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Supporting Information for

Stewartiacids A–N, C-23 carboxylated triterpenoids from the Chinese Stewartia and their inhibitory effects against ATP-citrate lyase and NF-*κ*B

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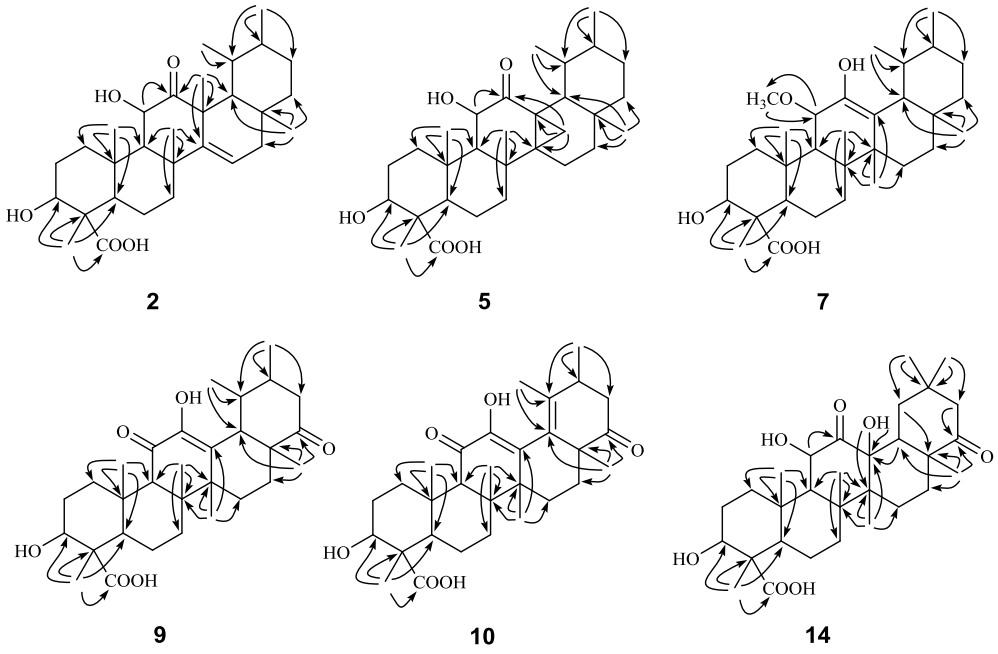


Fig. S1. HMBC correlations of compounds **2**, **5**, **7**, **9**, **10**, and **14**.

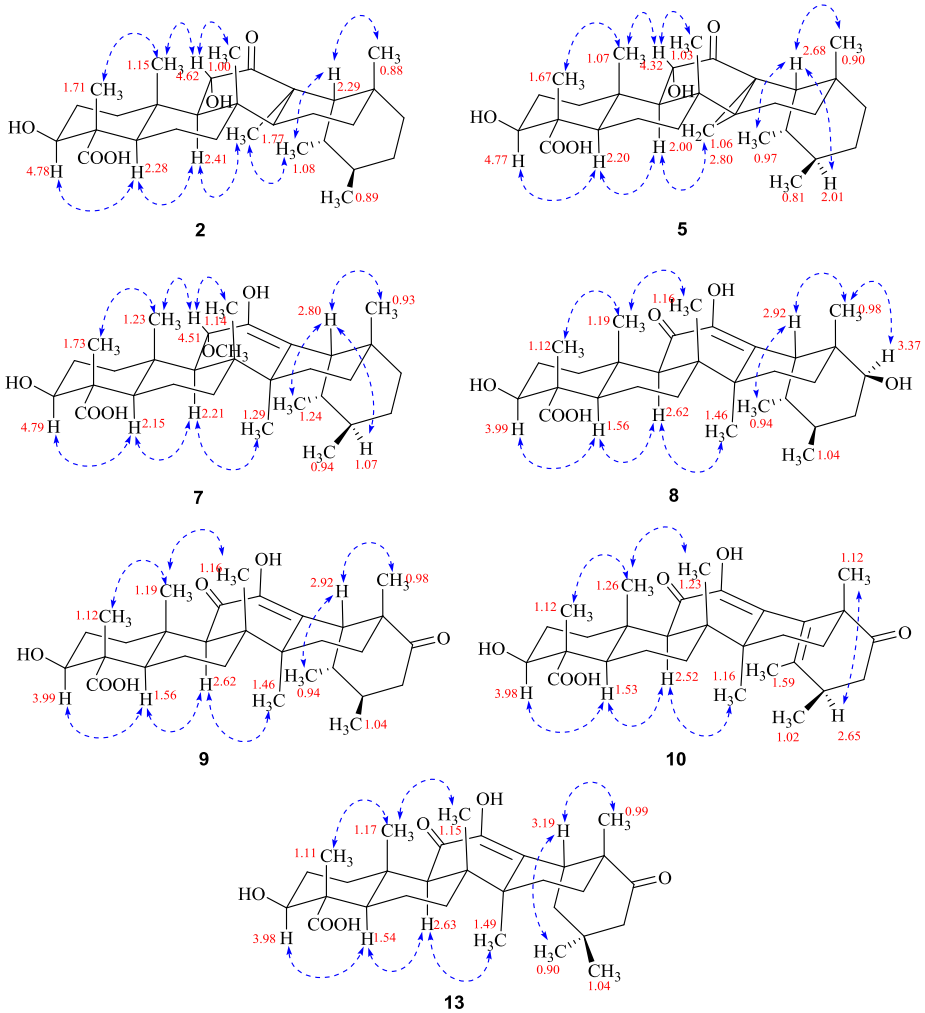


Fig.S2. Diagnostic ROE correlations of compounds **2**, **5**, **7**−**10**, and **13**.

Fig. S3. ^{1}H NMR spectrum of compound **1** in CD_3OD (400 MHz).

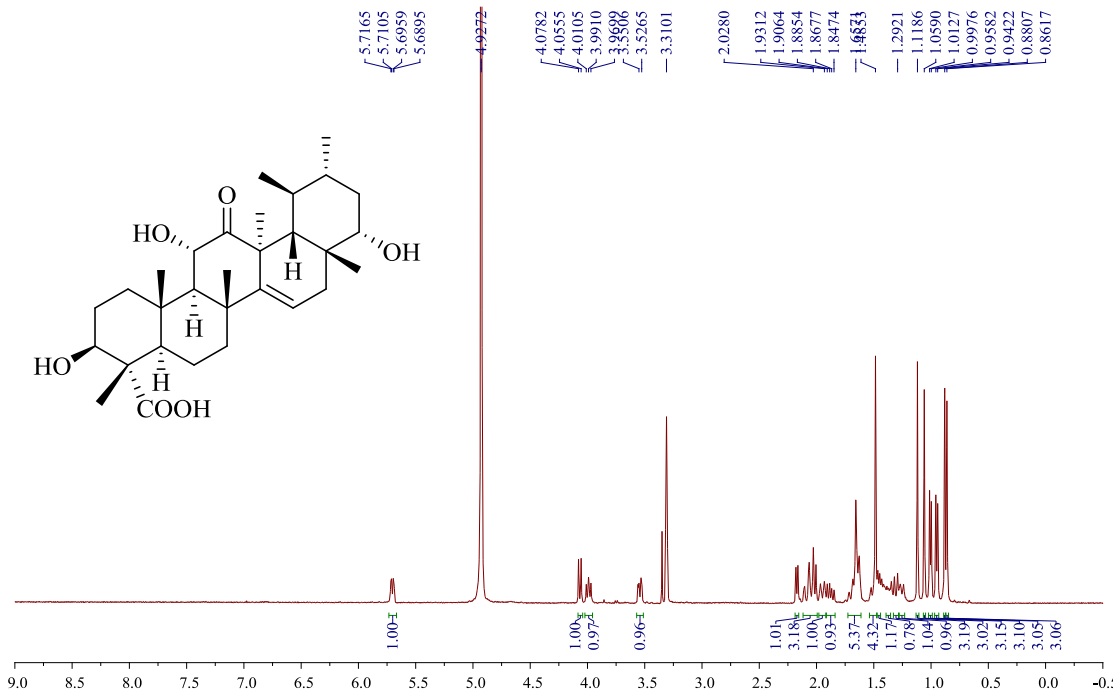


Fig. S4. ^{1}H NMR spectrum of compound **1** in CD_3OD–expansion.

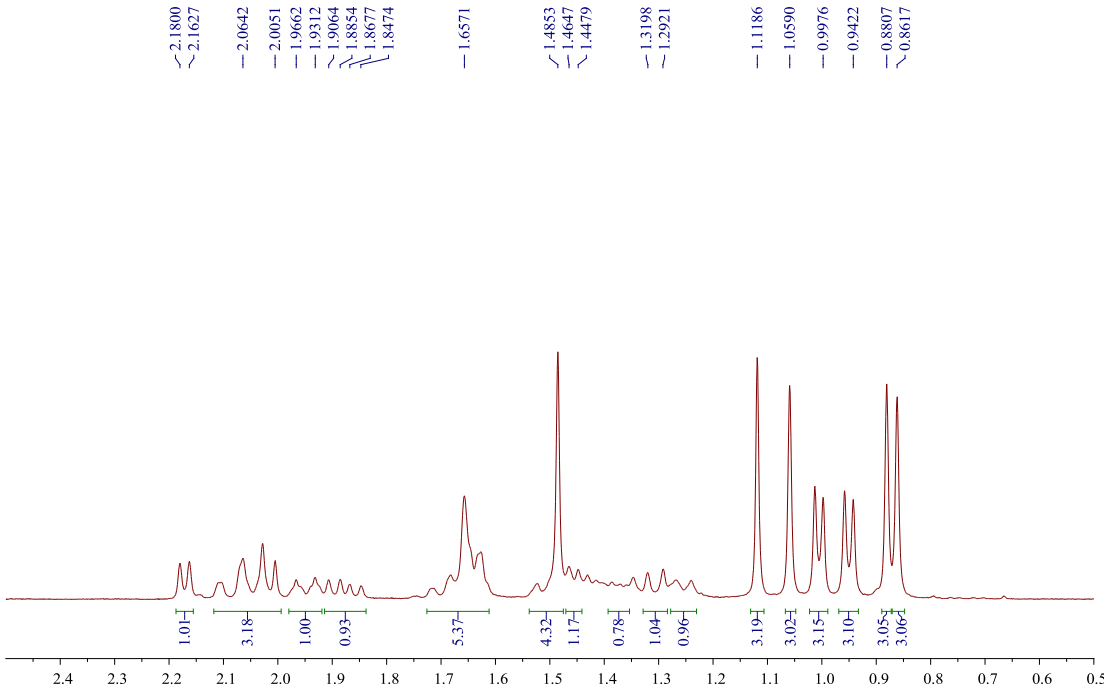


Fig. S5. ^{13}C NMR and DEPT 135 spectra of compound **1** in CD_3OD (150 MHz).

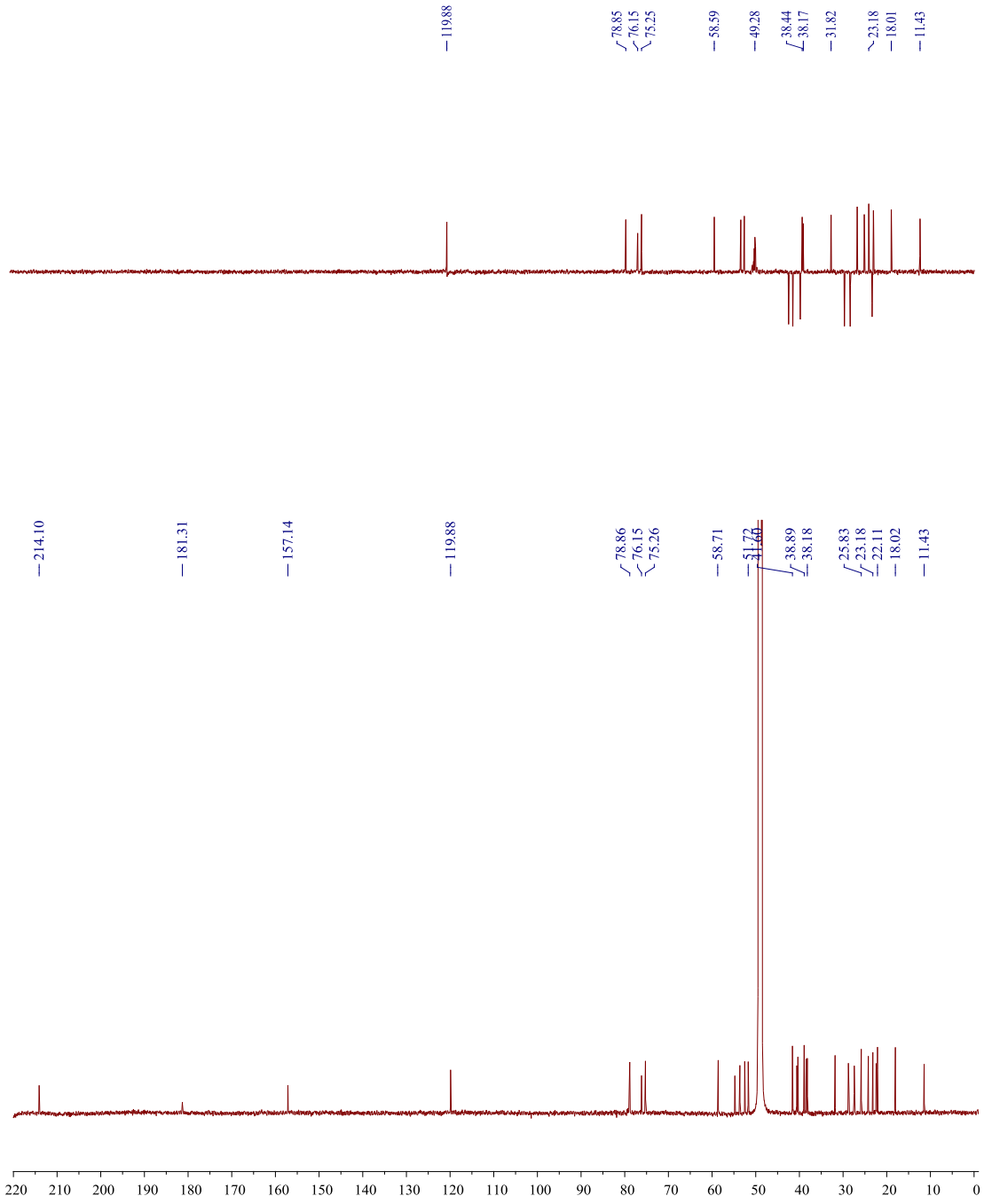


Fig. S6. ^{1}H-^{1}H COSY spectrum of compound **1** in CD_3OD (600 MHz).

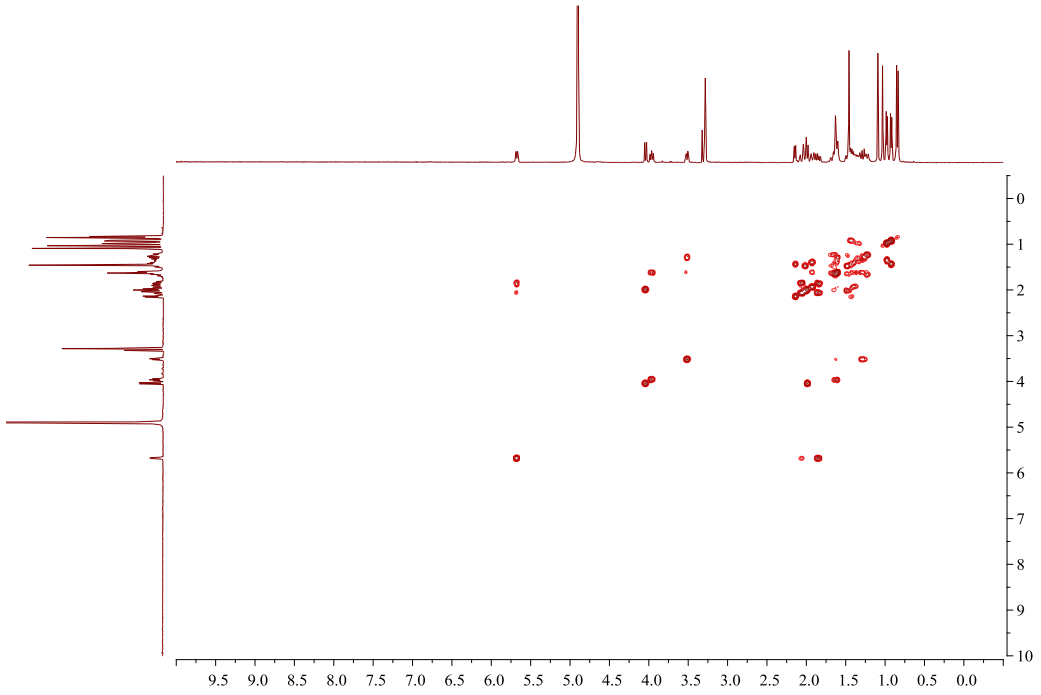


Fig. S7. ^{1}H-^{1}H COSY spectrum of compound **1**-expansion.

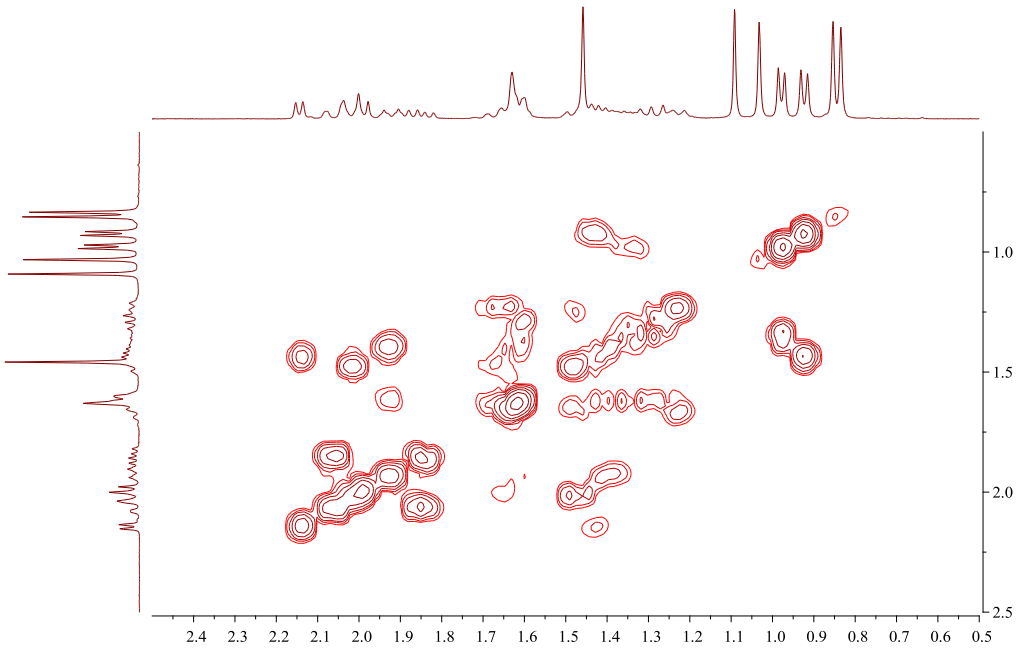


Fig. S8. HMBC spectrum of compound **1** in CD_3OD (600 MHz).

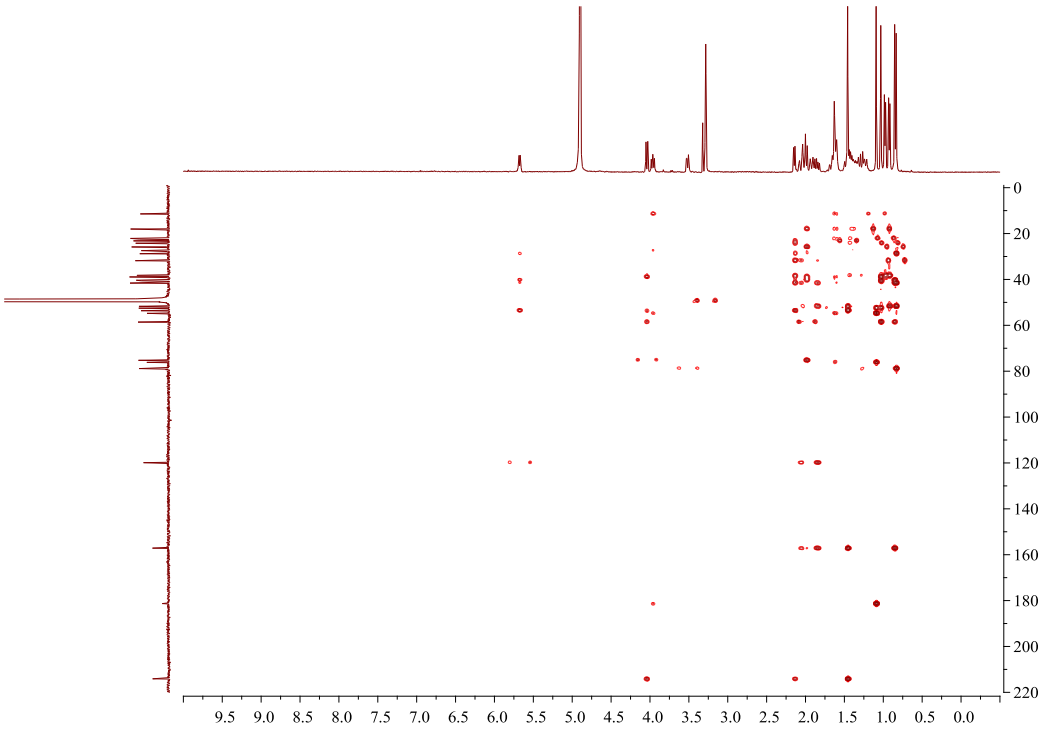


Fig. S9. HMBC spectrum of compound **1**-expansion.

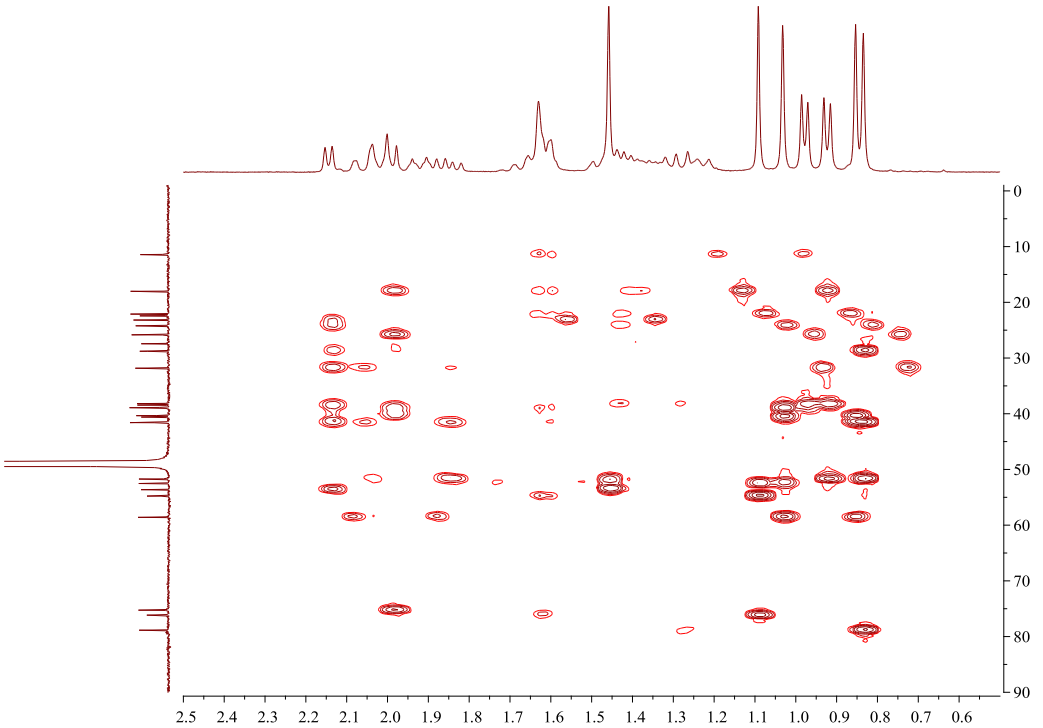


Fig. S10. ^{1}H NMR spectrum of compound **1** in C_5D_5N (600 MHz).

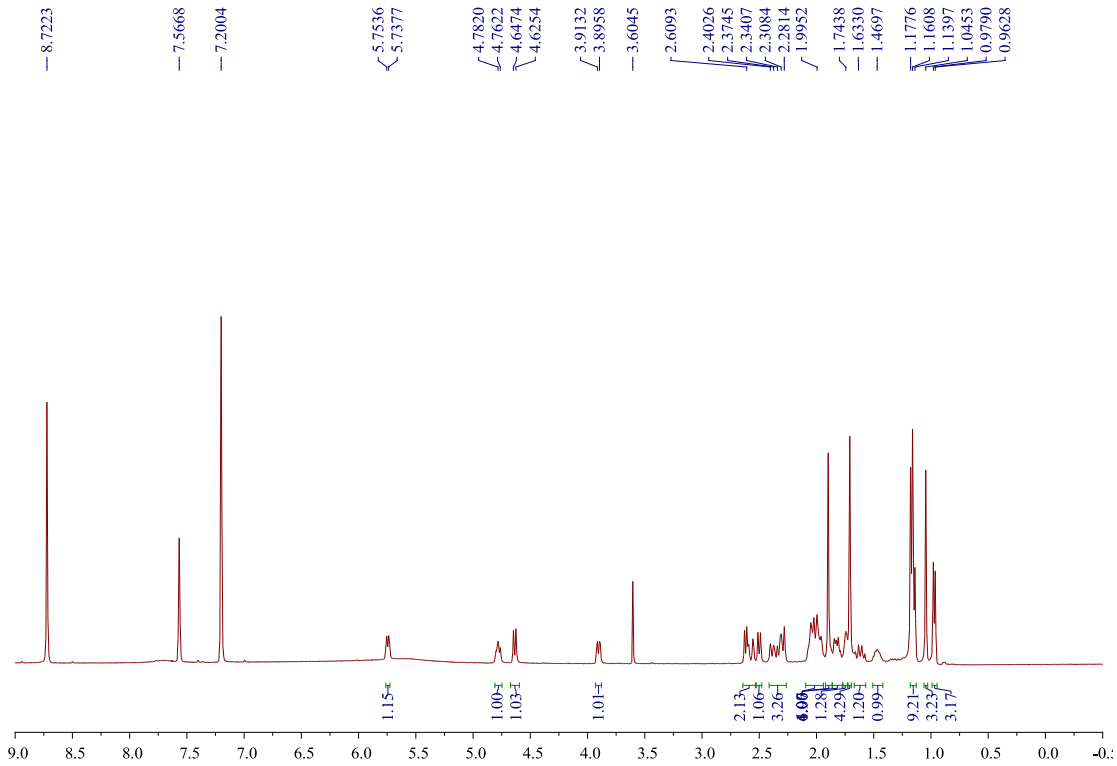


Fig. S11. ROESY spectrum of compound **1** inC_5D_5N (600 MHz).

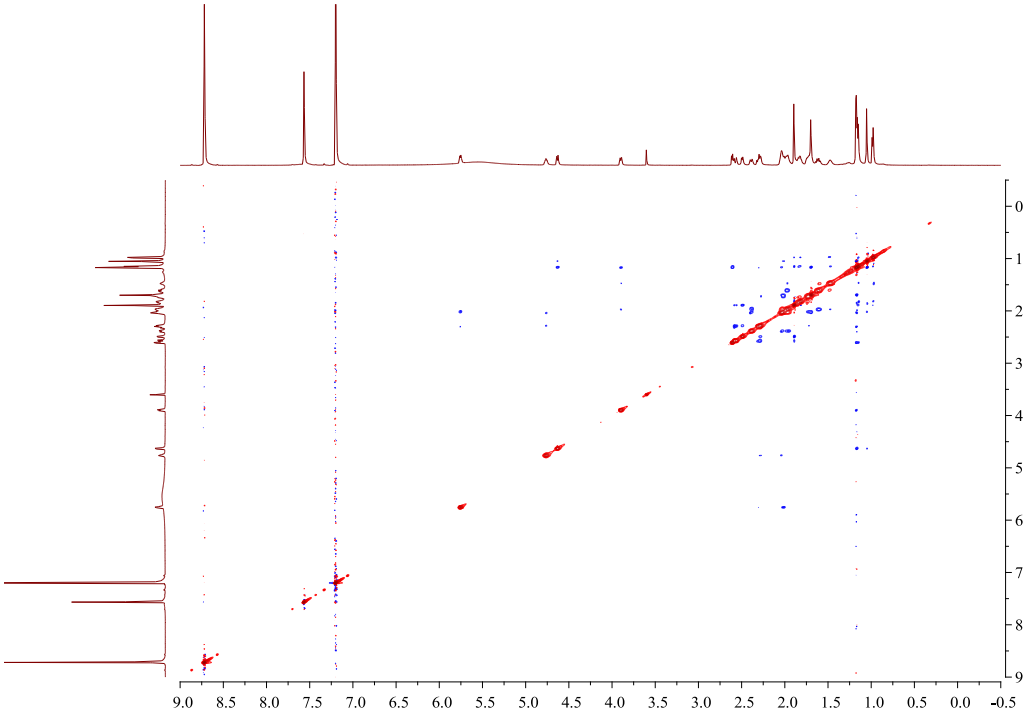


Fig. S12. ROESY spectrum of compound **1**–expansion.

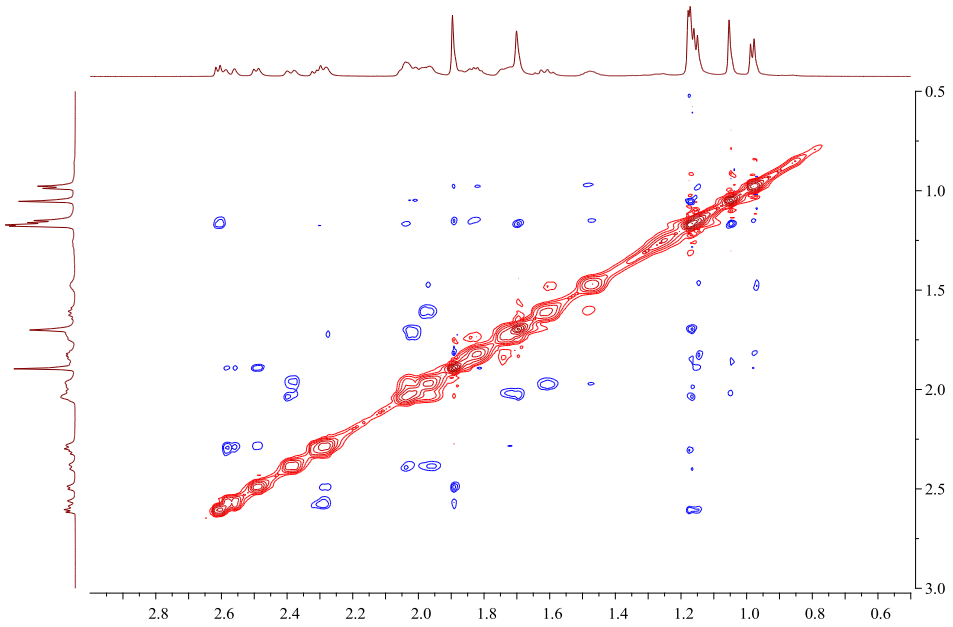


Fig. S13. HRESIMS report of compound **1**.

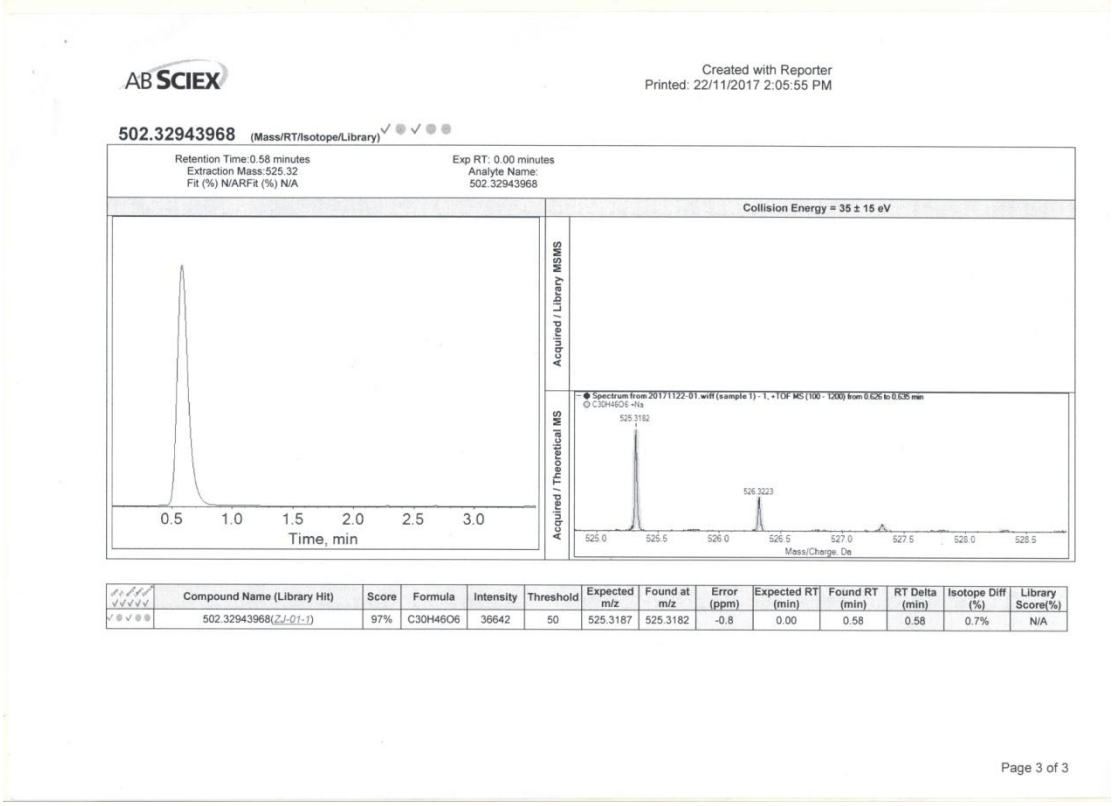


Fig. S14. ^{1}H NMR spectrum of compound **2** in C_5D_5N (400 MHz).

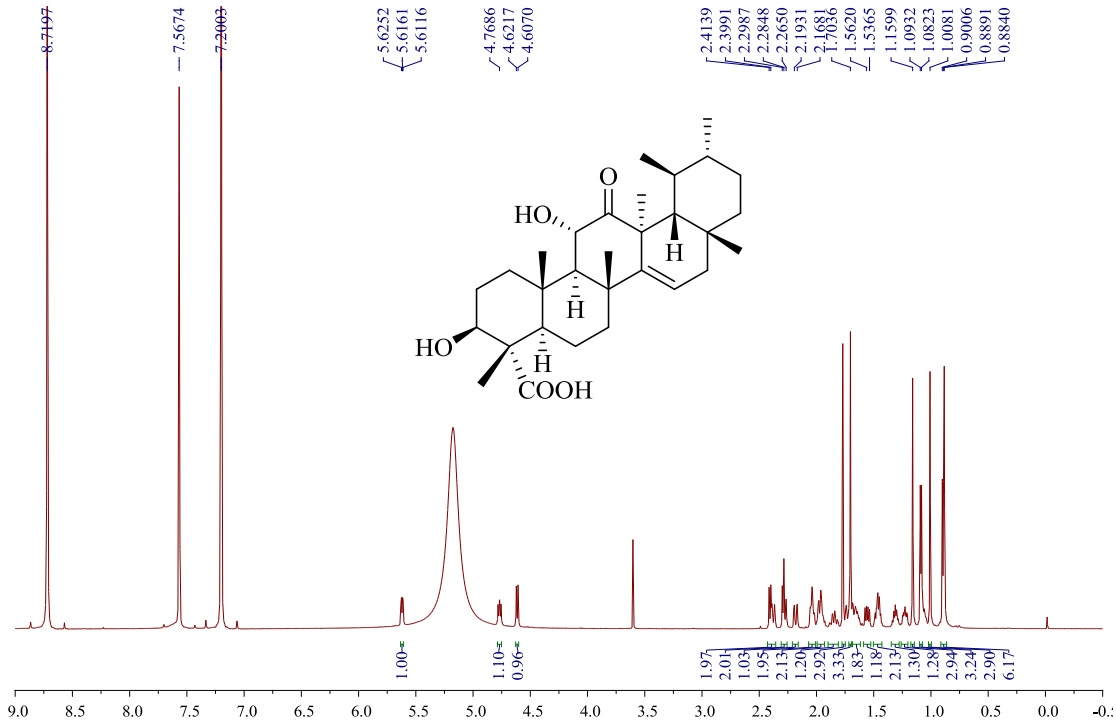


Fig. S15. ^{1}H NMR spectrum of compound **2**-expansion.

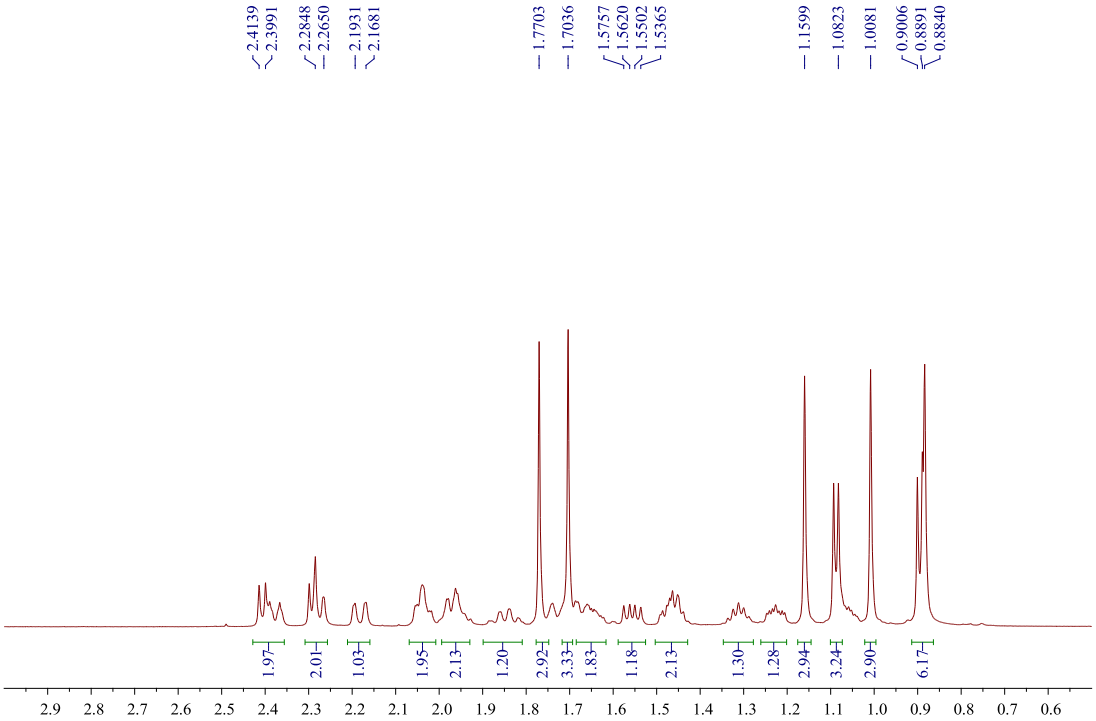


Fig. S16. ^{13}C NMR spectrum of compound **2** in C_5D_5N (150 MHz).

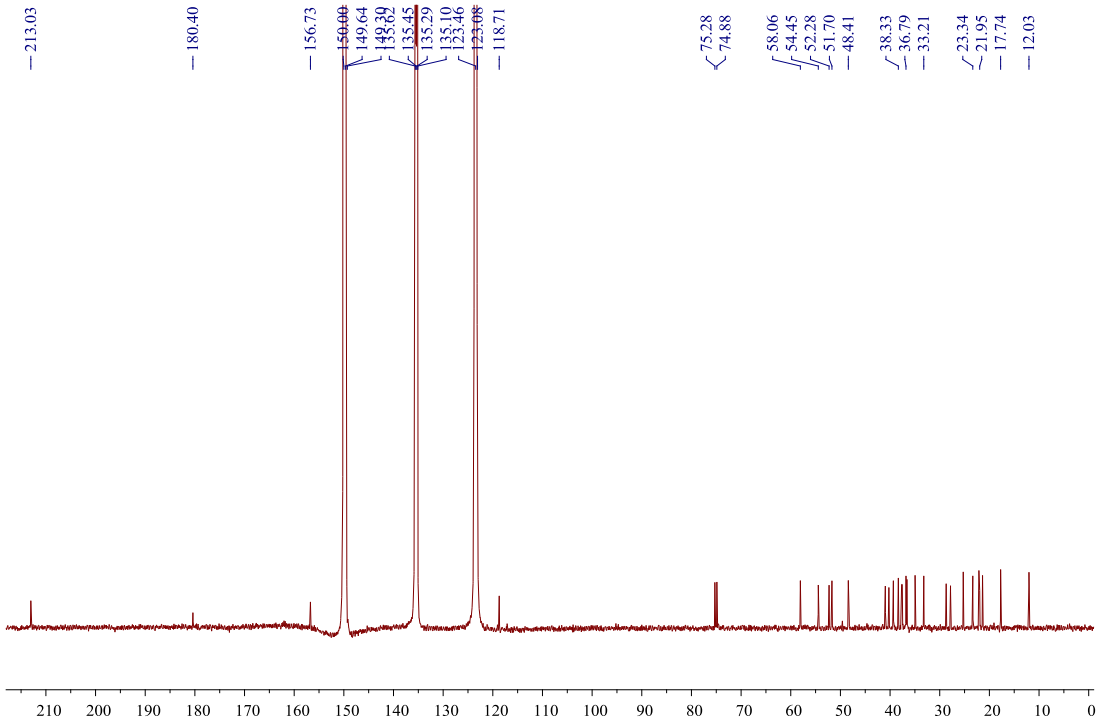


Fig. S17. ^{13}C NMR spectrum of compound **2** –expansion.

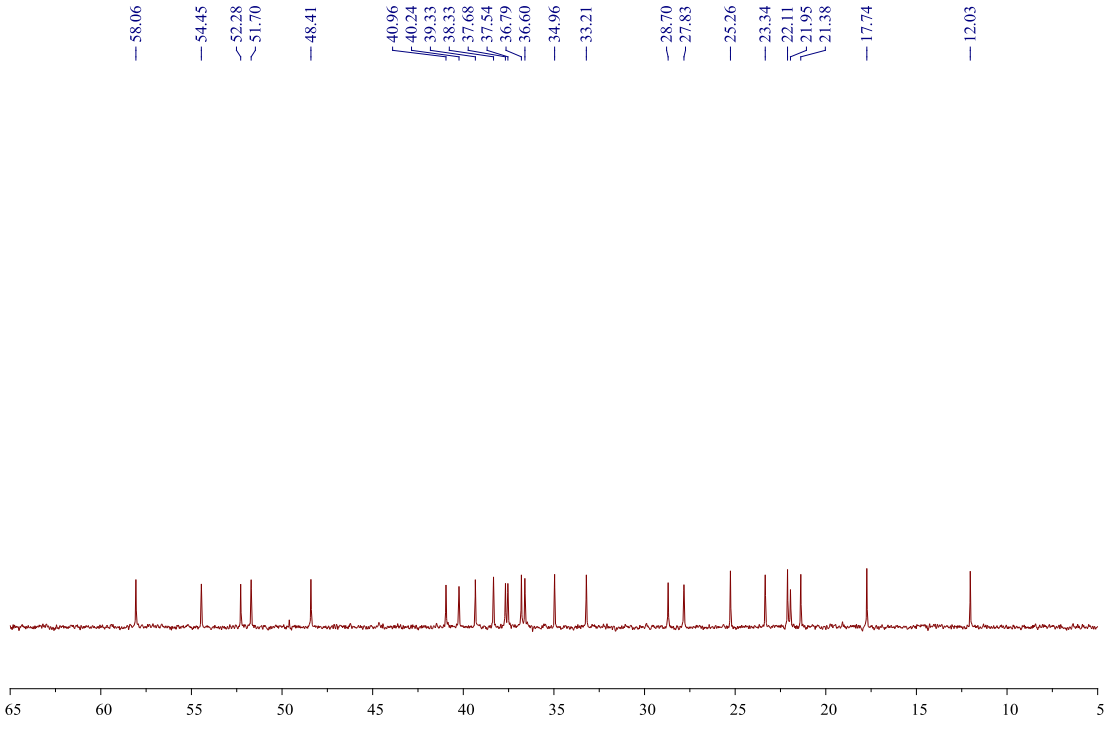


Fig. S18. HMBC spectrum of compound **2** in C_5D_5N (600 MHz).

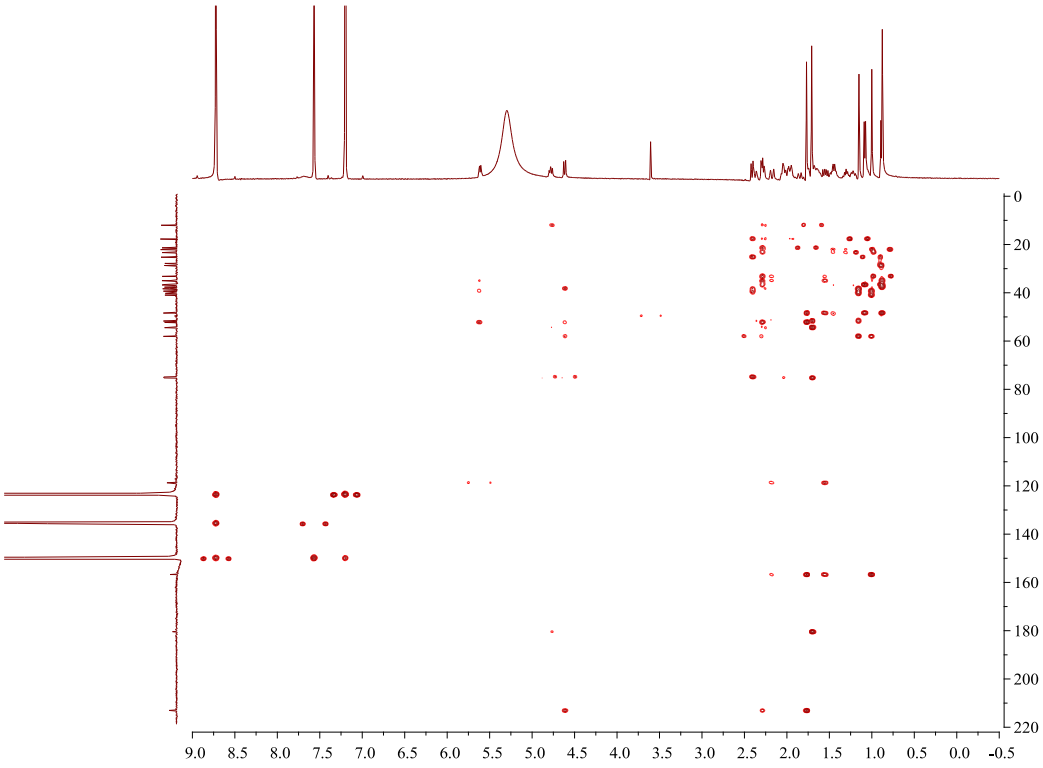


Fig. S19. HMBC spectrum of compound **2**-expansion.

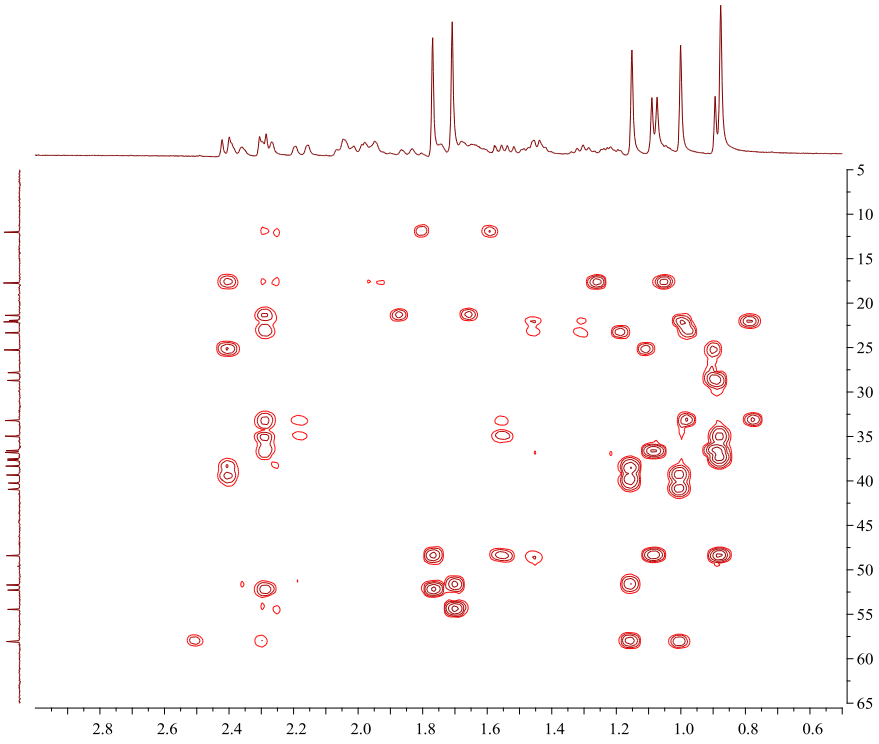


Fig. S20. ROESY spectrum of compound **2** in C_5D_5N (600 MHz).

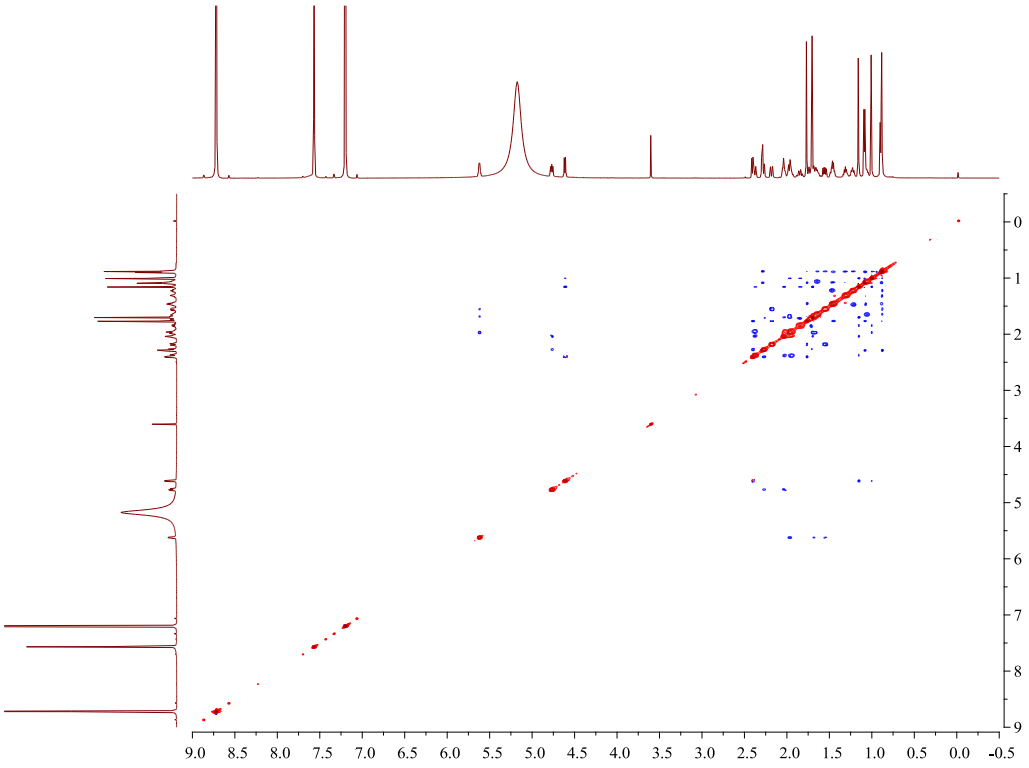


Fig. S21. ROESY spectrum of compound **2**-expansion.

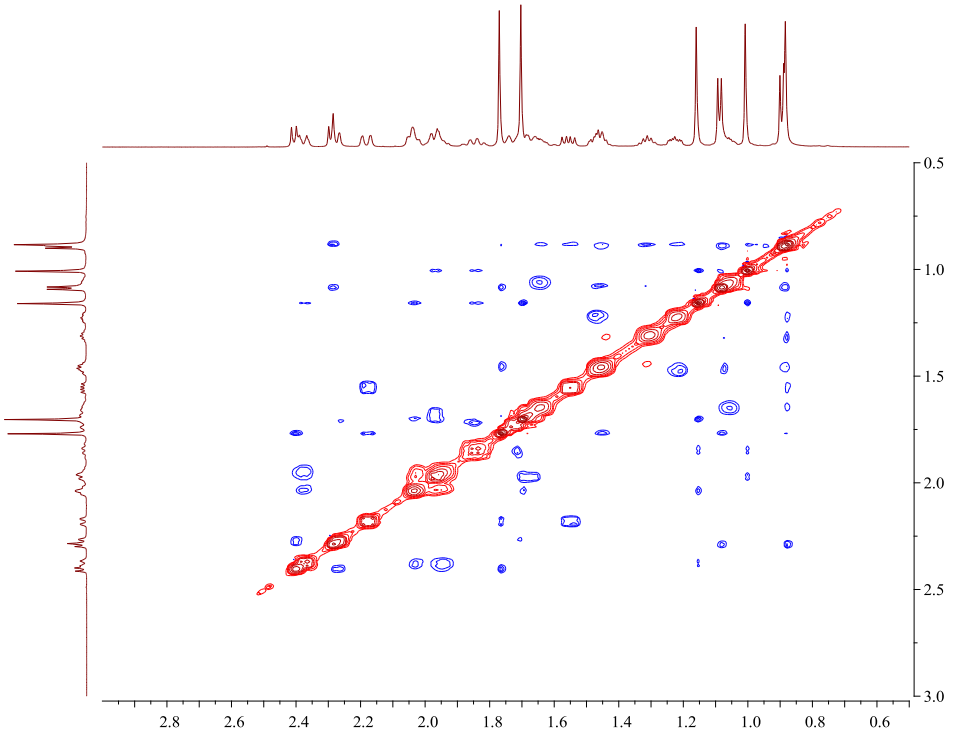


Fig. S22. HRESIMS report of compound **2**.

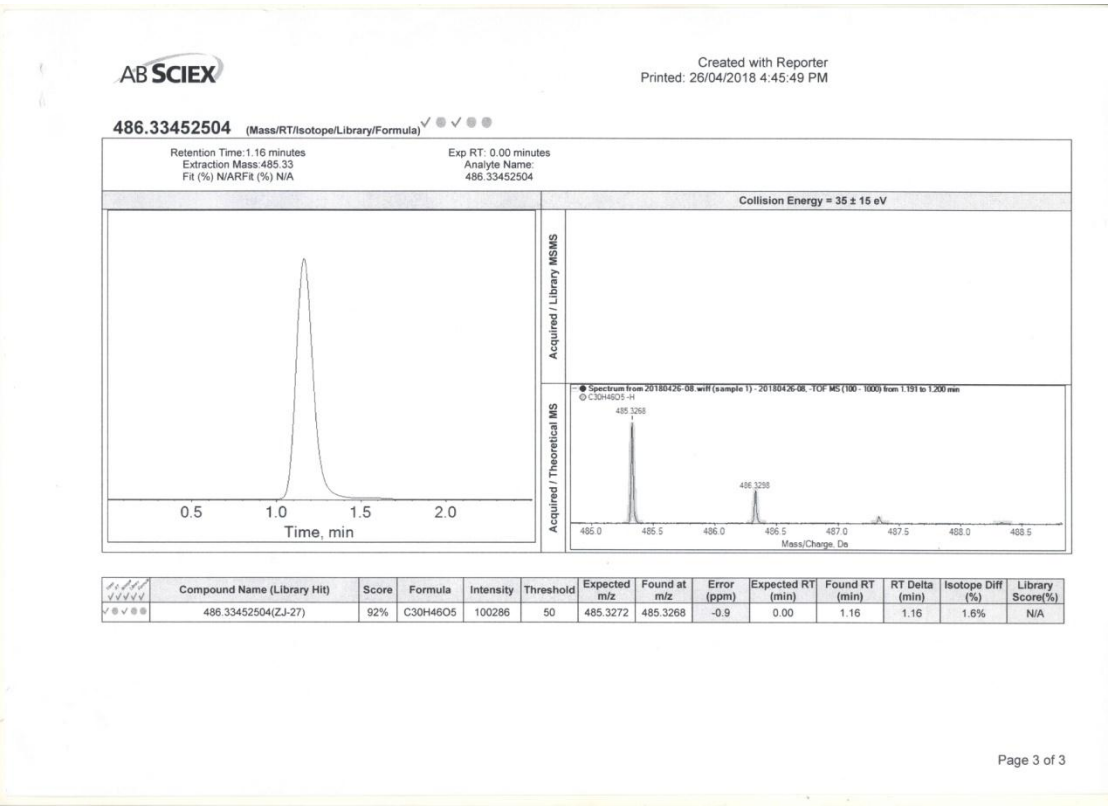


Fig. S23. Experimental ECD spectra of **1** (red curve) and **2** (black curve) in MeOH.

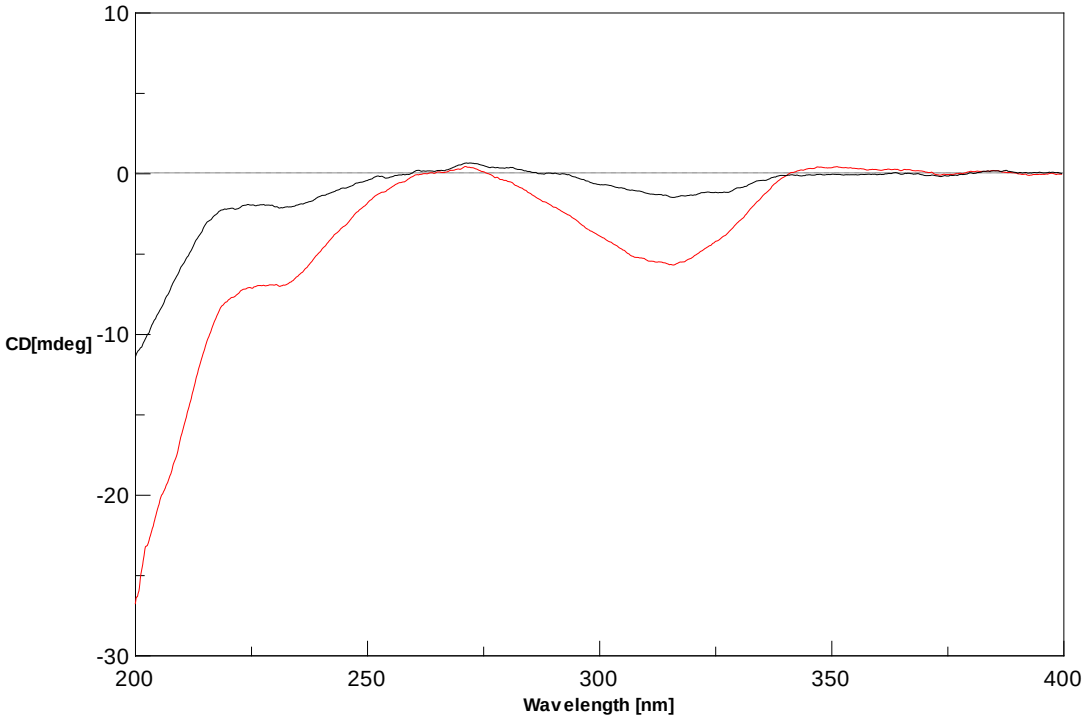


Fig. S24. ^{1}H NMR spectrum of compound **3** in CD_3OD (400 MHz).

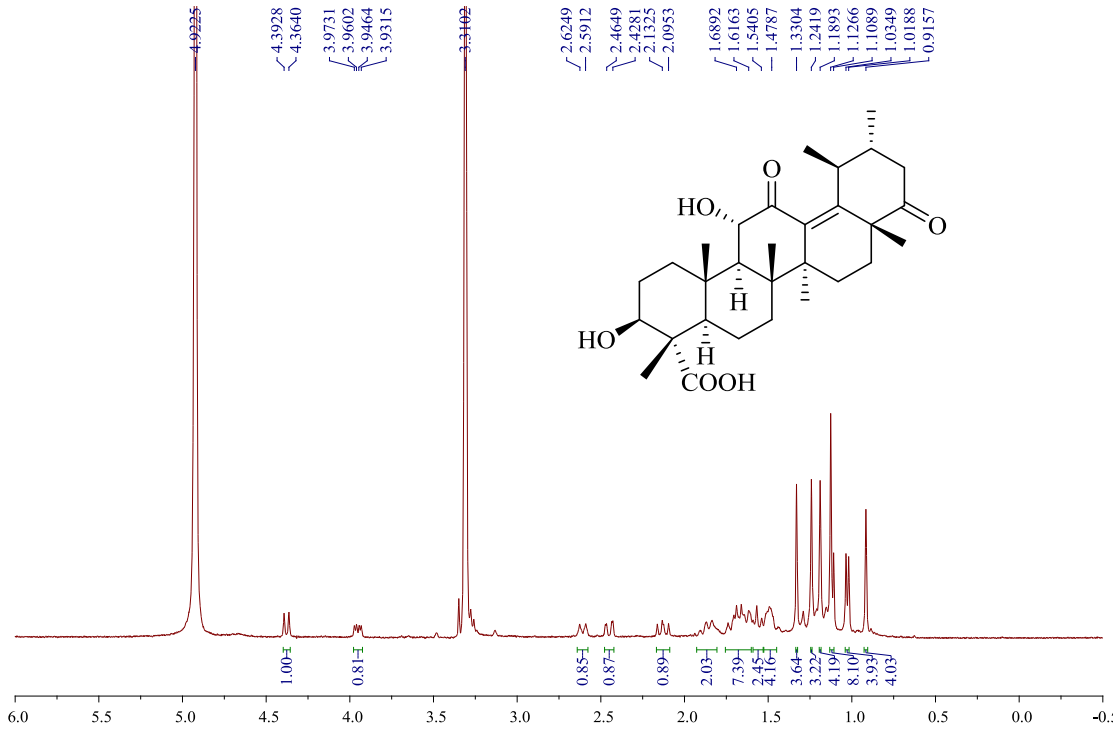


Fig. S25. ^{1}H NMR spectrum of compound **3**–expansion.

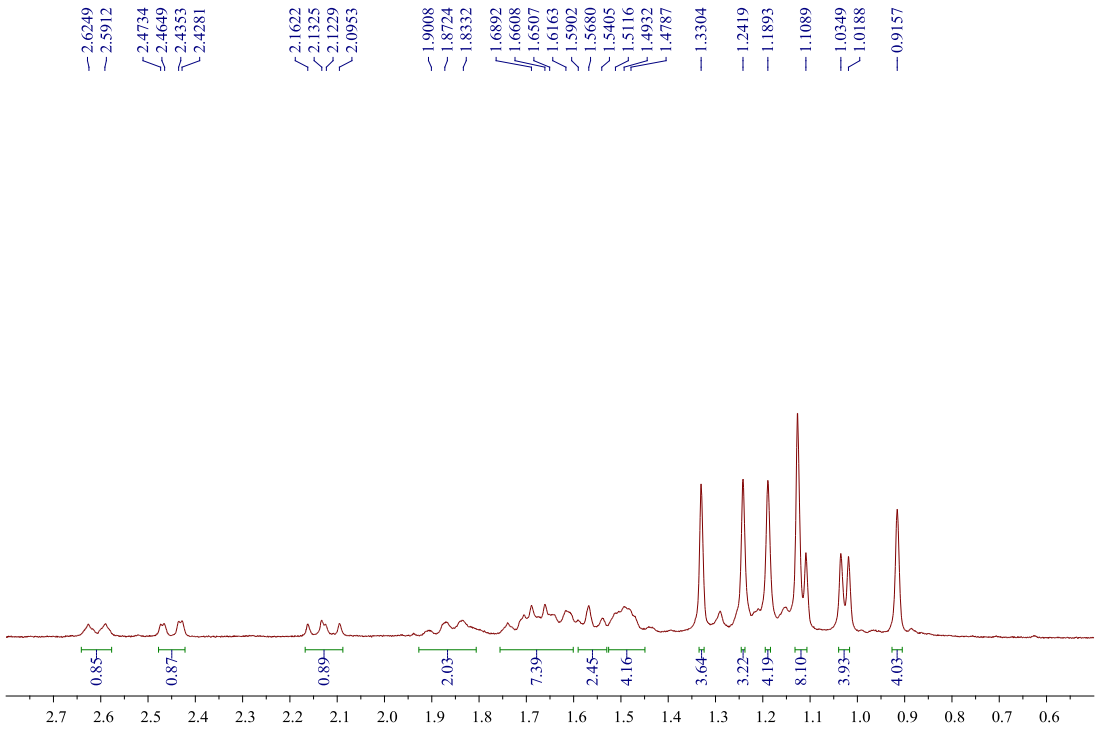


Fig. S26. ^{13}C NMR spectrum of compound **3** in CD_3OD (150 MHz).

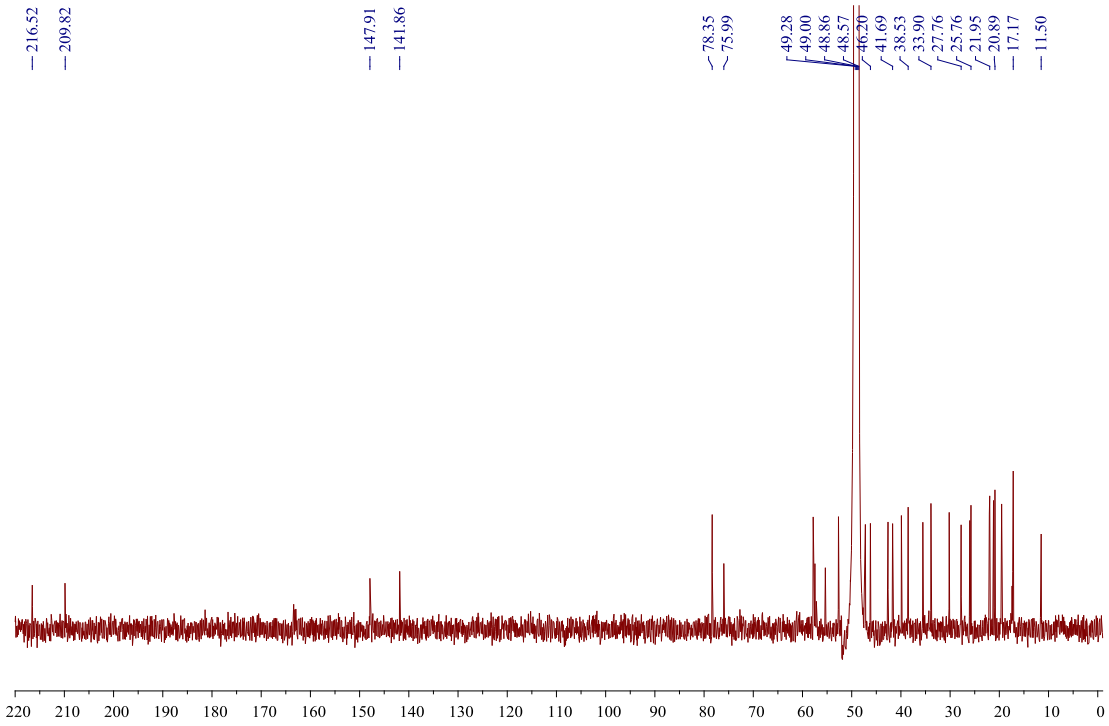


Fig. S27. ^{13}C NMR spectrum of compound **3**-expansion.

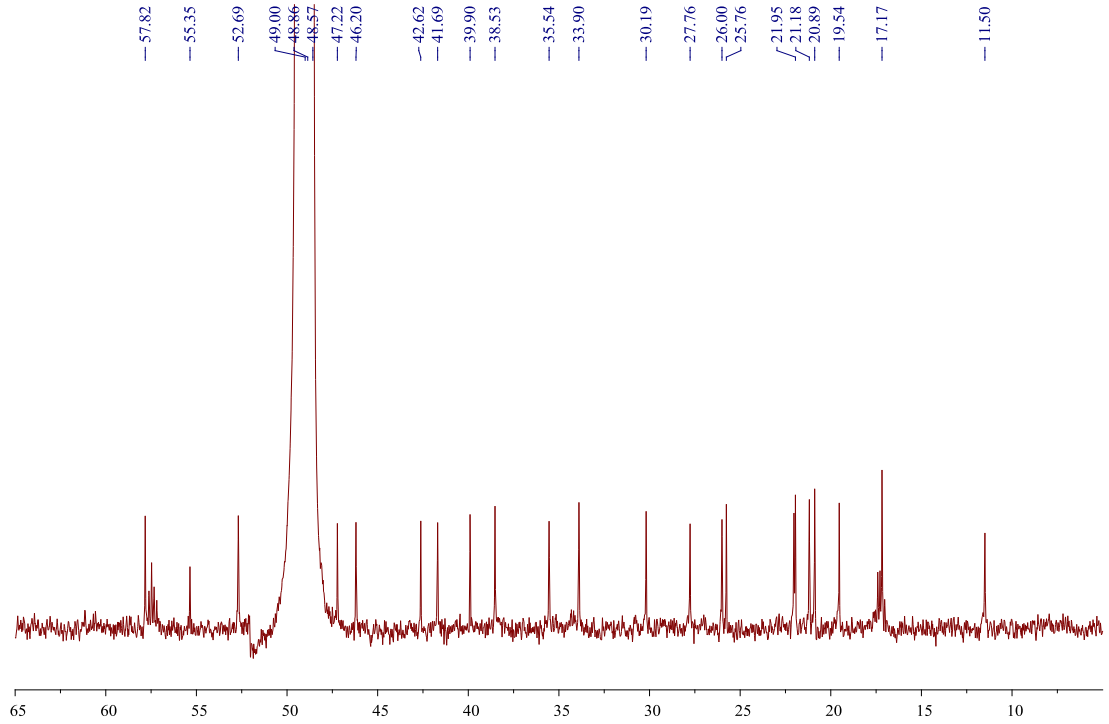


Fig. S28. HMBC spectrum of compound **3** in CD_3OD (600 MHz).

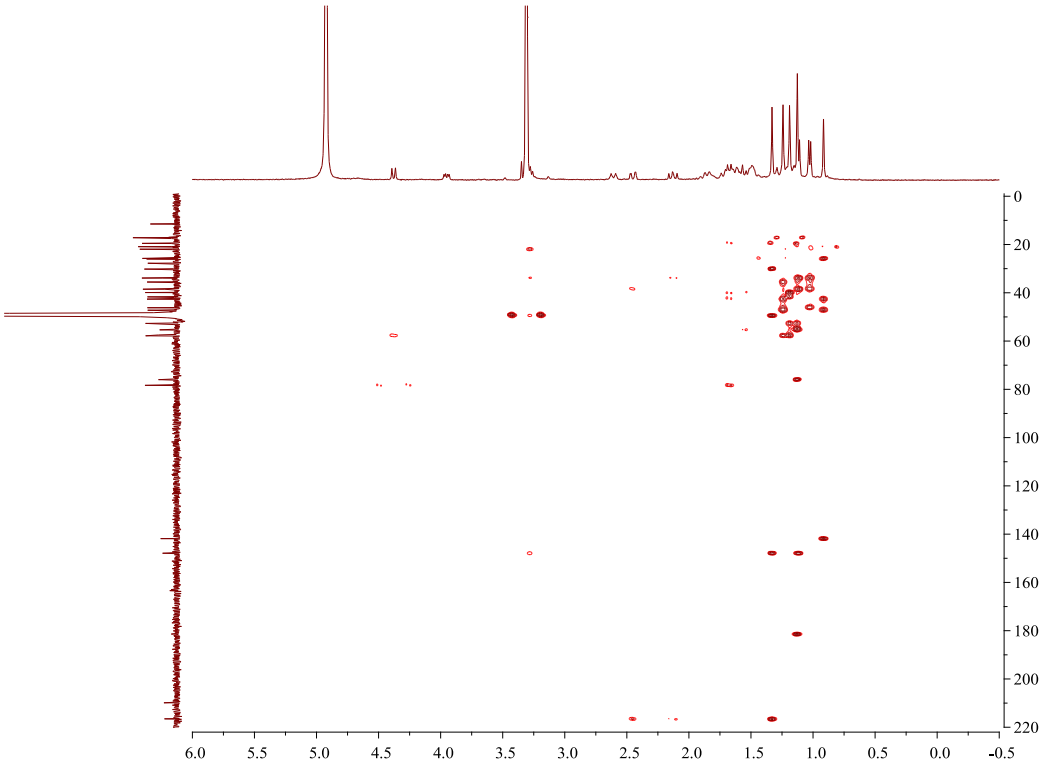


Fig. S29. HMBC spectrum of compound **3**–expansion.

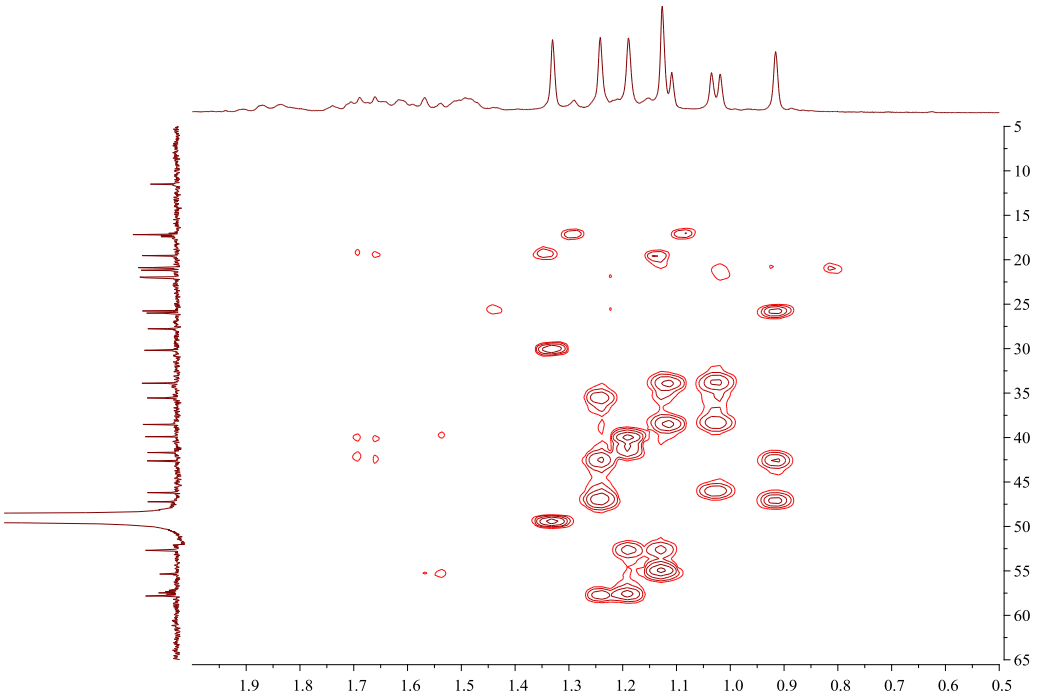


Fig. S30. ROESY spectrum of compound **3** in CD_3OD (600 MHz).

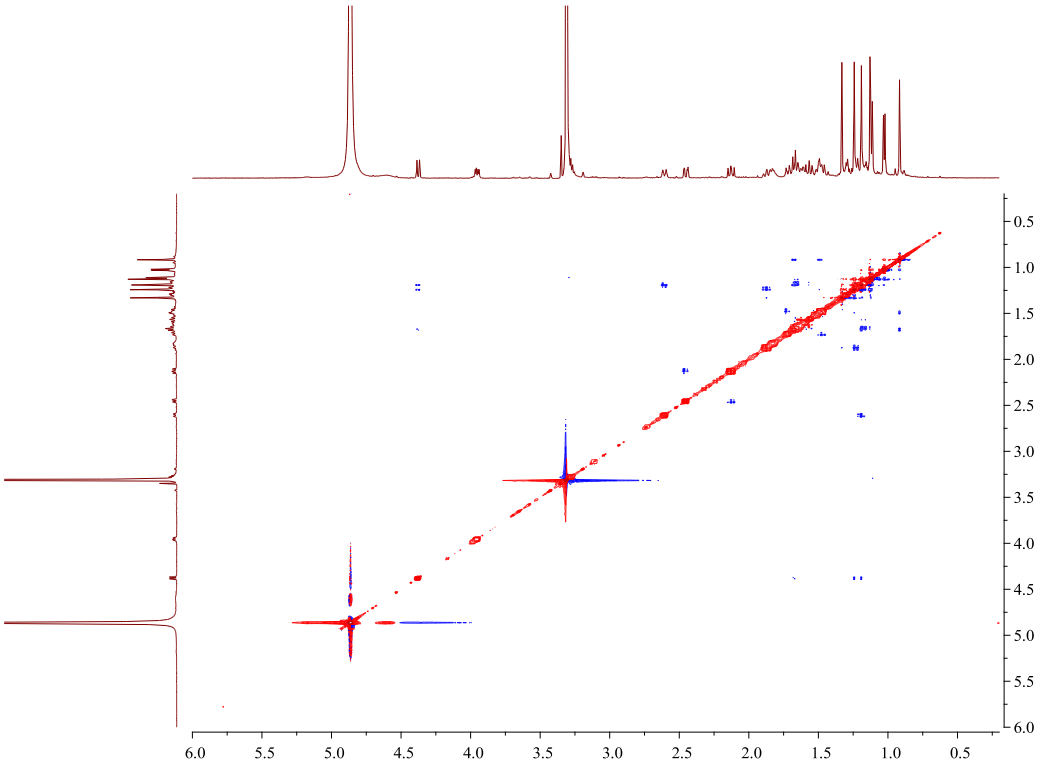


Fig. S31. HRESIMS report of compound **3**.

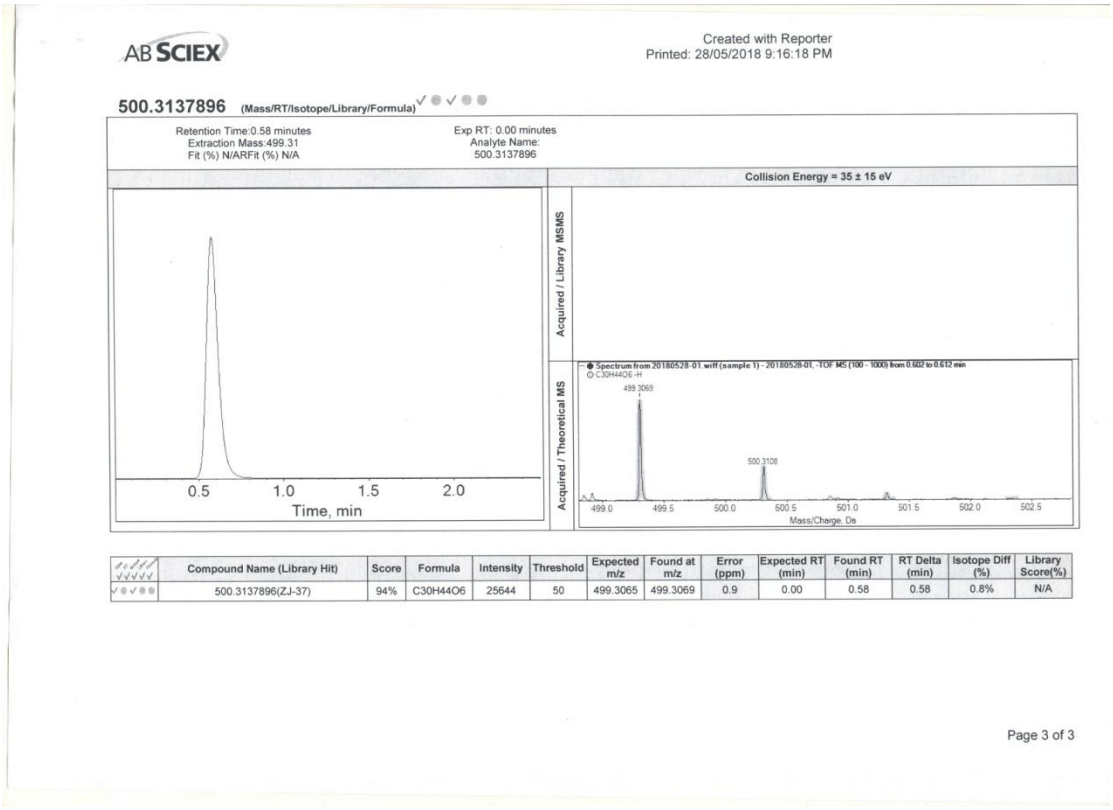


Fig. S32. Experimental ECD spectrum of **3** in MeOH.

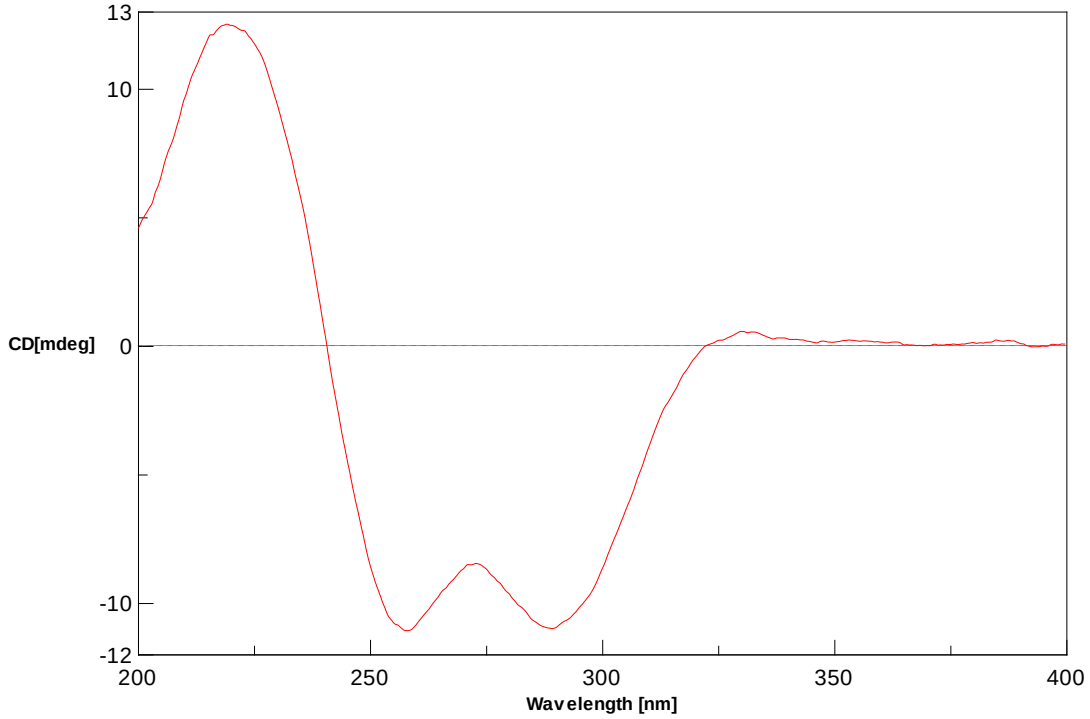


Fig. S33. ^{1}H NMR spectrum of compound **4** in C_5D_5N (400 MHz).

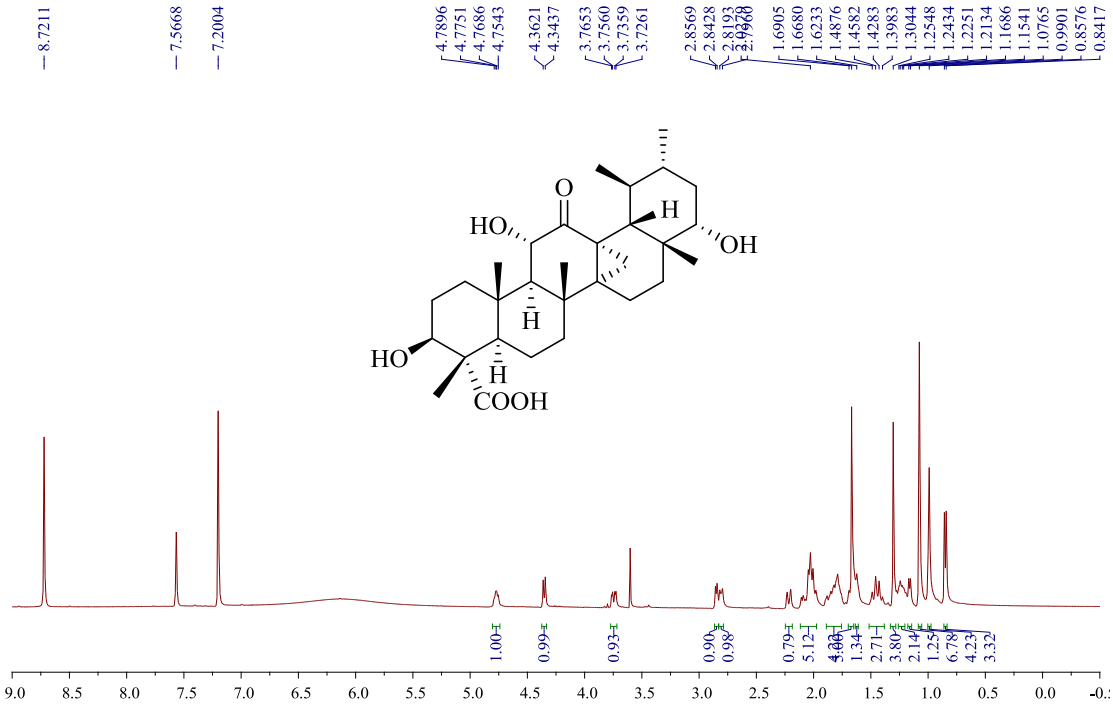


Fig. S34. ^{1}H NMR spectrum of compound **4**-expansion.

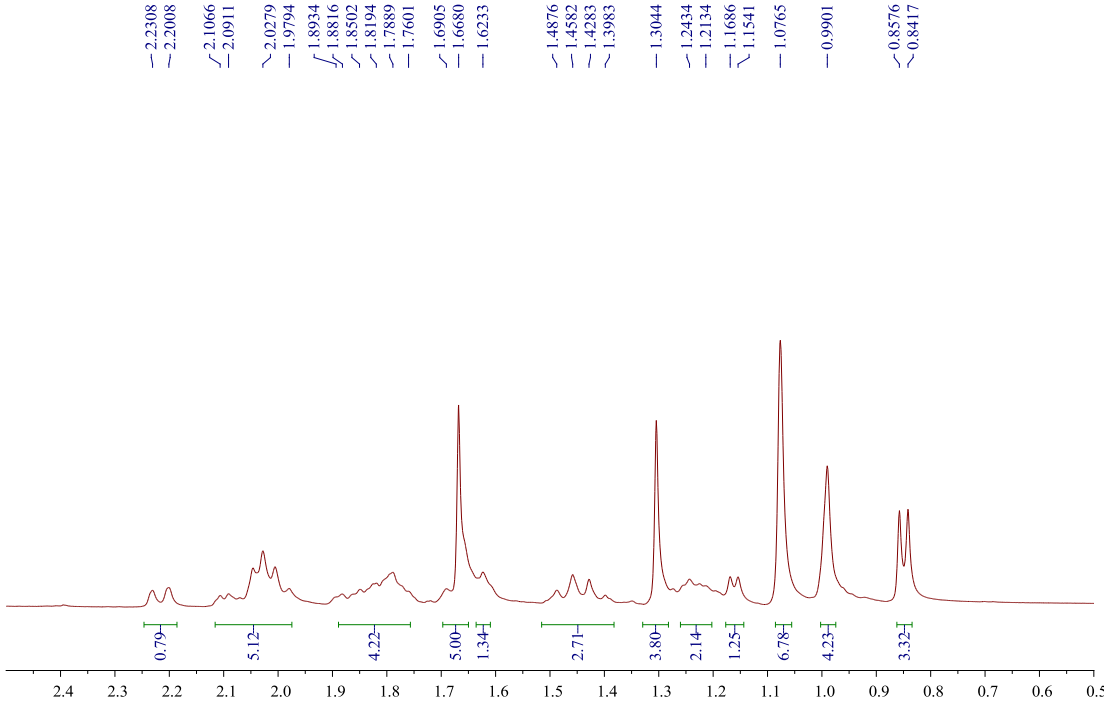


Fig. S35. ^{13}C NMR spectra of compound **4** in C_5D_5N (150 MHz).

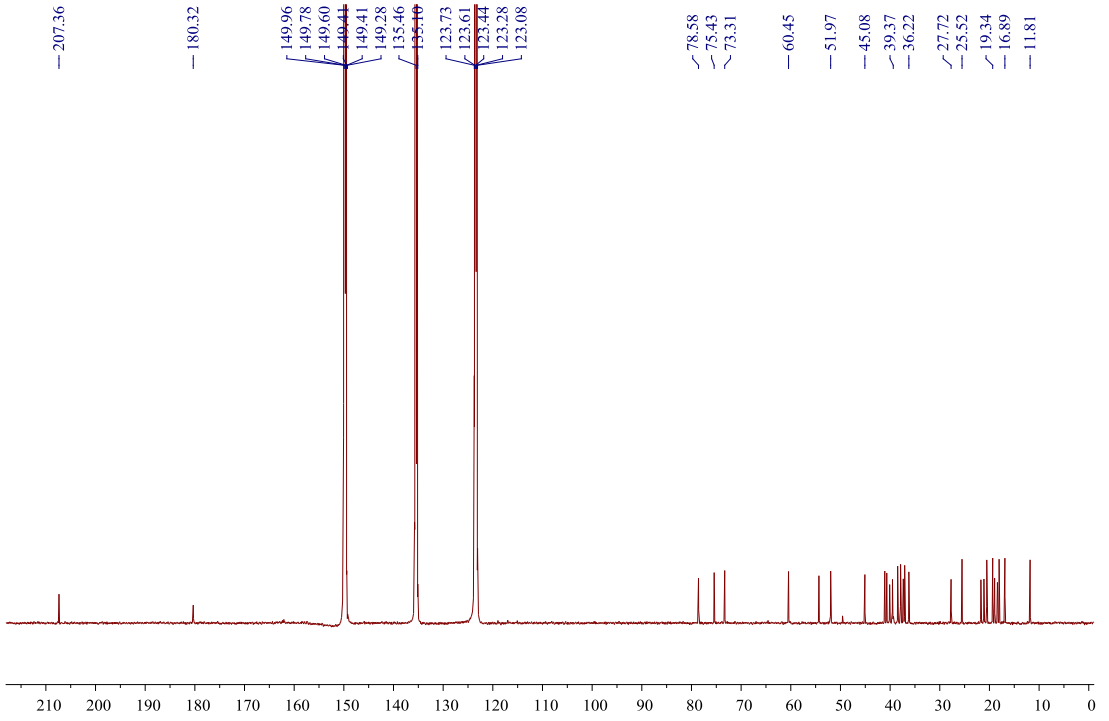


Fig. S36. ^{13}C NMR spectra of compound **4**-expansion.

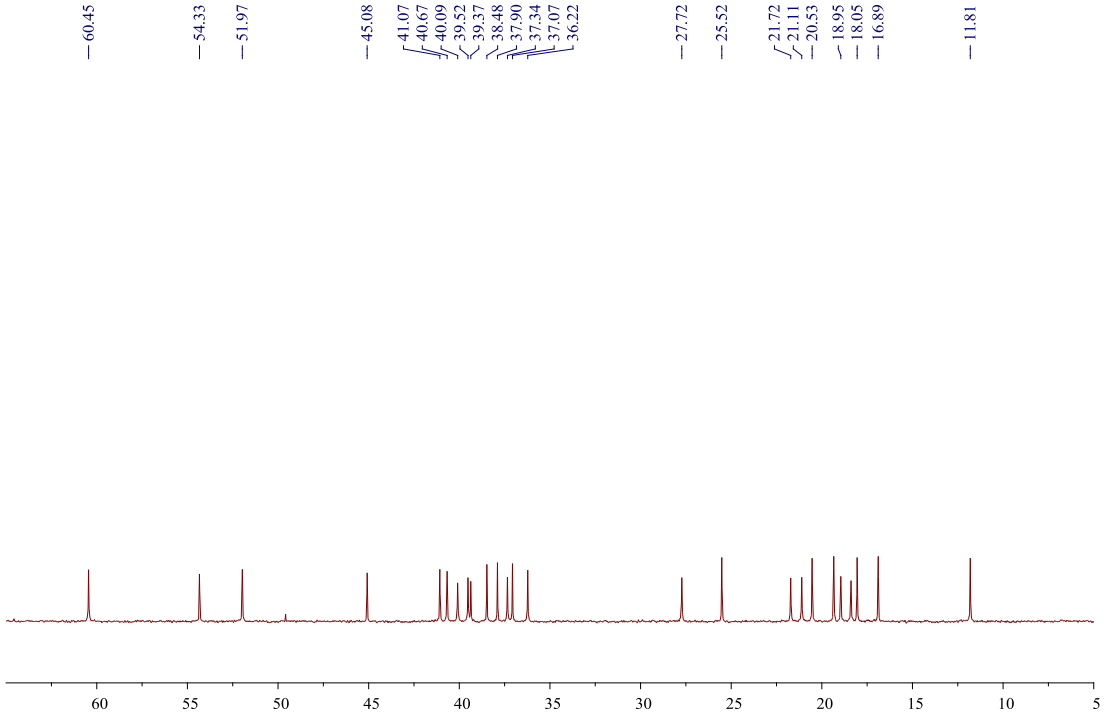


Fig. S37. DEPT 135 spectra of compound **4**.

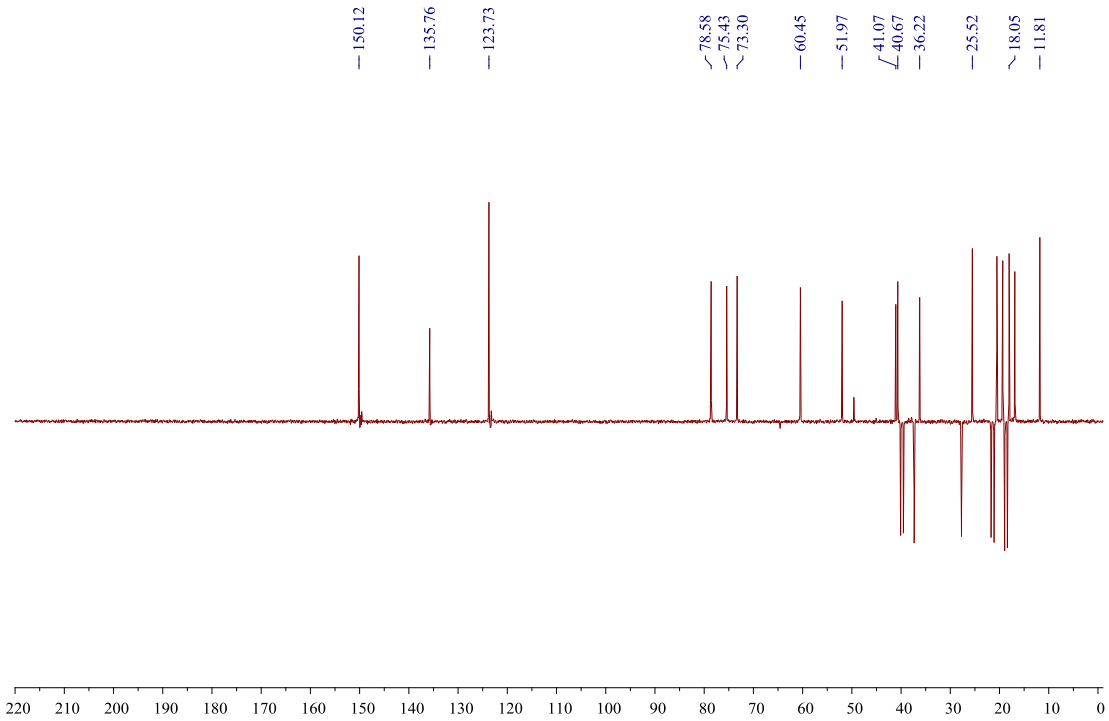


Fig. S38. HSQC spectrum of compound **4** in C_5D_5N (600 MHz).

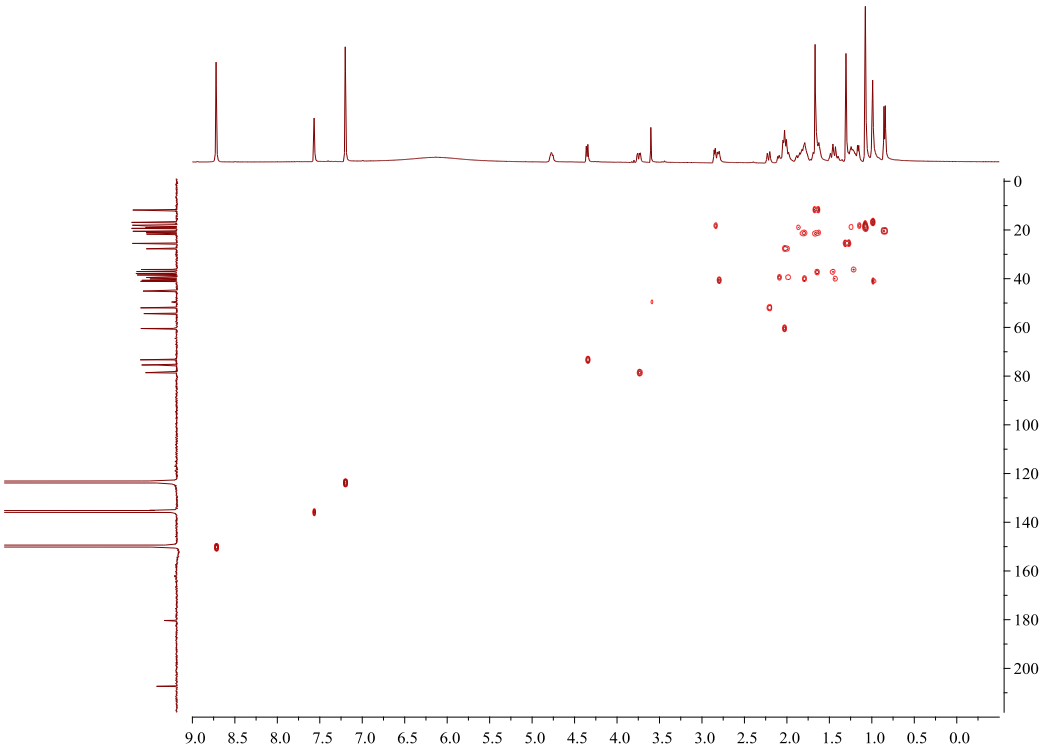


Fig. S39. ^{1}H-^{1}H COSY spectrum of compound **4** in C_5D_5N (600 MHz).

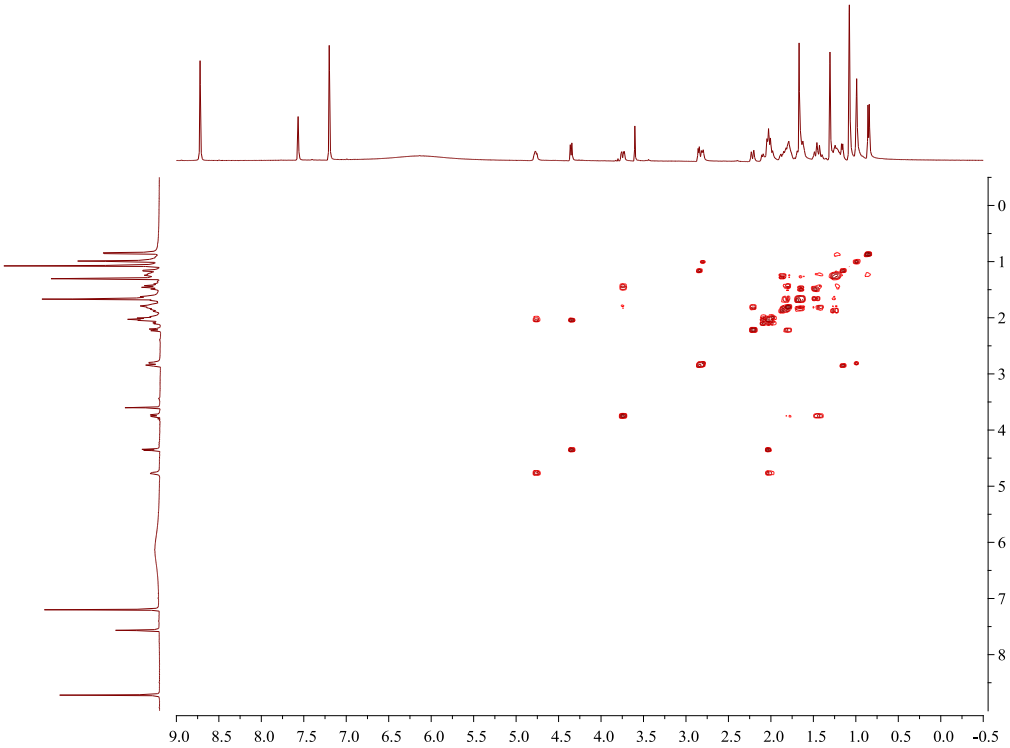


Fig. S40. HMBC spectrum of compound **4** in C_5D_5N (600 MHz).

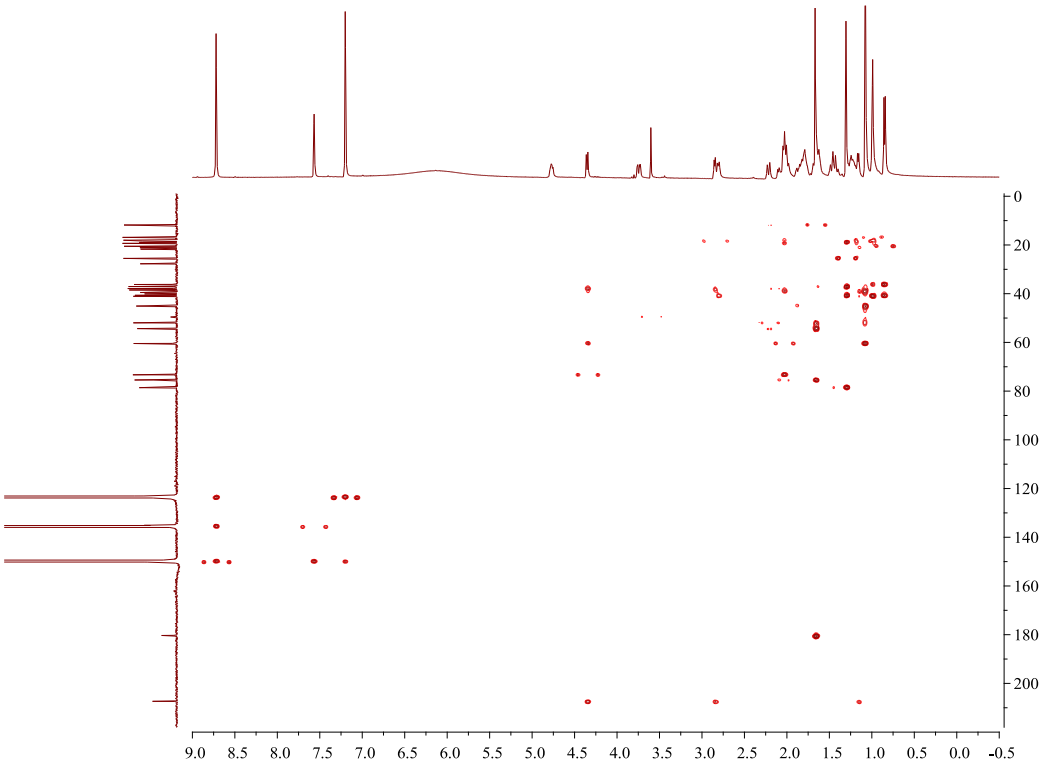


Fig. S41. HMBC spectrum of compound **4**-expansion.

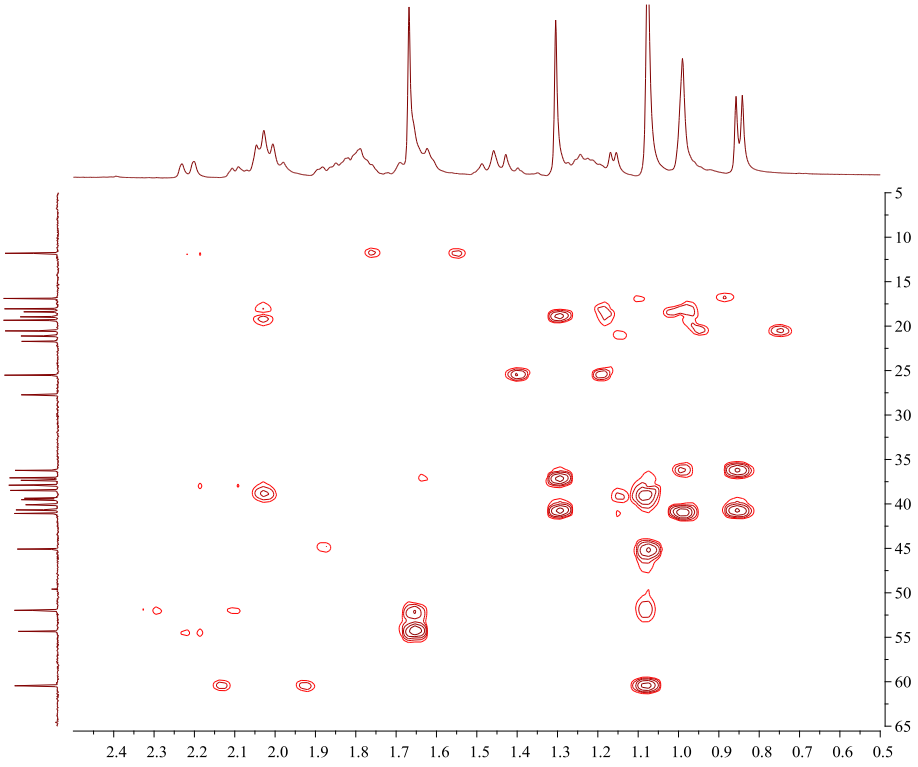


Fig. S42. ROESY spectrum of compound **4** in C_5D_5N (600 MHz).

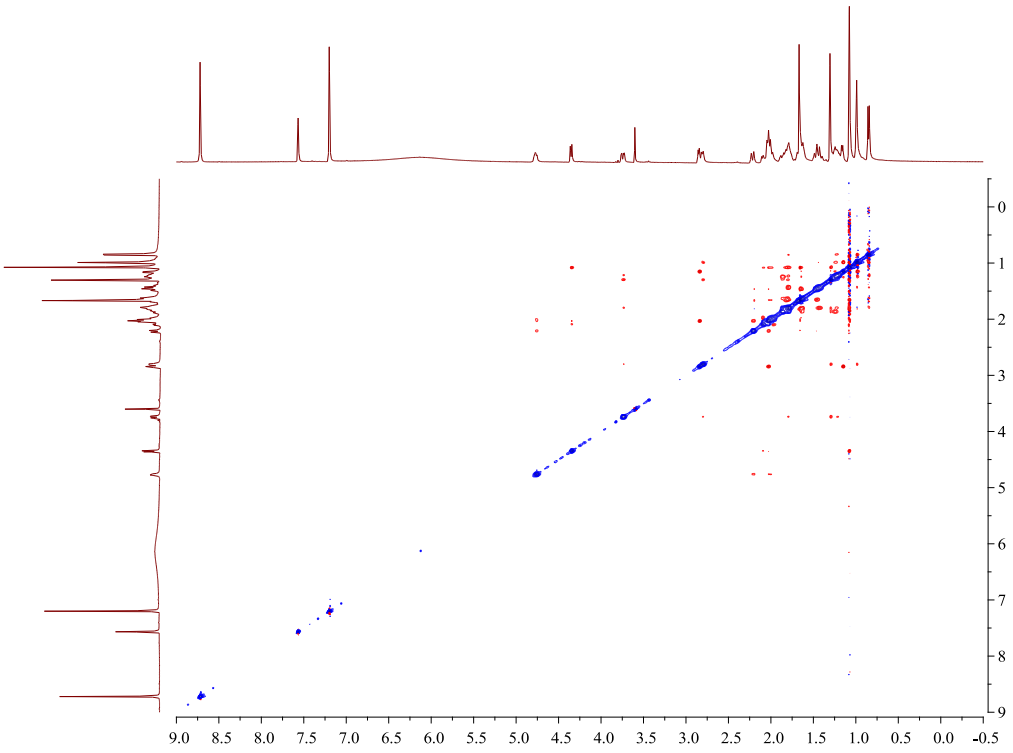


Fig. S43. HRESIMS report of compound **4**.

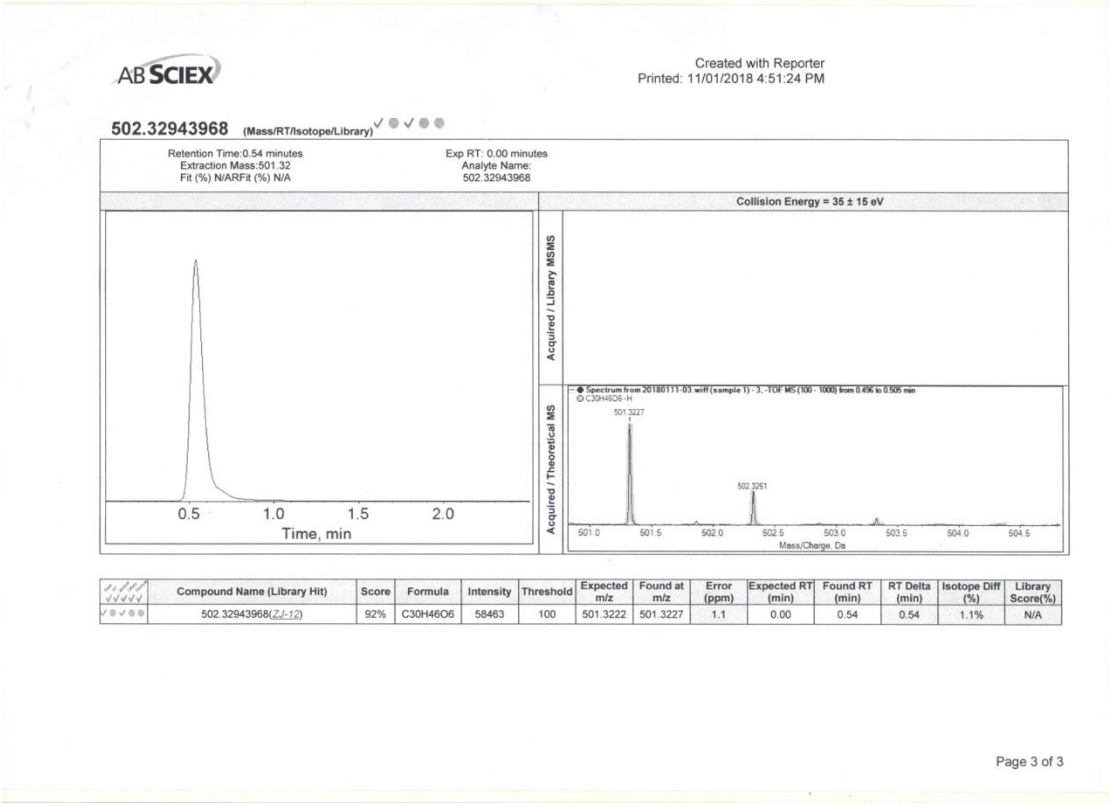


Fig. S44. ^{1}H NMR spectrum of compound **5** in C_5D_5N (400 MHz).

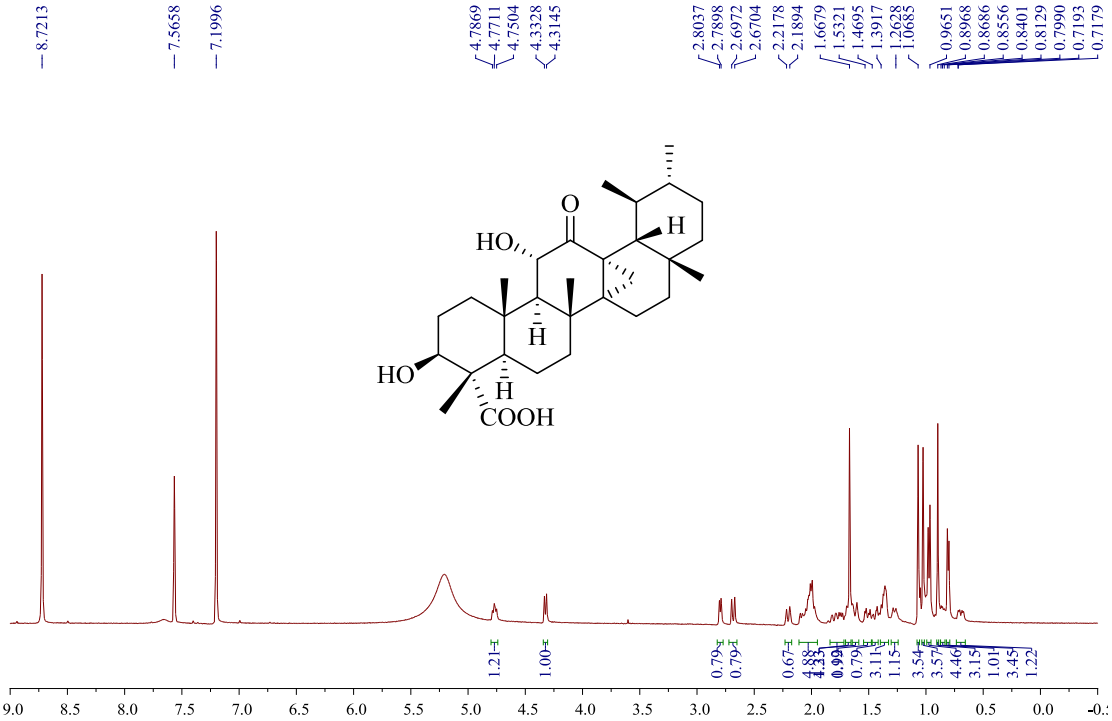


Fig. S45. ^{1}H NMR spectrum of compound **5**–expansion.

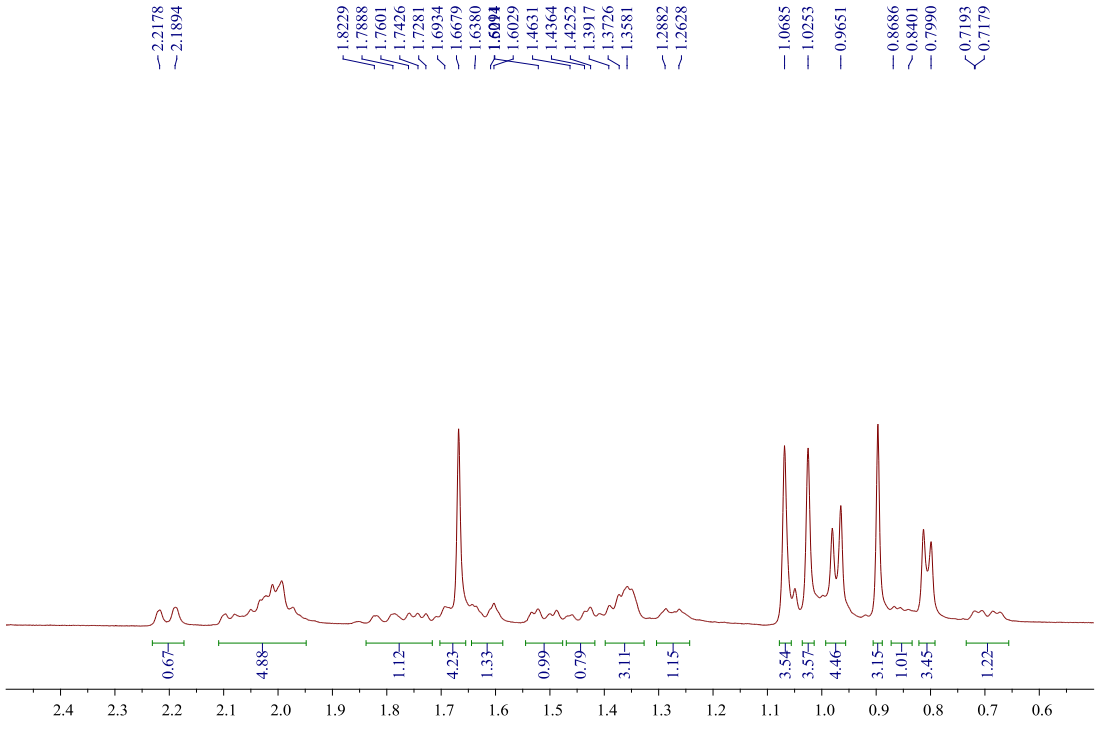


Fig. S46. ^{13}C NMR spectrum of compound **5** in C_5D_5N (150 MHz).

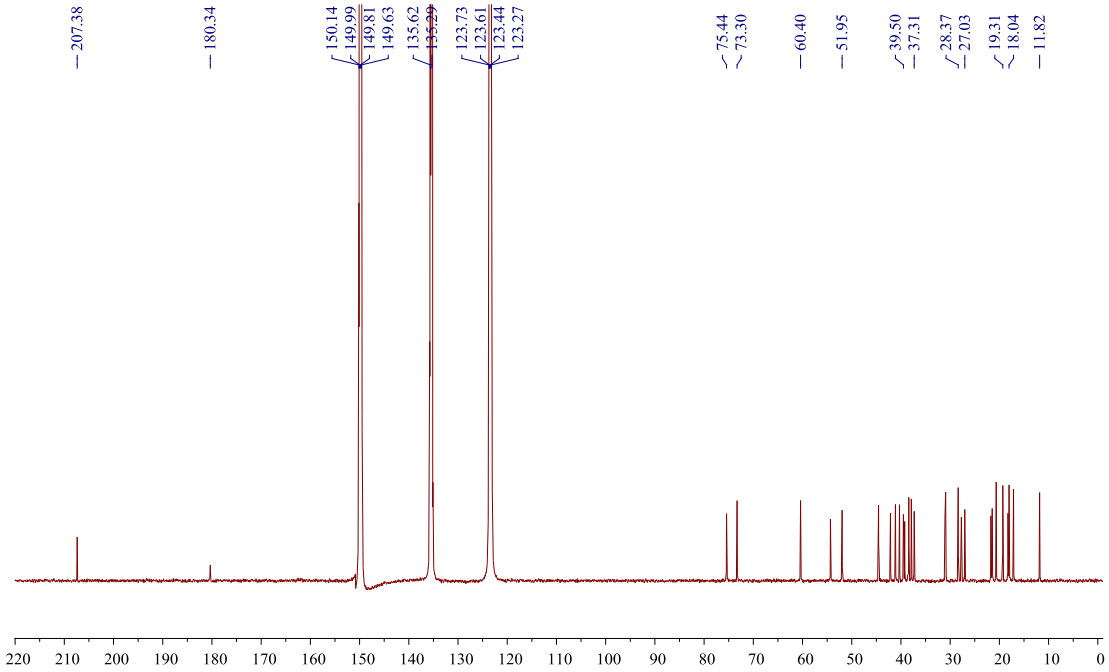


Fig. S47. ^{13}C NMR spectrum of compound **5**–expansion.

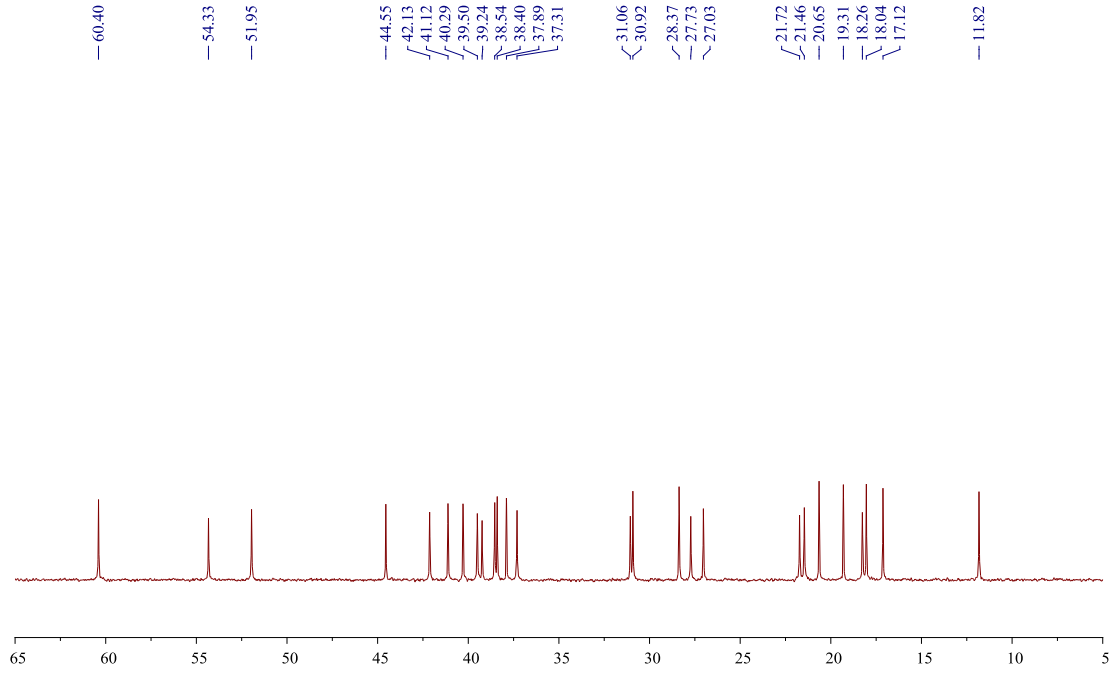


Fig. S48. HMBC spectrum of compound **5** in C_5D_5N (600 MHz).

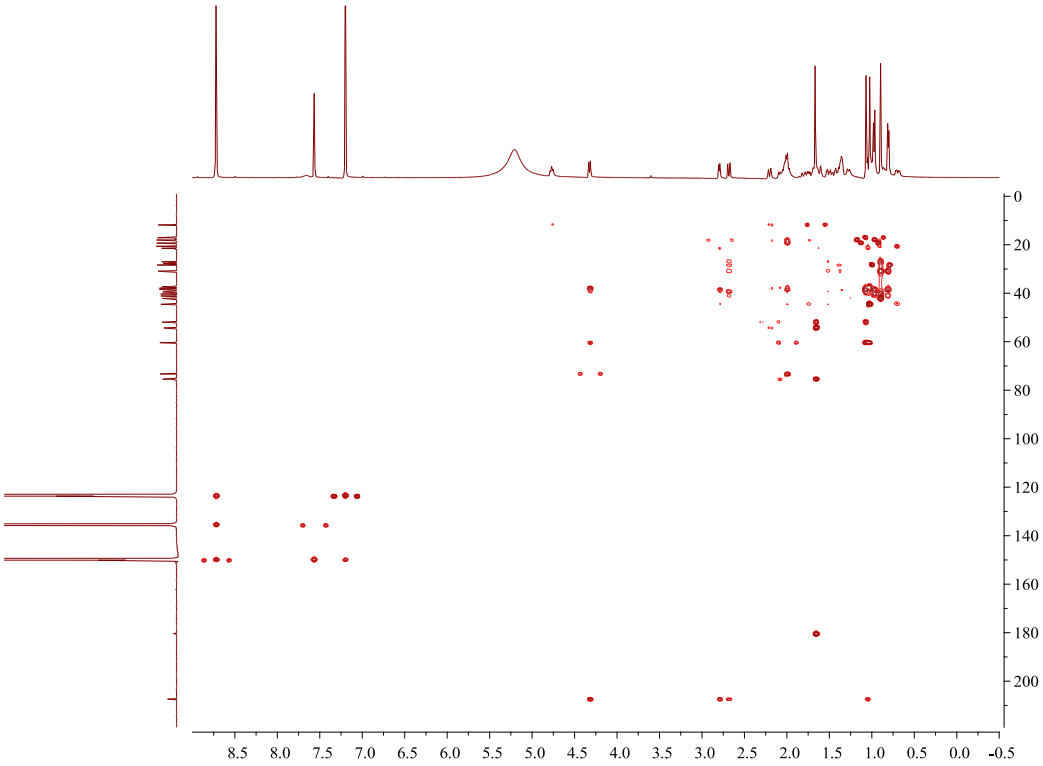


Fig. S49. HMBC spectrum of compound **5**–expansion.

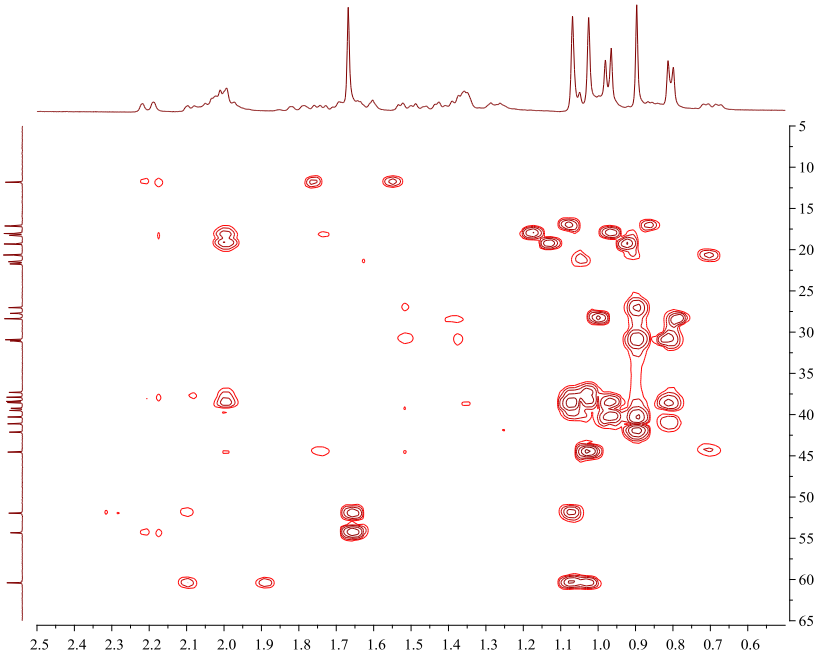


Fig. S50. ROESY spectrum of compound **5** in C_5D_5N (600 MHz).

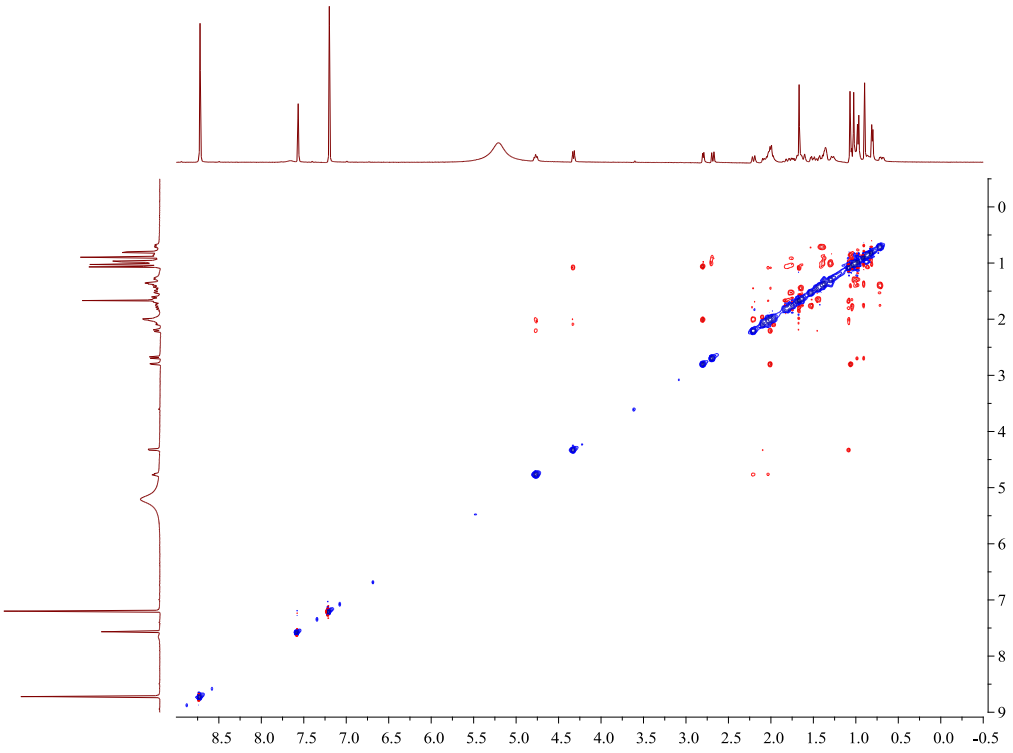


Fig. S51. HRESIMS report of compound **5**.

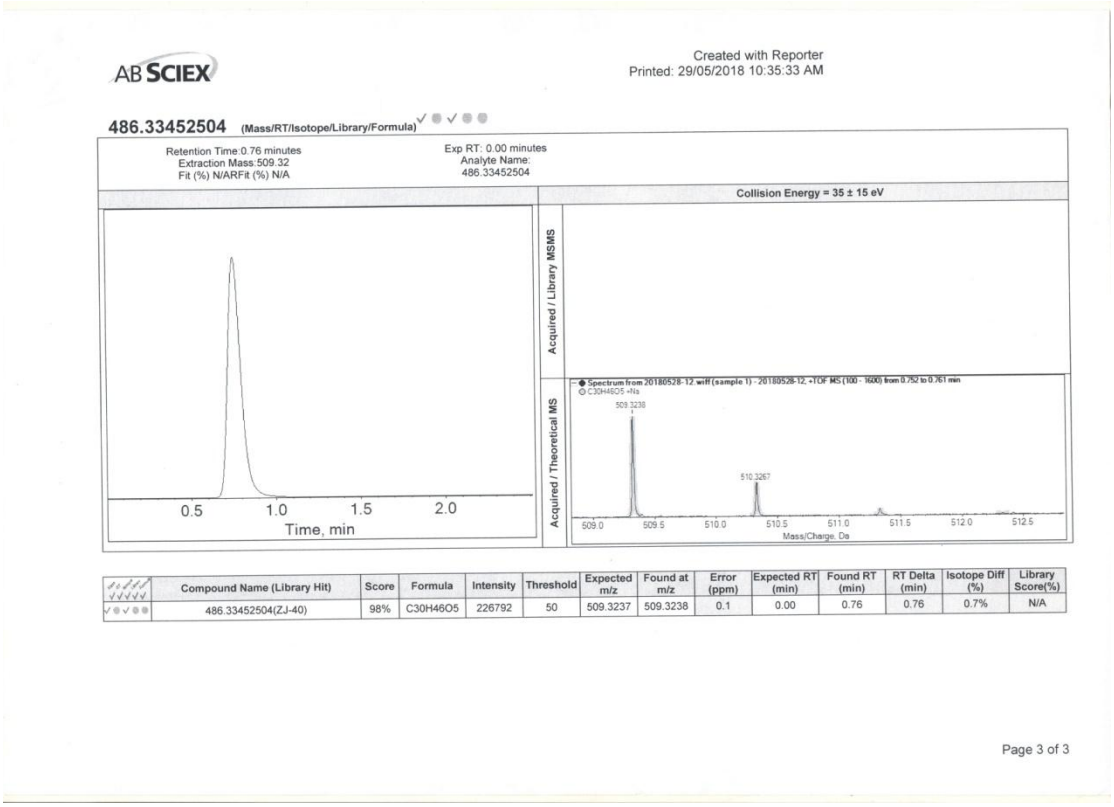


Fig. S52. Experimental ECD spectra of **4** (red curve) and **5** (black curve) in MeOH..

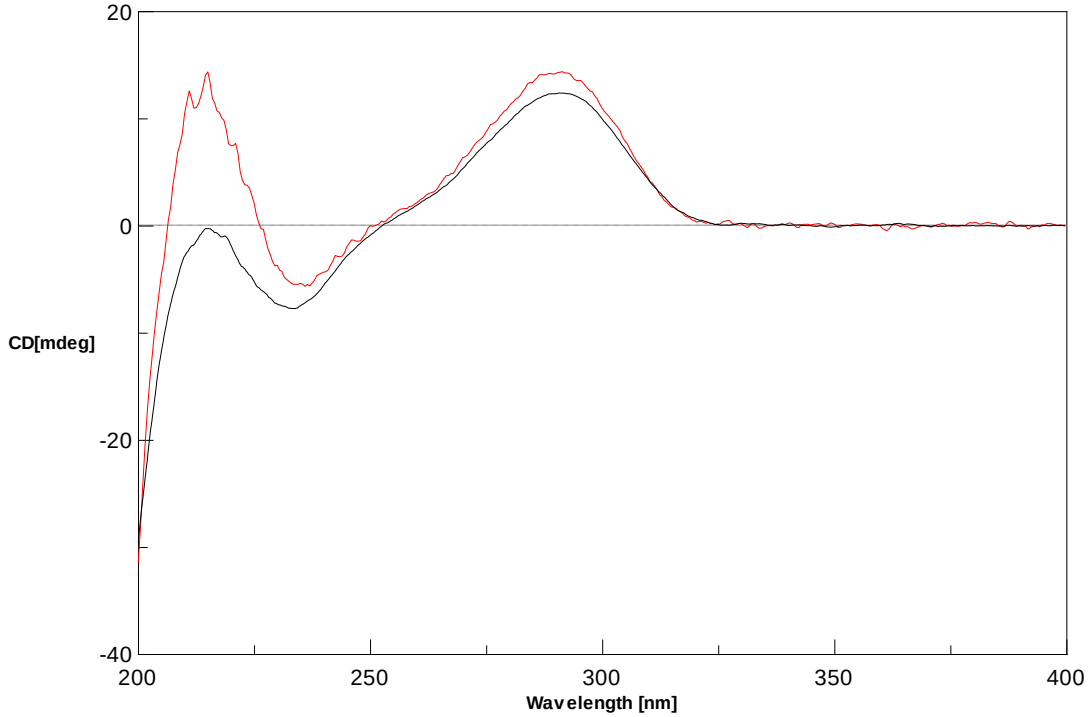


Fig. S53. ^{1}H NMR spectrum of compound **6** in C_5D_5N (400 MHz).

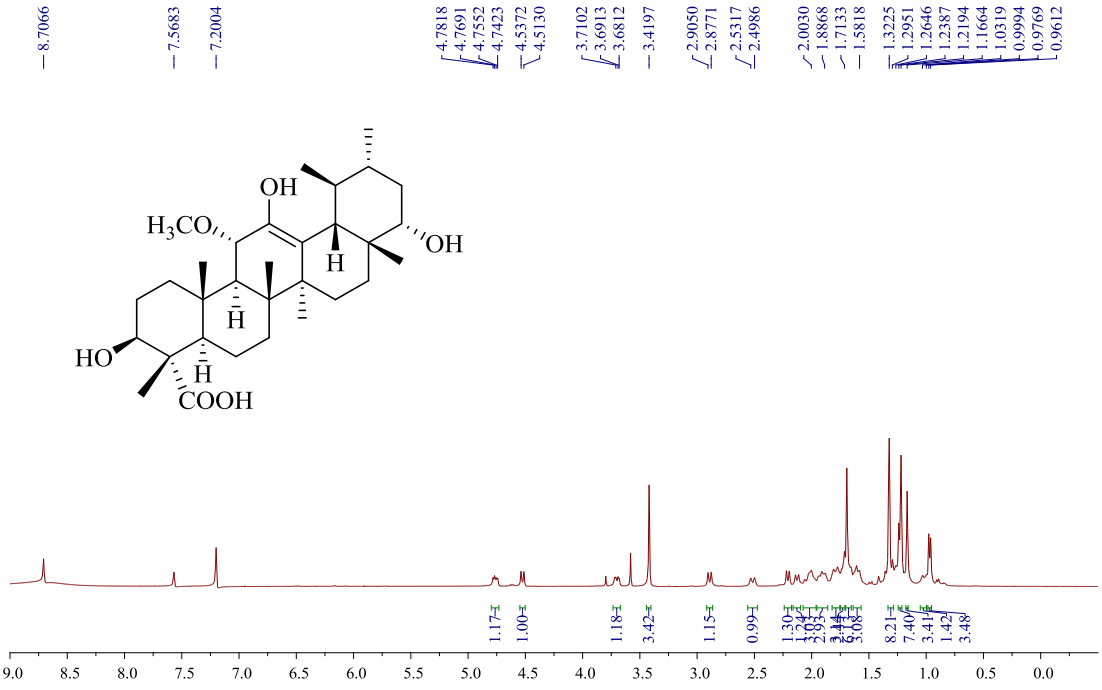


Fig. S54. ^{1}H NMR spectrum of compound **6**–expansion.

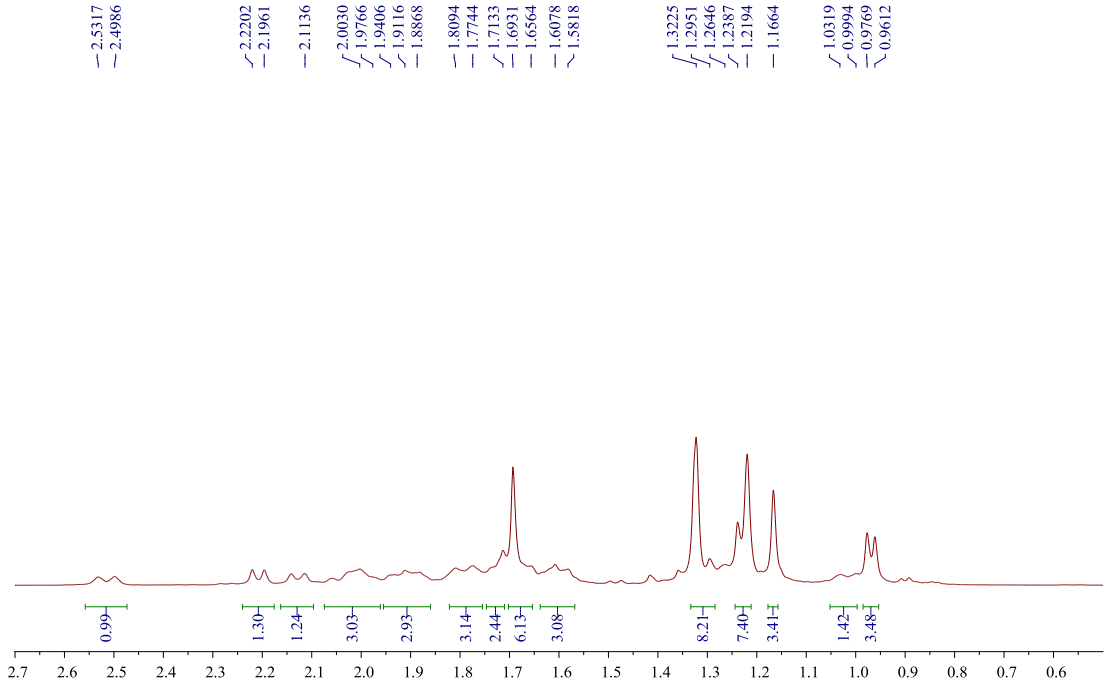


Fig. S55. ^{13}C NMR spectrum of compound **6** in C_5D_5N (150 MHz).

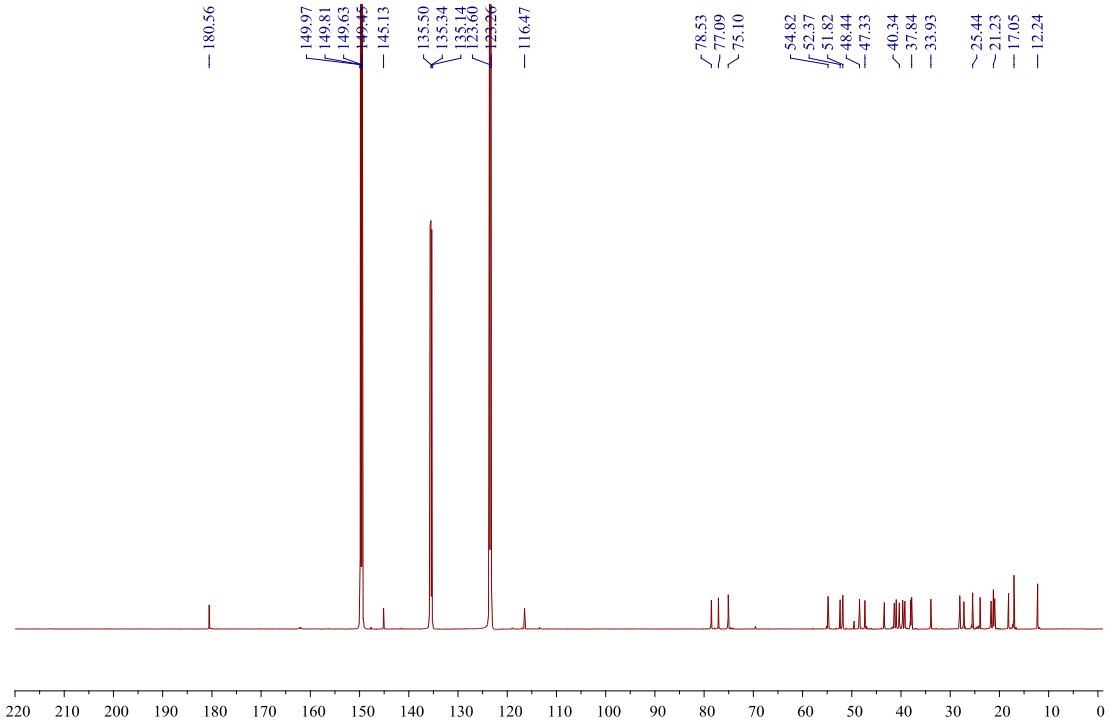


Fig. S56. ^{13}C NMR spectrum of compound **6**–expansion.

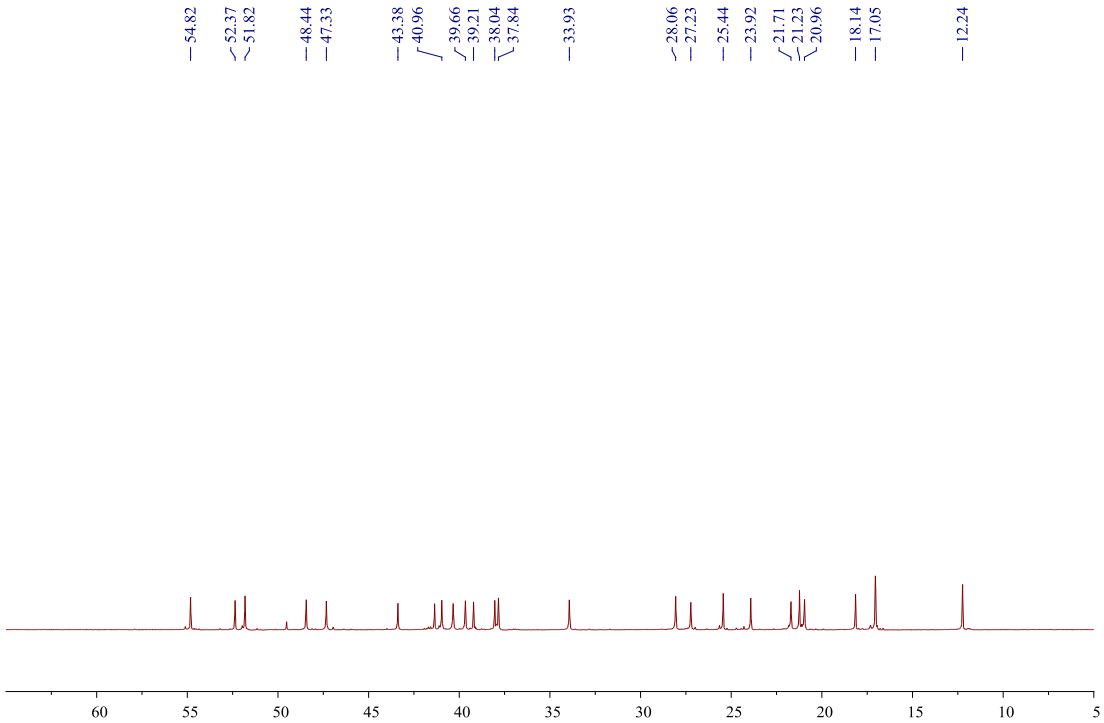


Fig. S57. HSQC spectrum of compound **6** in C_5D_5N (600 MHz).

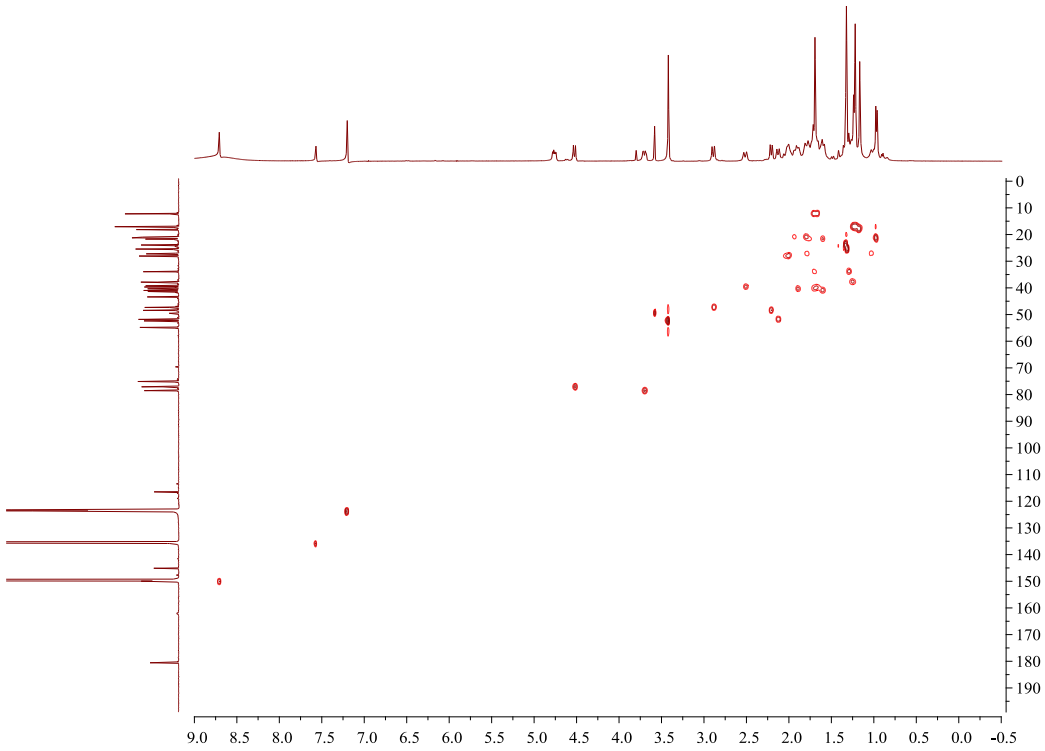


Fig. S58. HMBC spectrum of compound **6** in C_5D_5N (600 MHz).

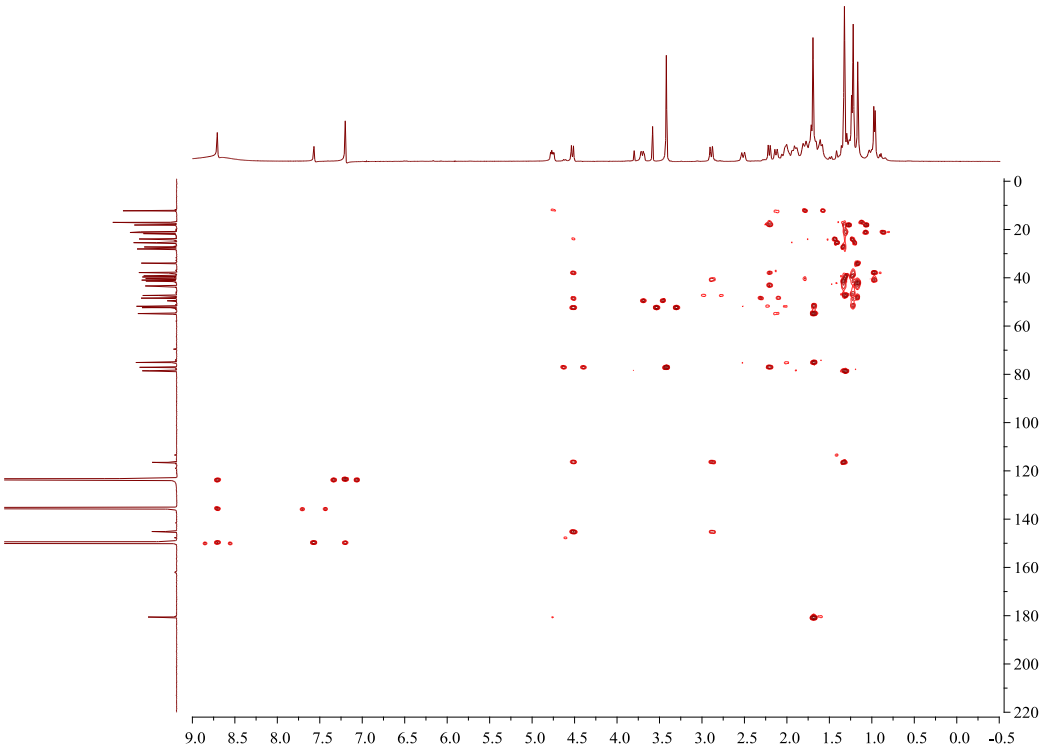


Fig. S59. HMBC spectrum of compound **6**–expansion.

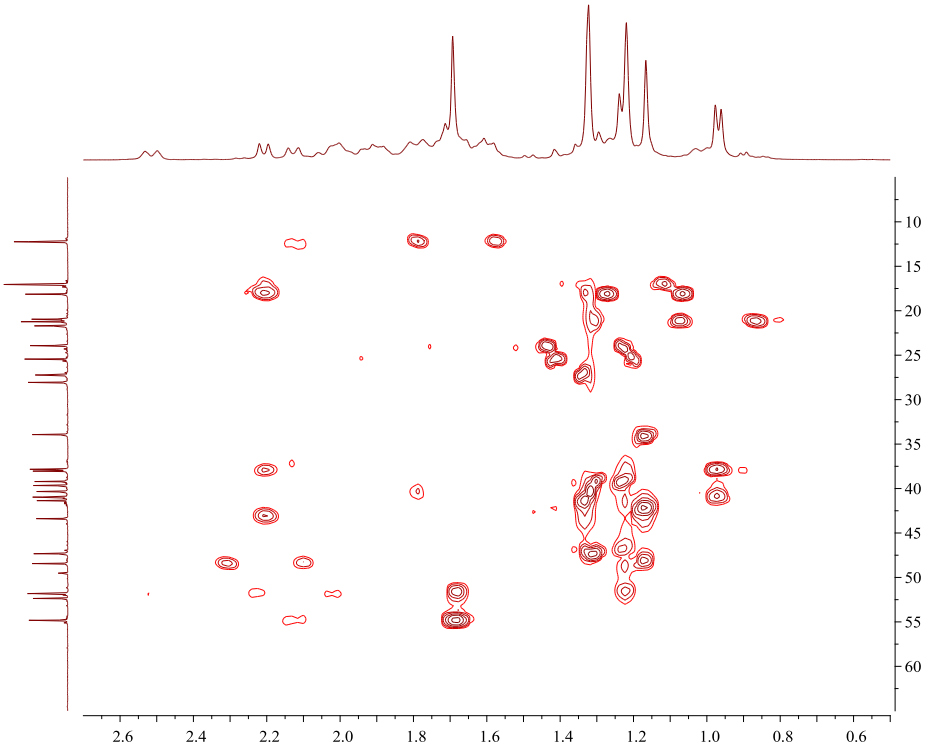


Fig. S60. ROESY spectrum of compound **6** in C_5D_5N (600 MHz).

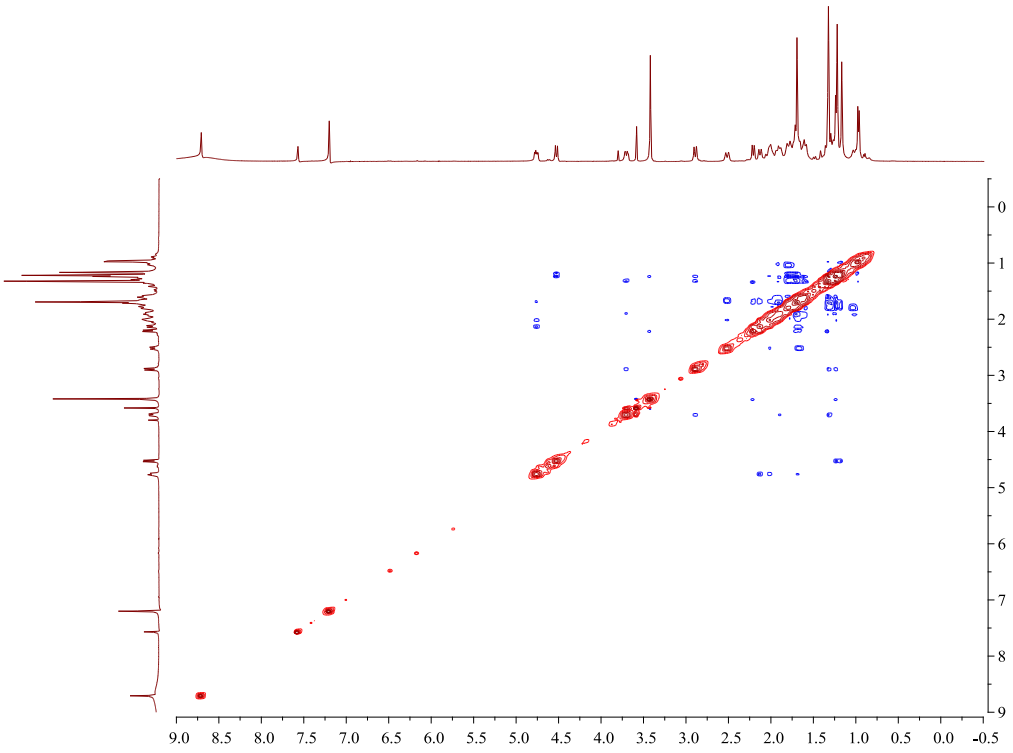


Fig. S61. HRESIMS report of compound **6**.

0

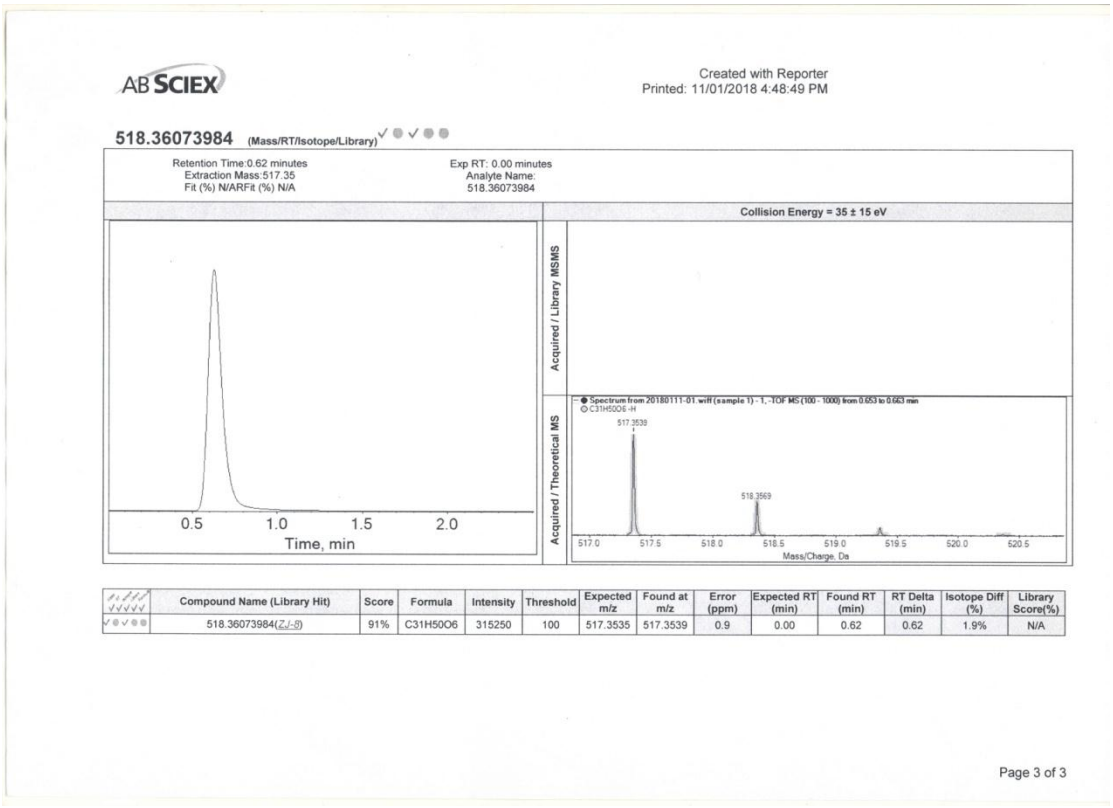


Fig. S62. ^{1}H NMR spectrum of compound **7** in C_5D_5N (400 MHz).

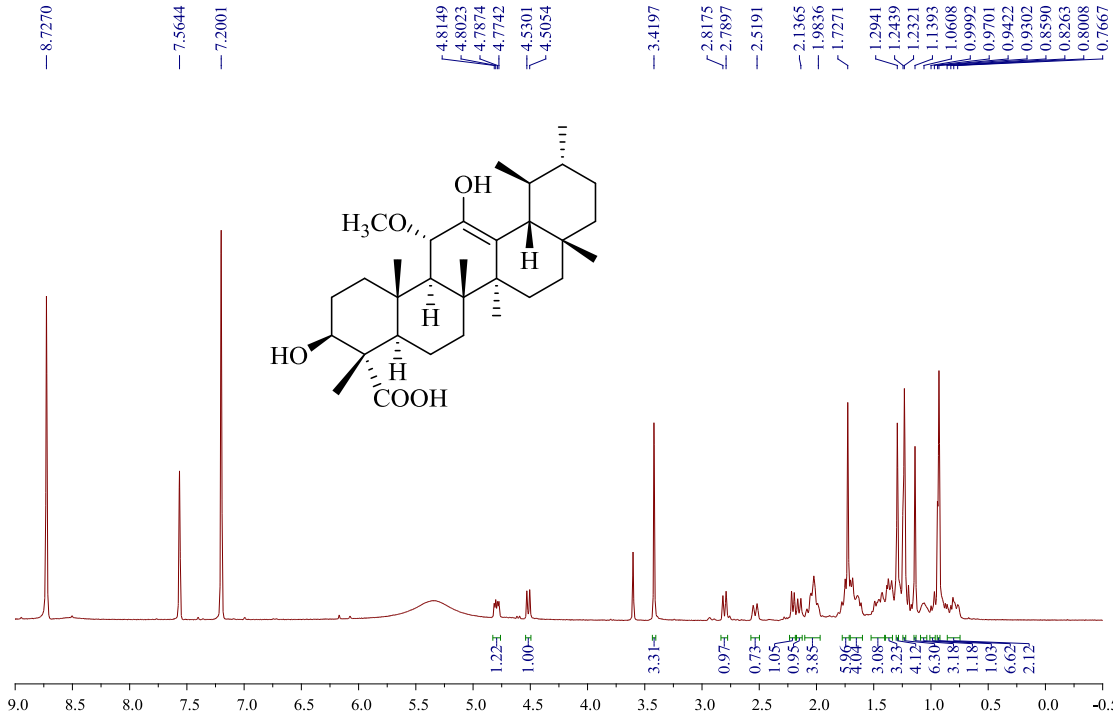


Fig. S63. ^{1}H NMR spectrum of compound **7**-expansion.

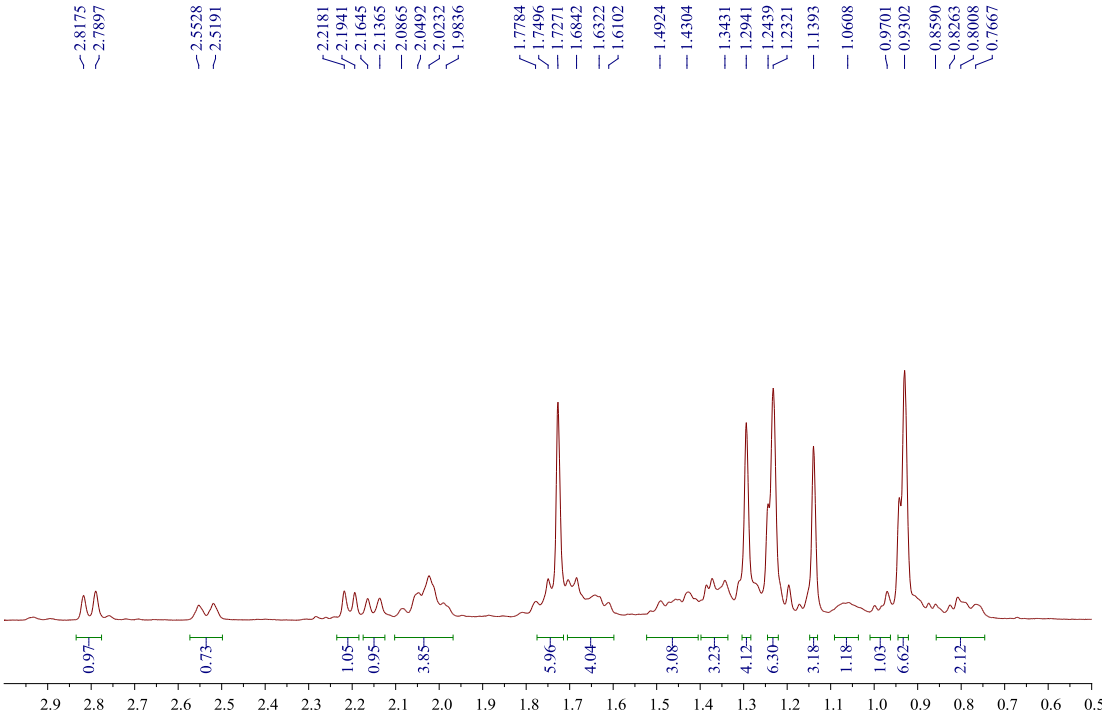


Fig. S64. ^{13}C NMR spectrum of compound **7** in C_5D_5N (150 MHz).

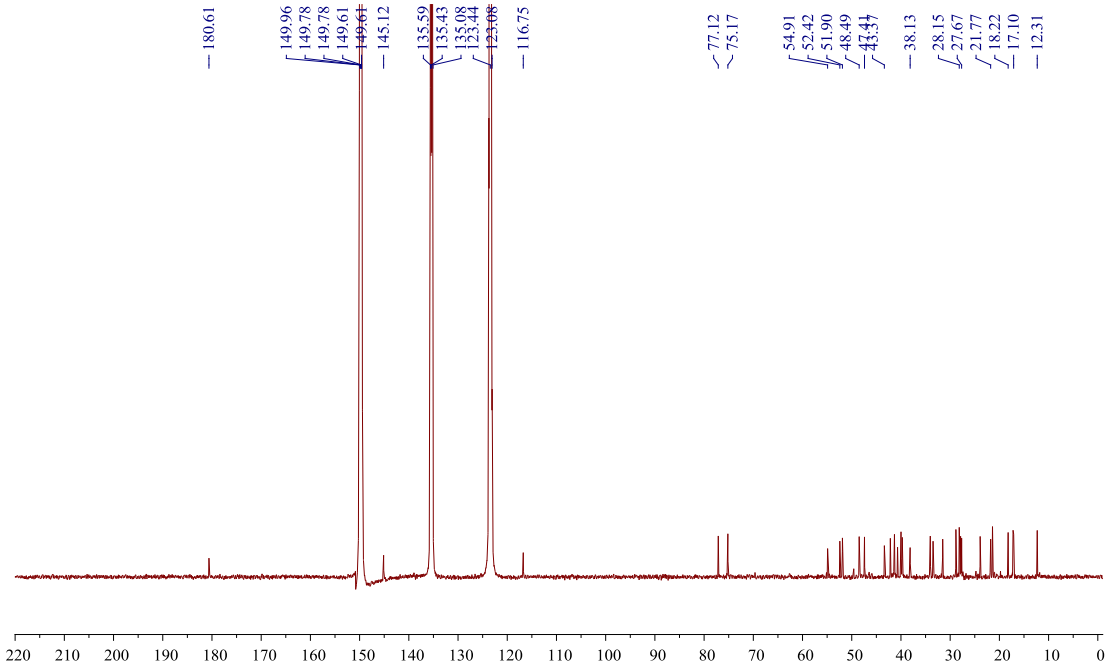


Fig. S65. ^{13}C NMR spectrum of compound **7** –expansion.

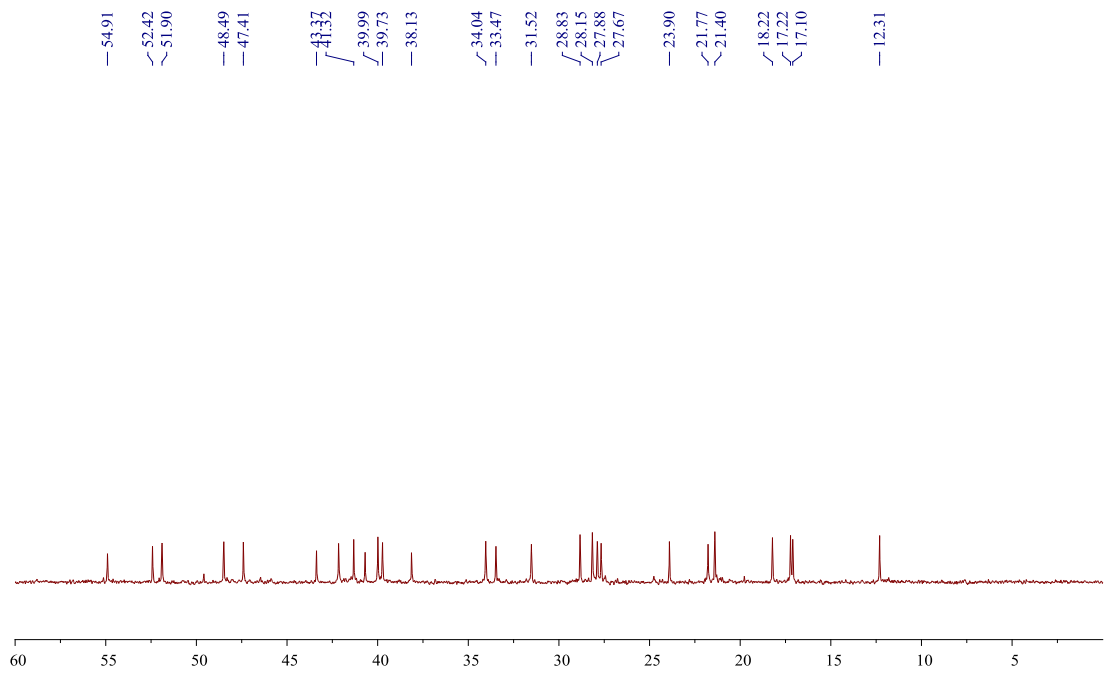


Fig. S66. HSQC spectrum of compound **7** in C_5D_5N (600 MHz).

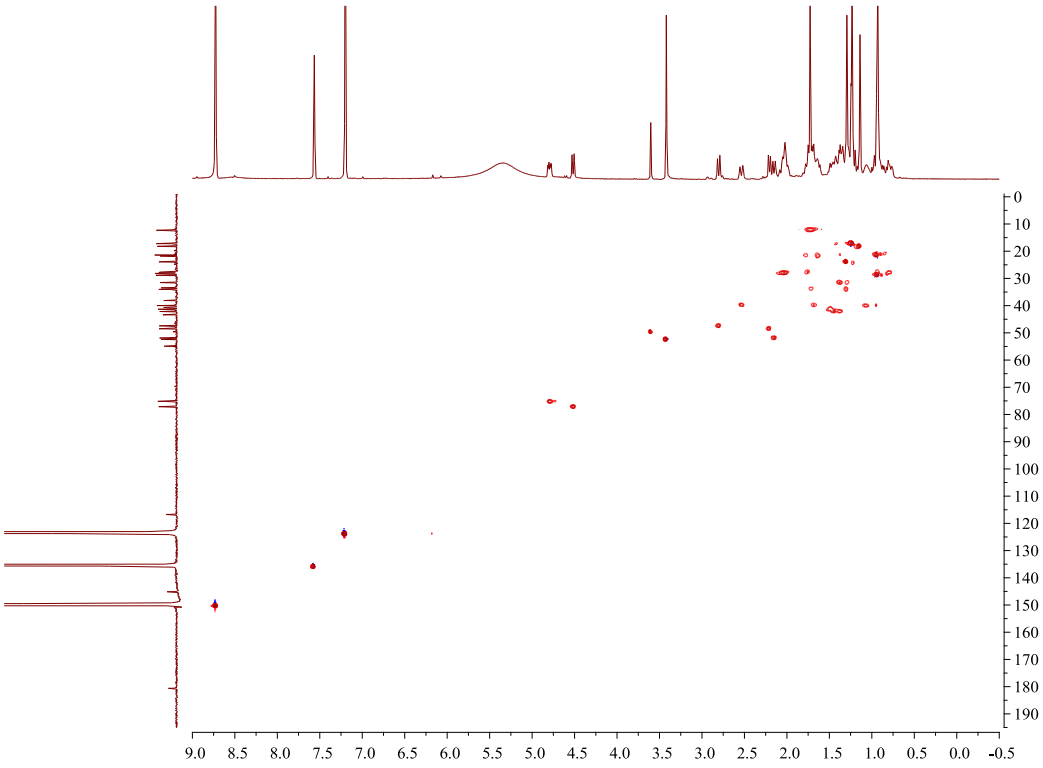


Fig. S67. HMBC spectrum of compound **7** in C_5D_5N (600 MHz).

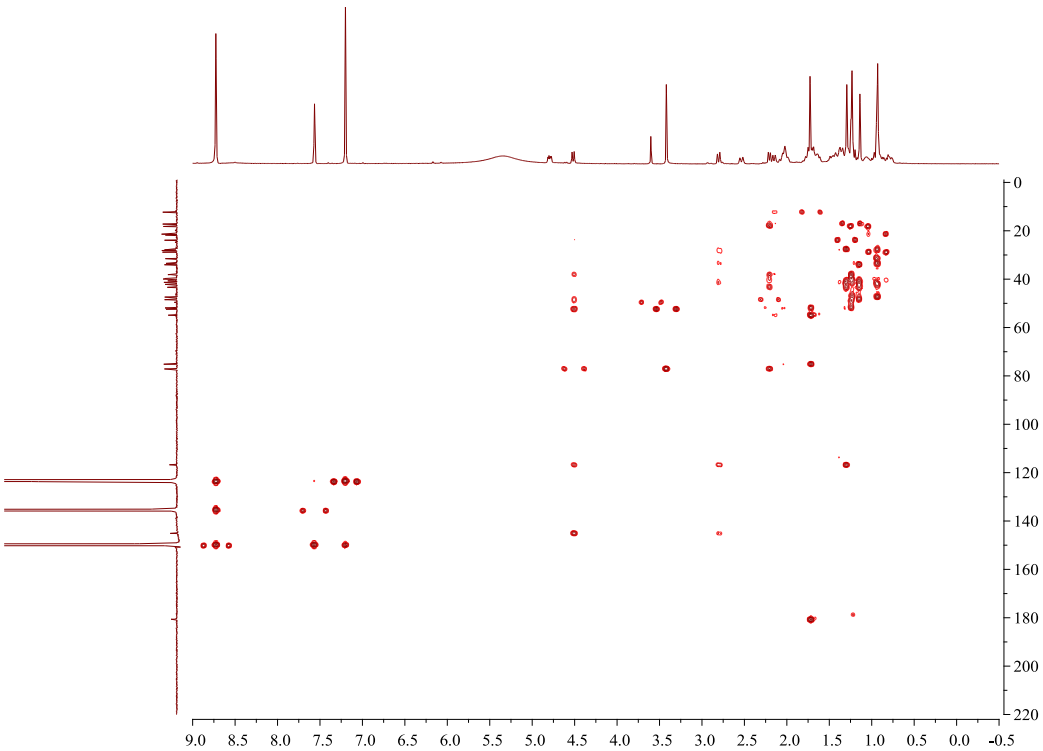


Fig. S68. ROESY spectrum of compound **7** in C_5D_5N (600 MHz).

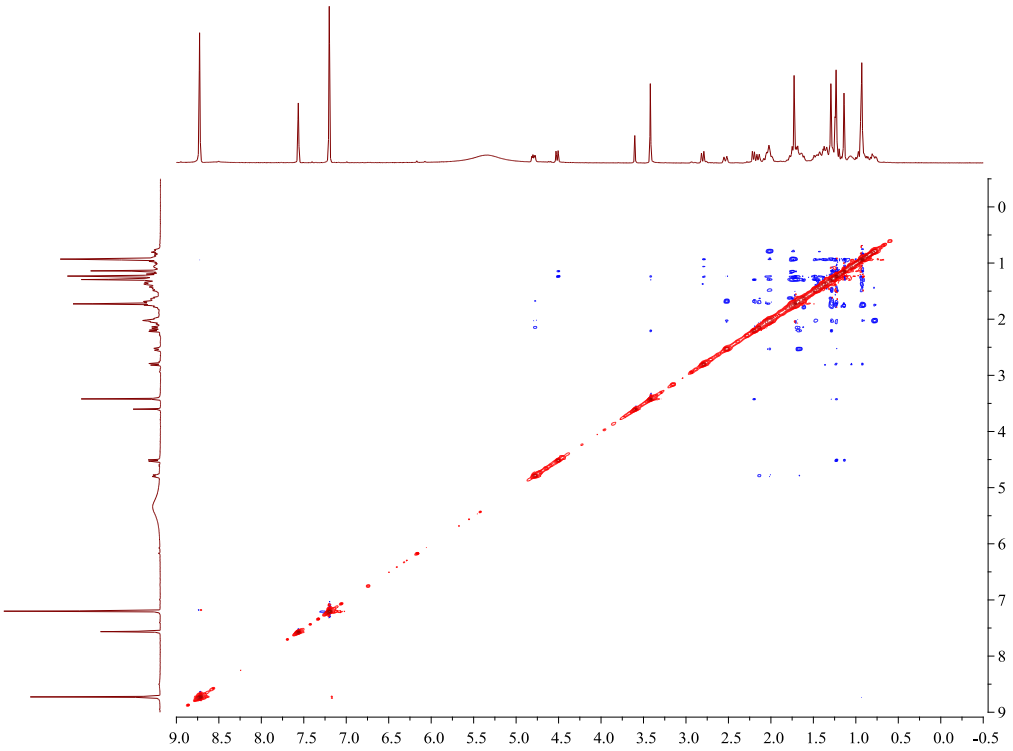


Fig. S69. ROESY spectrum of compound **7**-expansion.

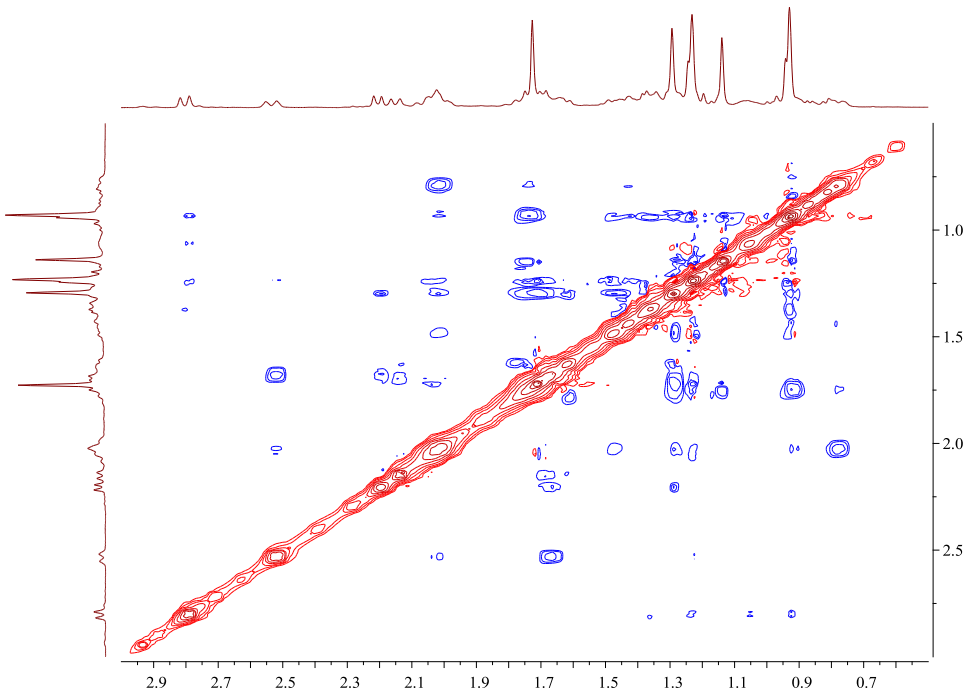


Fig. S70. HRESIMS report of compound **7**.

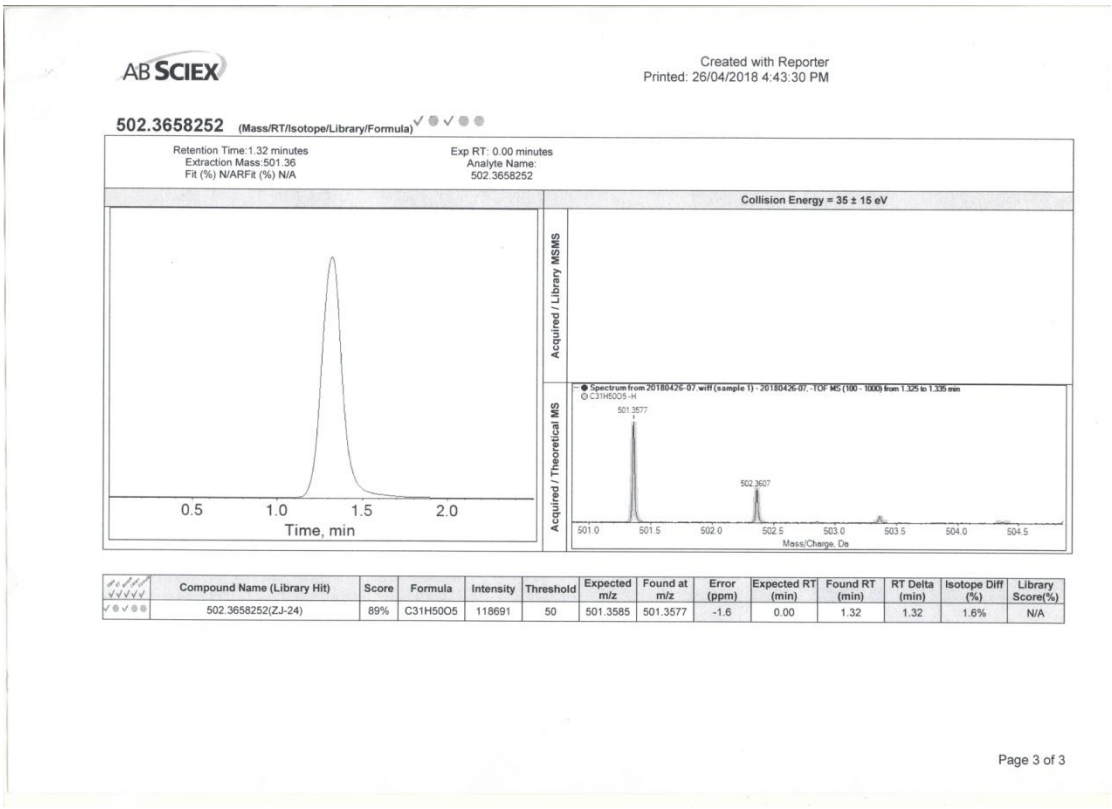


Fig. S71. Experimental ECD spectra of **6** (red curve) and **7** (black curve) in MeOH.

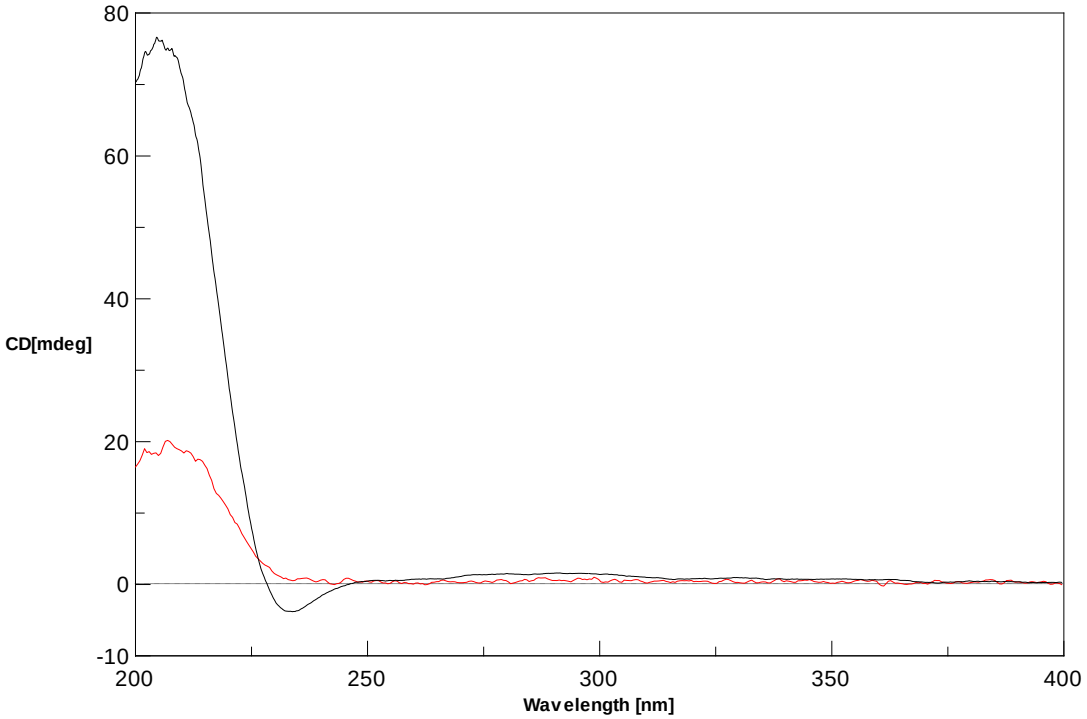


Fig. S72. ^{1}H NMR spectrum of compound **8** in CD_3OD (400 MHz).

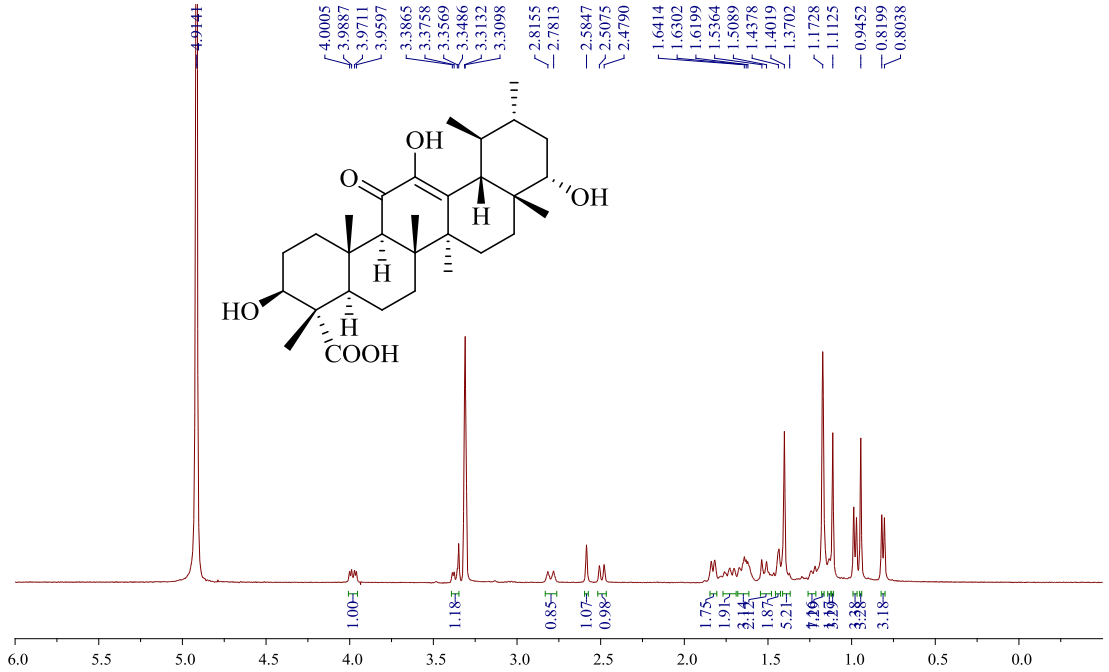


Fig. S73. ^{1}H NMR spectrum of compound **8**-expansion.

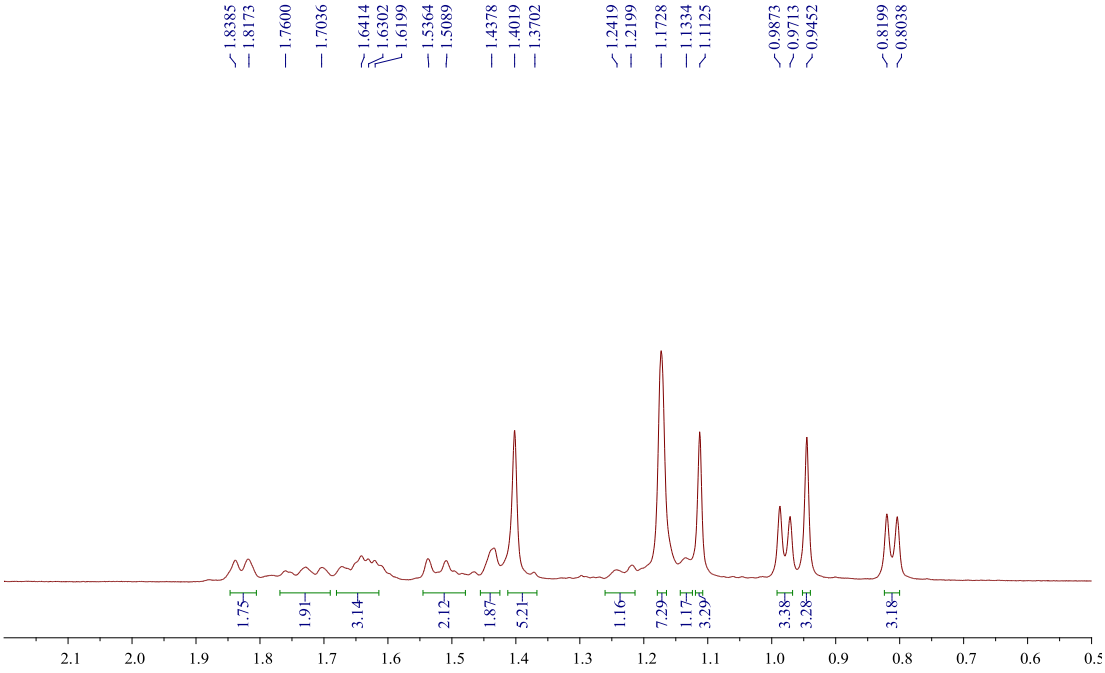


Fig. S74. ^{13}C NMR spectrum of compound **8** in CD_3OD (150 MHz).

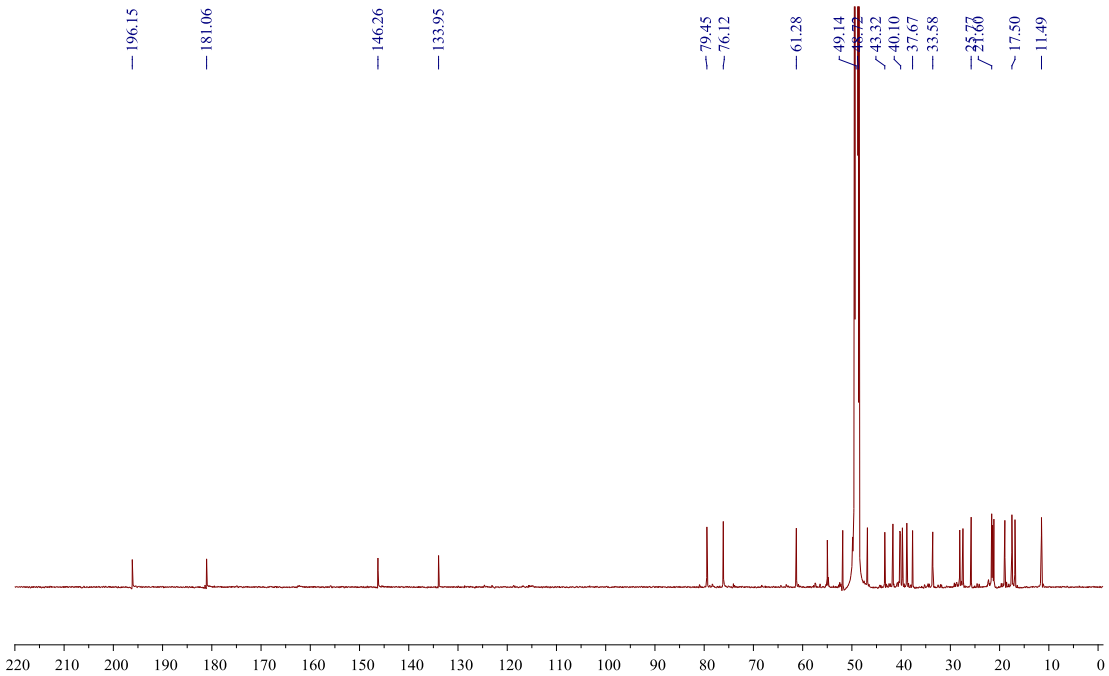


Fig. S75. ^{13}C NMR spectrum of compound **8**-expansion.

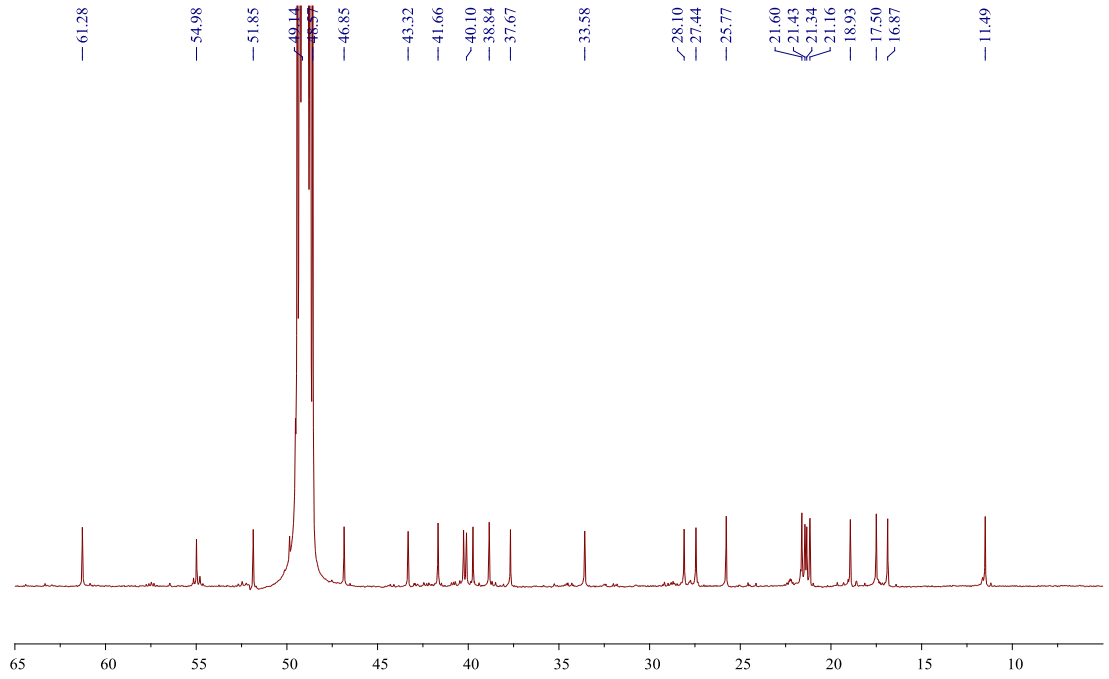


Fig. S76. ^{1}H-^{1}H COSY spectrum of compound **8** in CD_3OD (600 MHz).

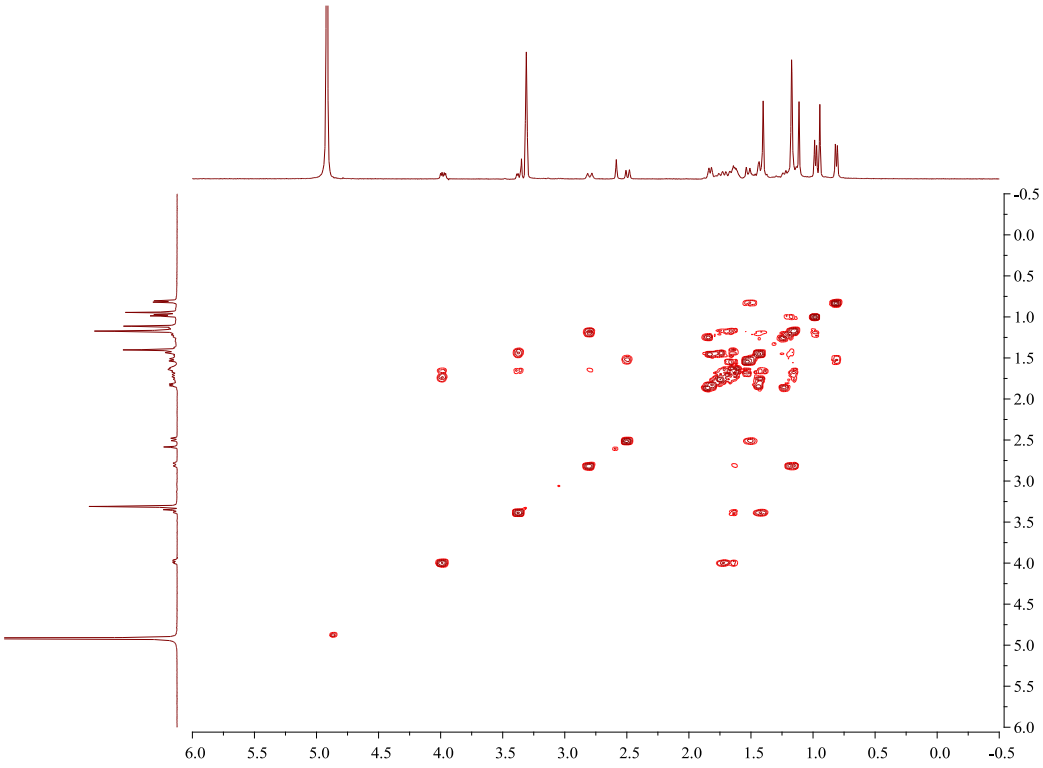


Fig. S77. HMBC spectrum of compound **8** in CD_3OD (600 MHz).

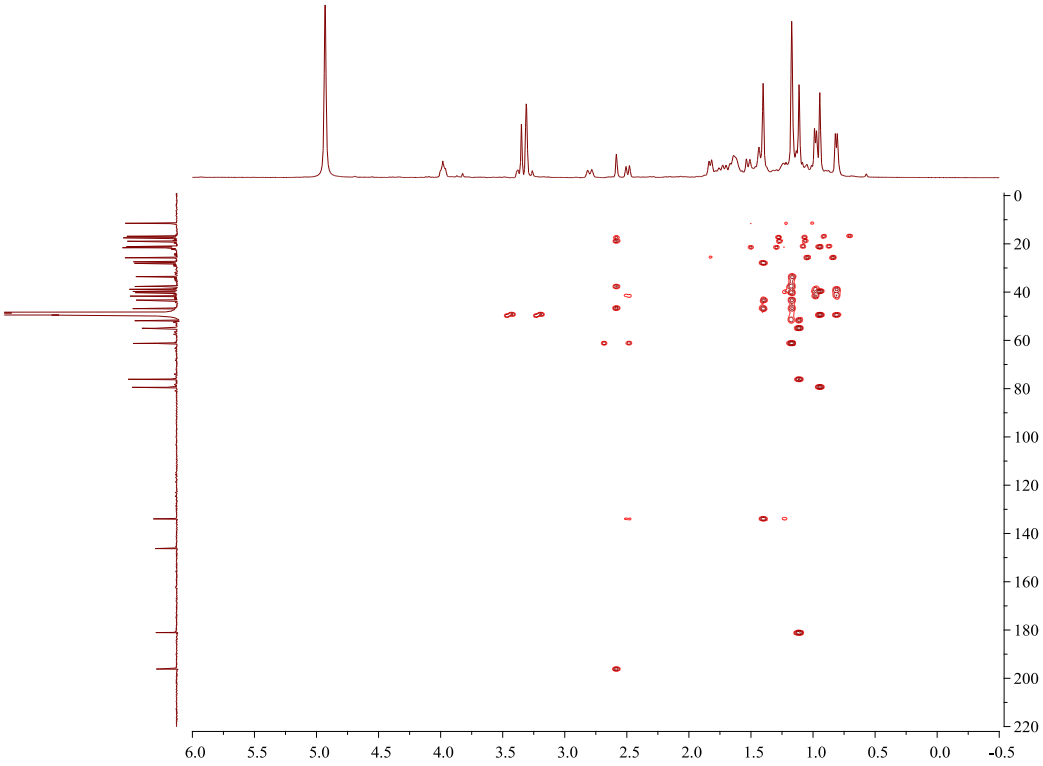


Fig. S78. HMBC spectrum of compound **8**–expansion.

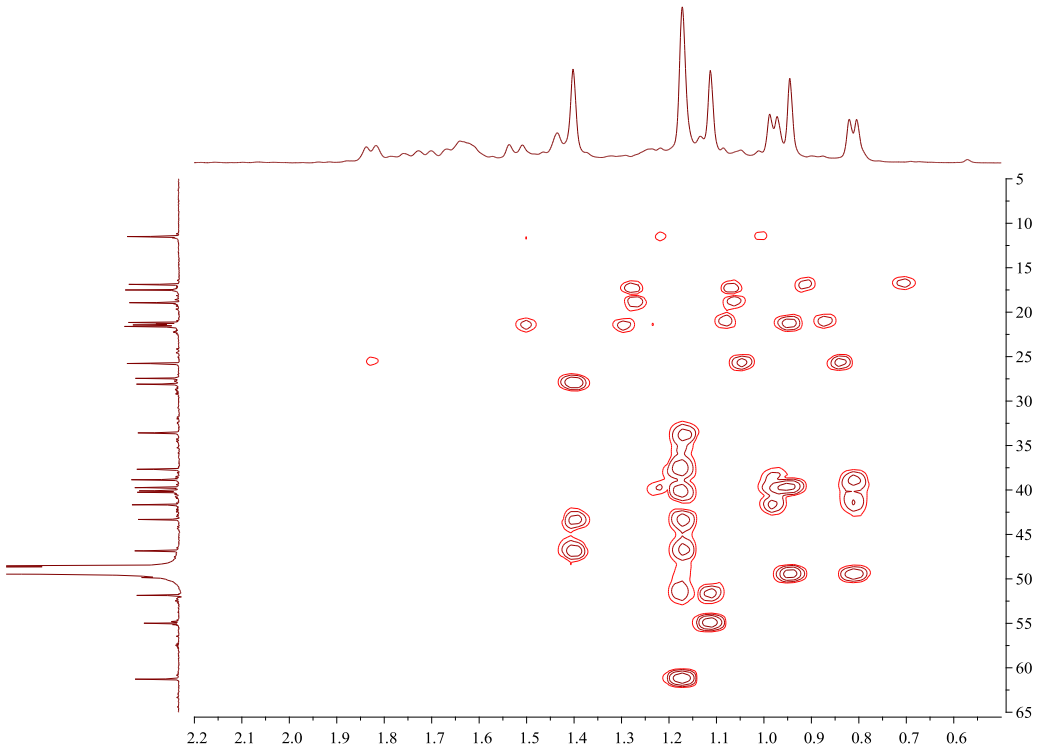


Fig. S79. ^{1}H NMR spectrum of compound **8** in C_5D_5N (600 MHz).

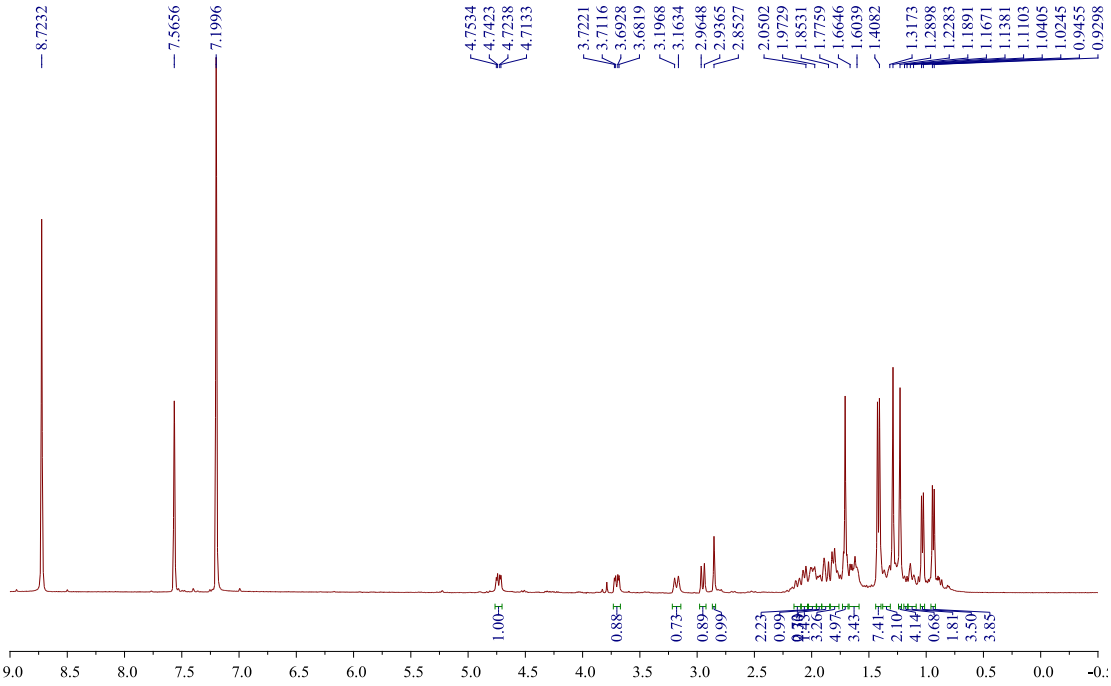


Fig. S80. ROESY spectrum of compound **8** in C_5D_5N (600 MHz).

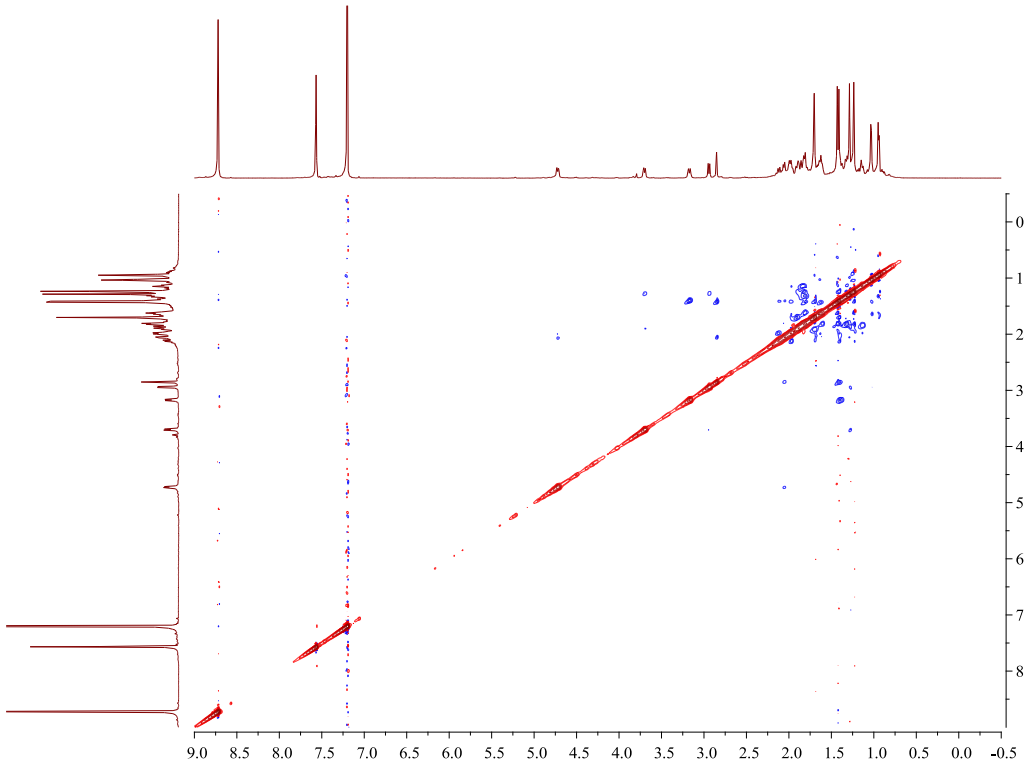


Fig. S81. HRESIMS report of compound **8**.

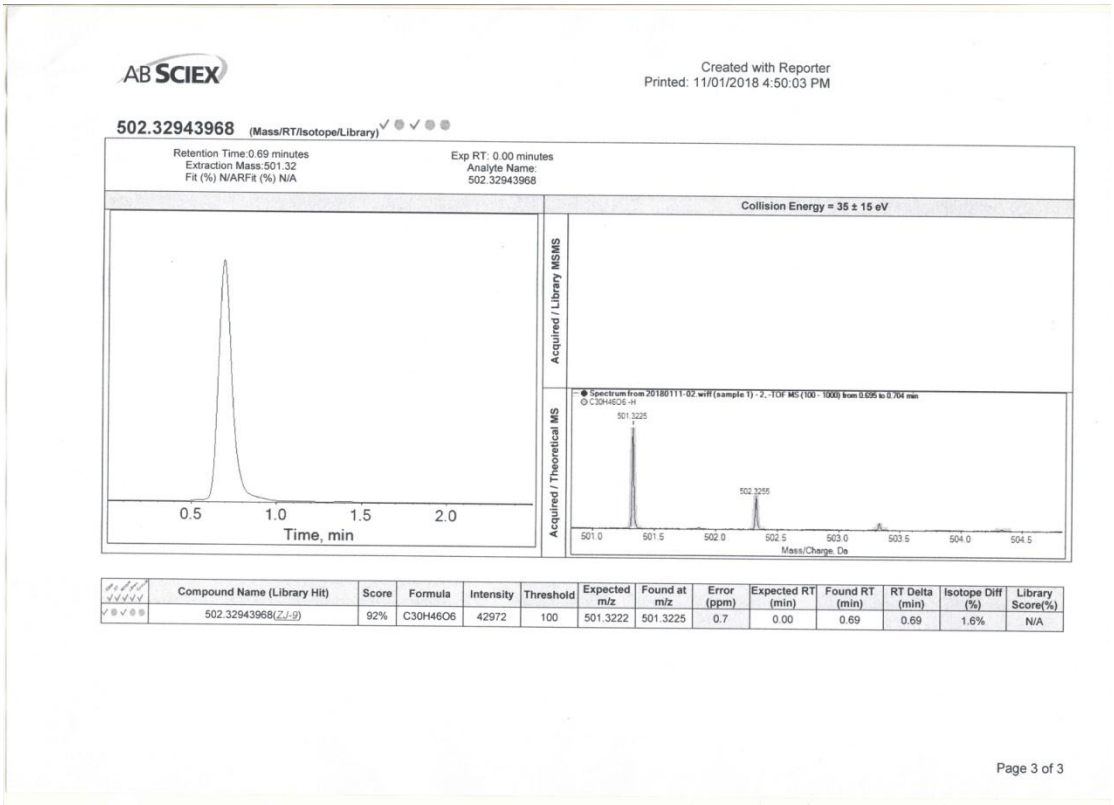


Fig. S82. ^{1}H NMR spectrum of compound **9** in CD_3OD (400 MHz).

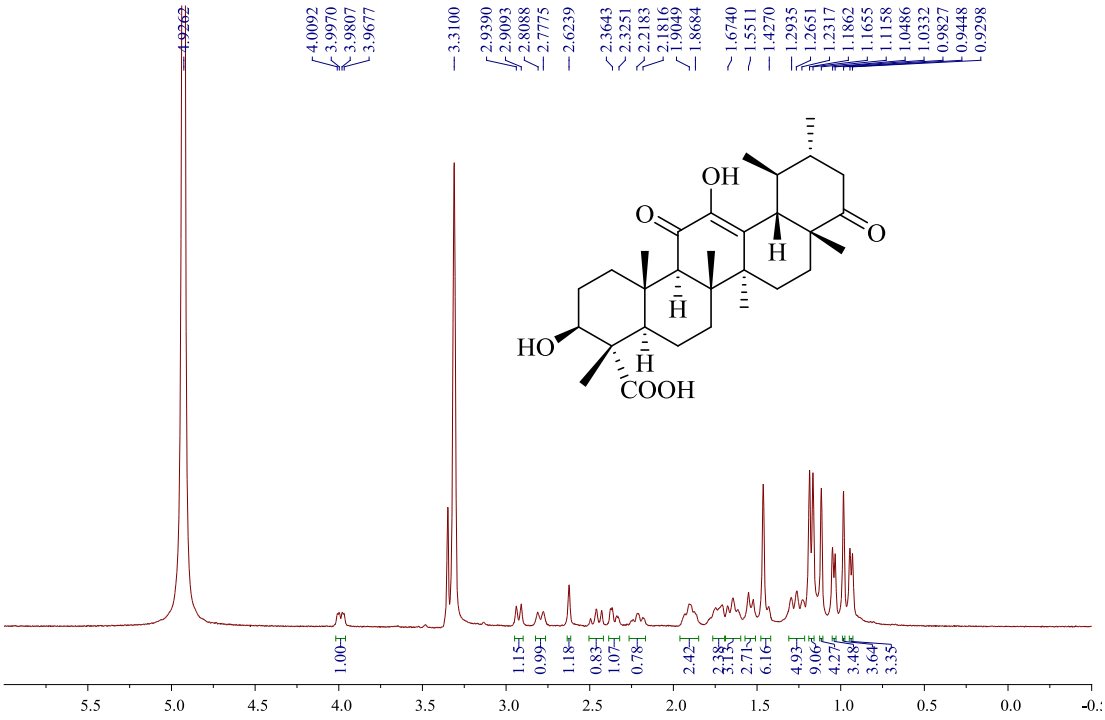


Fig. S83. ^{1}H NMR spectrum of compound **9**-expansion.

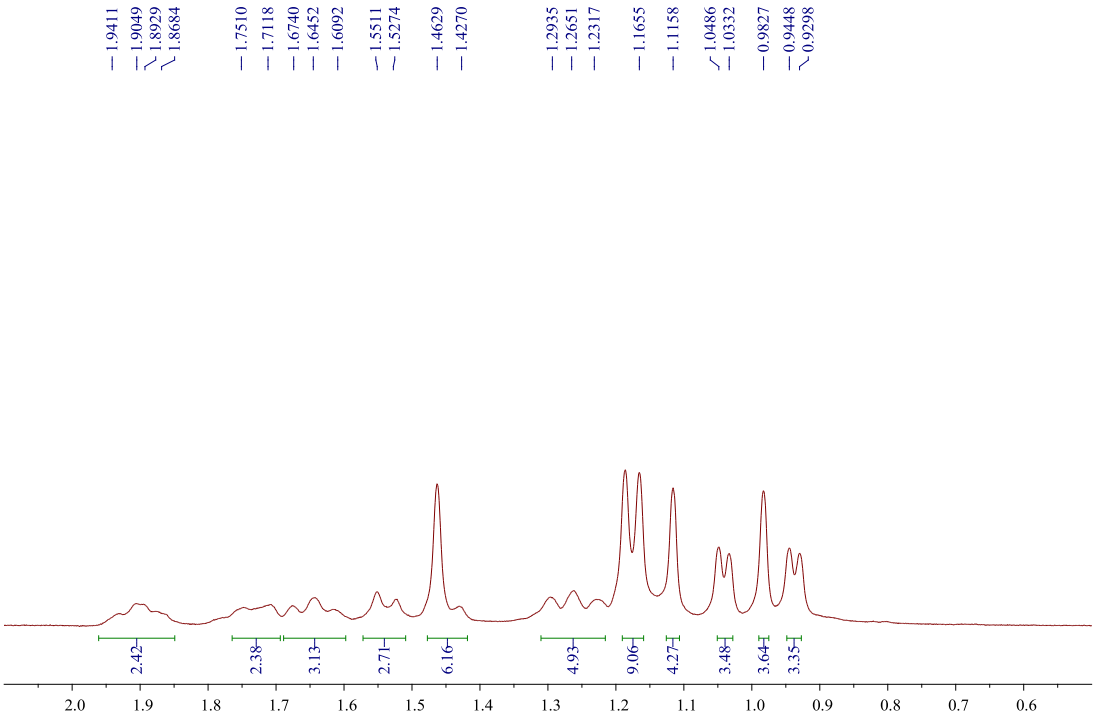


Fig. S84. ^{13}C NMR spectrum of compound **9** in CD_3OD (150 MHz).

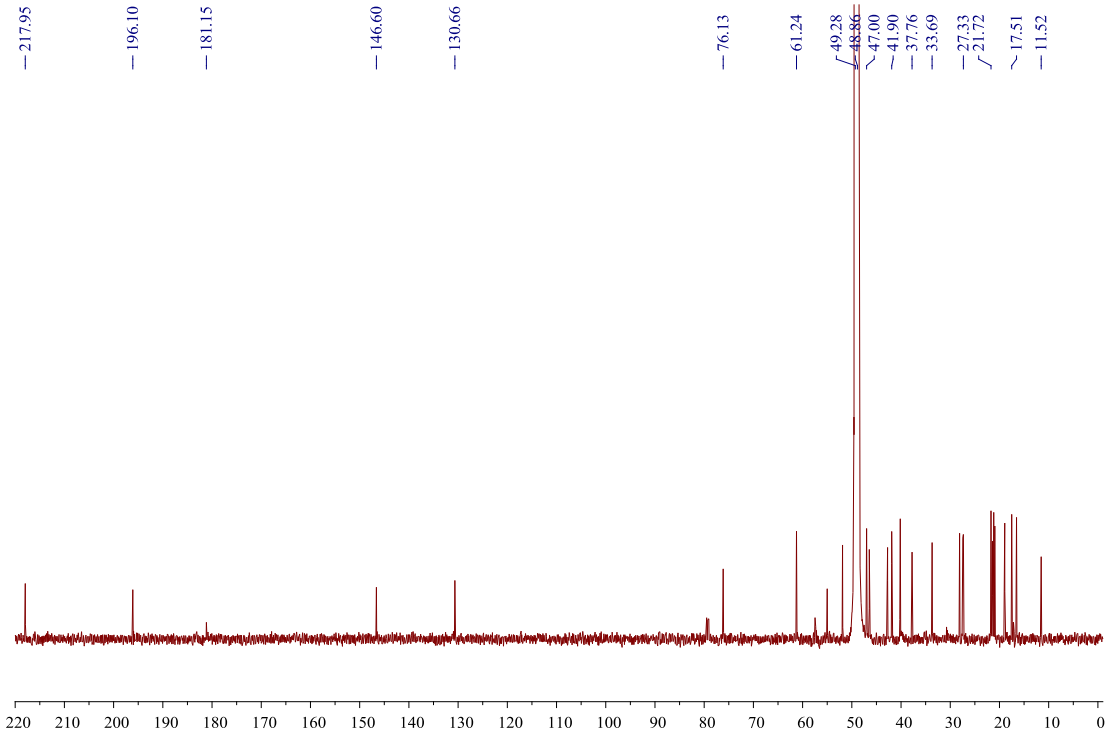


Fig. S85. ^{13}C NMR spectrum of compound **9**-expansion.

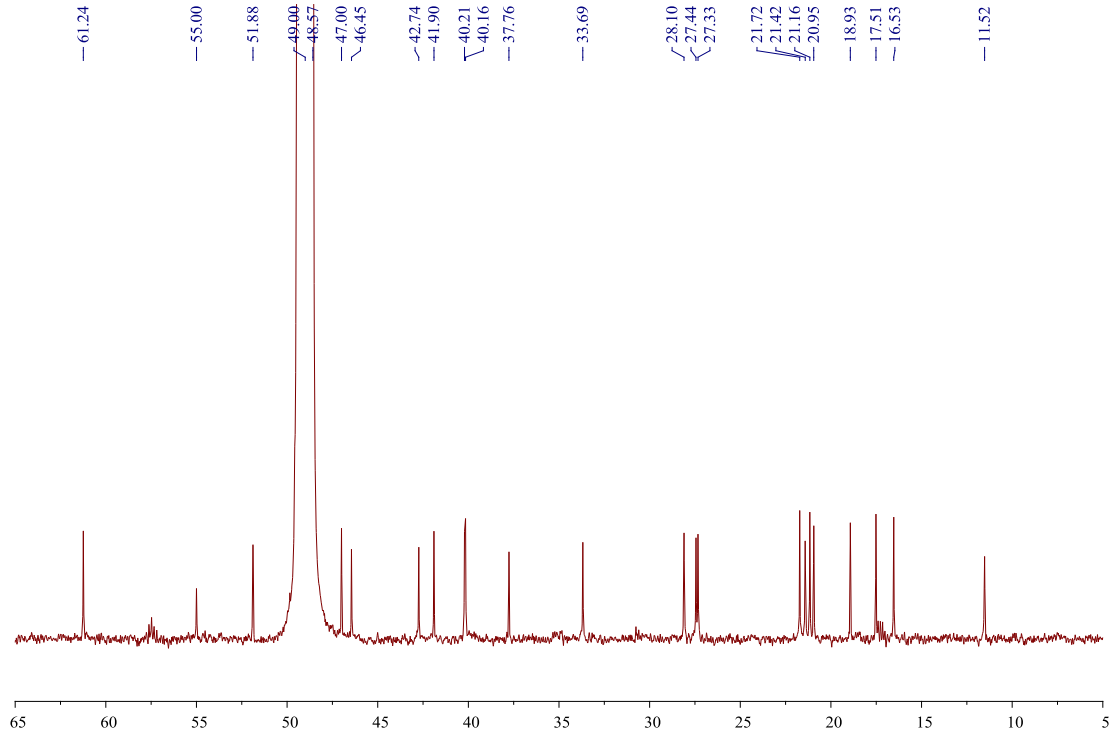


Fig. S86. HMBC spectrum of compound **9** in CD_3OD (600 MHz).

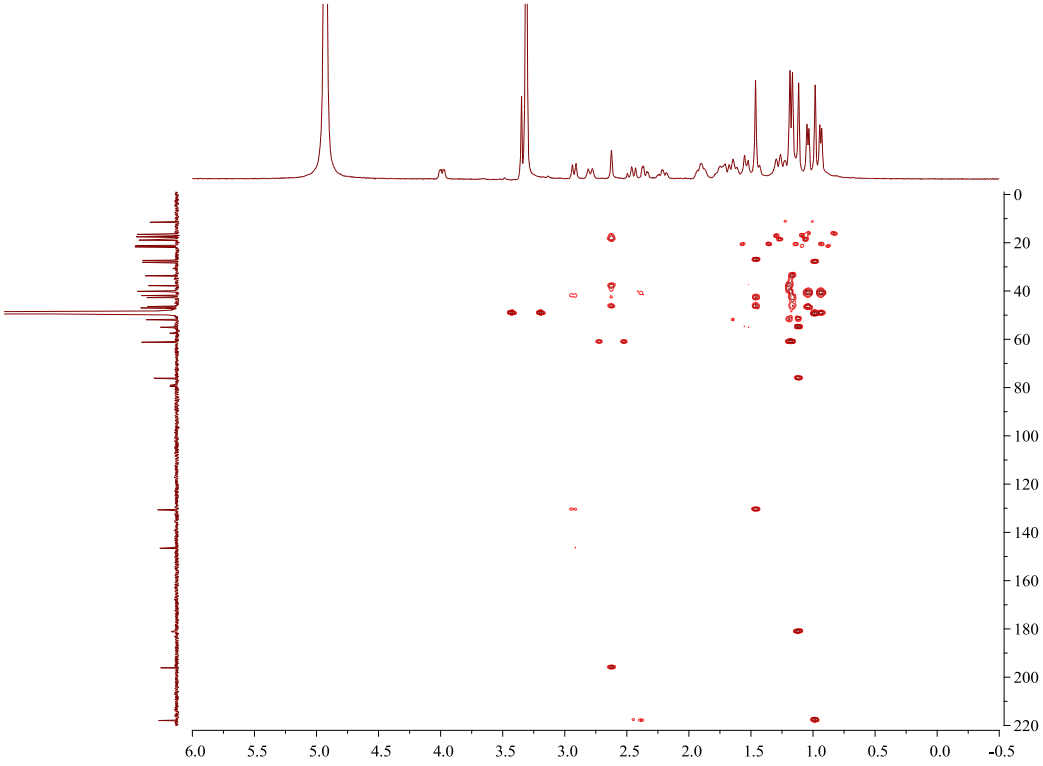


Fig. S87. HMBC spectrum of compound **9**-expansion.

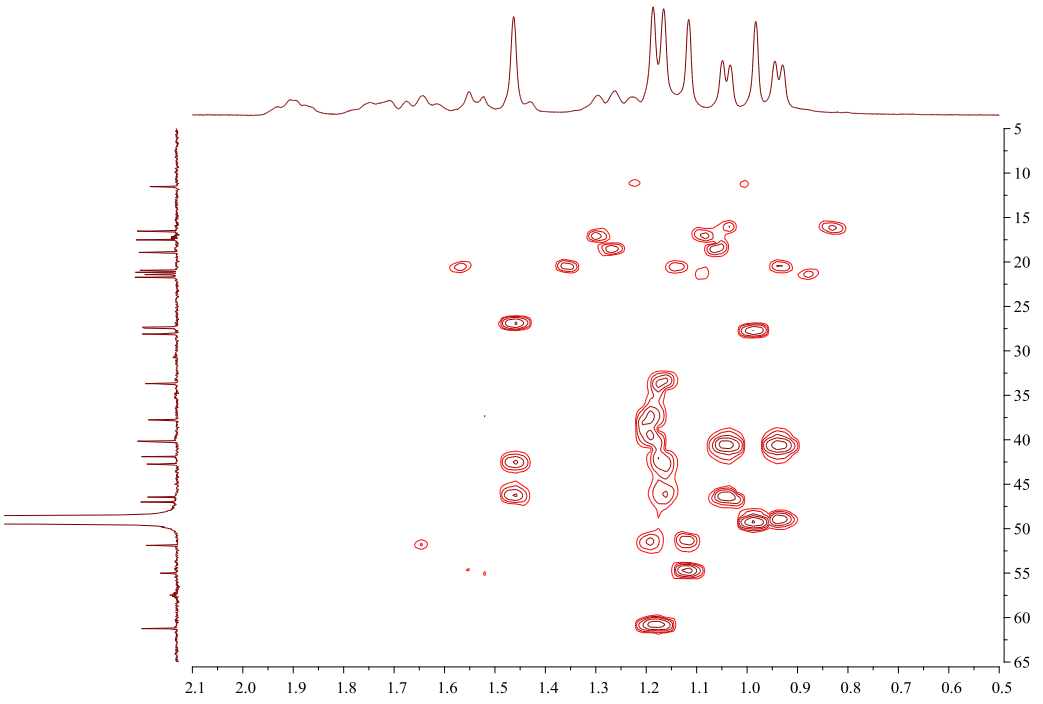


Fig. S88. ROESY spectrum of compound **9** in CD_3OD (600 MHz).

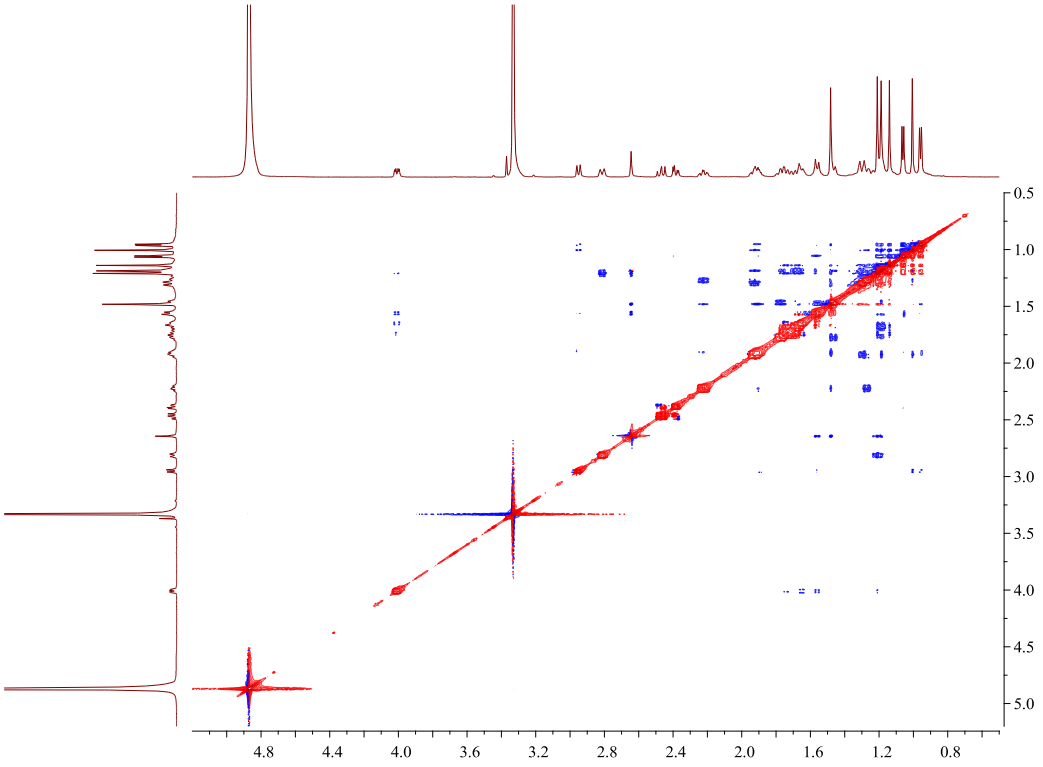


Fig. S89. HRESIMS report of compound **9**.

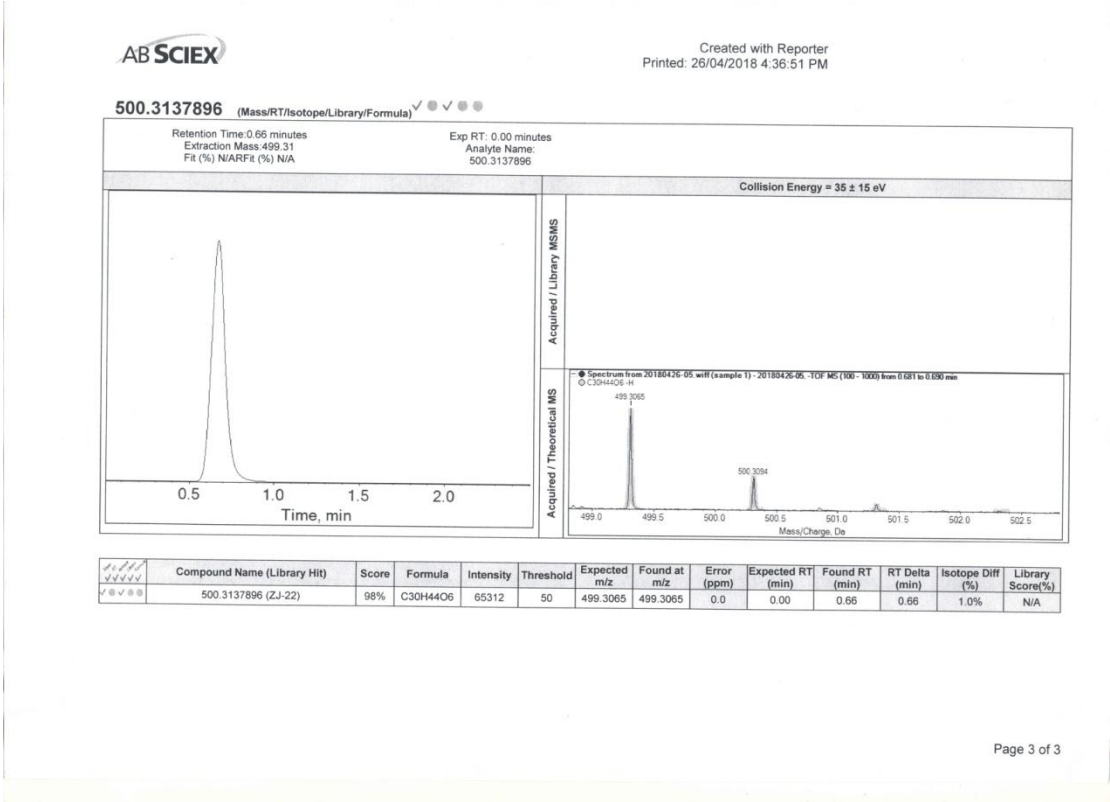


Fig. S90. ^{1}H NMR spectrum of compound **10** in CD_3OD (400 MHz).

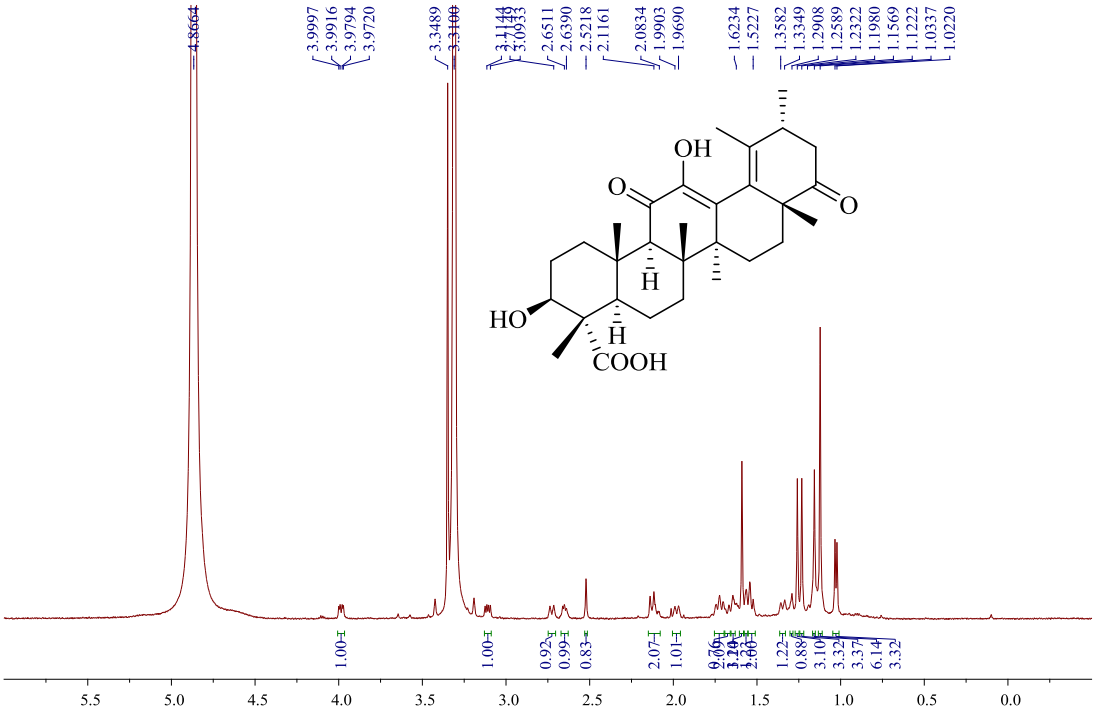


Fig. S91. ^{1}H NMR spectrum of compound **10**-expansion.

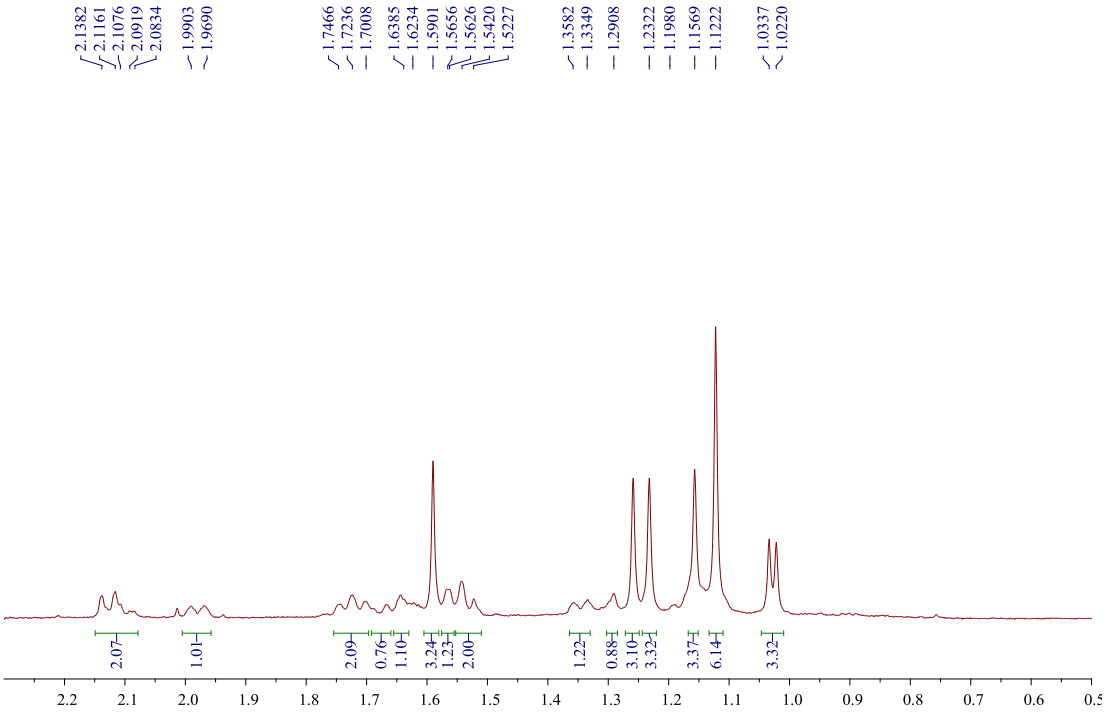


Fig. S92. ^{13}C NMR spectra of compound **10** in CD_3OD (150 MHz).

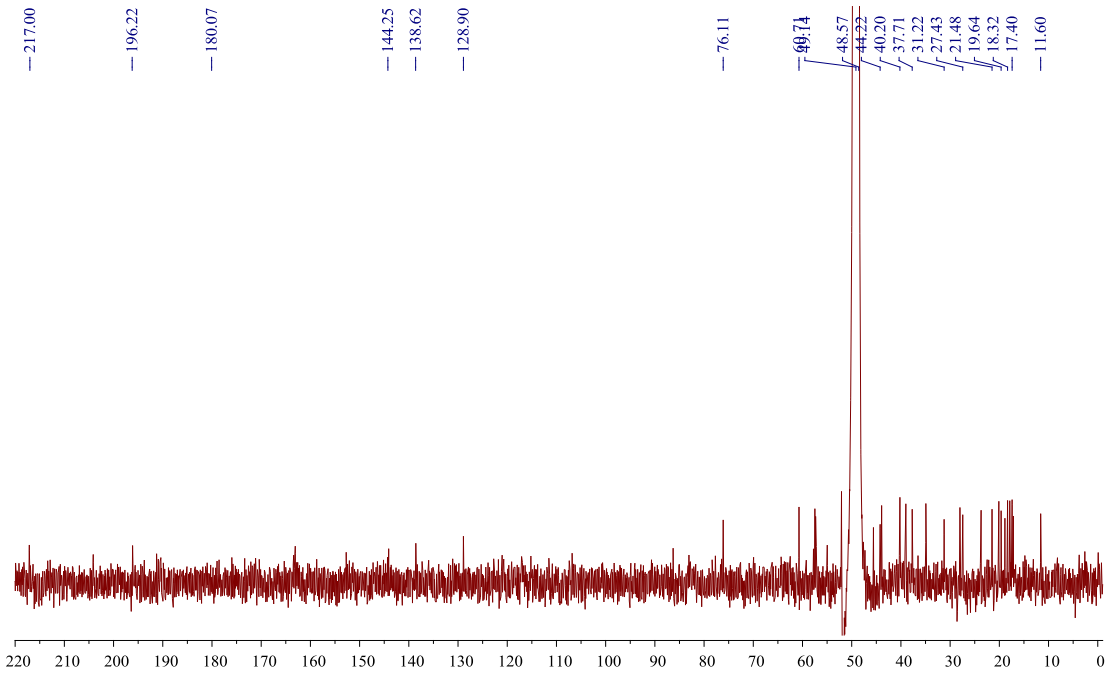


Fig. S93. HSQC spectrum of compound **10** in CD_3OD (600 MHz).

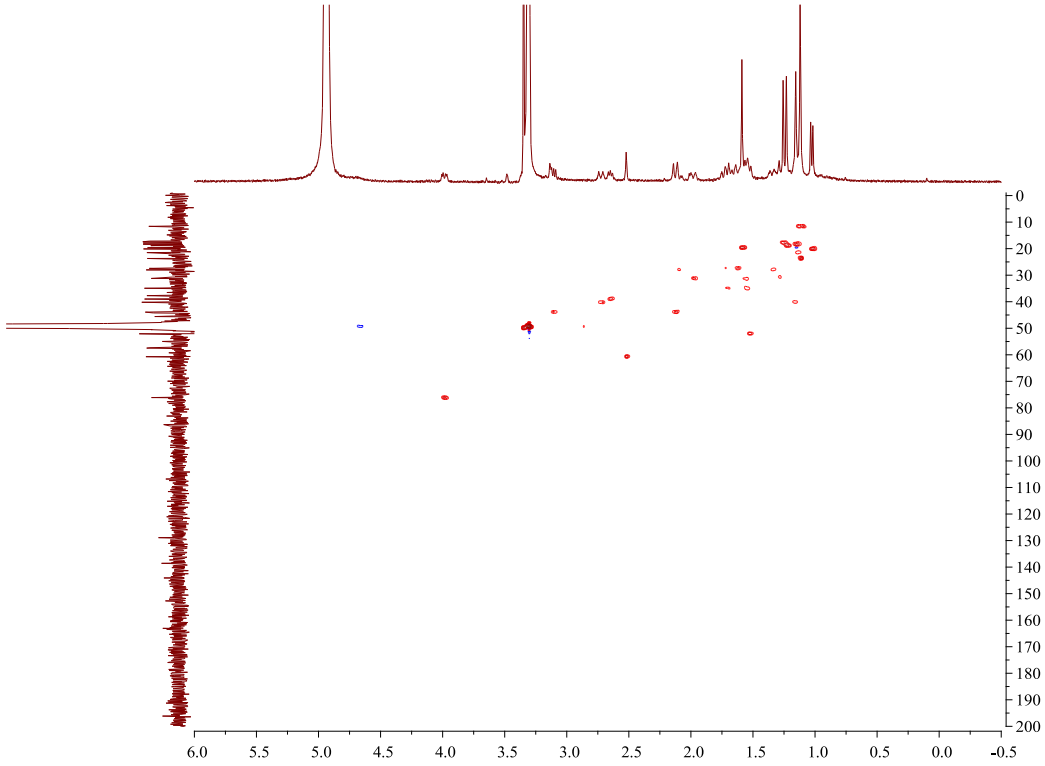


Fig. S94. HMBC spectrum of compound **10** in CD_3OD (600 MHz).

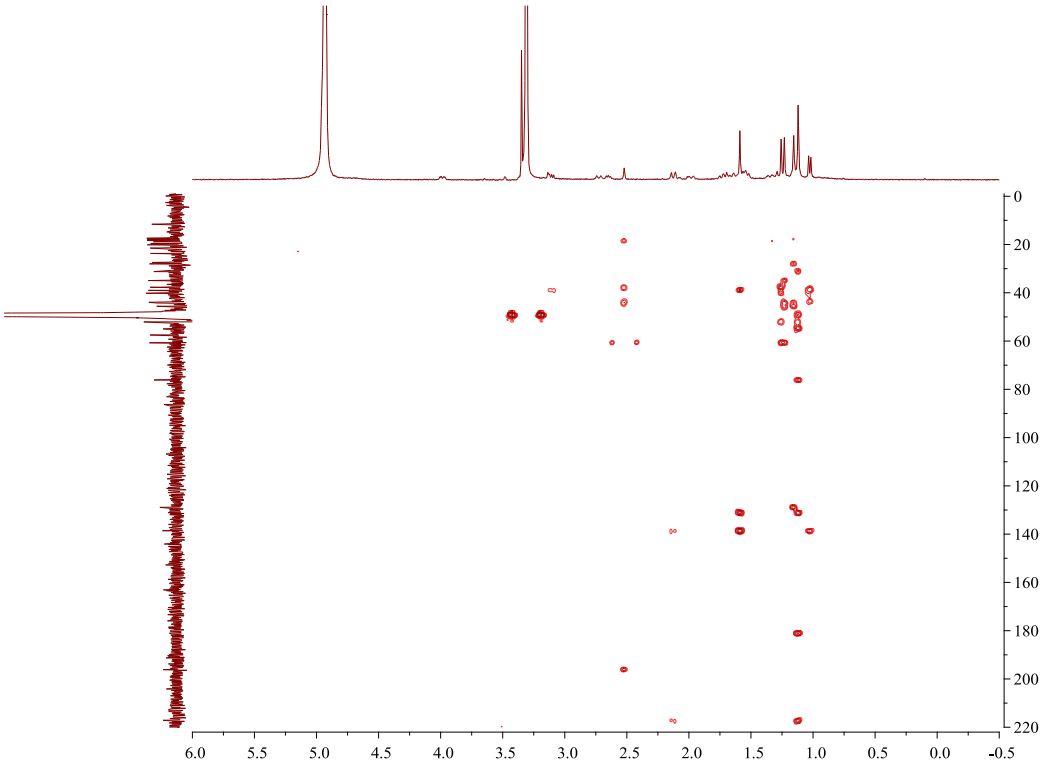


Fig. S95. HMBC spectrum of compound **10**–expansion.

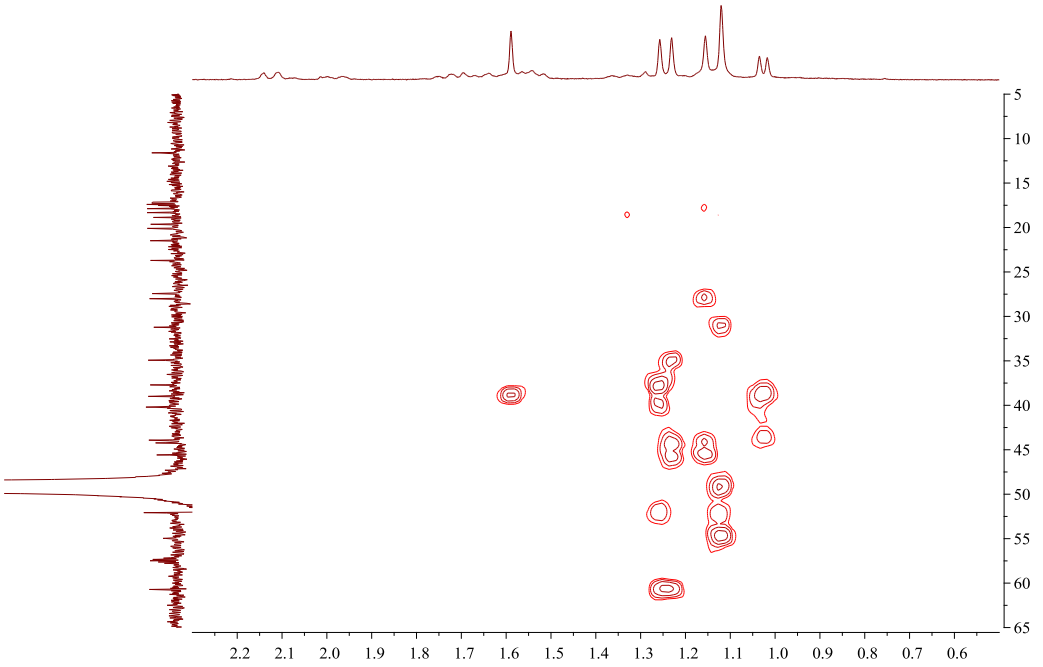


Fig. S96. ROESY spectrum of compound **10** in CD_3OD (600 MHz).

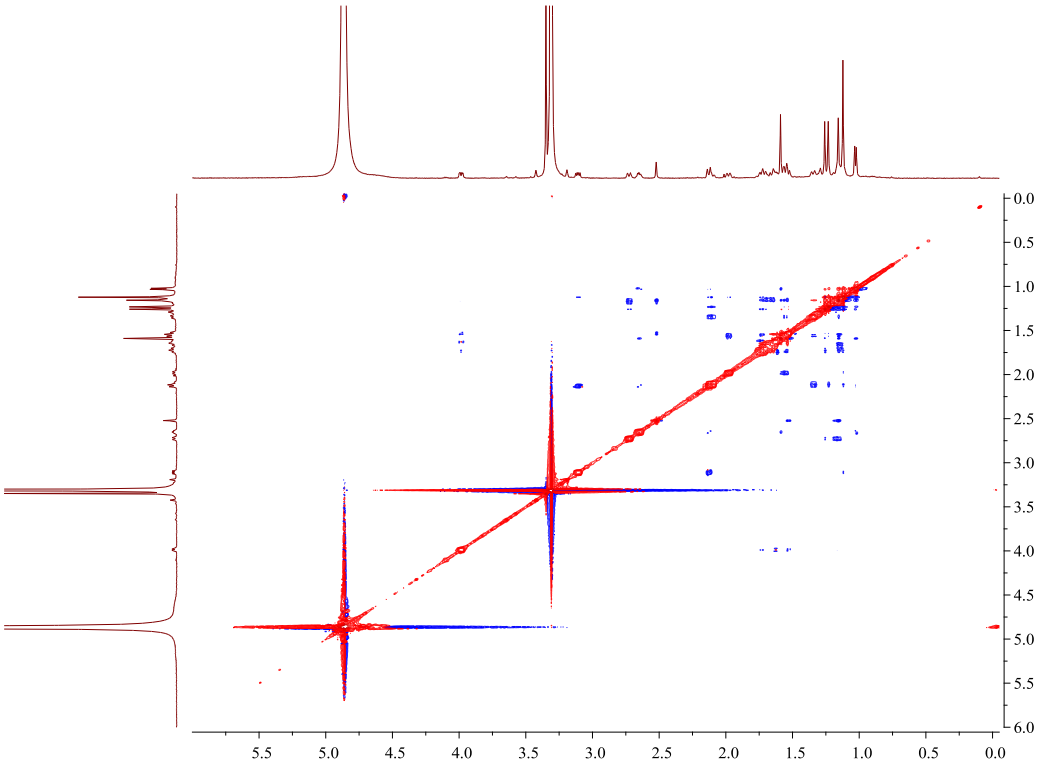


Fig. S97. HRESIMS report of compound **10**.

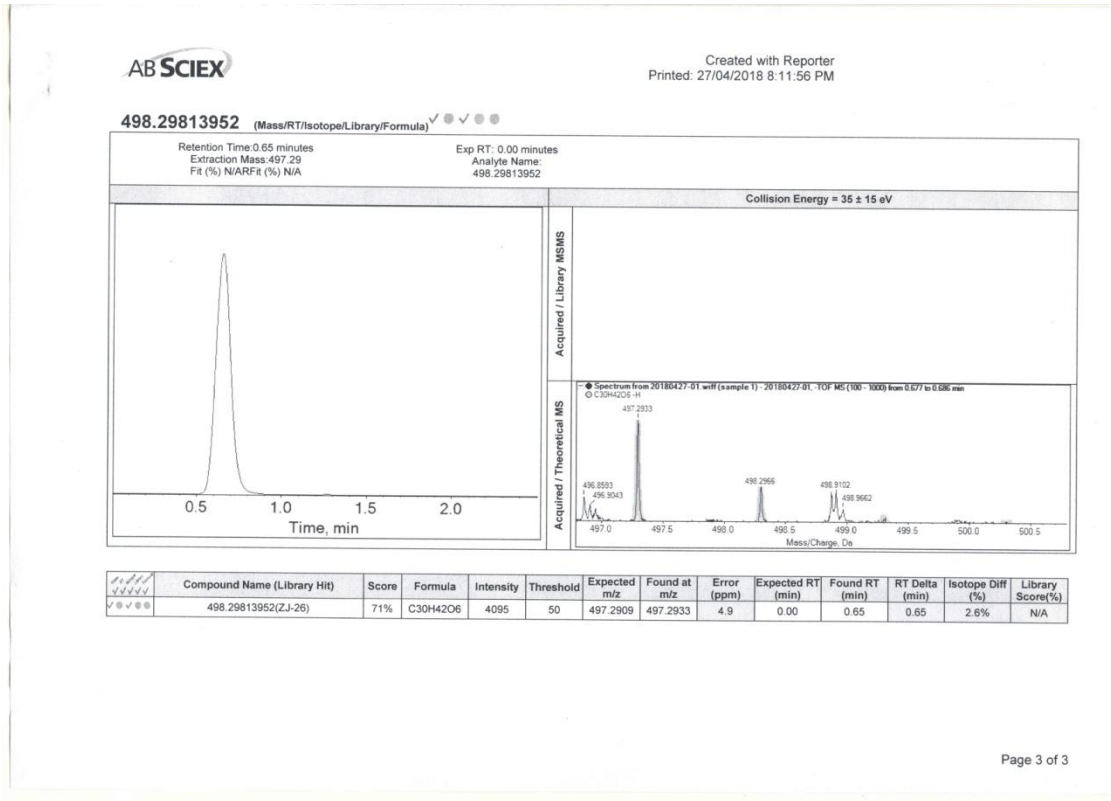


Fig. S98. ^{1}H NMR spectrum of compound **11** in C_5D_5N (400 MHz).

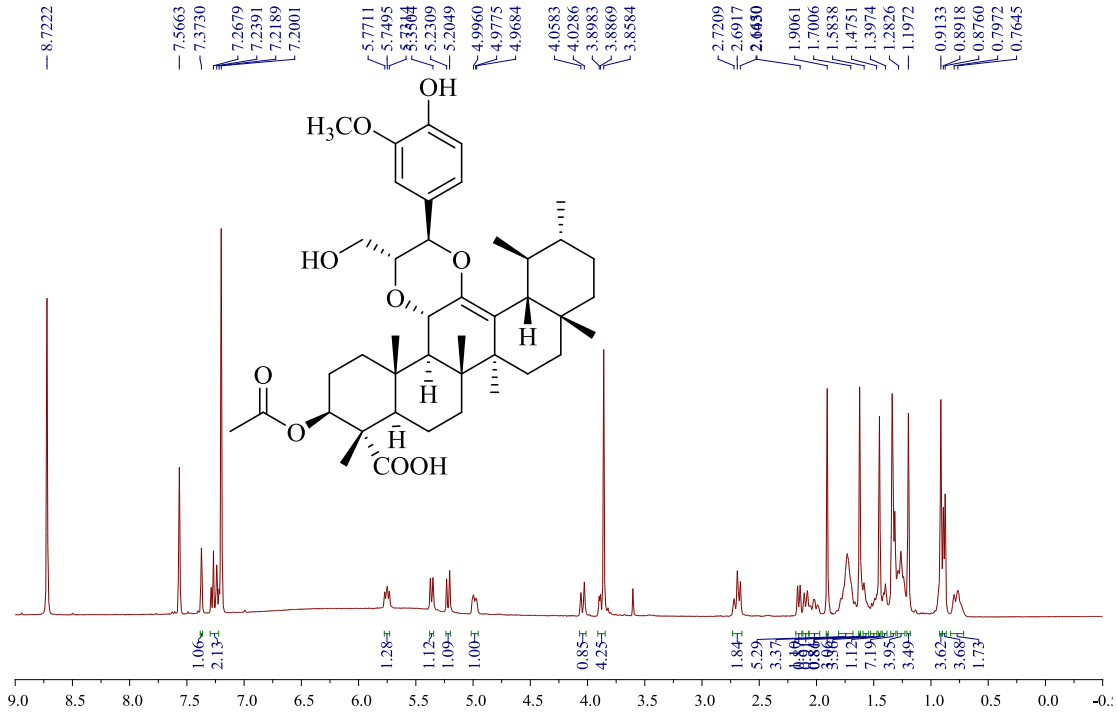


Fig. S99. ^{1}H NMR spectrum of compound **11**-expansion.

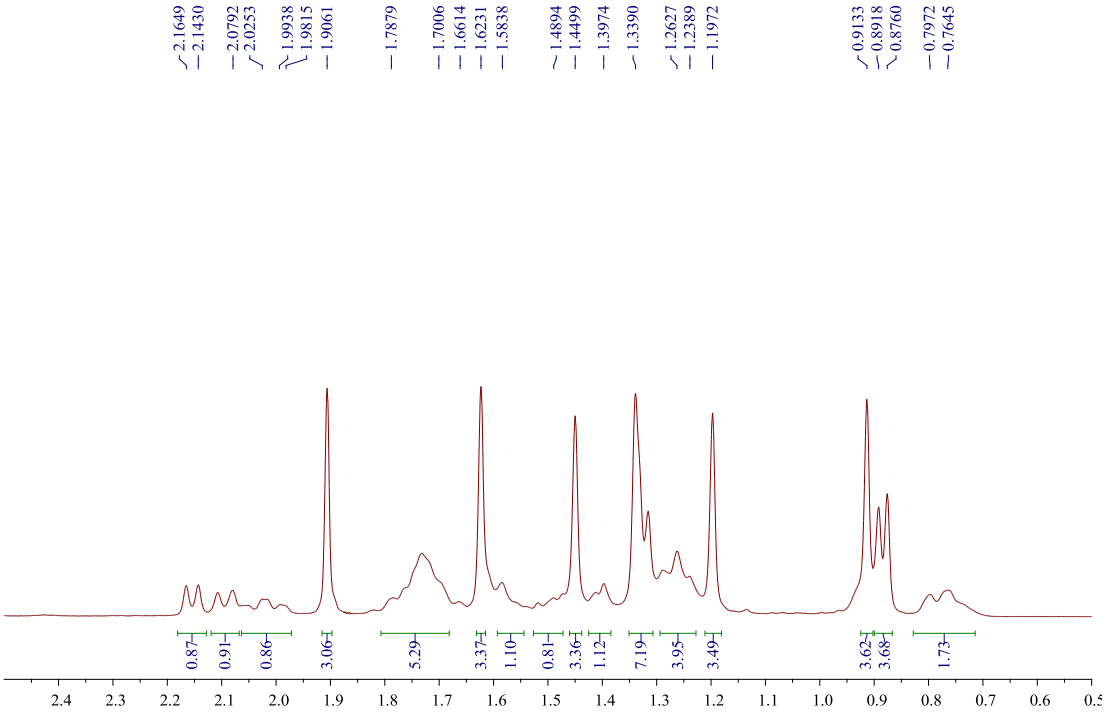


Fig. S100. ^{13}C NMR spectrum of compound **11** in C_5D_5N (150 MHz).

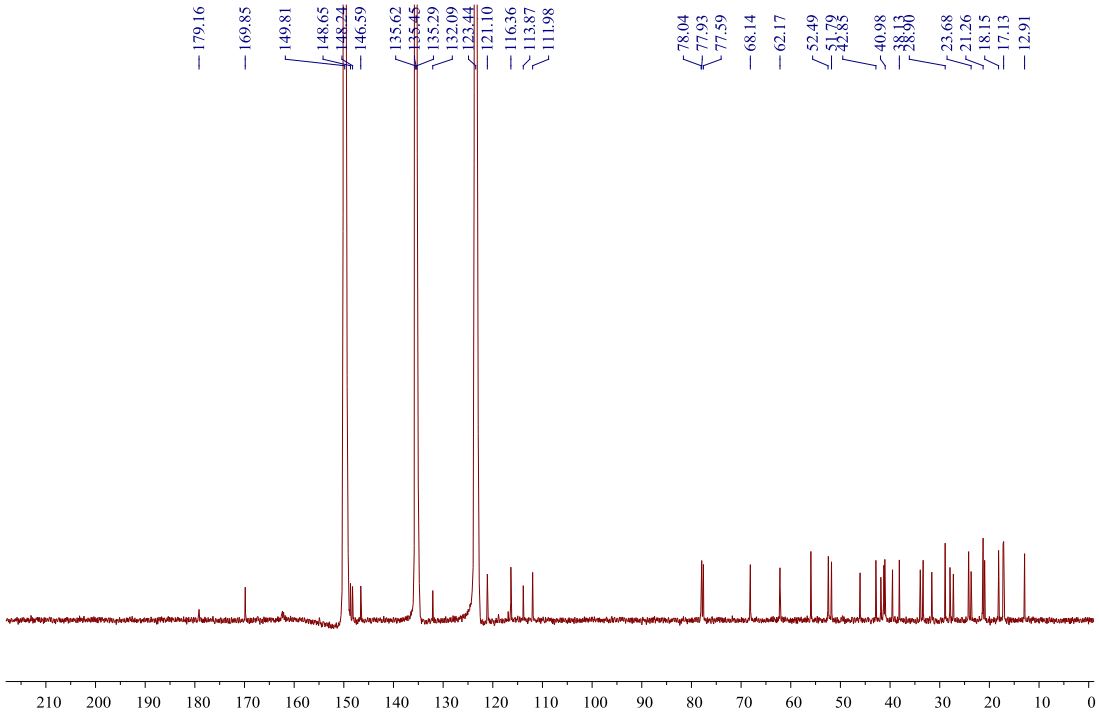


Fig. S101. ^{13}C NMR spectrum of compound **11**-expansion.

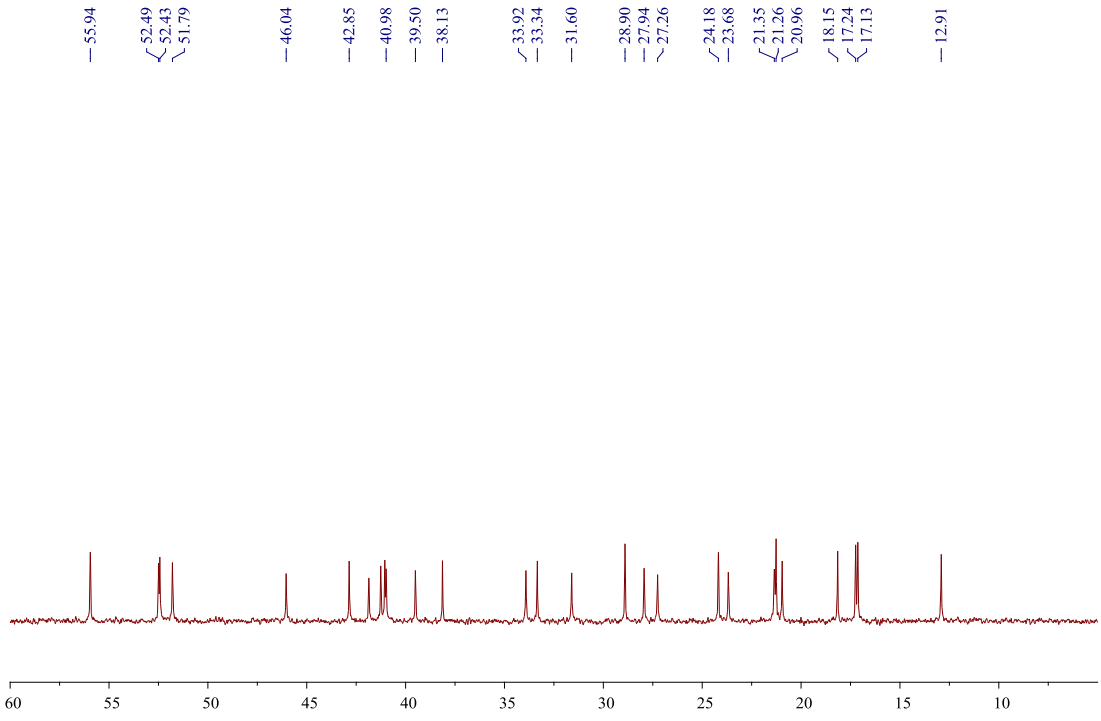


Fig. S102. HSQC spectrum of compound **11** in C_5D_5N (600 MHz).

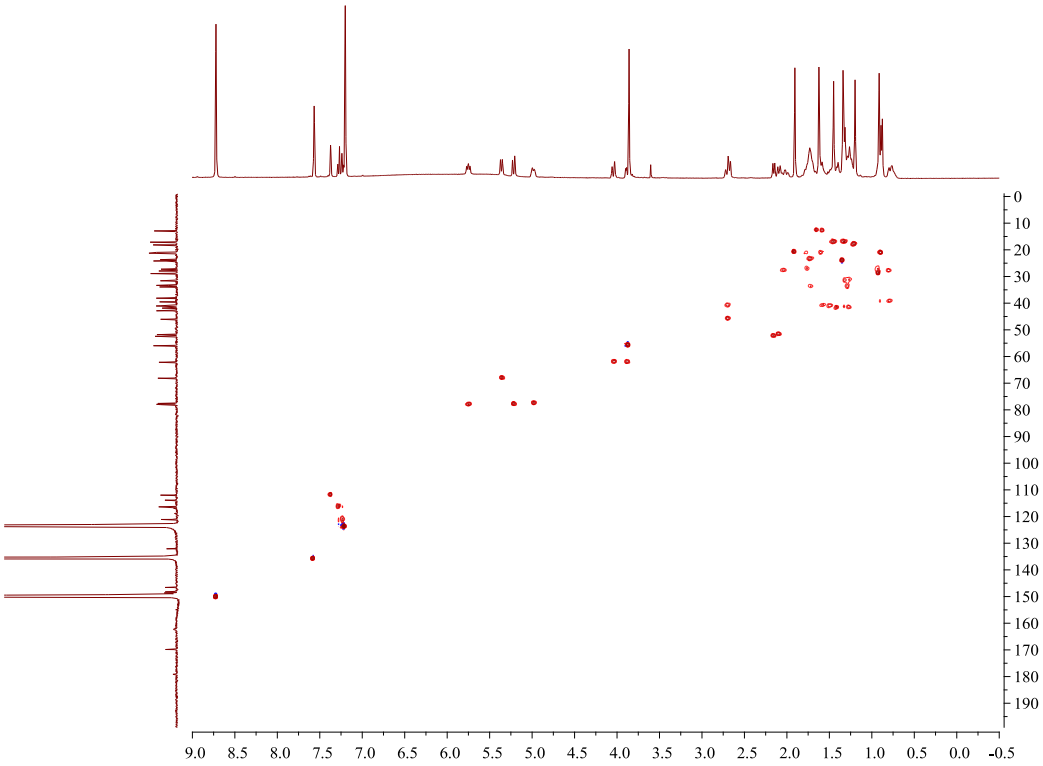


Fig. S103.^{1}H-^{1}H COSY spectrum of compound **11** in C_5D_5N (600 MHz).

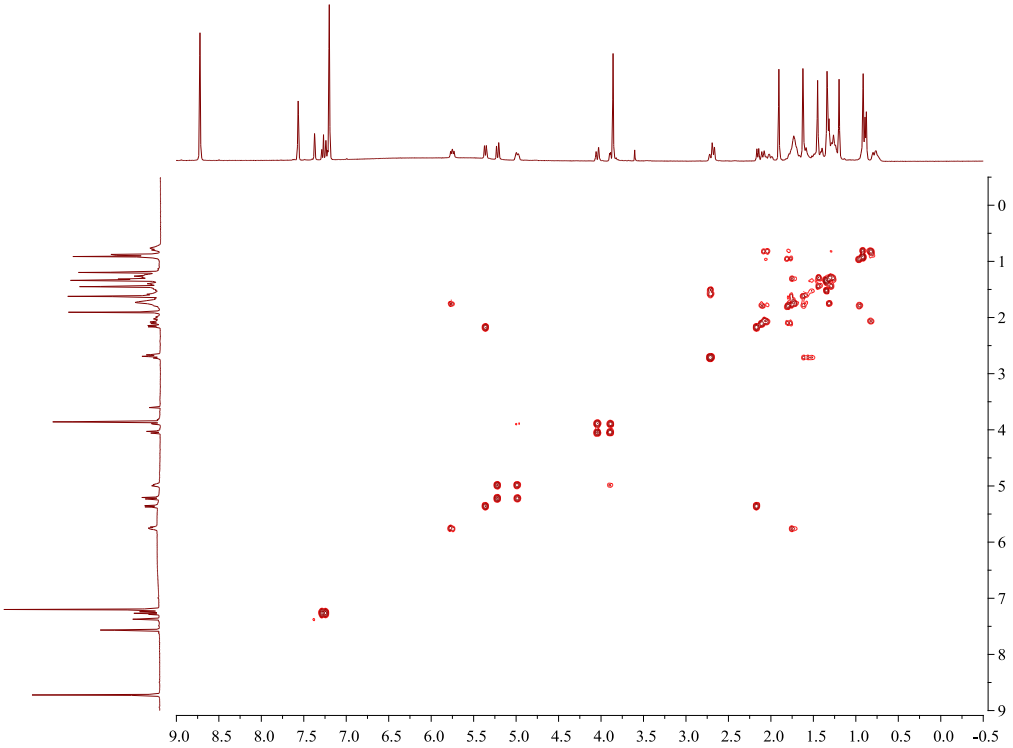


Fig. S104. HMBC spectrum of compound **11** in C_5D_5N (600 MHz).

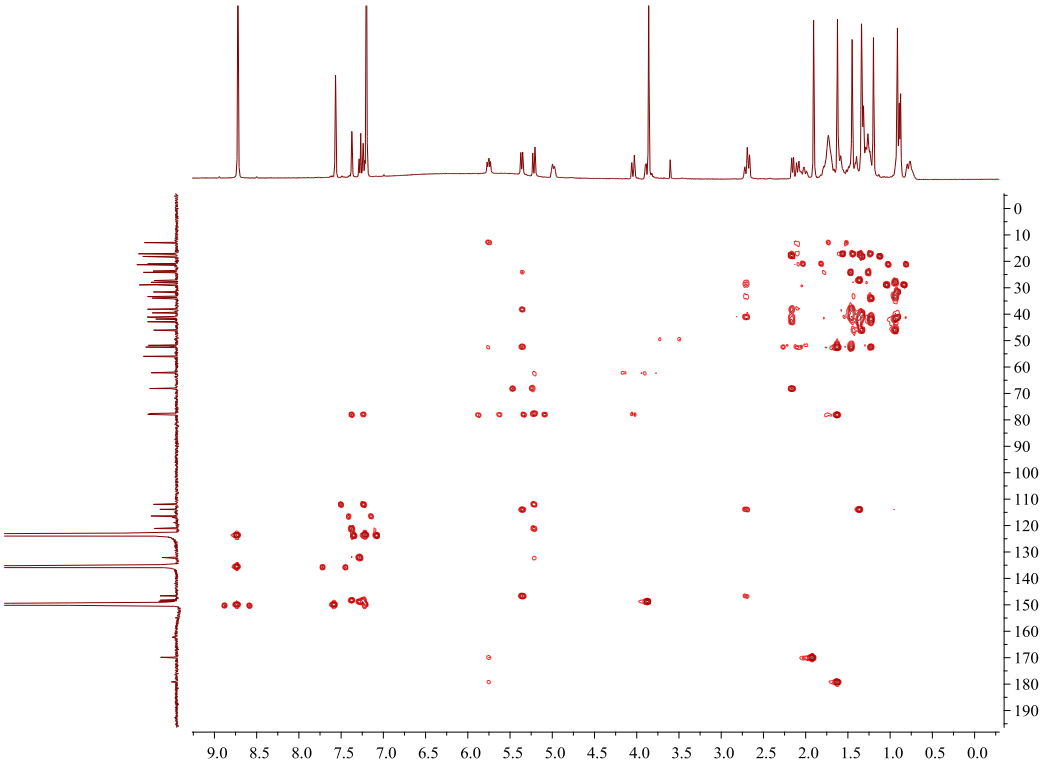


Fig. S105. HMBC spectrum of compound **11** –expansion.

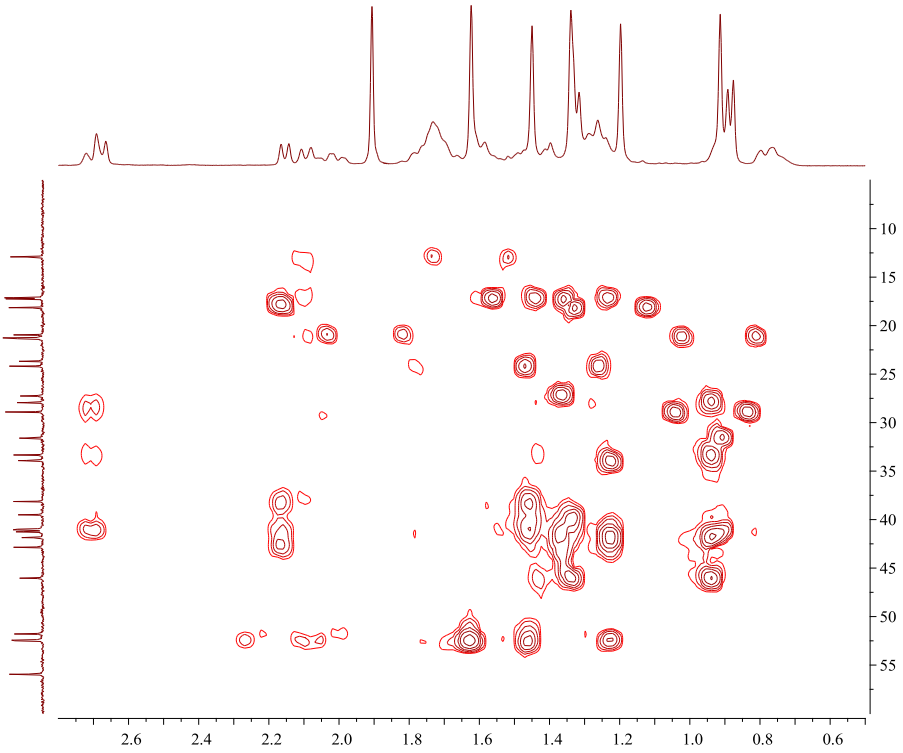


Fig. S106. ROESY spectrum of compound **11** in C_5D_5N (600 MHz).

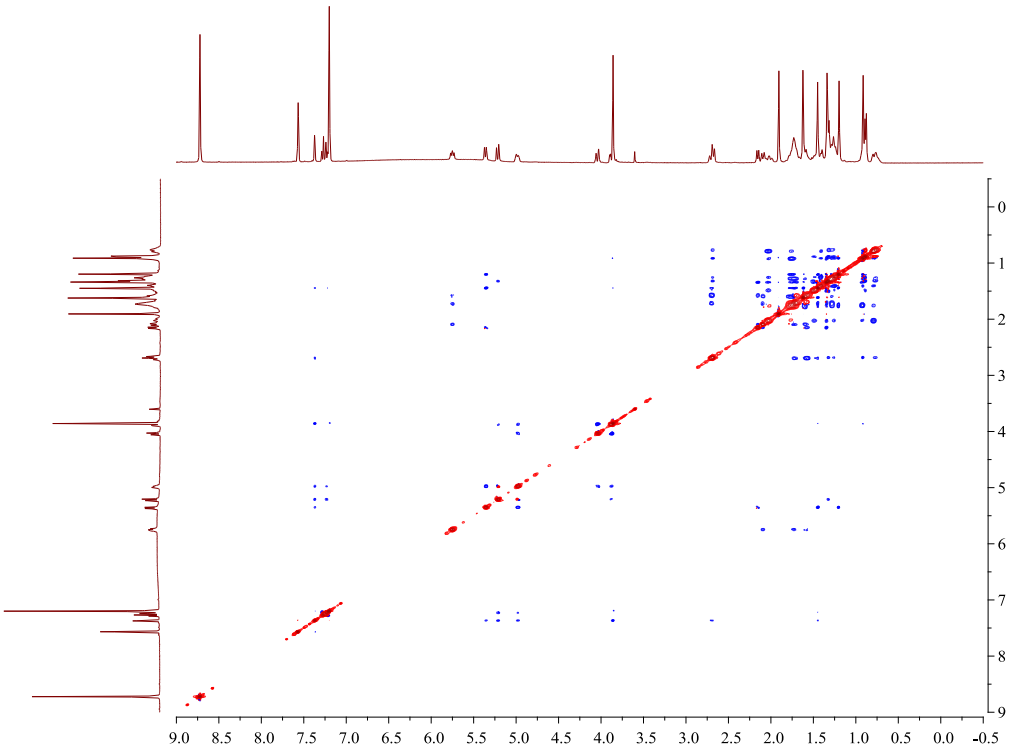


Fig. S107. ROESY spectrum of compound **11** –expansion.

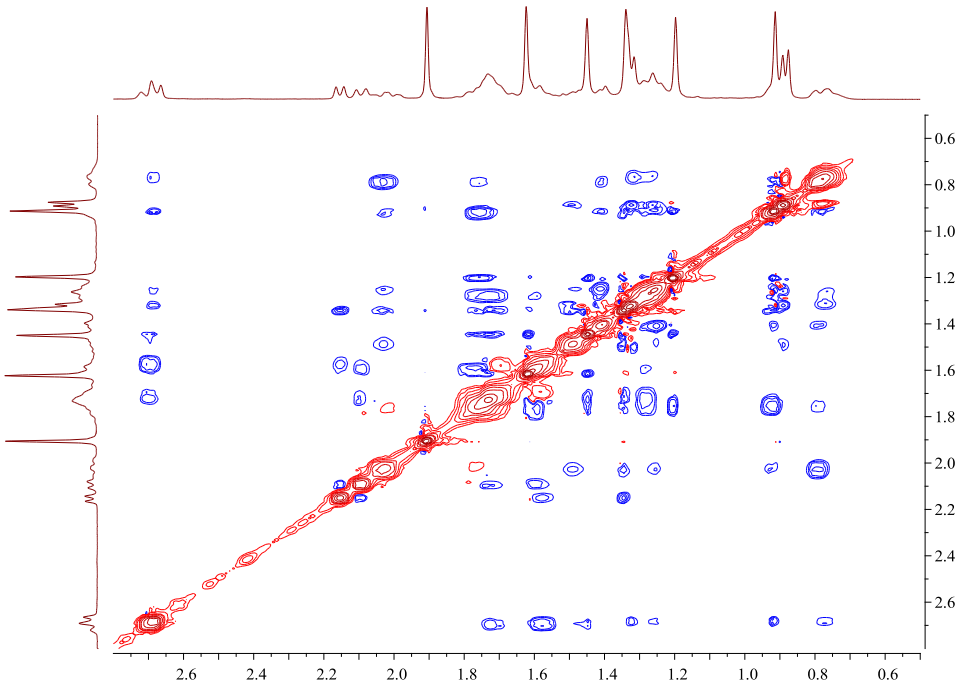


Fig. S108. HRESIMS report of compound **11**.

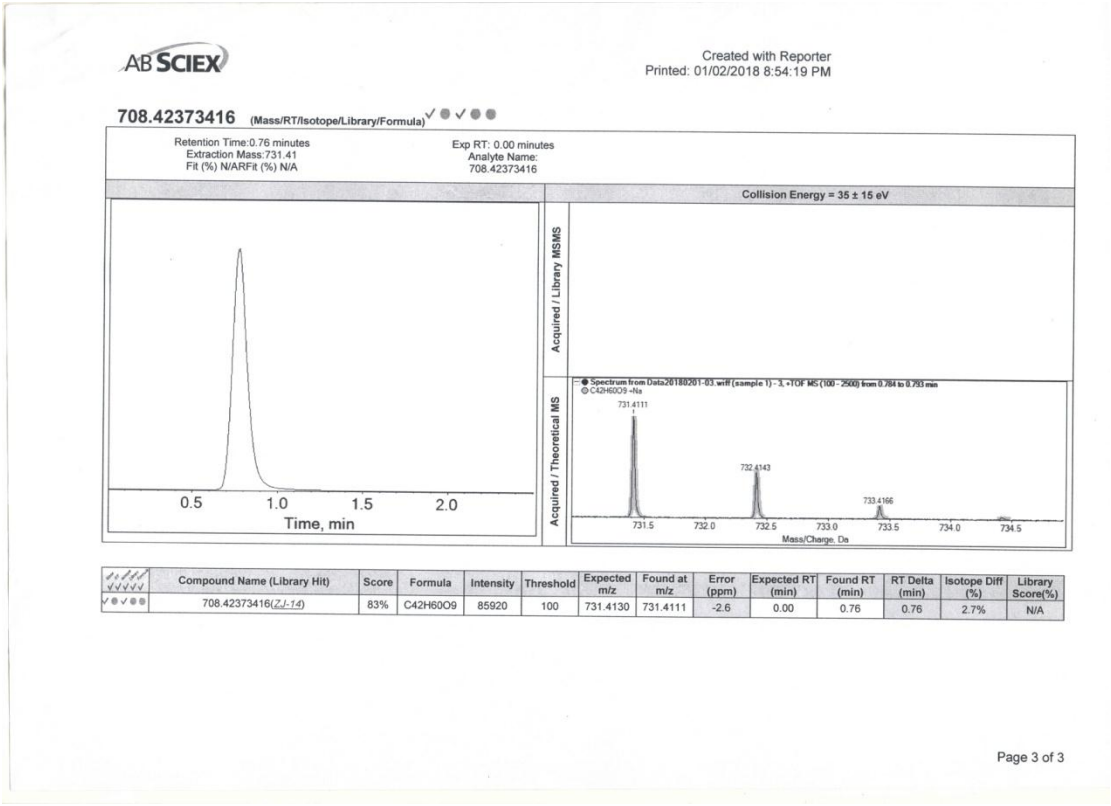


Fig. S109. ^{1}H NMR spectrum of compound **12** in C_5D_5N (400 MHz).

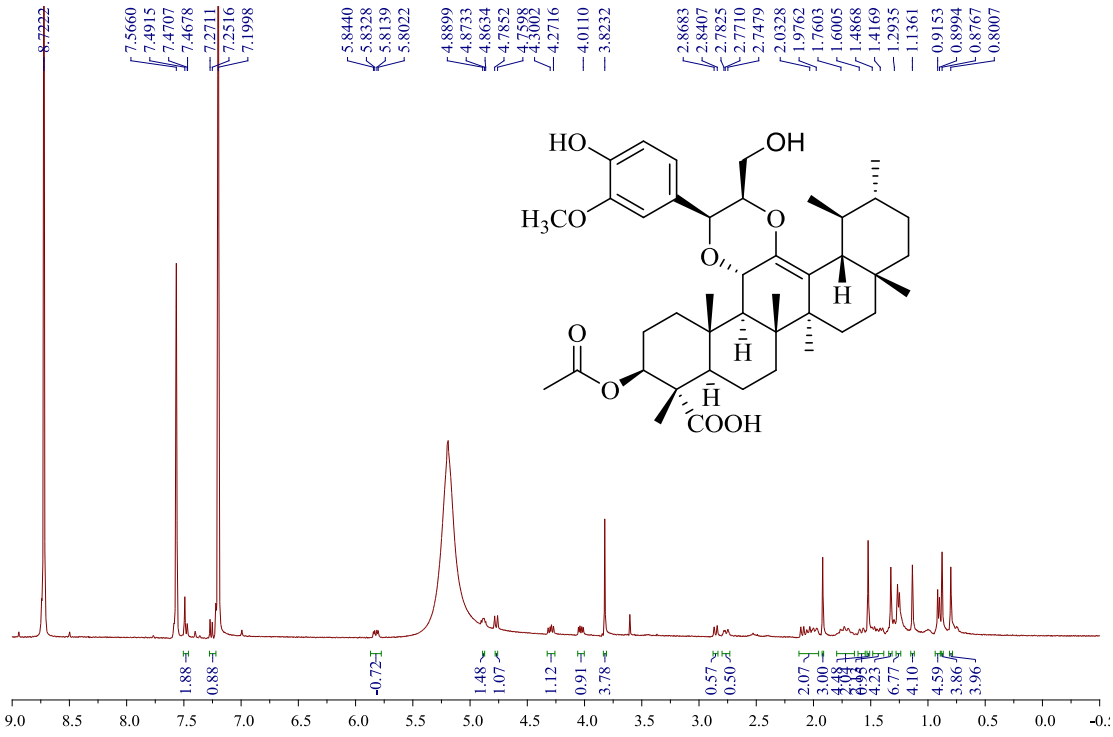


Fig. S110. ^{1}H NMR spectrum of compound **12**–expansion.

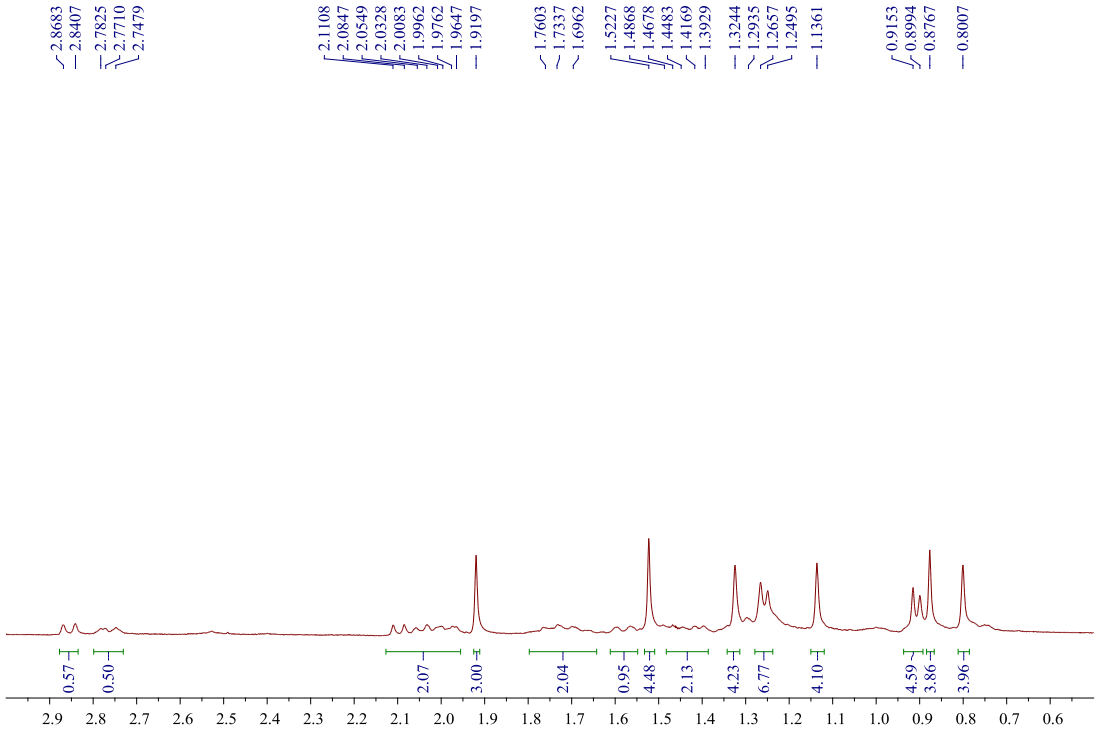


Fig. S111. ^{13}C NMR spectrum of compound **12** in C_5D_5N (150 MHz).

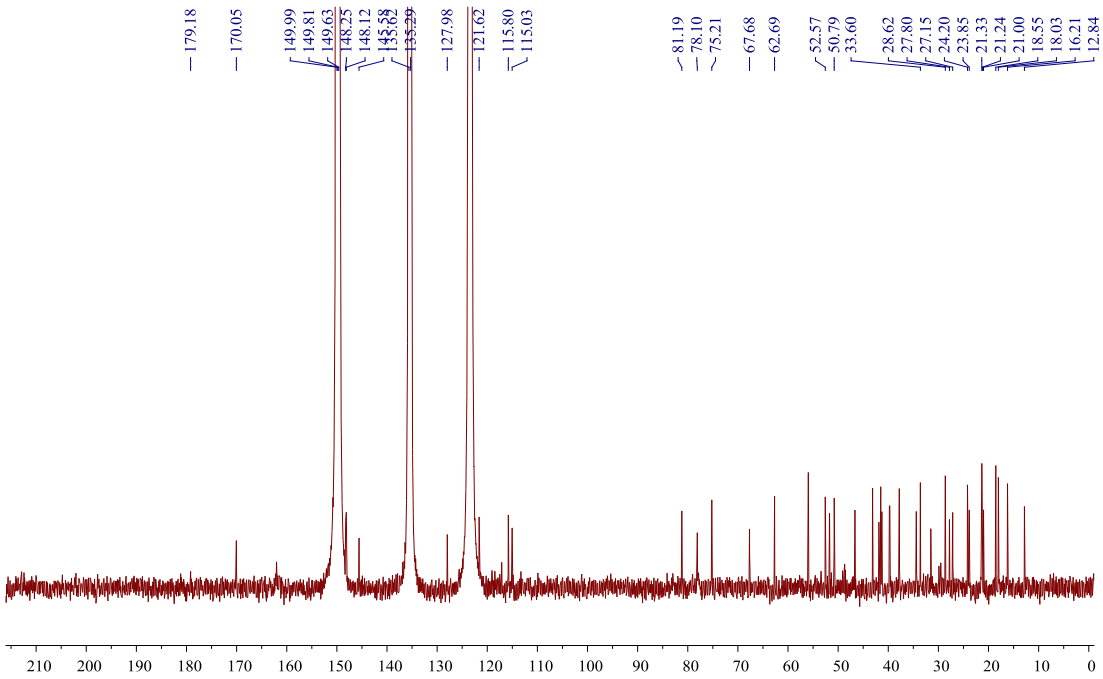


Fig. S112. ^{13}C NMR spectrum of compound **12**–expansion.

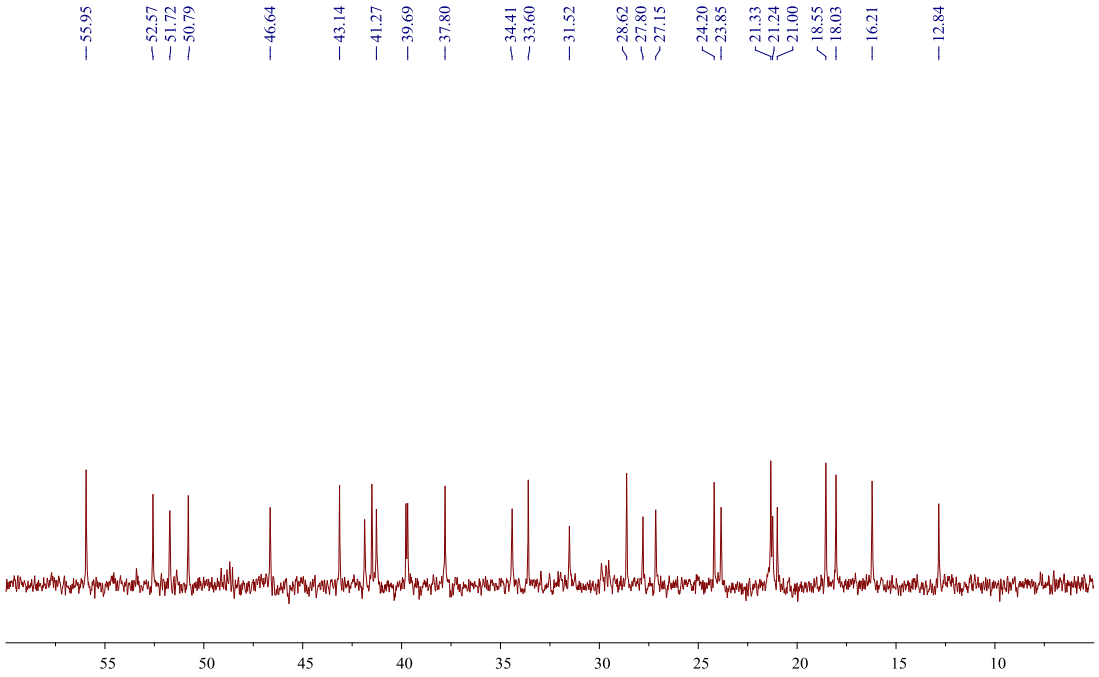


Fig. S113. ^{1}H-^{1}H COSY spectrum of compound **12** in C_5D_5N (600 MHz).

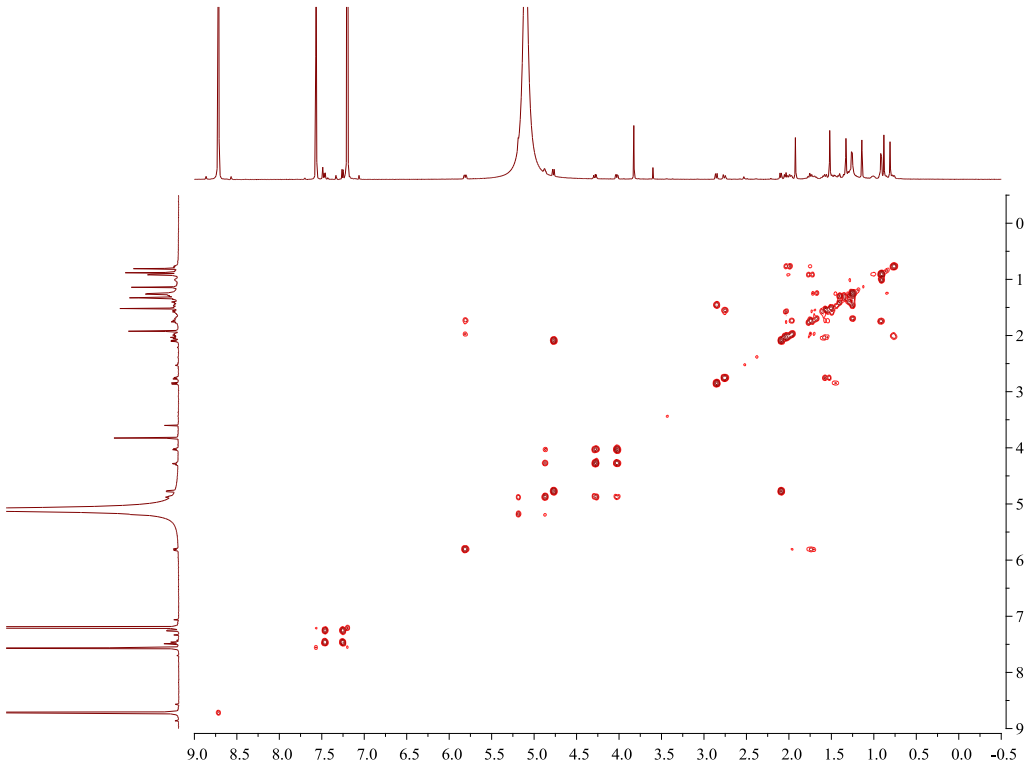


Fig. S114. HMBC spectrum of compound **12** in C_5D_5N (600 MHz).

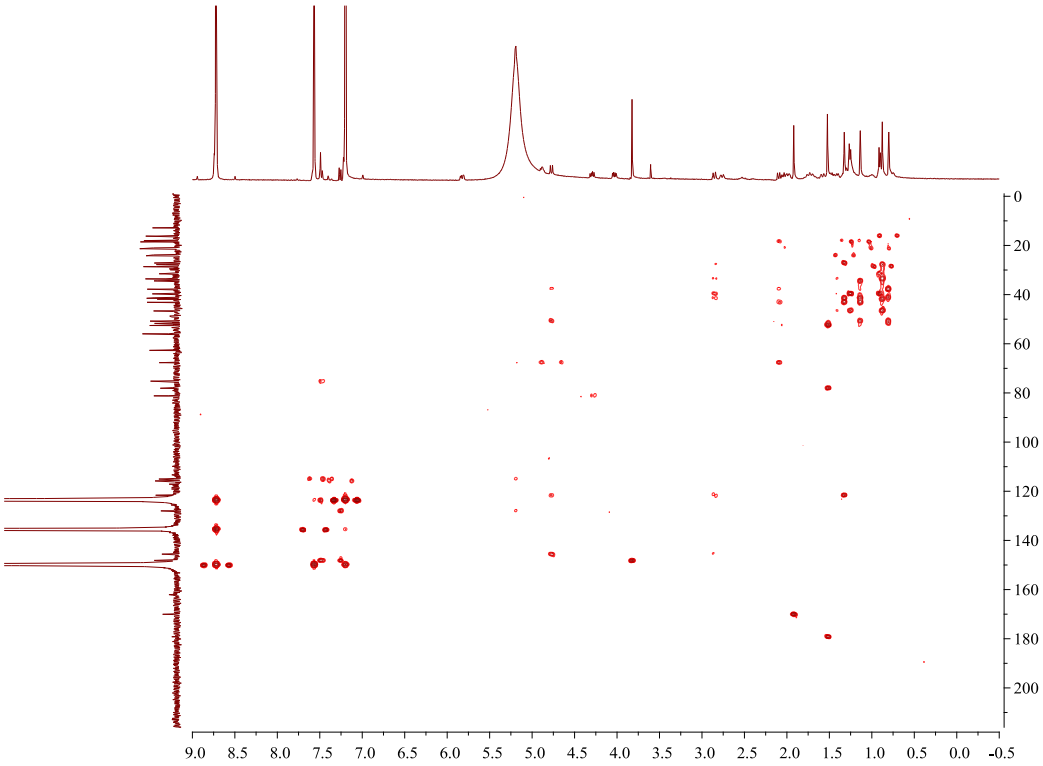


Fig. S115. ROESY spectrum of compound **12** in C_5D_5N (600 MHz).

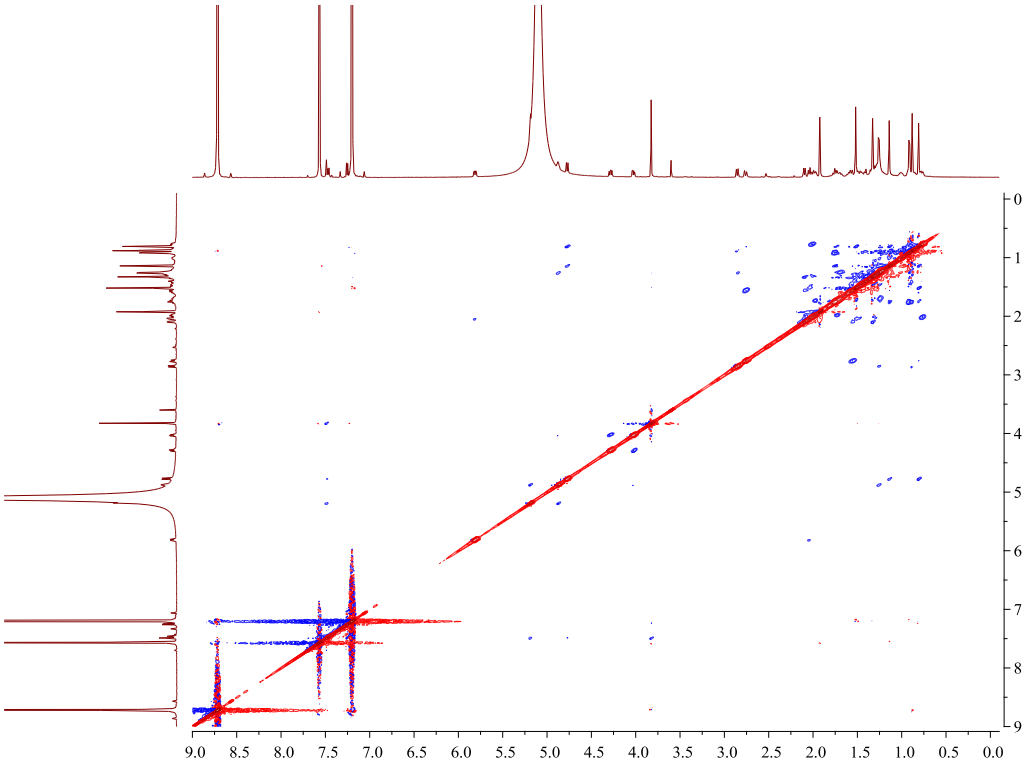


Fig. S116. HRESIMS report of compound **12**.

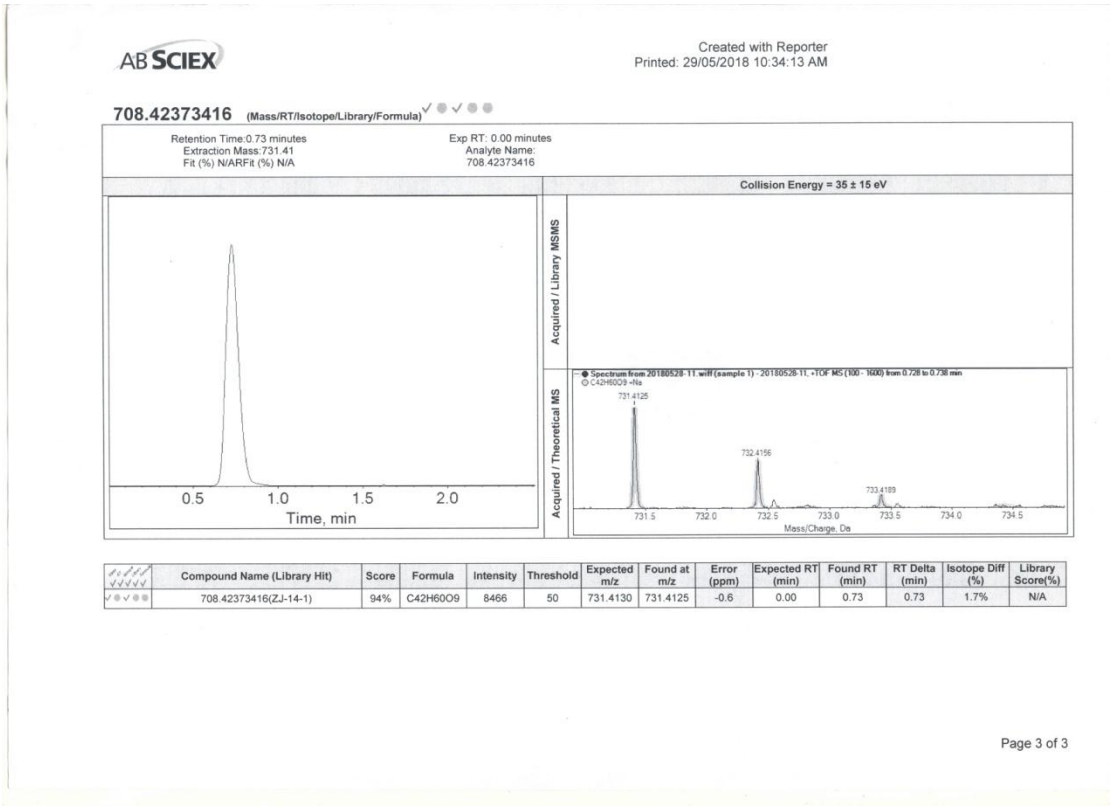


Fig. S117. ^{1}H NMR spectrum of compound **13** in CD_3OD (400 MHz)

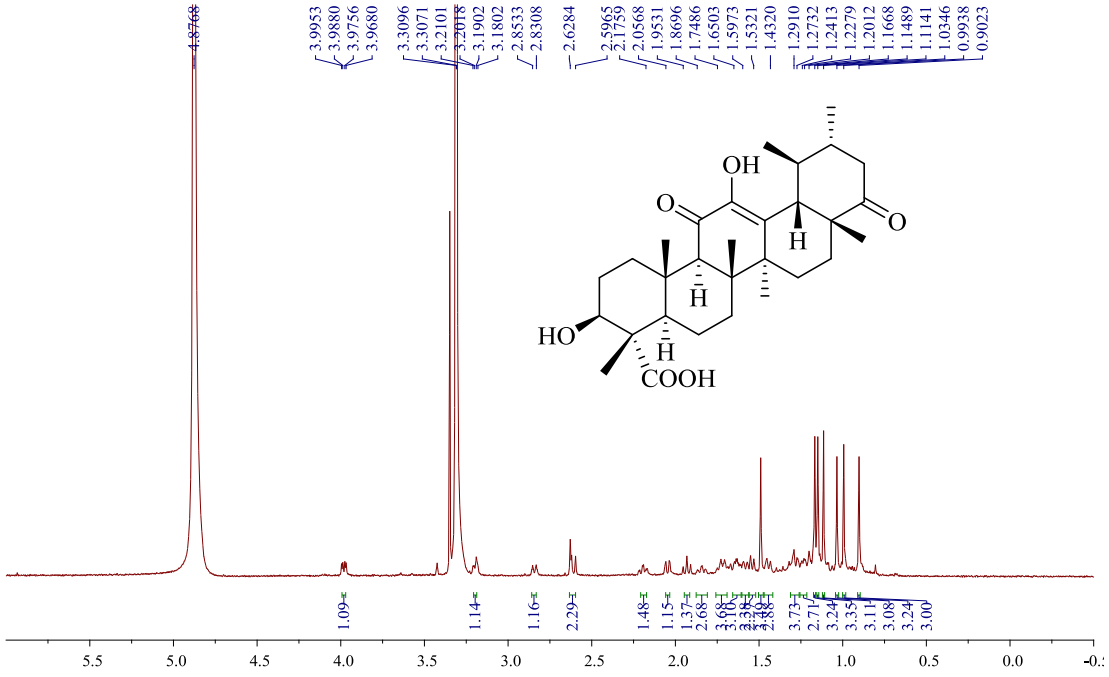


Fig. S118. ^{1}H NMR spectrum of compound **13** –expansion

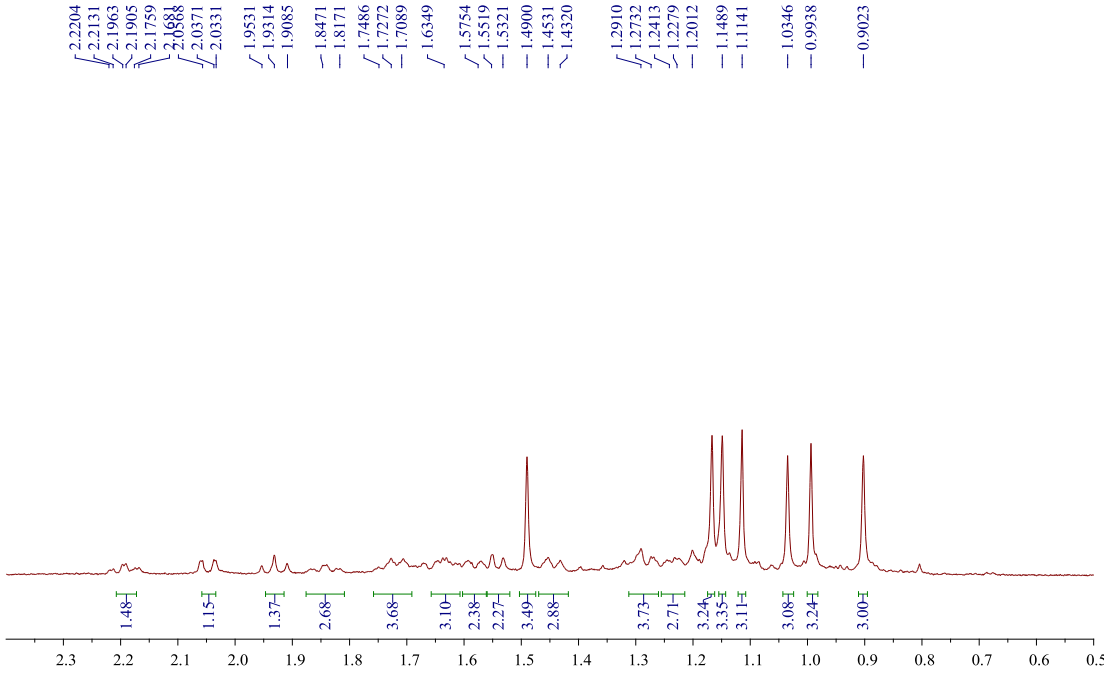


Fig. S119. ^{13}C NMR spectrum of compound **13** in CD_3OD (150 MHz)

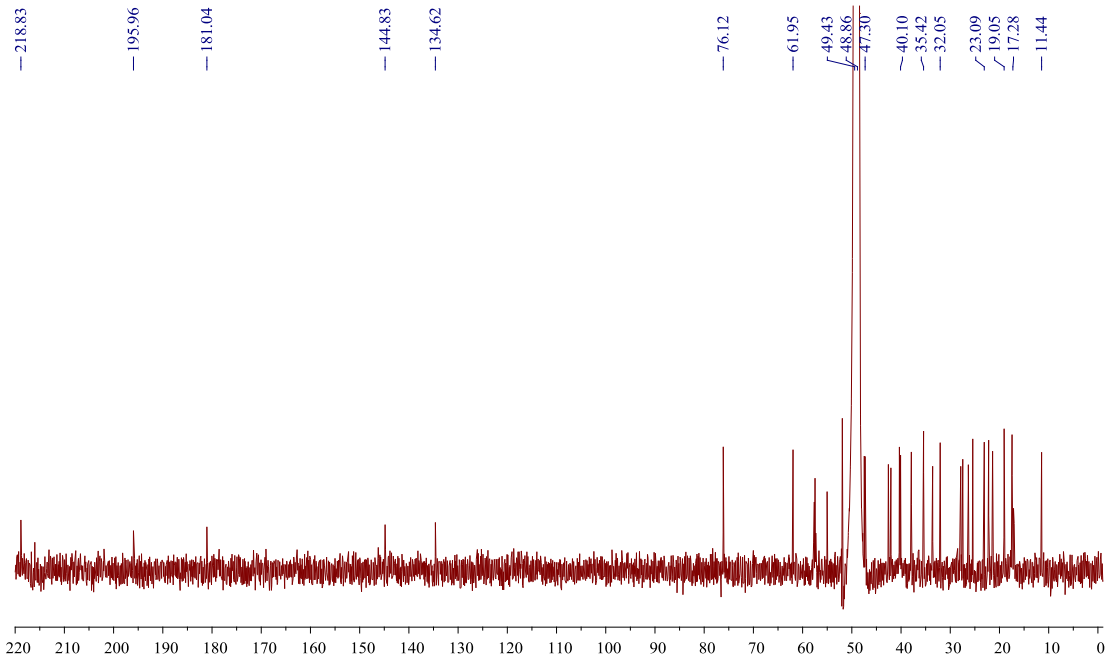


Fig. S120. ^{13}C NMR spectrum of compound **13** –expansion

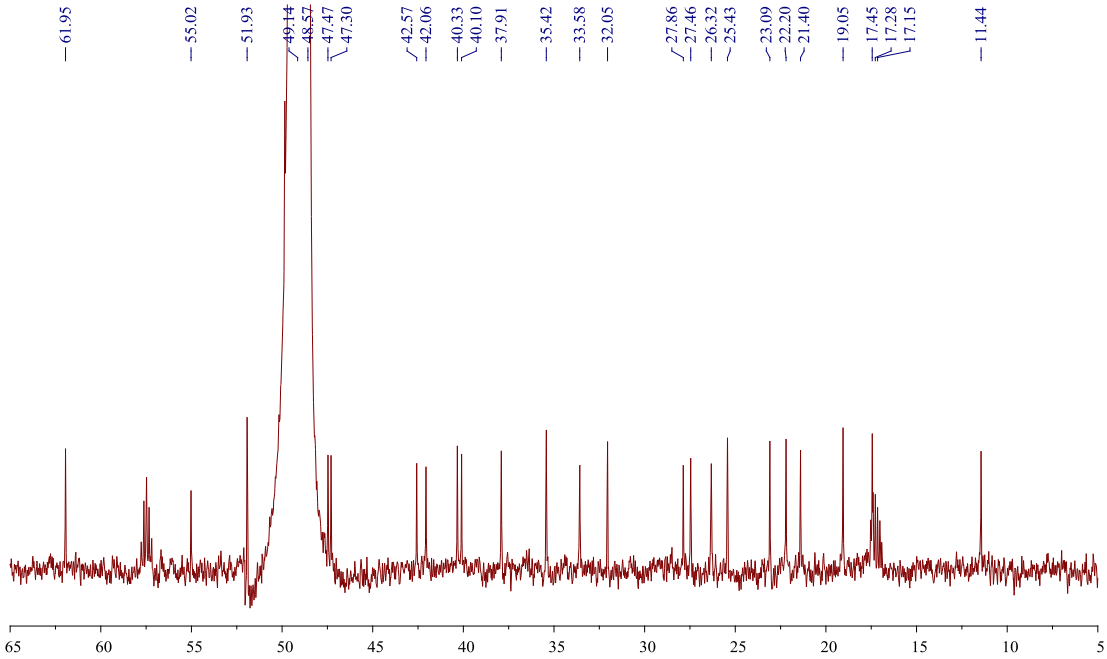


Fig. S121. HMBC spectrum of compound **13** in CD_3OD (600 MHz)

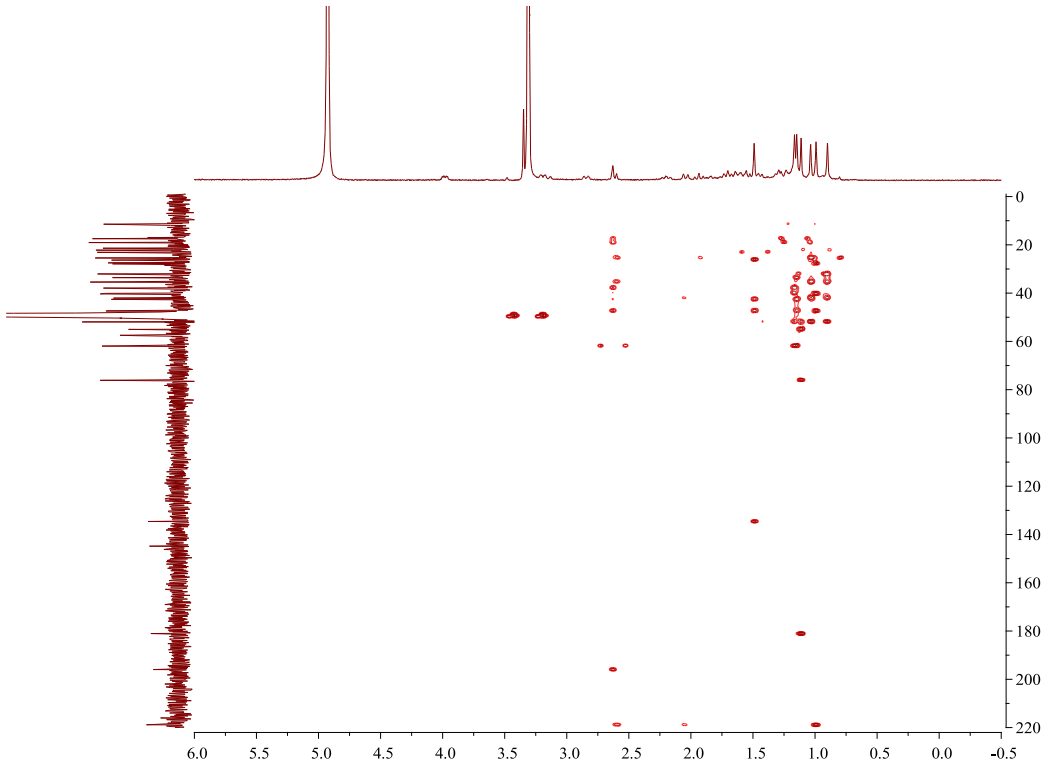


Fig. S122. HMBC spectrum of compound **13**-expansion

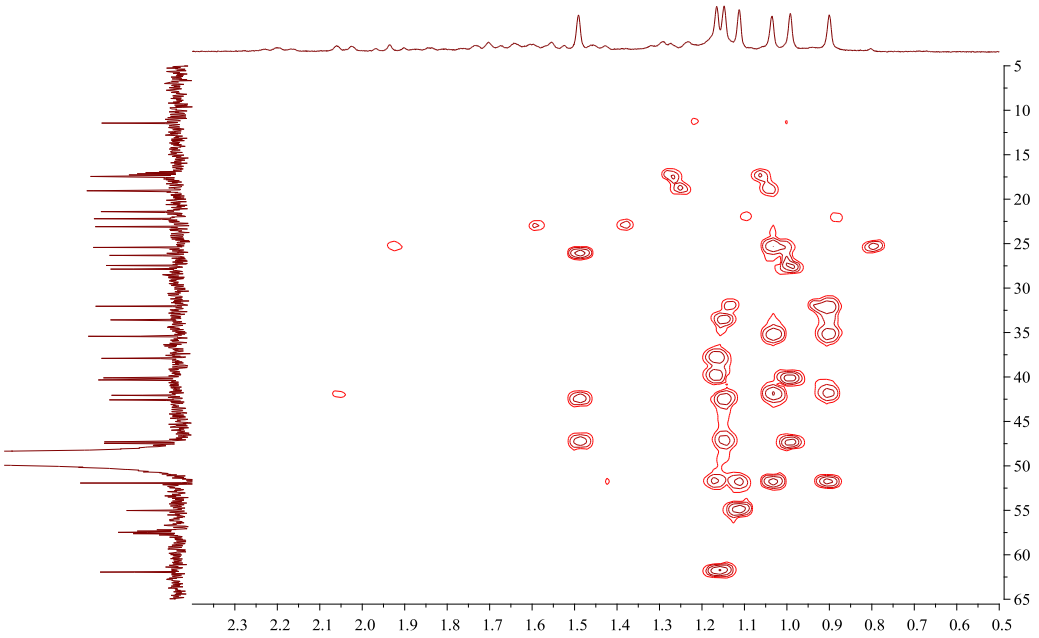


Fig. S123. ROESY spectrum of compound **13** in CD_3OD (600 MHz)

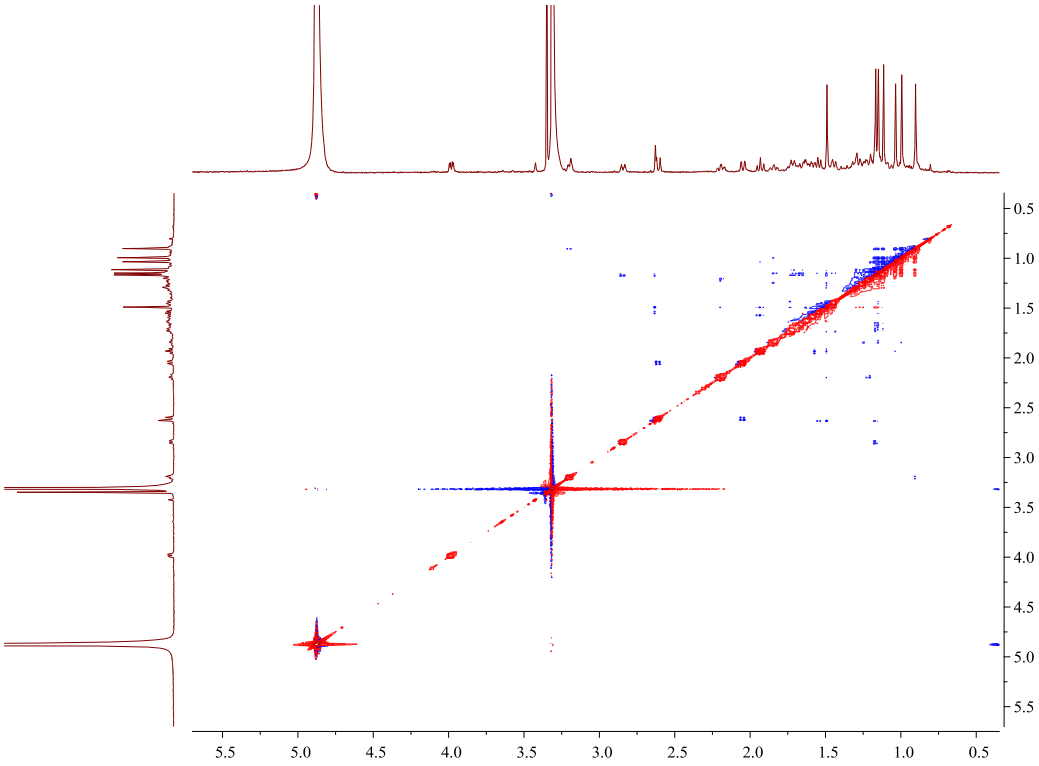


Fig. S124. HR-ESIMS report of compound **13**

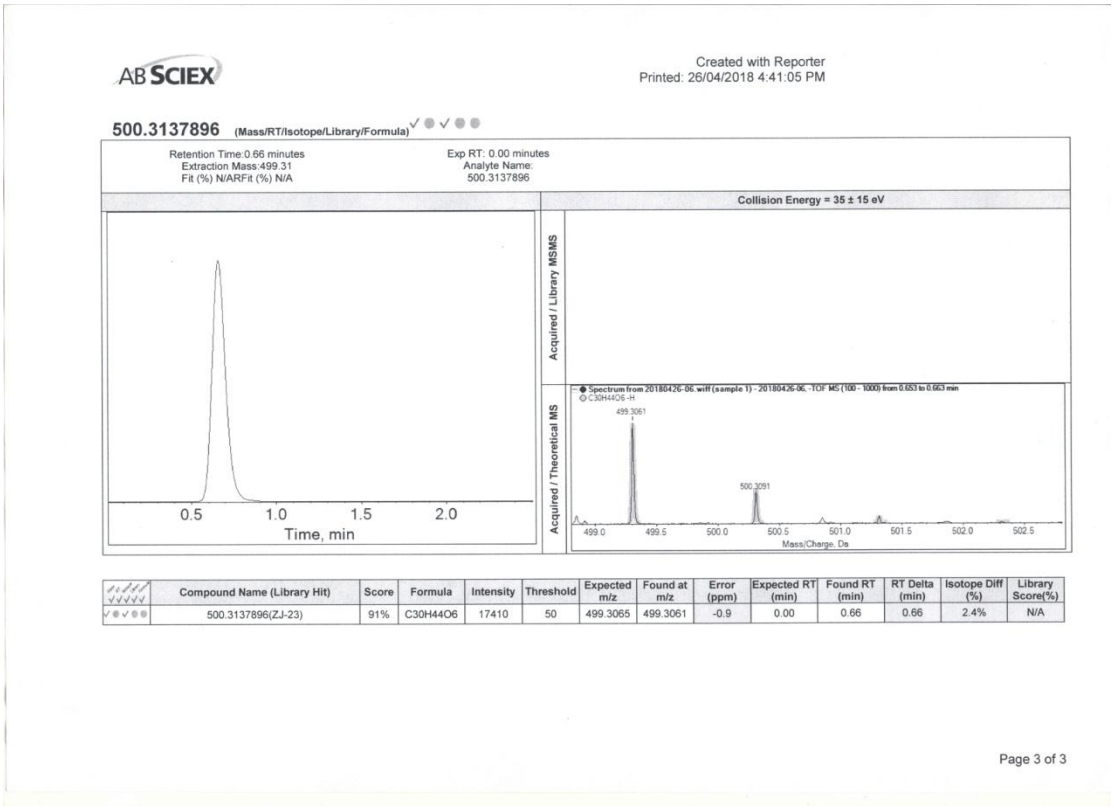


Fig. S125. ^{1}H NMR spectrum of compound **14** in C_5D_5N (400 MHz).

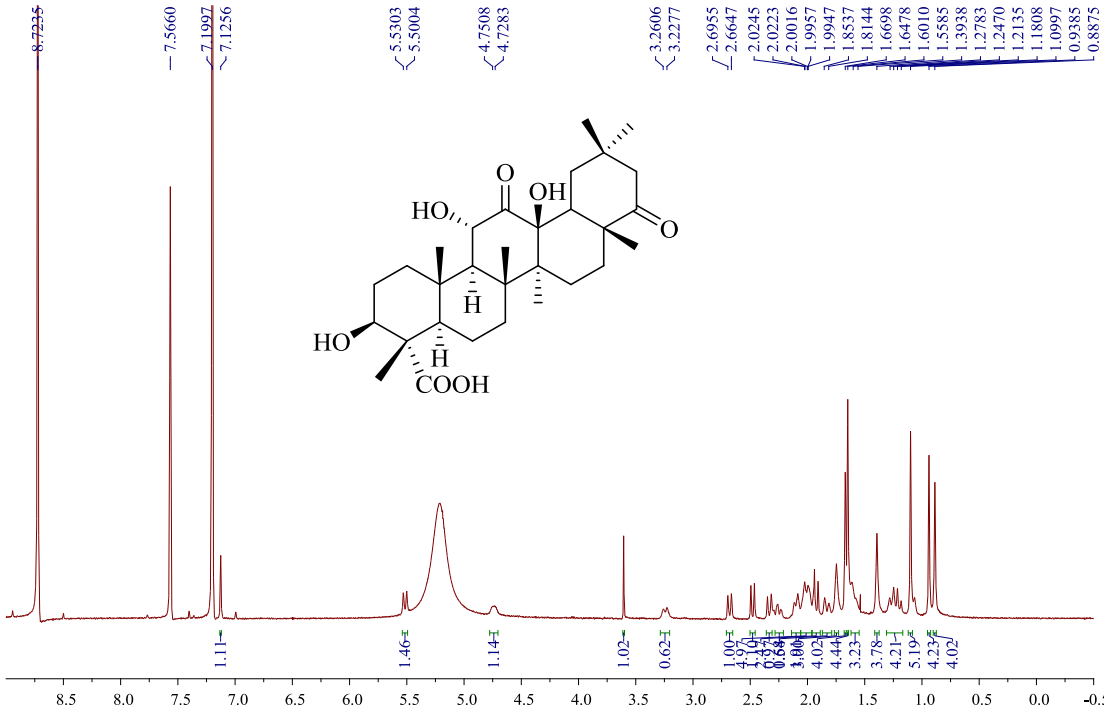


Fig. S126. ^{1}H NMR spectrum of compound **14** –expansion.

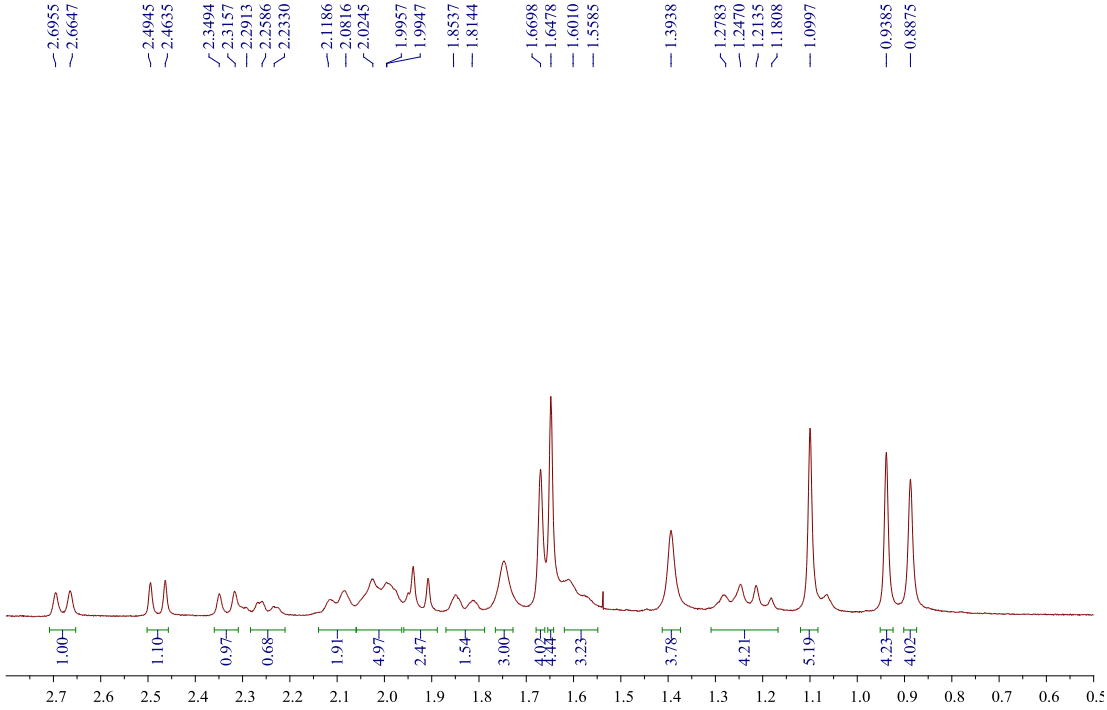


Fig. S127. ^{13}C NMR spectrum of compound **14** in C_5D_5N (150 MHz).

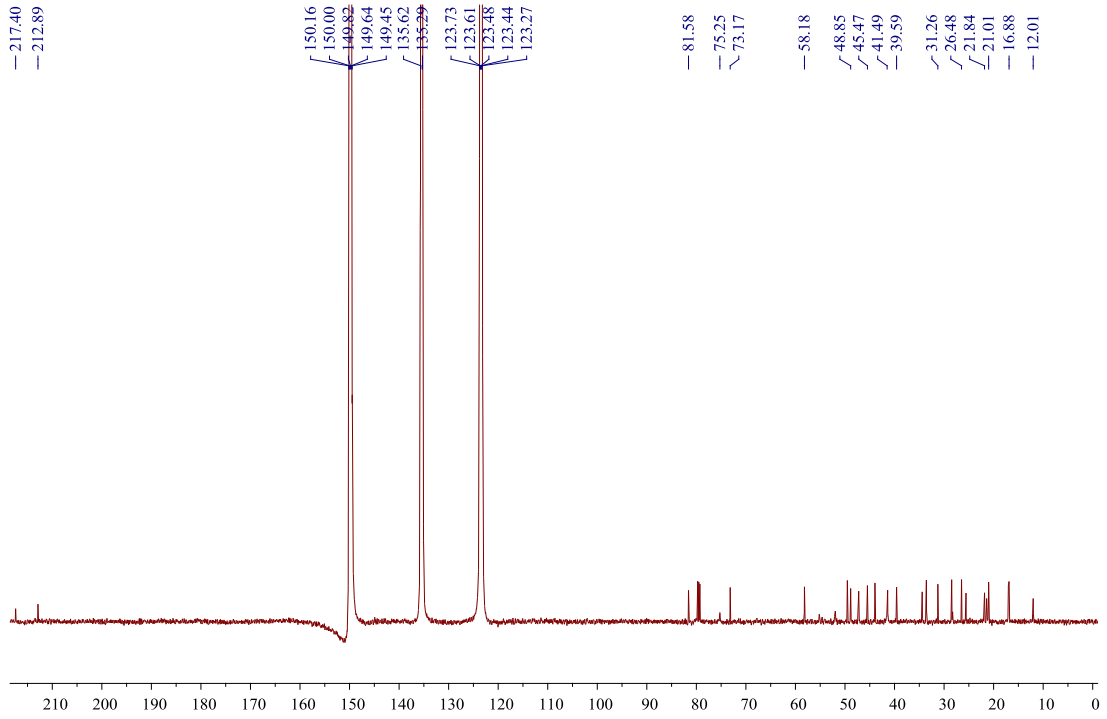


Fig. S128. ^{13}C NMR spectrum of compound **14**-expansion.

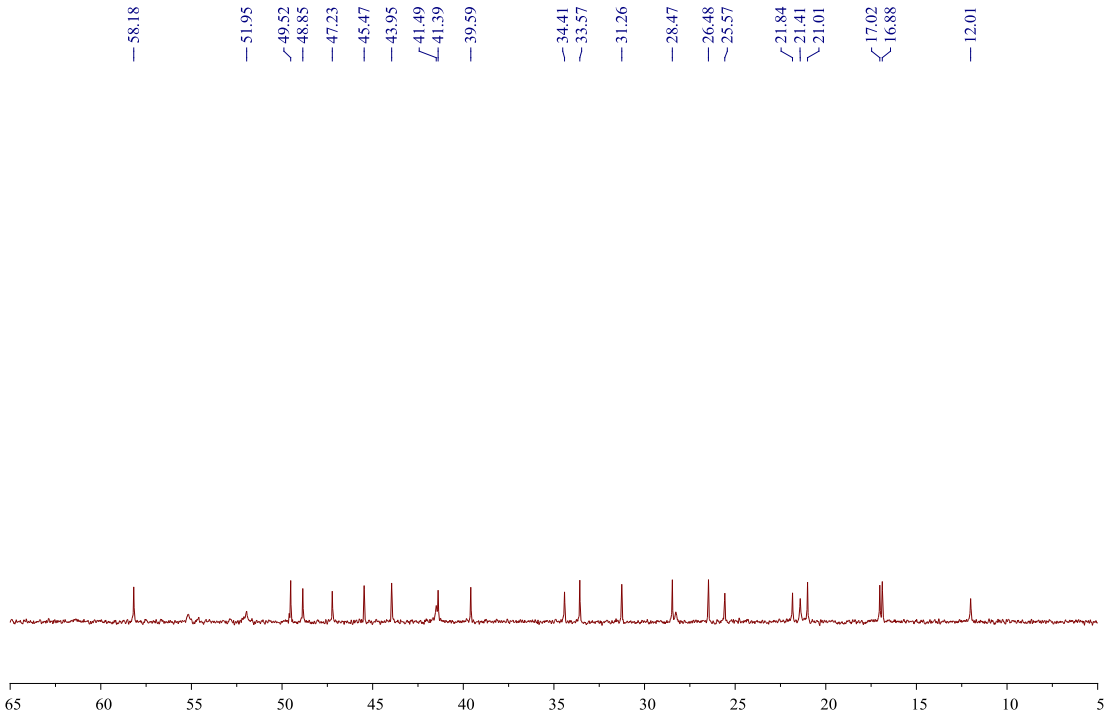


Fig. S129. HMBC spectrum of compound **14** in C_5D_5N (600 MHz).

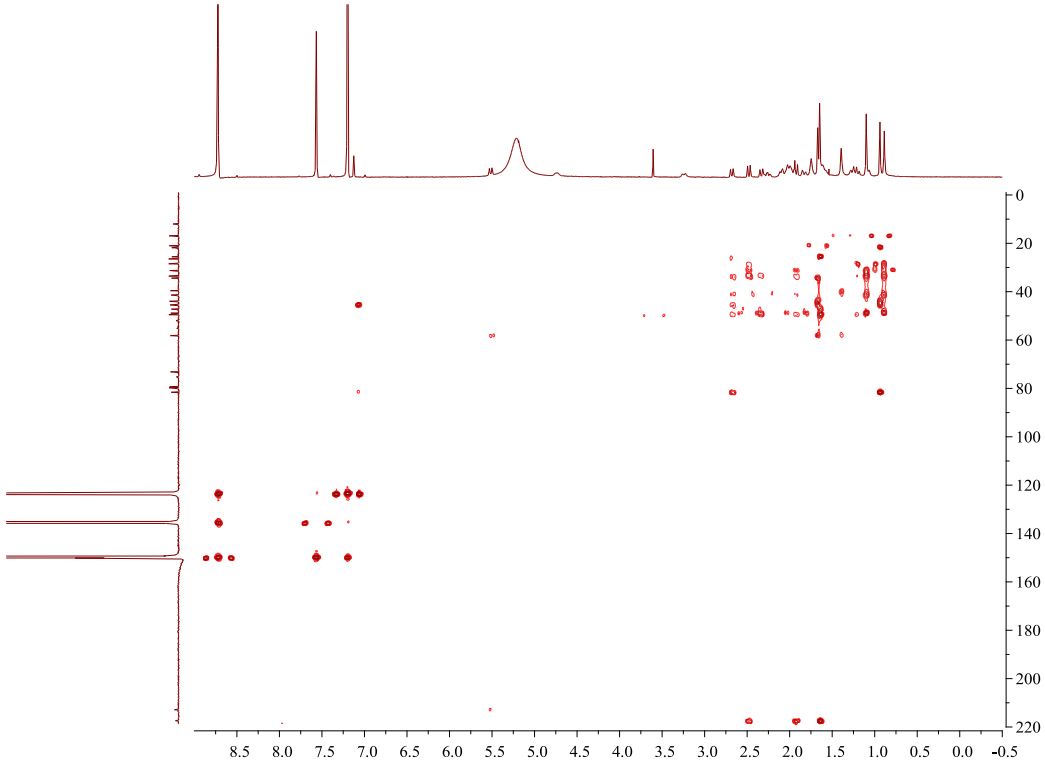


Fig. S130. HMBC spectrum of compound **14**-expansion.

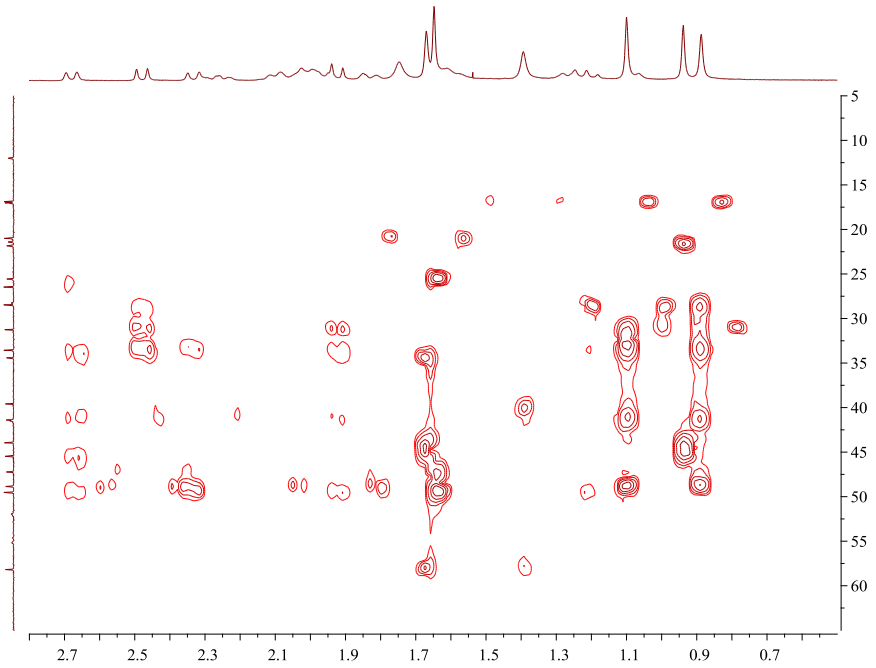


Fig. S131. ROESY spectrum of compound **14** in C_5D_5N (600 MHz).

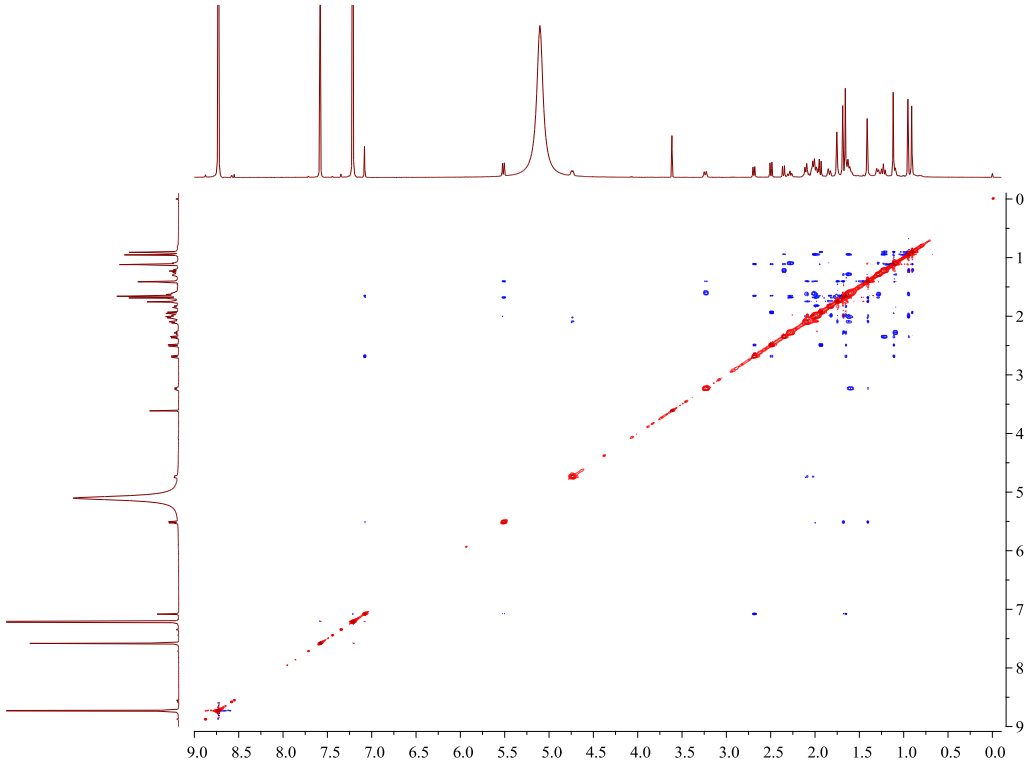
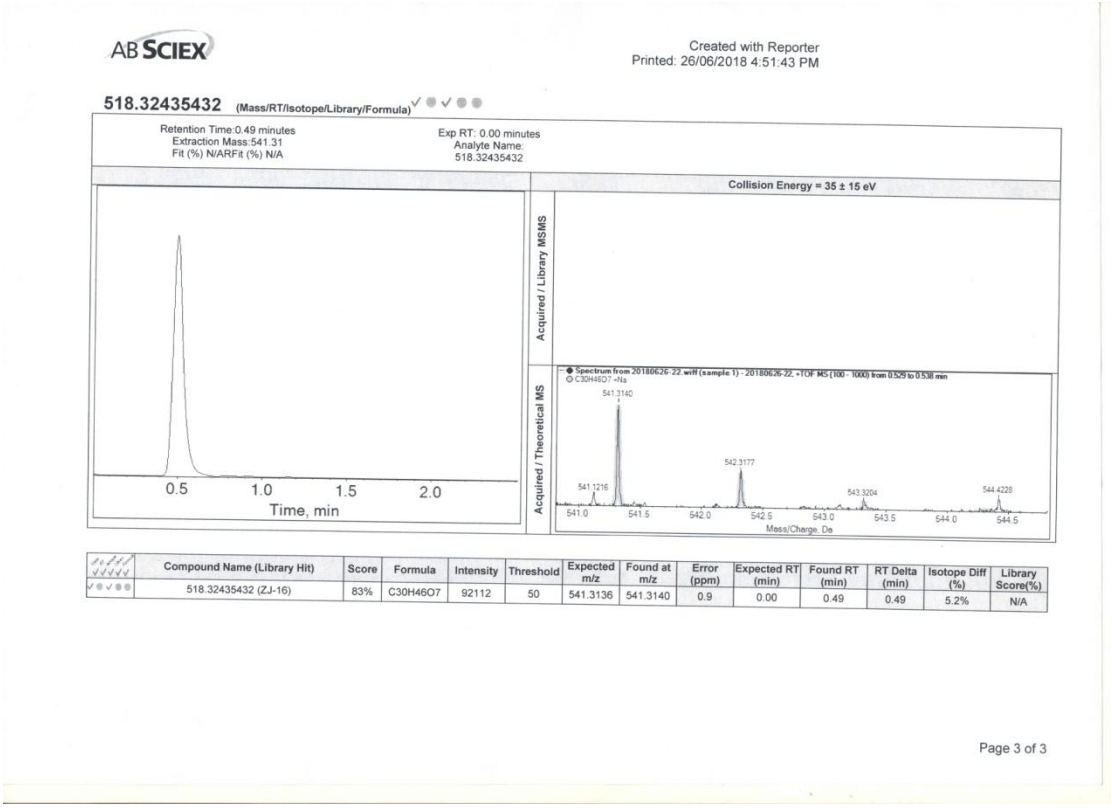


Fig. S132. HRESIMS report of compound **14**.



Compound Name (Library Hit)	Score	Formula	Intensity	Threshold	Expected m/z	Found at m/z	Error (ppm)	Expected RT (min)	Found RT (min)	RT Delta (min)	Isotope Diff (%)	Library Score(%)
518.32435432 (ZJ-16)	83%	C30H46O7	92112	50	541.3136	541.3140	0.9	0.00	0.49	0.49	5.2%	N/A

Table S1. Crystal data and structure refinement for stewartiacid A (**1**)

Identification code	mjr17084_0m	
Empirical formula	$C_{30}H_{46}O_6$	
Formula weight	502.67	
Temperature	170 K	
Wavelength	1.34139 Å	
Crystal system	Monoclinic	
Space group	P 1 21 1	
Unit cell dimensions	a = 14.2747(19) Å	α = 90 °
	b = 6.4197(9) Å	β = 105.303(9) °
	c = 14.897(2) Å	γ = 90 °
Volume	1316.7(3) $Å^3$	
Z	2	
Density (calculated)	1.268 Mg/m^3	
Absorption coefficient	0.444 mm^{-1}	
F(000)	548	
Crystal size	0.05 x 0.02 x 0.01 mm^3	
Theta range for data collection	3.319 to 55.147 °	
Index ranges	-17<=h<=17, -7<=k<=7, -16<=l<=18	
Reflections collected	14495	
Independent reflections	4786 [R(int) = 0.0521]	
Completeness to theta =	99.2%	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7508 and 0.4336	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4786 / 1 / 343	
Goodness-of-fit on F^2	1.061	
Final R indices [I>2sigma(I)]	R1 = 0.0683, wR2 = 0.1556	
R indices (all data)	R1 = 0.0866, wR2 = 0.1718	
Absolute structure parameter	0.19(17)	
Extinction coefficient	0.0051(14)	
Largest diff. peak and hole	0.323 and -0.320 e.$Å^{-3}$	

Table S2. Crystal data and structure refinement for stewartiacid C (**3**)

Identification code	191209wj_0m	
Empirical formula	$C_{30}H_{50}O_9$	
Formula weight	554.70	
Temperature	169.98 K	
Wavelength	1.34139 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 8.0649(6) Å	α = 90 °.
	b = 11.3973(8) Å	β = 90 °.
	c = 32.416(2) Å	γ = 90 °.
Volume	2979.6(4) $Å^3$	
Z	4	
Density (calculated)	1.237 Mg/m^3	
Absorption coefficient	0.471 mm^{-1}	
F (000)	1208	
Crystal size	0.15 x 0.1 x 0.008 mm^3	
Theta range for data collection	3.576 to 55.060 °.	
Index ranges	-9<=h<=7, -11<=k<=13, -39<=l<=39	
Reflections collected	21220	
Independent reflections	5558 [R (int) = 0.0705]	
Completeness to theta = 53.594 °	98.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7508 and 0.3675	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5558 / 0 / 372	
Goodness-of-fit on F^2	1.031	
Final R indices [I>2 sigma (I)]	R1 = 0.0949, wR2 = 0.2521	
R indices (all data)	R1 = 0.1371, wR2 = 0.2937	
Absolute structure parameter	-0.01(19)	
Extinction coefficient	0.029(4)	
Largest diff. peak and hole	0.292 and -0.310 e.$Å^{-3}$	

Table S3. Crystal data and structure refinement for **s**tewartiacid D (**4**).

Identification code	mjl18283_0m	
Empirical formula	$C_{30}H_{46}O_6$	
Formula weight	502.67	
Temperature	170.0 K	
Wavelength	1.34139 Å	
Crystal system	Monoclinic	
Space group	P 1 21 1	
Unit cell dimensions	a = 13.9664(4) Å	α = 90 °.
	b = 6.5552(2) Å	β = 104.366(2) °.
	c = 15.1284(5) Å	γ = 90 °.
Volume	1341.73(7) $Å^3$	
Z	2	
Density (calculated)	1.244 Mg/m^3	
Absorption coefficient	0.436 mm^{-1}	
F (000)	548	
Crystal size	0.1 x 0.02 x 0.01 mm^3	
Theta range for data collection	2.841 to 54.870 °.	
Index ranges	-17<=h<=17, -7<=k<=7, -18<=l<=18	
Reflections collected	20123	
Independent reflections	5048 [R(int) = 0.0530]	
Completeness to theta = 53.594 °	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7508 and 0.5858	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5048 / 1 / 335	
Goodness-of-fit on F^2	1.038	
Final R indices [I>2 sigma(I)]	R1 = 0.0534, wR2 = 0.1558	
R indices (all data)	R1 = 0.0595, wR2 = 0.1613	
Absolute structure parameter	-0.11(13)	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.397 and -0.327 e.$Å^{-3}$	

Table S4. Crystal data and structure refinement for **s**tewartiacid F (**6**).

Identification code	mjl18275_0m	
Empirical formula	$C_{31}H_{52}O_7$	
Formula weight	536.72	
Temperature	169.98 K	
Wavelength	1.34139 Å	
Crystal system	Monoclinic	
Space group	C 1 2 1	
Unit cell dimensions	a = 30.9220(6) Å	α= 90 °.
	b = 13.9294(3) Å	β= 107.9170(10) °.
	c = 14.7361(3) Å	γ= 90 °.
Volume	6039.4(2) $Å^3$	
Z	8	
Density (calculated)	1.181 Mg/m^3	
Absorption coefficient	0.421 mm^{-1}	
F(000)	2352	
Crystal size	0.15 x 0.1 x 0.02 mm^3	
Theta range for data collection	3.054 to 55.014 °.	
Index ranges	-37<=h<=37, -16<=k<=16, -17<=l<=18	
Reflections collected	48612	
Independent reflections	11459 [R(int) = 0.0507]	
Completeness to theta = 53.594 °	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7508 and 0.5610	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11459 / 13 / 710	
Goodness-of-fit on F^2	1.038	
Final R indices [I>2 sigma(I)]	R1 = 0.0875, wR2 = 0.2556	
R indices (all data)	R1 = 0.0955, wR2 = 0.2669	
Absolute structure parameter	0.10(8)	
Extinction coefficient	0.0029(7)	
Largest diff. peak and hole	1.152 and -0.472 e.$Å^{-3}$	