

Supplementary Information

Magnorolins A-L, sesquiterpenoids with diverse skeletons from the fruits of *Magnolia grandiflora* and their cytotoxic and anti-inflammatory

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Contents of Supplementary Information

Figure S1. ^1H NMR spectrum of magnolin A (1) in CDCl_3	1
Figure S2. ^{13}C NMR spectrum of magnolin A (1) in CDCl_3	1
Figure S3. HSQC spectrum of magnolin A (1) in CDCl_3	2
Figure S4. COSY spectrum of magnolin A (1) in CDCl_3	2
Figure S5. HMBC spectrum of magnolin A (1) in CDCl_3	3
Figure S6. ROESY spectrum of magnolin A (1) in CDCl_3	3
Figure S7. HR-ESI-MS spectrum of magnolin A (1).....	4
Figure S8. IR spectrum of magnolin A (1).....	5
Figure S9. UV spectrum of magnolin A (1).....	5
Figure S10. ^1H NMR spectrum of magnolin B (2) in CDCl_3	6
Figure S11. ^1H NMR spectrum of magnolin B (2) in CDCl_3	6
Figure S12. HSQC spectrum of magnolin B (2) in CDCl_3	7
Figure S13. COSY spectrum of magnolin B (2) in CDCl_3	7
Figure S14. HMBC spectrum of magnolin B (2) in CDCl_3	8
Figure S15. ROESY spectrum of magnolin B (2) in CDCl_3	8
Figure S16. HR-ESI-MS spectrum of magnolin B (2).....	9
Figure S17. IR spectrum of magnolin B (2).....	10
Figure S18. UV spectrum of magnolin B (2).....	10
Figure S19. ^1H NMR spectrum of magnolin C (3) in CDCl_3	11
Figure S20. ^{13}C NMR spectrum of magnolin C (3) in CDCl_3	11
Figure S21. HSQC spectrum of magnolin C (3) in CDCl_3	12
Figure S22. COSY spectrum of magnolin C (3) in CDCl_3	12
Figure S23. HMBC spectrum of magnolin C (3) in CDCl_3	13
Figure S24. ROESY spectrum of magnolin C (3) in CDCl_3	13
Figure S25. HR-ESI-MS spectrum of magnolin C (3).....	14
Figure S26. IR spectrum of magnolin C (3).....	15
Figure S27. UV spectrum of magnolin C (3).....	15
Figure S28. ^1H NMR spectrum of magnolin D (5) in CDCl_3	16

Figure S29. ^{13}C NMR spectrum of magnolin D (5) in CDCl_3	16
Figure S30. HSQC spectrum of magnolin D (5) in CDCl_3	17
Figure S31. COSY spectrum of magnolin D (5) in CDCl_3	17
Figure S32. HMBC spectrum of magnolin D (5) in CDCl_3	18
Figure S33. ROESY spectrum of magnolin D (5) in CDCl_3	18
Figure S34. HR-ESI-MS spectrum of magnolin D (5).....	19
Figure S35. IR spectrum of magnolin D (5).....	20
Figure S36. UV spectrum of magnolin D (5).....	20
Figure S37. ^1H NMR spectrum of magnolin E (6) in CDCl_3	21
Figure S38. ^{13}C NMR spectrum of magnolin E (6) in CDCl_3	21
Figure S39. HSQC spectrum of magnolin E (6) in CDCl_3	22
Figure S40. COSY spectrum of magnolin E (6) in CDCl_3	22
Figure S41. HMBC spectrum of magnolin E (6) in CDCl_3	23
Figure S42. ROESY spectrum of magnolin E (6) in CDCl_3	23
Figure S43. HR-ESI-MS spectrum of magnolin E (6)	24
Figure S44. IR spectrum of magnolin E (6)	25
Figure S45. UV spectrum of magnolin E (6)	25
Figure S46. ^1H NMR spectrum of magnorlin F (7) in CDCl_3	26
Figure S47. ^{13}C NMR spectrum of magnorlin F (7) in CDCl_3	26
Figure S48. HSQC spectrum of magnorlin F (7) in CDCl_3	27
Figure S49. COSY spectrum of magnorlin F (7) in CDCl_3	27
Figure S50. HMBC spectrum of magnorlin F (7) in CDCl_3	28
Figure S51. ROESY spectrum of magnorlin F (7) in CDCl_3	28
Figure S52. HR-ESI-MS spectrum of magnolin F (7)	29
Figure S53. IR spectrum of magnolin F (7)	30
Figure S54. UV spectrum of magnolin F (7).....	30
Figure S55. ^1H NMR spectrum of magnolin G (8) in CDCl_3	31
Figure S56. ^{13}C NMR spectrum of magnolin G (8) in CDCl_3	31
Figure S57. HSQC spectrum of magnolin G (8) in CDCl_3	32
Figure S58. COSY spectrum of magnolin G (8) in CDCl_3	32

Figure S59. HMBC spectrum of magnolin G (8) in CDCl ₃	33
Figure S60. ROESY spectrum of magnolin G (8) in CDCl ₃	33
Figure S61. HR-ESI-MS spectrum of magnolin G (8).....	34
Figure S62. IR spectrum of magnolin G (8).....	35
Figure S63. UV spectrum of magnolin G (8).....	35
Figure S64. ¹ H NMR spectrum of magnolin H (9) in CDCl ₃	36
Figure S65. ¹³ C NMR spectrum of magnolin H (9) in CDCl ₃	36
Figure S66. HSQC spectrum of magnolin H (9) in CDCl ₃	37
Figure S67. COSY spectrum of magnolin H (9) in CDCl ₃	37
Figure S68. HMBC spectrum of magnolin H (9) in CDCl ₃	38
Figure S69. ROESY spectrum of magnolin H (9) in CDCl ₃	38
Figure S70. HR-ESI-MS spectrum of magnolin H (9).....	39
Figure S71. IR spectrum of magnolin H (9).....	40
Figure S72. IR spectrum of magnolin H (9).....	40
Figure S73. ¹ H NMR spectrum of magnolin I (10) in CDCl ₃	41
Figure S74. ¹³ C NMR spectrum of magnolin I (10) in CDCl ₃	41
Figure S75. HSQC spectrum of magnolin I (10) in CDCl ₃	42
Figure S76. COSY spectrum of magnolin I (10) in CDCl ₃	42
Figure S77. HMBC spectrum of magnolin I (10) in CDCl ₃	43
Figure S78. ROESY spectrum of magnolin I (10) in CDCl ₃	43
Figure S79. HR-ESI-MS spectrum of magnolin I (10)	44
Figure S80. IR spectrum of magnolin I (10)	45
Figure S81. UV spectrum of magnolin I (10).....	45
Figure S82. ¹ H NMR spectrum of magnolin J (11) in CDCl ₃	46
Figure S83. ¹³ C NMR spectrum of magnolin J (11) in CDCl ₃	46
Figure S84. HSQC spectrum of magnolin J (11) in CDCl ₃	47
Figure S85. COSY spectrum of magnolin J (11) in CDCl ₃	47
Figure S86. HMBC spectrum of magnolin J (11) in CDCl ₃	48
Figure S87. ROESY spectrum of magnolin J (11) in CDCl ₃	48
Figure S88. HR-ESI-MS spectrum of magnolin J (11).....	49

Figure S89. IR spectrum of magnolin J (11)	50
Figure S90. UV spectrum of magnolin J (11)	50
Figure S91. ¹ H NMR spectrum of magnolin K (12) in CDCl ₃	51
Figure S92. ¹³ C NMR spectrum of magnolin K (12) in CDCl ₃	51
Figure S93. HSQC spectrum of magnolin K (12) in CDCl ₃	52
Figure S94. COSY spectrum of magnolin K (12) in CDCl ₃	52
Figure S95. HMBC spectrum of magnolin K (12) in CDCl ₃	53
Figure S96. ROESY spectrum of magnolin K (12) in CDCl ₃	53
Figure S97. HR-ESI-MS spectrum of magnolin K (12).....	54
Figure S98. IR spectrum of magnolin K (12).....	55
Figure S99. UV spectrum of magnolin K (12).....	55
Figure S100. ¹ H NMR spectrum of magnolin L (15) in CD ₃ OD	56
Figure S101. ¹³ C NMR spectrum of magnolin L (15) in CD ₃ OD	56
Figure S102. HSQC spectrum of magnolin L (15) in CD ₃ OD.....	57
Figure S103. COSY spectrum of magnolin L (15) in CD ₃ OD.....	57
Figure S104. HMBC spectrum of magnolin L (15) in CD ₃ OD.....	58
Figure S105. ROESY spectrum of magnolin L (15) in CD ₃ OD	58
Figure S106. HR-ESI-MS spectrum of magnolin L (15)	59
Figure S107. IR spectrum of magnolin L (15)	60
Figure S108. UV spectrum of magnolin L (15)	60
Figure S109. Conformers of isomer 1	61
Table S1. Important thermodynamic parameters and Boltzmann distributions of the optimized isomer 1 at B3LYP/6-31G (d, p) level in gas phase.....	61
Table S2. Optimized Z-matrixes of isomer 1 in the gas phase (Å) at B3LYP/6-31G (d) level.	61
Figure S110. Conformers of isomer 2	63
Table S3. Important thermodynamic parameters and Boltzmann distributions of the optimized isomer 2 at B3LYP/6-31G (d, p) level in gas phase.....	63
Table S4. Optimized Z-matrixes of isomer 2 in the gas phase (Å) at B3LYP/6-31G (d) level.	63

Figure S111. Conformers of isomer 5	67
Table S5. Important thermodynamic parameters and Boltzmann distributions of the optimized isomer 5 at B3LYP/6-31G (d, p) level in gas phase.....	67
Table S6. Optimized Z-matrixes of isomer 5 in the gas phase (Å) at B3LYP/6-31G (d) level.	67
Figure S112. Conformers of isomer 6	71
Table S7. Important thermodynamic parameters and Boltzmann distributions of the optimized isomer 6 at B3LYP/6-31G (d, p) level in gas phase.....	71
Table S8. Optimized Z-matrixes of isomer 6 in the gas phase (Å) at B3LYP/6-31G (d) level.	71
Figure S113. Conformers of isomer 7	74
Table S9. Important thermodynamic parameters and Boltzmann distributions of the optimized isomer 7 at B3LYP/6-31G (d, p) level in gas phase.....	75
Table S10. Optimized Z-matrixes of isomer 7 in the gas phase (Å) at B3LYP/6-31G (d) level.	75
Figure S114. Conformers of isomer 8	77
Table S11. Important thermodynamic parameters and Boltzmann distributions of the optimized isomer 8 at B3LYP/6-31G (d, p) level in gas phase.....	77
Table S12. Optimized Z-matrixes of isomer 8 in the gas phase (Å) at B3LYP/6-31G (d) level.	78
Figure S115. Conformers of isomer 9	80
Table S13. Important thermodynamic parameters and Boltzmann distributions of the optimized isomer 9 at B3LYP/6-31G (d, p) level in gas phase.....	80
Table S14. Optimized Z-matrixes of isomer 9 in the gas phase (Å) at B3LYP/6-31G (d) level.	80
Figure S116. Conformers of isomer 10	83
Table S15. Important thermodynamic parameters and Boltzmann distributions of the optimized isomer 10 at B3LYP/6-31G (d, p) level in gas phase.....	83
Table S16. Optimized Z-matrixes of isomer 10 in the gas phase (Å) at B3LYP/6-31G (d) level.	84

Figure S117. Conformers of isomer 11	88
Table S17. Important thermodynamic parameters and Boltzmann distributions of the optimized isomer 11 at B3LYP/6-31G (d, p) level in gas phase.....	88
Table S18. Optimized Z-matrixes of isomer 11 in the gas phase (Å) at B3LYP/6-31G (d) level.	89
Figure S118. Conformers of isomer 12	92
Table S19. Important thermodynamic parameters and Boltzmann distributions of the optimized isomer 12 at B3LYP/6-31G (d, p) level in gas phase.....	92
Table S20. Optimized Z-matrixes of isomer 12 in the gas phase (Å) at B3LYP/6-31G (d) level.	92
Figure S119. Conformers of isomer 15	95
Table S21. Important thermodynamic parameters and Boltzmann distributions of the optimized isomer 15 at B3LYP/6-31G (d, p) level in gas phase.....	95
Table S22. Optimized Z-matrixes of isomer 15 in the gas phase (Å) at B3LYP/6-31G (d) level.	95
Table S23. Energy analysis for (1 <i>R</i> , 4 <i>R</i> , 5 <i>S</i> , 6 <i>R</i> , 7 <i>R</i> , 10 <i>S</i> , 11 <i>R</i> [*])- 8a and (1 <i>R</i> , 4 <i>R</i> , 5 <i>S</i> , 6 <i>R</i> , 7 <i>R</i> , 10 <i>S</i> , 11 <i>S</i> [*])- 8b	98
Figure S120. mPW1PW91/6-311+G (d, p) (chloroform) optimized lowest energy conformers for (1 <i>R</i> , 4 <i>R</i> , 5 <i>S</i> , 6 <i>R</i> , 7 <i>R</i> , 10 <i>S</i> , 11 <i>R</i> [*])- 8a and (1 <i>R</i> , 4 <i>R</i> , 5 <i>S</i> , 6 <i>R</i> , 7 <i>R</i> , 10 <i>S</i> , 11 <i>S</i> [*])- 8b	99
Figure S121. DP4+ evaluation of theoretical and experimental data for (1 <i>R</i> , 4 <i>R</i> , 5 <i>S</i> , 6 <i>R</i> , 7 <i>R</i> , 10 <i>S</i> , 11 <i>R</i> [*])- 8a and (1 <i>R</i> , 4 <i>R</i> , 5 <i>S</i> , 6 <i>R</i> , 7 <i>R</i> , 10 <i>S</i> , 11 <i>S</i> [*])- 8b	99
Table S24. Calculated (calc.) and experimental (exp.) ¹³ C NMR chemical shift values of (1 <i>R</i> , 4 <i>R</i> , 5 <i>S</i> , 6 <i>R</i> , 7 <i>R</i> , 10 <i>S</i> , 11 <i>R</i> [*])- 8a and (1 <i>R</i> , 4 <i>R</i> , 5 <i>S</i> , 6 <i>R</i> , 7 <i>R</i> , 10 <i>S</i> , 11 <i>S</i> [*])- 8b at the mPW1PW91/6-311+G(d, p) level in chloroform.....	100
Table S25. Calculated (calc.) and experimental (exp.) ¹ H NMR chemical shift values of (1 <i>R</i> , 4 <i>R</i> , 5 <i>S</i> , 6 <i>R</i> , 7 <i>R</i> , 10 <i>S</i> , 11 <i>R</i> [*])- 8a and (1 <i>R</i> , 4 <i>R</i> , 5 <i>S</i> , 6 <i>R</i> , 7 <i>R</i> , 10 <i>S</i> , 11 <i>S</i> [*])- 8b at the mPW1PW91/6-311+G (d, p) level in chloroform.....	100
Figure S122. Linear correlations between the experimental and calculated ¹³ C NMR chemical shifts for two possible isomers of (1 <i>R</i> , 4 <i>R</i> , 5 <i>S</i> , 6 <i>R</i> , 7 <i>R</i> , 10 <i>S</i> , 11 <i>R</i> [*])- 8a and	

(1 <i>R</i> , 4 <i>R</i> , 5 <i>S</i> , 6 <i>R</i> , 7 <i>R</i> , 10 <i>S</i> , 11 <i>S</i> [*])- 8b at the PCM/ mPW1PW91/6-311+G (d, p) level.	101
Table S26. Energy analysis for (1 <i>R</i> , 4 <i>R</i> , 5 <i>S</i> , 6 <i>S</i> , 7 <i>R</i> , 11 <i>R</i> [*])- 11a and (1 <i>R</i> , 4 <i>R</i> , 5 <i>S</i> , 6 <i>S</i> , 7 <i>R</i> , 11 <i>S</i> [*])- 11b	101
Figure S123. mPW1PW91/6-311+G (d, p) (chloroform) optimized lowest energy conformers for (1 <i>R</i> , 4 <i>R</i> , 5 <i>S</i> , 6 <i>S</i> , 7 <i>R</i> , 11 <i>R</i> [*])- 11a and (1 <i>R</i> , 4 <i>R</i> , 5 <i>S</i> , 6 <i>S</i> , 7 <i>R</i> , 11 <i>S</i> [*])- 11b	102
Figure S124. DP4+ evaluation of theoretical and experimental data for (1 <i>R</i> , 4 <i>R</i> , 5 <i>S</i> , 6 <i>S</i> , 7 <i>R</i> , 11 <i>R</i> [*])- 11a and (1 <i>R</i> , 4 <i>R</i> , 5 <i>S</i> , 6 <i>S</i> , 7 <i>R</i> , 11 <i>S</i> [*])- 11b	102
Table S27. Calculated (calc.) and experimental (exp.) ¹³ C NMR chemical shift values of (1 <i>R</i> , 4 <i>R</i> , 5 <i>S</i> , 6 <i>S</i> , 7 <i>R</i> , 11 <i>R</i> [*])- 11a and (1 <i>R</i> , 4 <i>R</i> , 5 <i>S</i> , 6 <i>S</i> , 7 <i>R</i> , 11 <i>S</i> [*])- 11b at the mPW1PW91/6-311+G(d, p) level in chloroform.....	103
Table S28. Calculated (calc.) and experimental (exp.) ¹ H NMR chemical shift values of (1 <i>R</i> , 4 <i>R</i> , 5 <i>S</i> , 6 <i>S</i> , 7 <i>R</i> , 11 <i>R</i> [*])- 11a and (1 <i>R</i> , 4 <i>R</i> , 5 <i>S</i> , 6 <i>S</i> , 7 <i>R</i> , 11 <i>S</i> [*])- 11b at the mPW1PW91/6-311+G (d, p) level in chloroform.....	103
Figure S125. Linear correlations between the experimental and calculated ¹³ C NMR chemical shifts for two possible isomers of (1 <i>R</i> , 4 <i>R</i> , 5 <i>S</i> , 6 <i>S</i> , 7 <i>R</i> , 11 <i>R</i> [*])- 11a and (1 <i>R</i> , 4 <i>R</i> , 5 <i>S</i> , 6 <i>S</i> , 7 <i>R</i> , 11 <i>S</i> [*])- 11b at the PCM/ mPW1PW91/6-311+G (d, p) level.....	104
Table S29. Energy analysis for (1 <i>R</i> , 4 <i>R</i> , 5 <i>S</i> , 6 <i>S</i> , 7 <i>R</i> , 11 <i>R</i> [*])- 12a and (1 <i>R</i> , 4 <i>R</i> , 5 <i>S</i> , 6 <i>S</i> , 7 <i>R</i> , 11 <i>S</i> [*])- 12b	104
Figure S126. mPW1PW91/6-311+G (d, p) (chloroform) optimized lowest energy conformers for (1 <i>R</i> , 4 <i>R</i> , 5 <i>S</i> , 6 <i>S</i> , 7 <i>R</i> , 11 <i>R</i> [*])- 12a and (1 <i>R</i> , 4 <i>R</i> , 5 <i>S</i> , 6 <i>S</i> , 7 <i>R</i> , 11 <i>S</i> [*])- 12b	104
Figure S127. DP4+ evaluation of theoretical and experimental data for (1 <i>R</i> , 4 <i>R</i> , 5 <i>S</i> , 6 <i>S</i> , 7 <i>R</i> , 11 <i>R</i> [*])- 12a and (1 <i>R</i> , 4 <i>R</i> , 5 <i>S</i> , 6 <i>S</i> , 7 <i>R</i> , 11 <i>S</i> [*])- 12b	105
Table S30. Calculated (calc.) and experimental (exp.) ¹³ C NMR chemical shift values of (1 <i>R</i> , 4 <i>R</i> , 5 <i>S</i> , 6 <i>S</i> , 7 <i>R</i> , 11 <i>R</i> [*])- 12a and (1 <i>R</i> , 4 <i>R</i> , 5 <i>S</i> , 6 <i>S</i> , 7 <i>R</i> , 11 <i>S</i> [*])- 12b at the mPW1PW91/6-311+G(d, p) level in acetone	106
Table S31. Calculated (calc.) and experimental (exp.) ¹ H NMR chemical shift values of (1 <i>R</i> , 4 <i>R</i> , 5 <i>S</i> , 6 <i>S</i> , 7 <i>R</i> , 11 <i>R</i> [*])- 12a and (1 <i>R</i> , 4 <i>R</i> , 5 <i>S</i> , 6 <i>S</i> , 7 <i>R</i> , 11 <i>S</i> [*])- 12b at the mPW1PW91/6-311+G (d, p) level in acetone	106
Figure S128. Linear correlations between the experimental and calculated ¹³ C NMR chemical shifts for two possible isomers of (1 <i>R</i> , 4 <i>R</i> , 5 <i>S</i> , 6 <i>S</i> , 7 <i>R</i> , 11 <i>R</i> [*])- 12a and (1 <i>R</i> ,	

4*R*, 5*S*, 6*S*, 7*R*, 11*S**)-12b at the PCM/ mPW1PW91/6-311+G (d, p) level.....107

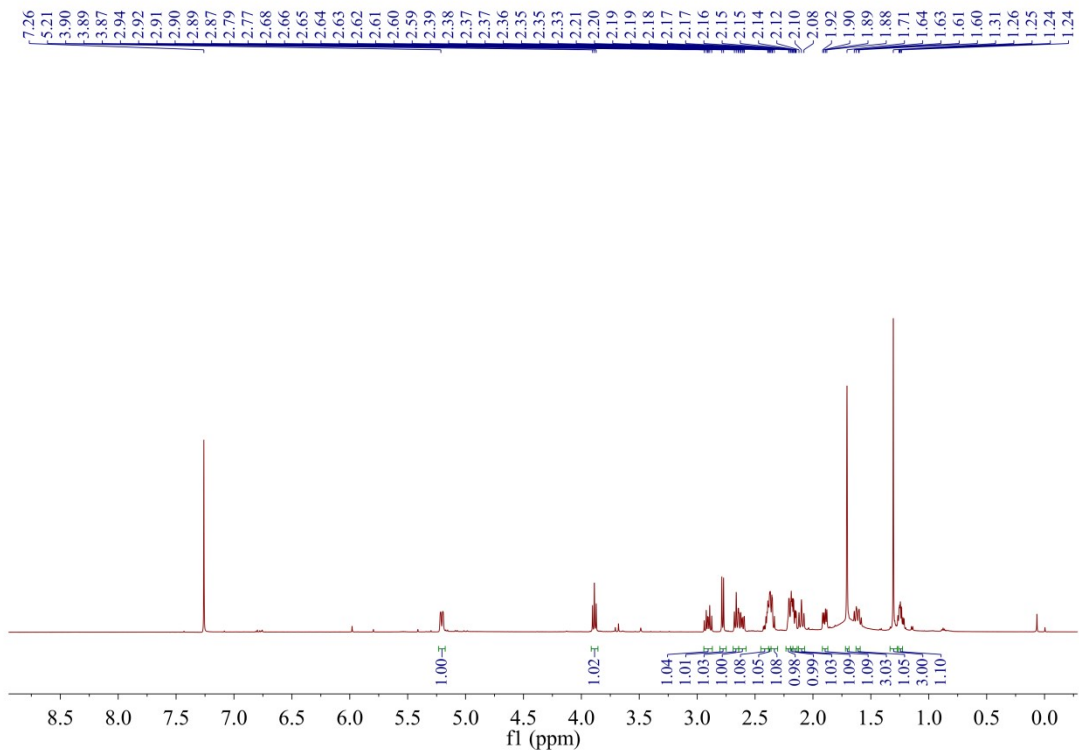


Figure S1. ^1H NMR spectrum of magnolin A (**1**) in CDCl_3

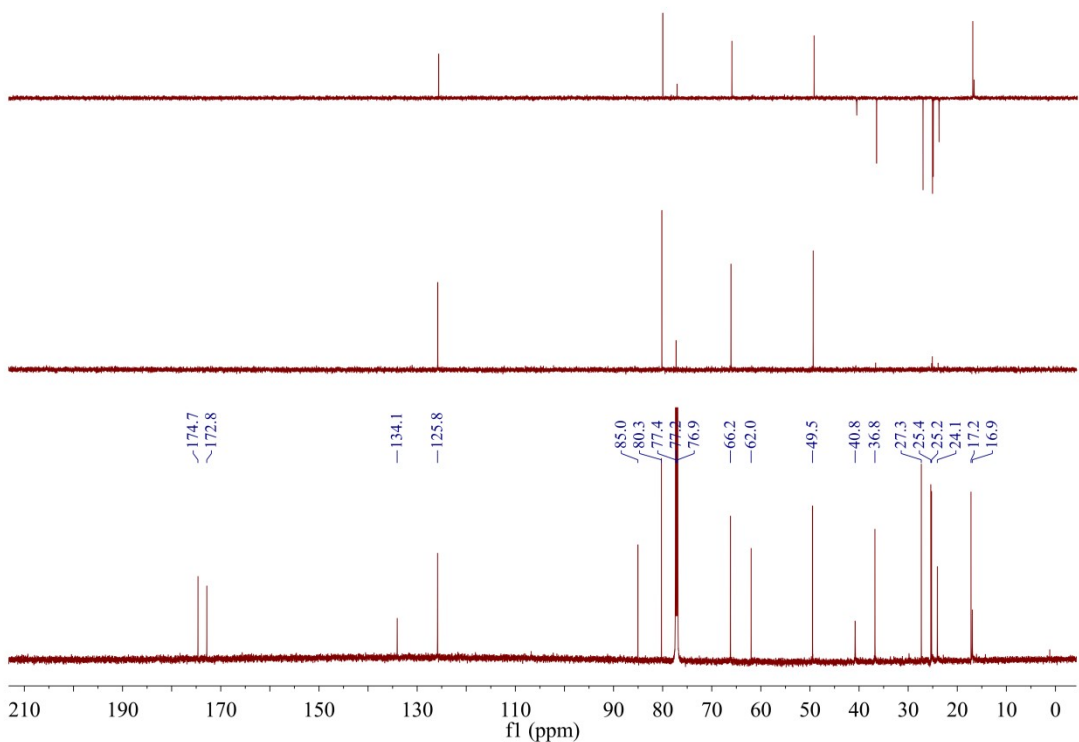


Figure S2. ^{13}C NMR spectrum of magnolin A (**1**) in CDCl_3

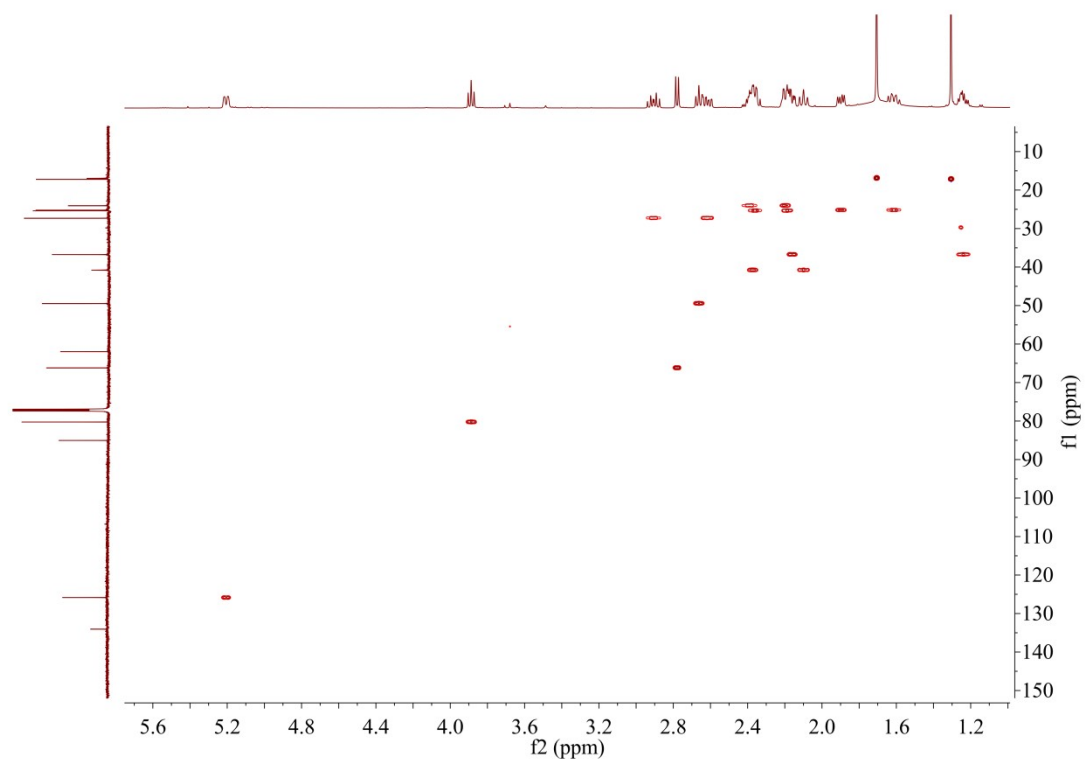


Figure S3. HSQC spectrum of magnolin A (**1**) in CDCl_3

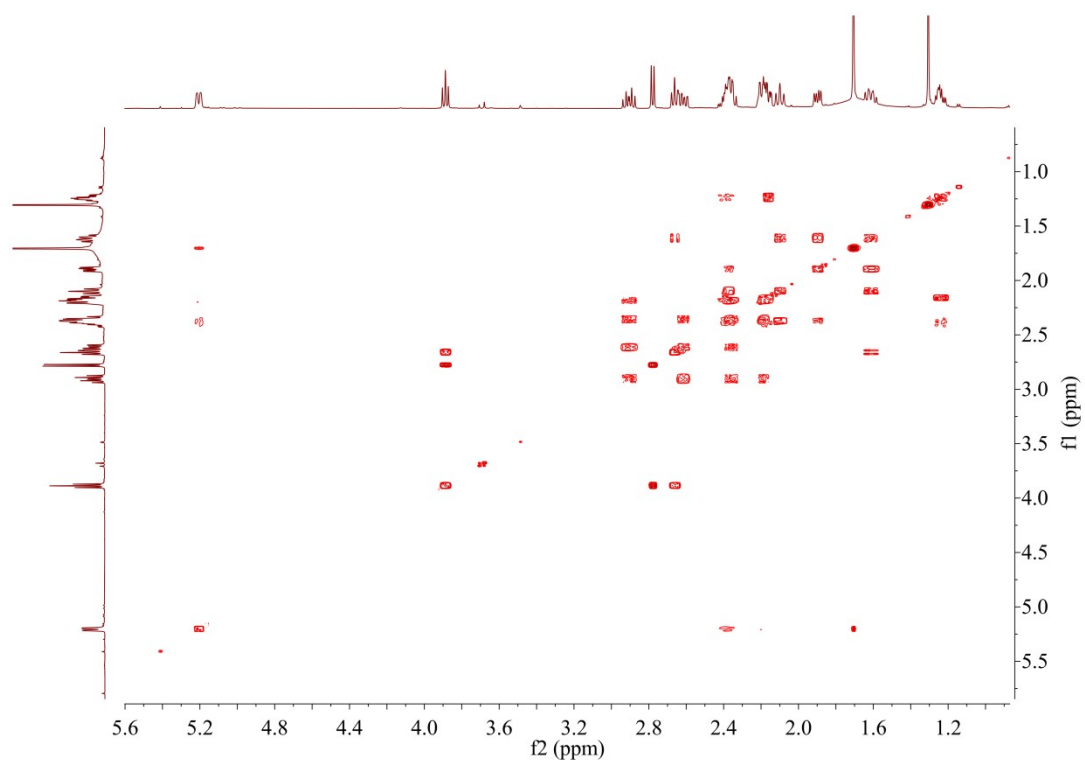


Figure S4. COSY spectrum of magnolin A (**1**) in CDCl_3

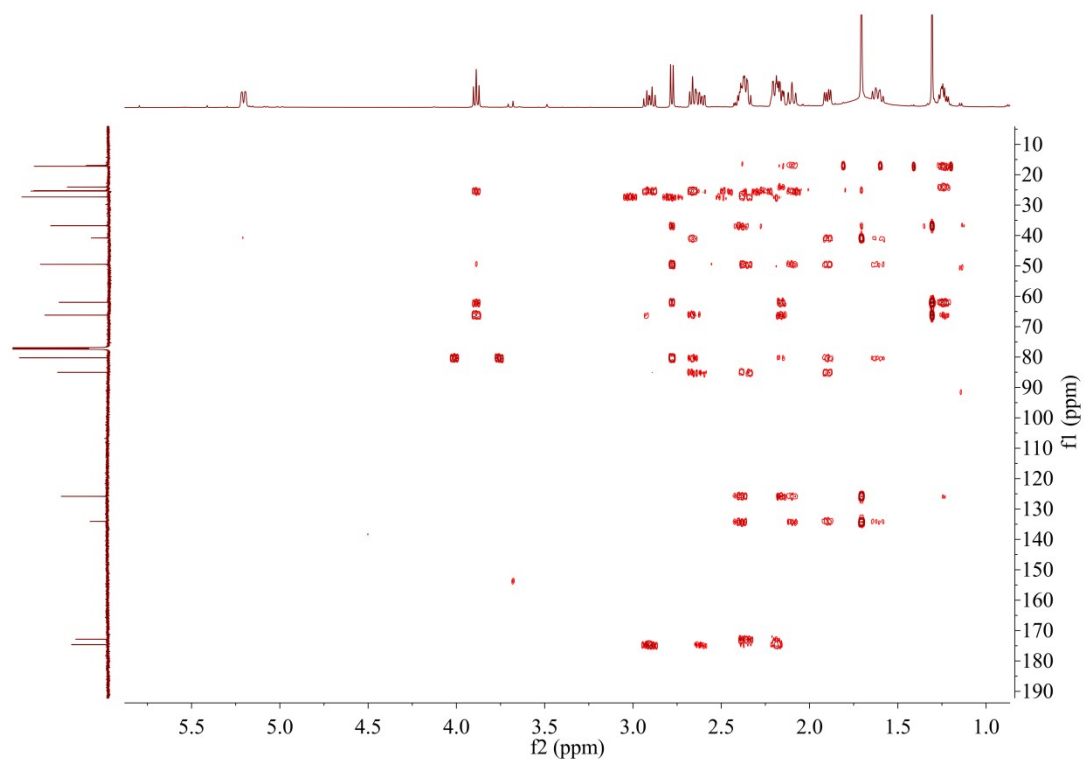


Figure S5. HMBC spectrum of magnolin A (**1**) in CDCl_3

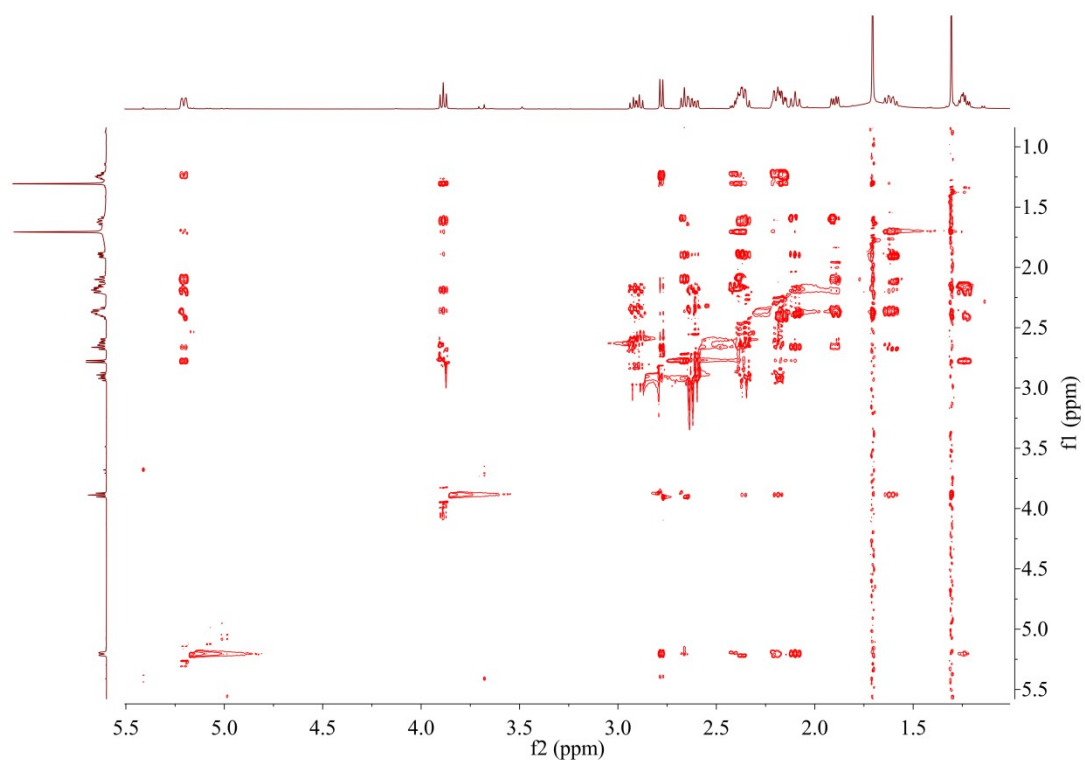


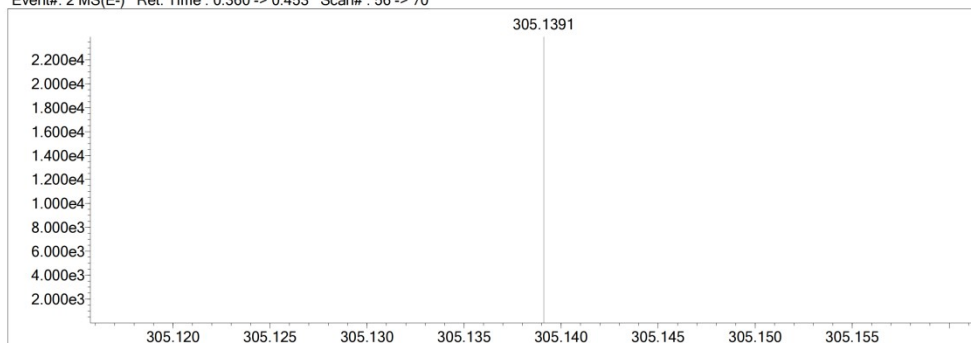
Figure S6. ROESY spectrum of magnolin A (**1**) in CDCl_3

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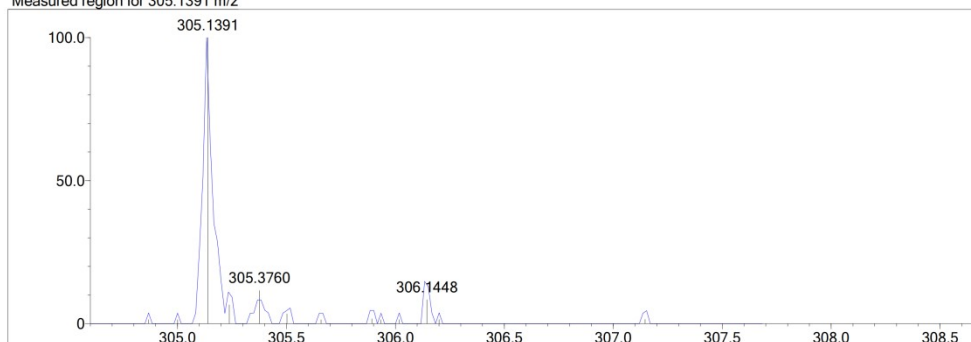
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H	1	5	100	N	3	0	10	Si	4	0	0	H
B	3	0	0	O	2	0	20	S	2	0	0	Cl
C	4	10	50	F	1	0	0	Cl	1	0	0	

Error Margin (ppm): 5
 DBE Range: -2.0 - 1000.0
 Electron Ions: both
 HC Ratio: unlimited
 Apply N Rule: no
 Use MSn Info: no
 Max Isotopes: all
 Isotope RI (%): 1.00
 Isotope Res: 10000
 MSn Iso RI (%): 75.00
 MSn Logic Mode: AND
 Max Results: 50

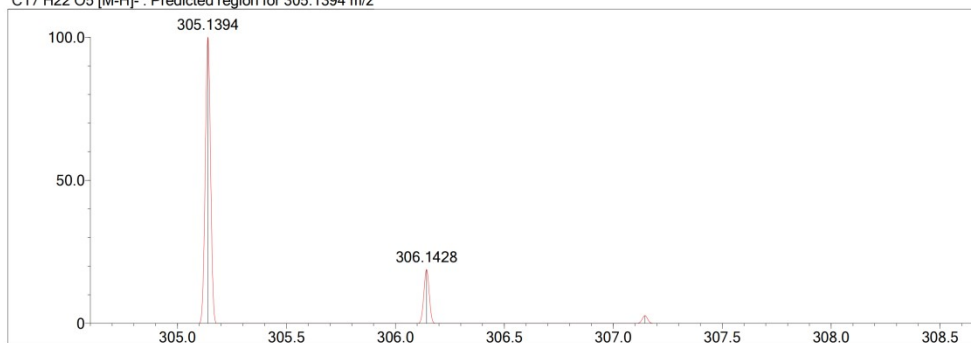
Event#: 2 MS(E-) Ret. Time : 0.360 -> 0.453 Scan# : 56 -> 70



Measured region for 305.1391 m/z



C17 H22 O5 [M-H]-: Predicted region for 305.1394 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C17 H22 O5	[M-H]-	305.1391	305.1394	-0.3	-0.98	7.0

Figure S7. HR-ESI-MS spectrum of magnolin A (1)

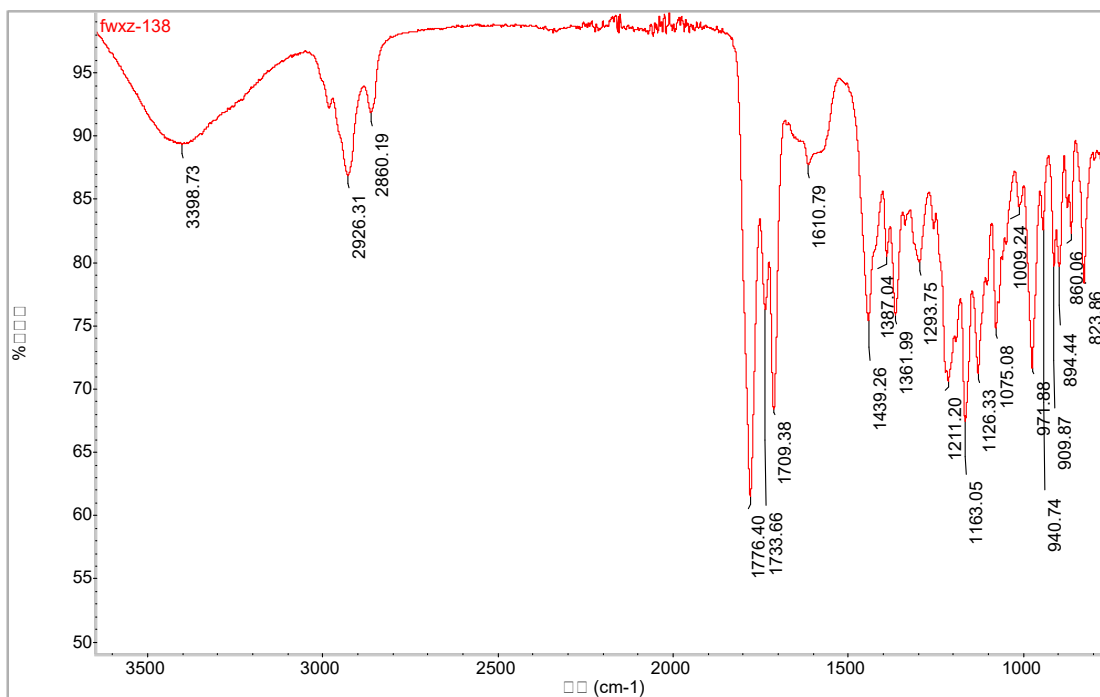


Figure S8. IR spectrum of magnolin A (1)

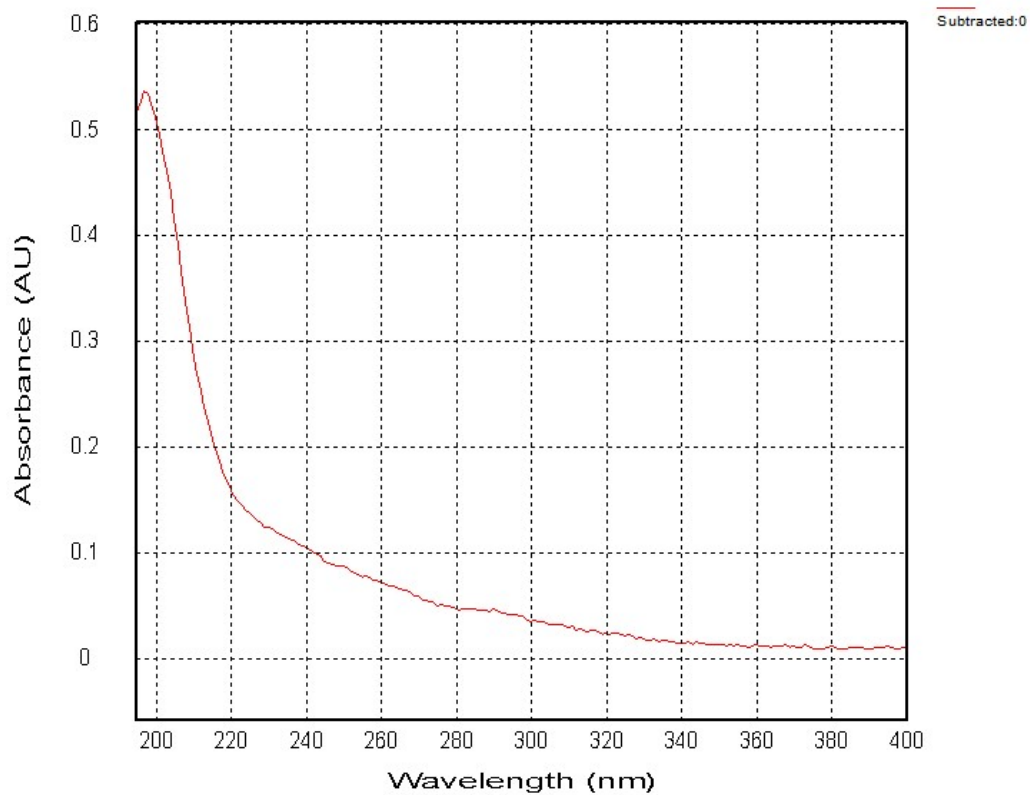


Figure S9. UV spectrum of magnolin A (1)

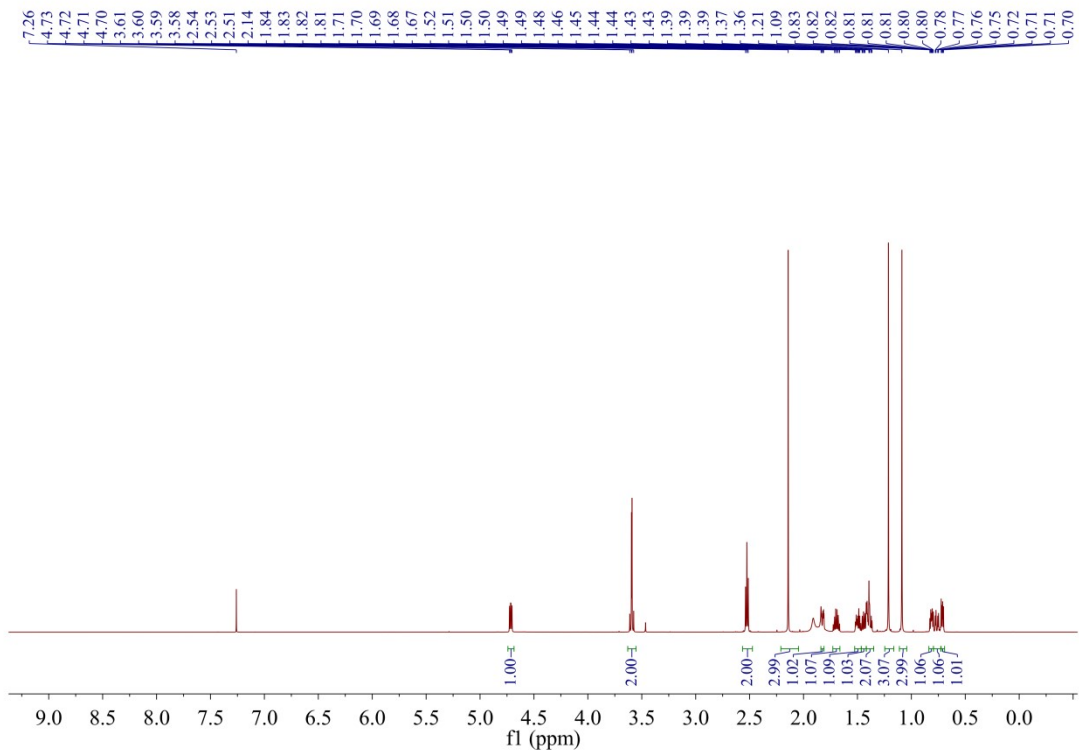


Figure S10. ^1H NMR spectrum of magnolin B (**2**) in CDCl_3

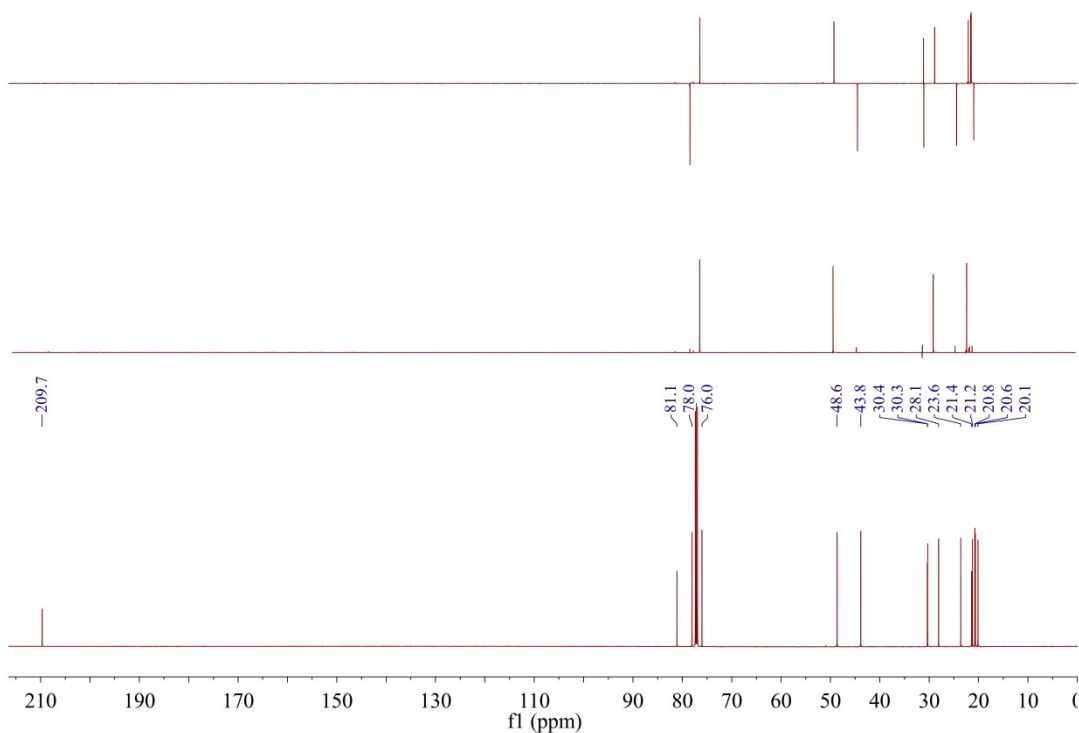


Figure S11. ^{13}C NMR spectrum of magnolin B (**2**) in CDCl_3

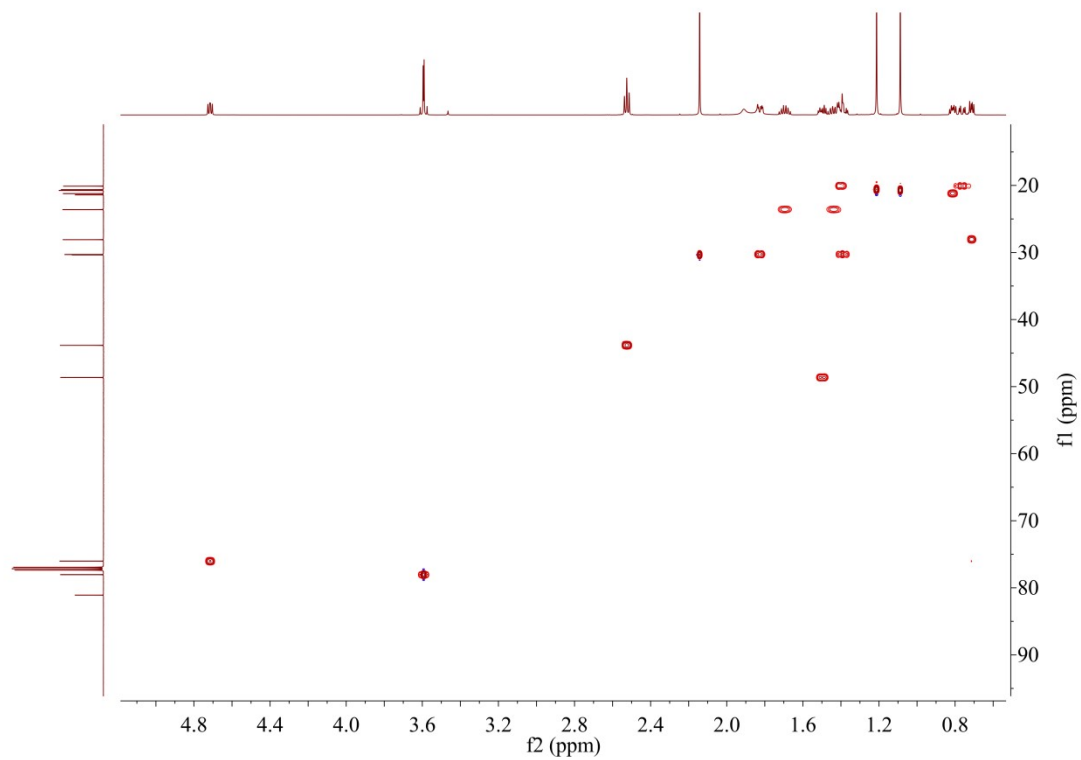


Figure S12. HSQC spectrum of magnolin B (**2**) in CDCl_3

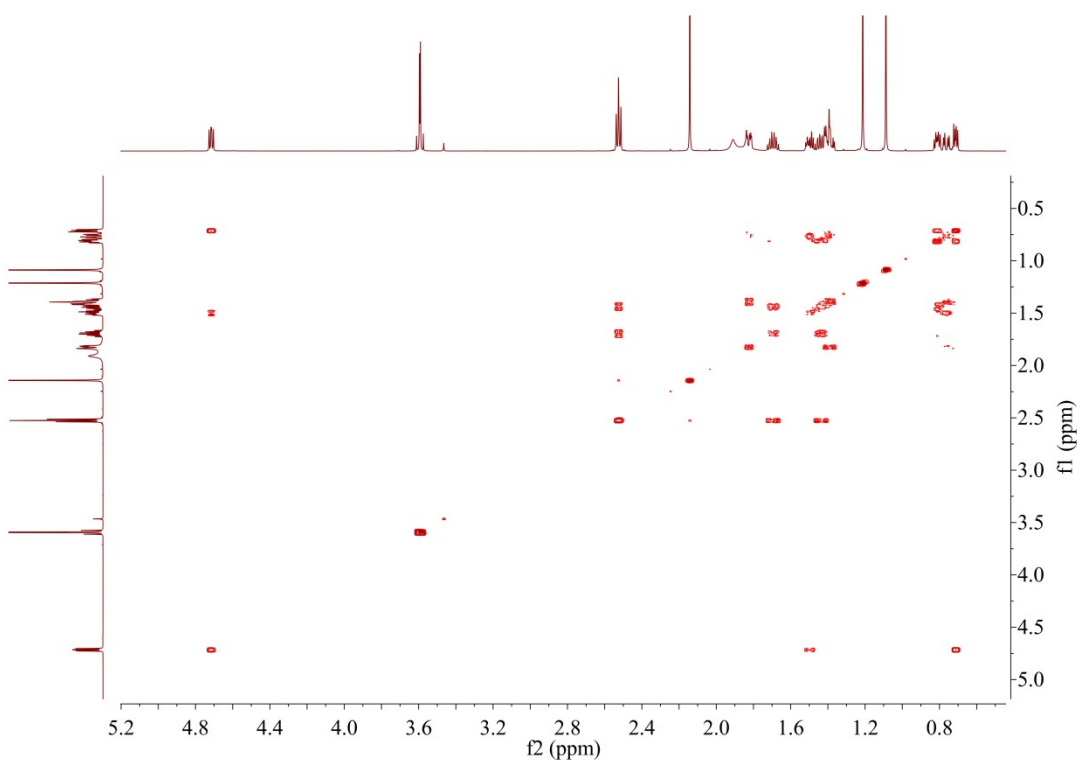


Figure S13. COSY spectrum of magnolin B (**2**) in CDCl_3

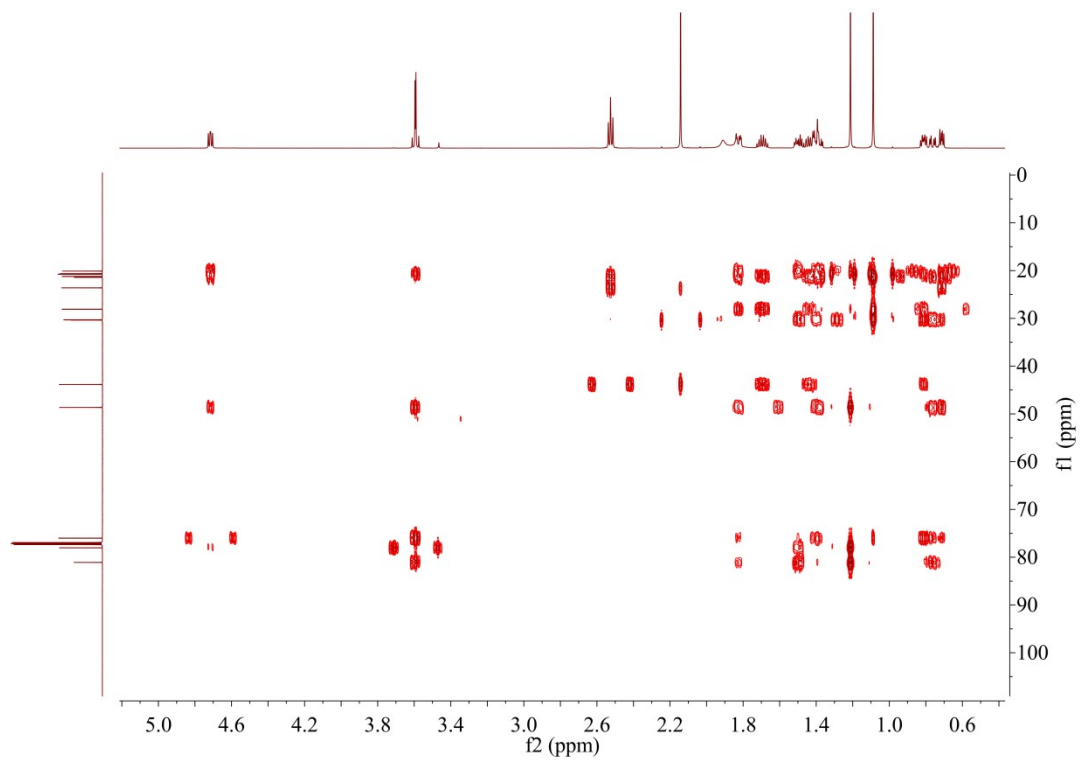


Figure S14. HMBC spectrum of magnolin B (2) in CDCl₃

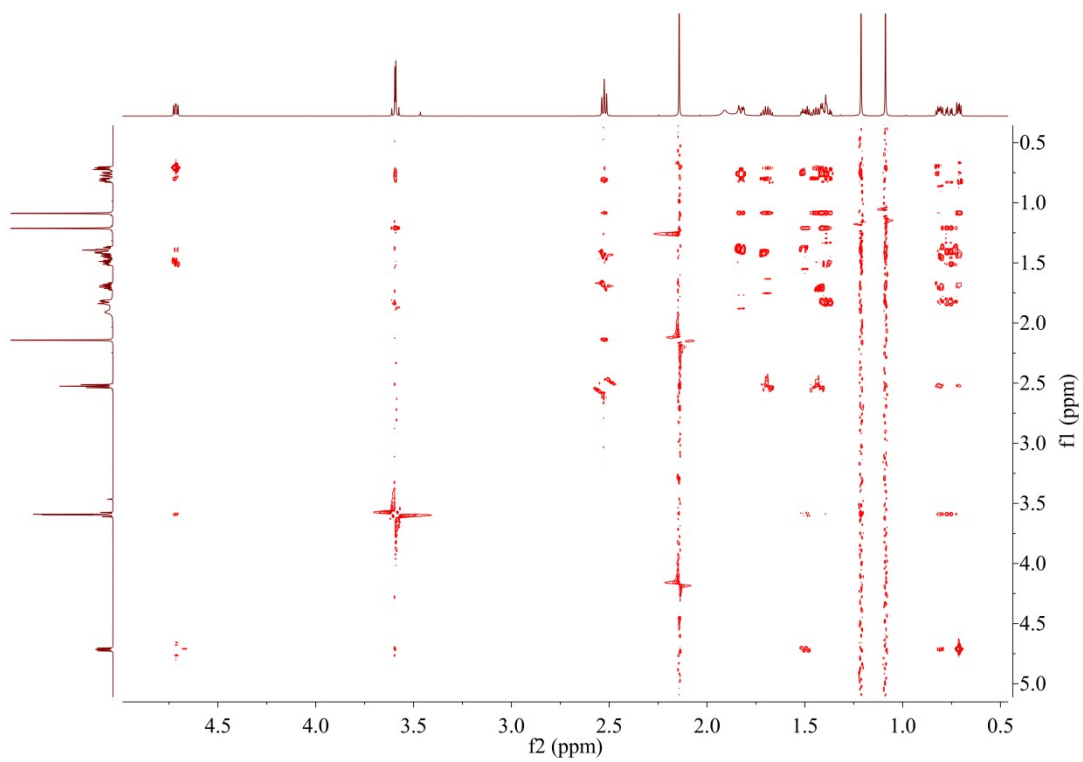


Figure S15. ROESY spectrum of magnolin B (2) in CDCl₃

Data File: D:\DATA\2025\1104\fwxz-132.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	5	100	N	3	0	10	Si	4	0	0	H
B	3	0	0	O	2	0	20	S	2	0	0	Na
C	4	10	50	F	1	0	0	Cl	1	0	0	

Error Margin (ppm): 5
HC Ratio: unlimited
Max Isotopes: all
MSn Iso RI (%): 75.00

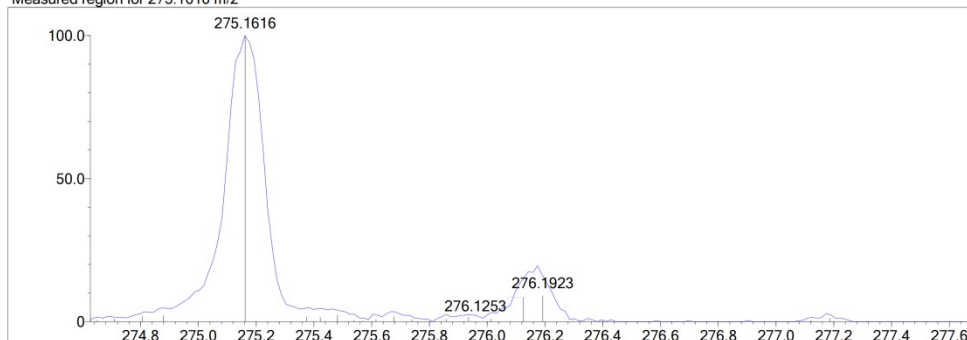
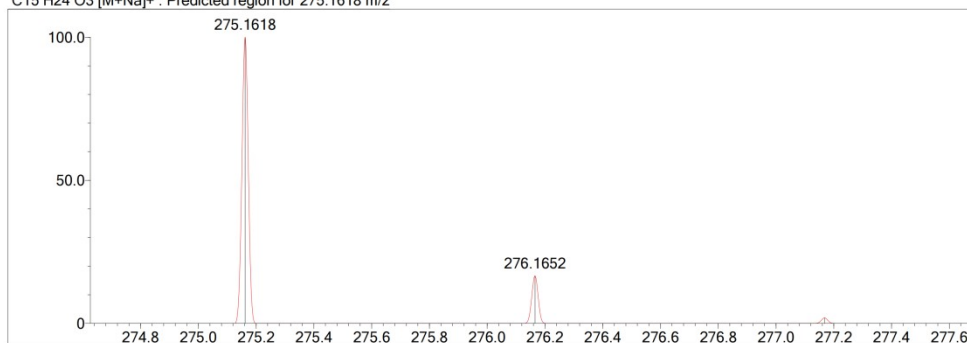
DBE Range: -2.0 - 1000.0
Apply N Rule: no
Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: both
Use MSn Info: no
Isotope Res: 10000
Max Results: 50

Event#: 1 MS(E+) Ret. Time : 0.440 -> 0.493 Scan#: 67 -> 75



Measured region for 275.1616 m/z

C15 H24 O3 [M+Na]⁺ : Predicted region for 275.1618 m/z

Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C15 H24 O3	[M+Na] ⁺	275.1616	275.1618	-0.2	-0.73	4.0

Figure S16. HR-ESI-MS spectrum of magnolin B (2)

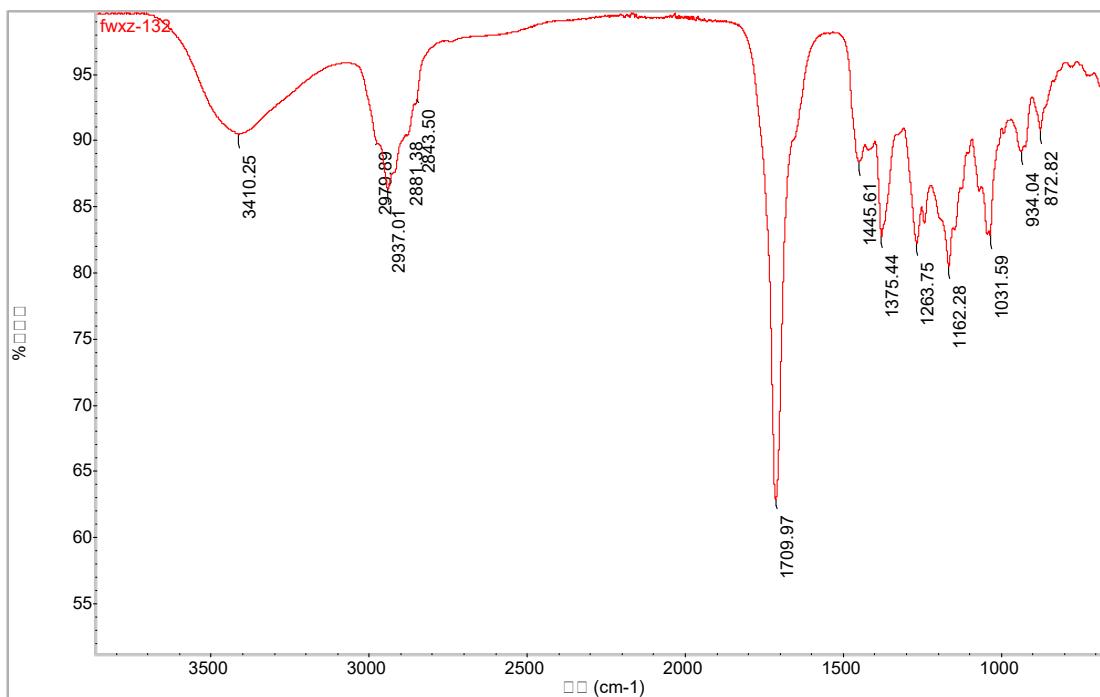


Figure S17. IR spectrum of magnolin B (2)

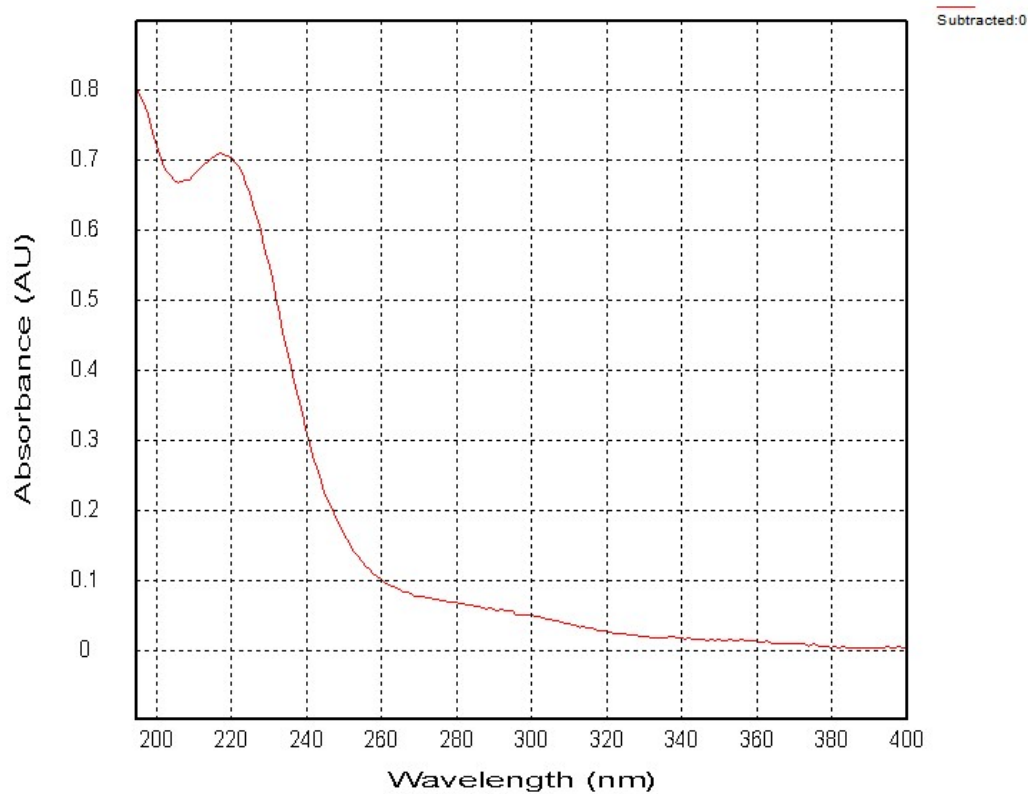


Figure S18. UV spectrum of magnolin B (2)

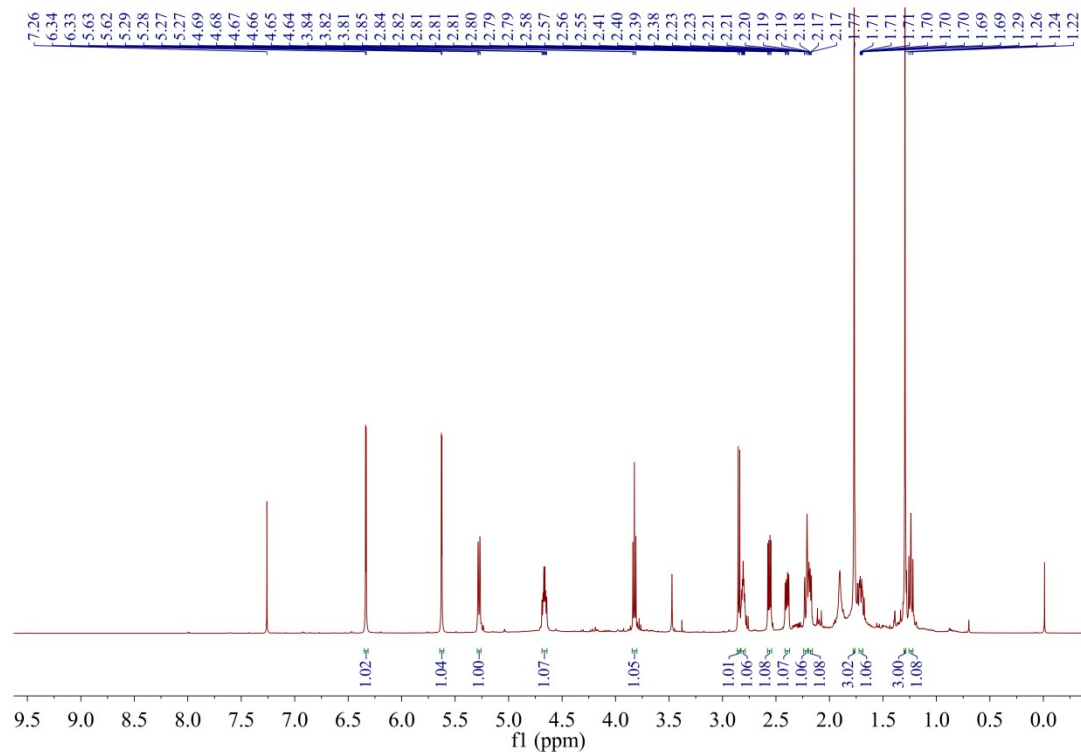


Figure S19. ^1H NMR spectrum of magnolin C (**3**) in CDCl_3

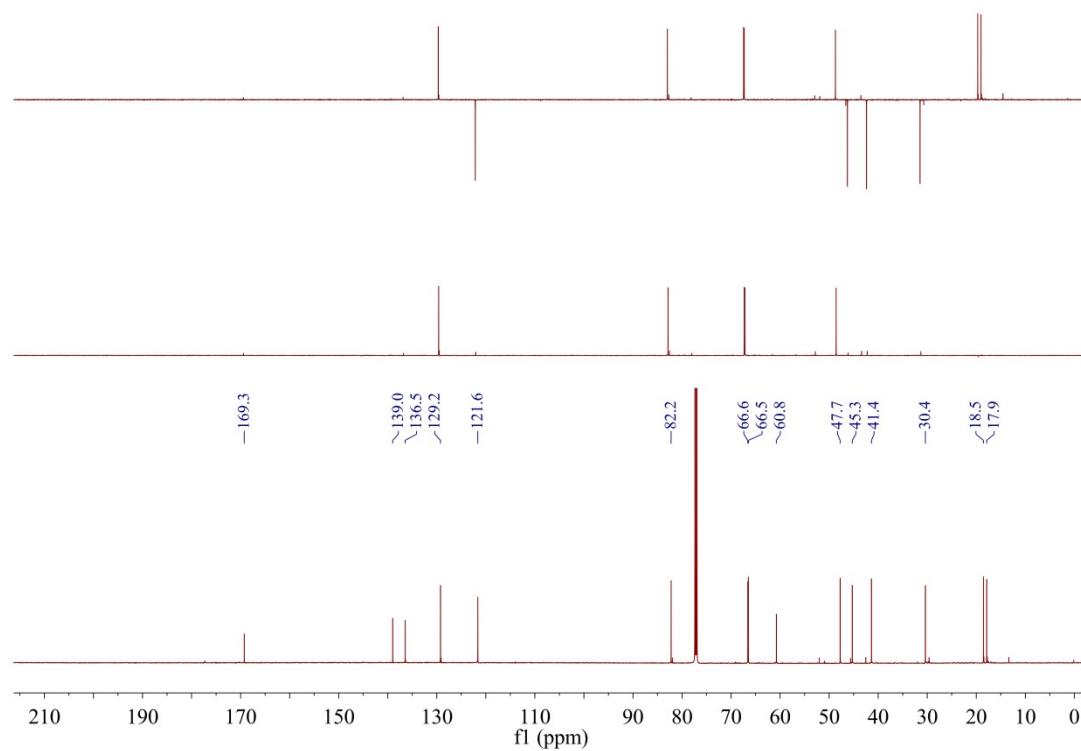


Figure S20. ^{13}C NMR spectrum of magnolin C (**3**) in CDCl_3

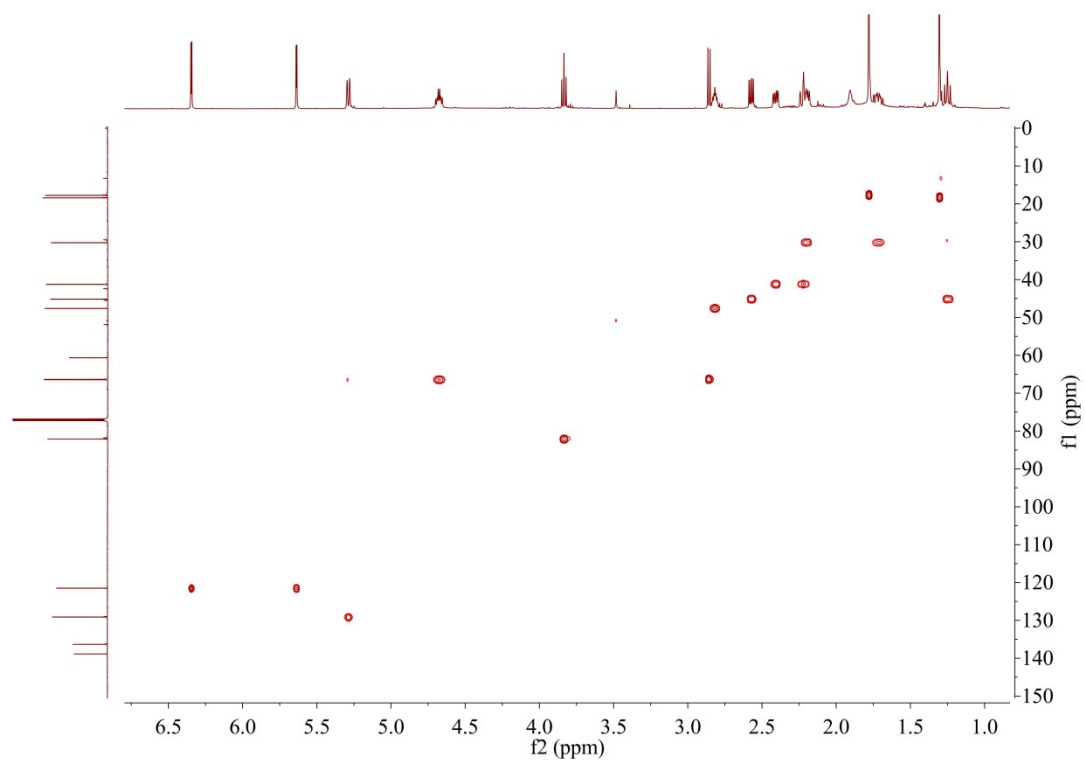


Figure S21. HSQC spectrum of magnolin C (**3**) in CDCl_3

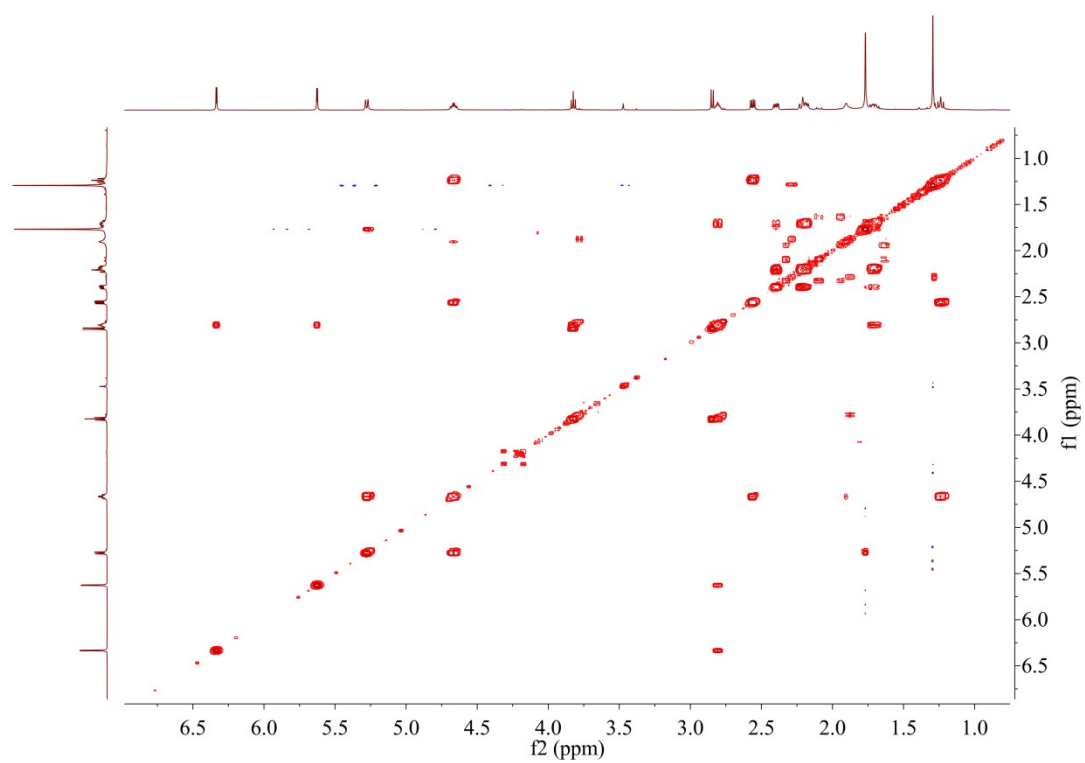


Figure S22. COSY spectrum of magnolin C (**3**) in CDCl_3

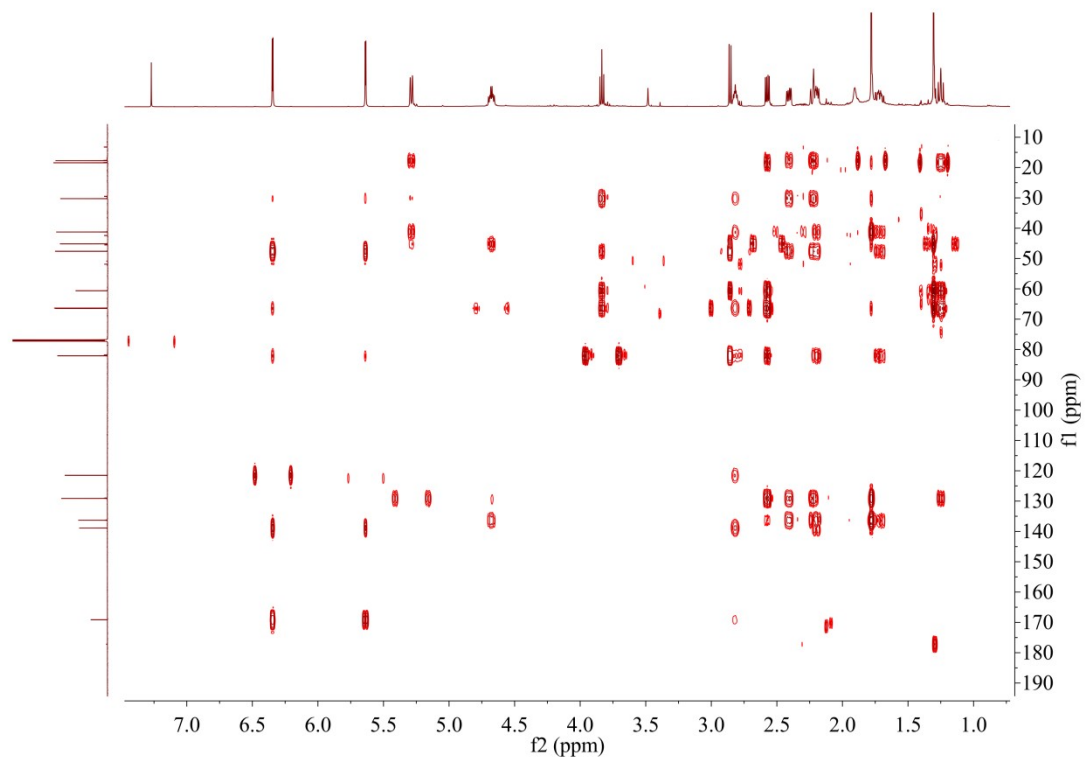


Figure S23. HMBC spectrum of magnolin C (**3**) in CDCl_3

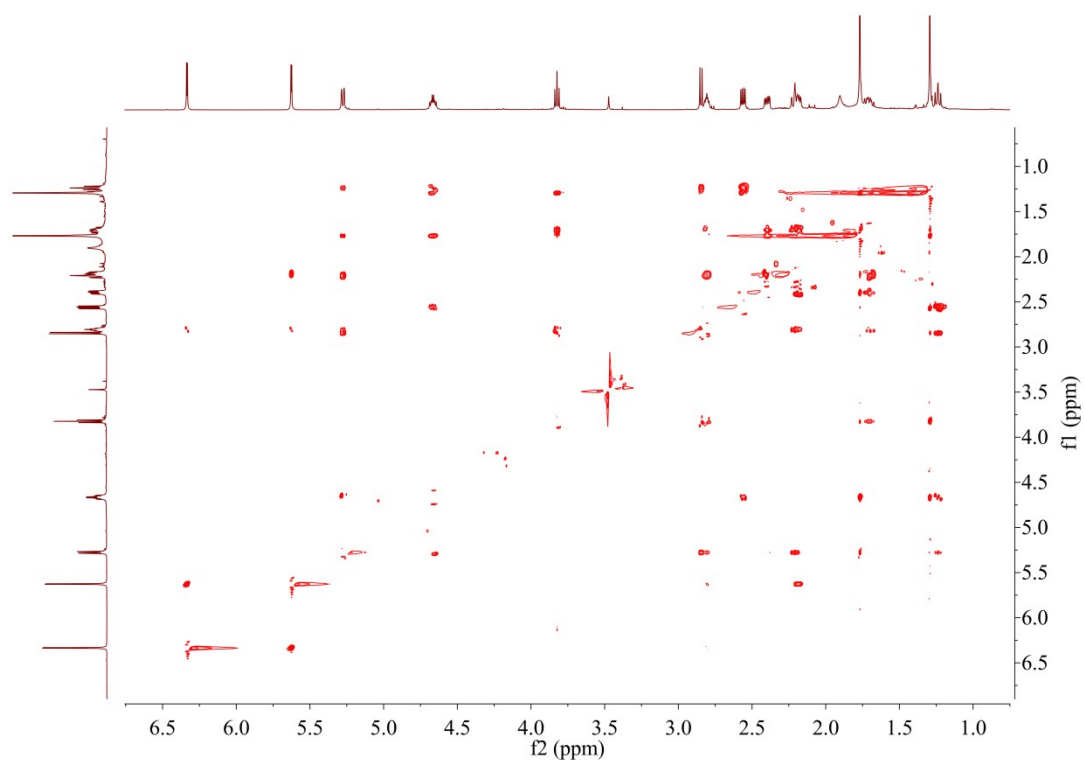


Figure S24. ROESY spectrum of magnolin C (**3**) in CDCl_3

Data File: D:\DATA\2025\1104\fwzx-125.lcd

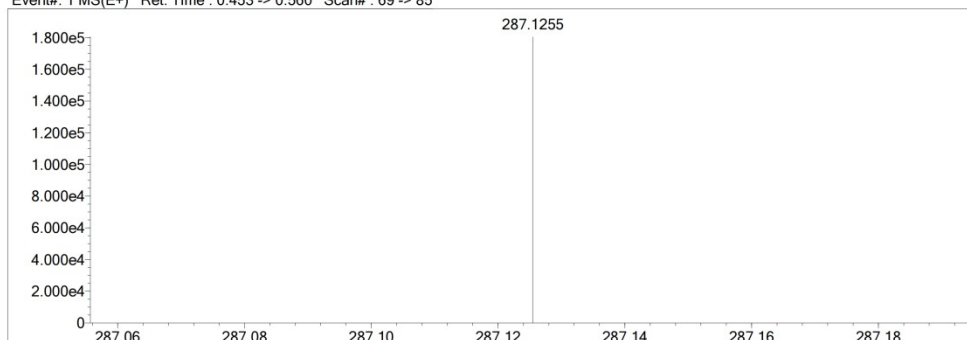
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	5	100	N	3	0	10	Si	4	0	0	H
B	3	0	0	O	2	0	20	S	2	0	0	Na
C	4	10	50	F	1	0	0	Cl	1	0	0	

Error Margin (ppm): 5
HC Ratio: unlimited
Max Isotopes: all
MSn Iso RI (%): 75.00

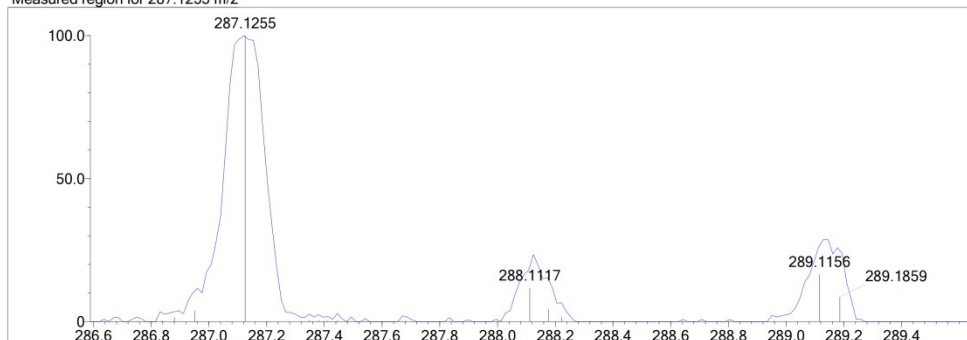
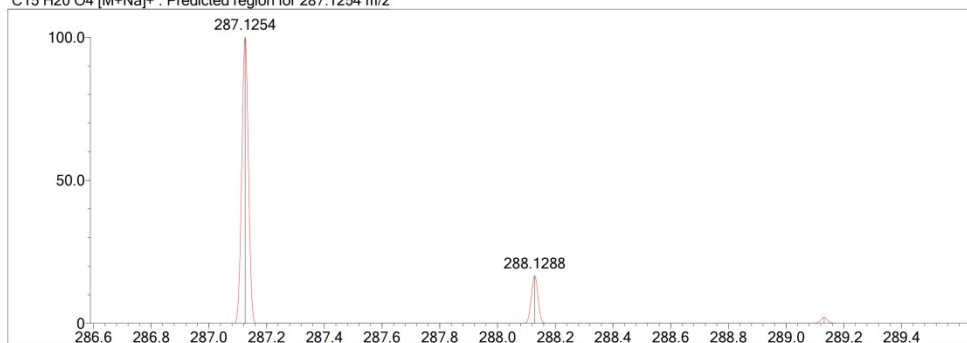
DBE Range: -2.0 - 1000.0
Apply N Rule: no
Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: both
Use MSn Info: no
Isotope Res: 10000
Max Results: 50

Event#: 1 MS(E+) Ret. Time : 0.453 -> 0.560 Scan#: 69 -> 85



Measured region for 287.1255 m/z

C15 H20 O4 [M+Na]⁺ : Predicted region for 287.1254 m/z

Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C15 H20 O4	[M+Na] ⁺	287.1255	287.1254	0.1	0.35	6.0

Figure S25. HR-ESI-MS spectrum of magnolin C (3)

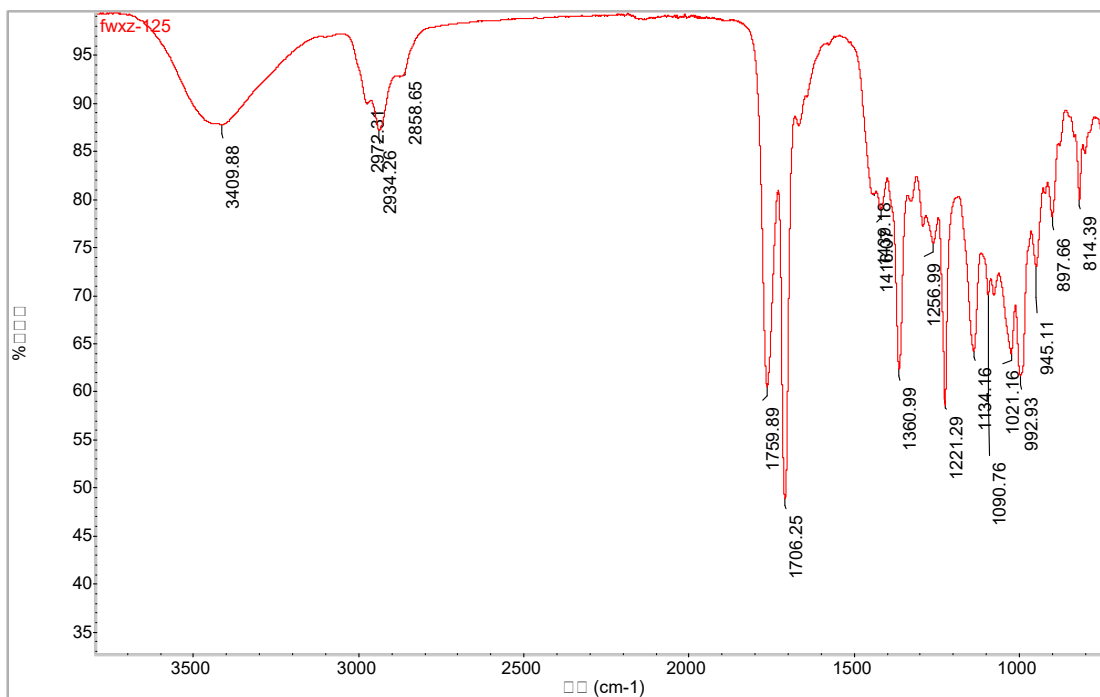


Figure S26. IR spectrum of magnolin C (3)

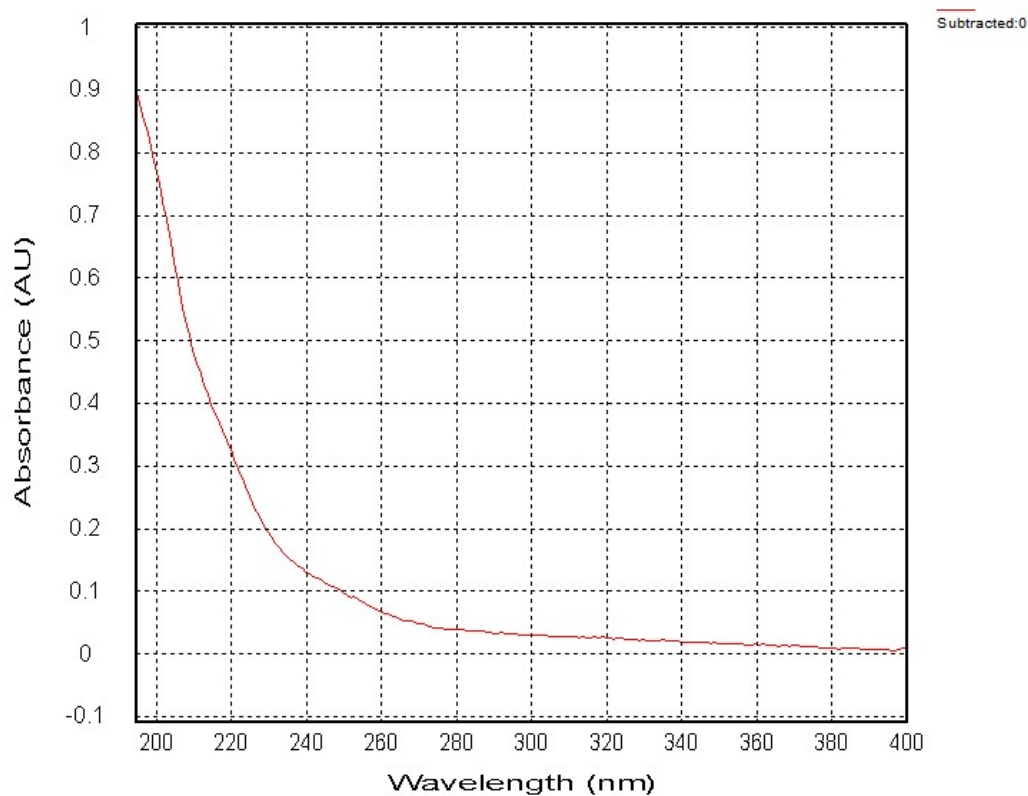


Figure S27. UV spectrum of magnolin C (3)

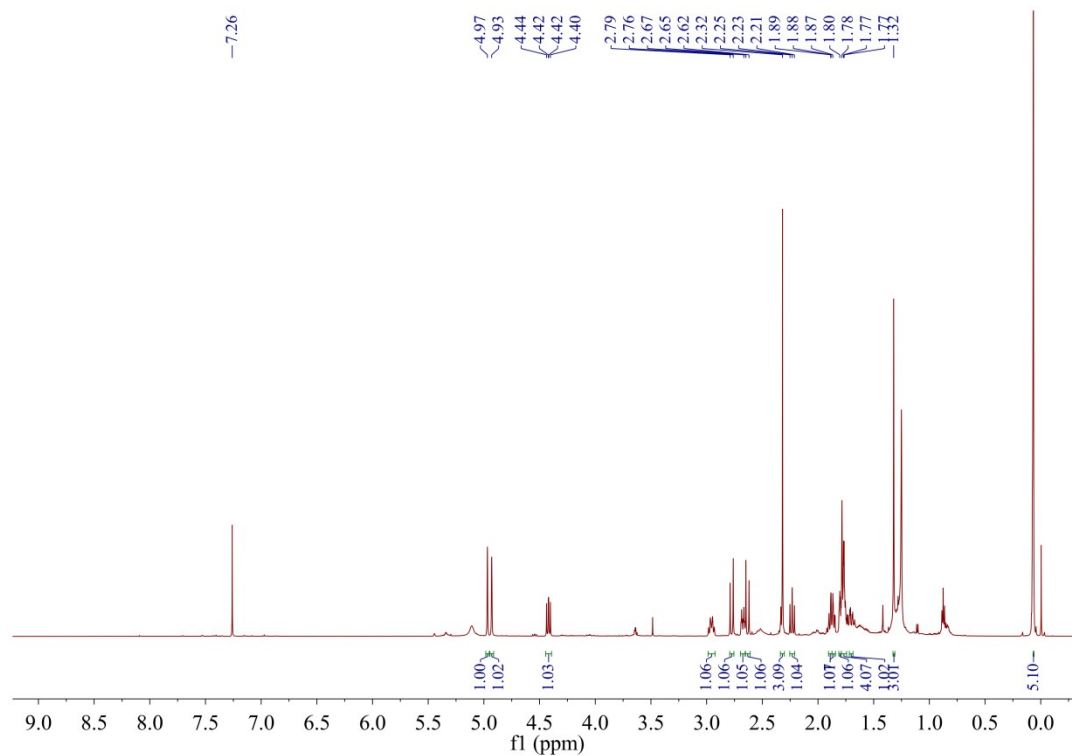


Figure S28. ^1H NMR spectrum of magnolin D (**5**) in CDCl_3

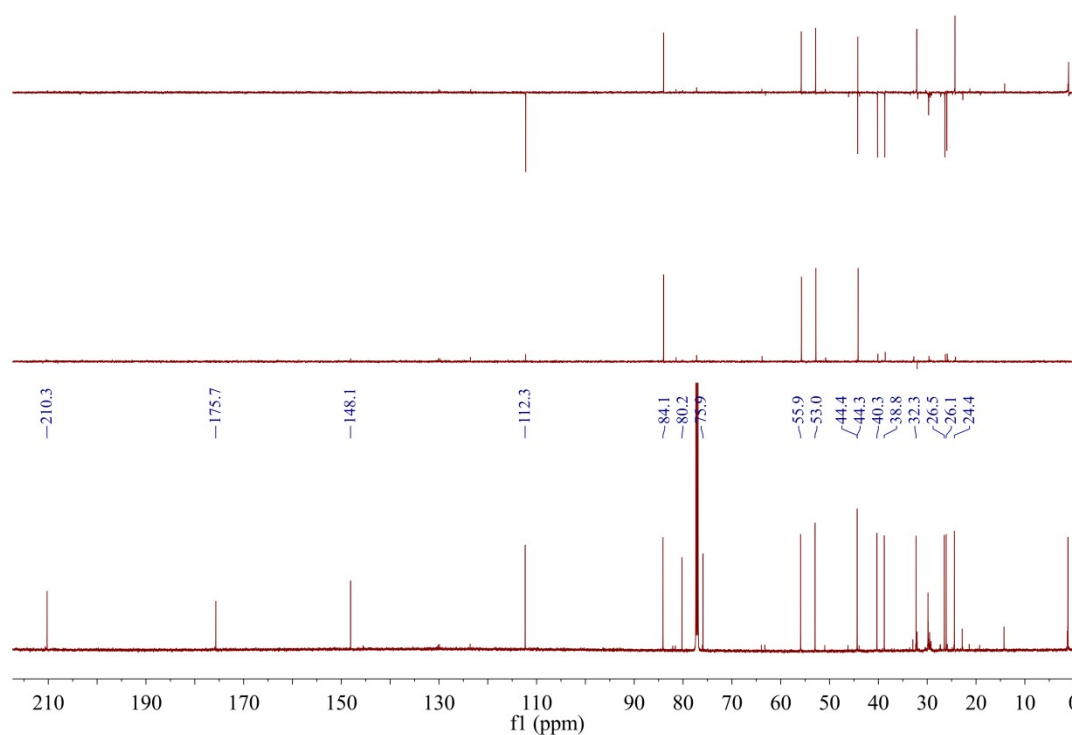


Figure S29. ^{13}C NMR spectrum of magnolin D (**5**) in CDCl_3

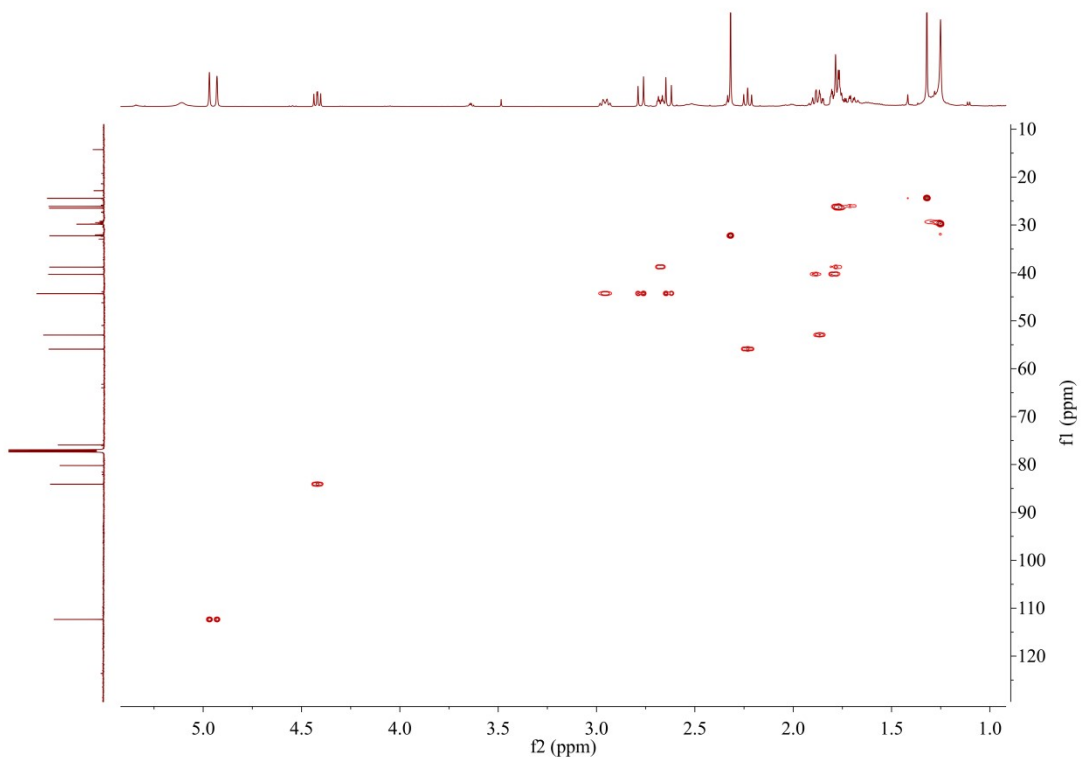


Figure S30. HSQC spectrum of magnolin D (**5**) in CDCl_3

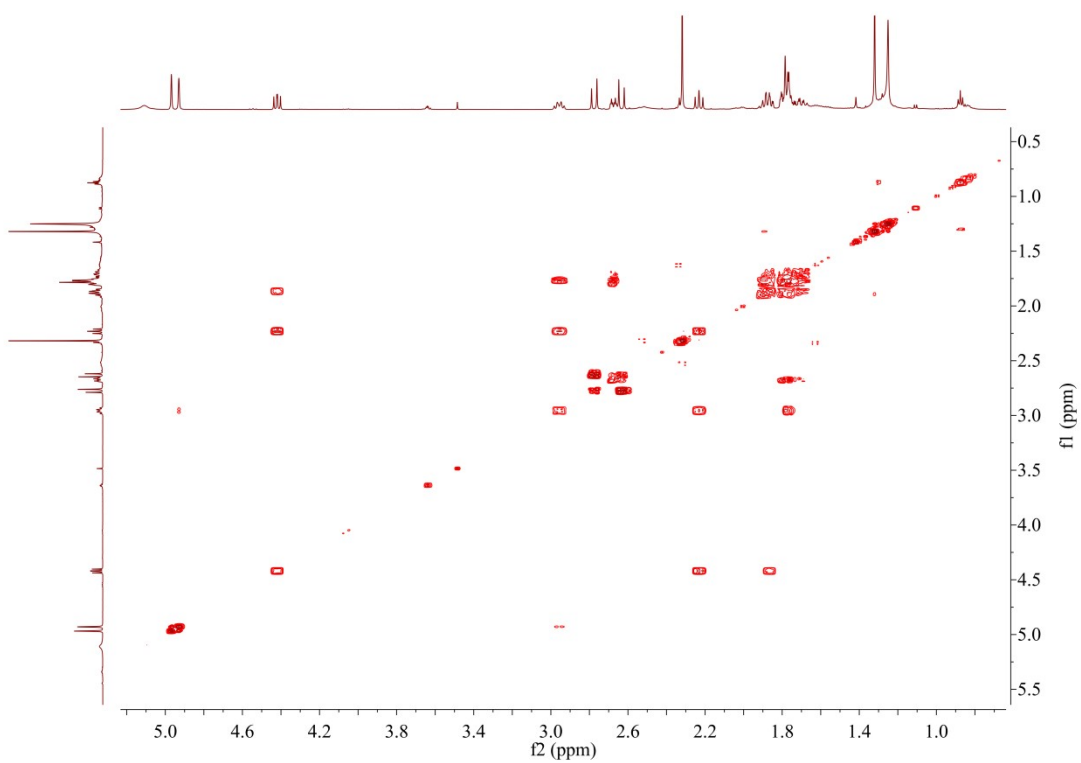


Figure S31. COSY spectrum of magnolin D (**5**) in CDCl_3

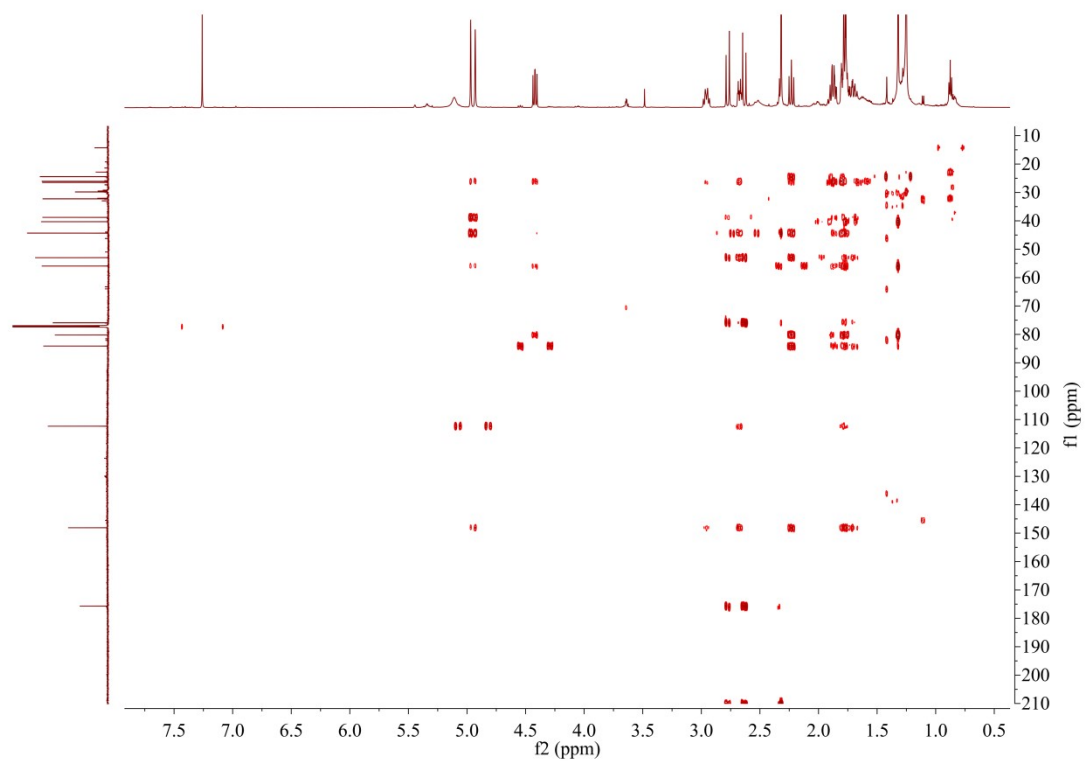


Figure S32. HMBC spectrum of magnolin D (**5**) in CDCl_3

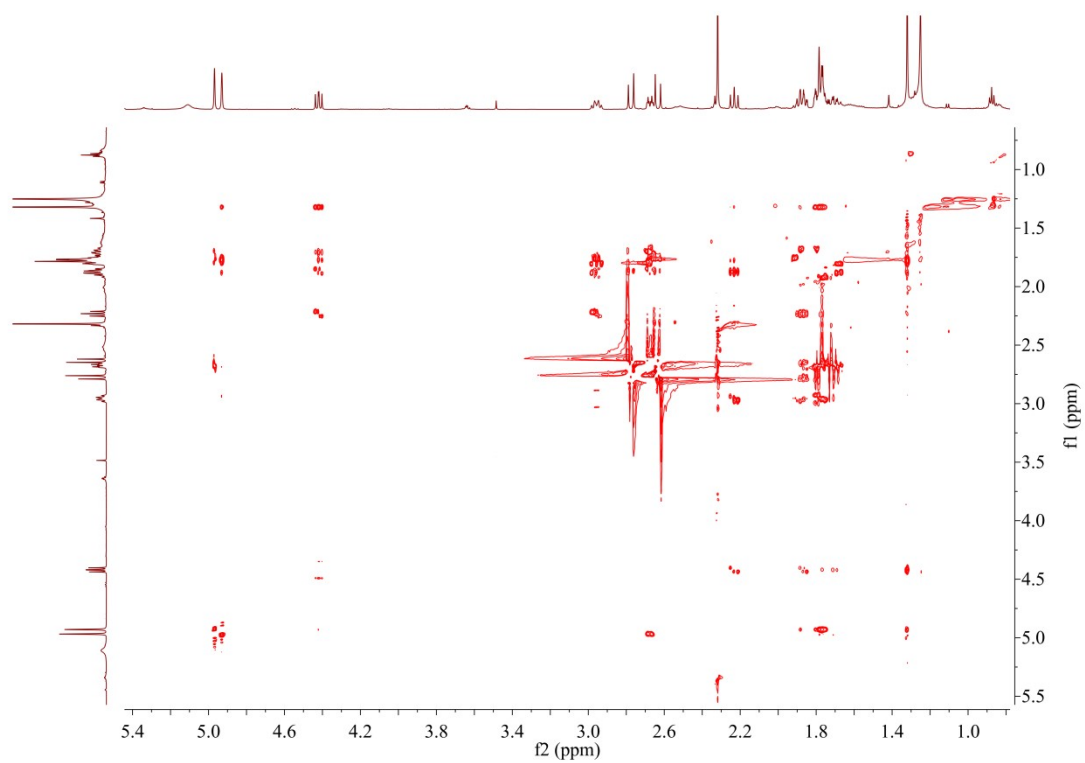


Figure S33. ROESY spectrum of magnolin D (**5**) in CDCl_3

Data File: D:\DATA\2025\0821\fwxz-112.lcd

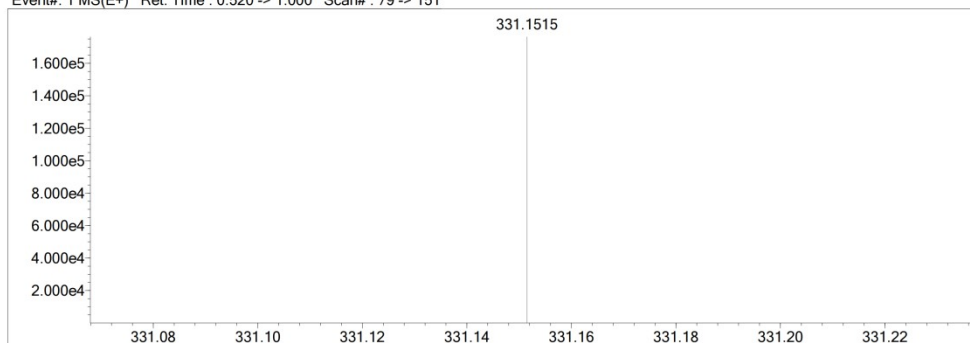
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	5	100	O	2	0	20	S	2	0	5	H
C	4	5	50	F	1	0	0	Cl	1	0	0	Na
N	3	0	10	Si	4	0	0	Br	1	0	0	

Error Margin (ppm): 5
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

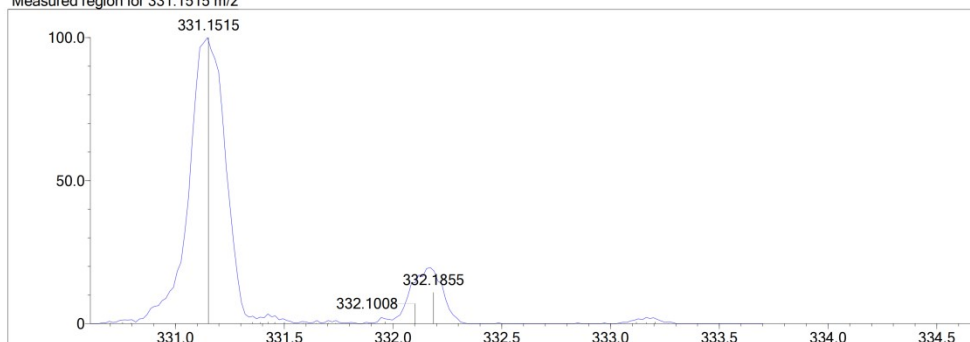
DBE Range: -2.0 - 1000.0
 Apply N Rule: no
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 50

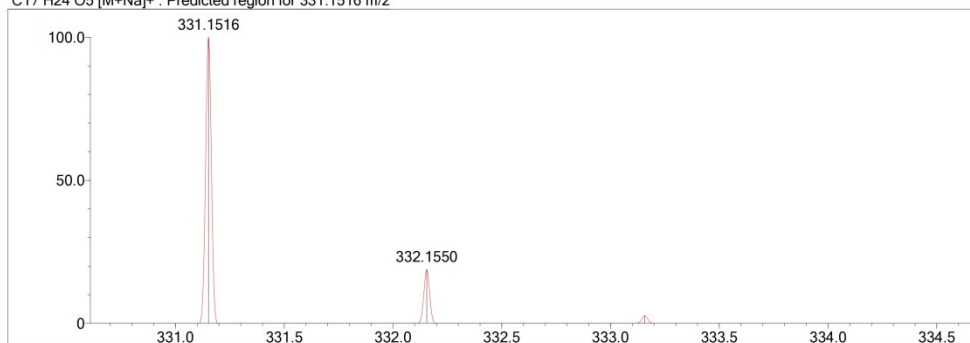
Event#: 1 MS(E+) Ret. Time : 0.520 -> 1.000 Scan#: 79 -> 151



Measured region for 331.1515 m/z



C17 H24 O5 [M+Na]+ : Predicted region for 331.1516 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C17 H24 O5	[M+Na]+	331.1515	331.1516	-0.1	-0.30	6.0

Figure S34. HR-ESI-MS spectrum of magnolin D (5)

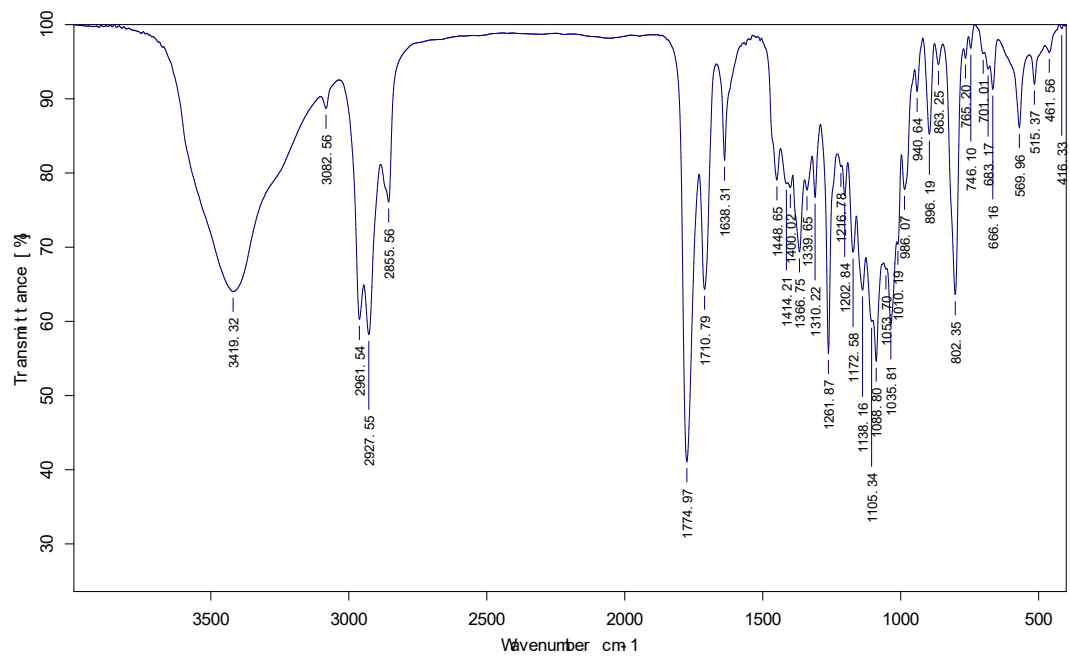


Figure S35. IR spectrum of magnolin D (5)

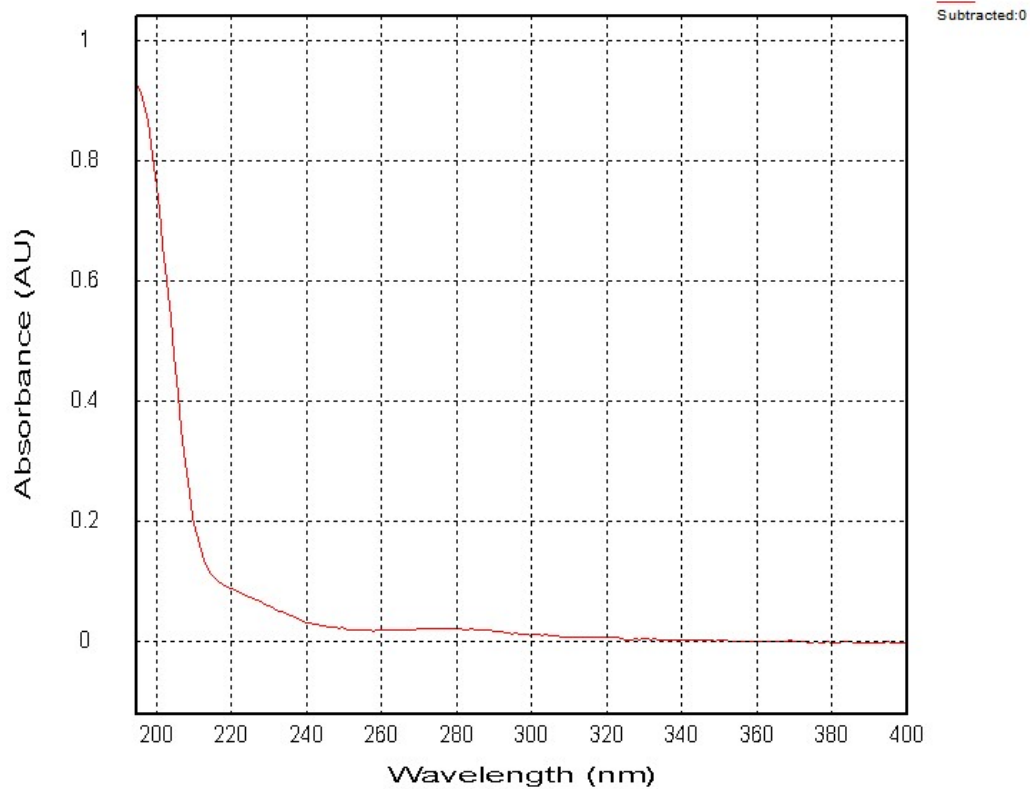


Figure S36. UV spectrum of magnolin D (5)

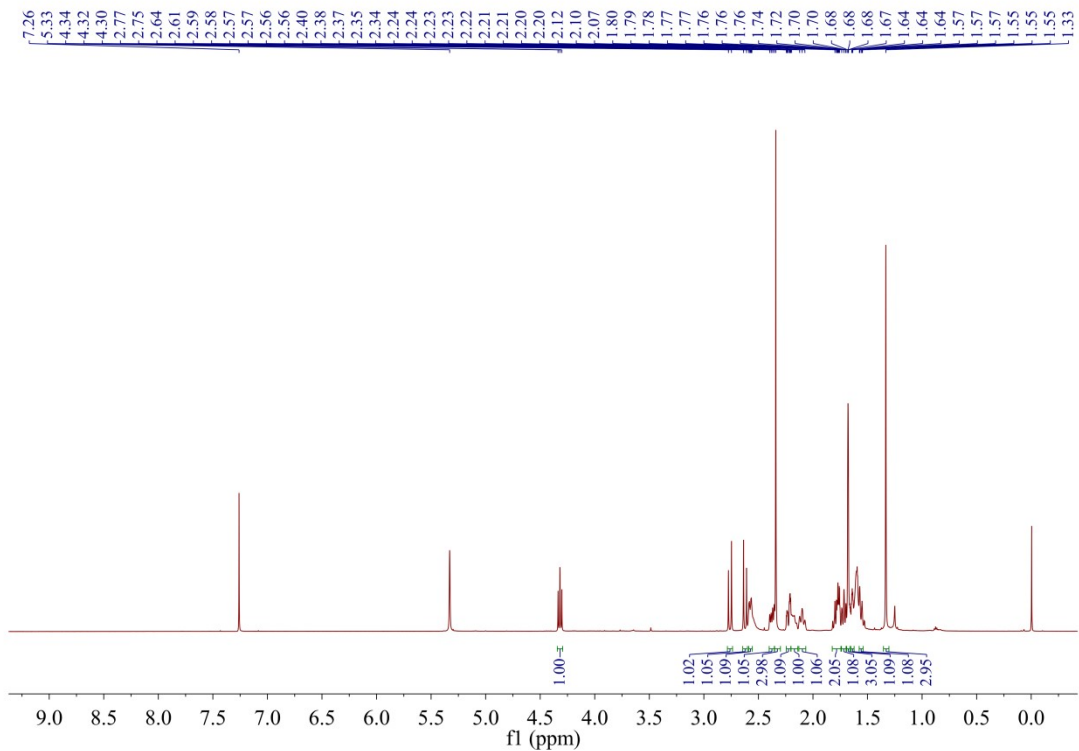


Figure S37. ^1H NMR spectrum of magnolin E (**6**) in CDCl_3

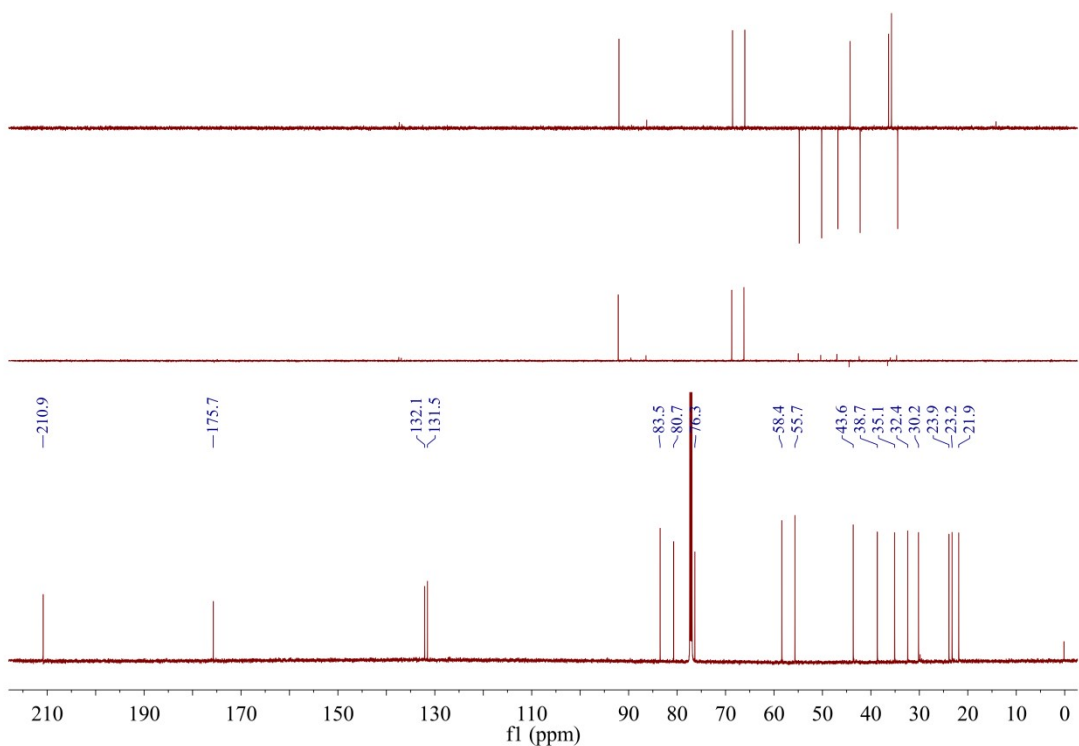


Figure S38. ^{13}C NMR spectrum of magnolin E (**6**) in CDCl_3

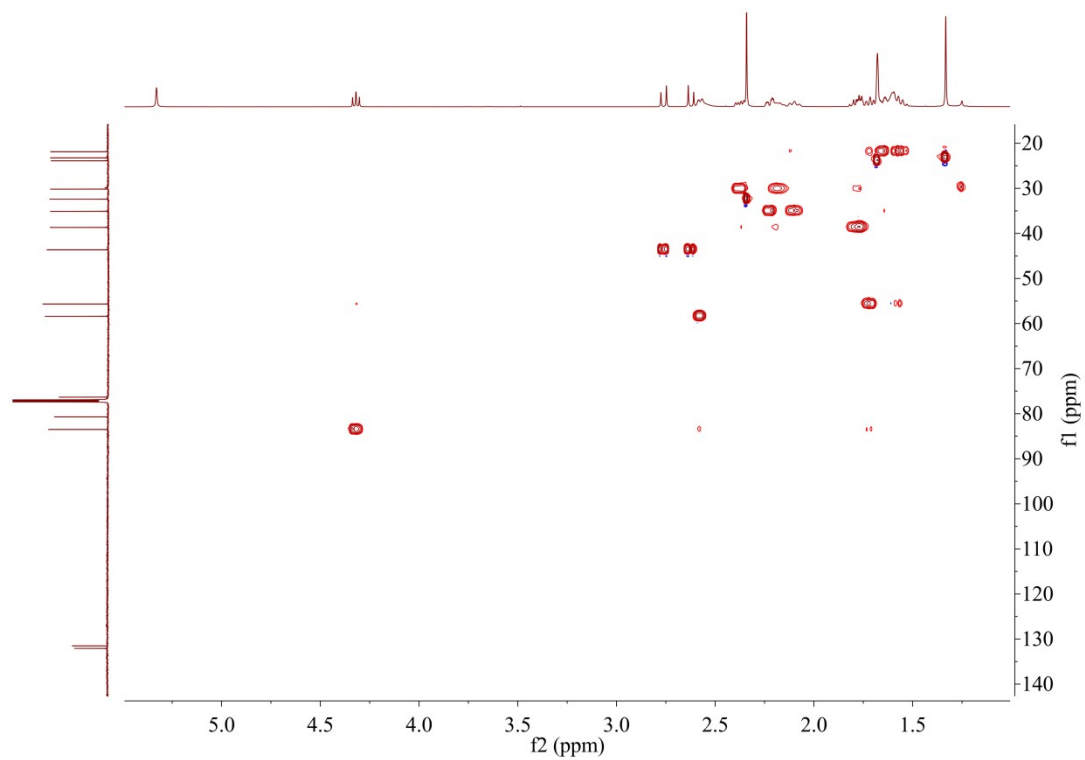


Figure S39. HSQC spectrum of magnolin E (**6**) in CDCl₃

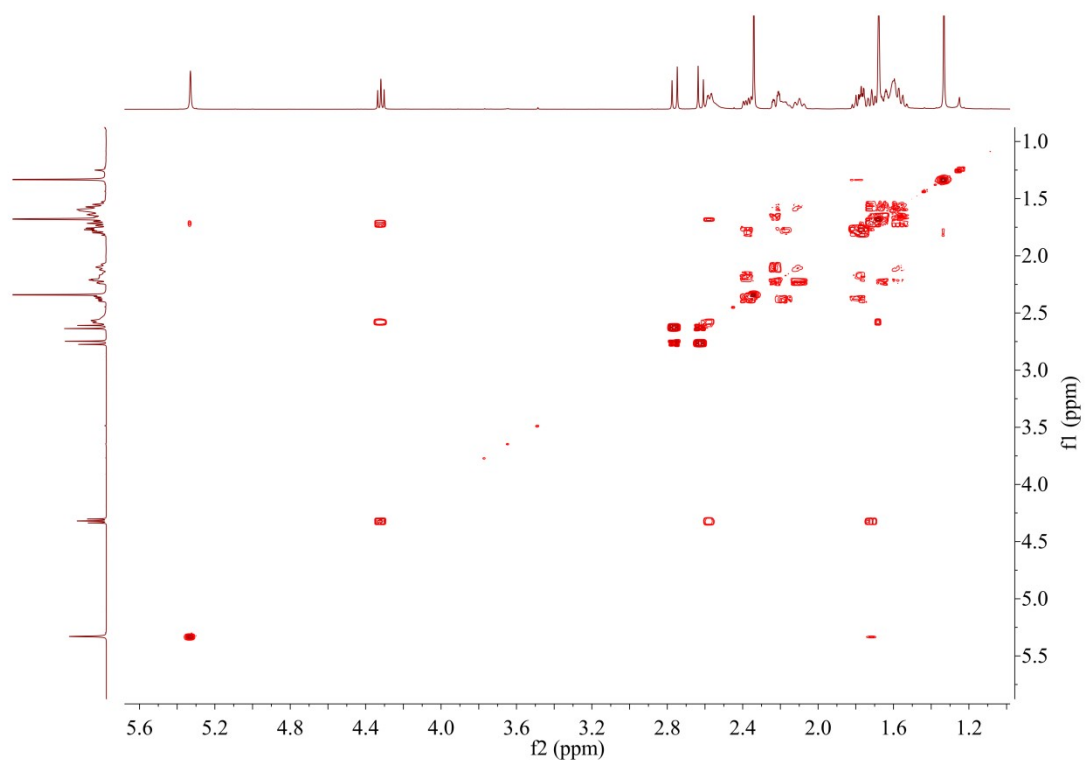


Figure S40. COSY spectrum of magnolin E (**6**) in CDCl₃

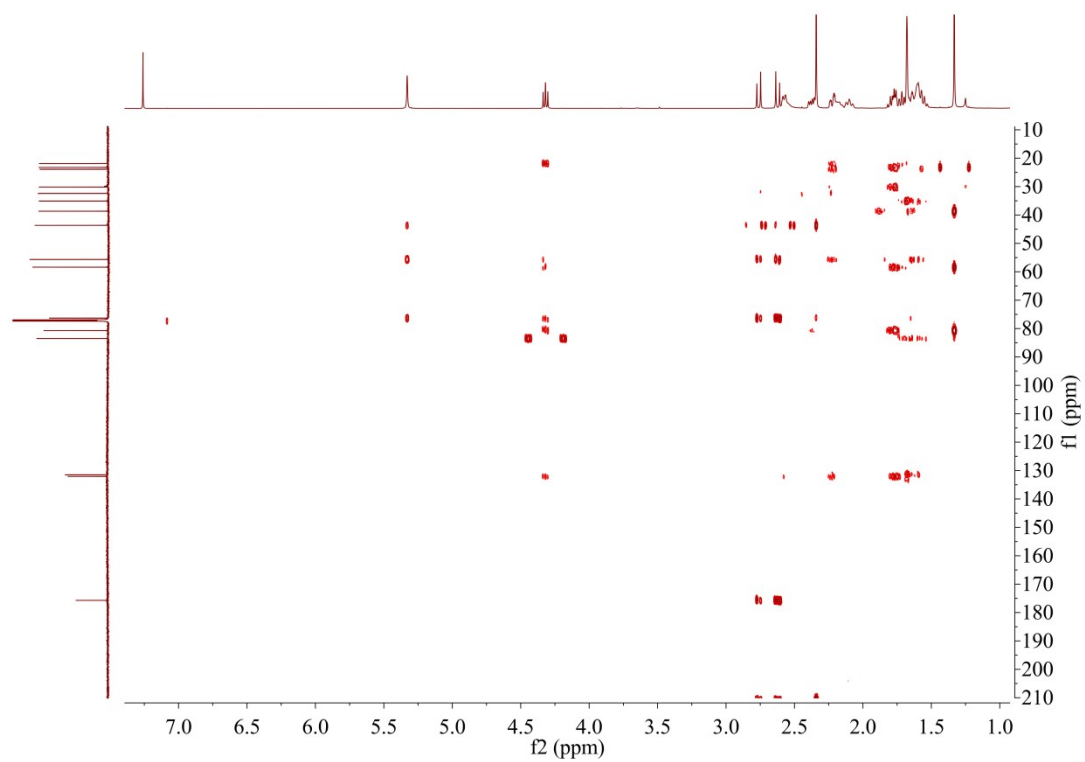


Figure S41. HMBC spectrum of magnolin E (**6**) in CDCl_3

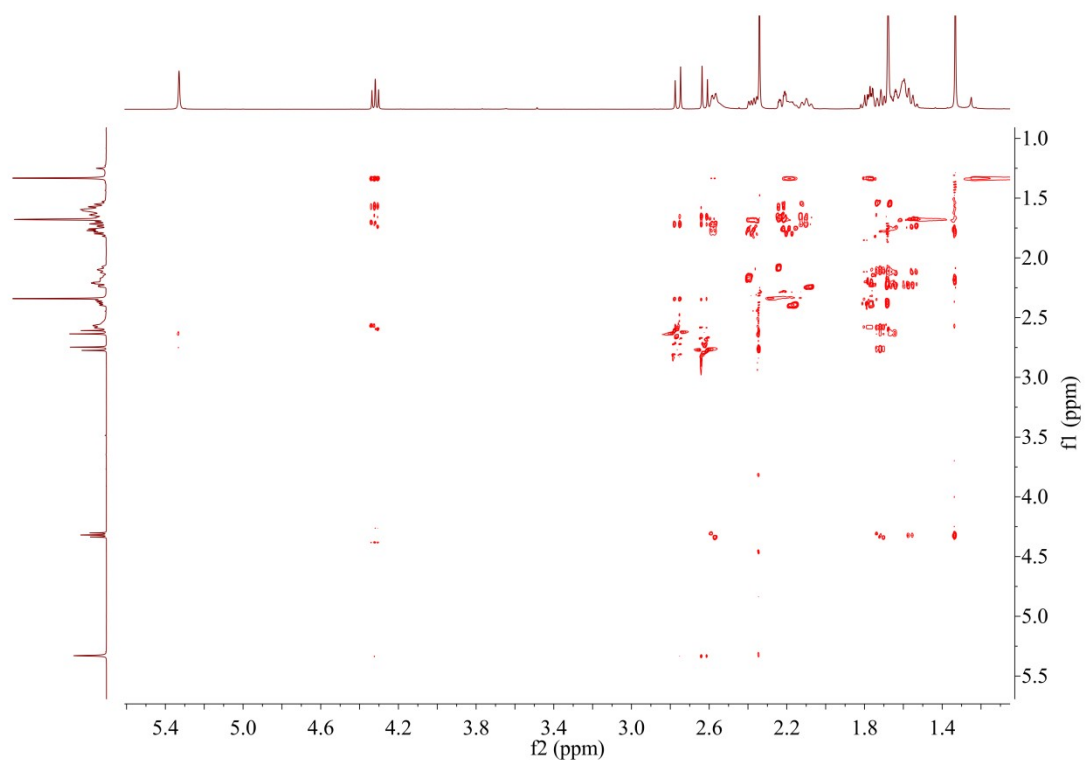


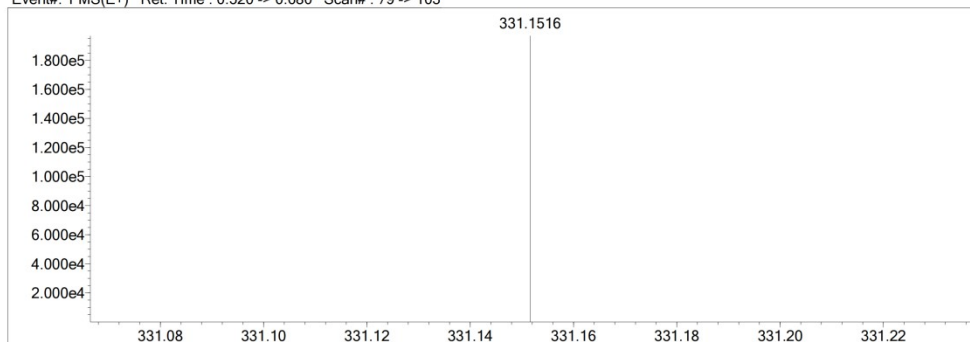
Figure S42. ROESY spectrum of magnolin E (**6**) in CDCl_3

Data File: D:\DATA\2025\0821\fwz-110.lcd

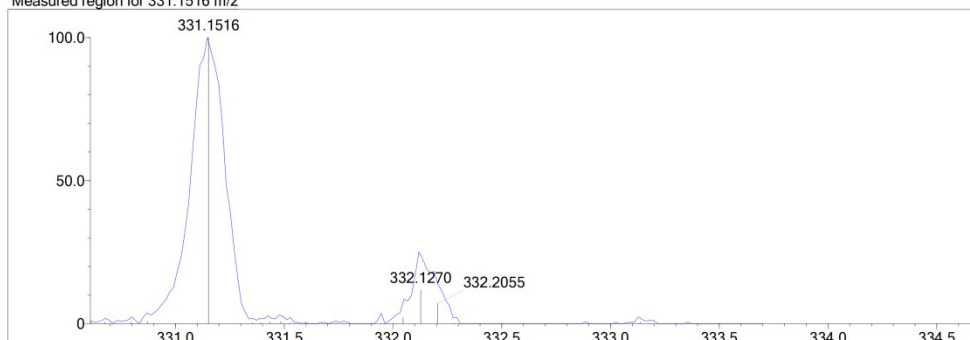
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	5	100	O	2	0	20	S	2	0	5	H
C	4	5	50	F	1	0	0	Cl	1	0	0	Na
N	3	0	10	Si	4	0	0	Br	1	0	0	

Error Margin (ppm): 5
 DBE Range: -2.0 - 1000.0
 Electron Ions: both
 HC Ratio: unlimited
 Apply N Rule: no
 Use MSn Info: no
 Max Isotopes: all
 Isotope RI (%): 1.00
 MSn Iso RI (%): 75.00
 MSn Logic Mode: AND
 Isotope Res: 10000
 Max Results: 50

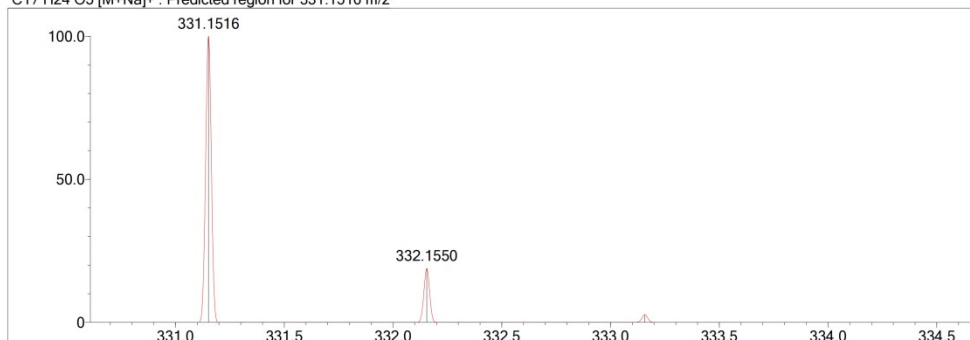
Event#: 1 MS(E+) Ret. Time : 0.520 -> 0.680 Scan#: 79 -> 103



Measured region for 331.1516 m/z



C17 H24 O5 [M+Na]+ : Predicted region for 331.1516 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C17 H24 O5	[M+Na]+	331.1516	331.1516	0.0	0.00	6.0

Figure S43. HR-ESI-MS spectrum of magnolin E (6)

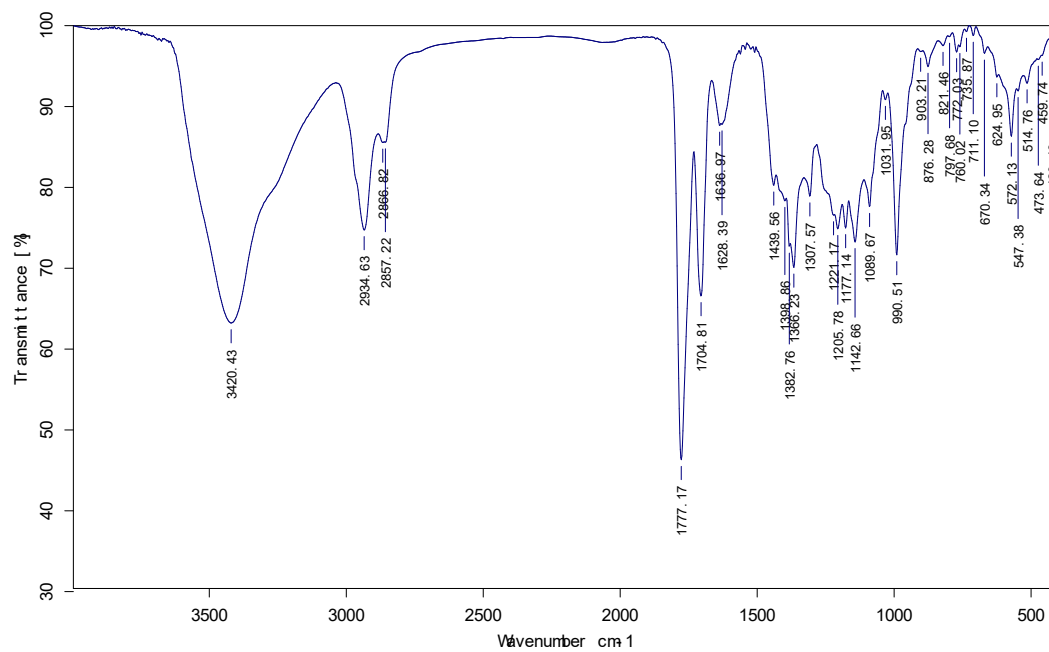


Figure S44. IR spectrum of magnolin E (6)

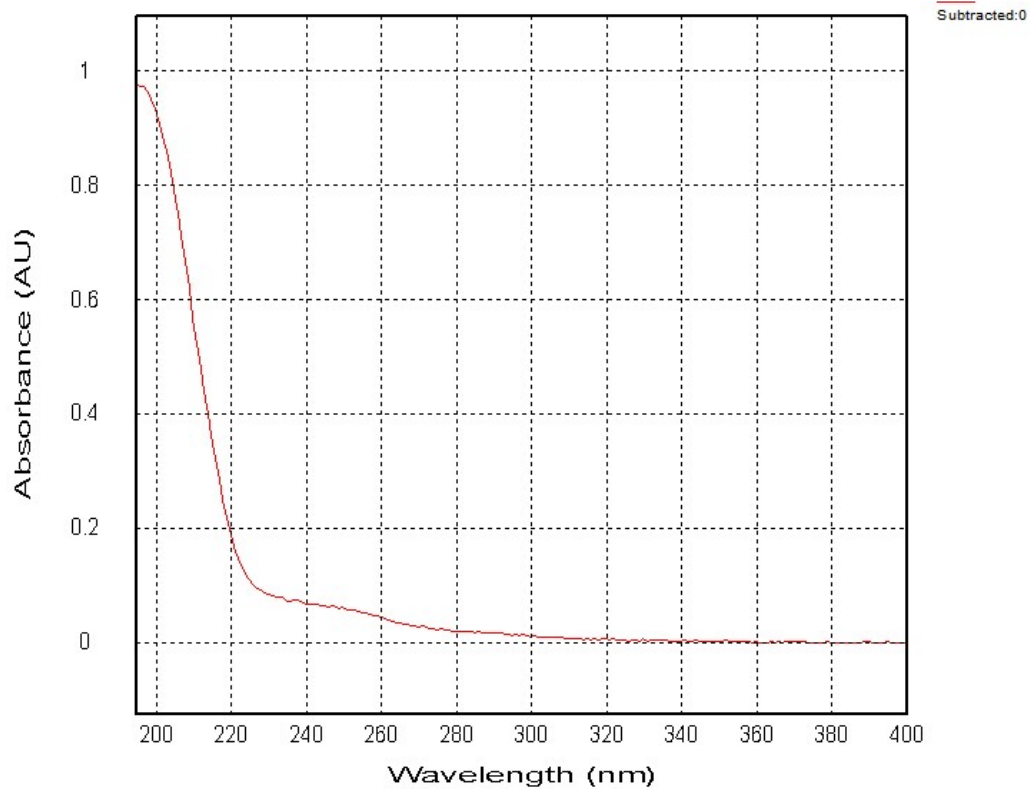


Figure S45. UV spectrum of magnolin E (6)

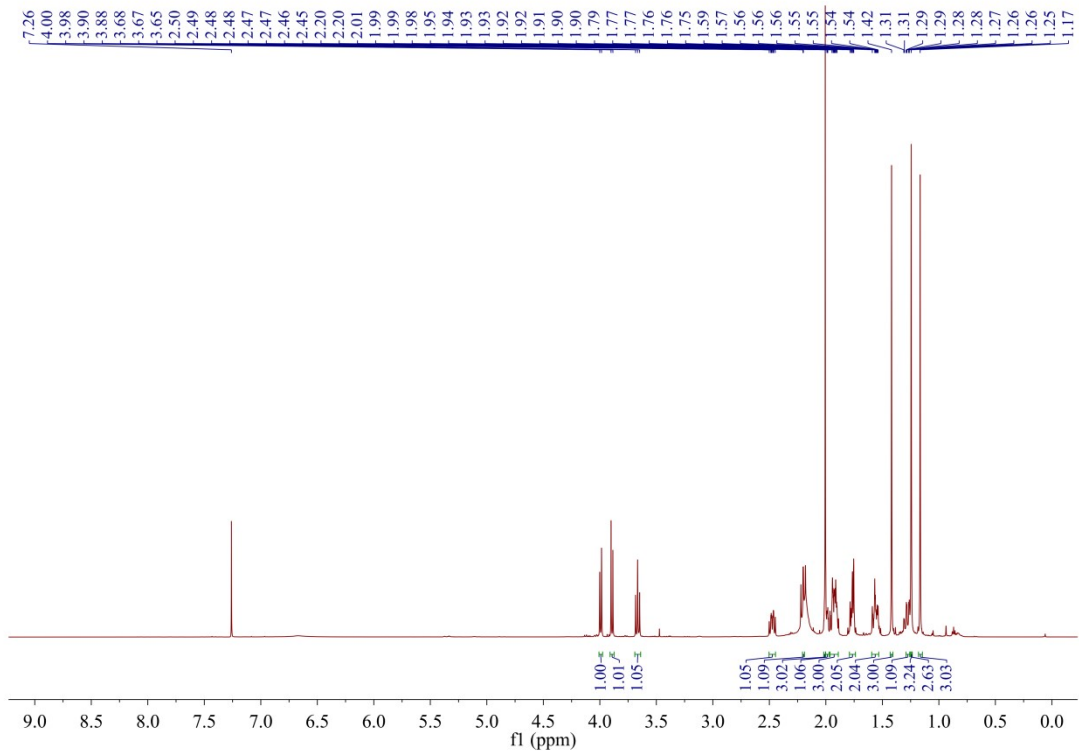


Figure S46. ^1H NMR spectrum of magnorlin F (7) in CDCl_3

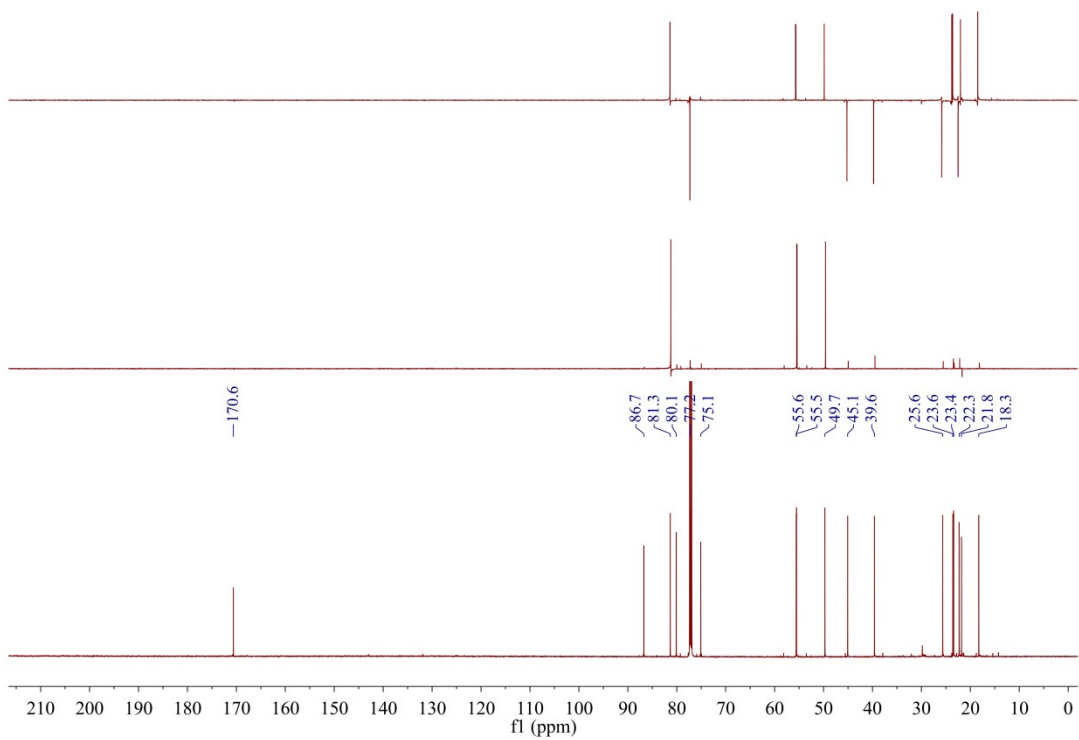


Figure S47. ^{13}C NMR spectrum of magnorlin F (7) in CDCl_3

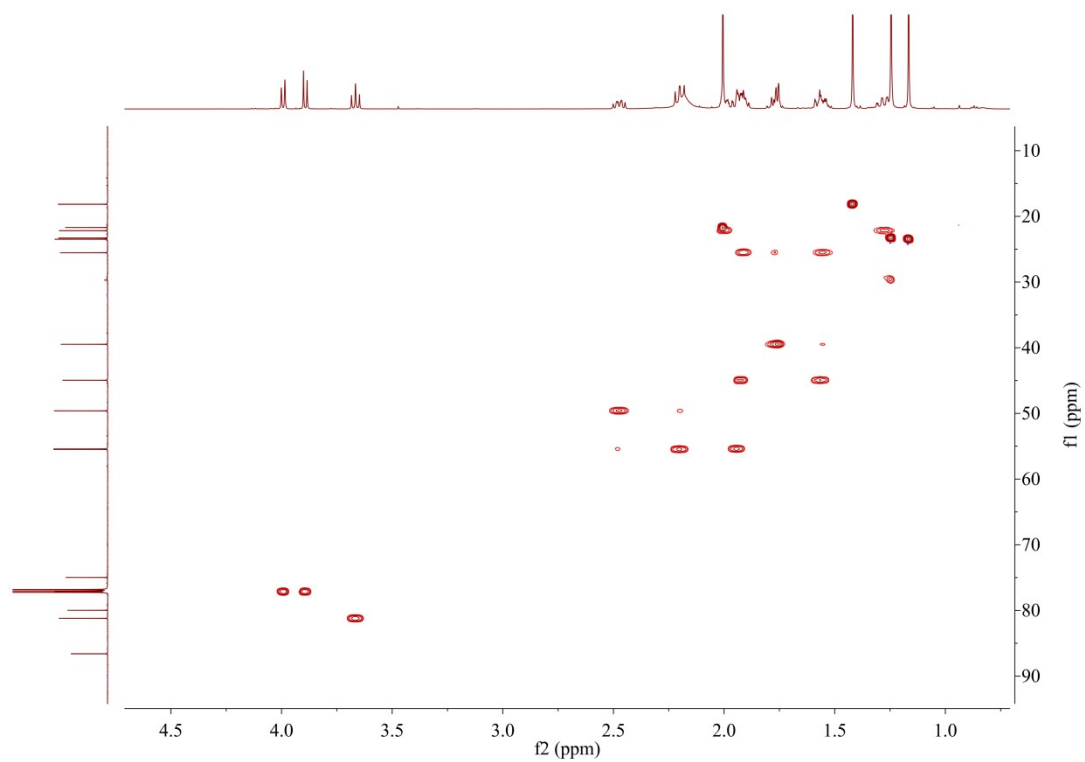


Figure S48. HSQC spectrum of magnorlin F (7) in CDCl_3

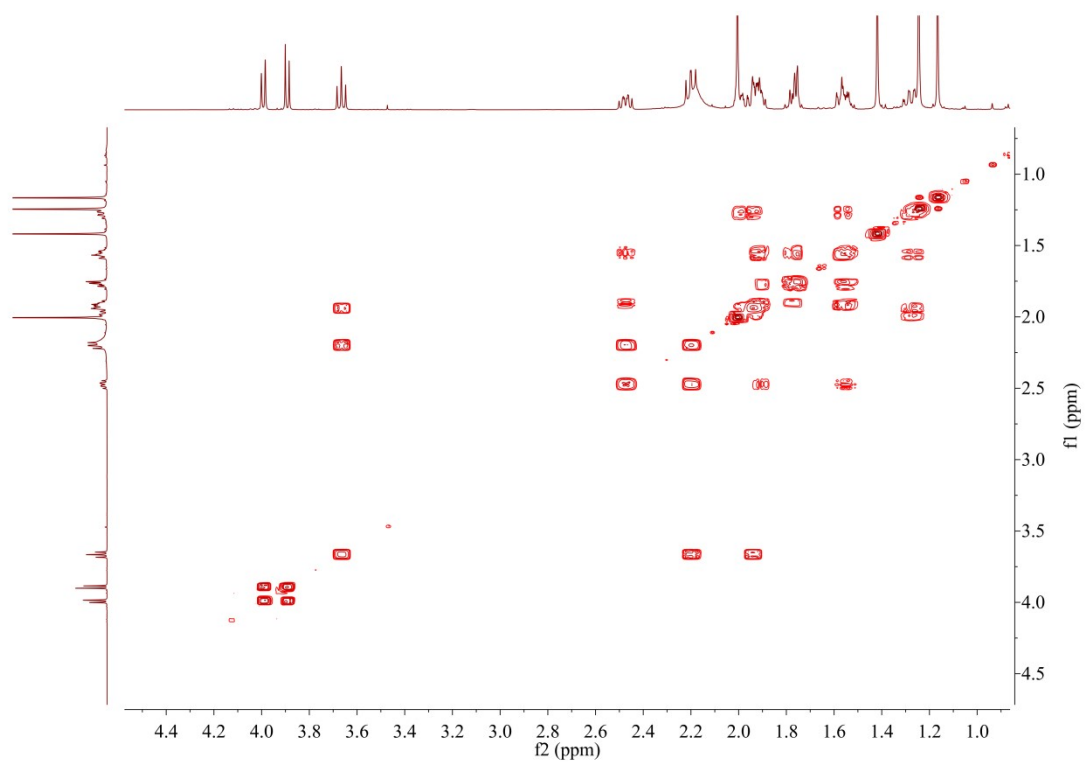


Figure S49. COSY spectrum of magnorlin F (7) in CDCl_3

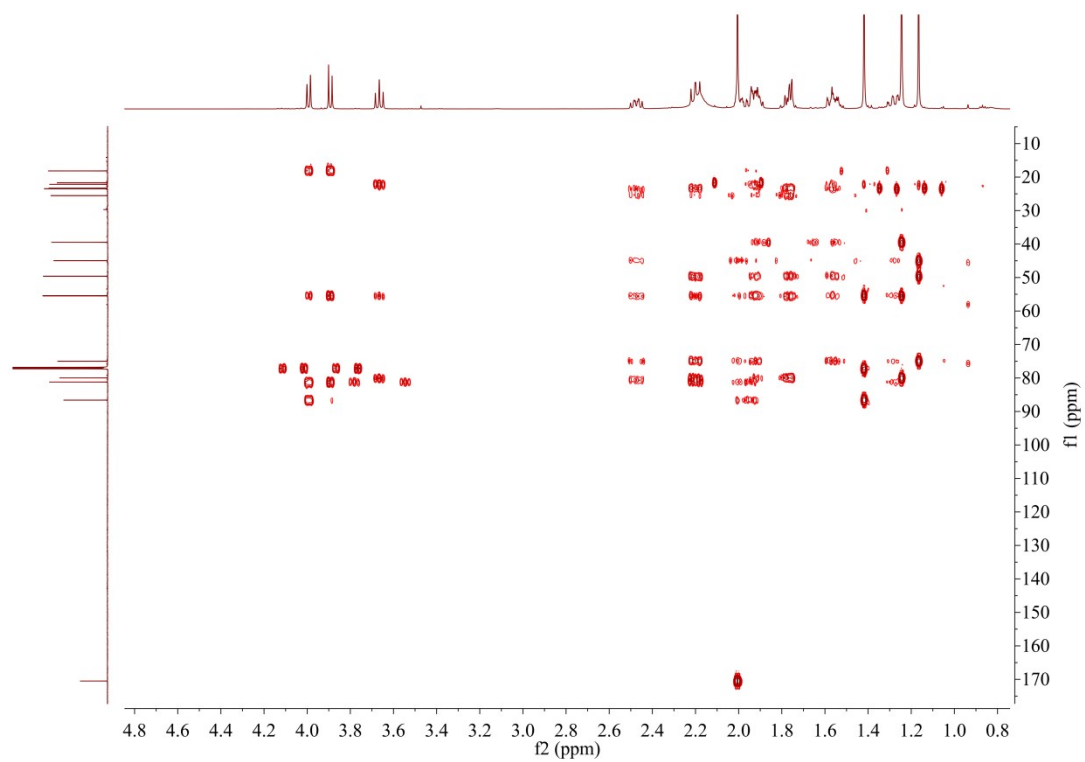


Figure S50. HMBC spectrum of magnorlin F (**7**) in CDCl_3

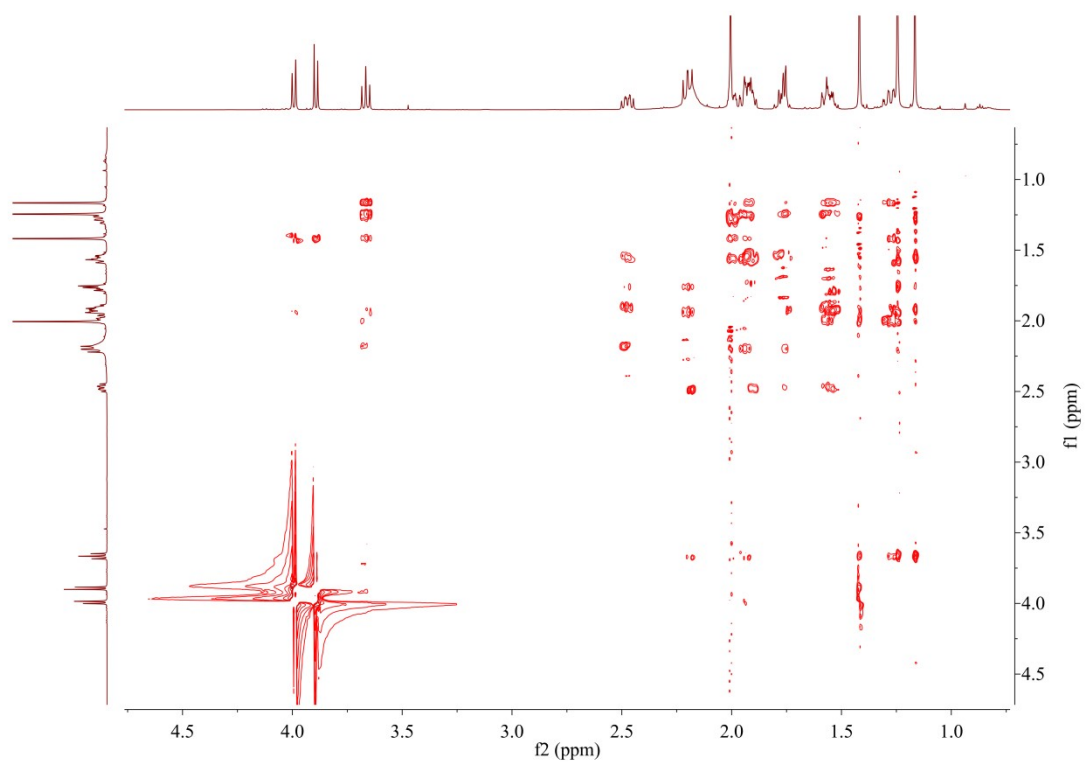


Figure S51. ROESY spectrum of magnorlin F (**7**) in CDCl_3

Data File: D:\DATA\2025\1208\fwxz-143.lcd

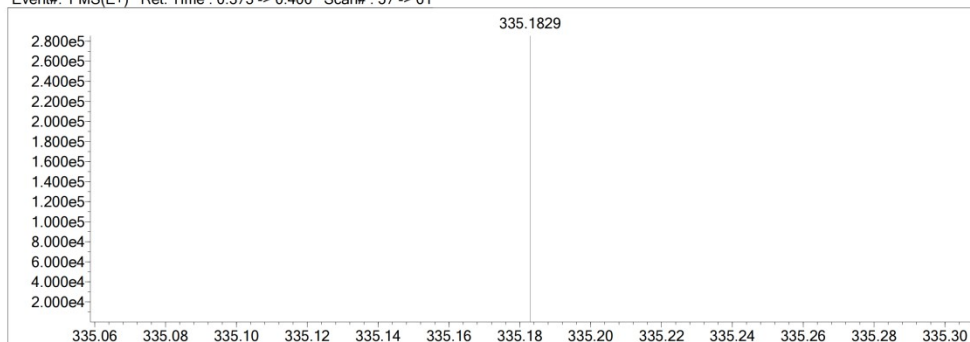
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	5	100	N	3	0	10	Si	4	0	0	Br	1	0	5	Na
B	3	0	0	O	2	0	30	S	2	0	0	I	3	0	0	
C	4	5	50	F	1	0	0	Cl	1	0	0					

Error Margin (ppm): 10
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

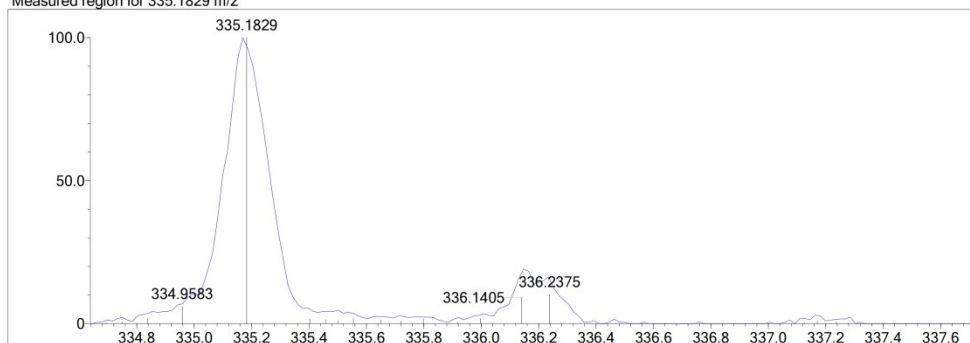
DBE Range: -2.0 - 1000.0
 Apply N Rule: no
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 50

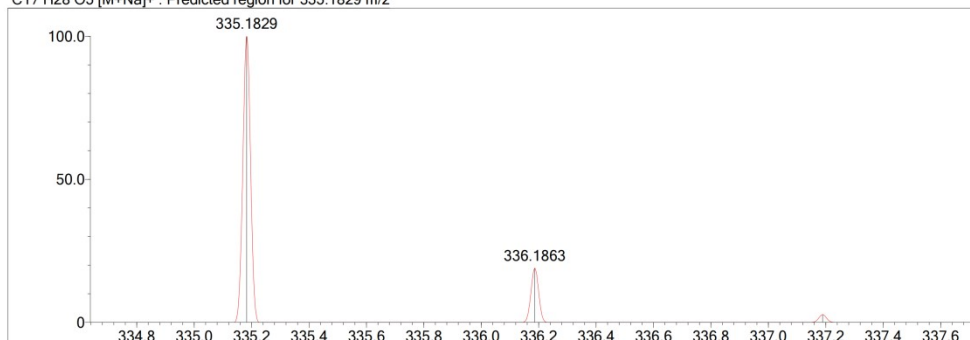
Event#: 1 MS(E+) Ret. Time : 0.373 -> 0.400 Scan#: 57 -> 61



Measured region for 335.1829 m/z



C17 H28 O5 [M+Na]+ : Predicted region for 335.1829 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C17 H28 O5	[M+Na]+	335.1829	335.1829	0.0	0.00	4.0

Figure S52. HR-ESI-MS spectrum of magnolin F (7)

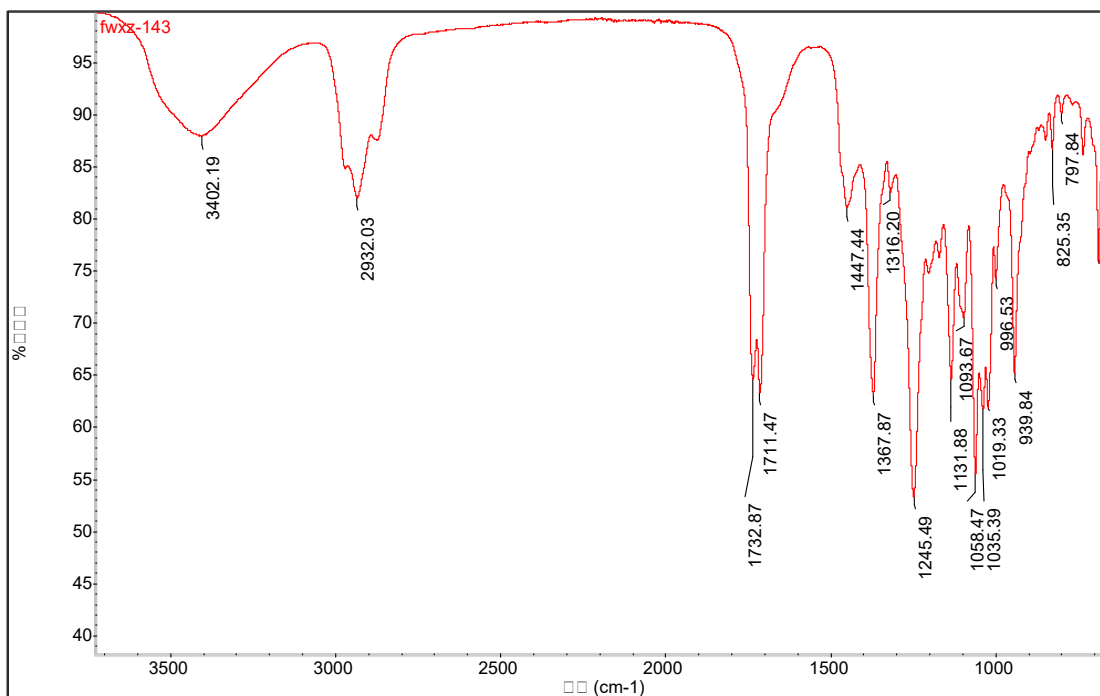


Figure S53. IR spectrum of magnolin F (7)

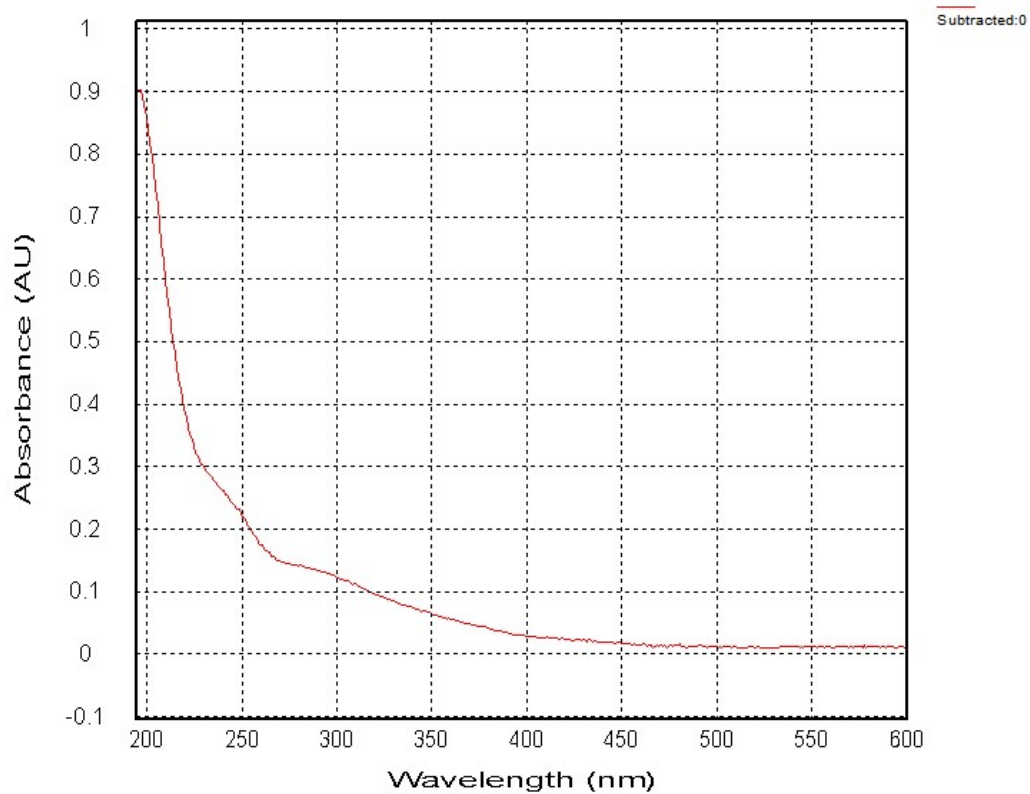


Figure S54. UV spectrum of magnolin F (7)

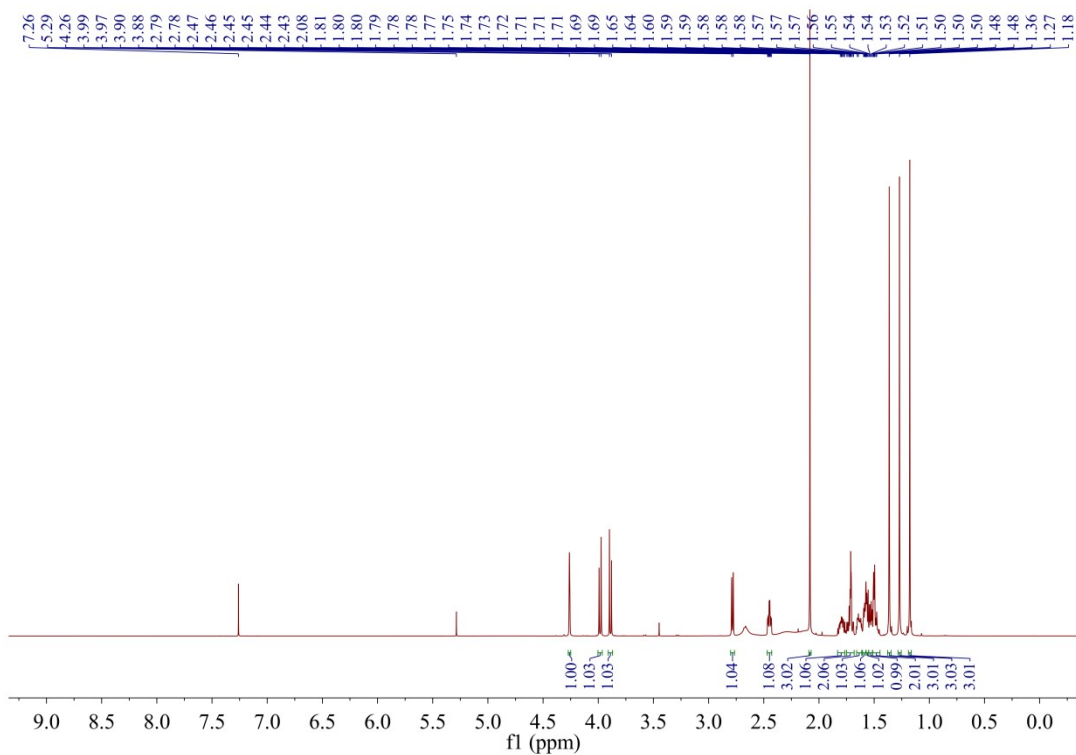


Figure S55. ^1H NMR spectrum of magnolin G (**8**) in CDCl_3

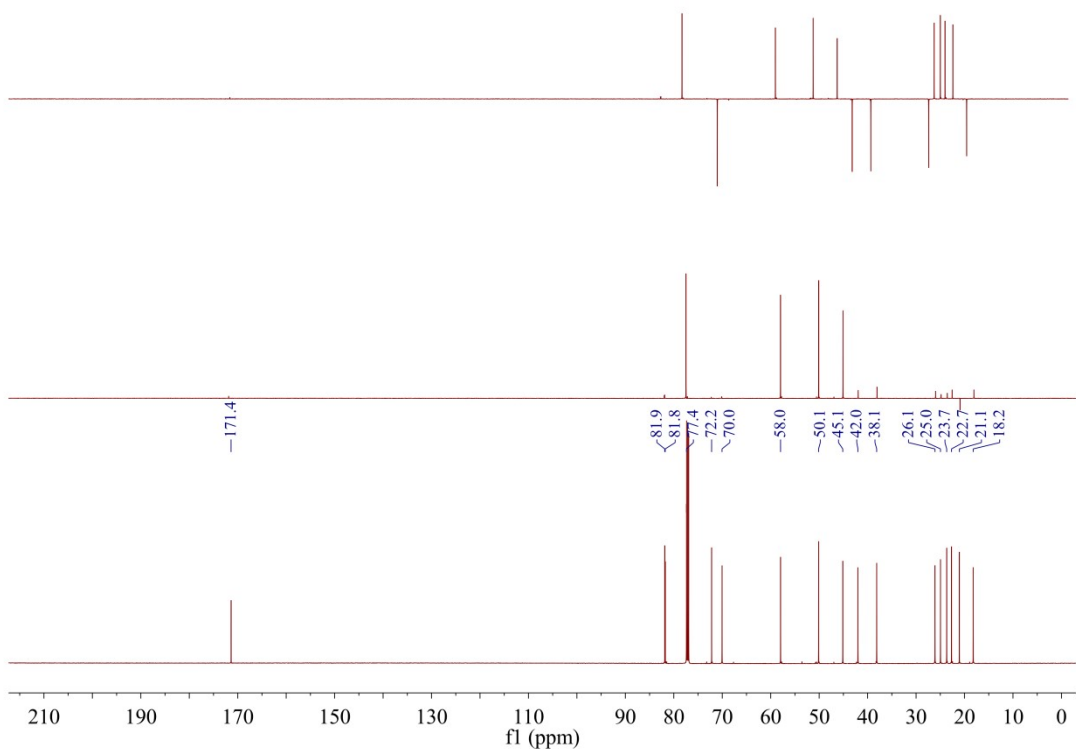


Figure S56. ^{13}C NMR spectrum of magnolin G (**8**) in CDCl_3

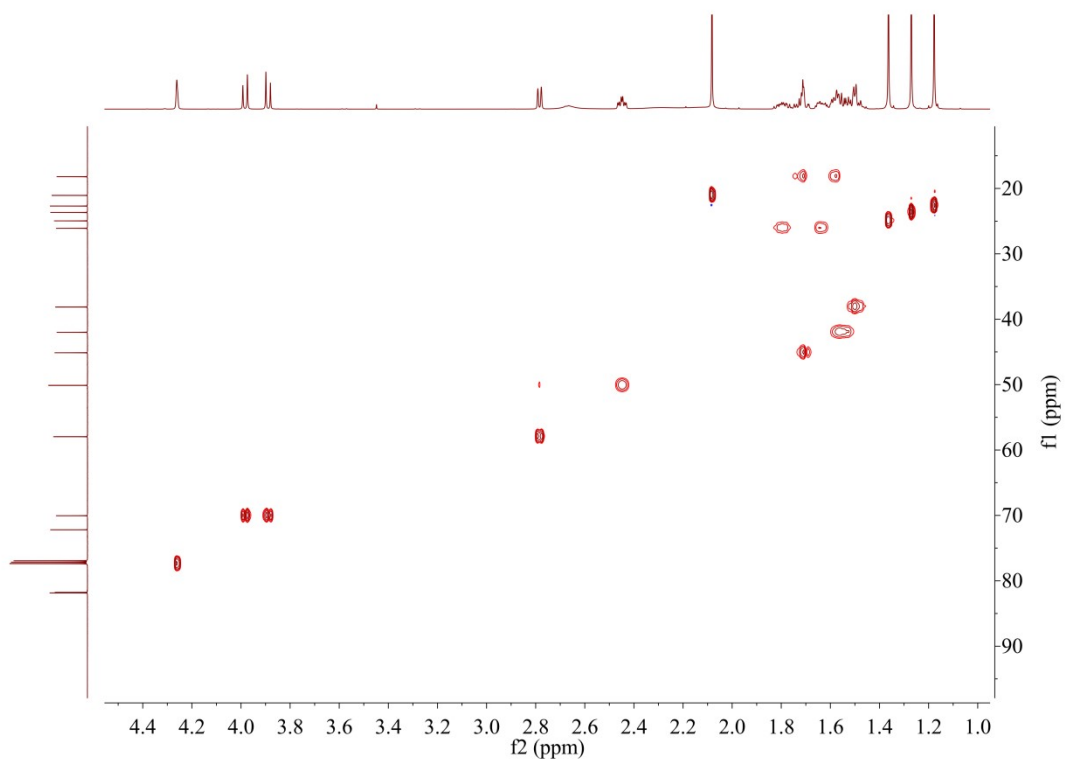


Figure S57. HSQC spectrum of magnolin G (**8**) in CDCl_3

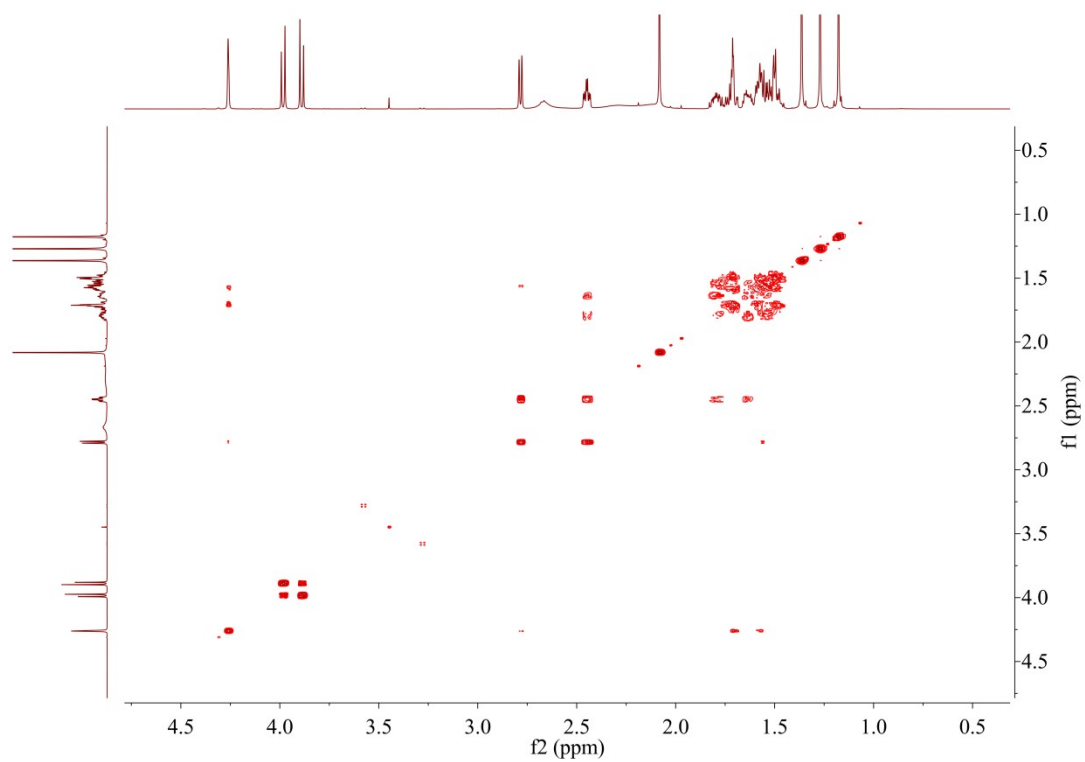


Figure S58. COSY spectrum of magnolin G (**8**) in CDCl_3

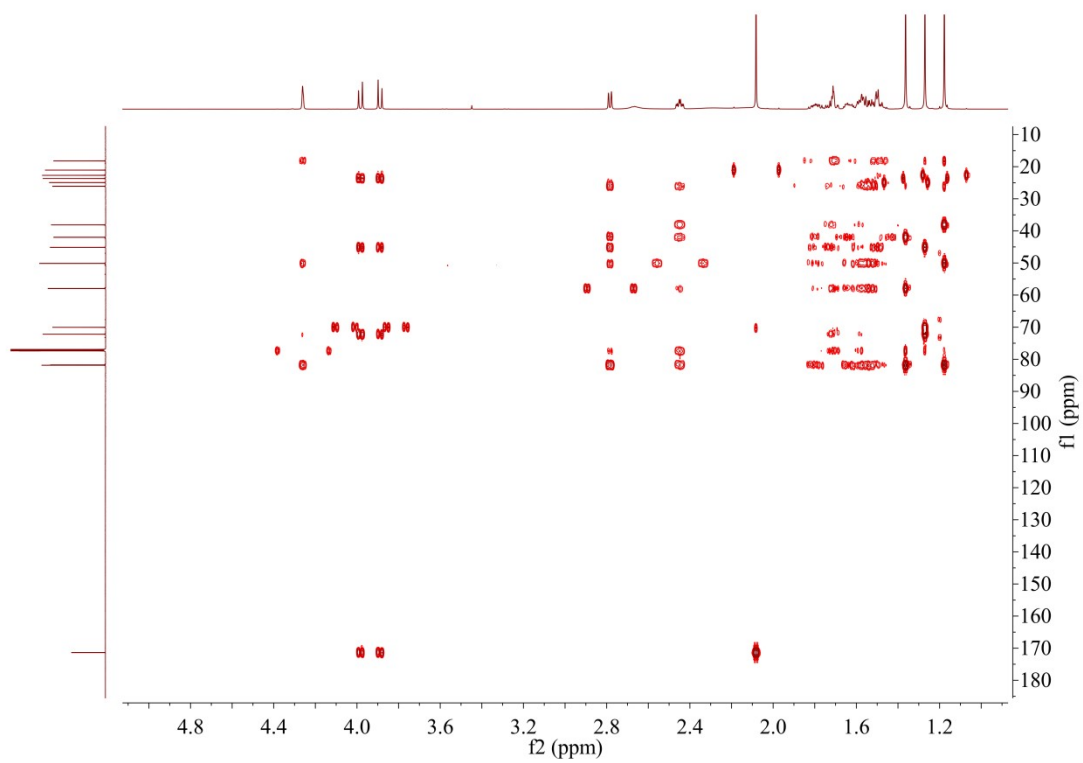


Figure S59. HMBC spectrum of magnolin G (**8**) in CDCl_3

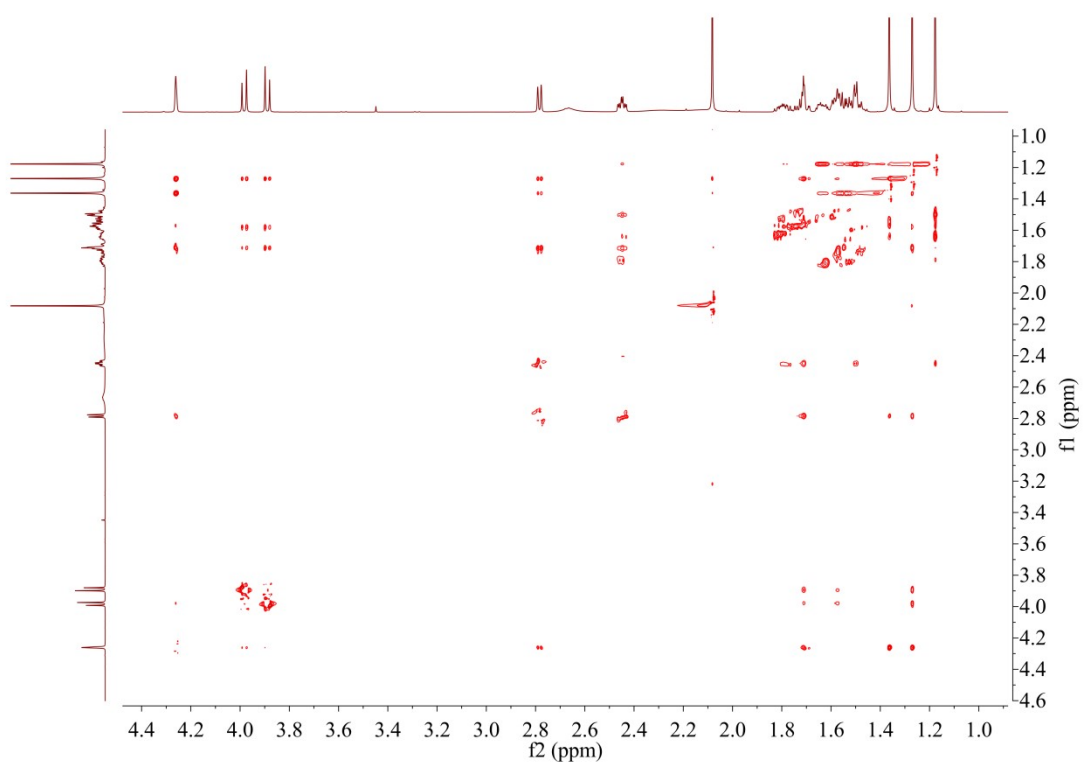


Figure S60. ROESY spectrum of magnolin G (**8**) in CDCl_3

Data File: D:\DATA\2025\1104\fwz-126.lcd

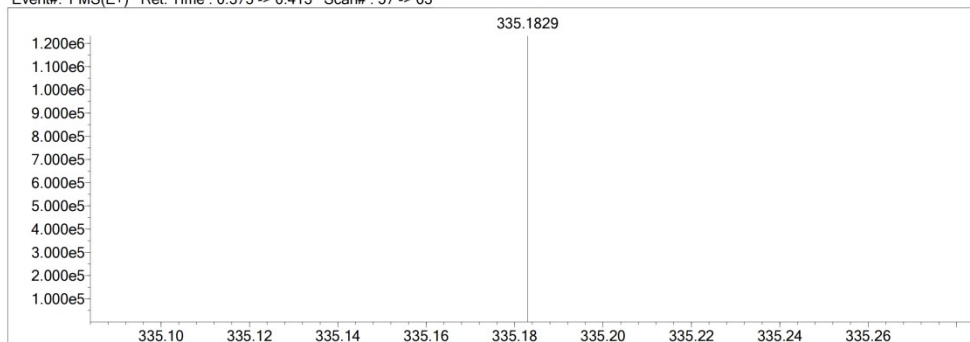
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	5	100	N	3	0	10	Si	4	0	0	H
B	3	0	0	O	2	0	20	S	2	0	0	Na
C	4	10	50	F	1	0	0	Cl	1	0	0	

Error Margin (ppm): 5
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

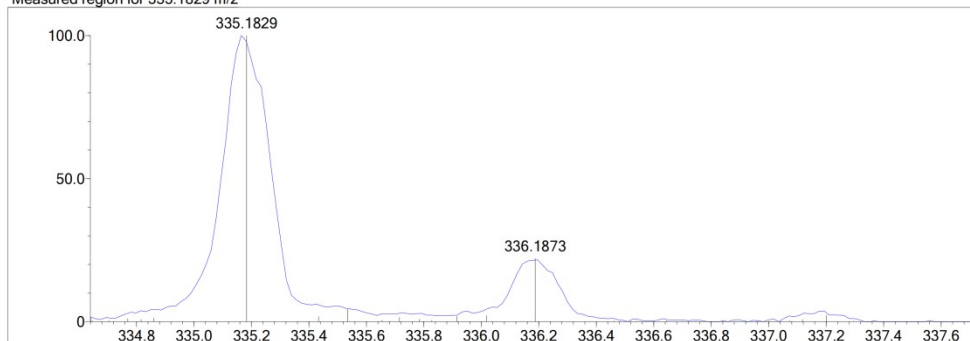
DBE Range: -2.0 - 1000.0
 Apply N Rule: no
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 50

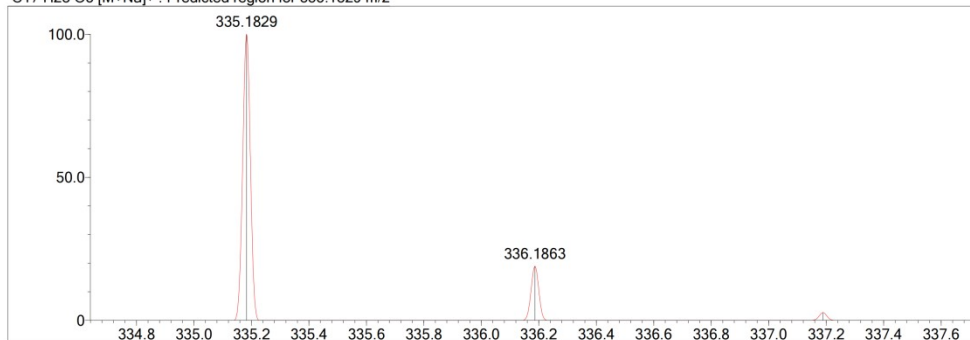
Event#: 1 MS(E+) Ret. Time : 0.373 -> 0.413 Scan#: 57 -> 63



Measured region for 335.1829 m/z



C17 H28 O5 [M+Na]+ : Predicted region for 335.1829 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C17 H28 O5	[M+Na]+	335.1829	335.1829	0.0	0.00	4.0

Figure S61. HR-ESI-MS spectrum of magnolin G (8)

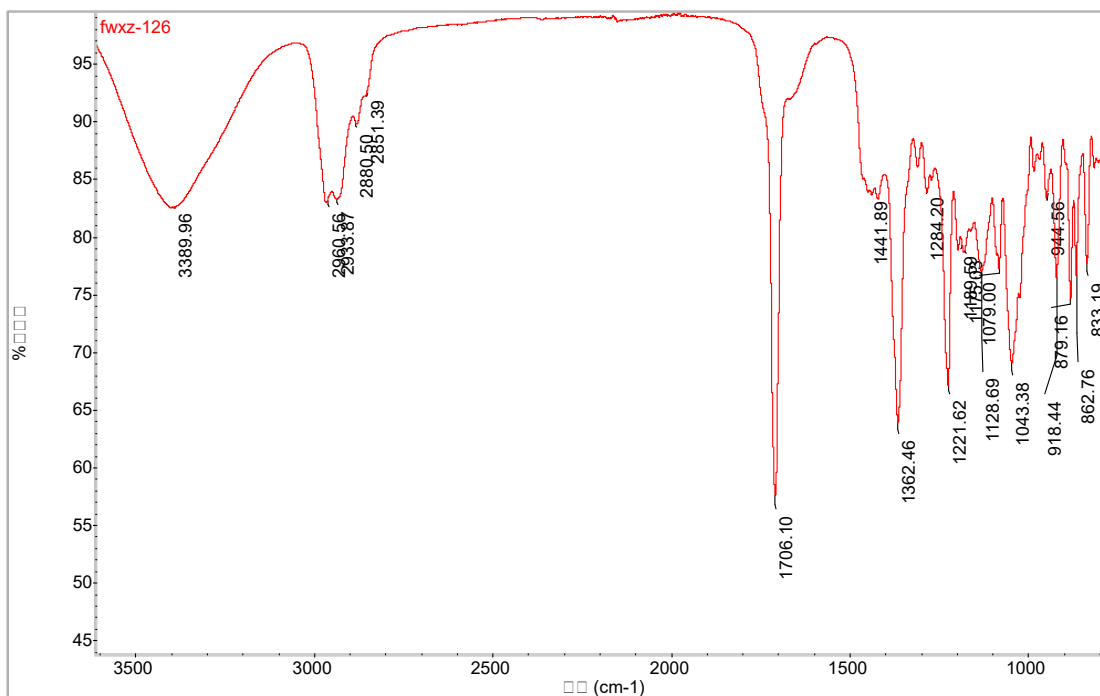


Figure S62. IR spectrum of magnolin G (**8**)

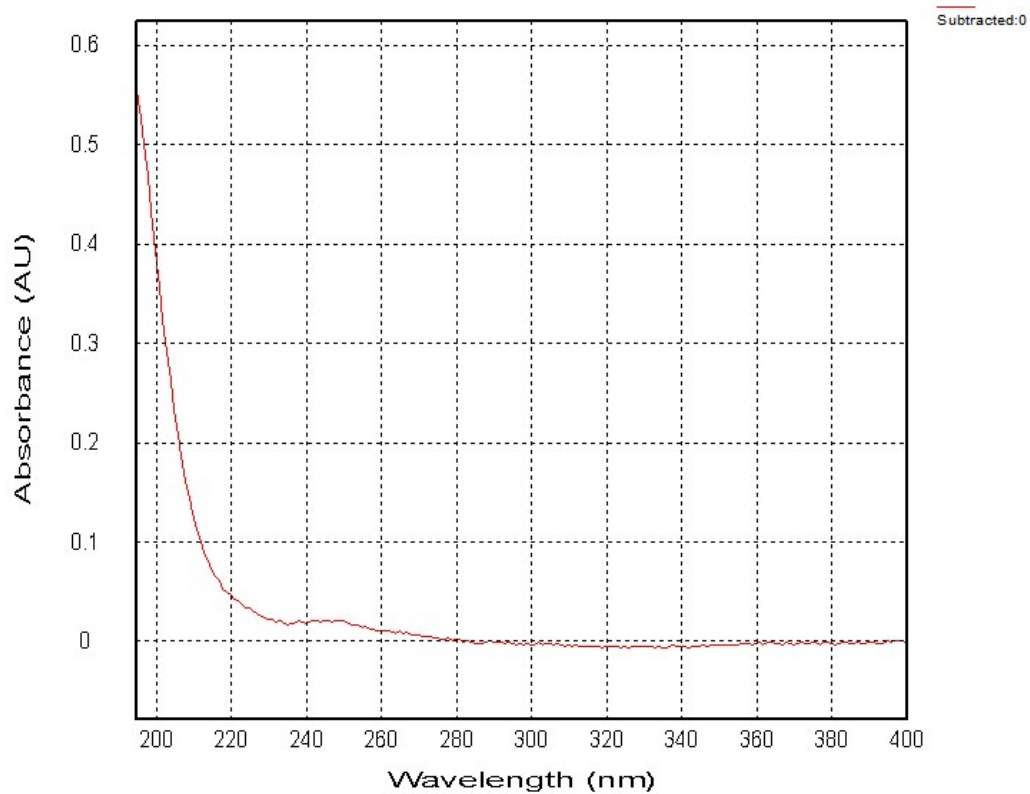


Figure S63. UV spectrum of magnolin G (**8**)

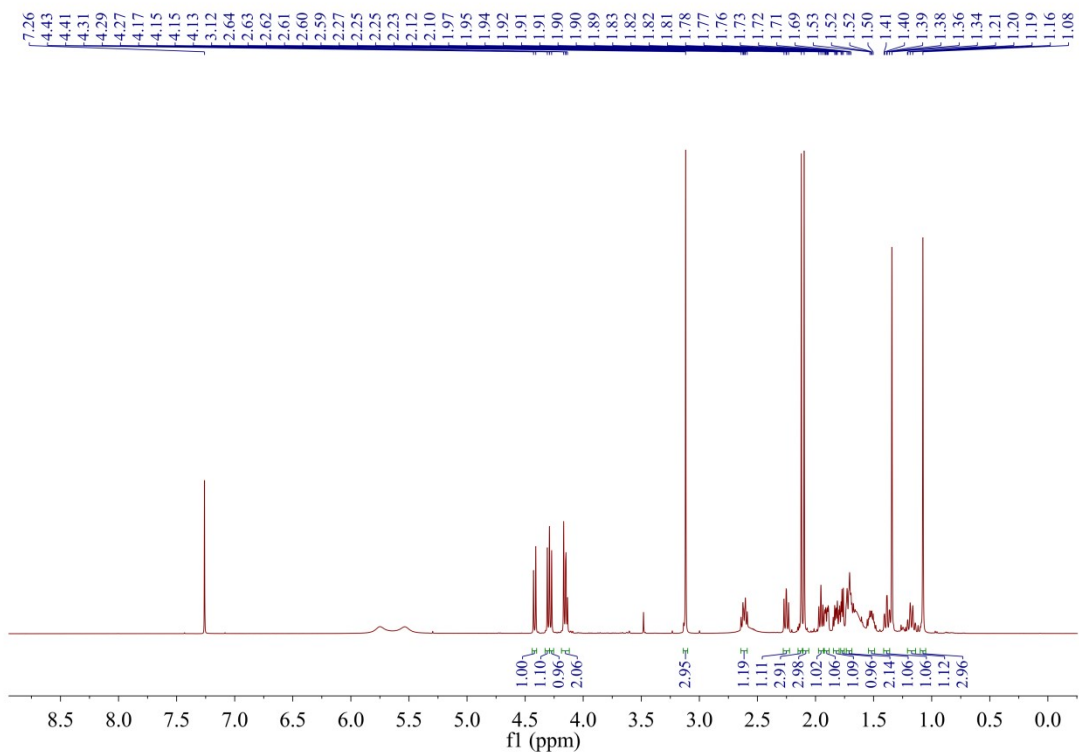


Figure S64. ^1H NMR spectrum of magnolin H (**9**) in CDCl_3

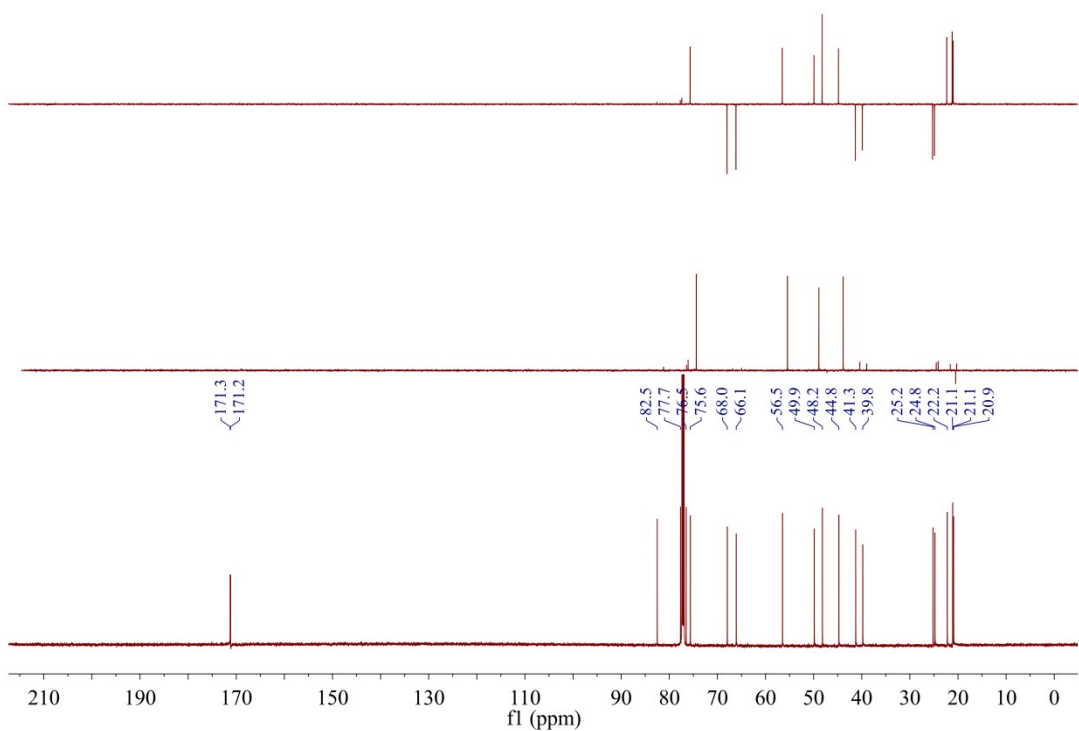


Figure S65. ^{13}C NMR spectrum of magnolin H (**9**) in CDCl_3

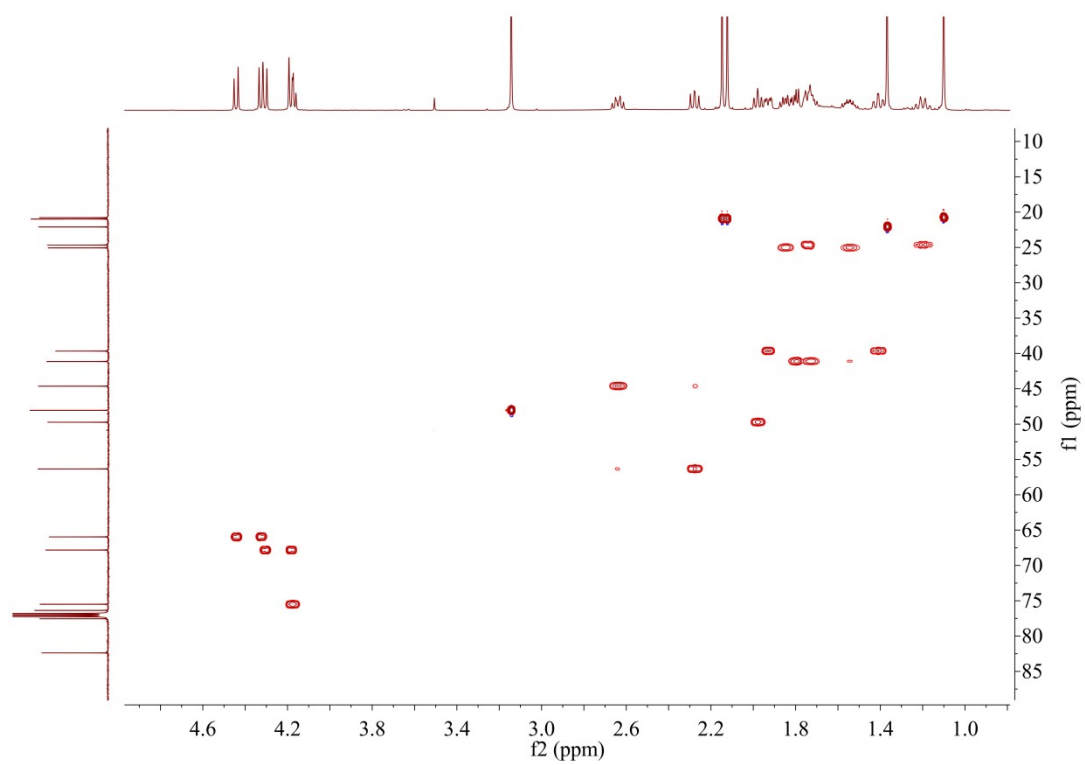


Figure S66. HSQC spectrum of magnolin H (**9**) in CDCl_3

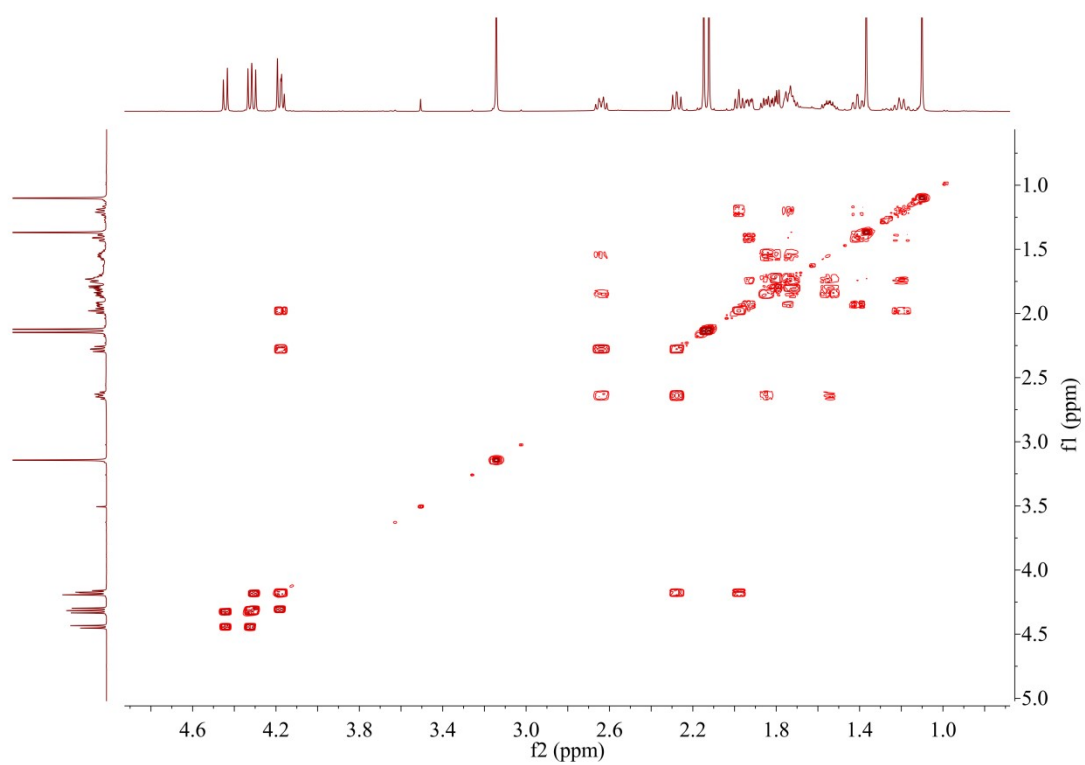


Figure S67. COSY spectrum of magnolin H (**9**) in CDCl_3

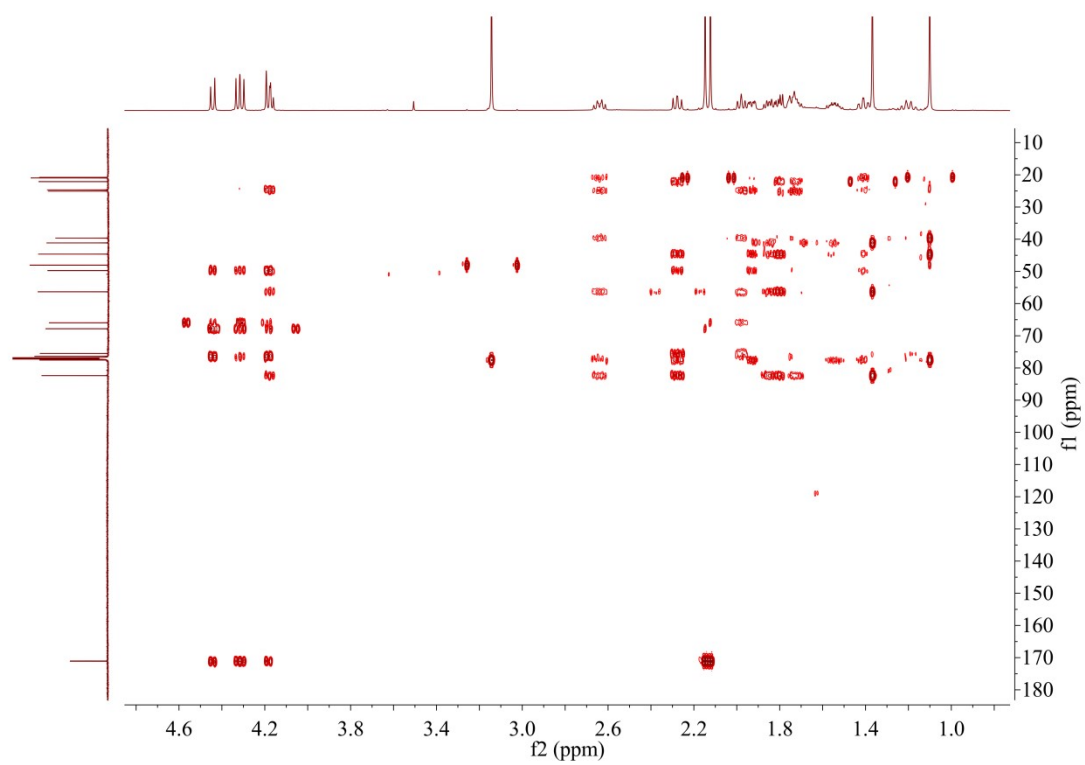


Figure S68. HMBC spectrum of magnolin H (**9**) in CDCl_3

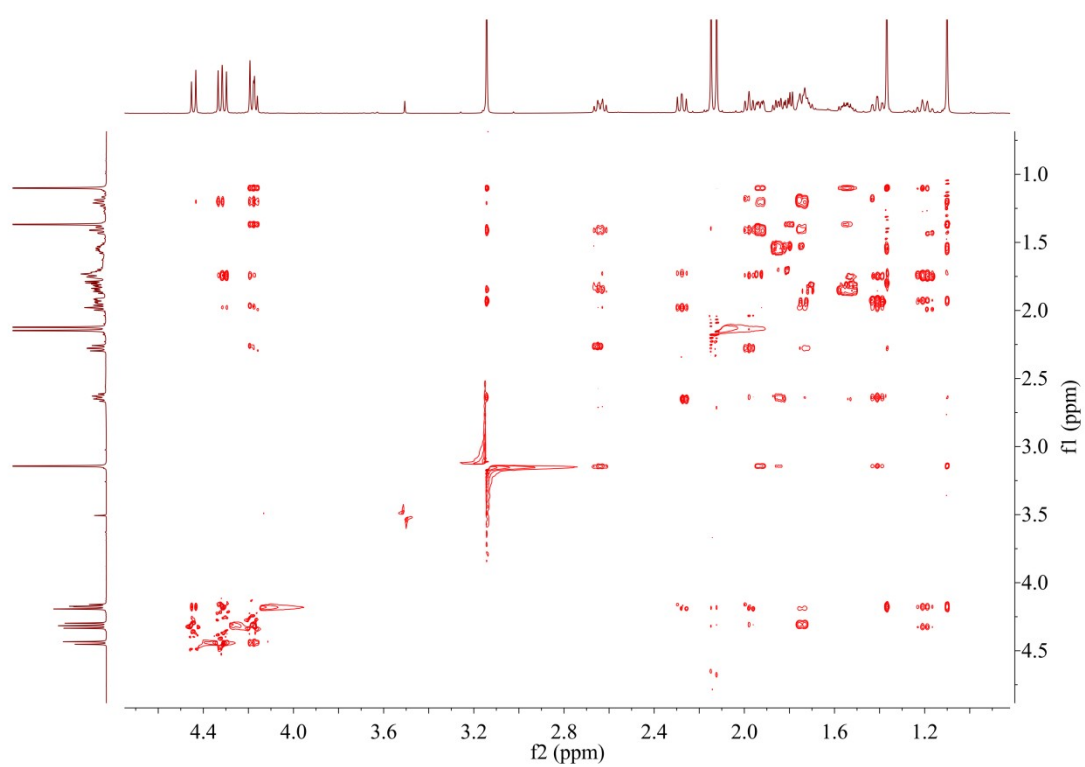


Figure S69. ROESY spectrum of magnolin H (**9**) in CDCl_3

Data File: D:\DATA\2025\1104\fwxz-130.lcd

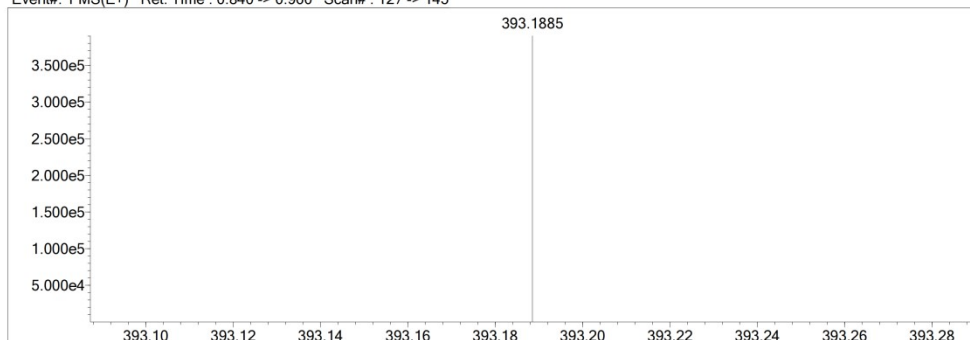
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	5	100	N	3	0	10	Si	4	0	0	H
B	3	0	0	O	2	0	20	S	2	0	0	Na
C	4	10	50	F	1	0	0	Cl	1	0	0	

Error Margin (ppm): 5
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

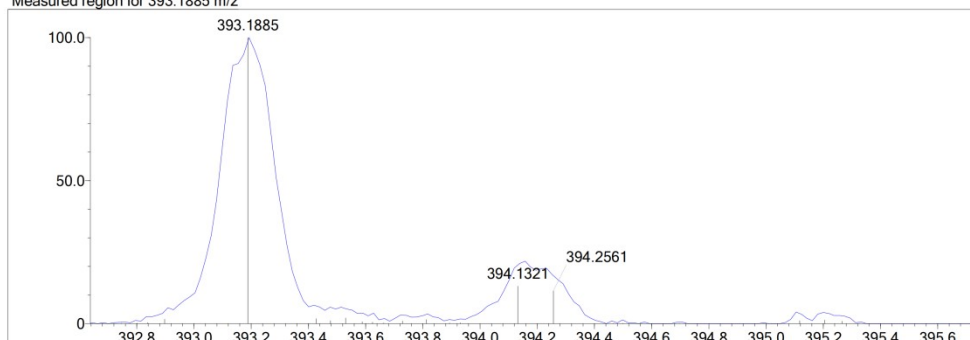
DBE Range: -2.0 - 1000.0
 Apply N Rule: no
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 50

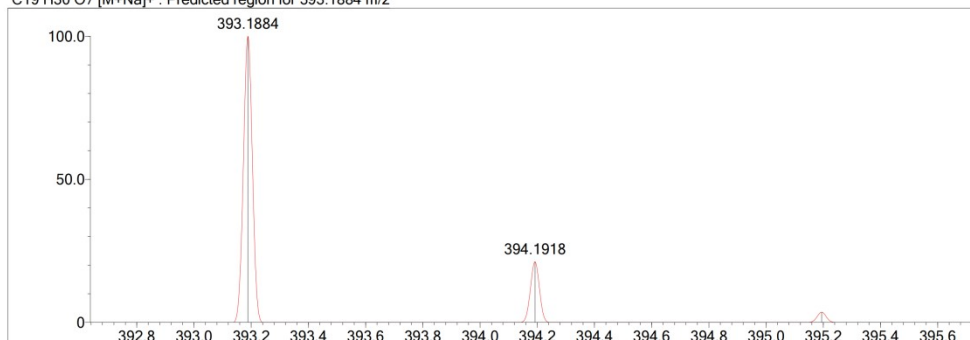
Event#: 1 MS(E+) Ret. Time : 0.840 -> 0.960 Scan#: 127 -> 145



Measured region for 393.1885 m/z



C19 H30 O7 [M+Na]+ : Predicted region for 393.1884 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C19 H30 O7	[M+Na]+	393.1885	393.1884	0.1	0.25	5.0

Figure S70. HR-ESI-MS spectrum of magnolin H (9)

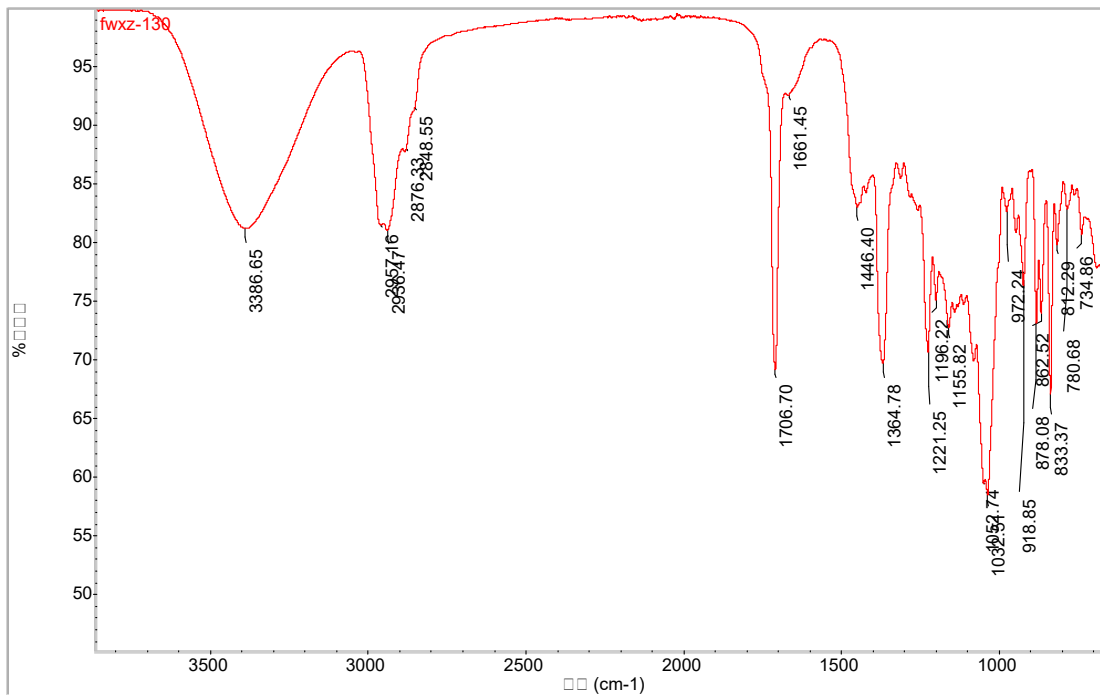


Figure S71. IR spectrum of magnolin H (9)

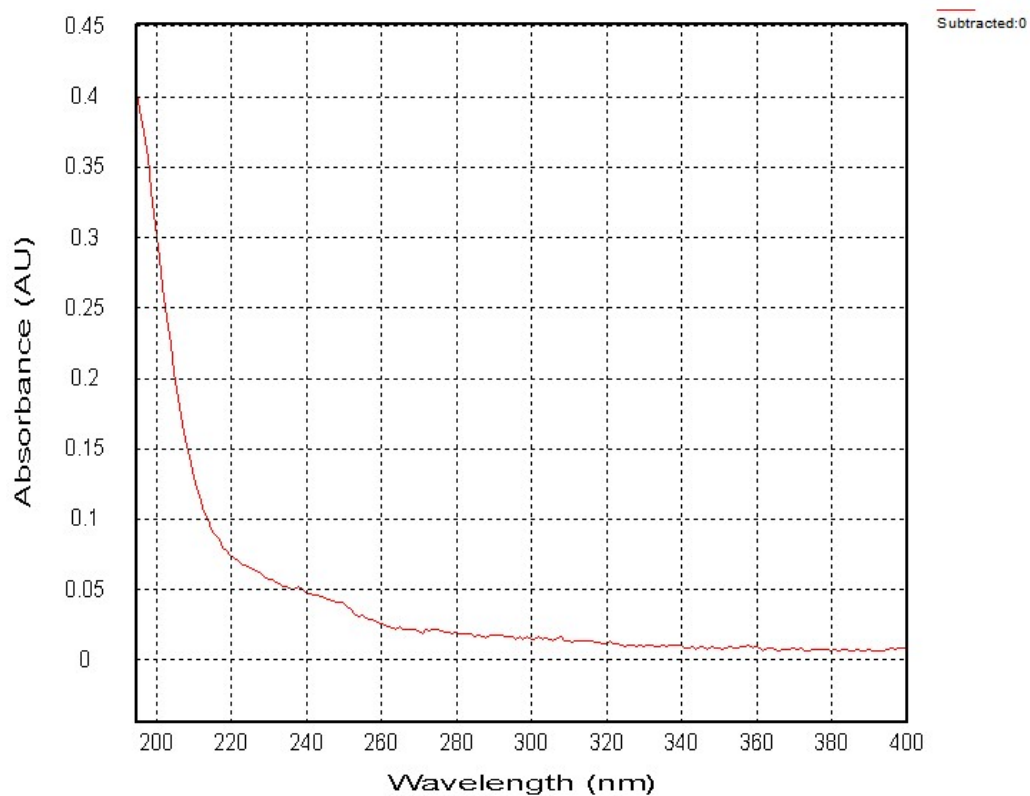


Figure S72. IR spectrum of magnolin H (9)



Figure S73. ¹H NMR spectrum of magnolin I (**10**) in CDCl₃



Figure S74. ¹³C NMR spectrum of magnolin I (**10**) in CDCl₃

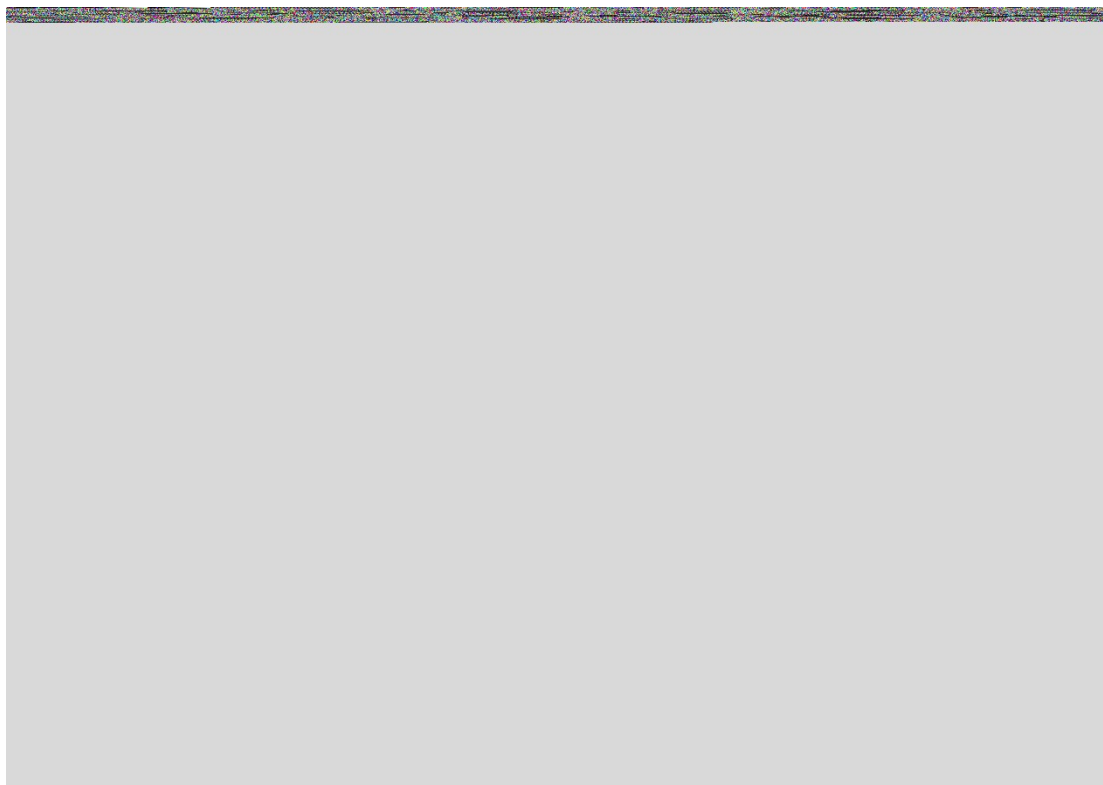


Figure S75. HSQC spectrum of magnolin I (**10**) in CDCl₃

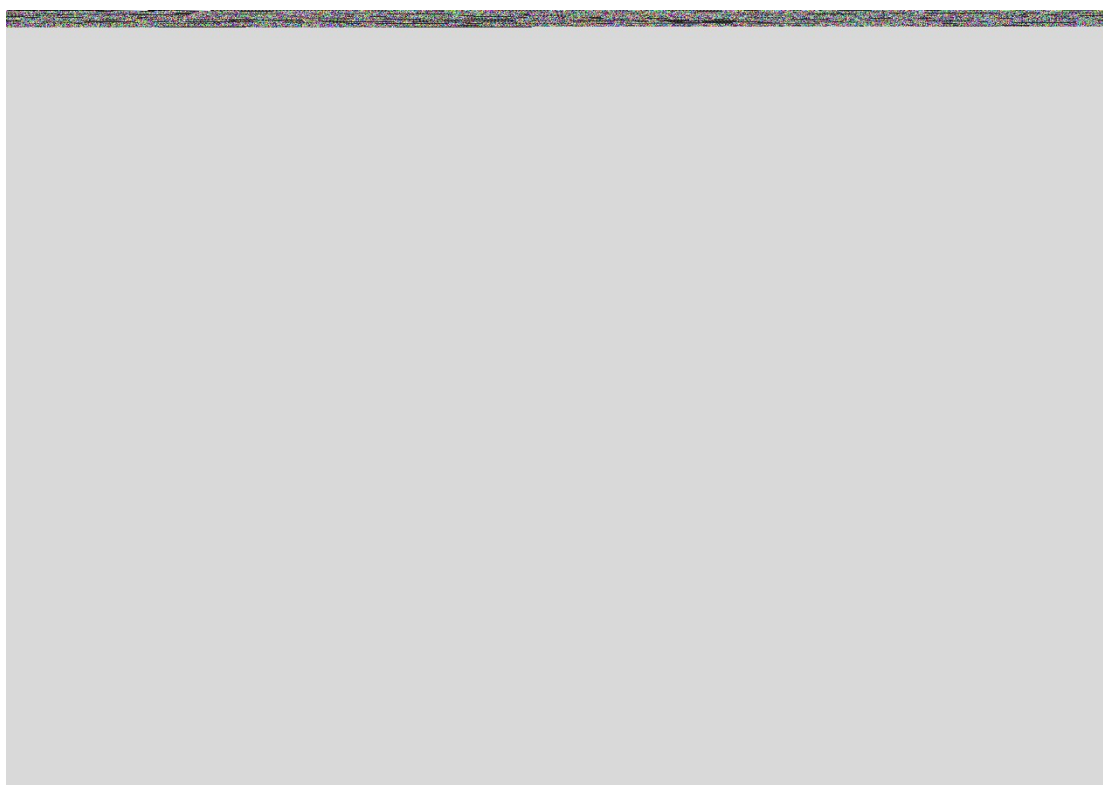


Figure S76. COSY spectrum of magnolin I (**10**) in CDCl₃



Figure S77. HMBC spectrum of magnolin I (**10**) in CDCl_3

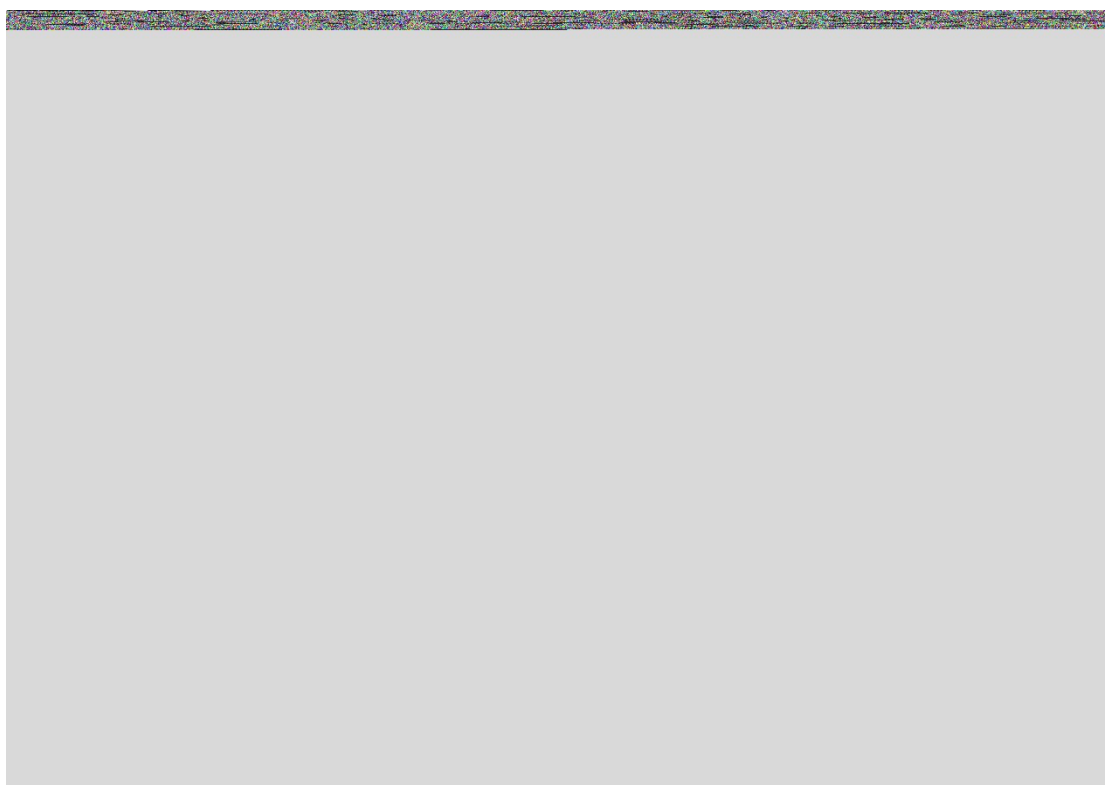


Figure S78. ROESY spectrum of magnolin I (**10**) in CDCl_3

Data File: D:\DATA\2025\1031\fwxz-133.lcd

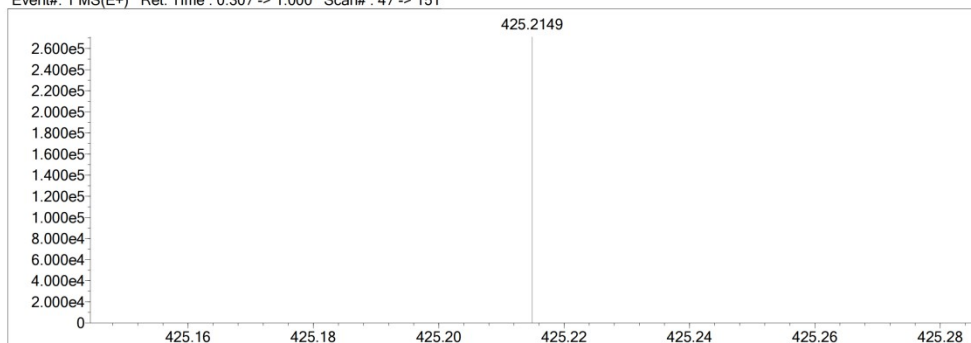
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	5	100	N	3	0	10	Si	4	0	0	H
B	3	0	0	O	2	0	20	S	2	0	0	Na
C	4	10	50	F	1	0	0	Cl	1	0	5	

Error Margin (ppm): 5
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

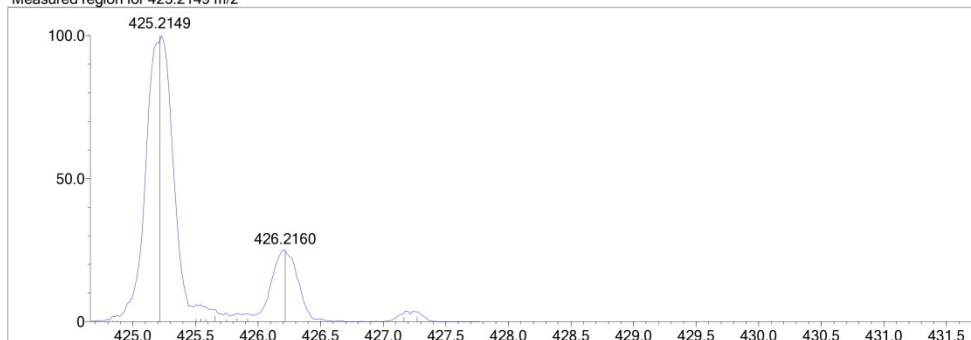
DBE Range: -2.0 - 1000.0
 Apply N Rule: no
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 50

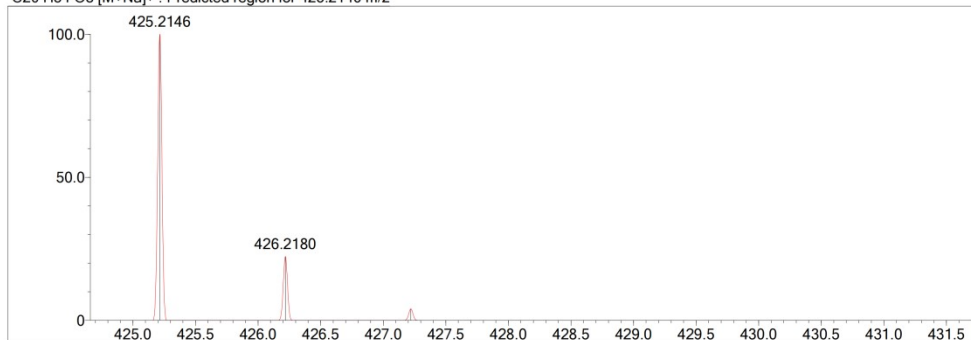
Event#: 1 MS(E+) Ret. Time : 0.307 -> 1.000 Scan#: 47 -> 151



Measured region for 425.2149 m/z



C20 H34 O8 [M+Na]+ : Predicted region for 425.2146 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C20 H34 O8	[M+Na]+	425.2149	425.2146	0.3	0.71	4.0

Figure S79. HR-ESI-MS spectrum of magnolin I (10)

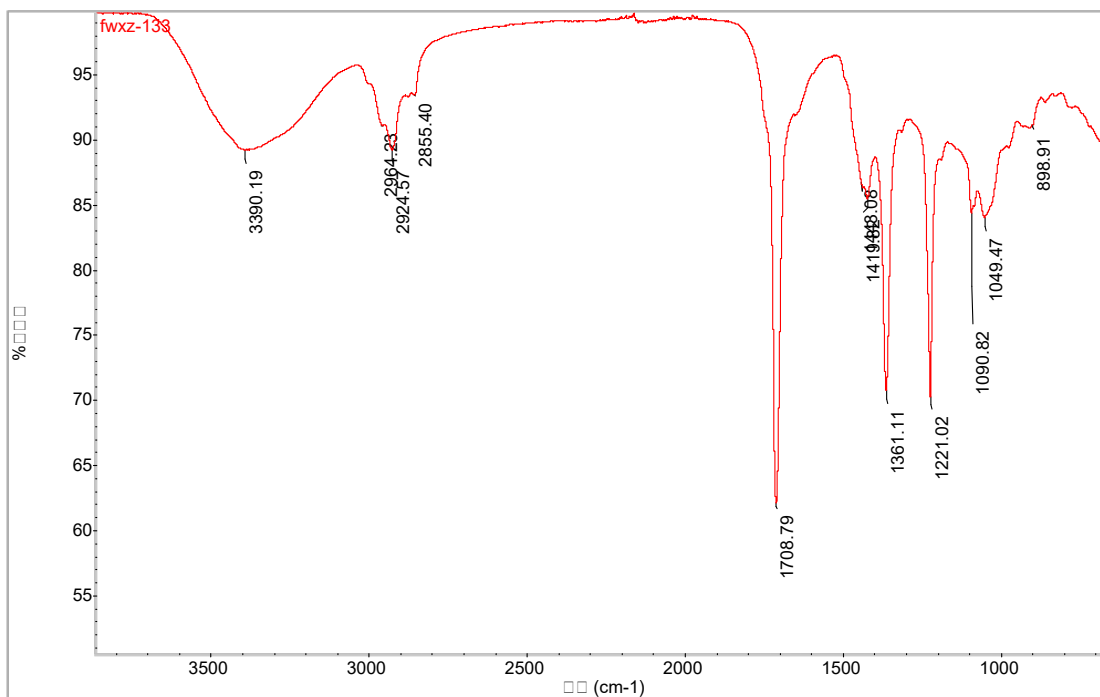


Figure S80. IR spectrum of magnolin I (10)

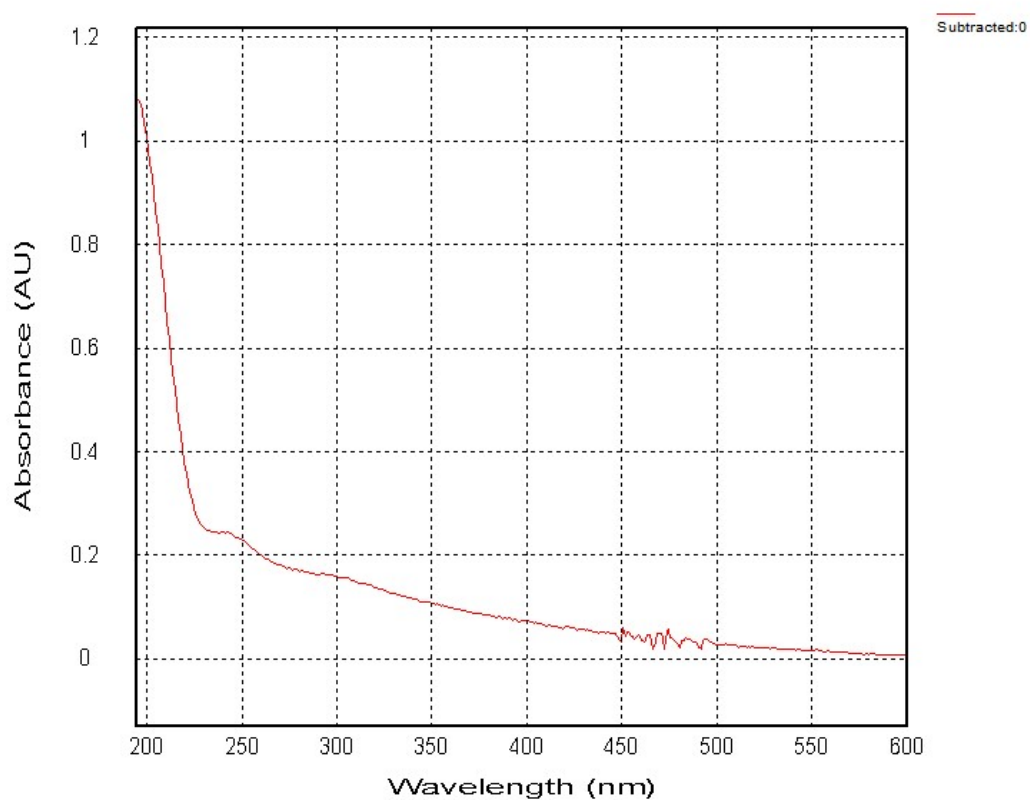


Figure S81. UV spectrum of magnolin I (10)

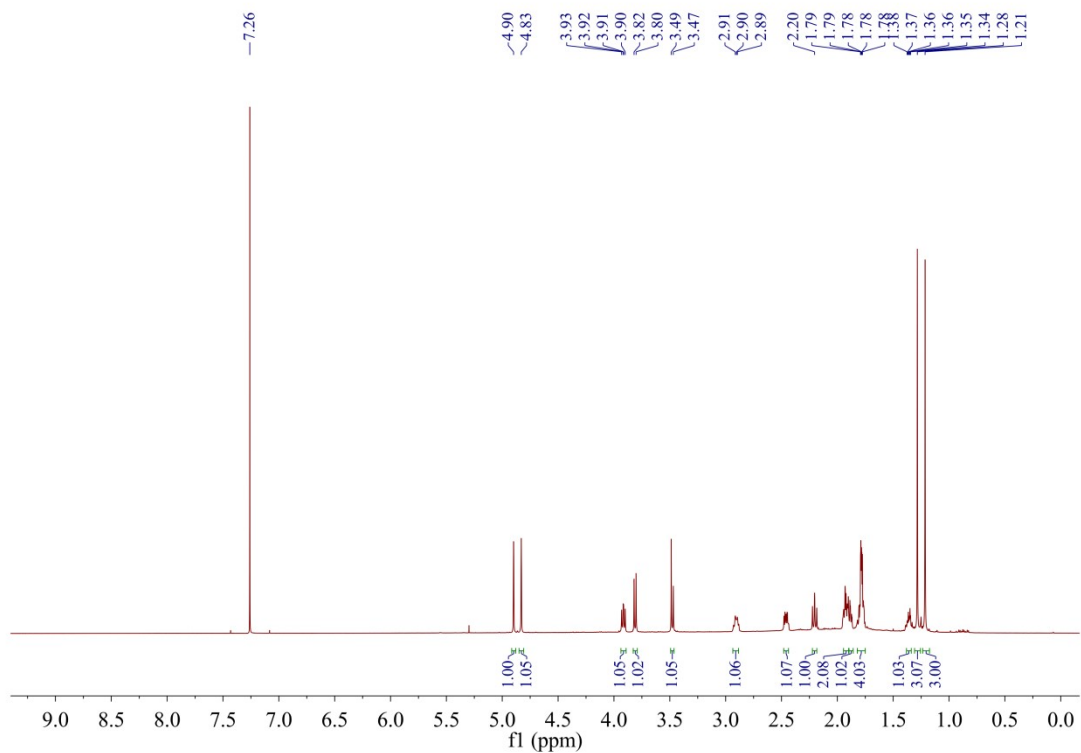


Figure S82. ^1H NMR spectrum of magnolin J (**11**) in CDCl_3

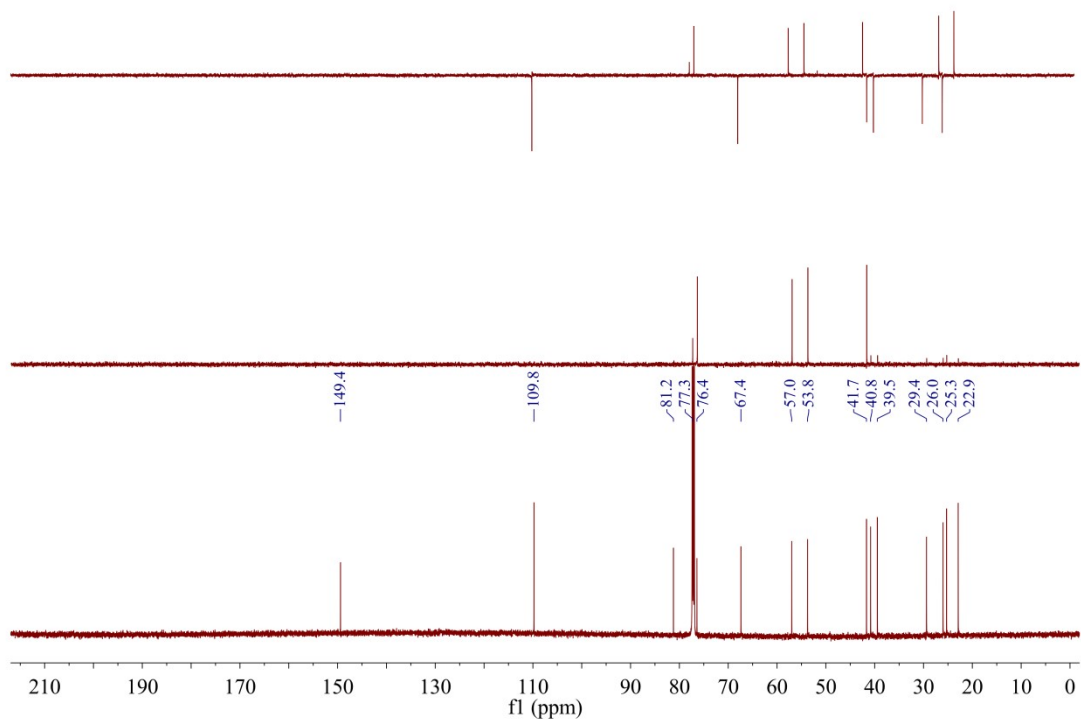


Figure S83. ^{13}C NMR spectrum of magnolin J (**11**) in CDCl_3

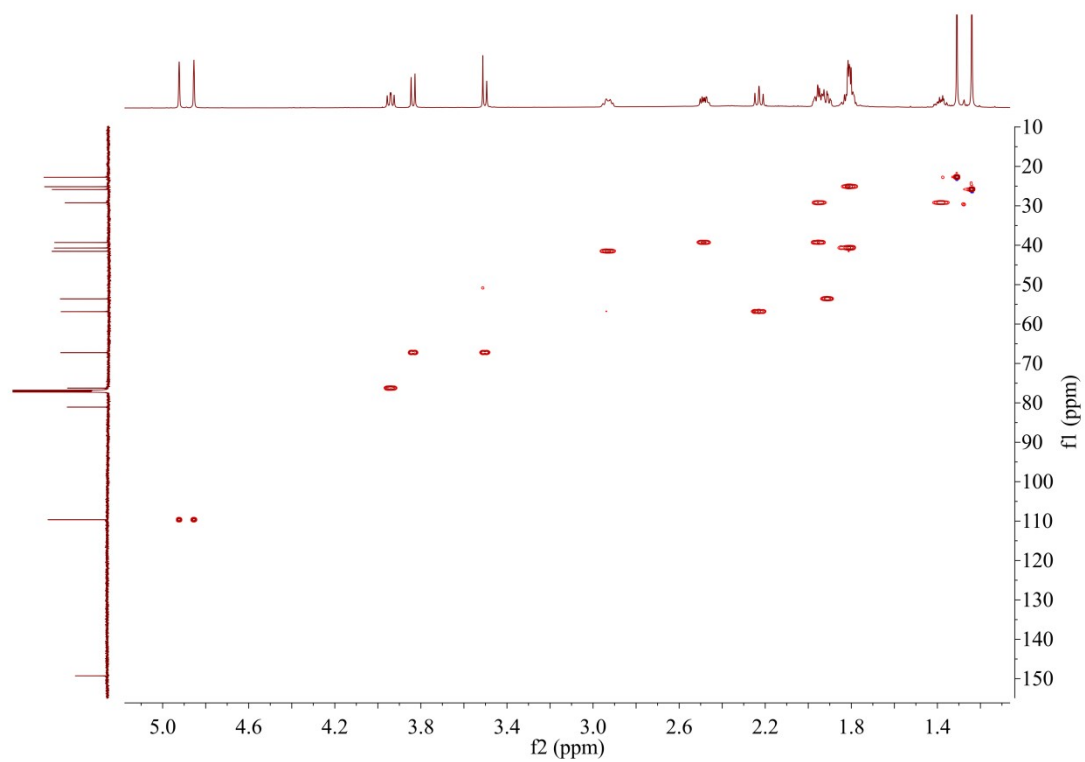


Figure S84. HSQC spectrum of magnolin J (**11**) in CDCl_3

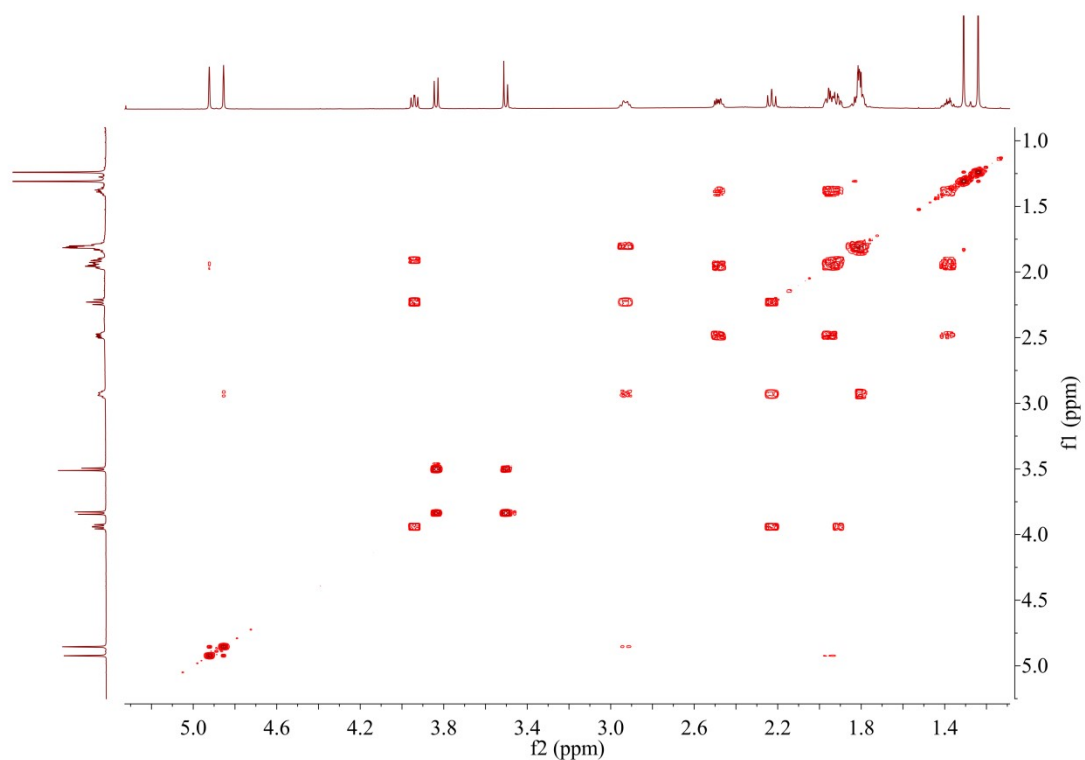


Figure S85. COSY spectrum of magnolin J (**11**) in CDCl_3

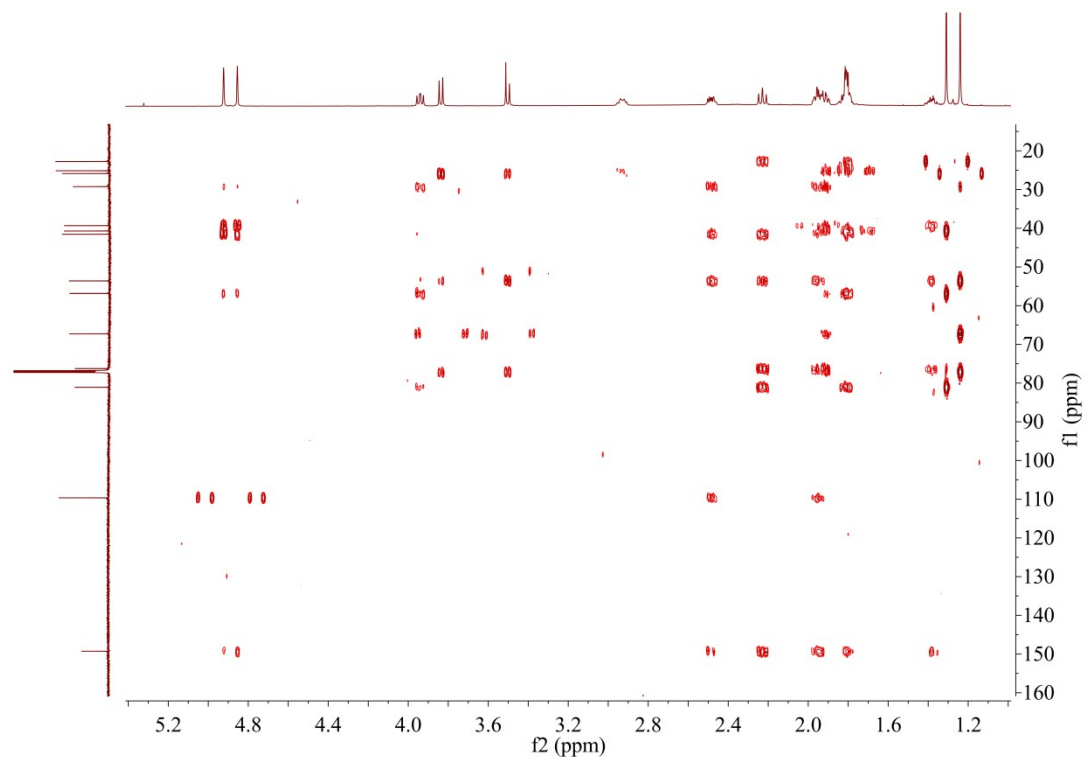


Figure S86. HMBC spectrum of magnolin J (**11**) in CDCl_3

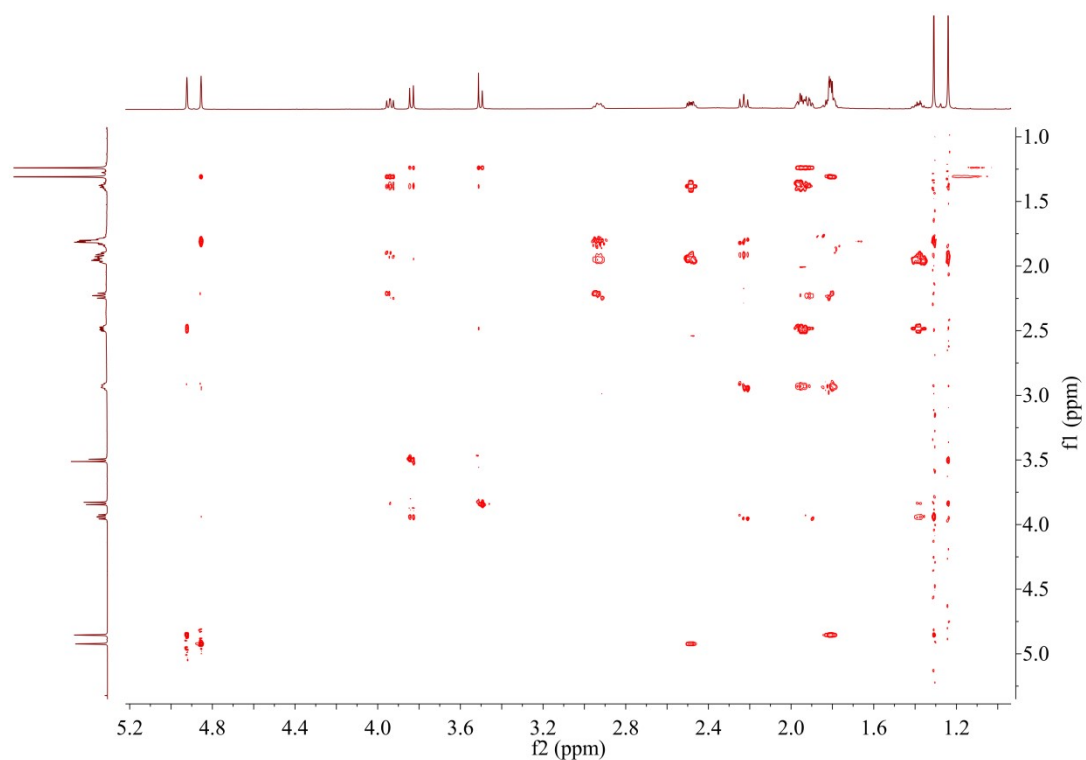


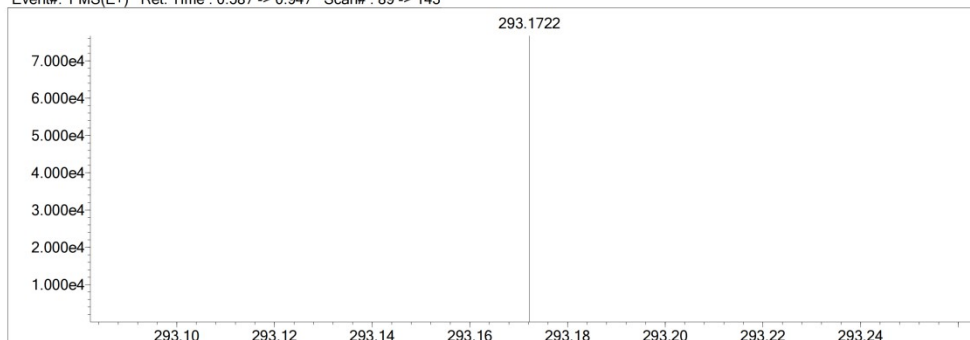
Figure S87. ROESY spectrum of magnolin J (**11**) in CDCl_3

Data File: D:\DATA\2025\1104\fwxz-134.lcd

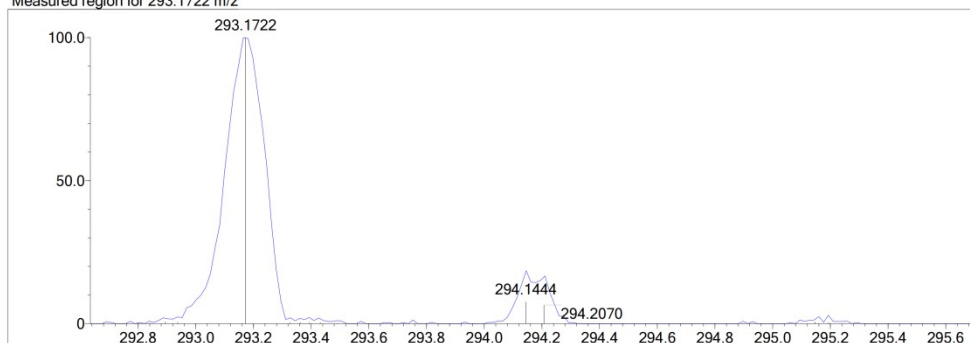
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	5	100	N	3	0	10	Si	4	0	0	H
B	3	0	0	O	2	0	20	S	2	0	0	Na
C	4	10	50	F	1	0	0	Cl	1	0	0	

Error Margin (ppm): 5
 DBE Range: -2.0 - 1000.0
 Electron Ions: both
 HC Ratio: unlimited
 Apply N Rule: no
 Use MSn Info: no
 Max Isotopes: all
 Isotope RI (%): 1.00
 MSn Iso RI (%): 75.00
 MSn Logic Mode: AND
 Isotope Res: 10000
 Max Results: 50

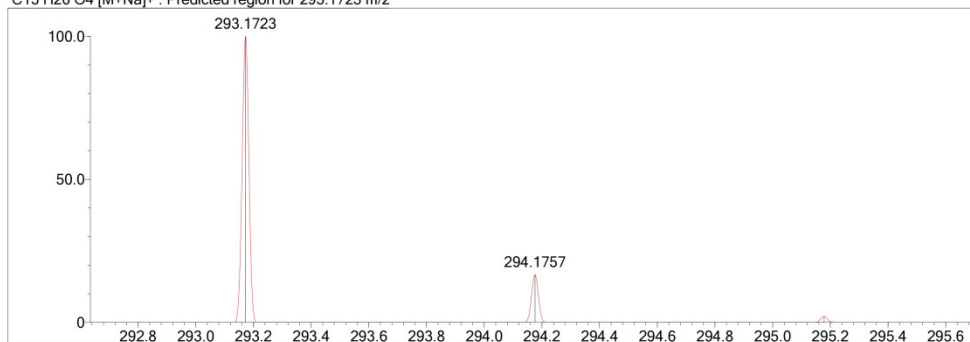
Event#: 1 MS(E+) Ret. Time : 0.587 -> 0.947 Scan#: 89 -> 143



Measured region for 293.1722 m/z



C15 H26 O4 [M+Na]+ : Predicted region for 293.1723 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C15 H26 O4	[M+Na]+	293.1722	293.1723	-0.1	-0.34	3.0

Figure S88. HR-ESI-MS spectrum of magnolin J (11)

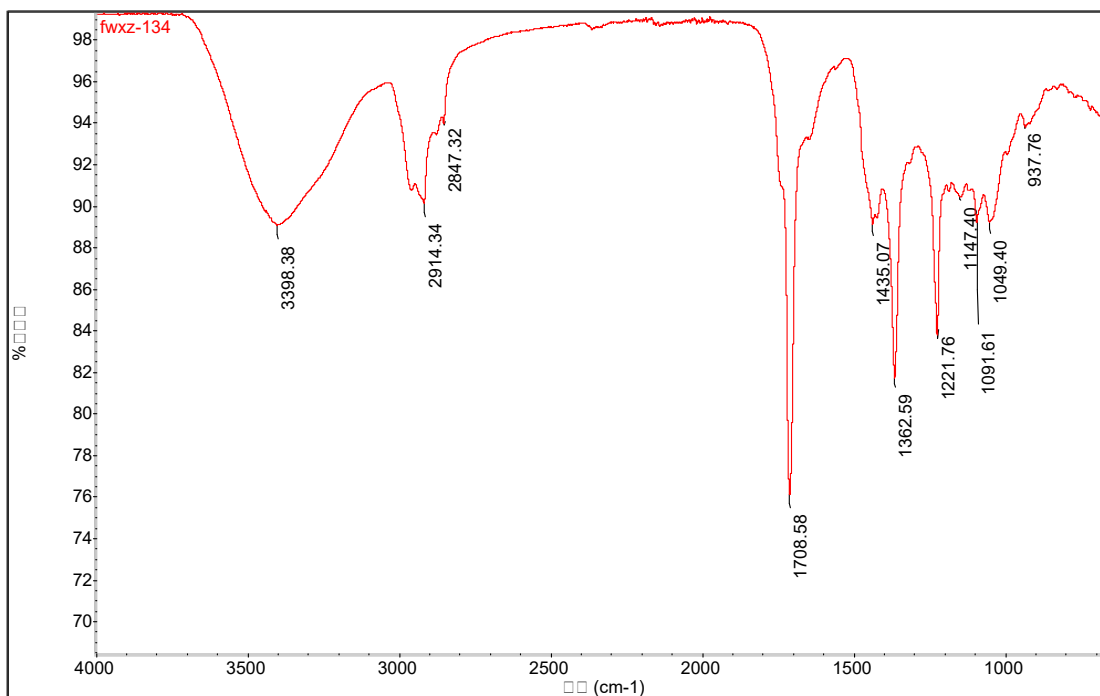


Figure S89. IR spectrum of magnolin J (**11**)

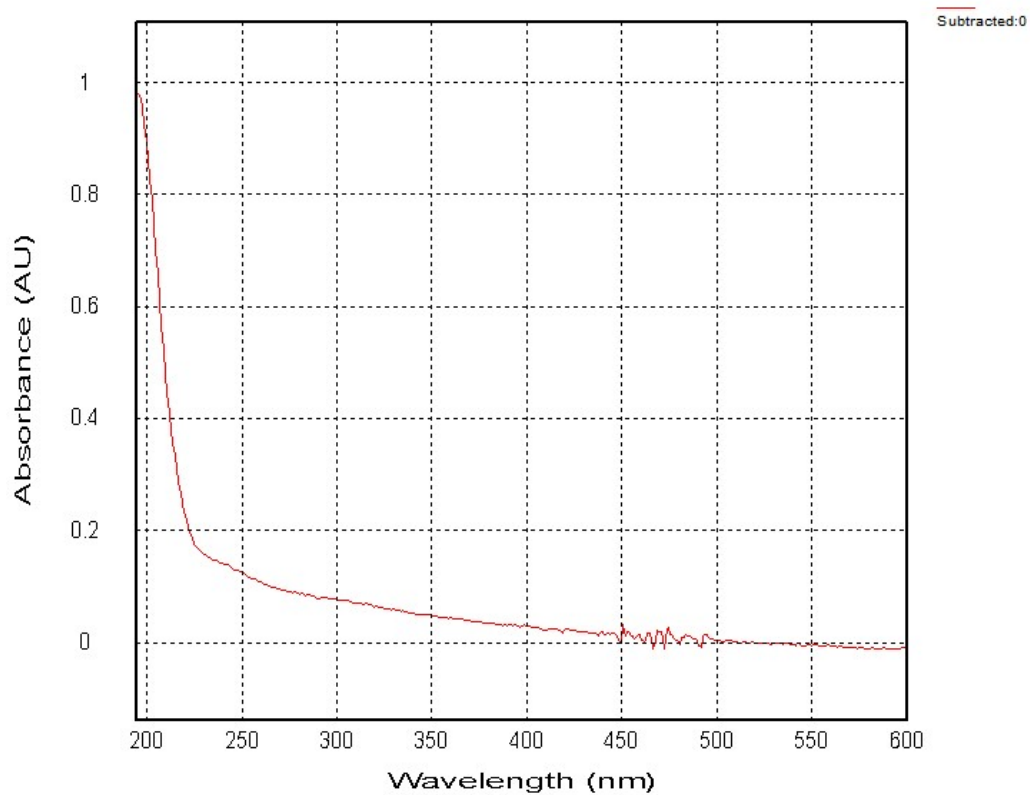


Figure S90. UV spectrum of magnolin J (**11**)

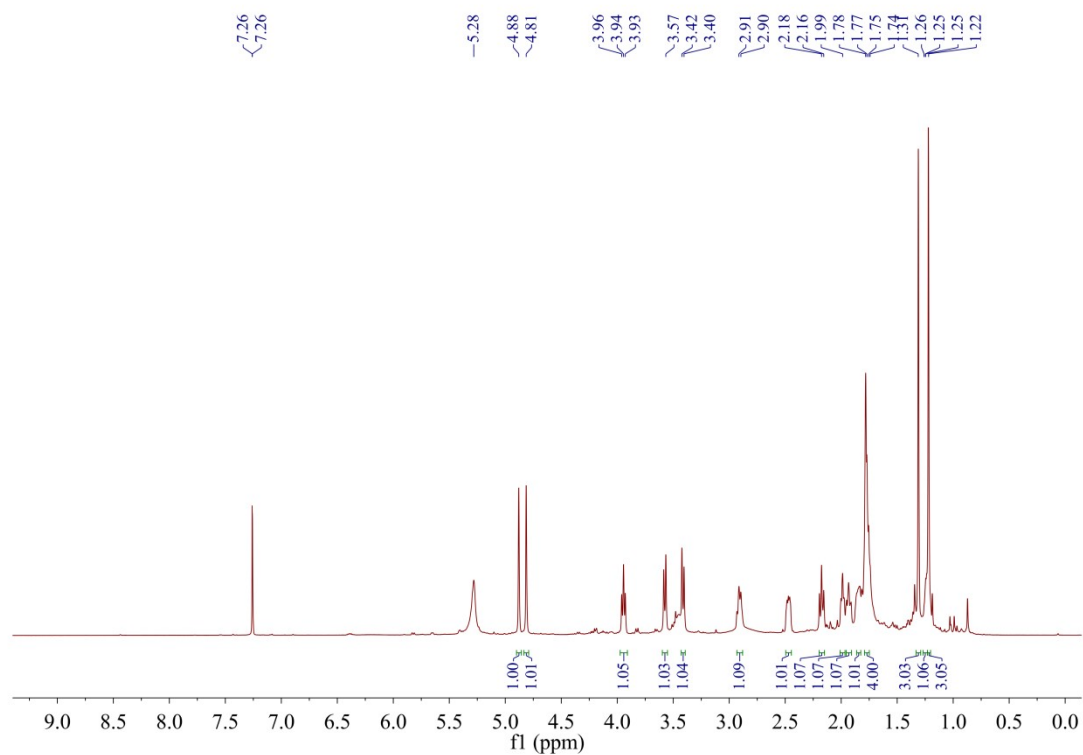


Figure S91. ^1H NMR spectrum of magnolin K (12) in CDCl_3

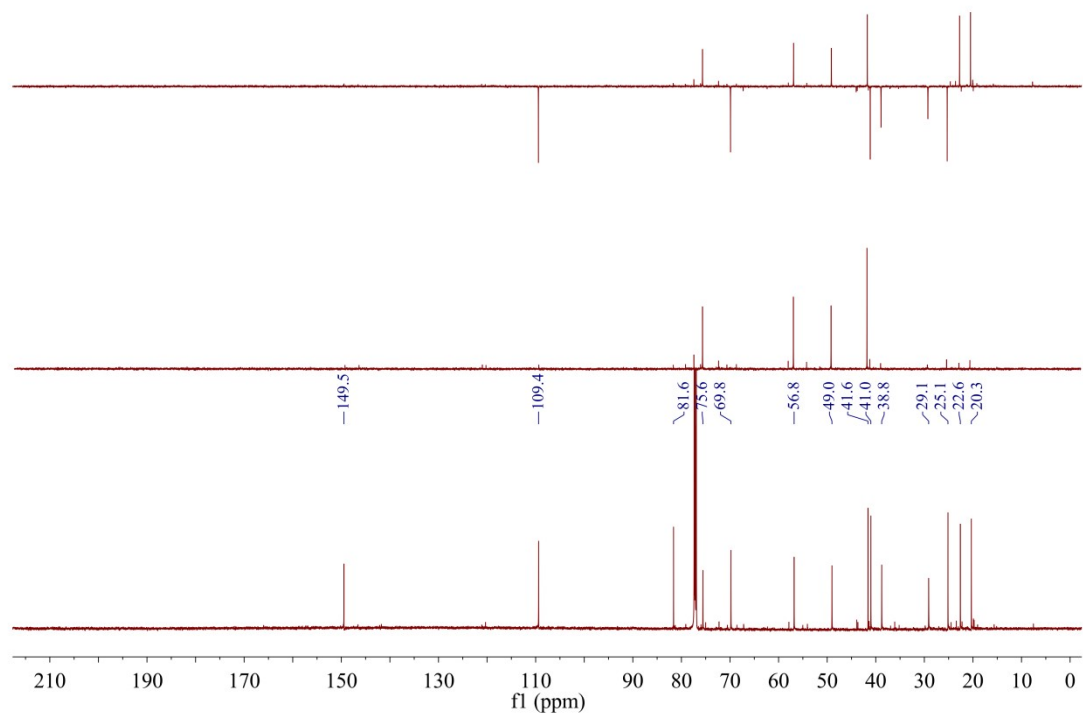


Figure S92. ^{13}C NMR spectrum of magnolin K (12) in CDCl_3

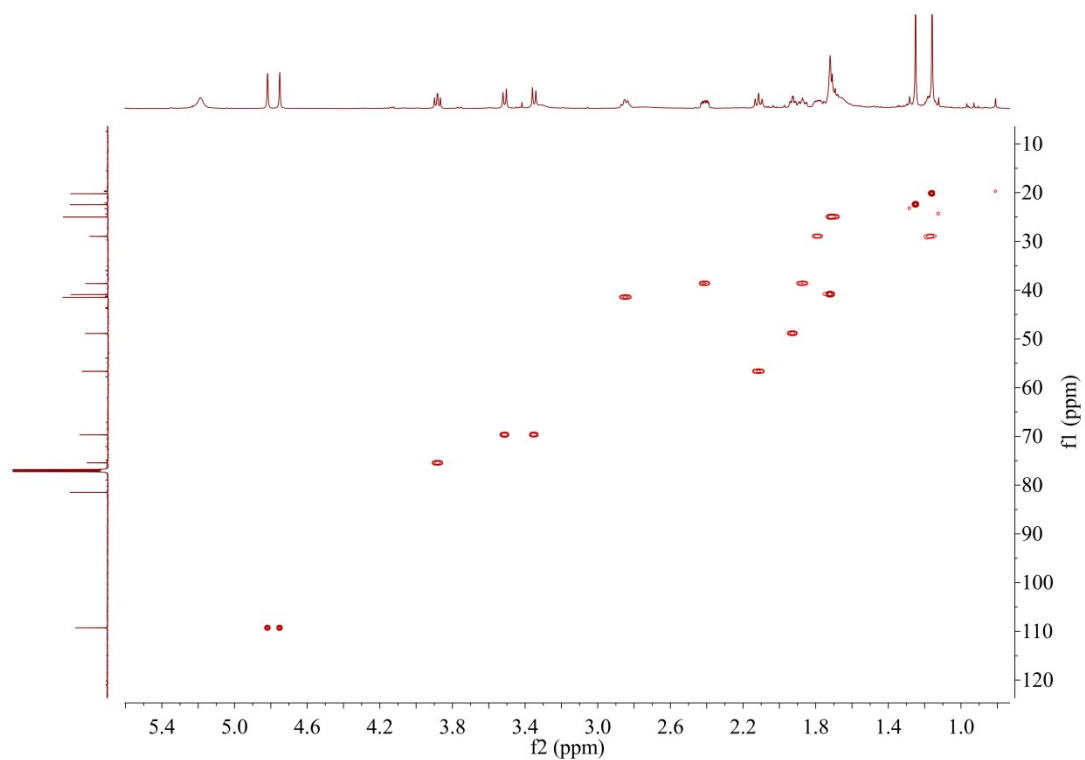


Figure S93. HSQC spectrum of magnolin K (**12**) in CDCl_3

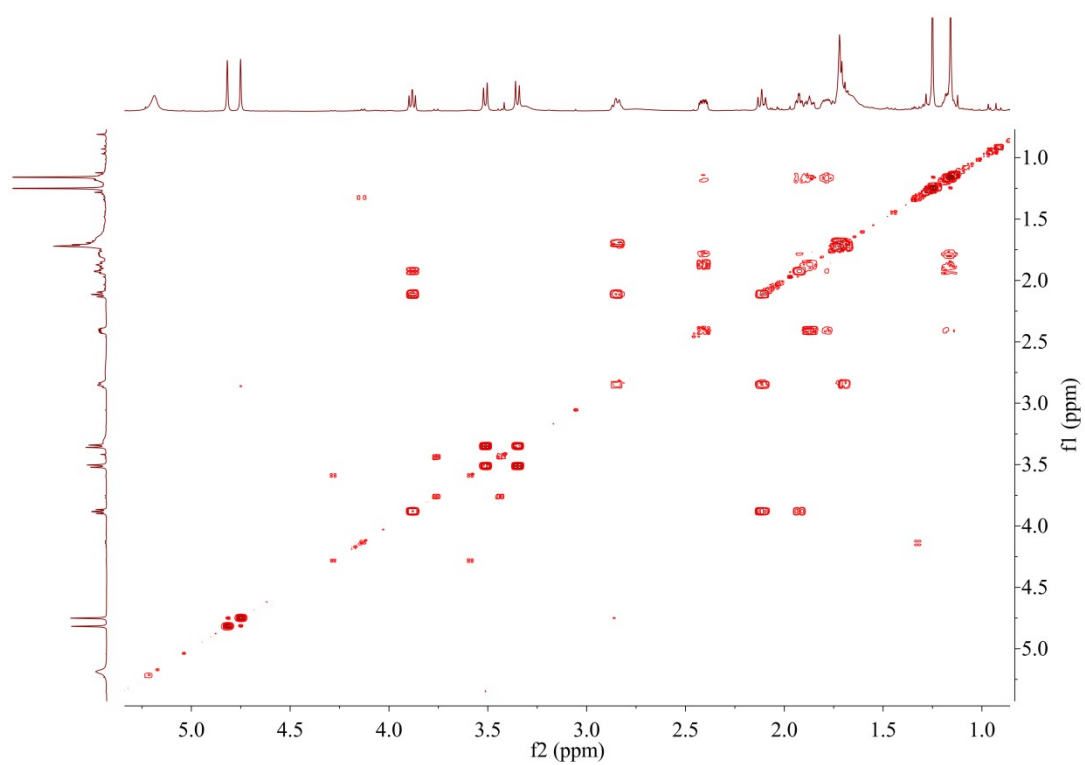


Figure S94. COSY spectrum of magnolin K (**12**) in CDCl_3

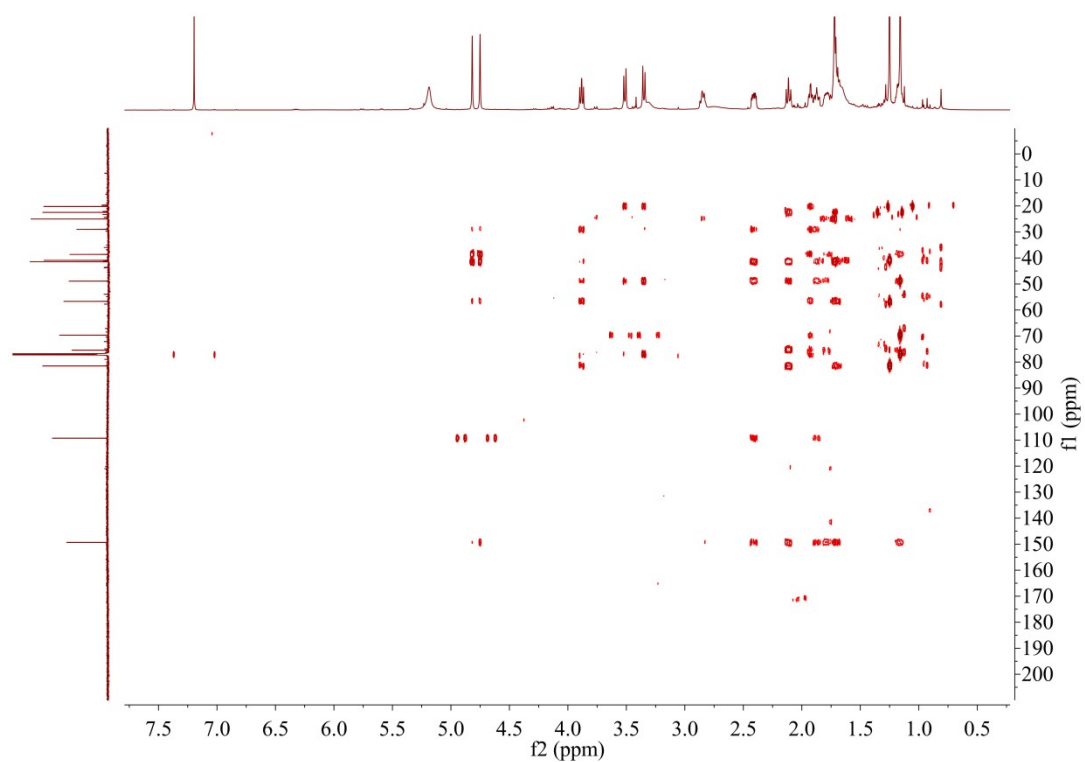


Figure S95. HMBC spectrum of magnolin K (12) in CDCl_3

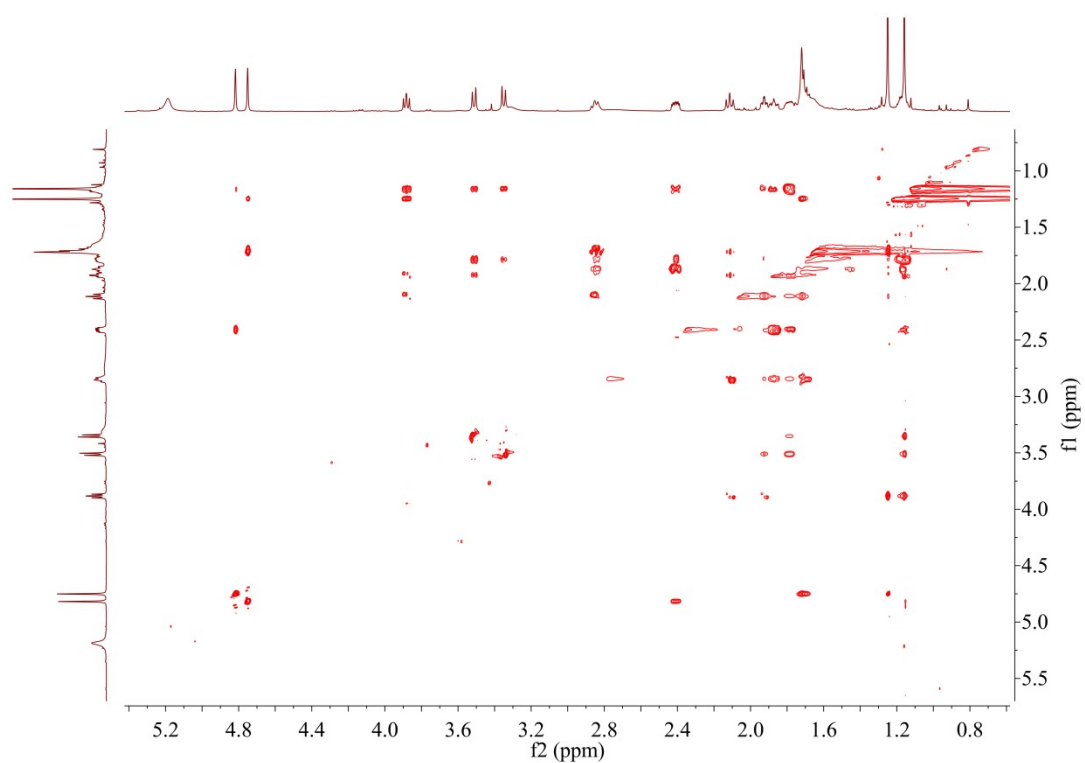


Figure S96. ROESY spectrum of magnolin K (12) in CDCl_3

Data File: D:\DATA\2025\1104\fwxz-135.lcd

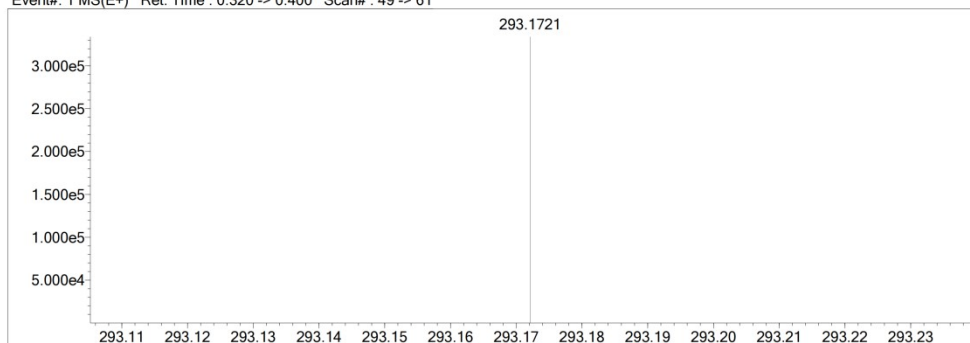
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	5	100	N	3	0	10	Si	4	0	0	H
B	3	0	0	O	2	0	20	S	2	0	0	Na
C	4	10	50	F	1	0	0	Cl	1	0	0	

Error Margin (ppm): 5
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

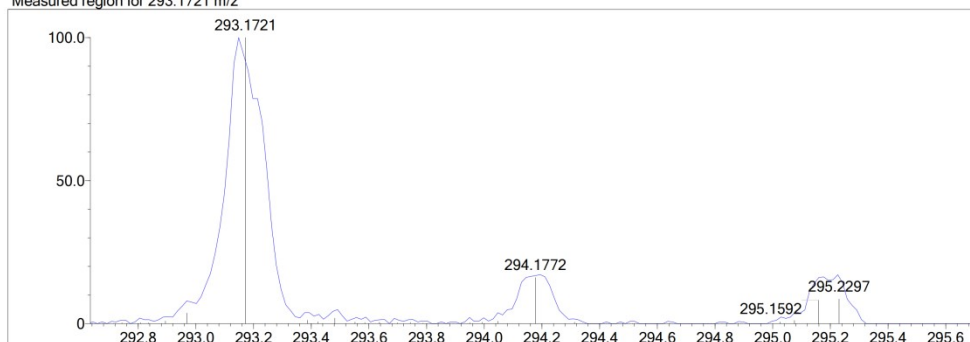
DBE Range: -2.0 - 1000.0
 Apply N Rule: no
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 50

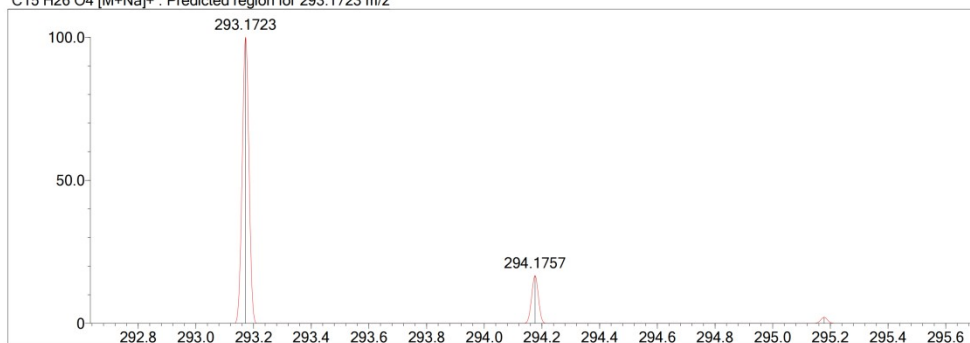
Event#: 1 MS(E+) Ret. Time : 0.320 -> 0.400 Scan#: 49 -> 61



Measured region for 293.1721 m/z



C15 H26 O4 [M+Na]+ : Predicted region for 293.1723 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C15 H26 O4	[M+Na]+	293.1721	293.1723	-0.2	-0.68	3.0

Figure S97. HR-ESI-MS spectrum of magnolin K (12)

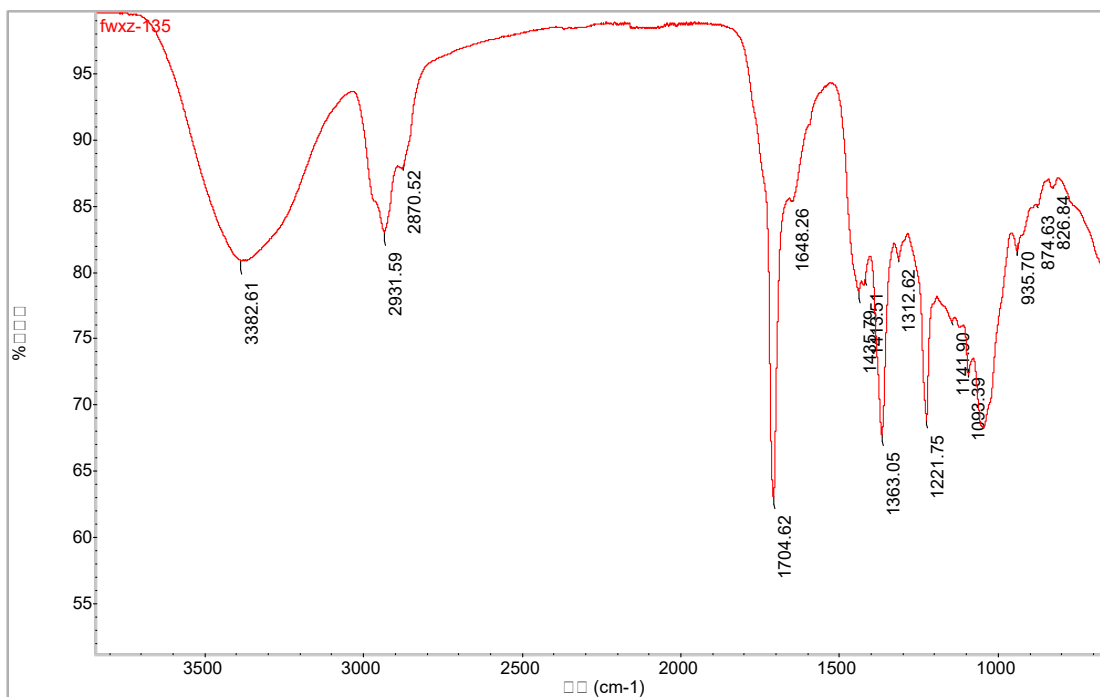


Figure S98. IR spectrum of magnolin K (12)

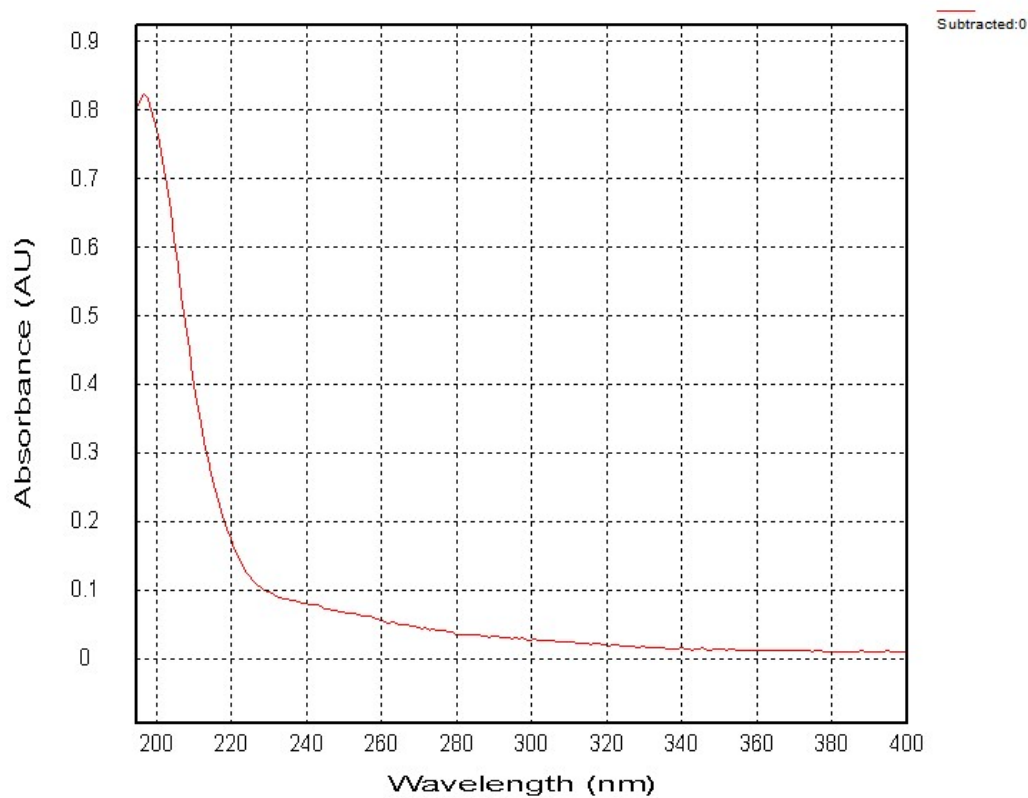


Figure S99. UV spectrum of magnolin K (12)

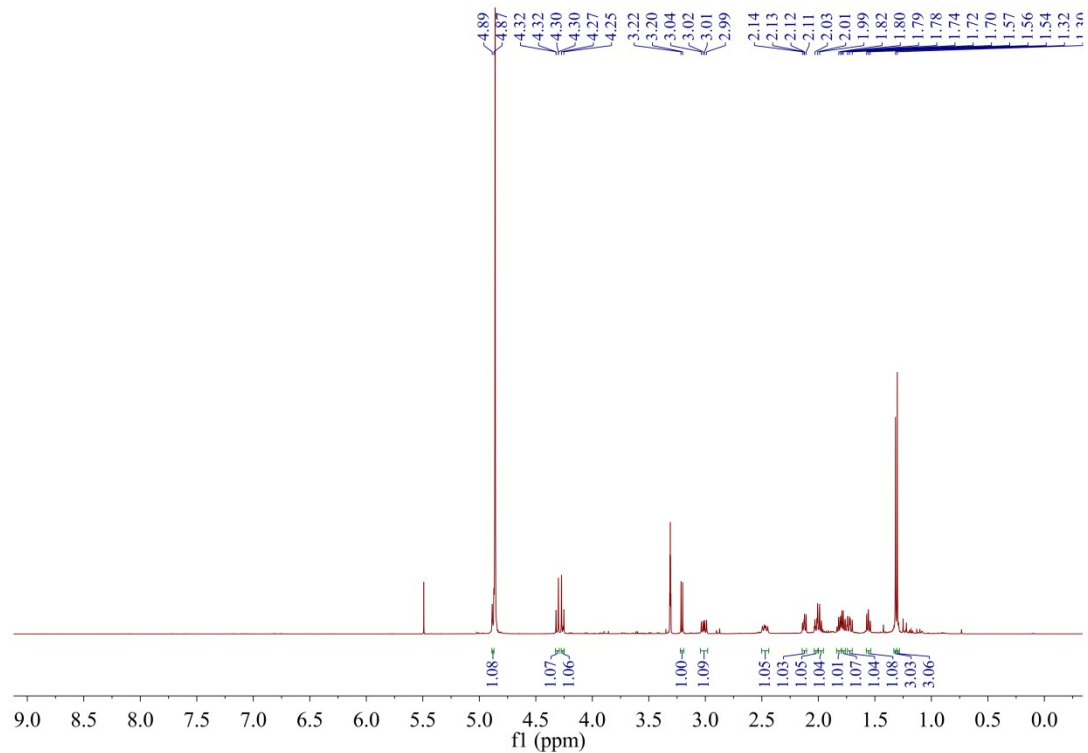


Figure S10. ^1H NMR spectrum of magnolin L (**15**) in CD_3OD

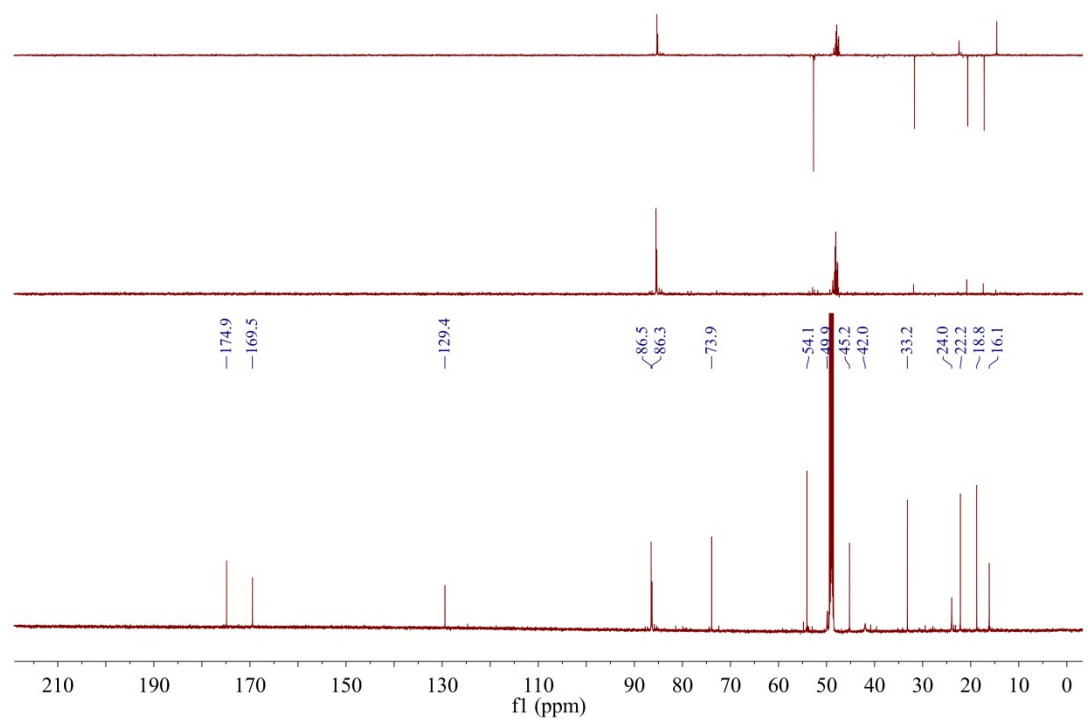


Figure S101. ^{13}C NMR spectrum of magnolin L (**15**) in CD_3OD

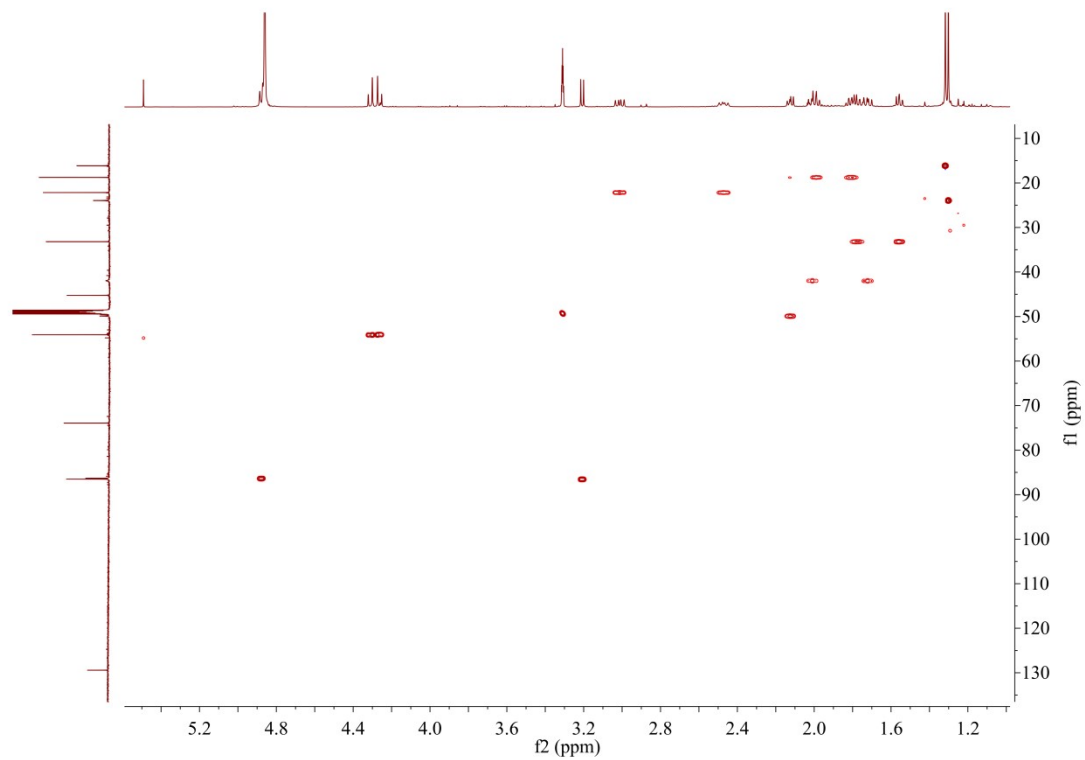


Figure S102. HSQC spectrum of magnolin L (**15**) in CD₃OD

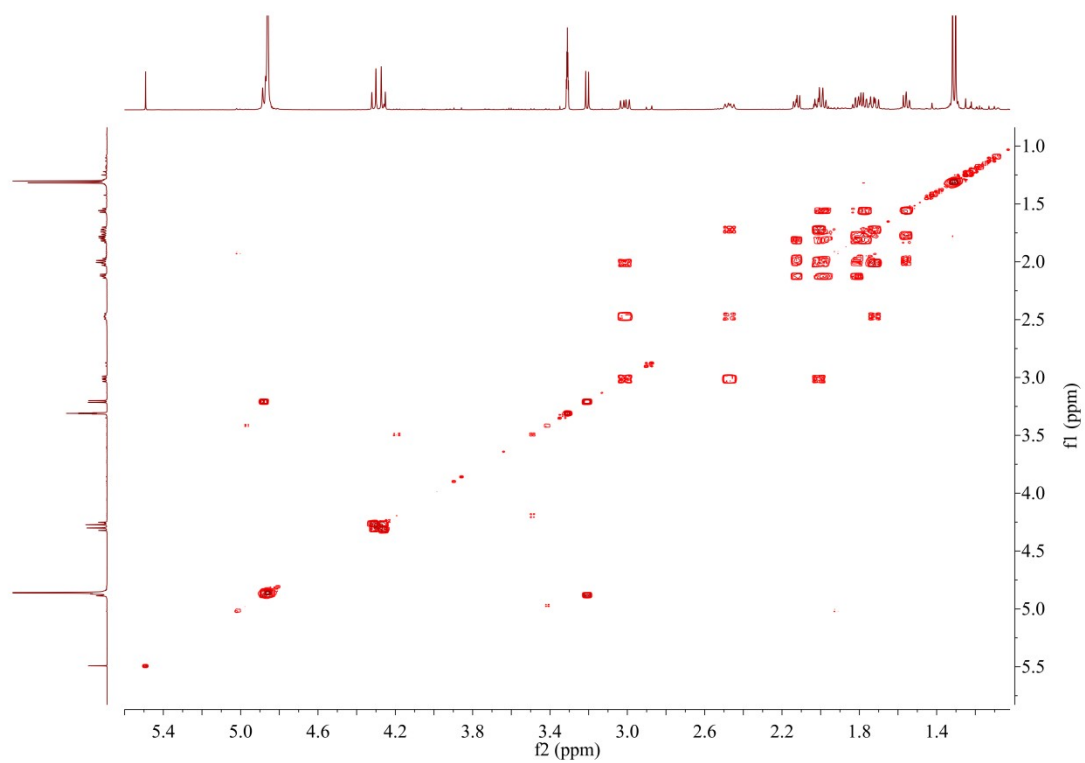


Figure S103. COSY spectrum of magnolin L (**15**) in CD₃OD

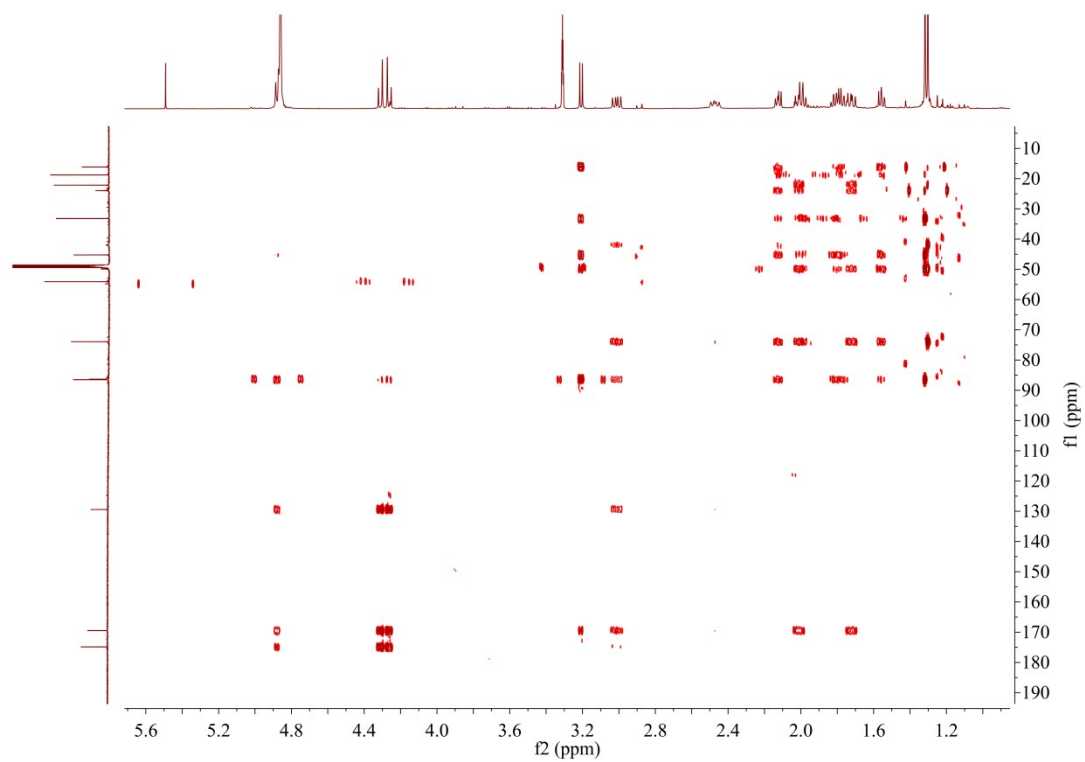


Figure S104. HMBC spectrum of magnolin L (**15**) in CD₃OD

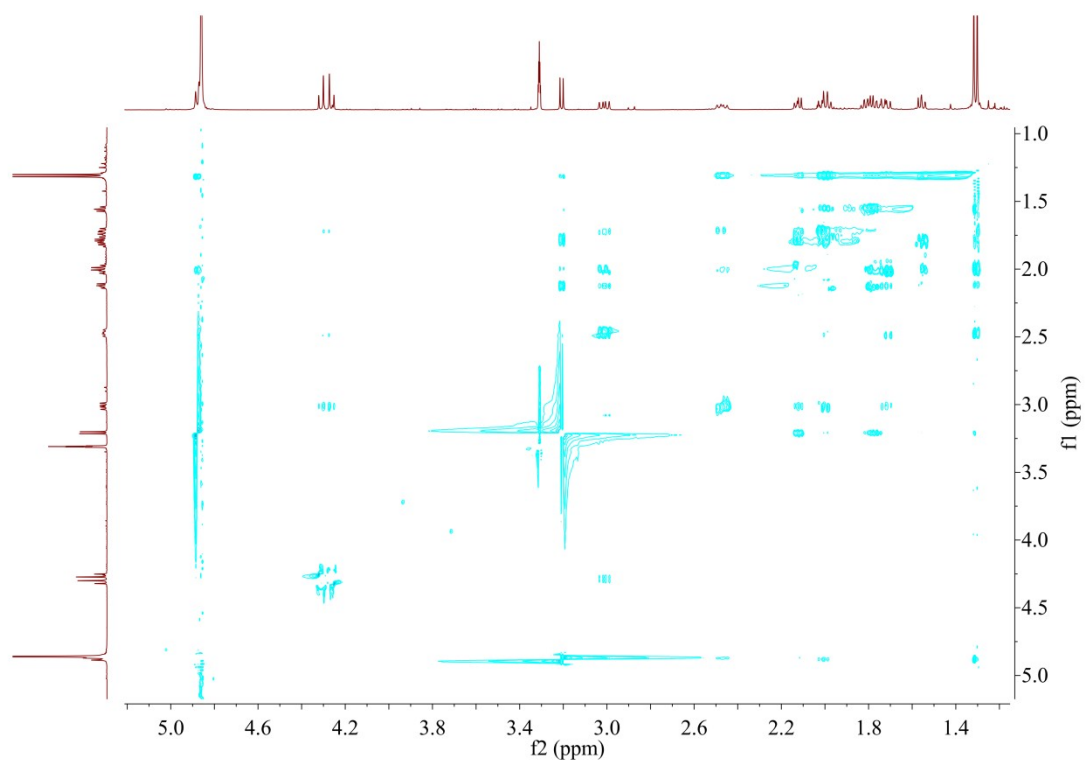


Figure S105. ROESY spectrum of magnolin L (**15**) in CD₃OD

Data File: D:\DATA\2025\0312\1\Fwxz-76.lcd

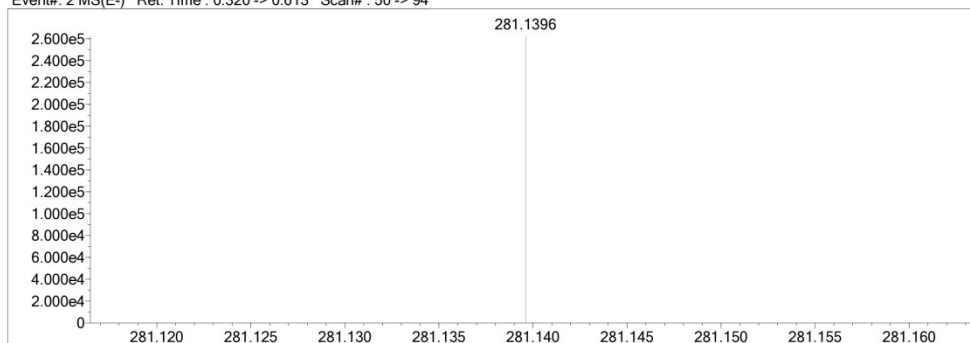
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	100	O	2	0	20	S	2	0	5	H
C	4	5	100	F	1	0	0	Cl	1	0	5	HCOO
N	3	0	10	Si	4	0	0	Br	1	0	0	Cl

Error Margin (ppm): 5
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

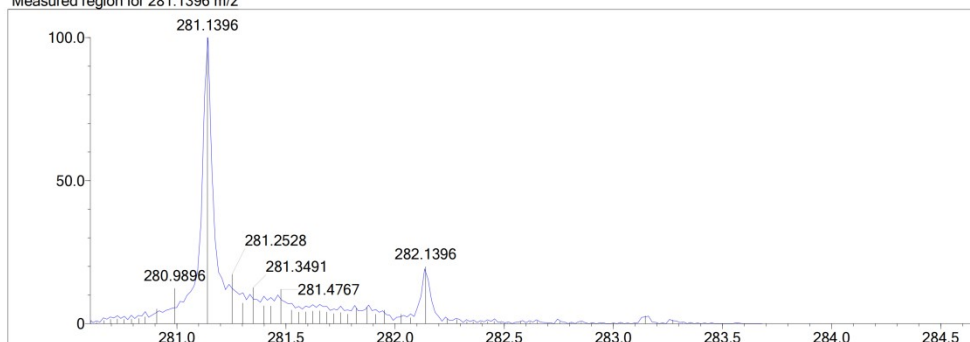
DBE Range: -2.0 - 1000.0
 Apply N Rule: no
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 50

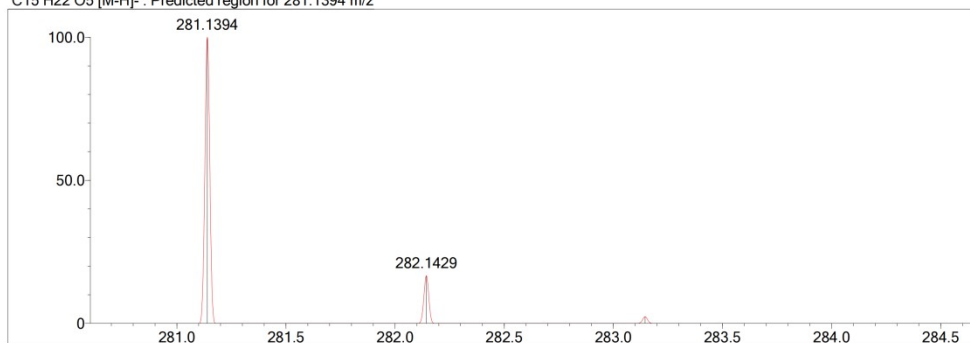
Event#: 2 MS(E-) Ret. Time : 0.320 -> 0.613 Scan# : 50 -> 94



Measured region for 281.1396 m/z



C15 H22 O5 [M-H]-: Predicted region for 281.1394 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C15 H22 O5	[M-H]-	281.1396	281.1394	0.2	0.71	5.0

Figure S106. HR-ESI-MS spectrum of magnolin L (15)

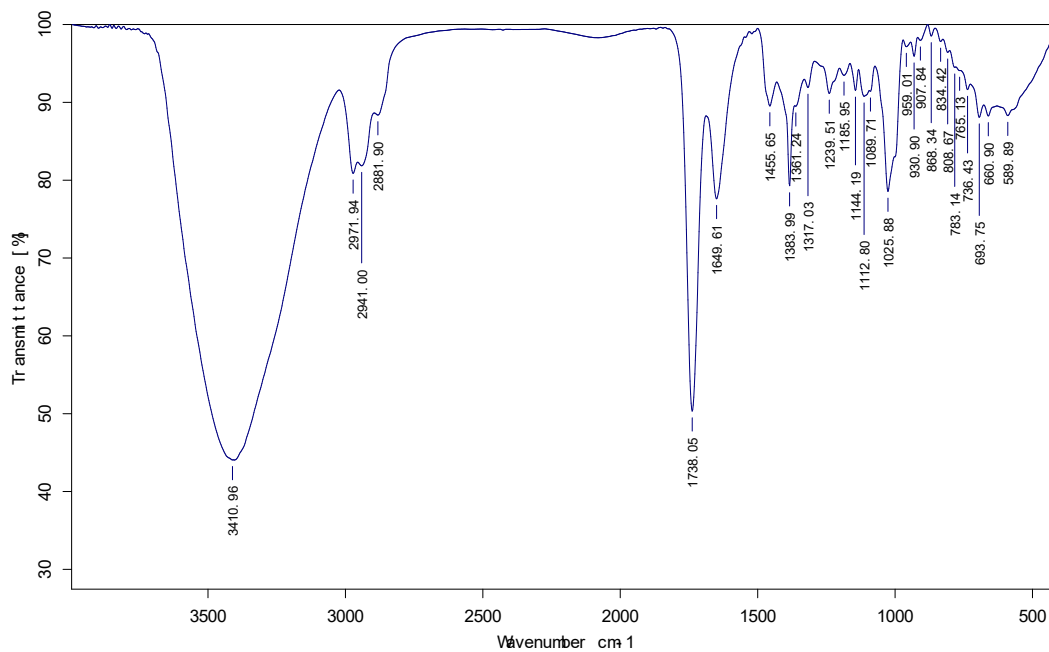


Figure S107. IR spectrum of magnolin L (15)

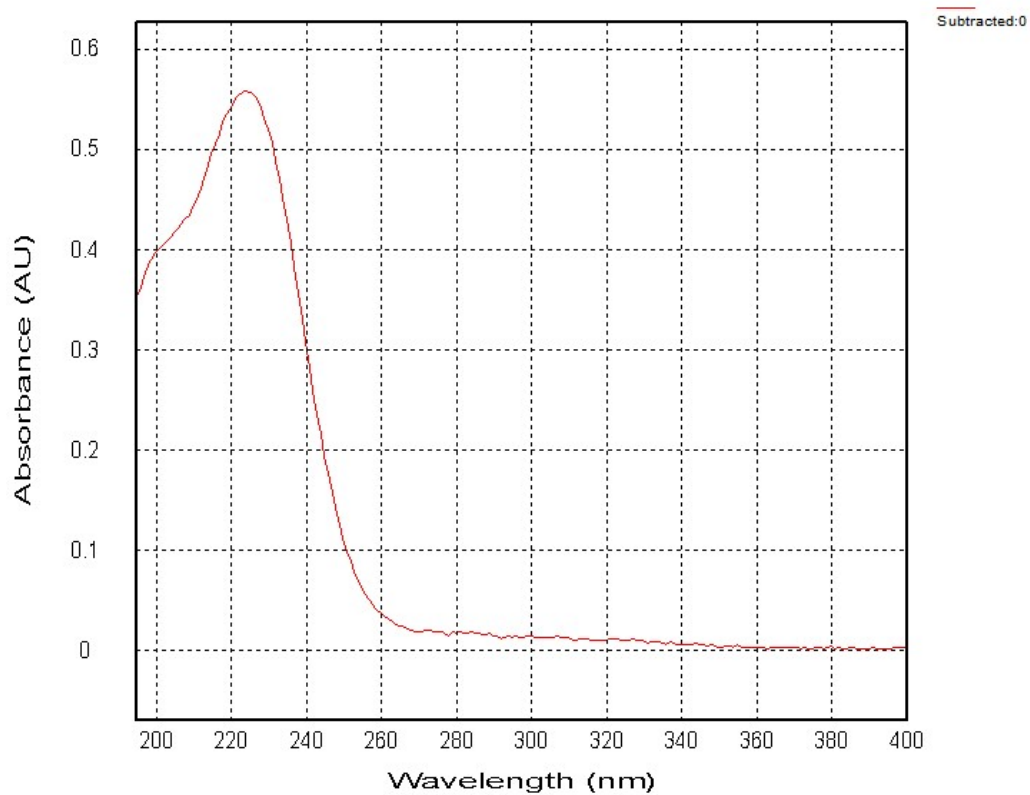


Figure S108. UV spectrum of magnolin L (15)

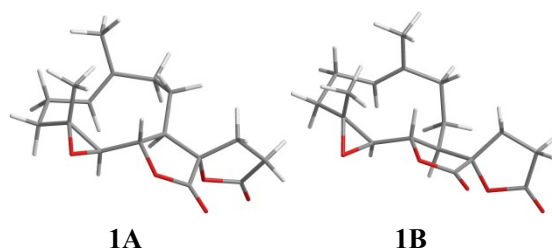


Figure S109. Conformers of isomer **1**

Table S1. Important thermodynamic parameters and Boltzmann distributions of the optimized isomer **1** at B3LYP/6-31G (d, p) level in gas phase.

Conformations	Energy (a.u)	$\Delta G(\text{kcal/mol})$	%	Number of imaginary frequencies
1A	-1036.722153	0.00	100.0	0
1B	-1036.711861	6.46	0.0	0

Table S2. Optimized Z-matrixes of isomer **1** in the gas phase (\AA) at B3LYP/6-31G (d) level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1A					
1	6	0	4.216437	0.457395	0.795873
2	6	0	3.912033	1.056771	0.734255
3	6	0	2.744564	1.336401	0.187364
4	6	0	1.406935	1.333607	0.427238
5	6	0	2.280929	2.017343	0.220119
6	6	0	2.941279	1.209164	1.054091
7	6	0	0.138183	0.958635	0.282689
8	6	0	0.577121	0.298757	0.261135
9	6	0	0.198319	1.688565	0.269387
10	6	0	0.871123	2.45187	0.539165
11	8	0	0.798393	2.05063	0.022302
12	6	0	2.028876	1.587655	0.199254
13	6	0	2.032988	0.079915	0.019413
14	8	0	2.033594	2.556621	0.050294
15	6	0	2.957763	1.005169	1.64316
16	8	0	2.963085	2.280107	0.488156
17	6	0	2.817228	2.55232	1.082804
18	8	0	2.931409	0.54716	0.888301
19	6	0	4.14786	0.744985	0.314292
20	6	0	4.099904	0.31589	1.134268
21	6	0	2.60366	0.212654	1.423286
22	8	0	5.06162	1.194859	0.940509
23	1	0	4.686085	0.77506	0.136066
24	1	0	4.942034	0.630398	1.595093
25	1	0	3.662698	1.42738	1.732309

26	1	0	4.794669	1.602068	0.388132
27	1	0	1.34995	1.197797	1.505906
28	1	0	2.445655	0.950452	1.990408
29	1	0	0.27109	0.905353	1.365
30	1	0	0.471864	0.288762	1.353901
31	1	0	1.110854	2.292163	0.237883
32	1	0	0.091115	1.624933	1.322961
33	1	0	0.758688	3.516278	0.310012
34	1	0	0.66547	2.327697	1.606124
35	1	0	3.908059	1.430646	1.975381
36	1	0	2.996468	0.07399	1.795098
37	1	0	2.164882	1.421251	2.2632
38	1	0	2.849216	3.645357	1.033443
39	1	0	3.820454	2.199736	1.316025
40	1	0	2.161396	2.298499	1.921094
41	1	0	4.603493	0.651114	1.205699
42	1	0	4.633593	1.030856	1.756402
43	1	0	2.216787	1.163887	1.787844
44	1	0	2.350508	0.564492	2.143765
1B					
1	6	0	4.119369	0.688611	0.663264
2	6	0	3.983593	0.852724	0.821557
3	6	0	2.807659	1.32942	0.0001
4	6	0	1.493325	1.256531	0.651635
5	6	0	2.049901	1.959123	0.149708
6	6	0	2.764084	1.33624	0.792805
7	6	0	0.265715	0.76829	0.084751
8	6	0	0.635953	0.121204	0.790459
9	6	0	0.211115	1.569365	1.097955
10	6	0	0.585588	2.329204	0.030493
11	8	0	0.588176	1.877363	0.46693
12	6	0	1.874481	1.521281	0.392368
13	6	0	1.978473	0.070266	0.090972
14	8	0	2.099812	2.515162	0.388626
15	6	0	2.941213	1.19021	1.494403
16	8	0	2.782761	2.249673	0.672421
17	6	0	2.585508	2.378888	1.494748
18	8	0	3.070117	0.035437	1.004521
19	6	0	4.201757	0.431004	0.36367
20	6	0	3.88063	0.746529	1.079559
21	6	0	2.35735	0.859495	1.075045
22	8	0	5.248898	0.493231	0.937852
23	1	0	4.580443	0.914542	0.298686

24	1	0	4.799888	1.0536	1.436911
25	1	0	3.808848	1.10731	1.87026
26	1	0	4.90953	1.340831	0.506649
27	1	0	1.477761	1.026636	1.71461
28	1	0	2.284141	1.138503	1.748155
29	1	0	0.547705	0.253898	1.008131
30	1	0	0.745302	0.405906	1.74591
31	1	0	0.339341	1.576446	2.039666
32	1	0	1.130208	2.125269	1.309823
33	1	0	0.105535	2.210284	0.947691
34	1	0	0.516944	3.401426	0.247429
35	1	0	3.811013	1.761586	1.828456
36	1	0	3.088453	0.149868	1.784974
37	1	0	2.060648	1.581323	2.005242
38	1	0	2.406264	3.449857	1.634848
39	1	0	3.653183	2.20116	1.612403
40	1	0	2.052985	1.867238	2.303385
41	1	0	4.233405	0.089931	1.687138
42	1	0	4.400884	1.648723	1.393255
43	1	0	2.060666	1.879287	0.826315
44	1	0	1.888269	0.57354	2.016041

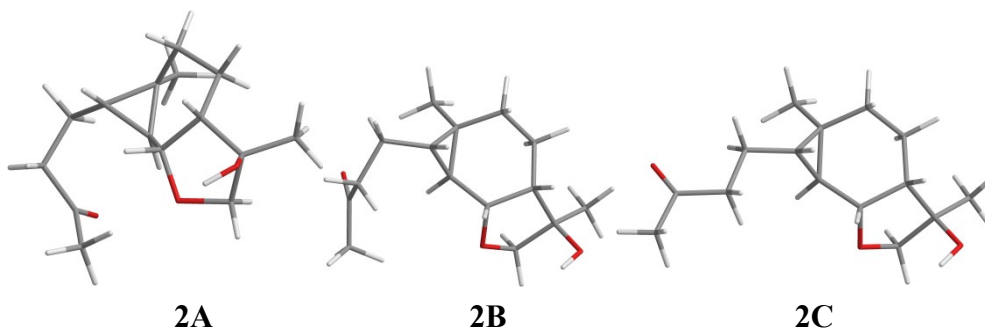


Figure S110. Conformers of isomer **2**

Table S3. Important thermodynamic parameters and Boltzmann distributions of the optimized isomer **2** at B3LYP/6-31G (d, p) level in gas phase.

Conformations	Energy (a.u)	ΔG (kcal/mol)	%	Number of imaginary frequencies
2A	-811.265185	0.00	31.1	0
2B	-811.265334	-0.09	36.4	0
2C	-811.265225	-0.03	32.5	0

Table S4. Optimized Z-matrixes of isomer **2** in the gas phase (Å) at B3LYP/6-31G (d) level.

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

2A					
1	6	0	0.400417	1.990276	0.025553
2	6	0	0.495287	0.573401	0.54314
3	6	0	-0.603298	-0.430377	0.321988
4	6	0	-1.726477	-0.000183	-0.633426
5	6	0	-2.048985	1.483213	-0.449855
6	6	0	-0.840689	2.355313	-0.791907
7	6	0	1.363222	1.012209	-0.605376
8	6	0	2.867233	1.098678	-0.460248
9	6	0	3.538307	-0.209647	-0.873904
10	6	0	3.299915	-1.355101	0.092187
11	6	0	3.357169	-2.742377	-0.491552
12	8	0	3.095251	-1.165243	1.271772
13	6	0	0.929828	3.10743	0.899764
14	1	0	1.020688	0.437918	1.483343
15	8	0	-1.273622	-0.678797	1.570693
16	6	0	-2.65407	-0.961489	1.337095
17	6	0	-2.859709	-0.943467	-0.183274
18	6	0	-4.262095	-0.543045	-0.597183
19	8	0	-2.658021	-2.249629	-0.736165
20	1	0	-1.471875	-0.204749	-1.677524
21	1	0	-0.149144	-1.373775	-0.018786
22	1	0	-2.892408	1.761016	-1.08597
23	1	0	-2.347958	1.669042	0.588708
24	1	0	-1.090363	3.403902	-0.609864
25	1	0	-0.628767	2.266761	-1.862506
26	1	0	1.042144	0.658393	-1.584827
27	1	0	3.255699	1.908588	-1.084945
28	1	0	3.138804	1.325723	0.572572
29	1	0	3.220352	-0.514643	-1.875343
30	1	0	4.628036	-0.09104	-0.926342
31	1	0	2.471842	-2.889279	-1.117718
32	1	0	4.229361	-2.844491	-1.141231
33	1	0	3.377286	-3.492599	0.296507
34	1	0	1.760332	2.779517	1.526483
35	1	0	1.272328	3.949062	0.289769
36	1	0	0.137499	3.473001	1.559495
37	1	0	-3.260618	-0.194471	1.827354
38	1	0	-2.912894	-1.939352	1.75152
39	1	0	-4.333119	-0.500765	-1.686175

40	1	0	-4.974935	-1.285398	-0.231765
41	1	0	-4.534012	0.429252	-0.187268
42	1	0	-1.803472	-2.59126	-0.453908
2B					
1	6	0	0.400417	1.990276	0.025553
2	6	0	0.495287	0.573401	0.54314
3	6	0	-0.603298	-0.430377	0.321988
4	6	0	-1.726477	-0.000183	-0.633426
5	6	0	-2.048985	1.483213	-0.449855
6	6	0	-0.840689	2.355313	-0.791907
7	6	0	1.363222	1.012209	-0.605376
8	6	0	2.867233	1.098678	-0.460248
9	6	0	3.538307	-0.209647	-0.873904
10	6	0	3.299915	-1.355101	0.092187
11	6	0	3.357169	-2.742377	-0.491552
12	8	0	3.095251	-1.165243	1.271772
13	6	0	0.929828	3.10743	0.899764
14	1	0	1.020688	0.437918	1.483343
15	8	0	-1.273622	-0.678797	1.570693
16	6	0	-2.65407	-0.961489	1.337095
17	6	0	-2.859709	-0.943467	-0.183274
18	6	0	-4.262095	-0.543045	-0.597183
19	8	0	-2.658021	-2.249629	-0.736165
20	1	0	-1.471875	-0.204749	-1.677524
21	1	0	-0.149144	-1.373775	-0.018786
22	1	0	-2.892408	1.761016	-1.08597
23	1	0	-2.347958	1.669042	0.588708
24	1	0	-1.090363	3.403902	-0.609864
25	1	0	-0.628767	2.266761	-1.862506
26	1	0	1.042144	0.658393	-1.584827
27	1	0	3.255699	1.908588	-1.084945
28	1	0	3.138804	1.325723	0.572572
29	1	0	3.220352	-0.514643	-1.875343
30	1	0	4.628036	-0.09104	-0.926342
31	1	0	2.471842	-2.889279	-1.117718
32	1	0	4.229361	-2.844491	-1.141231
33	1	0	3.377286	-3.492599	0.296507
34	1	0	1.760332	2.779517	1.526483
35	1	0	1.272328	3.949062	0.289769
36	1	0	0.137499	3.473001	1.559495

37	1	0	-3.260618	-0.194471	1.827354
38	1	0	-2.912894	-1.939352	1.75152
39	1	0	-4.333119	-0.500765	-1.686175
40	1	0	-4.974935	-1.285398	-0.231765
41	1	0	-4.534012	0.429252	-0.187268
42	1	0	-1.803472	-2.59126	-0.453908
2C					
1	6	0	0.400208	1.990168	0.025684
2	6	0	0.495261	0.573155	0.542826
3	6	0	-0.603435	-0.430525	0.32187
4	6	0	-1.726711	-0.000277	-0.633358
5	6	0	-2.049316	1.483072	-0.449375
6	6	0	-0.841142	2.355331	-0.791418
7	6	0	1.362872	1.012335	-0.605817
8	6	0	2.86689	1.098846	-0.461036
9	6	0	3.538078	-0.209528	-0.874391
10	6	0	3.300632	-1.354642	0.092287
11	6	0	3.358497	-2.742177	-0.490761
12	8	0	3.096309	-1.164348	1.271872
13	6	0	0.92961	3.107203	0.900021
14	1	0	1.021016	0.437473	1.482802
15	8	0	-1.273632	-0.678666	1.570657
16	6	0	-2.653914	-0.962371	1.337052
17	6	0	-2.85986	-0.943685	-0.183329
18	6	0	-4.262344	-0.543018	-0.596703
19	8	0	-2.658465	-2.249625	-0.736846
20	1	0	-1.472206	-0.204514	-1.677542
21	1	0	-0.149415	-1.374022	-0.018853
22	1	0	-2.892856	1.760945	-1.085301
23	1	0	-2.348144	1.668604	0.589278
24	1	0	-1.090835	3.403852	-0.609012
25	1	0	-0.629432	2.267111	-1.862085
26	1	0	1.04156	0.658847	-1.585303
27	1	0	3.255205	1.908525	-1.086133
28	1	0	3.138698	1.326307	0.571629
29	1	0	3.219809	-0.515022	-1.875572
30	1	0	4.627754	-0.090573	-0.927342
31	1	0	2.472876	-2.890034	-1.116287
32	1	0	4.230351	-2.844089	-1.140918
33	1	0	3.379575	-3.49194	0.297711

34	1	0	1.760542	2.779422	1.526248
35	1	0	1.271486	3.949166	0.290134
36	1	0	0.13745	3.47225	1.560246
37	1	0	-3.260904	-0.196111	1.827915
38	1	0	-2.911906	-1.940694	1.750903
39	1	0	-4.333626	-0.500171	-1.685659
40	1	0	-4.975078	-1.285593	-0.231524
41	1	0	-4.534199	0.429046	-0.186208
42	1	0	-1.80338	-2.590997	-0.45591

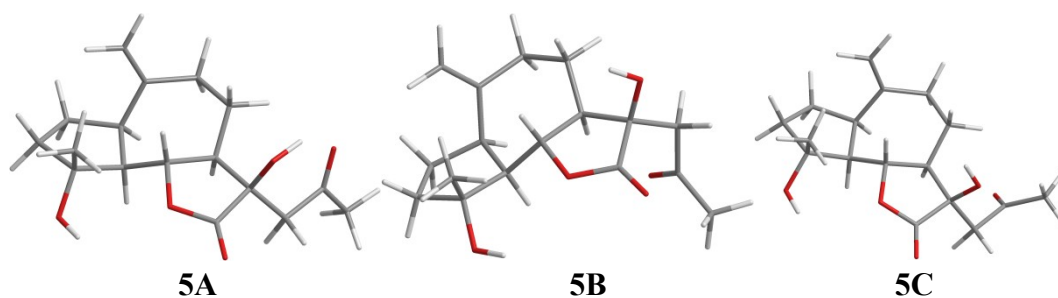


Figure S111. Conformers of isomer **5**

Table S5. Important thermodynamic parameters and Boltzmann distributions of the optimized isomer **5** at B3LYP/6-31G (d, p) level in gas phase.

Conformations	Energy (a.u)	ΔG (kcal/mol)	%	Number of imaginary frequencies
5A	-1037.927818	0.00	71.2	0
5B	-1037.926938	0.55	28.1	0
5C	-1037.923465	2.73	0.7	0

Table S6. Optimized Z-matrixes of isomer **5** in the gas phase (Å) at B3LYP/6-31G (d) level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
5A					
1	6	0	1.990095	-1.191849	-0.932876
2	6	0	1.660746	0.287951	-0.614552
3	6	0	0.455316	0.491683	0.277141
4	6	0	-0.805383	-0.30076	-0.090531
5	6	0	-0.850498	-1.647525	0.633505
6	6	0	0.223005	-2.656143	0.189901
7	6	0	1.65061	-2.148209	0.196131
8	6	0	3.46566	-1.112648	-1.361082
9	6	0	4.10479	-0.013288	-0.502018
10	6	0	2.974876	0.957329	-0.100029
11	8	0	0.087319	1.896821	0.18076

12	8	0	3.184915	2.18912	-0.803825
13	6	0	3.006927	1.237174	1.400208
14	6	0	-1.933401	0.683252	0.28922
15	6	0	2.527767	-2.560372	1.111229
16	6	0	-1.23757	2.049655	0.146808
17	8	0	-1.77041	3.118557	0.049043
18	6	0	-3.176283	0.647926	-0.595715
19	6	0	-4.097838	-0.534445	-0.370268
20	8	0	-2.259659	0.63049	1.668545
21	6	0	-5.022836	-0.881184	-1.499027
22	8	0	-4.100052	-1.150699	0.677802
23	1	0	1.381756	-1.50114	-1.787543
24	1	0	1.433445	0.773063	-1.570269
25	1	0	0.696168	0.30522	1.326416
26	1	0	-0.833163	-0.445411	-1.177444
27	1	0	-1.827823	-2.110982	0.485764
28	1	0	-0.743883	-1.461791	1.706229
29	1	0	-0.01328	-2.991807	-0.826295
30	1	0	0.148802	-3.529396	0.841567
31	1	0	3.974285	-2.073752	-1.271543
32	1	0	3.496593	-0.81979	-2.413646
33	1	0	4.885287	0.533085	-1.033553
34	1	0	4.55968	-0.433732	0.396794
35	1	0	2.435859	2.765999	-0.612771
36	1	0	3.987283	1.643027	1.65858
37	1	0	2.244084	1.964681	1.690266
38	1	0	2.852674	0.317915	1.971297
39	1	0	3.561426	-2.233511	1.111175
40	1	0	2.234044	-3.256939	1.889651
41	1	0	-3.774558	1.544599	-0.388878
42	1	0	-2.897879	0.700584	-1.651107
43	1	0	-2.855928	-0.125642	1.780652
44	1	0	-5.780054	-1.588132	-1.167284
45	1	0	-5.48634	0.022862	-1.899409
46	1	0	-4.431289	-1.324603	-2.305516
5B					
1	6	0	1.912951	0.79324	1.113657
2	6	0	1.29881	-0.482159	0.479686
3	6	0	0.27853	-0.202638	-0.6013
4	6	0	-0.776138	0.854462	-0.248167
5	6	0	-0.375527	2.247338	-0.728874
6	6	0	0.812185	2.846931	0.043671
7	6	0	2.038733	1.959923	0.14739

8	6	0	3.216793	0.255459	1.729079
9	6	0	3.717401	-0.847058	0.786073
10	6	0	2.481887	-1.404807	0.049074
11	8	0	-0.447291	-1.434475	-0.865222
12	8	0	2.246299	-2.73406	0.533342
13	6	0	2.729238	-1.46655	-1.456114
14	6	0	-2.063748	0.291723	-0.87512
15	6	0	3.146654	2.235719	-0.540682
16	6	0	-1.758664	-1.212426	-1.011011
17	8	0	-2.540574	-2.080788	-1.278596
18	6	0	-3.325908	0.528145	-0.066733
19	6	0	-3.33246	-0.150171	1.287717
20	8	0	-2.344743	0.798889	-2.172005
21	6	0	-4.488258	0.178129	2.19029
22	8	0	-2.448514	-0.913325	1.614292
23	1	0	1.249444	1.130885	1.914641
24	1	0	0.773327	-1.014657	1.280305
25	1	0	0.769115	0.07269	-1.539225
26	1	0	-0.911007	0.863682	0.836736
27	1	0	-1.230132	2.923262	-0.636852
28	1	0	-0.115884	2.206861	-1.791511
29	1	0	0.478587	3.08628	1.0598
30	1	0	1.088373	3.788524	-0.435358
31	1	0	3.95311	1.04393	1.891995
32	1	0	2.976048	-0.177536	2.703294
33	1	0	4.222552	-1.654731	1.317664
34	1	0	4.425786	-0.447667	0.057868
35	1	0	1.429856	-3.051656	0.12977
36	1	0	3.609274	-2.086203	-1.640658
37	1	0	1.879214	-1.9053	-1.98542
38	1	0	2.919579	-0.468959	-1.860703
39	1	0	4.045505	1.63549	-0.456595
40	1	0	3.189445	3.090766	-1.207346
41	1	0	-3.487909	1.603507	0.059071
42	1	0	-4.184166	0.148742	-0.632238
43	1	0	-1.563488	0.738324	-2.733218
44	1	0	-4.394048	1.217763	2.51631
45	1	0	-5.431696	0.092913	1.647607
46	1	0	-4.487191	-0.478404	3.057757
5C					
1	6	0	1.990095	-1.191849	-0.932876
2	6	0	1.660746	0.287951	-0.614552
3	6	0	0.455316	0.491683	0.277141

4	6	0	-0.805383	-0.30076	-0.090531
5	6	0	-0.850498	-1.647525	0.633505
6	6	0	0.223005	-2.656143	0.189901
7	6	0	1.65061	-2.148209	0.196131
8	6	0	3.46566	-1.112648	-1.361082
9	6	0	4.10479	-0.013288	-0.502018
10	6	0	2.974876	0.957329	-0.100029
11	8	0	0.087319	1.896821	0.18076
12	8	0	3.184915	2.18912	-0.803825
13	6	0	3.006927	1.237174	1.400208
14	6	0	-1.933401	0.683252	0.28922
15	6	0	2.527767	-2.560372	1.111229
16	6	0	-1.23757	2.049655	0.146808
17	8	0	-1.77041	3.118557	0.049043
18	6	0	-3.176283	0.647926	-0.595715
19	6	0	-4.097838	-0.534445	-0.370268
20	8	0	-2.259659	0.63049	1.668545
21	6	0	-5.022836	-0.881184	-1.499027
22	8	0	-4.100052	-1.150699	0.677802
23	1	0	1.381756	-1.50114	-1.787543
24	1	0	1.433445	0.773063	-1.570269
25	1	0	0.696168	0.30522	1.326416
26	1	0	-0.833163	-0.445411	-1.177444
27	1	0	-1.827823	-2.110982	0.485764
28	1	0	-0.743883	-1.461791	1.706229
29	1	0	-0.01328	-2.991807	-0.826295
30	1	0	0.148802	-3.529396	0.841567
31	1	0	3.974285	-2.073752	-1.271543
32	1	0	3.496593	-0.81979	-2.413646
33	1	0	4.885287	0.533085	-1.033553
34	1	0	4.55968	-0.433732	0.396794
35	1	0	2.435859	2.765999	-0.612771
36	1	0	3.987283	1.643027	1.65858
37	1	0	2.244084	1.964681	1.690266
38	1	0	2.852674	0.317915	1.971297
39	1	0	3.561426	-2.233511	1.111175
40	1	0	2.234044	-3.256939	1.889651
41	1	0	-3.774558	1.544599	-0.388878
42	1	0	-2.897879	0.700584	-1.651107
43	1	0	-2.855928	-0.125642	1.780652
44	1	0	-5.780054	-1.588132	-1.167284
45	1	0	-5.48634	0.022862	-1.899409
46	1	0	-4.431289	-1.324603	-2.305516

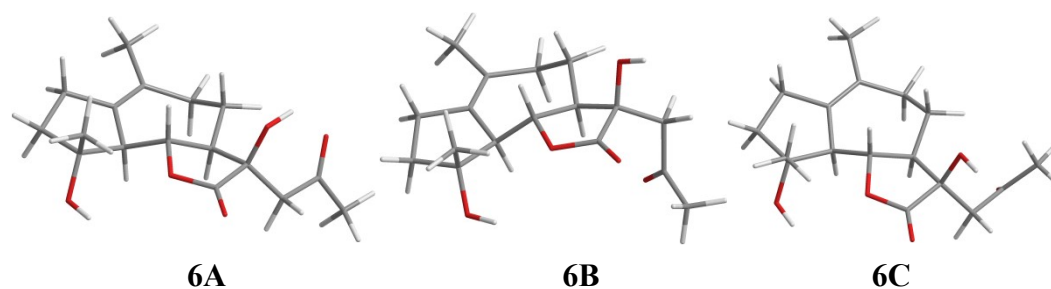


Figure S112. Conformers of isomer **6**

Table S7. Important thermodynamic parameters and Boltzmann distributions of the optimized isomer **6** at B3LYP/6-31G (d, p) level in gas phase.

Conformations	Energy (a.u)	$\Delta G(\text{kcal/mol})$	%	Number of imaginary frequencies
6A	-1037.938653	0.00	25.8	0
6B	-1037.939631	-0.61	72.8	0
6C	-1037.935918	1.72	1.4	0

Table S8. Optimized Z-matrixes of isomer **6** in the gas phase (\AA) at B3LYP/6-31G (d) level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
6A					
1	6	0	-2.335838	1.136603	-0.158632
2	6	0	-1.723039	-0.218588	-0.496477
3	6	0	-0.43187	-0.510525	0.232576
4	6	0	0.803105	0.255488	-0.223559
5	6	0	0.824182	1.695411	0.262442
6	6	0	-0.244785	2.556811	-0.421915
7	6	0	-1.705519	2.314346	-0.07716
8	6	0	-3.843936	0.948977	-0.003227
9	6	0	-4.10551	-0.451758	-0.564323
10	6	0	-2.854302	-1.238353	-0.183814
11	8	0	-0.072278	-1.909522	0.00571
12	8	0	-2.766577	-2.396219	-1.005451
13	6	0	-2.896508	-1.647465	1.289578
14	6	0	1.923993	-0.683732	0.252296
15	6	0	-2.451044	3.577856	0.275119
16	6	0	1.258766	-2.054349	0.01822
17	8	0	1.802398	-3.112591	-0.117226
18	6	0	3.246421	-0.604262	-0.50142
19	6	0	4.132901	0.571025	-0.138996
20	8	0	2.101659	-0.635274	1.659366
21	6	0	5.202968	0.922072	-1.13023

22	8	0	3.99637	1.180494	0.904105
23	1	0	-1.534823	-0.286406	-1.577523
24	1	0	-0.564539	-0.391147	1.3117
25	1	0	0.817016	0.243397	-1.321706
26	1	0	1.798365	2.136052	0.041111
27	1	0	0.695988	1.724415	1.349124
28	1	0	-0.124484	2.454287	-1.50845
29	1	0	-0.020251	3.601833	-0.196469
30	1	0	-4.406686	1.713417	-0.539958
31	1	0	-4.142385	1.007928	1.048662
32	1	0	-5.016673	-0.915253	-0.182486
33	1	0	-4.165143	-0.416004	-1.656128
34	1	0	-1.932965	-2.835029	-0.798524
35	1	0	-2.026079	-2.250646	1.556177
36	1	0	-2.92131	-0.774686	1.946897
37	1	0	-3.794733	-2.241635	1.468387
38	1	0	-2.419667	4.283811	-0.561923
39	1	0	-3.491904	3.402917	0.5407
40	1	0	-1.961195	4.072308	1.119708
41	1	0	3.830736	-1.506474	-0.279195
42	1	0	3.074906	-0.61008	-1.580968
43	1	0	2.662777	0.135139	1.836544
44	1	0	4.727511	1.384085	-2.000595
45	1	0	5.915563	1.616229	-0.69024
46	1	0	5.707488	0.019094	-1.479749
6B					
1	6	0	-2.423299	0.78289	-0.291886
2	6	0	-1.44183	-0.373621	-0.458473
3	6	0	-0.285134	-0.344976	0.511137
4	6	0	0.761755	0.732391	0.26454
5	6	0	0.336607	2.101233	0.764418
6	6	0	-0.761807	2.713799	-0.11167
7	6	0	-2.145212	2.07887	-0.098396
8	6	0	-3.836738	0.223047	-0.457777
9	6	0	-3.623489	-1.194609	-0.996918
10	6	0	-2.3238	-1.646273	-0.337726
11	8	0	0.460783	-1.597032	0.406399
12	8	0	-1.783189	-2.736703	-1.074407
13	6	0	-2.563134	-2.066161	1.113307
14	6	0	2.002353	0.113945	0.906377
15	6	0	-3.250862	3.096266	0.048282
16	6	0	1.75705	-1.387843	0.677211
17	8	0	2.5548	-2.275381	0.790953

18	6	0	3.343048	0.574927	0.361741
19	6	0	3.580047	0.250144	-1.100953
20	8	0	1.920297	0.336178	2.308751
21	6	0	4.797467	0.87049	-1.727442
22	8	0	2.826934	-0.470601	-1.718819
23	1	0	-1.035969	-0.375367	-1.480346
24	1	0	-0.649368	-0.284873	1.541004
25	1	0	0.944294	0.778719	-0.813501
26	1	0	1.200872	2.772032	0.746311
27	1	0	0.002861	2.034533	1.803059
28	1	0	-0.404678	2.735392	-1.14979
29	1	0	-0.877224	3.759506	0.182902
30	1	0	-4.437516	0.828645	-1.137169
31	1	0	-4.363316	0.198024	0.501933
32	1	0	-4.451766	-1.873257	-0.786357
33	1	0	-3.463278	-1.167765	-2.078739
34	1	0	-0.922293	-2.945385	-0.692515
35	1	0	-1.642234	-2.431245	1.573346
36	1	0	-2.938222	-1.233591	1.71397
37	1	0	-3.301265	-2.870212	1.135027
38	1	0	-3.207766	3.823221	-0.770088
39	1	0	-4.245136	2.654454	0.06502
40	1	0	-3.112174	3.661056	0.975402
41	1	0	3.458313	1.651142	0.52342
42	1	0	4.152133	0.092609	0.924851
43	1	0	2.644049	-0.128721	2.745231
44	1	0	5.666269	0.749453	-1.077722
45	1	0	4.985889	0.428501	-2.703554
46	1	0	4.622393	1.944318	-1.839325
6C					
1	6	0	-2.335838	1.136603	-0.158632
2	6	0	-1.723039	-0.218588	-0.496477
3	6	0	-0.43187	-0.510525	0.232576
4	6	0	0.803105	0.255488	-0.223559
5	6	0	0.824182	1.695411	0.262442
6	6	0	-0.244785	2.556811	-0.421915
7	6	0	-1.705519	2.314346	-0.07716
8	6	0	-3.843936	0.948977	-0.003227
9	6	0	-4.10551	-0.451758	-0.564323
10	6	0	-2.854302	-1.238353	-0.183814
11	8	0	-0.072278	-1.909522	0.00571
12	8	0	-2.766577	-2.396219	-1.005451
13	6	0	-2.896508	-1.647465	1.289578

14	6	0	1.923993	-0.683732	0.252296
15	6	0	-2.451044	3.577856	0.275119
16	6	0	1.258766	-2.054349	0.01822
17	8	0	1.802398	-3.112591	-0.117226
18	6	0	3.246421	-0.604262	-0.50142
19	6	0	4.132901	0.571025	-0.138996
20	8	0	2.101659	-0.635274	1.659366
21	6	0	5.202968	0.922072	-1.13023
22	8	0	3.99637	1.180494	0.904105
23	1	0	-1.534823	-0.286406	-1.577523
24	1	0	-0.564539	-0.391147	1.3117
25	1	0	0.817016	0.243397	-1.321706
26	1	0	1.798365	2.136052	0.041111
27	1	0	0.695988	1.724415	1.349124
28	1	0	-0.124484	2.454287	-1.50845
29	1	0	-0.020251	3.601833	-0.196469
30	1	0	-4.406686	1.713417	-0.539958
31	1	0	-4.142385	1.007928	1.048662
32	1	0	-5.016673	-0.915253	-0.182486
33	1	0	-4.165143	-0.416004	-1.656128
34	1	0	-1.932965	-2.835029	-0.798524
35	1	0	-2.026079	-2.250646	1.556177
36	1	0	-2.92131	-0.774686	1.946897
37	1	0	-3.794733	-2.241635	1.468387
38	1	0	-2.419667	4.283811	-0.561923
39	1	0	-3.491904	3.402917	0.5407
40	1	0	-1.961195	4.072308	1.119708
41	1	0	3.830736	-1.506474	-0.279195
42	1	0	3.074906	-0.61008	-1.580968
43	1	0	2.662777	0.135139	1.836544
44	1	0	4.727511	1.384085	-2.000595
45	1	0	5.915563	1.616229	-0.69024
46	1	0	5.707488	0.019094	-1.479749

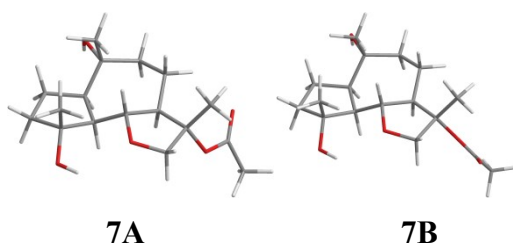


Figure S113. Conformers of isomer 7

Table S9. Important thermodynamic parameters and Boltzmann distributions of the optimized isomer **7** at B3LYP/6-31G (d, p) level in gas phase.

Conformations	Energy (a.u)	$\Delta G(\text{kcal/mol})$	%	Number of imaginary frequencies
7A	-1040.302256	0.00	30.9	0
7B	-1040.303017	-0.48	69.1	0

Table S10. Optimized Z-matrixes of isomer **7** in the gas phase (\AA) at B3LYP/6-31G (d) level.

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			X	Y	Z
7A					
1	6	0	-1.987903	0.672947	-0.849393
2	6	0	-1.223103	-0.652824	-0.530174
3	6	0	-0.126539	-0.626828	0.510767
4	6	0	1.023352	0.346356	0.226871
5	6	0	0.746755	1.755411	0.735908
6	6	0	-0.350716	2.484162	-0.0455
7	6	0	-1.791547	1.939315	0.022473
8	6	0	-3.472047	0.244454	-0.993975
9	6	0	-3.431499	-1.27125	-1.199308
10	6	0	-2.304342	-1.732718	-0.278611
11	8	0	-1.849311	-3.019346	-0.695469
12	6	0	-2.761432	-1.812446	1.177088
13	6	0	-2.271307	1.837718	1.466864
14	8	0	-2.645939	2.950293	-0.545809
15	8	0	0.490323	-1.918172	0.537097
16	6	0	1.674168	-1.728631	1.292103
17	6	0	2.260352	-0.385692	0.829904
18	6	0	3.003972	0.312217	1.956764
19	8	0	3.20024	-0.748224	-0.222369
20	8	0	3.528897	1.385129	-0.84443
21	6	0	3.76559	0.20779	-0.969573
22	6	0	4.713213	-0.381736	-1.974515
23	1	0	-1.641552	0.986639	-1.84095
24	1	0	-0.729644	-0.96506	-1.4579
25	1	0	-0.520837	-0.433351	1.517131
26	1	0	1.164957	0.384273	-0.857923
27	1	0	1.662021	2.343761	0.647183
28	1	0	0.489236	1.725177	1.800183
29	1	0	-0.056496	2.539144	-1.10186
30	1	0	-0.402149	3.513403	0.3214
31	1	0	-4.03252	0.483937	-0.088188

32	1	0	-3.962707	0.765326	-1.815653
33	1	0	-3.146262	-1.511652	-2.228257
34	1	0	-4.380188	-1.766021	-0.980478
35	1	0	-1.008701	-3.17364	-0.244537
36	1	0	-3.589357	-2.520462	1.253139
37	1	0	-1.948794	-2.164679	1.817502
38	1	0	-3.098665	-0.843839	1.552017
39	1	0	-1.758125	1.059731	2.028252
40	1	0	-2.086104	2.791933	1.966193
41	1	0	-3.343674	1.64378	1.505591
42	1	0	-2.36838	3.105821	-1.455632
43	1	0	1.427761	-1.671237	2.359458
44	1	0	2.354967	-2.559382	1.114933
45	1	0	3.466611	1.23791	1.619213
46	1	0	2.312852	0.541654	2.7696
47	1	0	3.778603	-0.353511	2.344708
48	1	0	5.493506	-0.940184	-1.455958
49	1	0	4.173988	-1.079071	-2.616954
50	1	0	5.154171	0.412688	-2.570536
7B					
1	6	0	-2.278332	0.581275	-0.797579
2	6	0	-1.359973	-0.662462	-0.555826
3	6	0	-0.158038	-0.523253	0.358755
4	6	0	0.846312	0.534544	-0.076135
5	6	0	0.517217	1.937443	0.413321
6	6	0	-0.717658	2.549678	-0.253205
7	6	0	-2.086327	1.889836	0.010166
8	6	0	-3.723519	0.021877	-0.739075
9	6	0	-3.570887	-1.485802	-0.948256
10	6	0	-2.301426	-1.831854	-0.173907
11	8	0	-1.783411	-3.077095	-0.639484
12	6	0	-2.566993	-1.931982	1.327955
13	6	0	-2.372404	1.797369	1.505609
14	8	0	-3.088329	2.805763	-0.470303
15	8	0	0.561358	-1.775605	0.34853
16	6	0	1.951658	-1.55332	0.109183
17	6	0	2.178484	-0.062497	0.403913
18	6	0	2.482204	0.20496	1.870282
19	8	0	3.198961	0.529575	-0.429737
20	8	0	4.717696	-1.023777	0.131884
21	6	0	4.423956	-0.014918	-0.460623
22	6	0	5.353939	0.791236	-1.319192
23	1	0	-2.093404	0.888925	-1.833441

24	1	0	-0.946165	-0.946028	-1.5305
25	1	0	-0.461866	-0.344431	1.394523
26	1	0	0.895433	0.537089	-1.173028
27	1	0	1.371103	2.588991	0.204078
28	1	0	0.387502	1.931923	1.500133
29	1	0	-0.559828	2.586245	-1.338704
30	1	0	-0.811471	3.58474	0.087673
31	1	0	-4.176239	0.219319	0.234666
32	1	0	-4.365534	0.48691	-1.486561
33	1	0	-3.393396	-1.709799	-2.004776
34	1	0	-4.436117	-2.062499	-0.61427
35	1	0	-0.869296	-3.122321	-0.327492
36	1	0	-3.321563	-2.700636	1.507878
37	1	0	-1.655729	-2.214037	1.861173
38	1	0	-2.928426	-0.987975	1.742222
39	1	0	-1.728982	1.082321	2.014381
40	1	0	-2.208961	2.779103	1.95699
41	1	0	-3.410859	1.516826	1.683687
42	1	0	-2.939931	2.950526	-1.411649
43	1	0	2.524482	-2.211348	0.759361
44	1	0	2.195857	-1.768963	-0.936973
45	1	0	2.607319	1.273977	2.048298
46	1	0	1.657848	-0.157113	2.489555
47	1	0	3.39097	-0.316683	2.169438
48	1	0	6.31092	0.282793	-1.398344
49	1	0	4.915509	0.932141	-2.307297
50	1	0	5.491344	1.776333	-0.870462

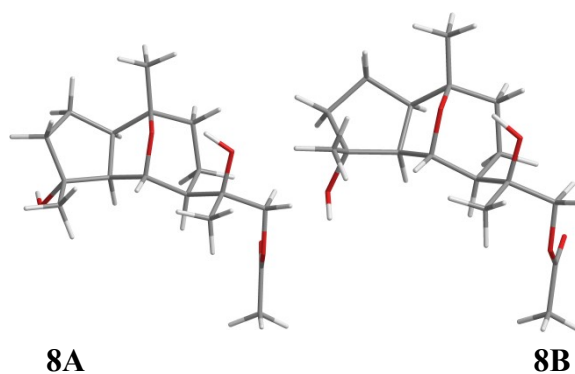


Figure S114. Conformers of isomer **8**

Table S11. Important thermodynamic parameters and Boltzmann distributions of the optimized isomer **8** at B3LYP/6-31G (d, p) level in gas phase.

Conformations	Energy (a.u)	ΔG (kcal/mol)	%	Number of imaginary frequencies
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8A	-1040.293872	0.00	77.5	0
8B	-1040.292702	0.73	22.5	0

Table S12. Optimized Z-matrixes of isomer **8** in the gas phase (Å) at B3LYP/6-31G (d) level.

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
8A					
1	6	0	2.247546	-0.306329	-1.110003
2	6	0	1.505078	0.861084	-0.378682
3	6	0	0.558751	0.134281	0.592012
4	6	0	-0.830537	-0.133022	-0.008564
5	6	0	-0.647066	-0.905876	-1.332086
6	6	0	0.401182	-2.024753	-1.231984
7	6	0	1.642549	-1.577705	-0.448183
8	6	0	3.749899	-0.064269	-0.858195
9	6	0	3.789735	0.742176	0.440117
10	6	0	2.620183	1.720901	0.279508
11	8	0	2.979291	2.772007	-0.624894
12	6	0	2.245007	2.437473	1.563917
13	6	0	-1.770298	-0.827574	1.012596
14	6	0	2.5949	-2.732579	-0.21383
15	6	0	-3.201636	-0.934294	0.476127
16	1	0	-1.279024	0.842123	-0.232935
17	1	0	0.934902	1.505478	-1.051692
18	6	0	-1.802611	-0.091571	2.357013
19	8	0	-1.409226	-2.186656	1.225151
20	1	0	2.033385	-0.33261	-2.180216
21	8	0	1.203178	-1.118484	0.848515
22	8	0	-3.815424	0.357411	0.384166
23	8	0	-3.491878	0.43844	-1.840216
24	6	0	-3.907785	0.933798	-0.828059
25	6	0	-4.59466	2.267555	-0.730417
26	1	0	0.473964	0.654626	1.542542
27	1	0	-0.339478	-0.186596	-2.097149
28	1	0	-1.594652	-1.309526	-1.685005
29	1	0	-0.029032	-2.894188	-0.730676
30	1	0	0.70533	-2.341711	-2.234445
31	1	0	4.171463	0.524484	-1.679946
32	1	0	4.333995	-0.983226	-0.819605
33	1	0	3.590187	0.083688	1.291236
34	1	0	4.729085	1.271514	0.610119
35	1	0	3.189192	2.391803	-1.482339

36	1	0	1.332343	3.023006	1.428031
37	1	0	2.104106	1.735797	2.386855
38	1	0	3.051968	3.122777	1.829043
39	1	0	3.042707	-3.057413	-1.156095
40	1	0	3.388556	-2.447904	0.478451
41	1	0	2.051647	-3.575709	0.217618
42	1	0	-3.791101	-1.500054	1.197488
43	1	0	-3.234065	-1.433769	-0.489519
44	1	0	-2.606491	-0.498883	2.972992
45	1	0	-0.866265	-0.239445	2.897558
46	1	0	-1.97402	0.97949	2.227318
47	1	0	-0.461428	-2.196606	1.414731
48	1	0	-4.038938	2.915469	-0.050998
49	1	0	-4.653218	2.71697	-1.717949
50	1	0	-5.594056	2.132888	-0.314906
8B					
1	6	0	2.282509	-0.330039	-1.067419
2	6	0	1.518203	0.83681	-0.373501
3	6	0	0.567151	0.112403	0.593434
4	6	0	-0.82446	-0.136131	-0.008011
5	6	0	-0.642097	-0.87774	-1.349482
6	6	0	0.396942	-2.006388	-1.273643
7	6	0	1.639809	-1.601151	-0.469777
8	6	0	3.769326	-0.077262	-0.755174
9	6	0	3.841028	1.439299	-0.60149
10	6	0	2.606058	1.768926	0.242189
11	8	0	2.298692	3.144311	0.034751
12	6	0	2.871408	1.522805	1.727083
13	6	0	-1.766651	-0.849772	0.997187
14	6	0	2.567005	-2.784167	-0.272827
15	6	0	-3.198523	-0.939522	0.459361
16	1	0	-1.269047	0.84573	-0.211441
17	1	0	0.960405	1.44207	-1.090903
18	6	0	-1.795329	-0.143476	2.357625
19	8	0	-1.410611	-2.214075	1.18069
20	1	0	2.13019	-0.308742	-2.149518
21	8	0	1.201415	-1.154524	0.83465
22	8	0	-3.808535	0.355954	0.396881
23	8	0	-3.490413	0.483488	-1.826156
24	6	0	-3.90368	0.957496	-0.80298
25	6	0	-4.591921	2.288254	-0.676334
26	1	0	0.491132	0.616305	1.554992
27	1	0	-0.325716	-0.143302	-2.096127

28	1	0	-1.591459	-1.26577	-1.715138
29	1	0	-0.045425	-2.886797	-0.802899
30	1	0	0.705293	-2.296228	-2.282898
31	1	0	4.431829	-0.467204	-1.529374
32	1	0	4.051634	-0.550925	0.188112
33	1	0	4.76311	1.80265	-0.144019
34	1	0	3.722646	1.93084	-1.572159
35	1	0	1.62804	3.411677	0.669159
36	1	0	2.03996	1.88326	2.340285
37	1	0	2.999489	0.460476	1.943979
38	1	0	3.768157	2.066731	2.029533
39	1	0	2.99756	-3.085886	-1.23083
40	1	0	3.376237	-2.545185	0.416702
41	1	0	2.009698	-3.6304	0.134292
42	1	0	-3.789621	-1.519795	1.167771
43	1	0	-3.232382	-1.416673	-0.517459
44	1	0	-0.856776	-0.302308	2.891242
45	1	0	-1.969735	0.929848	2.251848
46	1	0	-2.596615	-0.565417	2.967125
47	1	0	-0.461692	-2.231504	1.365183
48	1	0	-4.638752	2.764981	-1.651615
49	1	0	-5.596733	2.140953	-0.278321
50	1	0	-4.0465	2.917317	0.028513

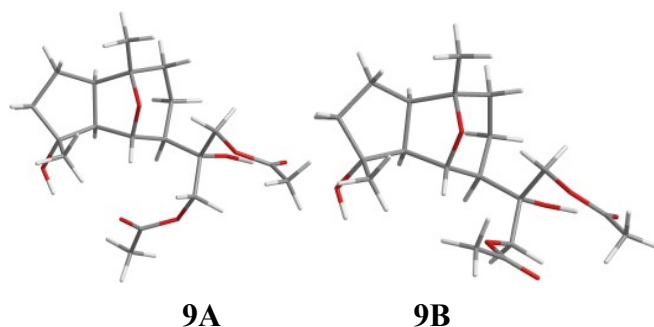


Figure S115. Conformers of isomer **9**

Table S13. Important thermodynamic parameters and Boltzmann distributions of the optimized isomer **9** at B3LYP/6-31G (d, p) level in gas phase.

Conformations	Energy (a.u)	ΔG (kcal/mol)	%	Number of imaginary frequencies
9A	-1268.136967	0.00	19.8	0
9B	-1268.138285	-0.83	80.2	0

Table S14. Optimized Z-matrixes of isomer **9** in the gas phase (\AA) at B3LYP/6-31G (d) level.

Center	Atomic	Atomic	Coordinates(Angstroms)
--------	--------	--------	------------------------

Number	Number	Type	X	Y	Z
9A					
1	6	0	3.122668	1.074939	0.302355
2	6	0	2.60961	0.063529	0.76586
3	6	0	1.127612	0.12991	0.390027
4	6	0	0.234029	0.823929	1.195417
5	6	0	0.684038	2.277938	0.938252
6	6	0	1.068052	2.547817	0.525156
7	6	0	1.865116	1.389396	1.143712
8	6	0	4.281654	0.351976	1.015135
9	6	0	4.816821	0.59365	0.057294
10	6	0	3.545198	1.178294	0.679278
11	8	0	3.882321	1.674598	1.976802
12	6	0	2.990055	2.322235	0.167853
13	6	0	1.291216	0.608514	1.051094
14	6	0	2.100757	1.635137	2.621285
15	6	0	1.692599	0.857578	1.281698
16	6	0	1.820256	1.091492	0.30947
17	8	0	1.845925	1.352206	2.131985
18	8	0	1.076936	0.189647	1.005316
19	8	0	1.438973	1.63601	0.106423
20	8	0	3.532572	2.457654	0.083467
21	6	0	2.450062	2.337932	0.433087
22	6	0	2.048068	2.917254	1.755726
23	8	0	3.061244	0.475683	0.721077
24	8	0	4.2521	1.617325	0.790586
25	6	0	4.20504	0.853678	0.150253
26	6	0	5.39066	0.215783	0.803548
27	1	0	3.498545	1.986881	0.1679
28	1	0	2.707206	0.459956	1.77852
29	1	0	0.794126	1.159773	0.494827
30	1	0	0.413145	0.599435	2.253008
31	1	0	1.554638	2.476595	1.569441
32	1	0	0.092785	2.971327	1.266209
33	1	0	0.177829	2.704504	1.140221
34	1	0	1.660111	3.465437	0.587486
35	1	0	5.033665	1.043933	1.396591
36	1	0	3.912904	0.233616	1.860341
37	1	0	5.486451	1.367714	0.323211
38	1	0	5.344406	0.027817	0.832042
39	1	0	3.107574	2.107618	2.350447
40	1	0	2.156429	2.816065	0.338657
41	1	0	2.626659	1.965067	1.133146

42	1	0	3.773328	3.065016	0.331624
43	1	0	2.777011	2.482774	2.755932
44	1	0	2.535143	0.760791	3.105797
45	1	0	1.154867	1.867476	3.115632
46	1	0	1.112231	1.279702	2.104622
47	1	0	2.751279	0.911667	1.53321
48	1	0	1.947964	2.176193	0.291785
49	1	0	1.124712	0.806376	1.092856
50	1	0	2.761418	1.573451	1.90535
51	1	0	1.06339	3.378364	1.684467
52	1	0	2.789602	3.640597	2.083919
53	1	0	1.985599	2.099932	2.478228
54	1	0	6.301453	0.539613	0.307762
55	1	0	5.414729	0.489918	1.858919
56	1	0	5.282677	0.86816	0.737311
9B					
1	6	0	-2.526179	-1.514811	0.729202
2	6	0	-2.184029	-0.03794	0.381115
3	6	0	-0.793583	-0.13475	-0.256393
4	6	0	0.28496	0.117247	0.806347
5	6	0	0.193171	-0.979708	1.894196
6	6	0	-0.207709	-2.370339	1.378587
7	6	0	-1.270574	-2.301932	0.273586
8	6	0	-3.856181	-1.79001	-0.003841
9	6	0	-4.50291	-0.405541	-0.101664
10	6	0	-3.335378	0.498081	-0.509628
11	8	0	-3.647177	1.852904	-0.182218
12	6	0	-3.059881	0.405208	-2.010997
13	6	0	1.686587	0.388829	0.220601
14	6	0	-1.533286	-3.680244	-0.301352
15	6	0	1.690861	1.682088	-0.609645
16	6	0	2.165644	-0.757839	-0.673209
17	8	0	2.612648	0.623306	1.276549
18	8	0	-0.721446	-1.470594	-0.76435
19	8	0	1.313937	2.815091	0.188061
20	8	0	-0.791456	2.825439	-0.599692
21	6	0	0.064807	3.289269	0.119576
22	6	0	-0.13006	4.441895	1.057443
23	8	0	3.496293	-0.516711	-1.160424
24	8	0	4.38333	-1.534977	0.630544
25	6	0	4.523395	-0.976777	-0.432974
26	6	0	5.834485	-0.709492	-1.106279
27	1	0	-2.673933	-1.640482	1.80463

28	1	0	-2.160778	0.590941	1.273603
29	1	0	-0.675556	0.529053	-1.106713
30	1	0	0.027179	1.053558	1.308833
31	1	0	-0.562545	-0.651926	2.613691
32	1	0	1.125889	-1.041335	2.458792
33	1	0	0.656853	-2.894054	0.959865
34	1	0	-0.575371	-2.97654	2.211619
35	1	0	-4.477165	-2.518669	0.519001
36	1	0	-3.675679	-2.174353	-1.010005
37	1	0	-5.337626	-0.356338	-0.80427
38	1	0	-4.857423	-0.082749	0.882687
39	1	0	-2.853028	2.378614	-0.355151
40	1	0	-2.30549	1.138677	-2.306362
41	1	0	-2.699579	-0.58431	-2.2981
42	1	0	-3.978468	0.624337	-2.559427
43	1	0	-2.036356	-4.304615	0.440998
44	1	0	-2.158074	-3.62572	-1.192876
45	1	0	-0.589771	-4.159066	-0.571866
46	1	0	2.709606	1.884614	-0.934433
47	1	0	1.03669	1.609649	-1.4771
48	1	0	2.145956	-1.701569	-0.128279
49	1	0	1.537672	-0.848592	-1.556667
50	1	0	3.010142	-0.215093	1.541518
51	1	0	0.652711	5.184095	0.902102
52	1	0	-1.111169	4.881241	0.899781
53	1	0	-0.046855	4.07687	2.083143
54	1	0	6.645344	-1.097635	-0.496402
55	1	0	5.84133	-1.17951	-2.090278
56	1	0	5.951623	0.365854	-1.248131

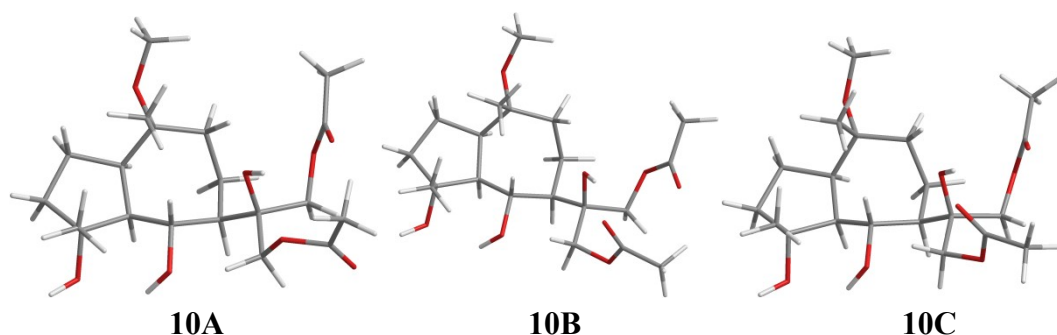


Figure S116. Conformers of isomer **10**

Table S15. Important thermodynamic parameters and Boltzmann distributions of the optimized isomer **10** at B3LYP/6-31G (d, p) level in gas phase.

Conformations	Energy (a.u)	ΔG (kcal/mol)	%	Number of imaginary frequencies
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10A	-1383.789542	0.00	72.2	0
10B	-1383.787995	0.97	14.0	0
10C	-1383.787977	0.98	13.8	0

Table S16. Optimized Z-matrixes of isomer **10** in the gas phase (Å) at B3LYP/6-31G (d) level.

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
10A					
1	6	0	-2.965436	0.479836	-0.459435
2	6	0	-2.412136	-0.982932	-0.621471
3	6	0	-4.341659	0.329803	0.23477
4	6	0	-4.732465	-1.127236	0.00133
5	6	0	-3.411643	-1.875961	0.16397
6	6	0	-0.946061	-1.326483	-0.317517
7	6	0	0.099433	-0.546727	-1.142933
8	6	0	-0.410755	0.785773	-1.71013
9	6	0	-0.85063	1.87996	-0.733217
10	6	0	-2.081293	1.579839	0.163643
11	6	0	1.449511	-0.431501	-0.398571
12	1	0	0.299243	-1.181717	-2.014007
13	6	0	2.009337	-1.823739	-0.072238
14	6	0	2.503505	0.303401	-1.264695
15	8	0	1.23006	0.26442	0.817672
16	1	0	-3.165898	0.845996	-1.470327
17	6	0	-3.050511	-2.067517	1.635762
18	1	0	-2.564843	-1.258332	-1.672622
19	8	0	-0.726399	-2.716781	-0.60434
20	8	0	-3.436272	-3.161083	-0.481896
21	6	0	-1.673575	1.329471	1.616137
22	8	0	2.403082	1.723541	-1.134433
23	8	0	3.773464	1.661885	0.642554
24	6	0	3.06456	2.285202	-0.112368
25	6	0	2.797045	3.758042	-0.035192
26	8	0	3.114202	-1.653803	0.833653
27	8	0	4.628342	-2.302062	-0.693932
28	6	0	4.36766	-1.892183	0.409164
29	6	0	5.365014	-1.54863	1.473721
30	8	0	-2.968226	2.721831	0.11984
31	6	0	-2.487089	3.917259	0.699356
32	1	0	-5.068241	1.031897	-0.171009
33	1	0	-4.267136	0.53326	1.304725

34	1	0	-5.07972	-1.271684	-1.026463
35	1	0	-5.505607	-1.490947	0.682422
36	1	0	-0.742688	-1.171888	0.744418
37	1	0	0.3675	1.213033	-2.345751
38	1	0	-1.235859	0.553955	-2.388812
39	1	0	-0.000424	2.173686	-0.116479
40	1	0	-1.122209	2.743828	-1.347907
41	1	0	1.271375	-2.419296	0.458119
42	1	0	2.333371	-2.348927	-0.970855
43	1	0	2.340705	0.084448	-2.31967
44	1	0	3.515406	0.004575	-0.998178
45	1	0	2.050916	0.23064	1.326559
46	1	0	-2.122746	-2.633554	1.741273
47	1	0	-3.849275	-2.619098	2.139775
48	1	0	-2.929292	-1.110219	2.144818
49	1	0	-1.569198	-3.188925	-0.541173
50	1	0	-3.995166	-3.755712	0.030674
51	1	0	-1.062211	2.159523	1.976776
52	1	0	-2.547437	1.24649	2.265329
53	1	0	-1.060133	0.438293	1.71244
54	1	0	2.89981	4.212328	-1.020152
55	1	0	1.766476	3.905174	0.29673
56	1	0	3.478406	4.21898	0.674728
57	1	0	5.356552	-0.464193	1.605616
58	1	0	5.078283	-2.006654	2.419943
59	1	0	6.355117	-1.87879	1.171574
60	1	0	-3.160039	4.712735	0.379527
61	1	0	-2.494092	3.872342	1.79256
62	1	0	-1.473852	4.161095	0.361951
10B					
1	6	0	-2.920612	0.629644	-0.375357
2	6	0	-2.442913	-0.840041	-0.665169
3	6	0	-4.259309	0.487663	0.391057
4	6	0	-4.722786	-0.937016	0.097203
5	6	0	-3.425677	-1.742222	0.12935
6	6	0	-0.975815	-1.249035	-0.47611
7	6	0	0.038333	-0.471842	-1.336357
8	6	0	-0.432821	0.927721	-1.759629
9	6	0	-0.763887	1.963535	-0.680842
10	6	0	-1.955742	1.651783	0.263632
11	6	0	1.446381	-0.475834	-0.687838
12	1	0	0.127302	-1.046734	-2.26543
13	6	0	1.915135	-1.924561	-0.469902

14	6	0	2.470943	0.229547	-1.623434
15	8	0	1.344629	0.21587	0.54769
16	1	0	-3.163276	1.071286	-1.345983
17	6	0	-2.980082	-2.035878	1.56067
18	1	0	-2.673718	-1.04182	-1.718983
19	8	0	-0.819458	-2.633495	-0.824541
20	8	0	-3.541198	-2.983767	-0.588012
21	6	0	-1.479537	1.296659	1.673162
22	8	0	2.56346	1.618315	-1.308258
23	8	0	4.118126	1.140395	0.240645
24	6	0	3.373158	1.932476	-0.285332
25	6	0	3.220882	3.37149	0.105765
26	8	0	3.330352	-2.028106	-0.200915
27	8	0	3.072328	-1.453925	1.949309
28	6	0	3.787205	-1.787701	1.02875
29	6	0	5.271429	-1.954681	1.112673
30	8	0	-2.797345	2.826579	0.341436
31	6	0	-2.239902	3.963299	0.9683
32	1	0	-4.97925	1.239909	0.072686
33	1	0	-4.113809	0.622687	1.464487
34	1	0	-5.139128	-1.004833	-0.912652
35	1	0	-5.466269	-1.312946	0.804238
36	1	0	-0.697605	-1.140559	0.57446
37	1	0	0.330049	1.370328	-2.404128
38	1	0	-1.304555	0.791407	-2.405534
39	1	0	0.133651	2.17764	-0.099339
40	1	0	-1.031614	2.879209	-1.217284
41	1	0	1.355726	-2.390781	0.341168
42	1	0	1.772458	-2.505643	-1.378475
43	1	0	2.141326	0.175241	-2.659787
44	1	0	3.458239	-0.217126	-1.539413
45	1	0	1.909962	-0.215442	1.204154
46	1	0	-2.066668	-2.634042	1.572028
47	1	0	-3.763766	-2.593769	2.081001
48	1	0	-2.795669	-1.116196	2.117615
49	1	0	-1.676306	-3.076825	-0.747586
50	1	0	-4.097125	-3.585107	-0.080028
51	1	0	-0.81576	2.079653	2.04612
52	1	0	-2.318342	1.20707	2.366235
53	1	0	-0.899172	0.378671	1.680783
54	1	0	4.044638	3.669762	0.748897
55	1	0	3.170993	4.004988	-0.778956
56	1	0	2.278188	3.474774	0.649039

57	1	0	5.578601	-1.990047	2.154467
58	1	0	5.589044	-2.850601	0.581673
59	1	0	5.72373	-1.086267	0.627893
60	1	0	-2.8964	4.801868	0.736288
61	1	0	-2.192266	3.847598	2.055291
62	1	0	-1.236656	4.191677	0.592675
10C					
1	6	0	-2.920816	0.629625	-0.375323
2	6	0	-2.443099	-0.840042	-0.665157
3	6	0	-4.259535	0.487655	0.391047
4	6	0	-4.723044	-0.937005	0.097049
5	6	0	-3.425951	-1.742217	0.129218
6	6	0	-0.976026	-1.249052	-0.475855
7	6	0	0.038282	-0.471898	-1.33595
8	6	0	-0.432796	0.927638	-1.759308
9	6	0	-0.764116	1.963544	-0.680656
10	6	0	-1.955979	1.651805	0.26372
11	6	0	1.446273	-0.475944	-0.687298
12	1	0	0.12735	-1.046804	-2.265007
13	6	0	1.914804	-1.924697	-0.468979
14	6	0	2.470949	0.229035	-1.623193
15	8	0	1.344195	0.215939	0.548066
16	1	0	-3.163421	1.071324	-1.345936
17	6	0	-2.98044	-2.035903	1.560587
18	1	0	-2.673771	-1.041761	-1.719015
19	8	0	-0.819606	-2.633482	-0.824314
20	8	0	-3.541425	-2.98375	-0.58815
21	6	0	-1.479846	1.296893	1.673303
22	8	0	2.563912	1.617897	-1.308446
23	8	0	4.117732	1.139681	0.241121
24	6	0	3.373451	1.93206	-0.285478
25	6	0	3.222186	3.371382	0.104835
26	8	0	3.330129	-2.028655	-0.200679
27	8	0	3.073595	-1.452517	1.949206
28	6	0	3.787812	-1.787325	1.028519
29	6	0	5.272041	-1.954509	1.111679
30	8	0	-2.797637	2.826608	0.341349
31	6	0	-2.240105	3.963601	0.967627
32	1	0	-4.979454	1.239914	0.072665
33	1	0	-4.114078	0.62262	1.464488
34	1	0	-5.139338	-1.004657	-0.912837
35	1	0	-5.466579	-1.312988	0.804
36	1	0	-0.698037	-1.140532	0.57477

37	1	0	0.330165	1.370269	-2.403683
38	1	0	-1.304418	0.791266	-2.405354
39	1	0	0.133352	2.177808	-0.099099
40	1	0	-1.03184	2.879125	-1.217267
41	1	0	1.355645	-2.390374	0.342573
42	1	0	1.771532	-2.506115	-1.377237
43	1	0	2.141086	0.174577	-2.65945
44	1	0	3.458156	-0.217857	-1.539309
45	1	0	1.911596	-0.213594	1.203918
46	1	0	-2.067162	-2.634289	1.571969
47	1	0	-3.764253	-2.593559	2.080963
48	1	0	-2.795716	-1.116238	2.117449
49	1	0	-1.676438	-3.076856	-0.747384
50	1	0	-4.097519	-3.585057	-0.080309
51	1	0	-0.816527	2.08026	2.046312
52	1	0	-2.318694	1.206934	2.366275
53	1	0	-0.898955	0.379236	1.68101
54	1	0	3.173862	4.004548	-0.780222
55	1	0	2.279042	3.475857	0.647079
56	1	0	4.045615	3.669137	0.74863
57	1	0	5.579563	-1.991522	2.153319
58	1	0	5.589618	-2.849453	0.579055
59	1	0	5.72408	-1.085139	0.628326
60	1	0	-2.896614	4.802075	0.735297
61	1	0	-2.192361	3.848421	2.054669
62	1	0	-1.236891	4.19178	0.59179

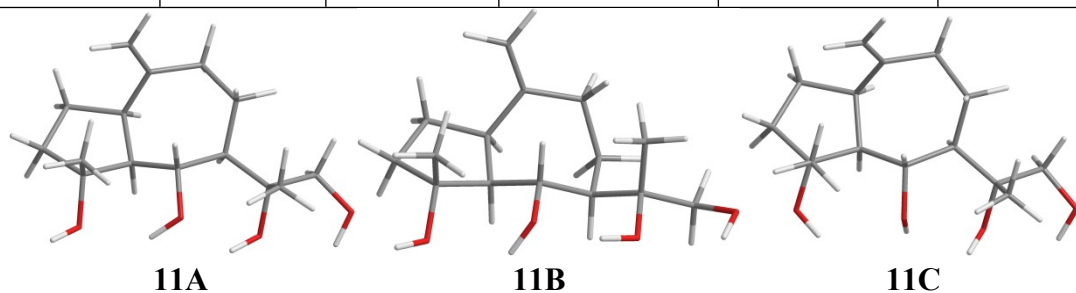


Figure S117. Conformers of isomer **11**

Table S17. Important thermodynamic parameters and Boltzmann distributions of the optimized isomer **11** at B3LYP/6-31G (d, p) level in gas phase.

Conformations	Energy (a.u)	$\Delta G(\text{kcal/mol})$	%	Number of imaginary frequencies
11A	-887.659169	0.00	47.5	0
11B	-887.657074	1.31	5.2	0
11C	-887.659166	0.00	47.3	0

Table S18. Optimized Z-matrixes of isomer **11** in the gas phase (Å) at B3LYP/6-31G (d) level.

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
11A					
1	6	0	-1.875621	1.002094	-0.820345
2	6	0	-1.228477	-0.398492	-0.542598
3	6	0	0.035689	-0.463089	0.32328
4	6	0	1.225111	0.349381	-0.258226
5	6	0	1.163148	1.80962	0.219157
6	6	0	-0.003067	2.649686	-0.315697
7	6	0	-1.369116	2.127865	0.059434
8	6	0	-3.40712	0.761995	-0.80346
9	6	0	-3.576155	-0.75611	-0.852728
10	6	0	-2.399627	-1.265824	-0.021852
11	1	0	-1.590149	1.27902	-1.839239
12	6	0	-2.638579	-1.114505	1.478538
13	1	0	-0.955783	-0.841207	-1.508485
14	6	0	-2.028142	2.661291	1.08732
15	6	0	2.611866	-0.278167	0.060027
16	6	0	2.851037	-0.492156	1.556064
17	6	0	3.749729	0.577351	-0.530206
18	8	0	4.957697	-0.144214	-0.561473
19	8	0	2.752025	-1.508334	-0.648664
20	1	0	1.150895	0.328671	-1.354582
21	8	0	0.400624	-1.841239	0.473597
22	8	0	-2.088837	-2.634607	-0.3226
23	1	0	-0.182403	-0.06815	1.32491
24	1	0	1.130212	1.828155	1.313916
25	1	0	2.077528	2.325874	-0.076922
26	1	0	0.074317	2.707424	-1.407378
27	1	0	0.109639	3.666931	0.066875
28	1	0	-3.856564	1.148143	0.110696
29	1	0	-3.897518	1.270601	-1.633683
30	1	0	-3.454117	-1.133846	-1.871889
31	1	0	-4.54236	-1.098113	-0.472271
32	1	0	-3.558358	-1.632357	1.767896
33	1	0	-1.806774	-1.541704	2.04224
34	1	0	-2.735087	-0.064229	1.76058
35	1	0	-3.006952	2.330487	1.410163
36	1	0	-1.590006	3.478106	1.651
37	1	0	2.144682	-1.214659	1.965729
38	1	0	2.756093	0.447772	2.105712

39	1	0	3.865863	-0.867217	1.698788
40	1	0	3.462085	0.900776	-1.541431
41	1	0	3.935864	1.460053	0.082196
42	1	0	4.731003	-1.026409	-0.879957
43	1	0	2.023719	-2.072878	-0.357499
44	1	0	-0.349035	-2.406845	0.238979
45	1	0	-2.772916	-3.202875	0.044526
11B					
1	6	0	1.78499	1.217256	0.604869
2	6	0	1.360128	0.298907	0.649199
3	6	0	0.028651	0.634539	0.022893
4	6	0	1.209665	0.121451	0.730773
5	6	0	1.016209	1.296256	1.300089
6	6	0	0.471021	2.379121	0.361469
7	6	0	0.8725	2.057579	0.267156
8	6	0	3.294643	1.217298	0.261276
9	6	0	3.750399	0.218987	0.528118
10	6	0	2.563684	1.04923	0.036358
11	1	0	1.682654	1.608538	1.621022
12	6	0	2.52587	1.119456	1.491177
13	1	0	1.313264	0.623002	1.696432
14	6	0	1.175923	2.513252	1.480886
15	6	0	2.501984	0.356973	0.099925
16	6	0	2.38637	0.041749	1.573007
17	6	0	3.704827	0.344084	0.543974
18	8	0	4.916068	0.109365	0.012402
19	8	0	2.85635	1.741614	0.025717
20	1	0	1.325056	0.780526	1.600396
21	8	0	0.131292	2.050105	0.193762
22	8	0	2.547988	2.373561	0.583969
23	1	0	0.050745	0.196943	1.024839
24	1	0	1.952612	1.650899	1.733777
25	1	0	0.334555	1.206327	2.150698
26	1	0	0.34147	3.288856	0.961106
27	1	0	1.193259	2.630134	0.418765
28	1	0	3.469524	1.466648	0.784948
29	1	0	3.83629	1.952828	0.856519
30	1	0	3.871622	0.399394	1.600384
31	1	0	4.686061	0.478586	0.026028
32	1	0	3.468514	1.529619	1.867103
33	1	0	1.705544	1.754446	1.827405
34	1	0	2.389712	0.129374	1.930586
35	1	0	2.136667	2.353763	1.953519

36	1	0	0.450269	3.086853	2.047865
37	1	0	1.968388	1.044635	1.692208
38	1	0	3.379189	0.017652	2.024416
39	1	0	1.74988	0.663563	2.111052
40	1	0	3.683513	0.158669	1.627088
41	1	0	3.660872	1.421903	0.370504
42	1	0	4.850619	1.071397	0.044623
43	1	0	2.053466	2.25869	0.175508
44	1	0	0.629079	2.515353	0.179723
45	1	0	3.248421	2.891954	0.175974
11C					
1	6	0	-1.875158	1.001962	-0.820671
2	6	0	-1.228331	-0.398633	-0.542473
3	6	0	0.035663	-0.463117	0.323625
4	6	0	1.225077	0.349467	-0.257825
5	6	0	1.163065	1.80959	0.220003
6	6	0	-0.002971	2.649766	-0.3151
7	6	0	-1.369115	2.127716	0.059435
8	6	0	-3.406683	0.761925	-0.804612
9	6	0	-3.57579	-0.756172	-0.853453
10	6	0	-2.399697	-1.265672	-0.021804
11	1	0	-1.589028	1.278852	-1.839383
12	6	0	-2.639178	-1.113808	1.478411
13	1	0	-0.955496	-0.841617	-1.508203
14	6	0	-2.028478	2.660876	1.087245
15	6	0	2.611864	-0.278176	0.059991
16	6	0	2.851442	-0.492269	1.555948
17	6	0	3.749575	0.577338	-0.530521
18	8	0	4.957512	-0.144241	-0.562114
19	8	0	2.75176	-1.508275	-0.648846
20	1	0	1.15064	0.329096	-1.35417
21	8	0	0.400692	-1.841225	0.474088
22	8	0	-2.088948	-2.634632	-0.32186
23	1	0	-0.182644	-0.068113	1.325174
24	1	0	1.129733	1.827775	1.31475
25	1	0	2.077576	2.325893	-0.075581
26	1	0	0.074849	2.707707	-1.406729
27	1	0	0.109504	3.666917	0.067765
28	1	0	-3.856606	1.148429	0.109156
29	1	0	-3.896637	1.270264	-1.635269
30	1	0	-3.453127	-1.134244	-1.872412
31	1	0	-4.542231	-1.097997	-0.473455
32	1	0	-3.558979	-1.631728	1.767646

33	1	0	-1.80752	-1.540765	2.042525
34	1	0	-2.73597	-0.063482	1.760135
35	1	0	-3.007317	2.329916	1.409833
36	1	0	-1.590561	3.47763	1.651188
37	1	0	2.145201	-1.214817	1.96572
38	1	0	2.756619	0.447632	2.105679
39	1	0	3.866317	-0.867309	1.698369
40	1	0	3.461661	0.900801	-1.54166
41	1	0	3.935927	1.460026	0.081836
42	1	0	4.730757	-1.026388	-0.880664
43	1	0	2.02336	-2.072719	-0.357709
44	1	0	-0.349127	-2.40685	0.239983
45	1	0	-2.772743	-3.202688	0.046126

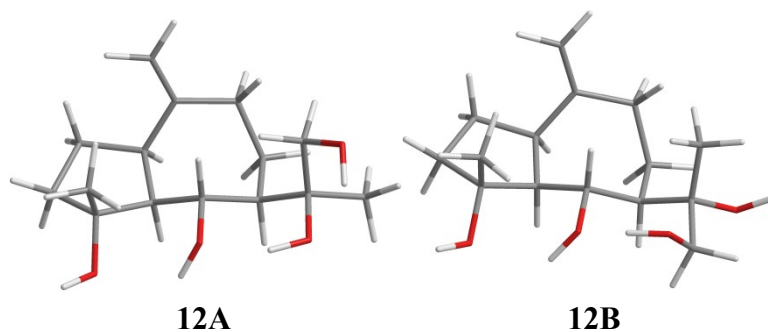


Figure S118. Conformers of isomer **12**

Table S19. Important thermodynamic parameters and Boltzmann distributions of the optimized isomer **12** at B3LYP/6-31G (d, p) level in gas phase.

Conformations	Energy (a.u)	ΔG (kcal/mol)	%	Number of imaginary frequencies
12A	-887.656212	0.00	85.0	0
12B	-887.654577	1.03	15.0	0

Table S20. Optimized Z-matrixes of isomer **12** in the gas phase (\AA) at B3LYP/6-31G (d) level.

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			X	Y	Z
12A					
1	6	0	1.697969	1.26484	0.571604
2	6	0	1.388284	0.275222	0.617047
3	6	0	0.027417	0.729031	0.080927
4	6	0	1.182114	0.292149	0.937832
5	6	0	1.028323	1.100054	1.58523
6	6	0	0.610184	2.291772	0.704689
7	6	0	0.620768	2.053069	0.138516

8	6	0	3.142072	1.390211	0.033986
9	6	0	3.743302	0.000723	0.237465
10	6	0	2.582436	0.930155	0.119738
11	6	0	2.38574	1.026809	1.632797
12	6	0	0.698777	2.513615	1.38533
13	6	0	2.538109	0.50419	0.208231
14	6	0	3.67563	0.665559	1.216926
15	6	0	2.865876	0.629151	0.777603
16	8	0	3.936557	0.268811	1.619604
17	8	0	2.523667	1.678835	0.60867
18	8	0	0.007386	2.163746	0.027348
19	8	0	2.743143	2.244088	0.432314
20	1	0	1.703691	1.617875	1.607533
21	1	0	1.464095	0.617736	1.656825
22	1	0	0.093779	0.363438	0.944358
23	1	0	1.184954	1.004929	1.772283
24	1	0	1.96059	1.361821	2.091594
25	1	0	0.290003	0.998491	2.386325
26	1	0	0.382412	3.120045	1.388136
27	1	0	1.425181	2.636421	0.069499
28	1	0	3.154966	1.64418	1.025911
29	1	0	3.692608	2.174027	0.554842
30	1	0	3.999831	0.165655	1.288278
31	1	0	4.633993	0.18502	0.368778
32	1	0	3.31325	1.361973	2.10755
33	1	0	2.11867	0.058515	2.060766
34	1	0	1.591001	1.733862	1.874044
35	1	0	1.578838	2.399038	2.005744
36	1	0	0.138953	3.040913	1.829151
37	1	0	3.762462	0.197073	1.881349
38	1	0	3.508326	1.56065	1.819734
39	1	0	4.617131	0.779068	0.677901
40	1	0	1.972932	0.872484	1.370831
41	1	0	3.18265	1.523192	0.236263
42	1	0	3.756075	0.635949	1.902723
43	1	0	1.770876	2.241734	0.384341
44	1	0	0.846764	2.53555	0.284764
45	1	0	3.425182	2.711873	0.05942
12B					
1	6	0	1.71068	1.30016	0.429218
2	6	0	1.247459	0.179489	0.688288
3	6	0	0.134469	0.584471	0.158948
4	6	0	1.320318	0.097868	0.872258

5	6	0	1.044305	1.548138	1.318072
6	6	0	0.480623	2.5471	0.292554
7	6	0	0.7453	2.066135	0.446196
8	6	0	3.179731	1.209711	0.043378
9	6	0	3.631482	0.183593	0.393703
10	6	0	2.398404	1.044455	0.116366
11	6	0	2.251529	1.346503	1.375405
12	6	0	0.912672	2.31346	1.743987
13	6	0	2.672808	0.053123	0.129678
14	6	0	2.791003	0.788931	1.141673
15	6	0	3.035622	1.515715	0.195337
16	8	0	2.387759	2.034215	1.333785
17	8	0	3.634331	0.390385	1.096314
18	8	0	0.295336	2.004361	0.313113
19	8	0	2.411778	2.271173	0.859708
20	1	0	1.710511	1.805782	1.399573
21	1	0	1.25297	0.363764	1.769821
22	1	0	0.172912	0.36806	0.914464
23	1	0	1.456549	0.47389	1.798137
24	1	0	1.972561	1.950781	1.726979
25	1	0	0.347427	1.498324	2.160488
26	1	0	0.191588	3.445397	0.853786
27	1	0	1.235152	2.86589	0.425092
28	1	0	3.259641	1.299277	1.126789
29	1	0	3.78418	2.009085	0.386111
30	1	0	3.829301	0.210607	1.469507
31	1	0	4.522044	0.540073	0.130542
32	1	0	3.160497	1.828775	1.748597
33	1	0	2.093249	0.432713	1.951354
34	1	0	1.404117	2.009394	1.554571
35	1	0	1.796568	2.018163	2.295674
36	1	0	0.148997	2.842919	2.303753
37	1	0	1.911595	0.695348	1.781211
38	1	0	2.937687	1.836592	0.879125
39	1	0	3.652969	0.456715	1.727763
40	1	0	4.109469	1.532457	0.415073
41	1	0	2.861819	2.136782	0.688752
42	1	0	1.534532	2.36691	1.027262
43	1	0	4.504899	0.370258	0.688183
44	1	0	0.517077	2.396914	0.660019
45	1	0	3.066543	2.864207	0.47846

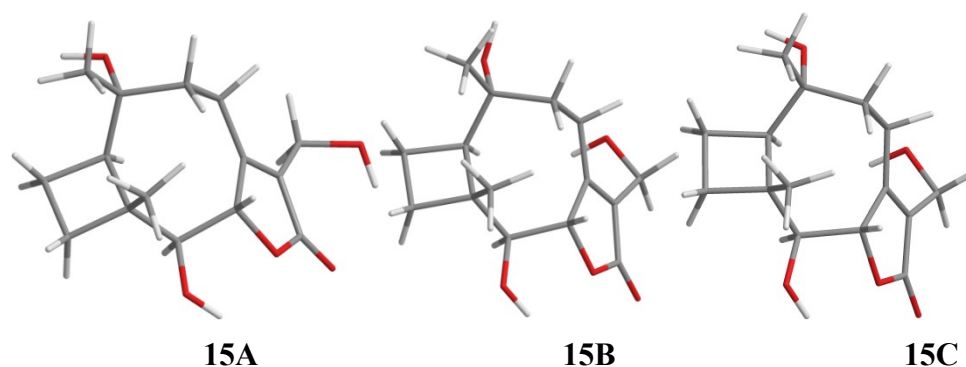


Figure S119. Conformers of isomer **15**

Table S21. Important thermodynamic parameters and Boltzmann distributions of the optimized isomer **15** at B3LYP/6-31G (d, p) level in gas phase.

Conformations	Energy (a.u)	$\Delta G(\text{kcal/mol})$	%	Number of imaginary frequencies
15A	-960.528658	0.00	57.2	0
15B	-960.527589	0.67	18.5	0
15C	-960.527849	0.51	24.3	0

Table S22. Optimized Z-matrixes of isomer **15** in the gas phase (\AA) at B3LYP/6-31G (d) level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
15A					
1	6	0	2.075908	0.200364	0.653288
2	6	0	1.666794	1.190969	0.076713
3	6	0	0.200706	1.579367	0.250909
4	6	0	0.810389	0.816821	0.633782
5	6	0	1.21447	0.564878	0.158963
6	6	0	0.351251	1.793227	0.119373
7	6	0	0.928831	1.778552	0.965446
8	6	0	2.206565	1.483828	0.175643
9	6	0	3.315979	0.464969	1.29617
10	6	0	2.58424	1.818648	1.164008
11	8	0	2.032147	1.578795	0.576262
12	6	0	3.026469	0.821355	0.065238
13	6	0	2.508508	0.527061	0.189191
14	8	0	4.142482	1.248852	0.10464
15	6	0	3.419165	1.58099	0.73962
16	8	0	2.330233	2.577671	0.751795
17	6	0	2.192627	1.529742	1.31735
18	8	0	0.116083	2.964348	0.033051
19	6	0	3.407299	1.525112	1.118033
20	8	0	4.633379	1.659638	0.007872

21	1	0	1.371489	0.428863	1.461231
22	1	0	0.090312	1.399101	1.29574
23	1	0	0.488242	0.816639	1.678366
24	1	0	0.093726	2.016215	0.92125
25	1	0	0.98411	2.62389	0.440941
26	1	0	0.845439	1.073682	1.796079
27	1	0	1.060073	2.765123	1.415921
28	1	0	3.599016	0.138705	2.296783
29	1	0	4.190478	0.424544	0.645702
30	1	0	3.172669	2.684161	0.857741
31	1	0	2.020719	2.064159	2.066375
32	1	0	3.62272	1.366156	1.795092
33	1	0	2.948449	2.562203	0.684935
34	1	0	3.0983	2.413959	1.309956
35	1	0	1.74688	0.9216	2.107989
36	1	0	3.274759	1.392972	1.360656
37	1	0	1.979785	2.577591	1.533847
38	1	0	0.802412	3.23596	0.069072
39	1	0	3.352336	0.756799	1.8887
40	1	0	3.433322	2.5012	1.607013
41	1	0	4.342427	1.398273	0.568253
42	1	0	5.056367	0.793707	0.057516
15B					
1	6	0	1.9471	0.205792	0.65214
2	6	0	1.543825	-1.232902	0.20156
3	6	0	0.066057	-1.59194	0.338268
4	6	0	-0.884609	-0.932172	-0.683205
5	6	0	-1.291811	0.495464	-0.395638
6	6	0	-0.418771	1.712824	-0.432942
7	6	0	0.905069	1.59749	-1.197767
8	6	0	2.135161	1.389648	-0.299543
9	6	0	3.140294	-0.400616	1.421572
10	6	0	2.395673	-1.753492	1.394416
11	8	0	-2.11928	-1.667559	-0.611886
12	6	0	-3.139841	-0.844118	-0.26309
13	6	0	-2.607723	0.518927	-0.136387
14	8	0	-4.262881	-1.251603	-0.118869
15	6	0	-3.464803	1.696968	0.21416
16	8	0	2.25302	2.509594	0.59527
17	6	0	2.138182	-1.72056	-1.119521
18	8	0	-0.019553	-3.000281	0.210915
19	6	0	3.391472	1.329497	-1.164626
20	8	0	-2.979554	2.412657	1.341973

21	1	0	1.208318	0.526753	1.39517
22	1	0	-0.278494	-1.291396	1.338239
23	1	0	-0.501125	-1.052816	-1.700178
24	1	0	-0.221212	2.035792	0.594488
25	1	0	-1.029306	2.514101	-0.859511
26	1	0	0.859691	0.805773	-1.950076
27	1	0	1.068449	2.524908	-1.754523
28	1	0	3.375871	0.031039	2.393441
29	1	0	4.047365	-0.437022	0.817442
30	1	0	2.98295	-2.653704	1.209773
31	1	0	1.782863	-1.897362	2.286709
32	1	0	-3.470838	2.41248	-0.611244
33	1	0	-4.492003	1.356719	0.373056
34	1	0	2.480921	3.289987	0.07793
35	1	0	1.745441	-1.195003	-1.992872
36	1	0	3.223021	-1.598648	-1.117214
37	1	0	1.922063	-2.783397	-1.237824
38	1	0	-0.947367	-3.250004	0.280273
39	1	0	3.365552	0.497117	-1.867116
40	1	0	3.470966	2.251822	-1.747938
41	1	0	4.284848	1.244088	-0.545083
42	1	0	-2.983648	1.821467	2.101448
15C					
1	6	0	1.941591	0.211797	0.640821
2	6	0	1.546292	1.23365	0.203668
3	6	0	0.068318	1.590736	0.342585
4	6	0	0.881367	0.931018	0.68062
5	6	0	1.291656	0.49635	0.393756
6	6	0	0.42337	1.71766	0.43236
7	6	0	0.899054	1.610473	1.201975
8	6	0	2.129755	1.395282	0.317084
9	6	0	3.139102	0.384503	1.418425
10	6	0	2.398425	1.739737	1.401704
11	8	0	2.114902	1.668467	0.611114
12	6	0	3.137284	0.847181	0.262457
13	6	0	2.607867	0.516787	0.135302
14	8	0	4.259539	1.257008	0.119089
15	6	0	3.46792	1.693068	0.214001
16	8	0	2.217526	2.584179	0.489915
17	6	0	2.140083	1.730428	1.113772
18	8	0	0.019536	2.999069	0.219771
19	6	0	3.379542	1.324253	1.191325
20	8	0	2.986177	2.409443	1.342869

21	1	0	1.199338	0.532612	1.380386
22	1	0	0.275442	1.286692	1.341767
23	1	0	0.496256	1.050901	1.697045
24	1	0	0.226911	2.041944	0.594454
25	1	0	1.037969	2.515814	0.858924
26	1	0	0.853756	0.822269	1.957429
27	1	0	1.064503	2.543609	1.745576
28	1	0	3.374662	0.051053	2.389332
29	1	0	4.046243	0.423677	0.814172
30	1	0	2.990961	2.638375	1.226848
31	1	0	1.785782	1.877318	2.29497
32	1	0	3.47399	2.408726	0.611277
33	1	0	4.494685	1.350699	0.371048
34	1	0	2.956821	2.480896	1.099019
35	1	0	1.747013	1.209222	1.989692
36	1	0	3.225025	1.609723	1.113
37	1	0	1.922628	2.793677	1.225328
38	1	0	0.947984	3.246996	0.287475
39	1	0	3.358545	0.472497	1.870467
40	1	0	3.442018	2.237539	1.786748
41	1	0	4.282562	1.25739	0.580568
42	1	0	2.991783	1.818409	2.102443

Table S23. Energy analysis for (1*R*, 4*R*, 5*S*, 6*R*, 7*R*, 10*S*, 11*R*^{*})-**8a** and (1*R*, 4*R*, 5*S*, 6*R*, 7*R*, 10*S*, 11*S*^{*})-**8b**

Conf.	G(Hartree)	$\Delta G(\text{kcal/mol})$	Boltzmann Distribution
a			
a1	0.395359	0.00	0.855
a2	0.39487	-0.31	0.103
b			
b1	0.393838	0.00	0.565
b2	0.393807	0.46	0.365

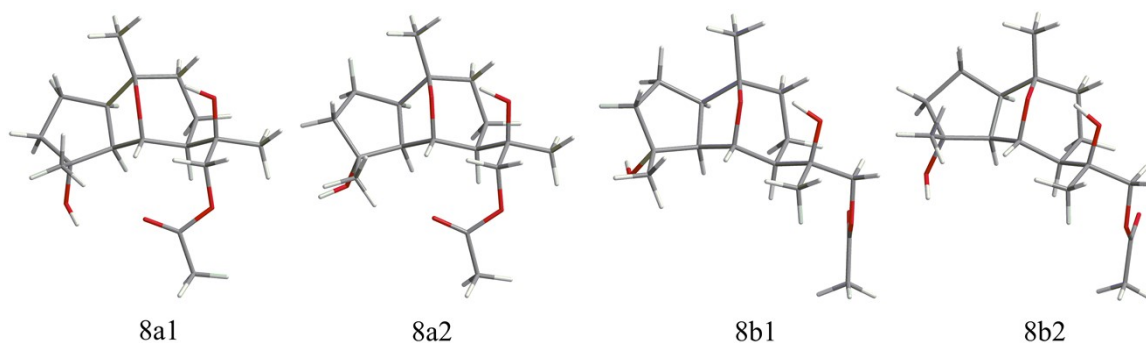


Figure S120. mPW1PW91/6-311+G (d, p) (chloroform) optimized lowest energy conformers for (1*R*, 4*R*, 5*S*, 6*R*, 7*R*, 10*S*, 11*R*^{*})-**8a** and (1*R*, 4*R*, 5*S*, 6*R*, 7*R*, 10*S*, 11*S*^{*})-**8b**

Functional		Solvent?		Basis Set		Type of Data	
mPW1PW91		PCI		6-311+G(d,p)		Unscaled Shifts	
		DP4+	0.00%	100.00%	-	-	-
Nuclei	sp2?	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5
C		50.1	54.36	54.54			
C		26.1	29.67	29.19			
C		42.0	45.12	44.52			
C		81.9	83.64	84.58			
C		58.0	66.25	65.91			
C		77.4	82.81	81.83			
C		45.1	39.85	43.20			
C		18.2	22.59	21.97			
C		38.1	38.65	39.53			
C		81.8	86.42	86.37			
C		72.2	77.86	78.40			
C		70.0	74.09	71.01			
C		23.7	26.69	29.06			
C		22.7	25.15	24.65			
C		25.0	26.28	25.50			
C		171.4	177.69	177.58			
C		21.1	23.86	23.32			
H		2.45	2.62	2.59			
H		1.79	1.77	1.88			
H		1.64	1.58	1.63			
H		1.58	1.81	1.63			
H		1.53	1.56	1.50			
H		2.78	2.19	2.22			
H		4.26	5.29	4.60			
H		1.70	0.74	0.81			
H		1.73	1.86	2.33			
H		1.58	1.81	1.69			
H		1.51	1.76	1.97			
H		1.48	1.32	1.28			
H		3.98	5.10	5.13			
H		3.89	3.37	3.23			
H		1.27	1.14	1.35			
H		1.27	1.48	1.50			
H		1.27	1.18	1.36			
H		1.18	1.09	1.14			
H		1.18	1.28	1.27			
H		1.18	1.15	1.19			
H		1.36	1.77	1.29			
H		1.36	1.65	1.28			
H		1.36	1.13	1.36			
H		2.08	1.72	2.04			
H		2.08	2.14	1.83			
H		2.08	2.22	2.18			

Functional	Solvent?		Basis Set		Type of Data	
mPW1PW91	PCI		6-311+G(d,p)		Unscaled Shifts	
	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)	1.76%	98.24%	-	-	-	-
sDP4+ (C data)	36.82%	63.18%	-	-	-	-
sDP4+ (all data)	1.03%	98.97%	-	-	-	-
uDP4+ (H data)	0.06%	99.94%	-	-	-	-
uDP4+ (C data)	31.28%	68.72%	-	-	-	-
uDP4+ (all data)	0.03%	99.97%	-	-	-	-
DP4+ (H data)	0.00%	100.00%	-	-	-	-
DP4+ (C data)	20.97%	79.03%	-	-	-	-
DP4+ (all data)	0.00%	100.00%	-	-	-	-

Figure S121. DP4+ evaluation of theoretical and experimental data for (1*R*, 4*R*, 5*S*, 6*R*, 7*R*, 10*S*, 11*R*^{*})-**8a** and (1*R*, 4*R*, 5*S*, 6*R*, 7*R*, 10*S*, 11*S*^{*})-**8b**

Table S24. Calculated (calc.) and experimental (exp.) ^{13}C NMR chemical shift values of (1*R*, 4*R*, 5*S*, 6*R*, 7*R*, 10*S*, 11*R**)-8a and (1*R*, 4*R*, 5*S*, 6*R*, 7*R*, 10*S*, 11*S**)-8b at the mPW1PW91/6-311+G(d, p) level in chloroform

Position	exp.	calc.a	calc. b
1	50.1	54.36	54.54
2	26.1	29.67	29.19
3	42.0	45.12	44.52
4	81.9	83.64	84.58
5	58.0	66.25	65.91
6	77.4	82.81	81.83
7	45.1	39.85	43.20
8	18.2	22.59	21.97
9	38.1	38.65	39.53
10	81.8	86.42	86.37
11	72.2	77.86	78.40
12	70.0	74.09	71.01
13	23.7	26.69	29.06
14	22.7	25.15	24.65
15	25.0	26.28	25.50
16	171.4	177.69	177.58
17	21.1	23.86	23.32

Table S25. Calculated (calc.) and experimental (exp.) ^1H NMR chemical shift values of (1*R*, 4*R*, 5*S*, 6*R*, 7*R*, 10*S*, 11*R**)-8a and (1*R*, 4*R*, 5*S*, 6*R*, 7*R*, 10*S*, 11*S**)-8b at the mPW1PW91/6-311+G (d, p) level in chloroform

Position	exp.	calc.a	calc. b
1	2.45	2.62	2.59
2a	1.79	1.77	1.88
2b	1.64	1.58	1.63
3a	1.58	1.81	1.63
3b	1.53	1.56	1.50
5	2.78	2.19	2.22
6	4.26	5.29	4.60
7	1.70	0.74	0.81
8a	1.73	1.86	2.33
8b	1.58	1.81	1.69
9a	1.51	1.76	1.97
9b	1.48	1.32	1.28
12a	3.98	5.10	5.13
12b	3.89	3.37	3.23
13a	1.27	1.14	1.35
13b	1.27	1.48	1.50

13c	1.27	1.18	1.36
14a	1.18	1.09	1.14
14b	1.18	1.28	1.27
14c	1.18	1.15	1.19
15a	1.36	1.77	1.29
15b	1.36	1.65	1.28
15c	1.36	1.13	1.36
17a	2.08	1.72	2.04
17b	2.08	2.14	1.83
17c	2.08	2.22	2.18

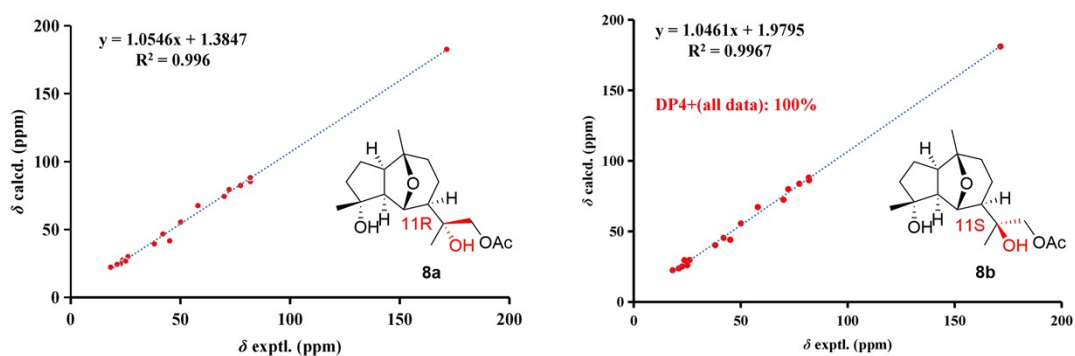


Figure S122. Linear correlations between the experimental and calculated ^{13}C NMR chemical shifts for two possible isomers of (1*R*, 4*R*, 5*S*, 6*R*, 7*R*, 10*S*, 11*R*^{*})-**8a** and (1*R*, 4*R*, 5*S*, 6*R*, 7*R*, 10*S*, 11*S*^{*})-**8b** at the PCM/ mPW1PW91/6-311+G (d, p) level.

Table S26. Energy analysis for (1*R*, 4*R*, 5*S*, 6*S*, 7*R*, 11*R*^{*})-**11a** and (1*R*, 4*R*, 5*S*, 6*S*, 7*R*, 11*S*^{*})-**11b**

Conf.	G(Hartree)	$\Delta\text{G}(\text{kcal/mol})$	Boltzann Distribution
a			
a1	0.359776	0.00	0.485
a2	0.360162	0.24	0.218
a3	0.359779	0.00	0.195
b			
b1	0.359062	0.00	0.603
b2	0.359062	0.00	0.133

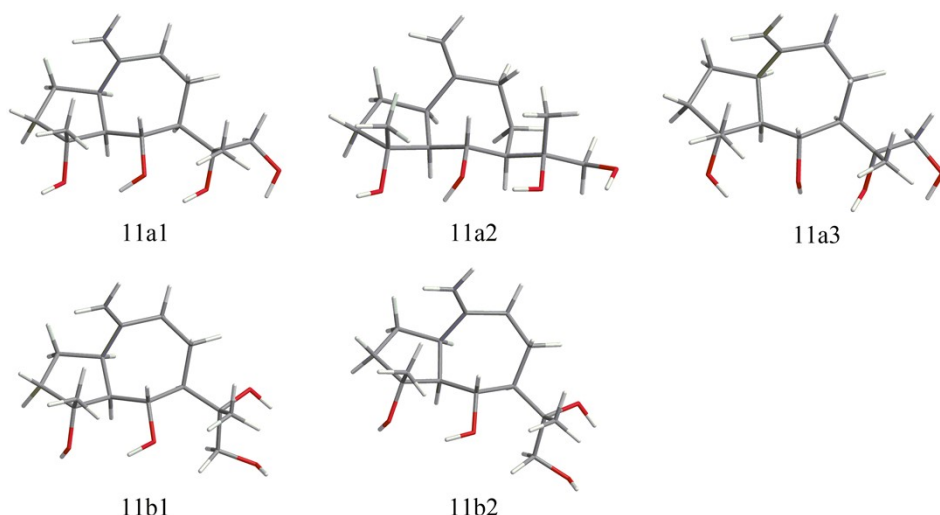


Figure S123. mPW1PW91/6-311+G (d, p) (chloroform) optimized lowest energy conformers for (1*R*, 4*R*, 5*S*, 6*S*, 7*R*, 11*R*^{*})-11a and (1*R*, 4*R*, 5*S*, 6*S*, 7*R*, 11*S*^{*})-11b

Functional mPW1PW91		Solvent? PCM		Basis Set 6-311+G(d, p)			Type of Data Unscaled Shifts	
		DP4+	100.00%	0.00%	-	-	-	-
Nuclei	sp2?	xperimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	
C		41.7	46.54	51.22				
C		25.3	28.86	32.93				
C		40.8	44.94	46.26				
C		81.2	85.74	87.06				
C		57.0	57.47	67.59				
C		76.4	79.06	78.23				
C		53.8	57.23	53.84				
C		29.4	32.14	34.12				
C		39.5	43.64	44.73				
C		149.4	162.47	165.72				
C		77.3	77.71	76.18				
C		67.4	72.78	75.29				
C		26.0	20.77	19.46				
C	x	109.8	115.28	114.23				
C		22.9	23.96	28.34				
H		2.91	3.06	2.83				
H		1.80	1.85	2.16				
H		1.76	1.70	1.79				
H		1.82	1.94	2.19				
H		1.78	1.71	1.81				
H		2.20	2.23	2.01				
H		3.92	4.10	3.72				
H		1.88	1.72	1.76				
H		1.92	1.64	2.73				
H		1.36	1.15	1.19				
H		2.46	2.53	2.46				
H		1.94	1.92	2.03				
H		3.81	3.44	4.76				
H		3.48	3.43	3.15				
H		1.21	1.39	1.01				
H		1.21	1.28	1.12				
H		1.21	1.48	1.43				
H		4.90	5.36	5.17				
H		4.83	5.23	4.94				
H		1.28	1.62	1.38				
H		1.28	1.02	1.38				
H		1.28	1.58	1.18				

Functional mPW1PW91		Solvent? PCM		Basis Set 6-311+G(d, p)			Type of Data Unscaled Shifts	
		Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6	
sDP4+ (H data)		99.64%	0.36%	-	-	-	-	
sDP4+ (C data)		100.00%	0.00%	-	-	-	-	
sDP4+ (all data)		100.00%	0.00%	-	-	-	-	
uDP4+ (H data)		85.57%	14.43%	-	-	-	-	
uDP4+ (C data)		100.00%	0.00%	-	-	-	-	
uDP4+ (all data)		100.00%	0.00%	-	-	-	-	
DP4+ (H data)		99.94%	0.06%	-	-	-	-	
DP4+ (C data)		100.00%	0.00%	-	-	-	-	
DP4+ (all data)		100.00%	0.00%	-	-	-	-	

Figure S124. DP4+ evaluation of theoretical and experimental data for (1*R*, 4*R*, 5*S*, 6*S*, 7*R*, 11*R*^{*})-11a and (1*R*, 4*R*, 5*S*, 6*S*, 7*R*, 11*S*^{*})-11b

Table S27. Calculated (calc.) and experimental (exp.) ^{13}C NMR chemical shift values of (1*R*, 4*R*, 5*S*, 6*S*, 7*R*, 11*R*^{*})-**11a** and (1*R*, 4*R*, 5*S*, 6*S*, 7*R*, 11*S*^{*})-**11b** at the mPW1PW91/6-311+G(d, p) level in chloroform

Position	exp.	calc.a	calc. b
1	41.7	46.54	51.22
2	25.3	28.86	32.93
3	40.8	44.94	46.26
4	81.2	85.74	87.06
5	57.0	57.47	67.59
6	76.4	79.06	78.23
7	53.8	57.23	53.84
8	29.4	32.14	34.12
9	39.5	43.64	44.73
10	149.4	162.47	165.72
11	77.3	77.71	76.18
12	67.4	72.78	75.29
13	26.0	20.77	19.46
14	109.8	115.28	114.23
15	22.9	23.96	28.34

Table S28. Calculated (calc.) and experimental (exp.) ^1H NMR chemical shift values of (1*R*, 4*R*, 5*S*, 6*S*, 7*R*, 11*R*^{*})-**11a** and (1*R*, 4*R*, 5*S*, 6*S*, 7*R*, 11*S*^{*})-**11b** at the mPW1PW91/6-311+G (d, p) level in chloroform

Position	exp.	calc.a	calc. b
1	2.91	3.06	2.83
2a	1.80	1.85	2.16
2b	1.76	1.70	1.79
3a	1.82	1.94	2.19
3b	1.78	1.71	1.81
5	2.20	2.23	2.01
6	3.92	4.10	3.72
7	1.88	1.72	1.76
8a	1.92	1.64	2.73
8b	1.36	1.15	1.19
9a	2.46	2.53	2.46
9b	1.94	1.92	2.03
12a	3.81	3.44	4.76
12b	3.48	3.43	3.15
13a	1.21	1.39	1.01
13b	1.21	1.28	1.12
13c	1.21	1.48	1.43
14a	4.90	5.36	5.17

14b	4.83	5.23	4.94
14c	1.28	1.62	1.38
15a	1.28	1.02	1.38
15b	1.28	1.58	1.18

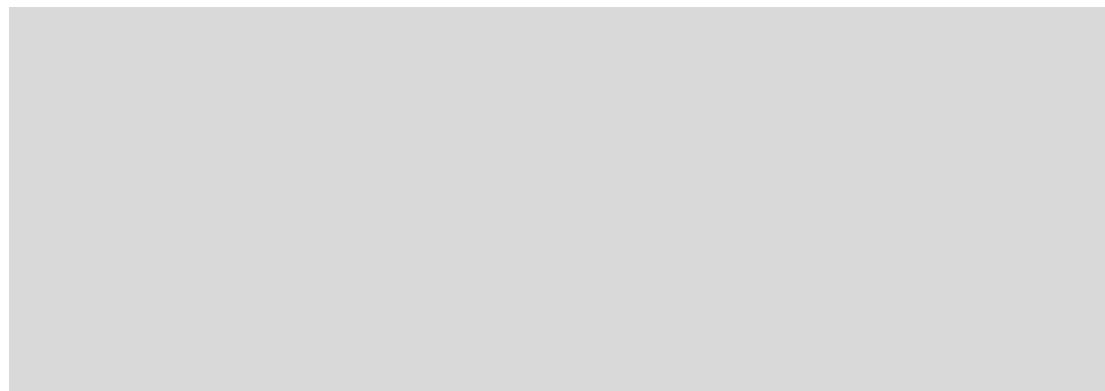


Figure S125. Linear correlations between the experimental and calculated ^{13}C NMR chemical shifts for two possible isomers of (1*R*, 4*R*, 5*S*, 6*S*, 7*R*, 11*R*^{*})-**11a** and (1*R*, 4*R*, 5*S*, 6*S*, 7*R*, 11*S*^{*})-**11b** at the PCM/ mPW1PW91/6-311+G (d, p) level.

Table S29. Energy analysis for (1*R*, 4*R*, 5*S*, 6*S*, 7*R*, 11*R*^{*})-**12a** and (1*R*, 4*R*, 5*S*, 6*S*, 7*R*, 11*S*^{*})-**12b**

Conf.	G(Hartree)	$\Delta\text{G}(\text{kcal/mol})$	Boltzmann Distribution
a			
a1	0.361596	0.00	0.739
a2	0.35926	-1.47	0.131
b			
b1	0.359382	0.00	0.684
b2	0.36001	0.39	0.116

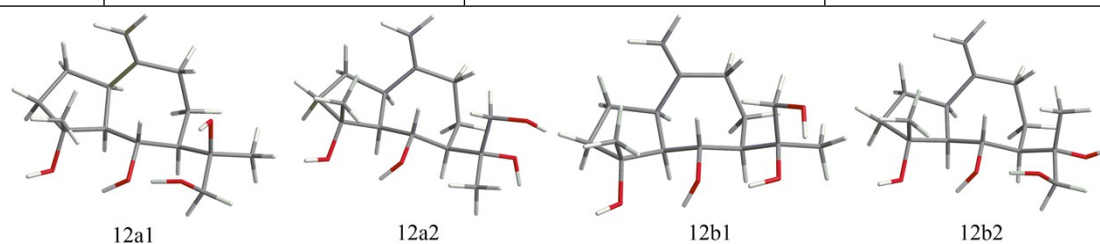


Figure S126. mPW1PW91/6-311+G (d, p) (chloroform) optimized lowest energy conformers for (1*R*, 4*R*, 5*S*, 6*S*, 7*R*, 11*R*^{*})-**12a** and (1*R*, 4*R*, 5*S*, 6*S*, 7*R*, 11*S*^{*})-**12b**

Functional mPW1PW91		Solvent? PCM		Basis Set 6-311+G(d,p)		Type of Data Unscaled Shifts	
		DP4+	0.00%	100.00%	-	-	-
Nuclei	sp2?	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5
C		41.6	45.35	44.96			
C		25.1	28.76	29.14			
C		41.0	44.96	44.86			
C		81.6	85.59	85.91			
C		56.8	54.36	53.96			
C		75.6	72.03	73.72			
C		49.0	59.24	58.18			
C		29.1	26.49	26.32			
C		38.8	39.25	41.26			
C		149.5	162.10	161.55			
C		77.3	77.69	78.30			
C		69.8	69.59	72.83			
C		20.3	29.98	27.01			
C	x	109.4	113.53	113.44			
C		22.6	23.93	23.93			
H		2.91	3.13	3.13			
H		1.79	1.86	1.89			
H		1.75	1.62	1.67			
H		1.77	1.91	1.96			
H		1.77	1.65	1.70			
H		2.18	2.11	2.22			
H		3.94	3.75	4.19			
H		1.99	1.79	1.84			
H		1.84	2.25	2.08			
H		1.23	1.85	1.89			
H		2.47	2.51	2.38			
H		1.93	2.24	2.23			
H		3.58	3.83	3.55			
H		3.41	3.46	3.49			
H		1.22	2.08	1.46			
H		1.22	1.83	0.90			
H		1.22	0.67	1.66			
H		4.88	5.33	5.33			
H		4.81	5.21	5.19			
H		1.31	1.59	1.73			
H		1.31	0.93	0.99			
H		1.31	1.69	1.65			

Functional mPW1PW91	Solvent? PCM		Basis Set 6-311+G(d,p)		Type of Data Unscaled Shifts	
	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)	0.02%	99.98%	-	-	-	-
sDP4+ (C data)	0.04%	99.96%	-	-	-	-
sDP4+ (all data)	0.00%	100.00%	-	-	-	-
uDP4+ (H data)	0.22%	99.78%	-	-	-	-
uDP4+ (C data)	0.01%	99.99%	-	-	-	-
uDP4+ (all data)	0.00%	100.00%	-	-	-	-
DP4+ (H data)	0.00%	100.00%	-	-	-	-
DP4+ (C data)	0.00%	100.00%	-	-	-	-
DP4+ (all data)	0.00%	100.00%	-	-	-	-

Figure S127. DP4+ evaluation of theoretical and experimental data for (1*R*, 4*R*, 5*S*, 6*S*, 7*R*, 11*R*^{*})-12a and (1*R*, 4*R*, 5*S*, 6*S*, 7*R*, 11*S*^{*})-12b

Table S30. Calculated (calc.) and experimental (exp.) ^{13}C NMR chemical shift values of (1*R*, 4*R*, 5*S*, 6*S*, 7*R*, 11*R*^{*})-**12a** and (1*R*, 4*R*, 5*S*, 6*S*, 7*R*, 11*S*^{*})-**12b** at the mPW1PW91/6-311+G(d, p) level in acetone

Position	exp.	calc.a	calc. b
1	41.6	45.35	44.96
2	25.1	28.76	29.14
3	41.0	44.96	44.86
4	81.6	85.59	85.91
5	56.8	54.36	53.96
6	75.6	72.03	73.72
7	49.0	59.24	58.18
8	29.1	26.49	26.32
9	38.8	39.25	41.26
10	149.5	162.10	161.55
11	77.3	77.69	78.30
12	69.8	69.59	72.83
13	20.3	29.98	27.01
14	109.4	113.53	113.44
15	22.6	23.93	23.93

Table S31. Calculated (calc.) and experimental (exp.) ^1H NMR chemical shift values of (1*R*, 4*R*, 5*S*, 6*S*, 7*R*, 11*R*^{*})-**12a** and (1*R*, 4*R*, 5*S*, 6*S*, 7*R*, 11*S*^{*})-**12b** at the mPW1PW91/6-311+G (d, p) level in acetone

Position	exp.	calc.a	calc. b
1	2.91	3.13	3.13
2a	1.79	1.86	1.89
2b	1.75	1.62	1.67
3a	1.77	1.91	1.96
3b	1.77	1.65	1.70
5	2.18	2.11	2.22
6	3.94	3.75	4.19
7	1.99	1.79	1.84
8a	1.84	2.25	2.08
8b	1.23	1.85	1.89
9a	2.47	2.51	2.38
9b	1.93	2.24	2.23
12a	3.58	3.83	3.55
12b	3.41	3.46	3.49
13a	1.22	2.08	1.46
13b	1.22	1.83	0.90
13c	1.22	0.67	1.66
14a	4.88	5.33	5.33

14b	4.81	5.21	5.19
15a	1.31	1.59	1.73
15b	1.31	0.93	0.99
15c	1.31	1.69	1.65

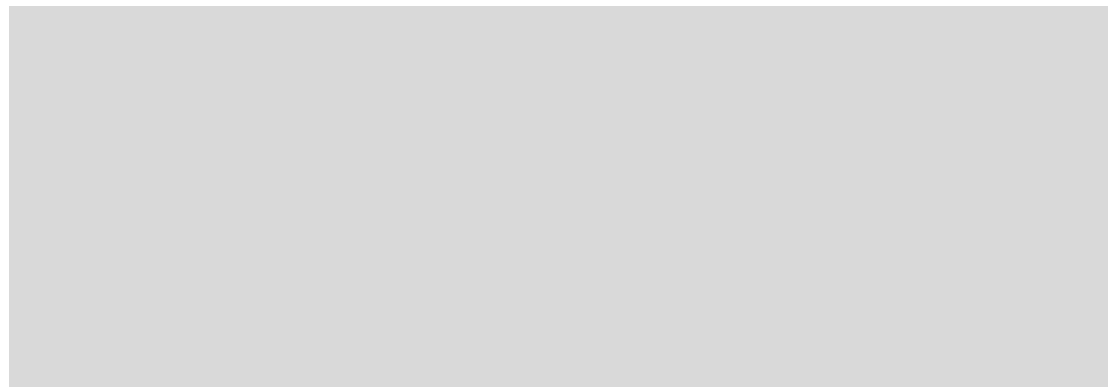


Figure S128. Linear correlations between the experimental and calculated ^{13}C NMR chemical shifts for two possible isomers of (1*R*, 4*R*, 5*S*, 6*S*, 7*R*, 11*R*^{*})-**12a** and (1*R*, 4*R*, 5*S*, 6*S*, 7*R*, 11*S*^{*})-**12b** at the PCM/ mPW1PW91/6-311+G (d, p) level.