

Supporting Information

Lignans and Isoflavonoids from the Stems of *Pisonia umbellifera*

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Table of Supplementary Tables

Table S1. Main conformers (> 1%) of **1a** in methanol.

Table S2. Main conformers (> 1%) of **2a** in methanol.

Table S3. Main conformers (> 1%) of **3a** in methanol.

Table of Supplementary Figures

Figure S1. ¹H NMR (600 MHz, CDCl₃) spectrum of **1**

Figure S2. ¹³C NMR (150 MHz, CDCl₃) spectrum of **1**

Figure S3. HSQC (600 MHz, CDCl₃) spectrum of **1**

Figure S4. HMBC (600 MHz, CDCl₃) spectrum of **1**

Figure S5. H-H COSY (600 MHz, CDCl₃) spectrum of **1**

Figure S6. NOESY (600 MHz, CDCl₃) spectrum of **1**

Figure S7. HRESIMS spectrum of **1**

Figure S8. Chiral-phase HPLC analytical chromatogram of **1**

Figure S9. ¹H NMR (600 MHz, CDCl₃) spectrum of **1a**

Figure S10. ¹H NMR (600 MHz, CDCl₃) spectrum of **1b**

Figure S11. Experimental ECD spectra of **1a**

Figure S12. Experimental ECD spectra of **1b**

Figure S13. ¹H NMR (600 MHz, MeOD) spectrum of **2**

Figure S14. ¹³C NMR (150 MHz, MeOD) spectrum of **2**

Figure S15. HSQC (600 MHz, MeOD) spectrum of **2**

Figure S16. HMBC (600 MHz, MeOD) spectrum of **2**

Figure S17. H-H COSY (600 MHz, MeOD) spectrum of **2**

Figure S18. NOESY (600 MHz, CDCl₃) spectrum of **2**

Figure S19. HRESIMS spectrum of **2**

Figure S20. Chiral-phase HPLC analytical chromatogram of **2**

Figure S21. ¹H NMR (600 MHz, MeOD) spectrum of **2a**

Figure S22. ¹H NMR (600 MHz, MeOD) spectrum of **2b**

Figure S23. Experimental ECD spectra of **2a**

Figure S24. Experimental ECD spectra of **2b**

Figure S25. ^1H NMR (600 MHz, MeOD) spectrum of **3**

Figure S26. ^{13}C NMR (150 MHz, MeOD) spectrum of **3**

Figure S27. HSQC (600 MHz, MeOD) spectrum of **3**

Figure S28. HMBC (600 MHz, MeOD) spectrum of **3**

Figure S29. H-H COSY (600 MHz, MeOD) spectrum of **3**

Figure S30. NOESY (600 MHz, CDCl_3) spectrum of **3**

Figure S31. HRESIMS spectrum of **3**

Figure S32. Chiral-phase HPLC analytical chromatogram of **3**

Figure S33. ^1H NMR (600 MHz, MeOD) spectrum of **3a**

Figure S34. ^1H NMR (600 MHz, MeOD) spectrum of **3b**

Figure S35. Experimental ECD spectra of **3a**

Figure S36. Experimental ECD spectra of **3b**

Figure S37. ^1H NMR (600 MHz, CDCl_3) spectrum of **5**

Figure S38. ^{13}C NMR (150 MHz, CDCl_3) spectrum of **5**

Figure S39. HSQC (600 MHz, CDCl_3) spectrum of **5**

Figure S40. HMBC (600 MHz, CDCl_3) spectrum of **5**

Figure S41. H-H COSY (600 MHz, CDCl_3) spectrum of **5**

Figure S42. NOESY (600 MHz, CDCl_3) spectrum of **5**

Figure S43. HRESIMS spectrum of **5**

Figure S44. ^1H NMR (600 MHz, CDCl_3) spectrum of **6**

Figure S45. ^{13}C NMR (150 MHz, CDCl_3) spectrum of **6**

Figure S46. HSQC (600 MHz, CDCl_3) spectrum of **6**

Figure S47. HMBC (600 MHz, CDCl_3) spectrum of **6**

Figure S48. H-H COSY (600 MHz, CDCl_3) spectrum of **6**

Figure S49. NOESY (600 MHz, CDCl_3) spectrum of **6**

Figure S50. HRESIMS spectrum of **6**

Figure S51. ^1H NMR (600 MHz, CDCl_3) spectrum of **7**

Figure S52. ^{13}C NMR (150 MHz, CDCl_3) spectrum of **7**

Figure S53. HSQC (600 MHz, CDCl₃) spectrum of **7**
Figure S54. HMBC (600 MHz, CDCl₃) spectrum of **7**
Figure S55. H-H COSY (600 MHz, CDCl₃) spectrum of **7**
Figure S56. NOESY (600 MHz, CDCl₃) spectrum of **7**
Figure S57. HRESIMS spectrum of **7**
Figure S58. ¹H NMR (600 MHz, CDCl₃) spectrum of **8**
Figure S59. ¹³C NMR (150 MHz, CDCl₃) spectrum of **8**
Figure S60. HSQC (600 MHz, CDCl₃) spectrum of **8**
Figure S61. HMBC (600 MHz, CDCl₃) spectrum of **8**
Figure S62. H-H COSY (600 MHz, CDCl₃) spectrum of **8**
Figure S63. NOESY (600 MHz, CDCl₃) spectrum of **8**
Figure S64. HRESIMS spectrum of **8**
Figure S65. ¹H NMR (600 MHz, CDCl₃) spectrum of **9**
Figure S66. ¹³C NMR (150 MHz, CDCl₃) spectrum of **9**
Figure S67. HSQC (600 MHz, CDCl₃) spectrum of **9**
Figure S68. HMBC (600 MHz, CDCl₃) spectrum of **9**
Figure S69. H-H COSY (600 MHz, CDCl₃) spectrum of **9**
Figure S70. NOESY (600 MHz, CDCl₃) spectrum of **9**
Figure S71. HRESIMS spectrum of **9**
Figure S72. ¹H NMR (600 MHz, CDCl₃) spectrum of **10**
Figure S73. ¹³C NMR (150 MHz, CDCl₃) spectrum of **10**
Figure S74. HSQC (600 MHz, CDCl₃) spectrum of **10**
Figure S75. HMBC (600 MHz, CDCl₃) spectrum of **10**
Figure S76. H-H COSY (600 MHz, CDCl₃) spectrum of **10**
Figure S77. NOESY (600 MHz, CDCl₃) spectrum of **10**
Figure S78. HRESIMS spectrum of **10**

Table S1. Main conformers (> 1%) of **1a** in methanol.

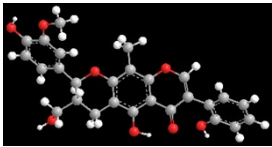
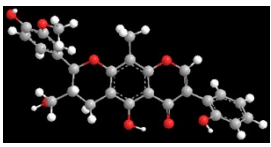
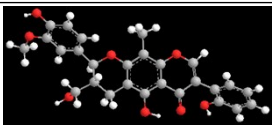
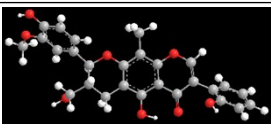
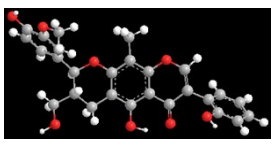
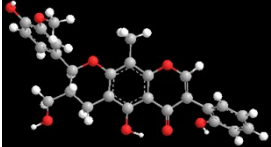
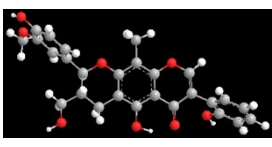
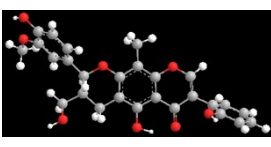
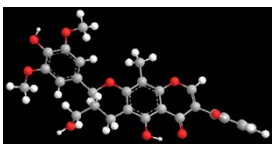
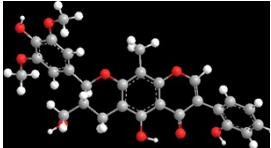
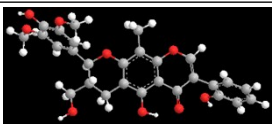
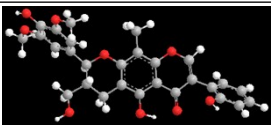
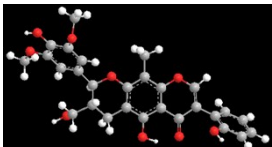
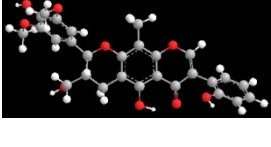
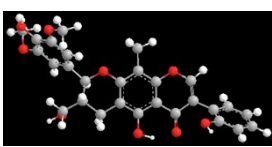
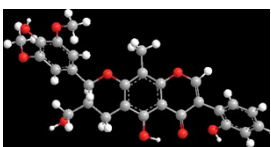
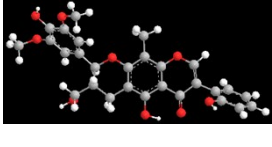
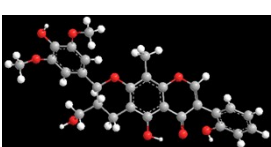
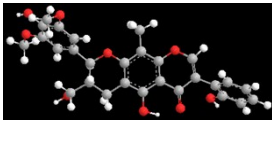
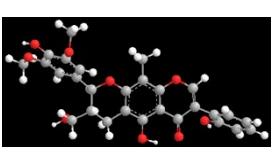
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|---|---|--|---|
|  |  |  |  |
| 1a C1 (22.23%) | 1a C2 (21.41%) | 1a C3 (18.01%) | 1a C4 (17.46%) |
|  |  |  |  |
| 1a C5 (5.94%) | 1a C6 (5.90%) | 1a C7 (3.51%) | 1a C8 (3.33%) |

Table S2. Main conformers (> 1%) of **2a** in methanol.

| | | | |
|---|---|--|---|
|  |  |  |  |
| 2a C1 (34.12%) | 2a C2 (16.89%) | 2a C3 (7.40%) | 2a C4 (7.31%) |
|  |  |  |  |
| 2a C5 (4.32%) | 2a C6 (4.23%) | 2a C7 (3.71%) | 2a C8 (3.19%) |
|  |  |  |  |
| 2a C9 (3.03%) | 2a C10 (2.15%) | 2a C11 (2.02%) | 2a C12 (1.96%) |

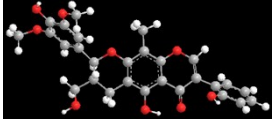
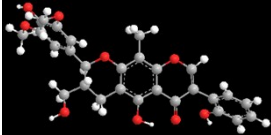
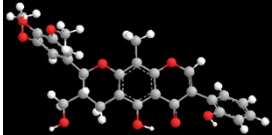
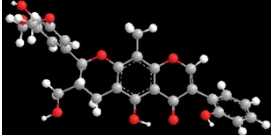
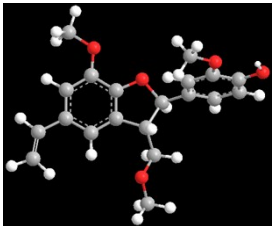
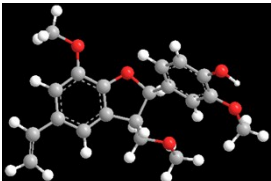
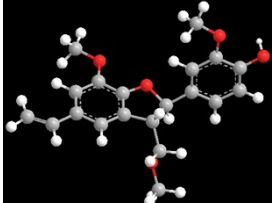
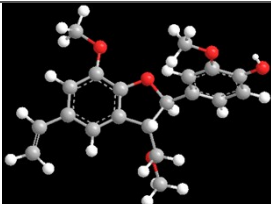
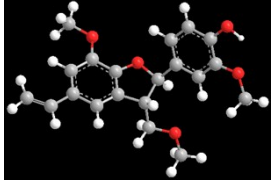
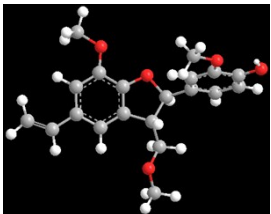
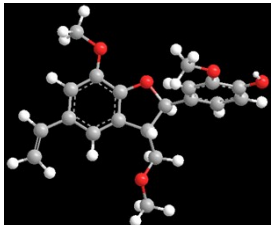
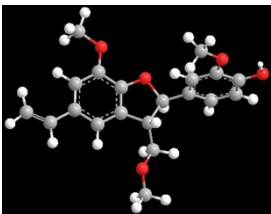
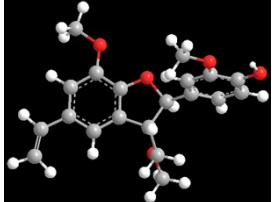
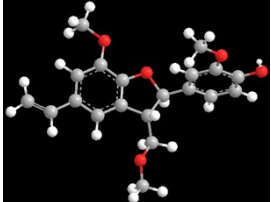
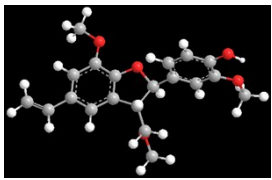
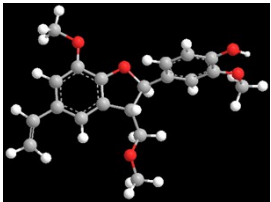
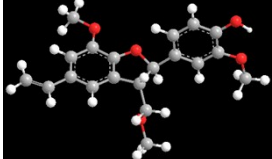
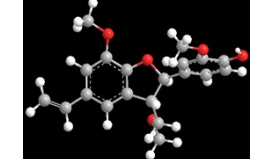
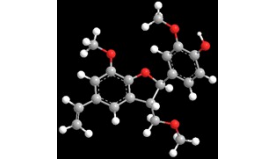
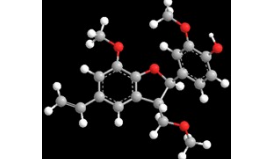
| | | | |
|---|---|--|---|
|  |  |  |  |
| 2a C13 (1.21%) | 2a C14 (1.08%) | 2a C15 (1.08%) | 2a C16 (1.07%) |

Table S3. Main conformers (> 1%) of **3a** in methanol.

| | | | |
|---|---|--|---|
|  |  |  |  |
| 3a C1 (5.66%) | 3a C2 (5.47%) | 3a C3 (4.67%) | 3a C4 (4.50%) |
|  |  |  |  |
| 3a C5 (4.49%) | 3a C6 (4.41%) | 3a C7 (4.27%) | 3a C8 (4.27%) |
|  |  |  |  |
| 3a C9 (4.00%) | 3a C10 (3.92%) | 3a C11 (3.65%) | 3a C12 (3.64%) |
|  |  |  |  |
| 3a C13 (3.61%) | 3a C14 (3.43%) | 3a C15 (3.38%) | 3a C16 (3.07%) |

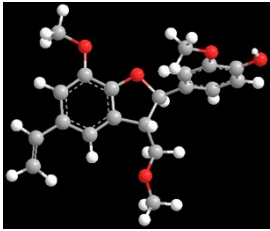
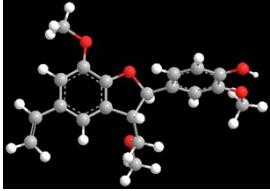
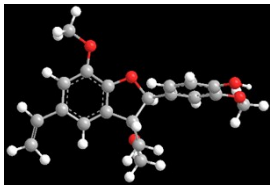
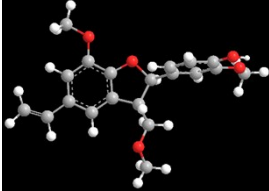
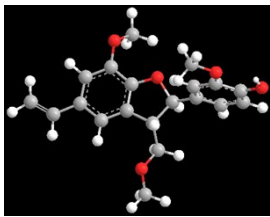
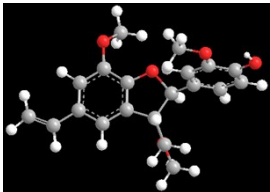
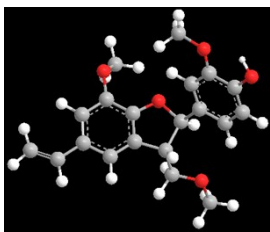
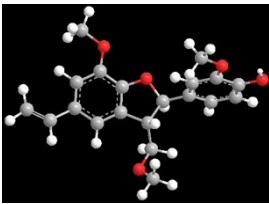
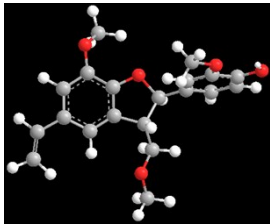
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|--|---|--|---|
|  |  |  |  |
| 3a C17 (2.95%) | 3a C18 (2.46%) | 3a C19 (2.45%) | 3a C20 (1.88%) |
|  |  |  |  |
| 3a C21 (1.82%) | 3a C22 (1.54%) | 3a C23 (1.32%) | 3a C24 (1.15%) |
|  | | | |
| 3a C25 (1.04%) | | | |

Figure S1. ^1H NMR (600 MHz, CDCl_3) spectrum of **1**

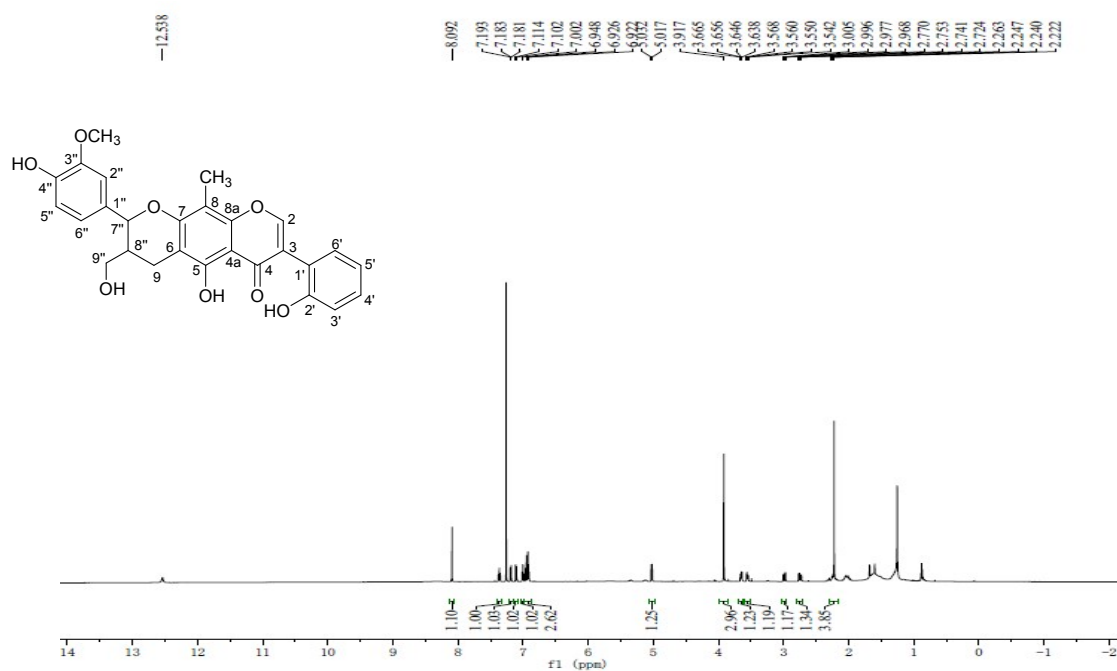


Figure S2. ^{13}C NMR (150 MHz, CDCl_3) spectrum of **1**

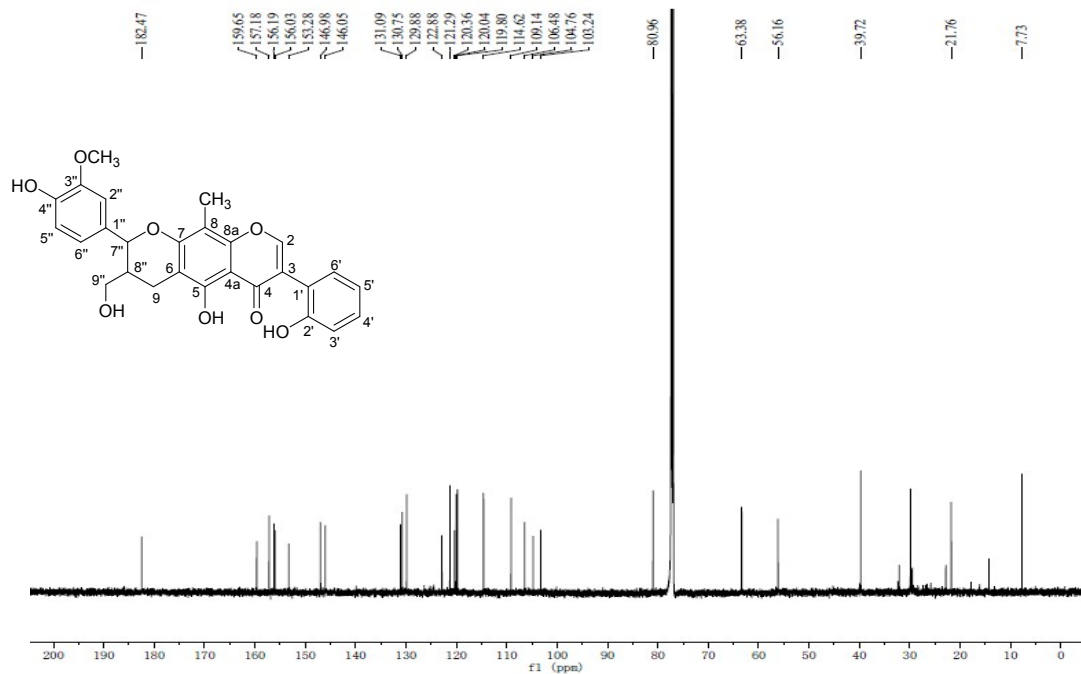


Figure S3. HSQC (600 MHz, CDCl₃) spectrum of **1**

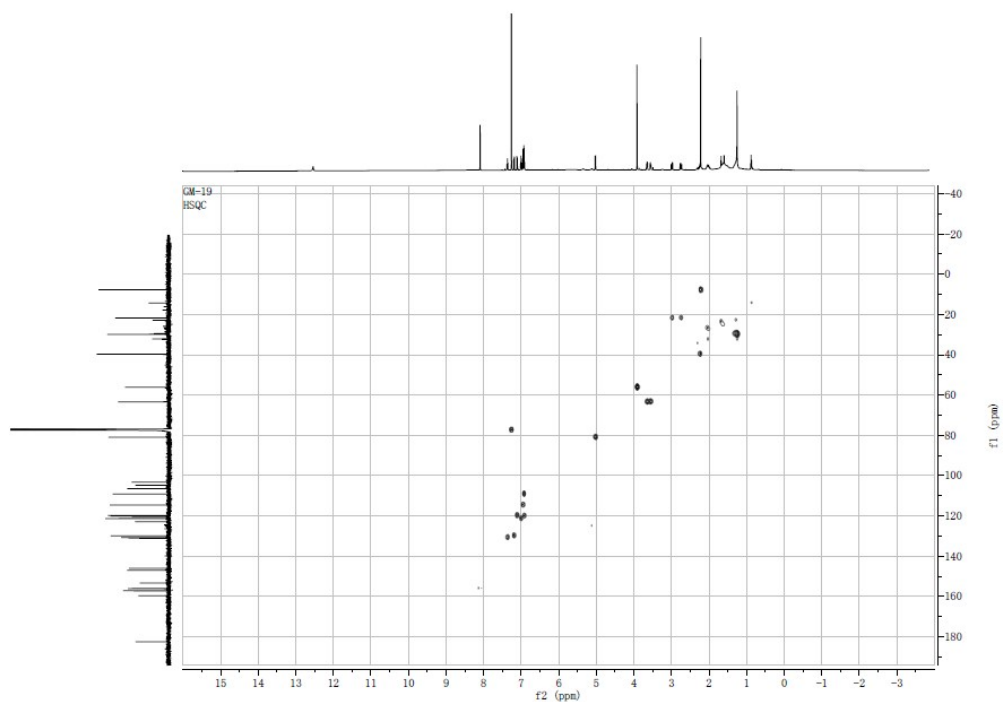


Figure S4. HMBC (600 MHz, CDCl₃) spectrum of **1**

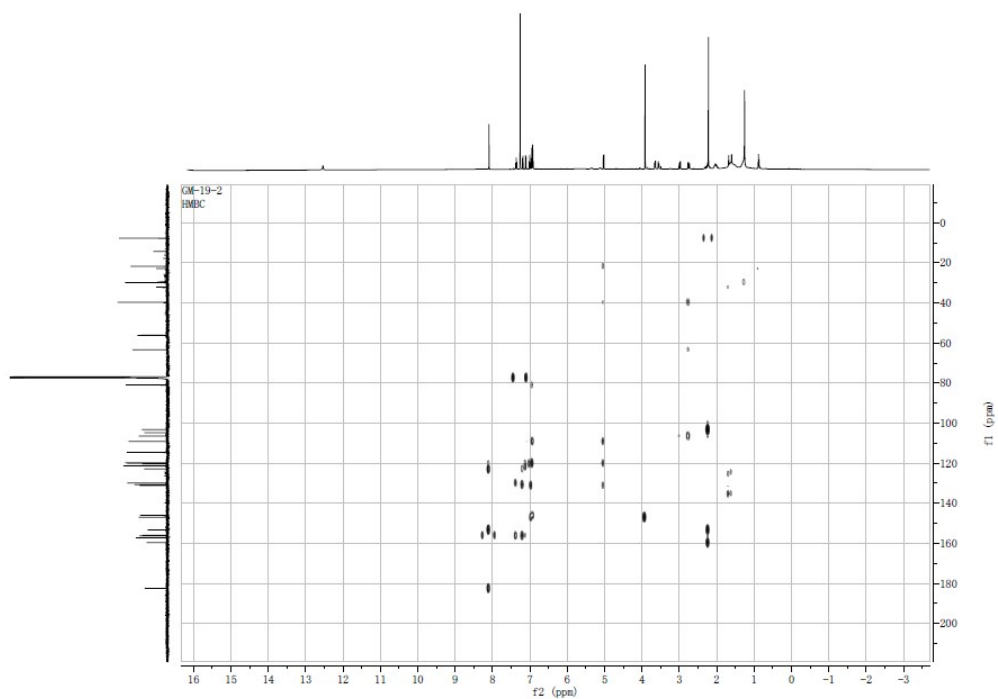


Figure S5. H-HCOSY (600 MHz, CDCl₃) spectrum of **1**

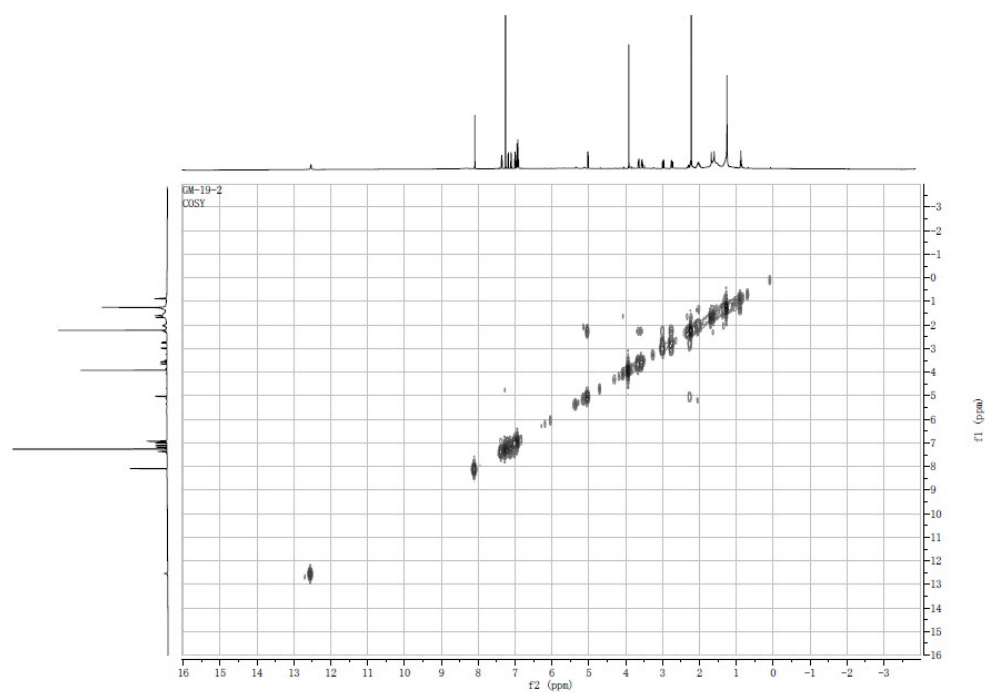


Figure S6. NOESY (600 MHz, CDCl₃) spectrum of **1**

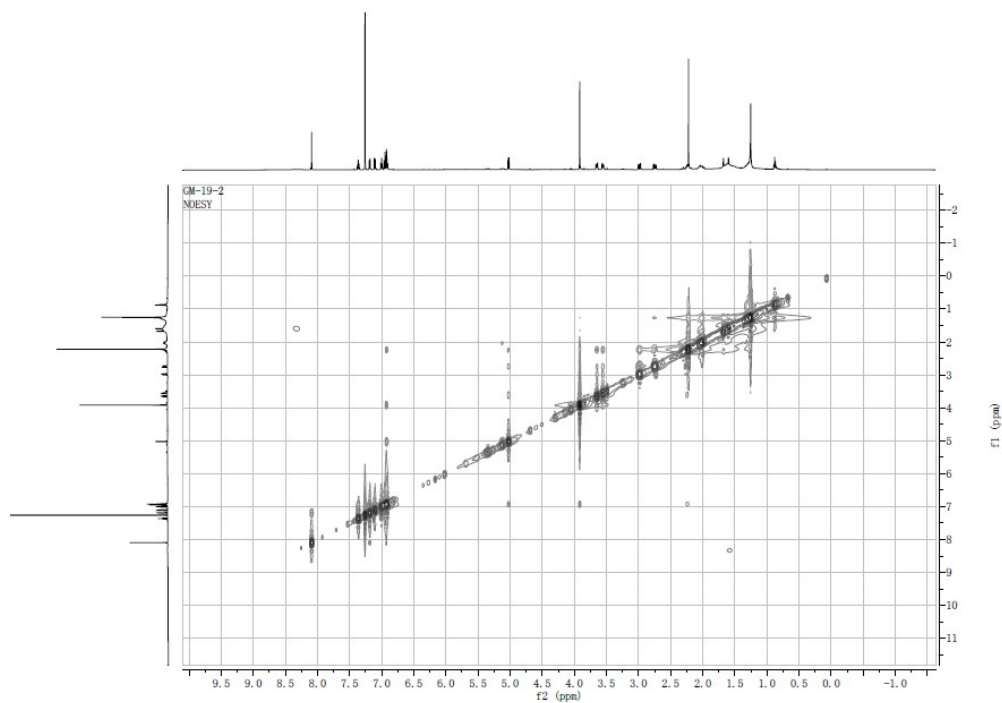
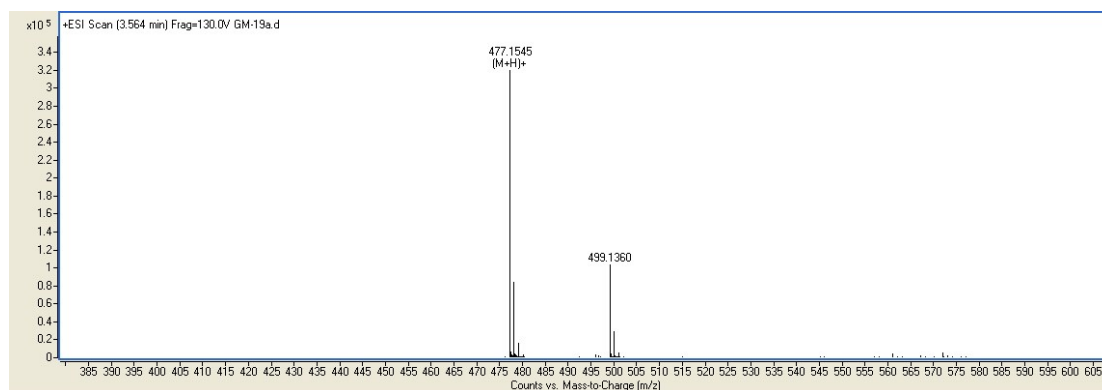


Figure S7. HRESIMS spectrum of **1**



| No. | Formula | Ion Formula | Measured m/z | Calc m/z | ppm |
|----------|-------------------|-------------------|--------------|----------|------|
| 1 | $C_{27}H_{24}O_8$ | $C_{27}H_{25}O_8$ | 477.1545 | 477.1544 | 0.21 |

Figure S8. Chiral-phase HPLC analytical chromatogram of **1**

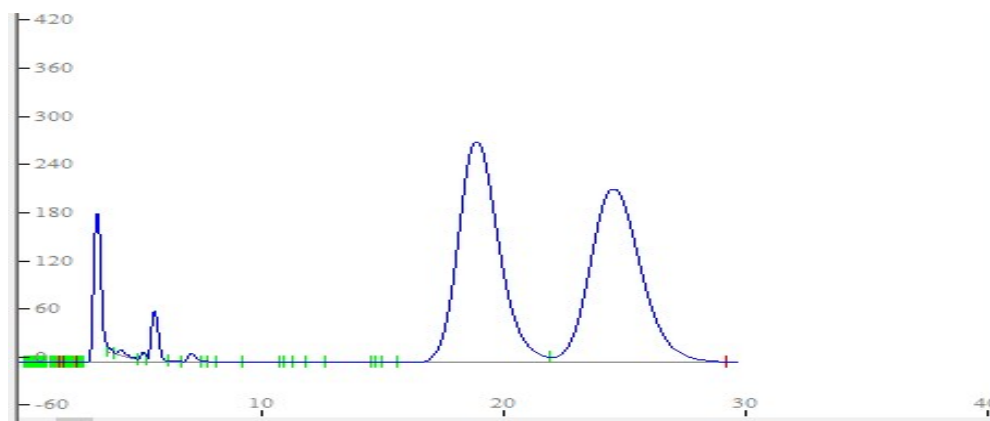


Figure S9. ^1H NMR (600 MHz, CDCl_3) spectrum of **1a**

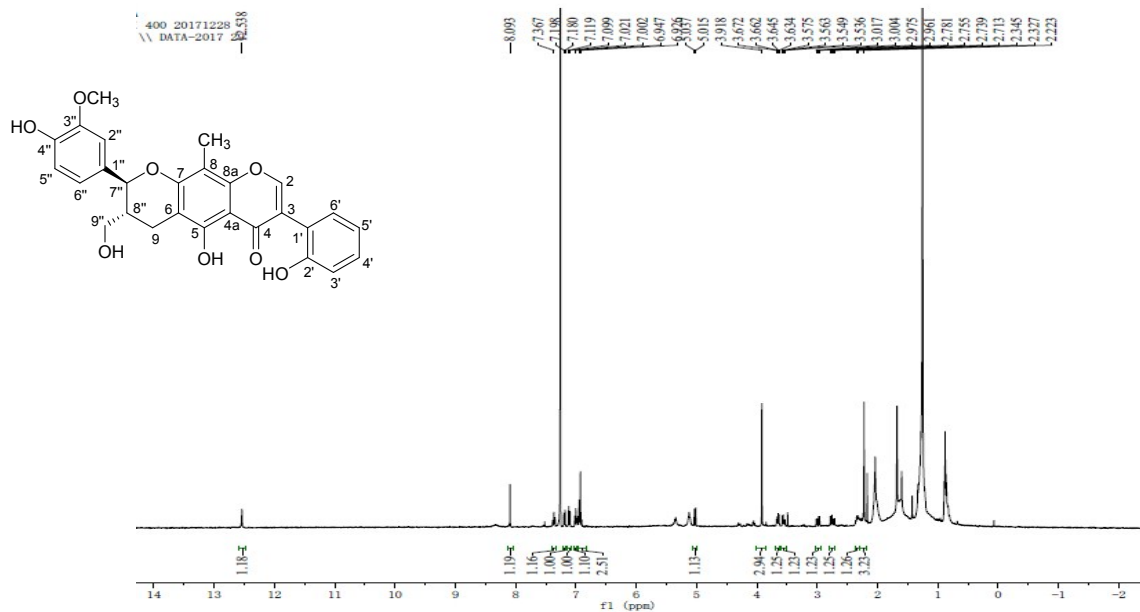


Figure S10. ^1H NMR (600 MHz, CDCl_3) spectrum of **1b**

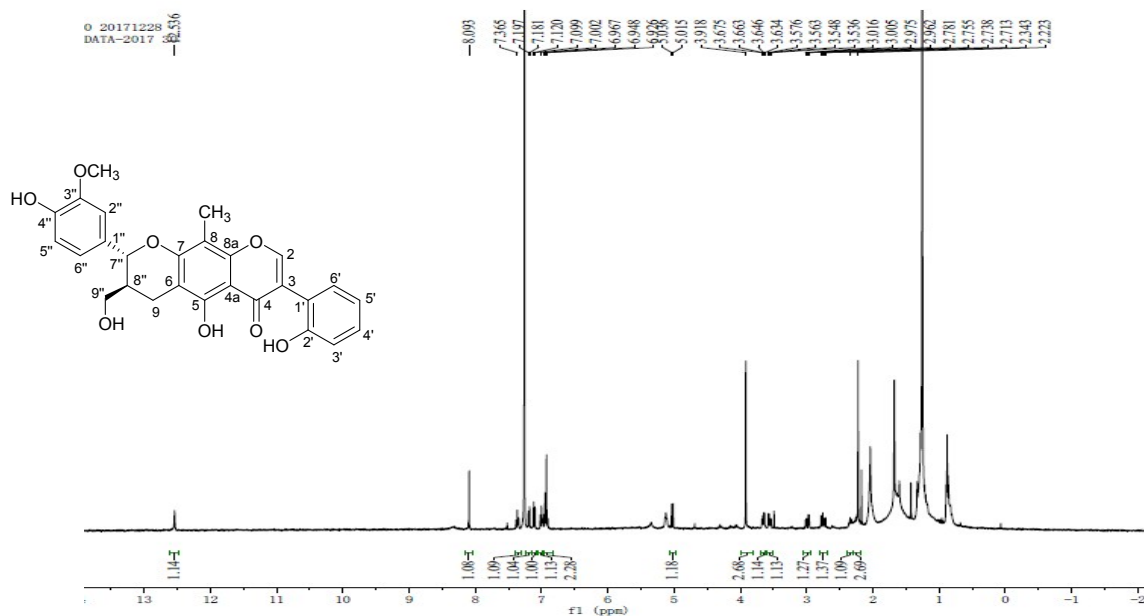


Figure S11. Experimental ECD spectra of **1a**

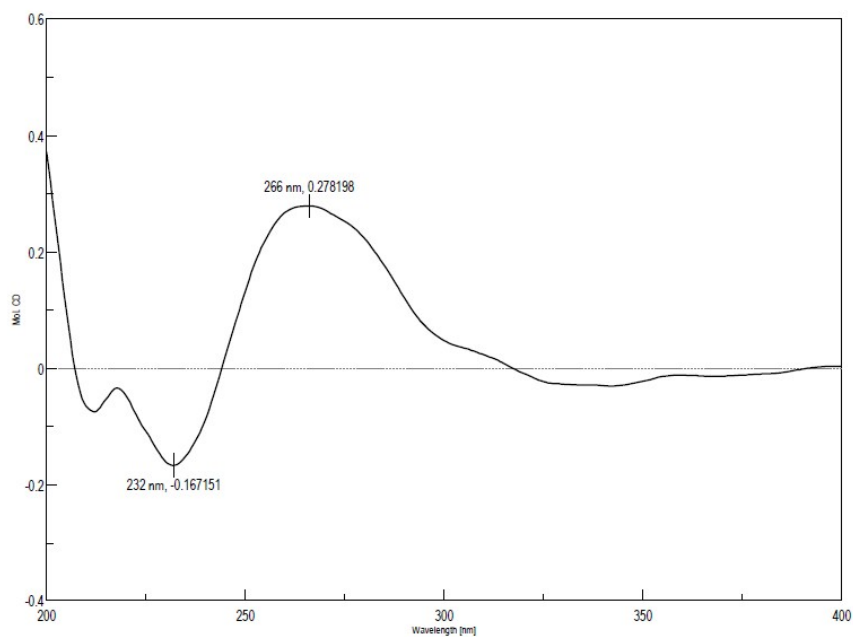


Figure S12. Experimental ECD spectra of **1b**

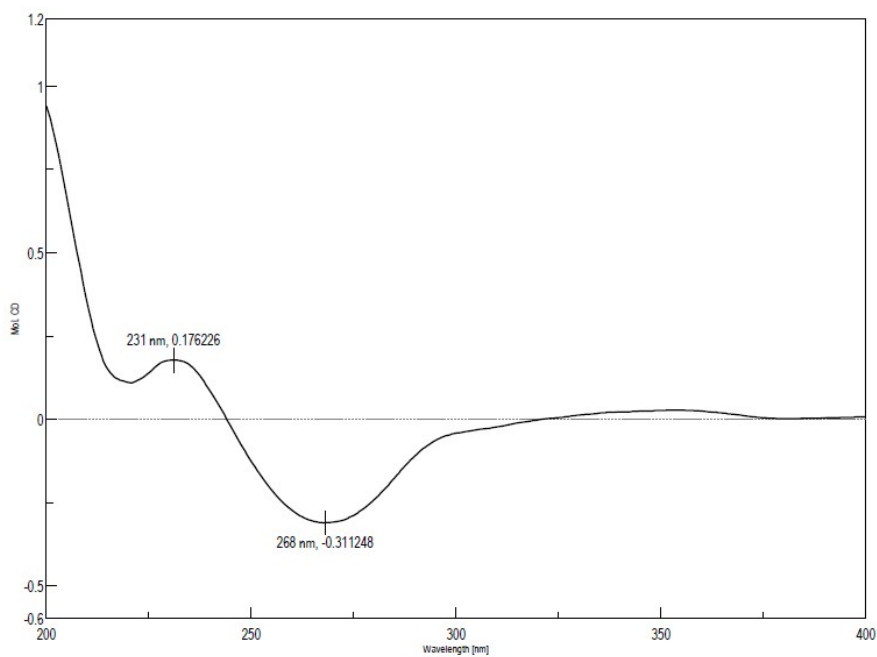


Figure S13. ¹H NMR (600 MHz, MeOD) spectrum of **2**

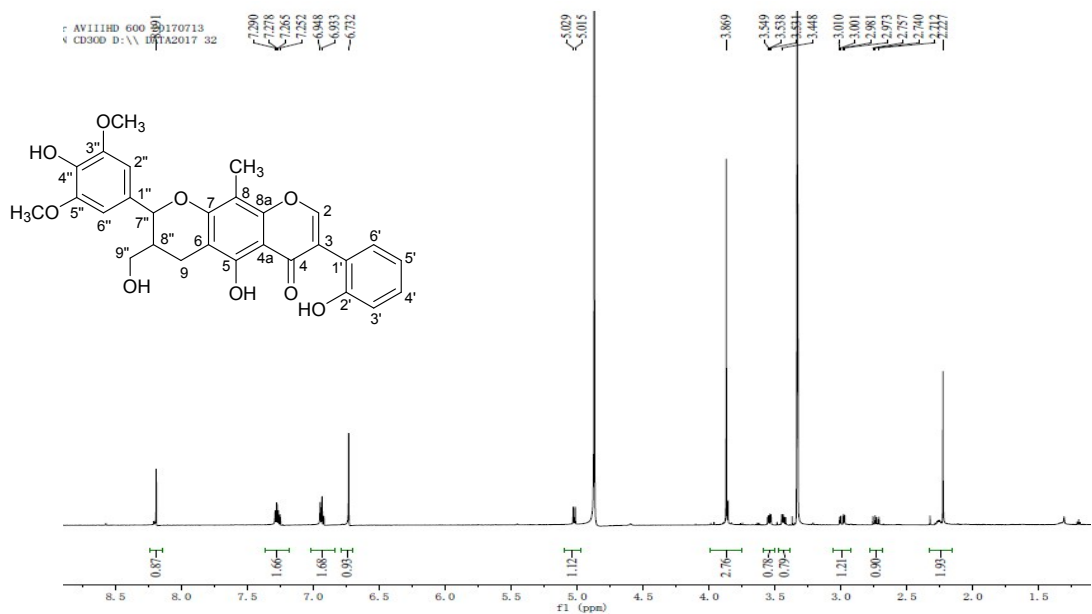


Figure S14. ^{13}C NMR (150 MHz, MeOD) spectrum of **2**

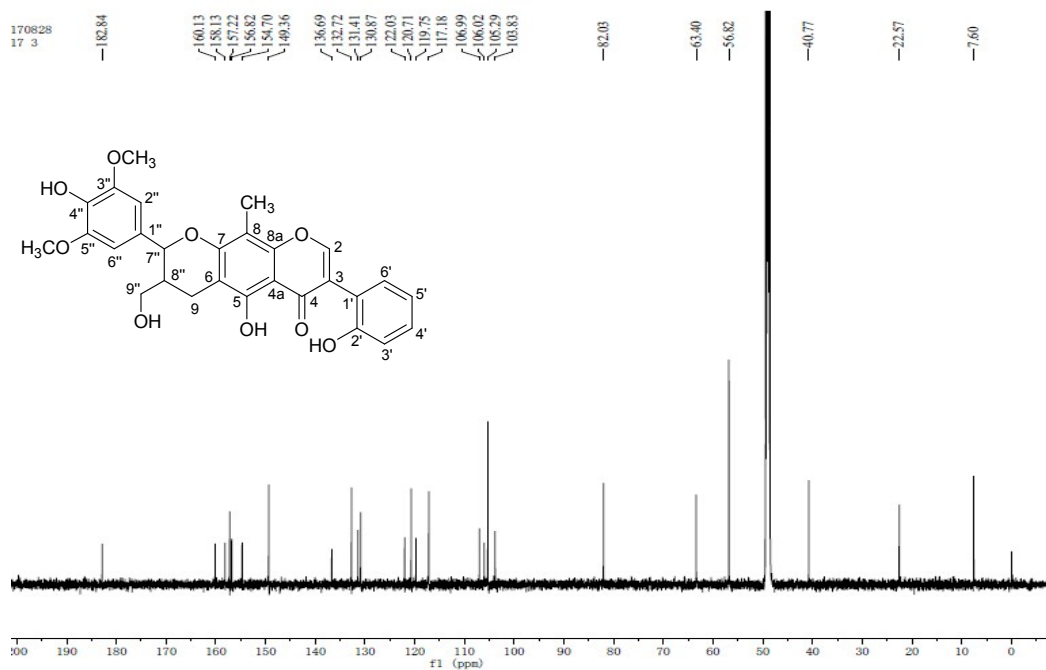


Figure S15. HSQC (600 MHz, MeOD) spectrum of **2**

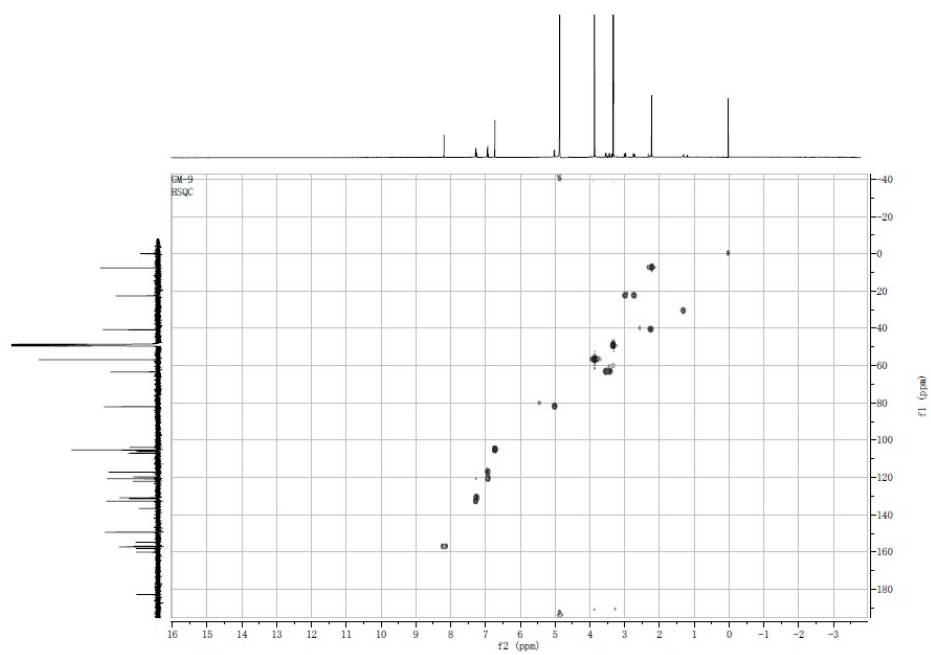


Figure S16. HMBC (600 MHz, MeOD) spectrum of **2**

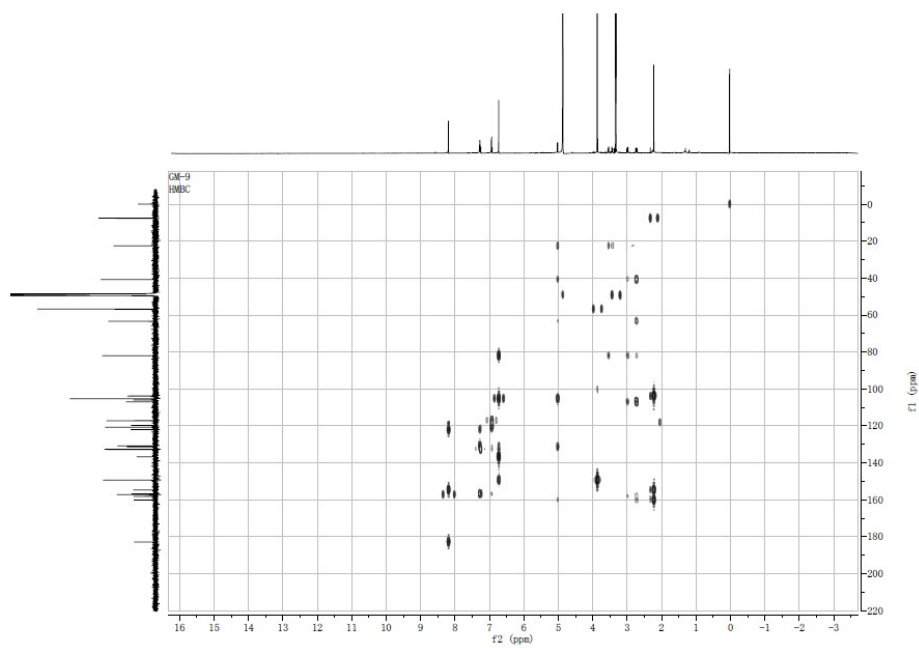


Figure S17. H-H COSY(600 MHz, MeOD) spectrum of **2**

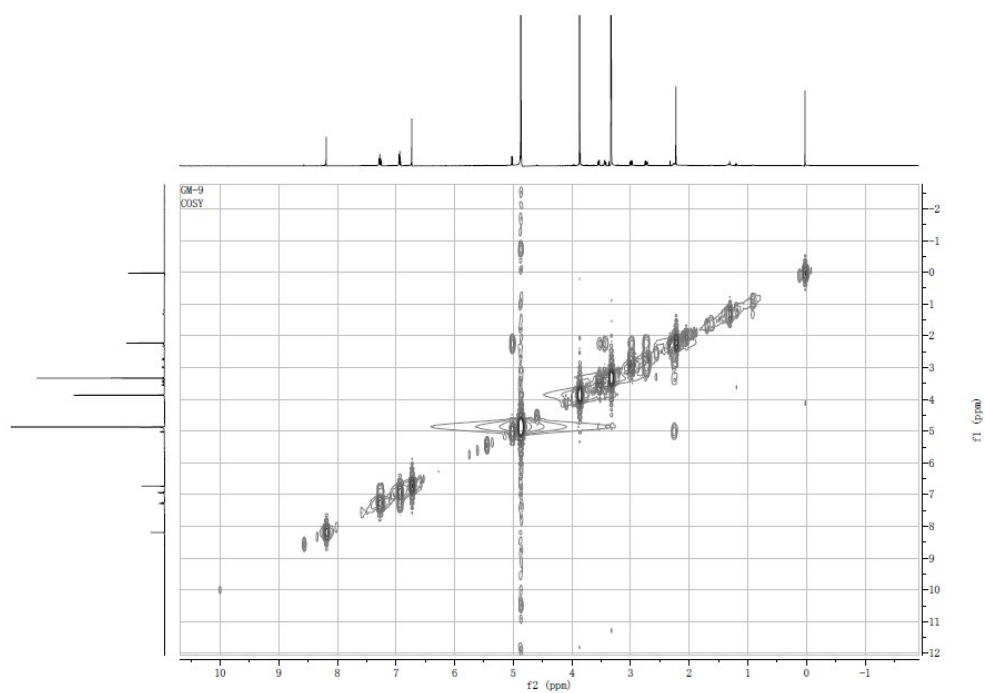


Figure S18. NOESY (600 MHz, MeOD) spectrum of **2**

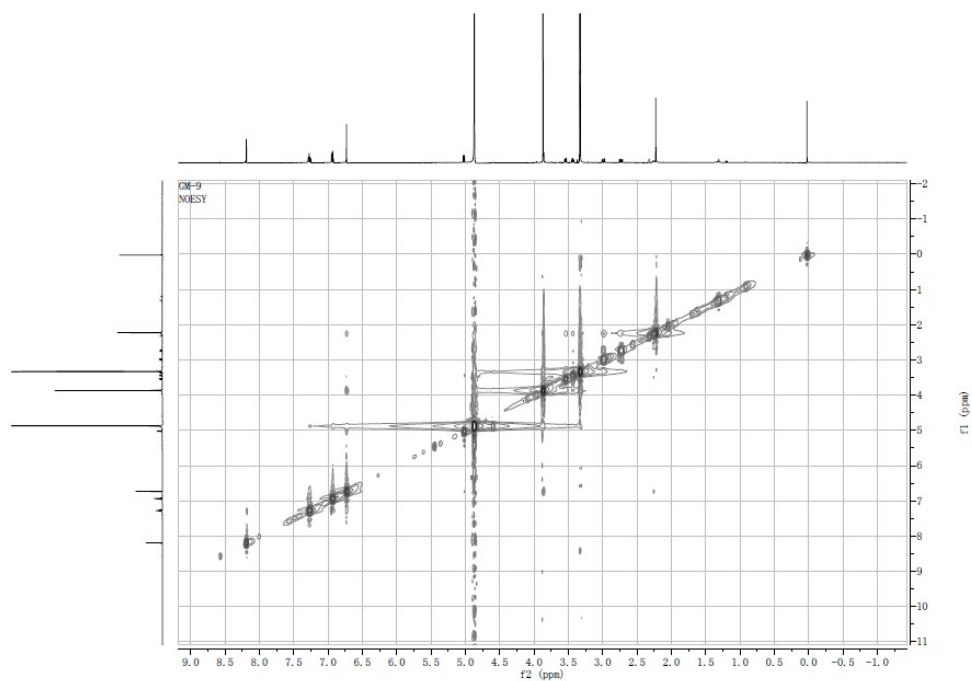
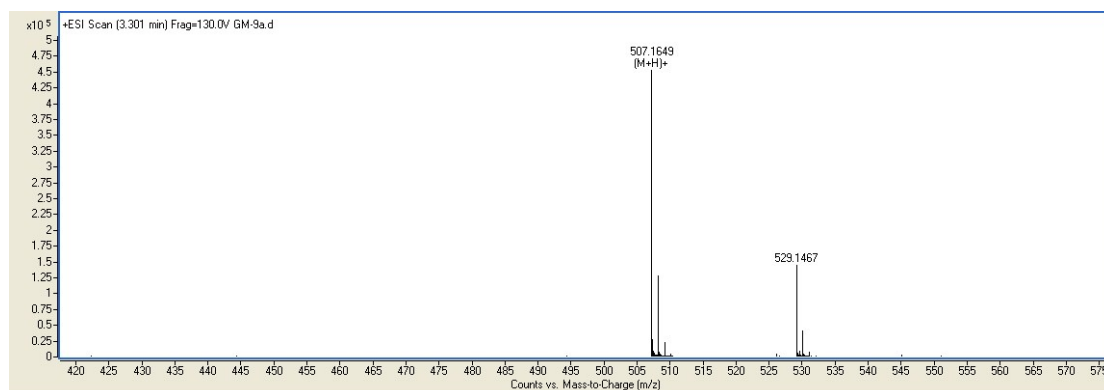


Figure S19. HRESIMS spectrum of **2**



| No. | Formula | Ion Formula | Measured m/z | Calc m/z | ppm |
|-----|--|--|--------------|----------|------|
| 2 | C ₂₈ H ₂₆ O ₉ | C ₂₈ H ₂₇ O ₉ | 507.1649 | 507.1650 | 0.20 |

Figure S20. Chiral-phase HPLC analytical chromatogram of **2**

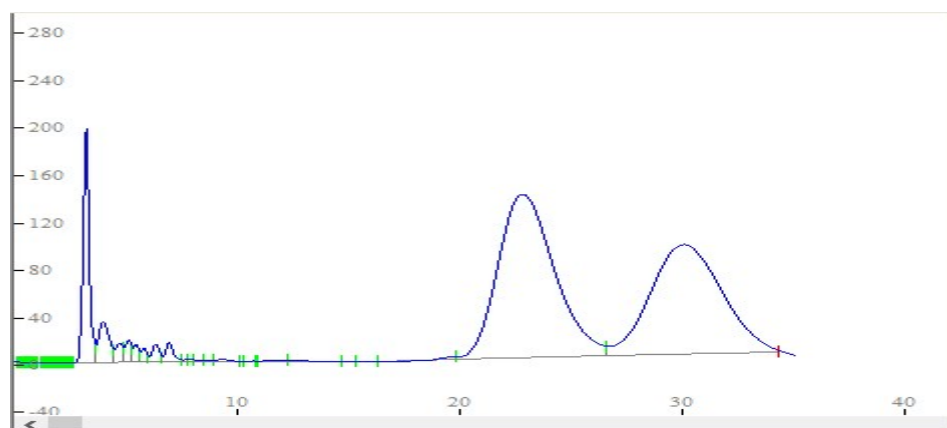


Figure S21. ¹H NMR (600 MHz, CDCl₃) spectrum of **2a**

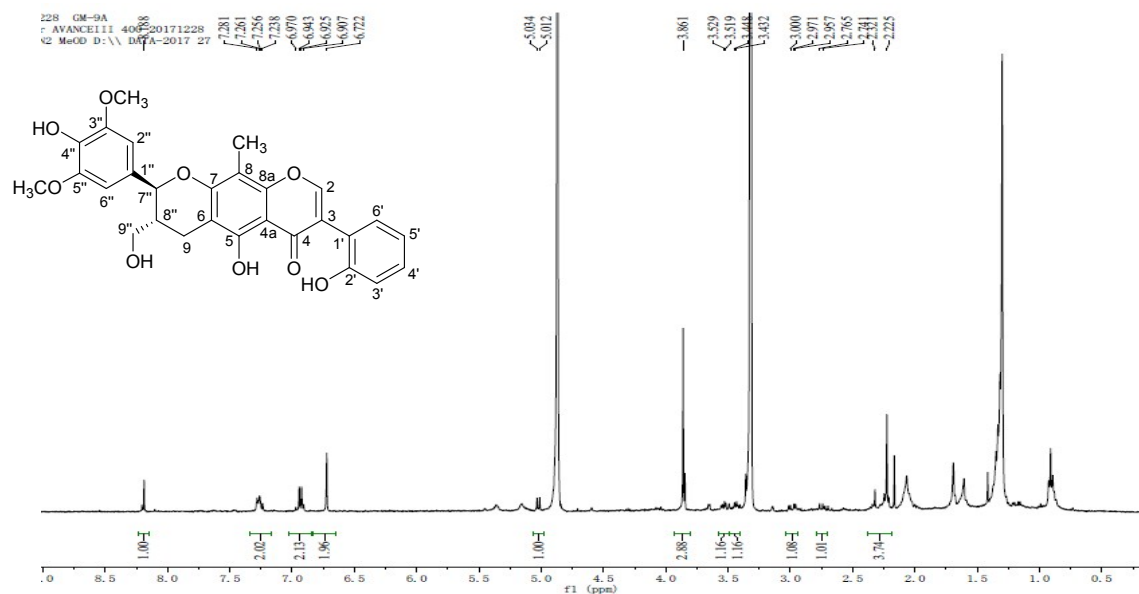


Figure S22. ^1H NMR (600 MHz, CDCl_3) spectrum of **2a**

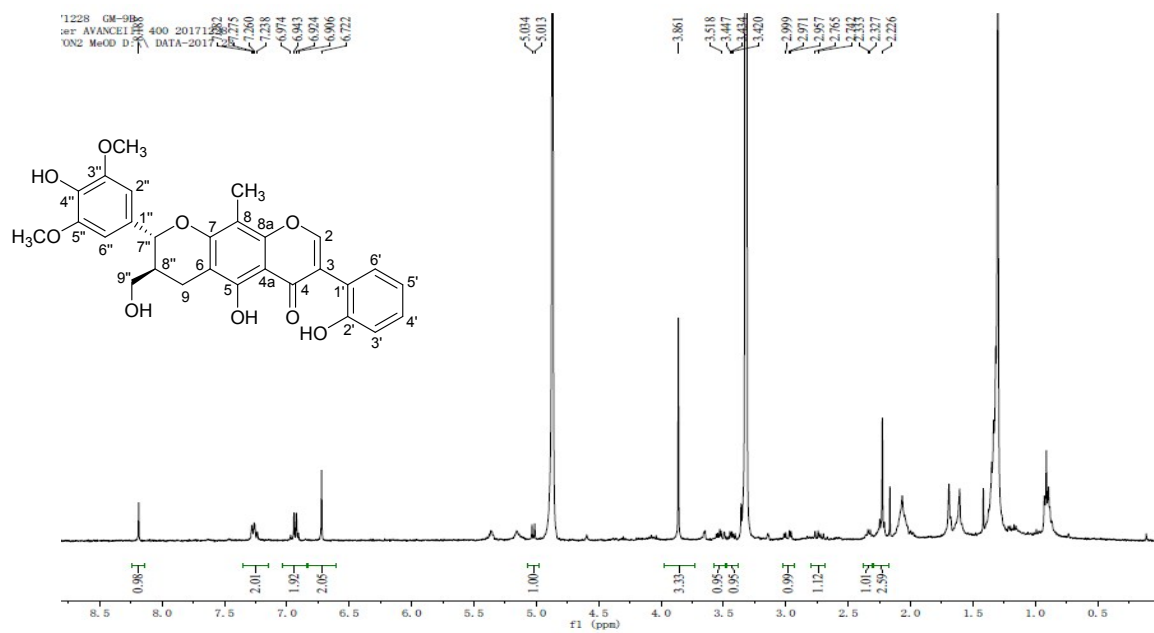


Figure S23. Experimental ECD spectra of **2a**

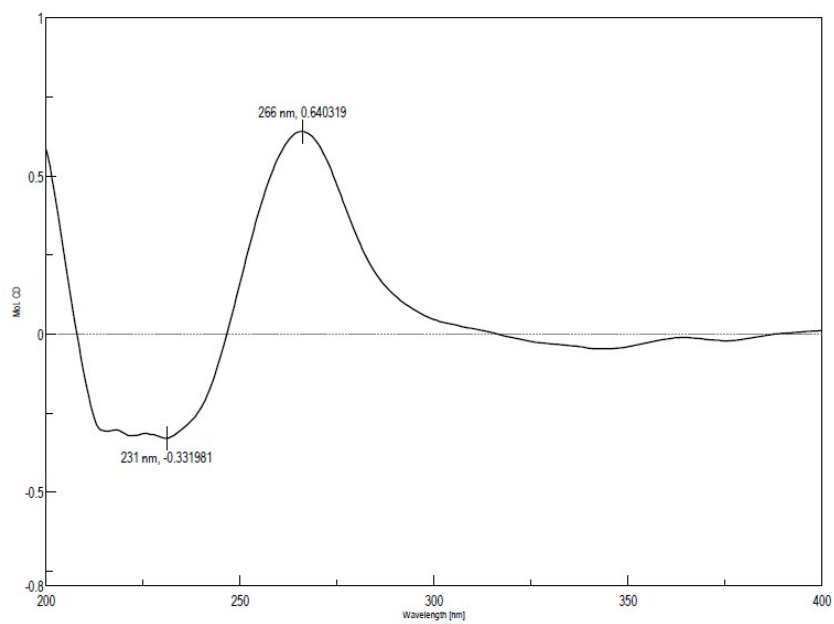


Figure S24. Experimental ECD spectra of **2b**

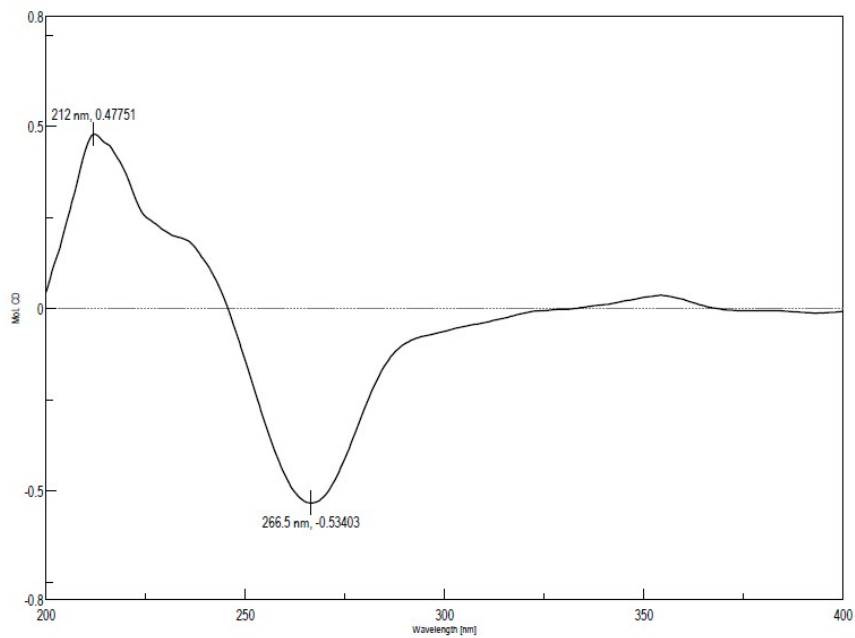


Figure S25. ^1H NMR (600 MHz, MeOD) spectrum of **3**

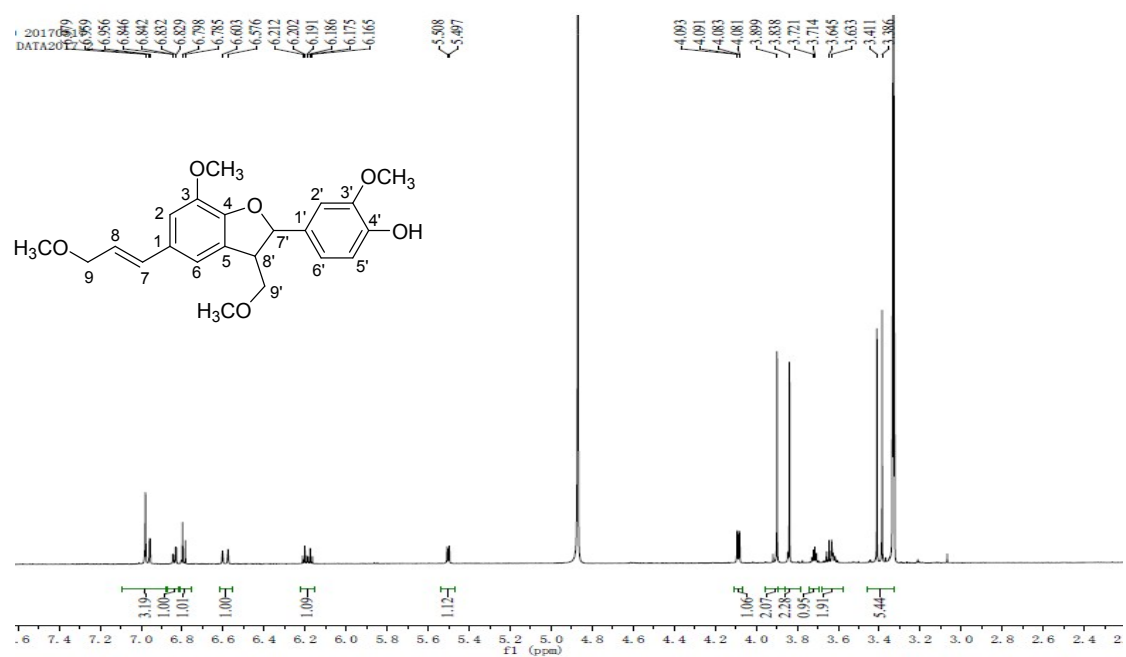


Figure S26. ¹³C NMR (150 MHz, MeOD) spectrum of **3**

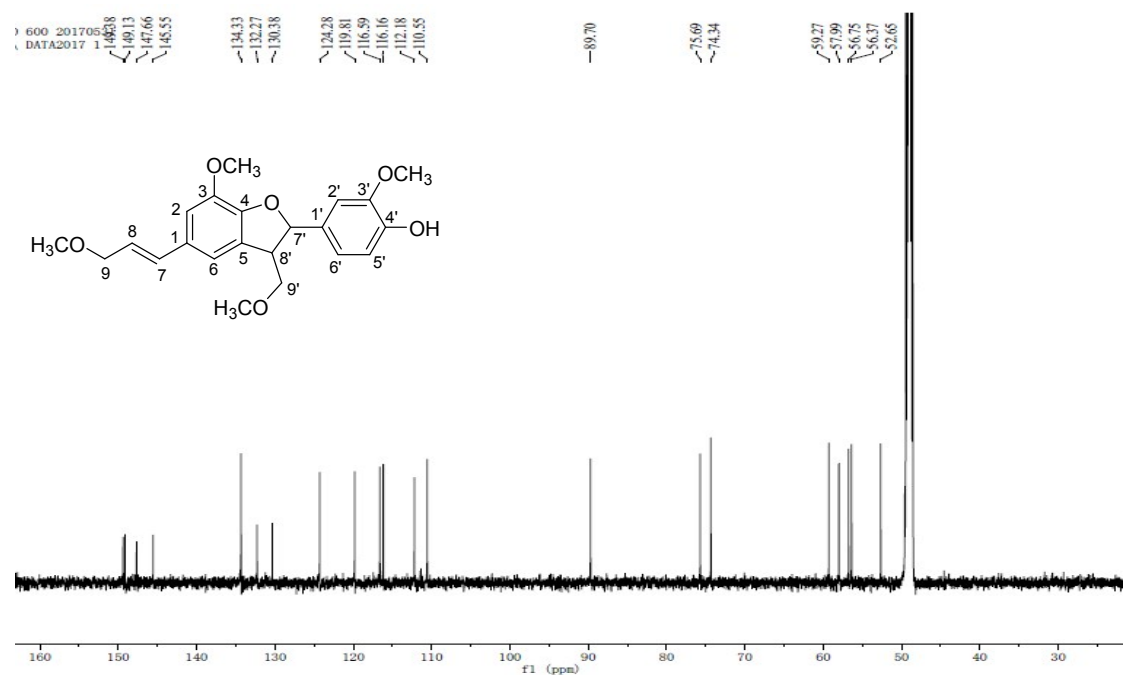


Figure S27. HSQC (600 MHz, MeOD) spectrum of **3**

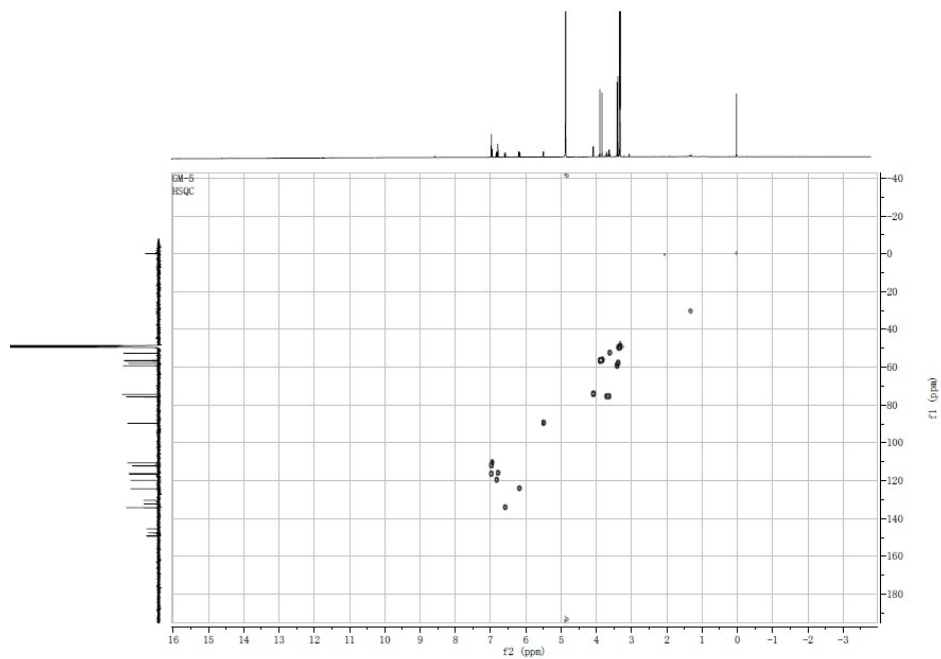


Figure S28. HMBC (600 MHz, MeOD) spectrum of **3**

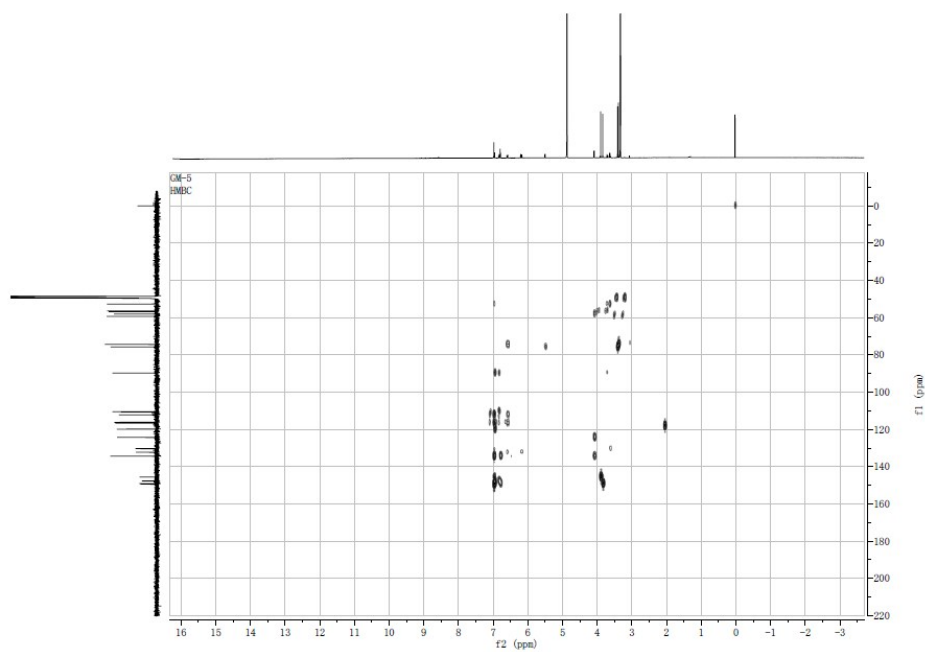


Figure S29. H-H COSY (600 MHz, MeOD) spectrum of **3**

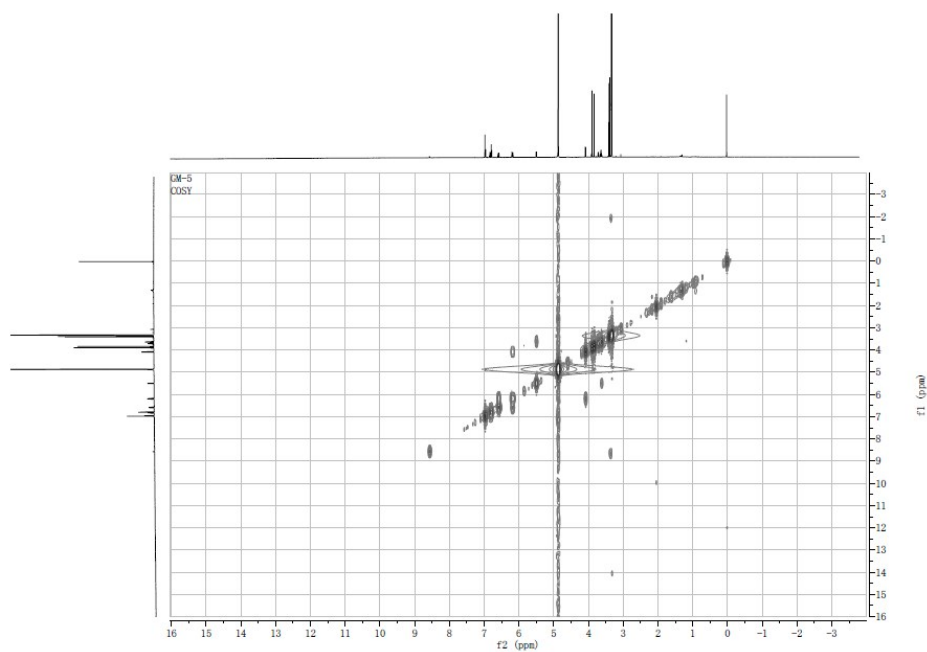


Figure S30. NOESY (600 MHz, MeOD) spectrum of **3**

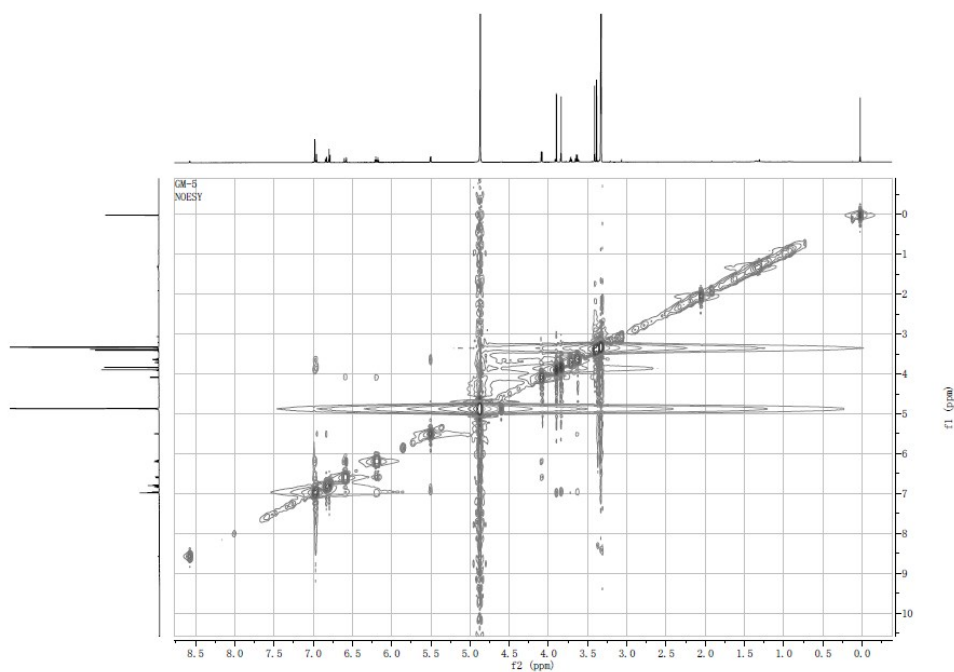
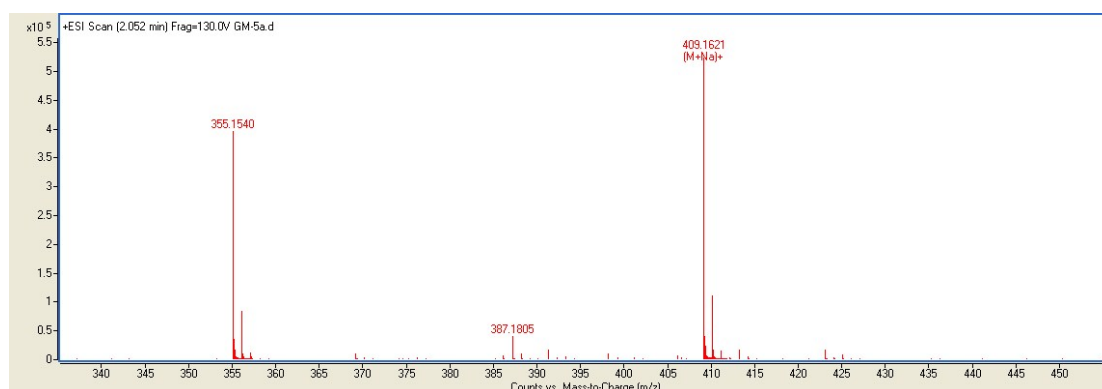


Figure S31. HRESIMS spectrum of **3**



| No. | Formula | Ion Formula | Measured m/z | Calc m/z | ppm |
|-----|--|--|--------------|----------|------|
| 3 | C ₂₂ H ₂₆ O ₆ | C ₂₂ H ₂₆ NaO ₆ | 409.1621 | 409.1622 | 0.24 |

Figure S32. Chiral-phase HPLC analytical chromatogram of **3**

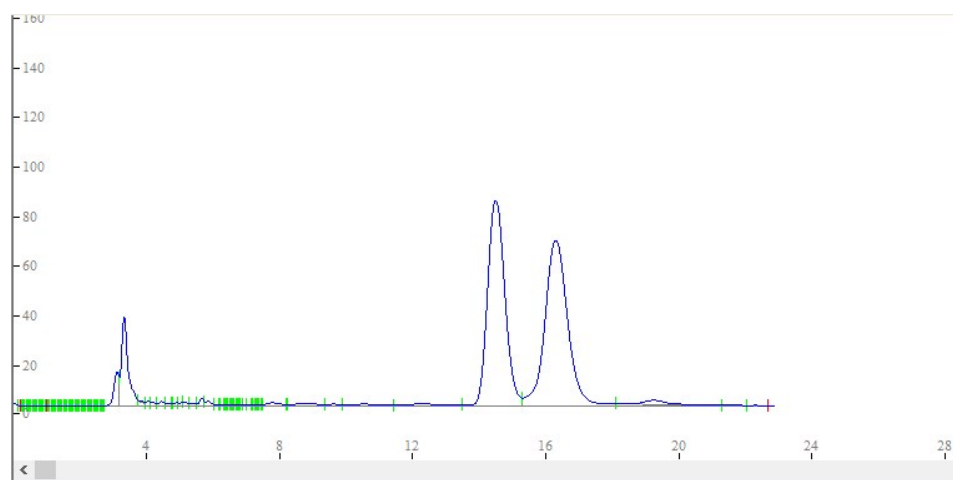


Figure S33. ¹H NMR (600 MHz, MeOD) spectrum of **3a**

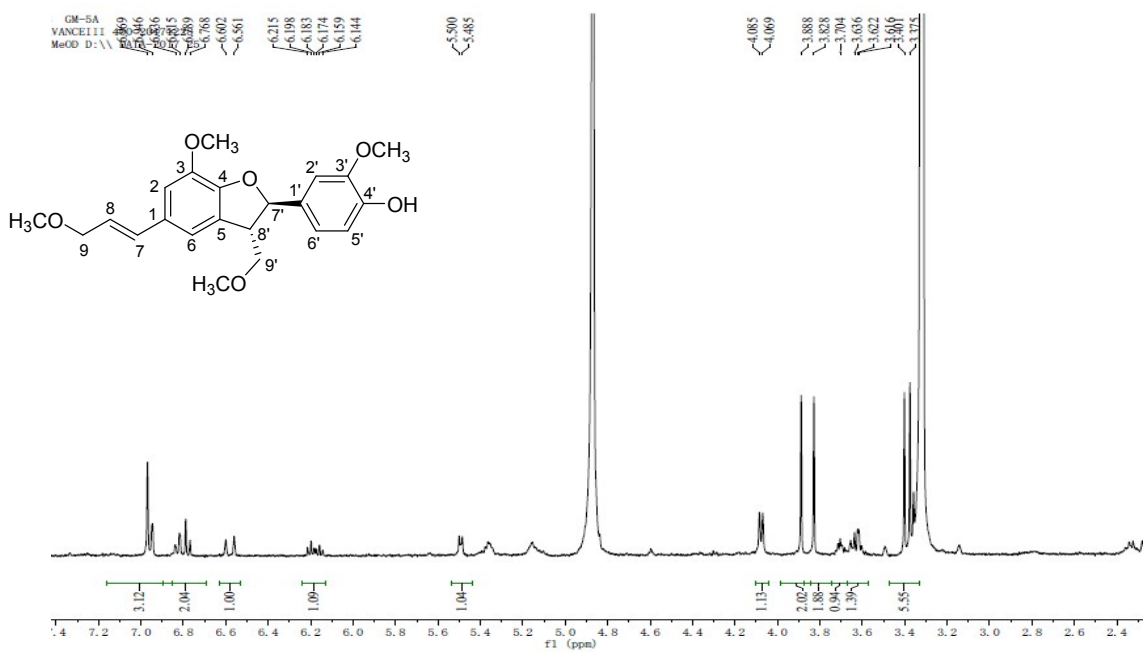


Figure S34. ^1H NMR (600 MHz, MeOD) spectrum of **3b**

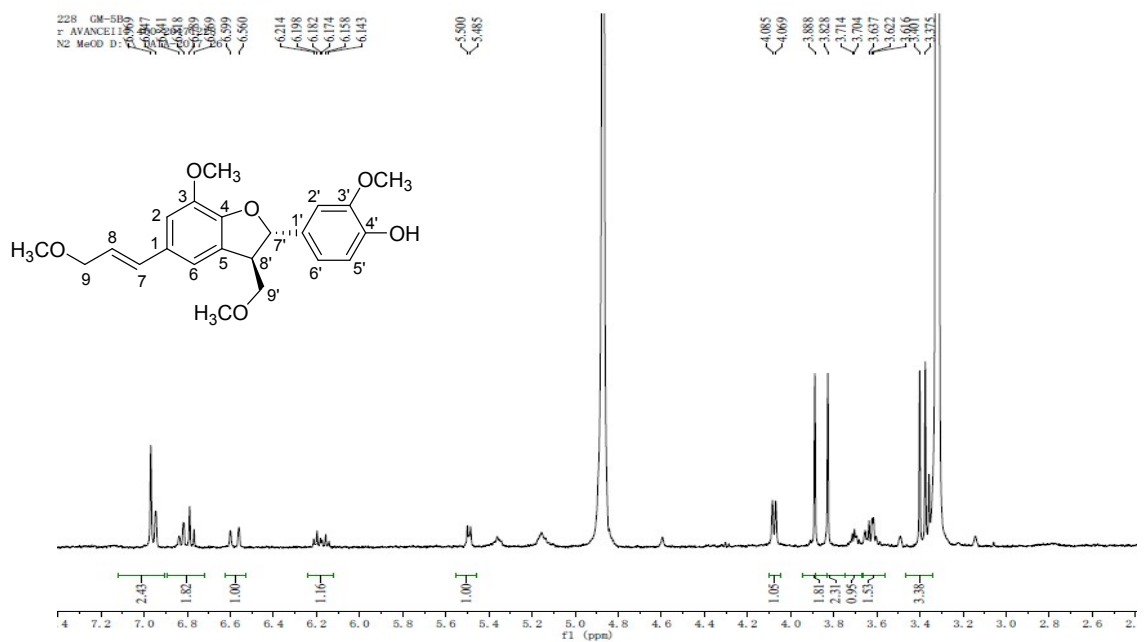


Figure S35. Experimental ECD spectra of **3a**

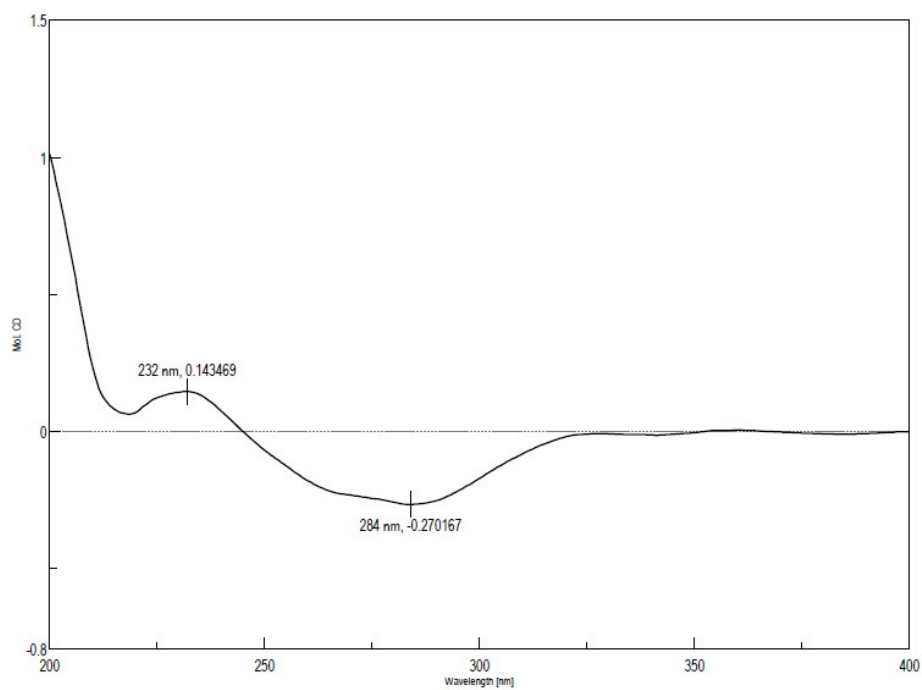


Figure S36. Experimental ECD spectra of **3b**

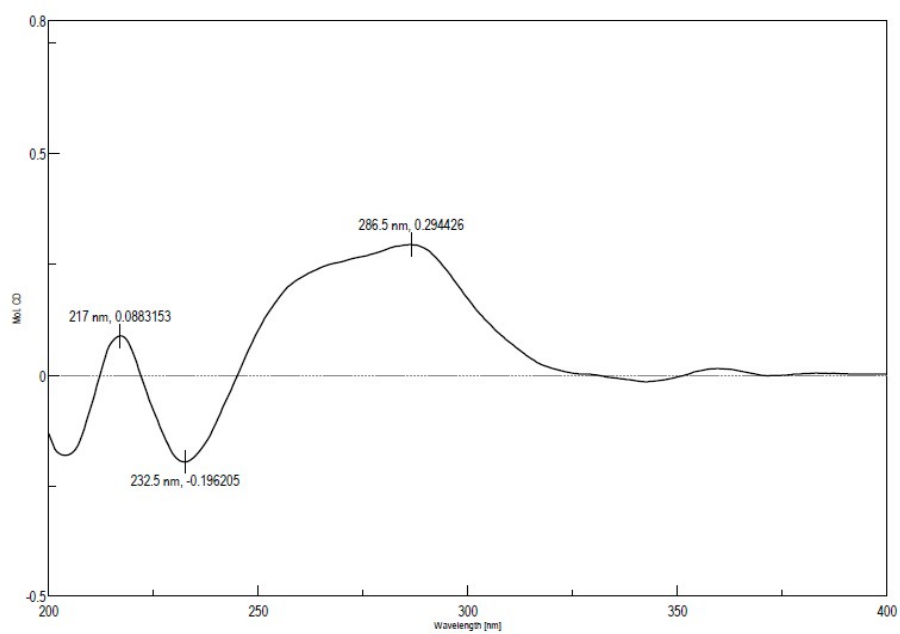


Figure S37. ¹H NMR (600 MHz, CDCl₃) spectrum of **5**

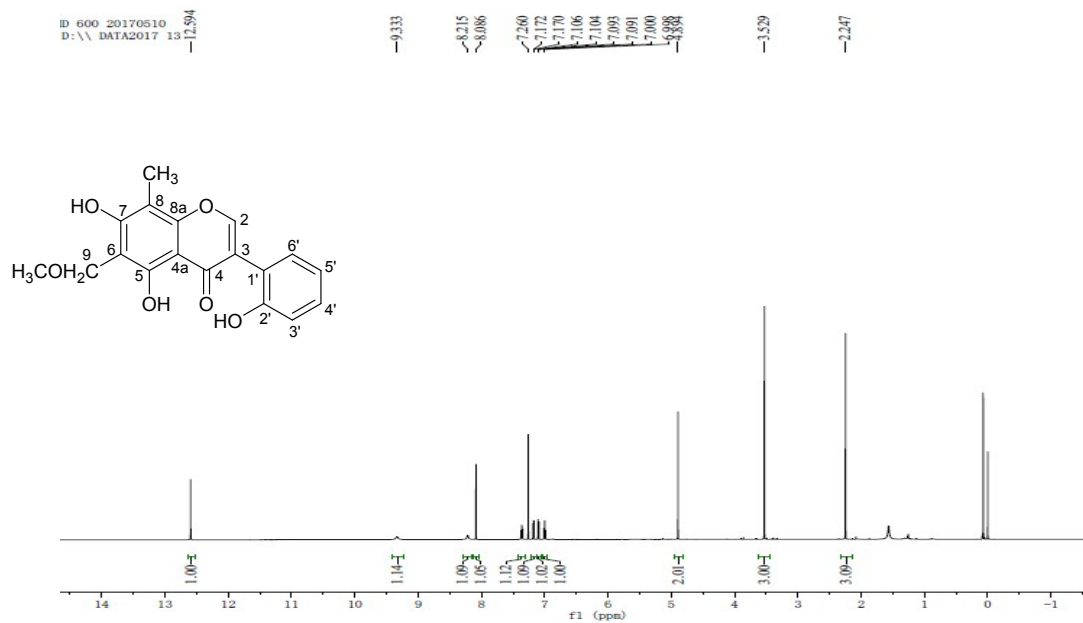


Figure S38. ^{13}C NMR (150 MHz, CDCl_3) spectrum of **5**

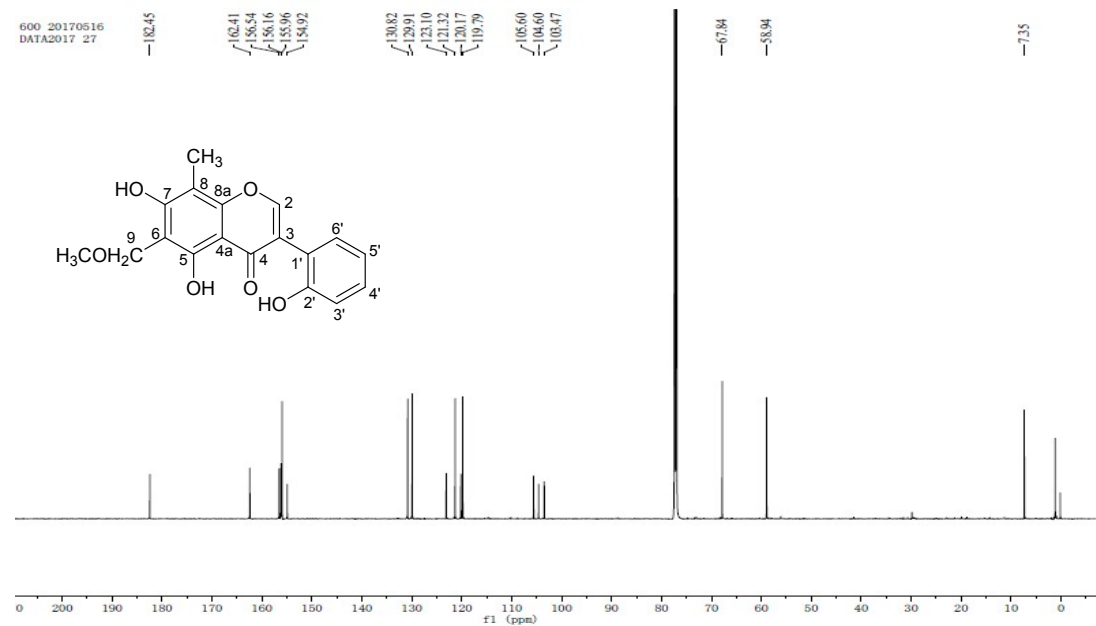


Figure S39. HSQC (600 MHz, CDCl_3) spectrum of **5**

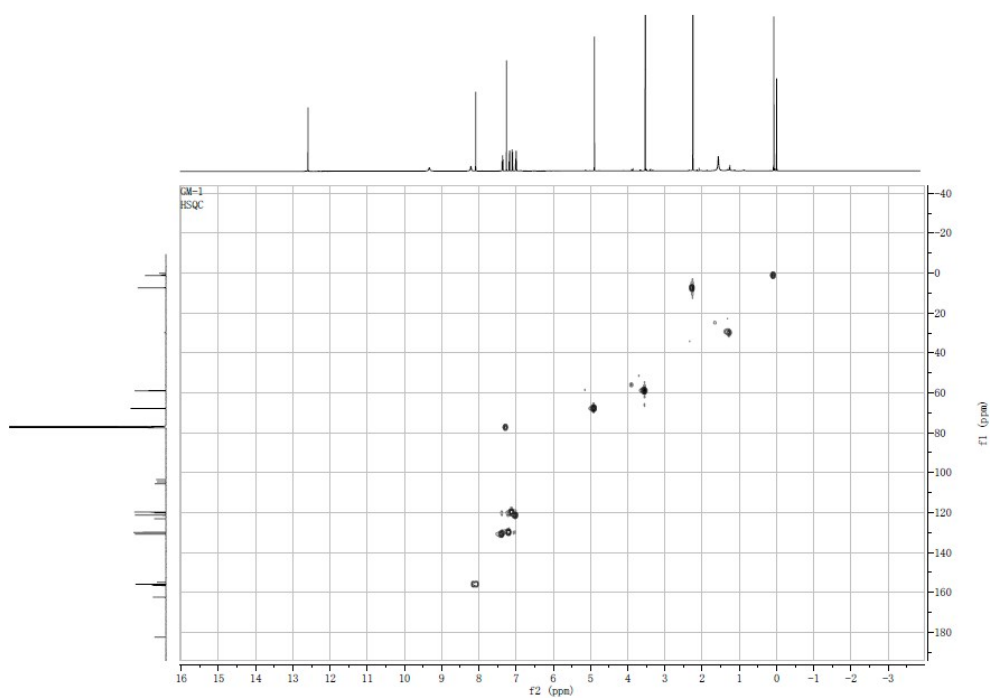


Figure S40. HMBC (600 MHz, CDCl₃) spectrum of **5**

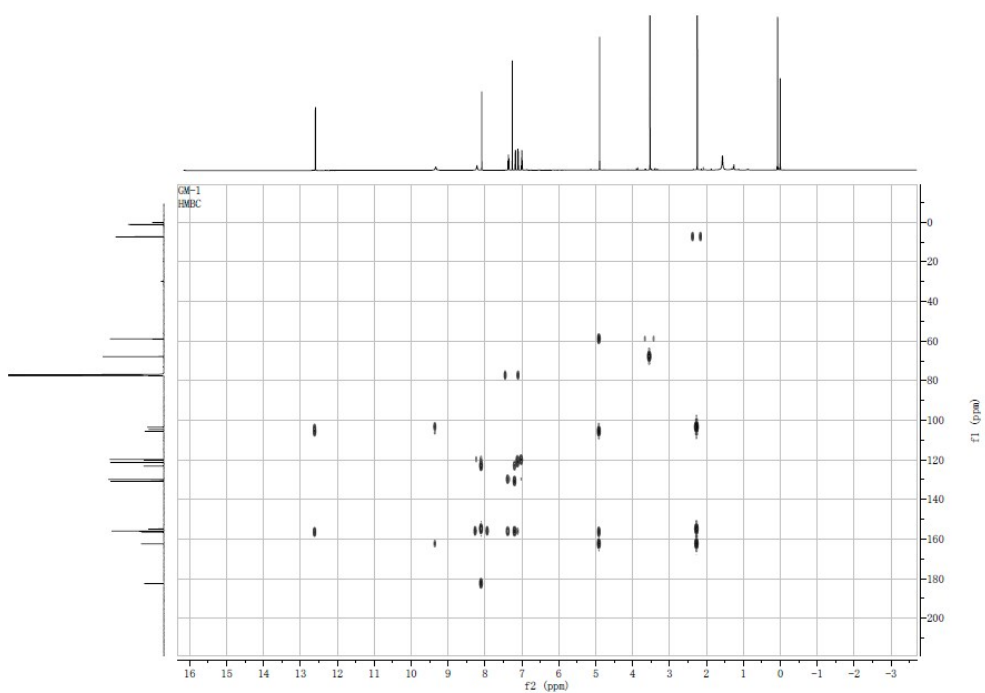


Figure S41. H-H COSY (600 MHz, CDCl₃) spectrum of **5**

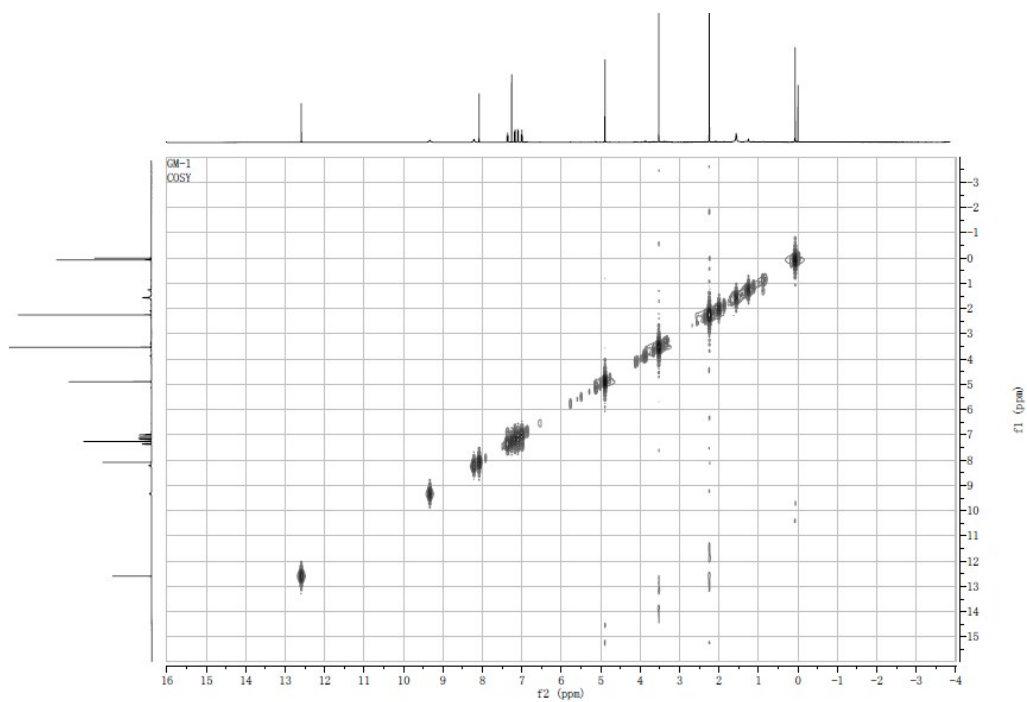


Figure S42. NOESY (600 MHz, CDCl₃) spectrum of **5**

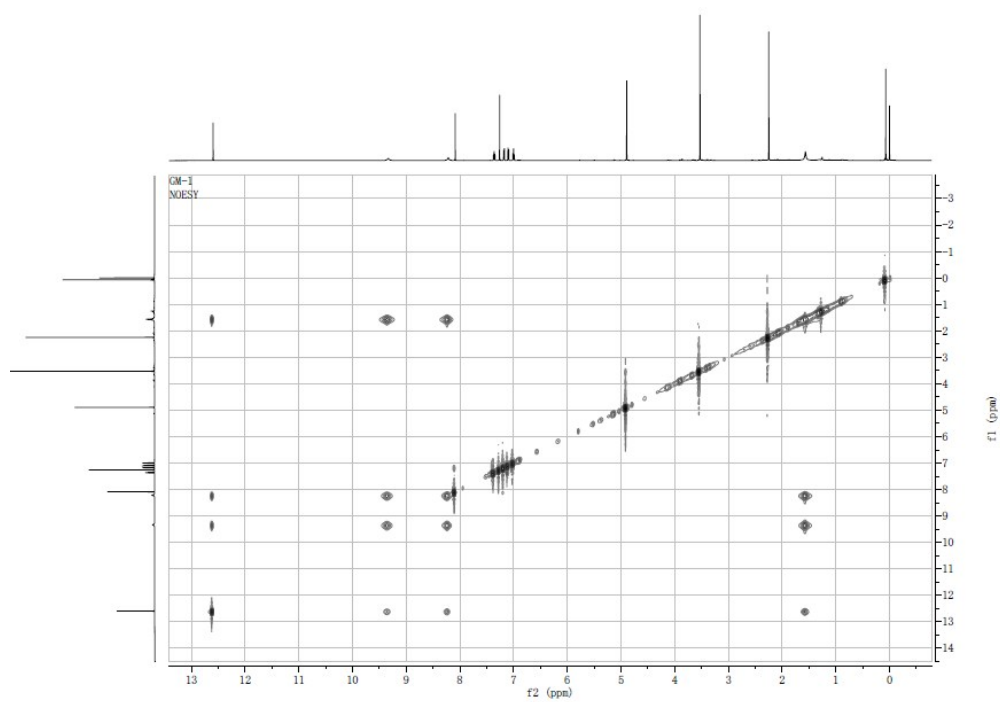
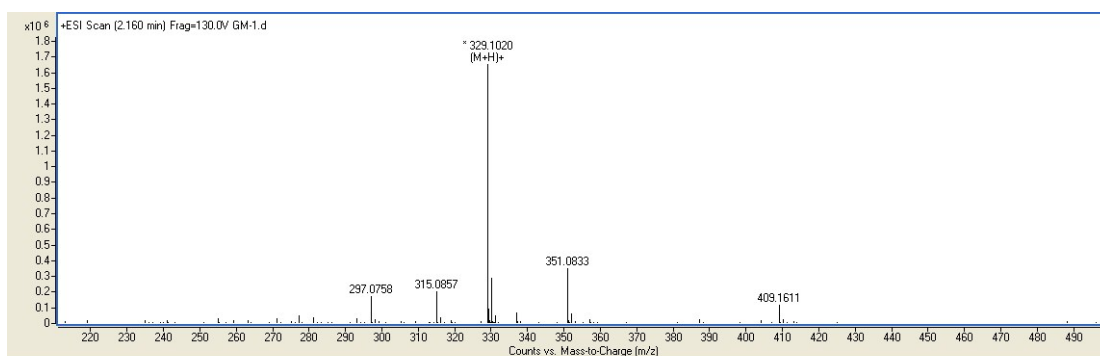


Figure S43. HRESIMS spectrum of **5**



| No. | Formula | Ion Formula | Measured m/z | Calc m/z | ppm |
|-----|--|--|--------------|----------|-----|
| 5 | C ₁₈ H ₁₆ O ₆ | C ₁₈ H ₁₇ O ₆ | 329.1020 | 329.1020 | 0 |

Figure S44. ¹H NMR (600 MHz, CDCl₃) spectrum of **6**

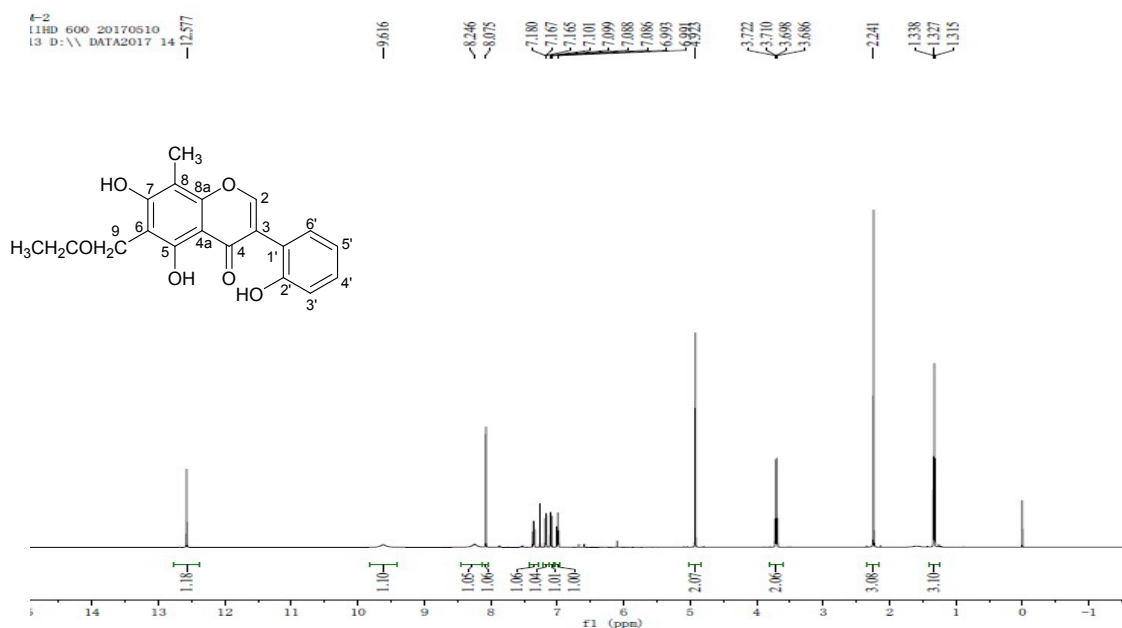


Figure S45. ¹³C NMR (150 MHz, CDCl₃) spectrum of **6**

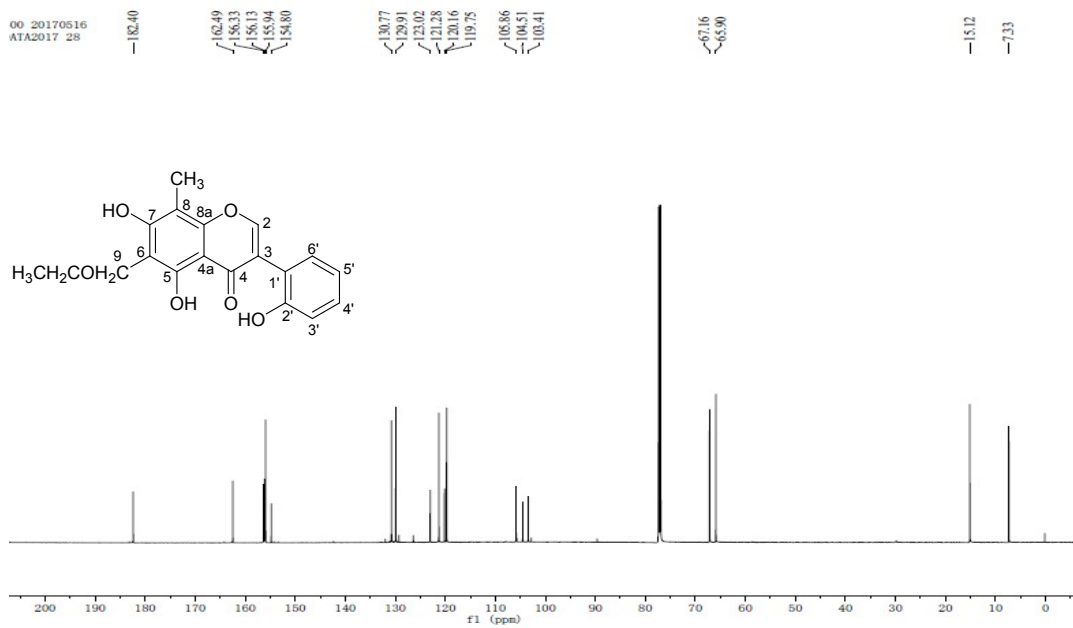


Figure S46. HSQC (600 MHz, CDCl₃) spectrum of **6**

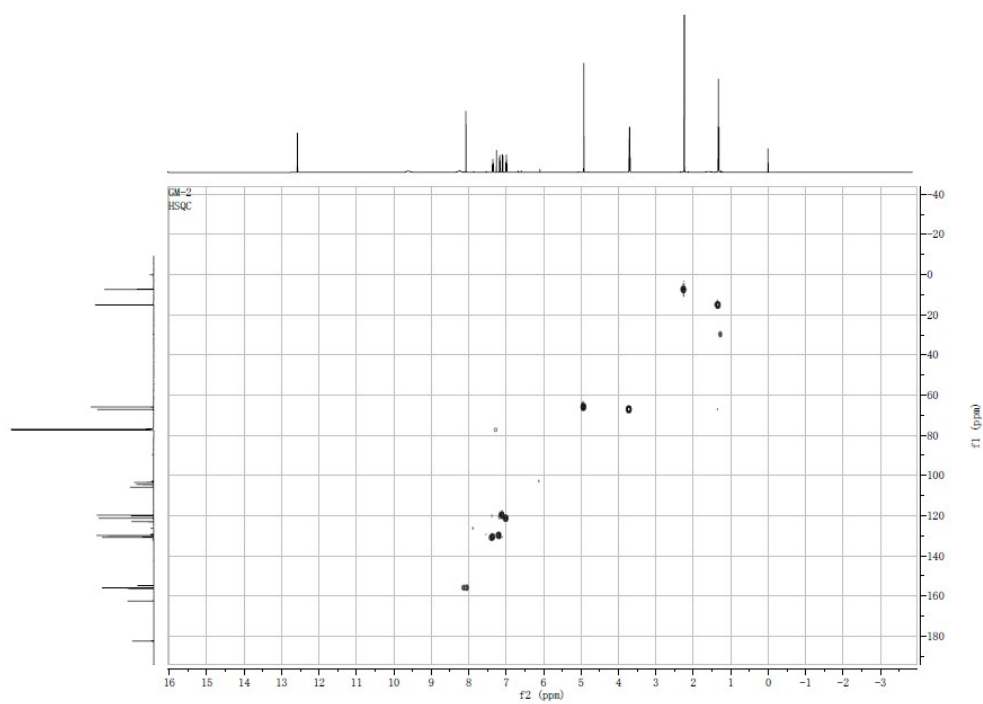


Figure S47. HMBC (600 MHz, CDCl₃) spectrum of **6**

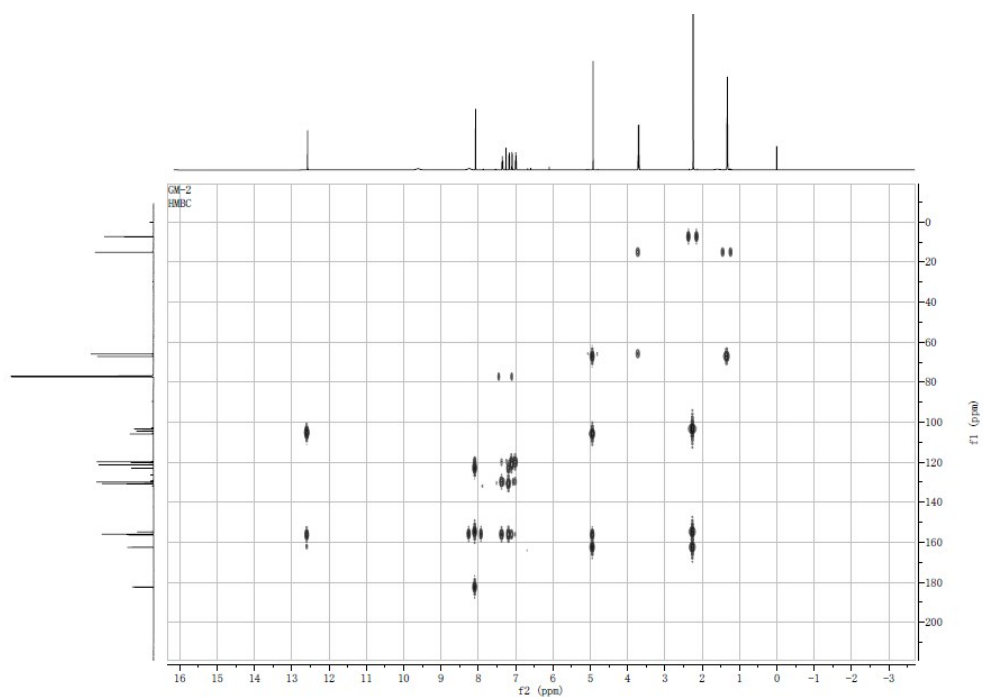


Figure S48. H-H COSY (600 MHz, CDCl₃) spectrum of **6**

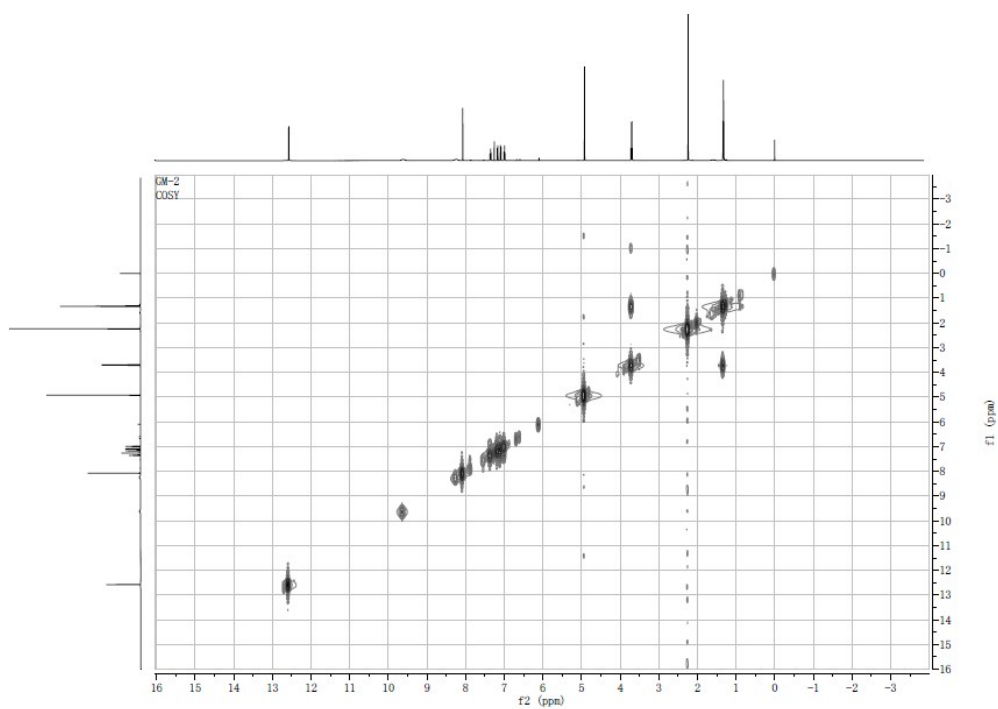


Figure S49. NOESY (600 MHz, CDCl₃) spectrum of **6**

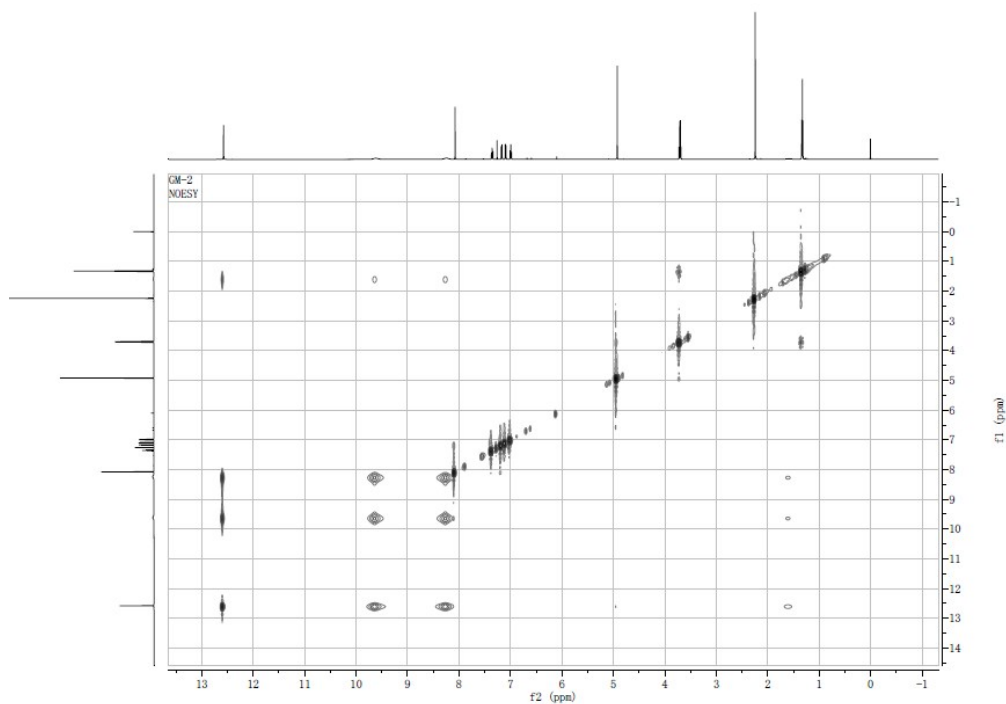
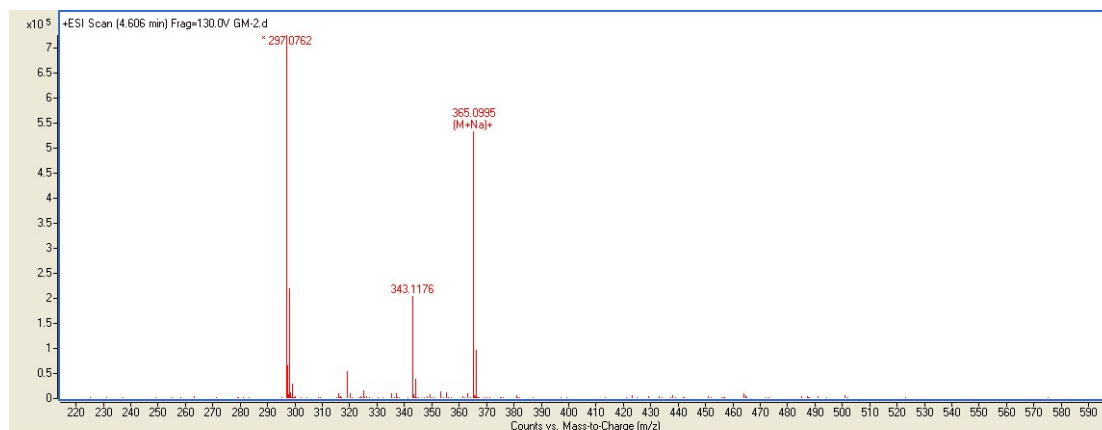


Figure S50. HRESIMS spectrum of **6**



| No. | Formula | Ion Formula | Measured m/z | Calc m/z | ppm |
|----------|-------------------|---------------------|--------------|----------|------|
| 6 | $C_{19}H_{18}O_6$ | $C_{19}H_{18}NaO_6$ | 365.0995 | 365.0996 | 0.27 |

Figure S51. ^1H NMR (600 MHz, CDCl_3) spectrum of **7**

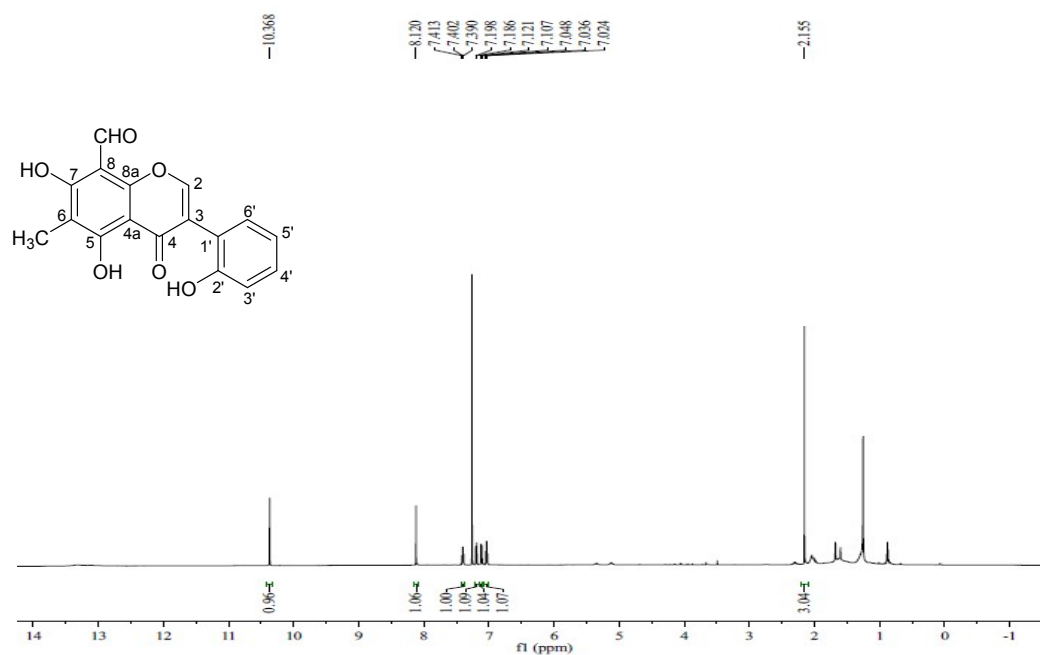


Figure S52. ^{13}C NMR (150 MHz, CDCl_3) spectrum of **7**

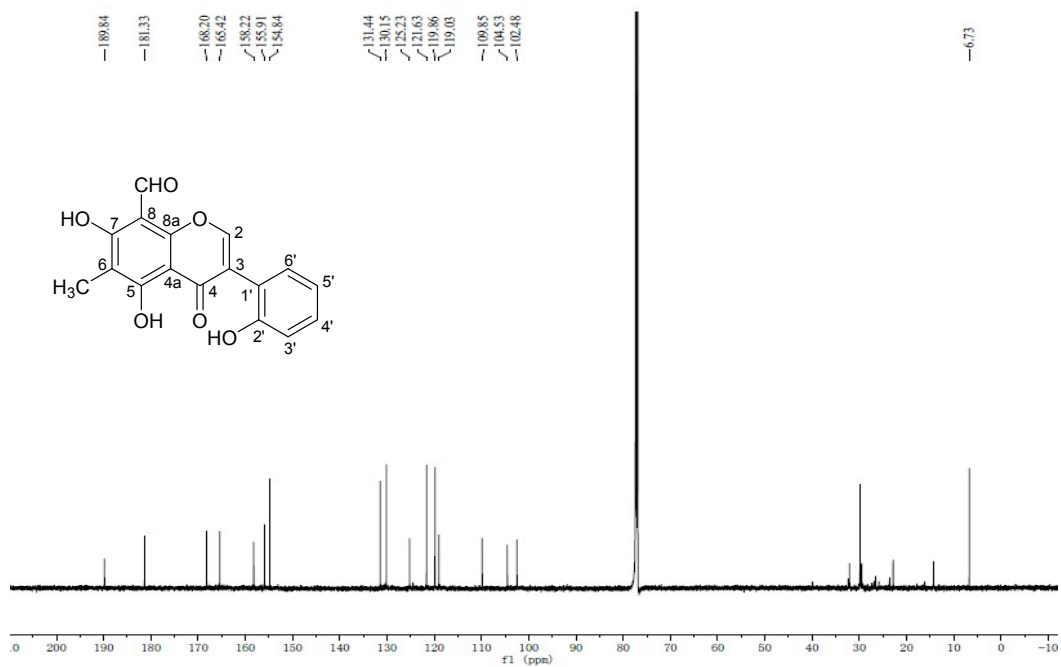


Figure S53. HSQC (600 MHz, CDCl₃) spectrum of **7**

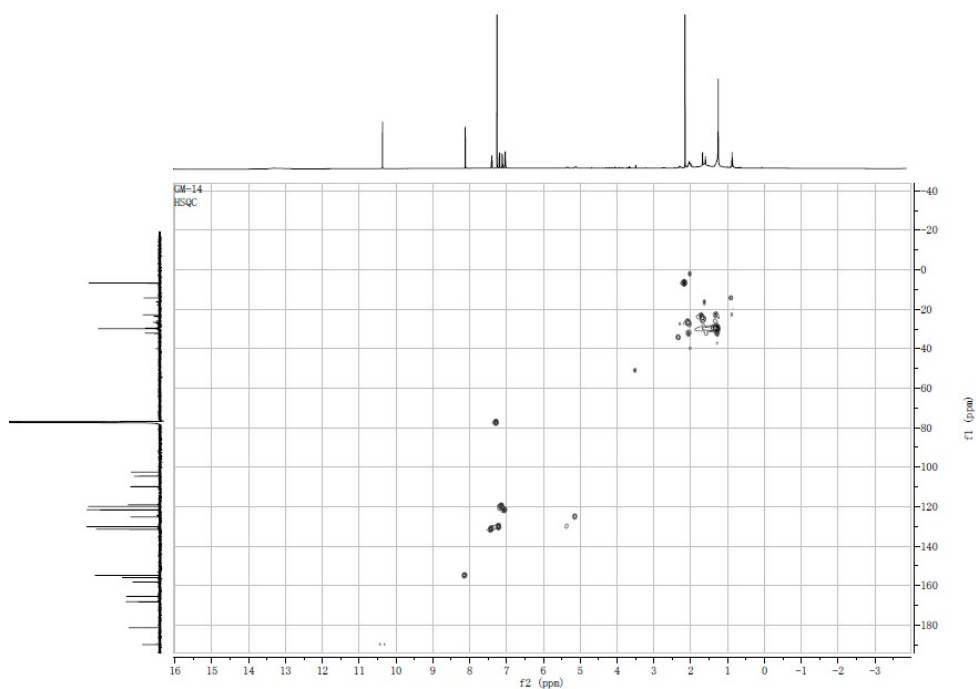


Figure S54. HMBC (600 MHz, CDCl₃) spectrum of **7**

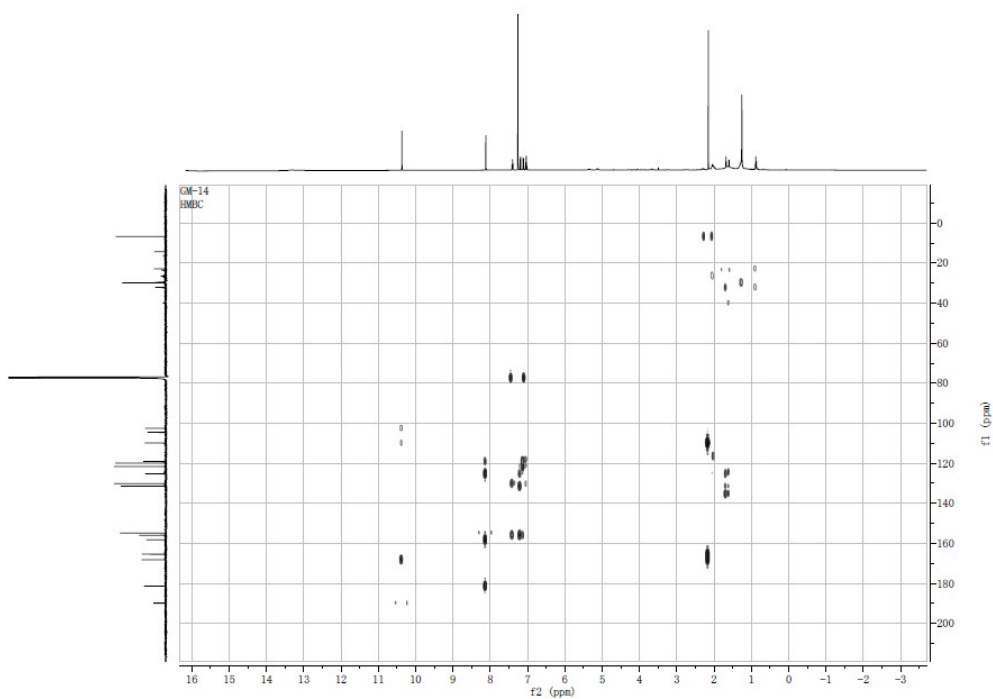


Figure S55. H-H COSY (600 MHz, CDCl₃) spectrum of **7**

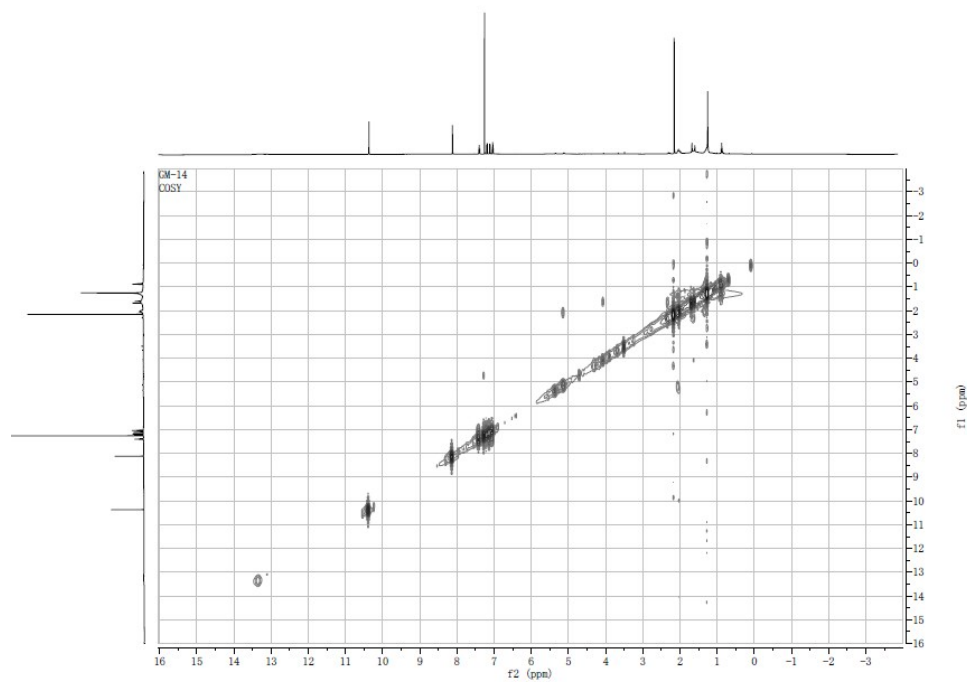


Figure S56. NOESY (600 MHz, CDCl₃) spectrum of **7**

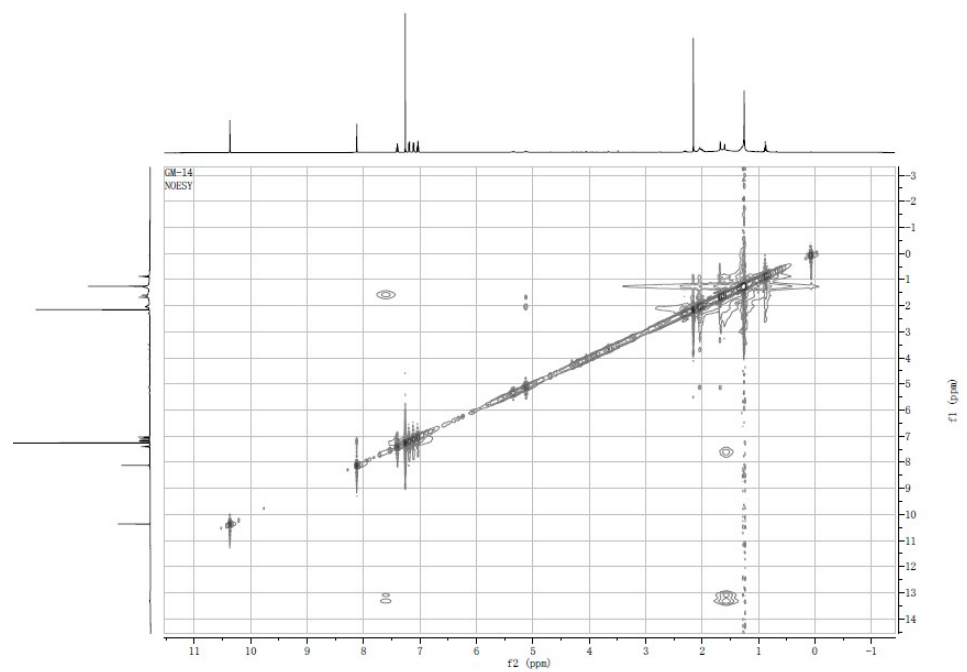
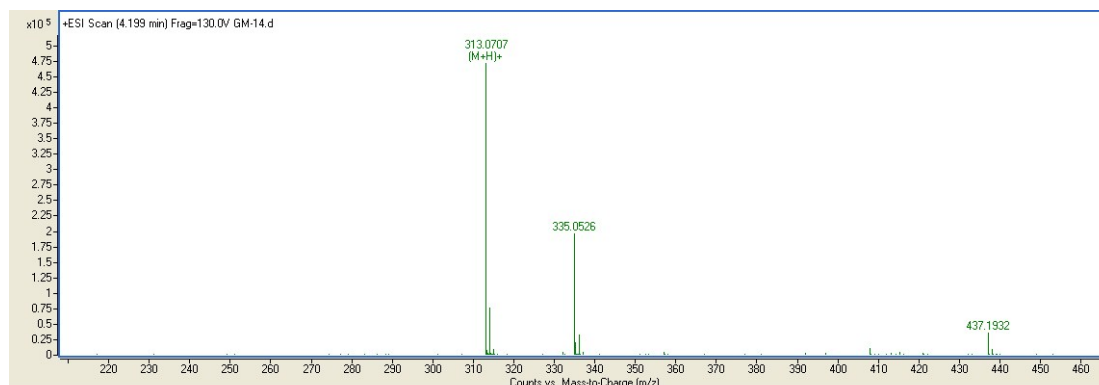


Figure S57. HRESIMS spectrum of **7**



| No. | Formula | Ion Formula | Measured m/z | Calc m/z | ppm |
|-----|--|--|--------------|----------|-----|
| 7 | C ₁₇ H ₁₂ O ₆ | C ₁₇ H ₁₃ O ₆ | 313.0707 | 313.0707 | 0 |

Figure S58. ¹H NMR (600 MHz, CDCl₃) spectrum of **8**

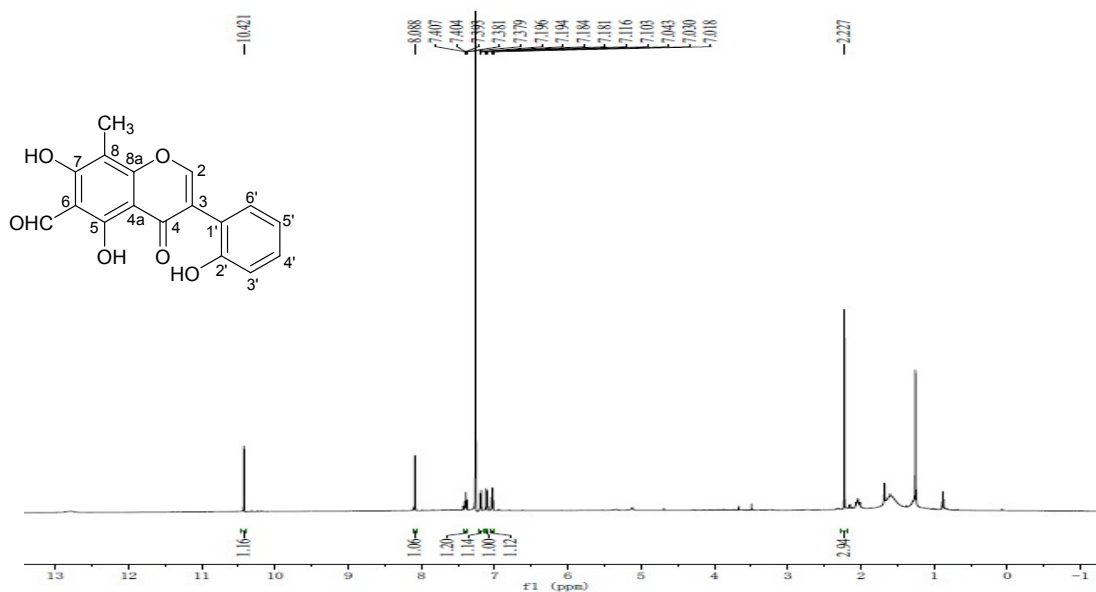


Figure S59. ^{13}C NMR (150 MHz, CDCl_3) spectrum of **8**

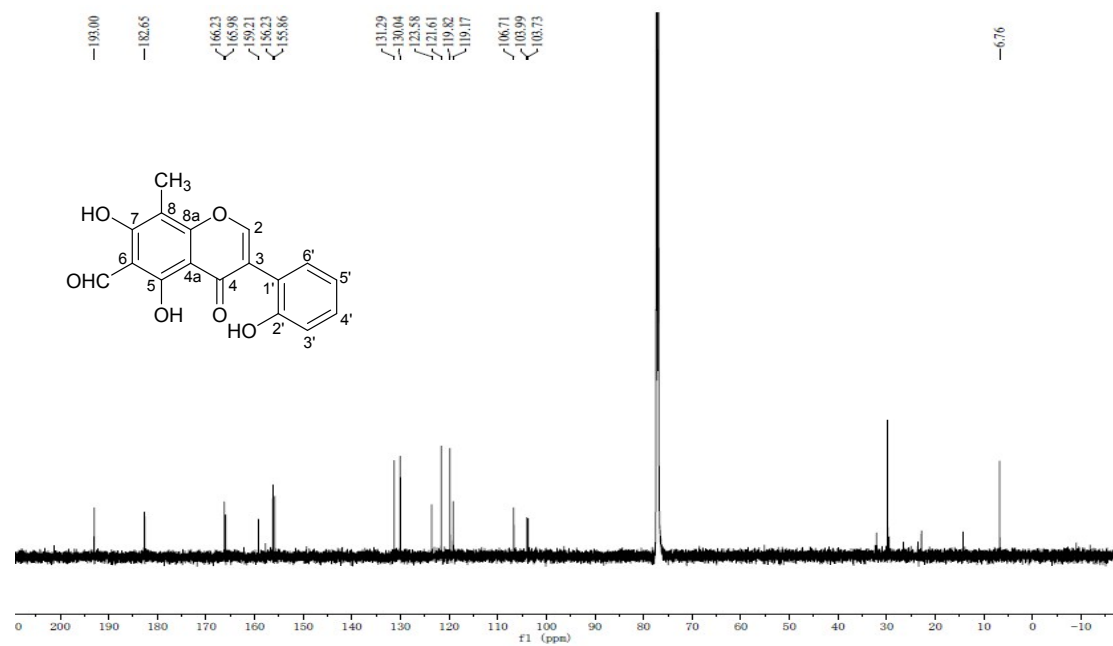


Figure S60. HSQC (600 MHz, CDCl_3) spectrum of **8**

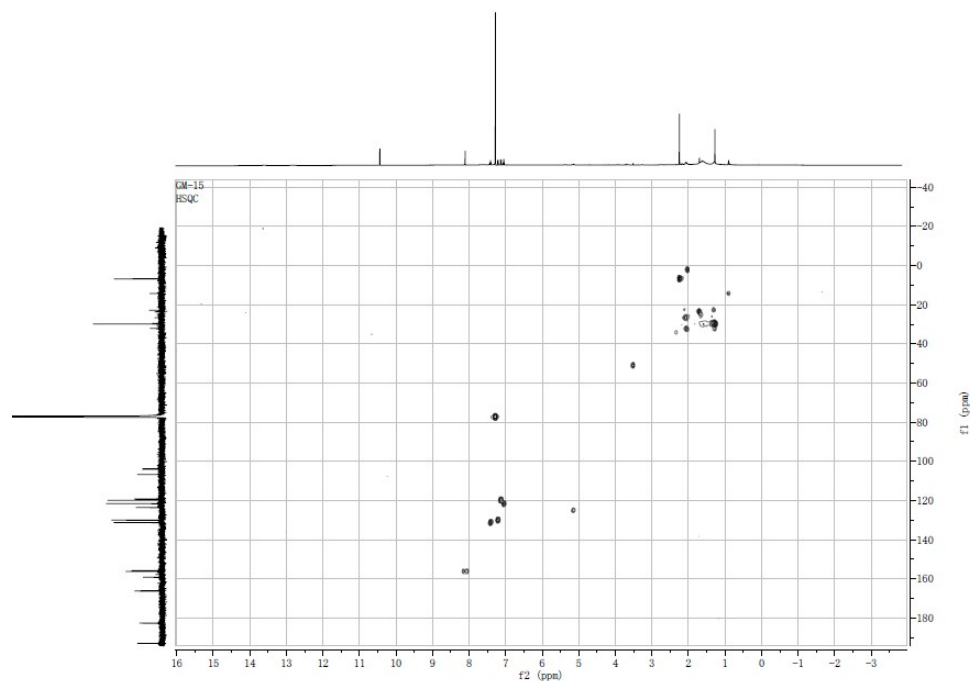


Figure S61. HMBC (600 MHz, CDCl₃) spectrum of **8**

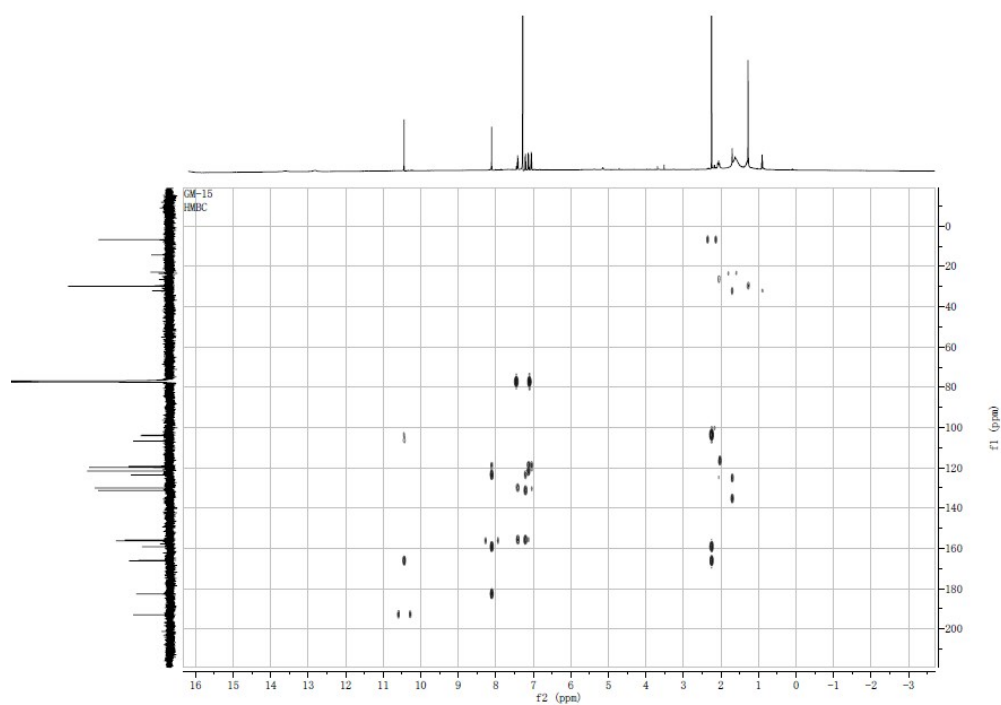


Figure S62. H-H COSY (600 MHz, CDCl₃) spectrum of **8**

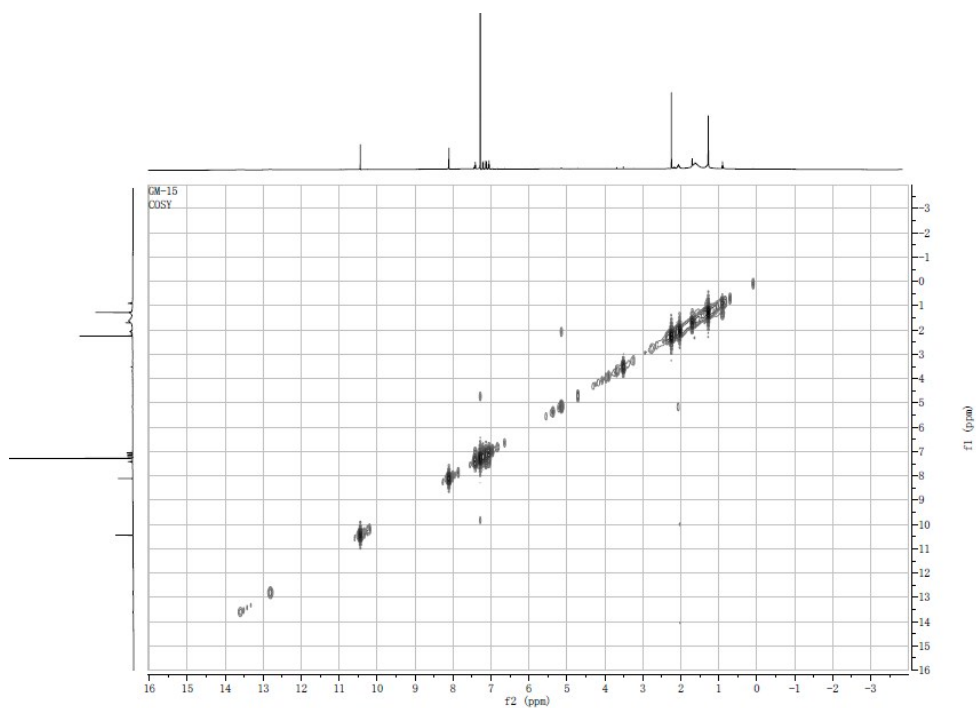


Figure S63. NOESY (600 MHz, CDCl₃) spectrum of **8**

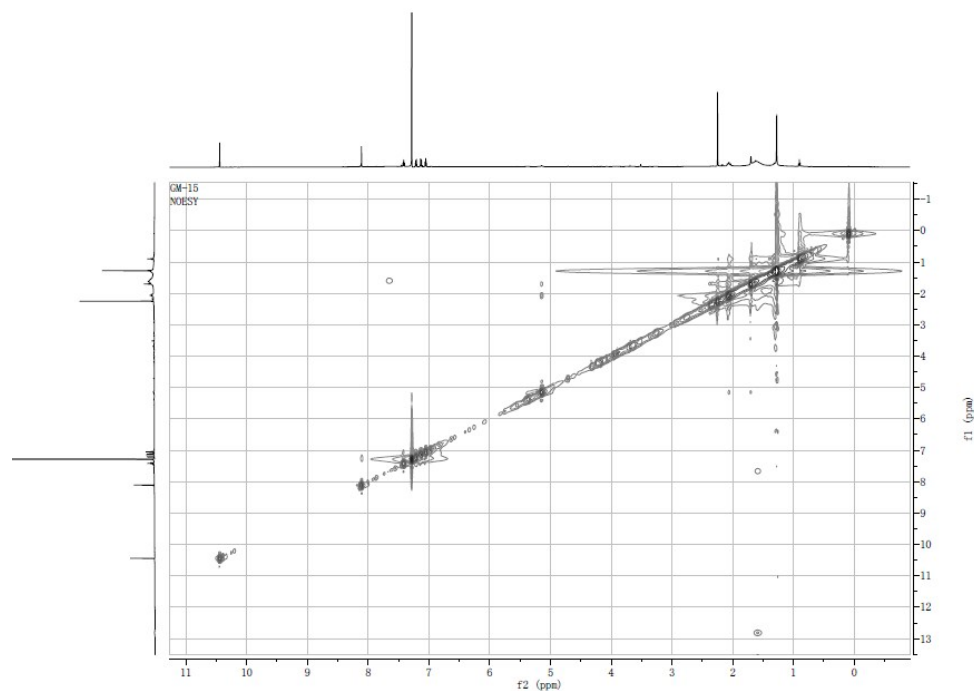
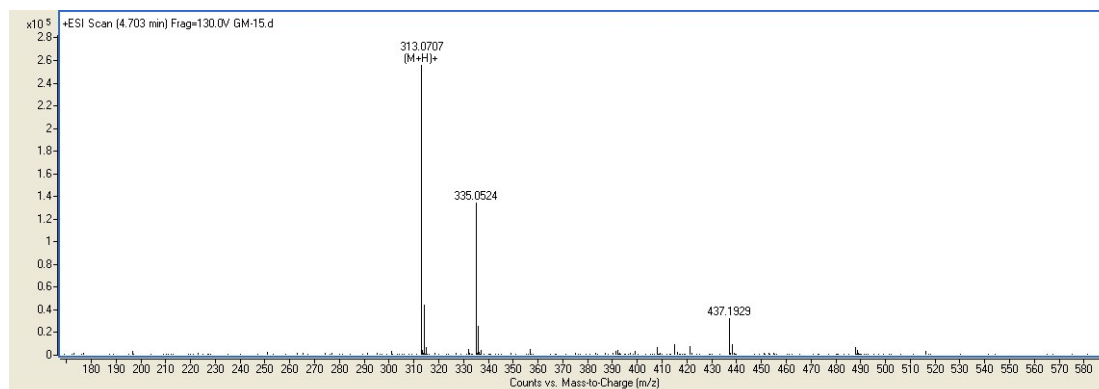


Figure S64. HRESIMS spectrum of **8**



| No. | Formula | Ion Formula | Measured m/z | Calc m/z | ppm |
|----------|--|--|--------------|----------|-----|
| 8 | C ₁₇ H ₁₂ O ₆ | C ₁₇ H ₁₃ O ₆ | 313.0707 | 313.0707 | 0 |

Figure S65. ^1H NMR (600 MHz, CDCl_3) spectrum of **9**

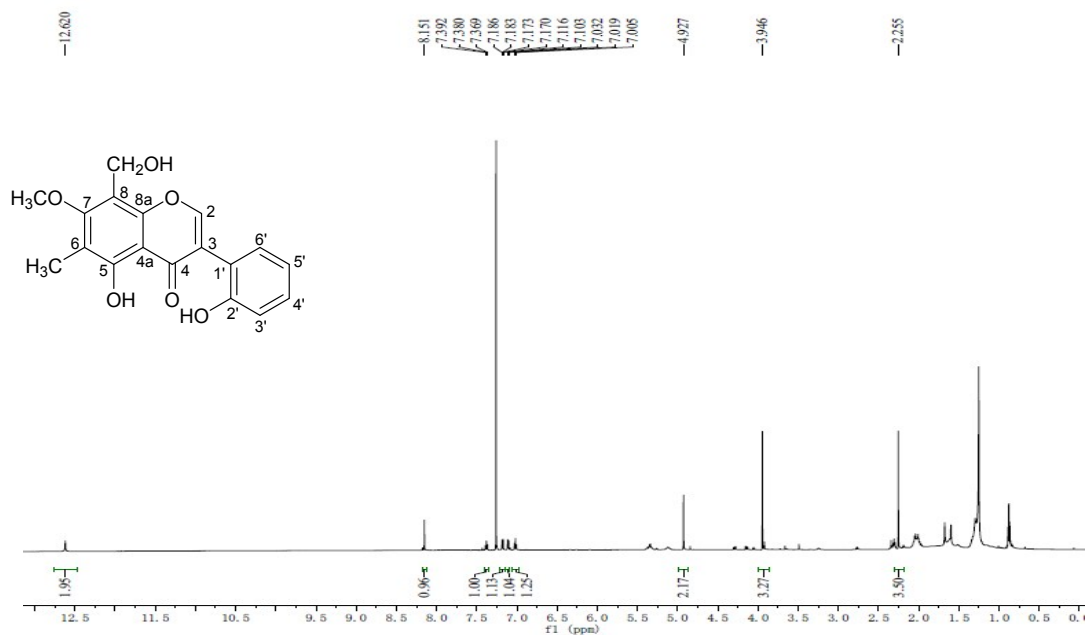


Figure S66. ^{13}C NMR (150 MHz, CDCl_3) spectrum of **9**

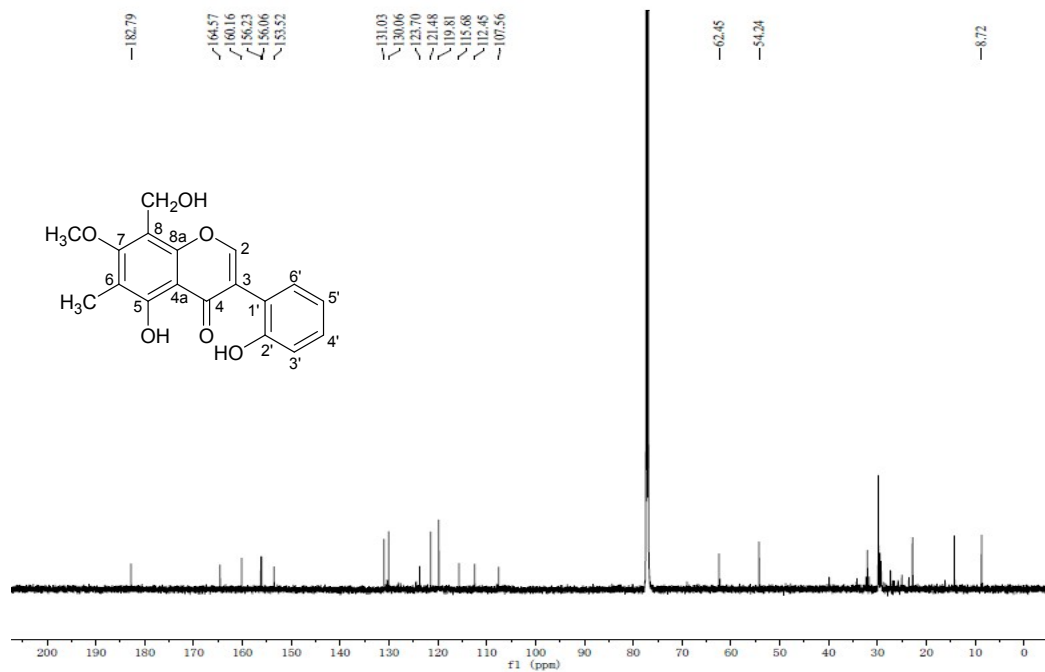


Figure S67. HSQC (600 MHz, CDCl₃) spectrum of **9**

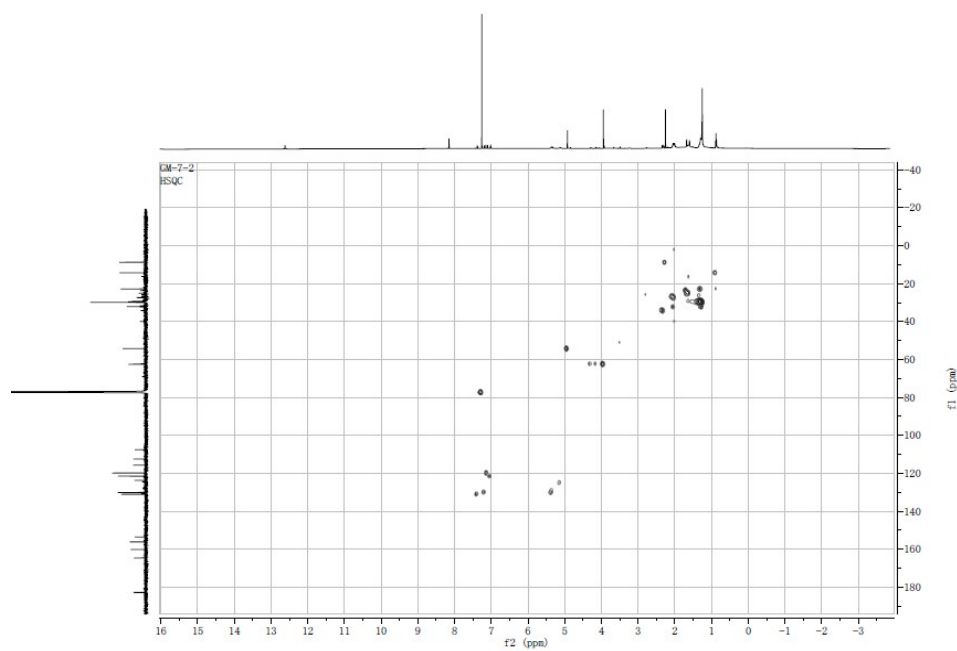


Figure S68. HMBC (600 MHz, CDCl₃) spectrum of **9**

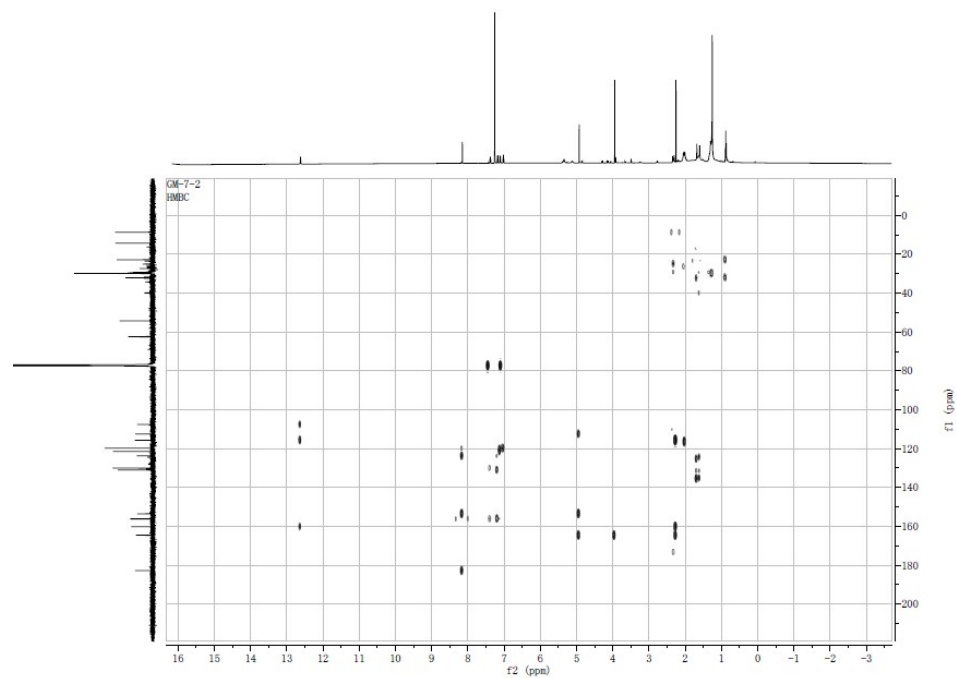


Figure S69. H-H COSY (600 MHz, CDCl₃) spectrum of **9**

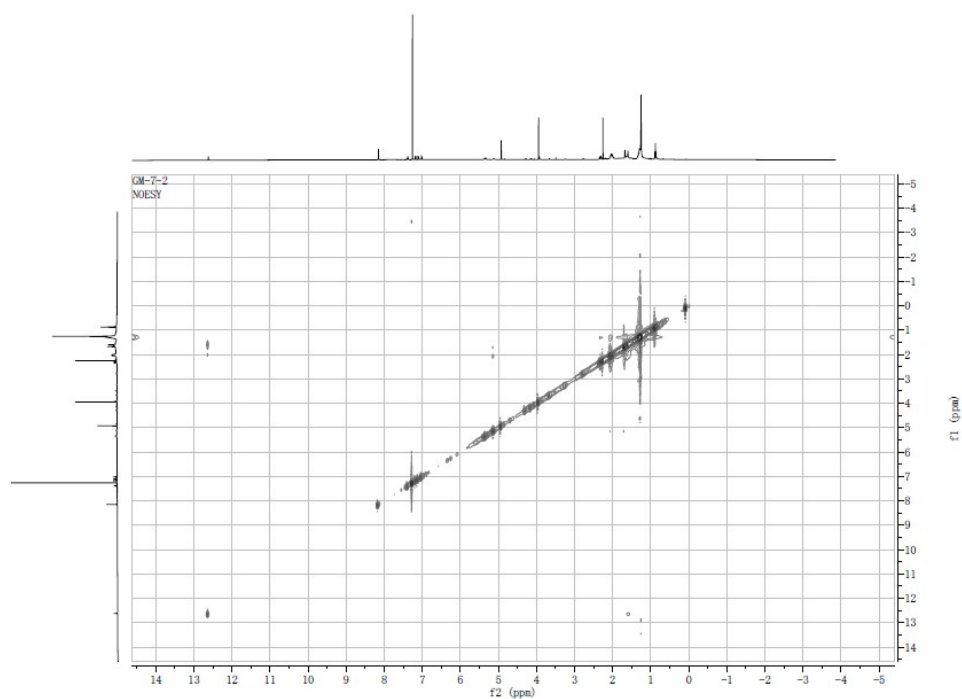


Figure S70. NOESY (600 MHz, CDCl₃) spectrum of **9**

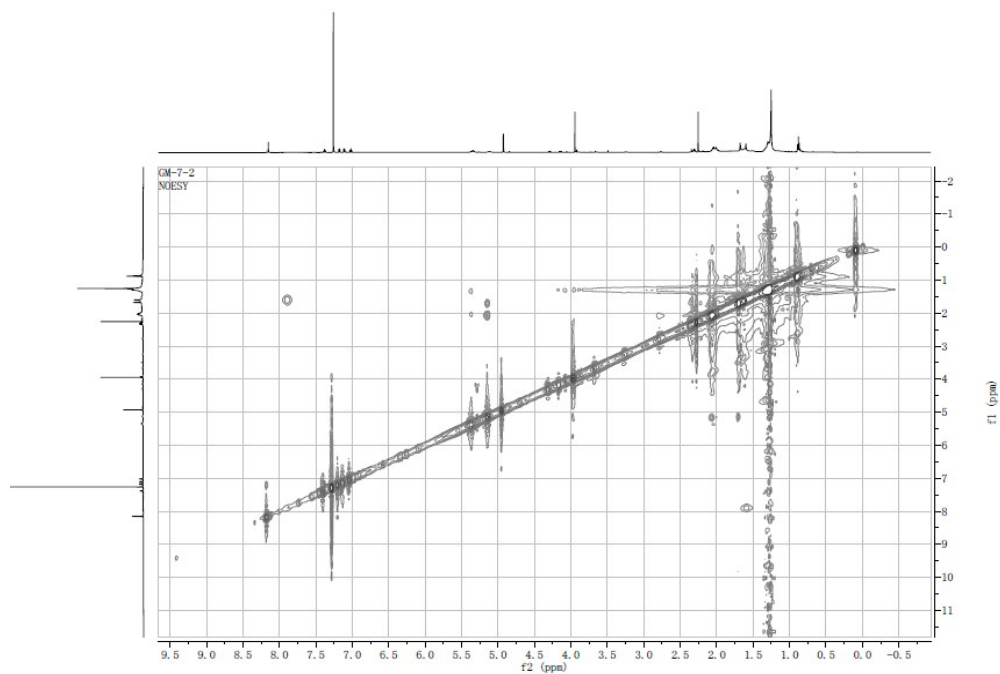
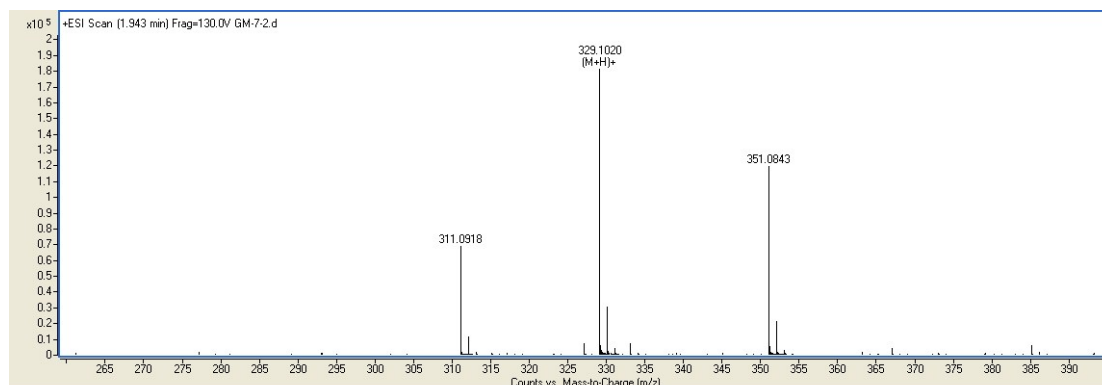


Figure S71. HRESIMS spectrum of **9**



| No. | Formula | Ion Formula | Measured m/z | Calc m/z | ppm |
|----------|--|--|--------------|----------|-----|
| 9 | C ₁₈ H ₁₆ O ₆ | C ₁₈ H ₁₇ O ₆ | 329.1020 | 329.1020 | 0 |

Figure S72. ¹H NMR (600 MHz, CDCl₃) spectrum of **10**

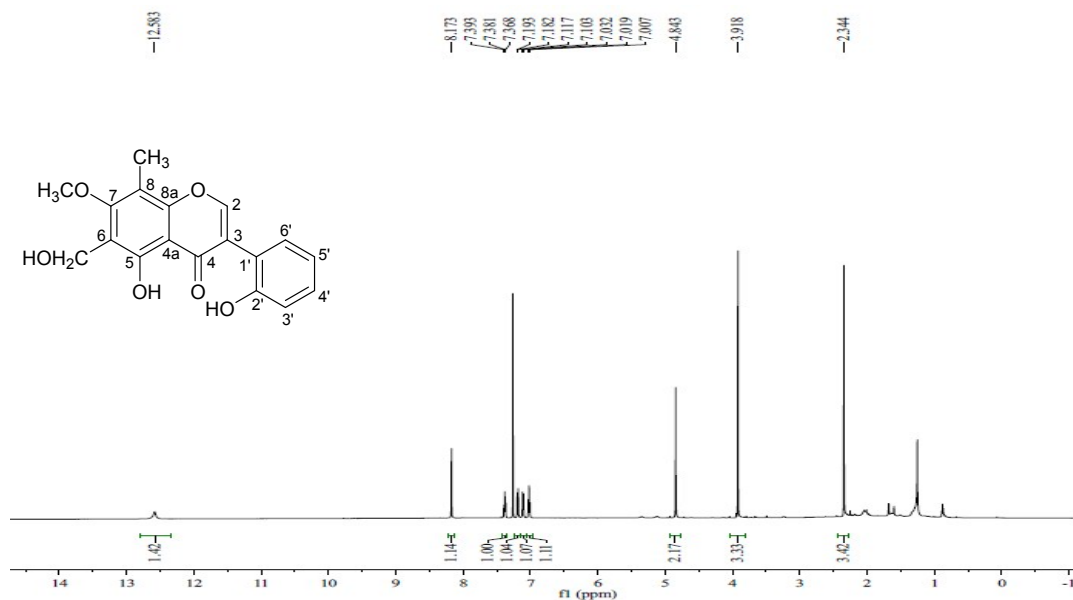


Figure S73. ^{13}C NMR (150 MHz, CDCl_3) spectrum of **10**

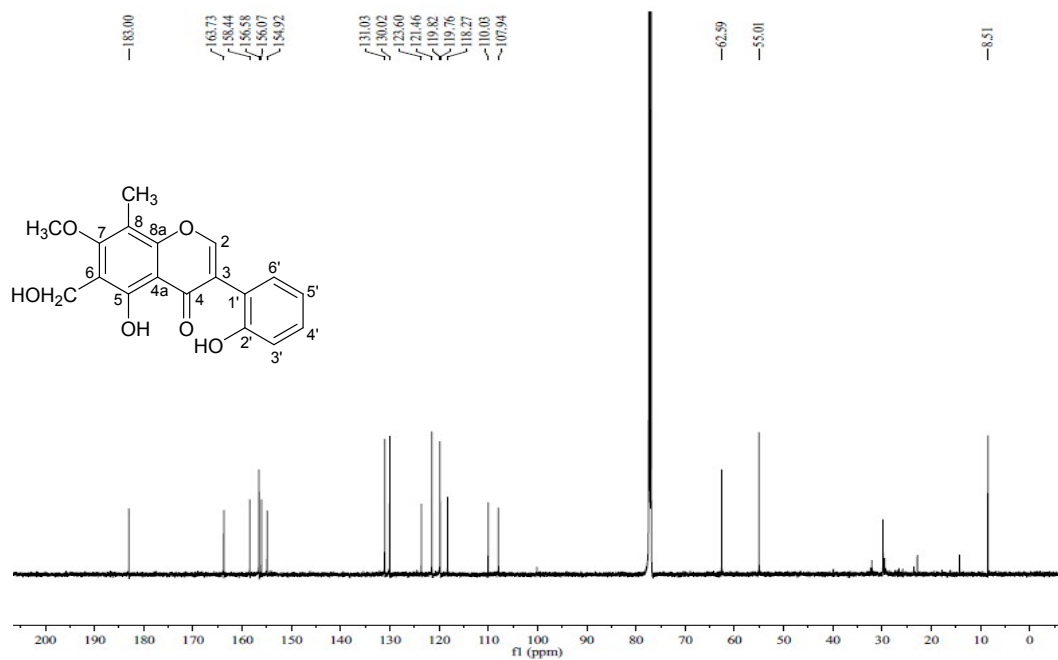


Figure S74. HSQC (600 MHz, CDCl_3) spectrum of **10**

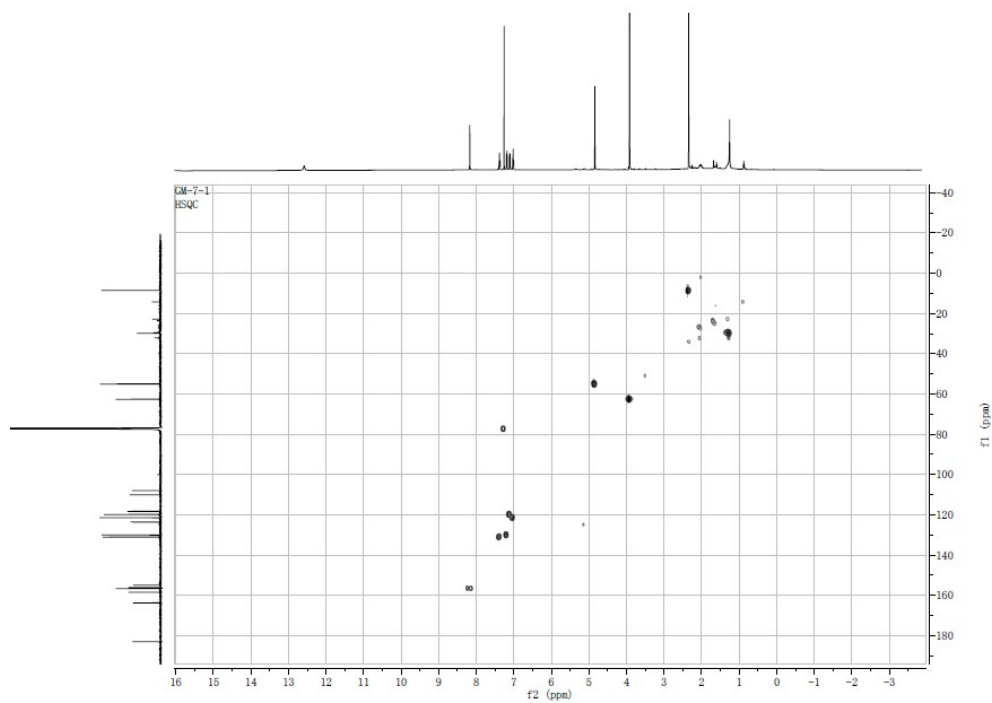


Figure S75. HMBC (600 MHz, CDCl₃) spectrum of **10**

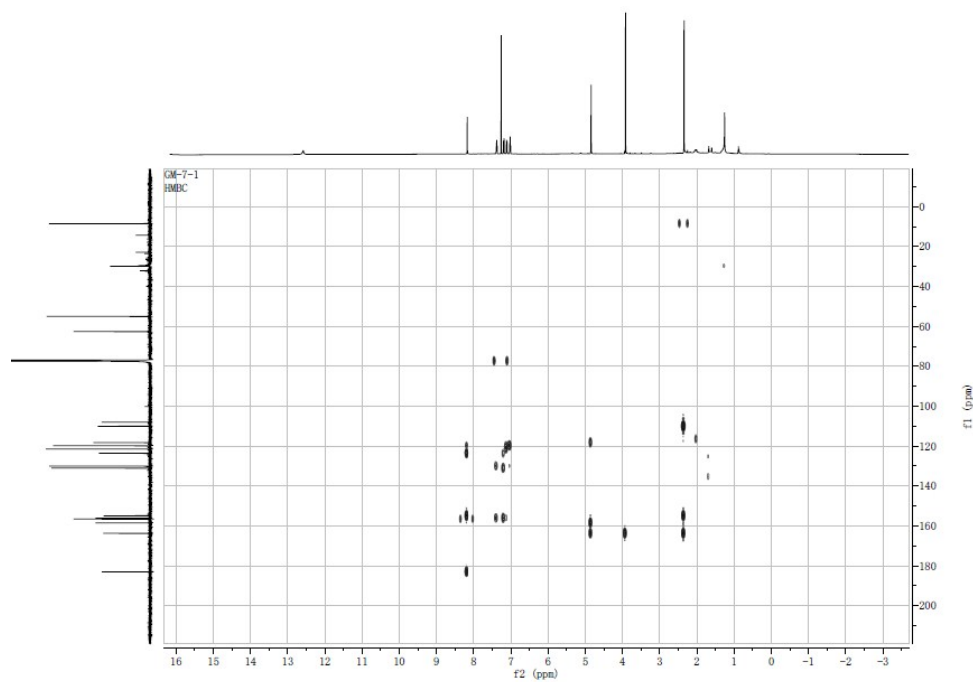


Figure S76. H-H COSY (600 MHz, CDCl₃) spectrum of **10**

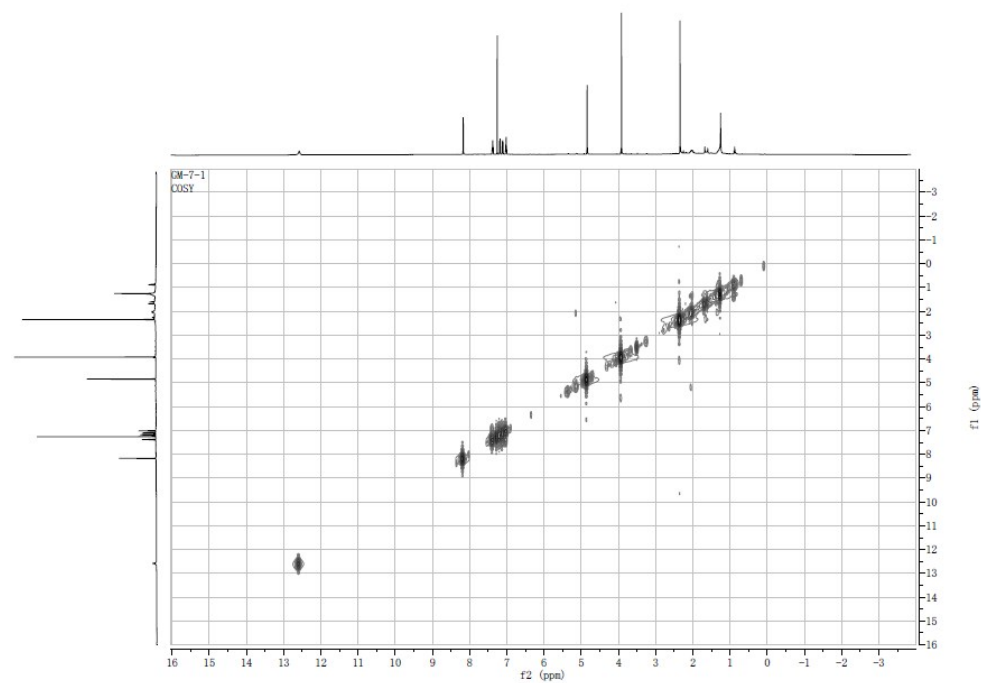


Figure S77. NOESY (600 MHz, CDCl₃) spectrum of **10**

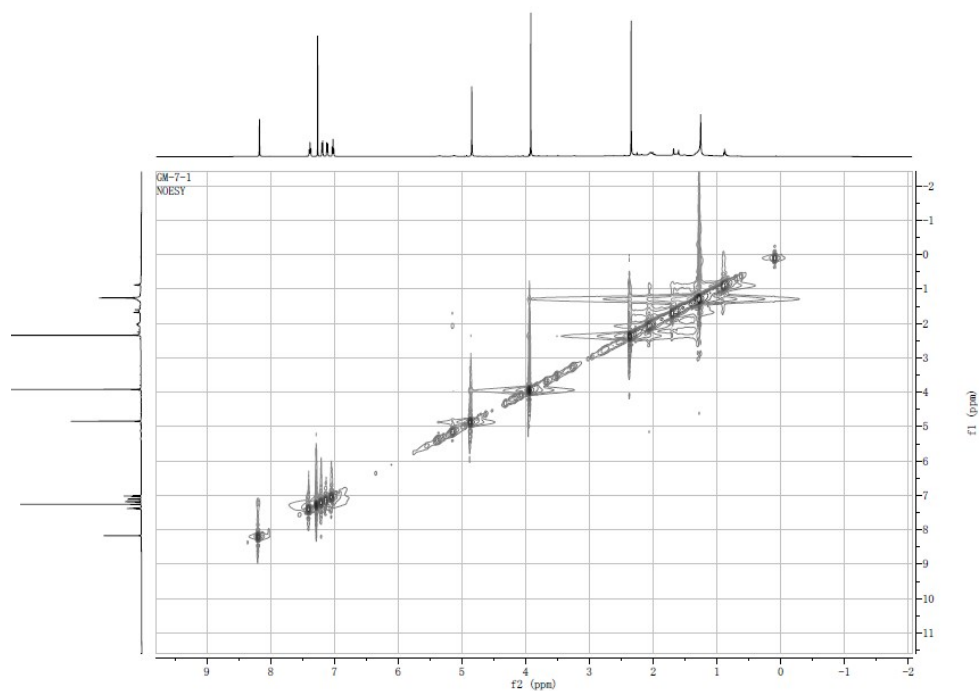
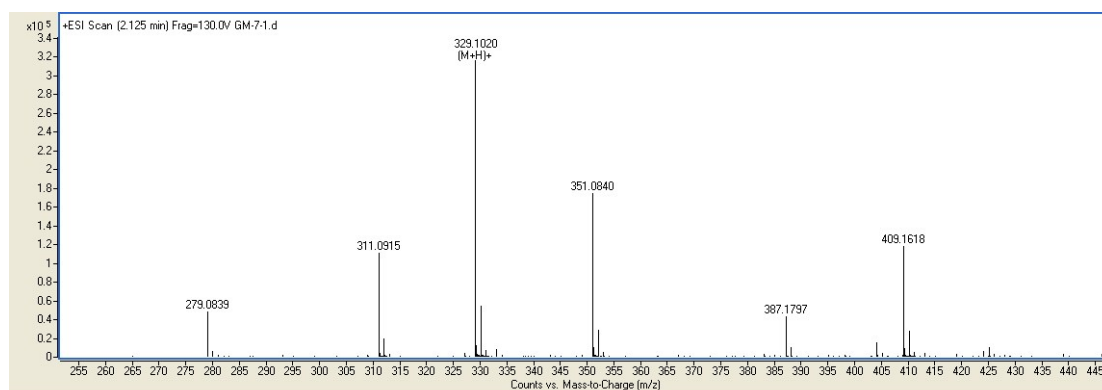


Figure S78. HRESIMS spectrum of **10**



| No. | Formula | Ion Formula | Measured m/z | Calc m/z | ppm |
|-----------|-------------------|-------------------|--------------|----------|-----|
| 10 | $C_{18}H_{16}O_6$ | $C_{18}H_{17}O_6$ | 329.1020 | 329.1020 | 0 |