

# Supplementary Materials

Figure S1.  $^1\text{H-NMR}$  spectrum of compound **1** in  $\text{CDCl}_3$ .

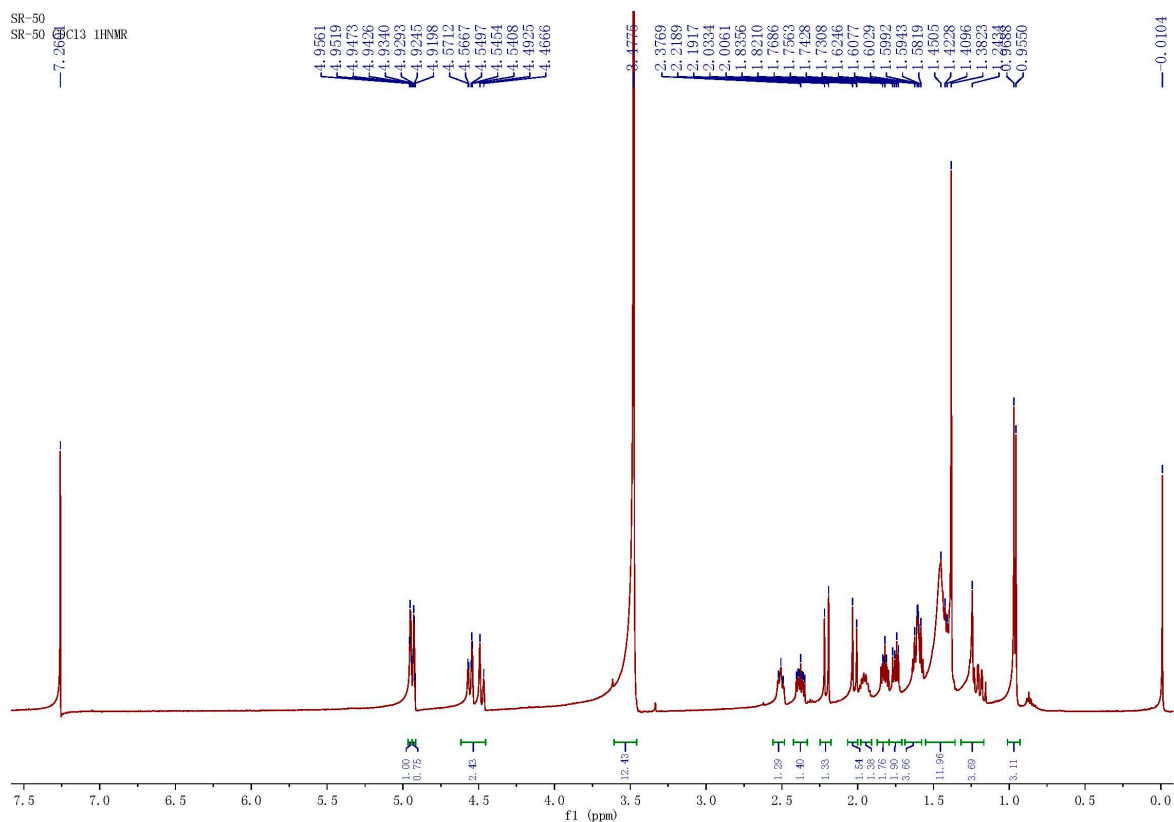
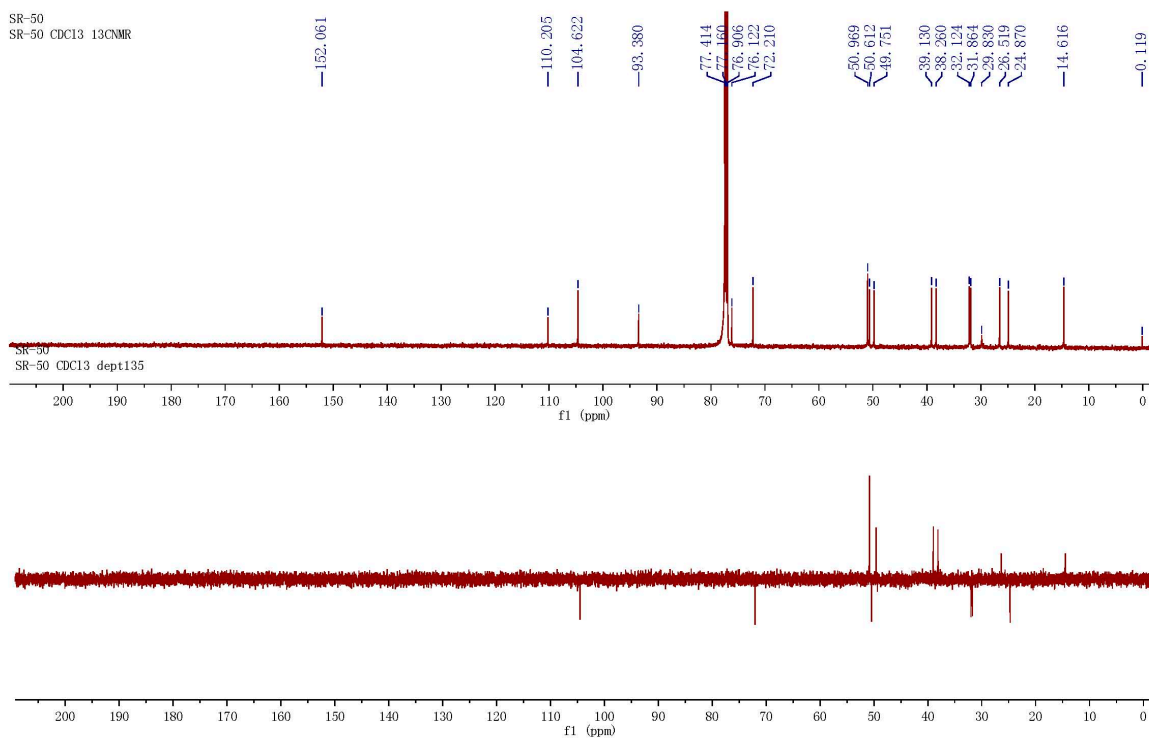
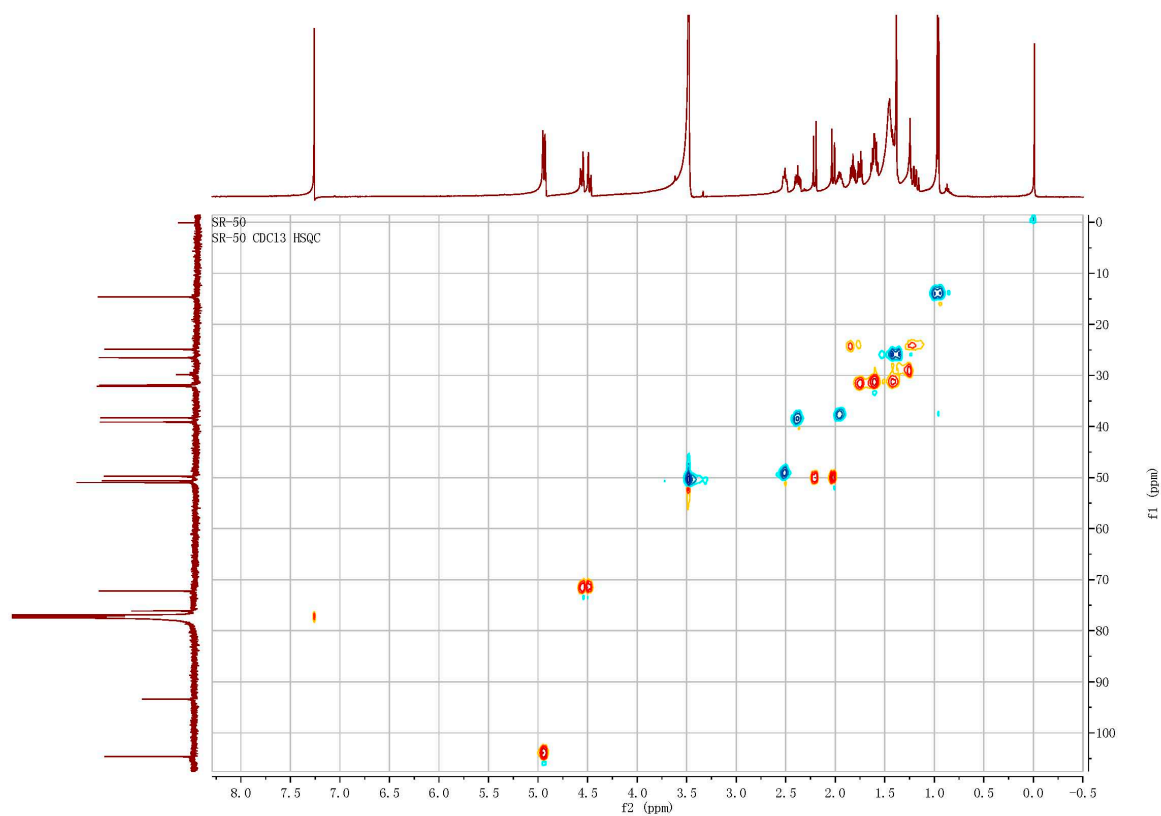
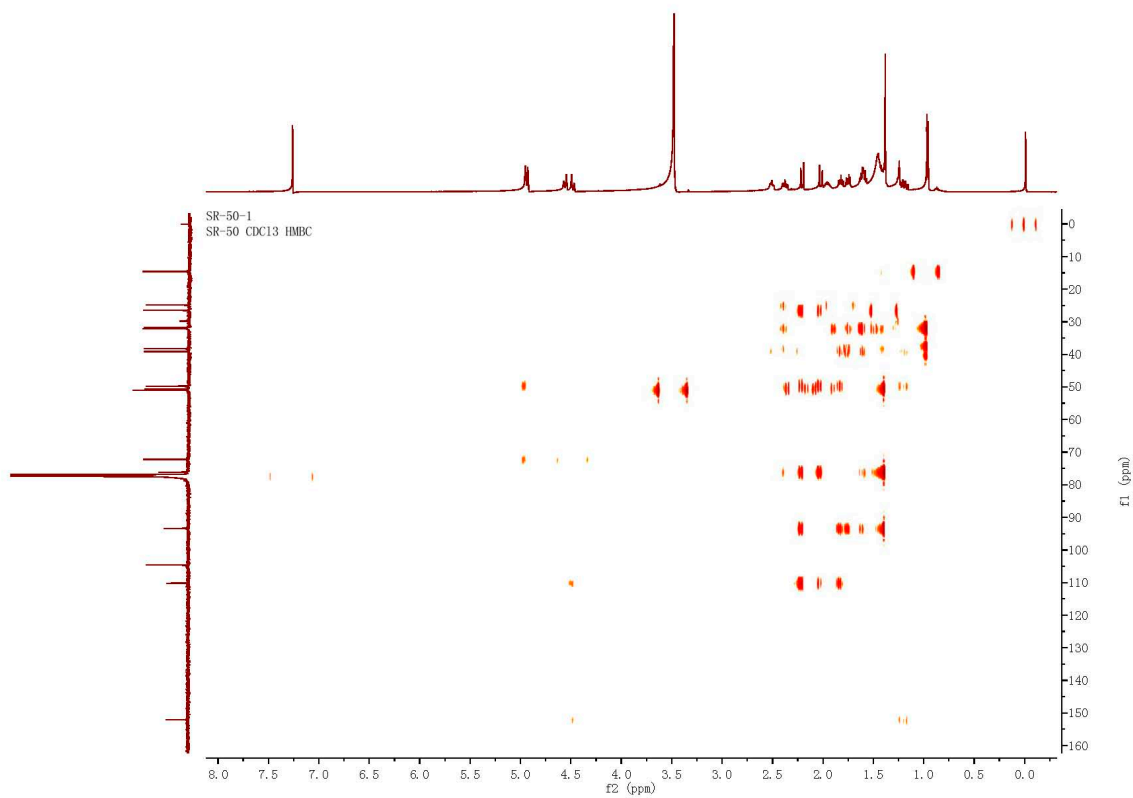


Figure S2.  $^{13}\text{C-NMR}$  and DEPT spectrum of compound **1** in  $\text{CDCl}_3$ .



**Figure S3.** HSQC spectrum of compound **1** in CDCl<sub>3</sub>.**Figure S4.** HMBC spectrum of compound **1** in CDCl<sub>3</sub>.

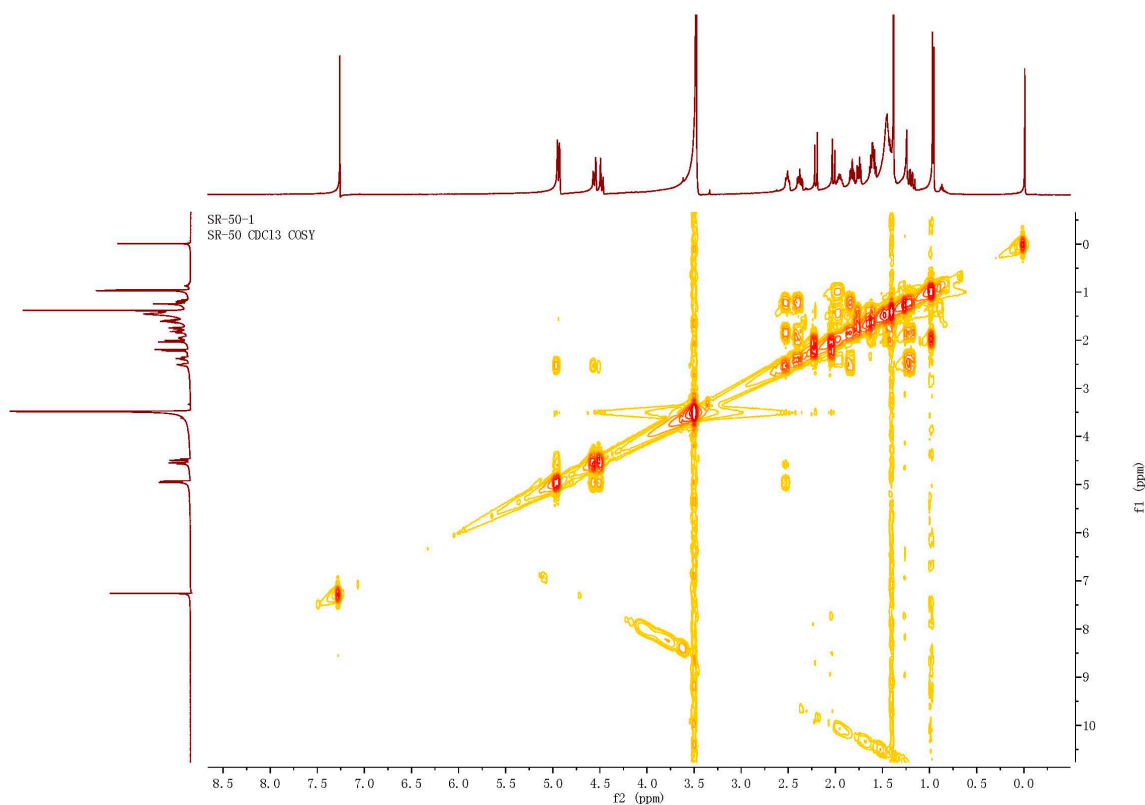
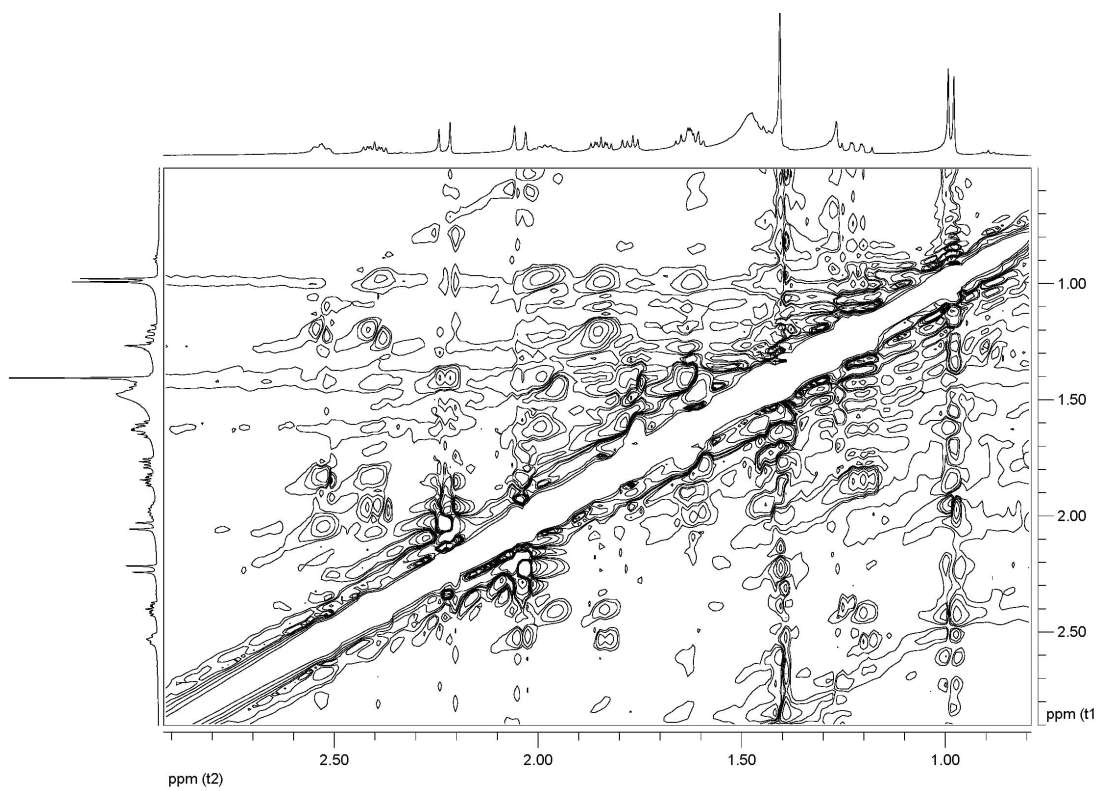
**Figure S5.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **1** in  $\text{CDCl}_3$ .**Figure S6.** ROESY spectrum of compound **1** in  $\text{CDCl}_3$ .

Figure S7. HREIMS spectrum of compound 1 in CHCl<sub>3</sub>.

## Elemental Composition Report

Page 1

## Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0  
 Selected filters: None

## Monoisotopic Mass, Odd and Even Electron Ions

13 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

## Elements Used:

C: 0-200 H: 0-400 O: 2-4

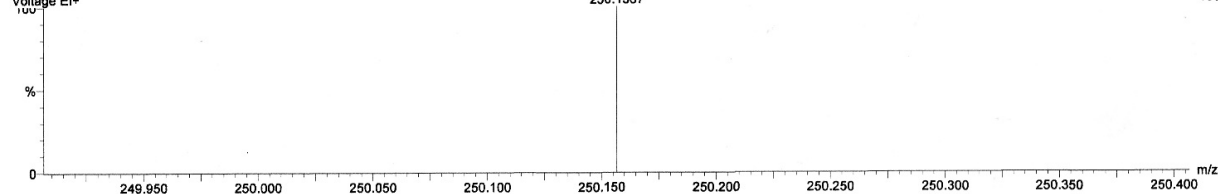
SR-50

11:08:52 02-Aug-2013

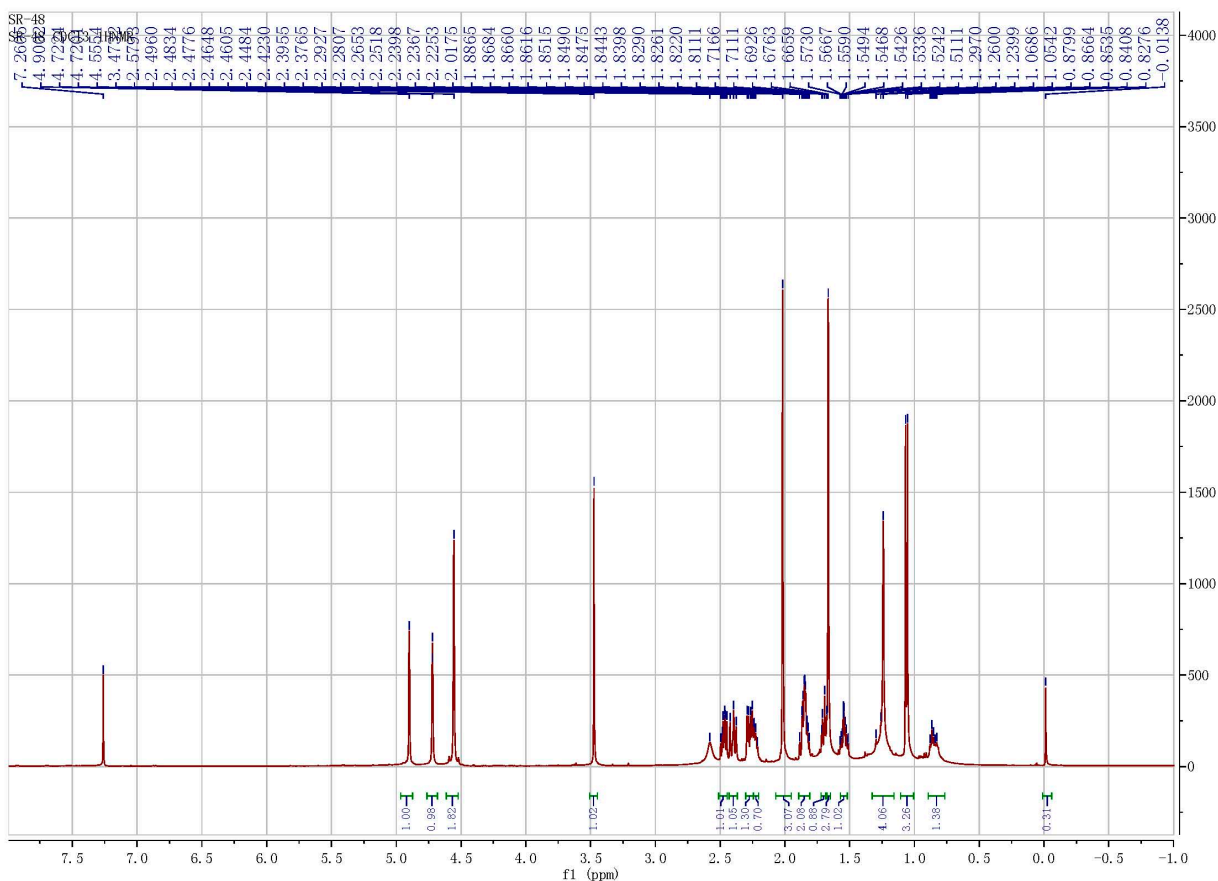
Voltage EI+

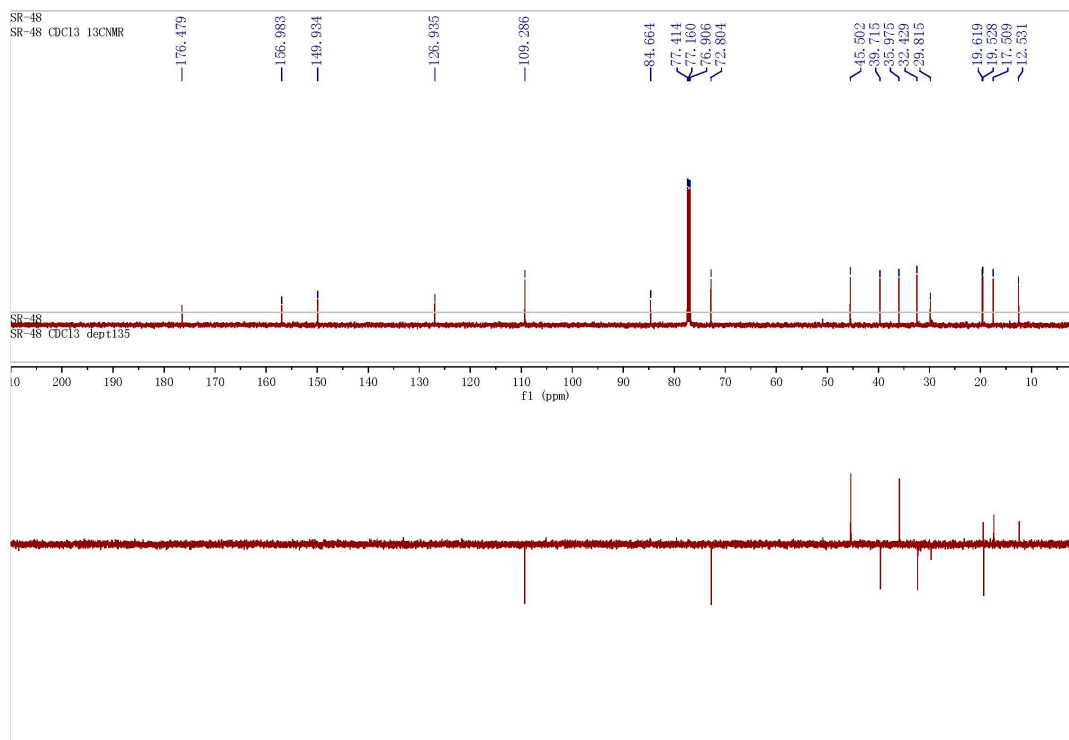
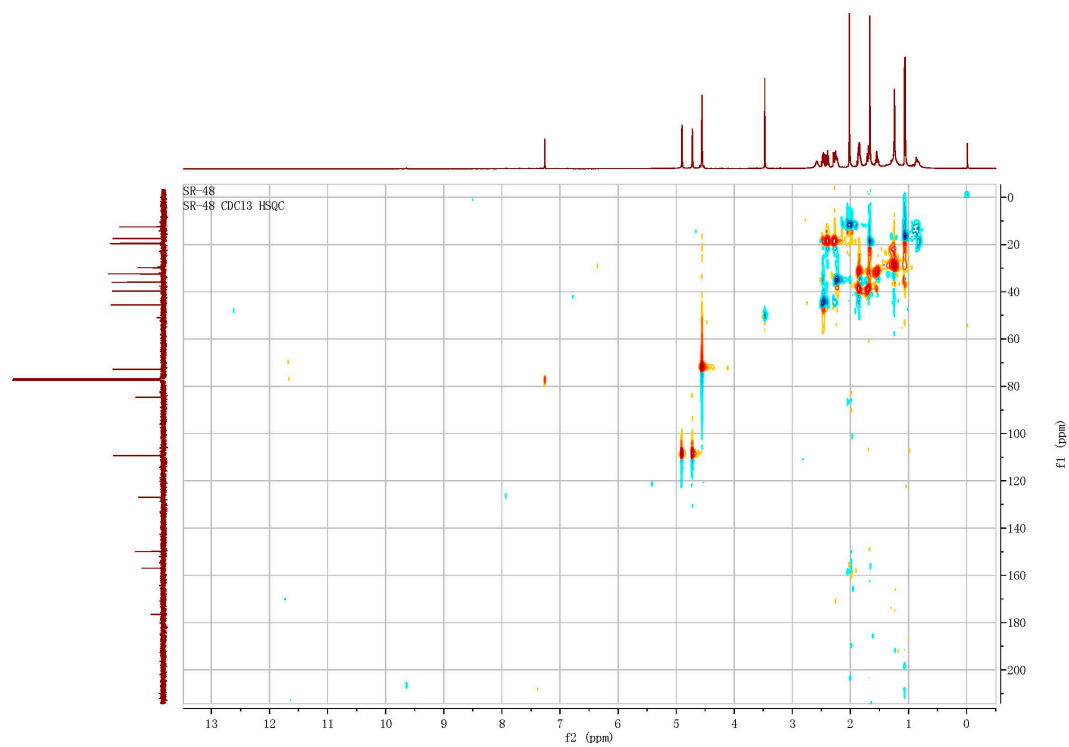
KIB  
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 250.1567

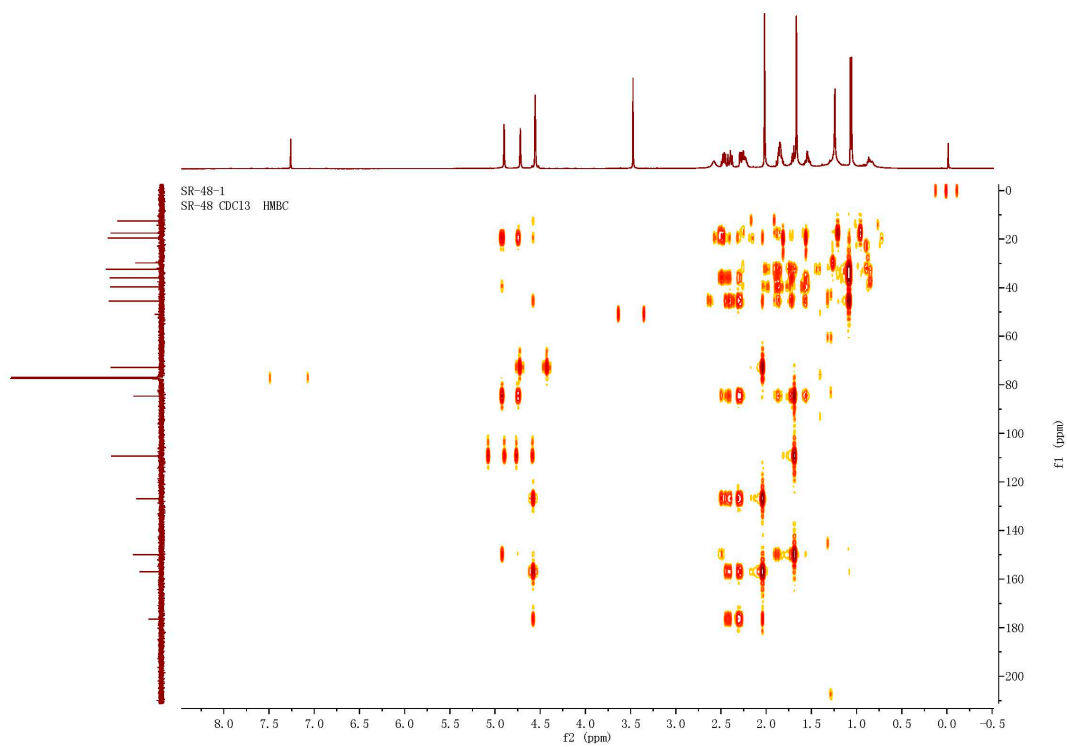
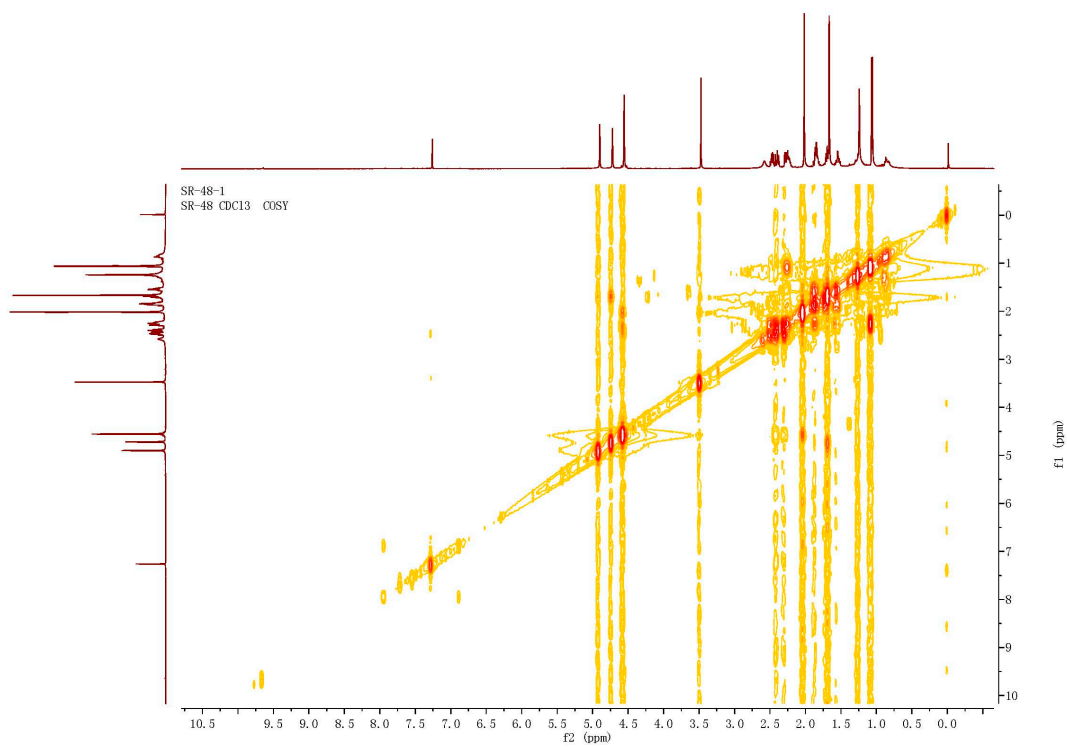
Autospec Premier  
 P776  
 199



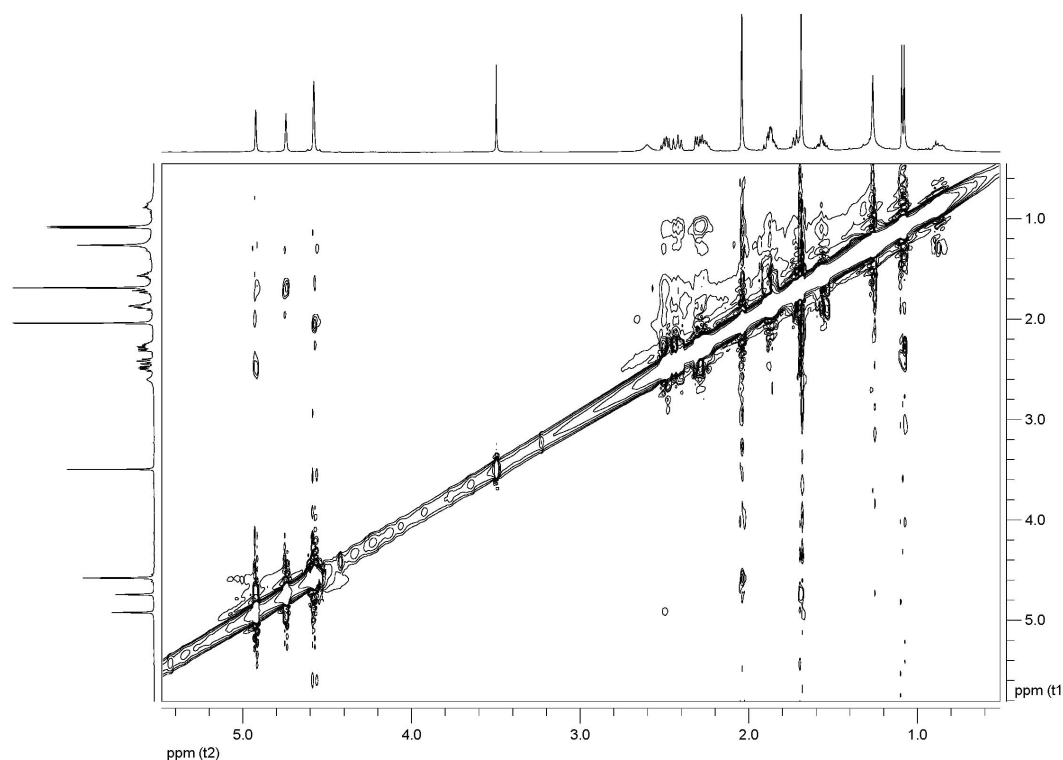
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
250.1567	250.1569	-0.2	-0.8	5.0	5546105.0	C15 H22 O3

Figure S8. <sup>1</sup>H-NMR spectrum of compound 2 in CDCl<sub>3</sub>.

**Figure S9.**  $^{13}\text{C}$ -NMR and DEPT spectrum of compound **2** in  $\text{CDCl}_3$ .**Figure S10.** HSQC spectrum of compound **2** in  $\text{CDCl}_3$ .

**Figure S11.** HMBC spectrum of compound **2** in CDCl<sub>3</sub>.**Figure S12.** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of compound **2** in CDCl<sub>3</sub>.

**Figure S13.** ROESY spectrum of compound **2** in CDCl<sub>3</sub>.



**Figure S14.** HREIMS spectrum of compound **2** in CHCl<sub>3</sub>.

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0  
Selected filters: None

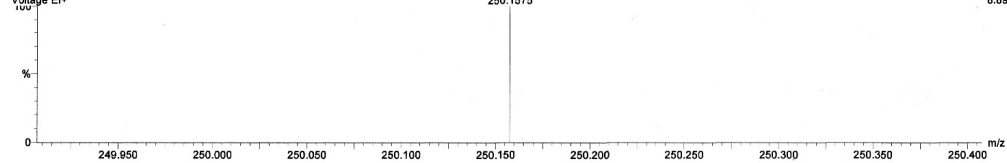
Monoisotopic Mass, Odd and Even Electron Ions  
13 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

Elements Used:  
C: 0-200 H: 0-400 O: 2-4

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11:04:14 02-Aug-2013  
Voltage Et+

KIB  
M130802EA-09AFAMM 7 (0.643)  
250.1575

Autospec Premier  
F776  
8.89



Mass	Calc. Mass	mDa	PPM	DBE	1-FIT	Formula
250.1575	250.1569	0.6	2.4	5.0	5546025.5	C15 H22 O3