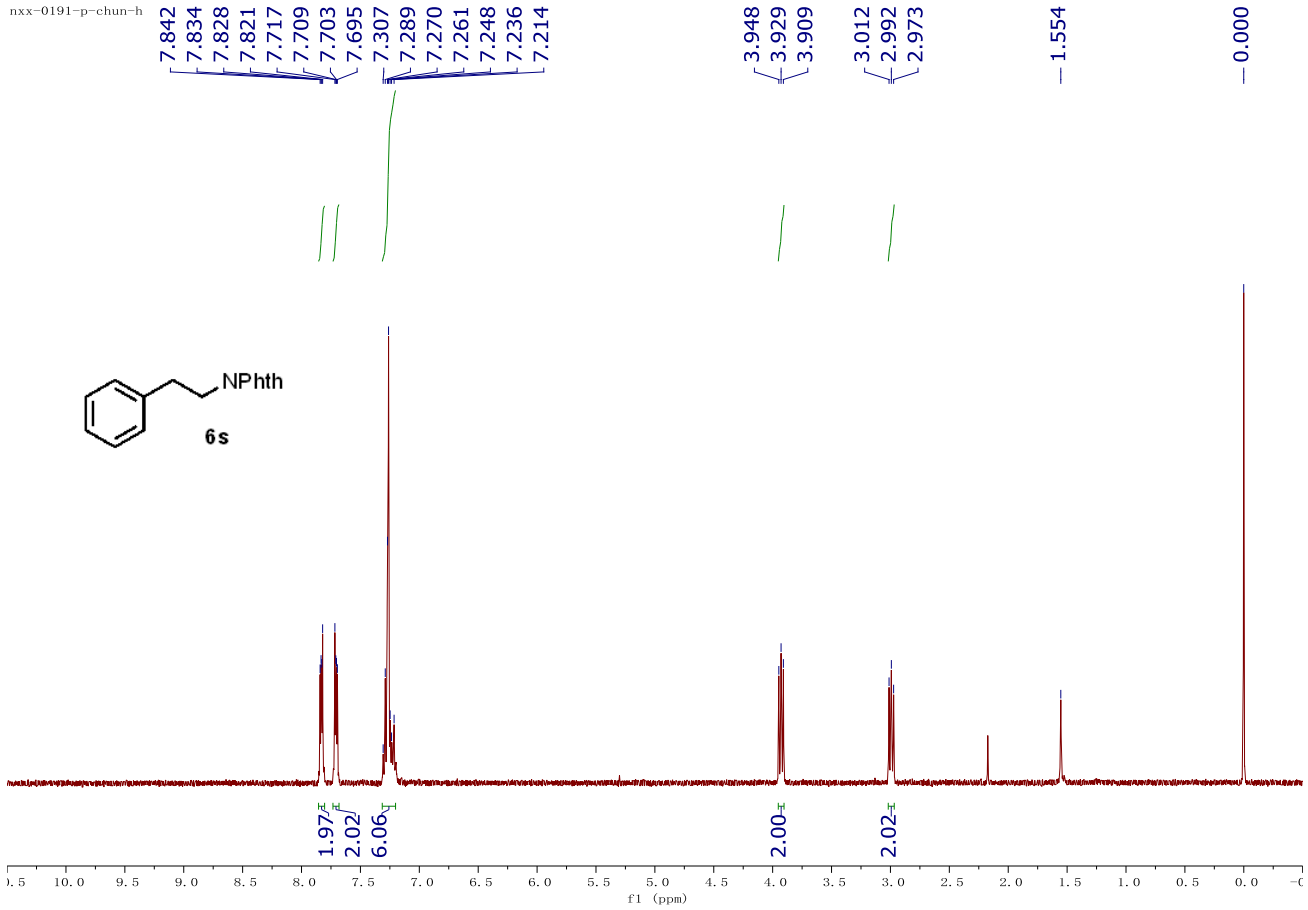
4. NMR Spectra

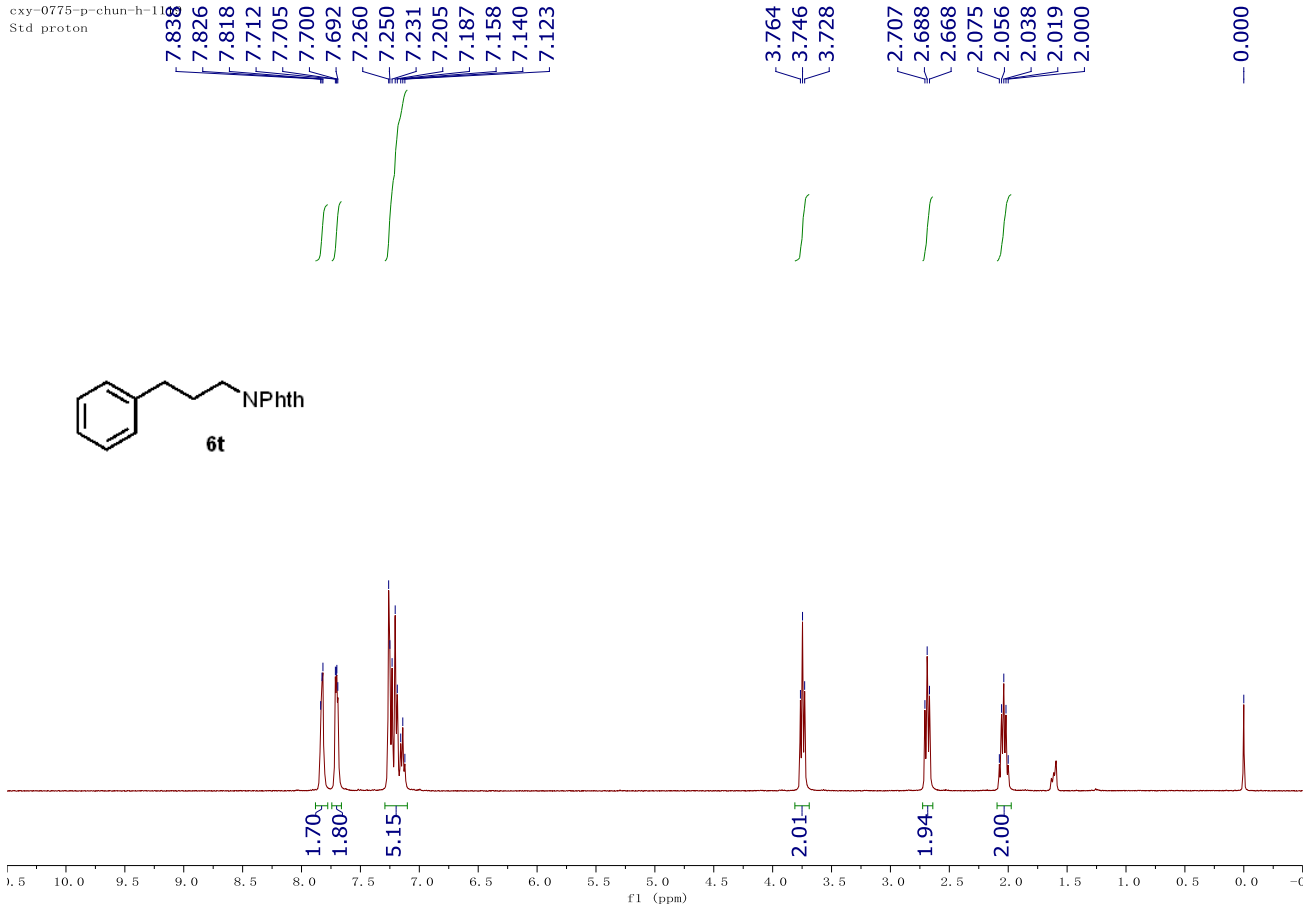
cxy-07104-p-chun-h

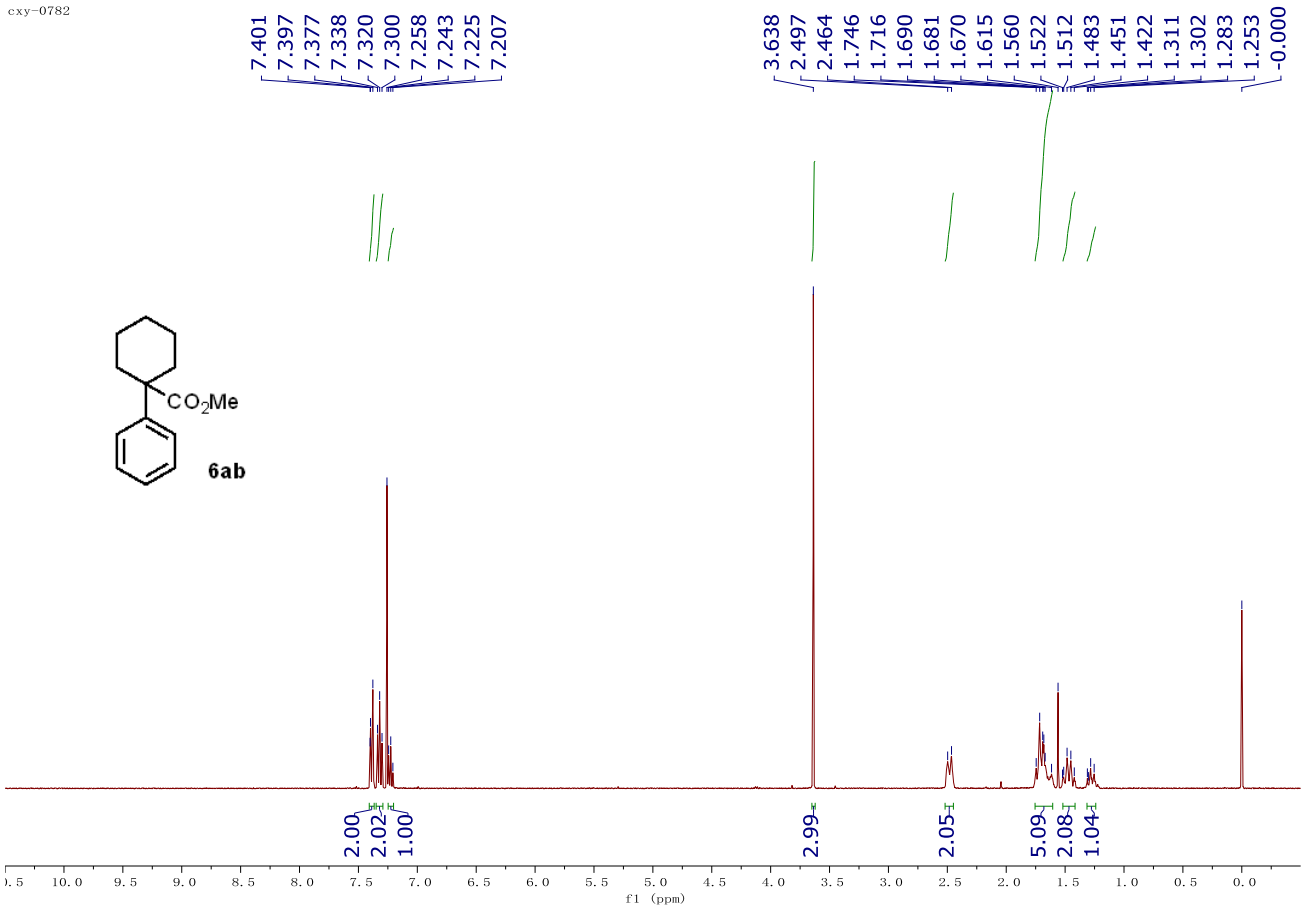


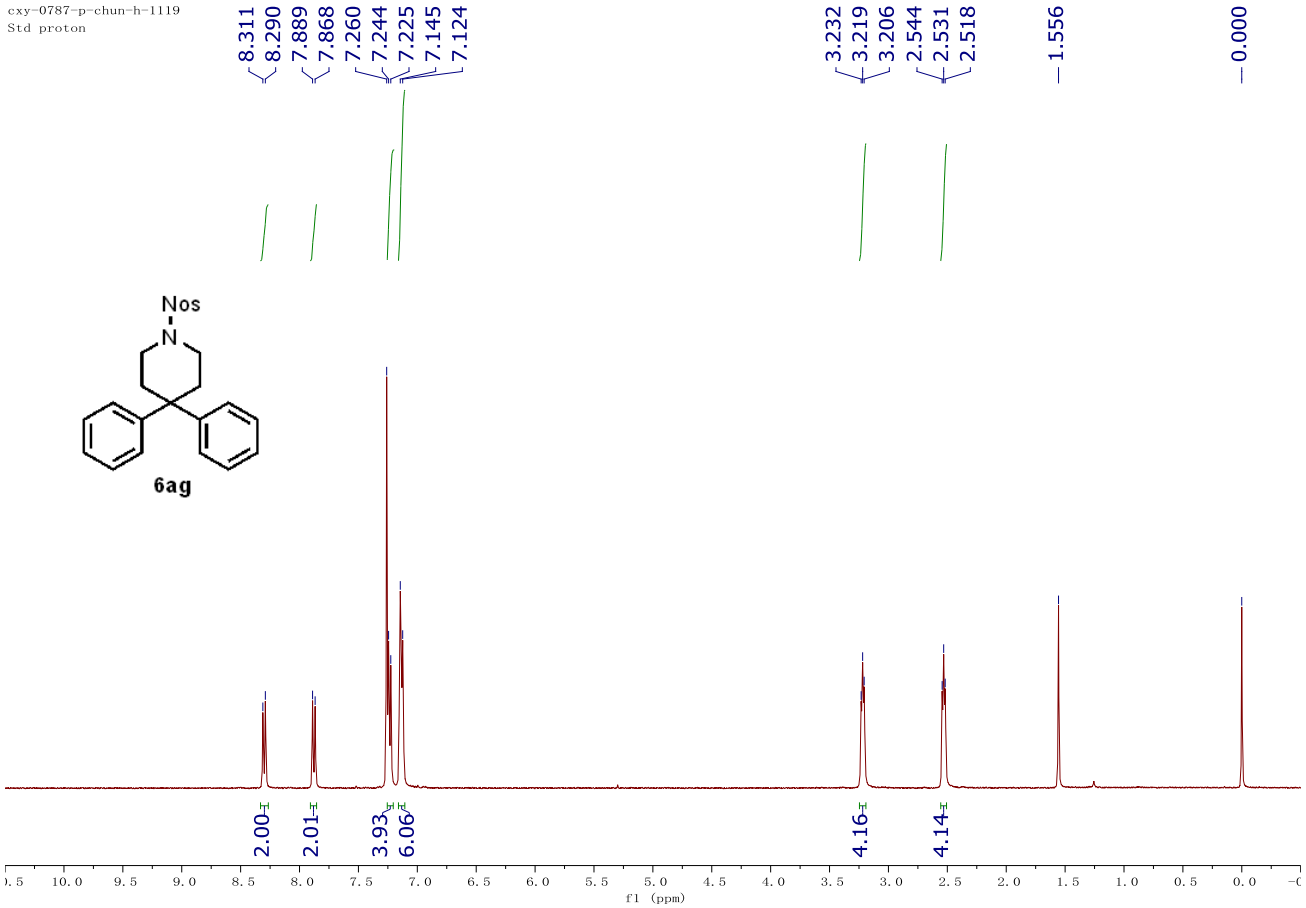
cxy-0589-p-h

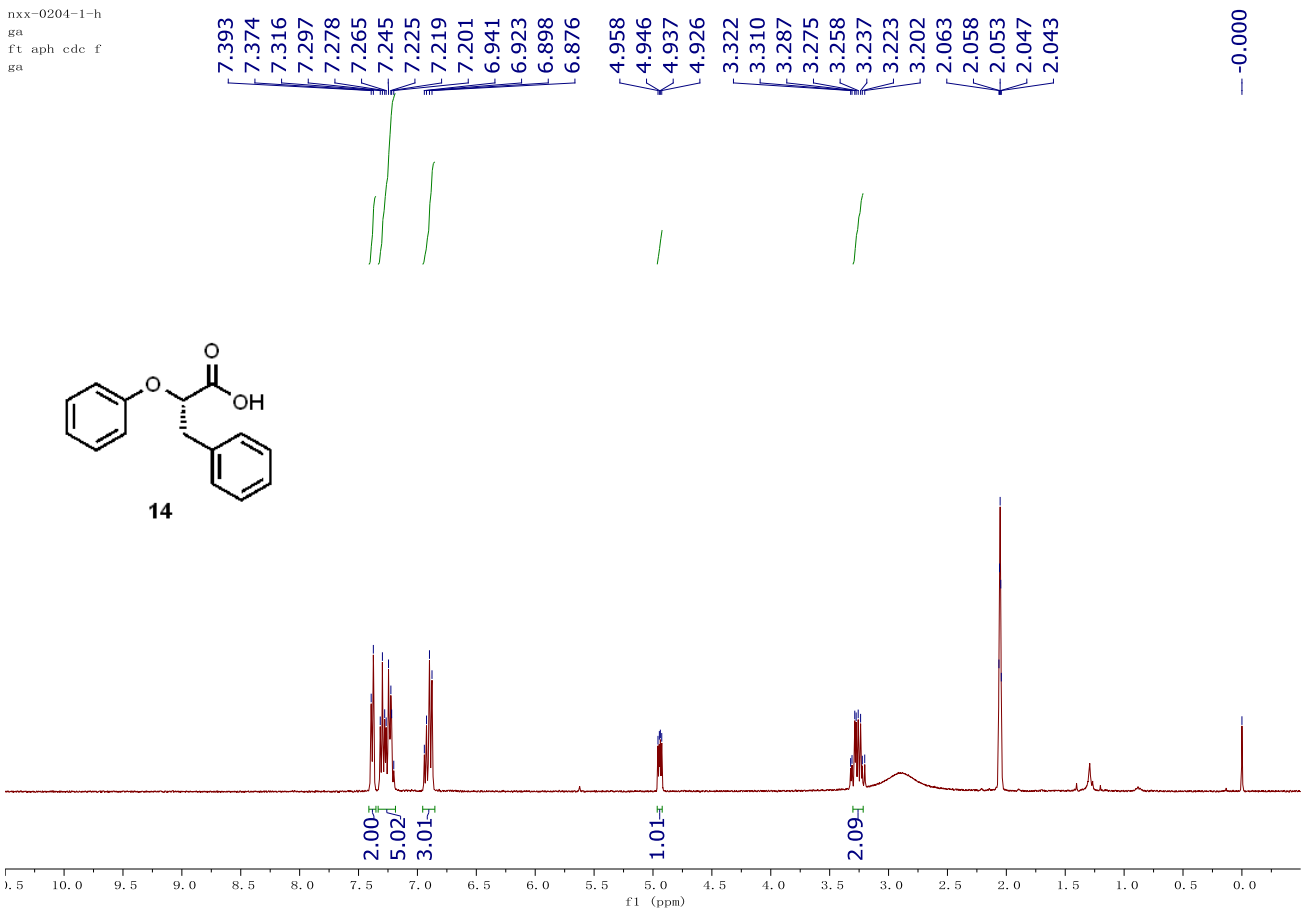


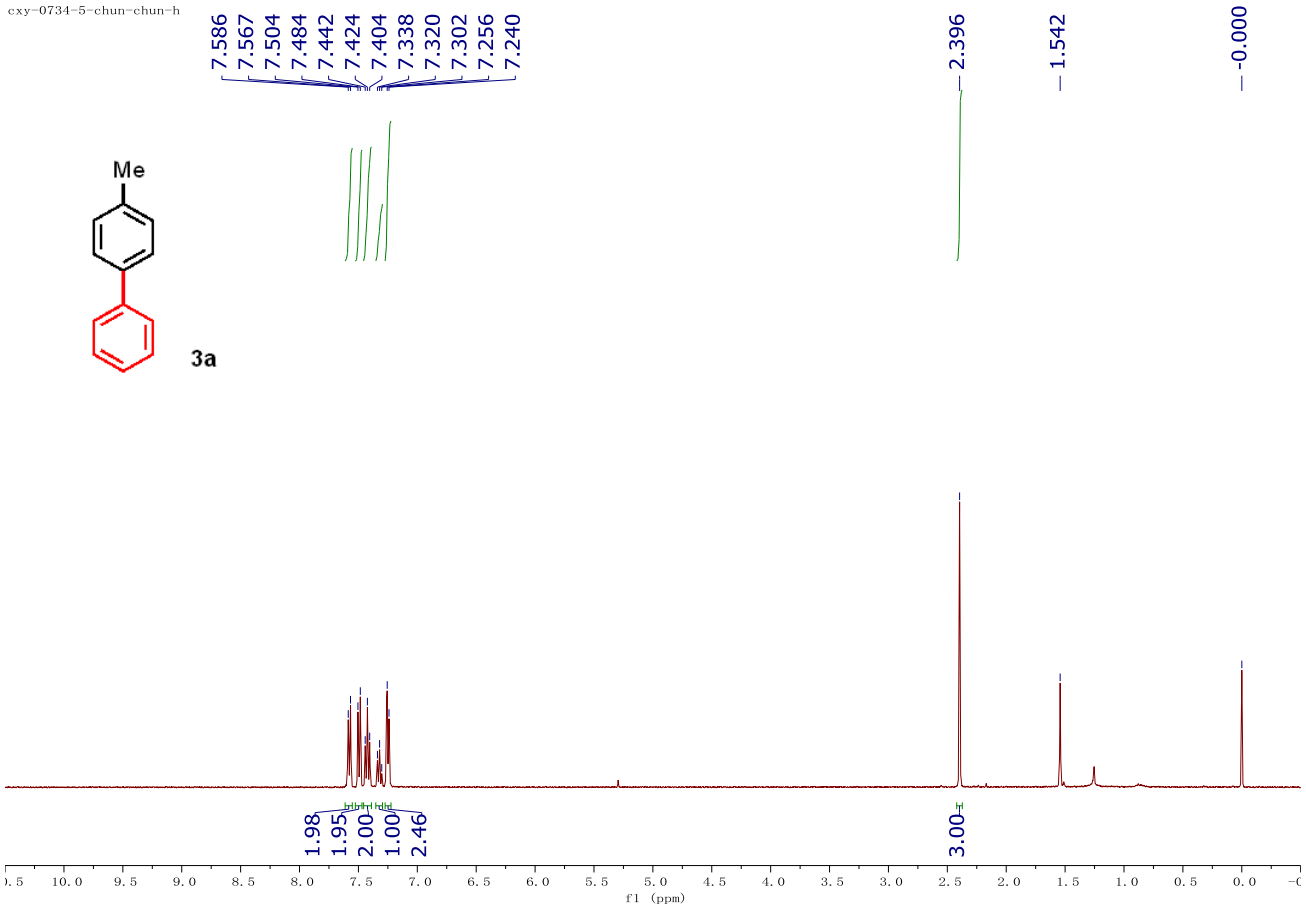

nxx-0191-p-chun-h
7.842
7.834
7.828
7.821
7.717
7.709
7.703
7.695
7.307
7.289
7.270
7.261
7.248
7.236
7.214
3.948
3.929
3.909
3.012
2.992
2.973
1.554
0.000
NPhth
6s
1.97
2.02
6.06
2.00
2.02
f1 (ppm)

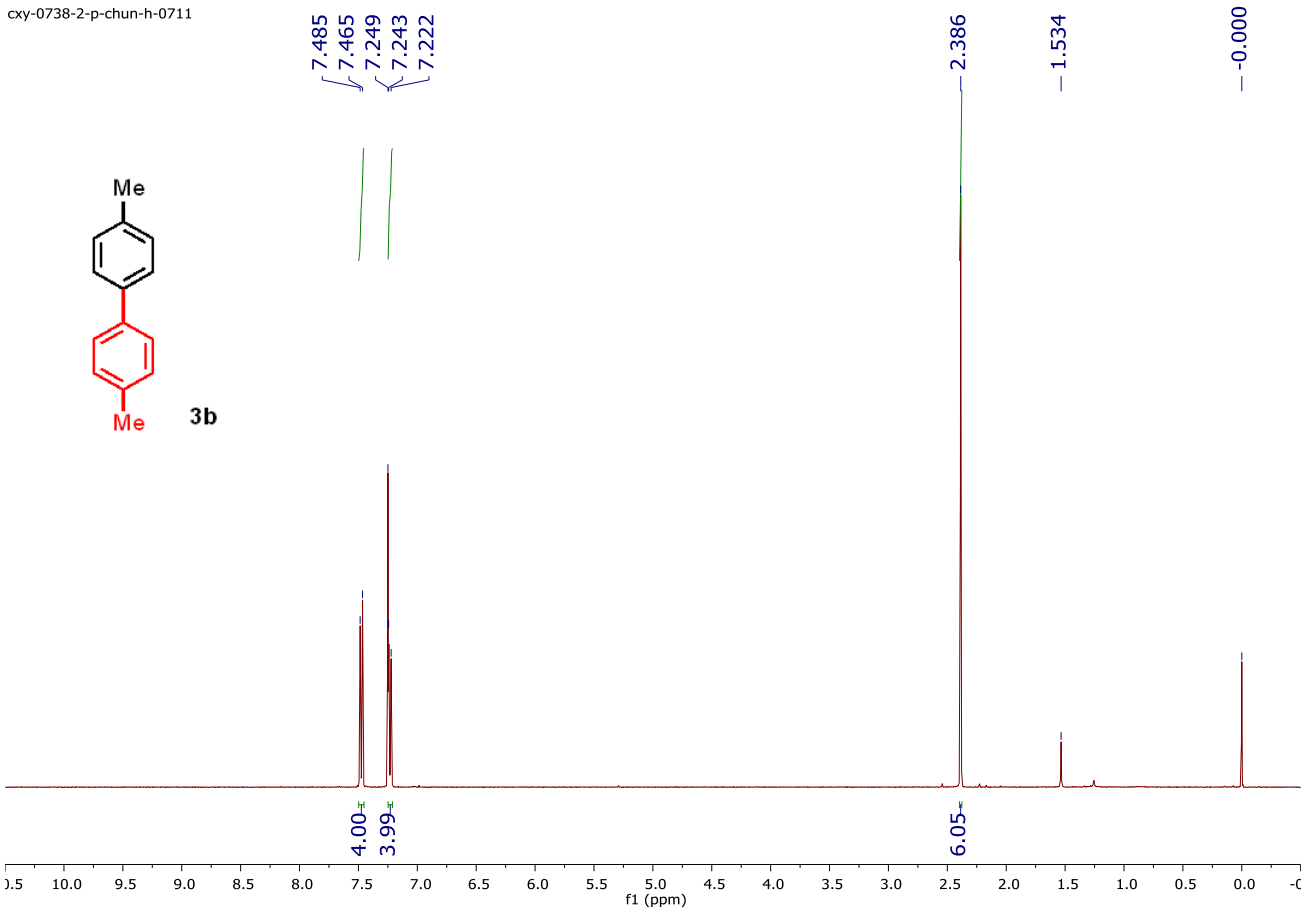

cxy-0775-p-chun-h-1H
Std proton
7.838
7.826
7.818
7.712
7.705
7.700
7.692
7.260
7.250
7.231
7.205
7.187
7.158
7.140
7.123
3.764
3.746
3.728
2.707
2.688
2.668
2.075
2.056
2.038
2.019
2.000
0.000
NPhth
6t
1.70
1.80
5.15
2.01
1.94
2.00
f1 (ppm)

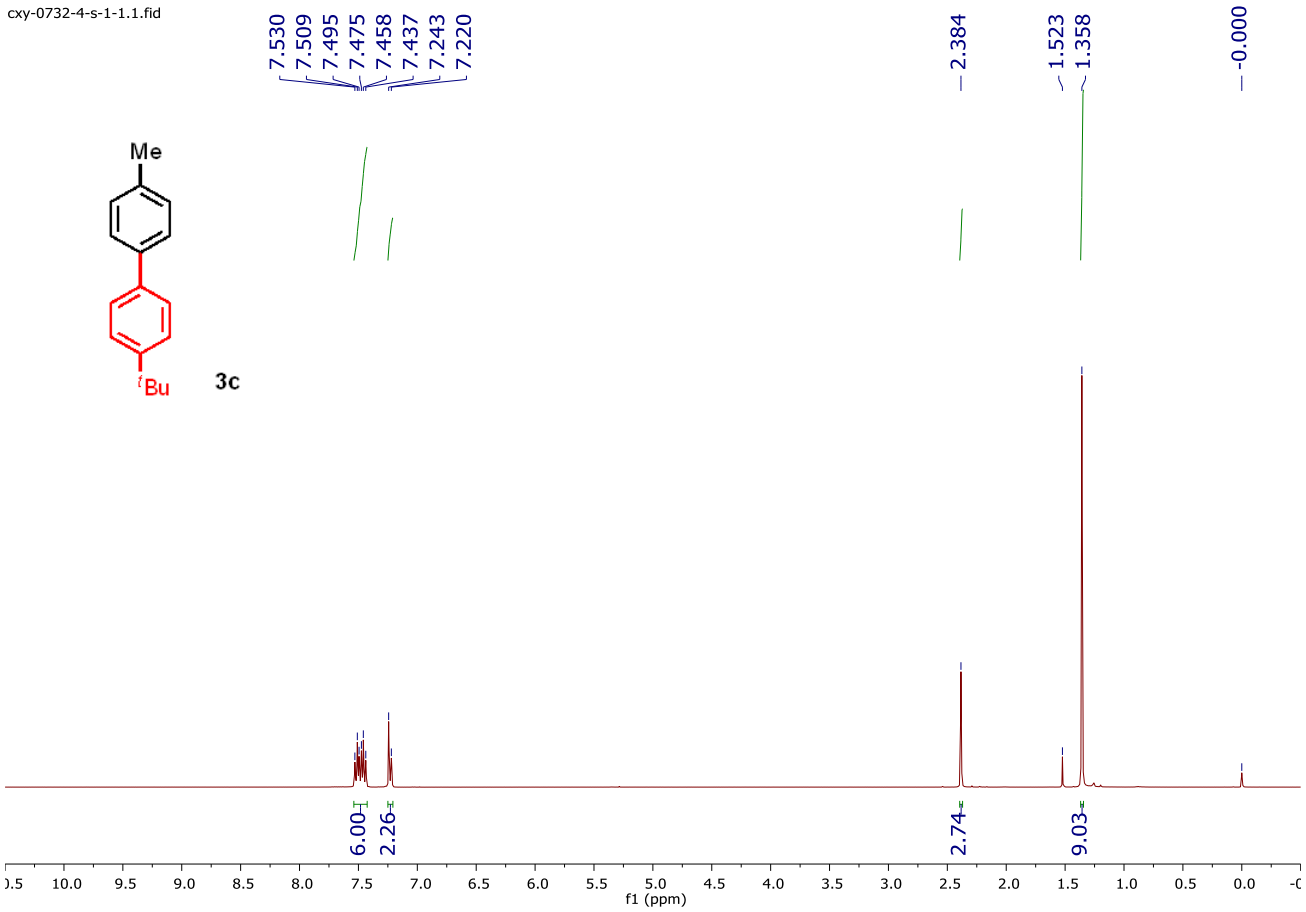

cxy-0782
7.401
7.397
7.377
7.338
7.320
7.300
7.258
7.243
7.225
7.207
3.638
2.497
2.464
1.746
1.716
1.690
1.681
1.670
1.615
1.560
1.522
1.512
1.483
1.451
1.422
1.311
1.302
1.283
1.253
-0.000
CO2Me
6ab
2.00
2.02
1.00
2.99
2.05
5.09
2.08
1.04
f1 (ppm)

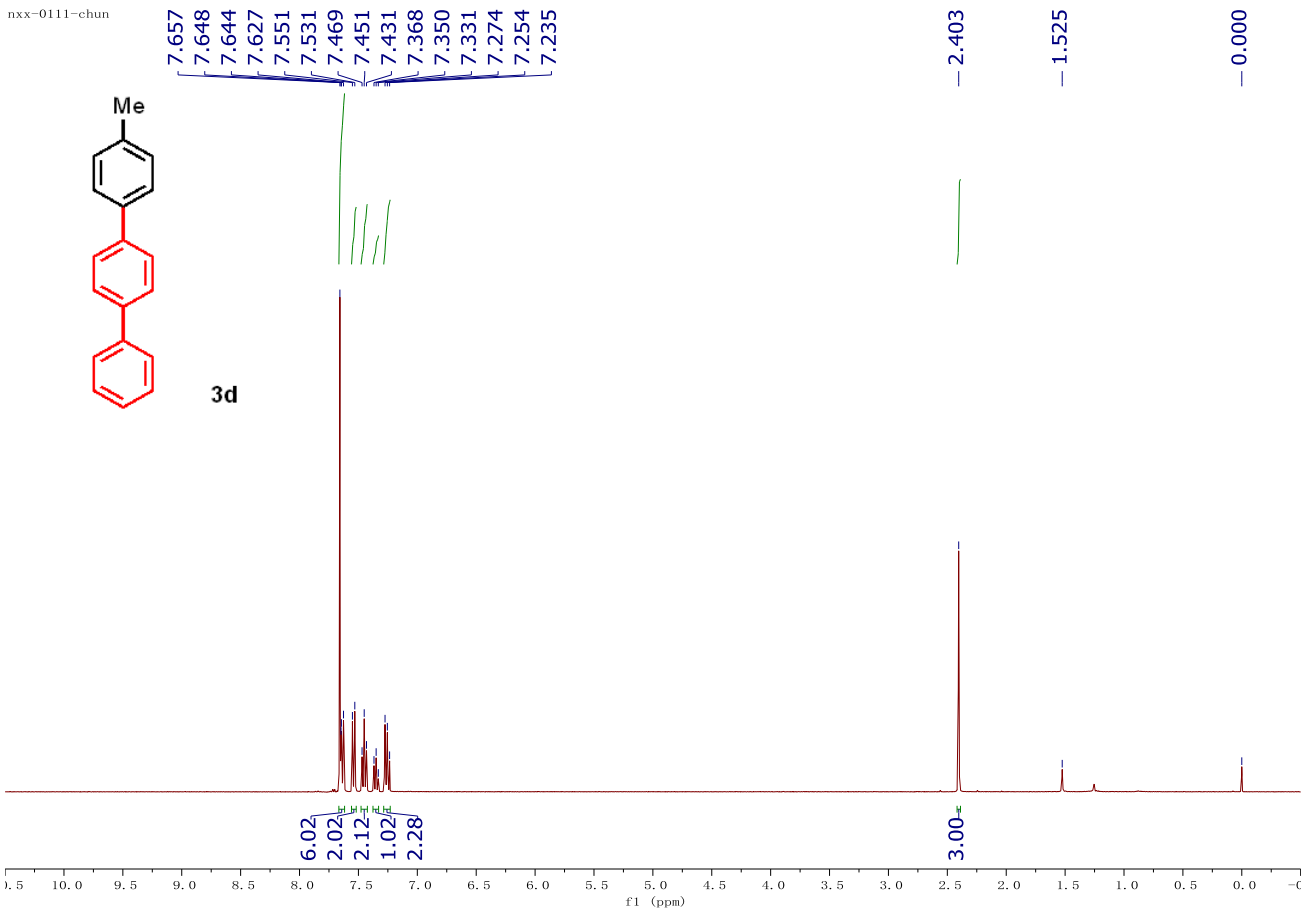

cxy-0787-p-chun-h-1119
Std proton
8.311
8.290
7.889
7.868
7.260
7.244
7.225
7.145
7.124
3.232
3.219
3.206
2.544
2.531
2.518
1.556
0.000
Nos
N
6ag
2.00
2.01
3.93
6.06
4.16
4.14
f1 (ppm)

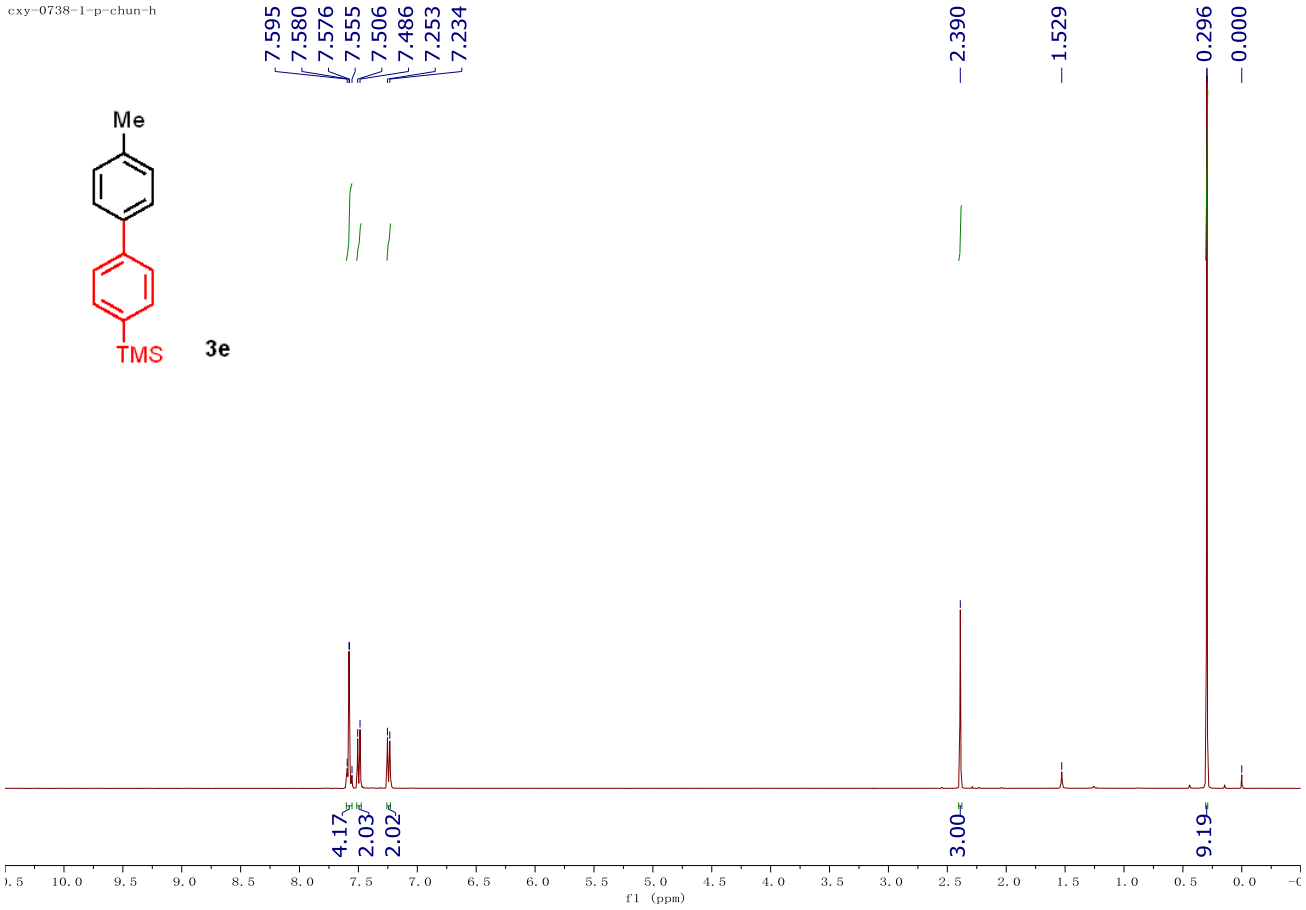

nxx-0204-1-h
ga
ft aph cdc f
ga
7.393
7.374
7.316
7.297
7.278
7.265
7.245
7.225
7.219
7.201
6.941
6.923
6.898
6.876
4.958
4.946
4.937
4.926
3.322
3.310
3.287
3.275
3.258
3.237
3.223
3.202
2.063
2.058
2.053
2.047
2.043
-0.000
O
O
OH
14
2.00
5.02
3.01
1.01
2.09
f1 (ppm)

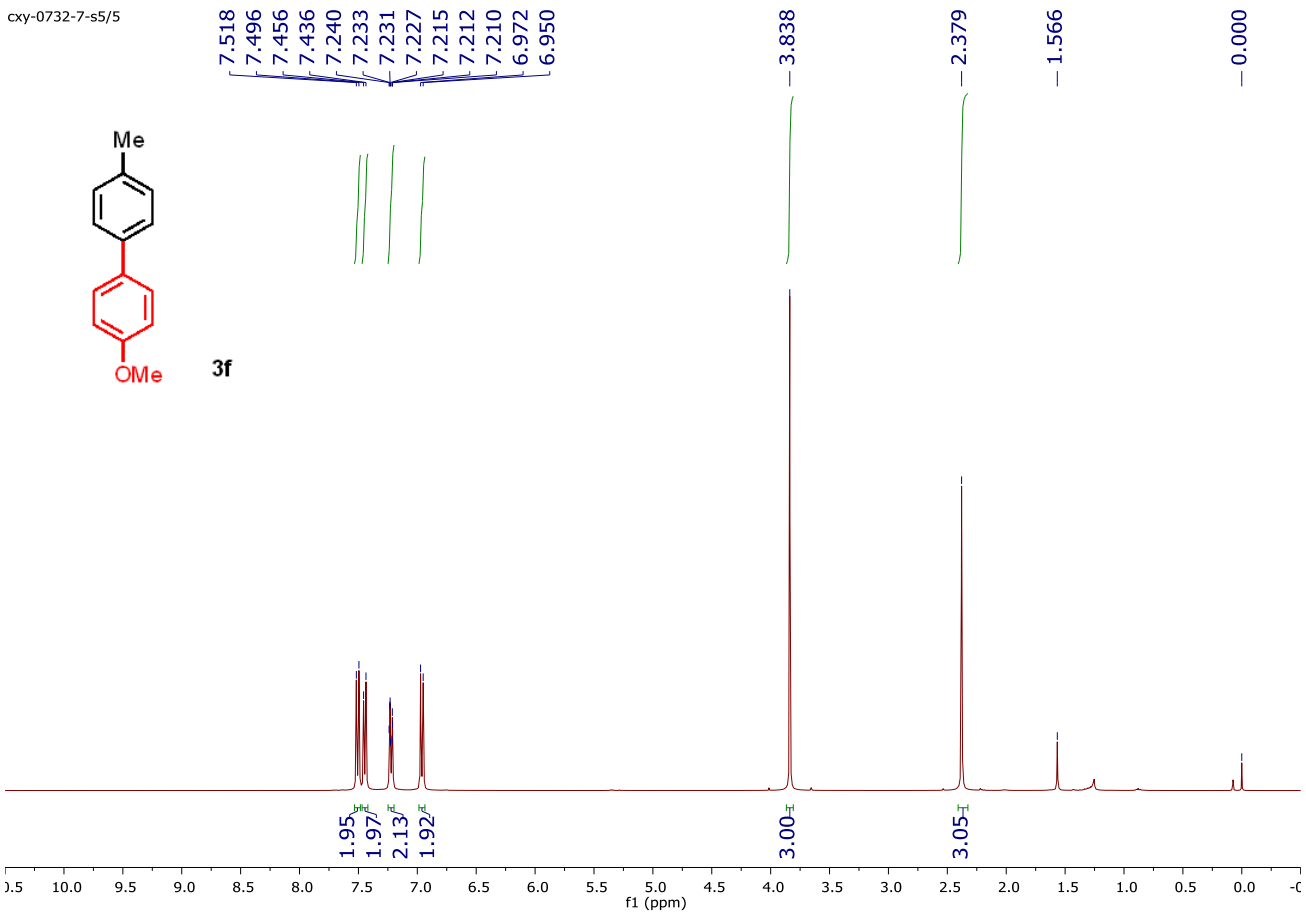

cxy-0734-5-chun-chun-h
7.586
7.567
7.504
7.484
7.442
7.424
7.404
7.338
7.320
7.302
7.256
7.240
2.396
1.542
-0.000
Me
3a
1.98
1.95
2.00
1.00
2.46
3.00
f1 (ppm)

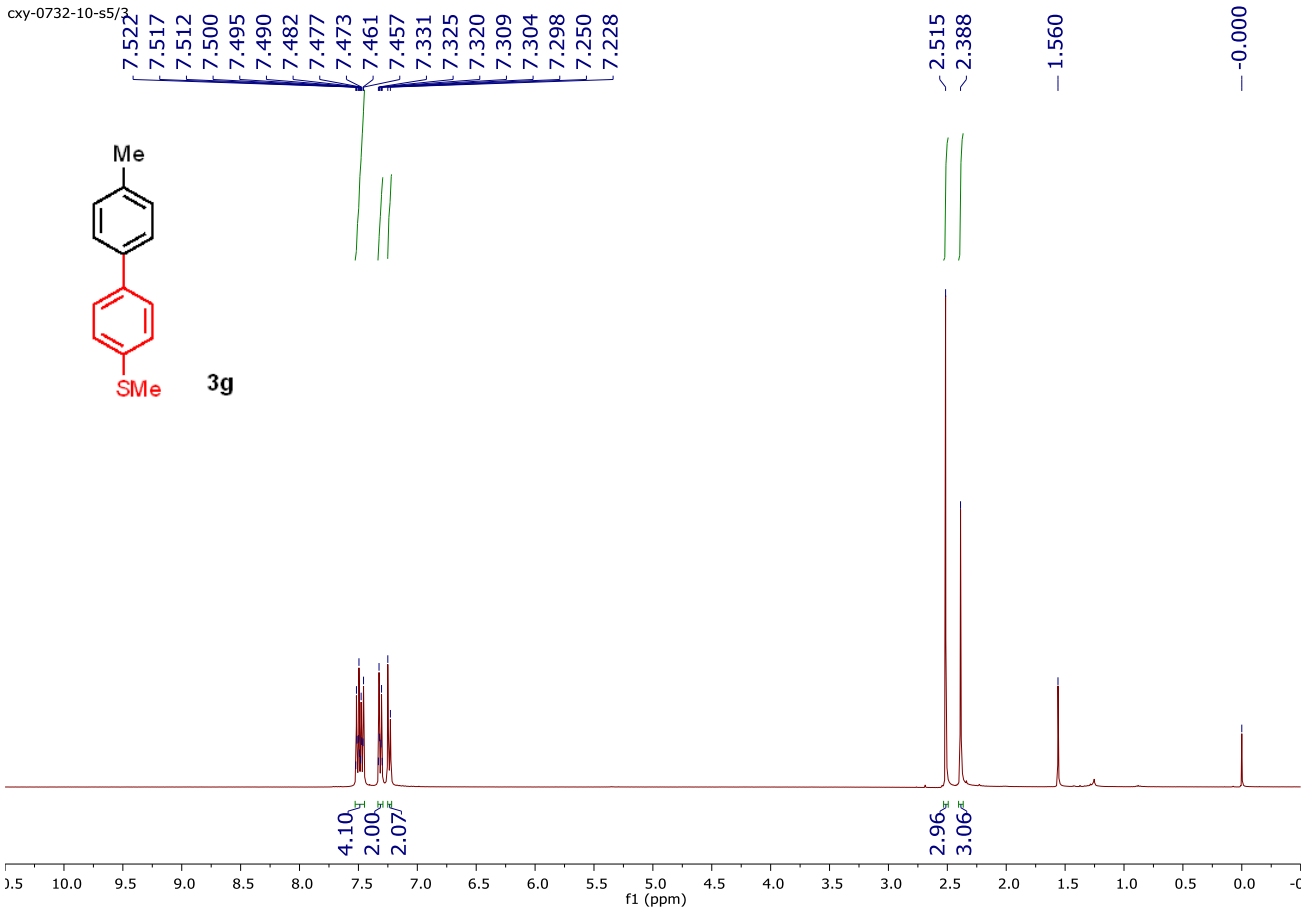

cxy-0738-2-p-chun-h-0711
7.485
7.465
7.249
7.243
7.222
2.386
1.534
-0.000
Me
Me
3b
4.00
3.99
6.05
f1 (ppm)

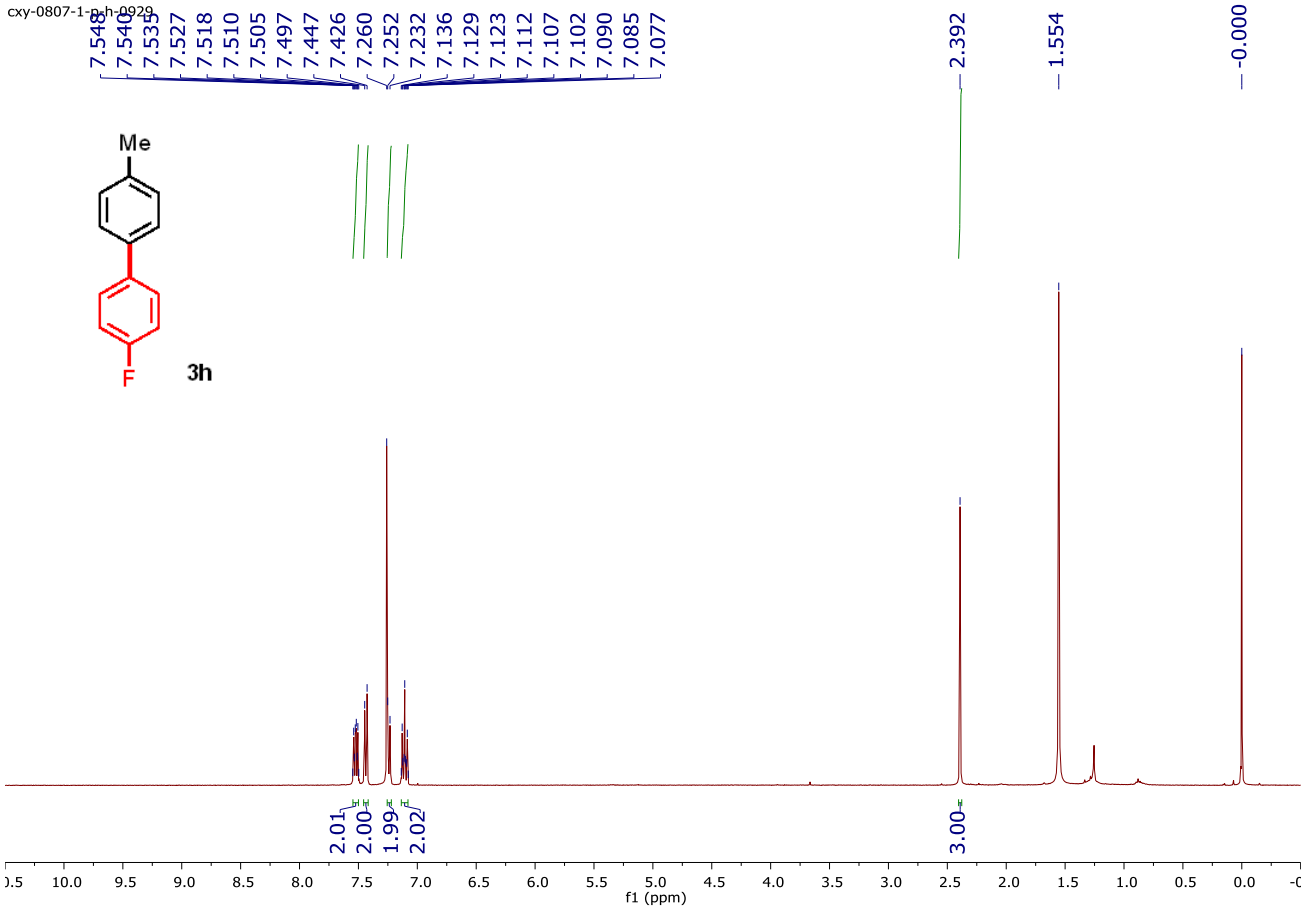

cxy-0732-4-s-1-1.1.fid
7.530
7.509
7.495
7.475
7.458
7.437
7.243
7.220
2.384
1.523
1.358
-0.000
Me
tBu
3c
6.00
2.26
2.74
9.03
f1 (ppm)

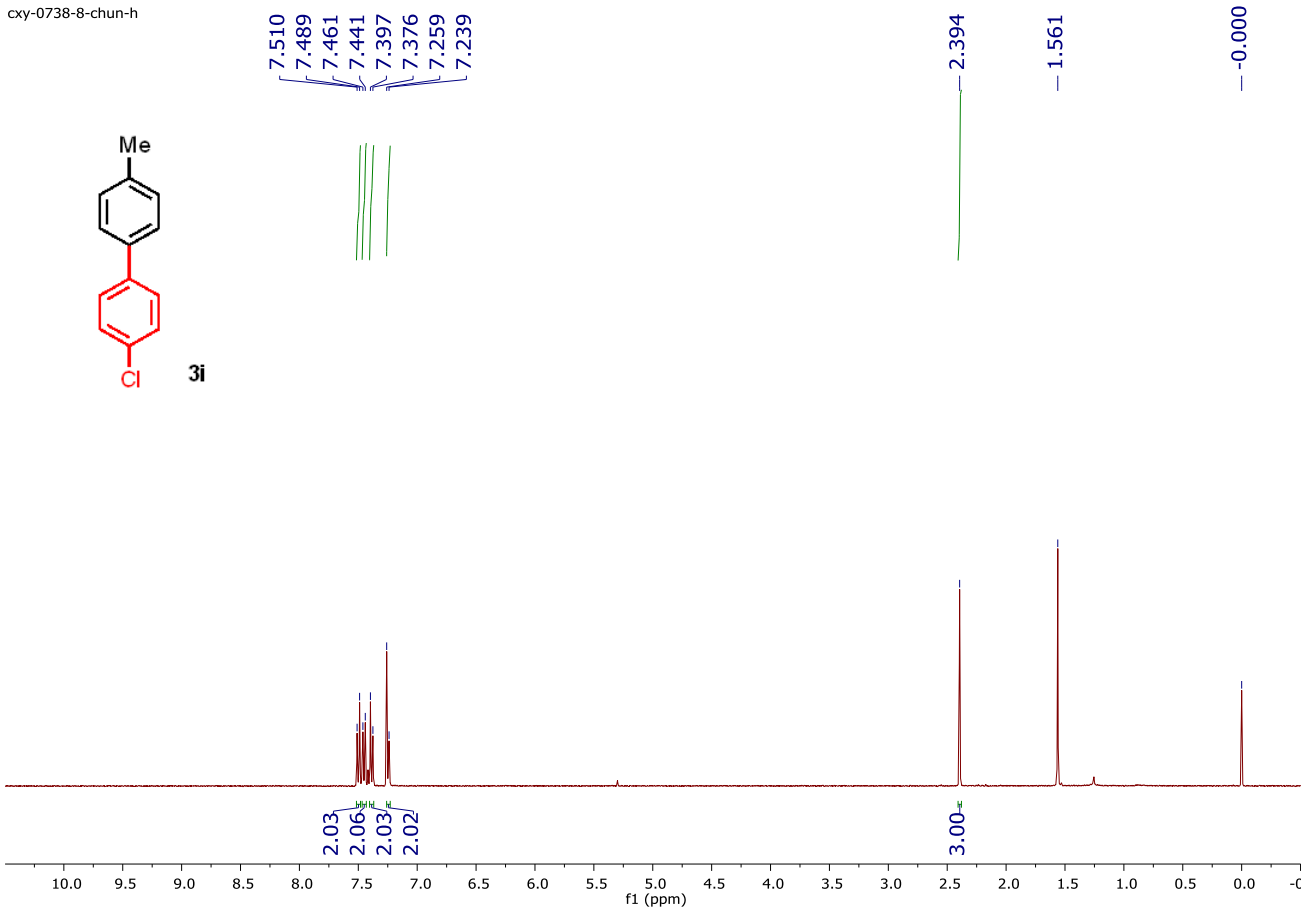

nxx-0111-chun
7.657
7.648
7.644
7.627
7.551
7.531
7.469
7.451
7.431
7.368
7.350
7.331
7.274
7.254
7.235
2.403
1.525
0.000
Me
3d
6.02
2.02
2.12
1.02
2.28
3.00
f1 (ppm)

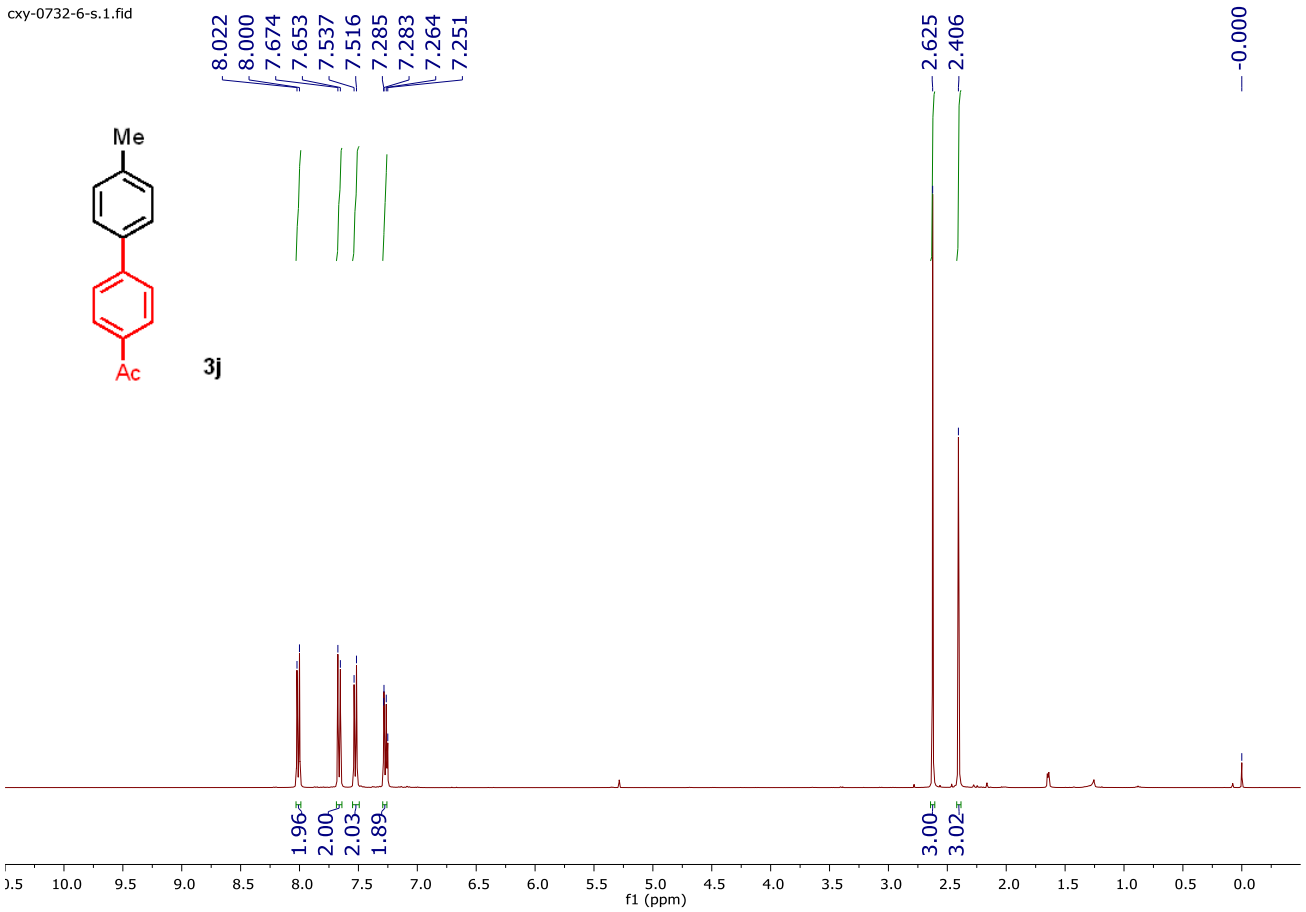

cxy-0738-1-p-chun-h
7.595
7.580
7.576
7.555
7.506
7.486
7.253
7.234
2.390
1.529
0.296
0.000
Me
TMS
3e
4.17
2.03
2.02
3.00
9.19
f1 (ppm)

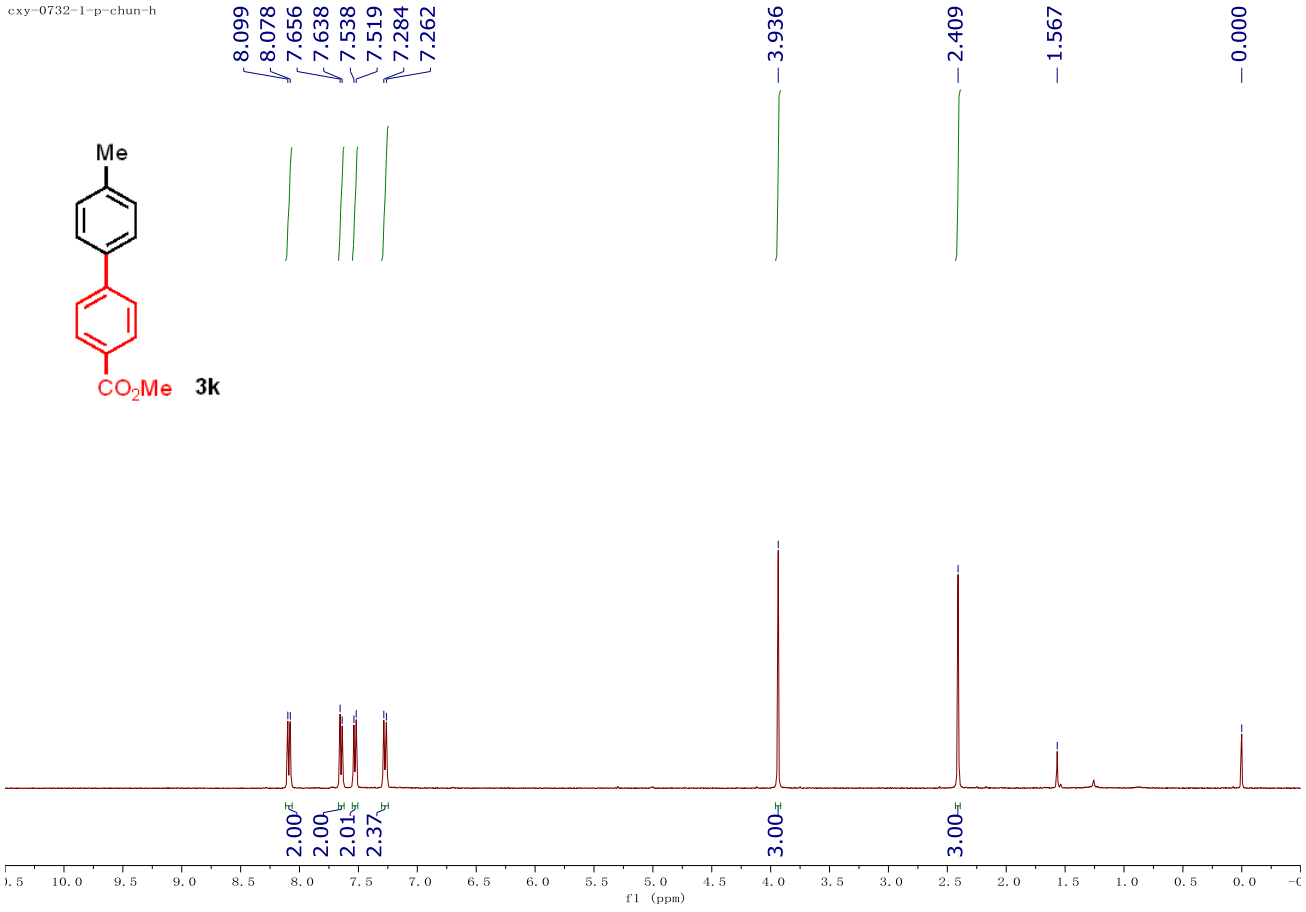

cxy-0732-7-s5/5
7.518
7.496
7.456
7.436
7.240
7.233
7.231
7.227
7.215
7.212
7.210
6.972
6.950
3.838
2.379
1.566
0.000
Me
OMe
3f
1.95
1.97
2.13
1.92
3.00
3.05
f1 (ppm)

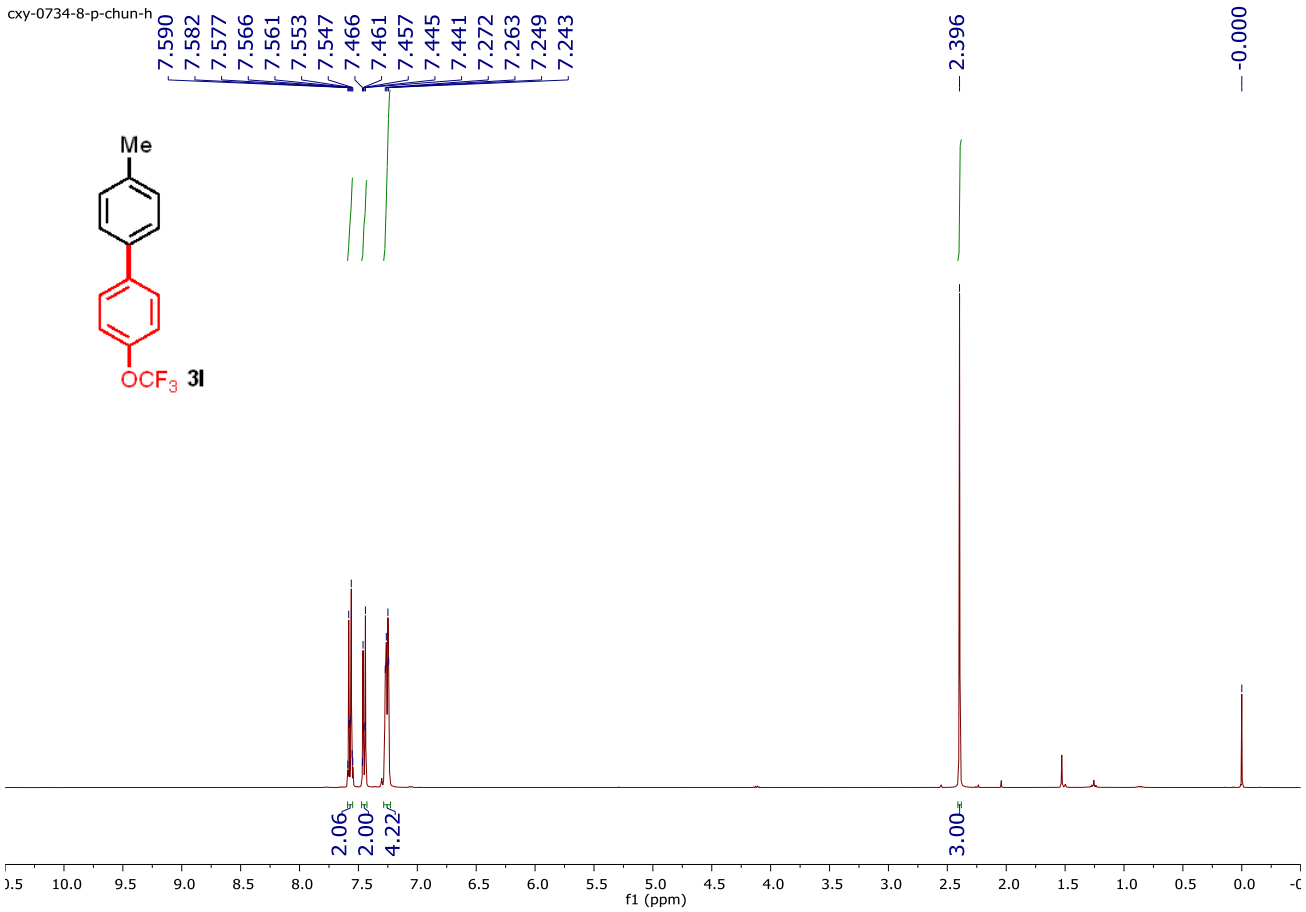

cxy-0732-10-s5/3
7.522
7.517
7.512
7.500
7.495
7.490
7.482
7.477
7.473
7.461
7.457
7.331
7.325
7.320
7.309
7.304
7.298
7.250
7.228
2.515
2.388
1.560
-0.000
Me
SMe
3g
4.10
2.00
2.07
2.96
3.06
f1 (ppm)

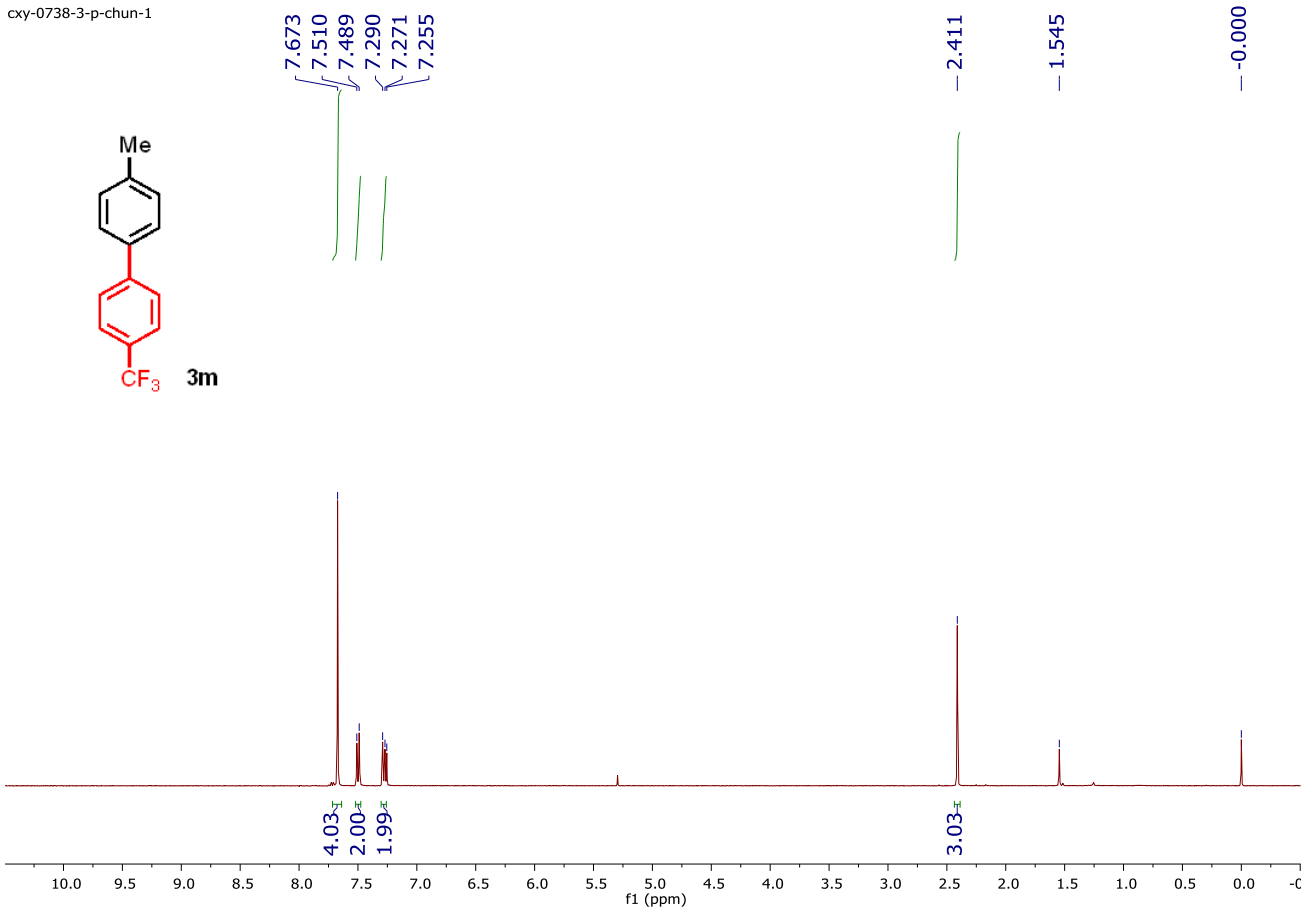

cxy-0807-1-p-h-0929
7.548
7.540
7.535
7.527
7.518
7.510
7.505
7.497
7.447
7.426
7.260
7.252
7.232
7.136
7.129
7.123
7.112
7.107
7.102
7.090
7.085
7.077
2.392
1.554
-0.000
Me
F
3h
2.01
2.00
1.99
2.02
3.00
f1 (ppm)

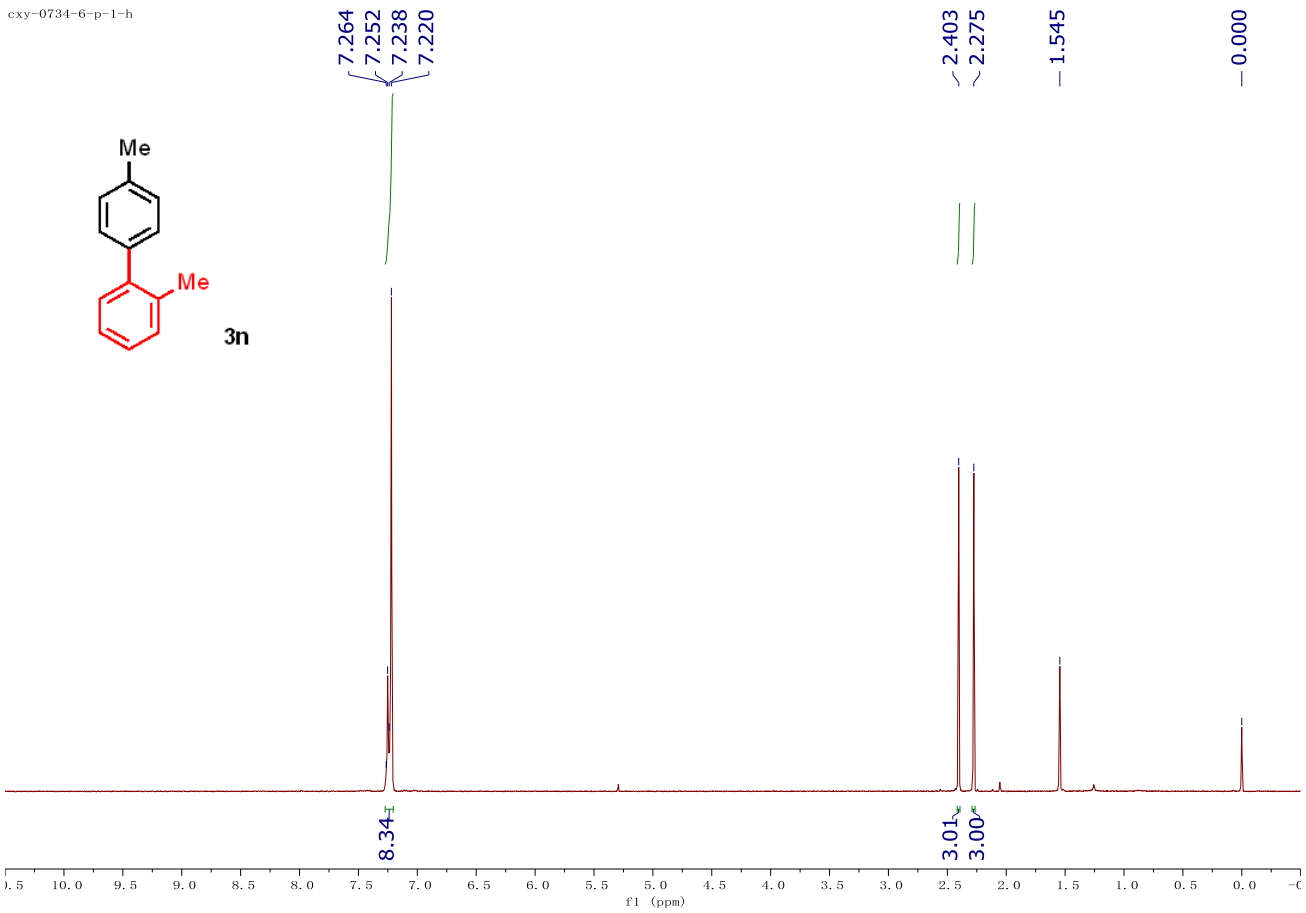

cxy-0738-8-chun-h
7.510
7.489
7.461
7.441
7.397
7.376
7.259
7.239
2.394
1.561
-0.000
Me
Cl
3i
2.03
2.06
2.03
2.02
3.00
f1 (ppm)

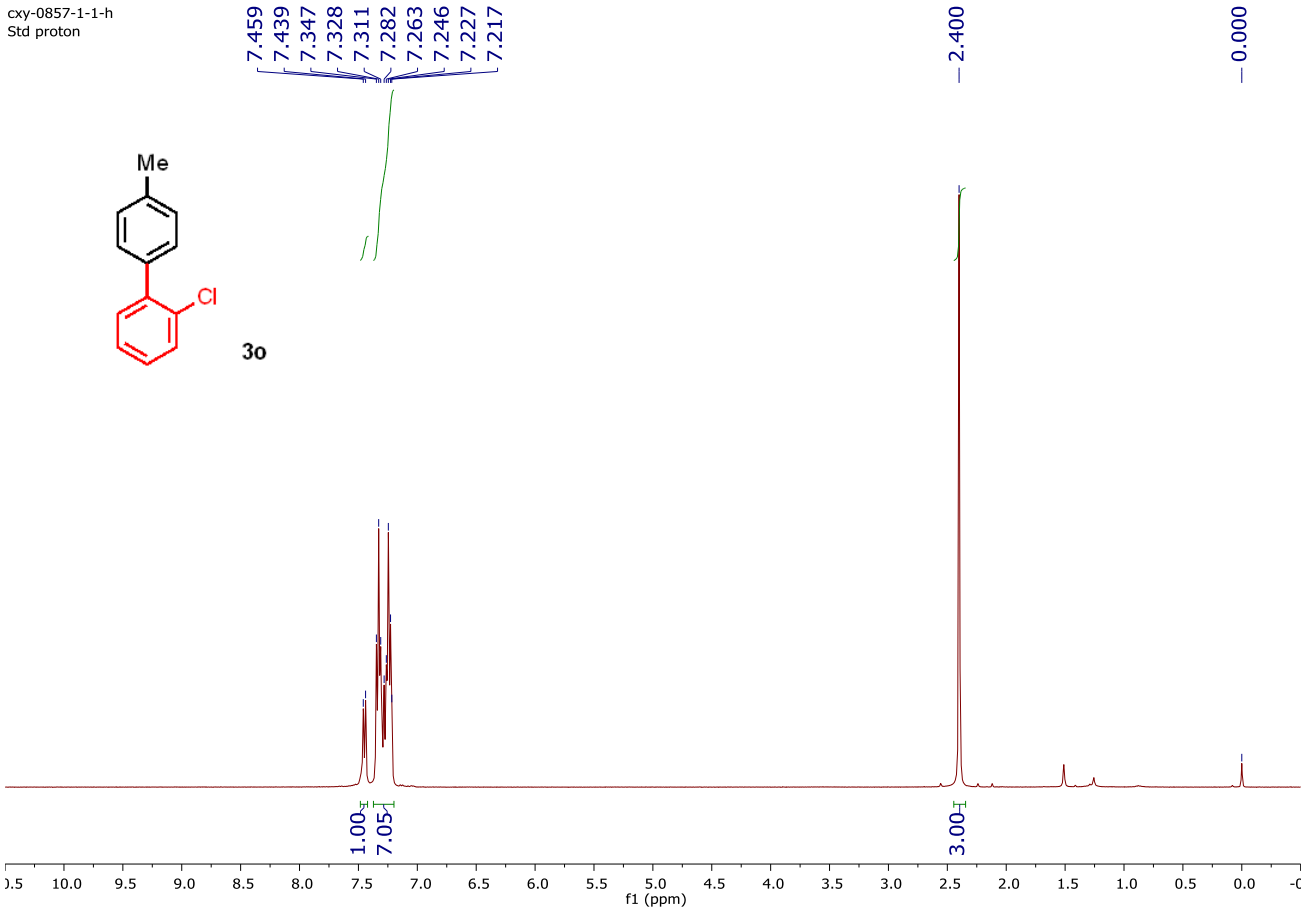

cxy-0732-6-s.1.fid
8.022
8.000
7.674
7.653
7.537
7.516
7.285
7.283
7.264
7.251
2.625
2.406
-0.000
Me
Ac
3j
1.96
2.00
2.03
1.89
3.00
3.02
f1 (ppm)

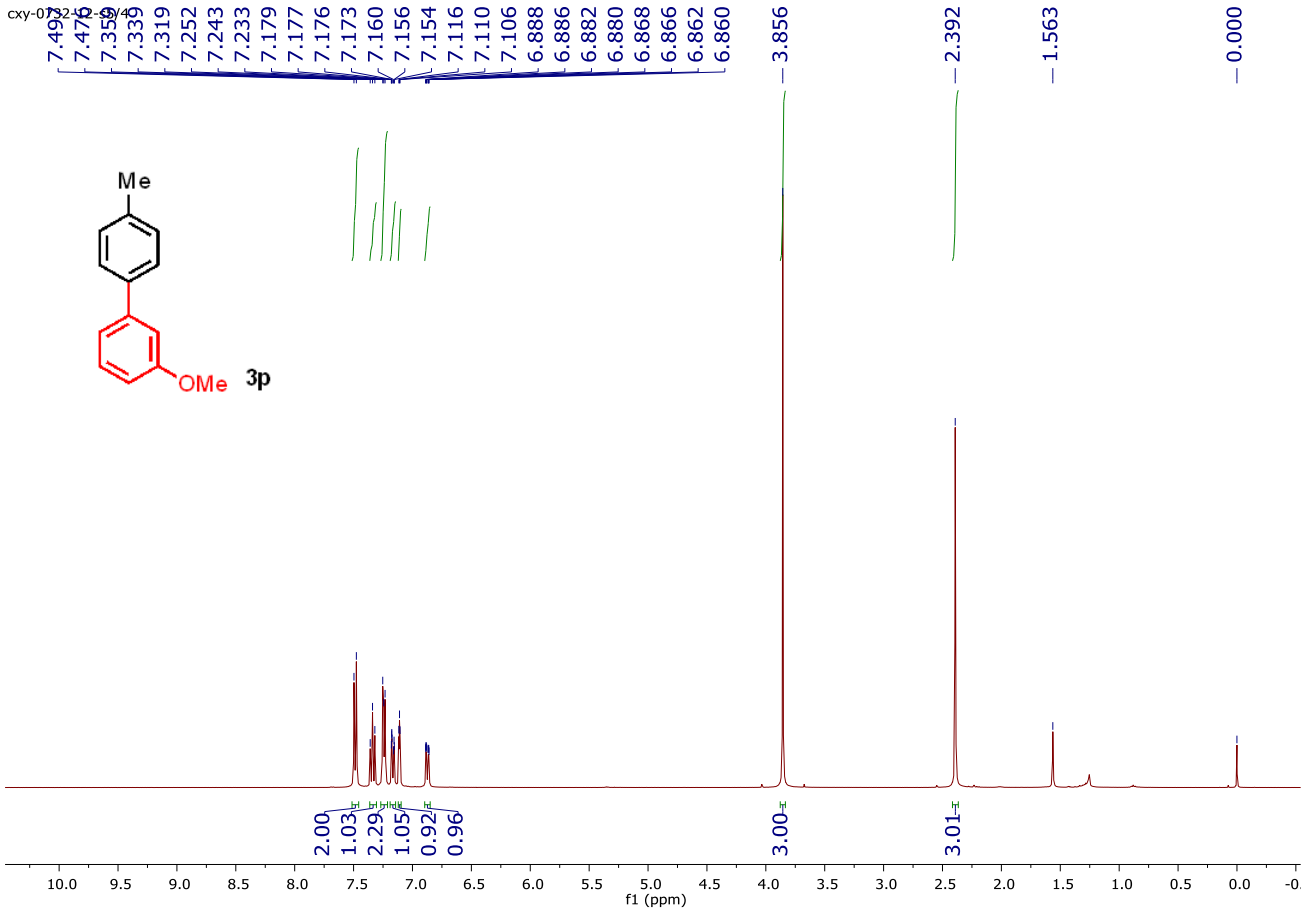

cxy-0732-1-p-chun-h
8.099
8.078
7.656
7.638
7.538
7.519
7.284
7.262
3.936
2.409
1.567
0.000
Me
CO2Me
3k
2.00
2.00
2.01
2.37
3.00
3.00
f1 (ppm)

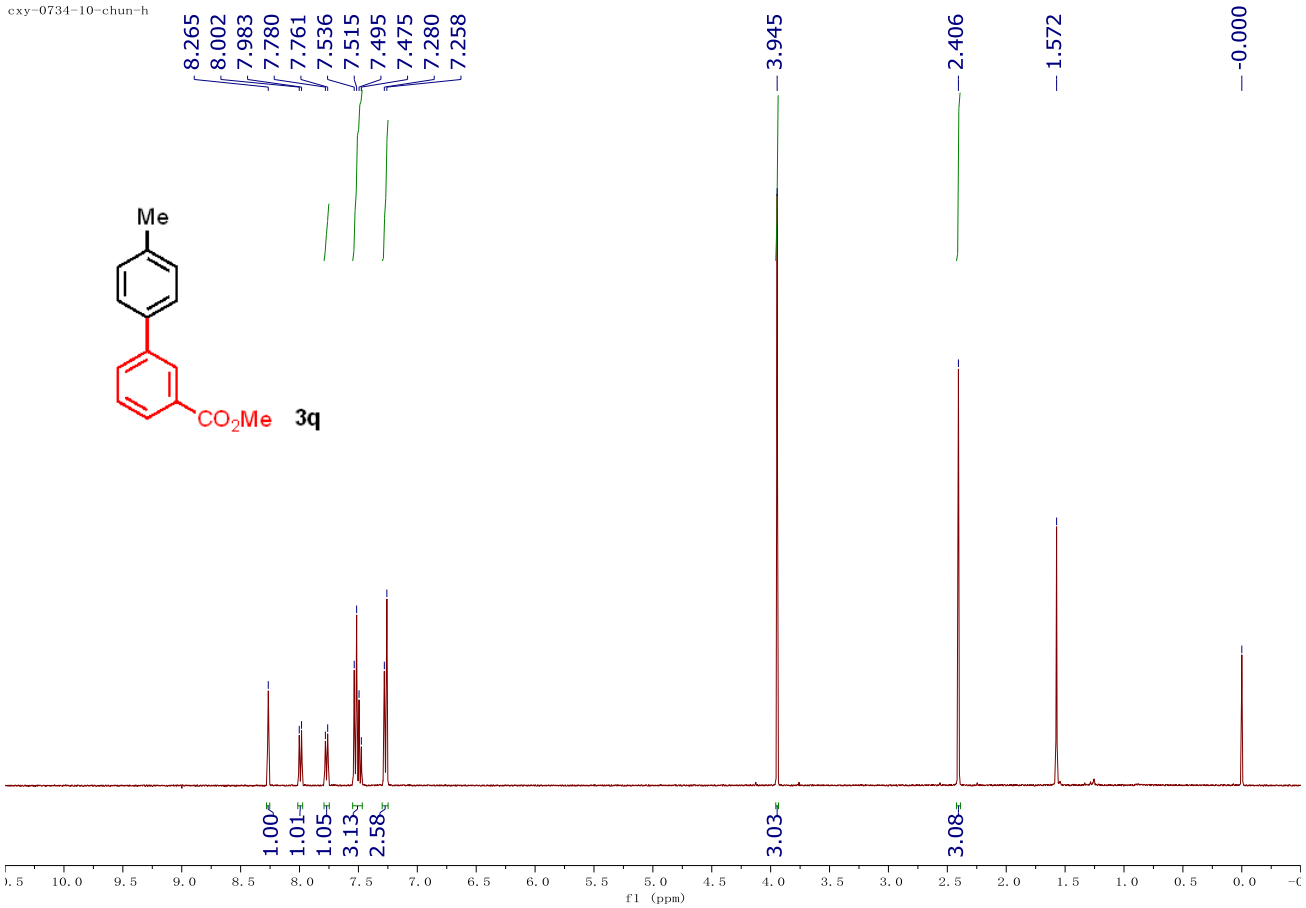

cxy-0734-8-p-chun-h
7.590
7.582
7.577
7.566
7.561
7.553
7.547
7.466
7.461
7.457
7.445
7.441
7.272
7.263
7.249
7.243
2.396
-0.000
Me
OCF3
3l
2.06
2.00
4.22
3.00
f1 (ppm)

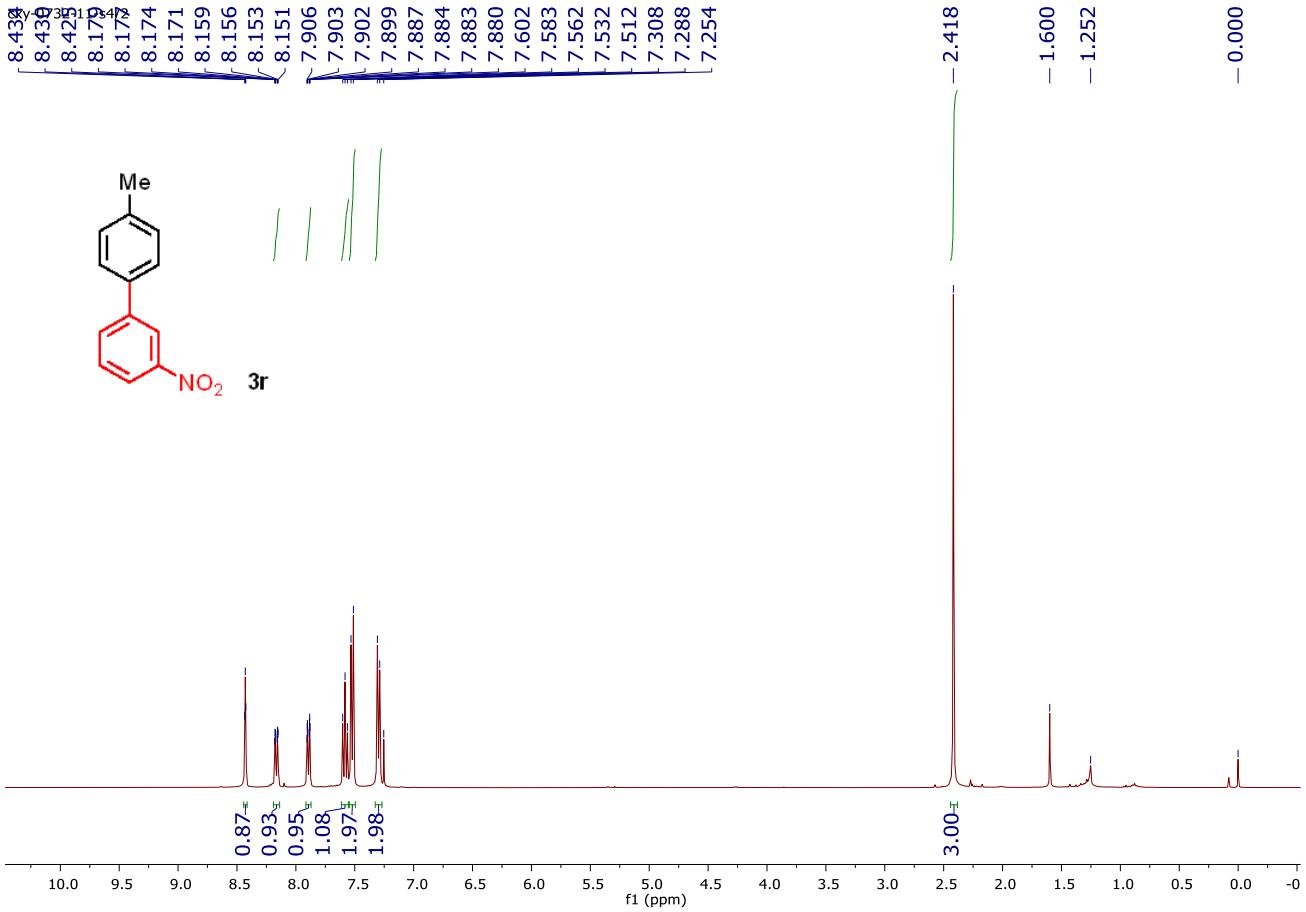

cxy-0738-3-p-chun-1
7.673
7.510
7.489
7.290
7.271
7.255
2.411
1.545
-0.000
Me
CF3
3m
4.03
2.00
1.99
3.03
f1 (ppm)

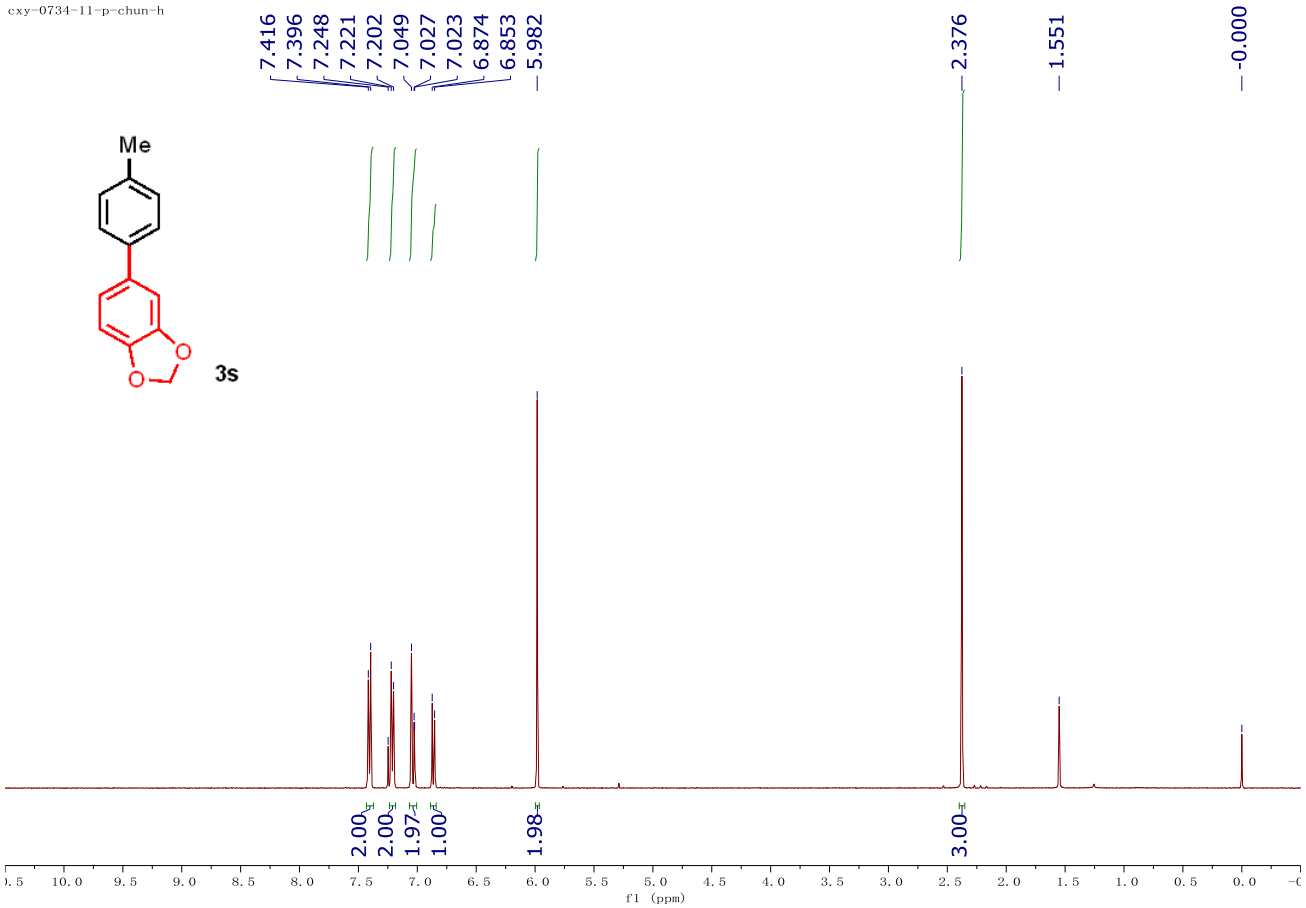

cxy-0734-6-p-1-h
7.264
7.252
7.238
7.220
2.403
2.275
1.545
0.000
Me
Me
3n
8.34
3.01
3.00
f1 (ppm)

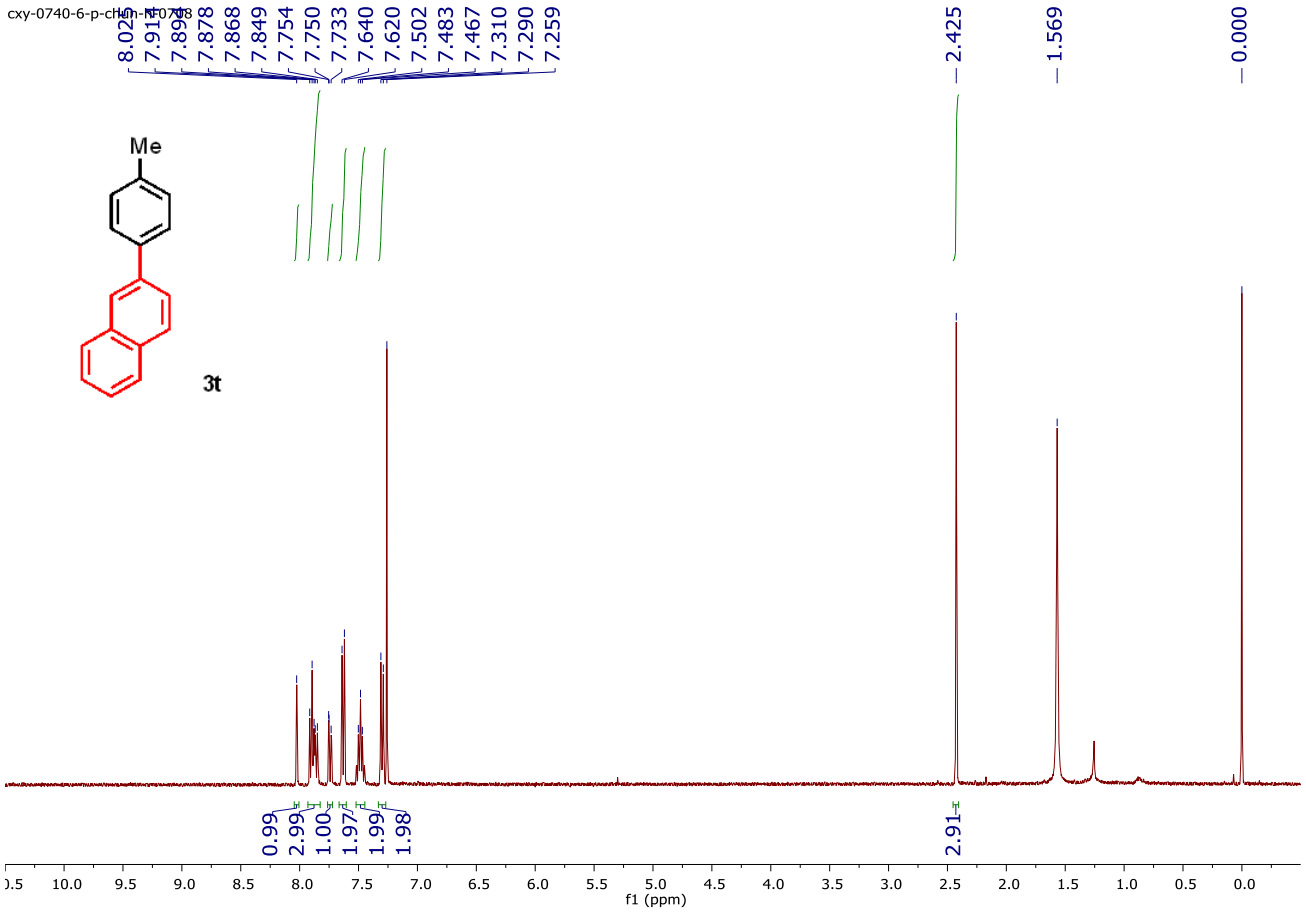

cxy-0857-1-1-h
Std proton
7.459
7.439
7.347
7.328
7.311
7.282
7.263
7.246
7.227
7.217
2.400
0.000
Me
Cl
3o
1.00
7.05
3.00
f1 (ppm)

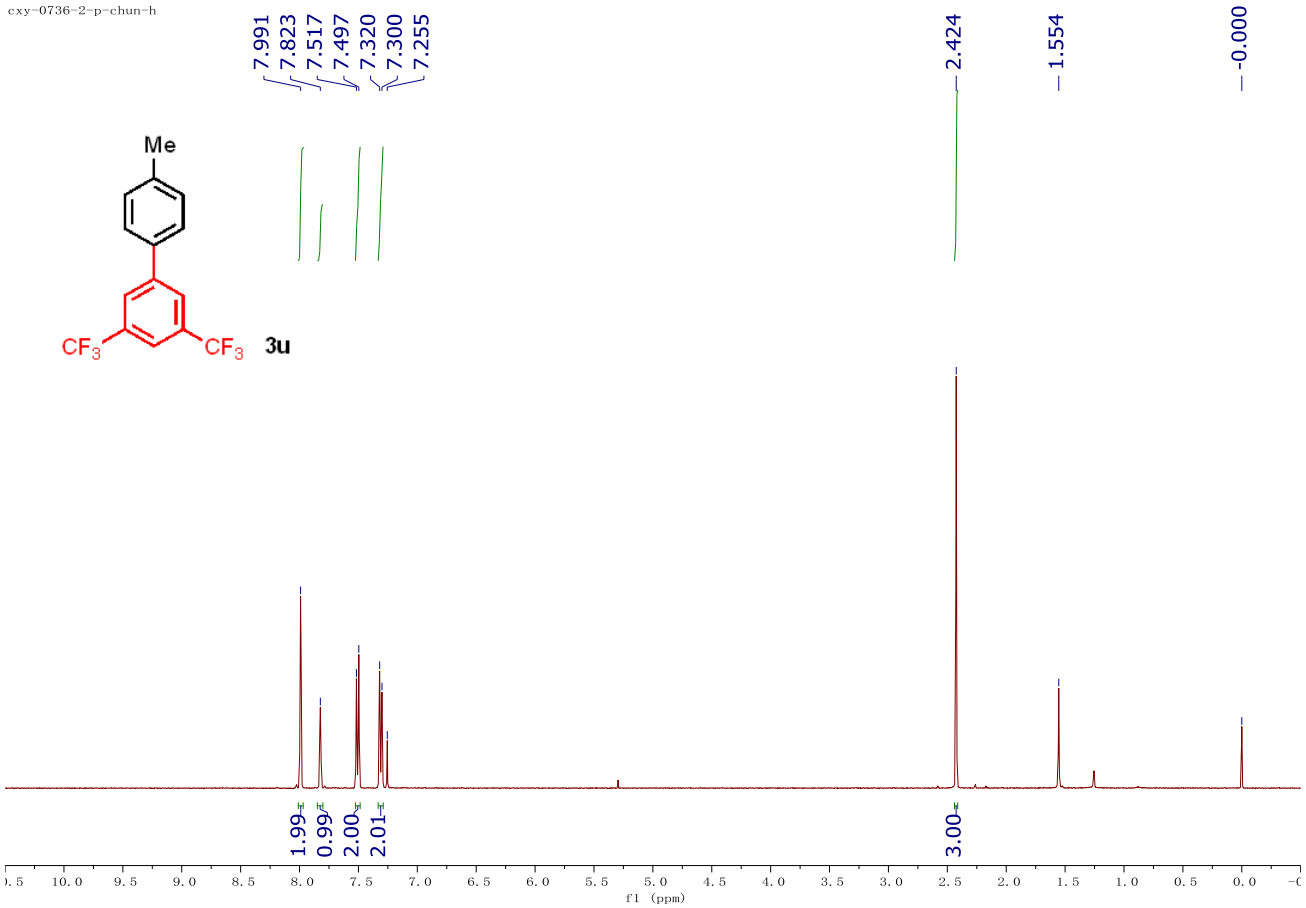

7.492
7.476
7.355
7.339
7.319
7.252
7.243
7.233
7.179
7.177
7.176
7.173
7.160
7.156
7.154
7.116
7.110
7.106
6.888
6.886
6.882
6.880
6.868
6.866
6.862
6.860
3.856
2.392
1.563
0.000
Me
OMe
3p
2.00
1.03
2.29
1.05
0.92
0.96
3.00
3.01
f1 (ppm)

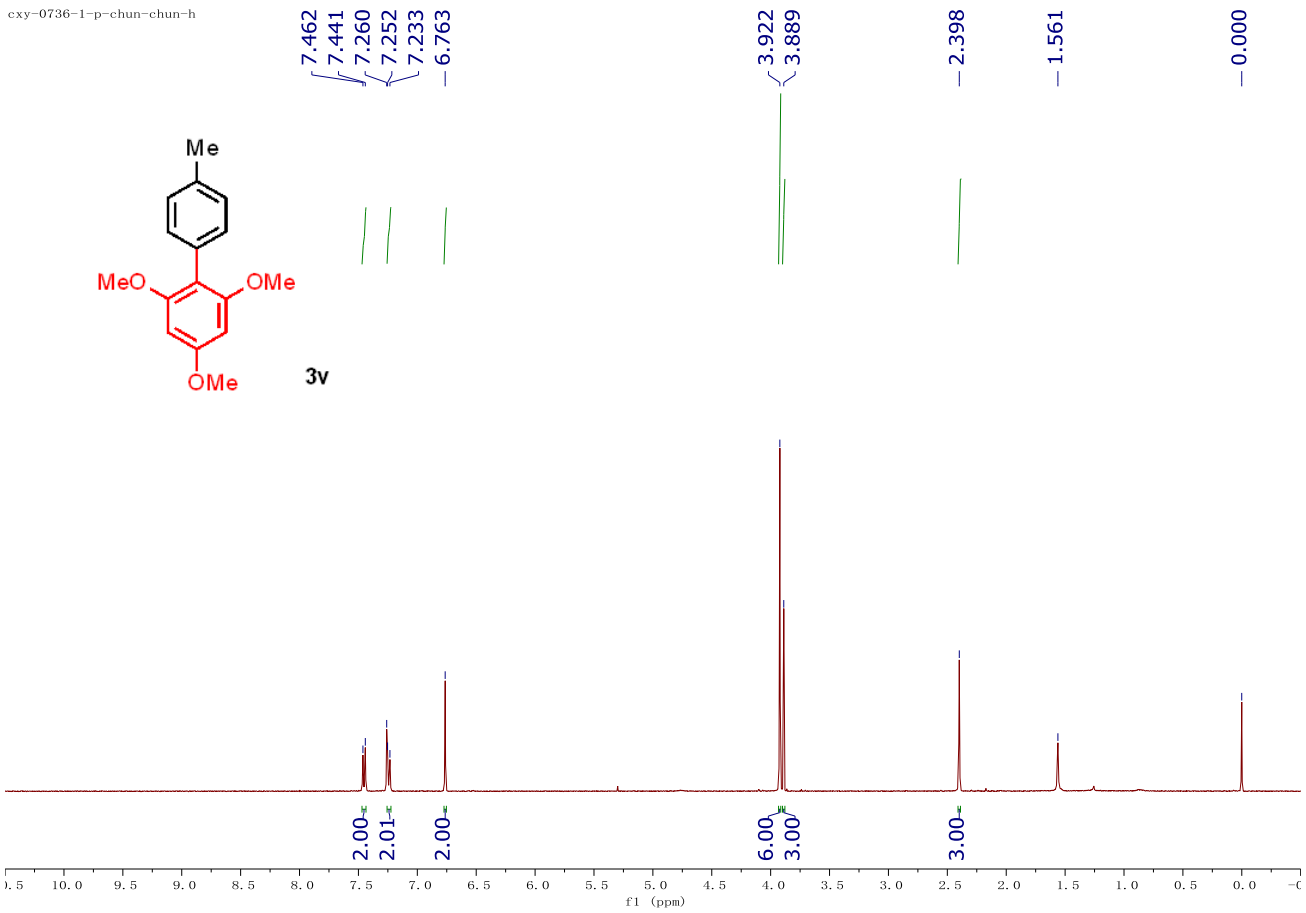

8.265
8.002
7.983
7.780
7.761
7.536
7.515
7.495
7.475
7.280
7.258
3.945
2.406
1.572
-0.000
Me
CO2Me
3q
1.00
1.01
1.05
3.13
2.58
3.03
3.08
f1 (ppm)

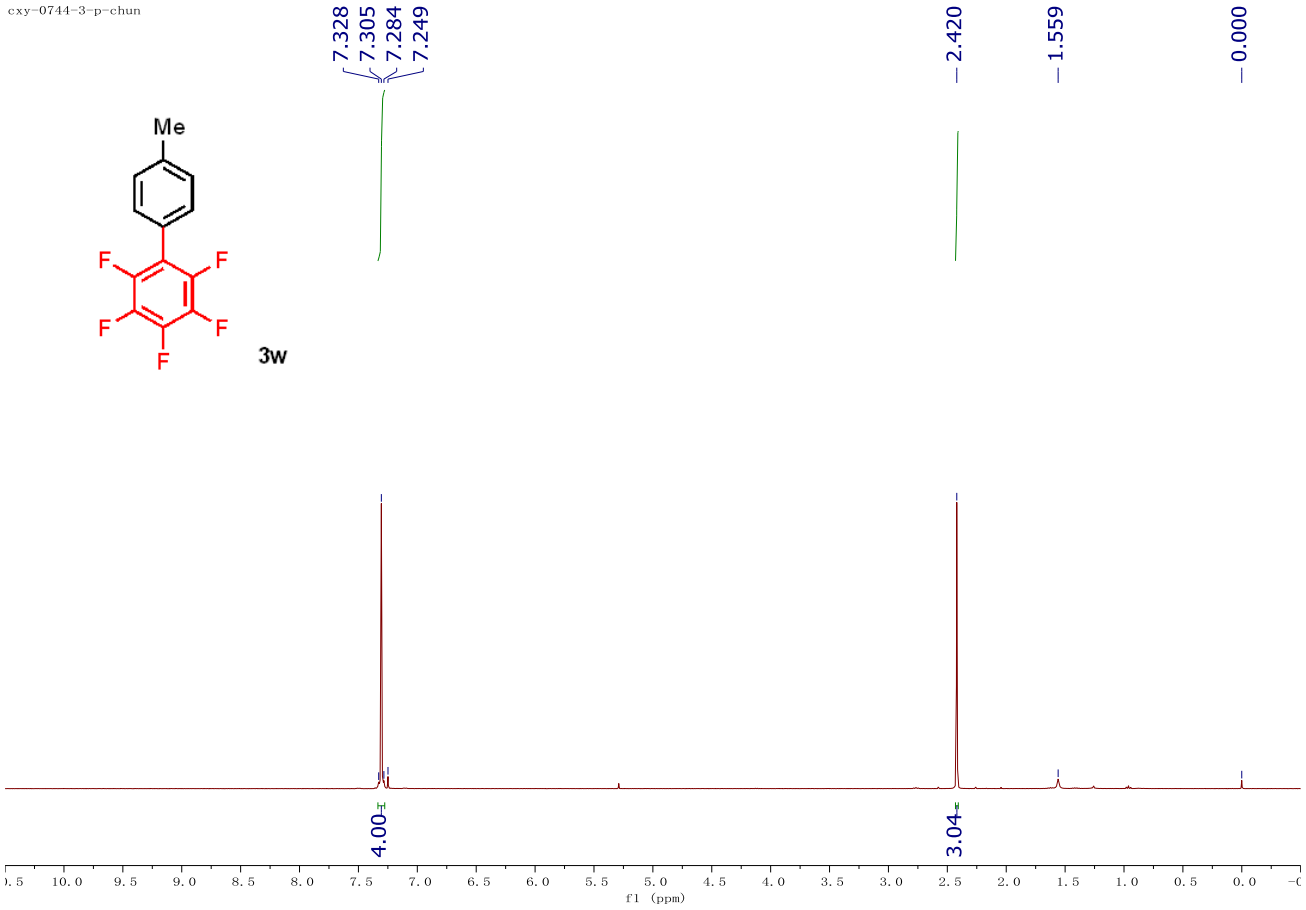

8.434
8.430
8.425
8.175
8.174
8.171
8.159
8.156
8.153
8.151
7.906
7.903
7.902
7.899
7.887
7.884
7.883
7.880
7.602
7.583
7.562
7.532
7.512
7.308
7.288
7.254
2.418
1.600
1.252
0.000
Me
NO2
3r
0.87
0.93
0.95
1.08
1.97
1.98
3.00
f1 (ppm)

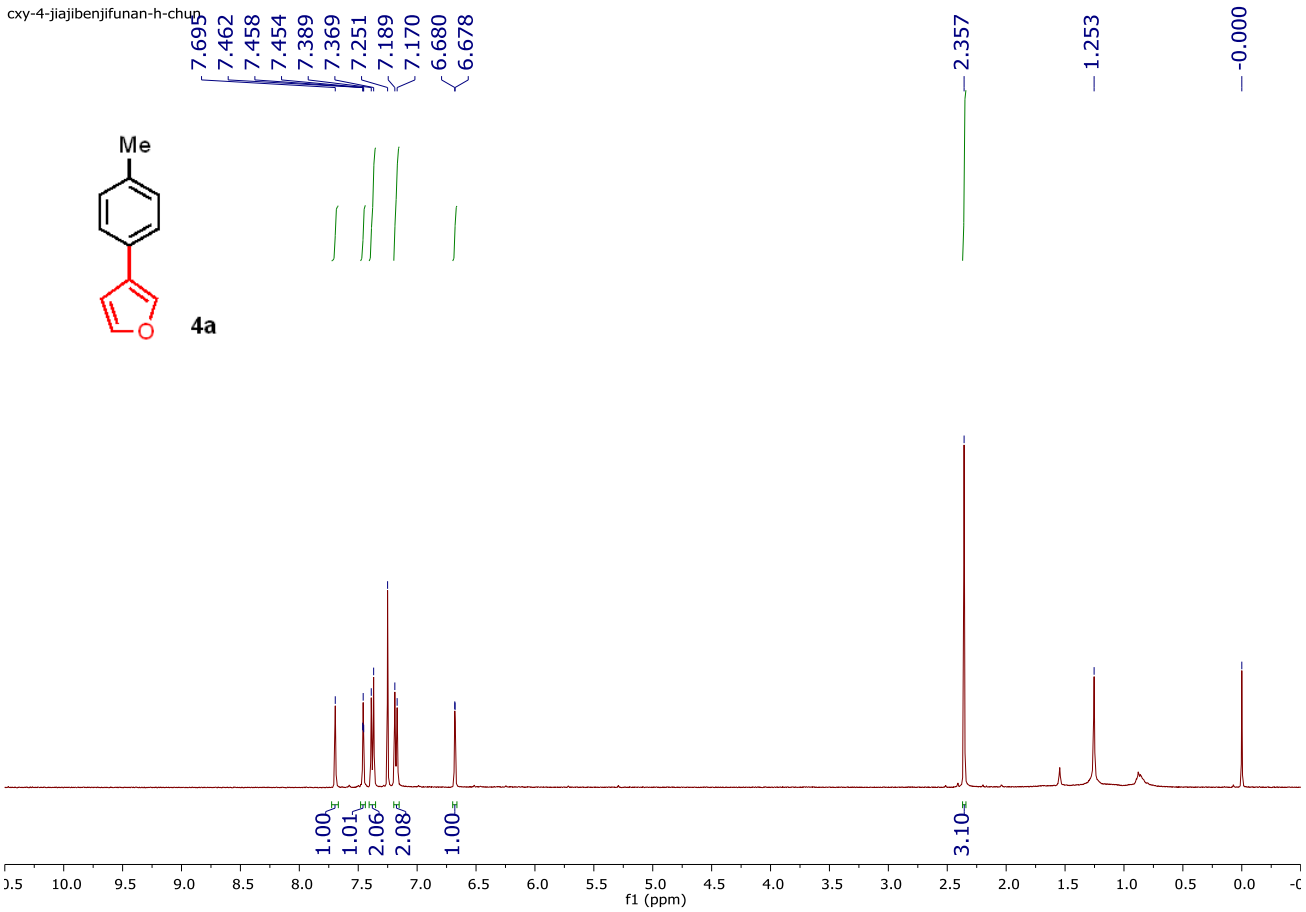

cxy-0734-11-p-chun-h
7.416
7.396
7.248
7.221
7.202
7.049
7.027
7.023
6.874
6.853
5.982
2.376
1.551
-0.000
Me
O
O
3s
2.00
2.00
1.97
1.00
1.98
3.00
f1 (ppm)

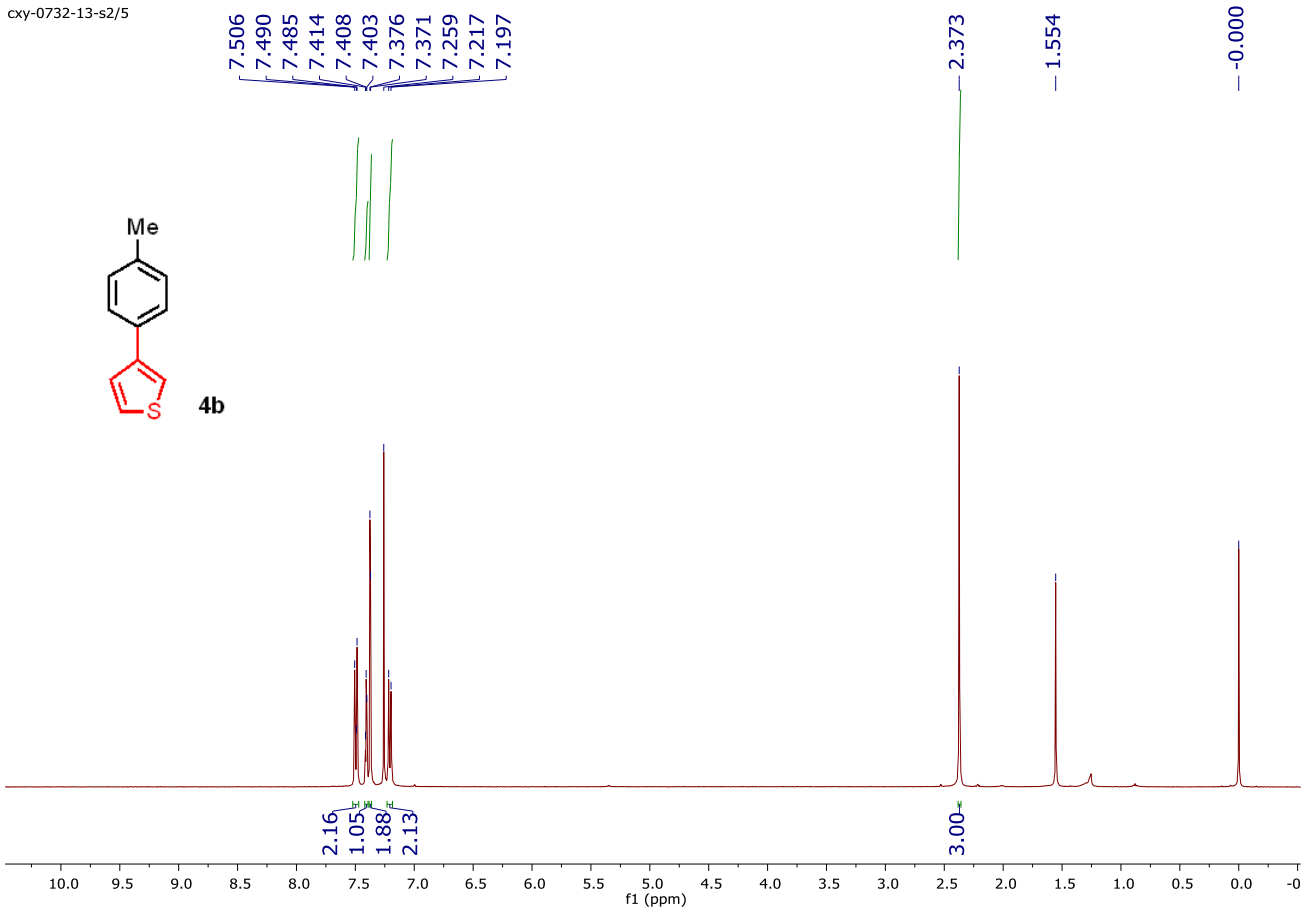

cxy-0740-6-p-chun-H708
8.025
7.915
7.898
7.878
7.868
7.849
7.754
7.750
7.733
7.640
7.620
7.502
7.483
7.467
7.310
7.290
7.259
2.425
1.569
0.000
Me
3t
0.99
2.99
1.00
1.97
1.99
1.98
2.91
f1 (ppm)

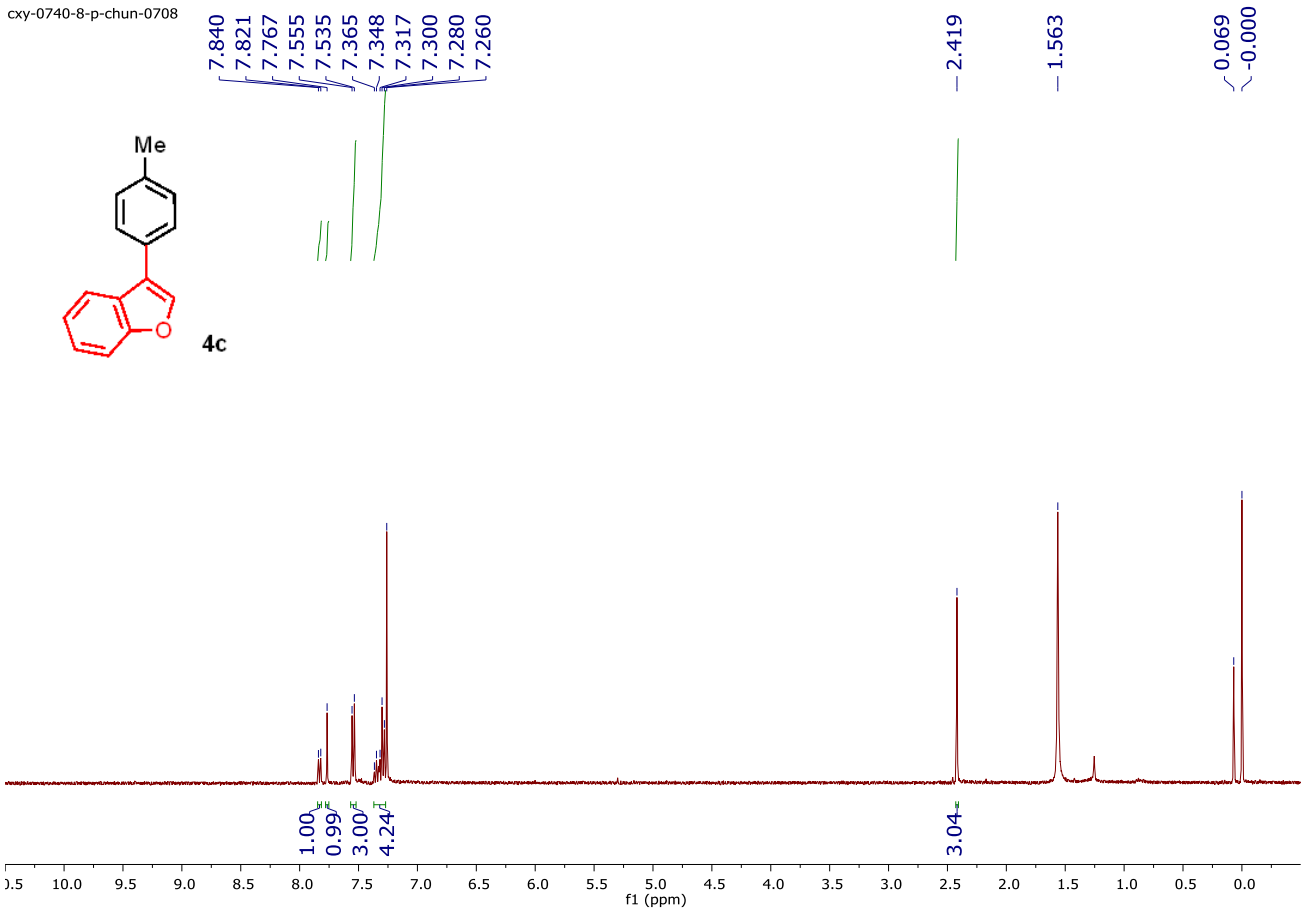

cxy-0736-2-p-chun-h
7.991
7.823
7.517
7.497
7.320
7.300
7.255
2.424
1.554
-0.000
Me
CF3
CF3
3u
1.99
0.99
2.00
2.01
3.00
f1 (ppm)

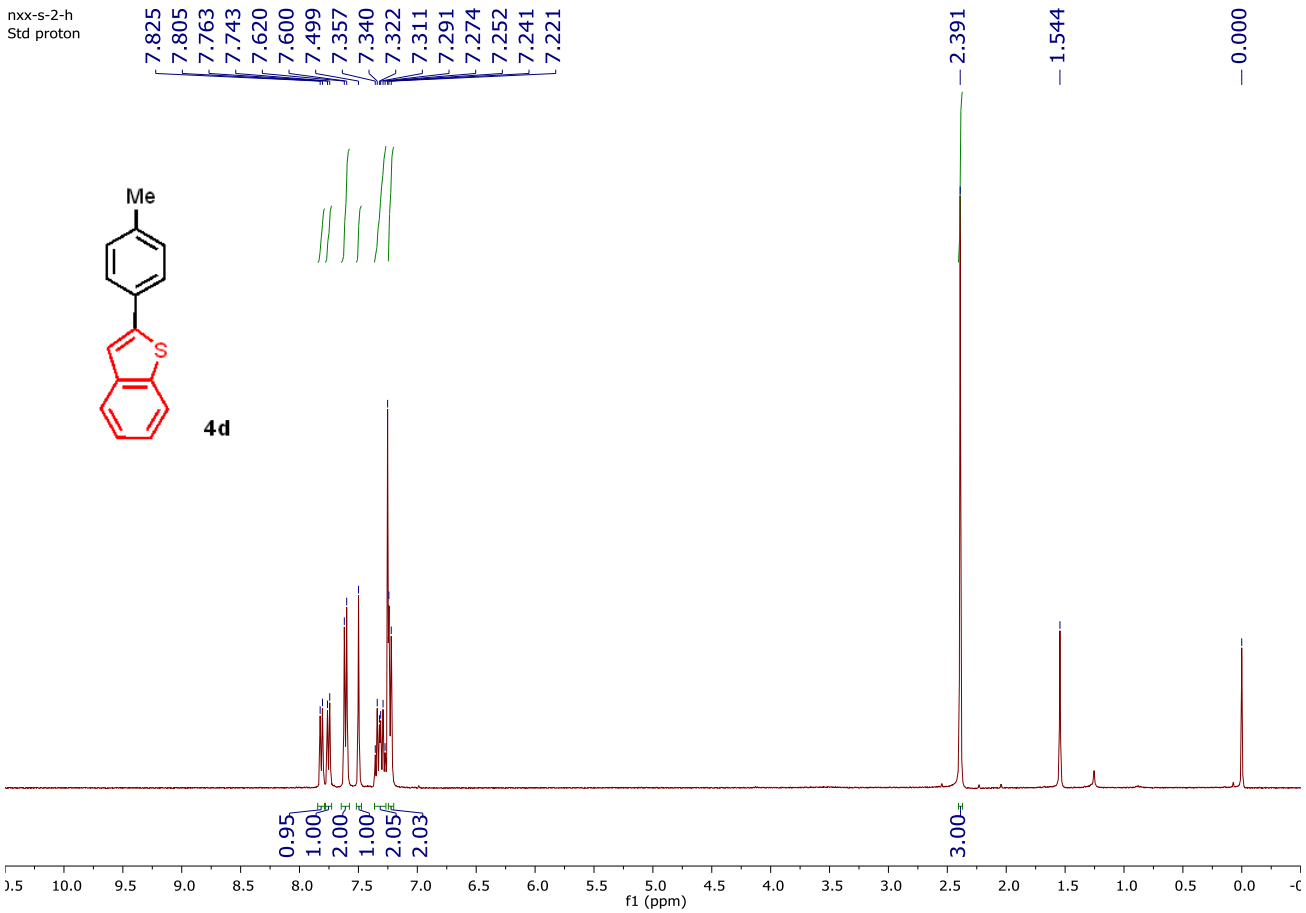

cxy-0736-1-p-chun-chun-h
7.462
7.441
7.260
7.252
7.233
6.763
3.922
3.889
2.398
1.561
0.000
Me
MeO
OMe
OMe
3v
2.00
2.01
2.00
6.00
3.00
3.00
f1 (ppm)

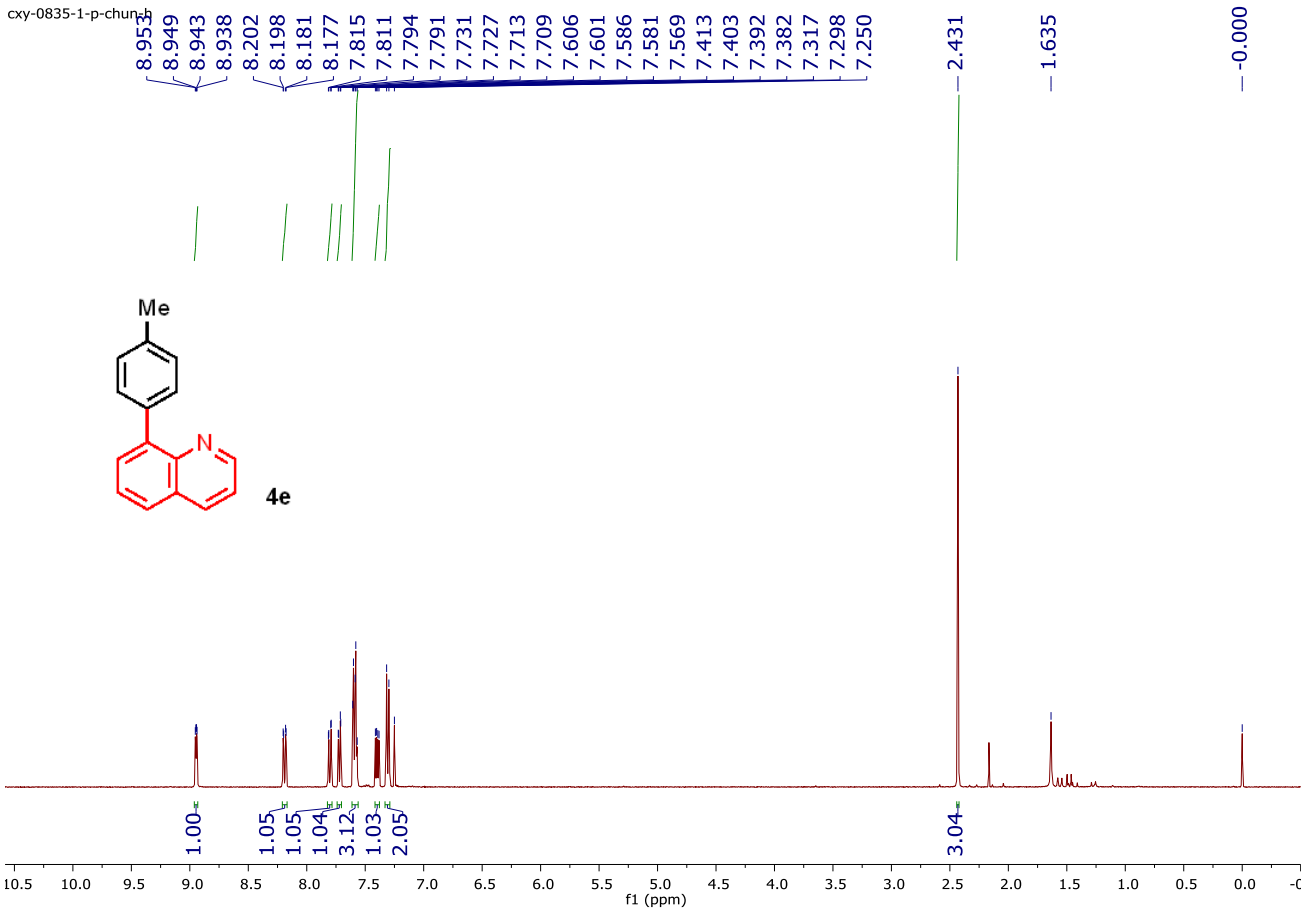

cxy-0744-3-p-chun
7.328
7.305
7.284
7.249
2.420
1.559
0.000
Me
F
F
F
F
F
3w
4.00
3.04
f1 (ppm)

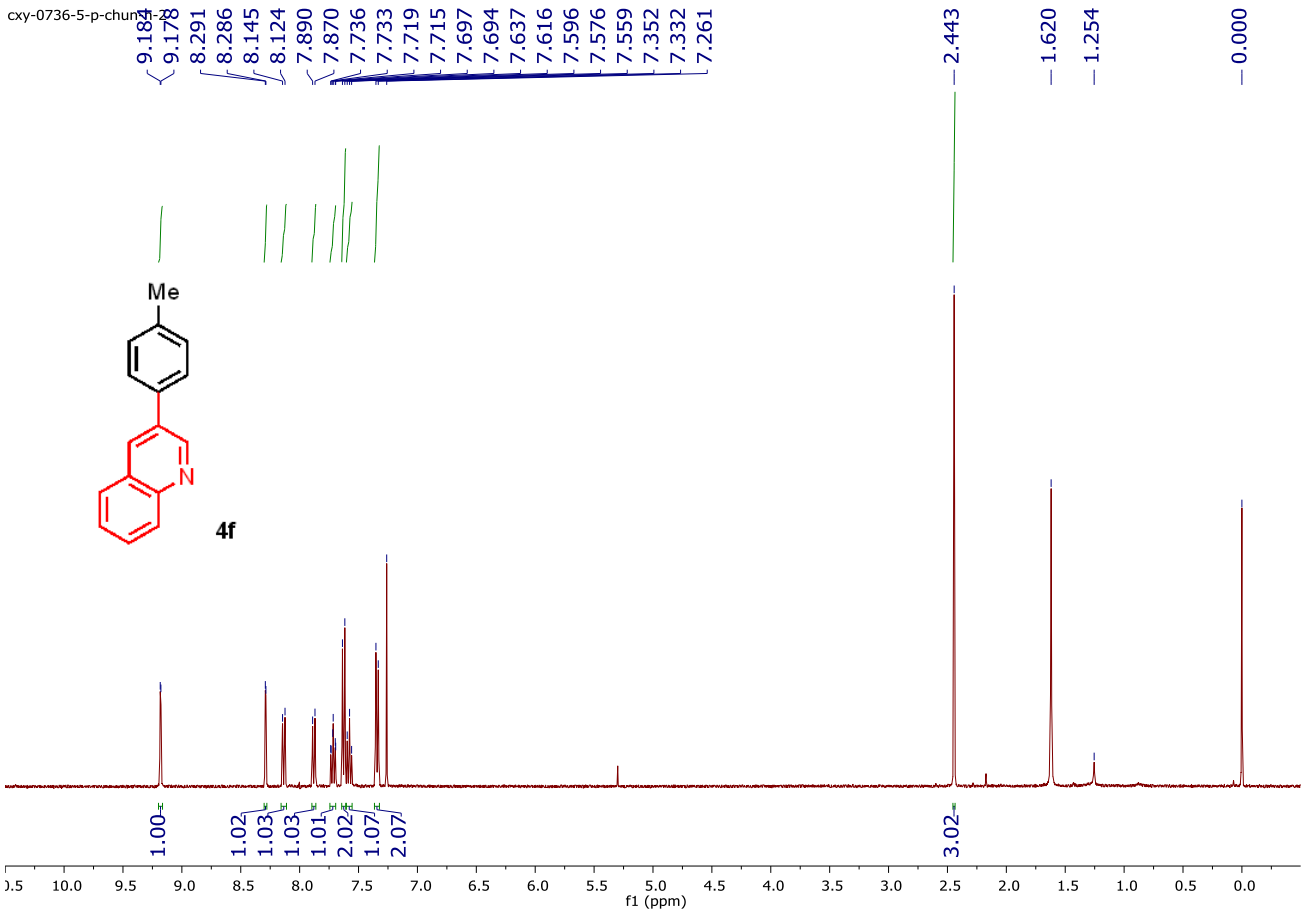

cxy-4-jiajibenjifunan-h-chun
7.695
7.462
7.458
7.454
7.389
7.369
7.251
7.189
7.170
6.680
6.678
2.357
1.253
-0.000
Me
O
4a
1.00
1.01
2.06
2.08
1.00
3.10
f1 (ppm)

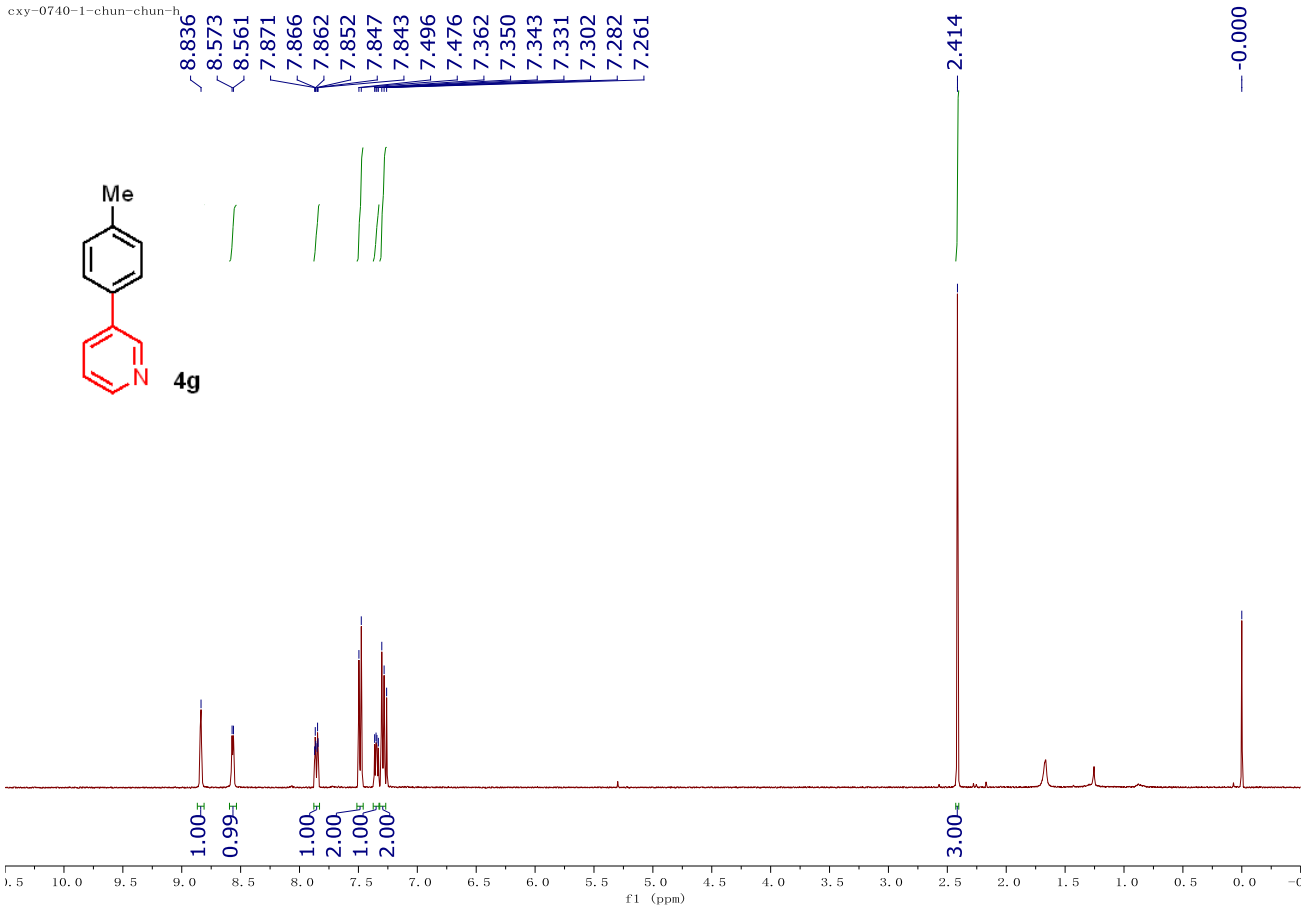

cxy-0732-13-s2/5
7.506
7.490
7.485
7.414
7.408
7.403
7.376
7.371
7.259
7.217
7.197
2.373
1.554
-0.000
Me
S
4b
2.16
1.05
1.88
2.13
3.00
f1 (ppm)

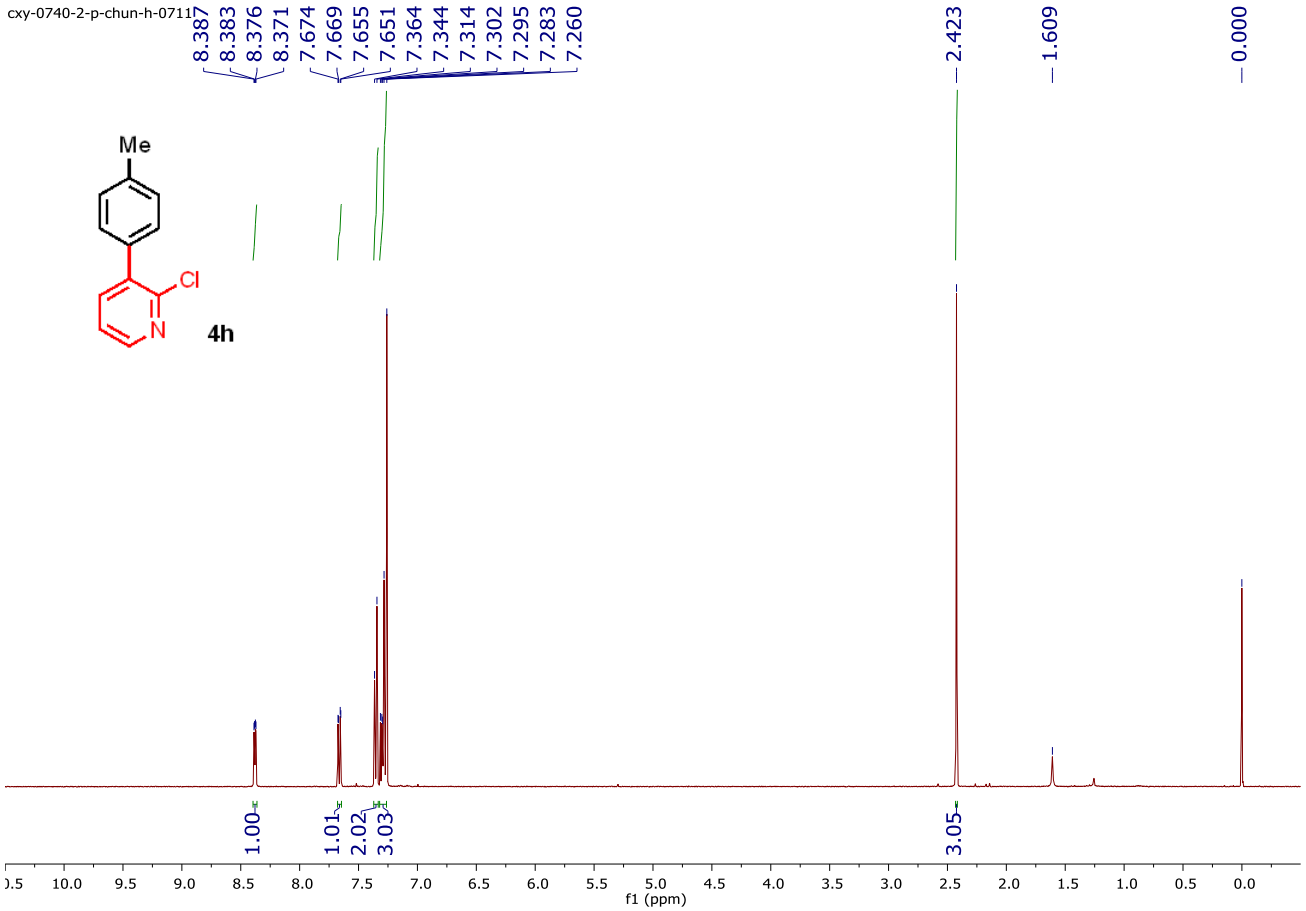

cxy-0740-8-p-chun-0708
7.840
7.821
7.767
7.555
7.535
7.365
7.348
7.317
7.300
7.280
7.260
2.419
1.563
0.069
-0.000
Me
O
4c
1.00
0.99
3.00
4.24
3.04
f1 (ppm)

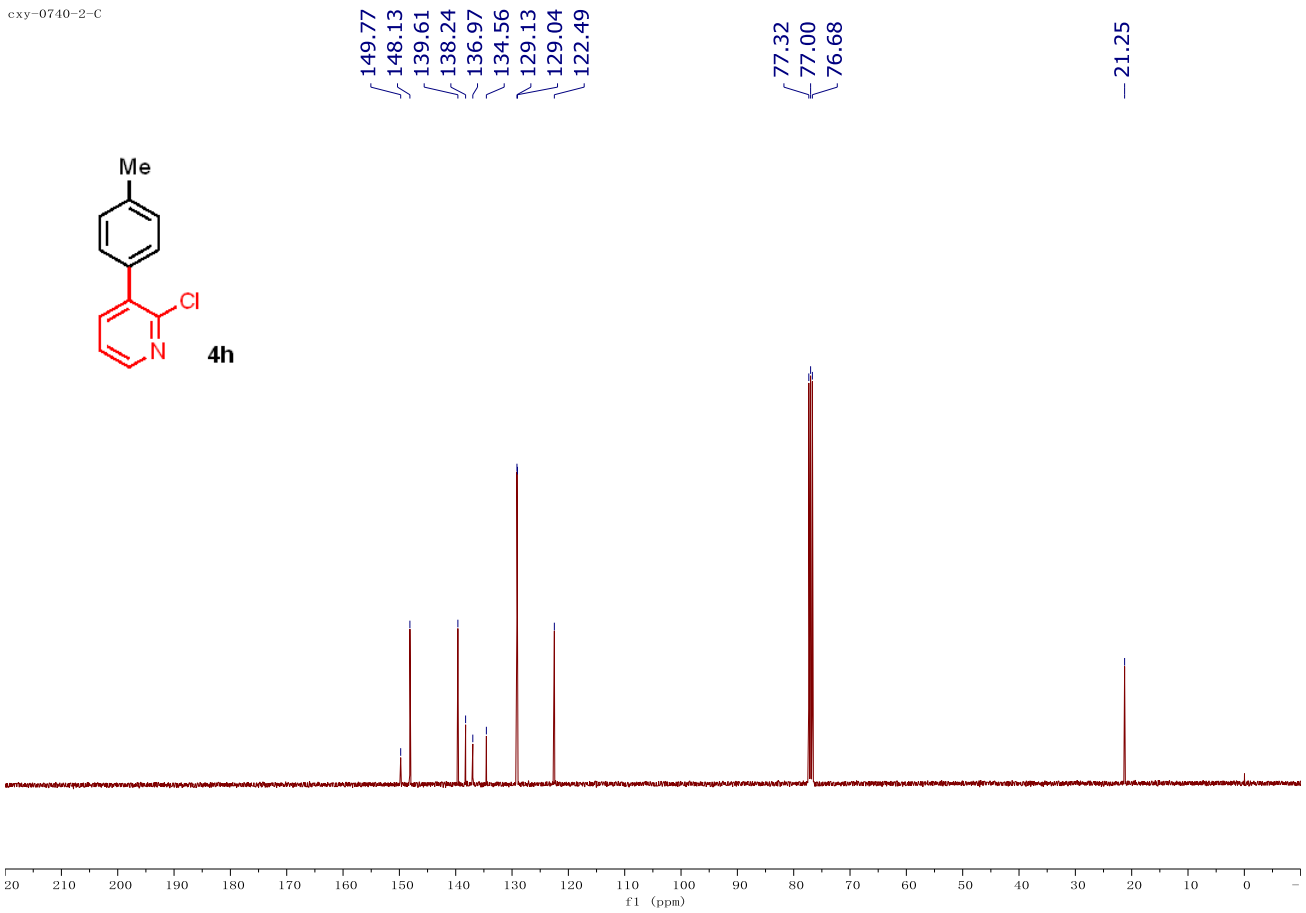

nxx-s-2-h
Std proton
7.825
7.805
7.763
7.743
7.620
7.600
7.499
7.357
7.340
7.322
7.311
7.291
7.274
7.252
7.241
7.221
2.391
1.544
0.000
Me
S
4d
0.95
1.00
2.00
1.00
2.05
2.03
3.00
f1 (ppm)

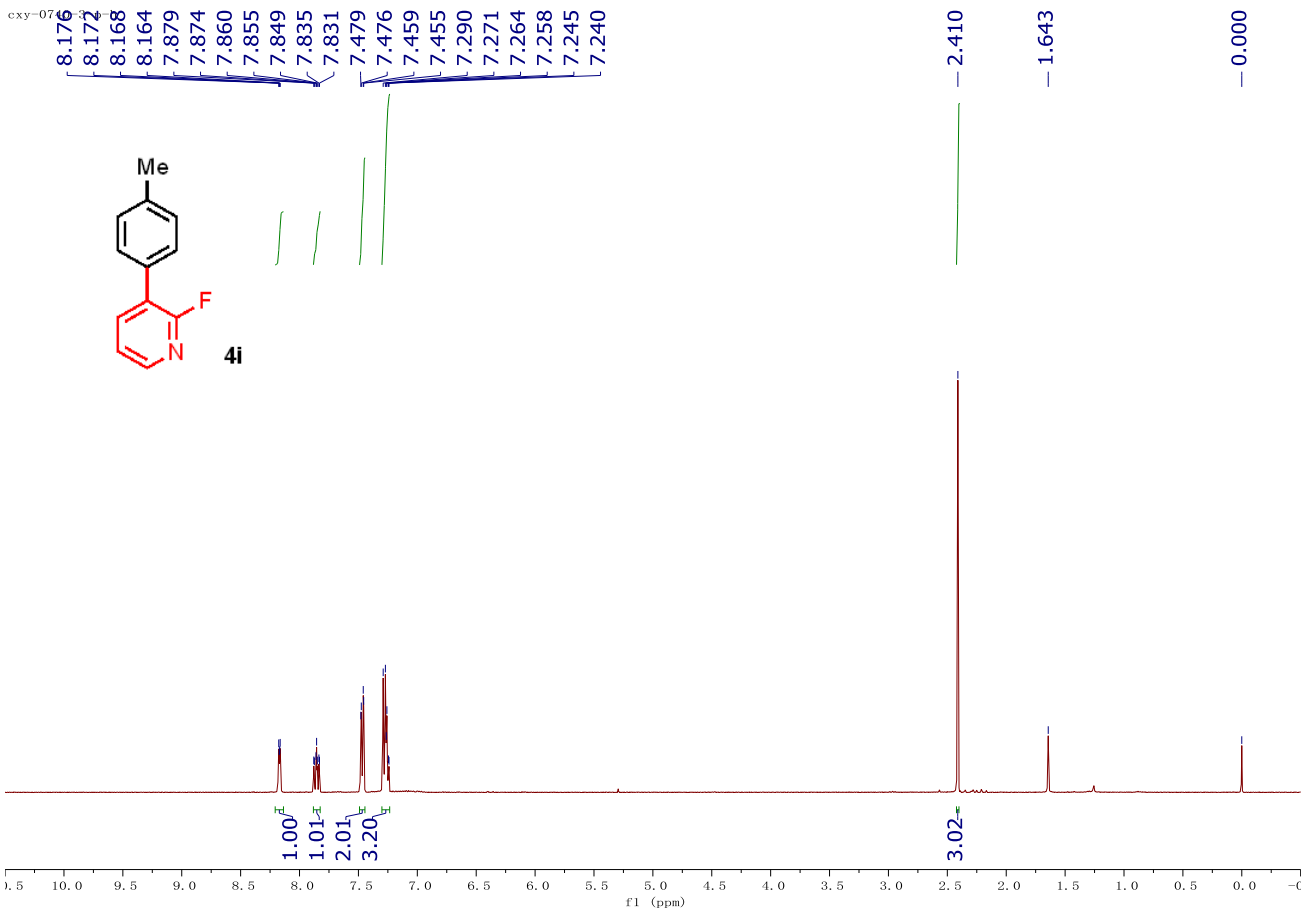

cxy-0835-1-p-chun-h
8.953
8.949
8.943
8.938
8.202
8.198
8.181
8.177
7.815
7.811
7.794
7.791
7.731
7.727
7.713
7.709
7.606
7.601
7.586
7.581
7.569
7.413
7.403
7.392
7.382
7.317
7.298
7.250
2.431
1.635
-0.000
Me
N
4e
1.00
1.05
1.05
1.04
3.12
1.03
2.05
3.04
f1 (ppm)

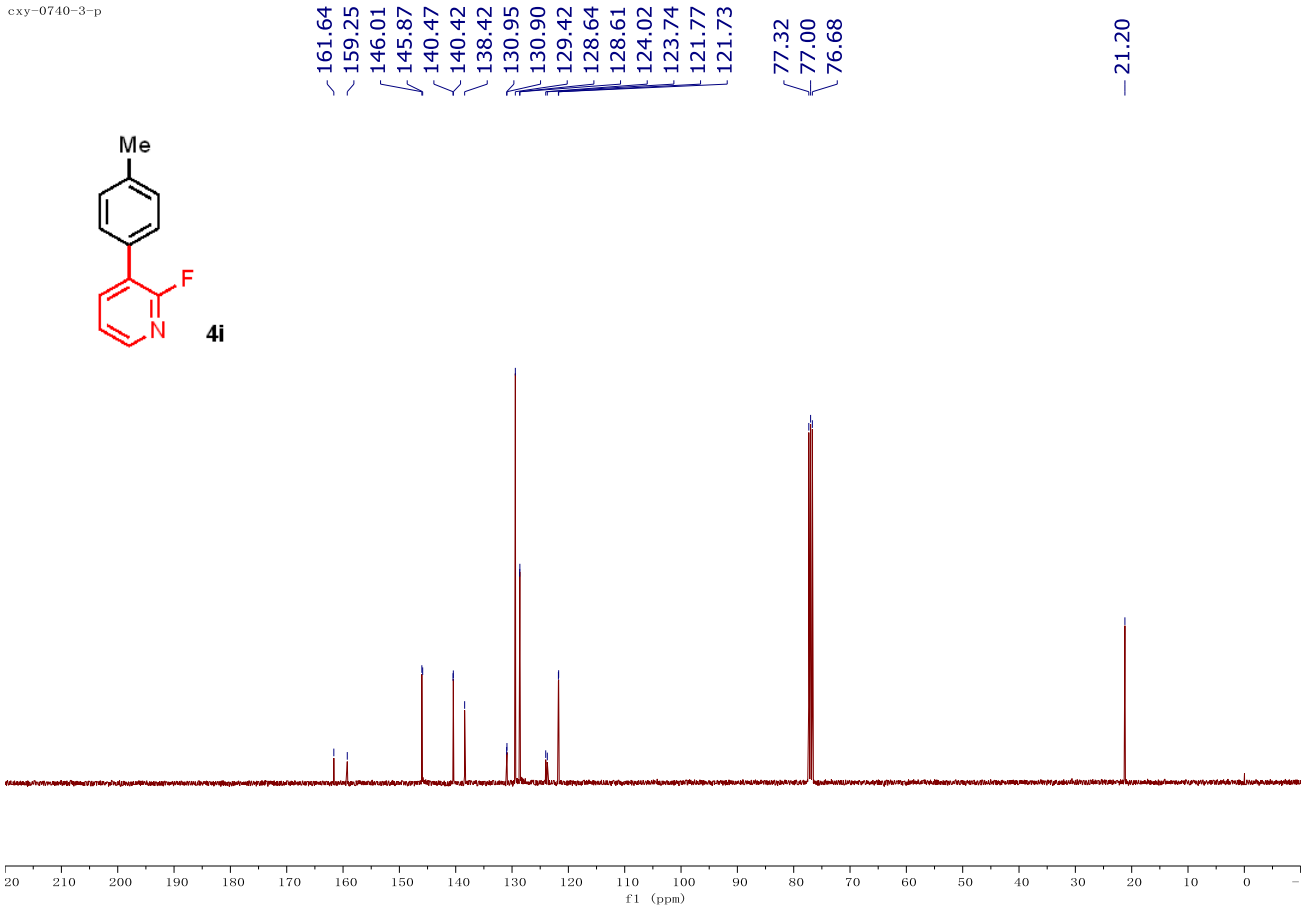

cxy-0736-5-p-chun-2
9.184
9.178
8.291
8.286
8.145
8.124
7.890
7.870
7.736
7.733
7.719
7.715
7.697
7.694
7.637
7.616
7.596
7.576
7.559
7.352
7.332
7.261
2.443
1.620
1.254
0.000
Me
N
4f
1.00
1.02
1.03
1.03
1.01
2.02
1.07
2.07
3.02
f1 (ppm)

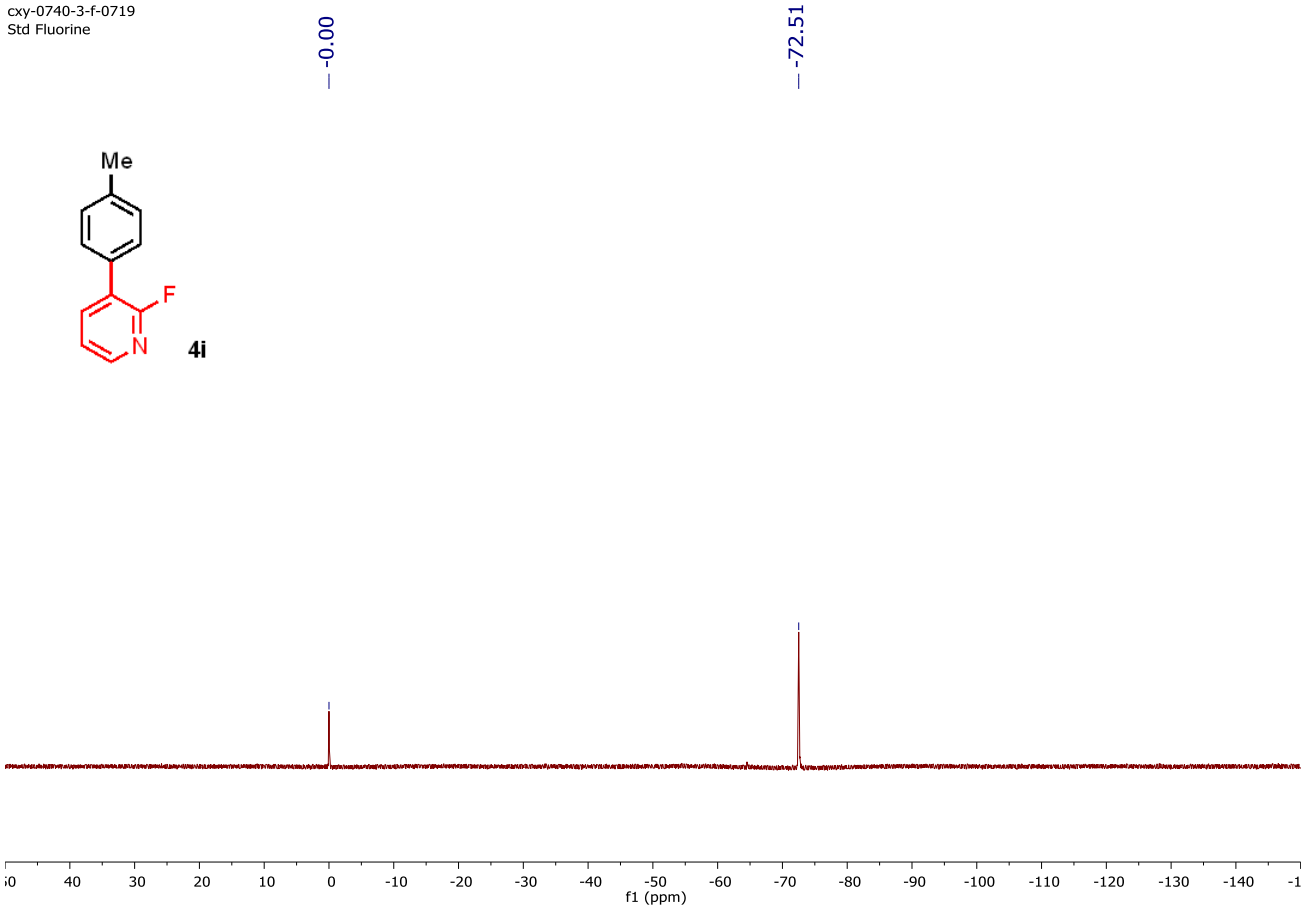

cxy-0740-1-chun-chun-h
8.836
8.573
8.561
7.871
7.866
7.862
7.852
7.847
7.843
7.496
7.476
7.362
7.350
7.343
7.331
7.302
7.282
7.261
2.414
-0.000
Me
N
4g
1.00
0.99
1.00
2.00
1.00
2.00
3.00
f1 (ppm)

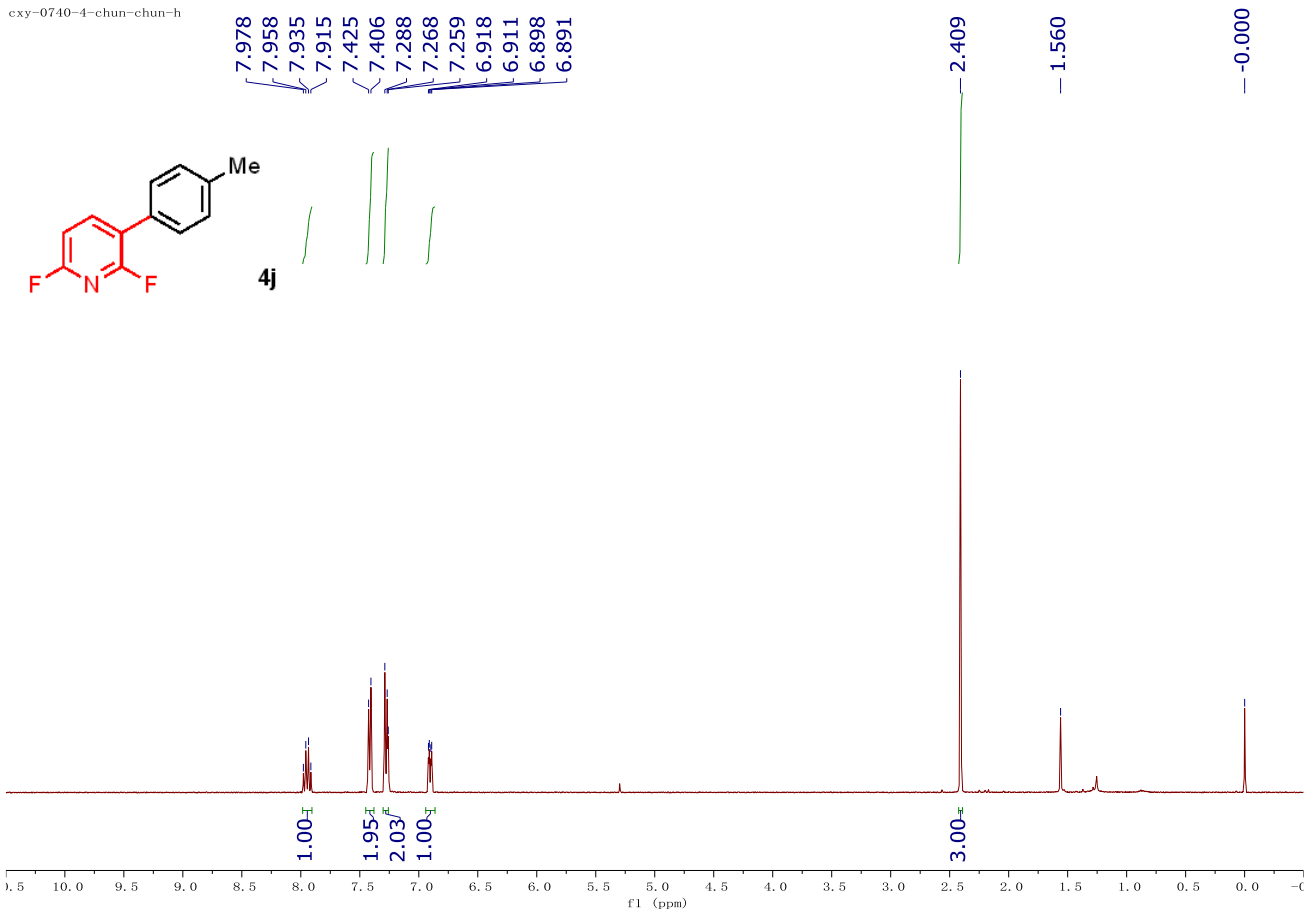

cxy-0740-2-p-chun-h-0711
8.387
8.383
8.376
8.371
7.674
7.669
7.655
7.651
7.364
7.344
7.314
7.302
7.295
7.283
7.260
2.423
1.609
0.000
Me
Cl
N
4h
1.00
1.01
2.02
3.03
3.05
f1 (ppm)

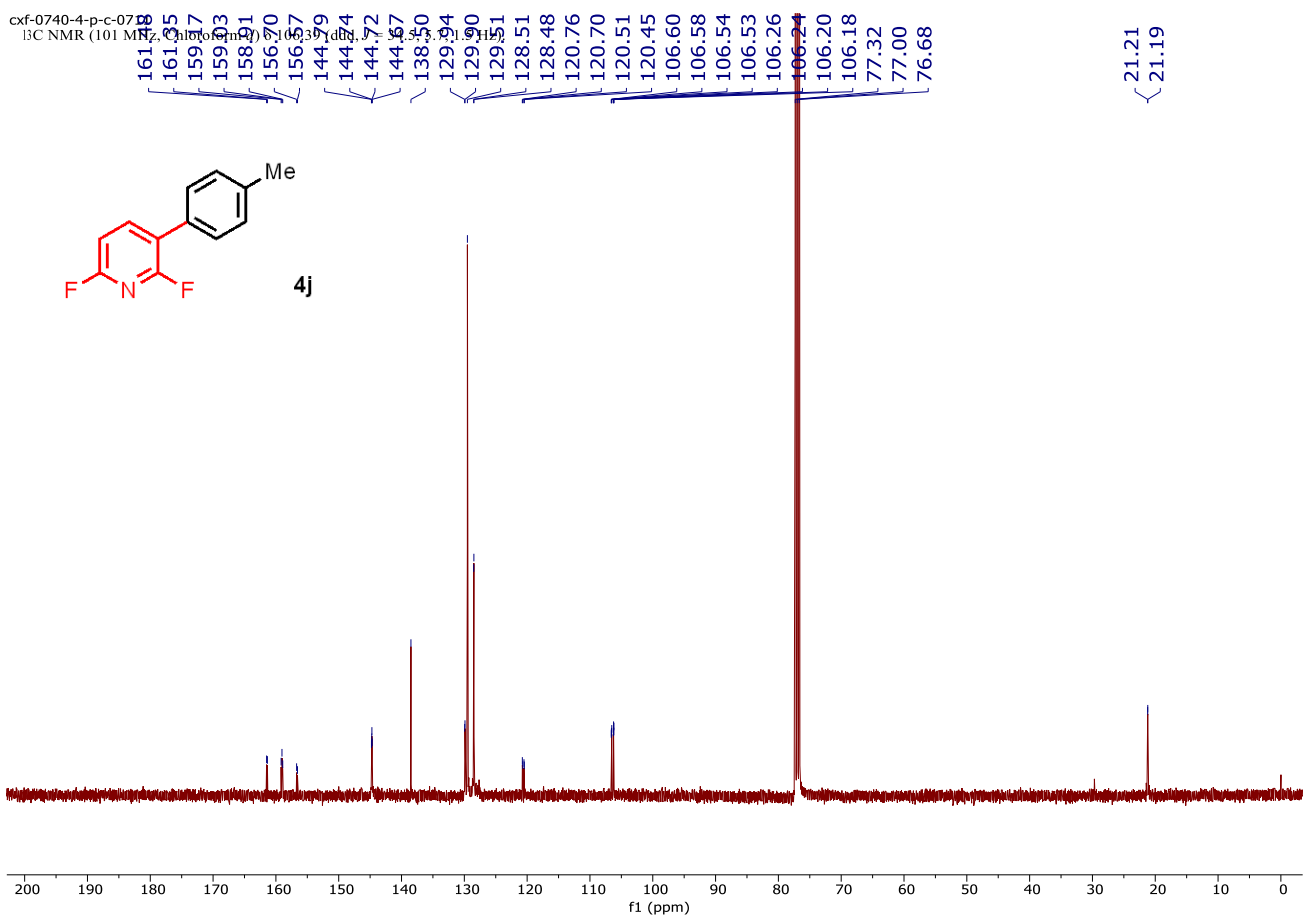

cxy-0740-2-C
149.77
148.13
139.61
138.24
136.97
134.56
129.13
129.04
122.49
77.32
77.00
76.68
21.25
Me
Cl
N
4h
f1 (ppm)

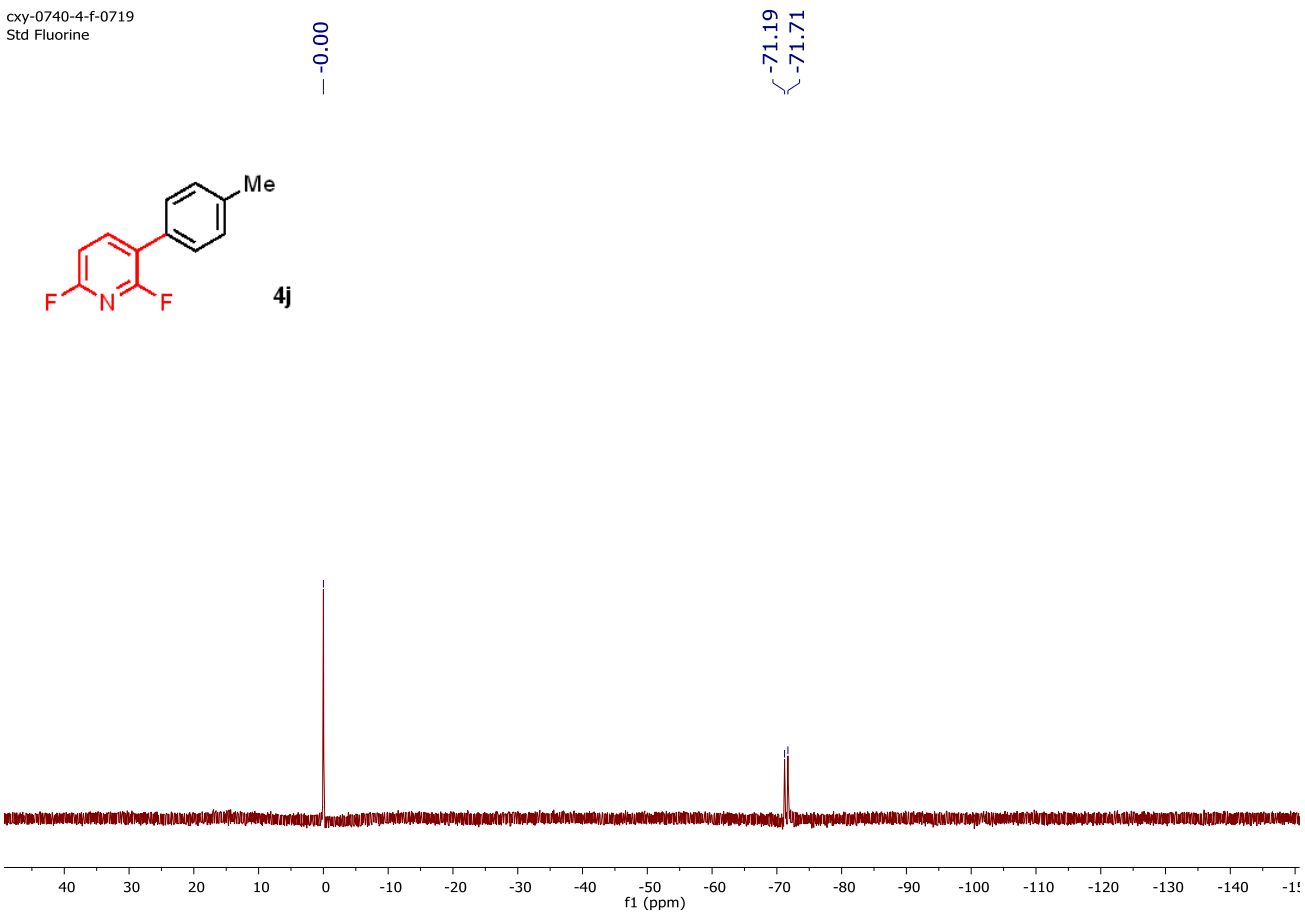

8.176
8.172
8.168
8.164
7.879
7.874
7.860
7.855
7.849
7.835
7.831
7.479
7.476
7.459
7.455
7.290
7.271
7.264
7.258
7.245
7.240
2.410
1.643
0.000
Me
F
N
4i
1.00
1.01
2.01
3.20
3.02
f1 (ppm)

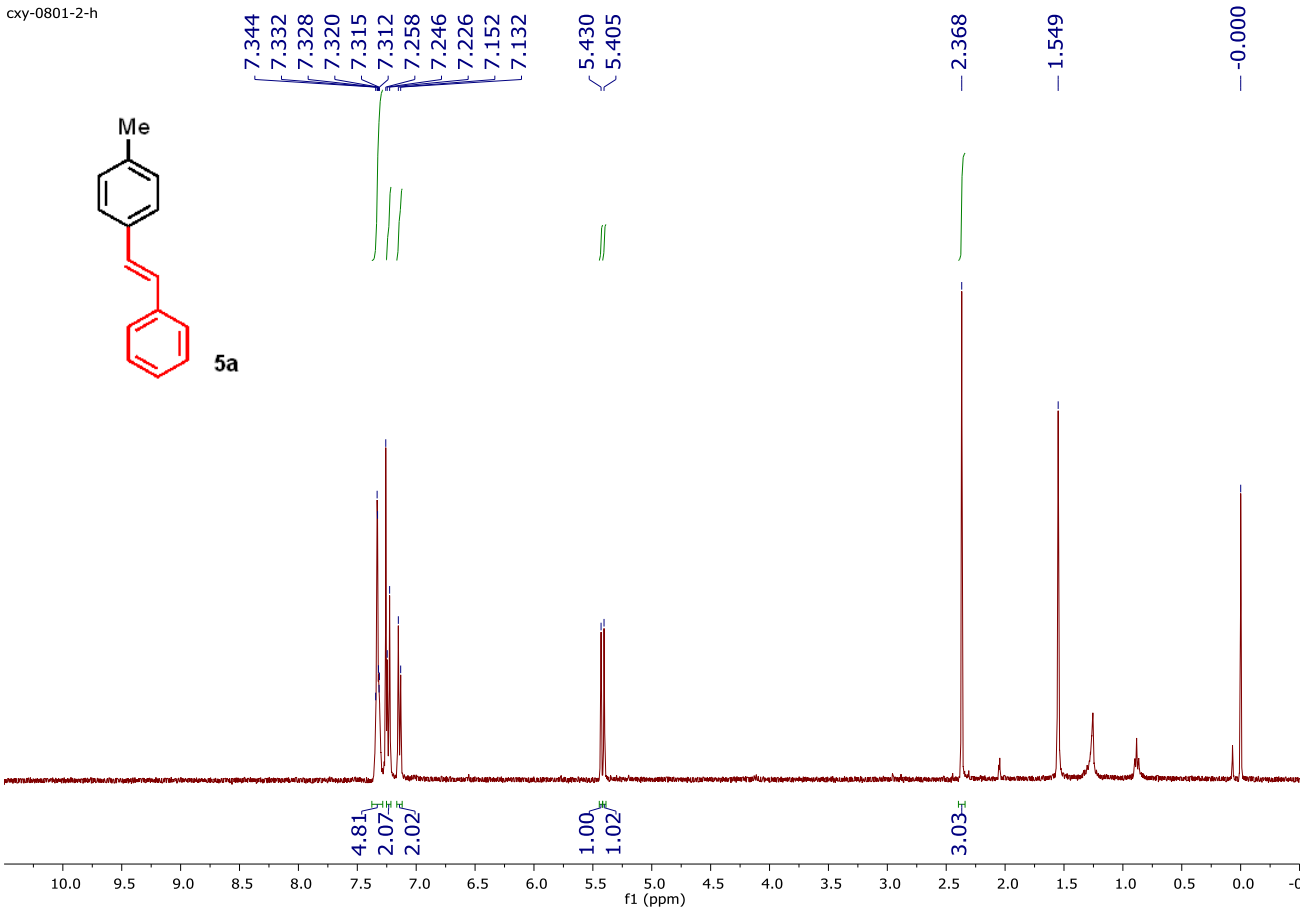

cxy-0740-3-p
161.64
159.25
146.01
145.87
140.47
140.42
138.42
130.95
130.90
129.42
128.64
128.61
124.02
123.74
121.77
121.73
77.32
77.00
76.68
21.20
Me
F
N
4i
f1 (ppm)

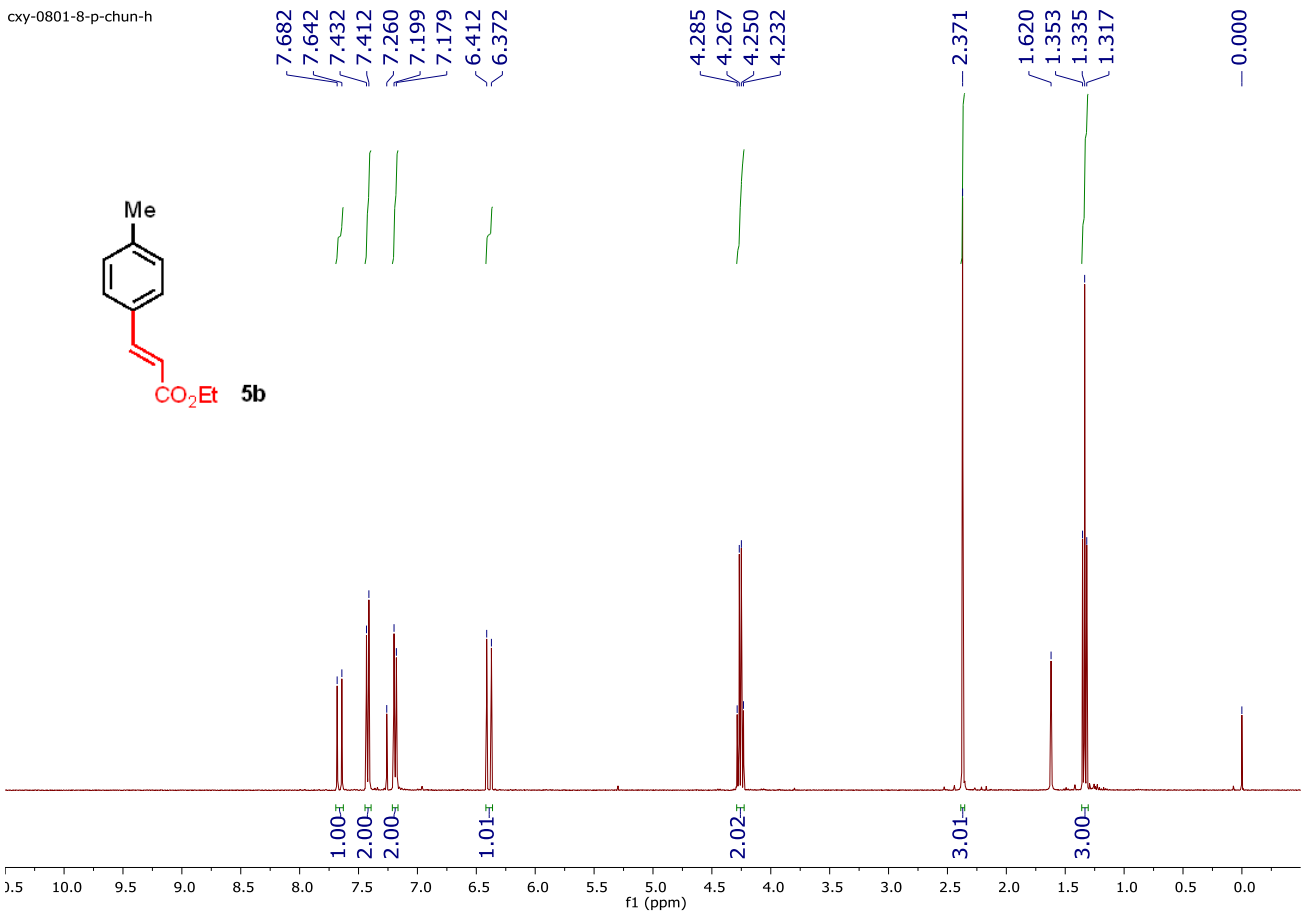

cxy-0740-3-f-0719
Std Fluorine
-0.00
-72.51
Me
F
N
4i
f1 (ppm)

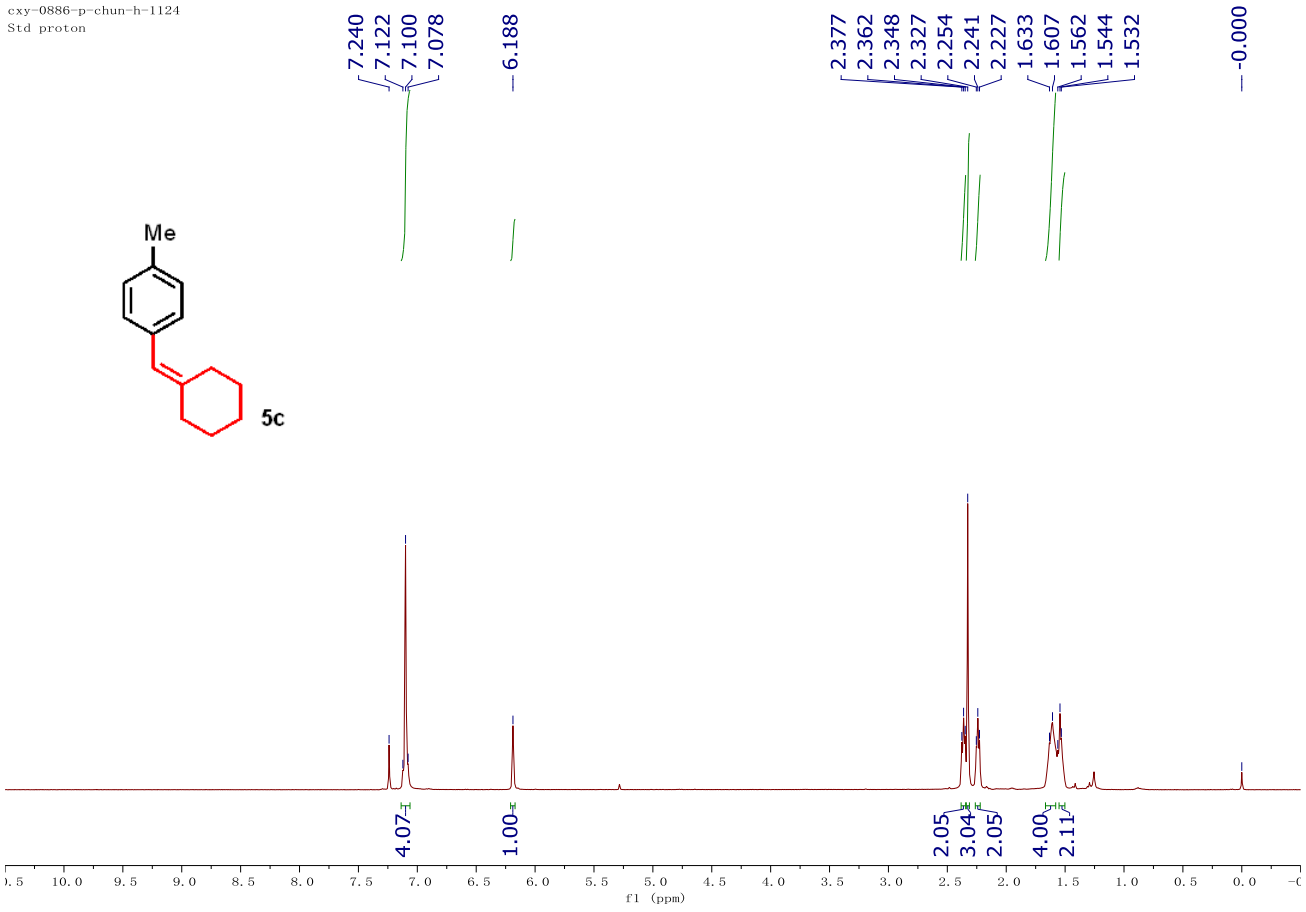

cxy-0740-4-chun-chun-h
7.978
7.958
7.935
7.915
7.425
7.406
7.288
7.268
7.259
6.918
6.911
6.898
6.891
2.409
1.560
-0.000
Me
F
N
F
4j
1.00
1.95
2.03
1.00
3.00
f1 (ppm)

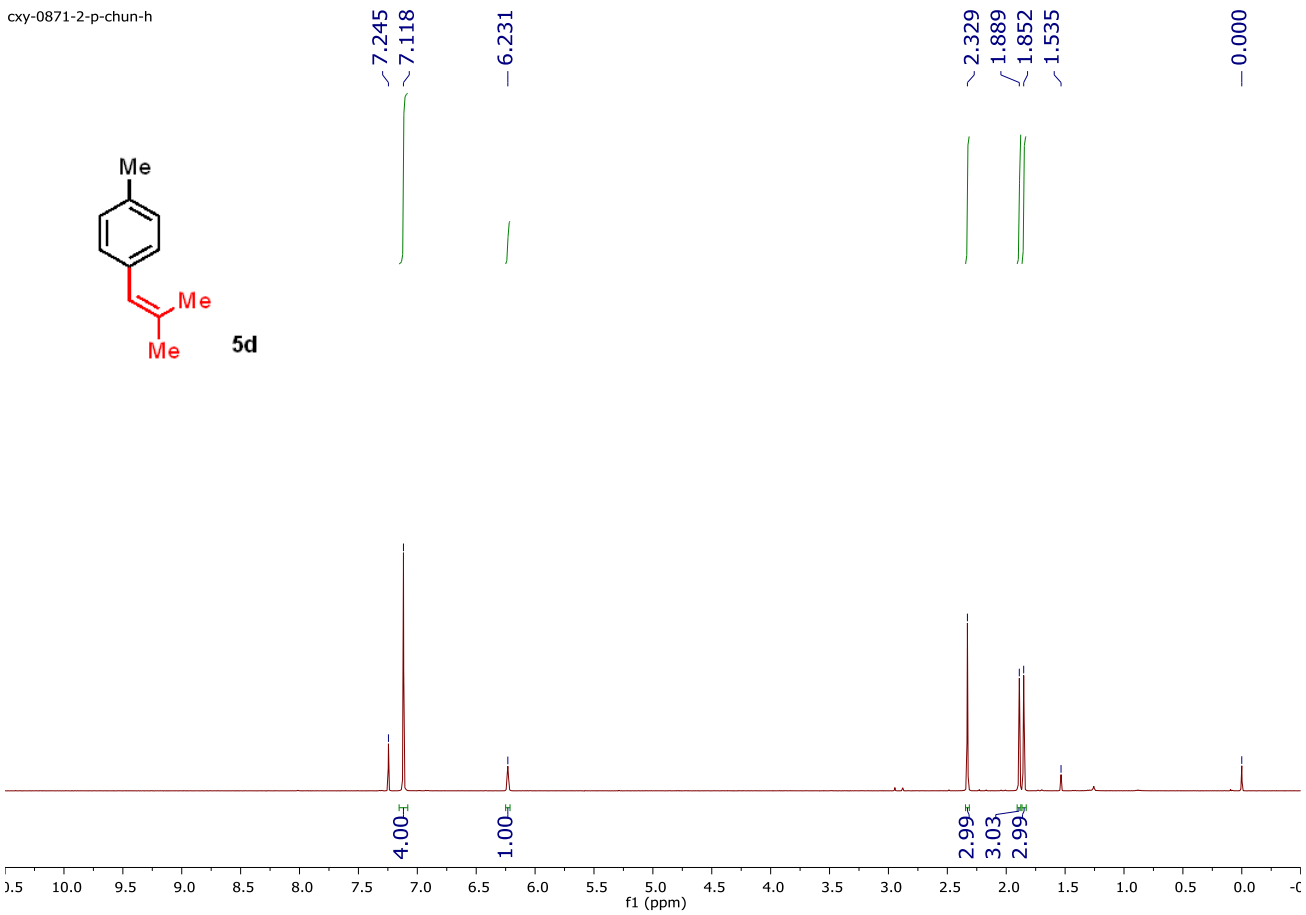

cxf-0740-4-p-c-0740
161.48
161.35
159.17
159.03
158.91
156.70
156.57
144.39
144.24
144.22
144.07
138.50
129.24
129.00
128.51
128.48
120.76
120.70
120.51
120.45
106.60
106.58
106.54
106.53
106.26
106.24
106.20
106.18
77.32
77.00
76.68
21.21
21.19
Me
F
N
F
4j
f1 (ppm)

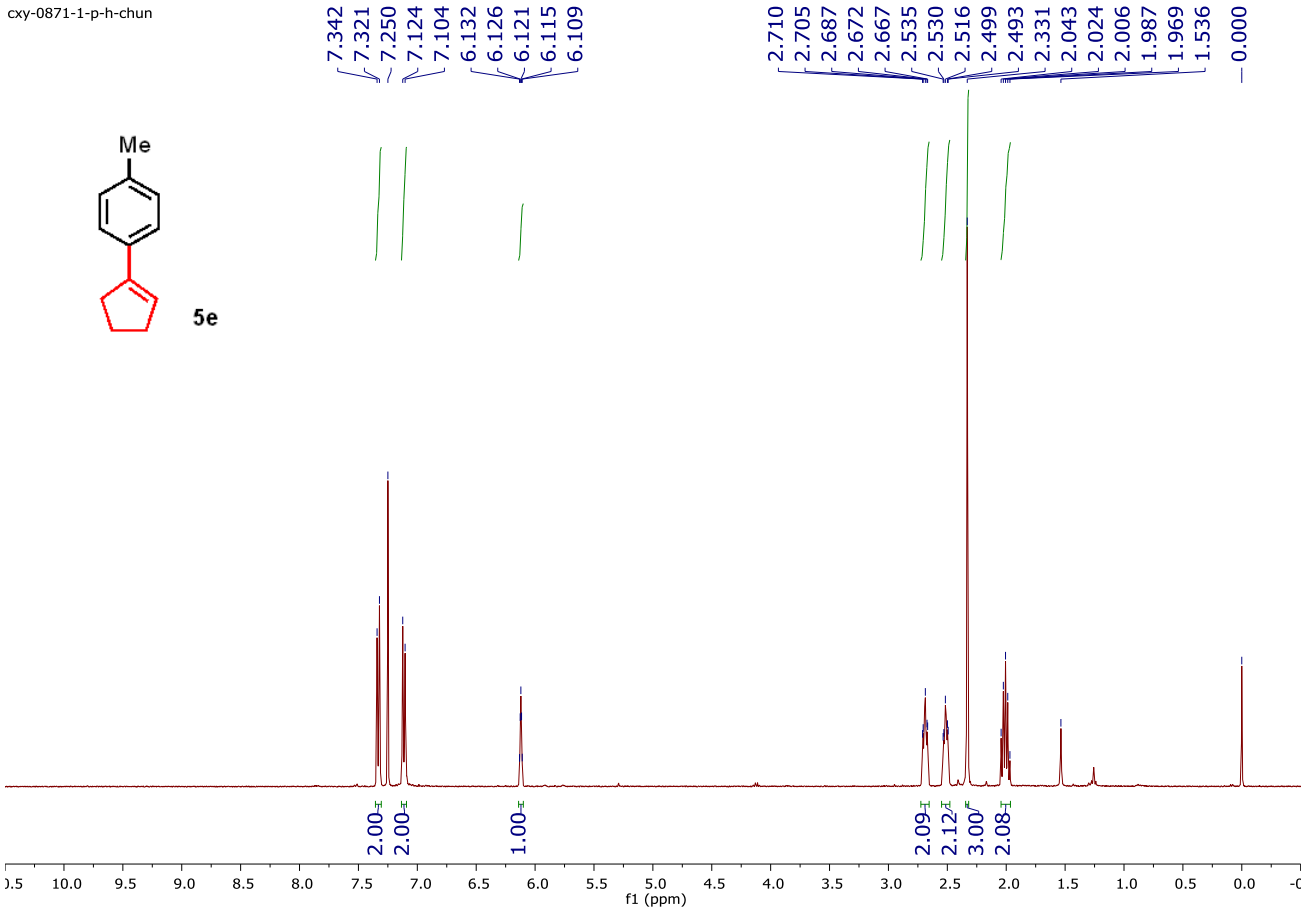

cxy-0740-4-f-0719
Std Fluorine
-0.00
-71.19
-71.71
Me
F
N
F
4j
f1 (ppm)

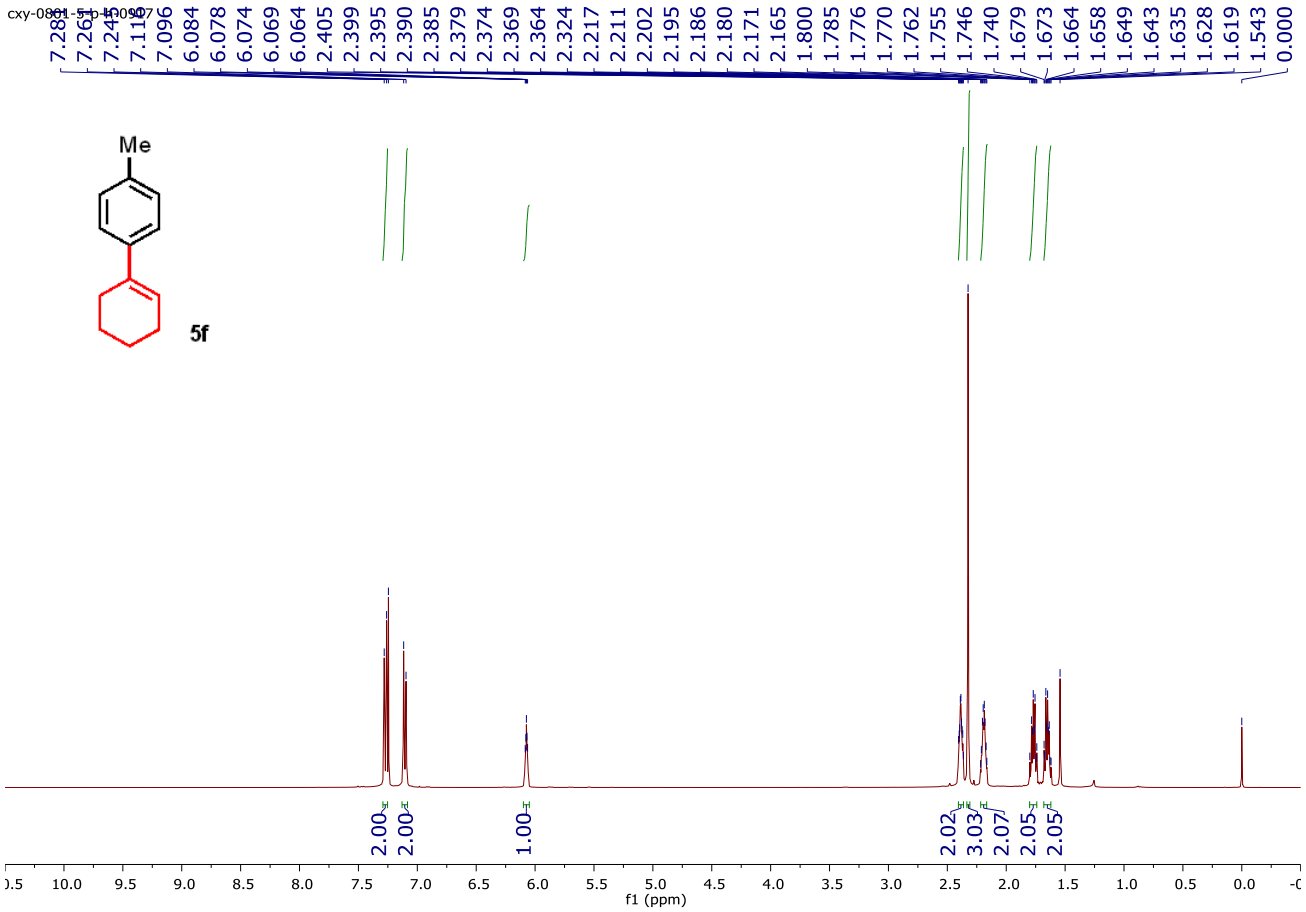

cxy-0801-2-h
7.344
7.332
7.328
7.320
7.315
7.312
7.258
7.246
7.226
7.152
7.132
5.430
5.405
2.368
1.549
-0.000
Me
5a
4.81
2.07
2.02
1.00
1.02
3.03
f1 (ppm)

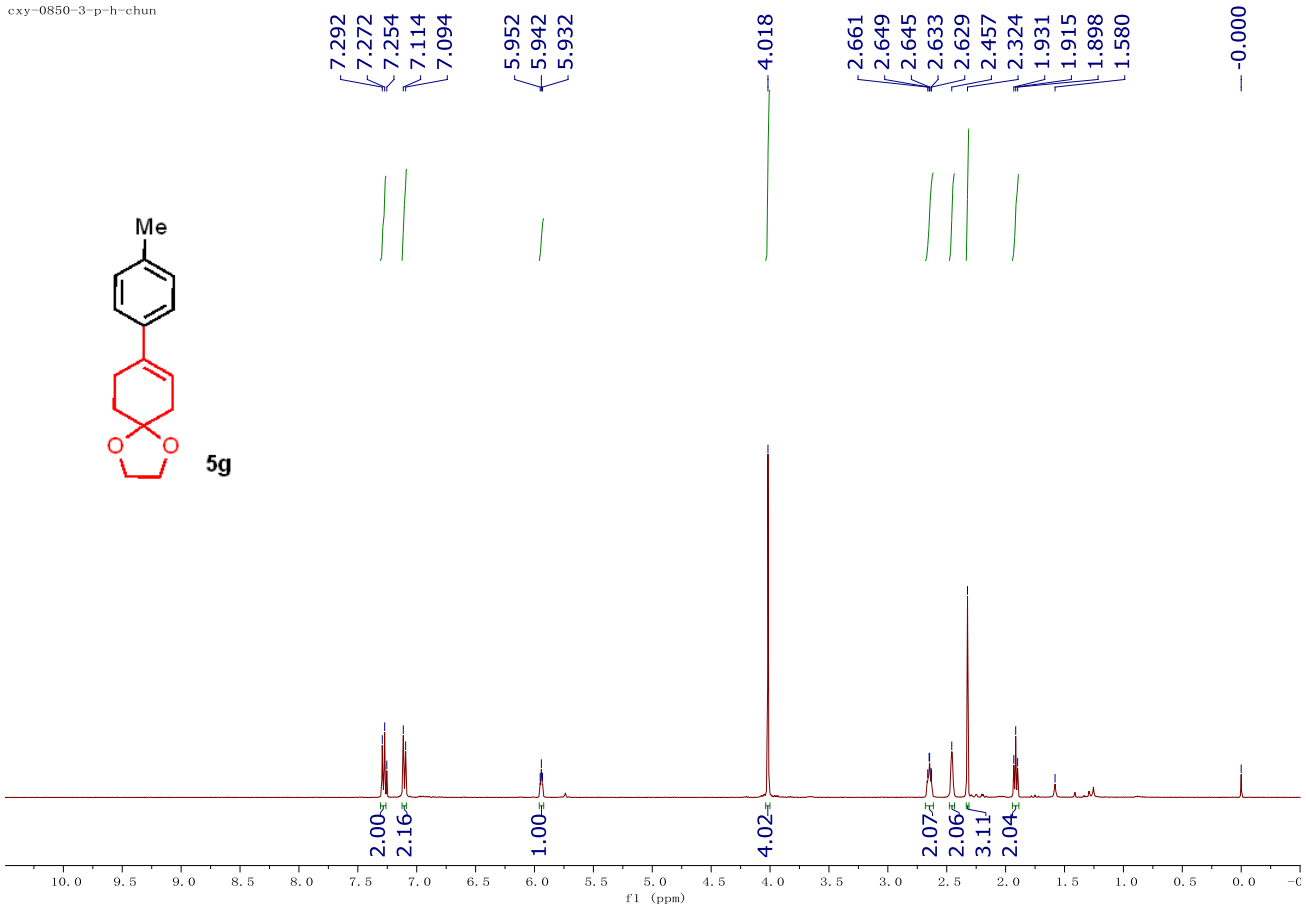

cxy-0801-8-p-chun-h
7.682
7.642
7.432
7.412
7.260
7.199
7.179
6.412
6.372
4.285
4.267
4.250
4.232
2.371
1.620
1.353
1.335
1.317
0.000
Me
CO2Et
5b
1.00
2.00
2.00
1.01
2.02
3.01
3.00
f1 (ppm)

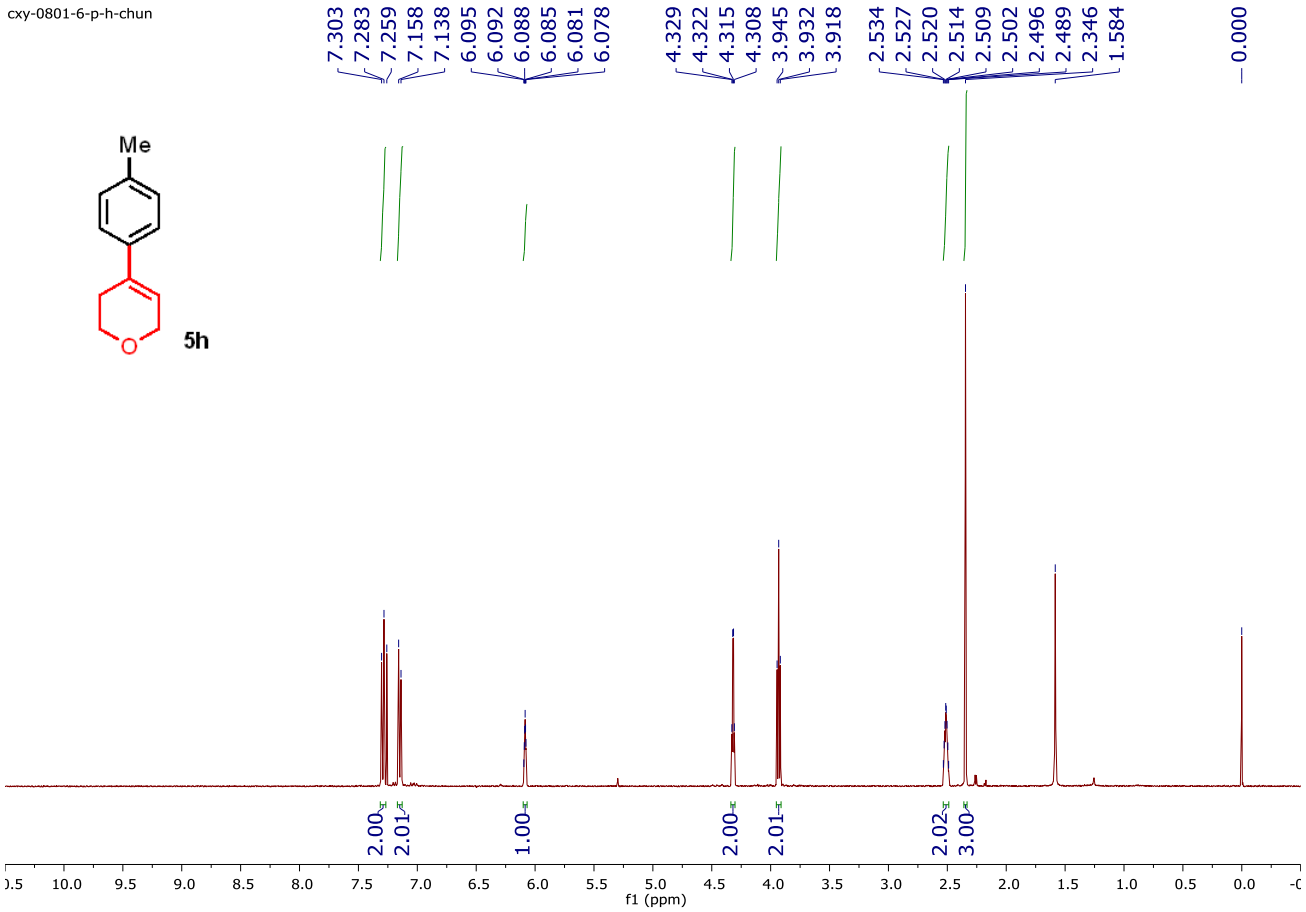

cxy-0886-p-chun-h-1124
Std proton
7.240
7.122
7.100
7.078
6.188
2.377
2.362
2.348
2.327
2.254
2.241
2.227
1.633
1.607
1.562
1.544
1.532
-0.000
Me
5c
4.07
1.00
2.05
3.04
2.05
4.00
2.11
f1 (ppm)

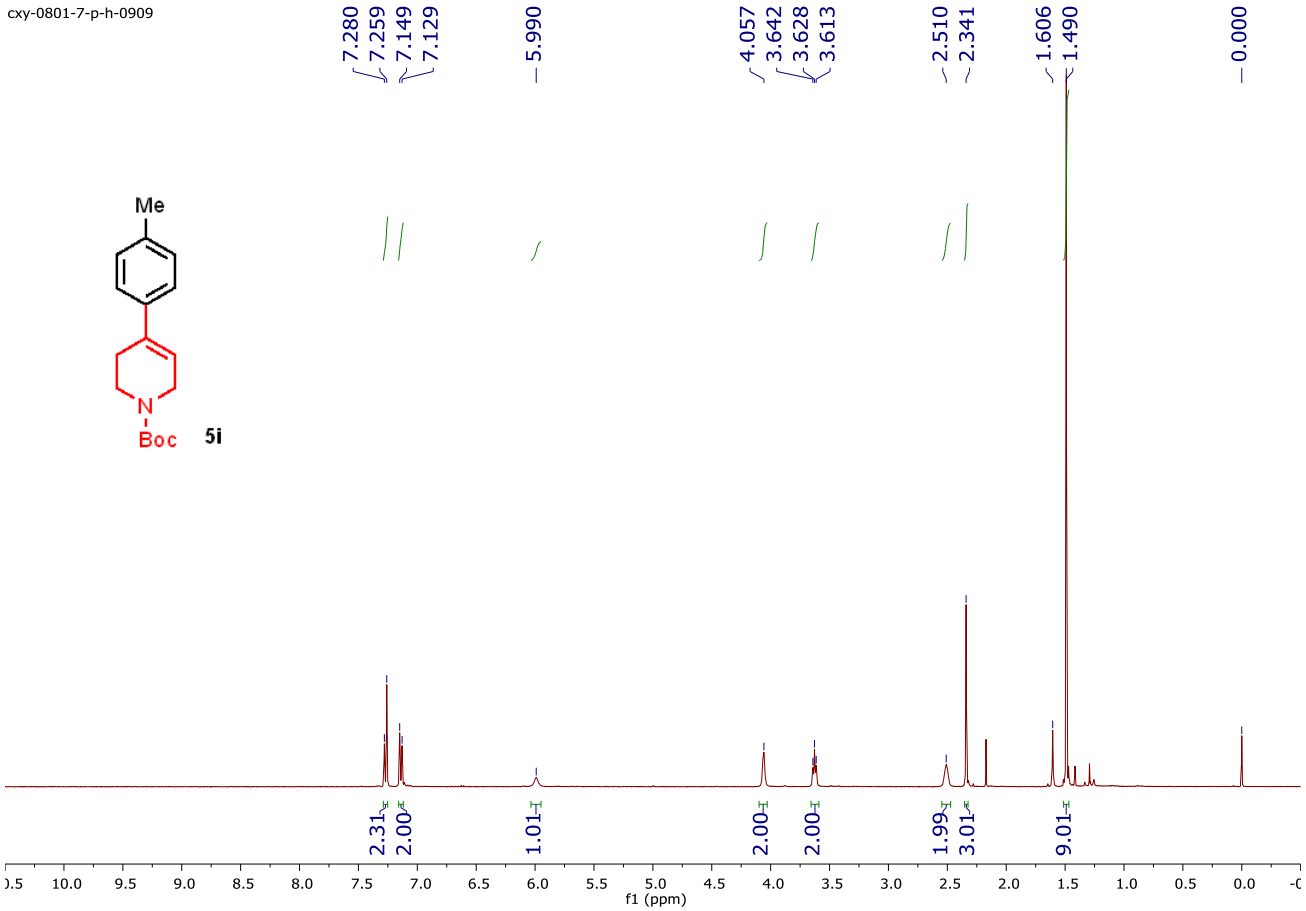

cxy-0871-2-p-chun-h
7.245
7.118
6.231
2.329
1.889
1.852
1.535
0.000
Me
Me
Me
5d
4.00
1.00
2.99
3.03
2.99
f1 (ppm)

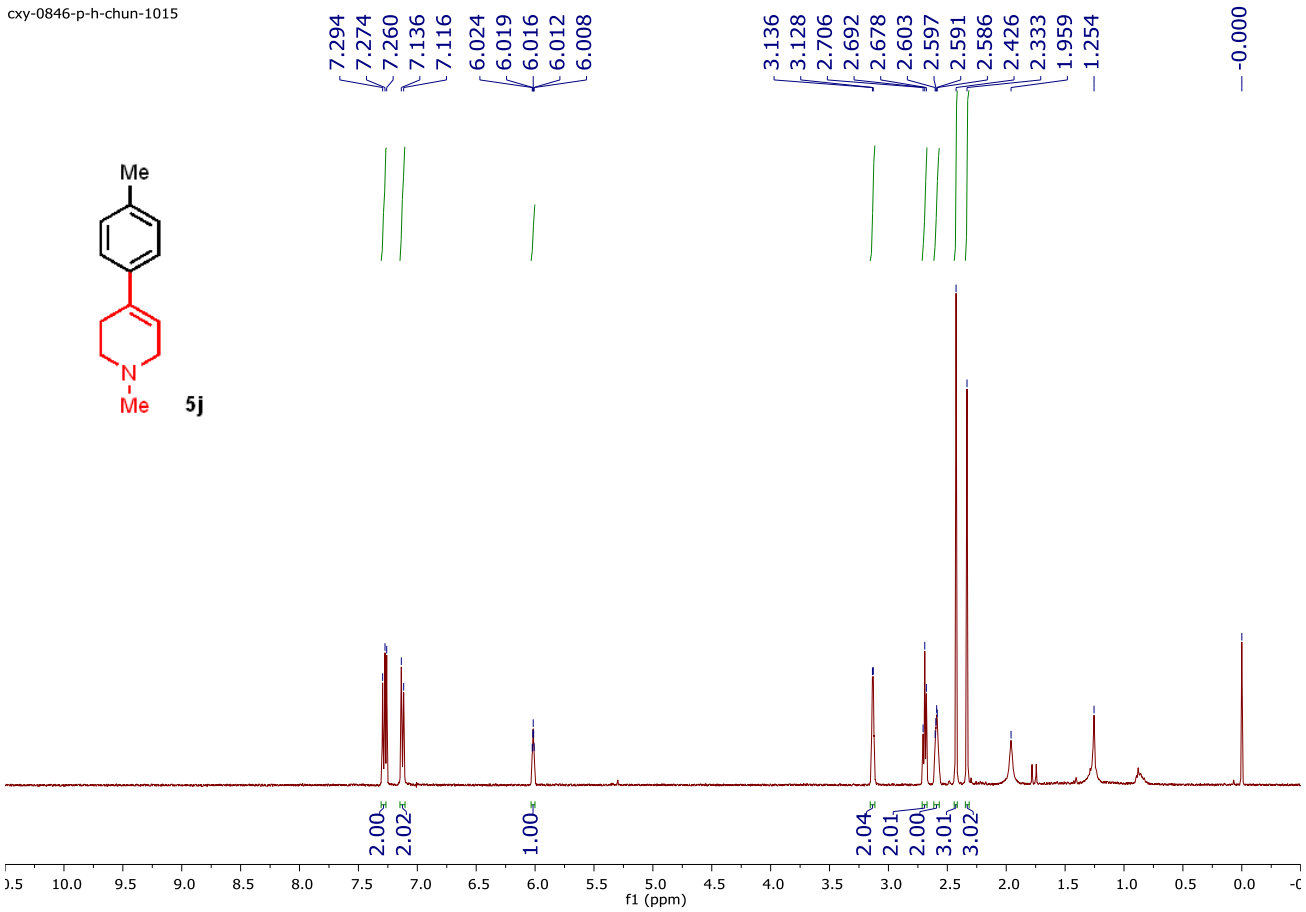

cxy-0871-1-p-h-chun
7.342
7.321
7.250
7.124
7.104
6.132
6.126
6.121
6.115
6.109
2.710
2.705
2.687
2.672
2.667
2.535
2.530
2.516
2.499
2.493
2.331
2.043
2.024
2.006
1.987
1.969
1.536
0.000
Me
5e
2.00
2.00
1.00
2.09
2.12
3.00
2.08
f1 (ppm)

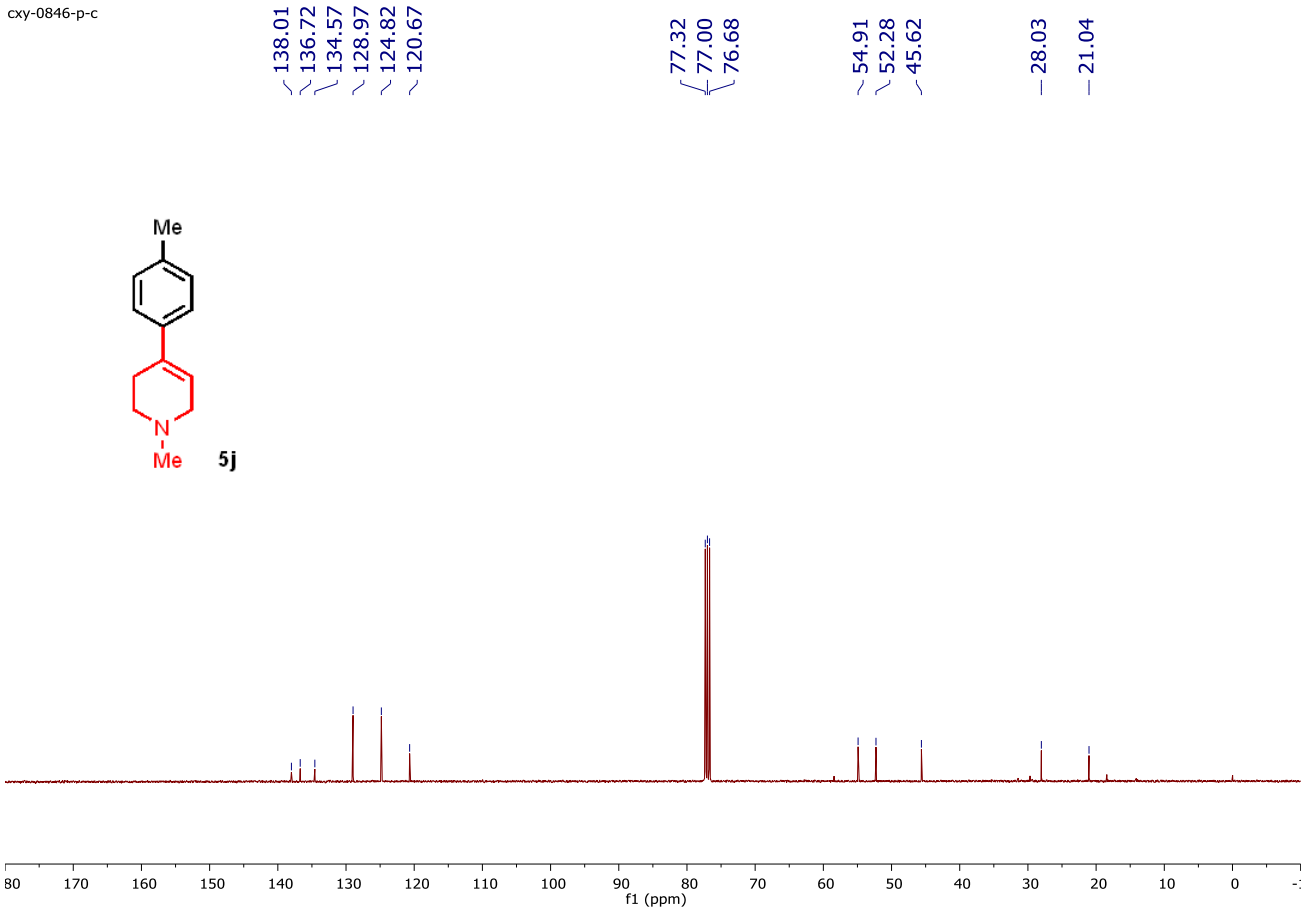

cxy-0861-51-h-090
7.285
7.261
7.241
7.117
7.096
6.084
6.078
6.074
6.069
6.064
2.405
2.399
2.395
2.390
2.385
2.379
2.374
2.369
2.364
2.324
2.217
2.211
2.202
2.195
2.186
2.180
2.171
2.165
1.800
1.785
1.776
1.770
1.762
1.755
1.746
1.740
1.679
1.673
1.664
1.658
1.649
1.643
1.635
1.628
1.619
1.543
0.000
Me
5f
2.00
2.00
1.00
2.02
3.03
2.07
2.05
2.05
f1 (ppm)

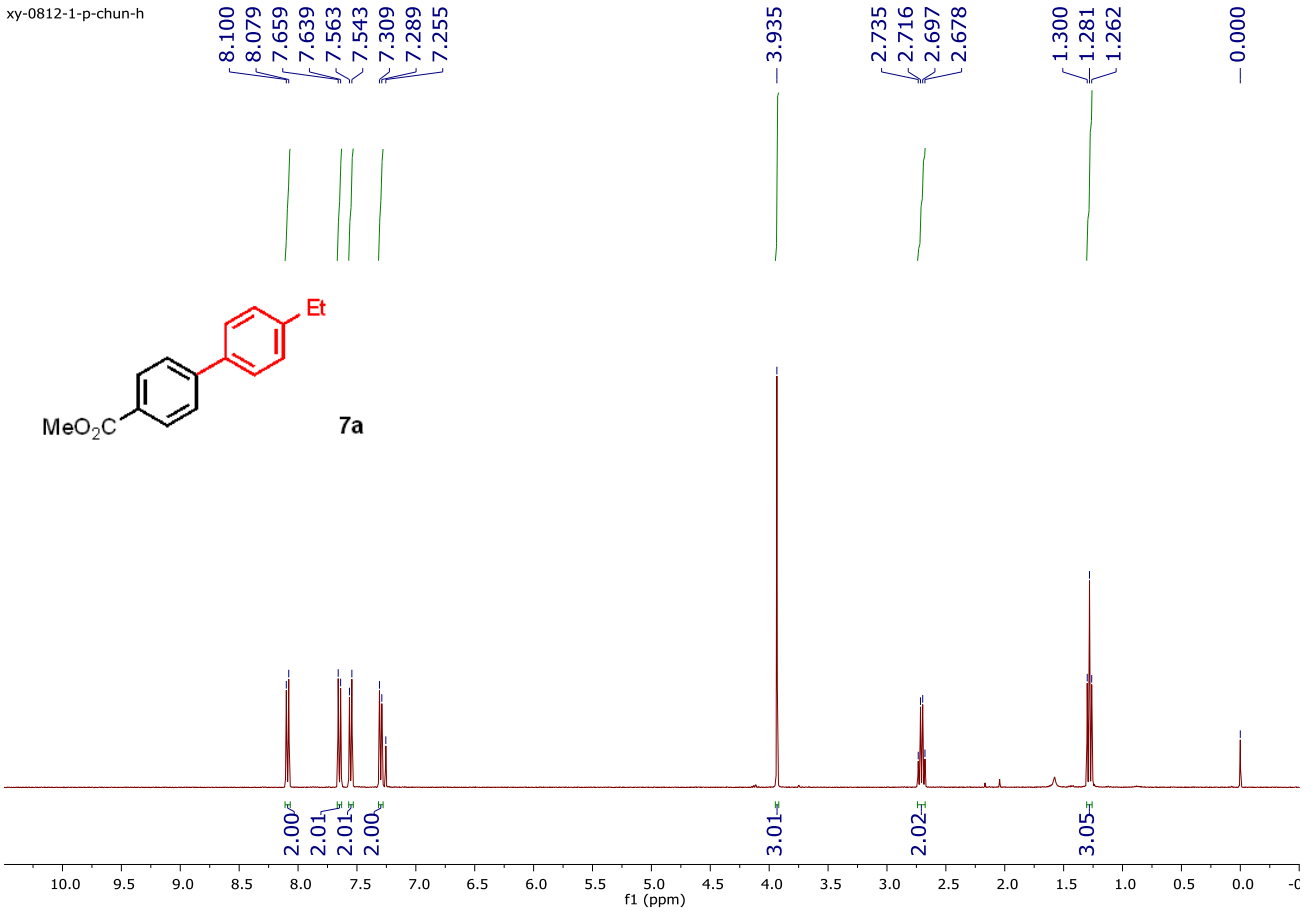

cxy-0850-3-p-h-chun
7.292
7.272
7.254
7.114
7.094
5.952
5.942
5.932
4.018
2.661
2.649
2.645
2.633
2.629
2.457
2.324
1.931
1.915
1.898
1.580
-0.000
Me
5g
2.00
2.16
1.00
4.02
2.07
2.06
3.11
2.04
f1 (ppm)

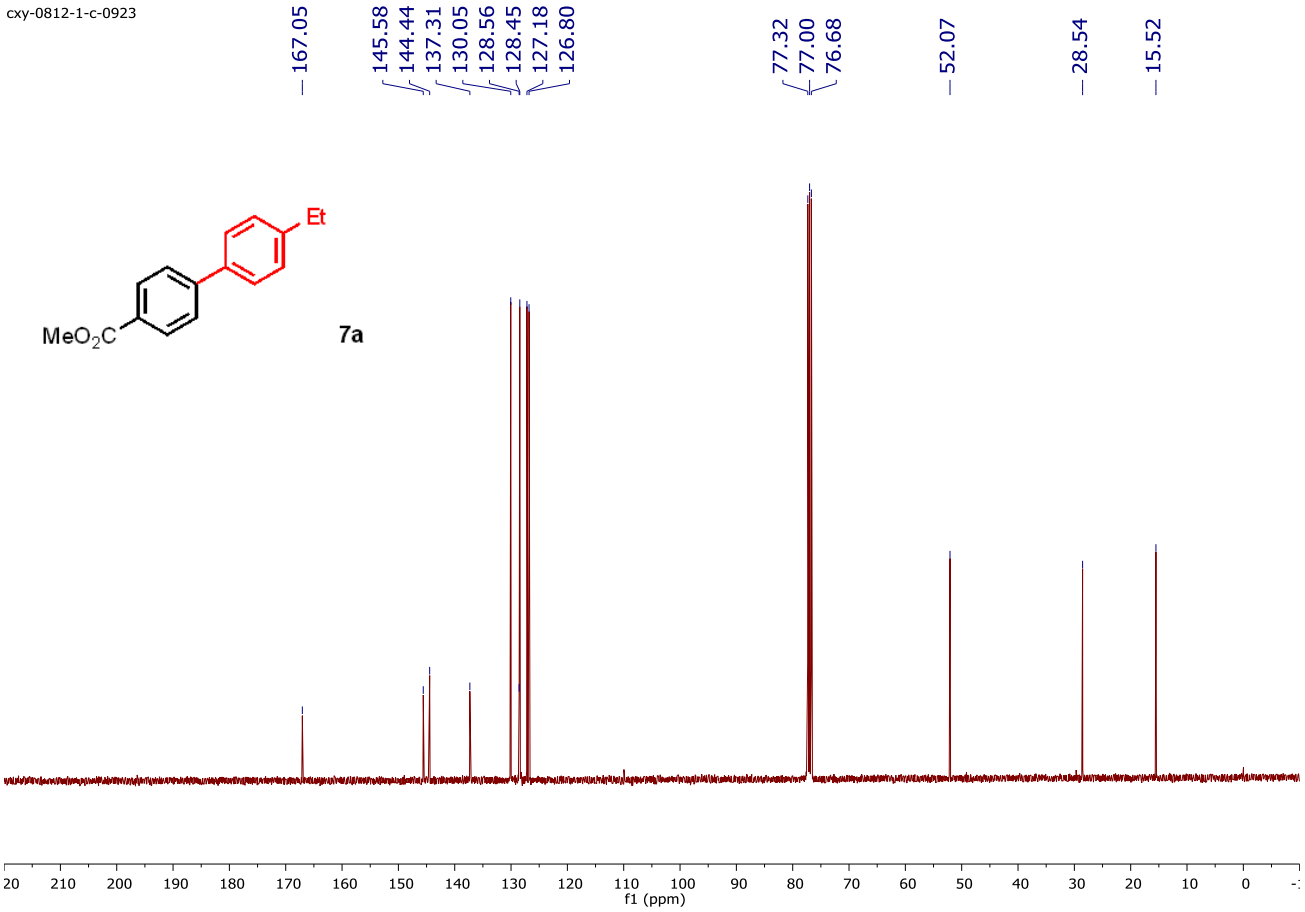

cxy-0801-6-p-h-chun
7.303
7.283
7.259
7.158
7.138
6.095
6.092
6.088
6.085
6.081
6.078
4.329
4.322
4.315
4.308
3.945
3.932
3.918
2.534
2.527
2.520
2.514
2.509
2.502
2.496
2.489
2.346
1.584
0.000
Me
O
5h
2.00
2.01
1.00
2.00
2.01
2.02
3.00
f1 (ppm)

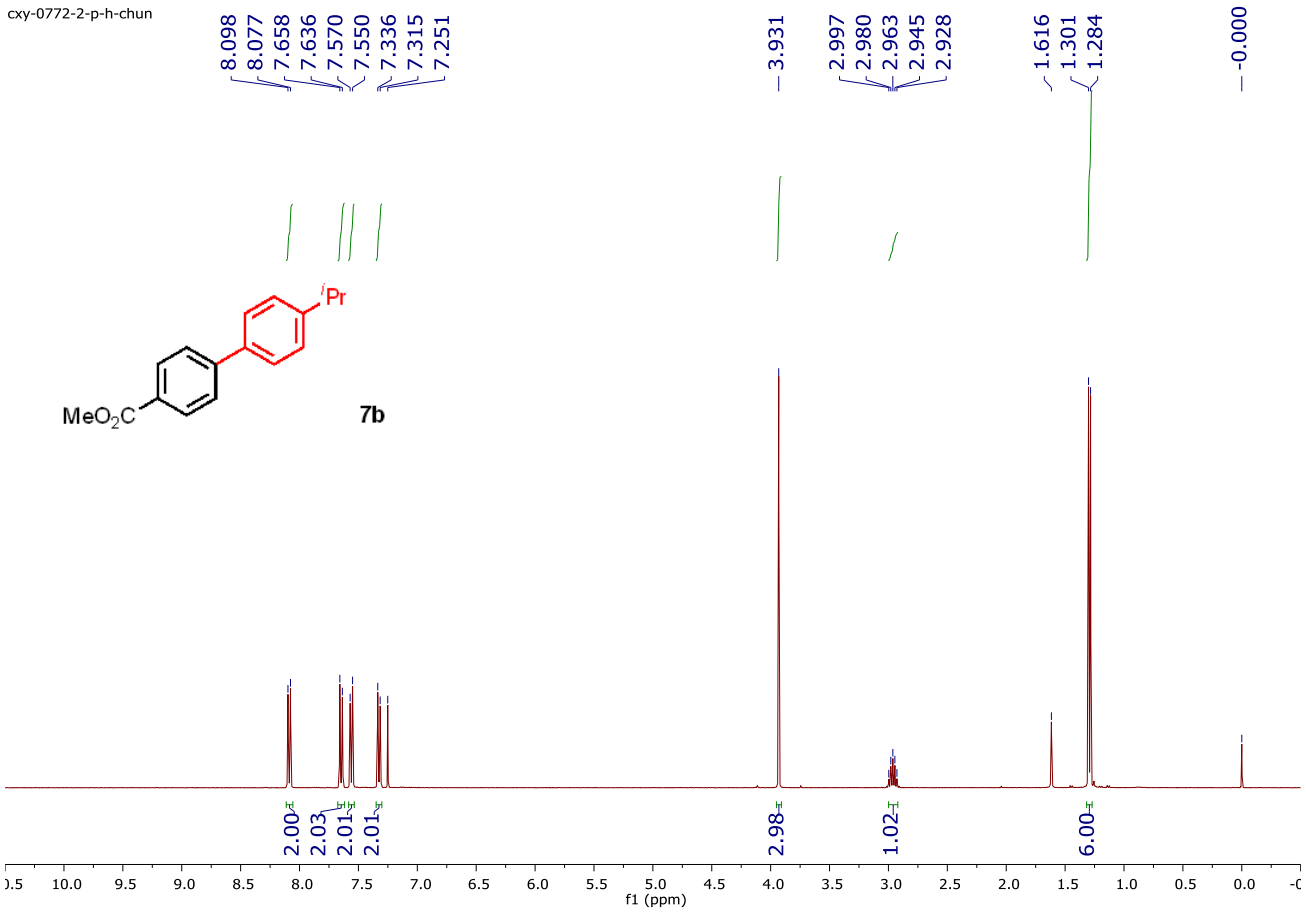

cxy-0801-7-p-h-0909
7.280
7.259
7.149
7.129
5.990
4.057
3.642
3.628
3.613
2.510
2.341
1.606
1.490
0.000
Me
N
Boc
5i
2.31
2.00
1.01
2.00
2.00
1.99
3.01
9.01
f1 (ppm)

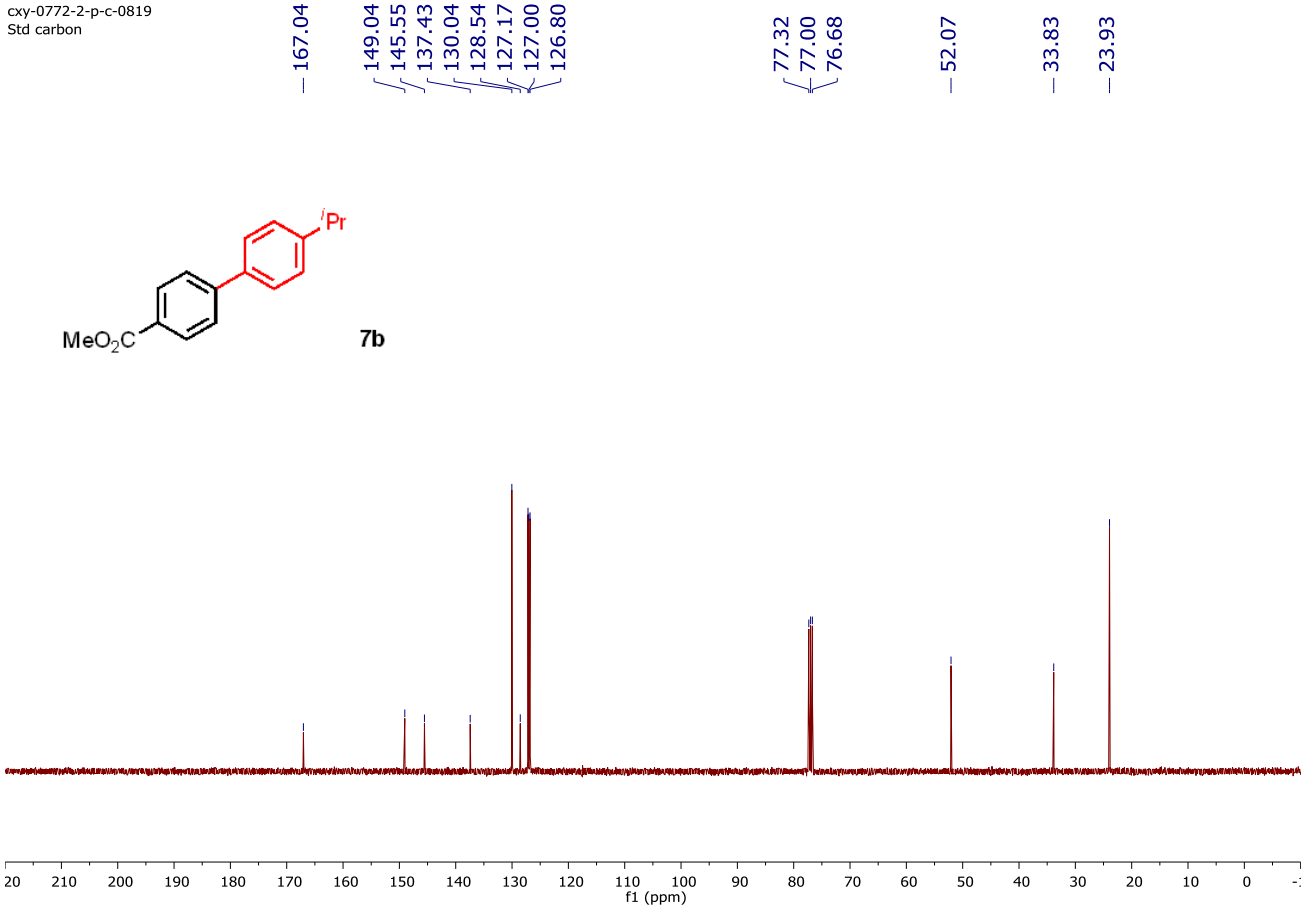

cxy-0846-p-h-chun-1015
7.294
7.274
7.260
7.136
7.116
6.024
6.019
6.016
6.012
6.008
3.136
3.128
2.706
2.692
2.678
2.603
2.597
2.591
2.586
2.426
2.333
1.959
1.254
-0.000
Me
N
Me
5j
2.00
2.02
1.00
2.04
2.01
2.00
3.01
3.02
f1 (ppm)

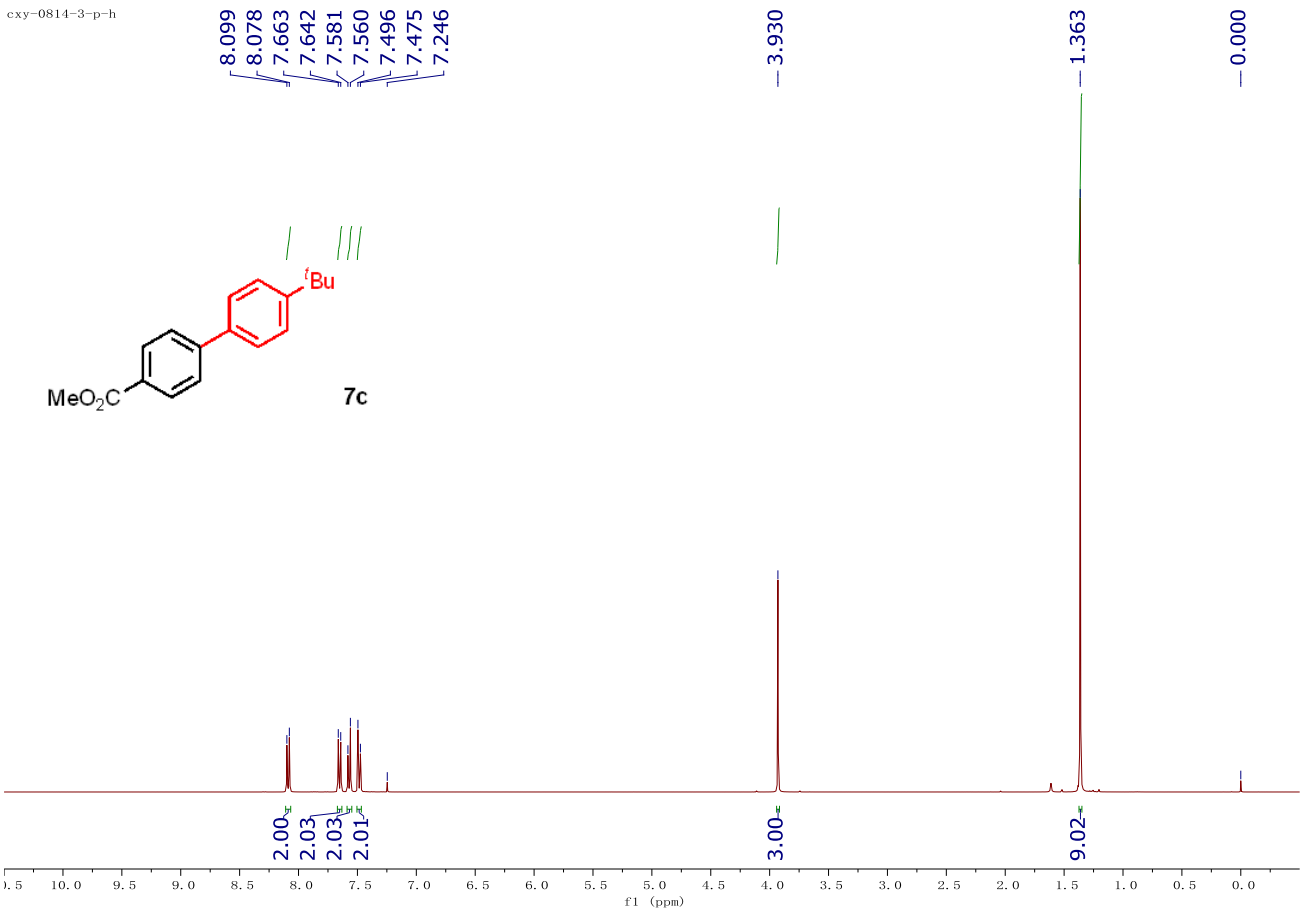

cxy-0846-p-c
138.01
136.72
134.57
128.97
124.82
120.67
77.32
77.00
76.68
54.91
52.28
45.62
28.03
21.04
Me
N
Me
5j
f1 (ppm)

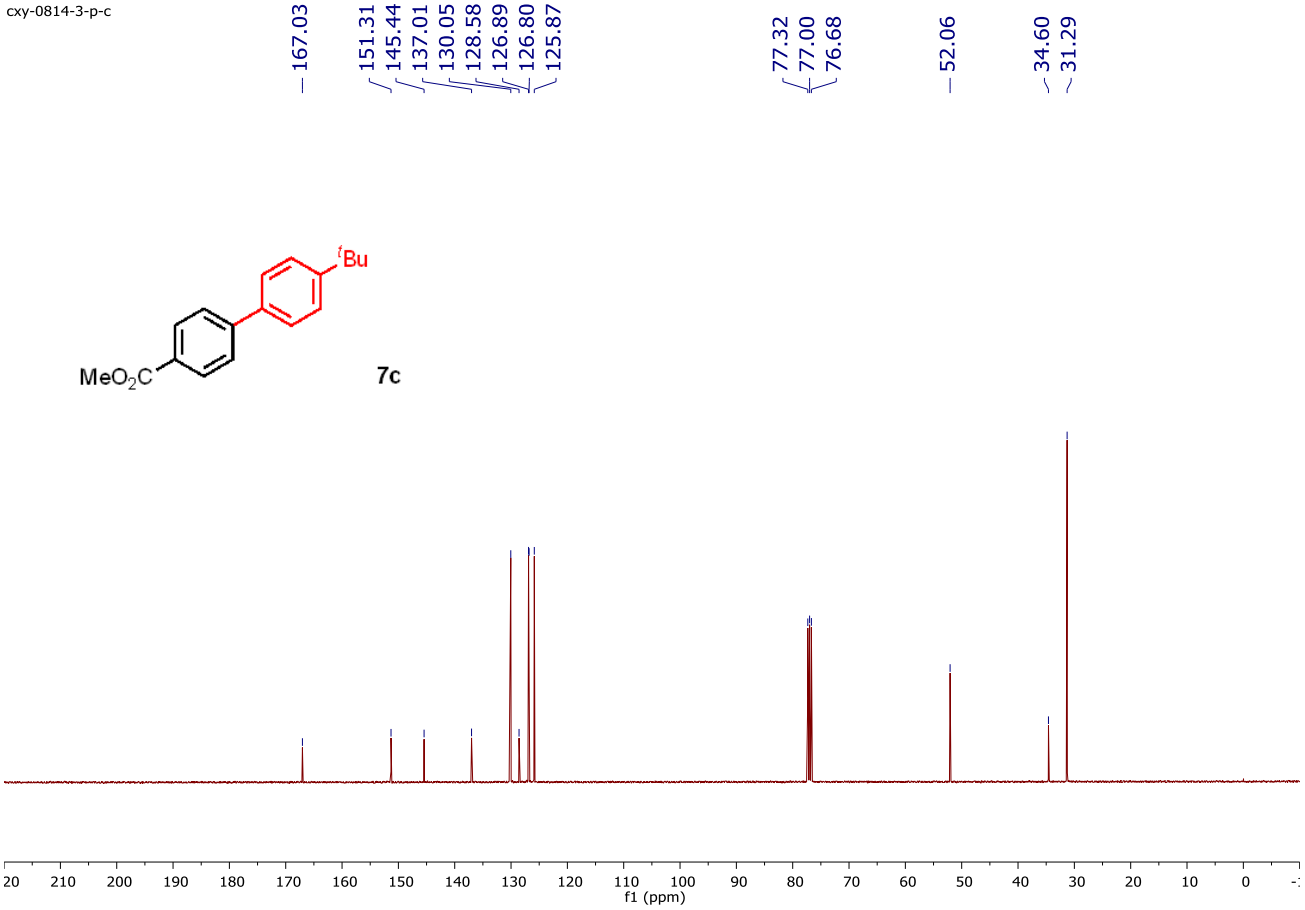

xy-0812-1-p-chun-h
8.100
8.079
7.659
7.639
7.563
7.543
7.309
7.289
7.255
3.935
2.735
2.716
2.697
2.678
1.300
1.281
1.262
0.000
Et
MeO2C
7a
2.00
2.01
2.01
2.00
3.01
2.02
3.05
f1 (ppm)

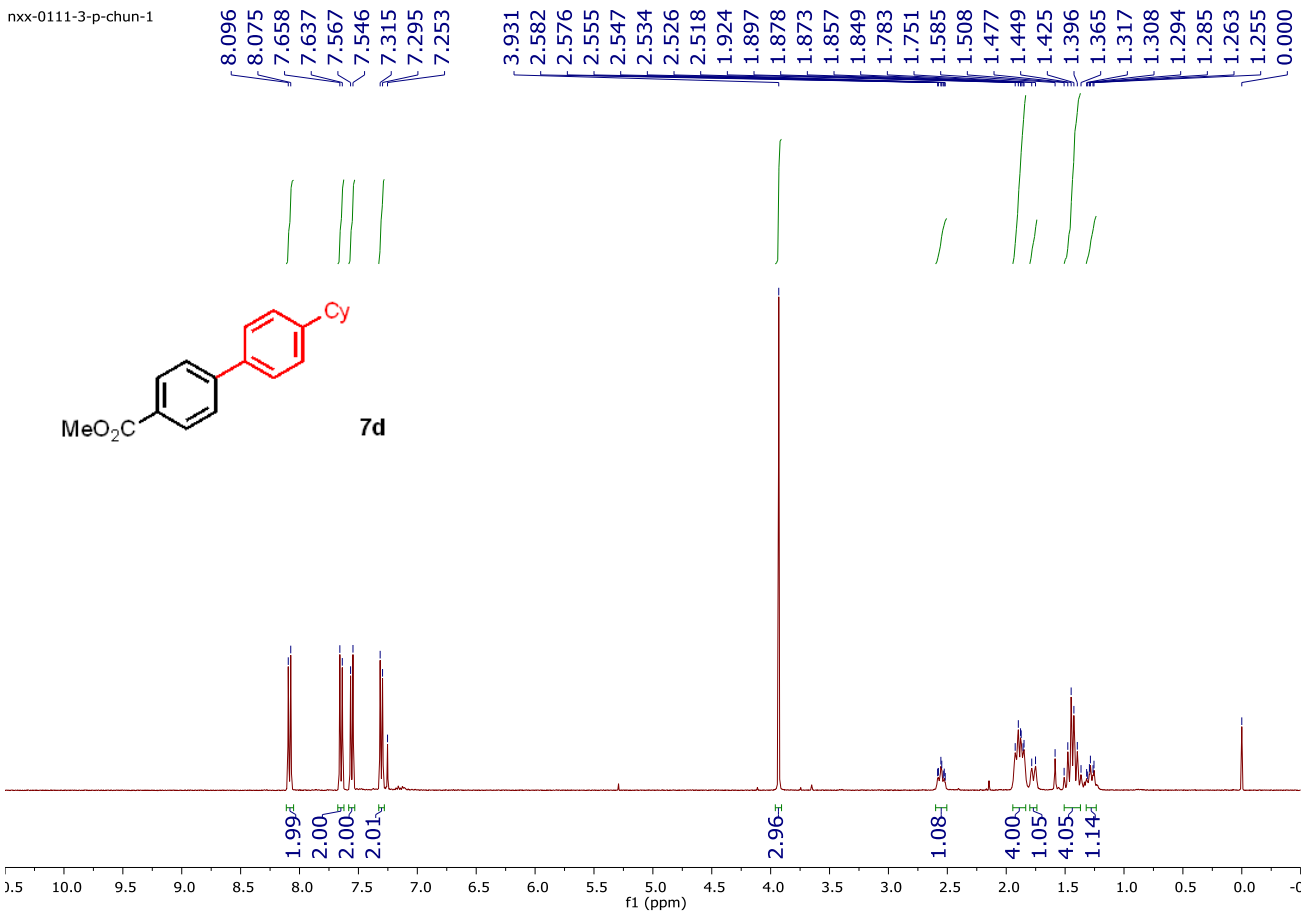

cxy-0812-1-c-0923
167.05
145.58
144.44
137.31
130.05
128.56
128.45
127.18
126.80
77.32
77.00
76.68
52.07
28.54
15.52
Et
MeO2C
7a
f1 (ppm)

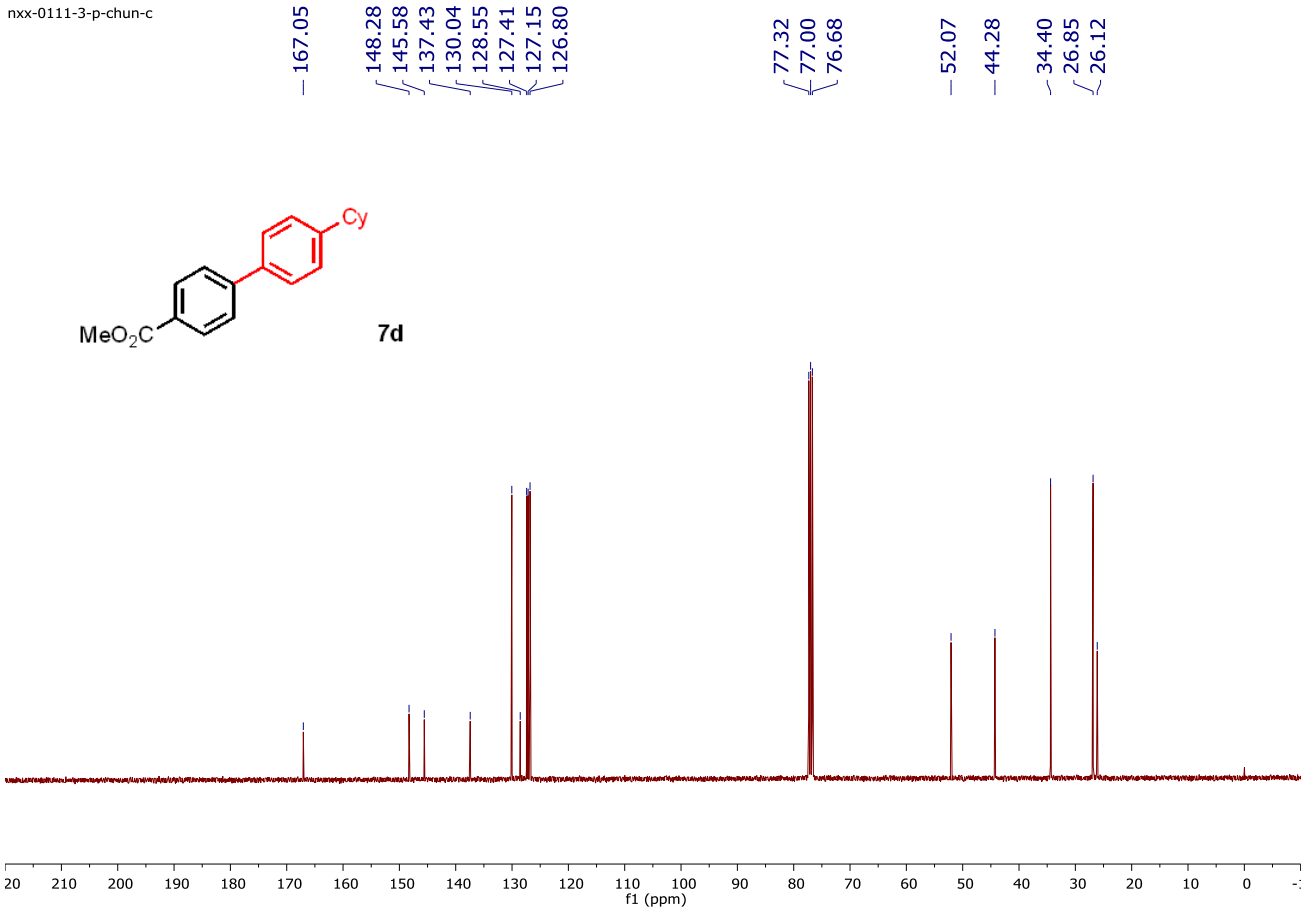

cxy-0772-2-p-h-chun
8.098
8.077
7.658
7.636
7.570
7.550
7.336
7.315
7.251
3.931
2.997
2.980
2.963
2.945
2.928
1.616
1.301
1.284
-0.000
iPr
MeO2C
7b
2.00
2.03
2.01
2.01
2.98
1.02
6.00
f1 (ppm)

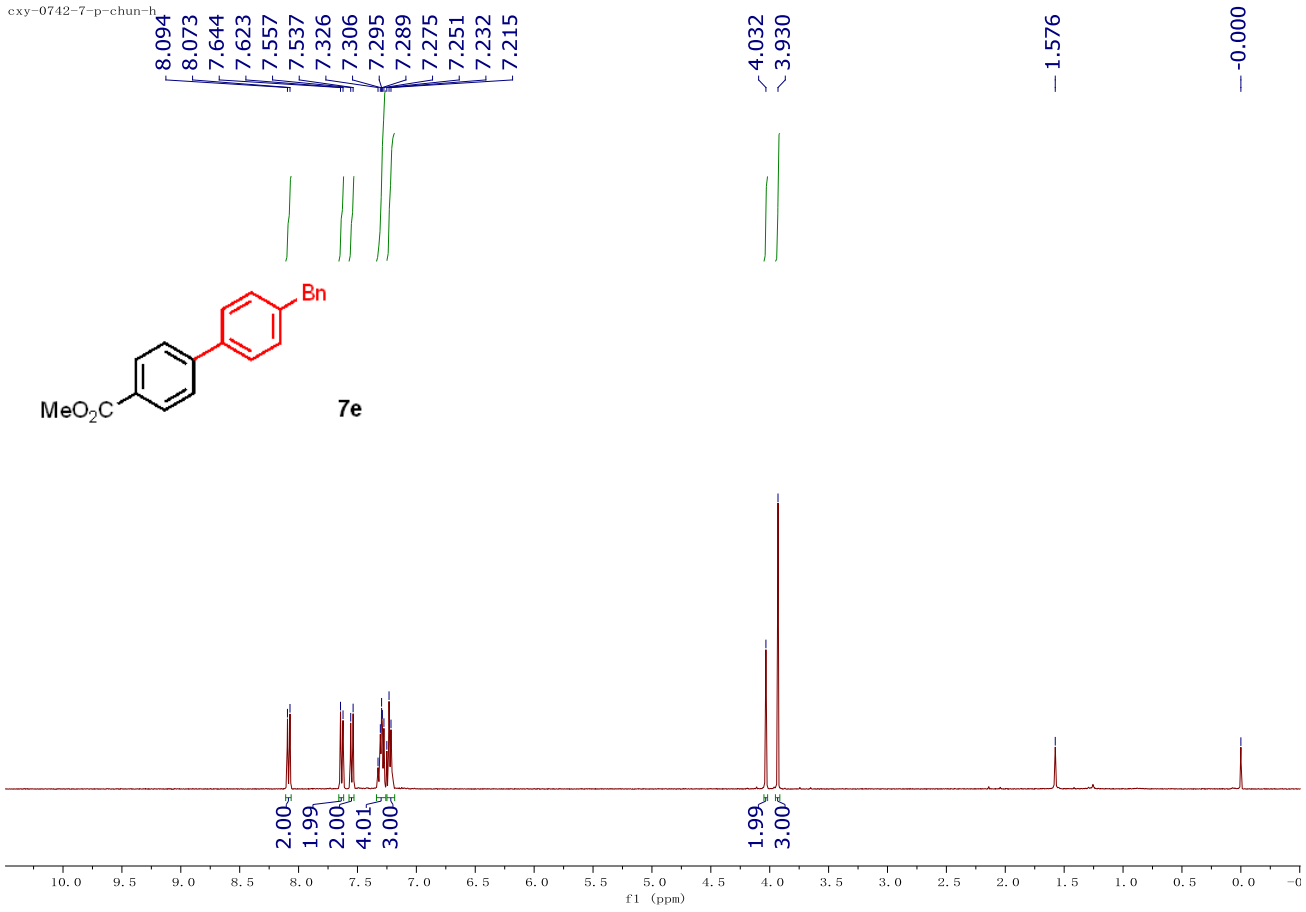

cxy-0772-2-p-c-0819
Std carbon
167.04
149.04
145.55
137.43
130.04
128.54
127.17
127.00
126.80
77.32
77.00
76.68
52.07
33.83
23.93
iPr
MeO2C
7b
f1 (ppm)

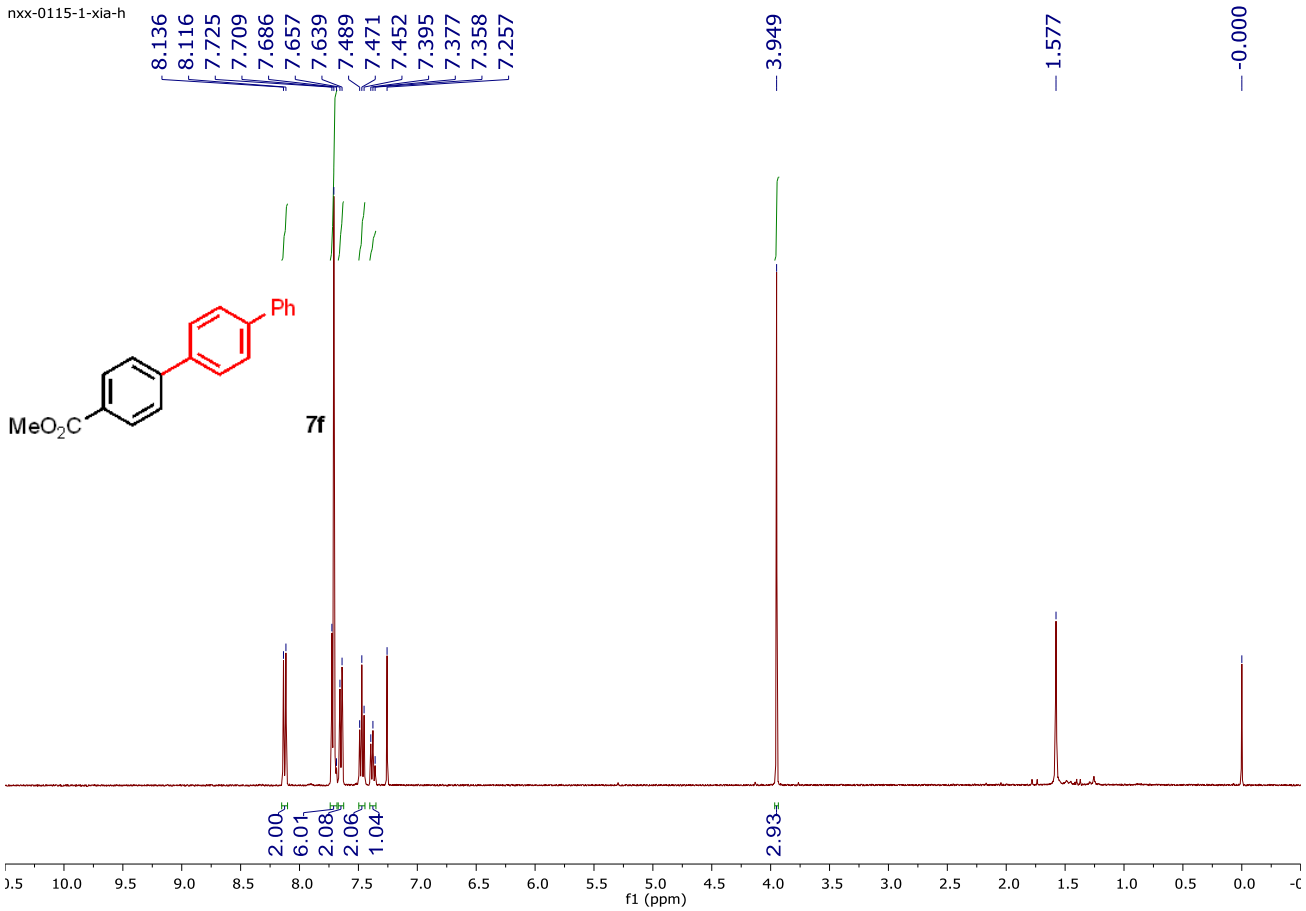

cxy-0814-3-p-h
8.099
8.078
7.663
7.642
7.581
7.560
7.496
7.475
7.246
3.930
1.363
0.000
tBu
MeO2C
7c
2.00
2.03
2.03
2.01
3.00
9.02
f1 (ppm)

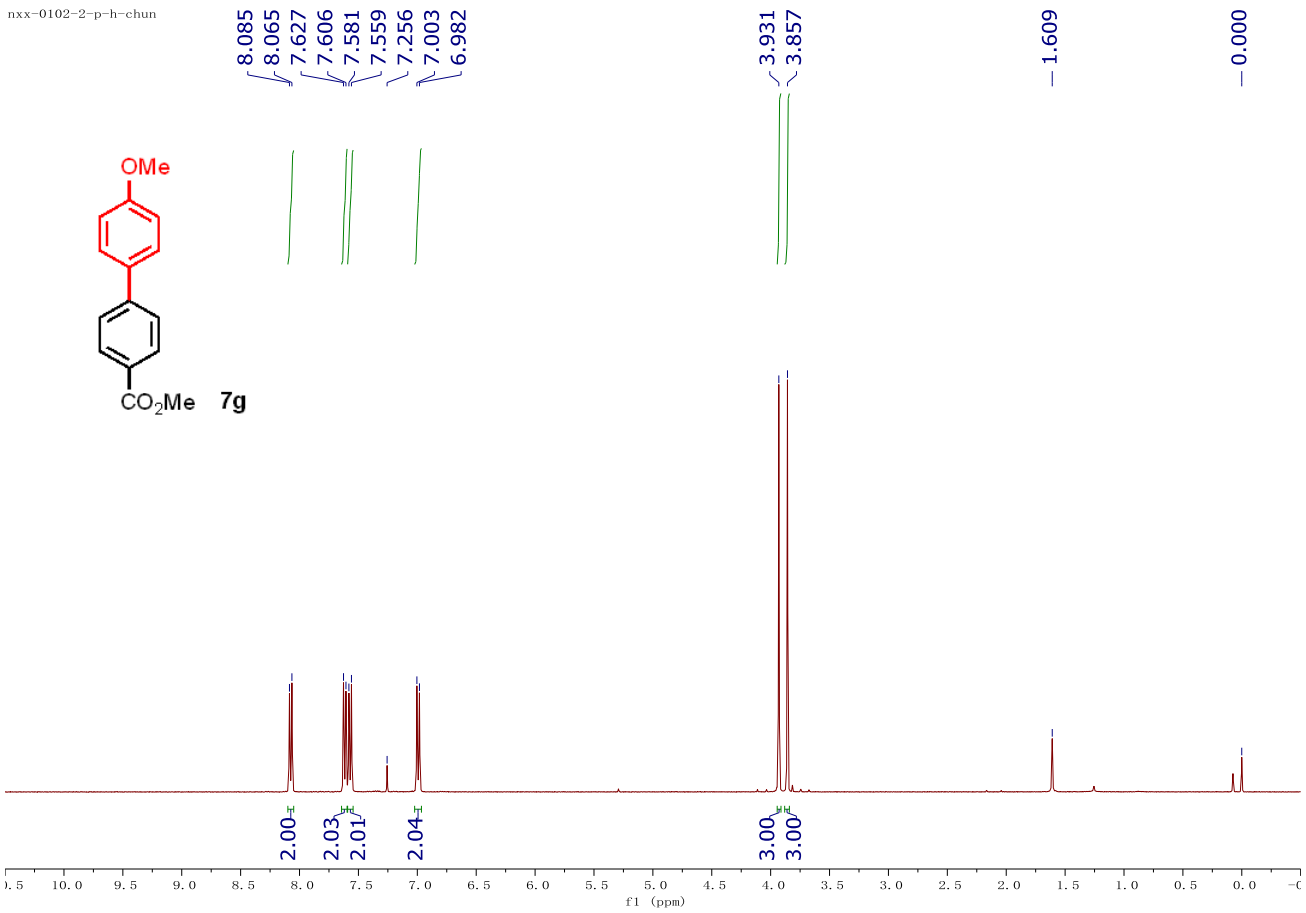

cxy-0814-3-p-c
167.03
151.31
145.44
137.01
130.05
128.58
126.89
126.80
125.87
77.32
77.00
76.68
52.06
34.60
31.29
tBu
MeO2C
7c
f1 (ppm)

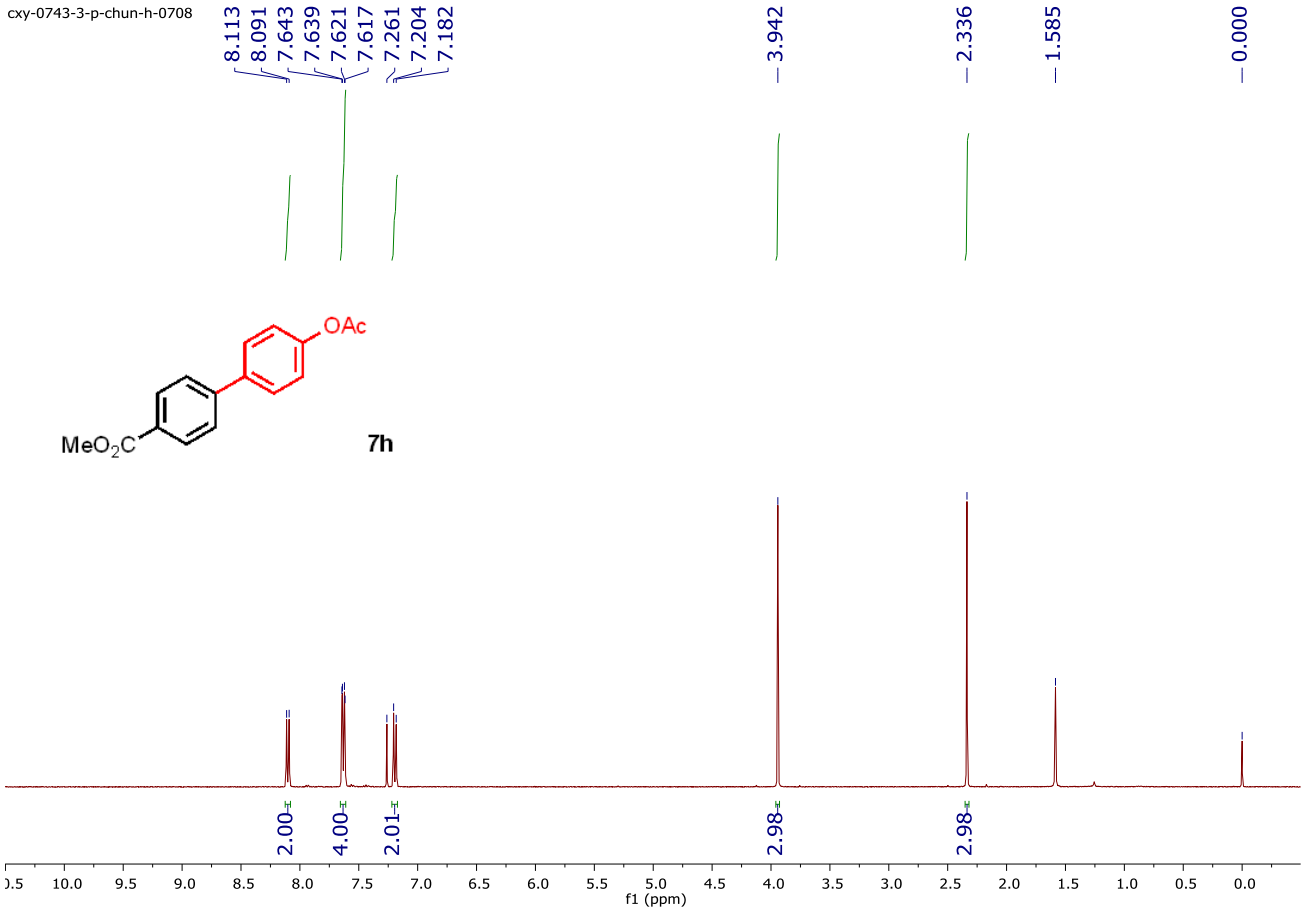

nxx-0111-3-p-chun-1
8.096
8.075
7.658
7.637
7.567
7.546
7.315
7.295
7.253
3.931
2.582
2.576
2.555
2.547
2.534
2.526
2.518
1.924
1.897
1.878
1.873
1.857
1.849
1.783
1.751
1.585
1.508
1.477
1.449
1.425
1.396
1.365
1.317
1.308
1.294
1.285
1.263
1.255
0.000
Cy
MeO2C
7d
1.99
2.00
2.00
2.01
2.96
1.08
4.00
1.05
4.05
1.14
f1 (ppm)

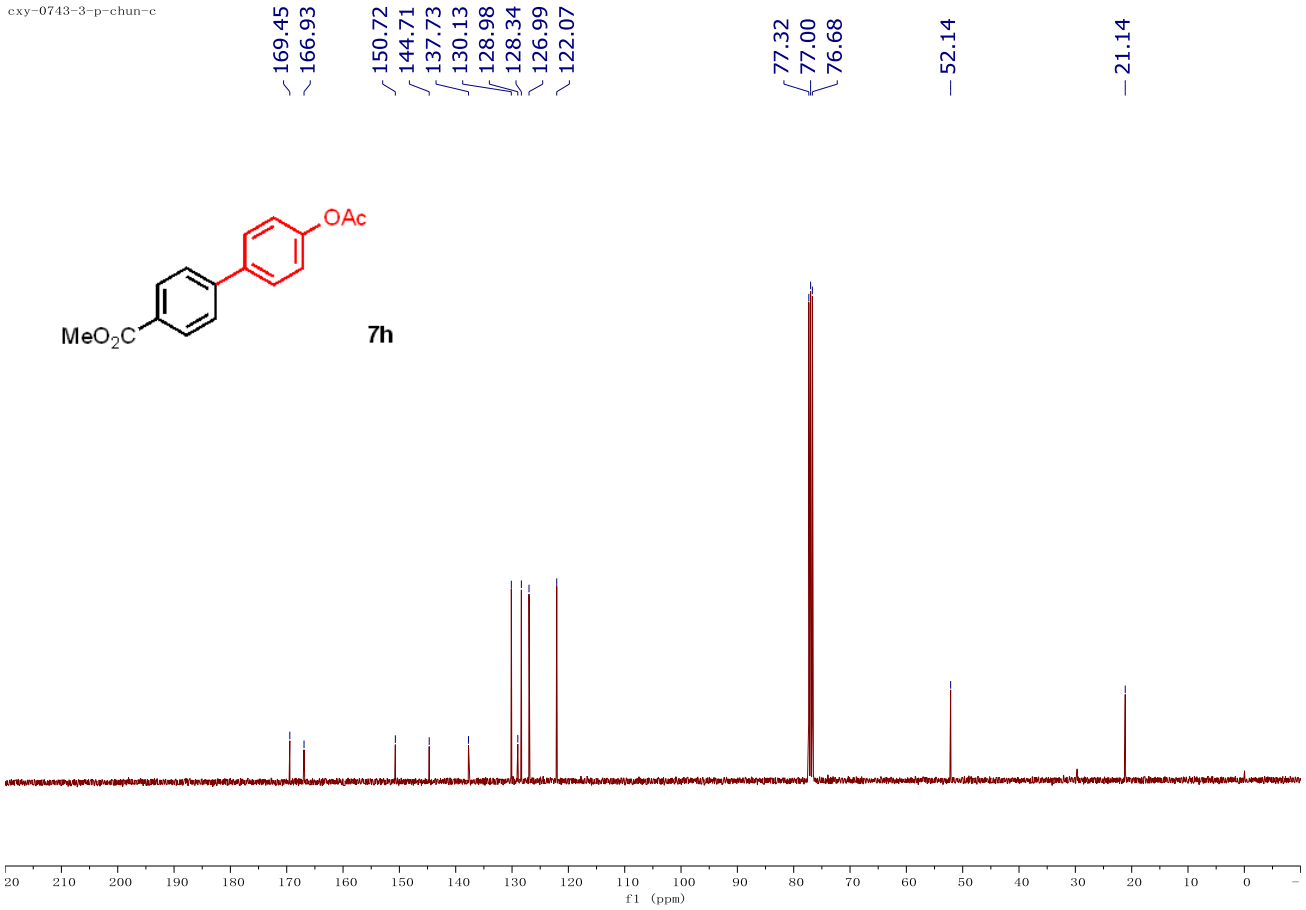

nxx-0111-3-p-chun-c
167.05
148.28
145.58
137.43
130.04
128.55
127.41
127.15
126.80
77.32
77.00
76.68
52.07
44.28
34.40
26.85
26.12
Cy
MeO2C
7d
f1 (ppm)

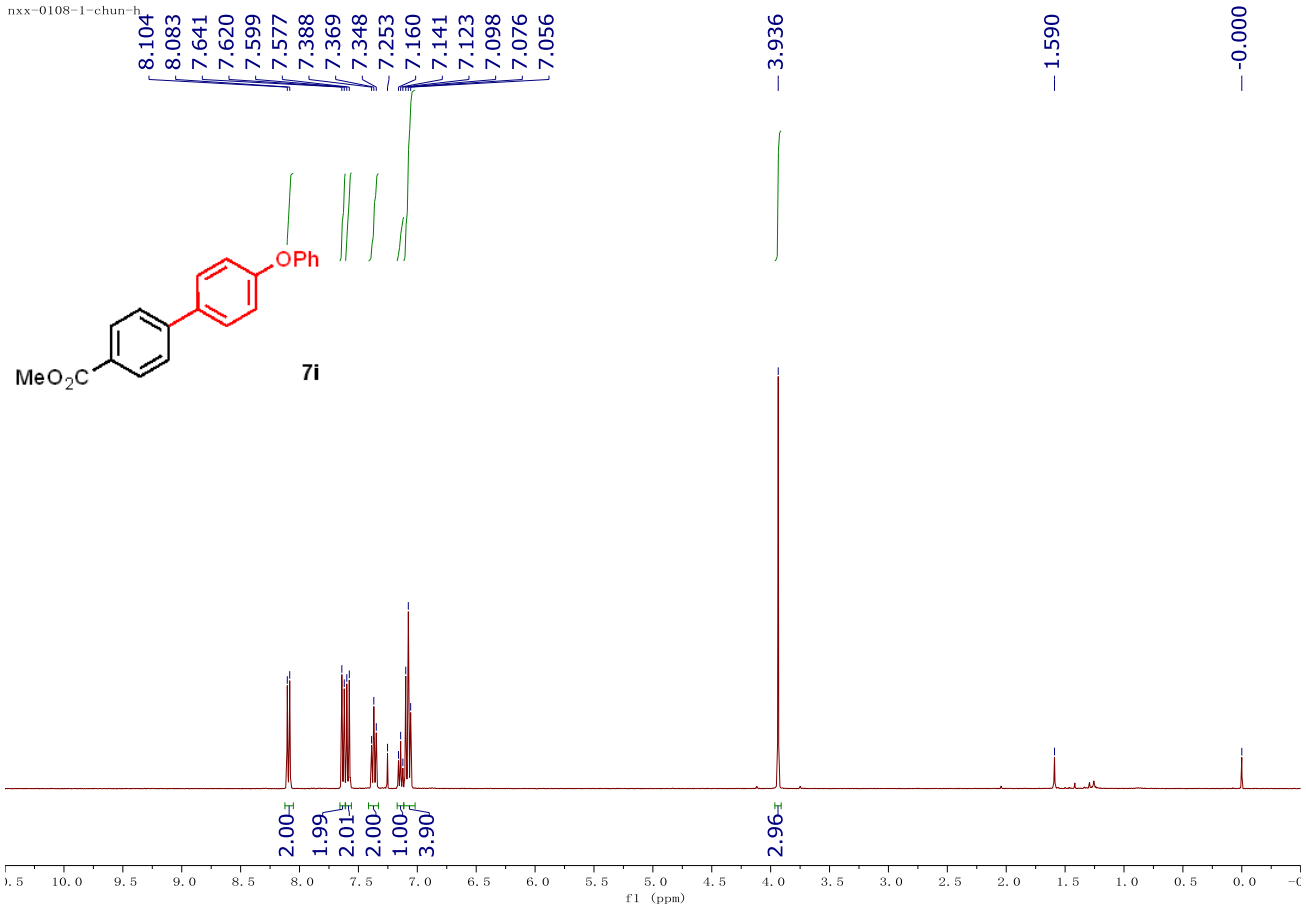

cxy-0742-7-p-chun-h
8.094
8.073
7.644
7.623
7.557
7.537
7.326
7.306
7.295
7.289
7.275
7.251
7.232
7.215
4.032
3.930
1.576
-0.000
Bn
MeO2C
7e
2.00
1.99
2.00
4.01
3.00
1.99
3.00
f1 (ppm)

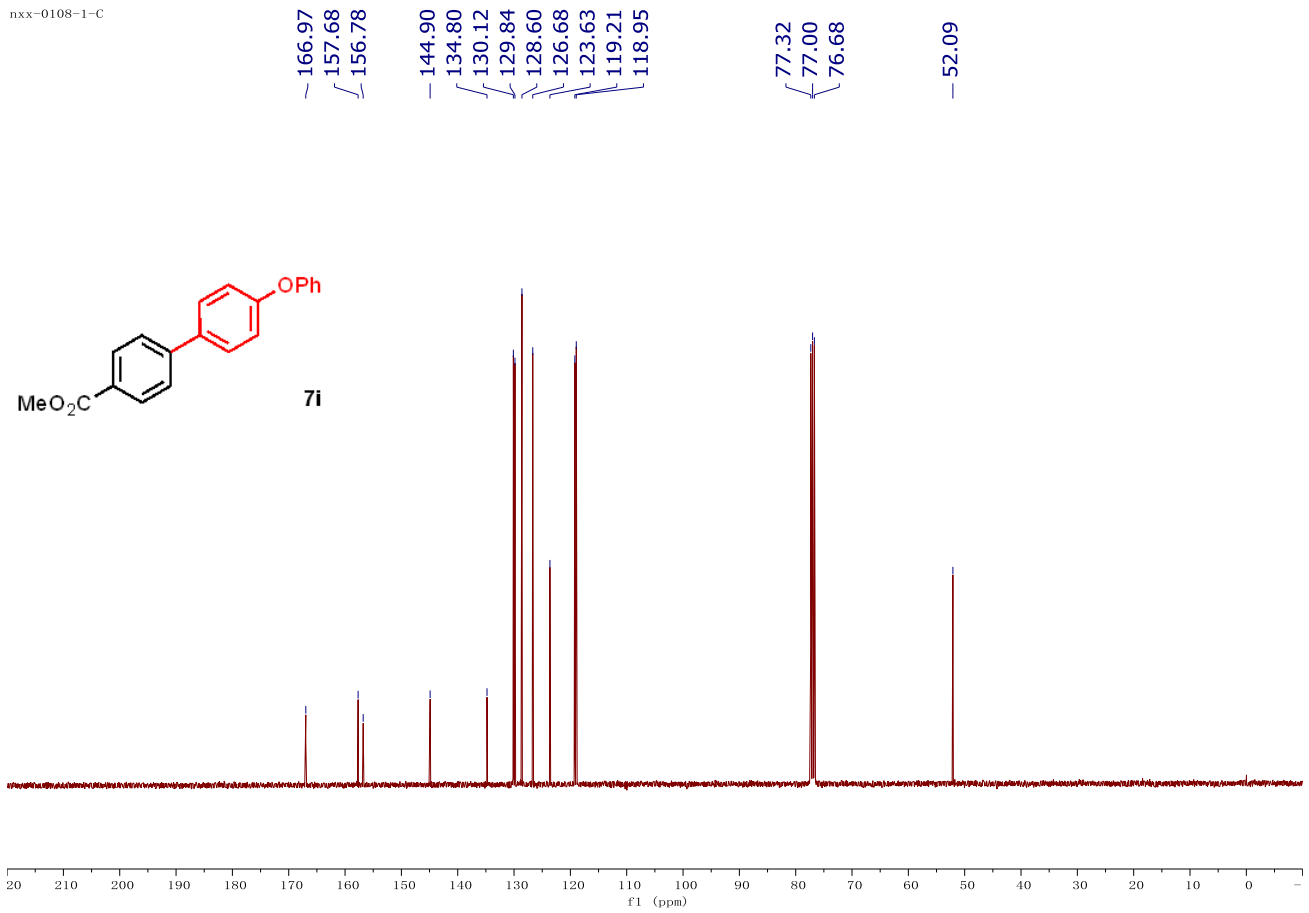

nxx-0115-1-xia-h
8.136
8.116
7.725
7.709
7.686
7.657
7.639
7.489
7.471
7.452
7.395
7.377
7.358
7.257
3.949
1.577
-0.000
Ph
MeO2C
7f
2.00
6.01
2.08
2.06
1.04
2.93
f1 (ppm)

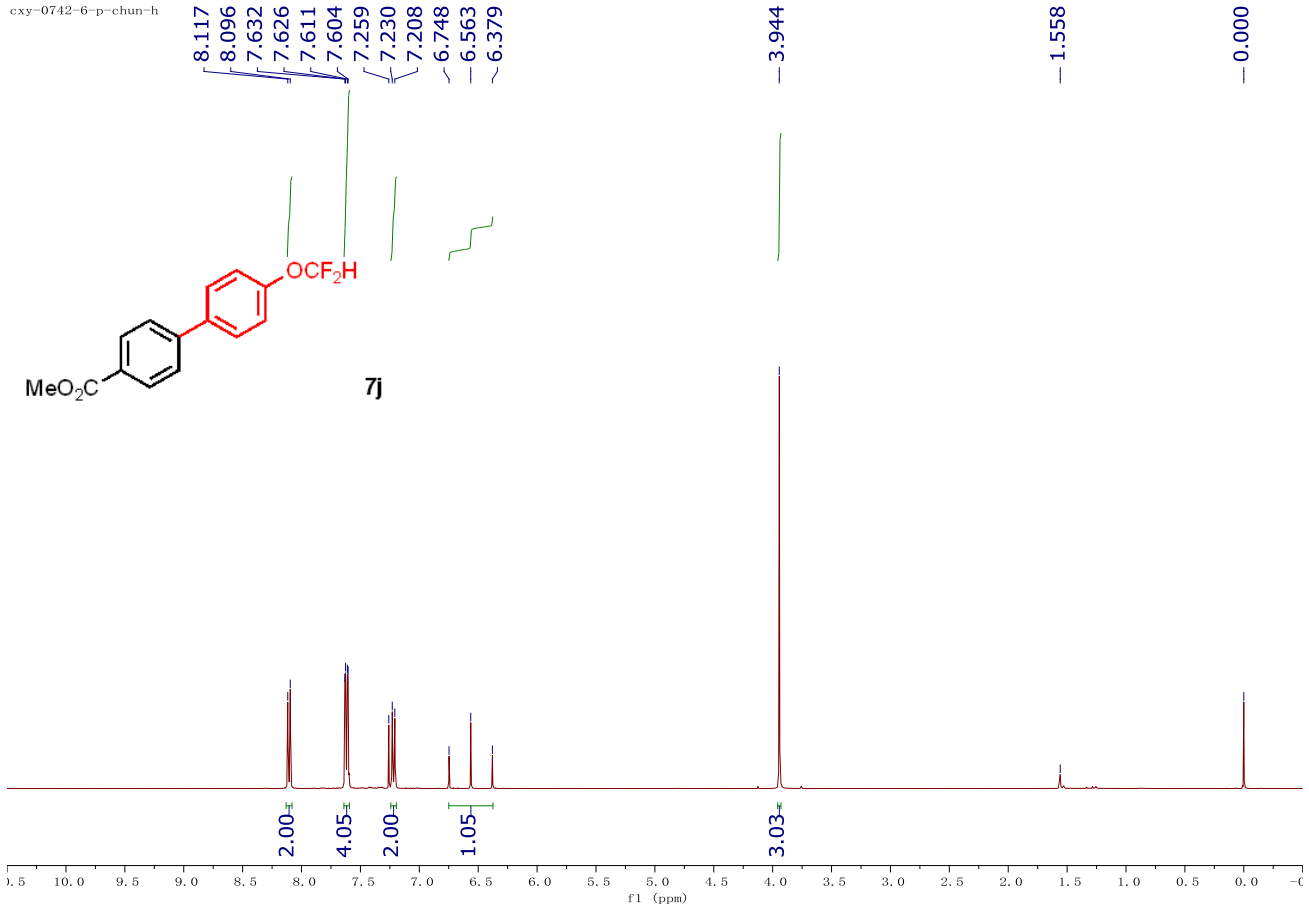

nxx-0102-2-p-h-chun
8.085
8.065
7.627
7.606
7.581
7.559
7.256
7.003
6.982
3.931
3.857
1.609
0.000
OMe
CO2Me
7g
2.00
2.03
2.01
2.04
3.00
3.00
f1 (ppm)

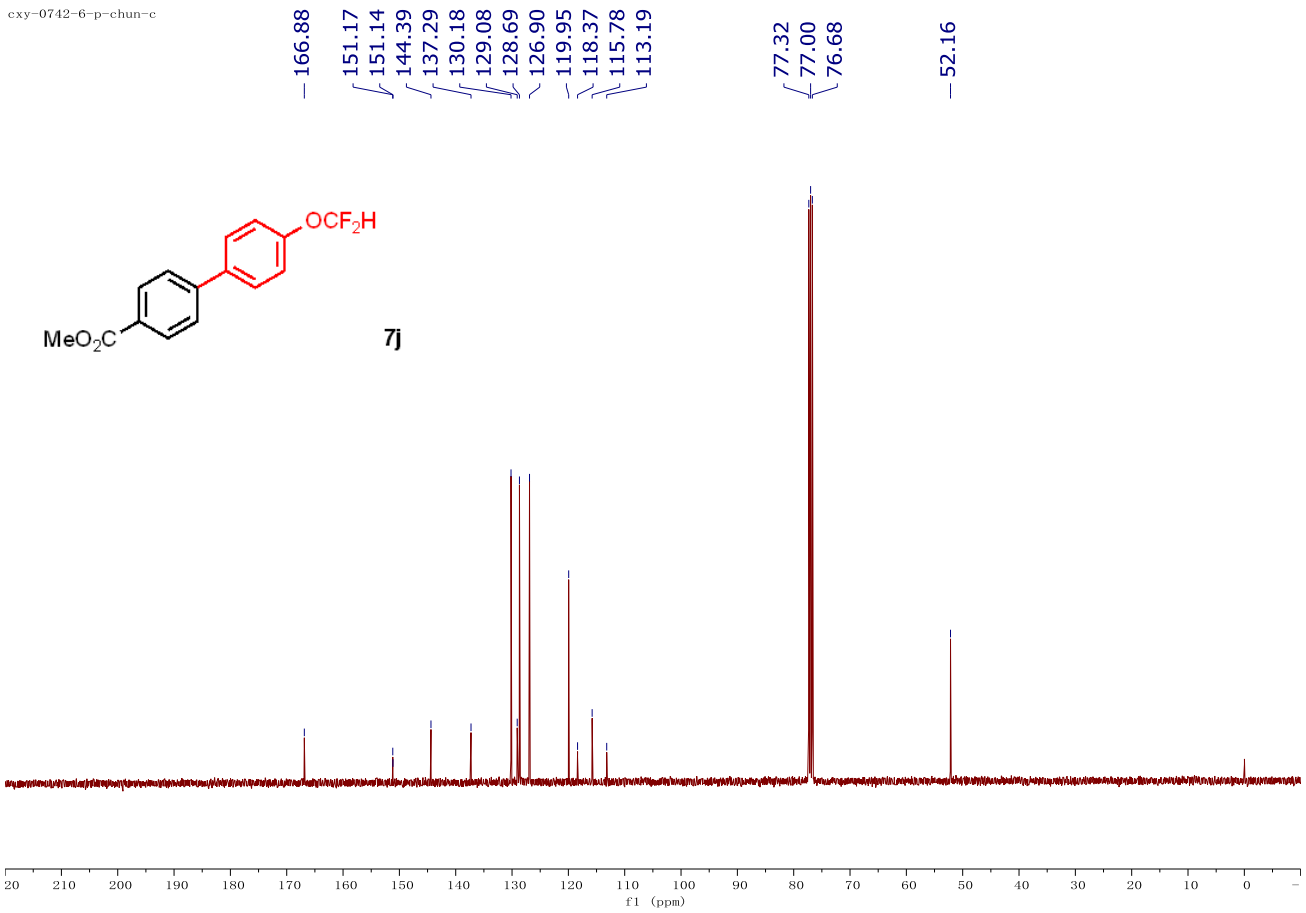

cxy-0743-3-p-chun-h-0708
8.113
8.091
7.643
7.639
7.621
7.617
7.261
7.204
7.182
3.942
2.336
1.585
0.000
OAc
MeO2C
7h
2.00
4.00
2.01
2.98
2.98
f1 (ppm)

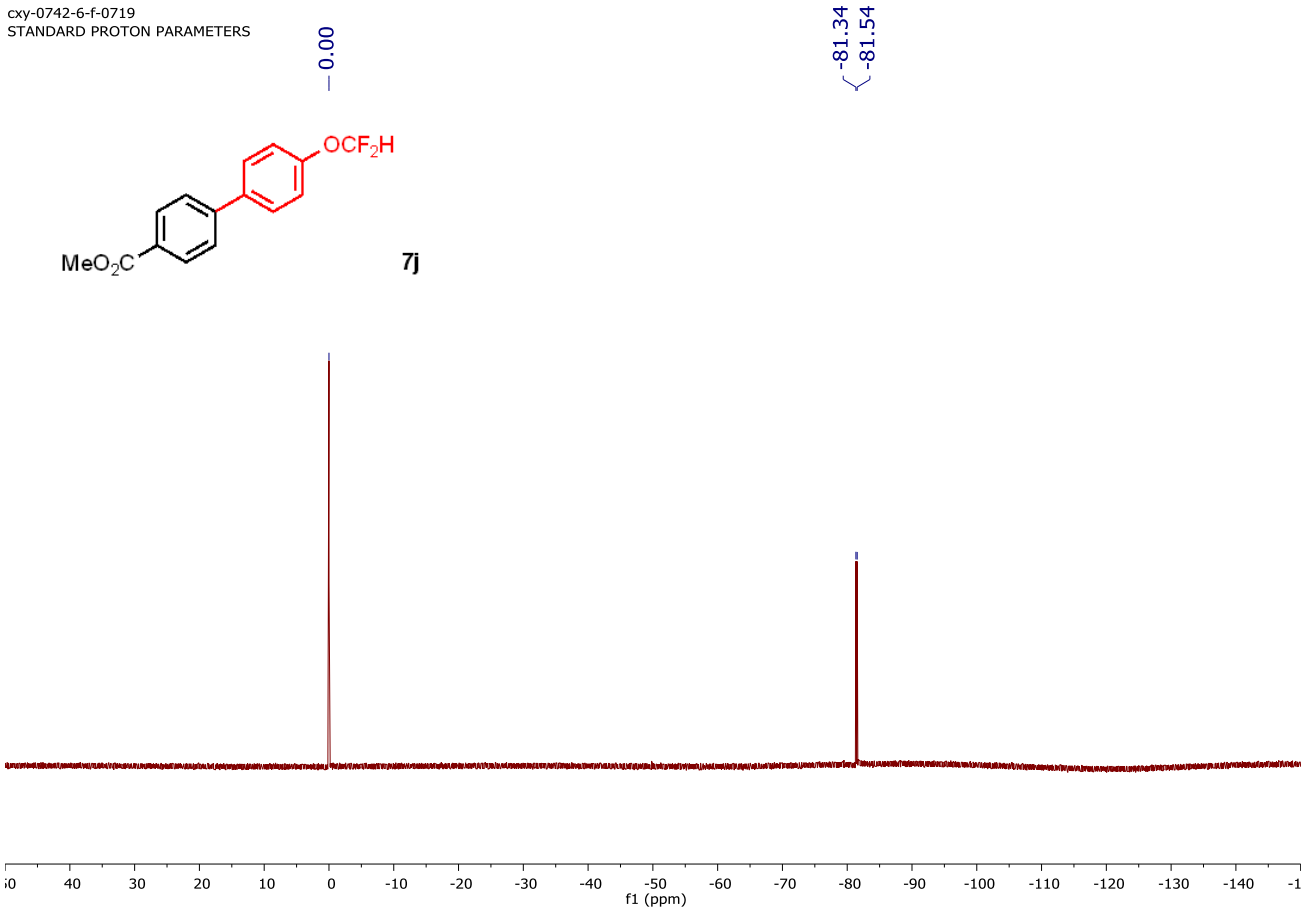

cxy-0743-3-p-chun-c
169.45
166.93
150.72
144.71
137.73
130.13
128.98
128.34
126.99
122.07
77.32
77.00
76.68
52.14
21.14
OAc
MeO2C
7h
f1 (ppm)

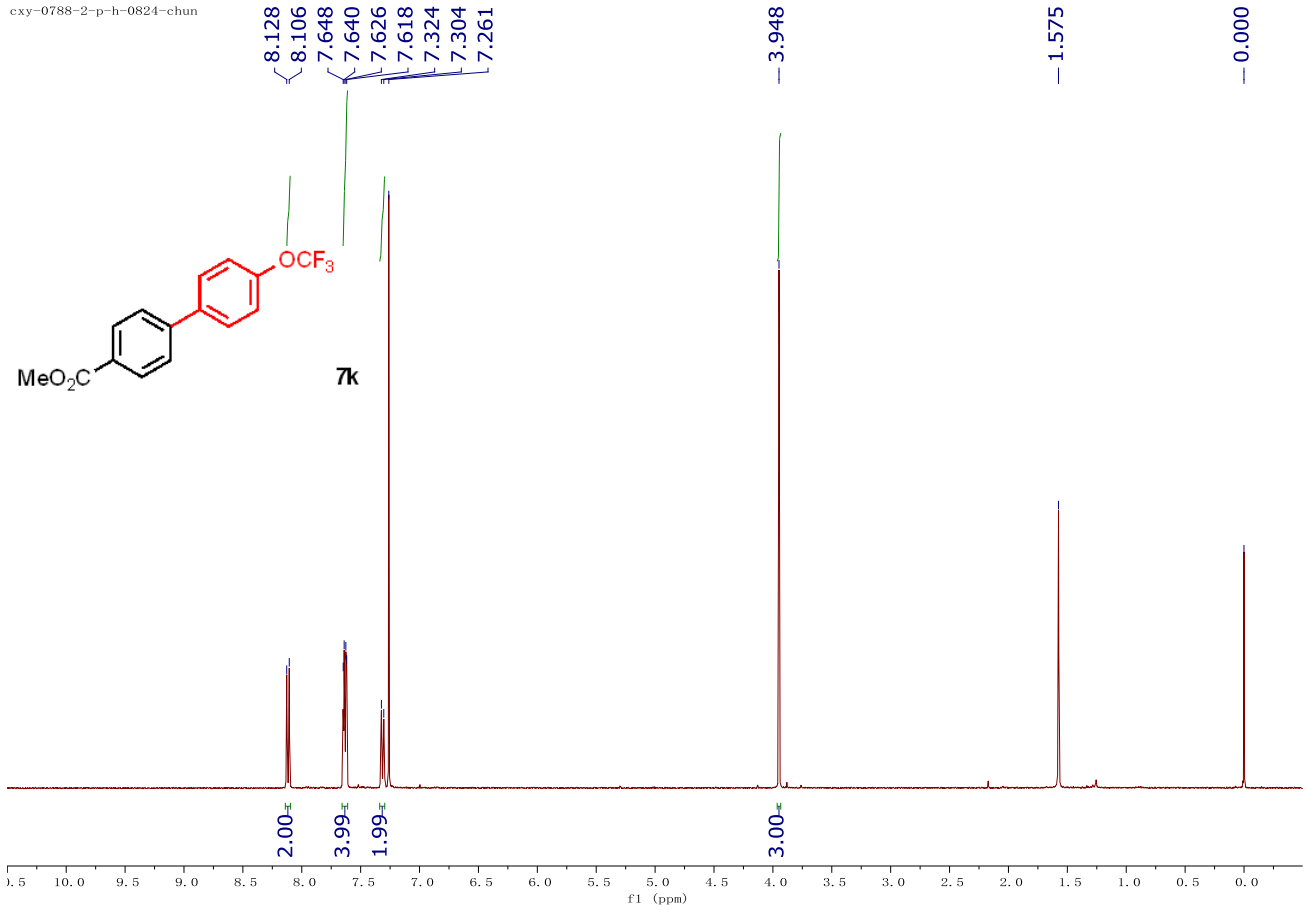

nxx-0108-1-chun-h
8.104
8.083
7.641
7.620
7.599
7.577
7.388
7.369
7.348
7.253
7.160
7.141
7.123
7.098
7.076
7.056
3.936
1.590
-0.000
OPh
MeO2C
7i
2.00
1.99
2.01
2.00
1.00
3.90
2.96
f1 (ppm)

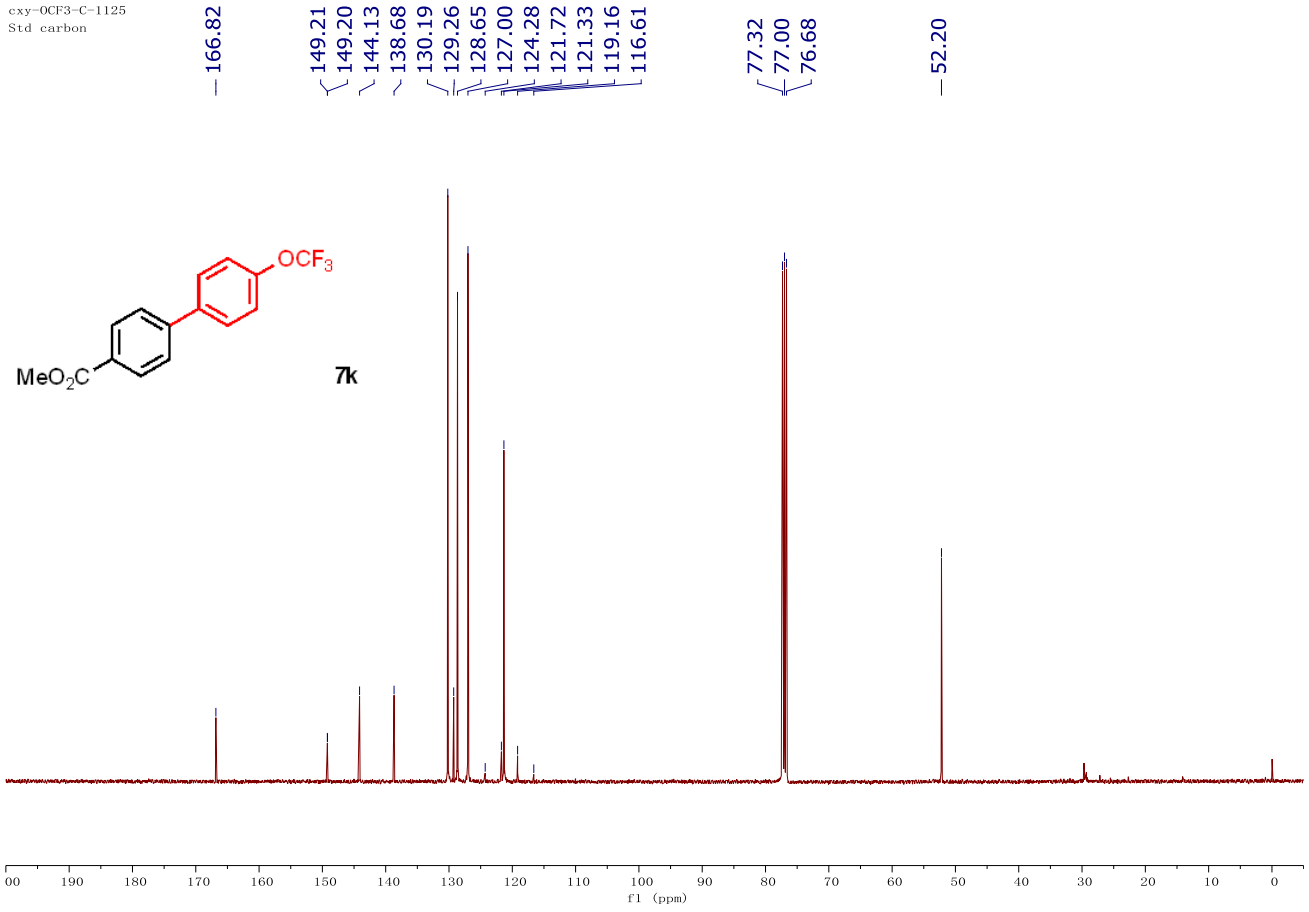

nxx-0108-1-C
166.97
157.68
156.78
144.90
134.80
130.12
129.84
128.60
126.68
123.63
119.21
118.95
77.32
77.00
76.68
52.09
OPh
MeO2C
7i
f1 (ppm)

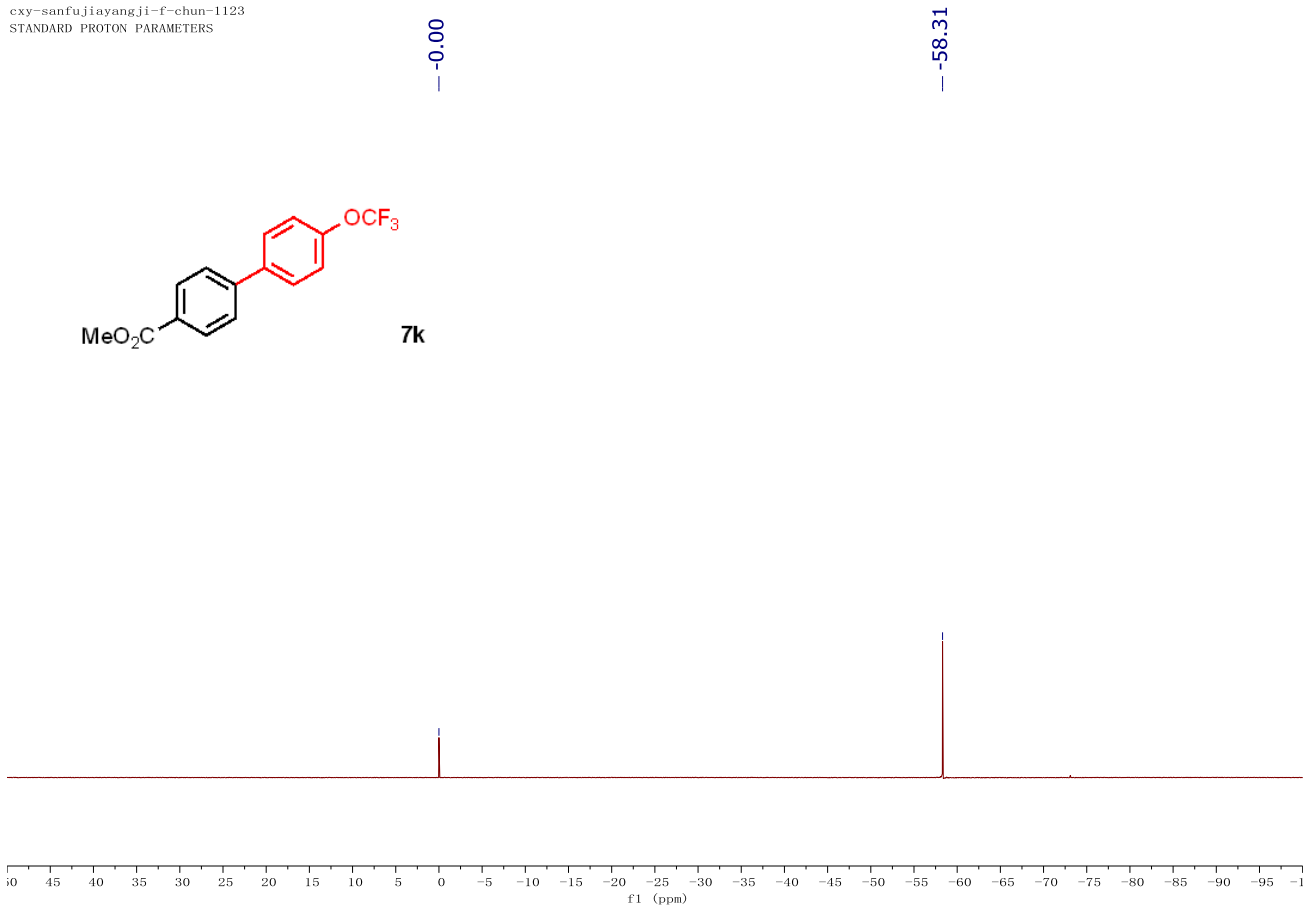

cxy-0742-6-p-chun-h
8.117
8.096
7.632
7.626
7.611
7.604
7.259
7.230
7.208
6.748
6.563
6.379
3.944
1.558
0.000
OCF2H
MeO2C
7j
2.00
4.05
2.00
1.05
3.03
f1 (ppm)

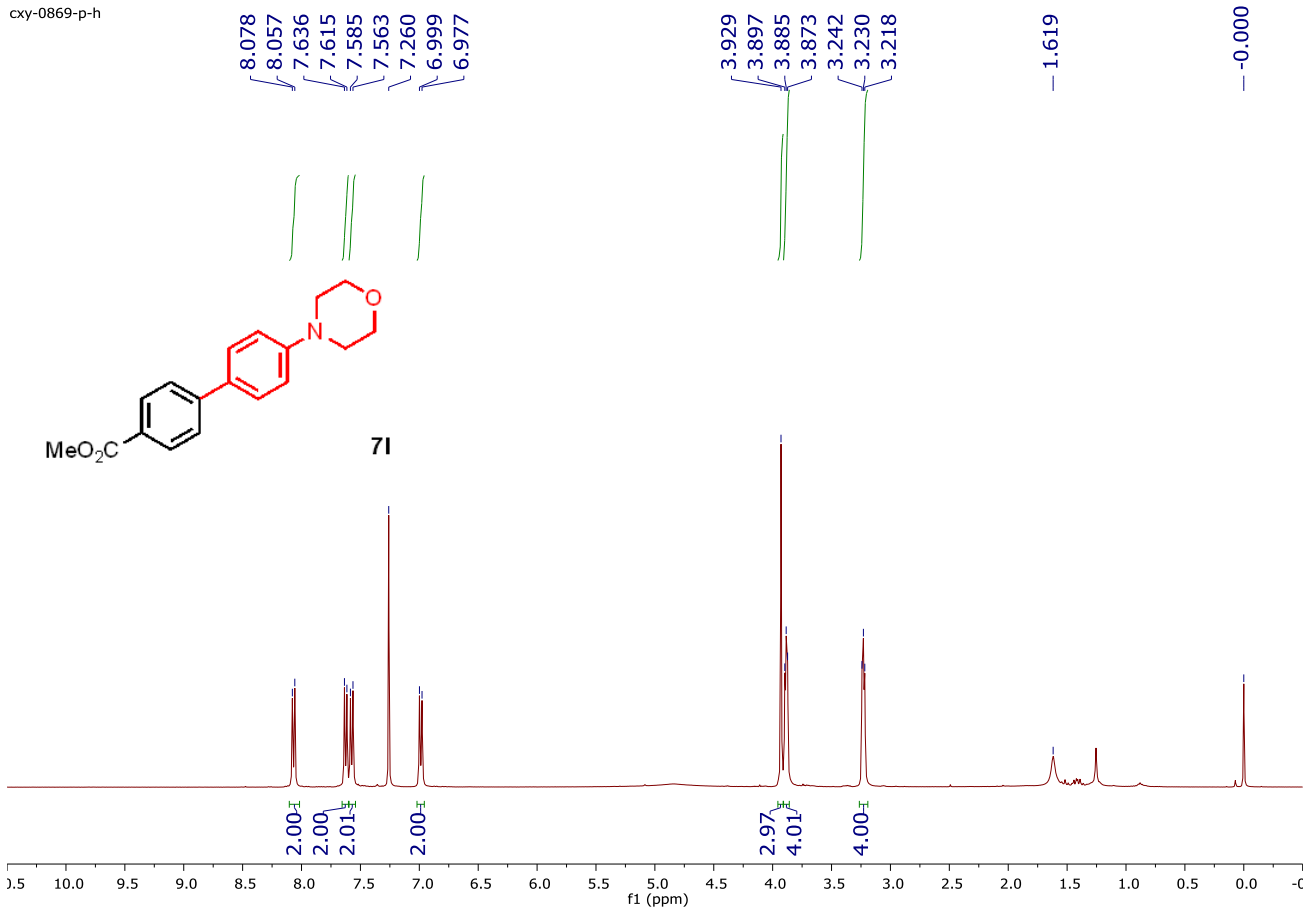

cxy-0742-6-p-chun-c
166.88
151.17
151.14
144.39
137.29
130.18
129.08
128.69
126.90
119.95
118.37
115.78
113.19
77.32
77.00
76.68
52.16
OCF2H
MeO2C
7j
f1 (ppm)

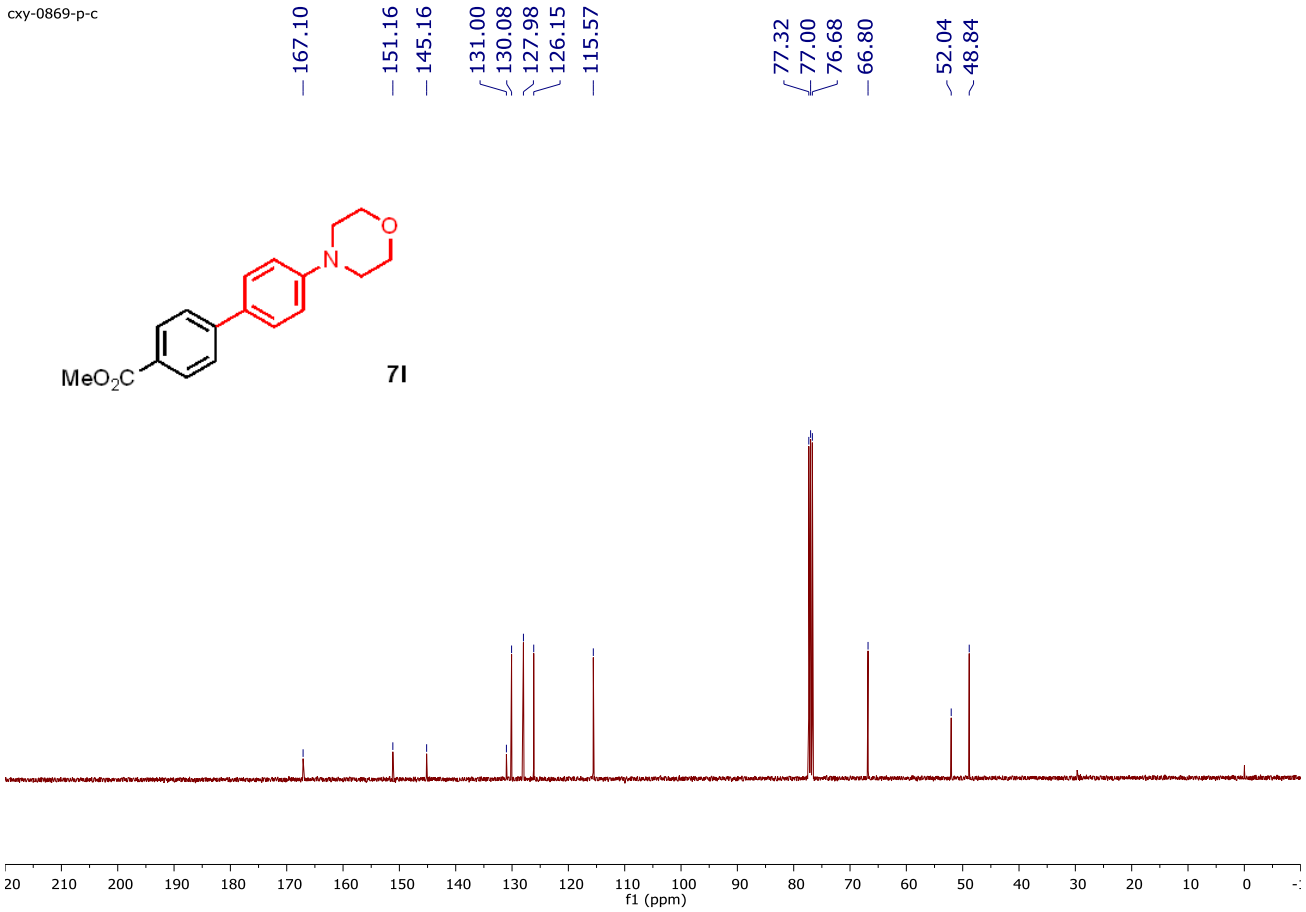

cxy-0742-6-f-0719
STANDARD PROTON PARAMETERS
0.00
-81.34
-81.54
OCF2H
MeO2C
7j
f1 (ppm)

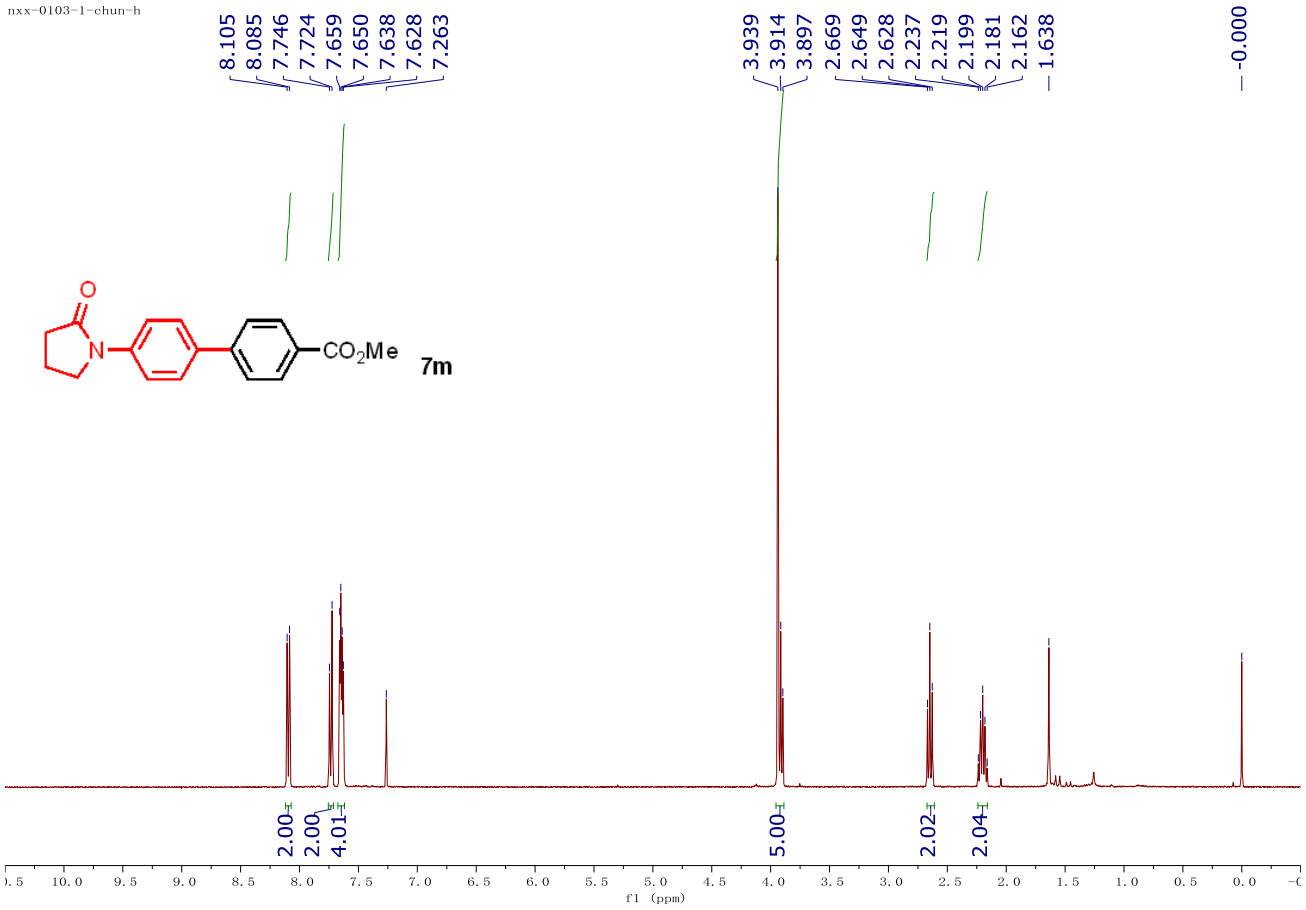

cxy-0788-2-p-h-0824-chun
8.128
8.106
7.648
7.640
7.626
7.618
7.324
7.304
7.261
3.948
1.575
0.000
OCF3
MeO2C
7k
2.00
3.99
1.99
3.00
f1 (ppm)

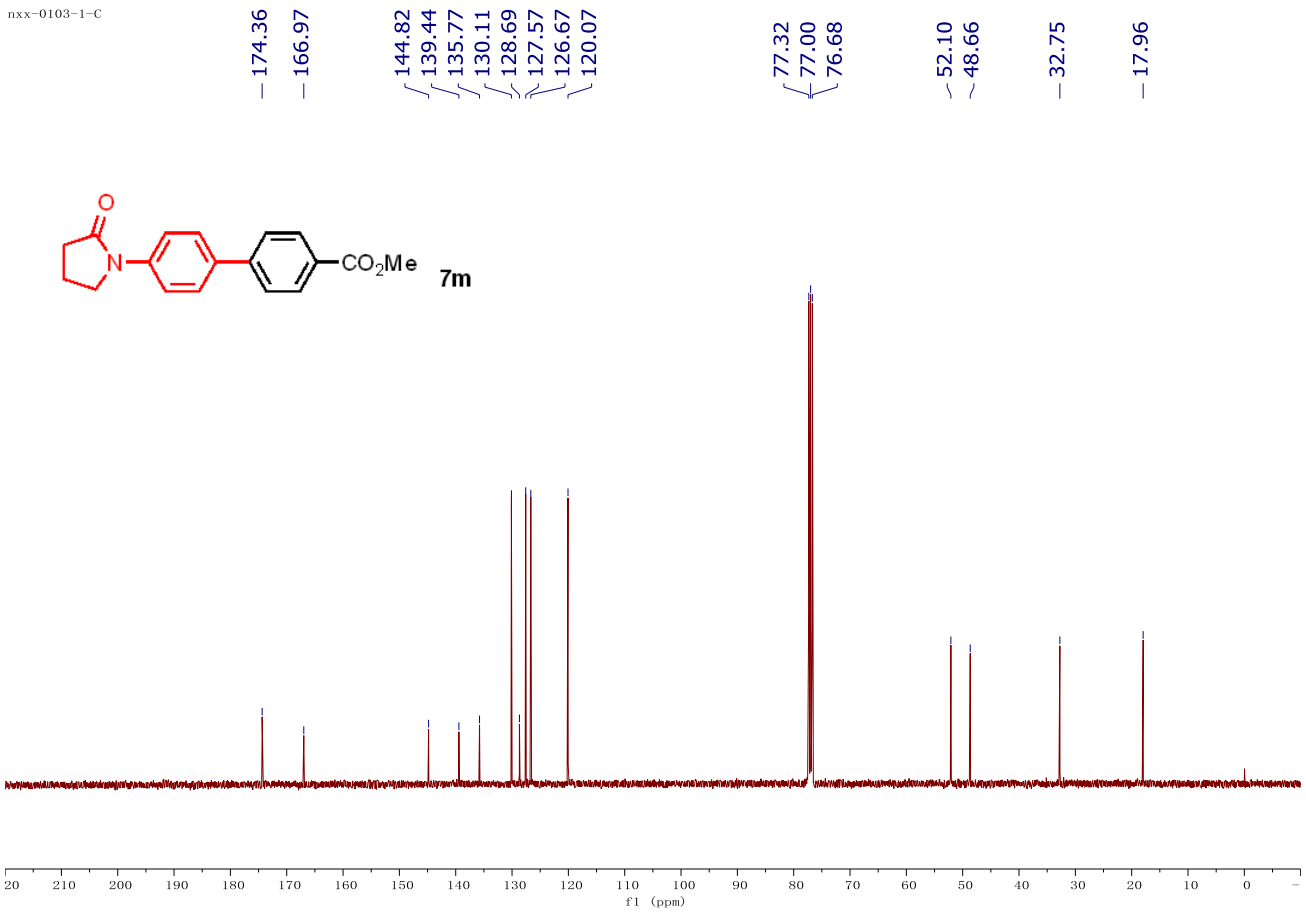

cxy-OCF3-C-1125
Std carbon
166.82
149.21
149.20
144.13
138.68
130.19
129.26
128.65
127.00
124.28
121.72
121.33
119.16
116.61
77.32
77.00
76.68
52.20
OCF3
MeO2C
7k
f1 (ppm)

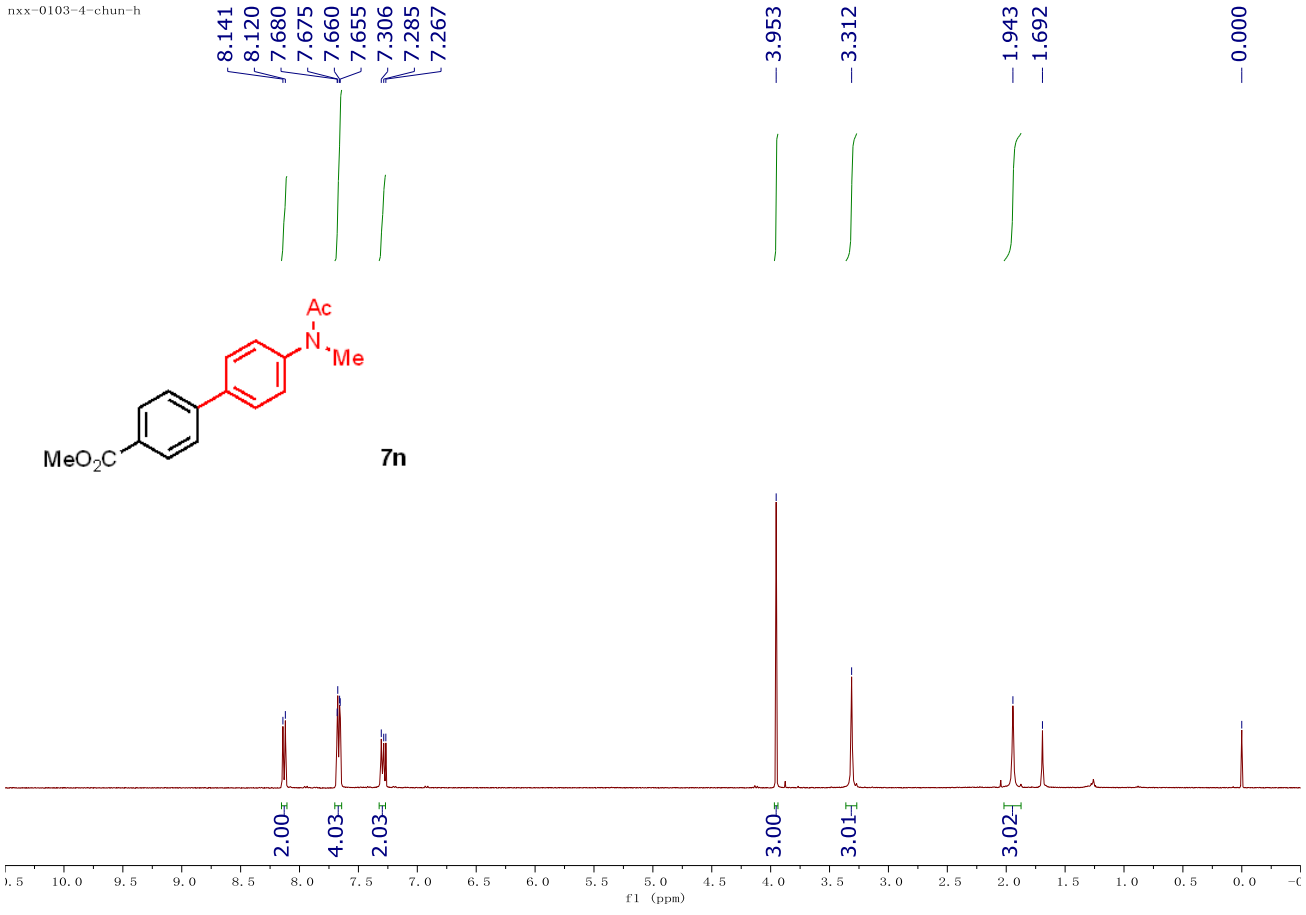

cxy-sanfujiayangji-f-chun-1123
STANDARD PROTON PARAMETERS
-0.00
-58.31
OCF3
MeO2C
7k
f1 (ppm)

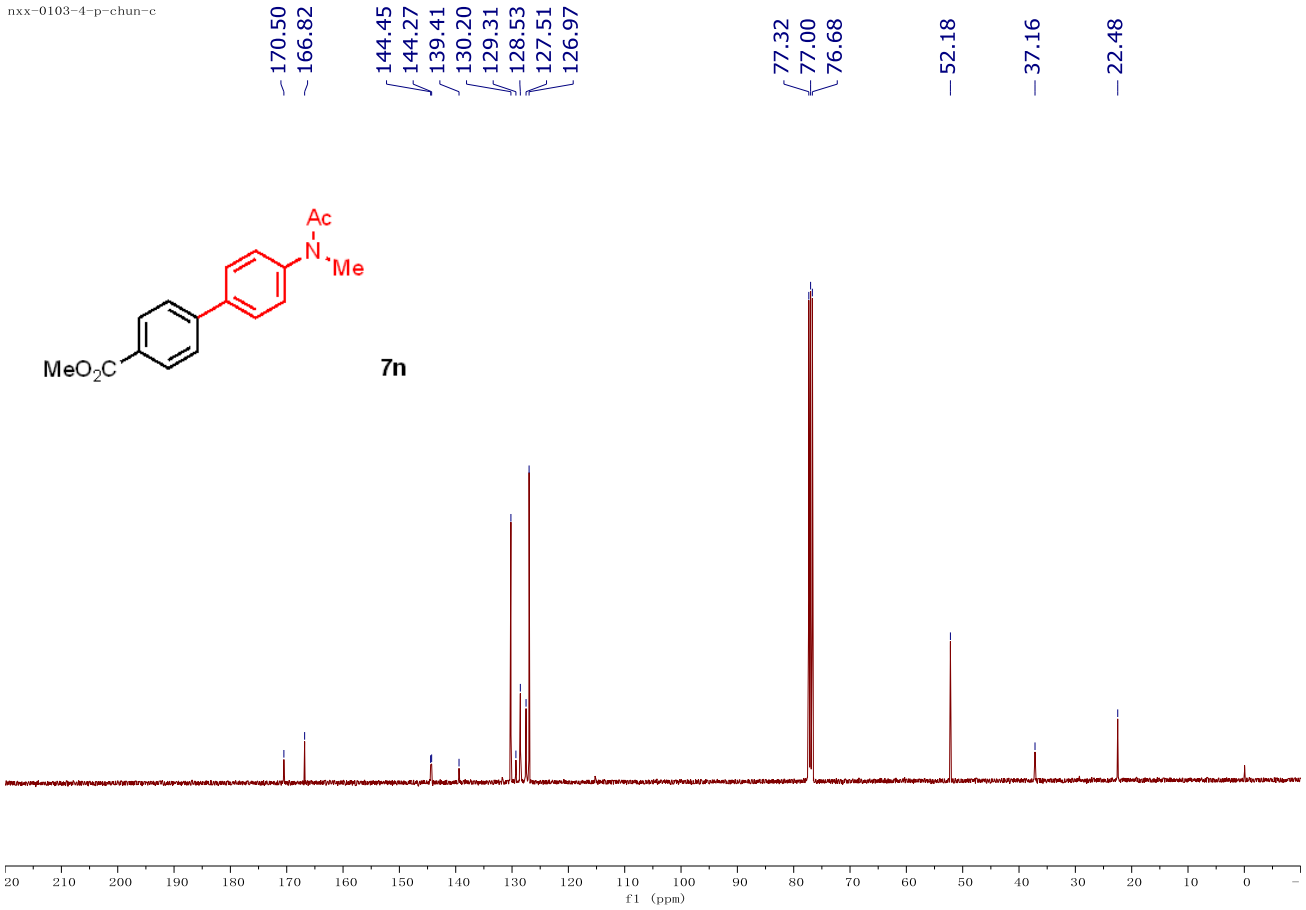

cxy-0869-p-h
8.078
8.057
7.636
7.615
7.585
7.563
7.260
6.999
6.977
3.929
3.897
3.885
3.873
3.242
3.230
3.218
1.619
0.000
O
N
MeO2C
7l
2.00
2.00
2.01
2.00
2.97
4.01
4.00
f1 (ppm)

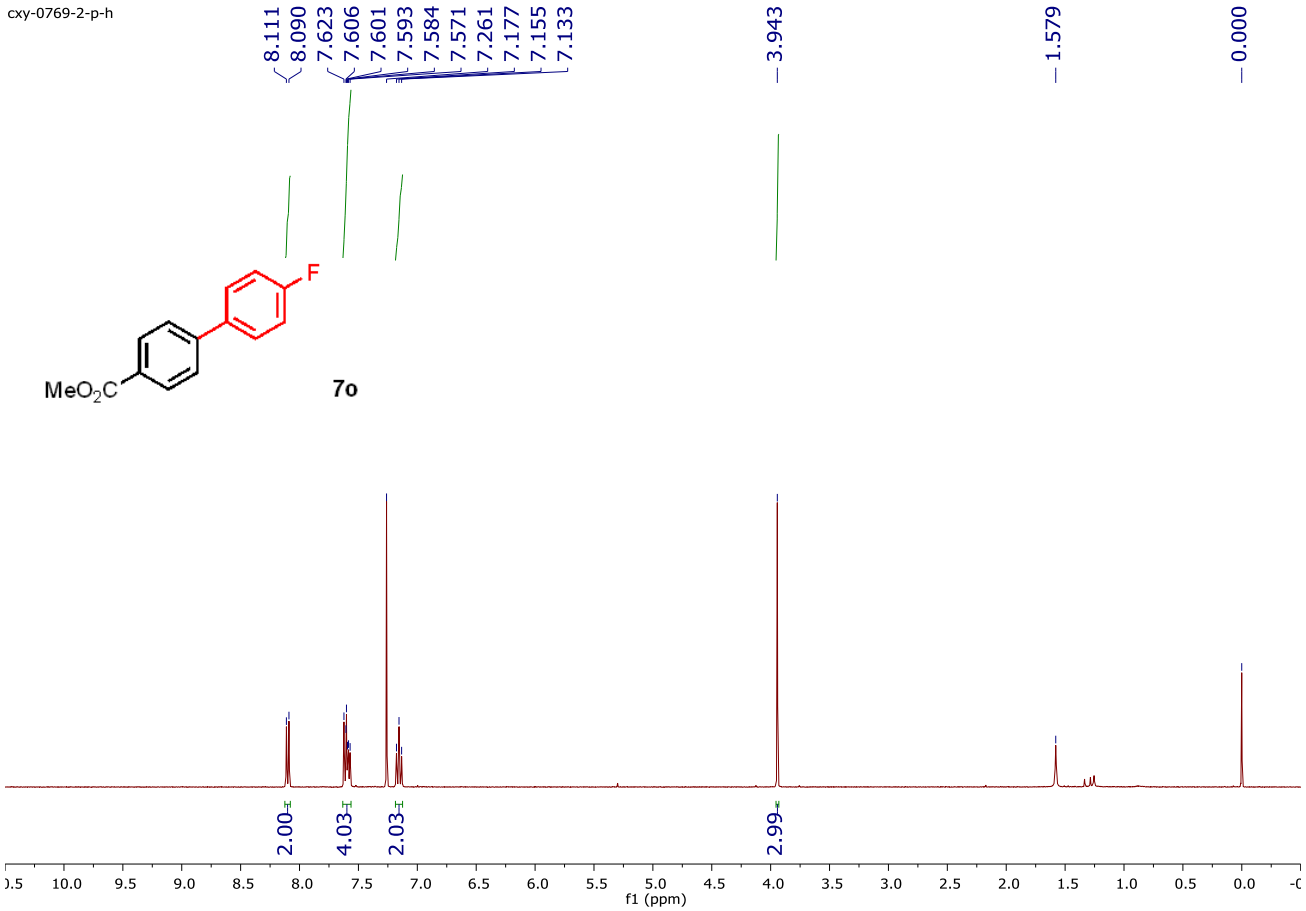

cxy-0869-p-c
167.10
151.16
145.16
131.00
130.08
127.98
126.15
115.57
77.32
77.00
76.68
66.80
52.04
48.84
MeO2C
7l
f1 (ppm)


nxx-0103-1-chun-h
8.105
8.085
7.746
7.724
7.659
7.650
7.638
7.628
7.263
3.939
3.914
3.897
2.669
2.649
2.628
2.237
2.219
2.199
2.181
2.162
1.638
-0.000
CO2Me
7m
2.00
2.00
4.01
5.00
2.02
2.04
f1 (ppm)

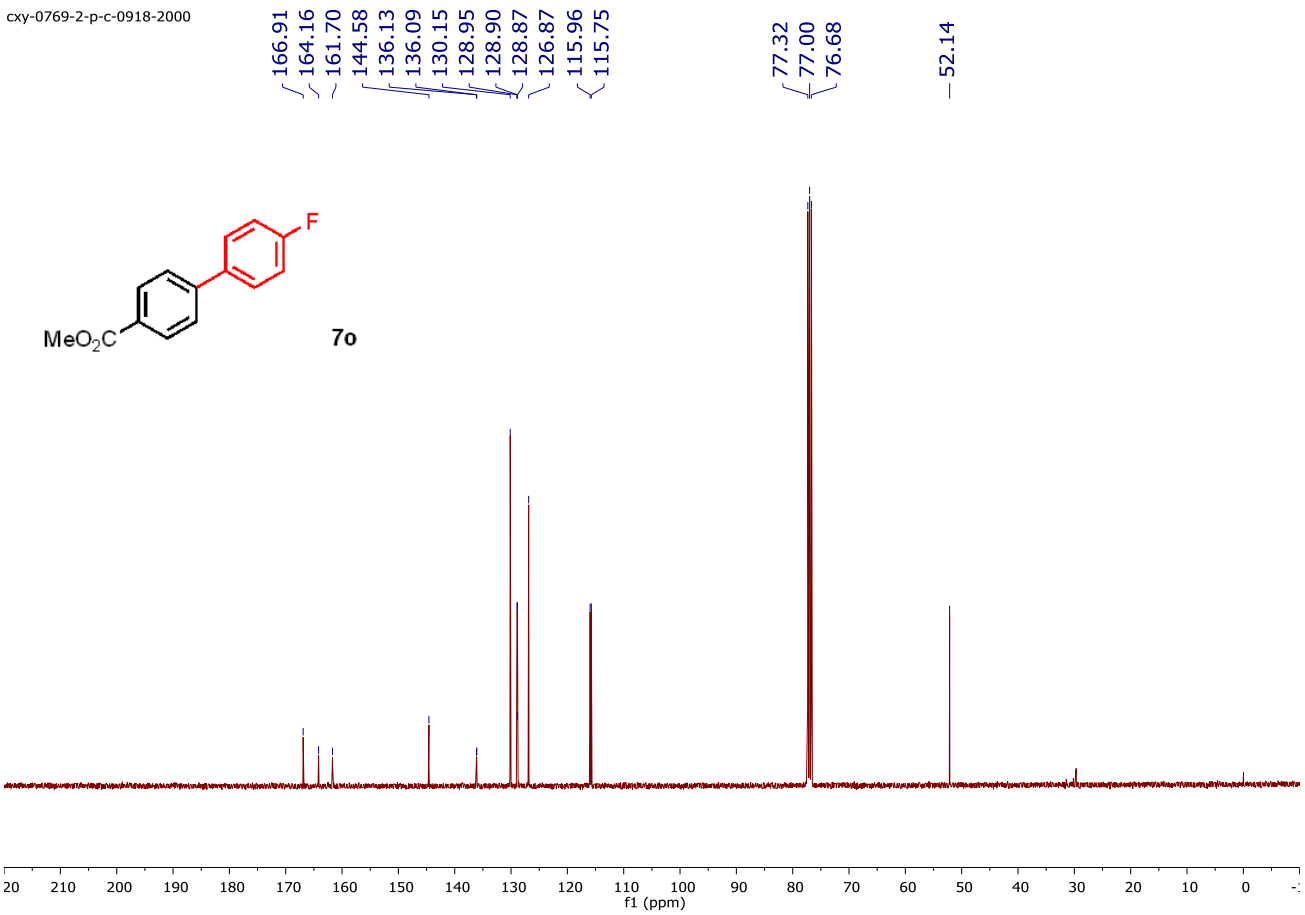

nxx-0103-1-C
174.36
166.97
144.82
139.44
135.77
130.11
128.69
127.57
126.67
120.07
77.32
77.00
76.68
52.10
48.66
32.75
17.96
O
N
CO2Me
7m
f1 (ppm)


nxx-0103-4-chun-h
8.141
8.120
7.680
7.675
7.660
7.655
7.306
7.285
7.267
3.953
3.312
1.943
1.692
0.000
Ac
N
Me
MeO2C
7n
2.00
4.03
2.03
3.00
3.01
3.02
f1 (ppm)

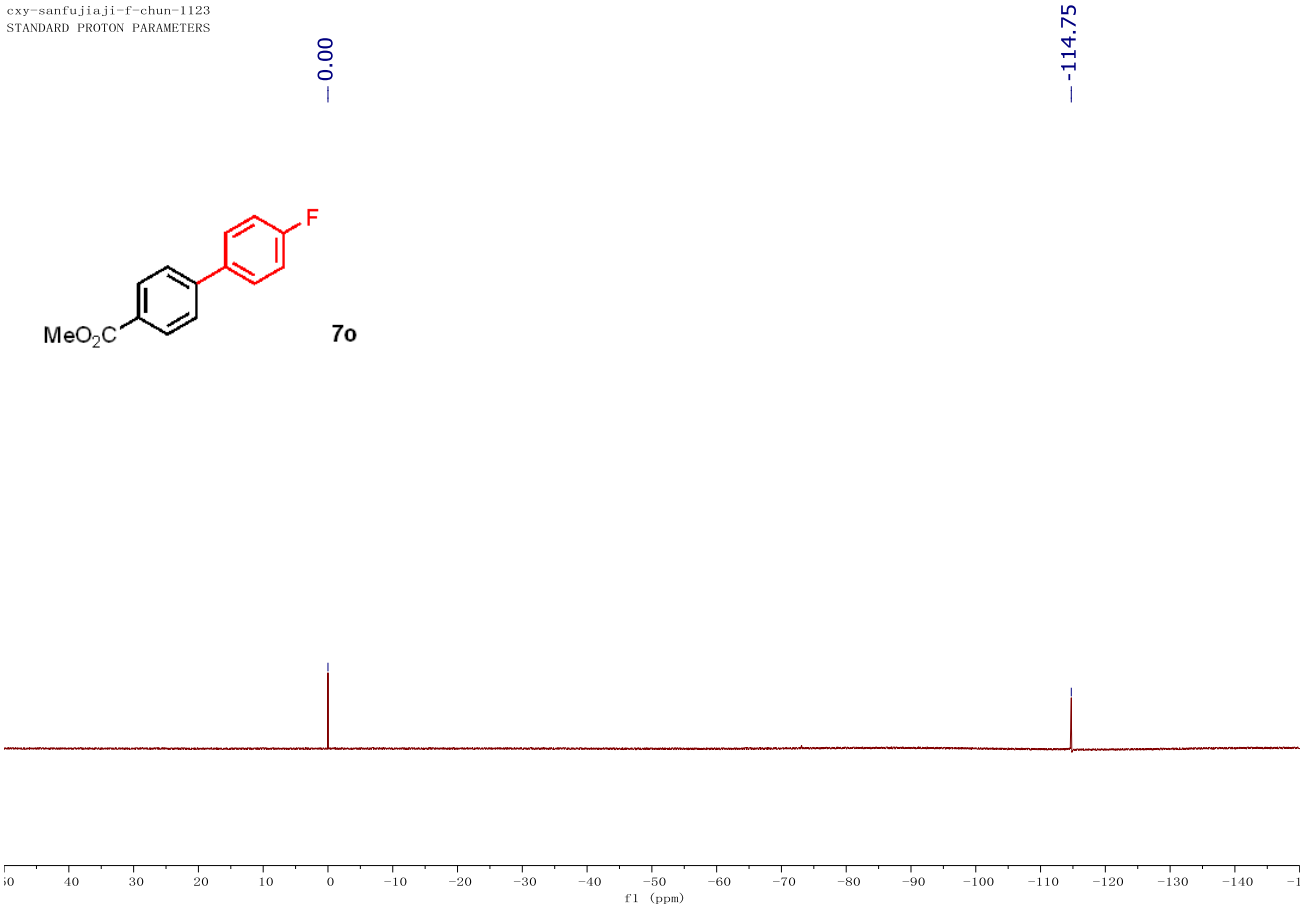

nxx-0103-4-p-chun-c
170.50
166.82
144.45
144.27
139.41
130.20
129.31
128.53
127.51
126.97
77.32
77.00
76.68
52.18
37.16
22.48
Ac
N
Me
MeO2C
7n
f1 (ppm)

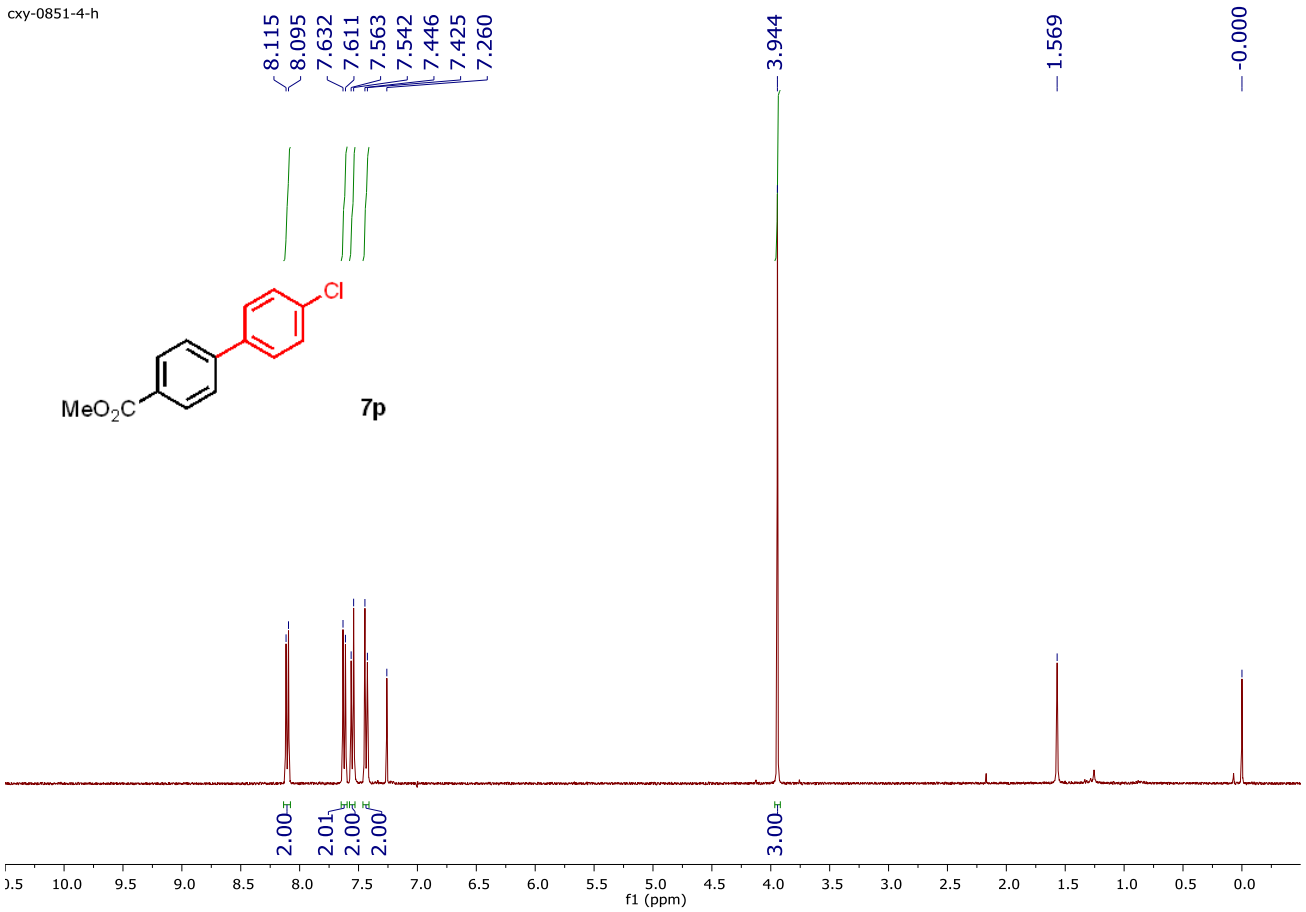

cxy-0769-2-p-h
8.111
8.090
7.623
7.606
7.601
7.593
7.584
7.571
7.261
7.177
7.155
7.133
3.943
1.579
0.000
F
MeO2C
7o
2.00
4.03
2.03
2.99
f1 (ppm)

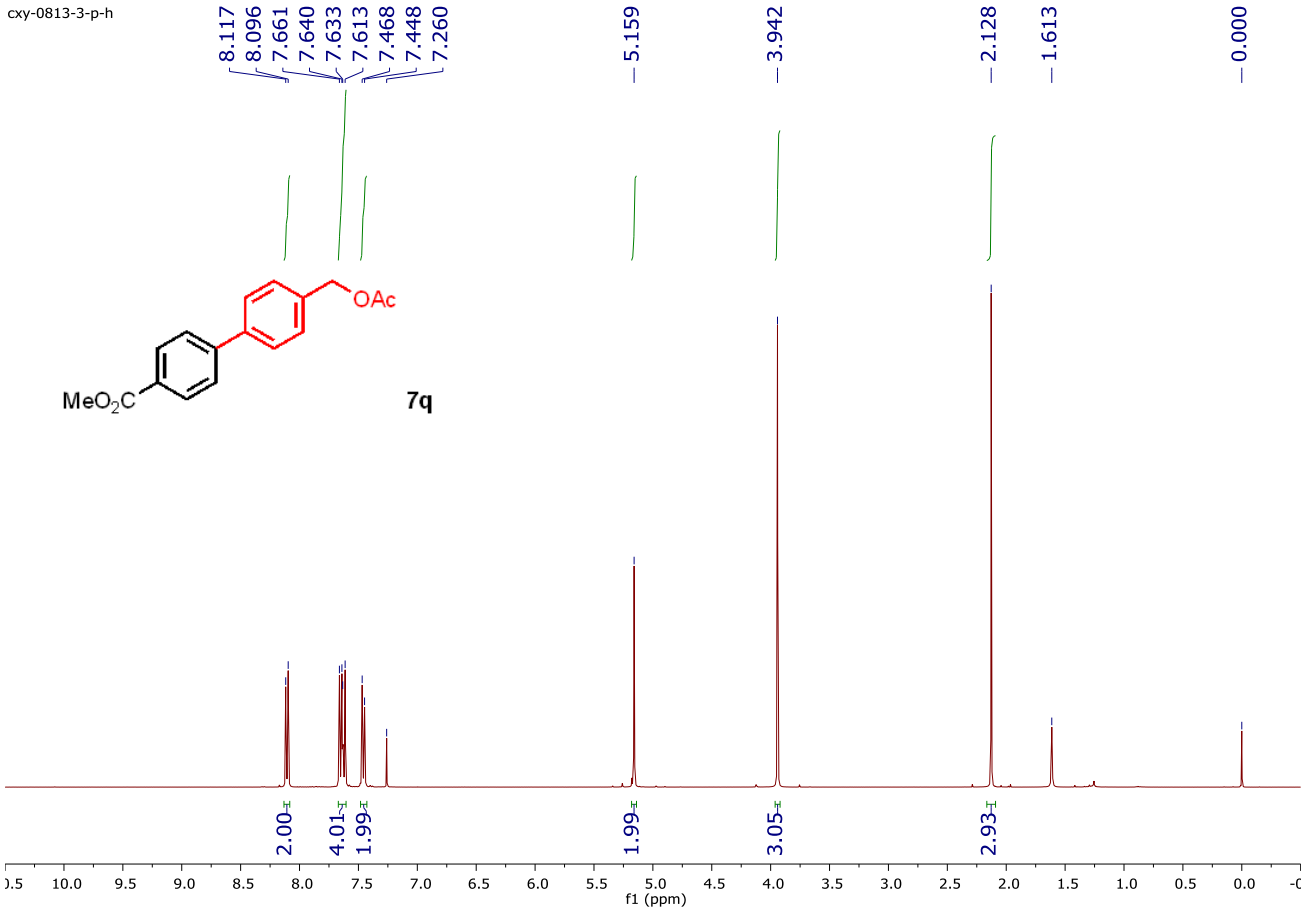
cxy-0769-2-p-c-0918-2000

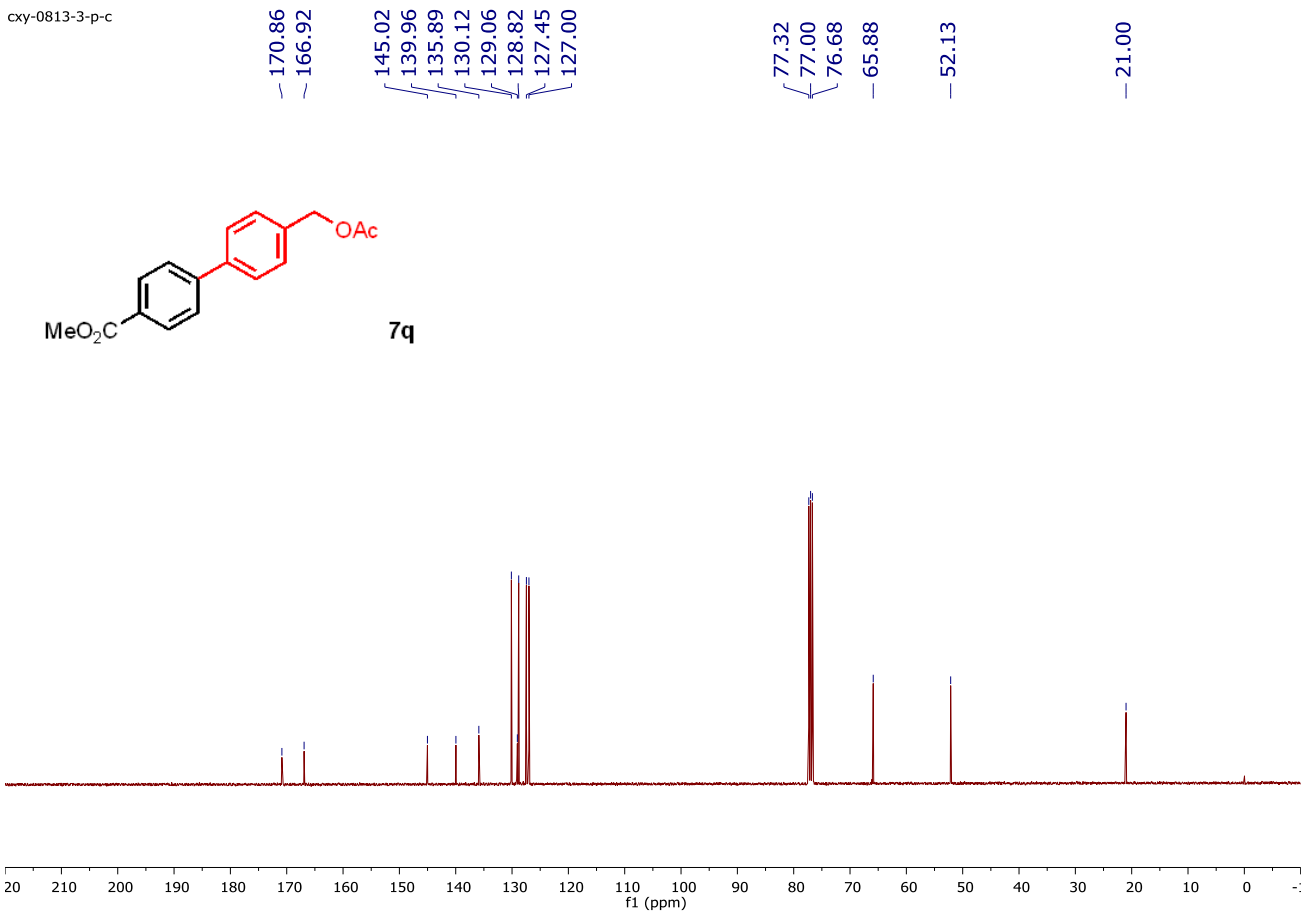


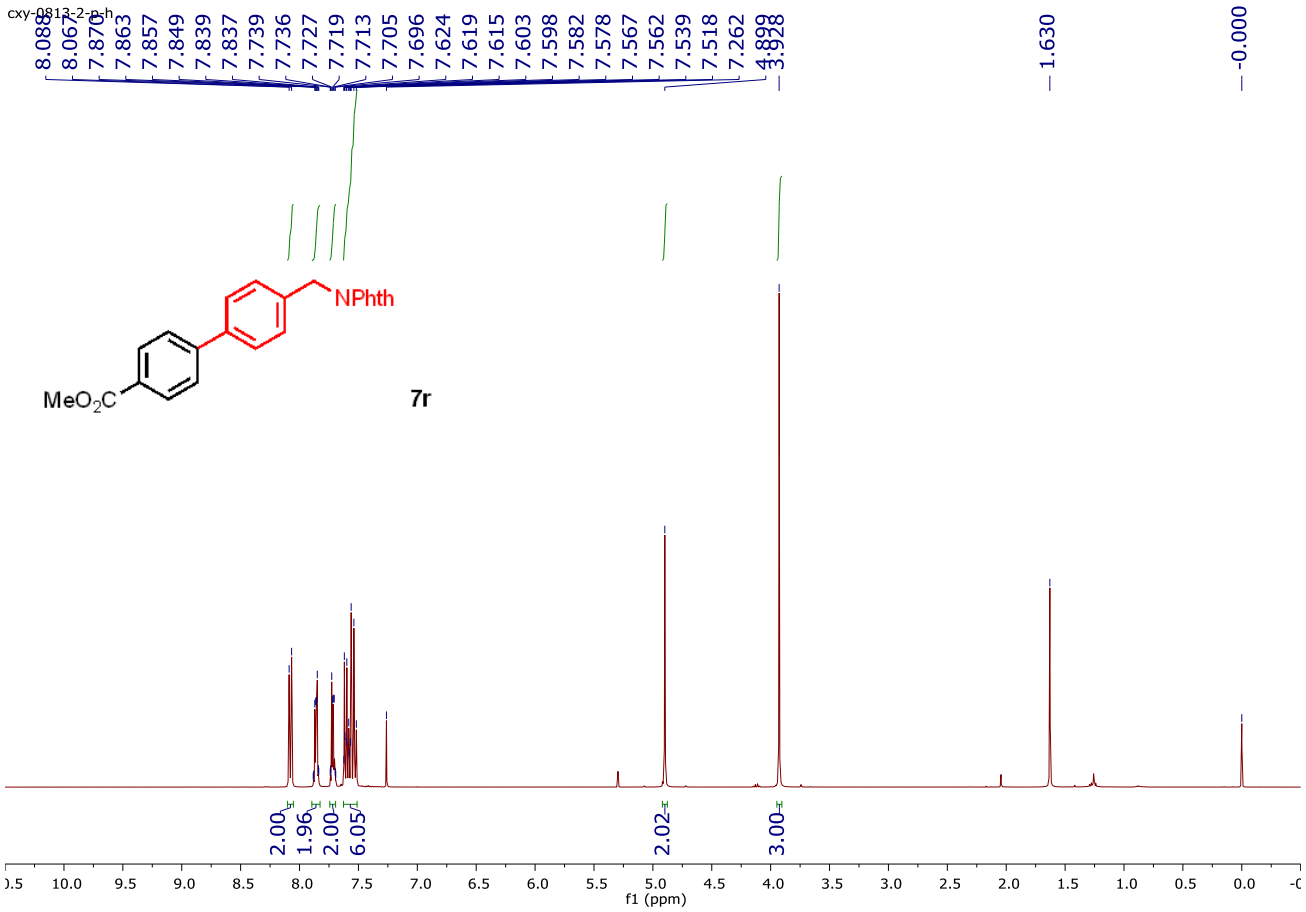
cxy-sanfujiaji-f-chun-1123
STANDARD PROTON PARAMETERS

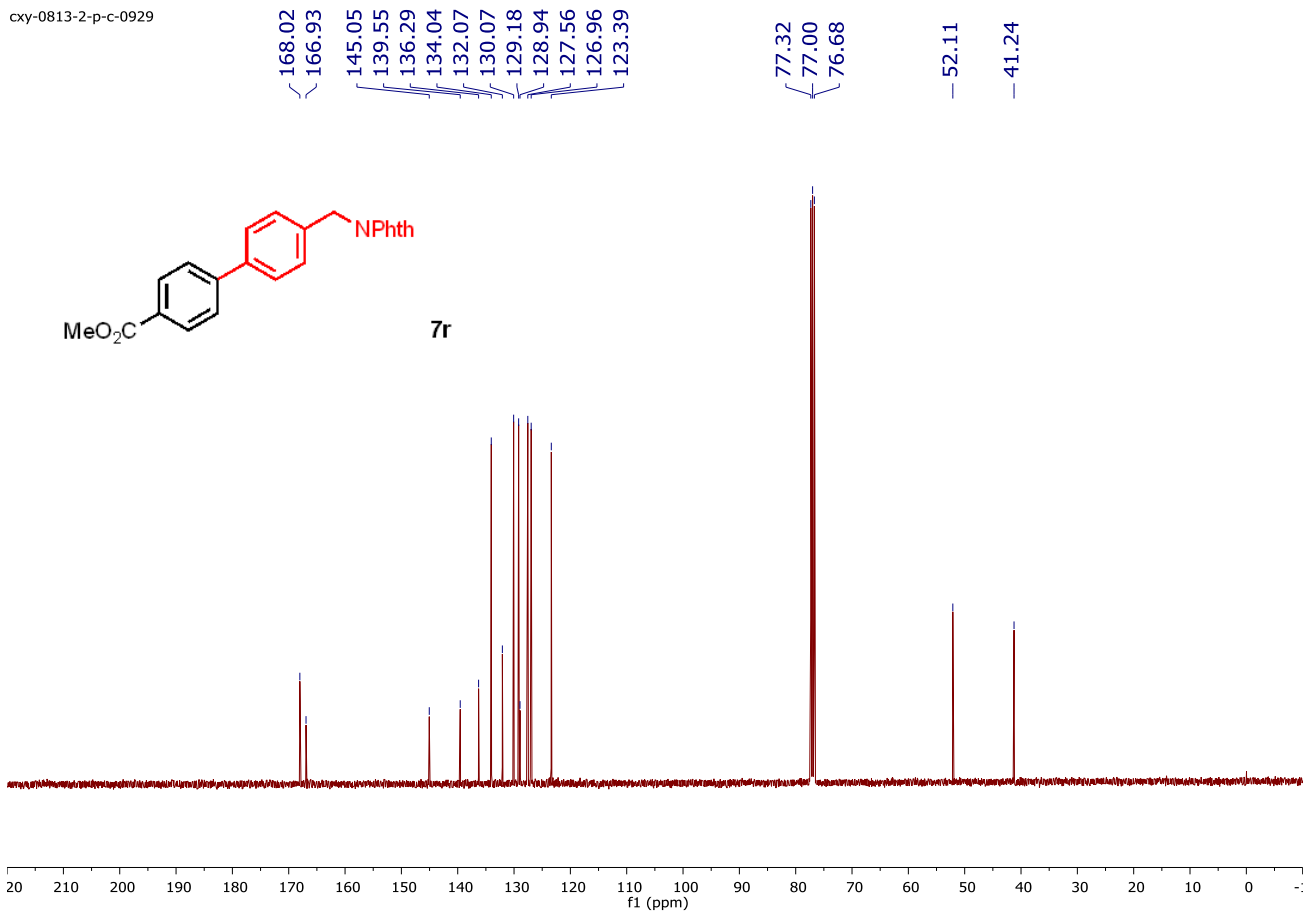


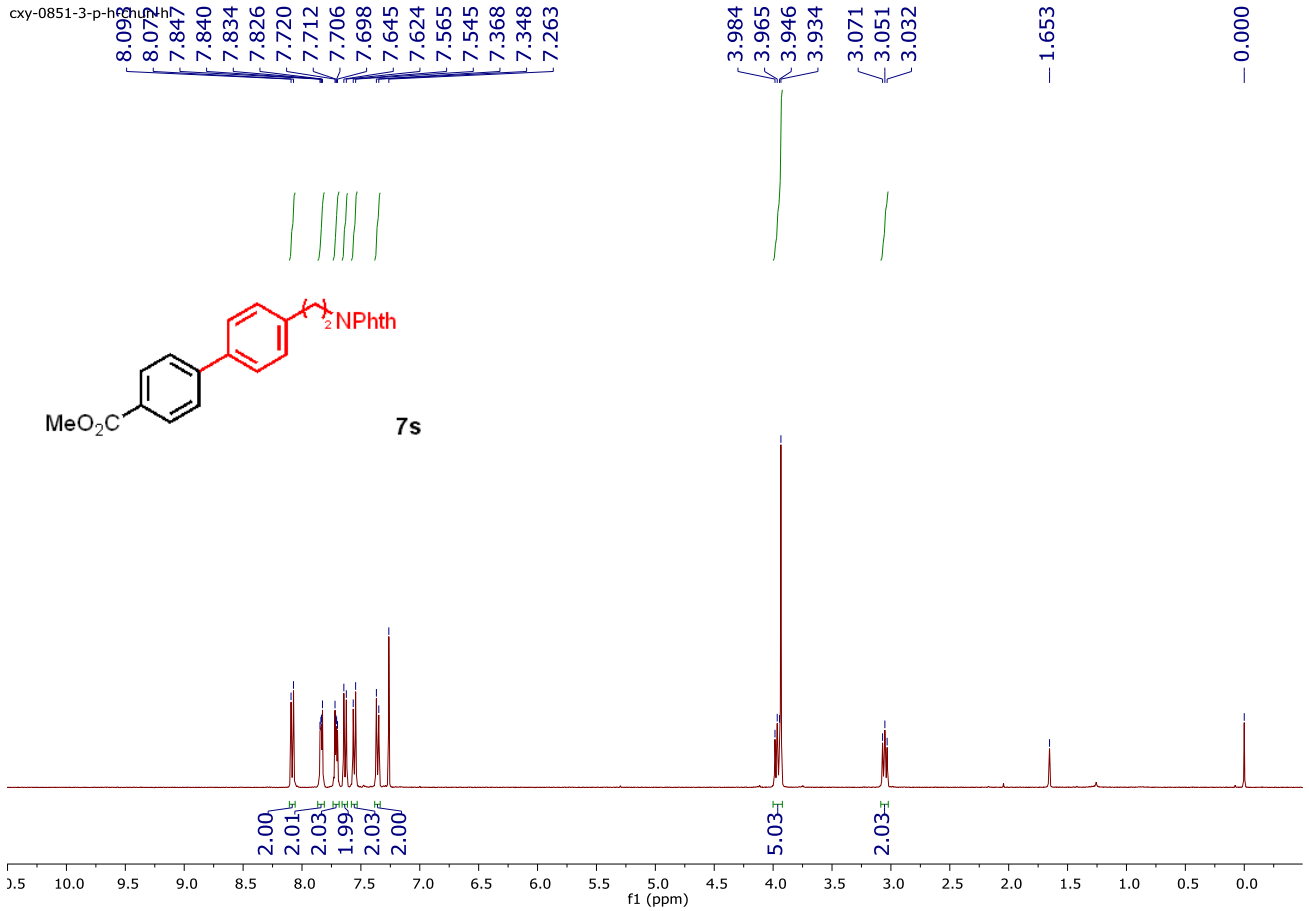

cxy-0851-4-h
8.115
8.095
7.632
7.611
7.563
7.542
7.446
7.425
7.260
3.944
1.569
-0.000
Cl
MeO2C
7p
2.00
2.01
2.00
2.00
3.00
f1 (ppm)


cxy-0813-3-p-h
8.117
8.096
7.661
7.640
7.633
7.613
7.468
7.448
7.260
5.159
3.942
2.128
1.613
0.000
OAc
MeO2C
7q
2.00
4.01
1.99
1.99
3.05
2.93
f1 (ppm)


cxy-0813-3-p-c
170.86
166.92
145.02
139.96
135.89
130.12
129.06
128.82
127.45
127.00
77.32
77.00
76.68
65.88
52.13
21.00
OAc
MeO2C
7q
f1 (ppm)

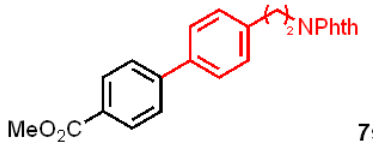

cxy-0813-2-p-h
8.088
8.067
7.870
7.863
7.857
7.849
7.839
7.837
7.739
7.736
7.727
7.719
7.713
7.705
7.696
7.624
7.619
7.615
7.603
7.598
7.582
7.578
7.567
7.562
7.539
7.518
7.262
4.899
3.928
1.630
-0.000
NPhth
MeO2C
7r
2.00
1.96
2.00
6.05
2.02
3.00
f1 (ppm)


cxy-0813-2-p-c-0929
168.02
166.93
145.05
139.55
136.29
134.04
132.07
130.07
129.18
128.94
127.56
126.96
123.39
77.32
77.00
76.68
52.11
41.24
NPhth
MeO2C
7r
f1 (ppm)

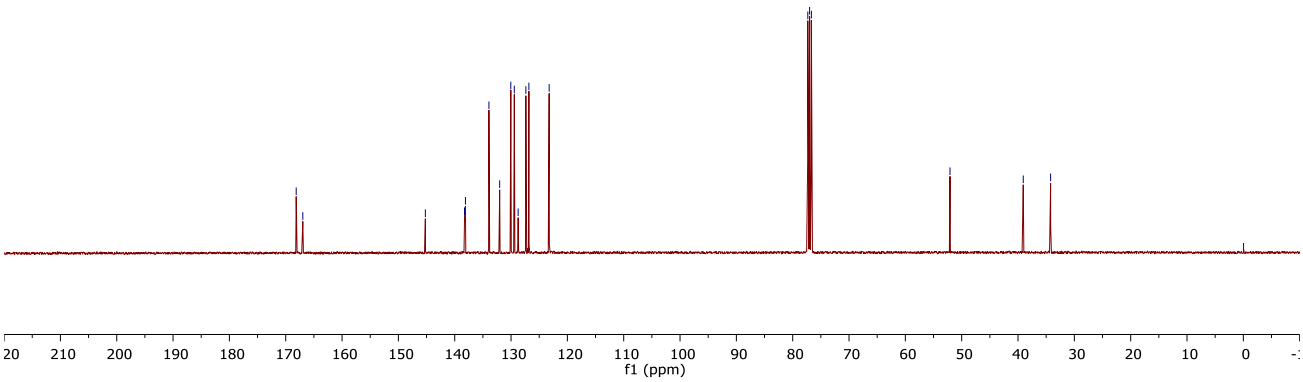

8.09
8.07
7.847
7.840
7.834
7.826
7.720
7.712
7.706
7.698
7.645
7.624
7.565
7.545
7.368
7.348
7.263
3.984
3.965
3.946
3.934
3.071
3.051
3.032
1.653
0.000
NPhth
MeO2C
7s
2.00
2.01
2.03
1.99
2.03
2.00
5.03
2.03
f1 (ppm)

cxy-0835-3-p-c

168.14
166.97
145.21
138.26
138.10
133.93
132.02
130.04
129.42
128.74
127.37
126.83
123.23
77.32
77.00
76.68
52.08
39.07
34.22

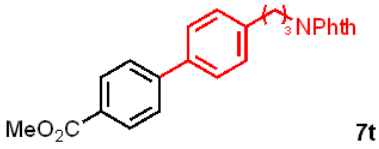


7s



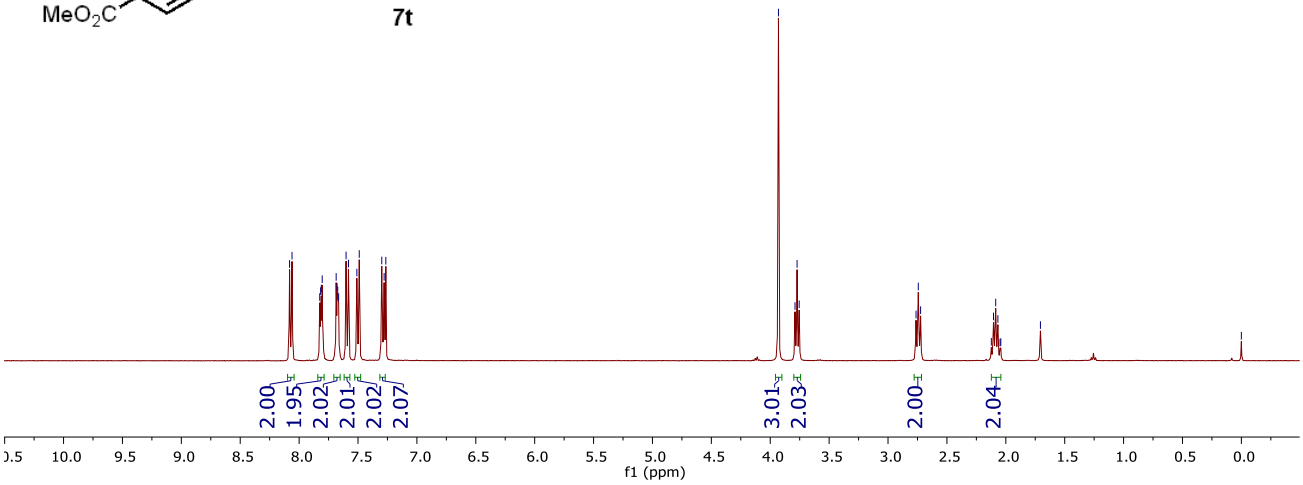
cxy-0848-2-p-chm

8.089
8.066
7.825
7.817
7.811
7.804
7.685
7.678
7.672
7.664
7.601
7.581
7.510
7.489
7.298
7.278
7.264
3.930
3.790
3.772
3.754
2.762
2.743
2.723
2.123
2.104
2.086
2.067
2.049
2.042
1.706
0.000



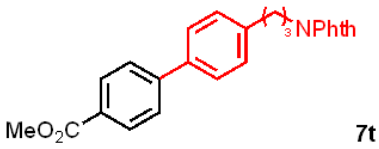
7t

2.00
1.95
2.02
2.01
2.02
2.07
3.01
2.03
2.00
2.04

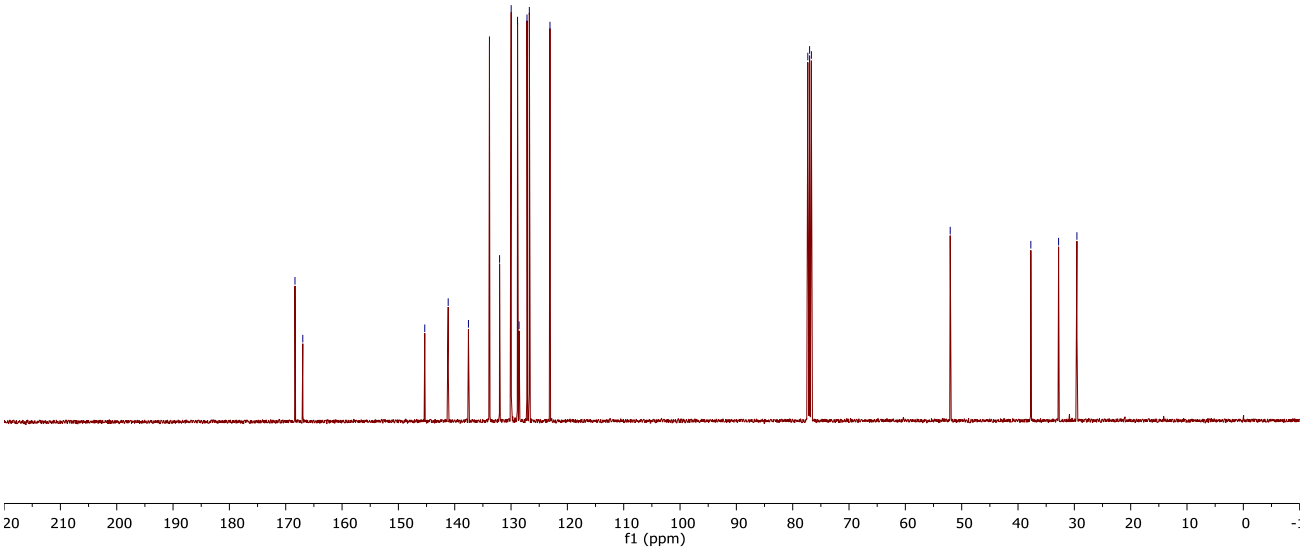


cxy-0848-2-p-c

168.36
166.97
145.32
141.16
137.56
133.83
132.04
129.98
128.84
128.58
127.17
126.75
123.09
77.32
77.00
76.68
52.04
37.72
32.80
29.54

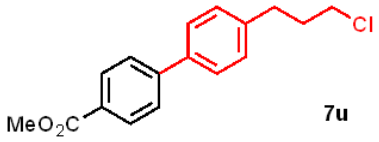


7t

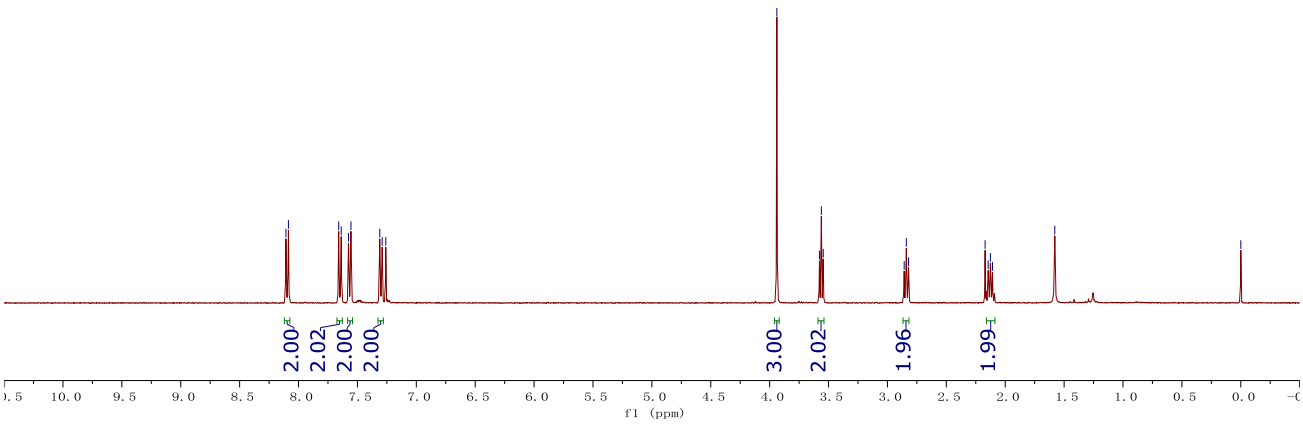


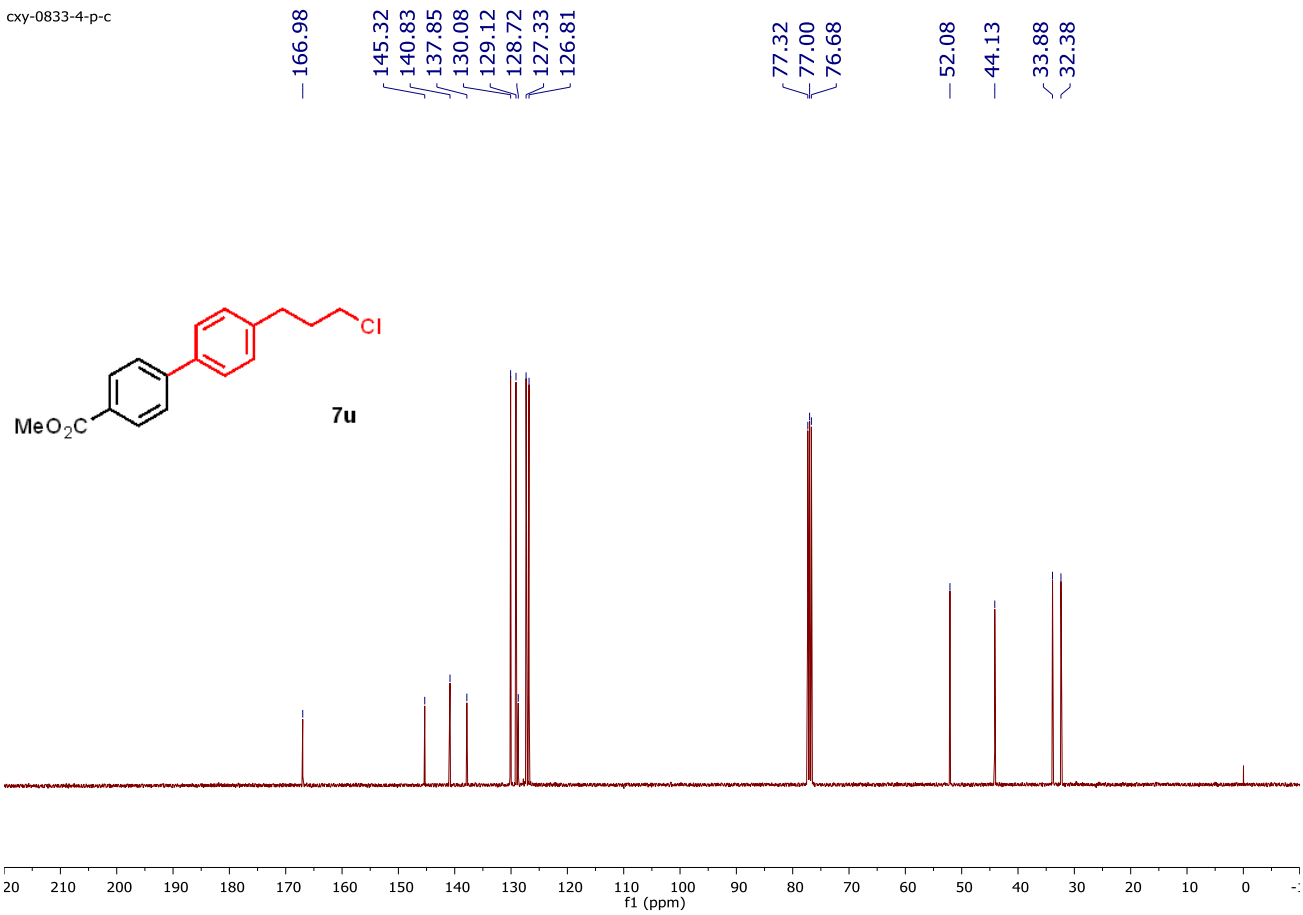
cxy-0826-2-p-chun-h

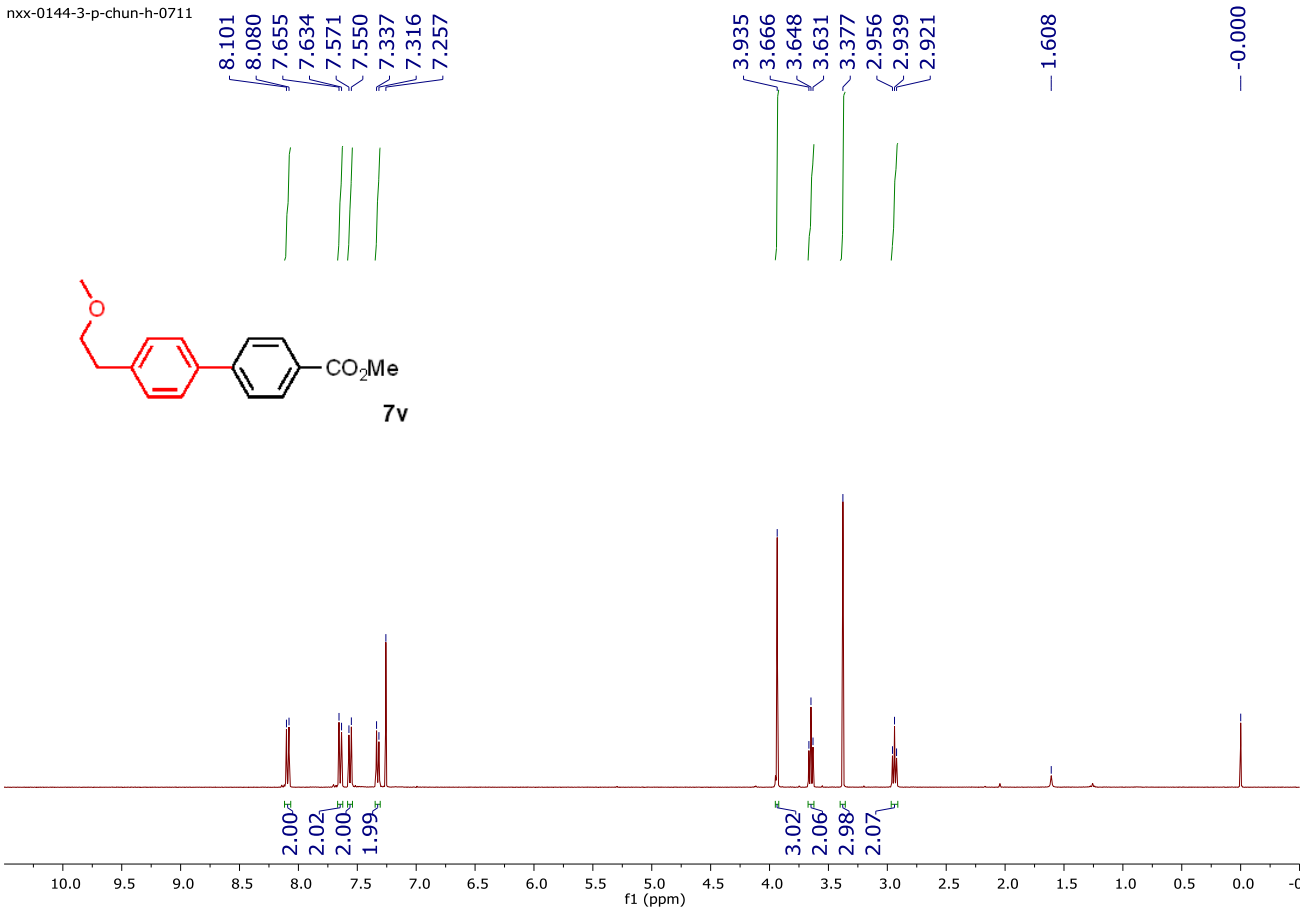
8.107
8.086
7.659
7.638
7.575
7.555
7.310
7.290
7.259
3.939
3.577
3.561
3.545
2.858
2.840
2.821
2.171
2.145
2.126
2.108
1.579
-0.000

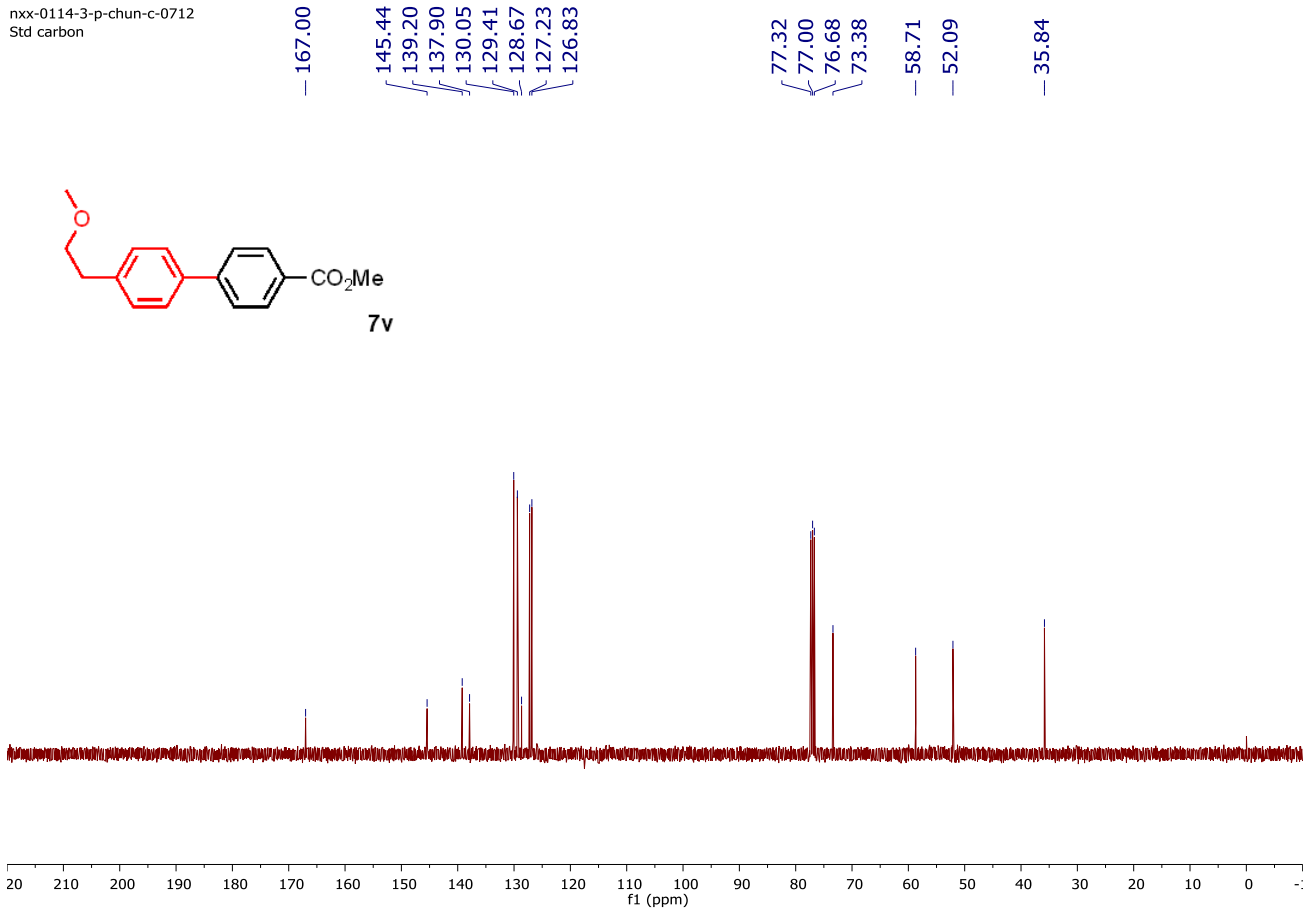


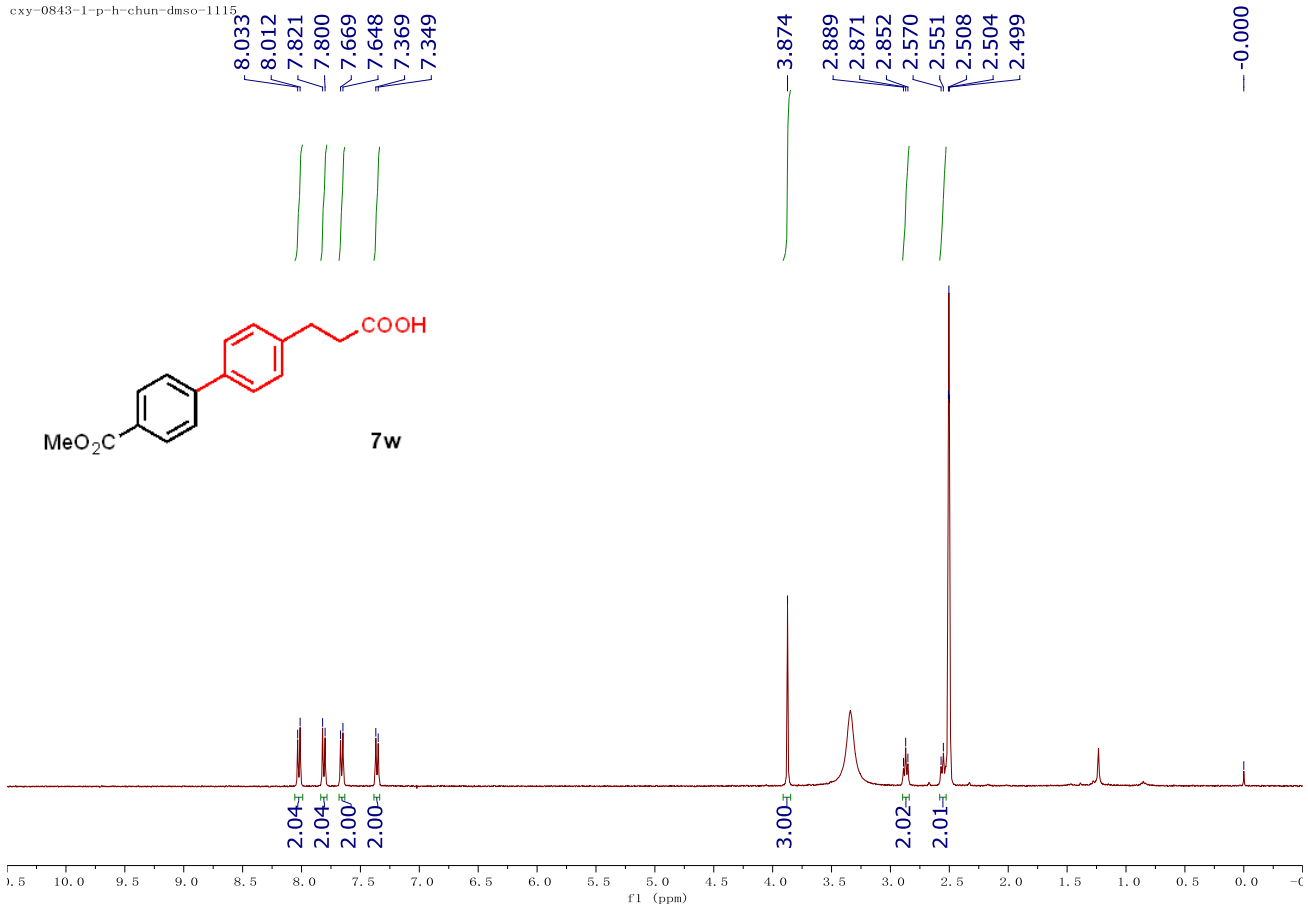
7u

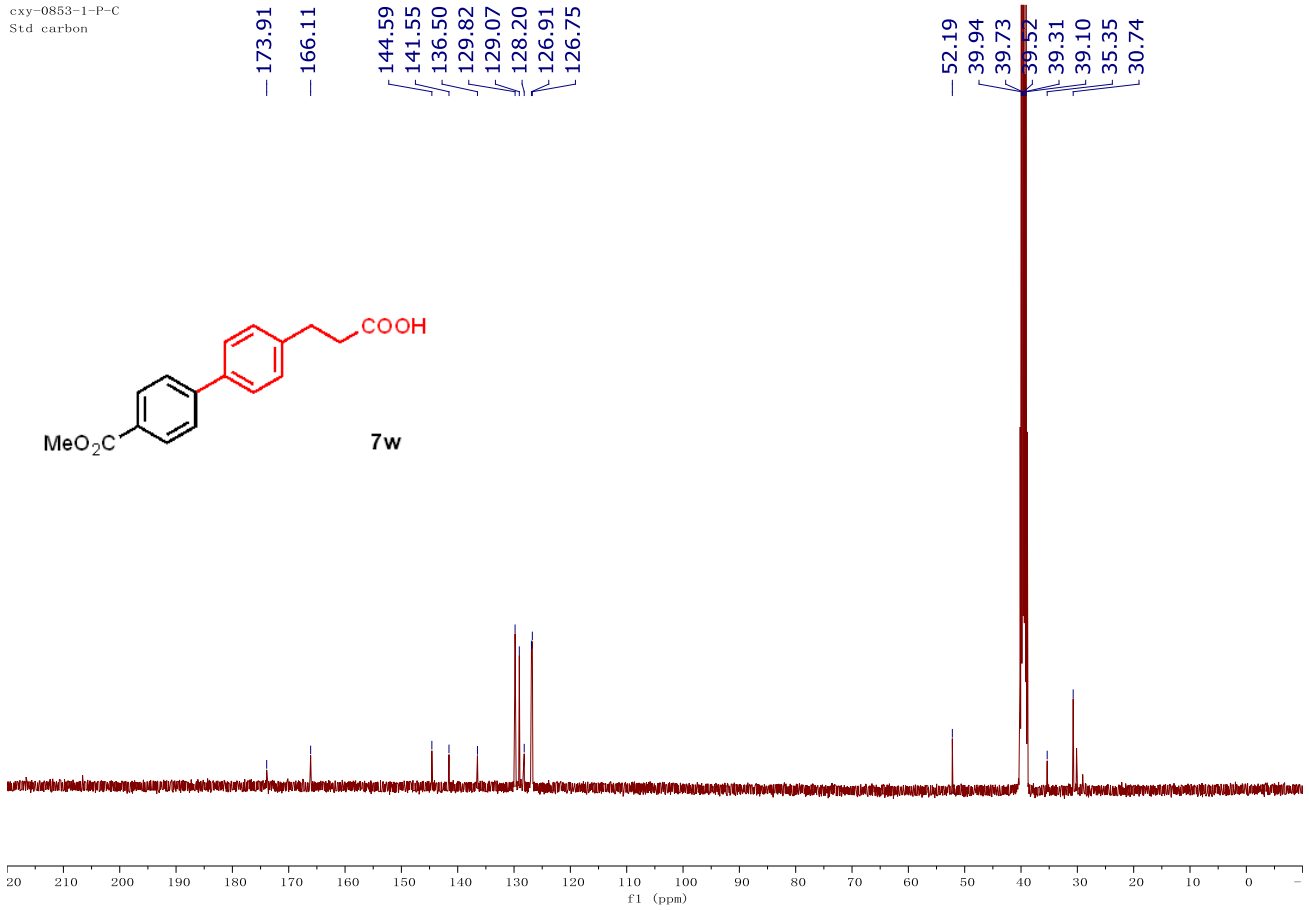


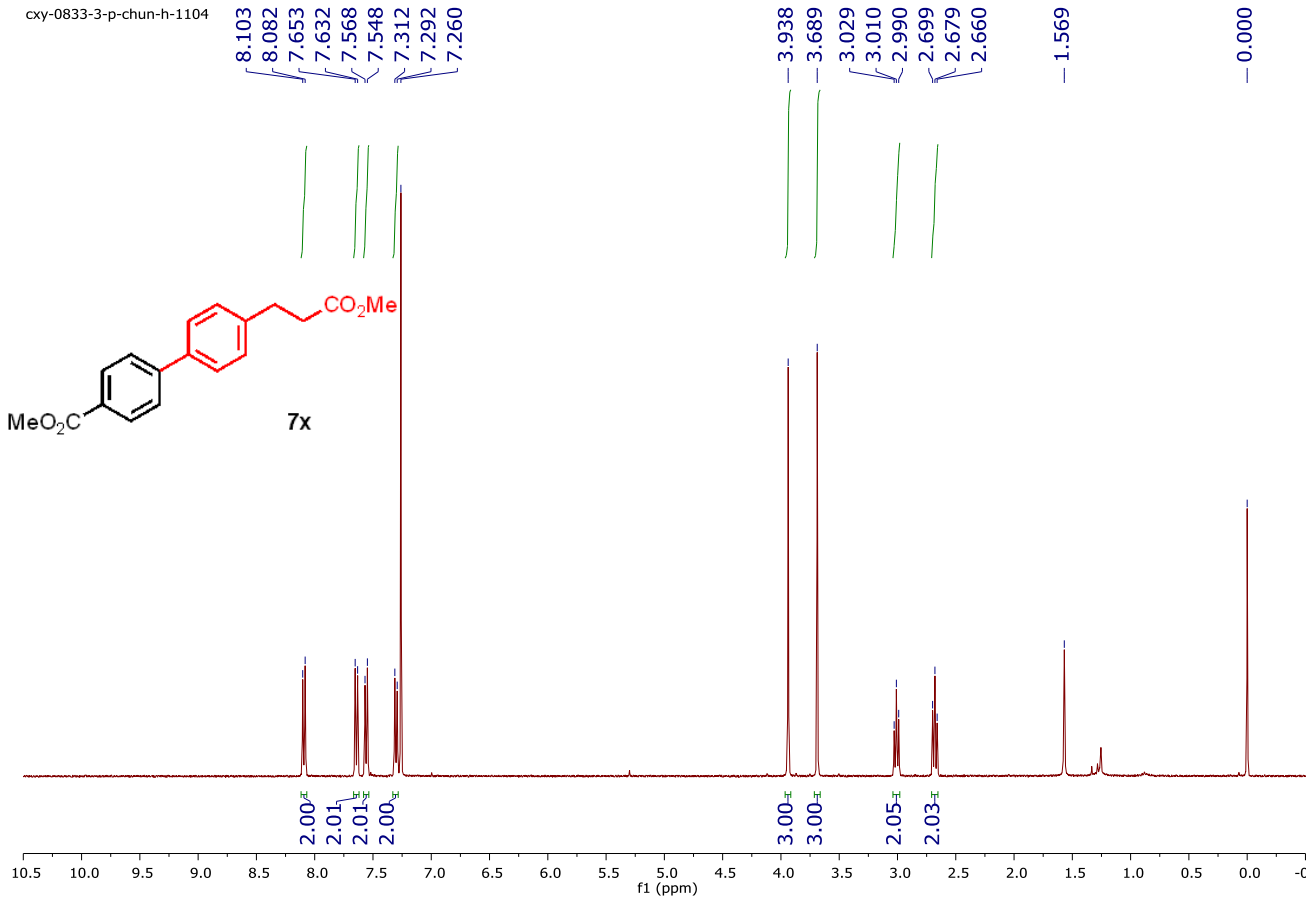

cxy-0833-4-p-c
166.98
145.32
140.83
137.85
130.08
129.12
128.72
127.33
126.81
77.32
77.00
76.68
52.08
44.13
33.88
32.38
Cl
MeO2C
7u
f1 (ppm)

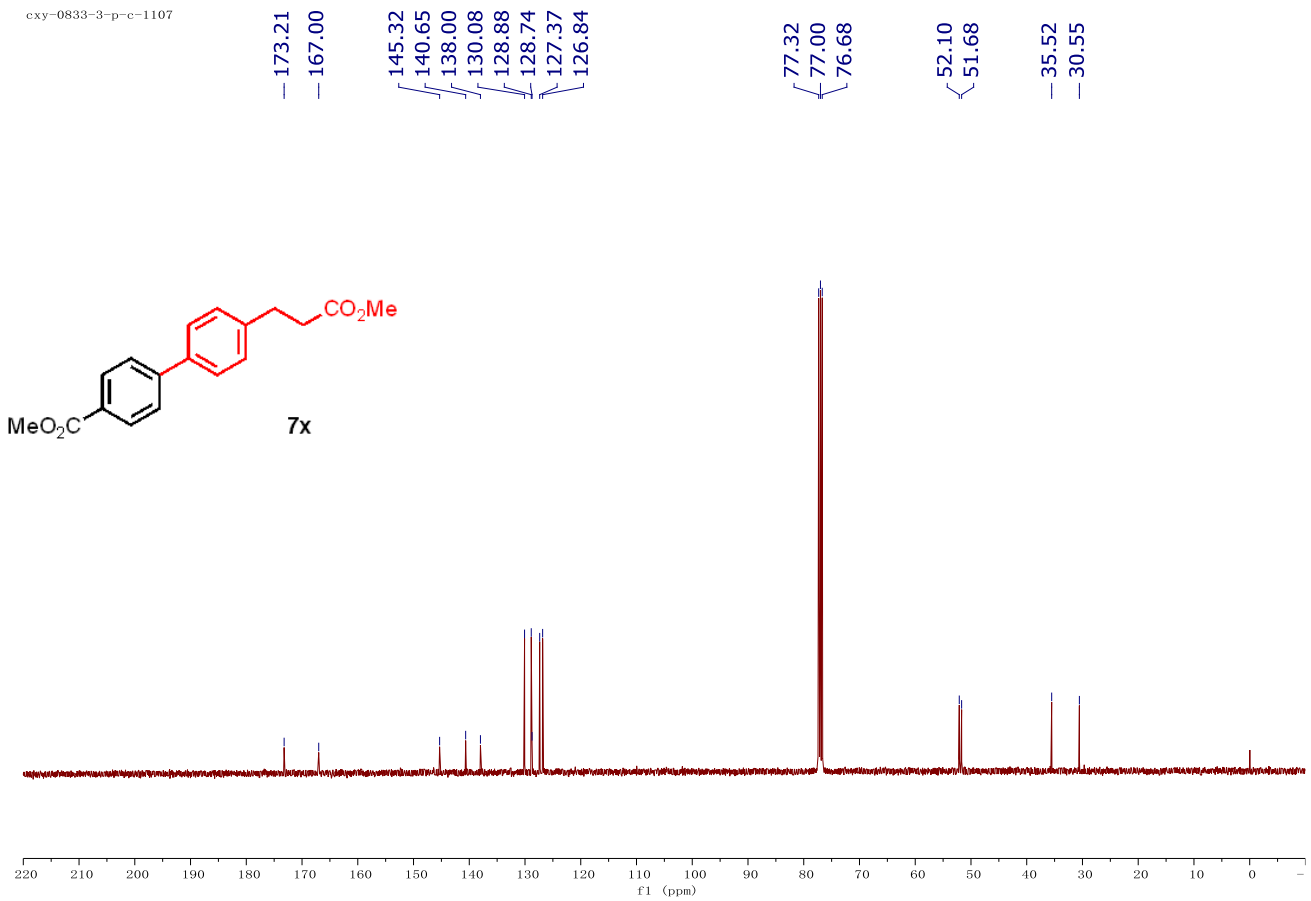

nxx-0144-3-p-chun-h-0711
8.101
8.080
7.655
7.634
7.571
7.550
7.337
7.316
7.257
3.935
3.666
3.648
3.631
3.377
2.956
2.939
2.921
1.608
-0.000
O
CO2Me
7v
2.00
2.02
2.00
1.99
3.02
2.06
2.98
2.07
f1 (ppm)

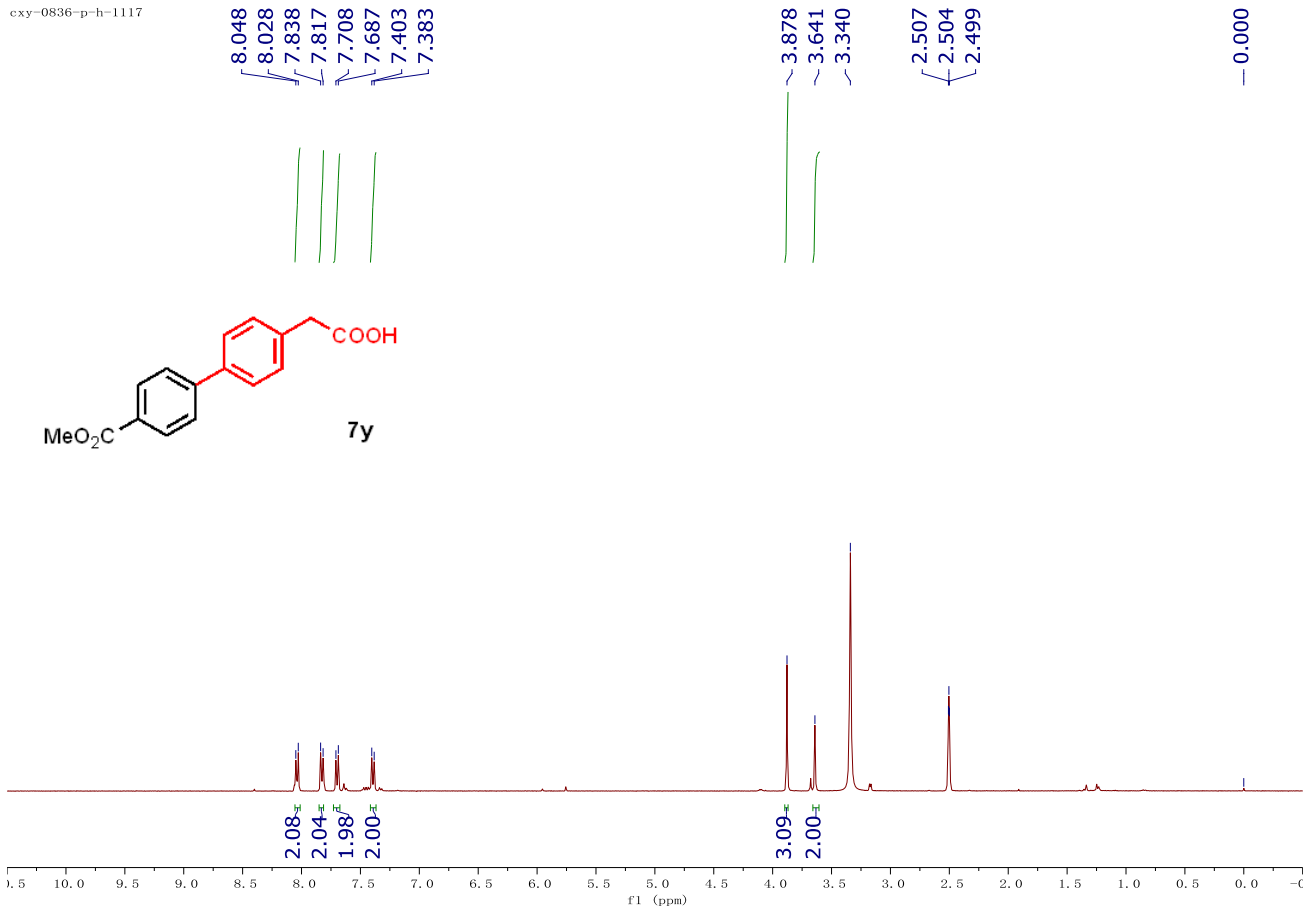

nxx-0114-3-p-chun-c-0712
Std carbon
167.00
145.44
139.20
137.90
130.05
129.41
128.67
127.23
126.83
77.32
77.00
76.68
73.38
58.71
52.09
35.84
O
CO2Me
7v
f1 (ppm)

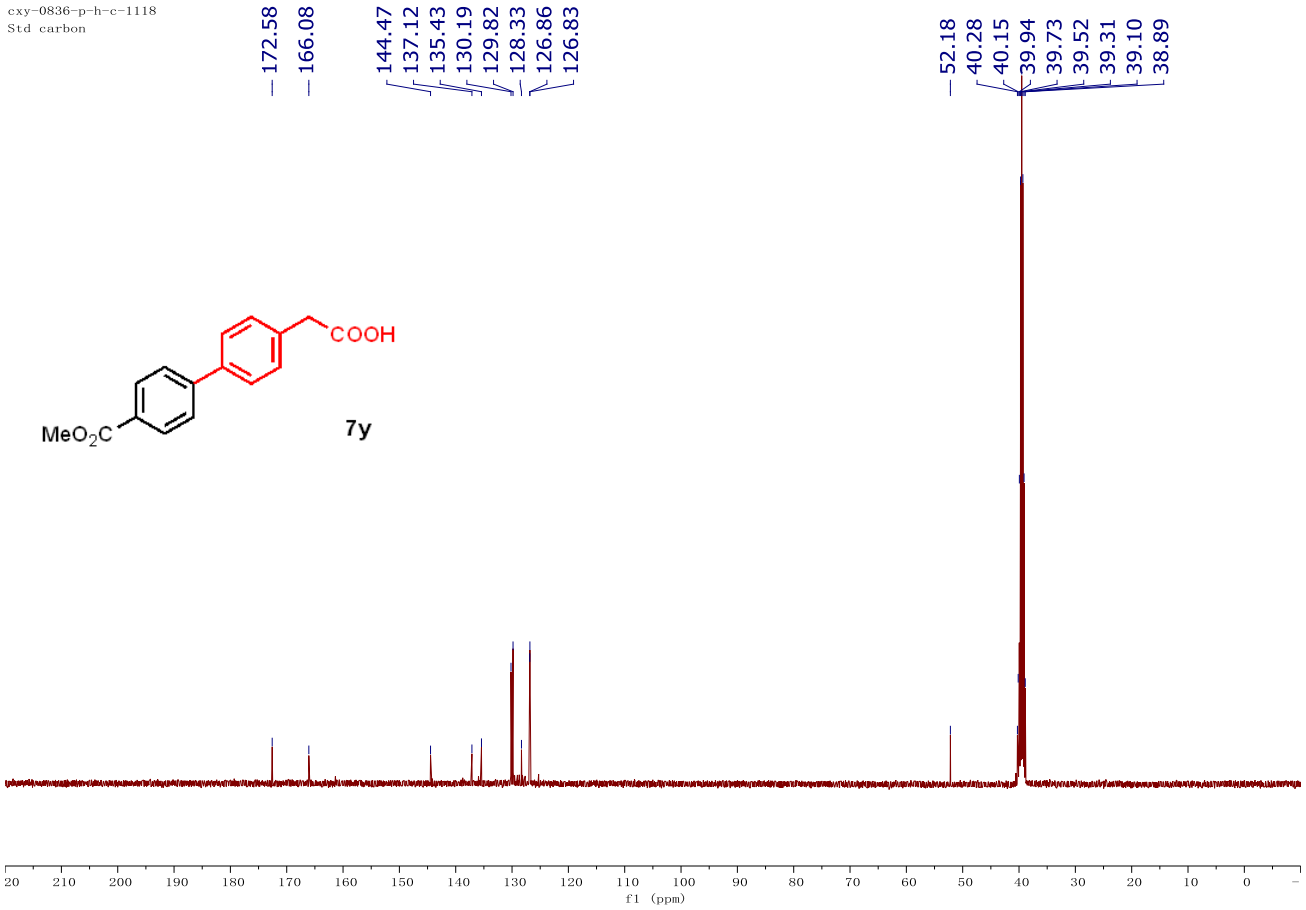

cxy-0843-1-p-h-chun-dmso-1115
8.033
8.012
7.821
7.800
7.669
7.648
7.369
7.349
3.874
2.889
2.871
2.852
2.570
2.551
2.508
2.504
2.499
-0.000
COOH
MeO2C
7w
2.04
2.04
2.00
2.00
3.00
2.02
2.01
f1 (ppm)

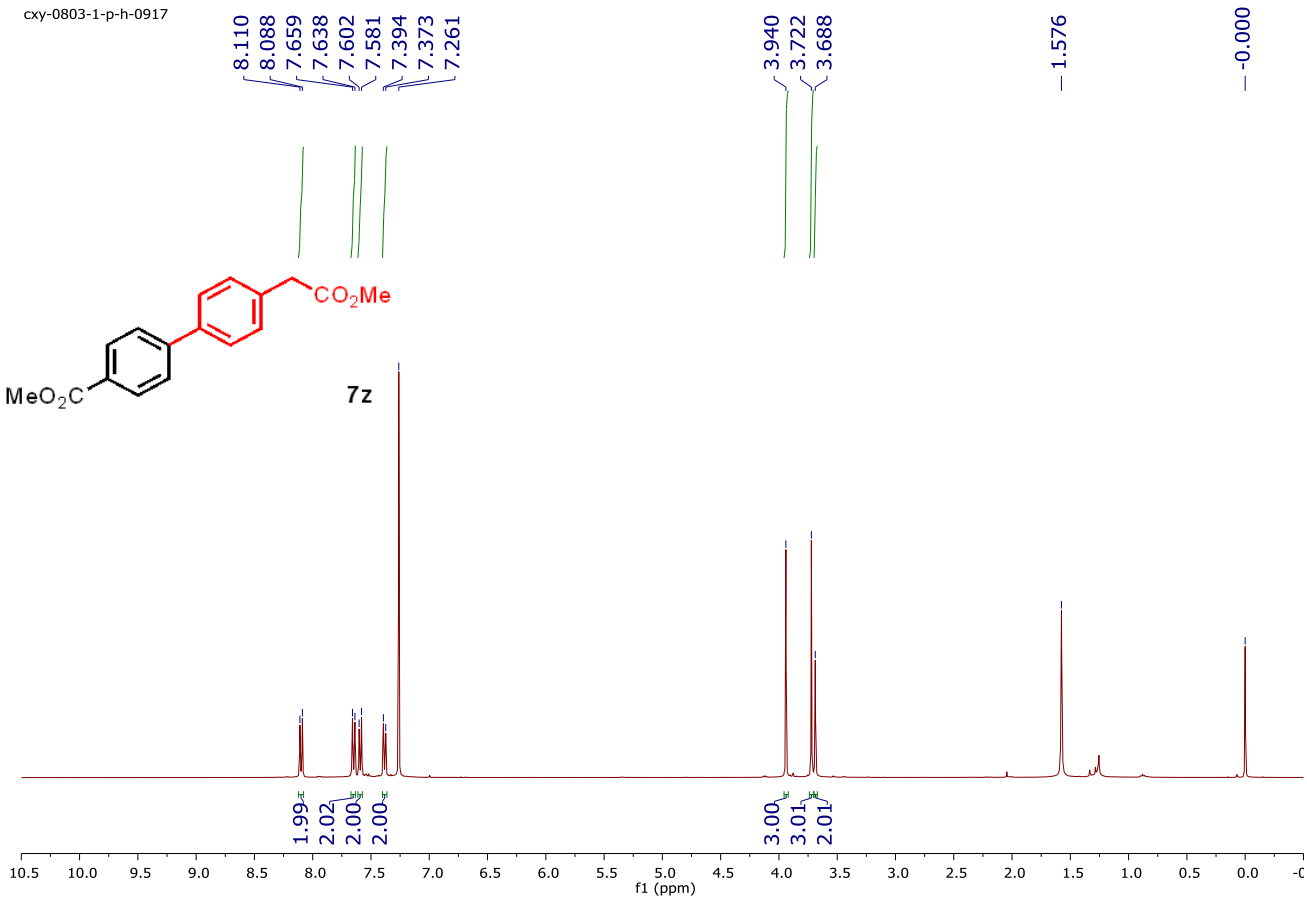

cxy-0853-1-P-C
Std carbon
173.91
166.11
144.59
141.55
136.50
129.82
129.07
128.20
126.91
126.75
52.19
39.94
39.73
39.52
39.31
39.10
35.35
30.74
COOH
MeO2C
7w
f1 (ppm)

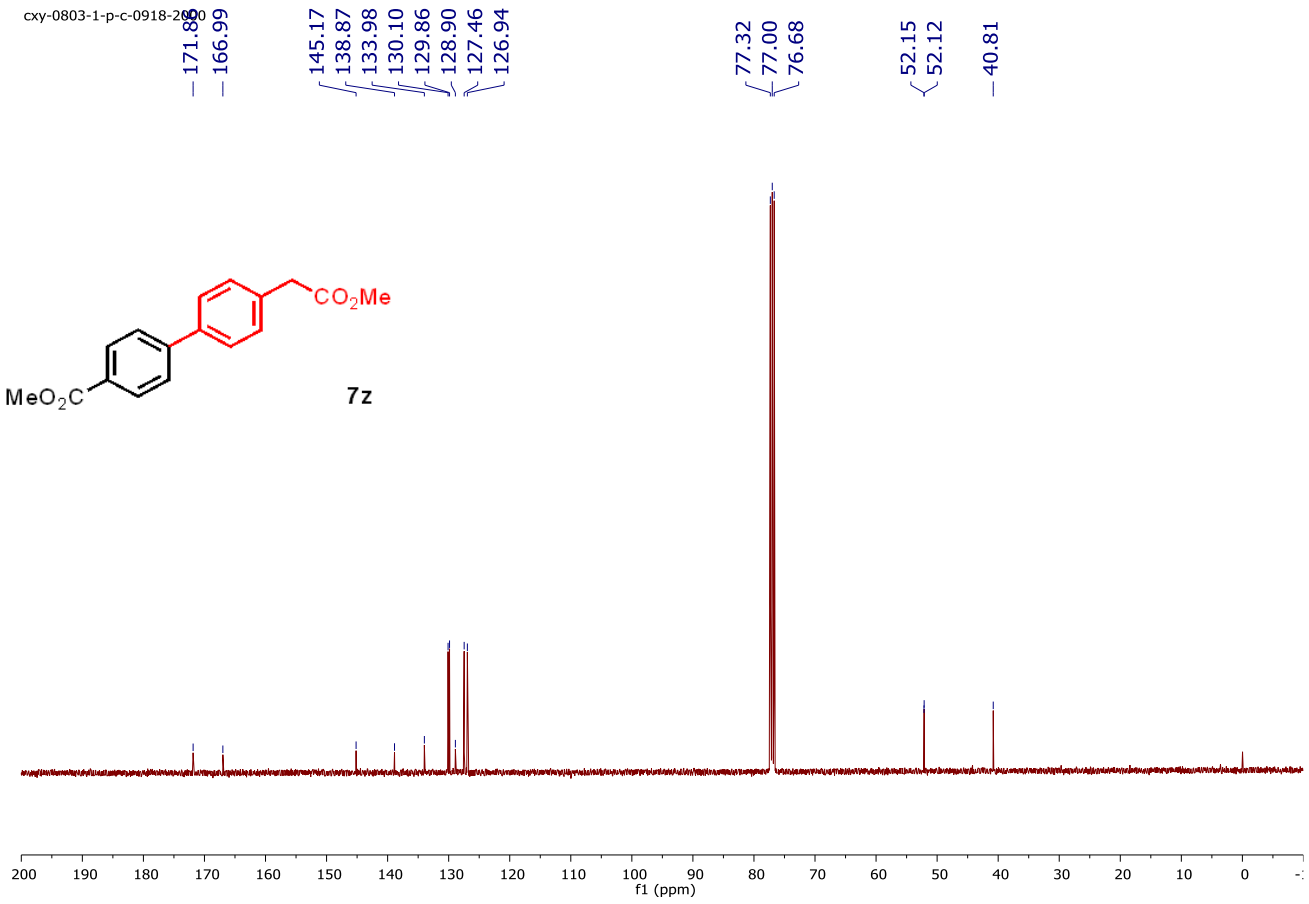

cxy-0833-3-p-chun-h-1104
8.103
8.082
7.653
7.632
7.568
7.548
7.312
7.292
7.260
3.938
3.689
3.029
3.010
2.990
2.699
2.679
2.660
1.569
0.000
CO2Me
MeO2C
7x
2.00
2.01
2.01
2.00
3.00
3.00
2.05
2.03
f1 (ppm)

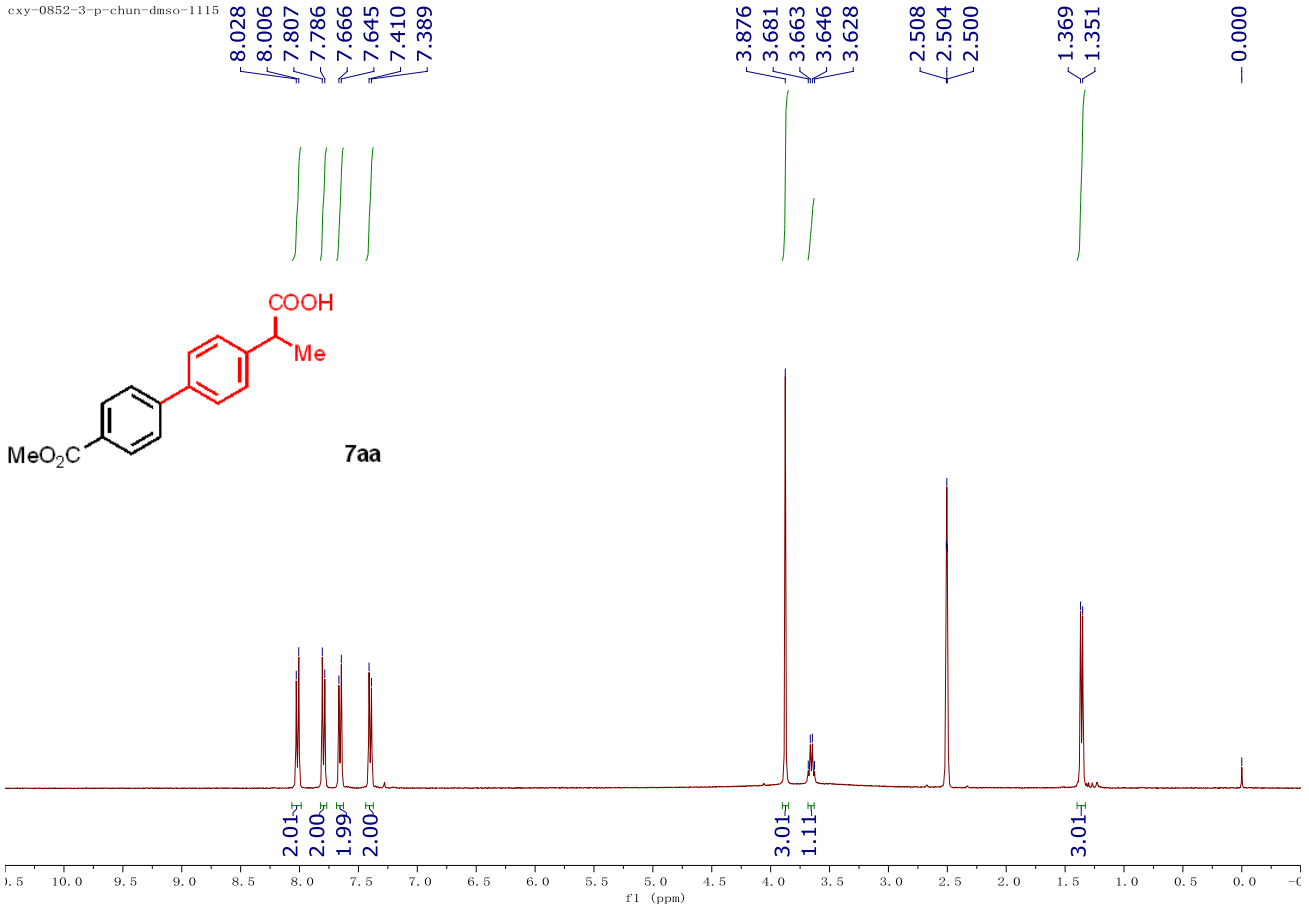

cxy-0833-3-p-c-1107
173.21
167.00
145.32
140.65
138.00
130.08
128.88
128.74
127.37
126.84
77.32
77.00
76.68
52.10
51.68
35.52
30.55
CO2Me
MeO2C
7x
f1 (ppm)

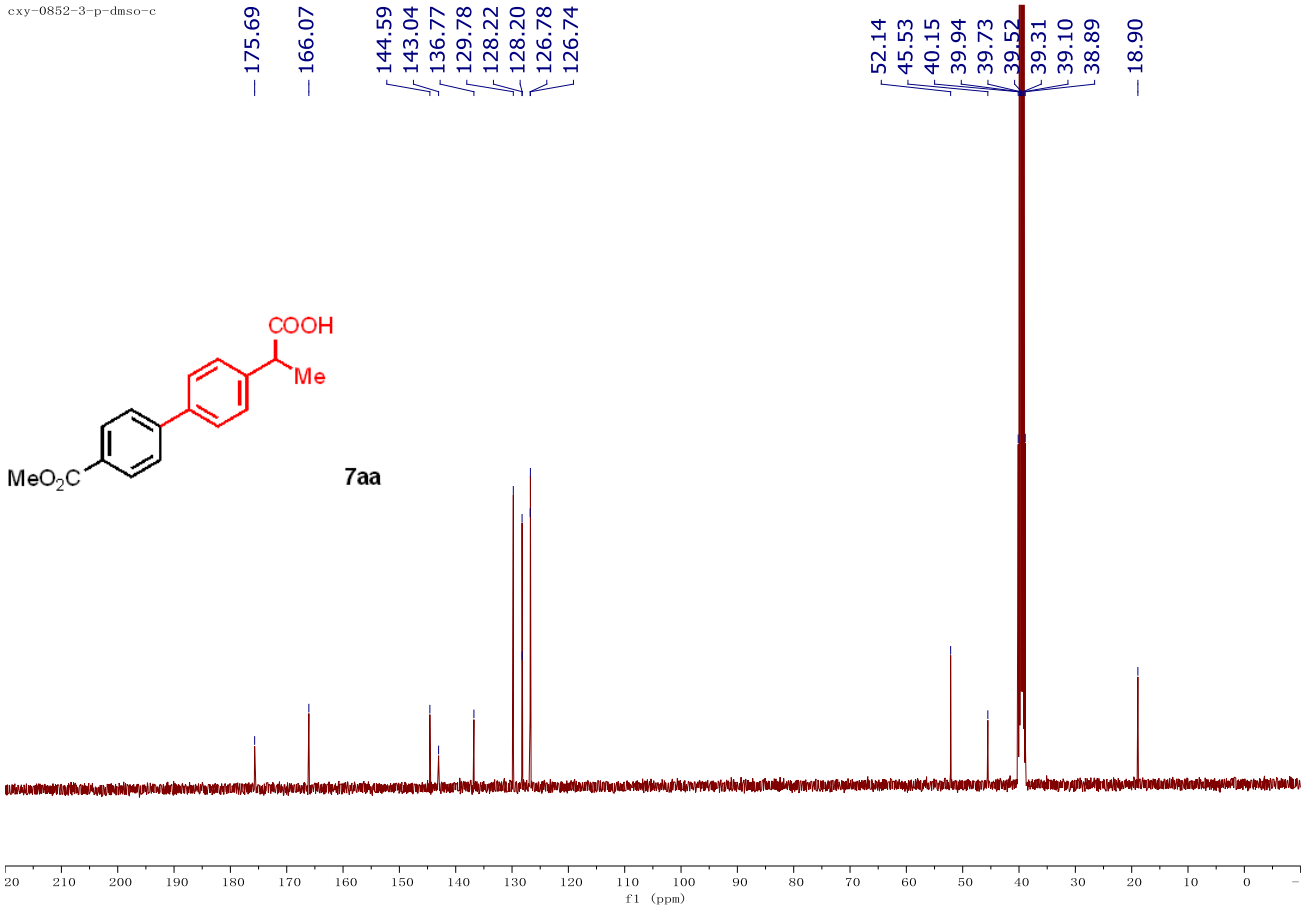

cxy-0836-p-h-1117
8.048
8.028
7.838
7.817
7.708
7.687
7.403
7.383
3.878
3.641
3.340
2.507
2.504
2.499
0.000
COOH
MeO2C
7y
2.08
2.04
1.98
2.00
3.09
2.00
f1 (ppm)

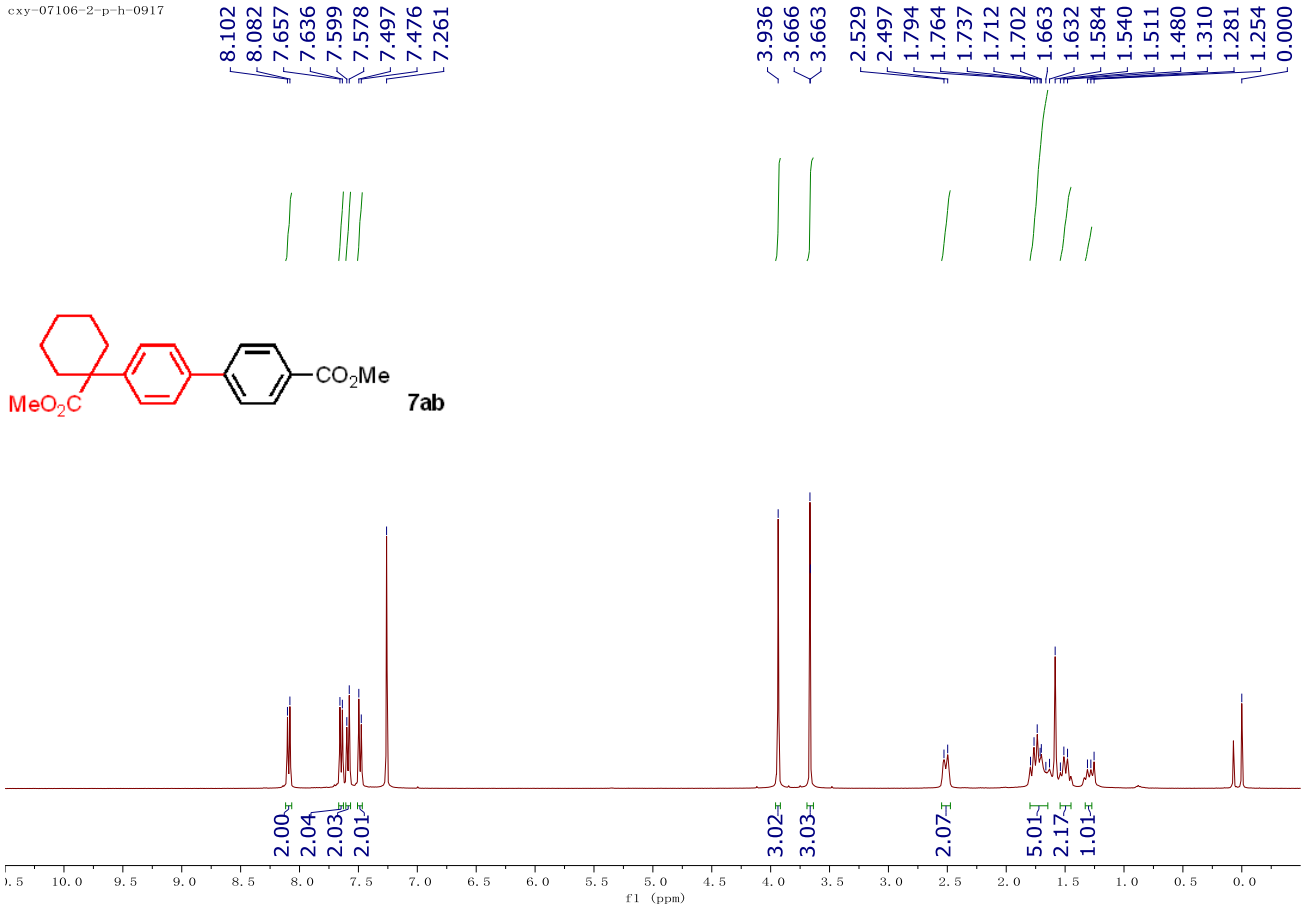

cxy-0836-p-h-c-1118
Std carbon
172.58
166.08
144.47
137.12
135.43
130.19
129.82
128.33
126.86
126.83
52.18
40.28
40.15
39.94
39.73
39.52
39.31
39.10
38.89
COOH
MeO2C
7y
f1 (ppm)

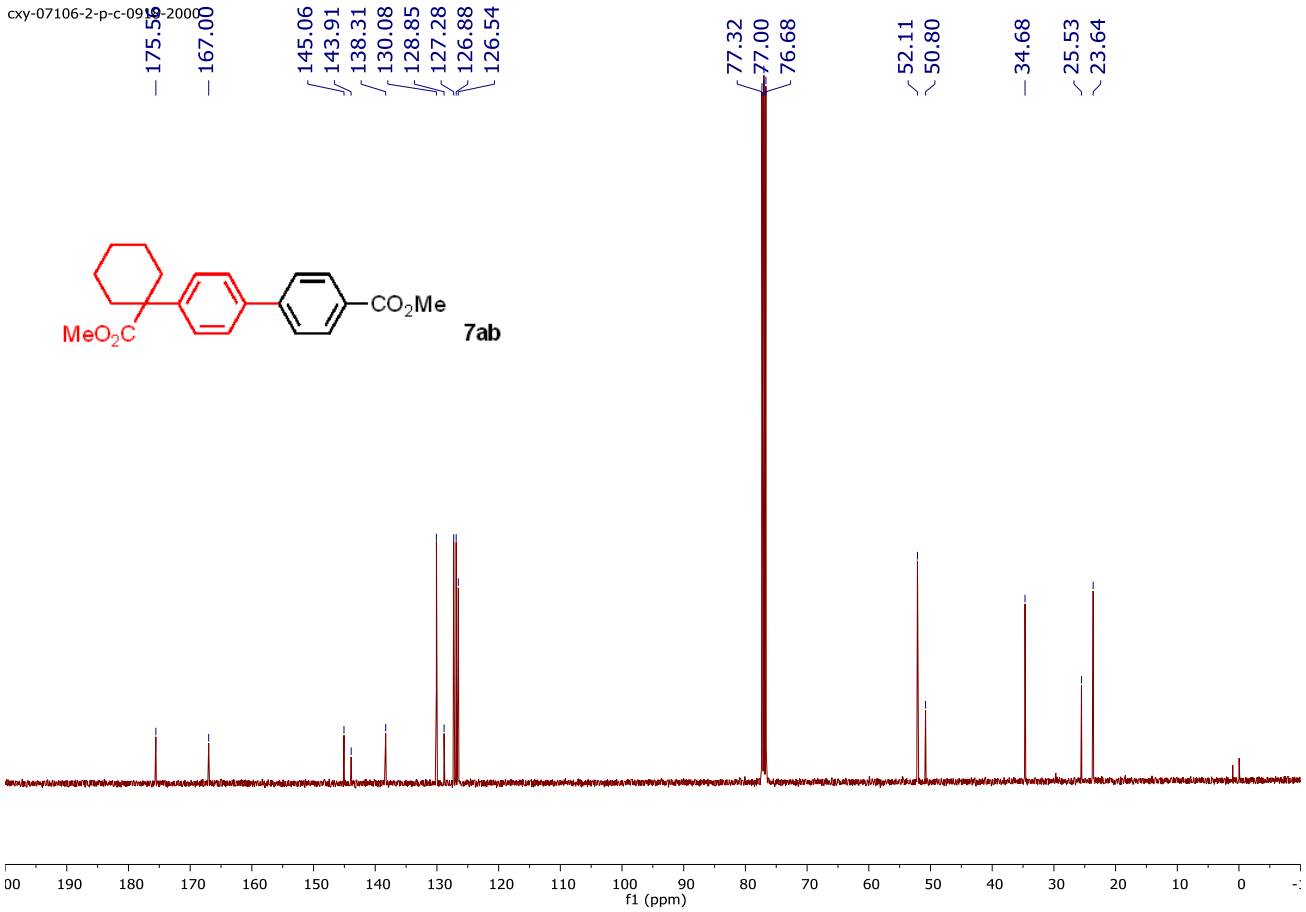

cxy-0803-1-p-h-0917
8.110
8.088
7.659
7.638
7.602
7.581
7.394
7.373
7.261
3.940
3.722
3.688
1.576
-0.000
CO2Me
MeO2C
7z
1.99
2.02
2.00
2.00
3.00
3.01
2.01
f1 (ppm)

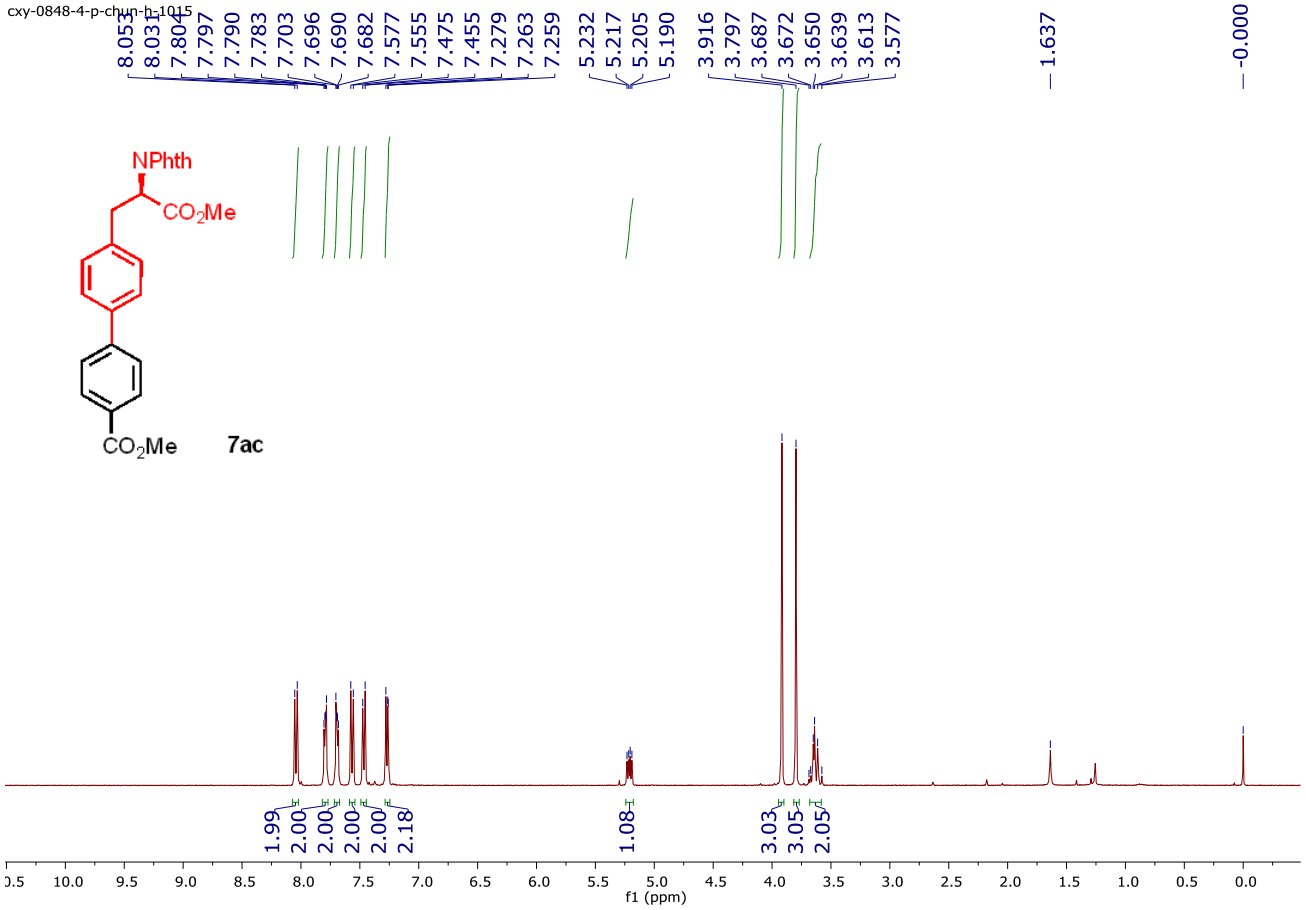

cxy-0803-1-p-c-0918-2000
171.80
166.99
145.17
138.87
133.98
130.10
129.86
128.90
127.46
126.94
77.32
77.00
76.68
52.15
52.12
40.81
CO2Me
MeO2C
7z
f1 (ppm)

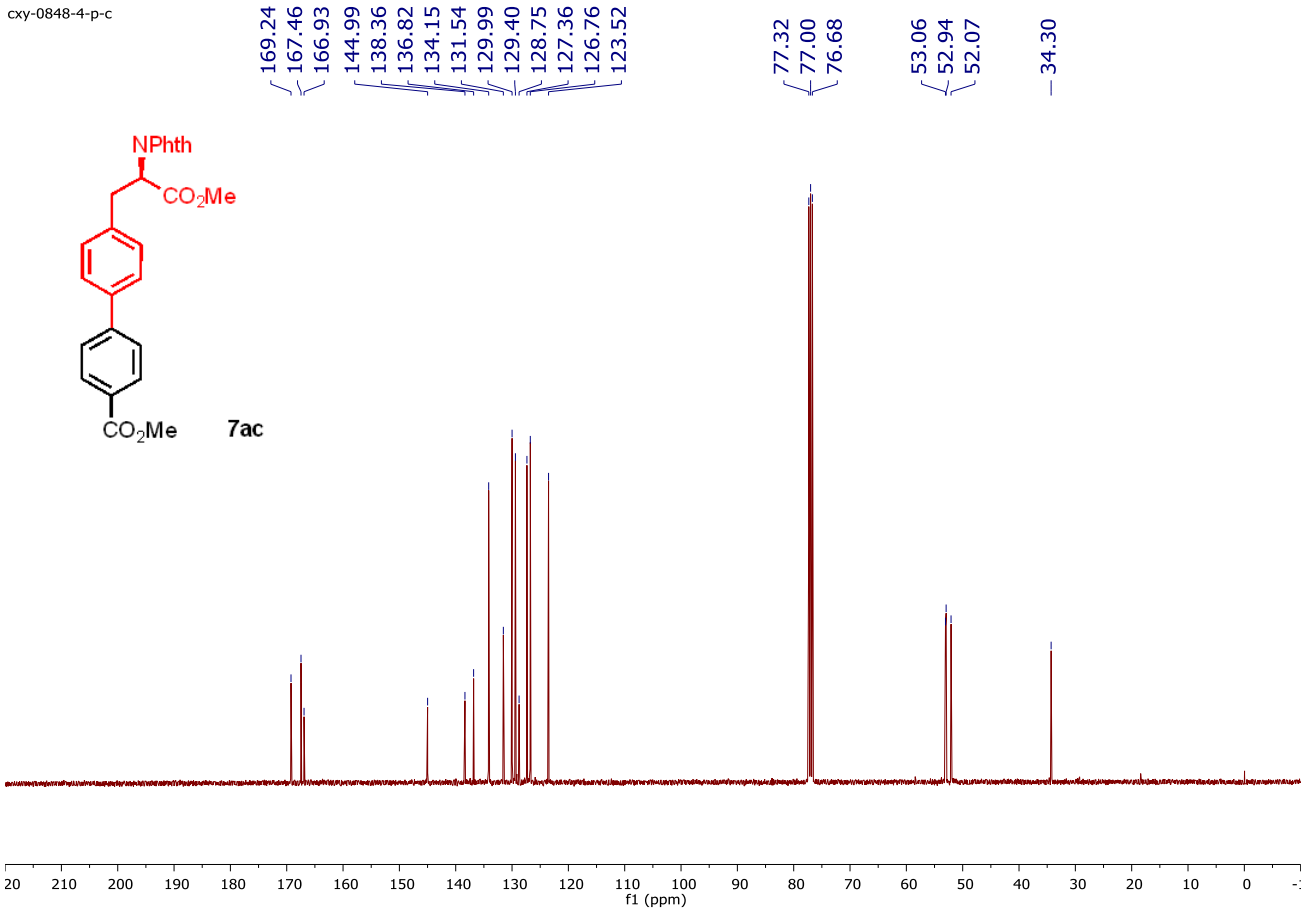

cxy-0852-3-p-chun-dmso-1115
8.028
8.006
7.807
7.786
7.666
7.645
7.410
7.389
3.876
3.681
3.663
3.646
3.628
2.508
2.504
2.500
1.369
1.351
0.000
COOH
Me
MeO2C
7aa
2.01
2.00
1.99
2.00
3.01
1.11
3.01
f1 (ppm)

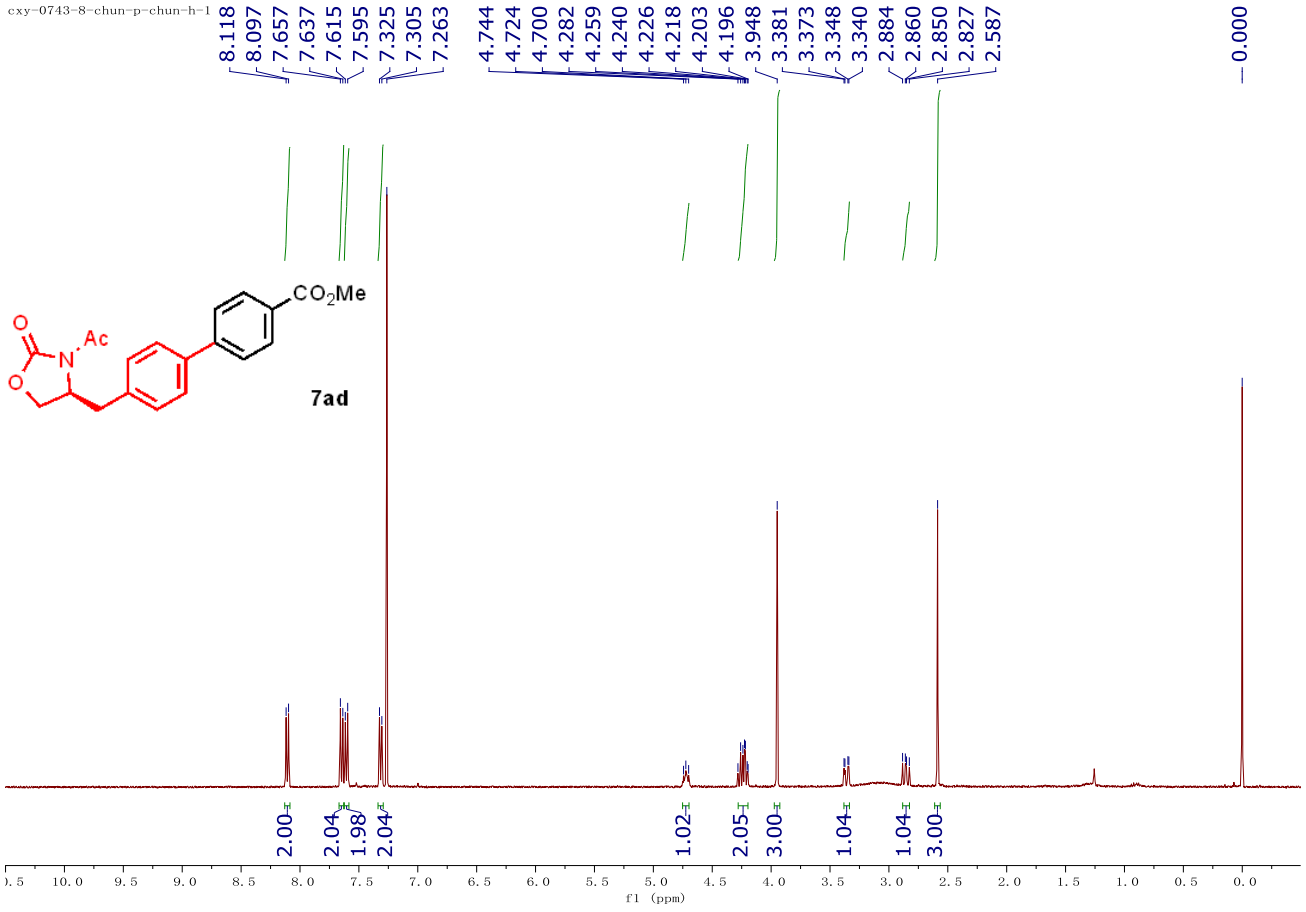

cxy-0852-3-p-dmso-c
175.69
166.07
144.59
143.04
136.77
129.78
128.22
128.20
126.78
126.74
52.14
45.53
40.15
39.94
39.73
39.52
39.31
39.10
38.89
18.90
COOH
Me
MeO2C
7aa
f1 (ppm)

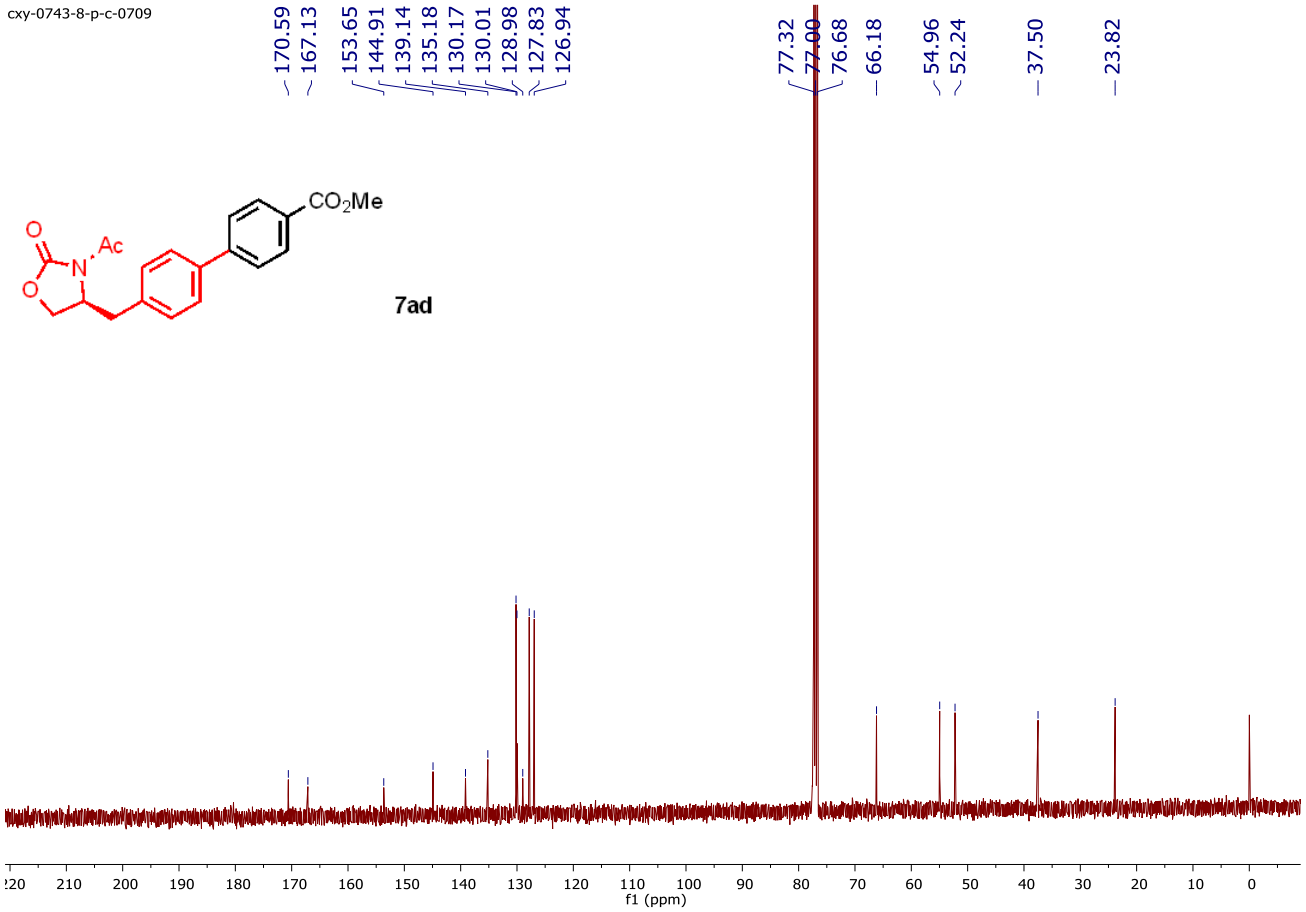

cxy-07106-2-p-h-0917
8.102
8.082
7.657
7.636
7.599
7.578
7.497
7.476
7.261
3.936
3.666
3.663
2.529
2.497
1.794
1.764
1.737
1.712
1.702
1.663
1.632
1.584
1.540
1.511
1.480
1.310
1.281
1.254
0.000
MeO2C
CO2Me
7ab
2.00
2.04
2.03
2.01
3.02
3.03
2.07
5.01
2.17
1.01
f1 (ppm)

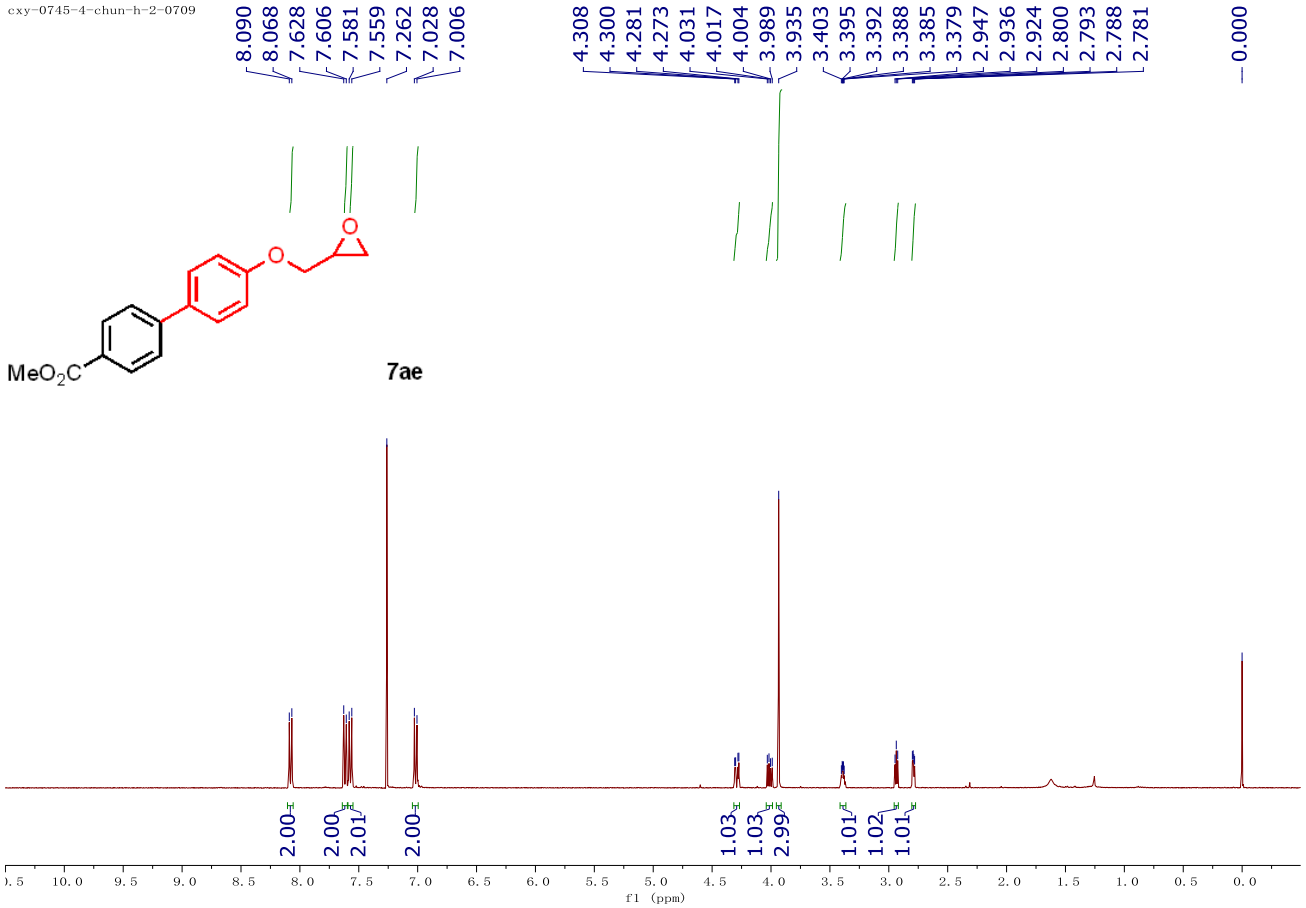

cxy-07106-2-p-c-0919-2000
175.59
167.00
145.06
143.91
138.31
130.08
128.85
127.28
126.88
126.54
77.32
77.00
76.68
52.11
50.80
34.68
25.53
23.64
MeO2C
CO2Me
7ab
f1 (ppm)

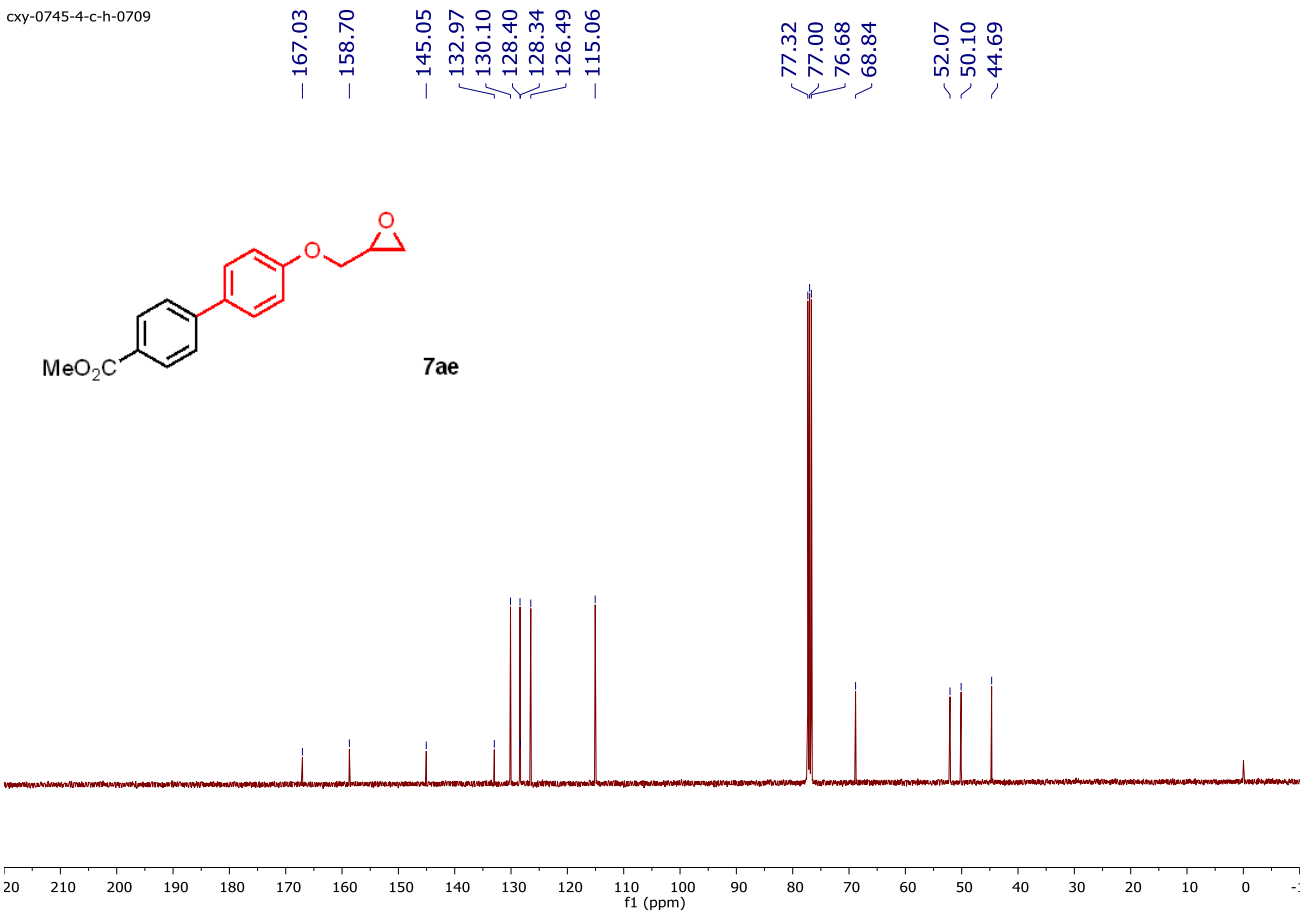

cxy-0848-4-p-chun-h-1015
8.053
8.031
7.804
7.797
7.790
7.783
7.703
7.696
7.690
7.682
7.577
7.555
7.475
7.455
7.279
7.263
7.259
5.232
5.217
5.205
5.190
3.916
3.797
3.687
3.672
3.650
3.639
3.613
3.577
1.637
-0.000
NPhth
CO2Me
CO2Me
7ac
1.99
2.00
2.00
2.00
2.00
2.18
1.08
3.03
3.05
2.05
f1 (ppm)

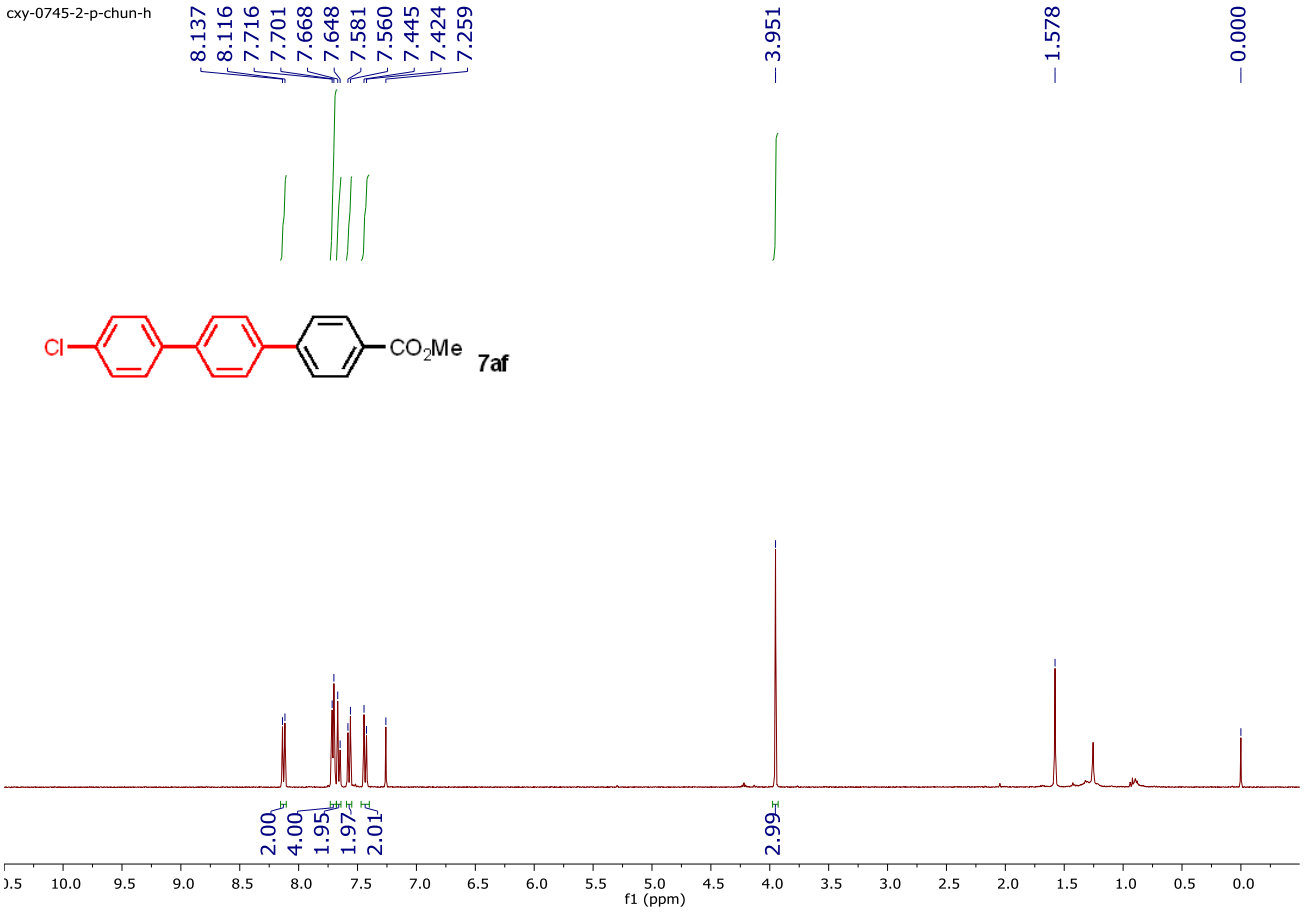

cxy-0848-4-p-c
169.24
167.46
166.93
144.99
138.36
136.82
134.15
131.54
129.99
129.40
128.75
127.36
126.76
123.52
77.32
77.00
76.68
53.06
52.94
52.07
34.30
NPhth
CO2Me
CO2Me
7ac
f1 (ppm)

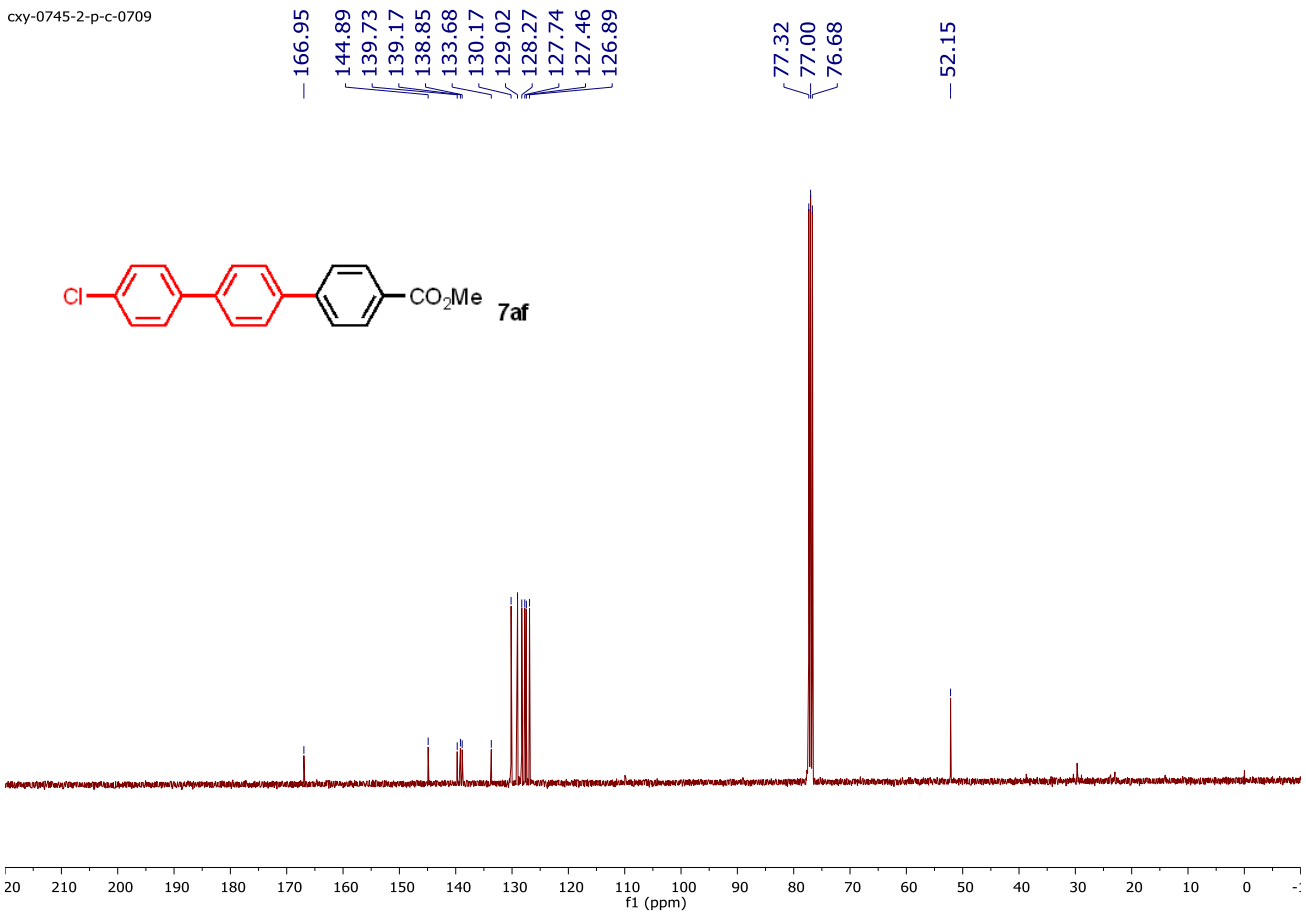

cxy-0743-8-chun-p-chun-h-1
8.118
8.097
7.657
7.637
7.615
7.595
7.325
7.305
7.263
4.744
4.724
4.700
4.282
4.259
4.240
4.226
4.218
4.203
4.196
3.948
3.381
3.373
3.348
3.340
2.884
2.860
2.850
2.827
2.587
0.000
CO2Me
O
N
Ac
O
7ad
2.00
2.04
1.98
2.04
1.02
2.05
3.00
1.04
1.04
3.00
f1 (ppm)

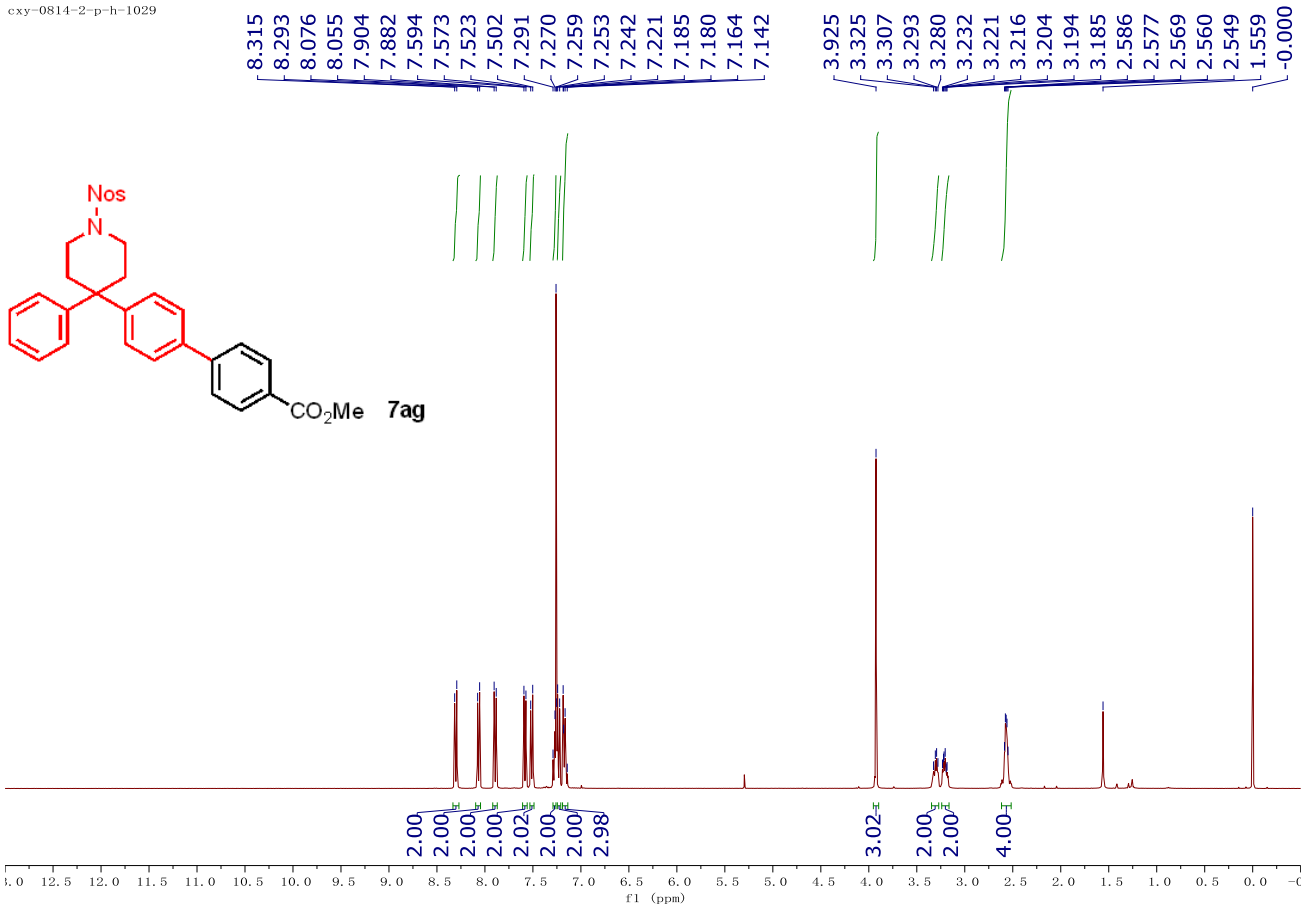

cxy-0743-8-p-c-0709
170.59
167.13
153.65
144.91
139.14
135.18
130.17
130.01
128.98
127.83
126.94
77.32
77.00
76.68
66.18
54.96
52.24
37.50
23.82
CO2Me
Ac
O
N
O
7ad
f1 (ppm)

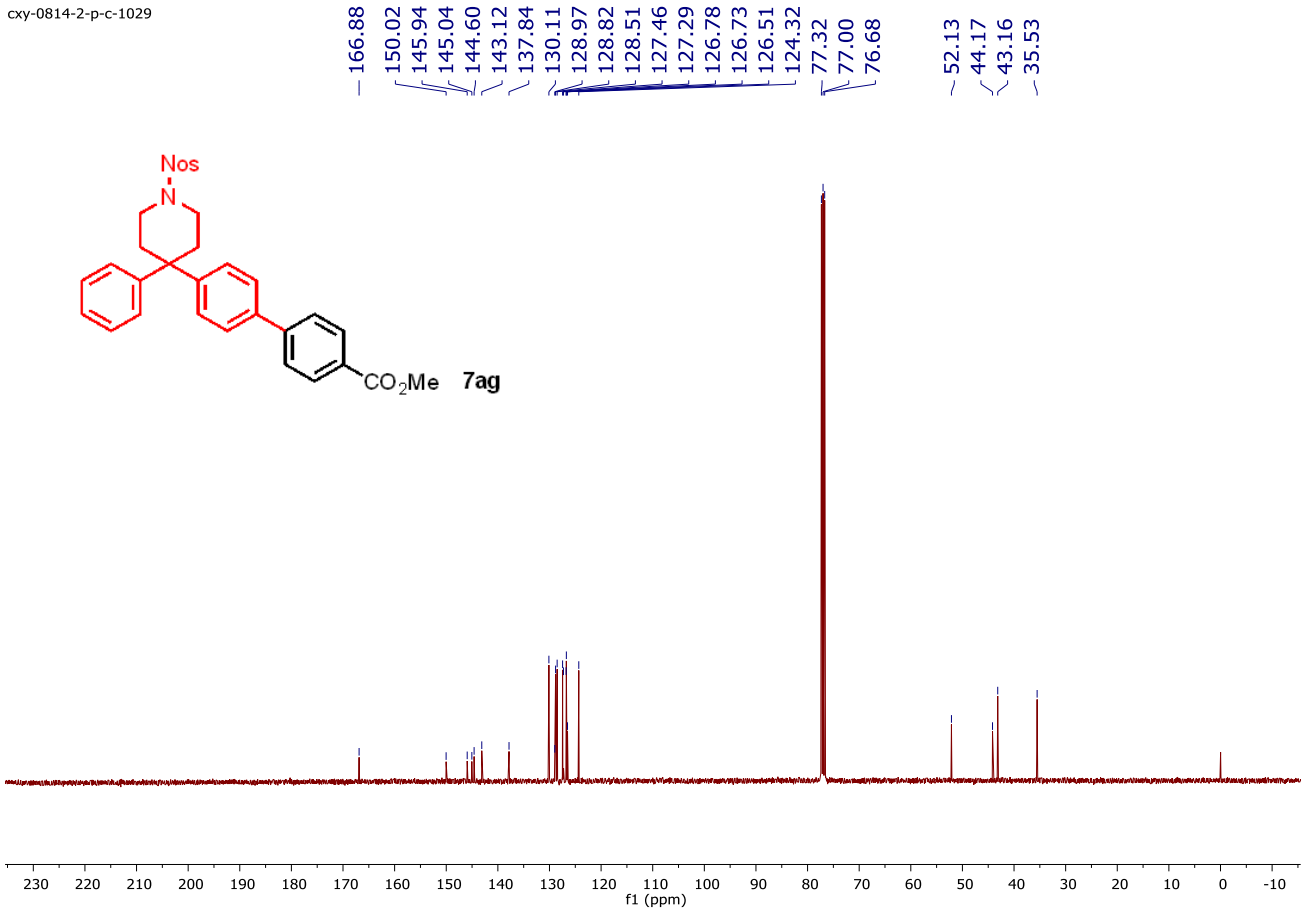

cxy-0745-4-chun-h-2-0709
8.090
8.068
7.628
7.606
7.581
7.559
7.262
7.028
7.006
4.308
4.300
4.281
4.273
4.031
4.017
4.004
3.989
3.935
3.403
3.395
3.392
3.388
3.385
3.379
2.947
2.936
2.924
2.800
2.793
2.788
2.781
0.000
O
O
MeO2C
7ae
2.00
2.00
2.01
2.00
1.03
1.03
2.99
1.01
1.02
1.01
f1 (ppm)

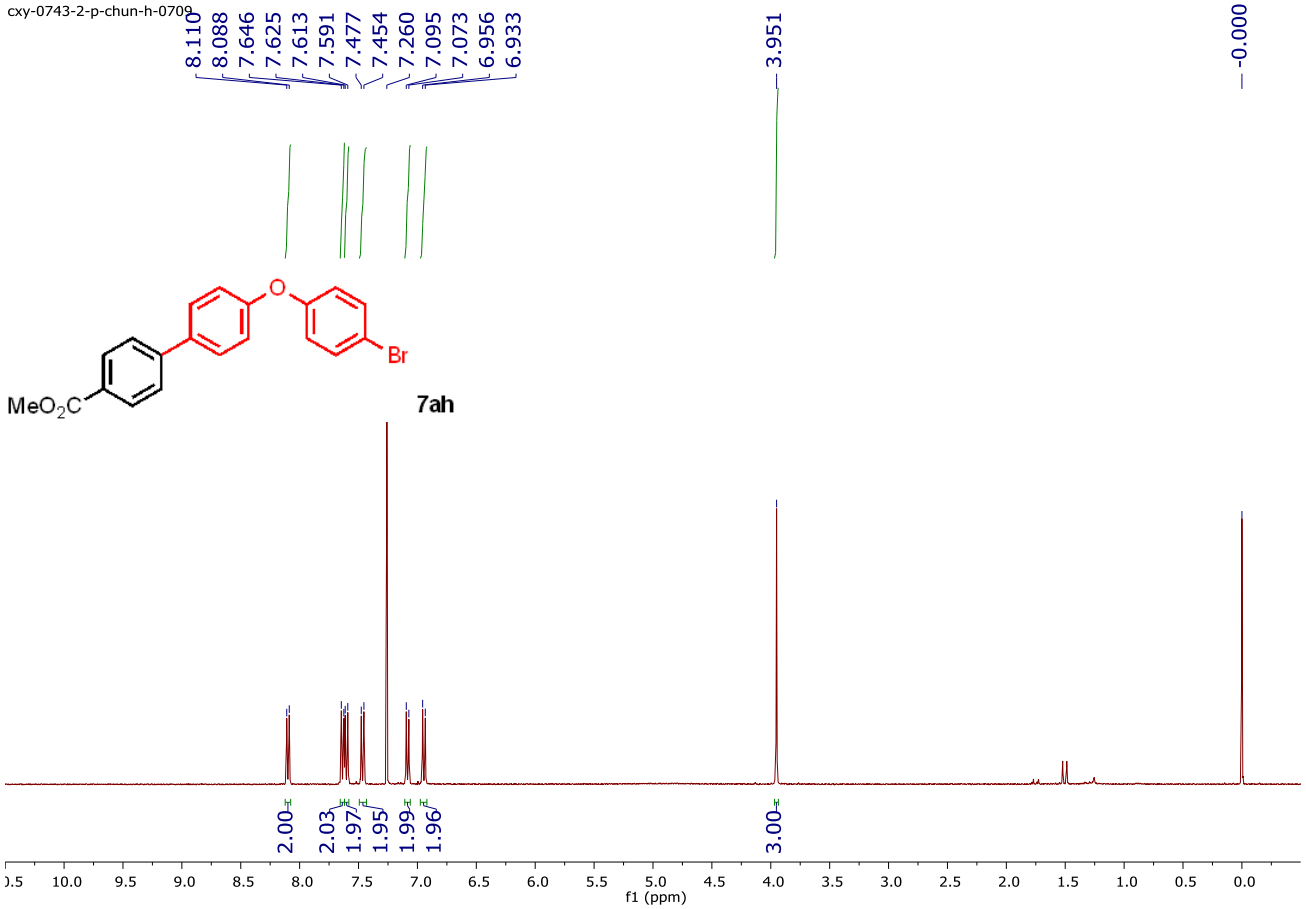

cxy-0745-4-c-h-0709
167.03
158.70
145.05
132.97
130.10
128.40
128.34
126.49
115.06
77.32
77.00
76.68
68.84
52.07
50.10
44.69
MeO2C
7ae
f1 (ppm)

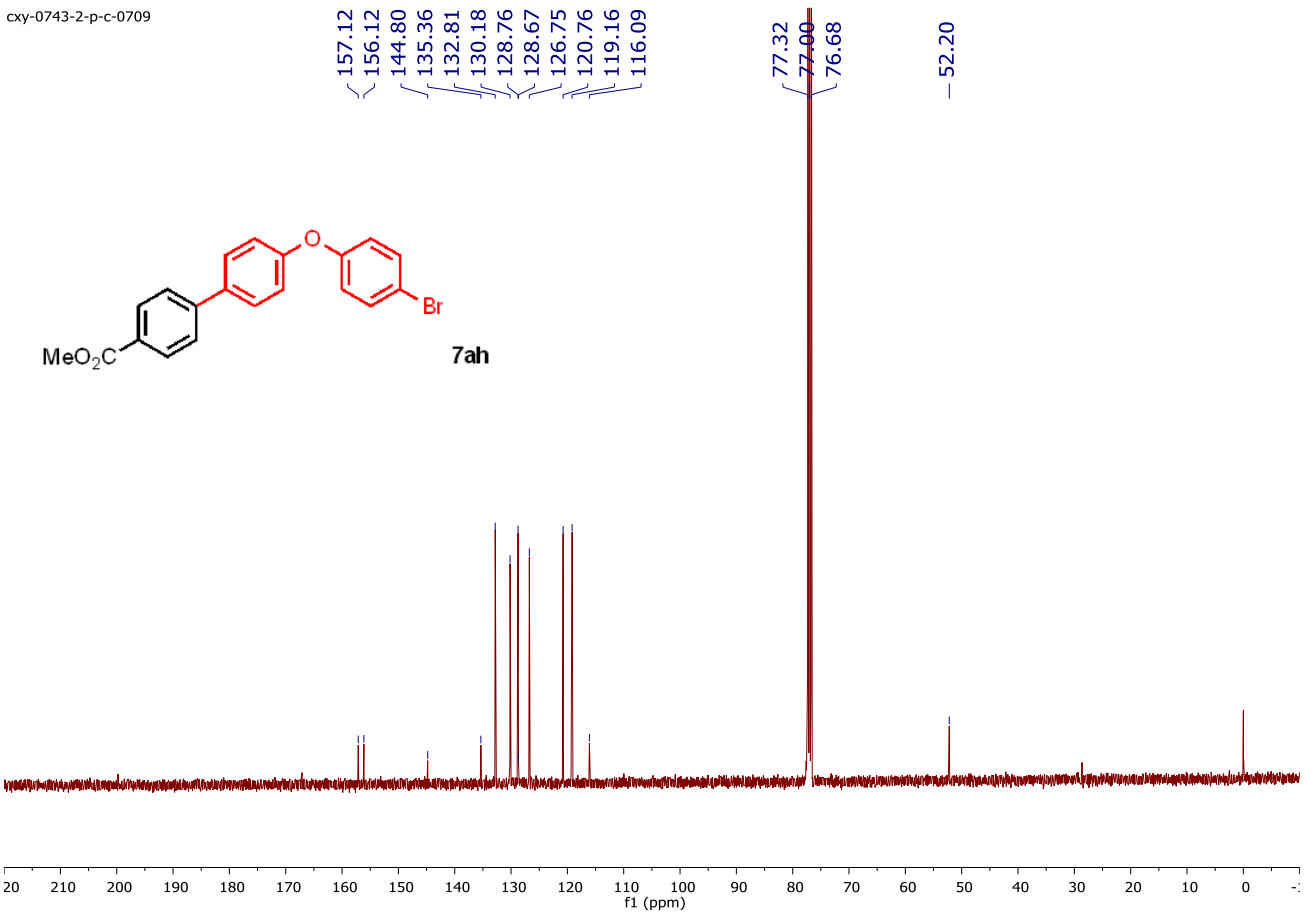

cxy-0745-2-p-chun-h
8.137
8.116
7.716
7.701
7.668
7.648
7.581
7.560
7.445
7.424
7.259
3.951
1.578
0.000
Cl
CO2Me
7af
2.00
4.00
1.95
1.97
2.01
2.99
f1 (ppm)

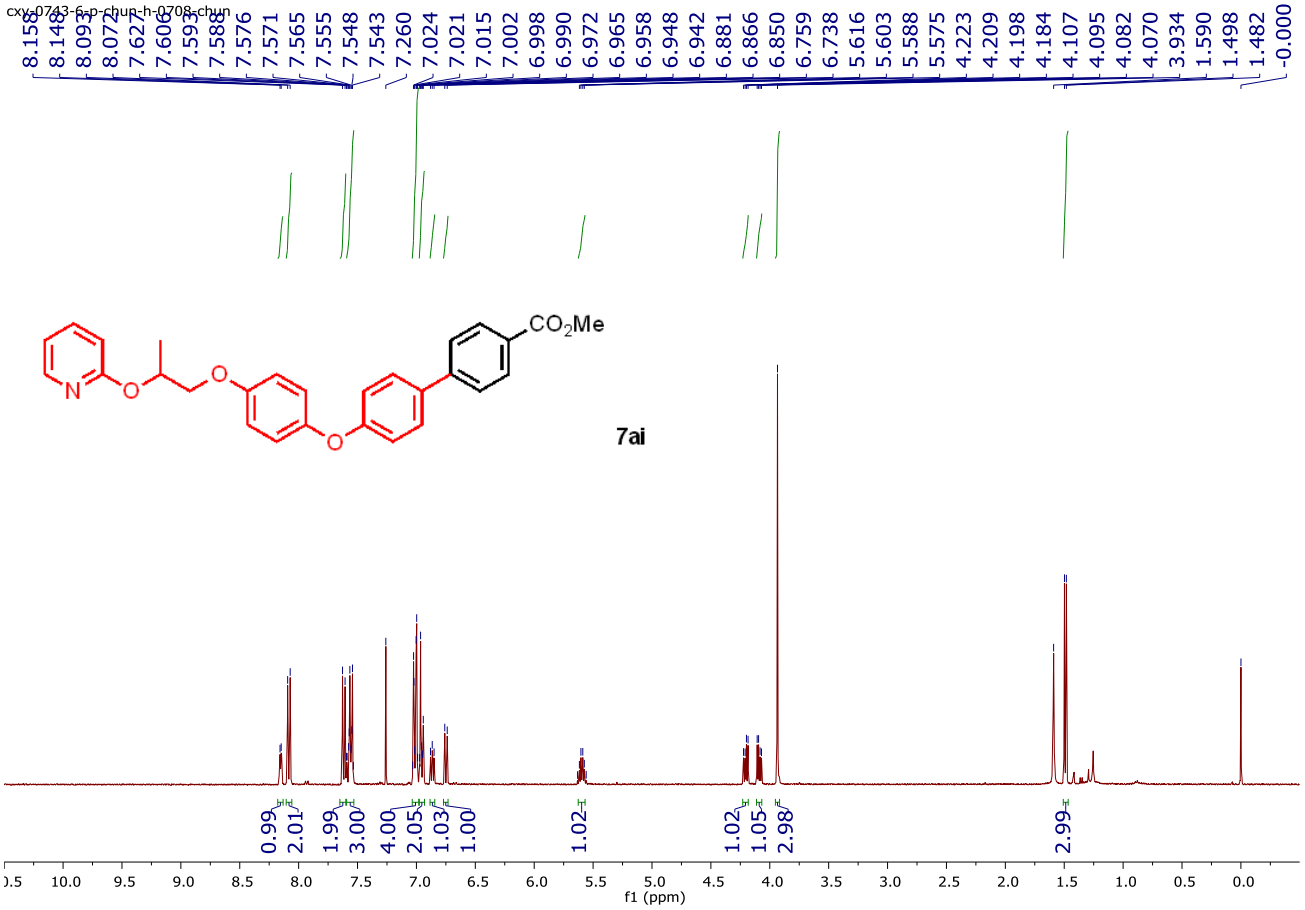

cxy-0745-2-p-c-0709
166.95
144.89
139.73
139.17
138.85
133.68
130.17
129.02
128.27
127.74
127.46
126.89
77.32
77.00
76.68
52.15
Cl
CO2Me
7af
f1 (ppm)

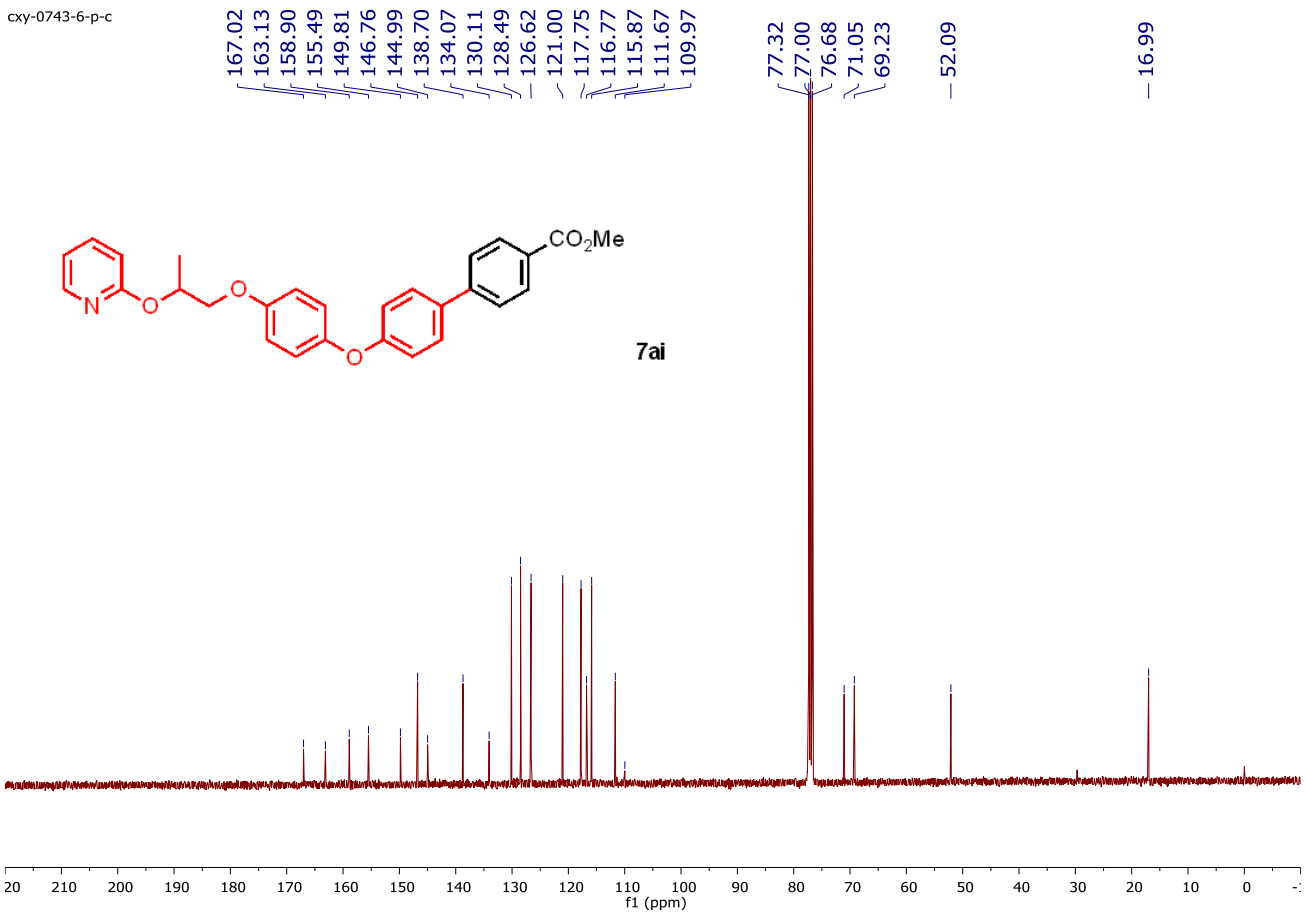

cxy-0814-2-p-h-1029
8.315
8.293
8.076
8.055
7.904
7.882
7.594
7.573
7.523
7.502
7.291
7.270
7.259
7.253
7.242
7.221
7.185
7.180
7.164
7.142
3.925
3.325
3.307
3.293
3.280
3.232
3.221
3.216
3.204
3.194
3.185
2.586
2.577
2.569
2.560
2.549
1.559
-0.000
Nos
N
CO2Me
7ag
2.00
2.00
2.00
2.00
2.02
2.00
2.00
2.98
3.02
2.00
2.00
4.00
f1 (ppm)

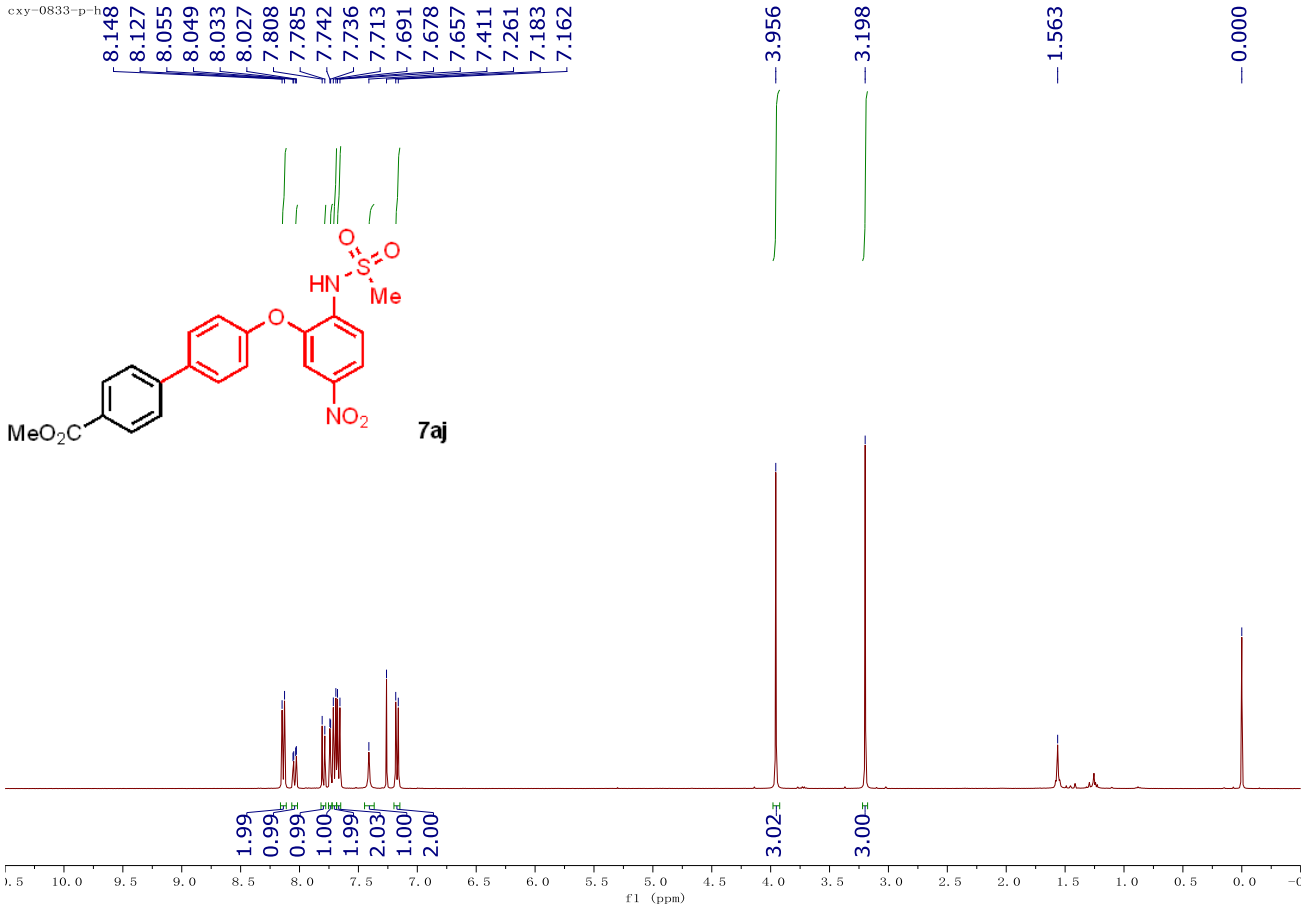

cxy-0814-2-p-c-1029
166.88
150.02
145.94
145.04
144.60
143.12
137.84
130.11
128.97
128.82
128.51
127.46
127.29
126.78
126.73
126.51
124.32
77.32
77.00
76.68
52.13
44.17
43.16
35.53
Nos
N
CO2Me
7ag
f1 (ppm)

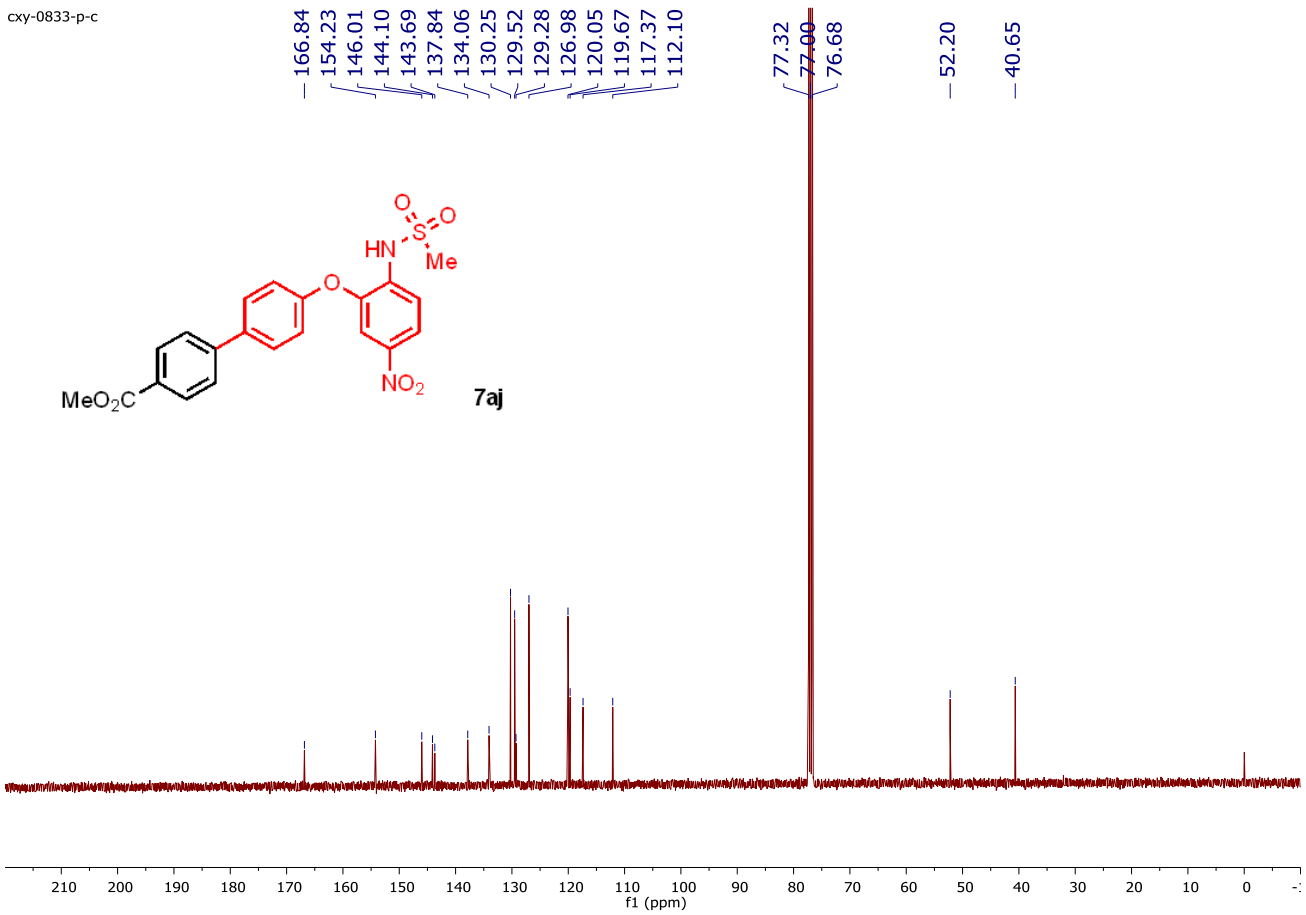

cxy-0743-2-p-chun-h-0709
8.110
8.088
7.646
7.625
7.613
7.591
7.477
7.454
7.260
7.095
7.073
6.956
6.933
3.951
-0.000
O
Br
MeO2C
7ah
2.00
2.03
1.97
1.95
1.99
1.96
3.00
f1 (ppm)

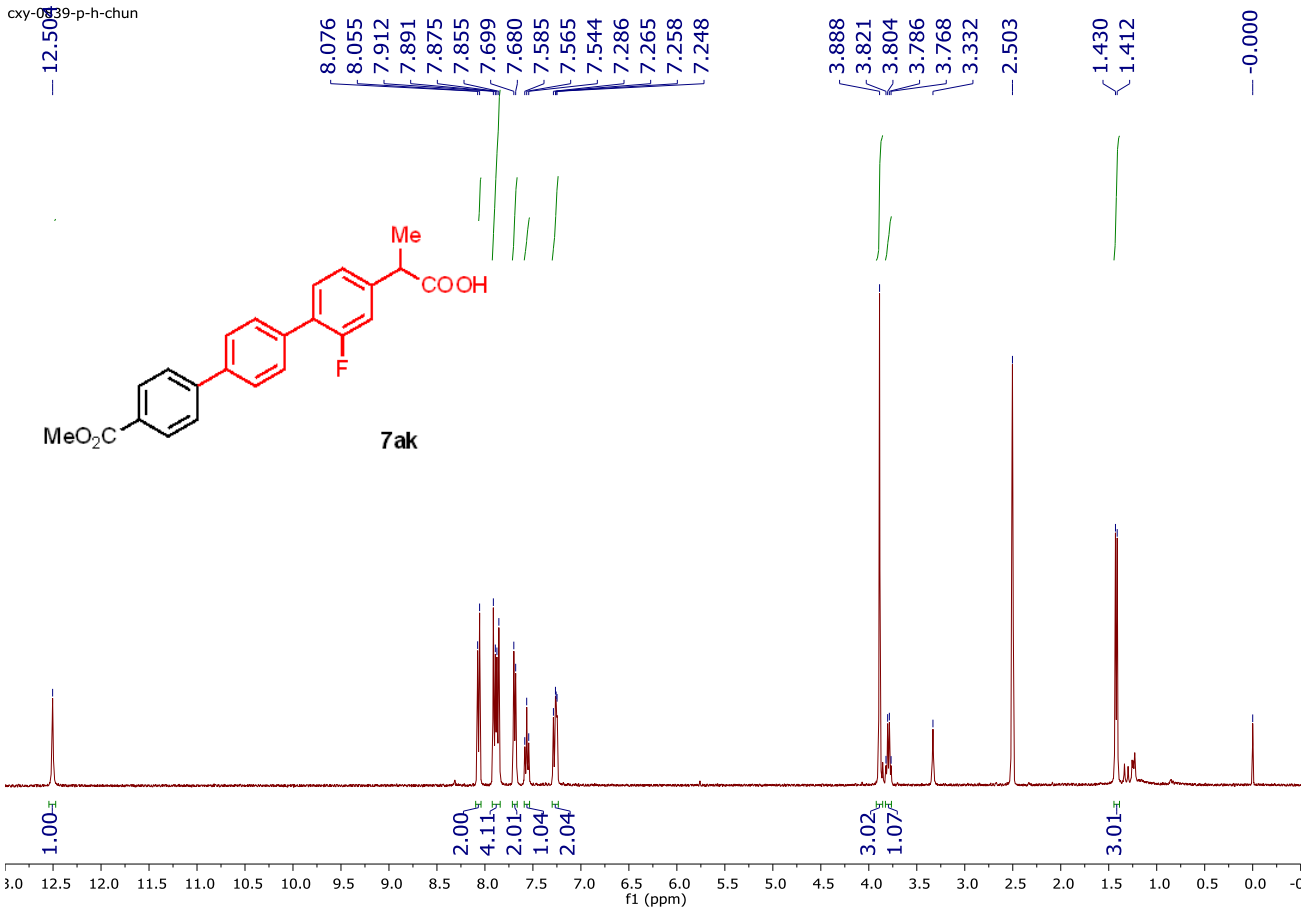

cxy-0743-2-p-c-0709
157.12
156.12
144.80
135.36
132.81
130.18
128.76
128.67
126.75
120.76
119.16
116.09
77.32
77.00
76.68
52.20
O
Br
MeO2C
7ah
f1 (ppm)

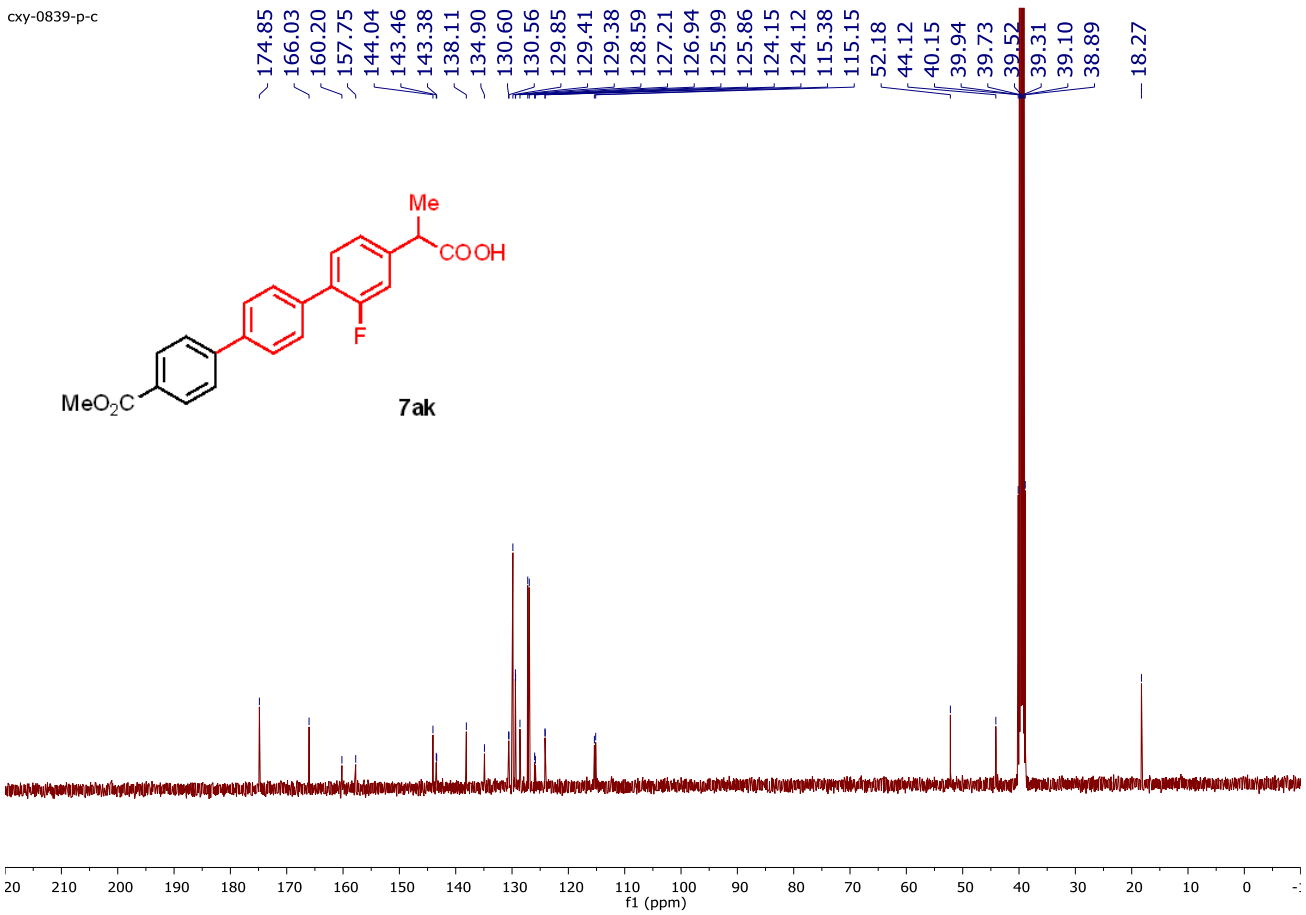

cxy-0743-6-p-chun-h-0708.chun
8.158
8.146
8.097
8.072
7.627
7.608
7.597
7.588
7.576
7.571
7.565
7.555
7.548
7.543
7.260
7.024
7.021
7.015
7.002
6.998
6.990
6.972
6.965
6.958
6.948
6.942
6.881
6.866
6.850
6.759
6.738
5.616
5.603
5.588
5.575
4.223
4.209
4.198
4.184
4.107
4.095
4.082
4.070
3.934
1.590
1.498
1.482
-0.000
CO2Me
N
O
O
O
7ai
0.99
2.01
1.99
3.00
4.00
2.05
1.03
1.00
1.02
1.02
1.05
2.98
2.99
f1 (ppm)

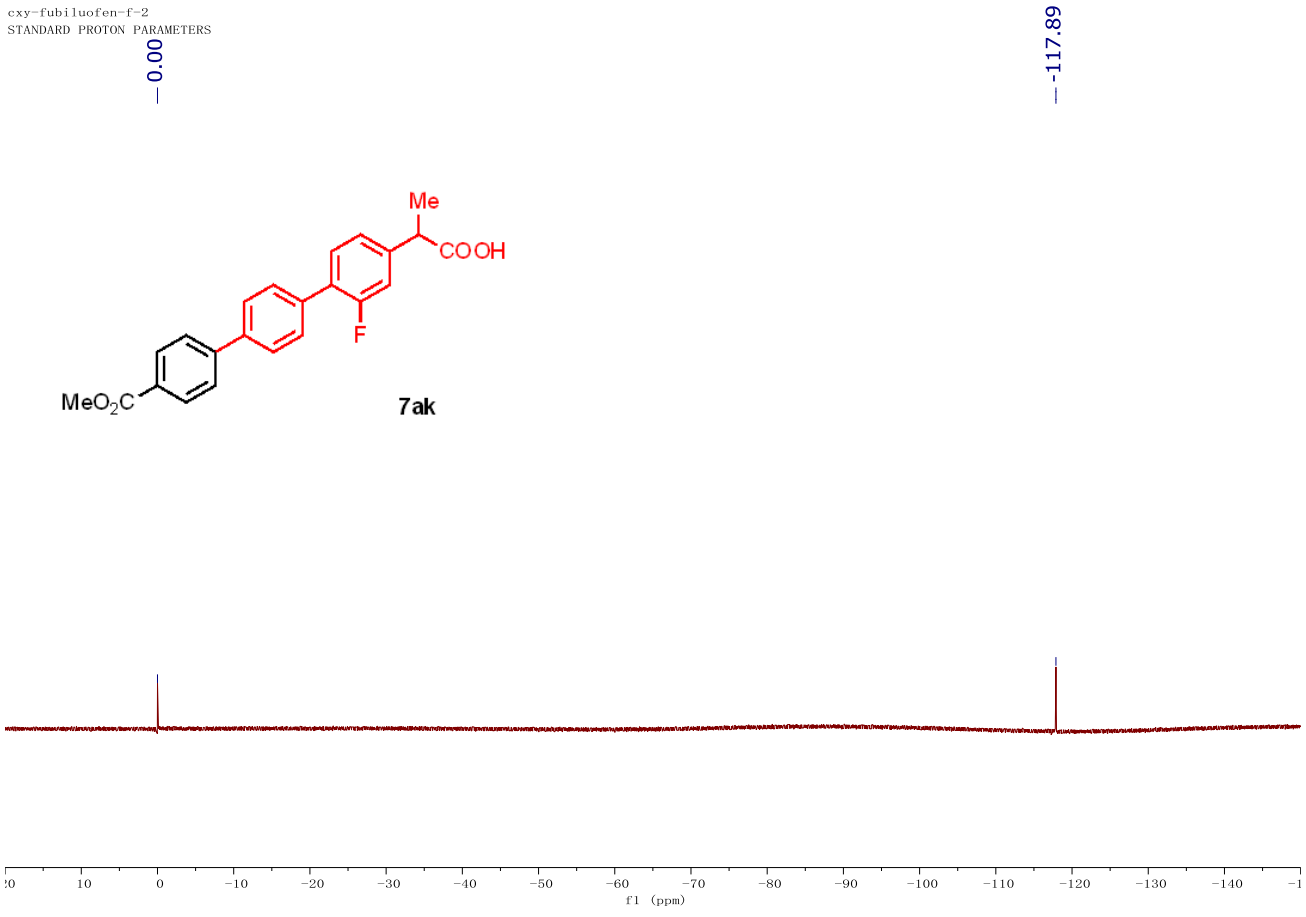

cxy-0743-6-p-c
167.02
163.13
158.90
155.49
149.81
146.76
144.99
138.70
134.07
130.11
128.49
126.62
121.00
117.75
116.77
115.87
111.67
109.97
77.32
77.00
76.68
71.05
69.23
52.09
16.99
CO2Me
7ai
f1 (ppm)

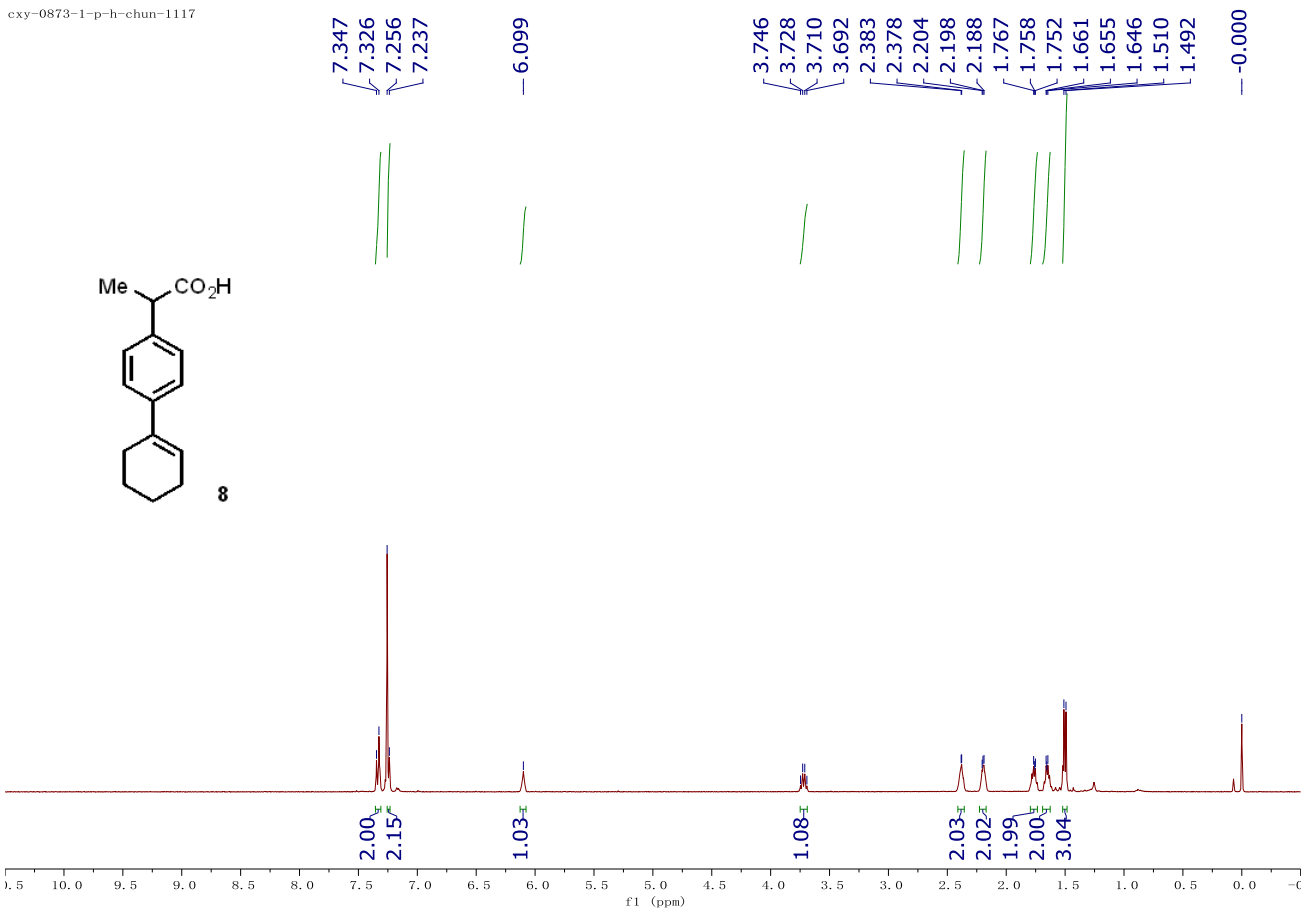

cxy-0833-p-h
8.148
8.127
8.055
8.049
8.033
8.027
7.808
7.785
7.742
7.736
7.713
7.691
7.678
7.657
7.411
7.261
7.183
7.162
3.956
3.198
1.563
0.000
HN
S
O
Me
NO2
MeO2C
7aj
1.99
0.99
0.99
1.00
1.99
2.03
1.00
2.00
3.02
3.00
f1 (ppm)

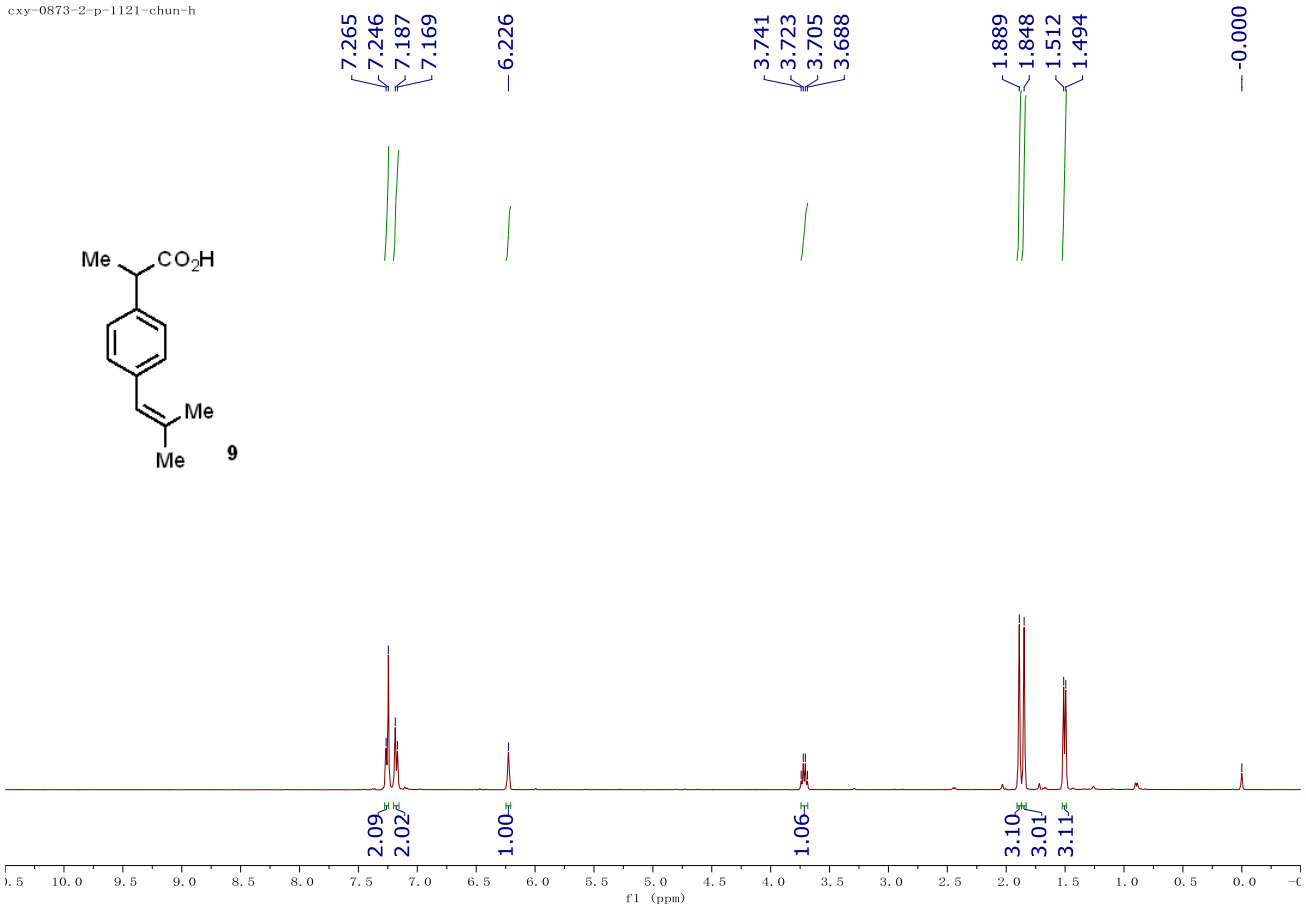

cxy-0833-p-c
166.84
154.23
146.01
144.10
143.69
137.84
134.06
130.25
129.52
129.28
126.98
120.05
119.67
117.37
112.10
77.32
77.00
76.68
52.20
40.65
HN
Me
O
NO2
MeO2C
7aj
f1 (ppm)

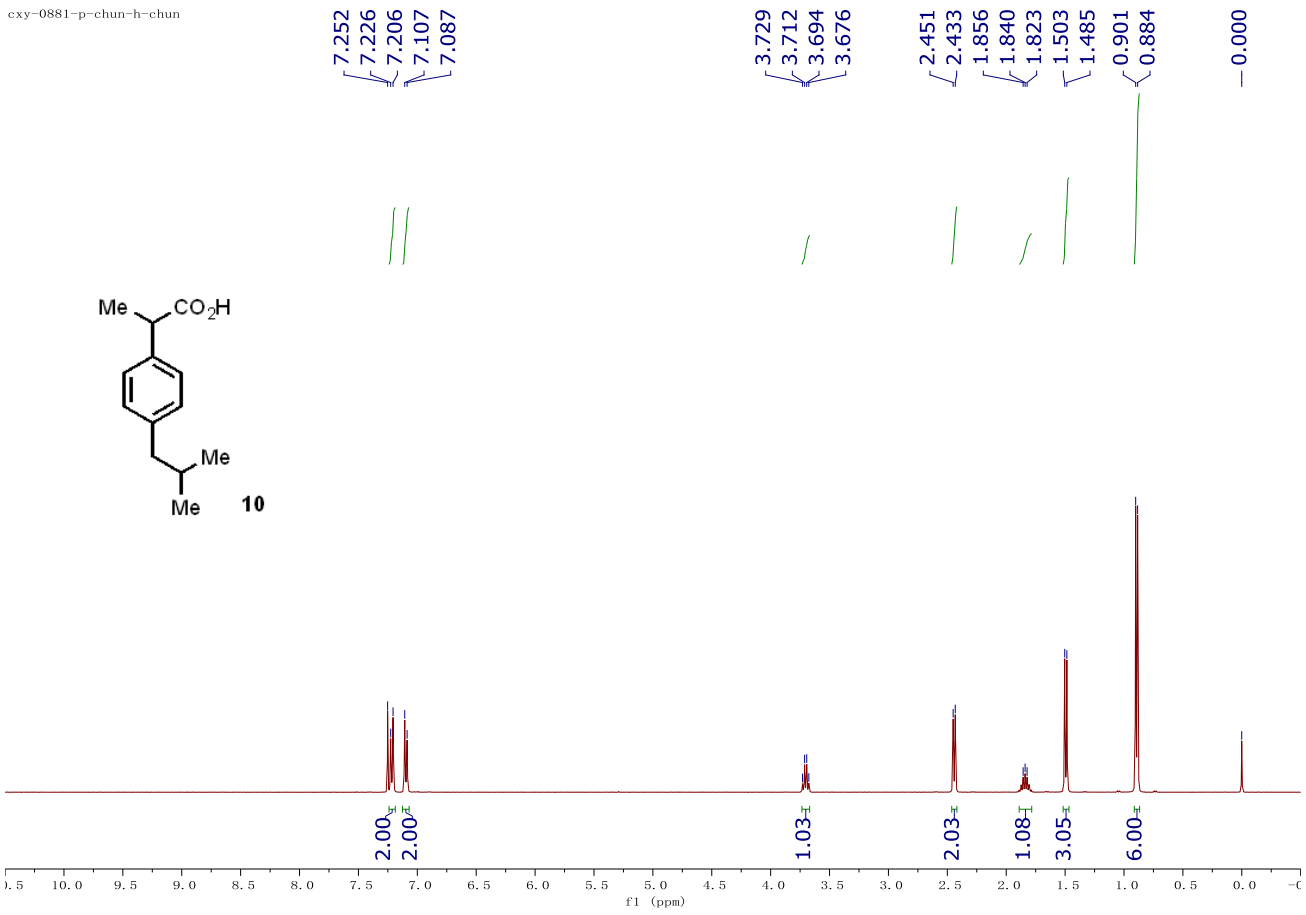

cxy-0839-p-h-chun
12.50
8.076
8.055
7.912
7.891
7.875
7.855
7.699
7.680
7.585
7.565
7.544
7.286
7.265
7.258
7.248
3.888
3.821
3.804
3.786
3.768
3.332
2.503
1.430
1.412
-0.000
Me
COOH
F
MeO2C
7ak
1.00
2.00
4.11
2.01
1.04
2.04
3.02
1.07
3.01
f1 (ppm)

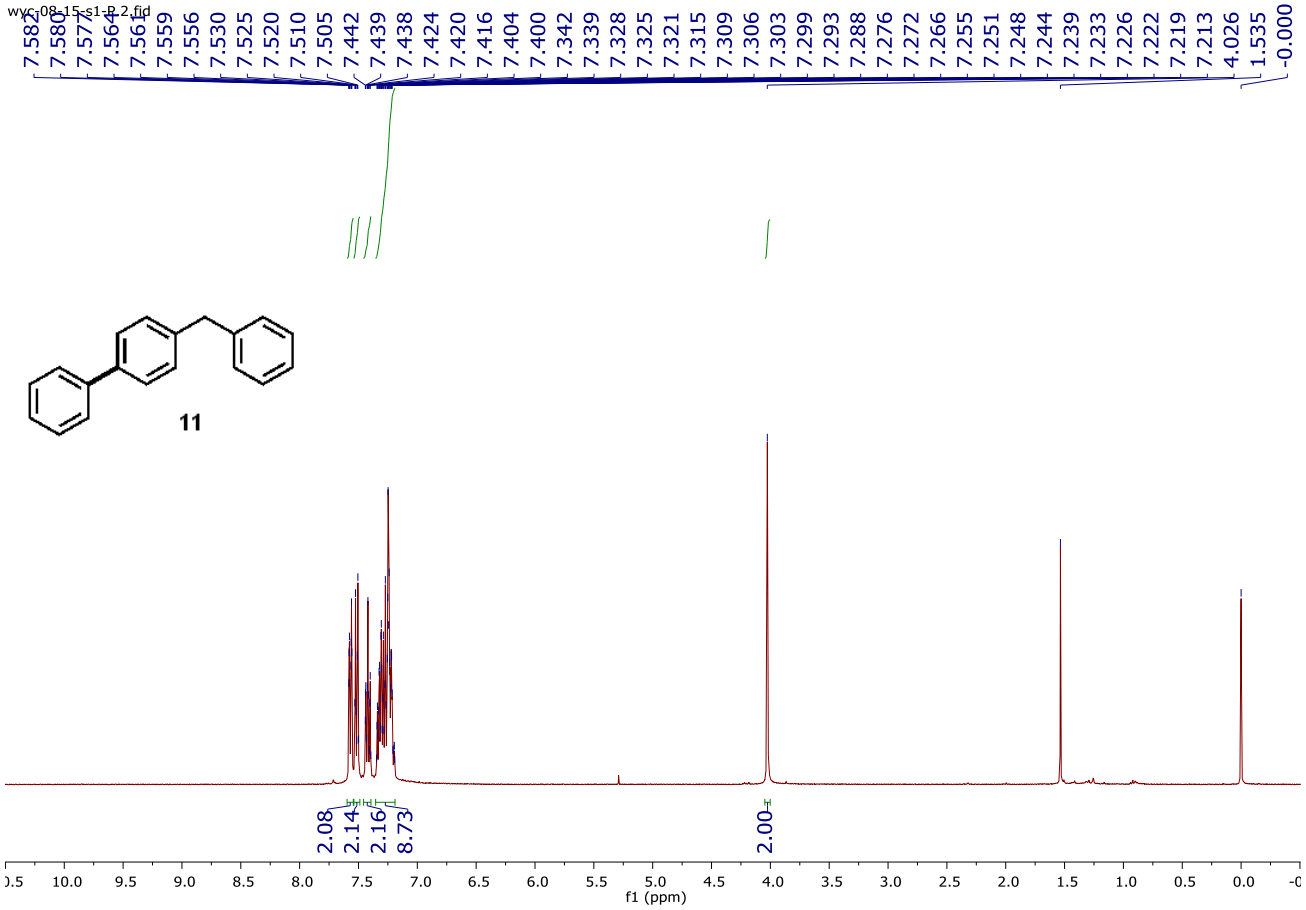

cxy-0839-p-c
174.85
166.03
160.20
157.75
144.04
143.46
143.38
138.11
134.90
130.60
130.56
129.85
129.41
129.38
128.59
127.21
126.94
125.99
125.86
124.15
124.12
115.38
115.15
52.18
44.12
40.15
39.94
39.73
39.52
39.31
39.10
38.89
18.27
Me
COOH
F
MeO2C
7ak
f1 (ppm)

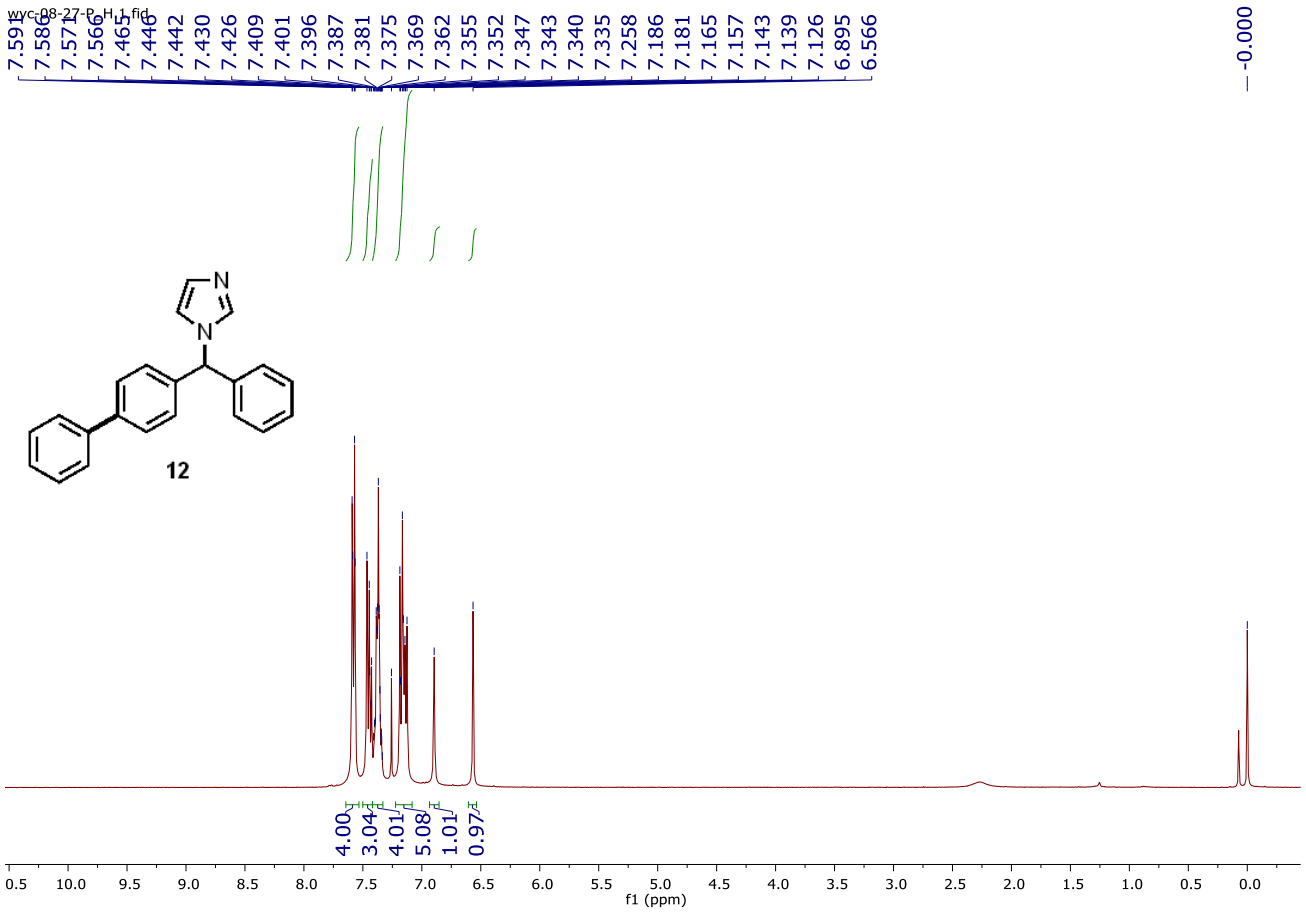

cxy-fubiluofen-f-2
STANDARD PROTON PARAMETERS
0.00
-117.89
Me
COOH
F
MeO2C
7ak
f1 (ppm)

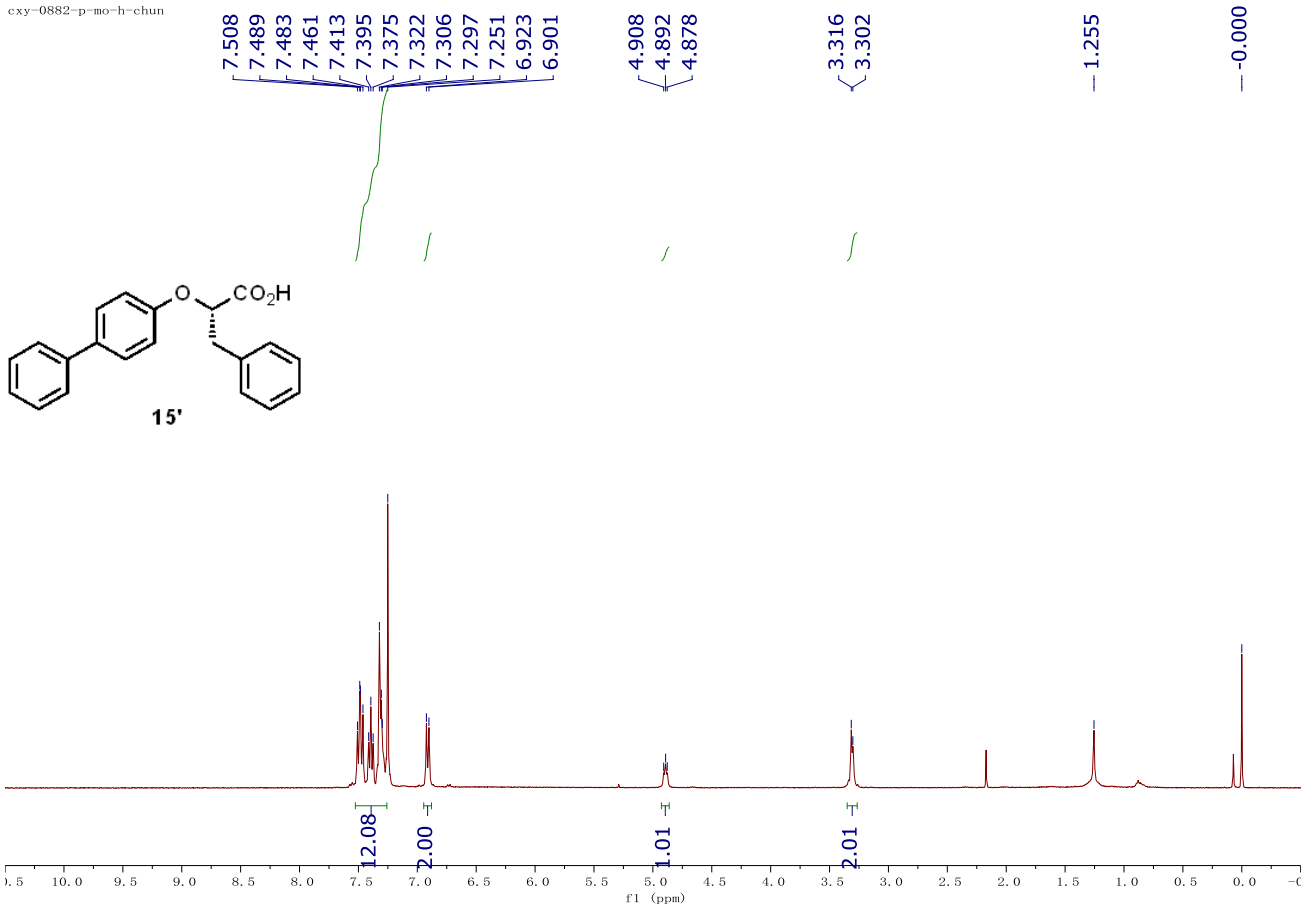

cxy-0873-1-p-h-chun-1117
7.347
7.326
7.256
7.237
6.099
3.746
3.728
3.710
3.692
2.383
2.378
2.204
2.198
2.188
1.767
1.758
1.752
1.661
1.655
1.646
1.510
1.492
-0.000
Me
CO2H
8
2.00
2.15
1.03
1.08
2.03
2.02
1.99
2.00
3.04
f1 (ppm)

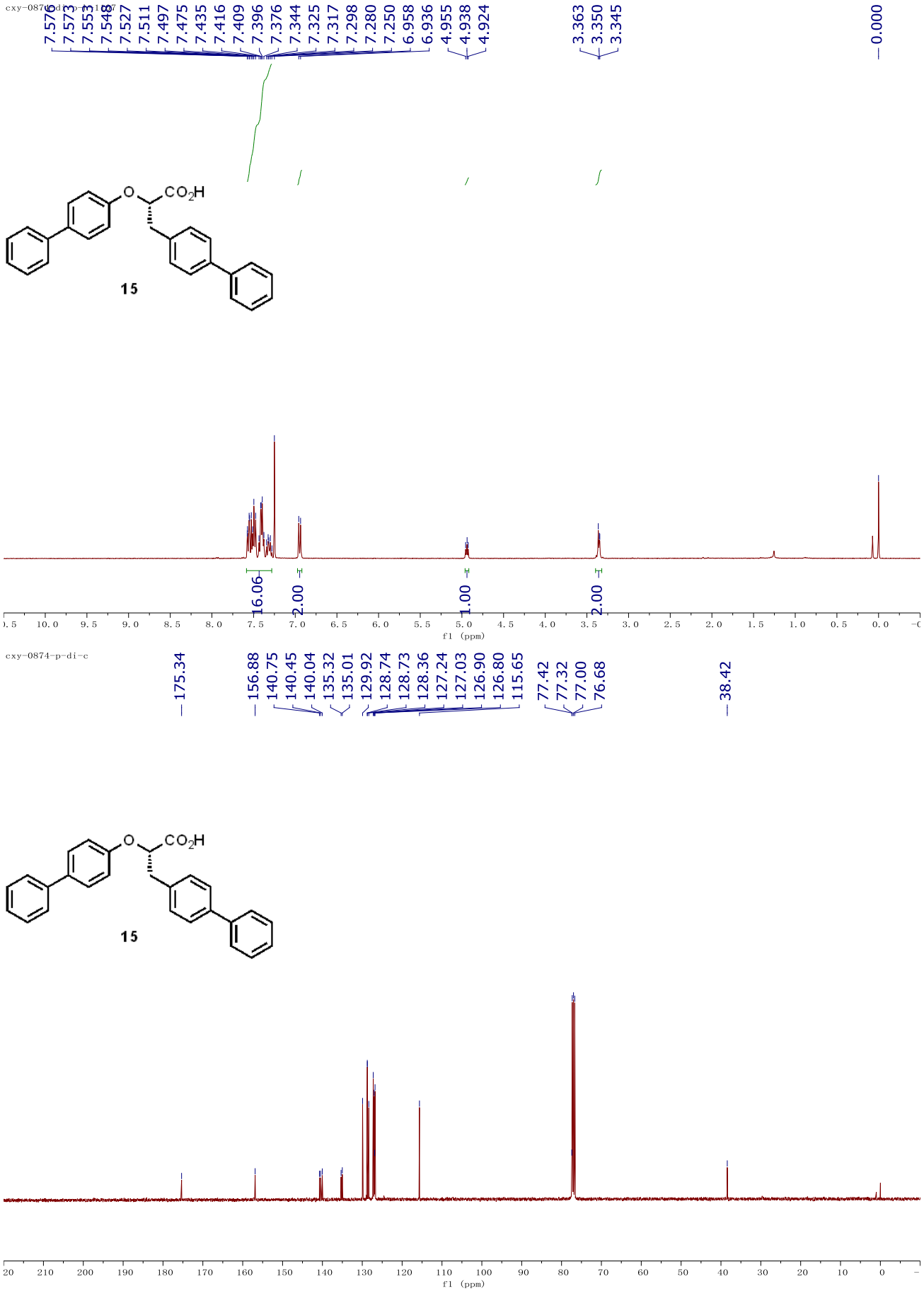

cxy-0873-2-p-1121-chun-h
7.265
7.246
7.187
7.169
6.226
3.741
3.723
3.705
3.688
1.889
1.848
1.512
1.494
-0.000
Me
CO2H
Me
Me
9
2.09
2.02
1.00
1.06
3.10
3.01
3.11
f1 (ppm)


cxy-0881-p-chun-h-chun
7.252
7.226
7.206
7.107
7.087
3.729
3.712
3.694
3.676
2.451
2.433
1.856
1.840
1.823
1.503
1.485
0.901
0.884
0.000
Me
CO2H
Me
Me
10
2.00
2.00
1.03
2.03
1.08
3.05
6.00
f1 (ppm)


wyc-08-15-s1-B-2.fid
7.582
7.580
7.577
7.564
7.561
7.559
7.556
7.530
7.525
7.520
7.510
7.505
7.442
7.439
7.438
7.424
7.420
7.416
7.404
7.400
7.342
7.339
7.328
7.325
7.321
7.315
7.309
7.306
7.303
7.299
7.293
7.288
7.276
7.272
7.266
7.255
7.251
7.248
7.244
7.239
7.233
7.226
7.222
7.219
7.213
4.026
1.535
-0.000
11
2.08
2.14
2.16
8.73
2.00
f1 (ppm)


wyc-08-27-P_H_1.fid
7.591
7.586
7.571
7.566
7.465
7.446
7.442
7.430
7.426
7.409
7.401
7.396
7.387
7.381
7.375
7.369
7.362
7.355
7.352
7.347
7.343
7.340
7.335
7.258
7.186
7.181
7.165
7.157
7.143
7.139
7.126
6.895
6.566
-0.000
12
4.00
3.04
4.01
5.08
1.01
0.97
f1 (ppm)


cxy-0882-p-mo-h-chun
7.508
7.489
7.483
7.461
7.413
7.395
7.375
7.322
7.306
7.297
7.251
6.923
6.901
4.908
4.892
4.878
3.316
3.302
1.255
-0.000
CO2H
15'
12.08
2.00
1.01
2.01
f1 (ppm)


7.576
7.573
7.553
7.548
7.527
7.511
7.497
7.475
7.435
7.416
7.409
7.396
7.376
7.344
7.325
7.317
7.298
7.280
7.250
6.958
6.936
4.955
4.938
4.924
3.363
3.350
3.345
0.000
CO2H
O
15
16.06
2.00
1.00
2.00
f1 (ppm)
cxy-0874-p-di-c
175.34
156.88
140.75
140.45
140.04
135.32
135.01
129.92
128.74
128.73
128.36
127.24
127.03
126.90
126.80
115.65
77.42
77.32
77.00
76.68
38.42
CO2H
O
15
f1 (ppm)