

The Triterpenoids and Their Anti-proliferative Effects from *Munronia pinnata*

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Table S1. Partial $^3J_{\text{H,H}}$ and $^2,3J_{\text{C,H}}$ data for munropenes A-F (1-6).

Position	1	2	3	4	5	6
3J (H-24,H-23)	8.6	8.5	9.5	7.8	8.7	6.9
3J (H-24,C-22)	2.2	3.1	3.3	-1.5	1.7	2.3
3J (C-25,H-23)	6.5	5.9	4.9	2.8	4.7	3.7
3J (H-24,C-23)	-3.2	-3.4	-3.2	3.2	-3.2	-3.2
3J (H-23, H-22a)	8.2	12.0	8.6	8.8	9.1	6.7
3J (H-23, H-22b)	6.5	4.0	5.4	2.8	9.0	6.7
3J (H-23, C-20)	5.5	4.0	2.5	2.6	4.5	2.8
3J (C-24, H-22a)	2.1	-1.6	2.0	0.6	-1.9	Nd
3J (C-24, H-22b)	1.9	-1.7	2.0	1.0	1.6	1.2
2J (C-23, H-22a)	-6.0	6.8	-6.8	-5.5	4.8	5.3
2J (C-23, H-22b)	-1.7	3.3	-2.0	-3.9	-2.5	-3.7
3J (H-20,H-22a)	5.8	8.0	11.0	6.7	4.7	3.4
3J (H-20,H-22b)	6.1	5.0	4.9	4.9	4.1	4.3
3J (H-20,C-23)	3.1	5.8	3.1	2.7	Nd	Nd
3J (C-17, H-22a)	-2.3	3.5	2.1	2.5	6.5	2.4
3J (C-17, H-22b)	1.6	3.5	-3.3	-4.3	3.5	-1.7
2J (C-20, H-22a)	2.6	5.0	5.1	5.6	6.5	5.4
2J (C-20, H-22b)	2.3	3.5	-1.7	-4.0	3.4	3.5
3J (H-17,H-20)	16.0	8.1	13.7	12.2	8.8	9.8
3J (H-17,C-21)	3.7	4.2	-5.9	1.6	2.8	3.9
3J (H-17,C-22)	3.8	5.2	2.9	3.5	2.6	2.2
3J (C-16,H-20)	Nd	Nd	Nd	Nd	Nd	Nd
3J (C-13,H-20)	2.8	2.9	2.6	3.6	2.9	2.9
3J (H-1,C-5)		7.3	4.2			
3J (H-1,C-9)		6.1	6.2			
3J (H-1,C-19)		1.2	4.1			
3J (H-1,H-2a)		7.8	11.2			
3J (H-1,H-2b)		4.0	6.4			
3J (H-1,C-3)		6.2	4.6			
2J (C-10, H-2a)		9.0	4.8			
2J (C-10, H-2b)		Nd	Nd			

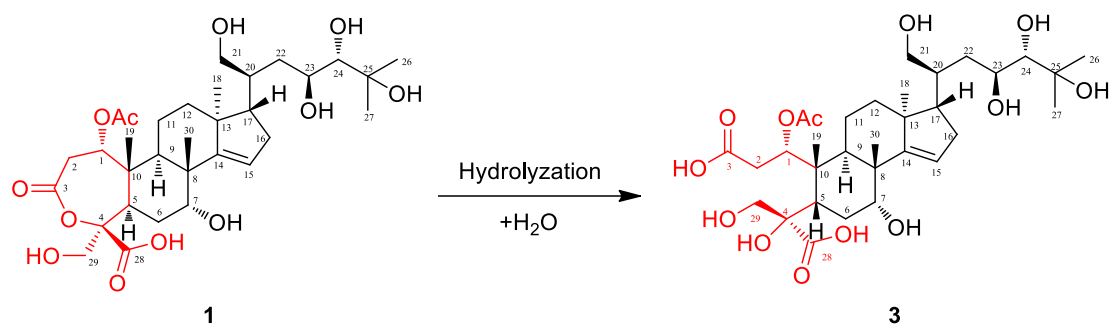


Figure S1. Possible biogenetic pathway of munropene C (3).

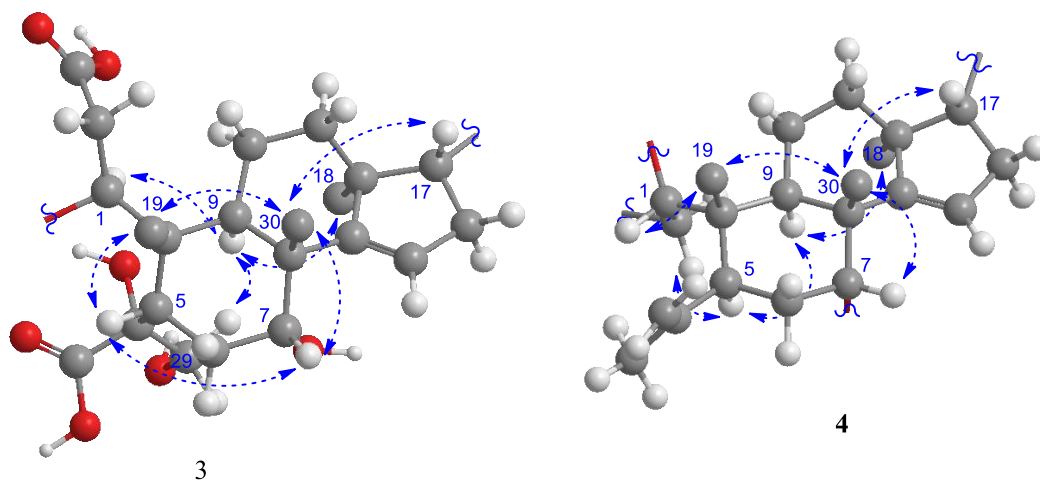


Figure S2. Key NOESY correlations and relative configuration for munropenes C-D (3-4) (protons of methyl groups are omitted).

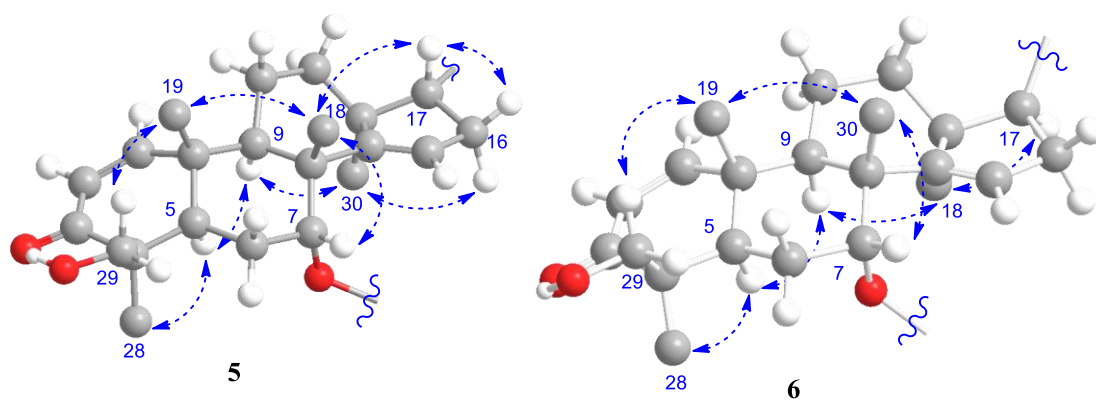
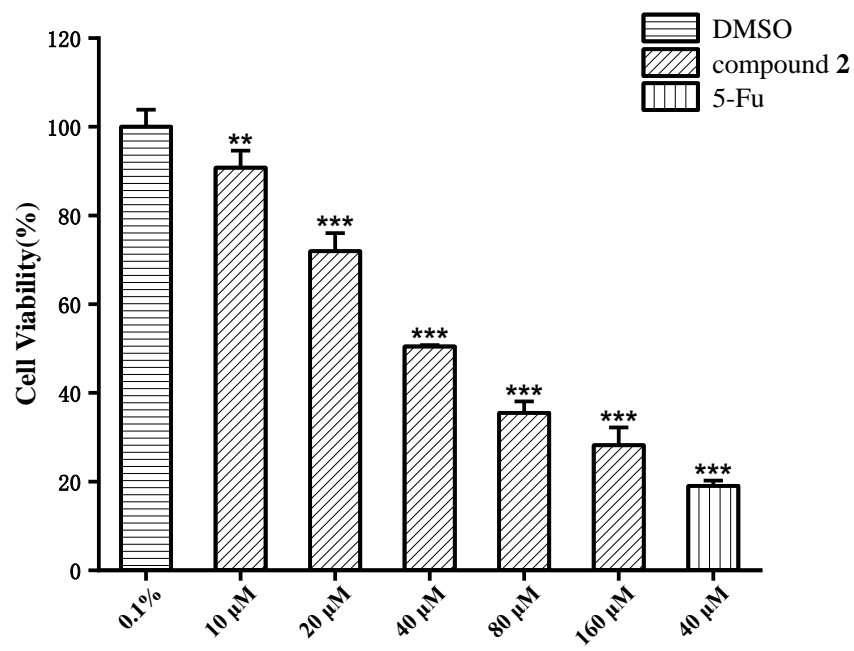
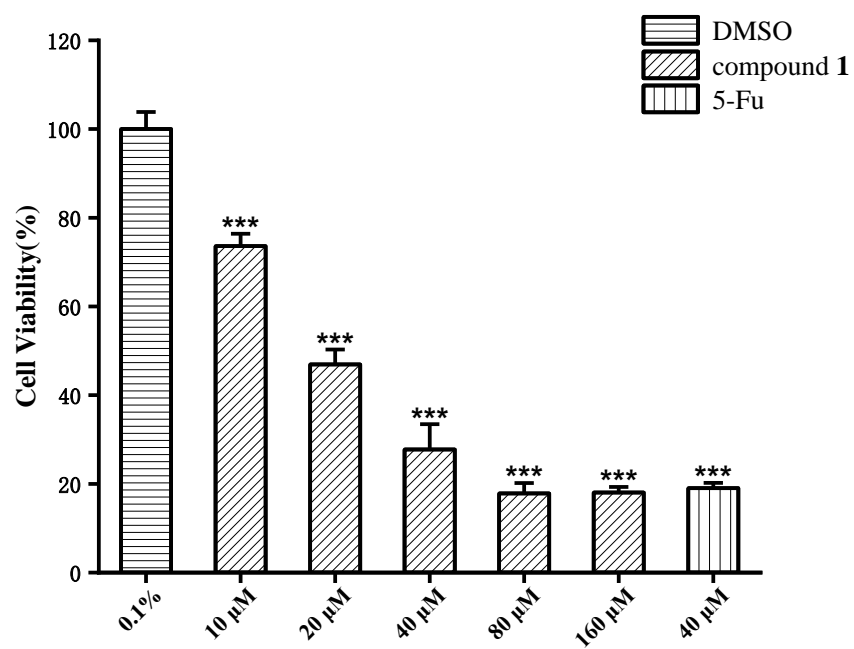
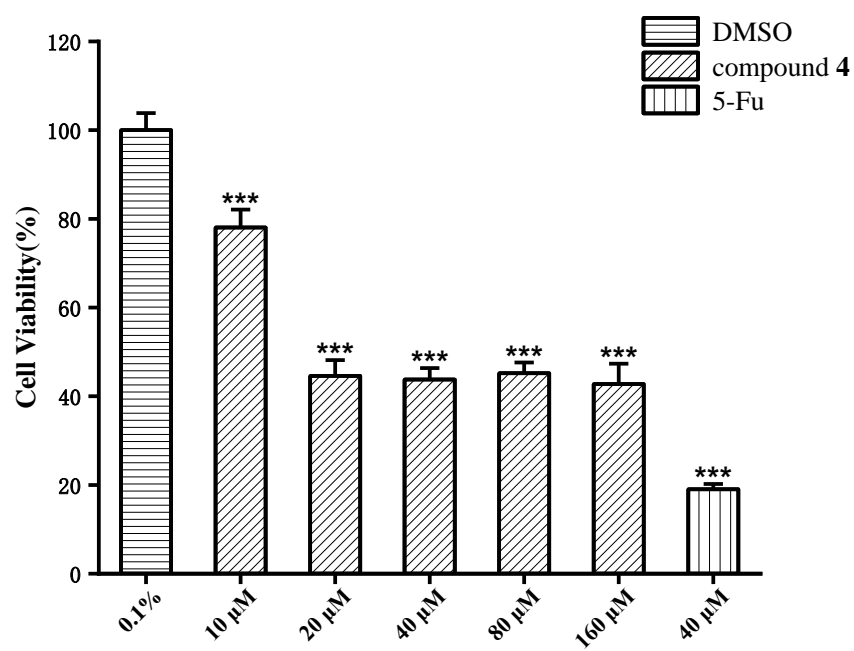
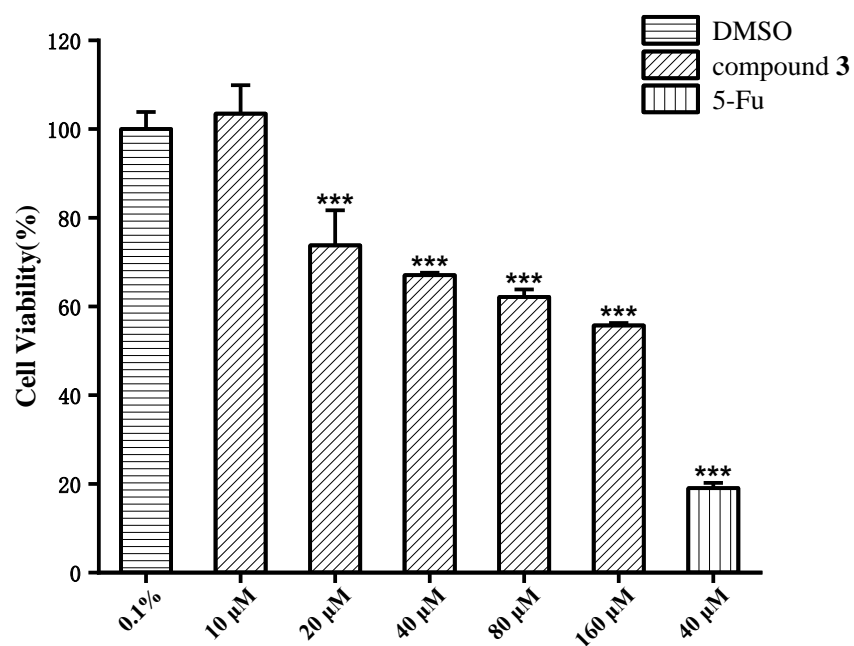


Figure S3. Key NOESY correlations and relative configuration for munropenes E-F (5-6) (protons of methyl groups are omitted).





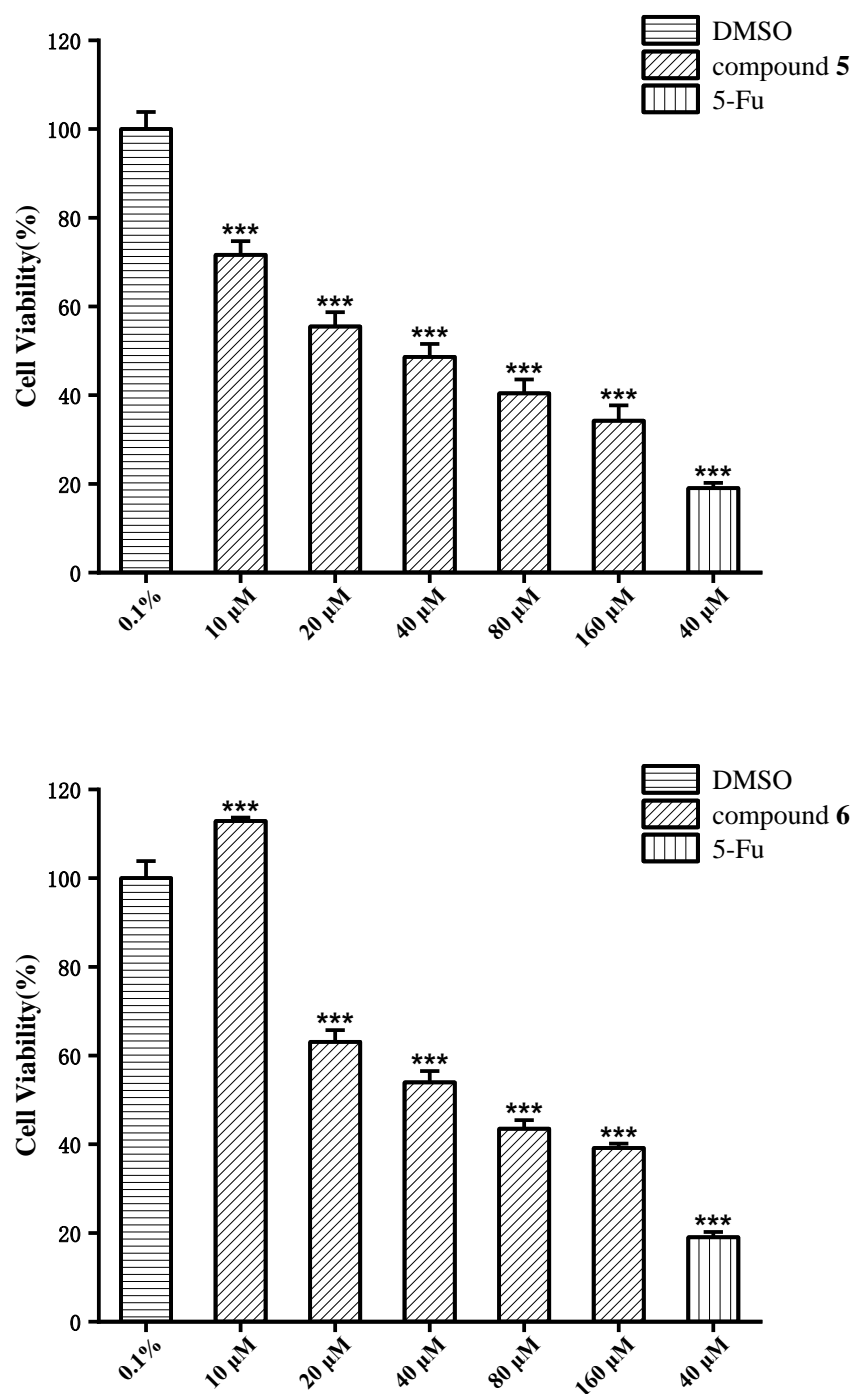


Figure S4. Effects of different concentrations of munropenes A-F (compounds 1-6) proliferation in HCT116 cells at 72 h. Compounds 1-6 were tested at concentration ranges from 10 to 160 μ M, respectively, and 5-Fu (40 μ M) was used as a positive control. Data are represented as the mean \pm SD (n = 3). **p < 0.01, ***p < 0.001 compared to control cells that treated by DMSO. (p < 0.01).

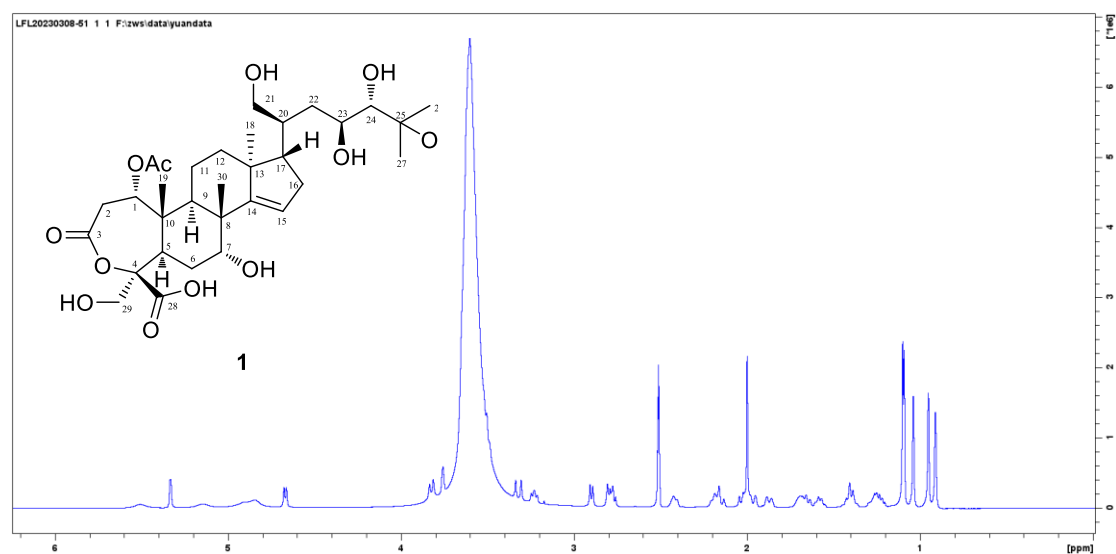


Figure S5. ^1H NMR spectrum of munropene A (**1**) in CD_3OD .

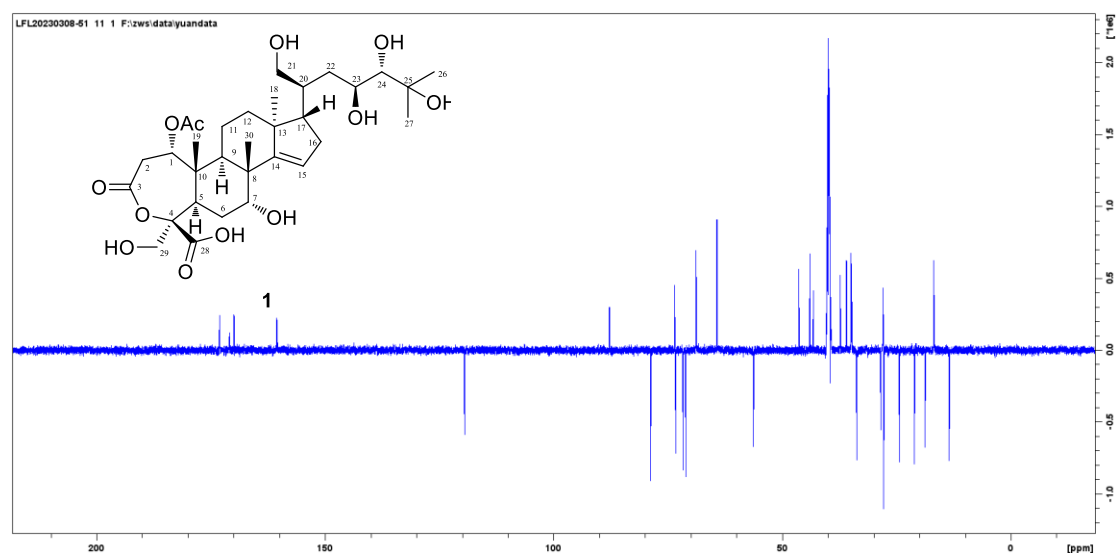


Figure S6. ^{13}C NMR spectrum of munropene A (**1**) in CD_3OD .

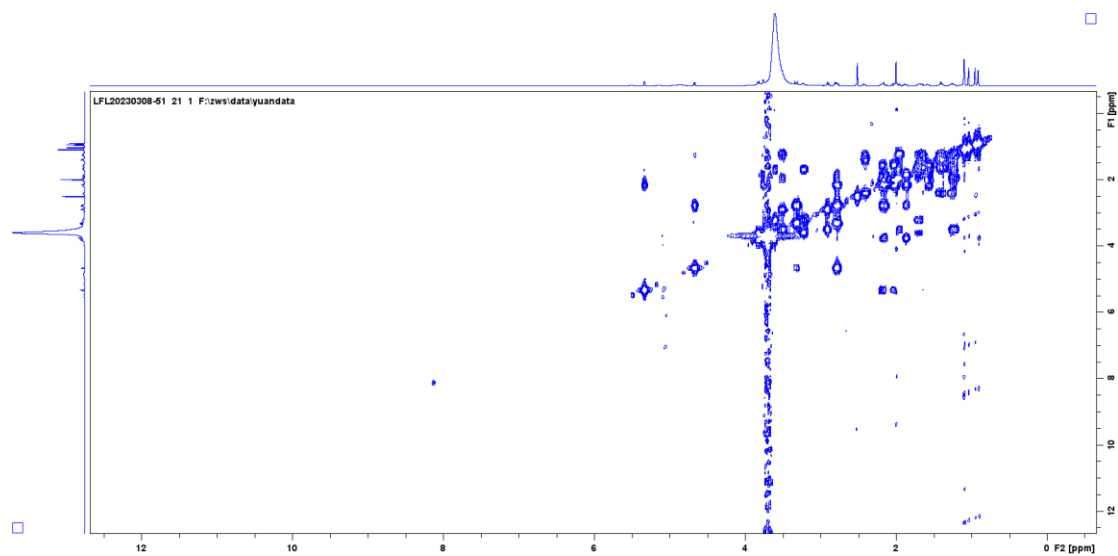


Figure S7. ^1H - ^1H COSY spectrum of munropene A (**1**) in CD_3OD .

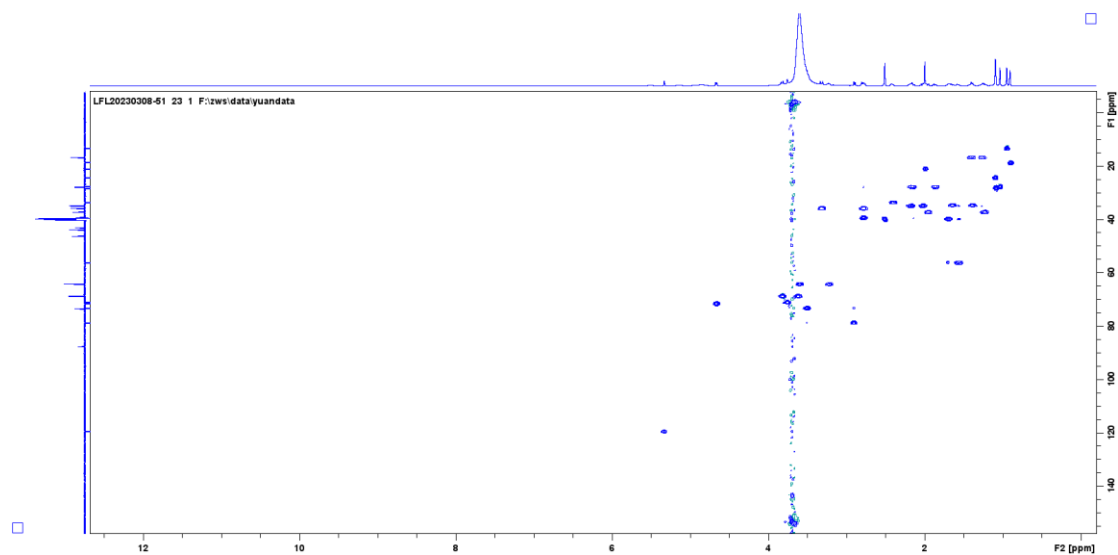


Figure S8. HSQC spectrum of munropene A (**1**) in CD_3OD .

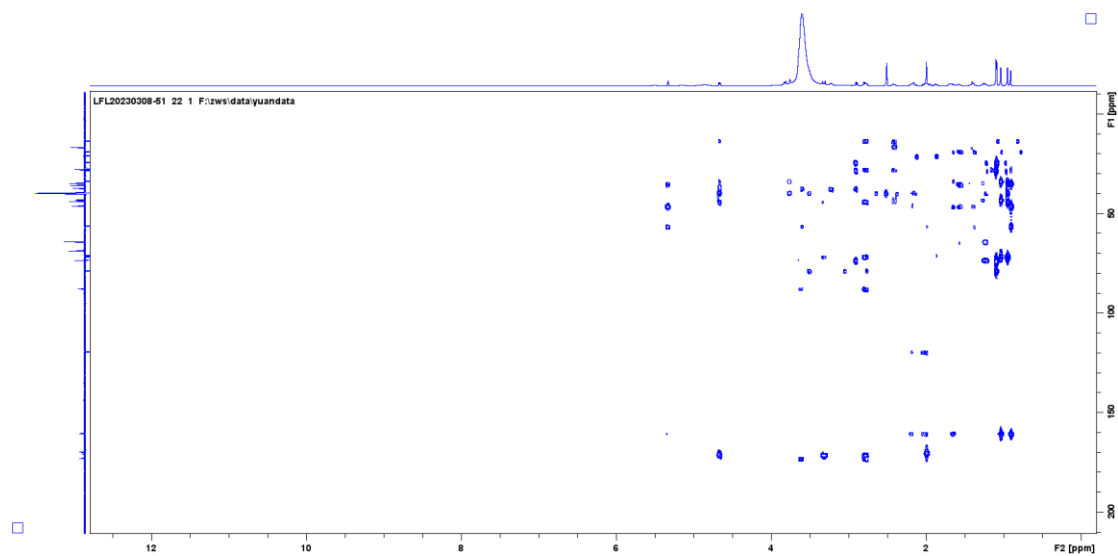


Figure S9. HMBC spectrum of munropene A (1) in CD₃OD.

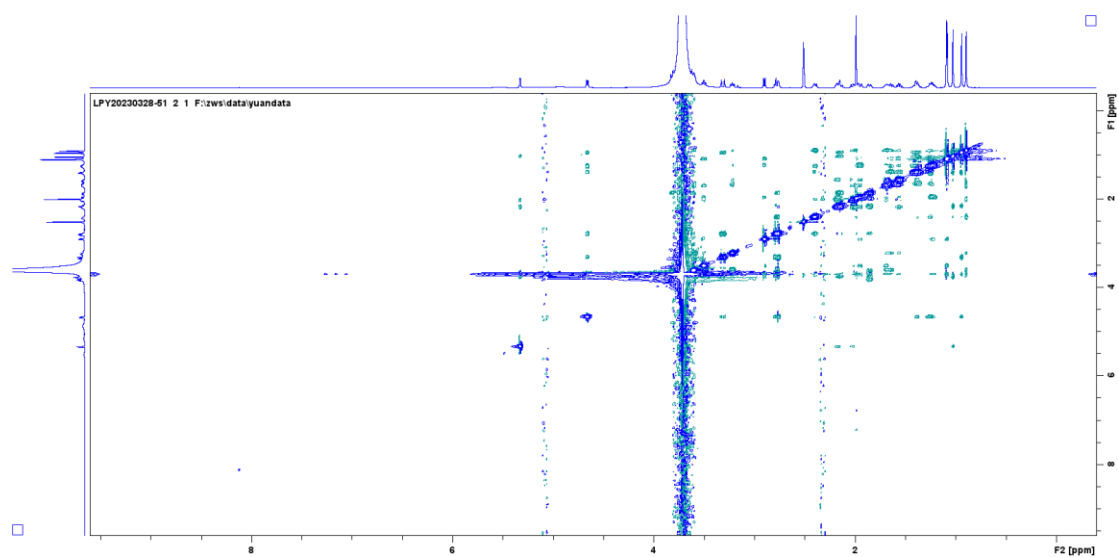


Figure S10. ROESY spectrum of munropene A (1) in CD₃OD.

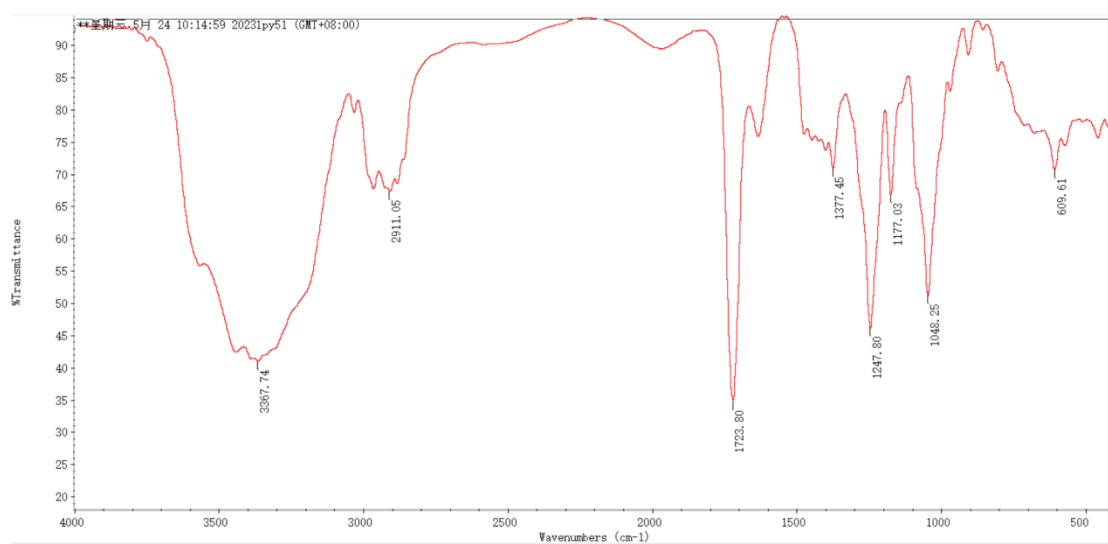


Figure S11. IR spectrum of munropene A (**1**).

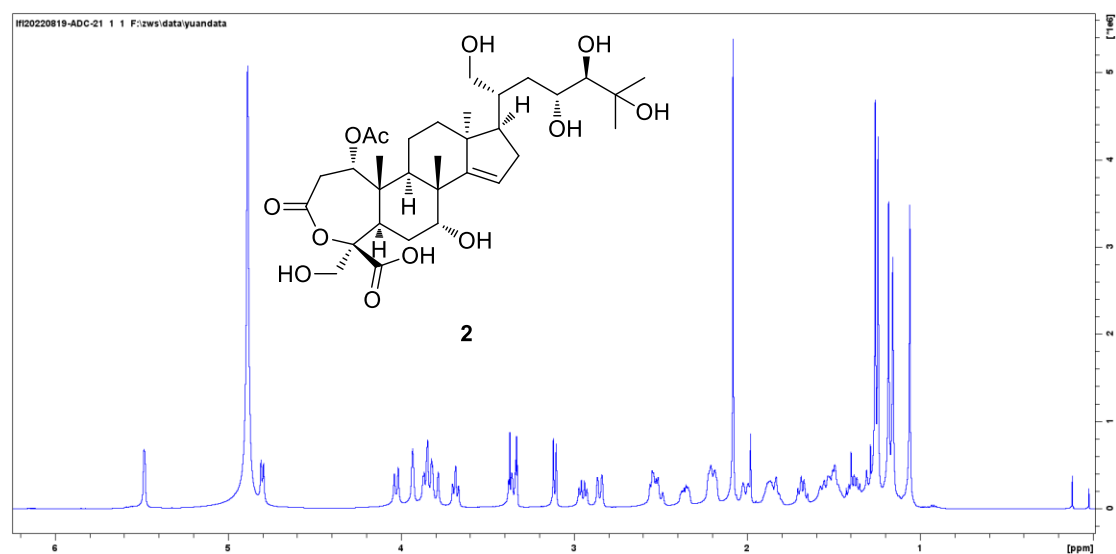


Figure S12. ^1H NMR spectrum of munropene B (2) in CD_3OD .

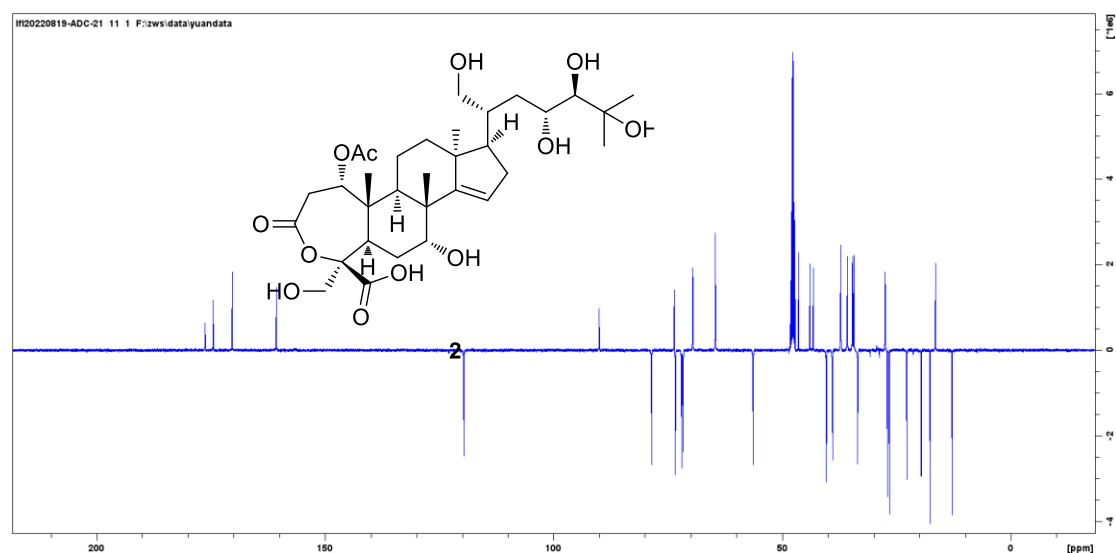


Figure S13. ^{13}C NMR spectrum of munropene B (2) in CD_3OD .

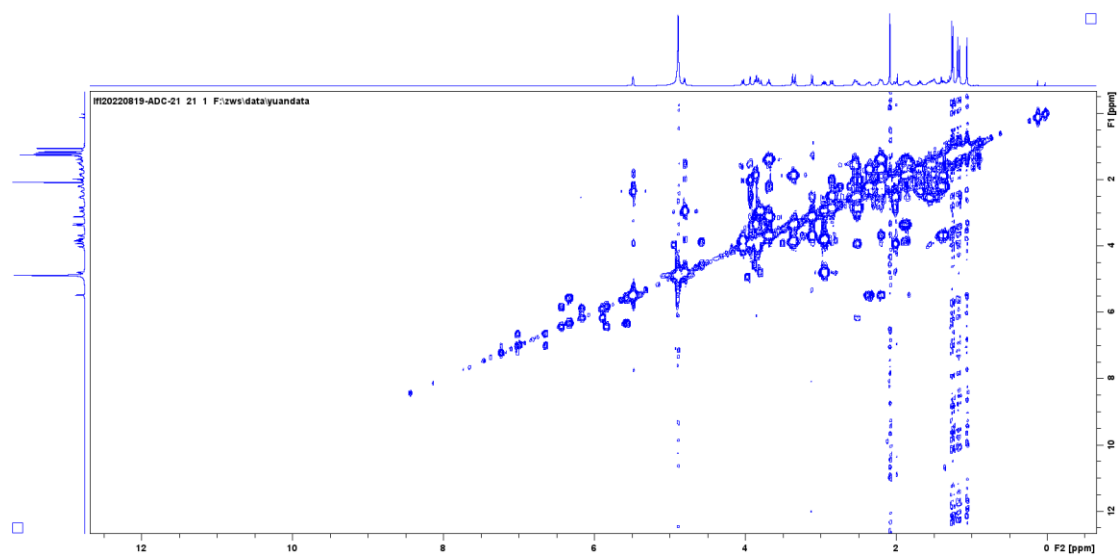


Figure S14. ^1H - ^1H COSY spectrum of munropene B (2) in CD_3OD .

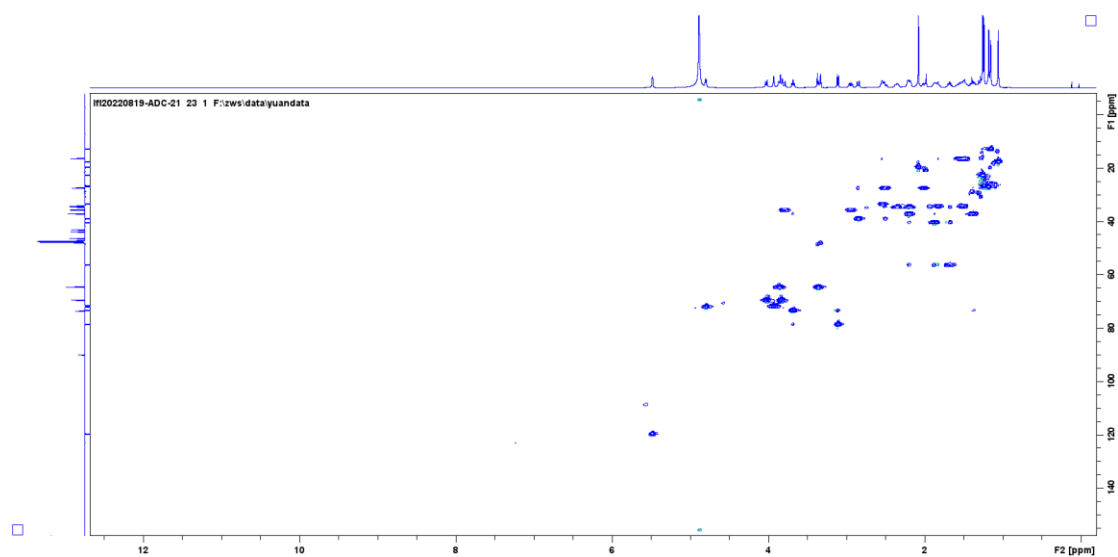


Figure S15. HSQC spectrum of munropene B (2) in CD_3OD .

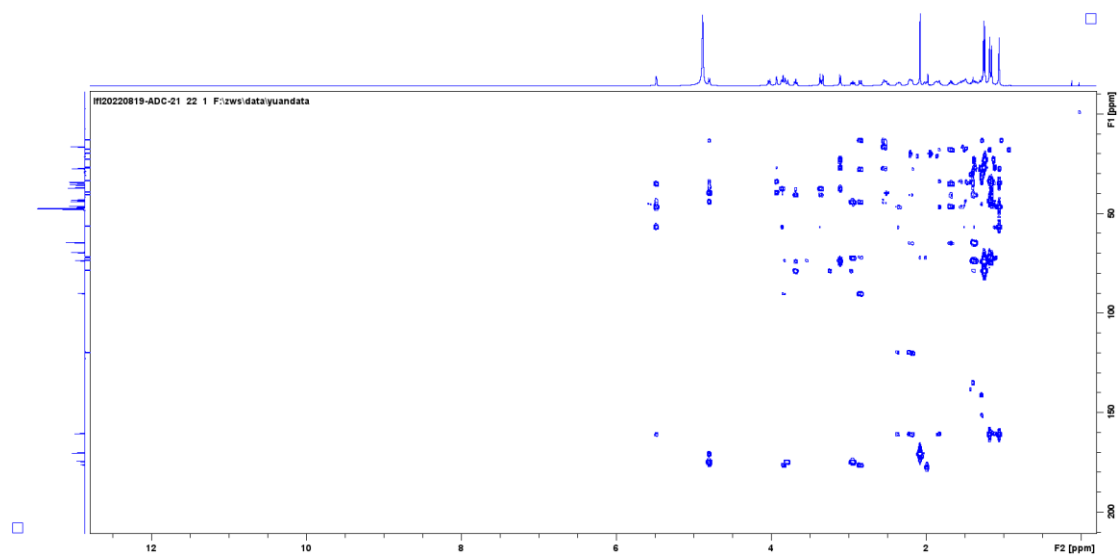


Figure S16. HMBC spectrum of munropene B (2) in CD₃OD.

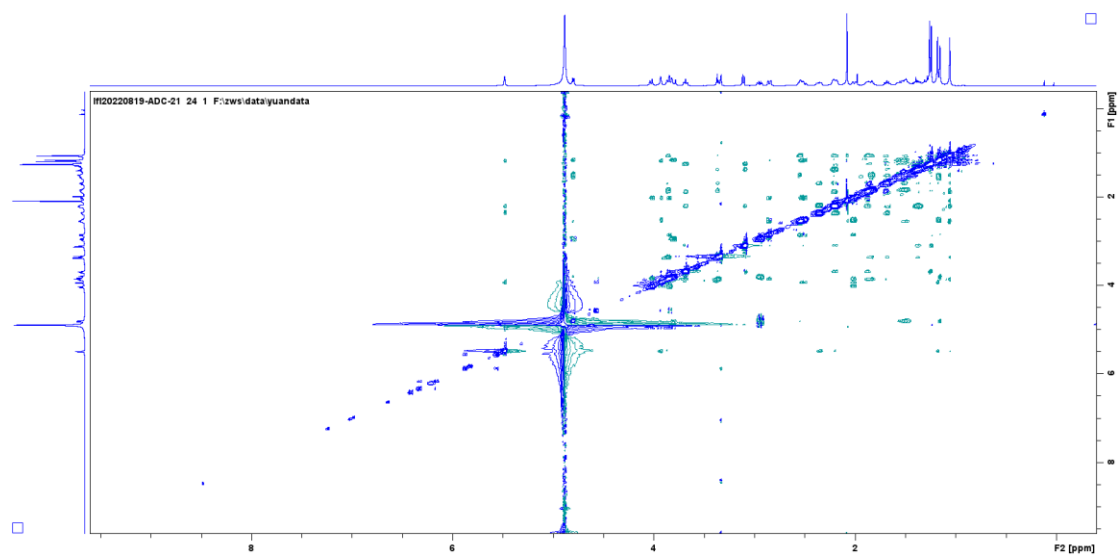


Figure S17. ROESY spectrum of munropene B (2) in CD₃OD.

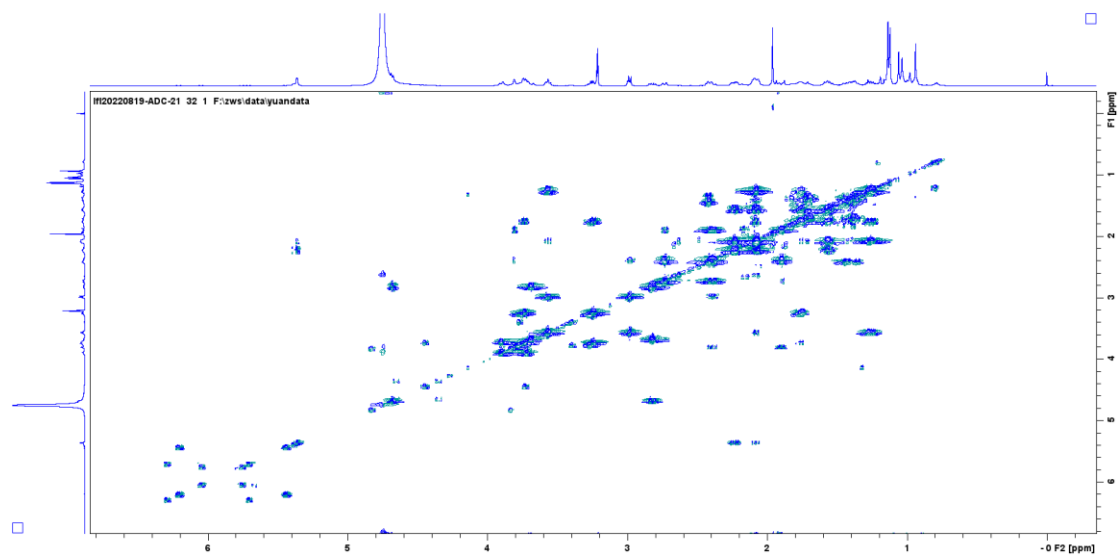


Figure S18. HETLOC spectrum of munropene B (2) in CD₃OD.

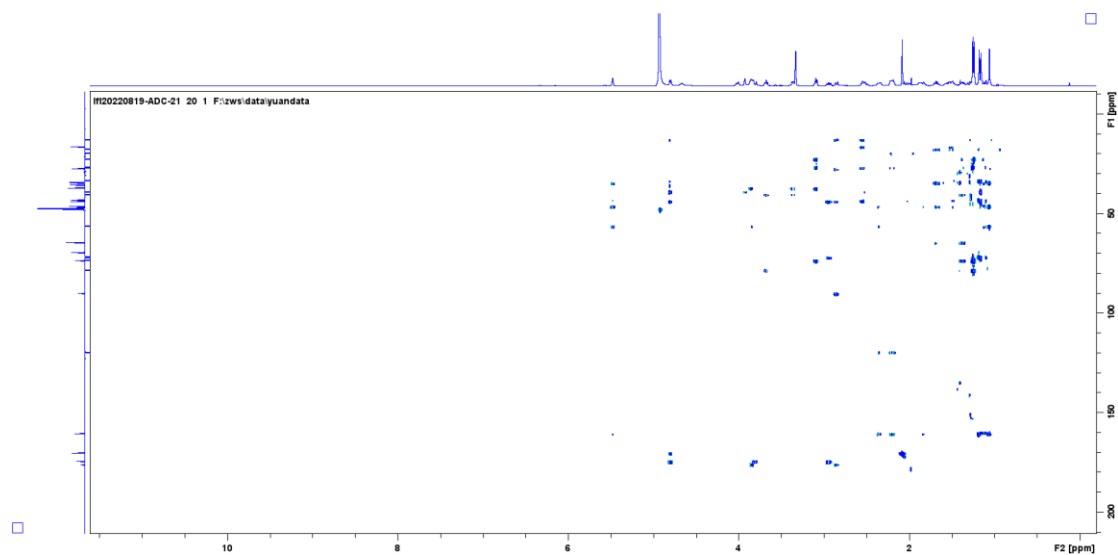


Figure S19. PS-HMBC spectrum of munropene B (2) in CD₃OD.

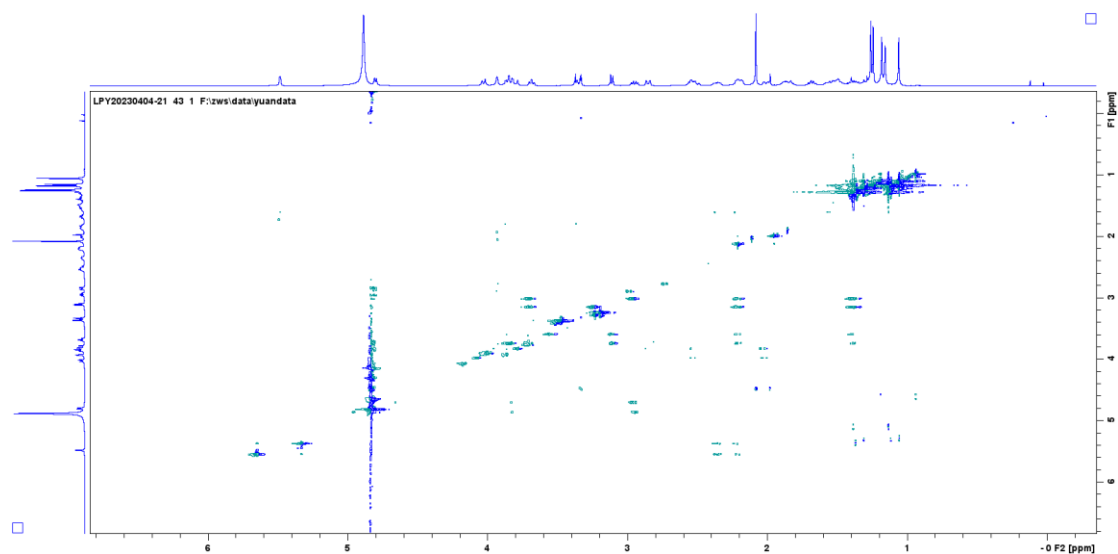
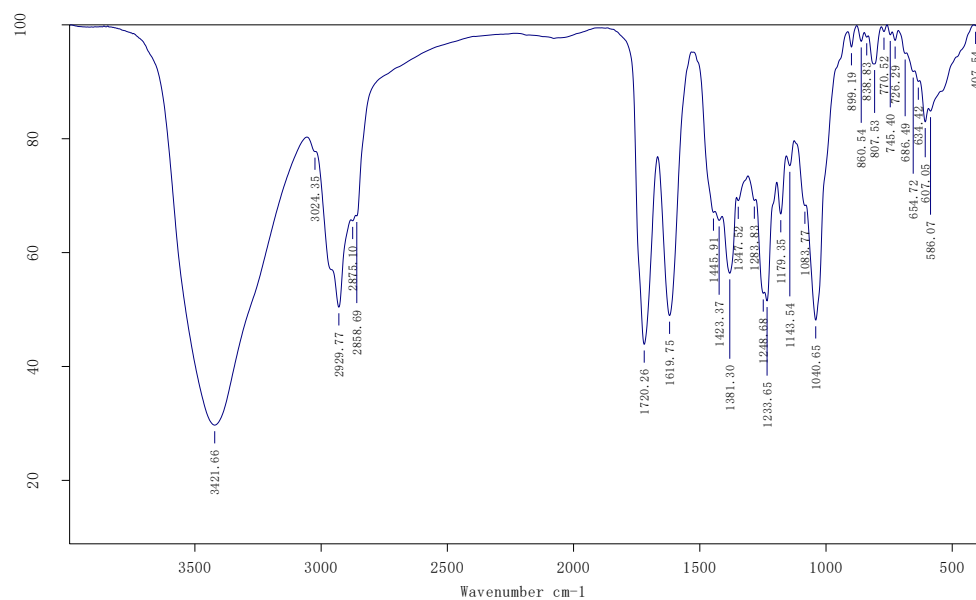


Figure S20. PS-COSY spectrum of munropene B (**2**) in CD₃OD.



Sample Name: 21	Resolution: 4	Beamsplitter Setting: KBr
Sample Form: KBr	Aperture Setting: 6 mm	Source Setting: MIR
Path of File: E:\data	Number of Background Scans: 16	Instrument Type: BRUKER VERTEX 70
Date of Measurement: 2023/1/16	Number of Sample Scans: 16	Soft Version: OPUS8.1

Figure S21. IR spectrum of munropene B (**2**).

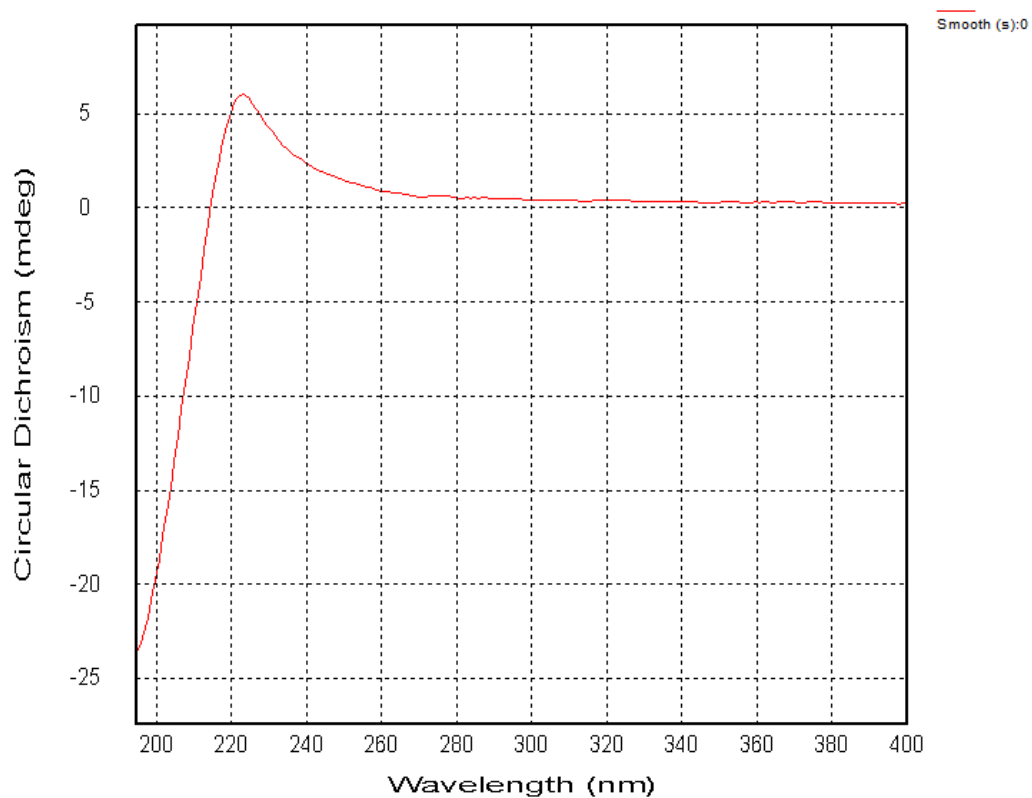


Figure S22. CD spectrum of munropene B (2).

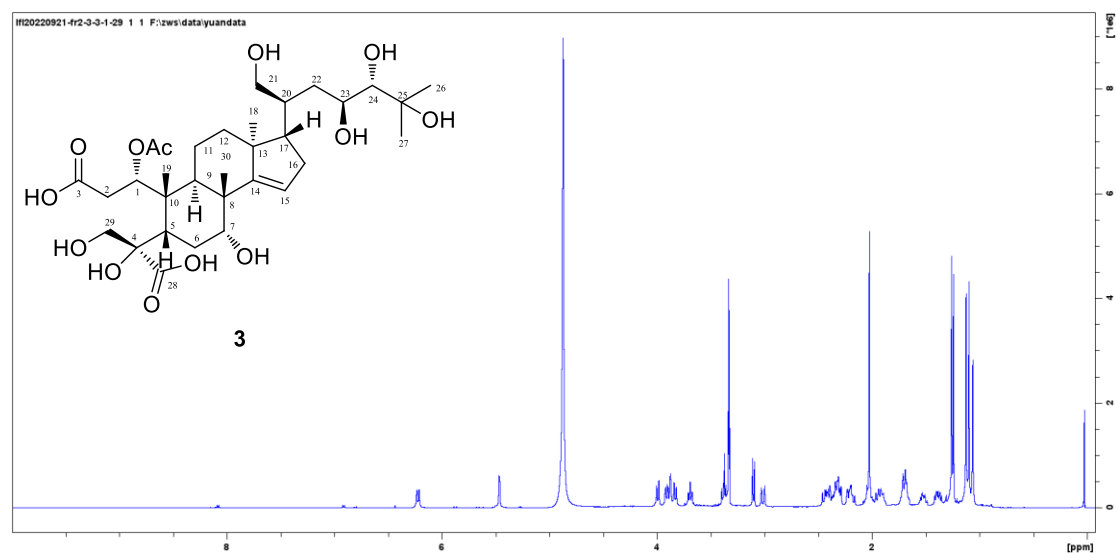


Figure S23. ^1H NMR spectrum of munropene C (3) in CD_3OD .

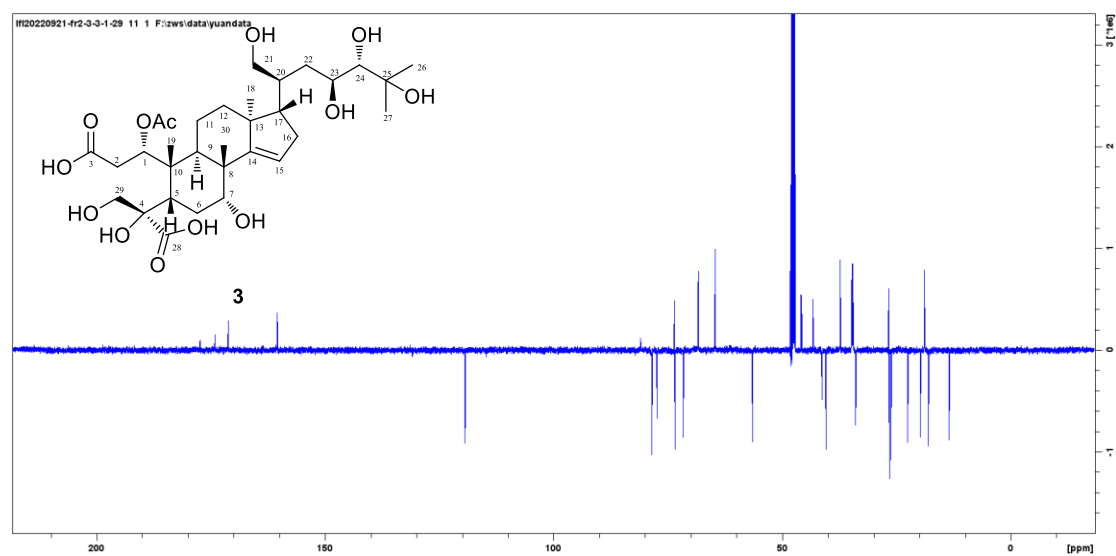


Figure S24. ^{13}C NMR spectrum of munropene C (3) in CD_3OD .

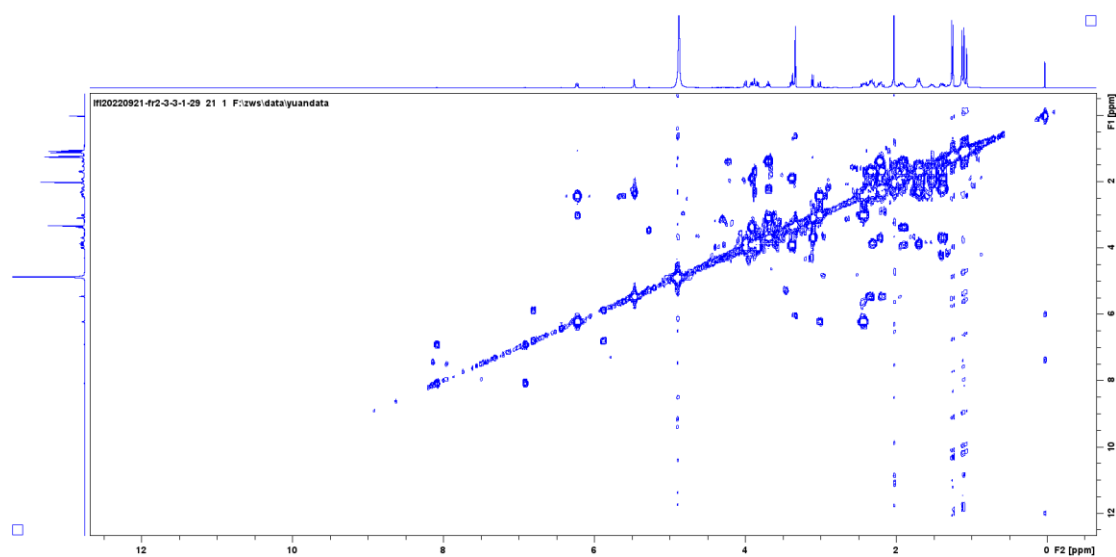


Figure S25. ^1H - ^1H COSY spectrum of munropene C (3) in CD_3OD .

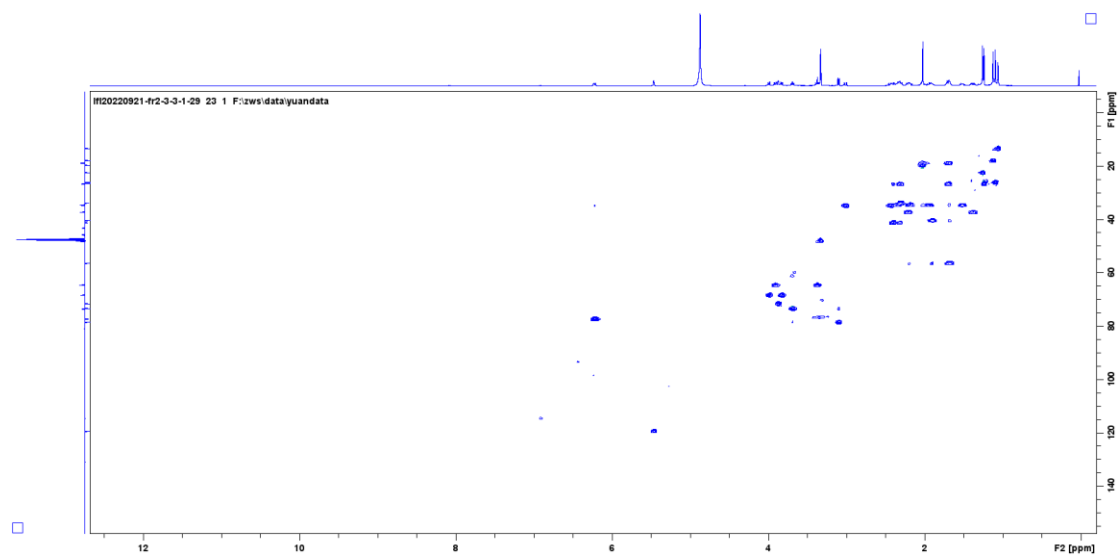


Figure S26. HSQC spectrum of munropene C (3) in CD₃OD.

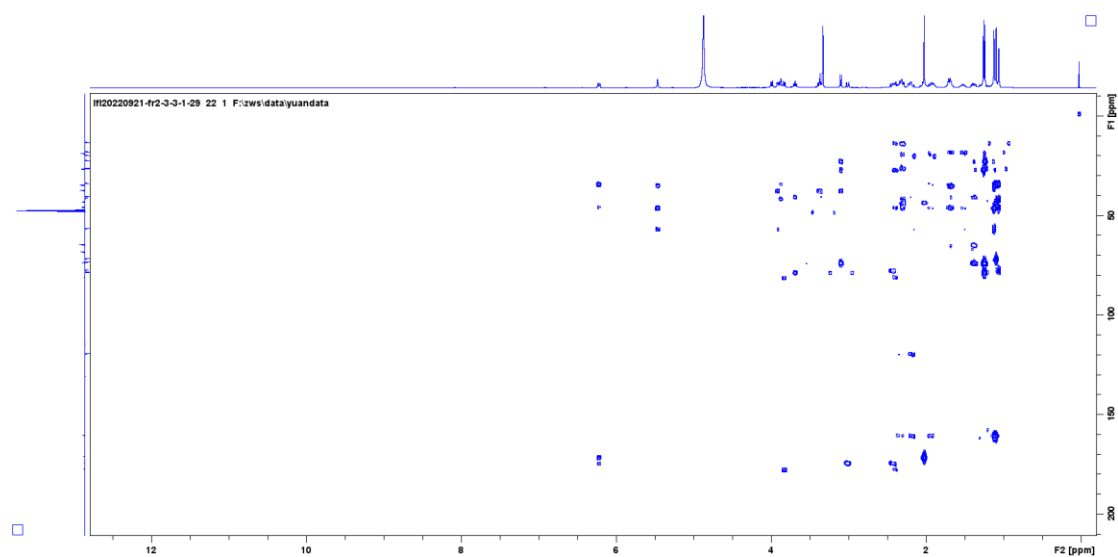


Figure S27. HMBC spectrum of munropene C (3) in CD₃OD.

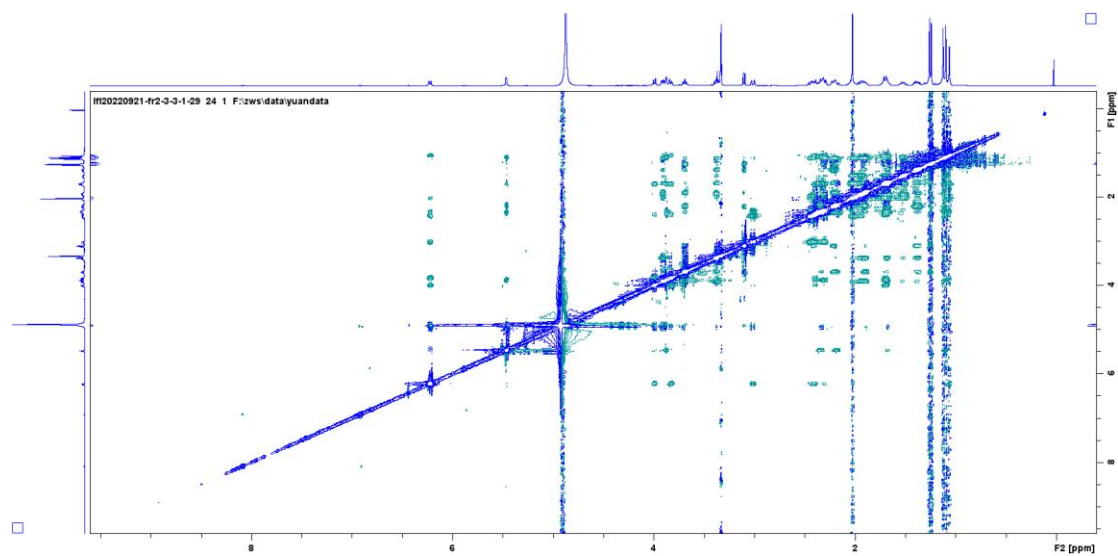


Figure S28. ROESY spectrum of munropene C (3) in CD₃OD.

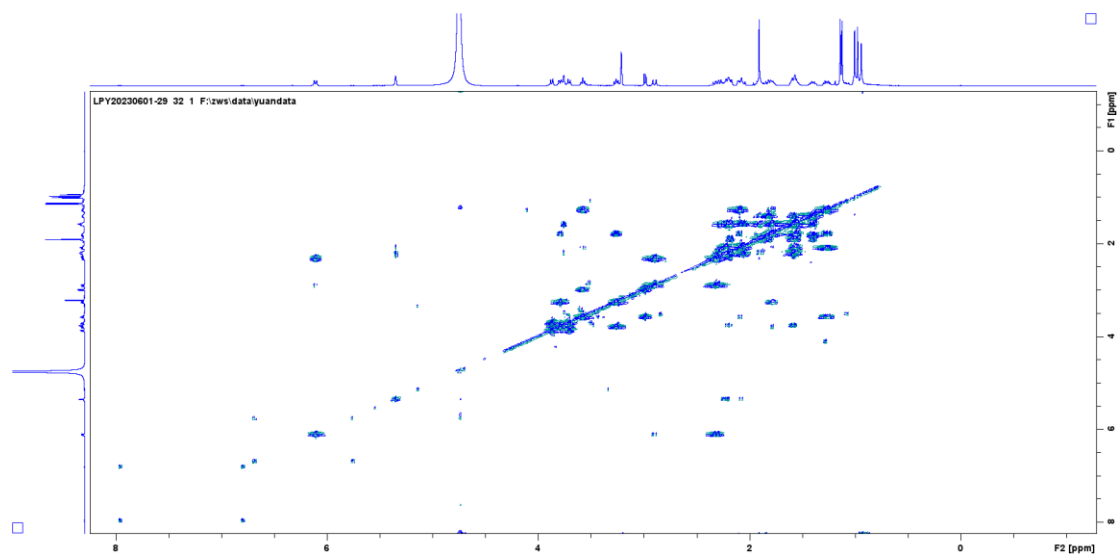


Figure S29. HETLOC spectrum of munropene C (3) in CD₃OD.

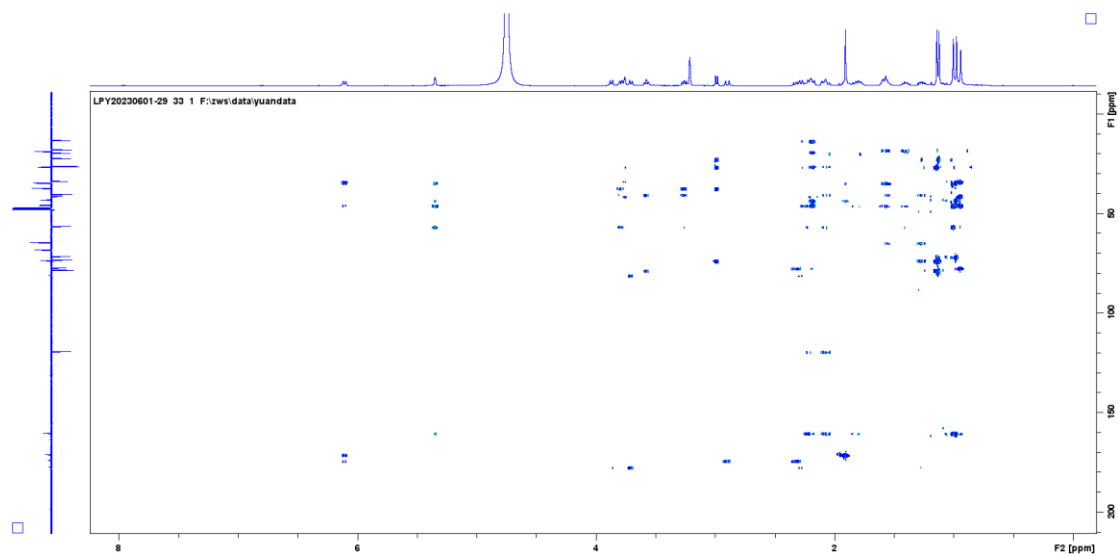


Figure S30. PS-HMBC spectrum of munropene C (3) in CD₃OD.

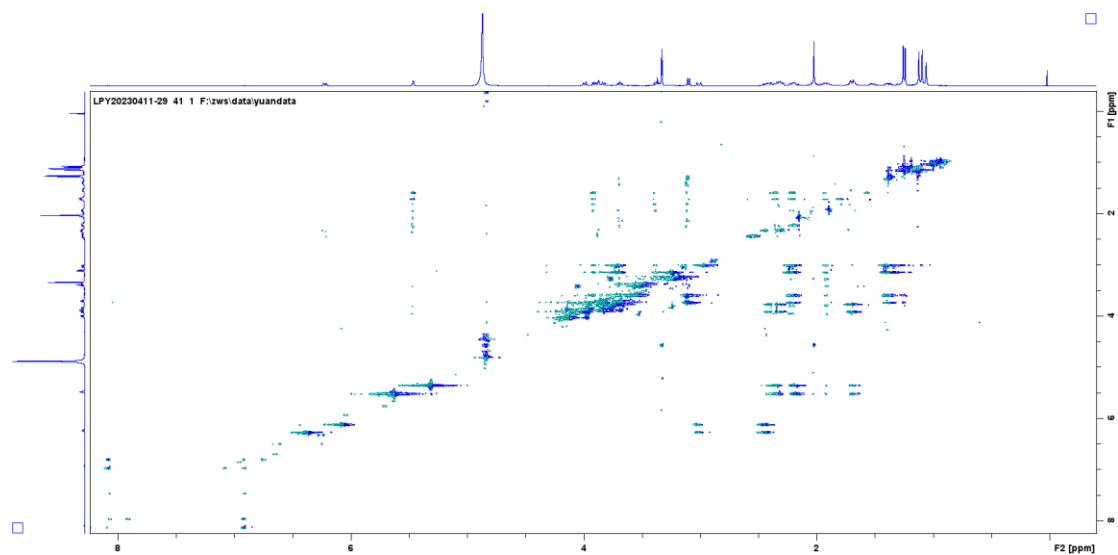


Figure S31. PS-COSY spectrum of munropene C (3) in CD₃OD.

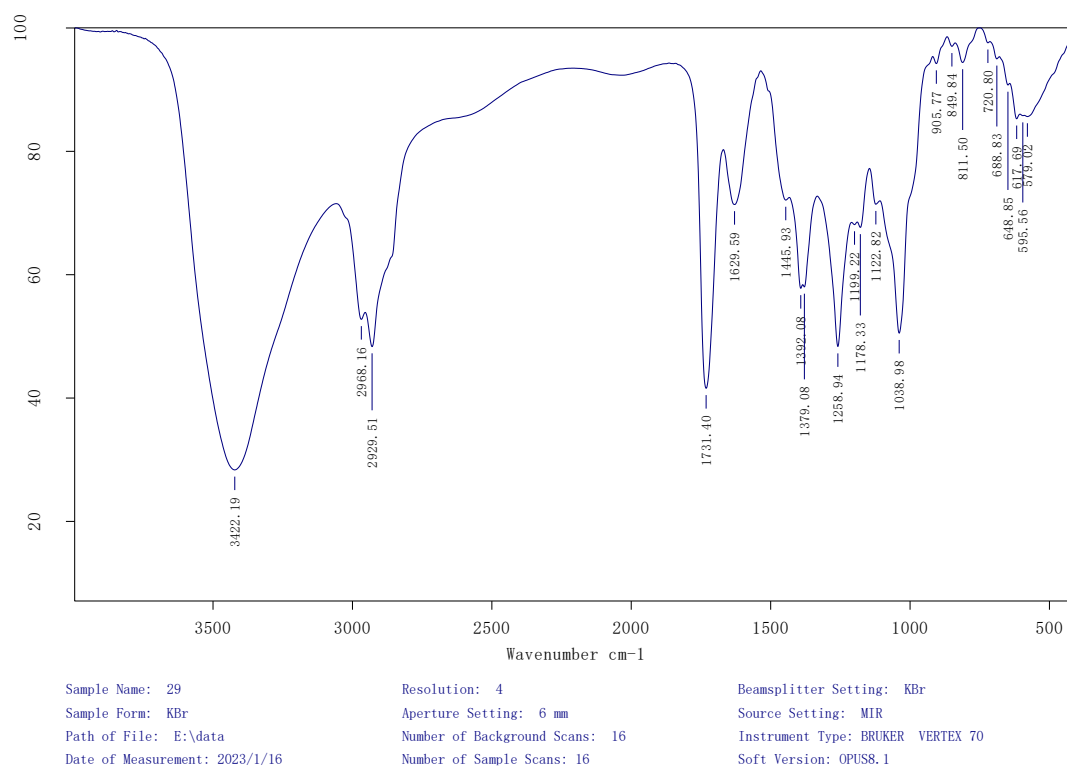


Figure S32. IR spectrum of munropene C (3).

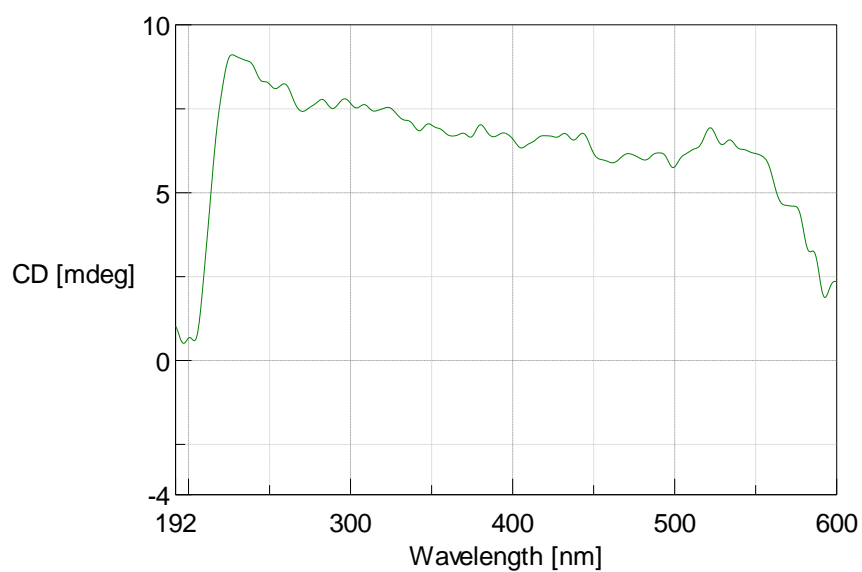


Figure S33. CD spectrum of munropene C (3).

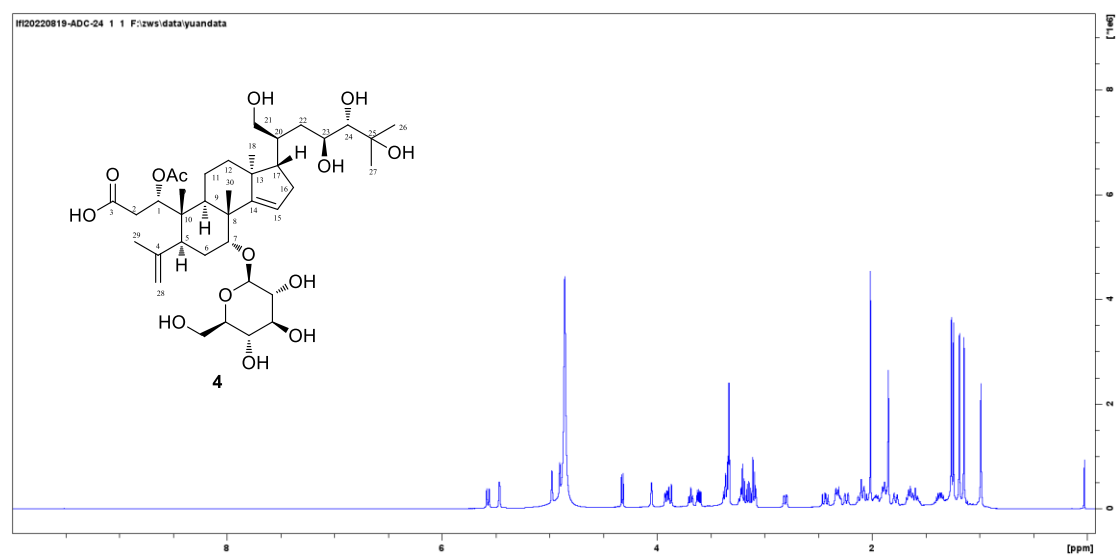


Figure S34. ^1H NMR spectrum of munropene D (**4**) in CD_3OD .

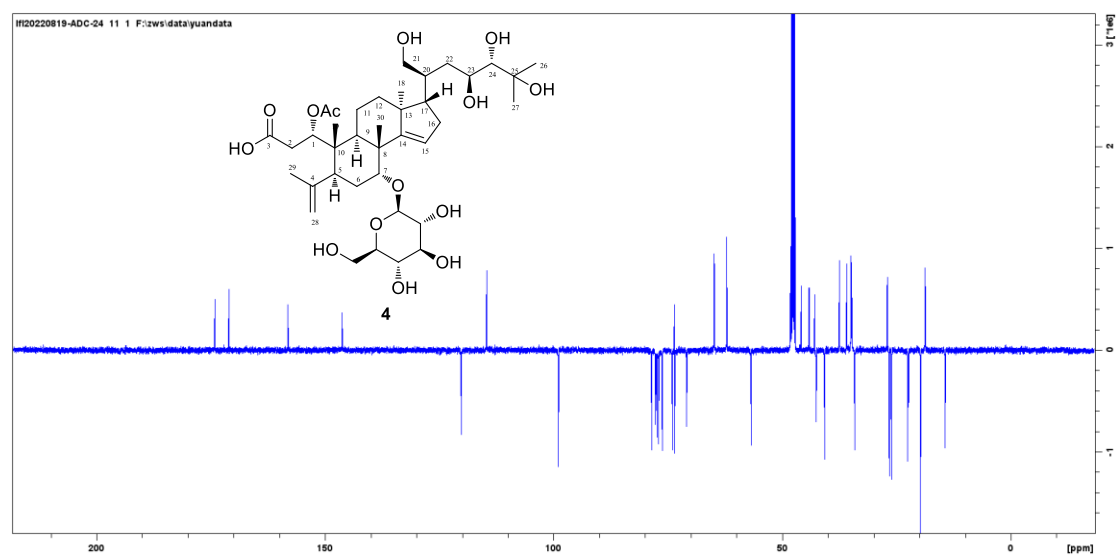


Figure S35. ^{13}C NMR spectrum of munropene D (**4**) in CD_3OD .

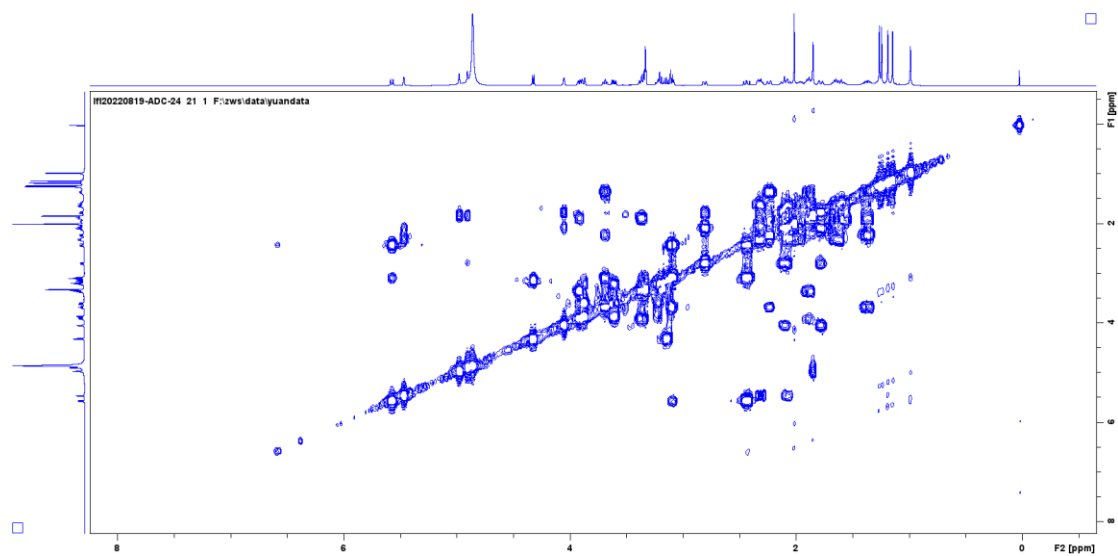


Figure S36. ^1H – ^1H COSY spectrum of munropene D (**4**) in CD_3OD .

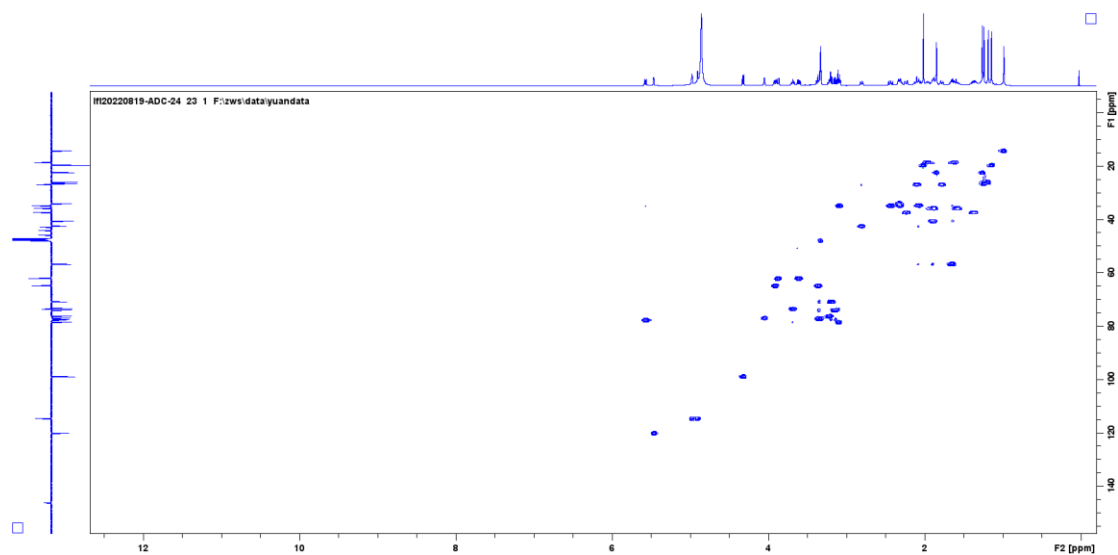


Figure S37. HSQC spectrum of munropene D (**4**) in CD_3OD .

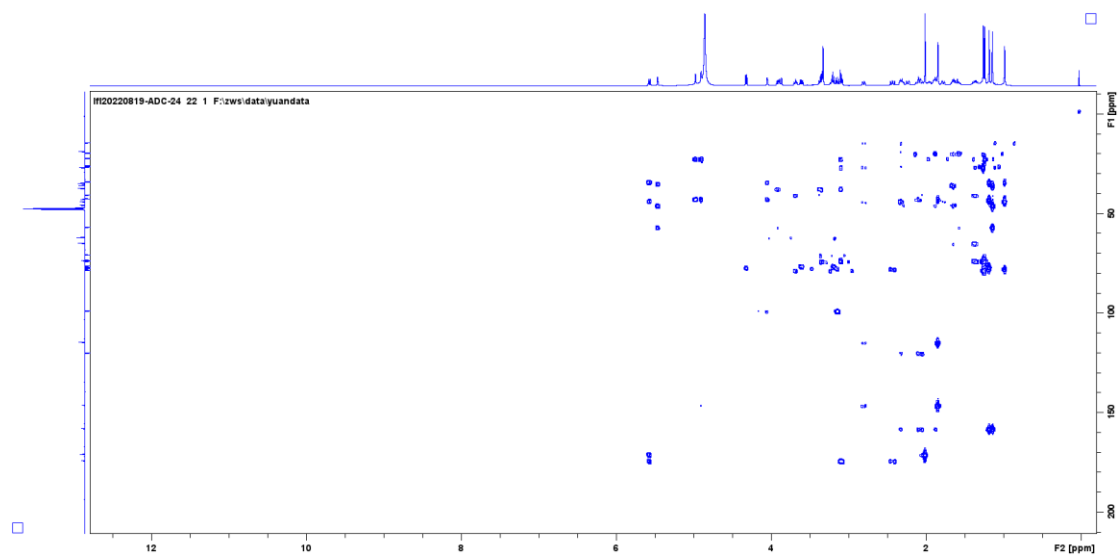


Figure S38. HMBC spectrum of munropene D (4) in CD₃OD.

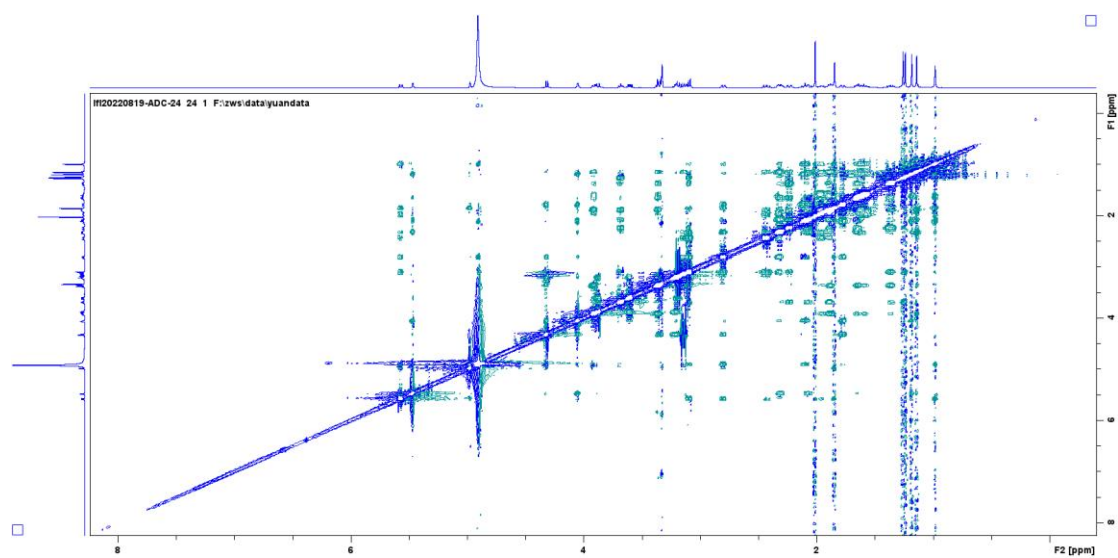


Figure S39. ROESY spectrum of munropene D (4) in CD₃OD.

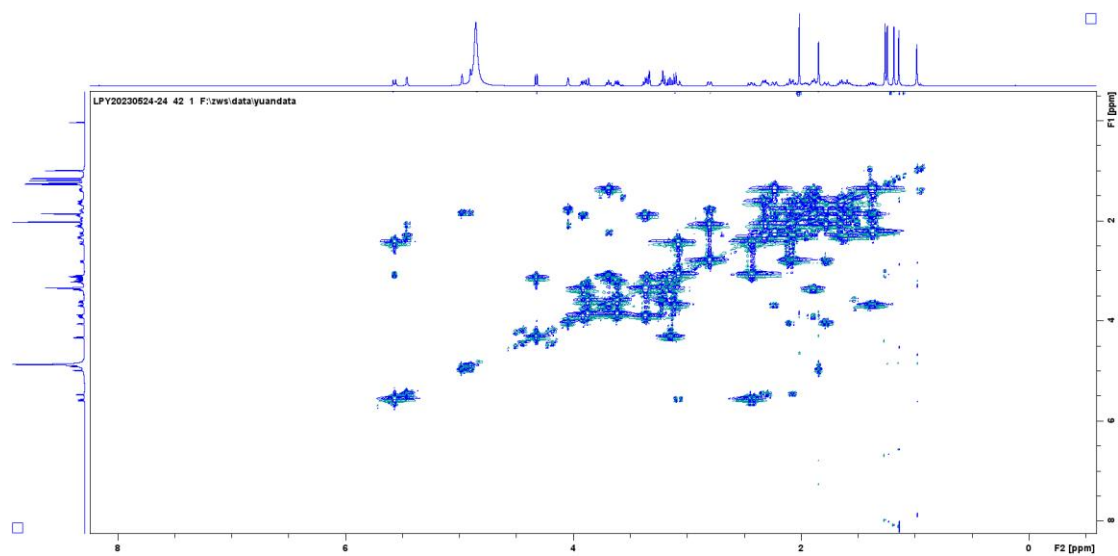


Figure S40. HETLOC spectrum of munropene D (4) in CD₃OD.

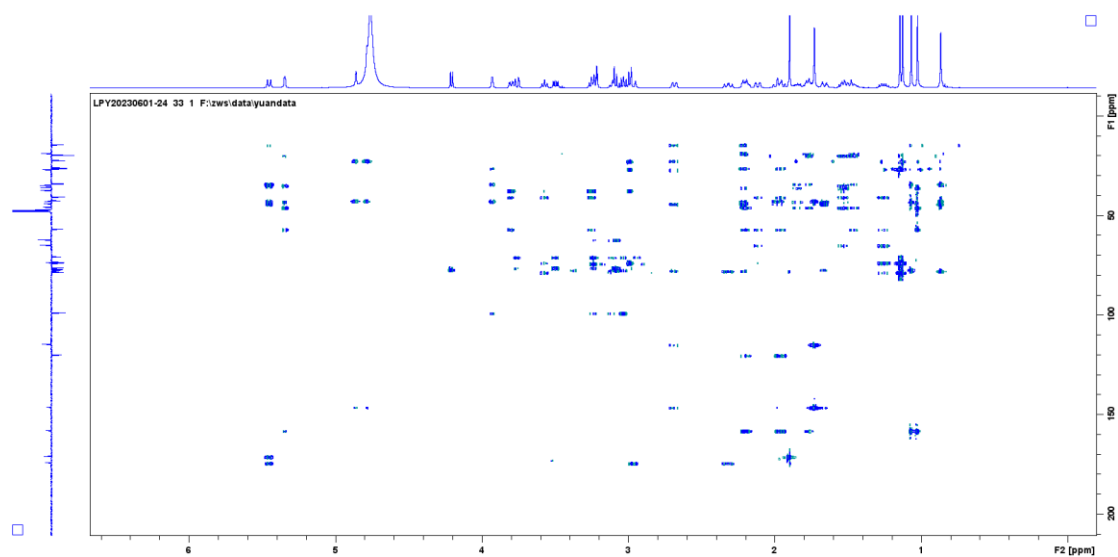


Figure S41. PS-HMBC spectrum of munropene D (4) in CD₃OD.

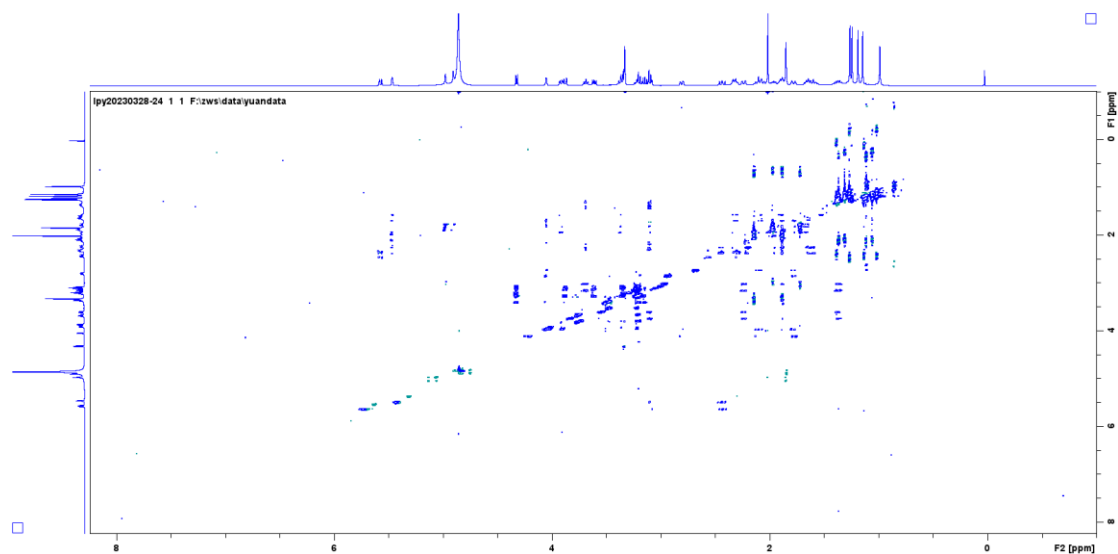
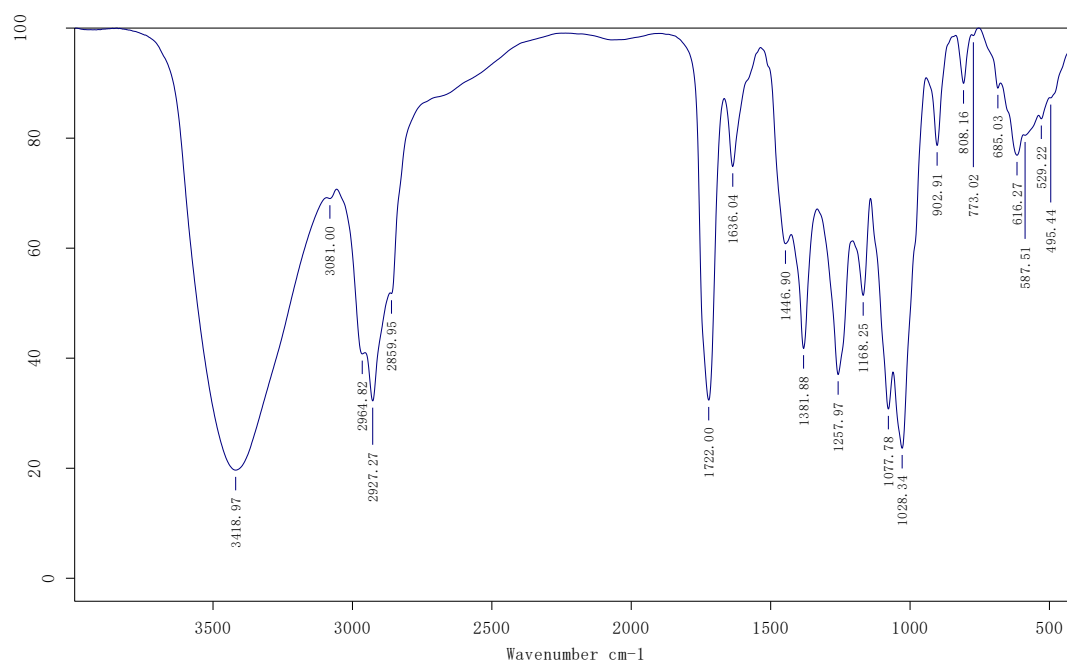


Figure S42. PS-COSY spectrum of munropene D (**4**) in CD₃OD.



Sample Name: 24

Sample Form: KBr

Path of File: E:\data

Date of Measurement: 2023/1/16

Resolution: 4

Aperture Setting: 6 mm

Number of Background Scans: 16

Number of Sample Scans: 16

Beamsplitter Setting: KBr

Source Setting: MIR

Instrument Type: BRUKER VERTEX 70

Soft Version: OPUS8.1

Figure S43. IR spectrum of munropene D (**4**).

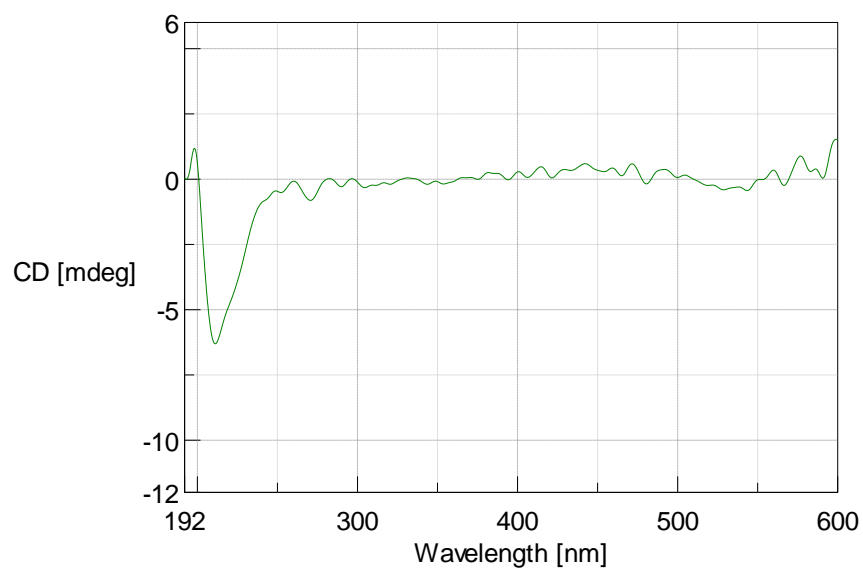


Figure S44. CD spectrum of munropene D (**4**).

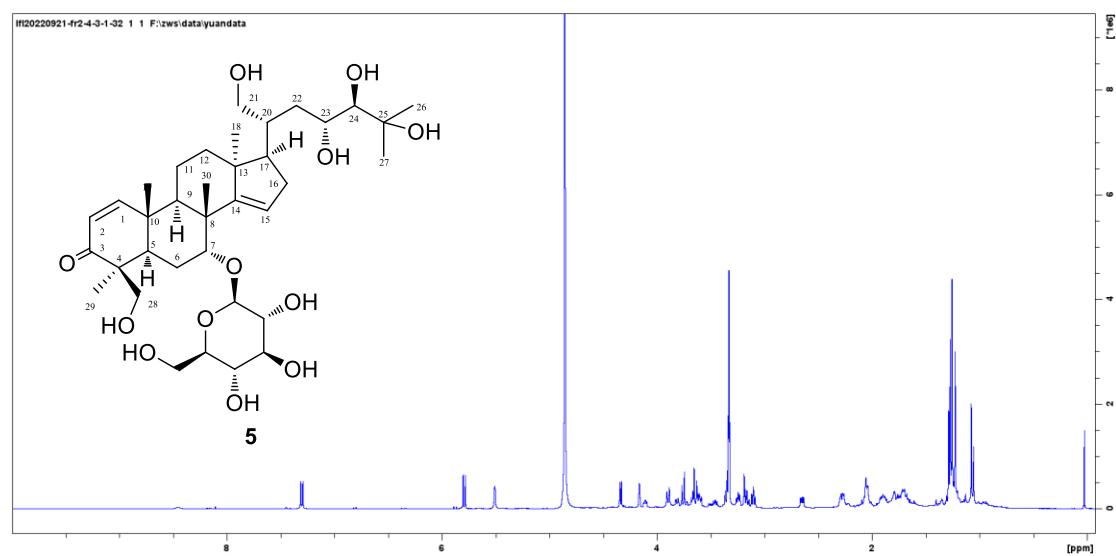


Figure S45. ^1H NMR spectrum of munropene E (5) in CD_3OD .

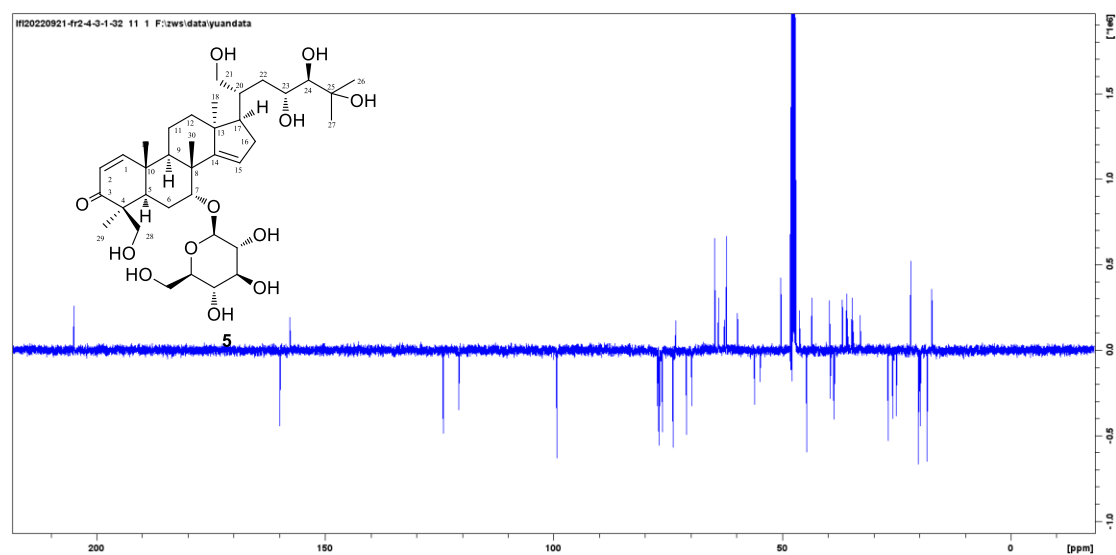


Figure S46. ^{13}C NMR spectrum of munropene E (5) in CD_3OD .

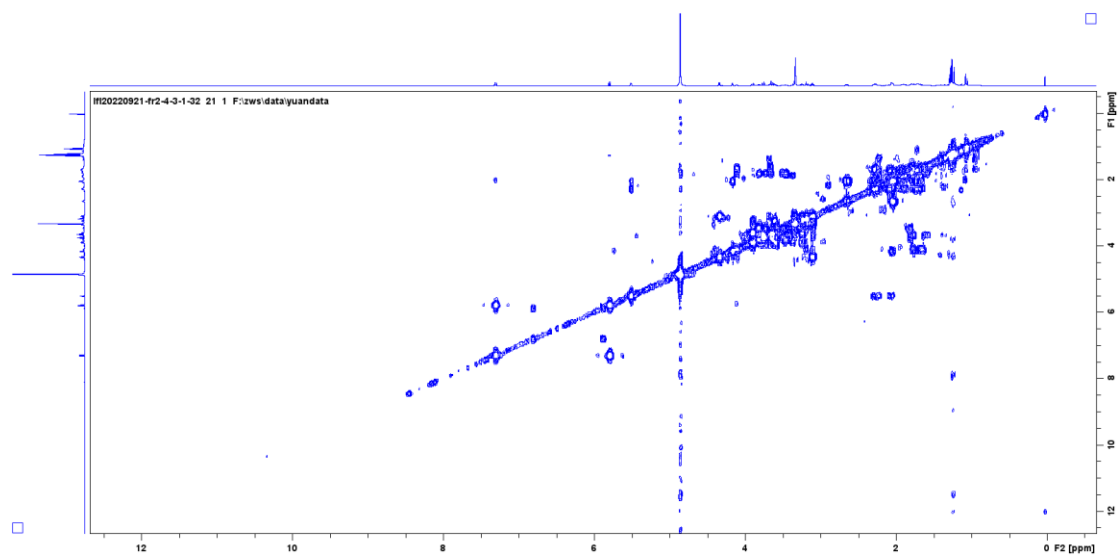


Figure S47. ^1H - ^1H COSY spectrum of munropene E (5) in CD_3OD .

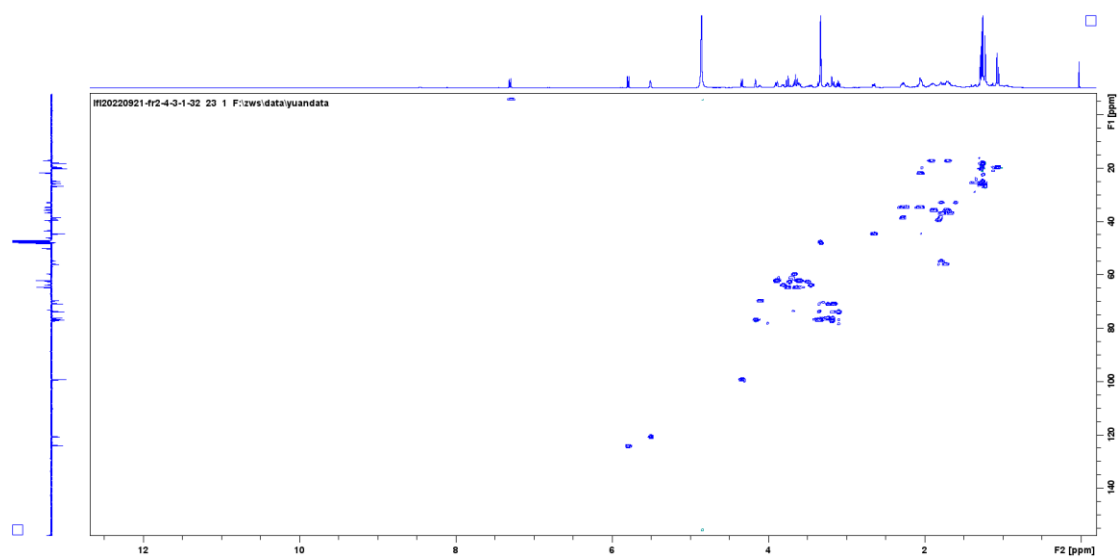


Figure S48. HSQC spectrum of munropene E (5) in CD_3OD .

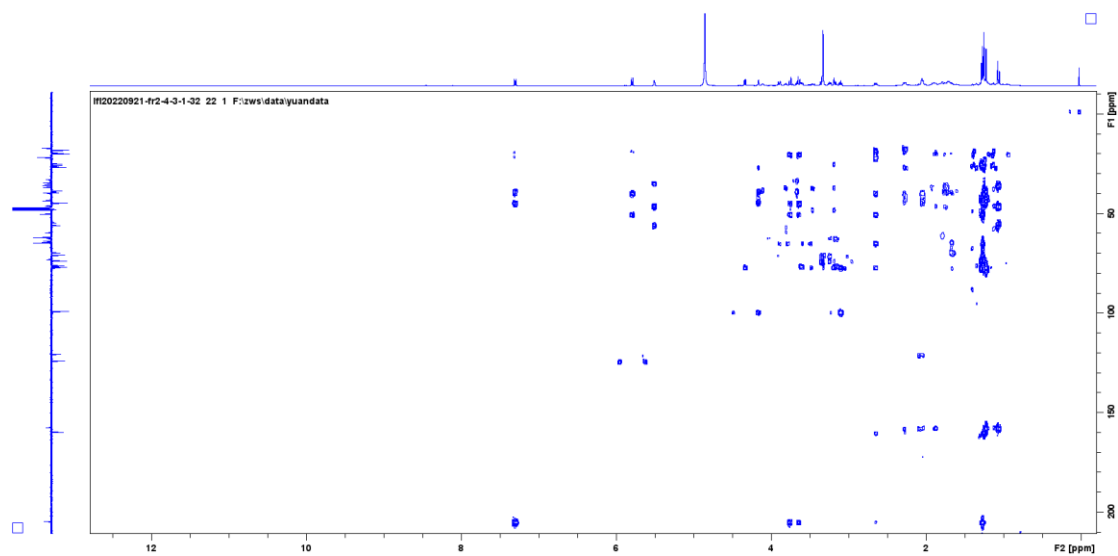


Figure S49. HMBC spectrum of munropene E (5) in CD₃OD.

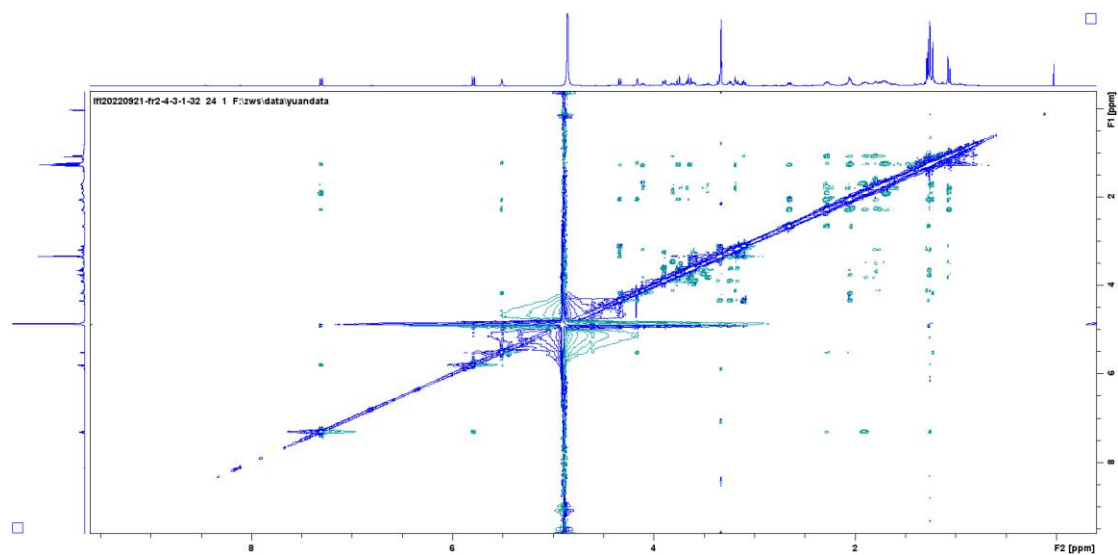


Figure S50. ROESY spectrum of munropene E (5) in CD₃OD.

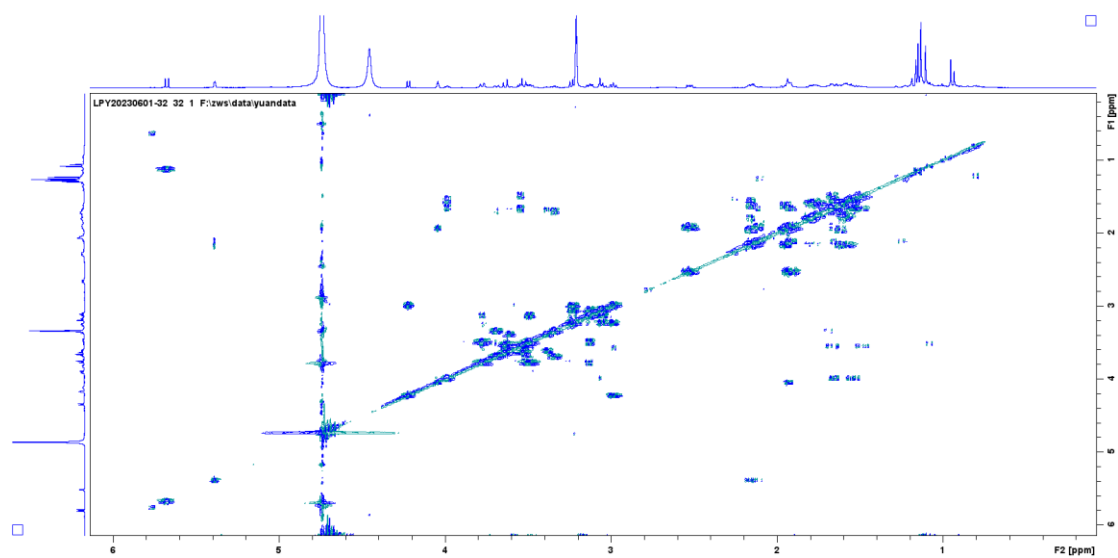


Figure S51. HETLOC spectrum of munropene E (5) in CD₃OD.

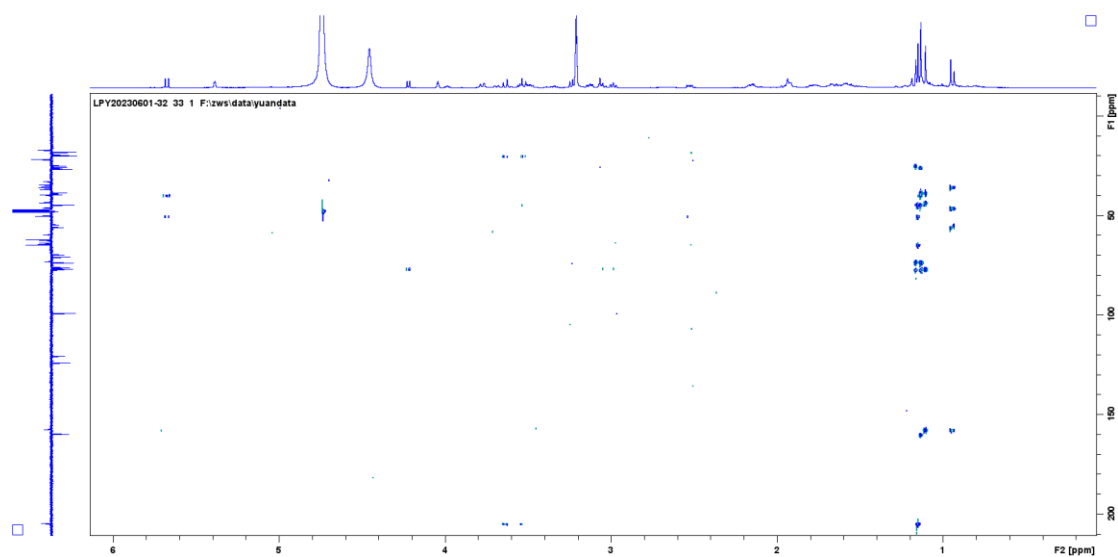


Figure S52. PS-HMBC spectrum of munropene E (5) in CD₃OD.

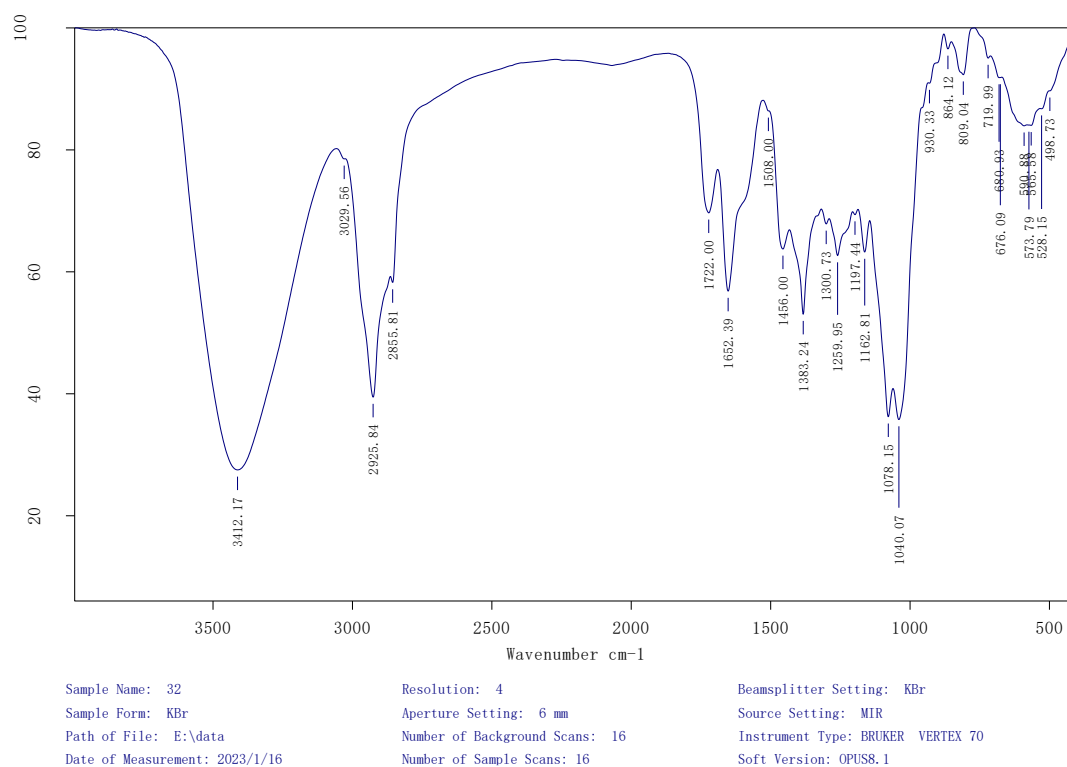
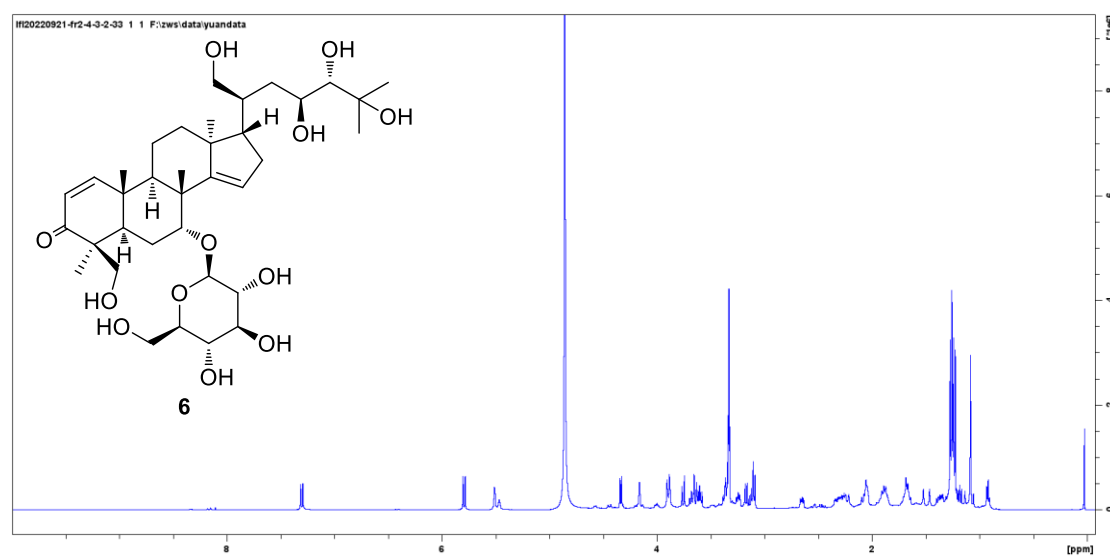


Figure S53. IR spectrum of munropene E (5).



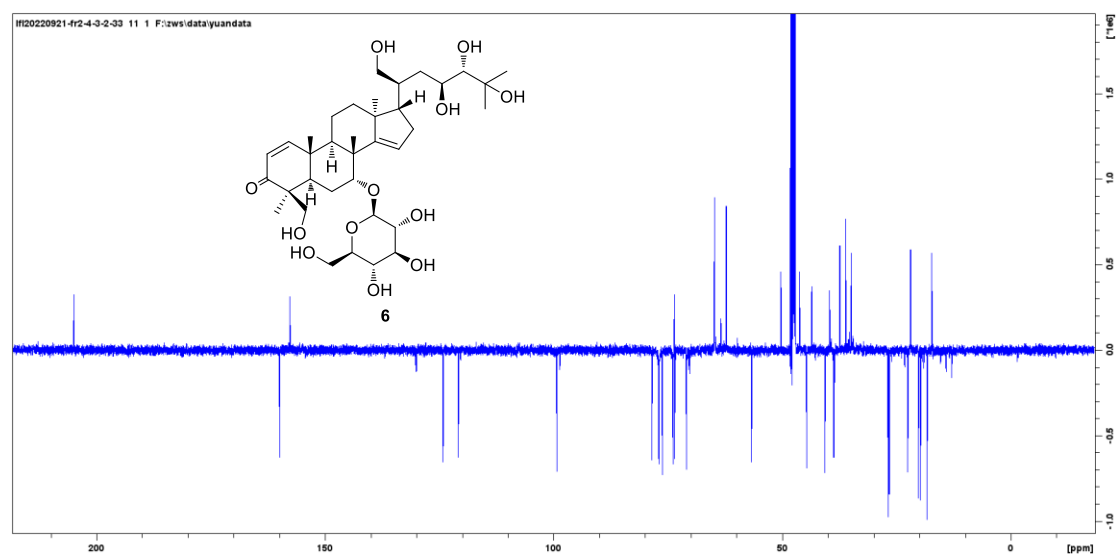


Figure S55. ^{13}C NMR spectrum of munropene F (6) in CD_3OD .

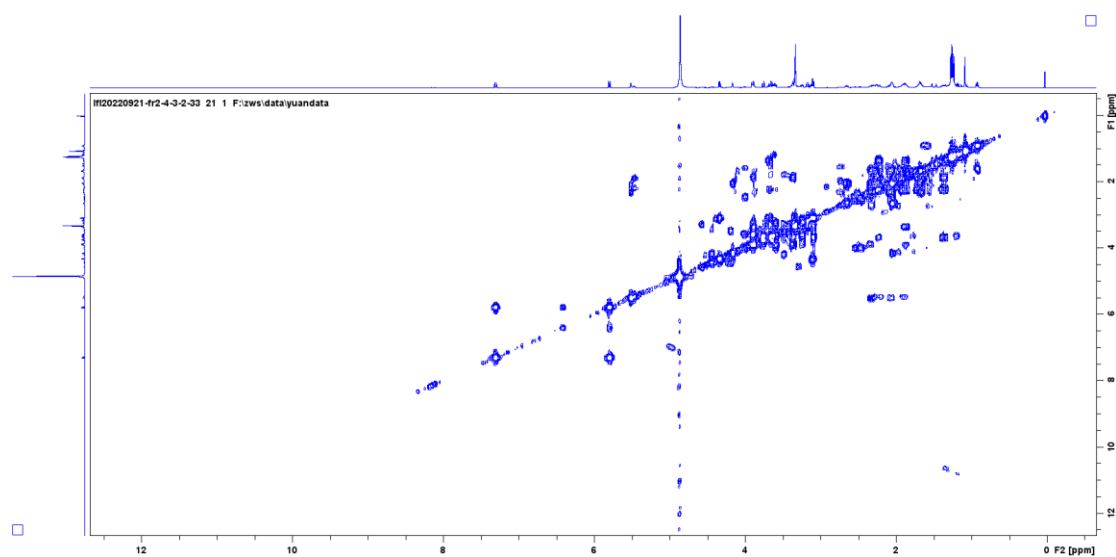


Figure S56. ^1H - ^1H COSY spectrum of munropene F (6) in CD_3OD .

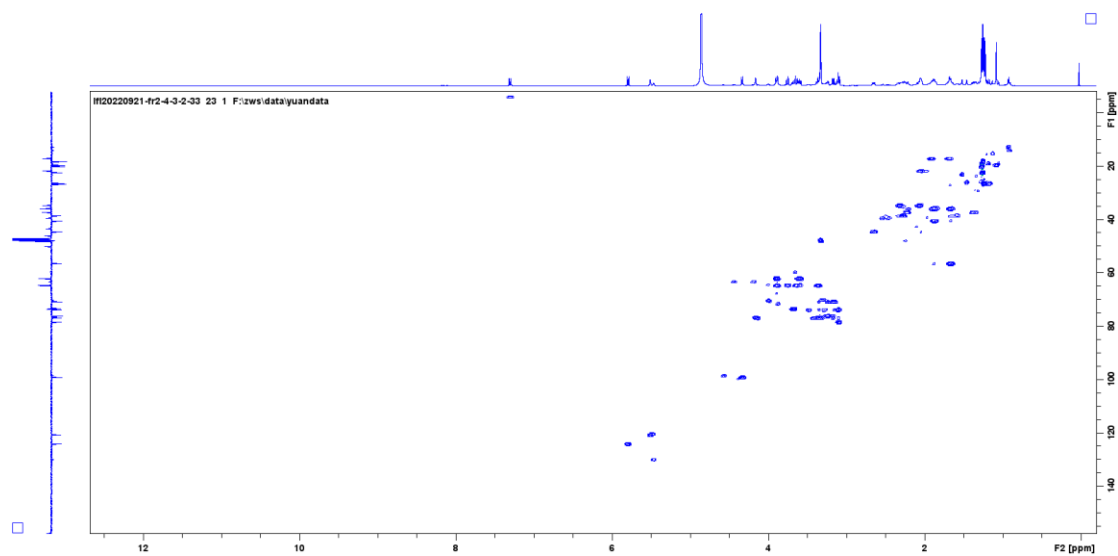


Figure S57. HSQC spectrum of munropene F (6) in CD₃OD.

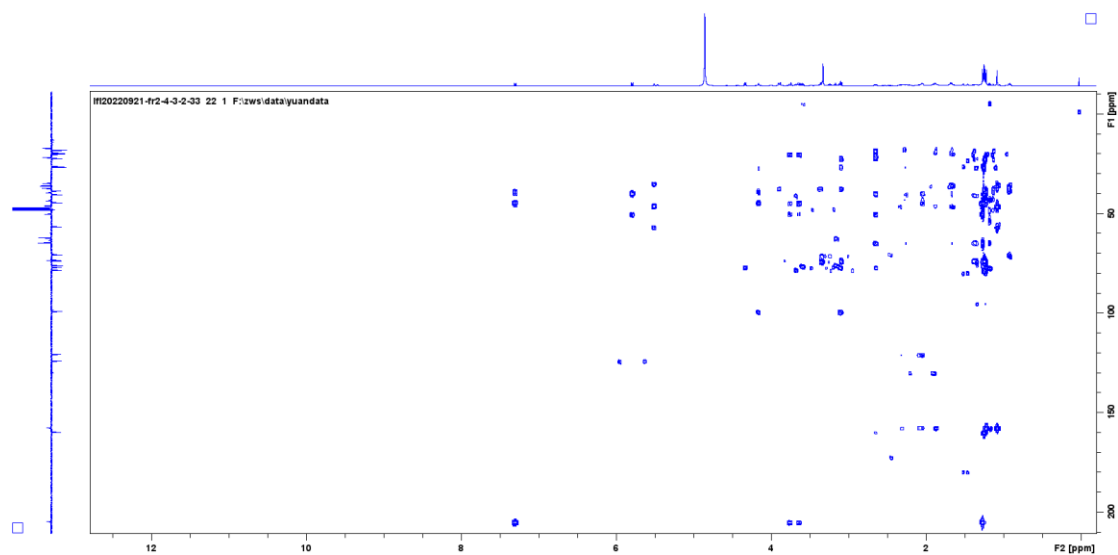


Figure S58. HMBC spectrum of munropene F (6) in CD₃OD.

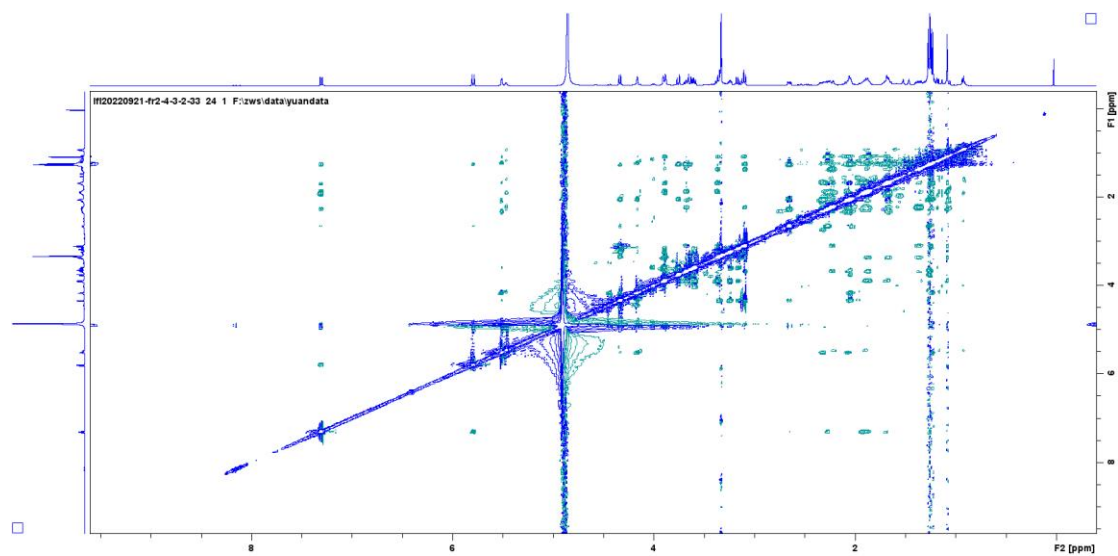


Figure S59. ROESY spectrum of munropene F (6) in CD₃OD.

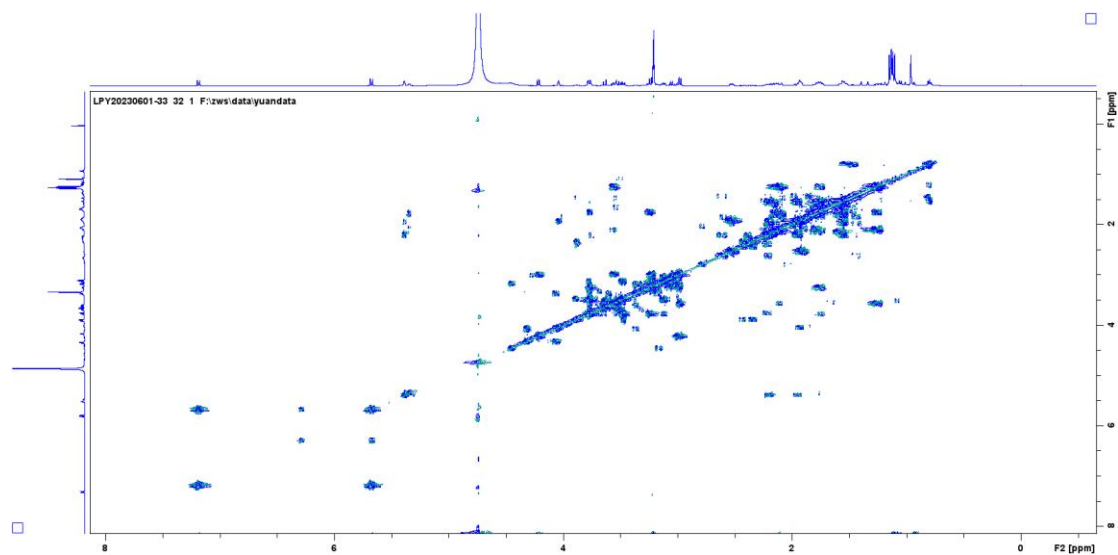


Figure S60. HETLOC spectrum of munropene F (6) in CD₃OD.

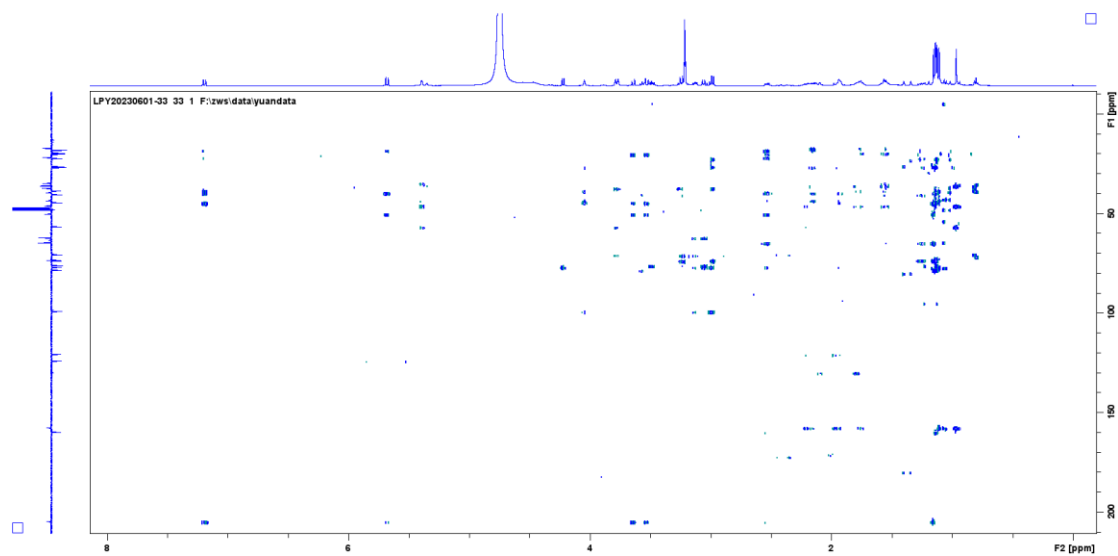
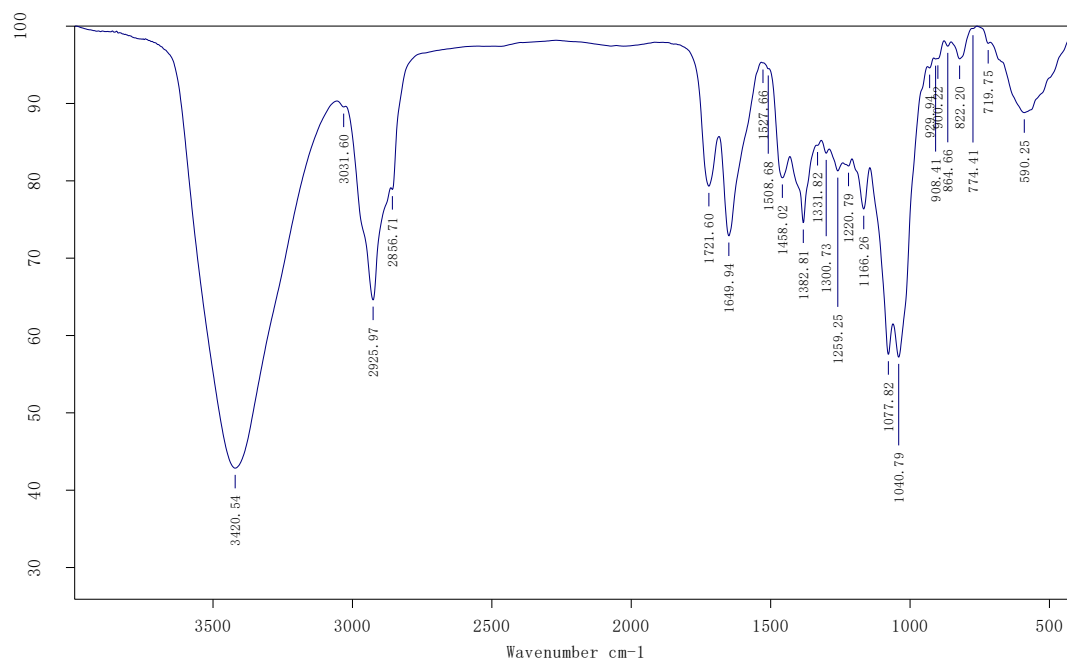


Figure S61. PS-HMBC spectrum of munropene F (6) in CD₃OD.



Sample Name: 33
 Sample Form: KBr
 Path of File: E:\data
 Date of Measurement: 2023/1/17

Resolution: 4
 Aperture Setting: 6 mm
 Number of Background Scans: 16
 Number of Sample Scans: 16

Beamsplitter Setting: KBr
 Source Setting: MIR
 Instrument Type: BRUKER VERTEX 70
 Soft Version: OPUS8.1

Figure S62. IR spectrum of munropene F (6).