Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Successive Cu/Pd Transmetalation Relay Catalysis in Stereoselective Synthesis of Tetraarylethenes

Chuanling Song,[†] Yihua Sun,[‡] Jianwu Wang,[†] Hui Chen,*[,‡] Jiannian Yao,[‡] Chen-Ho Tung[†] and Zhenghu Xu*[,†,§]

[†]Key Lab of Colloid and Interface Chemistry of Ministry of Education, School of Chemistry and Chemical Engineering, Shandong University, No. 27 South Shanda Road, Jinan, Shandong 250100, China

[‡]Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Photochemistry, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China

[§]State Key Laboratory of Organometallic Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai 200032, China

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Part I. General

^{1}H and ^{13}C NMR spectra were recorded using Bruker AV 400 MHz spectrometers. ^{1}H NMR spectra were referenced to tetramethylsilane (TMS, 0 ppm) and ^{13}C NMR spectra were referenced to $CDCl_3$ solvent (77 ppm). HRMS were measured on the Q-TOF6510 instruments. Routine monitoring of the reaction was performed by TLC using precoated silica gel plates. UV-vis absorption spectra were measured on a Milton Roy Spectronic 3000 Array spectrophotometer. Photoluminescence (PL) spectra were recorded on a Perkin-Elmer LS 55 spectrofluorometer. Fluorescence quantum yields were calculated using Fluorescein (0.1 M NaOH) as the standards. All the reagents and solvents used in this reaction such as CH_3CN were purchased from Acros or local company and used directly. All the reactions don't require inert atmosphere.

Part II. Synthesis of Substrates

Diazomalonates and cyclopropenes were synthesized from the procedures reported in the literature.[S1]

General Procedure for Synthesis of Alkynes: To a solution of the corresponding arylhalide (1 eq.), $PdCl_2(PPh_3)_2$ (1 ~ 10 mol%), CuI (1 ~ 10 mol%) in solvent (amine and THF) was added slowly terminal alkyne (1.0 ~ 2.0 eq) at 0℃ and the reaction mixture was stirred at indicated temperature and time. After the reaction was complete as monitored by TLC, to the reaction mixture was added n-hexane and precipitation was removed by filtration through celite. After the mixture was evaporated under reduced pressure, purification by silica-gel chromatography.

Part III. Optimization of reaction conditions

1. Bases and acids

Entry	Catalyst	Oxidant	Base	Additive	Solvent	Temperature	Yield/%[b]
1[c]	$Pd(OAc)_2$	$Cu(OAc)_2$	CsF	DMSO	CH_3CN	60℃	< 5%
2	$Pd(OAc)_2$	$Cu(OAc)_2$	/	DMSO	CH_3CN	60℃	< 5%
3	$Pd(OAc)_2$	$Cu(OAc)_2$	CsF	DMSO	CH_3CN	60℃	20
4	$Pd(OAc)_2$	$Cu(OAc)_2$	KF	DMSO	CH_3CN	60℃	8
5	$Pd(OAc)_2$	$Cu(OAc)_2$	Cs_2CO_3	DMSO	CH_3CN	60℃	55
6	$Pd(OAc)_2$	$Cu(OAc)_2$	TBAB	DMSO	CH_3CN	60℃	0
7	$Pd(OAc)_2$	$Cu(OAc)_2$	TBAF	DMSO	CH_3CN	60℃	0
8	$Pd(OAc)_2$	$Cu(OAc)_2$	K_2CO_3	DMSO	CH_3CN	60℃	20
9	$Pd(OAc)_2$	$Cu(OAc)_2$	Na_2CO_3	DMSO	CH_3CN	60℃	18
10	$Pd(OAc)_2$	$Cu(OAc)_2$	NaOAc	DMSO	CH_3CN	60℃	10
11	$Pd(OAc)_2$	$Cu(OAc)_2$	PivONa	DMSO	CH_3CN	60℃	8
12	$Pd(OAc)_2$	$Cu(OAc)_2$	K_3PO_4	DMSO	CH_3CN	60℃	18
13	$Pd(OAc)_2$	$Cu(OAc)_2$	KI	DMSO	CH_3CN	60℃	0
14	$Pd(OAc)_2$	$Cu(OAc)_2$	CsOAc	DMSO	CH_3CN	60℃	30
15	$Pd(OAc)_2$	$Cu(OAc)_2$	tBuOLi	DMSO	CH_3CN	60℃	27
16	$Pd(OAc)_2$	$Cu(OAc)_2$	tBuOK	DMSO	CH_3CN	60℃	0
17	$Pd(OAc)_2$	$Cu(OAc)_2$	Et_3N	DMSO	CH_3CN	60℃	10
18	$Pd(OAc)_2$	$Cu(OAc)_2$	Py	DMSO	CH_3CN	60℃	0
19	$Pd(OAc)_2$	$Cu(OAc)_2$	DBU	DMSO	CH_3CN	60℃	0
20	$Pd(OAc)_2$	$Cu(OAc)_2$	HOAc	DMSO	CH_3CN	60℃	messy
21	$Pd(OAc)_2$	$Cu(OAc)_2$	PivOH	DMSO	CH_3CN	60℃	messy
22[d]	$Pd(OAc)_2$	$Cu(OAc)_2$	Cs_2CO_3	DMSO	CH_3CN	60℃	28
23[e]	$Pd(OAc)_2$	$Cu(OAc)_2$	Cs_2CO_3	DMSO	CH_3CN	60℃	22
24[f]	$Pd(OAc)_2$	$Cu(OAc)_2$	Cs_2CO_3	DMSO	CH_3CN	60℃	20
25[g]	$Pd(OAc)_2$	$Cu(OAc)_2$	Cs_2CO_3	DMSO	CH_3CN	60℃	18
26[h]	$Pd(OAc)_2$	$Cu(OAc)_2$	Cs_2CO_3	DMSO	CH_3CN	60℃	22

[a]Reaction conditions: Cyclopropene 1b (0.2 mmol), Diphenylacetylene 2a (0.1 mmol), catalyst (5 % mmol, 0.005 mmol), oxidant (2 eq., 0.2 mmol), base (1 eq., 0.1 mmol), additive (6 eq., 0.6 mmol), CH_3CN (1 ml), 60 °C. [b]Isolated yield. [c]CsF (2 eq., 0.2 mmol). [d]Cs_2CO_3 (0.5 eq., 0.2 mmol). [e]Cs_2CO_3 (0.8 eq., 0.2 mmol). [f]Cs_2CO_3 (1.2 eq., 0.2 mmol). [g]Cs_2CO_3 (1.5 eq., 0.2 mmol). [h]Cs_2CO_3 (2.0 eq., 0.2 mmol).

2. Solvents and additives

Entry	Catalyst	Oxidant	Base	Additive	Solvent	Temperature	Yield/%[b]
1	$Pd(OAc)_2$	$Cu(OAc)_2$	Cs_2CO_3	/	CH_3OH	60℃	0
2	$Pd(OAc)_2$	$Cu(OAc)_2$	Cs_2CO_3	/	Acetone	60℃	0
3	$Pd(OAc)_2$	$Cu(OAc)_2$	Cs_2CO_3	/	xylene	60℃	NR
4	$Pd(OAc)_2$	$Cu(OAc)_2$	Cs_2CO_3	/	DMF	60℃	0
5	$Pd(OAc)_2$	$Cu(OAc)_2$	Cs_2CO_3	/	EtOAc	60℃	NR
6	$Pd(OAc)_2$	$Cu(OAc)_2$	Cs_2CO_3	/	CH_3NO_2	60℃	NR
7[c]	$Pd(OAc)_2$	$Cu(OAc)_2$	Cs_2CO_3	DMSO	CH_3CN	60℃	18
8[d]	$Pd(OAc)_2$	$Cu(OAc)_2$	Cs_2CO_3	DMSO	CH_3CN	60℃	22
9[e]	$Pd(OAc)_2$	$Cu(OAc)_2$	Cs_2CO_3	DMSO	CH_3CN	60℃	10
10	$Pd(OAc)_2$	$Cu(OAc)_2$	Cs_2CO_3	DMSO	CH_3CN	60℃	55
11[f]	$Pd(OAc)_2$	$Cu(OAc)_2$	Cs_2CO_3	DMSO	CH_3CN	60℃	18
12[g]	$Pd(OAc)_2$	$Cu(OAc)_2$	Cs_2CO_3	DMSO	CH_3CN	60℃	20
13	$Pd(OAc)_2$	$Cu(OAc)_2$	Cs_2CO_3	DMSO	/	60℃	20
14	$Pd(OAc)_2$	$Cu(OAc)_2$	Cs_2CO_3	/	CH_3CN	60℃	8
15	$Pd(OAc)_2$	$Cu(OAc)_2$	Cs_2CO_3	DMF	CH_3CN	60℃	10
16	$Pd(OAc)_2$	$Cu(OAc)_2$	Cs_2CO_3	$(CH_3)_2S$	CH_3CN	60℃	10
17[h]	$Pd(OAc)_2$	$Cu(OAc)_2$	Cs_2CO_3	iPr_2S	CH_3CN	60℃	22

[a]Reaction conditions: Cyclopropene 1b (0.2 mmol), Diphenylacetylene 2a (0.1 mmol), catalyst (5 % mmol, 0.005 mmol), oxidant (2 eq., 0.2 mmol), base (1 eq., 0.1 mmol), additive (6 eq., 0.6 mmol), CH_3CN (1 ml), 60 ºC. [b]Isolated yield. [c]DMSO (1 eq., 0.1 mmol). [d]DMSO (2 eq., 0.1 mmol). [e]DMSO (3 eq., 0.1 mmol). [f]DMSO (10 eq., 0.1 mmol). [g]DMSO (15 eq., 0.1 mmol). [h]iPr_2S (3 eq., 0.1 mmol).

3. Ligand

Entry	Catalyst	Oxidant	Base	Ligand	Additive	Solvent	Yield/%[b]
1	$Pd(OAc)_2$	$Cu(OAc)_2$	Cs_2CO_3	1,10-phen	DMSO	CH_3CN	20
2	$Pd(OAc)_2$	$Cu(OAc)_2$	Cs_2CO_3	DPPB	DMSO	CH_3CN	20
3	$Pd(OAc)_2$	$Cu(OAc)_2$	Cs_2CO_3	/	DMSO	CH_3CN	55
4	$Pd(OAc)_2$	$Cu(OAc)_2$	Cs_2CO_3	PPh_3	DMSO	CH_3CN	20
5	$Pd(OAc)_2$	$Cu(OAc)_2$	Cs_2CO_3	DPEphos	DMSO	CH_3CN	28
6	$Pd(OAc)_2$	$Cu(OAc)_2$	Cs_2CO_3	Xantphos	DMSO	CH_3CN	20
7	$Pd(OAc)_2$	$Cu(OAc)_2$	Cs_2CO_3	PCy_3	DMSO	CH_3CN	20
8	$Pd(OAc)_2$	$Cu(OAc)_2$	Cs_2CO_3	L-Boc-Valine	DMSO	CH_3CN	20
9	$Pd(OAc)_2$	$Cu(OAc)_2$	Cs_2CO_3	L-Boc-Proline	DMSO	CH_3CN	22

[a]Reaction conditions: Cyclopropene 1b (0.2 mmol), Diphenylacetylene 2a (0.1 mmol), catalyst (5 % mmol, 0.005 mmol), ligand (10% mmol, 0.01 mmol), oxidant (2 eq., 0.2 mmol), base (1 eq., 0.1 mmol), additive (6 eq., 0.6 mmol), CH_3CN (1 ml), 60 ºC. [b]Isolated yield.

4. Catalyst

Entry	Catalyst	Oxidant	Base	Additive	Solvent	Temperature	Yield/%[b]
1	$PdCl_2$	$Cu(OAc)_2$	Cs_2CO_3	DMSO	CH_3CN	60℃	12
2	$Pd(TFA)_2$	$Cu(OAc)_2$	Cs_2CO_3	DMSO	CH_3CN	60℃	15
3	$Pd(OAc)_2$	$Cu(OAc)_2$	Cs_2CO_3	DMSO	CH_3CN	60℃	55
4	$PdCl_2(CH_3CN)_2$	$Cu(OAc)_2$	Cs_2CO_3	DMSO	CH_3CN	60℃	40
5	$PdCl_2(PPh_3)_2$	$Cu(OAc)_2$	Cs_2CO_3	DMSO	CH_3CN	60℃	37
6	$Pd_2(dba)_3$	$Cu(OAc)_2$	Cs_2CO_3	DMSO	CH_3CN	60℃	42
7	$Pd(PPh_3)_4$	$Cu(Oac)_2$	Cs_2CO_3	DMSO	CH_3CN	60℃	20

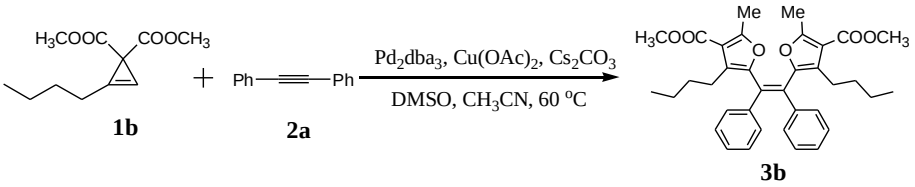
[a]Reaction conditions: Cyclopropene 1b (0.2 mmol), Diphenylacetylene 2a (0.1 mmol), catalyst (5 % mmol, 0.005 mmol), oxidant (2 eq., 0.2 mmol), base (1 eq., 0.1 mmol), additive (6 eq., 0.6 mmol), CH_3CN (1 ml), 60 °C. [b]Isolated yield.

5. Ratio of substrates

1a:2a	Catalyst	Oxidant	Base	Additive	Solvent	Temperature	Yield/%[b]
2:1	$Pd_2(dba)_3$	$Cu(OAc)_2$	Cs_2CO_3	DMSO	CH_3CN	60℃	42
2.2:1	$Pd_2(dba)_3$	$Cu(OAc)_2$	Cs_2CO_3	DMSO	CH_3CN	60℃	60
2.5:1	$Pd_2(dba)_3$	$Cu(OAc)_2$	Cs_2CO_3	DMSO	CH_3CN	60℃	72
3:1	$Pd_2(dba)_3$	$Cu(OAc)_2$	Cs_2CO_3	DMSO	CH_3CN	60℃	58
2.5:1[c]	$Pd_2(dba)_3$	$Cu(Oac)_2$	Cs_2CO_3	DMSO	CH_3CN	60℃	73

[a]Reaction conditions: Cyclopropene 1b, Diphenylacetylene 2a, catalyst (5 % mmol, 0.005 mmol), oxidant (2 eq., 0.2 mmol), base (1 eq., 0.1 mmol), additive (6 eq., 0.6 mmol), CH_3CN (1 ml), 60 °C. [b]Isolated yield. [c]Catalyst(10% mmol).

Part IV. General procedure of the oxidative coupling reactions



1b **2a** **3b**

A mixture of catalyst (5% mmol), $Cu(OAc)_2$ (0.2 mmol) and Cs_2CO_3 (0.1 mmol)was dissolved in CH_3CN (1 mL), DMSO (0.6 mmol,), cyclopropene **1b** (0.25 mmol) and alkyne **2a** (0.1 mmol) were added to the reaction system. The resulting mixture was stirred at 60℃ until the reaction was completed (monitored by TLC). The reaction mixture was filtered and evaporated under reduced pressure and purified by column chromatography (silica gel) to give the pure product **3b**.

Part V. Data of UV and fluorescence spectra

a) b)

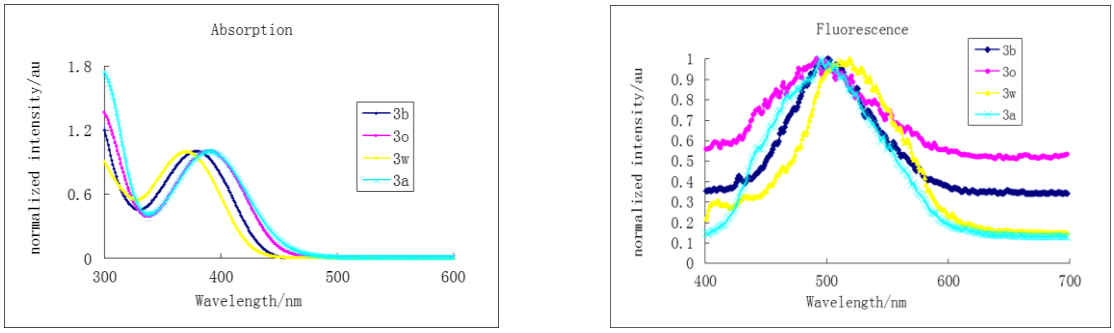


Figure S1. Absorption (a) and fluorescence (b) spectra of products 3a, 3b, 3o, 3w in THF.

a) b)

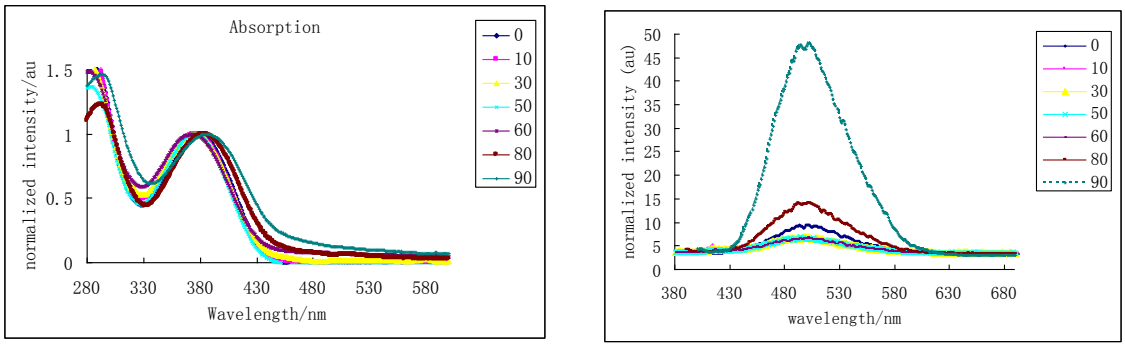


Figure S2. Absorption (a) and fluorescence (b) spectra of 3b in THF/water with different fraction of water (f_w %).

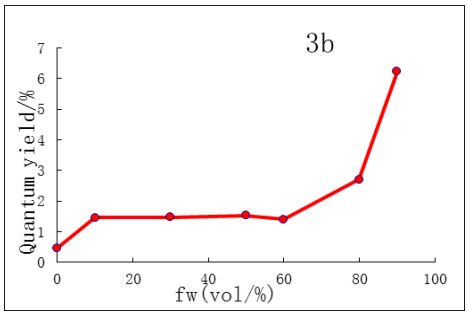
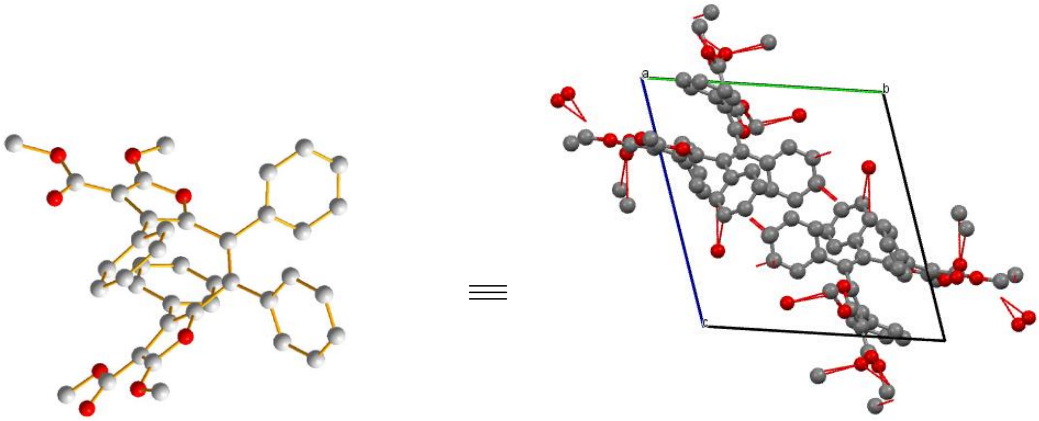


Figure S3. Variations of fluorescence quantum yields of 3b with water fractions in THF/water mixtures.

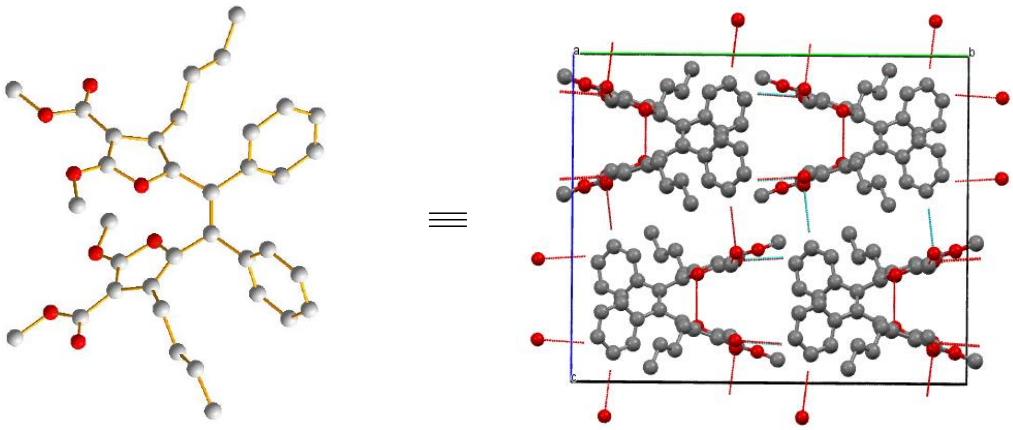
a) b)

Pictures S1. a) 3b in water fractions in THF/water mixtures. From left to right, fw = 0, 10% ⟶ 80%, 90%. b) 3b in solid state. (365 nm)

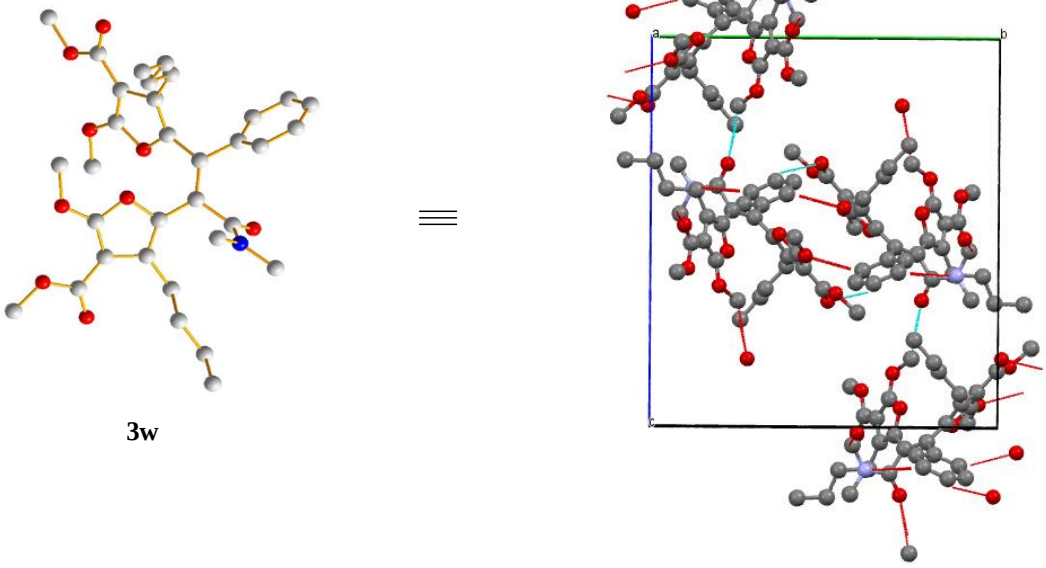
Part VI. Crystal structures and packings of 3a, 3b, 3w



3a

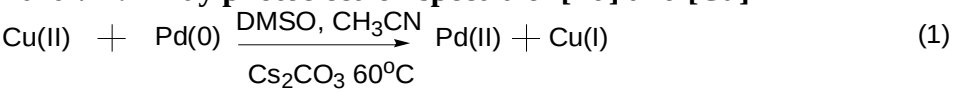


3b



3w

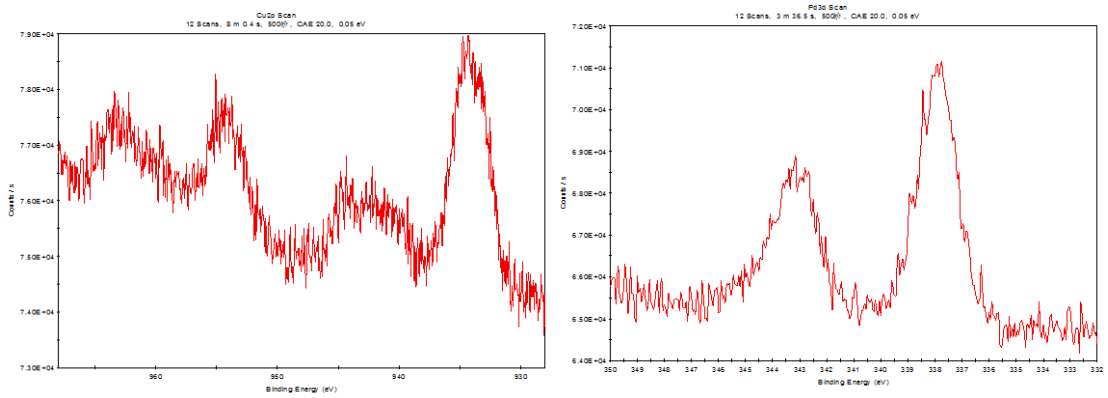
Part VII. X-ray photoelectron spectra of [Pd] and [Cu]



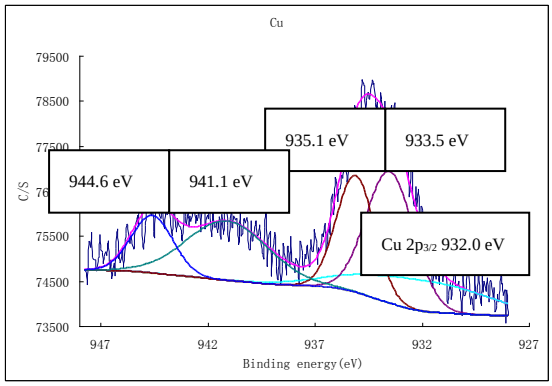
(1)

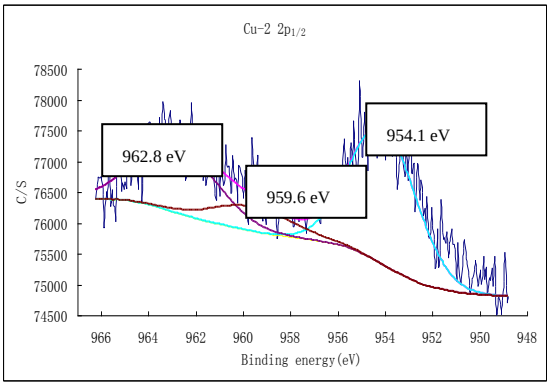
In a 25 mL Schlenk tube under N_2 atmosphere, Pd_2dba_3 (0.01 mmol), $Cu(OAc)_2$ (0.04 mmol), Cs_2CO_3 (0.02 mmol) were added to 1 mL CH_3CN and 43 μL DMSO. Then the mixture was exchanged with N_2 for three times and heated to 60 °C for 0.5 h. After remove the CH_3CN under reduced pressure distillation, a black solid resident was obtained.

XPS data for Cu and Pd

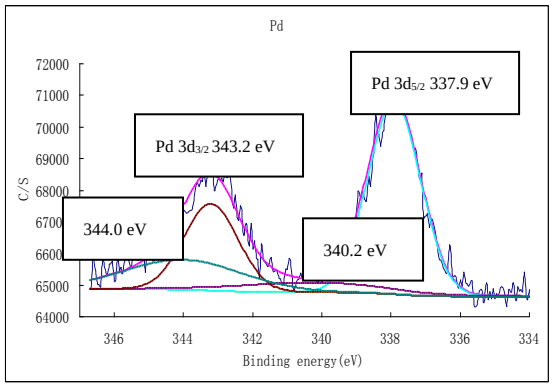


a) XPS data for Cu $2p_{3/2}$ b) XPS data for Cu $2p_{1/2}$





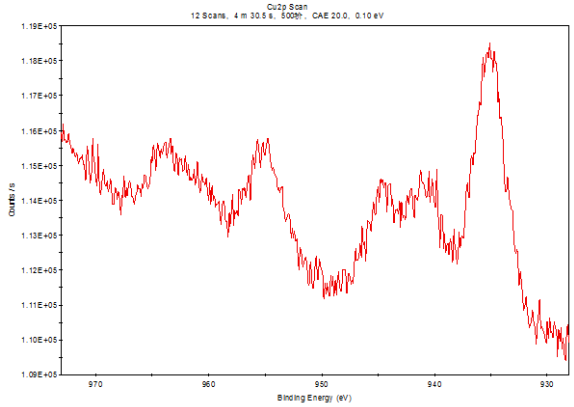
c) XPS data for Cu $2p_{1/2}$

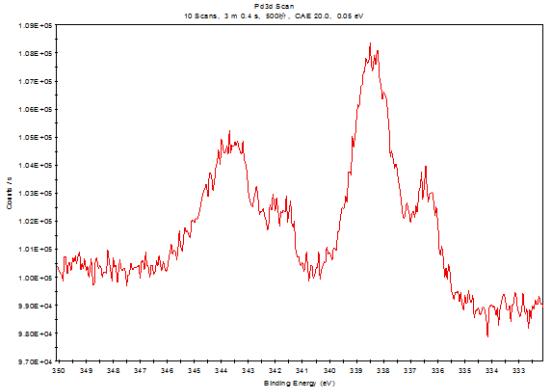


$$Cu(II) + Pd(0) \xrightarrow[60^{o}C]{DMSO,\ CH_3CN} Pd(II) + Cu(I) \qquad (2)$$

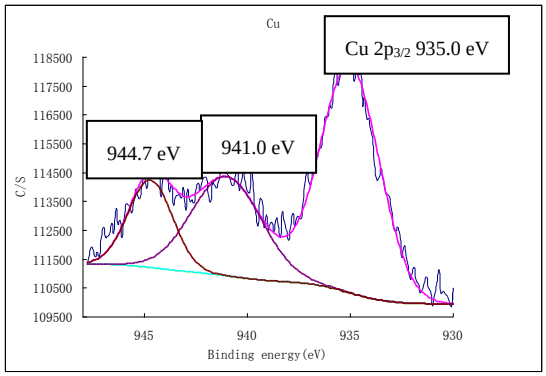
In a 25 mL Schlenk tube under N_2 atmosphere, Pd_2dba_3 (0.01 mmol), $Cu(OAc)_2$ (0.04 mmol) were added to 1 mL CH_3CN and 43 μL DMSO. Then the mixture was exchanged with N_2 for three times and heated to 60 °C for 0.5 h. After remove the CH_3CN under reduced pressure distillation, a black solid resident was obtained.

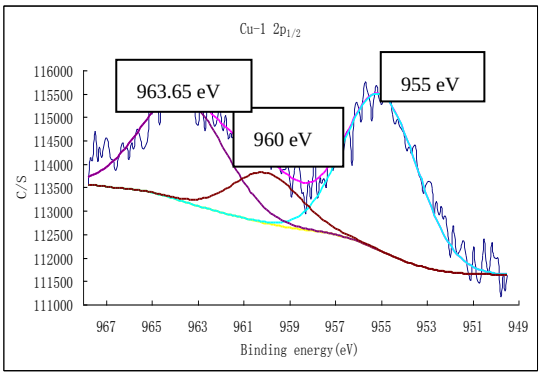
XPS data for Cu and Pd



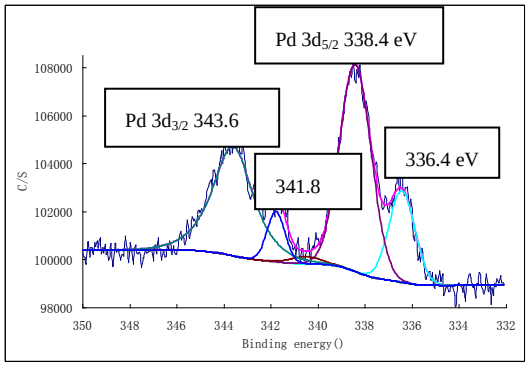


a) XPS data for Cu $2p_{3/2}$ b) XPS data for Cu $2p_{1/2}$





c) XPS data for Pd



Part VIII. Computational details

All DFT calculations were carried out with Gaussian 09 program[S2] using B3LYP hybrid functional[S3]. For modeling the reactions involving the closed-shell Cu(I) and Pd(II) centers, restricted DFT method was employed for the singlet spin states, while for modeling the reactions involving the open-shell Cu(II) center, unrestricted DFT method was employed for the doublet spin state. For considering the relativistic effect of Pd, the relativistic effective core potential (ECP)[S4] was utilized. Geometries were fully optimized in gas phase consistently using polarized double-ζ def2-SVP basis set[S5] on all atoms, with Grimme's DFT-D3[S6] empirical dispersion correction (with zero short range damping) considered. Vibrational analyses were performed on all optimized geometries to verify the identities of minima, transition state, and high-order saddle point. Larger polarized triple-ζ def2-TZVP basis set[S5] was utilized in single point calculations to refine the calculated electronic energies of these optimized structures. The solvent effect was accounted for in these single point calculations with SMD continuum solvation model[S7] with acetonitrile as the solvent, which is the main solvent used in the experimental studies. Reported energies (in kcal/mol) are the Gibbs free energies which include thermal free energy correction, solvent effect correction, and DFT-D3 empirical dispersion correction.

References

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Part IX. DFT optimized Cartesian coordinates of structures in DFT modeling

A

C	-1.03871900	0.43027600	-0.07744000
C	0.21819600	0.48330500	-0.55706400
C	-0.47063800	1.82444800	-0.33178700
C	-0.08689900	2.62583700	0.88339300
O	0.44015500	2.11950300	1.85702000
O	-0.44540600	3.90342500	0.83251100
C	-0.96554400	2.52199700	-1.57717100
O	-1.90010600	2.13481300	-2.23983200
O	-0.20310600	3.57040000	-1.91002800
C	-0.15595200	4.69618300	1.99092500
H	0.92680000	4.71345500	2.18520500
H	-0.52271700	5.70472000	1.76595100
H	-0.66490800	4.28631800	2.87619600
C	-0.59389800	4.29048200	-3.08143800
H	0.12498300	5.11188300	-3.18912700
H	-0.56847200	3.63809200	-3.96794800
H	-1.61529800	4.68630700	-2.97182100
C	-2.37458000	-0.22735800	-0.08044500
C	-2.29134600	-1.75271800	0.04353200
H	-2.87054800	0.07900000	-1.01828000
H	-2.97644000	0.18799900	0.74501900
C	-3.66224100	-2.42940700	-0.01043800
H	-1.64913000	-2.14784000	-0.76431300
H	-1.78932300	-2.00128100	0.99488800
H	-4.30007500	-2.01461900	0.79101900
H	-4.16302400	-2.16965700	-0.96099800
C	-3.57982900	-3.94919600	0.13411800
H	-3.10987900	-4.23032600	1.09125400
H	-4.57734800	-4.41540200	0.09947300
H	-2.97435000	-4.39381500	-0.67368300
Cu	0.30494200	-0.16554300	1.35117600
C	0.87589800	-1.66555700	3.09594800
O	1.77161600	-1.26493900	2.29836200
O	-0.32338400	-1.26237600	2.96789300
C	1.21373100	-2.64744300	4.19282000
H	0.81873600	-3.63834800	3.91565000
H	2.29980300	-2.71940700	4.33264900
H	0.71936200	-2.34779600	5.12811600
H	0.91241600	0.08757800	-1.29831300

TS_{A-B}

C	-1.38628500	0.87378100	0.19398400
C	-0.24683200	0.58495600	-0.34713600
C	-1.04729500	2.31551500	-0.00483500
C	-0.29492000	2.98543500	1.03317300
O	0.35857500	2.40484200	1.93587700
O	-0.32393800	4.31202700	1.02643300
C	-1.78019300	2.93933300	-1.12200900
O	-2.61350700	2.33229100	-1.76991500
O	-1.43668700	4.21061900	-1.39904800
C	0.43933200	4.99358100	2.02343200
H	1.50501900	4.72763200	1.95278800
H	0.29894300	6.06324900	1.82524600
H	0.08258000	4.74060800	3.03328900
C	-2.14431100	4.82274800	-2.47416400
H	-3.22836100	4.83475800	-2.27954700
H	-1.75994400	5.84823000	-2.54795200
H	-1.97442000	4.28202300	-3.41870100
C	-2.53760900	0.16003800	0.81297000
C	-3.19710300	-0.82581400	-0.16366700
H	-3.26248100	0.90620700	1.17263000
H	-2.15534900	-0.38433300	1.69706800
C	-4.36984800	-1.58343600	0.46052000
H	-3.53267800	-0.25898700	-1.04802500
H	-2.42651700	-1.53364700	-0.50991900
H	-4.01655200	-2.13210400	1.35319500
H	-5.12139400	-0.86069200	0.82826700
C	-5.02944900	-2.55850800	-0.51543000
H	-4.30669400	-3.31066200	-0.87343000
H	-5.87064700	-3.09578100	-0.04880300
H	-5.41822500	-2.02898100	-1.40120900
Cu	0.72971900	0.52261900	1.88365600
C	0.68017900	-2.00017000	0.82509900
O	1.08456100	-1.32401100	1.83137800
O	0.07553900	-1.54581000	-0.17278500
C	0.95848000	-3.49192800	0.88920800
H	0.34845100	-3.93105500	1.69479200
H	0.71492300	-3.97809900	-0.06358700
H	2.01310300	-3.66045500	1.15295600
H	0.58851600	0.61149600	-1.02696000

B

C	-0.96254500	0.77595900	0.12272500
C	0.13980000	0.04999400	-0.15837500
C	-0.90214800	2.25937200	0.01920900
C	-0.03394700	2.99373800	0.86234400
O	0.73056400	2.52185500	1.77477300
O	-0.02111400	4.32800900	0.72750000
C	-1.90704900	2.80565100	-0.88200600
O	-2.69315400	2.10094100	-1.50681700
O	-1.94254200	4.15385400	-1.00591300
C	0.77369500	5.07550500	1.63622200
H	1.83997500	4.81104400	1.55357900
H	0.62625000	6.12912200	1.36377900
H	0.46037600	4.90994600	2.67955300
C	-2.92878400	4.66198200	-1.89161800
H	-3.94518500	4.38759400	-1.56460500
H	-2.81275300	5.75440600	-1.88386900
H	-2.79113900	4.27393800	-2.91412500
C	-2.23064500	0.09365600	0.61353800
C	-2.89800700	-0.85450000	-0.39317900
H	-2.94694500	0.87399900	0.90482800
H	-1.98351100	-0.46104900	1.54113300
C	-4.17842200	-1.48887000	0.15372700
H	-3.11991000	-0.27000100	-1.29828000
H	-2.19126000	-1.64879300	-0.68778100
H	-3.94995700	-2.04588400	1.08259800
H	-4.88077000	-0.68869800	0.44953500
C	-4.85787600	-2.42090700	-0.85015900
H	-4.19045300	-3.25074300	-1.13966000
H	-5.78089800	-2.86174500	-0.44012300
H	-5.12458300	-1.87902300	-1.77258300
Cu	0.84041000	0.67266700	2.10620200
C	0.52746200	-1.90991100	1.15206700
O	0.88380700	-1.26976800	2.14378000
O	0.15876300	-1.36632200	0.00378600
C	0.44277800	-3.40416800	1.14451700
H	-0.62143800	-3.69088600	1.13020300
H	0.90119900	-3.80365500	0.22878100
H	0.92393300	-3.81374600	2.03985900
H	1.05328400	0.44008500	-0.61083100

B'

C	-2.05365800	0.62346400	-0.42804800
C	-1.49027800	-0.12959300	-1.38417600
C	-1.94512300	2.11024900	-0.50549100
C	-0.66419600	2.65839900	-0.80354200
O	0.40941300	2.01151900	-0.83606200
O	-0.59524900	4.00418900	-1.06073300
C	-3.14824000	2.84889900	-0.24535700
O	-4.26487000	2.36423400	-0.03870900
O	-3.02396300	4.23205400	-0.18449800
C	0.69594600	4.51243700	-1.32083900
H	1.18141700	3.99537800	-2.16944600
H	0.56474900	5.58334700	-1.54625800
H	1.36911800	4.39621800	-0.45246600
C	-4.21640500	4.92282500	0.07631300
H	-4.65718800	4.65253500	1.05464300
H	-3.96481500	5.99669800	0.07187500
H	-4.99472100	4.72445600	-0.68404800
C	-2.72882200	-0.03756700	0.76458700
C	-4.02631200	-0.77902500	0.41651200
H	-2.95335100	0.72880500	1.52294400
H	-2.00897300	-0.74665900	1.20933100
C	-4.70684600	-1.40803800	1.63447900
H	-4.71067200	-0.05986700	-0.06163800
H	-3.79768300	-1.56531000	-0.32370300
H	-4.00131500	-2.09672600	2.13722500
H	-4.93302000	-0.61562400	2.37318000
C	-5.99428800	-2.16038000	1.28901500
H	-5.79339500	-2.98131200	0.57865900
H	-6.47775700	-2.59936700	2.18058800
H	-6.72501700	-1.48778000	0.80700800
Cu	1.50526400	1.27605100	-2.24319100
C	-0.35110300	-2.14658800	-0.83813700
O	0.11208200	-1.84716100	0.23498100
O	-1.46193500	-1.52596000	-1.36532600
C	0.18839100	-3.15742900	-1.79176600
H	-0.61836300	-3.68551400	-2.32165100
H	0.72896900	-2.49287100	-2.53318400
H	0.87835800	-3.85147000	-1.29150700
C	2.24017000	-0.48873100	-3.82938400
O	2.78619100	-1.26308500	-4.63482300
O	1.16666300	-0.78779800	-3.12953500
O	2.72479600	0.73744500	-3.60081800
H	-0.94824500	0.25988000	-2.24928000

TS_{B-C}

C	-1.72700400	0.71061500	-0.40336200
C	-1.02576100	-0.05562600	-1.27114500
C	-1.74564300	2.21028900	-0.50538200
C	-0.51735800	2.90626300	-0.40611800
O	0.64297200	2.40790300	-0.37878800
O	-0.55914100	4.27890900	-0.28433100
C	-3.04644200	2.82285300	-0.57400000
O	-4.12890600	2.23431700	-0.53839800
O	-3.07938300	4.20977500	-0.70242200
C	0.68869400	4.92745400	-0.32133800
H	1.27712000	4.64824700	-1.21293700
H	0.47354200	6.00944400	-0.33859700
H	1.31319400	4.69307000	0.56049400
C	-4.36473100	4.76459000	-0.77444400
H	-4.97094100	4.54913100	0.12612600
H	-4.23138800	5.85553400	-0.87320100
H	-4.94235700	4.38542300	-1.63827700
C	-2.45472100	0.08353400	0.78600500
C	-3.71171500	-0.72434800	0.42571800
H	-2.73996900	0.87794500	1.49802800
H	-1.75192500	-0.58814200	1.31593500
C	-4.41470600	-1.32880000	1.64390200
H	-4.40149600	-0.05560000	-0.11133100
H	-3.42338800	-1.53060600	-0.26843200
H	-3.70836900	-1.97791500	2.19730000
H	-4.69182100	-0.51940300	2.34706300
C	-5.66588500	-2.13412700	1.28298600
H	-5.41447700	-2.96978700	0.60672400
H	-6.16688600	-2.56018500	2.17183000
H	-6.39948400	-1.50159700	0.75349800
Cu	1.16342300	1.07023800	-1.67584600
C	-0.01565500	-2.22463100	-1.08716200
O	1.04980000	-1.93172000	-0.59225100
O	-1.12429600	-1.47637100	-1.00149600
C	-0.25336400	-3.46662300	-1.91405100
H	-1.25757300	-3.88238300	-1.73839200
H	-0.20168300	-3.10102100	-2.95645000
H	0.52967600	-4.21637100	-1.73174700
C	1.21394700	-0.64036500	-3.87457200
O	1.72109900	-1.30820600	-4.78732900
O	-0.07841500	-0.76772000	-3.57720800
O	1.92154700	0.21406200	-3.16377200
H	-0.47930900	-0.17392100	-2.54700000

C'

C	-1.75003200	0.77657800	-0.30632500
C	-0.95334500	0.05058400	-1.13167100
C	-1.78576200	2.27928100	-0.33430200
C	-0.59994100	2.99998800	-0.71593300
O	0.40097900	2.56742700	-1.30515300
O	-0.55580300	4.34102300	-0.34972800
C	-3.04021100	2.91279400	-0.04034100
O	-4.11885400	2.35753700	0.20767900
O	-3.06024200	4.31342100	-0.06923000
C	0.55895100	5.05141800	-0.82167000
H	0.65661200	5.00326300	-1.92186300
H	0.41487800	6.10064300	-0.50994900
H	1.51046000	4.67143500	-0.40553700
C	-4.31391600	4.88770000	0.16676300
H	-4.72420500	4.62707800	1.16157400
H	-4.17490400	5.98150500	0.10581900
H	-5.07549500	4.57462600	-0.57340200
C	-2.56780000	0.06007700	0.77176200
C	-3.82185200	-0.66517800	0.26233600
H	-2.87399400	0.77730200	1.54793500
H	-1.91304600	-0.68488600	1.26120100
C	-4.63819300	-1.31442100	1.38278600
H	-4.44817900	0.07002200	-0.26518500
H	-3.51637500	-1.43519900	-0.46612100
H	-3.99569300	-2.01192500	1.95514700
H	-4.94948000	-0.53120300	2.09953900
C	-5.87553700	-2.06275500	0.87977500
H	-5.59192100	-2.86925300	0.18071500
H	-6.45780500	-2.52007900	1.70107600
H	-6.54838000	-1.38180200	0.32982900
Cu	0.40549400	0.55559000	-2.38172100
C	-0.07664900	-2.14392600	-0.57003100
O	0.85226400	-1.77202200	0.11678500
O	-1.10701800	-1.41075500	-0.96085100
C	-0.13420700	-3.53136900	-1.19108800
H	-1.16961400	-3.88311200	-1.31136600
H	0.31585600	-3.43313400	-2.19562000
H	0.46073100	-4.24287800	-0.60028500
C	1.88196900	-0.72117500	-4.44249700
O	2.76629900	-1.00846000	-5.23973700

O	0.91687800	-1.70550700	-4.19208200
O	1.71912900	0.38205300	-3.80932500
H	0.28351700	-1.29520500	-3.56606700

C

C	-1.01118800	0.71373600	0.73656000
C	0.05643200	-0.04793600	1.13936000
C	-0.92003200	2.15231700	0.33353500
C	0.20482100	3.00712600	0.41152900
O	1.35954600	2.83151400	0.92795600
O	0.05821000	4.21653700	-0.24965200
C	-2.11497100	2.72229000	-0.31721500
O	-2.78247500	2.22248300	-1.20962400
O	-2.51897000	3.92301700	0.21889700
C	1.06472300	5.17374800	-0.04118800
H	2.05063700	4.83301100	-0.40363400
H	0.75792100	6.07191200	-0.60097000
H	1.18236000	5.43436700	1.02702800
C	-3.53782400	4.59263900	-0.48999700
H	-4.47140300	4.00429700	-0.52581600
H	-3.71625300	5.54313900	0.03619200
H	-3.24015100	4.79859900	-1.53377800
C	-2.40264100	0.07494900	0.73608000
C	-2.68944900	-0.79052300	-0.49987300
H	-3.18820700	0.84142900	0.82129400
H	-2.49603700	-0.56179700	1.63208500
C	-4.10854800	-1.36220300	-0.52026700
H	-2.53115200	-0.17454500	-1.39819500
H	-1.95615300	-1.61527300	-0.52838300
H	-4.28935400	-1.94038600	0.40649800
H	-4.83008400	-0.52446900	-0.50109700
C	-4.38899000	-2.24692400	-1.73656700
H	-3.69977500	-3.10897900	-1.76794200
H	-5.41983200	-2.64250800	-1.73763500
H	-4.24495200	-1.68260600	-2.67380400
Cu	1.60962000	0.96412000	1.37914000
C	0.54487600	-2.21284500	2.07652300
O	1.62403800	-1.93480500	2.55252300
O	-0.29707900	-1.39442000	1.44952100
C	-0.03503000	-3.62056200	2.09631000
H	0.02989400	-4.05549100	1.08477500
H	0.53485300	-4.24588000	2.79643400
H	-1.09985000	-3.59891200	2.37268900

TS(2)$_{C\text{-}M1}$

C	-1.30056000	0.89098800	0.94295200
C	-0.17733500	0.37785500	1.47270100
C	-1.28405400	2.30293100	0.48013600
C	-0.02606000	3.00364000	0.49403900
O	1.03029900	2.63536600	1.02231000
O	0.00799500	4.17687100	-0.24237700
C	-2.49922000	2.90535000	-0.03350500
O	-3.47936500	2.34070600	-0.51782800
O	-2.54669400	4.28004700	0.09542300
C	1.22714600	4.87444000	-0.20751300
H	2.05903600	4.28878400	-0.63985000
H	1.07842900	5.79253800	-0.79829000
H	1.52666300	5.14390600	0.82183300
C	-3.64121700	4.90766900	-0.52684400
H	-4.60529500	4.60392400	-0.08051600
H	-3.49777100	5.99177800	-0.39438500
H	-3.69830100	4.67210400	-1.60500800
C	-2.56253600	0.04602800	0.82659000
C	-2.68495700	-0.63665900	-0.54048600
H	-3.44456900	0.67932400	0.98539000
H	-2.54562300	-0.72489700	1.60675600
C	-4.00784100	-1.38406800	-0.71417700
H	-2.59974900	0.13042500	-1.32635600
H	-1.83802100	-1.33590300	-0.65654900
H	-4.12974600	-2.11509900	0.10777700
H	-4.83681700	-0.66090500	-0.60864100
C	-4.12517600	-2.10327900	-2.05937100
H	-3.32093800	-2.84963500	-2.18268500
H	-5.08971200	-2.62939700	-2.16853600
H	-4.03671800	-1.38906000	-2.89602400
Cu	1.63352700	0.11492700	1.81513700
C	0.53024400	-2.27446100	2.05462200
O	1.72704100	-1.87830300	2.18564600
O	-0.48997800	-1.58691200	1.76174200
C	0.27297000	-3.76972700	2.24157600
H	0.09446800	-4.22531700	1.25343500
H	1.13685300	-4.25883300	2.71318100
H	-0.63688400	-3.92297800	2.84098600

M1

C	-1.72211200	1.58594300	0.61995800
C	-0.42891400	1.26164400	0.94813100
C	-1.76461200	2.97677400	0.17463000
C	-0.45112100	3.40863800	0.27686100
O	0.34377800	2.44515400	0.71883400
O	0.09639700	4.60356600	0.01204000
C	-2.91675000	3.73505900	-0.27703900
O	-4.06453600	3.33559100	-0.36474700
O	-2.60177000	5.02376500	-0.62408600
C	1.49335000	4.72190700	0.21223300
H	2.05742600	4.01649700	-0.42201600
H	1.75608800	5.75487600	-0.05668600
H	1.77262000	4.52745500	1.26211800
C	-3.68366100	5.81152200	-1.07905200
H	-4.46956900	5.90862600	-0.31025700
H	-3.26908600	6.80202700	-1.31679200
H	-4.15558200	5.37693700	-1.97701600
C	-2.87000200	0.60970700	0.70180000
C	-2.75859900	-0.55453500	-0.29703800
H	-3.82188500	1.14129900	0.55862900
H	-2.88683400	0.17794800	1.71920300
C	-3.85416200	-1.60924900	-0.13187200
H	-2.77165700	-0.15474300	-1.32846900
H	-1.78464600	-1.05220300	-0.16103200
H	-3.86685100	-1.93795200	0.92384800
H	-4.84704200	-1.15770300	-0.32446500
C	-3.63402700	-2.83285000	-1.02474100
H	-2.67449100	-3.30901300	-0.76834100
H	-4.43952600	-3.57916200	-0.90589000
H	-3.60169700	-2.54600100	-2.09124000
Cu	0.29585900	-0.42337100	1.41699300
C	0.32472300	-3.19545500	1.35489400
O	0.91766200	-2.16551600	1.84948700
O	-0.63830200	-3.20260700	0.58563100
C	0.93637100	-4.52574000	1.82106200
H	2.00946100	-4.54958000	1.56999000
H	0.86405200	-4.59921900	2.91881800
H	0.42158200	-5.37806900	1.35570600

Transition state alternative to **$TS_{A\text{-}B}$** for cleaving C-C bond without migrating acetate ligand to C2 position, which is higher in energy than **$TS_{A\text{-}B}$**

C	-0.95290100	0.58970700	0.93788000
C	-0.26160600	-0.24557200	1.89397700
C	-0.22682200	1.49694200	0.18182700
C	1.22473400	1.45199500	0.37642400
O	1.73131700	0.76040800	1.25506000
O	1.96547300	2.15716100	-0.48467100
C	-0.88607800	2.48768800	-0.71138600
O	-1.90209700	2.29800000	-1.34684300
O	-0.24949800	3.67396400	-0.71676600
C	3.37902900	2.09509800	-0.30081400
H	3.74500200	1.06192600	-0.40697600
H	3.81458000	2.73607600	-1.07735700
H	3.66134200	2.46021800	0.69893000
C	-0.78434000	4.66767900	-1.58776900
H	-0.13055800	5.54359400	-1.49020100
H	-0.79516200	4.31274300	-2.63031300
H	-1.81653900	4.92680800	-1.30406600
C	-2.46539600	0.51627800	0.88550800
C	-2.96963200	-0.45913100	-0.19335200
H	-2.87865000	1.51345600	0.68098100
H	-2.82904000	0.19191200	1.86970800
C	-4.48423200	-0.65932100	-0.11643200
H	-2.69218400	-0.05552500	-1.17897500
H	-2.46724800	-1.42920900	-0.06412800
H	-4.74445200	-1.05524900	0.88285600
H	-4.98898300	0.32048000	-0.19840800
C	-5.01290700	-1.60371200	-1.19612600
H	-4.54380200	-2.59883500	-1.11639000
H	-6.10386400	-1.73990300	-1.12041000
H	-4.79231600	-1.21572100	-2.20453700
Cu	-0.66221300	-0.10155900	3.73030900
H	0.41416300	-1.03766900	1.56630400
C	-2.13421500	-2.15560000	3.27194500
O	-1.63529100	-1.90666000	2.13665700
O	-1.94239700	-1.46999900	4.32437700
C	-3.07527800	-3.34023300	3.36993100
H	-2.83266000	-4.09108600	2.60694100
H	-3.04385800	-3.77442300	4.37806900
H	-4.09999900	-2.97810100	3.18416300

$A(Cu^{II})$

C	-1.10942900	0.34344600	-0.07236200
C	0.13399200	0.00622200	-0.03511200
C	-0.12833100	1.49562500	0.08476100
C	-0.03443800	2.09304000	1.45966900
O	-0.73497100	1.72616600	2.39353900
O	0.92300700	3.00046200	1.60726300
C	0.14430200	2.36484400	-1.11727200
O	0.53217800	1.95093100	-2.18238000
O	-0.16902700	3.65488100	-0.89207800
C	1.04725300	3.60349000	2.90735000
H	1.25167600	2.83796500	3.66961300
H	1.87821300	4.31449500	2.82757900
H	0.11745000	4.12849900	3.17201400
C	0.04001300	4.55137300	-1.98262900
H	-0.24803100	5.54703700	-1.62240200
H	1.09601100	4.54855300	-2.29483000
H	-0.57526800	4.26474000	-2.84987100
C	-2.56130700	0.08019400	-0.08741900
C	-2.90382100	-1.40879400	-0.19326800
H	-3.02816000	0.65864700	-0.90554800
H	-2.96414600	0.49585800	0.85267300
C	-4.40185600	-1.68128200	-0.04387900
H	-2.54384100	-1.80072700	-1.16120300
H	-2.35862100	-1.94349900	0.59971600
H	-4.74156000	-1.27242300	0.92513000
H	-4.96122600	-1.12738800	-0.82025600
C	-4.74752300	-3.16851200	-0.11810300
H	-4.22888100	-3.73357100	0.67445300
H	-5.82946200	-3.34218300	-0.00295600
H	-4.44011800	-3.60124600	-1.08492200
Cu	-0.40303300	-0.15840400	3.56685800
C	1.96429200	0.05051900	3.45779500
O	1.32450200	-0.61617800	2.58597100
O	1.31405800	0.54902400	4.42618200
C	3.43594300	0.30218800	3.29908400
H	3.55974900	1.16580500	2.62456100
H	3.89555300	0.54097500	4.26674800
H	3.92396100	-0.56378700	2.83179400
H	0.94888200	-0.70464000	0.03082700
C	-2.66310500	-0.75215400	3.88938800
O	-2.00625900	-1.19079700	2.89184700
O	-2.04878800	-0.04348400	4.73983100
C	-4.13274200	-1.03066900	4.01782900
H	-4.67926100	-0.27401100	3.43136800
H	-4.37045900	-2.01882300	3.60121000
H	-4.45037100	-0.95567600	5.06587300

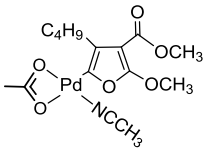
$TS_{A\text{-}B}(Cu^{II})$

C	-1.51772300	0.64791200	0.57136700
C	-0.44232400	-0.01621900	0.84750500
C	-0.66908600	1.83399900	0.26558100
C	-0.35633600	2.68257300	1.38645100
O	-0.60939800	2.37438900	2.58113400
O	0.20343200	3.85553300	1.13324200
C	-0.51528800	2.11864200	-1.17082800
O	-1.04382000	1.43276300	-2.02668400
O	0.26189200	3.17614300	-1.46627400
C	0.65442300	4.61373900	2.26253100
H	1.35360200	4.01495600	2.86545800
H	1.15611400	5.49484000	1.84415100
H	-0.19306800	4.91974300	2.89397400
C	0.40648900	3.47040200	-2.85309700
H	1.04982000	4.35779500	-2.91121400
H	0.86873700	2.62743800	-3.39086600
H	-0.57027900	3.67620900	-3.31881700
C	-2.99335800	0.46054400	0.62355800
C	-3.46392400	-0.82836100	-0.06429800
H	-3.46836200	1.34331800	0.16869100
H	-3.27795100	0.45856100	1.69203500
C	-4.96777100	-1.06359500	0.08618800
H	-3.19181200	-0.77026400	-1.13178400
H	-2.90507700	-1.68059600	0.35428400
H	-5.22440200	-1.09524600	1.16181900
H	-5.51955700	-0.19971700	-0.32712000
C	-5.43852200	-2.35026200	-0.59237600
H	-4.92487800	-3.23086100	-0.17133200
H	-6.52268100	-2.50268600	-0.46947500
H	-5.22242300	-2.33014000	-1.67353000
Cu	0.04388800	0.69716900	3.39339100
C	2.31103500	0.33268400	3.99671200
O	1.96307800	1.36605500	3.34130000
O	1.40803000	-0.49933500	4.31079100
C	3.73884500	0.12441400	4.40879700
H	4.41564800	0.51726900	3.63765100
H	3.92020000	0.68880500	5.33810800
H	3.93247100	-0.93879300	4.60094800

H	0.57290700	-0.36886900	0.77033400
C	-1.65383700	-1.45247600	2.99039400
O	-1.01590400	-1.72359200	1.94771900
O	-1.52760200	-0.38225600	3.67822200
C	-2.71824500	-2.42569300	3.45796900
H	-3.64319900	-2.21307000	2.89602800
H	-2.41266400	-3.45435000	3.22440000
H	-2.92221800	-2.30631500	4.52954800

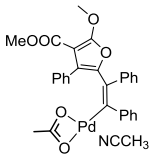
B(Cu^{II})

C	-1.22090300	0.68540300	0.72373100
C	-0.34096100	-0.21875300	1.44563900
C	-0.72914700	1.82953600	0.09870100
C	0.60212600	2.34603700	0.40868500
O	1.24844200	2.11113300	1.44548500
O	1.12758800	3.14267600	-0.51221800
C	-1.57862900	2.59092100	-0.86298500
O	-2.32549900	2.09455300	-1.67810600
O	-1.46252200	3.92428800	-0.70785800
C	2.37675500	3.77198100	-0.20627600
H	3.16400800	3.01883200	-0.05382300
H	2.61105900	4.40501800	-1.07029800
H	2.28999100	4.37967600	0.70670300
C	-2.19308600	4.72895700	-1.63158500
H	-1.96052100	5.77150400	-1.38049900
H	-1.89205100	4.50788000	-2.66769200
H	-3.27530600	4.54643700	-1.54206600
C	-2.68319100	0.32075500	0.63937500
C	-2.94390700	-0.82046000	-0.36078800
H	-3.28610300	1.19120500	0.35377700
H	-3.01938300	0.02270300	1.64269600
C	-4.42011400	-1.21845800	-0.41647000
H	-2.61201500	-0.48564900	-1.35643500
H	-2.33363200	-1.69665400	-0.08386500
H	-4.75527600	-1.51934700	0.59335200
H	-5.02272500	-0.33224100	-0.68508700
C	-4.69446800	-2.34773400	-1.40988600
H	-4.12791700	-3.25680300	-1.14616800
H	-5.76297700	-2.61528500	-1.43680500
H	-4.39527400	-2.05803700	-2.43101100
Cu	0.72717800	0.78756700	2.85467200
C	1.64293500	0.18959600	4.97372300
O	1.68809400	1.38835000	4.57610700
O	1.15719300	-0.70354200	4.20817800
C	2.12022200	-0.18508800	6.35223000
H	2.82618000	0.56380300	6.73394900
H	1.24651300	-0.21930300	7.02360900
H	2.57504600	-1.18531800	6.34054100
H	0.51828100	-0.57638500	0.85969400
C	-1.50322000	-1.16677200	3.28168200
O	-0.93889500	-1.34661300	2.06375200
O	-1.67849700	-0.07443800	3.76943400
C	-1.82202700	-2.47901200	3.93508300
H	-2.15924800	-3.22282800	3.20058600
H	-0.88278700	-2.83811200	4.38642600
H	-2.56842900	-2.33140600	4.72495800



C	-1.37892000	1.44979600	1.32810700
C	-0.42342600	1.73397700	2.26445400
C	-1.31013700	2.51186900	0.32952000
C	-0.31749900	3.36582200	0.76702200
O	0.22047100	2.92959400	1.91337200
O	0.15513900	4.49339900	0.24442100
C	-2.13672900	2.61932700	-0.87112000
O	-2.96877500	1.80690100	-1.22358900
O	-1.88030300	3.74363600	-1.58193700
C	1.23779800	5.12886100	0.90544800
H	2.11369200	4.46287800	0.97927500
H	1.49009400	6.00978100	0.30142000
H	0.95464900	5.44851900	1.92369600
C	-2.64029400	3.90903900	-2.77305500
H	-2.30549500	4.85326700	-3.22227800
H	-2.47168900	3.07425000	-3.47227400
H	-3.71931300	3.95363100	-2.55404100
C	-2.28827800	0.25664200	1.29463900
C	-1.77837100	-0.85875800	0.36963400
H	-3.28496100	0.57388900	0.95231800
H	-2.39016800	-0.14461300	2.31350600
C	-2.64790400	-2.11523300	0.42558600
H	-1.74282200	-0.47448700	-0.66388400
H	-0.74807100	-1.11667800	0.66622000
H	-2.67407400	-2.48230500	1.46806000

H	-3.68942500	-1.85145500	0.16565500
C	-2.15358600	-3.22945700	-0.49762400
H	-1.12460700	-3.53145100	-0.23759200
H	-2.79129300	-4.12683600	-0.43753700
H	-2.14127300	-2.89743900	-1.54959200
C	0.08213600	-1.68435700	4.35926800
O	0.56989100	-0.93915400	5.24948300
O	-0.33034900	-1.15602900	3.26495800
C	-0.04831900	-3.17053700	4.53827300
H	0.38110800	-3.68614000	3.66644600
H	0.45036300	-3.49161200	5.46139000
H	-1.11690800	-3.43425800	4.58055300
Pd	0.16812000	0.75643200	3.85893900
C	1.44319500	4.77141500	5.67812400
H	0.71919000	5.09073500	6.44332800
H	2.44085000	4.69933600	6.13739800
H	1.47064400	5.52494800	4.87589700
C	1.05124900	3.48428000	5.12621900
N	0.73613100	2.47089300	4.67438400



C	-2.14859500	5.65324700	0.54016900
C	-2.02052200	5.39724800	1.88113800
C	-3.39686800	6.39683200	0.38177300
C	-3.89144800	6.54700900	1.66683900
O	-3.07206000	5.99430100	2.56371500
O	-4.98444300	7.13537200	2.11266300
C	-3.99789200	6.90790300	-0.85040100
O	-3.45698700	6.97048000	-1.93394200
O	-5.28220600	7.30369500	-0.66091600
C	-5.36315100	6.87160700	3.47054400
H	-4.64544200	7.32691200	4.17119600
H	-6.35120900	7.33087600	3.59707600
H	-5.40787700	5.78620100	3.64430200
C	-5.94123100	7.83694600	-1.80519500
H	-6.94936100	8.11779900	-1.47430700
H	-5.40780600	8.71857000	-2.19414800
H	-5.99886500	7.08970400	-2.61252100
C	-5.56657200	3.55846500	1.31454800
O	-4.81276700	3.75240000	2.33834600
O	-5.19465200	2.77404700	0.40650900
C	-6.83917700	4.35350900	1.19763800
H	-7.53265600	3.86524900	0.50065800
H	-7.30650300	4.48669100	2.18339200
H	-6.57624600	5.35021700	0.80432900
Pd	-3.17980100	2.69292200	1.50272900
C	-0.04810600	0.89860200	-1.34869700
H	0.89197200	1.44959800	-1.20015300
H	0.11723100	-0.17882900	-1.19651900
H	-0.39190400	1.08126000	-2.37685600
C	-1.04167700	1.39253400	-0.41118700
N	-1.82448800	1.78163900	0.34256800
C	-1.23384500	4.44581000	2.70485900
C	-1.70894000	3.17521000	2.76475200
C	-1.22549500	5.13204800	-0.48561600
C	-1.68826300	4.61507000	-1.70973400
C	0.15712300	5.09373700	-0.22304100
C	-0.79271200	4.10089400	-2.64883700
H	-2.75475600	4.62286500	-1.92787200
C	1.05184100	4.57084500	-1.16044600
H	0.53373800	5.49575700	0.71949700
C	0.58196600	4.08195200	-2.38392000
H	-1.17288800	3.72220100	-3.60176900
H	2.12277700	4.56708300	-0.93997700
H	1.28258500	3.69555400	-3.12957300
C	-0.06536800	4.97356200	3.46166800
C	-0.04713300	6.31653400	3.88693400
C	1.06776900	4.17946700	3.72611500
C	1.05128500	6.83810000	4.57407000
H	-0.91078700	6.95320900	3.68404400
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H	3.02410200	6.44203400	5.37625400
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C	-1.48336300	2.44116800	5.12220100
C	-0.51120600	-0.06476200	4.37166000
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C	-1.14921300	1.50223400	6.09781900
H	-1.86232500	3.42434700	5.40829700
C	-0.65647200	0.24619600	5.72796700

H	-0.13235800	-1.04606100	4.07363300
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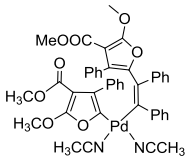

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C	-3.79066100	6.89740200	1.74140900
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O	-3.98371400	6.55597600	-1.89201000
O	-4.92318400	8.08106000	-0.53581800
C	-4.83811400	7.82605800	3.63183200
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H	-0.62133000	-0.97827600	-0.83730600
H	-1.20133900	0.23754200	-2.03031300
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C	-1.34403300	4.49407400	2.74255100
C	-1.69009500	3.22304600	3.05990000
C	-1.81544200	4.66309300	-0.46492300
C	-2.53661200	4.04116900	-1.49946600
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H	0.15444000	4.95255000	0.37965300
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H	-2.46021000	2.81850800	-3.27292900
H	1.32138800	3.59565500	-1.33443600
H	0.02315600	2.53817500	-3.19337500
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H	-7.87029300	2.18664900	2.94383000
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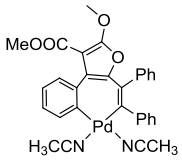

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C	-4.01742600	0.33368800	3.12423700
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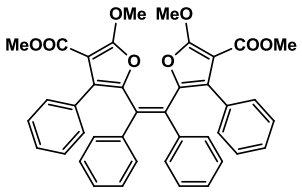
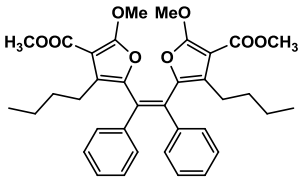
Part X. NMR spectra for the products



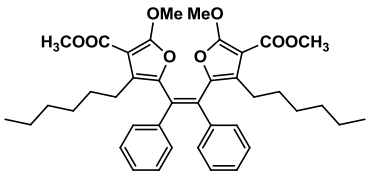
3a

(3a) Yield:64 % ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.58 (s, 6H), δ 3.65 (s, 6H), δ 6.93-7.22 (m, 20H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 50.84, 57.03, 91.25, 125.90, 126.98, 127.17, 127.21, 127.71, 129.86, 130.05, 130.51, 132.06, 138.73, 141.40, 162.39, 163.38; HRMS exact mass calcd. for $(C_{40}H_{32}O_8+H)^+$ requires m/z 641.2170, found m/z 641.2169.



3b

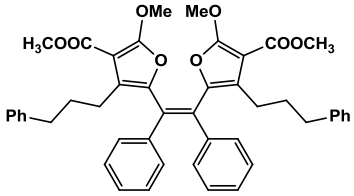
(3b) Yield:72 % ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.72 (t, *J* = 7.30 Hz, 6H), δ 1.06-1.12 (m, 4H), δ 1.24-1.28 (m, 4H), δ 2.07 (t, *J* = 7.82 Hz, 4H), δ 3.77 (s, 6H), δ 3.81 (s, 6H), δ 7.09-7.11 (m, 10H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.67, 22.69, 24.12, 32.03, 50.87, 57.15, 91.74, 127.19, 127.20, 127.86, 130.08, 131.05, 139.10, 141.21, 162.03, 163.67; HRMS exact mass calcd. for $(C_{36}H_{40}O_8+Na)^+$ requires m/z 623.2615, found m/z 623.2608.



3c

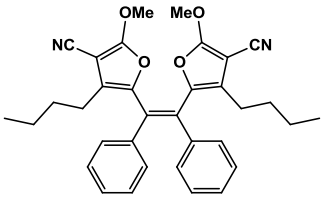
(3c) Yield:62 % ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.72 (t, *J* = 7.30 Hz, 6H), δ 1.05-1.07 (m, 8H), δ 1.14-1.25 (m, 8H), δ 2.06 (t, *J* = 7.84 Hz, 4H), δ 3.77 (s, 6H), δ 3.80 (s, 6H), δ 7.09-7.12 (m, 10H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.05, 22.61, 24.42, 29.39, 29.89, 31.46, 50.92, 57.21, 91.79, 127.21, 127.87, 130.12, 131.05,

131.06, 139.11, 141.20, 162.04, 163.70; HRMS exact mass calcd. for $(C_{40}H_{48}O_8+H)^+$ requires m/z 657.3422, found m/z 657.3433.



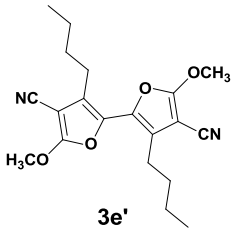
3d

(3d) Yield:67 % ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.59-1.65 (m, 4H), δ 2.13 (t, *J* = 7.80 Hz, 4H), δ 2.34 (t, *J* = 7.76 Hz, 4H), δ 3.73 (s, 6H), δ 3.78 (s, 6H), δ 7.00-7.22 (m, 20H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 24.52, 31.33, 36.06, 50.97, 57.27, 91.80, 125.57, 126.70, 127.33, 127.97, 128.19, 128.29, 130.13, 131.04, 139.00, 141.25, 142.25, 162.08, 163.63; HRMS exact mass calcd. for $(C_{46}H_{44}O_8+H)^+$ requires m/z 725.3109, found m/z 725.3124.



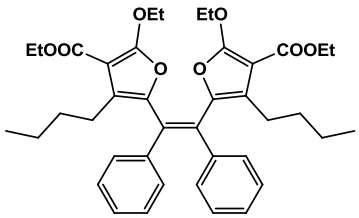
3e

(3e) Yield:62 % When cyclopropene 1e was reacted with diphenylacetylene 2a, we got the mixture of target product 3e and bifuran 3e′ with the ratio 3e: 3e′ =1:1.8. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.74-0.78 (t, *J* = 7.28 Hz, 6H), δ 1.08-1.14 (m, 4H), δ 1.15-1.25 (m, 4H), δ 1.79-1.83 (t, *J* = 7.80 Hz, 4H), δ 3.96 (s, 6H), δ 7.03-7.31 (m, 10H); HRMS exact mass calcd. for $(C_{34}H_{34}N_2O_4+H)^+$ requires m/z 535.2591, found m/z 535.2591.



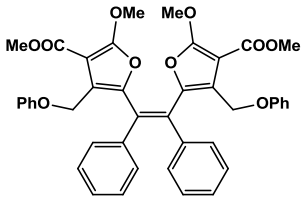
3e'

(3e′) Yield:62 % ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.91 (t, *J* = 7.28 Hz, 6H), δ 1.32-1.38 (m, 4H), δ 1.58-1.60 (m, 4H), δ 2.49 (t, *J* = 7.70 Hz, 4H), δ 4.16 (s, 6H); HRMS exact mass calcd. for $(C_{20}H_{24}N_2O_4+H)^+$ requires m/z 357.1809, found m/z 357.1805.



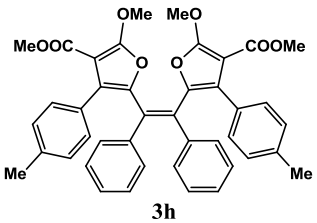
3f

(3f) Yield:54 % ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.73 (t, *J* = 7.28 Hz, 6H), δ 1.09-1.13 (m, 4H), δ 1.24-1.32 (m, 16H), δ 2.10 (t, *J* = 7.82 Hz, 4H), δ 4.11-4.17 (q, *J* = 14.20 Hz, *J* = 7.08 Hz，4H), δ 4.21-4.26 (q, *J* = 14.24 Hz, *J* = 7.12 Hz，4H), δ 7.06-7.11 (m, 10H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.78, 14.34, 14.81, 22.81, 24.36, 32.12, 59.52, 66.90, 92.70, 126.64, 127.12, 127.81, 130.19, 131.07, 139.38, 141.02, 162.02, 163.51; HRMS exact mass calcd. for $(C_{40}H_{48}O_8+H)^+$ requires m/z 657.3422, found m/z 657.3435.



3g

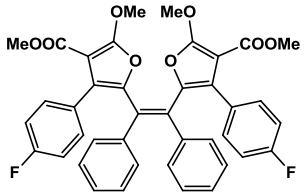
(3g) Yield:51 % ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.70 (s, 6H), δ 3.74 (s, 6H), δ4.56 (s, 4H), δ 6.66-6.69 (d, *J* = 8.16 Hz, 4H), δ 6.86-6.84 (d, *J* = 7.40 Hz, 4H), δ 7.12 (s, 2H), δ 7.12-7.23 (m, 10H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 51.14, 57.54, 60.05, 91.86, 114.70, 120.47, 121.28, 127.64, 127.95, 129.09, 129.35, 130.90, 138.35, 143.51, 158.66, 162.25, 163.21; HRMS exact mass calcd. for $(C_{42}H_{36}O_{10}+Na)^+$ requires m/z 723.2001, found m/z 723.2008.



3h

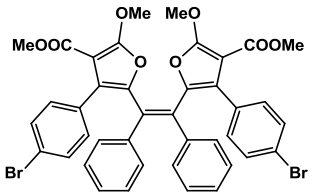
(3h) Yield:67 % ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.27 (s, 6H), δ 3.56 (s, 6H), δ 3.66 (s, 6H), δ6.91-7.08 (m, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.25, 50.90, 56.77, 91.20, 125.84, 127.11, 127.72, 128.03, 129.01, 129.52, 130.00, 130.53, 136.33,

138.87, 141.33, 162.33, 163.50; HRMS exact mass calcd. for $(C_{42}H_{36}O_8+H)^+$ requires m/z 669.2483, found m/z 669.2481.



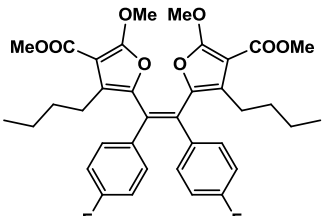
3i

(3i) Yield:83 % ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.63 (s, 6H), δ 3.67 (s, 6H), δ 6.91-7.18 (m, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 51.00, 56.99, 91.03, 114.23, 114.45, 124.99, 127.45, 127.89, 127.93, 127.97, 129.85, 130.40, 131.23, 131.32, 138.42, 141.55, 160.93, 162.43, 163.31, 163.37; HRMS exact mass calcd. for $(C_{40}H_{30}F_2O_8+H)^+$ requires m/z 677.1982, found m/z 677.1982.



3j

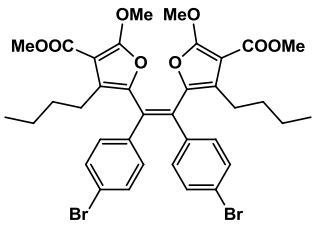
(3j) Yield:65 % ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.64 (s, 6H), δ 3.67 (s, 6H), δ6.91-7.39 (m, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 50.97, 57.35, 90.98, 121.41, 124.82, 127.54, 127.96, 129.87, 130.33, 130.55, 130.98, 131.26, 138.40, 141.42, 162.57, 163.20; HRMS exact mass calcd. for $(C_{40}H_{30}Br_2O_8+H)^+$ requires m/z 797.0380, found m/z 6797.0371.



3k

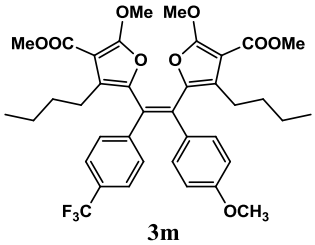
(3k) Yield:64 % ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.73 (t, *J* = 7.22 Hz, 6H), δ 1.08-1.14 (m, 4H), δ 1.24-1.28 (m, 4H), δ 2.04-2.10 (t, *J* = 7.93 Hz, 4H), δ 3.77 (s, 6H), δ 3.80 (s, 6H), δ 6.81-7.06 (m, 8H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.66, 22.70, 24.16, 32.08, 50.95, 57.21, 91.86, 115.01, 115.22, 127.52, 128.94, 128.98, 132.61，

132.69，134.91, 134.95, 140.79, 160.69, 162.08, 163.59; HRMS exact mass calcd. for $(C_{36}H_{38}F_2O_8+H)^+$ requires m/z 637.2608, found m/z 637.2603.



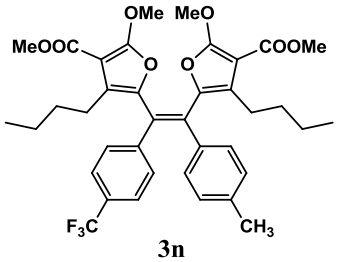
3l

(3l) Yield:65 % ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.74 (t, *J* = 7.28 Hz, 6H), δ 0.85-0.96 (m, 4H), δ 1.09-1.14 (m, 4H), δ 2.07 (t, *J* = 7.76 Hz, 4H), δ 3.77 (s, 6H), δ 3.80 (s, 6H), δ 6.94-6.96 (d, *J* = 8.40 Hz, 4H), δ 7.27-7.29 (d, *J* = 8.44 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.61, 22.70, 24.23, 32.03, 50.96, 57.24, 91.98, 121.62, 127.94, 129.19, 131.36, 132.56, 137.80, 140.47, 162.15, 163.51; HRMS exact mass calcd. for $(C_{36}H_{38}Br_2O_8+H)^+$ requires m/z 757.1006, found m/z 757.0988.



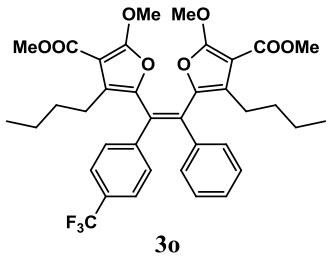
3m

(3m) Yield:43 % ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.72-0.74 (m, 6H), δ 0.86-0.88 (m, 2H), δ 1.06-1.13 (m, 4H), δ 1.21-1.28 (m, 2H), δ 2.04-2.09 (m, 4H), δ 3.76 (s, 3H), δ 3.77 (s, 6H), δ 3.80 (s, 6H), δ 6.66-6.69 (d, *J* = 8.68 Hz, 2H), δ 6.98-7.00 (d, *J* = 8.68 Hz, 2H), δ 7.18-7.20 (d, *J* = 8.12 Hz, 2H), δ 7.36-7.38 (d, *J* = 8.24 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.59, 13.68, 22.71, 24.20, 24.23, 29.69, 31.87, 32.16, 50.95, 53.70, 55.20, 57.20, 57.26, 91.77, 92.01, 113.63, 124.49, 124.82, 124.86, 126.83, 126.96, 128.49, 130.59, 130.86, 131.20, 131.69, 132.36, 140.75, 140.91, 143.51, 159.27, 162.09, 162.15, 163.61; HRMS exact mass calcd. for $(C_{38}H_{41}F_3O_9+H)^+$ requires m/z 699.2775, found m/z 699.2777.



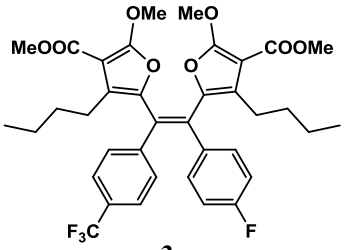
3n

(3n) Yield:59 % ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.71 (t, *J* = 7.22 Hz, 6H), δ 0.83-0.88 (m, 4H), δ 1.07-1.11 (m, 4H), δ 2.03-2.09 (m, 4H), δ 2.28 (s, 3H), δ 3.77 (s, 6H), δ 3.80 (s, 6H), δ 6.92-6.94 (d, *J* = 8.56 Hz, 2H), δ 6.95-6.97 (d, *J* = 8.48 Hz, 2H), δ 7.18-7.20 (d, *J* = 8.12 Hz, 2H), δ 7.35-7.37 (d, *J* = 8.20 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.58, 13.63, 21.21, 22.69, 22.71, 24.19, 24.23, 31.87, 32.08, 50.92, 50.94, 57.19, 57.25, 91.79, 92.01, 124.76, 124.80, 126.98, 127.48, 128.42, 128.90, 128.97, 129.47, 129.82, 130.97, 131.20, 132.10, 135.33, 137.77. 140.76, 140.85, 162.11, 162.13, 163.59; HRMS exact mass calcd. for $(C_{38}H_{41}F_3O_8+H)^+$ requires m/z 683.2826, found m/z 683.2826.



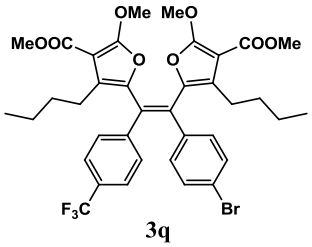
3o

(3o) Yield:64 % ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.68-0.75 (m, 6H), δ 0.83-0.89 (m, 4H), δ 1.04-1.12 (m, 4H), δ 2.02-2.10 (m, 4H), δ 3.76 (s, 3H), δ 3.77 (s, 3H), δ 3.80 (s, 3H), δ 3.81 (s, 3H), δ 7.07-7.36 (m, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.59, 13.64, 22.68, 22.71, 24.18, 24.24, 31.89, 32.08, 50.96, 50.97, 57.20, 57.27, 91.82, 92.02, 124.80, 124.81, 127.29, 127.84, 128.00, 128.16, 128.55, 128.57, 131.10, 131.26, 132.01, 132.06, 138.38, 140.63, 140.69, 162.15, 162.16, 163.57, 163.58; HRMS exact mass calcd. for $(C_{37}H_{39}F_3O_8+Na)^+$ requires m/z 691.2489, found m/z 691.2482.



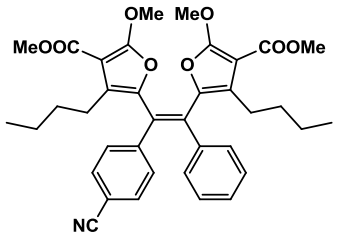
3p

(3p) Yield:70 % ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.69-0.71 (m, 6H), δ 0.86-0.88 (m, 4H), δ 1.06-1.13 (m, 4H), δ 2.05-2.08 (t, *J* = 7.64 Hz, 4H), δ 3.78 (s, 6H), δ 3.81 (s, 6H), δ 6.83-6.87 (m, 2H), δ 7.06-7.08 (m, 2H), δ 7.17-7.19 (d, *J* = 8.04 Hz, 2H), δ 7.38-7.40 (d, *J* = 8.08 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.54, 13.60, 22.68, 24.19, 24.24, 29.66, 31.89, 32.10, 50.93, 53.35, 57.21, 57.26, 91.98, 92.13, 115.18, 115.39, 124.91, 124.94, 125.33, 127.55, 128.27, 128.59, 129.34, 130.64, 131.24, 132.70, 132.78, 134.43, 134.46, 140.41, 140.49, 143.00, 160.98, 162.16, 162.20, 163.47, 163.48; HRMS exact mass calcd. for $(C_{37}H_{38}F_4O_8+H)^+$ requires m/z 687.2576, found m/z 687.2576.



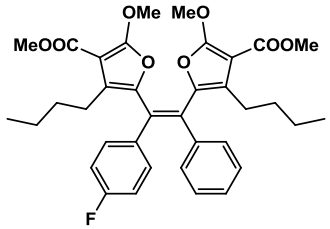
3q

(3q) Yield:75 % ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.68-0.73 (m, 6H), δ 0.75-0.89 (m, 4H), δ 1.04-1.18 (m, 4H), δ 2.02-2.09 (m, 4H), δ 3.77 (s, 6H), δ 3.80 (s, 6H), δ 6.94-6.96 (d, *J* = 8.40 Hz, 2H), δ 7.19-7.21 (d, *J* = 8.08 Hz, 2H), δ 7.26-7.28 (d, *J* = 8.44 Hz, 2H), δ 7.39-7.41 (d, *J* = 8.16 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.56, 13.65, 22.69, 24.25, 24.27, 29.69, 31.89, 32.06, 50.75, 51.03, 56.85, 57.29, 91.98, 92.04, 121.94, 125.04, 125.08, 127.97, 128.54, 128.72, 129.52, 130.29, 131.26, 131.42, 132.60, 135.07, 137.47, 140.24, 140.38, 142.76, 162.18, 162.22, 163.47; HRMS exact mass calcd. for $(C_{37}H_{38}BrF_3O_8+H)^+$ requires m/z 747.1775, found m/z 747.1773.



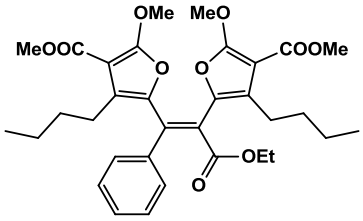
3r

(3r) Yield:41 % ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.73 (t, *J* = 7.28 Hz, 3H), δ 0.85-0.89 (m, 5H), δ 1.05-1.11 (m, 2H), δ 1.14-1.42 (m, 4H), δ 2.06 (t, *J* = 7.70 Hz, 2H), δ 2.85 (t, *J* = 7.80 Hz, 2H), δ 3.77 (s, 3H), δ 3.79 (s, 3H), δ 3.80 (s, 3H), δ 3.84 (s, 3H), δ 7.13-7.59 (m, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.65, 13.85, 22.55, 22.92, 24.23, 24.34, 29.69, 32.15, 32.29, 50.95, 57.20, 57.24, 88.85, 91.81, 92.29, 93.90, 109.61, 123.28, 126.55, 127.92, 128.16, 128.24, 128.66, 129.65, 130.47, 131.17, 137.12, 137.46, 138.38, 139.44, 161.82, 162.47, 163.48; HRMS exact mass calcd. for $(C_{37}H_{39}NO_8+H)^+$ requires m/z 626.2748, found m/z 626.2750.



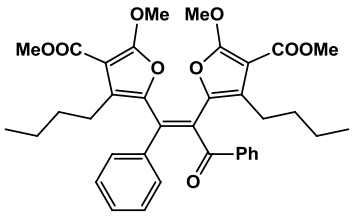
3s

(3s) Yield:58 % ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.67-0.72 (t, *J* = 7.32 Hz, 3H), δ 0.72-0.75 (t, *J* = 7.28 Hz, 3H), δ 1.05-1.15 (m, 4H), δ 1.20-1.28 (m, 4H), δ 2.03-2.11 (m, 4H), δ 3.76 (s, 3H), δ 3.77 (s, 3H), δ 3.79 (s, 3H), δ 3.80 (s, 3H), δ 6.78-6.82 (m, 2H), δ 7.03-7.14 (m, 7H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.65, 13.66, 22.67, 22.70, 24.13, 24.15, 32.05, 32.06, 50.89, 50.91, 57.18, 57.21, 91.84, 91.88, 114.82, 115.04, 127.25, 127.34, 127.44, 128.00, 128.76, 130.32, 131.03, 132.62, 132.70, 135.13, 135.16, 138.93, 141.00, 141.02, 160.63, 162.04, 162.08, 163.10, 163.62, 163.64; HRMS exact mass calcd. for $(C_{36}H_{39}FO_8+H)^+$ requires m/z 619.2707, found m/z 619.2703.



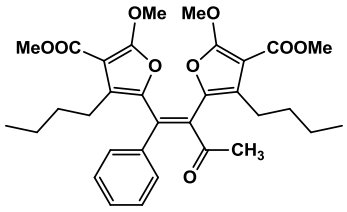
3t

(3t) Yield:53 % ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.85-0.88 (t, *J* = 7.04 Hz, 3H), δ 0.90-1.05 (m, 6H), δ 1.19-1.22 (m, 4H), δ 1.30-1.36 (m, 2H), δ 1.42-1.47 (m, 2H), δ 1.97-2.00 (t, *J* = 7.70 Hz, 2H), δ 2.39-2.43 (t, *J* = 7.64 Hz, 2H),δ 3.76 (s, 3H), δ 3.77 (s, 3H), δ 3.78 (s, 3H), δ 3.85 (s, 3H), δ 3.90-3.93 (q, *J* = 7.12 Hz, 2H), δ 7.33-7.36 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.52, 13.60, 13.80, 22.56, 22.83, 24.17, 24.51, 29.70, 31.75, 32.24, 50.97, 51.01, 57.23, 61.13, 91.63, 92.56, 120.52, 127.15, 127.16, 128.35, 129.04, 129.23, 132.26, 136.83, 137.69, 138.57, 162.21, 162.60, 163.30, 163.54, 168.11; HRMS exact mass calcd. for $(C_{33}H_{40}O_{10}+H)^+$ requires m/z 597.2695, found m/z 597.2695.



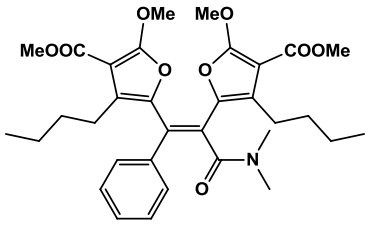
3u

(3u) Yield:54 % ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.65-0.70 (m, 6H), δ 1.03-1.17 (m, 4H), δ 1.20-1.32 (m, 4H), δ 2.03-2.07 (t, *J* = 7.76 Hz, 2H), δ 2.25-2.29 (t, *J* = 7.88 Hz, 2H), δ 3.75 (s, 3H), δ 3.77 (s, 3H), δ 3.81 (s, 3H), δ 3.83 (s, 3H), δ 7.09-7.36 (m, 8H), δ 7.76-7.77 (d, *J* = 7.36 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.61, 13.62, 22.58, 22.73, 24.23, 24.60, 31.92, 32.26, 50.93, 51.12, 57.24, 57.35, 91.81, 92.57, 127.39, 127.49, 128.08, 128.23, 129.06, 129.14, 130.21, 131.41, 132.58, 135.84, 137.87, 138.07, 138.81, 139.18, 162.32, 162.66, 163.35, 163.45, 196.04; HRMS exact mass calcd. for $(C_{37}H_{40}O_9+H)^+$ requires m/z 629.2745, found m/z 629.2739.



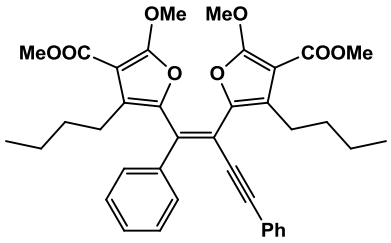
3v

(3v) Yield:50 % ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.64-0.68 (t, *J* = 7.32 Hz, 3H), δ 0.84-0.88 (t, *J* = 7.20 Hz, 3H), δ 0.99-1.02 (m, 2H), δ 1.17-1.20 (m, 2H), δ 1.28-1.42 (m, 4H), δ 1.88 (s, 3H), δ 1.96-2.00 (t, *J* = 7.84 Hz, 2H), δ 2.31-2.34 (t, *J* = 7.68 Hz, 2H), δ 3.74 (s, 3H), δ 3.76 (s, 6H), δ 3.84 (s, 3H), δ 7.28-7.42 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.55, 13.80, 22.61, 22.85, 24.22, 24.68, 30.63, 31.74, 32.23, 50.94, 50.99, 57.24, 57.28, 91.66, 92.76, 126.83, 128.79, 129.43, 129.85, 130.10, 132.61, 136.82, 138.01, 138.78, 138.87, 162.33, 162.66, 163.23, 163.51, 202.54; HRMS exact mass calcd. for $(C_{32}H_{38}O_9+H)^+$ requires m/z 567.2589, found m/z 567.2586.



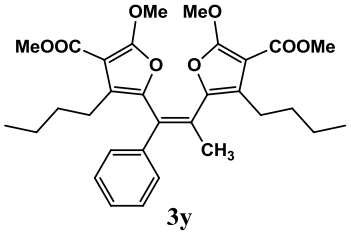
3w

(3w) Yield:56 % ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.67-0.70 (t, *J* = 7.28 Hz, 3H), δ 0.86-0.90 (t, *J* = 7.24 Hz, 3H), δ 1.06-1.14 (m, 2H), δ 1.19-1.28 (m, 2H), δ 1.29-1.55 (m, 4H), δ 2.16-2.37 (m, 2H), δ 2.42-2.49 (m, 2H), δ 2.72 (s, 3H), δ 2.77 (s, 3H), δ 3.75 (s, 3H), δ 3.76 (s, 3H), δ 3.77 (s, 3H), δ 3.79 (s, 3H), δ 7.30-7.37 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.63, 13.83, 22.64, 23.20, 24.17, 24.51, 32.13, 32.27, 34.64, 38.01, 50.95, 51.00, 57.10, 57.29, 91.68, 92.07, 123.84, 127.78, 128.24, 128.75, 128.85, 129.14, 130.19, 137.010, 137.79, 139.23, 162.21, 162.33, 163.48, 168.04, 168.05; HRMS exact mass calcd. for $(C_{33}H_{41}NO_9+H)^+$ requires m/z 596.2854, found m/z 596.2850.



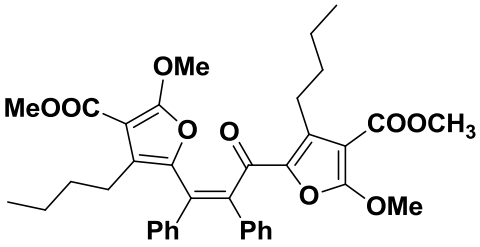
3x

(3x) Yield:53 % ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.69-0.73 (t, *J* = 7.28 Hz, 3H), δ 0.85-0.88 (t, *J* = 7.28 Hz, 3H), δ 1.07-1.11 (m, 2H), δ 1.34-1.39 (m, 4H), δ 1.56-1.61 (m, 2H), δ 2.04-2.08 (t, *J* = 7.70 Hz, 2H), δ 2.83-2.87 (t, *J* = 7.80 Hz, 2H), δ 3.77 (s, 3H), δ 3.79 (s, 3H), δ 3.80 (s, 3H), δ 3.84 (s, 3H), δ 7.13-7.58 (m, 10H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.65, 13.83, 19.18, 22.55, 22.92, 24.23, 24.35, 29.69, 32.15, 32.29, 50.96, 57.20, 88.85, 91.80, 92.29, 93.90, 109.61, 123.28, 126.55, 127.92, 128.16, 128.24, 128.66, 129.65, 130.47, 131.17, 137.12, 137.46, 138.37, 139.44, 162.45, 162.47, 163.49, 163.64; HRMS exact mass calcd. for $(C_{38}H_{40}O_8+H)^+$ requires m/z 625.2796, found m/z 625.2796.



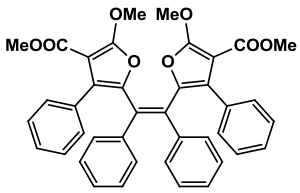
3y

(3y) Yield:39 % ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.70-0.78 (t, *J* = 6.96 Hz, 3H), δ 0.88-0.90 (m, 5H), δ 1.05-1.12 (m, 2H), δ 1.28-1.37 (m, 4H), δ 2.00-2.04 (m, 5H), δ 2.39-2.42 (t, *J* = 7.28 Hz, 2H), δ 3.74 (s, 3H), δ 3.77 (s, 3H), δ 3.78 (s, 3H), δ 3.99 (s, 3H), δ 7.23-7.36 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.67, 13.89, 19.88, 22.69, 22.88, 24.02, 24.16, 31.19, 31.98, 50.80, 50.87, 57.08, 57.32, 91.52, 91.64, 123.34, 125.62, 125.87, 127.57, 128.26, 129.81, 131.04, 139.37, 140.32, 141.56, 161.91, 161.92, 163.76, 163.82; HRMS exact mass calcd. for $(C_{31}H_{38}O_8+H)^+$ requires m/z 539.2639, found m/z 539.2631.

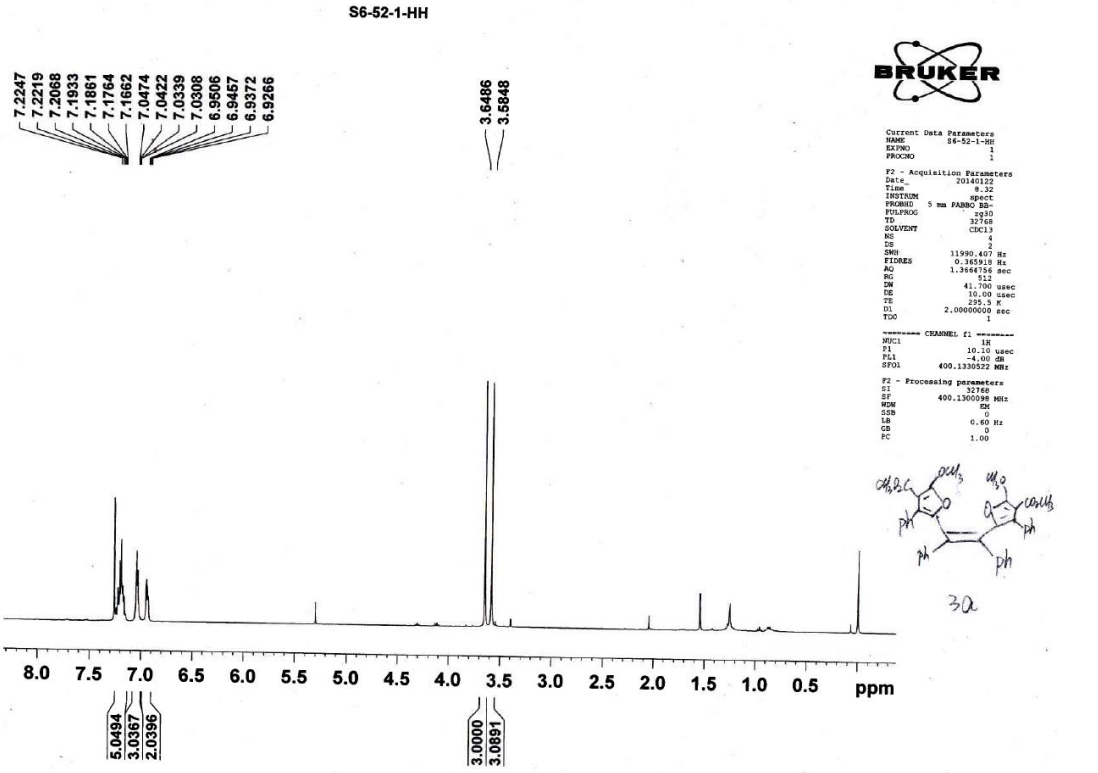


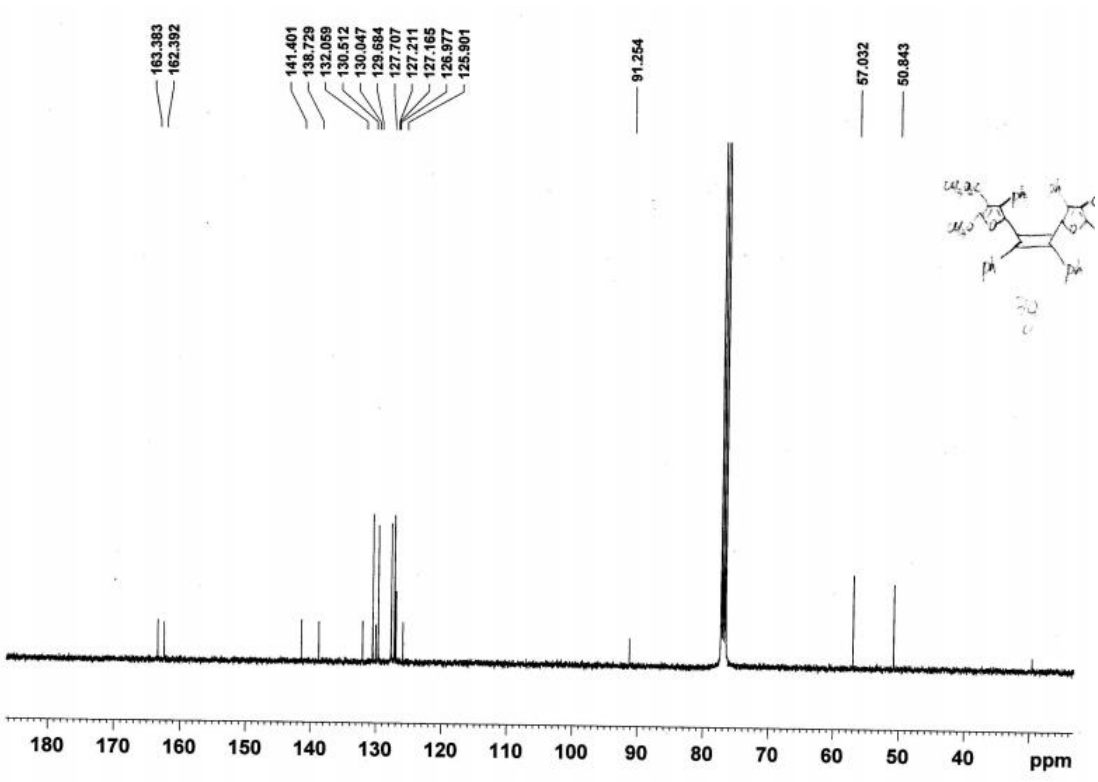
5a

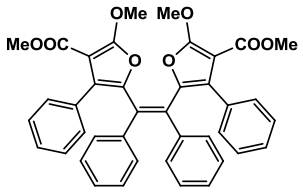
(5a) Yield:15 % ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.78-0.81 (t, *J* = 7.32 Hz, 3H), δ 0.0.84-0.88 (t, *J* = 7.26 Hz, 3H), δ 1.28-1.33 (m, 4H), δ 1.42-1.48 (m, 4H), δ 2.44-2.47 (t, *J* = 7.84 Hz, 2H), δ 2.71-2.75 (t, *J* = 7.54 Hz, 2H), δ 3.45 (s, 3H), δ 3.62 (s, 3H), δ 3.77 (s, 3H), δ 3.78 (s, 3H), δ 7.05-7.22 (m, 10H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.69, 13.86, 22.59, 24.04, 31.10, 31.12, 32.31, 32.53, 50.94, 52.12, 52.16, 57.25, 109.65, 111.71, 124.76, 126.26, 127.03, 127.52, 127.72, 128.22, 128.75, 129.83, 130.50, 131.63, 131.99, 138.76, 142.22, 143.37, 145.69, 147.21, 162.25, 163.58, 165.34; HRMS exact mass calcd. for $(C_{37}H_{40}O_9+H)^+$ requires m/z 629.2745, found m/z 629.2758.


OMe MeO
MeOOC
COOMe
O
O

3a


S6-52-1-HH
7.2247
7.2219
7.2068
7.1933
7.1861
7.1764
7.1662
7.0474
7.0422
7.0339
7.0308
6.9506
6.9457
6.9372
6.9266
3.6486
3.5848
BRUKER
Current Data Parameters
NAME S6-52-1-HH
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140122
Time 8.32
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 4
DS 2
SWH 11990.407 Hz
FIDRES 0.365919 Hz
AQ 1.3664756 sec
RG 512
DW 41.700 usec
DE 10.00 usec
TE 295.5 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.10 usec
PL1 -4.00 dB
SFO1 400.1330522 MHz
F2 - Processing parameters
SI 32768
SF 400.1300098 MHz
WDW EM
SSB 0
LB 0.60 Hz
GB 0
PC 1.00
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
5.0494
3.0367
2.0396
3.0000
3.0691
3a


163.383
162.392
141.401
138.729
132.059
130.512
130.047
129.684
127.707
127.211
127.165
126.977
126.901
91.254
57.032
50.843
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 ppm



3a

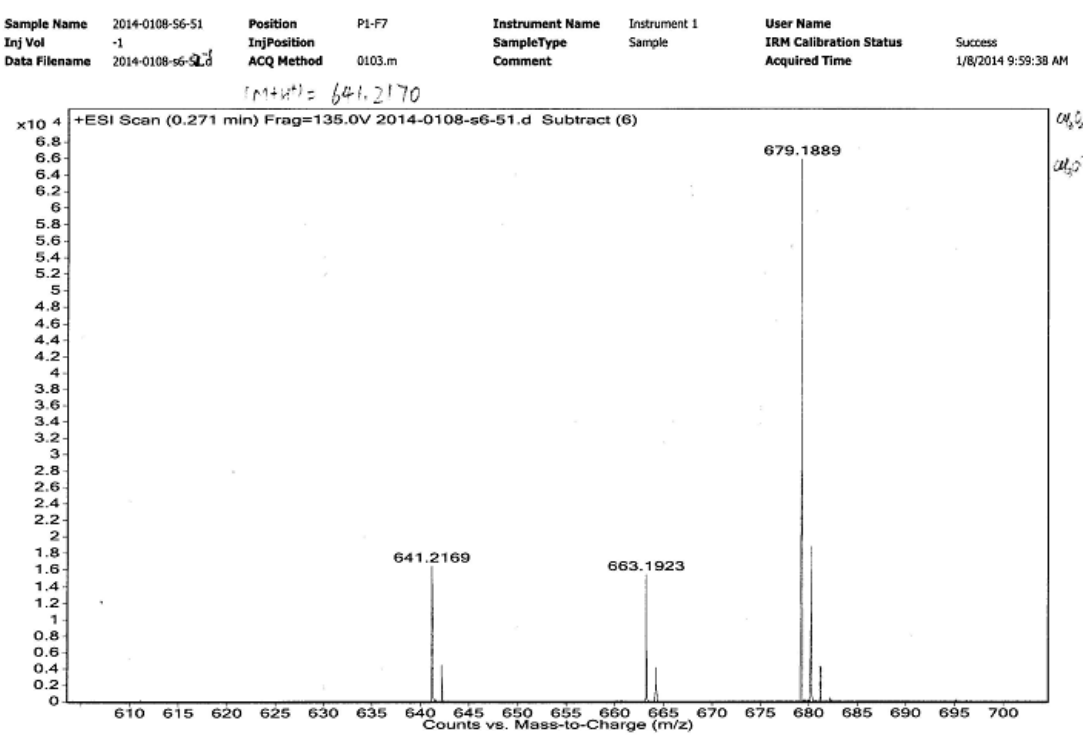
Chemical Formula: $C_{40}H_{32}O_8$

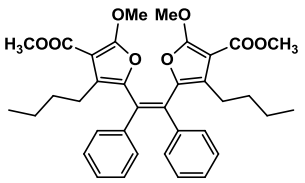
Exact Mass: 640.21

Molecular Weight: 640.68

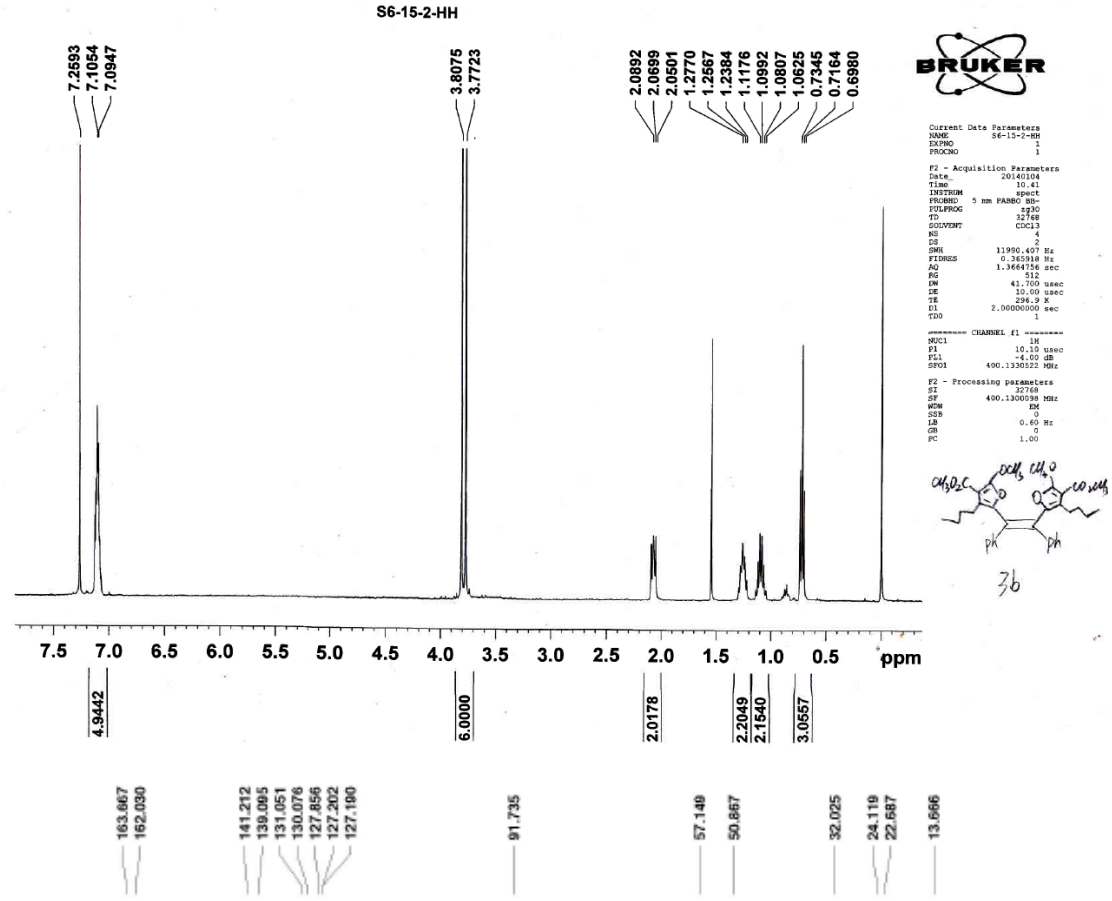
m/z: 640.21 (100.0%), 641.21 (43.6%), 642.22 (9.4%), 643.22 (2.0%), 642.21 (1.6%)

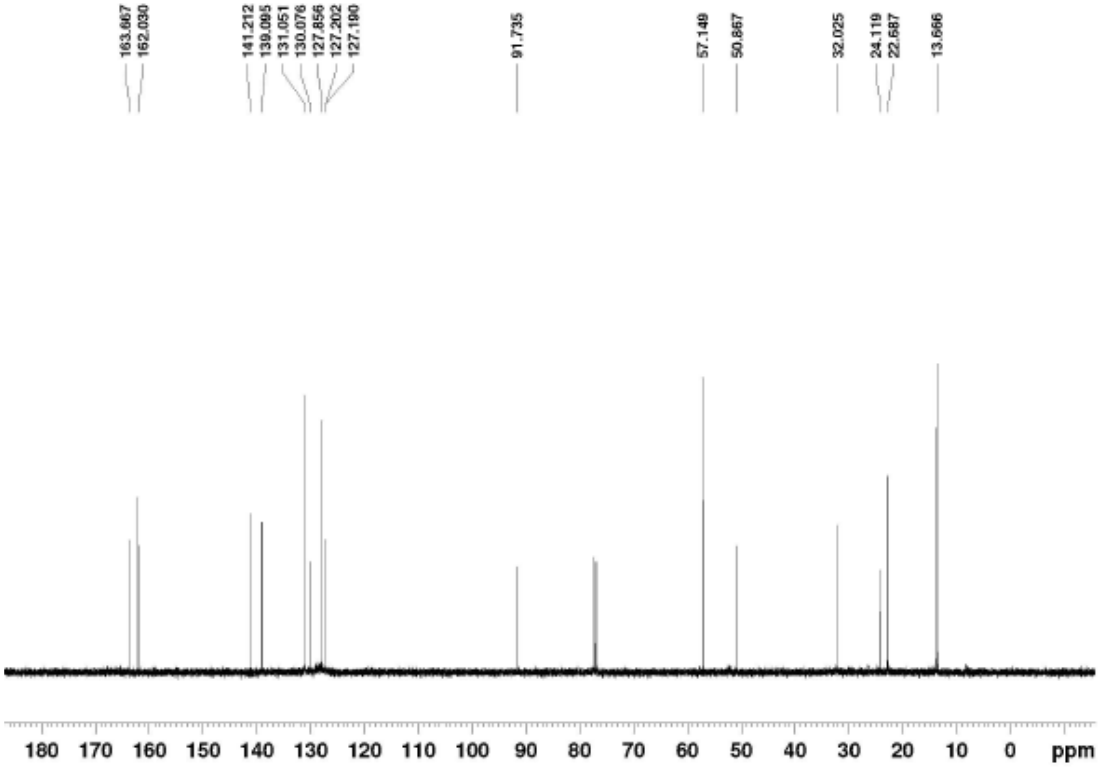
Elemental Analysis: C, 74.99; H, 5.03; O, 19.98

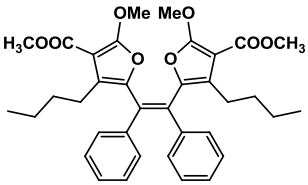



OMe MeO
H3COOC
COOCH3
O
O

3b


S6-15-2-HH
7.2593
7.1054
7.0947
3.8075
3.7723
2.0892
2.0699
2.0501
1.2770
1.2567
1.2384
1.1176
1.0992
1.0807
1.0625
0.7345
0.7164
0.6980
BRUKER
Current Data Parameters
NAME S6-15-2-HH
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140104
Time 10.41
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 4
DS 2
SWH 11990.407 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 512
DW 41.700 usec
DE 10.00 usec
TE 296.9 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.10 usec
PL1 -4.00 dB
SFO1 400.1330522 MHz
F2 - Processing parameters
SI 32768
SF 400.1300098 MHz
WDW EM
SSB 0
LB 0.60 Hz
GB 0
PC 1.00
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
4.9442
6.0000
2.0178
2.2049
2.1540
3.0557


163.667
162.030
141.212
139.095
131.051
130.076
127.856
127.202
127.190
91.735
57.149
50.867
32.025
24.119
22.687
13.666
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm



3b

Chemical Formula: $C_{36}H_{40}O_8$

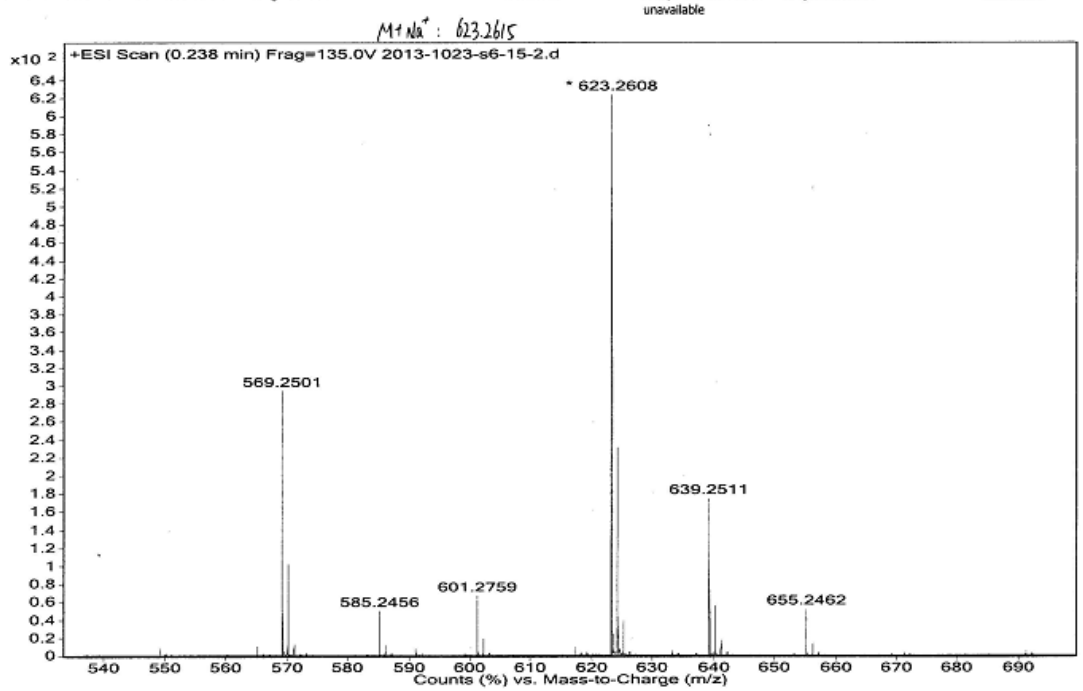
Exact Mass: 600.27

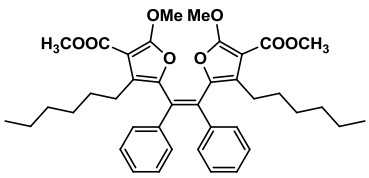
Molecular Weight: 600.70

m/z: 600.27 (100.0%), 601.28 (39.7%), 602.28 (9.3%), 603.28 (1.6%)

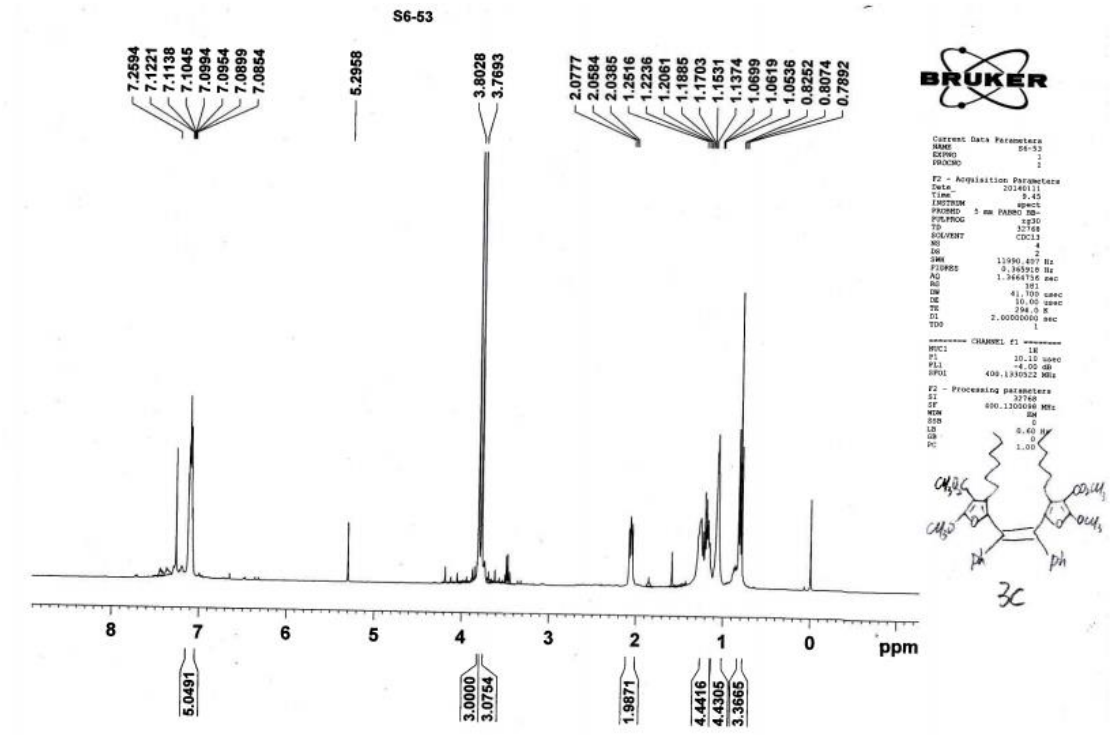
Elemental Analysis: C, 71.98; H, 6.71; O, 21.31

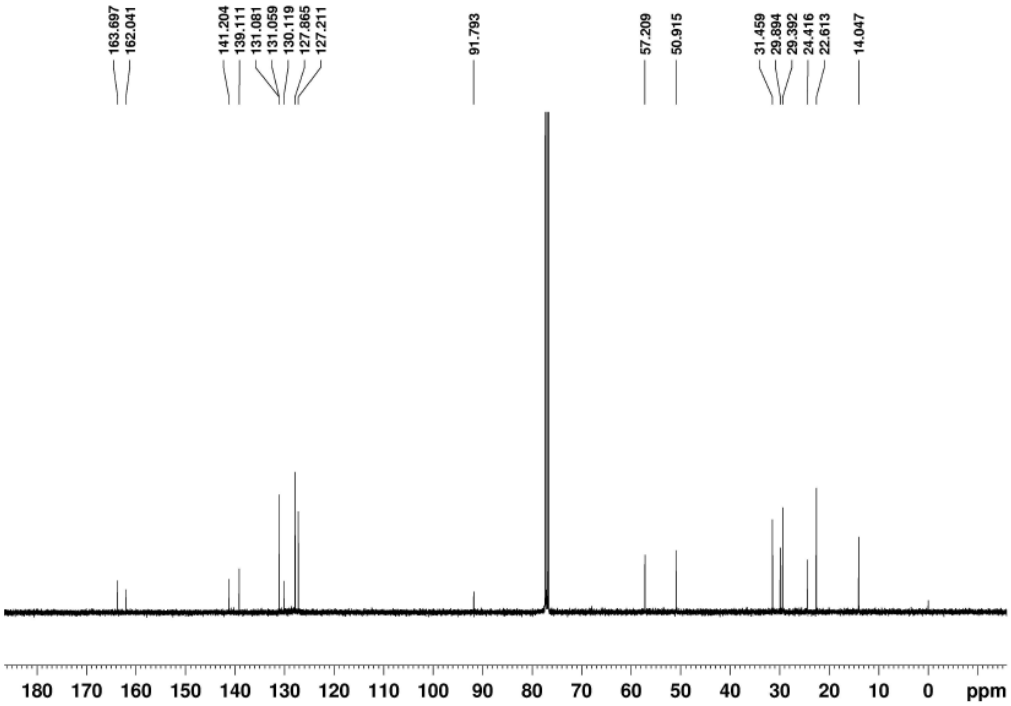
Sample Name	Unavailable	**Position**	Unavailable	**Instrument Name**	Unavailable	**User Name**	Unavailable
Inj Vol	Unavailable	**InjPosition**	Unavailable	**SampleType**	Unavailable	**IRM Calibration Status**	Success
Data Filename	2013-1023-s6-15-2.d	**ACQ Method**		**Comment**	Sample information is unavailable	**Acquired Time**	Unavailable

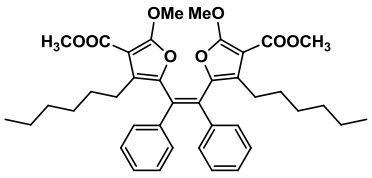



OMe MeO
H3COOC
COOCH3
O
O

3c


S6-53
7.2594
7.1221
7.1138
7.1045
7.0994
7.0954
7.0899
7.0854
5.2958
3.8028
3.7693
2.0777
2.0584
2.0385
1.2516
1.2236
1.2061
1.1885
1.1703
1.1531
1.1374
1.0699
1.0619
1.0536
0.8252
0.8074
0.7892
BRUKER
8
7
6
5
4
3
2
1
0
ppm
5.0491
3.0000
3.0764
1.9871
4.4416
4.4305
3.3665


163.697
162.041
141.204
139.111
131.081
131.059
130.119
127.865
127.211
91.793
57.209
50.915
31.459
29.894
29.392
24.416
22.613
14.047
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm



3c

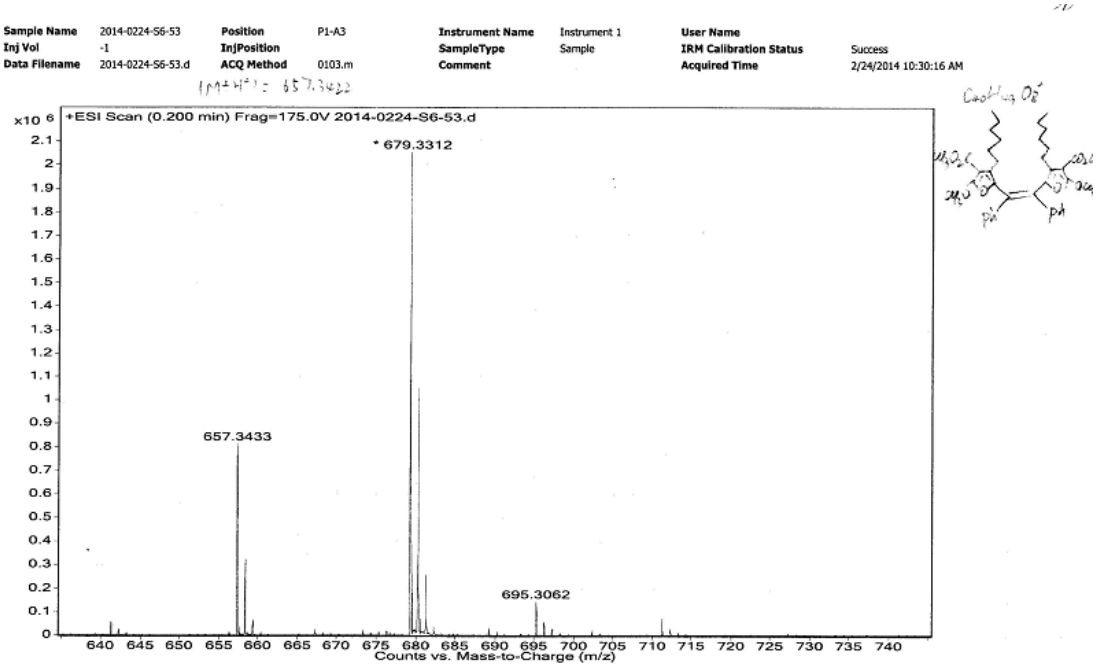
Chemical Formula: $C_{40}H_{48}O_8$

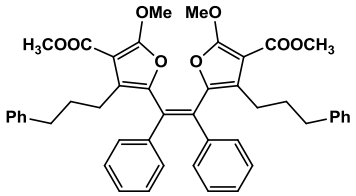
Exact Mass: 656.33

Molecular Weight: 656.80

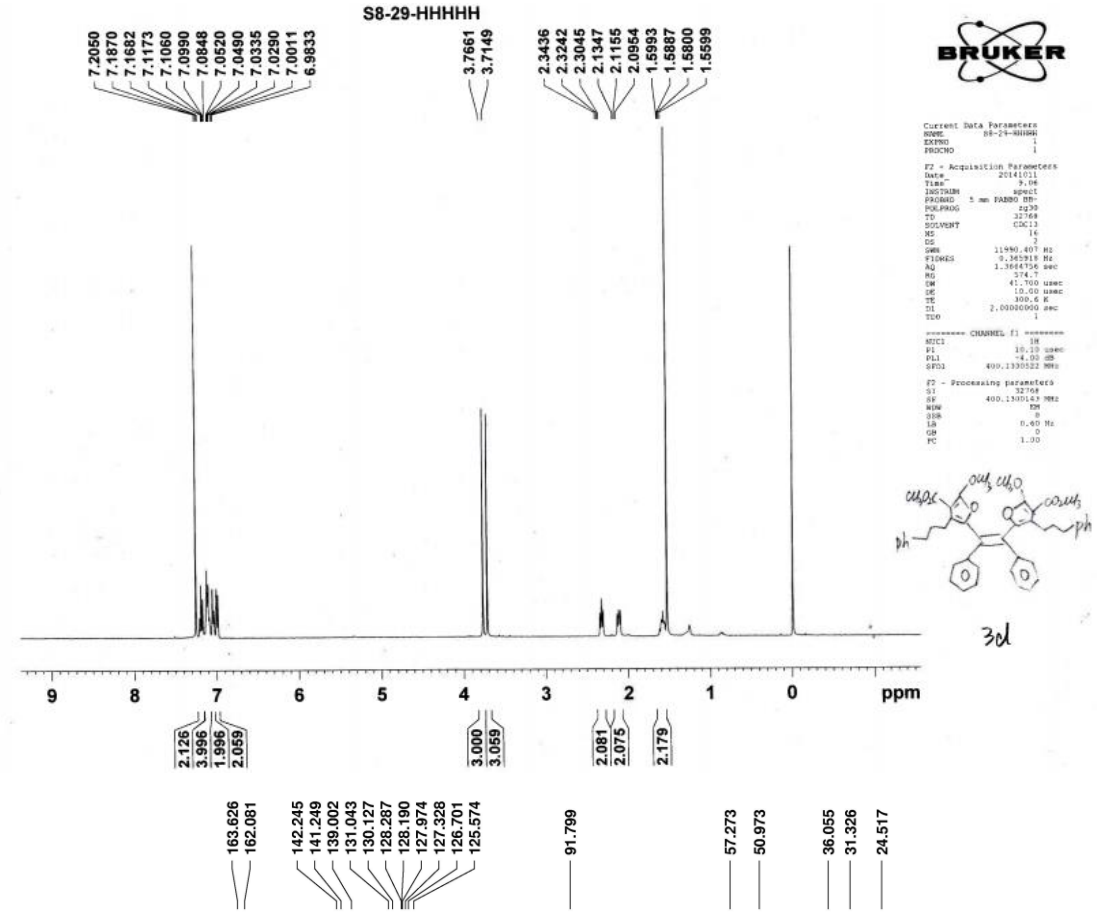
m/z: 656.33 (100.0%), 657.34 (44.1%), 658.34 (11.1%), 659.34 (2.0%)

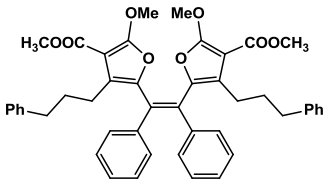
Elemental Analysis: C, 73.15; H, 7.37; O, 19.49




OMe
MeO
H3COOC
COOCH3
O
O
Ph
Ph

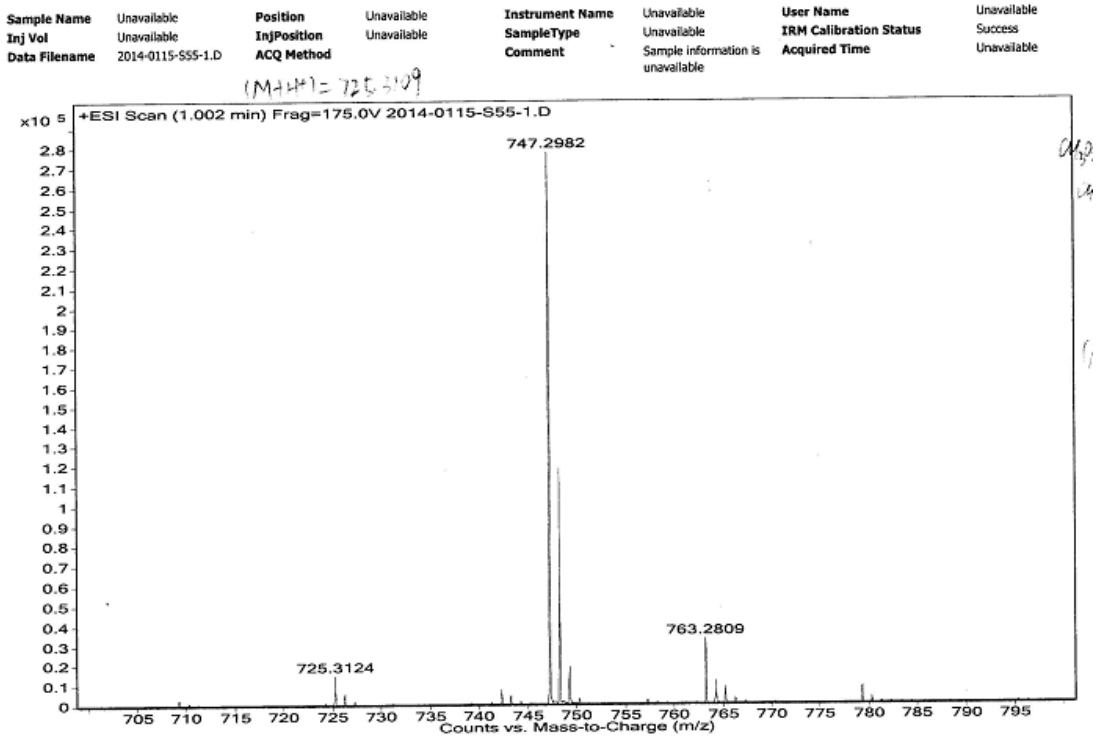
3d

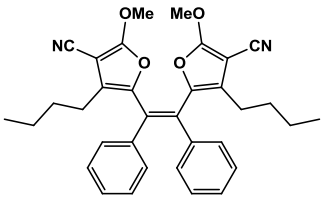

S8-29-HHHHH
7.2050
7.1870
7.1682
7.1173
7.1060
7.0990
7.0848
7.0520
7.0490
7.0335
7.0290
7.0011
6.9833
3.7661
3.7149
2.3436
2.3242
2.3045
2.1347
2.1155
2.0954
1.5993
1.5887
1.5800
1.5599
BRUKER
3d
9
8
7
6
5
4
3
2
1
0
ppm
2.126
3.996
1.996
2.059
3.000
3.059
2.081
2.075
2.179
163.626
162.081
142.245
141.249
139.002
131.043
130.127
128.287
128.190
127.974
127.328
126.701
125.574
91.799
57.273
50.973
36.055
31.326
24.517
200
180
160
140
120
100
80
60
40
20
0
ppm



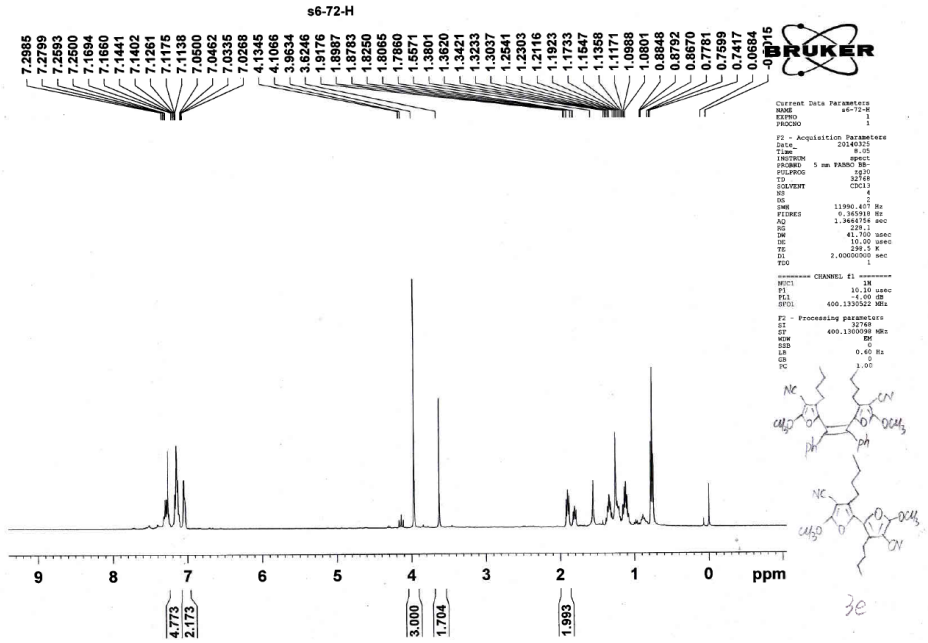
3d

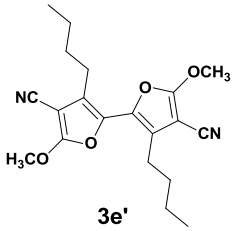
Chemical Formula: $C_{46}H_{44}O_8$
Exact Mass: 724.30
Molecular Weight: 724.84
m/z: 724.30 (100.0%), 725.31 (50.6%), 726.31 (14.2%), 727.31 (2.8%)
Elemental Analysis: C, 76.22; H, 6.12; O, 17.66



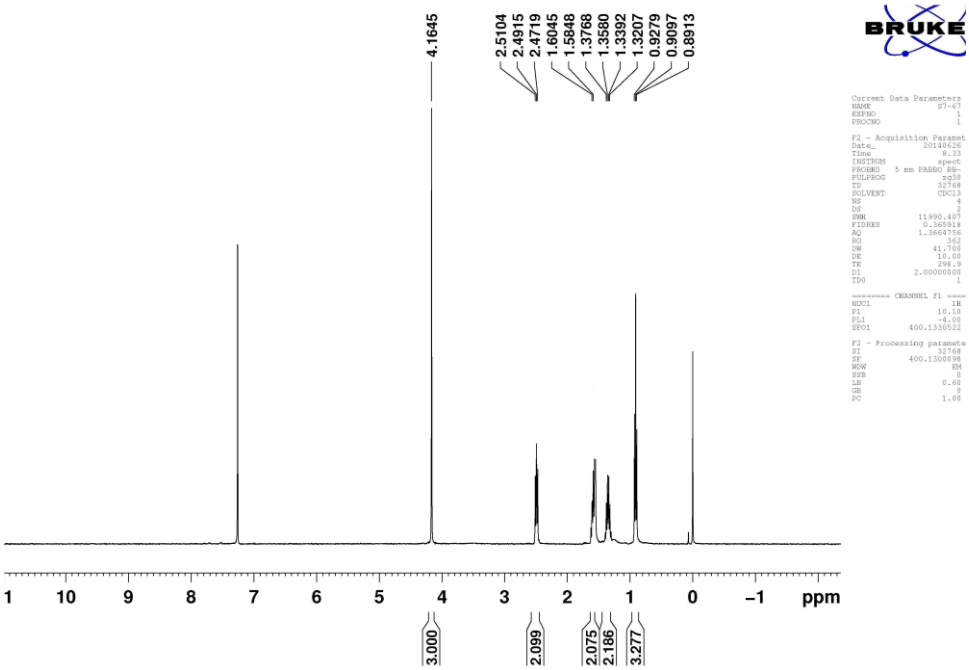

OMe
MeO
NC
CN
O
O

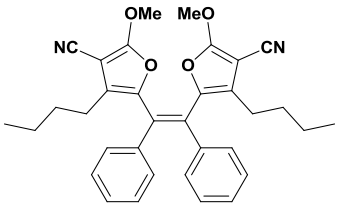
3e


s6-72-H
BRUKER
ppm
4.773
2.173
3.000
1.704
1.993
3e


NC
OCH3
O
CN
H3CO
O

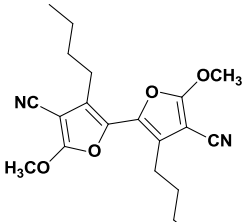
3e'


BRUKER
4.1645
2.5104
2.4915
2.4719
1.6045
1.5848
1.3768
1.3580
1.3392
1.3207
0.9279
0.9097
0.8913
ppm
3.000
2.099
2.075
2.186
3.277



3e

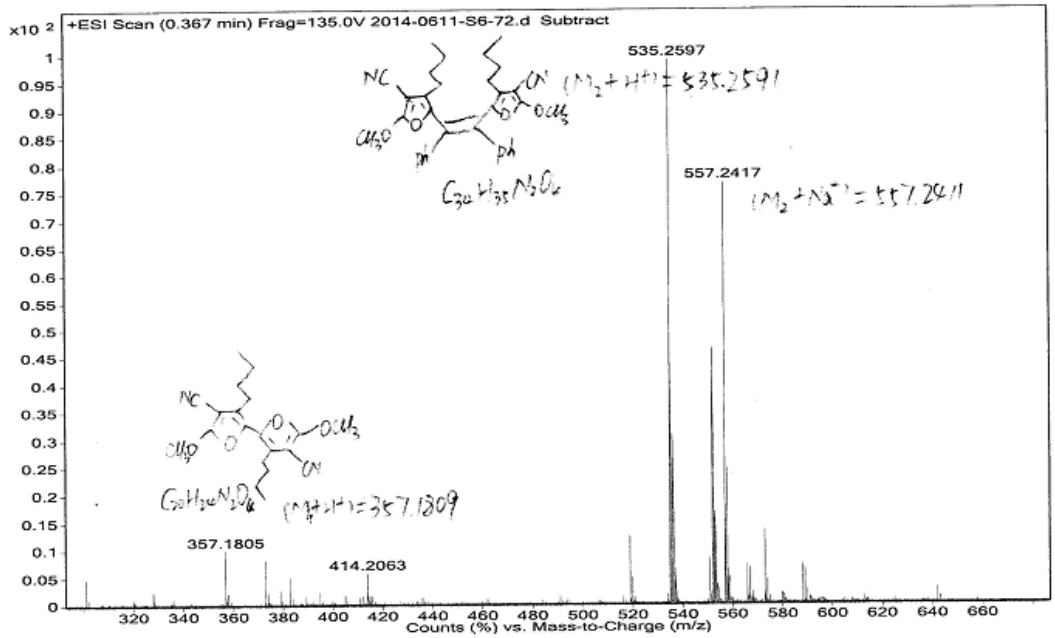
Chemical Formula: $C_{34}H_{34}N_2O_4$
Exact Mass: 534.25
Molecular Weight: 534.64
m/z: 534.25 (100.0%), 535.26 (37.3%), 536.26 (7.6%), 537.26 (1.1%)
Elemental Analysis: C, 76.38; H, 6.41; N, 5.24; O, 11.97

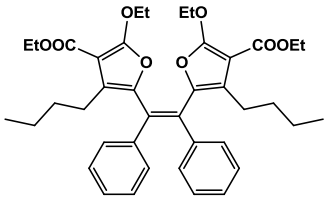


3e'

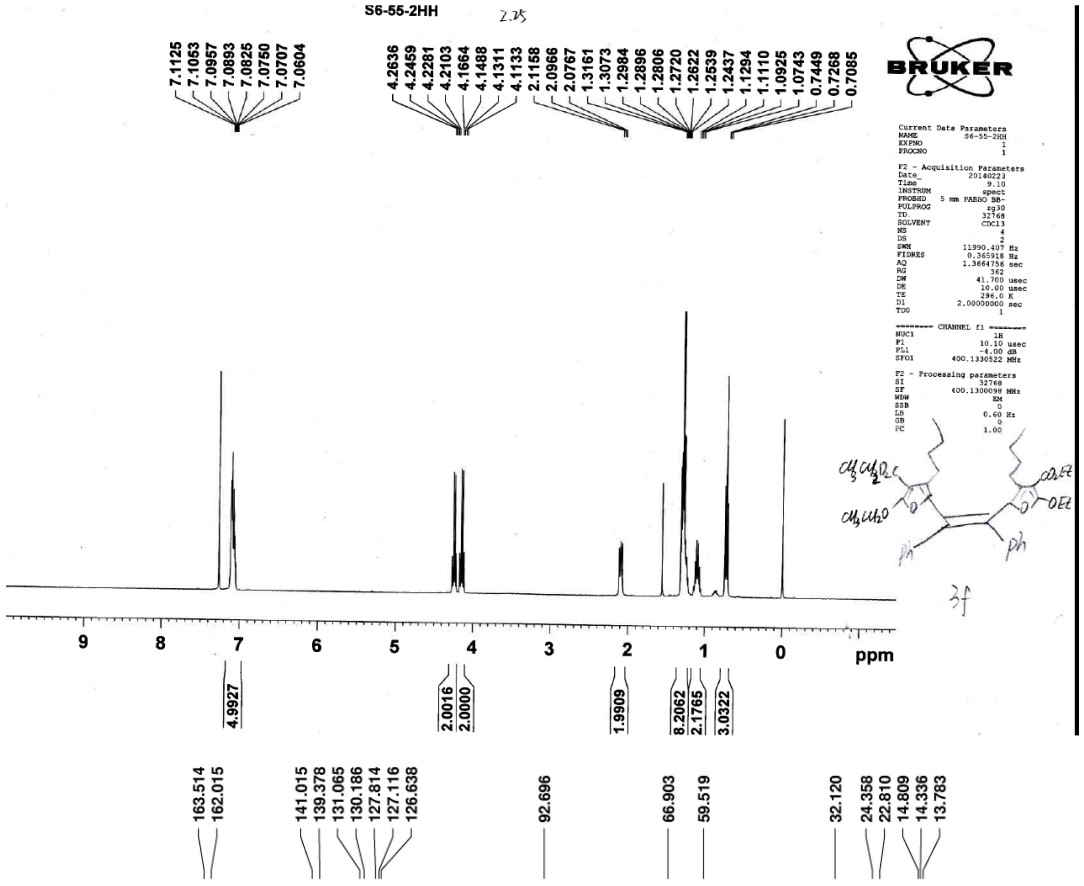
Chemical Formula: $C_{20}H_{24}N_2O_4$
Exact Mass: 356.17
Molecular Weight: 356.42
m/z: 356.17 (100.0%), 357.18 (22.1%), 358.18 (3.1%)
Elemental Analysis: C, 67.40; H, 6.79; N, 7.86; O, 17.96

Sample Name	Unavailable	**Position**	Unavailable	**Instrument Name**	Unavailable	**User Name**	Unavailable
Inj Vol	Unavailable	**InjPosition**	Unavailable	**SampleType**	Unavailable	**IRM Calibration Status**	Success
Data Filename	2014-0611-S6-72.d	**ACQ Method**		**Comment**	Sample information is unavailable	**Acquired Time**	Unavailable

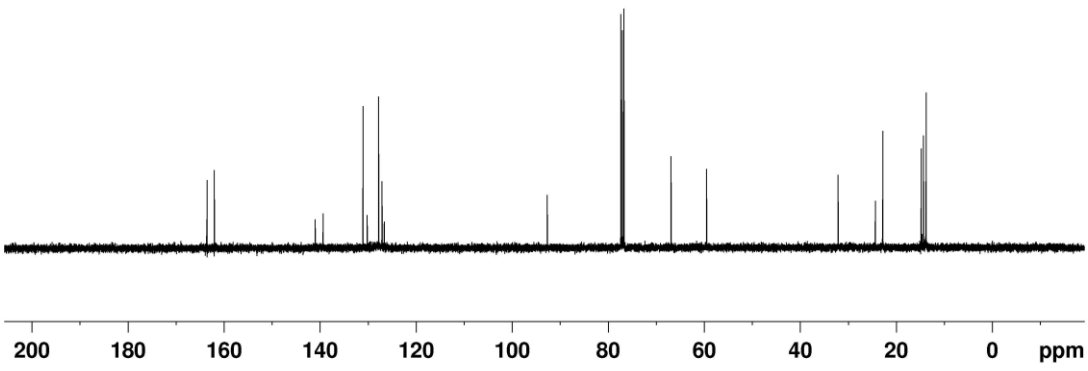


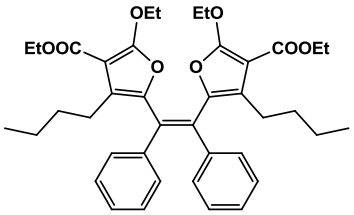

OEt
EtO
EtOOC
COOEt
O
O

3f


S6-55-2HH
7.1125
7.1053
7.0957
7.0893
7.0825
7.0750
7.0707
7.0604
4.2636
4.2459
4.2281
4.2103
4.1664
4.1488
4.1311
4.1133
2.1158
2.0966
2.0767
2.0539
1.2437
1.1294
1.1110
1.0925
1.0743
0.7449
0.7268
0.7085
BRUKER
9
8
7
6
5
4
3
2
1
0
ppm
4.9927
2.0016
2.0000
1.9909
8.2062
2.1765
3.0322

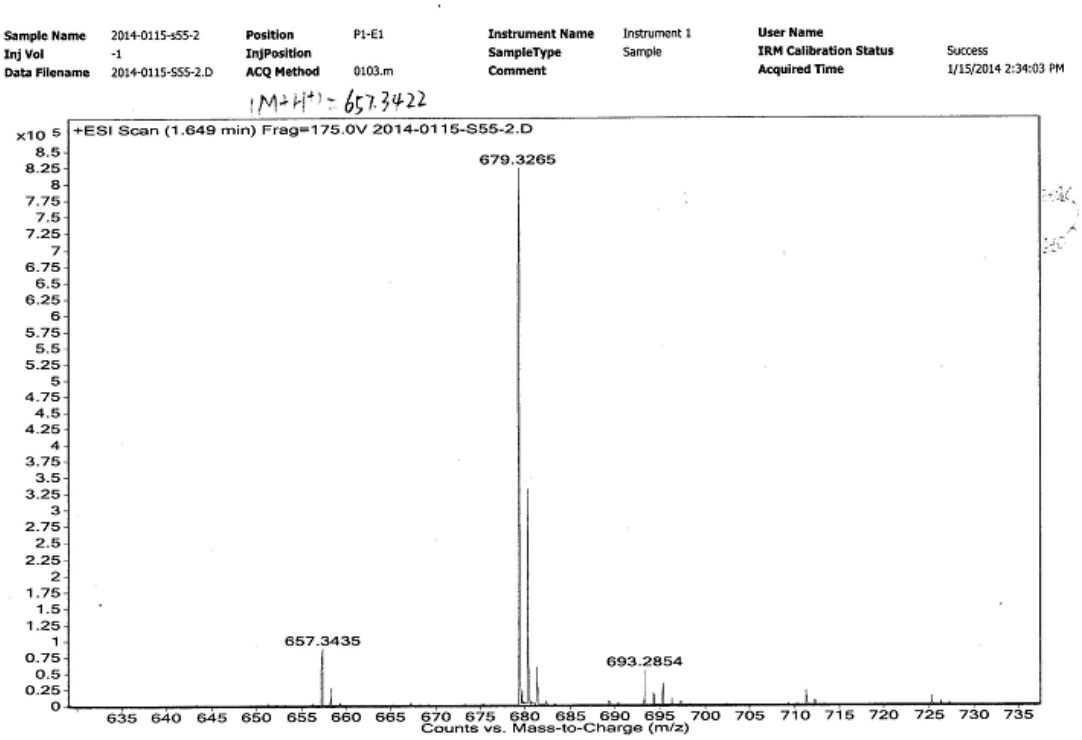
163.514
162.015
141.015
139.378
131.065
130.186
127.814
127.116
126.638
92.696
66.903
59.519
32.120
24.358
22.810
14.809
14.336
13.783

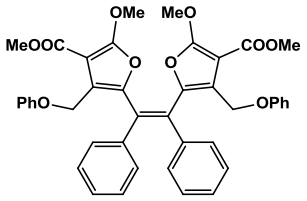

200
180
160
140
120
100
80
60
40
20
0
ppm



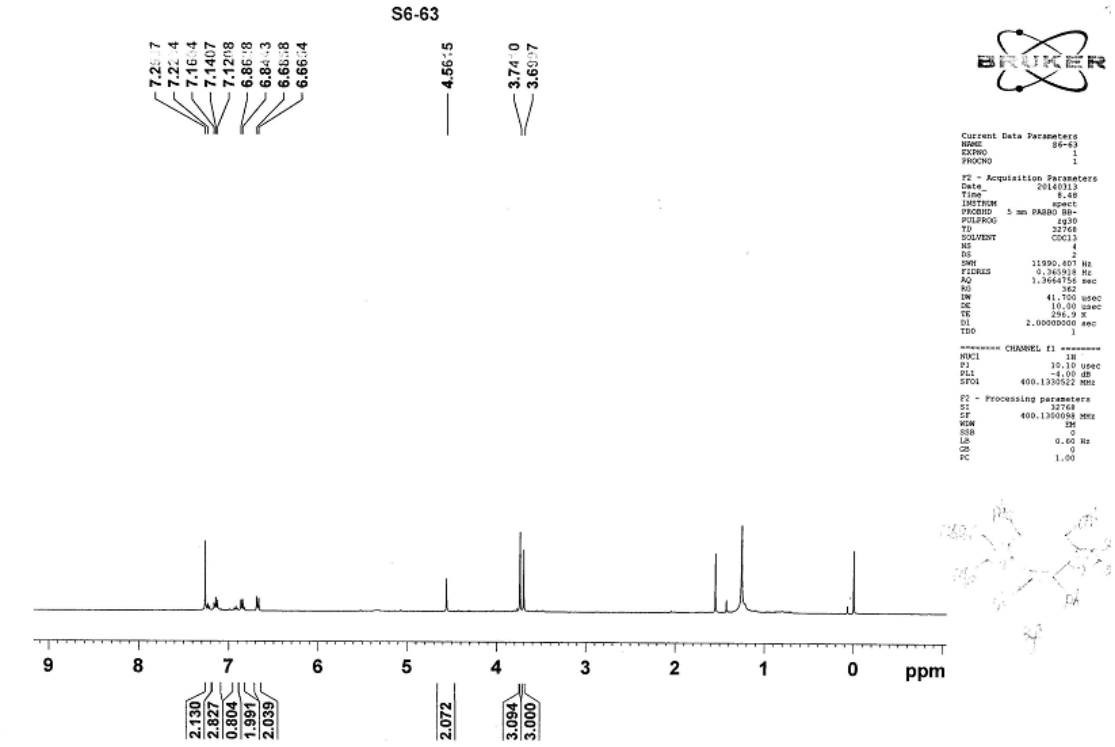
3f

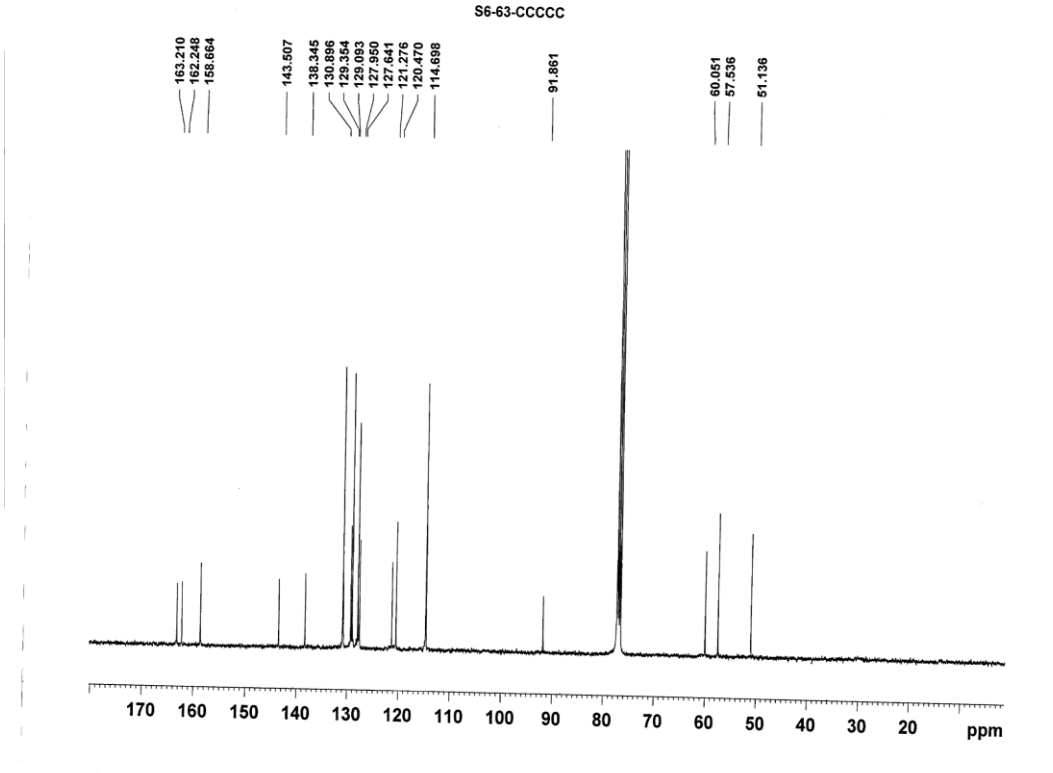
Chemical Formula: $C_{40}H_{48}O_8$
Exact Mass: 656.33
Molecular Weight: 656.80
m/z: 656.33 (100.0%), 657.34 (44.1%), 658.34 (11.1%), 659.34 (2.0%)
Elemental Analysis: C, 73.15; H, 7.37; O, 19.49

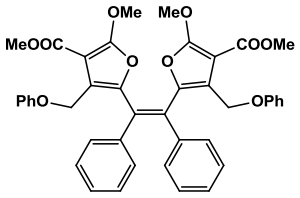



OMe
MeO
MeOOC
COOMe
O
O
PhO
OPh

3g


S6-63
7.2
7.2
7.1
7.14
7.12
6.86
6.84
6.66
6.66
4.56
3.74
3.69
BRUKER
Current Data Parameters
NAME 86-63
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140313
Time 8.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 4
DS 2
SWH 11990.407 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 362
DW 41.700 usec
DE 10.00 usec
TE 296.9 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.10 usec
PL1 -4.00 dB
SFO1 400.1330522 MHz
F2 - Processing parameters
SI 32768
SF 400.1300098 MHz
WDW EM
SSB 0
LB 0.60 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
ppm
2.130
2.827
0.804
1.991
2.039
2.072
3.094
3.000

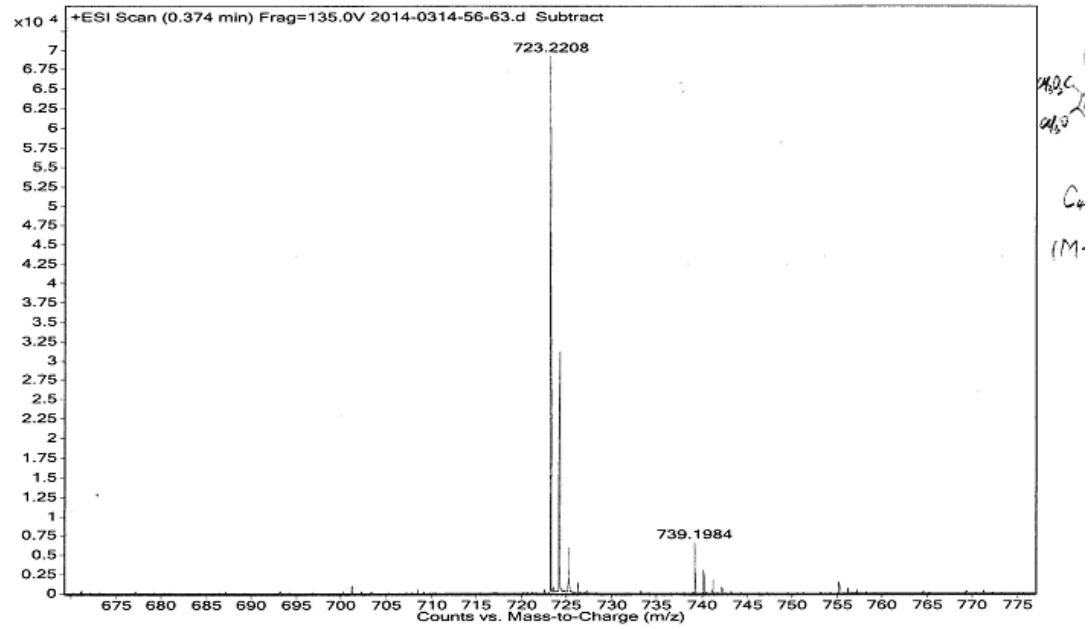

S6-63-CCCCC
163.210
162.248
158.664
143.507
138.345
130.896
129.354
129.093
127.950
127.641
121.276
120.470
114.698
91.861
60.051
57.536
51.136
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

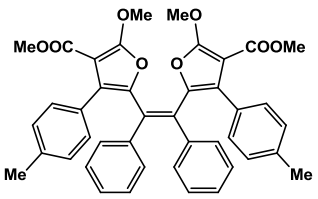


3g

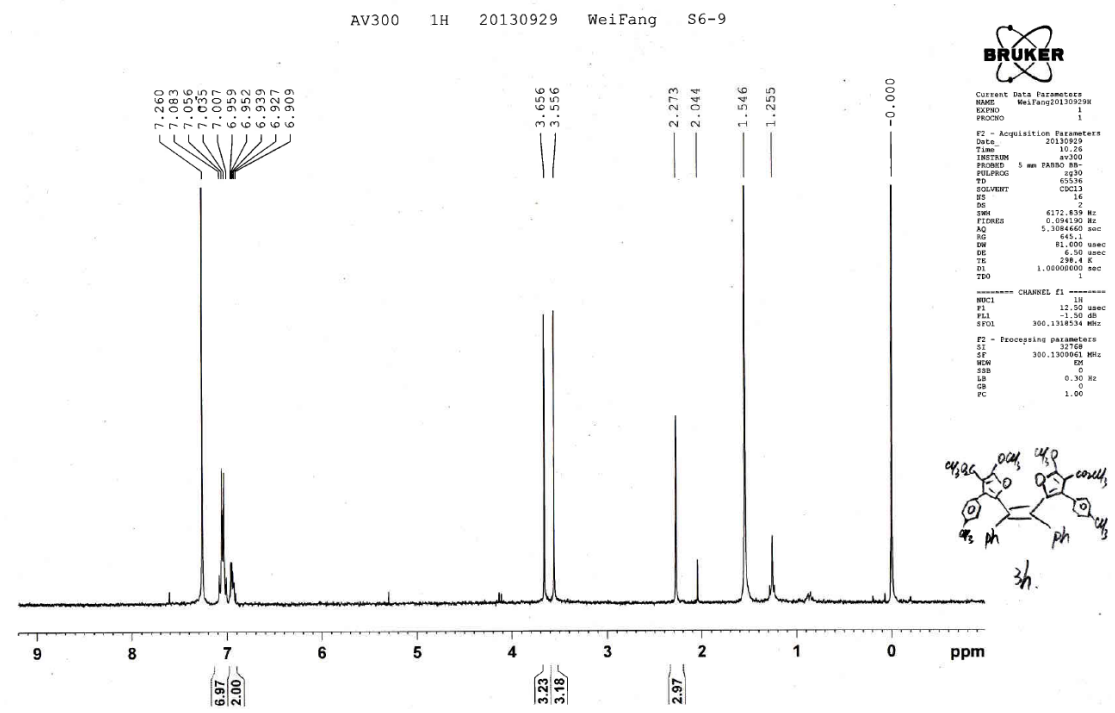
Chemical Formula: $C_{42}H_{36}O_{10}$
Exact Mass: 700.23
Molecular Weight: 700.73
m/z: 700.23 (100.0%), 701.23 (45.4%), 702.24 (12.5%), 703.24 (2.5%)
Elemental Analysis: C, 71.99; H, 5.18; O, 22.83

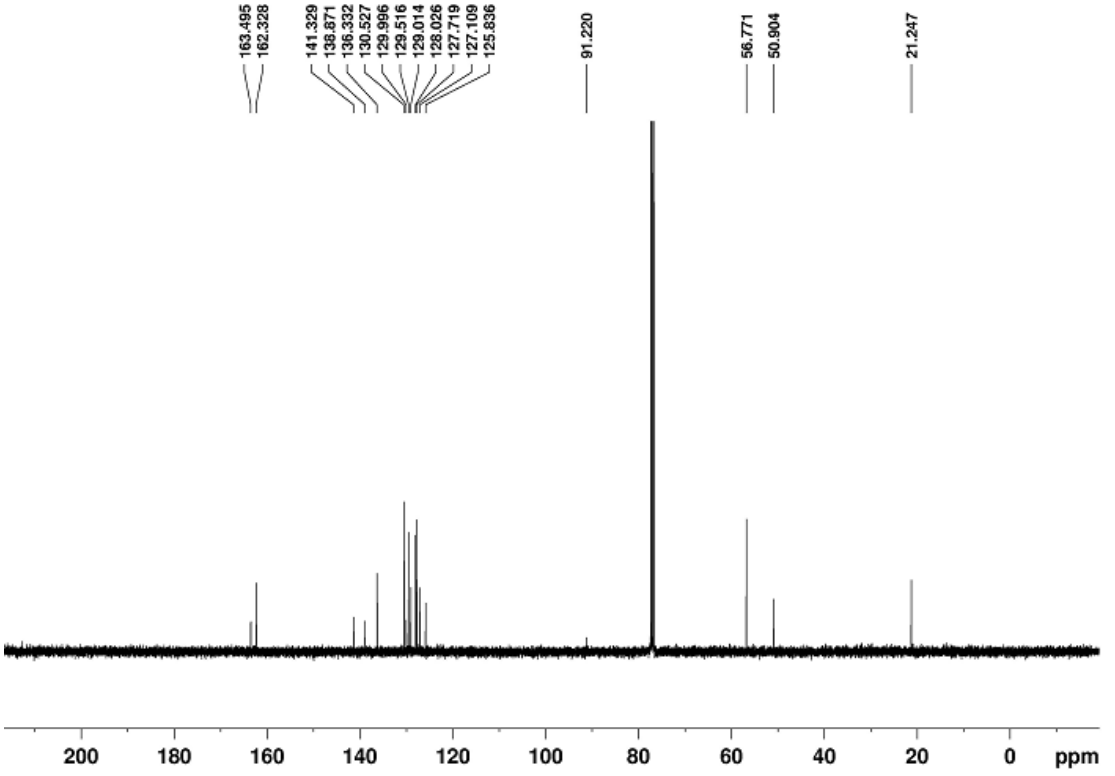
Sample Name	2014-0314-56-63	**Position**	P1-D2	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	2014-0314-56-63.d	**ACQ Method**	0103.m	**Comment**		**Acquired Time**	3/15/2014 10:43:07 AM

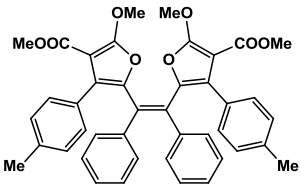



OMe
MeO
MeOOC
COOMe
O
O
Me
Me

3h

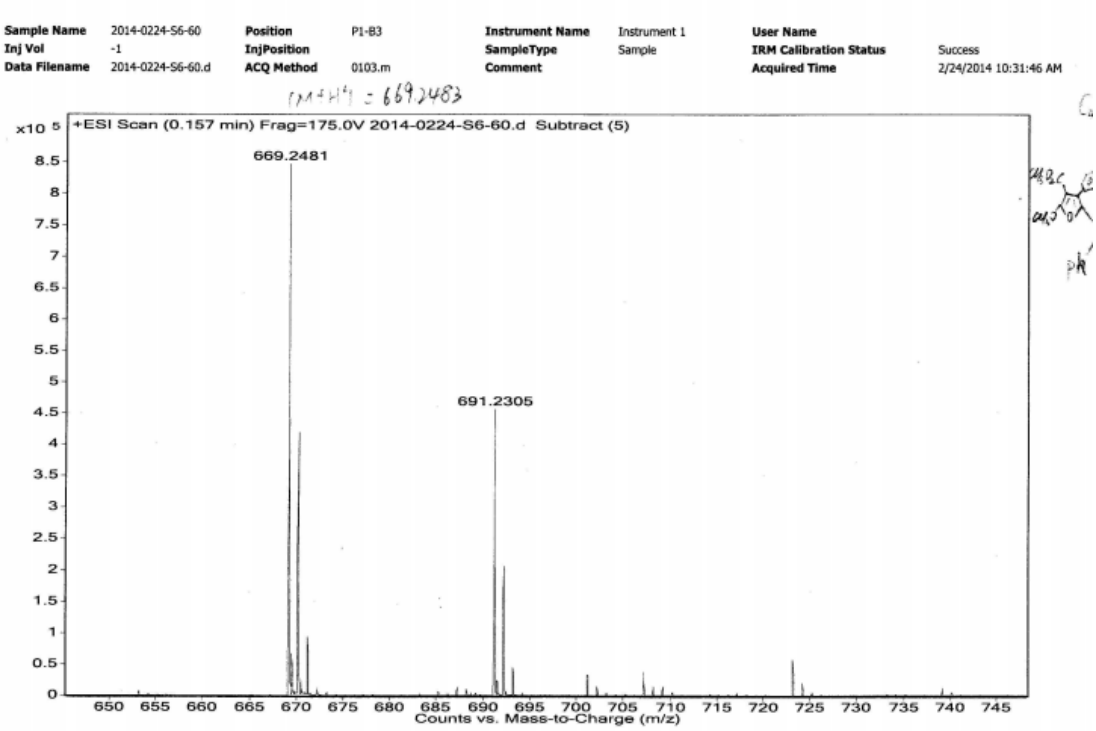

AV300 1H 20130929 WeiFang S6-9
BRUKER
7.260
7.083
7.056
7.035
7.007
6.959
6.952
6.939
6.927
6.909
3.656
3.556
2.273
2.044
1.546
1.255
0.000
9
8
7
6
5
4
3
2
1
0
ppm
6.97
2.00
3.23
3.18
2.97

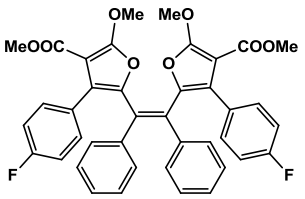

163.495
162.328
141.329
138.871
136.332
130.527
129.996
129.516
129.014
128.026
127.719
127.109
125.836
91.220
56.771
50.904
21.247
200
180
160
140
120
100
80
60
40
20
0
ppm



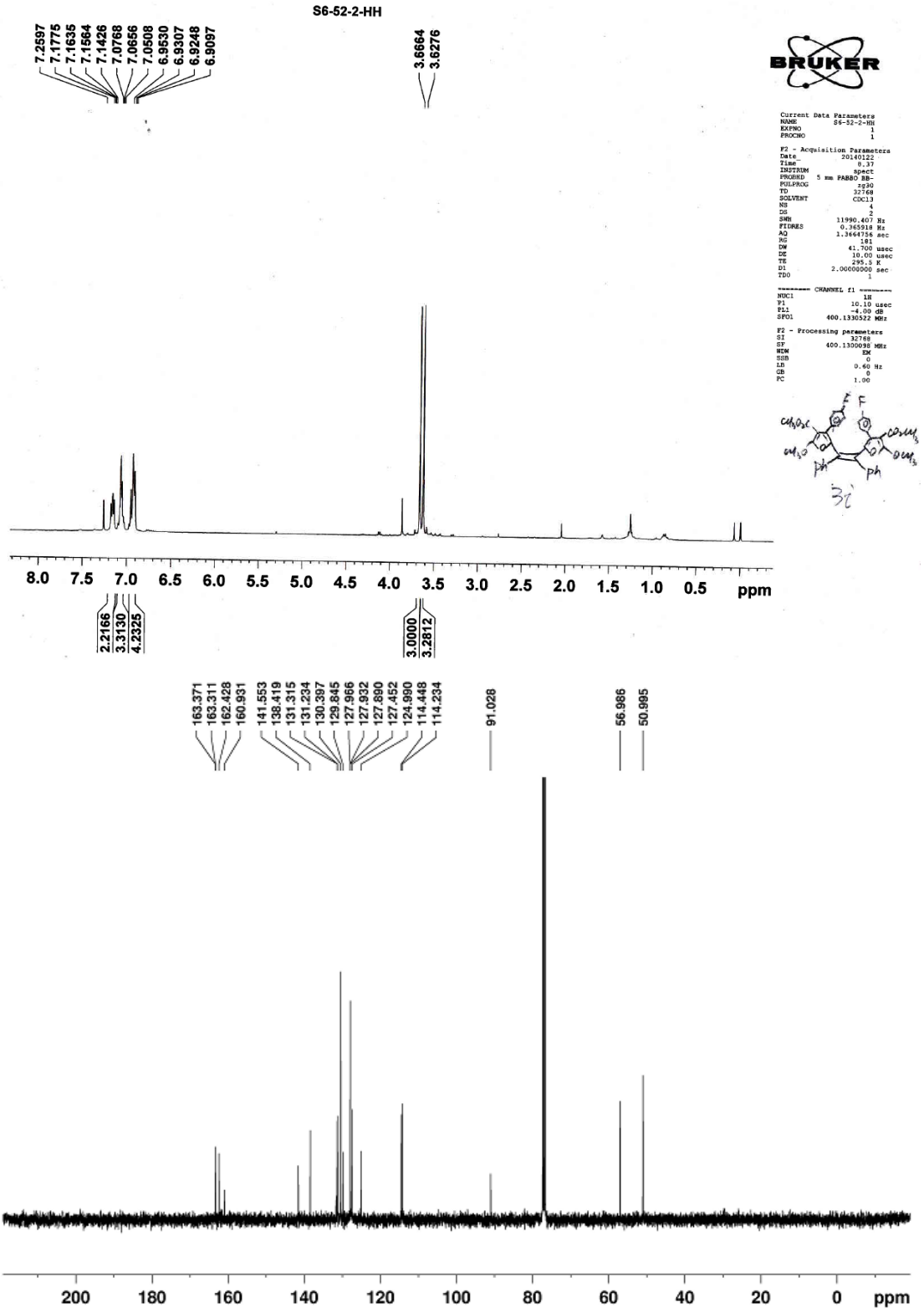
3h

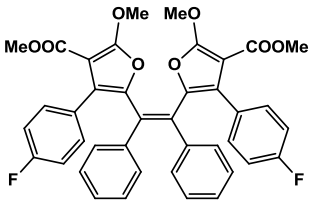
Chemical Formula: $C_{42}H_{36}O_8$
Exact Mass: 668.24
Molecular Weight: 668.73
m/z: 668.24 (100.0%), 669.24 (45.4%), 670.25 (12.0%), 671.25 (2.3%)
Elemental Analysis: C, 75.43; H, 5.43; O, 19.14




OMe
MeO
MeOOC
COOMe
O
O
F
F

3i

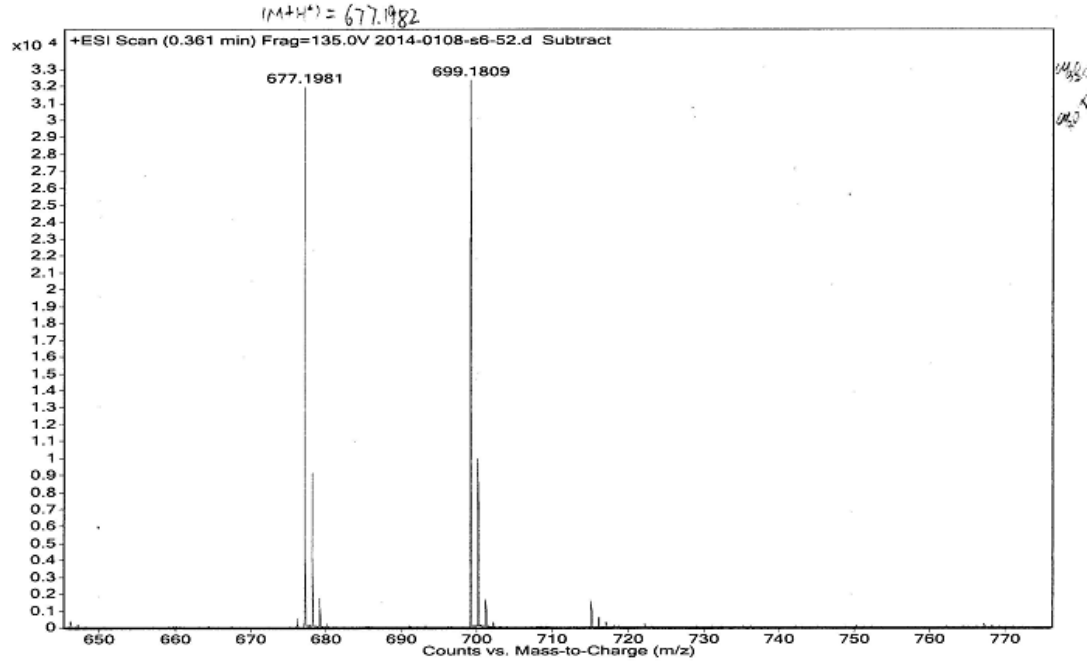

S6-52-2-HH
7.2597
7.1775
7.1635
7.1564
7.1426
7.0768
7.0656
7.0508
6.9530
6.9307
6.9248
6.9097
3.6664
3.6276
BRUKER
Current Data Parameters
NAME S6-52-2-HH
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date 20140122
Time 8.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 4
DS 2
SWH 11990.407 Hz
FIRES 0.365918 Hz
AQ 1.3664756 sec
RG 181
DW 41.700 usec
DE 10.00 usec
TE 295.1 K
D1 2.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 10.10 usec
PL1 -4.00 dB
SFO1 400.1330522 MHz
F2 - Processing parameters
SI 32768
SF 400.1300098 MHz
WDW EM
SSB 0
LB 0.60 Hz
GB 0
PC 1.00
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.2166
3.3130
4.2325
3.0000
3.2812
163.371
163.311
162.428
160.931
141.553
138.419
131.315
131.234
130.397
129.845
127.966
127.932
127.890
127.452
124.990
114.448
114.234
91.028
56.986
50.995
200 180 160 140 120 100 80 60 40 20 0 ppm

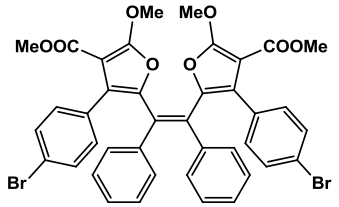


3i

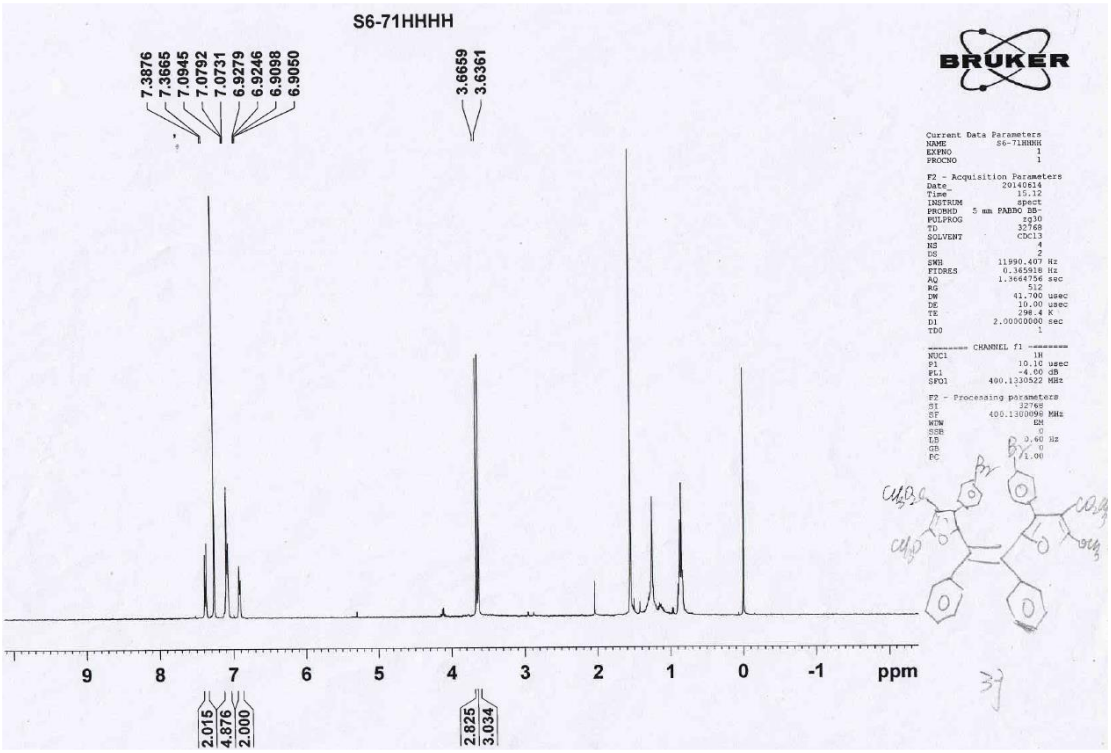
Chemical Formula: $C_{40}H_{30}F_2O_8$
Exact Mass: 676.19
Molecular Weight: 676.66
m/z: 676.19 (100.0%), 677.19 (43.3%), 678.20 (11.1%), 679.20 (2.0%)
Elemental Analysis: C, 71.00; H, 4.47; F, 5.62; O, 18.92

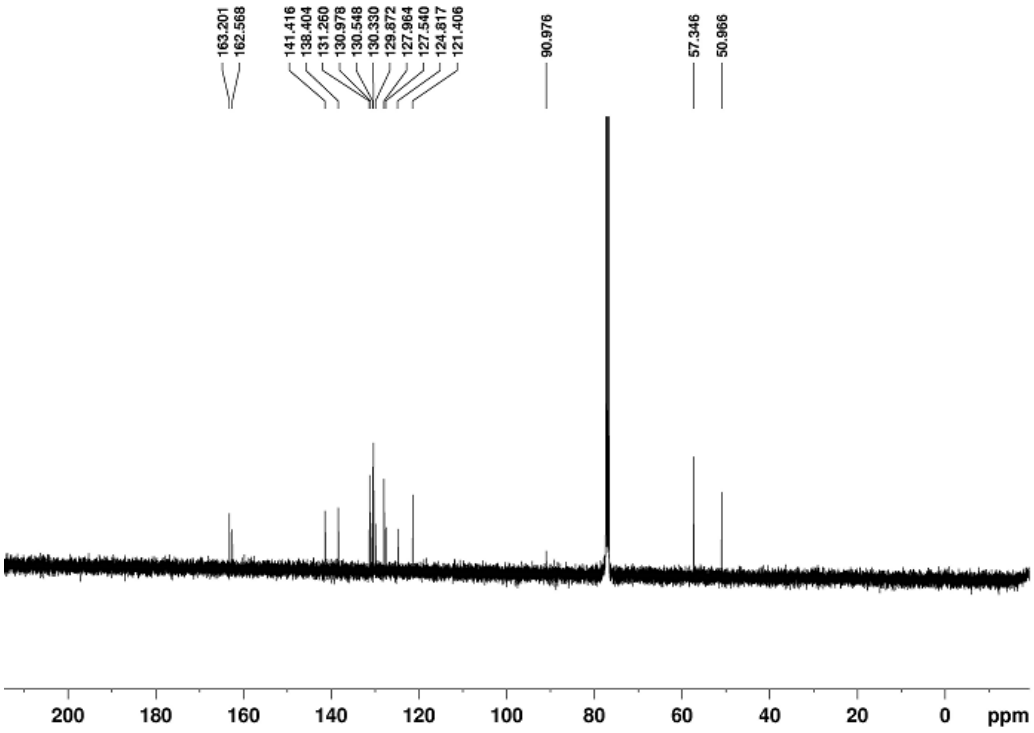
Sample Name	2014-0108-S6-52	**Position**	P1-E7	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	2014-0108-s6-52.d	**ACQ Method**	0103.m	**Comment**		**Acquired Time**	1/8/2014 10:07:41 AM

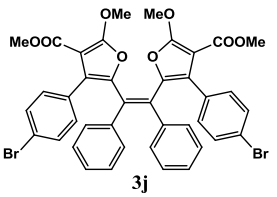



OMe
MeO
MeOOC
COOMe
O
O
Br
Br

3j


S6-71HHHH
7.3876
7.3665
7.0945
7.0792
7.0731
6.9279
6.9246
6.9098
6.9050
3.6659
3.6361
BRUKER
9
8
7
6
5
4
3
2
1
0
-1
ppm
2.015
4.876
2.000
2.825
3.034

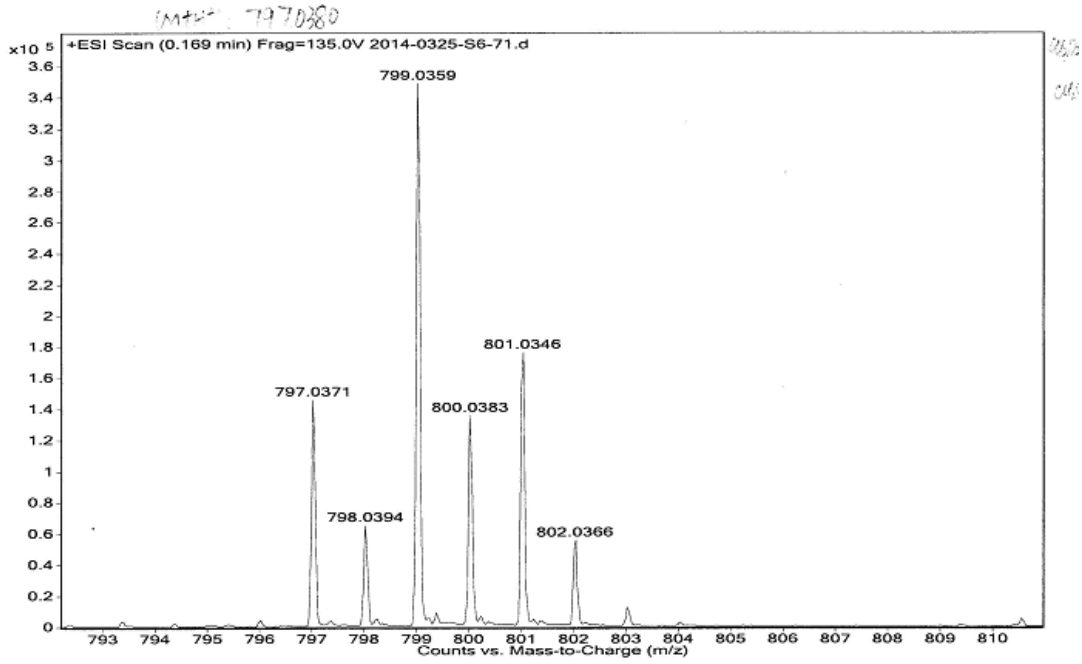

163.201
162.568
141.416
138.404
131.250
130.978
130.548
130.330
129.872
127.964
127.540
124.817
121.406
90.976
57.346
50.966
200
180
160
140
120
100
80
60
40
20
0
ppm

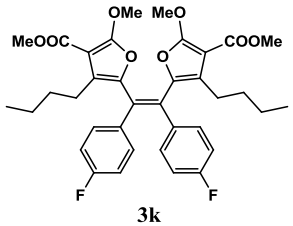


3j

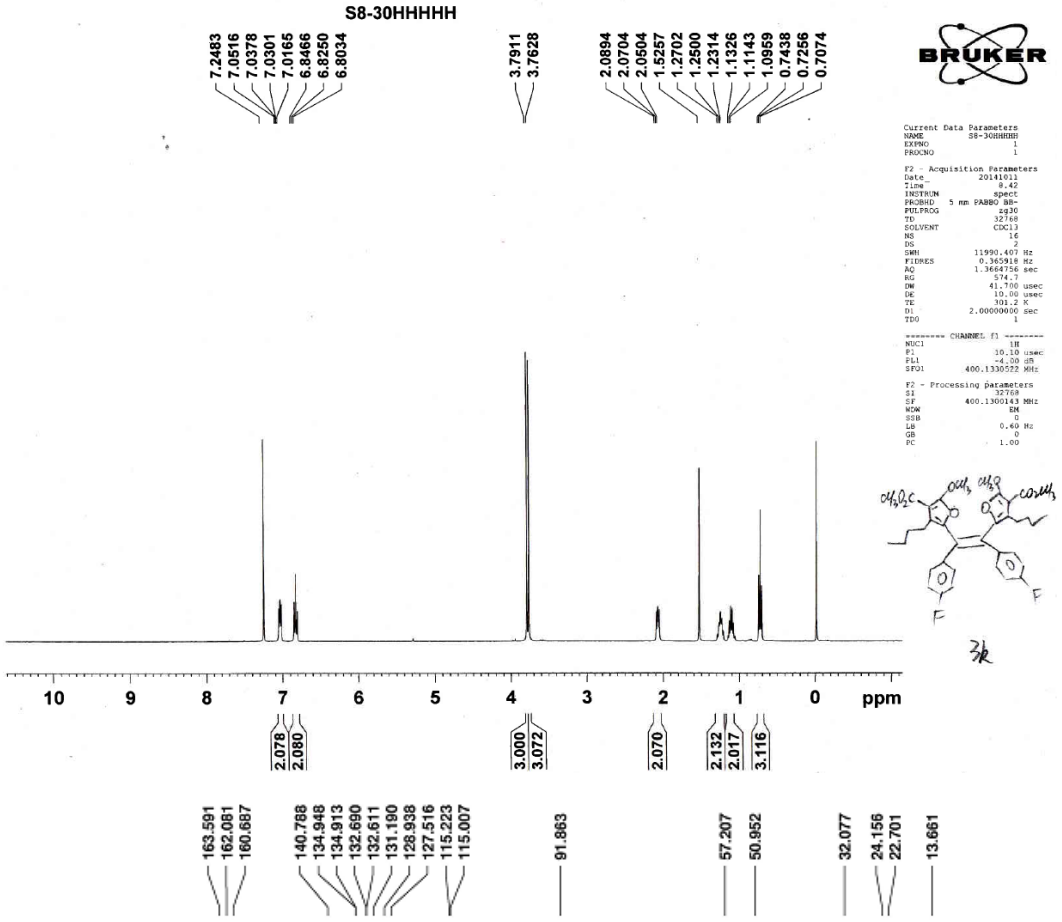
Chemical Formula: $C_{40}H_{30}Br_2O_8$
Exact Mass: 796.03
Molecular Weight: 798.47
m/z: 798.03 (100.0%), 796.03 (51.0%), 800.03 (49.9%), 799.03 (43.5%), 797.03 (22.2%), 801.03 (21.2%), 800.04 (9.5%), 802.03 (5.3%), 798.04 (4.8%), 801.04 (2.0%), 799.04 (1.0%)
Elemental Analysis: C, 60.17; H, 3.79; Br, 20.01; O, 16.03

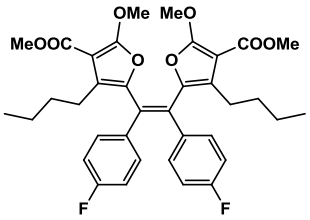
Sample Name	2014-0325-S6-71	**Position**	P1-F4	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	2014-0325-S6-71.d	**ACQ Method**	0103.m	**Comment**		**Acquired Time**	3/26/2014 9:43:31 AM




OMe
MeO
MeOOC
COOMe
O
O
F
F

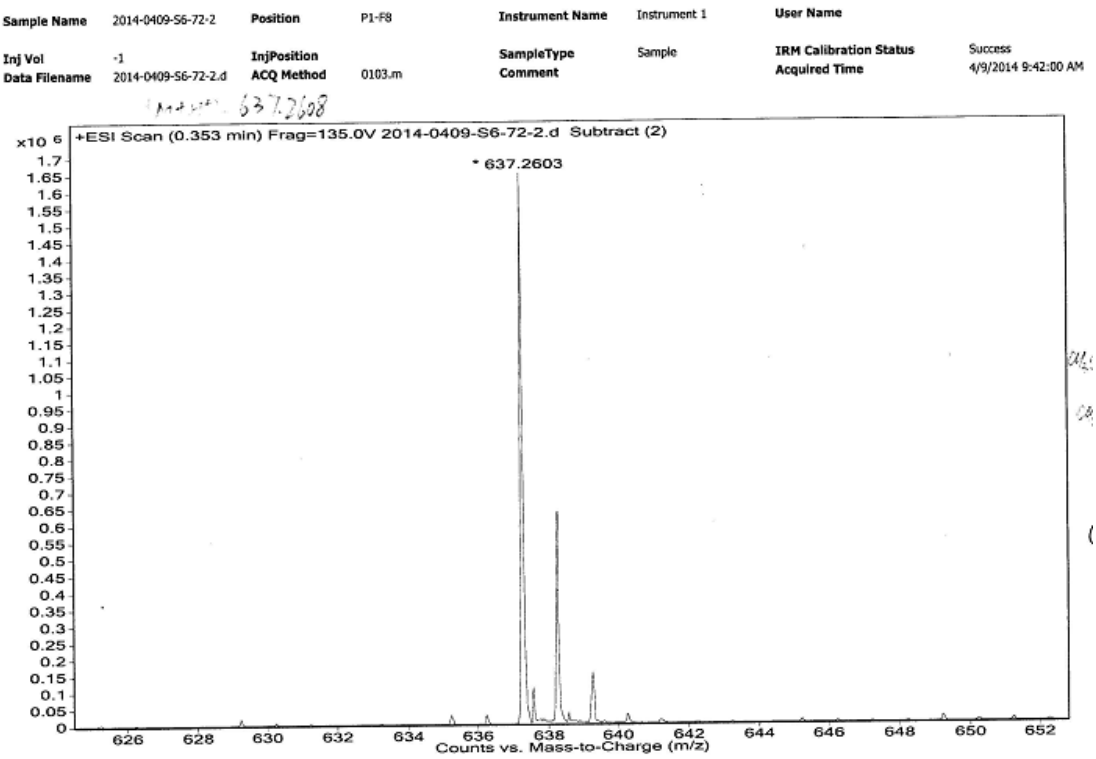
3k

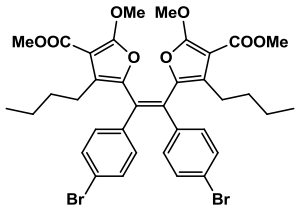

S8-30HHHHH
7.2483
7.0516
7.0378
7.0301
7.0165
6.8466
6.8250
6.8034
3.7911
3.7628
2.0894
2.0704
2.0504
1.5257
1.2702
1.2500
1.2314
1.1326
1.1143
1.0959
0.7438
0.7256
0.7074
BRUKER
Current Data Parameters
NAME S8-30HHHHH
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141011
Time 8.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 11990.407 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 574.7
DW 41.700 usec
DE 10.00 usec
TE 301.2 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.10 usec
PL1 -4.00 dB
SFO1 400.1330522 MHz
F2 - Processing parameters
SI 32768
SF 400.1300143 MHz
WDW EM
SSB 0
LB 0.60 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
2.078
2.080
3.000
3.072
2.070
2.132
2.017
3.116
163.591
162.061
160.687
140.788
134.948
134.913
132.690
132.611
131.190
128.938
127.516
115.223
115.007
91.863
57.207
50.952
32.077
24.156
22.701
13.661
200
180
160
140
120
100
80
60
40
20
0
ppm



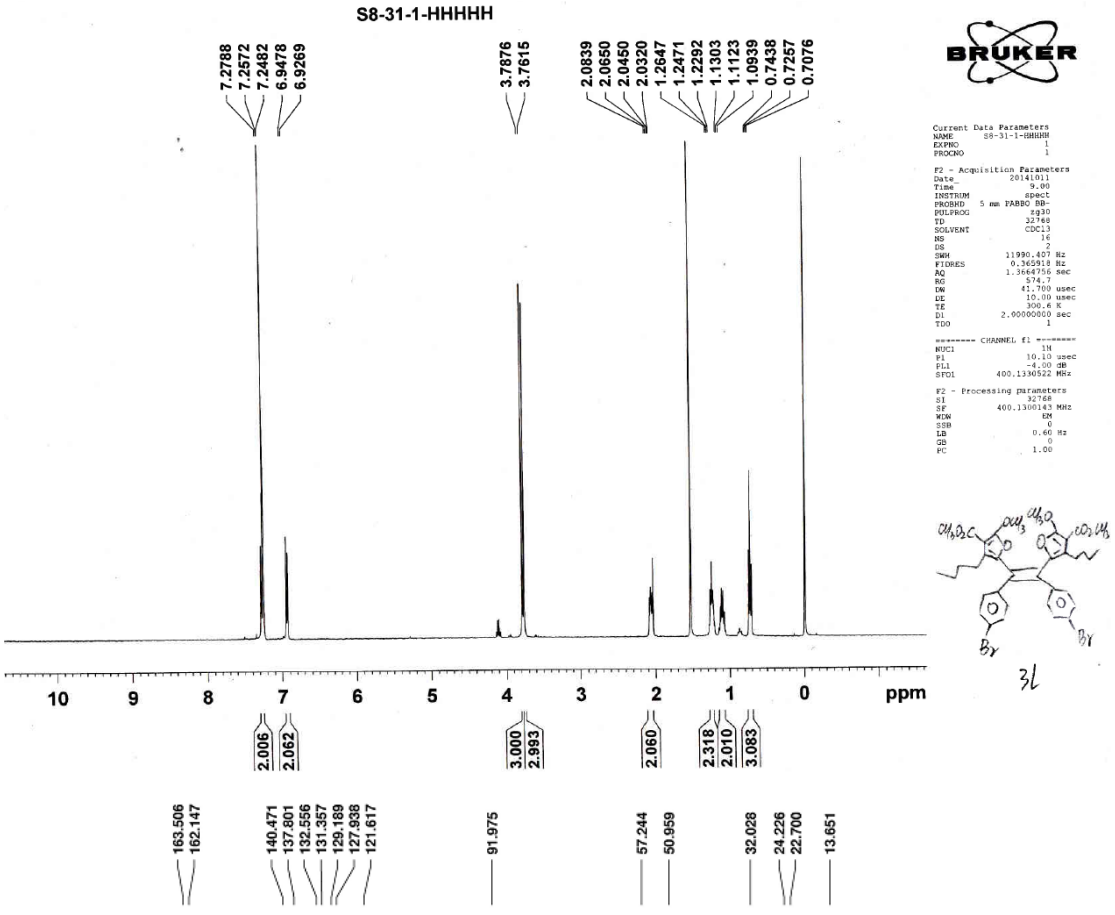
3k

Chemical Formula: $C_{36}H_{38}F_2O_8$
Exact Mass: 636.25
Molecular Weight: 636.68
m/z: 636.25 (100.0%), 637.26 (39.7%), 638.26 (9.3%), 639.26 (1.6%)
Elemental Analysis: C, 67.91; H, 6.02; F, 5.97; O, 20.10

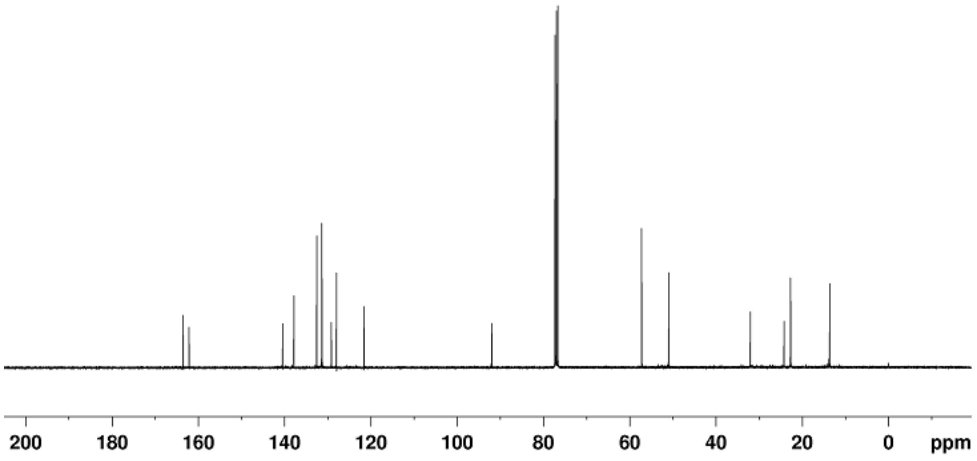


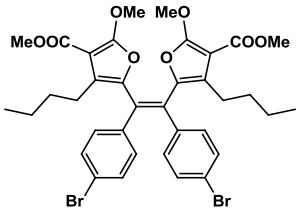

OMe
MeO
MeOOC
COOMe
O
O
Br
Br

3l


S8-31-1-HHHHH
7.2788
7.2572
7.2482
6.9478
6.9269
3.7876
3.7615
2.0839
2.0650
2.0450
2.0320
1.2647
1.2471
1.2292
1.1303
1.1123
1.0939
0.7438
0.7257
0.7076
BRUKER
Current Data Parameters
NAME S8-31-1-HHHHH
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141011
Time 9.00
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 11990.407 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 574.7
DW 41.700 usec
DE 10.00 usec
TE 300.6 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.10 usec
PL1 -4.00 dB
SFO1 400.1330522 MHz
F2 - Processing parameters
SI 32768
SF 400.1300143 MHz
WDW EM
SSB 0
LB 0.60 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
2.006
2.062
3.000
2.993
2.060
2.318
2.010
3.083
3l

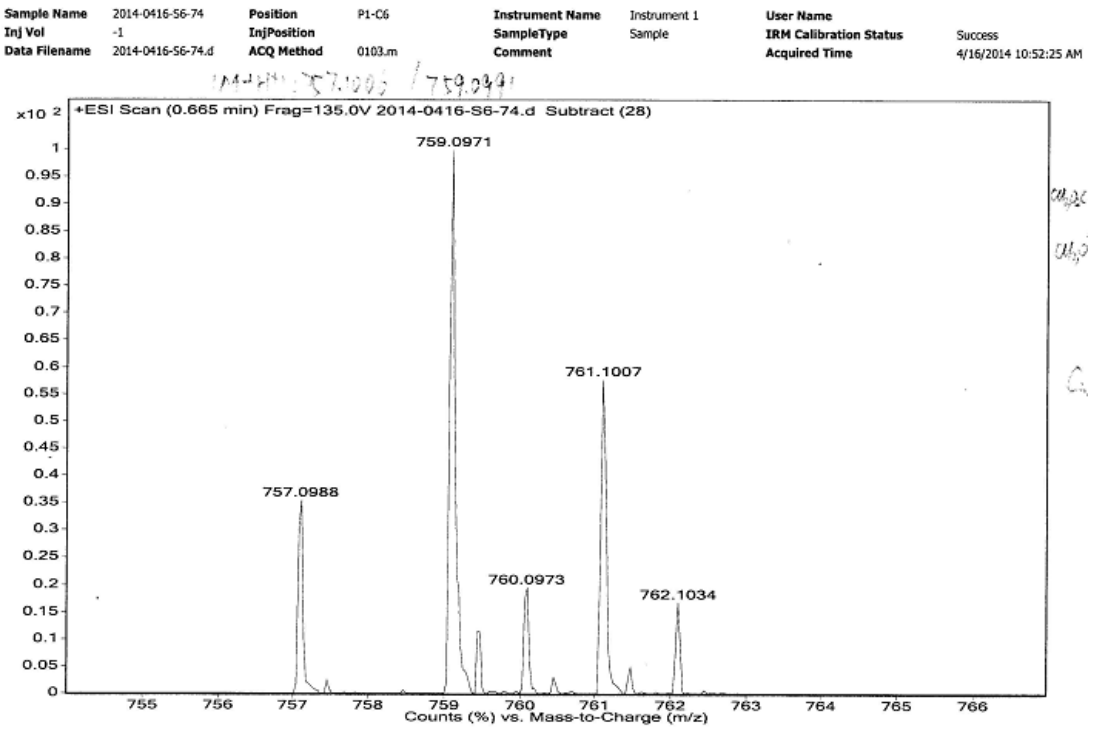
163.506
162.147
140.471
137.801
132.556
131.357
129.189
127.938
121.617
91.975
57.244
50.959
32.028
24.226
22.700
13.651

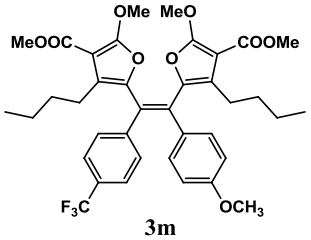

200
180
160
140
120
100
80
60
40
20
0
ppm



3l

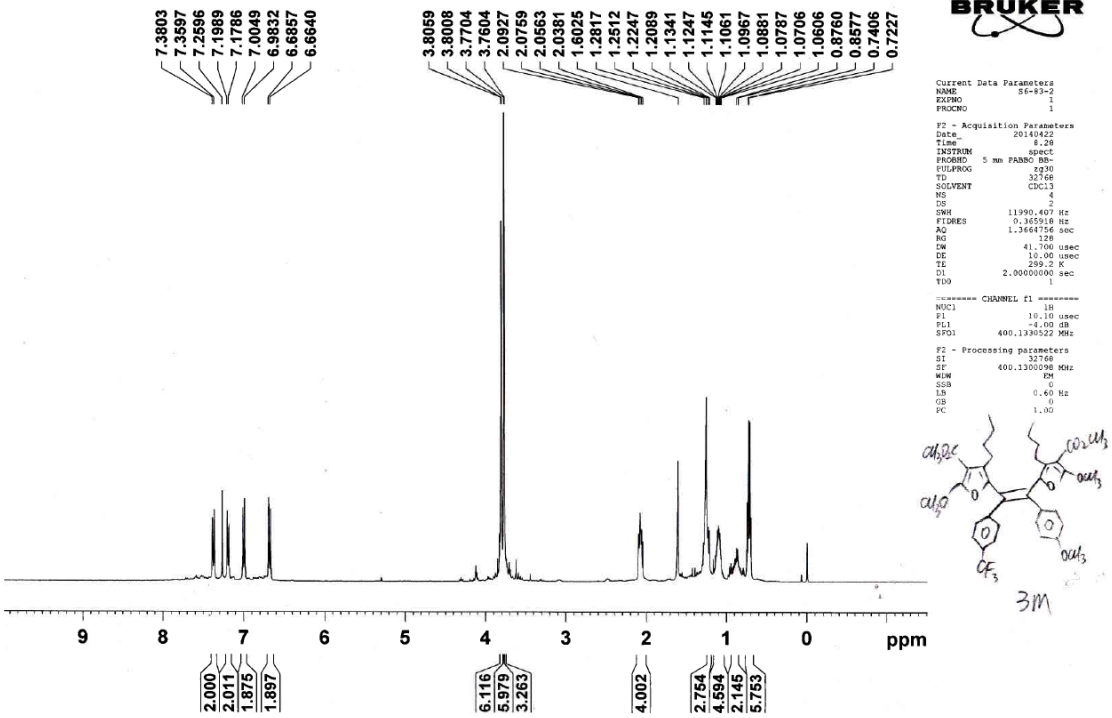
Chemical Formula: $C_{36}H_{38}Br_2O_8$
Exact Mass: 756.09
Molecular Weight: 758.49
m/z: 758.09 (100.0%), 756.09 (51.4%), 760.09 (48.6%), 759.09 (38.9%), 757.10 (20.4%), 761.09 (19.1%), 760.10 (9.4%), 758.10 (4.8%), 762.10 (3.9%), 761.10 (1.8%), 759.10 (1.6%)
Elemental Analysis: C, 57.01; H, 5.05; Br, 21.07; O, 16.87



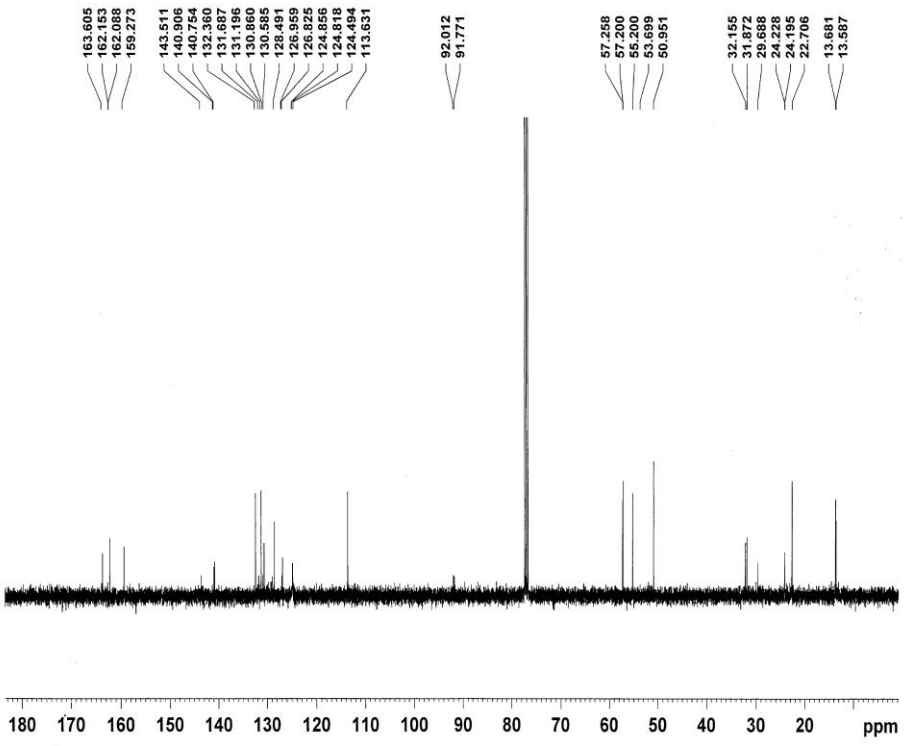


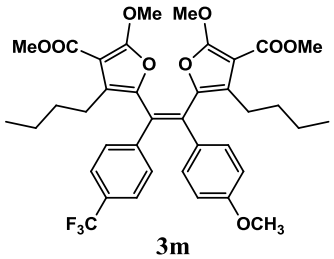
3m

S6-83-2



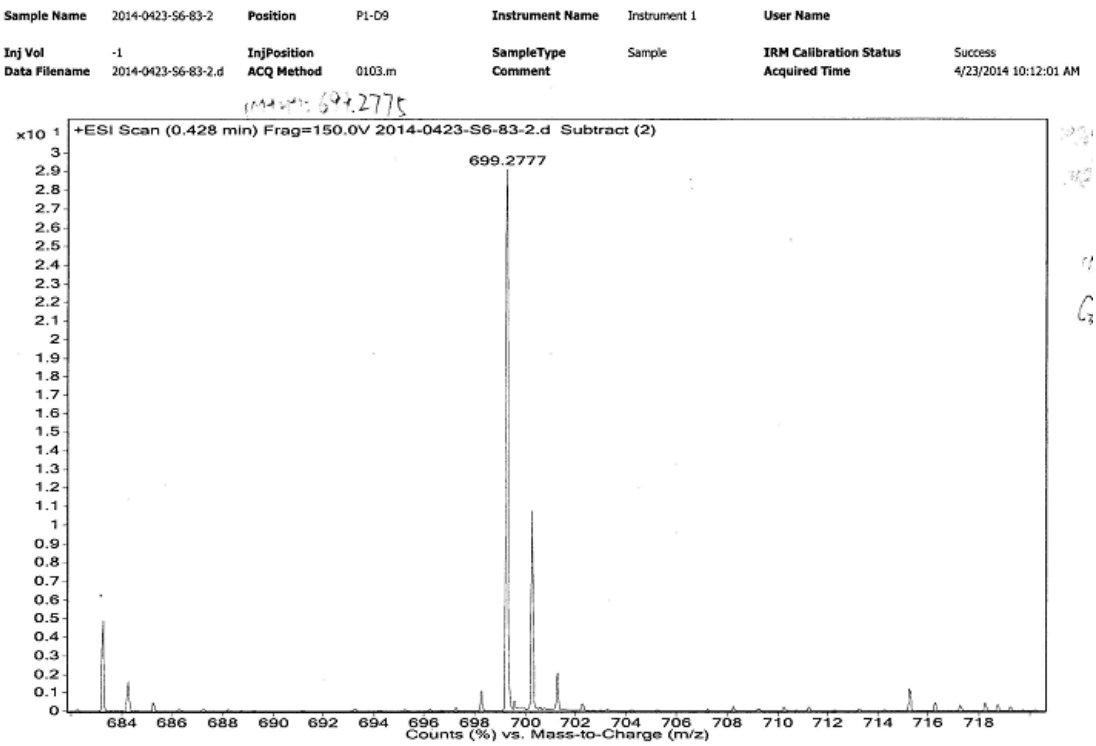
S6-83-2-C13

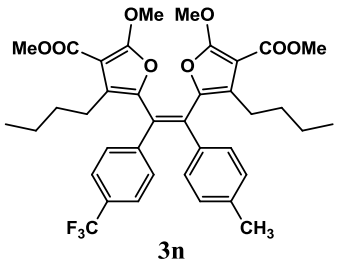




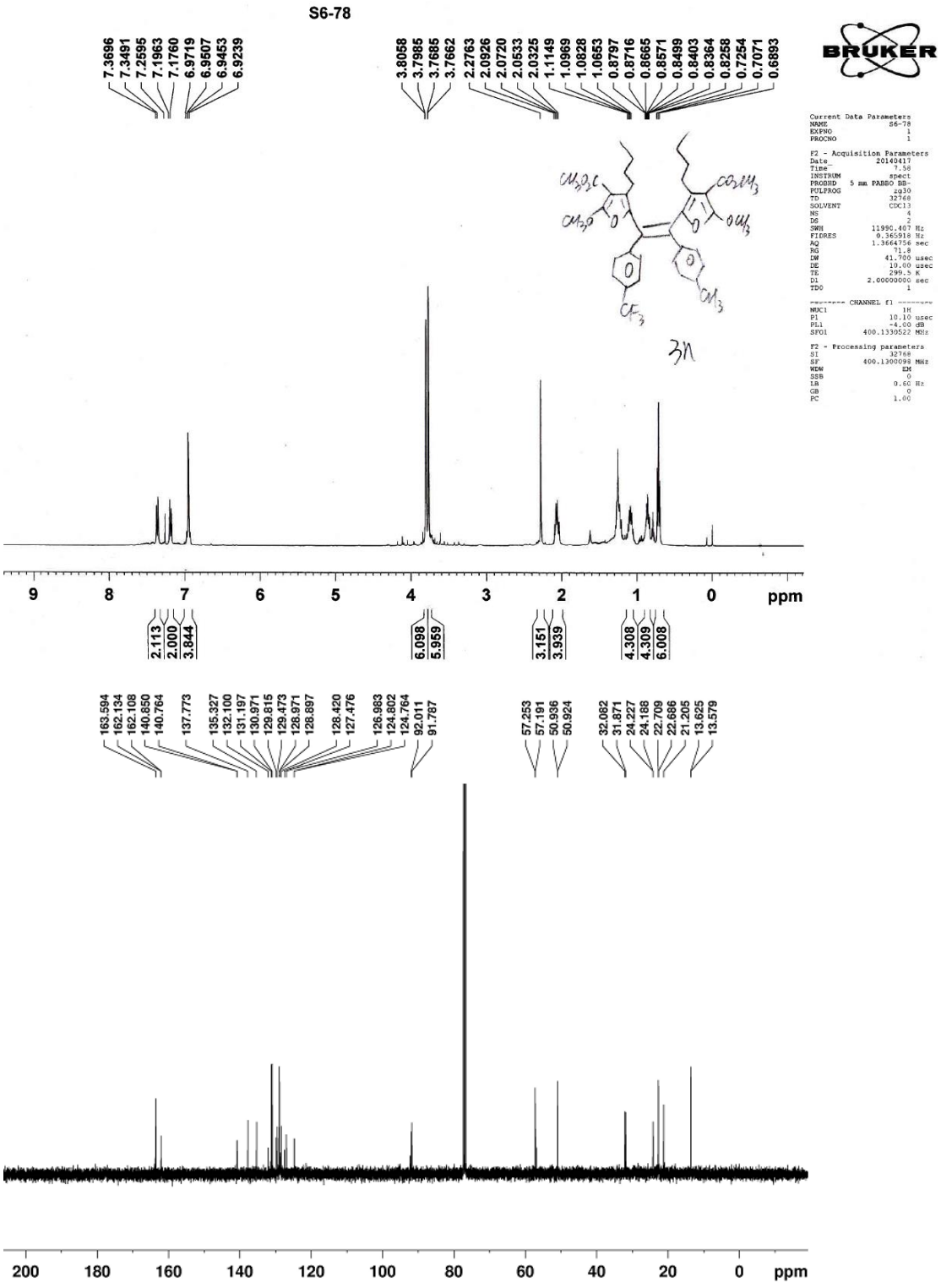
3m

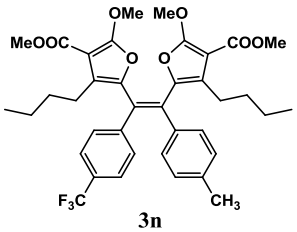
Chemical Formula: $C_{38}H_{41}F_3O_9$
Exact Mass: 698.27
Molecular Weight: 698.72
m/z: 698.27 (100.0%), 699.27 (41.4%), 700.28 (8.6%), 701.28 (1.9%), 700.27 (1.8%)
Elemental Analysis: C, 65.32; H, 5.91; F, 8.16; O, 20.61




OMe
MeO
MeOOC
COOMe
O
O
F3C
CH3

3n

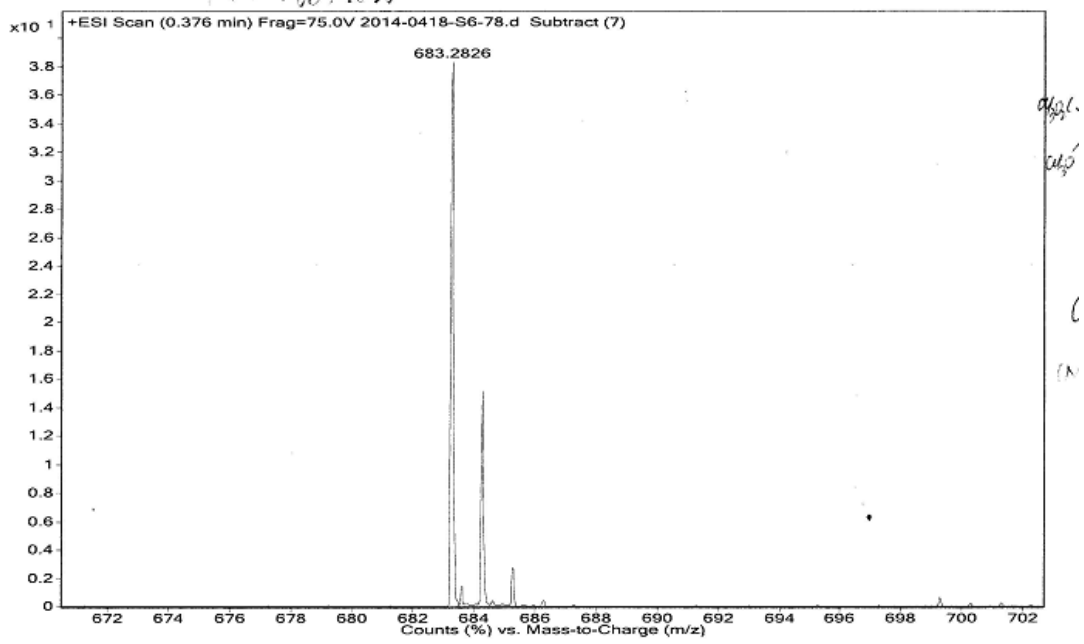

S6-78
7.3696
7.3491
7.2595
7.1963
7.1760
6.9719
6.9507
6.9453
6.9239
3.8058
3.7985
3.7685
3.7662
2.2763
2.0926
2.0720
2.0533
2.0325
1.1149
1.0969
1.0828
1.0653
0.8797
0.8716
0.8665
0.8571
0.8499
0.8403
0.8364
0.8258
0.7254
0.7071
0.6893
BRUKER
Current Data Parameters
NAME S6-78
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140417
Time 7.56
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 4
DS 2
SWH 11990.407 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 71.8
DW 41.700 usec
DE 10.00 usec
TE 299.5 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.10 usec
PL1 -4.00 dB
SFO1 400.1330522 MHz
F2 - Processing parameters
SI 32768
SF 400.1300098 MHz
WDW EM
SSB 0
LB 0.60 Hz
GB 0
PC 1.00
3n
9
8
7
6
5
4
3
2
1
0
ppm
2.113
2.000
3.844
6.098
5.959
3.151
3.939
4.308
4.309
6.008
163.594
162.134
162.108
140.850
140.764
137.773
135.327
132.100
131.197
130.971
129.815
129.473
128.971
128.897
128.420
127.476
126.983
124.802
124.764
92.011
91.787
57.253
57.191
50.936
50.924
32.082
31.871
24.227
24.188
22.709
22.686
21.205
13.625
13.579
200
180
160
140
120
100
80
60
40
20
0
ppm

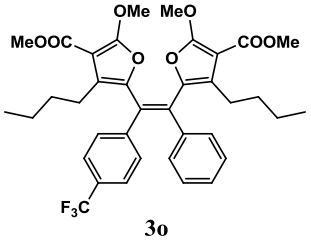


3n

Chemical Formula: $C_{38}H_{41}F_3O_8$
Exact Mass: 682.28
Molecular Weight: 682.72
m/z: 682.28 (100.0%), 683.28 (41.9%), 684.28 (10.2%), 685.29 (1.1%)
Elemental Analysis: C, 66.85; H, 6.05; F, 8.35; O, 18.75

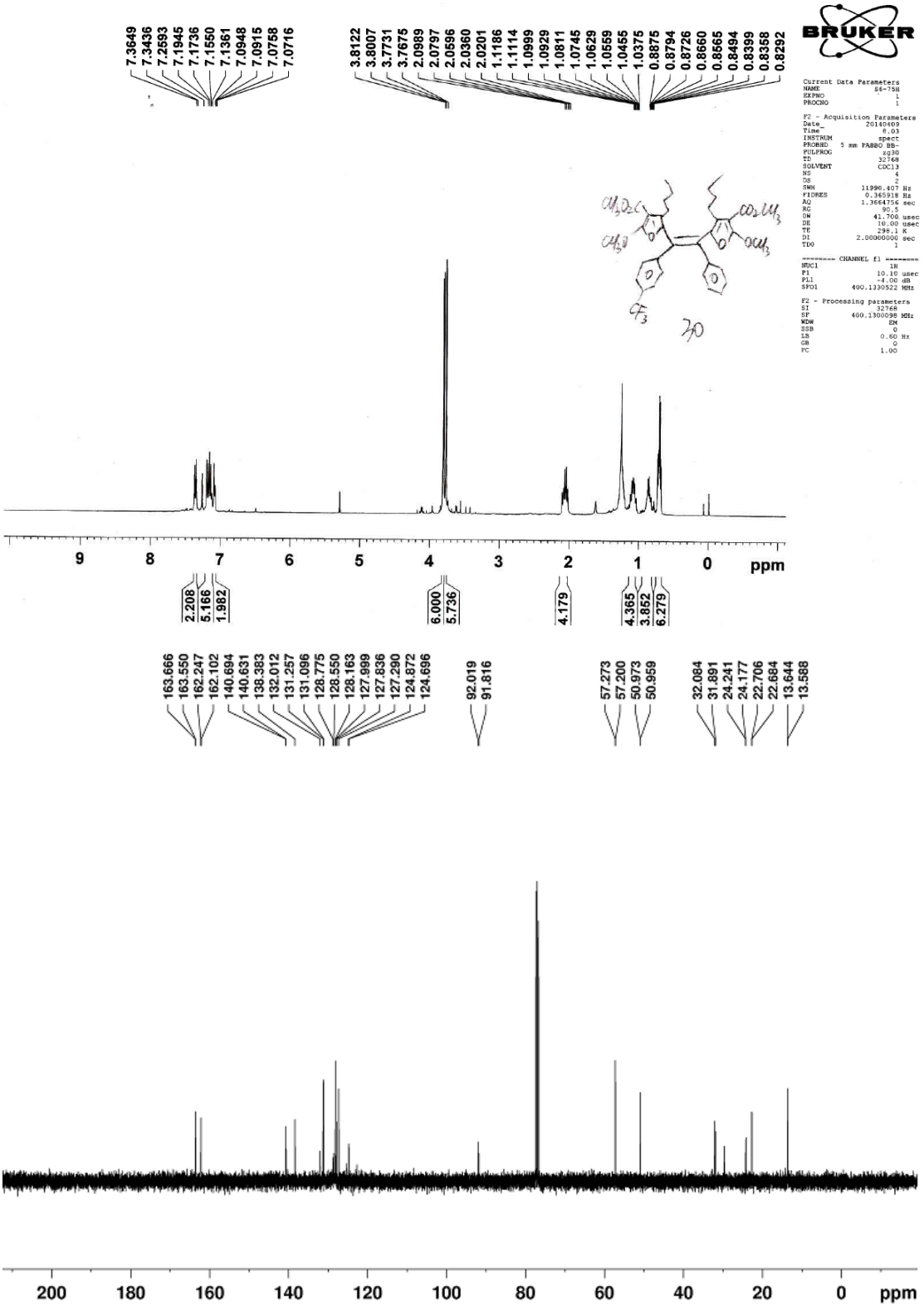
Sample Name	2014-0418-S6-78	**Position**	P1-E9	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	2014-0418-S6-78.d	**ACQ Method**	0103.m	**Comment**		**Acquired Time**	4/18/2014 9:43:04 AM

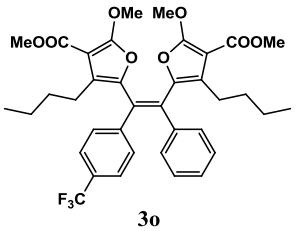



OMe MeO
MeOOC
COOMe
O
O
F3C

3o

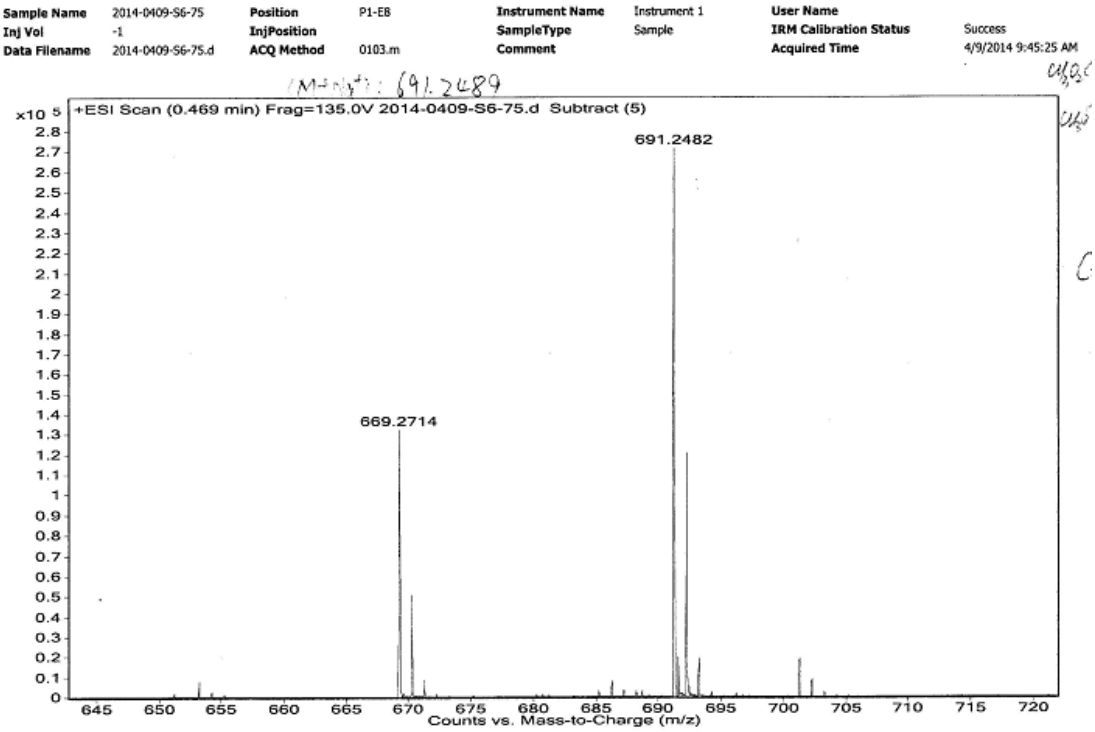
S6-75H

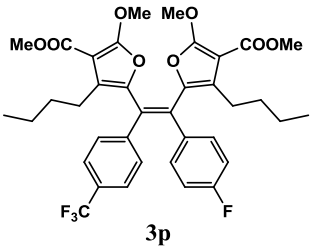

7.3649 7.3436 7.2593 7.1945 7.1736 7.1550 7.1361 7.0948 7.0915 7.0758 7.0716
3.8122 3.8007 3.7731 3.7675 2.0989 2.0797 2.0596 2.0360 2.0201 1.1186 1.1114 1.0999 1.0929 1.0811 1.0745 1.0629 1.0559 1.0455 1.0375 0.8875 0.8794 0.8726 0.8660 0.8565 0.8494 0.8399 0.8358 0.8292
BRUKER
Current Data Parameters
NAME 86-75H
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140409
Time 8.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 4
DS 2
SWH 11990.407 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 90.5
DW 41.700 usec
DE 10.00 usec
TE 296.1 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.10 usec
PL1 -4.00 dB
SFO1 400.1330522 MHz
F2 - Processing parameters
SI 32768
SF 400.1300098 MHz
WDW EM
SSB 0
LB 0.60 Hz
GB 0
PC 1.00
9 8 7 6 5 4 3 2 1 0 ppm
2.208 5.166 1.982 6.000 5.736 4.179 4.365 3.852 6.279
163.666 163.550 162.247 162.102 140.694 140.631 138.383 132.012 131.257 131.096 128.775 128.550 128.163 127.999 127.836 127.290 124.872 124.696 92.019 91.816 57.273 57.200 50.973 50.959 32.084 31.891 24.241 24.177 22.706 22.684 13.644 13.588
200 180 160 140 120 100 80 60 40 20 0 ppm



3o

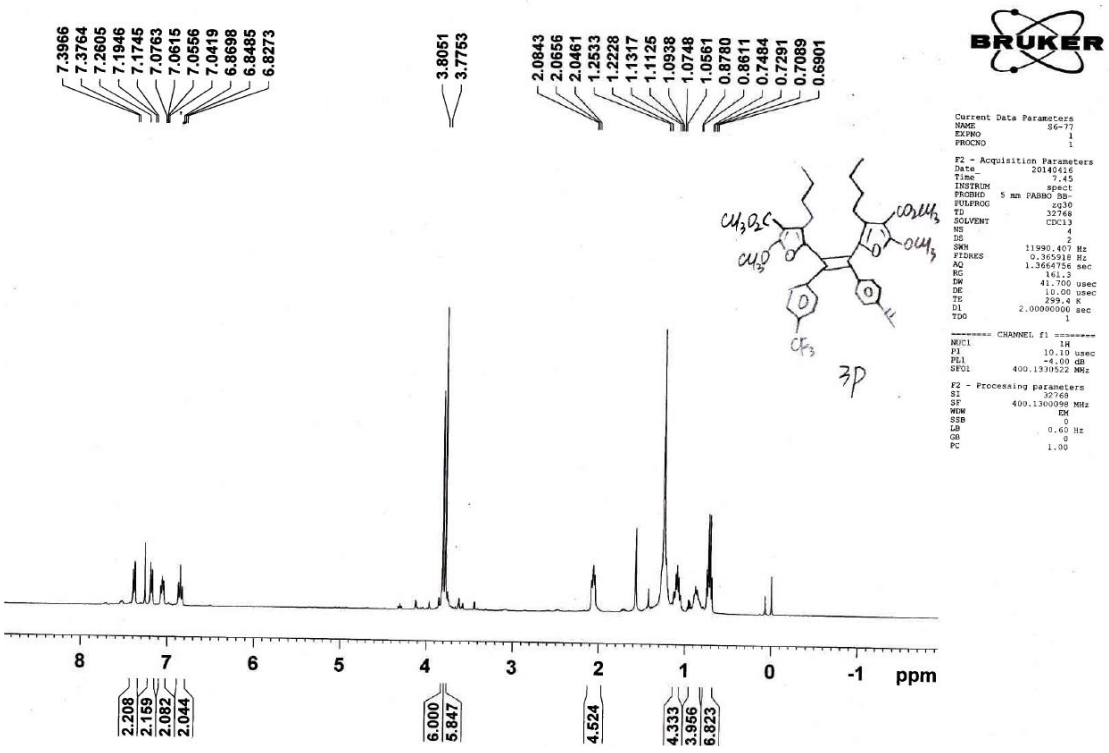
Chemical Formula: $C_{37}H_{39}F_3O_8$
Exact Mass: 668.26
Molecular Weight: 668.70
m/z: 668.26 (100.0%), 669.26 (40.3%), 670.27 (8.1%), 671.27 (1.7%), 670.26 (1.6%)
Elemental Analysis: C, 66.46; H, 5.88; F, 8.52; O, 19.14



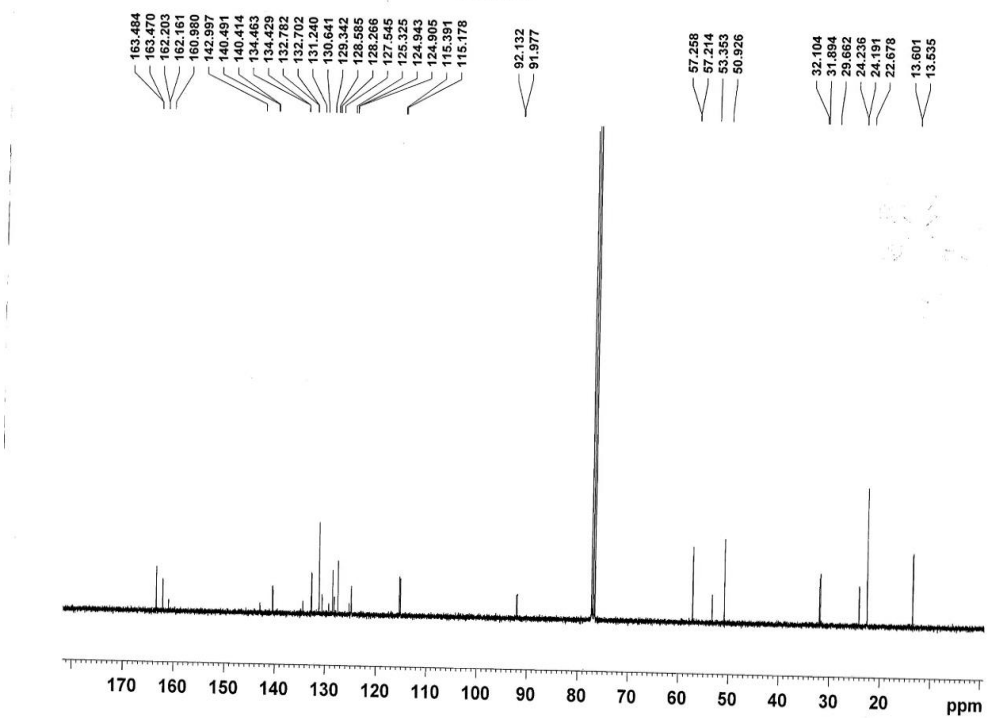


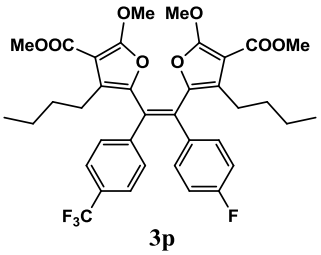
3p

S6-77



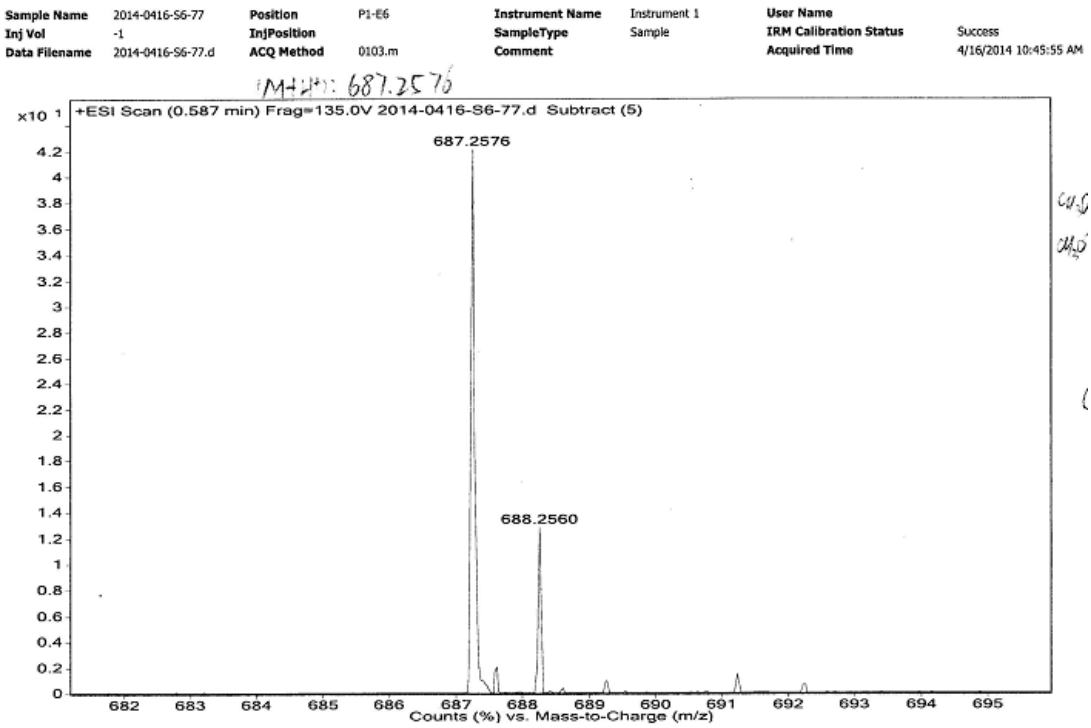
SS6-77-C13

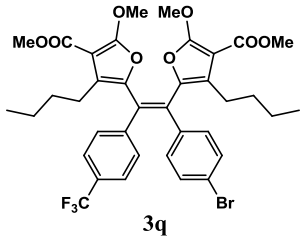




3p

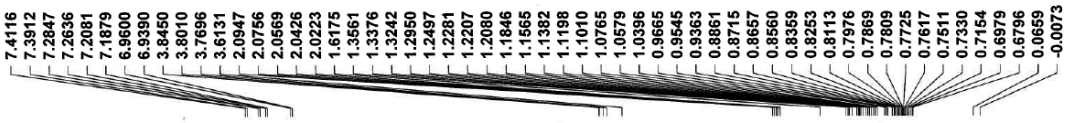
Chemical Formula: $C_{37}H_{38}F_4O_8$
Exact Mass: 686.25
Molecular Weight: 686.69
m/z: 686.25 (100.0%), 687.25 (40.3%), 688.26 (8.1%), 689.26 (1.7%), 688.25 (1.6%)
Elemental Analysis: C, 64.72; H, 5.58; F, 11.07; O, 18.64




OMe
MeO
MeOOC
COOMe
O
O
F3C
Br

3q

S6-76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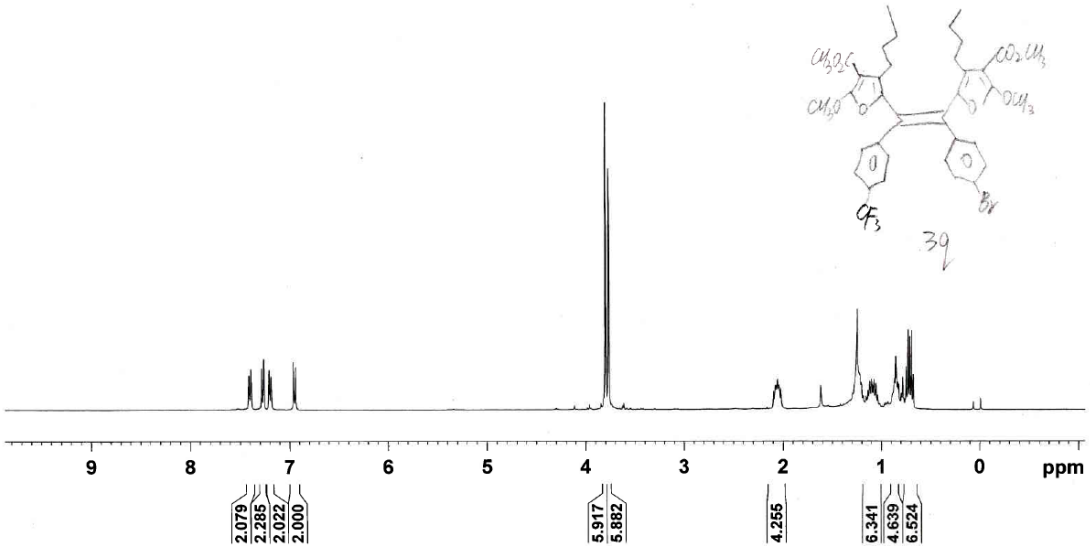
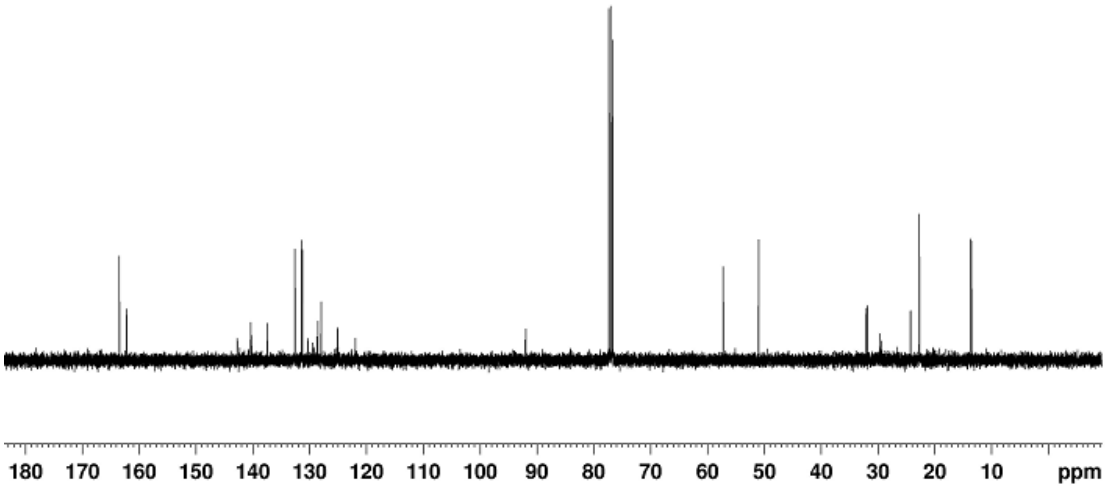
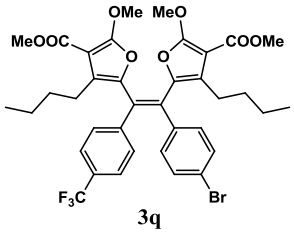
7.2081
7.1879
7.1600
6.9390
3.8450
3.8010
3.7696
3.6131
2.0947
2.0756
2.0569
2.0426
2.0223
1.6175
1.3561
1.3376
1.3242
1.2950
1.2497
1.2281
1.2207
1.2080
1.1846
1.1565
1.1382
1.1198
1.1010
1.0765
1.0579
1.0396
0.9665
0.9545
0.9363
0.8861
0.8715
0.8657
0.8560
0.8359
0.8253
0.8113
0.7976
0.7869
0.7809
0.7725
0.7617
0.7511
0.7330
0.7154
0.6979
0.6796
0.0659
-0.0073


9
8
7
6
5
4
3
2
1
0
ppm
2.079
2.285
2.022
2.000
5.917
5.882
4.255
6.341
4.639
6.524

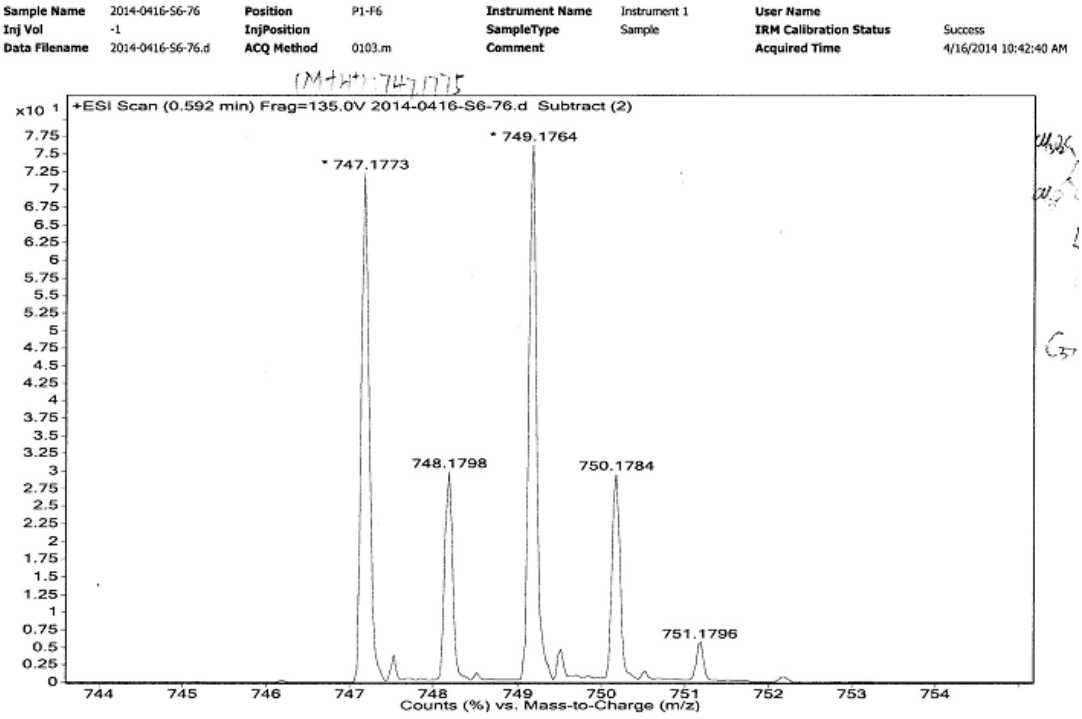

163.470
162.219
162.183
142.755
140.376
140.237
137.467
135.072
132.600
131.422
131.262
130.293
129.516
128.742
128.542
127.974
125.077
125.041
121.940
92.038
91.976
57.293
56.854
51.028
50.750
32.056
31.894
29.689
24.270
24.249
22.694
13.652
13.557

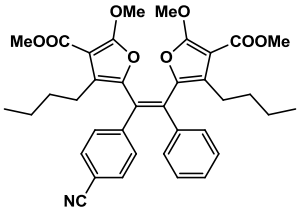

180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm



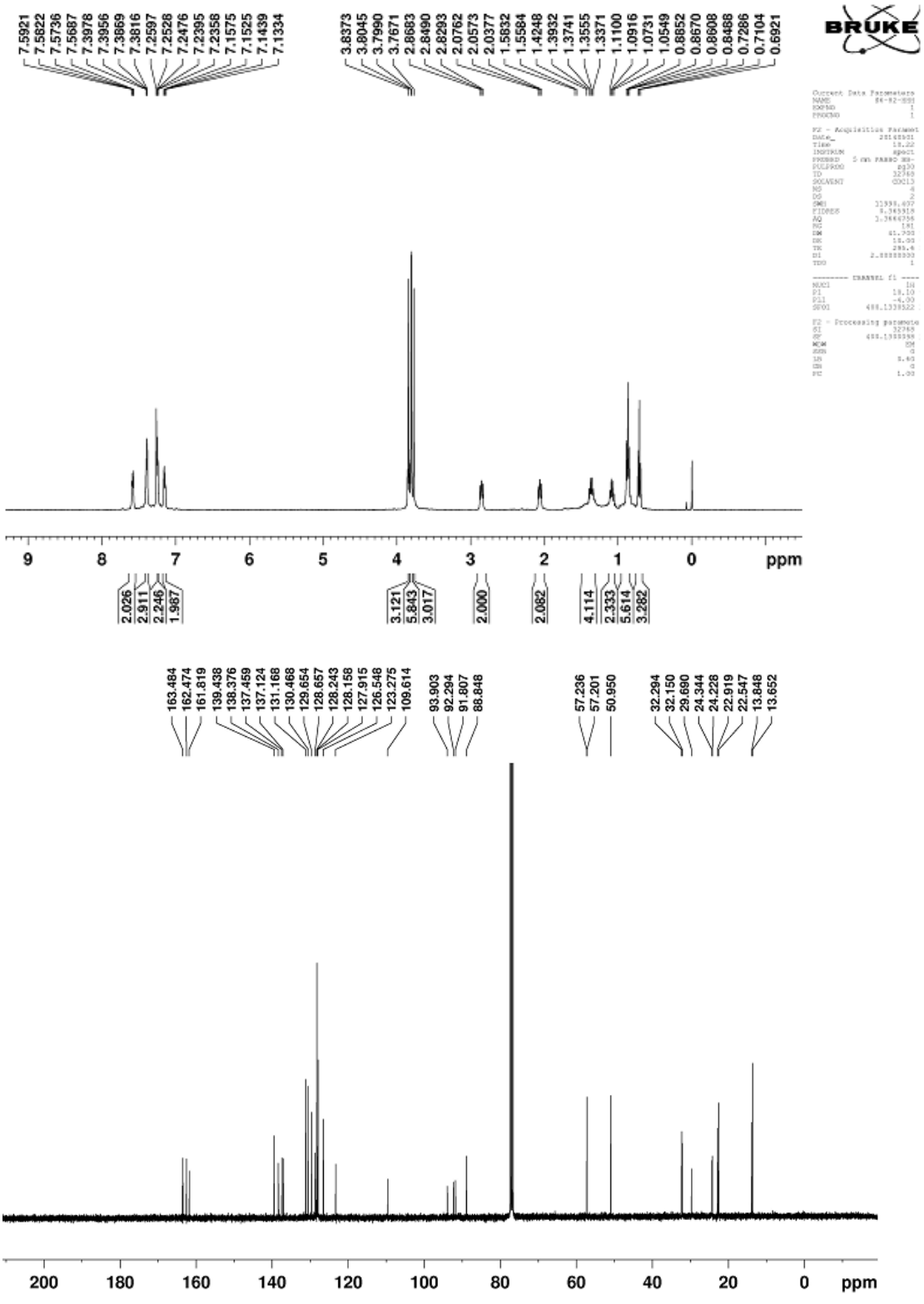
3q

Chemical Formula: $C_{37}H_{38}BrF_3O_8$
Exact Mass: 746.17
Molecular Weight: 747.59
m/z: 746.17 (100.0%), 748.17 (98.9%), 747.17 (40.3%), 749.17 (39.7%), 750.17 (9.2%), 748.18 (8.1%), 749.18 (1.7%), 751.18 (1.7%)
Elemental Analysis: C, 59.44; H, 5.12; Br, 10.69; F, 7.62; O, 17.12




OMe
MeO
MeOOC
COOMe
O
O
NC

3r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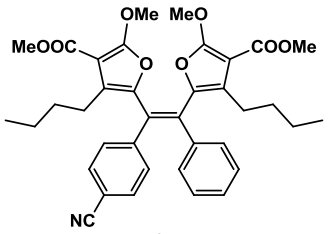
7.3978
7.3956
7.3869
7.3816
7.2597
7.2526
7.2476
7.2395
7.2358
7.1575
7.1525
7.1439
7.1334
3.8373
3.8045
3.7990
3.7671
2.8683
2.8490
2.8293
2.0762
2.0573
2.0377
1.5832
1.5584
1.4248
1.3932
1.3741
1.3555
1.3371
1.1100
1.0916
1.0731
1.0549
0.8852
0.8670
0.8608
0.8488
0.7286
0.7104
0.6921
BRUKE
9
8
7
6
5
4
3
2
1
0
ppm
2.026
2.911
2.246
1.967
3.121
5.843
3.017
2.000
2.062
4.114
2.333
5.614
3.282
163.484
162.474
161.819
139.438
138.376
137.459
137.124
131.166
130.468
129.654
128.657
128.243
128.156
127.915
126.548
123.275
109.614
93.903
92.294
91.807
88.848
57.236
57.201
50.950
32.294
32.150
29.690
24.344
24.228
22.919
22.547
13.848
13.652
200
180
160
140
120
100
80
60
40
20
0
ppm



3r

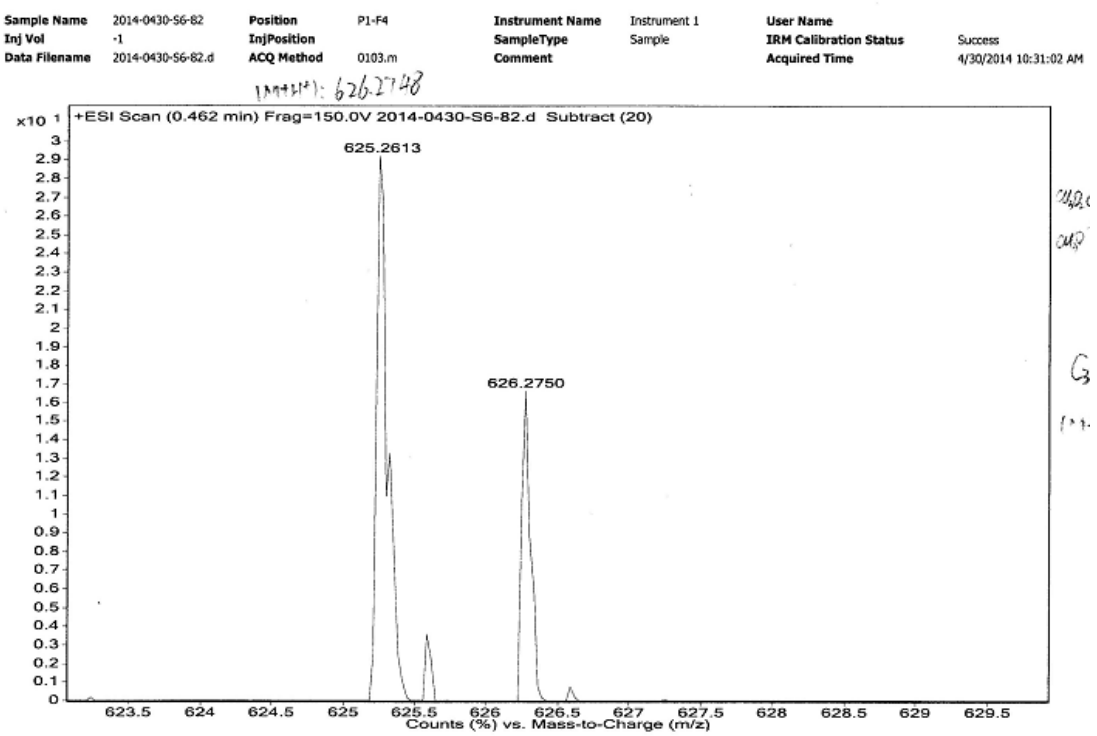
Chemical Formula: $C_{37}H_{39}NO_8$

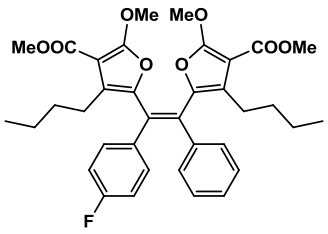
Exact Mass: 625.27

Molecular Weight: 625.71

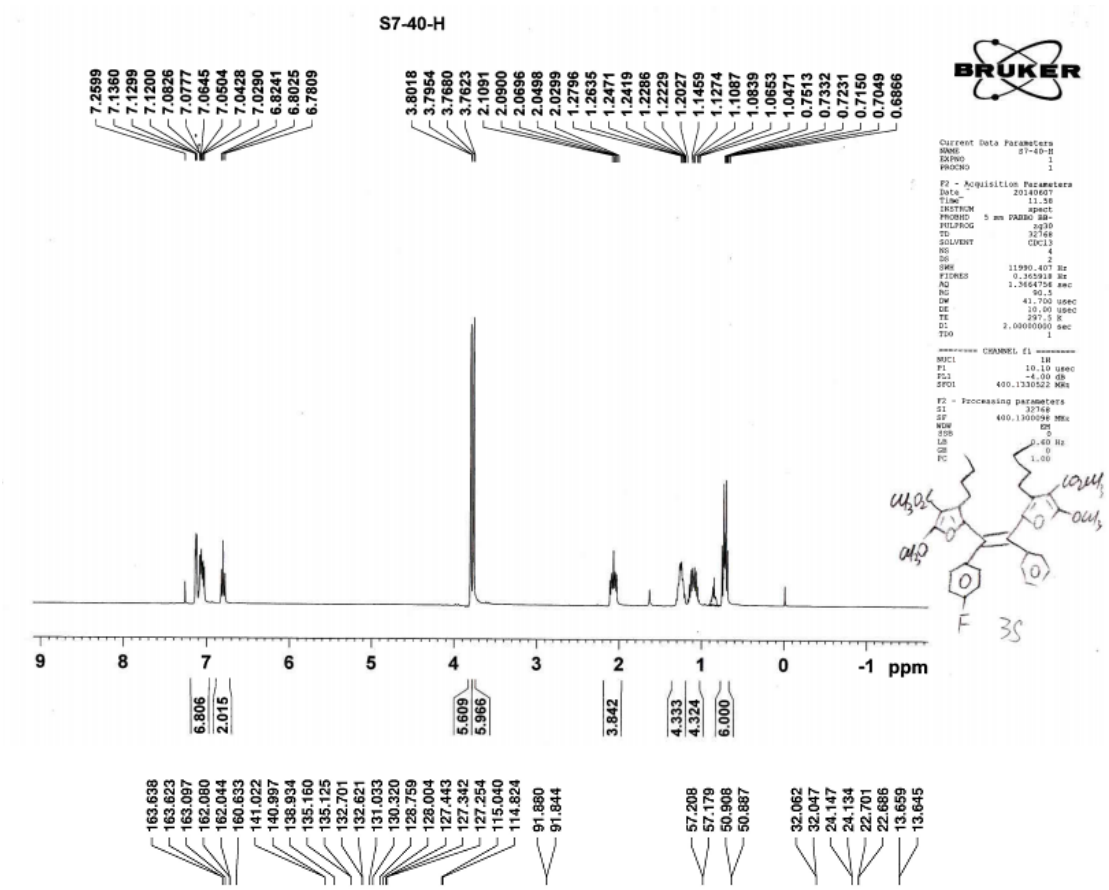
m/z: 625.27 (100.0%), 626.27 (40.8%), 627.27 (9.6%), 628.28 (1.7%)

Elemental Analysis: C, 71.02; H, 6.28; N, 2.24; O, 20.46




OMe
MeO
MeOOC
COOMe
O
O
F

3s


S7-40-H
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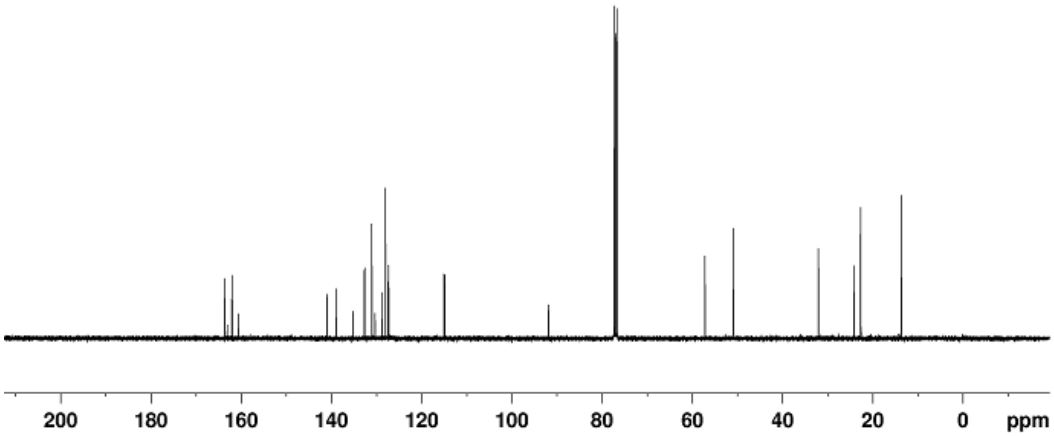
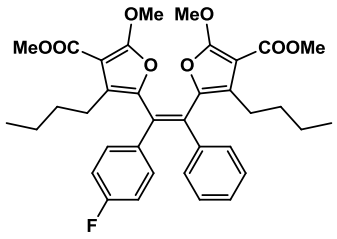
7.1299
7.1200
7.0826
7.0777
7.0645
7.0504
7.0428
7.0290
6.8241
6.8025
6.7809
3.8018
3.7954
3.7680
3.7623
2.1091
2.0900
2.0696
2.0498
2.0299
1.2796
1.2635
1.2471
1.2419
1.2286
1.2229
1.2027
1.1459
1.1274
1.1087
1.0839
1.0653
1.0471
0.7513
0.7332
0.7231
0.7150
0.7049
0.6866
9
8
7
6
5
4
3
2
1
0
-1 ppm
6.806
2.015
5.609
5.966
3.842
4.333
4.324
6.000

163.638
163.623
163.097
162.080
162.044
160.633
141.022
140.997
138.934
135.160
135.125
132.701
132.621
131.033
130.320
128.759
128.004
127.443
127.342
127.254
115.040
114.824
91.880
91.844
57.208
57.179
50.908
50.887
32.062
32.047
24.147
24.134
22.701
22.686
13.659
13.645

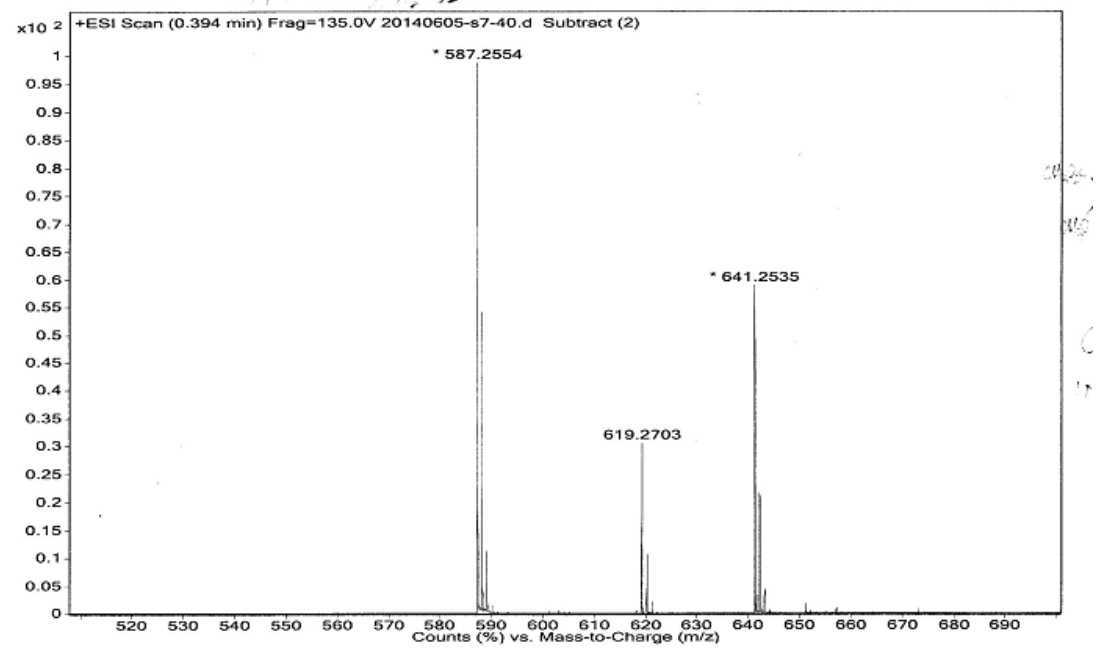

200
180
160
140
120
100
80
60
40
20
0
ppm

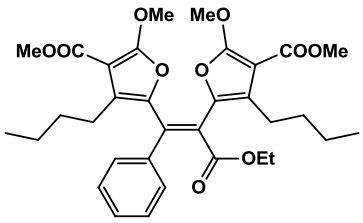


3s

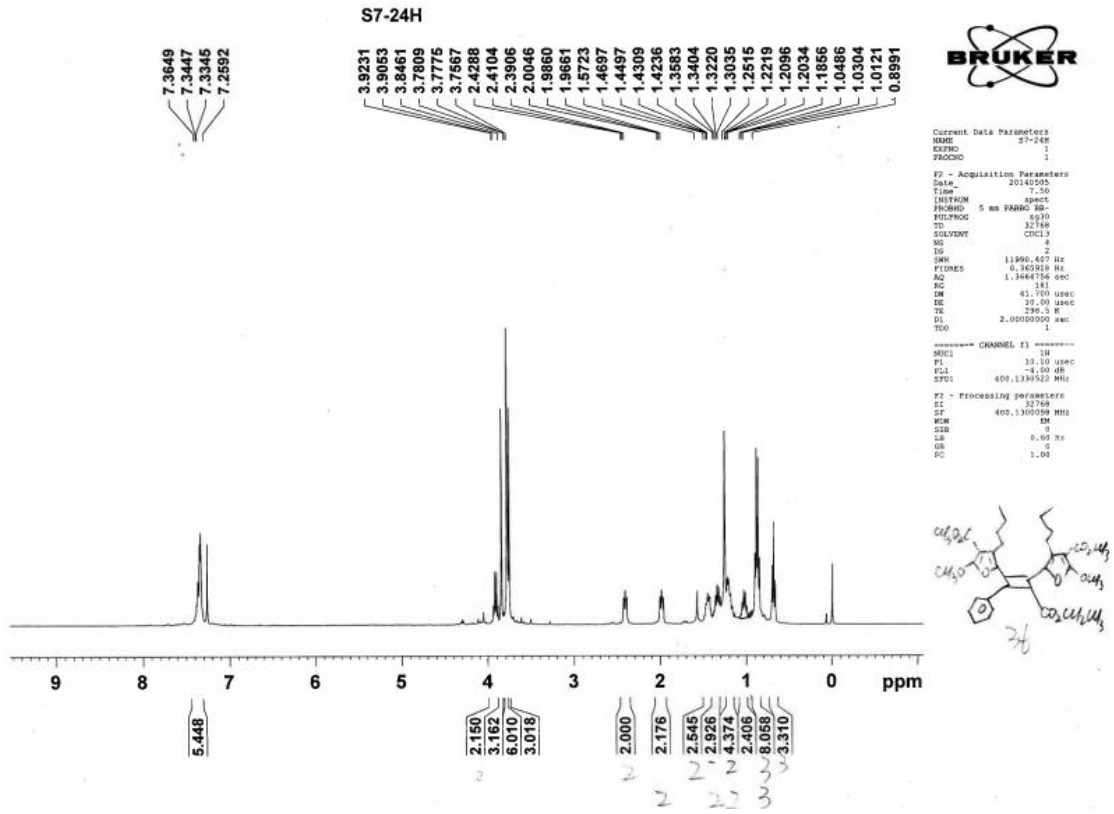
Chemical Formula: $C_{36}H_{39}FO_8$
Exact Mass: 618.26
Molecular Weight: 618.69
m/z: 618.26 (100.0%), 619.27 (39.7%), 620.27 (9.3%), 621.27 (1.6%)
Elemental Analysis: C, 69.89; H, 6.35; F, 3.07; O, 20.69

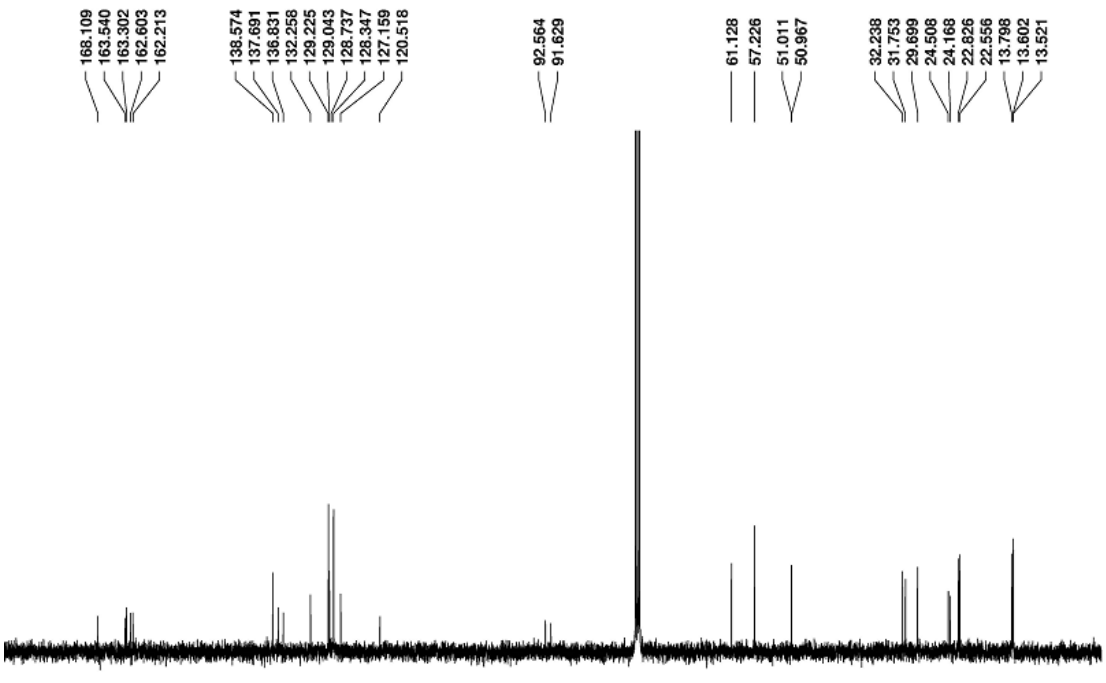
Sample Name	20140605-s7-40	**Position**	P1-F4	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	20140605-s7-40.d	**ACQ Method**	0103.m	**Comment**		**Acquired Time**	6/5/2014 9:12:08 AM

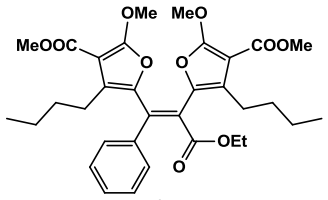



OMe
MeO
MeOOC
COOMe
O
O
OEt
O

3t

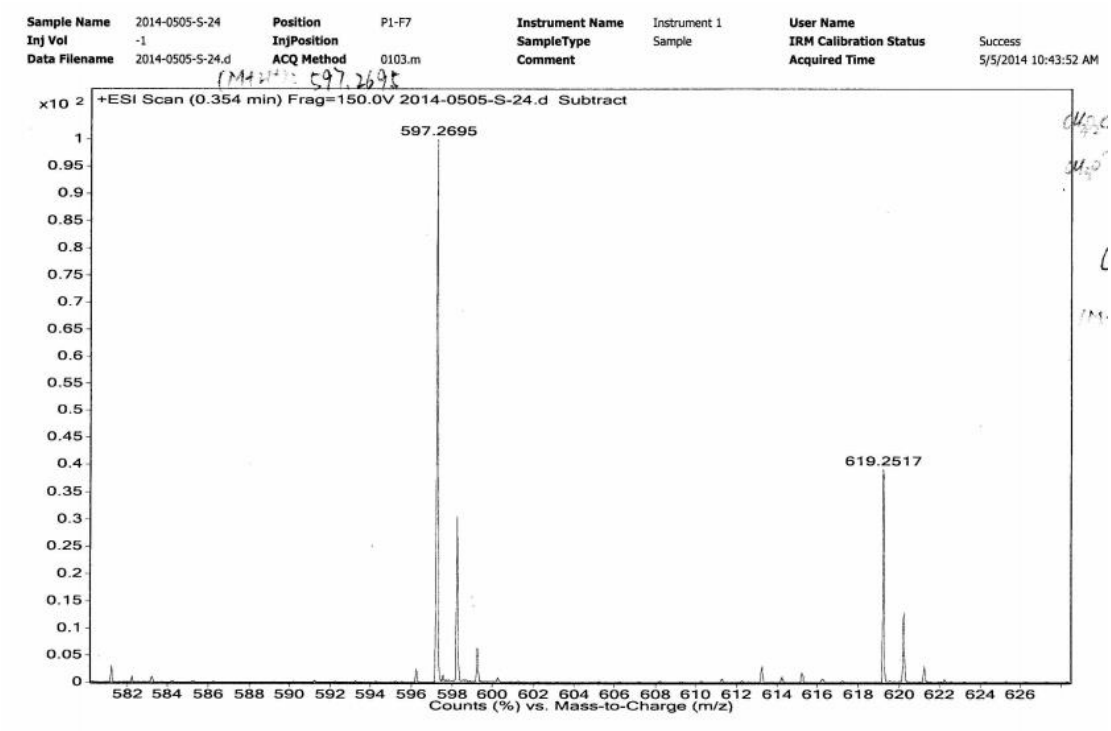

S7-24H
BRUKER
7.3649
7.3447
7.3345
7.2592
3.9231
3.9053
3.8461
3.7809
3.7775
3.7567
2.4288
2.4104
2.3906
2.0046
1.9860
1.9661
1.5723
1.4697
1.4497
1.4309
1.4236
1.3583
1.3404
1.3220
1.3035
1.2515
1.2219
1.2096
1.2034
1.1856
1.0486
1.0304
1.0121
0.8991
9
8
7
6
5
4
3
2
1
0
ppm
5.448
2.150
3.162
6.010
3.018
2.000
2.176
2.545
2.926
4.374
2.406
8.058
3.310

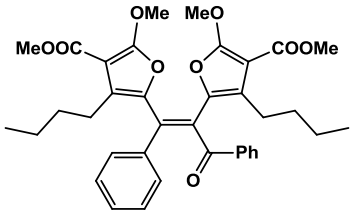

168.109
163.540
163.302
162.603
162.213
138.574
137.691
136.831
132.258
129.225
129.043
128.737
128.347
127.159
120.518
92.564
91.629
61.128
57.226
51.011
50.967
32.238
31.753
29.699
24.508
24.168
22.826
22.556
13.798
13.602
13.521



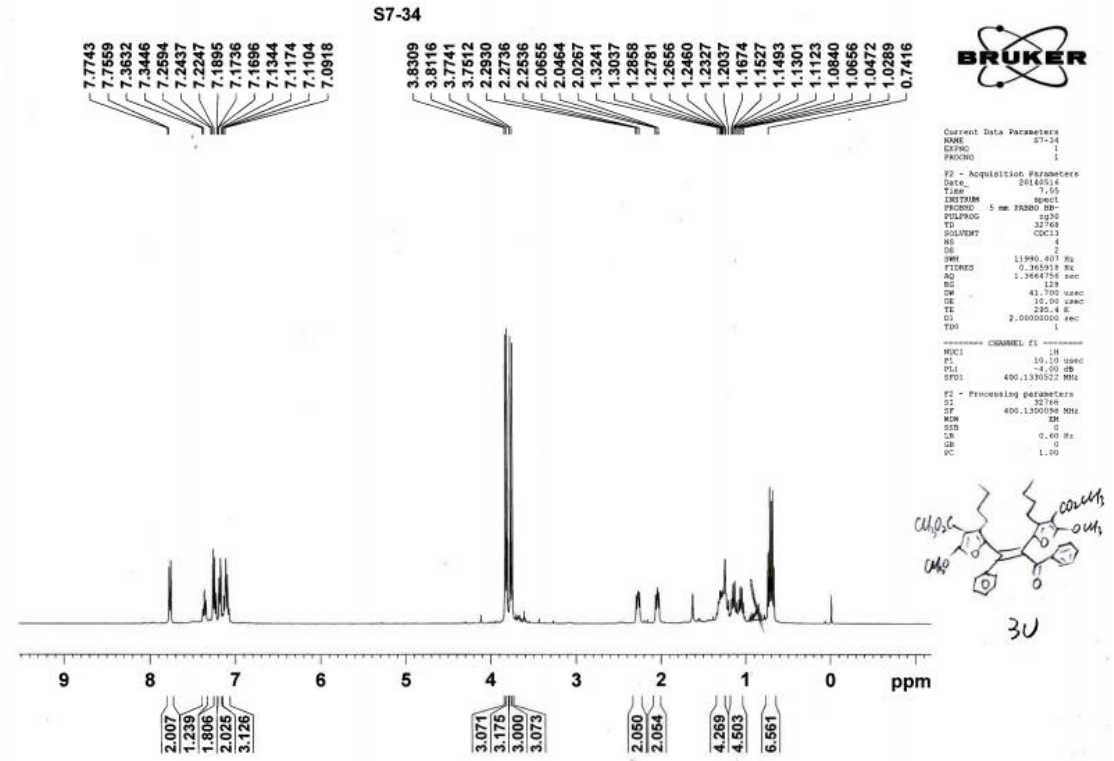
3t

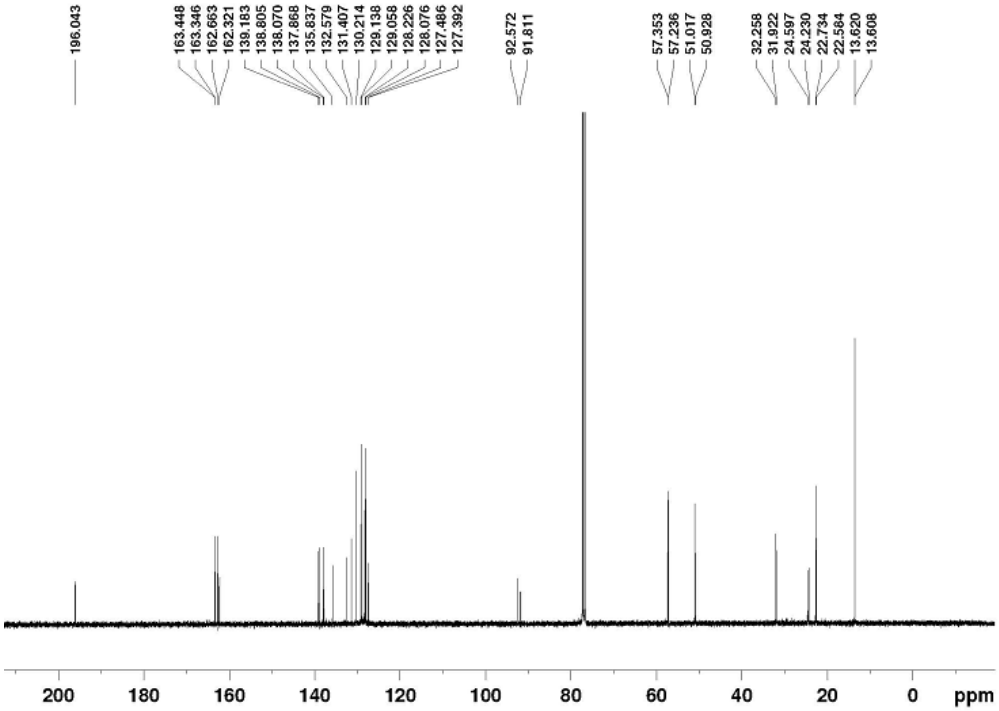
Chemical Formula: $C_{33}H_{40}O_{10}$
Exact Mass: 596.26
Molecular Weight: 596.66
m/z: 596.26 (100.0%), 597.27 (36.5%), 598.27 (8.5%), 599.27 (1.5%)
Elemental Analysis: C, 66.43; H, 6.76; O, 26.81

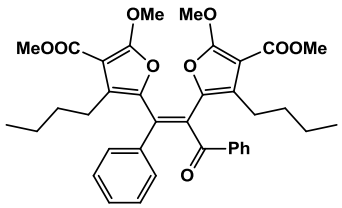



OMe
MeO
MeOOC
COOMe
O
O
Ph
O

3u


S7-34
BRUKER
7.7743 7.7559 7.3632 7.3446 7.2594 7.2437 7.2247 7.1895 7.1736 7.1696 7.1344 7.1174 7.1104 7.0918
3.8309 3.8116 3.7741 3.7512 2.2930 2.2736 2.2536 2.0655 2.0464 2.0267 1.3241 1.3037 1.2858 1.2781 1.2656 1.2460 1.2327 1.2037 1.1674 1.1527 1.1493 1.1301 1.1123 1.0840 1.0656 1.0472 1.0289 0.7416
9 8 7 6 5 4 3 2 1 0 ppm
2.007 1.239 1.806 2.025 3.126
3.071 3.175 3.000 3.073
2.050 2.054
4.269 4.503
6.561
3U

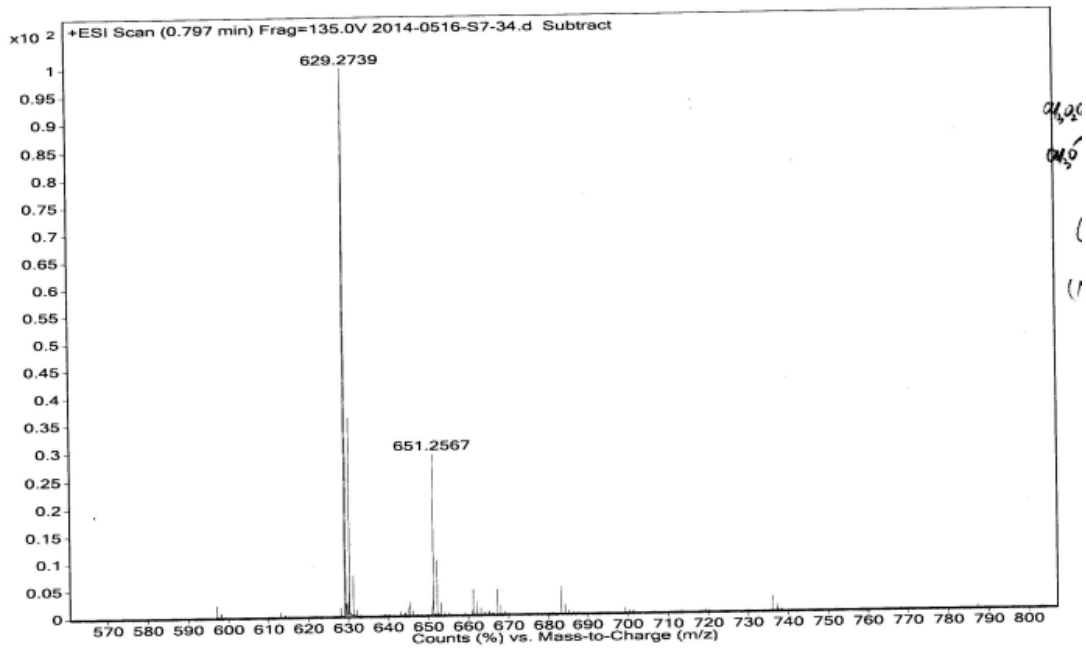

196.043
163.448 163.346 162.663 162.321 139.183 138.805 138.070 137.668 135.637 132.579 131.407 130.214 129.138 129.058 128.226 128.076 127.486 127.392
92.572 91.811
57.353 57.236 51.017 50.928
32.258 31.922 24.597 24.230 22.734 22.584 13.620 13.608
200 180 160 140 120 100 80 60 40 20 0 ppm

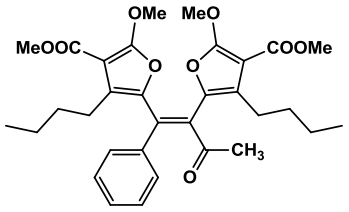


3u

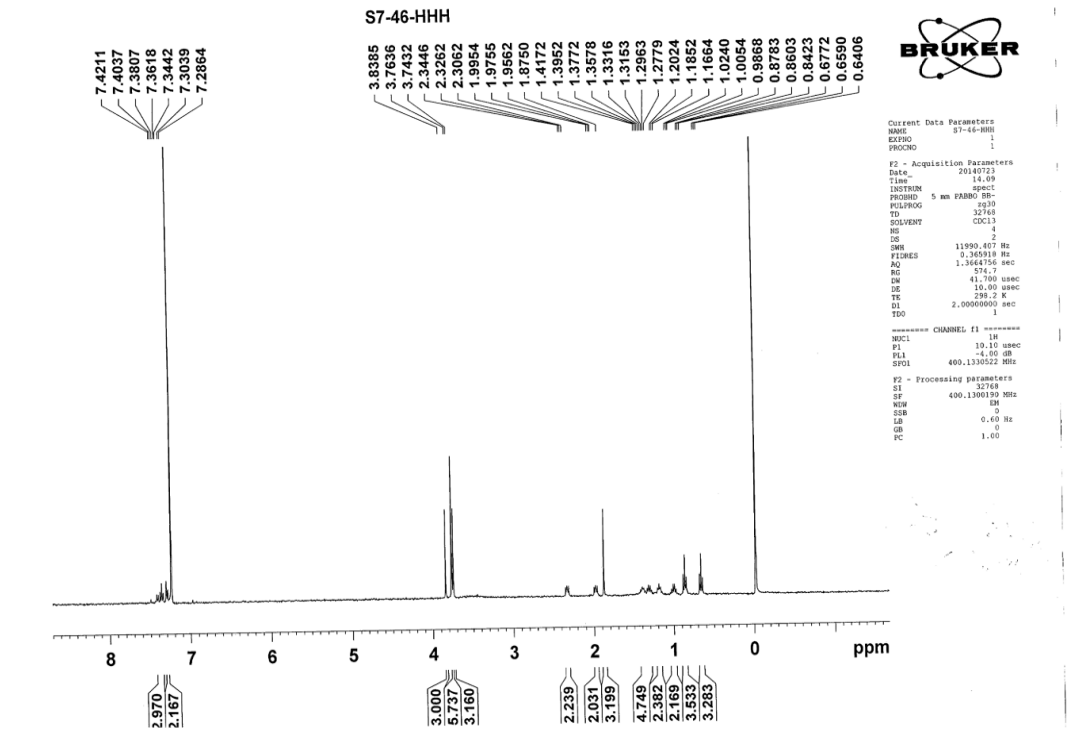
Chemical Formula: $C_{37}H_{40}O_9$
Exact Mass: 628.27
Molecular Weight: 628.71
m/z: 628.27 (100.0%), 629.27 (40.8%), 630.27 (9.8%), 631.28 (1.1%)
Elemental Analysis: C, 70.68; H, 6.41; O, 22.90

Sample Name	Unavailable	**Position**	Unavailable	**Instrument Name**	Unavailable	**User Name**	Unavailable
Inj Vol	Unavailable	**InjPosition**	Unavailable	**SampleType**	Unavailable	**IRM Calibration Status**	Success
Data Filename	2014-0516-S7-34.d	**ACQ Method**		**Comment**	Sample information is unavailable	**Acquired Time**	Unavailable




OMe
MeO
MeOOC
COOMe
O
O
O
CH3
O

3v


S7-46-HHH
BRUKER
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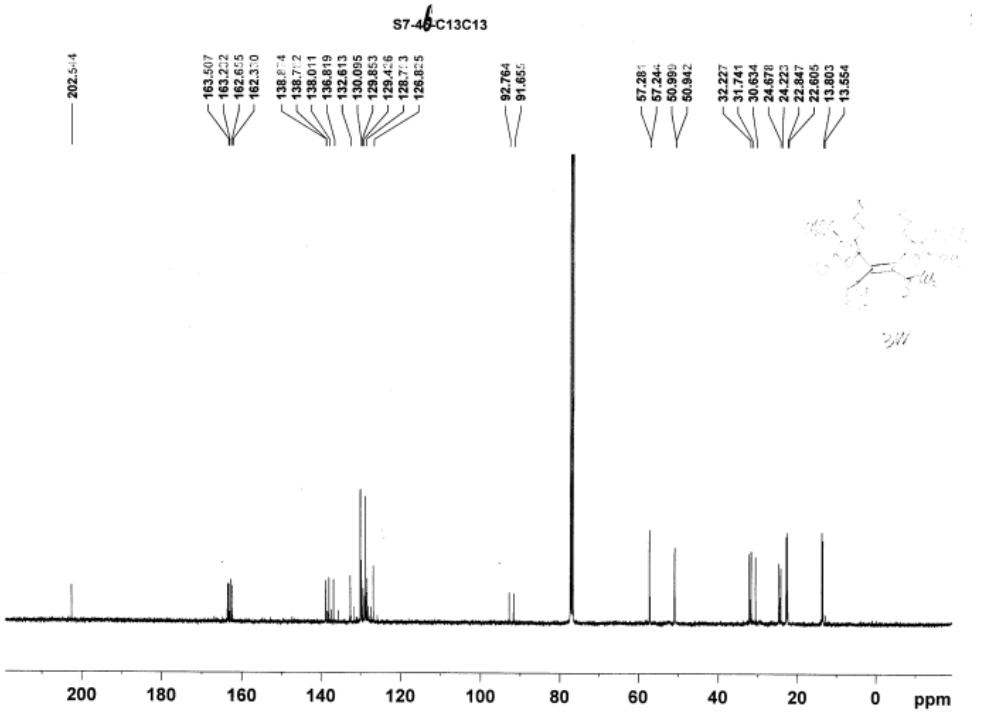
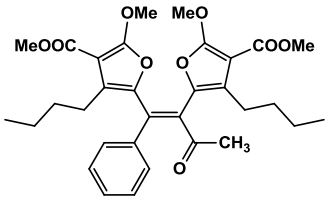
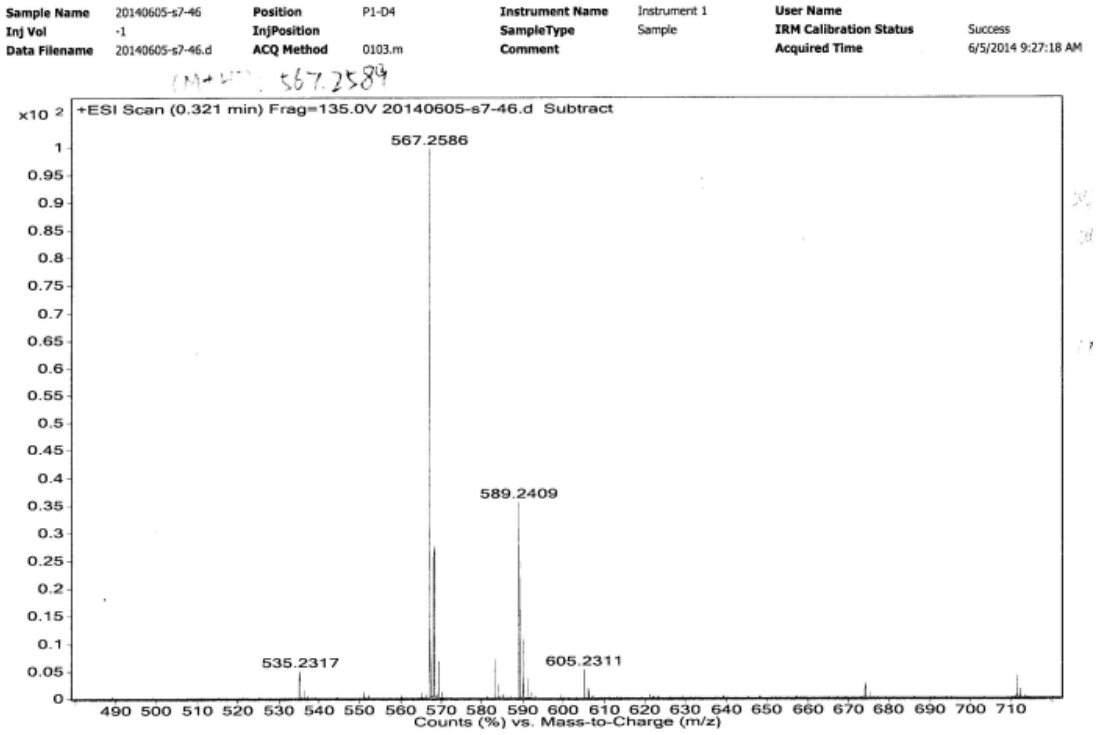
7.4037
7.3807
7.3618
7.3442
7.3039
7.2864
3.8385
3.7636
3.7432
2.3446
2.3262
2.3062
1.9954
1.9755
1.9562
1.8750
1.4172
1.3952
1.3772
1.3578
1.3316
1.3153
1.2963
1.2779
1.2024
1.1852
1.1664
1.0240
1.0054
0.9888
0.8783
0.8603
0.8423
0.6772
0.6590
0.6406
Current Data Parameters
NAME S7-46-HHH
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140723
Time 14.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 4
DS 2
SWH 11990.407 Hz
FIDRES 0.365919 Hz
AQ 1.3664756 sec
RG 574.7
DW 41.700 usec
DE 10.00 usec
TE 298.2 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.10 usec
PL1 -4.00 dB
SFO1 400.1330522 MHz
F2 - Processing parameters
SI 32768
SF 400.1300190 MHz
WDW EM
SSB 0
LB 0.60 Hz
GB 0
PC 1.00
8
7
6
5
4
3
2
1
0
ppm
2.970
2.167
3.000
5.737
3.160
2.239
2.031
3.199
4.749
2.382
2.169
3.533
3.283

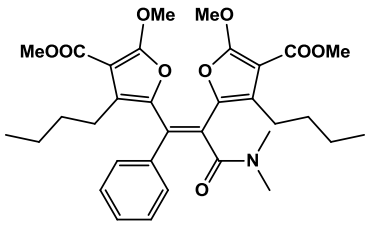

S7-46-C13C13
202.544
163.507
163.222
162.655
162.310
138.874
138.712
138.011
136.819
132.613
130.095
129.853
129.426
128.713
128.625
92.764
91.655
57.281
57.244
50.999
50.942
32.227
31.741
30.634
24.678
24.223
22.847
22.605
13.803
13.554
200
180
160
140
120
100
80
60
40
20
0
ppm



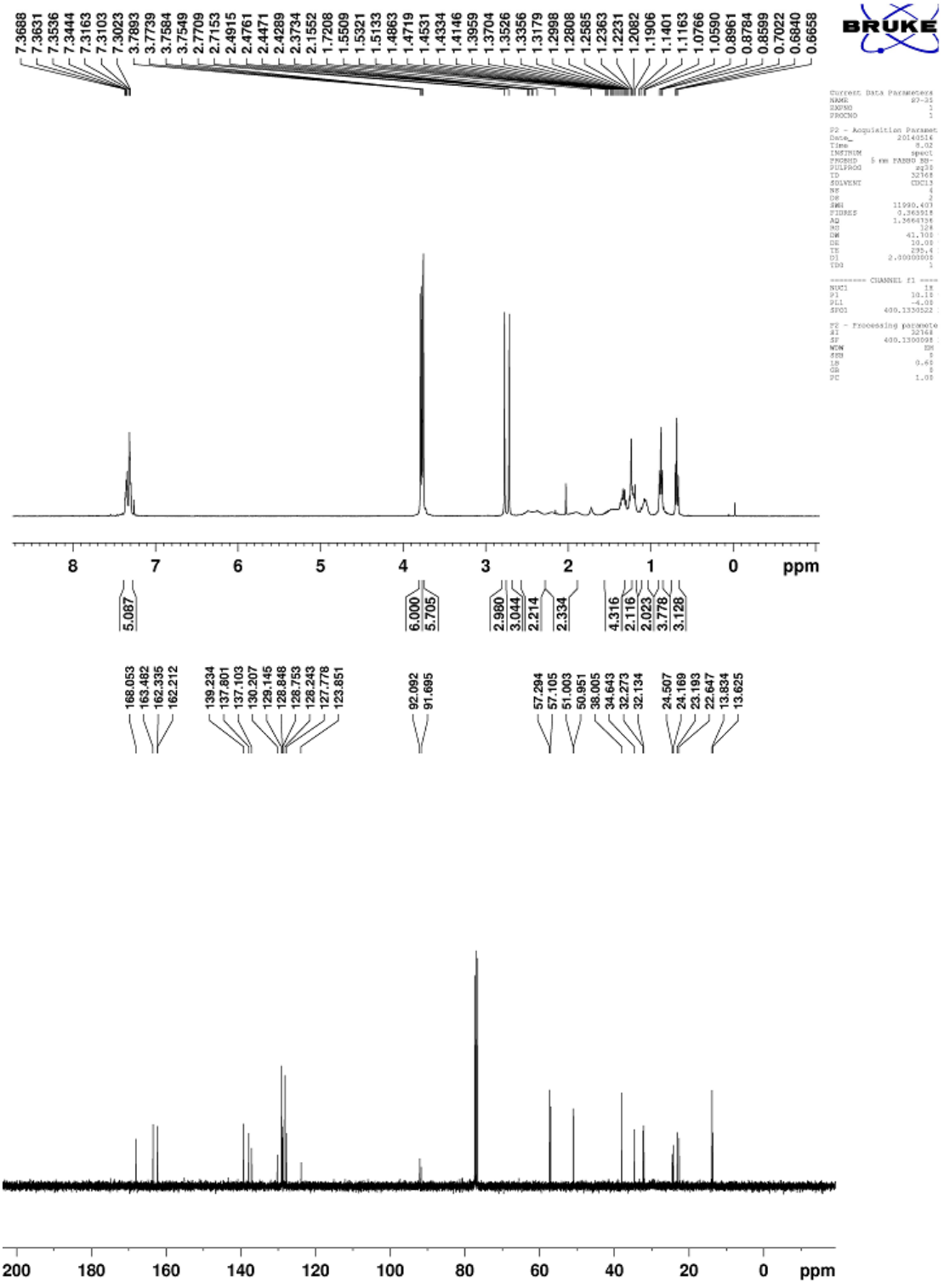
3v

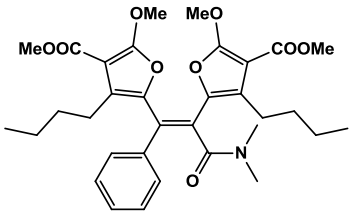
Chemical Formula: $C_{32}H_{38}O_9$
Exact Mass: 566.25
Molecular Weight: 566.64
m/z: 566.25 (100.0%), 567.25 (34.6%), 568.26 (7.9%), 569.26 (1.3%)
Elemental Analysis: C, 67.83; H, 6.76; O, 25.41




OMe
MeO
MeOOC
COOMe
O
O
N
O

3w


7.3688
7.3631
7.3536
7.3444
7.3163
7.3103
7.3023
3.7893
3.7739
3.7584
3.7549
2.7709
2.7153
2.4915
2.4761
2.4471
2.4289
2.3734
2.1552
1.7208
1.5509
1.5321
1.5133
1.4863
1.4719
1.4531
1.4334
1.4146
1.3959
1.3704
1.3526
1.3356
1.3179
1.2998
1.2808
1.2585
1.2363
1.2231
1.2082
1.1906
1.1401
1.1163
1.0766
1.0590
0.8961
0.8784
0.8599
0.7022
0.6840
0.6658
BRUKER
8
7
6
5
4
3
2
1
0
ppm
5.087
6.000
5.705
2.980
3.044
2.214
2.334
4.316
2.116
2.023
3.778
3.128
168.053
163.482
162.335
162.212
139.234
137.801
137.103
130.207
129.145
128.848
128.753
128.243
127.778
123.851
92.092
91.695
57.294
57.105
51.003
50.951
38.005
34.643
32.273
32.134
24.507
24.169
23.193
22.647
13.834
13.625
200
180
160
140
120
100
80
60
40
20
0
ppm



3w

Chemical Formula: $C_{33}H_{41}NO_9$

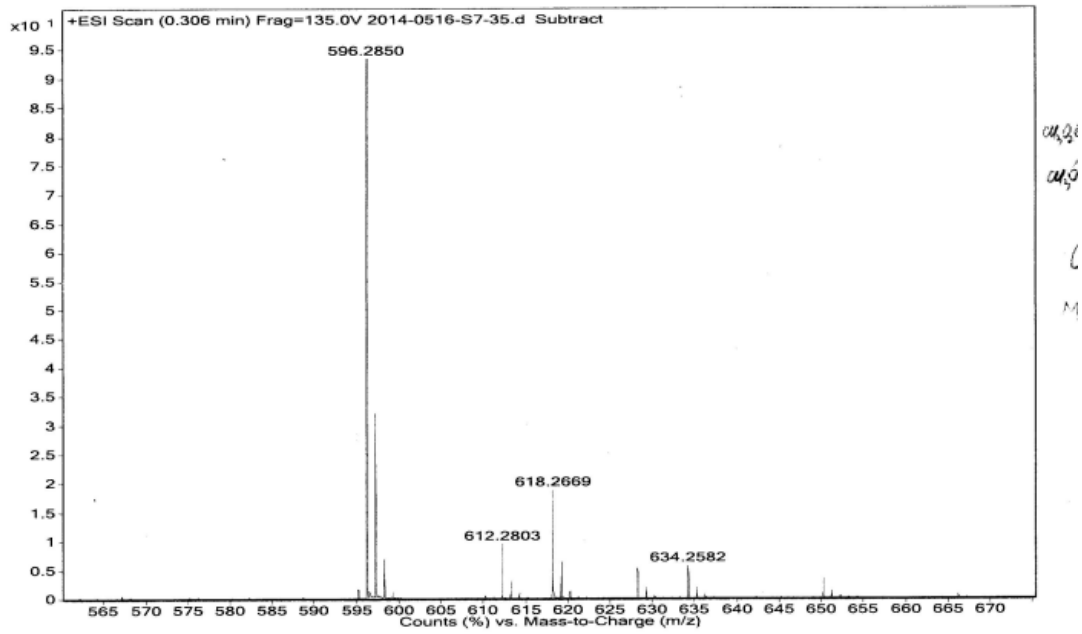
Exact Mass: 595.28

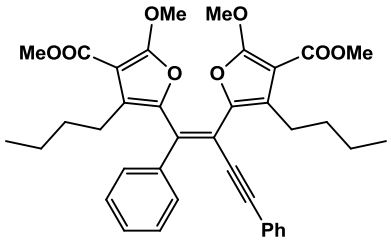
Molecular Weight: 595.68

m/z: 595.28 (100.0%), 596.28 (36.9%), 597.28 (8.2%), 598.29 (1.4%)

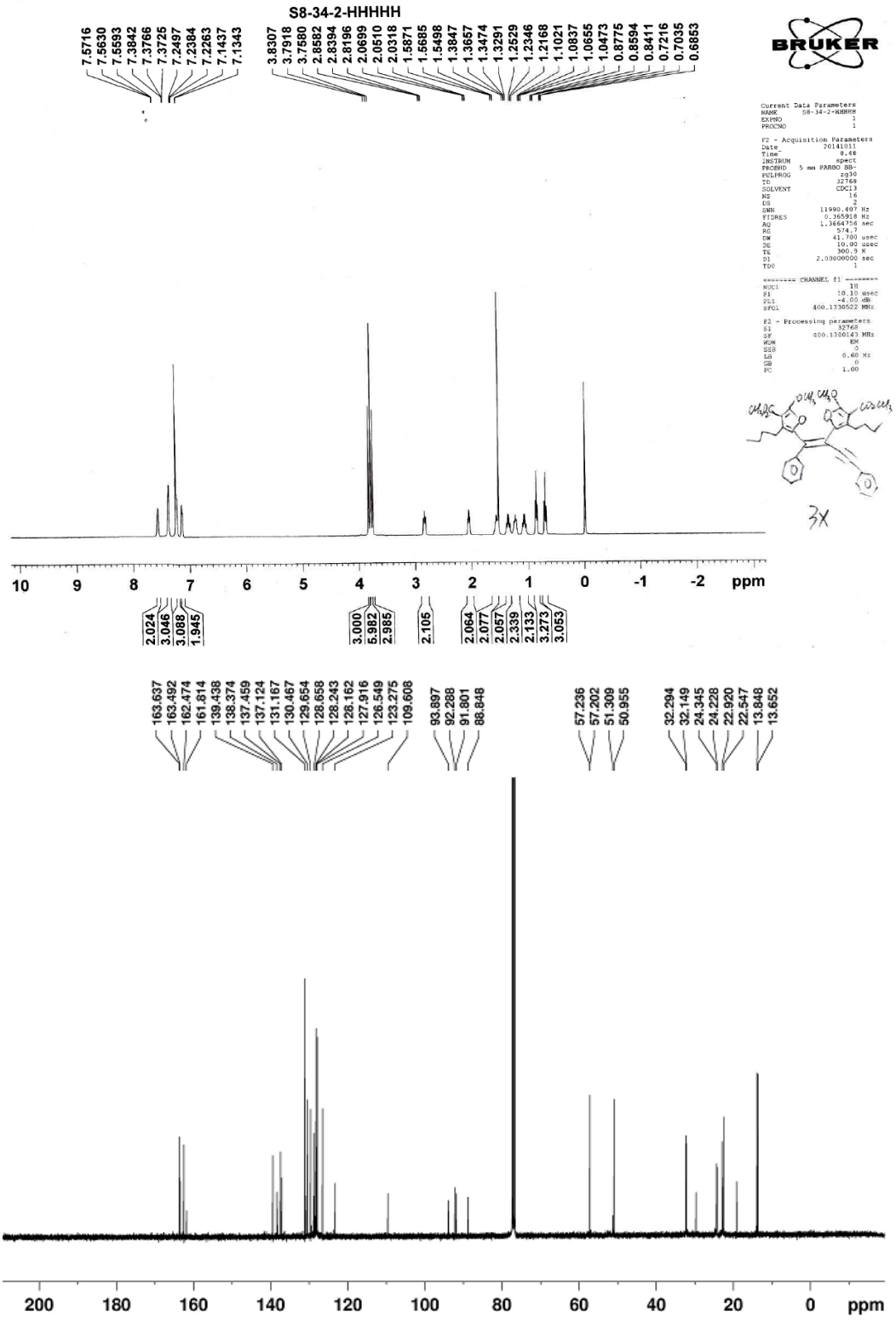
Elemental Analysis: C, 66.54; H, 6.94; N, 2.35; O, 24.17

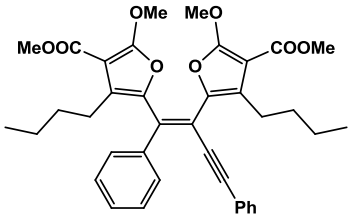
Sample Name	2014-0516-S7-35	**Position**	P1-D1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	2014-0516-S7-35.d	**ACQ Method**	0103.m	**Comment**		**Acquired Time**	5/16/2014 2:21:14 PM





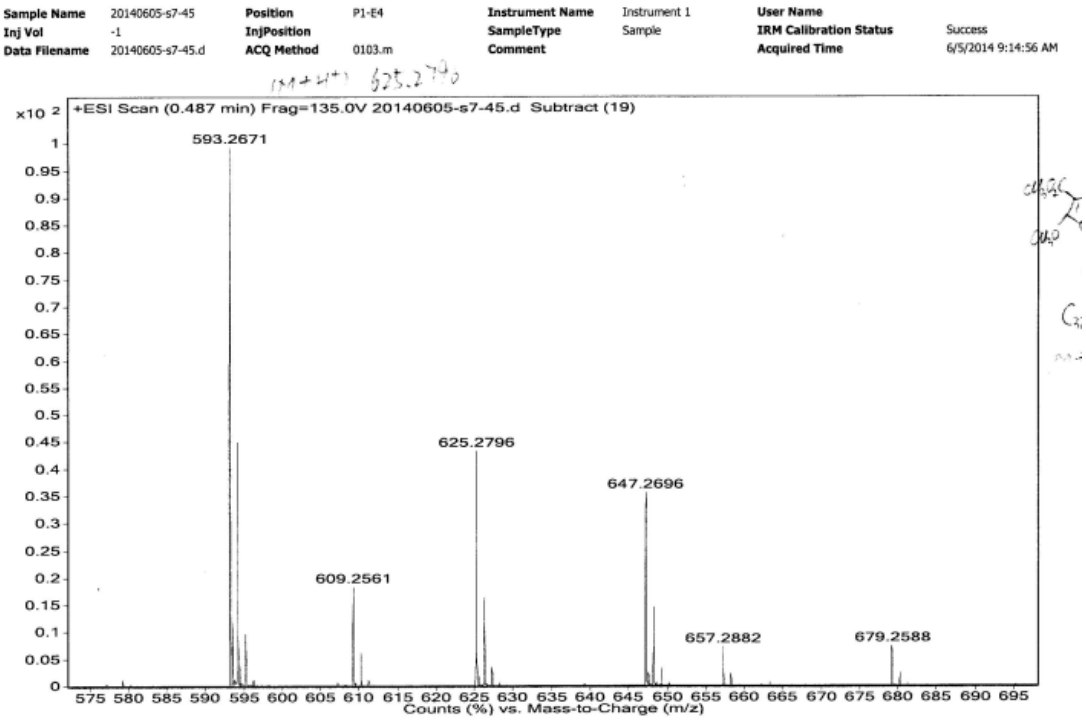
3x

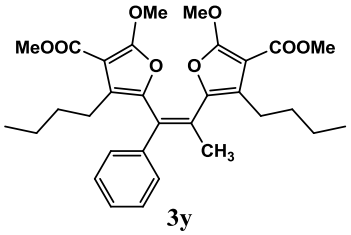




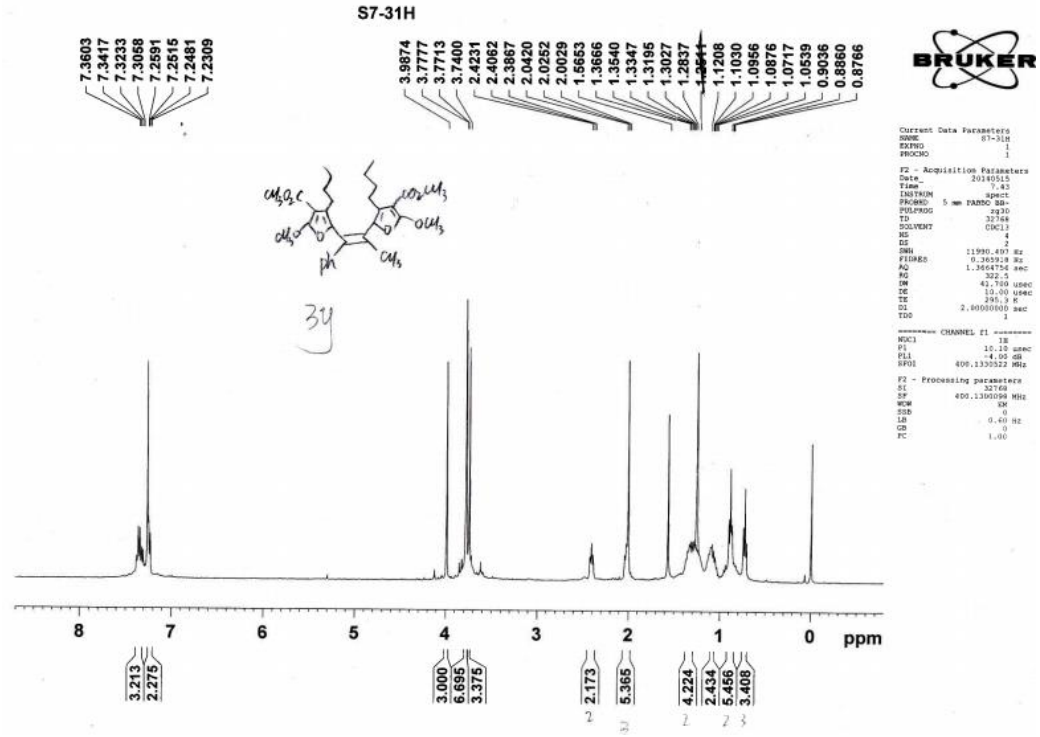
3x

Chemical Formula: $C_{38}H_{40}O_8$
Exact Mass: 624.27
Molecular Weight: 624.72
m/z: 624.27 (100.0%), 625.28 (41.9%), 626.28 (10.2%), 627.28 (1.8%)
Elemental Analysis: C, 73.06; H, 6.45; O, 20.49




OMe
MeO
MeOOC
COOMe
O
O
CH3

3y


S7-31H
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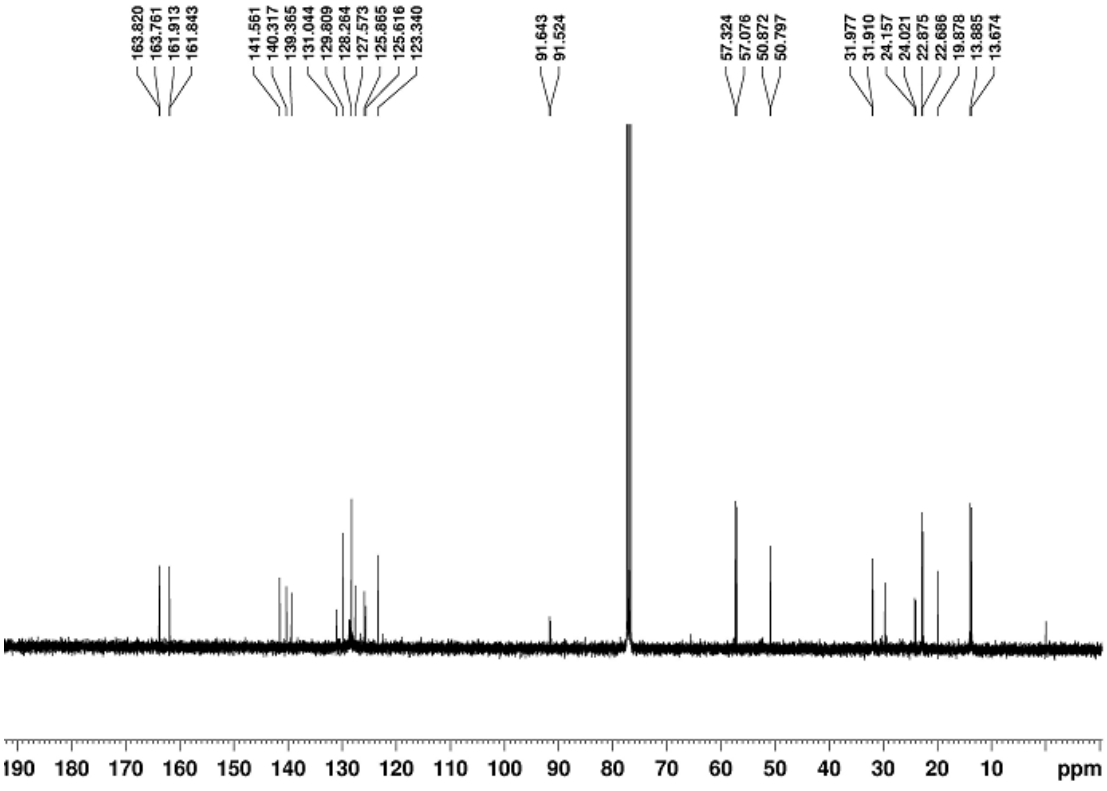
7.3417
7.3233
7.3058
7.2591
7.2515
7.2481
7.2309
3.9874
3.7777
3.7713
3.7400
2.4231
2.4062
2.3867
2.0420
2.0252
2.0029
1.6653
1.3666
1.3540
1.3347
1.3195
1.3027
1.2837
1.1208
1.1030
1.0956
1.0876
1.0717
1.0539
0.9036
0.8860
0.8766
BRUKER
3y
8
7
6
5
4
3
2
1
0
ppm
3.213
2.275
3.000
6.695
3.375
2.173
5.365
4.224
2.434
5.456
3.408


163.820
163.761
161.913
161.843
141.561
140.317
139.365
131.044
129.809
128.264
127.573
125.865
125.616
123.340
91.643
91.524
57.324
57.076
50.872
50.797
31.977
31.910
24.157
24.021
22.875
22.686
19.878
13.885
13.674
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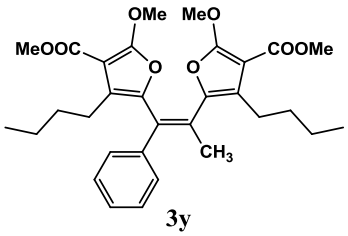
90
80
70
60
50
40
30
20
10
ppm



3y

Chemical Formula: $C_{31}H_{38}O_8$
Exact Mass: 538.26
Molecular Weight: 538.63
m/z: 538.26 (100.0%), 539.26 (34.3%), 540.26 (7.2%)
Elemental Analysis: C, 69.13; H, 7.11; O, 23.76

Position	P1-F1	**Instrument Name**	Instrument 1	**User Name**			
InjPosition		**SampleType**	Sample	**IRM Calibration Status**	Success		
ACQ Method	0103.m	**Comment**		**Acquired Time**	5/16/2014 2:16:06 PM