

# Supporting Information

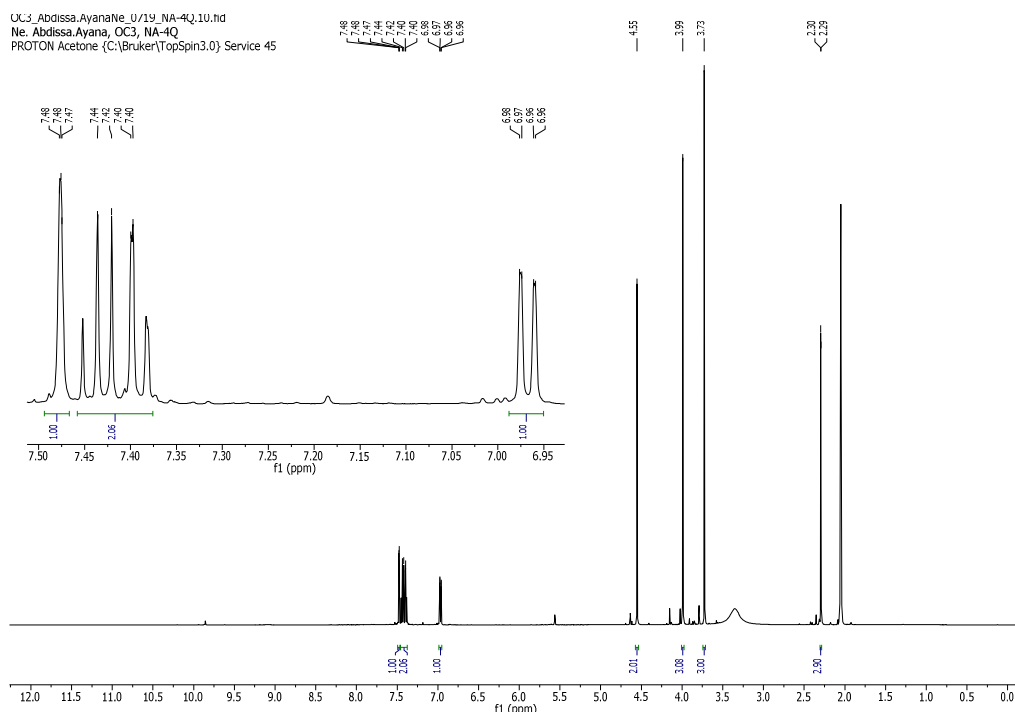
## Cytotoxic Compounds from *Aloe megalacantha*

Negera Abdissa, Sebastian Gohlke, Marcel Frese, and Norbert Sewald

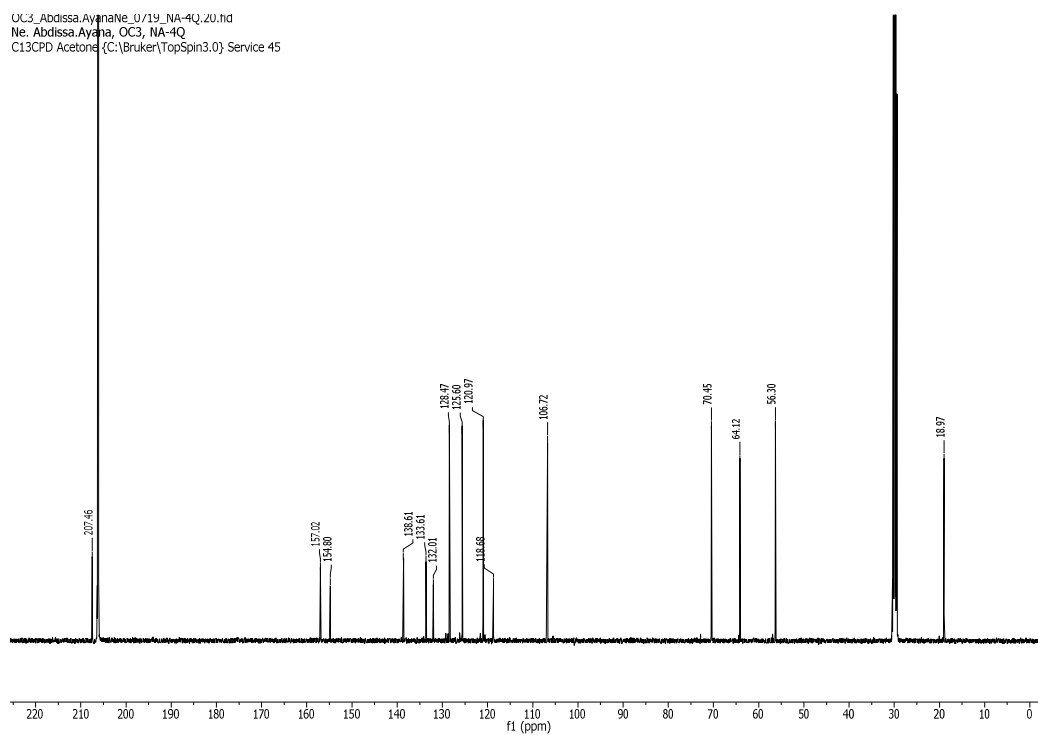
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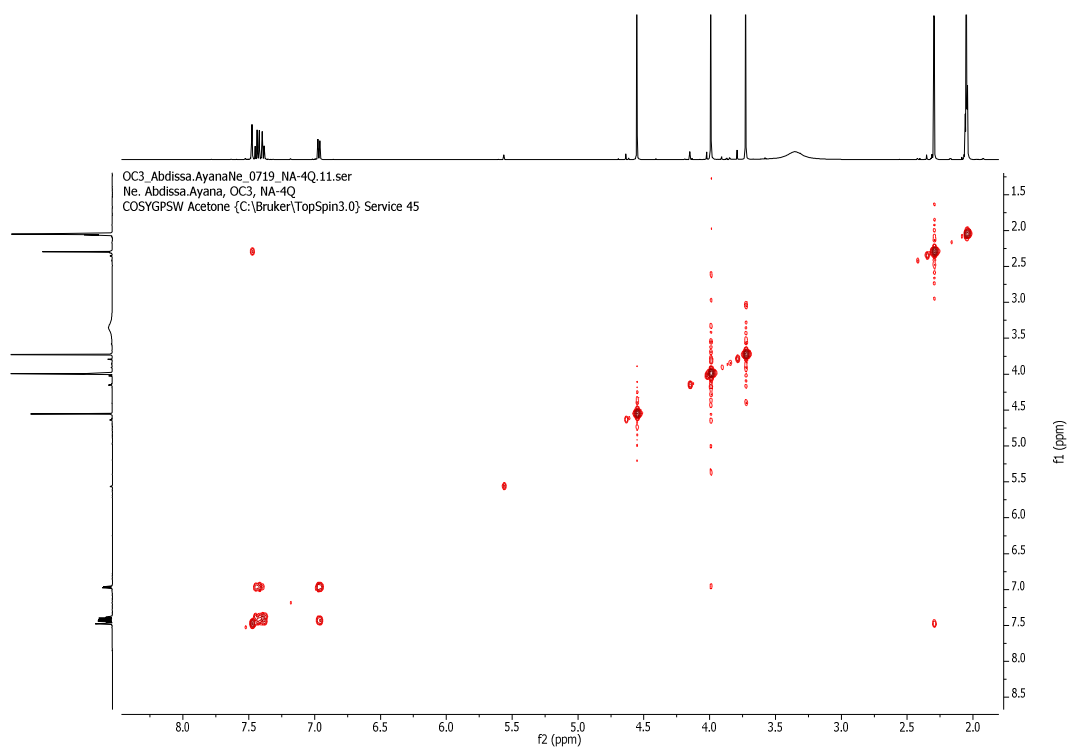
## Spectroscopic data for 1,8-dimethoxynepodiol (1)



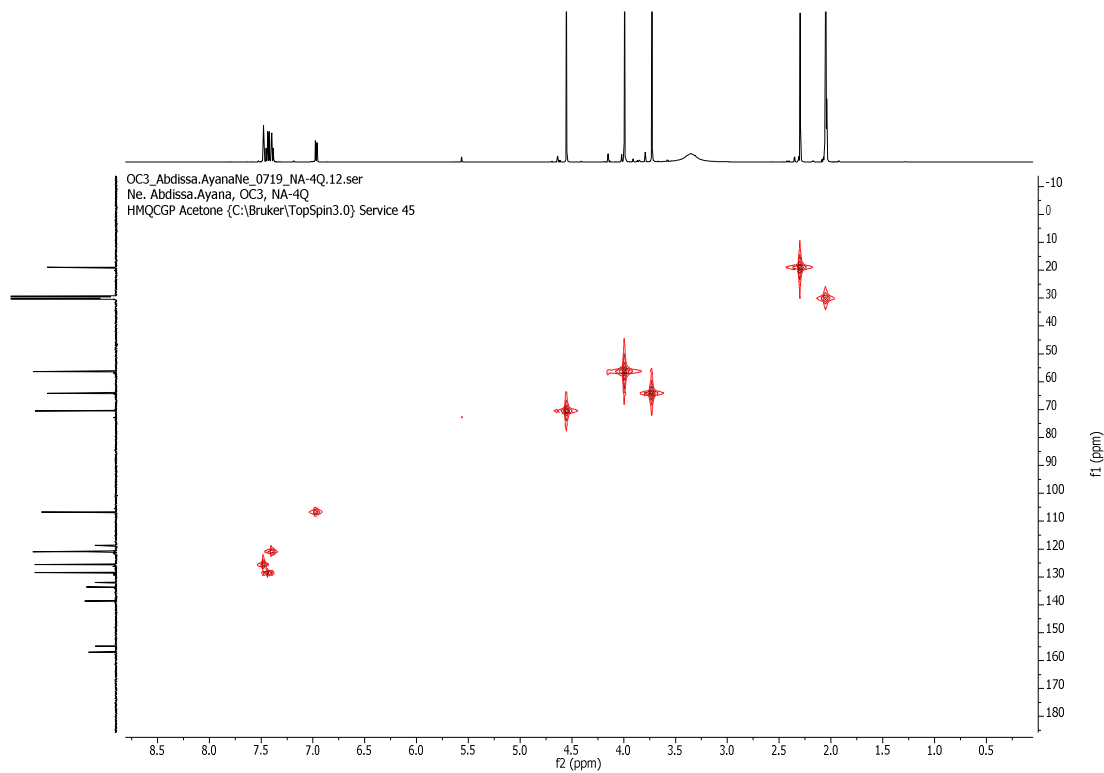
**Figure S1.** The  $^1\text{H}$  NMR spectrum of 1,8-dimethoxynepodiol (1) observed at 500 MHz in acetone- $d_6$  at 25 °C. Assignments are given in Table 1.



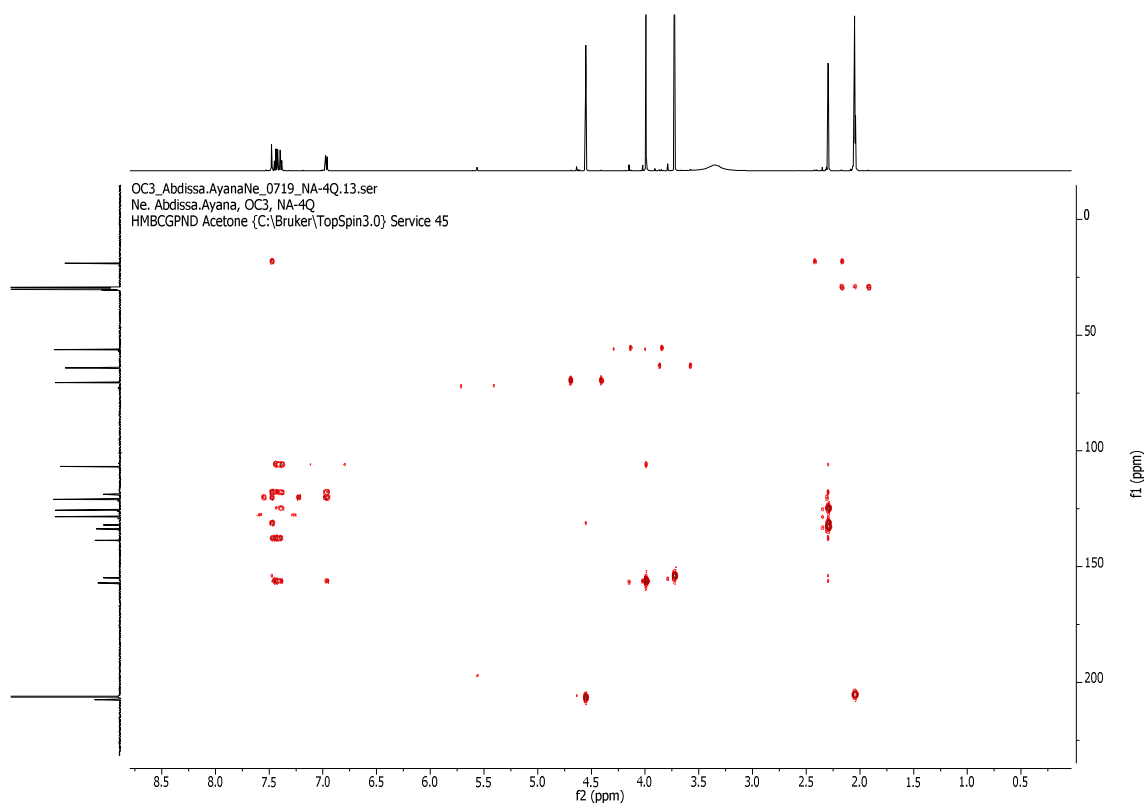
**Figure S2.** The  $^{13}\text{C}$  NMR spectrum of 1,8-dimethoxynepodiol (1) observed at 125 MHz for acetone- $d_6$  solution at 25 °C. Assignments are given in Table 1.



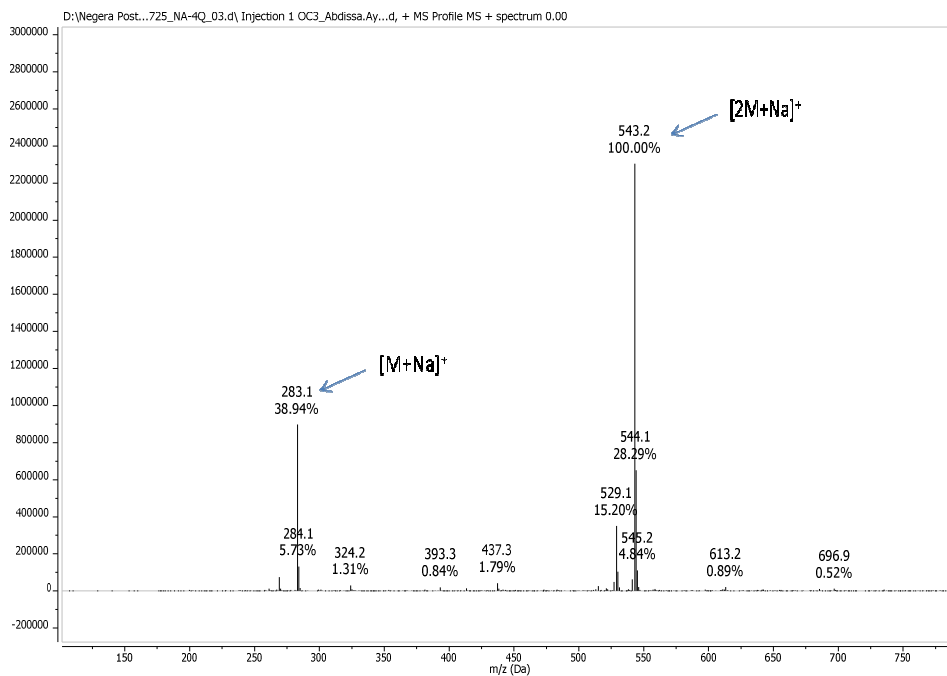
**Figure S3.** The COSY spectrum of 1,8-dimethoxynepodiol (**1**) observed at 500 MHz in acetone- $d_6$  solution at 25 °C.



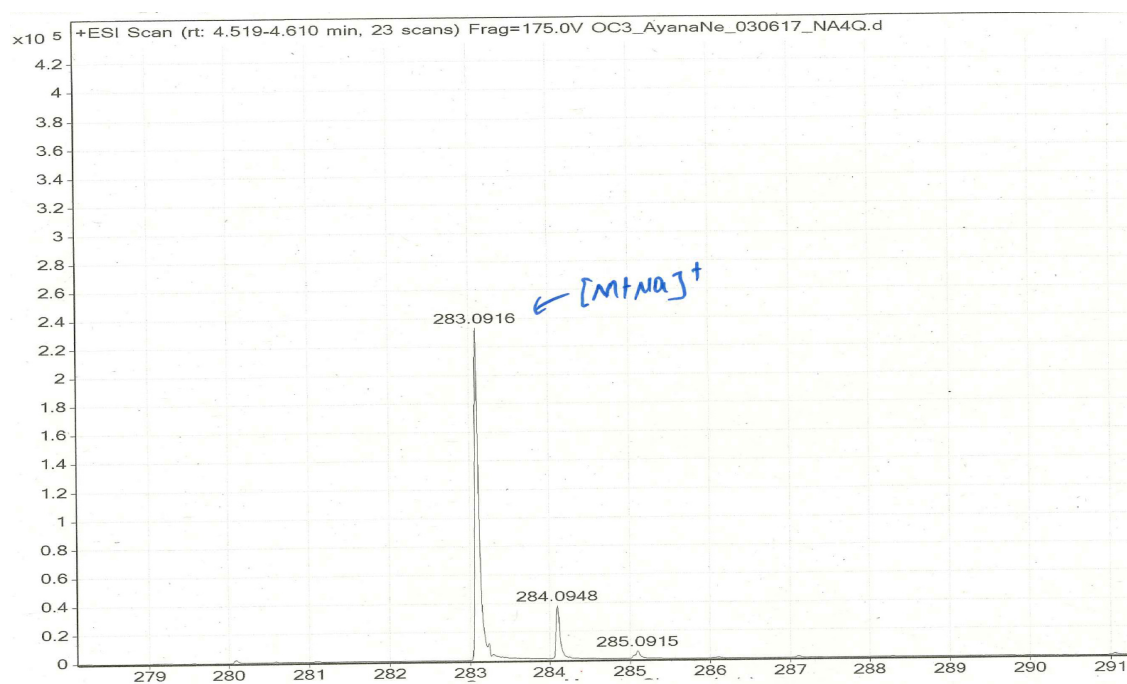
**Figure S4.** The HSQC spectrum of 1,8-dimethoxynepodiol (**1**) observed at 500 and 125 MHz for acetone- $d_6$  solution at 25 °C.



**Figure S 5.** The HMBC spectrum of 1,8-dimethoxynepodiol (**1**) observed at 500 and 125 MHz for acetone- $d_6$  solution at 25 °C.



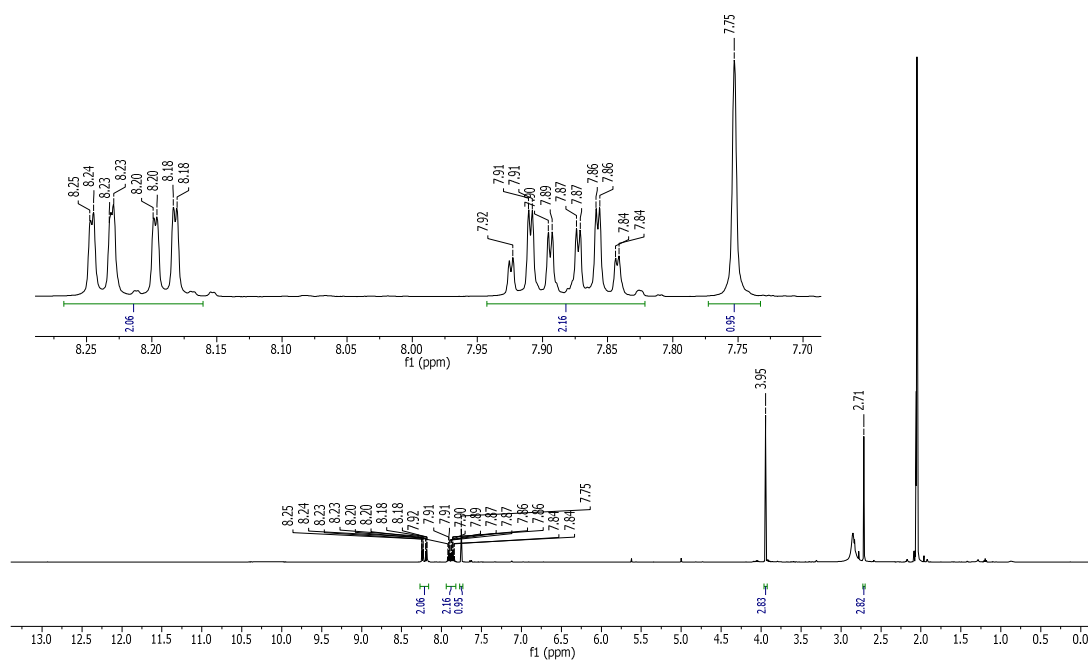
**Figure S 6.** The ESI-MS of 1,8-dimethoxynepodiol (**1**).



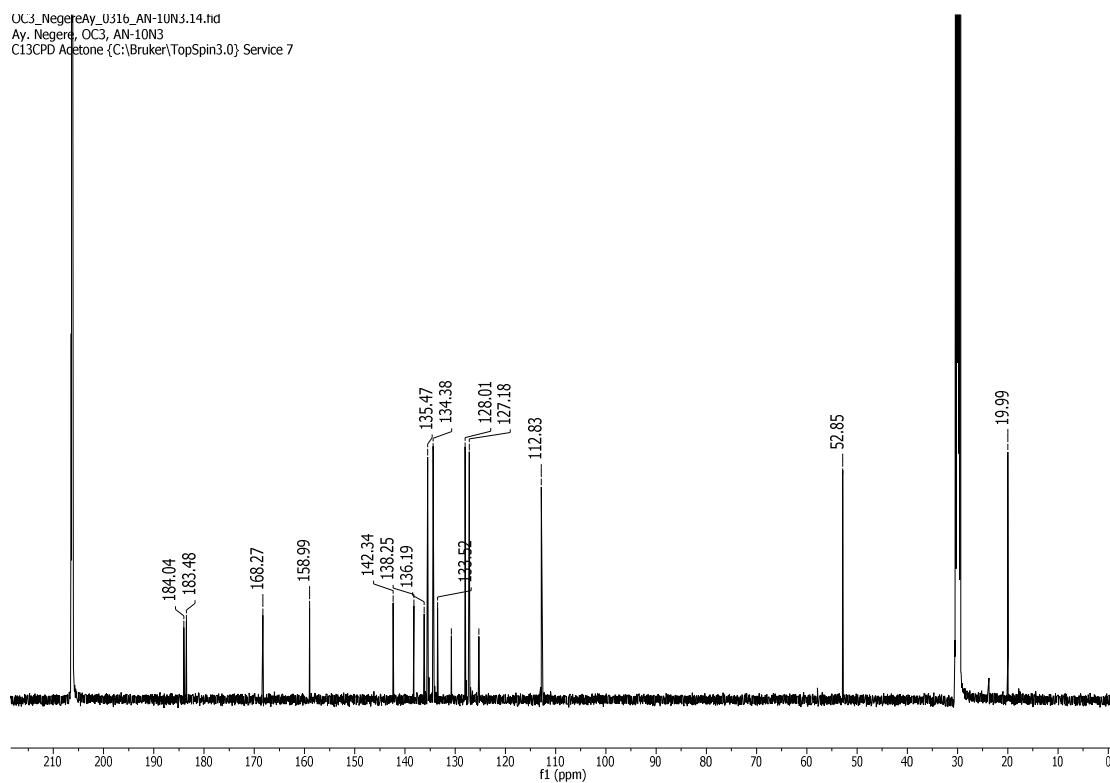
**Figure S7.** The HRESIMS of 1,8-dimethoxynepodiol (**1**).

### Spectroscopic data for aloesaponarin III B (**2**)

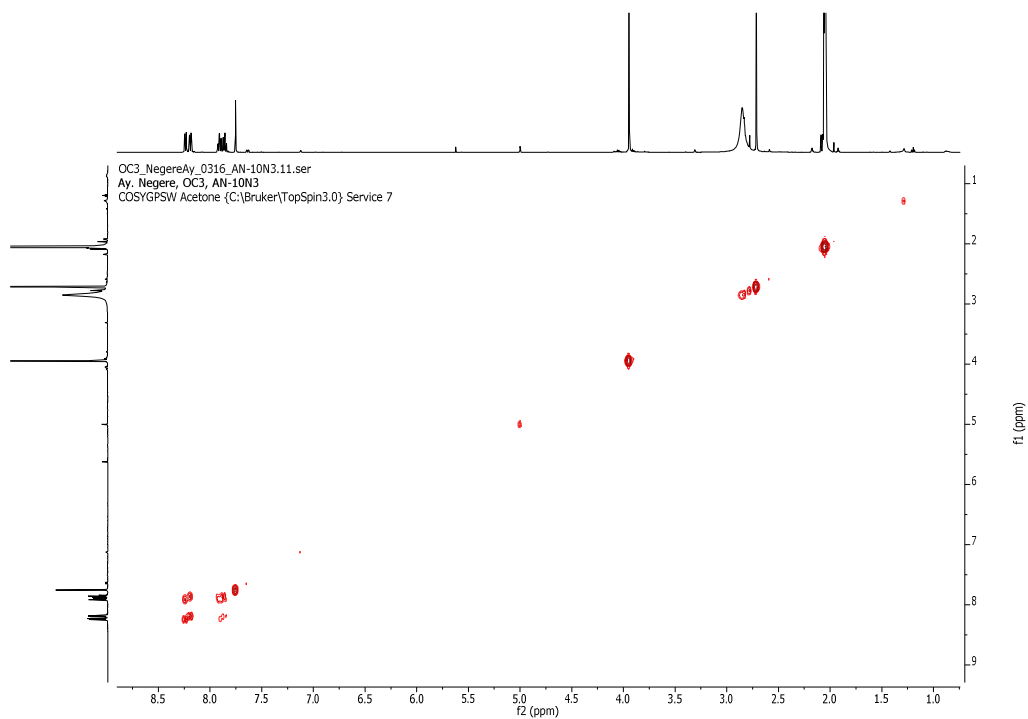
OC3\_NegereAy\_0316\_AN-10N3.10.hd  
 Ay. Negere, OC3, AN-10N3  
 PROTON Acetone (C:\Bruker\TopSpin3.0) Service 7



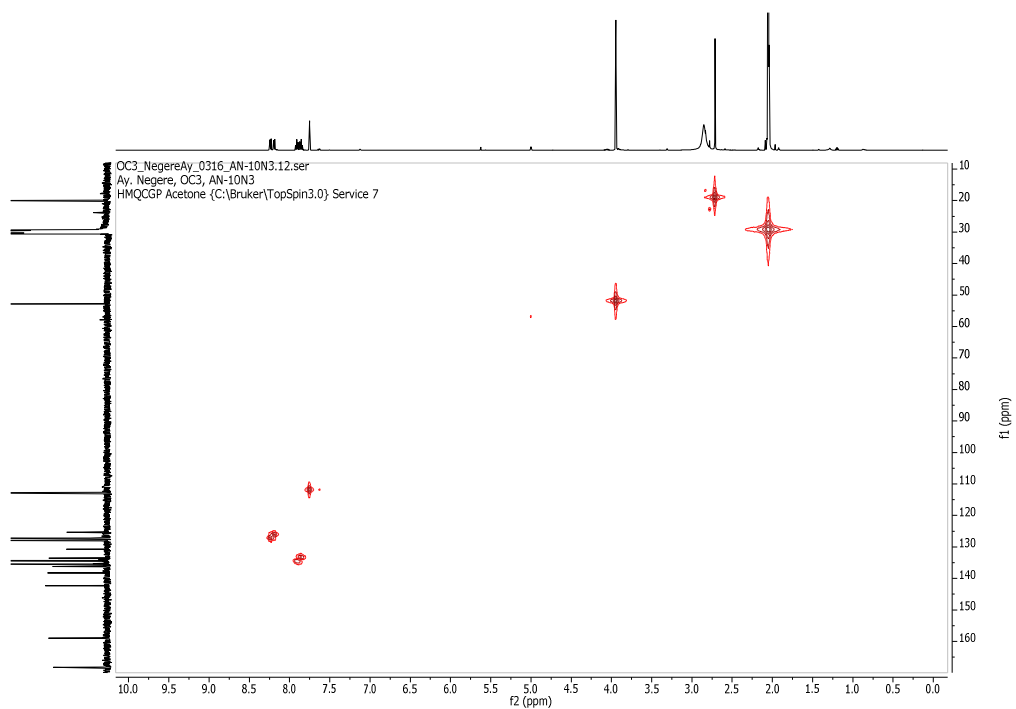
**Figure S8.** The <sup>1</sup>H NMR of aloesaponarin III (**2**) observed at 500 MHz in acetone-*d*<sub>6</sub> solution at 25 °C. Assignments are given in Table 1.



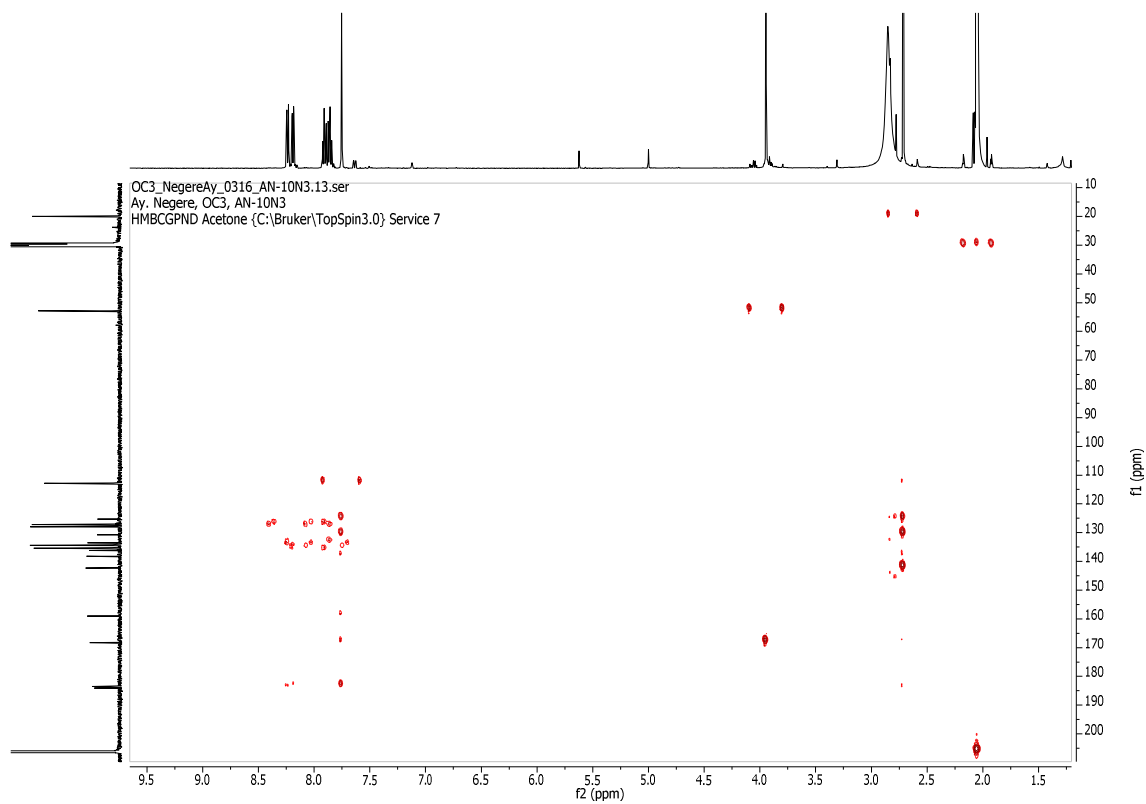
**Figure S9.** The  $^{13}\text{C}$  NMR spectrum of aloesaponarin III (**2**) observed at 125 MHz for acetone- $d_6$  solution at 25 °C. Assignments are given in Table 1.



**Figure S10.** The COSY spectrum of aloesaponarin III (**2**) observed at 500 MHz in acetone- $d_6$  solution at 25 °C.



**Figure S11.** The HSQC spectrum of aloesaponarin III (**2**) observed at 500 and 125 MHz for acetone- $d_6$  solution at 25 °C.



**Figure S12.** The HMBC spectrum of aloesaponarin III (**2**) observed at 500 and 125 MHz for acetone- $d_6$  solution at 25 °C.

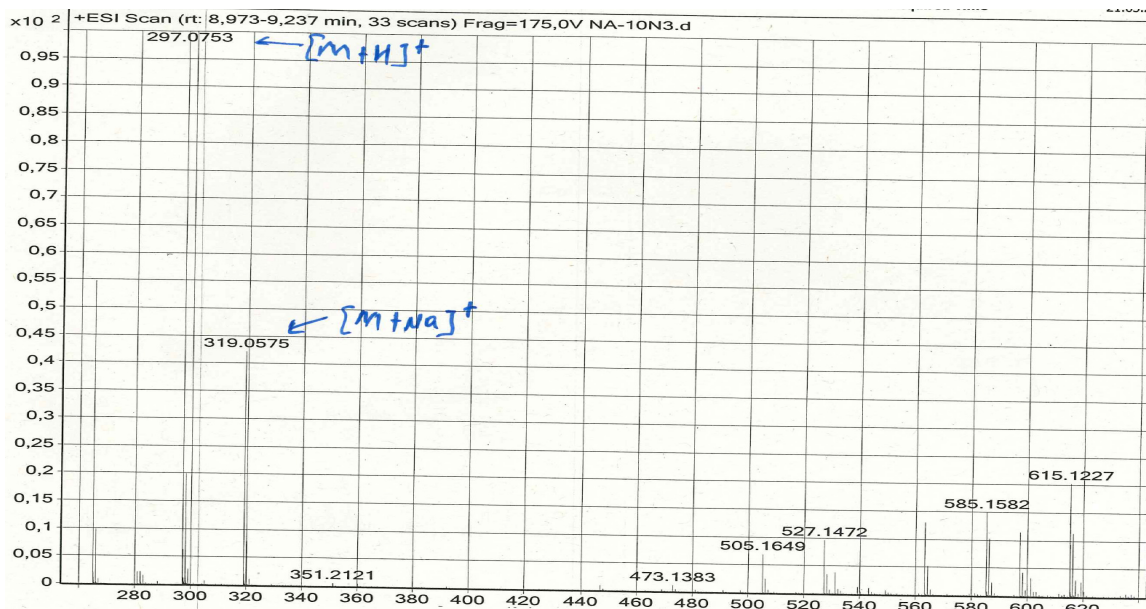


Figure S13. The HRESIMS of aloesaponarin III (**2**)

### Spectroscopic data for 10-*O*-methylchrysalodin (**3**)

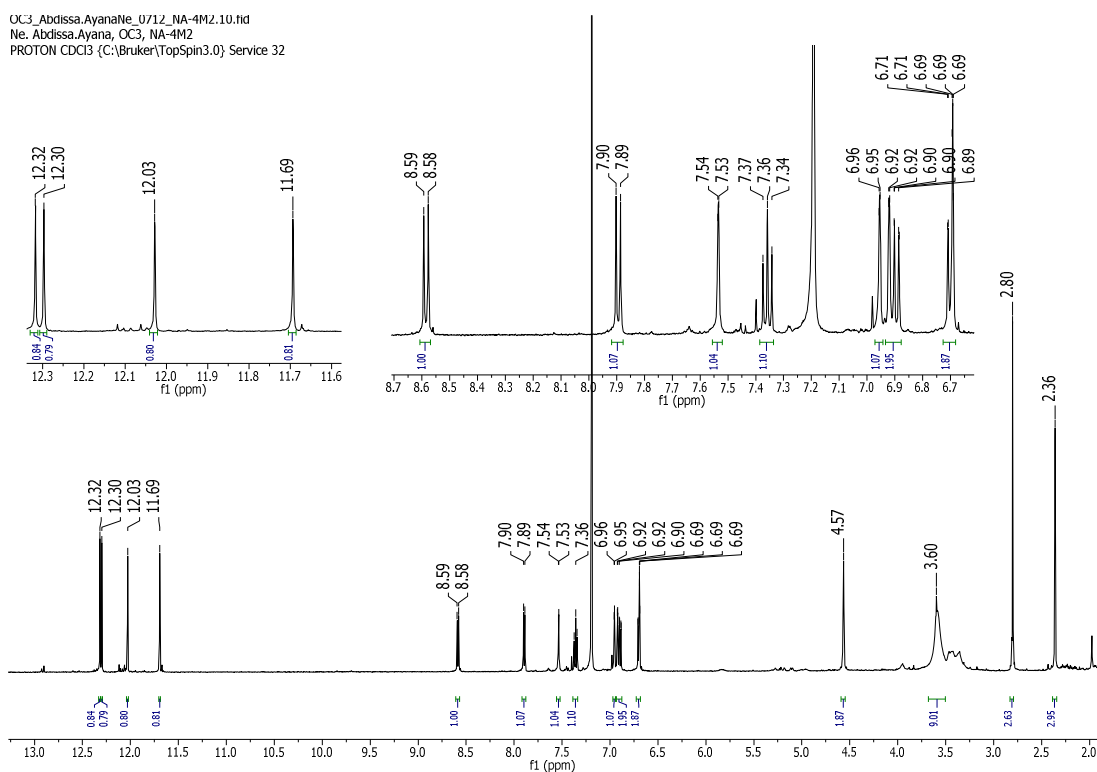
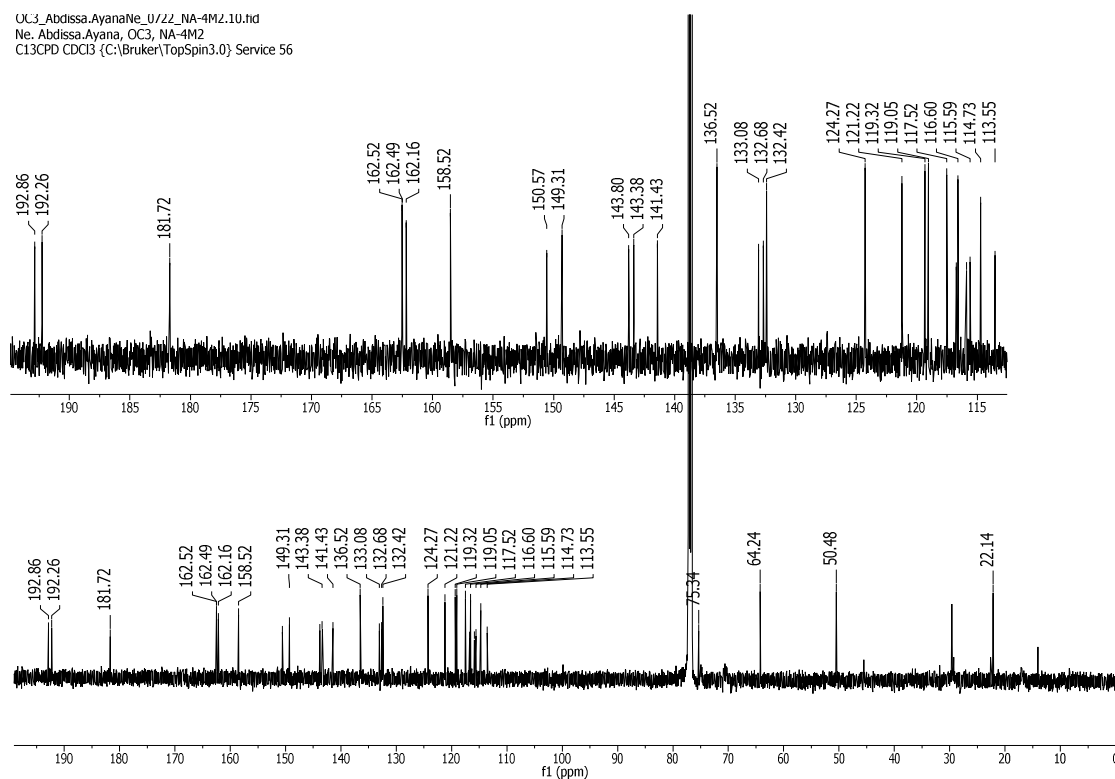
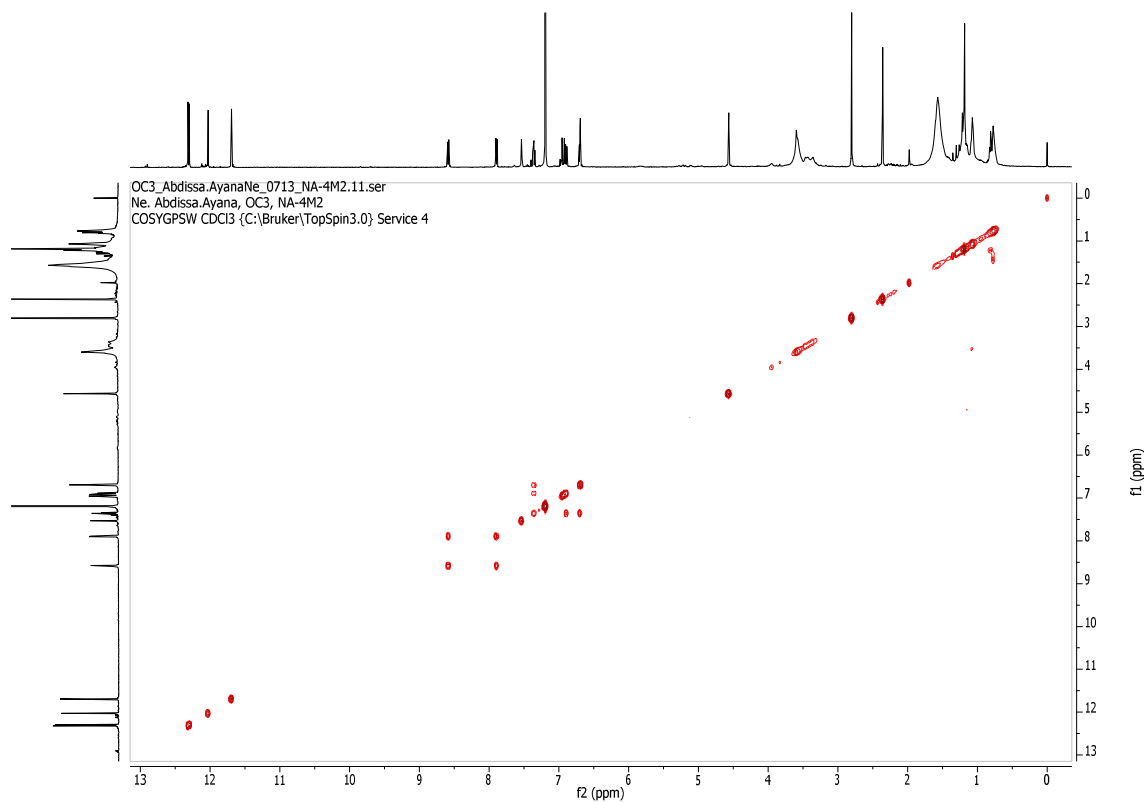


Figure S14. The <sup>1</sup>H NMR of 10-*O*-methylchrysalodin (**3**) observed at 500 MHz for CDCl<sub>3</sub> solution at 25 °C. Assignment is given in Table 1.

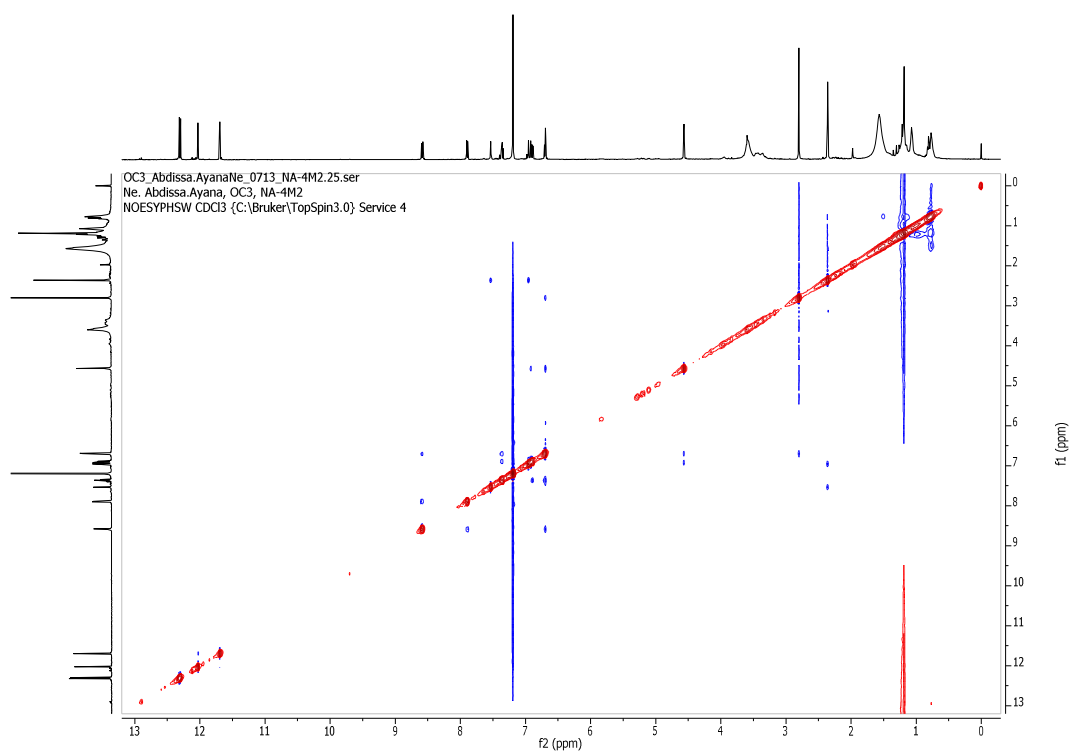




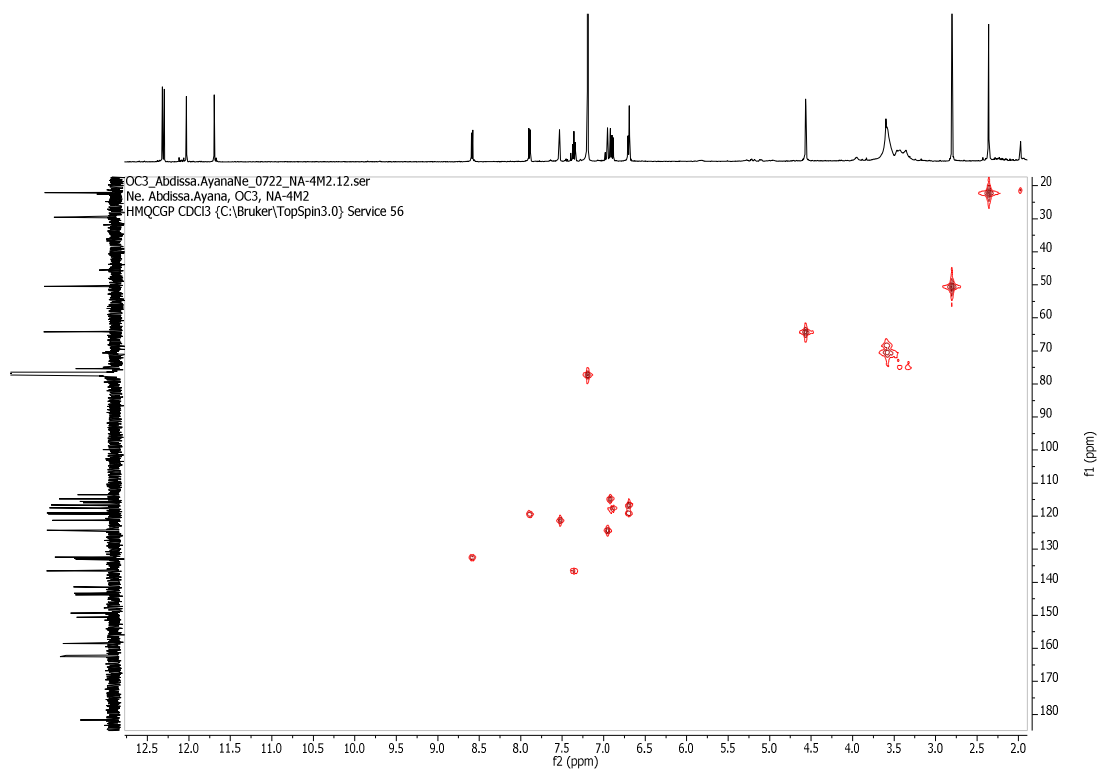
**Figure S15.** The  $^{13}\text{C}$  NMR spectrum of 10-*O*-methylchrysalodin (**3**) observed at 125 MHz for  $\text{CDCl}_3$  solution at 25 °C. Assignment is given in Table 1.



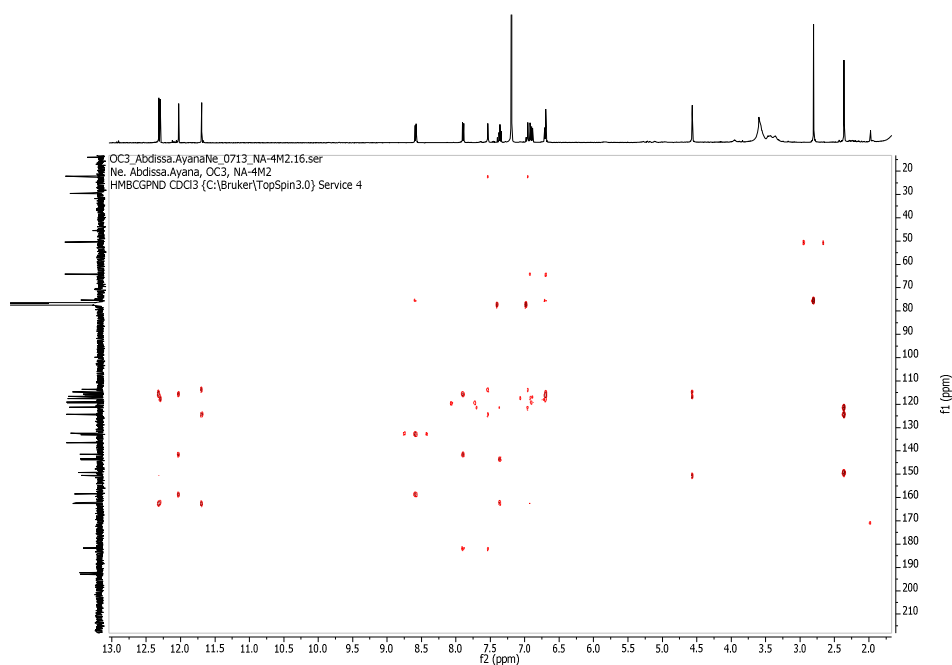
**Figure S16.** The COSY spectrum of 10-*O*-methylchrysalodin (**3**) observed at 500 MHz for  $\text{CDCl}_3$  solution at 25 °C.



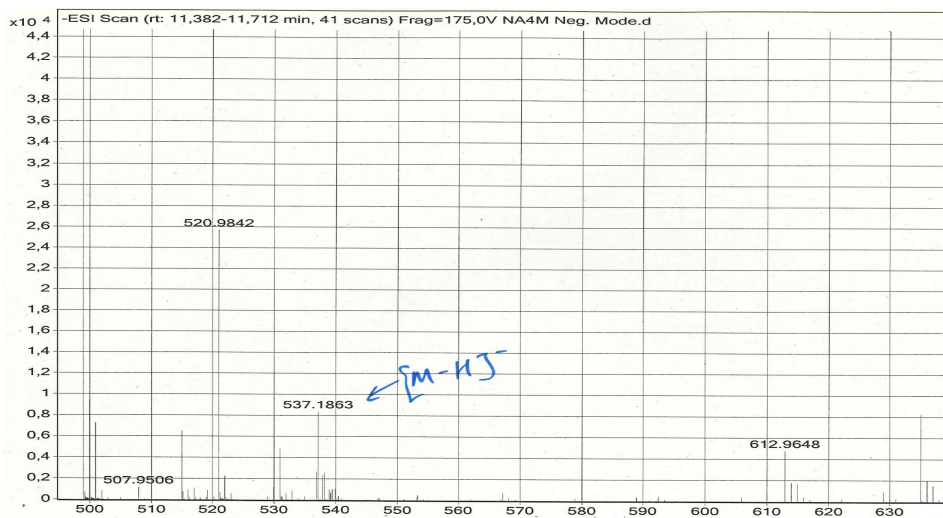
**Figure S17.** The NOESY spectrum of 10-*O*-methylchrysalodin (**3**) observed at 500 MHz for CDCl<sub>3</sub> solution at 25 °C.



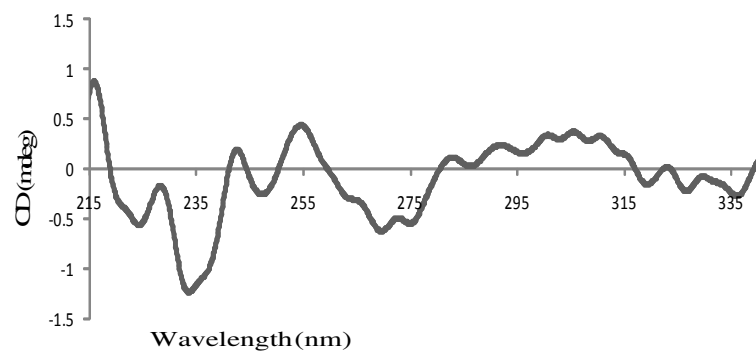
**Figure S18.** The HSQC spectrum of 10-*O*-methylchrysalodin (**3**) observed at 500 and 125 MHz for CDCl<sub>3</sub> solution at 25 °C.



**Figure S19.** The HMBC spectrum of 10-*O*-methylchrysalodin (**3**) observed at 500 and 125 MHz for CDCl<sub>3</sub> solution at 25 °C.



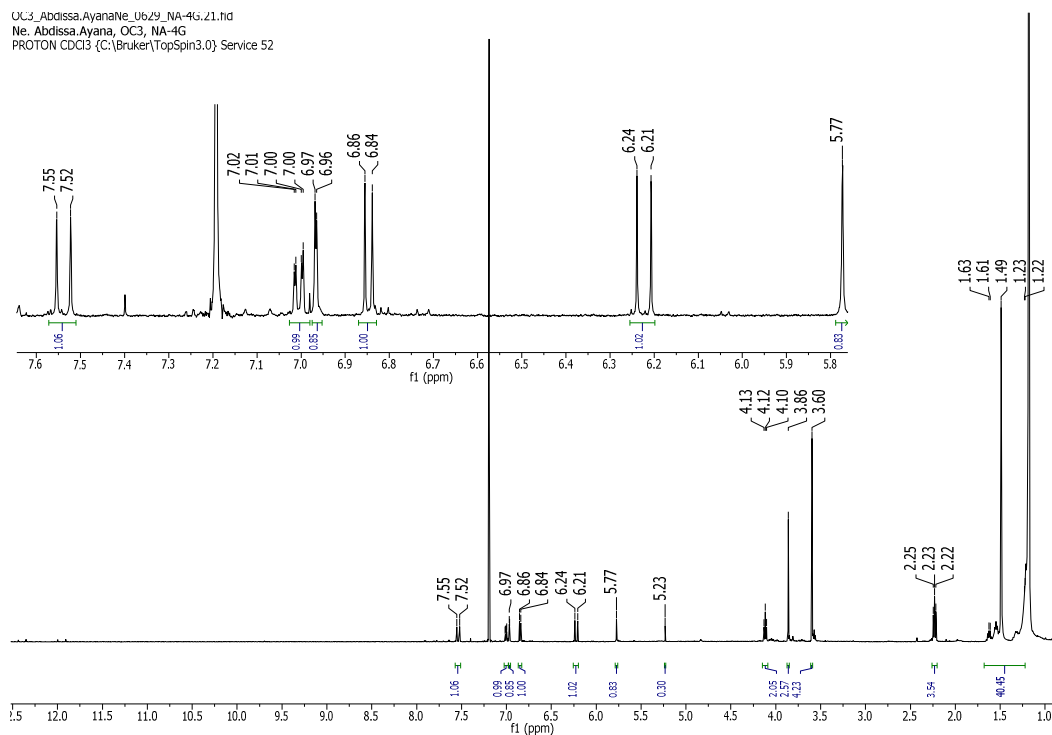
**Figure S20.** The HRESIMS of 10-*O*-methylchrysalodin (**3**).



**Figure21.** The CD spectrum of 10-*O*-methylchrysalodin (**3**) in acetonitril

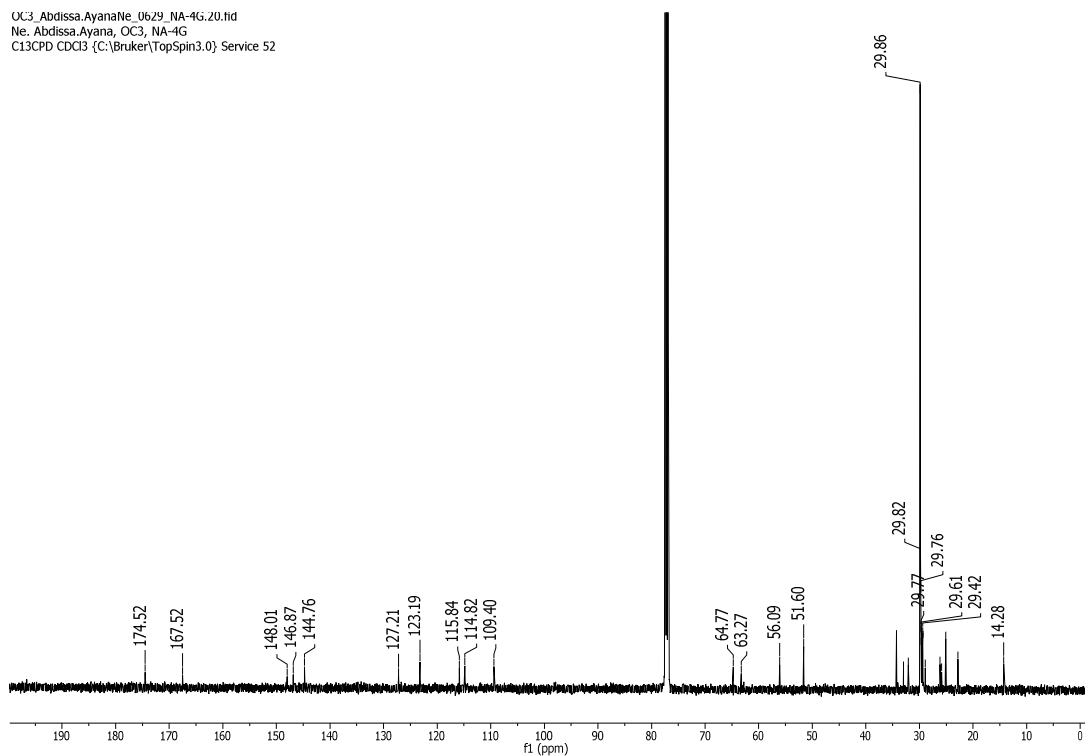
## Spectroscopic data for methyl 26-*O*-feruloyl-oxyhexacosanoate (**4**)

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Ne. Abdissa.Ayana, OC3, NA-4G  
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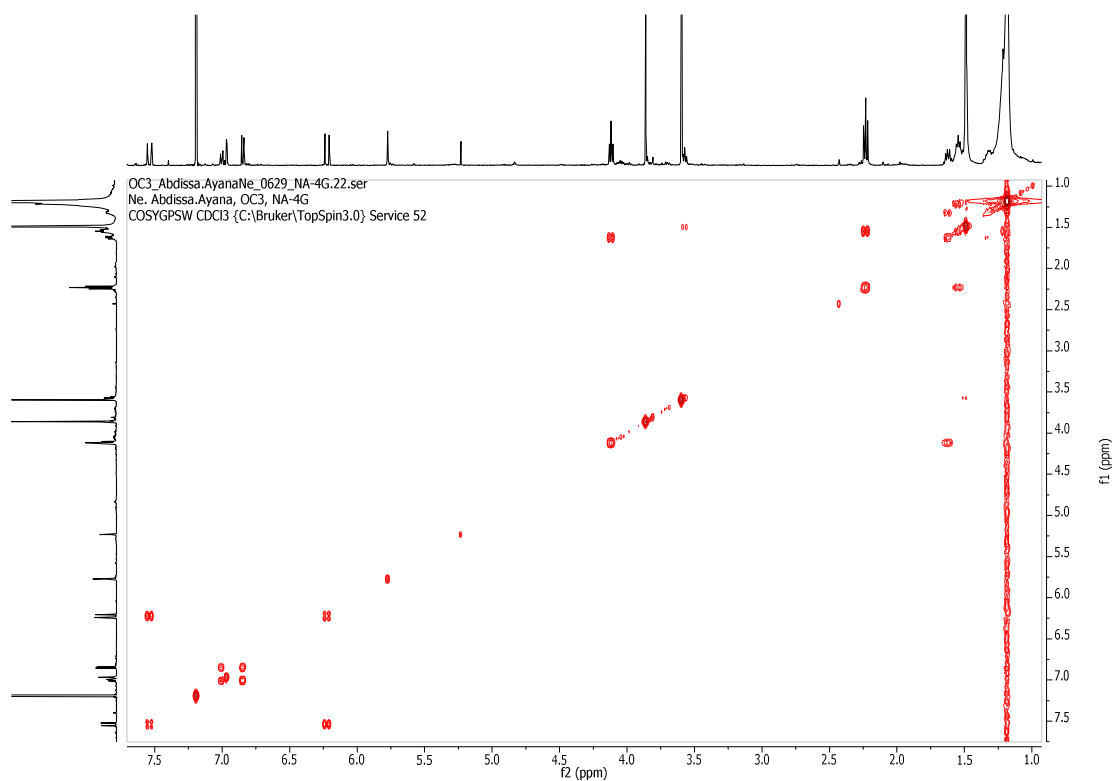


**Figure S22.** The <sup>1</sup>H NMR of methyl 26-*O*-feruloyl-oxyhexacosanoate (**4**) observed at 500 MHz for CDCl<sub>3</sub> solution at 25 °C. Assignment is given in section 3.3.

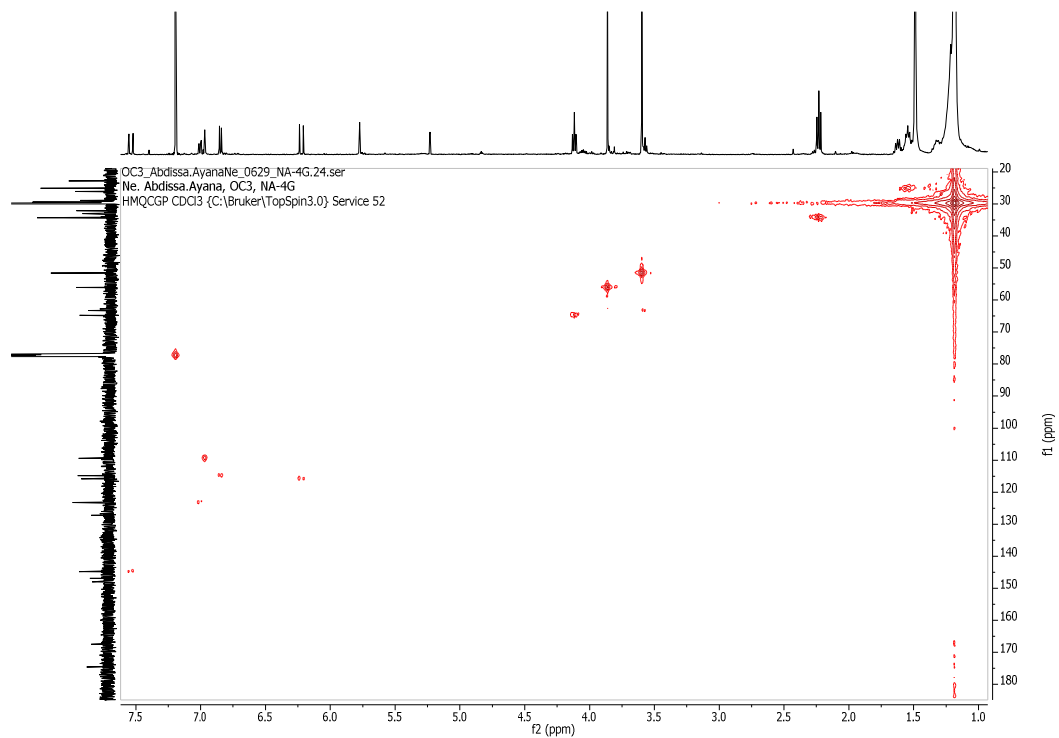
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C13CPD CDCl3 (C:\Bruker\TopSpin3.0) Service 52



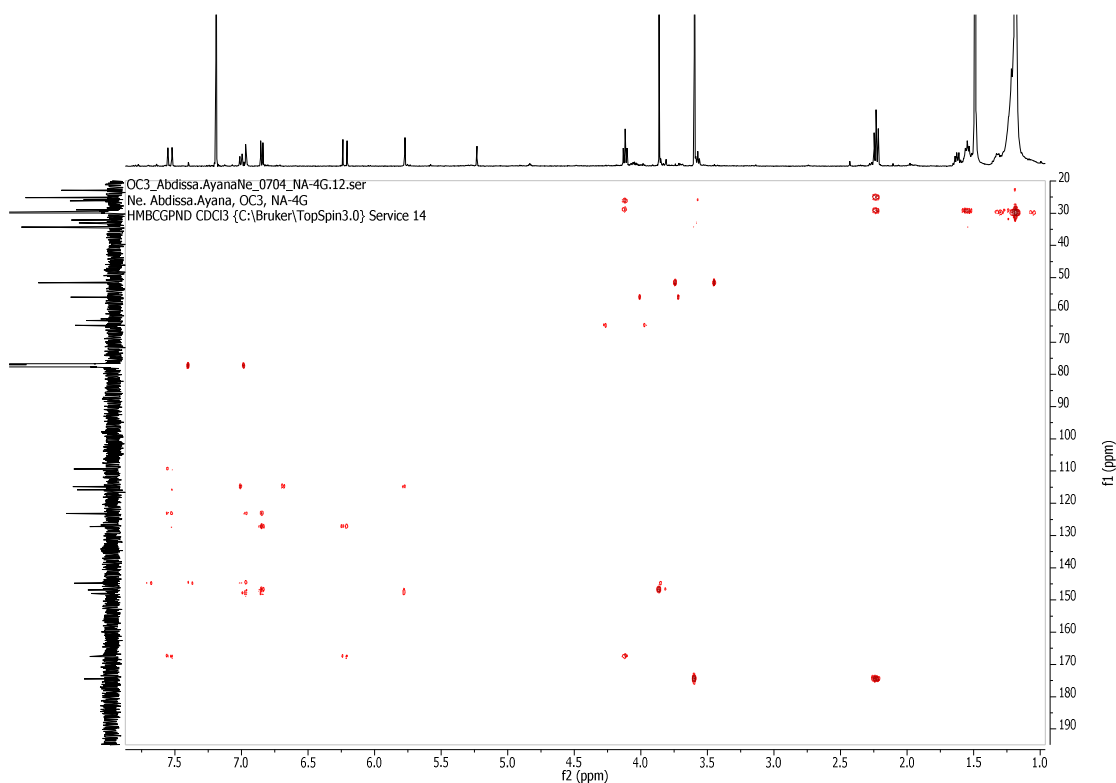
**Figure S23.** The <sup>13</sup>C NMR spectrum methyl 26-*O*-feruloyl-oxyhexacosanoate (**4**) observed at 125 MHz for CDCl<sub>3</sub> solution at 25 °C. Assignment is given in section 3.3.



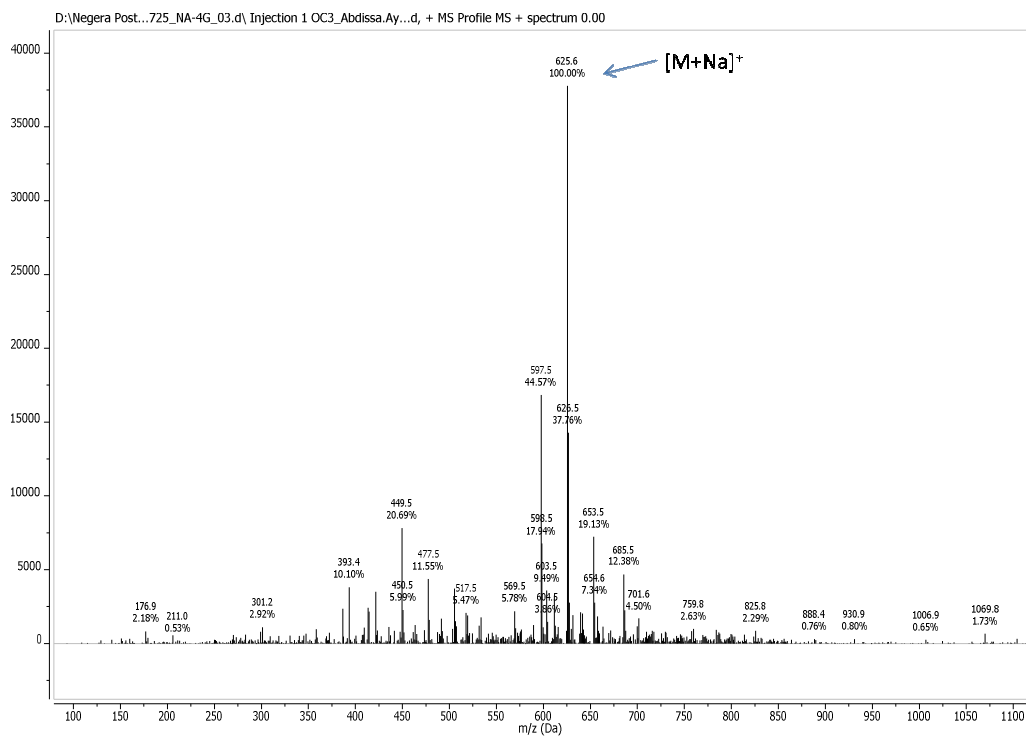
**Figure S24.** The COSY spectrum of methyl 26-*O*-feruloyl-oxyhexacosanoate (**4**) observed at 500 MHz for CDCl<sub>3</sub> solution at 25 °C.



**Figure S25.** The HSQC spectrum of methyl 26-*O*-feruloyl-oxyhexacosanoate (**4**) observed at 500 and 125 MHz for CDCl<sub>3</sub> solution at 25 °C.



**Figure S26.** The HMBC spectrum of methyl 26-*O*-feruloyl-oxyhexacosanoate (**4**) observed at 500 and 125 MHz for CDCl<sub>3</sub> solution at 25 °C.



**Figure S27.** The ESI-MS of methyl 26-*O*-feruloyl-oxyhexacosanoate (**4**)