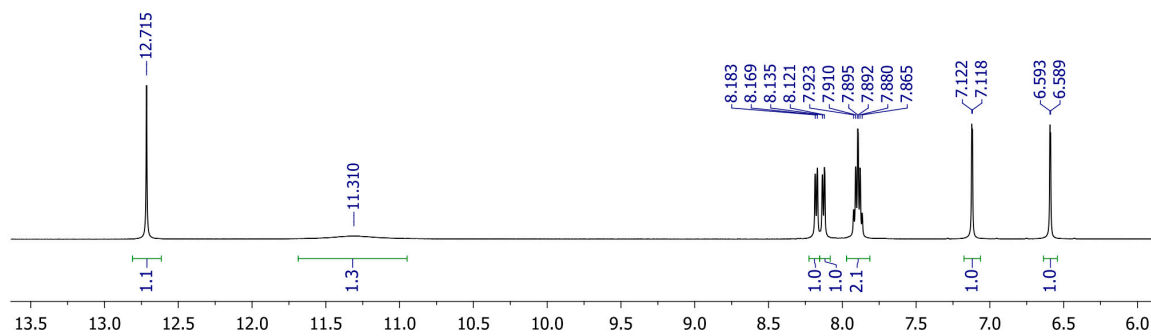


# Supplementary Materials: 1-Hydroxy-3-(3-methylbut-2-enyloxy)anthracene-9,10-dione

Siti Nurbayti, Didin Mujahidin and Yana M. Syah



1,3-Dihydroxyanthracene-9,10-dione,  $^{13}\text{C}$  NMR

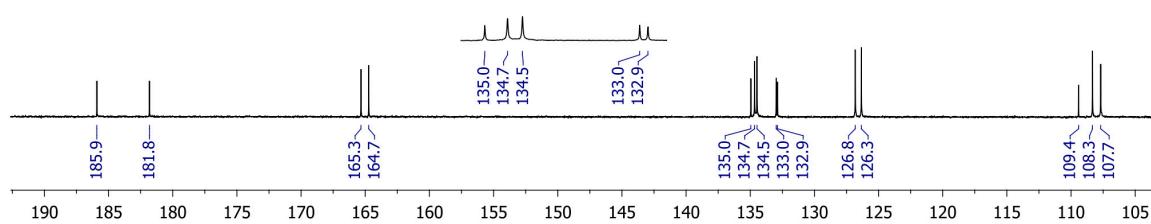


Figure S1.  $^1\text{H}$  and  $^{13}\text{C}$ -NMR spectra of 1,3-Dihydroxyanthracene-9,10-dione (3).

1,3-Dihydroxyanthracene-9,10-dione, HSQC

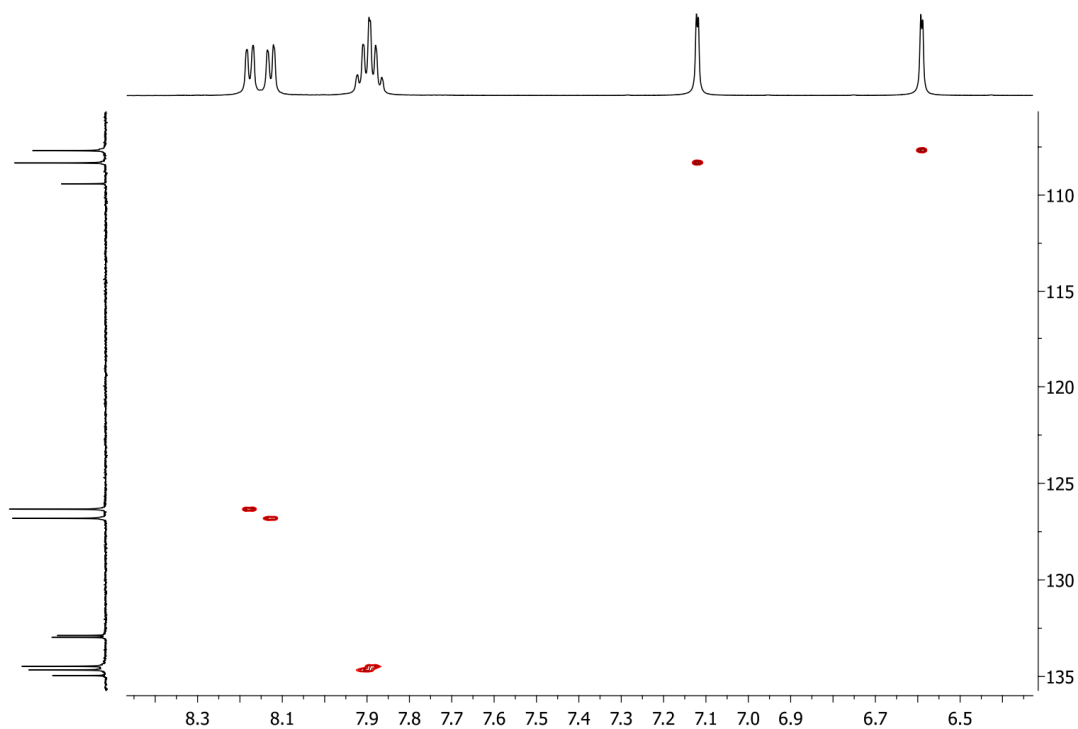
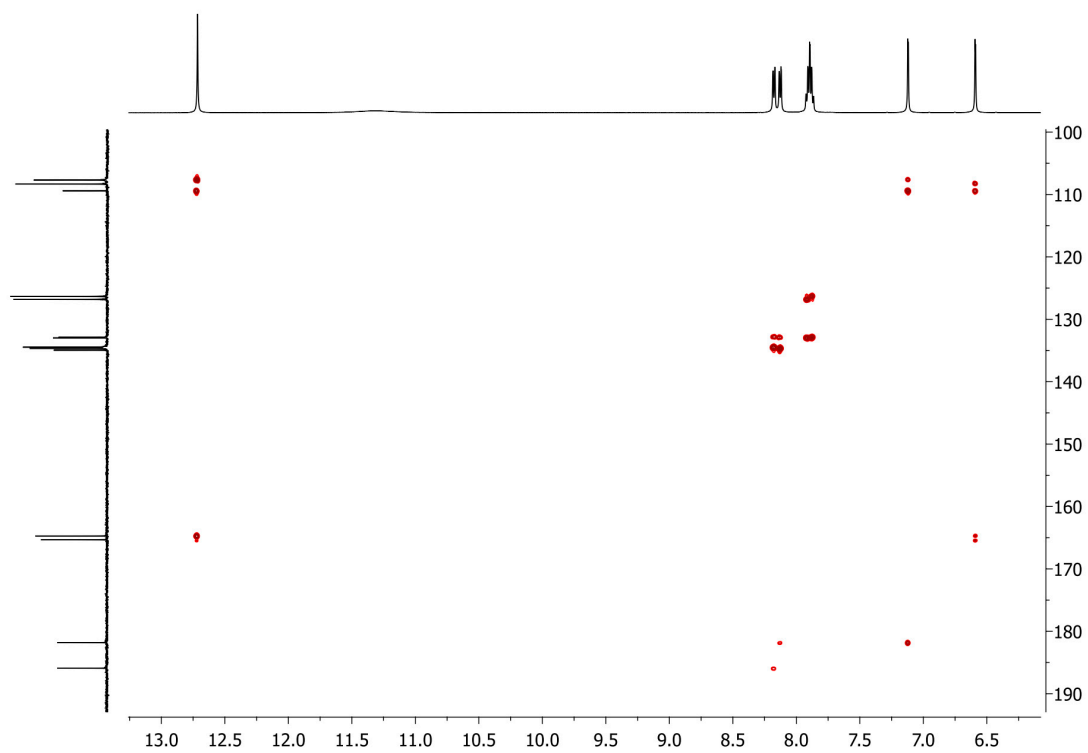
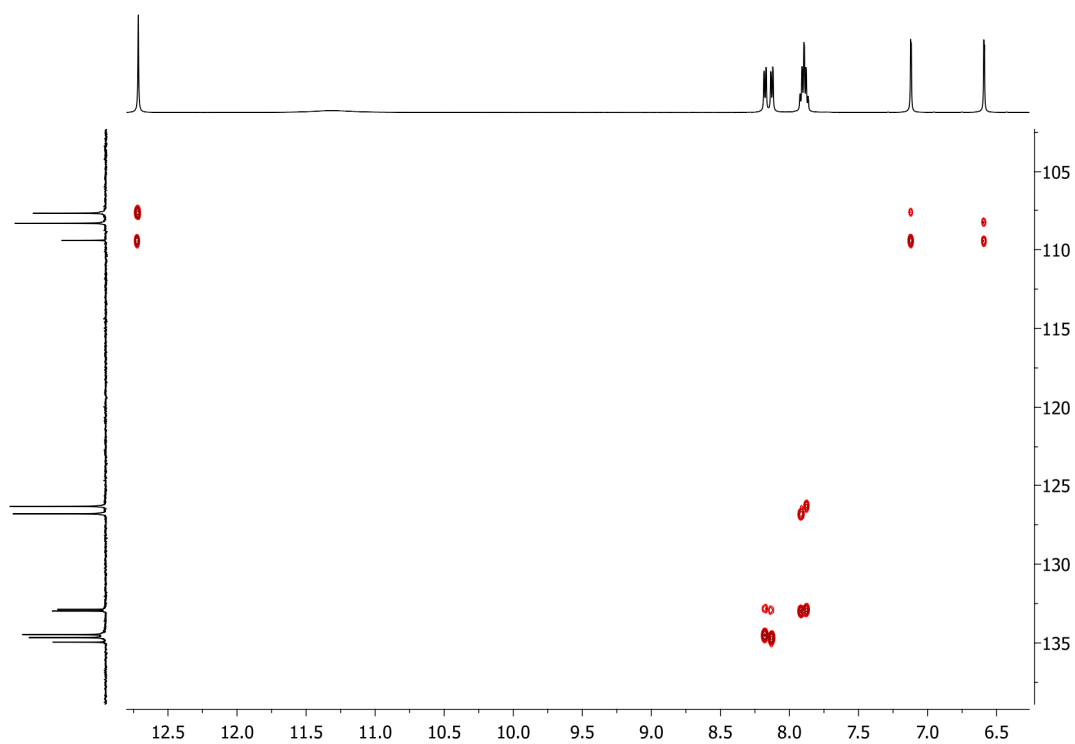


Figure S2. HSQC spectrum of 1,3-Dihydroxyanthracene-9,10-dione (3).

## 1,3-Dihydroxyanthracene-9,10-dione, HMBC

**Figure S3.** HMBC spectrum of 1,3-Dihydroxyanthracene-9,10-dione (3).

## 1,3-Dihydroxyanthracene-9,10-dione, HMBC

**Figure S4.** HMBC spectrum of 1,3-Dihydroxyanthracene-9,10-dione (3).

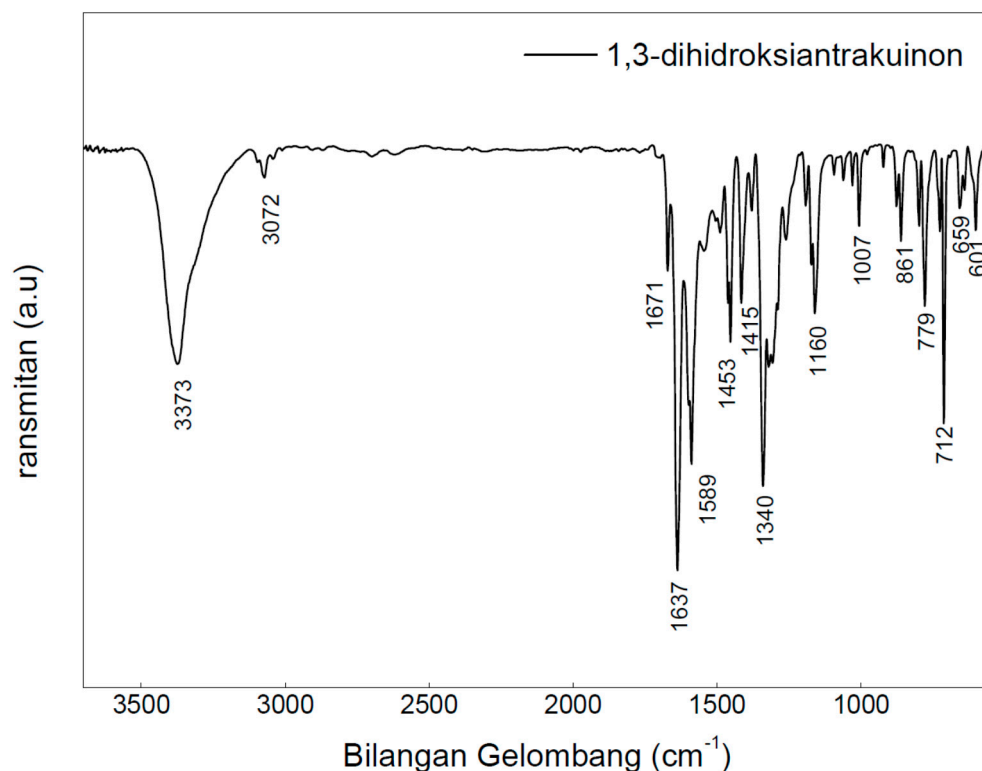


Figure S5. IR spectrum of 1,3-Dihydroxyanthracene-9,10-dione (3).

### Elemental Composition Report

Page 1

#### Single Mass Analysis (displaying only valid results)

Tolerance = 10.0 mDa / DBE: min = 1.0, max = 30.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

62 formula(e) evaluated with 3 results within limits (up to 1 best isotopic matches for each mass)

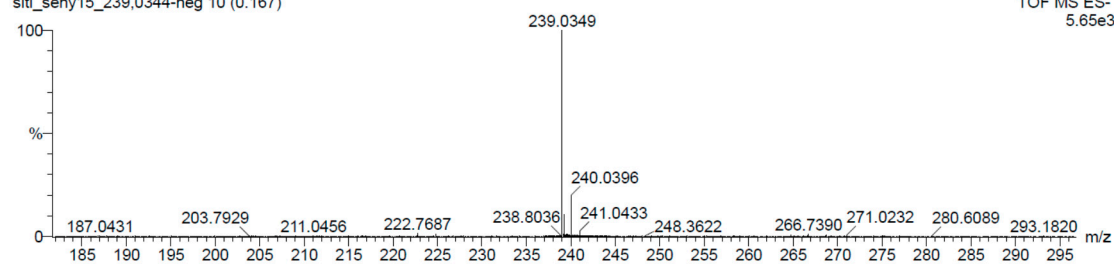
Elements Used:

C: 0-500 H: 0-1000 O: 0-20 Na: 0-1

standar

siti\_seny15\_239.0344-neg 10 (0.167)

TOF MS ES-  
5.65e3



Minimum: 1.0  
Maximum: 10.0 10.0 30.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
239.0349	239.0344	0.5	2.1	11.5	22.7	C14 H7 O4

Figure S6. HRESI-TOF mass spectrum (negative mode) of 1,3-Dihydroxyanthracene-9,10-dione (3).

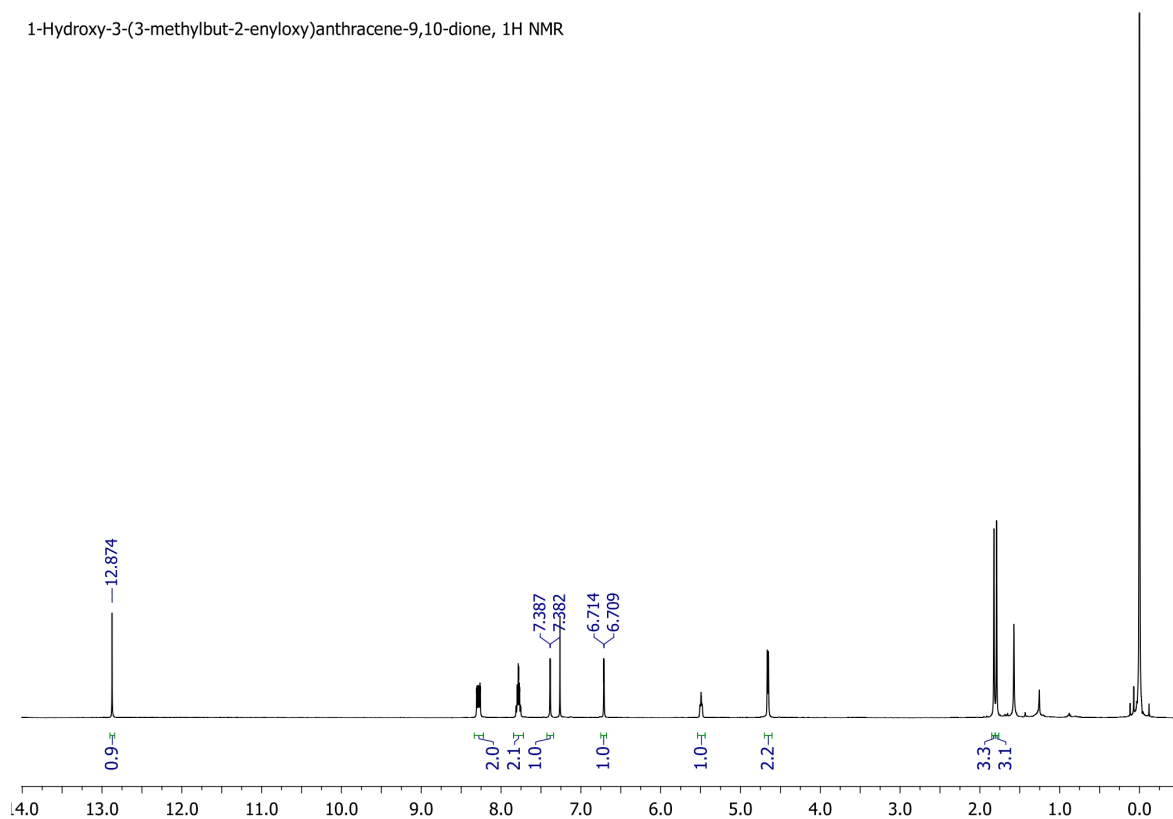
1-Hydroxy-3-(3-methylbut-2-enyloxy)anthracene-9,10-dione, <sup>1</sup>H NMR

Figure S7. <sup>1</sup>H-NMR spectrum of 1-Hydroxy-3-(3-methylbut-2-enyloxy)anthracene-9,10-dione (4).

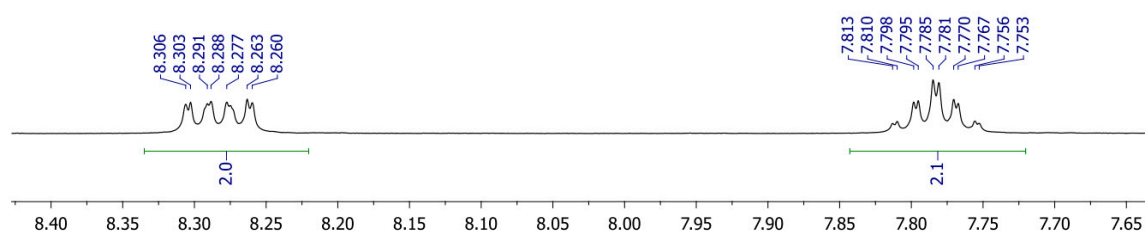


Figure S8. <sup>1</sup>H-NMR spectrum of 1-Hydroxy-3-(3-methylbut-2-enyloxy)anthracene-9,10-dione (4).

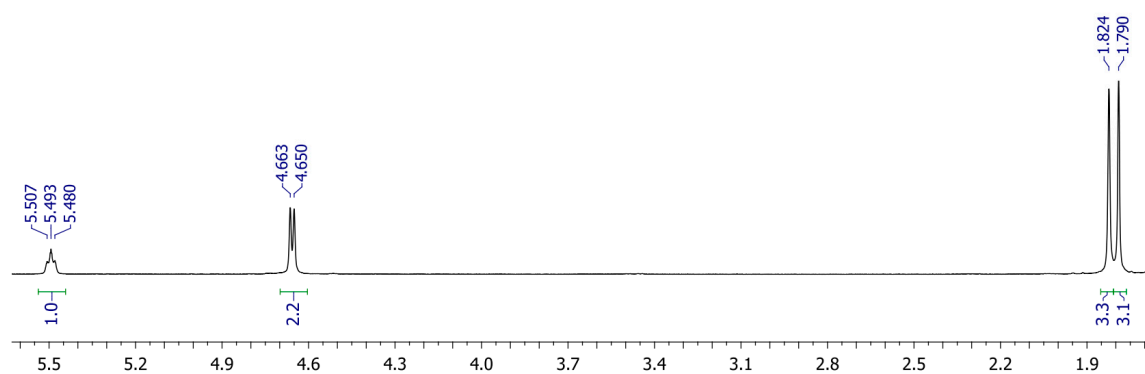


Figure S9. <sup>1</sup>H-NMR spectrum of 1-Hydroxy-3-(3-methylbut-2-enyloxy)anthracene-9,10-dione (4).

1-Hydroxy-3-(3-methylbut-2-enyloxy)anthracene-9,10-dione, <sup>13</sup>C NMR

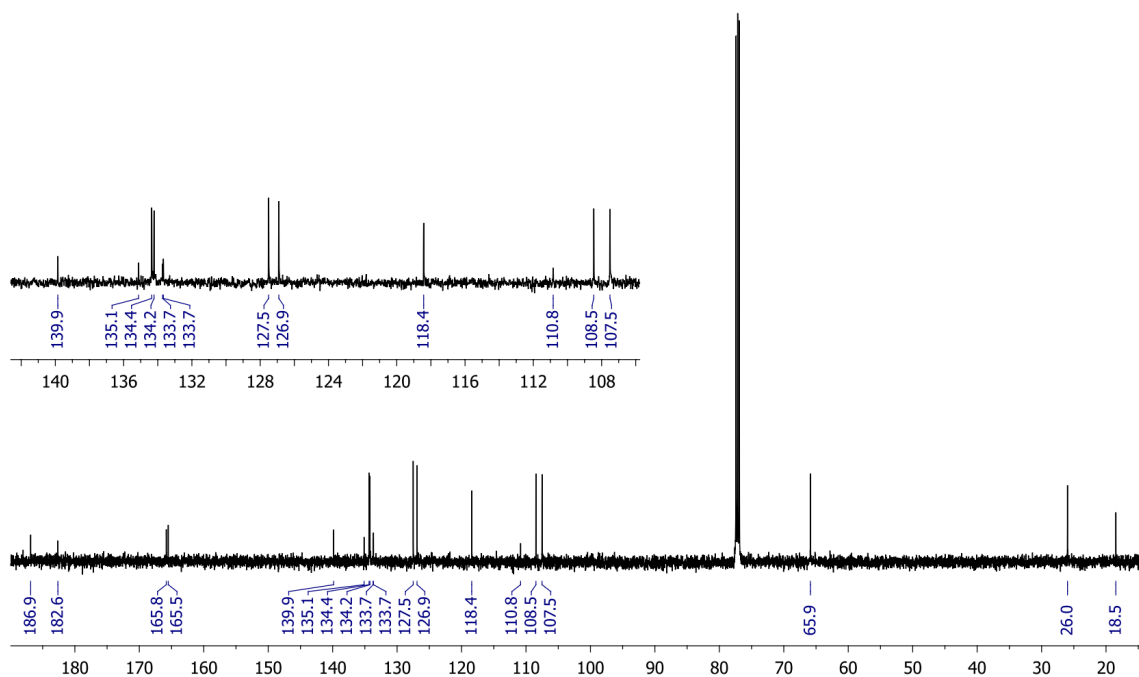


Figure S10. <sup>13</sup>C-NMR spectrum of 1-Hydroxy-3-(3-methylbut-2-enyloxy)anthracene-9,10-dione (4).

1-Hydroxy-3-(3-methylbut-2-enyloxy)anthracene-9,10-dione, HSQC

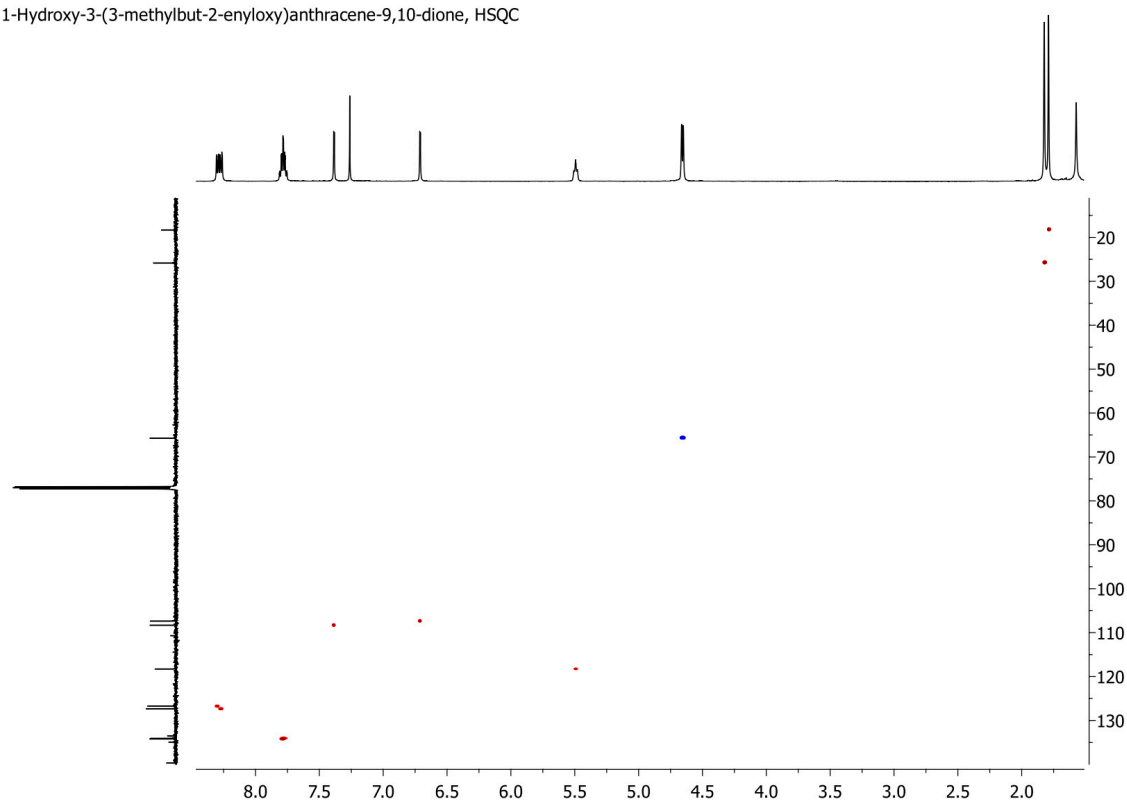
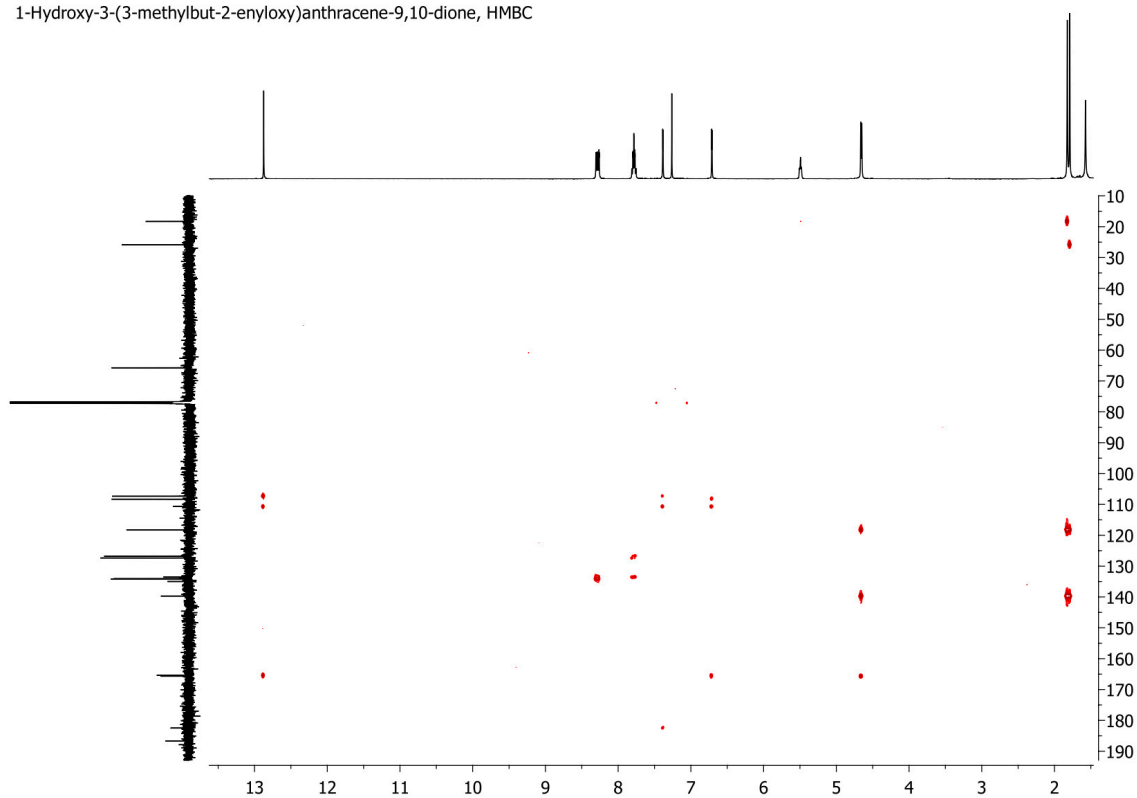
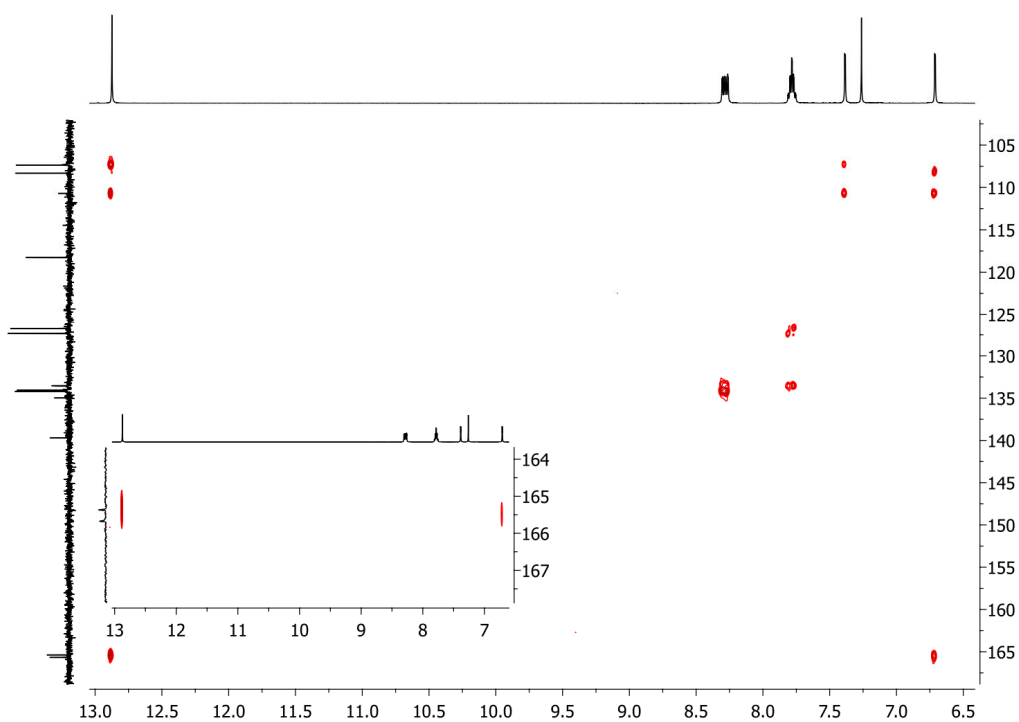


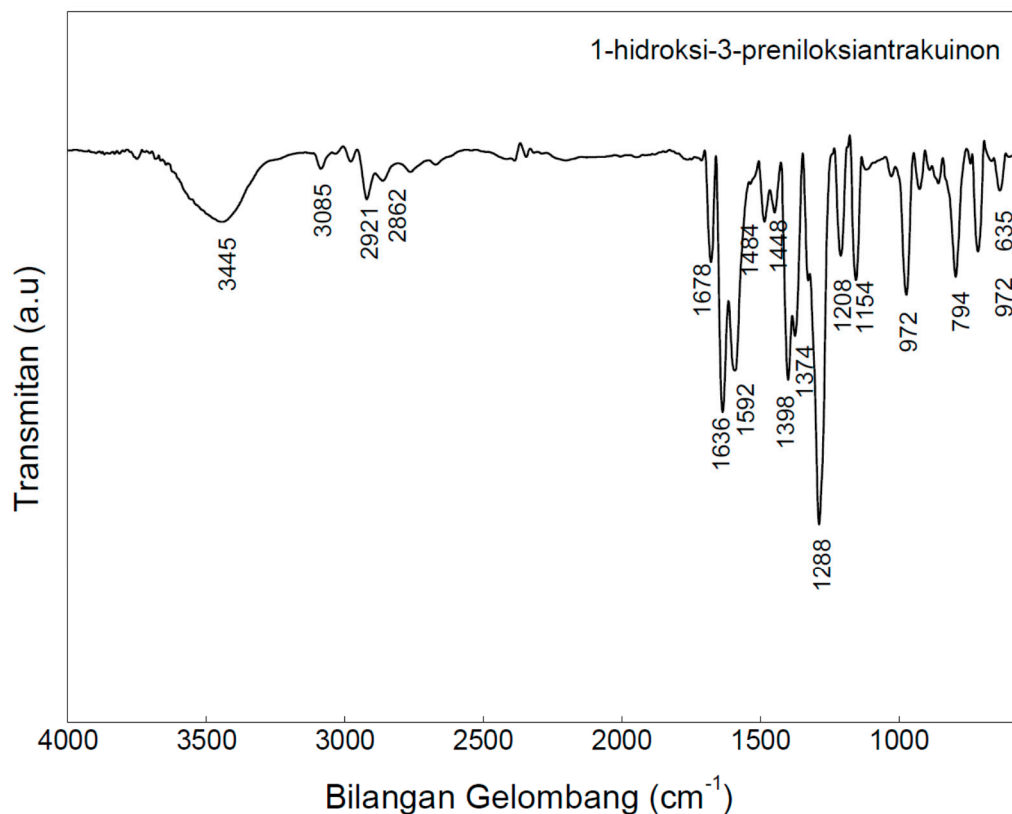
Figure S11. HSQC spectrum of 1-Hydroxy-3-(3-methylbut-2-enyloxy)anthracene-9,10-dione (4).

1-Hydroxy-3-(3-methylbut-2-enyloxy)anthracene-9,10-dione, HMBC

**Figure S12.** HMBC spectrum of 1-Hydroxy-3-(3-methylbut-2-enyloxy)anthracene-9,10-dione (4).

1-Hydroxy-3-(3-methylbut-2-enyloxy)anthracene-9,10-dione, HMBC

**Figure S13.** HMBC spectrum of 1-Hydroxy-3-(3-methylbut-2-enyloxy)anthracene-9,10-dione (4).



**Figure S14.** IR spectrum of 1-Hydroxy-3-(3-methylbut-2-enyloxy)anthracene-9,10-dione (**4**).

### Elemental Composition Report

Page 1

#### Single Mass Analysis (displaying only valid results)

Tolerance = 10.0 mDa / DBE: min = 1.0, max = 30.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

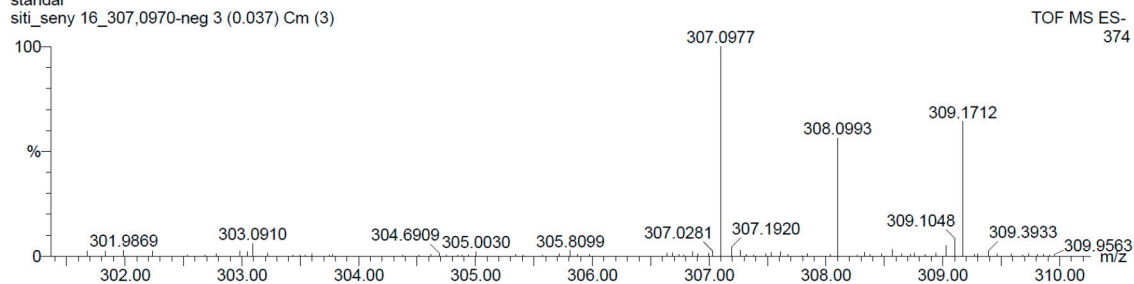
96 formula(e) evaluated with 3 results within limits (up to 1 best isotopic matches for each mass)

Elements Used:

C: 0-500 H: 0-1000 O: 0-20 Na: 0-1

standar

siti\_seny 16\_307.0970-neg 3 (0.037) Cm (3)



Minimum: 1.0  
Maximum: 10.0 10.0 30.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
307.0977	307.0970	0.7	2.3	12.5	42.1	C19 H15 O4

**Figure S15.** HRESI-TOF mass spectrum of 1-Hydroxy-3-(3-methylbut-2-enyloxy)anthracene-9,10-dione (**4**).