

Supplementary Materials

Scalarane-type sesterterpenoids from the marine sponge *Lendenfeldia* sp. alleviate inflammation in human neutrophils

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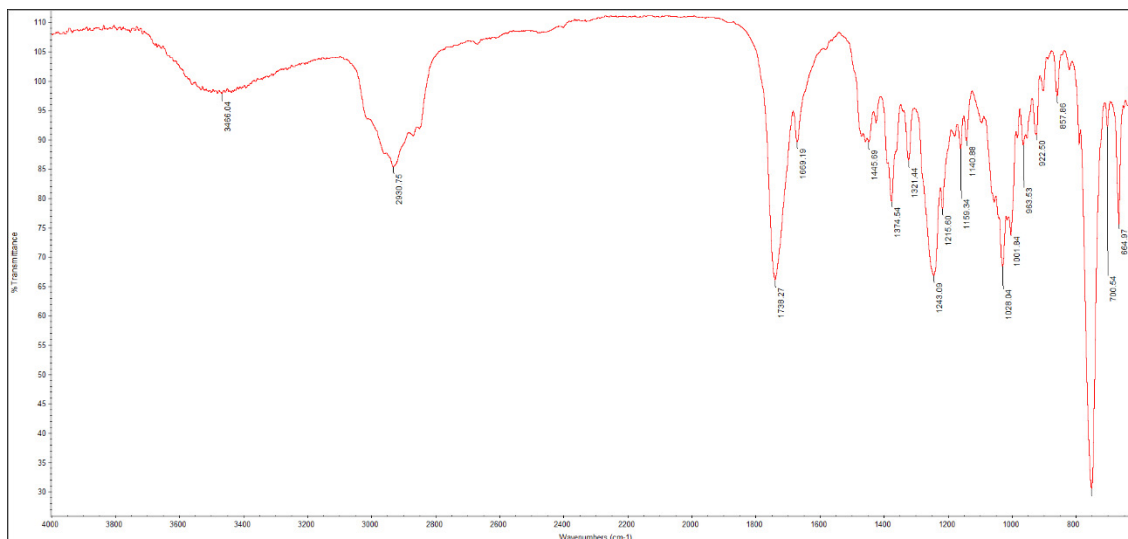


Figure S1. IR spectrum of compound 1.

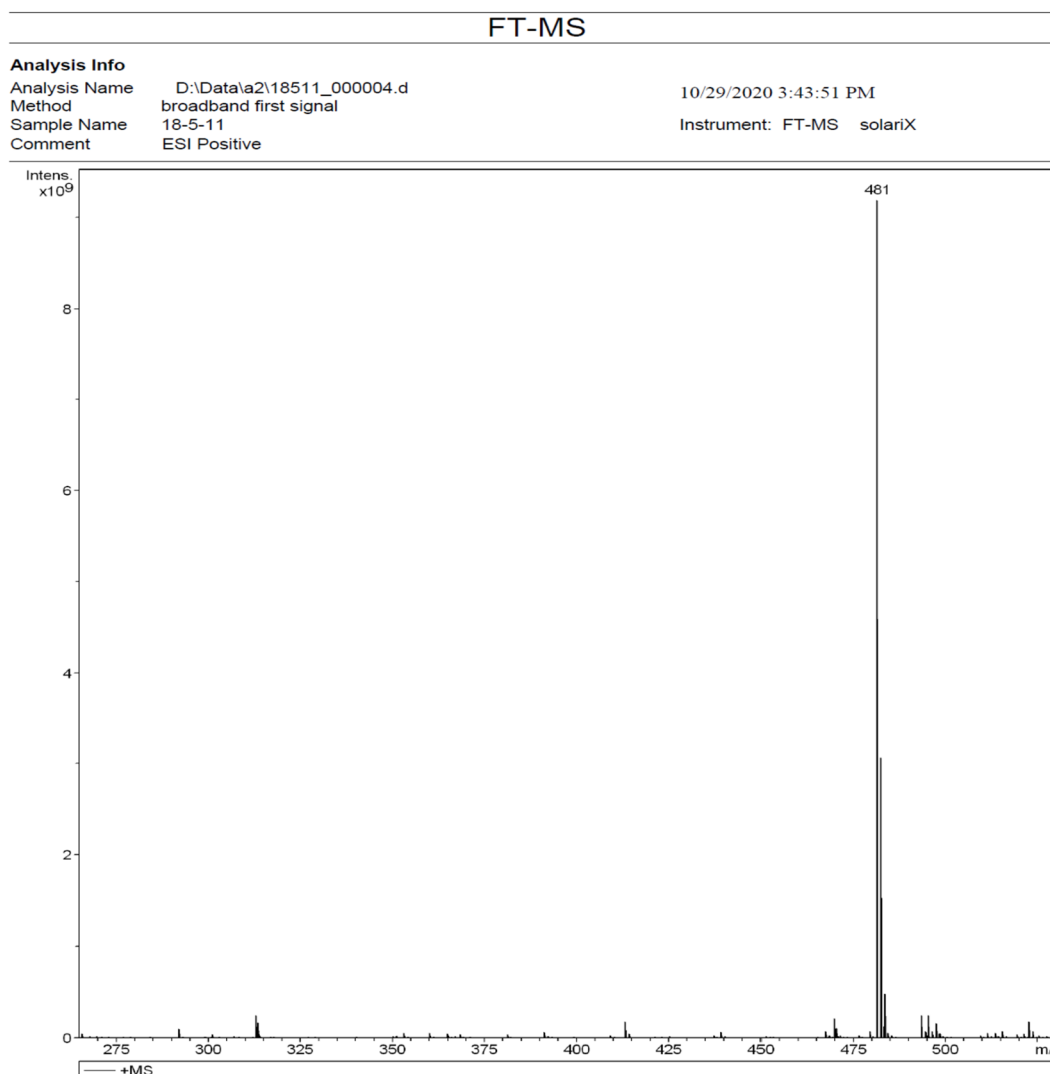


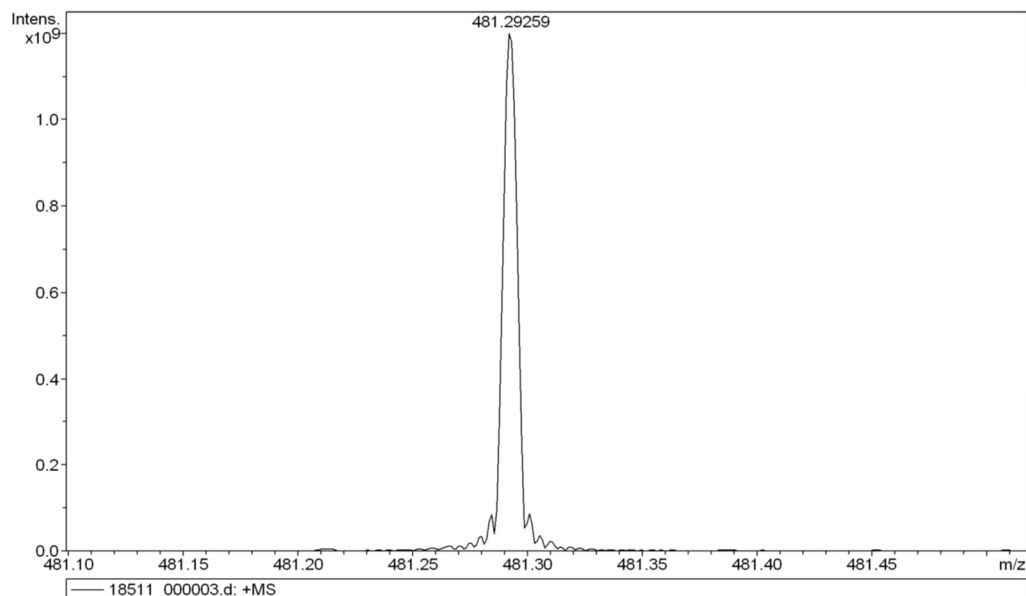
Figure S2. ESIMS spectrum of compound 1.

Mass Spectrum SmartFormula Report

Analysis Info

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 Method broadband first signal
 Sample Name 18-5-11
 Comment ESI Positive

10/29/2020 3:42:39 PM
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 Instrument: BRUKER FT-MS solariX



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Figure S3. HRESIMS spectrum of compound **1**.

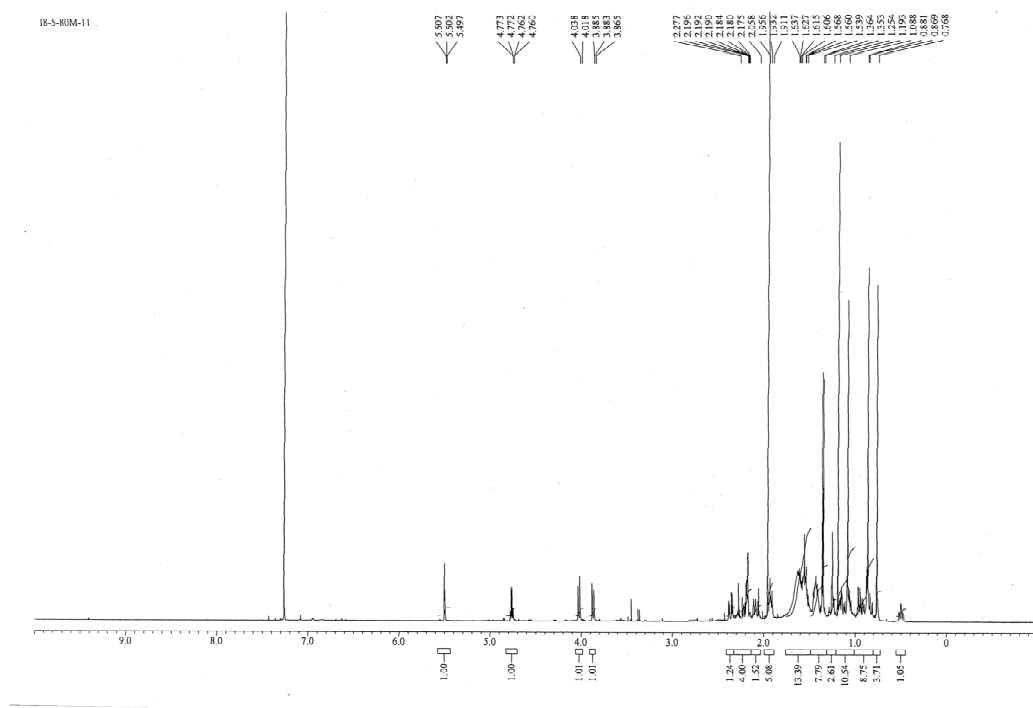


Figure S4. ¹H NMR spectrum (600 MHz) of compound **1** in CDCl₃.

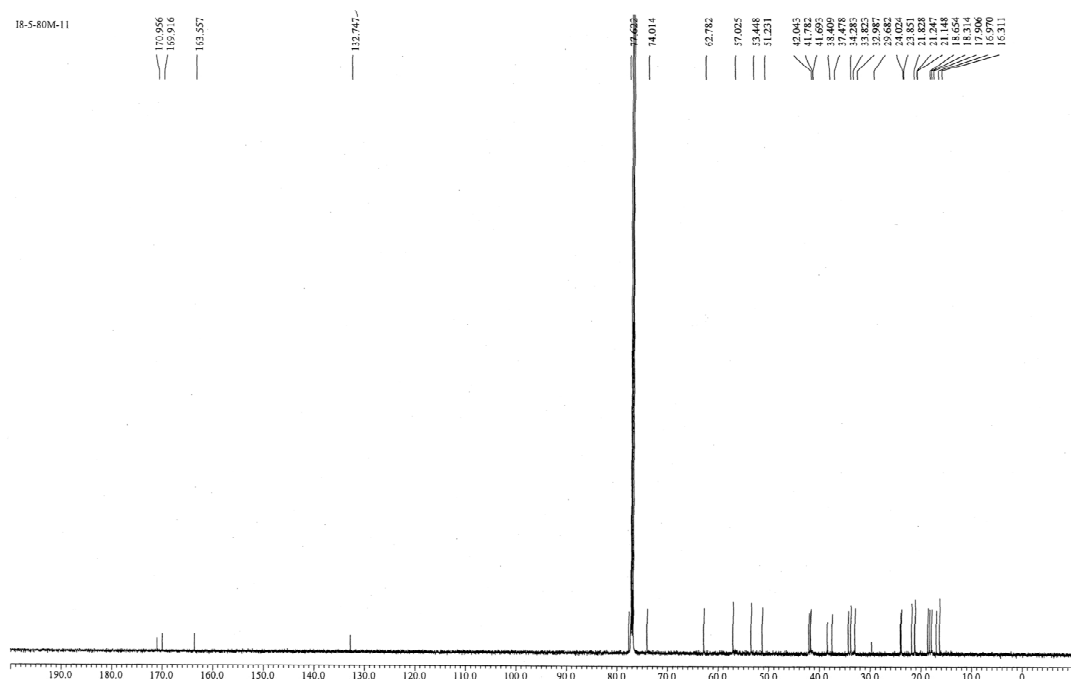


Figure S5. ^{13}C NMR spectrum (150 MHz) of compound **1** in CDCl_3 .

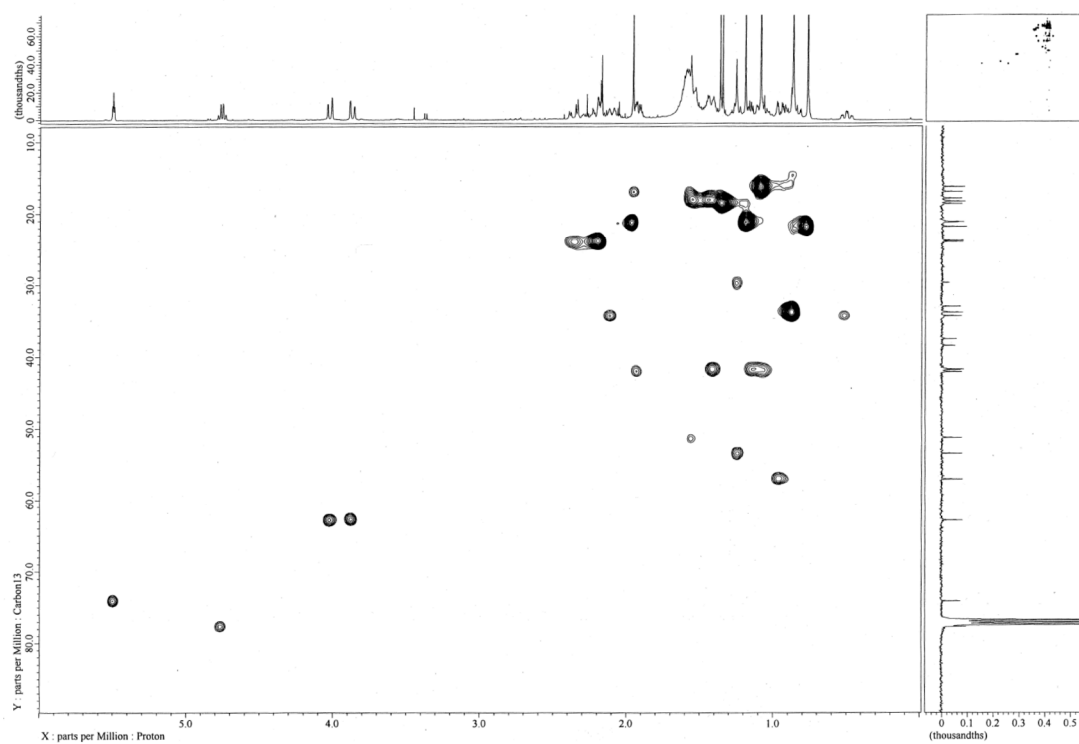


Figure S6. HSQC spectrum of compound **1** in CDCl_3 .

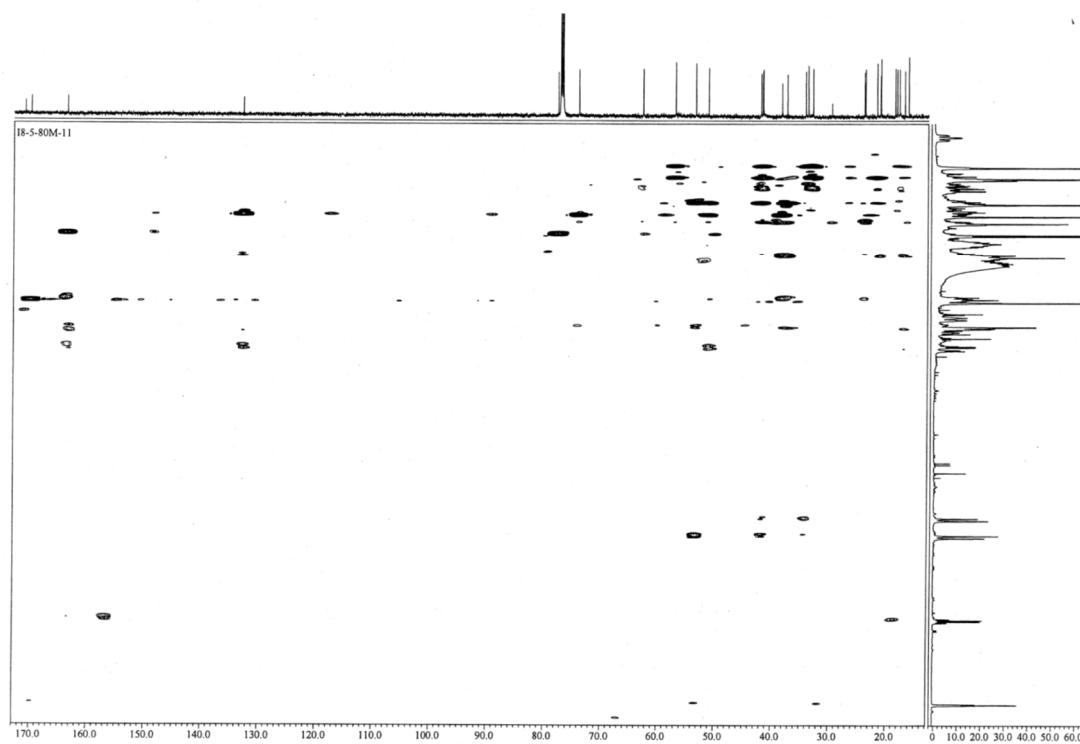


Figure S7. HMBC spectrum of compound **1** in CDCl₃.

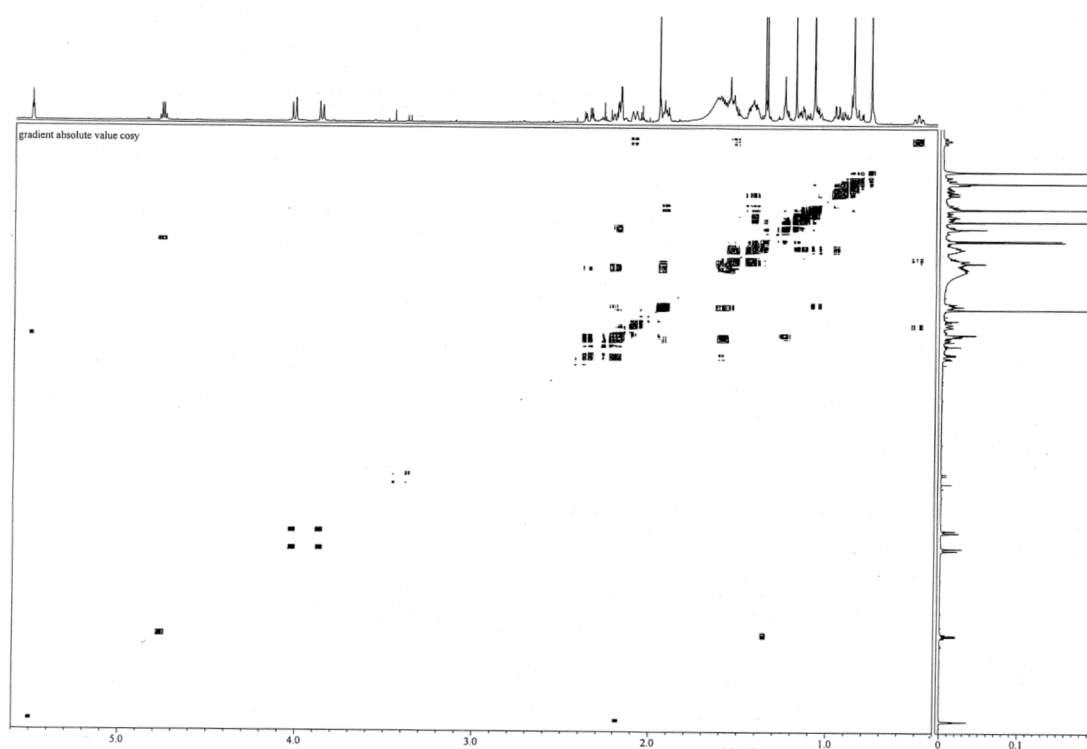


Figure S8. ¹H-¹H COSY spectrum of compound **1** in CDCl₃.

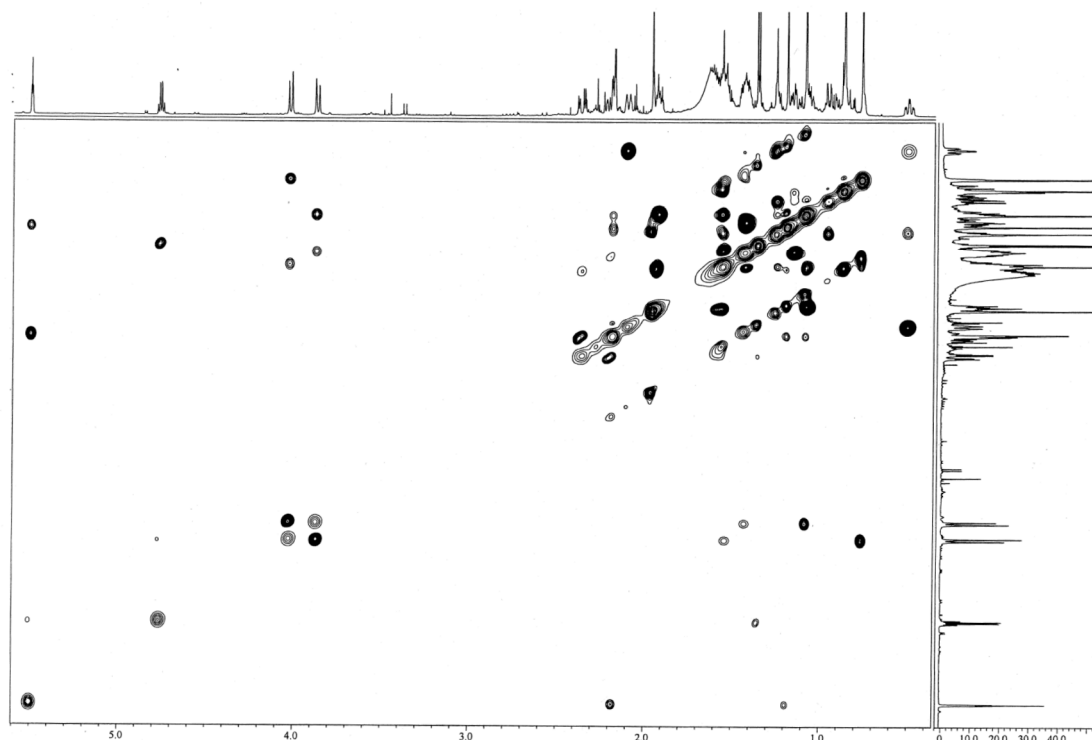


Figure S9. NOESY spectrum of compound **1** in CDCl₃

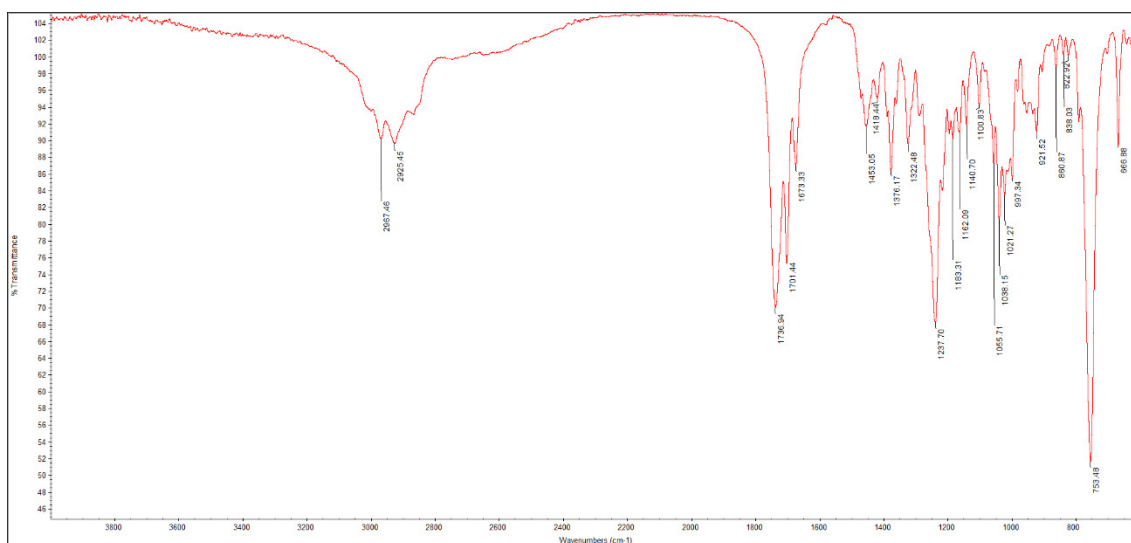


Figure S10. IR spectrum of compound **2**.

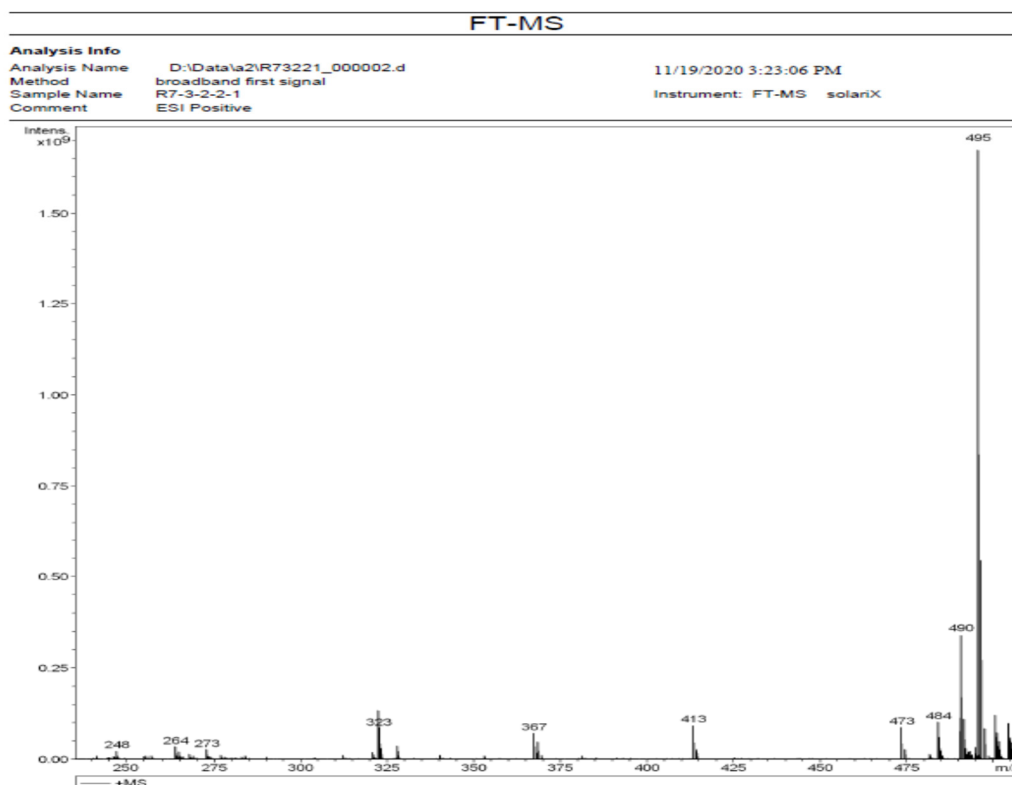


Figure S11. ESIMS spectrum of compound 2.

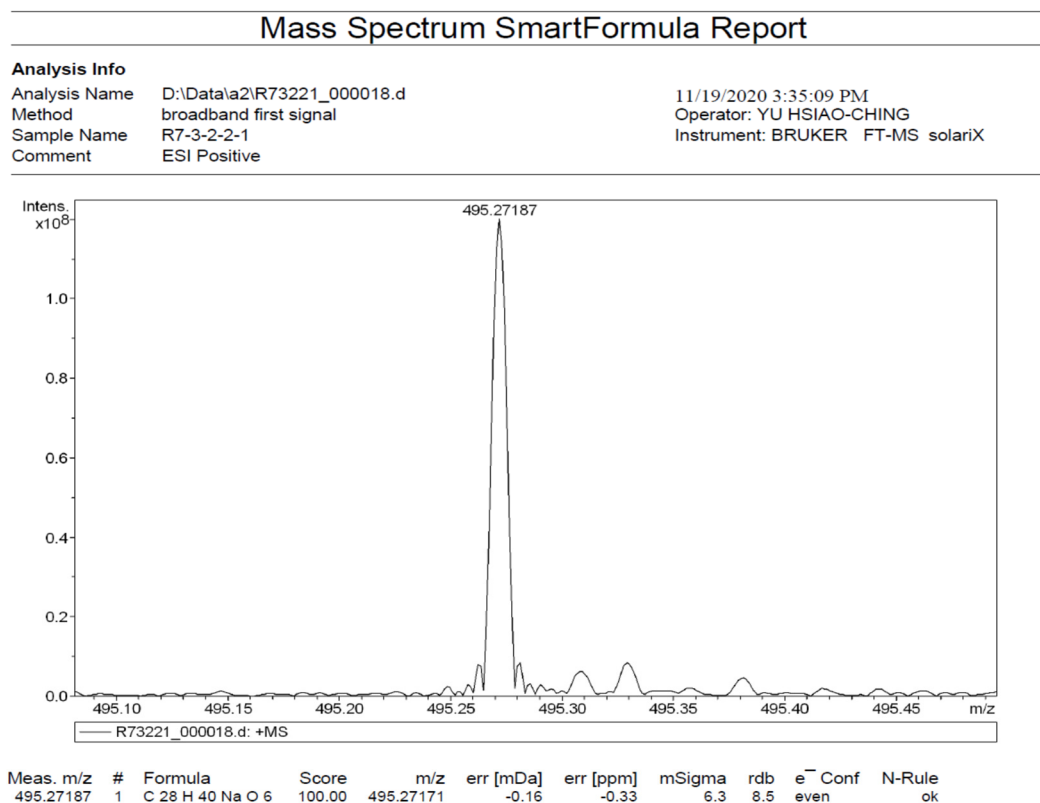


Figure S12. HRESIMS spectrum of compound 2.

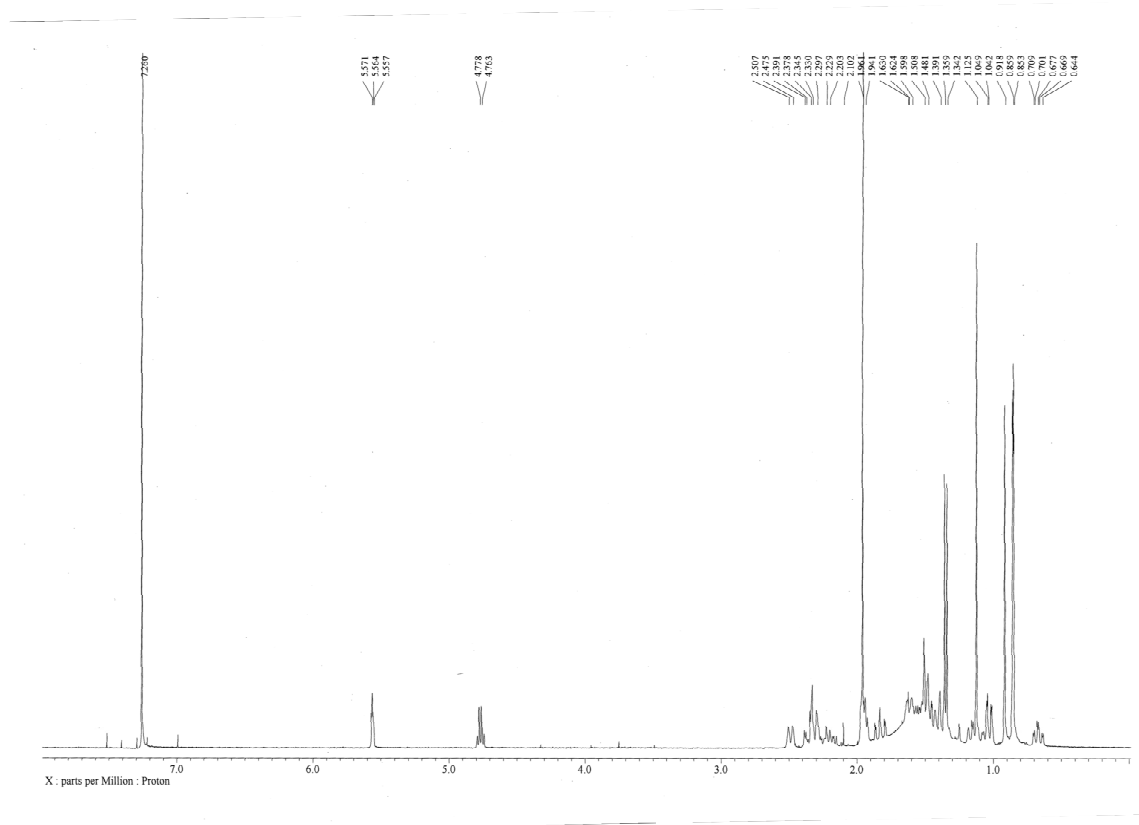


Figure S13. ^1H NMR spectrum (400 MHz) of compound **2** in CDCl_3 .

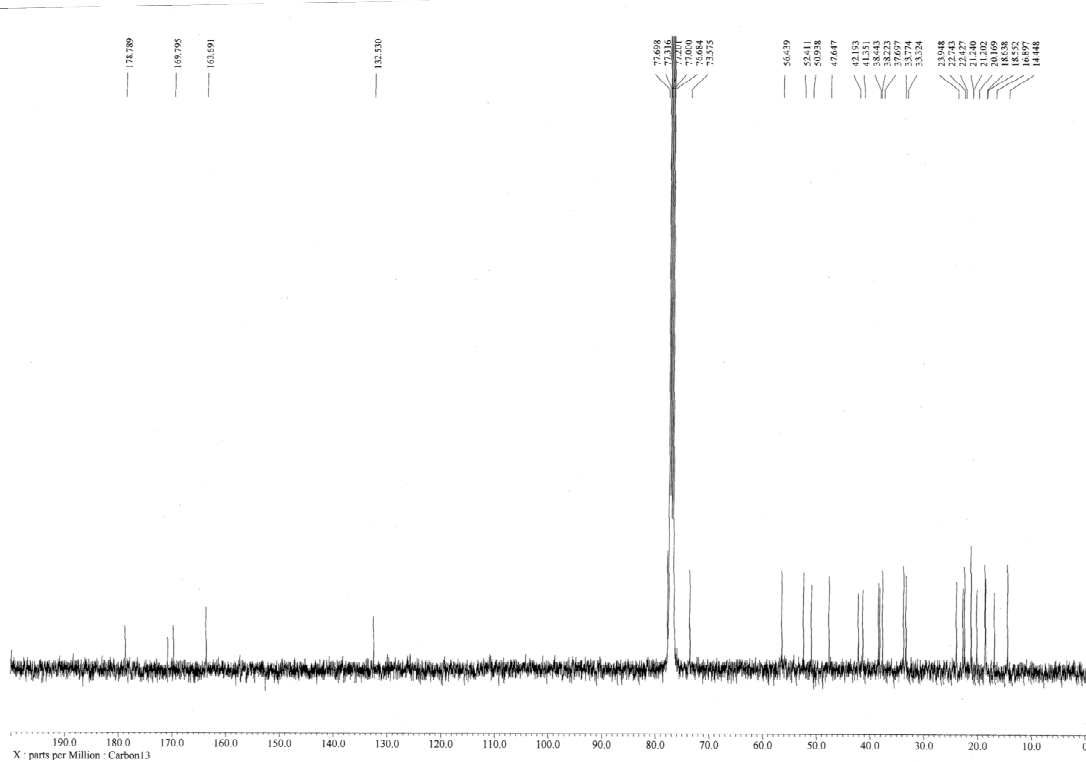


Figure S14. ^{13}C NMR spectrum (100 MHz) of compound **2** in CDCl_3 .

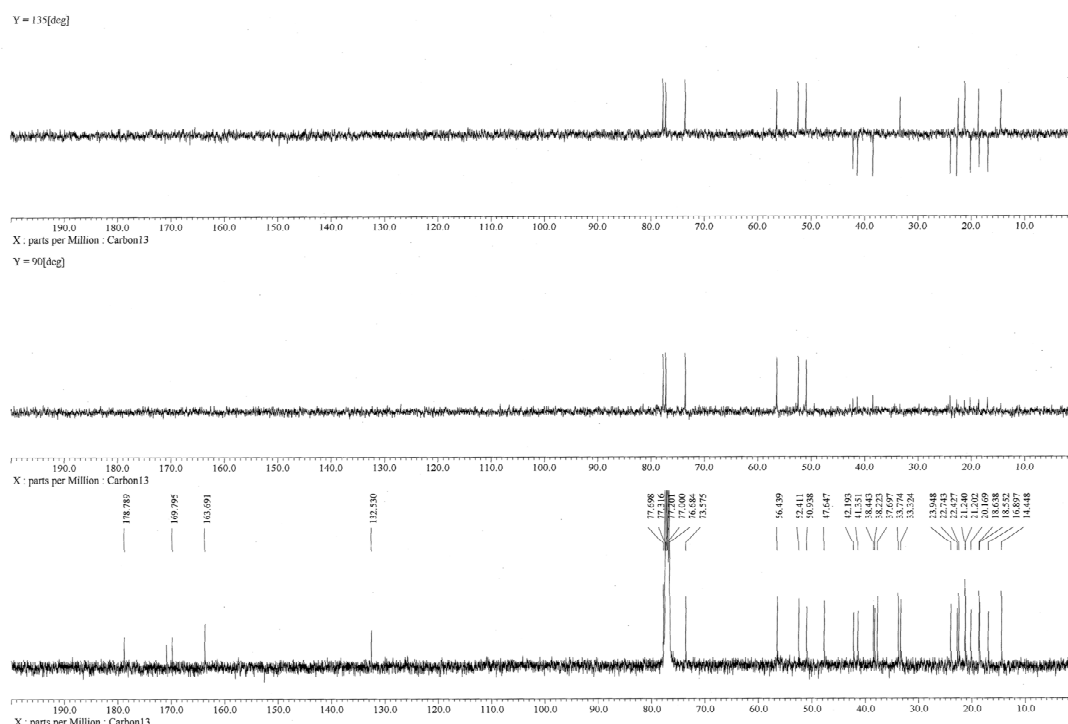


Figure S15. DEPT spectrum of compound 2 in CDCl₃.

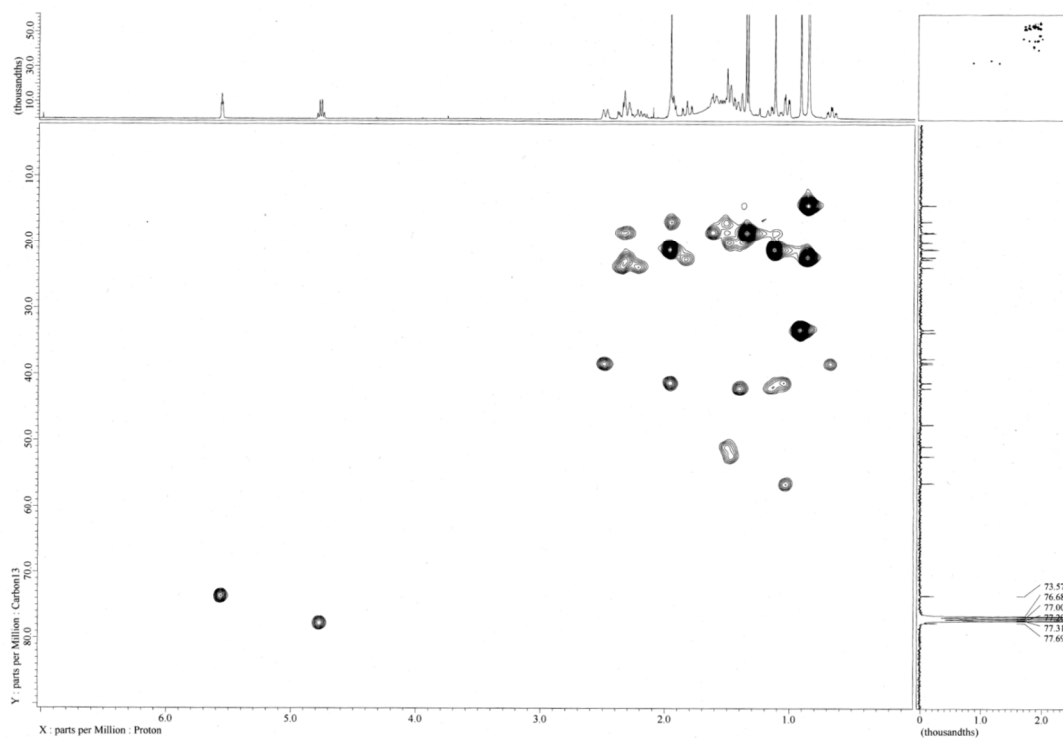


Figure S16. HSQC spectrum of compound 2 in CDCl₃.

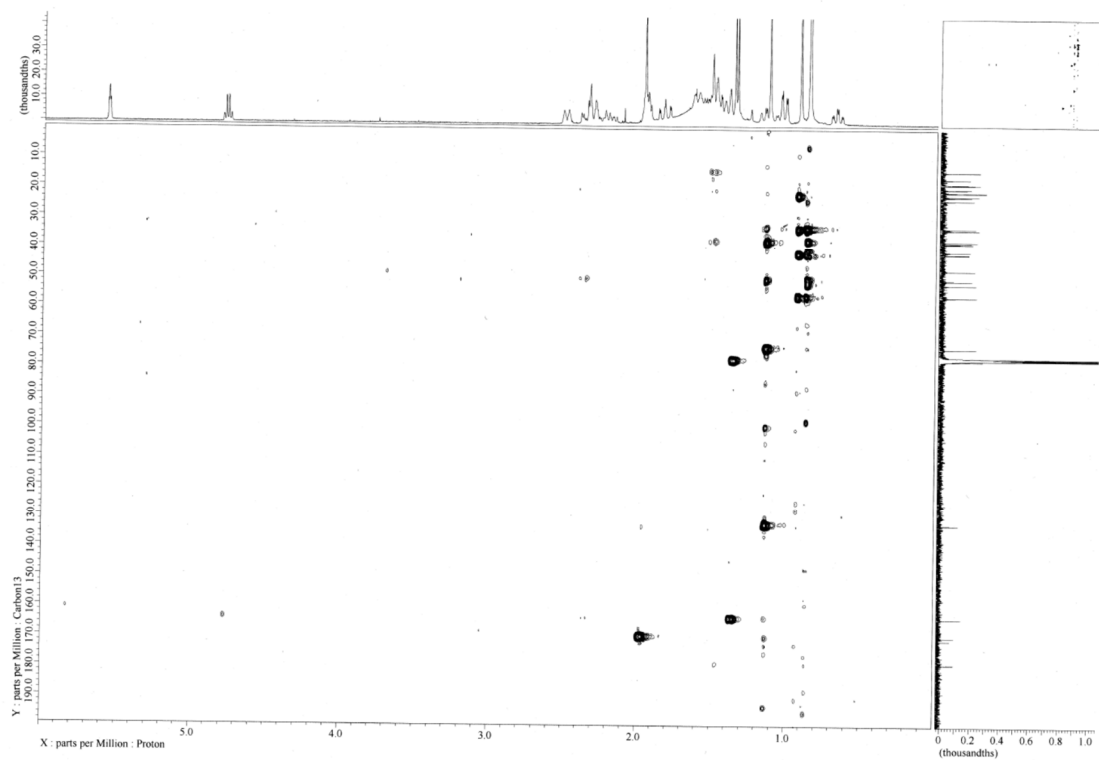


Figure S17. HMBC spectrum of compound **2** in CDCl₃.

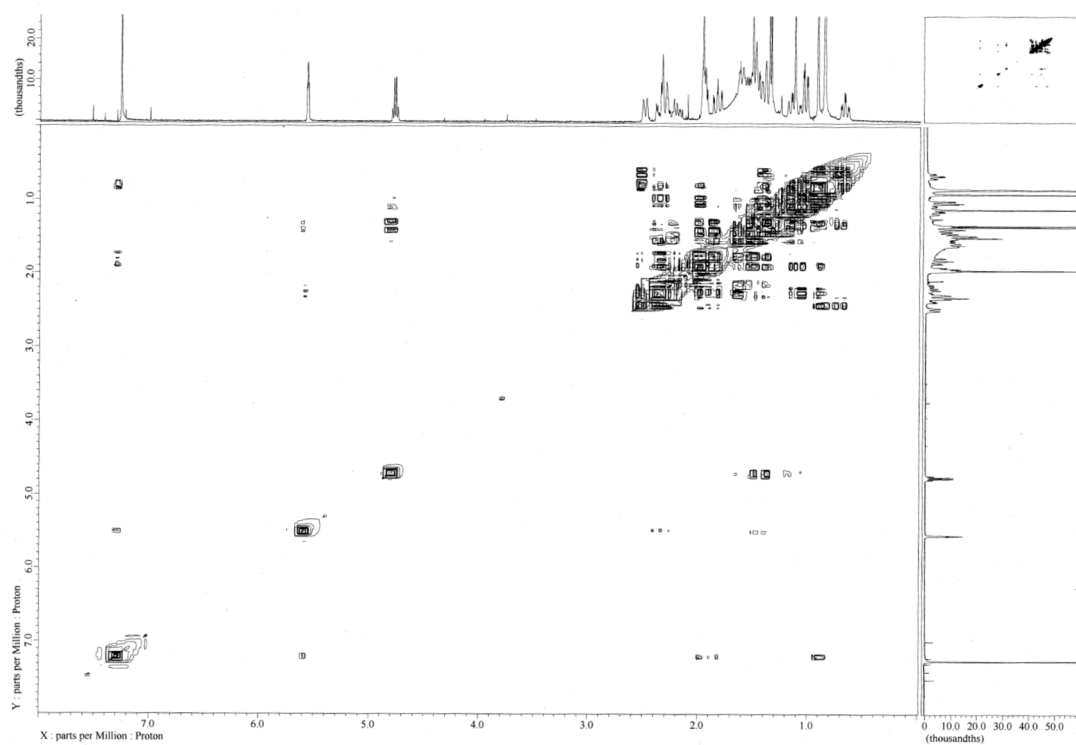


Figure S18. ¹H-¹H COSY spectrum of compound **2** in CDCl₃.

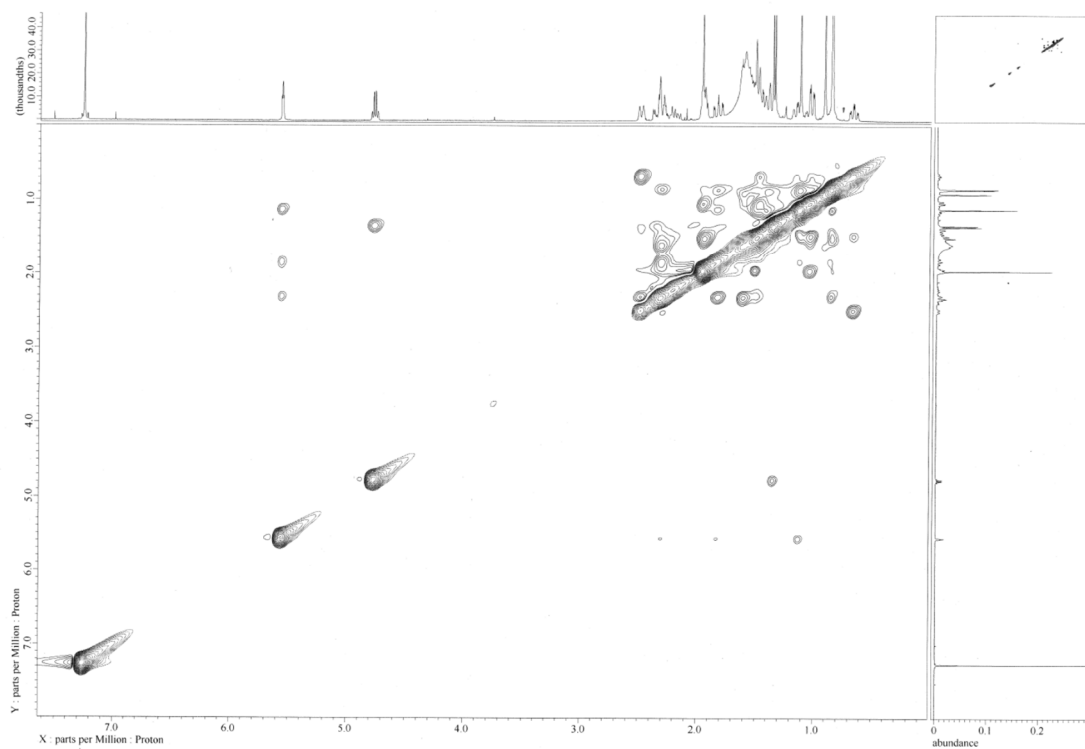


Figure S19. NOESY spectrum of compound **2** in CDCl_3

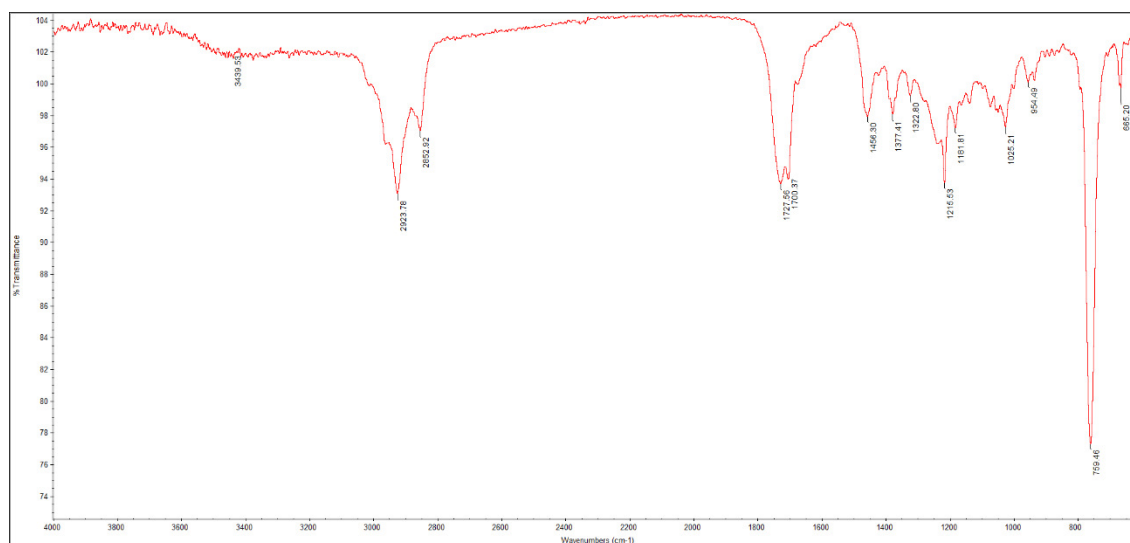


Figure S20. IR spectrum of compound **3**.

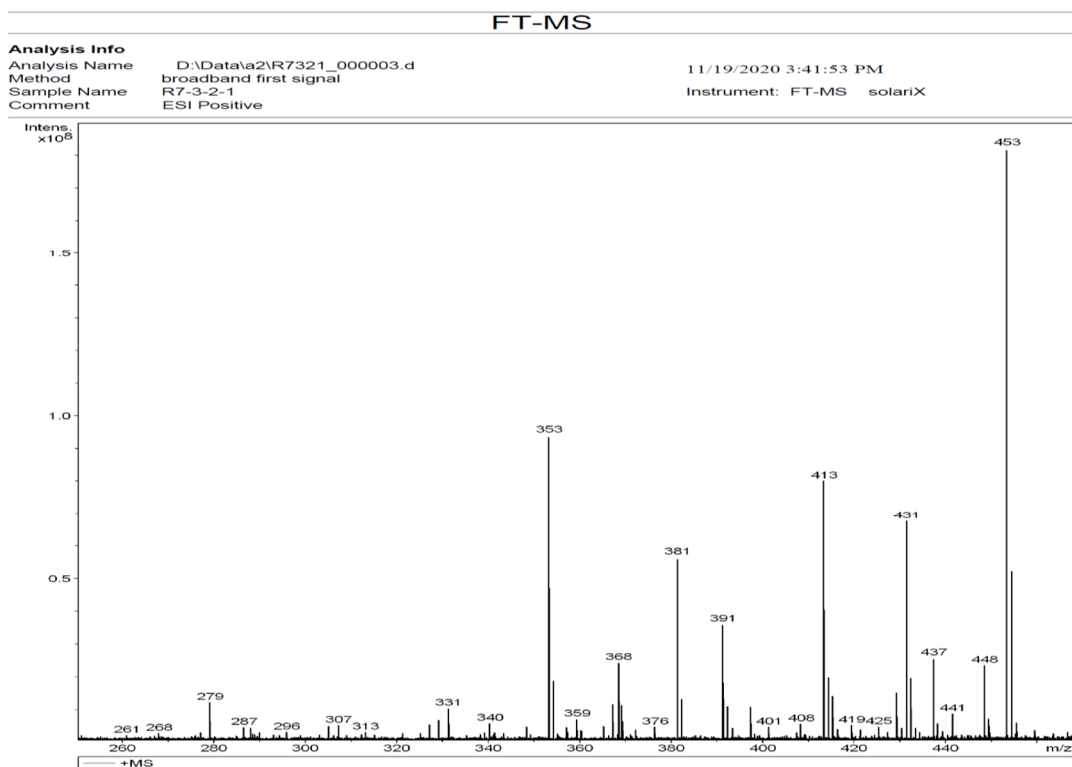


Figure S21. ESIMS spectrum of compound 3.

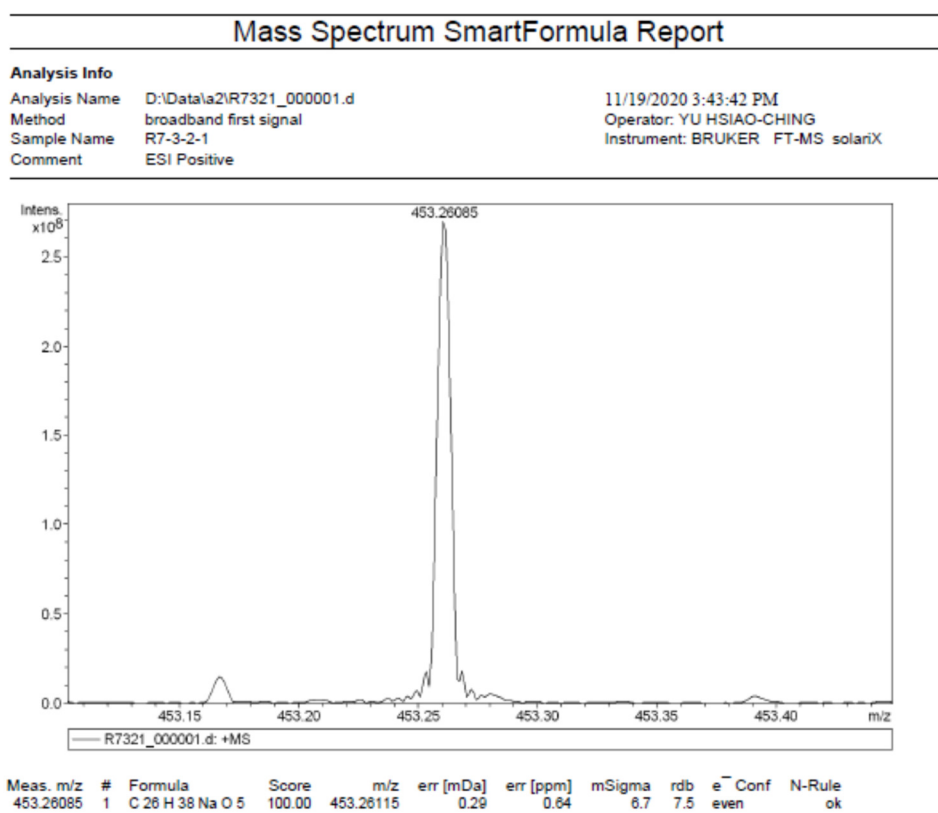


Figure S22. HRESIMS spectrum of compound 3.

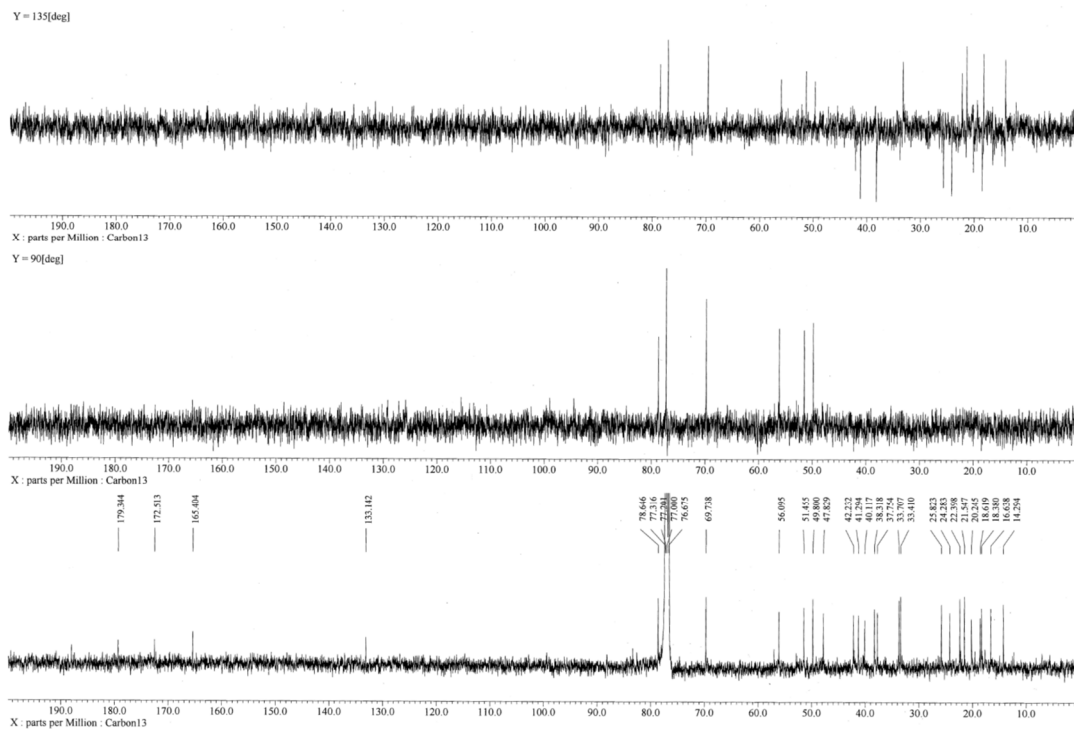


Figure S25. DEPT spectrum of compound 3 in CDCl₃.

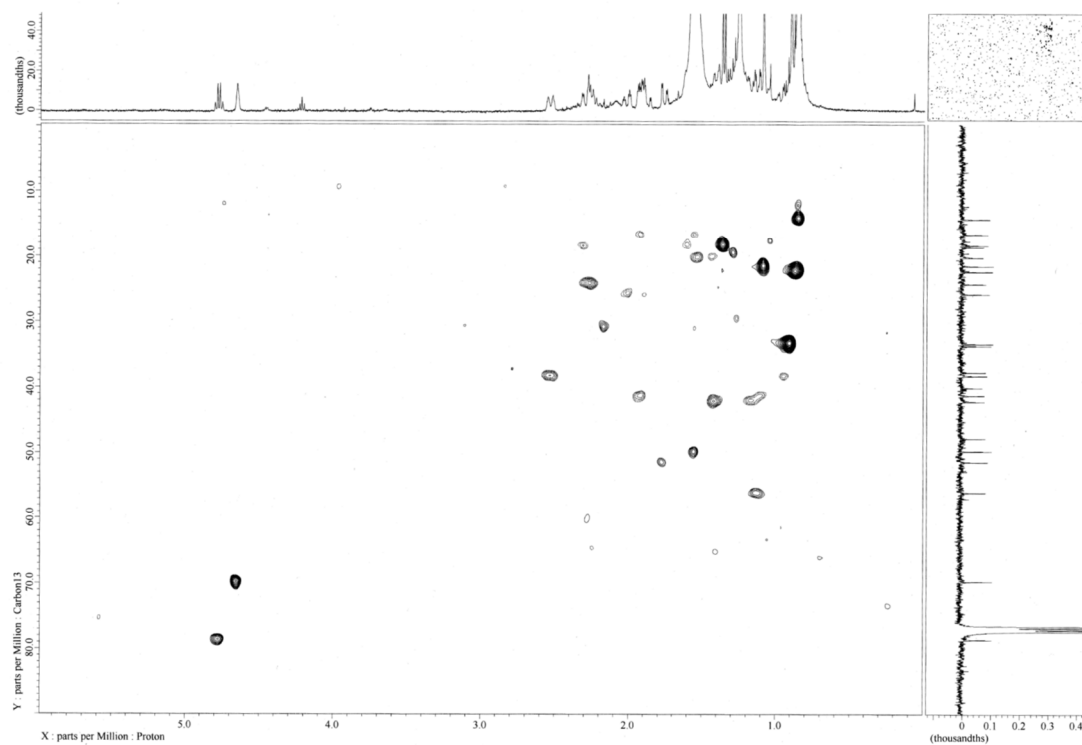


Figure S26. HSQC spectrum of compound 3 in CDCl₃.

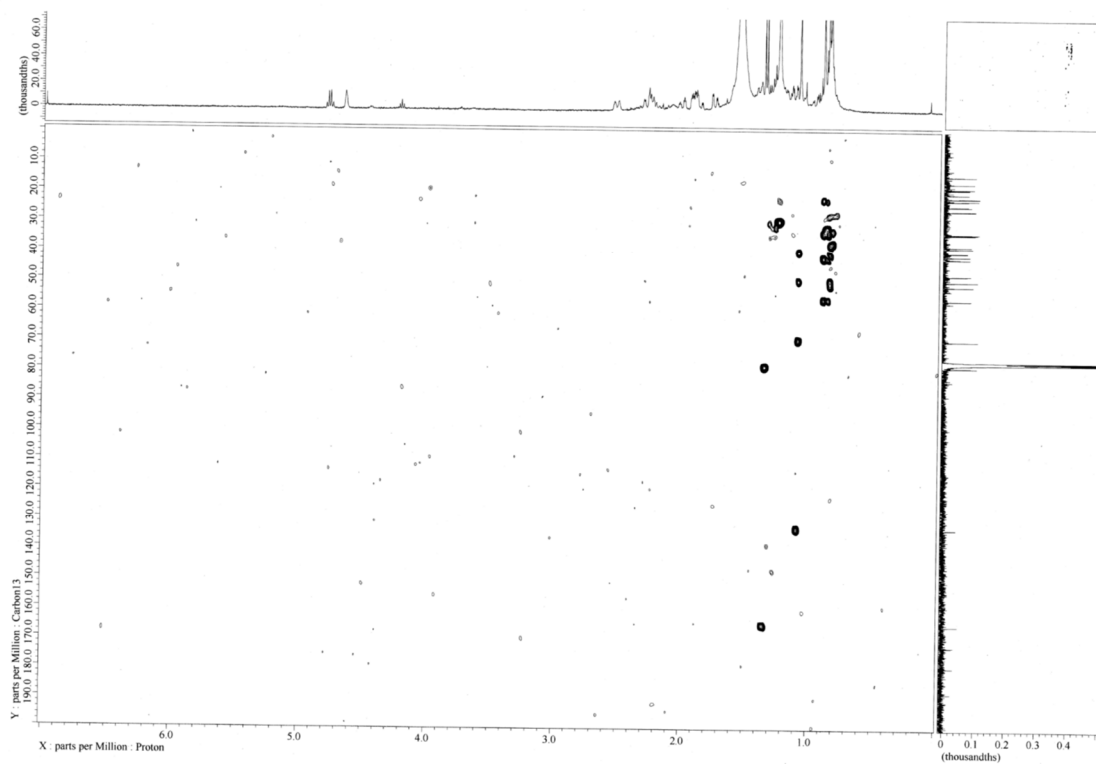


Figure S27. HMBC spectrum of compound **3** in CDCl₃.

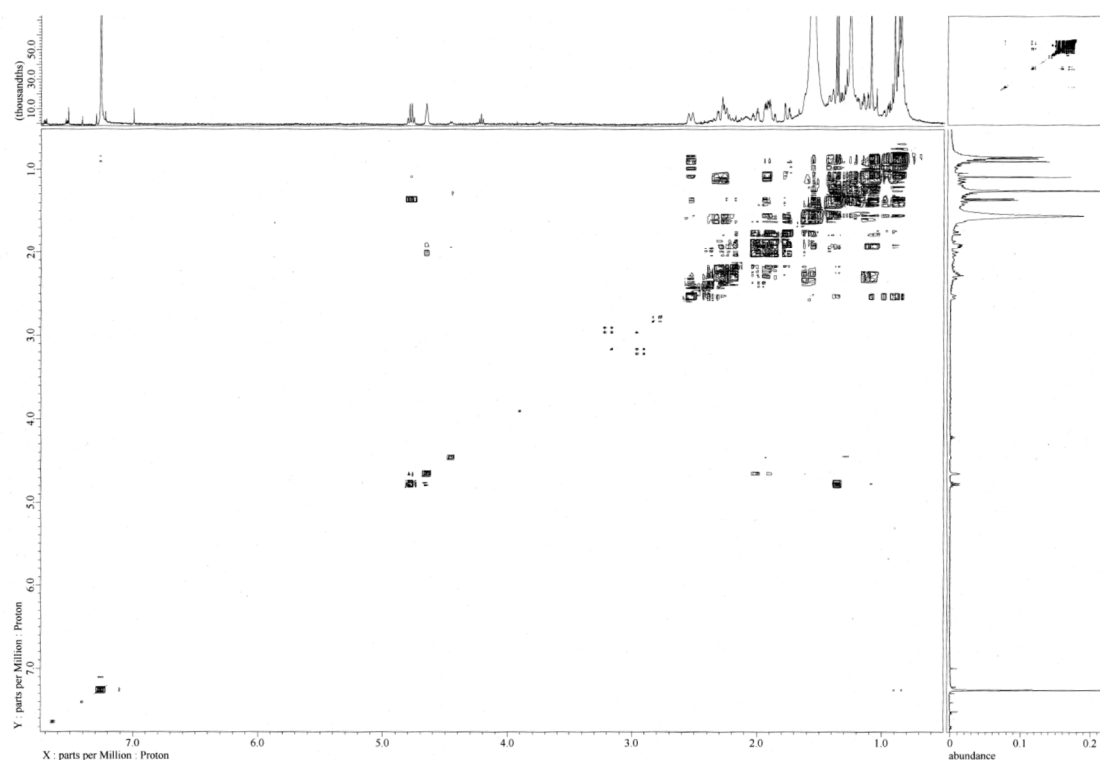


Figure S28. ¹H-¹H COSY spectrum of compound **3** in CDCl₃.

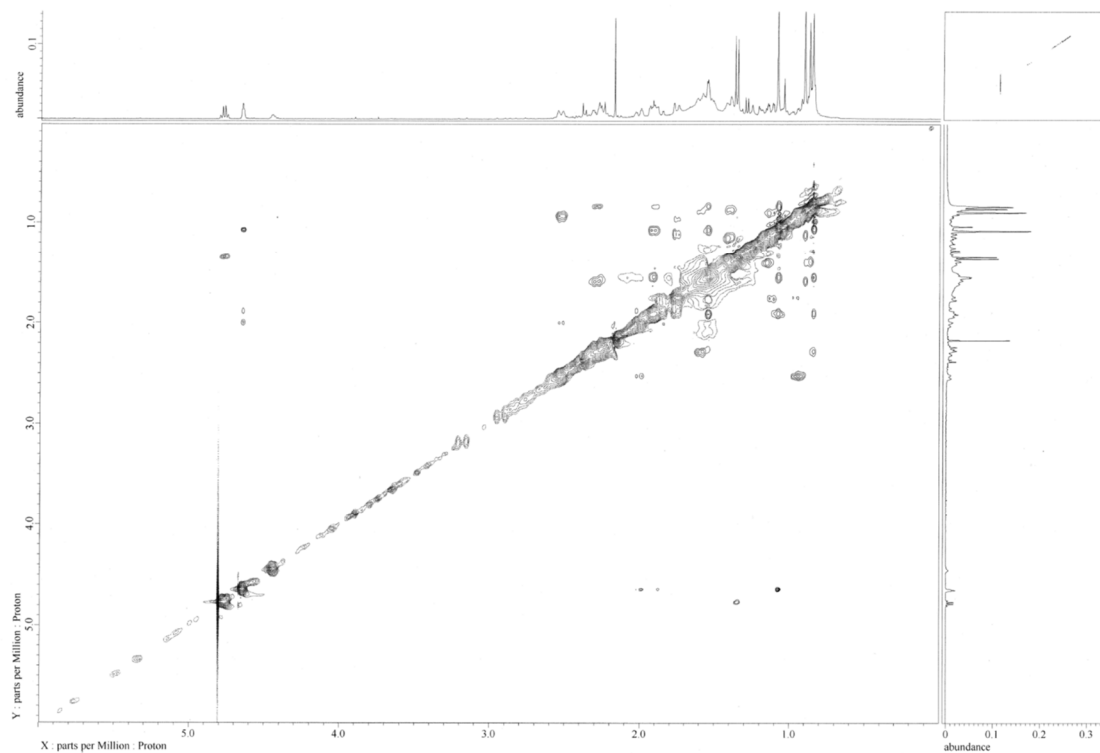


Figure S29. NOESY spectrum of compound **3** in CDCl_3



Figure S30. IR spectrum of compound **4**.

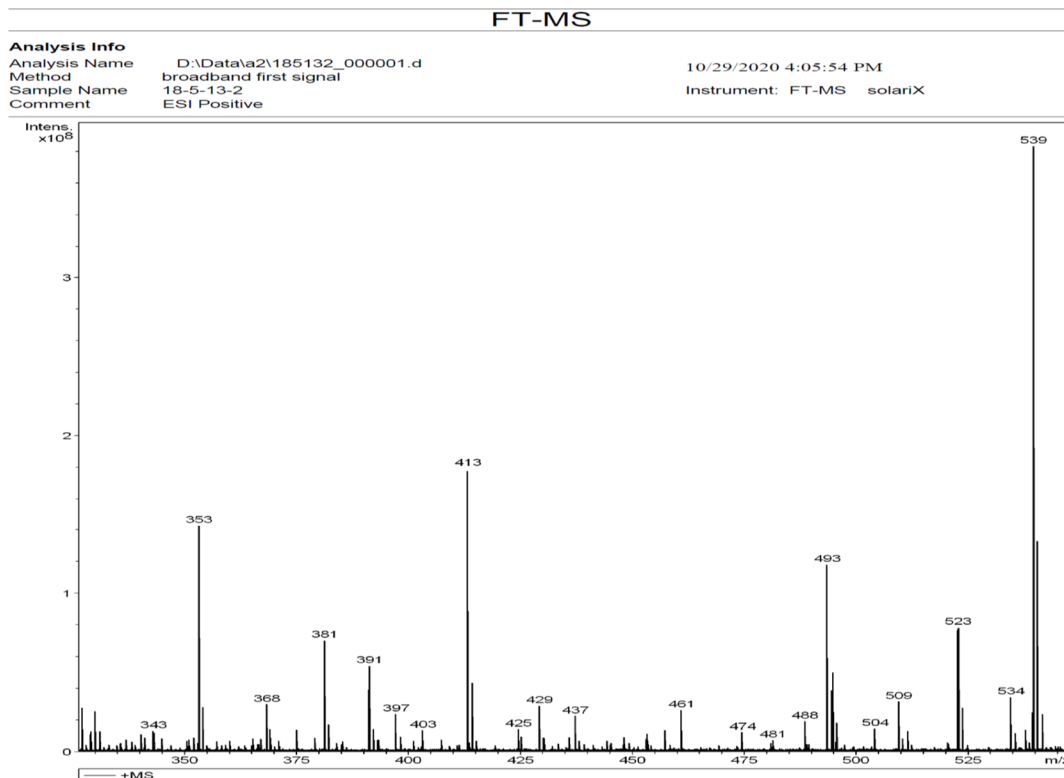


Figure S31. ESIMS spectrum of compound **4**.

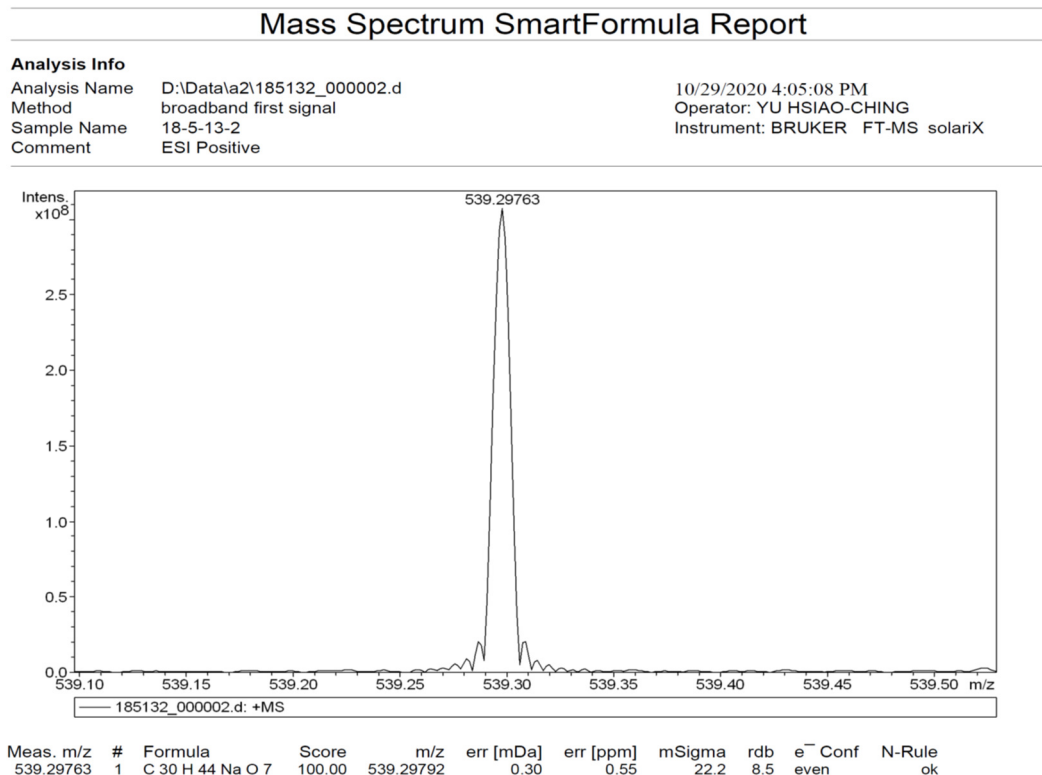


Figure S32. HRESIMS spectrum of compound **4**.

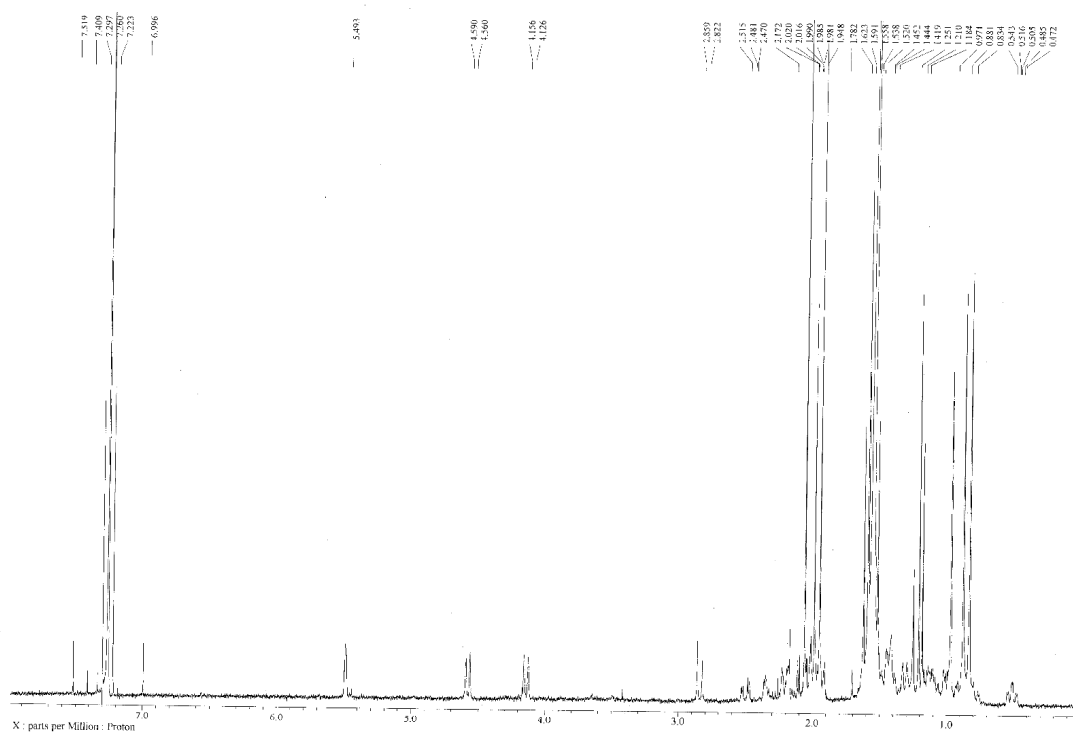


Figure S33. ^1H NMR spectrum (400 MHz) of compound **4** in CDCl_3 .

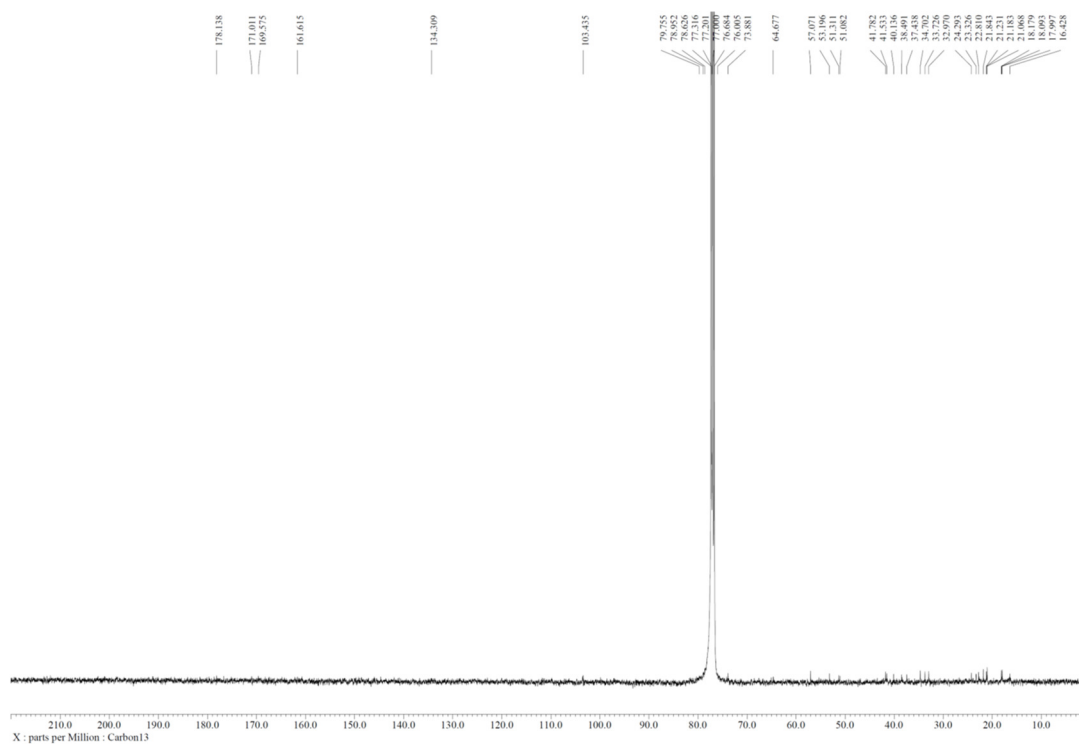


Figure S34. ^{13}C NMR spectrum (100 MHz) of compound **4** in CDCl_3 .

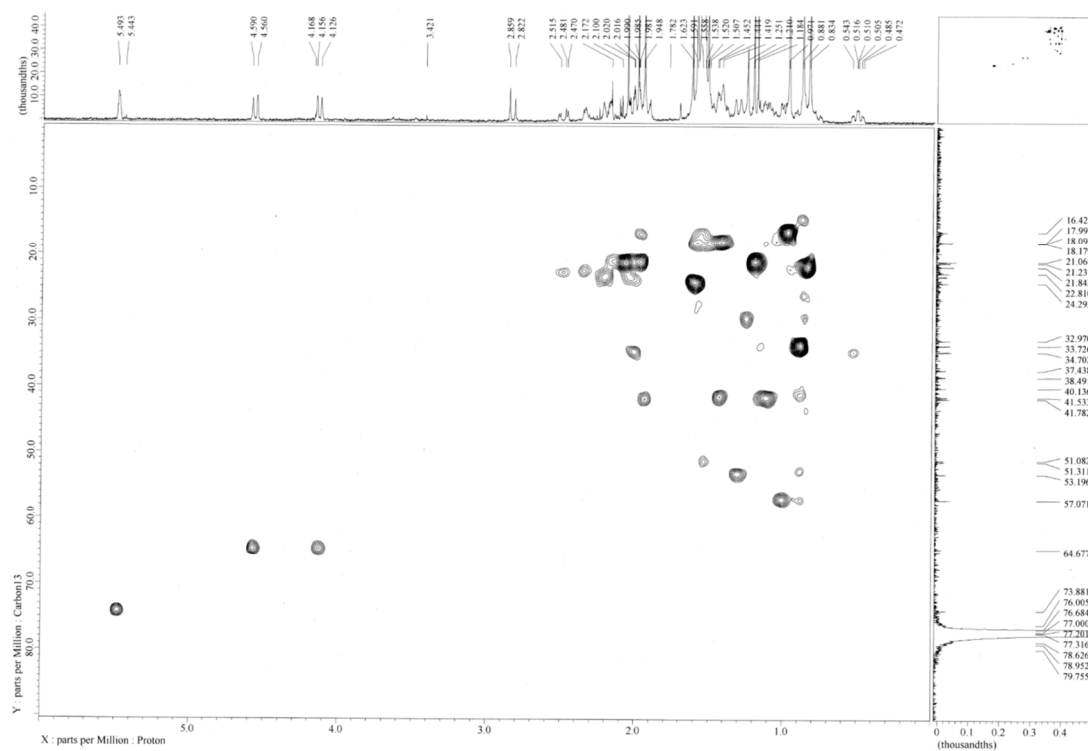


Figure S35. HSQC spectrum of compound **4** in CDCl₃.

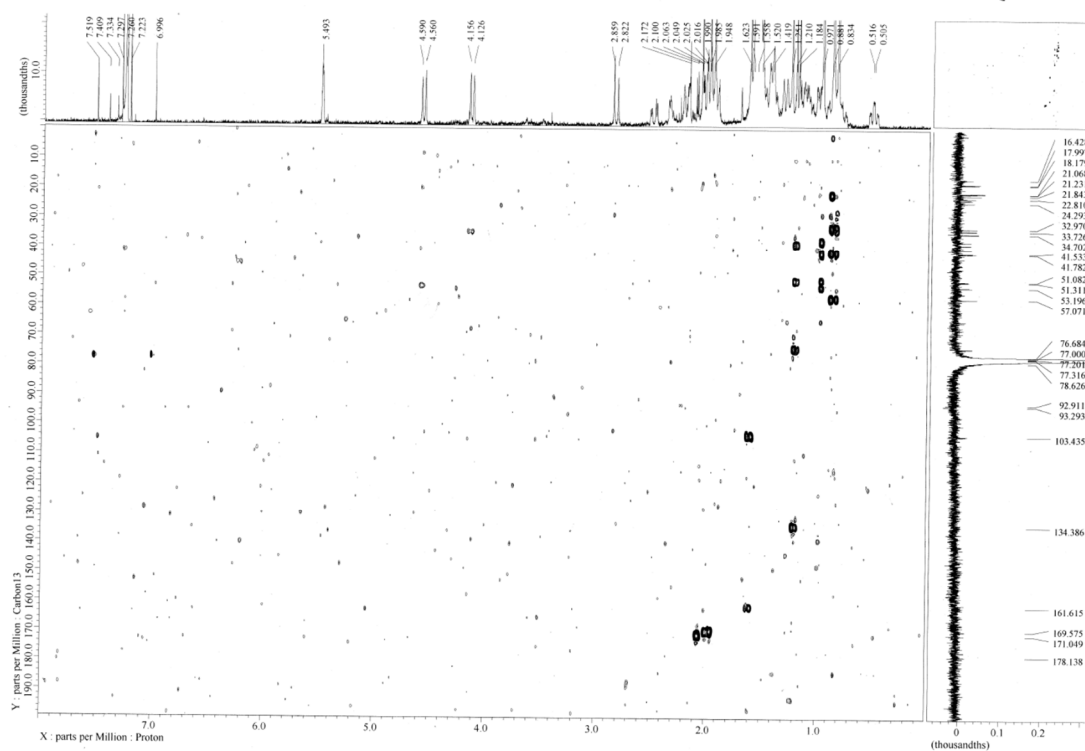


Figure S36. HMBC spectrum of compound **4** in CDCl₃.

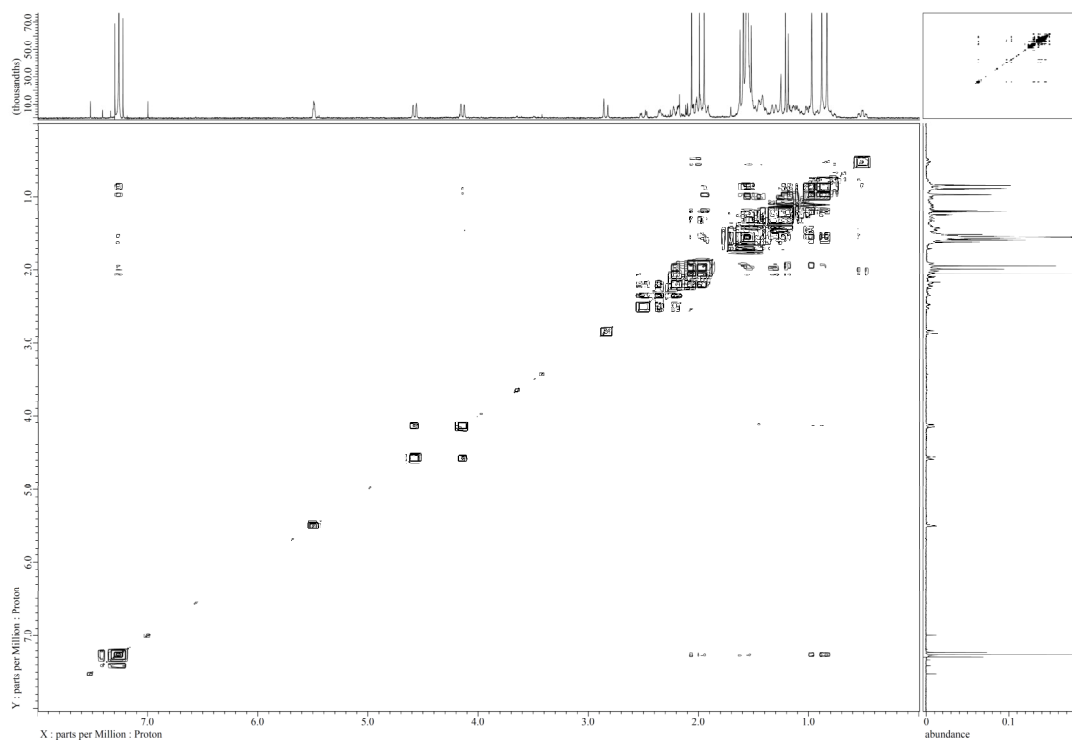


Figure S37. ^1H - ^1H COSY spectrum of compound **4** in CDCl_3 .

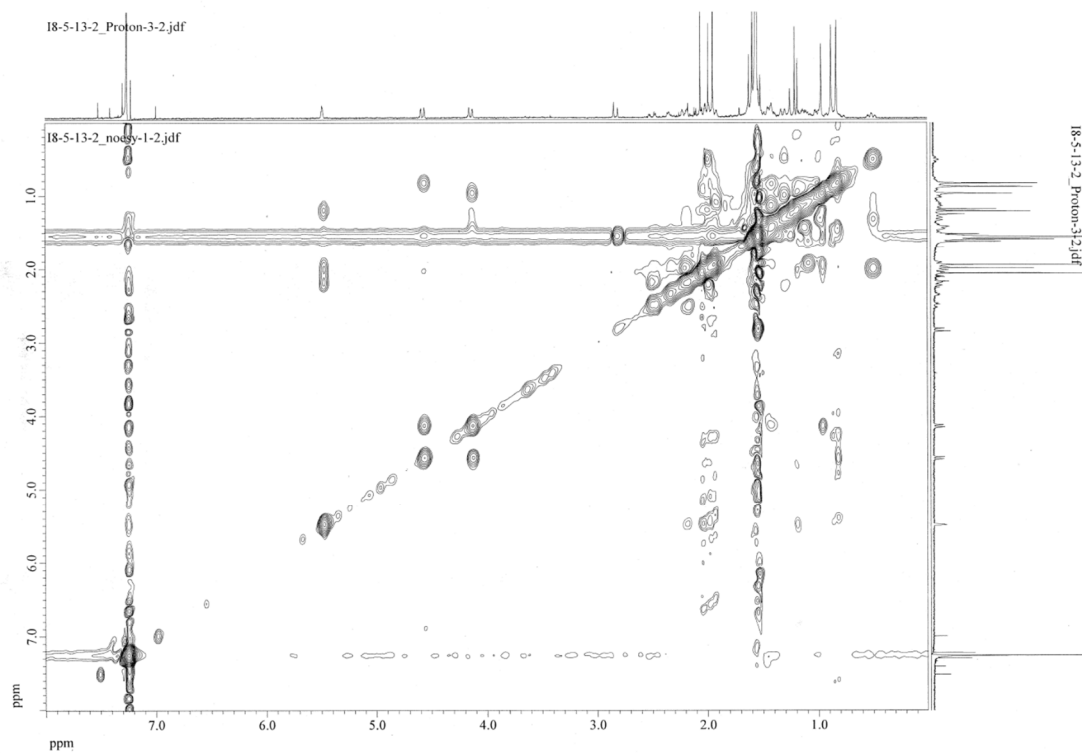


Figure S38. NOESY spectrum of compound **4** in CDCl_3

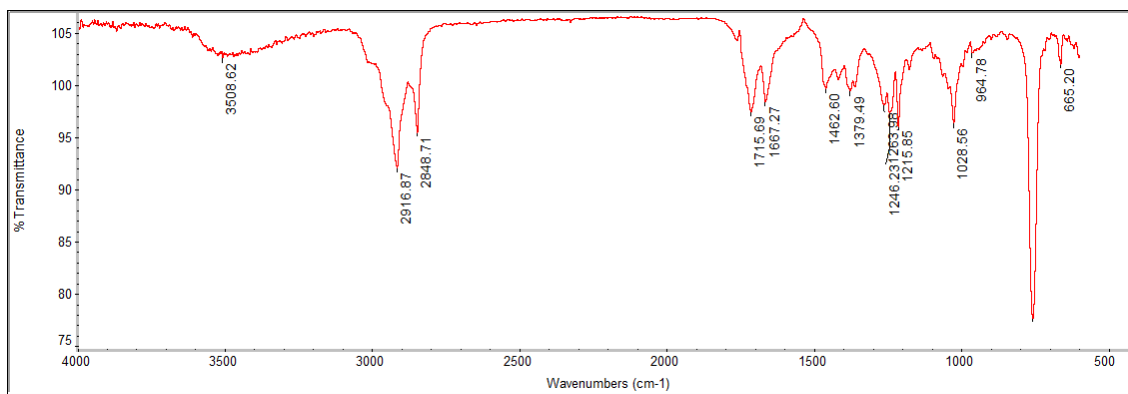


Figure S39. IR spectrum of compound 5.

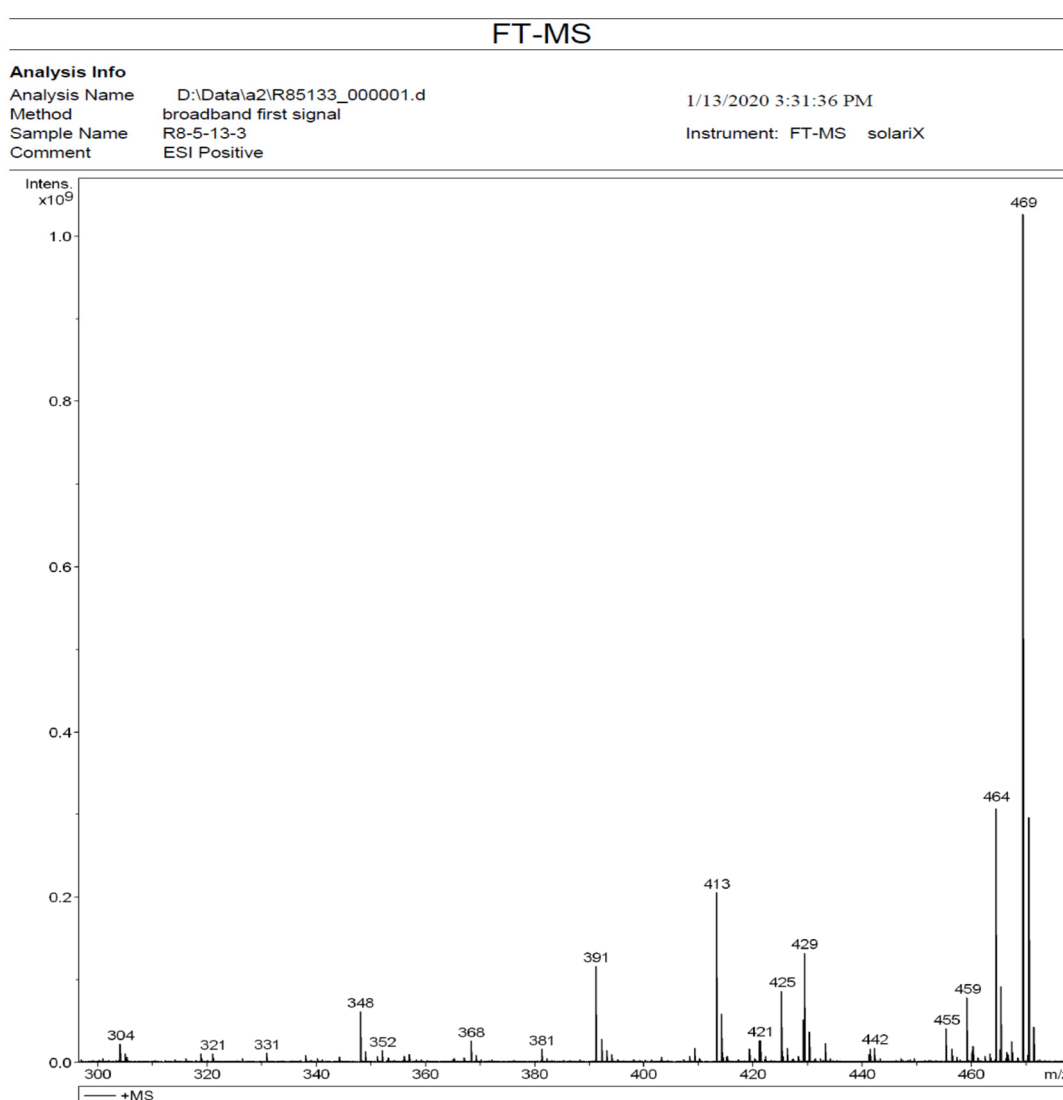


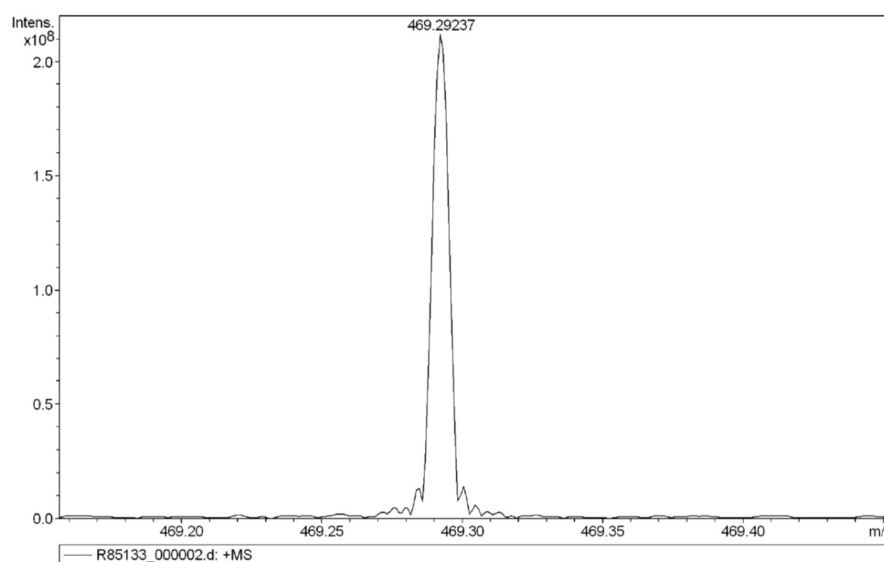
Figure S40. ESIMS spectrum of compound 5.

Mass Spectrum SmartFormula Report

Analysis Info

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 Method broadband first signal
 Sample Name R8-5-13-3
 Comment ESI Positive

1/13/2020 3:30:43 PM
 Operator: YU HSIAO-CHING
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Figure S41. HRESIMS spectrum of compound **5**.

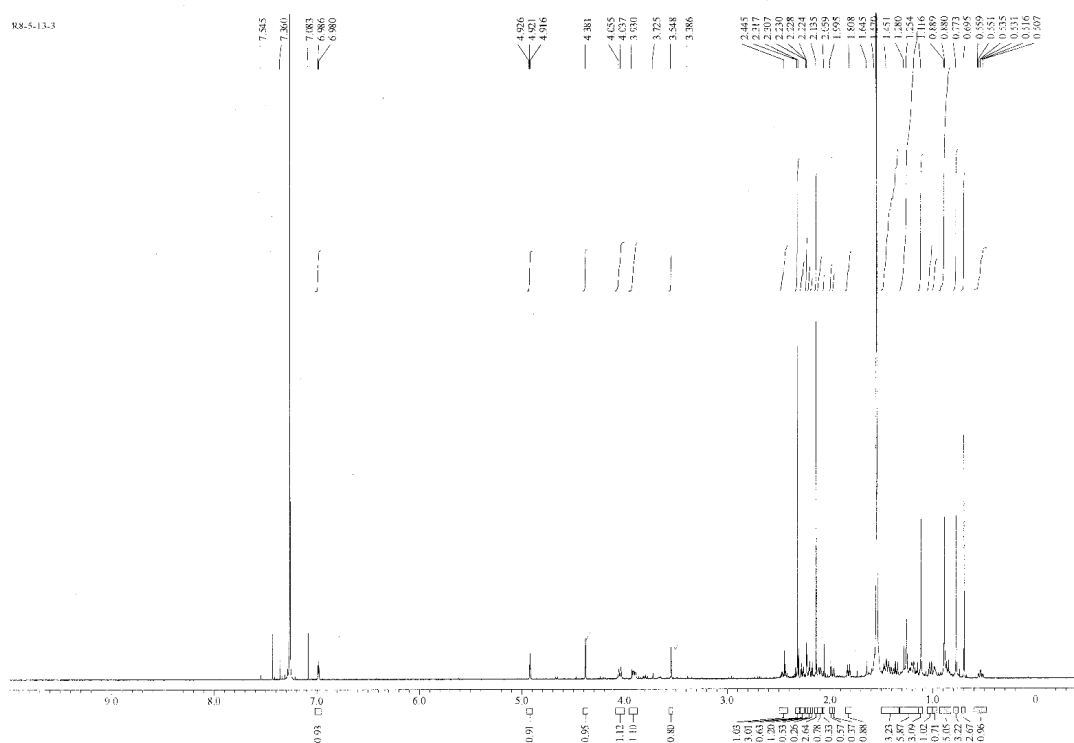


Figure S42. ¹H NMR spectrum (600 MHz) of compound **5** in CDCl₃.

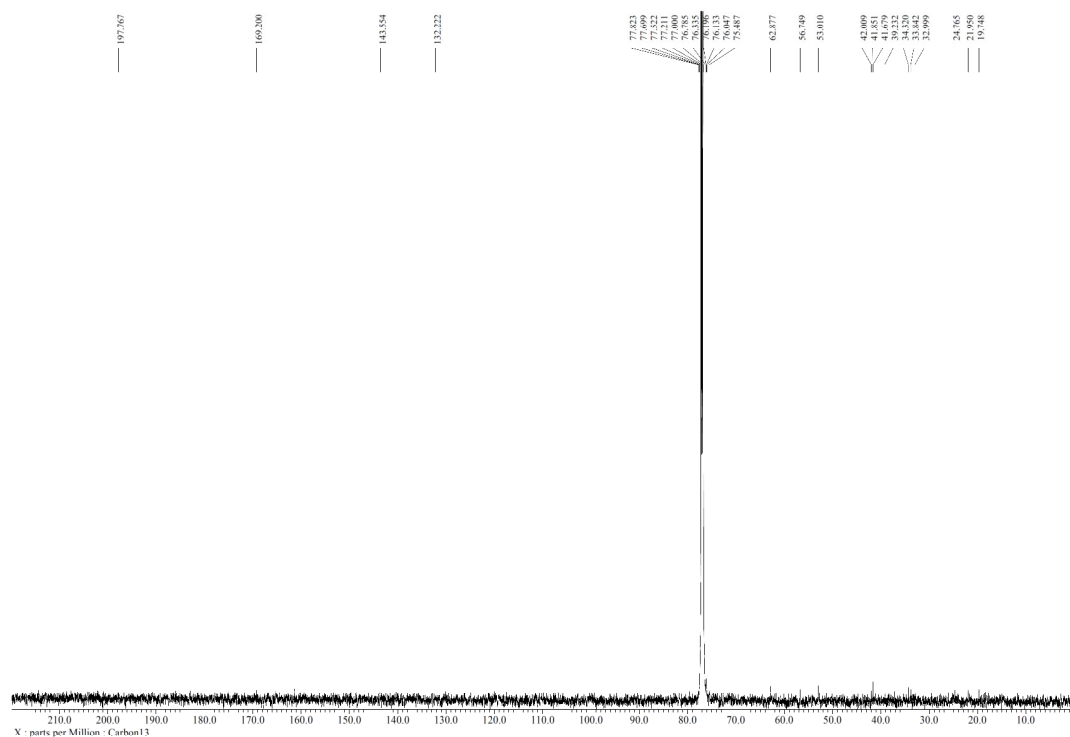


Figure S43. ^{13}C NMR spectrum (150 MHz) of compound **5** in CDCl_3 .

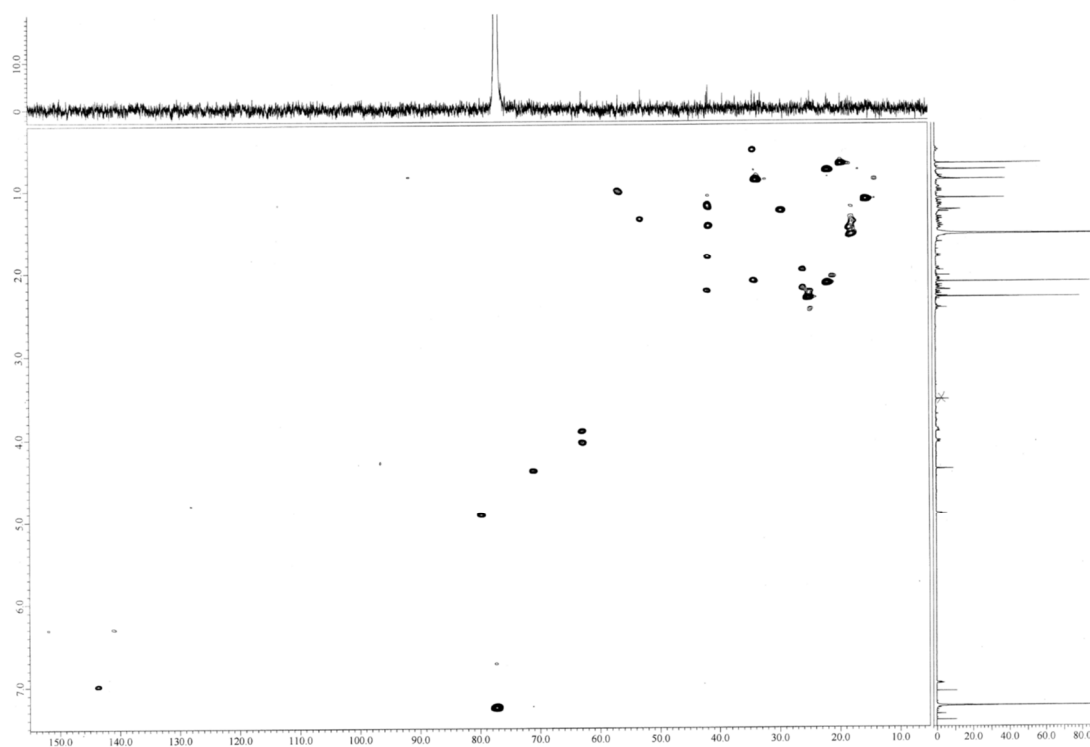


Figure S44. HSQC spectrum of compound **5** in CDCl_3 .

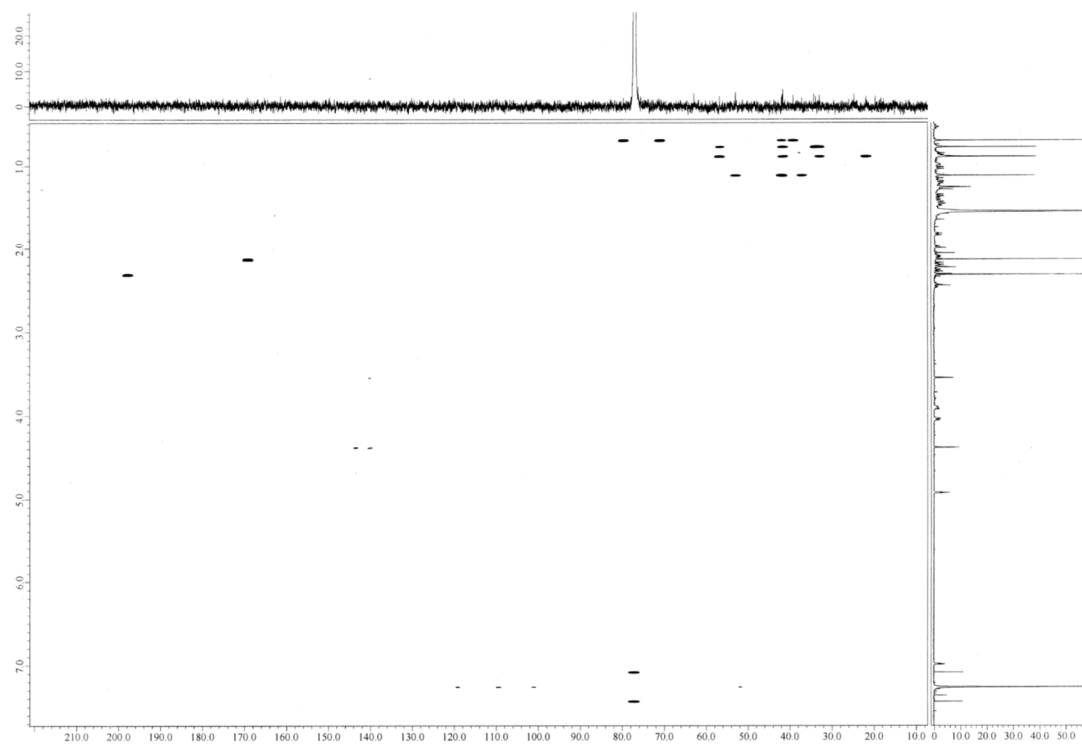


Figure S45. HMBC spectrum of compound **5** in CDCl₃.

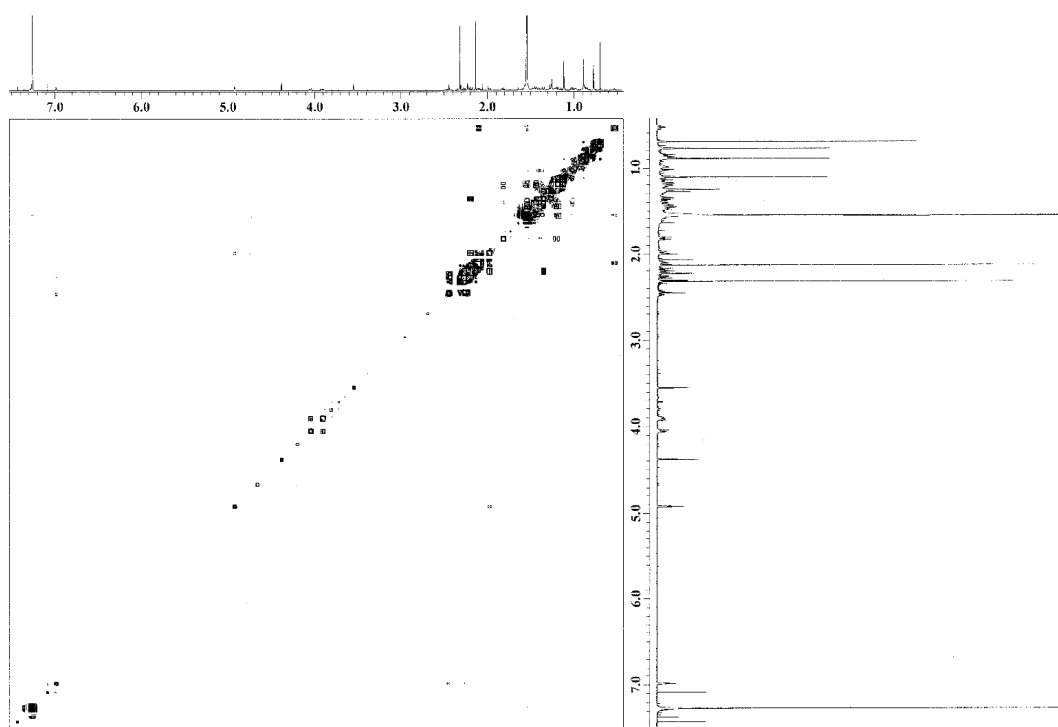


Figure S46. ¹H-¹H COSY spectrum of compound **5** in CDCl₃.

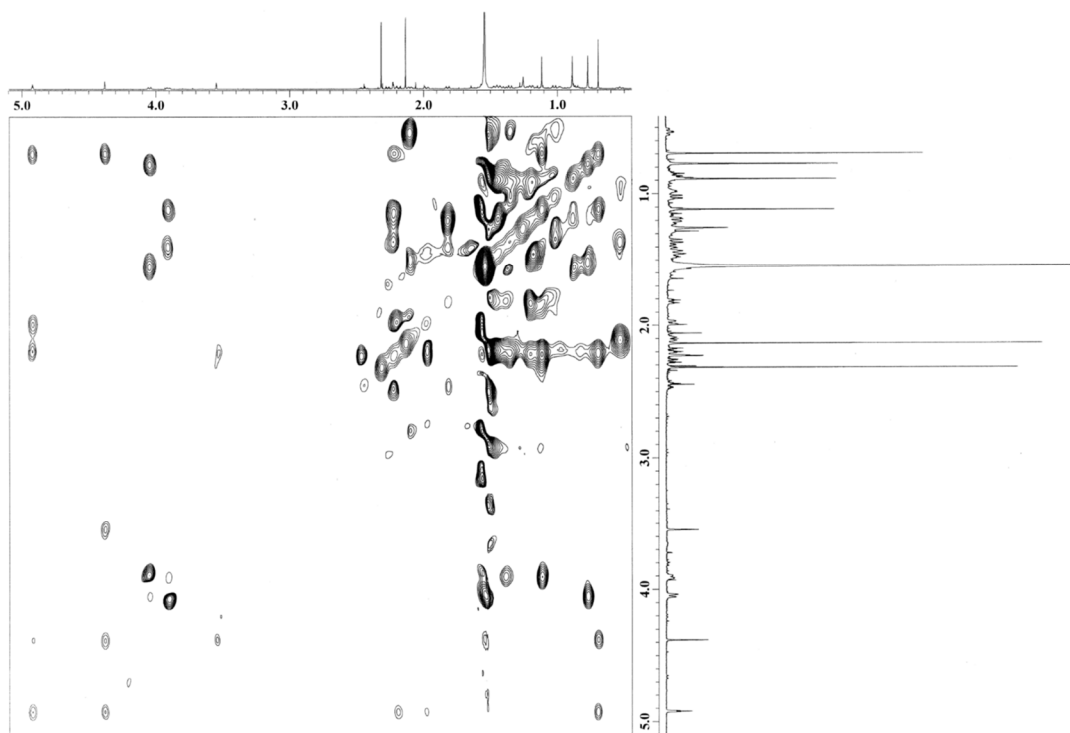


Figure S47. NOESY spectrum of compound **5** in CDCl₃



Figure S48. IR spectrum of compound **6**.

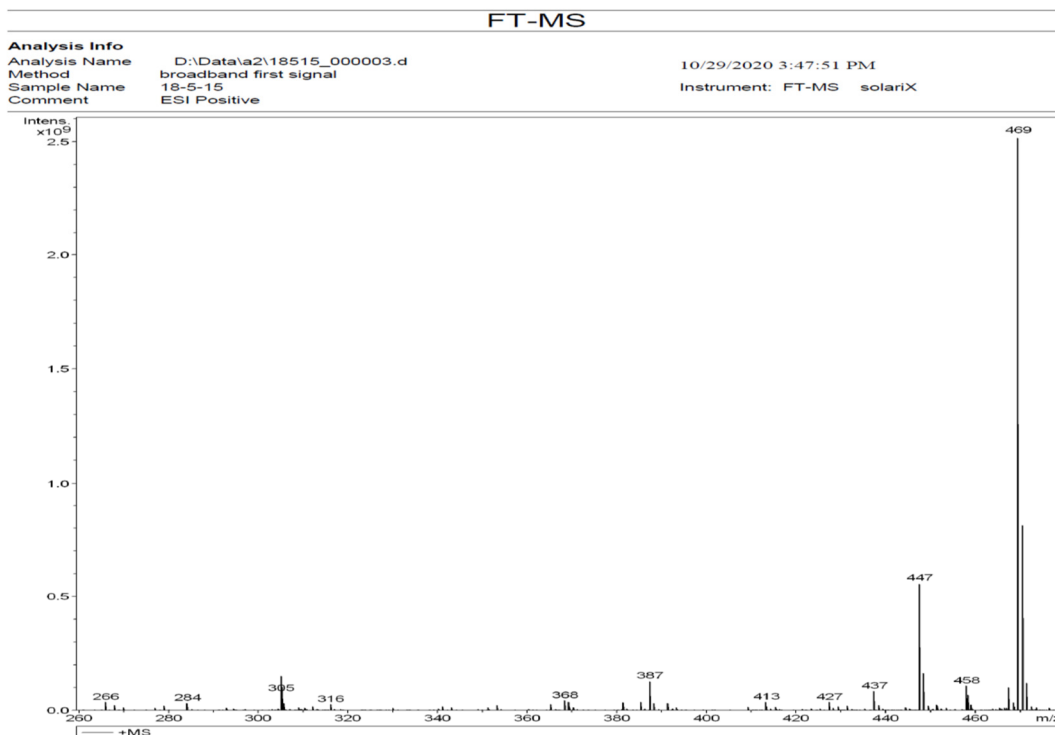


Figure S49. ESIMS spectrum of compound 6.

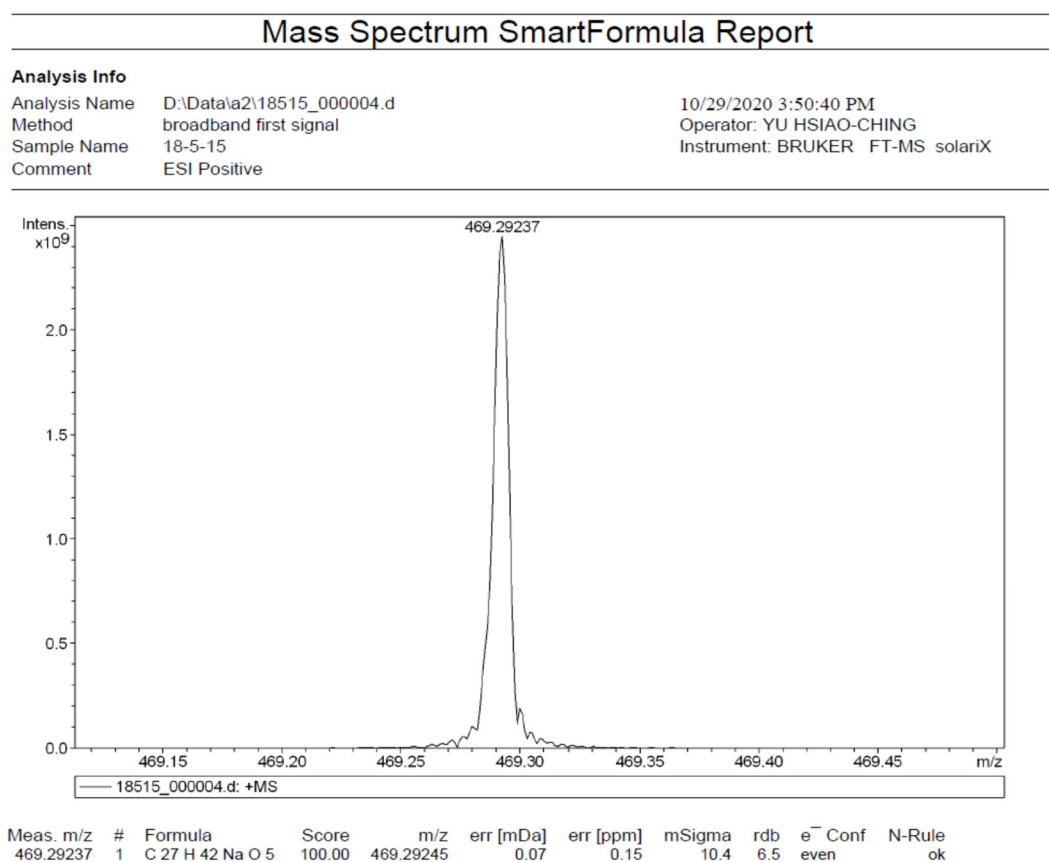


Figure S50. HRESIMS spectrum of compound 6.

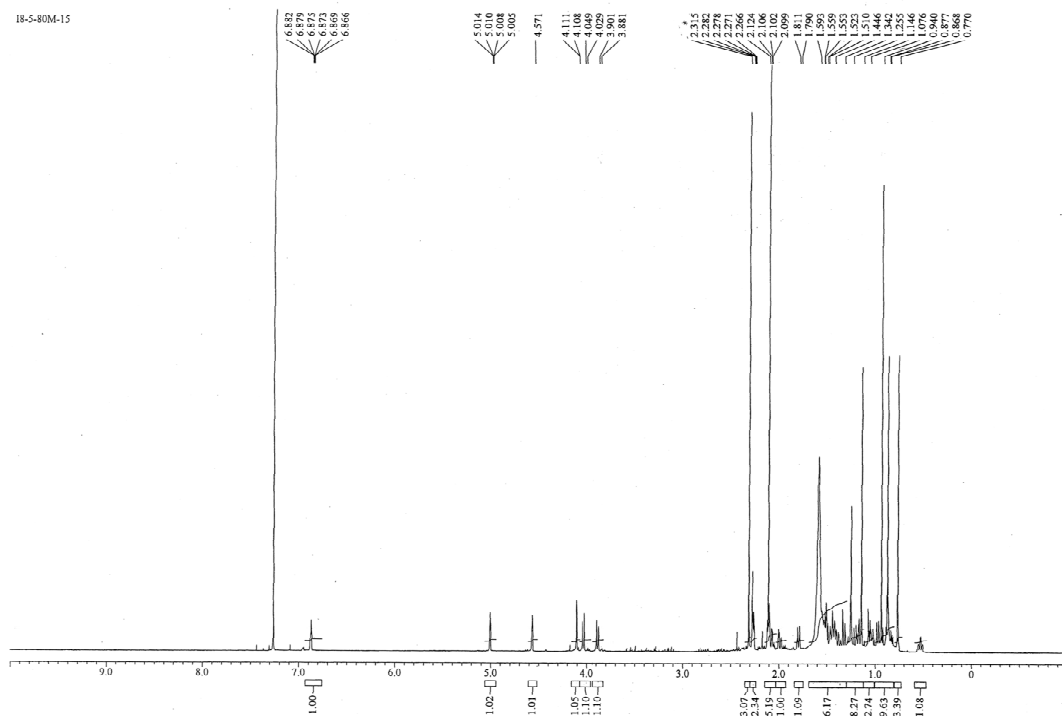


Figure S51. ^1H NMR spectrum (600 MHz) of compound **6** in CDCl_3 .

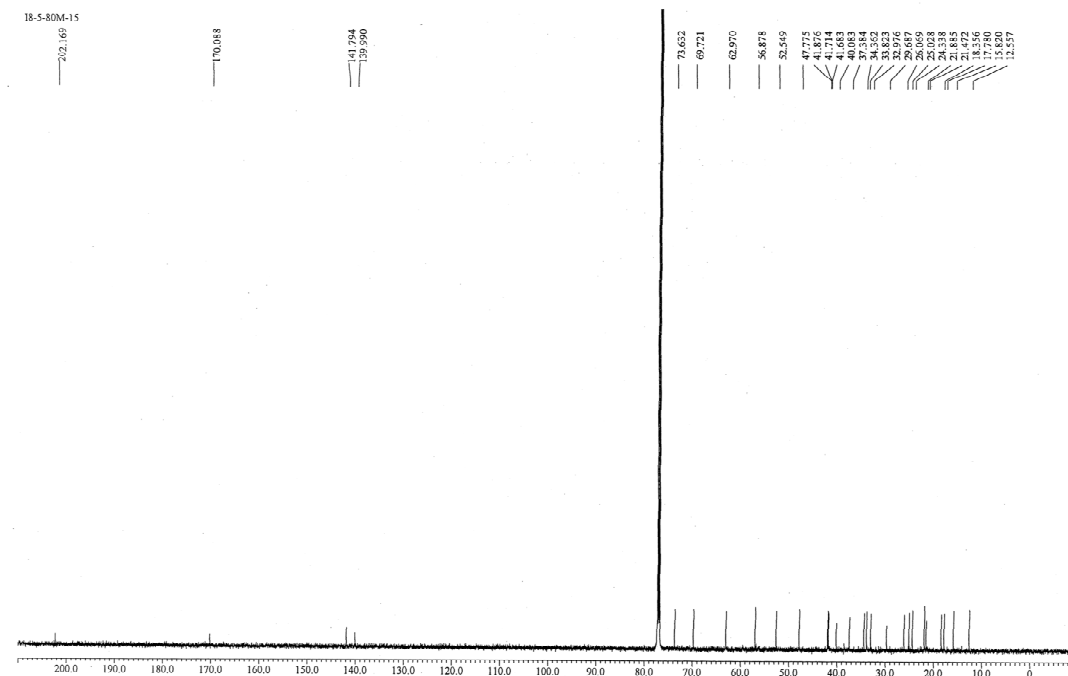


Figure S52. ^{13}C NMR spectrum (150 MHz) of compound **6** in CDCl_3 .

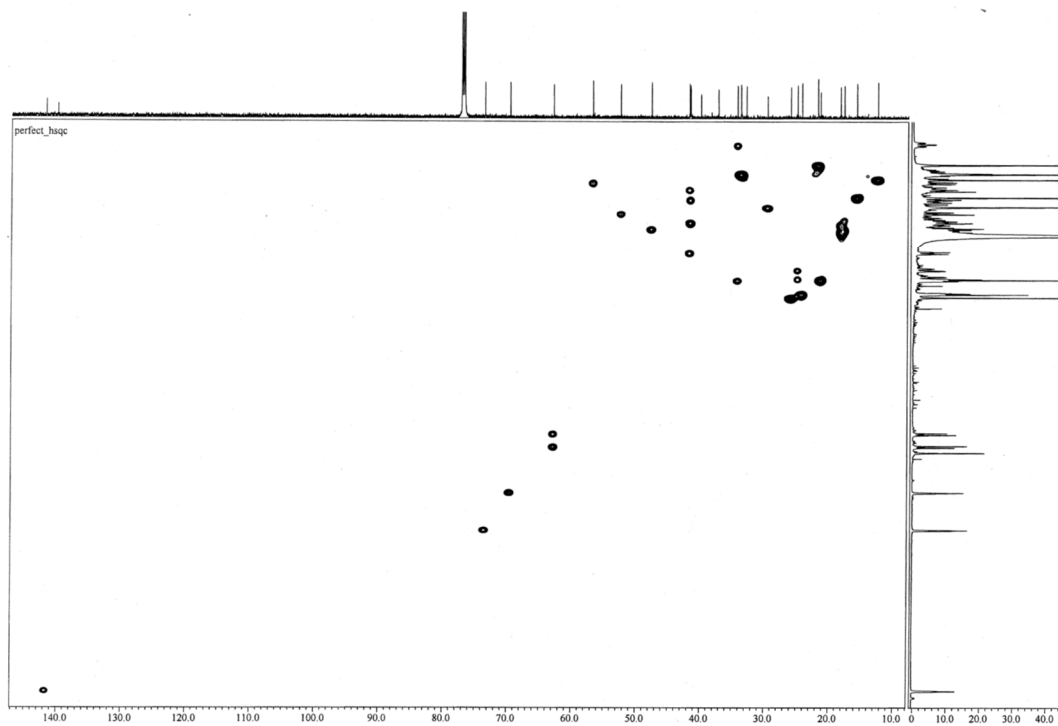


Figure S53. HSQC spectrum of compound **6** in CDCl_3 .

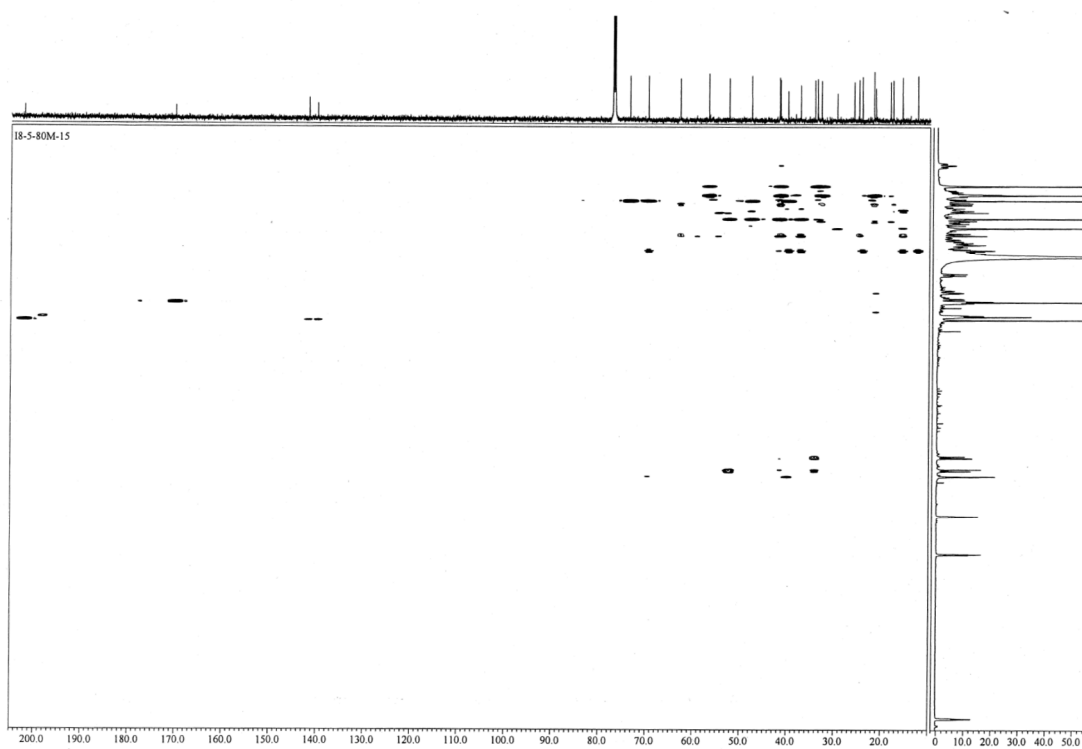


Figure S54. HMBC spectrum of compound **6** in CDCl_3 .

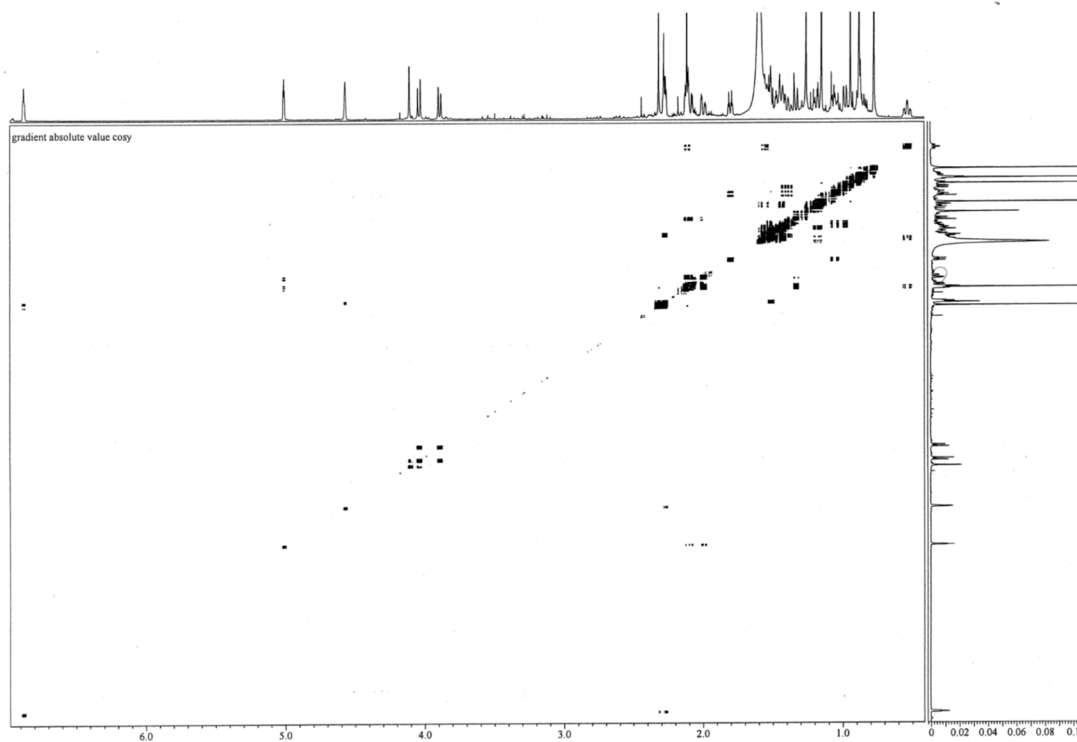


Figure S55. ^1H - ^1H COSY spectrum of compound **6** in CDCl_3 .

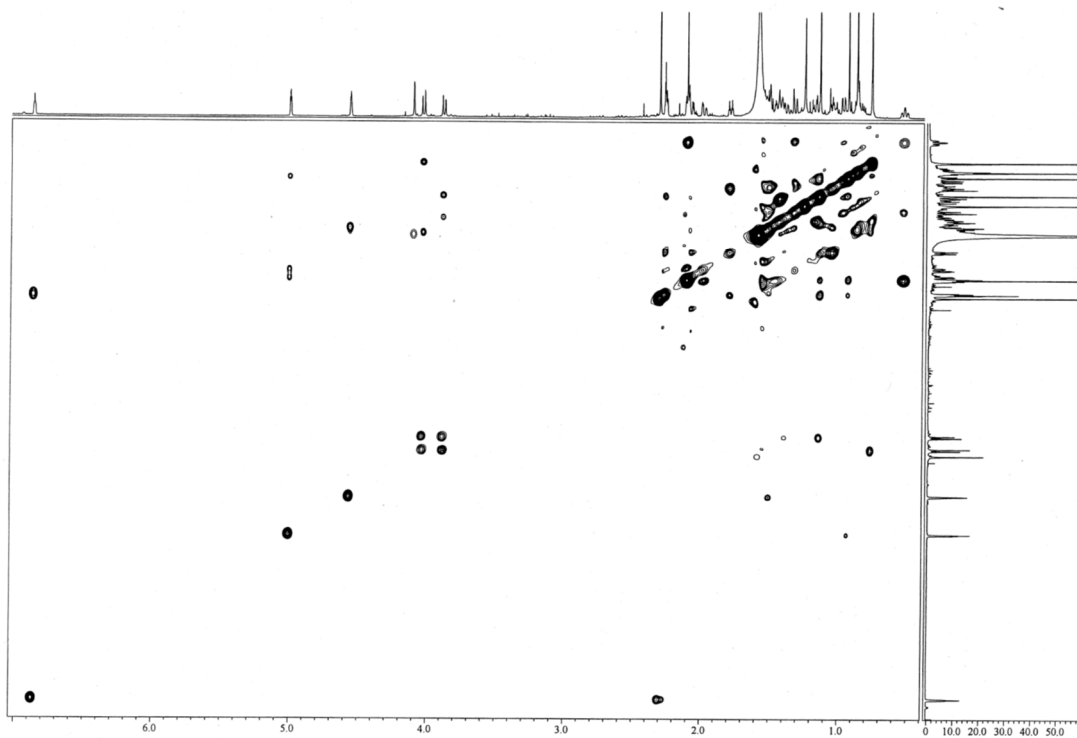


Figure S56. NOESY spectrum of compound **6** in CDCl_3

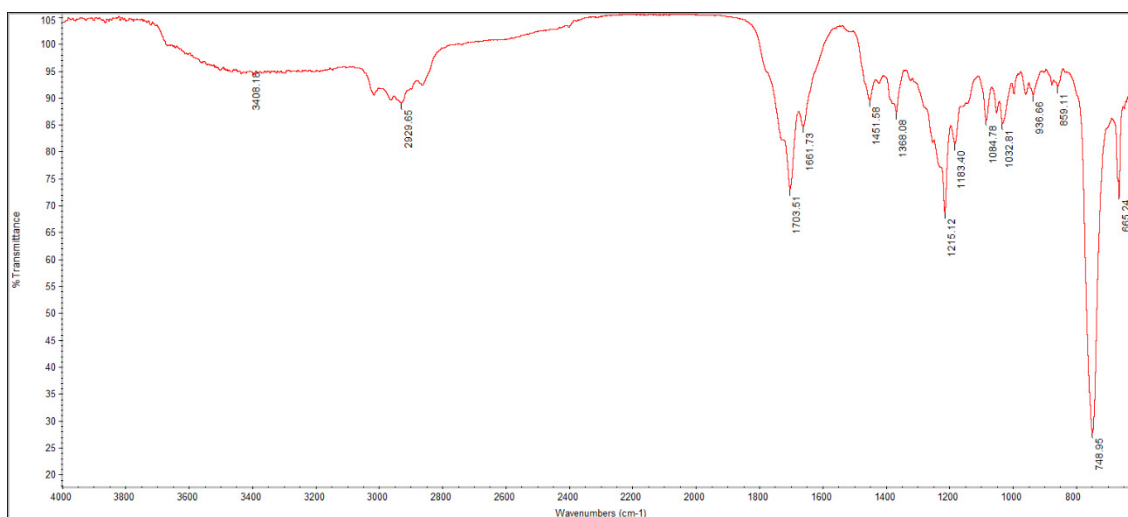


Figure S57. IR spectrum of compound 7.

FT-MS

Analysis Info

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 Method broadband first signal
 Sample Name 18-4-4
 Comment ESI Positive

10/29/2020 4:17:55 PM

Instrument: FT-MS solarix

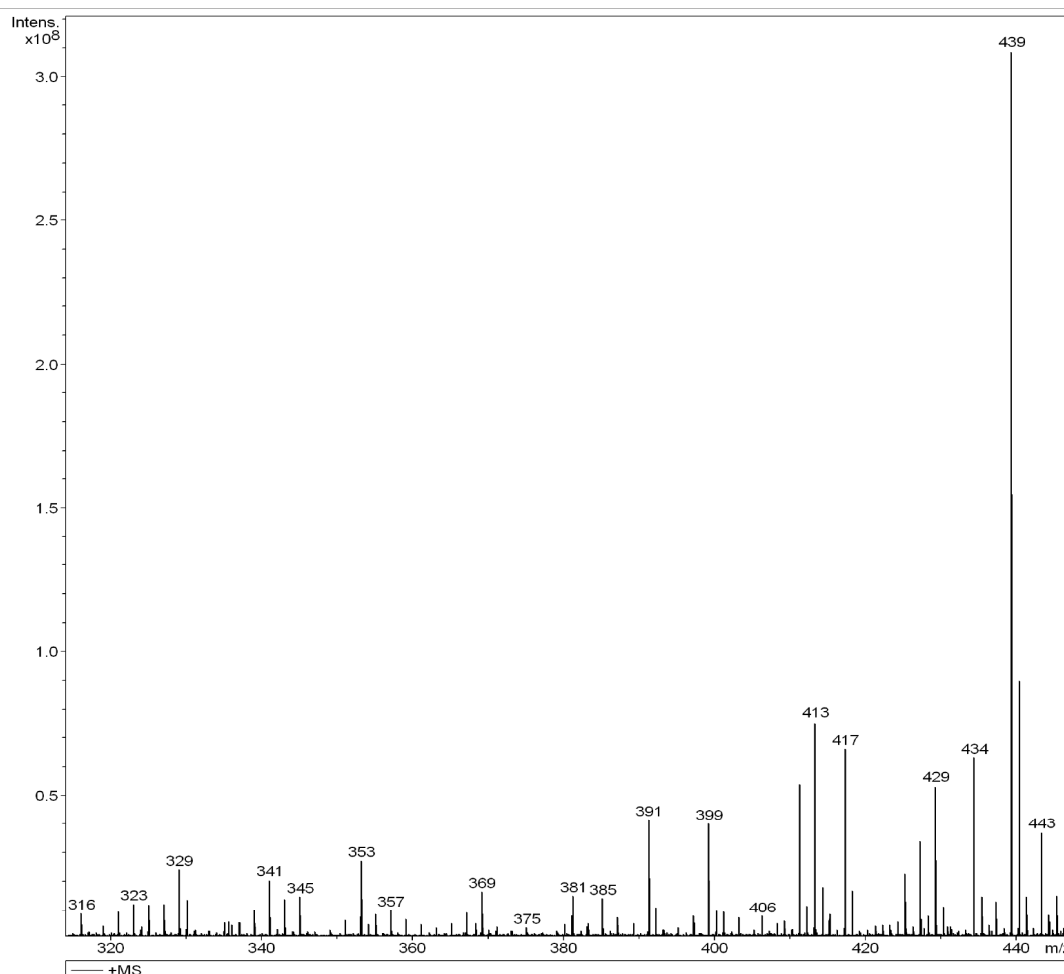


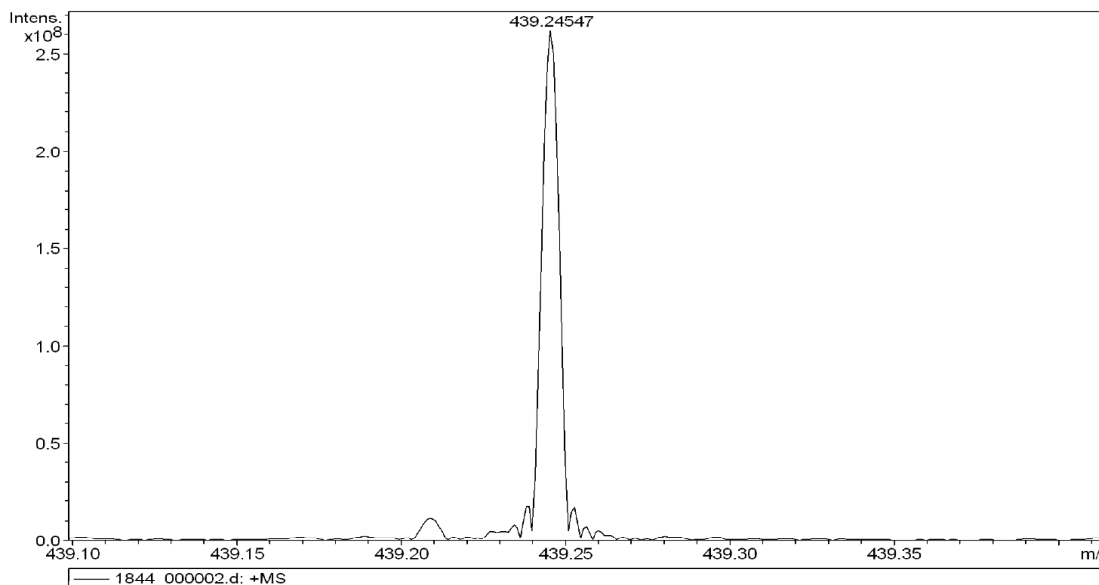
Figure S58. ESIMS spectrum of compound 7.

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\Data\1844_000002.d
Method broadband first signal
Sample Name 18-4-4
Comment ESI Positive

10/29/2020 4:16:52 PM
Operator: YU HSIAO-CHING
Instrument: BRUKER FT-MS solariX



| Meas. m/z | # | Formula | Score | m/z | err [mDa] | err [ppm] | mSigma | rdb | e ⁻ | Conf | N-Rule |
|-----------|---|------------------|--------|-----------|-----------|-----------|--------|-----|----------------|------|--------|
| 439.24547 | 1 | C 25 H 36 Na O 5 | 100.00 | 439.24550 | 0.03 | 0.07 | 4.9 | 7.5 | even | | ok |

Figure S59. HRESIMS spectrum of compound 7.

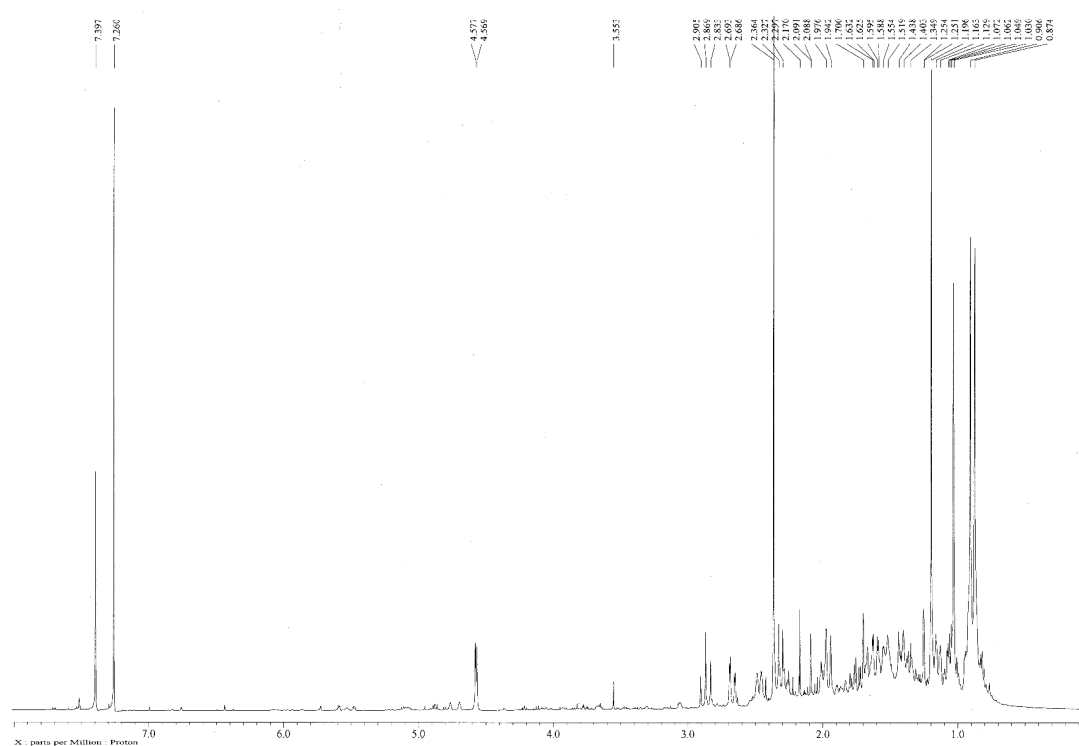


Figure S60. ¹H NMR spectrum (400 MHz) of compound 7 in CDCl₃.

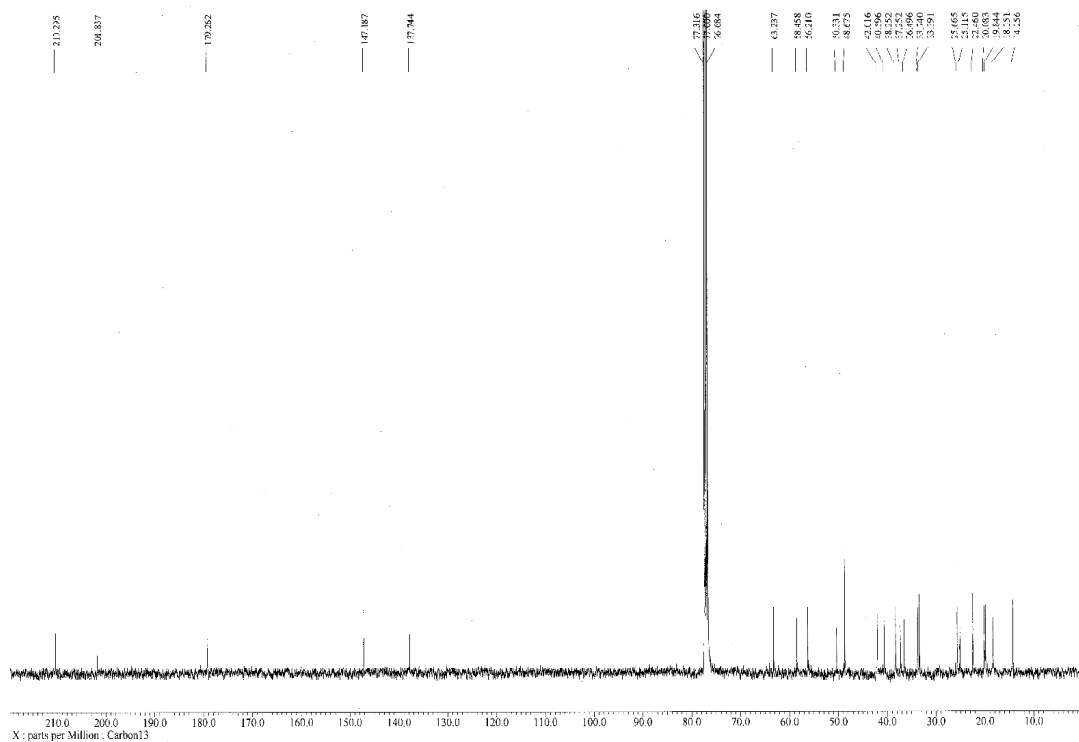


Figure S61. ^{13}C NMR spectrum (100 MHz) of compound **7** in CDCl_3 .

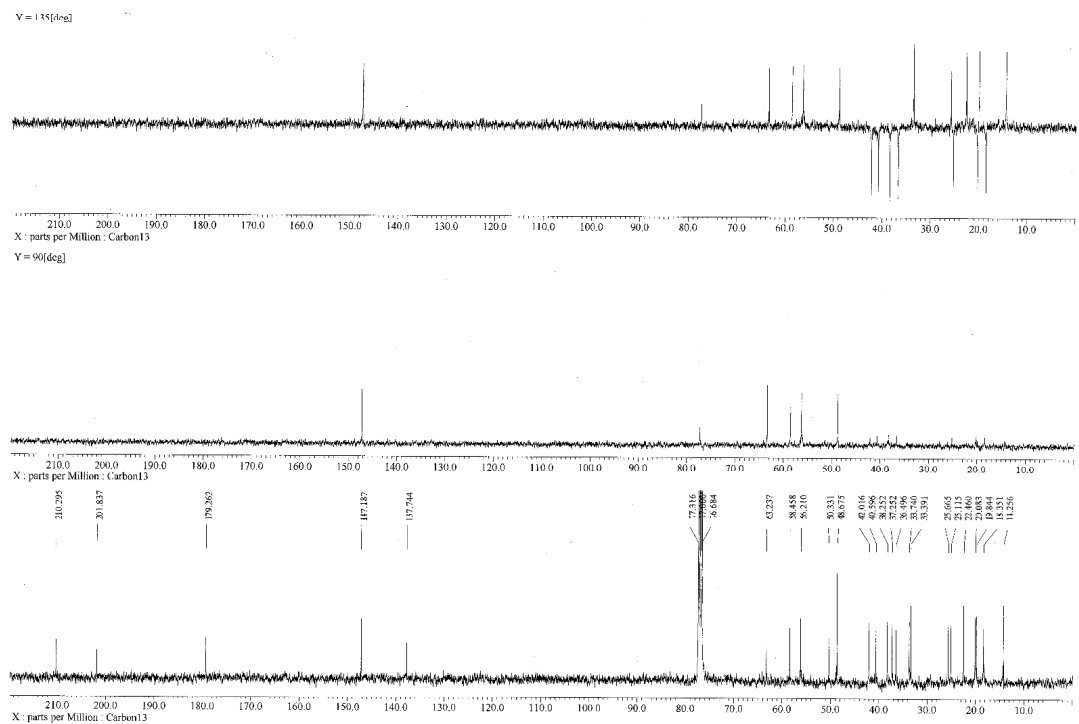


Figure S62. DEPT spectrum of compound **7** in CDCl_3 .

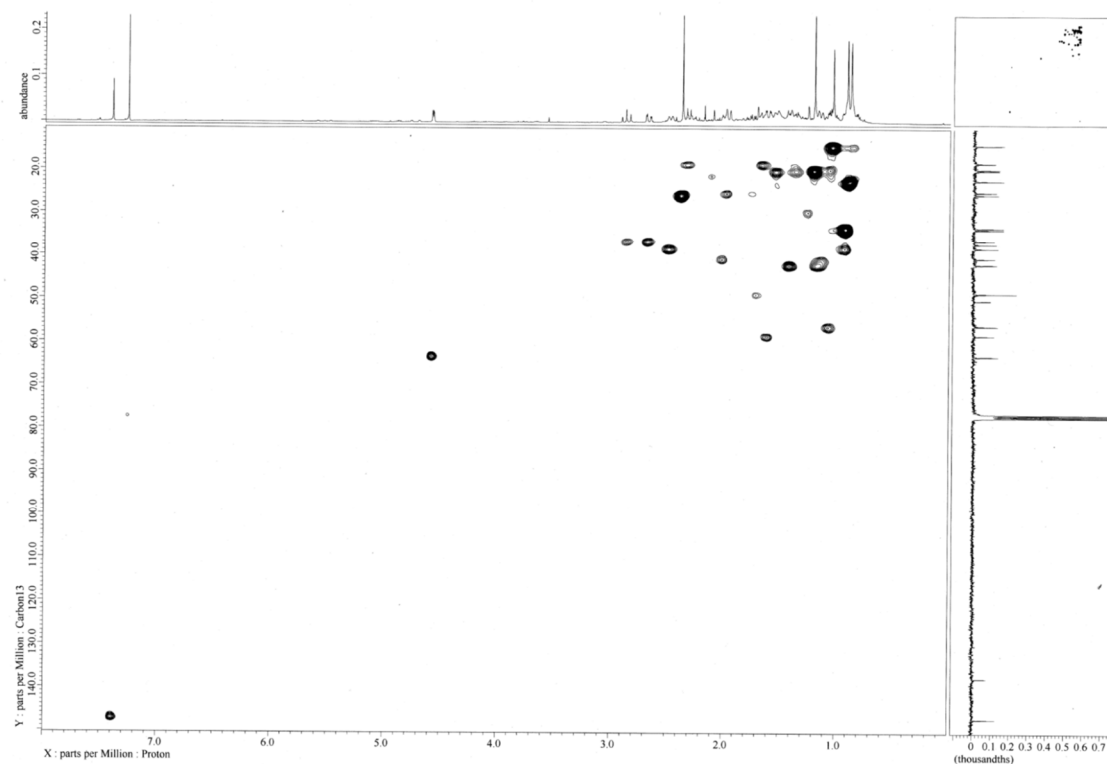


Figure S63. HSQC spectrum of compound **7** in CDCl_3 .

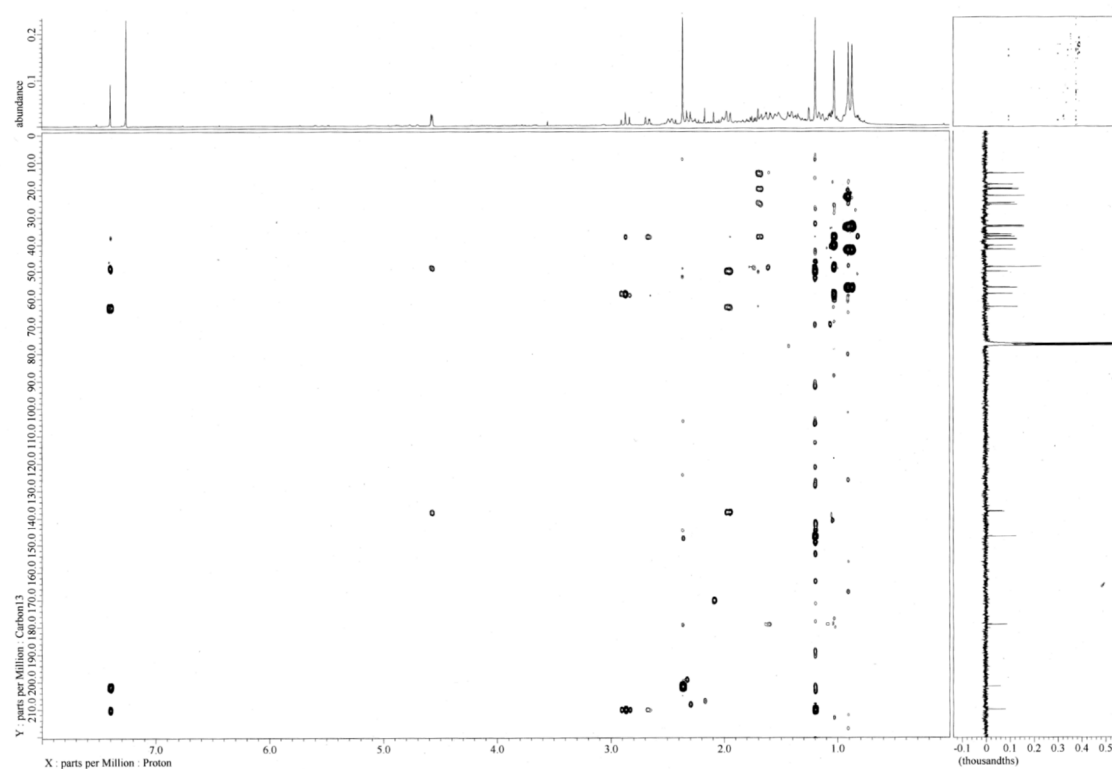


Figure S64. HMBC spectrum of compound **7** in CDCl_3 .

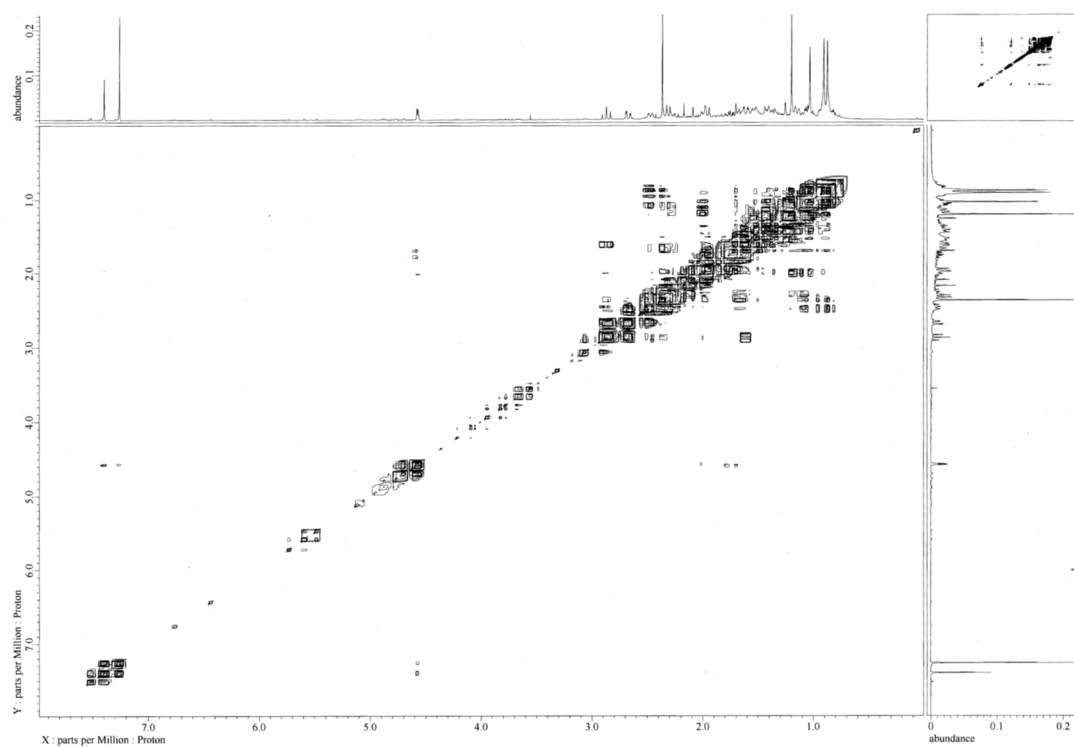


Figure S65. ^1H - ^1H COSY spectrum of compound 7 in CDCl_3 .

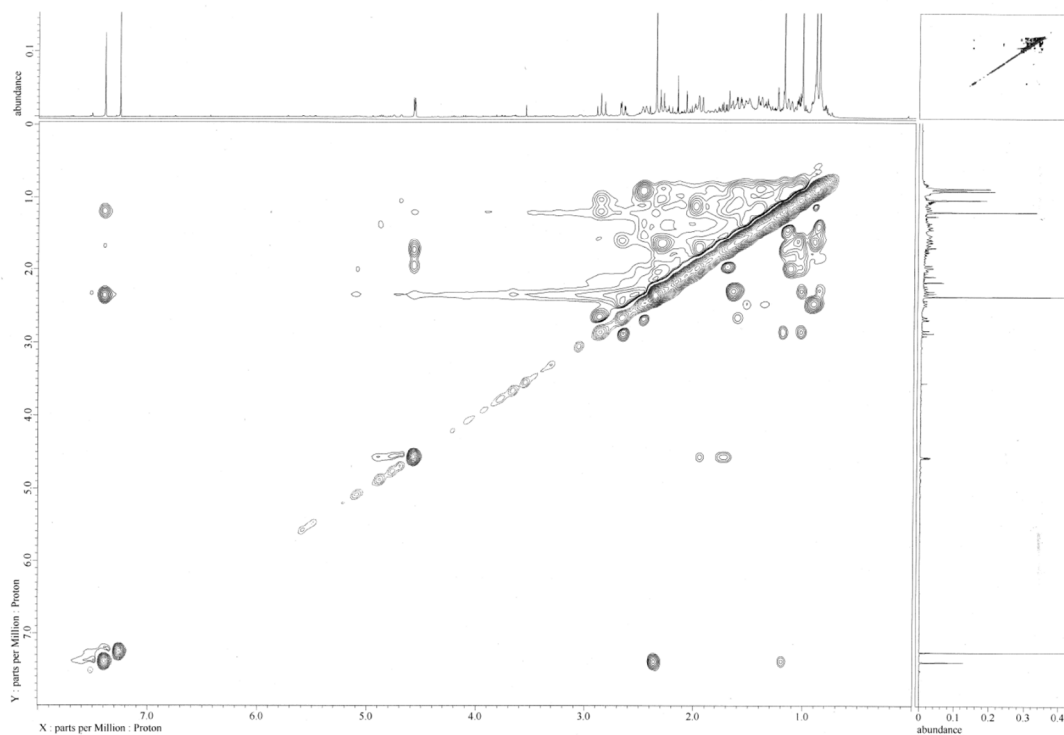


Figure S66. NOESY spectrum of compound 7 in CDCl_3