

**Supplementary Information for**

**Chemical constituents from *Carica papaya* Linn. leaves as potential cytotoxic, EGFR<sup>wt</sup> and Aromatase (CYP19A) inhibitors; a study supported by molecular docking**

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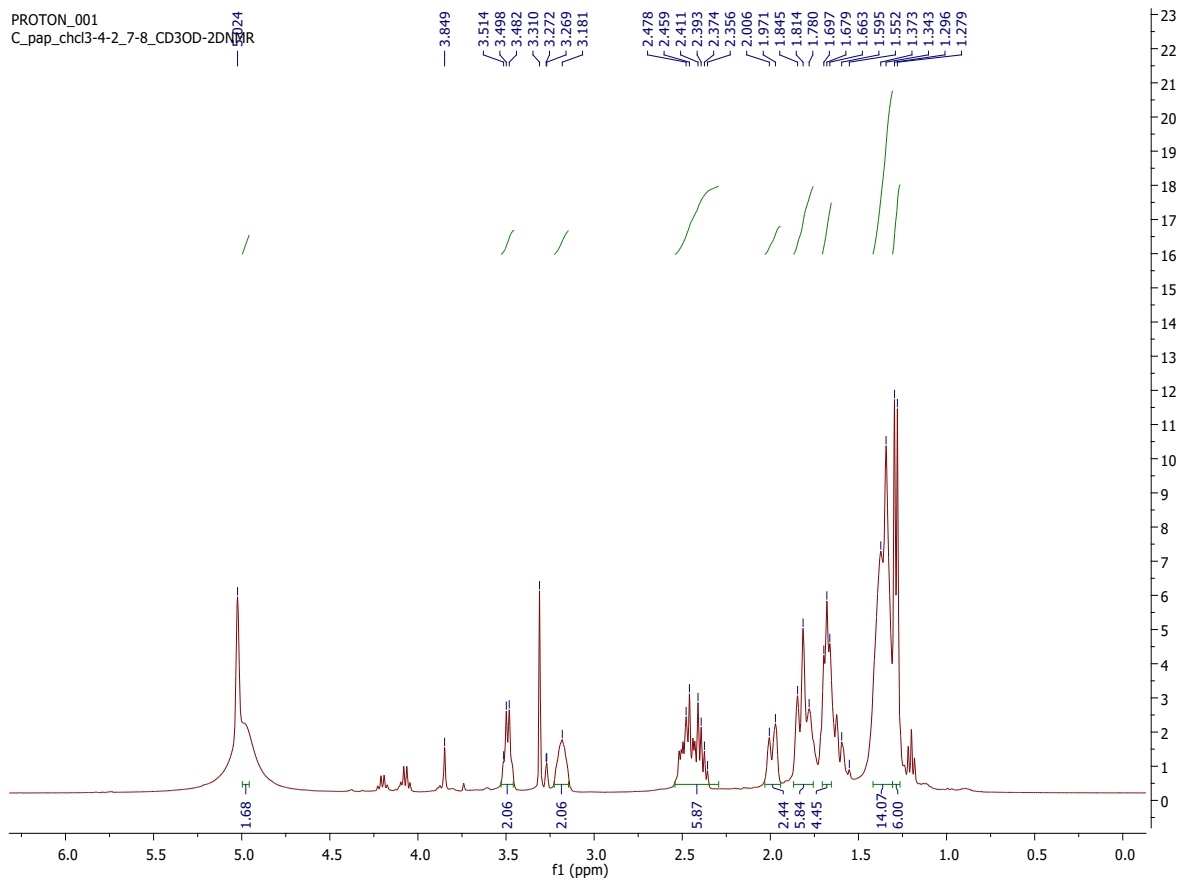
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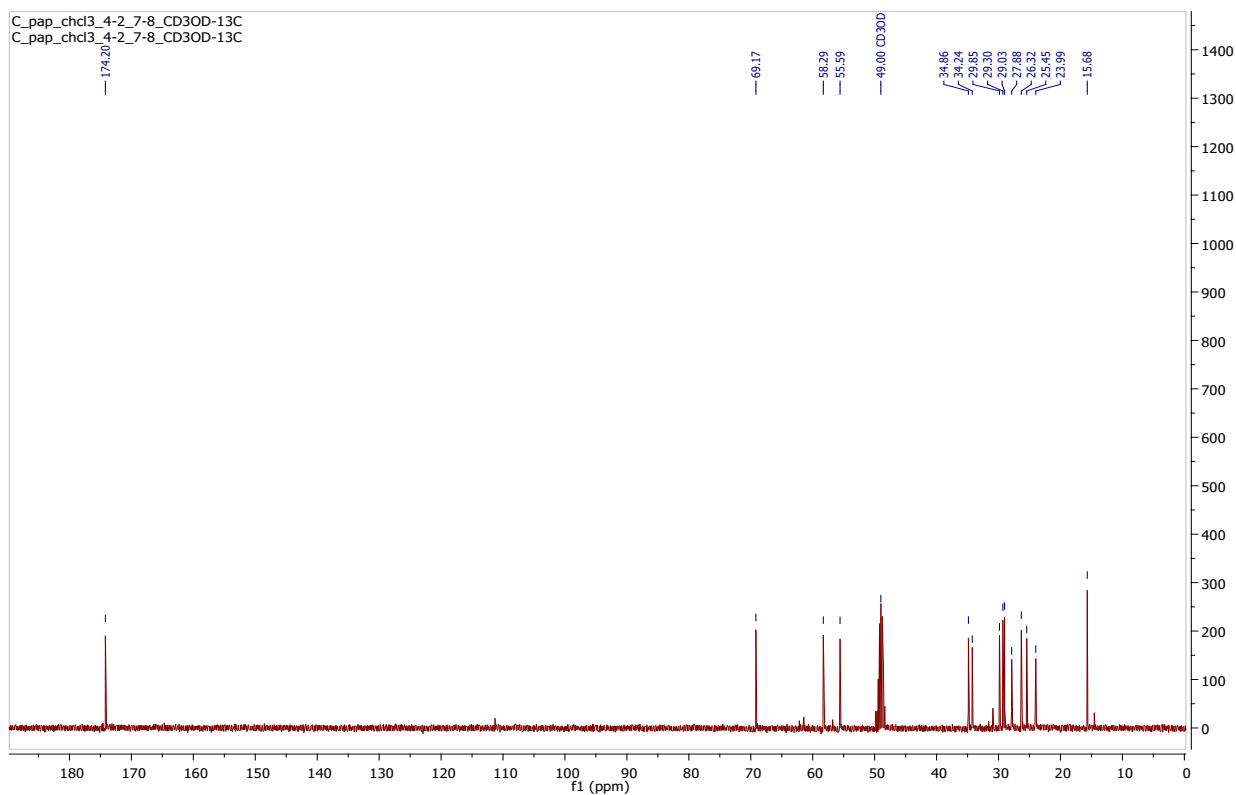
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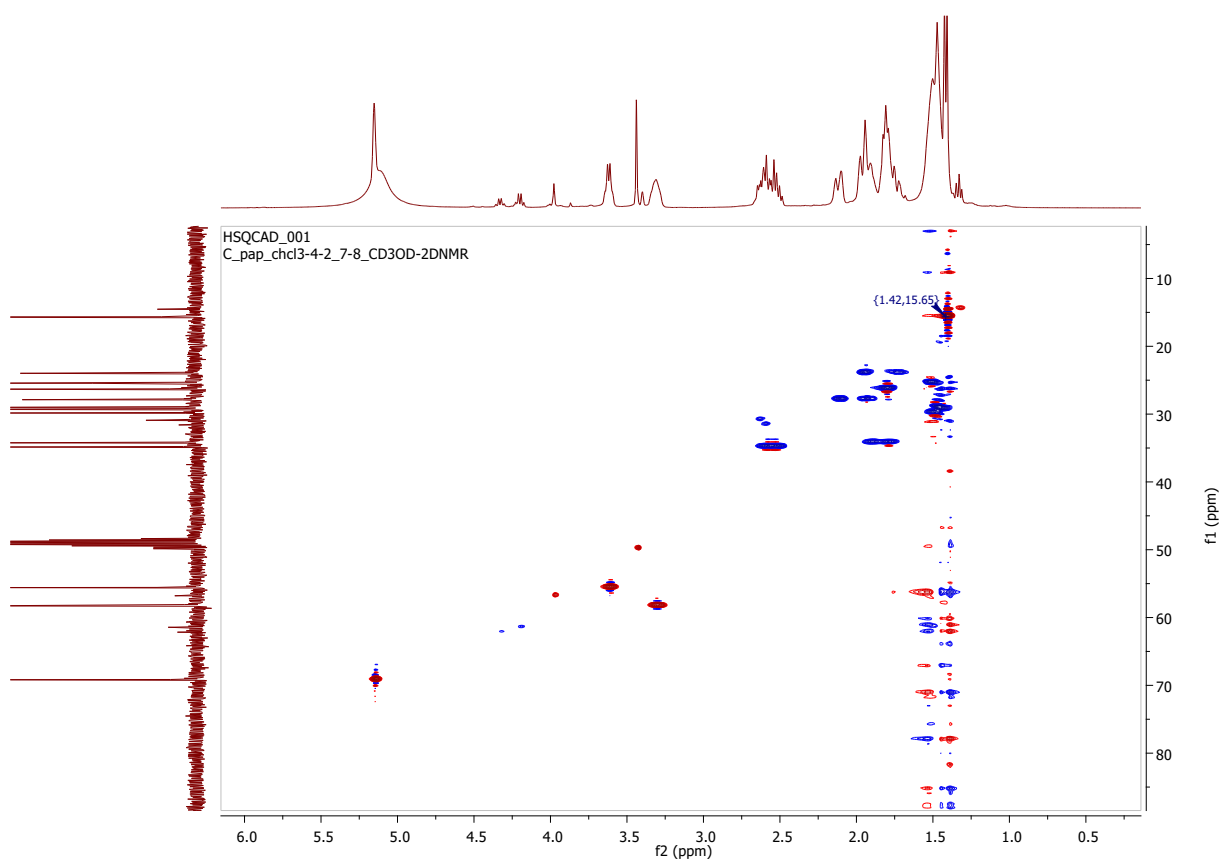
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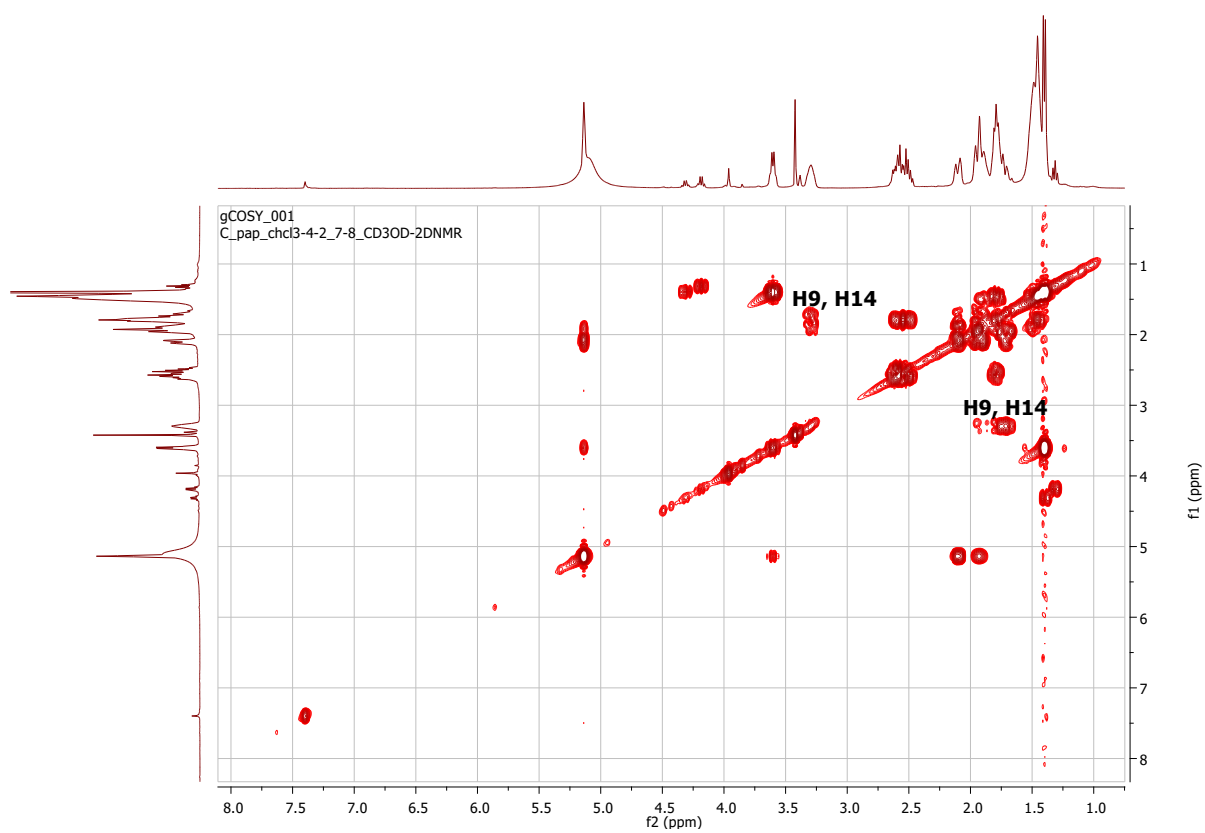
**Fig. S1**  $^1\text{H}$ -NMR spectrum of compound **1** (400 MHz,  $\text{CD}_3\text{OD}$ ).



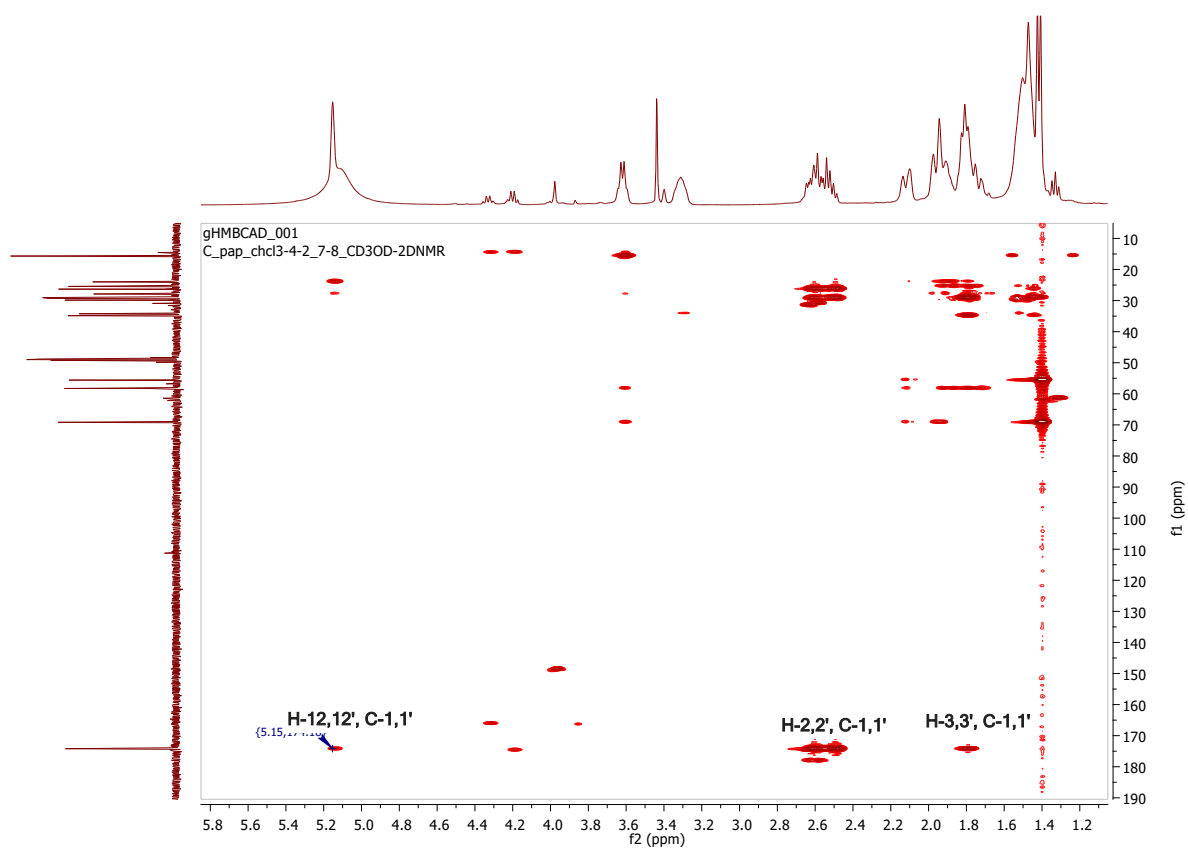
**Fig. S2**  $^{13}\text{C}$ -NMR spectrum of compound **1** (100 MHz,  $\text{CD}_3\text{OD}$ ).



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

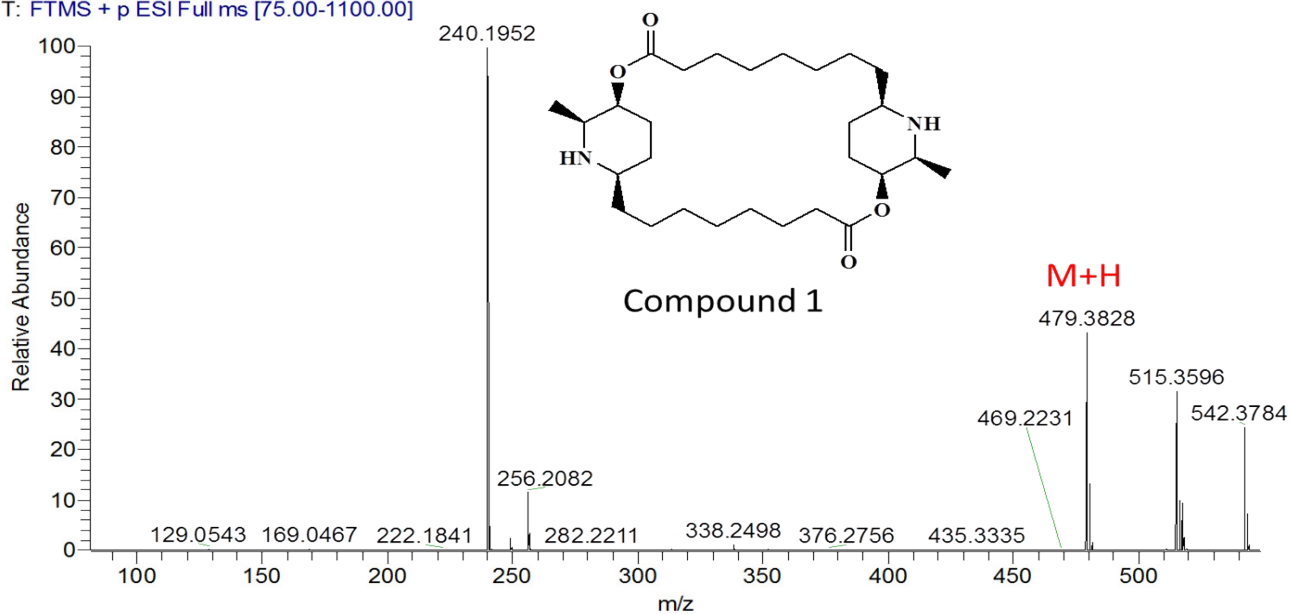


**Fig. S4.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **1**.

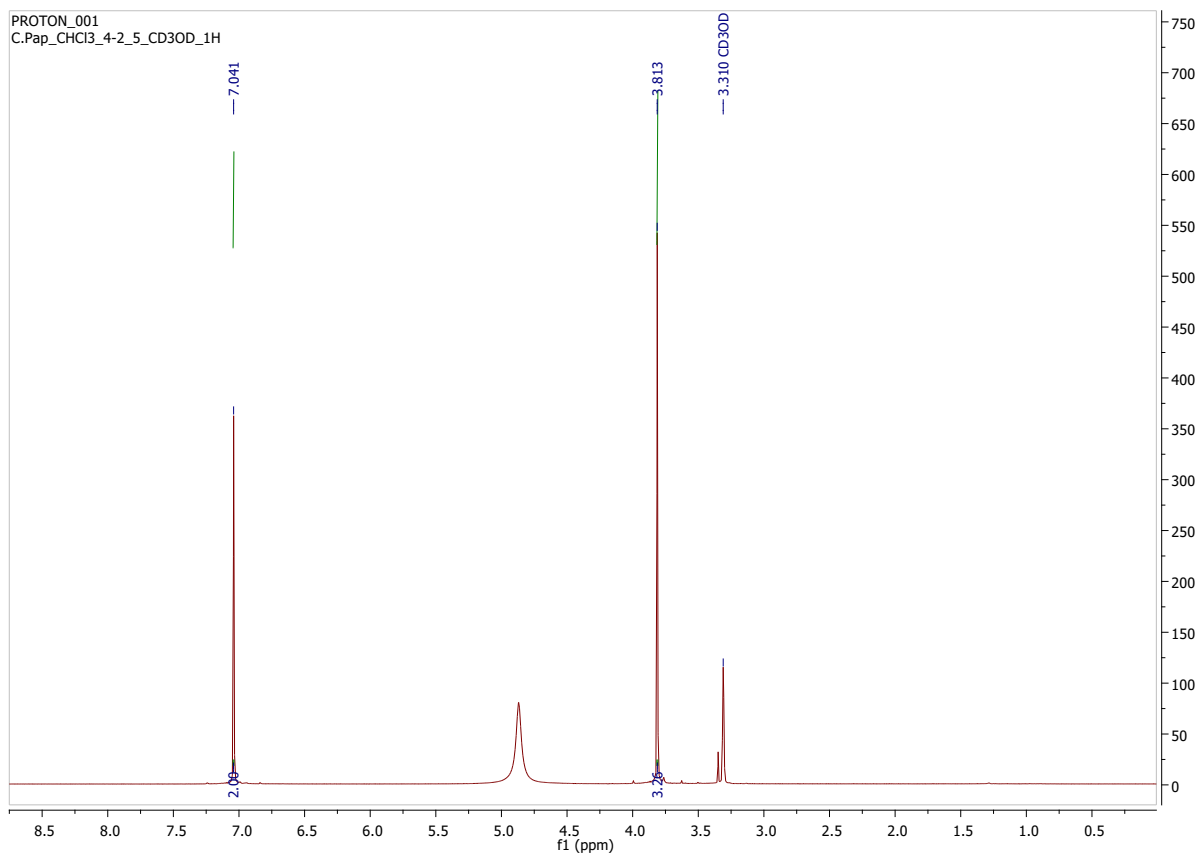


**Fig. S5** HMBC spectrum of compound **1**.

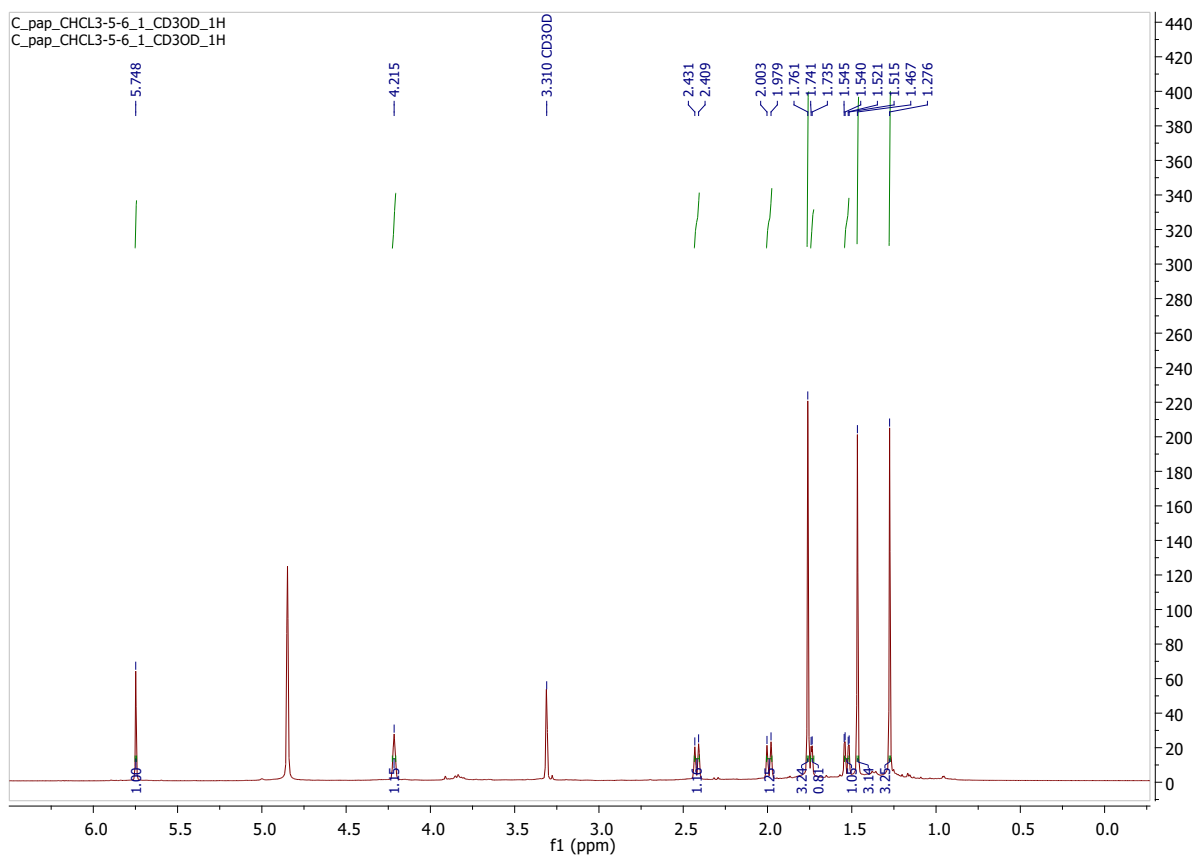
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T: FTMS + p ESI Full ms [75.00-1100.00]



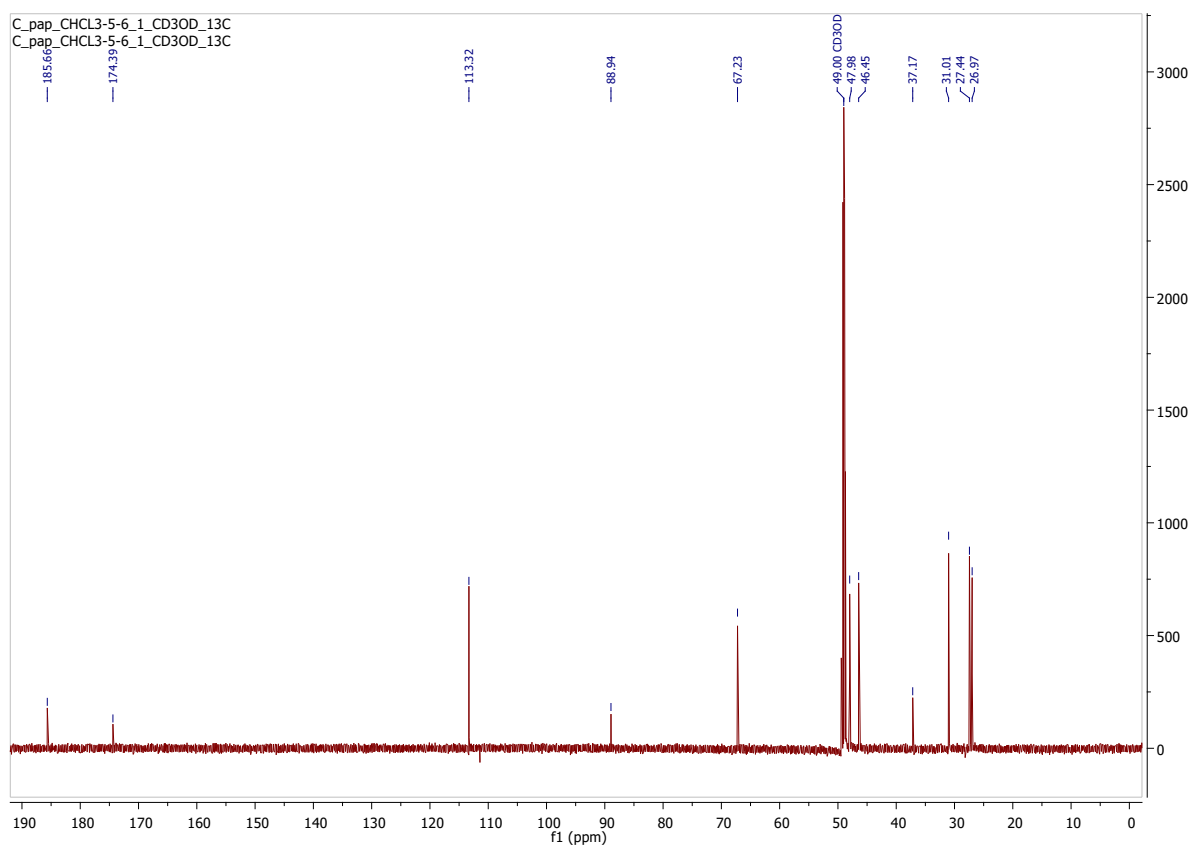
**Fig. S6** Positive HR-ESI-MS spectrum of compound **1**.



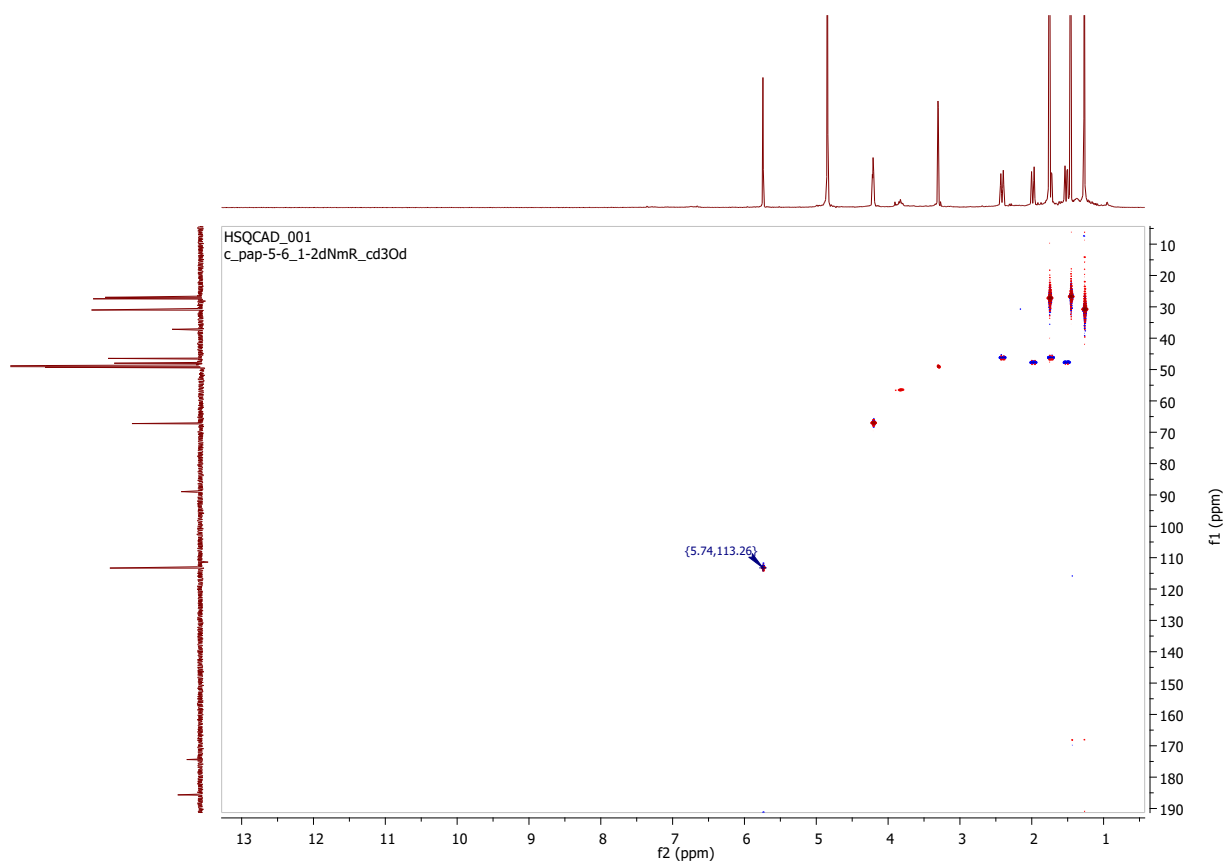
**Fig. S7**  $^1\text{H-NMR}$  spectrum of compound **2** (400 MHz,  $\text{CD}_3\text{OD}$ ).



**Fig. S8**  $^1\text{H-NMR}$  spectrum of compound **3** (400 MHz,  $\text{CD}_3\text{OD}$ ).

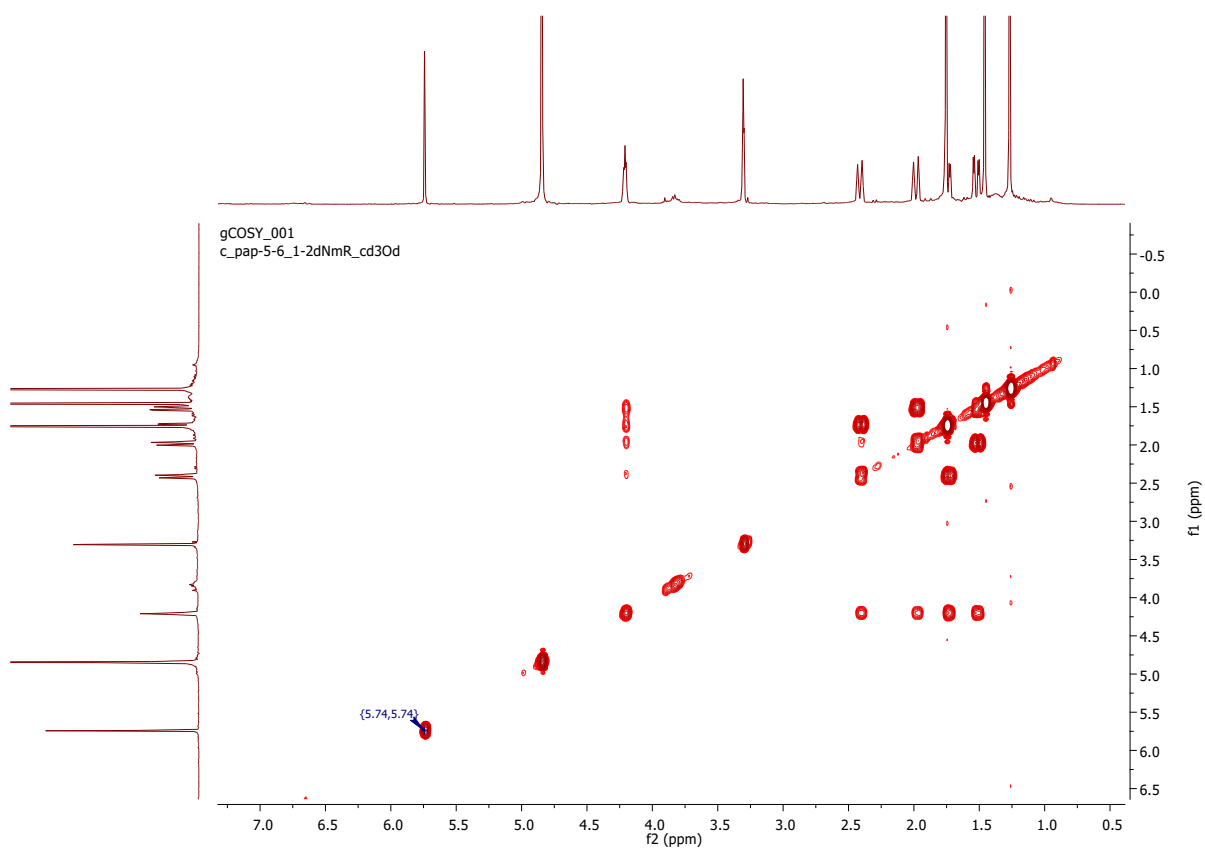


**Fig. S9**  $^{13}\text{C}$ -NMR spectrum of compound **3** (100 MHz,  $\text{CD}_3\text{OD}$ ).

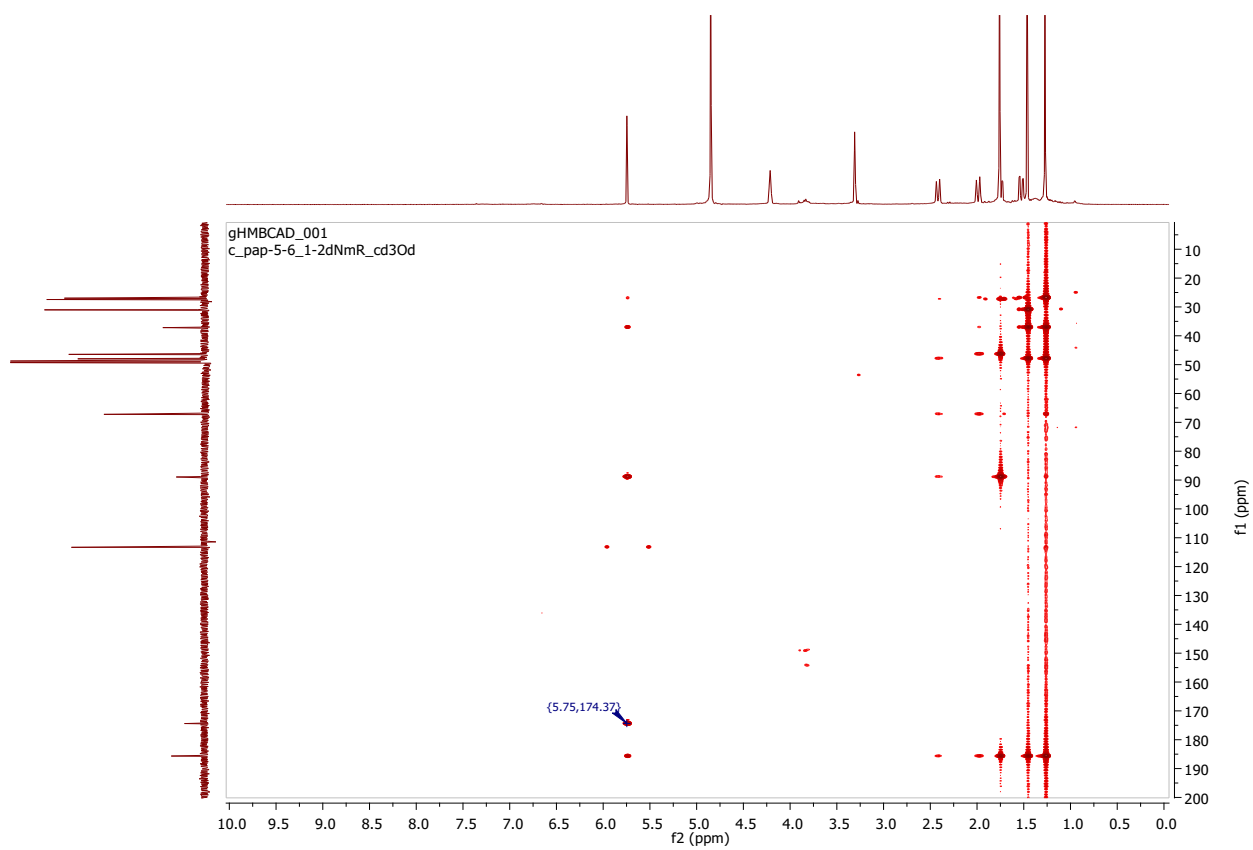


**Fig. S10** HSQC spectrum of compound **3**.

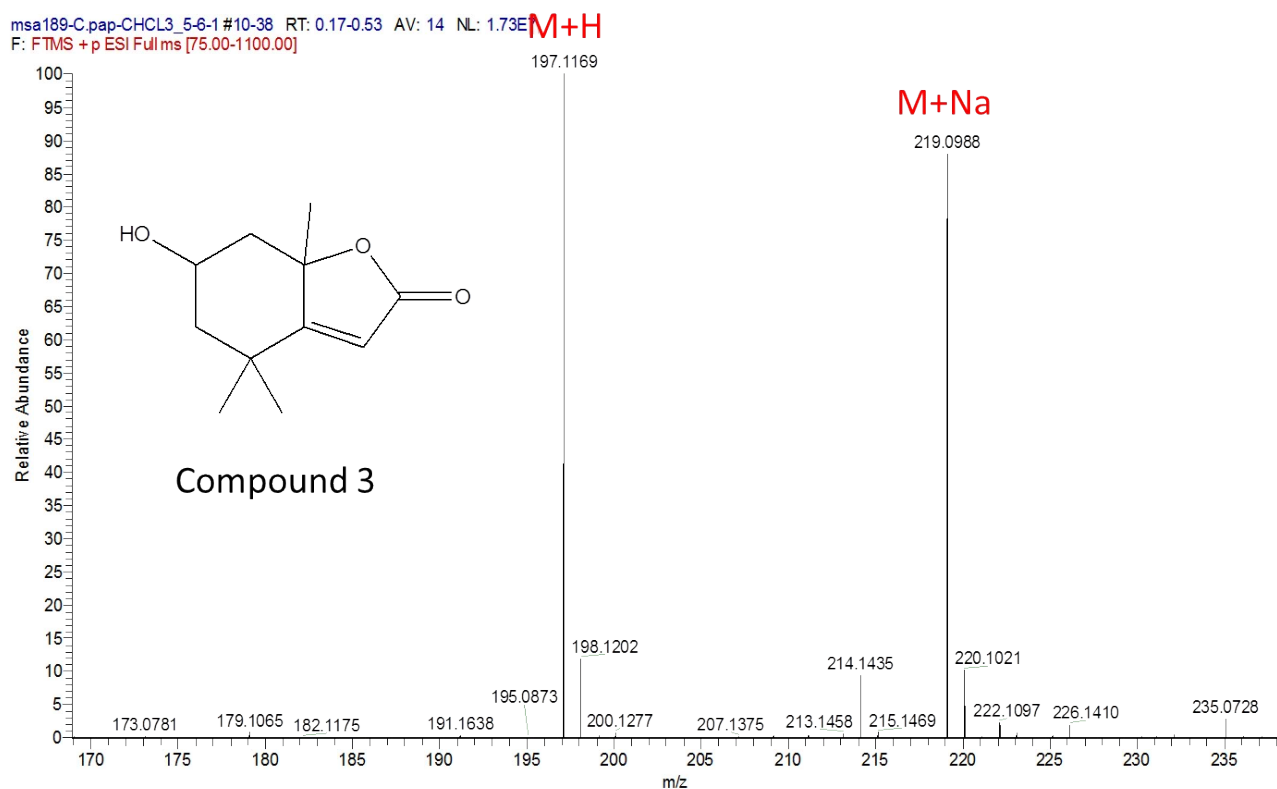




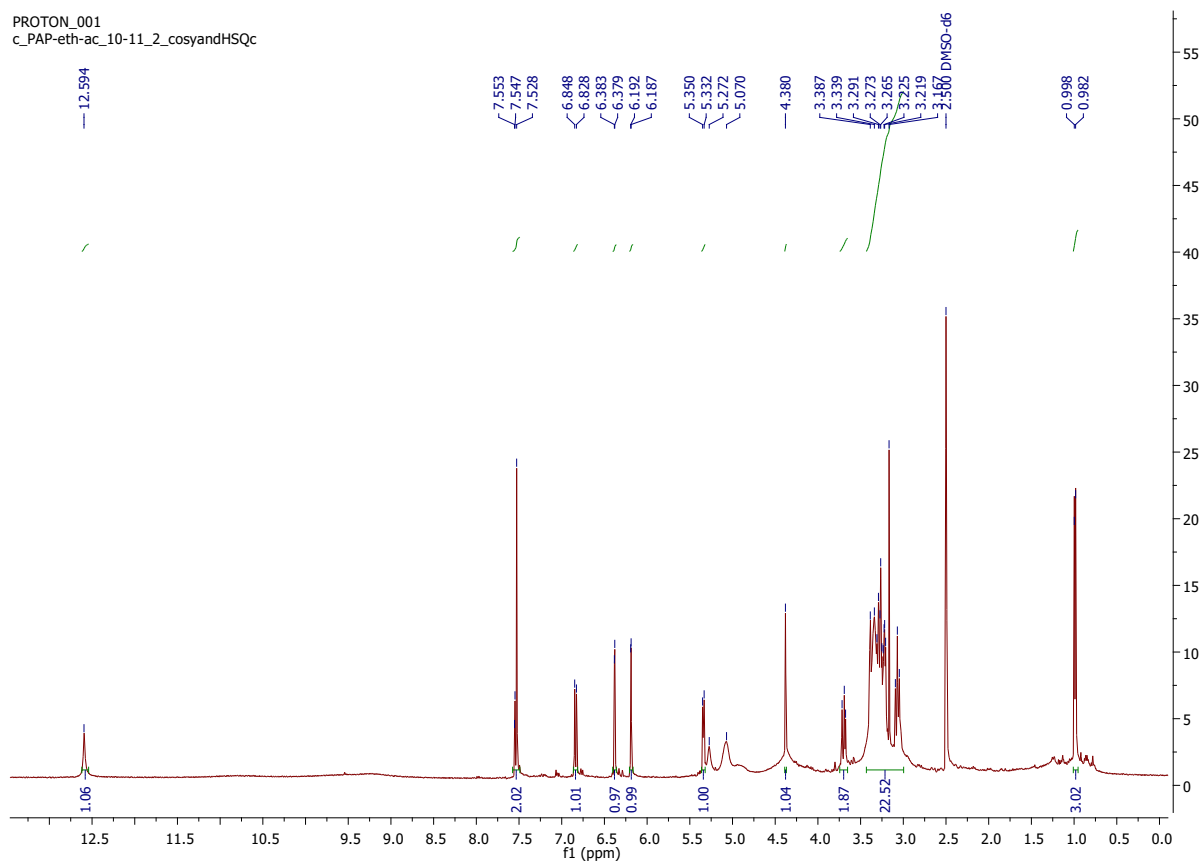
**Fig. S11.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **3**.



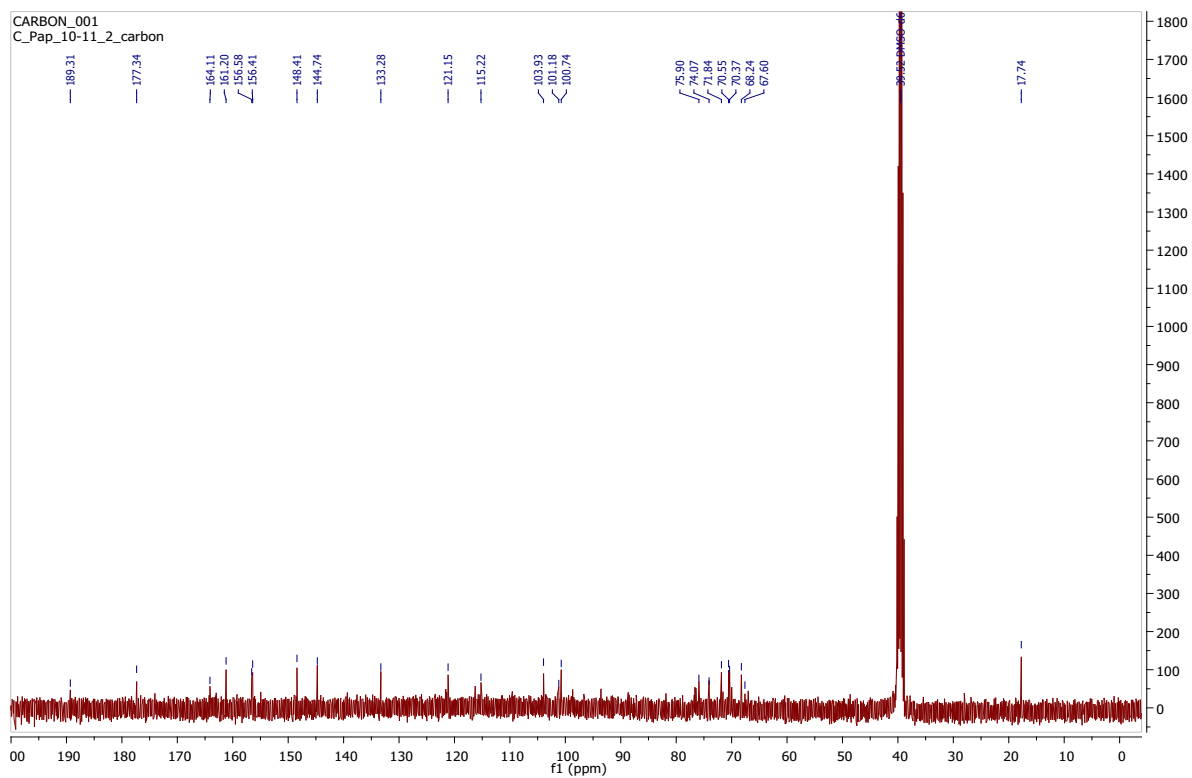
**Fig. S12** HMBC spectrum of compound **3**.



**Fig. S13** Positive HR-ESI-MS spectrum of compound **3**.



**Fig. S14.**  $^1\text{H-NMR}$  spectrum of compound **4** (400 MHz,  $\text{DMSO-}d_6$ ).



**Fig. S15.**  $^{13}\text{C-NMR}$  spectrum of compound **4** (100 MHz,  $\text{DMSO-}d_6$ ).

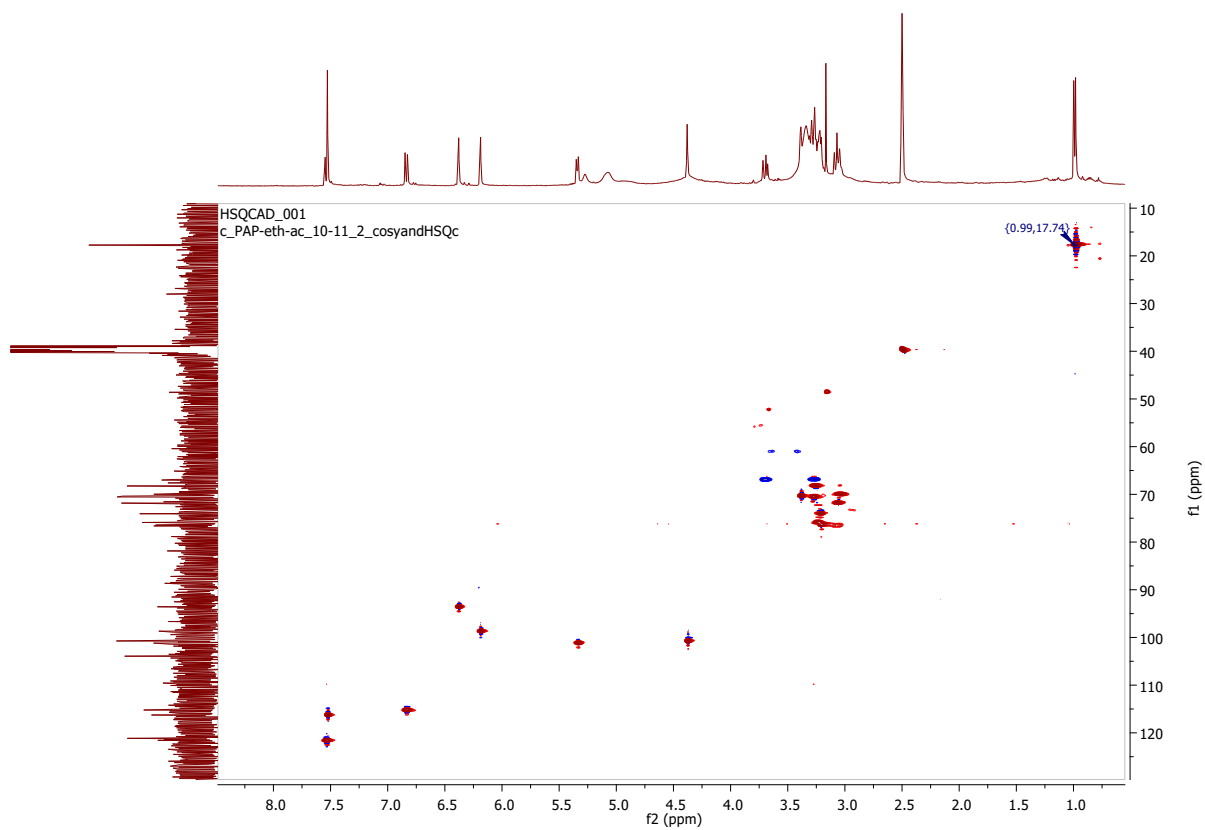


Fig. S16 HSQC spectrum of compound 4.

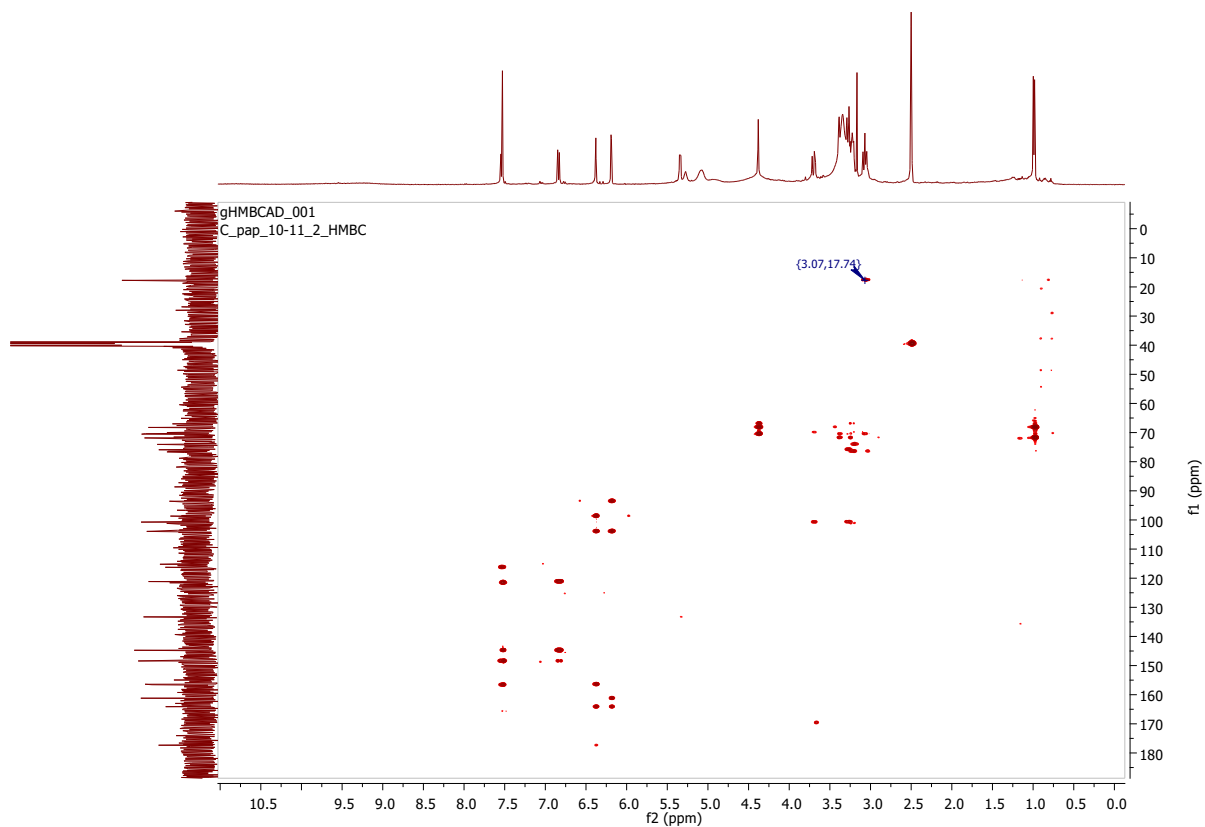
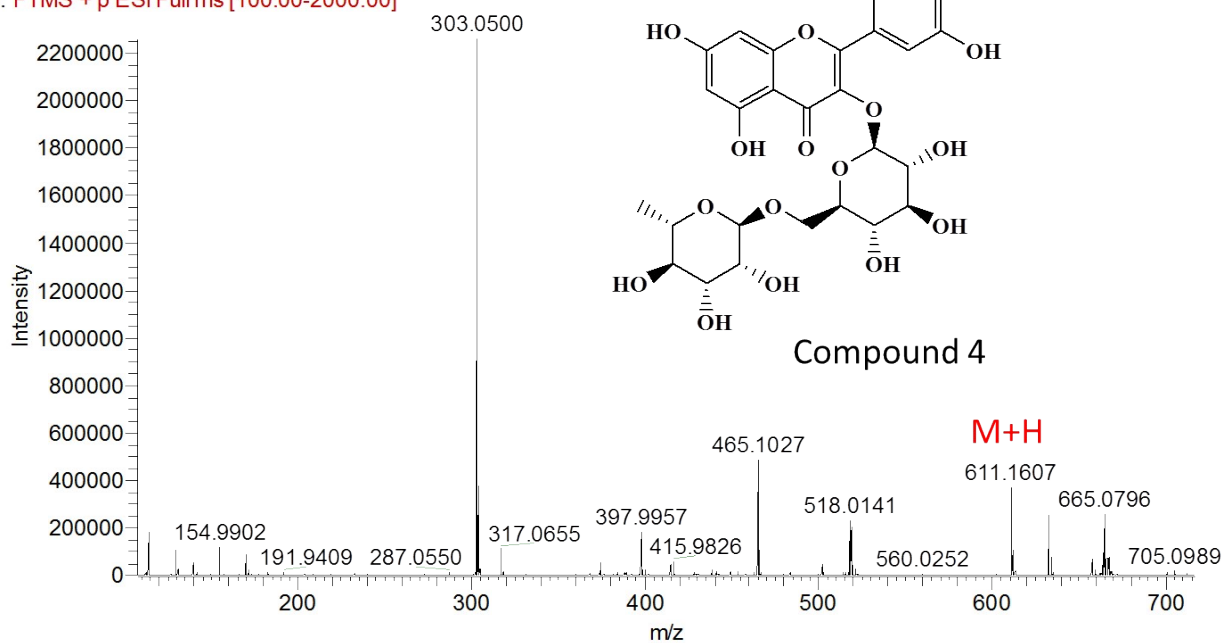
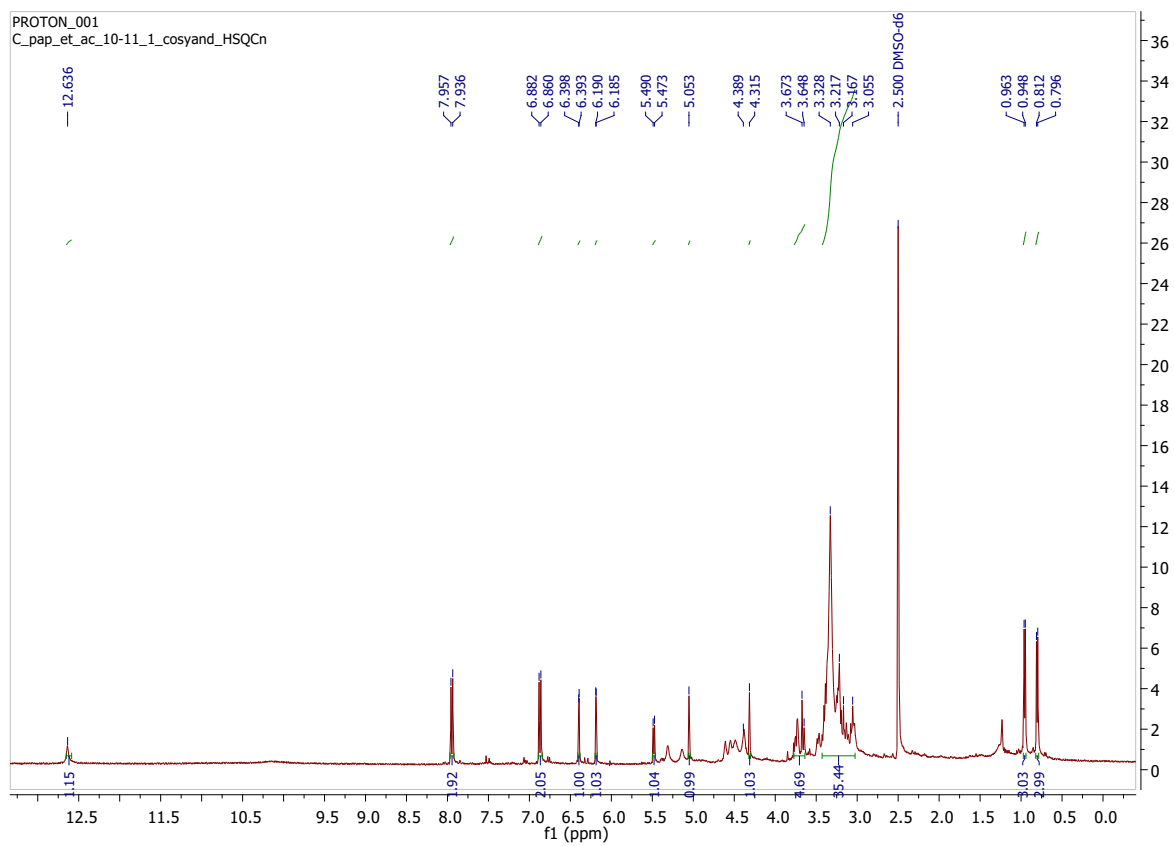


Fig. S17 HMBC spectrum of compound 4.

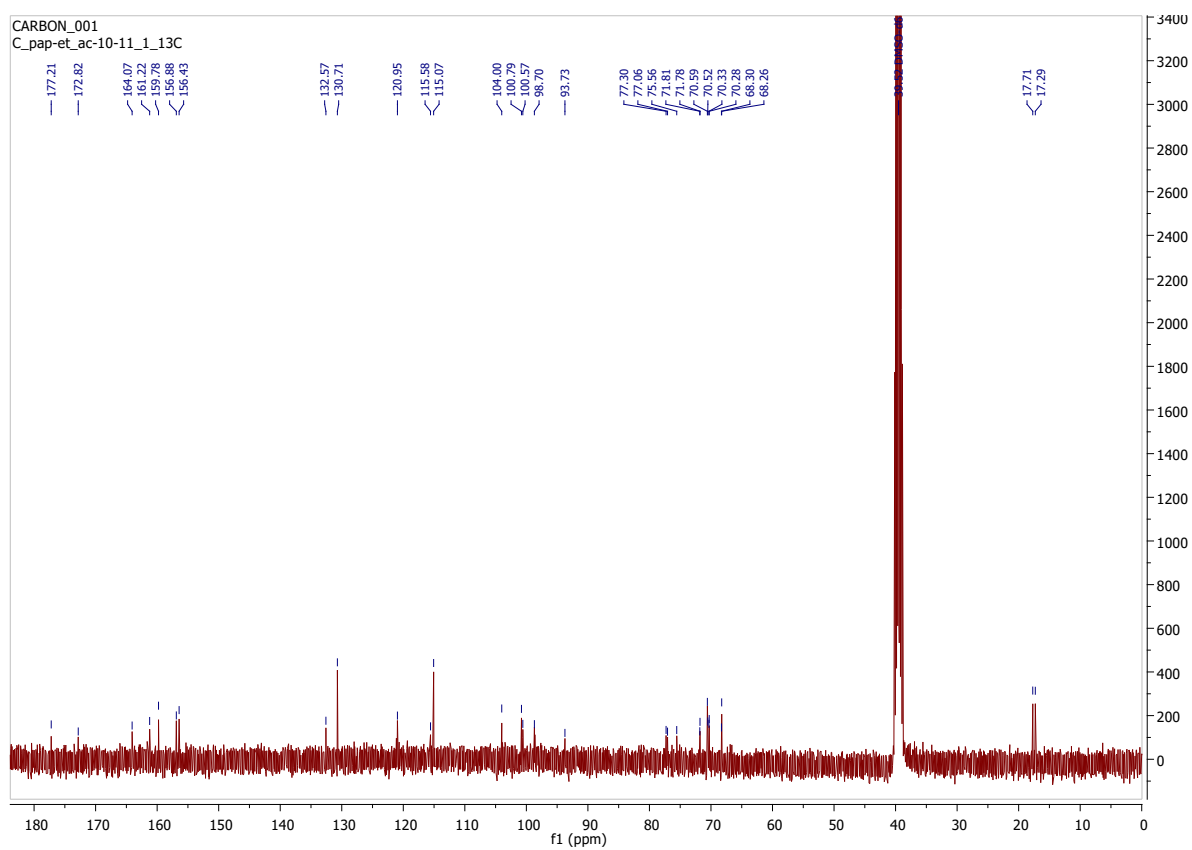
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F: FTMS + p ESI Full ms [100.00-2000.00]



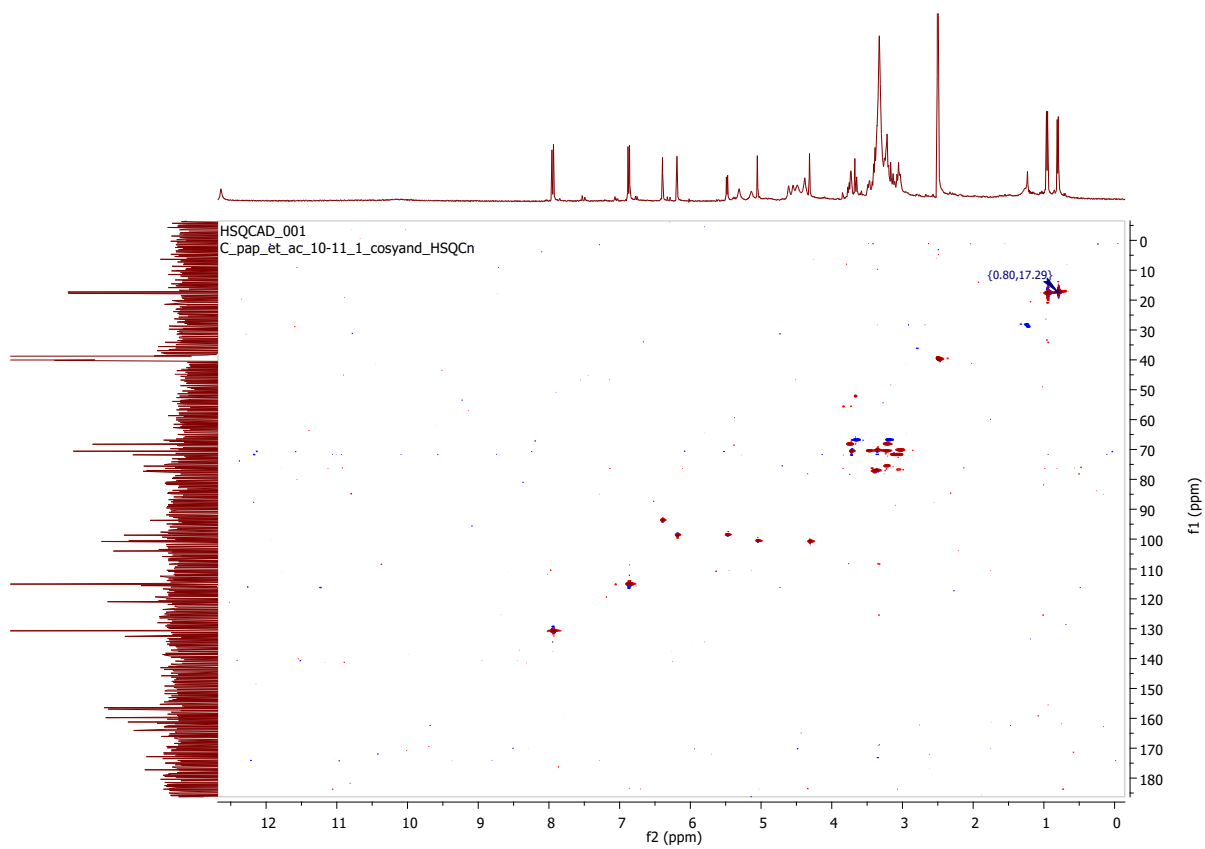
**Fig. S18** Positive HR-ESI-MS spectrum of compound **4**.



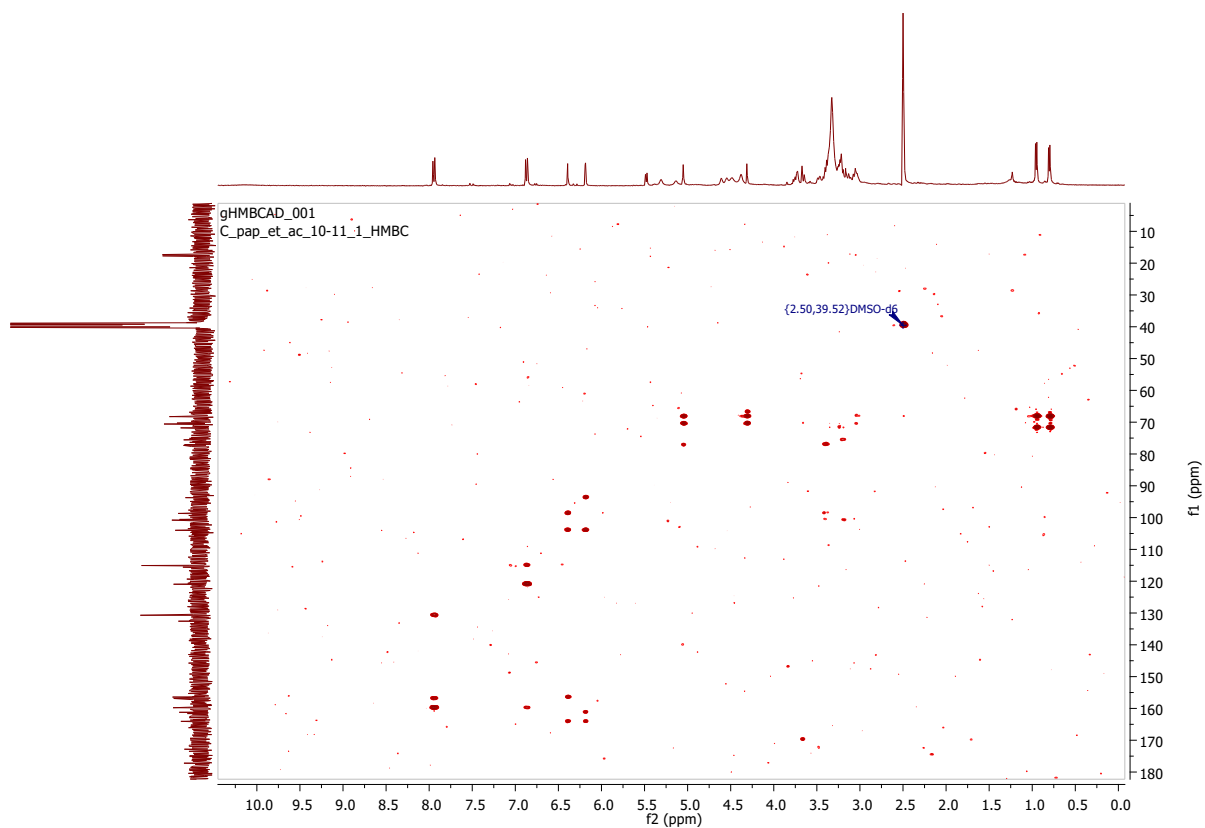
**Fig. S19**  $^1\text{H-NMR}$  spectrum of compound **5** (400 MHz,  $\text{DMSO-}d_6$ ).



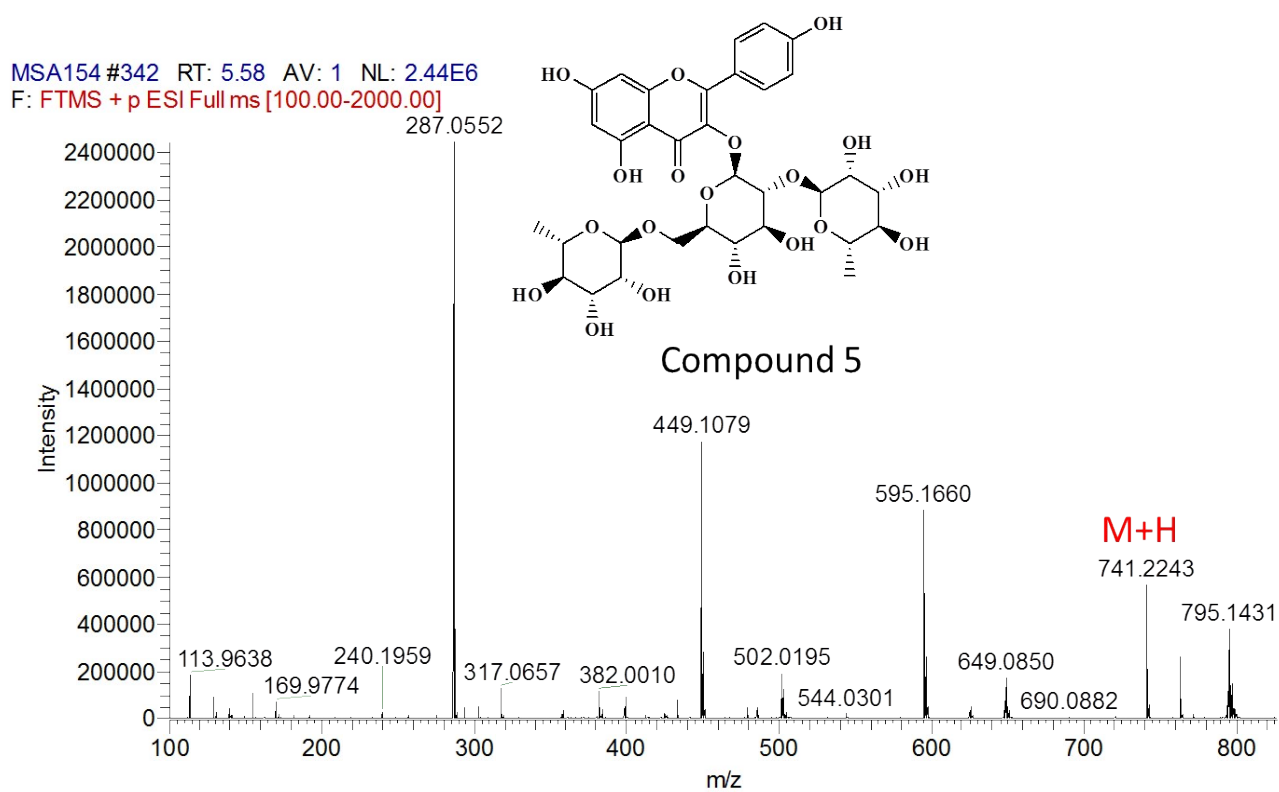
**Fig. S20**  $^{13}\text{C}$ -NMR spectrum of compound **5** (100 MHz,  $\text{DMSO-}d_6$ ).



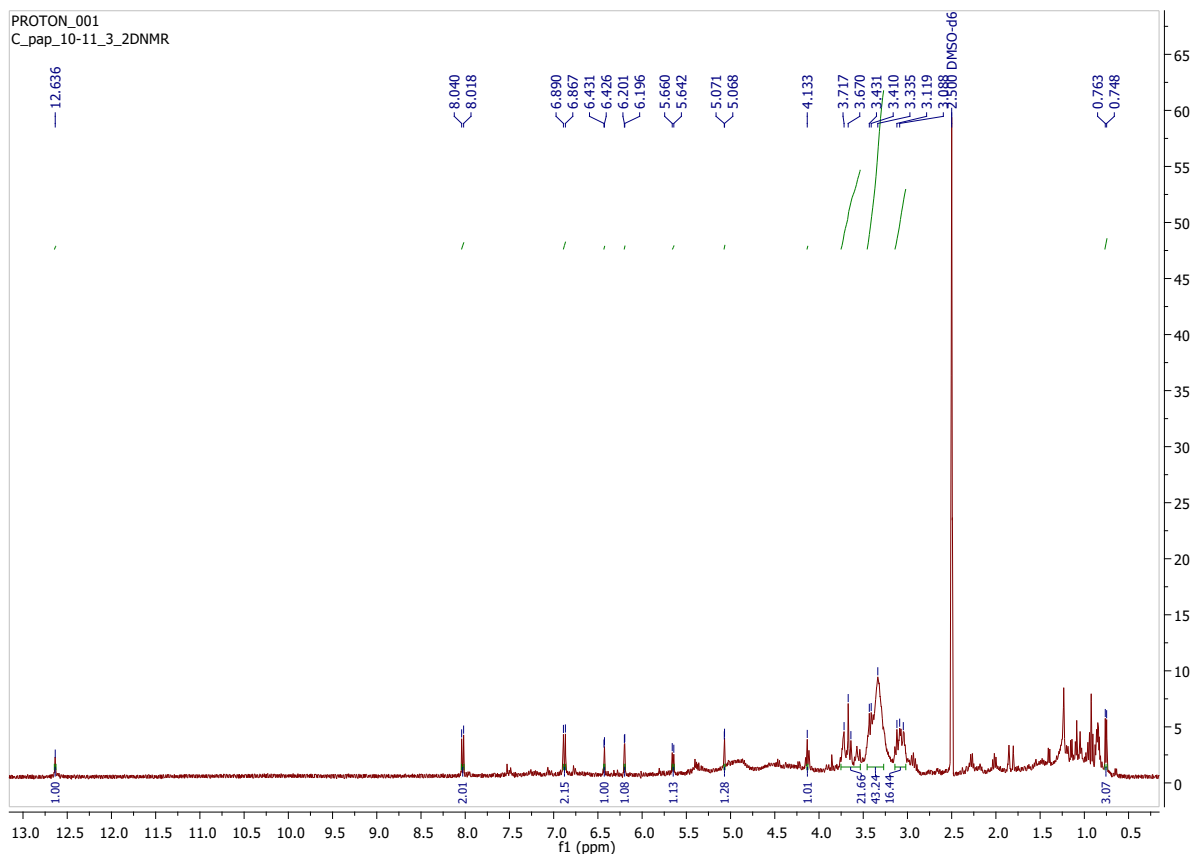
**Fig. S21** HSQC spectrum of compound **5**.



**Fig. S22** HMBC spectrum of compound **5**.

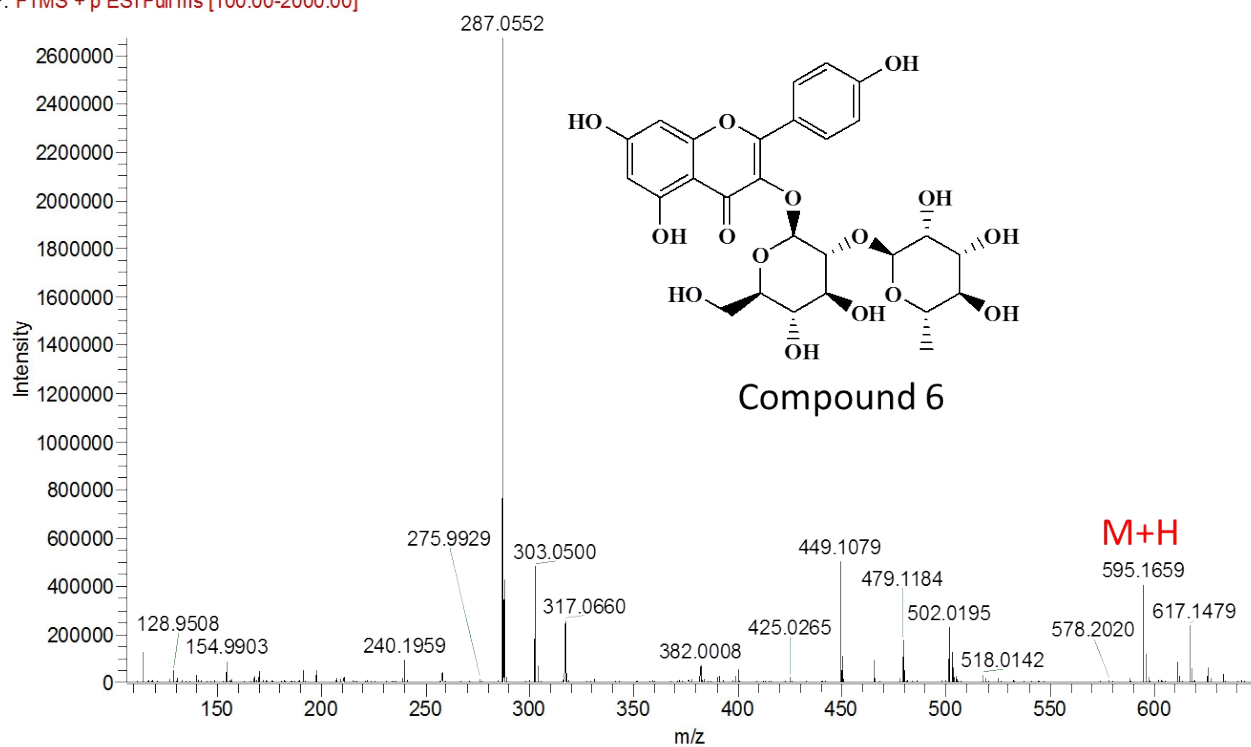


**Fig. S23** Positive HR-ESI-MS spectrum of compound **5**.



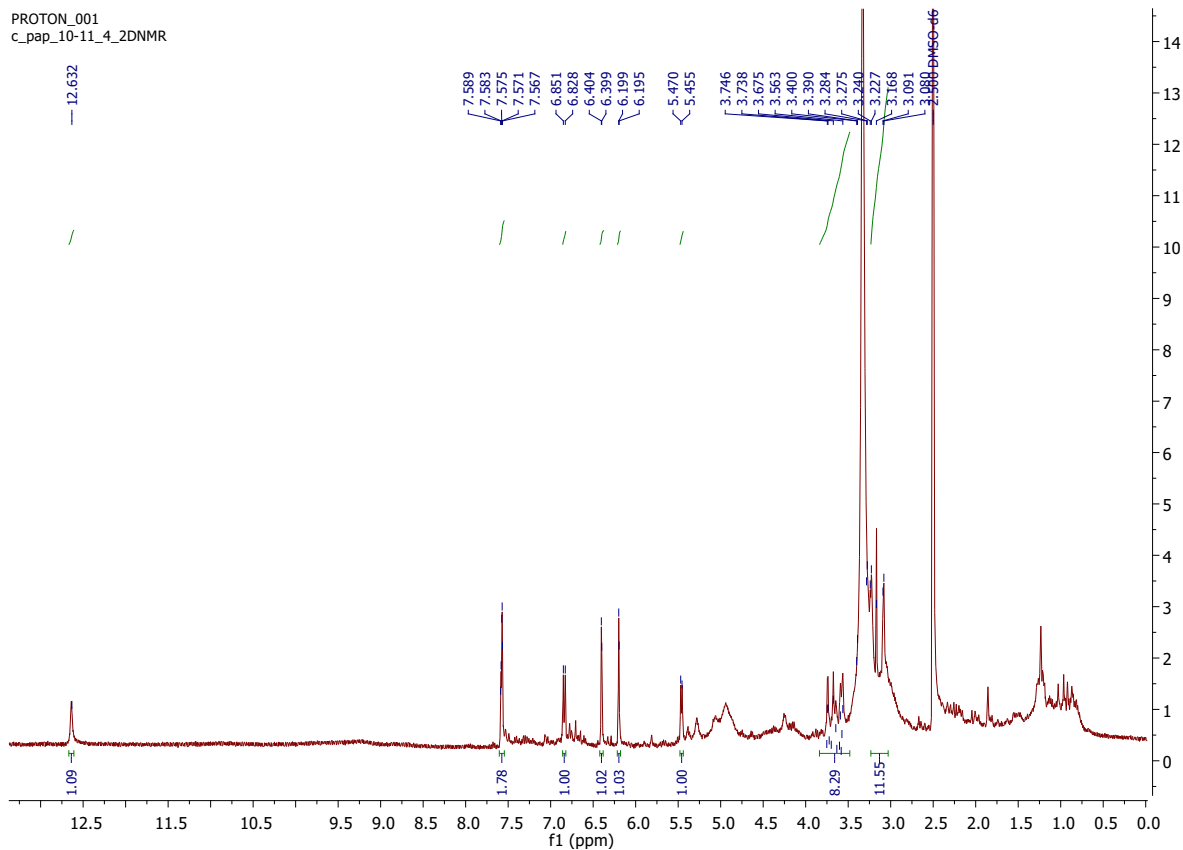
**Fig. S24**  $^1\text{H-NMR}$  spectrum of compound **6** (400 MHz,  $\text{DMSO-}d_6$ ).

MSA156 #381 RT: 6.18 AV: 1 NL: 2.67E6  
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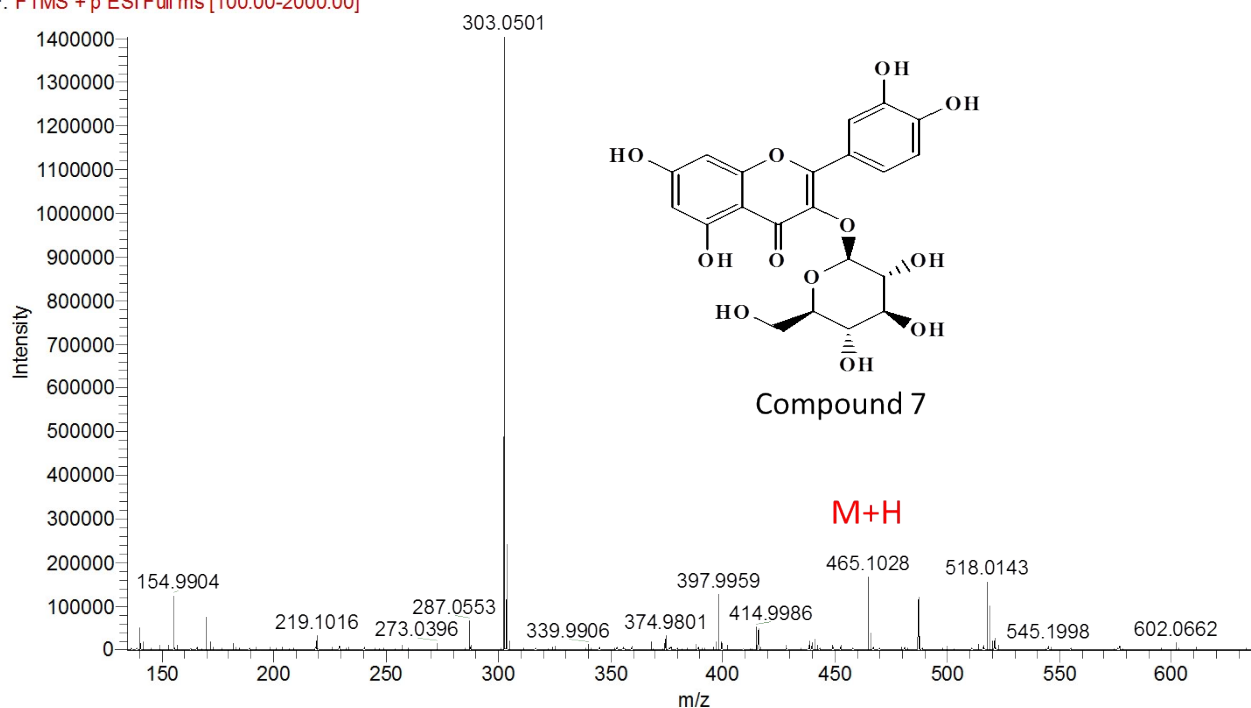
**Fig. S25** Positive HR-ESI-MS spectrum of compound **6**.



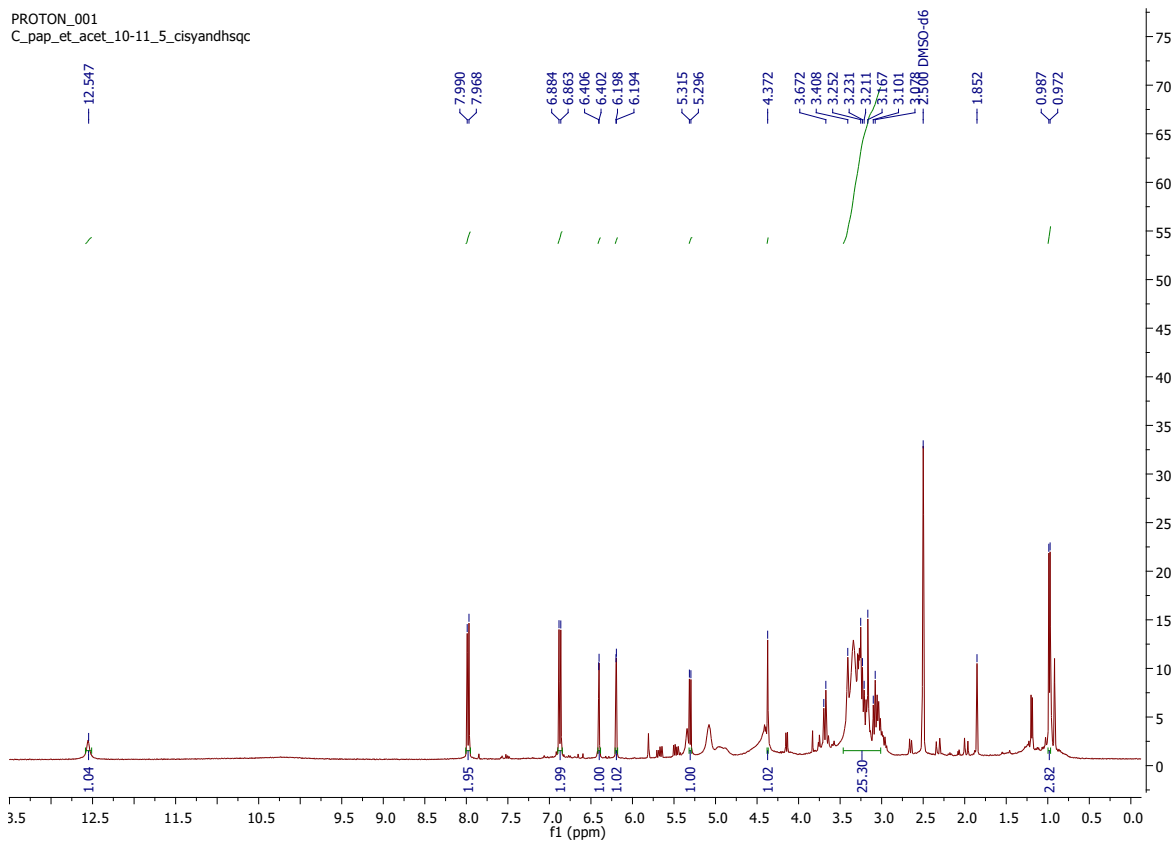


**Fig. S26**  $^1\text{H-NMR}$  spectrum of compound **7** (400 MHz,  $\text{DMSO-d}_6$ ).

MSA157 #375 RT: 5.98 AV: 1 NL: 1.40E6  
F: FTMS + p ESI Full ms [100.00-2000.00]

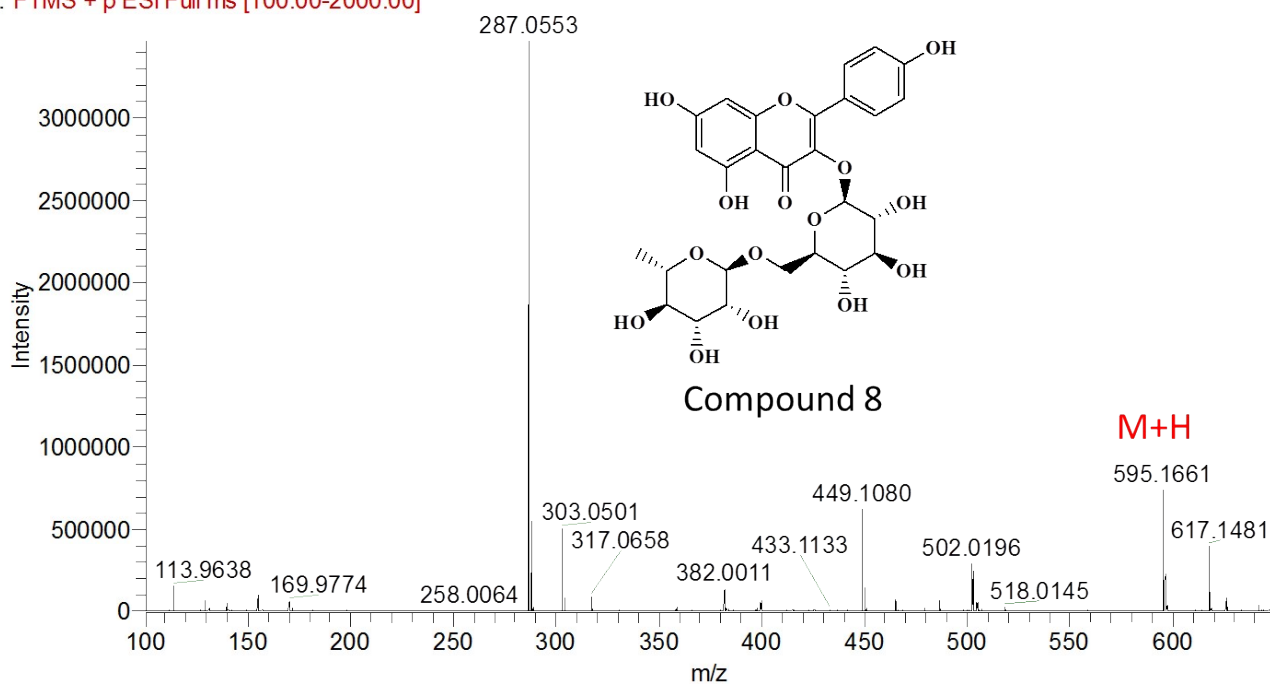


**Fig. S27** Positive HR-ESI-MS spectrum of compound **7**.



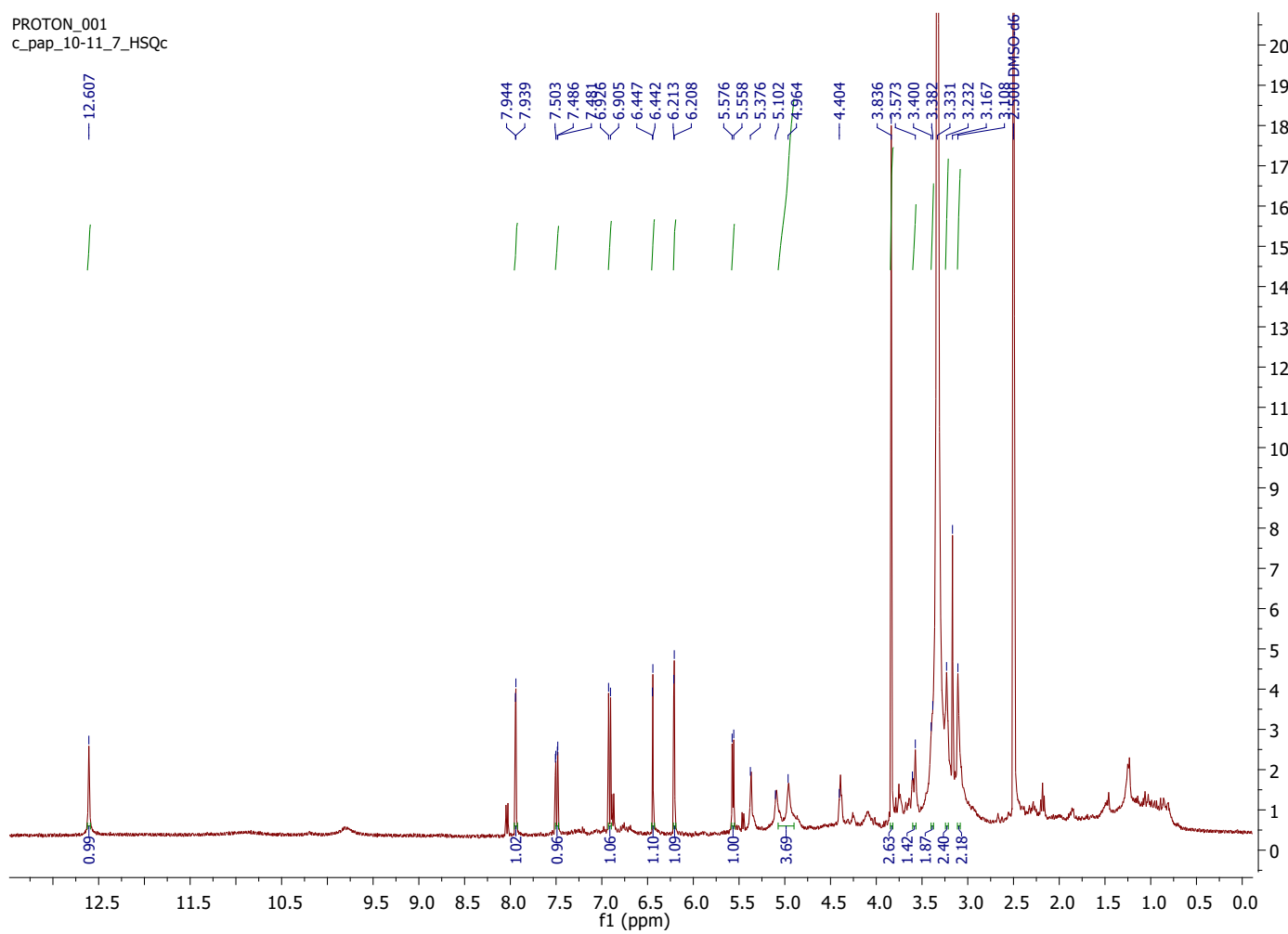
**Fig. S28**  $^1\text{H-NMR}$  spectrum of compound **8** (400 MHz,  $\text{DMSO-d}_6$ ).

MSA158 #384 RT: 6.20 AV: 1 NL: 3.47E6  
F: FTMS + p ESI Full ms [100.00-2000.00]



**Fig. S29** Positive HR-ESI-MS spectrum of compound **8**.

PROTON\_001  
c\_pap\_10-11\_7\_HSQC



**Fig. S30**  $^1\text{H-NMR}$  spectrum of compound **9** (400 MHz,  $\text{DMSO-}d_6$ ).

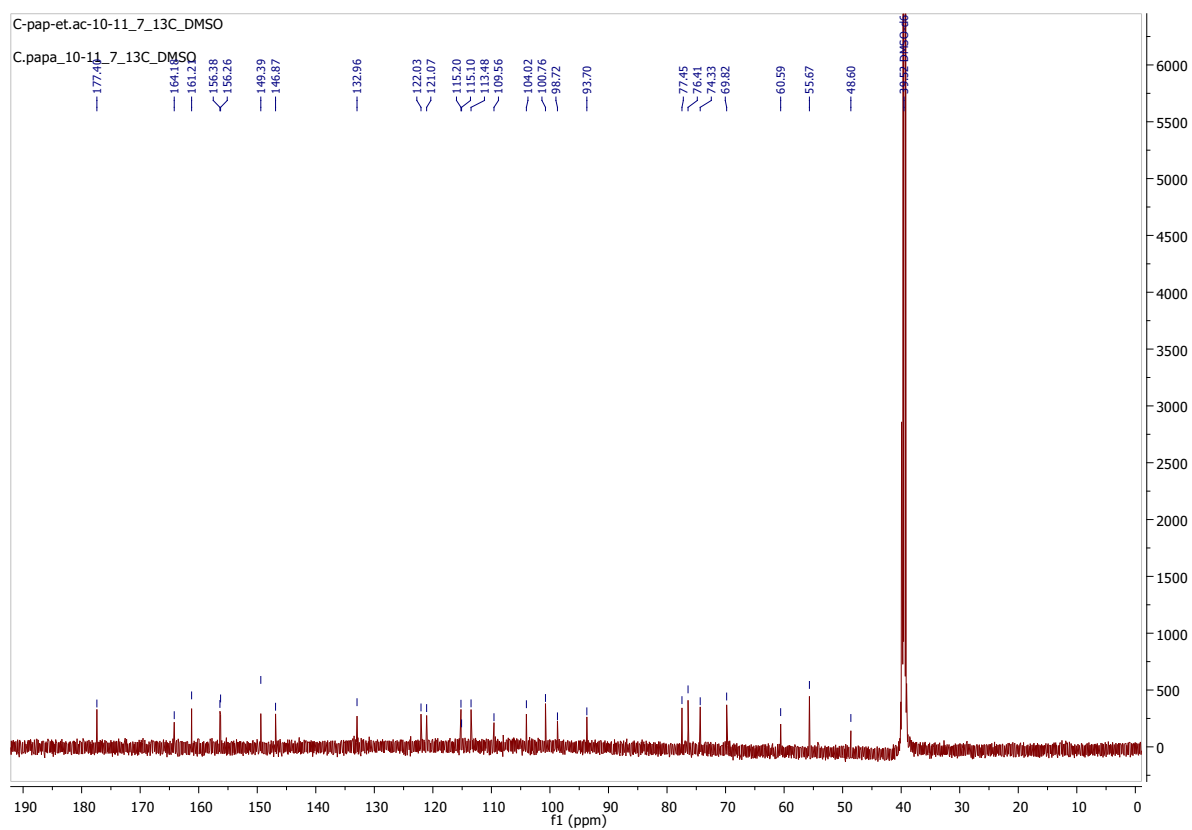


Fig. S31  $^{13}\text{C}$ -NMR spectrum of compound **9** (100 MHz,  $\text{DMSO-}d_6$ ).

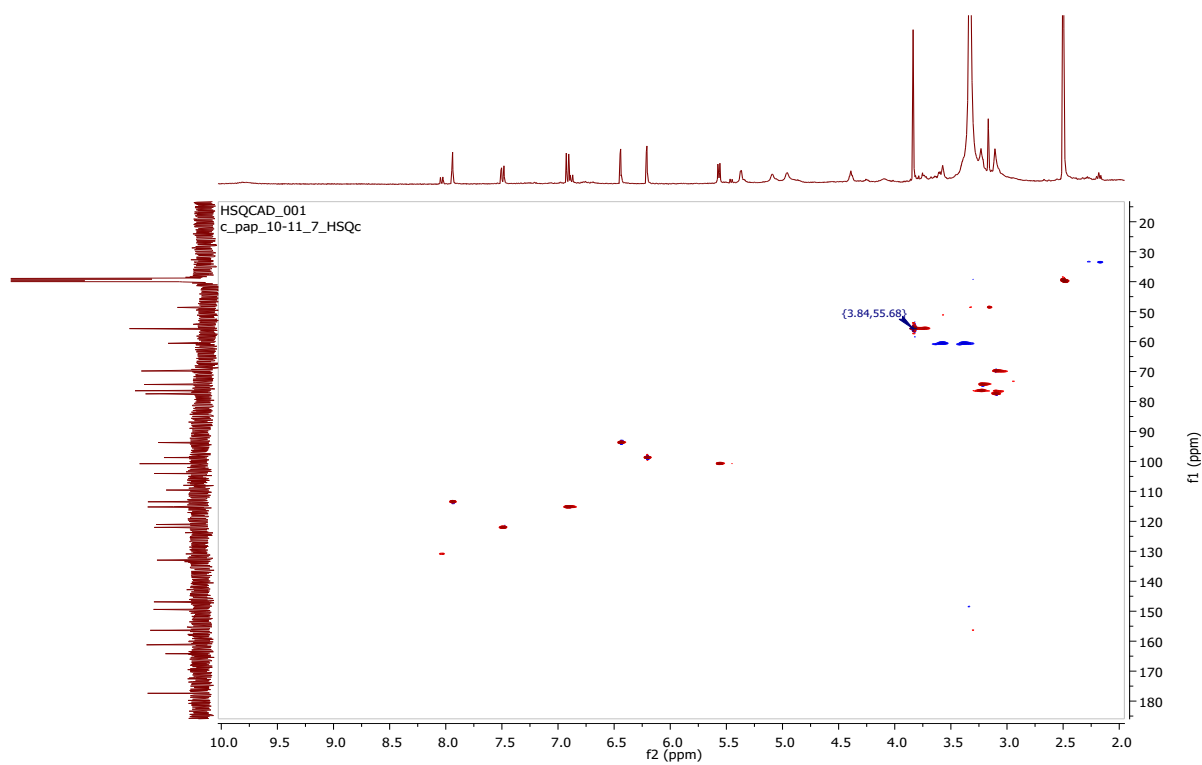
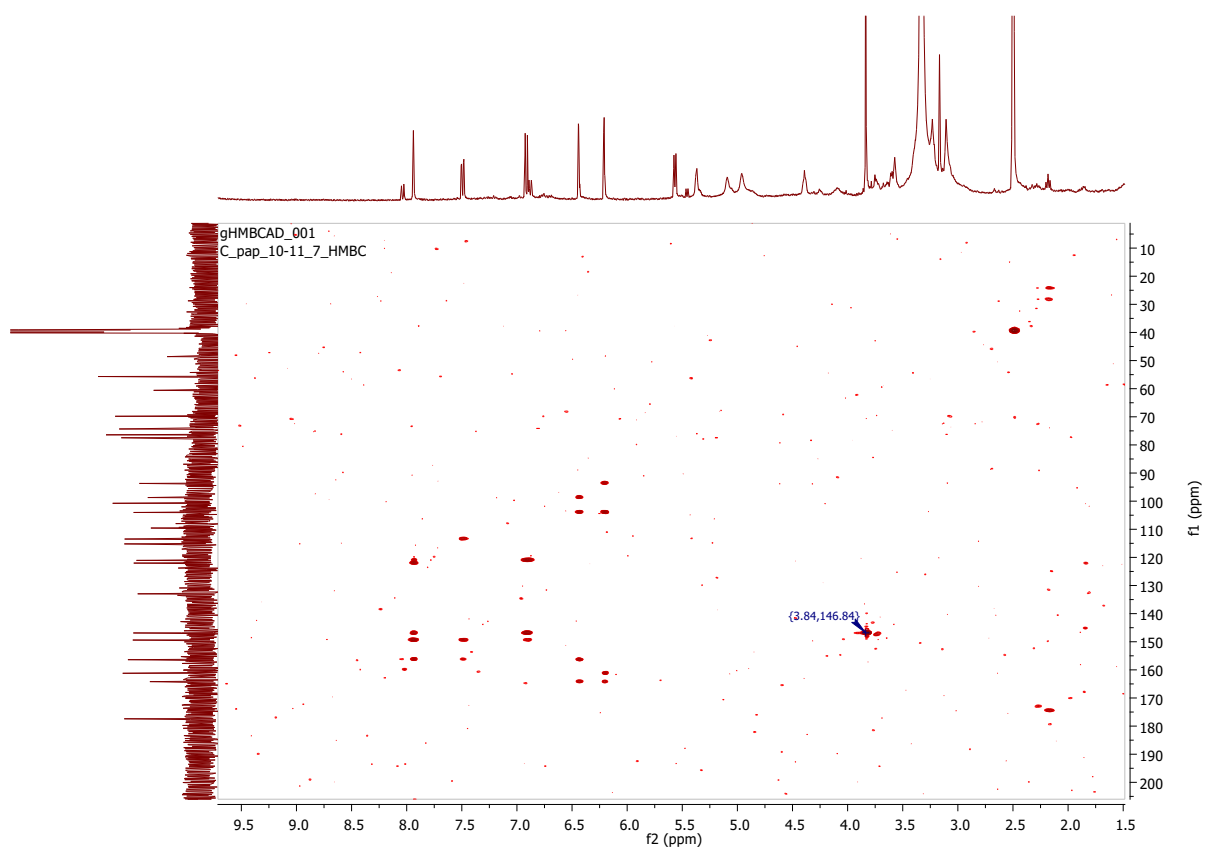
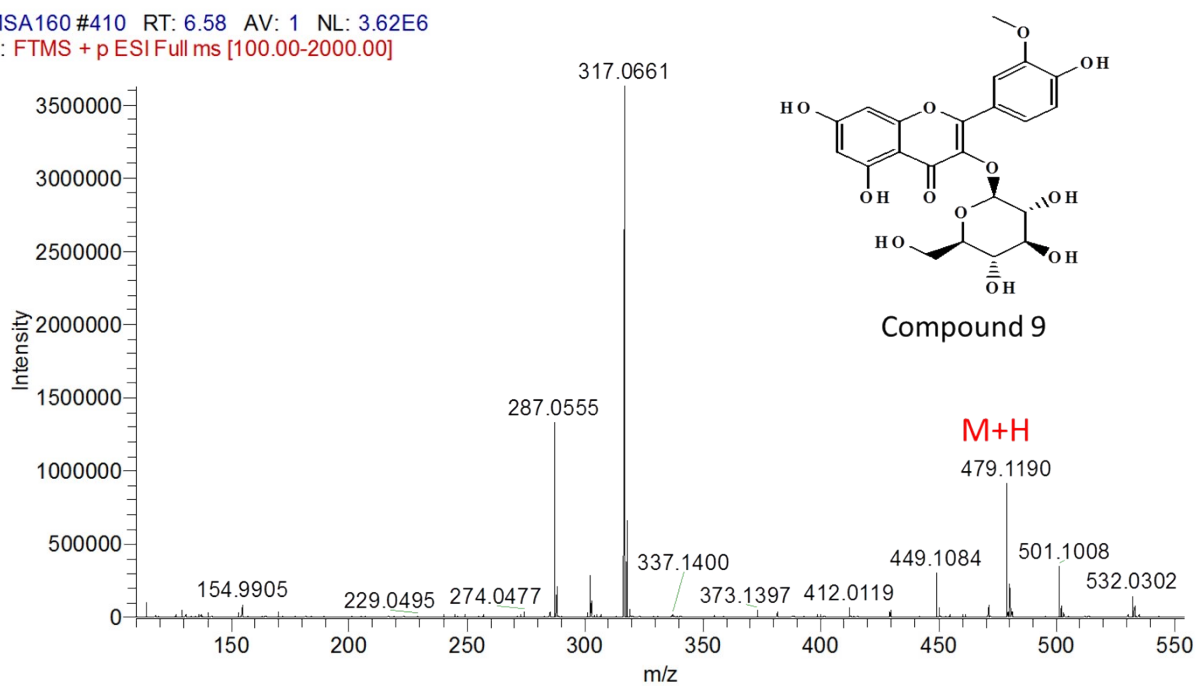


Fig. S32 HSQC spectrum of compound **9**.



**Fig. S33** HMBC spectrum of compound **9**.

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F: FTMS + p ESI Full ms [100.00-2000.00]



**Fig. S34** Positive HR-ESI-MS spectrum of compound **9**.