Electronic Supplementary Material (ESI) for RSC Advances.

Sesquiterpenoids and Monoterpenoid Coumarins from *Parasenecio rubescens*

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Figure S1. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of pararunine A (**1**)

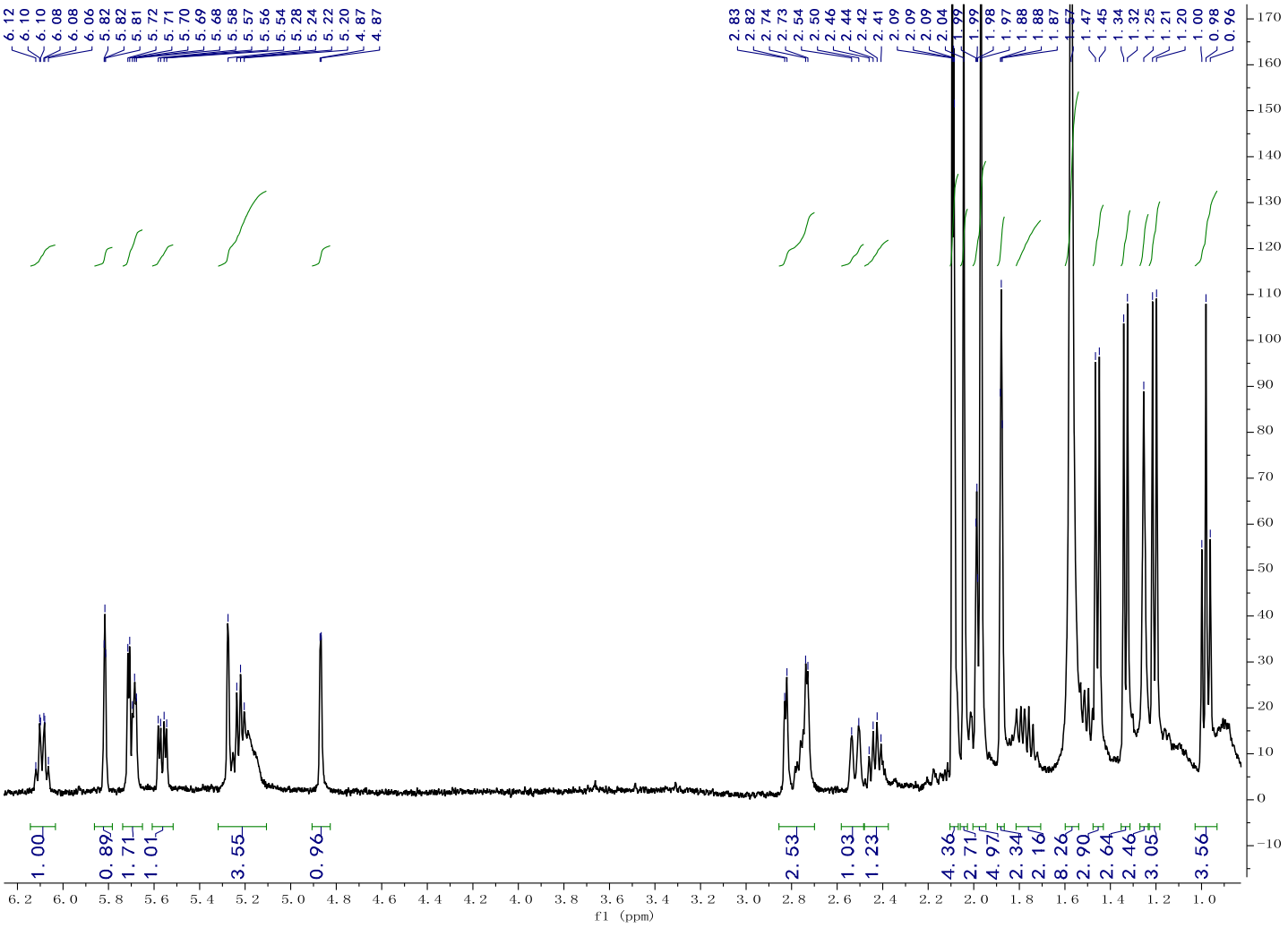


Figure S2. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of pararunine A (**1**)

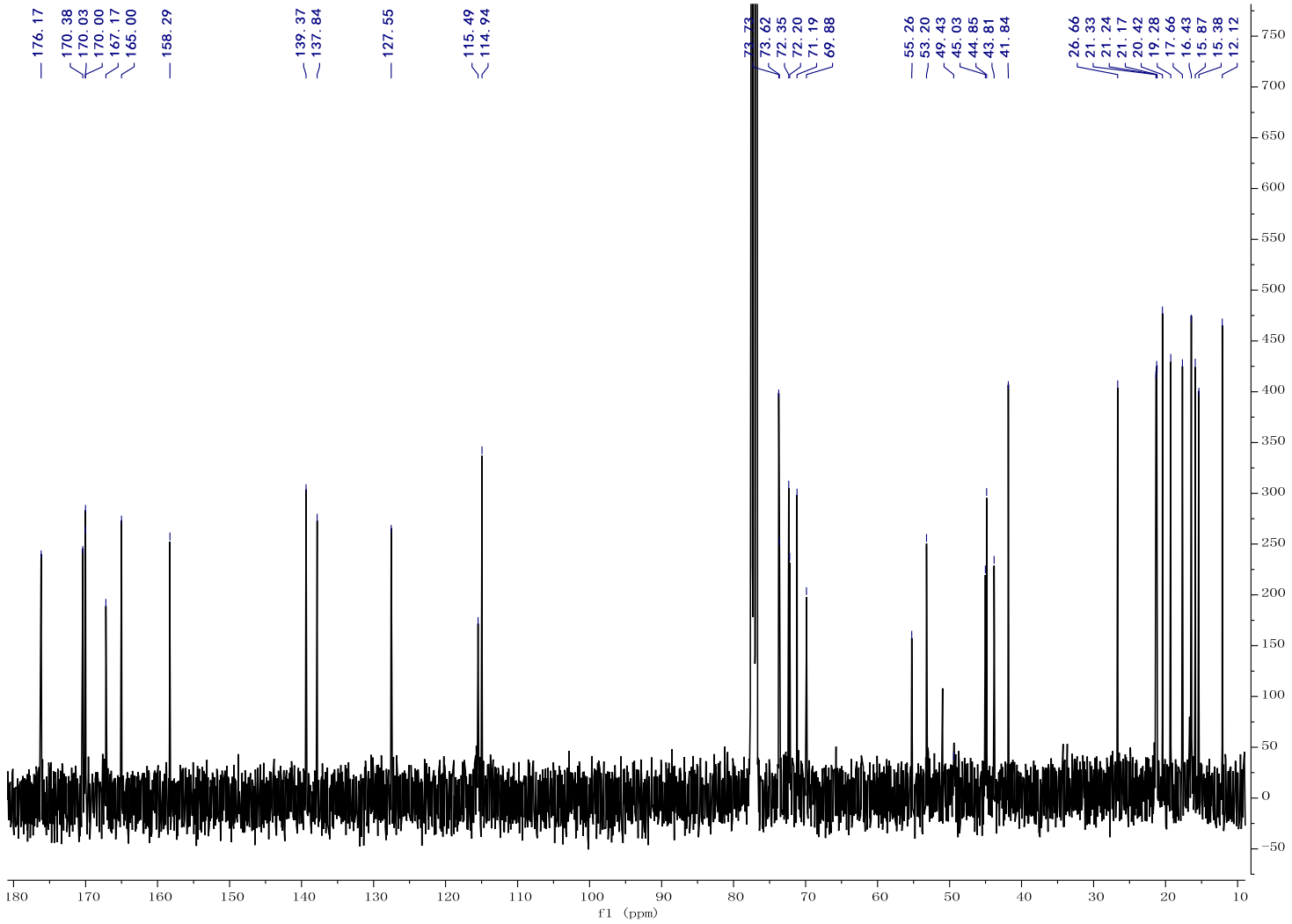


Figure S3. HSQC (400 MHz, $CDCl_3$) spectrum of pararunine A (**1**)

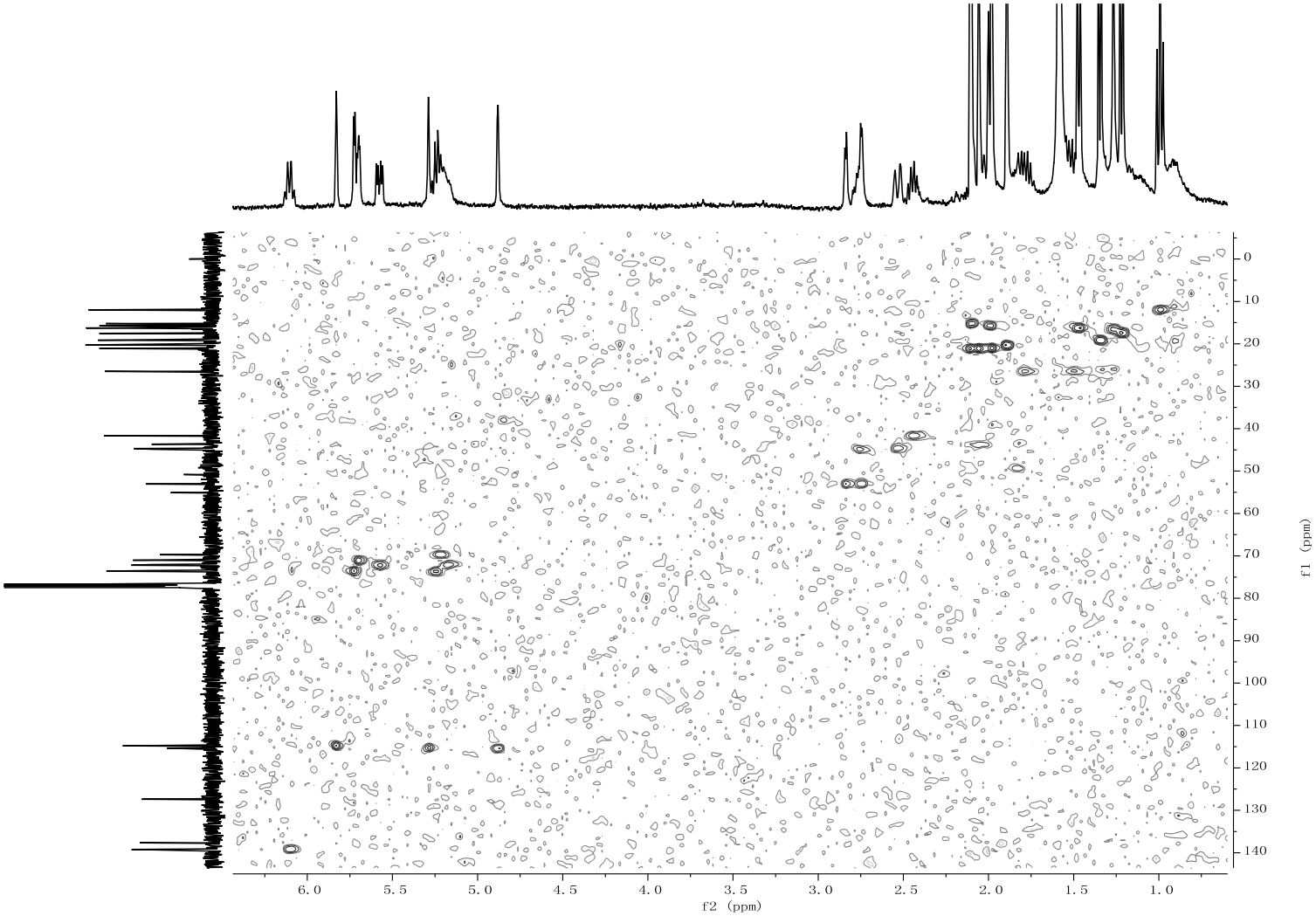


Figure S4. ^{1}H-^{1}H COSY (400 MHz, $CDCl_3$) spectrum of pararunine A (**1**)

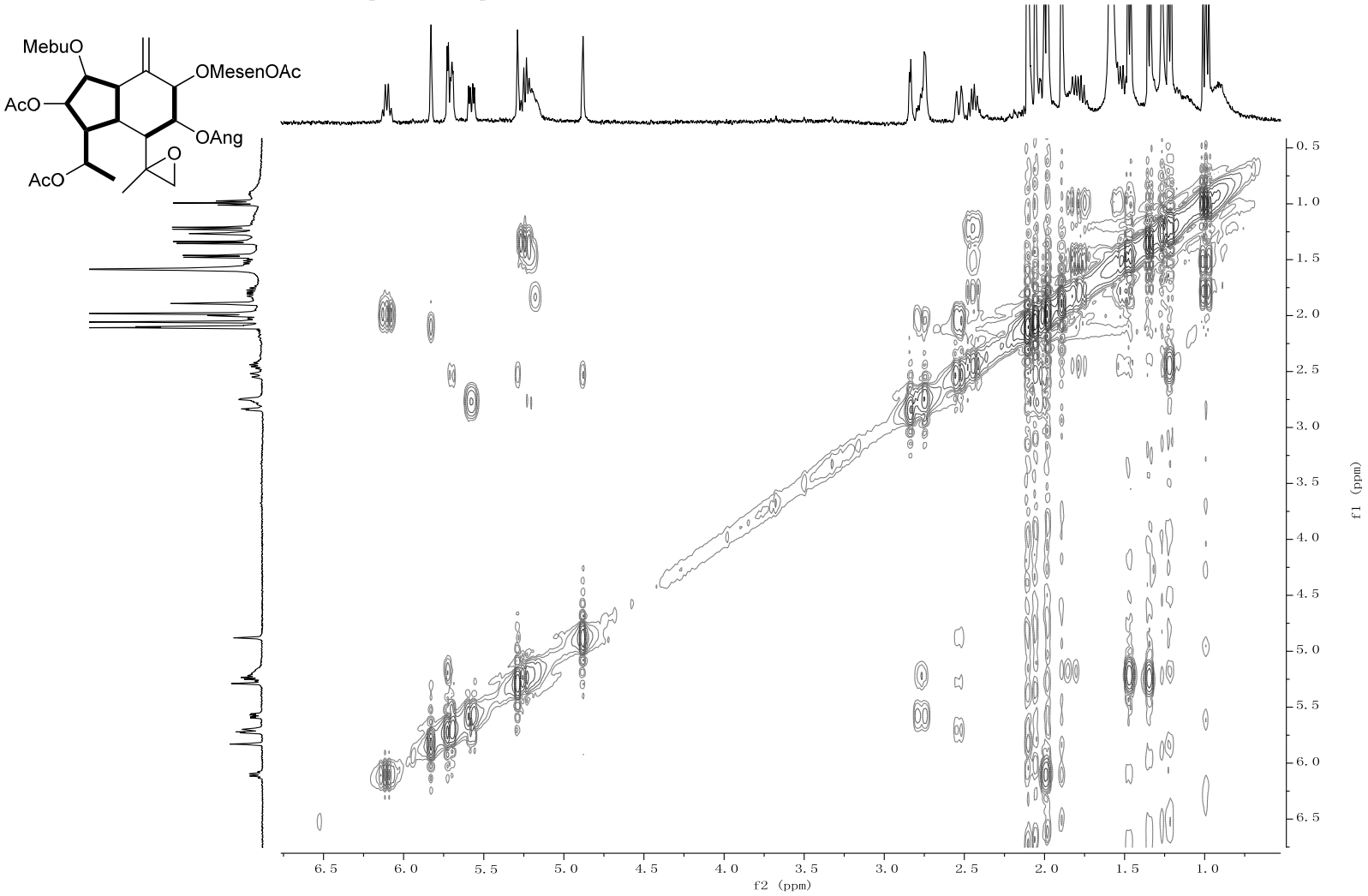


Figure S5. HMBC (400 MHz, $CDCl_3$) spectrum of pararunine A (**1**)

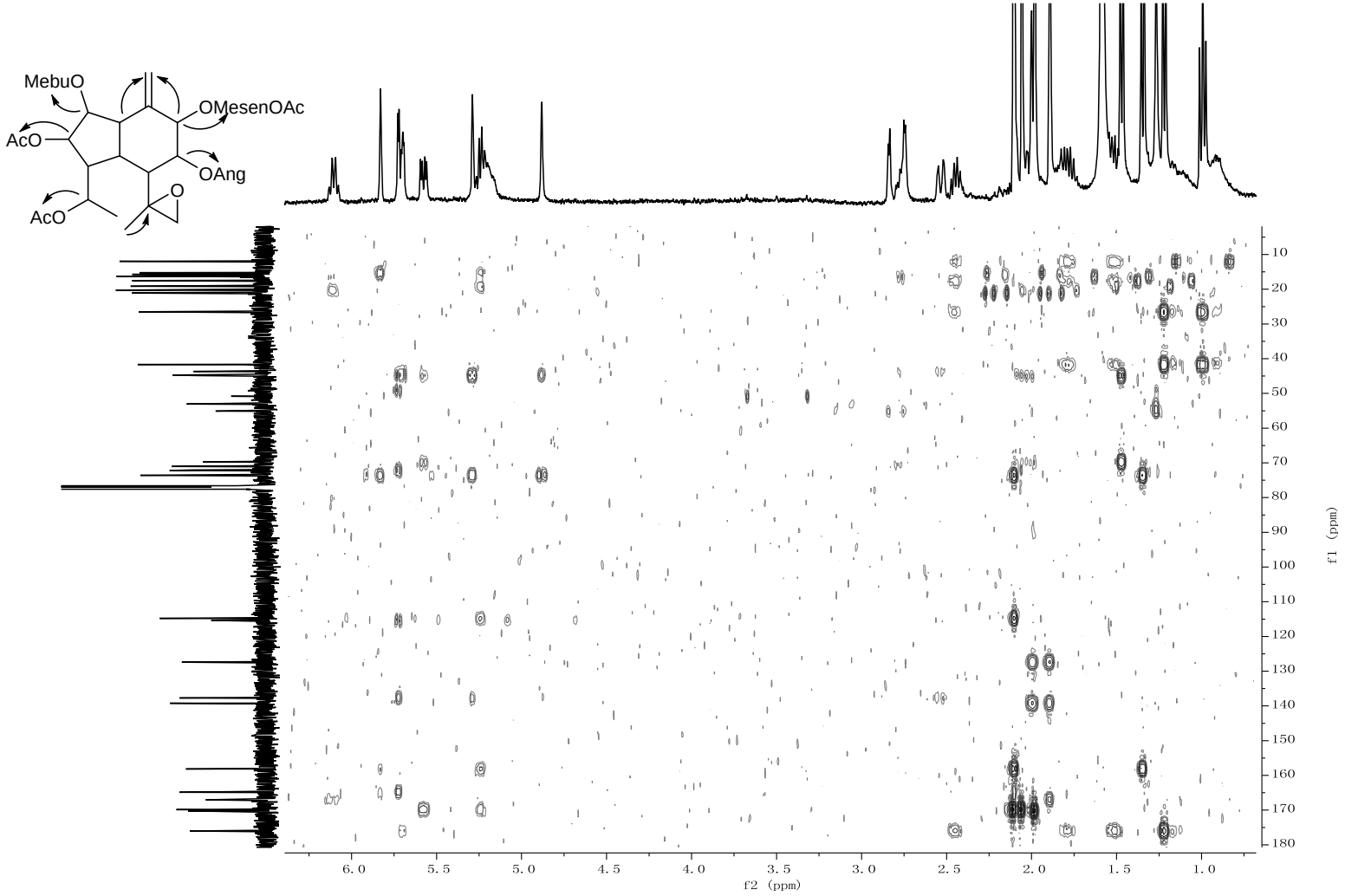


Figure S6. NOESY (400 MHz, $CDCl_3$) spectrum of pararunine A (**1**)

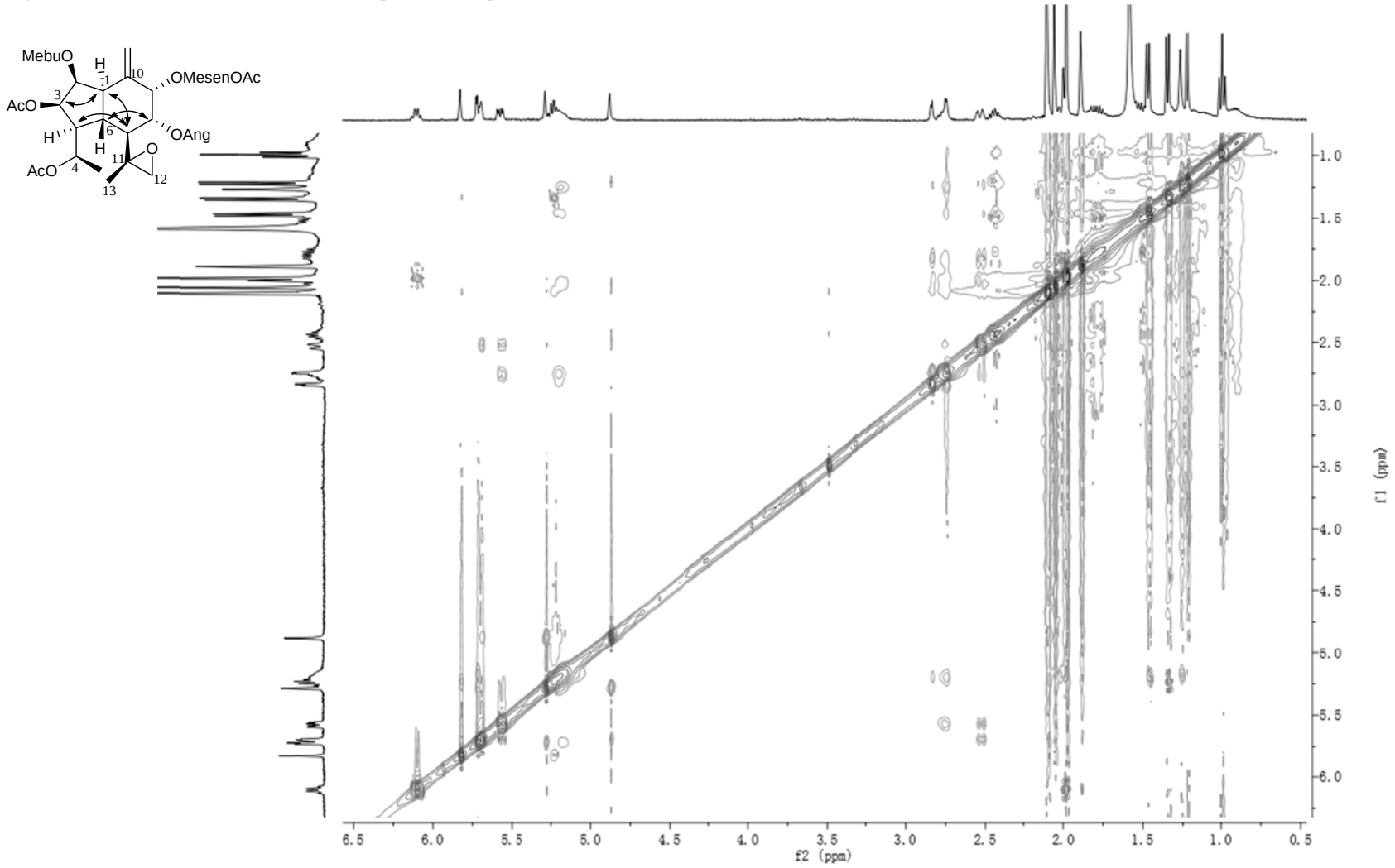


Figure S7. HRESIMS spectrum of pararunine A (**1**)

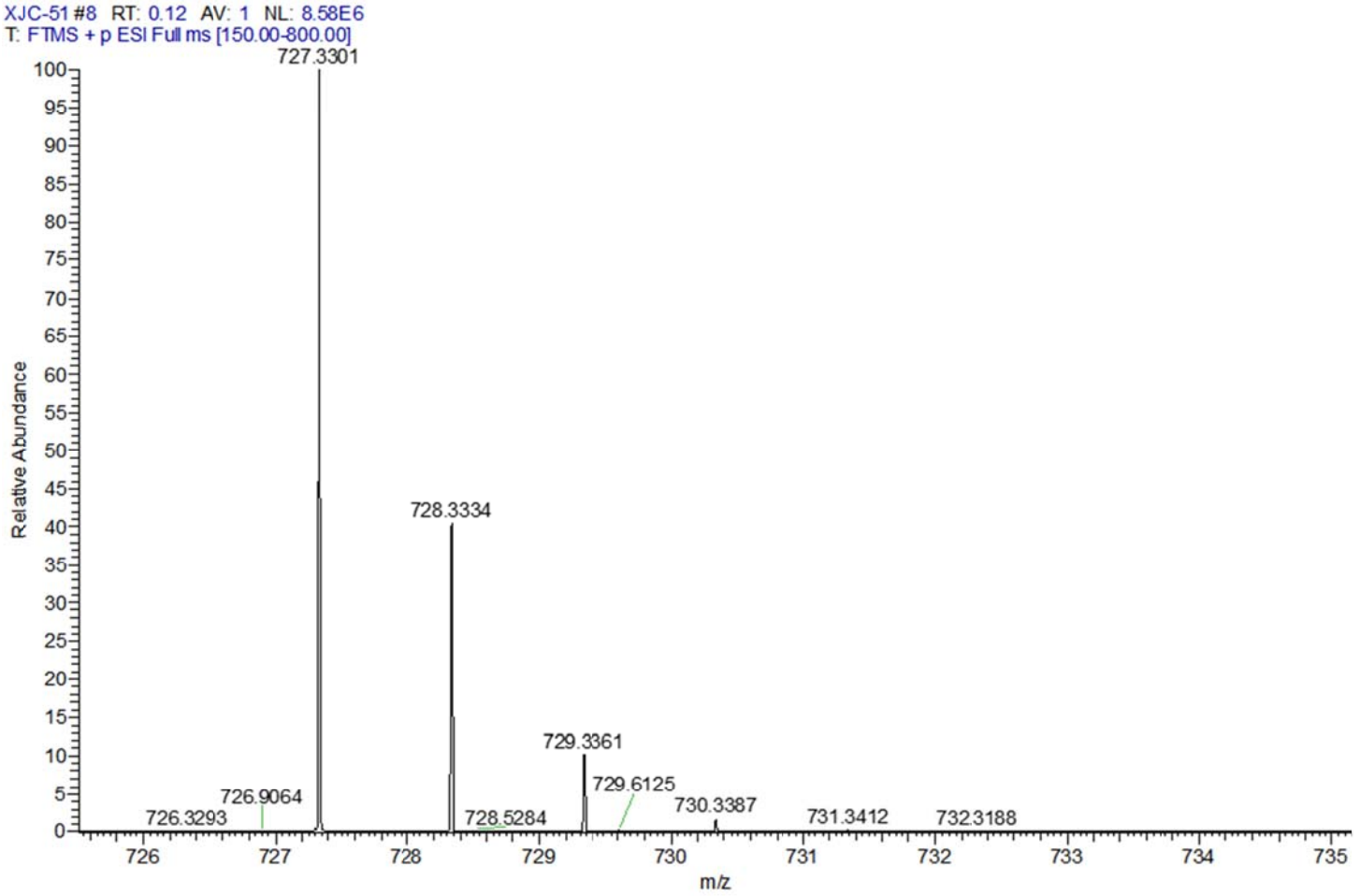


Figure S8. IR spectrum of pararunine A (**1**)

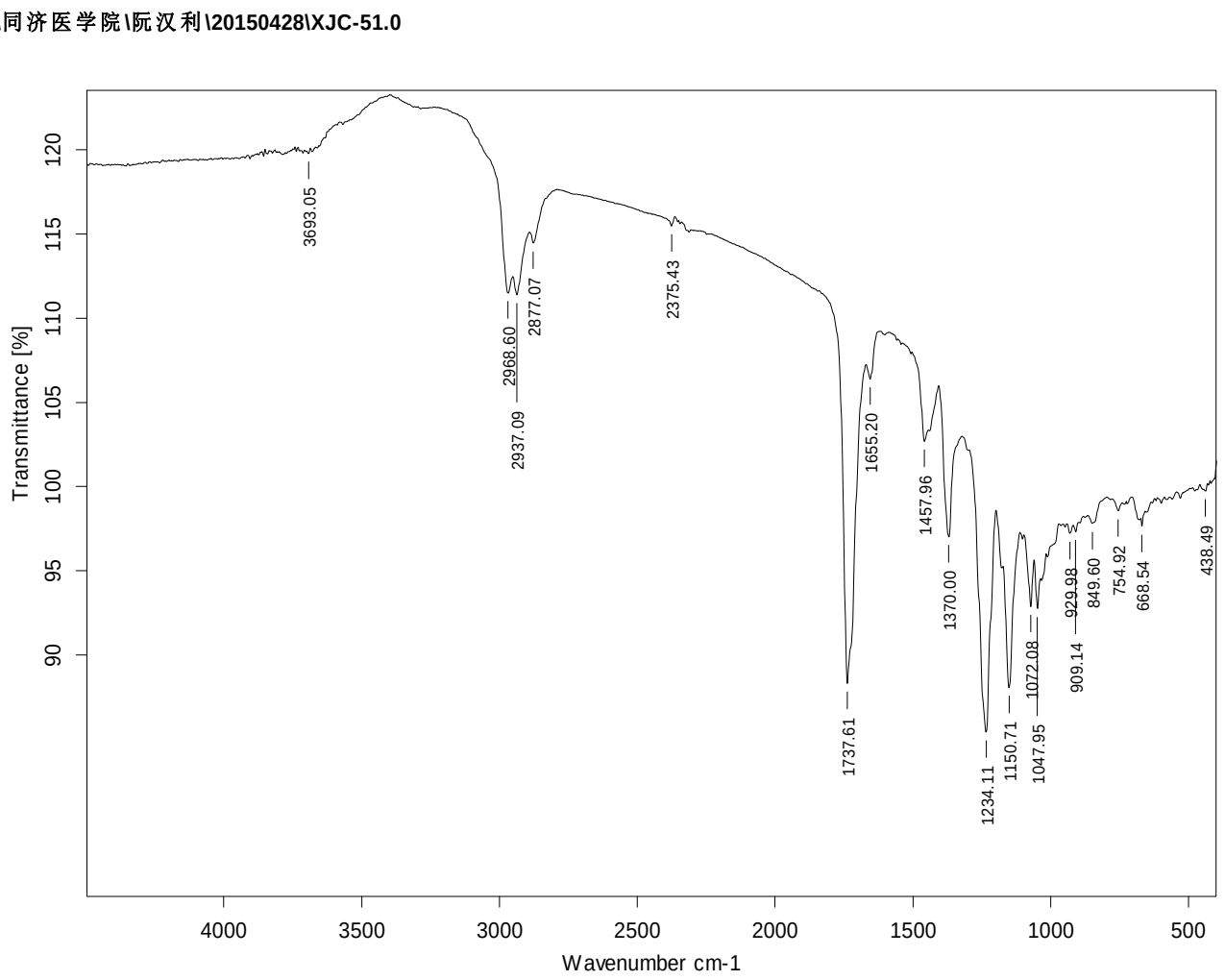


Figure S9. CD spectrum of pararunine A (**1**)

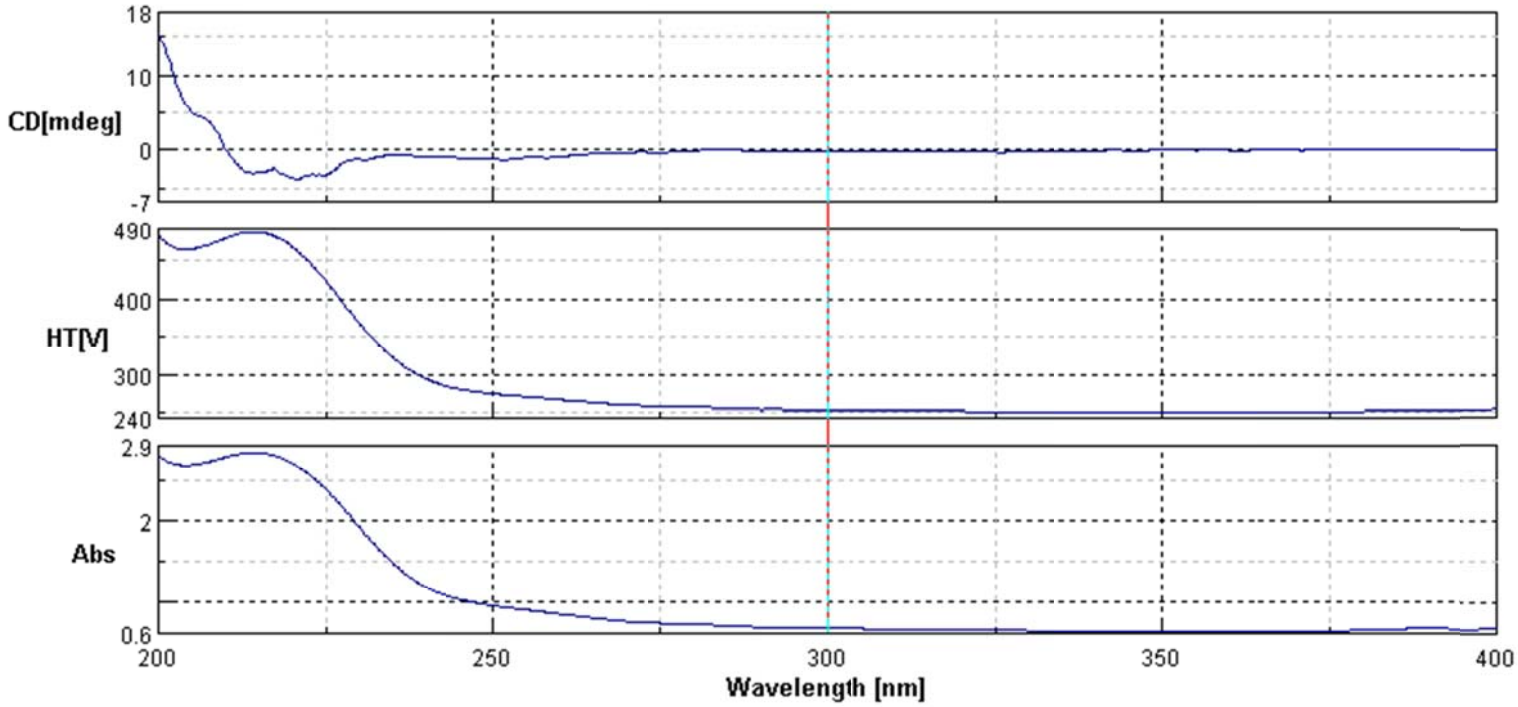


Figure S10. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of pararunine B (**2**)

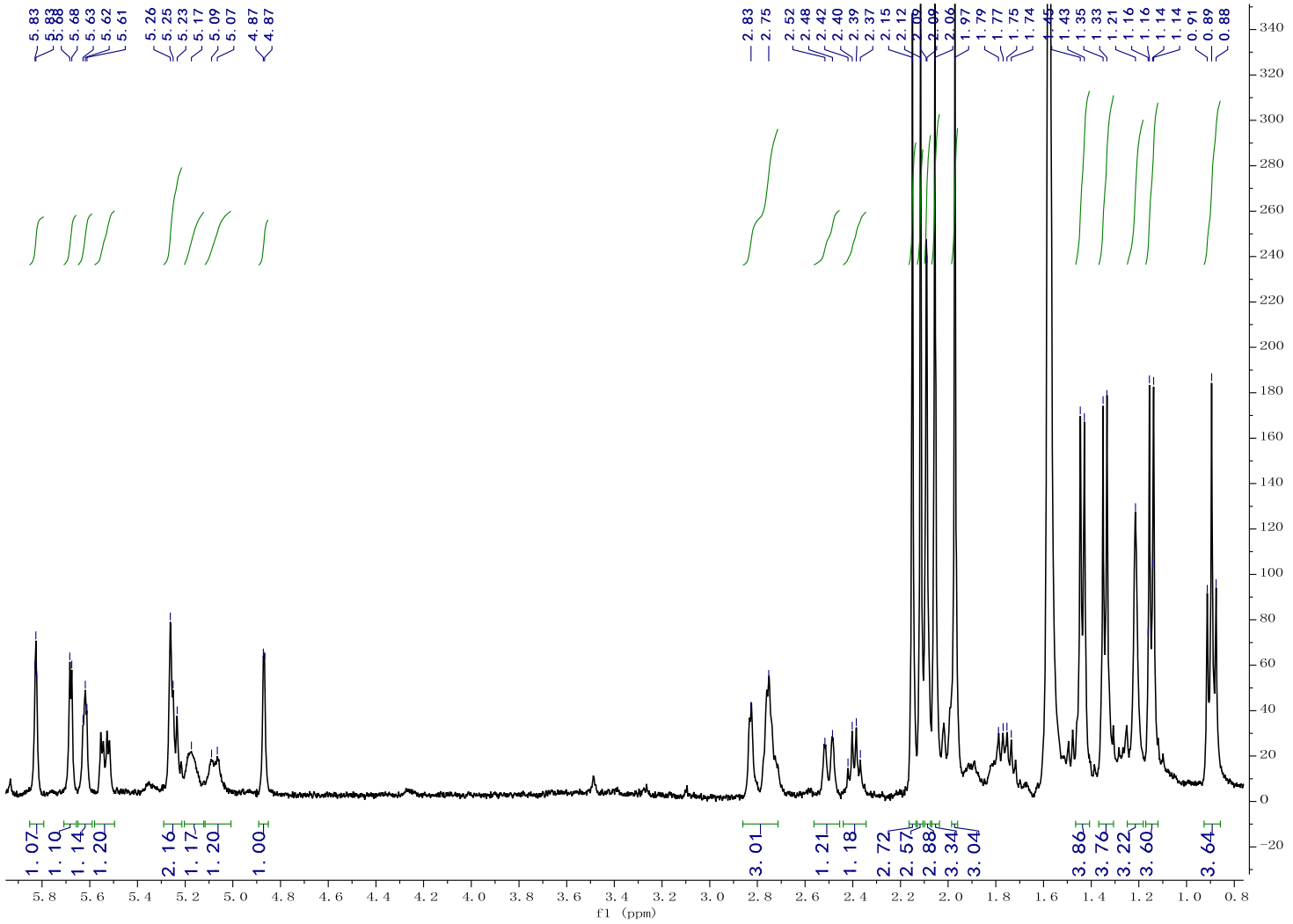


Figure S11. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of pararunine B (**2**)

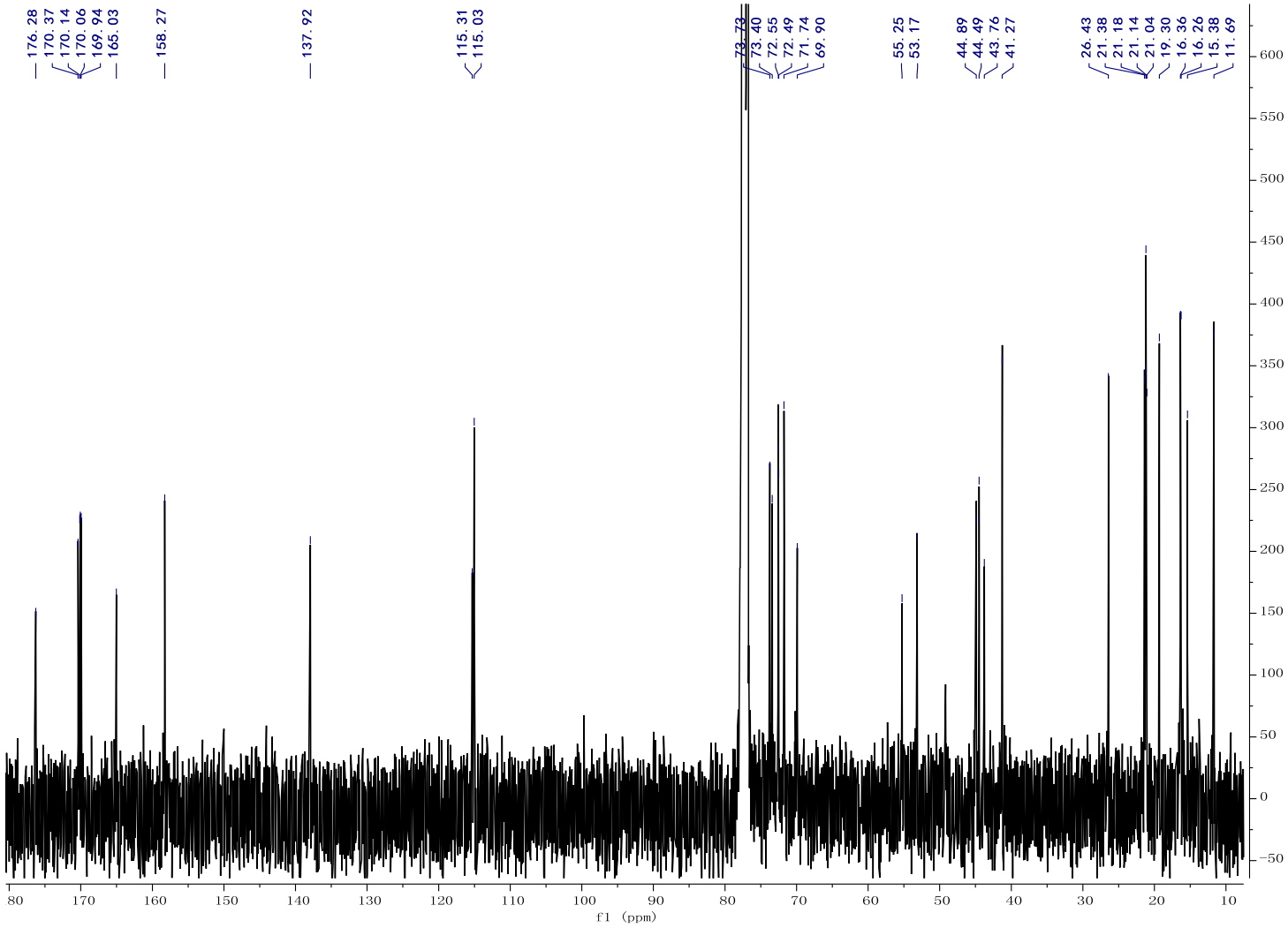


Figure S12. HSQC (400 MHz, $CDCl_3$) spectrum of pararunine B (**2**)

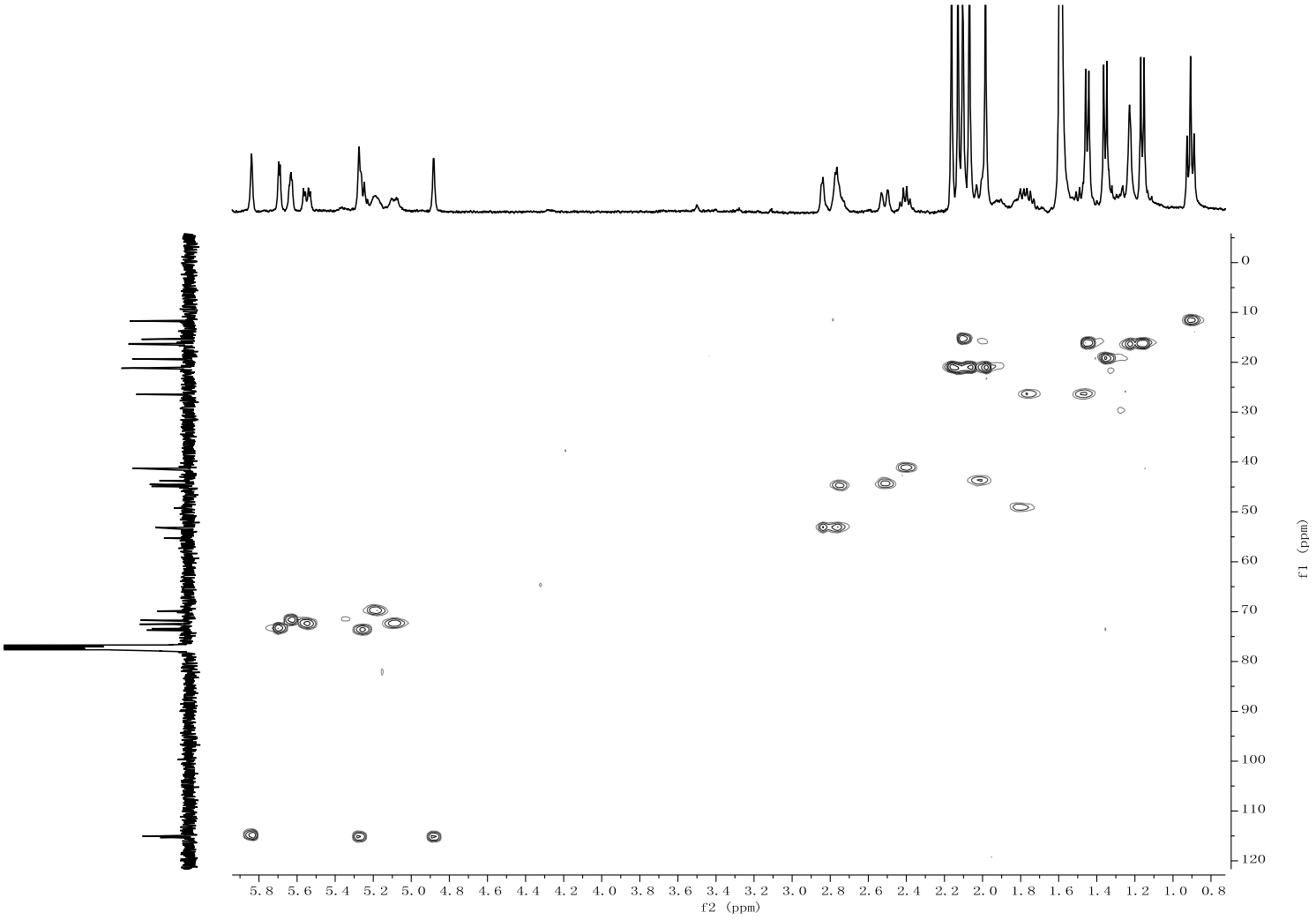


Figure S13. ^{1}H-^{1}H COSY (400 MHz, $CDCl_3$) spectrum of pararunine B (**2**)

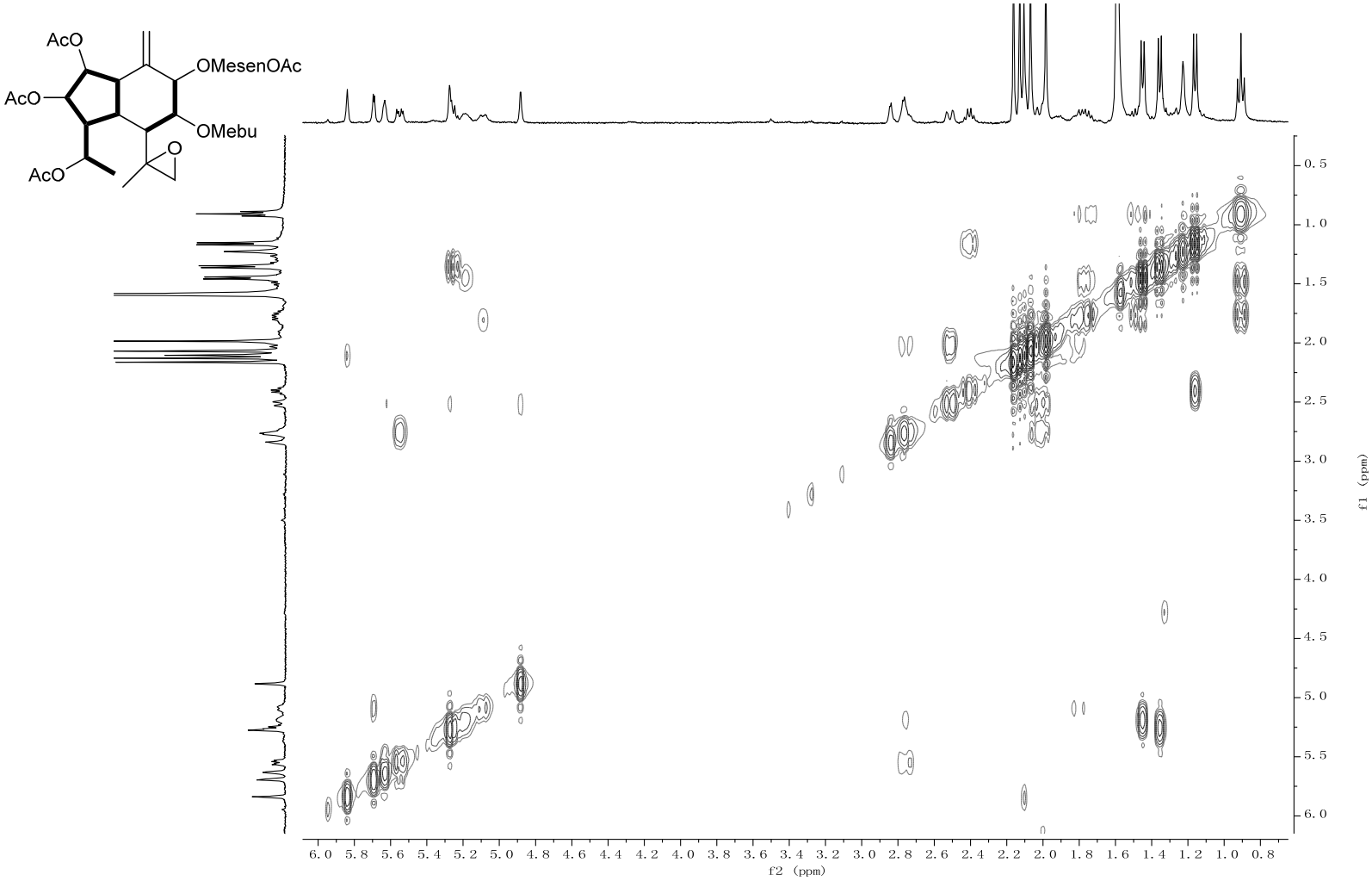


Figure S14. HMBC (400 MHz, $CDCl_3$) spectrum of pararunine B (**2**)

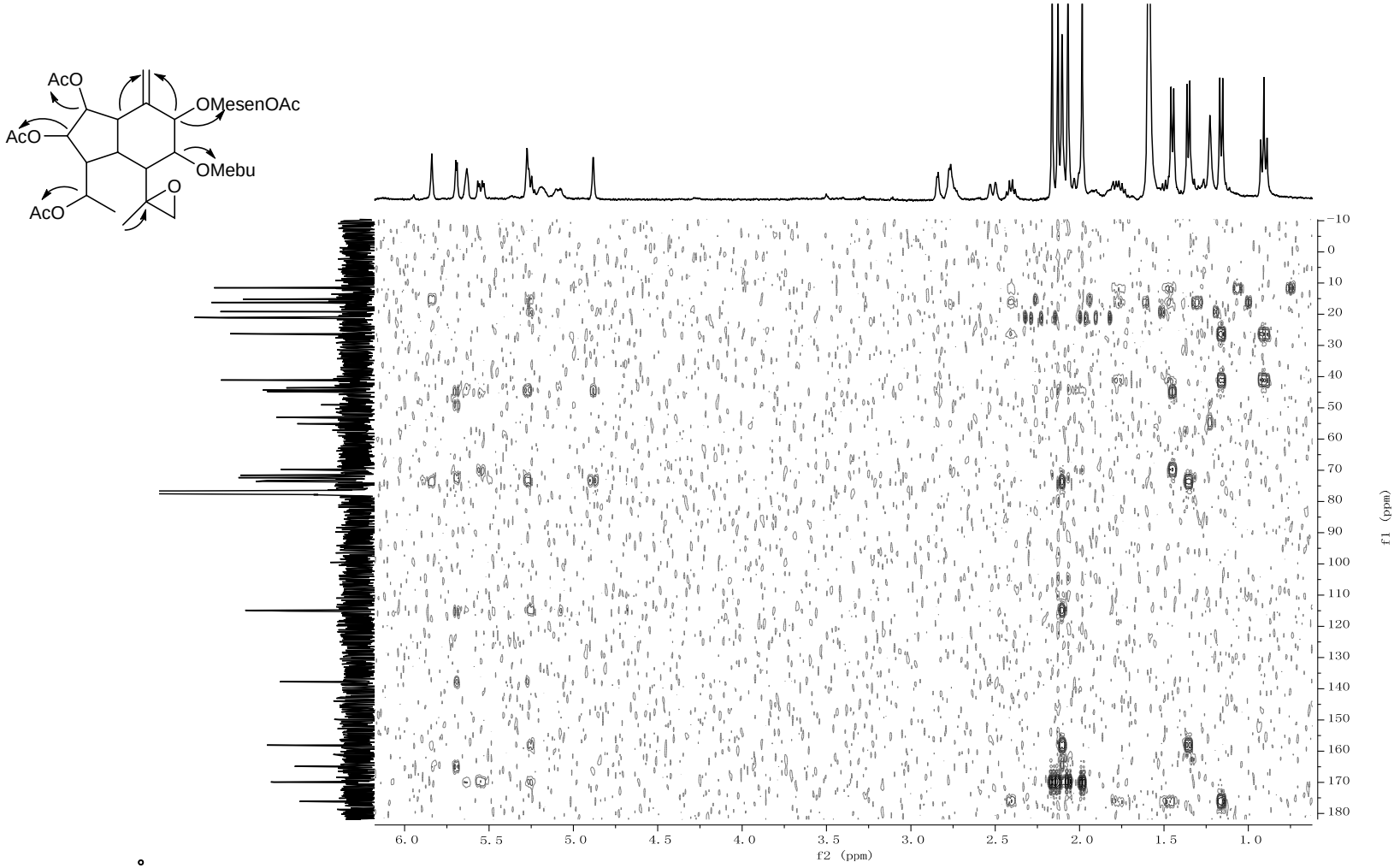


Figure S15. NOESY (400 MHz, $CDCl_3$) spectrum of pararunine B (**2**)

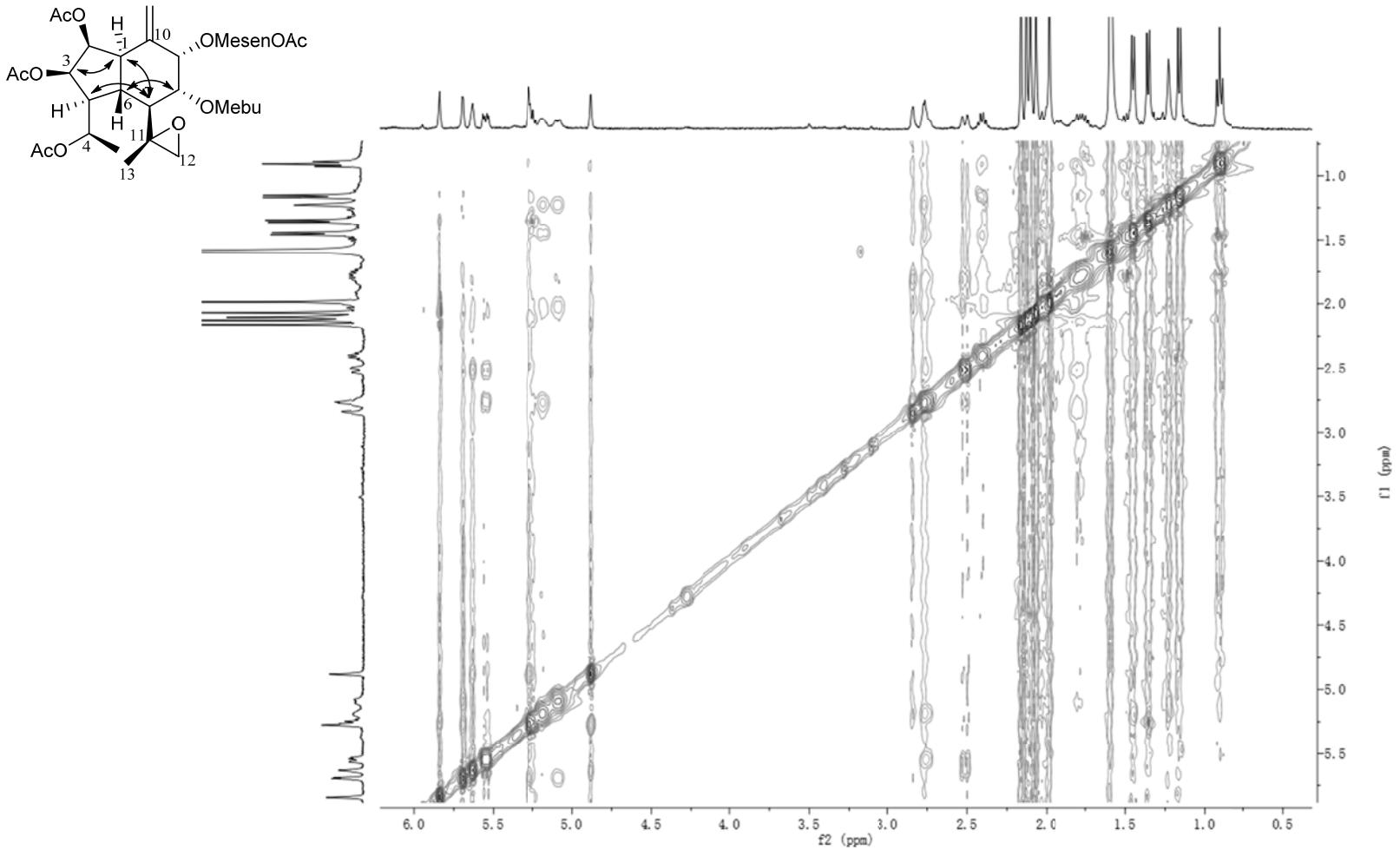


Figure S16. HRESIMS spectrum of pararunine B (**2**)

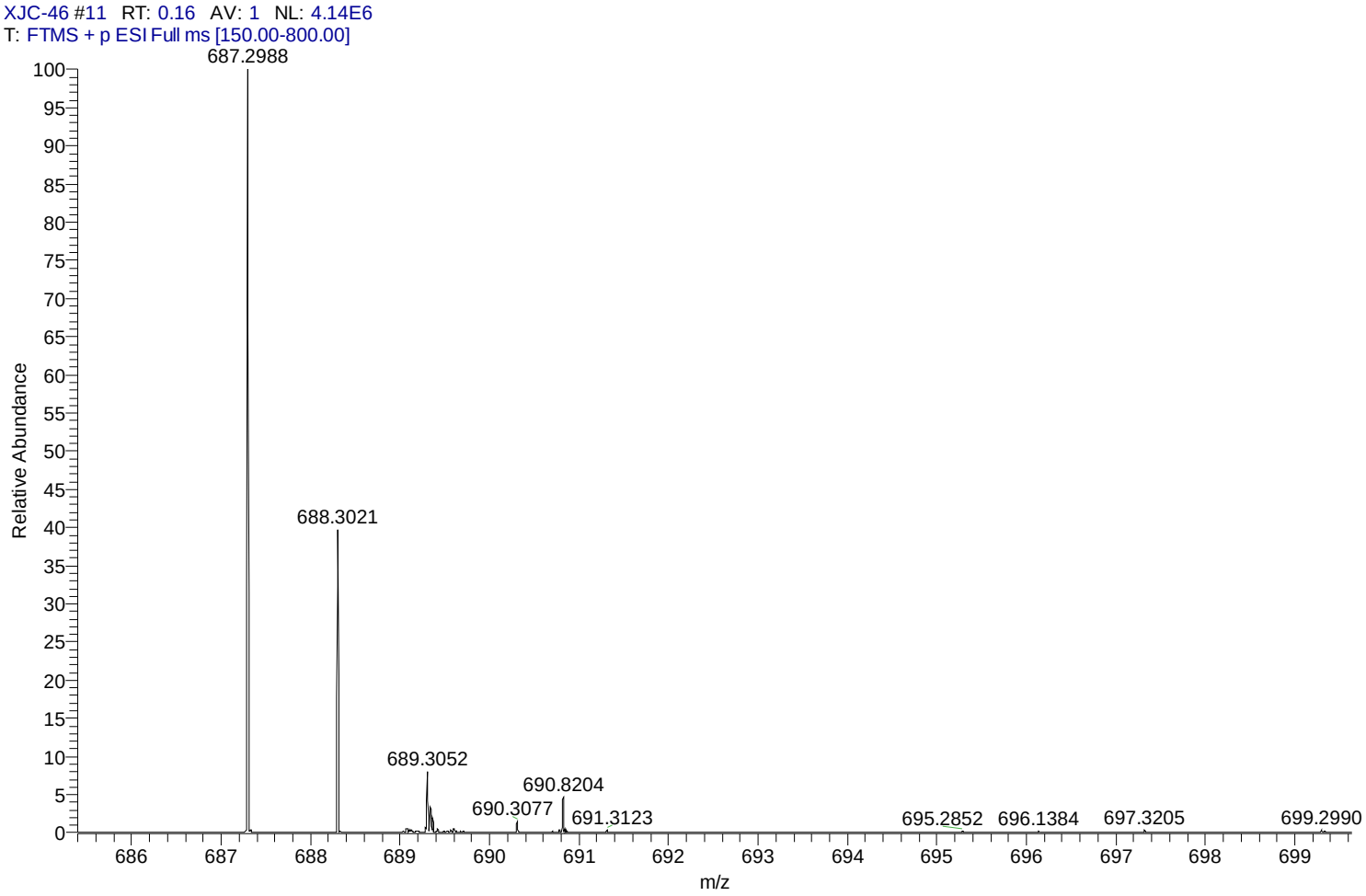


Figure S17. IR spectrum of pararunine B (**2**)

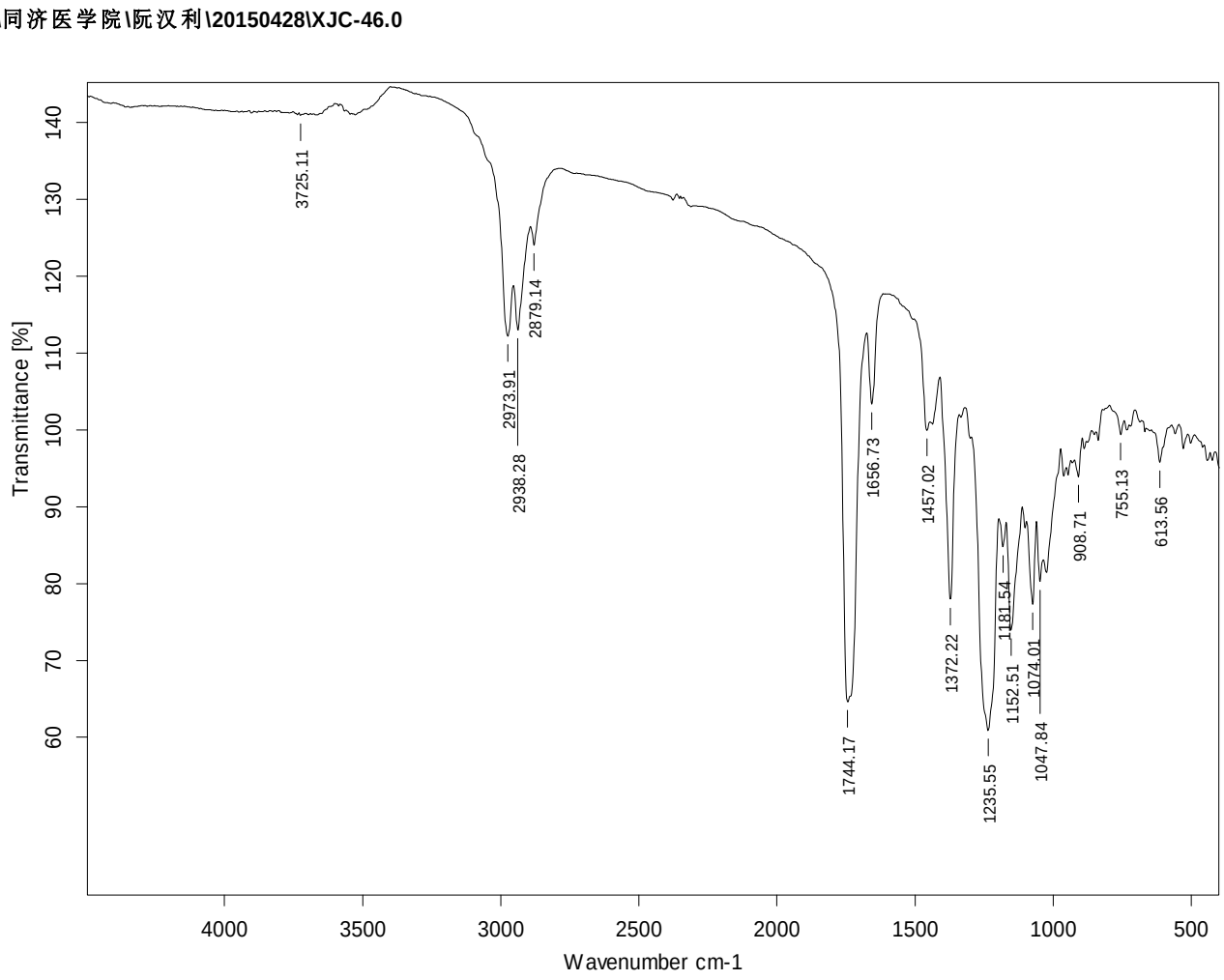


Figure S18. CD spectrum of pararunine B (**2**)

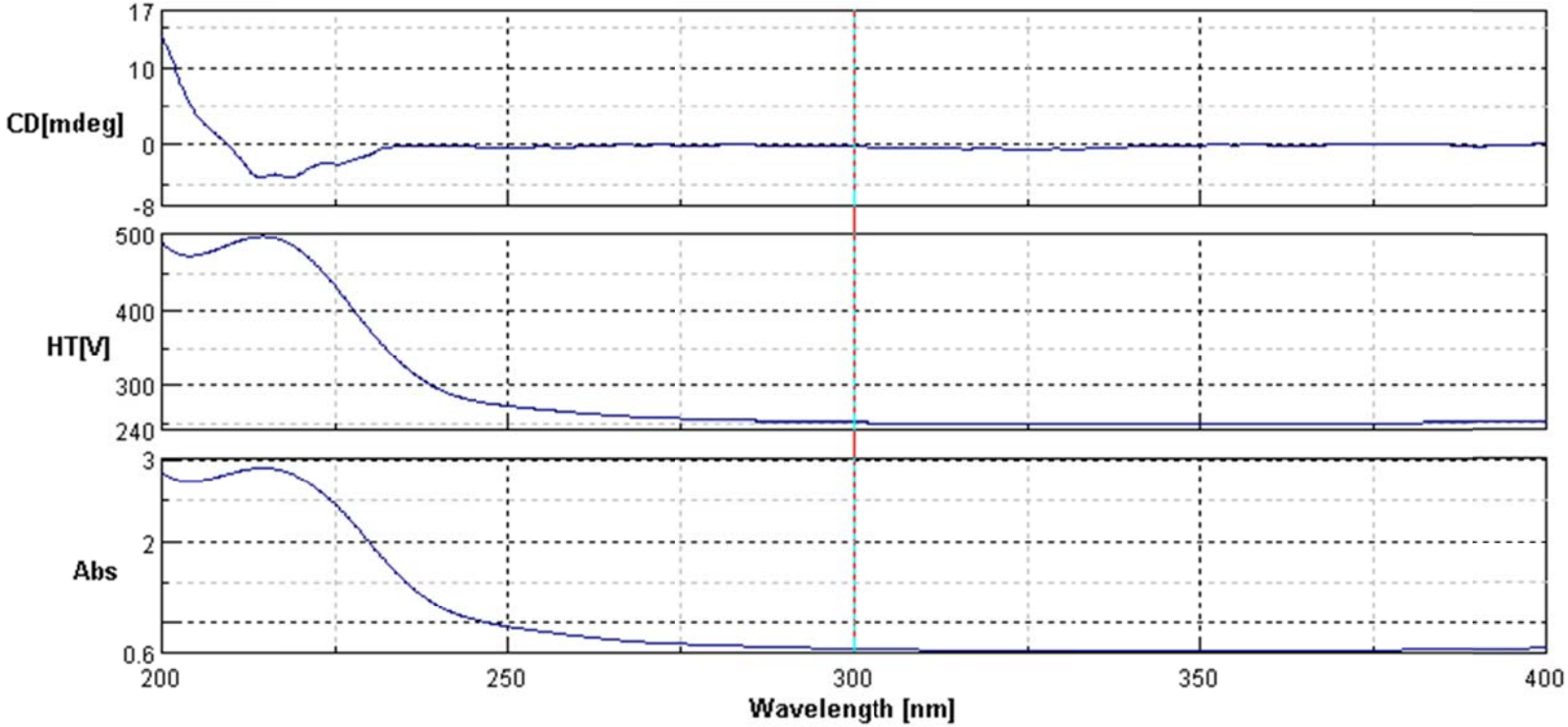


Figure S19. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of pararunine C (**5**)

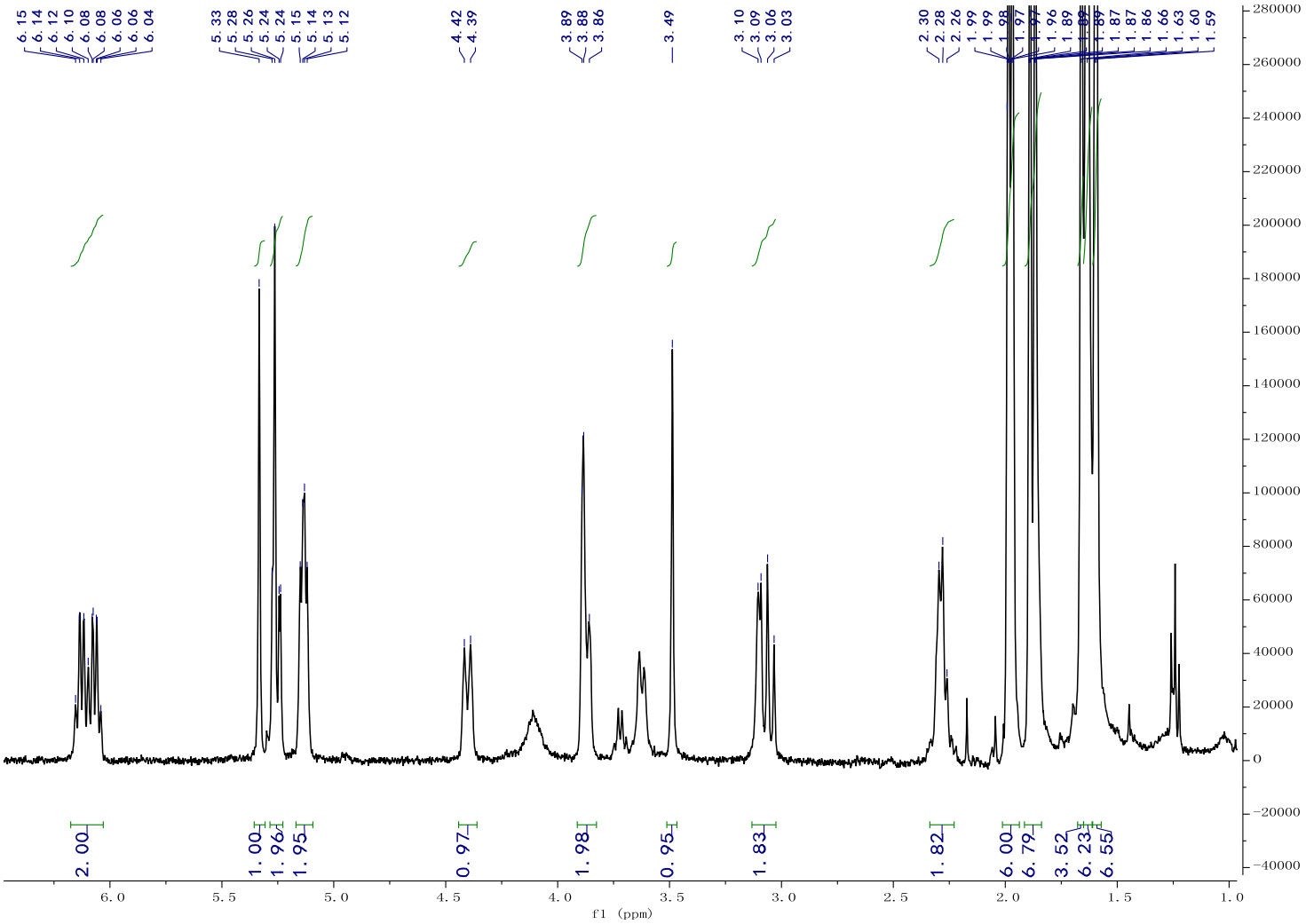


Figure S20. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of pararunine C (**5**)

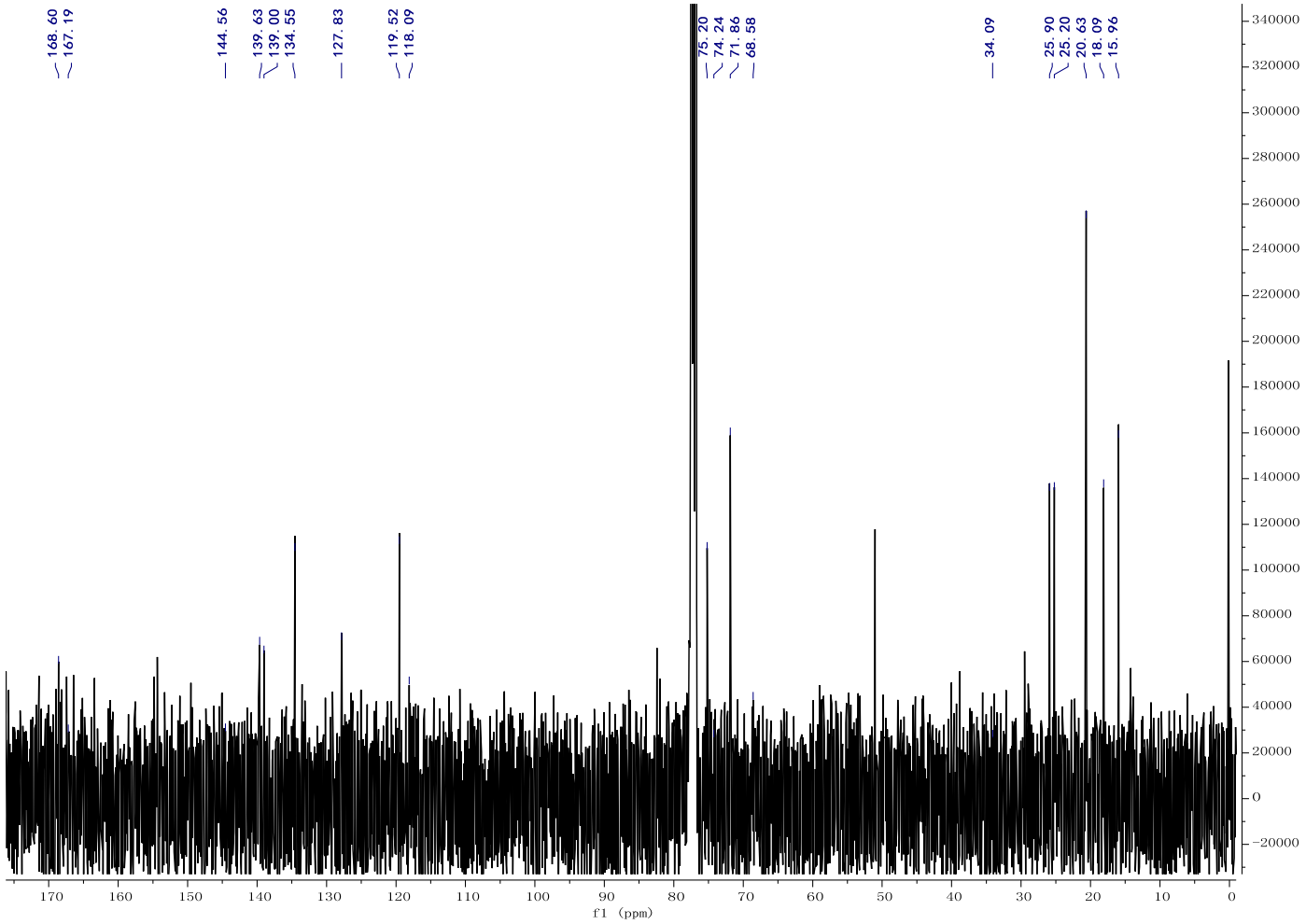


Figure S21. HSQC (400 MHz, $CDCl_3$) spectrum of pararunine C (5)

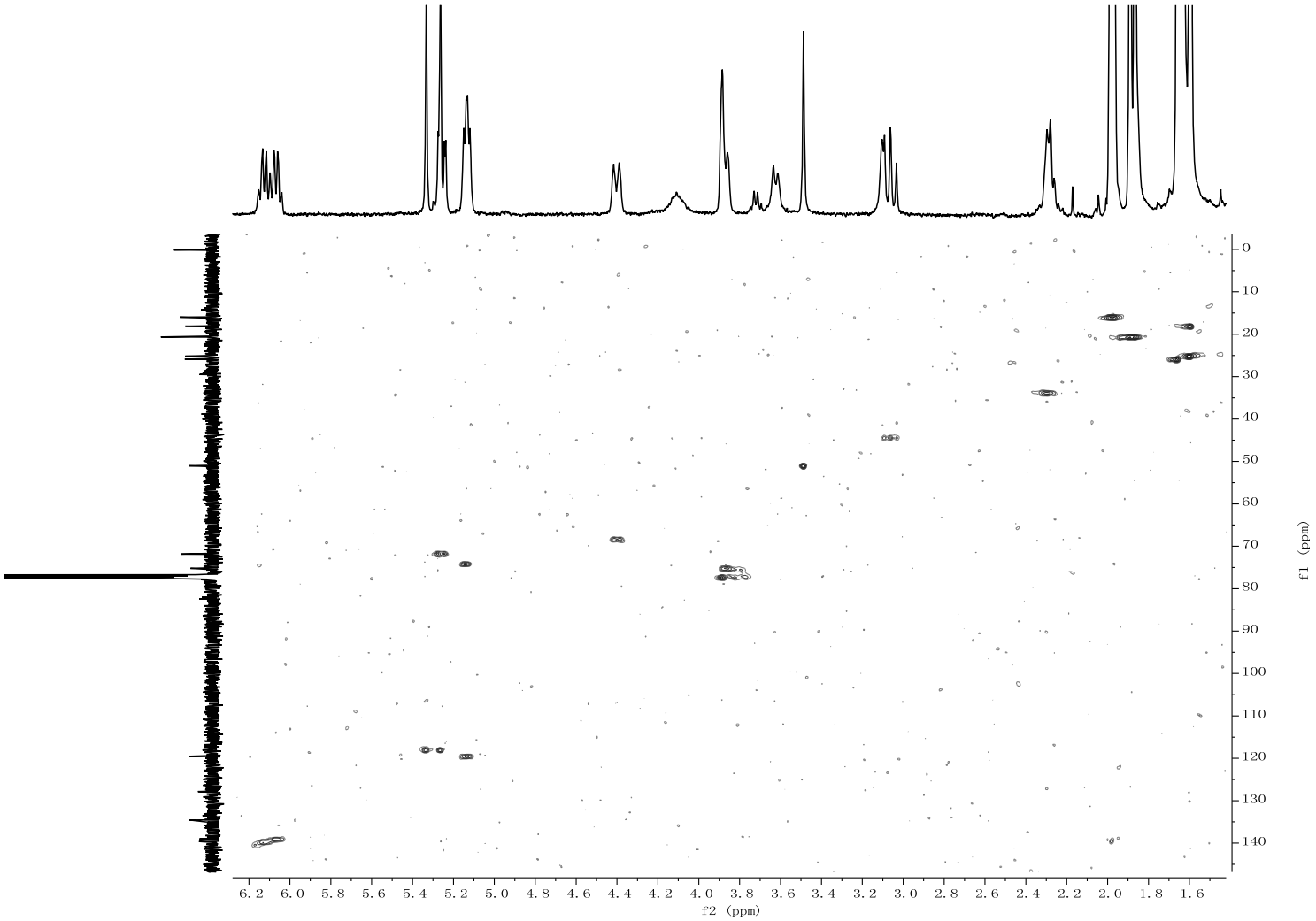


Figure S22. ^{1}H-^{1}H COSY (400 MHz, $CDCl_3$) spectrum of pararunine C (**5**)

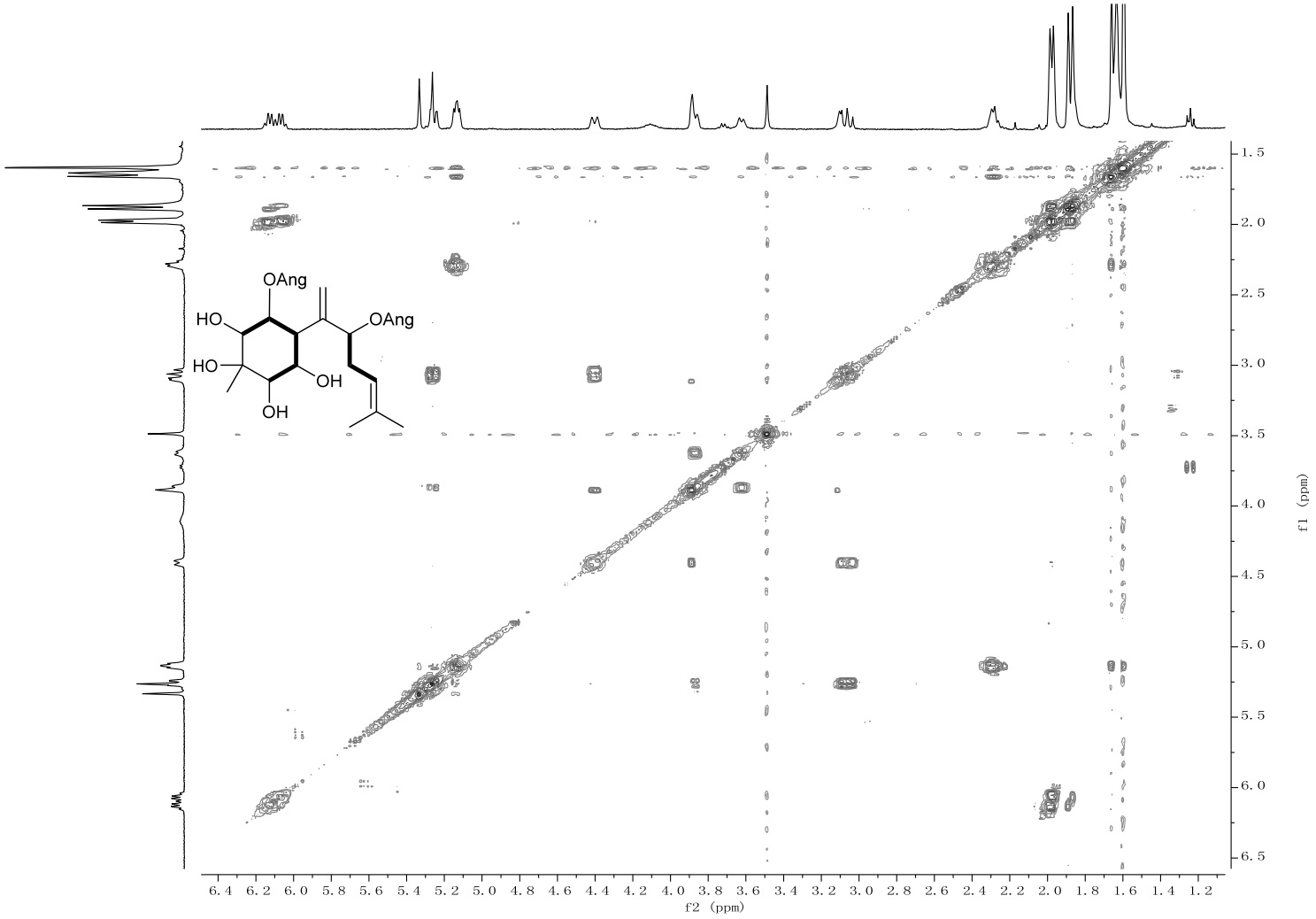


Figure S23. HMBC (400 MHz, $CDCl_3$) spectrum of pararunine C (**5**)

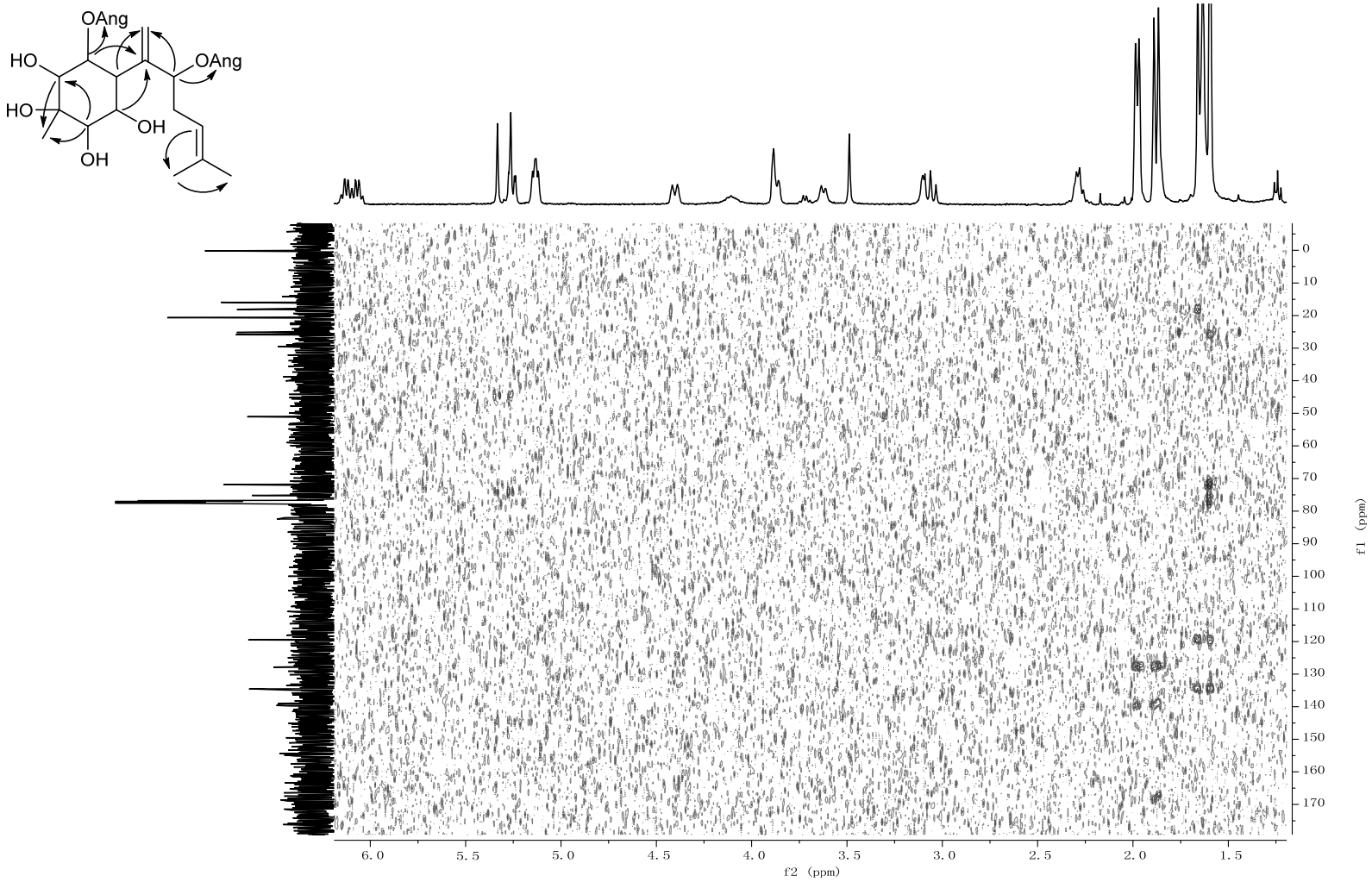


Figure S24. NOESY (400 MHz, $CDCl_3$) spectrum of pararunine C (**5**)

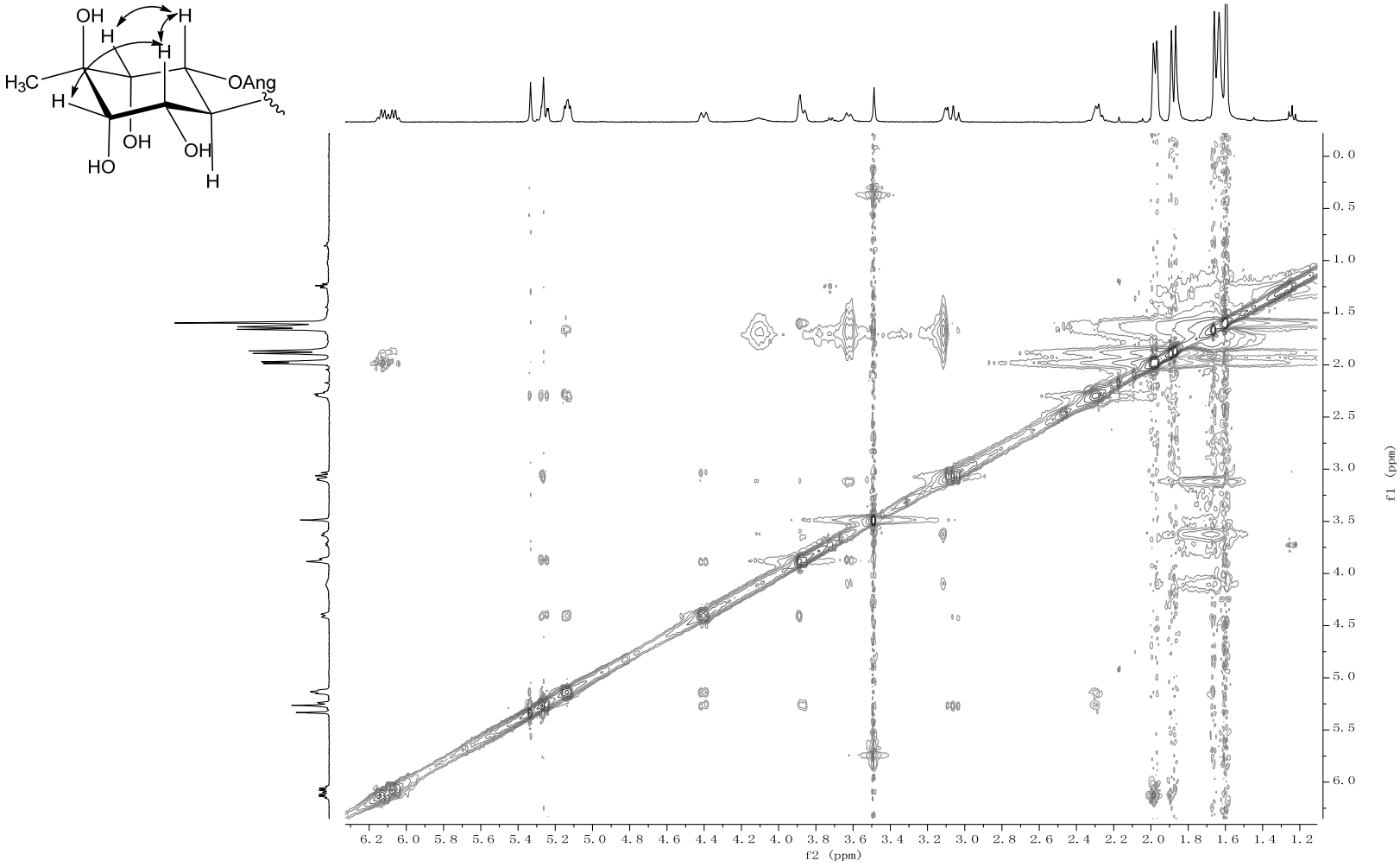


Figure S25. HRESIMS spectrum of pararunine C (**5**)

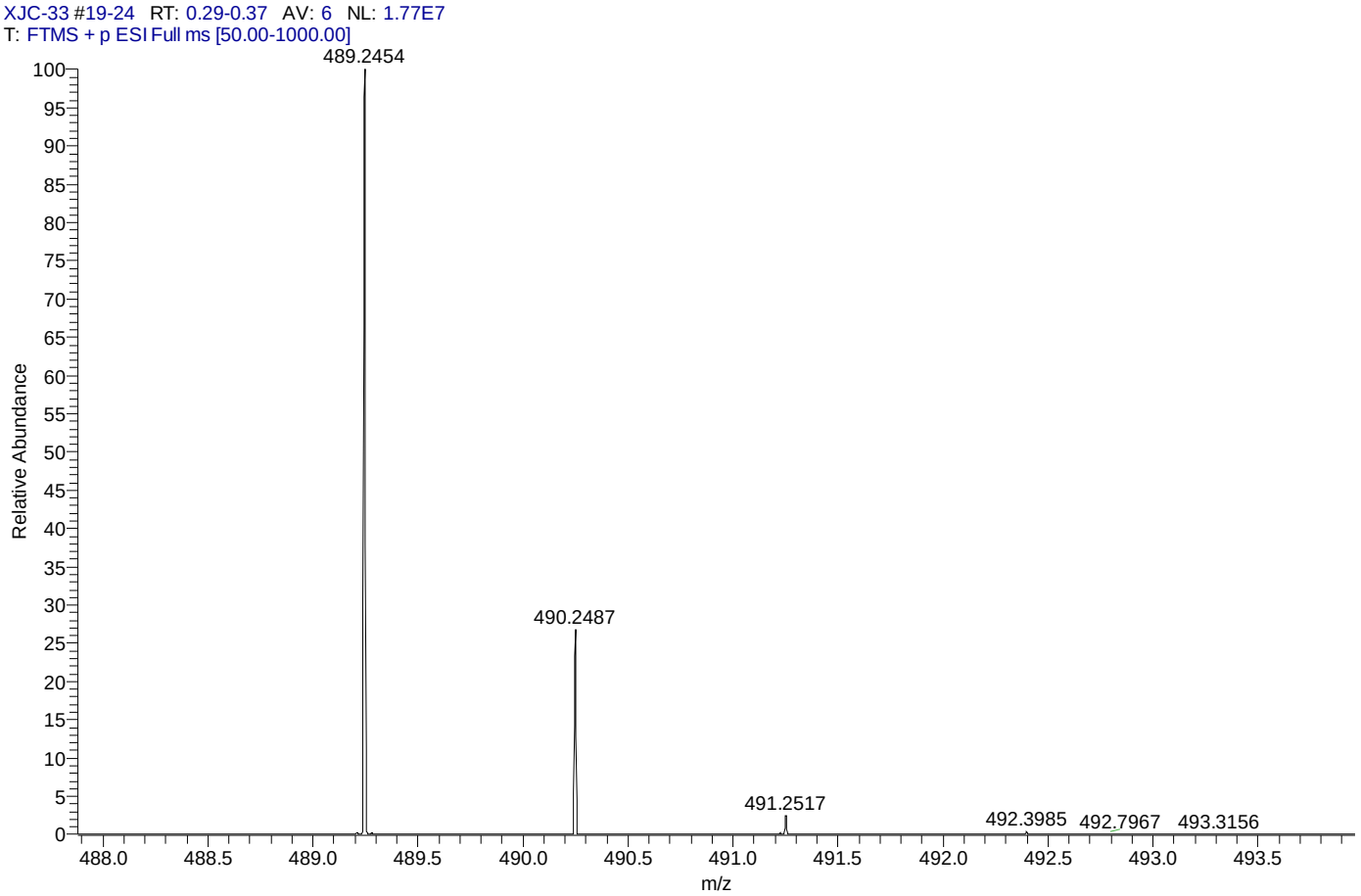


Figure S26. IR spectrum of pararunine C (**5**)

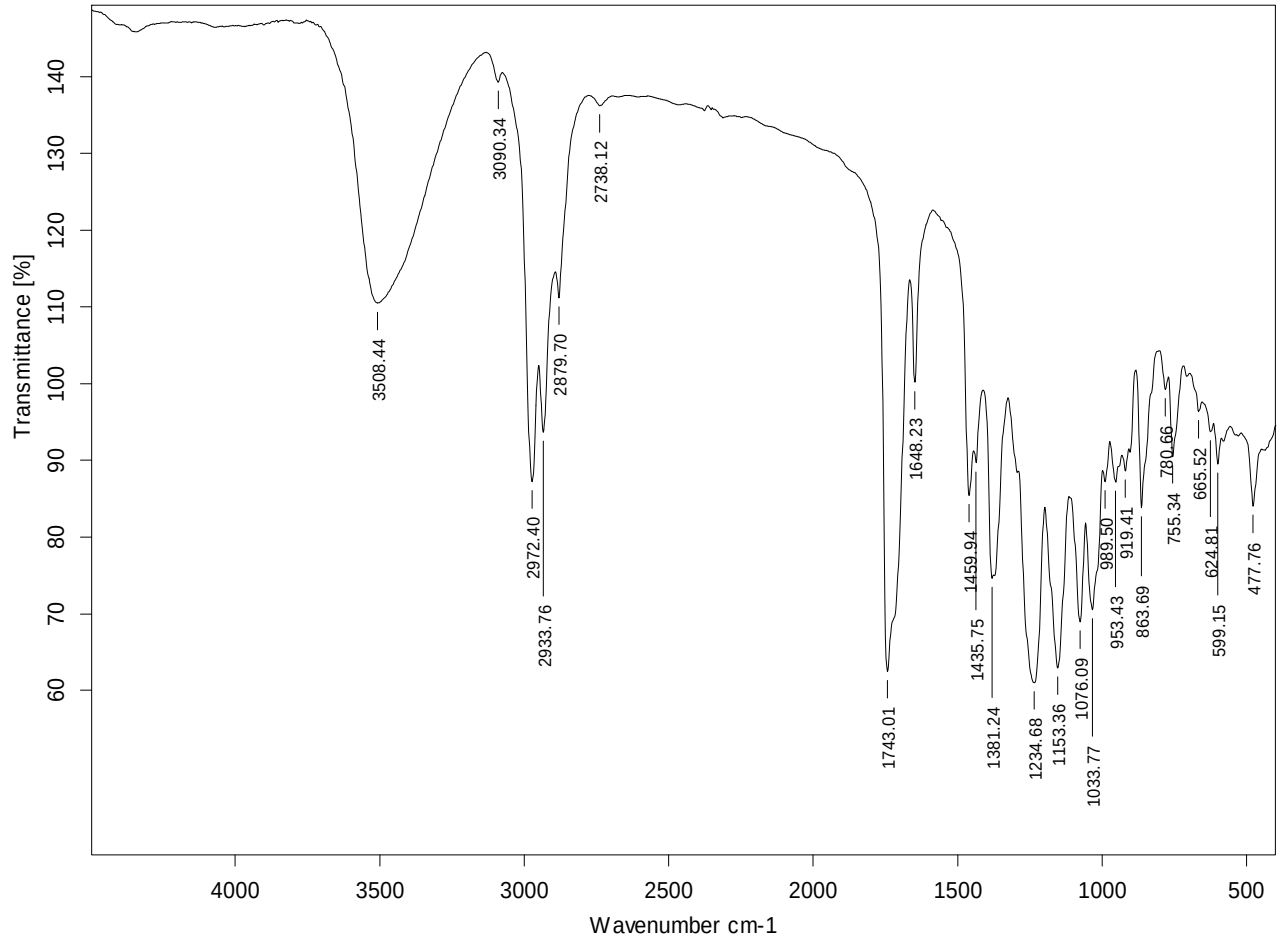


Figure S27. CD spectrum of pararunine C (**5**)

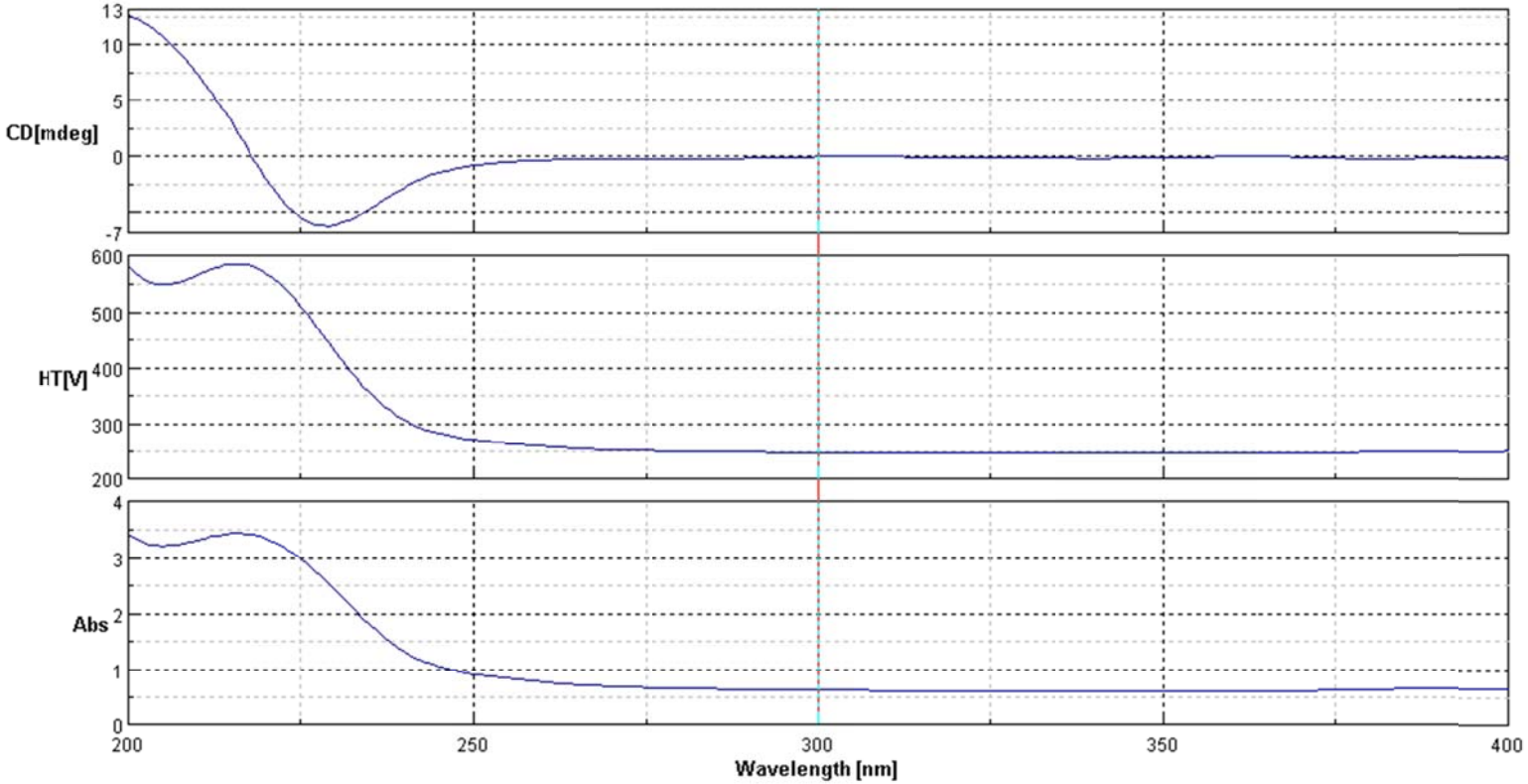


Figure S28. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of pararunine D (**6**)

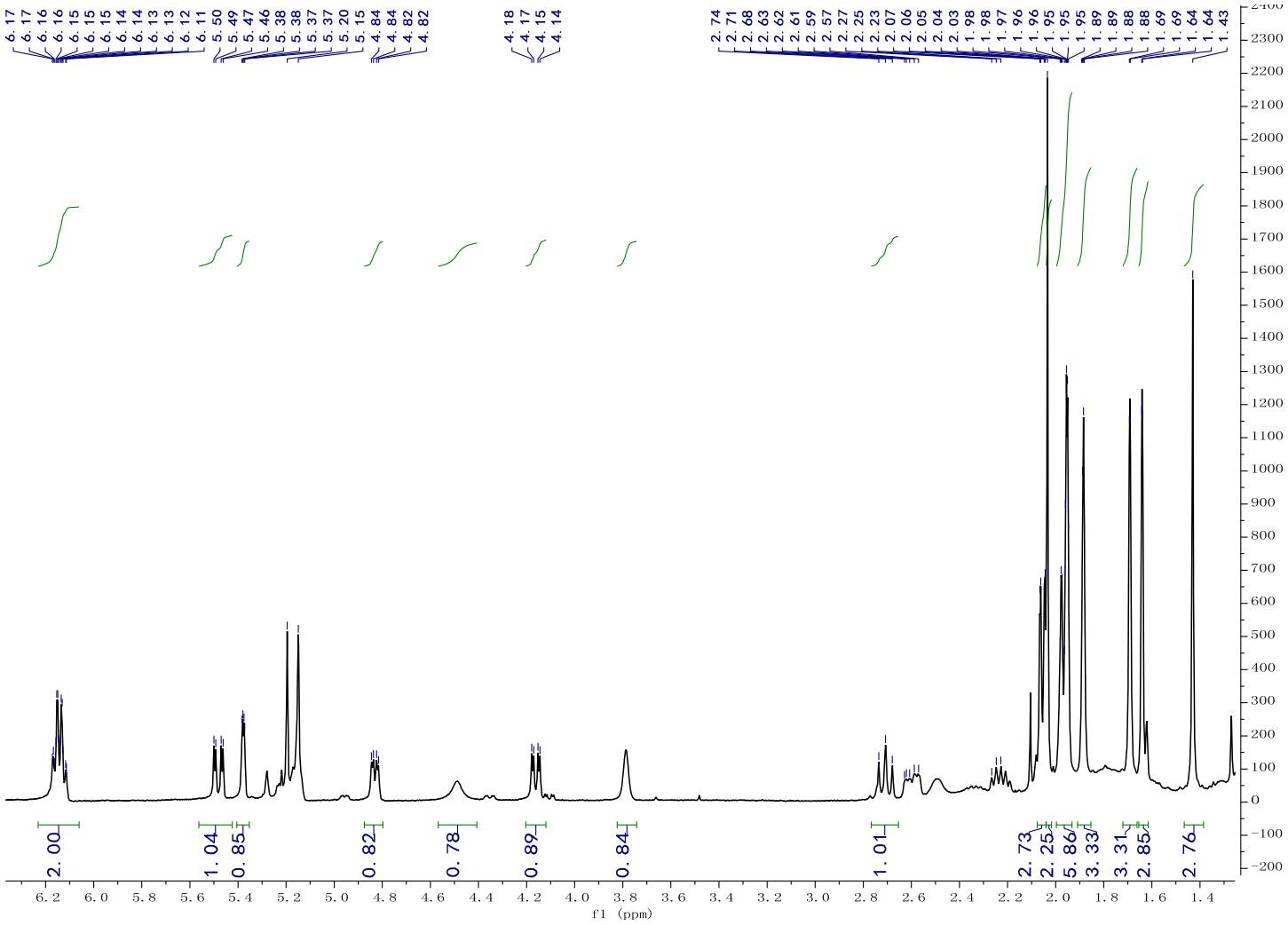


Figure S29. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of pararunine D (**6**)

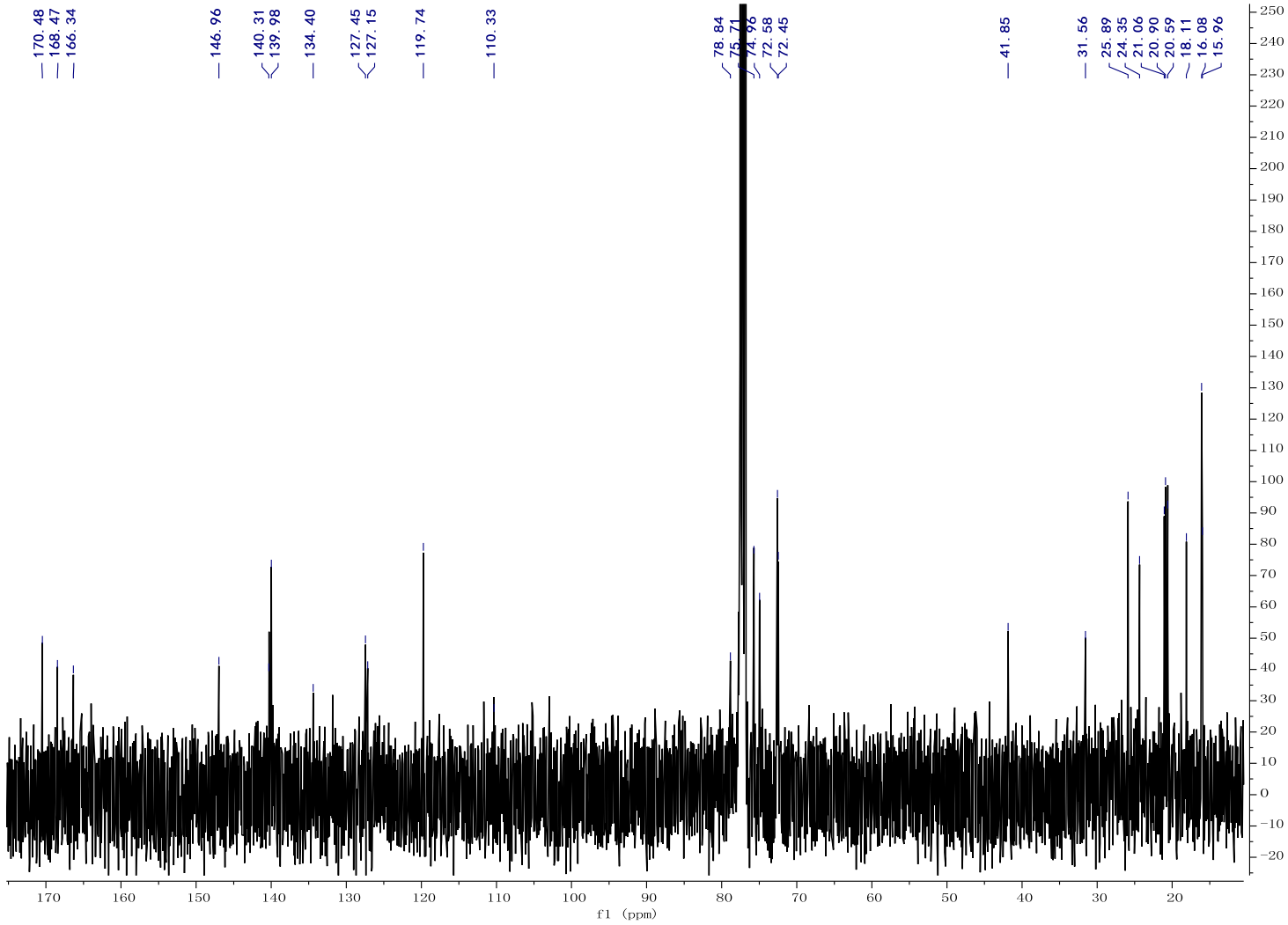


Figure S30. HSQC (400 MHz, $CDCl_3$) spectrum of pararunine D (**6**)

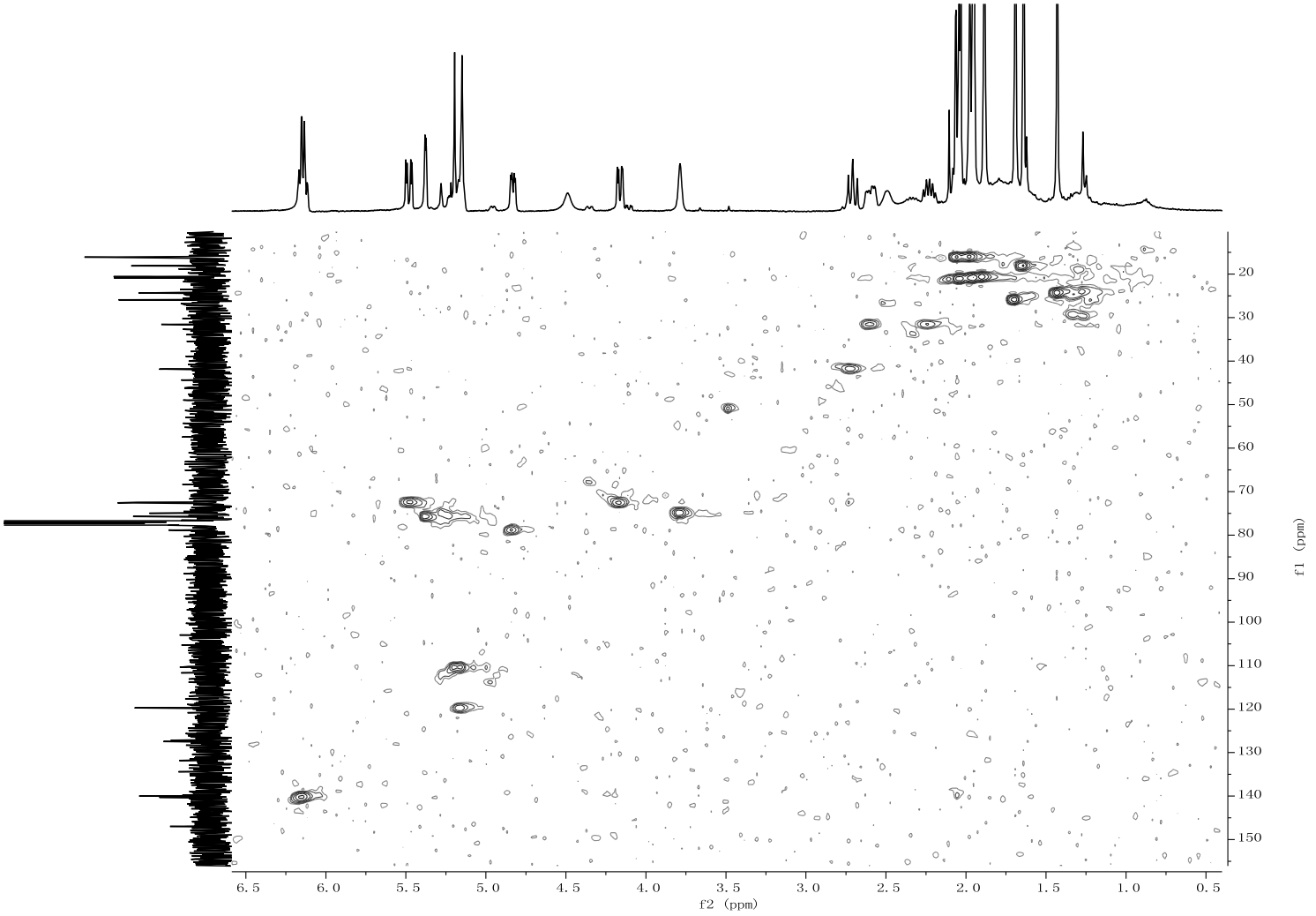


Figure S31. ^{1}H-^{1}H COSY (400 MHz, $CDCl_3$) spectrum of pararunine D (**6**)

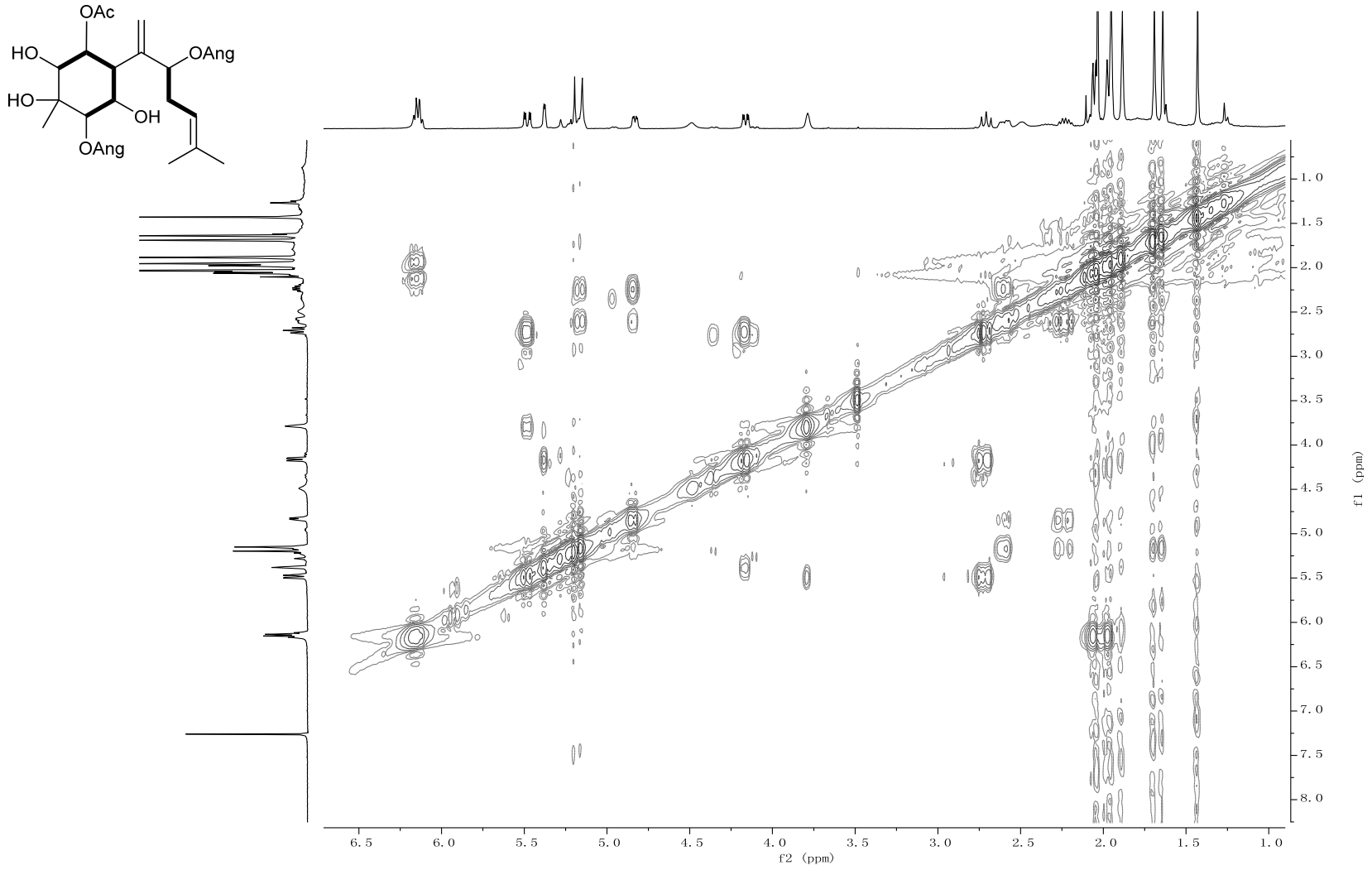


Figure S32. HMBC (400 MHz, $CDCl_3$) spectrum of pararunine D (**6**)

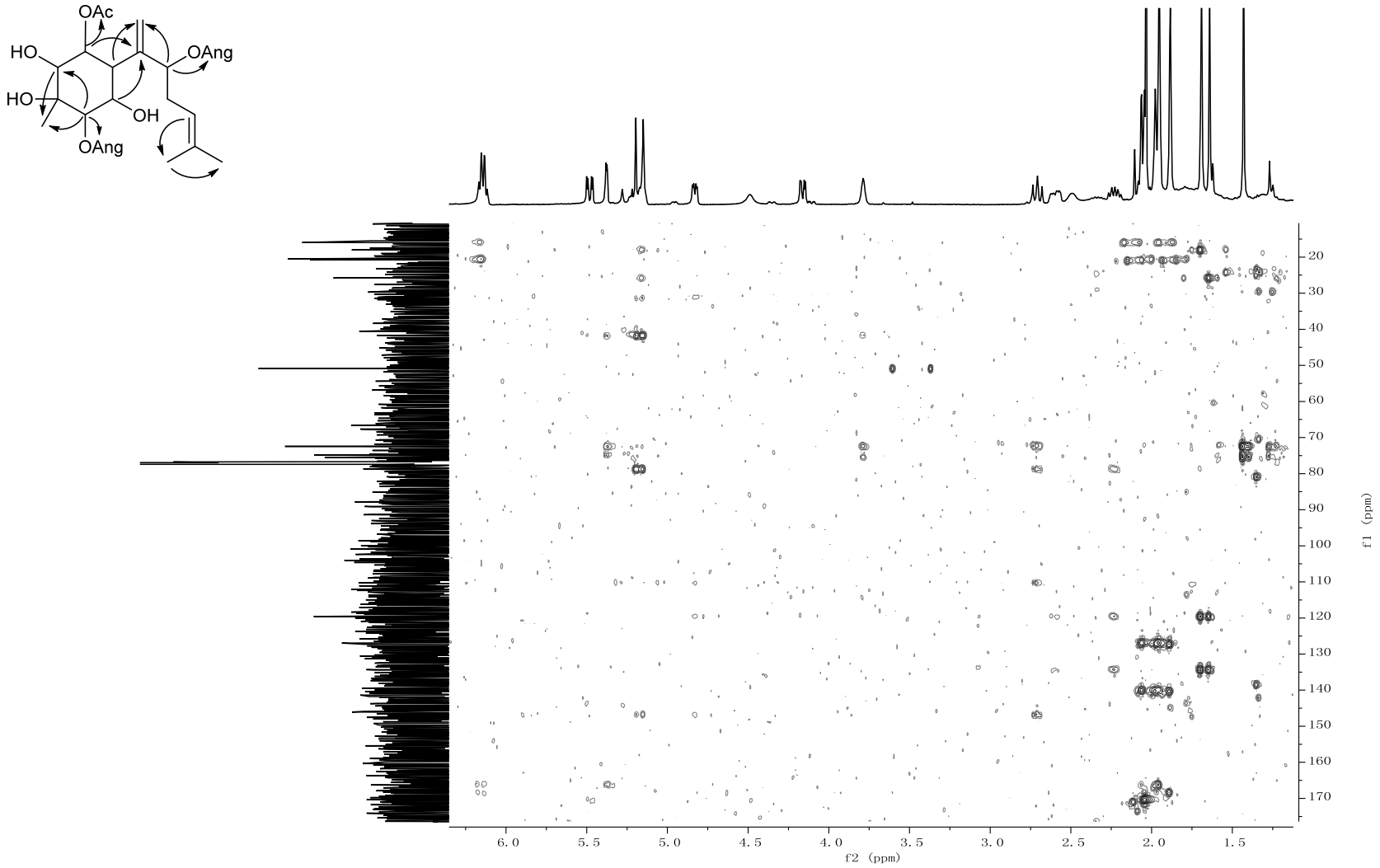


Figure S33. NOESY (400 MHz, $CDCl_3$) spectrum of pararunine D (**6**)

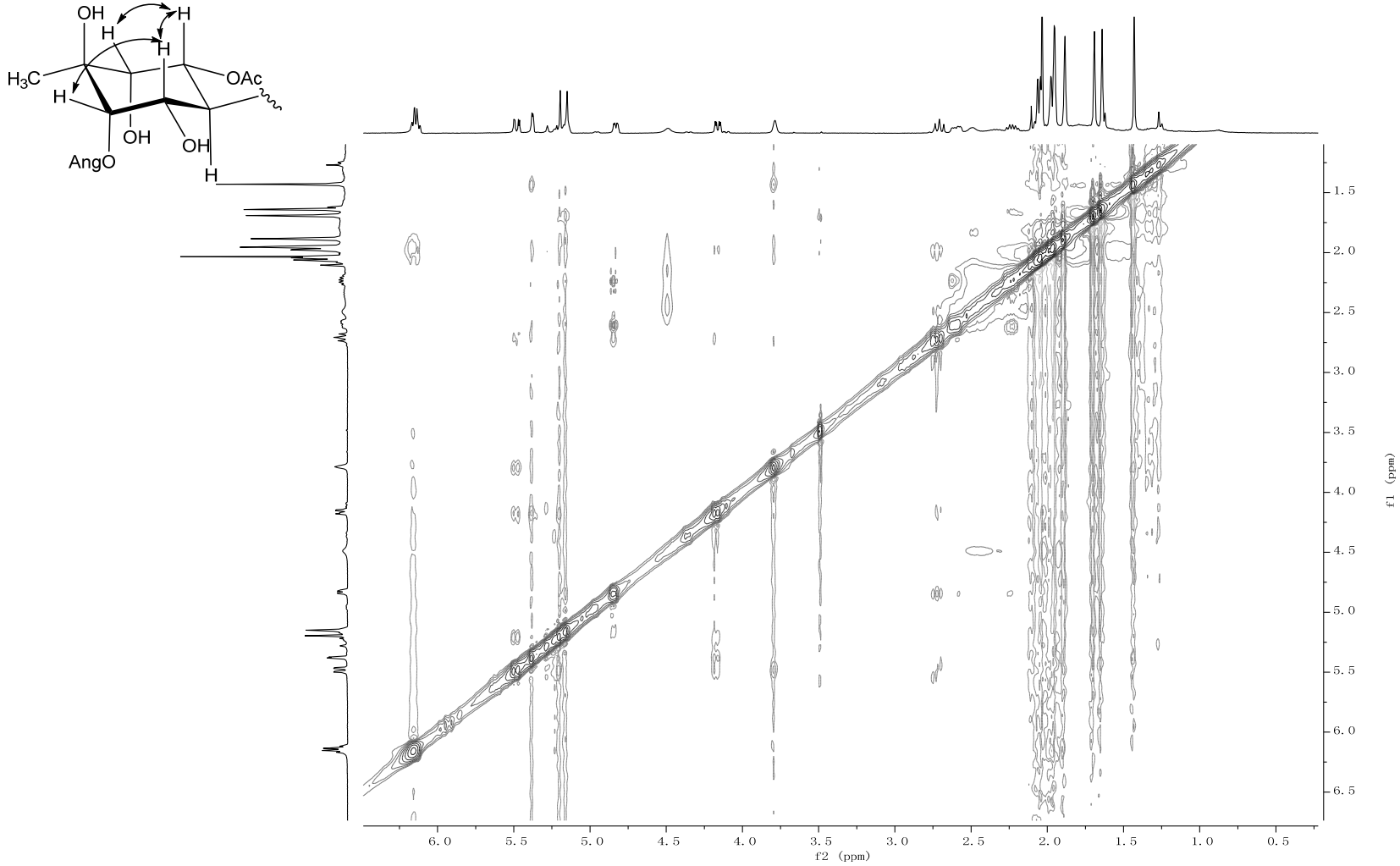


Figure S34. HRESIMS spectrum of pararunine D (**6**)

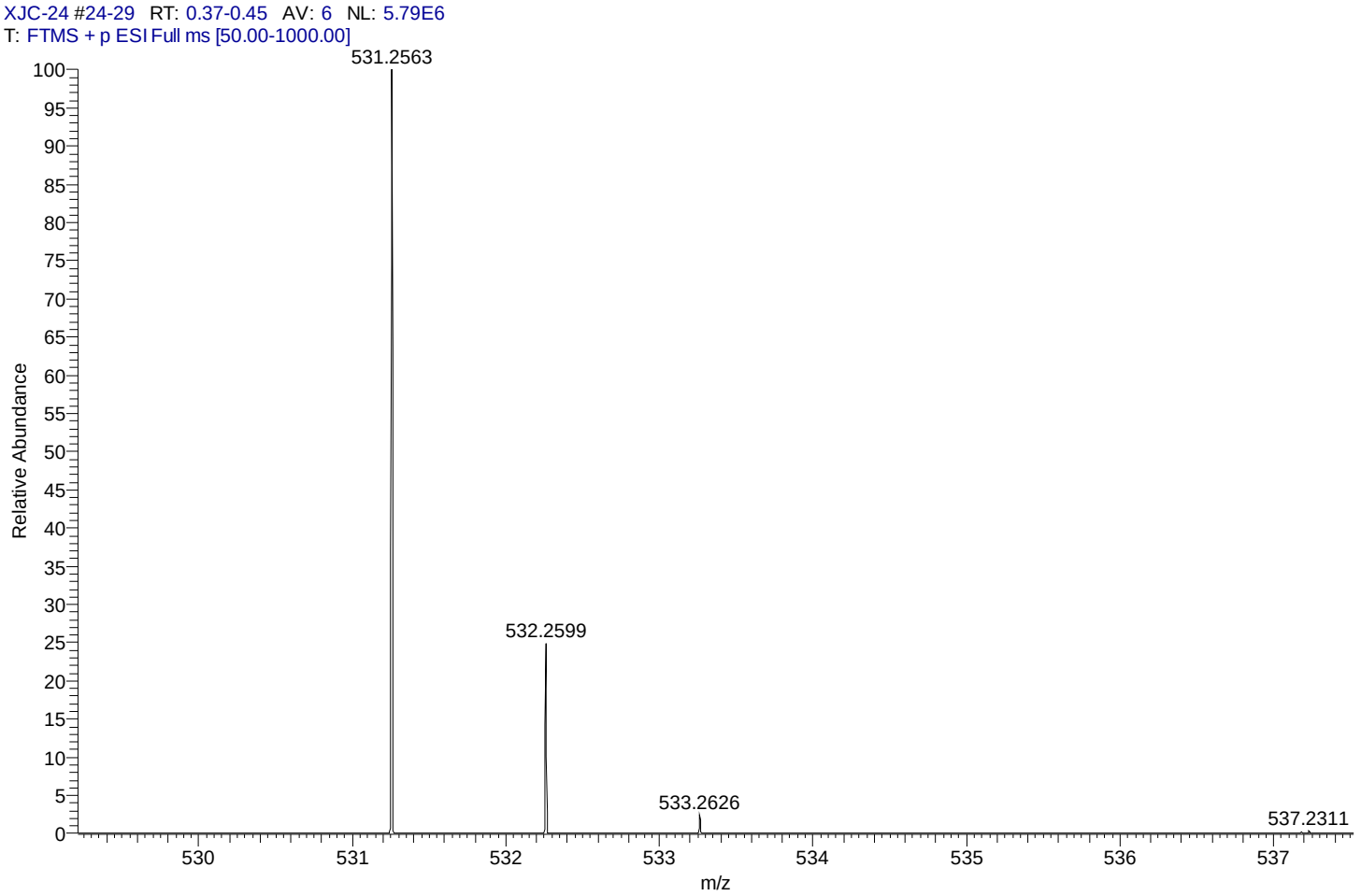


Figure S35. IR spectrum of pararunine D (**6**)

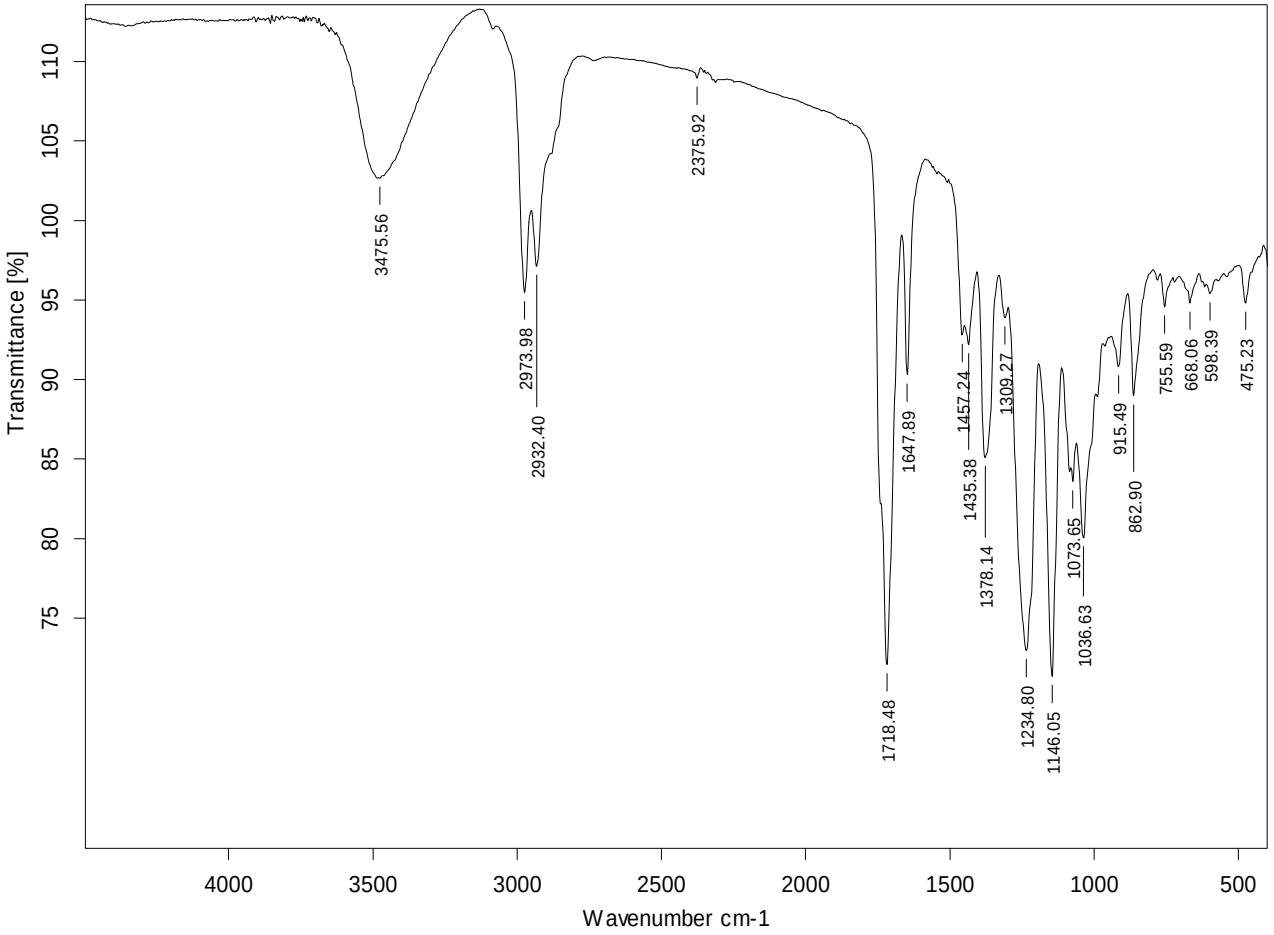


Figure S36. CD spectrum of pararunine D (**6**)

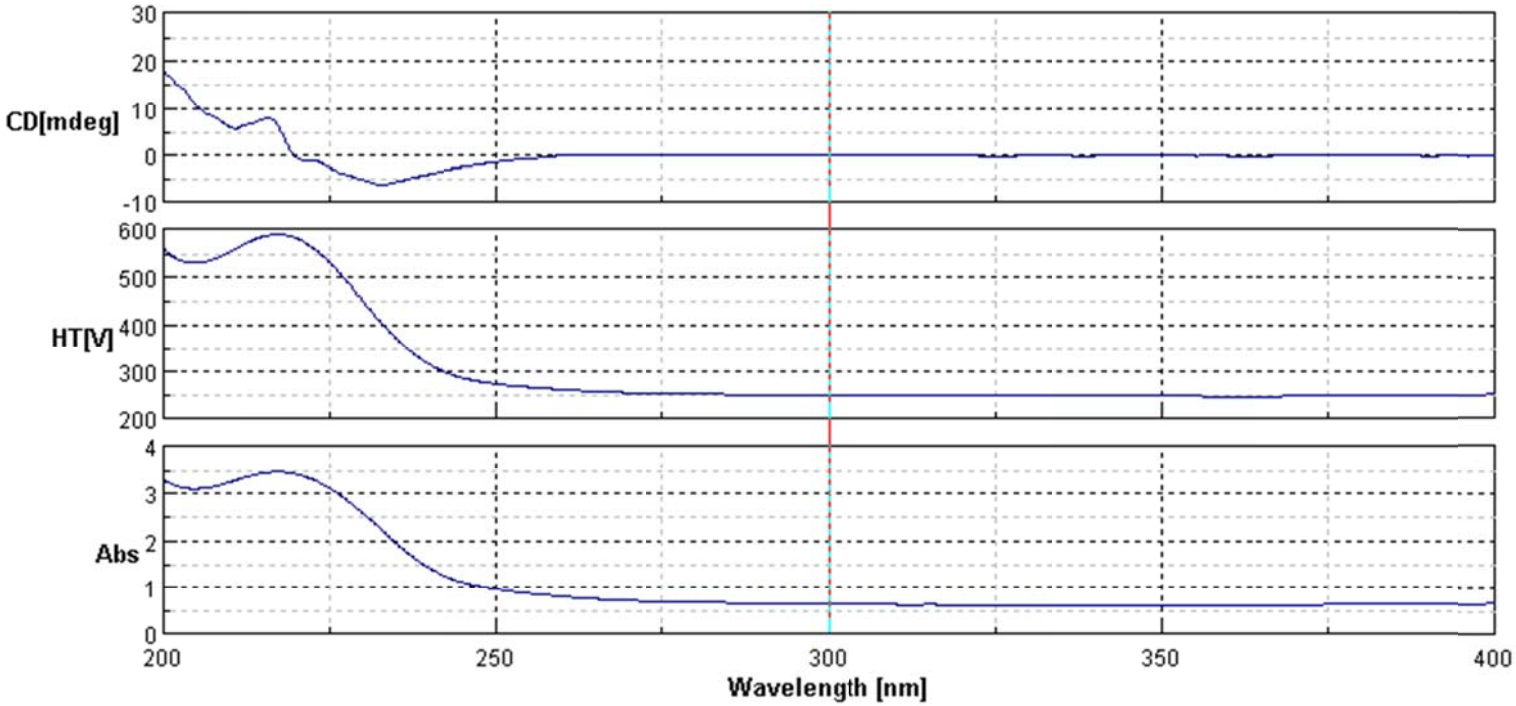


Figure S37. ^{1}H NMR (400 MHz, CD_3OD) spectrum of pararunine E (**7**)

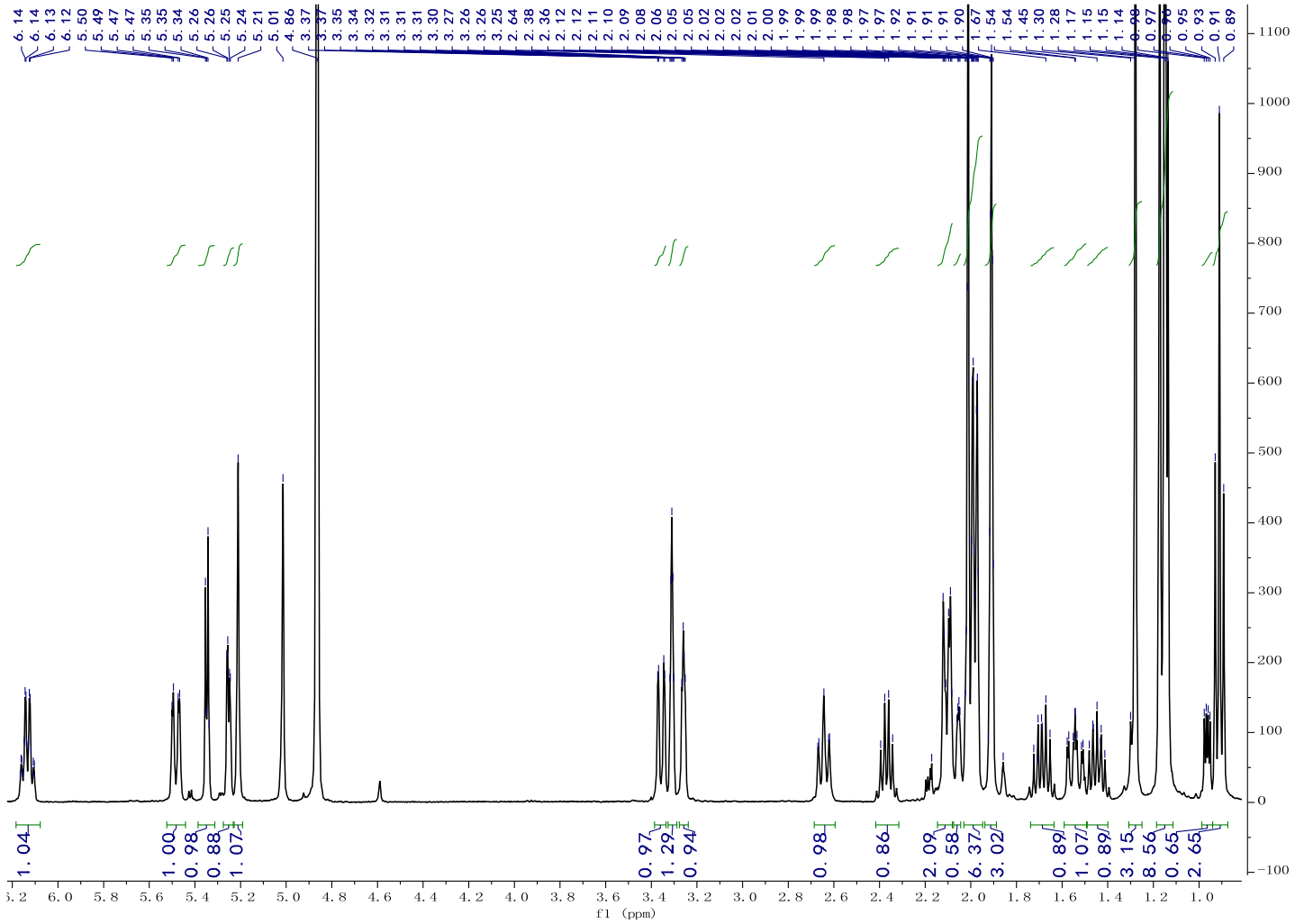


Figure S38. ^{13}C NMR (100 MHz, CD_3OD) spectrum of pararunine E (**7**)

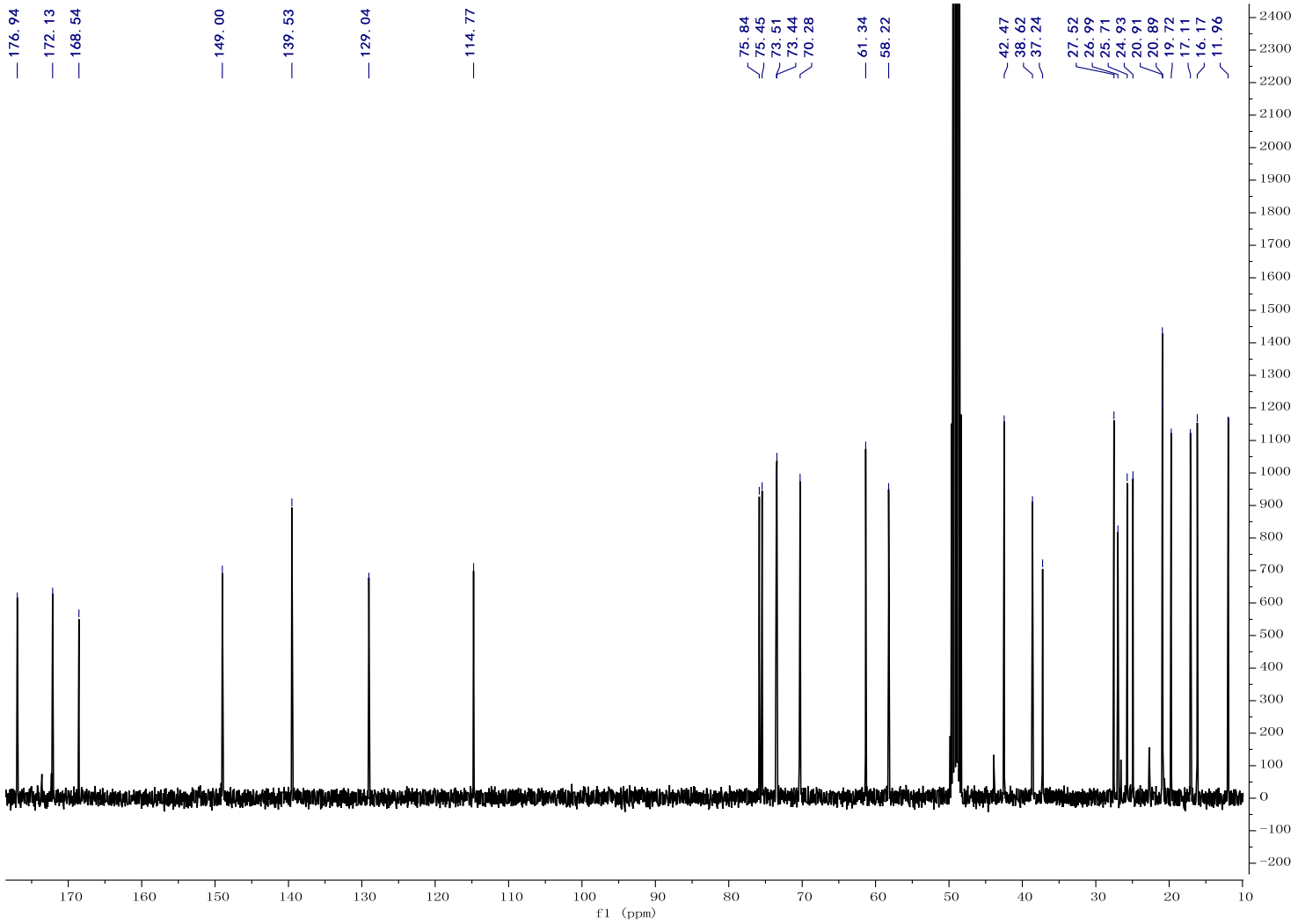


Figure S39. HSQC (400 MHz, CD_3OD) spectrum of pararunine E (**7**)

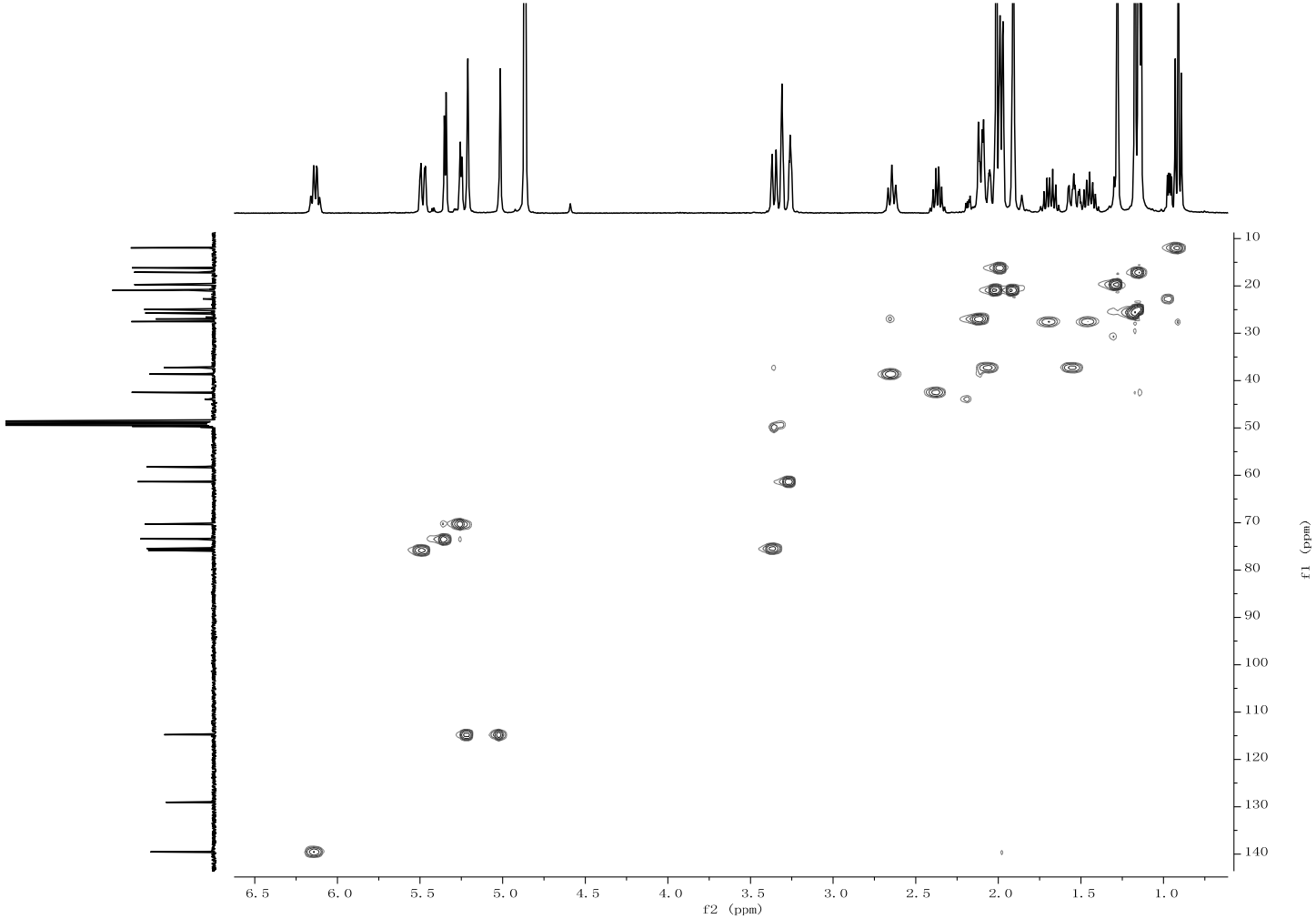


Figure S40. ^{1}H-^{1}H COSY (400 MHz, CD_3OD) spectrum of pararunine E (**7**)

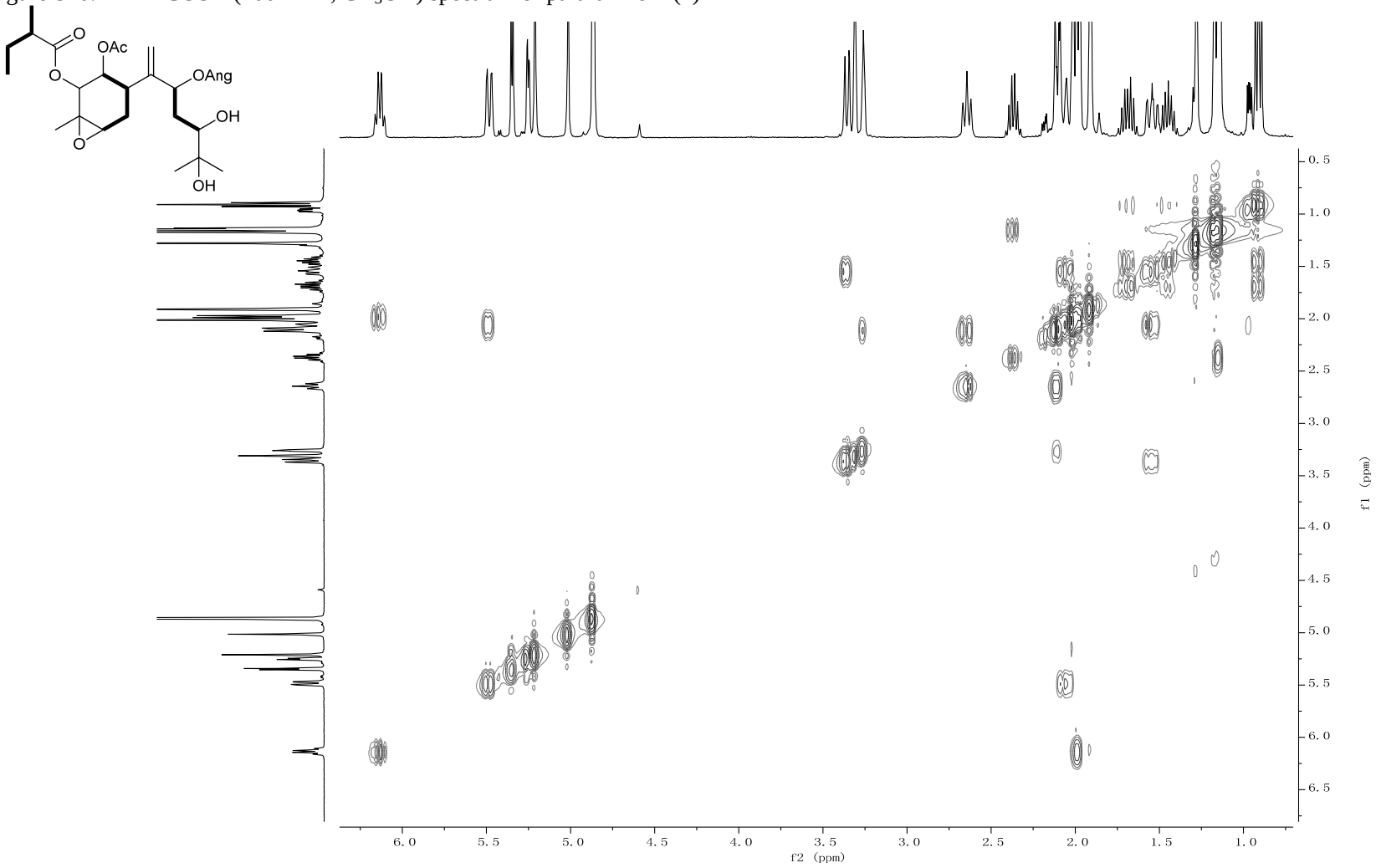


Figure S41. HMBC (400 MHz, CD_3OD) spectrum of pararunine E (**7**)

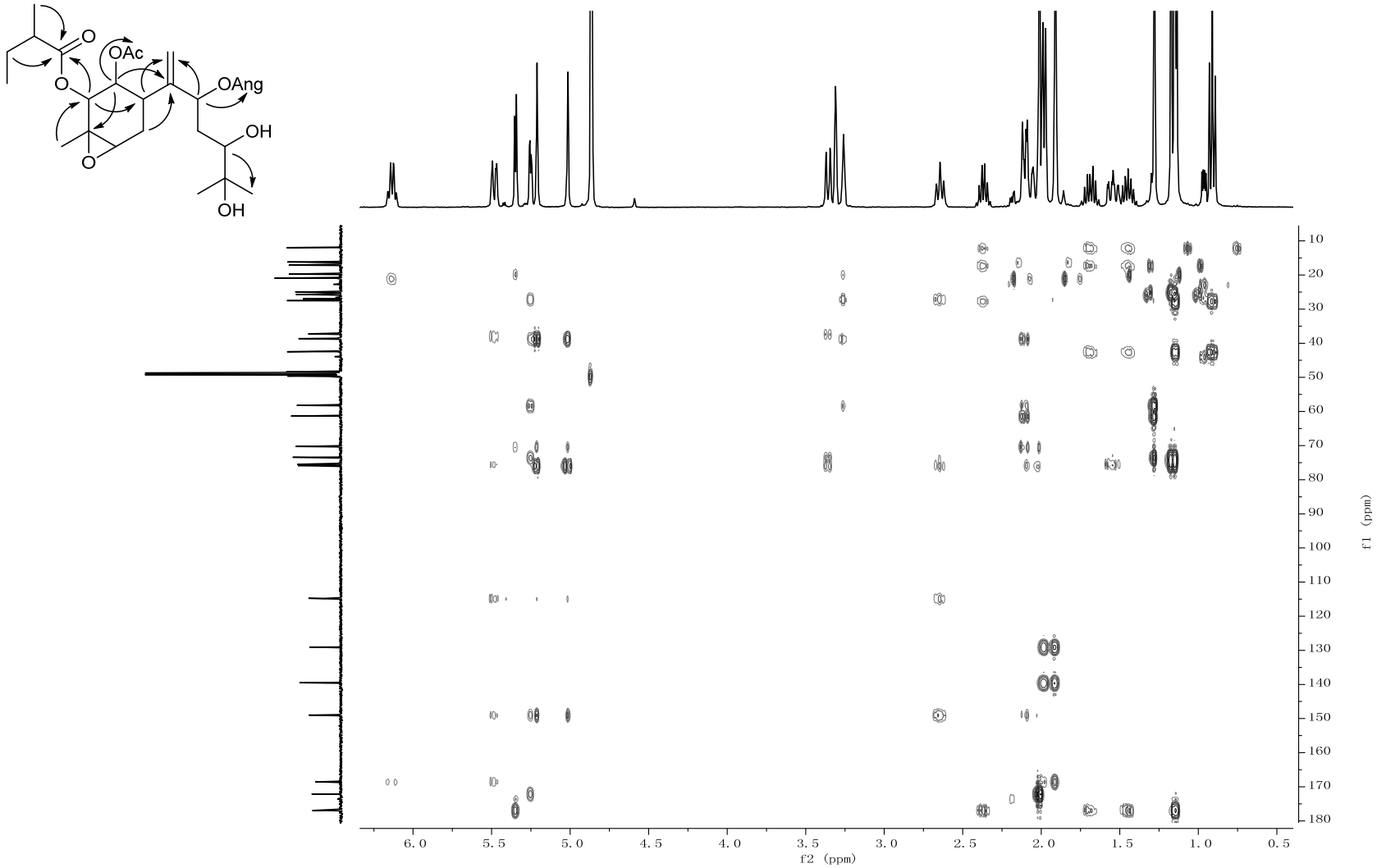


Figure S42. NOESY (400 MHz, CD_3OD) spectrum of pararunine E (**7**)

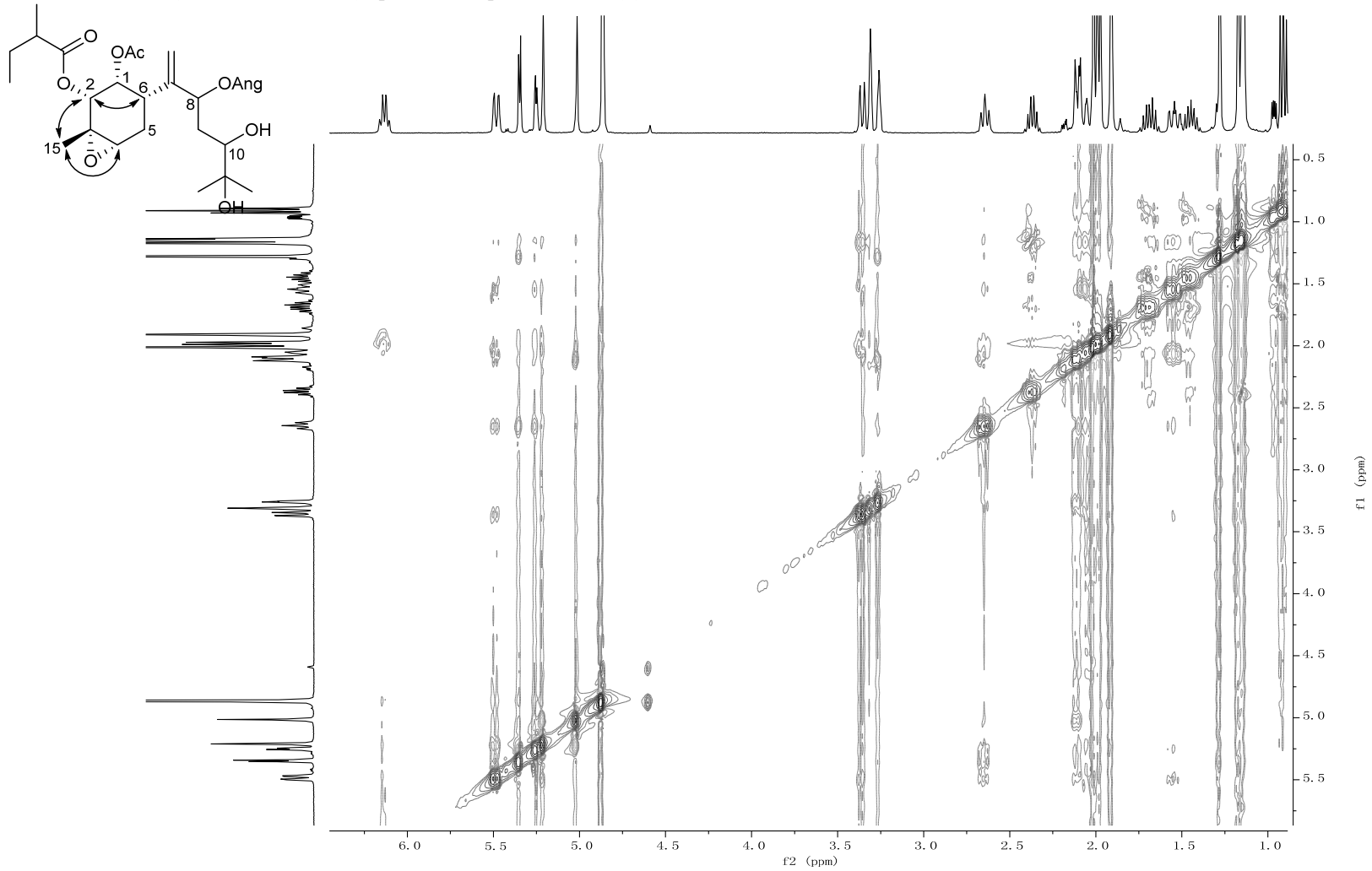


Figure S43. HRESIMS spectrum of pararunine E (**7**)

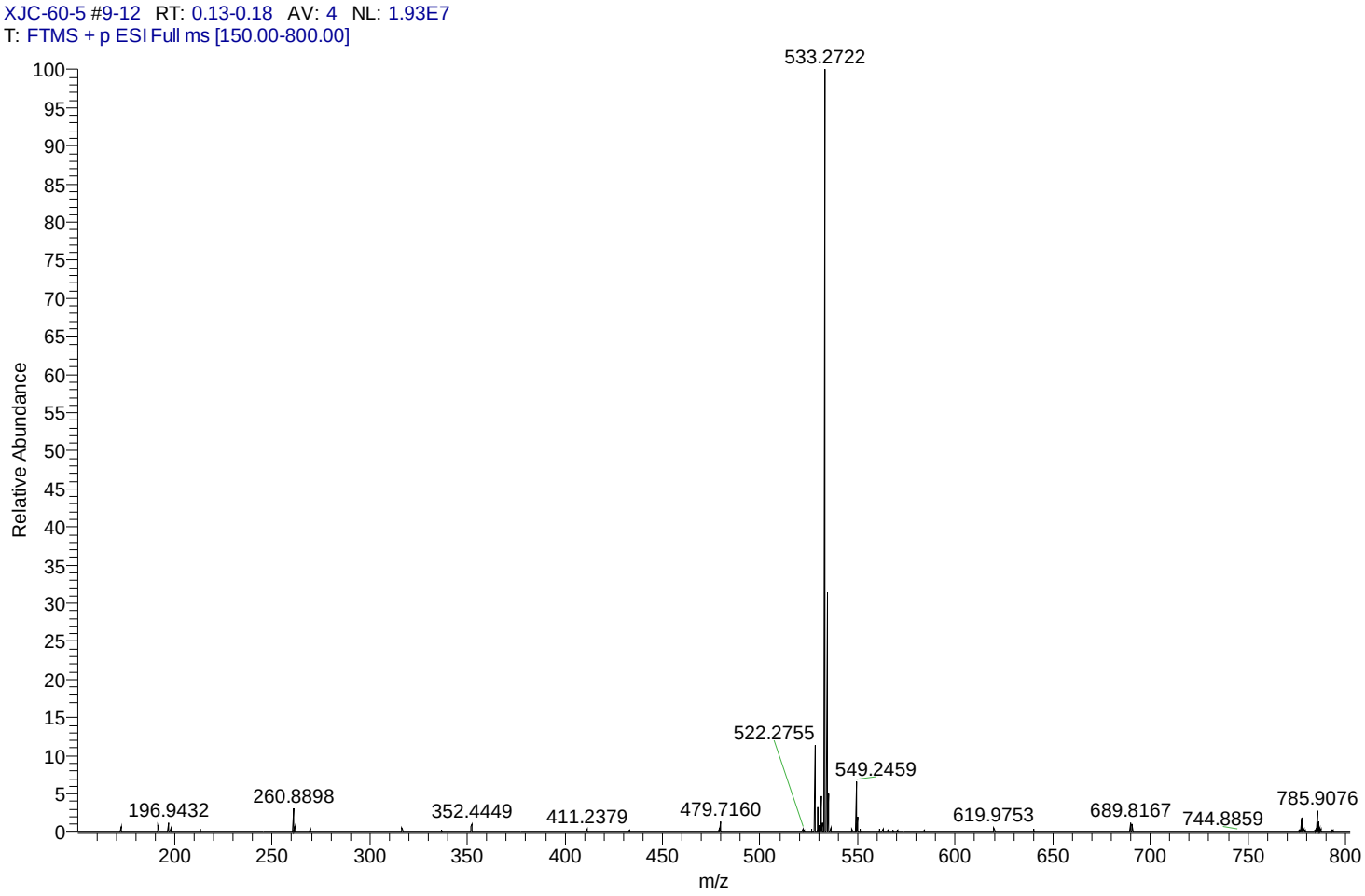


Figure S44. IR spectrum of pararunine E (**7**)

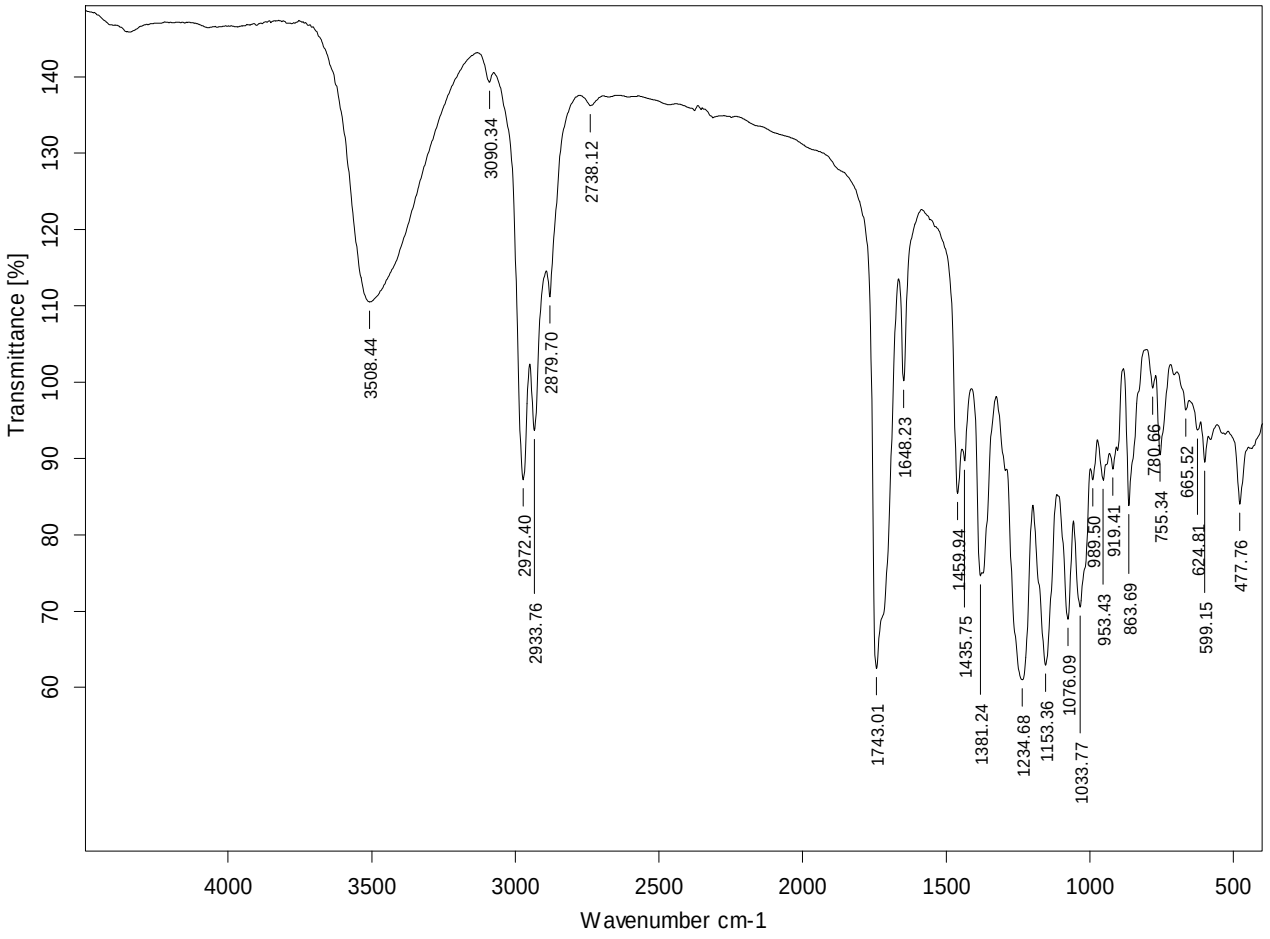


Figure S45. CD spectrum of pararunine E (**7**)

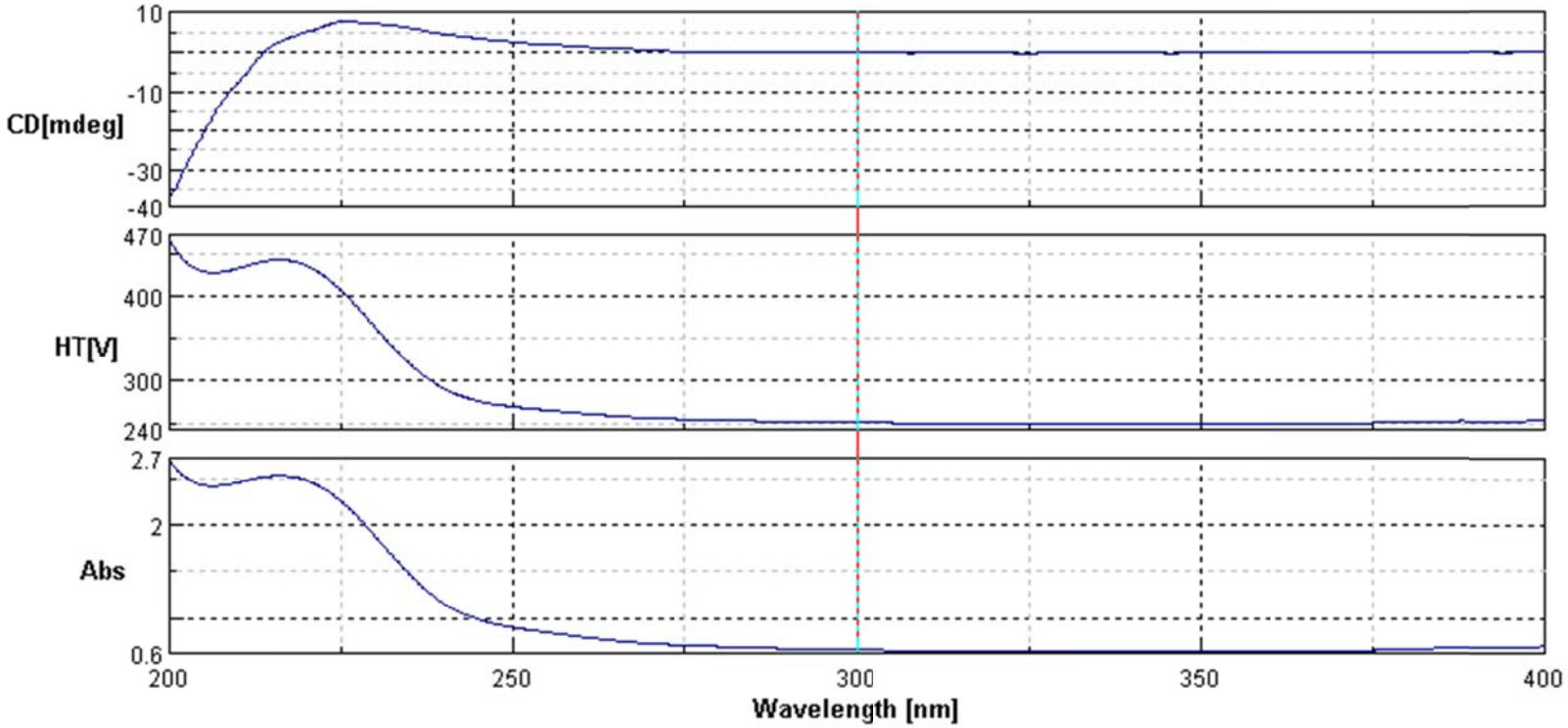


Figure S46. ^{1}H NMR (400 MHz, CD_3OD) spectrum of pararunine F (**8**)

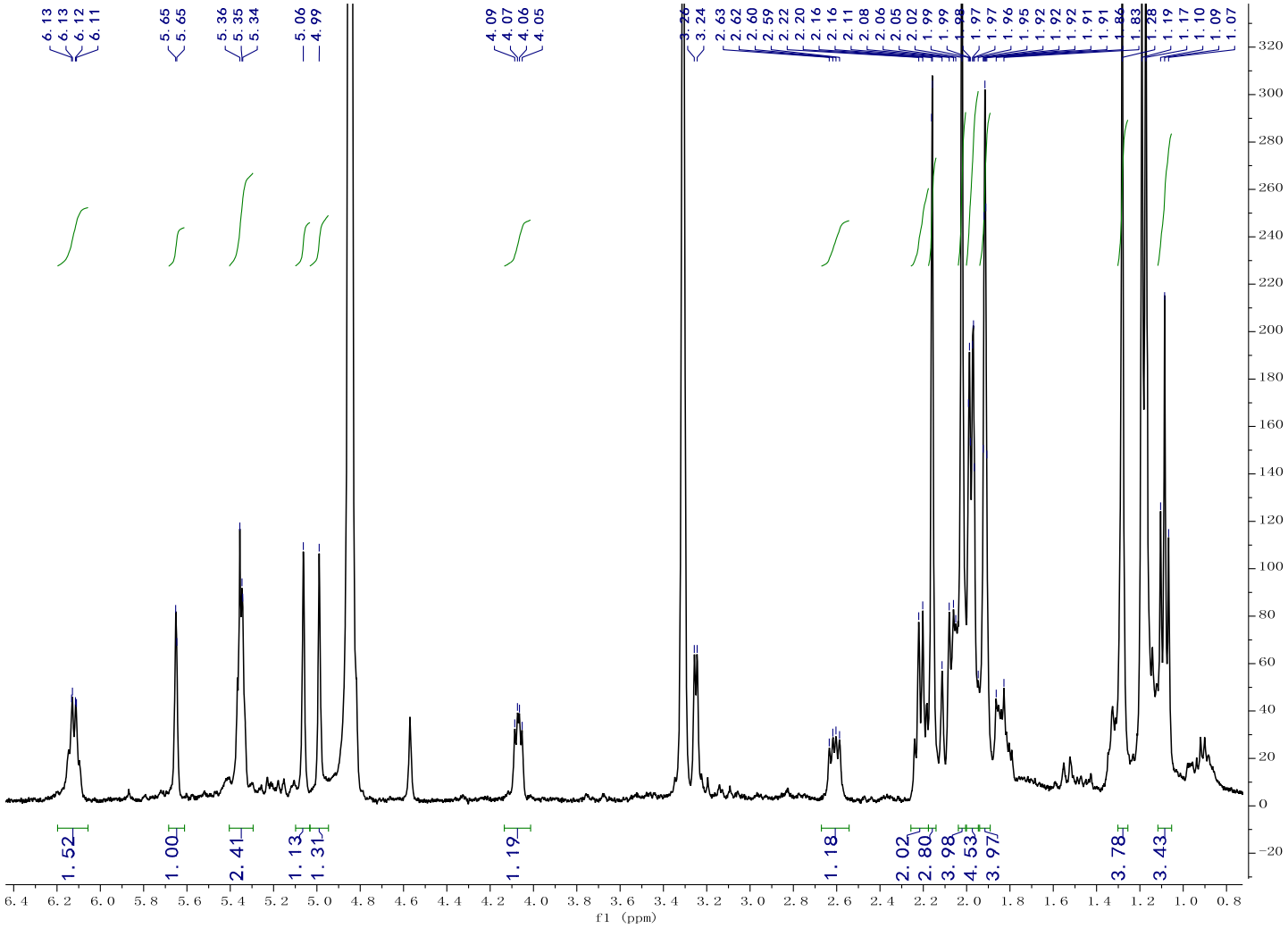


Figure S47. ^{13}C NMR (100 MHz, CD_3OD) spectrum of pararunine F (**8**)

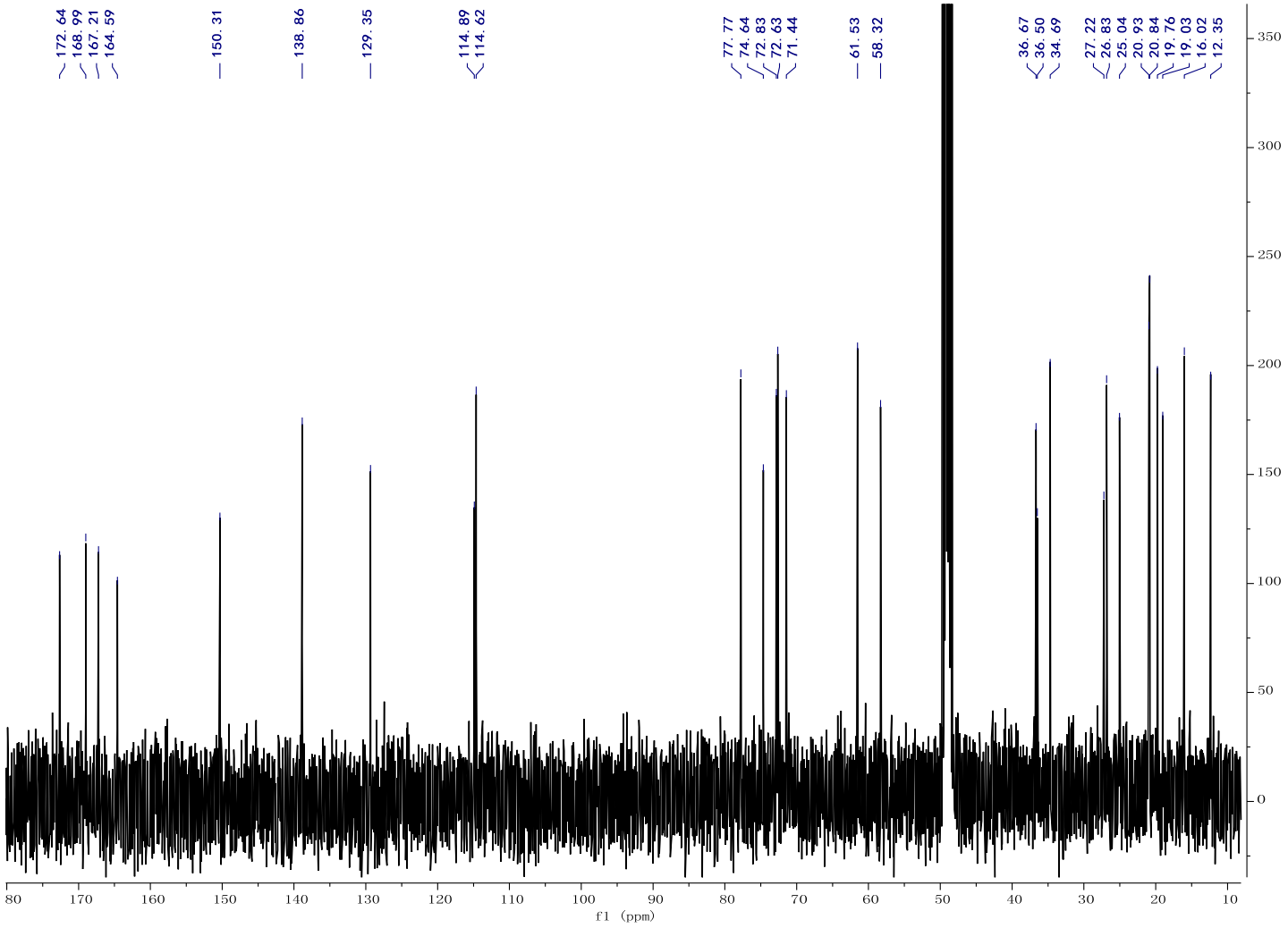


Figure S48. HSQC (400 MHz, CD_3OD) spectrum of pararunine F (**8**)

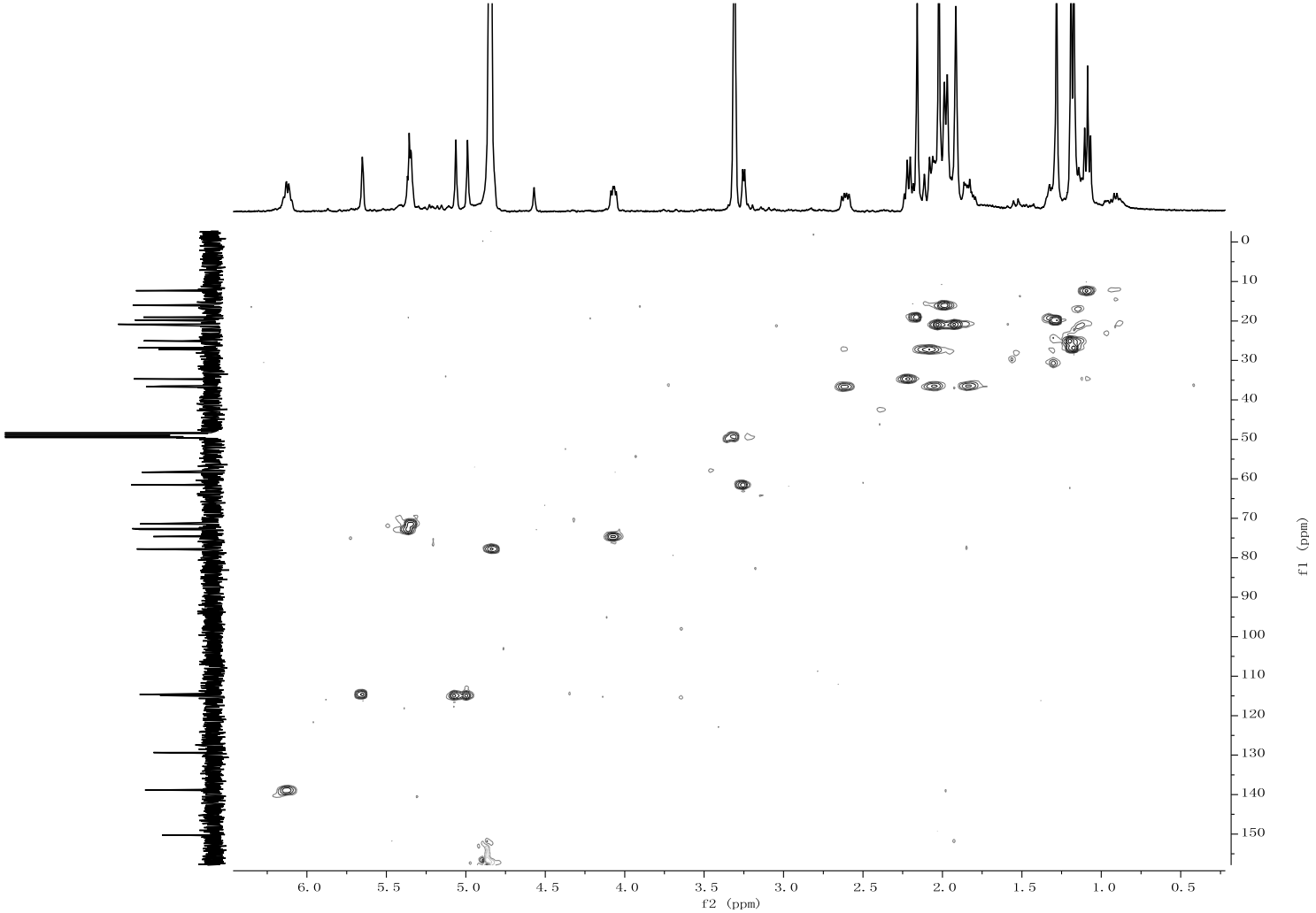


Figure S49. ^{1}H-^{1}H COSY (400 MHz, CD_3OD) spectrum of pararunine F (**8**)

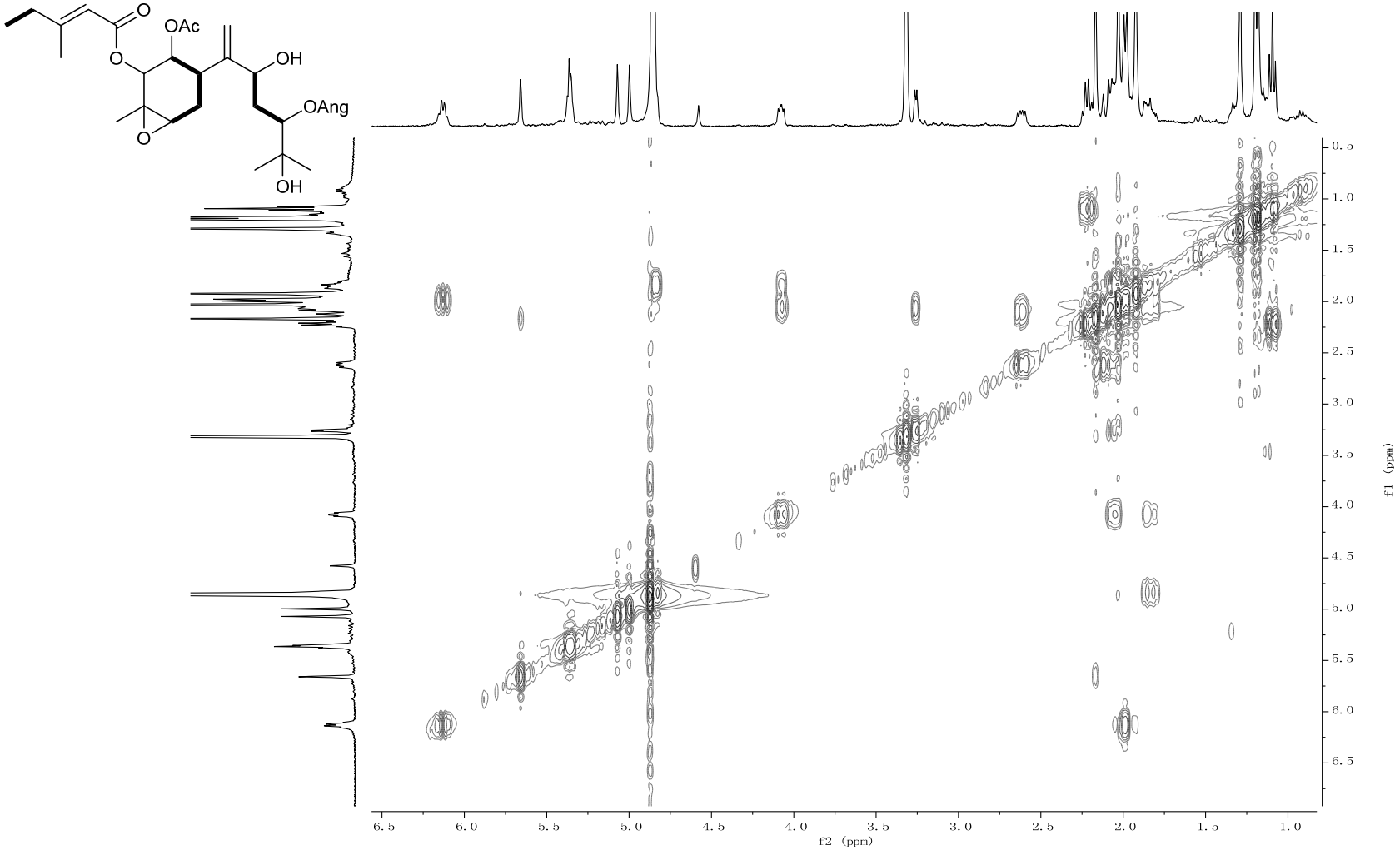


Figure S50. HMBC (400 MHz, CD_3OD) spectrum of pararunine F (**8**)

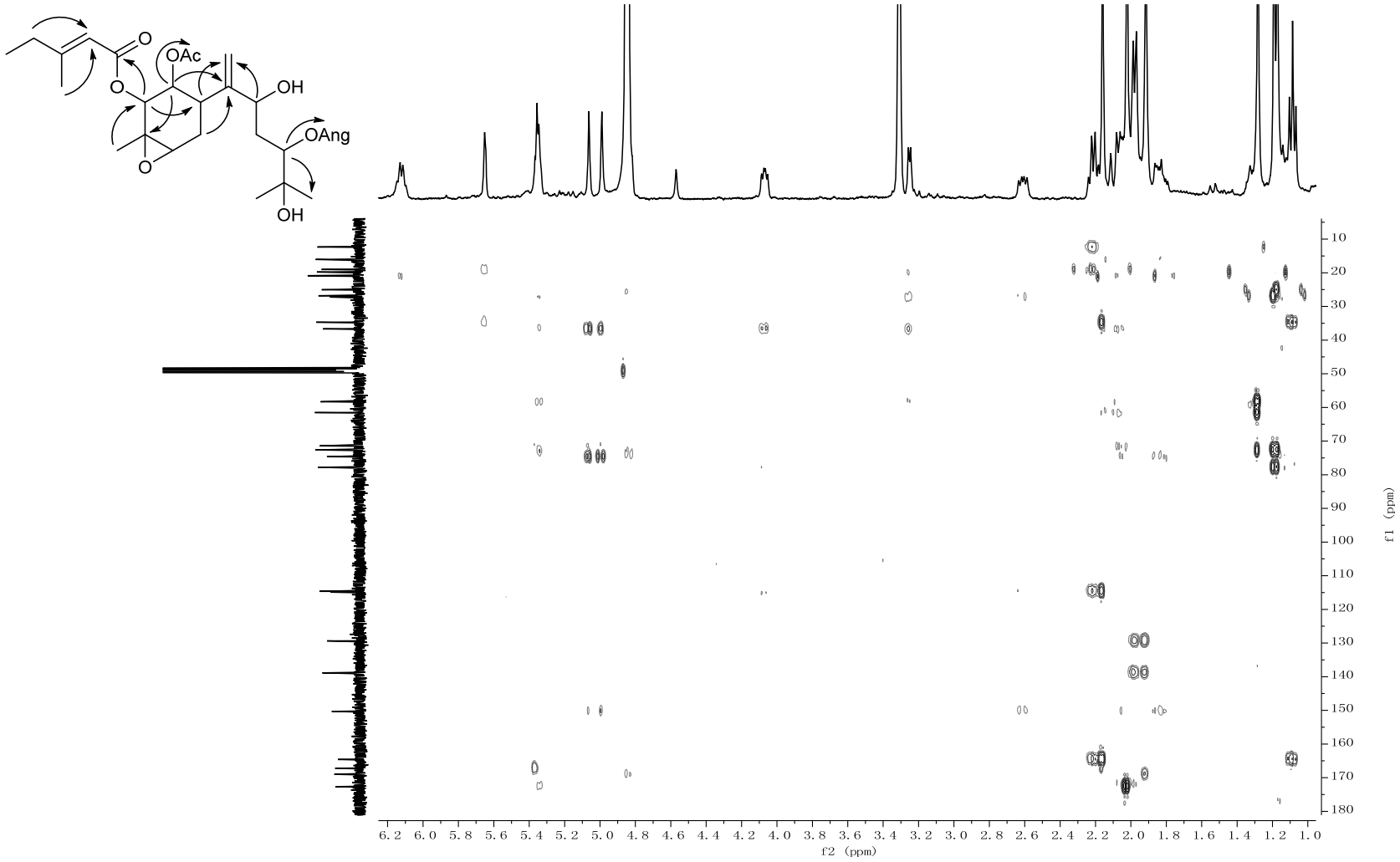


Figure S51. NOESY (400 MHz, CD_3OD) spectrum of pararunine F (**8**)

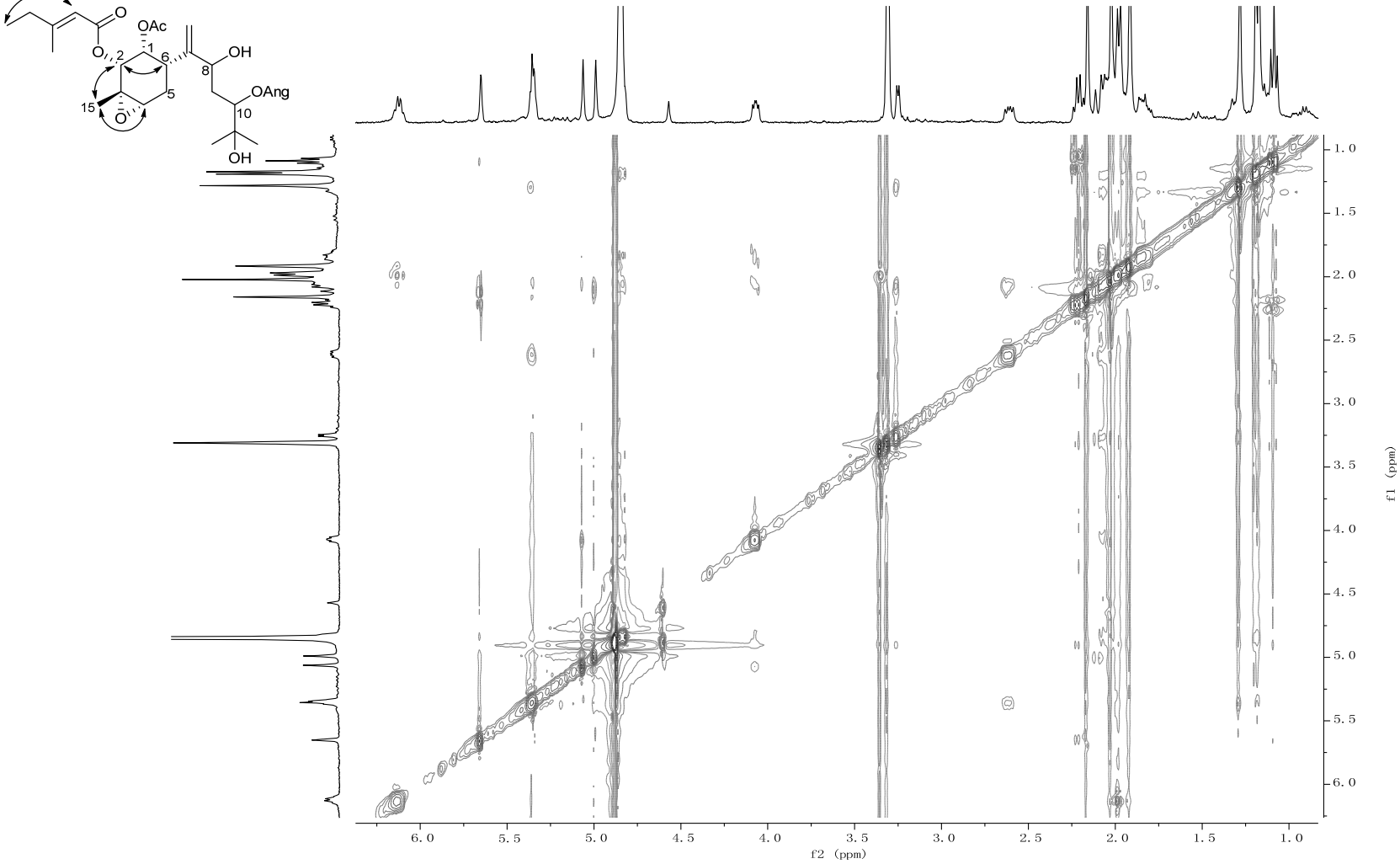


Figure S52. HRESIMS spectrum of pararunine F (**8**)

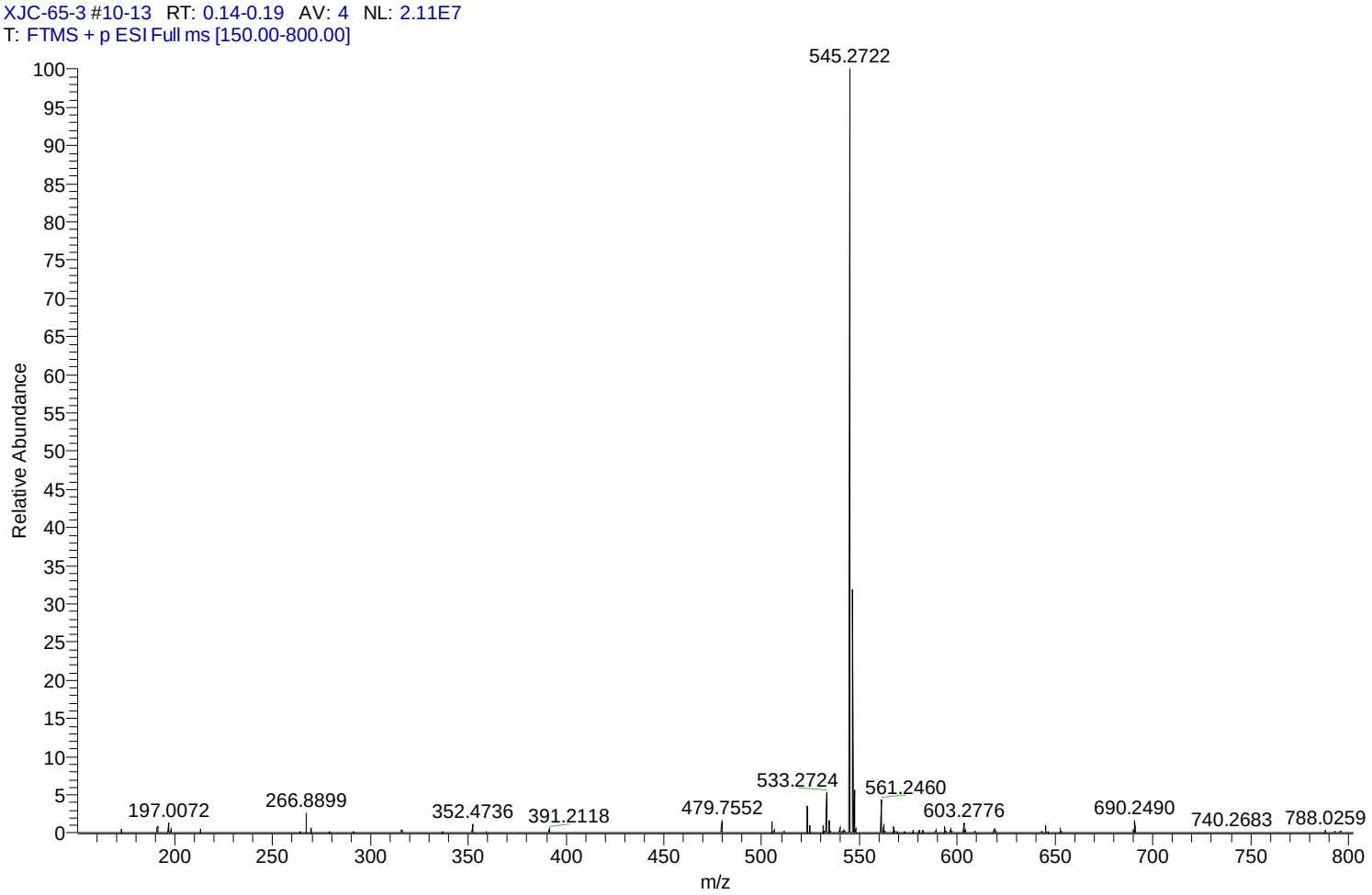


Figure S53. IR spectrum of pararunine F (**8**)

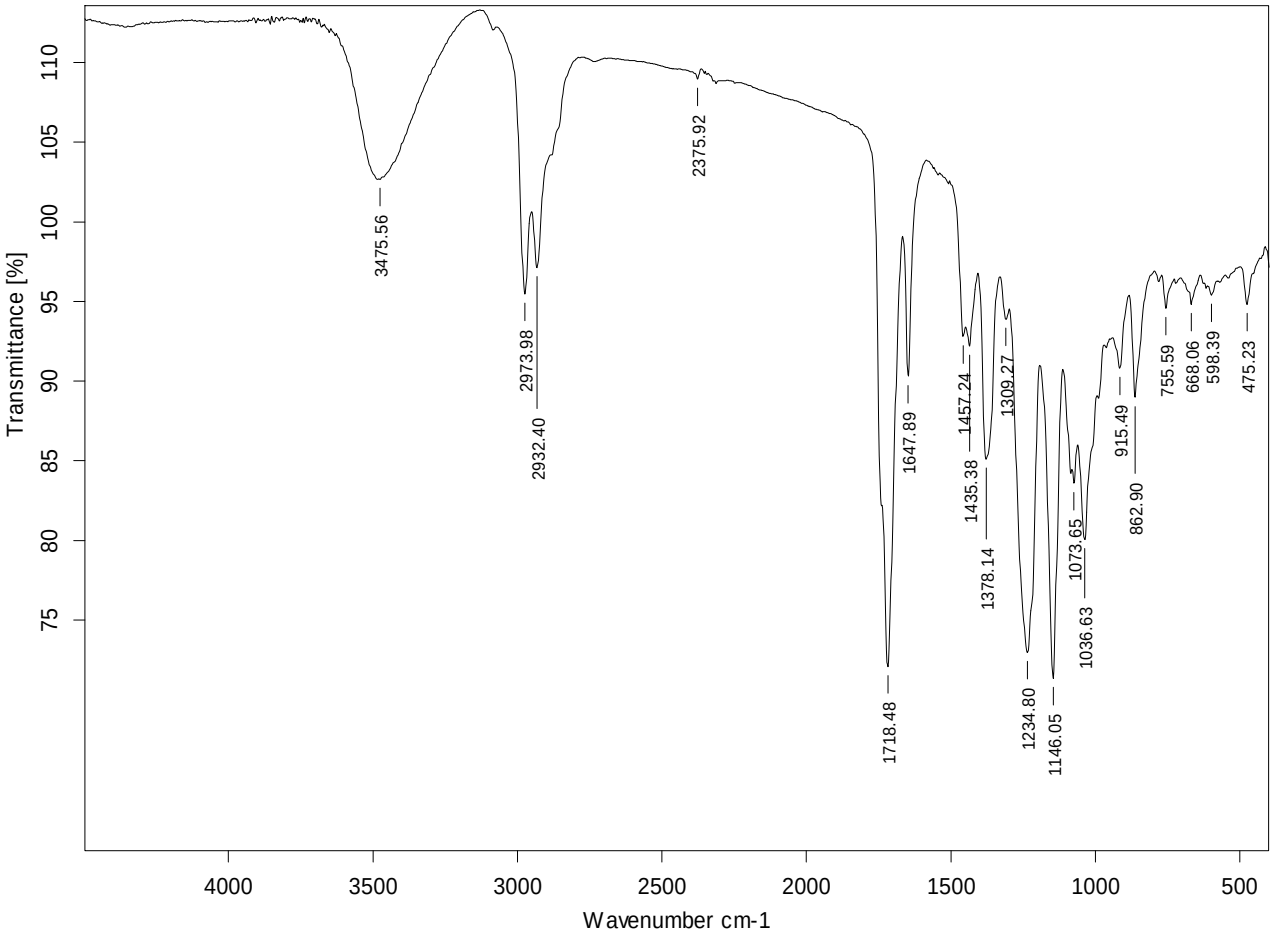


Figure S54. CD spectrum of pararunine F (**8**)

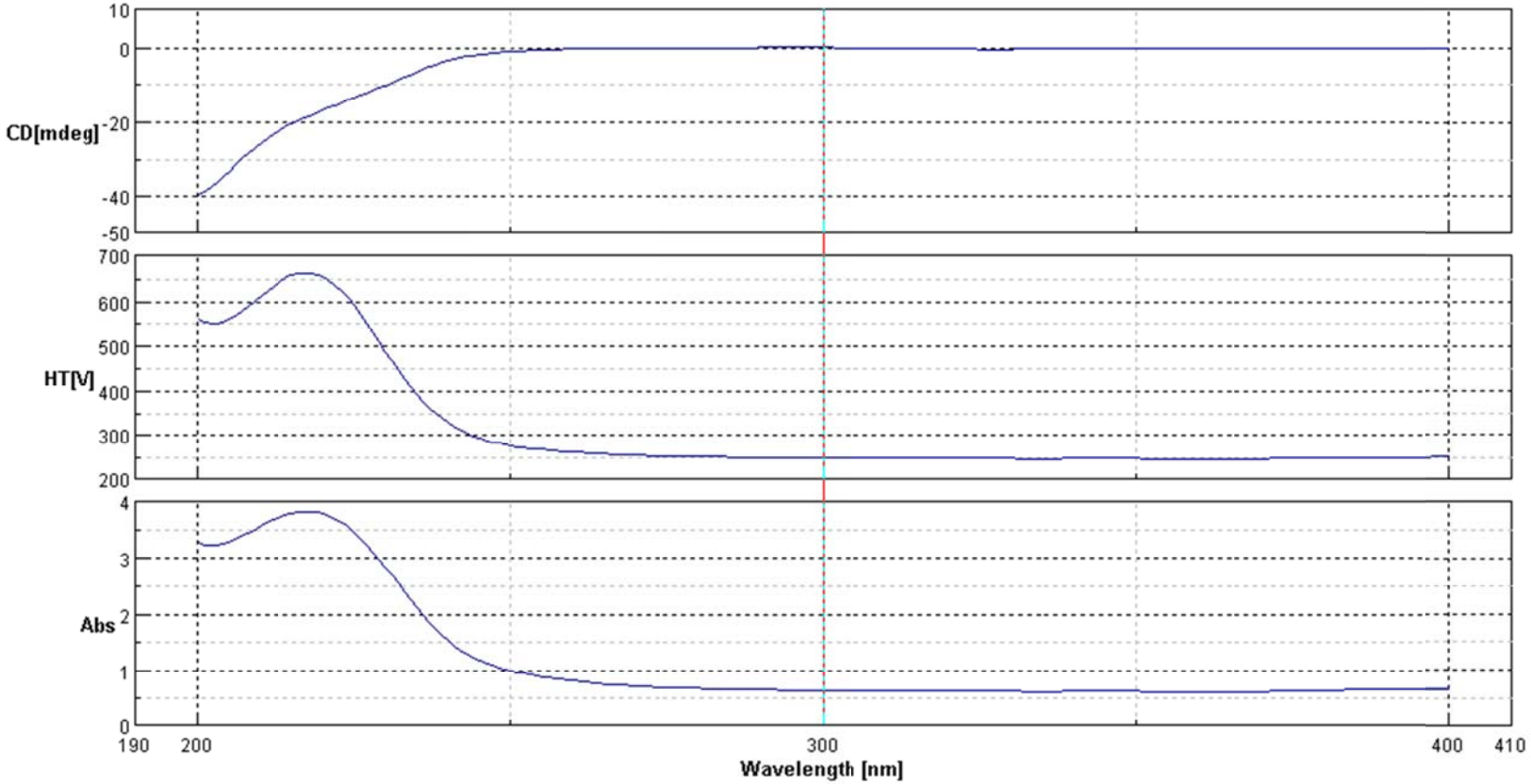


Figure S55. ^{1}H NMR (400 MHz, CD_3OD) spectrum of pararunine G (**9**)

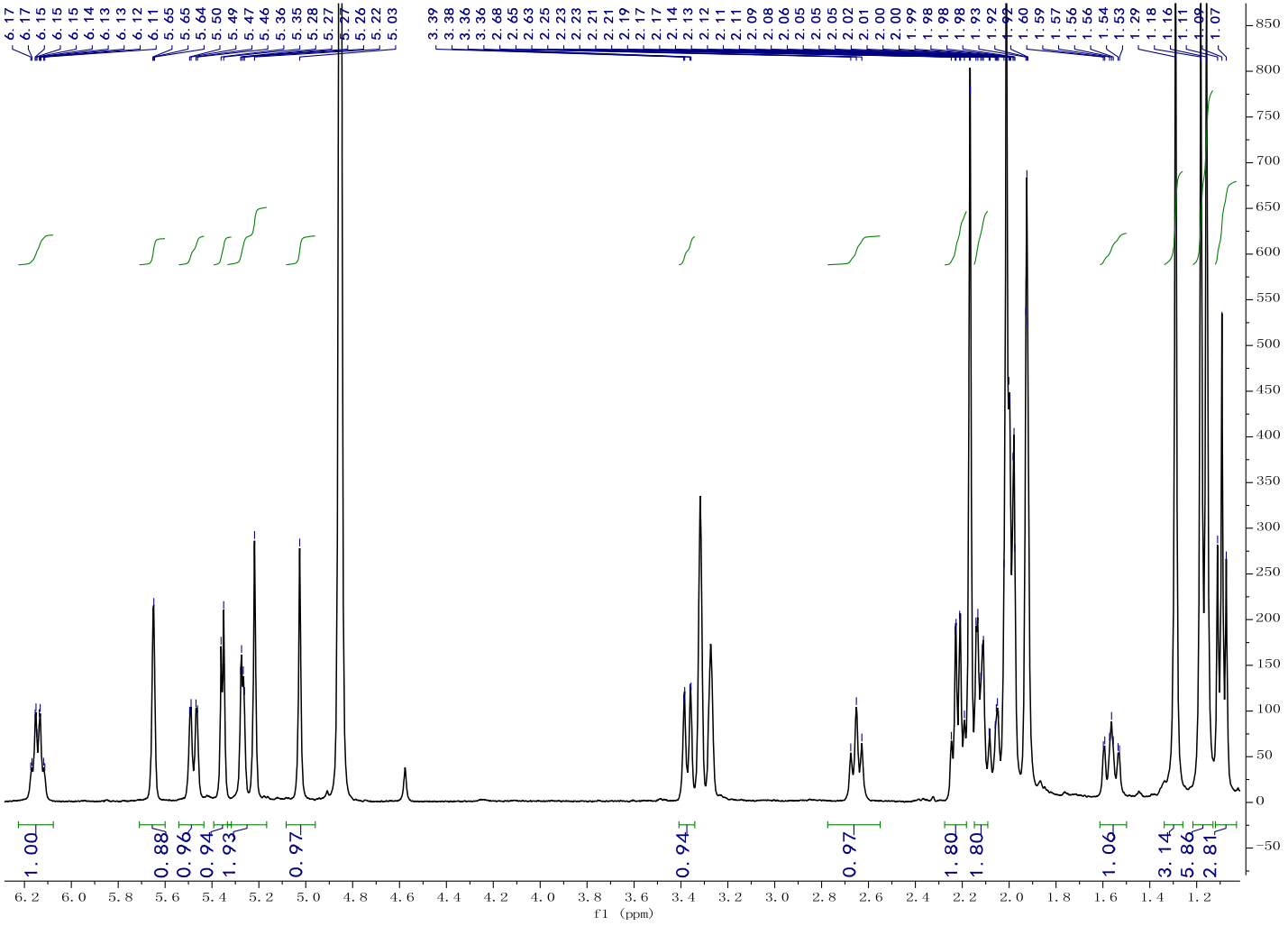


Figure S56. ^{13}C NMR (100 MHz, CD_3OD) spectrum of pararunine G (**9**)

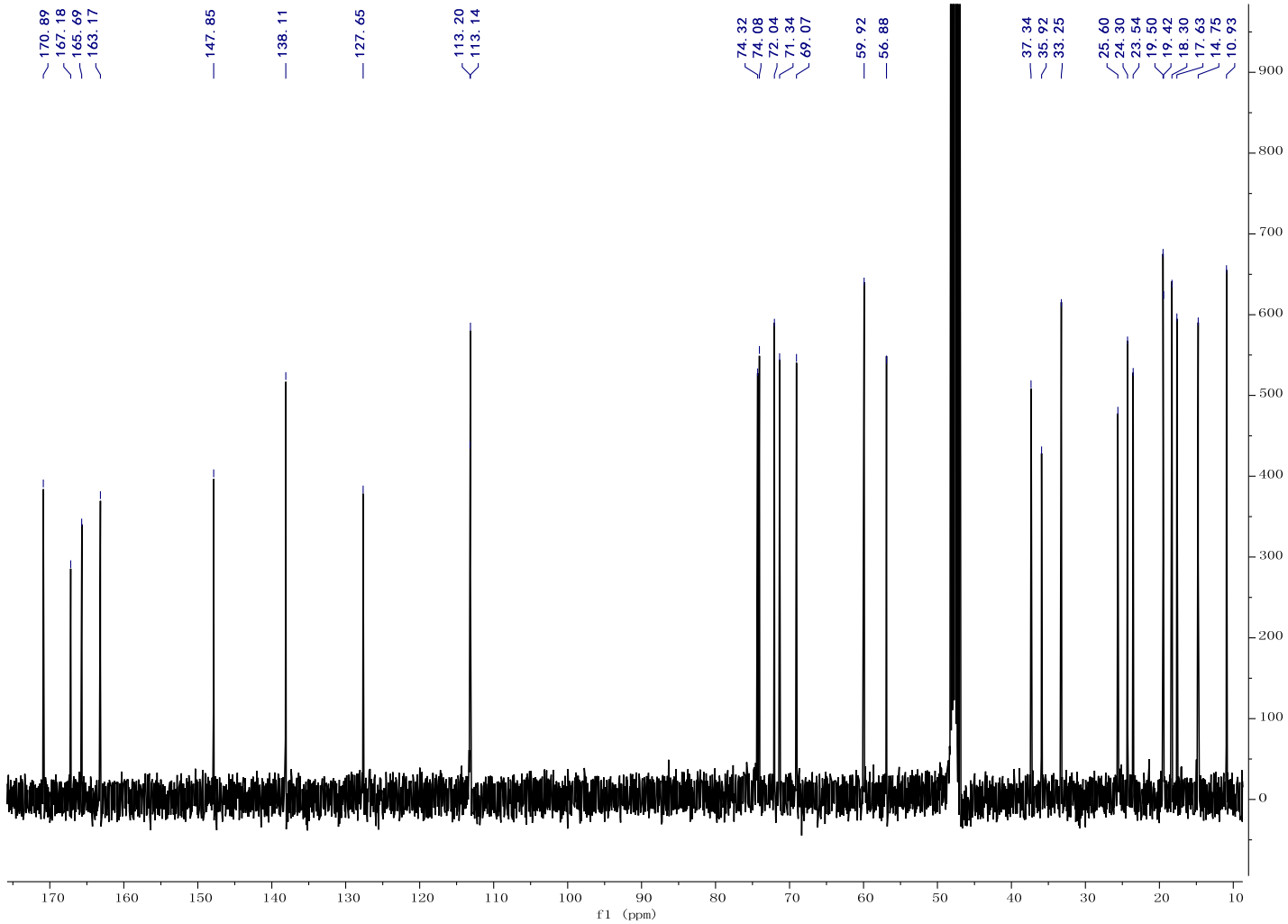


Figure S57. HSQC (400 MHz, CD_3OD) spectrum of pararunine G (**9**)

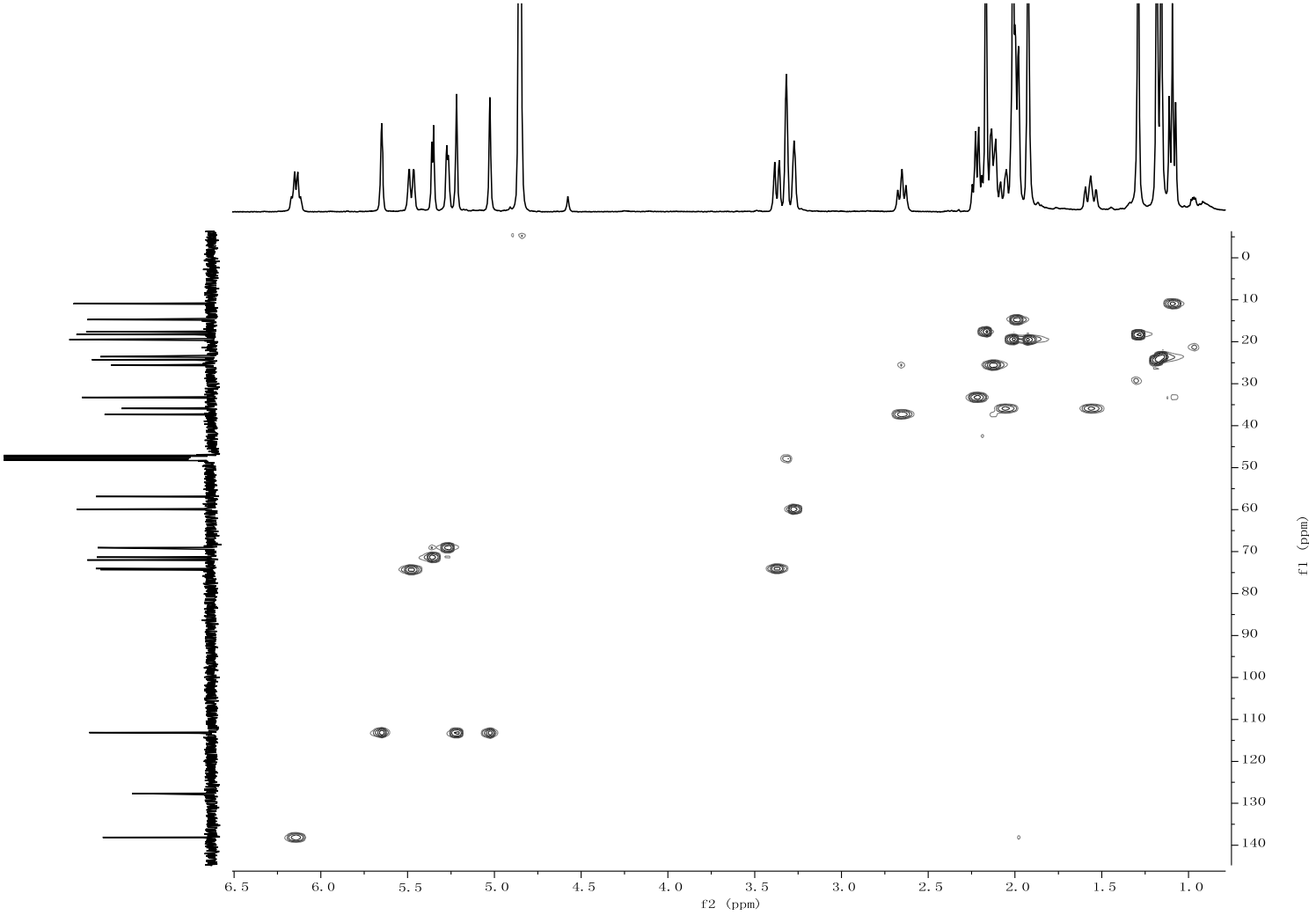


Figure S58. ^{1}H-^{1}H COSY (400 MHz, CD_3OD) spectrum of pararunine G (**9**)

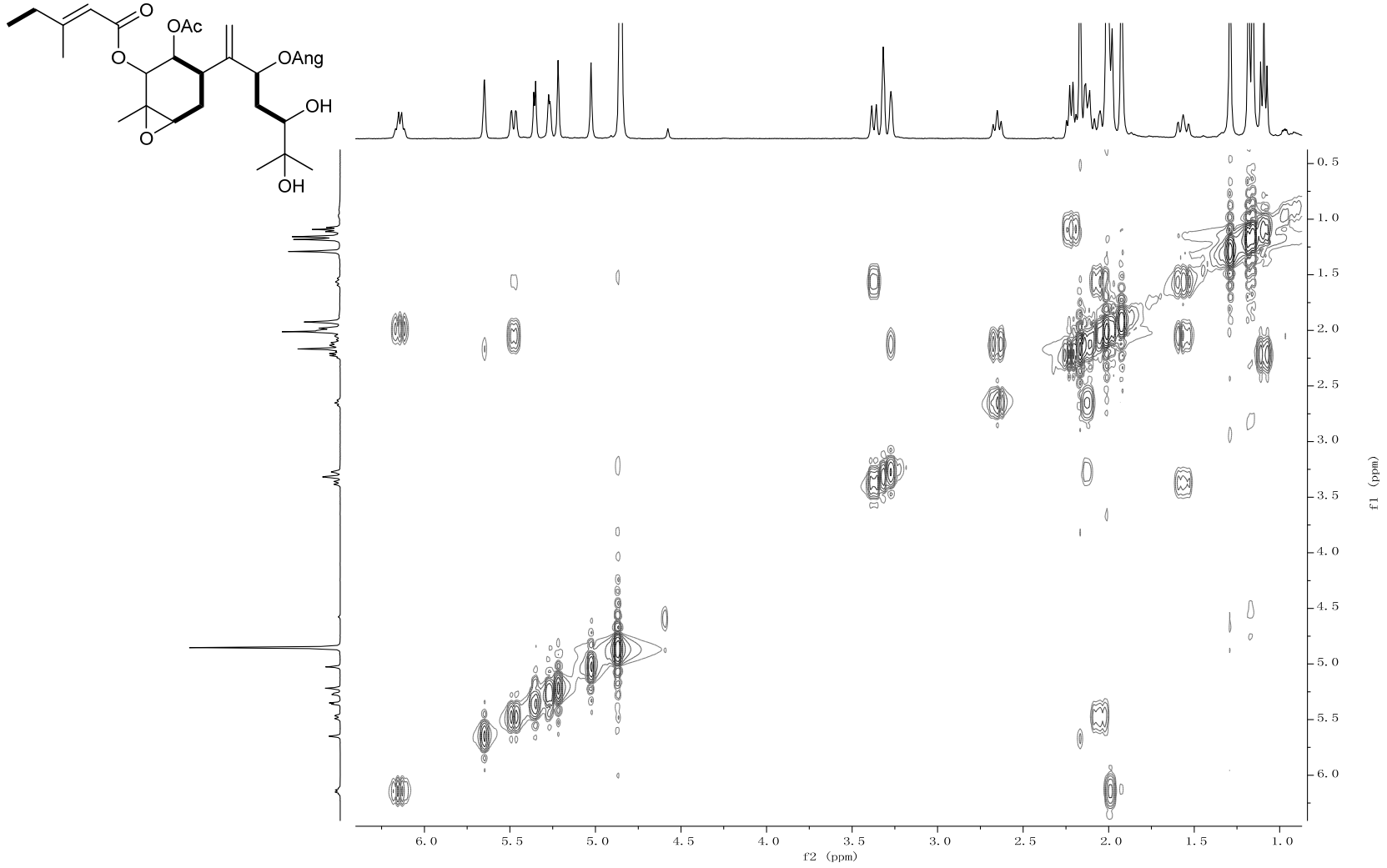


Figure S59. HMBC (400 MHz, CD_3OD) spectrum of pararunine G (**9**)

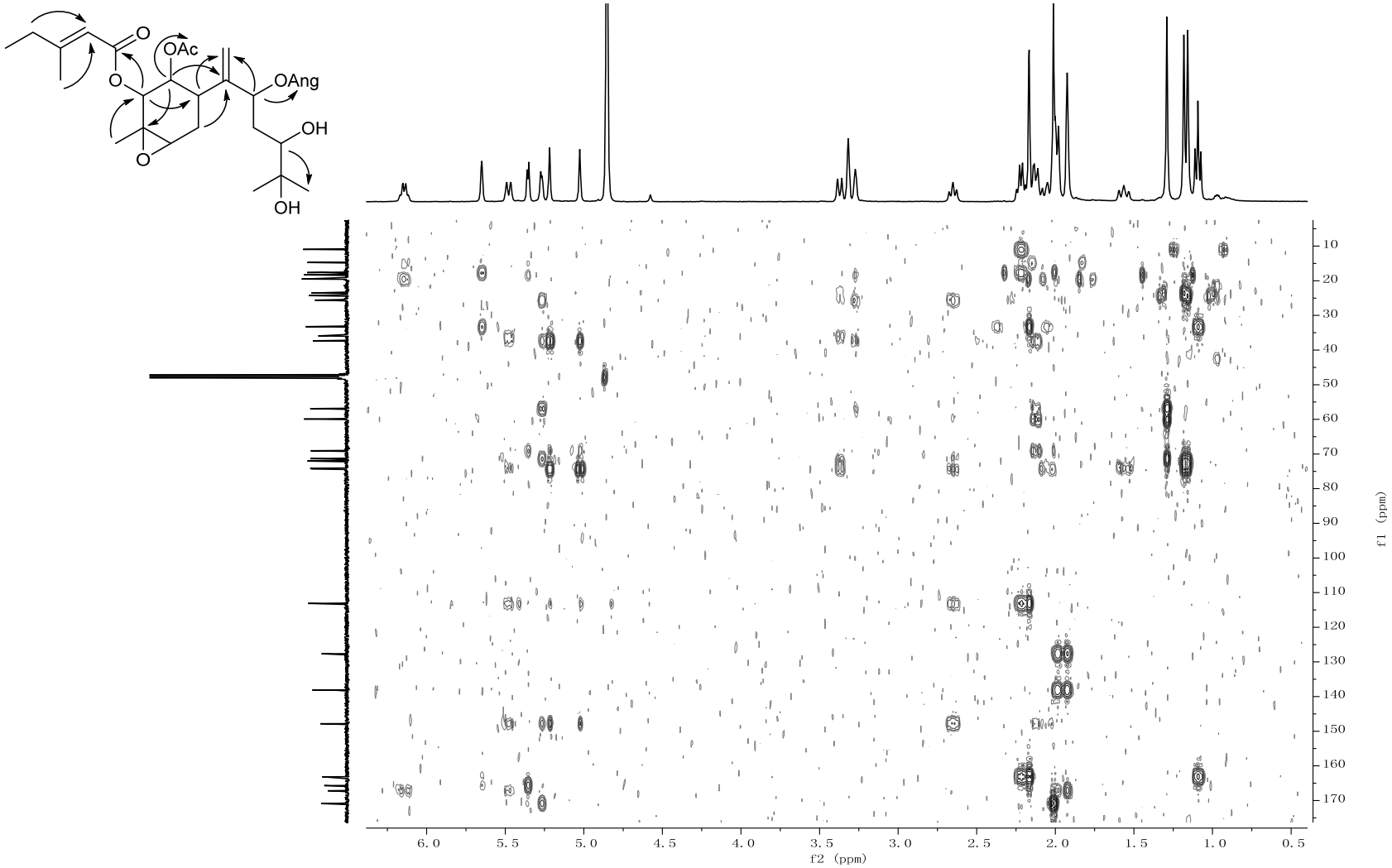


Figure S60. NOESY (400 MHz, CD_3OD) spectrum of pararunine G (**9**)

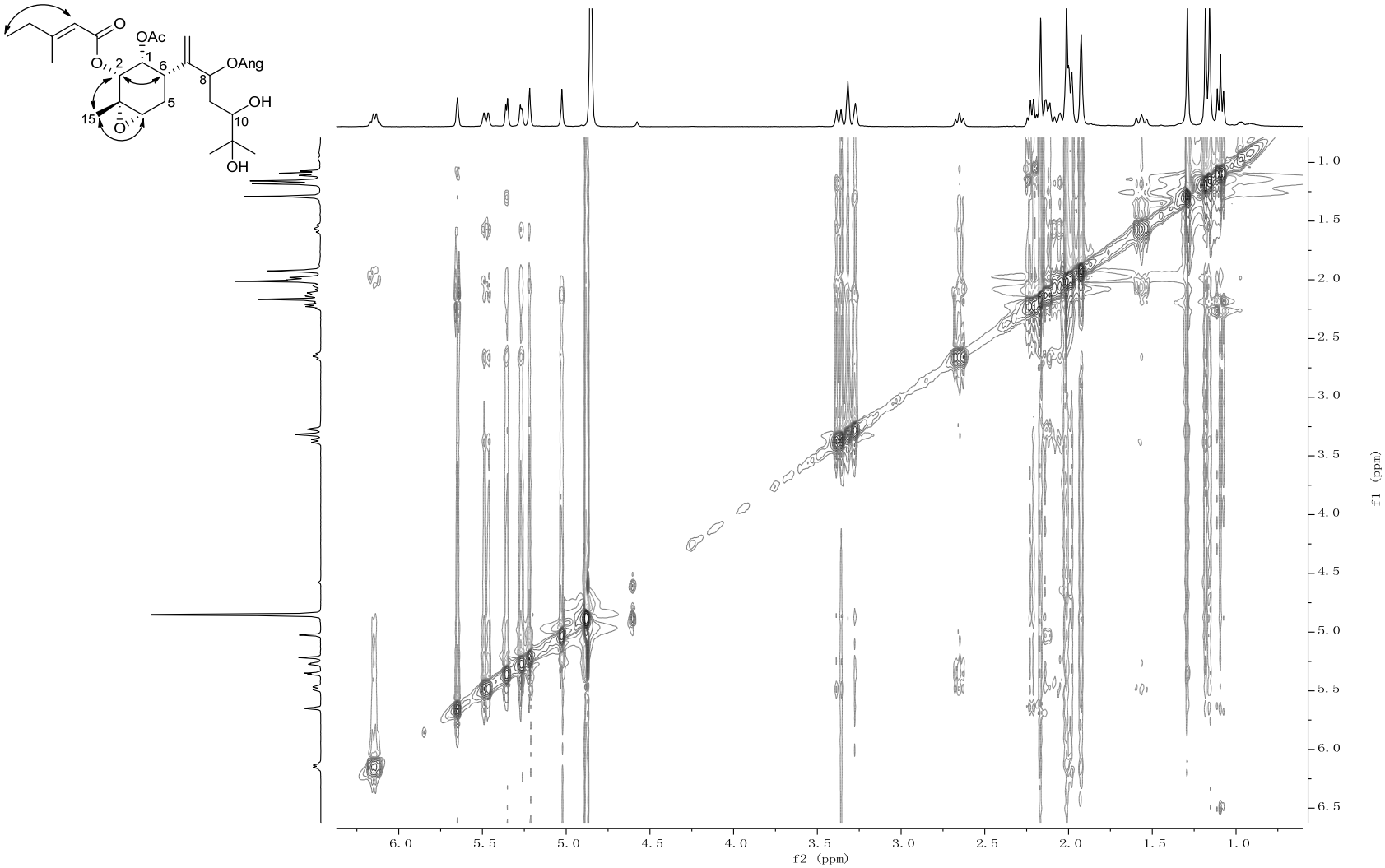


Figure S61. HRESIMS spectrum of pararunine G (**9**)

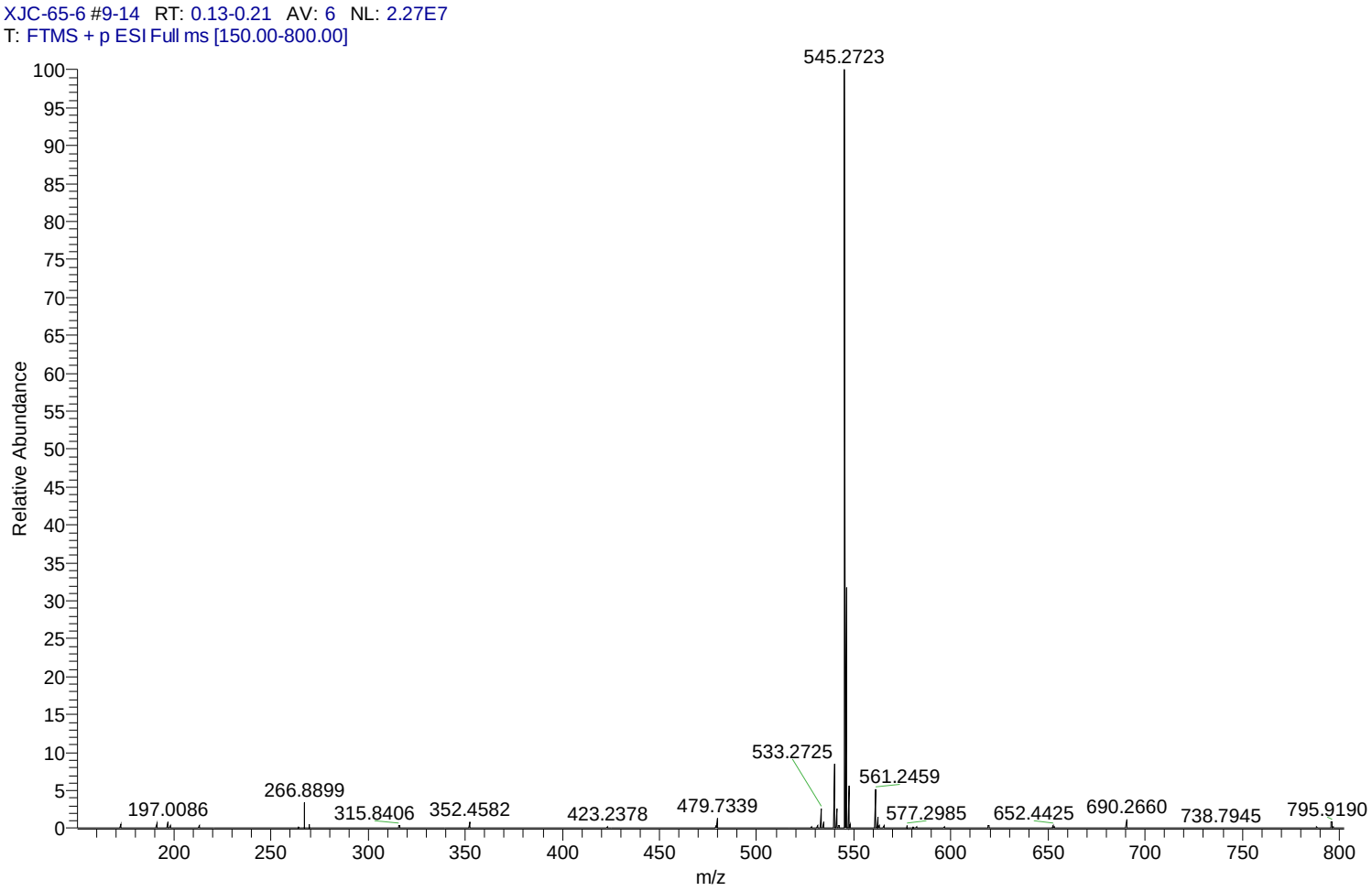


Figure S62. IR spectrum of pararunine G (**9**)

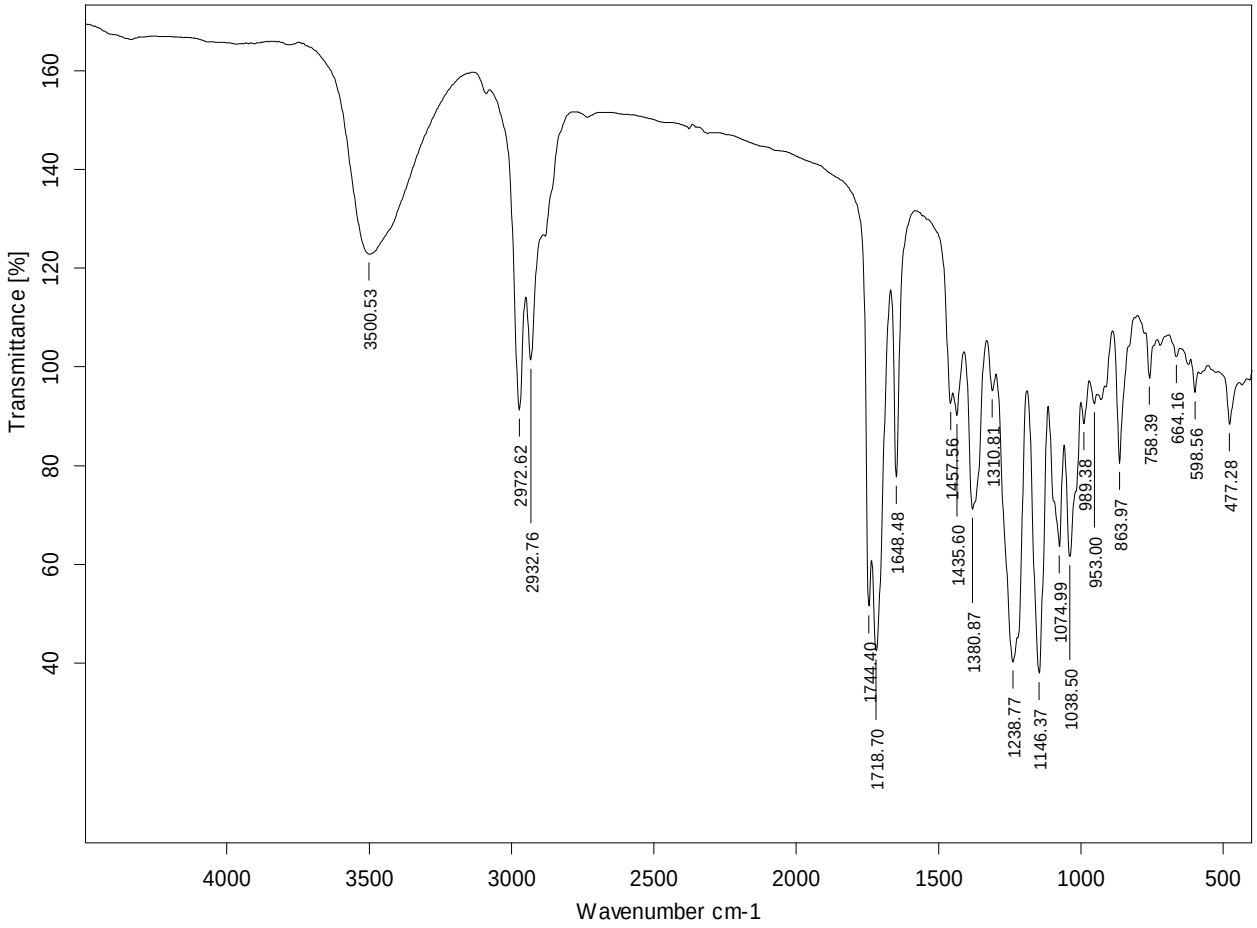


Figure S63. CD spectrum of pararunine G (**9**)

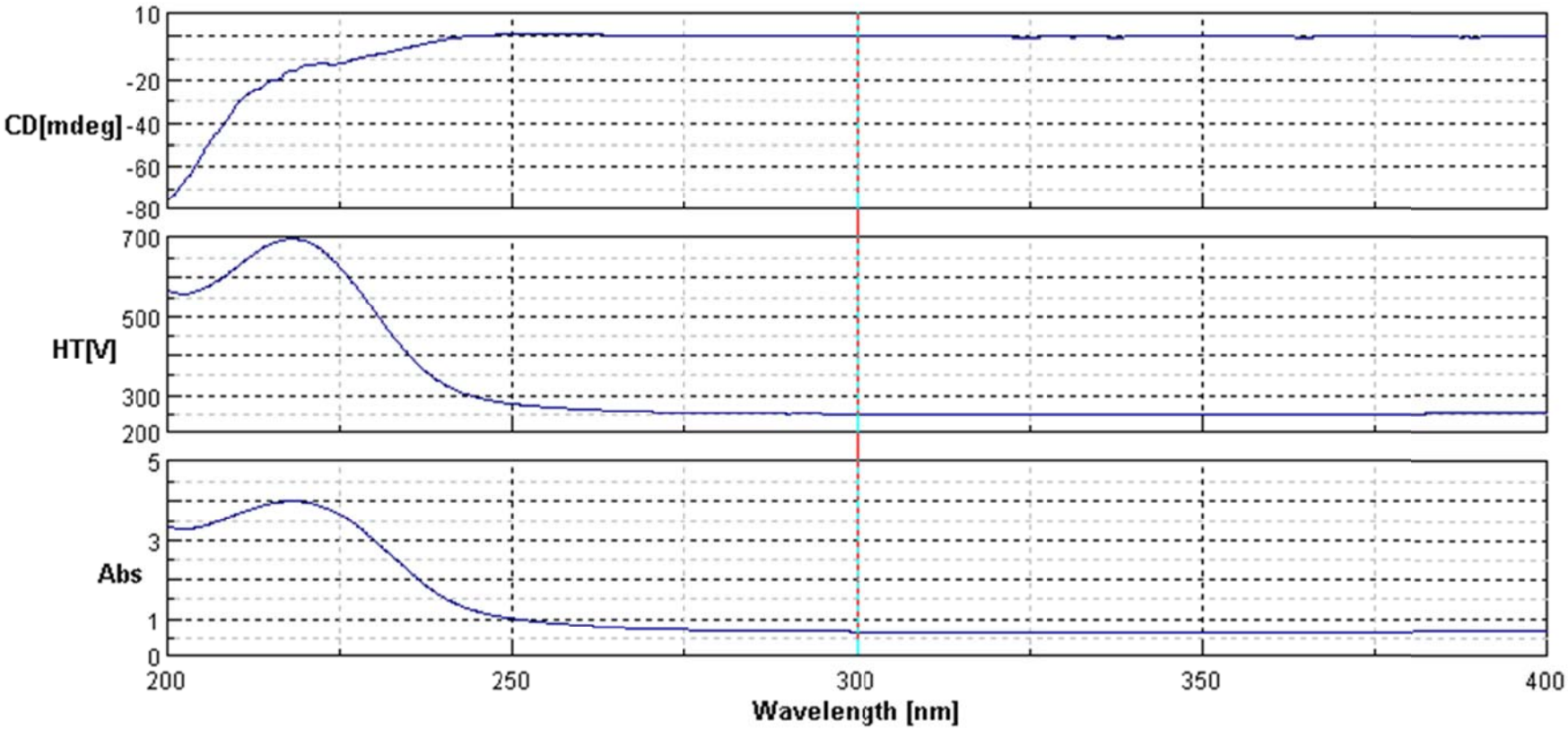


Figure S64. ^{1}H NMR (400 MHz, CD_3OD) spectrum of pararunine H (**12**)

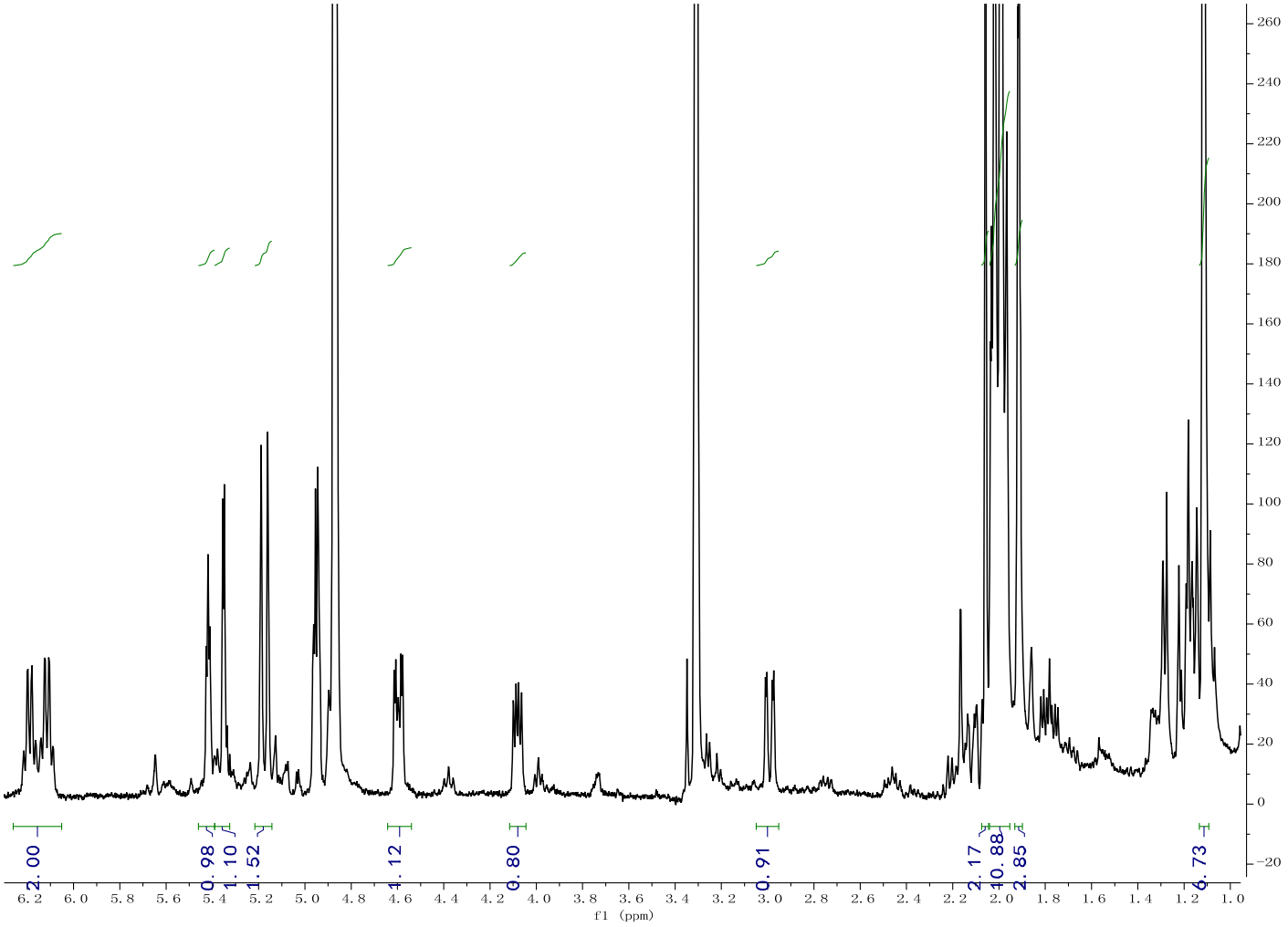


Figure S65. ^{13}C NMR (100 MHz, CD_3OD) spectrum of pararunine H (**12**)

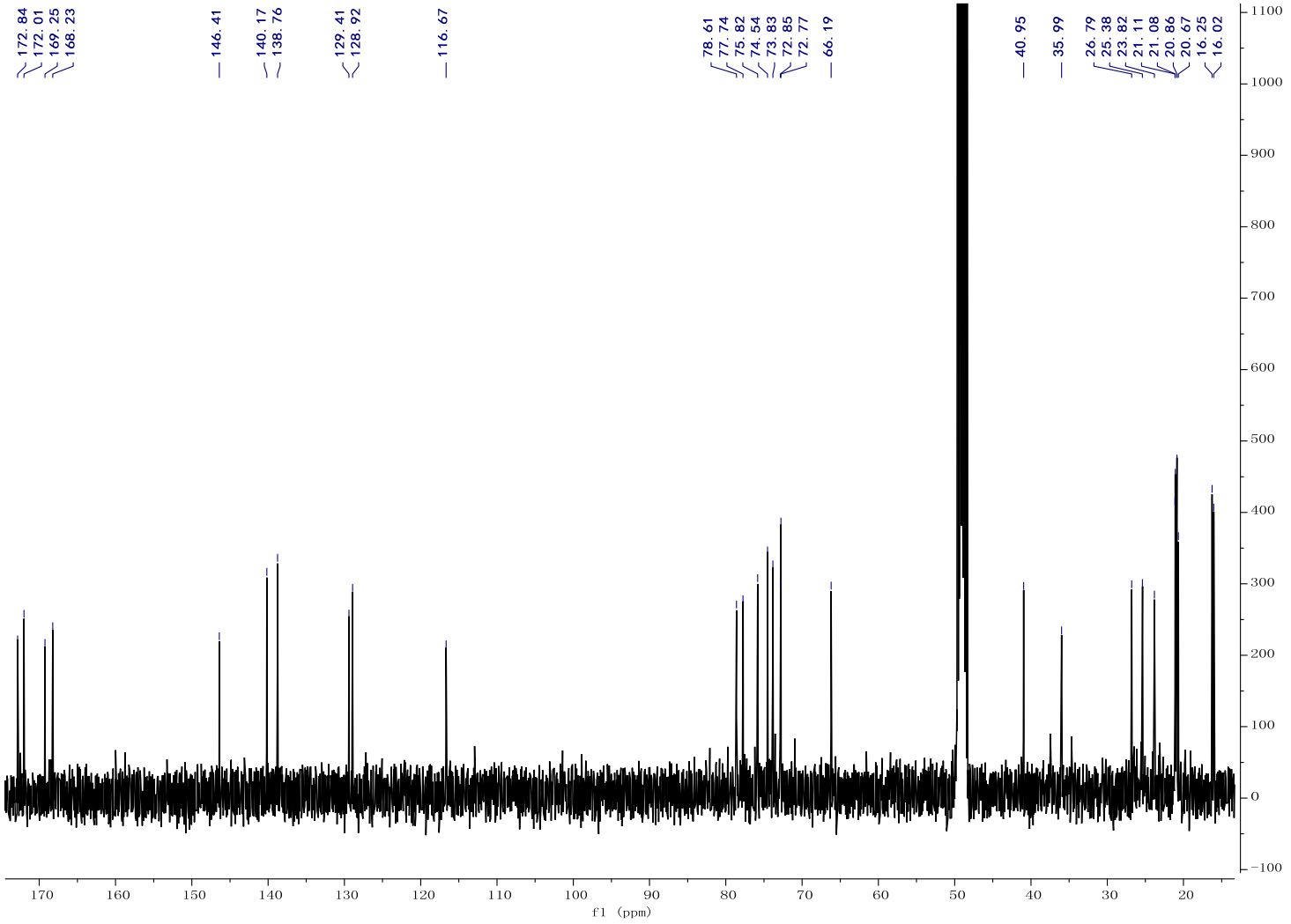


Figure S66. HSQC (400 MHz, CD_3OD) spectrum of pararunine H (**12**)

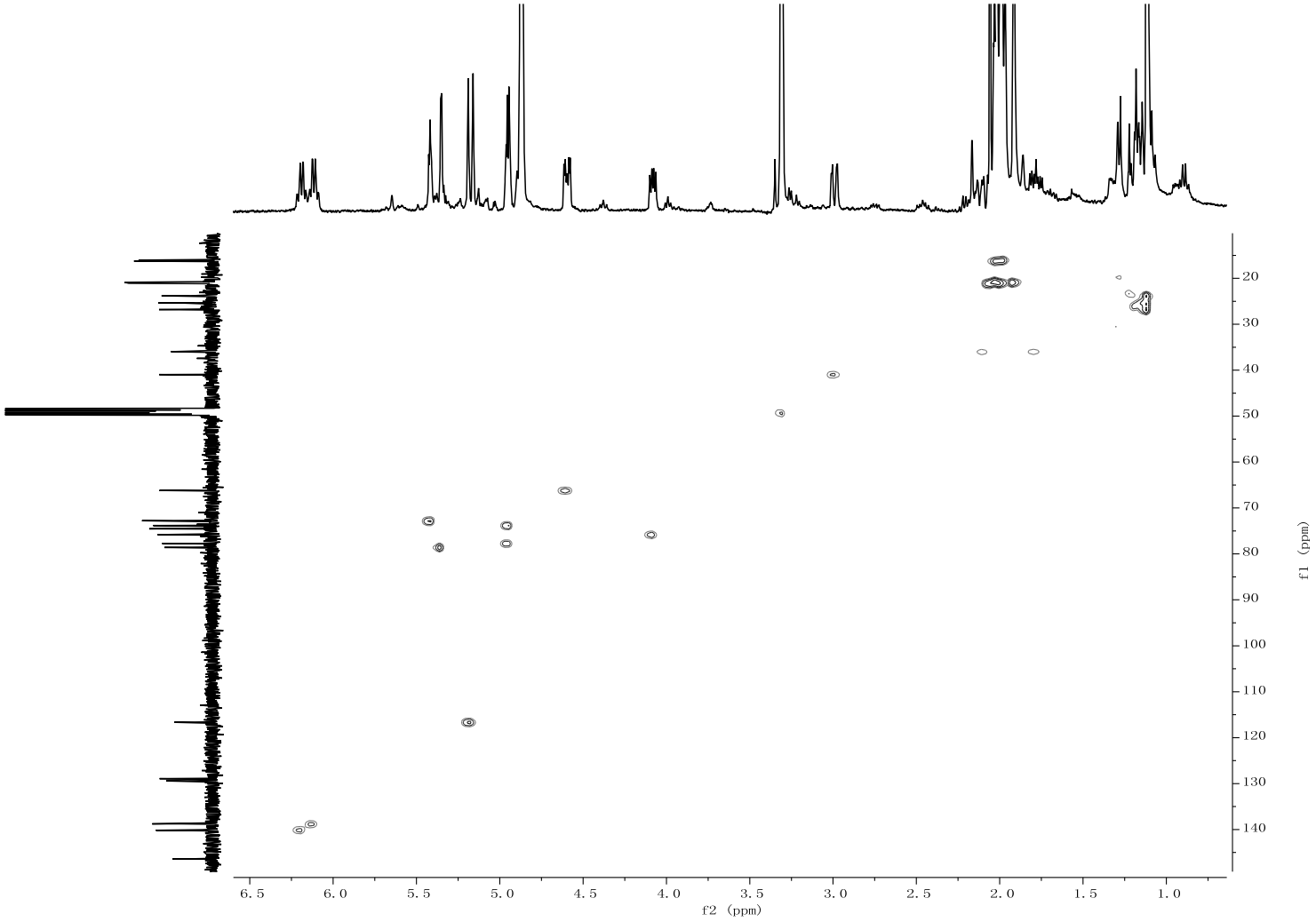


Figure S67. ^{1}H-^{1}H COSY (400 MHz, CD_3OD) spectrum of pararunine H (**12**)

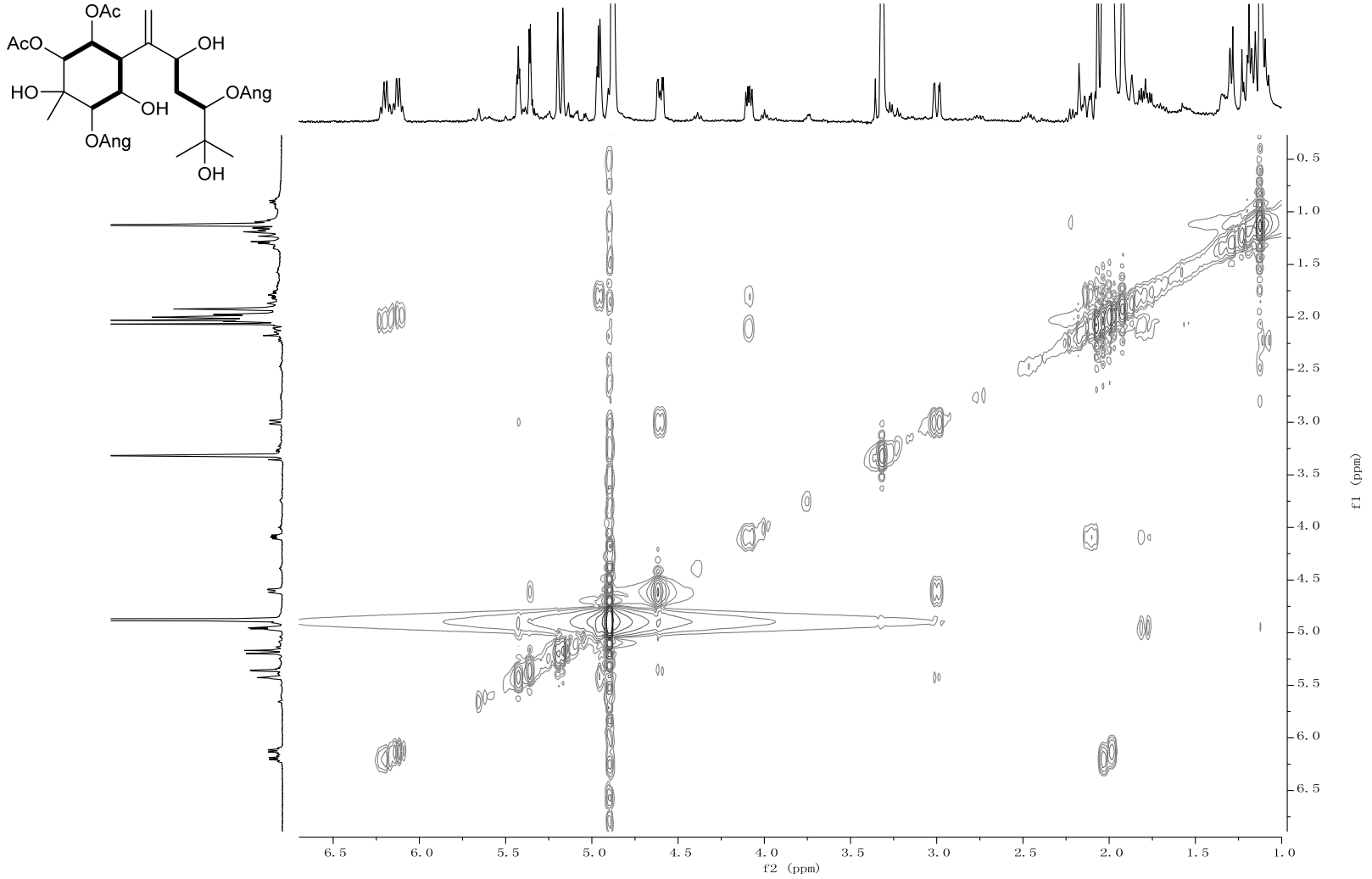


Figure S68. HMBC (400 MHz, CD_3OD) spectrum of pararunine H (**12**)

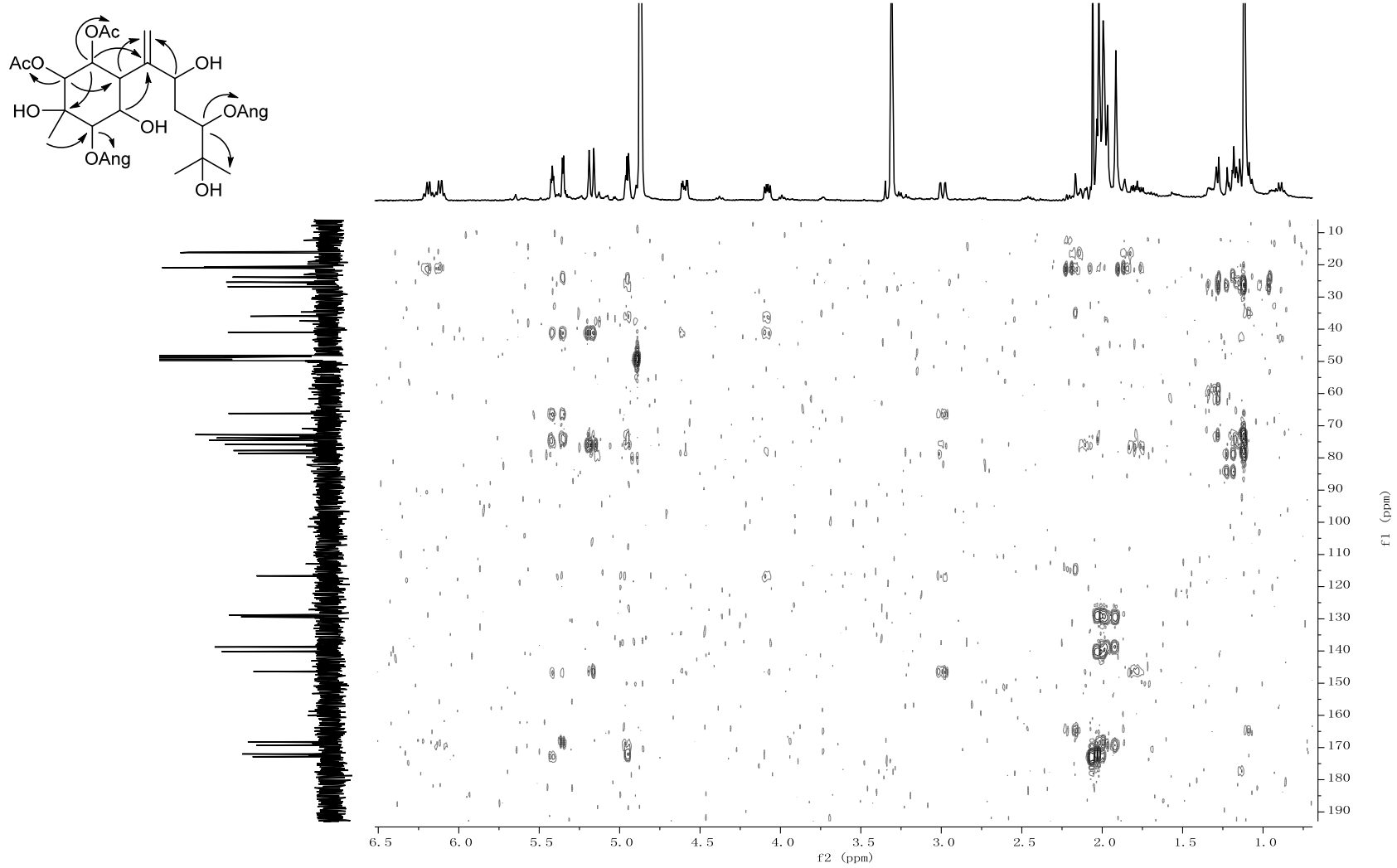


Figure S69. NOESY (400 MHz, CD_3OD) spectrum of pararunine H (**12**)

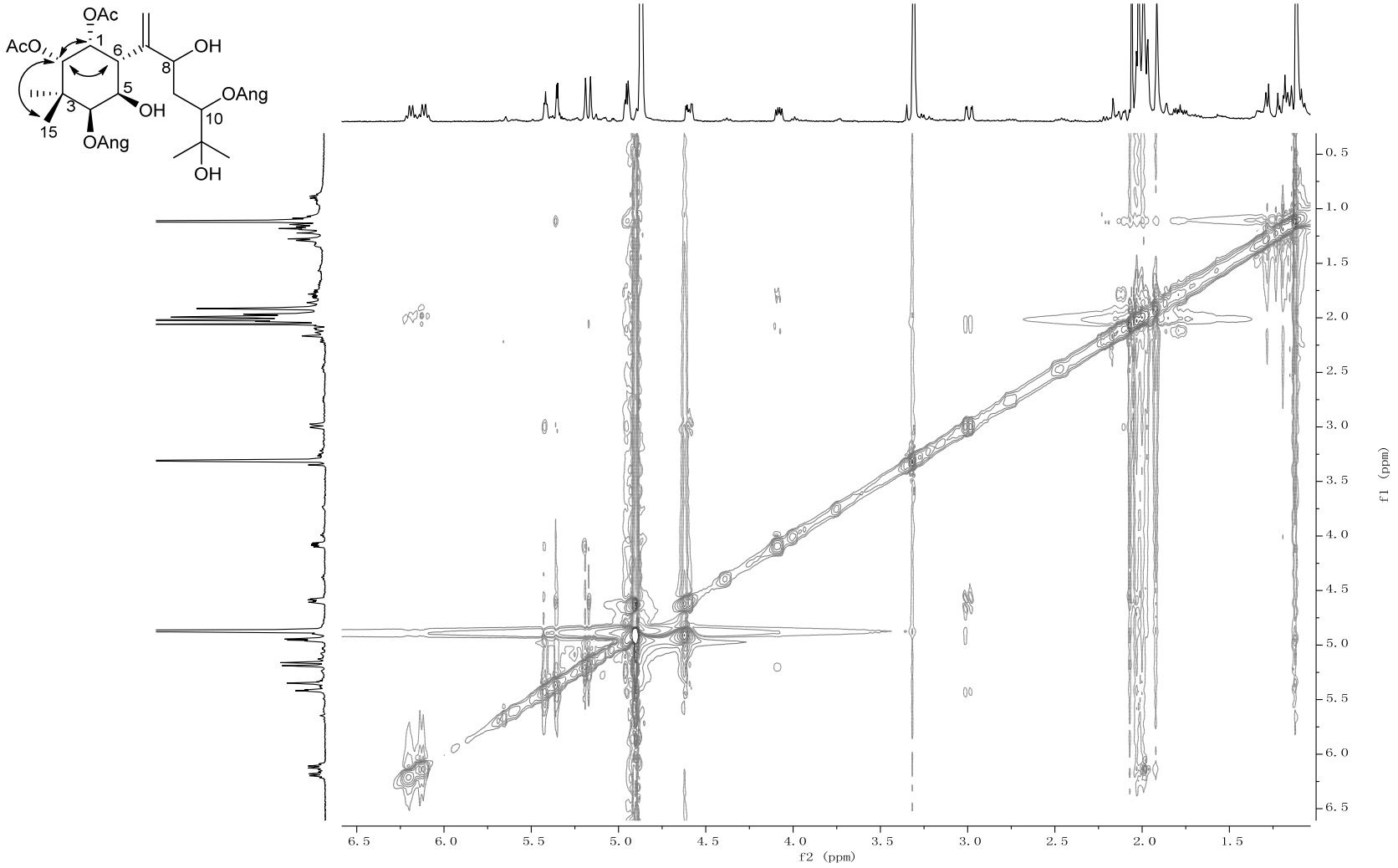


Figure S70. HRESIMS spectrum of pararunine H (**12**)

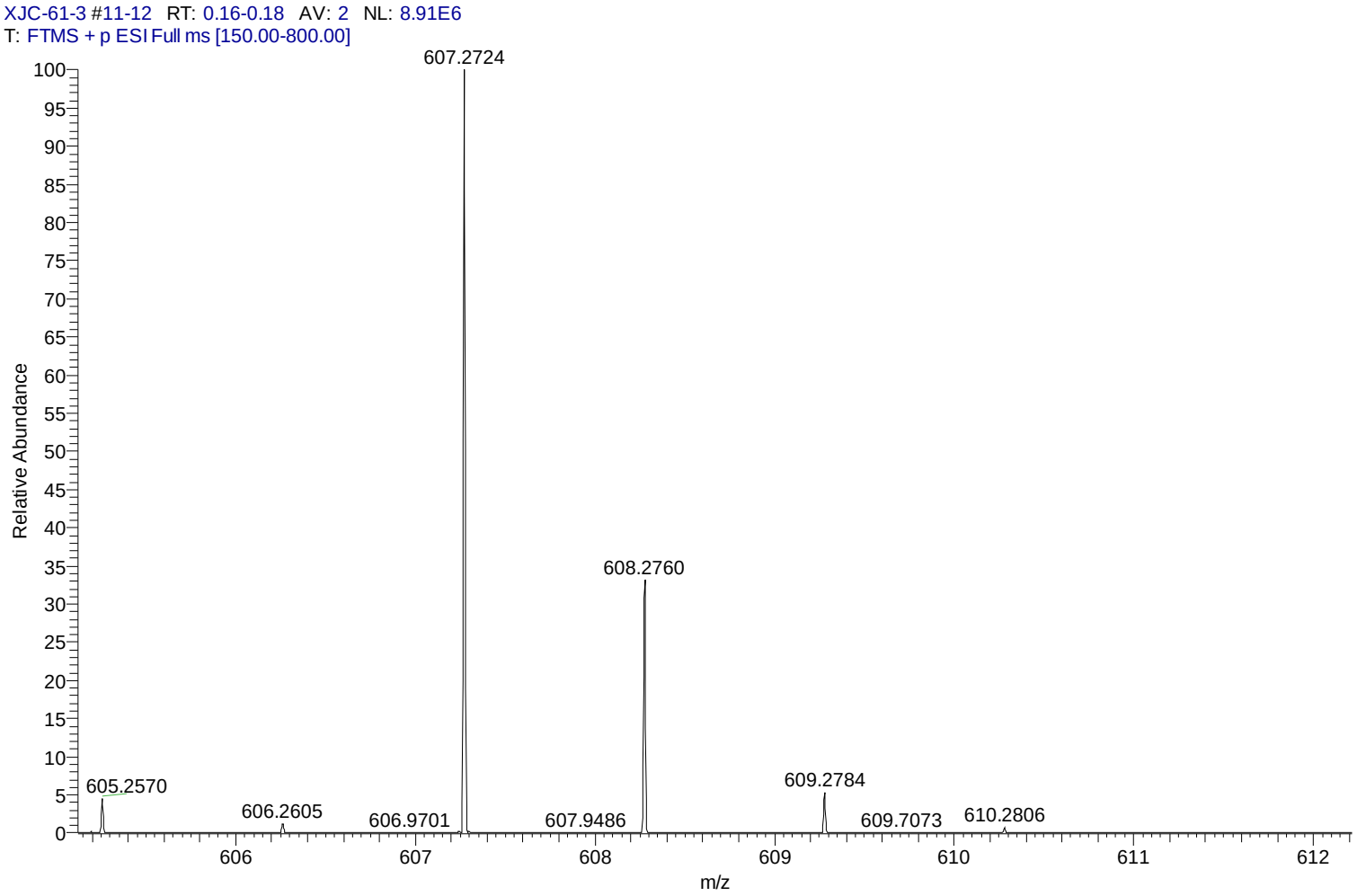


Figure S71. IR spectrum of pararunine H (**12**)

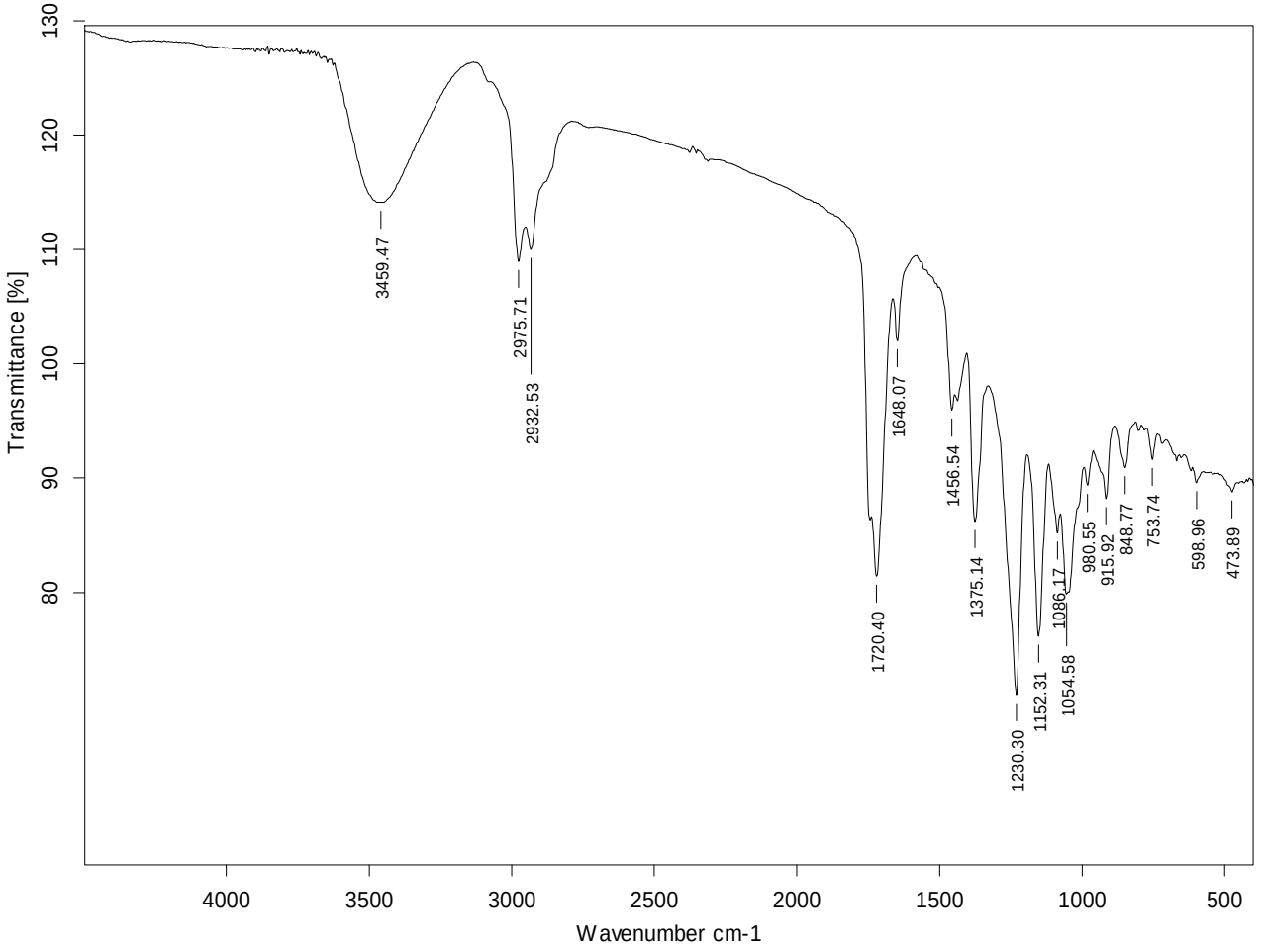


Figure S72.CD spectrum of pararunine H (**12**)

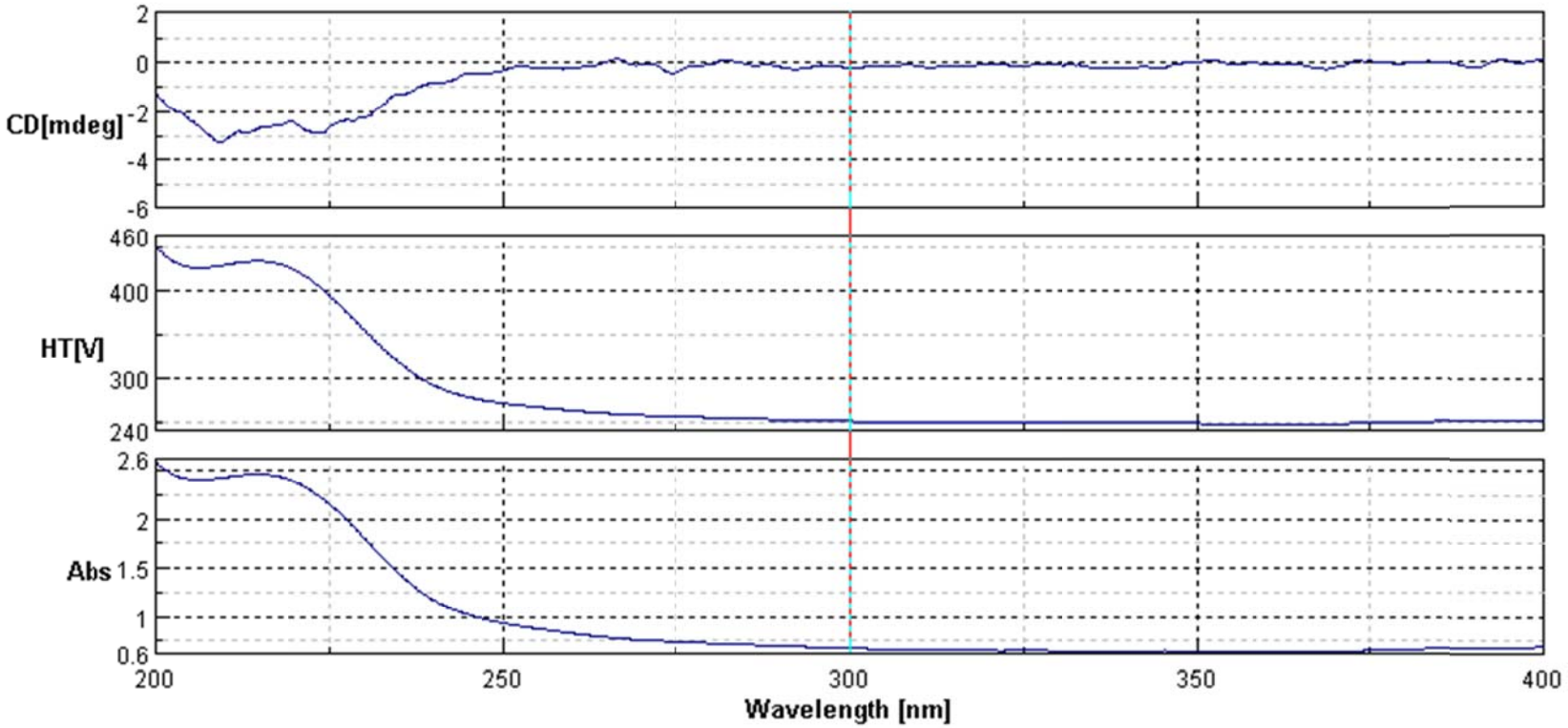


Figure S73. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of pararunine I (**13**)

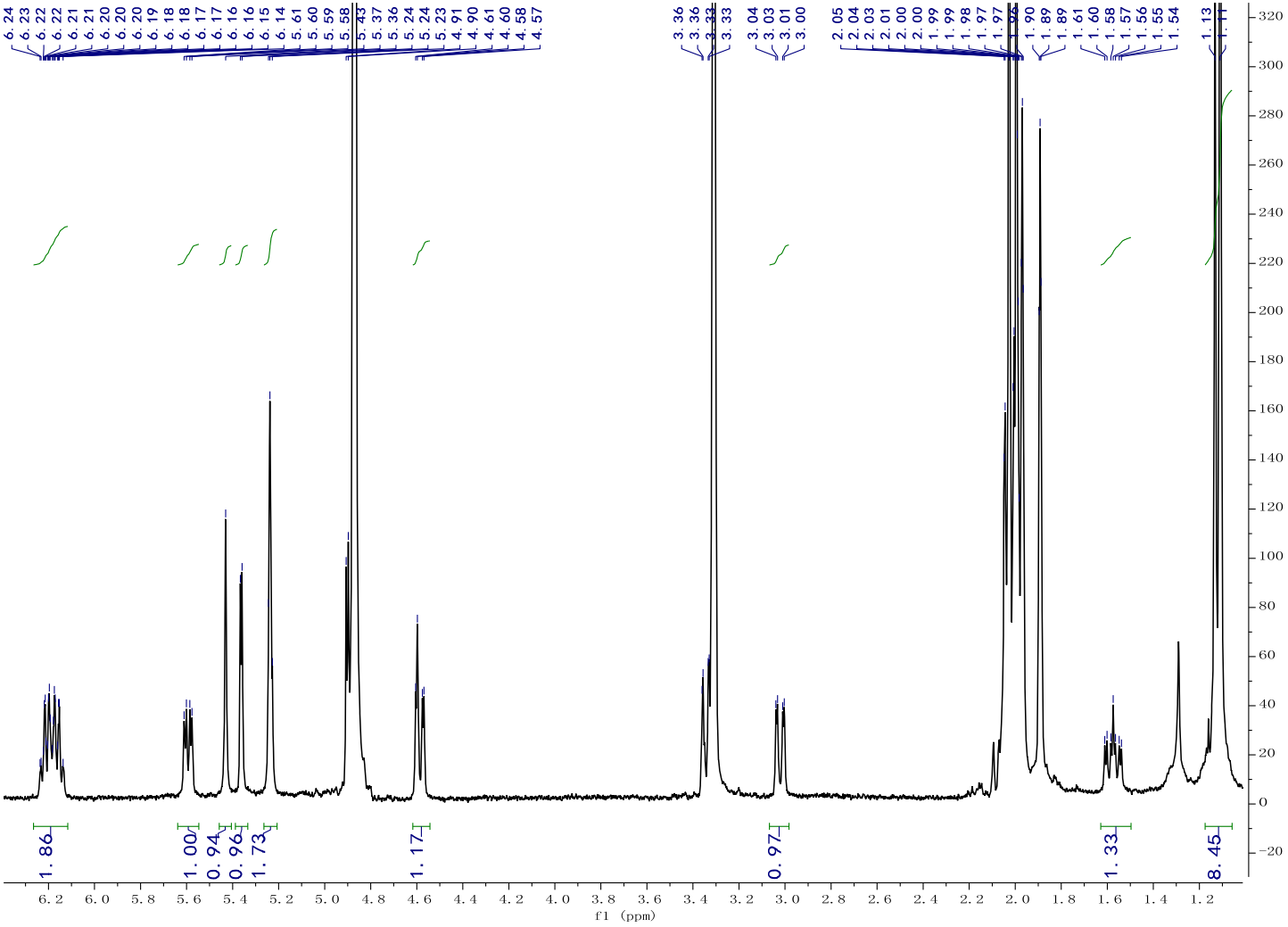


Figure S74. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of pararunine I (**13**)

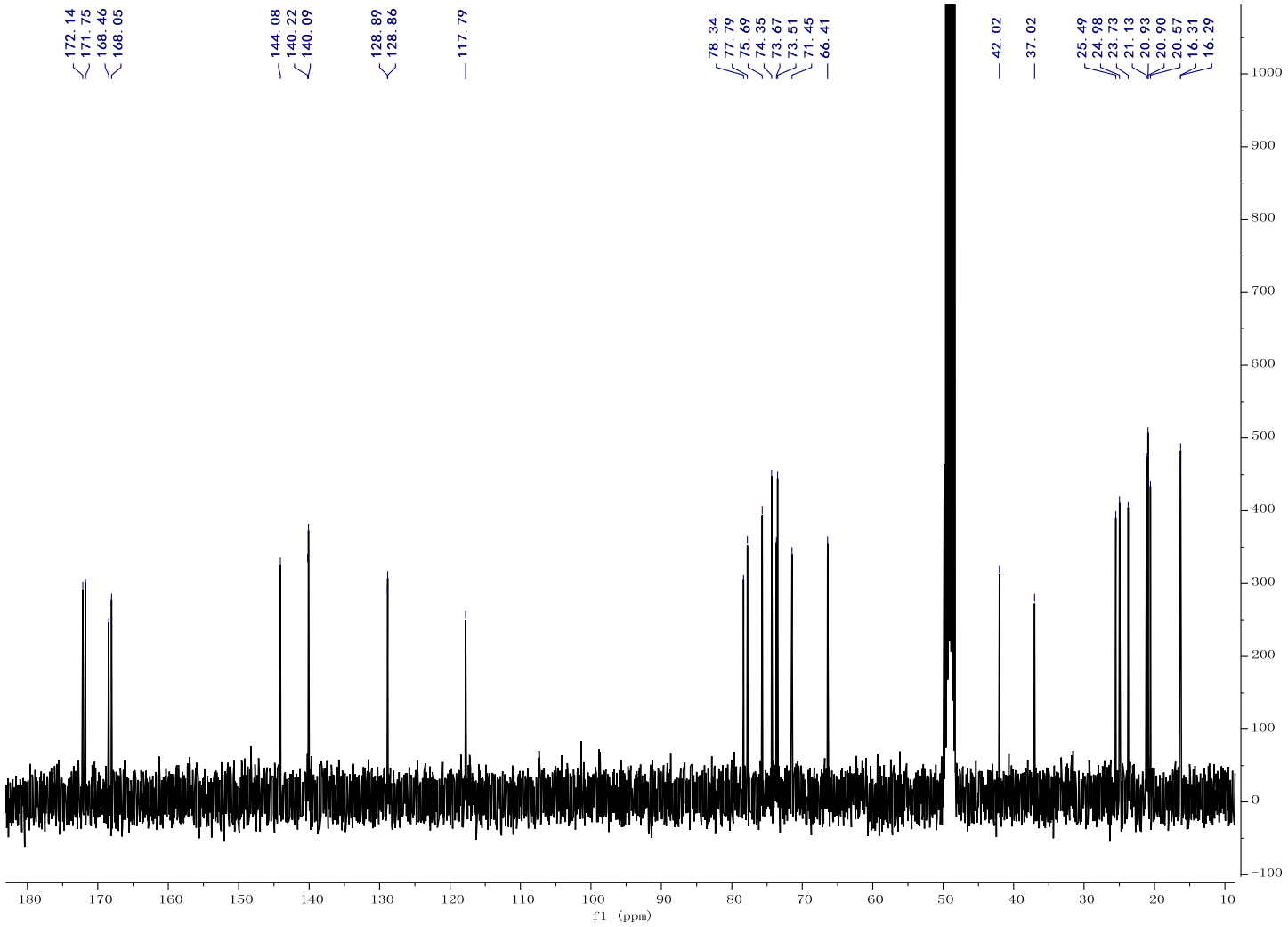


Figure S75. HSQC (400 MHz, $CDCl_3$) spectrum of pararunine I (1**3**)

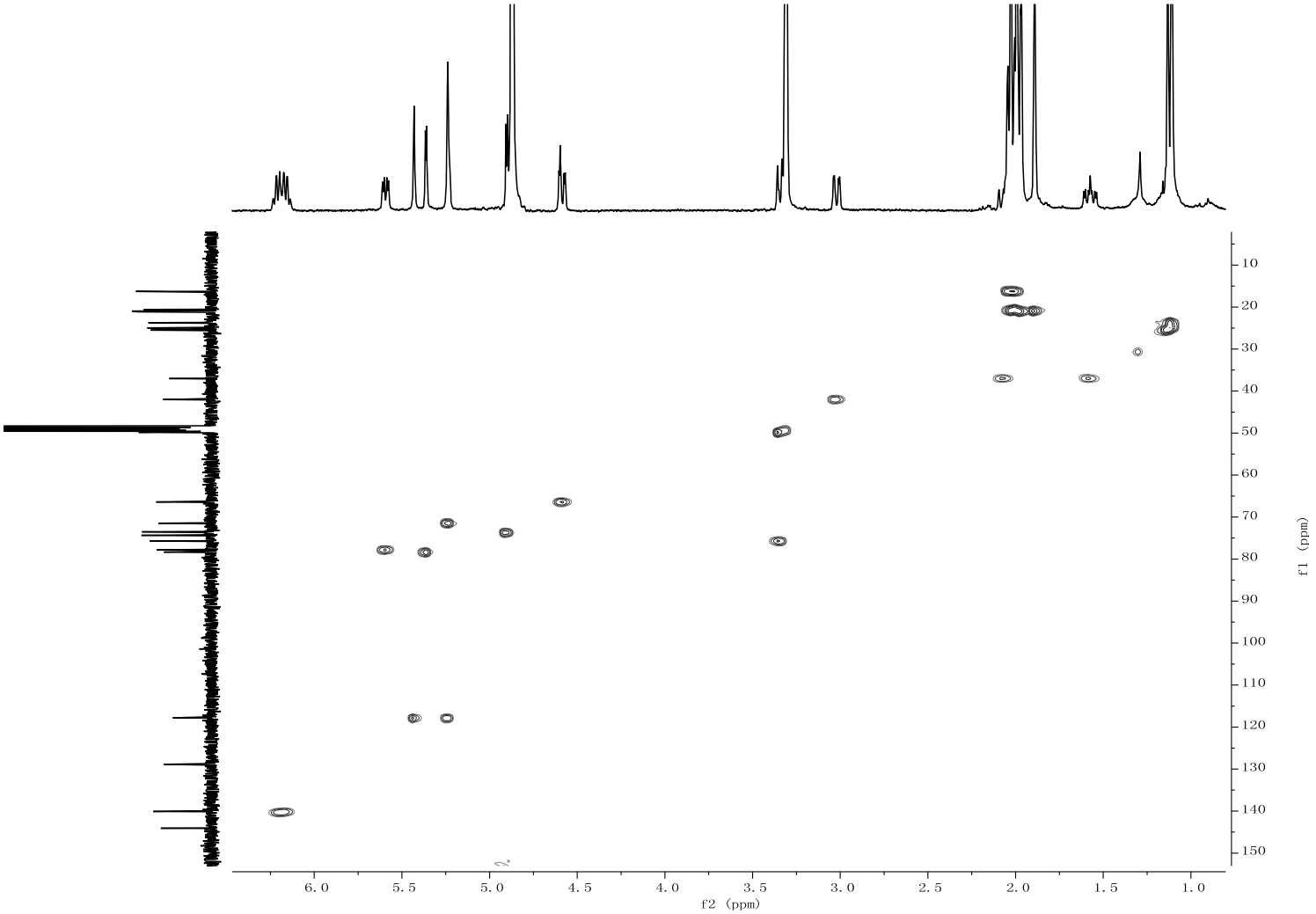


Figure S76. ^{1}H-^{1}H COSY (400 MHz, $CDCl_3$) spectrum of pararunine I (**13**)

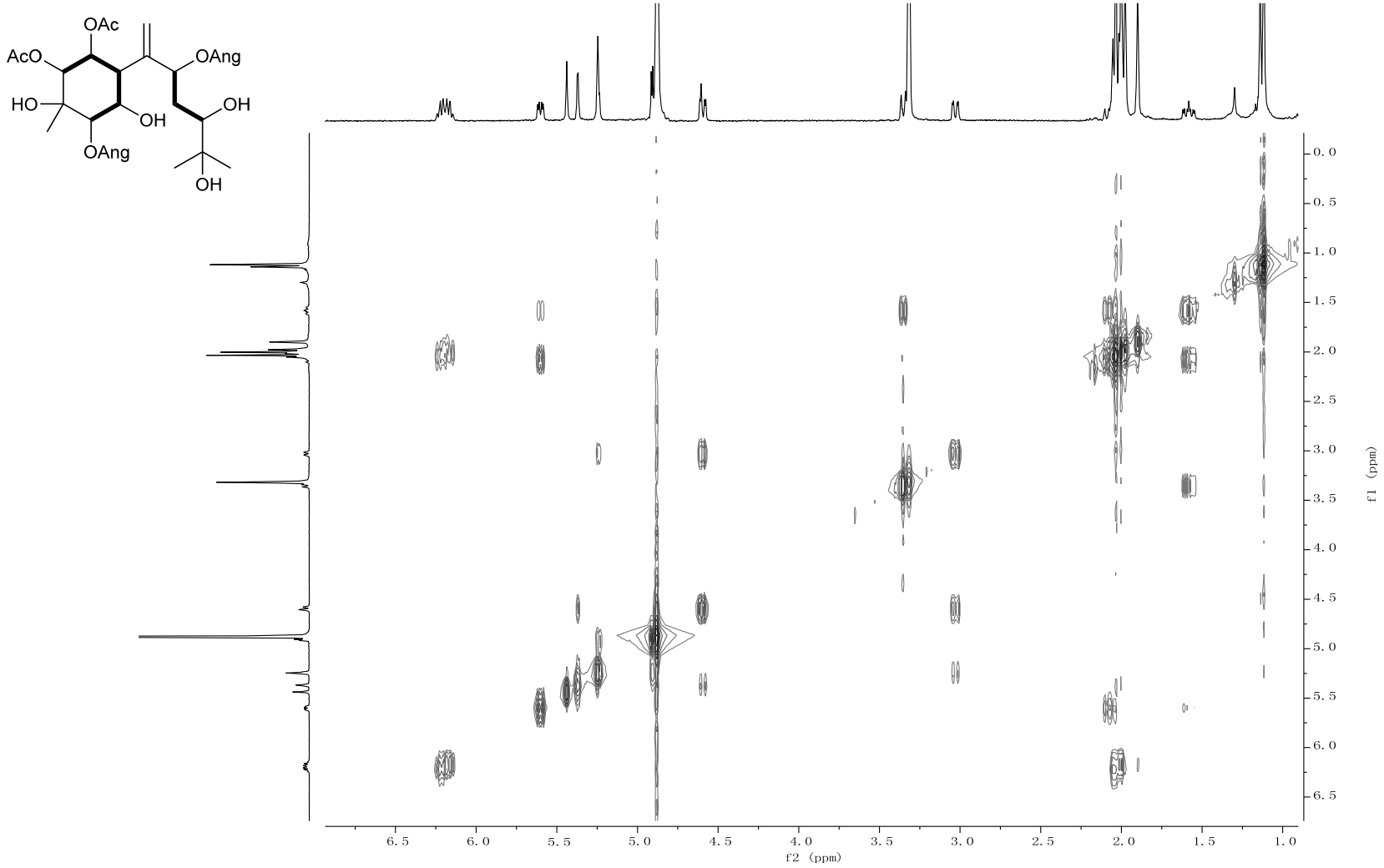


Figure S77. HMBC (400 MHz, $CDCl_3$) spectrum of pararunine I (**13**)

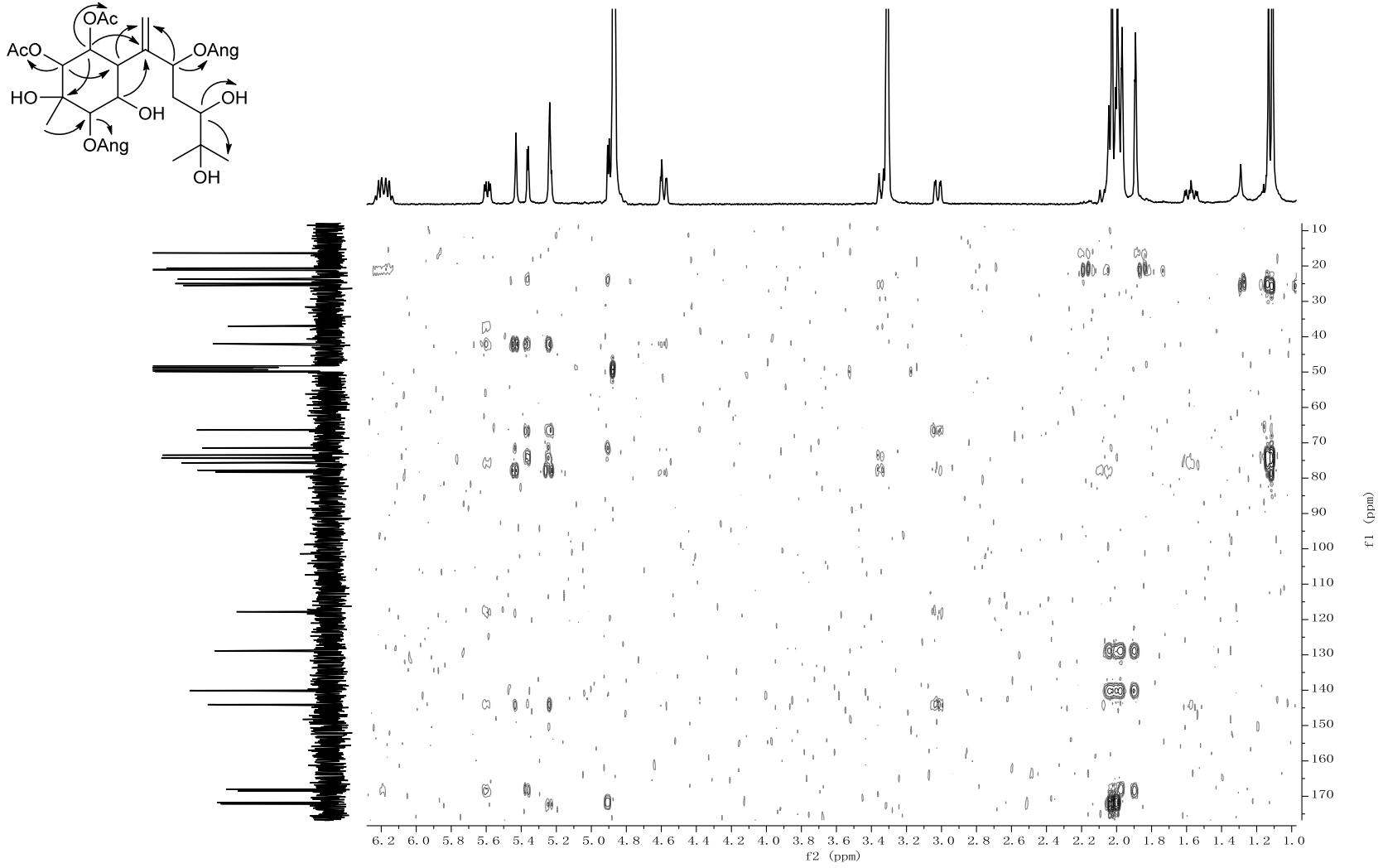


Figure S78. NOESY (400 MHz, $CDCl_3$) spectrum of pararunine I (**13**)

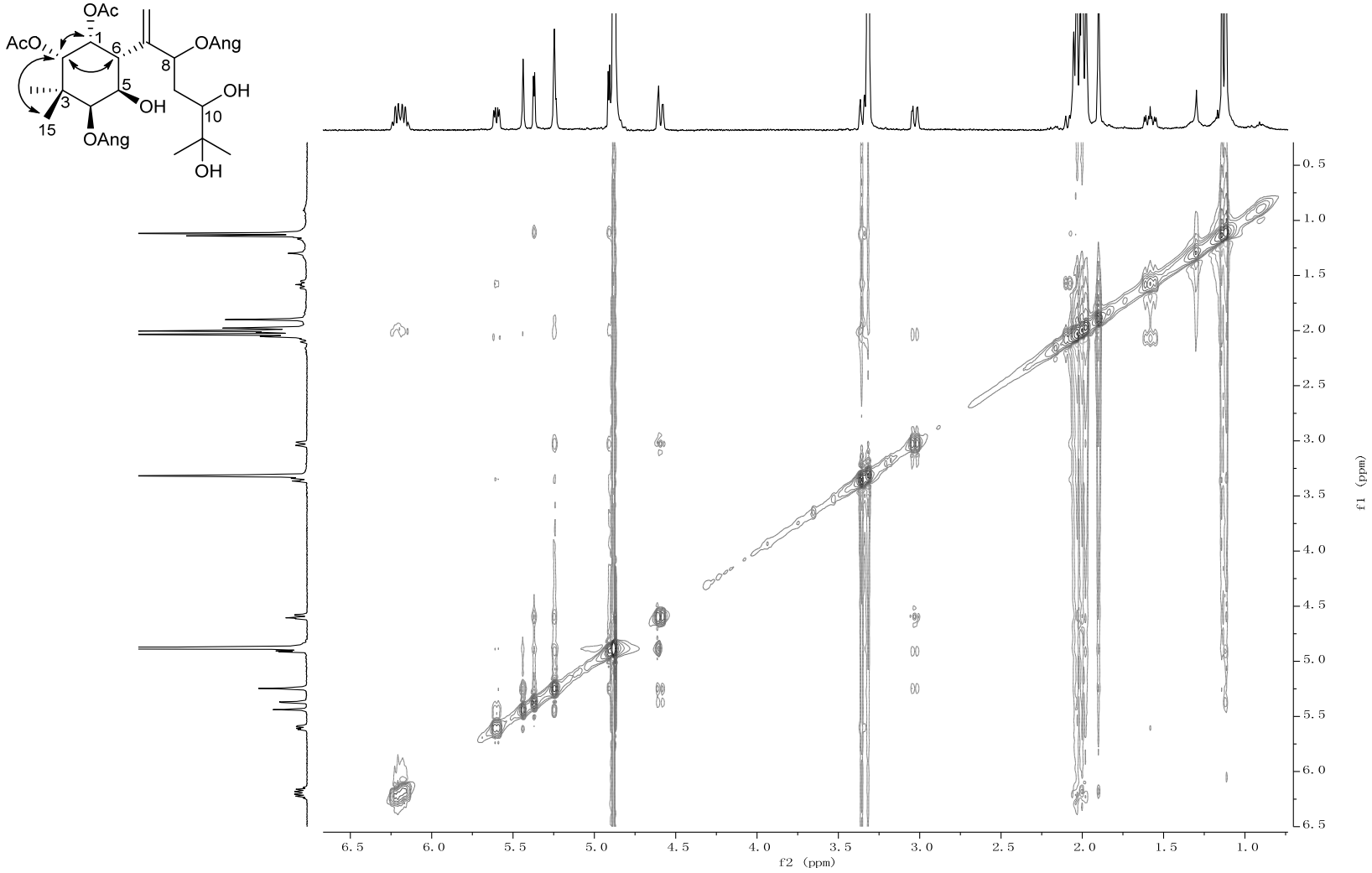


Figure S79. HRESIMS spectrum of pararunine I (**13**)

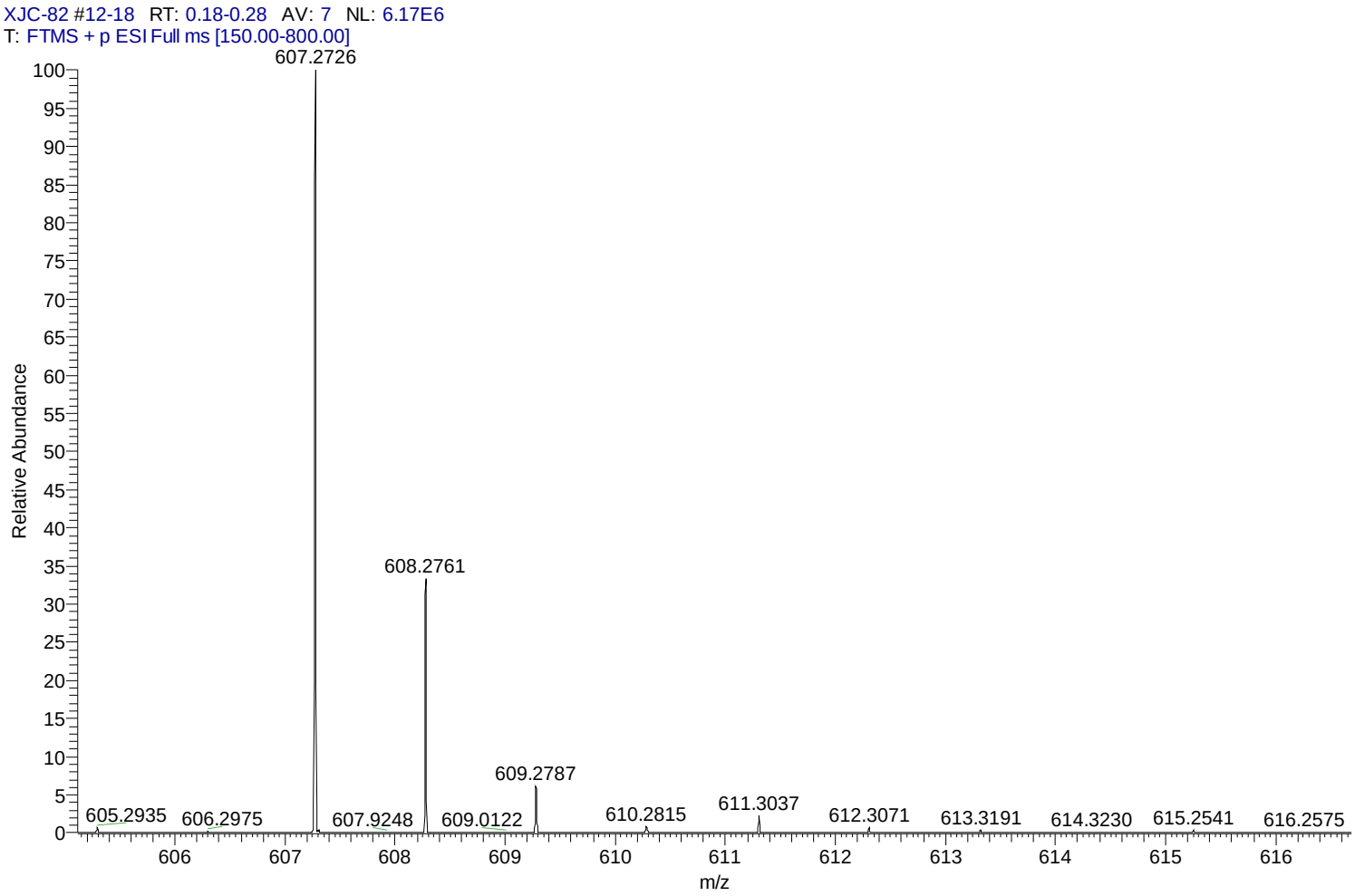


Figure S80. IR spectrum of pararunine I (**13**)

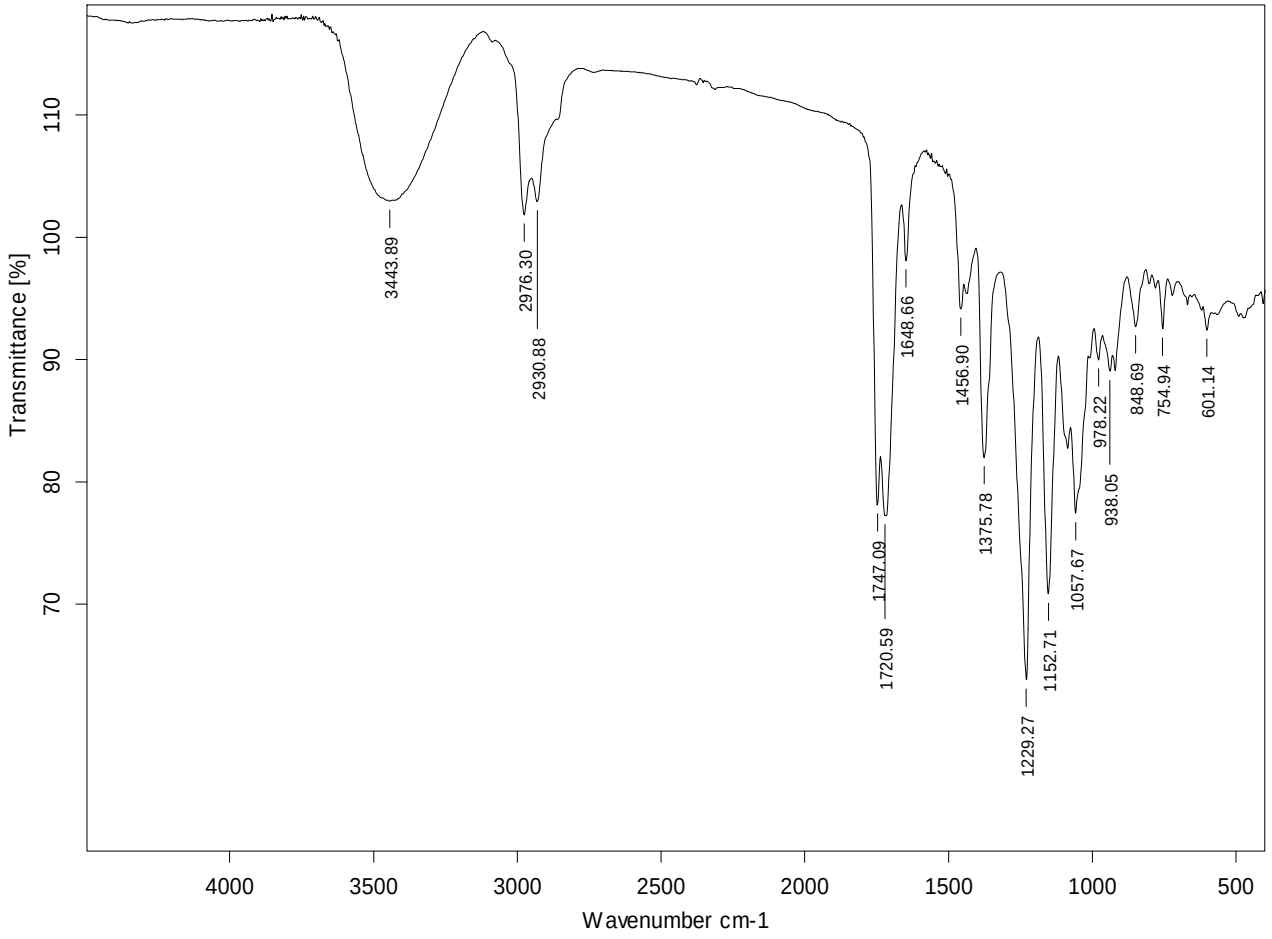


Figure S81. CD spectrum of pararunine I (**13**)

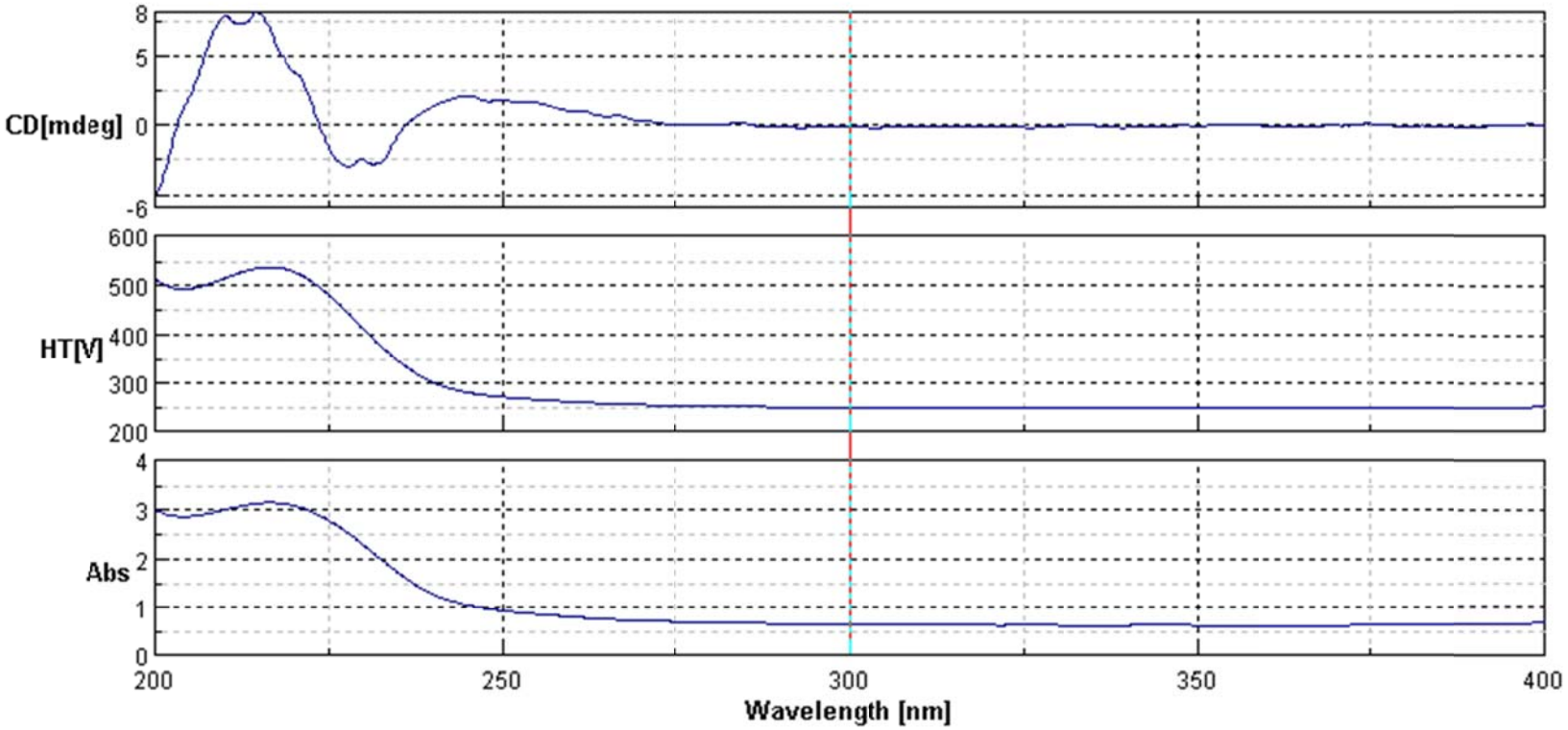


Figure S82. ^{1}H NMR (400 MHz, CD_3OD) spectrum of pararunine J (**14**)

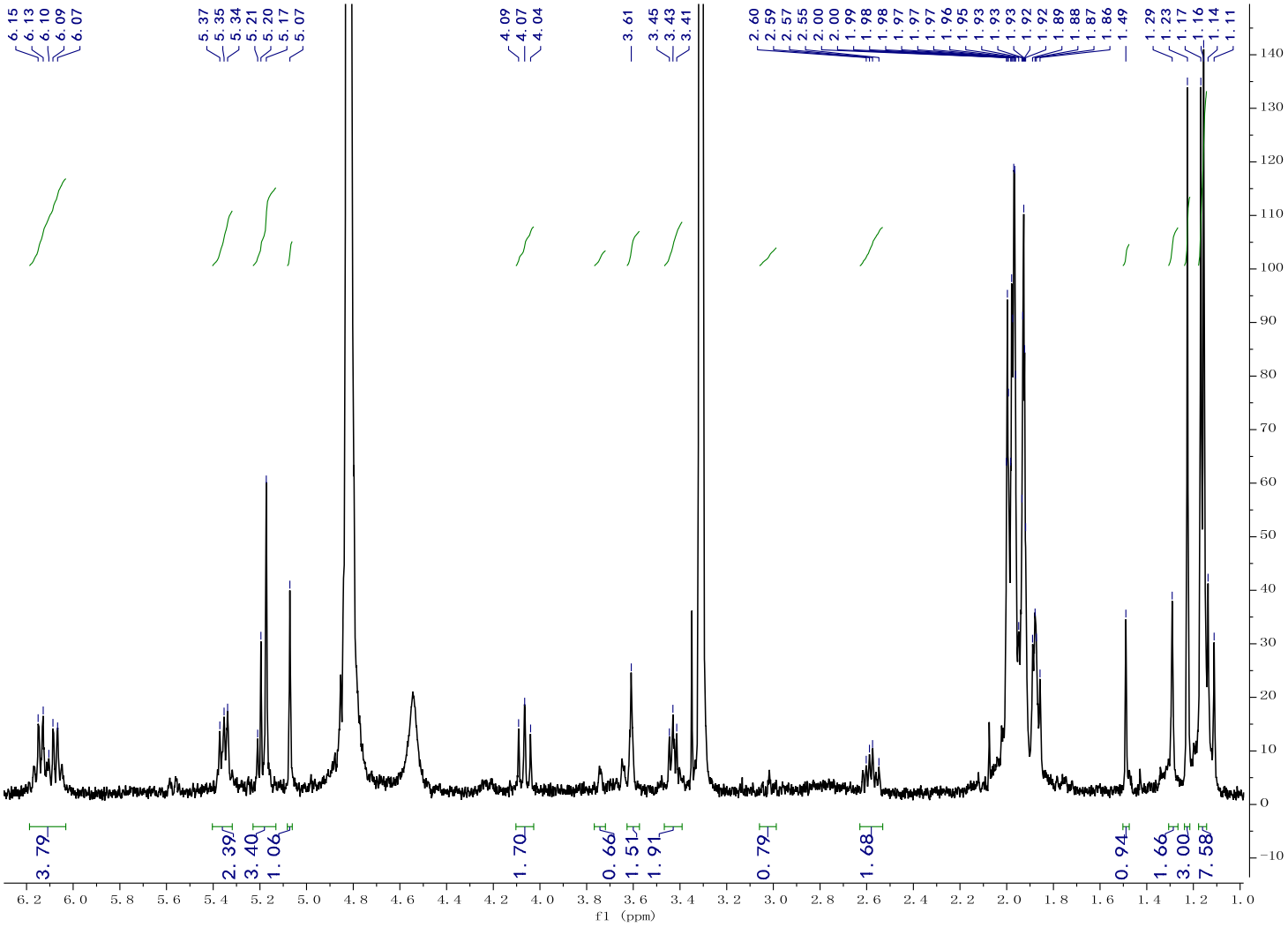


Figure S83. ^{13}C NMR (100 MHz, CD_3OD) spectrum of pararunine J (**14**)

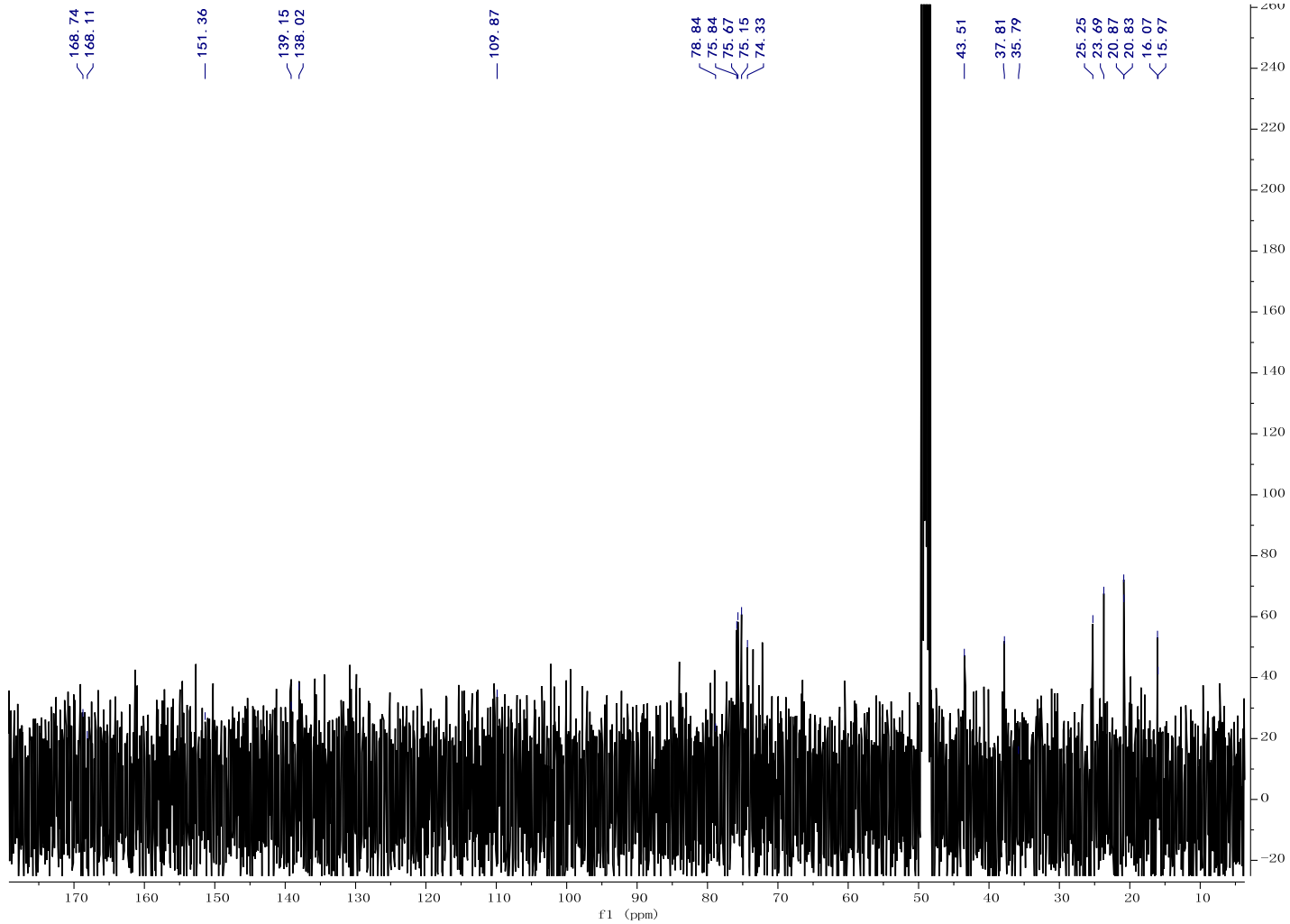


Figure S84. HSQC (400 MHz, CD_3OD) spectrum of pararunine J (**14**)

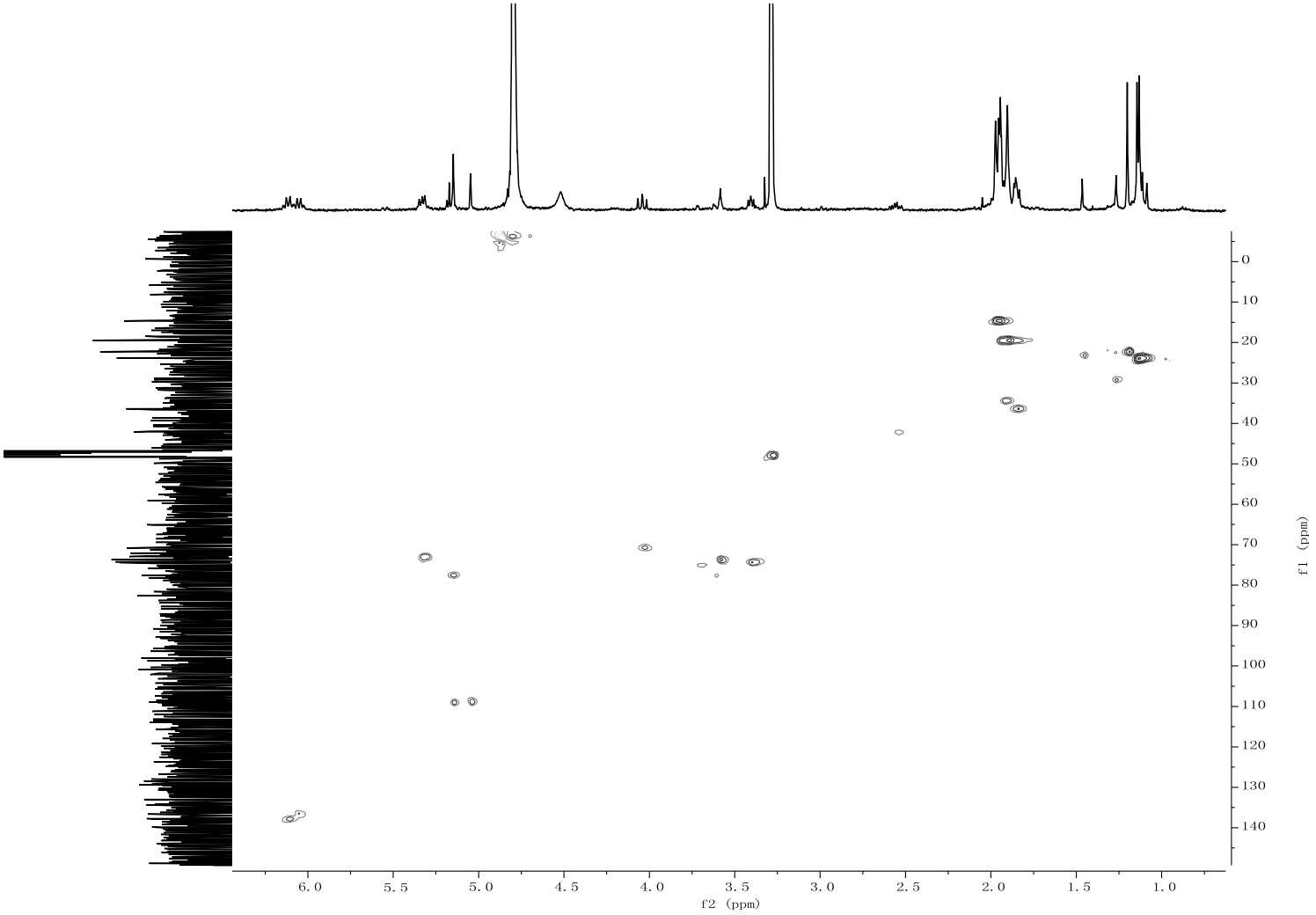


Figure S85. ^{1}H-^{1}H COSY (400 MHz, CD_3OD) spectrum of pararunine J (**14**)

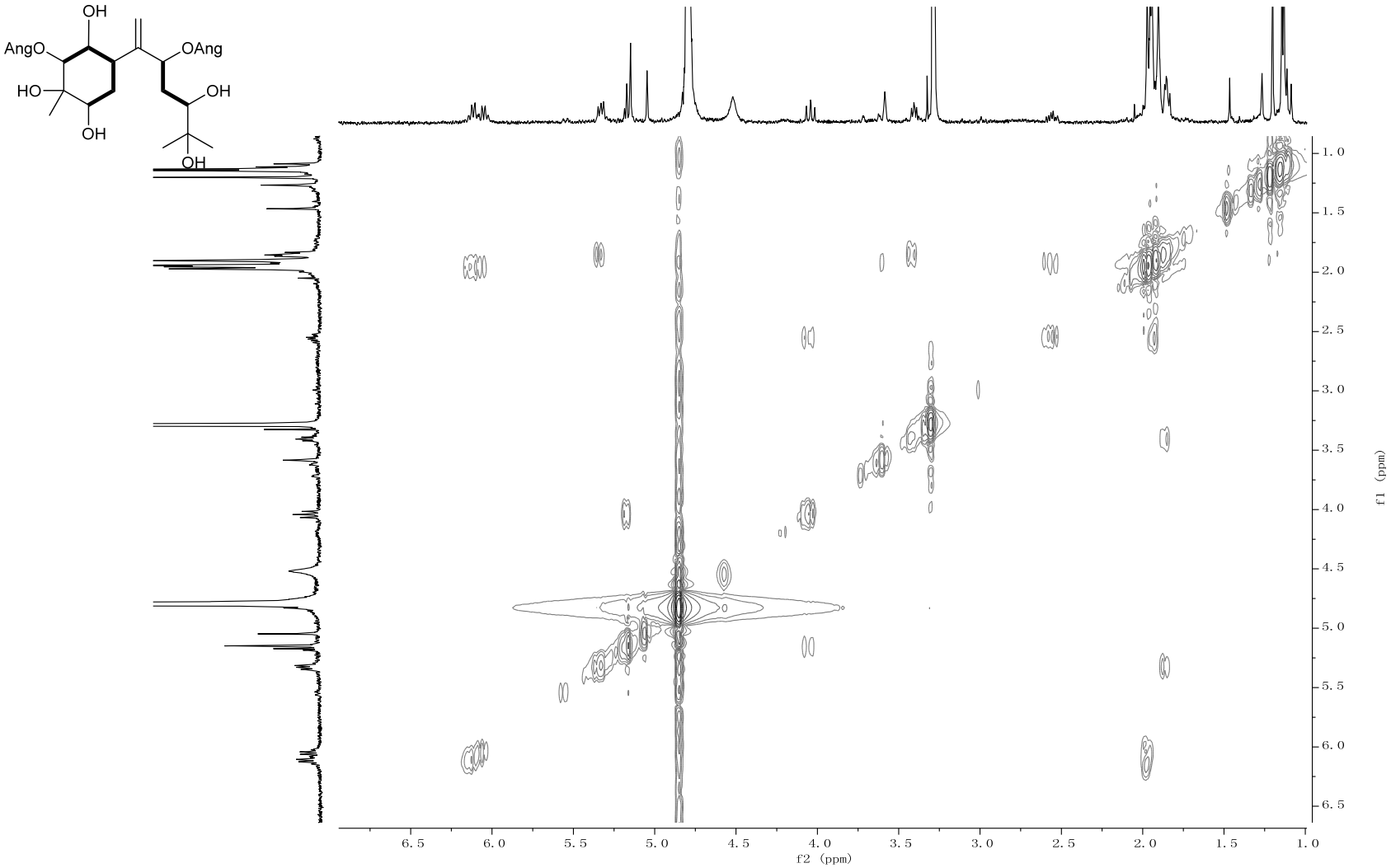


Figure S86. HMBC (400 MHz, CD_3OD) spectrum of pararunine J (**14**)

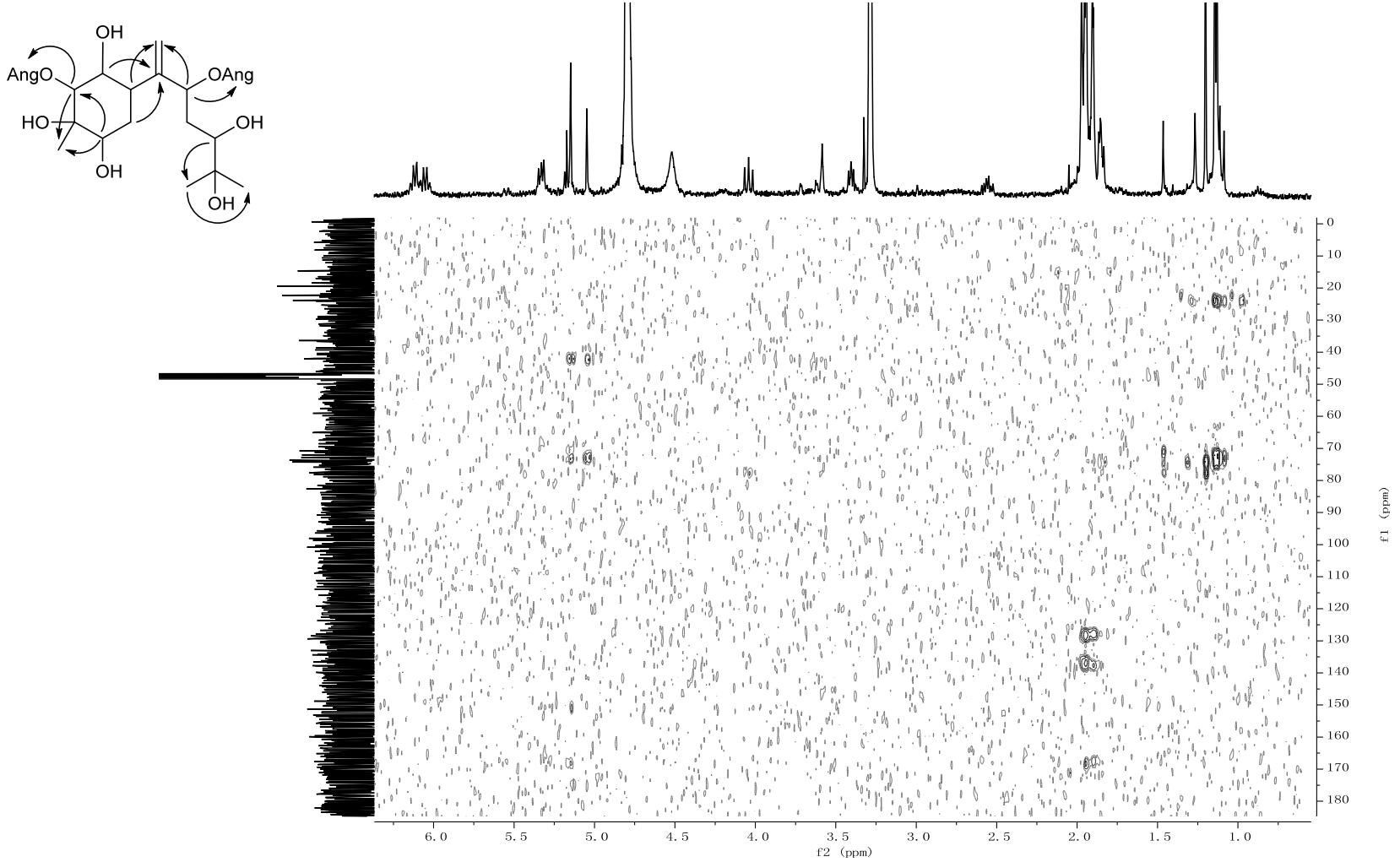


Figure S87. NOESY (400 MHz, CD_3OD) spectrum of pararunine J (**14**)

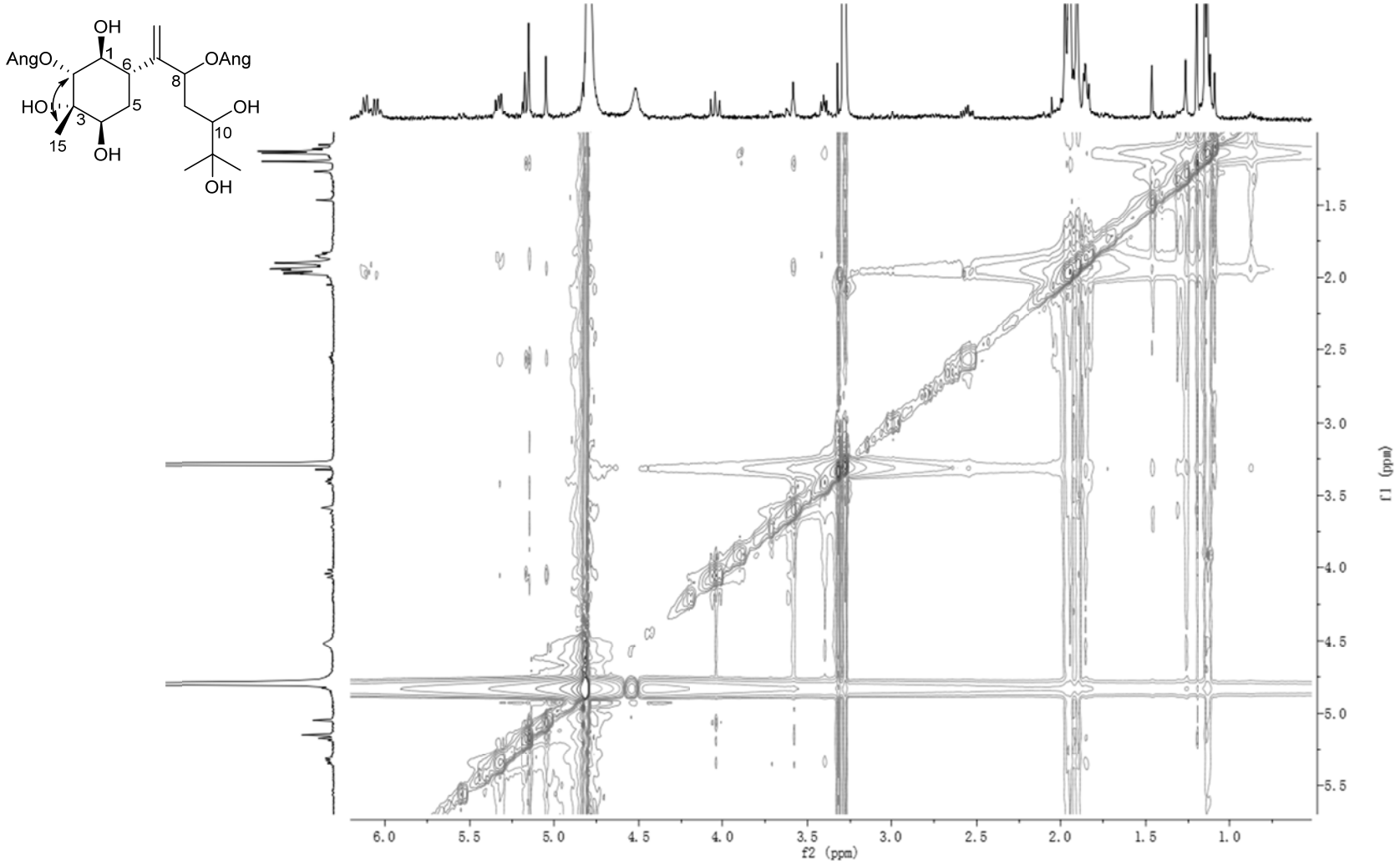


Figure S88. HRESIMS spectrum of pararunine J (**14**)

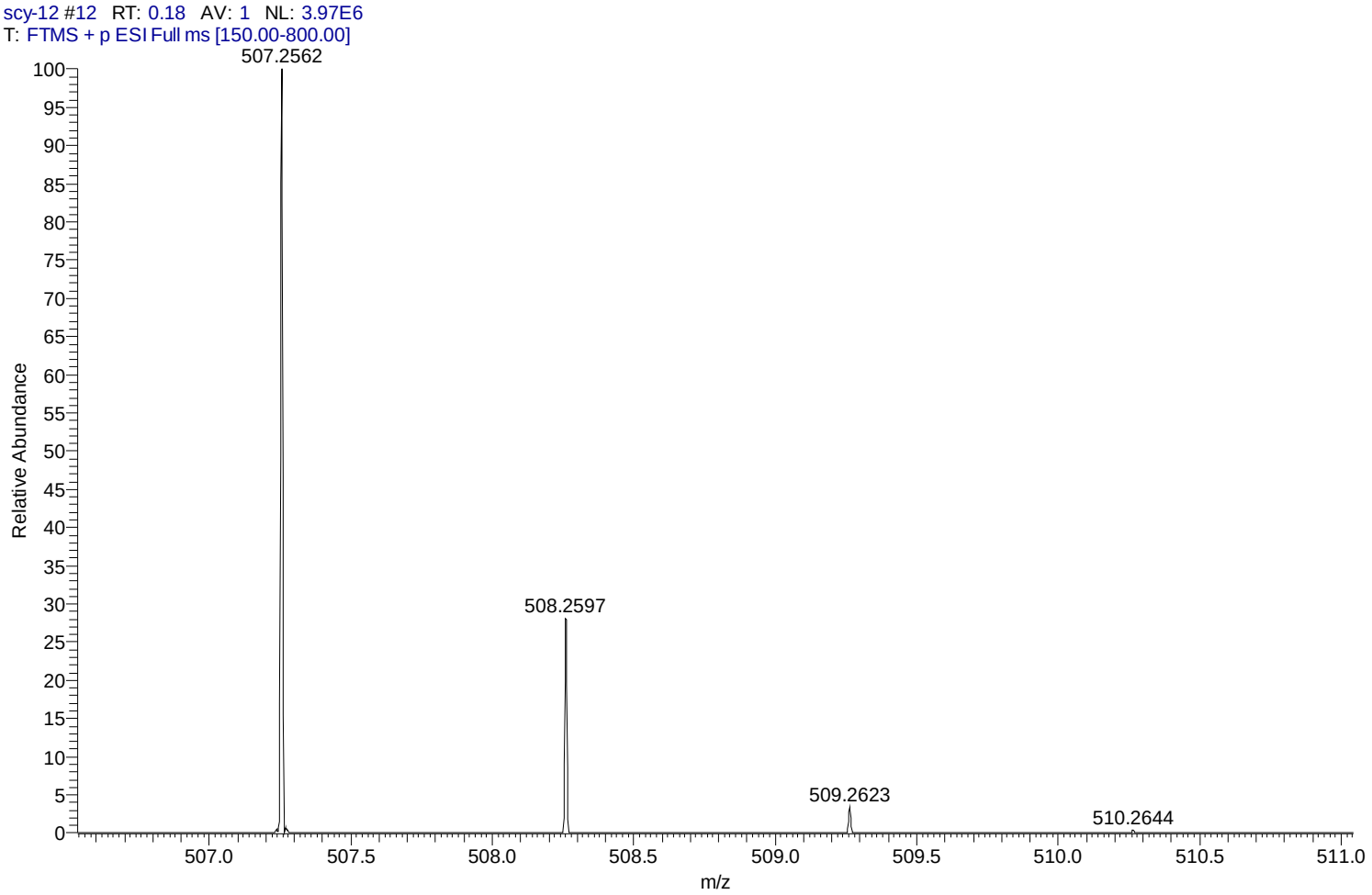


Figure S89. IR spectrum of pararunine J (**14**)

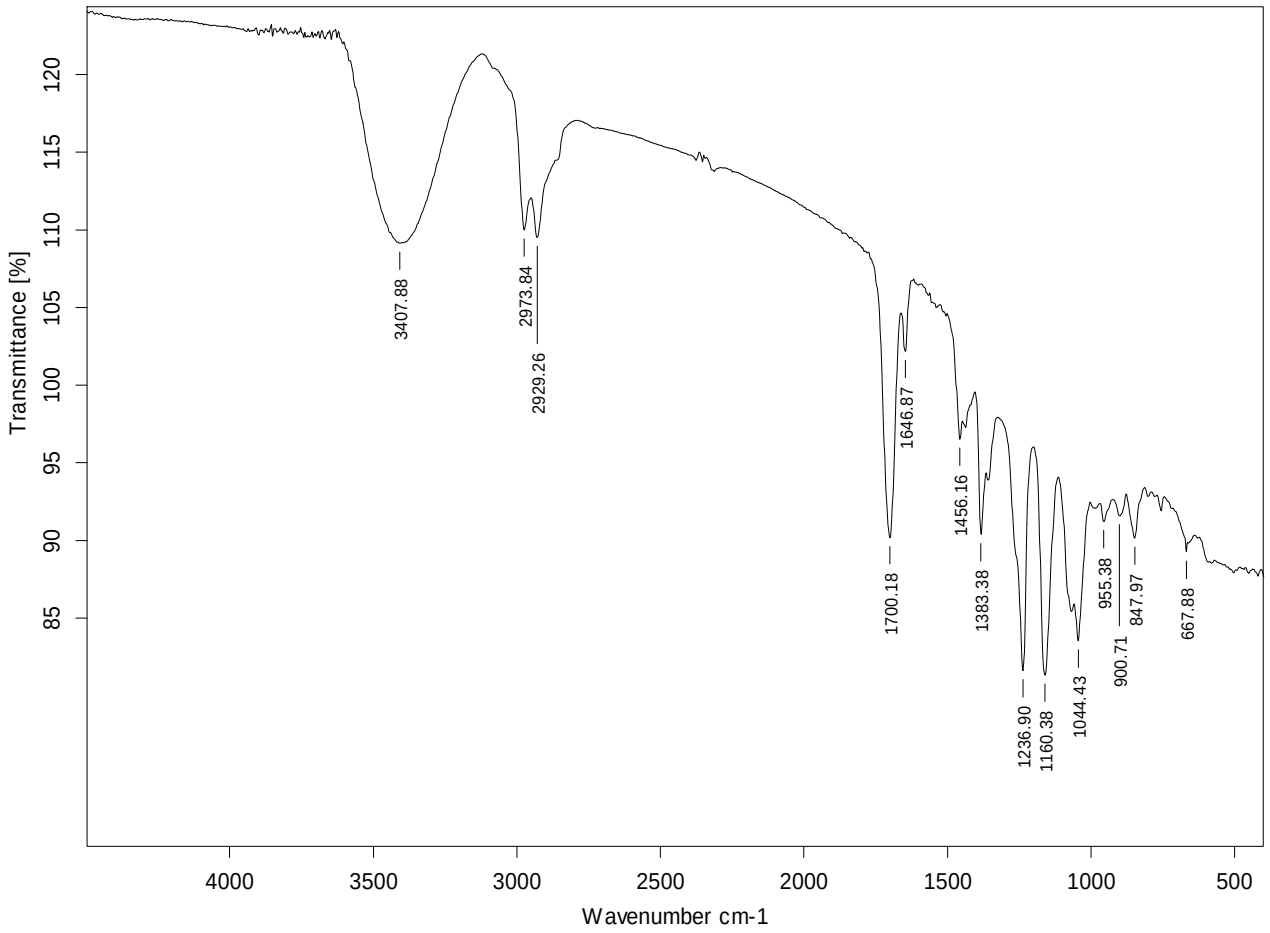


Figure S90. CD spectrum of pararunine J (**14**)

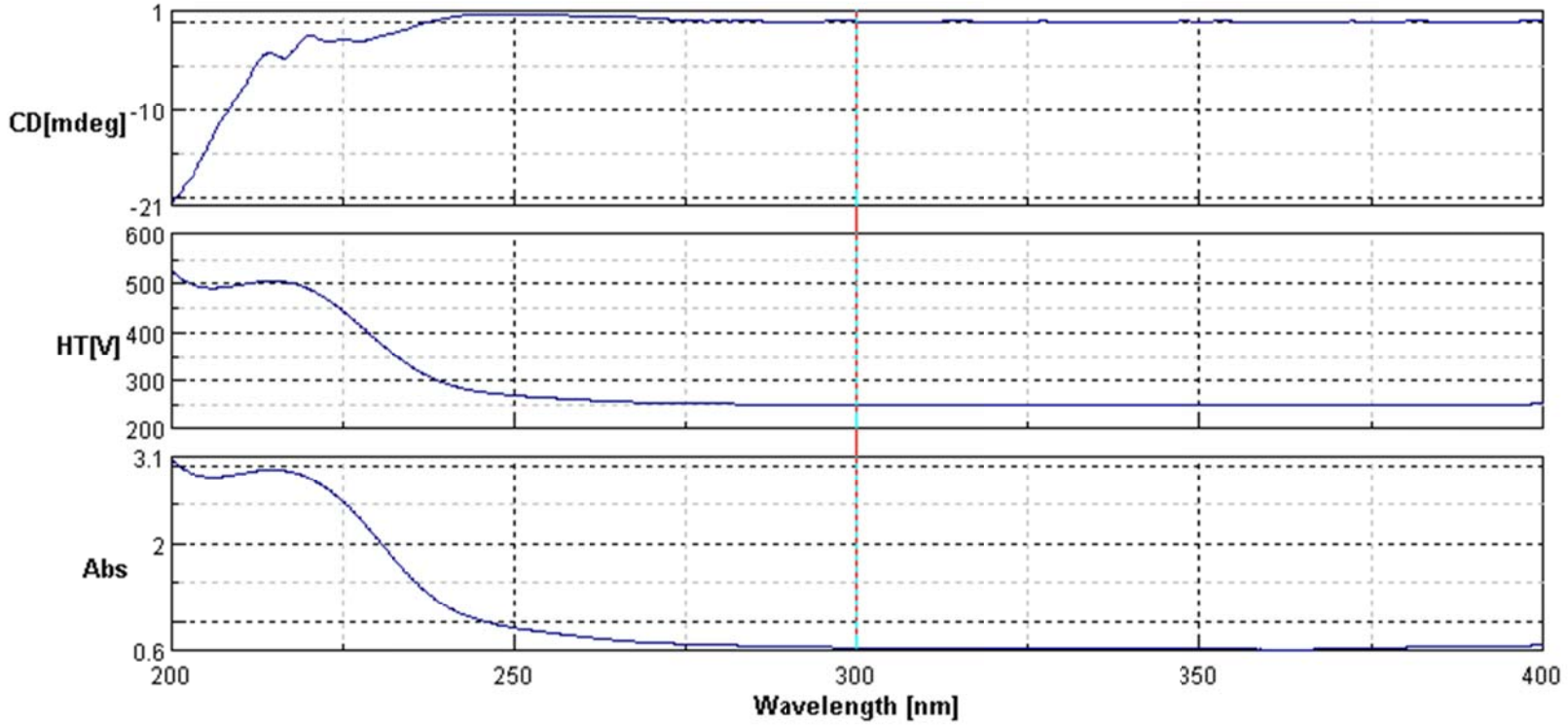


Figure S91. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of pararubcoumarin A (**15**)

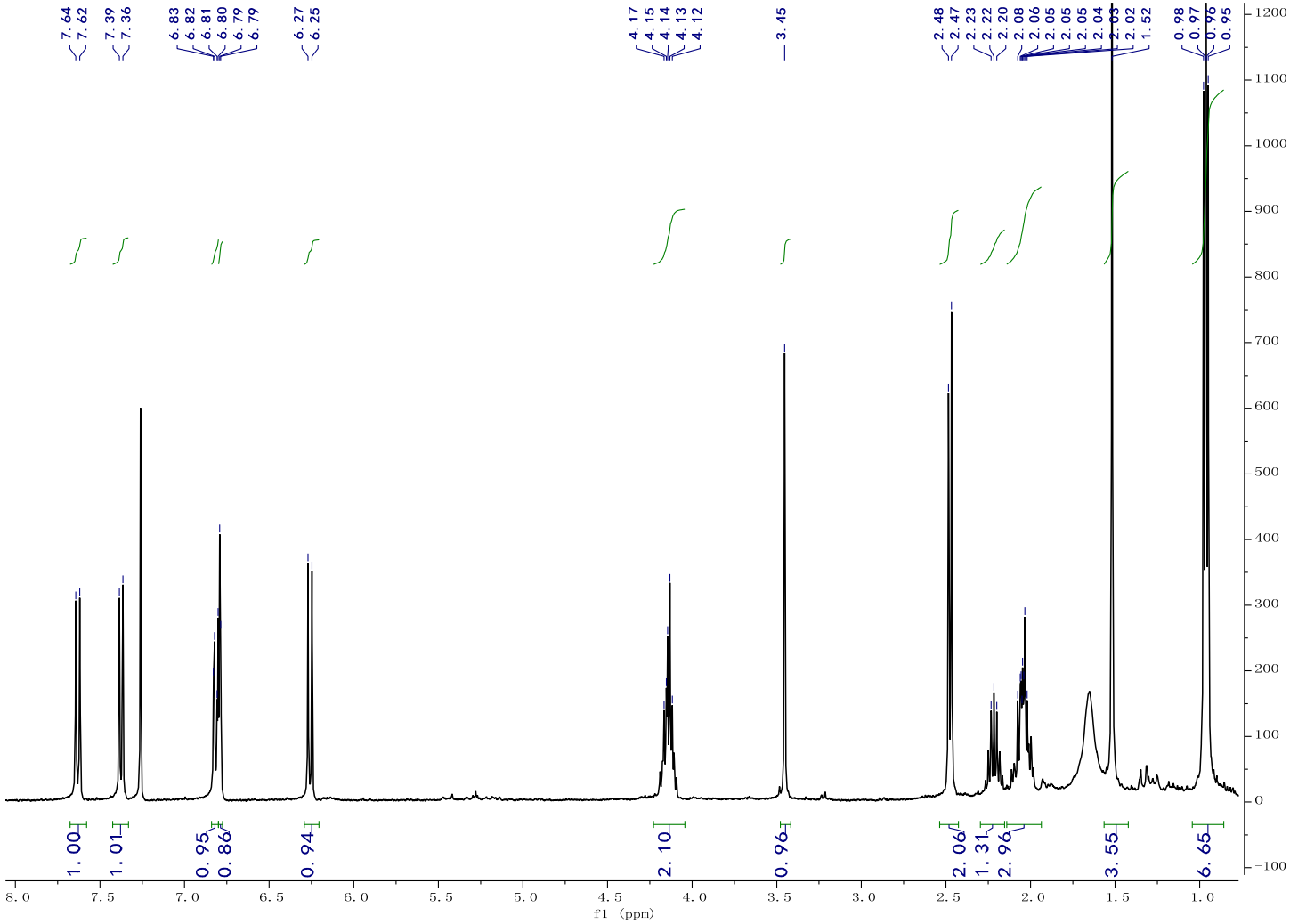


Figure S92. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of pararubcoumarin A (**15**)

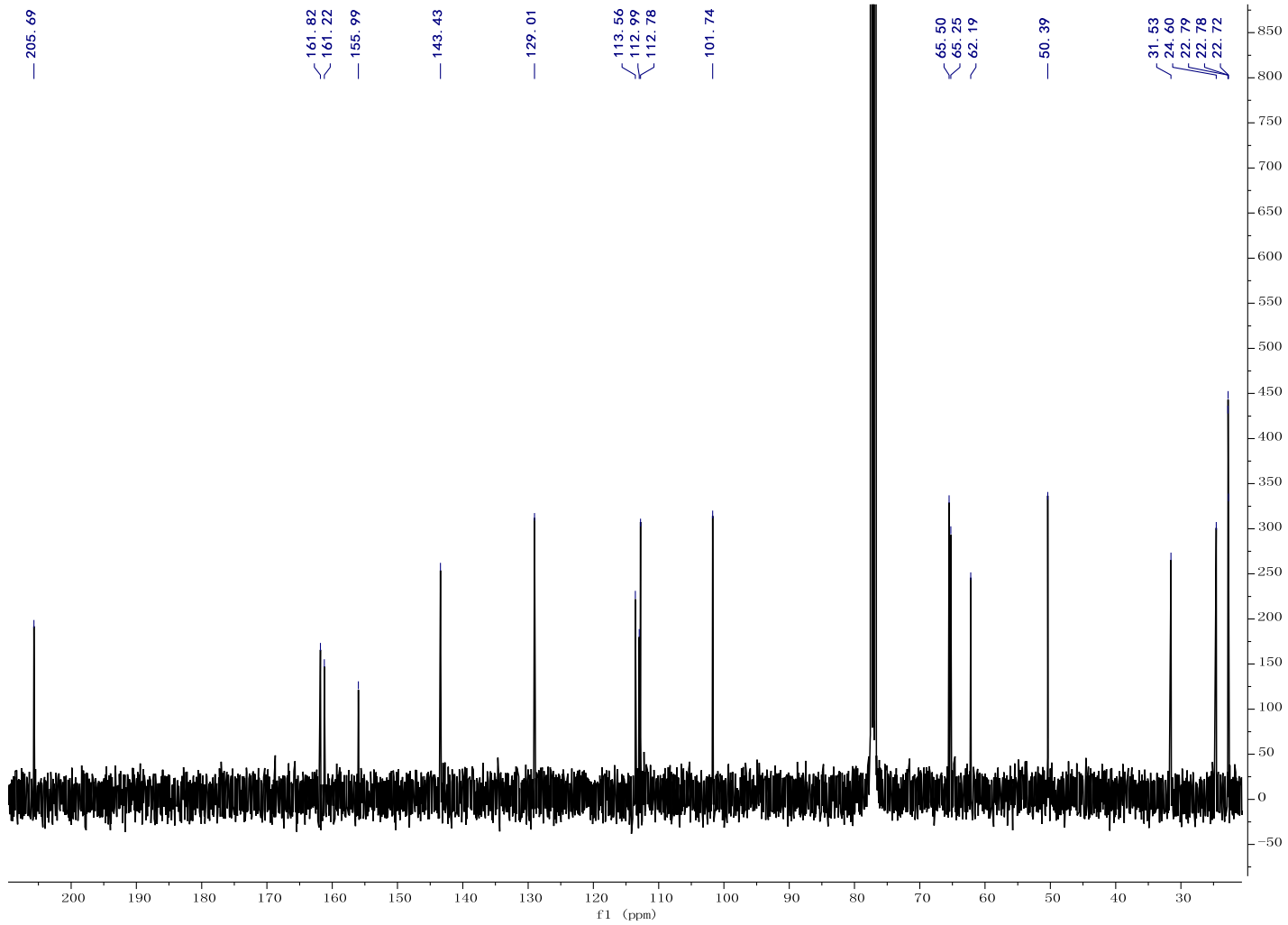


Figure S93. HSQC (400 MHz, $CDCl_3$) spectrum of pararubcoumarin A (**15**)

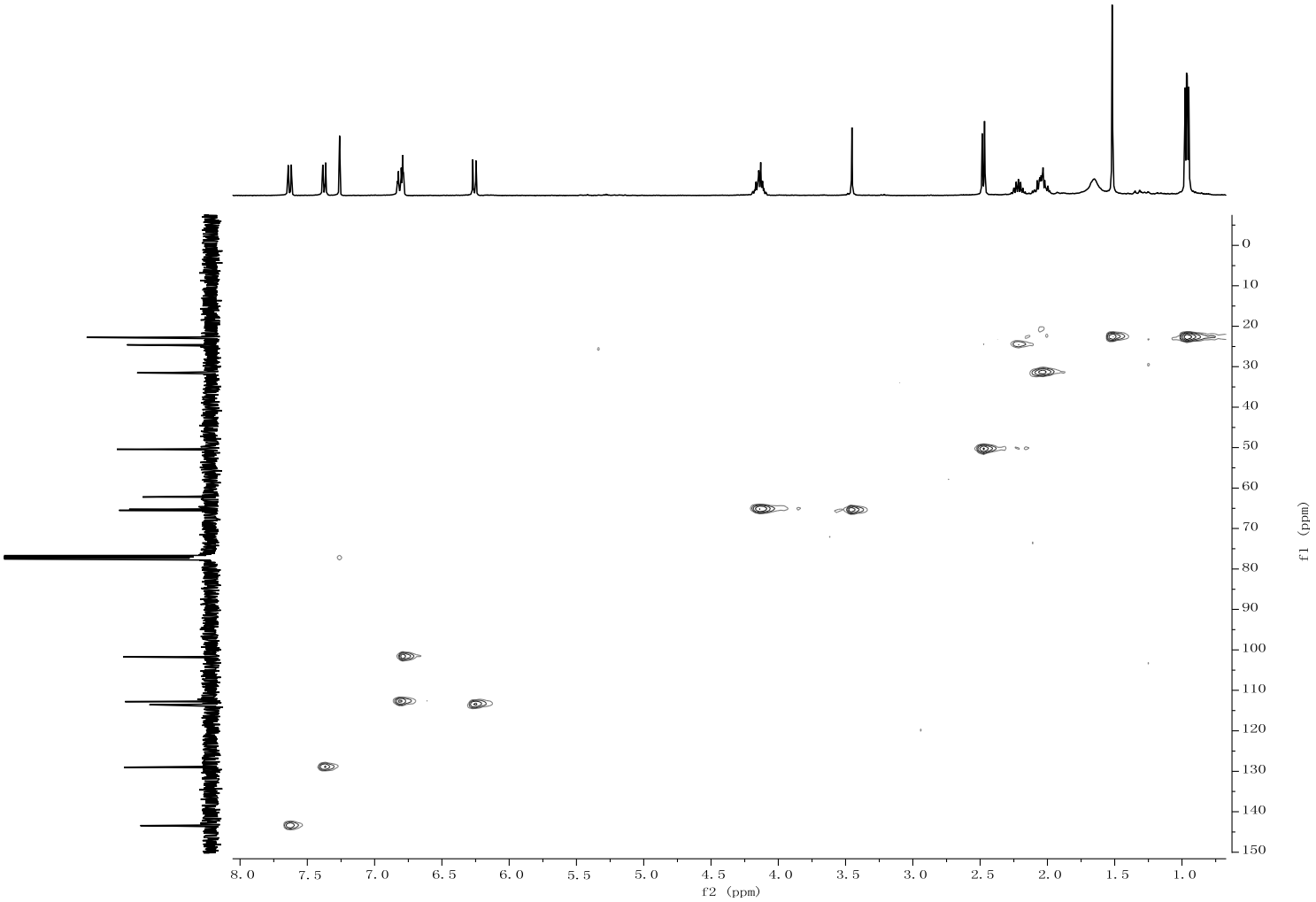


Figure S94. ^{1}H-^{1}H COSY (400 MHz, $CDCl_3$) spectrum of pararubcoumarin A (**15**)

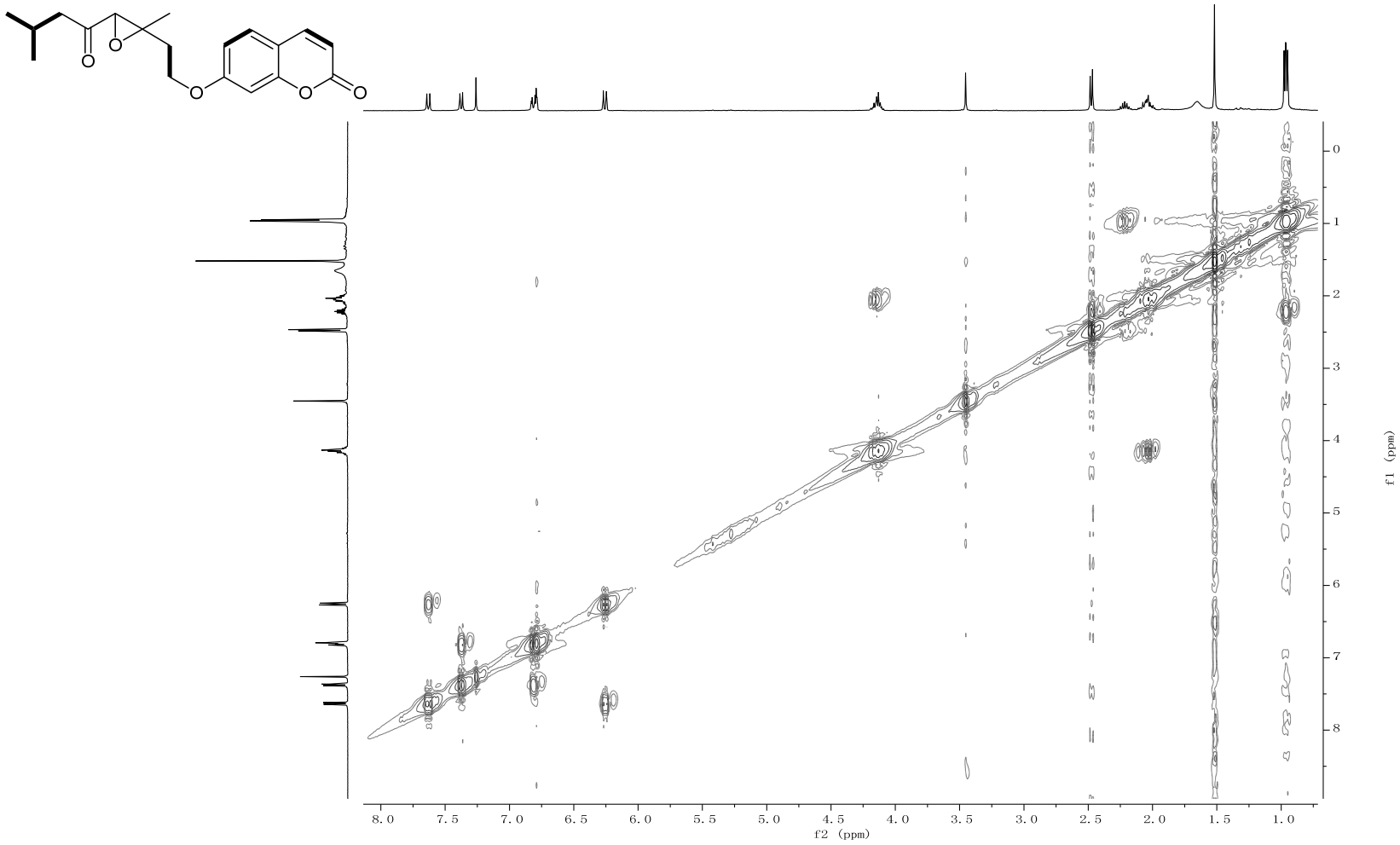


Figure S95. HMBC (400 MHz, $CDCl_3$) spectrum of pararubcoumarin A (**15**)

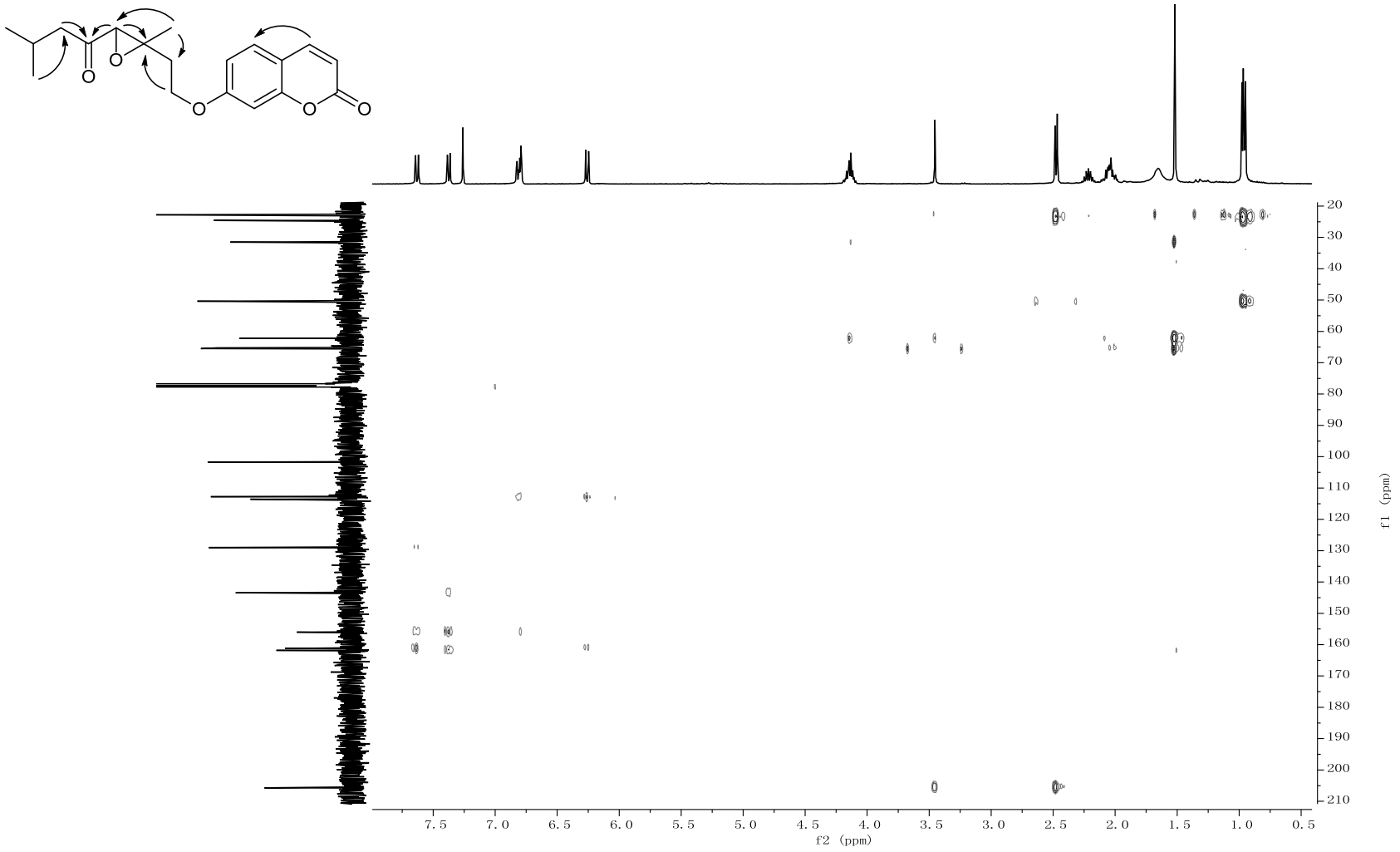


Figure S96. NOESY (400 MHz, $CDCl_3$) spectrum of pararubcoumarin A (**15**)

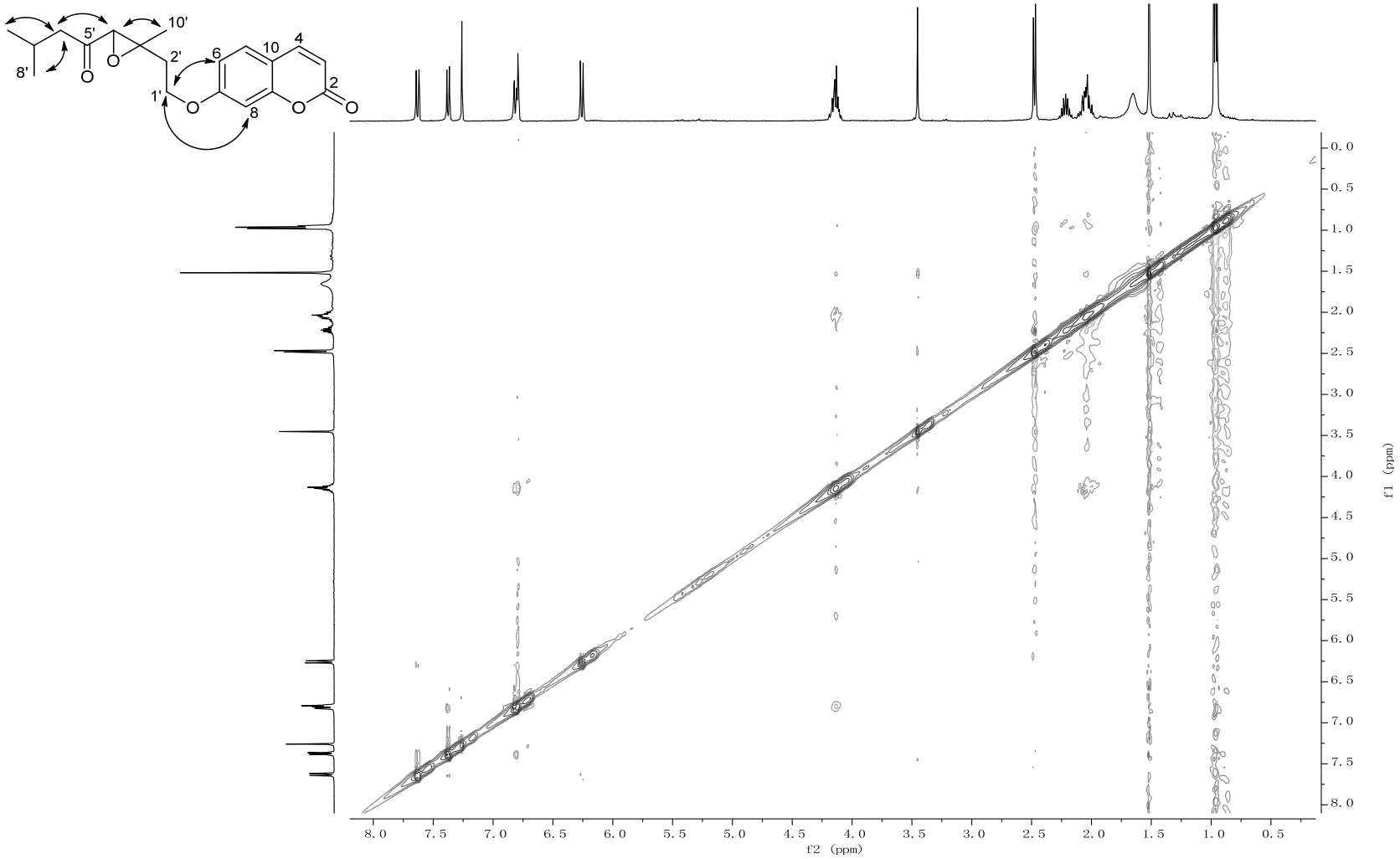


Figure S97. HRESIMS spectrum of pararubcoumarin A (**15**)

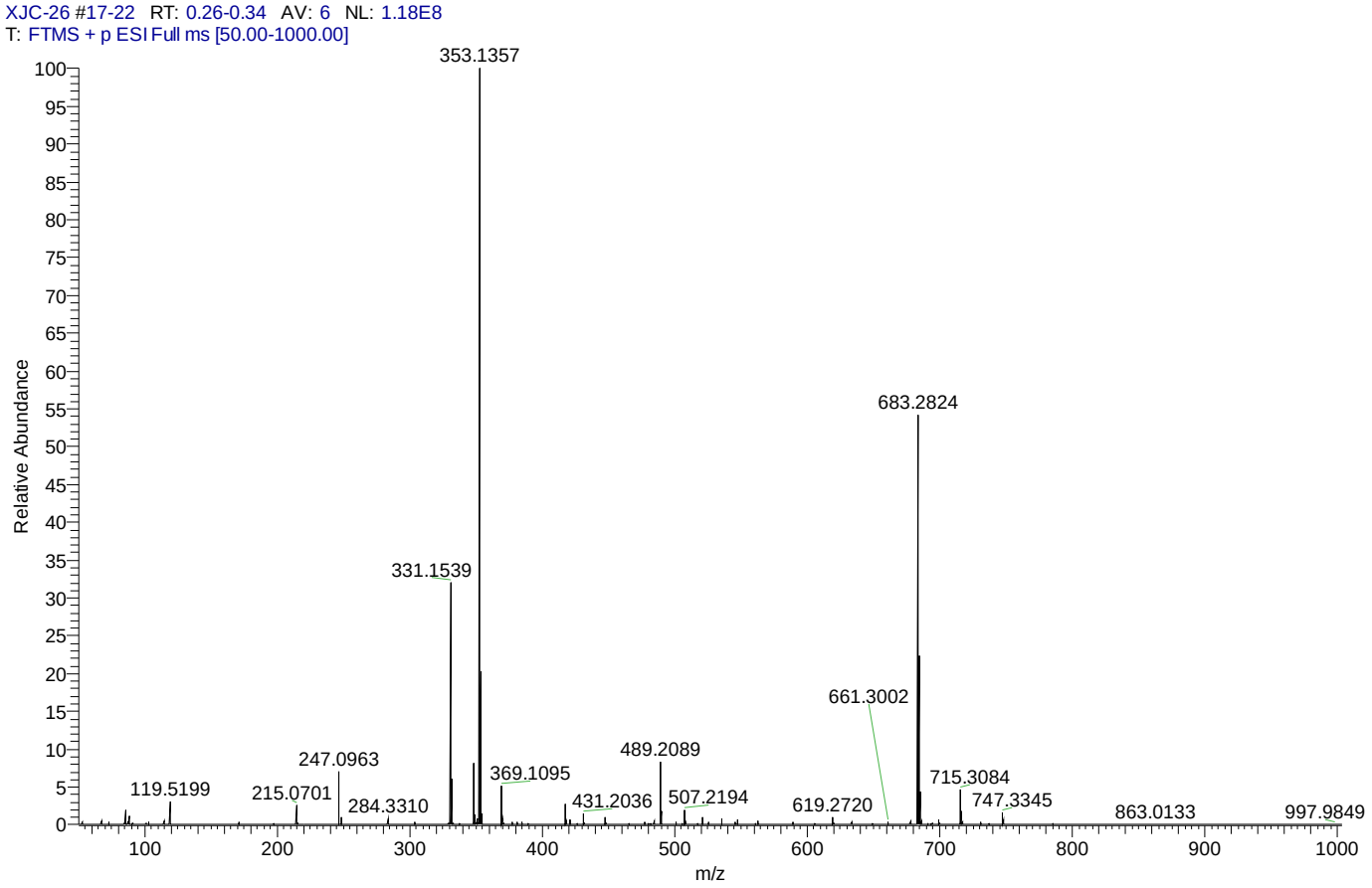


Figure S98. IR spectrum of pararubcoumarin A (**15**)

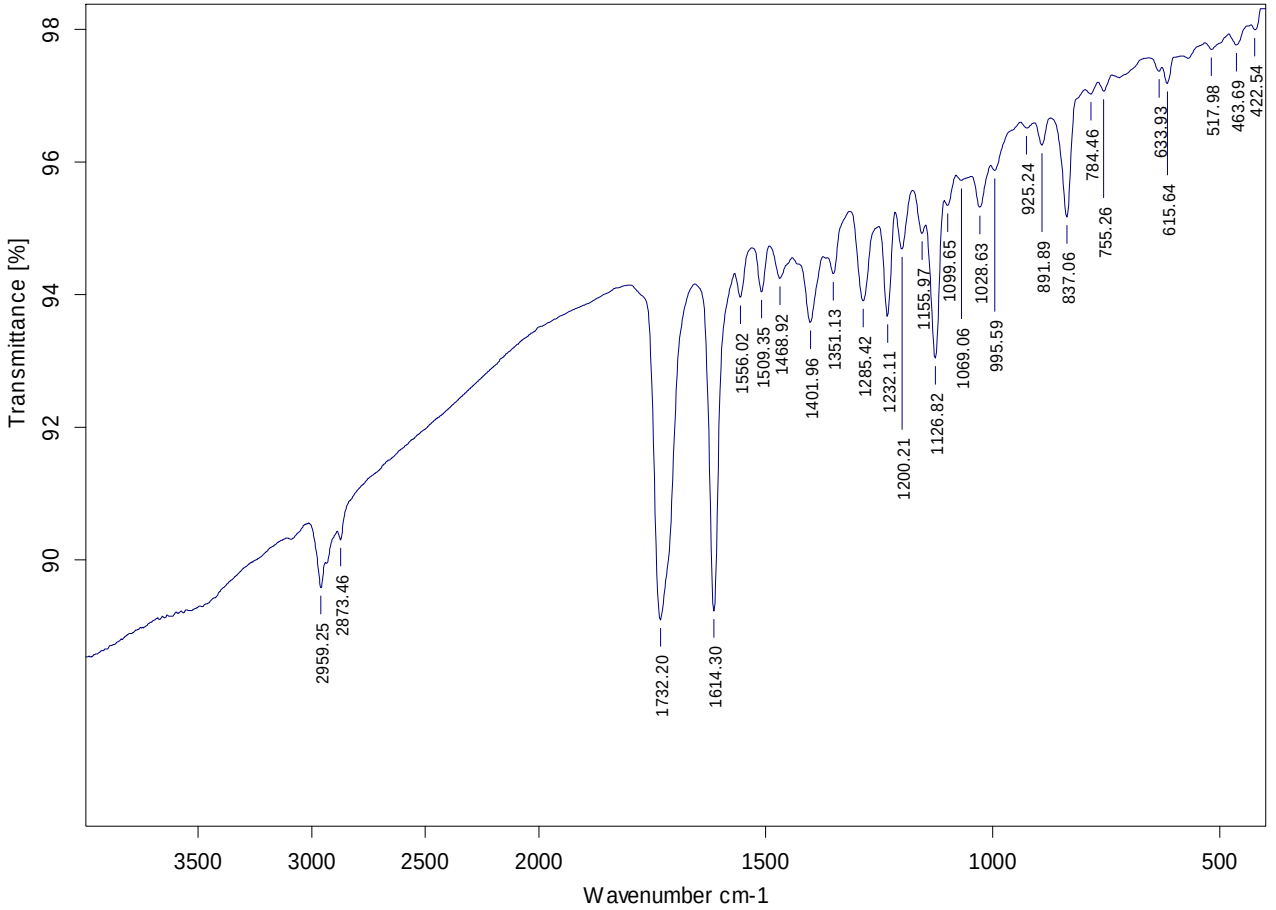


Figure S99. CD spectrum of pararubcoumarin A (**15**)

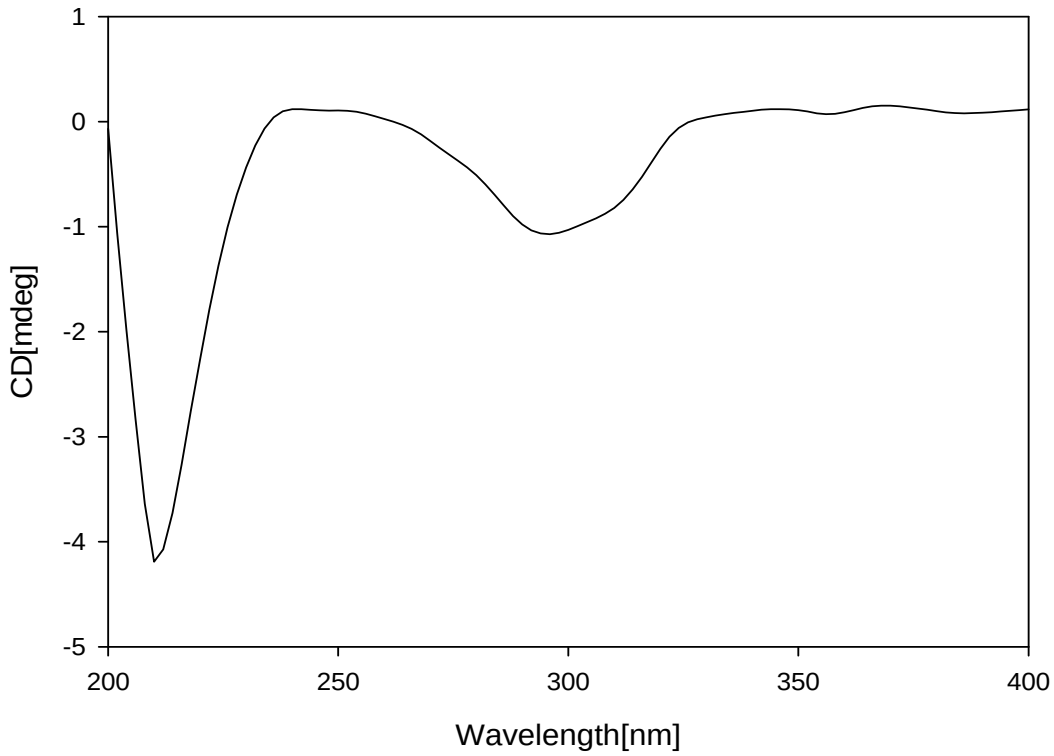


Figure S100. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of pararubcoumarin B (**16**)

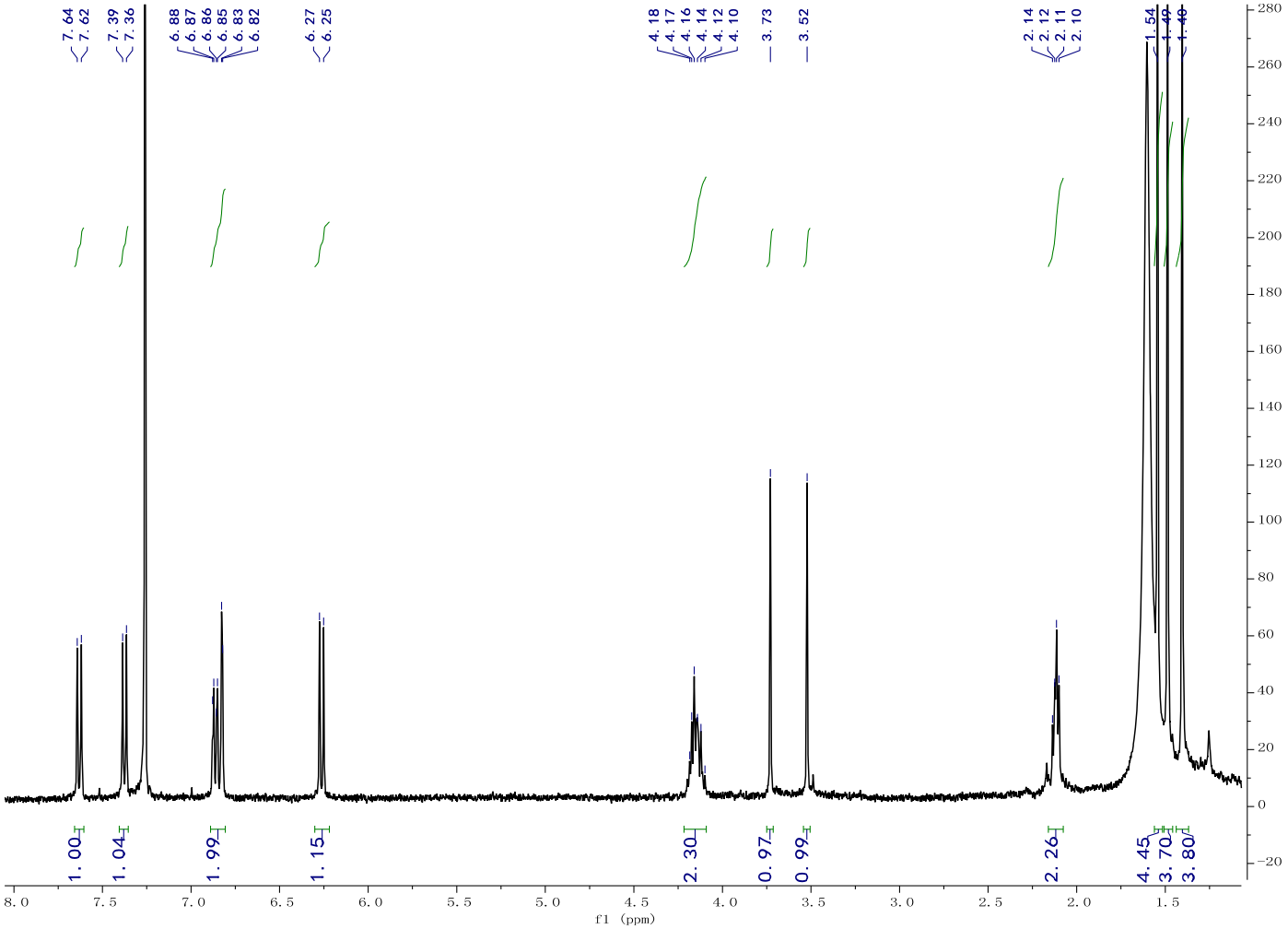


Figure S101. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of pararubcoumarin B (**16**)

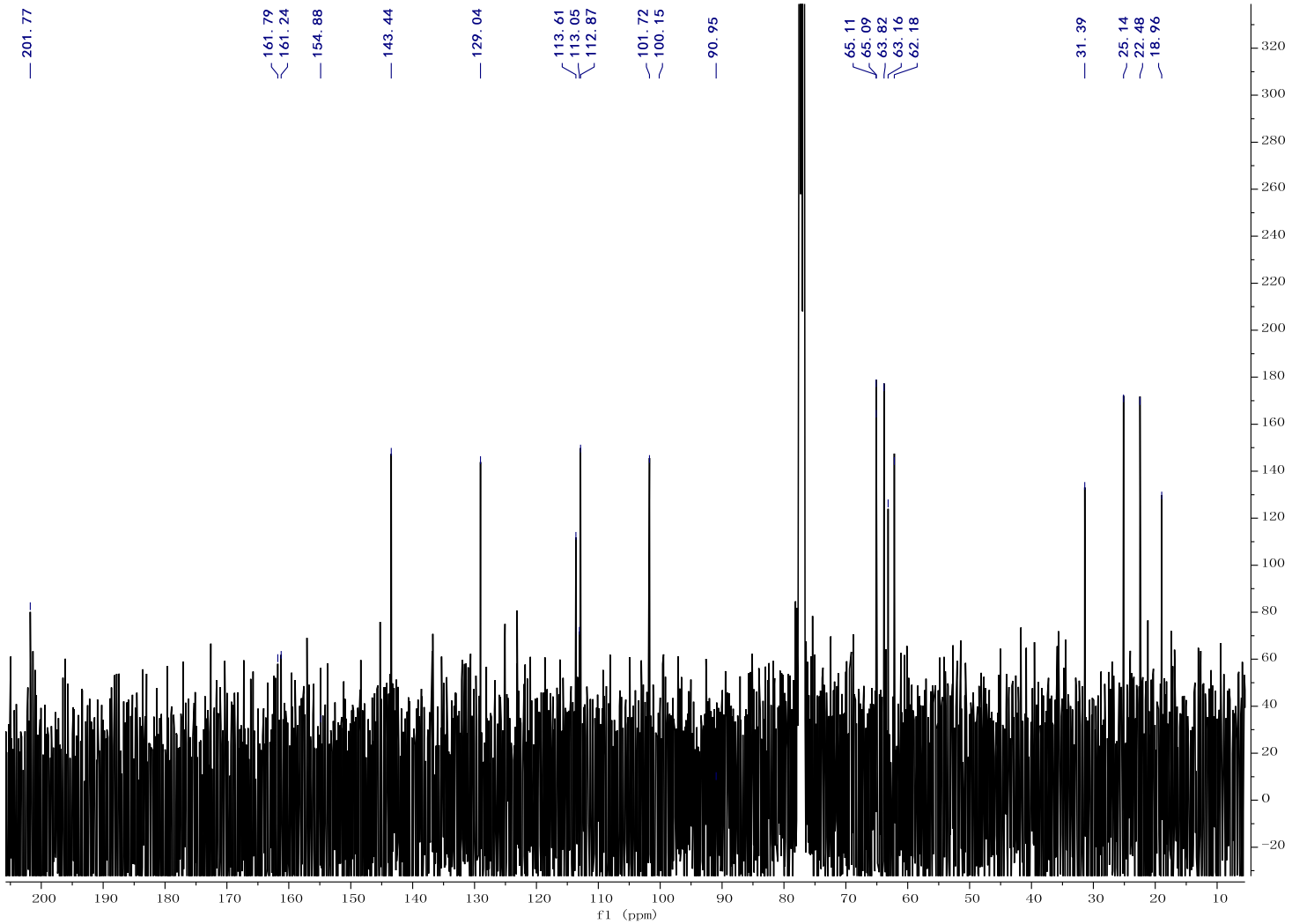


Figure S102. HSQC (400 MHz, $CDCl_3$) spectrum of pararubcoumarin B (**16**)

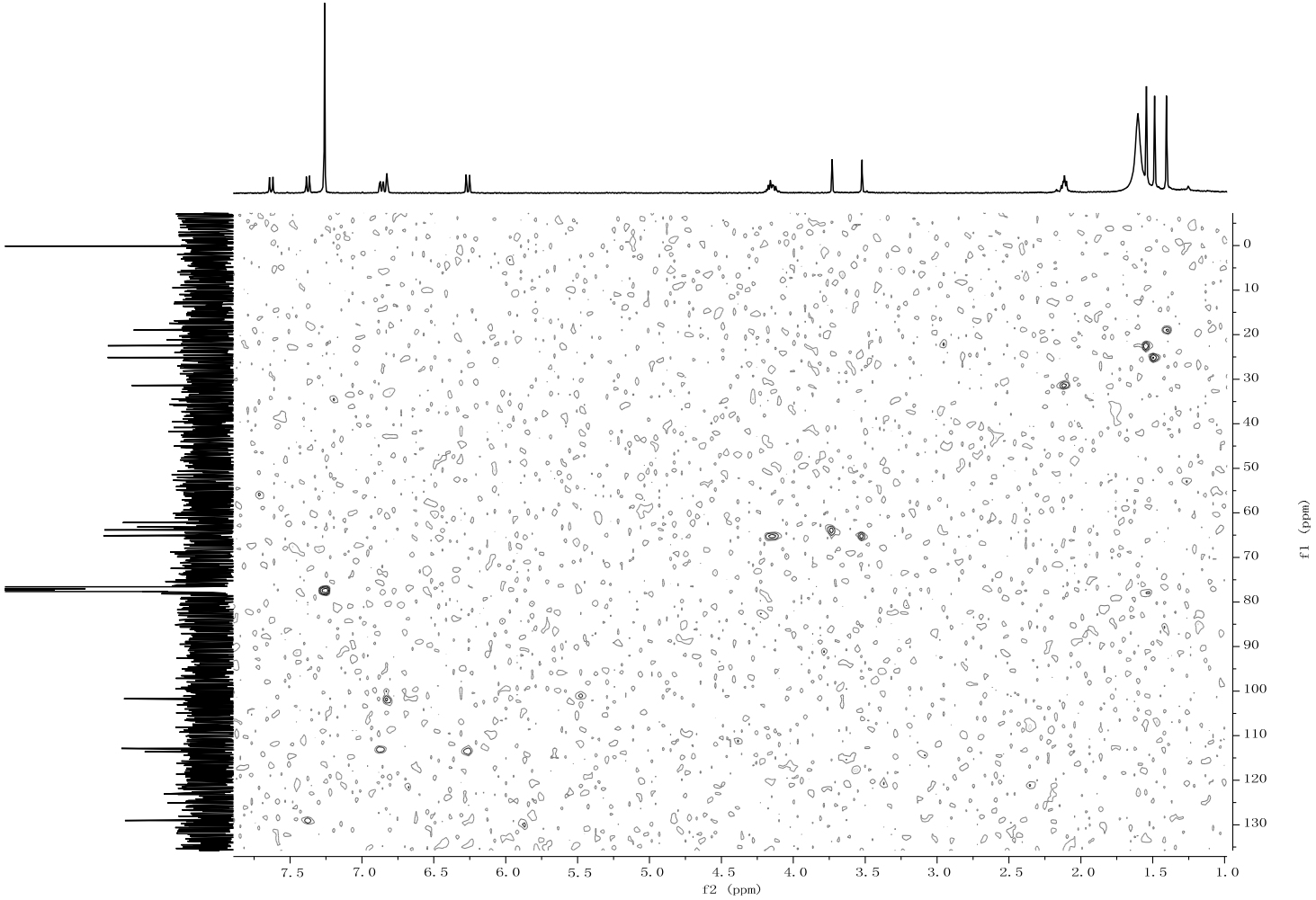


Figure S103. ^{1}H-^{1}H COSY (400 MHz, $CDCl_3$) spectrum of pararubcoumarin B (**16**)

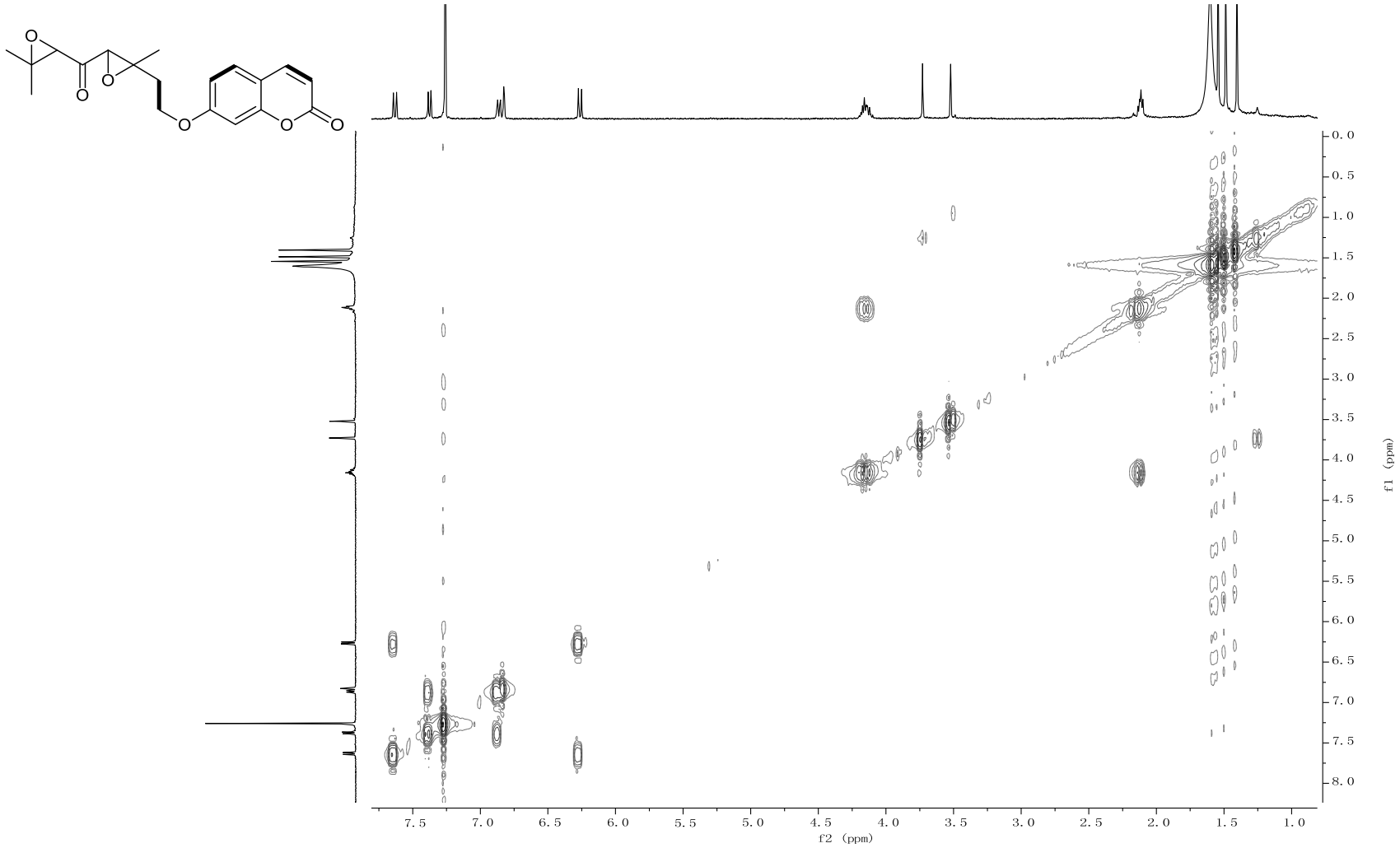


Figure S104. HMBC (400 MHz, $CDCl_3$) spectrum of pararubcoumarin B (**16**)

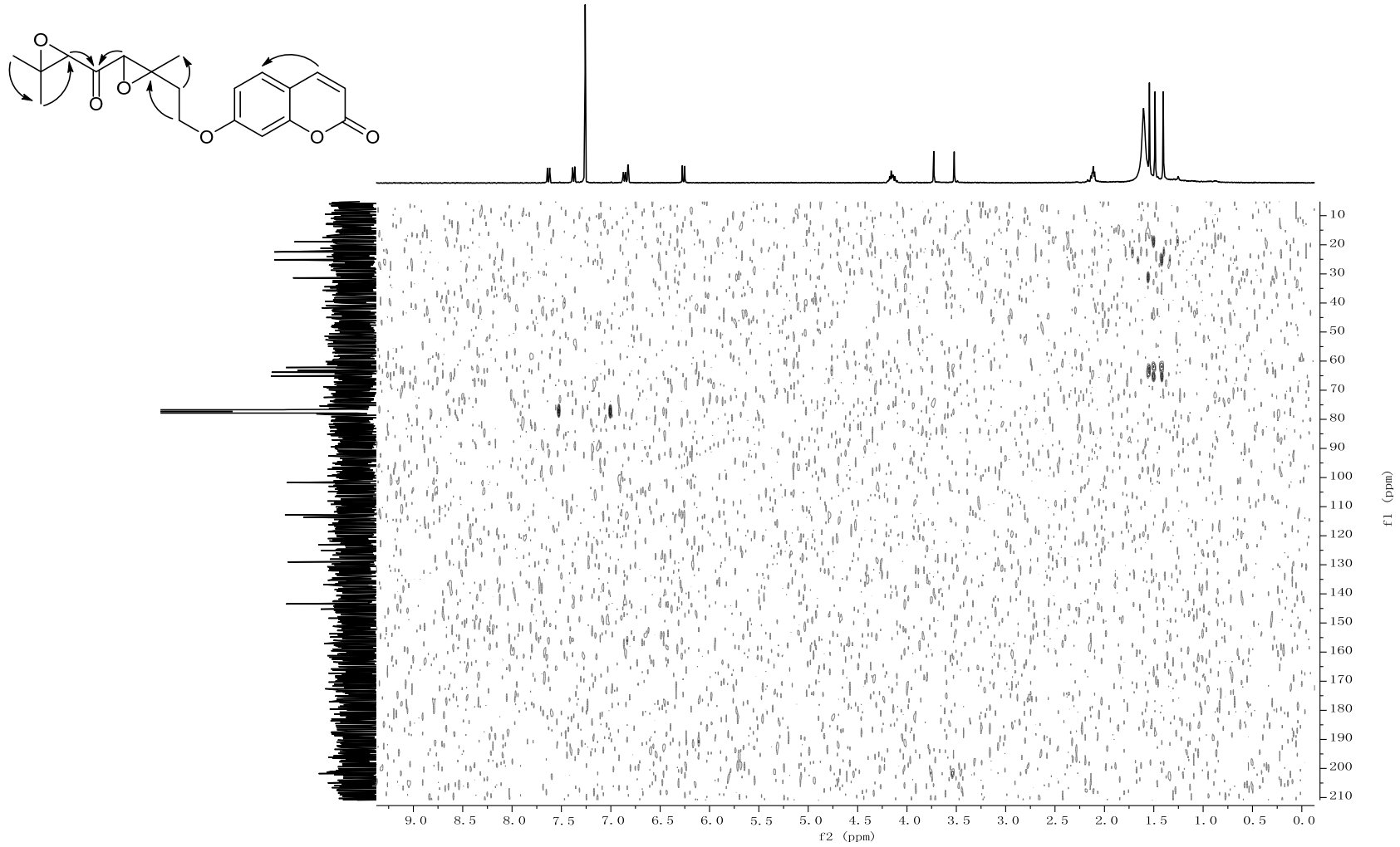


Figure S105. NOESY (400 MHz, $CDCl_3$) spectrum of pararubcoumarin B (**16**)

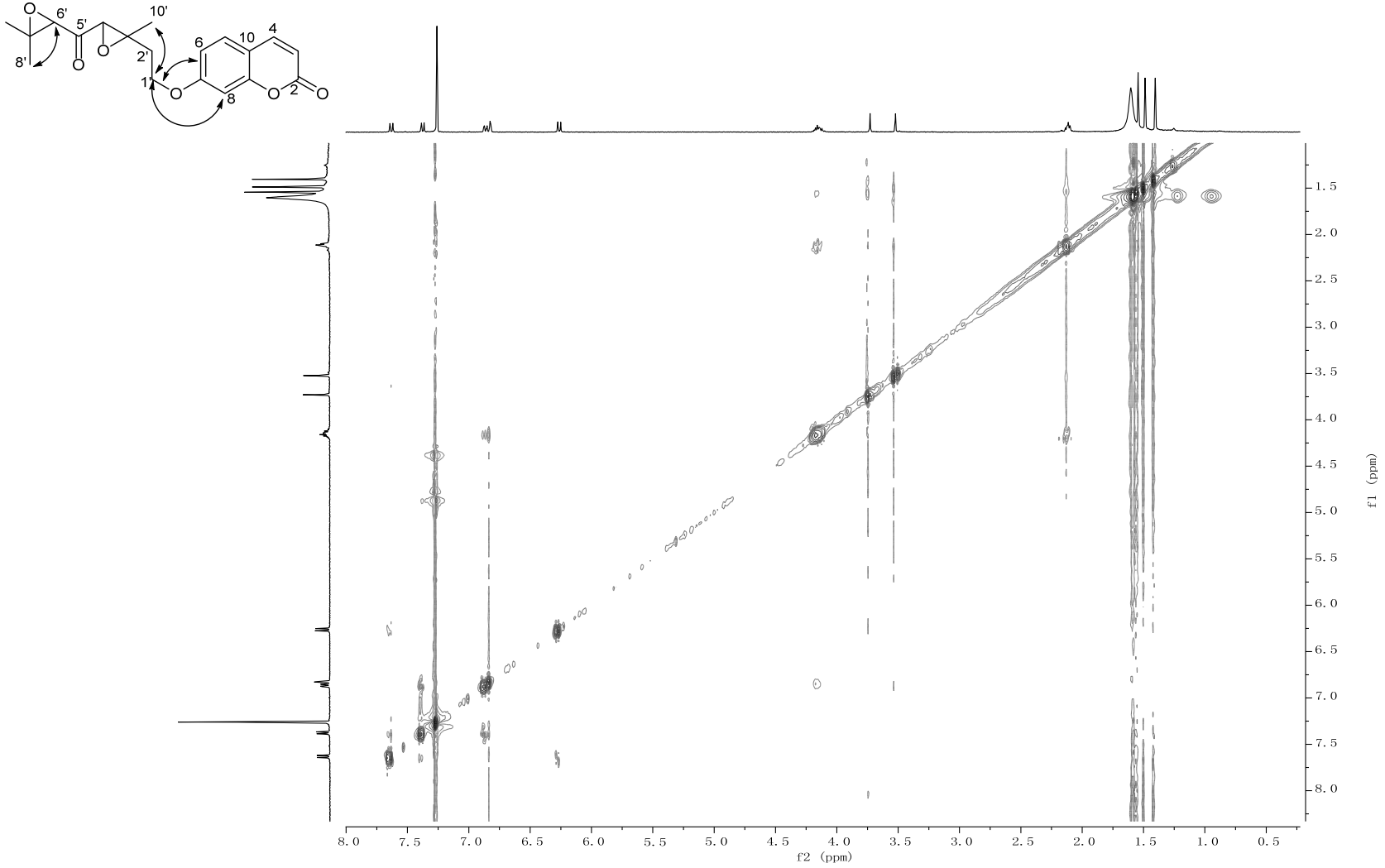


Figure S106. HRESIMS spectrum of pararubcoumarin B (**16**)

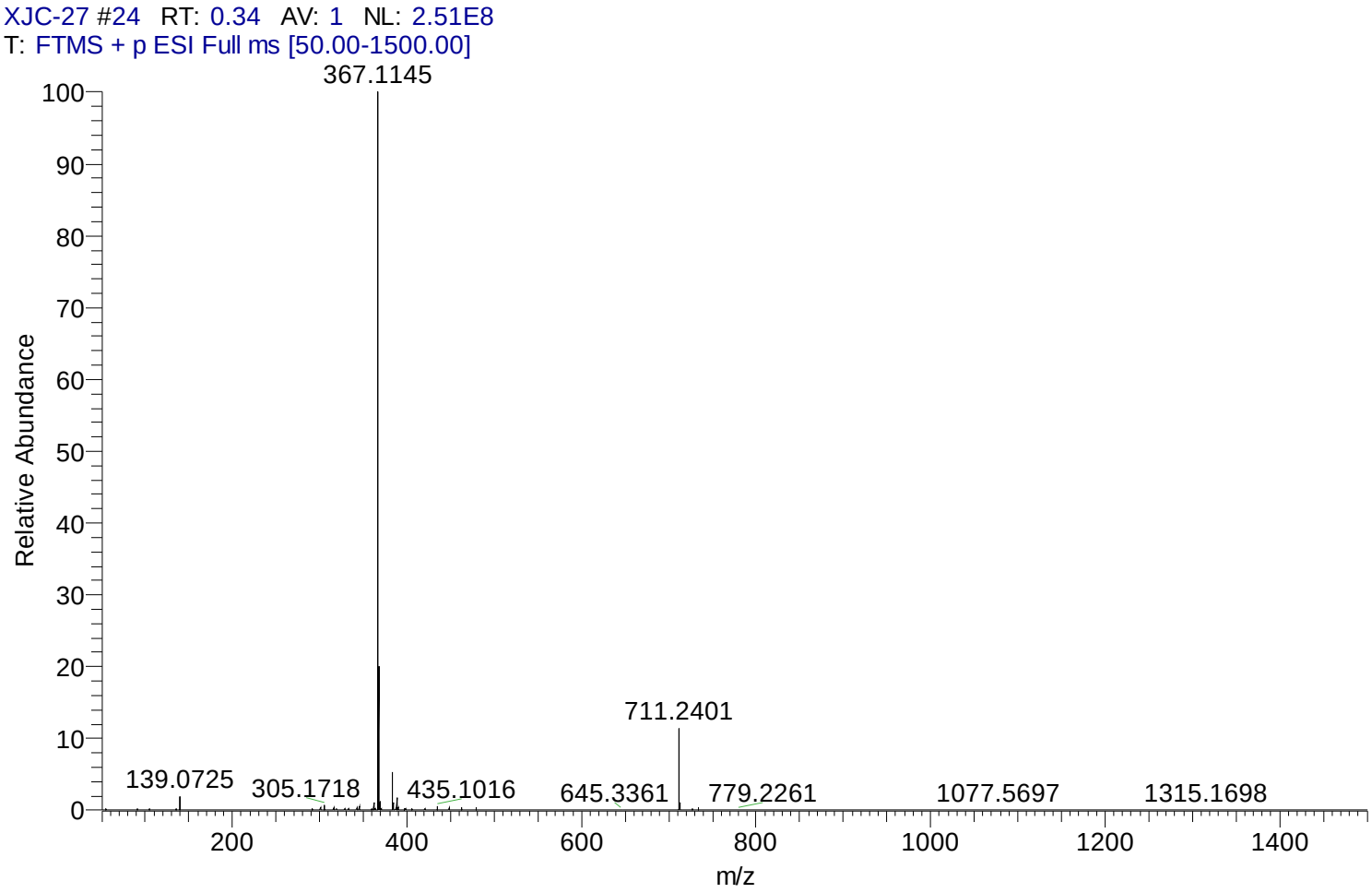


Figure S107. IR spectrum of pararubcoumarin B (**16**)

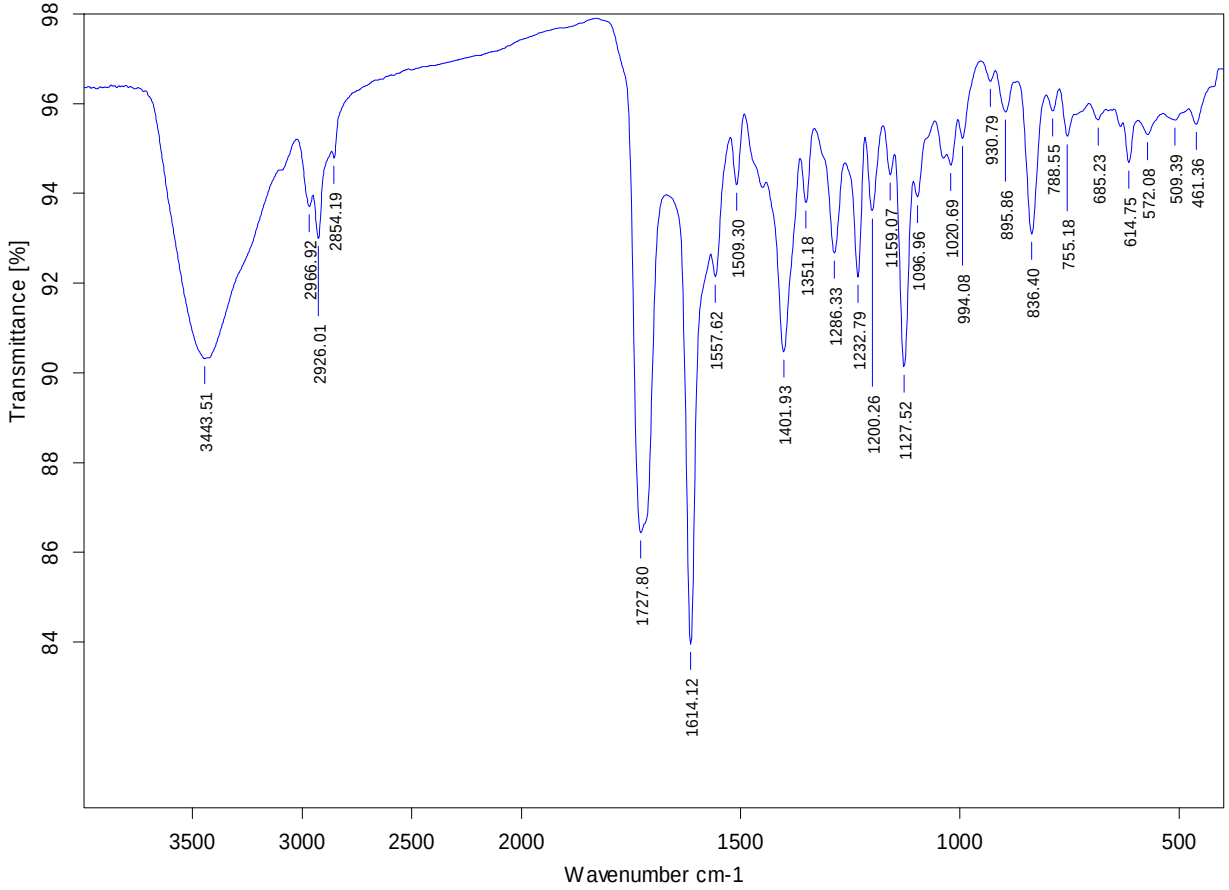


Figure S108. CD spectrum of pararubcoumarin B (**16**)

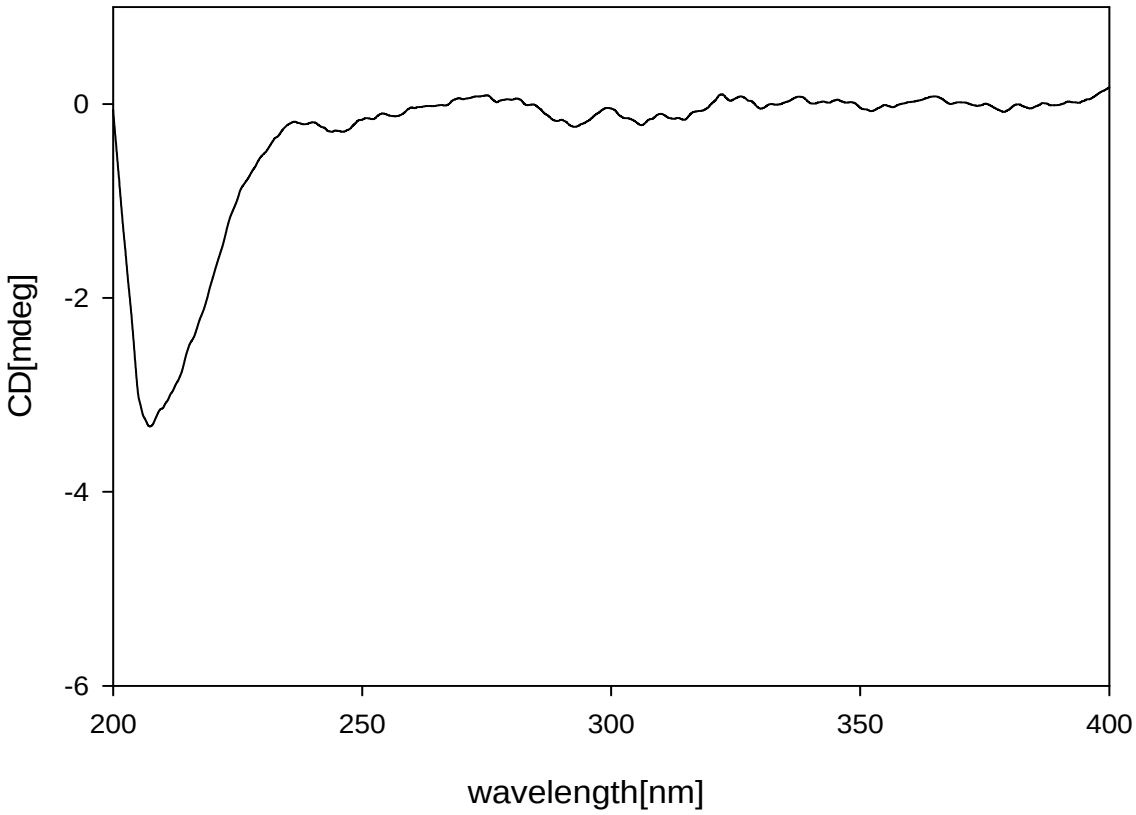


Figure S109. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of pararubcoumarin C (**17**)

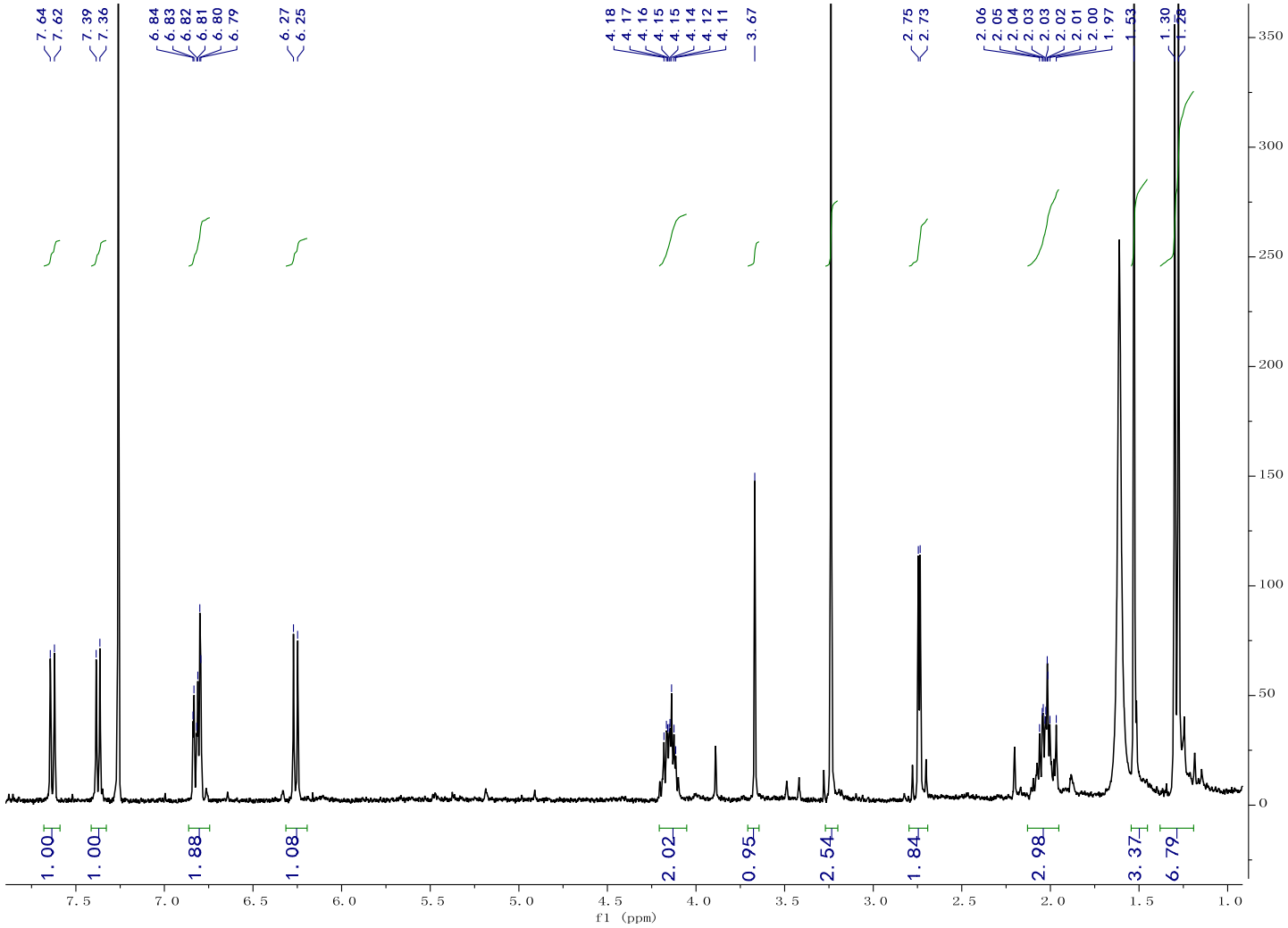


Figure S110. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of pararubcoumarin C (**17**)

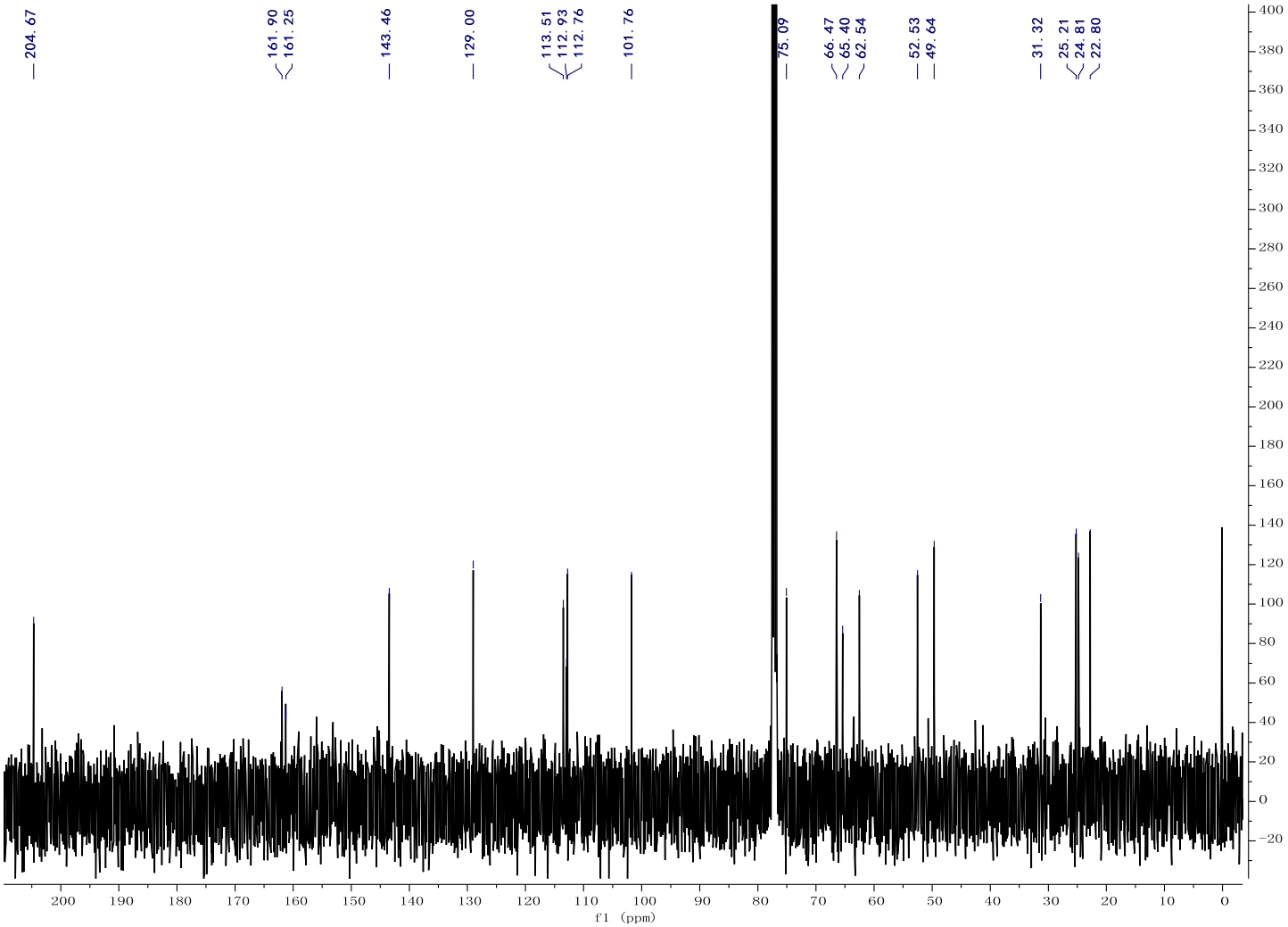


Figure S111. HSQC (400 MHz, $CDCl_3$) spectrum of pararubcoumarin C (**17**)

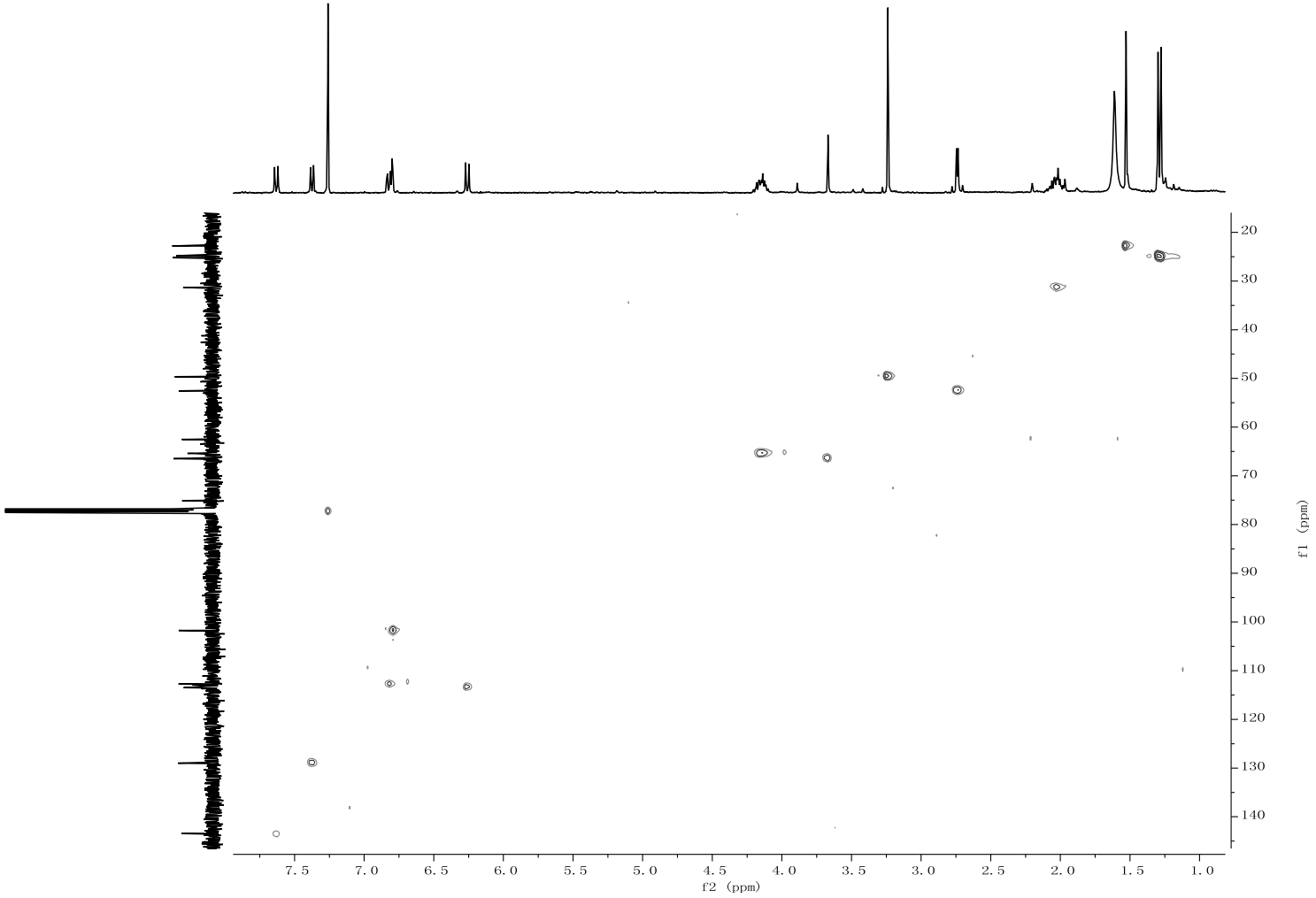


Figure S112. ^{1}H-^{1}H COSY (400 MHz, $CDCl_3$) spectrum of pararubcoumarin C (**17**)

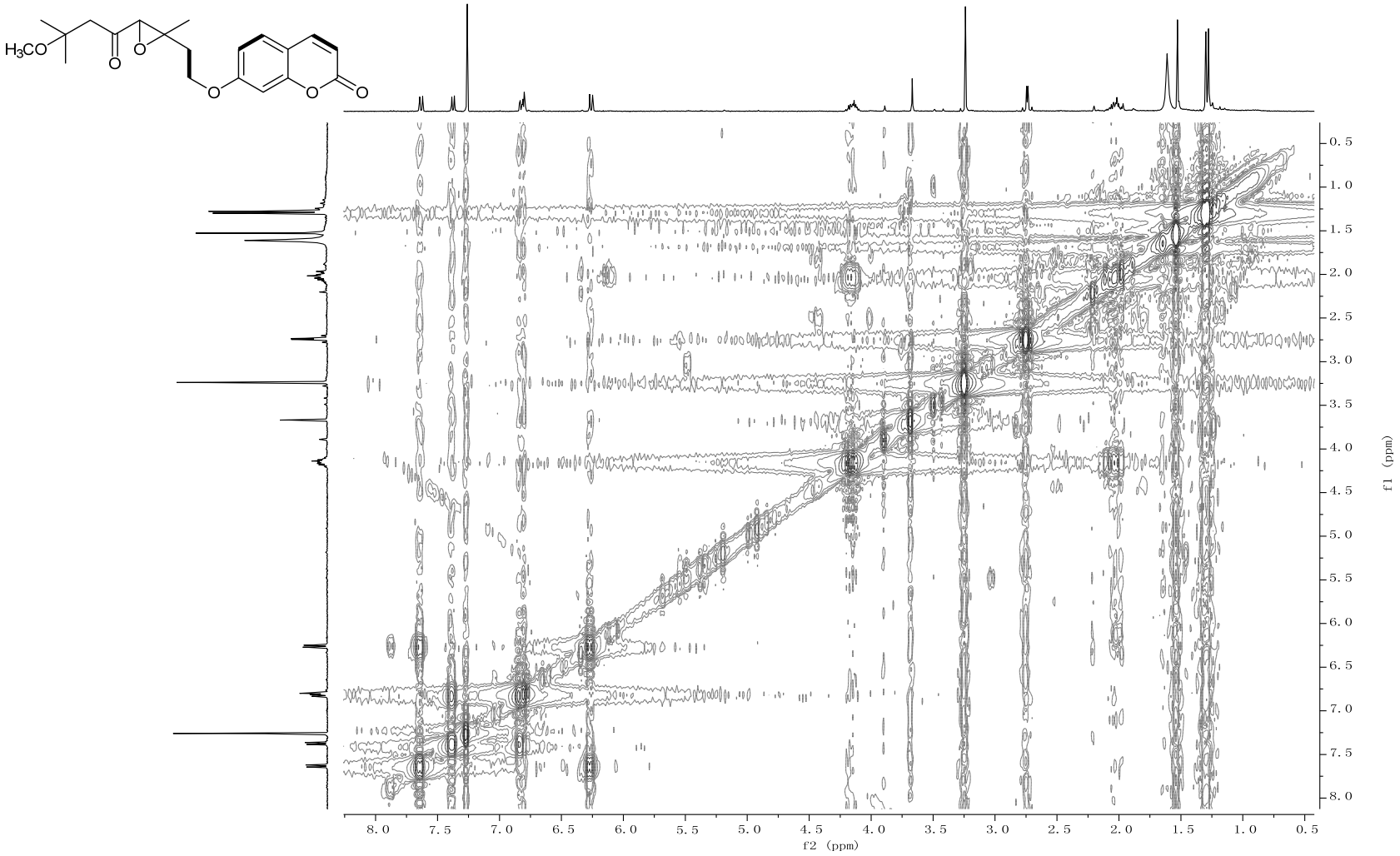


Figure S113. HMBC (400 MHz, $CDCl_3$) spectrum of pararubcoumarin C (**17**)

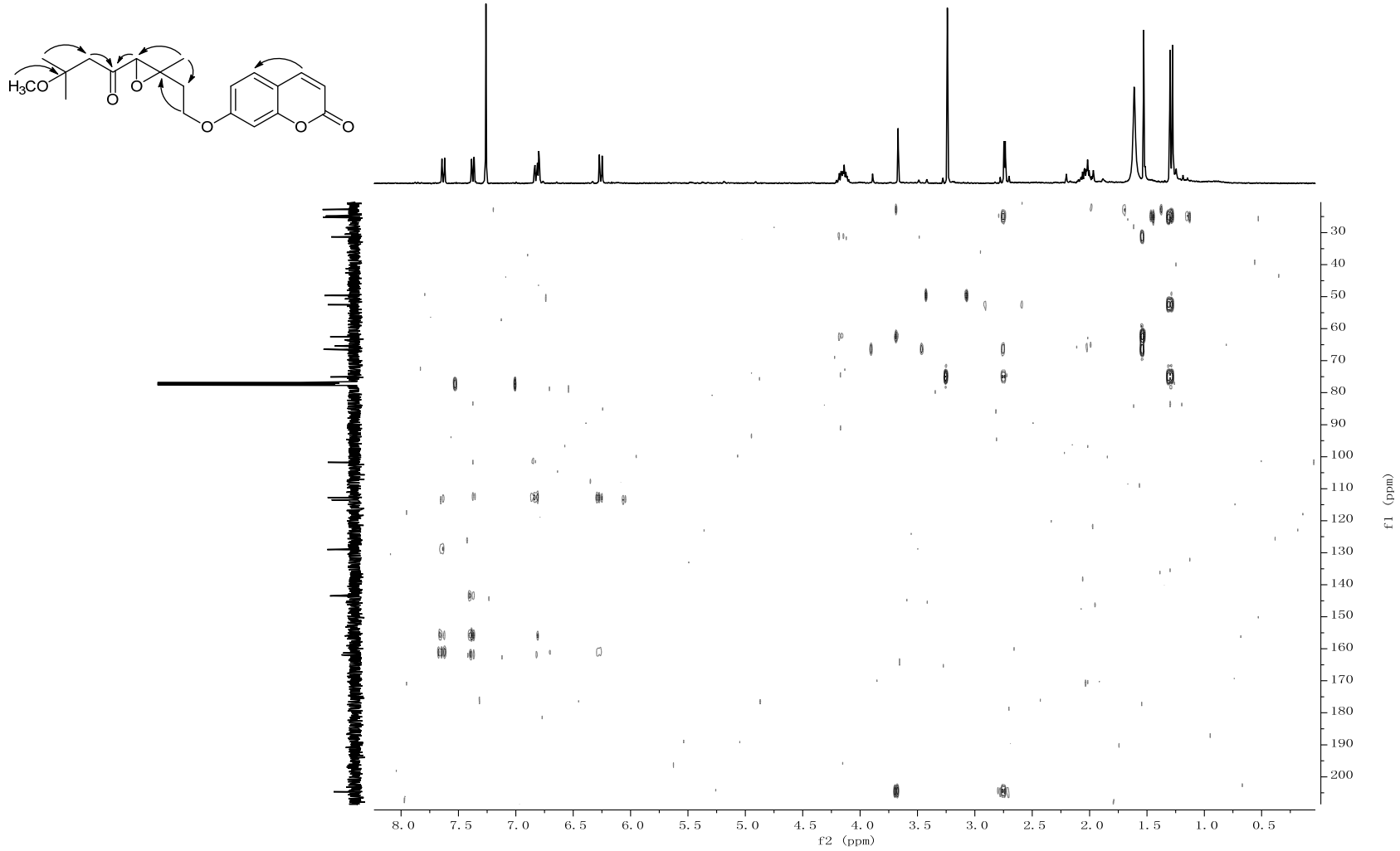


Figure S114. NOESY (400 MHz, $CDCl_3$) spectrum of pararubcoumarin C (**17**)

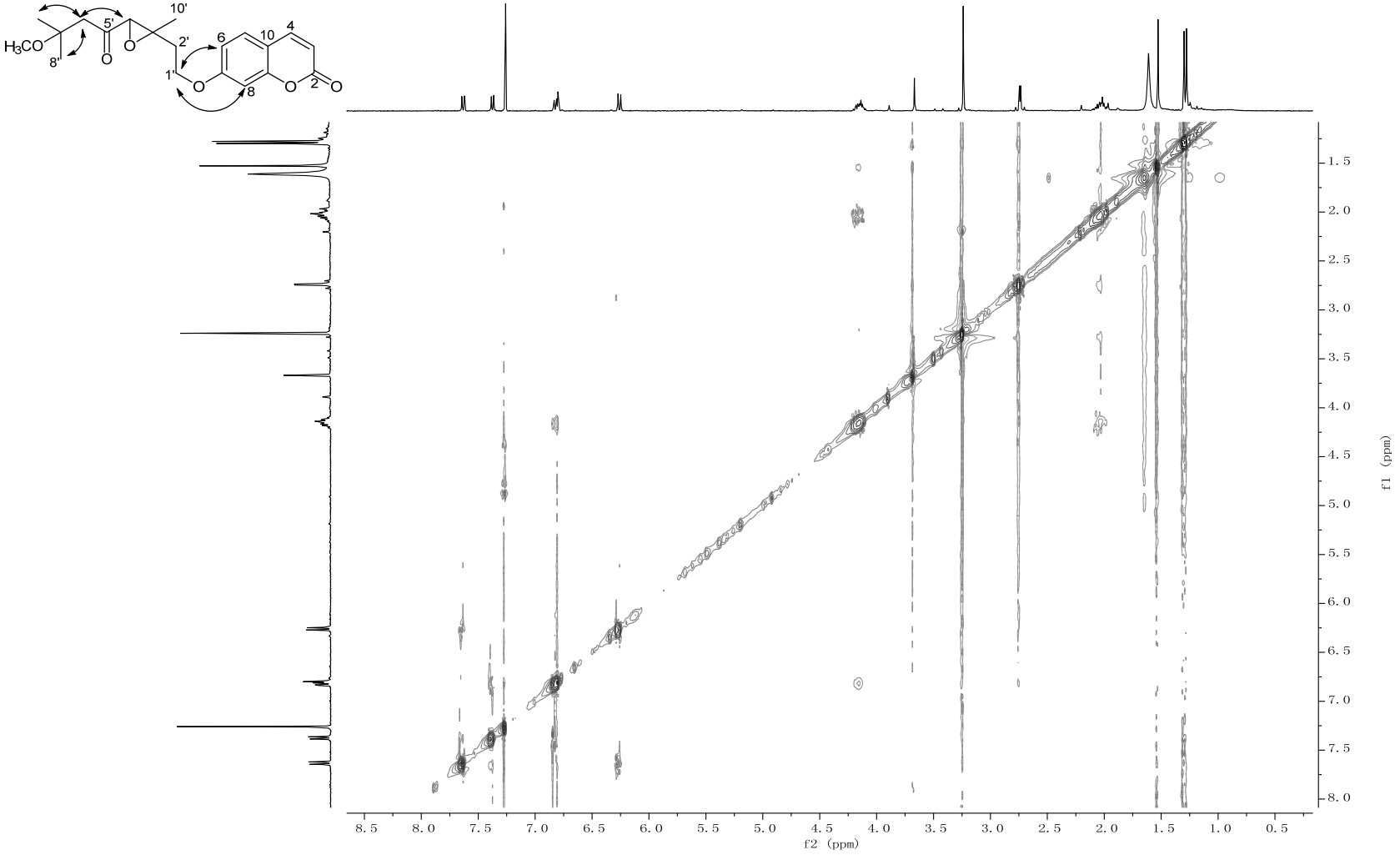


Figure S115. HRESIMS spectrum of pararubcoumarin C (**17**)

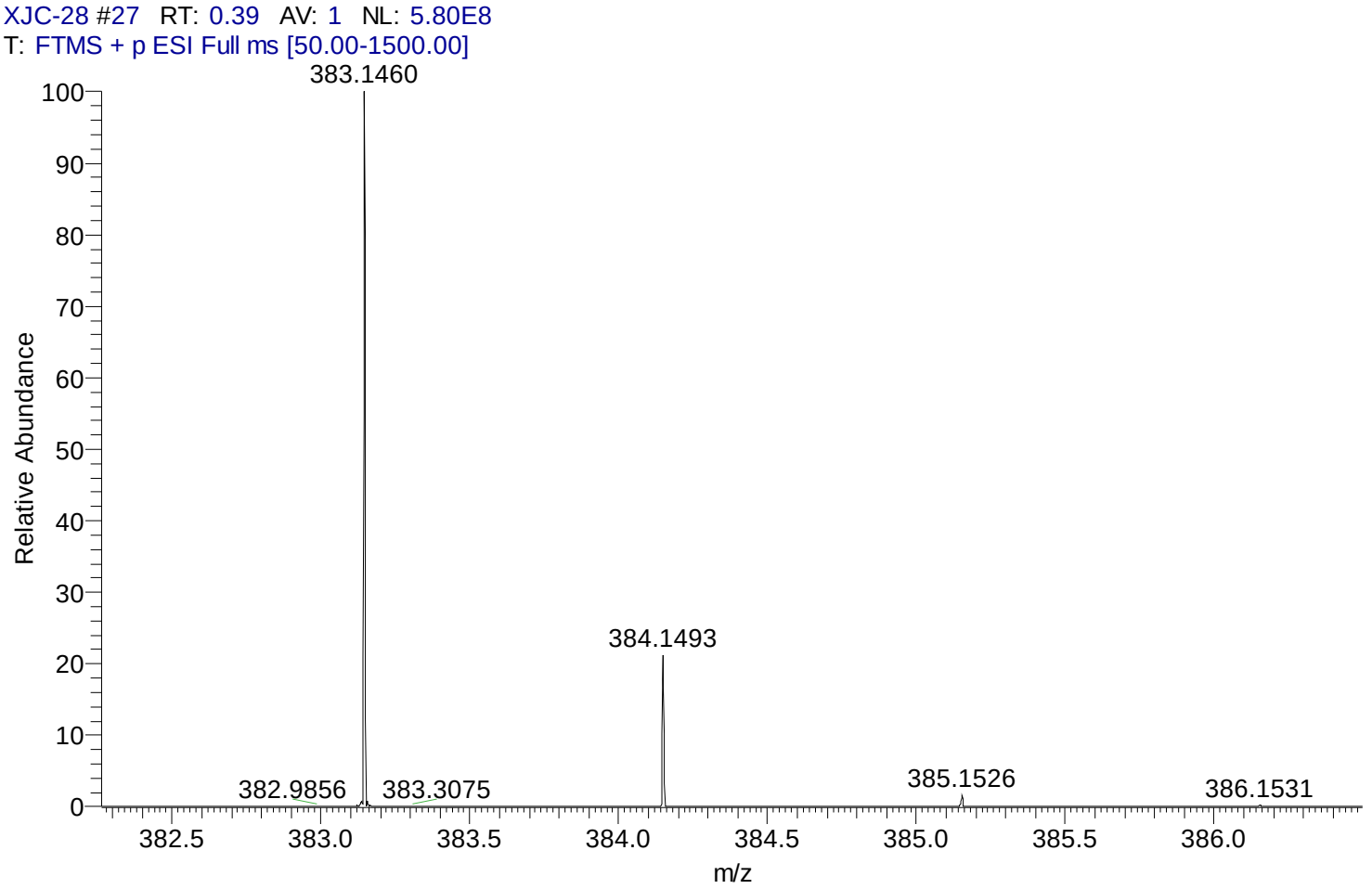


Figure S116. IR spectrum of pararubcoumarin C (**17**)

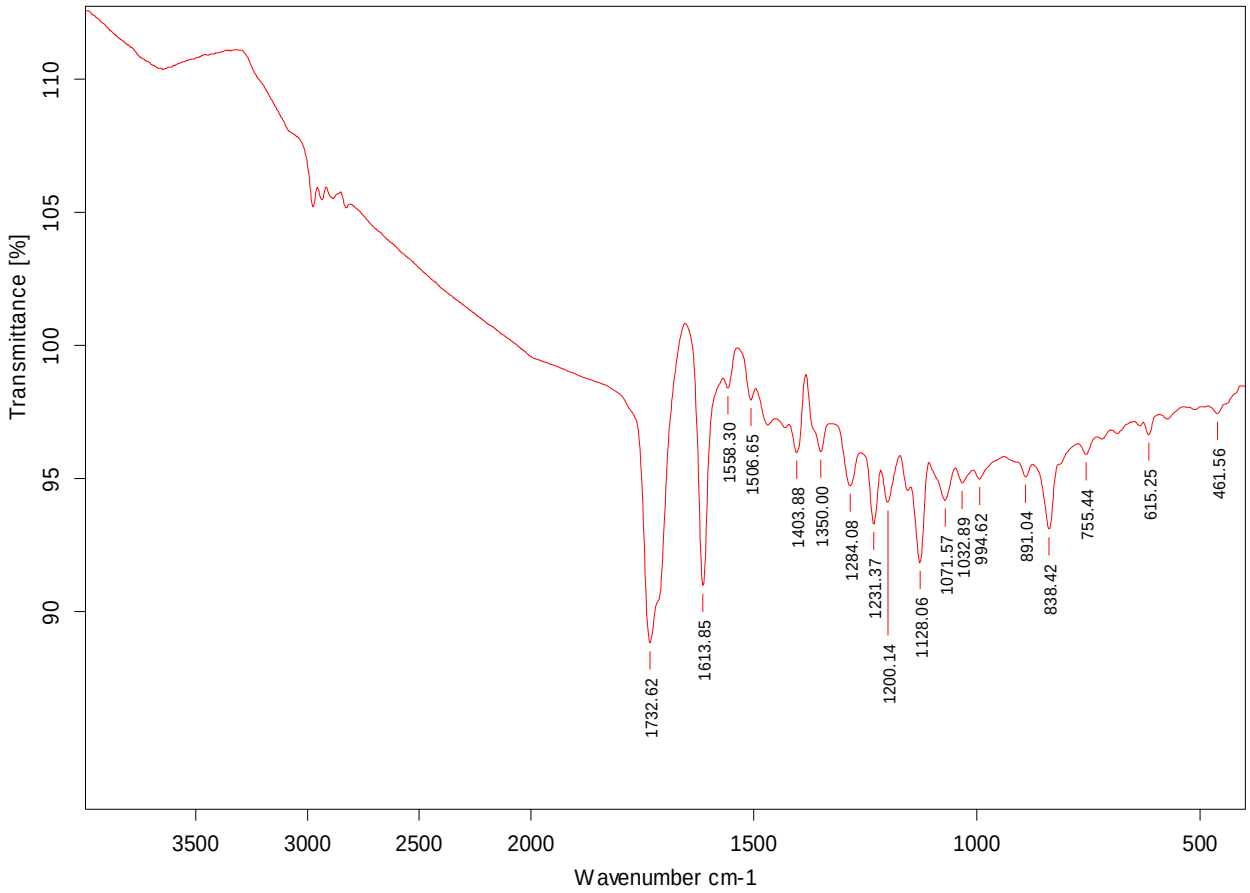


Figure S117. CD spectrum of pararubcoumarin C (**17**)

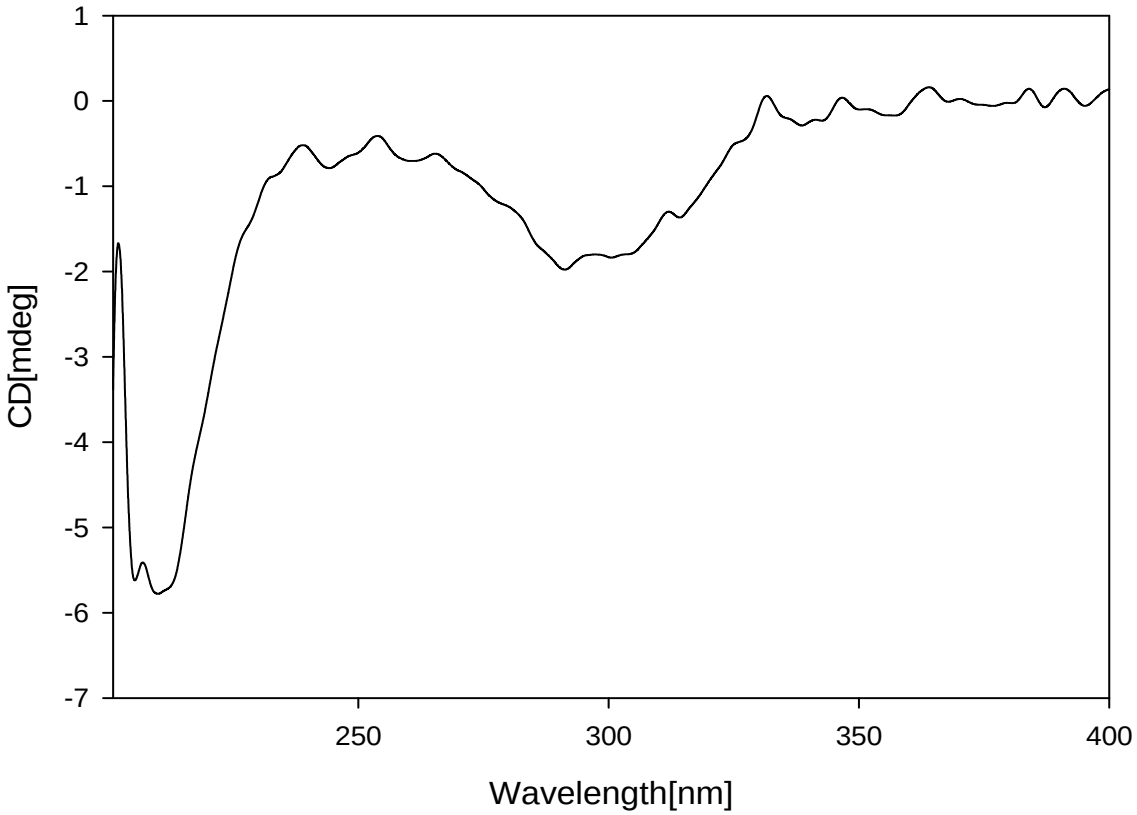


Figure S118. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of pararubcoumarin D (**18**)

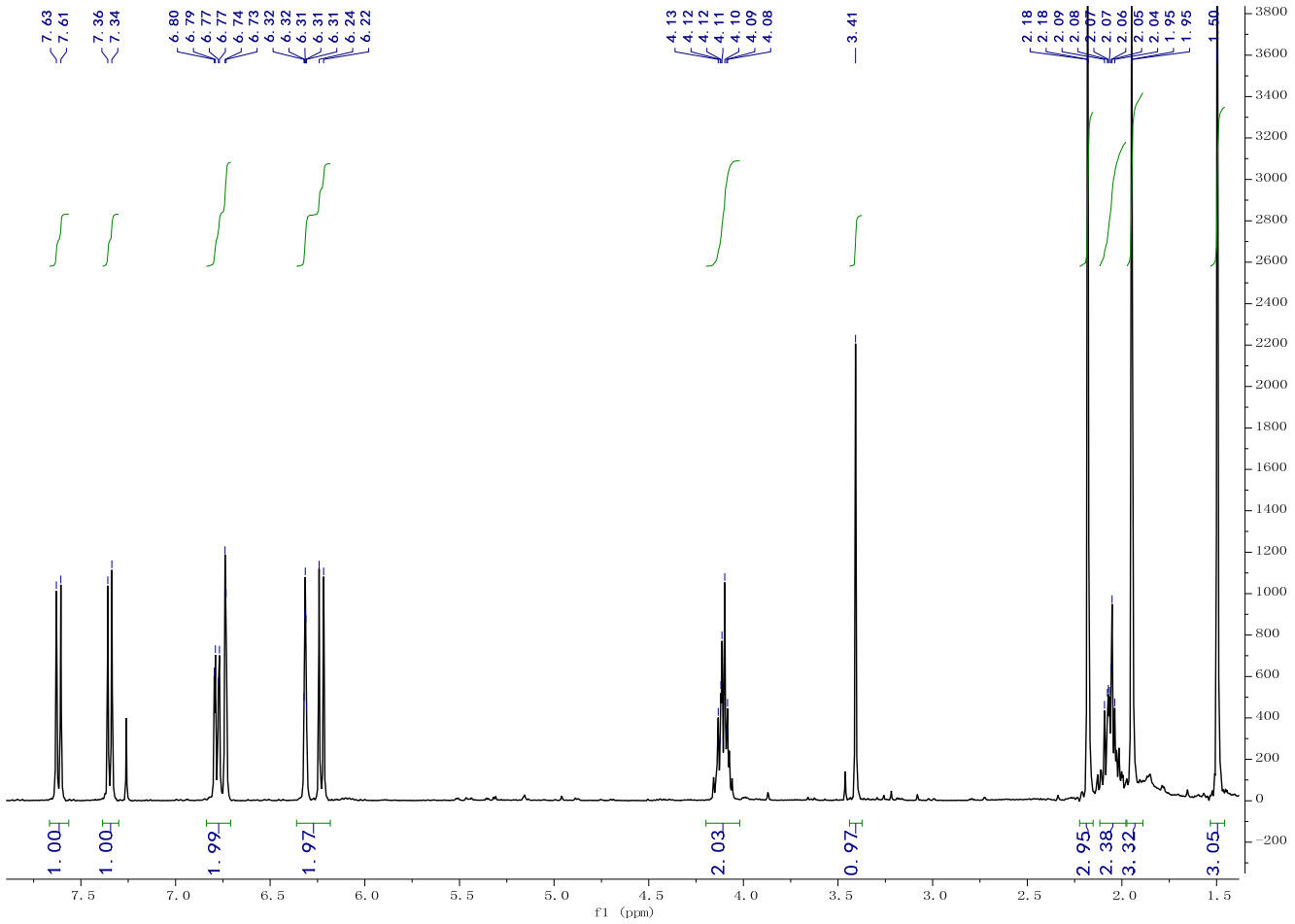


Figure S119. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of pararubcoumarin D (**18**)

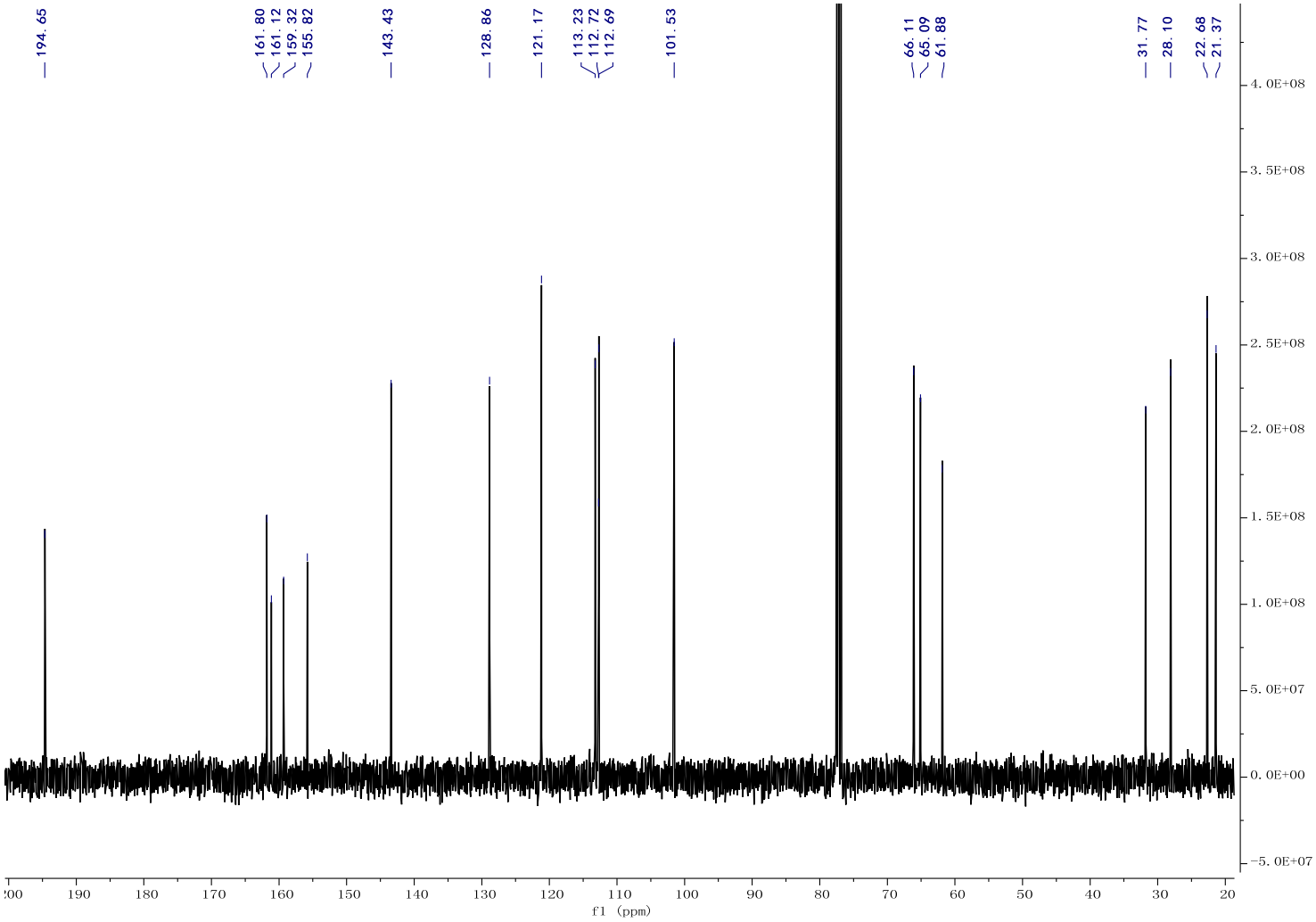


Figure S120. HSQC (400 MHz, $CDCl_3$) spectrum of pararubcoumarin D (**18**)

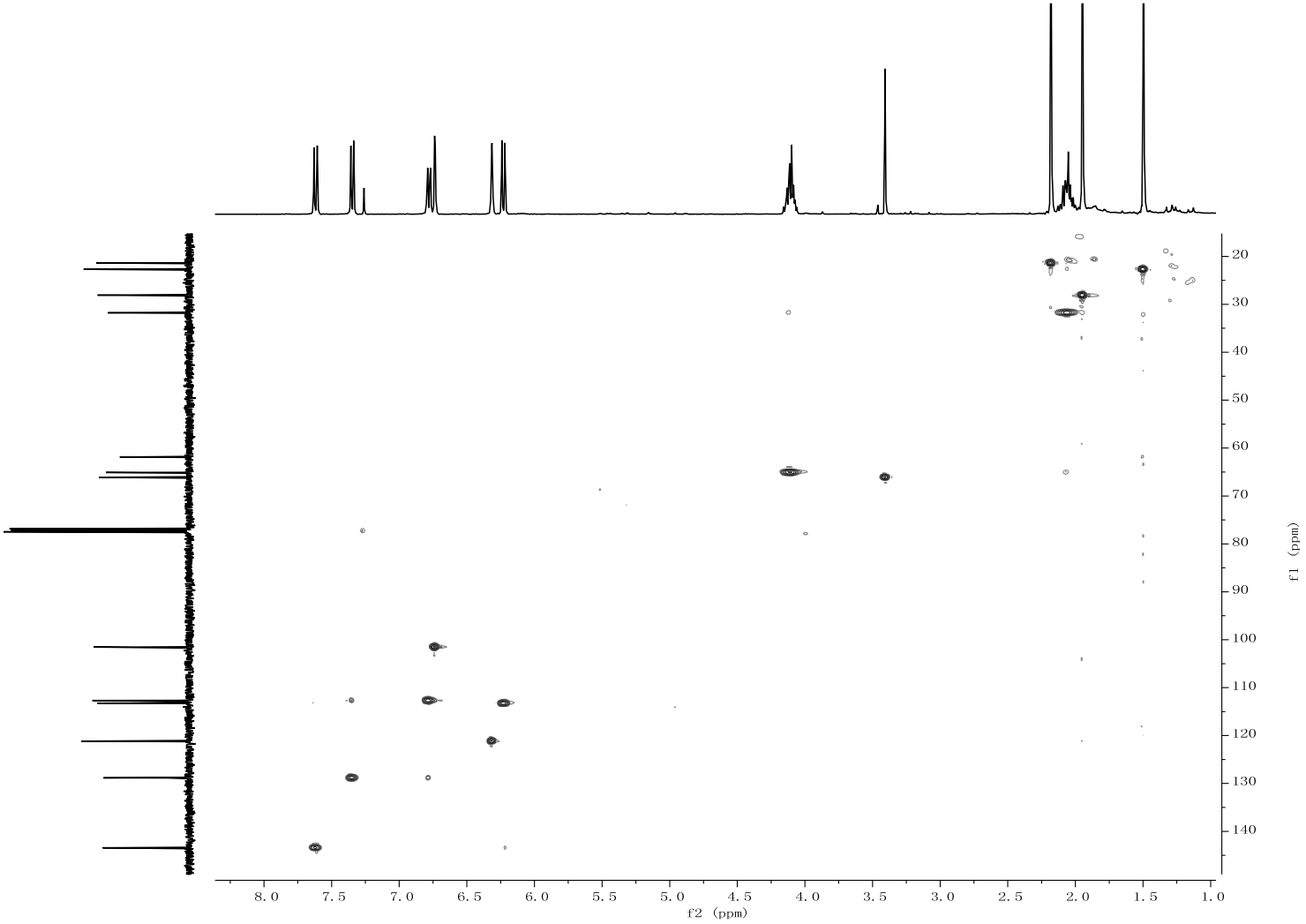


Figure S121. ^{1}H-^{1}H COSY (400 MHz, $CDCl_3$) spectrum of pararubcoumarin D (**18**)

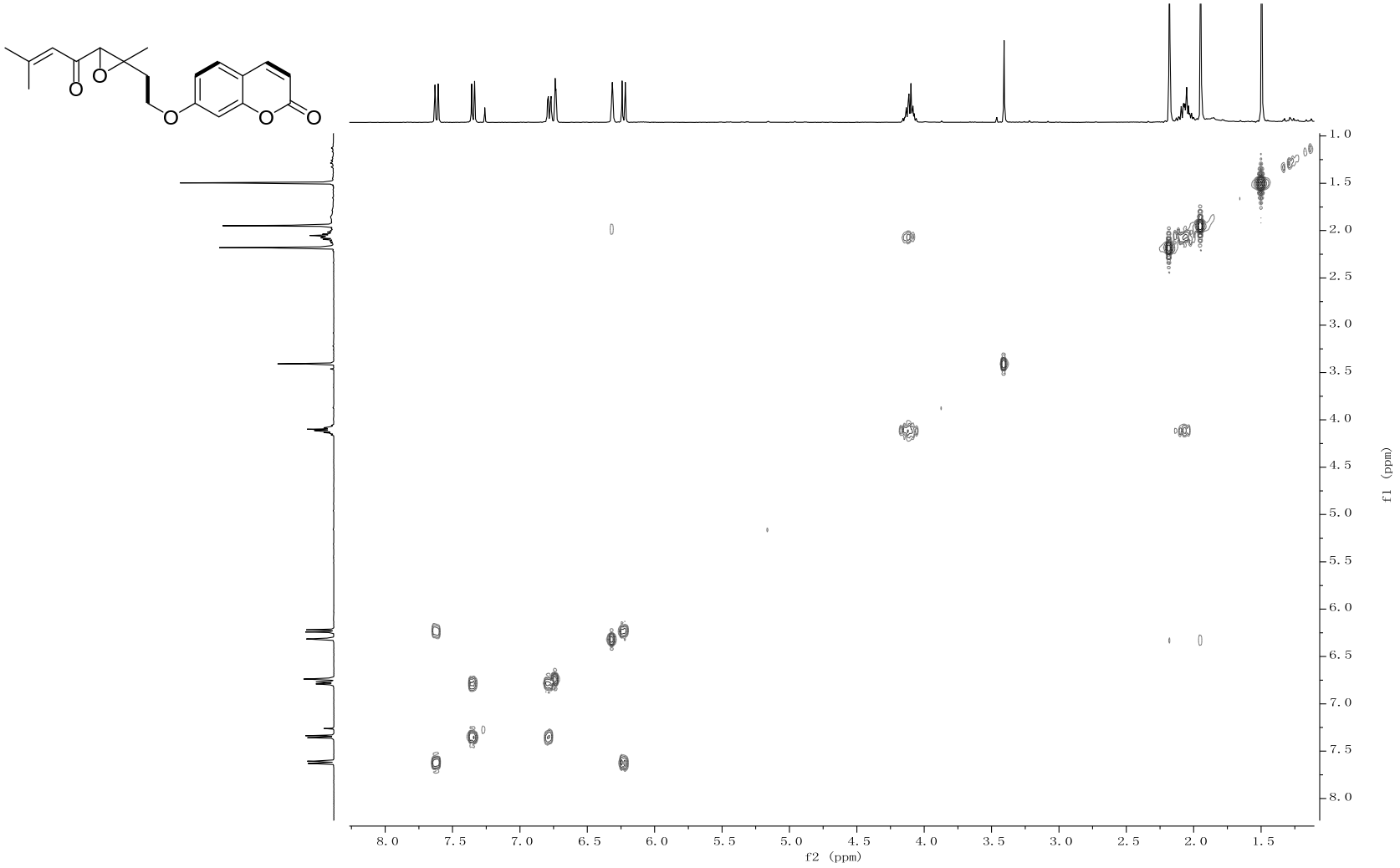


Figure S122. HMBC (400 MHz, $CDCl_3$) spectrum of pararubcoumarin D (**18**)

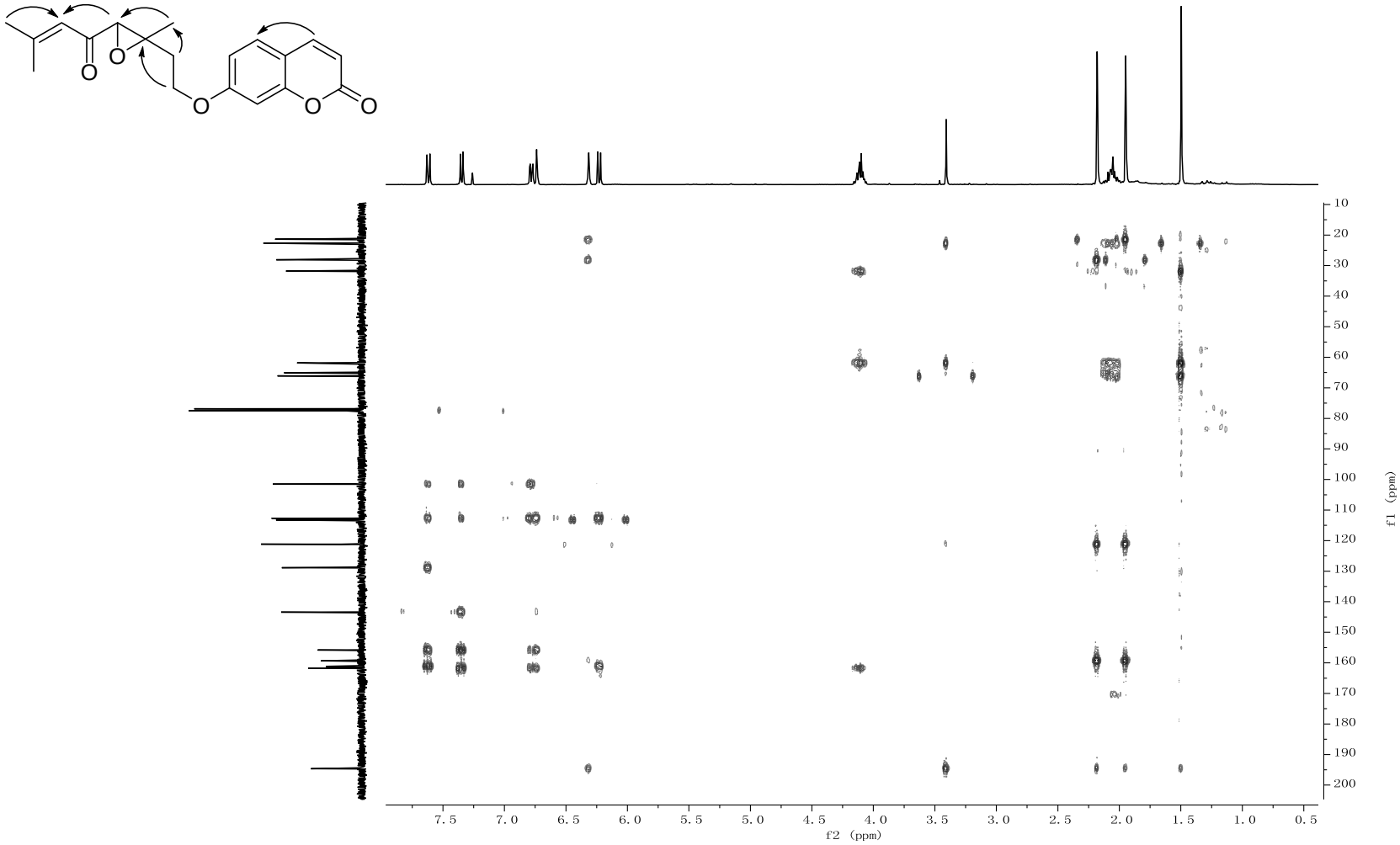


Figure S123. NOESY (400 MHz, $CDCl_3$) spectrum of pararubcoumarin D (**18**)

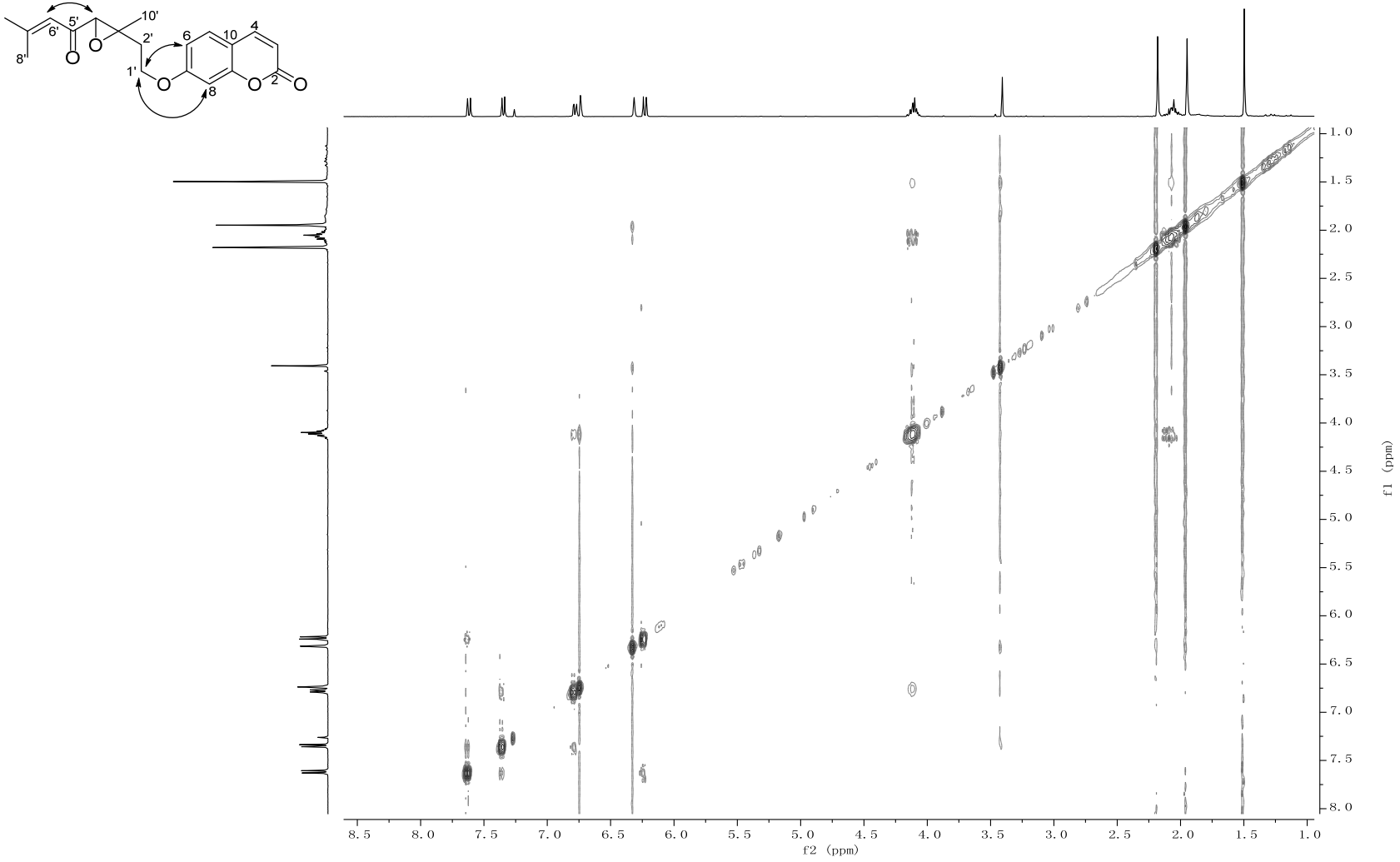


Figure S124 HRESIMS spectrum of pararubcoumarin D (**18**)

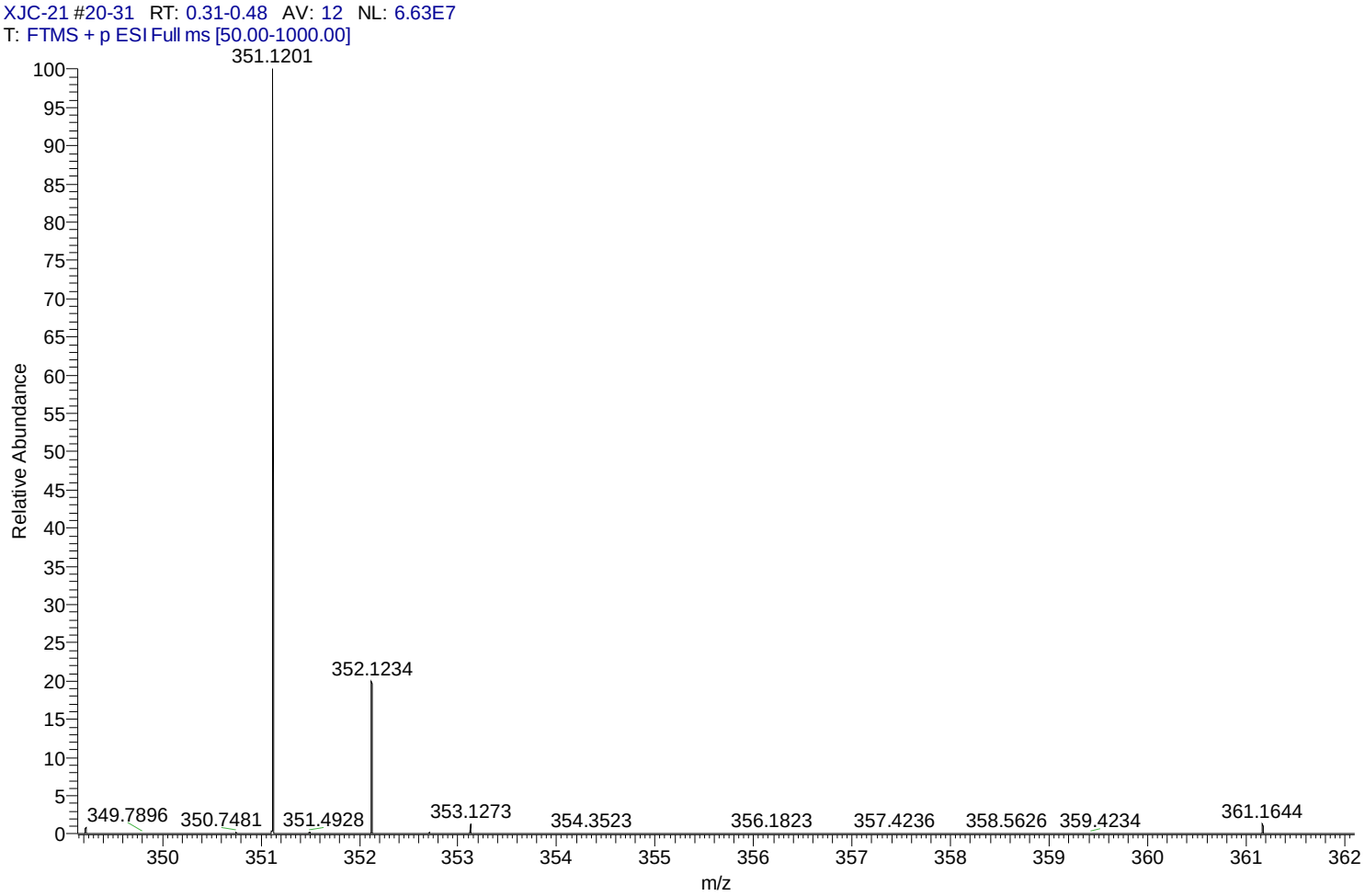


Figure S125. IR spectrum of pararubcoumarin D (**18**)

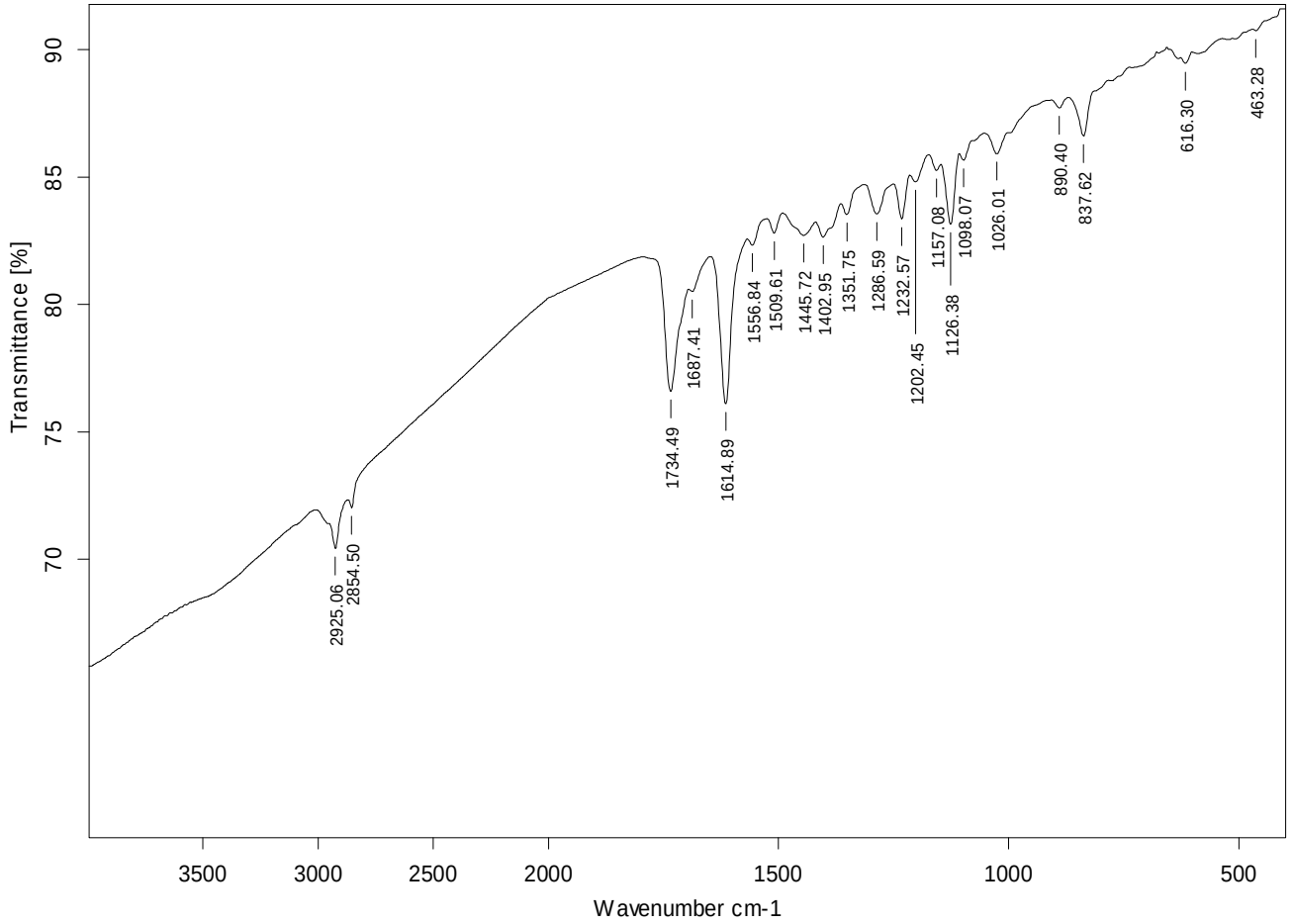
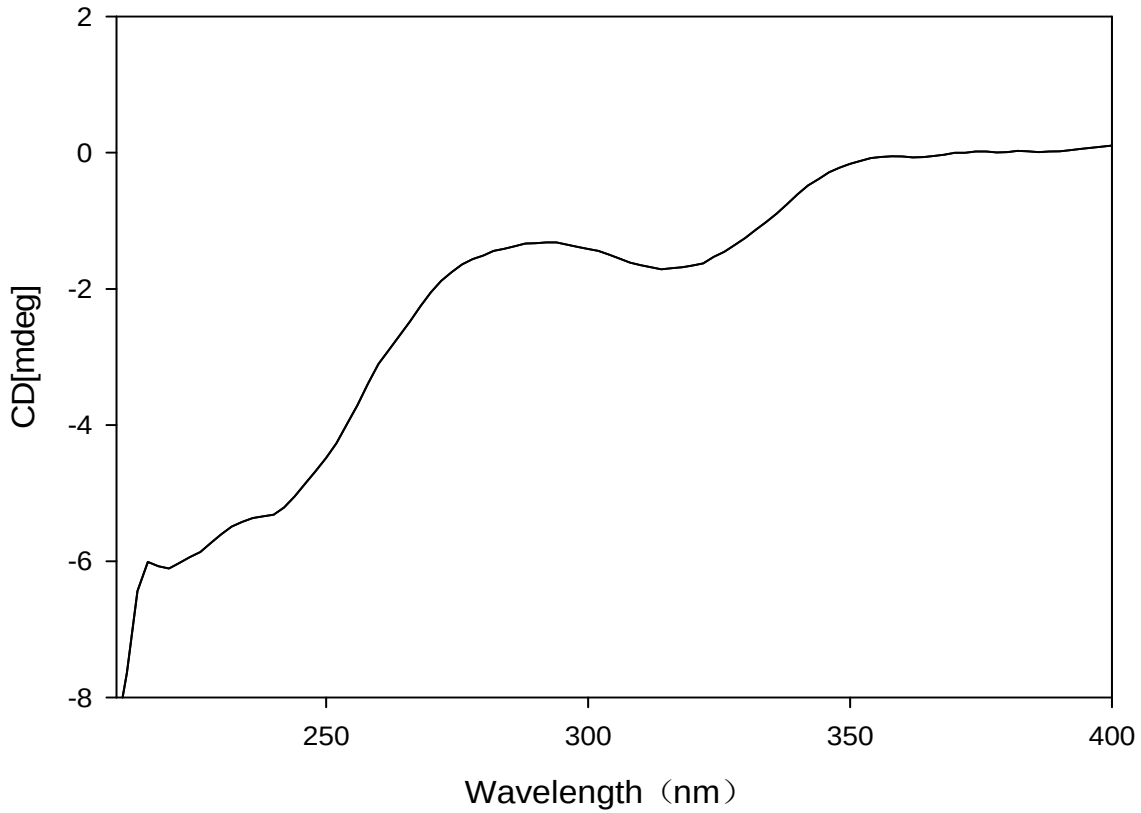


Figure S126. CD spectrum of pararubcoumarin D (**18**)



checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: g__141230a_work_cu_141230a_0m

```
Bond precision:  C-C = 0.0041 A          Wavelength=1.54178

Cell:            a=12.2069(2)     b=14.3991(2)     c=22.2180(4)
                 alpha=90         beta=90          gamma=90
Temperature:     100 K
```

	Calculated	Reported
Volume	3905.22(11)	3905.22(11)
Space group	P 21 21 21	P2(1)2(1)2(
Hall group	P 2ac 2ab	?
Moiety formula	C37 H52 O13	?
Sum formula	C37 H52 O13	C37 H52 O13
Mr	704.79	704.79
Dx,g cm-3	1.199	1.199
Z	4	4
Mu (mm-1)	0.749	0.749
F000	1512.0	1512.0
F000’	1517.08	
h,k,lmax	14,17,26	14,17,26
Nref	7039[3938]	6906
Tmin,Tmax	0.898,0.928	0.896,0.929
Tmin’	0.894	

```
Correction method= # Reported T Limits: Tmin=0.896 Tmax=0.929
AbsCorr = NONE

Data completeness= 1.75/0.98      Theta(max)= 67.500

R(reflections)= 0.0520( 6646)     wR2(reflections)= 0.1686( 6906)

S = 1.055                 Npar= 501
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

```
PLAT031_ALERT_4_B Refined Extinction Parameter within Range ......      1.500 Sigma
PLAT035_ALERT_1_B _chemical_absolute_configuration info  Not given     Please Do !
PLAT230_ALERT_2_B Hirshfeld Test Diff for    O7     --  C11     ..       14.7 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for    O7     --  C12     ..       20.3 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for    C11    --  C12     ..       10.0 s.u.
PLAT241_ALERT_2_B High   'MainMol' Ueq as Compared to Neighbors of         O7 Check
```

Alert level C

```
ABSTY03_ALERT_1_C  The _exptl_absorpt_correction_type has been given as none.
            However values have been given for Tmin and Tmax. Remove
            these if an absorption correction has not been applied.
  From the CIF: _exptl_absorpt_correction_T_min   0.896
  From the CIF: _exptl_absorpt_correction_T_max   0.929
PLAT220_ALERT_2_C Non-Solvent Resd 1   C   Ueq(max)/Ueq(min) Range        3.5 Ratio
PLAT222_ALERT_3_C Non-Solvent Resd 1   H Uiso(max)/Uiso(min) Range        4.4 Ratio
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C1B Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C2D Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C7E Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C11 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C12 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.00411 Ang.
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         9 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         4 Report
PLAT005_ALERT_5_G No Embedded Refinement Details found  in the CIF     Please Do !
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical         ? Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large      0.13 Report
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as      mixed Check
PLAT230_ALERT_2_G Hirshfeld Test Diff for    C2A    --  C3A     ..       5.7 s.u.
PLAT301_ALERT_3_G Main Residue  Disorder ..... Percentage =          8 Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........        37 Note
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        90 Check
              C2A  -C1A  -C2F     1.555   1.555   1.555            17.00 Deg.
PLAT791_ALERT_4_G The Model has Chirality at C1      (Chiral SPGR)         R Verify
PLAT791_ALERT_4_G The Model has Chirality at C2      (Chiral SPGR)         S Verify
PLAT791_ALERT_4_G The Model has Chirality at C2A     (Chiral SPGR)         S Verify
PLAT791_ALERT_4_G The Model has Chirality at C3      (Chiral SPGR)         R Verify
PLAT791_ALERT_4_G The Model has Chirality at C4      (Chiral SPGR)         R Verify
PLAT791_ALERT_4_G The Model has Chirality at C4E     (Chiral SPGR)         S Verify
PLAT791_ALERT_4_G The Model has Chirality at C5      (Chiral SPGR)         S Verify
PLAT791_ALERT_4_G The Model has Chirality at C6      (Chiral SPGR)         R Verify
PLAT791_ALERT_4_G The Model has Chirality at C7      (Chiral SPGR)         S Verify
PLAT791_ALERT_4_G The Model has Chirality at C8      (Chiral SPGR)         R Verify
PLAT791_ALERT_4_G The Model has Chirality at C9      (Chiral SPGR)         S Verify
PLAT791_ALERT_4_G The Model has Chirality at C11     (Chiral SPGR)         R Verify
PLAT791_ALERT_4_G The Model has Chirality at C2F     (Chiral SPGR)         S Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        30 Note
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL       2014 Note
```

---

0 **ALERT level A** = Most likely a serious problem - resolve or explain
6 **ALERT level B** = A potentially serious problem, consider carefully
9 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
25 **ALERT level G** = General information/check it is not something unexpected

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

```
  14 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 ALERT type 3 Indicator that the structure quality may be low
  17 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_ABSTY03_g__141230a_work_cu_141230a_0m
;
PROBLEM: The _exptl_absorpt_correction_type has been given as none.
RESPONSE: ...
;
_vrf_PLAT220_g__141230a_work_cu_141230a_0m
;
PROBLEM: Non-Solvent Resd 1   C   Ueq(max)/Ueq(min) Range        3.5 Ratio
RESPONSE: ...
;
_vrf_PLAT222_g__141230a_work_cu_141230a_0m
;
PROBLEM: Non-Solvent Resd 1   H Uiso(max)/Uiso(min) Range        4.4 Ratio
RESPONSE: ...
;
_vrf_PLAT242_g__141230a_work_cu_141230a_0m
;
PROBLEM: Low    'MainMol' Ueq as Compared to Neighbors of        C1B Check
RESPONSE: ...
;
_vrf_PLAT340_g__141230a_work_cu_141230a_0m
;
PROBLEM: Low Bond Precision on  C-C Bonds ..............    0.00411 Ang.
RESPONSE: ...
;
# end Validation Reply Form
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 30/03/2016; check.def file version of 30/03/2016

Datablock g__141230a_work_cu_141230a_0m - ellipsoid plot