

## Supplementary Data

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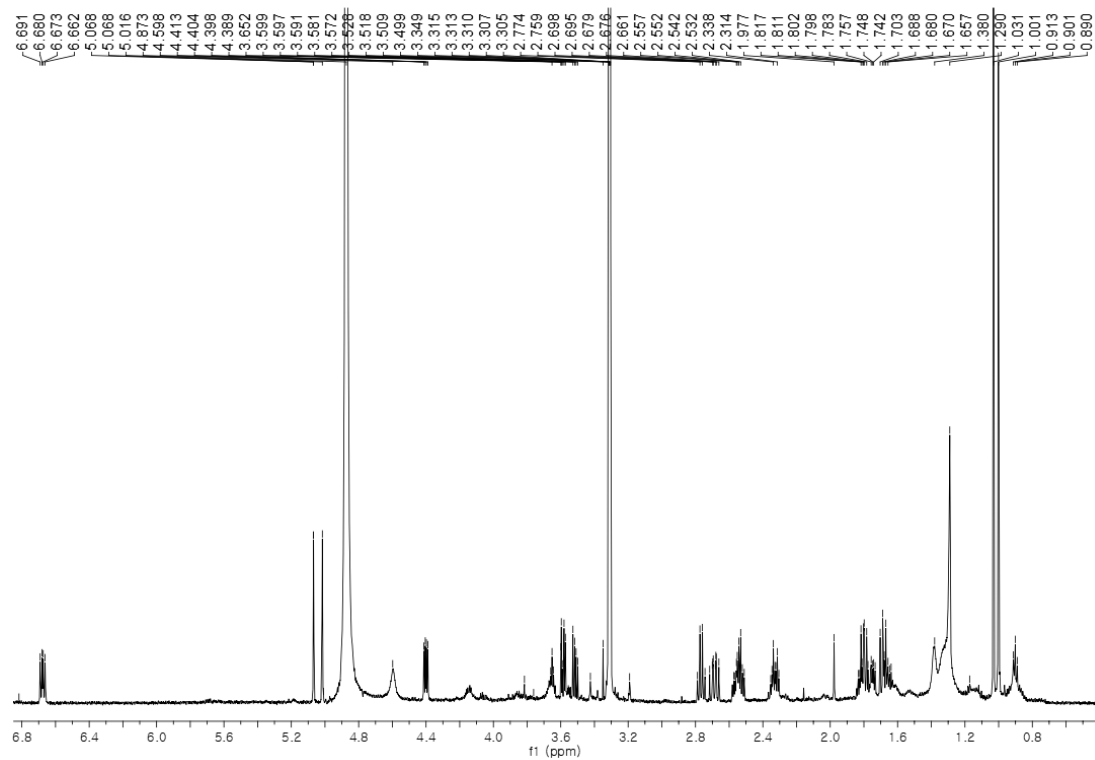


Figure S1.  $^1\text{H}$  NMR (600 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound 2.

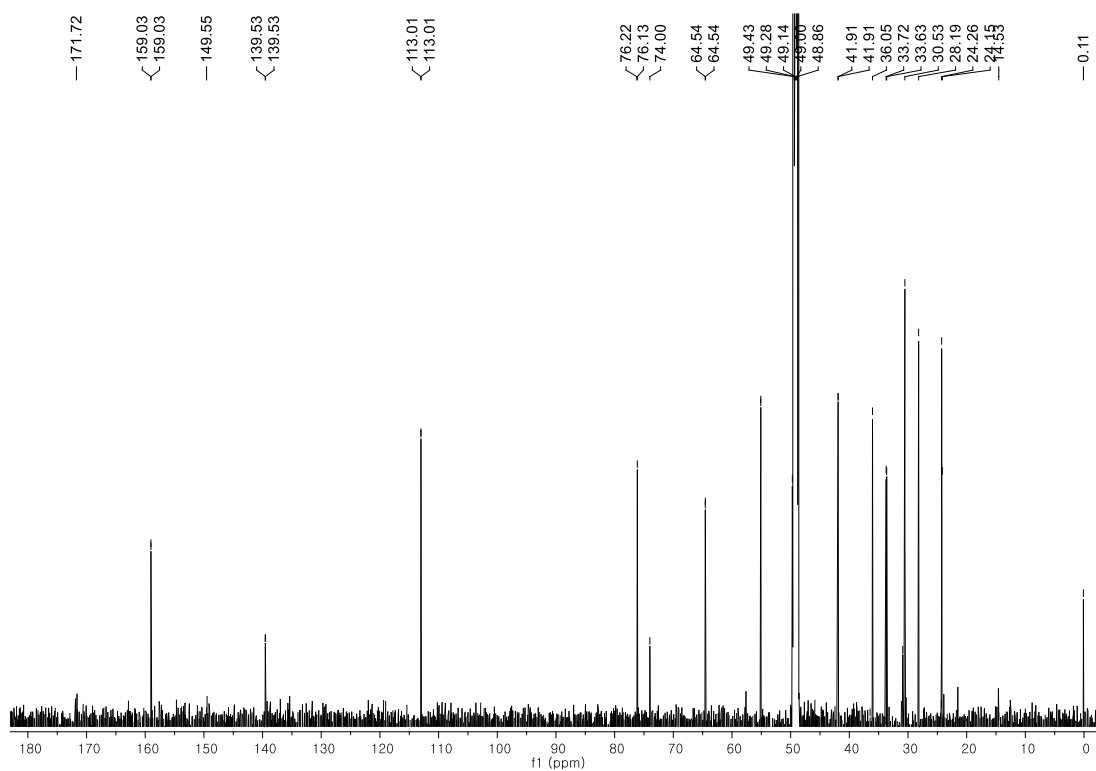


Figure S2.  $^{13}\text{C}$  NMR (150 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound 2.

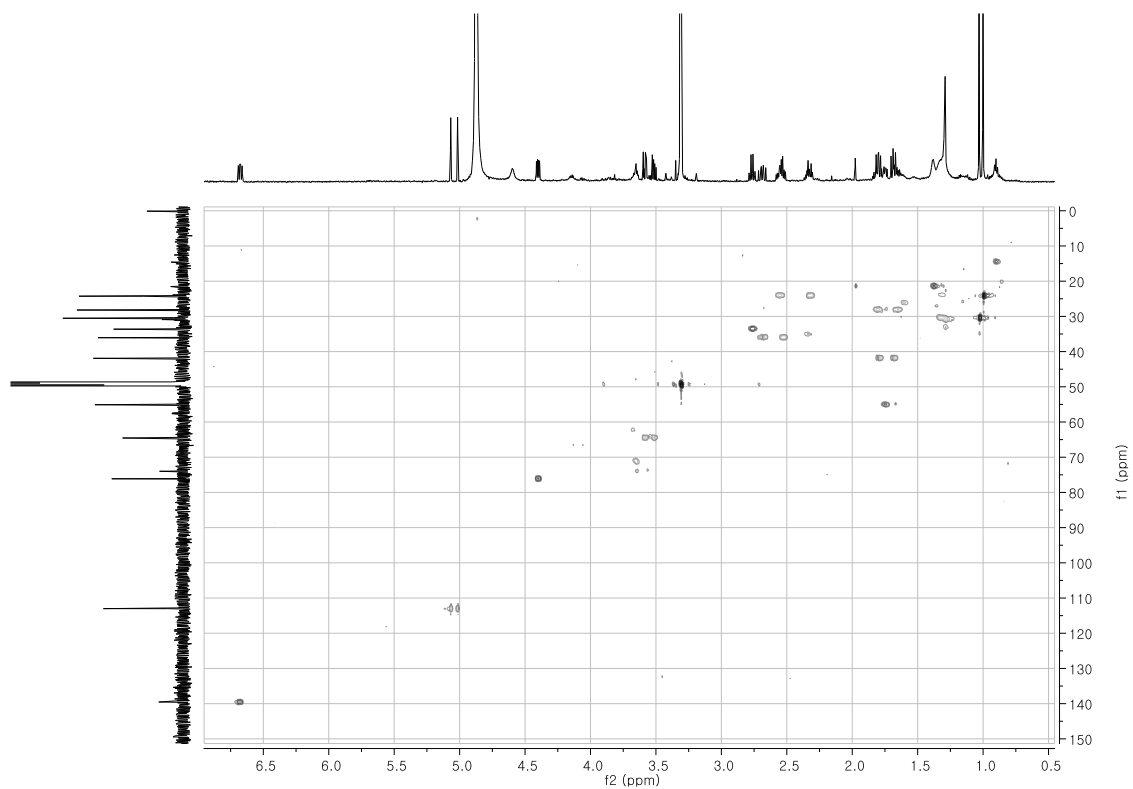


Figure S3. HSQC spectrum of compound **1**.

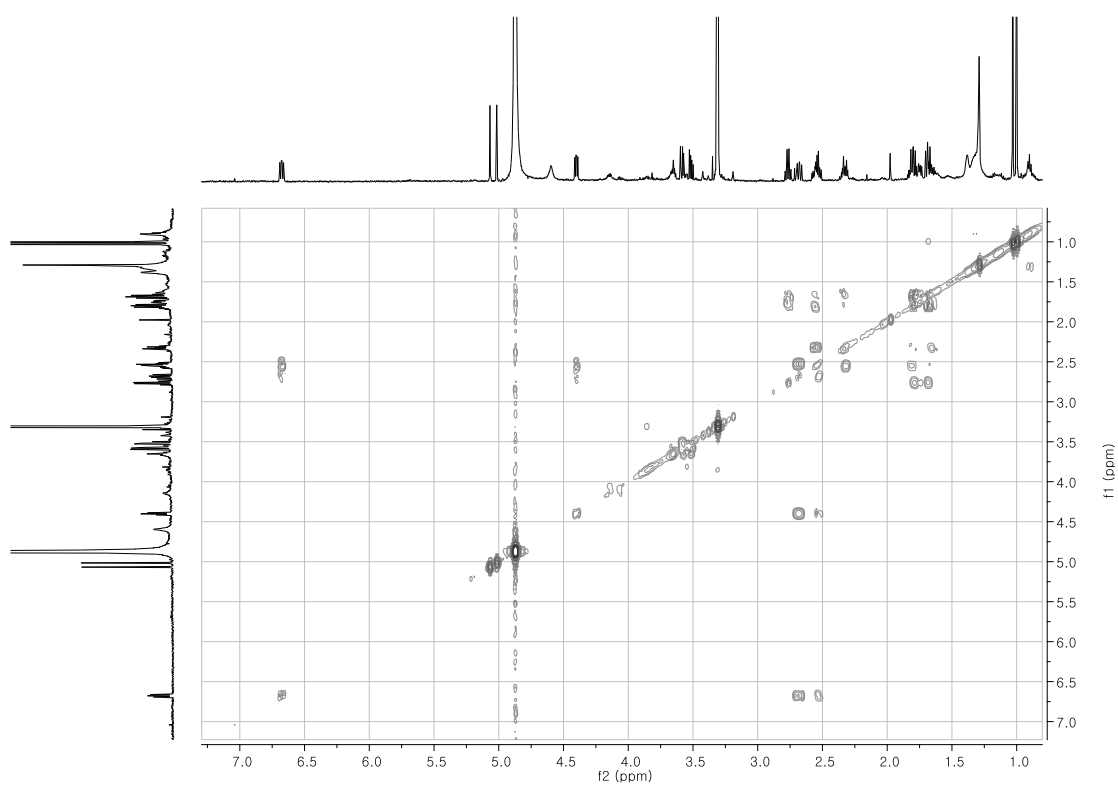


Figure S4.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **1**.

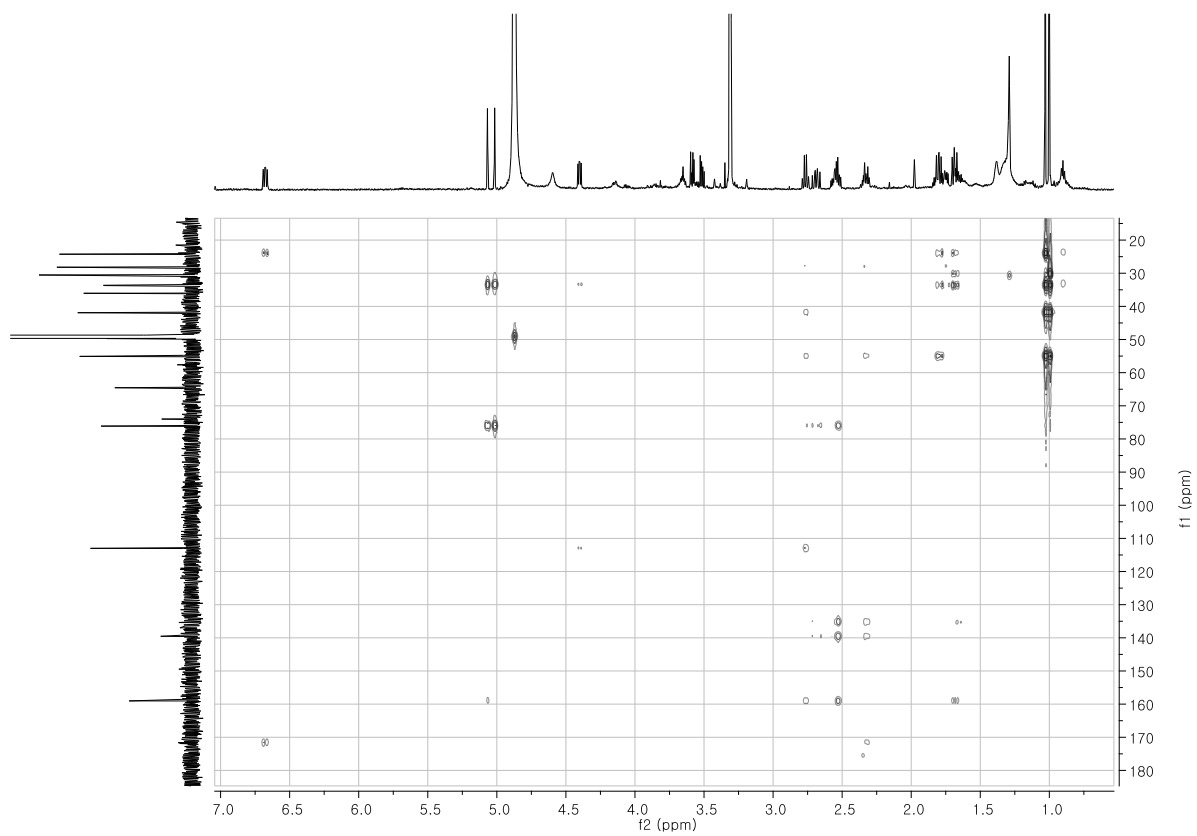


Figure S5. HMBC spectrum of compound **1**.

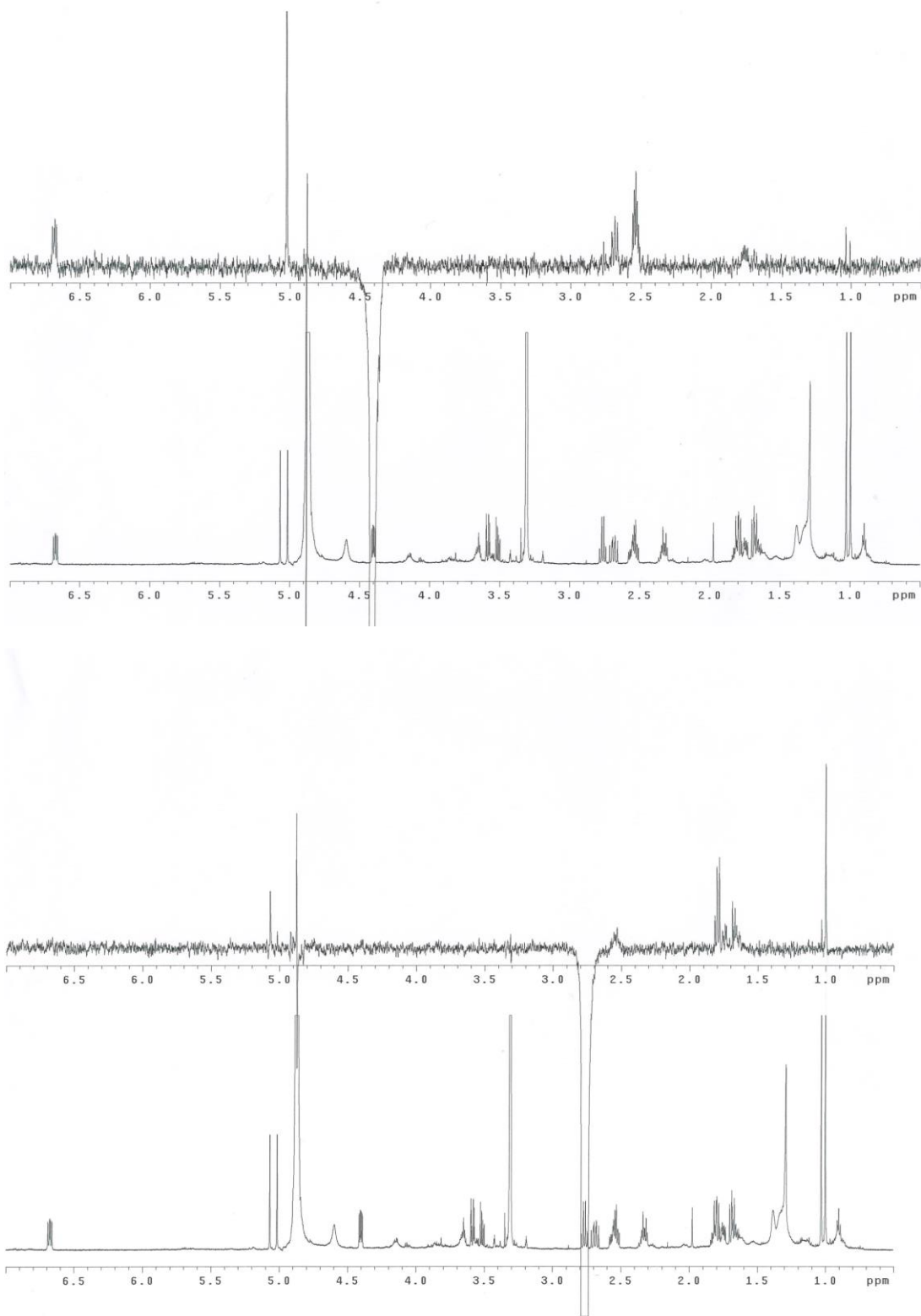


Figure S6. NOE spectra of compound 2.

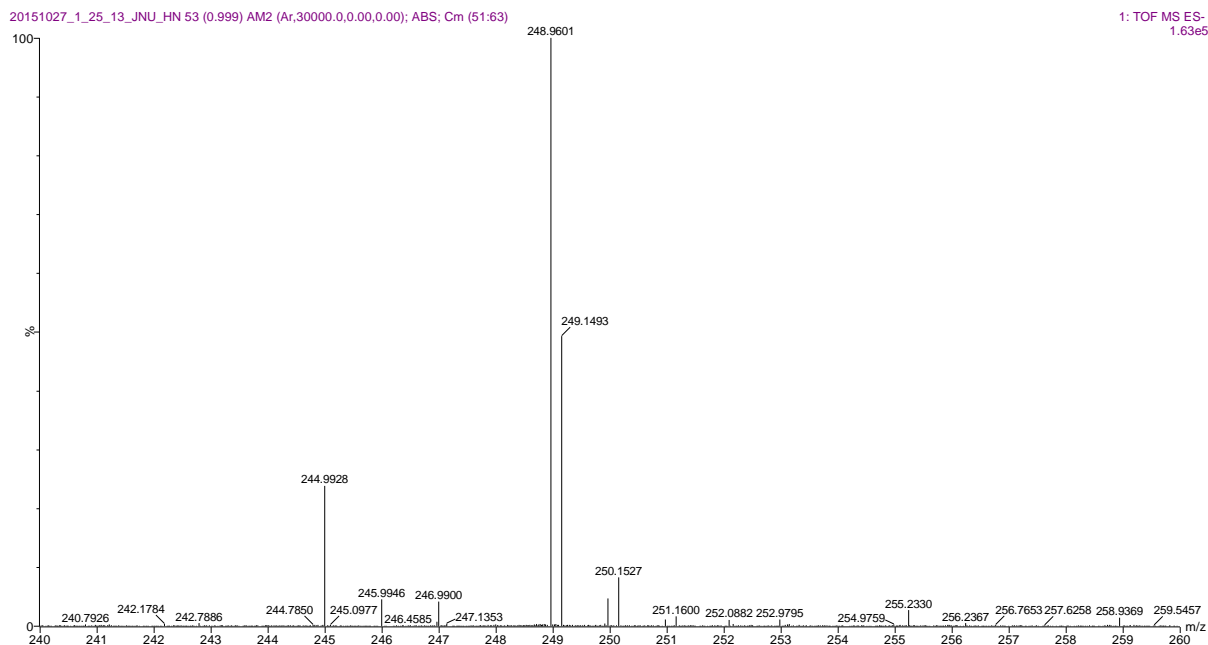


Figure S7. ESI-MS spectrum of compound **2**.

### Elemental Composition Report

#### Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

100 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 1-50 H: 1-50 O: 1-30

Minimum: -1.5

Maximum: 500.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
249.1493	249.1491	0.2	0.8	5.5	716.6	n/a	n/a	C15 H21 O3

Figure S8. HRESI-MS data of compound **2**.

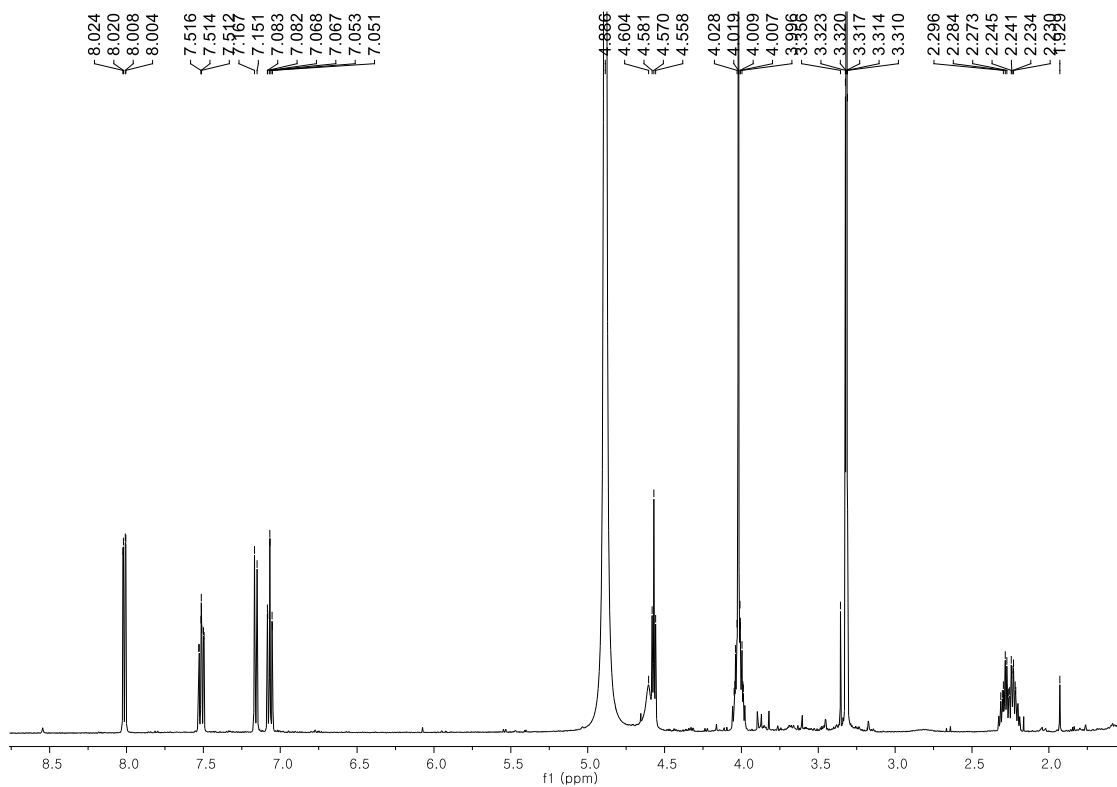


Figure S9.  $^1\text{H}$  NMR (500 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound **8**.

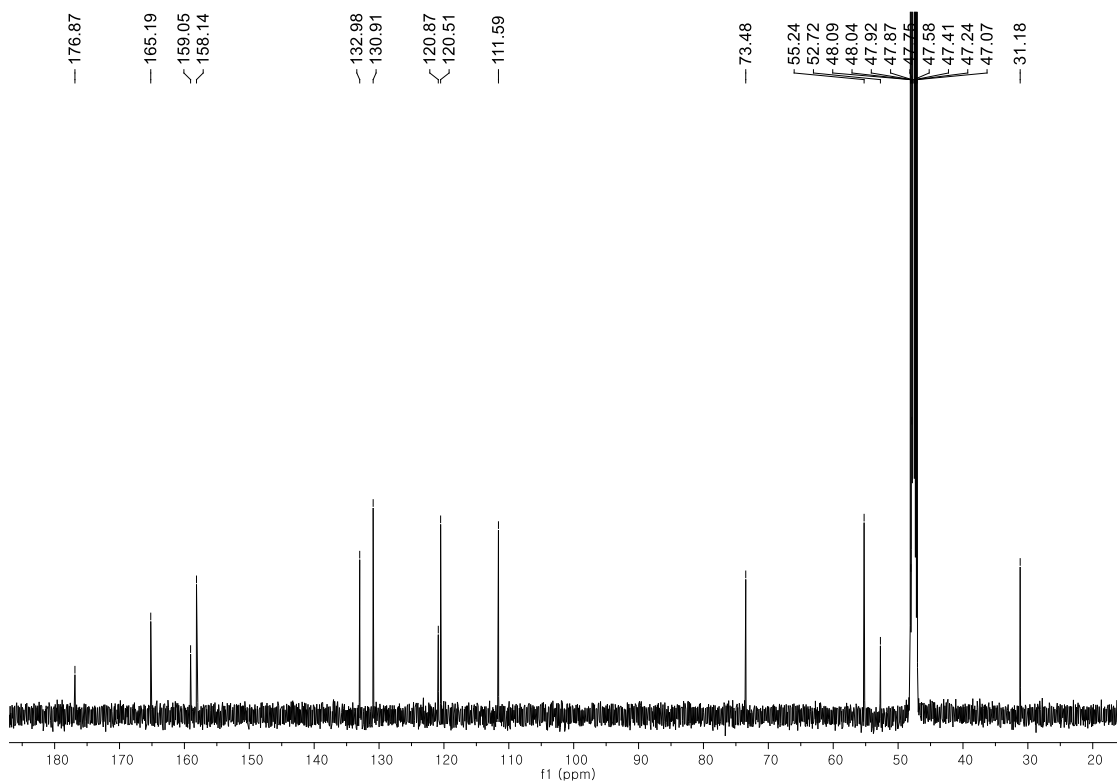


Figure S10.  $^{13}\text{C}$  NMR (125 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound **8**.

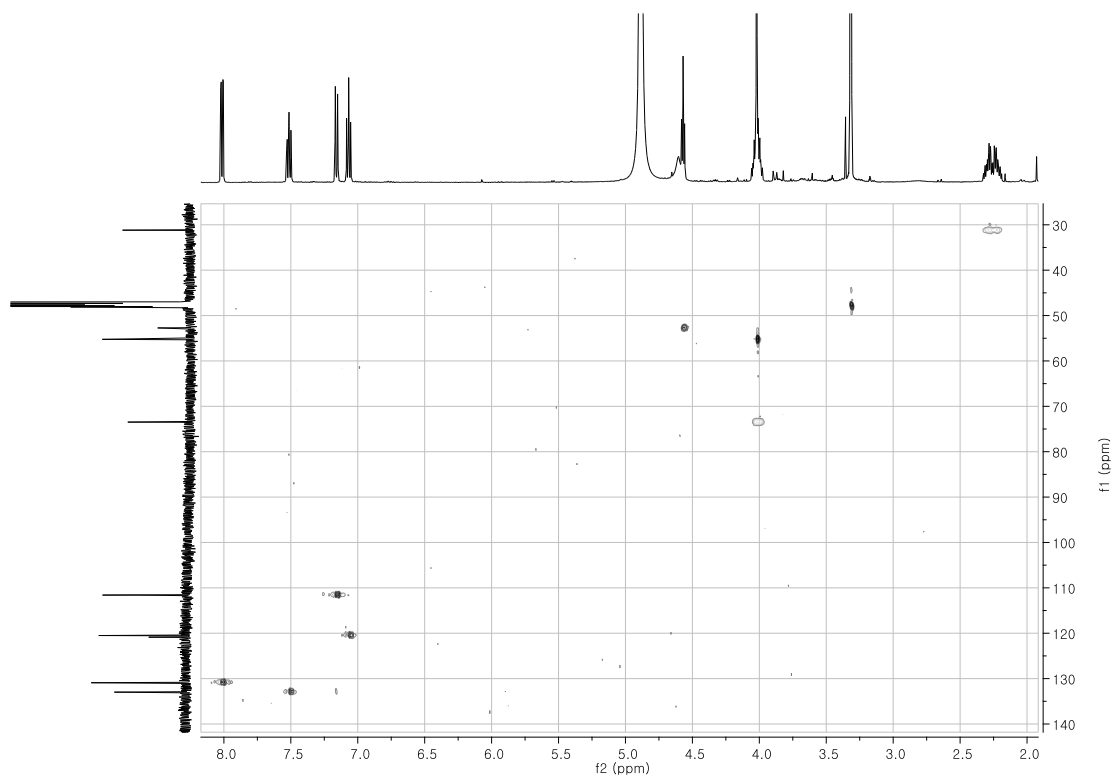


Figure S11. HSQC spectrum of compound **8**.

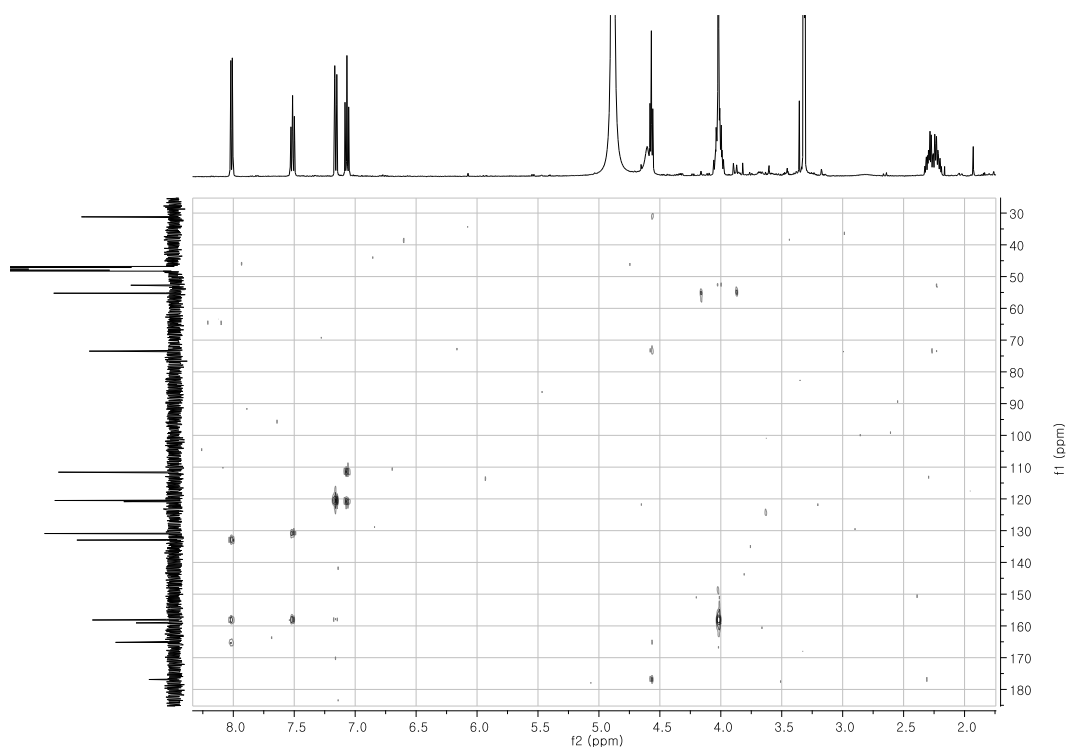


Figure S12. HMBC spectrum of compound **8**.



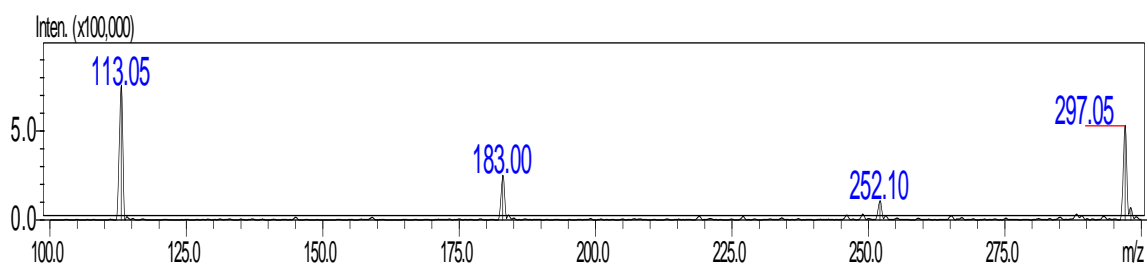


Figure S13. ESI-MS (negative) spectrum of compound **8**.

### Elemental Composition Report

#### Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

115 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 1-50 H: 1-50 O: 1-30

Minimum: -1.5

Maximum: 500.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
254.1041	254.1023	1.8	1.6	6.5	362.7	n/a	n/a	C12 H16 N1O5

Figure S14. HRESI-MS of compound **8**.

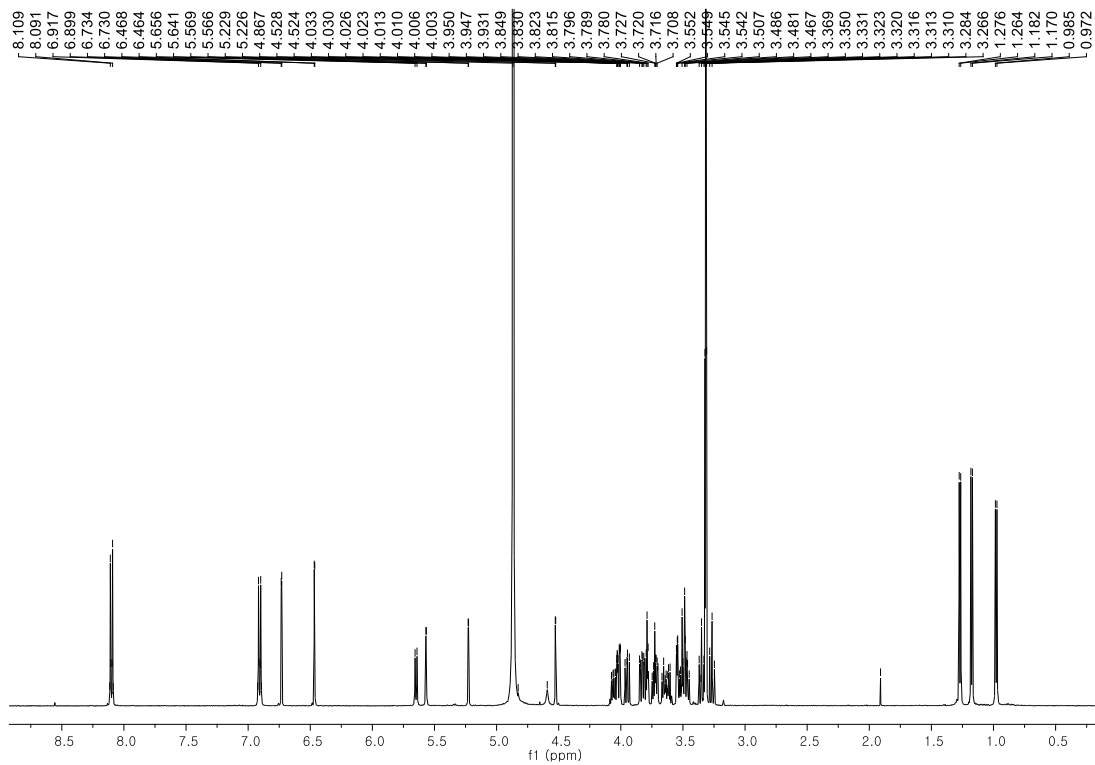


Figure S15.  $^1\text{H}$  NMR (500 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound **9**.

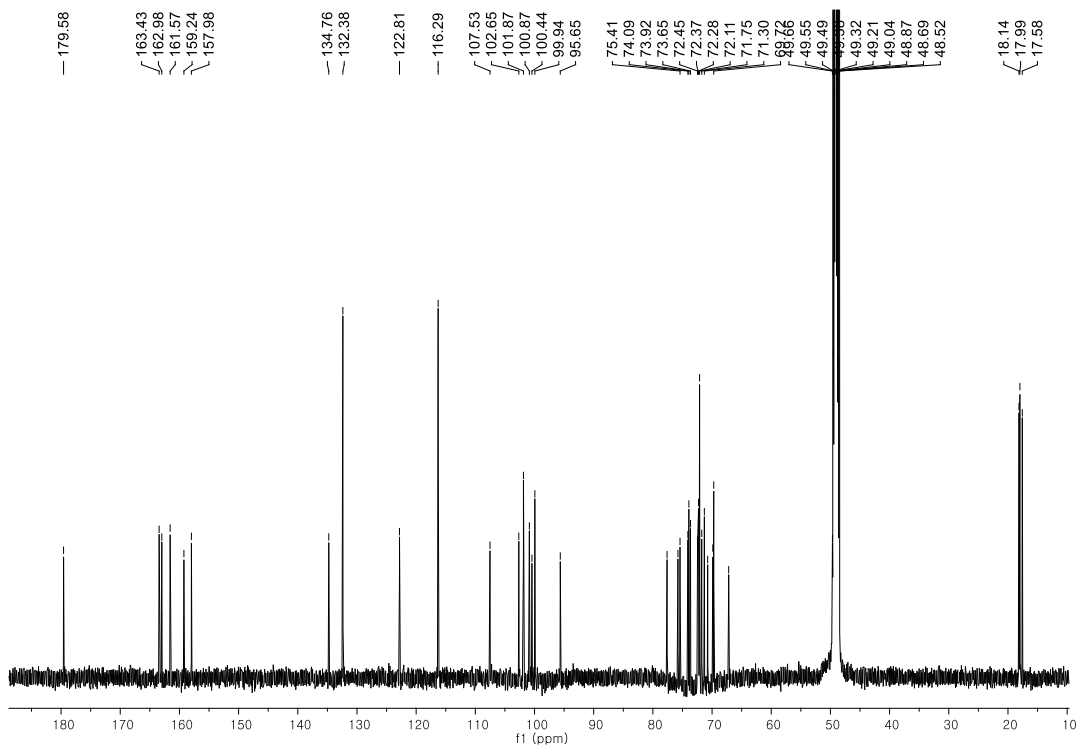


Figure S16.  $^{13}\text{C}$  NMR (125 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound **9**.

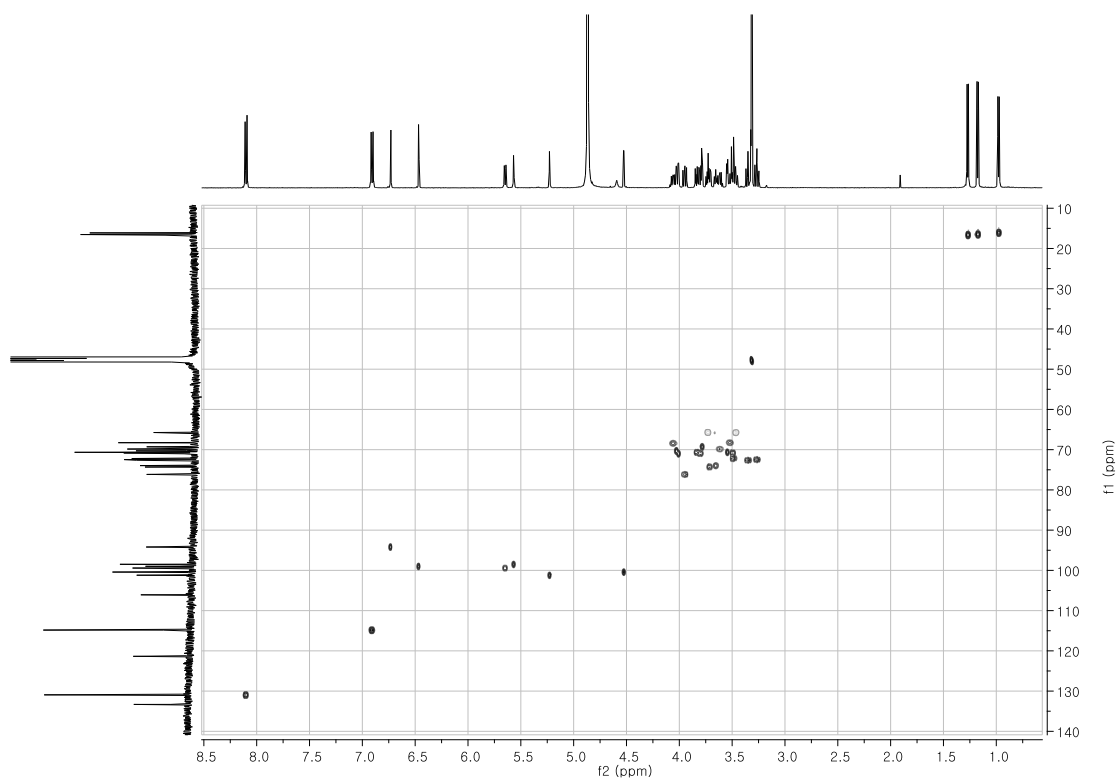


Figure S17. HSQC spectrum of compound **9**.

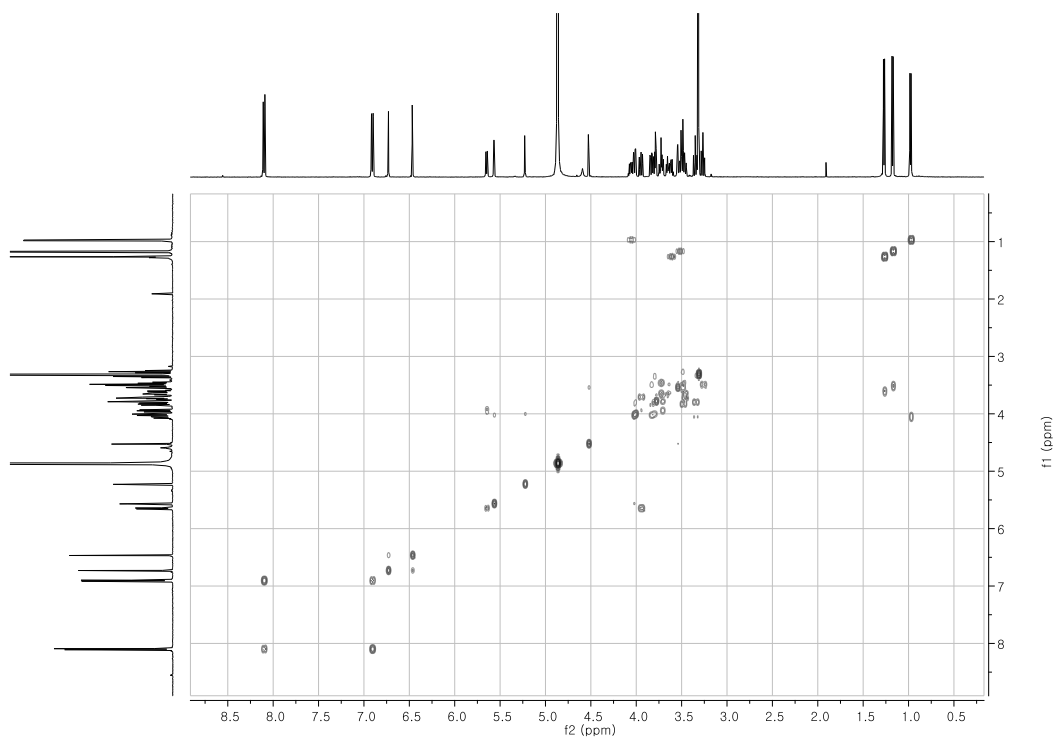


Figure S18.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **9**.

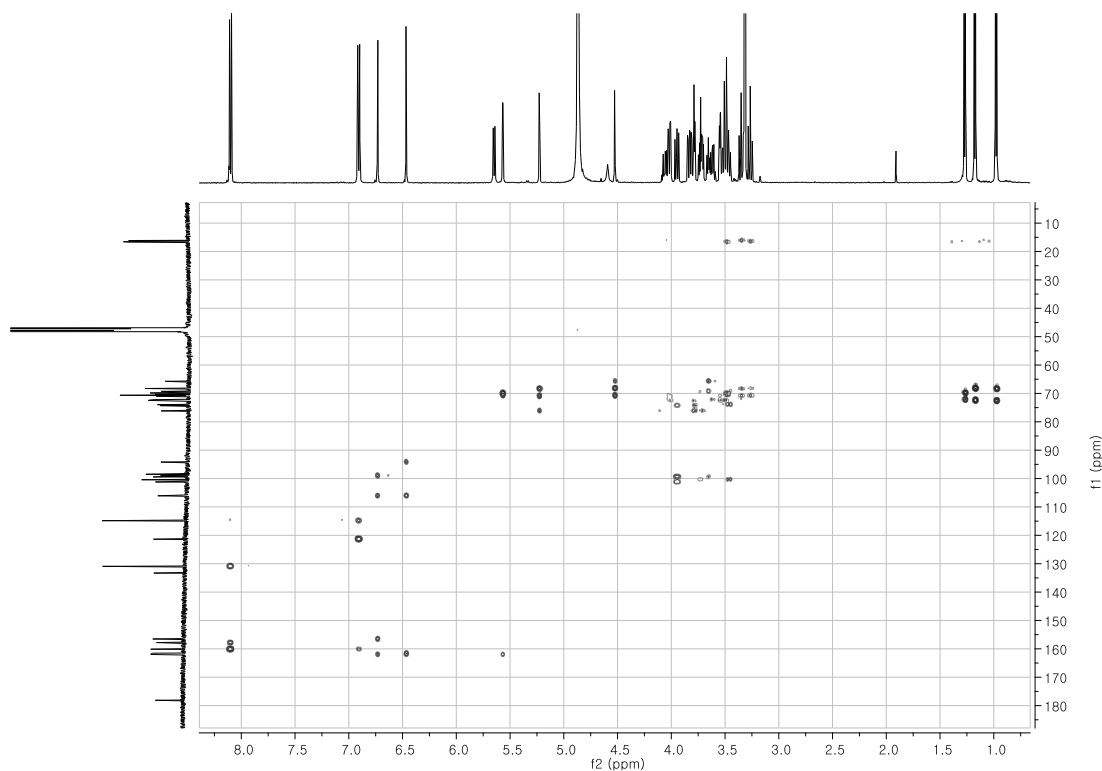


Figure S19. HMBC spectrum of compound **9**.

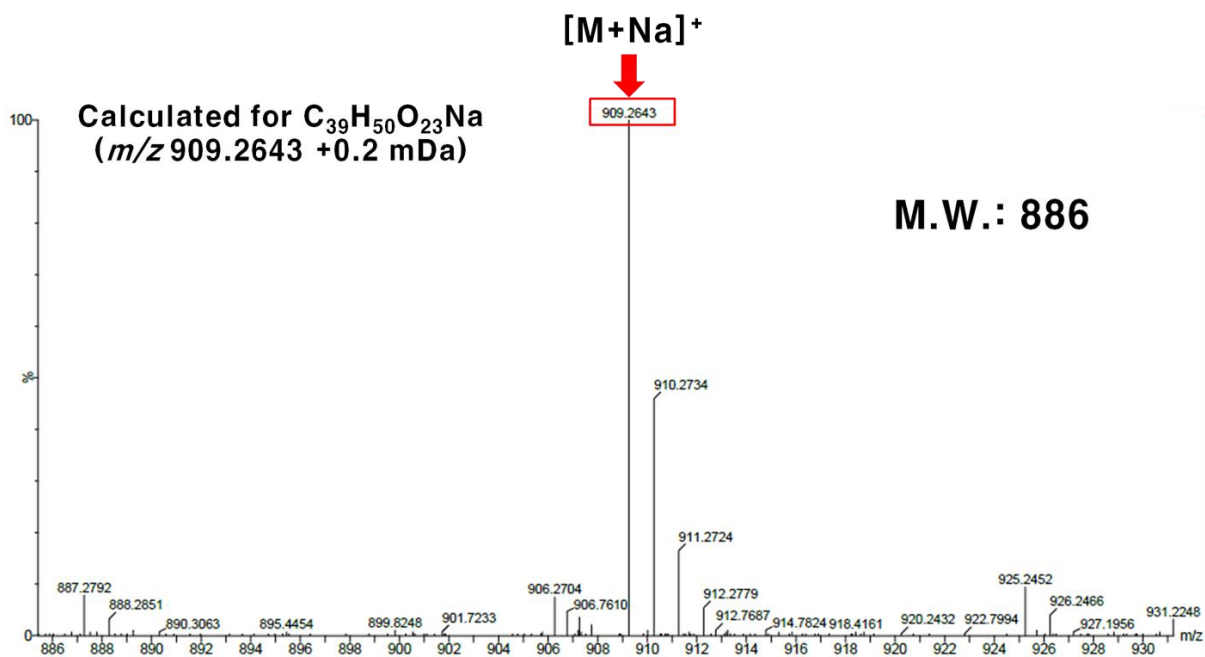


Figure S19. ESI-MS spectrum of compound **9**.

### Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

100 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 1-50 H: 1-50 O: 1-30

Minimum: -1.5

Maximum: 500.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
909.2643	909.2641	0.2	0.6	14.5	308.2	0.009	99.11	C39 H50O23Na

Figure S20. HRESI-MS data of compound **9**.