

Study on the Anti-*Mycobacterium marinum* Activity of a Series of Marine-Derived 14-Membered Resorcylic Acid Lactone Derivatives

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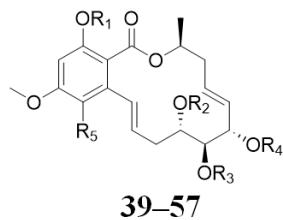
Figure S45. HR-ESI-MS spectrum of compound 37.

Figure S46. ^1H NMR (400 MHz, Chloroform-*d*) spectrum of compound 38.

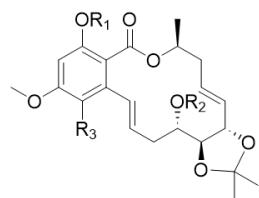
Figure S47. ^{13}C NMR (100 MHz, Chloroform-*d*) spectrum of compound 38.

Figure S48. HR-ESI-MS spectrum of compound 38.

Table S1. The derivatives 39 – 97 of zeaenol (**1**)



| No. | R ₁ | R ₂ | R ₃ | R ₄ | R ₅ | No. | R ₁ | R ₂ | R ₃ | R ₄ | R ₅ |
|-----------|----------------|----------------|----------------|----------------|----------------|-----------|----------------|----------------|----------------|----------------|----------------|
| 39 | | H | H | H | H | 49 | | H | H | H | H |
| 40 | | H | H | H | H | 50 | | H | H | H | H |
| 41 | | H | H | H | H | 51 | | H | H | H | H |
| 42 | | H | H | H | H | 52 | | H | H | H | H |
| 43 | | H | H | H | H | 53 | | H | H | H | H |
| 44 | | H | H | H | H | 54 | | H | H | H | H |
| 45 | | H | H | H | H | 55 | | H | H | H | Cl |
| 46 | | H | H | H | H | 56 | | H | H | H | Cl |
| 47 | | H | H | H | H | 57 | | H | H | H | Cl |
| 48 | | H | H | H | H | | | | | | |



| No. | R ₁ | R ₂ | R ₃ | No. | R ₁ | R ₂ | R ₃ | No. | R ₁ | R ₂ | R ₃ |
|-----------|----------------|----------------|----------------|-----------|----------------|----------------|----------------|-----------|----------------|----------------|----------------|
| 58 | | H | H | 66 | | H | H | 74 | | H | H |
| 59 | | | H | 67 | | H | H | 75 | | H | H |

| | | | | | | | | | | | |
|-----------|---|---|---|-----------|--|---|---|-----------|--|---|---|
| 60 | | H | H | 68 | | H | H | 76 | | H | H |
| 61 | | | H | 69 | | H | H | 77 | | H | H |
| 62 | | H | H | 70 | | H | H | 78 | | H | H |
| 63 | | H | H | 71 | | H | H | 79 | | H | H |
| 64 | H | | H | 72 | | H | H | 80 | | H | H |
| 65 | | H | H | 73 | | H | H | 81 | | H | H |

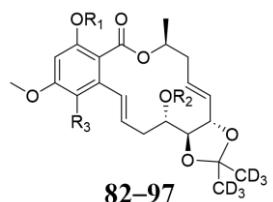


Table S2. Anhydride, acyl chloride reagents or carboxylic acid reagents used to generate compounds **24–38^a**.

| No. | reagents | Yield | No. | reagents | Yield | No. | reagents | Yield |
|-----------|-----------------------|-------|-----------|----------------------|-------|-----------|-----------------------------|-------|
| 24 | 2-Methoxybenzoic acid | 83.2% | 29 | Benzoyl chloride | 77.8% | 34 | Nicotinic acid | 85.6% |
| 25 | 2-Furoic acid | 70.3% | 30 | 2-Fluorobenzoic acid | 83.5% | 35 | Nicotinic acid | 72.4% |
| 26 | 2-Furoic acid | 60.6% | 31 | 2-Fluorobenzoic acid | 87.2% | 36 | Acetic anhydride | 63.7% |
| 27 | 2-Furoic acid | 73.4% | 32 | 2-Fluorobenzoic acid | 73.9% | 37 | Thiophene-2-carboxylic acid | 85.2% |
| 28 | Benzoyl chloride | 63.7% | 33 | Nicotinic acid | 67.7% | 38 | Thiophene-2-carboxylic acid | 87.7% |

^a All reagents used in this study are commercial reagents.

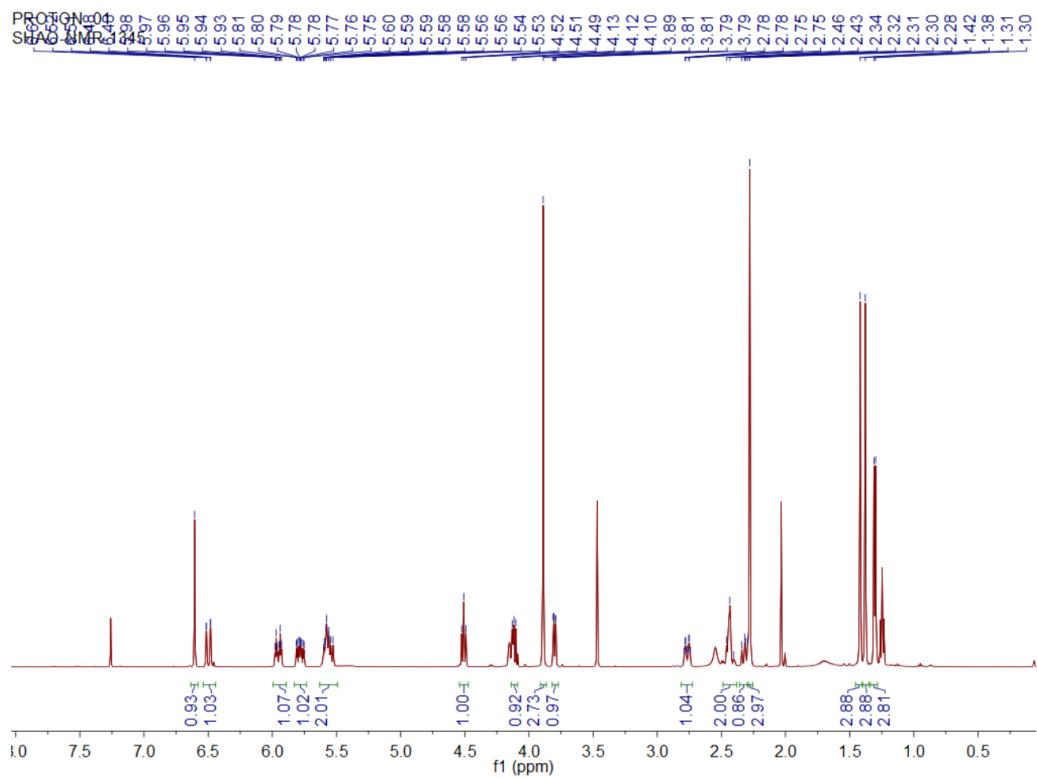


Figure S1. ^1H NMR (400 MHz, Chloroform-*d*) spectrum of compound **19**.

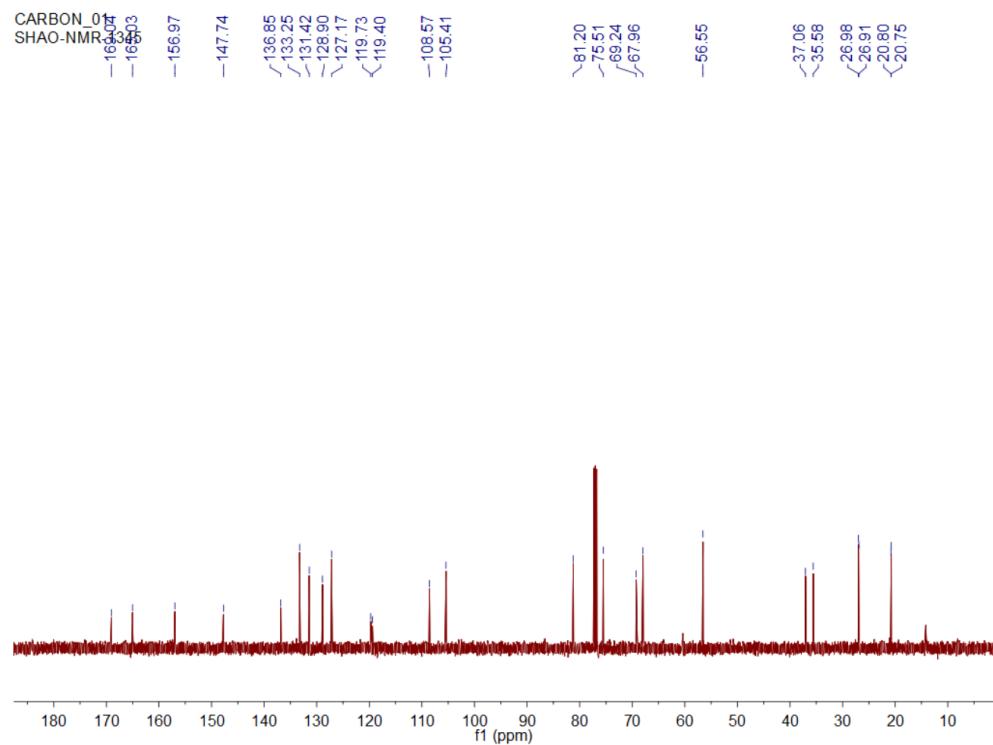


Figure S2. ^{13}C NMR (100 MHz, Chloroform-*d*) spectrum of compound **19**.

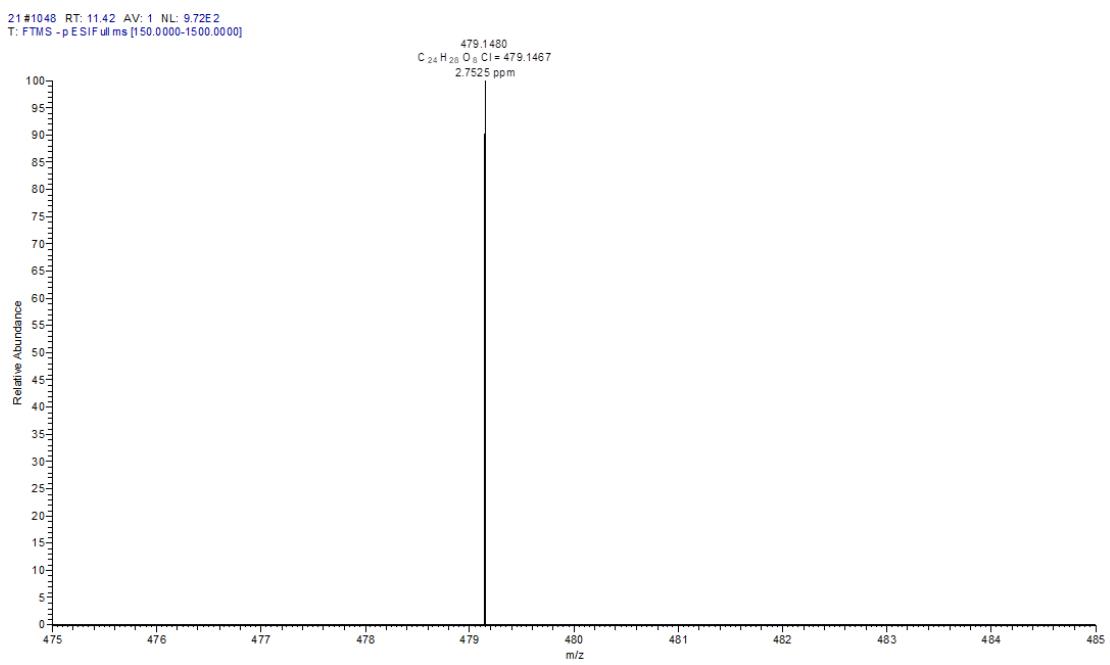


Figure S3. HR-ESI-MS spectrum of compound **19**.

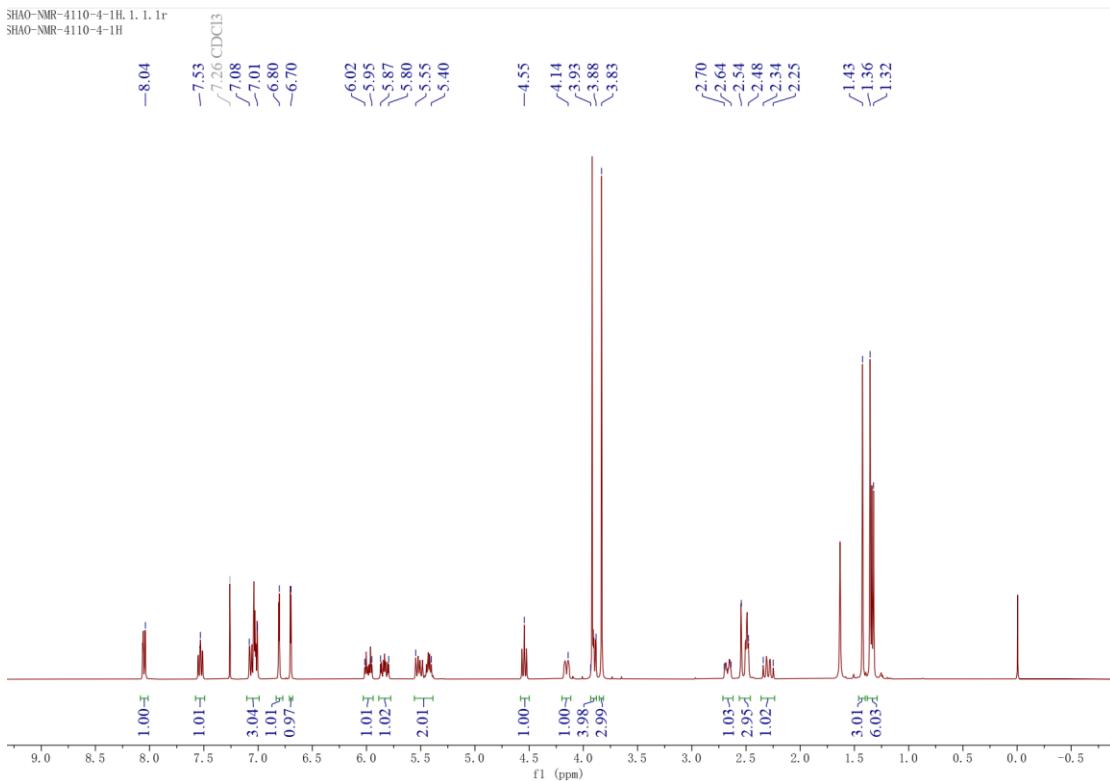


Figure S4. 1H NMR (400 MHz, Chloroform-*d*) spectrum of compound **24**.

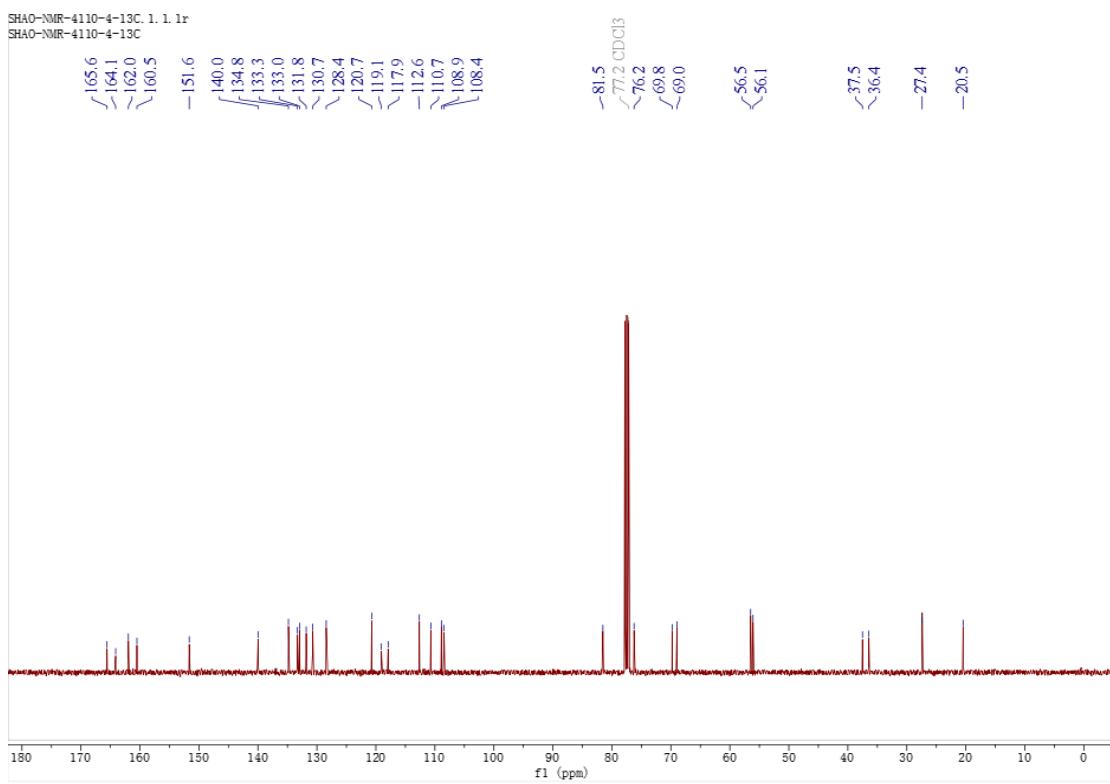


Figure S5. ^{13}C NMR (100 MHz, Chloroform- d) spectrum of compound **24**.

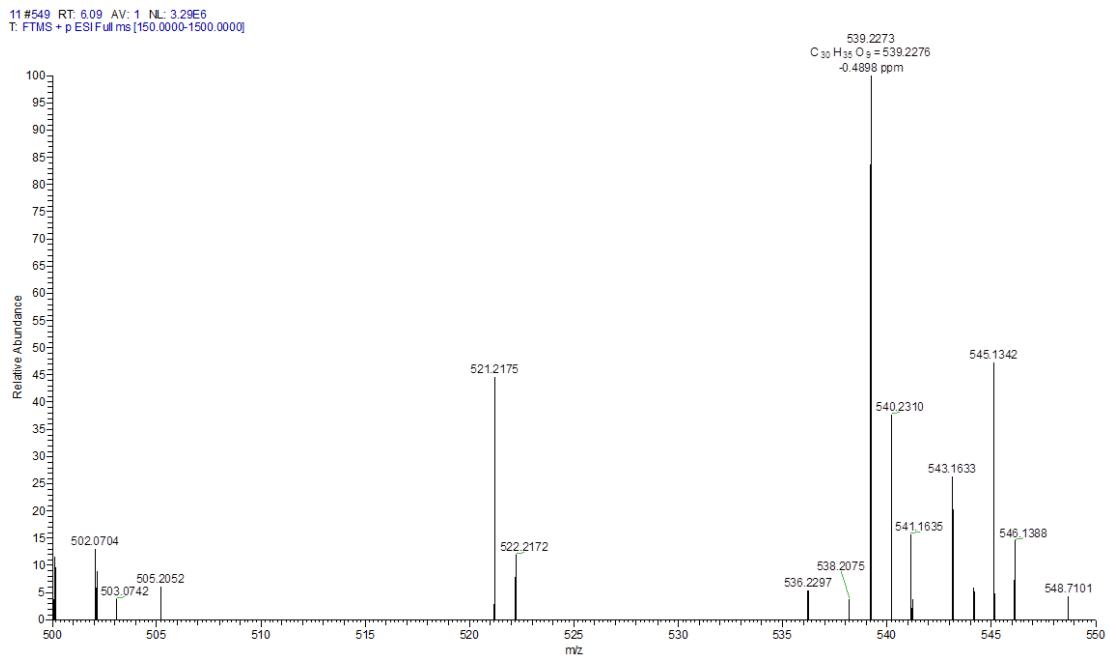


Figure S6. HR-ESI-MS spectrum of compound **24**.

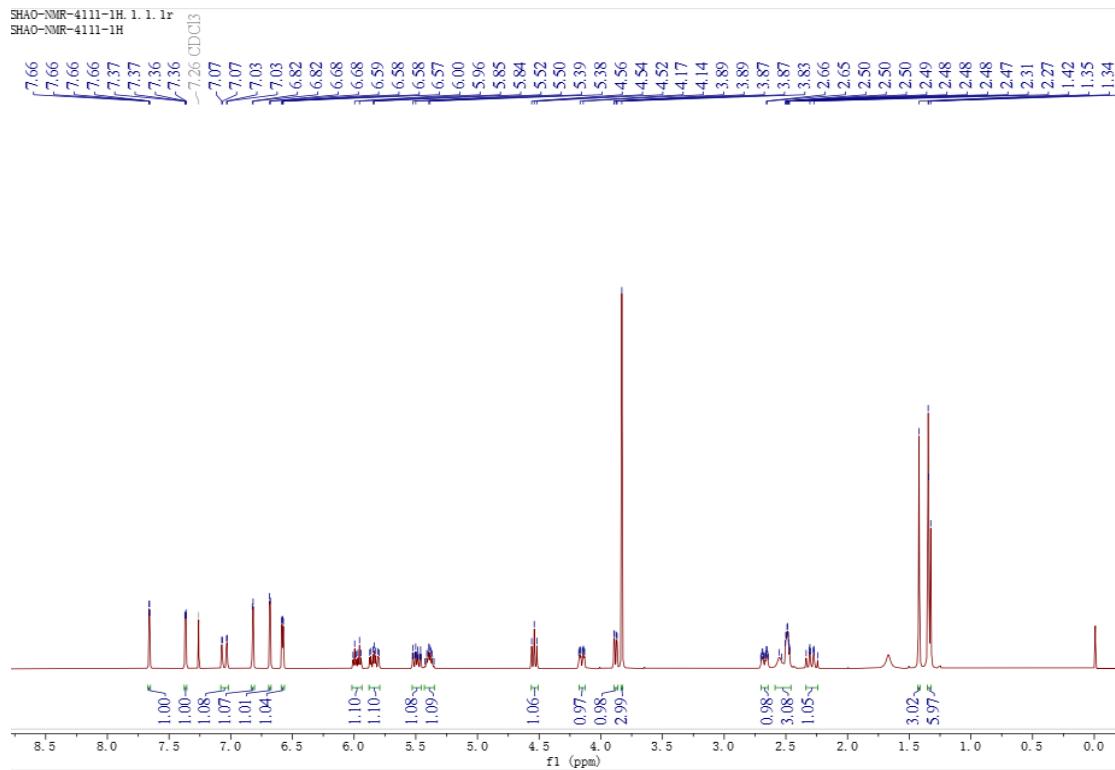


Figure S7. ^1H NMR (400 MHz, Chloroform-*d*) spectrum of compound 25.

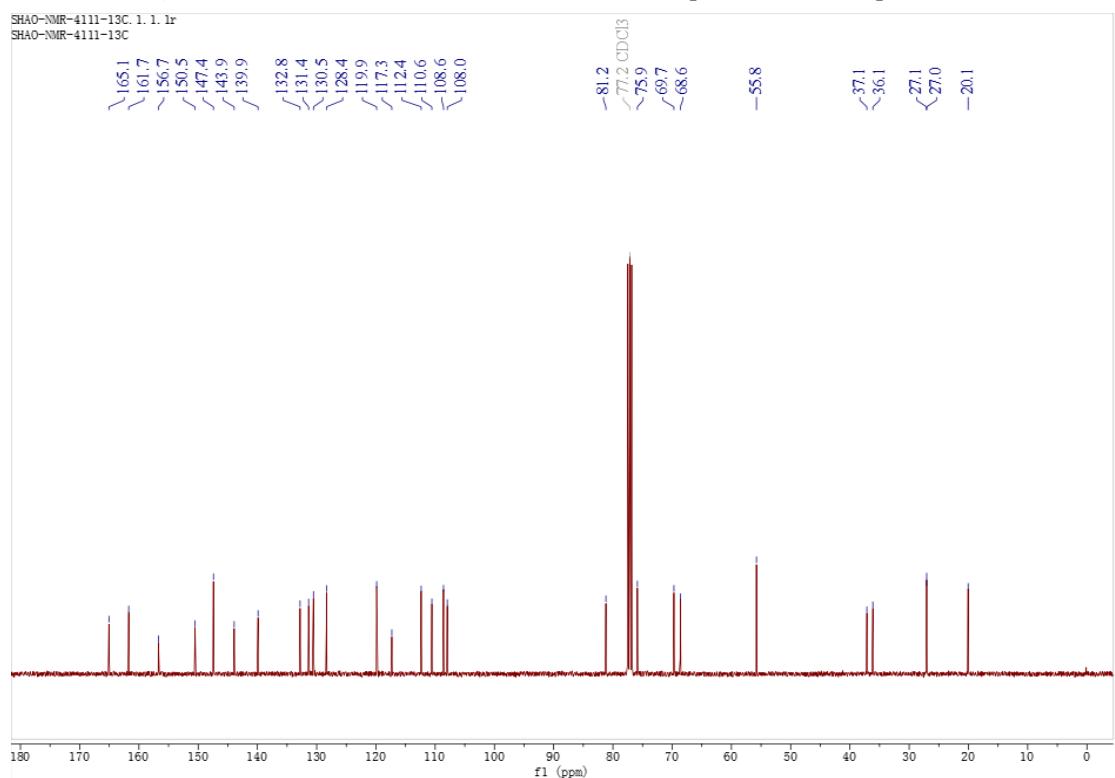


Figure S8. ^{13}C NMR (100 MHz, Chloroform-*d*) spectrum of compound 25.

11#493 RT: 5.50 AV: 1 NL: 1.59E6
T: FTMS + p ESI Full ms[150.0000-1500.0000]

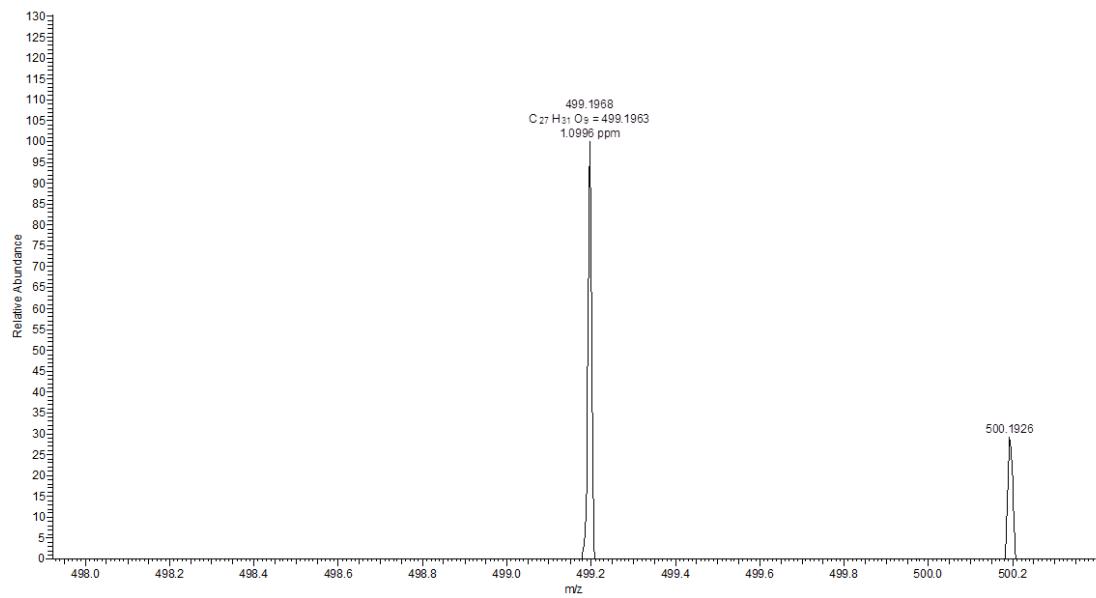


Figure S9. HR-ESI-MS spectrum of compound **25**.

SHAO-NMR-4114-1-1H. 1. 1. lr
SHAO-NMR-4114-1-1H

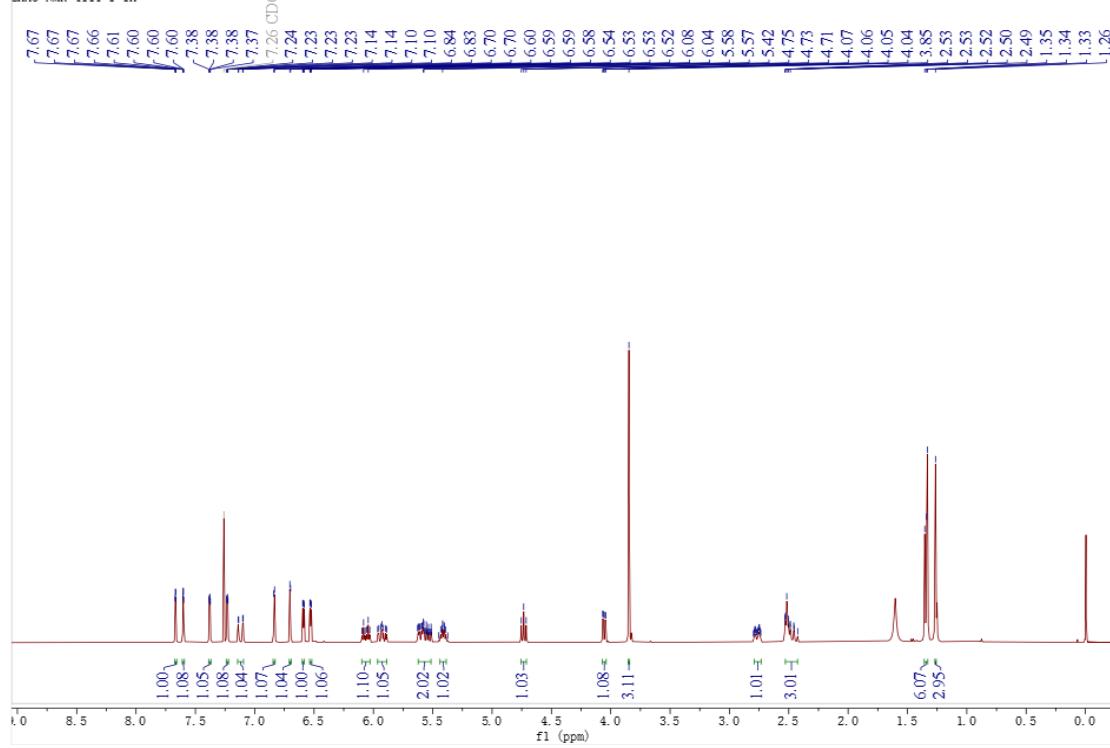


Figure S10. ¹H NMR (400 MHz, Chloroform-*d*) spectrum of compound **26**.

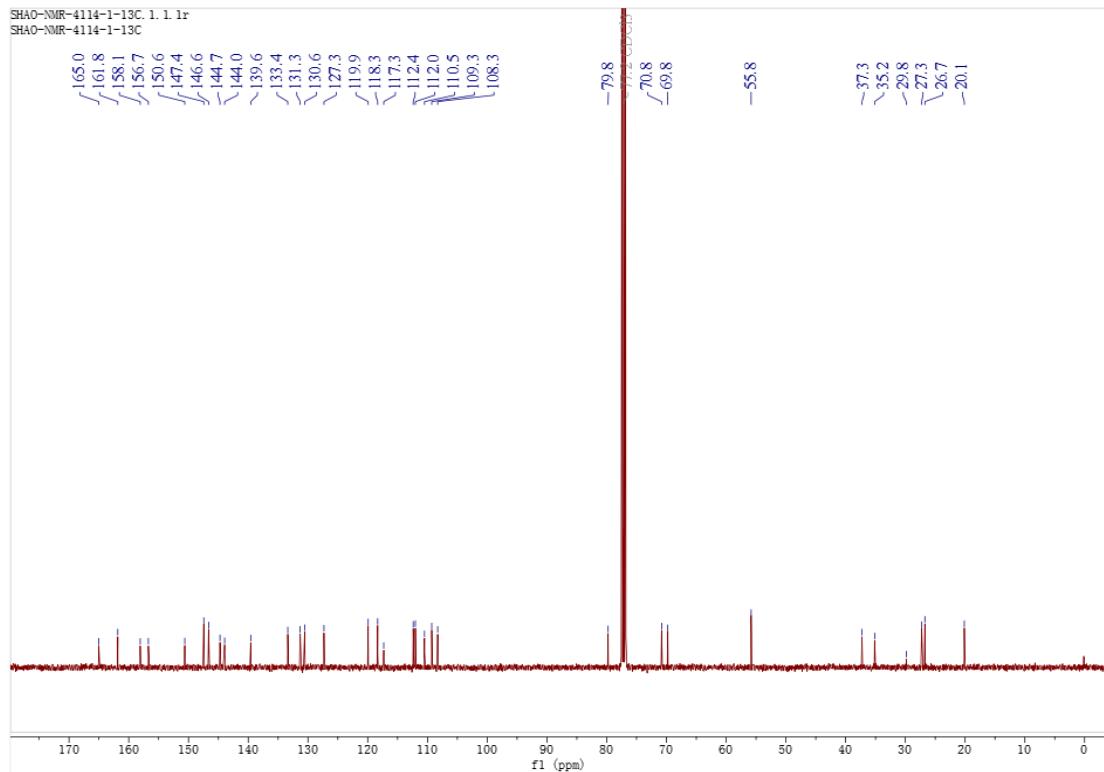


Figure S11. ^{13}C NMR (100 MHz, Chloroform-*d*) spectrum of compound **26**.

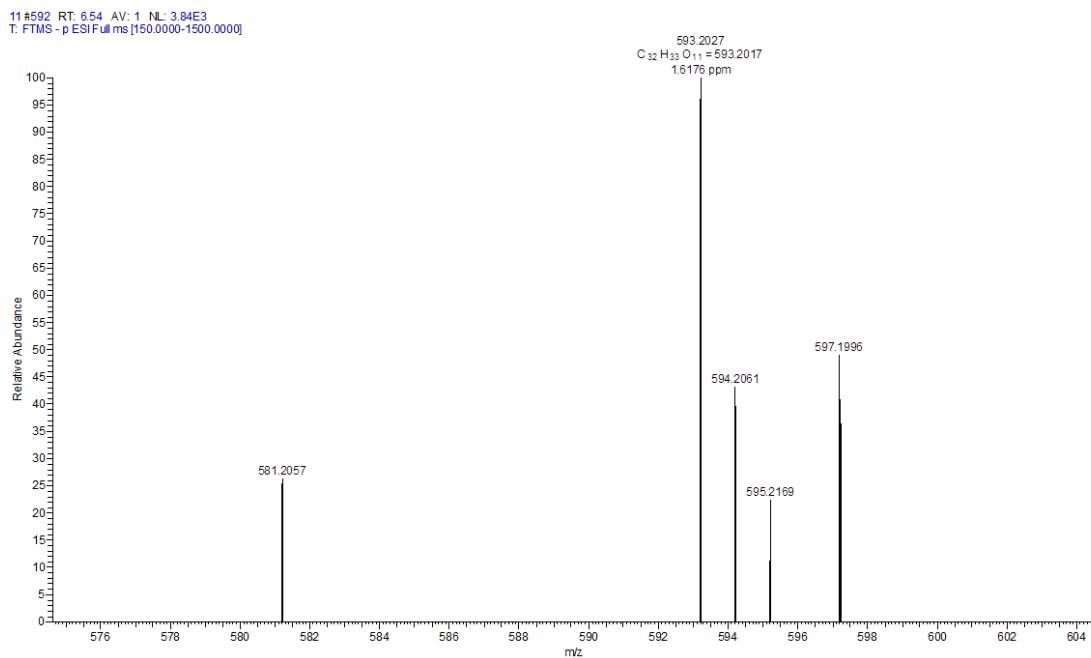


Figure S12. HR-ESI-MS spectrum of compound **26**.

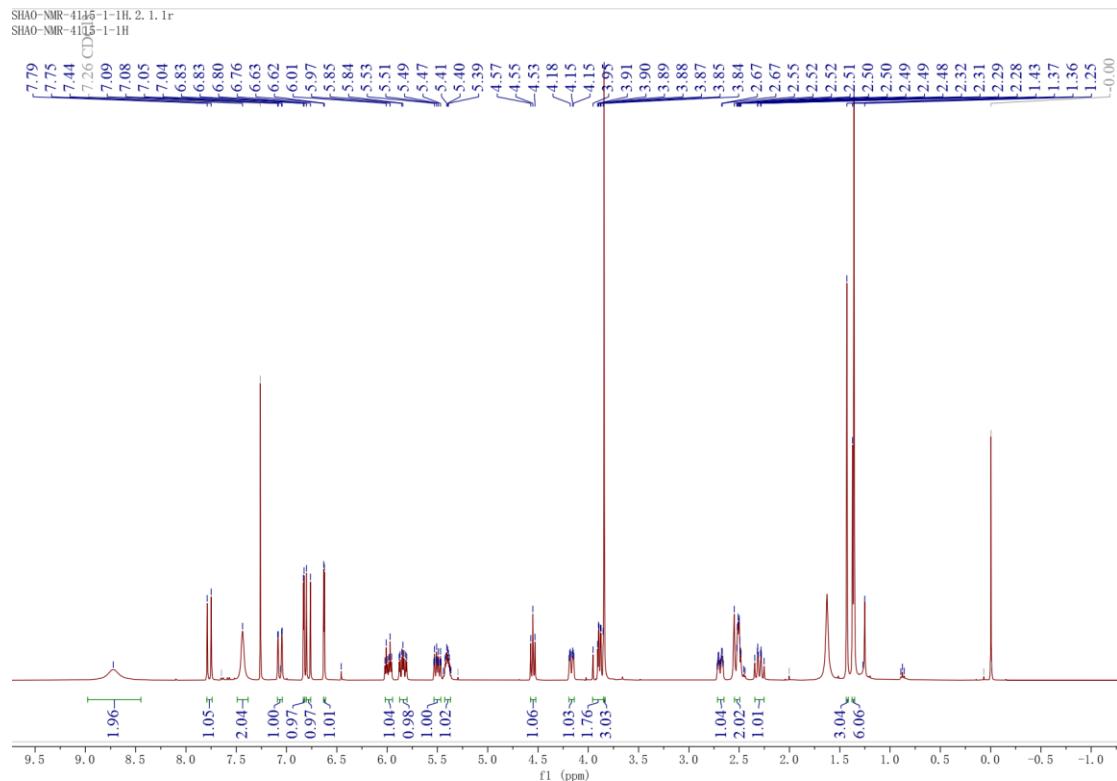


Figure S13. ¹H NMR (400 MHz, Chloroform-*d*) spectrum of compound 27.

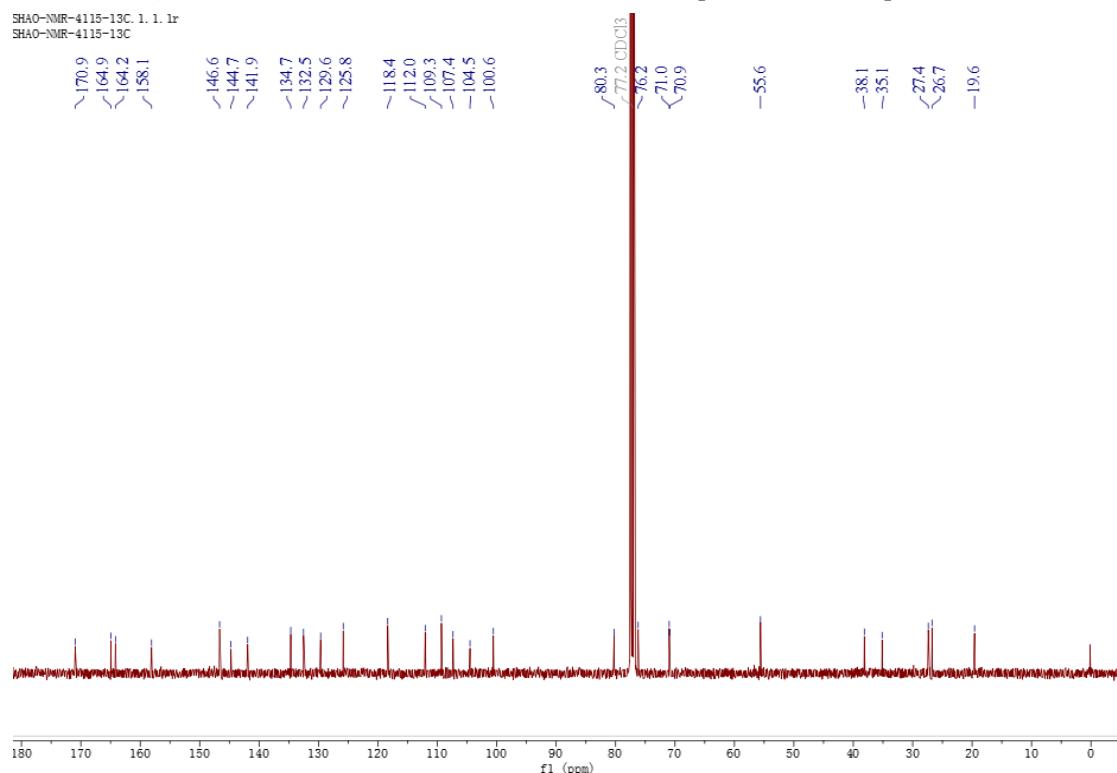


Figure S14. ¹³C NMR (100 MHz, Chloroform-*d*) spectrum of compound 27.

12 #695 RT: 7.55 AV: 1 NL: 4.21E7
T: FTMS + p ESI Full ms [150.0000-1500.0000]

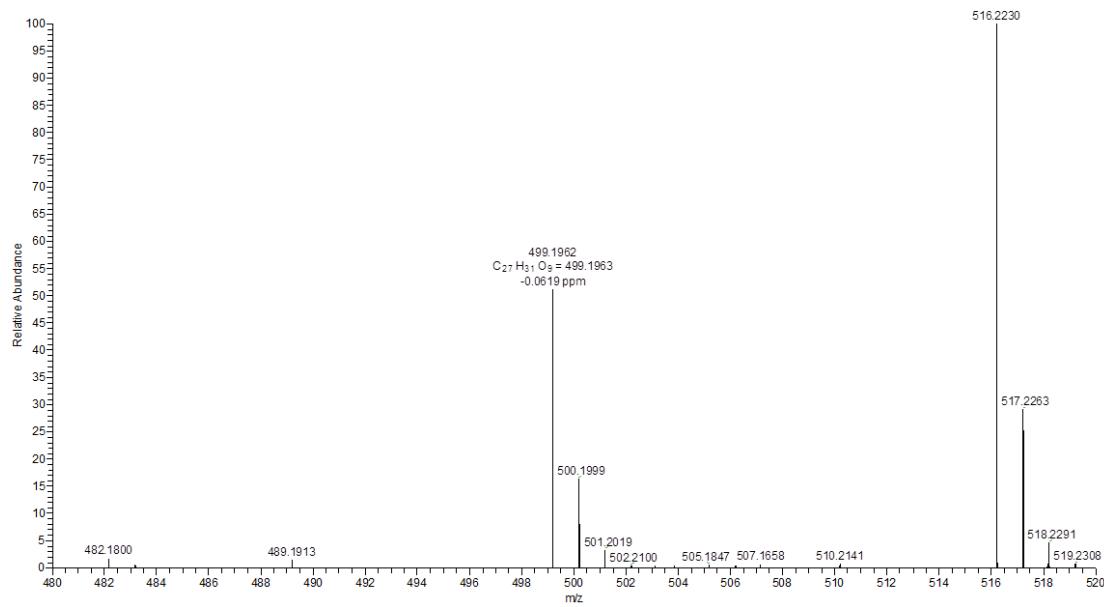


Figure S15. HR-ESI-MS spectrum of compound 27.

SHAO-NMR-4111-5-1H, 1, 1, 1r
SHAO-NMR-4111-5-1H

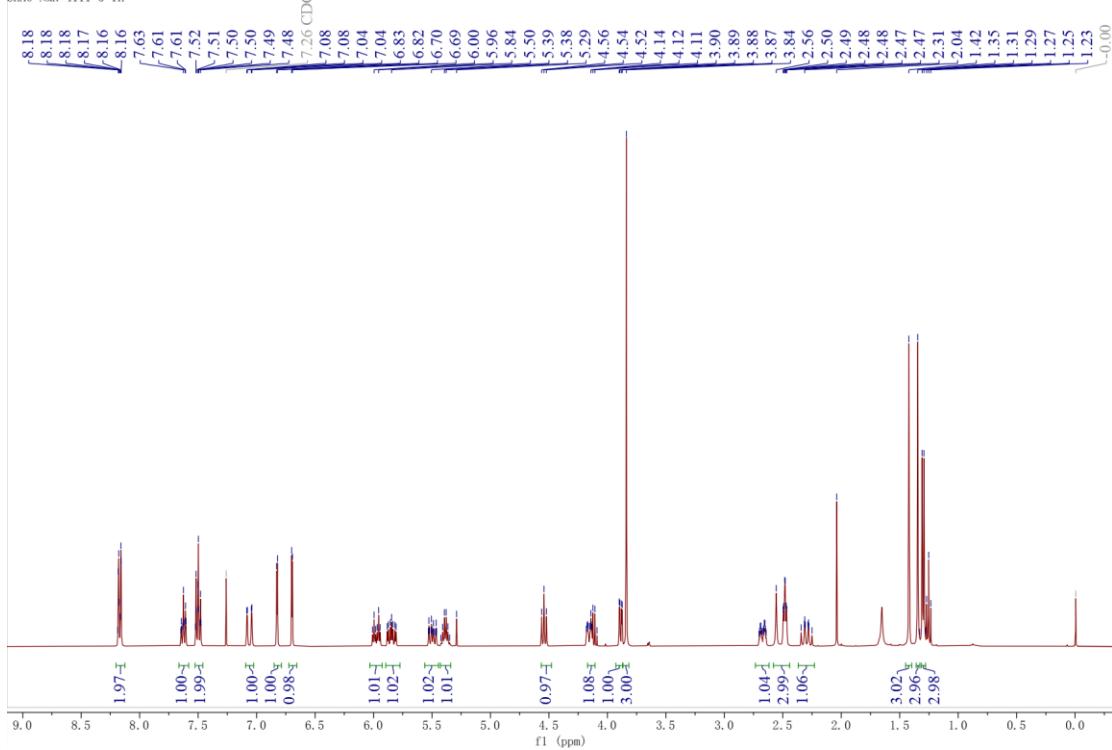


Figure S16. ¹H NMR (400 MHz, Chloroform-*d*) spectrum of compound 28.

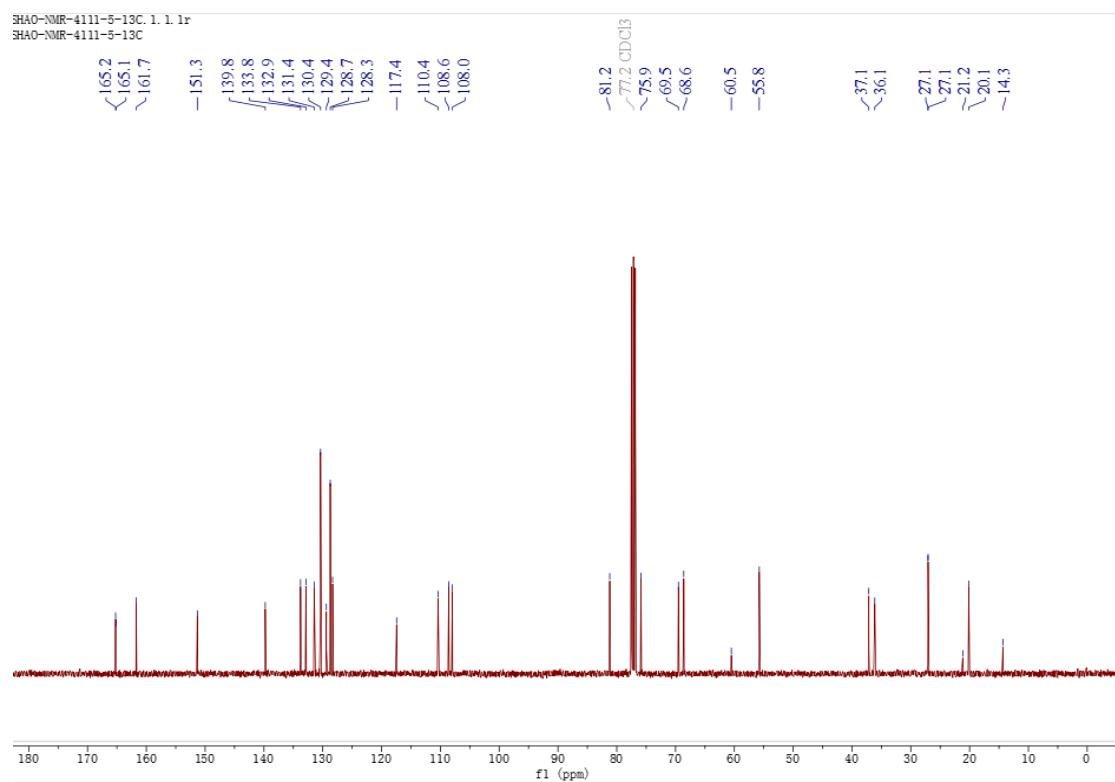


Figure S17. ^{13}C NMR (100 MHz, Chloroform-*d*) spectrum of compound **28**.

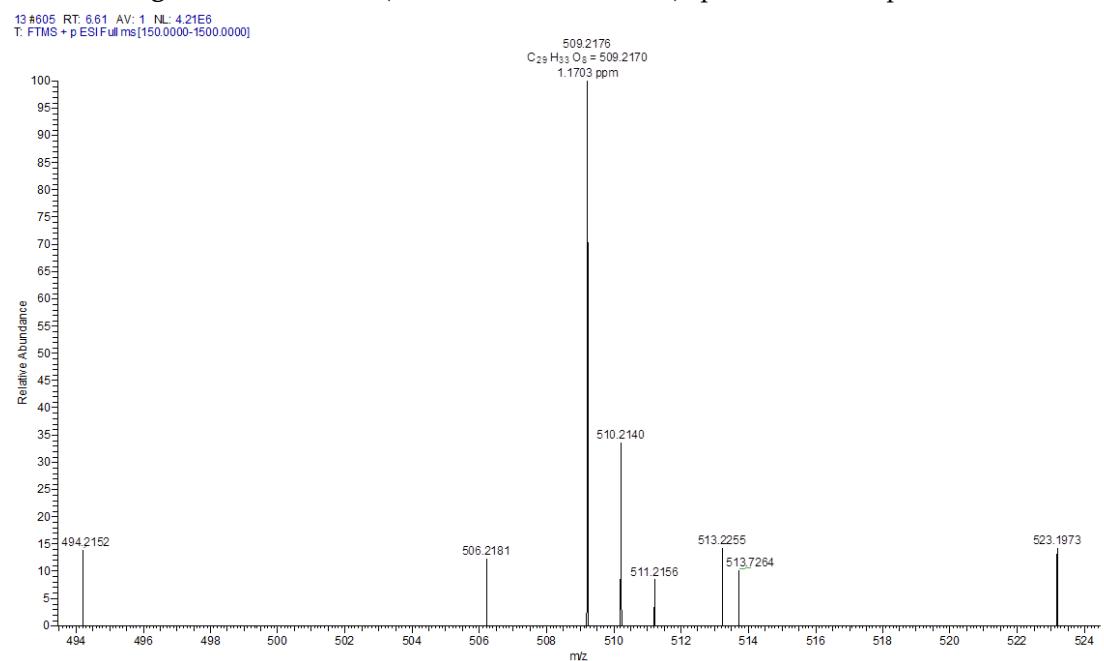


Figure S18. HR-ESI-MS spectrum of compound **28**.

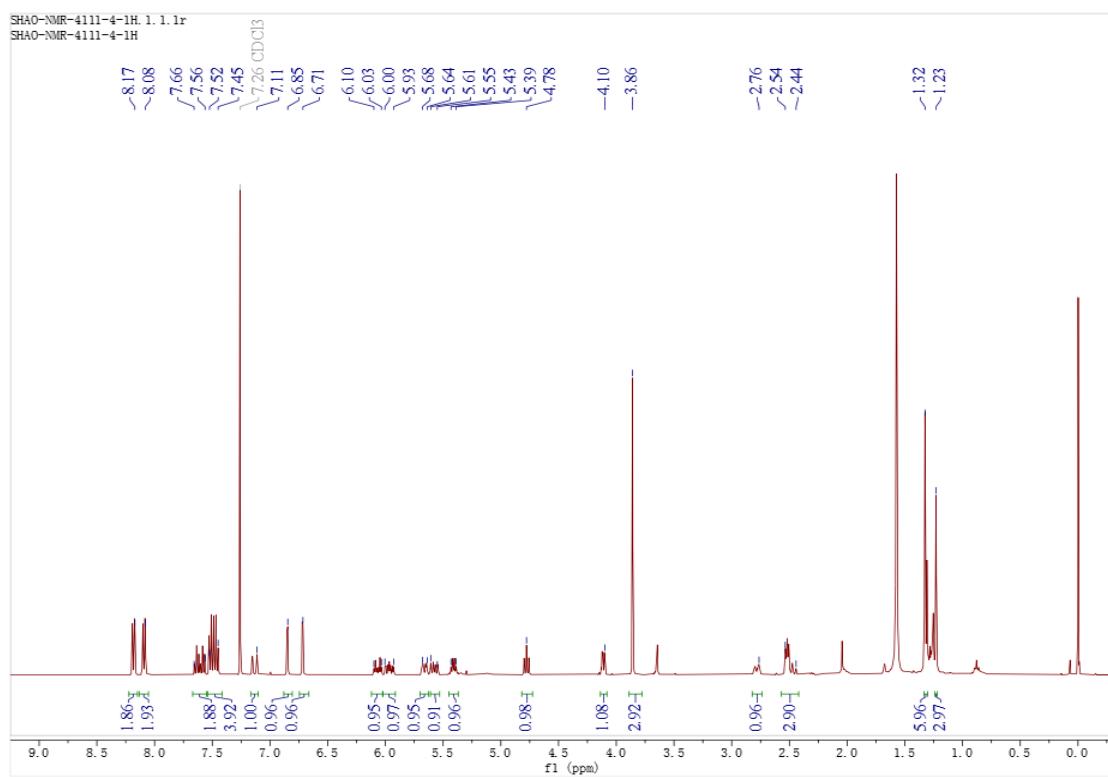


Figure S19. ^1H NMR (400 MHz, Chloroform-*d*) spectrum of compound **29**.

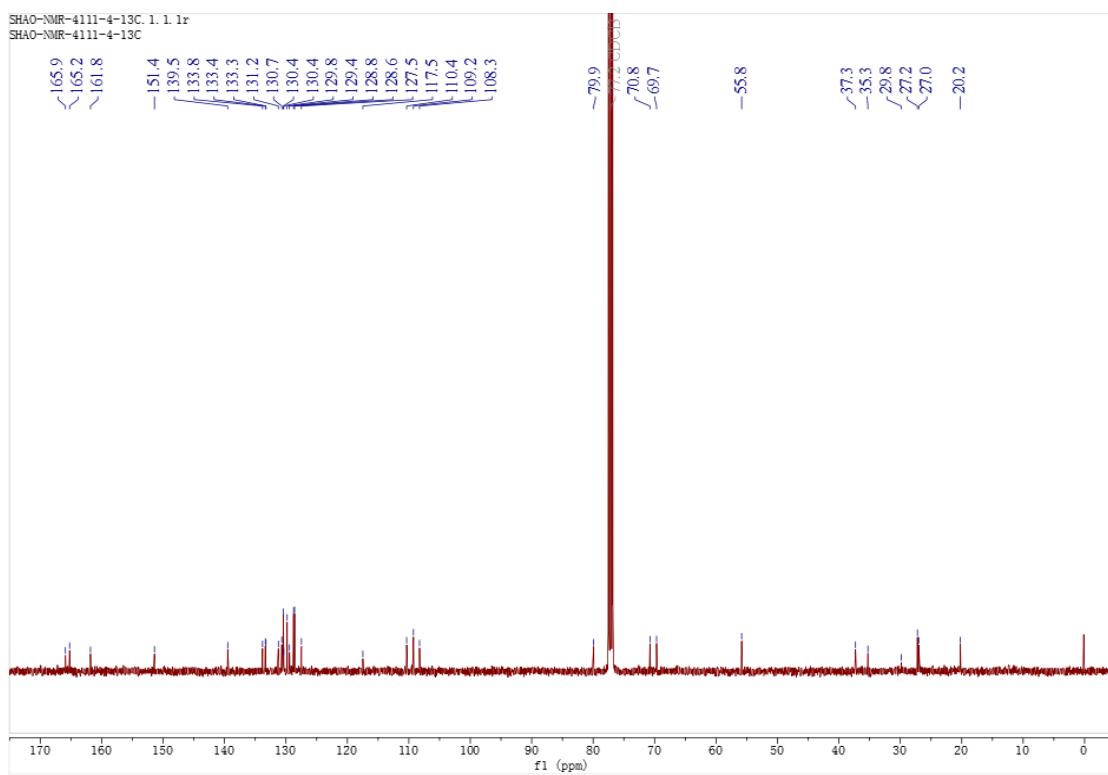


Figure S20. ^{13}C NMR (100 MHz, Chloroform-*d*) spectrum of compound 29.

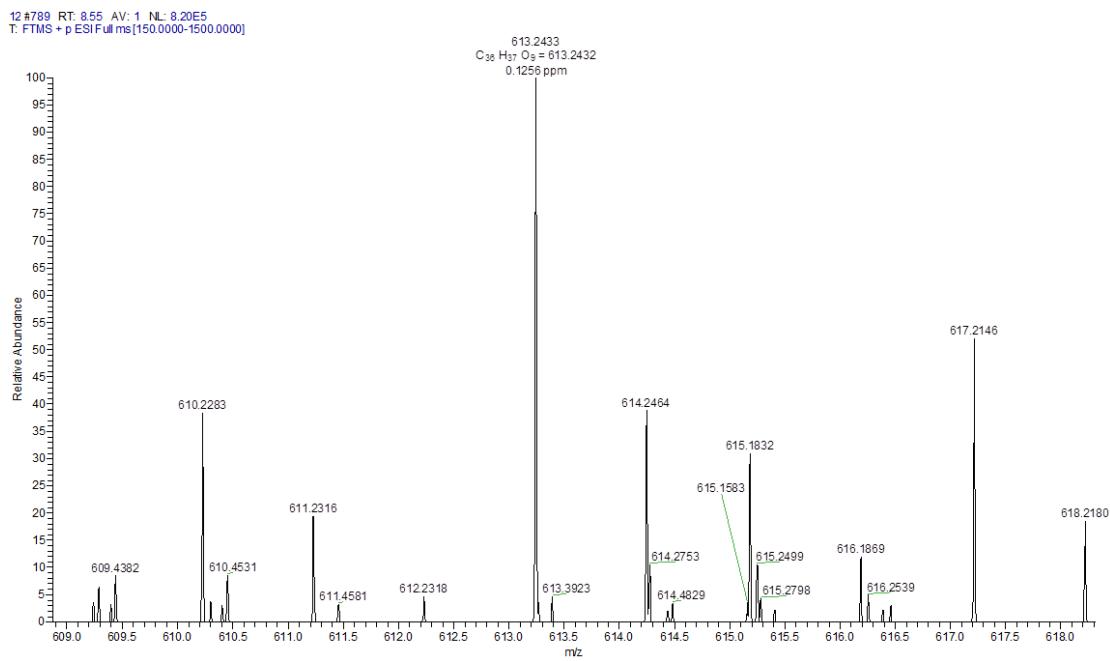


Figure S21. HR-ESI-MS spectrum of compound **29**.

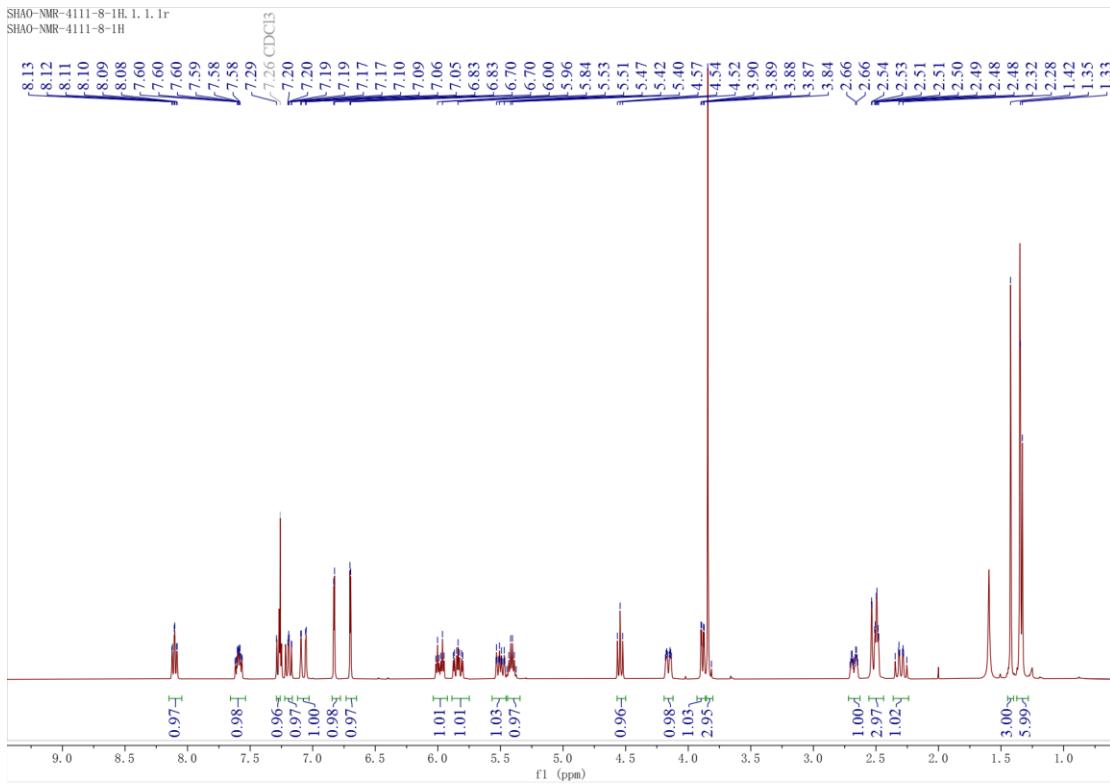


Figure S22. ^1H NMR (400 MHz, Chloroform-*d*) spectrum of compound 30.

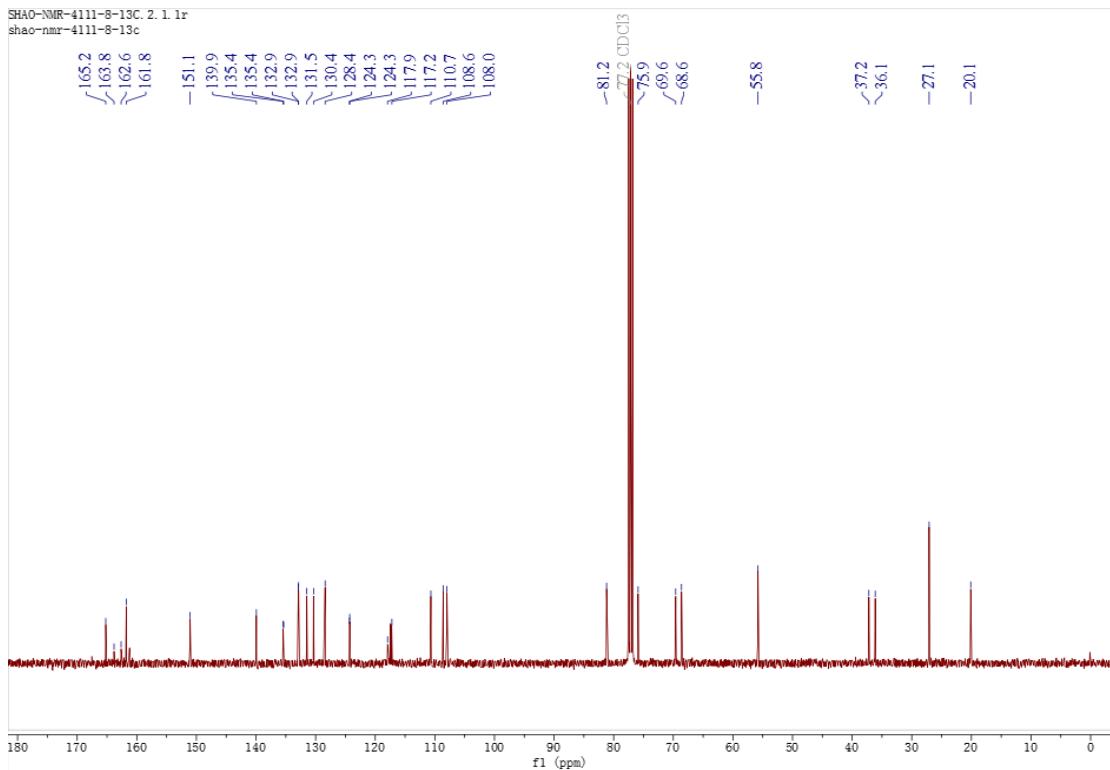


Figure S23. ¹³C NMR (100 MHz, Chloroform-*d*) spectrum of compound 30.

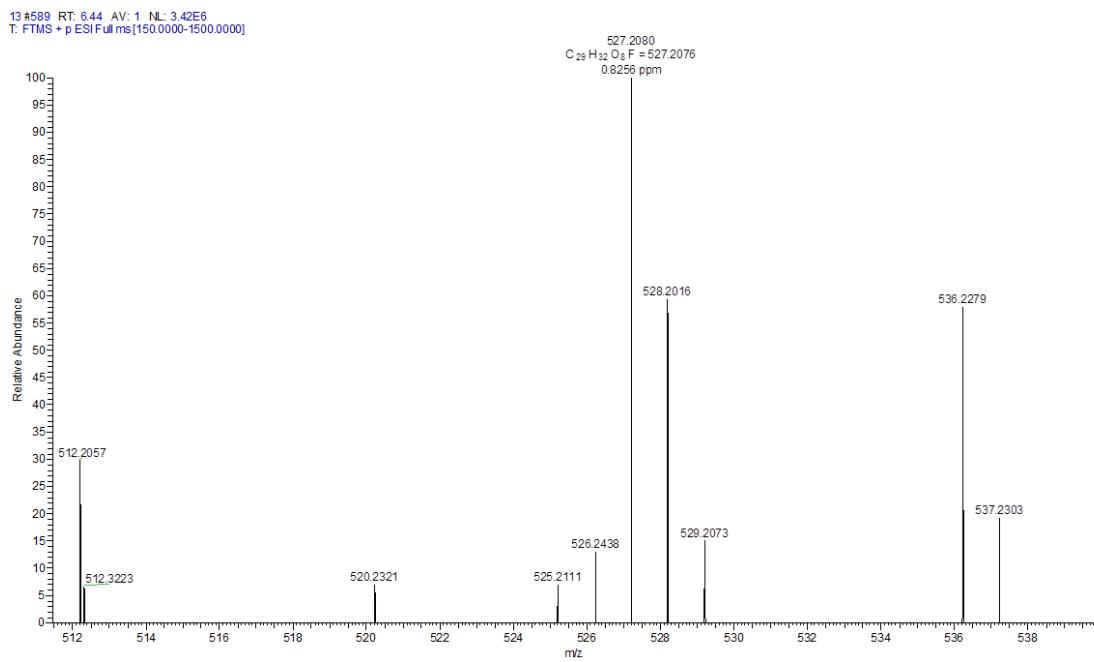


Figure S24. HR-ESI-MS spectrum of compound 30.

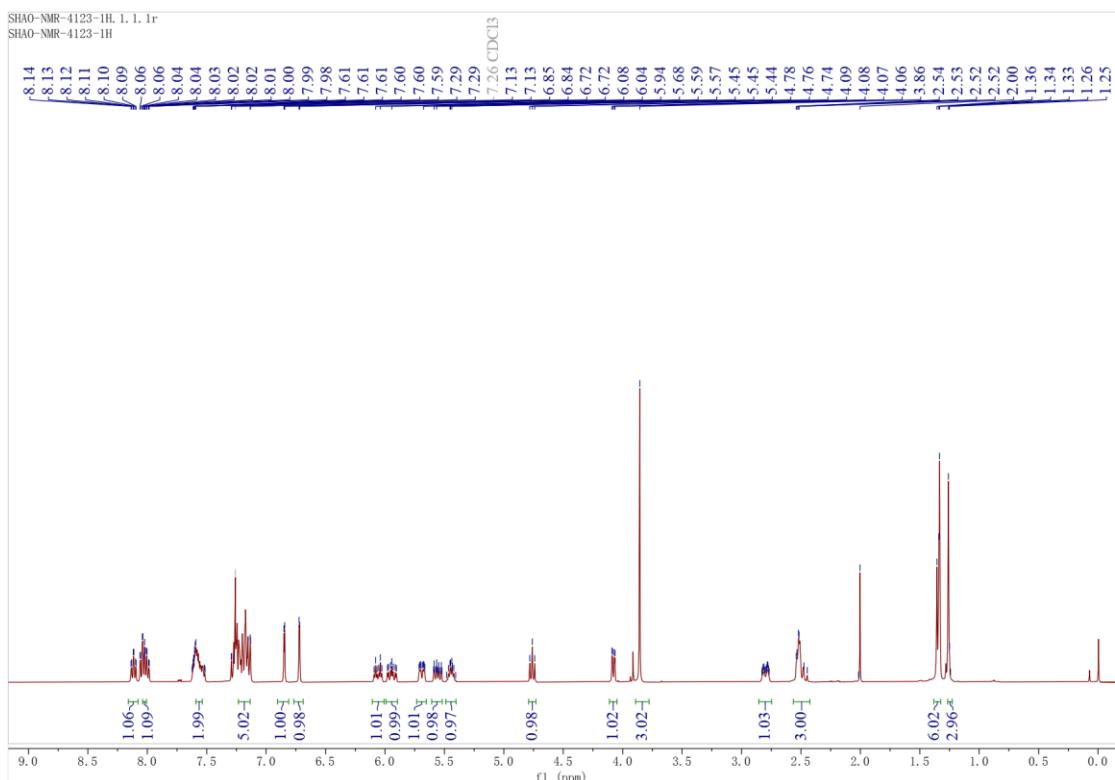


Figure S25. ^1H NMR (400 MHz, Chloroform-*d*) spectrum of compound 31.

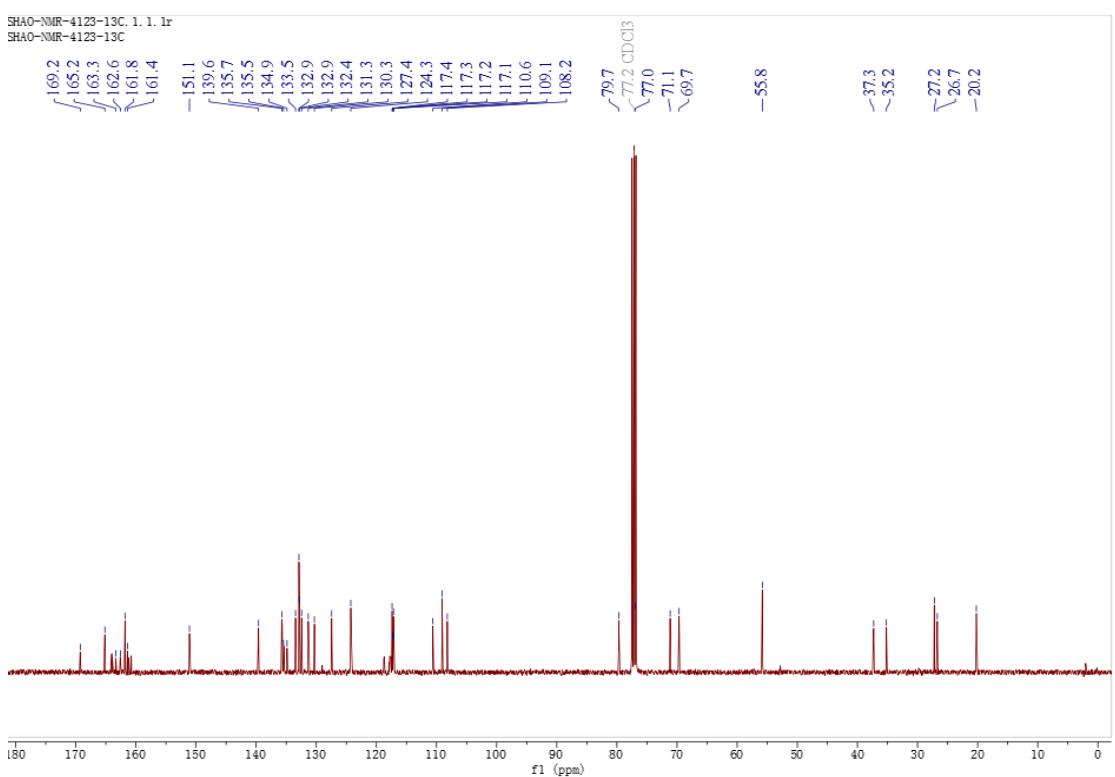


Figure S26. ^{13}C NMR (100 MHz, Chloroform-*d*) spectrum of compound 31.

11 #759 RT: 8.30 AV: 1 NL: 2.42E5
T: FTMS + p ESI Full ms[150.0000-1500.0000]

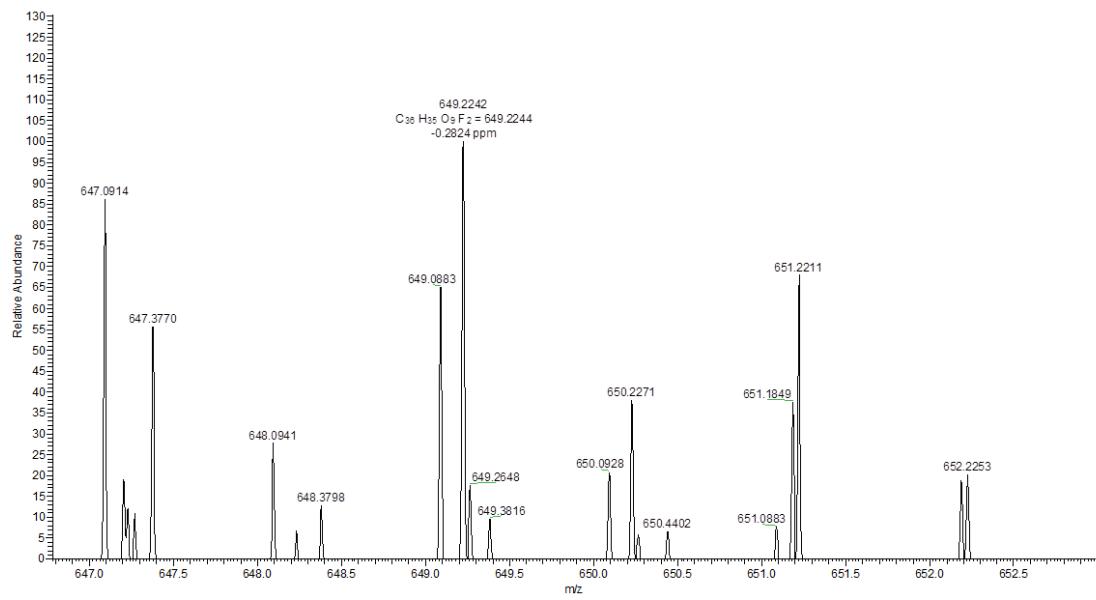


Figure S27. HR-ESI-MS spectrum of compound 31.

SHAO-NMR-4111-6-1H, 1, 1, 1r
SHAO-NMR-4111-6-1H

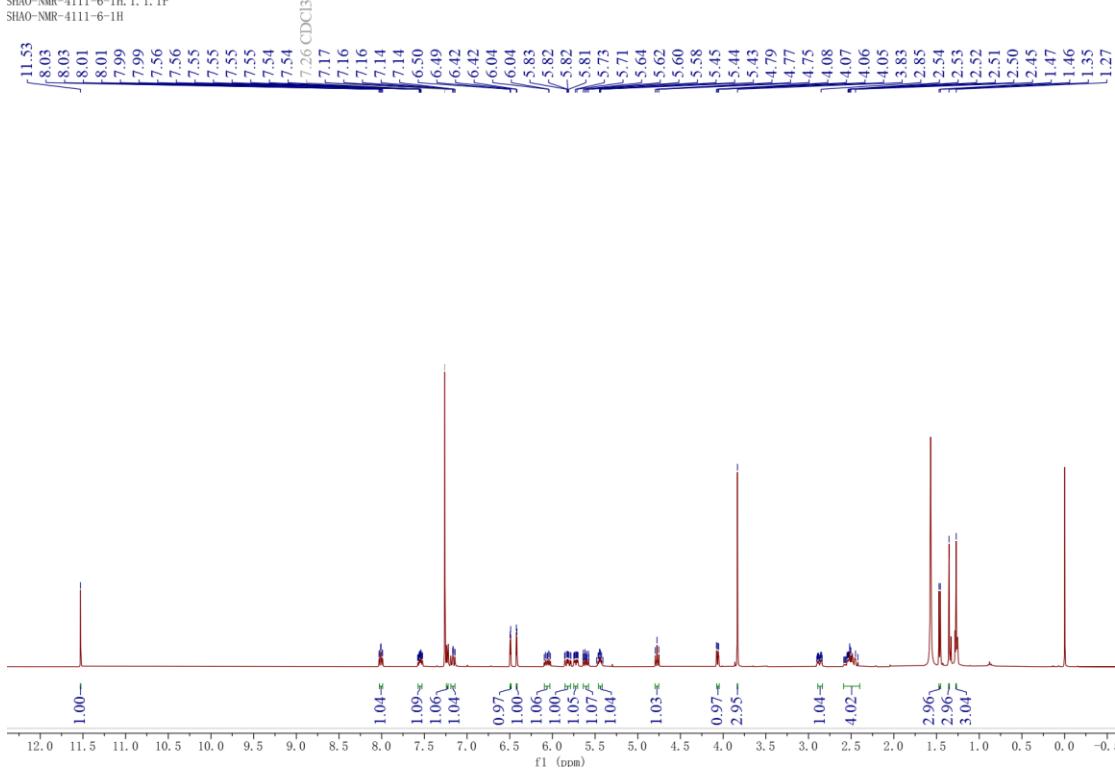


Figure S28. ^1H NMR (400 MHz, Chloroform-*d*) spectrum of compound 32.

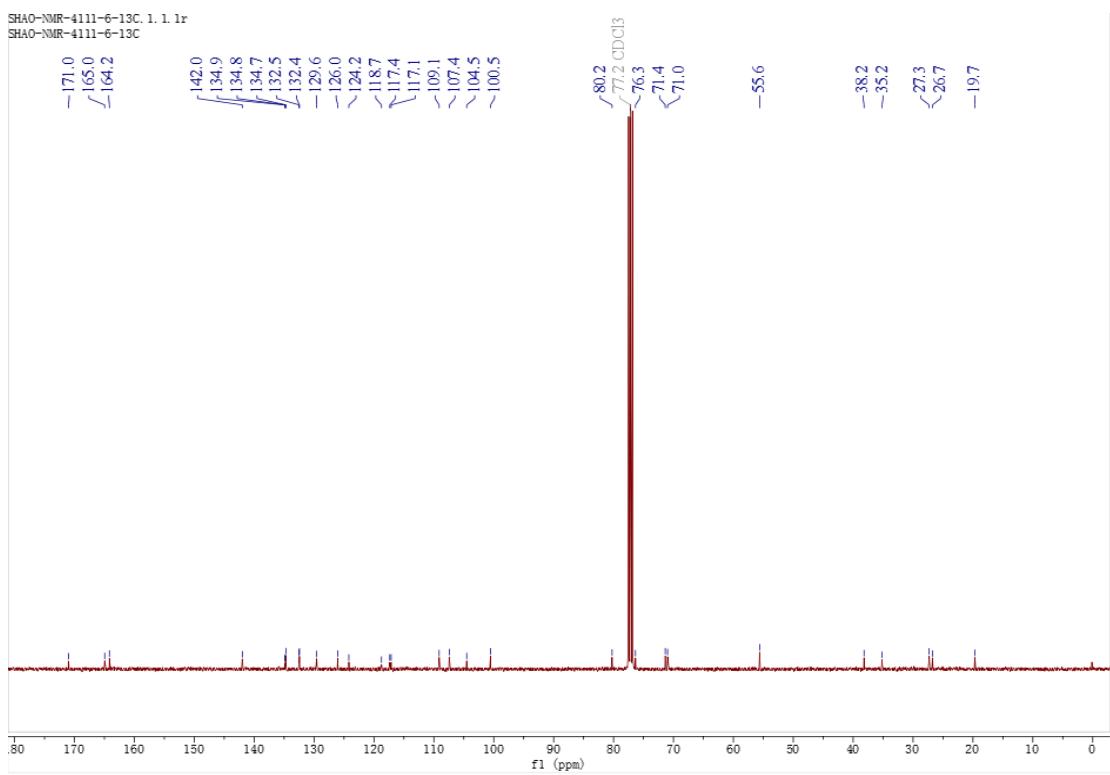


Figure S29. ¹³C NMR (100 MHz, Chloroform-*d*) spectrum of compound 32.

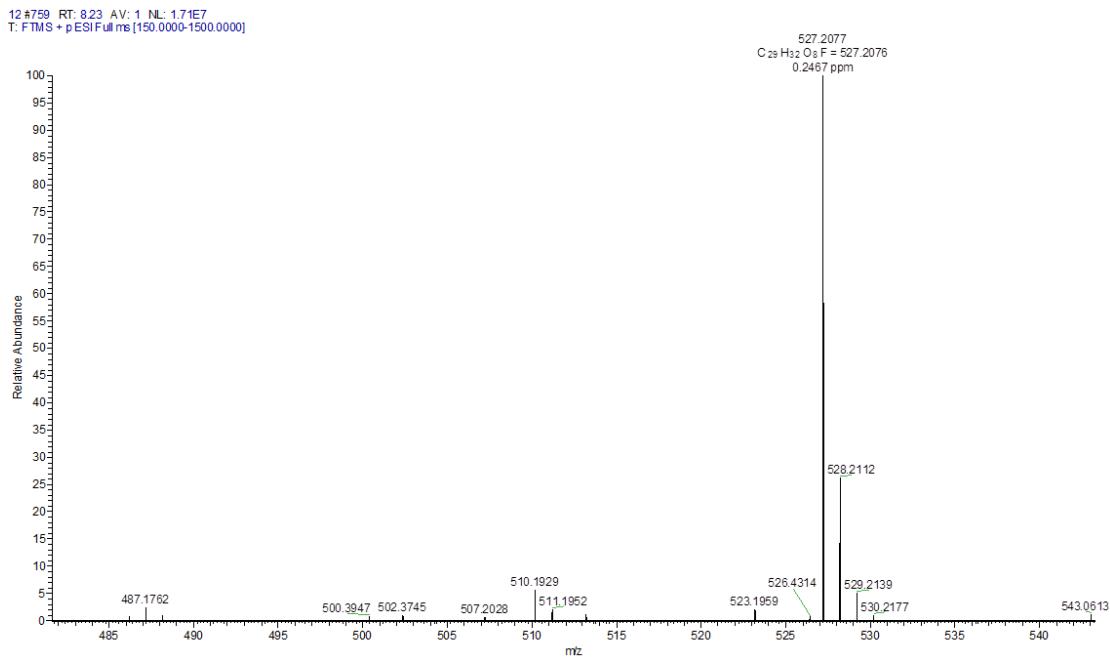


Figure S30. HR-ESI-MS spectrum of compound 32.

SHAO-NMR-4110-2-1H. 1. 1. 1r
SHAO-NMR-4110-2-1H

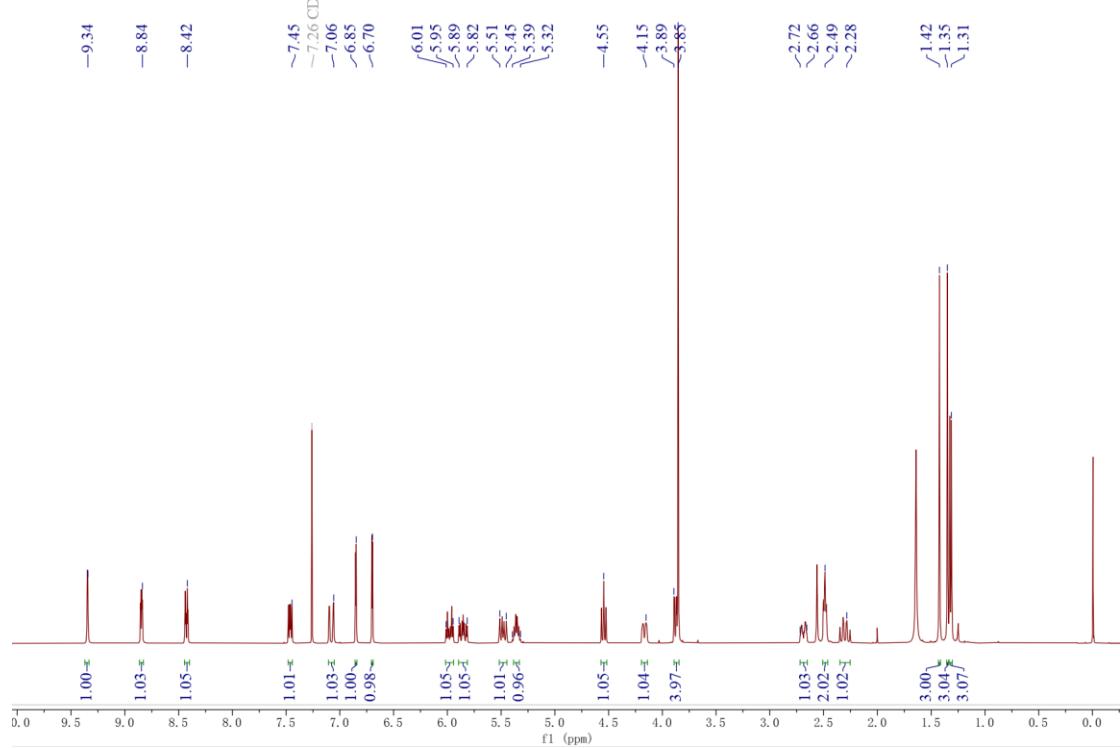


Figure S31. ¹H NMR (400 MHz, Chloroform-*d*) spectrum of compound 33.

SHAO-NMR-4110-2-13C. 1. 1. 1r
SHAO-NMR-4110-2-13C

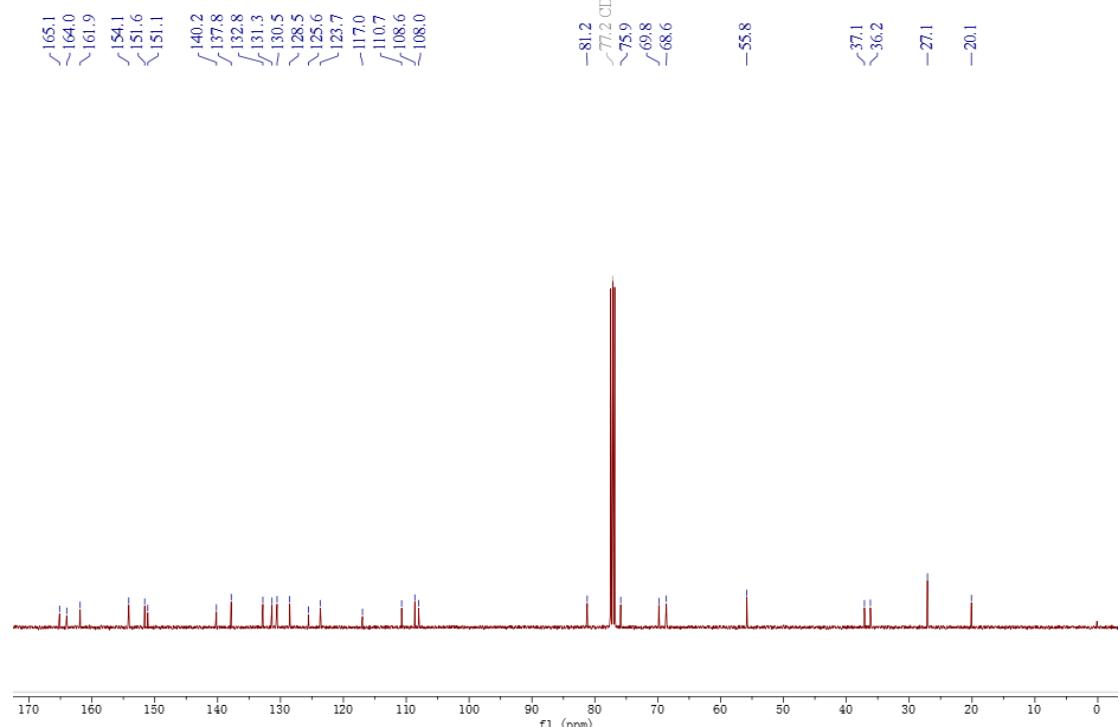


Figure S32. ¹³C NMR (100 MHz, Chloroform-*d*) spectrum of compound 33.

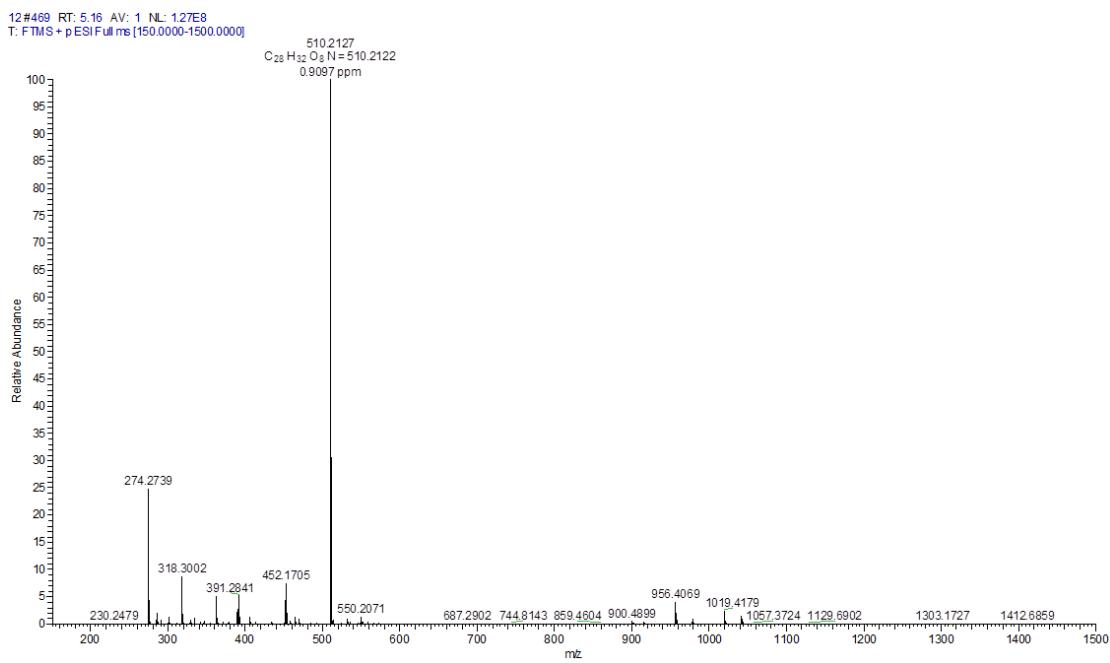


Figure S33. HR-ESI-MS spectrum of compound 33.

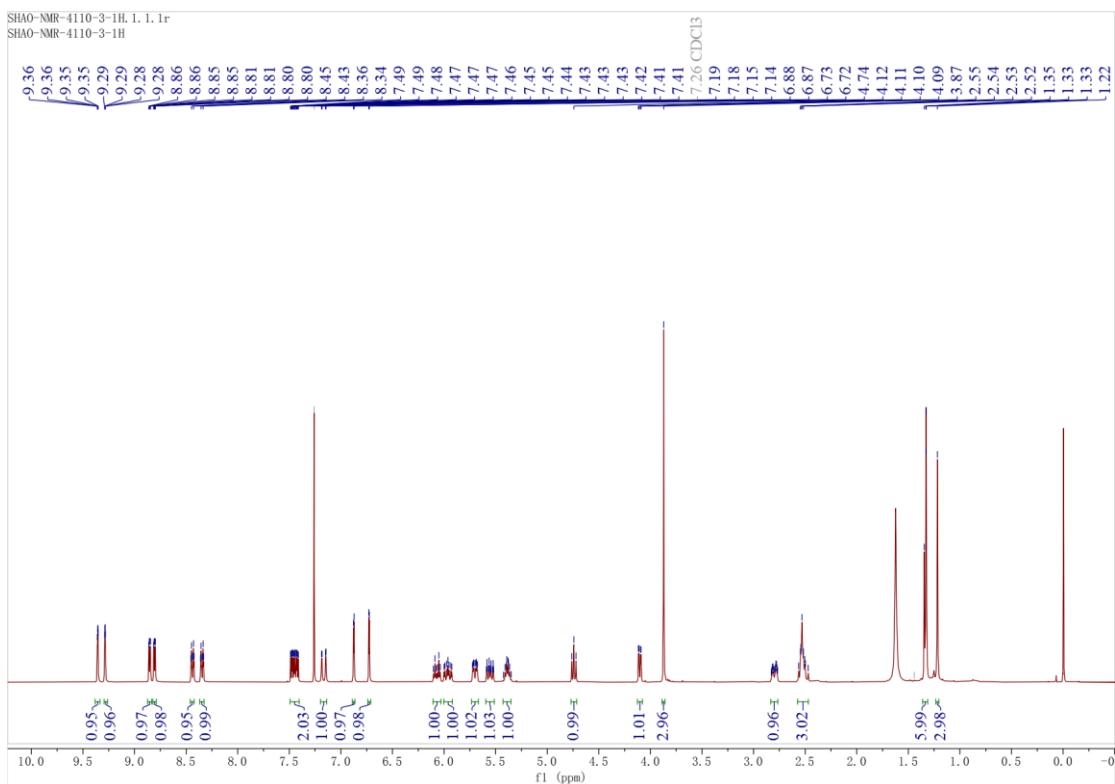


Figure S34. 1H NMR (400 MHz, Chloroform-*d*) spectrum of compound 34.

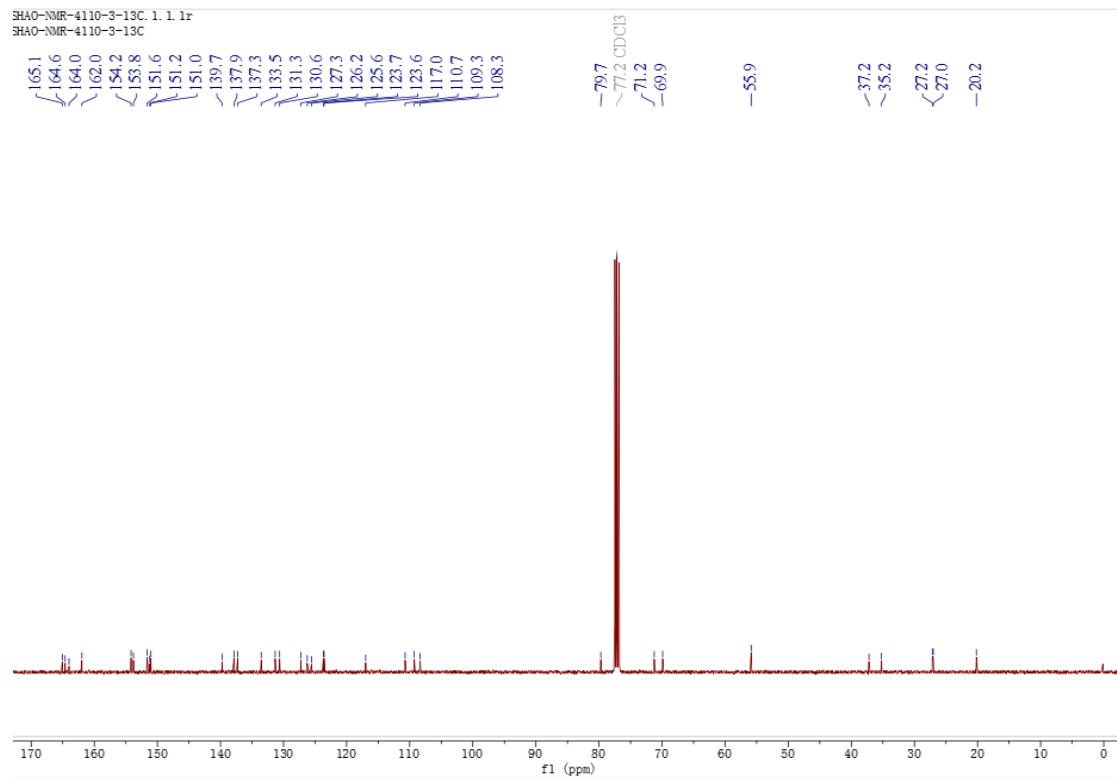


Figure S35. ¹³C NMR (100 MHz, Chloroform-*d*) spectrum of compound 34.

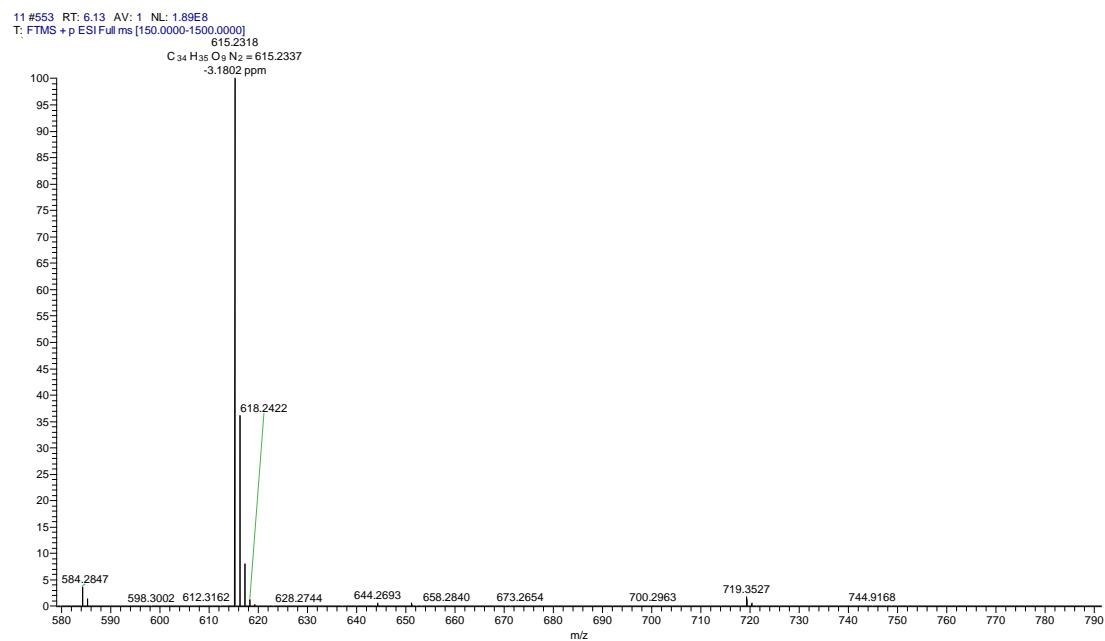


Figure S36. HR-ESI-MS spectrum of compound 34.

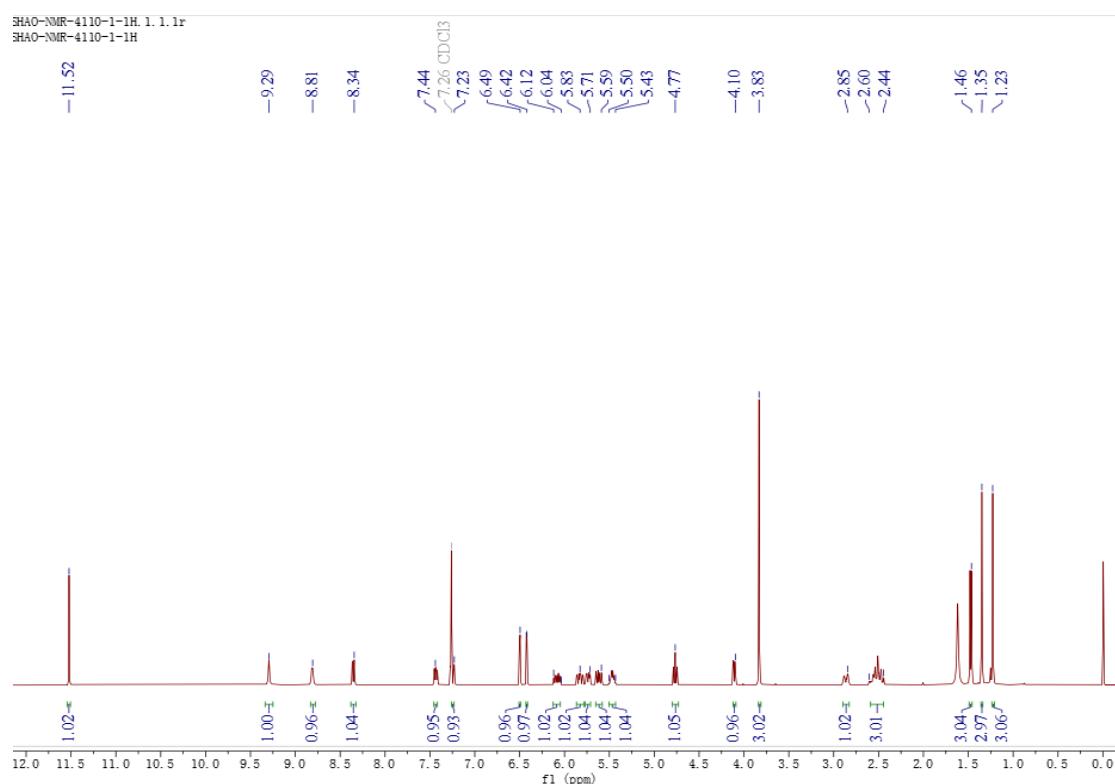


Figure S37. ^1H NMR (400 MHz, Chloroform-*d*) spectrum of compound 35.

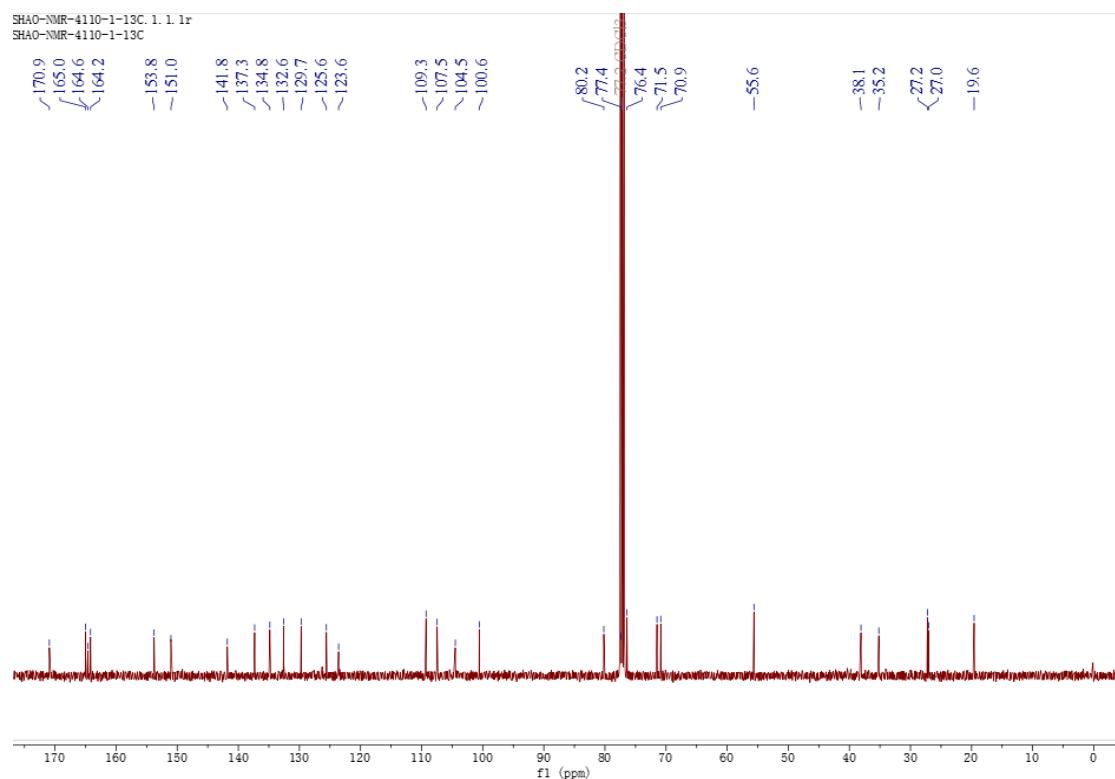


Figure S38. ^{13}C NMR (100 MHz, Chloroform-*d*) spectrum of compound 35.

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T: FTMS + p ESI Full ms [150.0000-1500.0000]

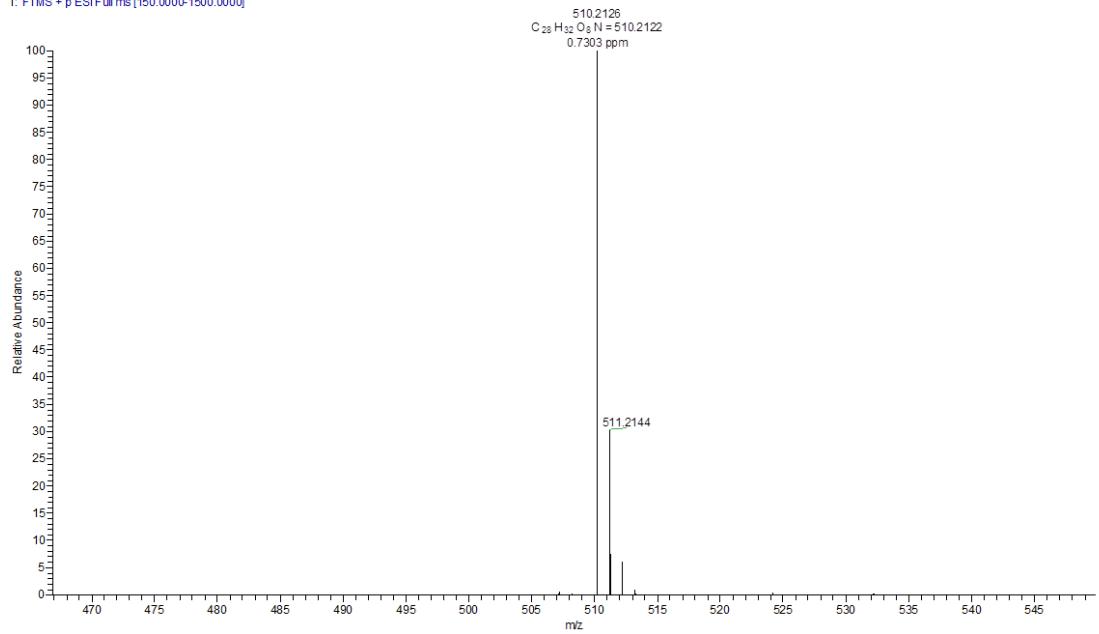


Figure S39. HR-ESI-MS spectrum of compound 35.

SHDQ-NMR-4111-3-1H, 1, 1, 1r
SHDQ-NMR-4111-3-1H

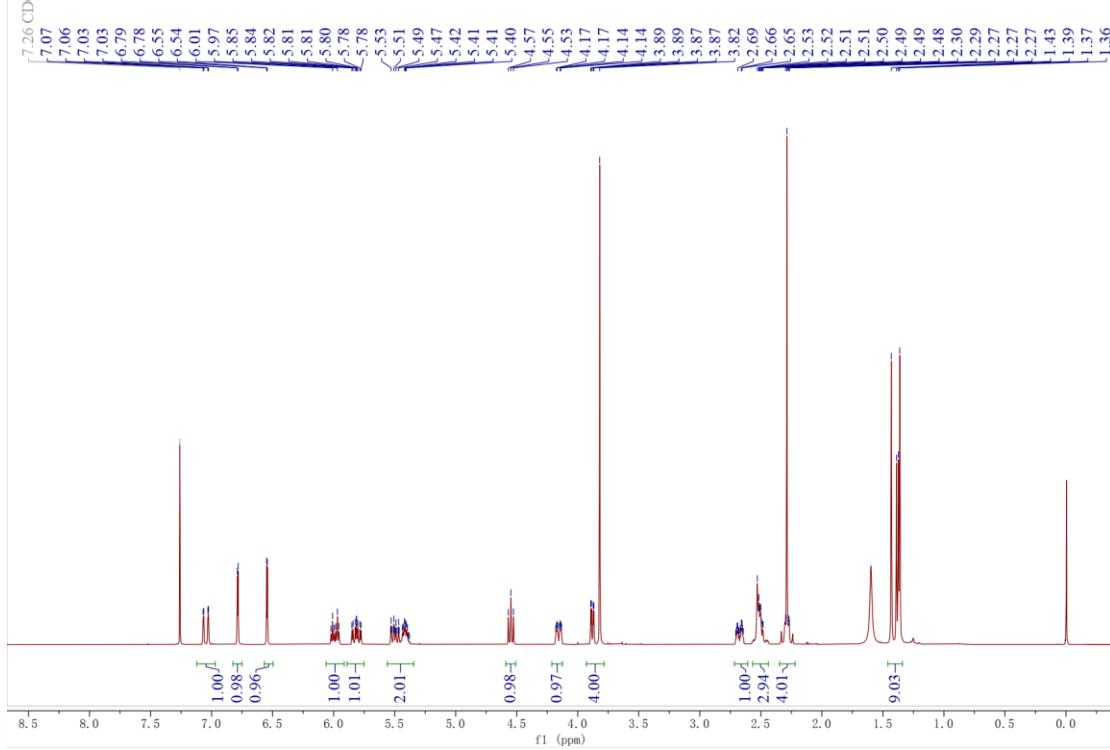


Figure S40. ¹H NMR (400 MHz, Chloroform-*d*) spectrum of compound 36.

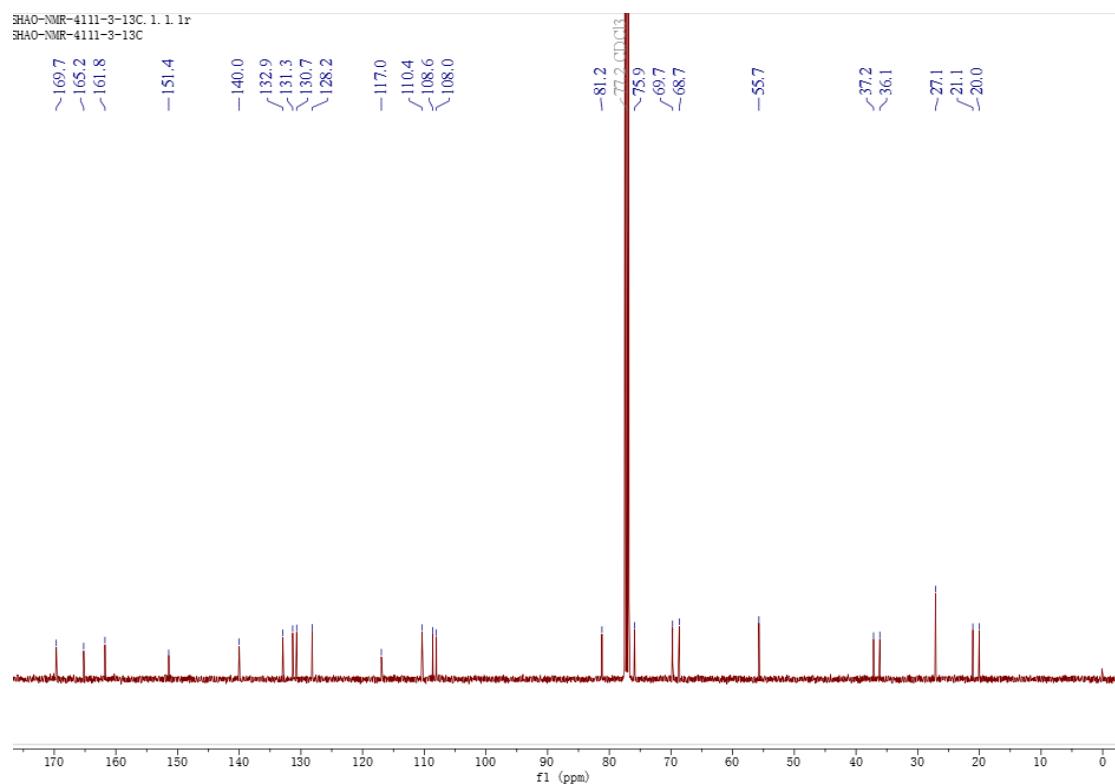


Figure S41. ^{13}C NMR (100 MHz, Chloroform-*d*) spectrum of compound 36.

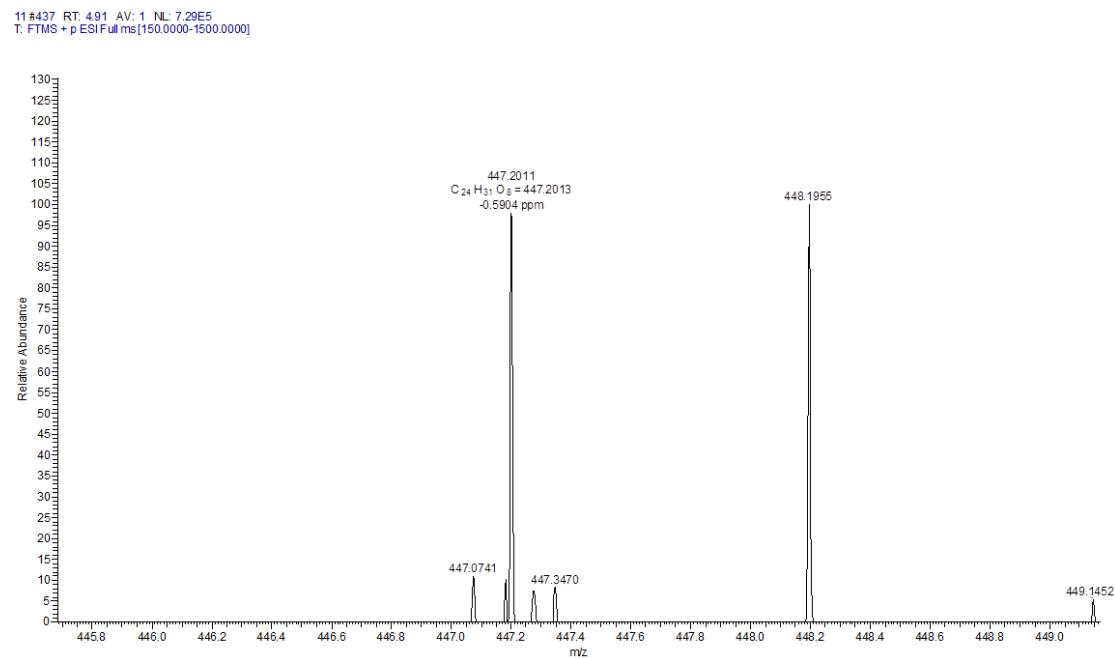


Figure S42. HR-ESI-MS spectrum of compound 36

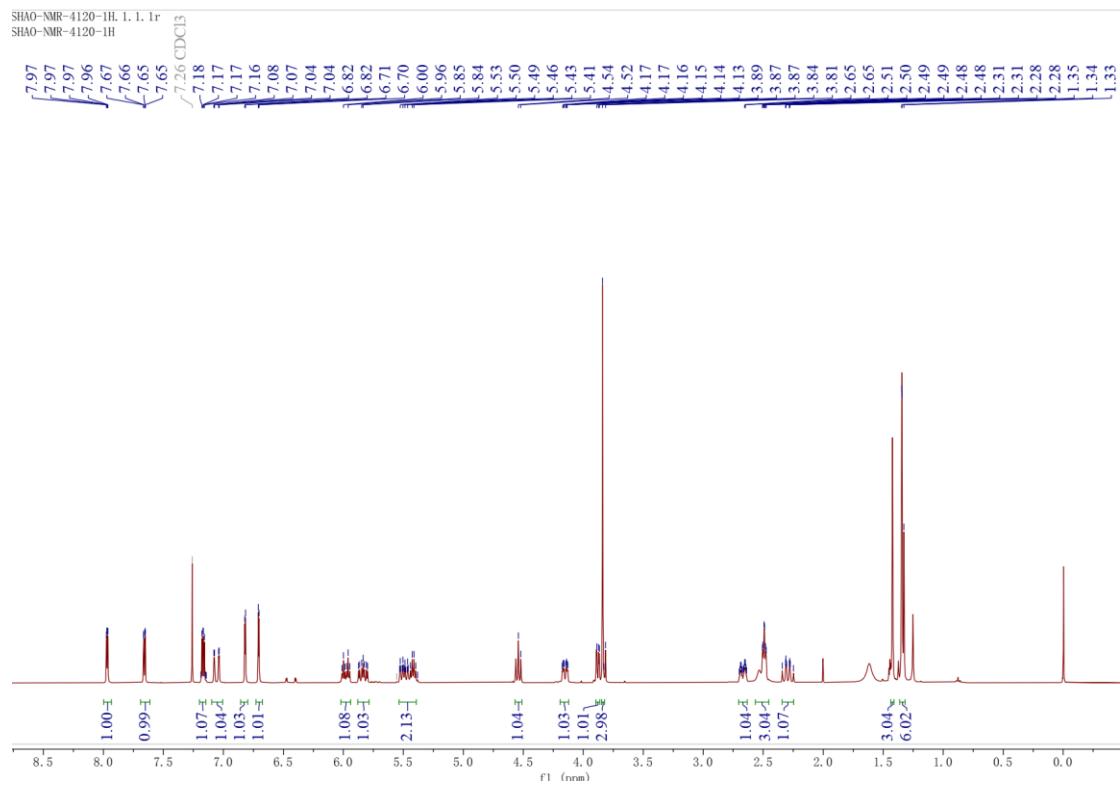


Figure S43. ^1H NMR (400 MHz, Chloroform-*d*) spectrum of compound 37.

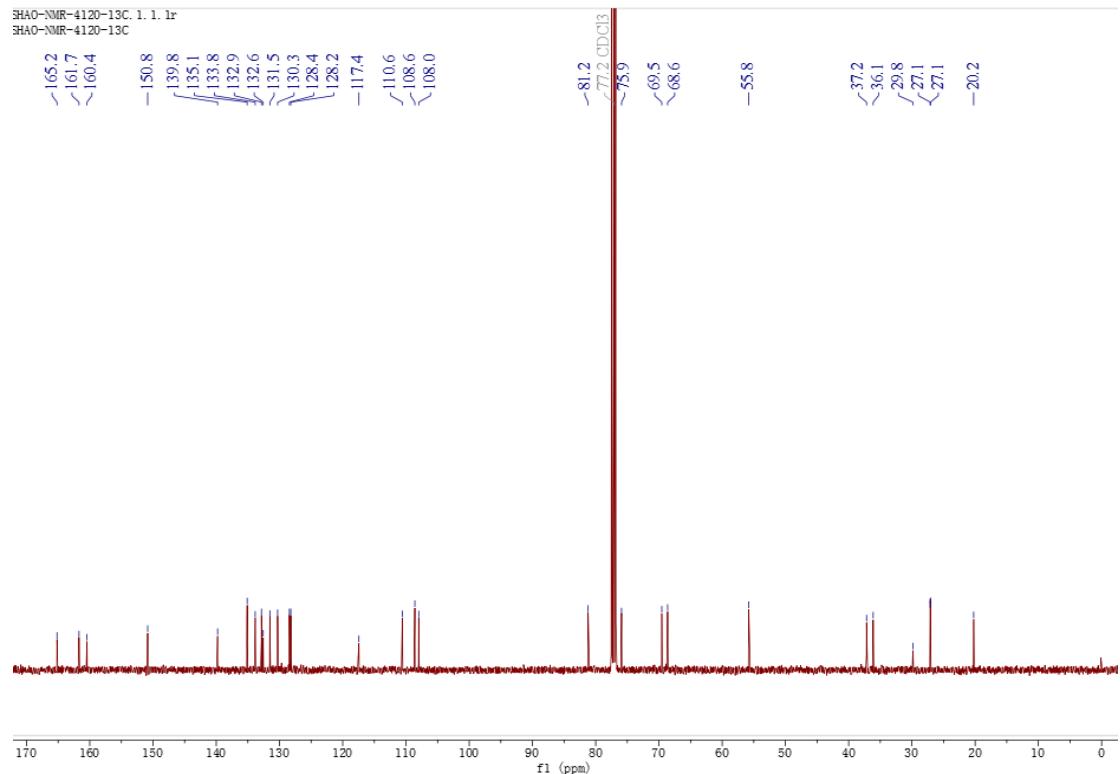


Figure S44. ^{13}C NMR (100 MHz, Chloroform-*d*) spectrum of compound 37.

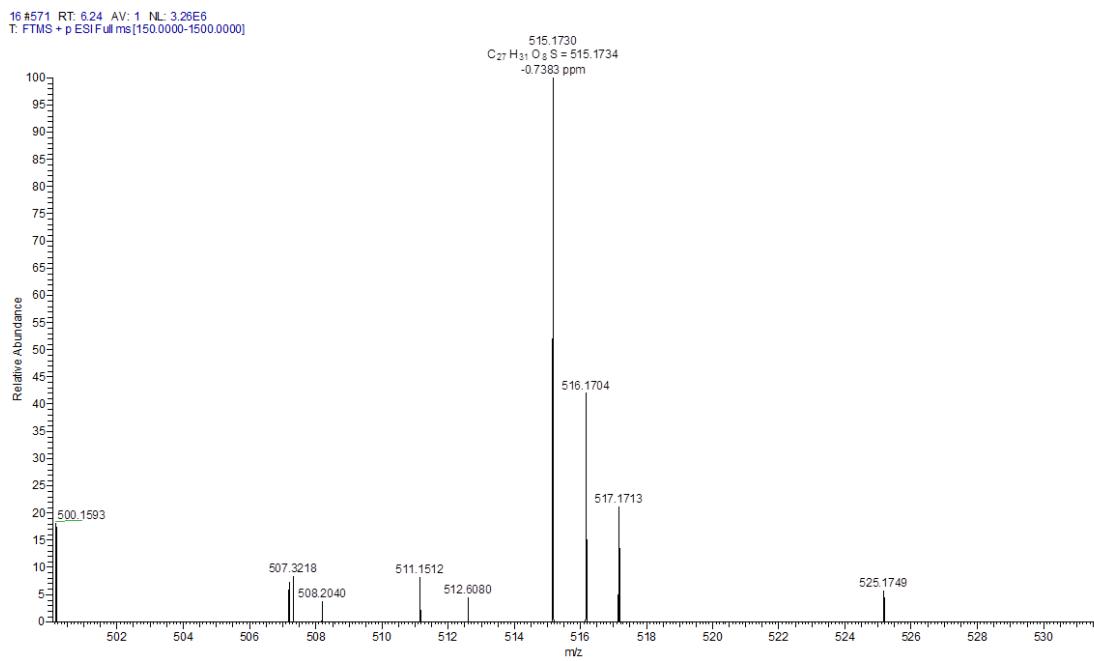


Figure S45. HR-ESI-MS spectrum of compound 37.

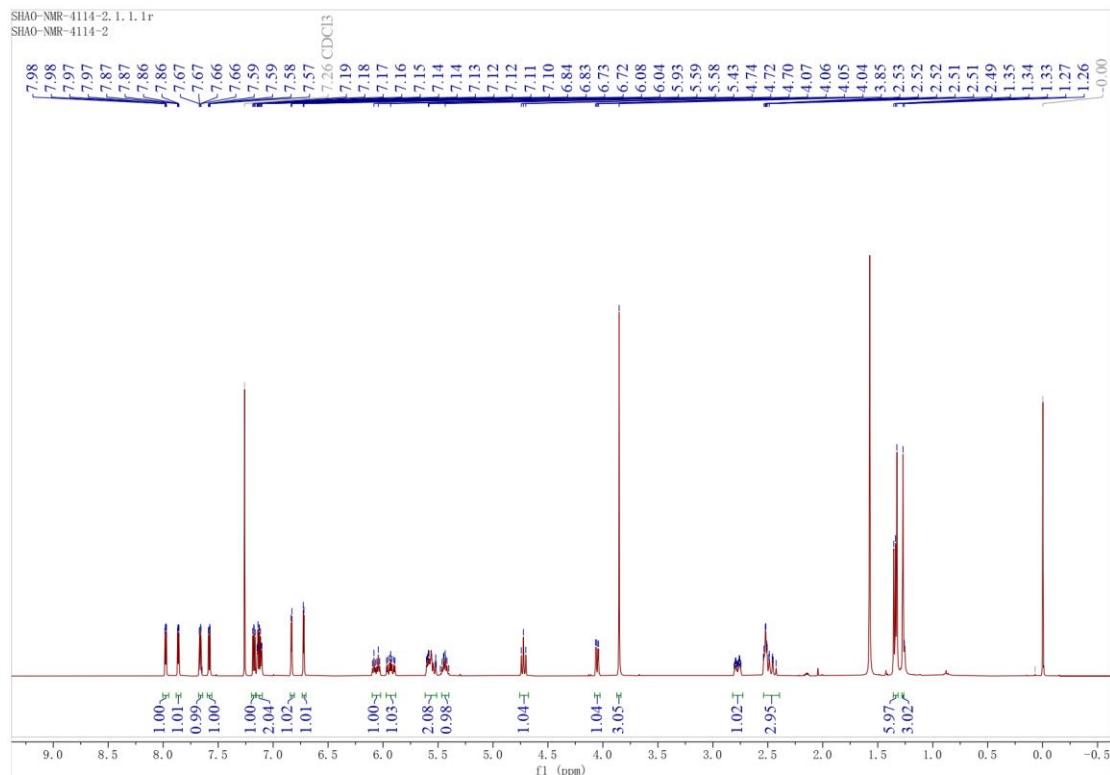


Figure S46. ^1H NMR (400 MHz, Chloroform-*d*) spectrum of compound 38.

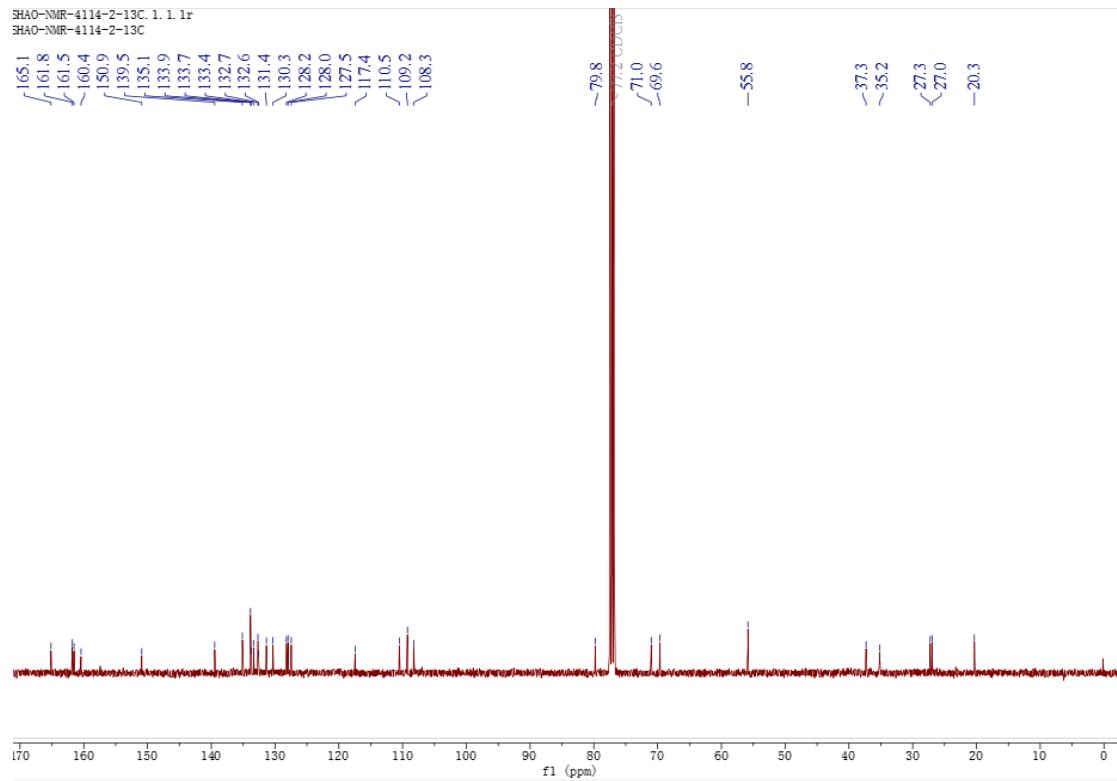


Figure S47. ^{13}C NMR (100 MHz, Chloroform-*d*) spectrum of compound 38.

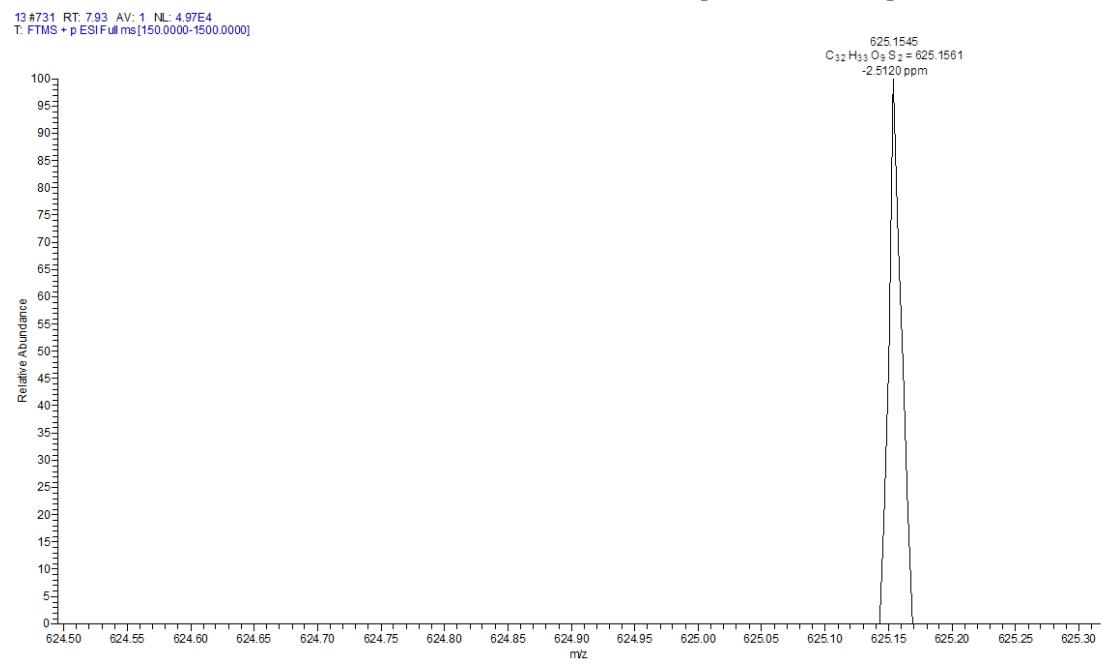


Figure S48. HR-ESI-MS spectrum of compound 38.