

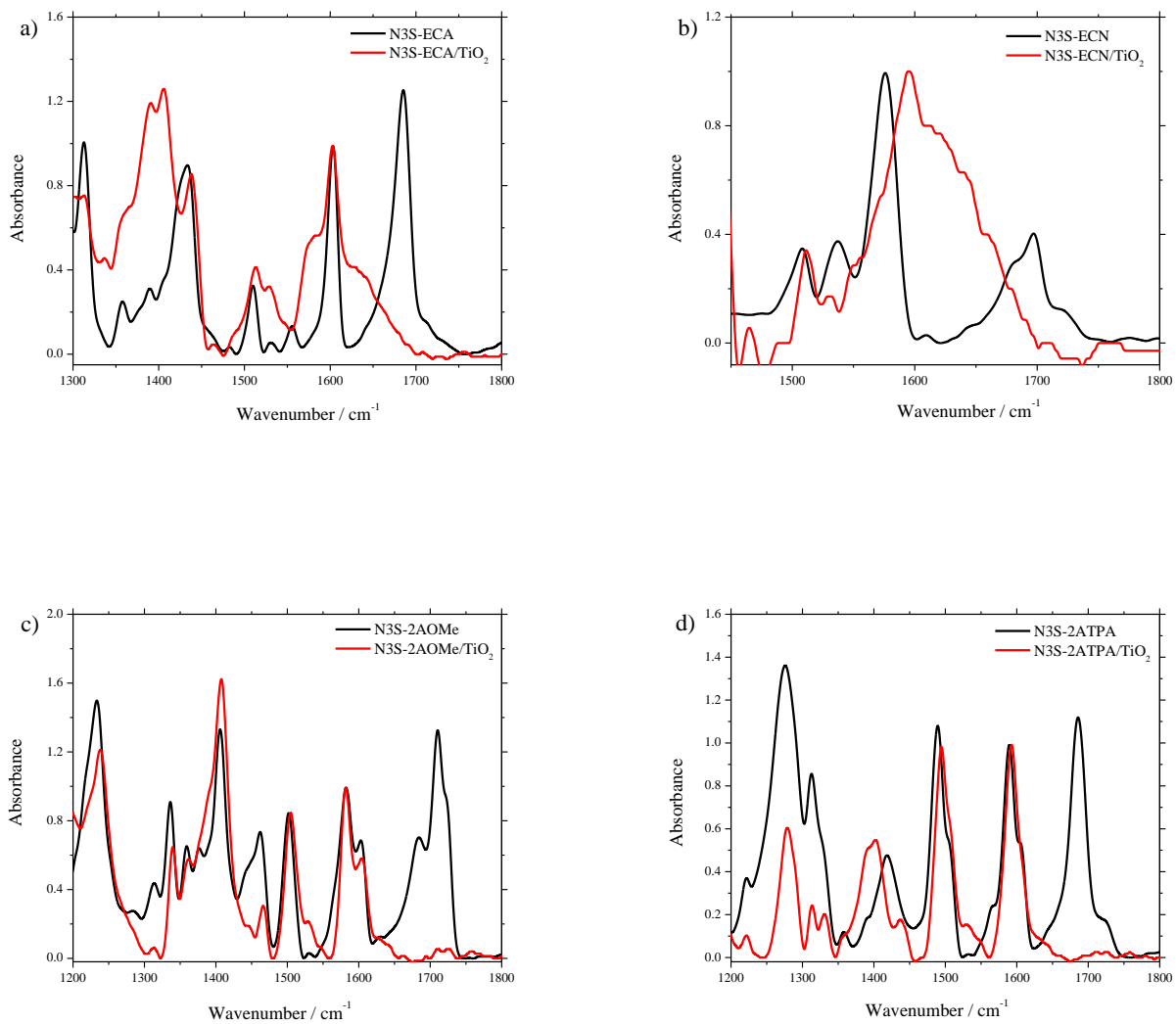
## Supporting information

### **Synthesis of Carboxylate functionalized A<sub>3</sub>B and A<sub>2</sub>B<sub>2</sub> Thiaporphyrins and their application in Dye-Sensitized Solar Cells**

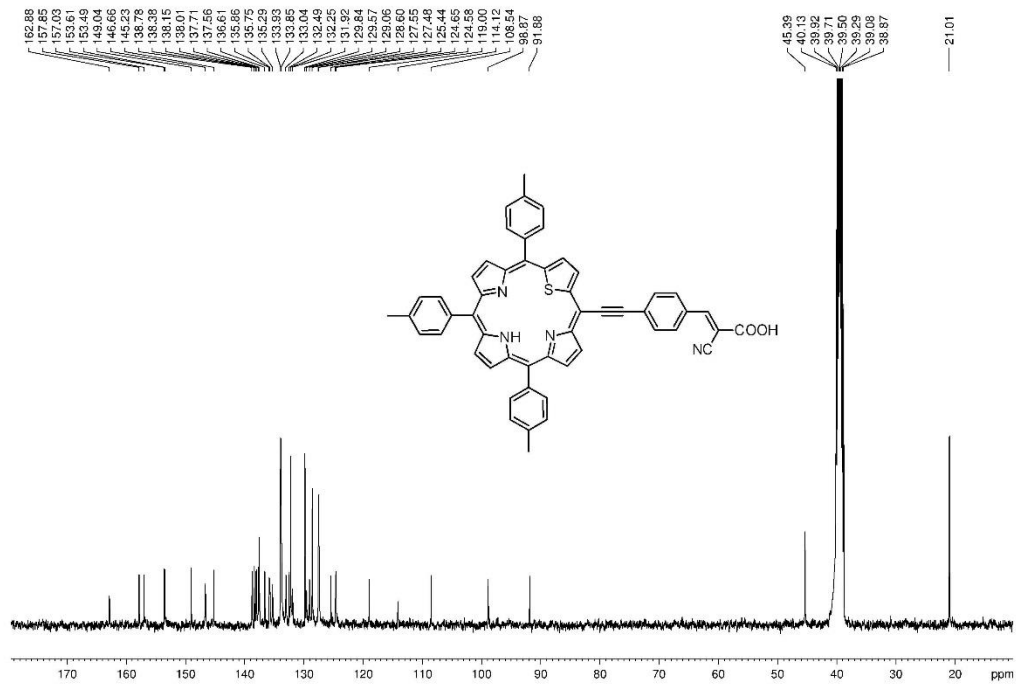
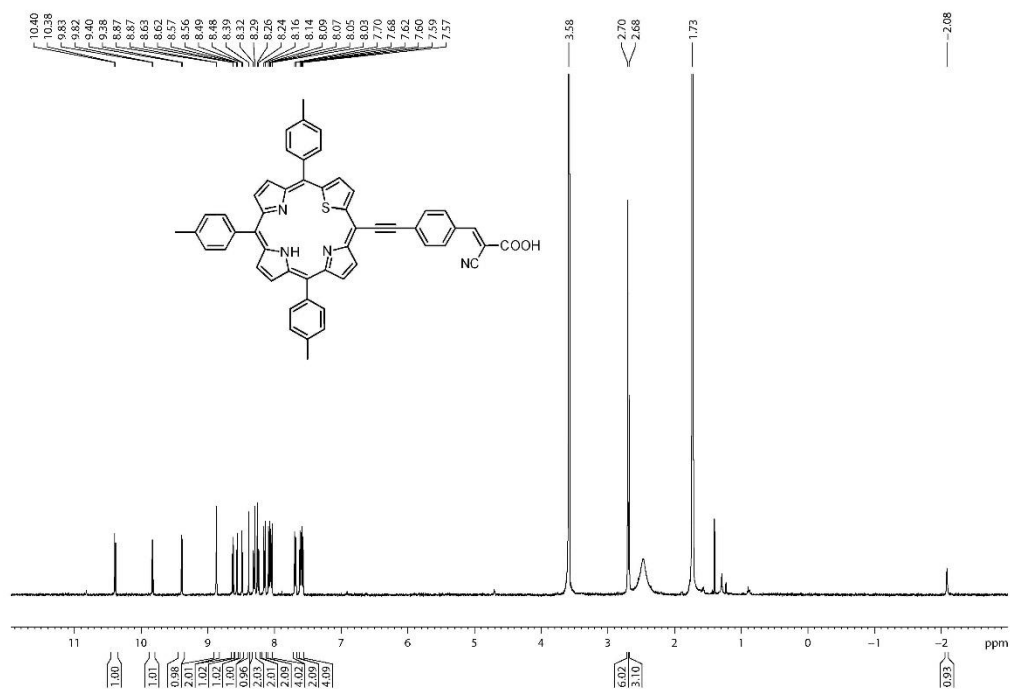
Sandeep B. Mane and Chen-Hsiung Hung\*

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1. Figure S1: ATR-FTIR spectra of neat thiaporphyrins contrasted with thiaporphyrins on  $\text{TiO}_2$  for N3S-ECA, N3S-ECN, N3S-2AOMe, and N3S-2ATPA
2.  $^1\text{H}$ ,  $^{13}\text{C}$  NMR spectra and HR-Mass Spectra for N3S-ECN, N3S-CA, N3S-2AOMe, N3S-2ATol, and N3S-2ATPA



**Figure S1.** ATR-FTIR spectra of neat thiaporphyrins contrasted with thiaporphyrins on  $\text{TiO}_2$ . a) N3S-ECA, b) N3S-ECN, c) N3S-2AOMe, and d) N3S-2ATPA



san211 (HR-ESI)

### Elemental Composition Report

#### Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 1000.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

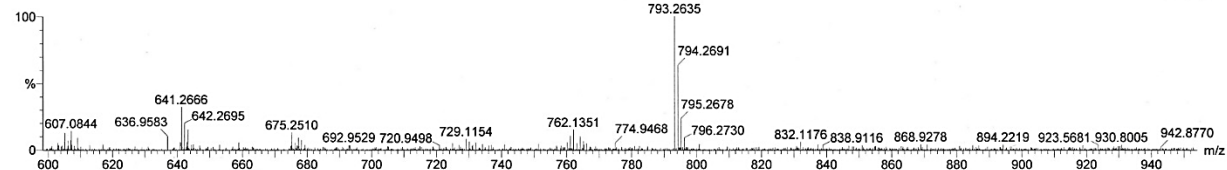
10 formula(e) evaluated with 1 results within limits (up to 100 closest results for each mass)

Elements Used:

C: 0-8000 H: 0-4000 N: 4-4 O: 2-2 S: 1-1

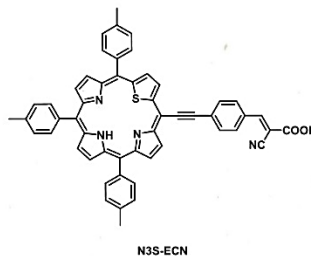
san211

0901\_san211 29 (2.857) Cm (29-100)

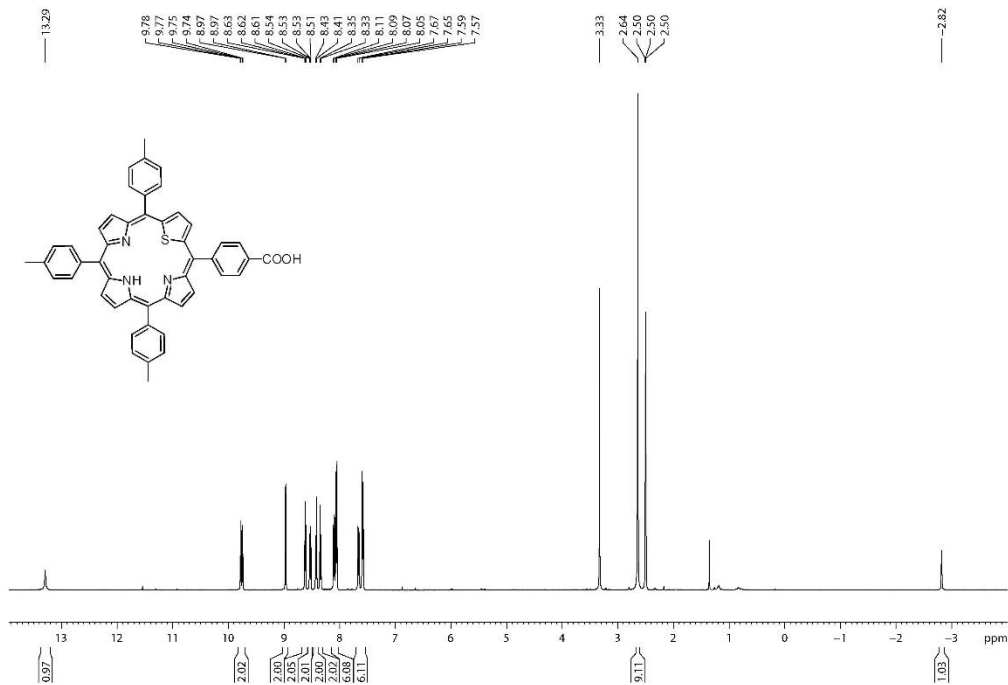


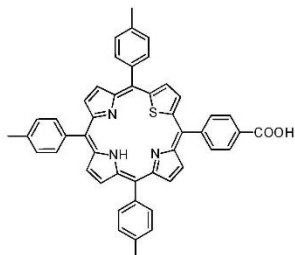
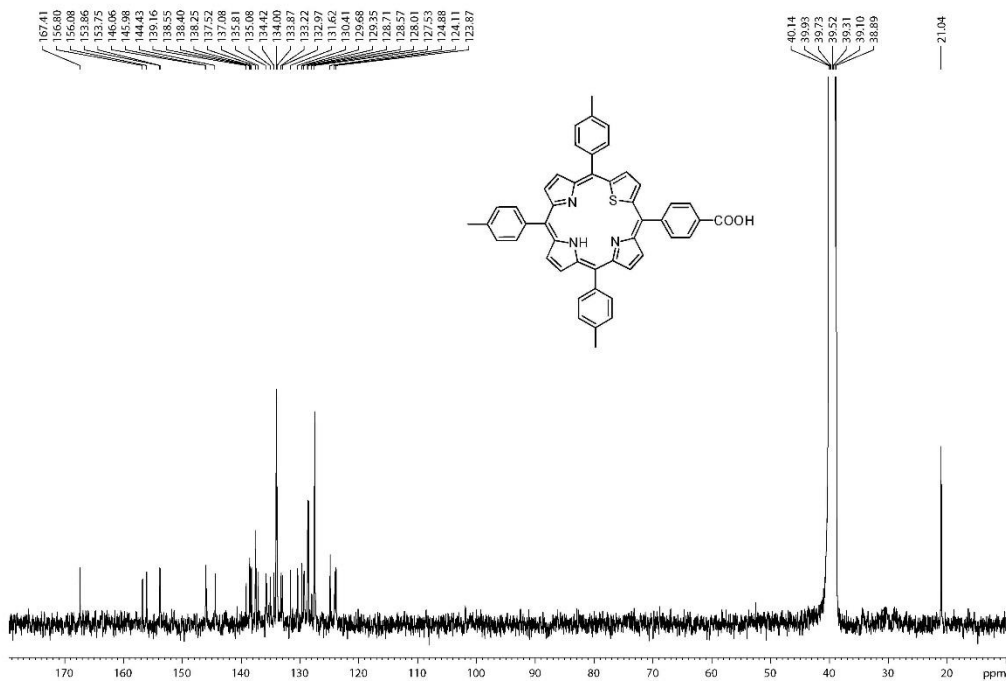
Minimum: -1.5  
Maximum: 5.0 100.0 1000.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
793.2635	793.2637	-0.2	-0.3	37.5	27.8	0.0	C53 H37 N4 O2 S



01-Sep-2010  
18:36:27  
1: TOF MS ES+  
5.91e+002





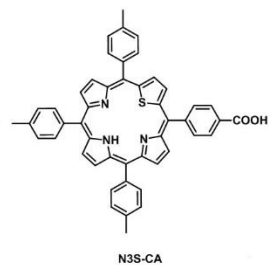
san-377 (HR-ESI)

Elemental Composition Report

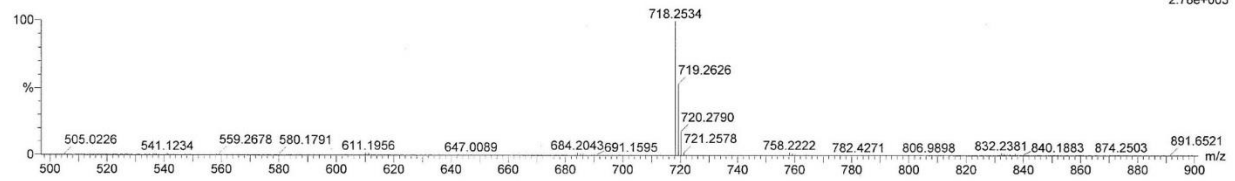
Single Mass Analysis  
 Tolerance = 50.0 PPM / DBE: min = -100.0, max = 1000.0  
 Element prediction: Off  
 Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions  
 23 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)  
 Elements Used:  
 C: 0-400 H: 0-1000 N: 3-3 O: 2-2 S: 1-1  
 san-377

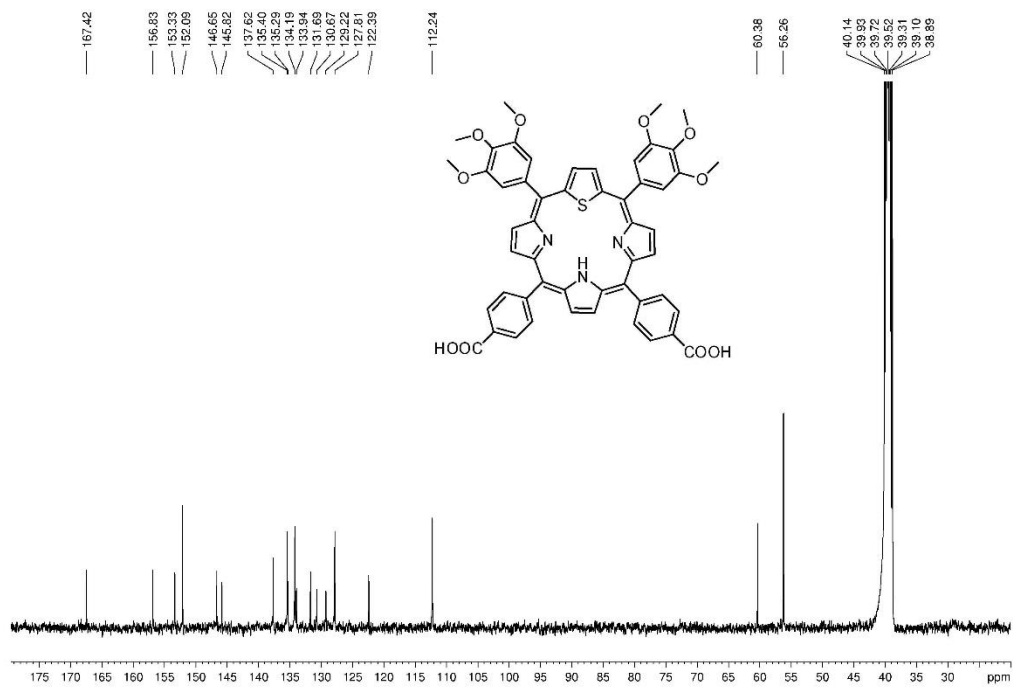
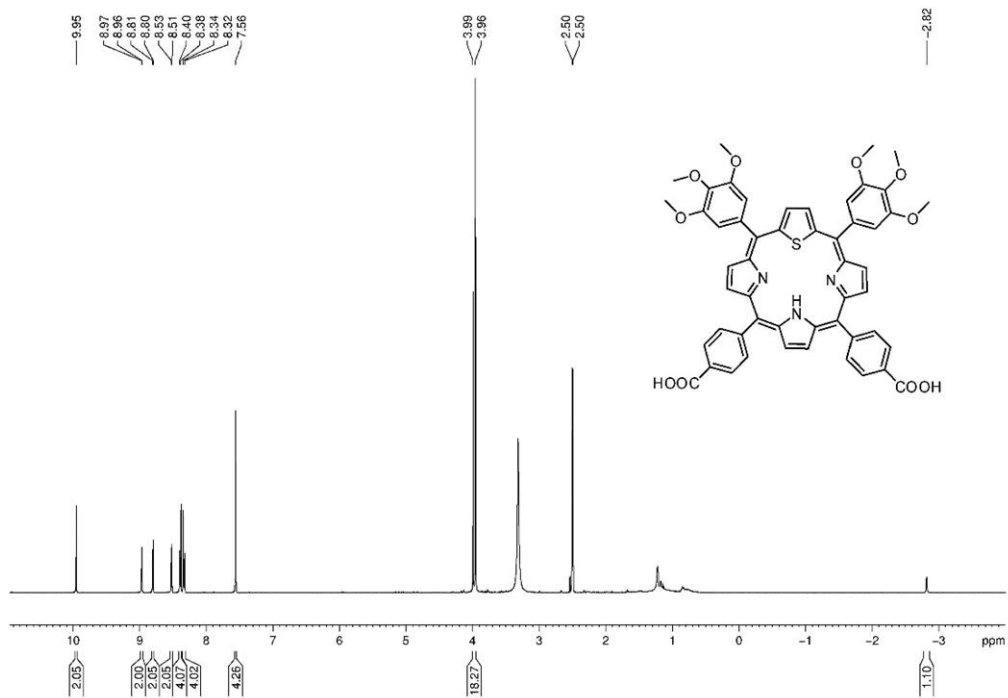
1016\_san-377 34 (1.897) Cm (34-1x10.000)



17-Oct-2012  
 11:20:49  
 1: TOF MS ES+  
 2.78e+003



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
718.2534	718.2528	0.6	0.8	32.5	35.5	0.0	C <sub>48</sub> H <sub>36</sub> N <sub>3</sub> O <sub>2</sub> S



san-283 (HR-ESI)

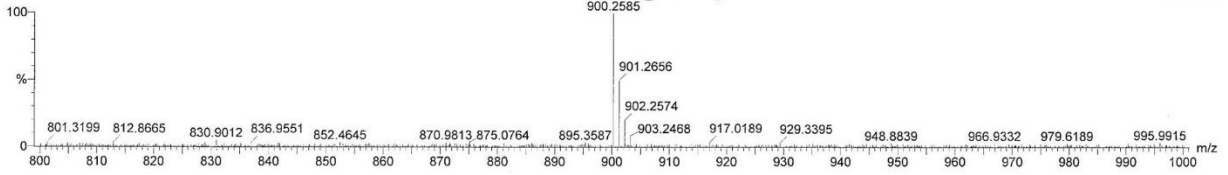
### Elemental Composition Report

#### Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -100.0, max = 1000.0  
Element prediction: Off  
Number of isotope peaks used for i-FIT = 2

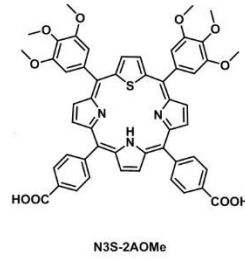
Monoisotopic Mass, Even Electron Ions  
23 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)  
Elements Used:  
C: 0-400 H: 0-1000 N: 3-3 O: 10-10 S: 1-1  
san-283

1016\_san-283.95 (5.299)

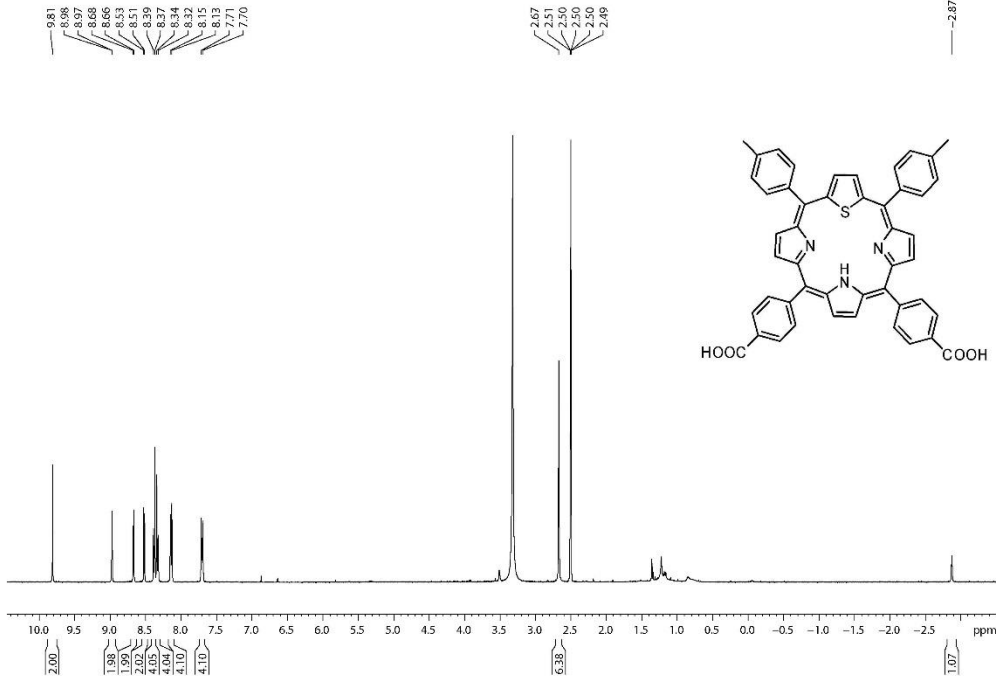


Minimum: -100.0  
Maximum: 50.0 50.0 1000.0

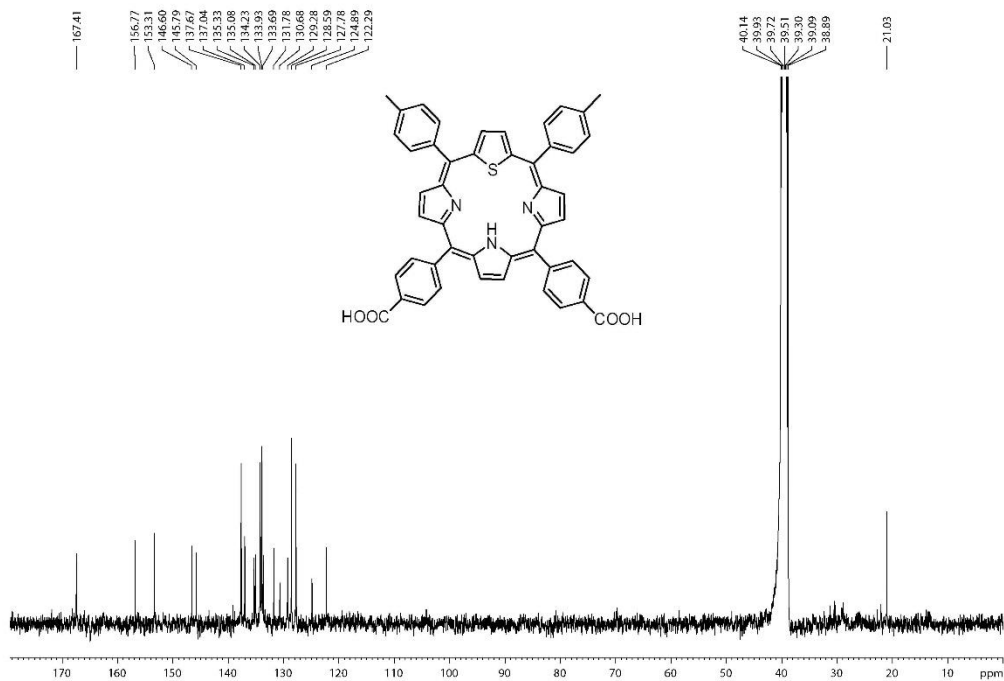
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
900.2585	900.2591	-0.6	-0.7	33.5	19.6	0.0	C52 H42 N3 O10 S



17-Oct-2012  
10:46:59  
1: TOF MS ES+  
1.84e+002







san411 (HR-ESI)

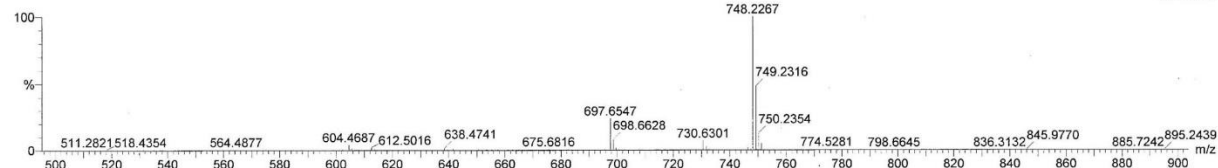
Elemental Composition Report

Single Mass Analysis

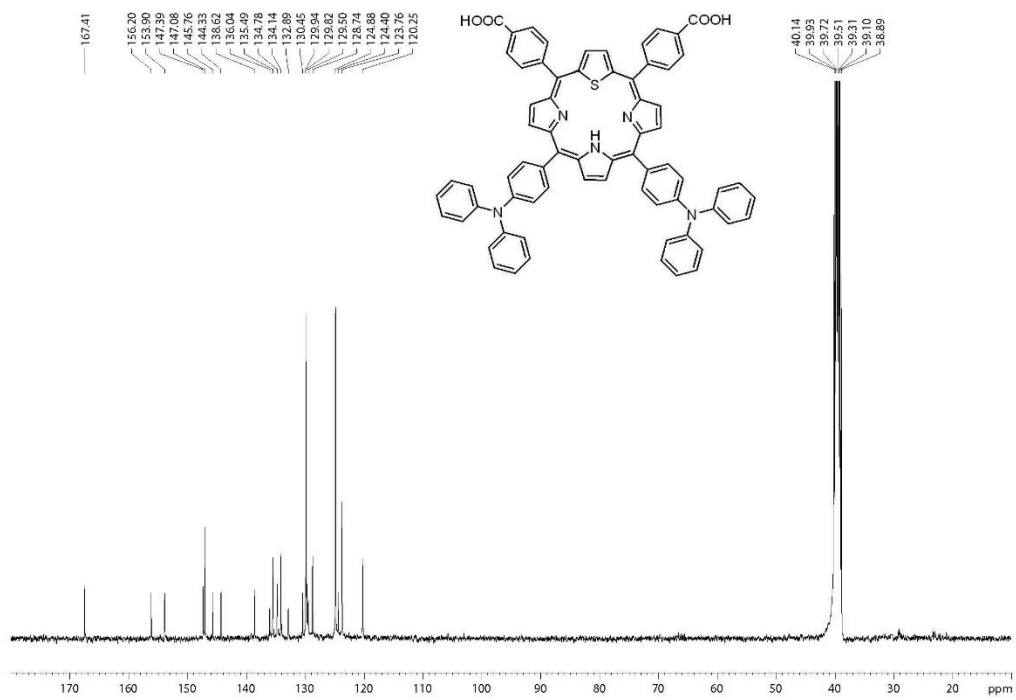
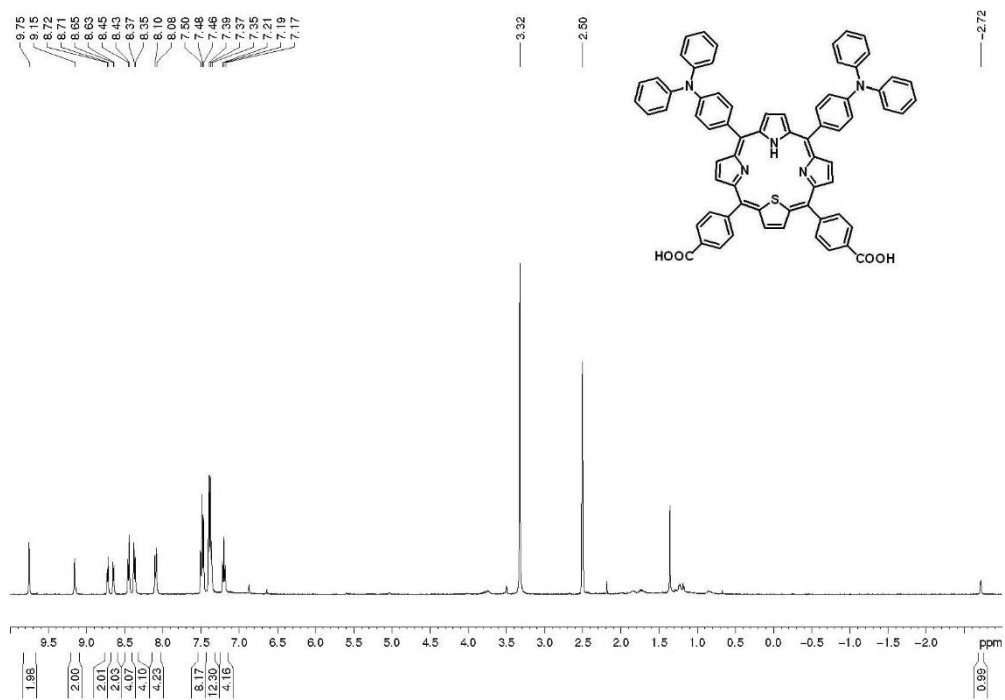
Tolerance = 20.0 PPM / DBE: min = -100.0, max = 1000.0  
 Element prediction: Off  
 Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions  
 22 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)  
 Elements Used:  
 C: 0-400 H: 0-1000 N: 3-3 O: 4-4 S: 1-1  
 san411

0912\_san411 20 (1.089)



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
748.2267	748.2270	-0.3	-0.4	33.5	53.0	0.0	C48 H34 N3 O4 S



San 482 (HR-ESI)

### Elemental Composition Report

#### Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 1000.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

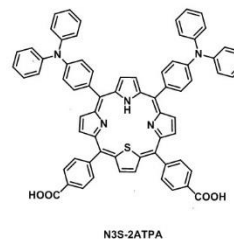
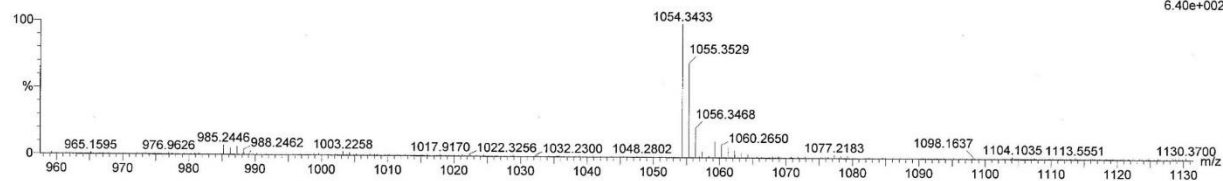
12 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-1000 H: 0-1000 N: 5-5 O: 4-4 S: 1-1

san 482

0930\_san 482 34 (1.896)



30-Sep-2013  
17:13:52  
1: TOF MS ES+  
6.40e+002

Minimum: -1.5  
Maximum: 5.0 20.0 1000.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
1054.3433	1054.3427	0.6	0.6	49.5	23.0	0.0	C70 H48 N5 O4 S