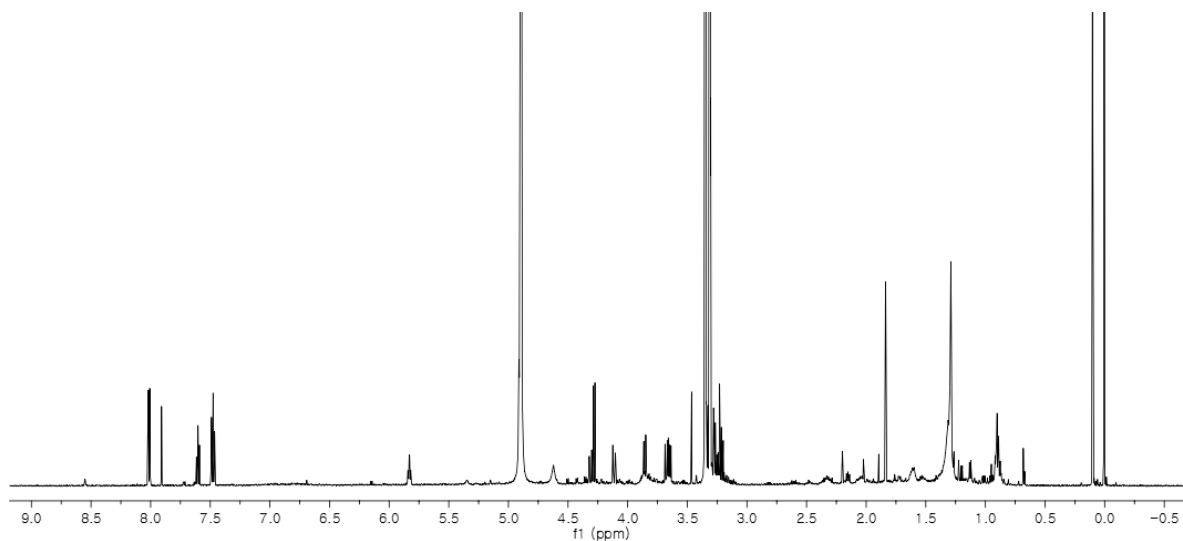


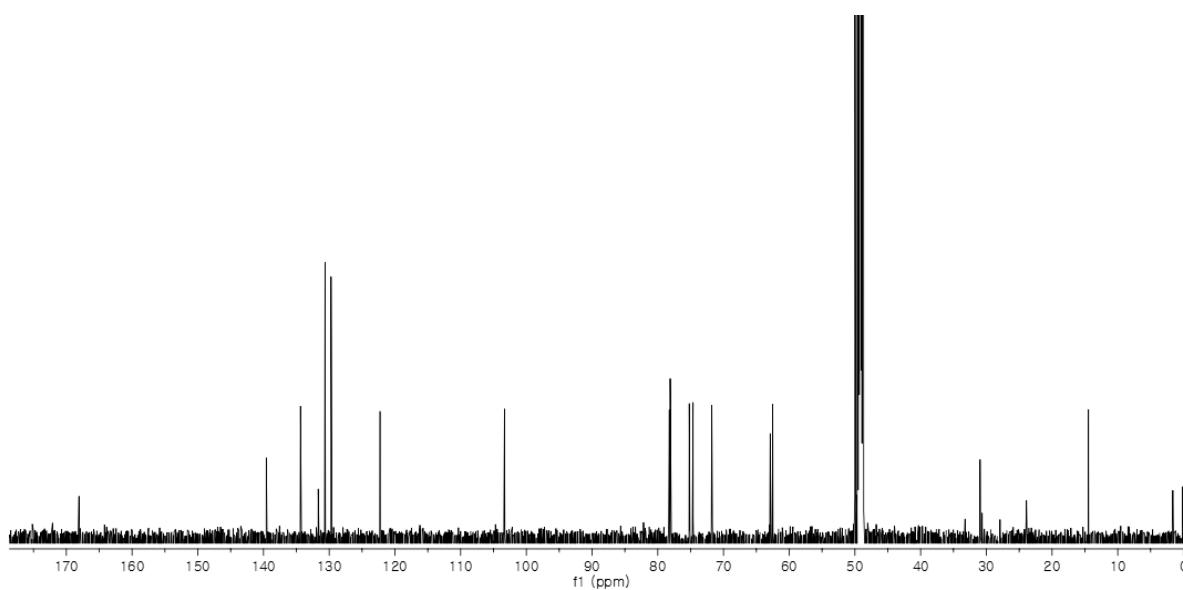
Supplementary Informations

NMR and MS Spectra of 2

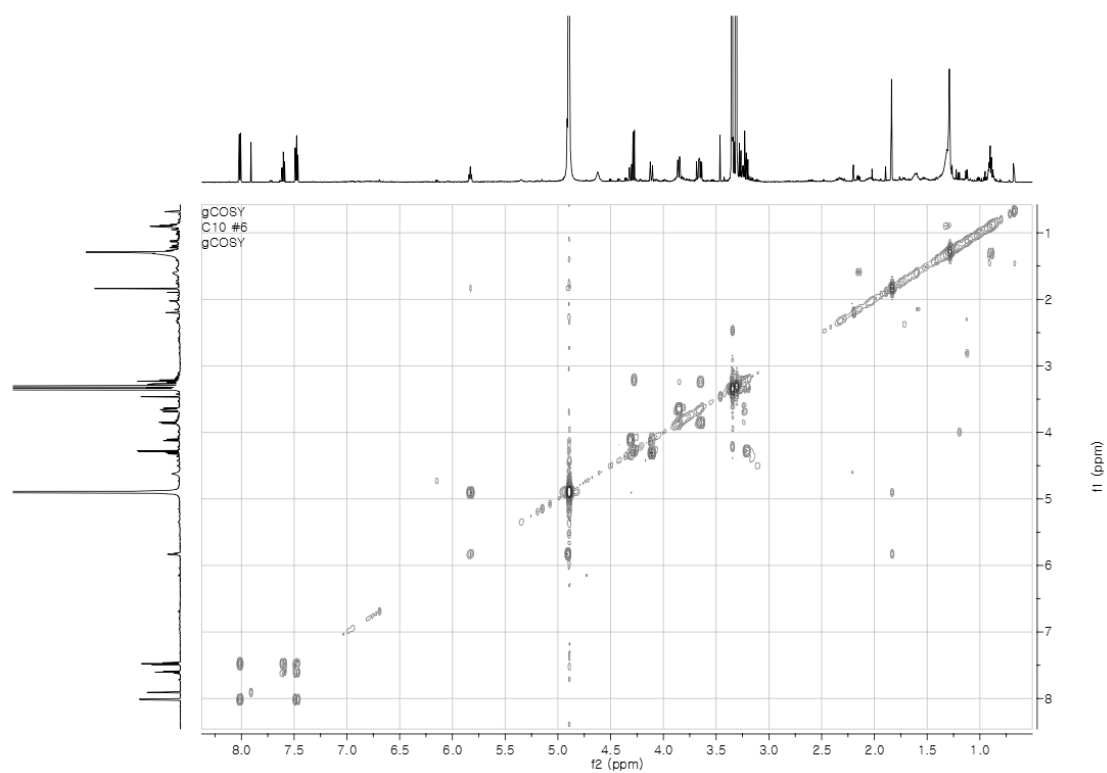
$^1\text{H-NMR}$ Spectrum (500 MHz, CD_3OD)



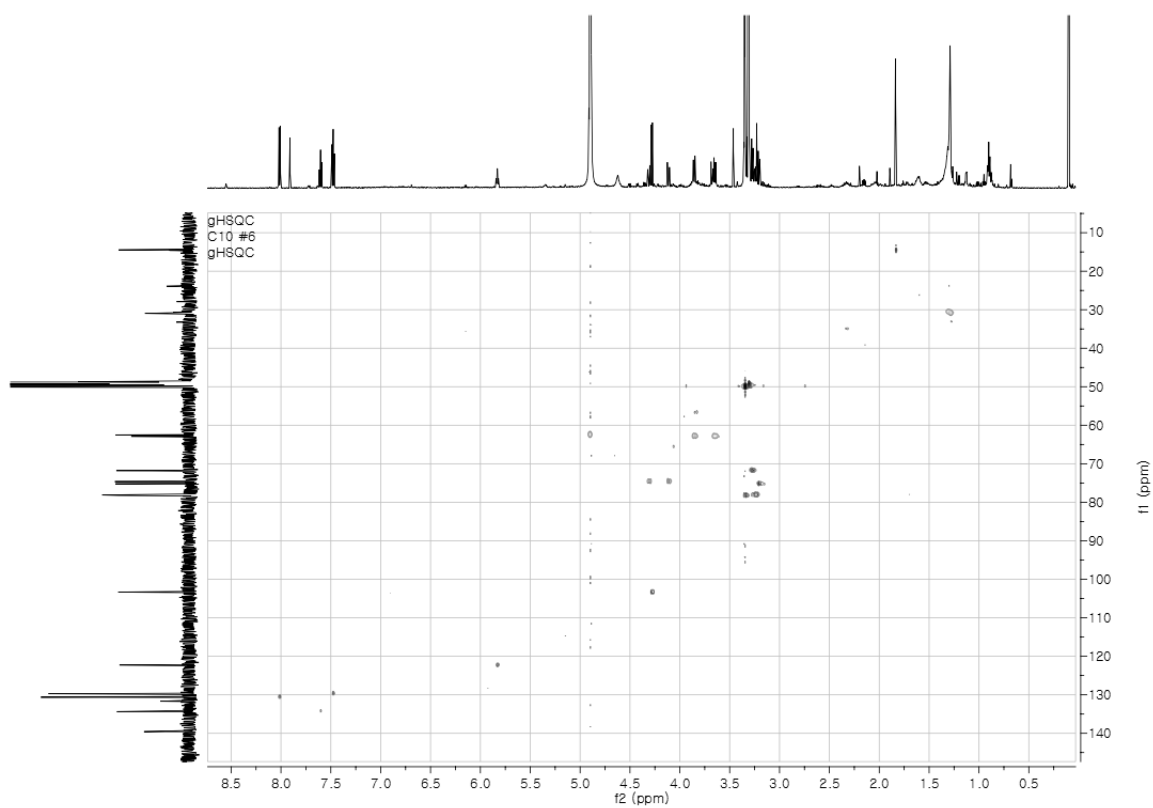
$^{13}\text{C-NMR}$ Spectrum (125 MHz, CD_3OD)



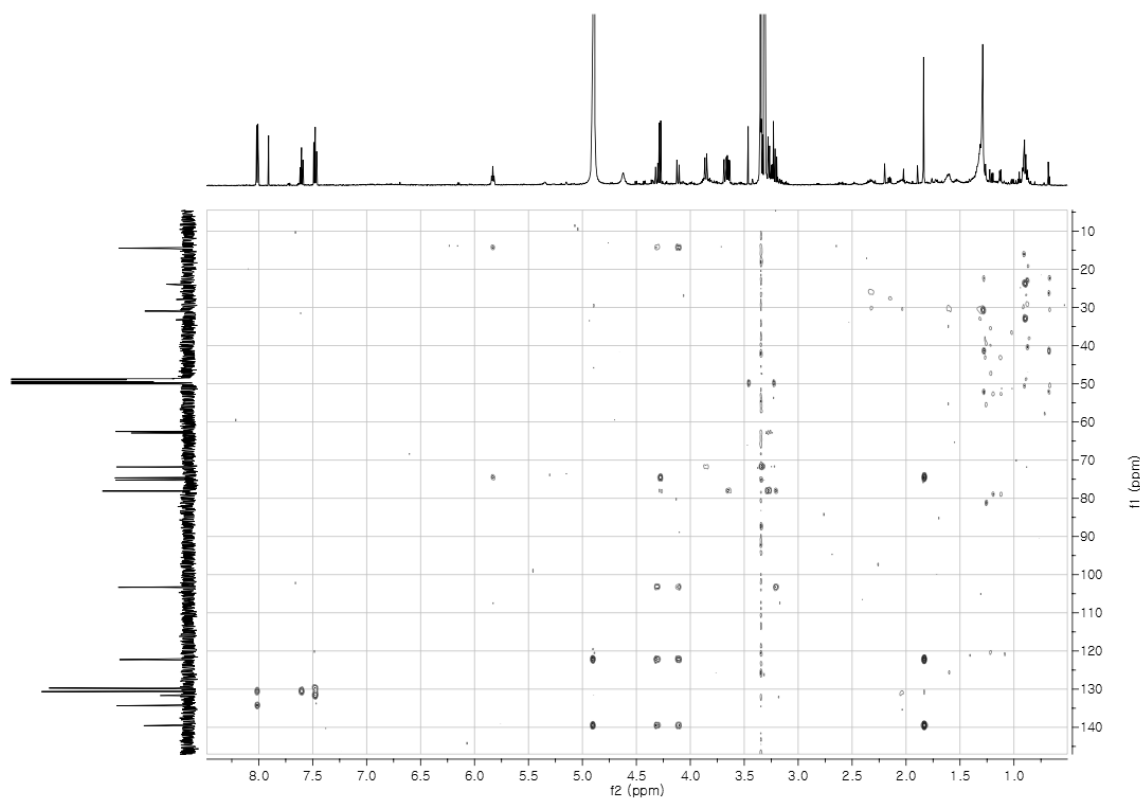
^1H - ^1H COSY Spectrum



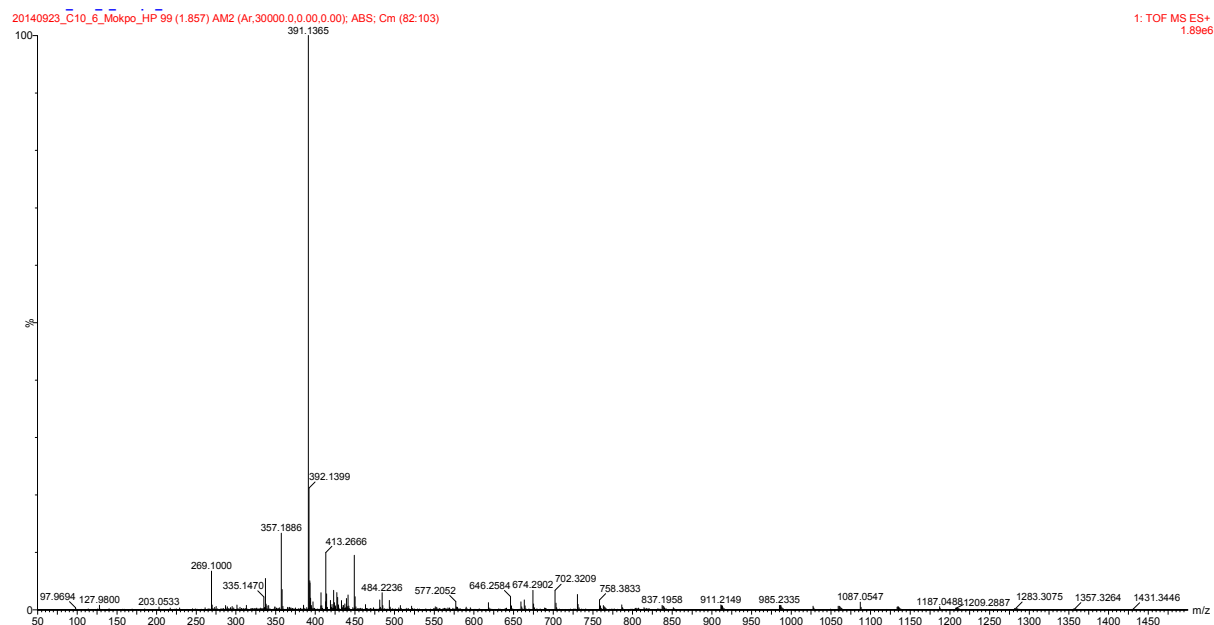
HSQC Spectrum



HMBC Spectrum



ESI-MS (Positive) Spectrum



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 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

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

Elements Used:

Elements Used: C: 1-20 H: 1-30 O: 1-10 Na: 1-1

Minimum -1.5

Maximum 5.0 5.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf(%) | Formula |
|----------|------------|------|------|-----|--------|------|---------|---------------|
| 391.1365 | 391.1369 | -0.4 | -1.0 | 6.5 | 1078.1 | n/a | n/a | C18 H24 O8 Na |