

SUPPORTING INFORMATION

**SYNTHESIS AND CYTOTOXIC ACTIVITY OF MADECASSIC ACID – SILYBIN
CONJUGATE COMPOUNDS IN LIVER CANCER CELLS**

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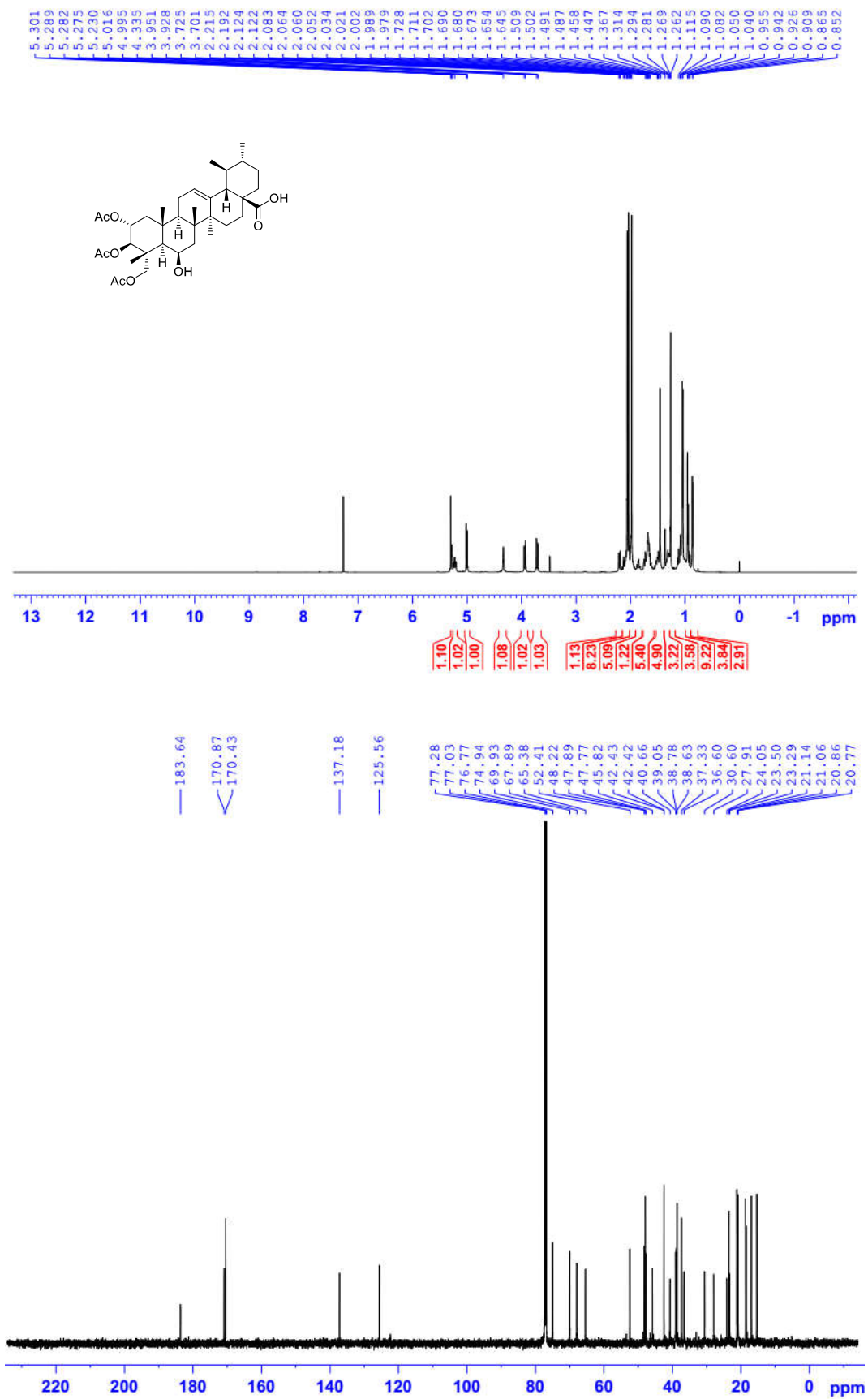


Figure S1. ¹H and ¹³C NMR (CDCl₃, 500 MHz) spectra of compound 3

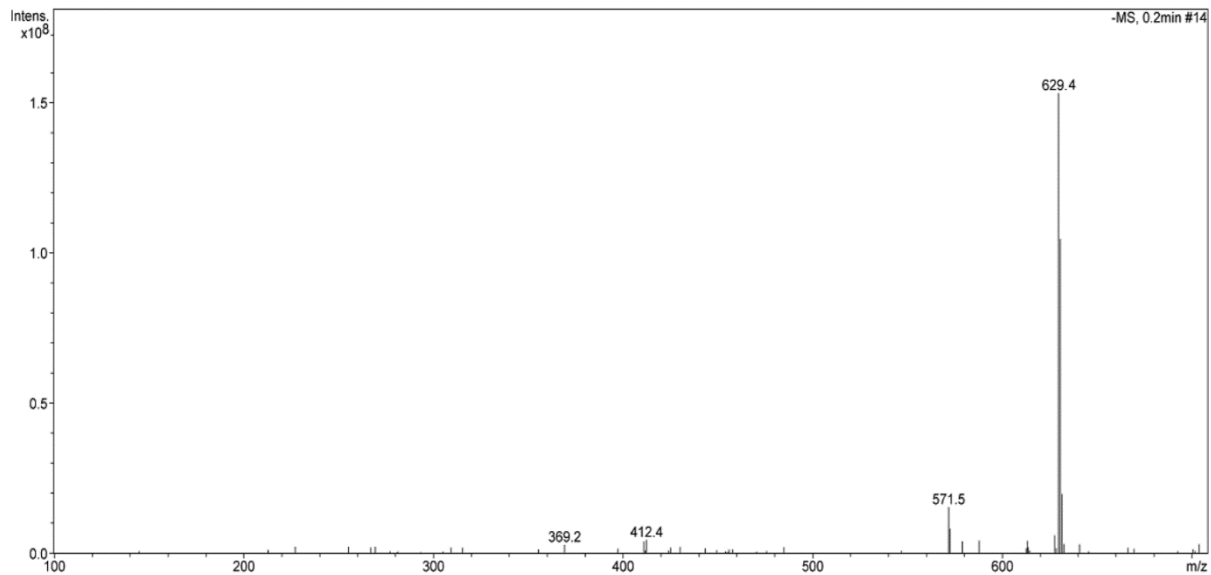
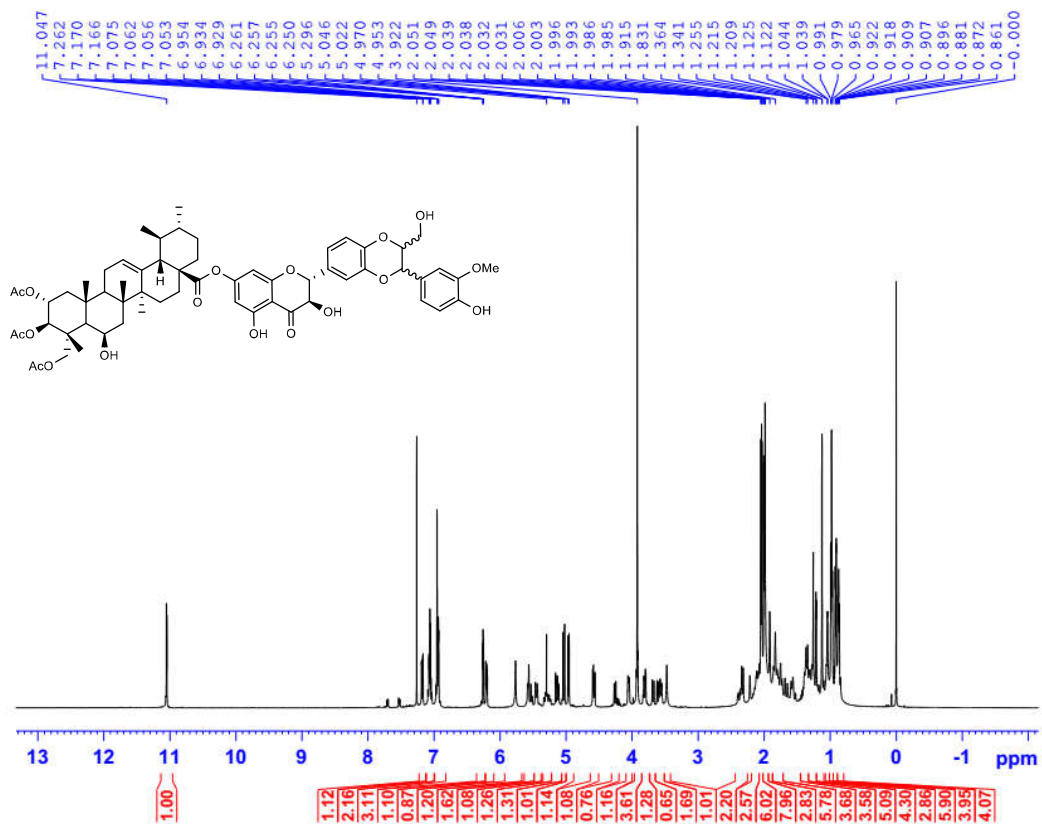


Figure S2. ESI-MS spectrum of compound 3



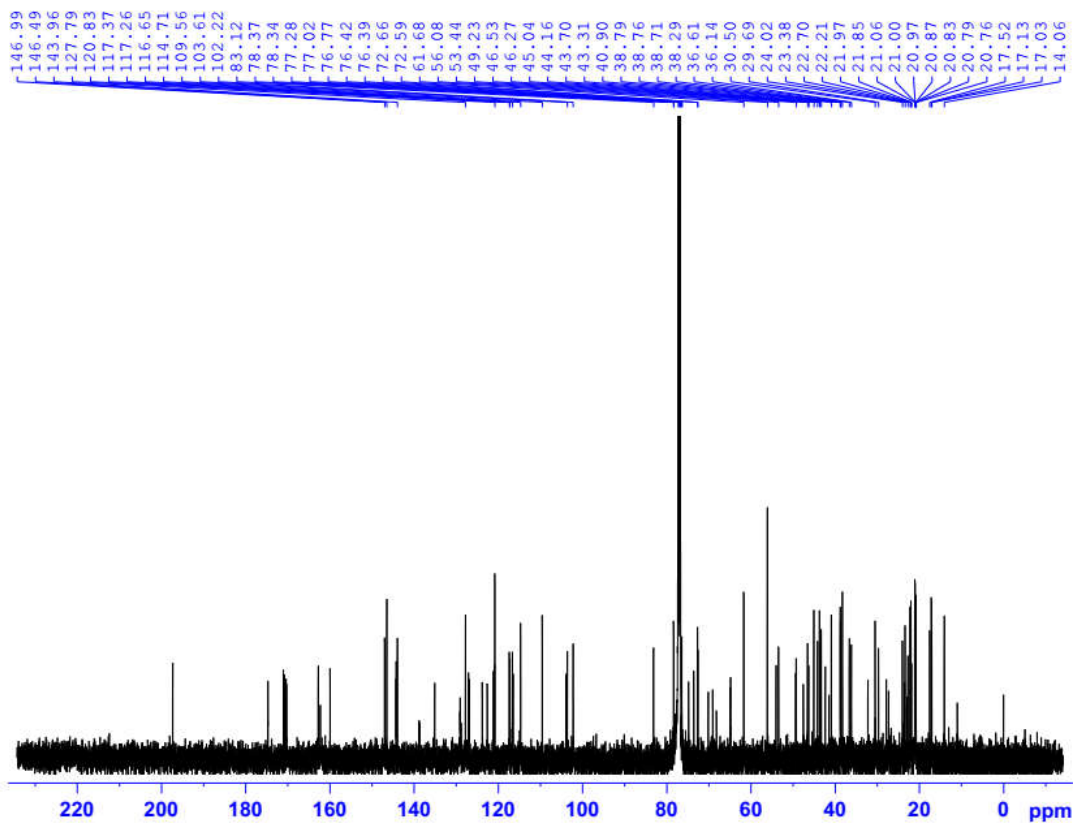


Figure S3. ¹H and ¹³C NMR (CDCl₃, 500 MHz) spectra of compound **4**

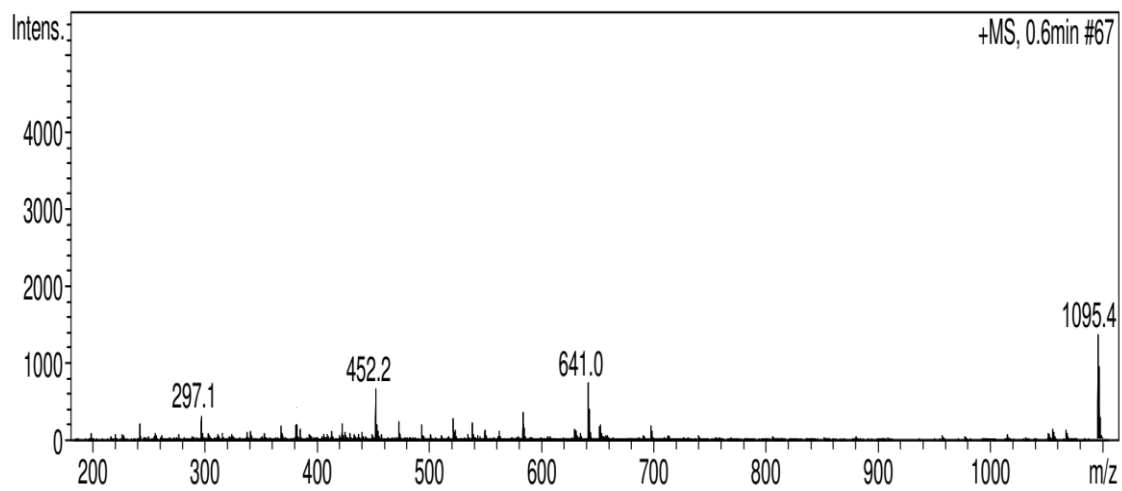


Figure S4. ESI-MS spectrum of compound **4**

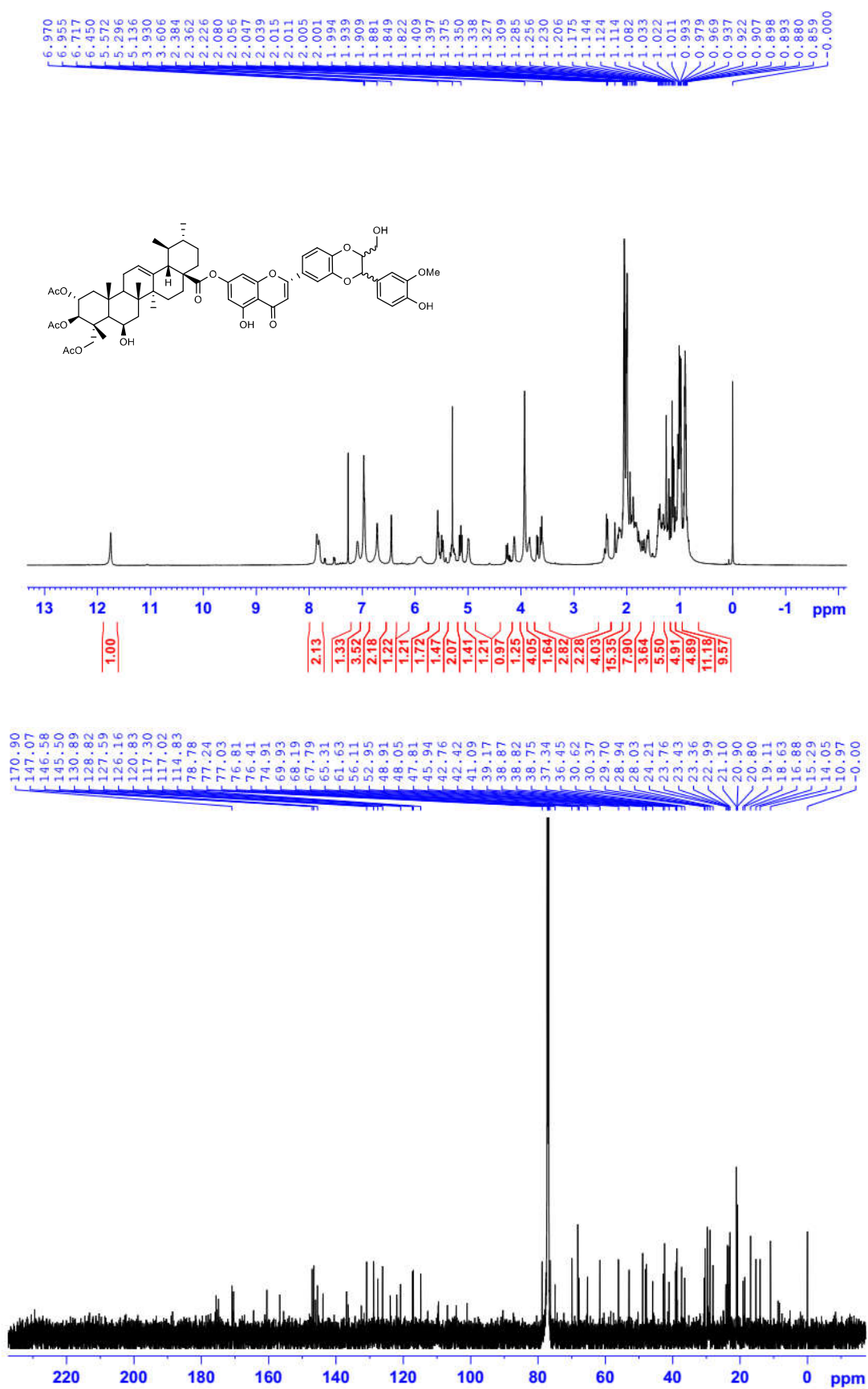


Figure S5. ¹H and ¹³C NMR (CDCl₃, 500 MHz) spectra of compound 5

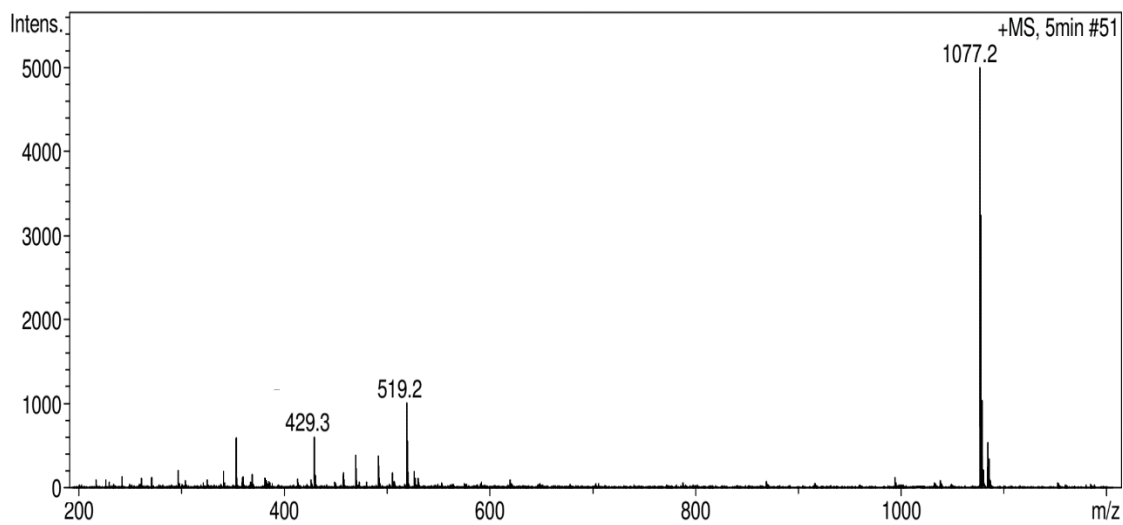
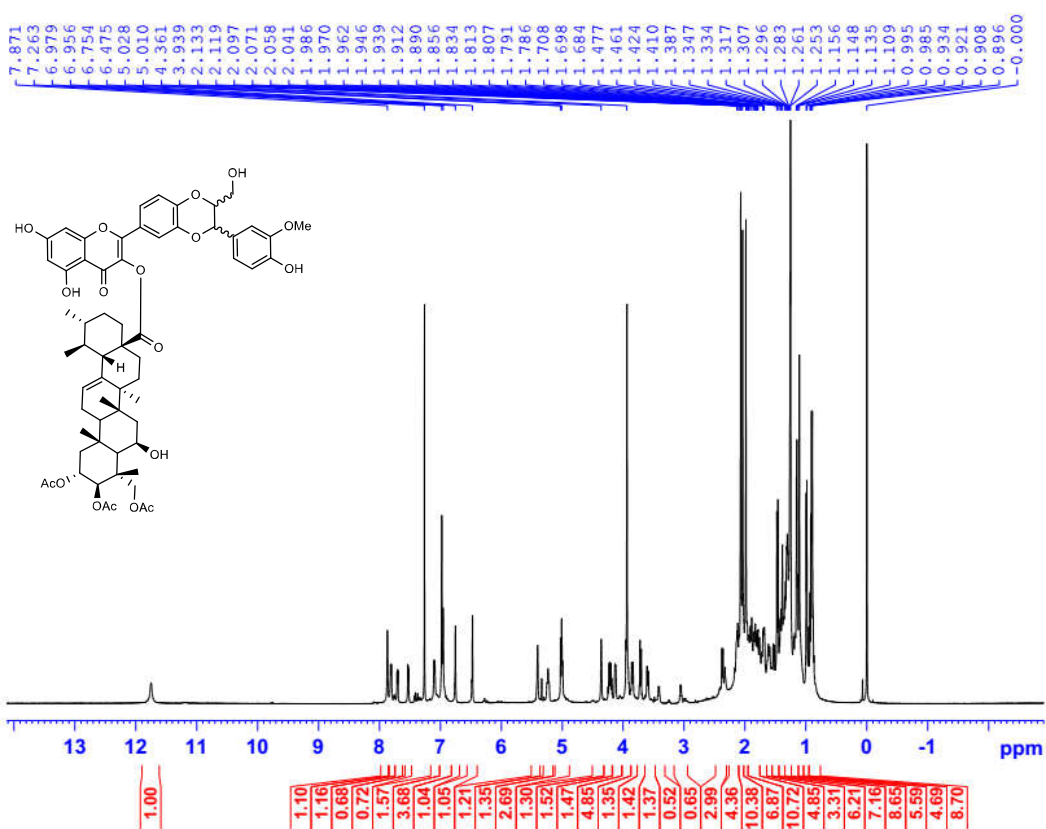


Figure S6. ESI-MS spectrum of compound 5



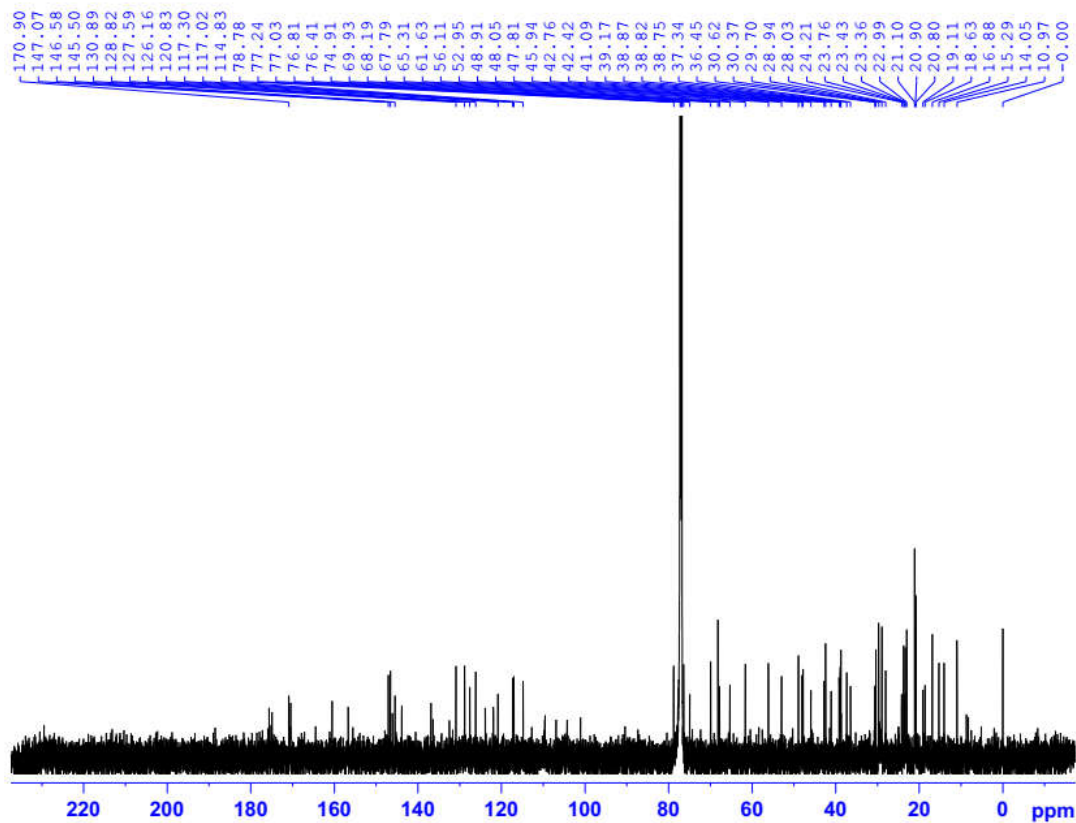


Figure S7. ^1H and ^{13}C NMR (CDCl_3 , 600 MHz) spectra of compound **6**

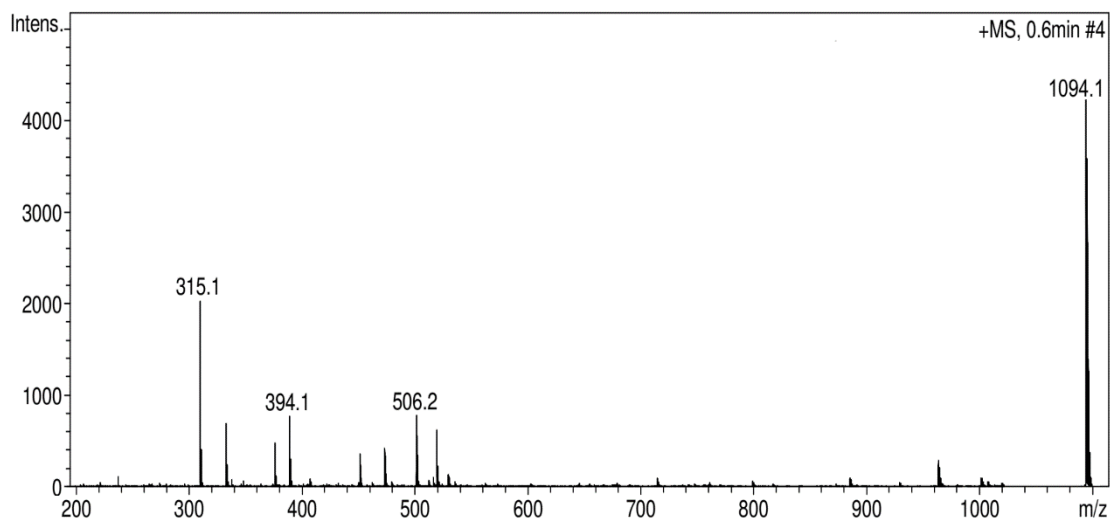


Figure S8. ESI-MS spectrum of compound **6**

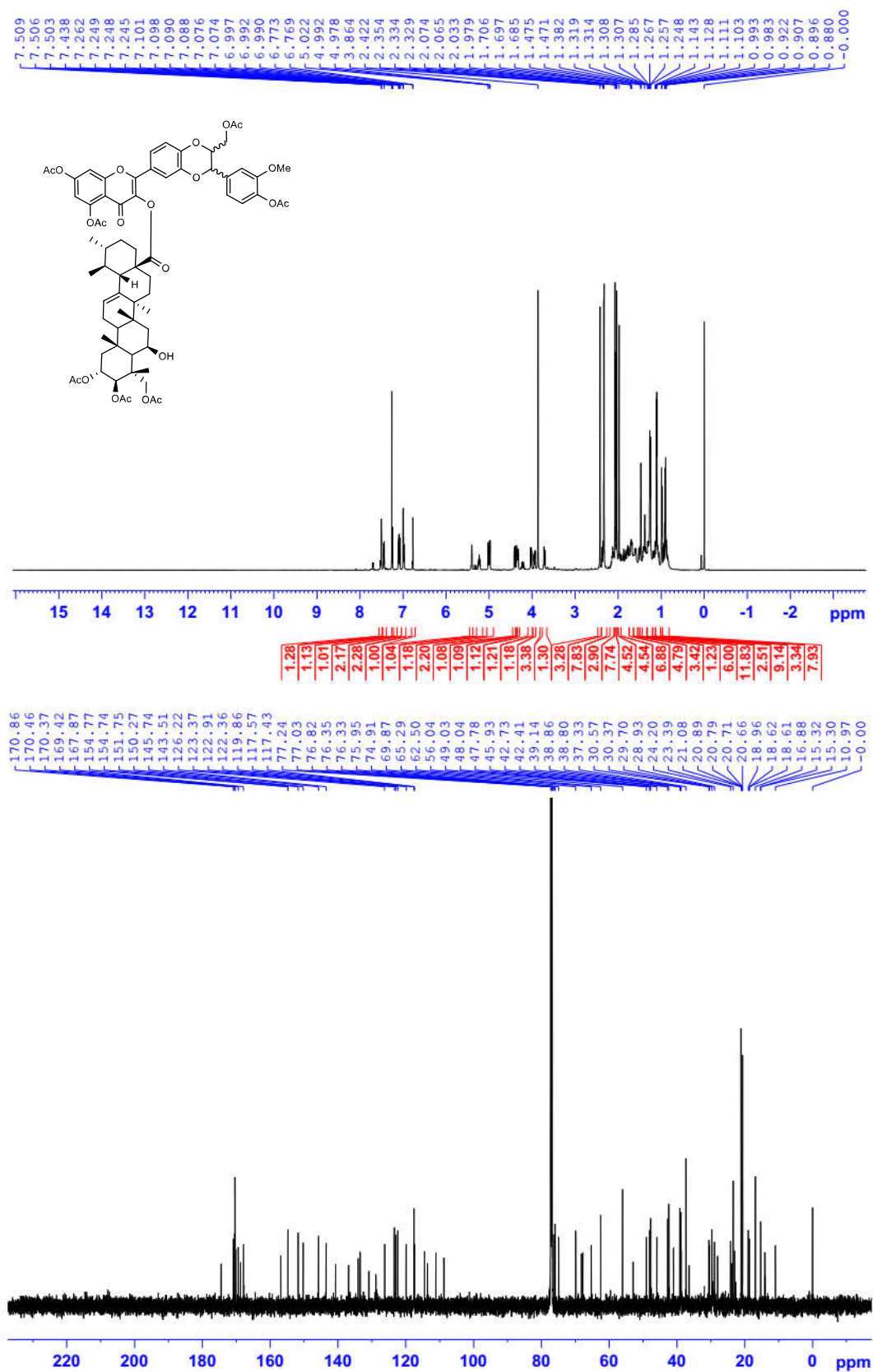


Figure S9. ¹H and ¹³C NMR (CDCl₃, 600 MHz) spectra of compound 7

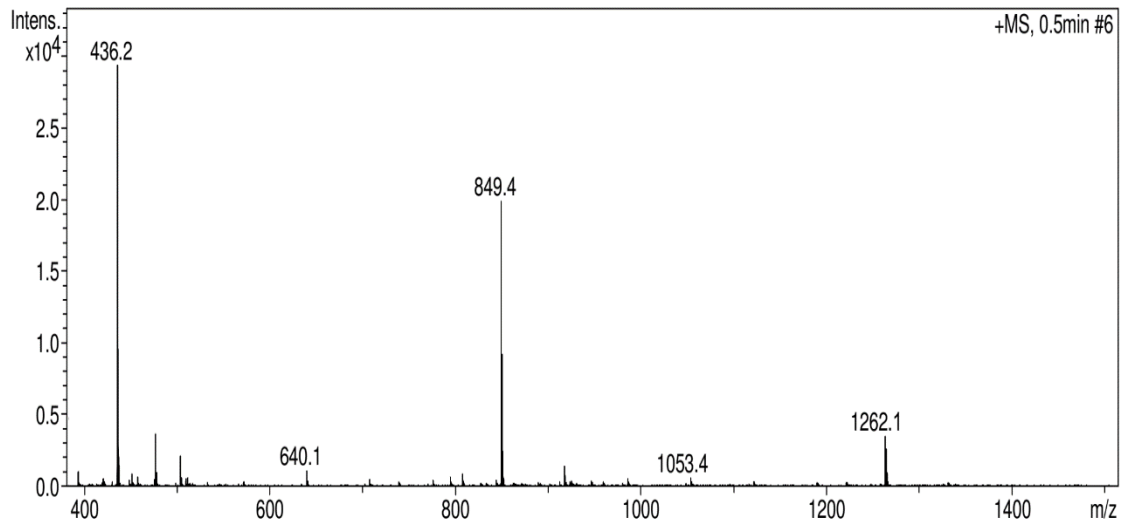
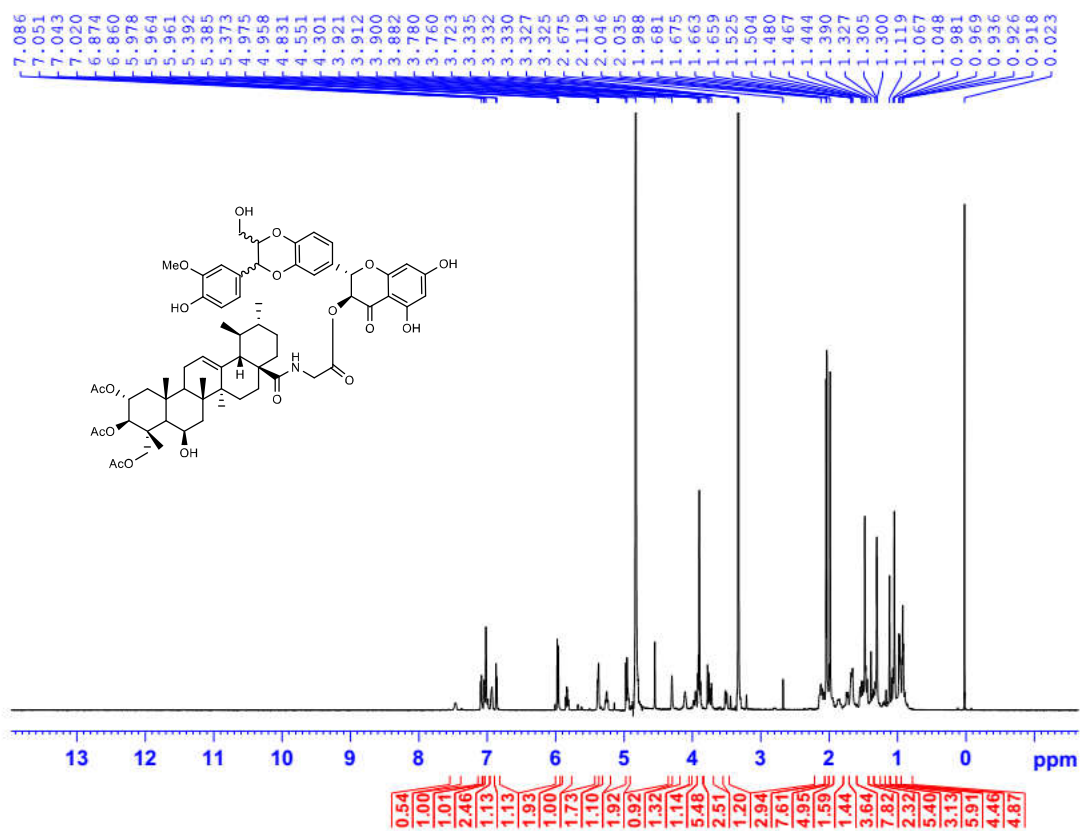


Figure S10. ESI-MS spectrum of compound 7



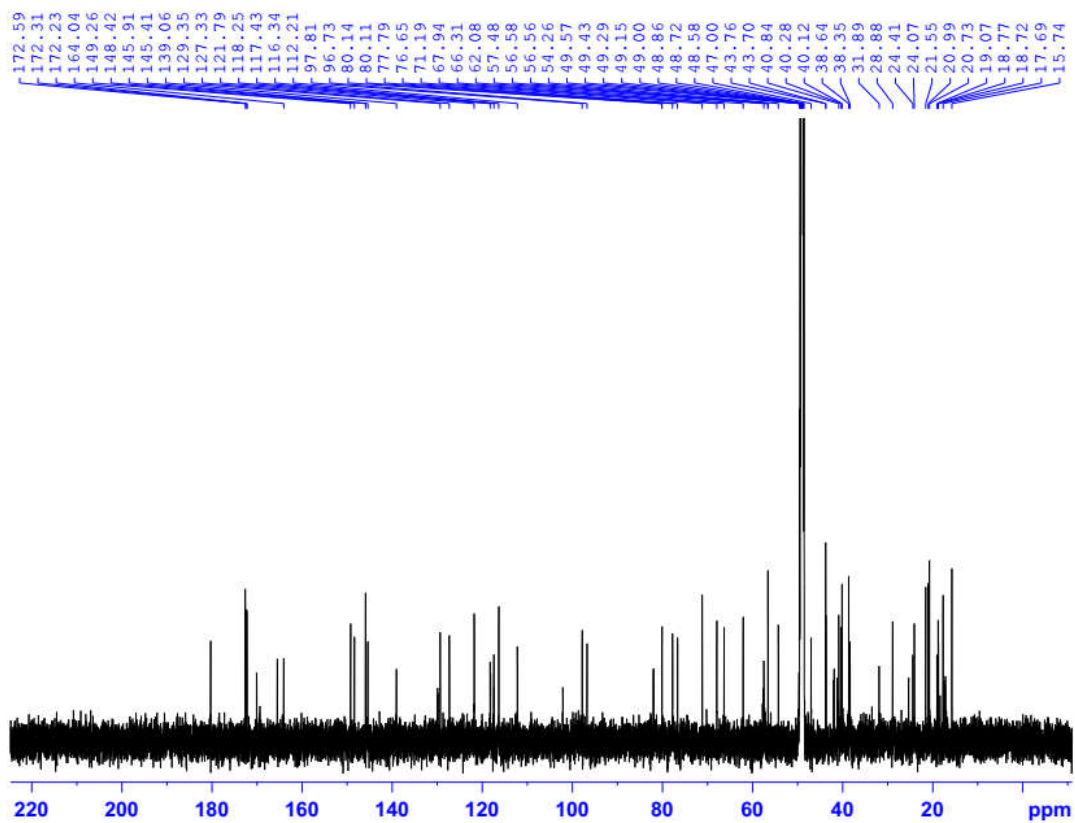


Figure S11. ^1H and ^{13}C NMR (CD_3OD , 600 MHz) spectra of compound **8**

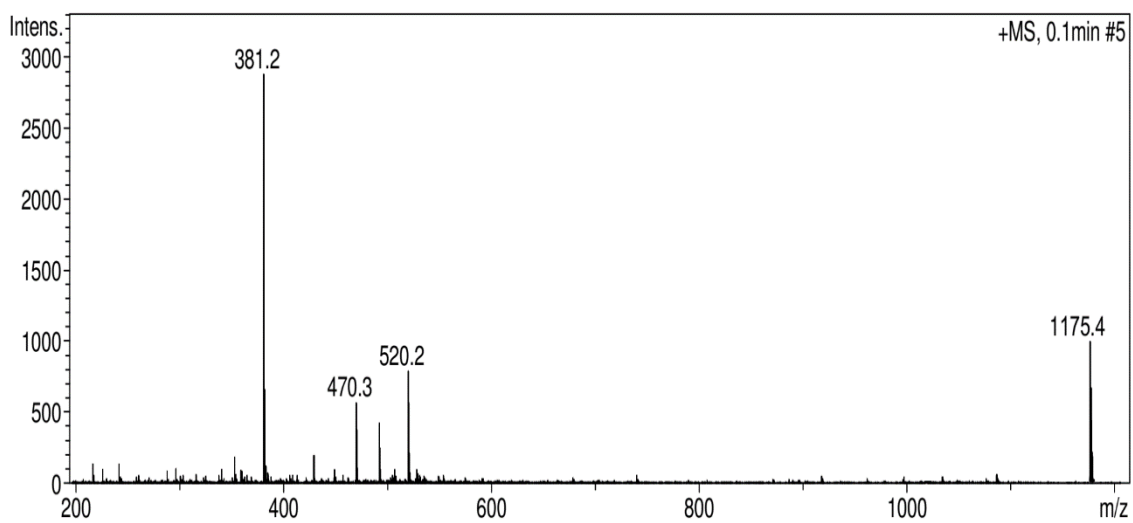
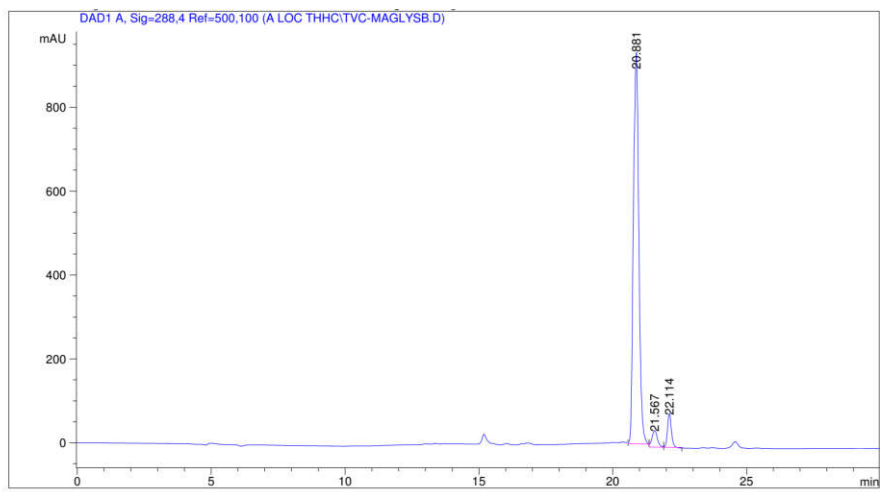


Figure S12. ESI-MS spectrum of compound **8**



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Area Percent Report
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Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

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2	21.567	VV	0.2272	343.86725	41.41860	2.2359
3	22.114	VB	0.1622	394.74591	82.19529	2.5668

Totals : 1.53789e4 1066.81726

Figure S13. HPLC analysis of compound **8**

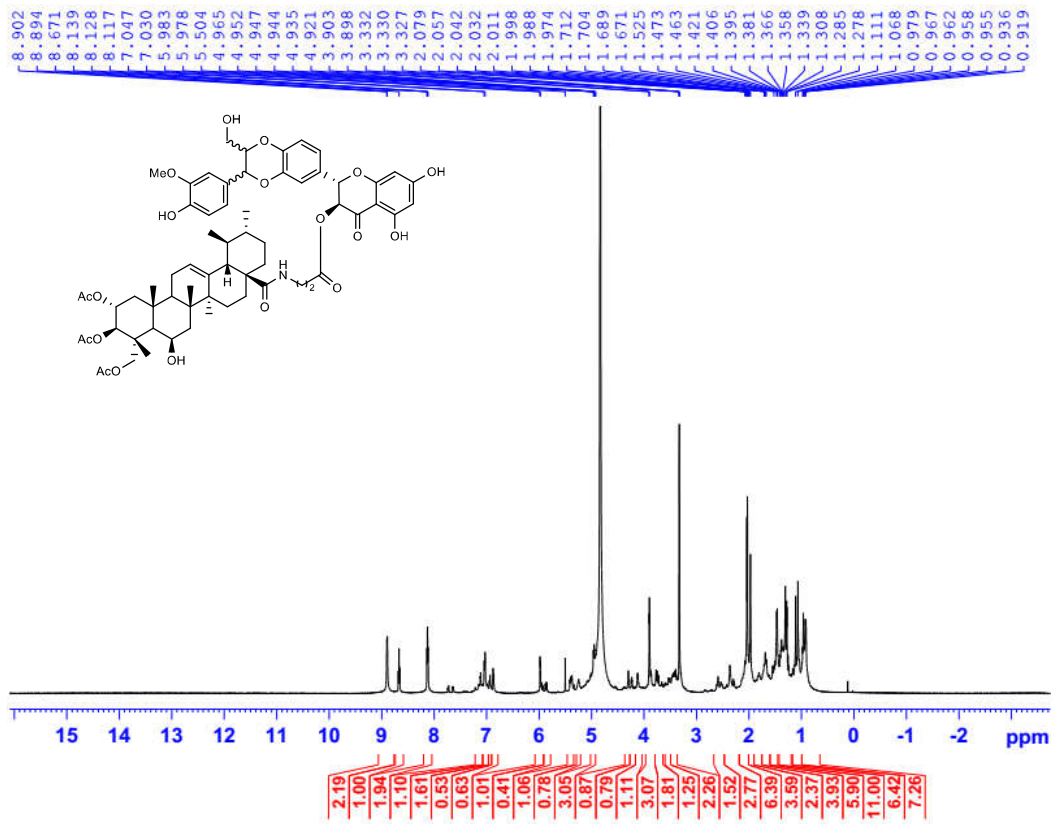


Figure S14. ¹H NMR (CD₃OD, 600 MHz) spectrum of compound **9**

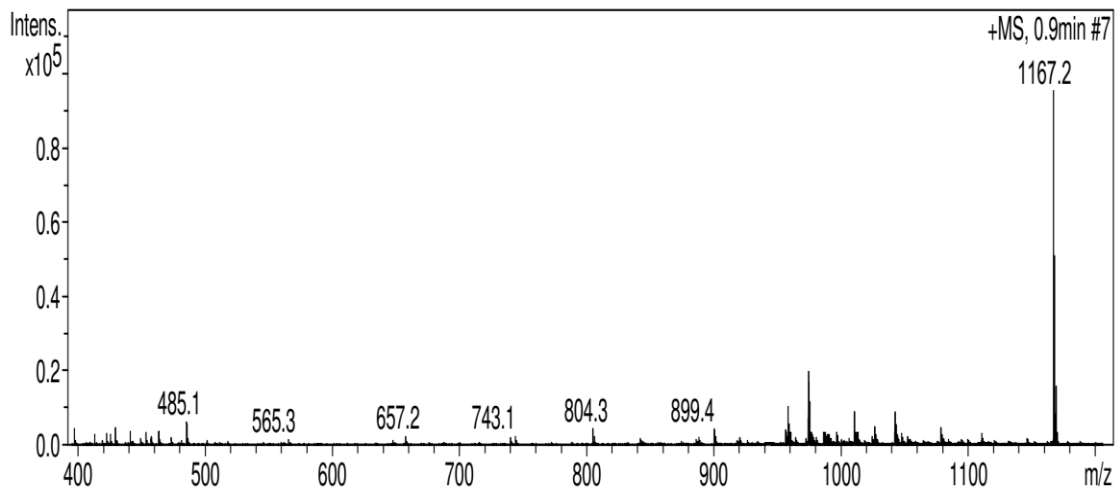
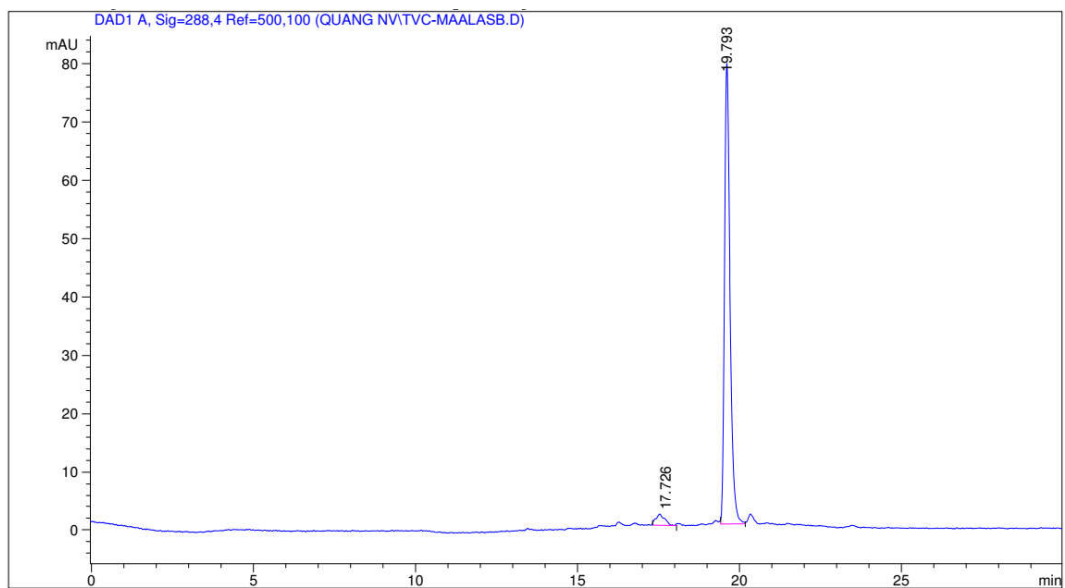


Figure S15. ESI-MS spectrum of compound 9



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Peak RetTime Type Width Area Height Area
# [min] [min] [min] [mAU*s] [mAU] %
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Figure S16. HPLC analysis of compound 9

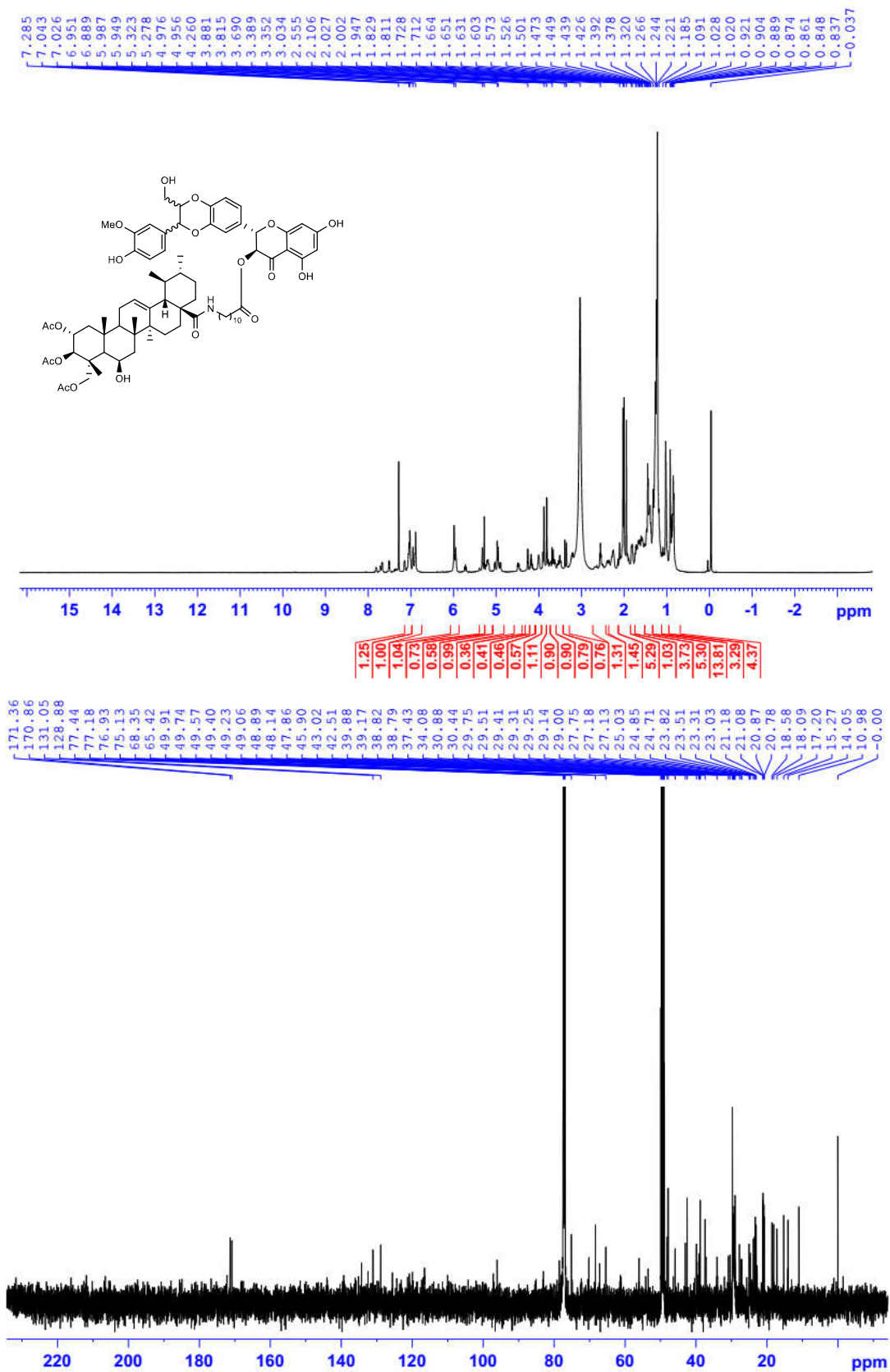


Figure S17. ¹H and ¹³C NMR (CDCl₃, 500 MHz) spectra of compound 10

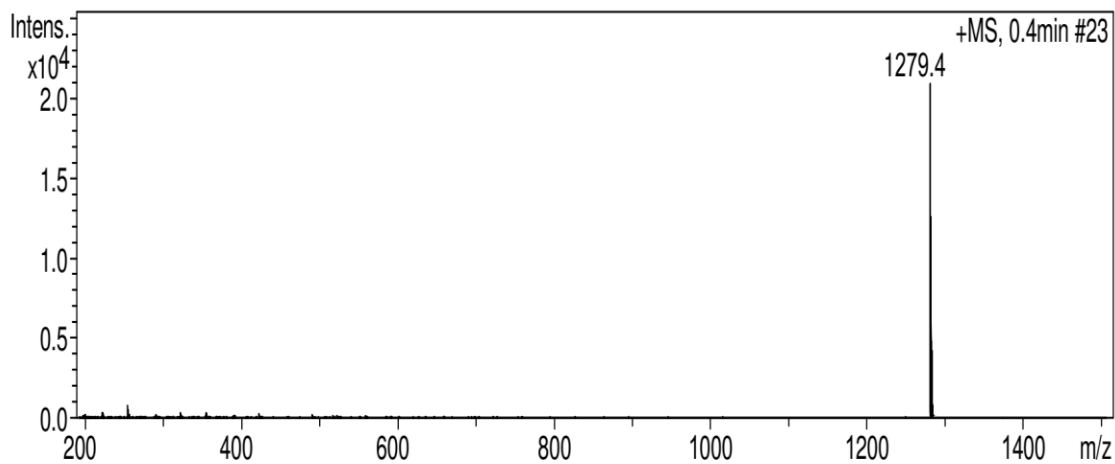
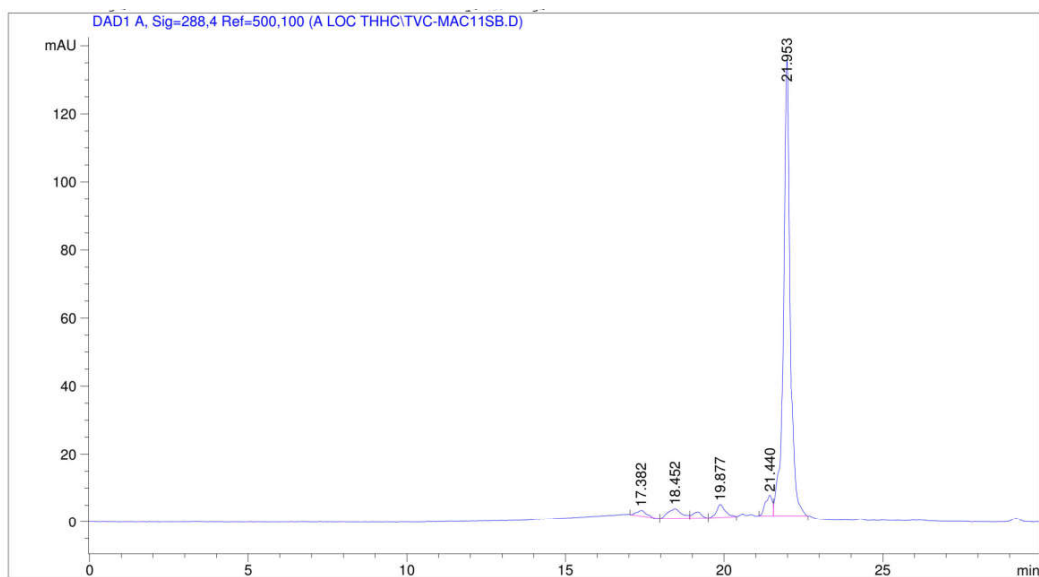


Figure S18. ESI-MS spectrum of compound 10



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Dilution      :      1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=288,4 Ref=500,100

Peak RetTime Type  Width   Area   Height   Area
#   [min]         [min] [mAU*s] [mAU]    %
-----|-----|-----|-----|-----|-----
  1  17.382  BB    0.2435  23.43523  1.68535  0.6321
  2  18.452  BV    0.3712  58.01112  2.87418  1.5647
  3  19.877  VV    0.2672  64.86910  3.87856  1.7497
  4  21.440  BV    0.2092  74.20120  6.13362  2.0015
  5  21.953  VV    0.2035 3486.84570 134.15177 94.0519

Totals :                               3707.36235  148.72348

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Figure S19. HPLC analysis of compound 10

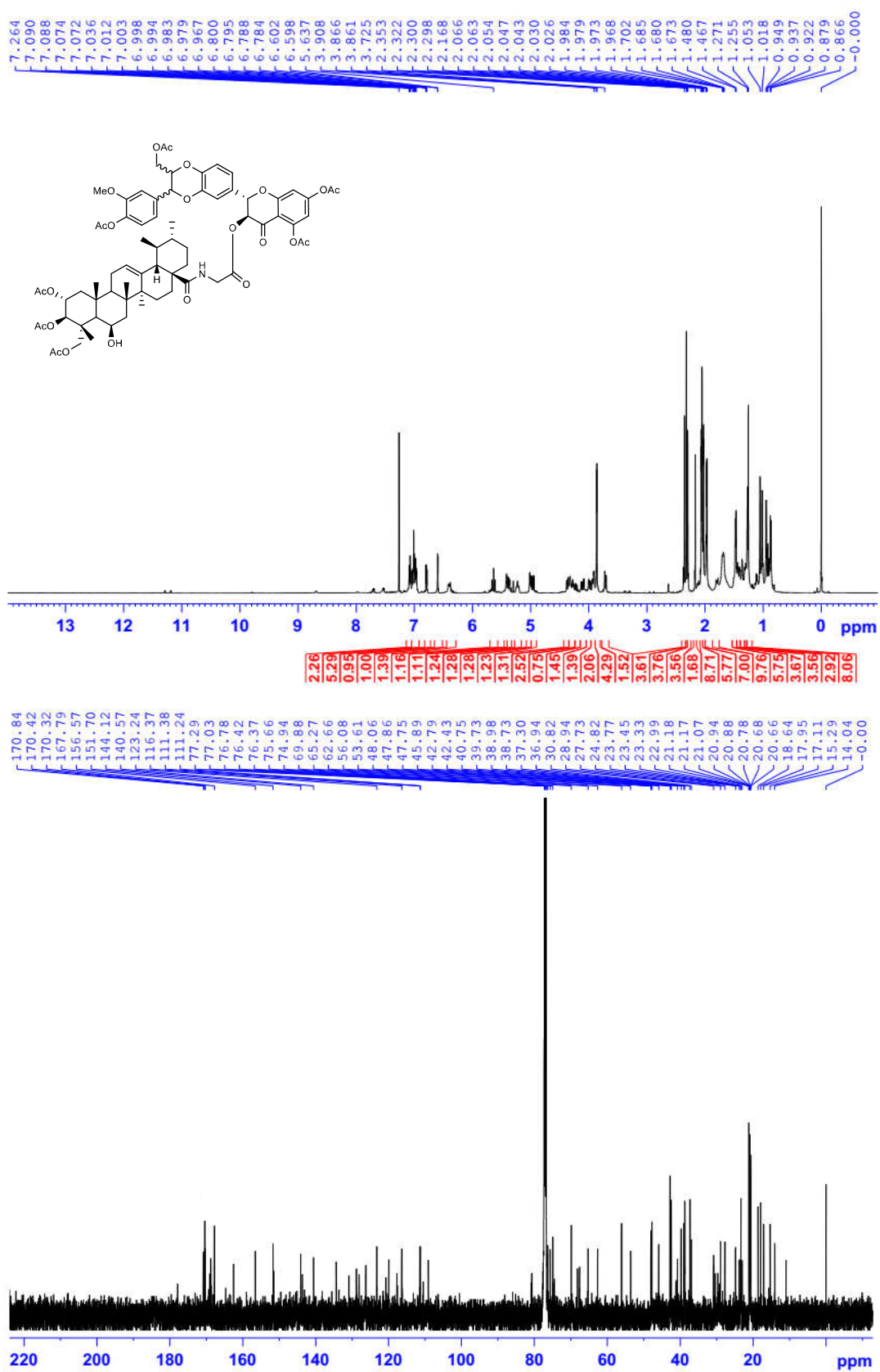


Figure S20. ¹H and ¹³C NMR (CDCl₃, 500 MHz) spectra of compound **11**

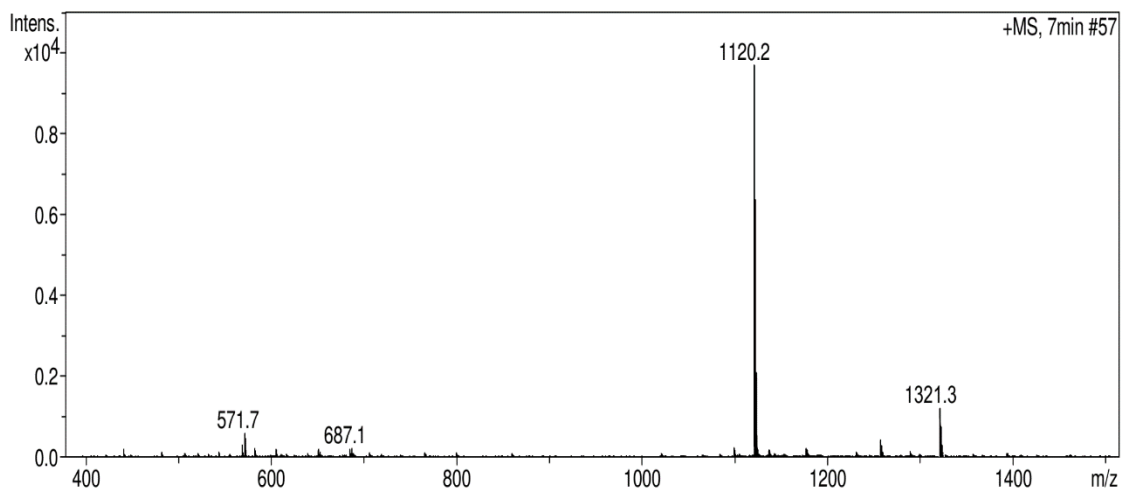
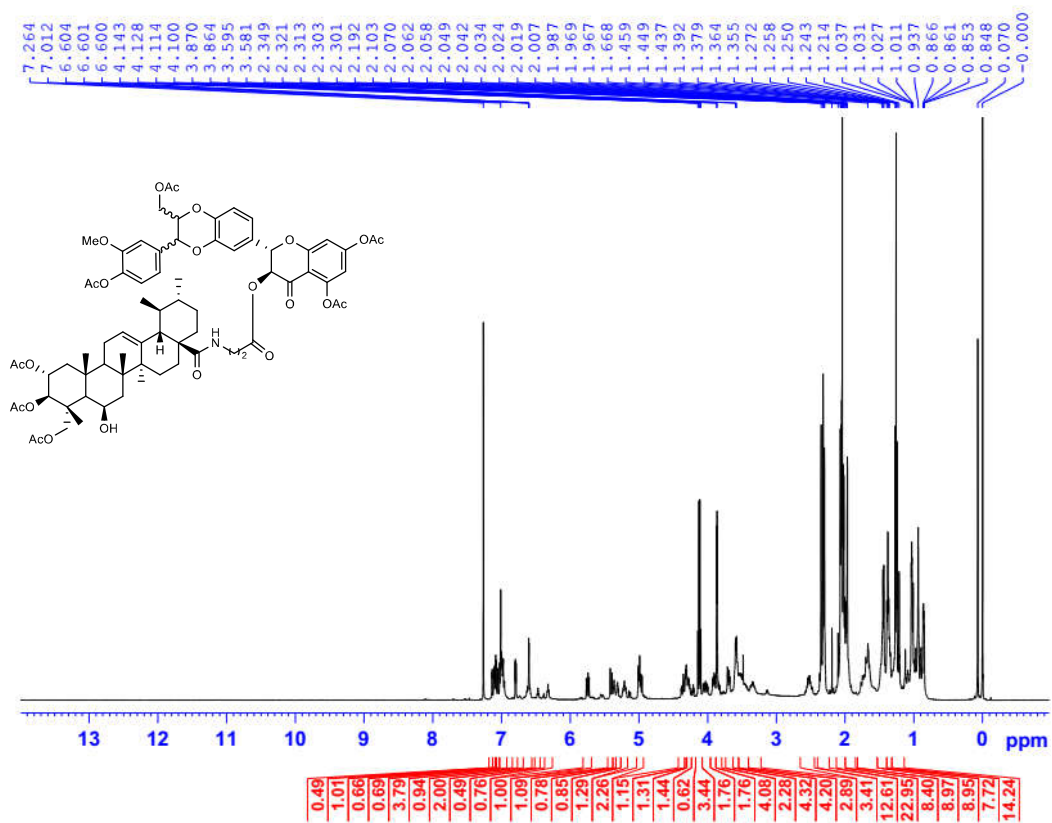


Figure S21. ESI-MS spectrum of compound 11



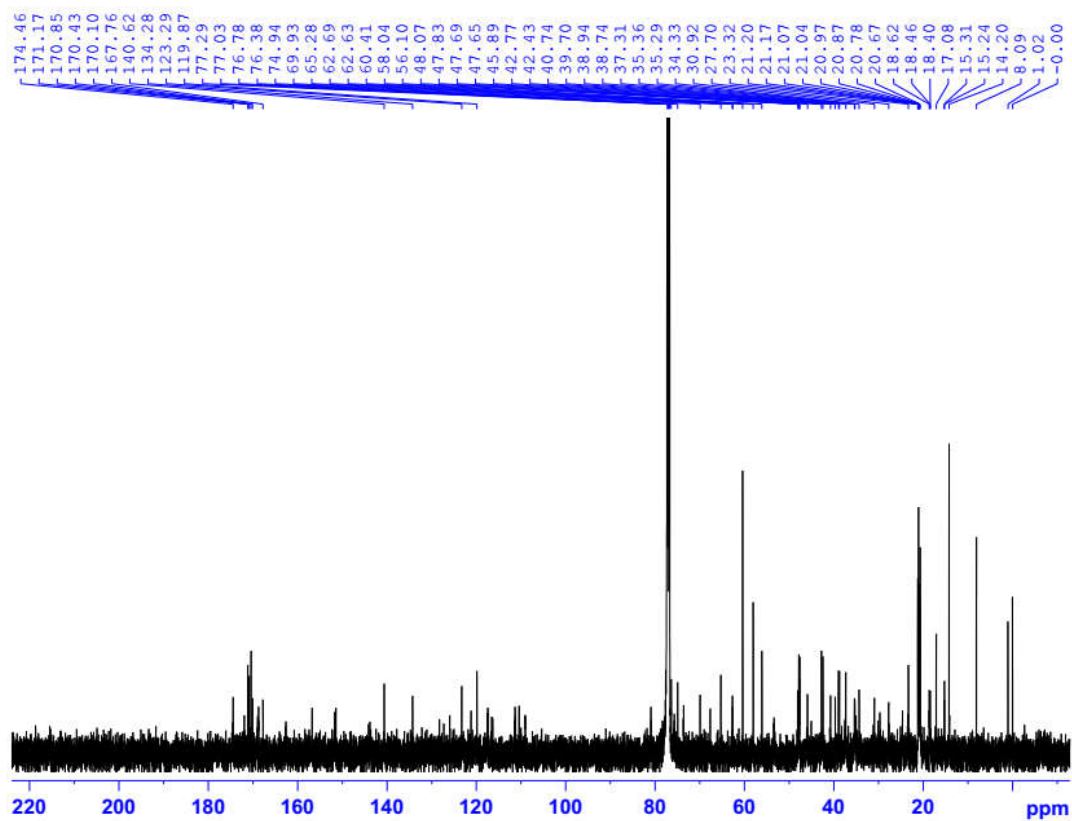


Figure S22. ^1H and ^{13}C NMR (CDCl_3 , 500 MHz) spectra of compound **12**

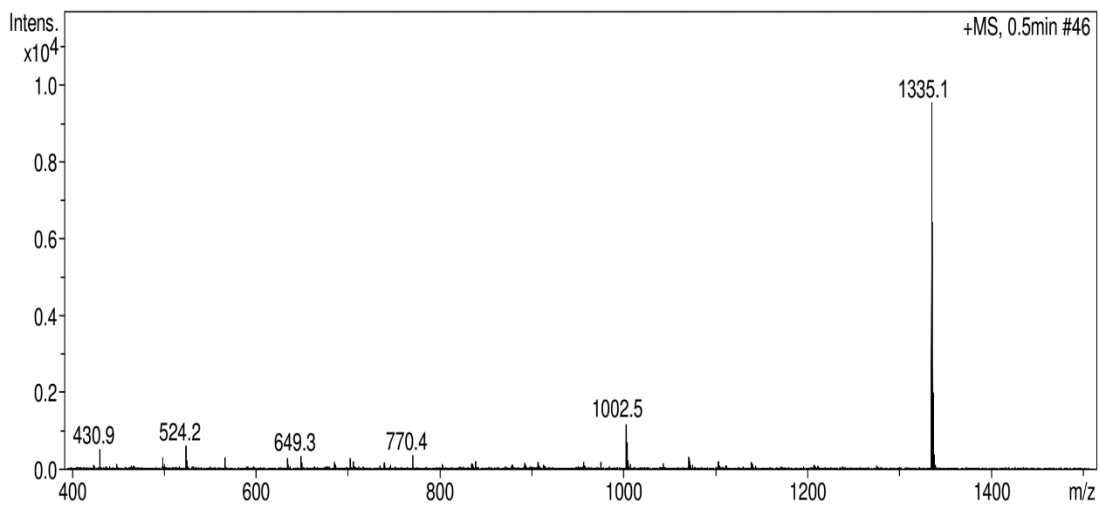


Figure S23. ESI-MS spectrum of compound **12**

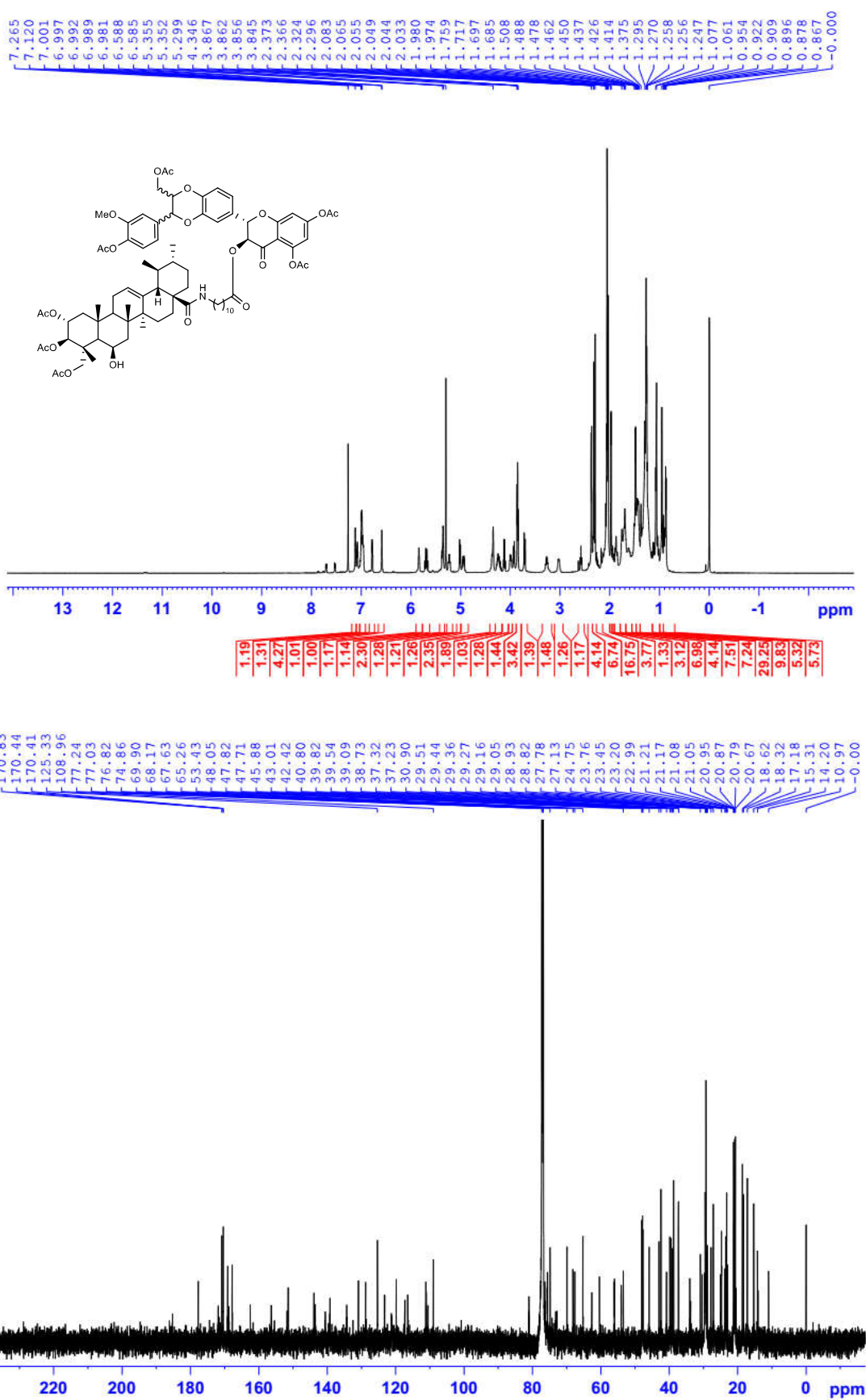


Figure S24. ¹H and ¹³C NMR (CDCl₃, 500 MHz) spectra of compound **13**

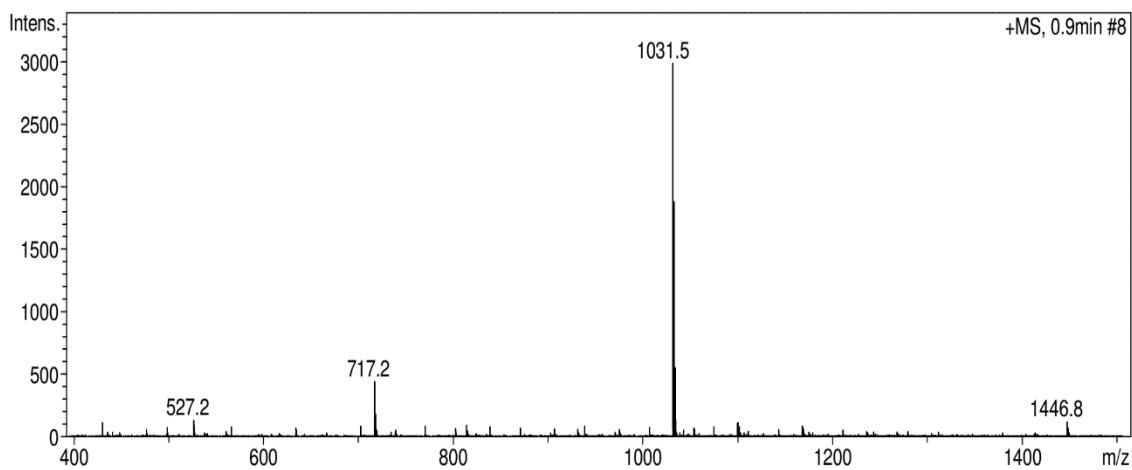
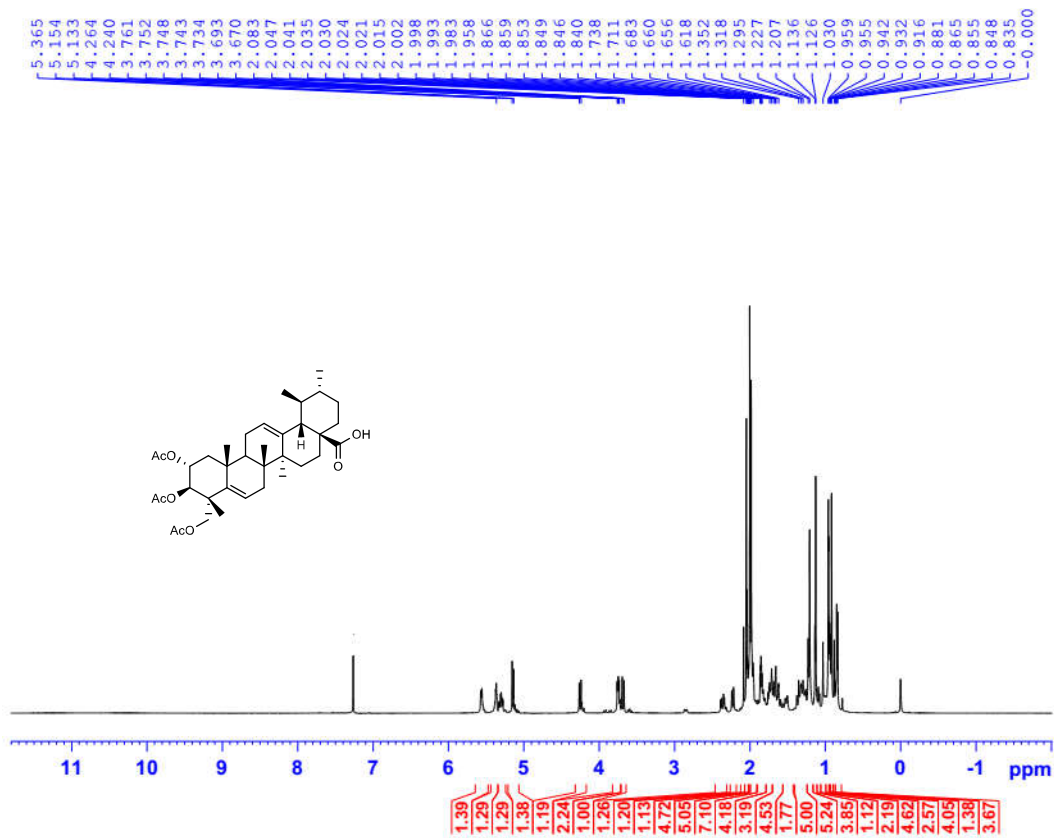


Figure S25. ESI-MS spectrum of compound 13



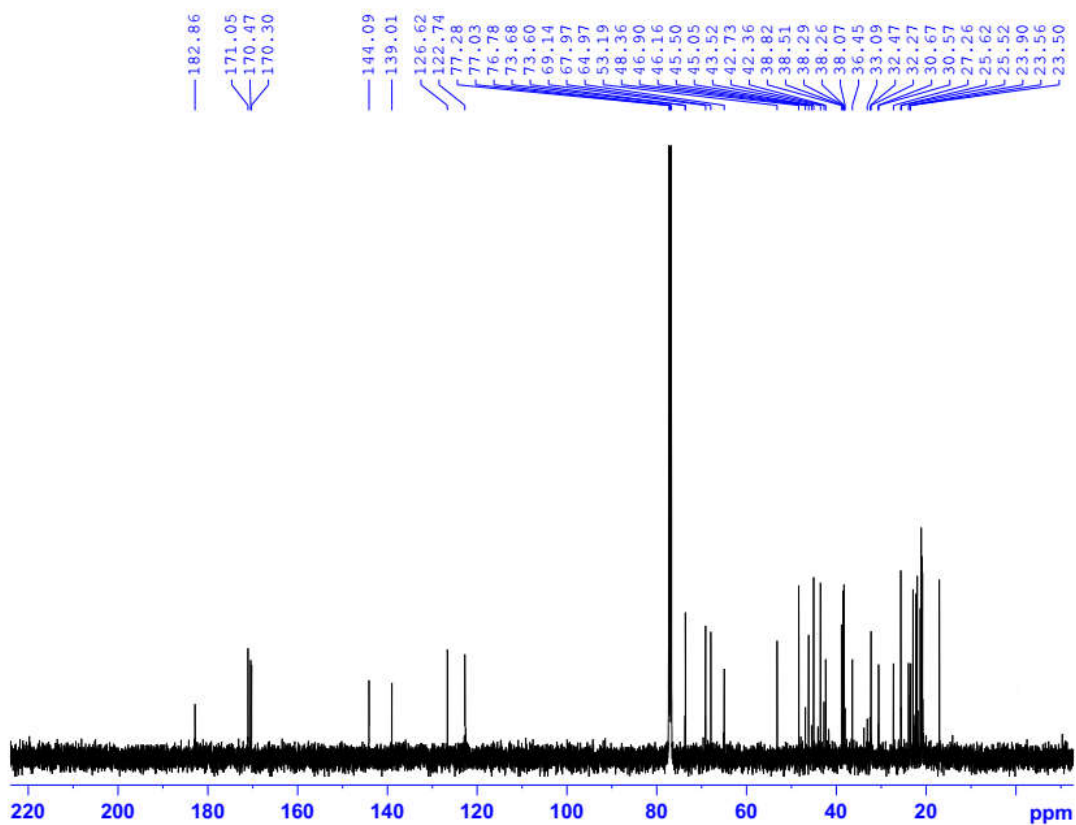


Figure S26. ^1H and ^{13}C NMR (CDCl_3 , 500 MHz) spectra of compound **14**

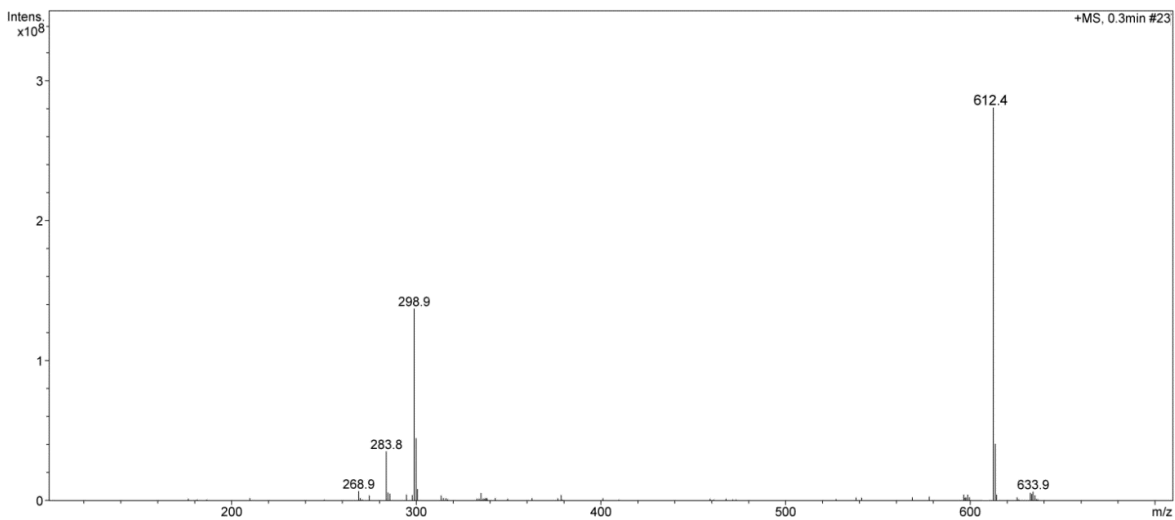


Figure S27. ESI-MS spectrum of compound **14**

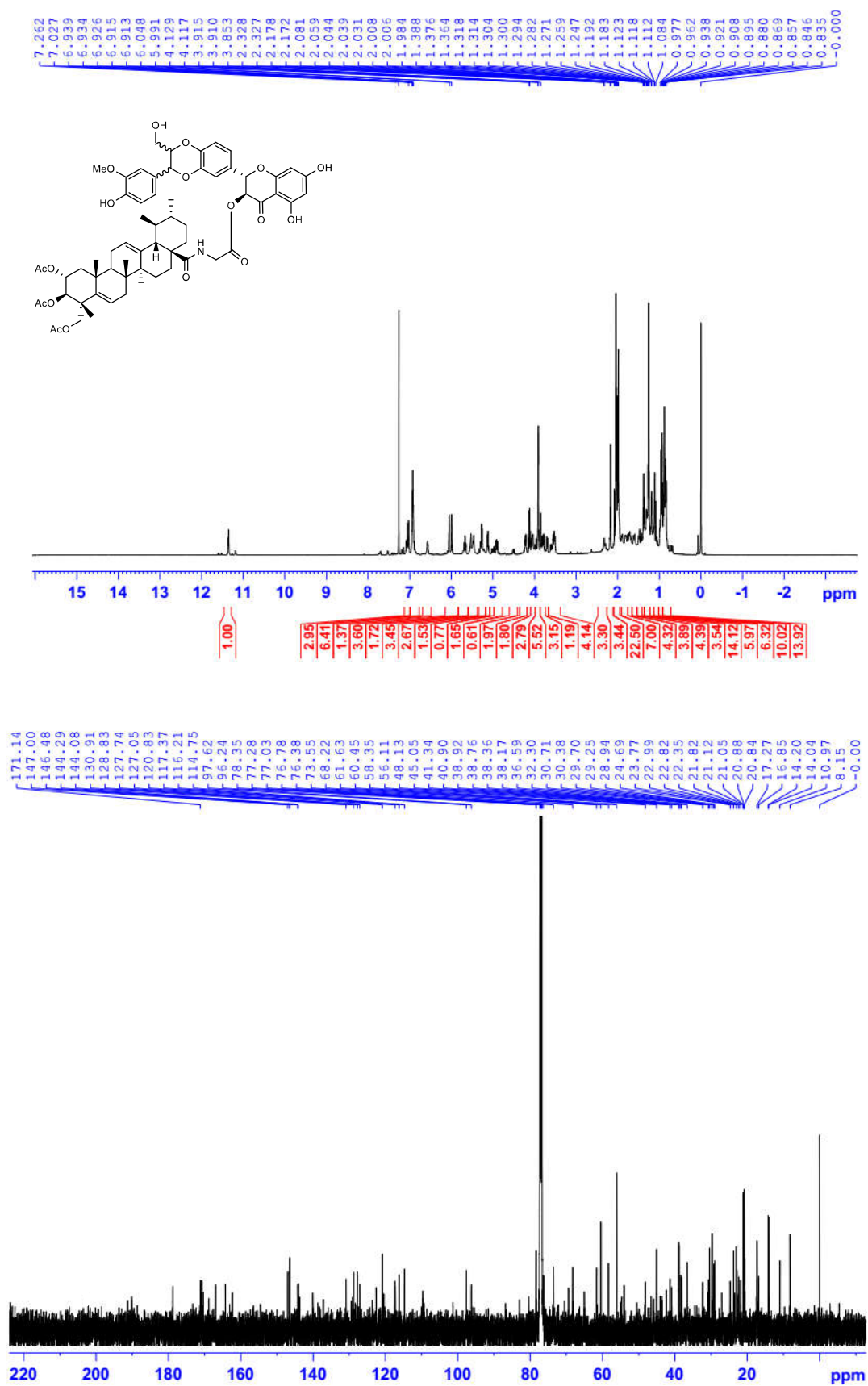


Figure S28. ¹H and ¹³C NMR (CDCl₃, 500 MHz) spectra of compound 15

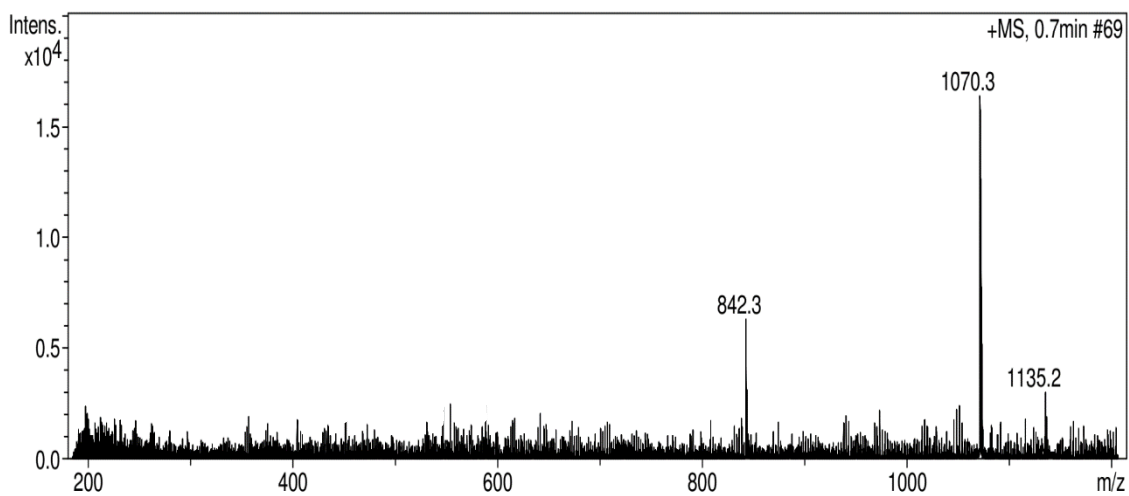
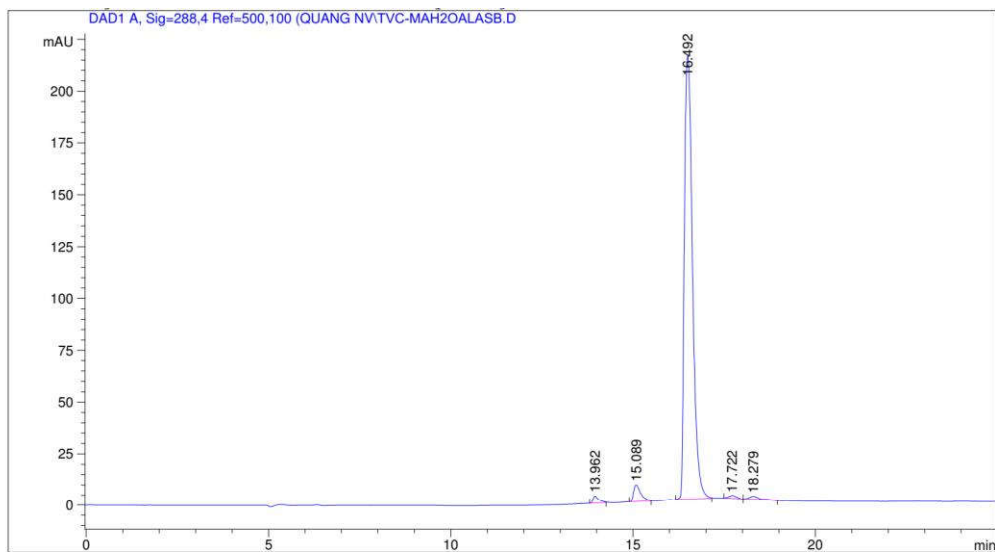


Figure S29. ESI-MS spectrum of compound 15



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 Use Multiplier & Dilution Factor with ISTDs

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2	15.089	BB	0.2027	110.67388	7.26386	3.1445
3	16.492	BB	0.2468	3316.17288	213.93143	94.2195
4	17.722	BV	0.2370	23.55582	1.36626	0.6693
5	18.279	VB	0.2751	28.97230	1.56911	0.8232
Totals :				3519.62529	228.70263	

Figure S30. HPLC analysis of compound 15

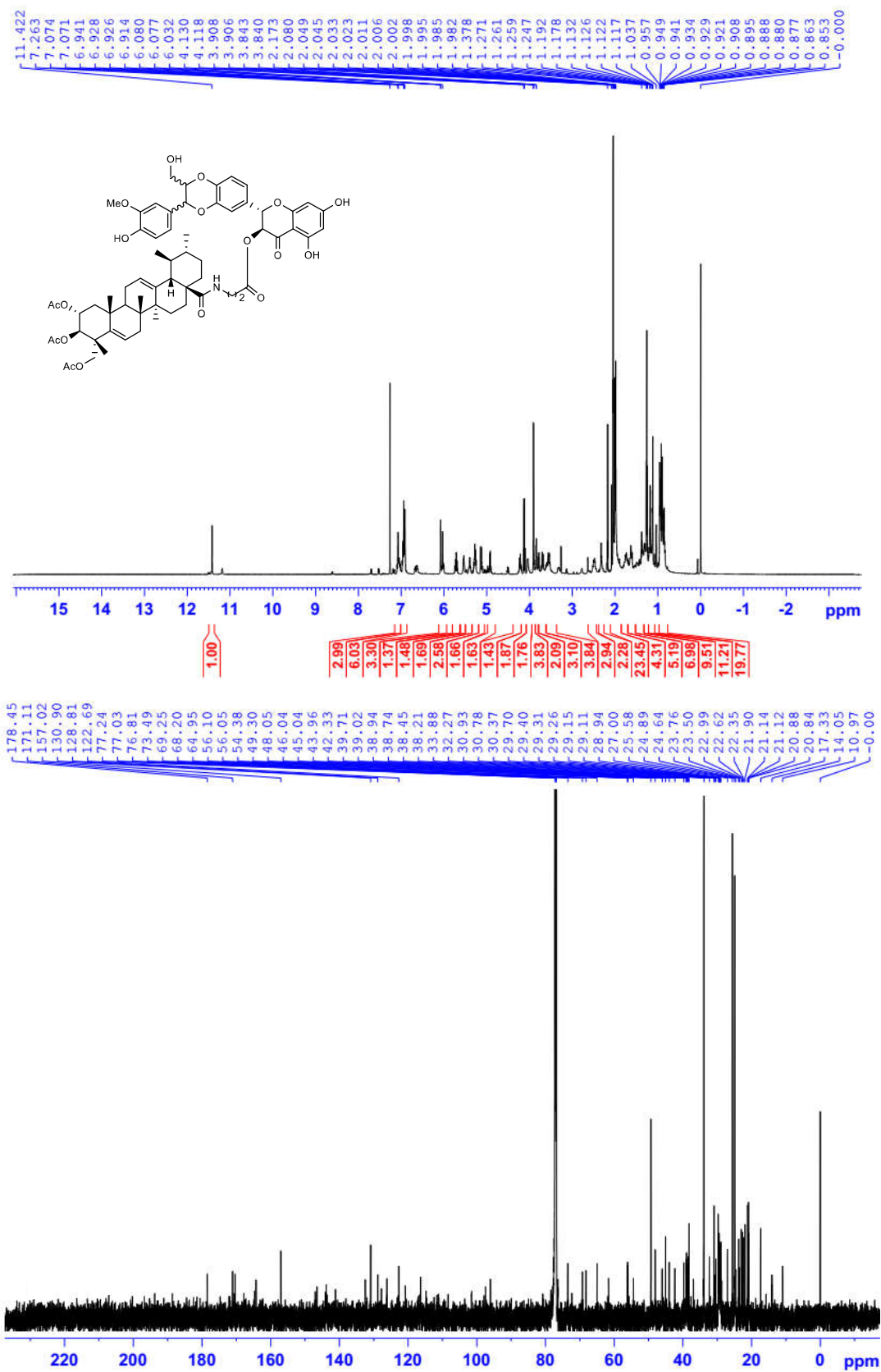


Figure S31. ¹H and ¹³C NMR (CDCl₃, 500 MHz) spectra of compound 16

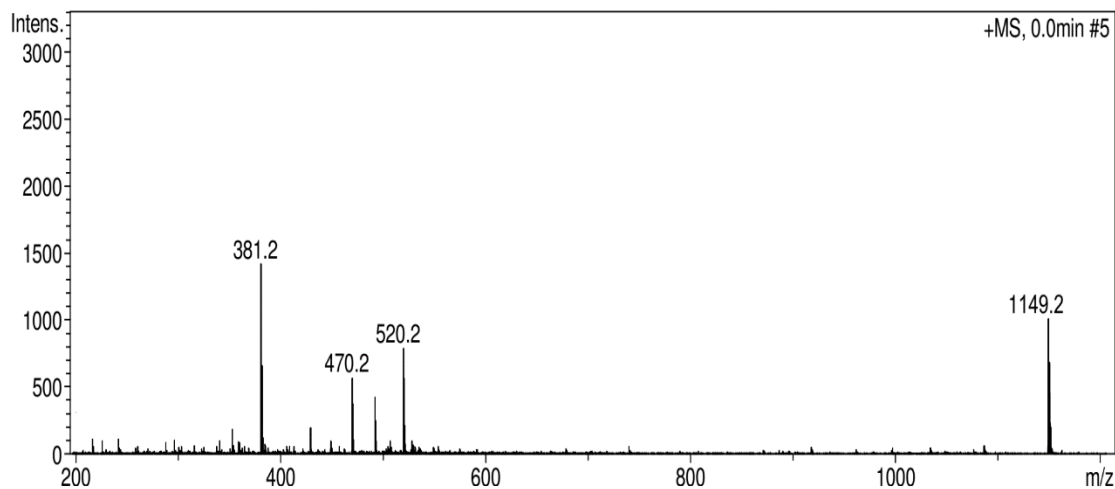
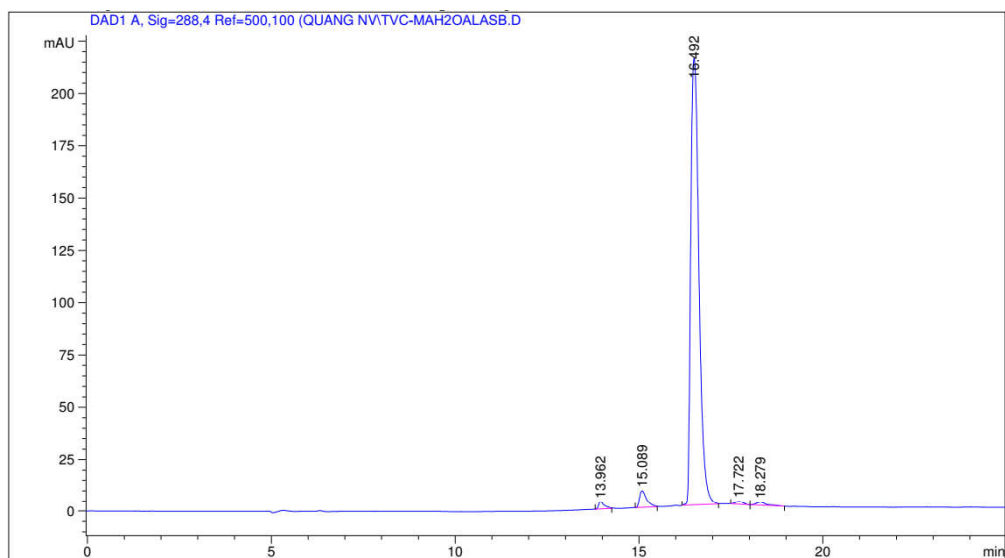


Figure S32. ESI-MS spectrum of compound 16



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 Area Percent Report
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1	13.962	BB	0.1643	40.25041	4.57196	1.1436
2	15.089	BB	0.2027	110.67388	7.26386	3.1445
3	16.492	BB	0.2468	3316.17288	213.93143	94.2195
4	17.722	BV	0.2370	23.55582	1.36626	0.6693
5	18.279	VB	0.2751	28.97230	1.56911	0.8232

Totals : 3519.62529 228.70263

Figure S33. HPLC analysis of compound 16

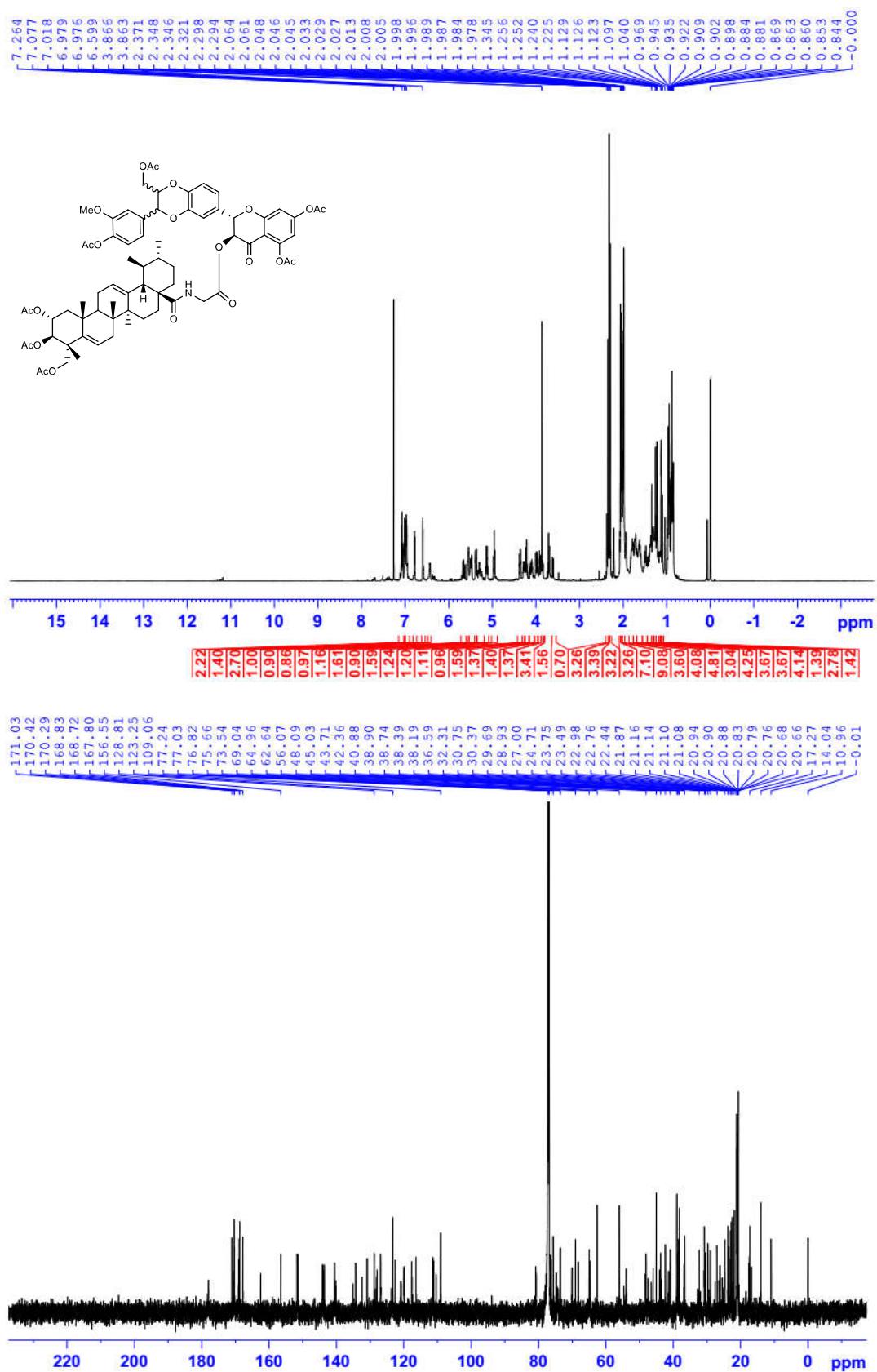


Figure S 34. ¹H and ¹³C NMR (CDCl₃, 500 MHz) spectra of compound 17

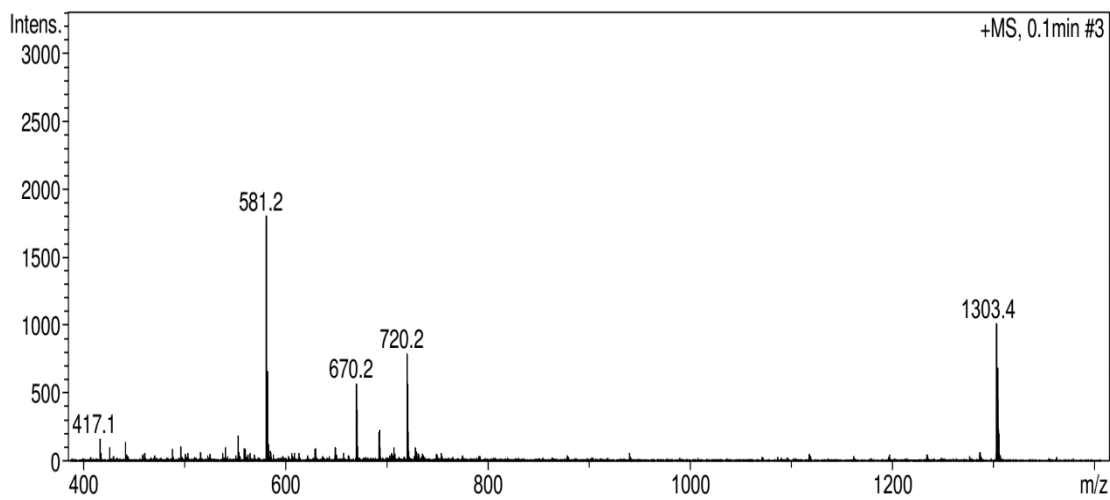
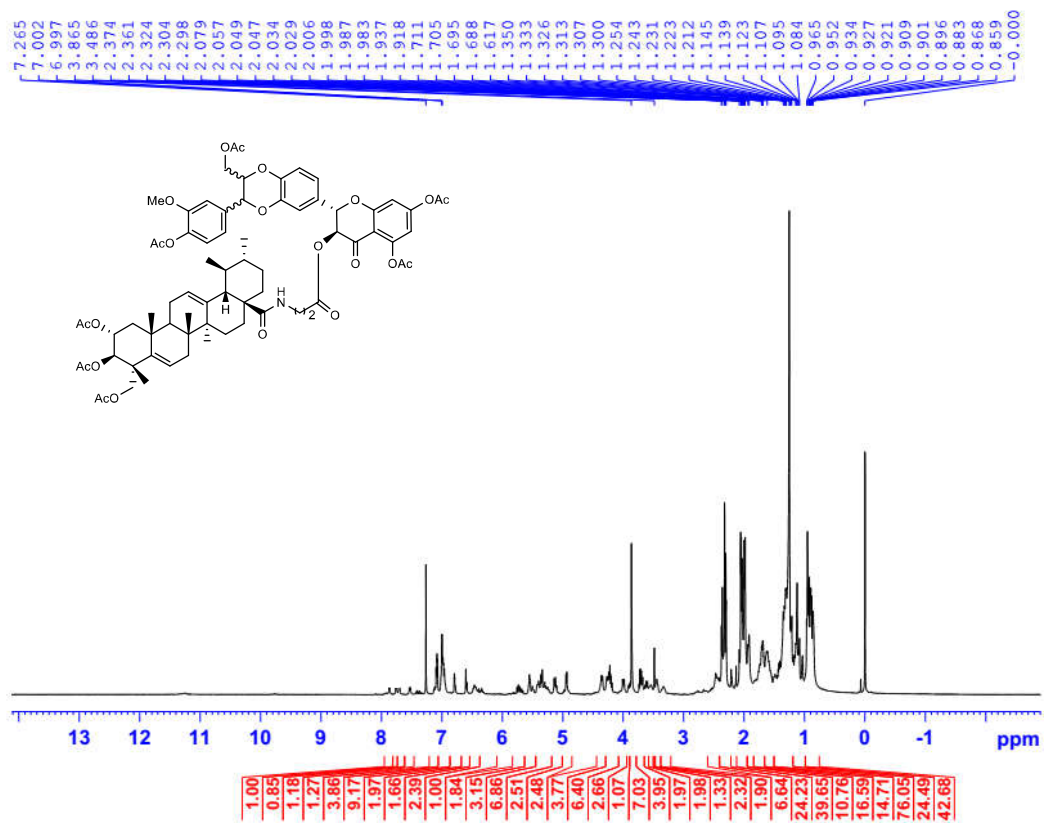


Figure S35. ESI-MS spectrum of compound 17



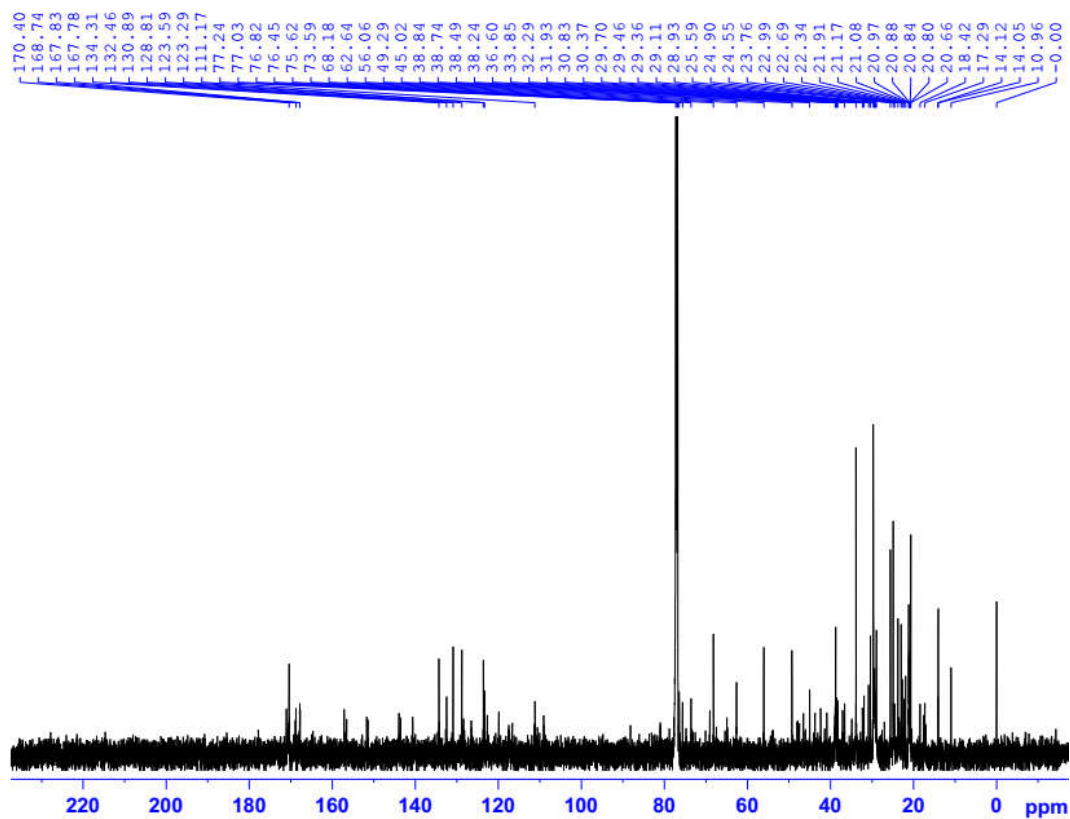


Figure S36. ¹H and ¹³C NMR (CDCl₃, 500 MHz) spectra of compound **18**

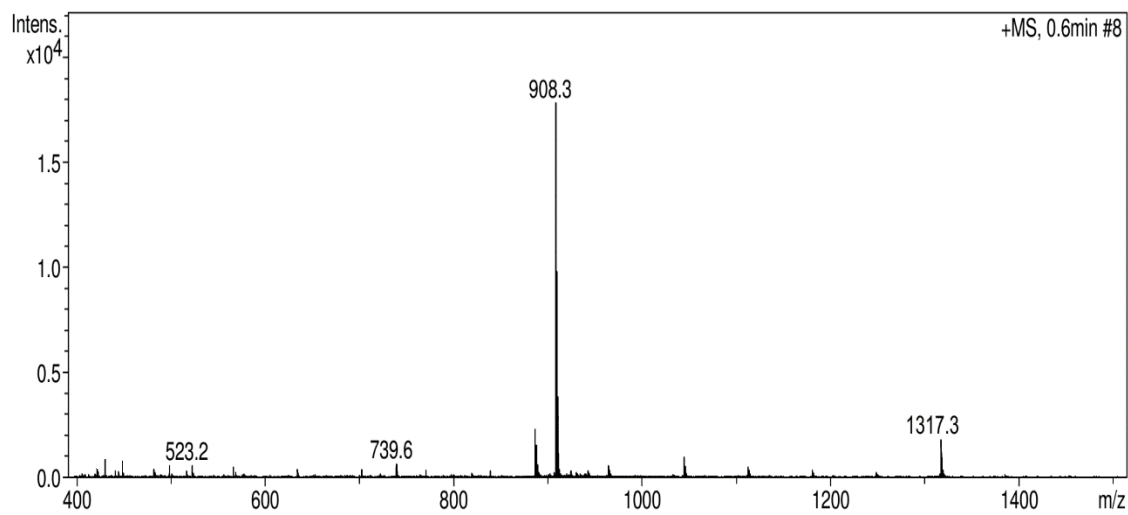


Figure S37. ESI-MS spectrum of compound **18**