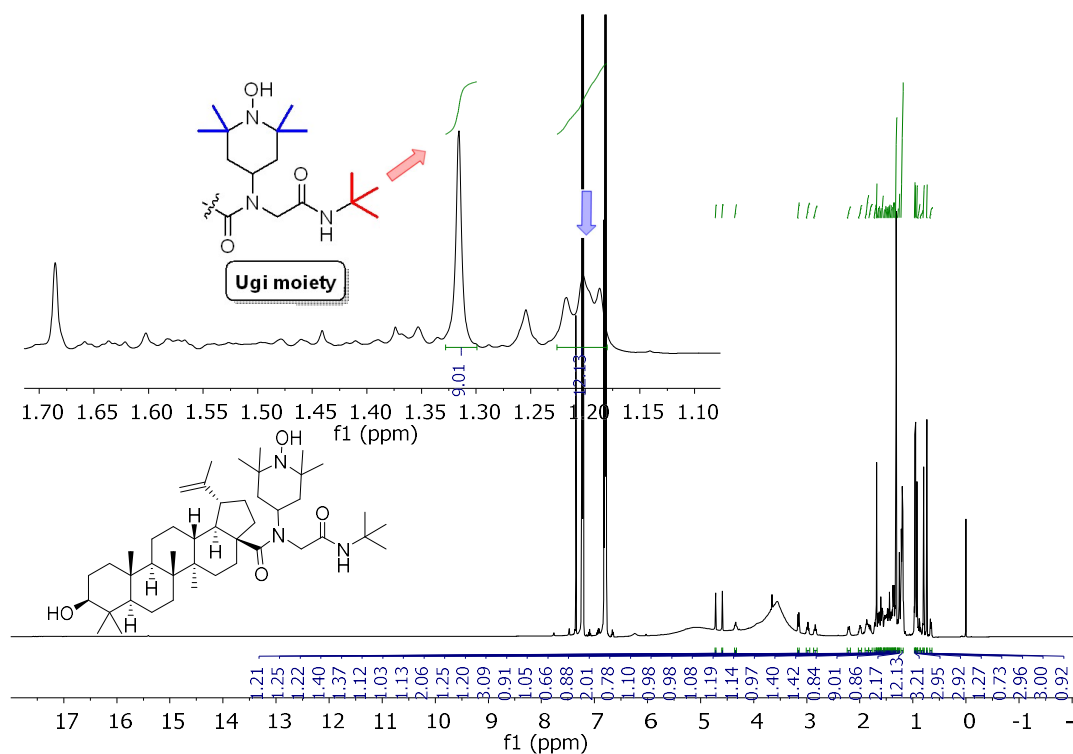


## Supplementary Materials for

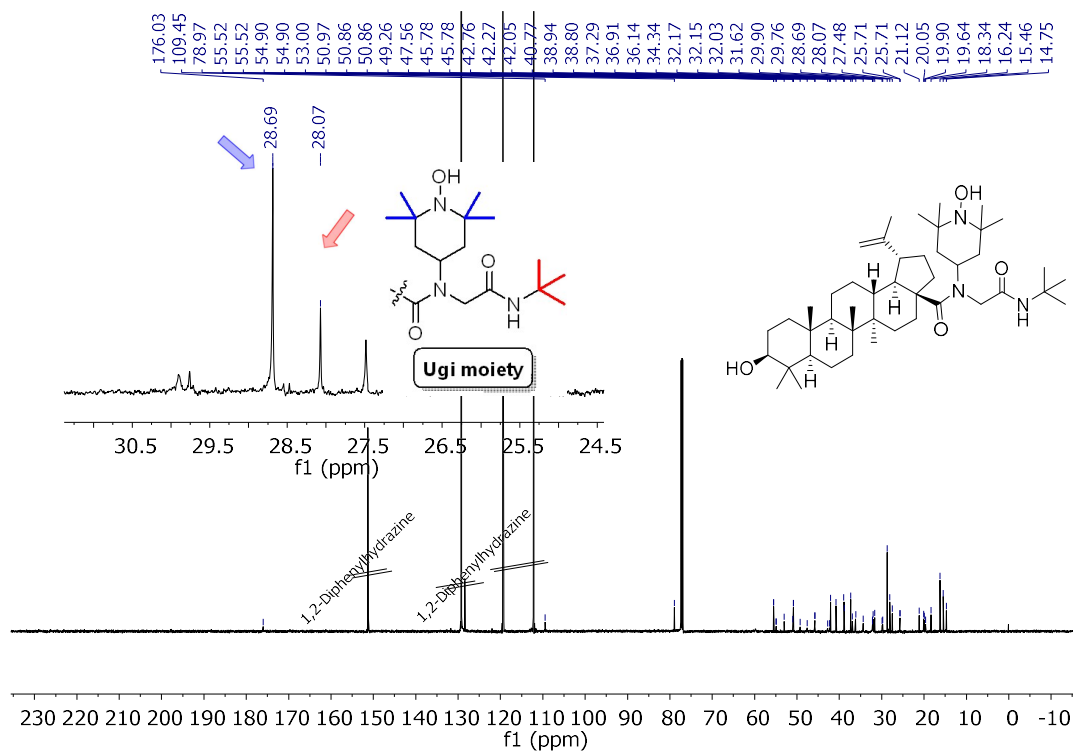
### Access to new cytotoxic triterpene and steroidal acid-TEMPO conjugates by Ugi multicomponent-reactions

**Table S1.** Numerical values of EPR characteristics ( $A_{\text{iso}}$  and  $\tau_c$  (ns)) for the nitroxide conjugated compounds, obtained by simulations.

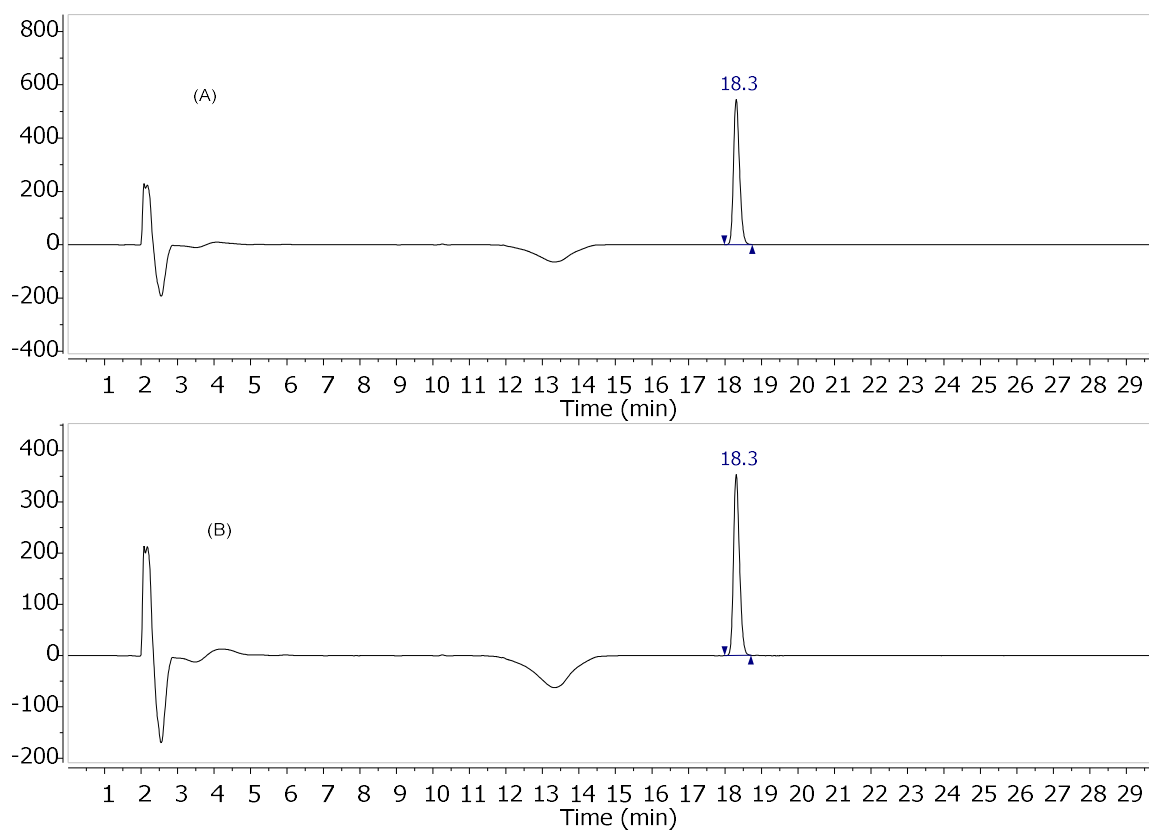
Compound	$\tau_c(\text{ns})$	$A_{\text{iso}}(\text{MHz})$
6	1,10	45,33
7	1,39	45,33
8	2,00	47,33
9	2,52	47,33
10	2,00	47,67
11	2,28	47,67
12	2,44	45,33
14	1,30	45,33
16	1,93	45,33
17	2,07	45,33
18	2,68	45,33



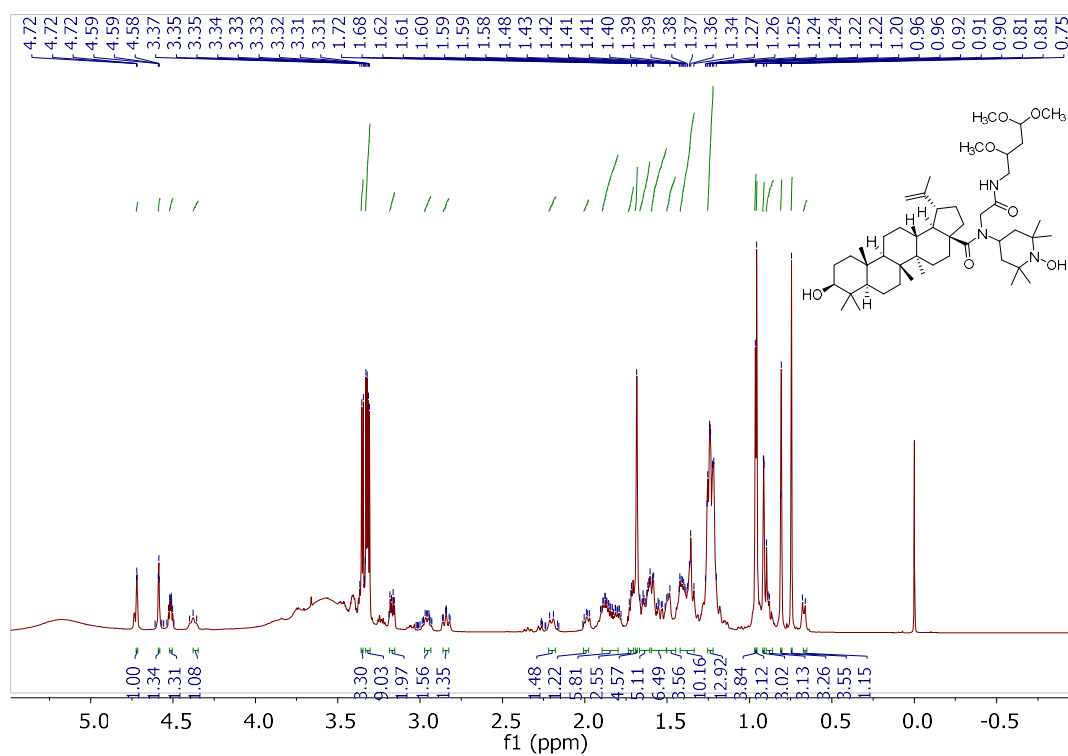
**Figure S2.**  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of compound **6**.



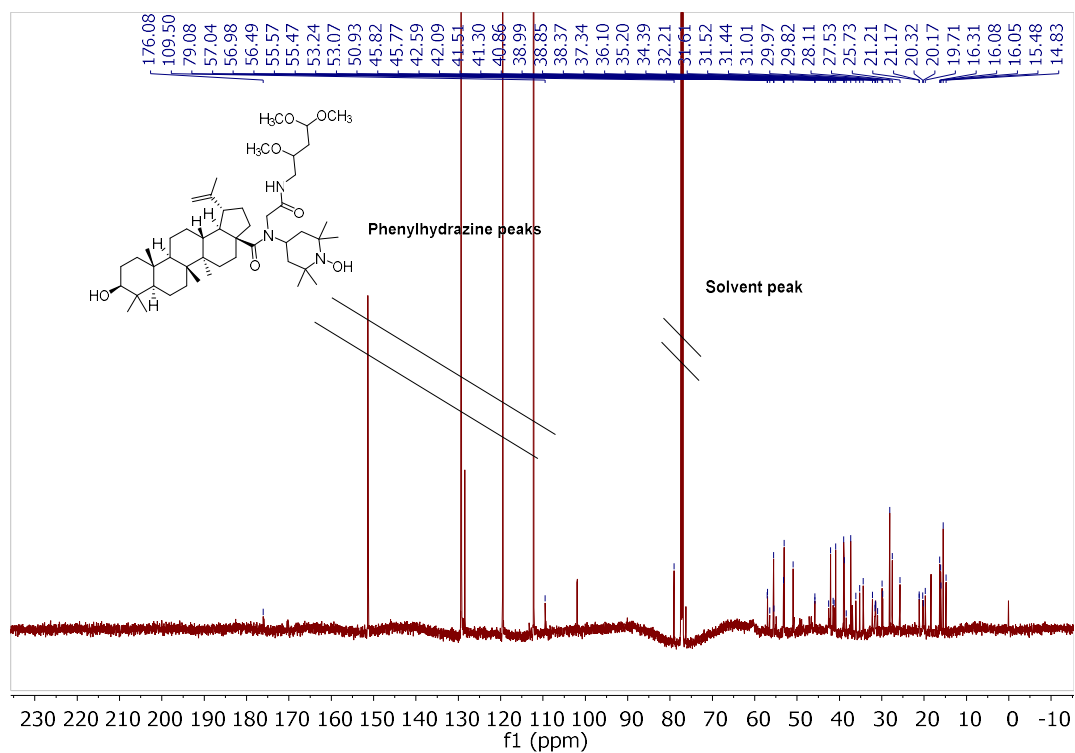
**Figure S3.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{CDCl}_3$ ) spectrum of compound **6**.



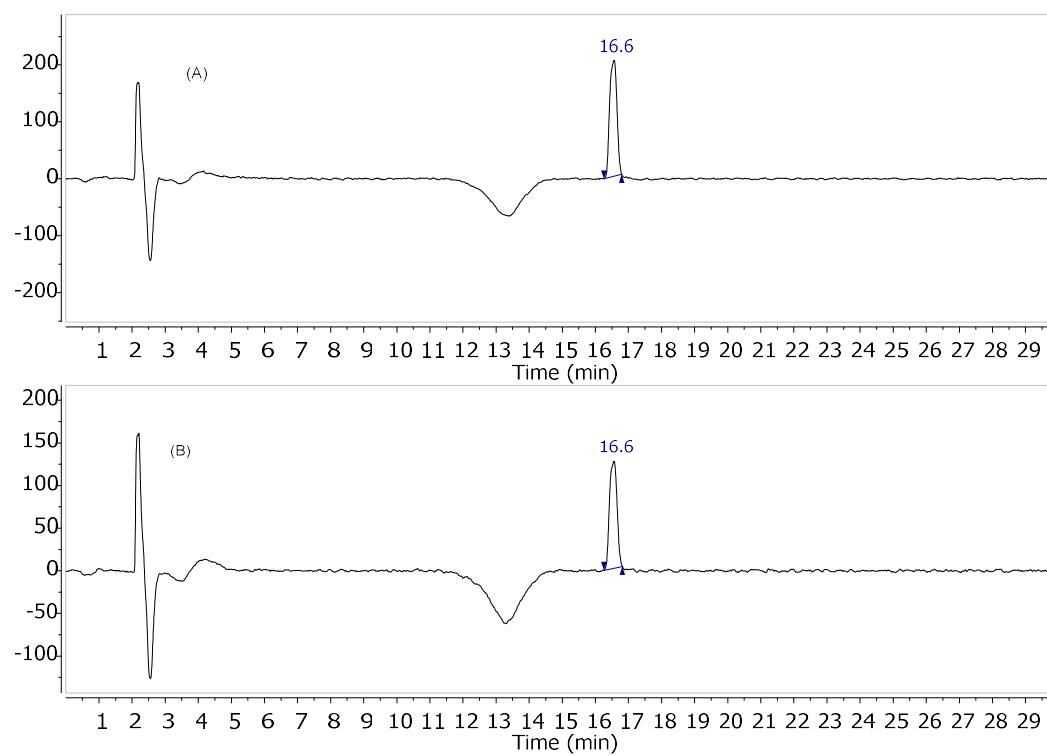
**Figure S4.** RP-HPLC chromatogram of compound **6** a) 210 nm, b) 215 nm.



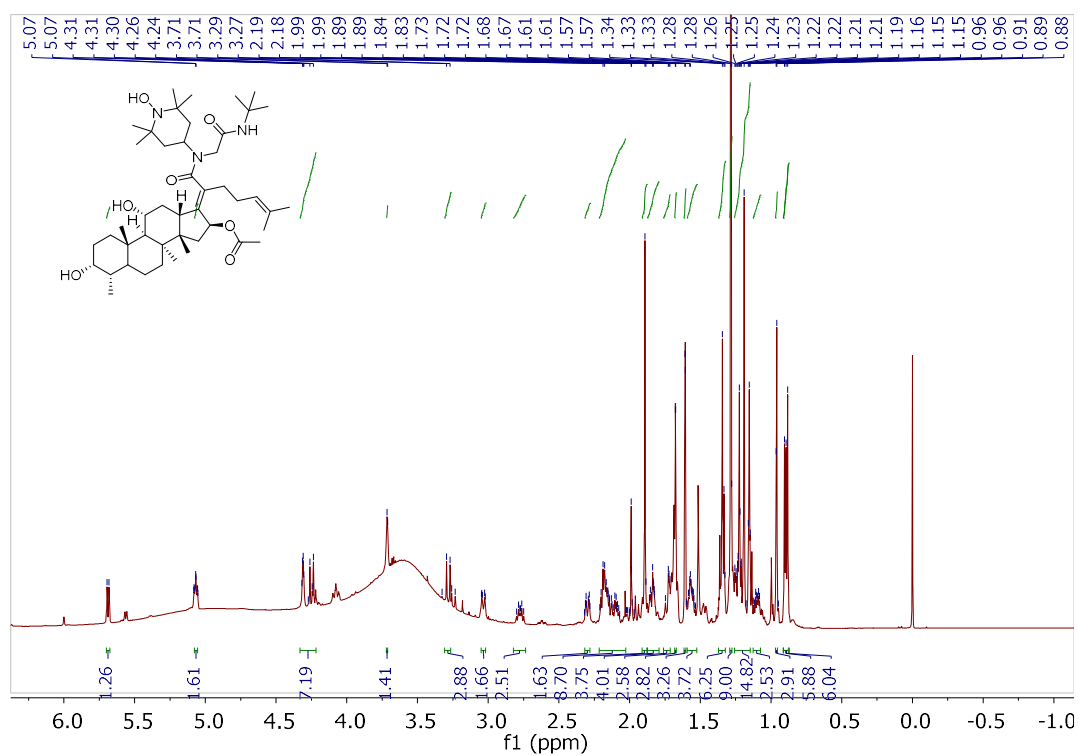
**Figure S5.**  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of compound 7.



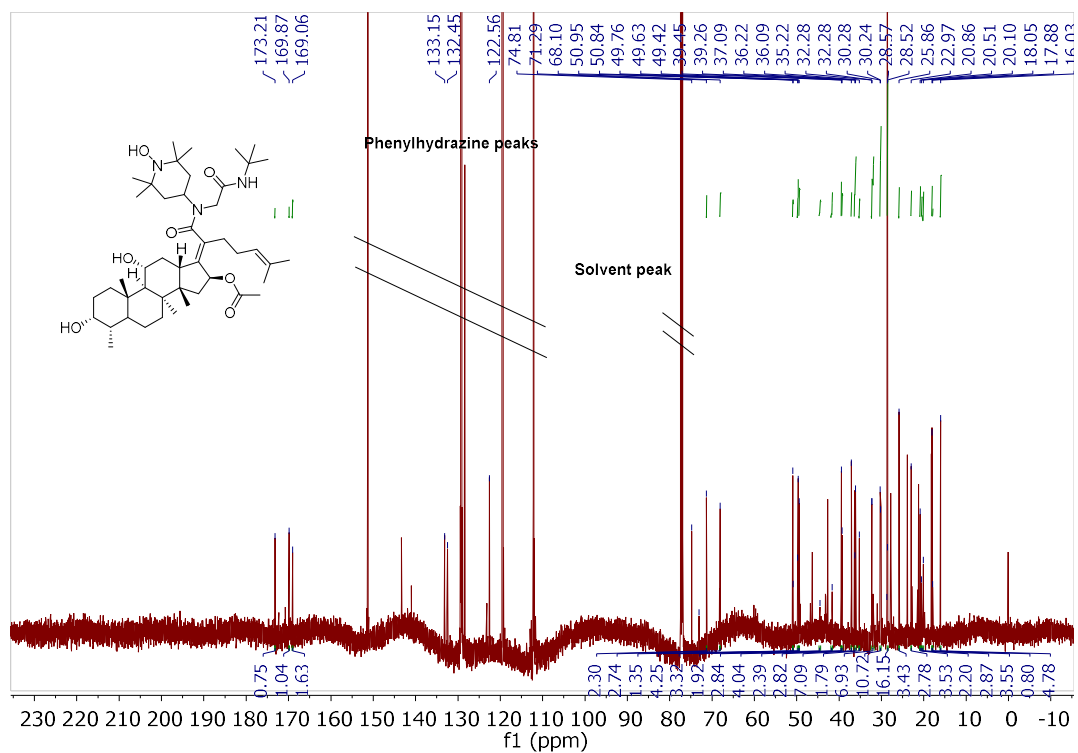
**Figure S6.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{CDCl}_3$ ) spectrum of compound 7.



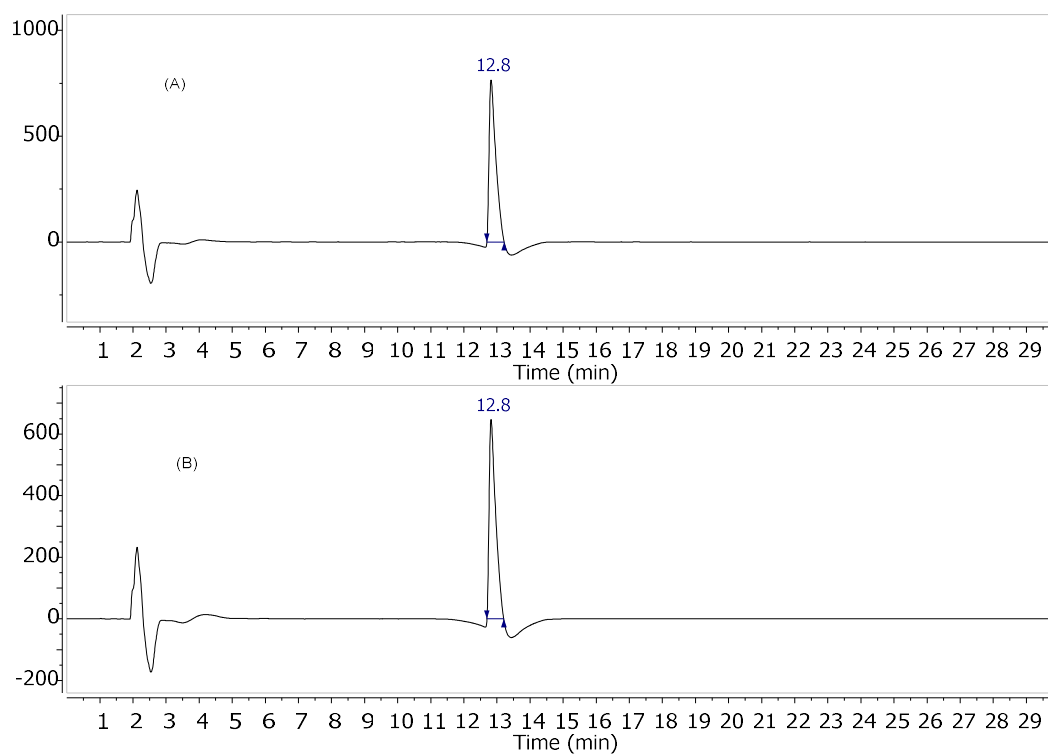
**Figure S7.** RP-HPLC chromatogram of compound 7 a) 210 nm, b) 215 nm.



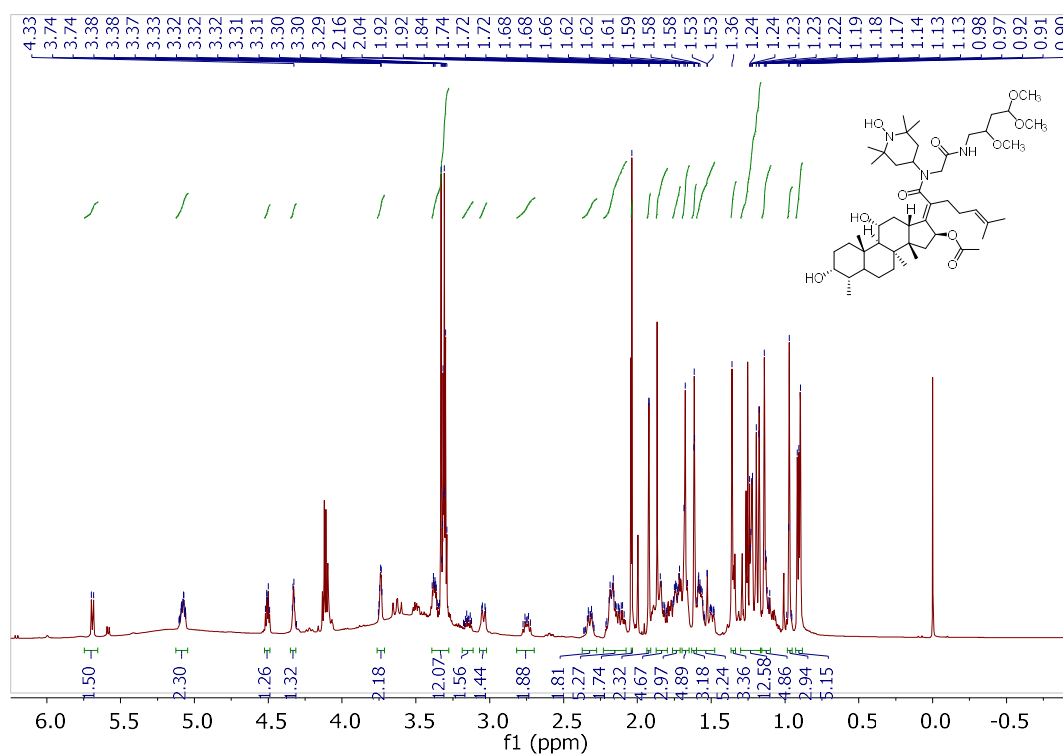
**Figure S8.**  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of compound **8**.



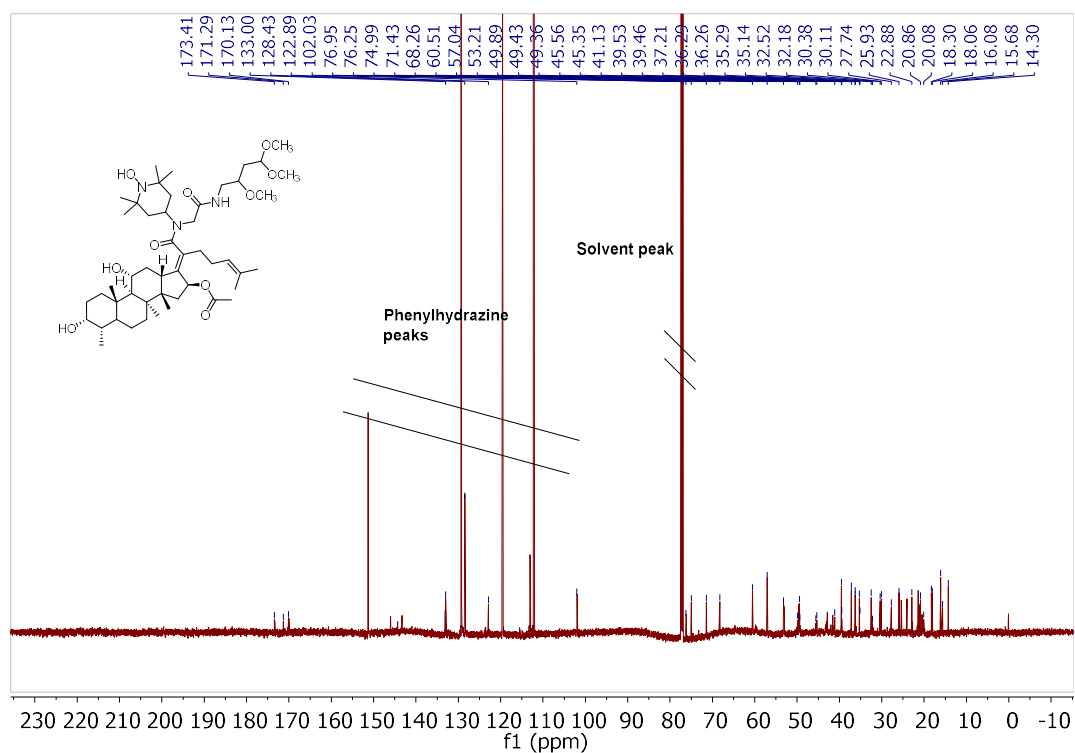
**Figure S9.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{CDCl}_3$ ) spectrum of compound **8**.



**Figure S10.** RP-HPLC chromatogram of compound **8** a) 210 nm, b) 215 nm.

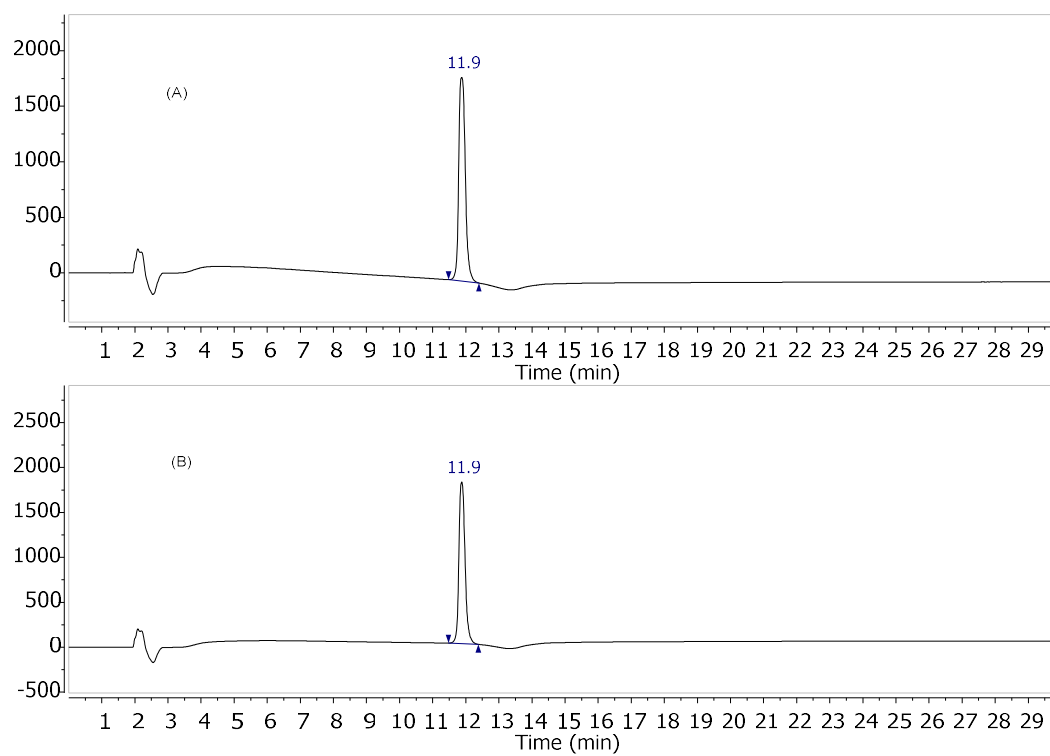


**Figure S11.**  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of compound **9**.

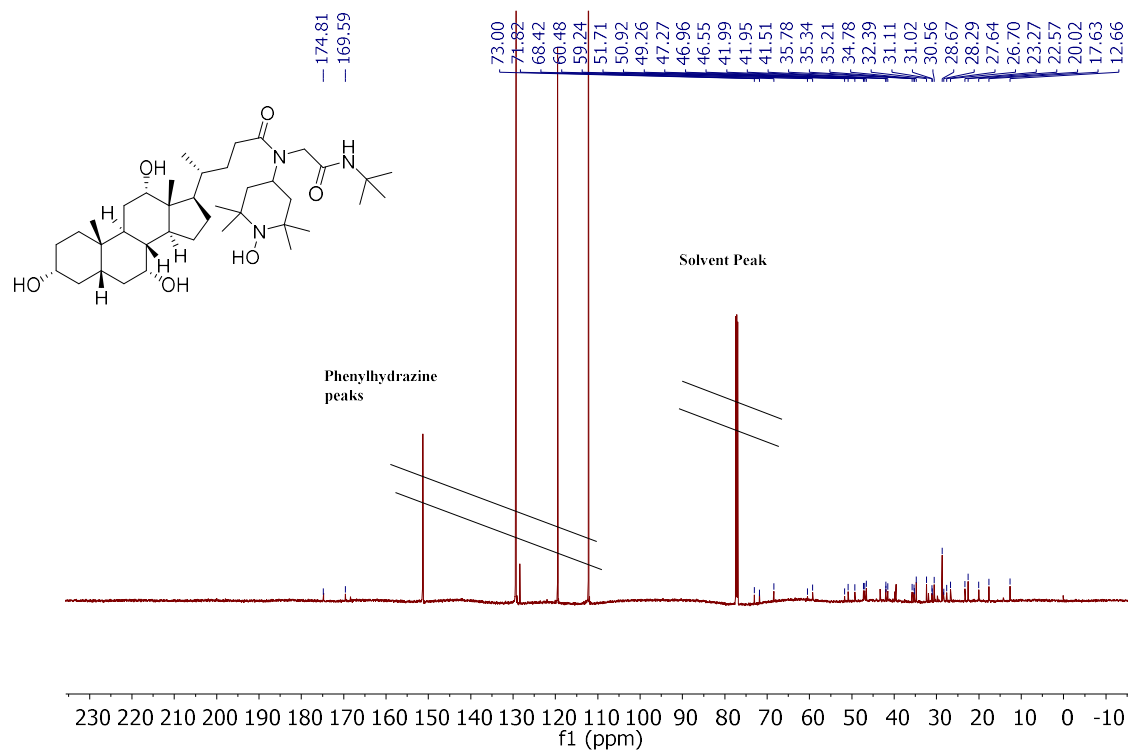
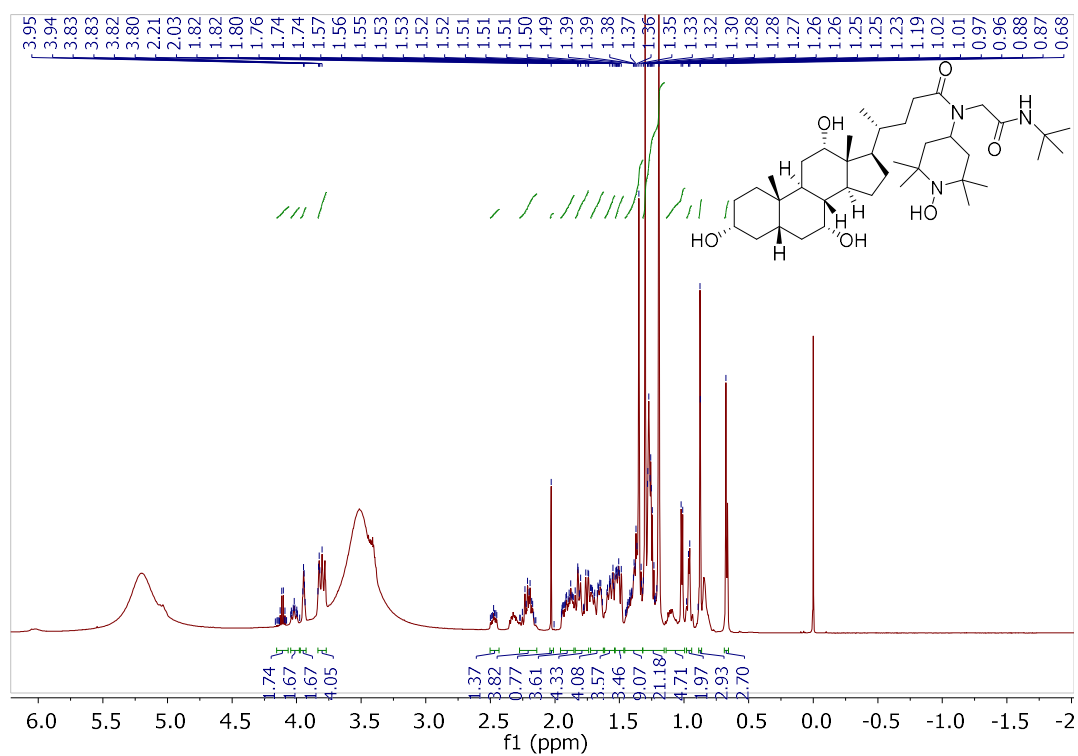


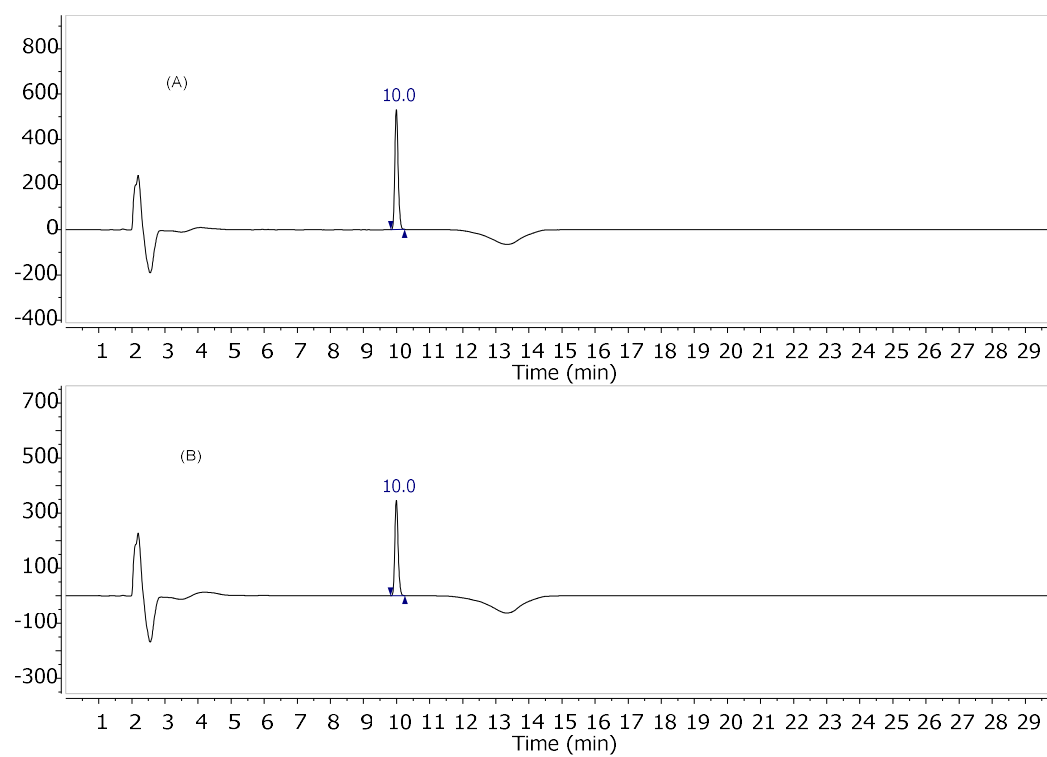
**Figure S12.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{CDCl}_3$ ) spectrum of compound **9**.



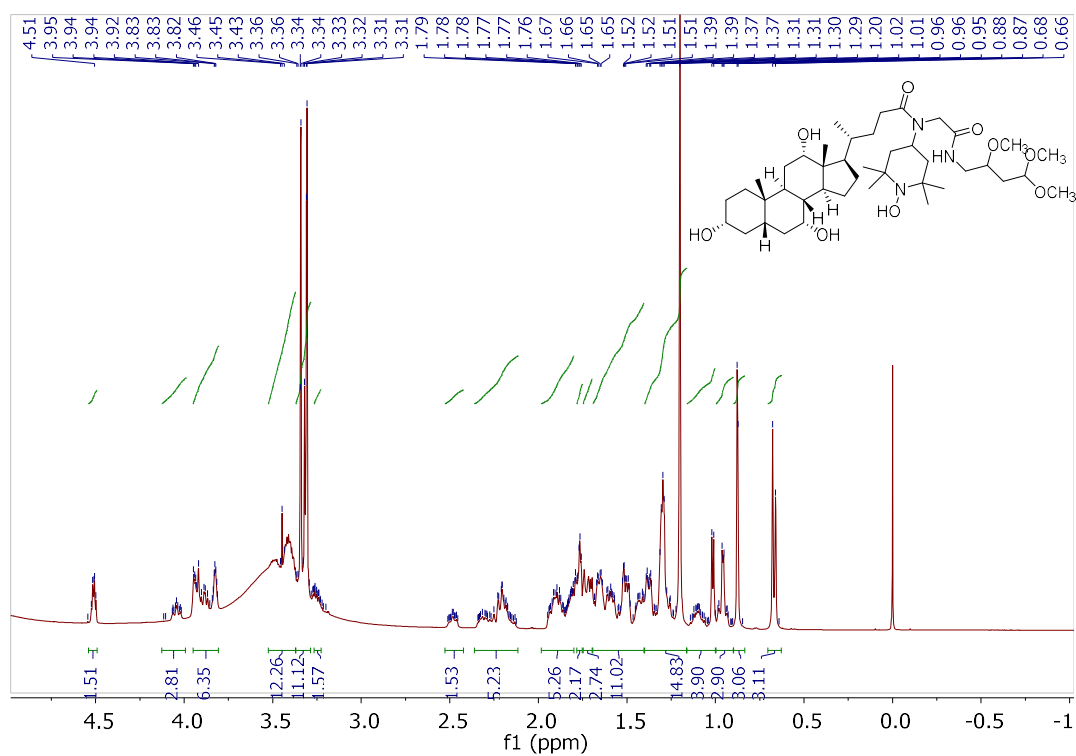


**Figure S13.** RP-HPLC chromatogram of compound **9** a) 210 nm, b) 215 nm.

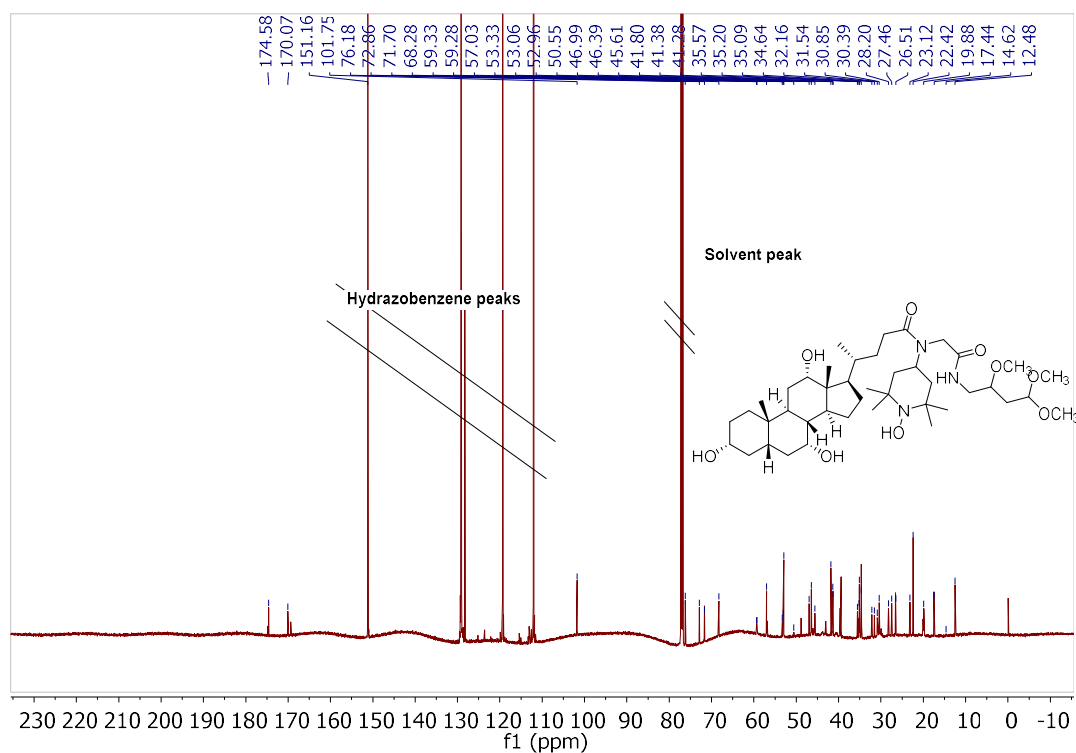




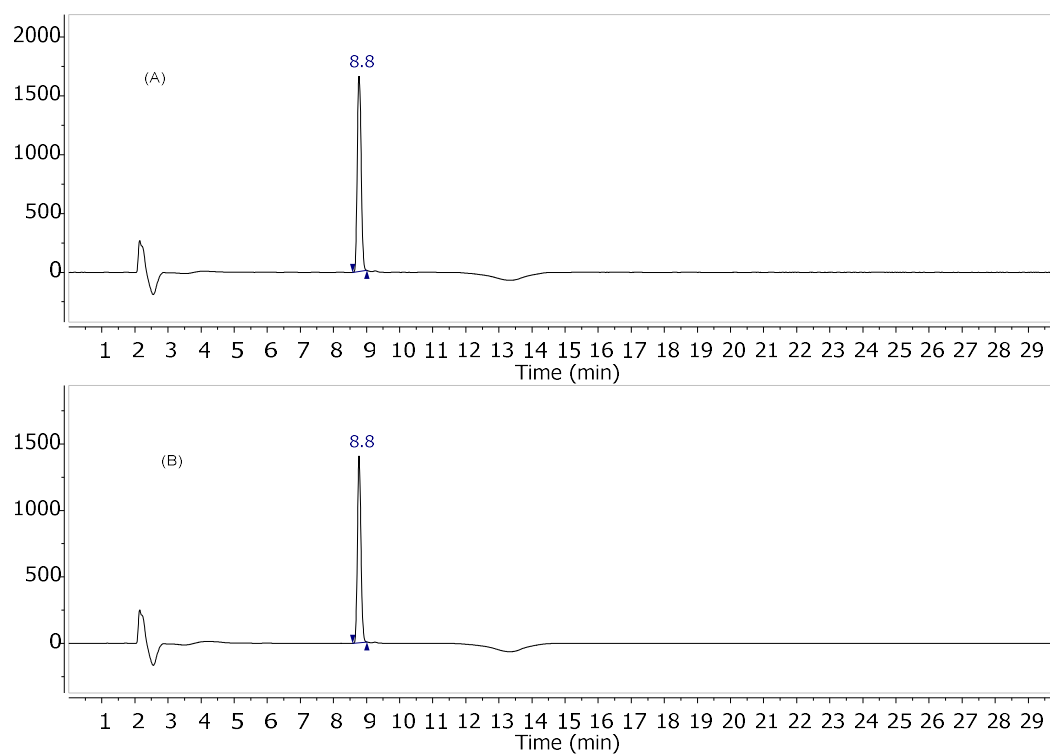
**Figure S16.** RP-HPLC chromatogram of compound **10** a) 210 nm, b) 215 nm.



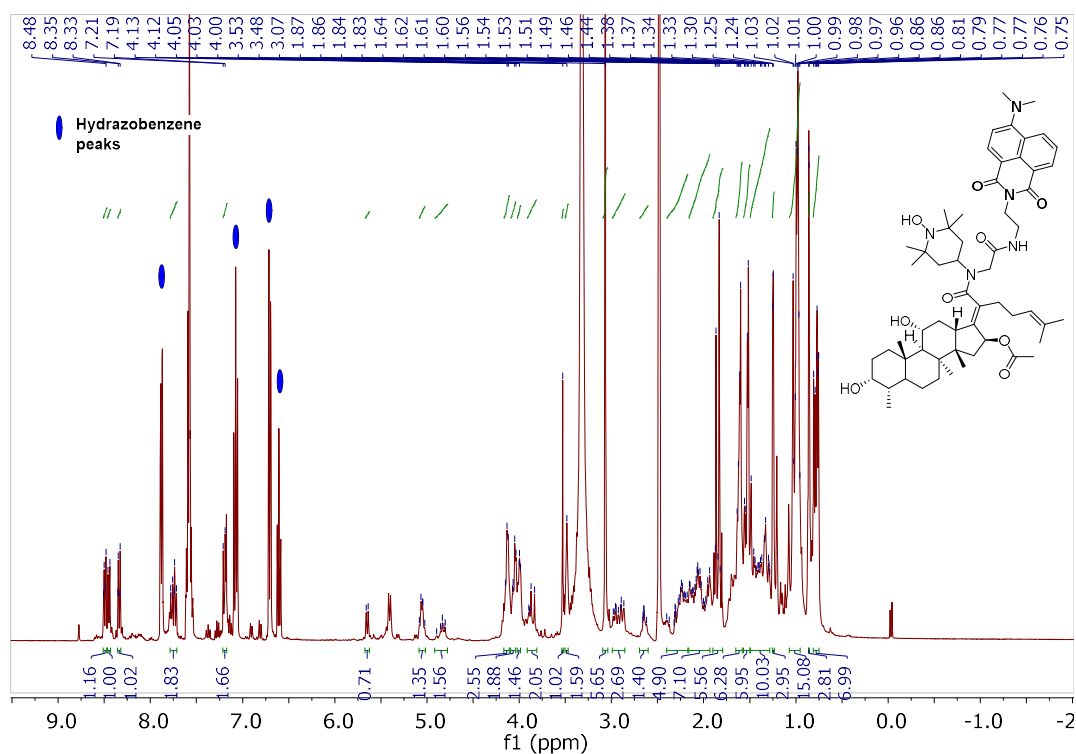
**Figure S17.** <sup>13</sup>C NMR (151 MHz, CDCl<sub>3</sub>) spectrum of compound **11**.



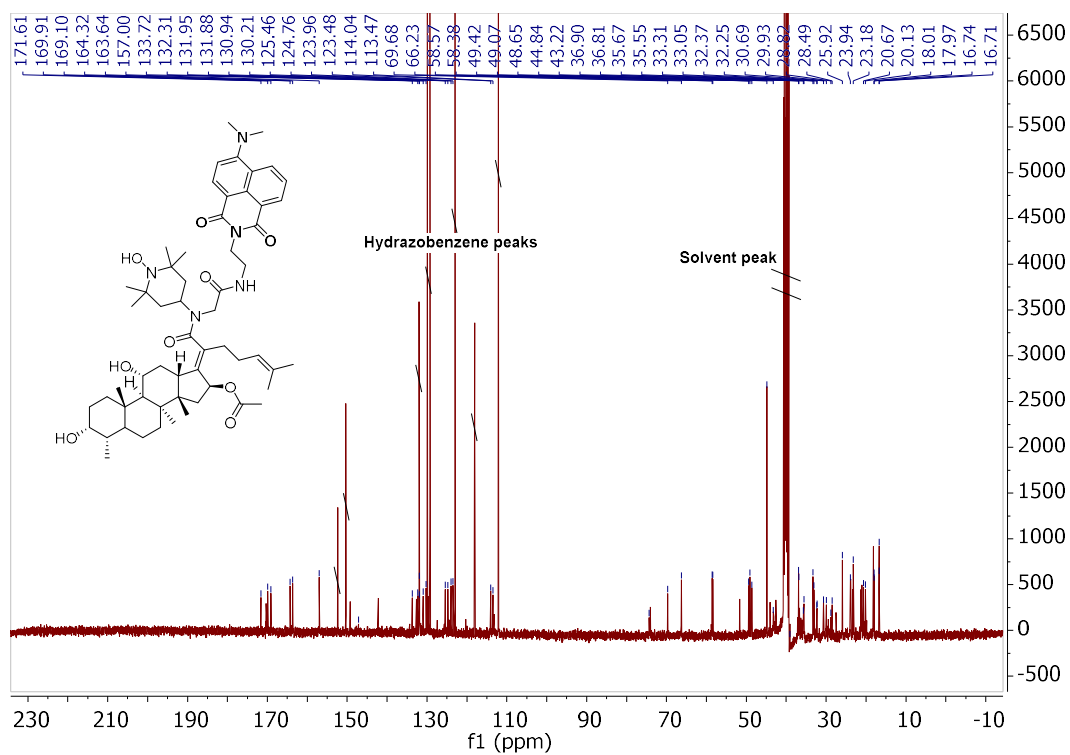
**Figure S18.** <sup>13</sup>C NMR (151 MHz, CDCl<sub>3</sub>) spectrum of compound **11**.



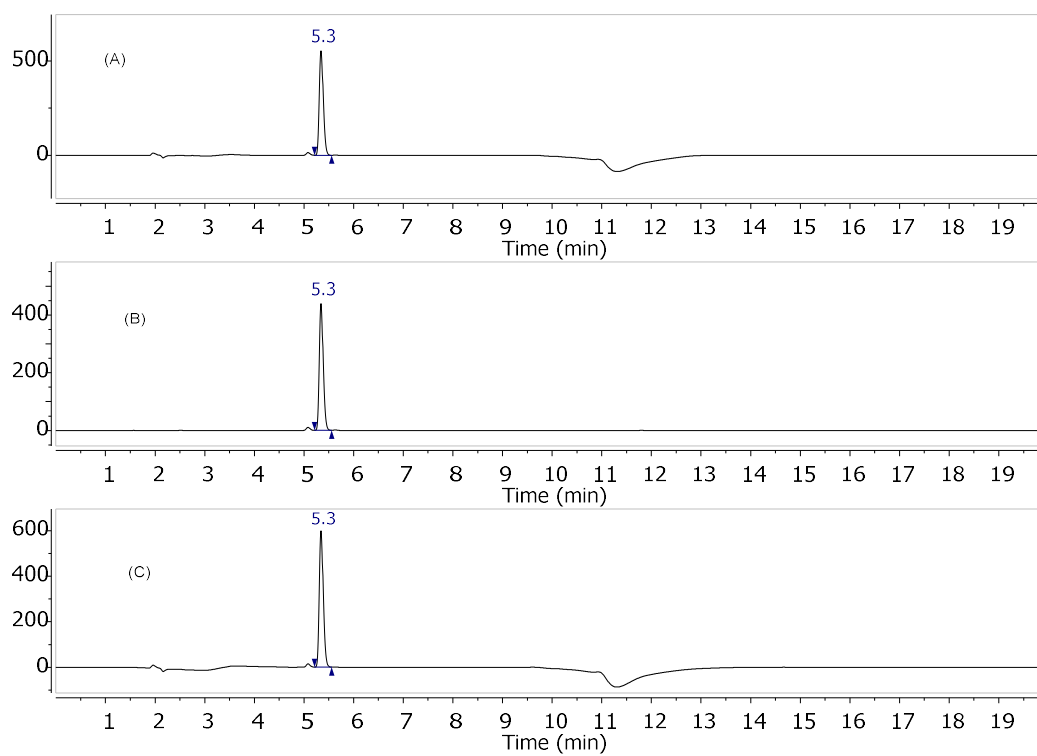
**Figure S19.** RP-HPLC chromatogram of compound **11** a) 210 nm, b) 215 nm.



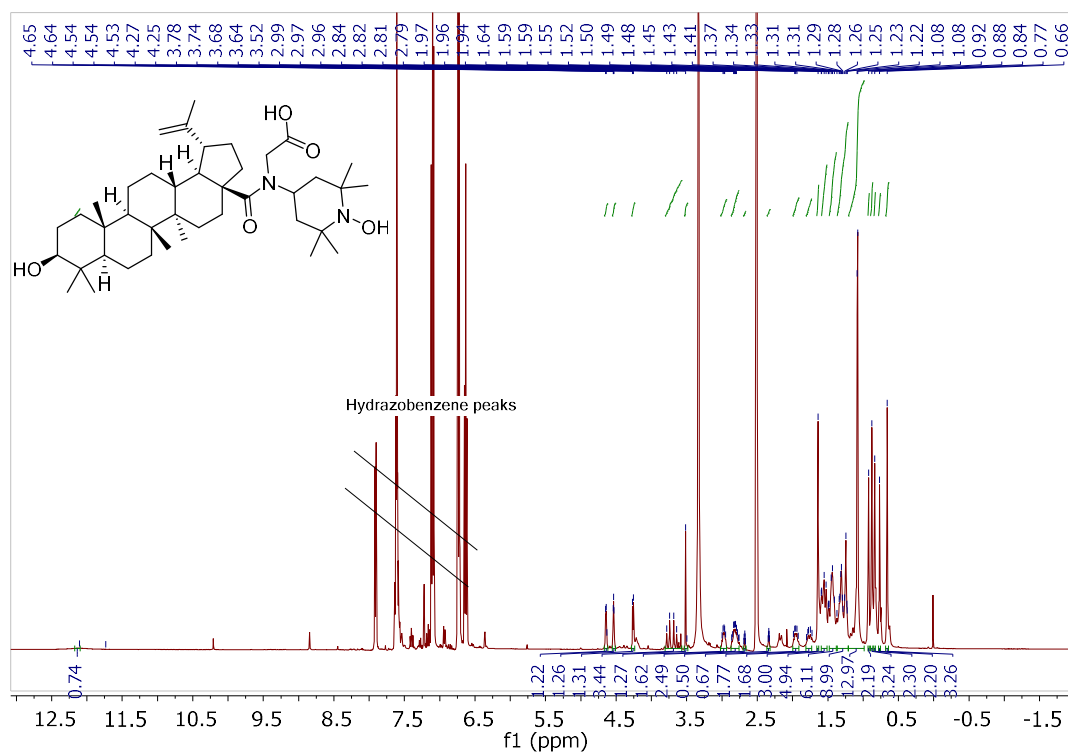
**Figure S20.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of compound **12**.



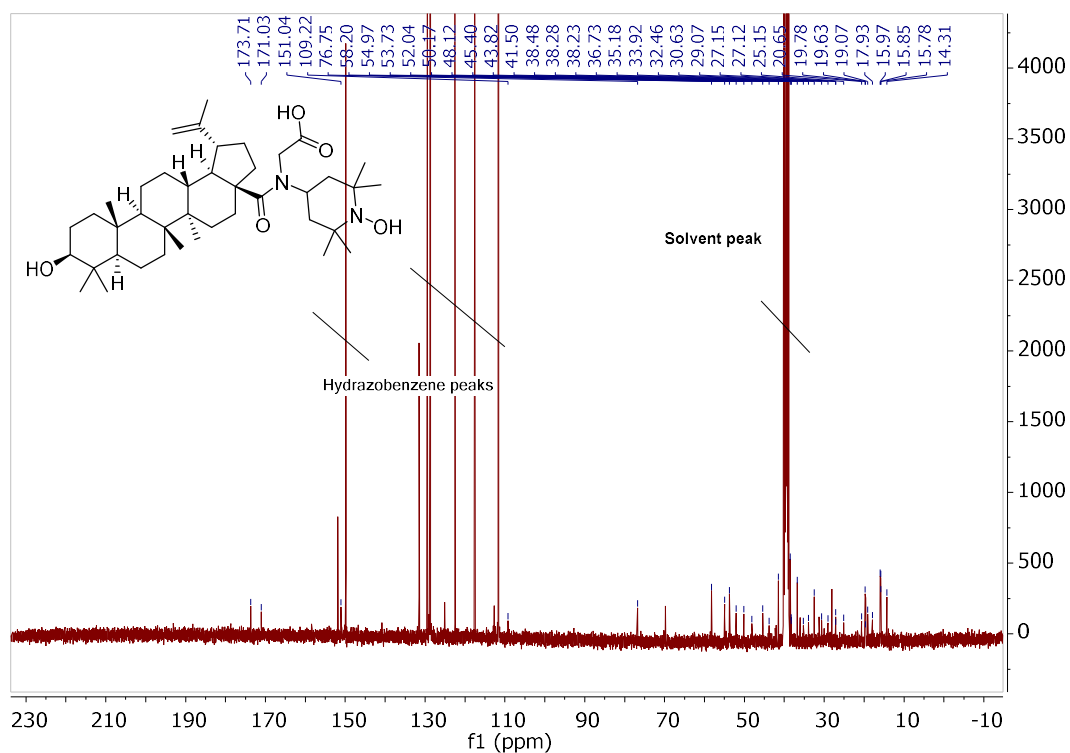
**Figure S21.**  $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO}-d_6$ ) spectrum of compound **12**.



**Figure S22.** RP-HPLC chromatogram of compound **12** a) 210 nm, b) 215 nm, c) 254 nm.

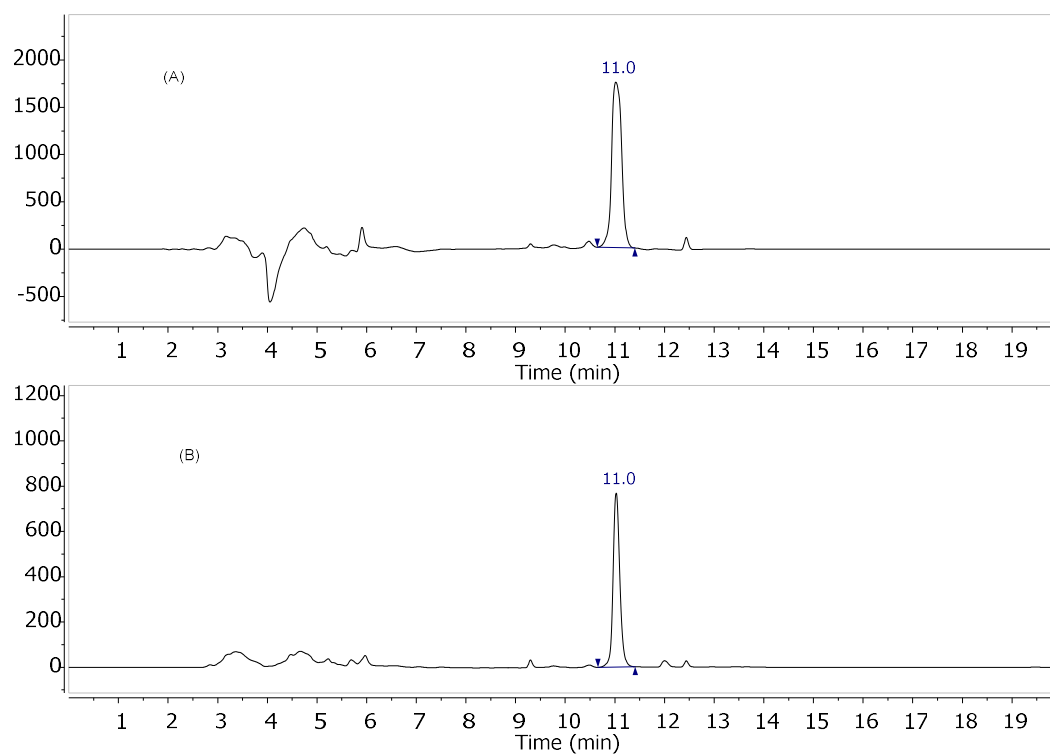


**Figure S23.** <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound **14**.

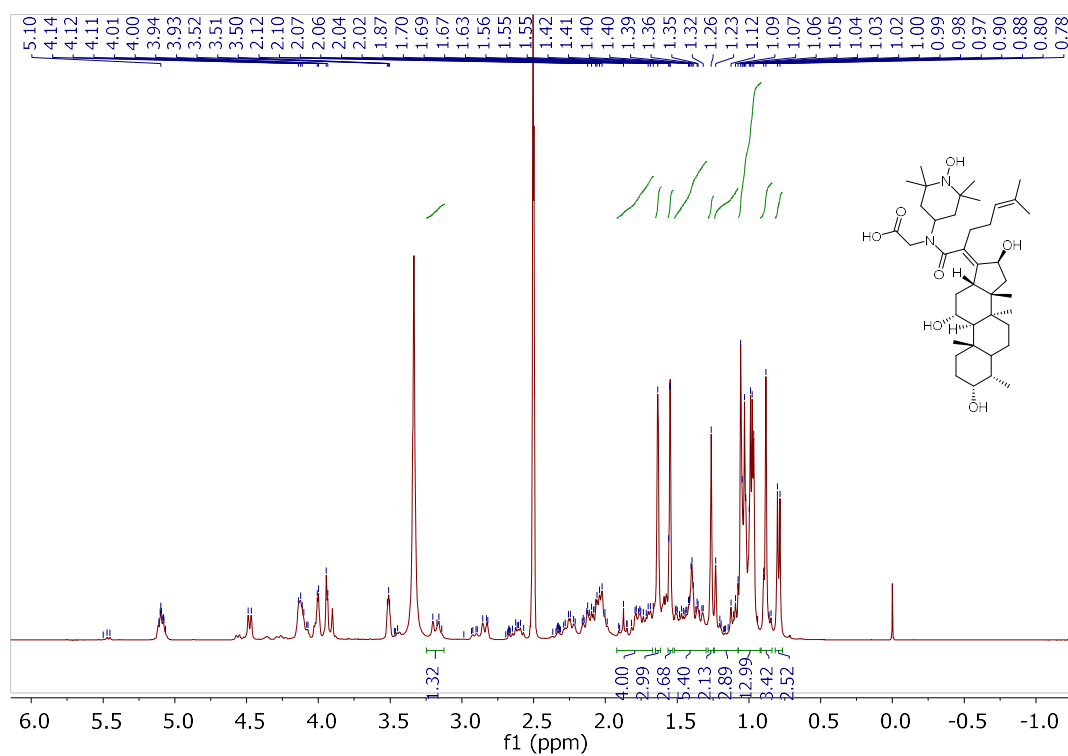


**Figure S24.** <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound **14**.

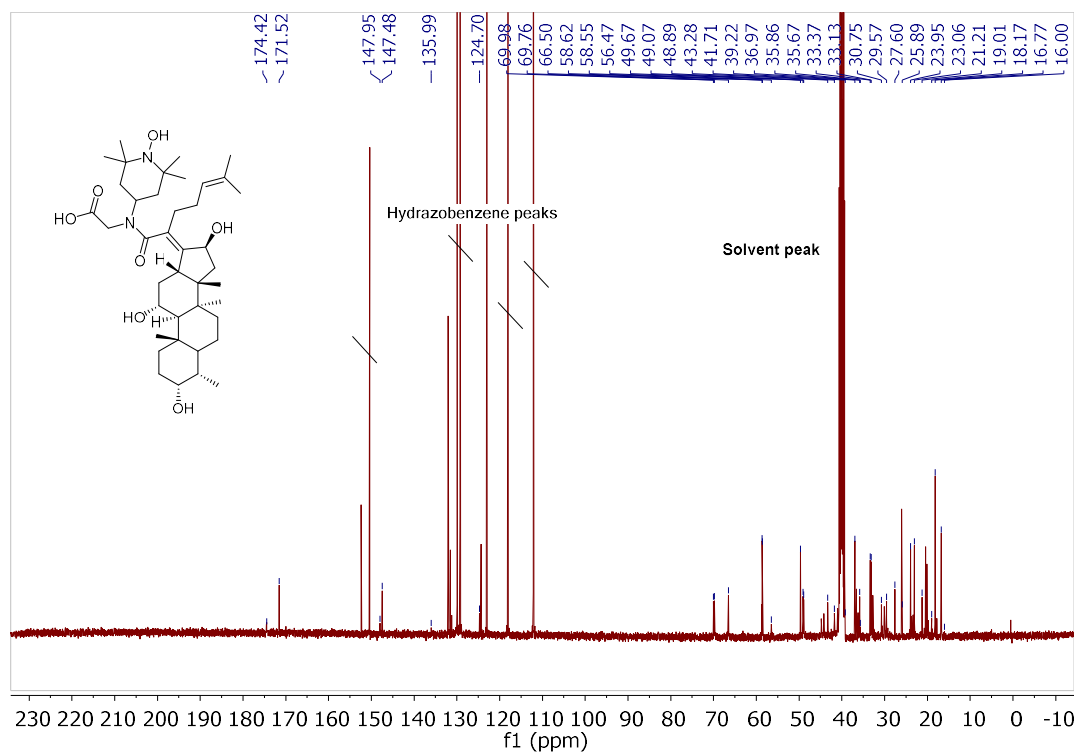




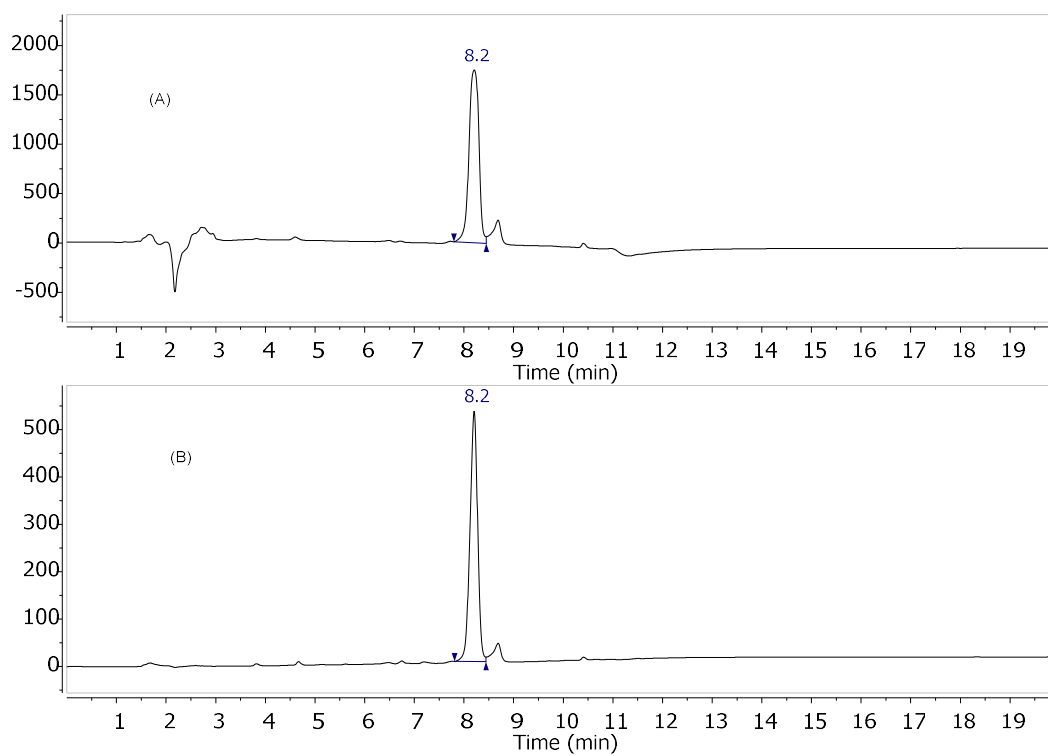
**Figure S25.** RP-HPLC chromatogram of compound **14** a) 210 nm, b) 215 nm.



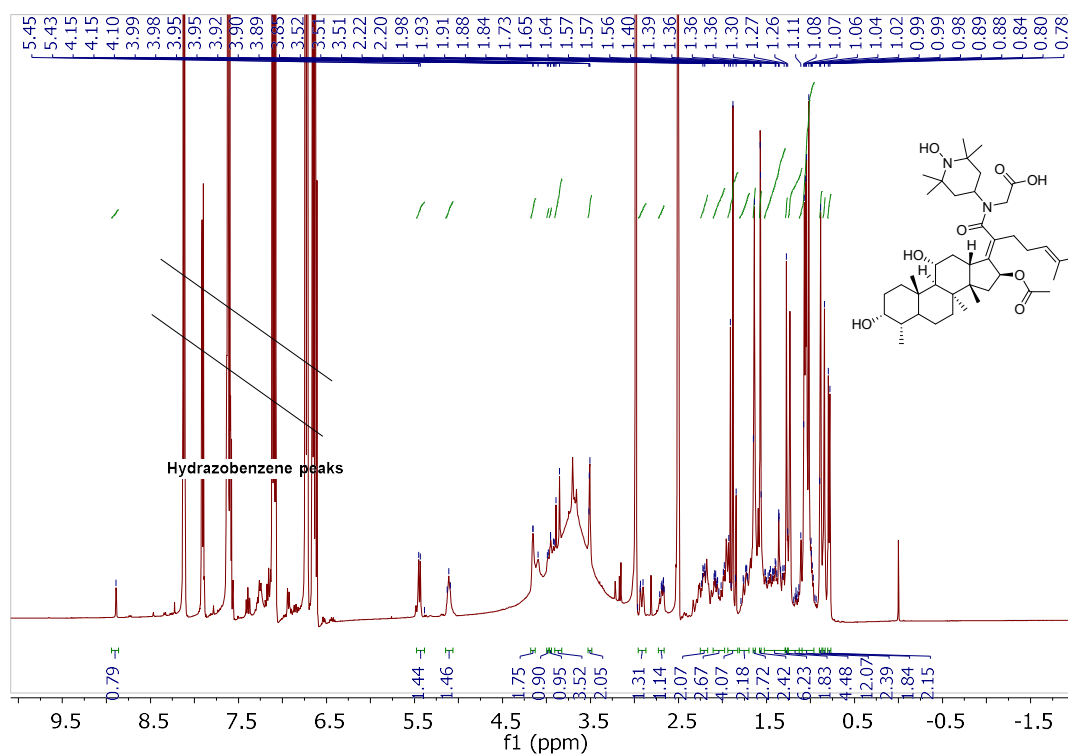
**Figure S26.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of compound **16**.



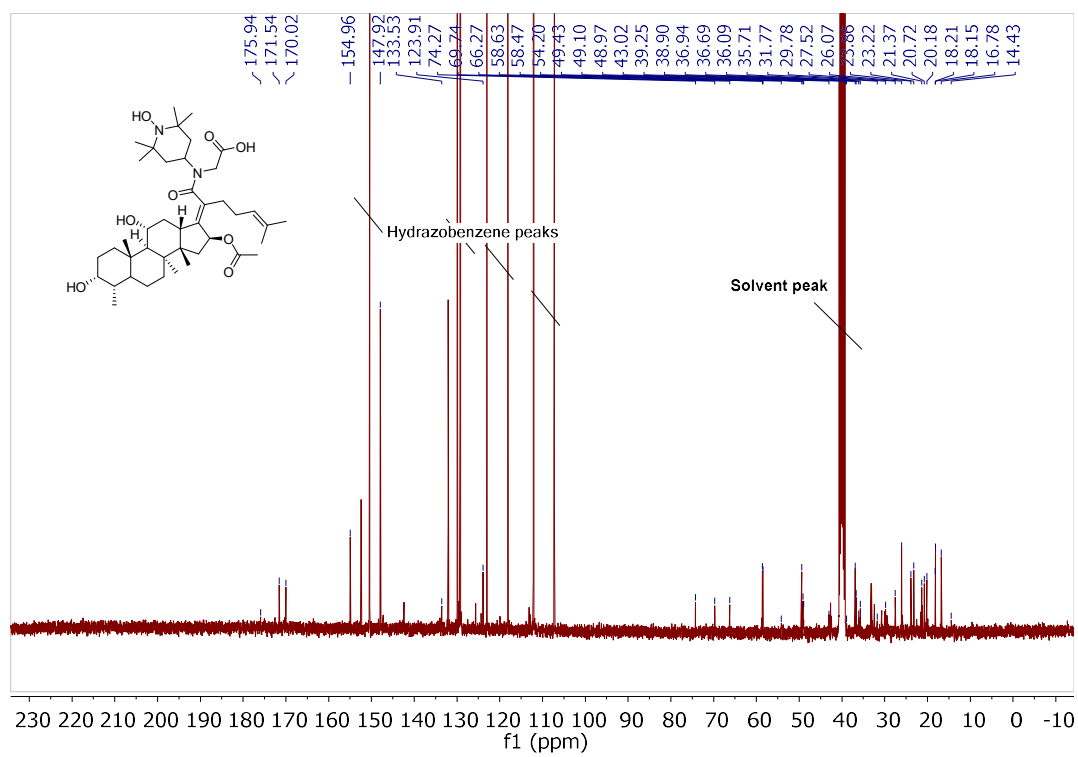
**Figure S27.**  $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO}-d_6$ ) spectrum of compound **16**.



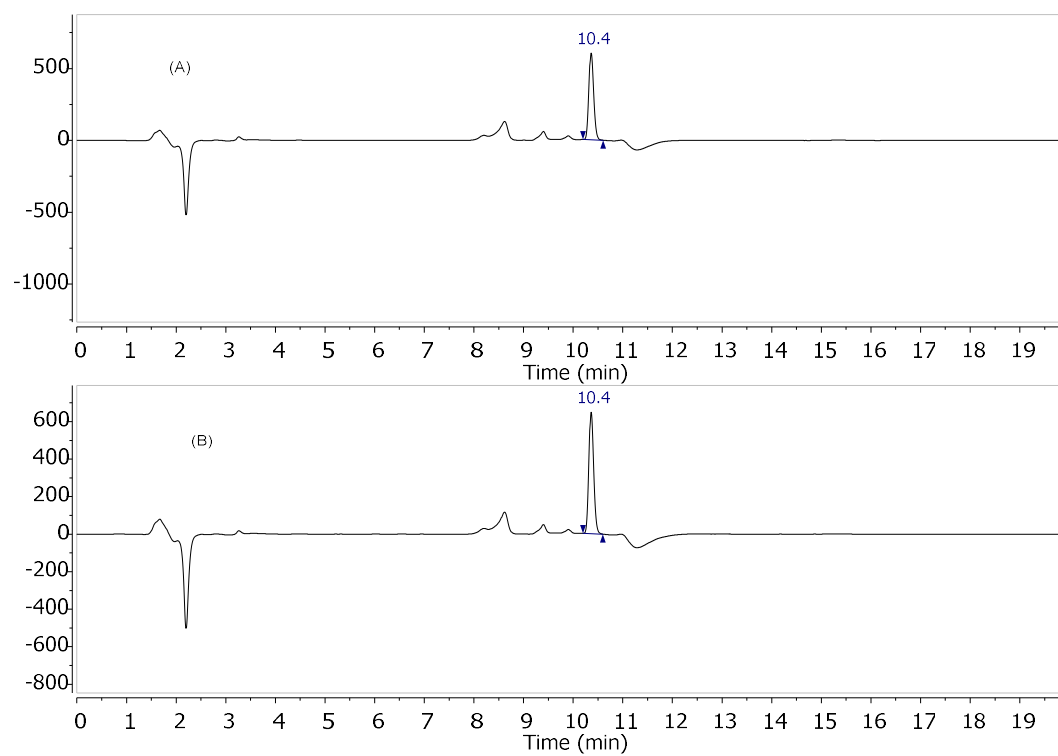
**Figure S28.** RP-HPLC chromatogram of compound **16** a) 210 nm, b) 215 nm.



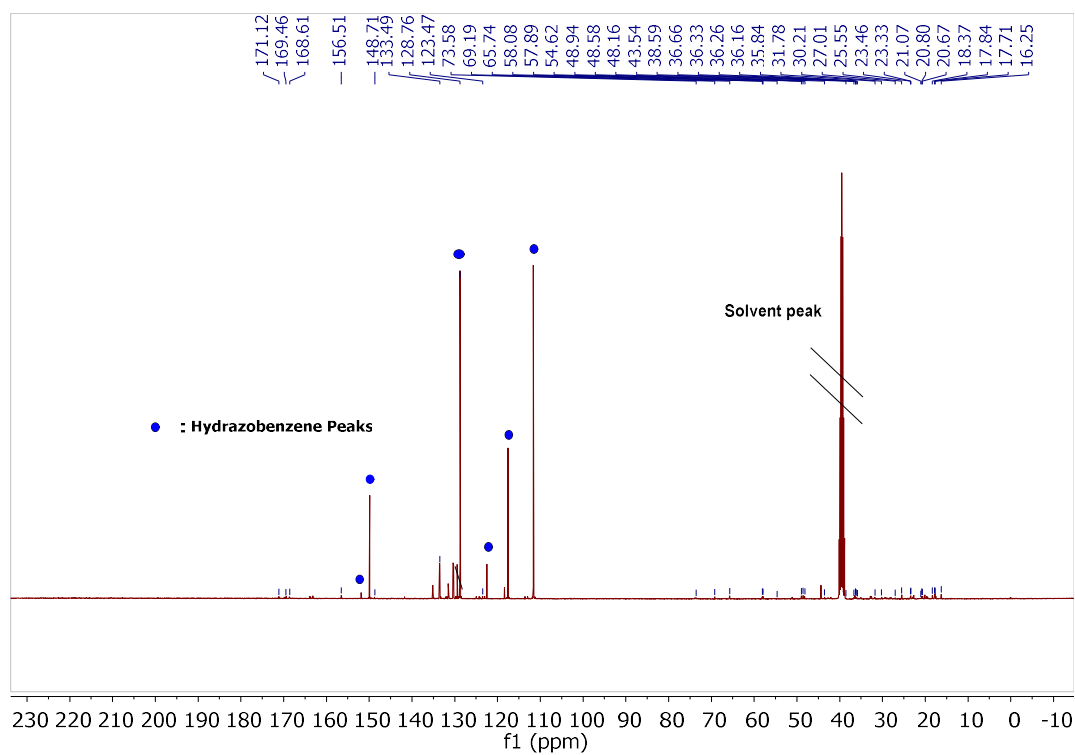
**Figure S29.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of compound **17**.

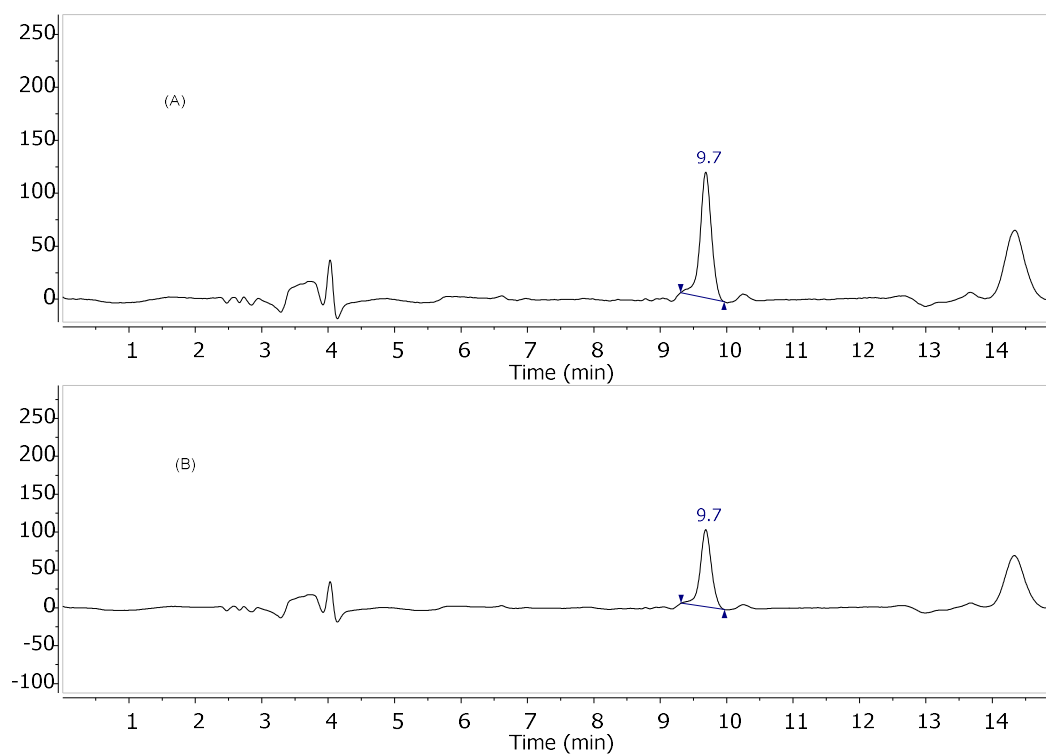


**Figure S30.**  $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO}-d_6$ ) spectrum of compound **17**.



**Figure S31.** RP-HPLC chromatogram of compound **17** a) 210 nm, b) 215 nm.





**Figure S34.** RP-HPLC chromatogram of compound **18** a) 210 nm, b) 215 nm.