SUPPORTING INFORMATION

Secondary Metabolites from the Chinese Liverwort *Cephaloziella kiaeri*

Rui-Juan Li,[†] Rong-Xiu Zhu,[‡] Yao-Yao Li,[†] Jin-Chuan Zhou,[†] Jiao-Zhen Zhang,[†] Song Wang,[†] Jian-Ping Ye,[§] Yue-Hu Wang,[Δ] Susan L. Morris-Natschke,[Δ] Kuo-Hsiung Lee,[Δ] and Hong-Xiang Lou[*,†]

[†]*Department of Natural Products Chemistry, Key Lab of Chemical Biology of Ministry of Education, School of Pharmaceutical Science, Shandong University, Jinan 250012, People's Republic of China*

[‡]*School of Chemistry and Chemical Engineering, Shandong University, Jinan 250100, People's Republic of China*

[§]*Guangxi Mount. Maoer National Nature Reserve, Guilin 541001, People's Republic of China*

[Δ]*Natural Products Research Laboratories, UNC Eshelman School of Pharmacy, University of North Carolina, Chapel Hill, North Carolina 27599-7568, United States*

[*]To whom correspondence should be addressed.

Tel.: +86-531-8838-2012. Fax: +86-531-88382019.

E-mail: louhongxiang@sdu.edu.cn

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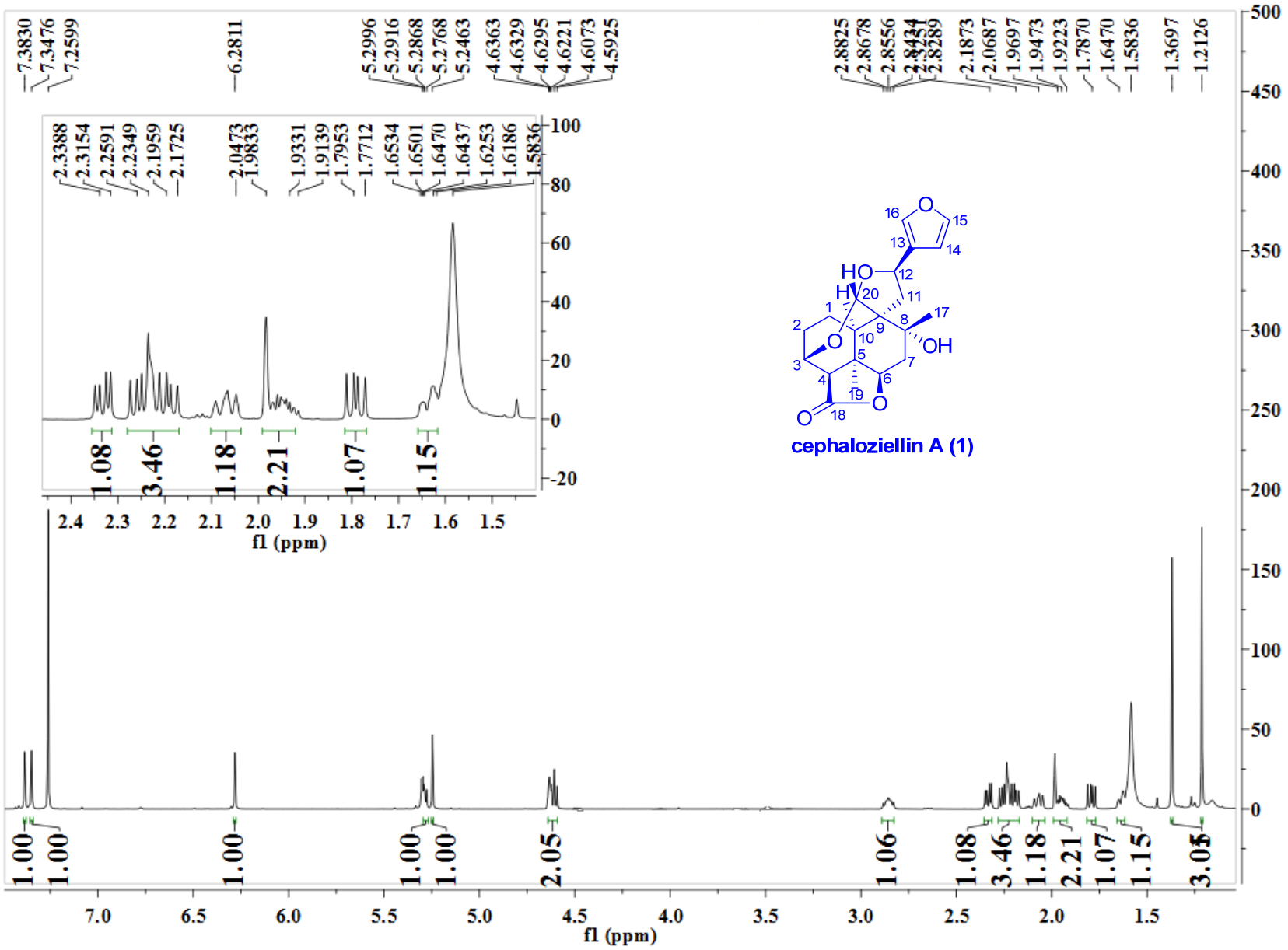
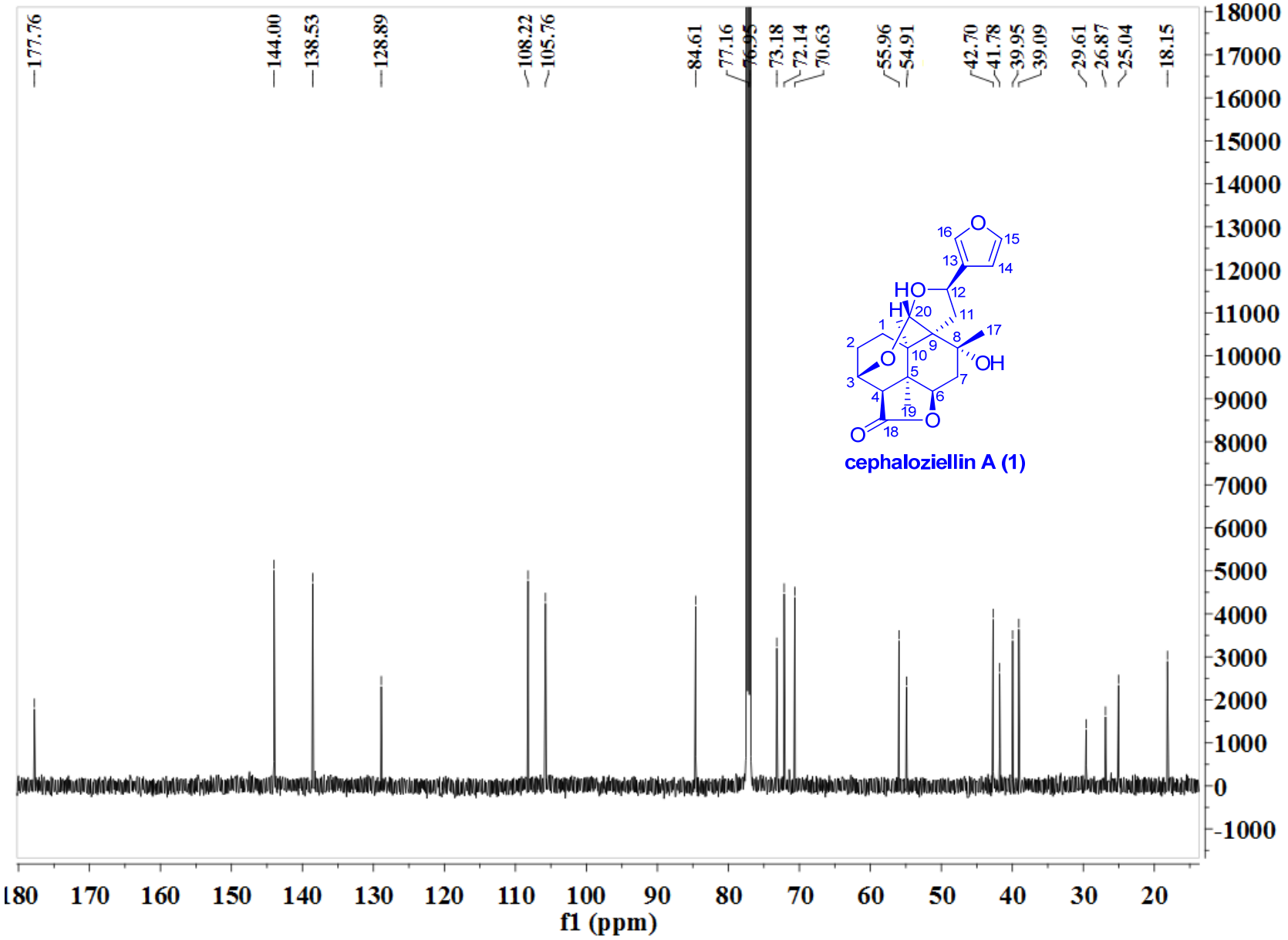
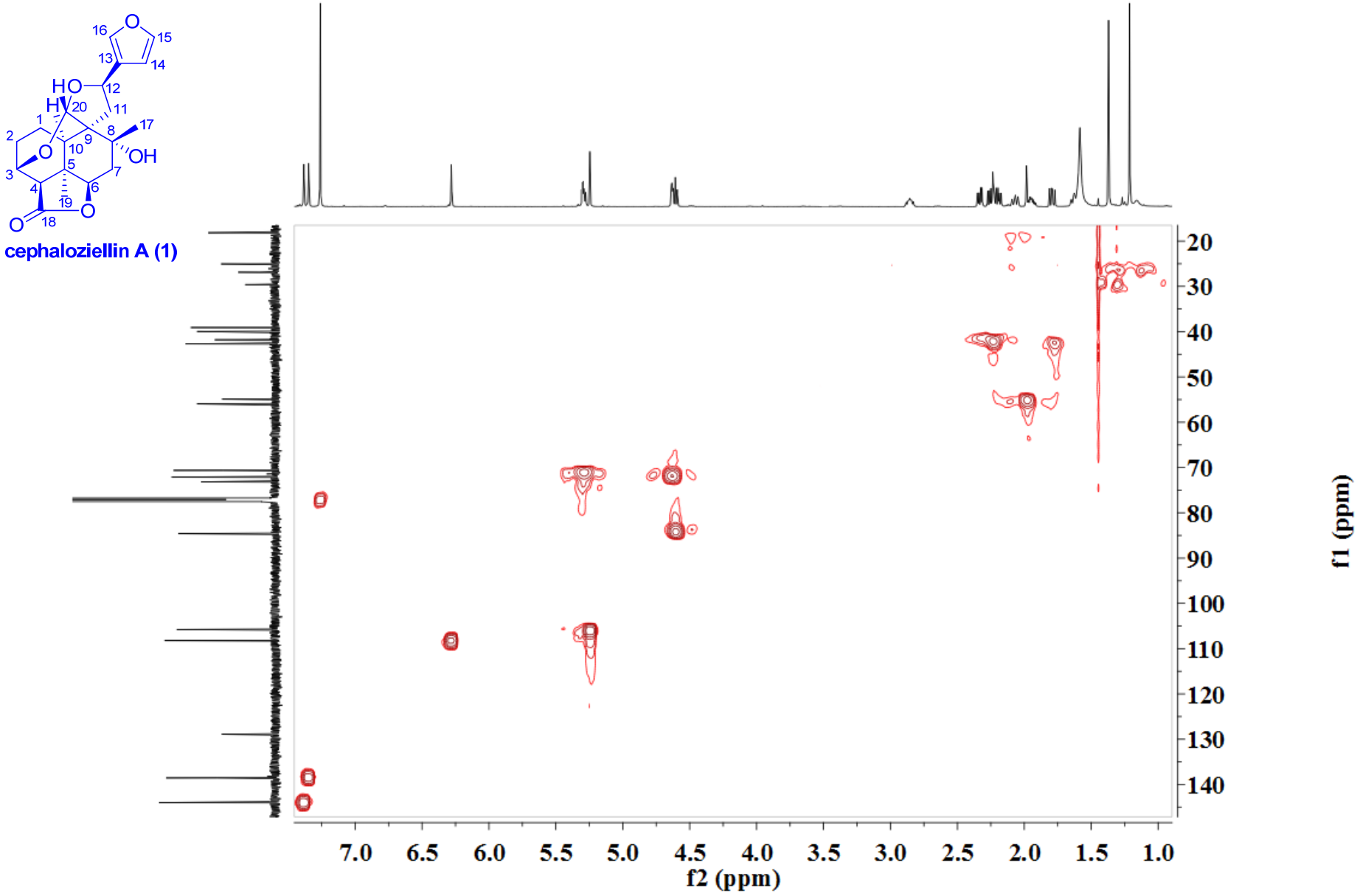


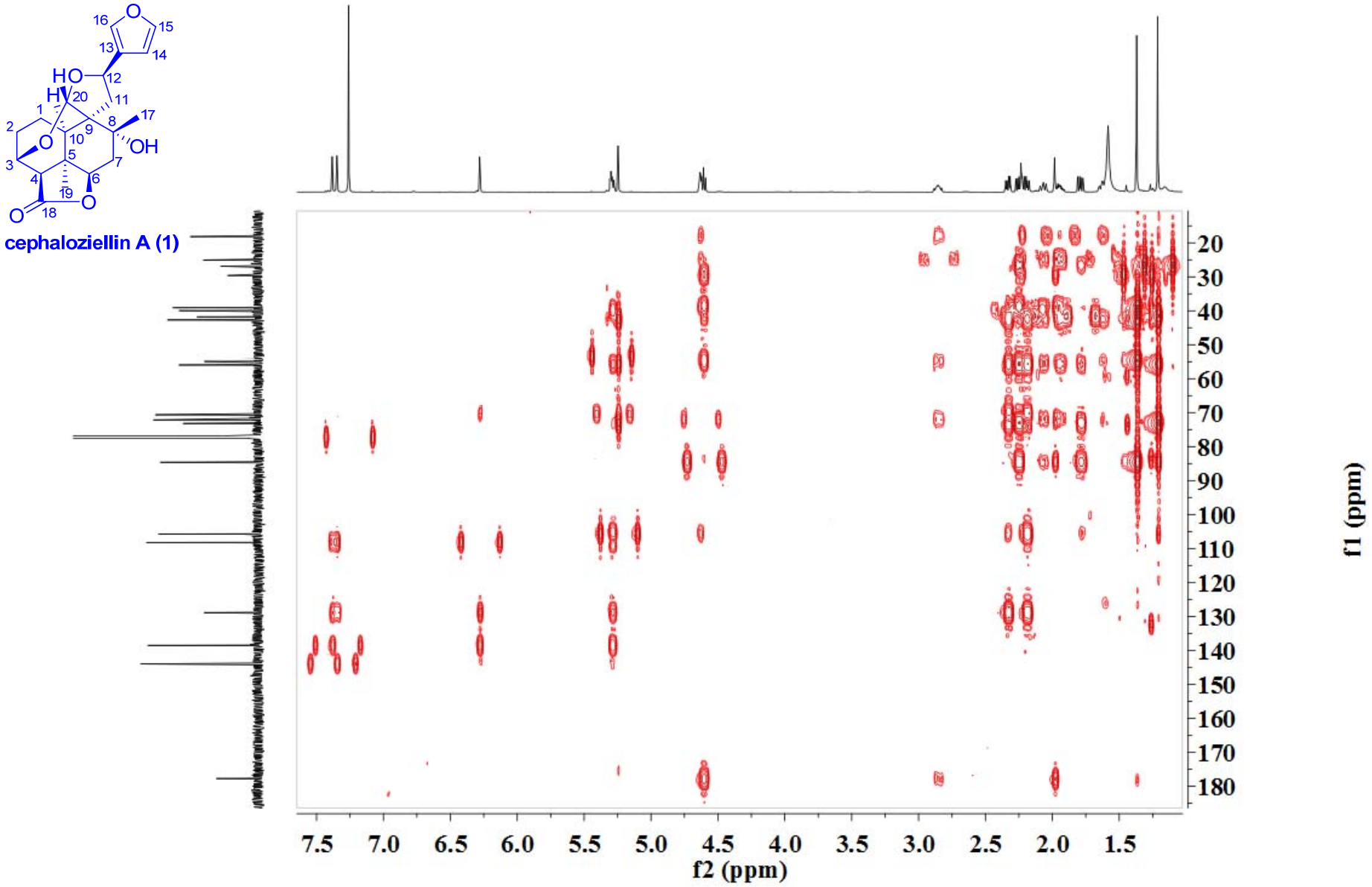
S2. ^{13}C NMR spectrum (150 MHz) of cephaloziellin A (**1**) in $CDCl_3$.



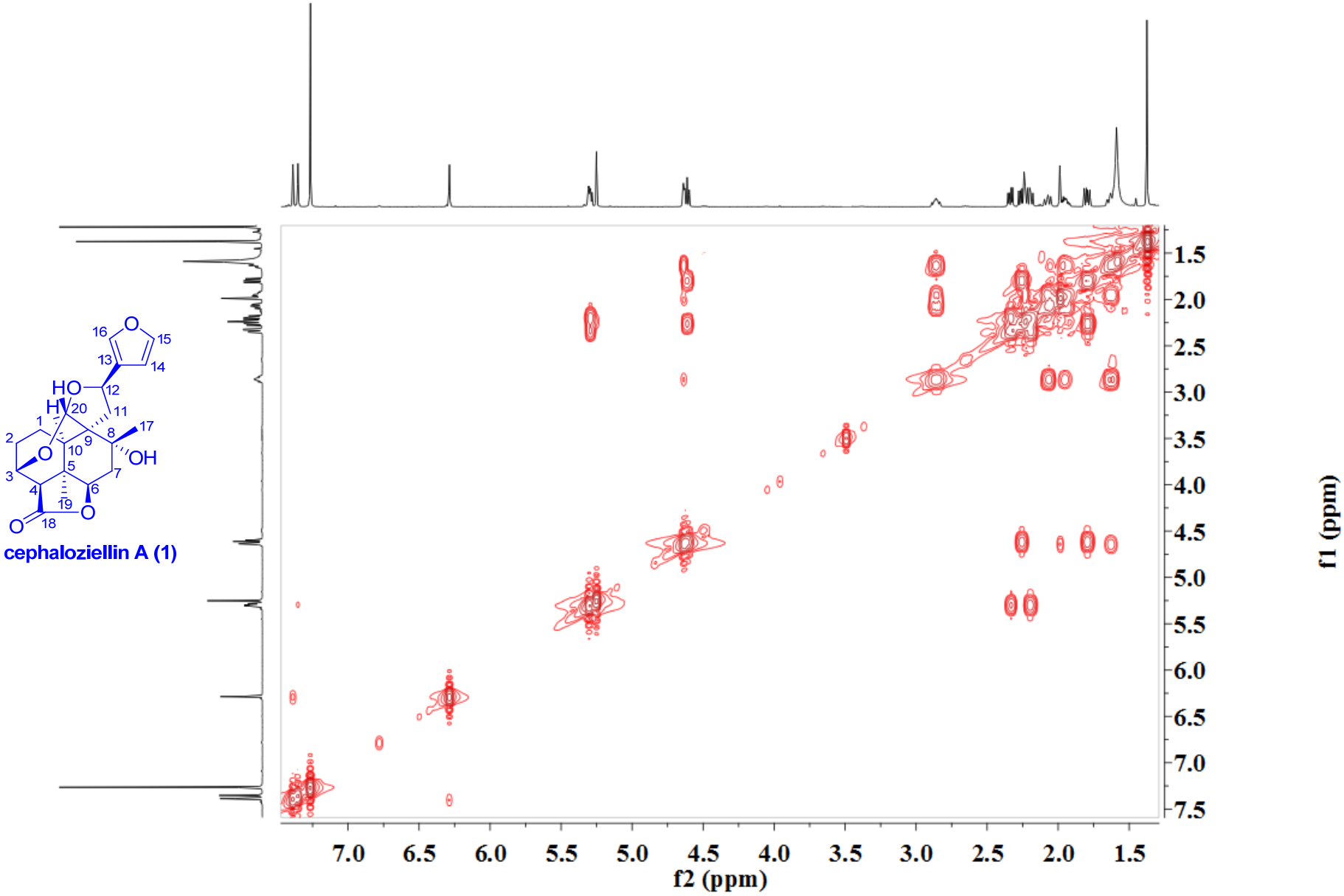
S3. HSQC spectrum (600 MHz) of cephaloziellin A (**1**) in $CDCl_3$.



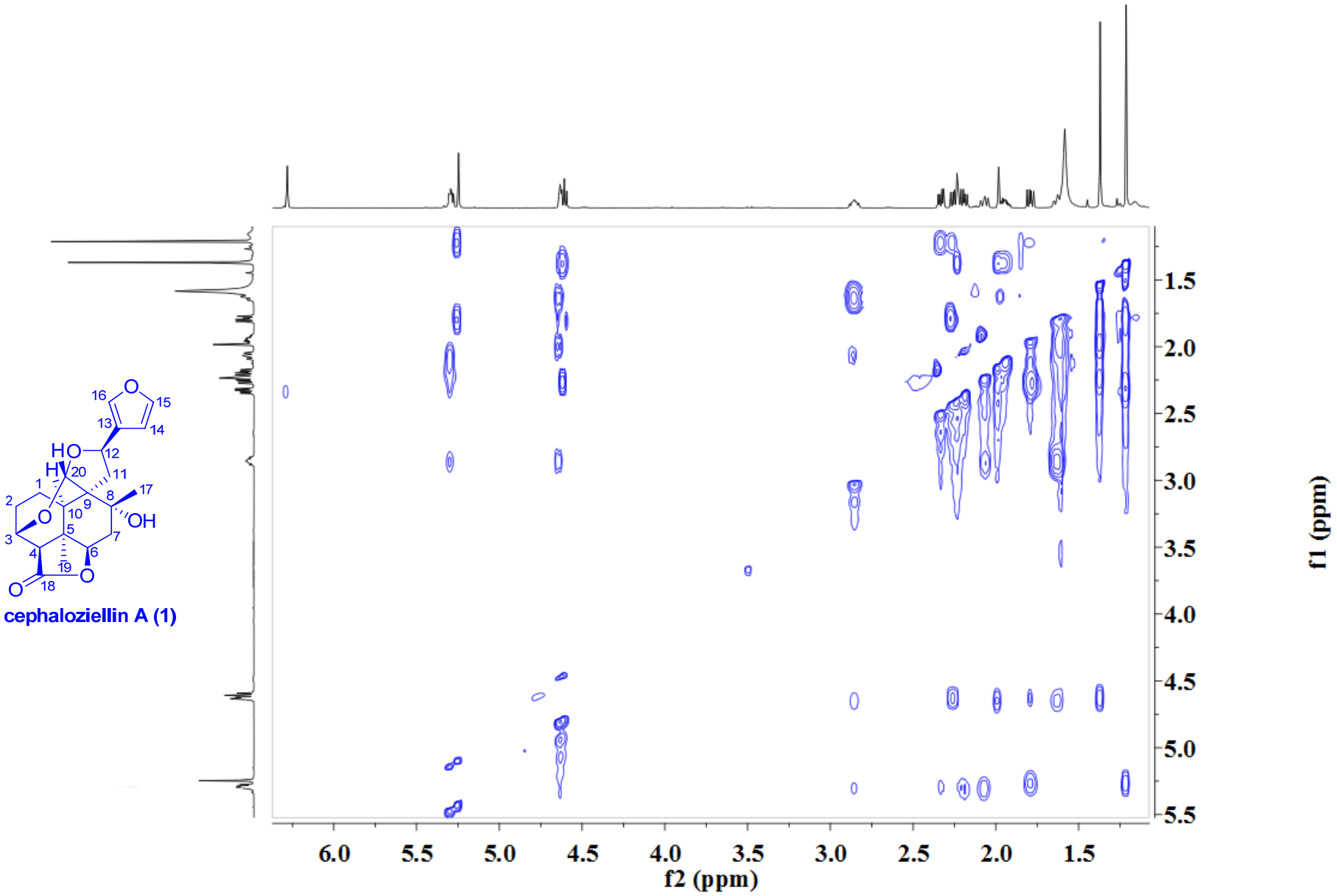
S4. HMBC spectrum (600 MHz) of cephaloziellin A (**1**) in $CDCl_3$.



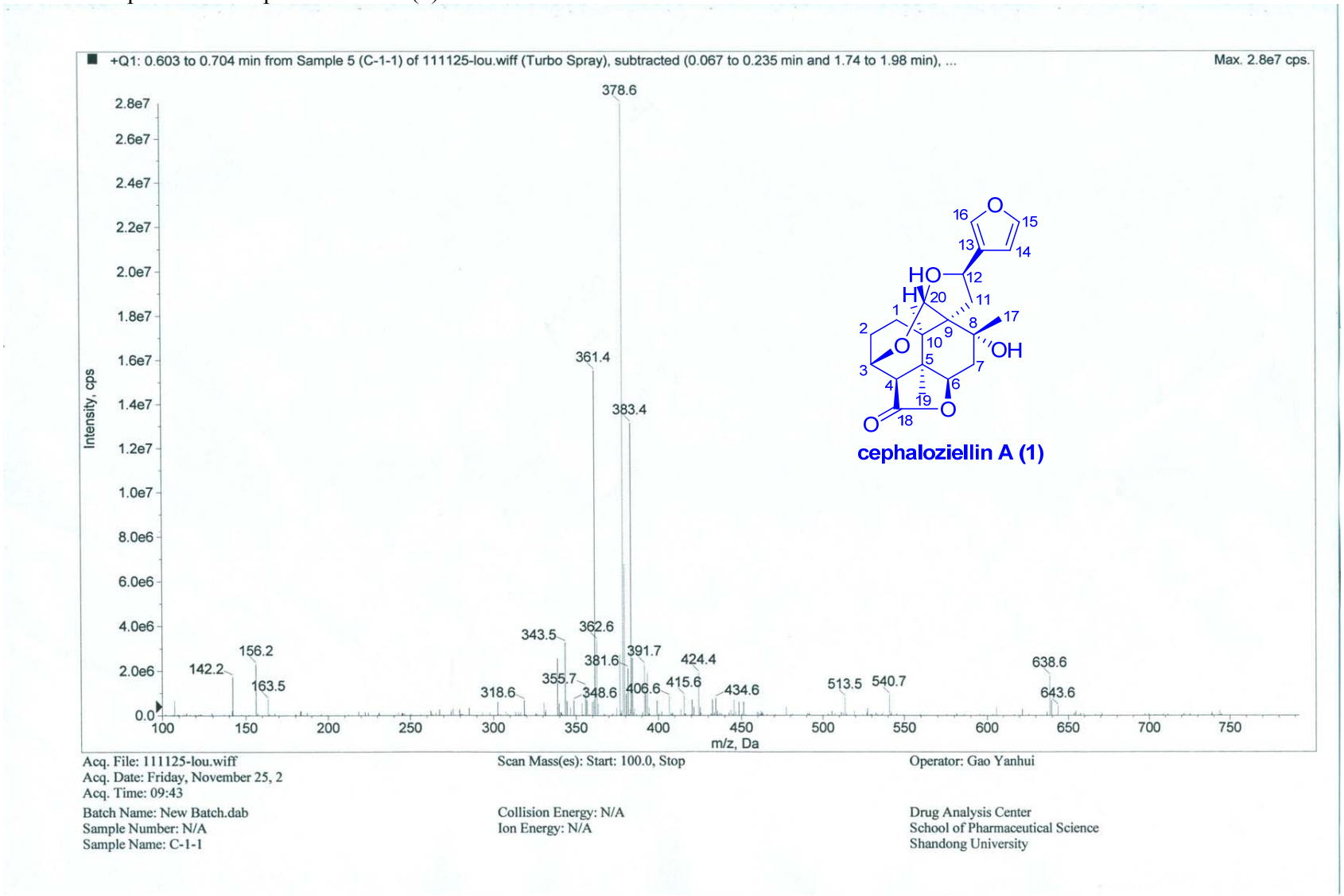
S5. ^{1}H-^{1}H COSY spectrum (600 MHz) of cephaloziellin A (**1**) in $CDCl_3$.



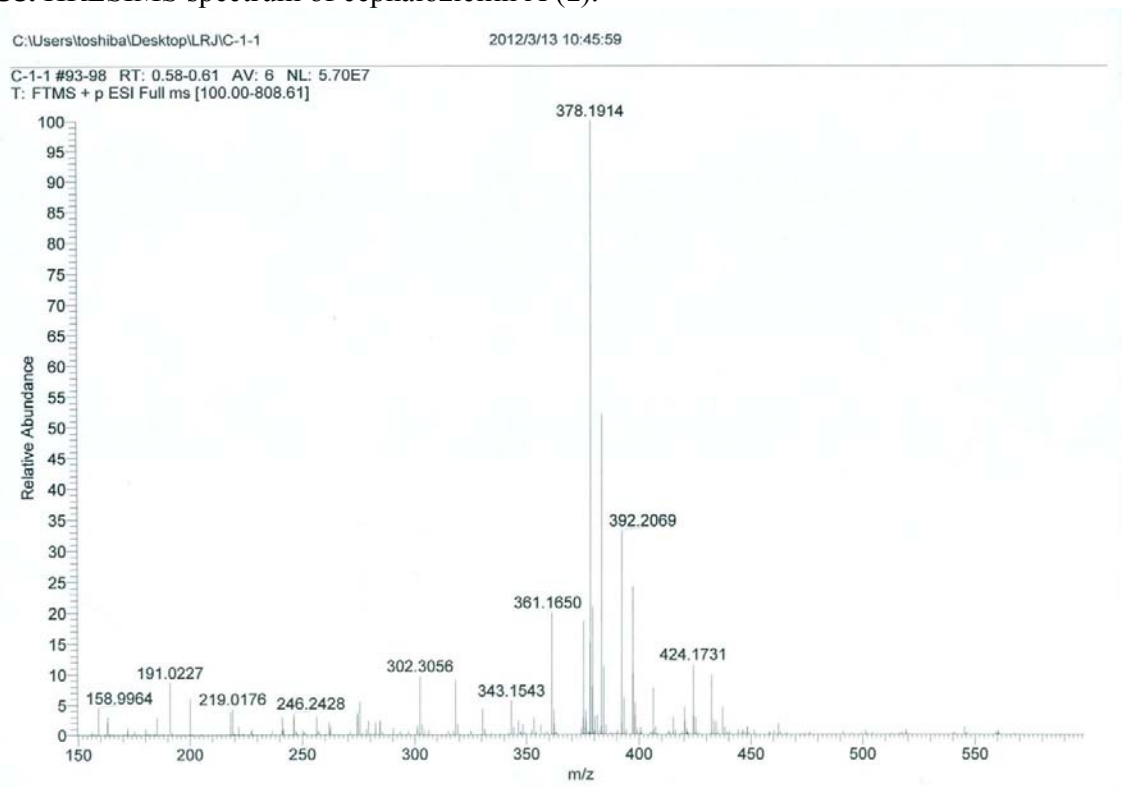
S6. NOESY spectrum (600 MHz) of cephaloziellin A (**1**) in $CDCl_3$.

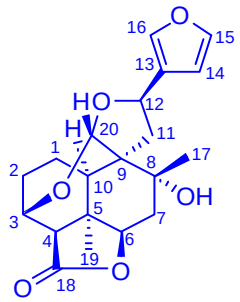


S7. ESIMS spectrum of cephaloziellin A (**1**).



S8. HRESIMS spectrum of cephaloziellin A (**1**).



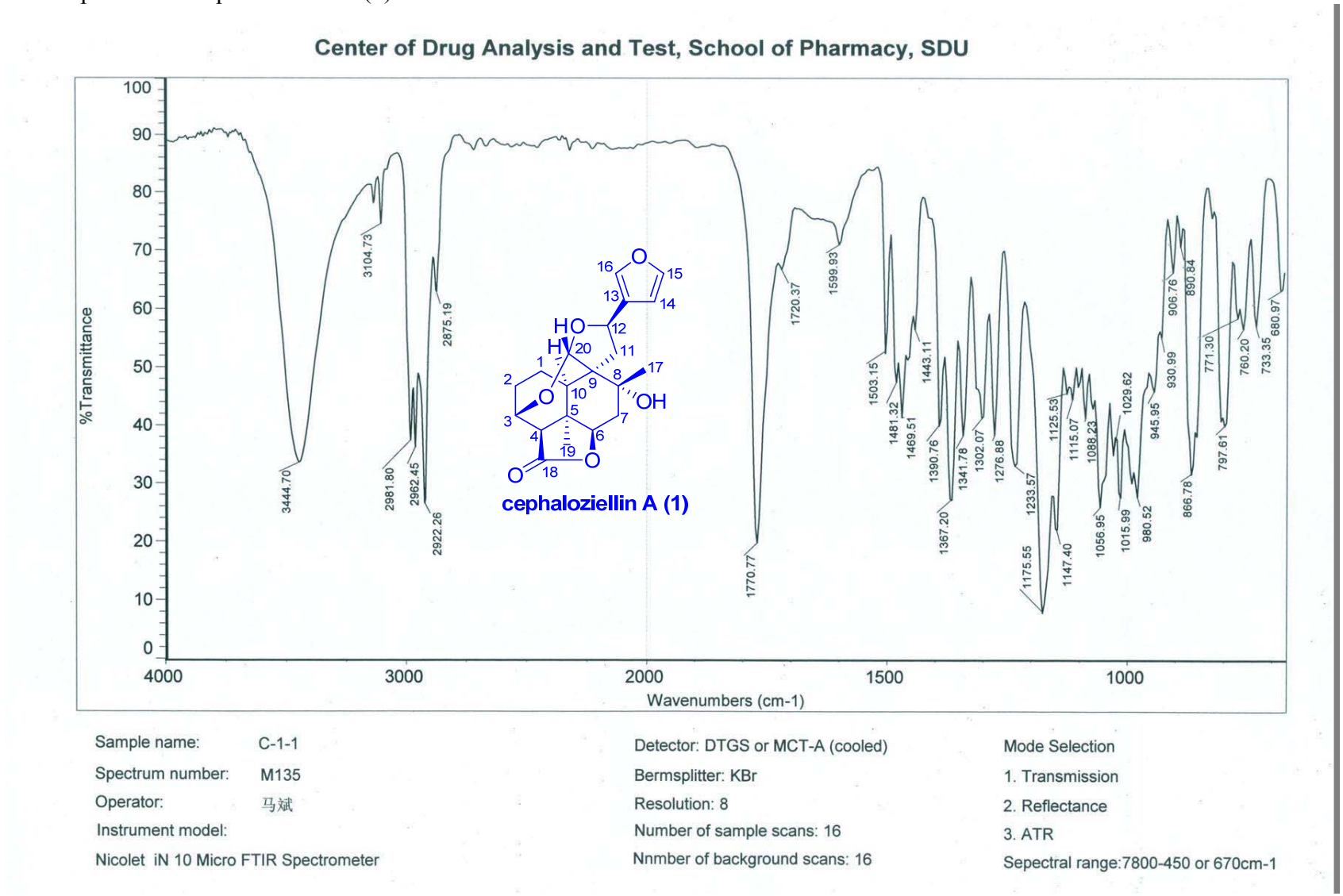


cephaloziellin A (1)

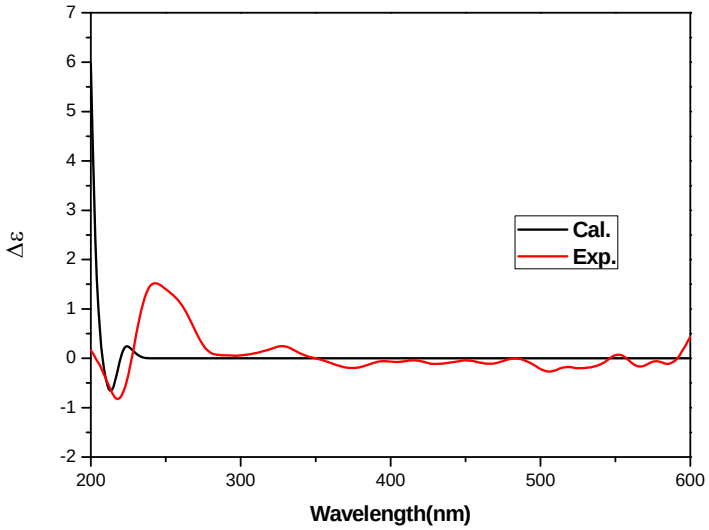
SPECTRUM - simulation :

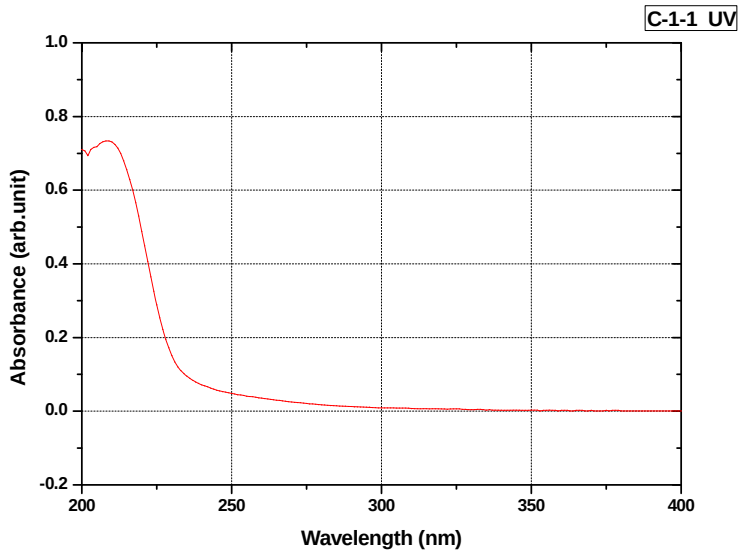
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
378.1914	378.1911	0.86	7.5	$^{12}C_{20}H_{28}O_6N_1$

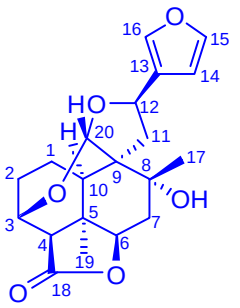
S9. IR spectrum of cephaloziellin A (**1**).



S10. Experimental ECD and calculated ECD, and UV spectra of cephaloziellin A **(1)**.

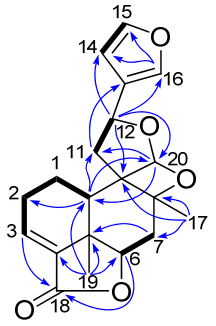






cephaloziellin A (1)

S11. Key HMBC and ^{1}H-^{1}H COSY correlations (in figure) of cephaloziellin B (**2**).

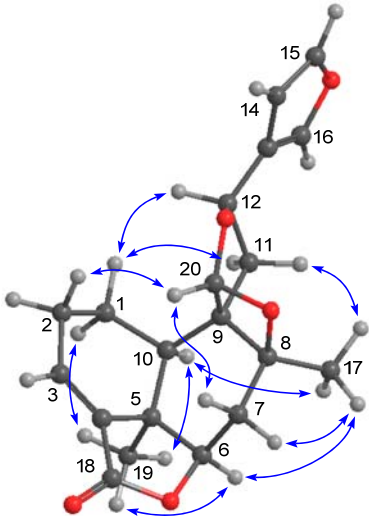


2

HMBC

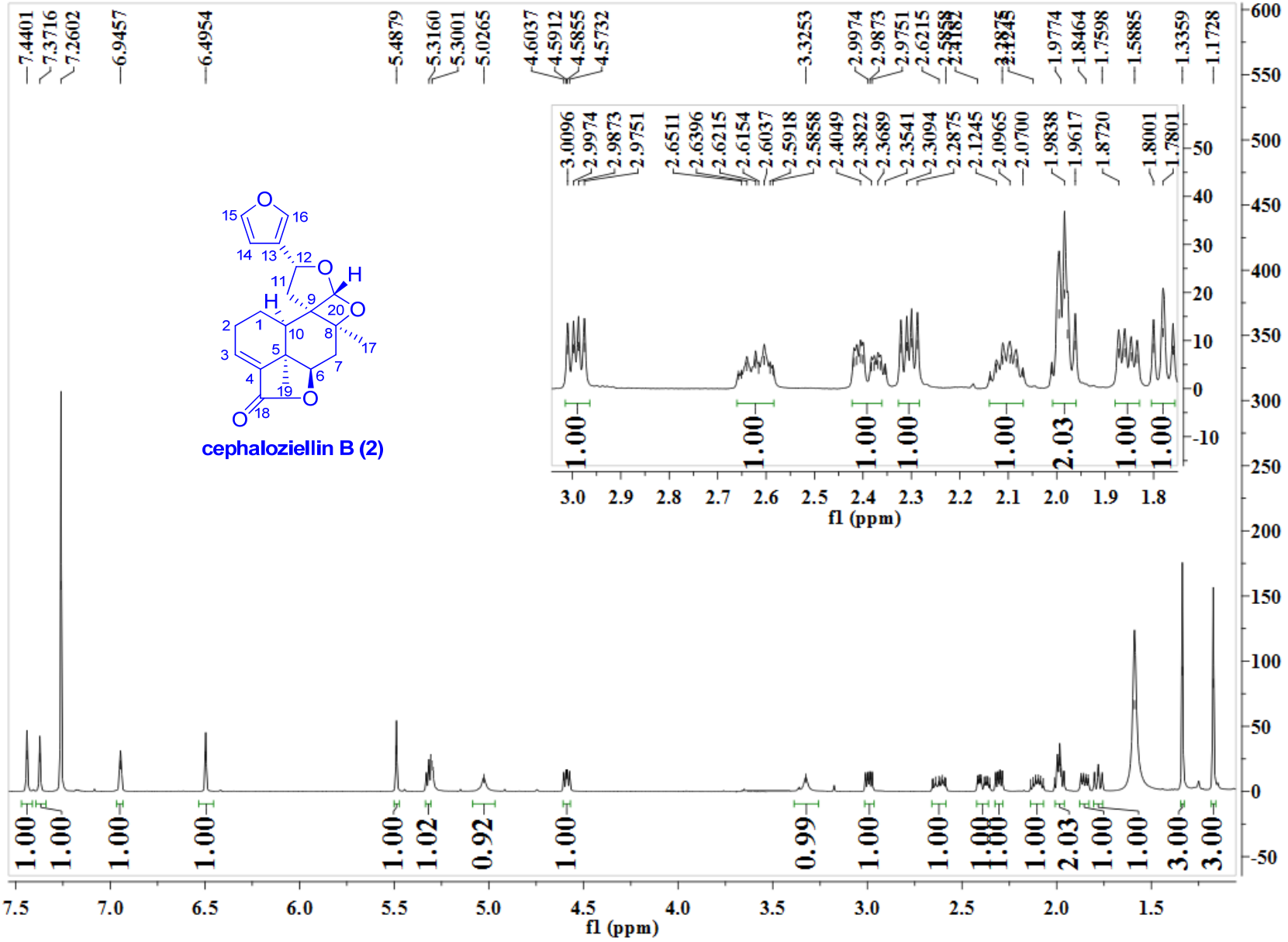
^{1}H-^{1}H COSY

S12. Key NOESY correlations (in figure) of cephaloziellin B (**2**).

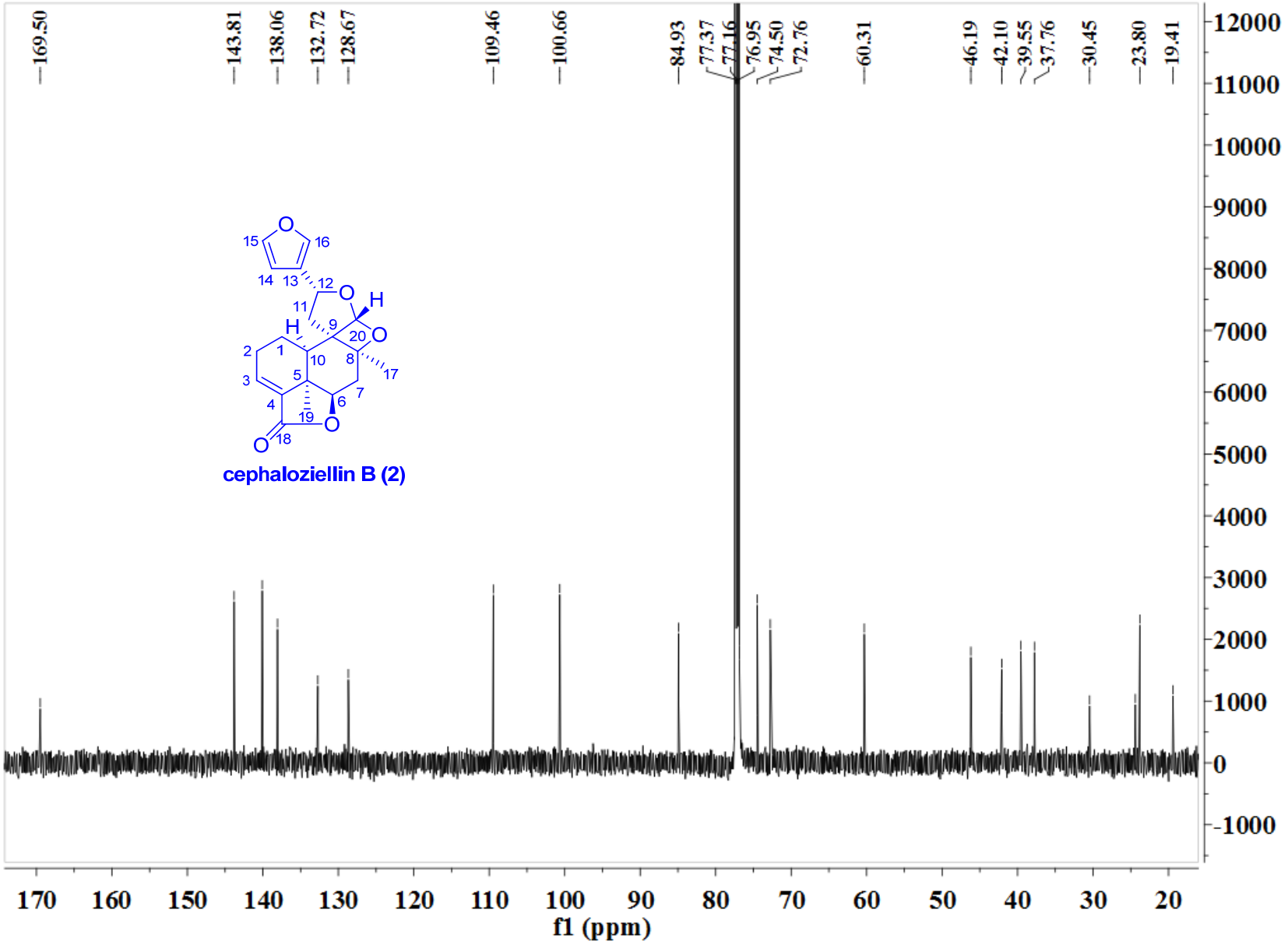


2 NOESY

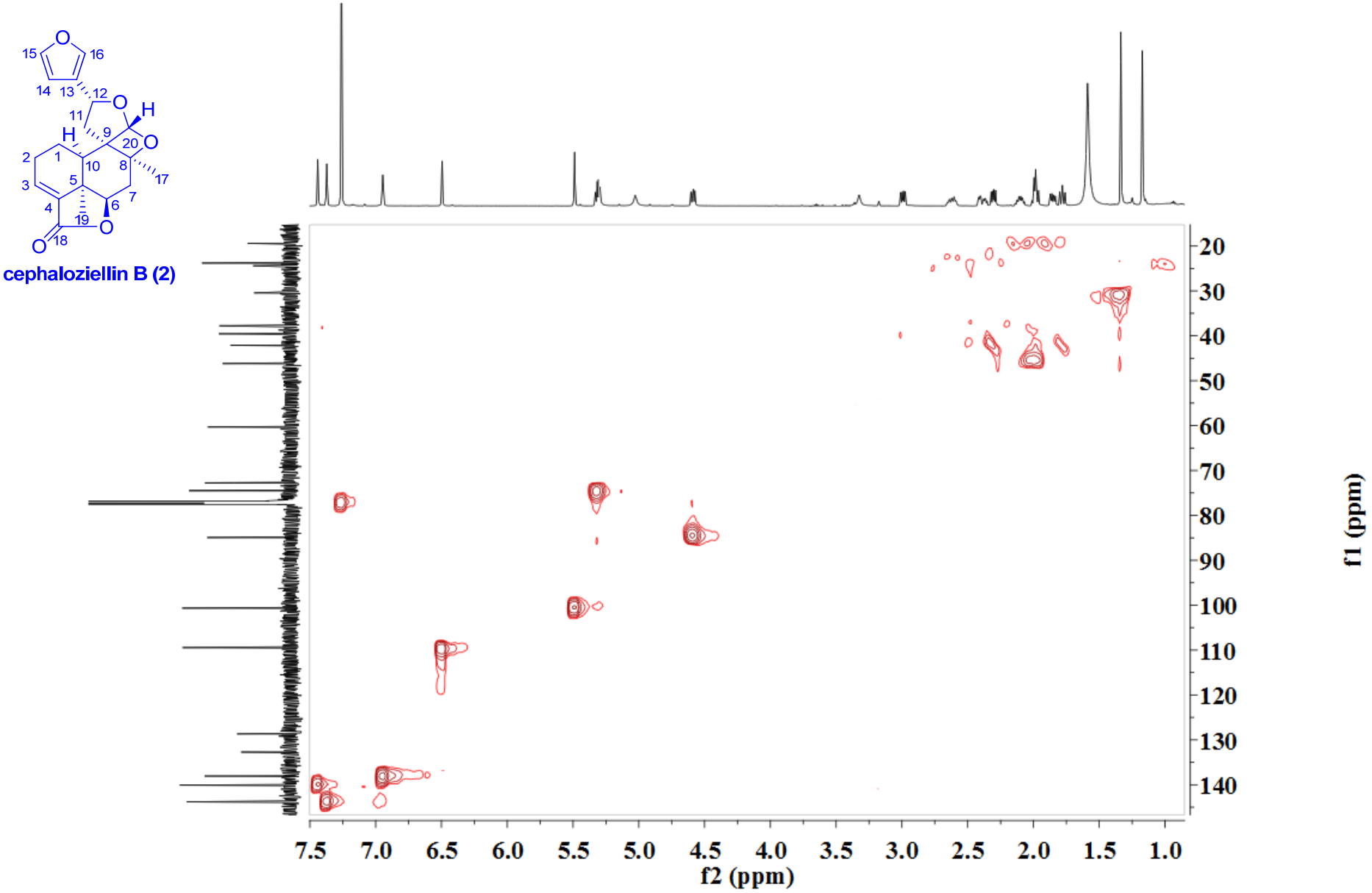
S13. ^{1}H NMR spectrum (600 MHz) of cephaloziellin B (**2**) in $CDCl_3$.



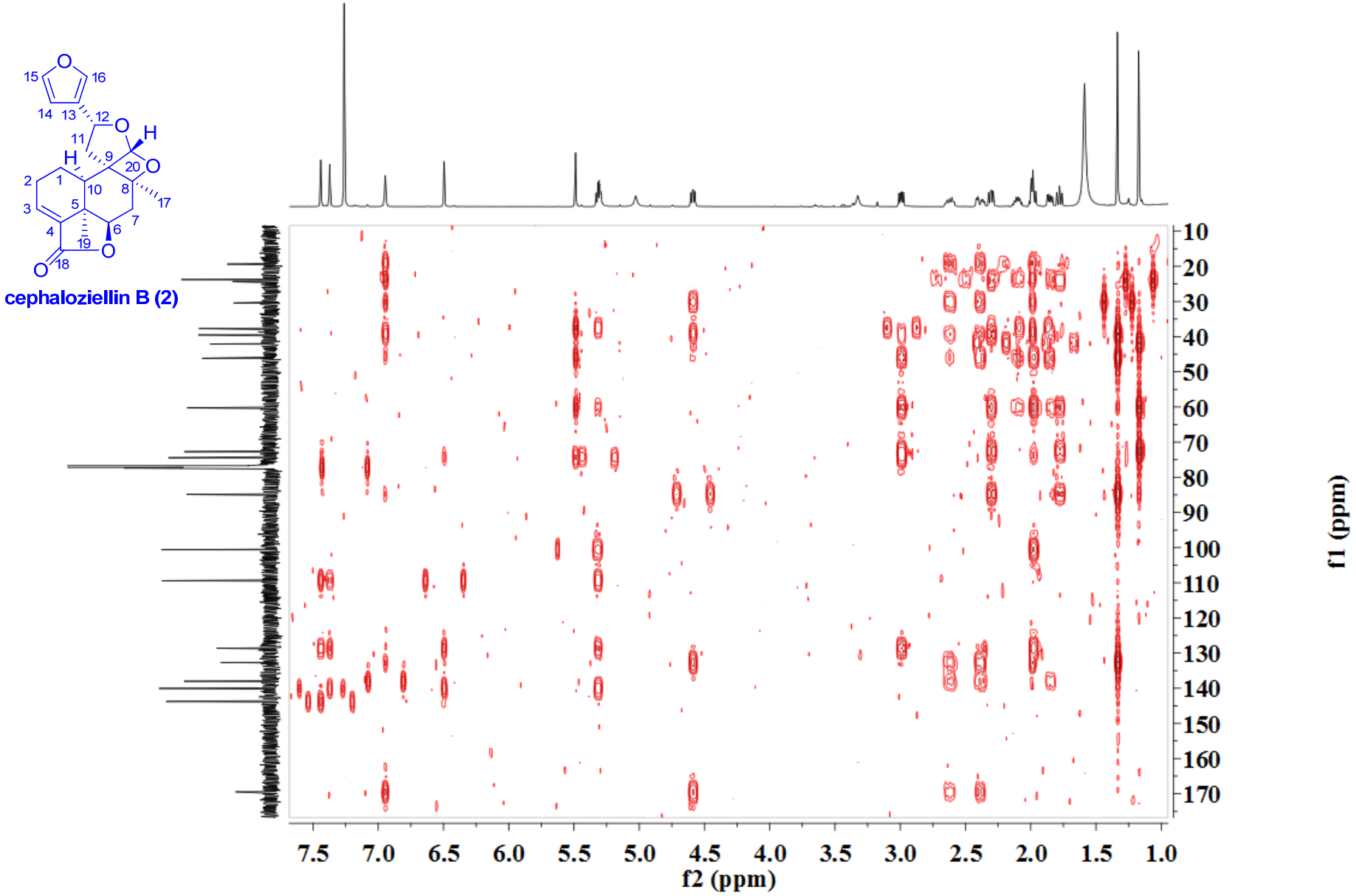
S14. ^{13}C NMR spectrum (150 MHz) of cephaloziellin B (**2**) in $CDCl_3$.



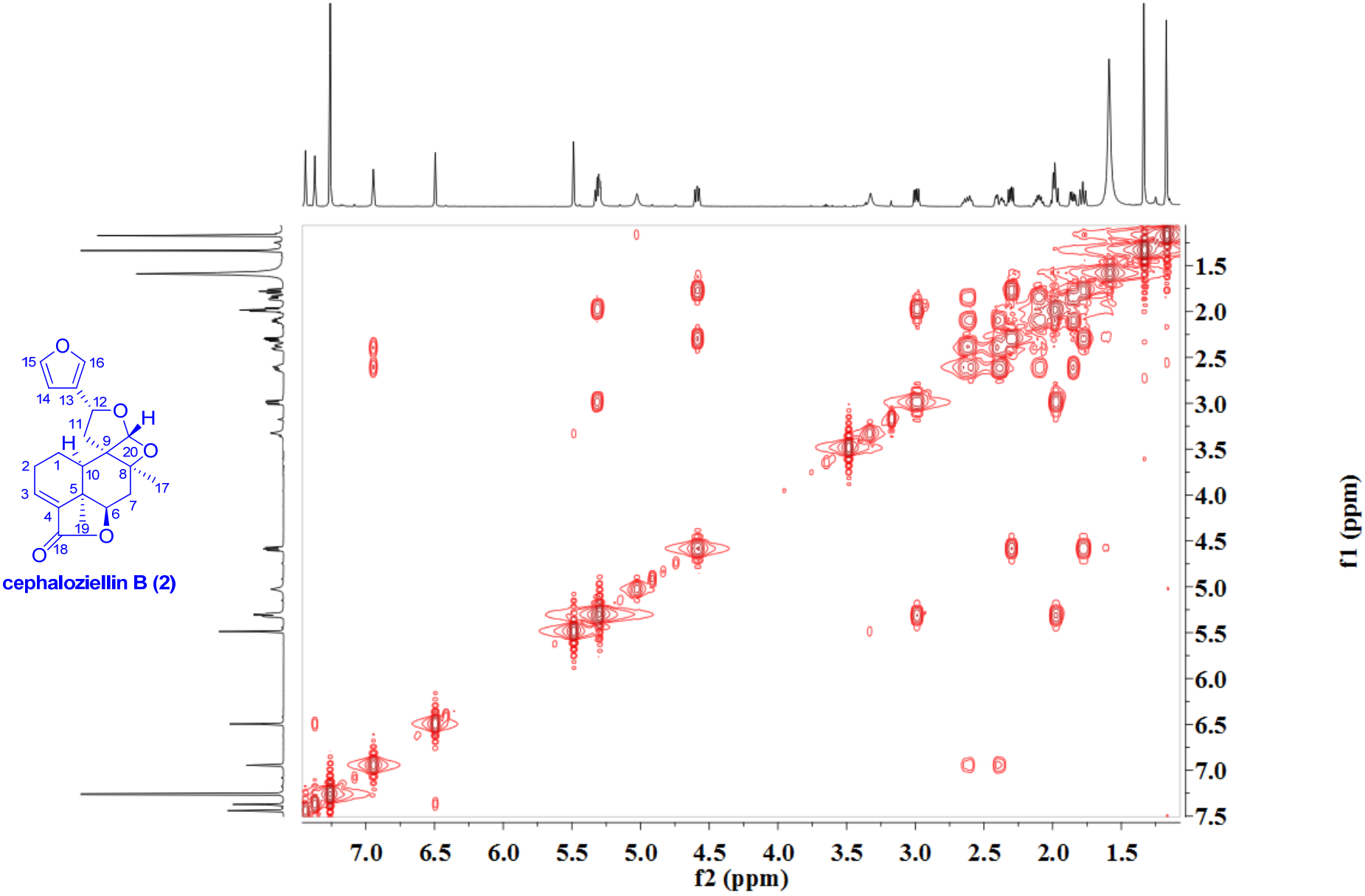
S15. HSQC spectrum (600 MHz) of cephaloziellin B (**2**) in $CDCl_3$.



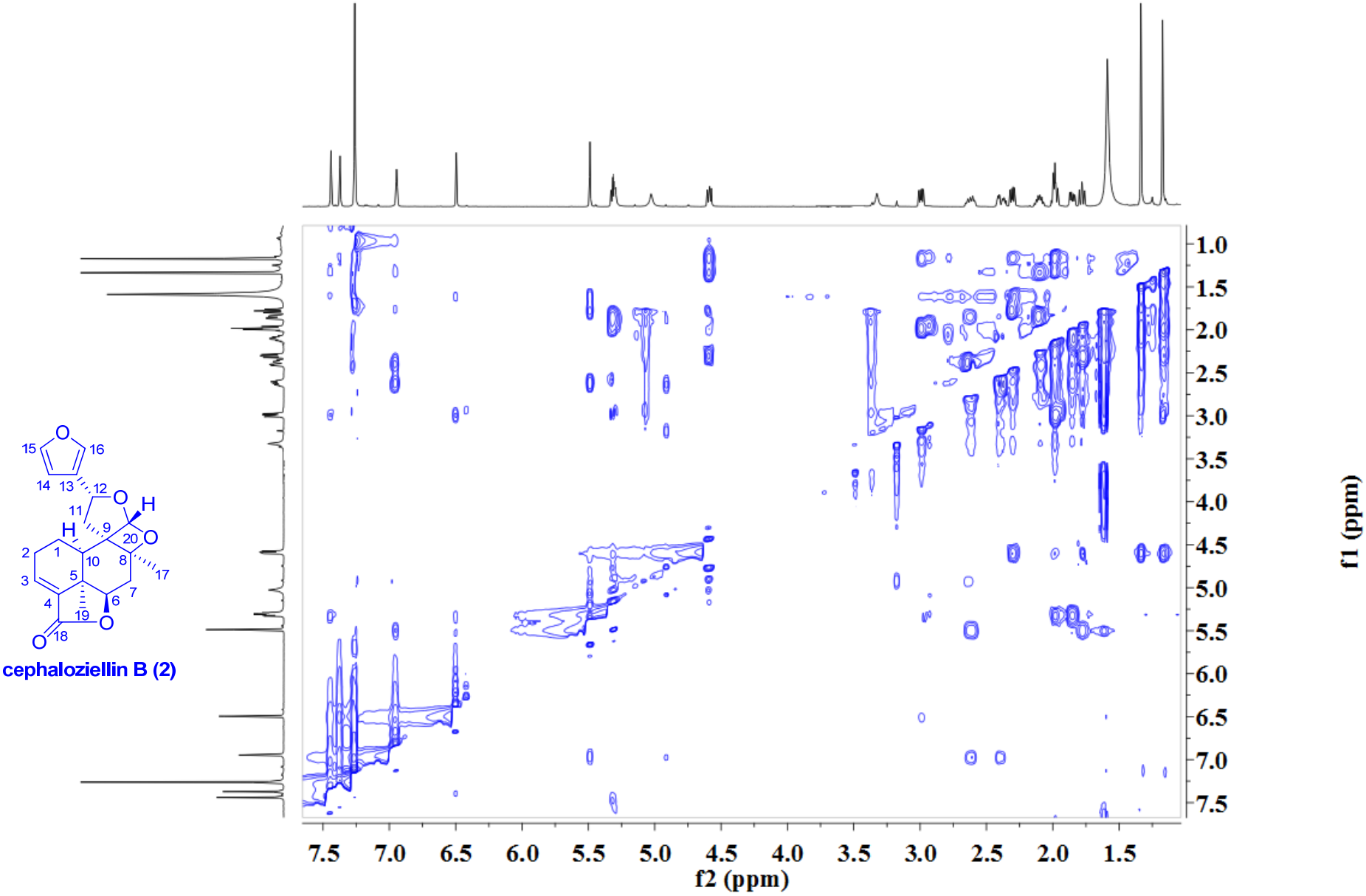
S16. HMBC spectrum (600 MHz) of cephaloziellin B (**2**) in $CDCl_3$.



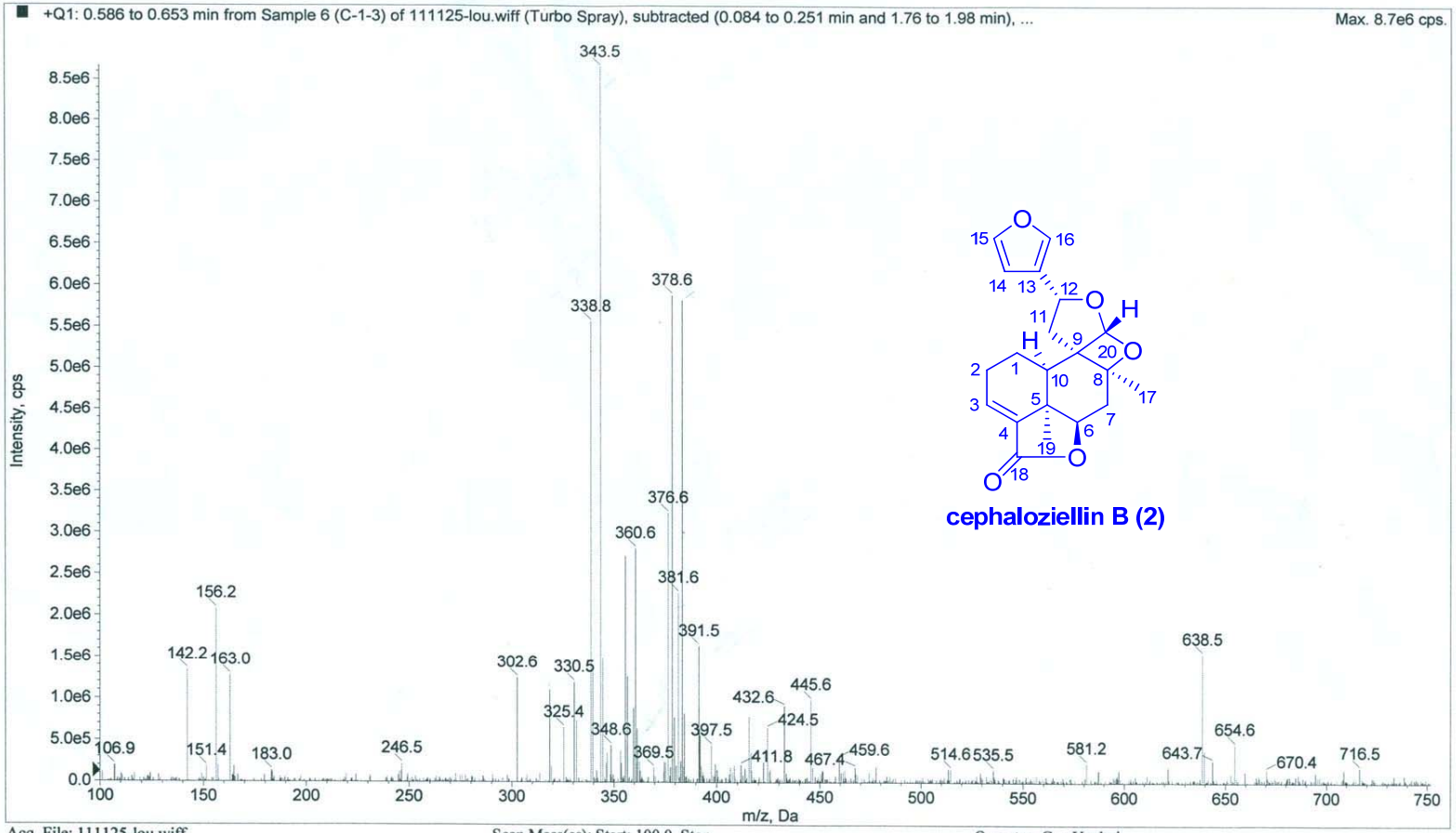
S17. ^{1}H-^{1}H COSY spectrum (600 MHz) of cephaloziellin B (**2**) in $CDCl_3$.



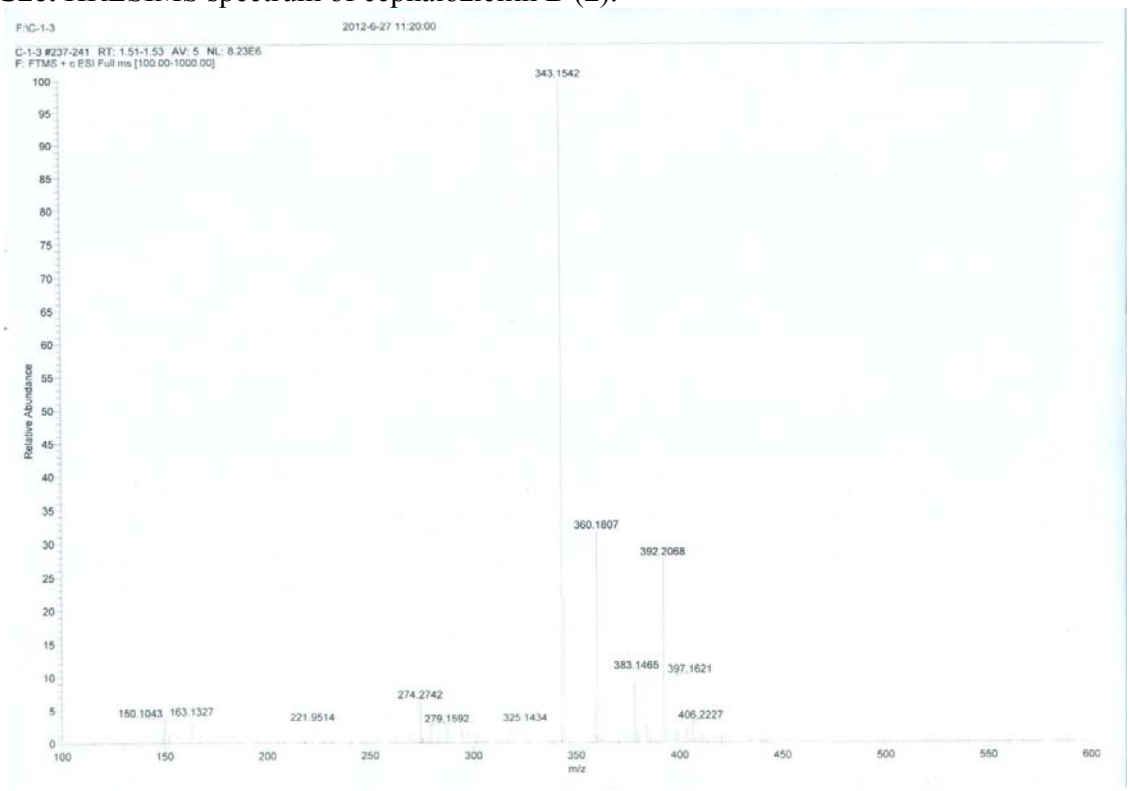
S18. NOESY spectrum (600 MHz) of cephaloziellin B (**2**) in $CDCl_3$.

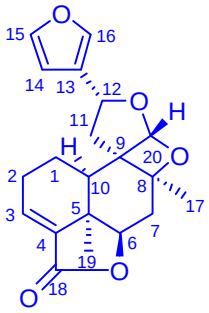


S19. ESIMS spectrum of cephaloziellin B (**2**).



S20. HRESIMS spectrum of cephaloziellin B (**2**).



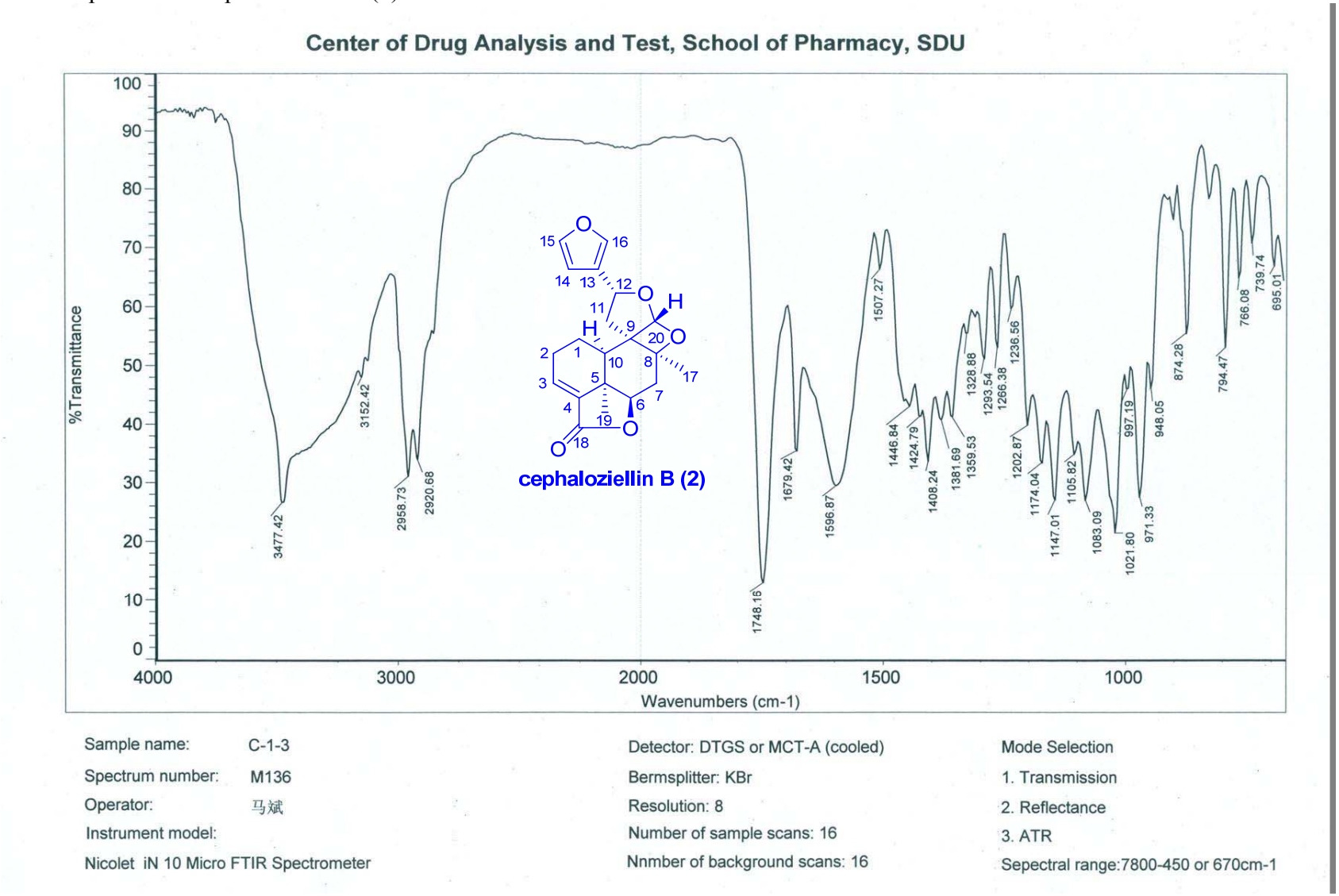


cephaloziellin B (2)

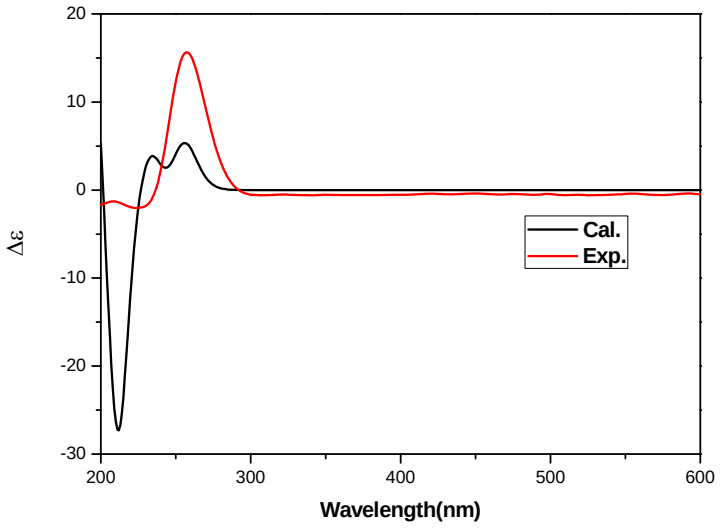
SPECTRUM - simulation :

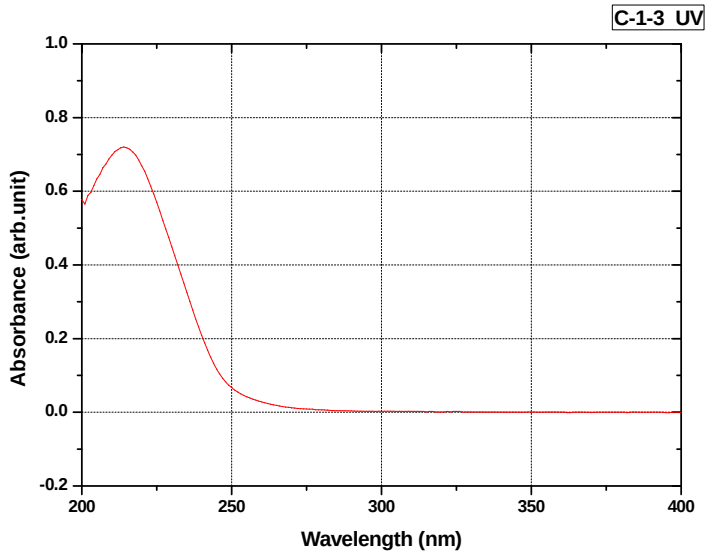
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
343.1542	343.1540	0.44	9.5	$^{12}C_{20}H_{23}O_5$

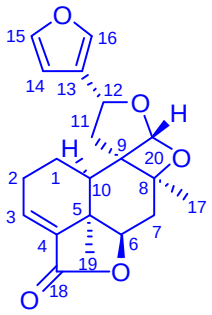
S21. IR spectrum of cephaloziellin B (**2**).



S22. Experimental ECD and calculated ECD, and UV spectra of cephaloziellin B (**2**).

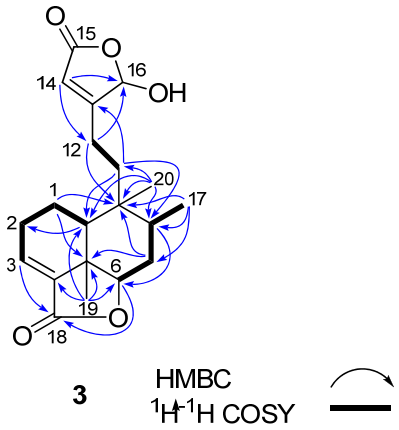




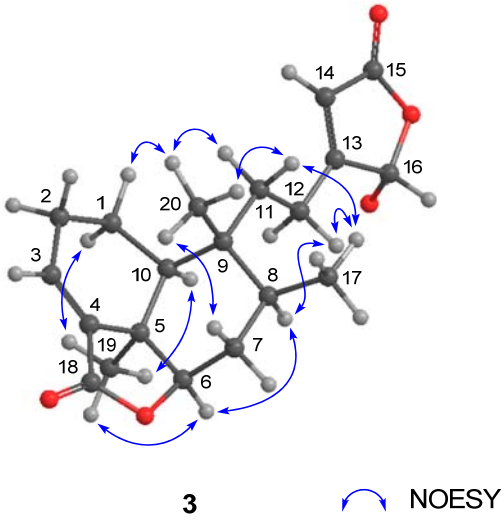


cephaloziellin B (2)

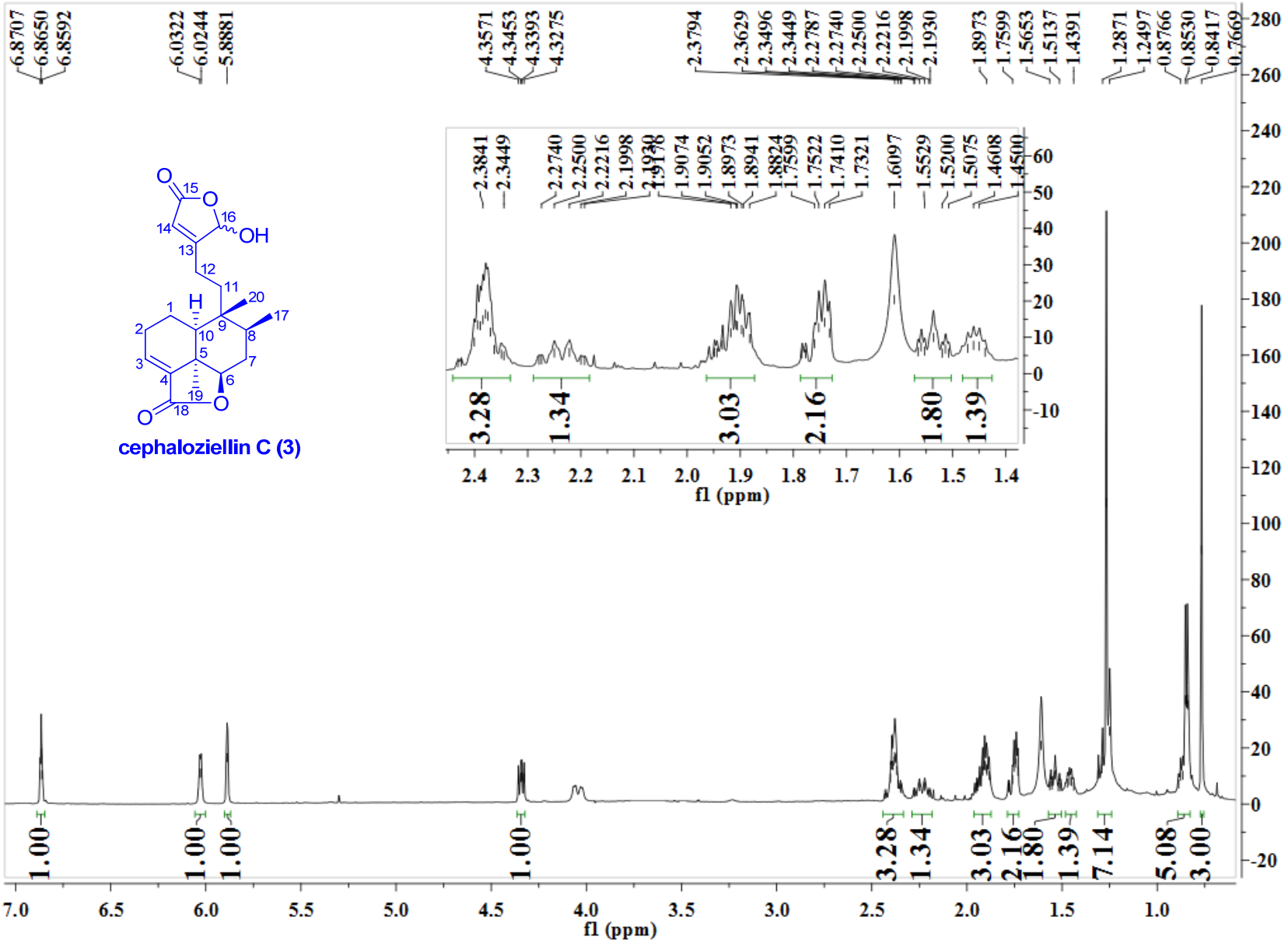
S23. Key HMBC and ^{1}H-^{1}H COSY correlations (in figure) of cephaloziellin C (**3**).



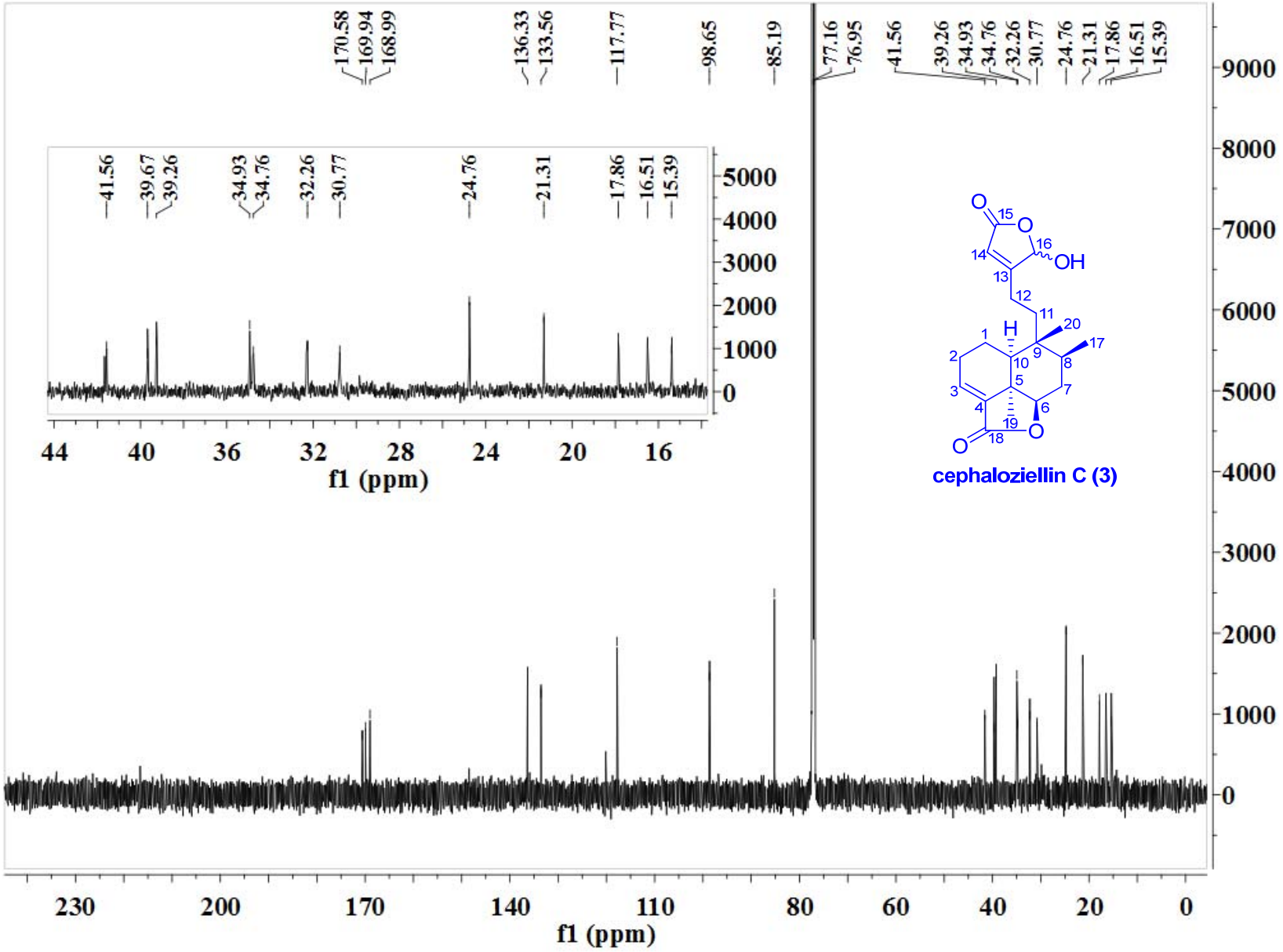
S24. Key NOESY correlations (in figure) of cephaloziellin C (**3**).



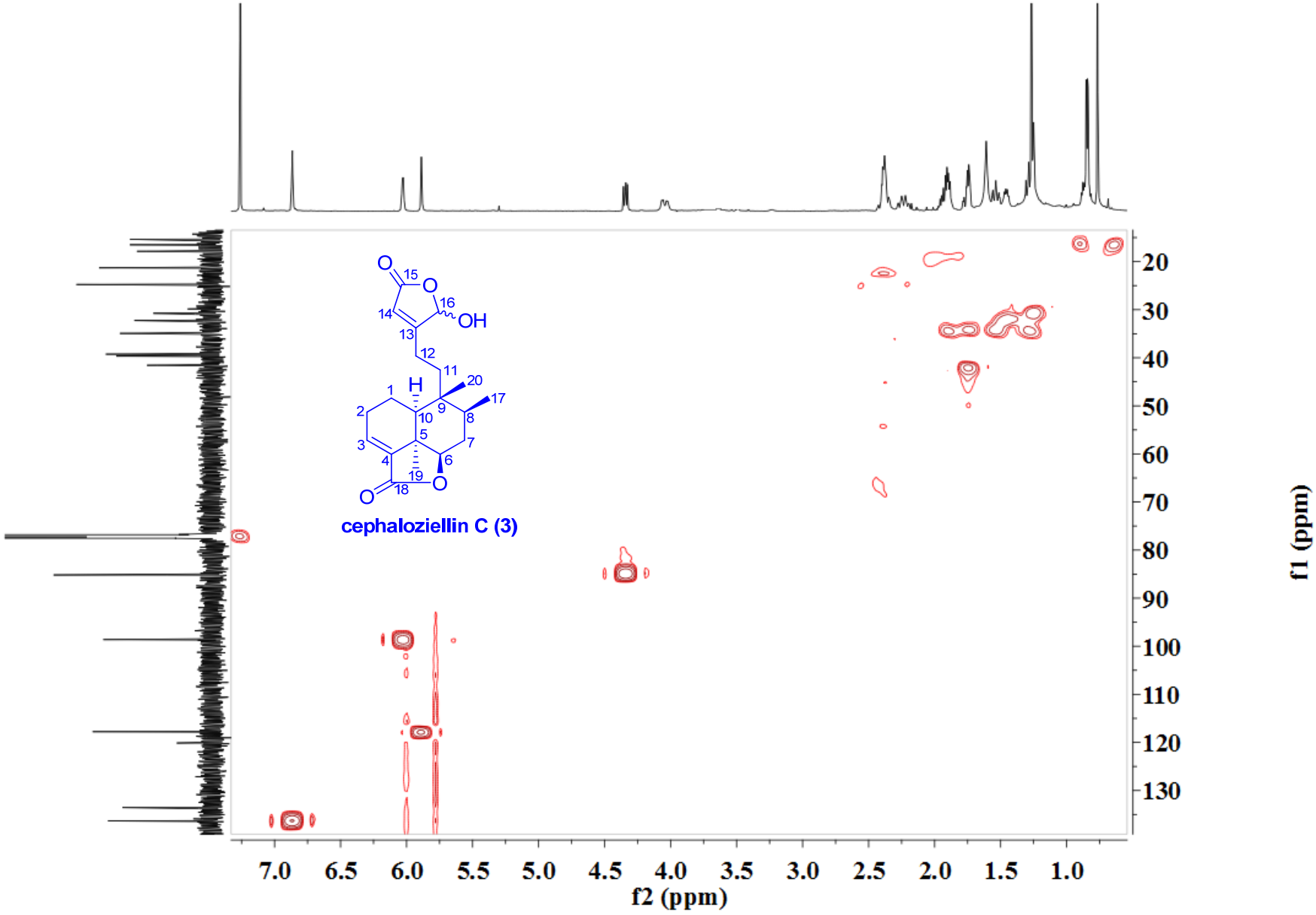
S25. ^{1}H NMR spectrum (600 MHz) of cephaloziellin C (**3**) in $CDCl_3$.



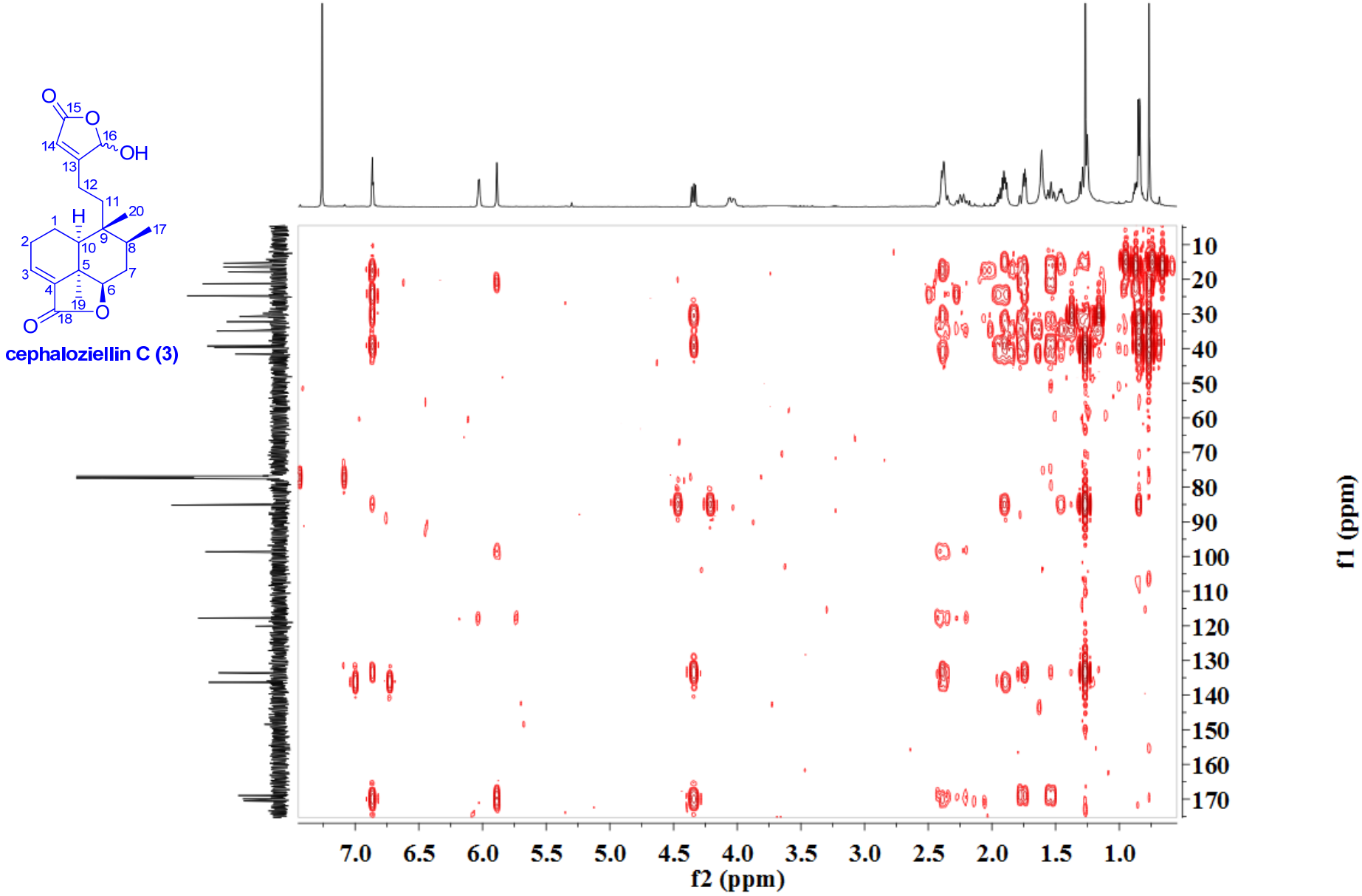
S26. ^{13}C NMR spectrum (150 MHz) of cephaloziellin C (**3**) in $CDCl_3$.



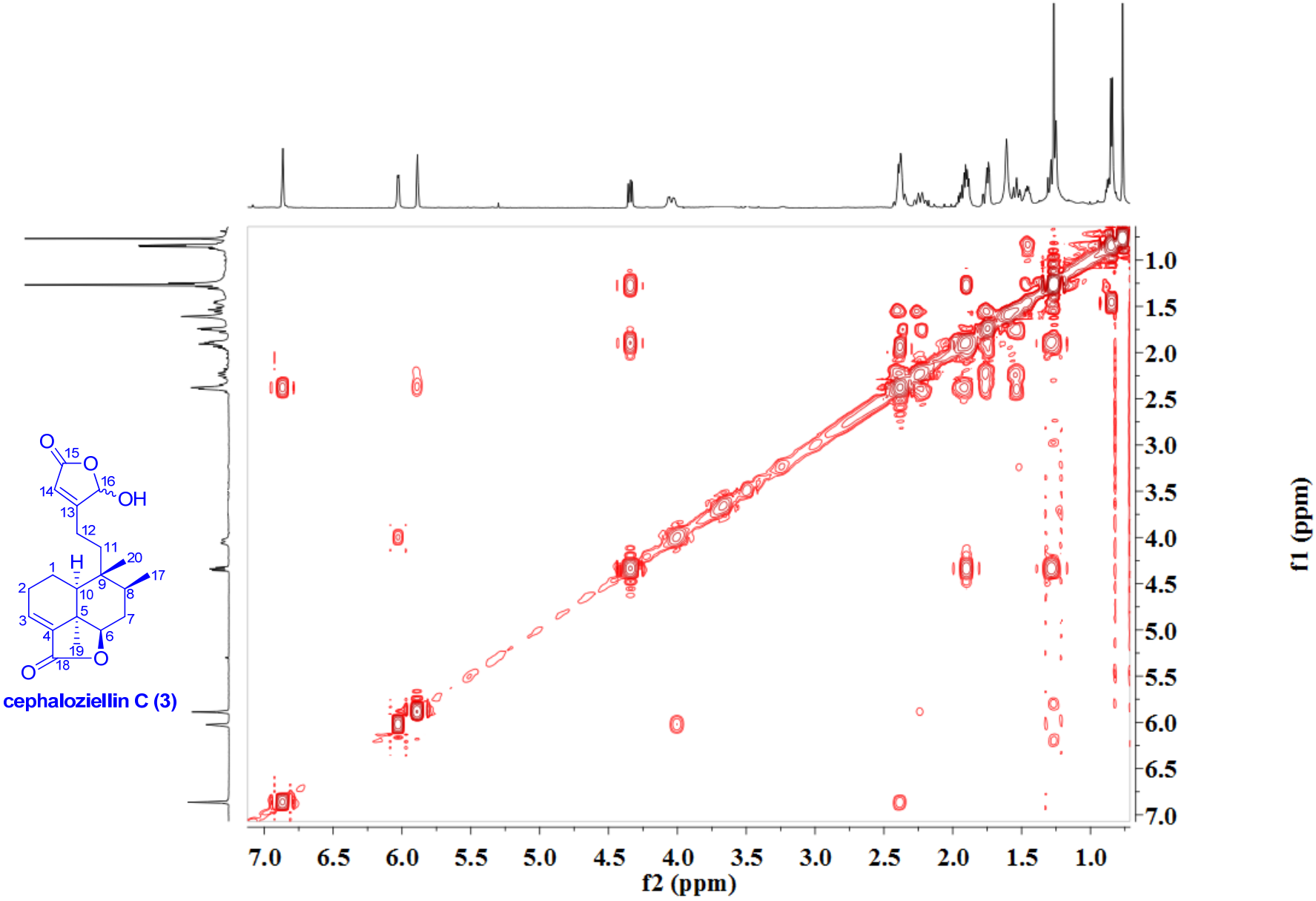
S27. HSQC spectrum (600 MHz) of cephaloziellin C (**3**) in $CDCl_3$.



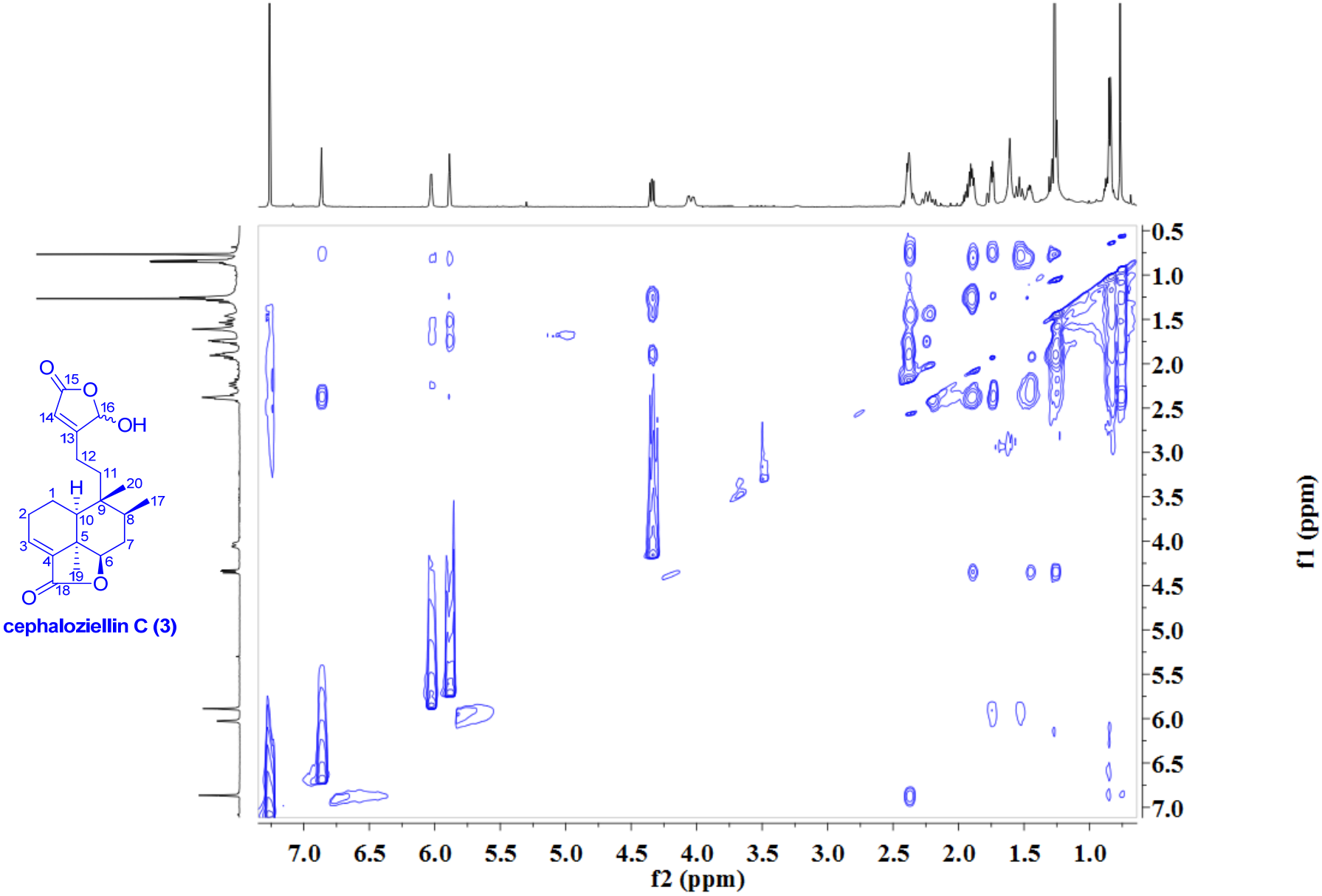
S28. HMBC spectrum (600 MHz) of cephaloziellin C (**3**) in $CDCl_3$.



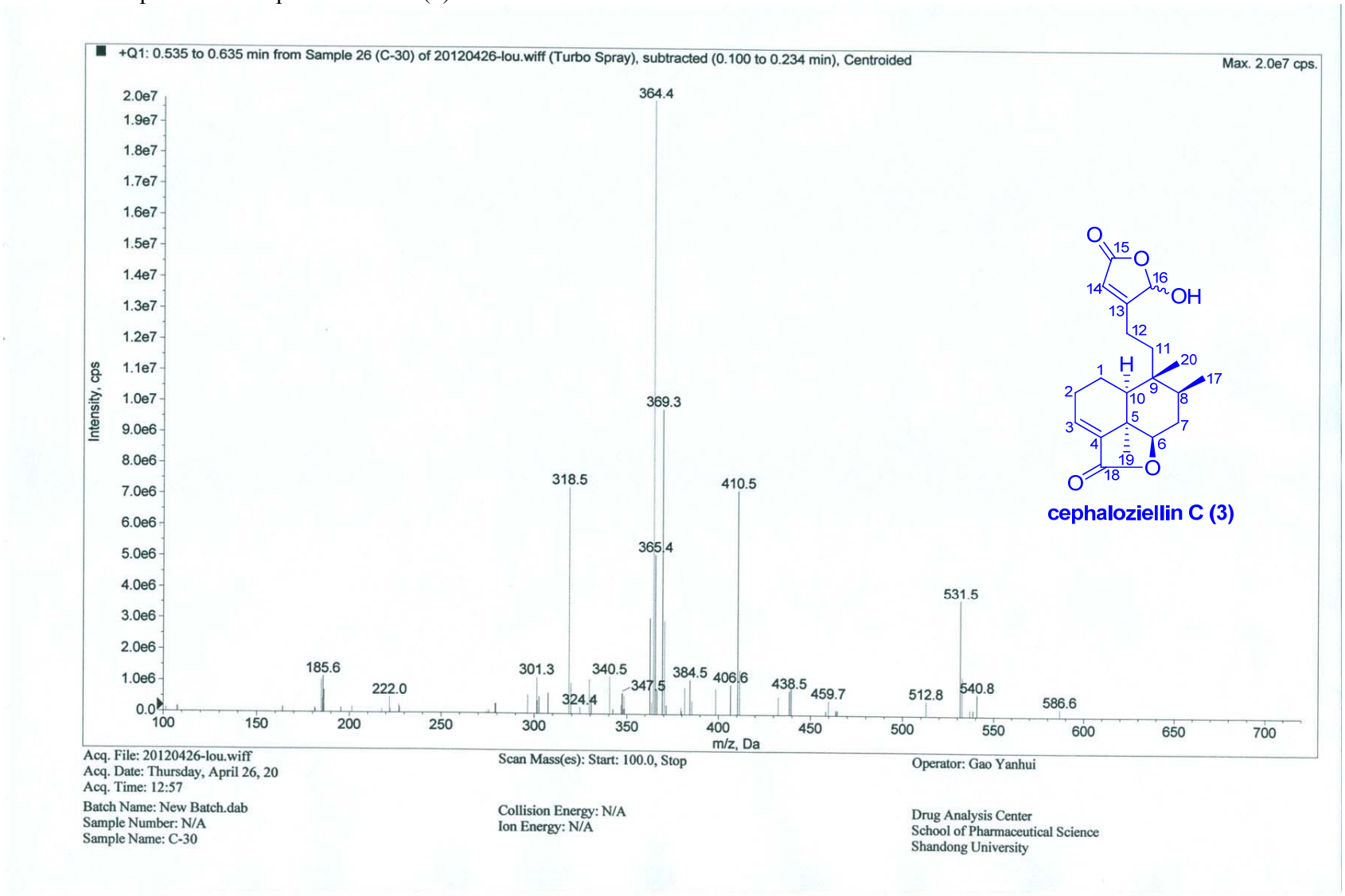
S29. ^{1}H-^{1}H COSY spectrum (600 MHz) of cephaloziellin C (**3**) in $CDCl_3$.



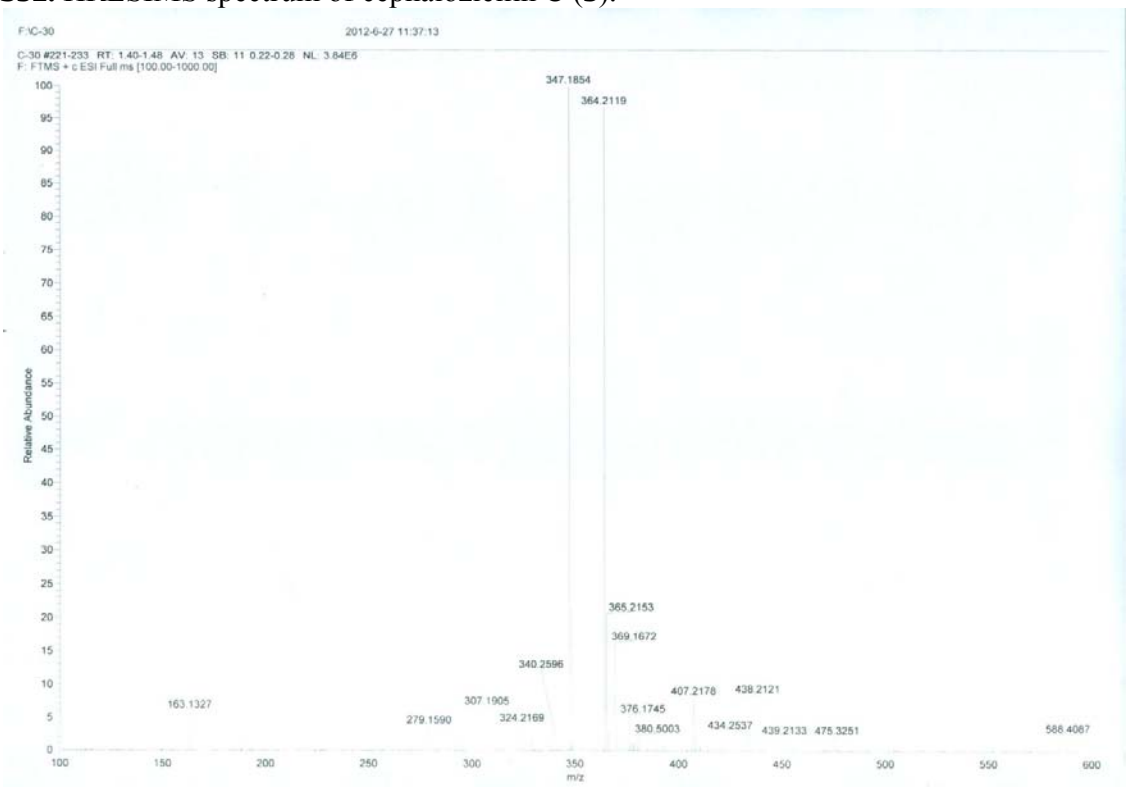
S30. NOESY spectrum (600 MHz) of cephaloziellin C (**3**) in $CDCl_3$.

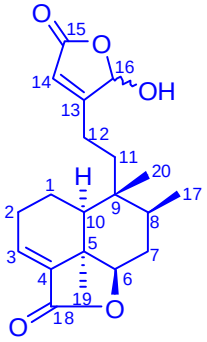


S31. ESIMS spectrum of cephaloziellin C (**3**).



S32. HRESIMS spectrum of cephaloziellin C (**3**).



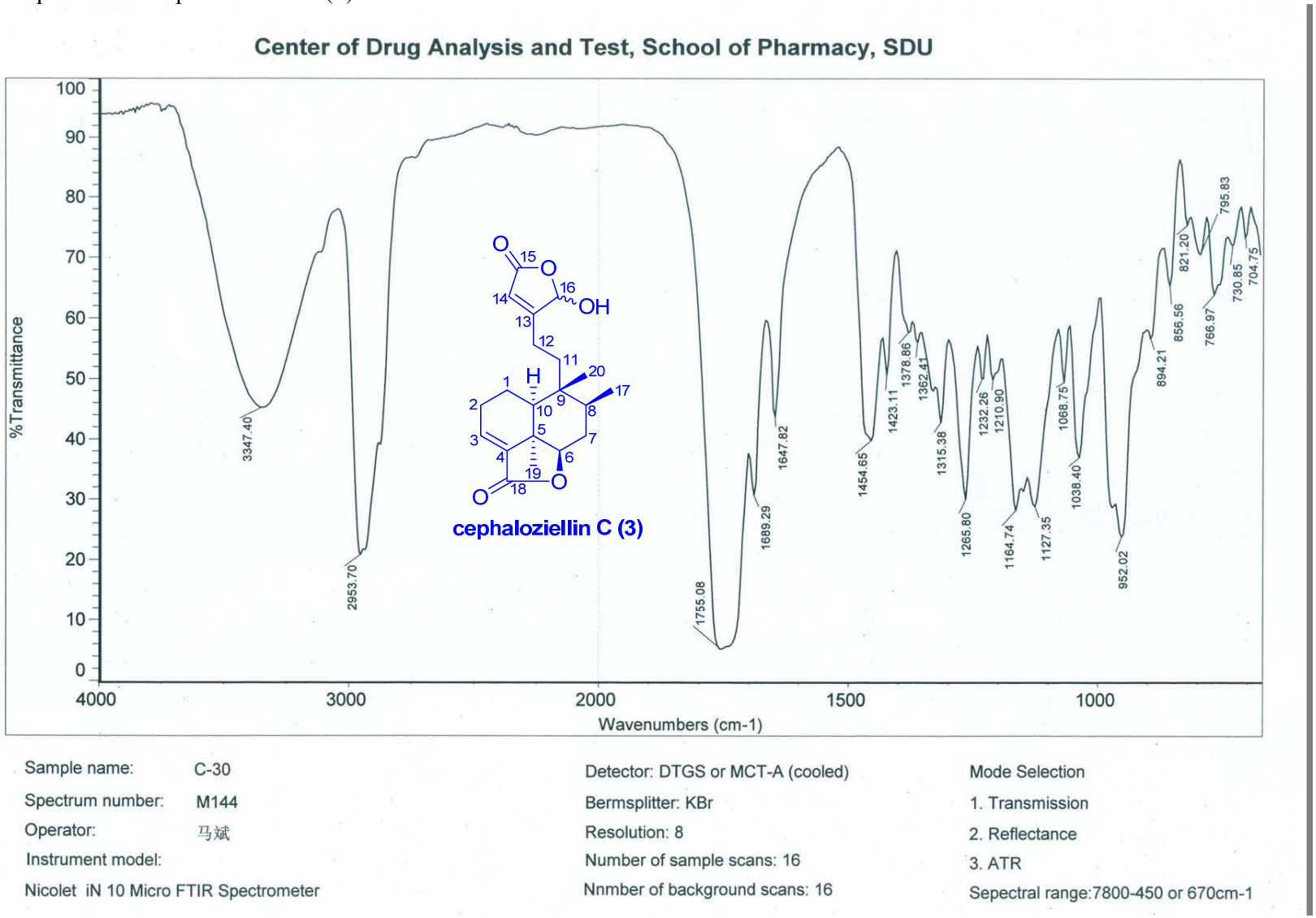


cephaloziellin C (3)

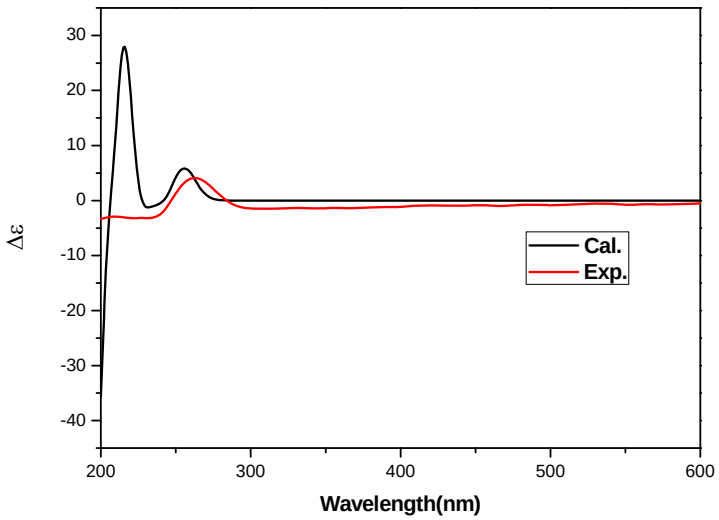
SPECTRUM - simulation :

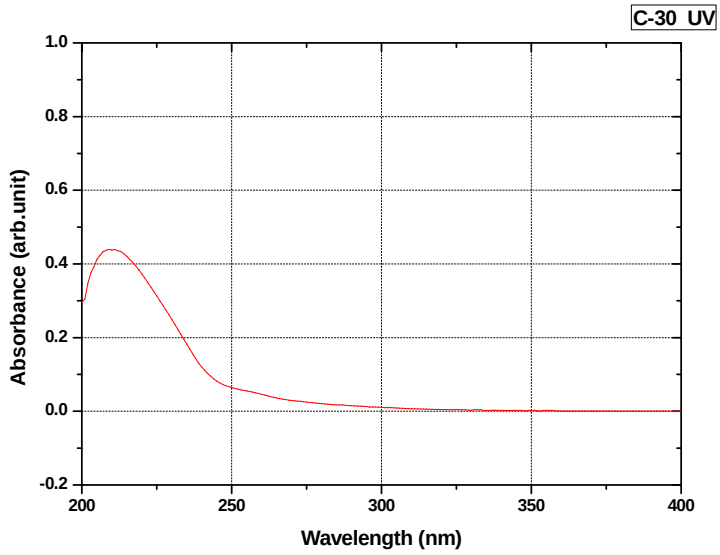
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
347.1854	347.1853	0.14	7.5	$^{12}C_{20}H_{27}O_5$

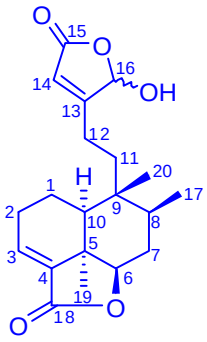
S33. IR spectrum of cephaloziellin C (**3**).



S34. Experimental ECD and calculated ECD, and UV spectra of cephaloziellin C (**3**).

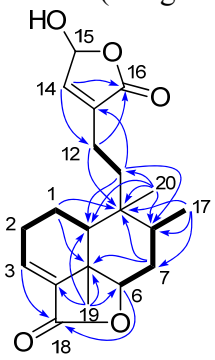






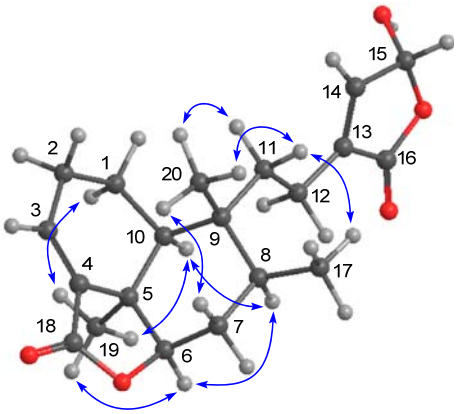
cephaloziellin C (3)

S35. Key HMBC and ^{1}H-^{1}H COSY correlations (in figure) of cephaloziellin D (**4**).



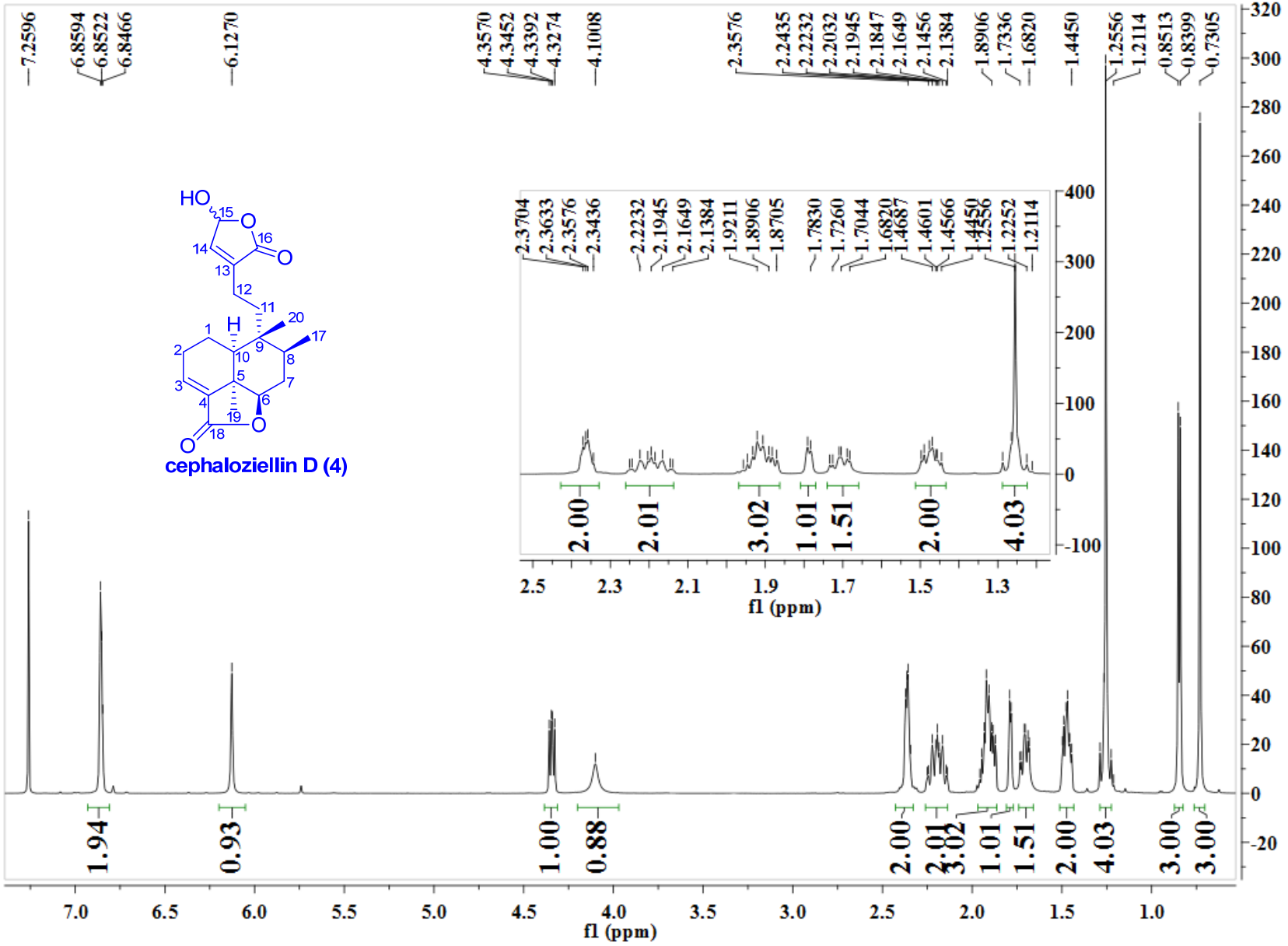
4 HMBC ^{1}H-^{1}H COSY

S36. Key NOESY correlations (in figure) of cephaloziellin D (**4**).

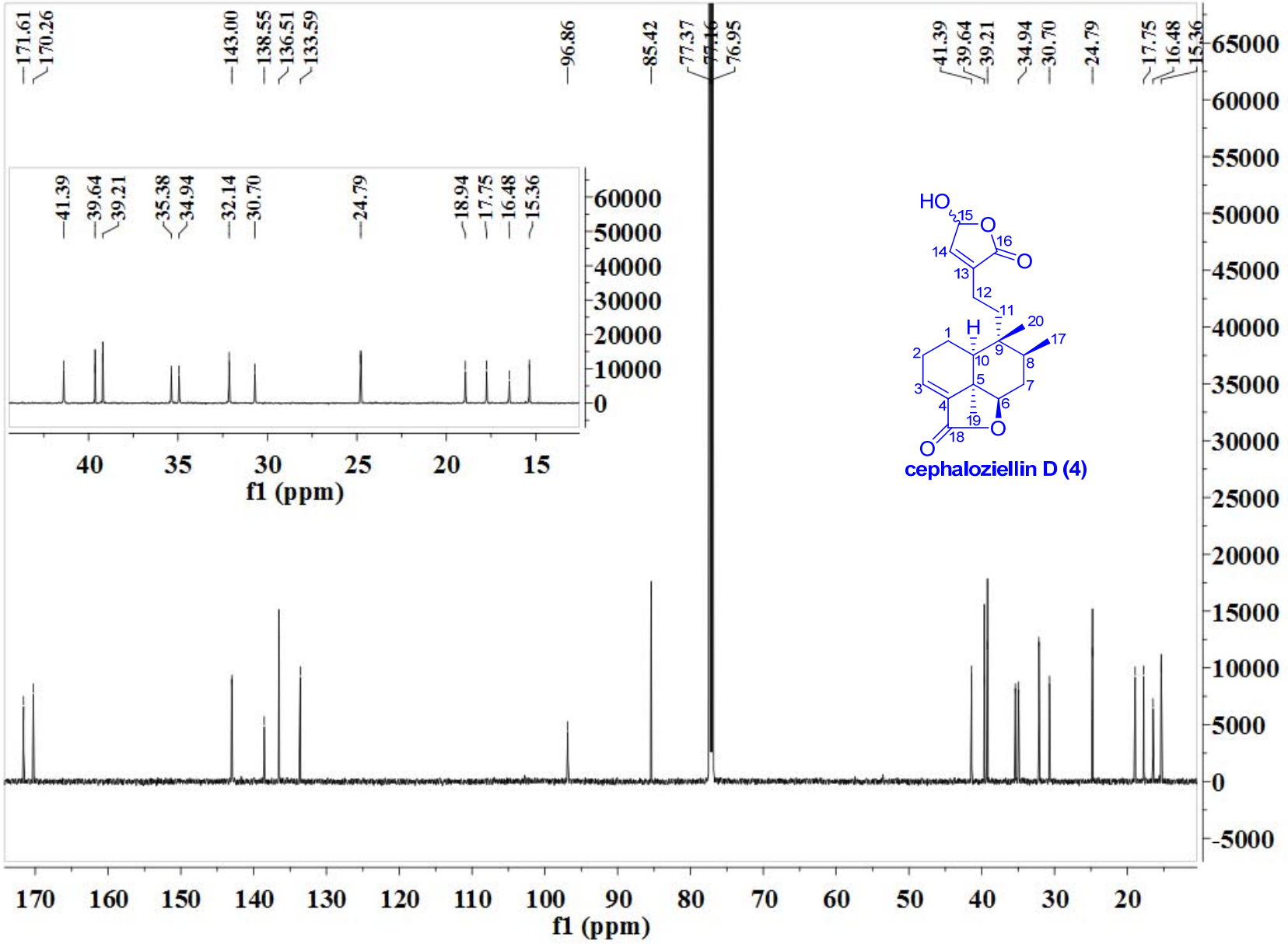


4 NOESY

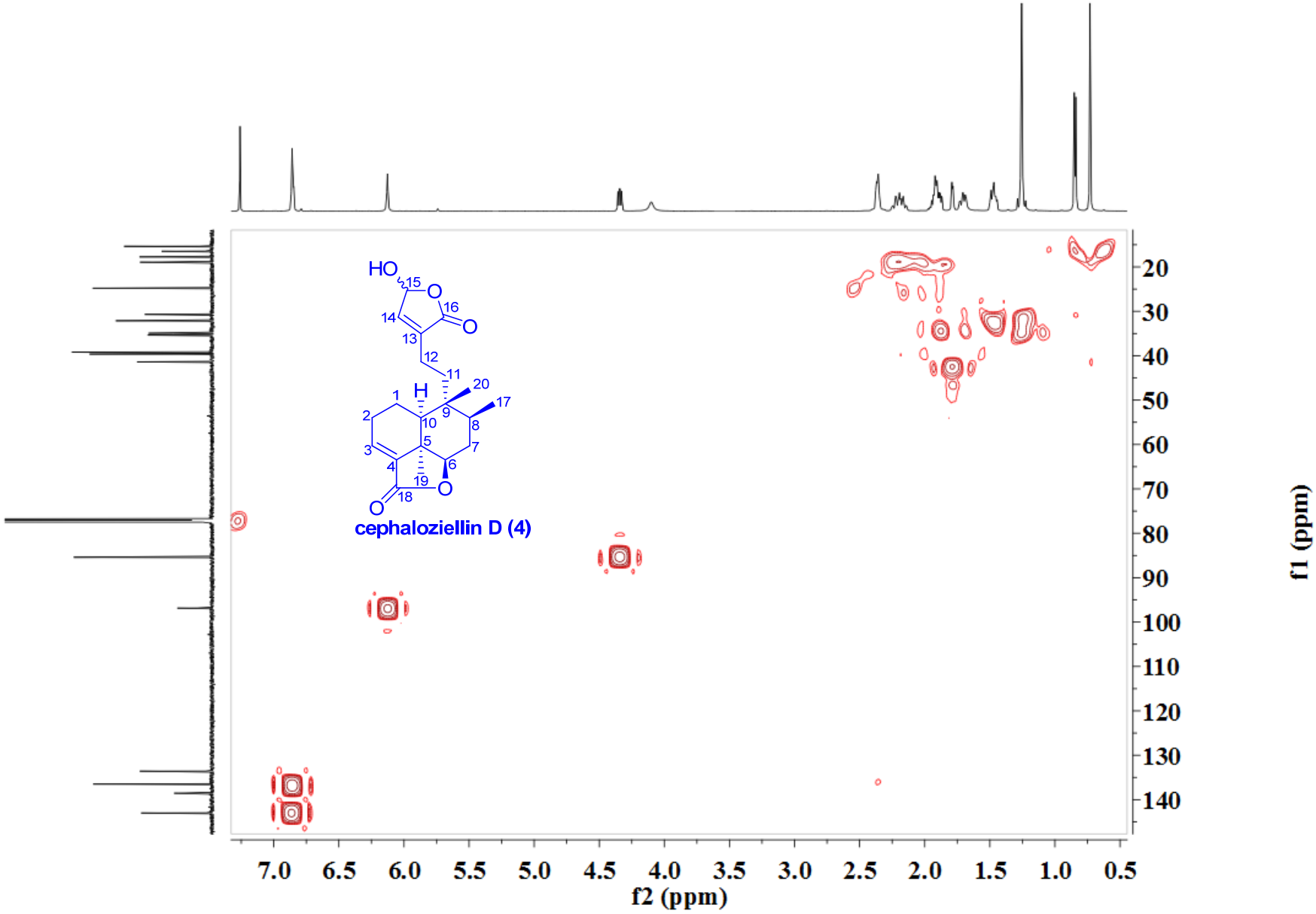
S37. ^{1}H NMR spectrum (600 MHz) of cephaloziellin D (**4**) in $CDCl_3$.



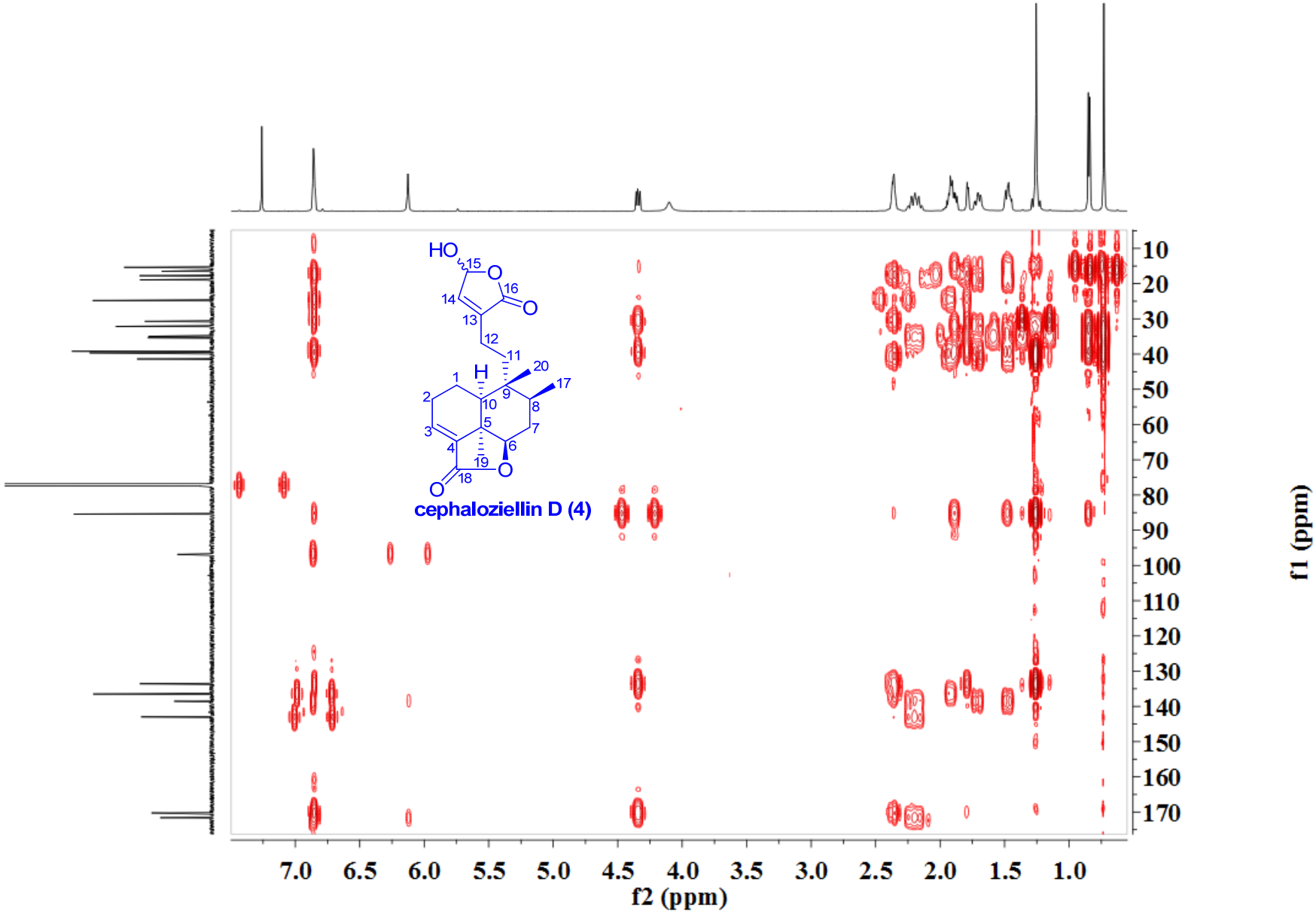
S38. ^{13}C NMR spectrum (150 MHz) of cephaloziellin D (**4**) in $CDCl_3$.



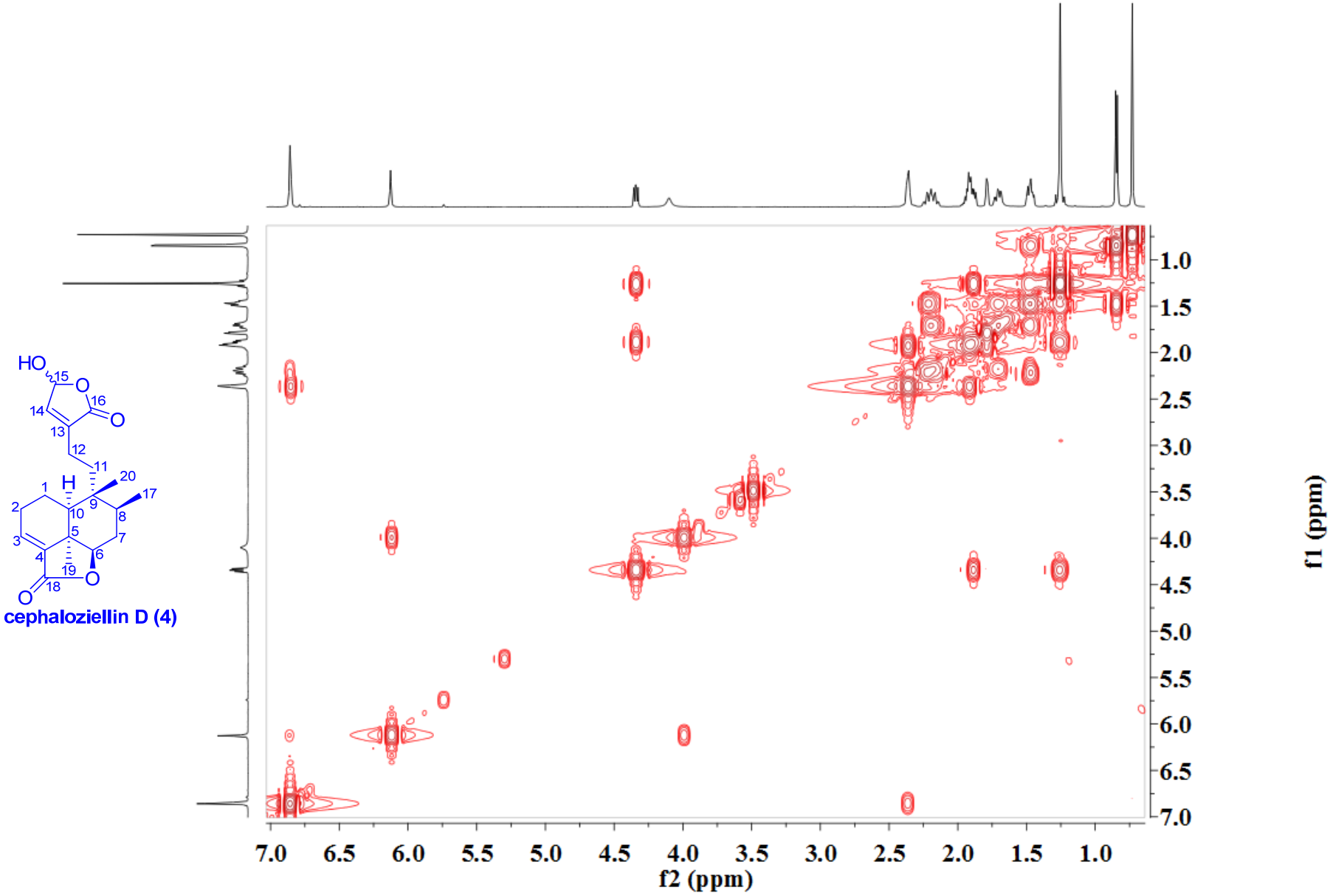
S39. HSQC spectrum (600 MHz) of cephaloziellin D (**4**) in $CDCl_3$.



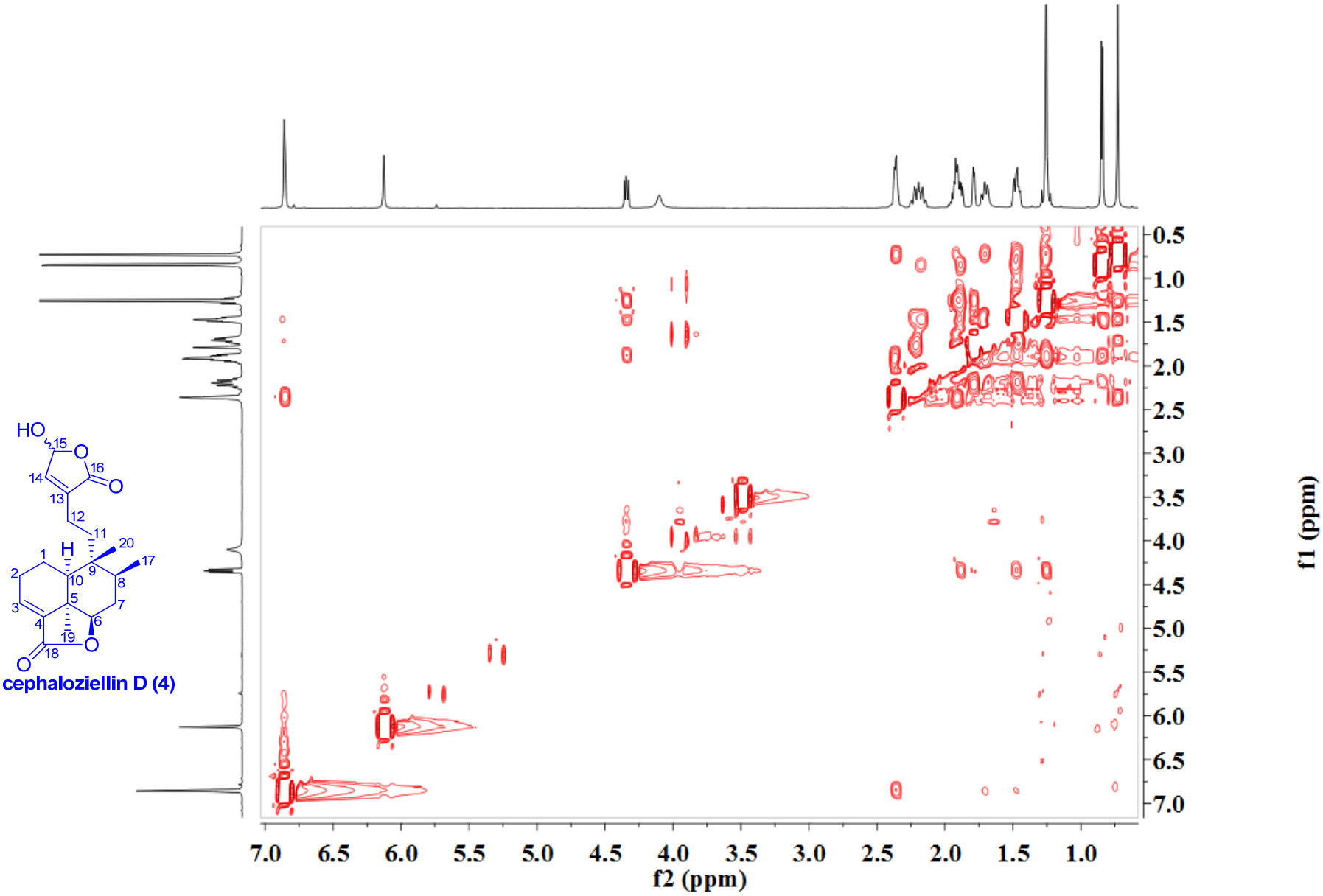
S40. HMBC spectrum (600 MHz) of cephaloziellin D (**4**) in $CDCl_3$.



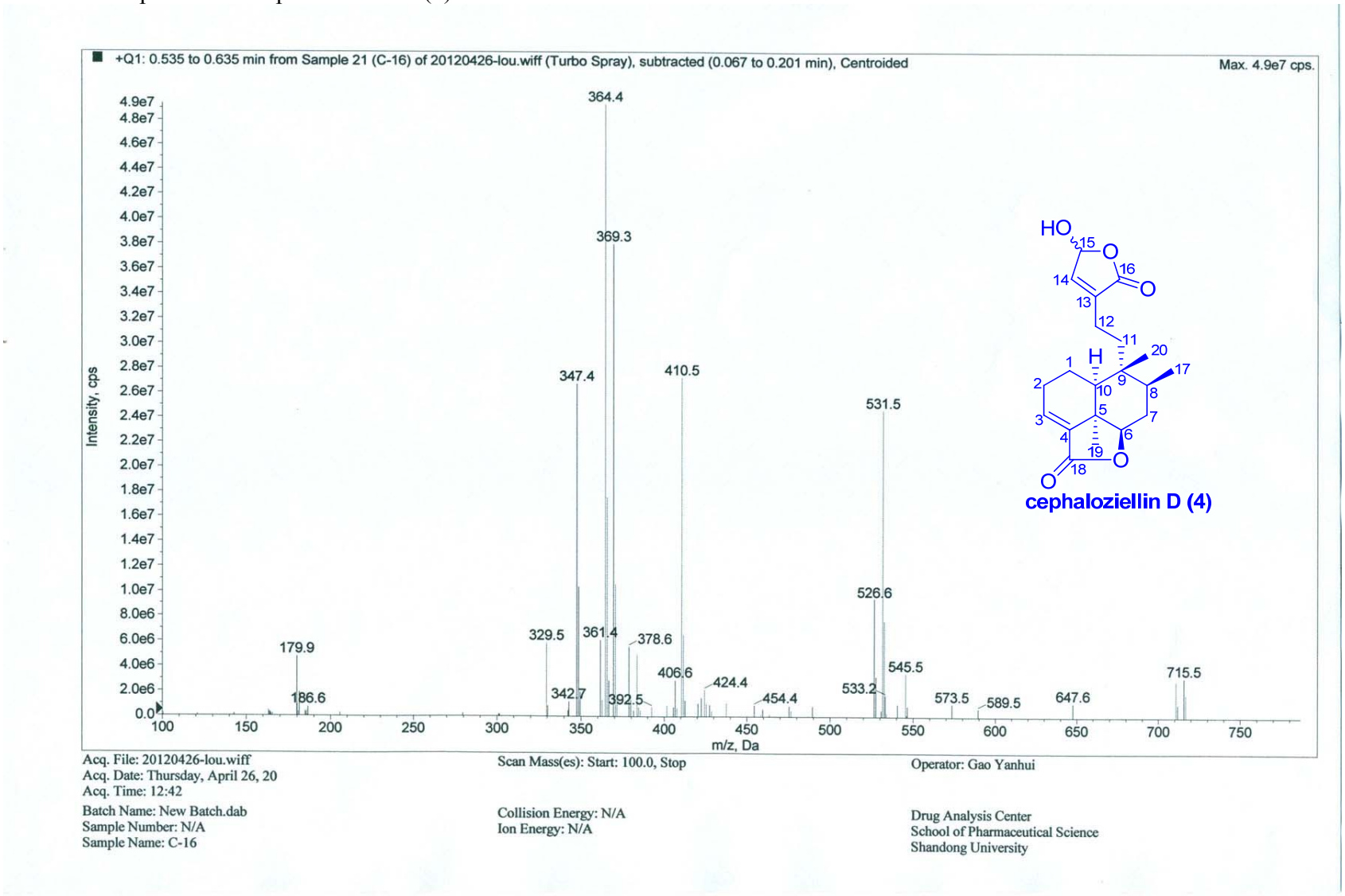
S41. ^{1}H-^{1}H COSY spectrum (600 MHz) of cephaloziellin D (**4**) in $CDCl_3$.



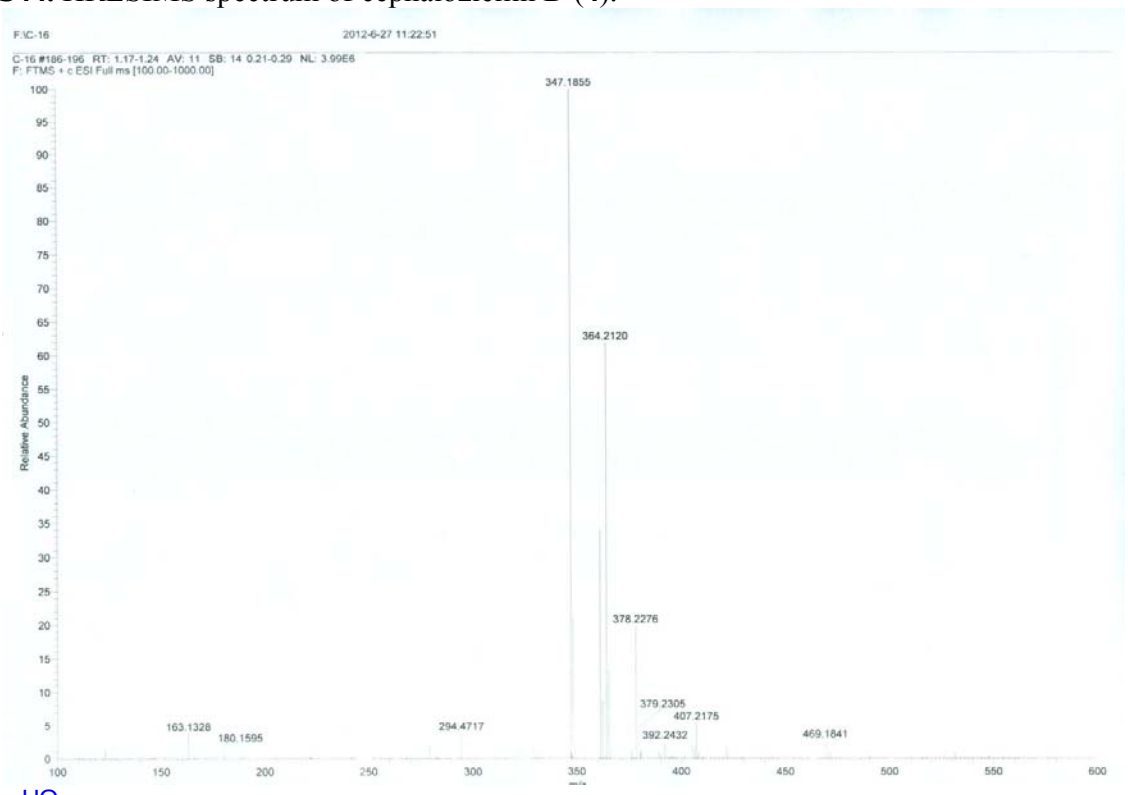
S42. NOESY spectrum (600 MHz) of cephaloziellin D (**4**) in $CDCl_3$.

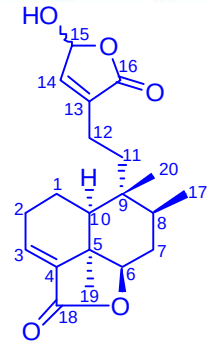


S43. ESIMS spectrum of cephaloziellin D (**4**).



S44. HRESIMS spectrum of cephaloziellin D (**4**).



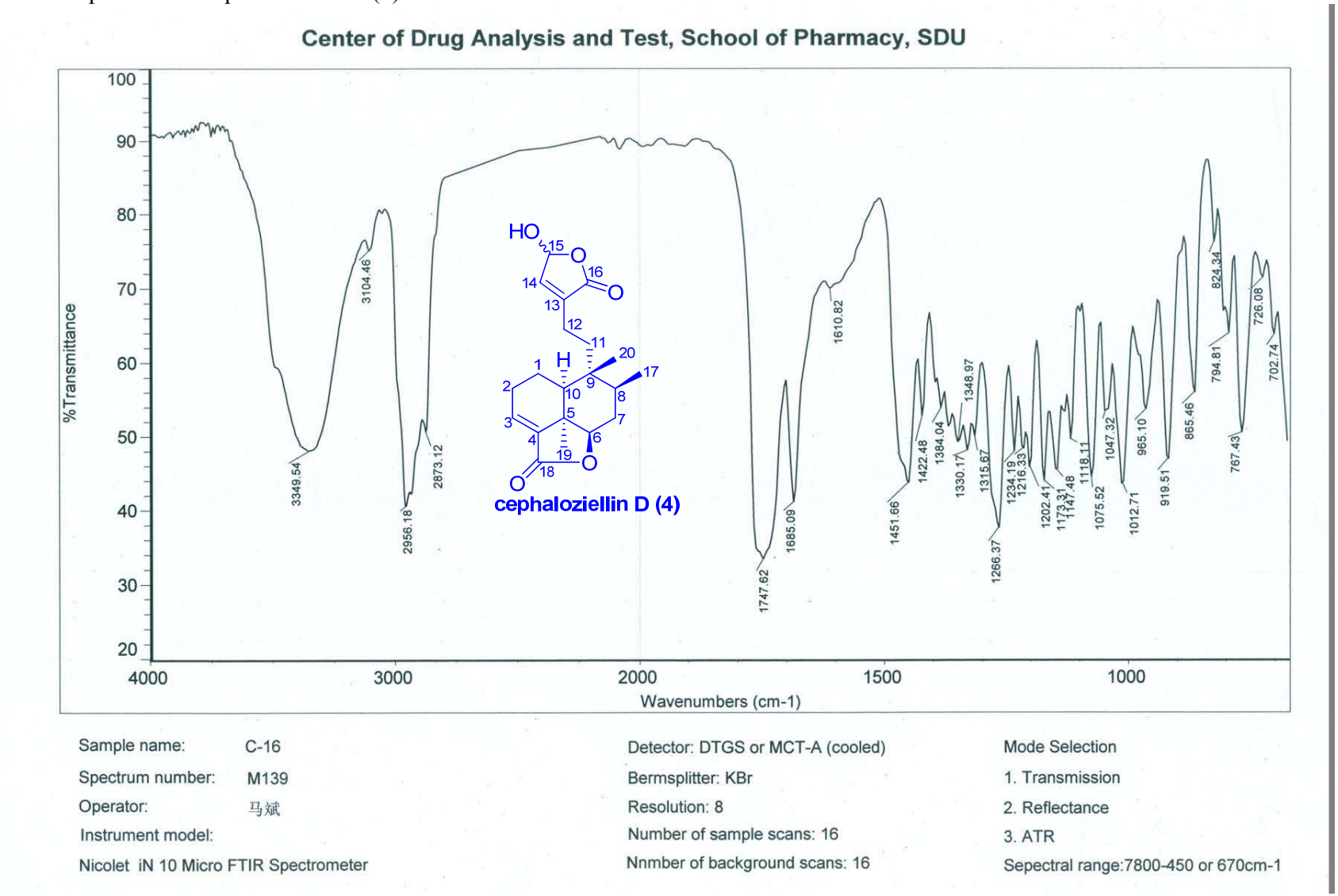


cephaloziellin D (4)

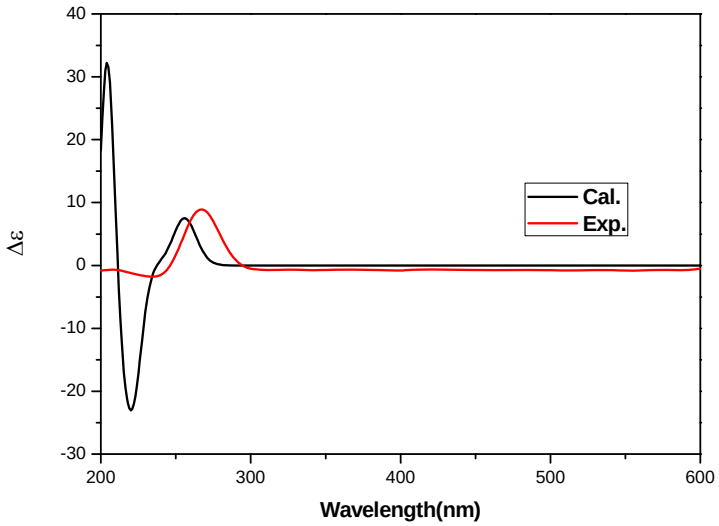
SPECTRUM - simulation :

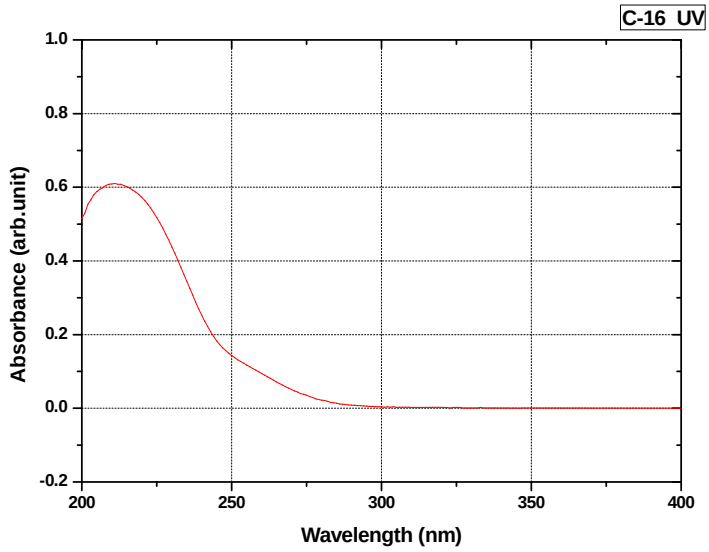
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
347.1855	347.1853	0.69	7.5	$^{12}C_{20}H_{27}O_5$

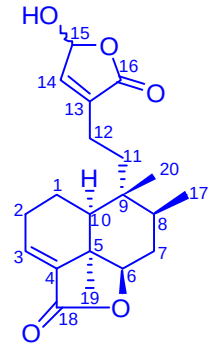
S45. IR spectrum of cephaloziellin D (**4**).



S46. Experimental ECD and calculated ECD, and UV spectra of cephaloziellin D (**4**).

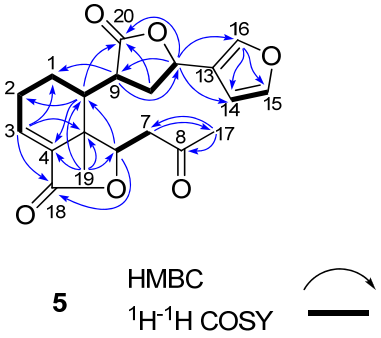






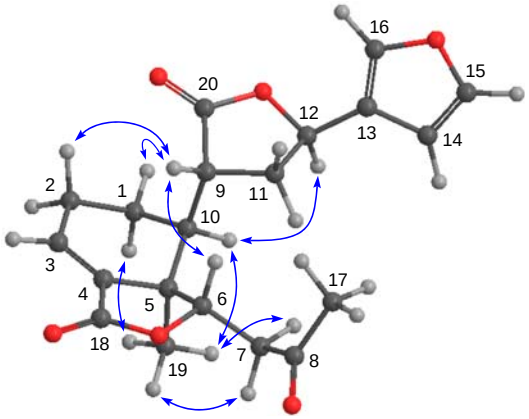
cephaloziellin D (4)

S47. Key HMBC and ^{1}H-^{1}H COSY correlations (in figure) of cephaloziellin E (**5**).



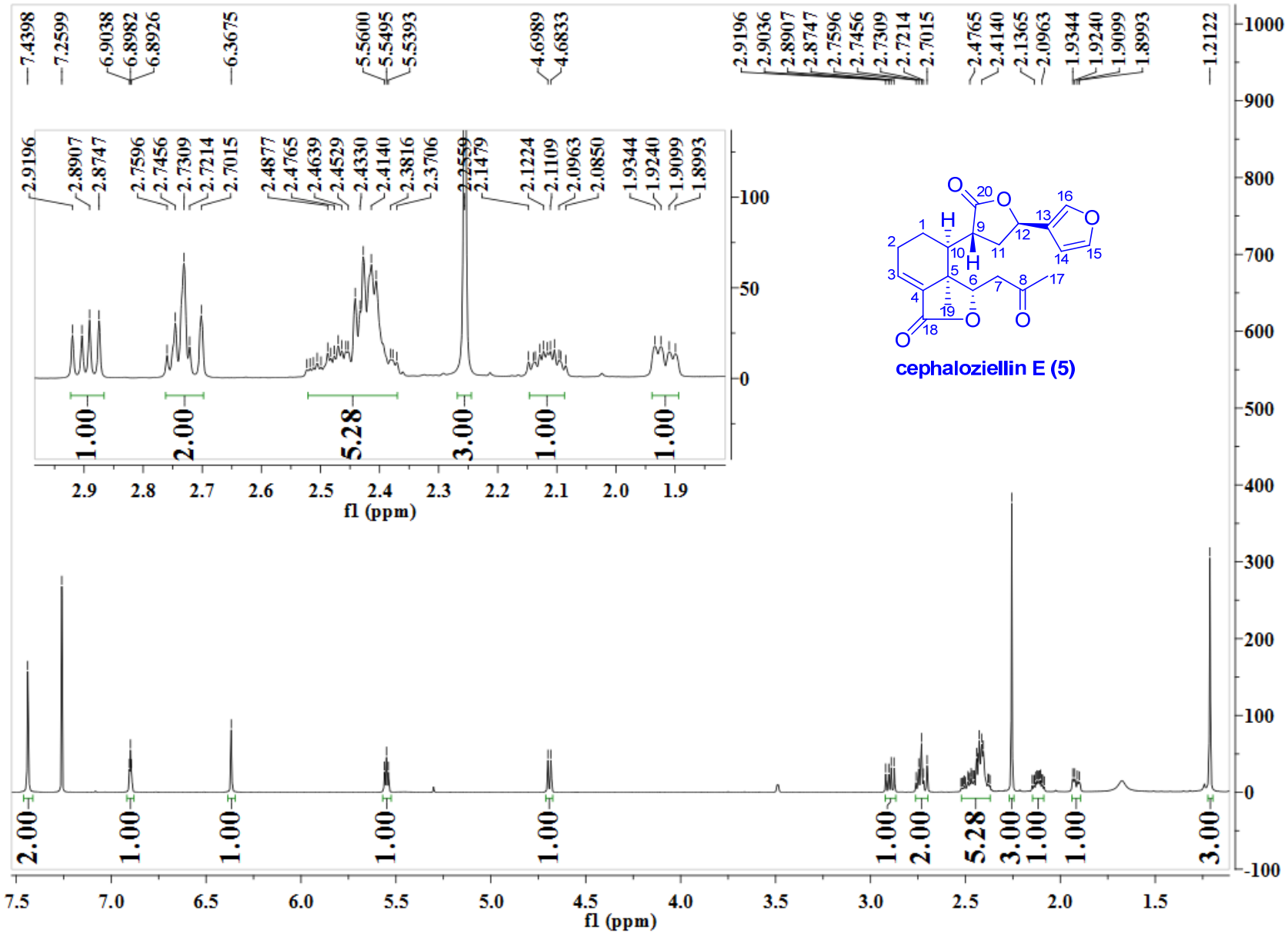
5 HMBC, ^{1}H-^{1}H COSY

S48. Key NOESY correlations (in figure) of cephaloziellin E (**5**).

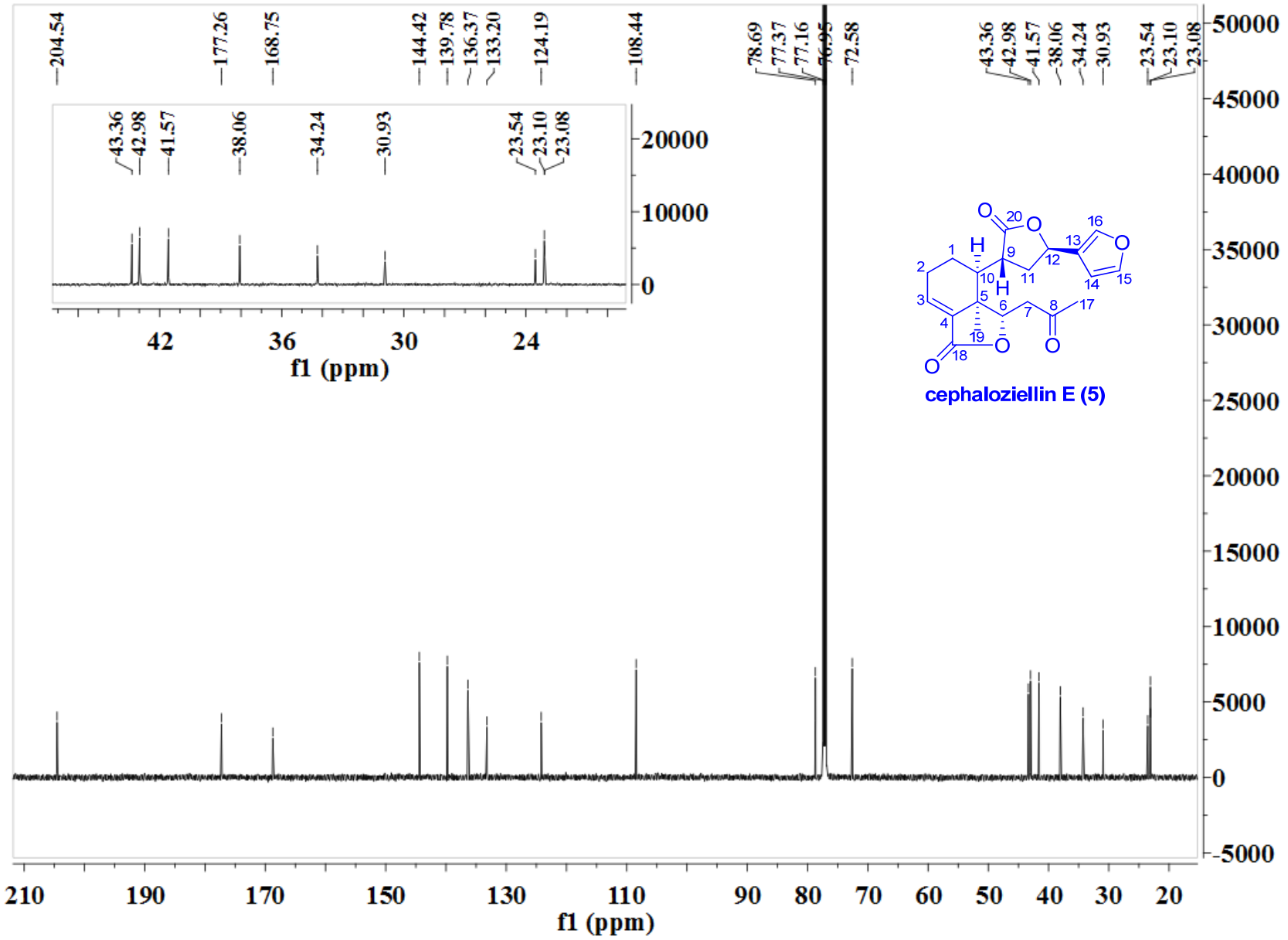


5 NOESY

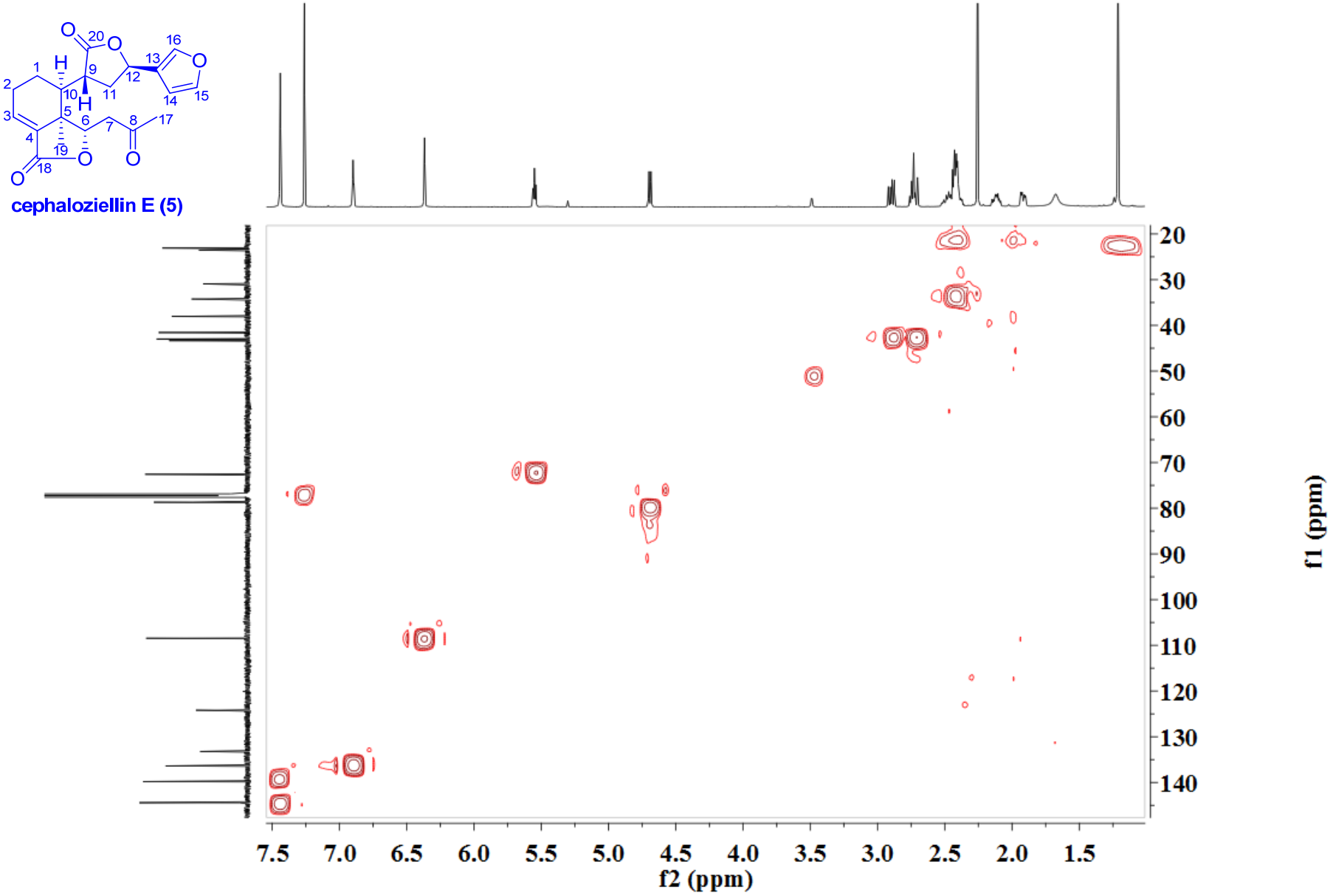
S49. ^{1}H NMR spectrum (600 MHz) of cephaloziellin E (**5**) in $CDCl_3$.



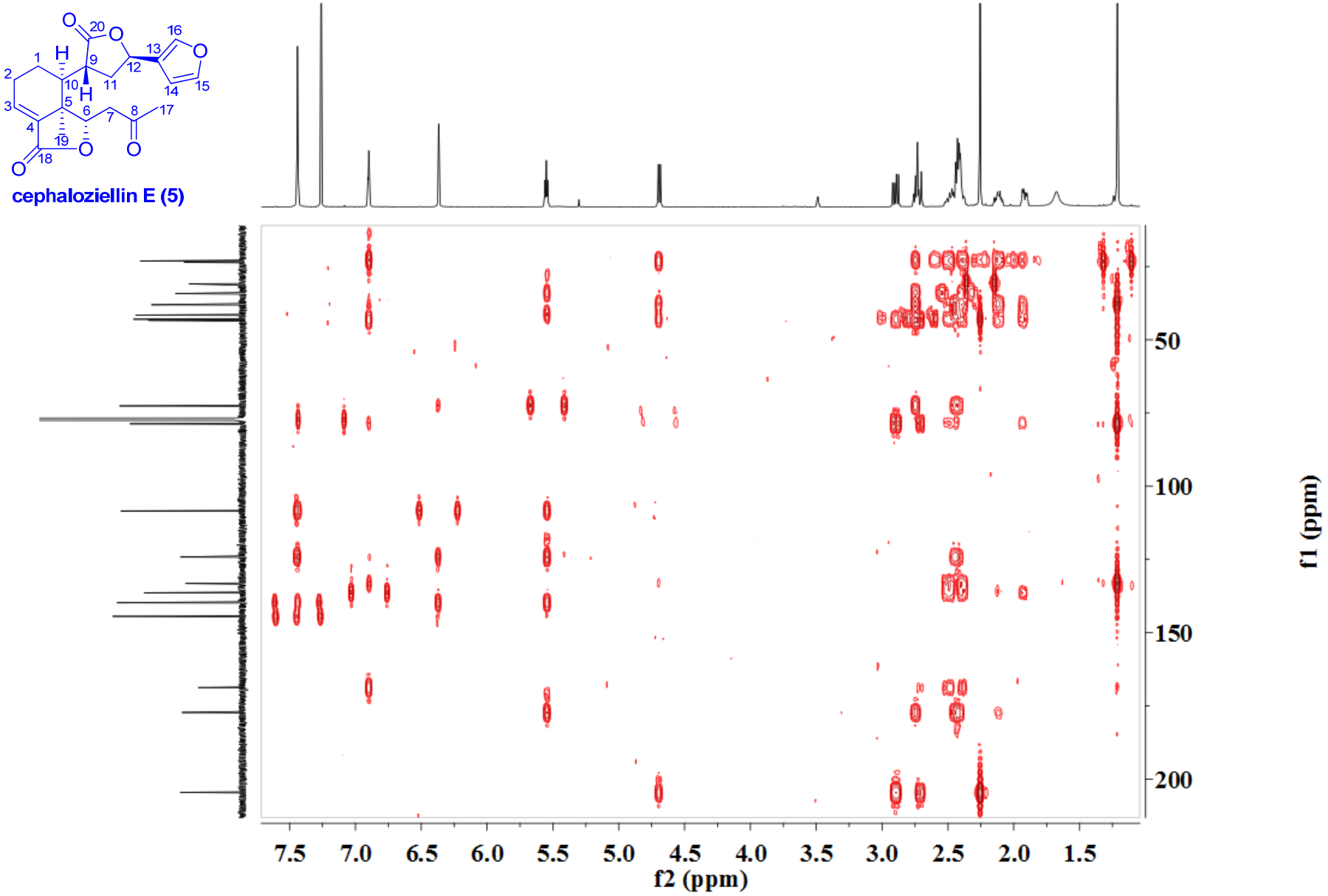
S50. ^{13}C NMR spectrum (150 MHz) of cephaloziellin E (**5**) in $CDCl_3$.



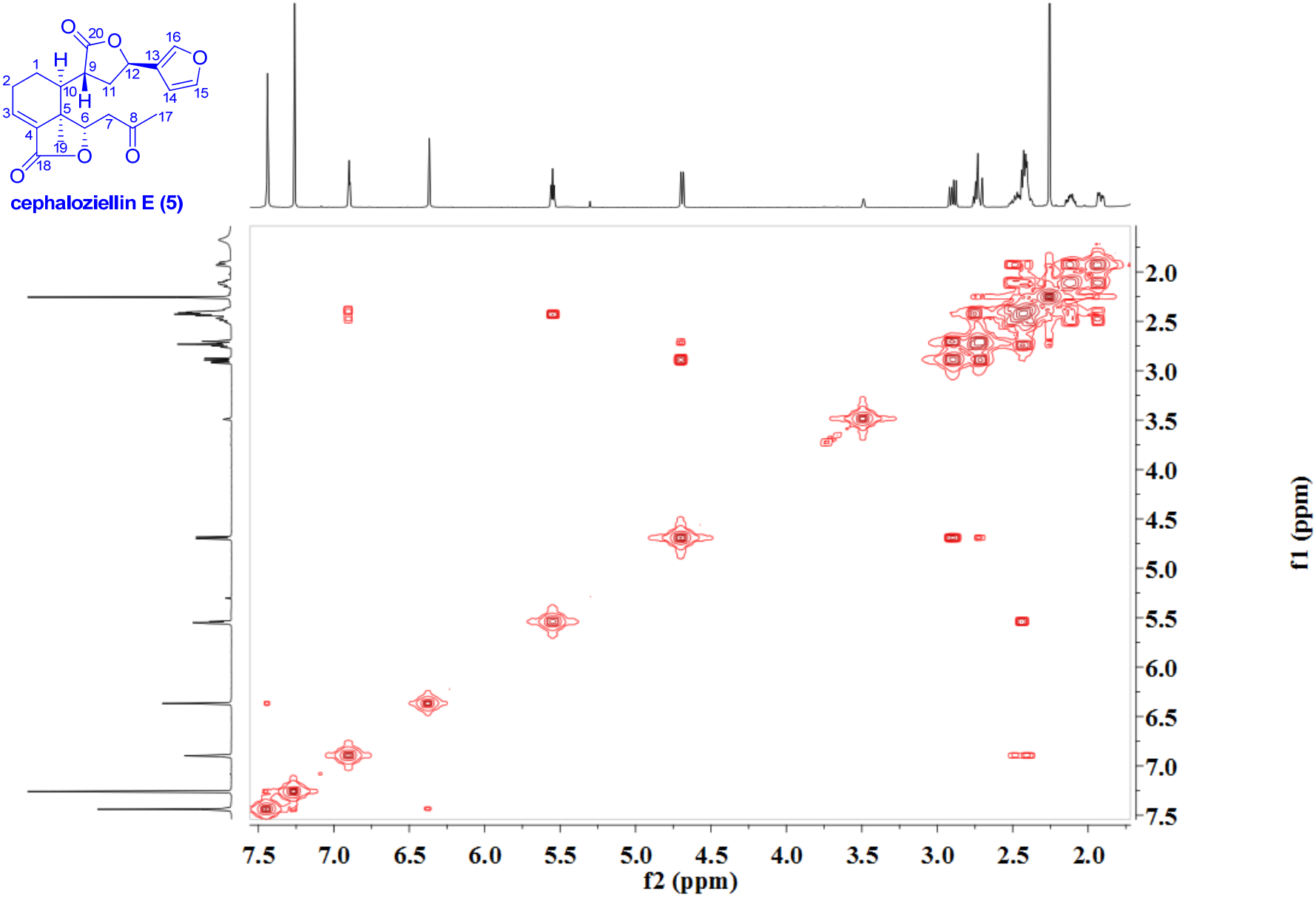
S51. HSQC spectrum (600 MHz) of cephaloziellin E (**5**) in $CDCl_3$.



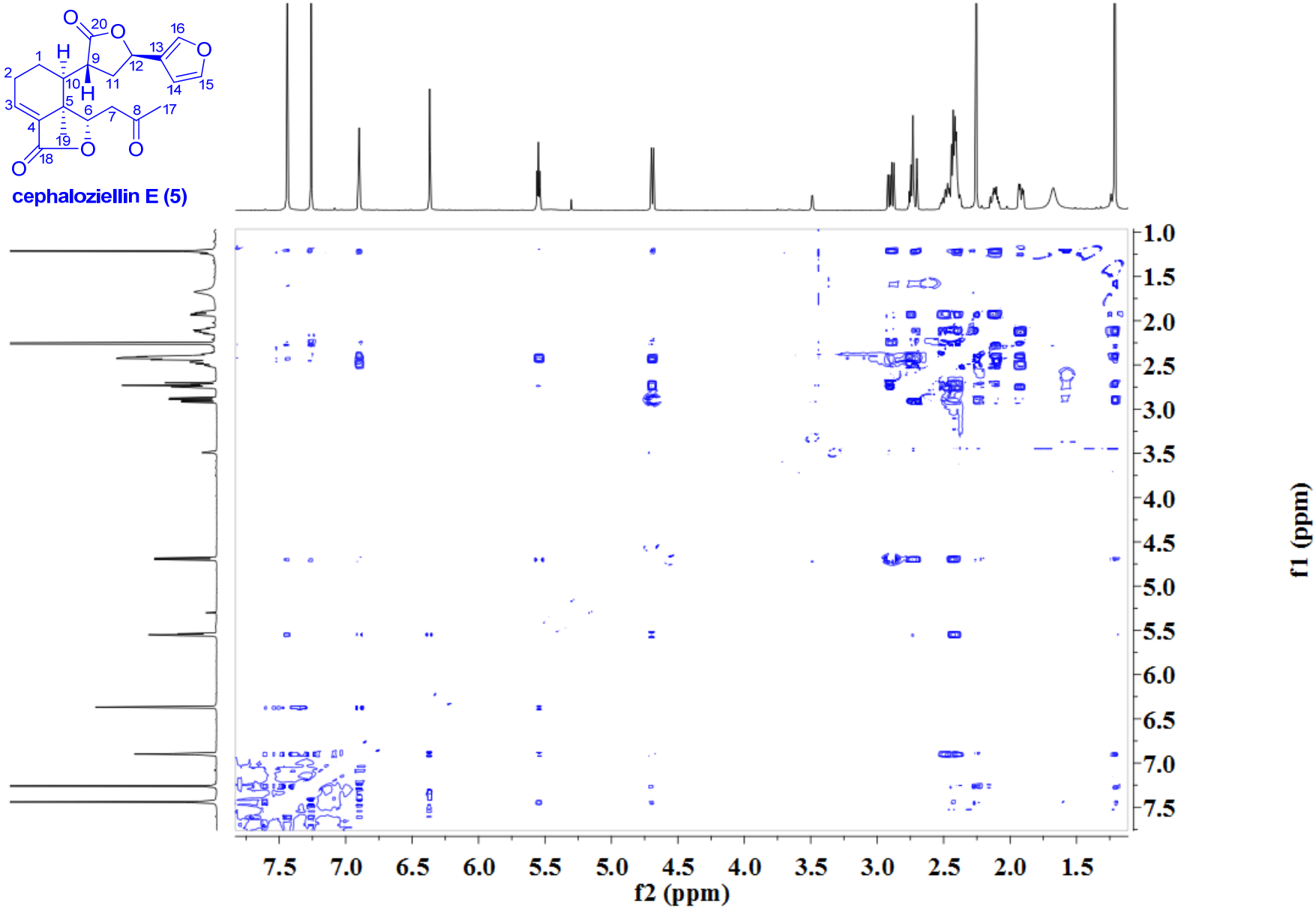
S52. HMBC spectrum (600 MHz) of cephaloziellin E (**5**) in $CDCl_3$.



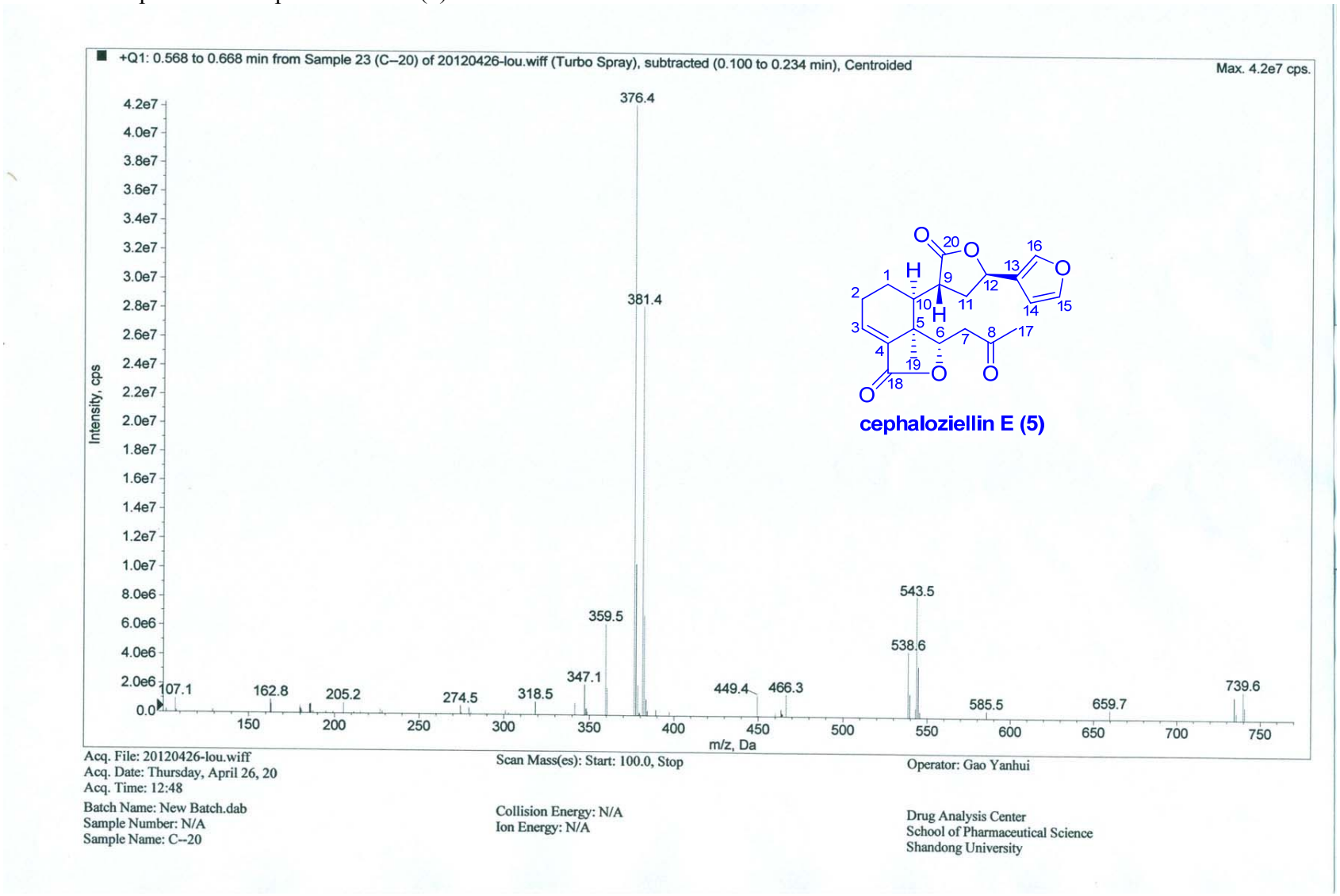
S53. ^{1}H-^{1}H COSY spectrum (600 MHz) of cephaloziellin E (**5**) in $CDCl_3$.



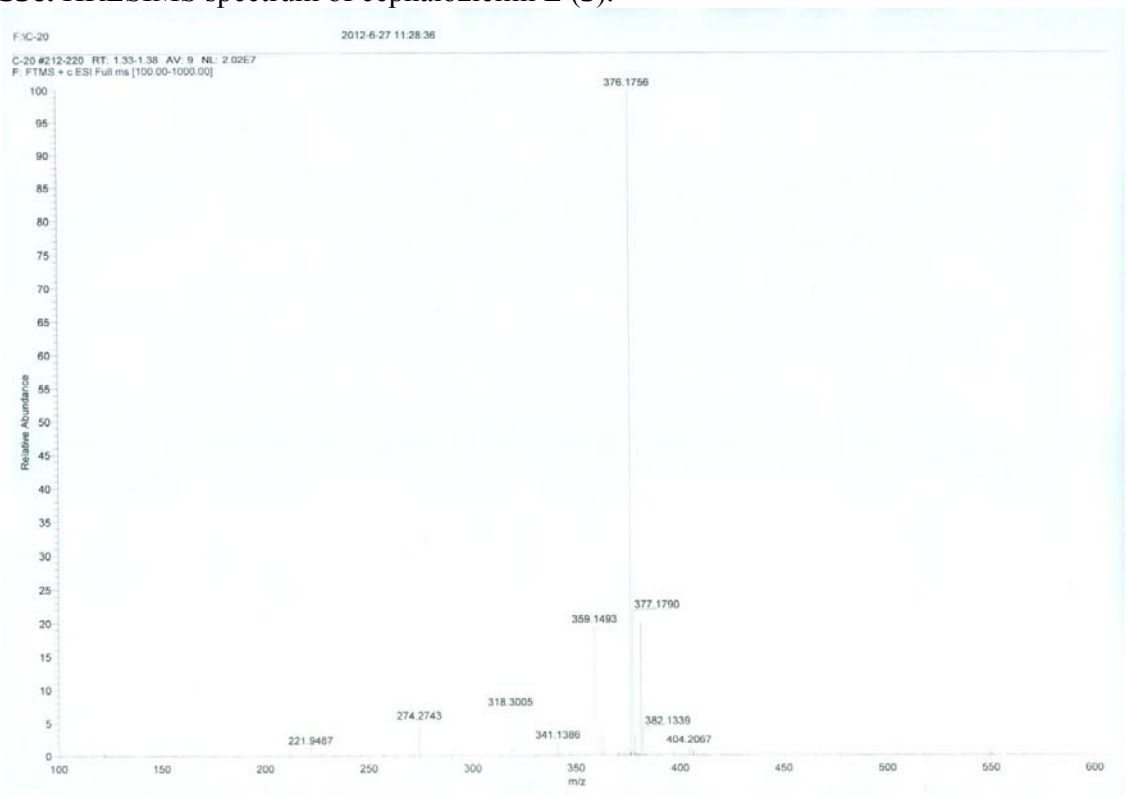
S54. NOESY spectrum (600 MHz) of cephaloziellin E (**5**) in $CDCl_3$.

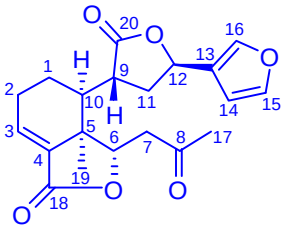


S55. ESIMS spectrum of cephaloziellin E (**5**).



S56. HRESIMS spectrum of cephaloziellin E (**5**).



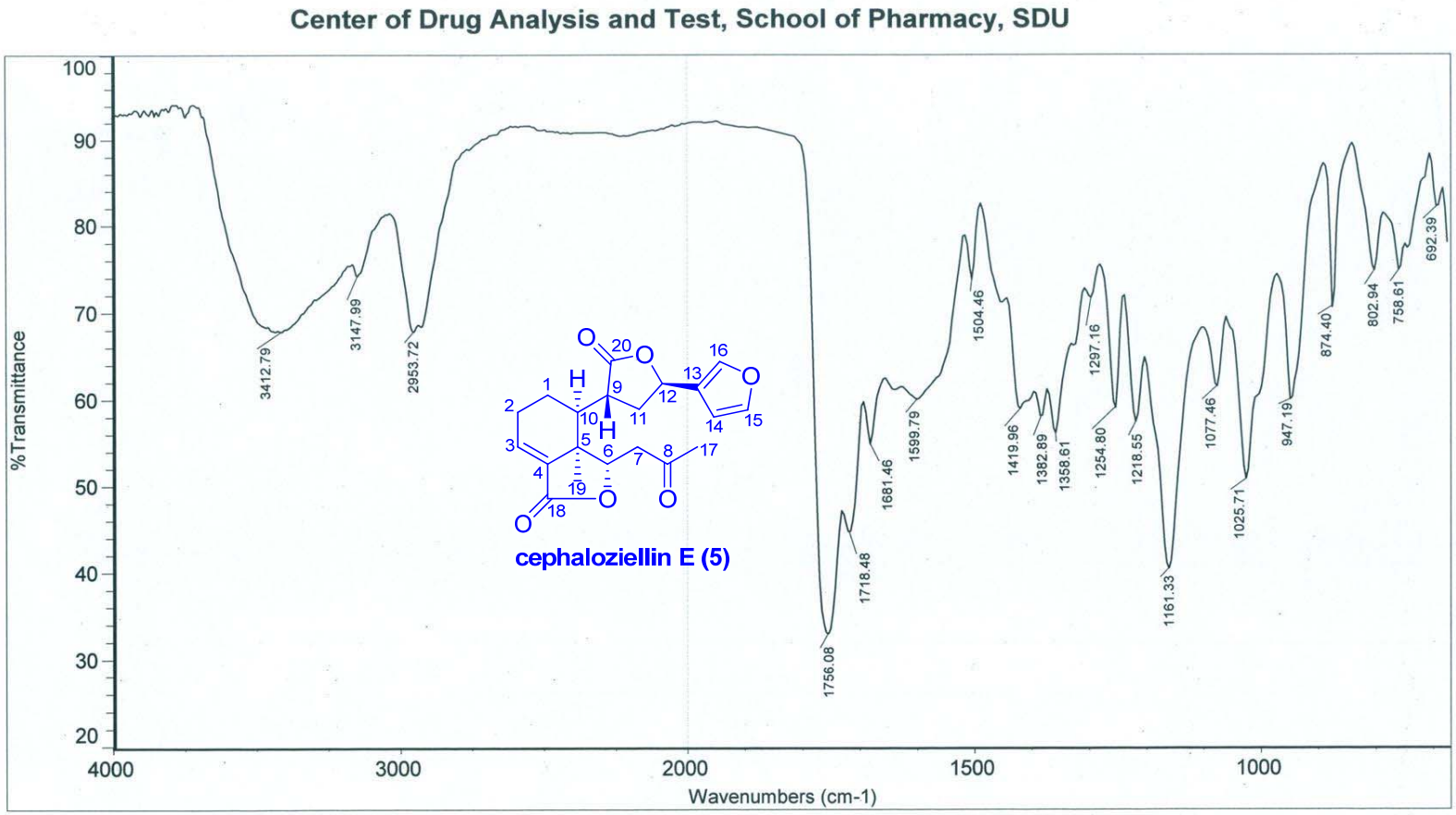


cephaloziellin E (5)

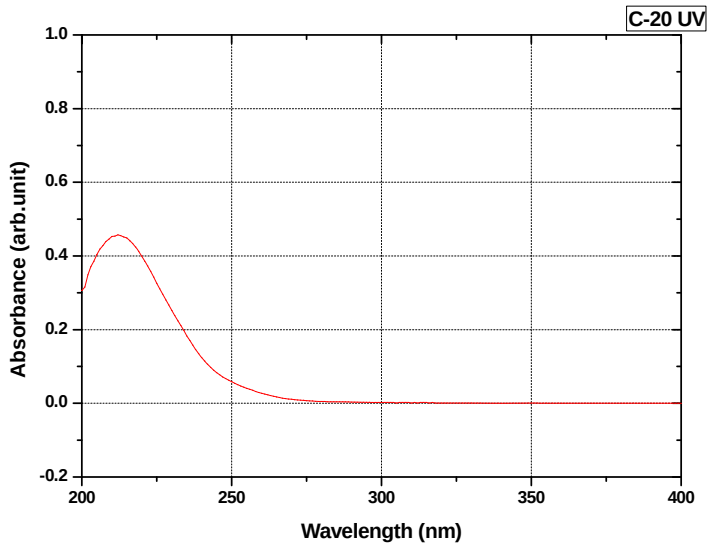
SPECTRUM - simulation :

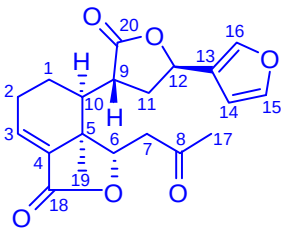
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
376.1756	376.1755	0.39	8.5	$^{12}C_{20}H_{26}O_6N$

S57. IR spectrum of cephaloziellin E (**5**).



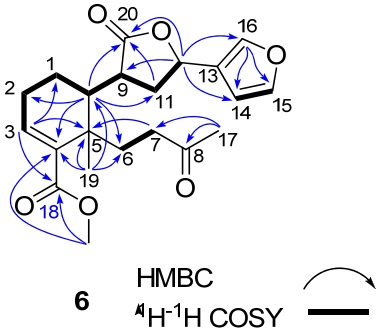
S58. UV spectra of cephaloziellin E (**5**).





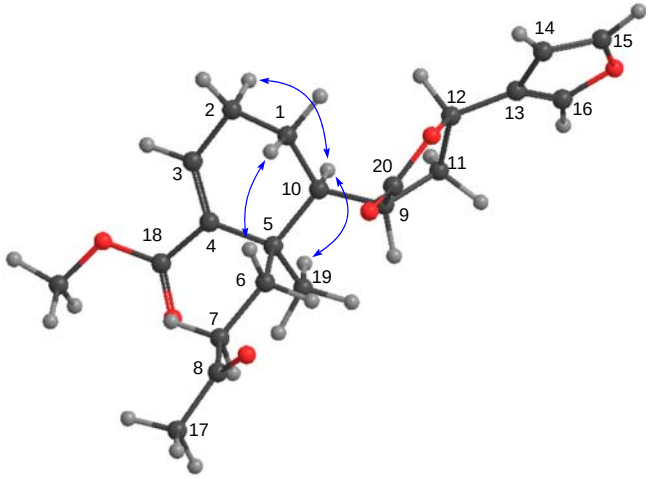
cephaloziellin E (5)

S59. Key HMBC and ^{1}H-^{1}H COSY correlations (in figure) of cephaloziellin F (**6**).



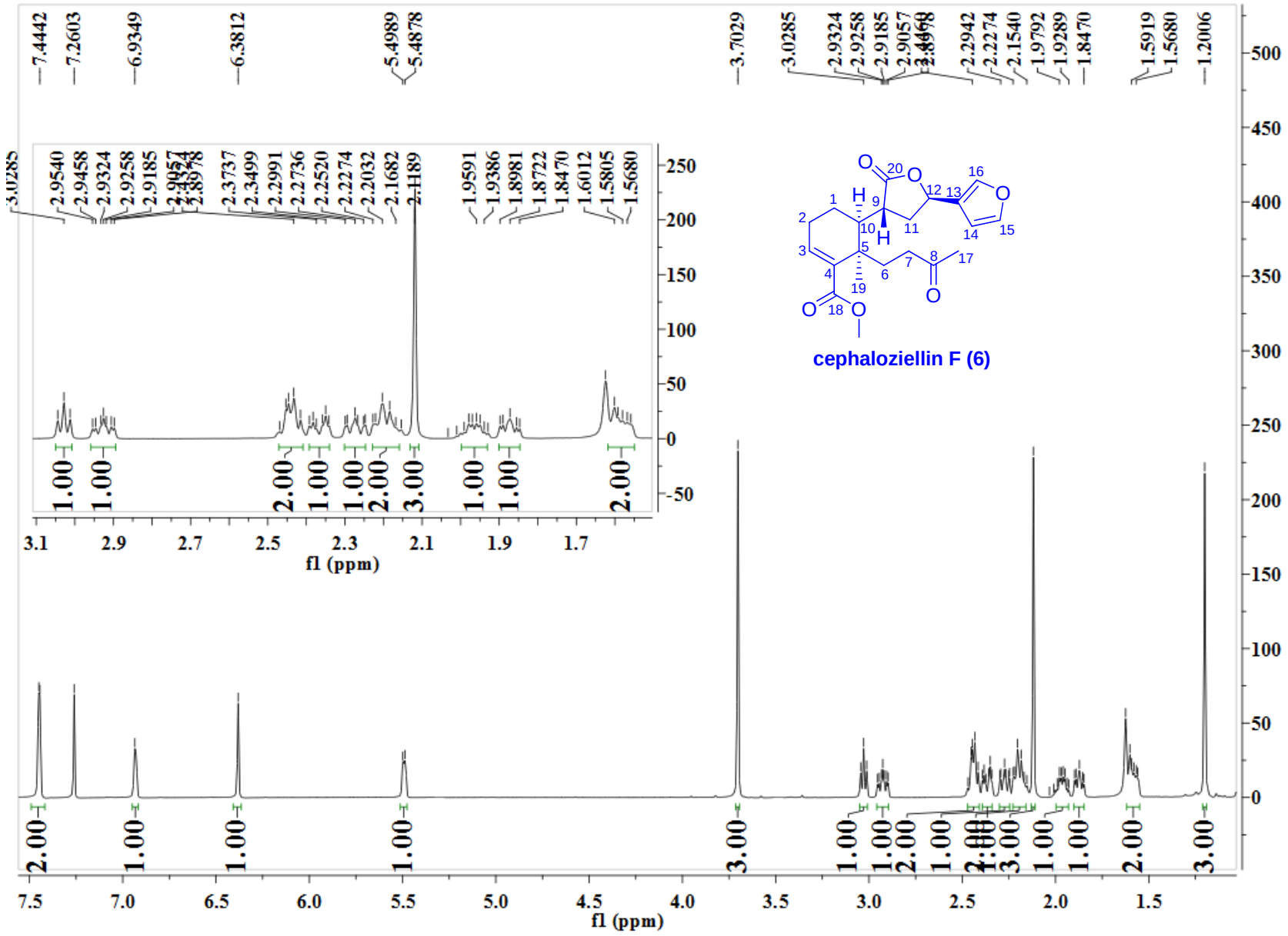
6 HMBC ^{1}H-^{1}H COSY

S60 Key NOESY correlations (in figure) of cephaloziellin F (**6**).

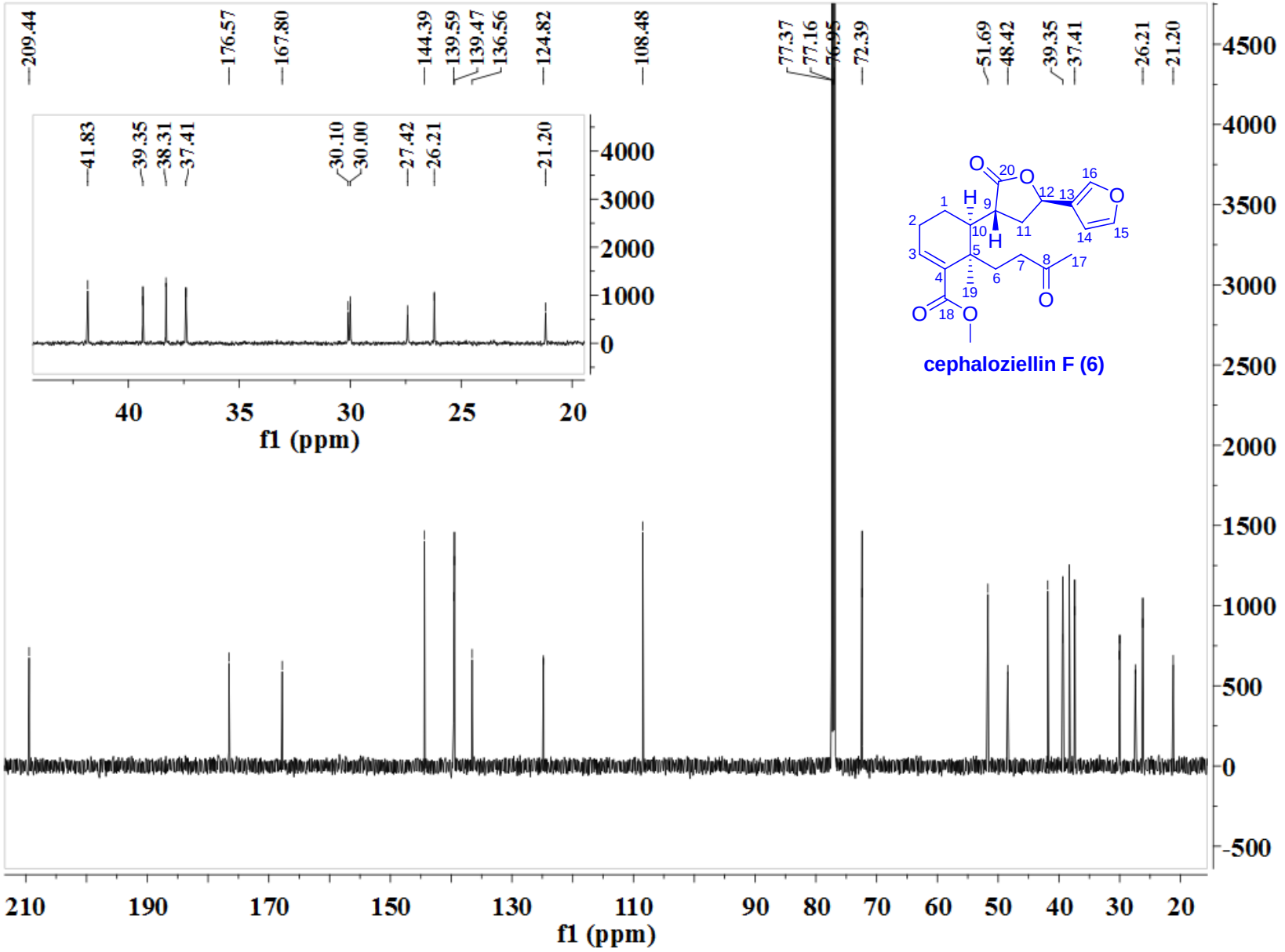


6 NOESY

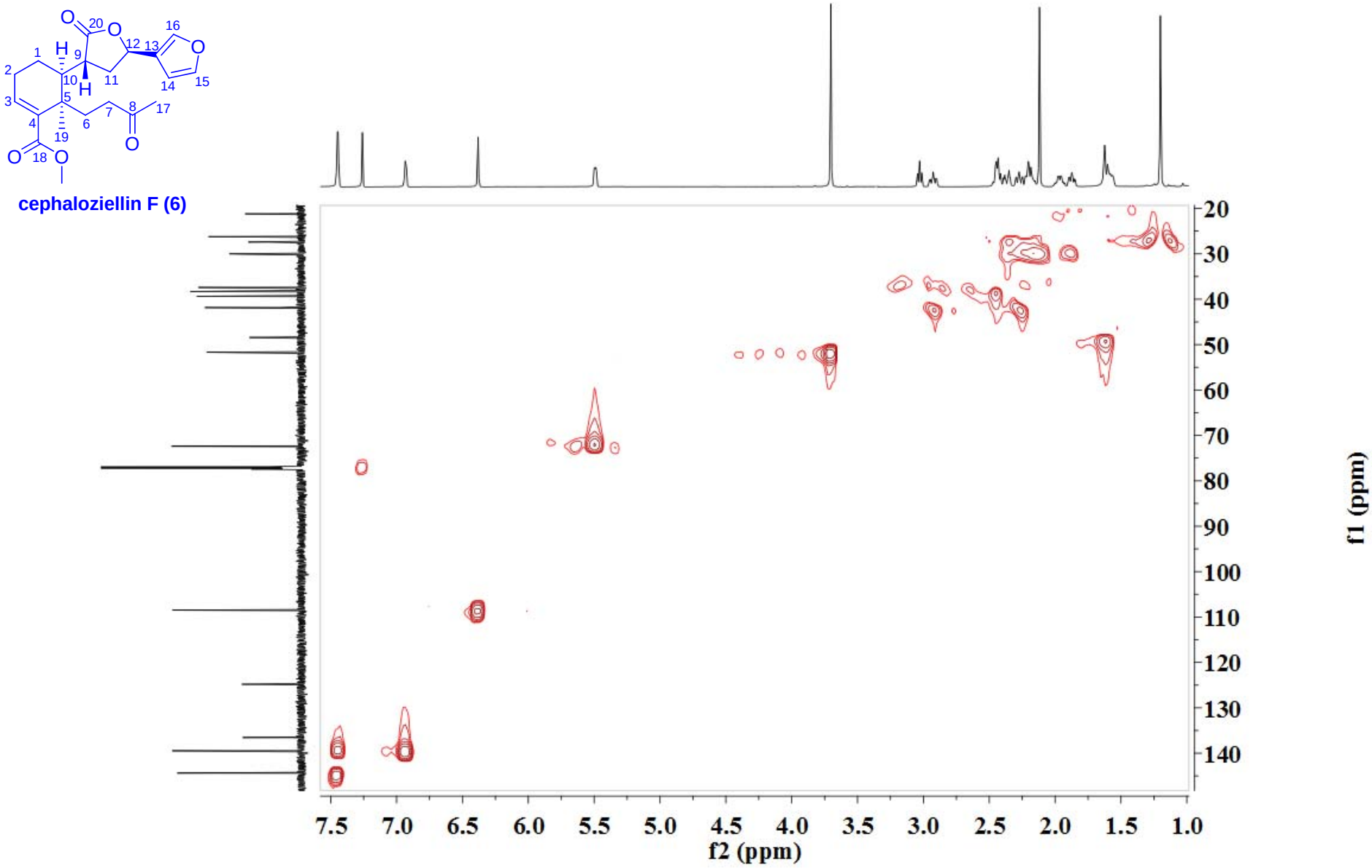
S61 ^{1}H NMR spectrum (600 MHz) of cephaloziellin F (**6**) in $CDCl_3$.



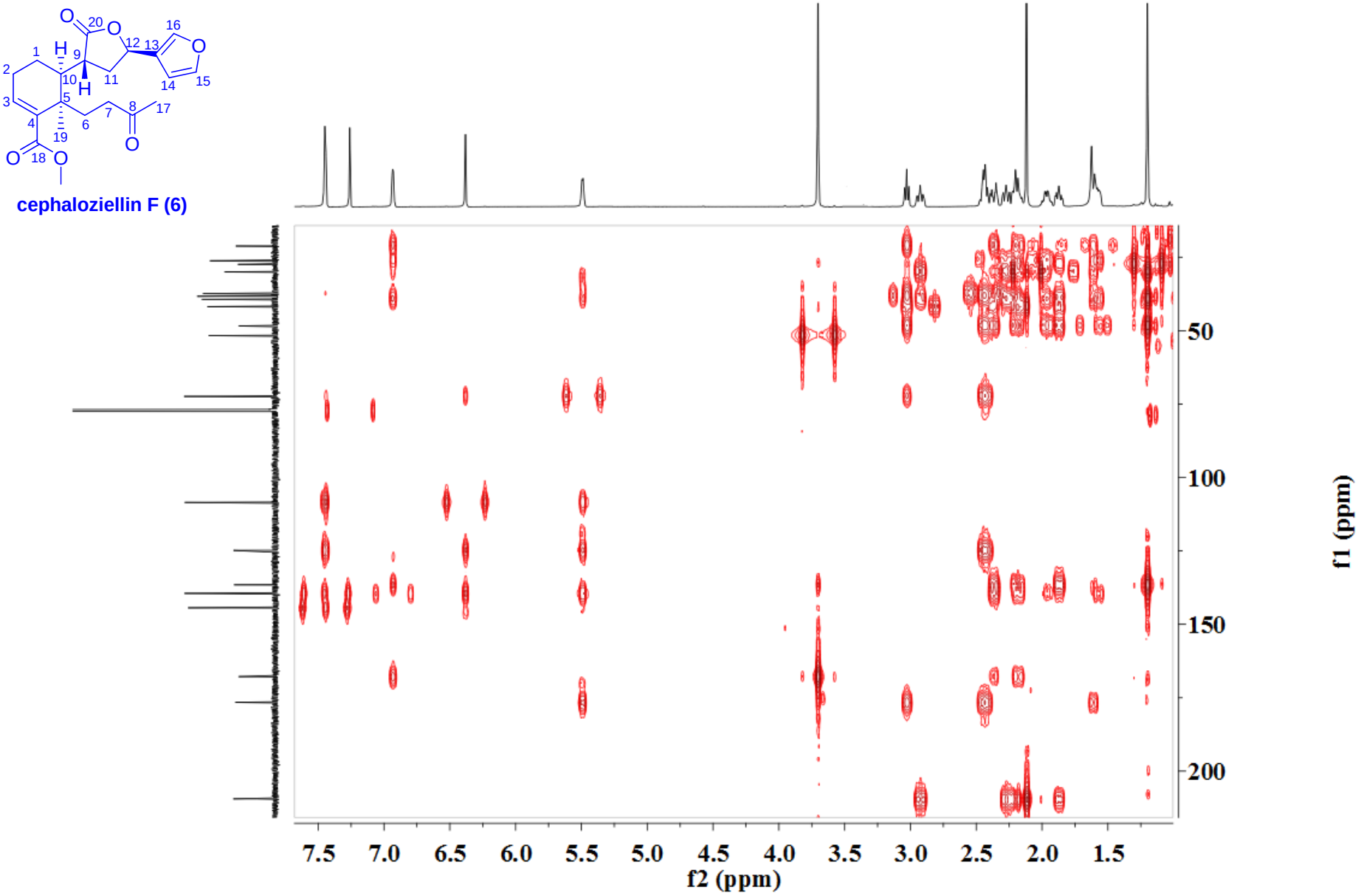
S62 ^{13}C NMR spectrum (150 MHz) of cephaloziellin F (**6**) in $CDCl_3$.



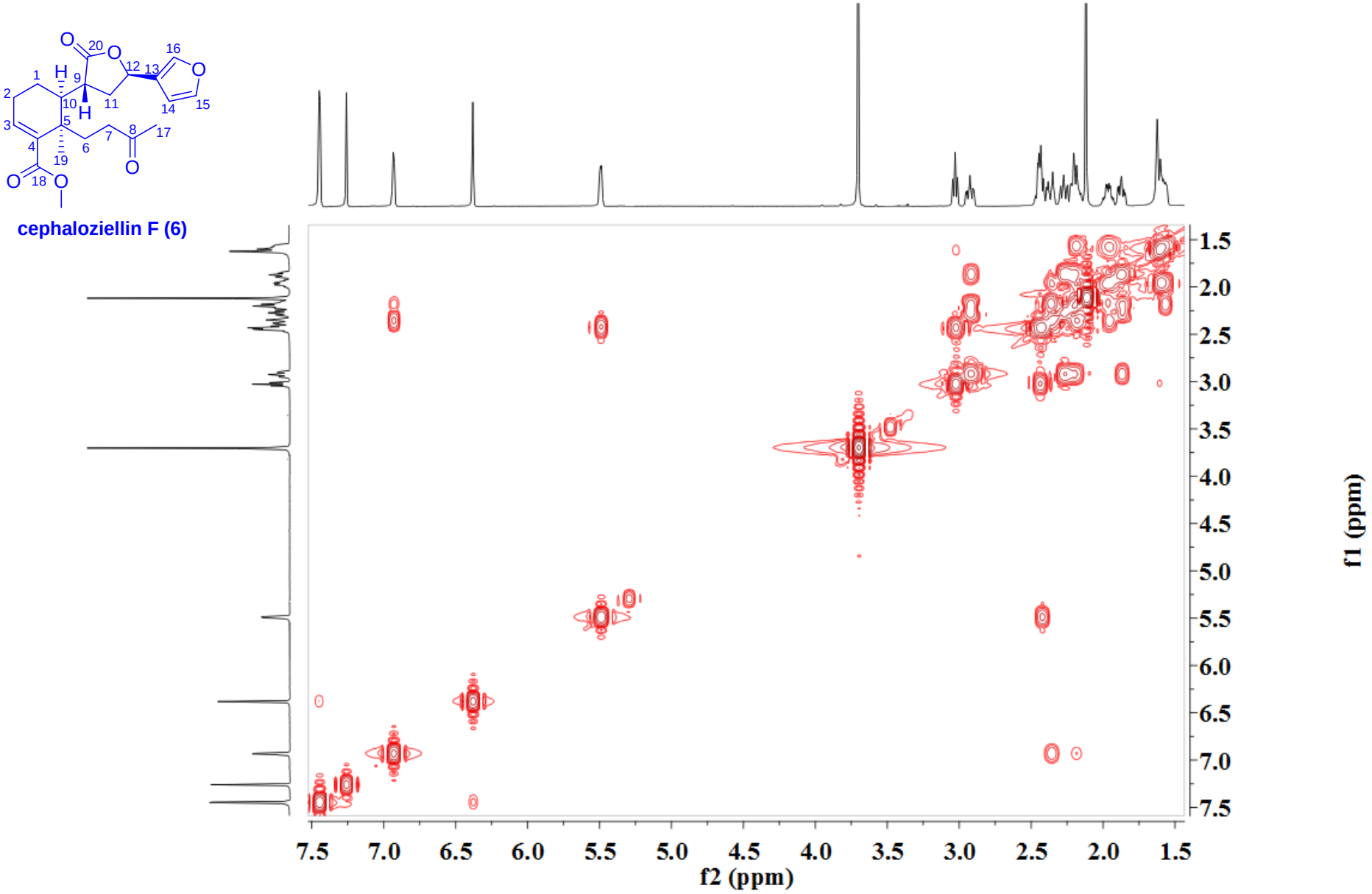
S63. HSQC spectrum (600 MHz) of cephaloziellin F (**6**) in $CDCl_3$.



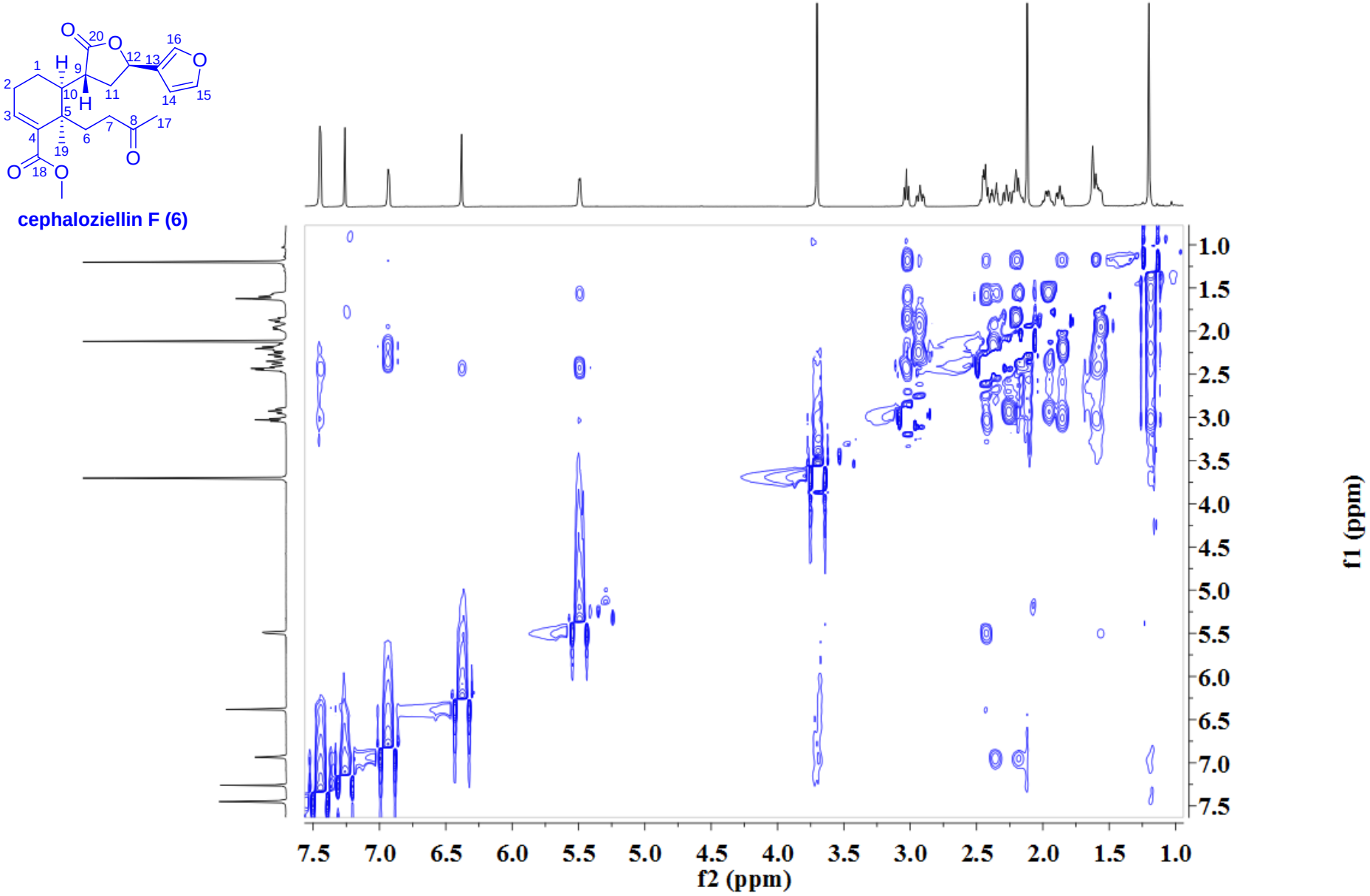
S64. HMBC spectrum (600 MHz) of cephaloziellin F (**6**) in $CDCl_3$.



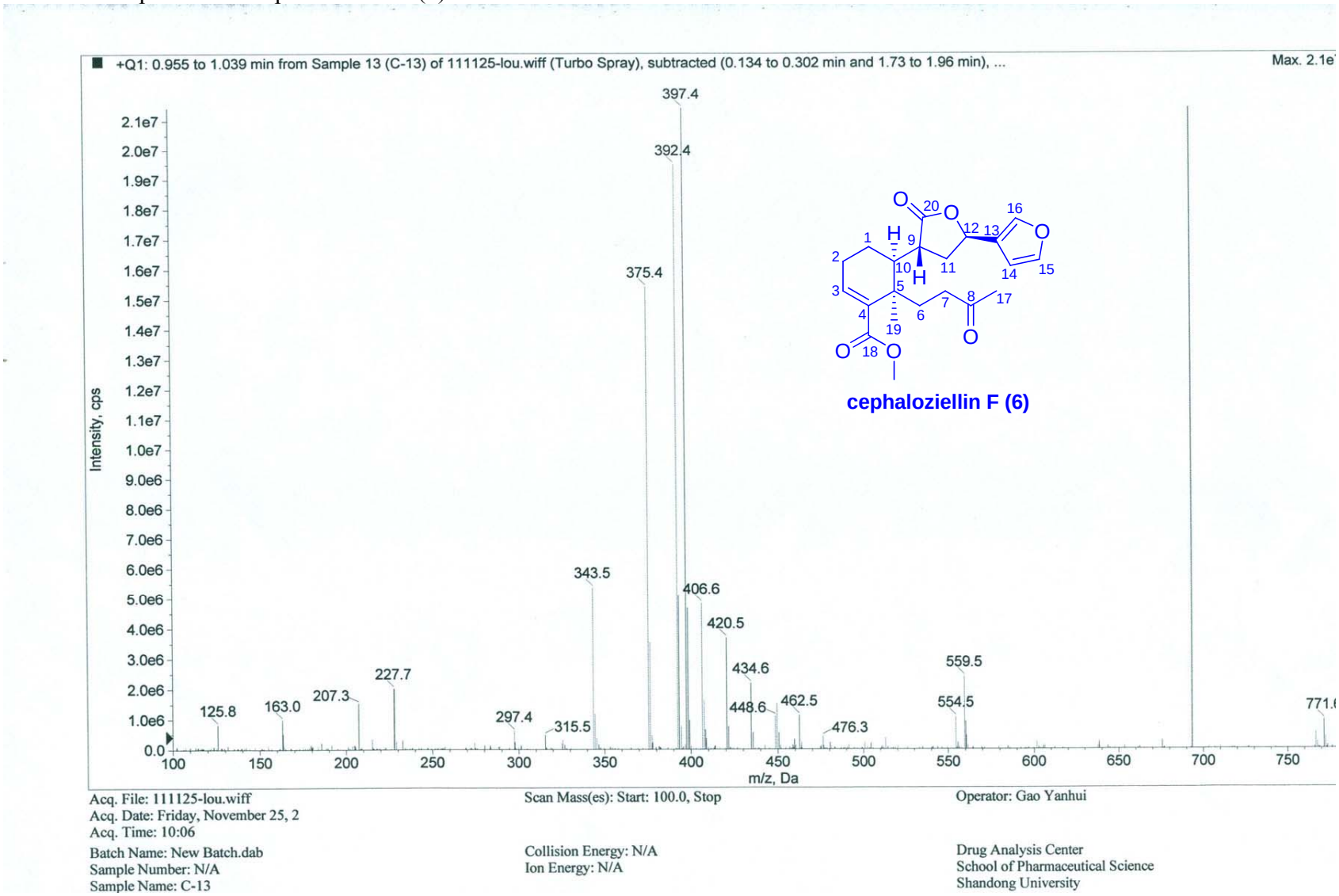
S65. ^{1}H-^{1}H COSY spectrum (600 MHz) of cephaloziellin F (**6**) in $CDCl_3$.



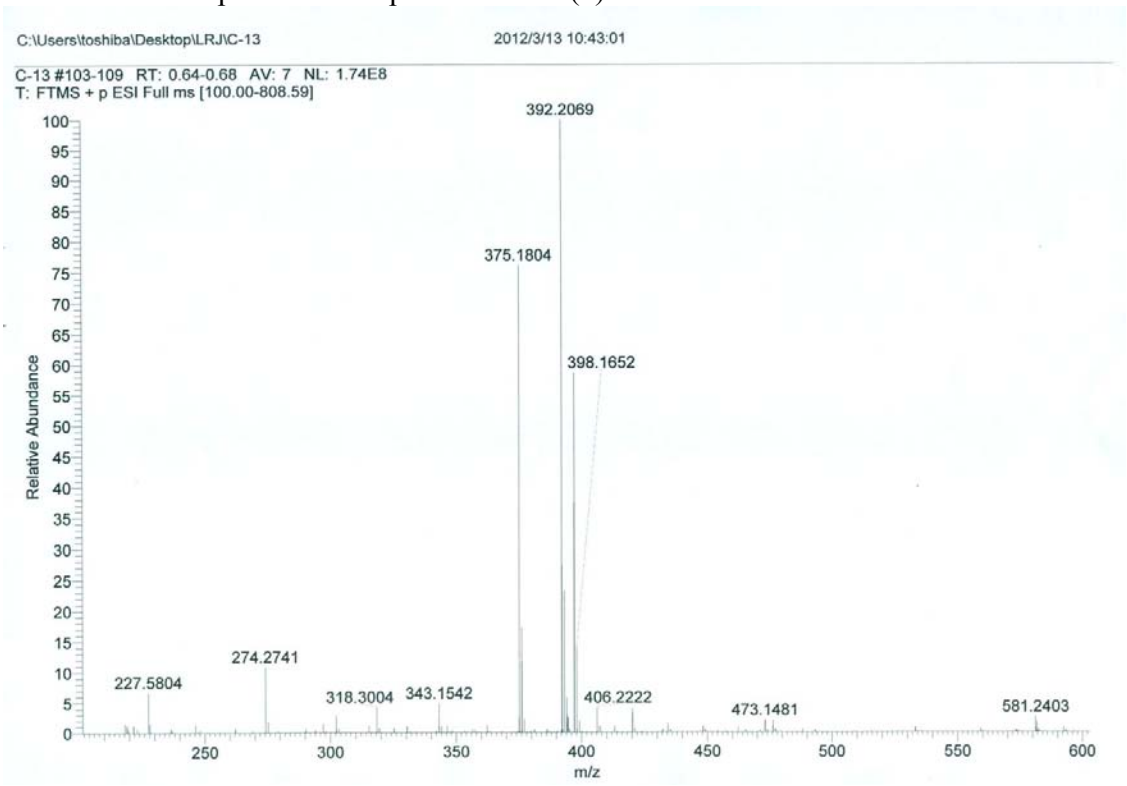
S66. NOESY spectrum (600 MHz) of cephaloziellin F (**6**) in $CDCl_3$.

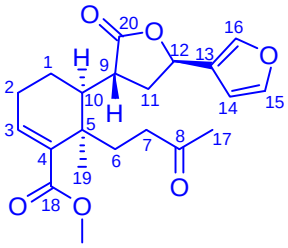


S67. ESIMS spectrum of cephaloziellin F (**6**).



S68. HRESIMS spectrum of cephaloziellin F (**6**).



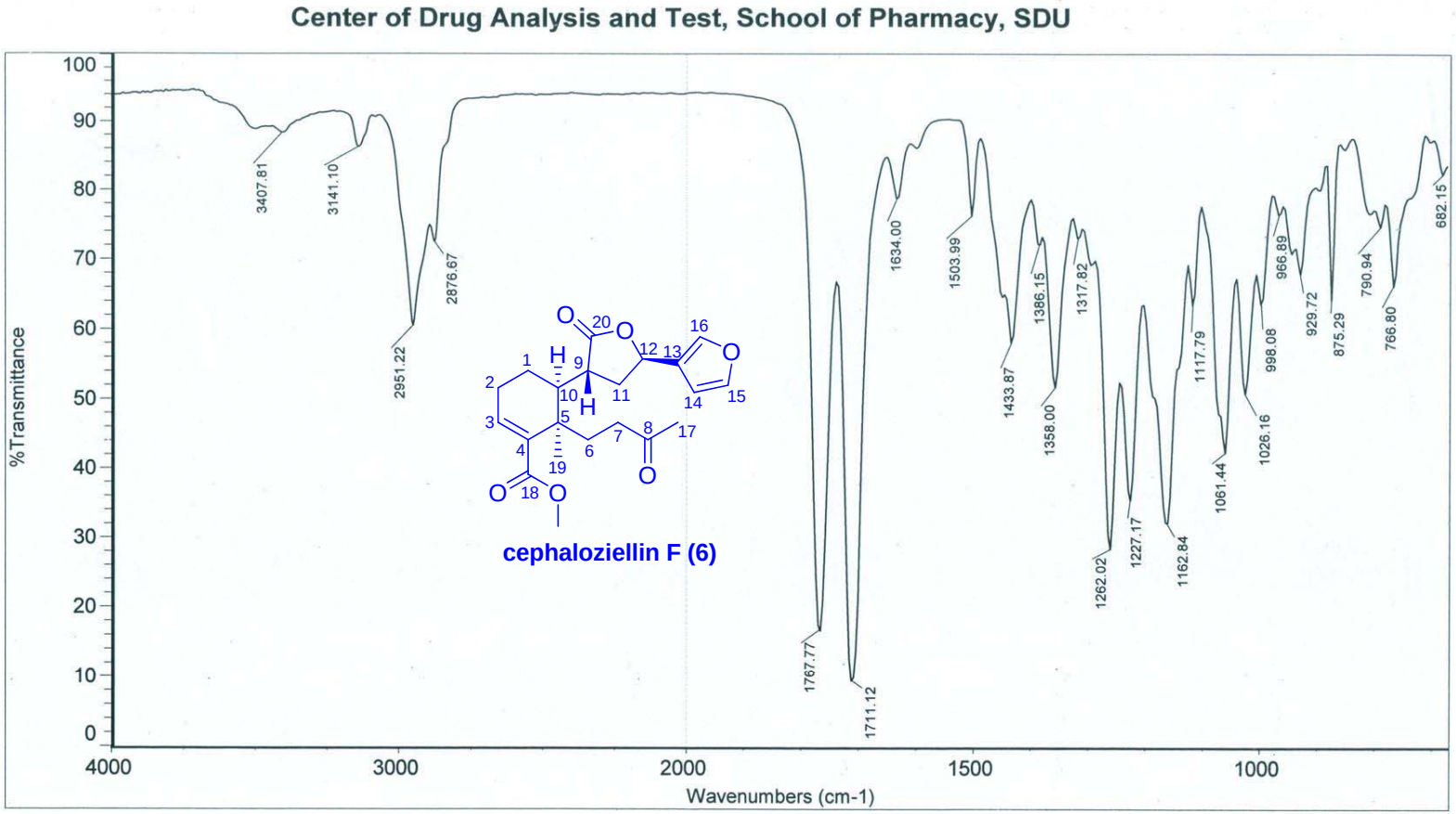


cephaloziellin F (6)

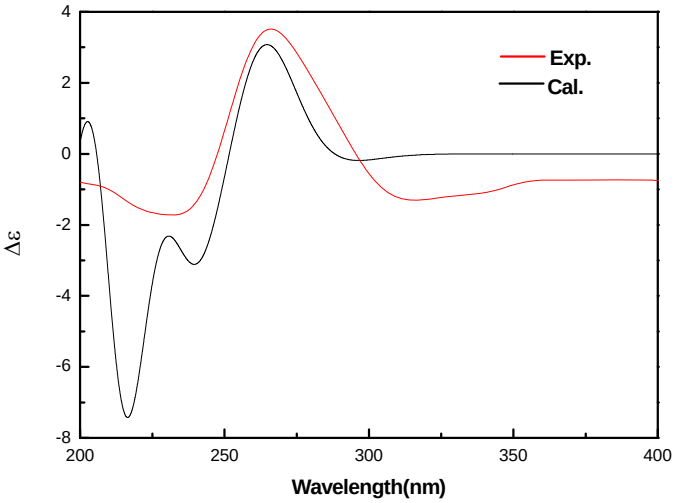
SPECTRUM - simulation :

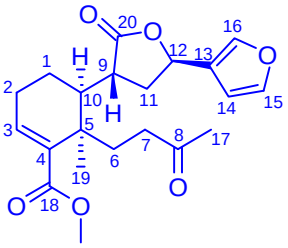
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
375.1804	375.1802	0.55	8.5	$^{12}C_{21}H_{27}O_6$

S69. IR spectrum of cephaloziellin F (**6**).

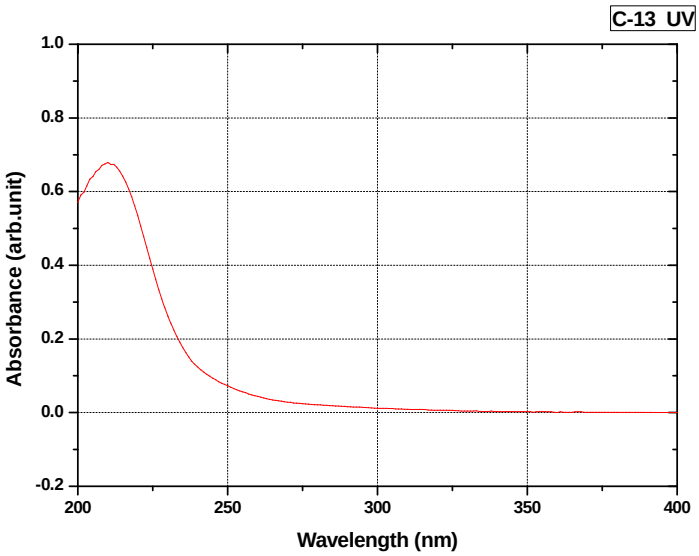


S70. Experimental ECD and calculated ECD, and UV spectra of cephaloziellin F (**6**).

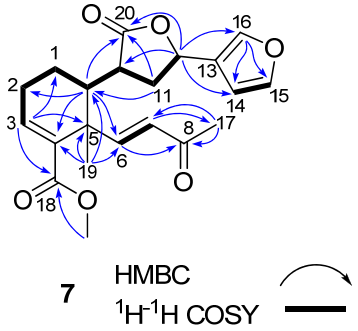




cephaloziellin F (6)

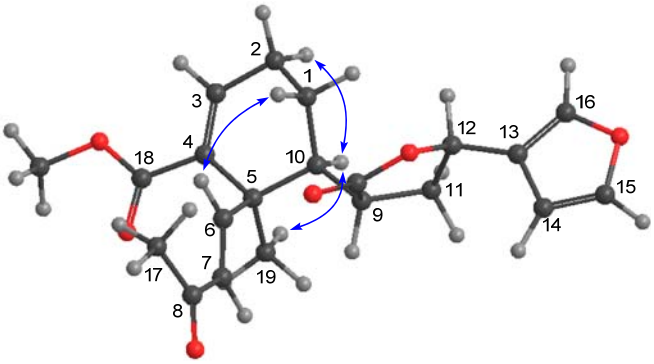


S71. Key HMBC and ^{1}H-^{1}H COSY correlations (in figure) of cephaloziellin G (**7**).



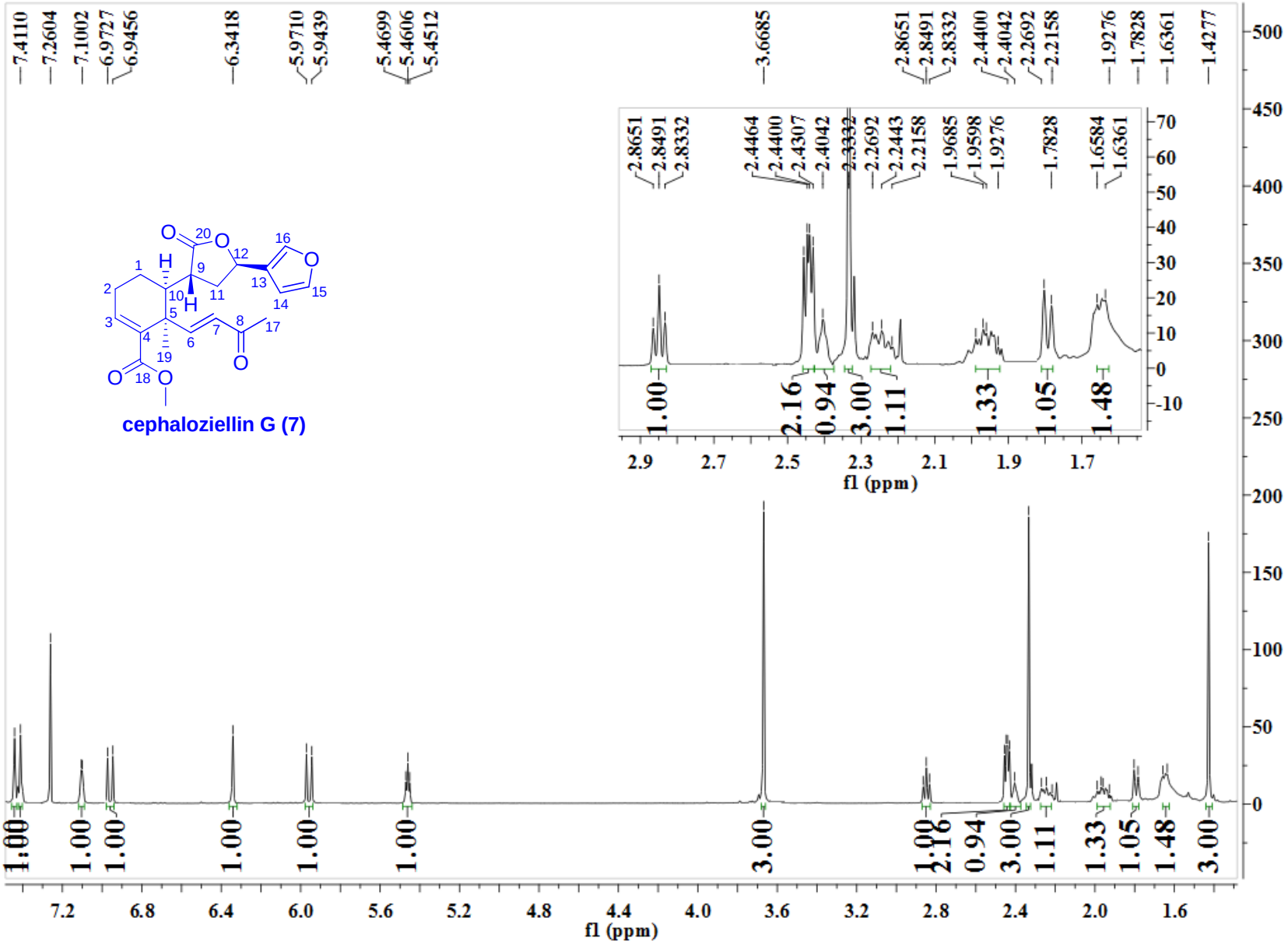
7 HMBC
^{1}H-^{1}H COSY

S72. Key NOESY correlations (in figure) of cephaloziellin G (**7**).

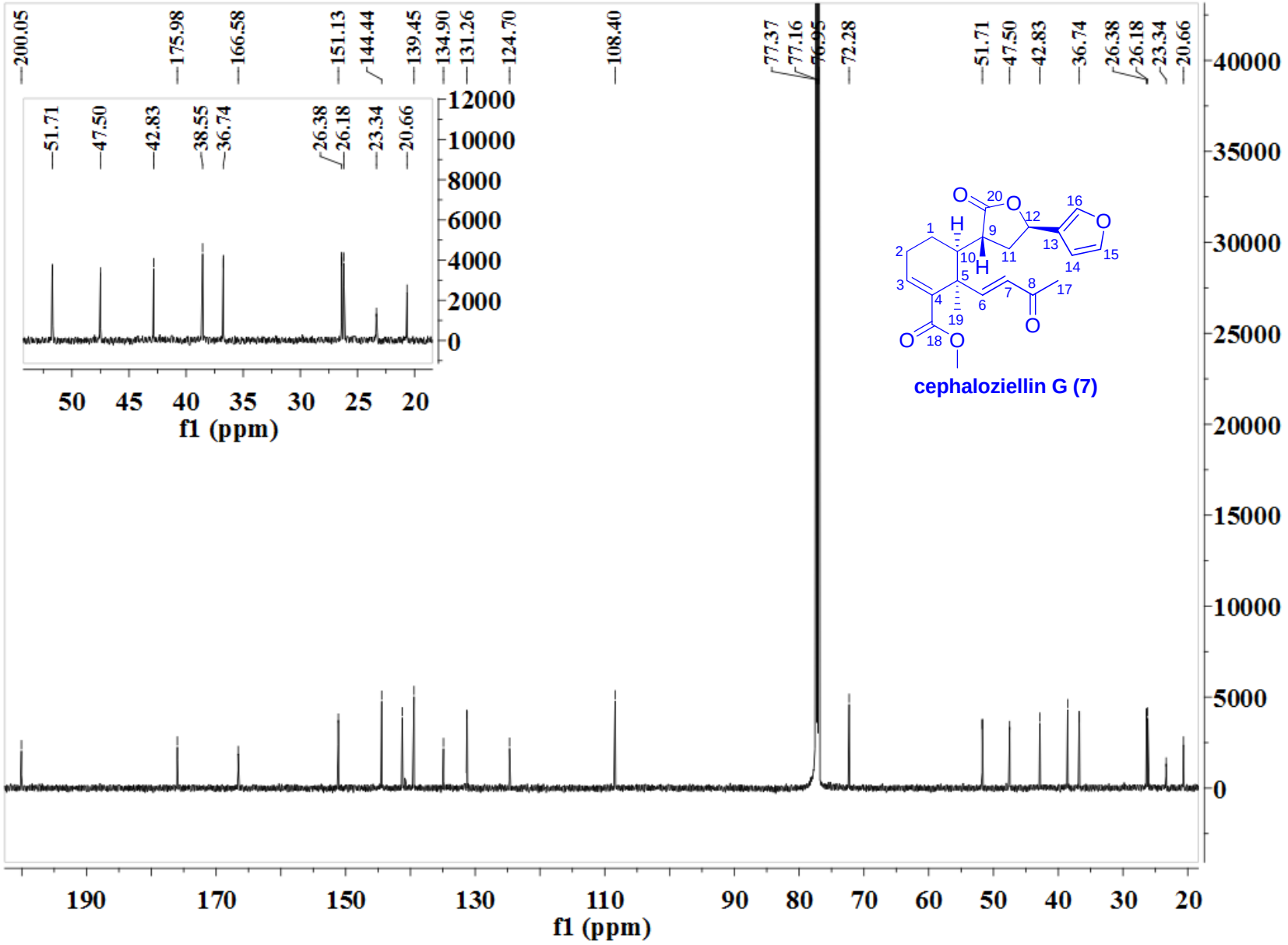


7 NOESY

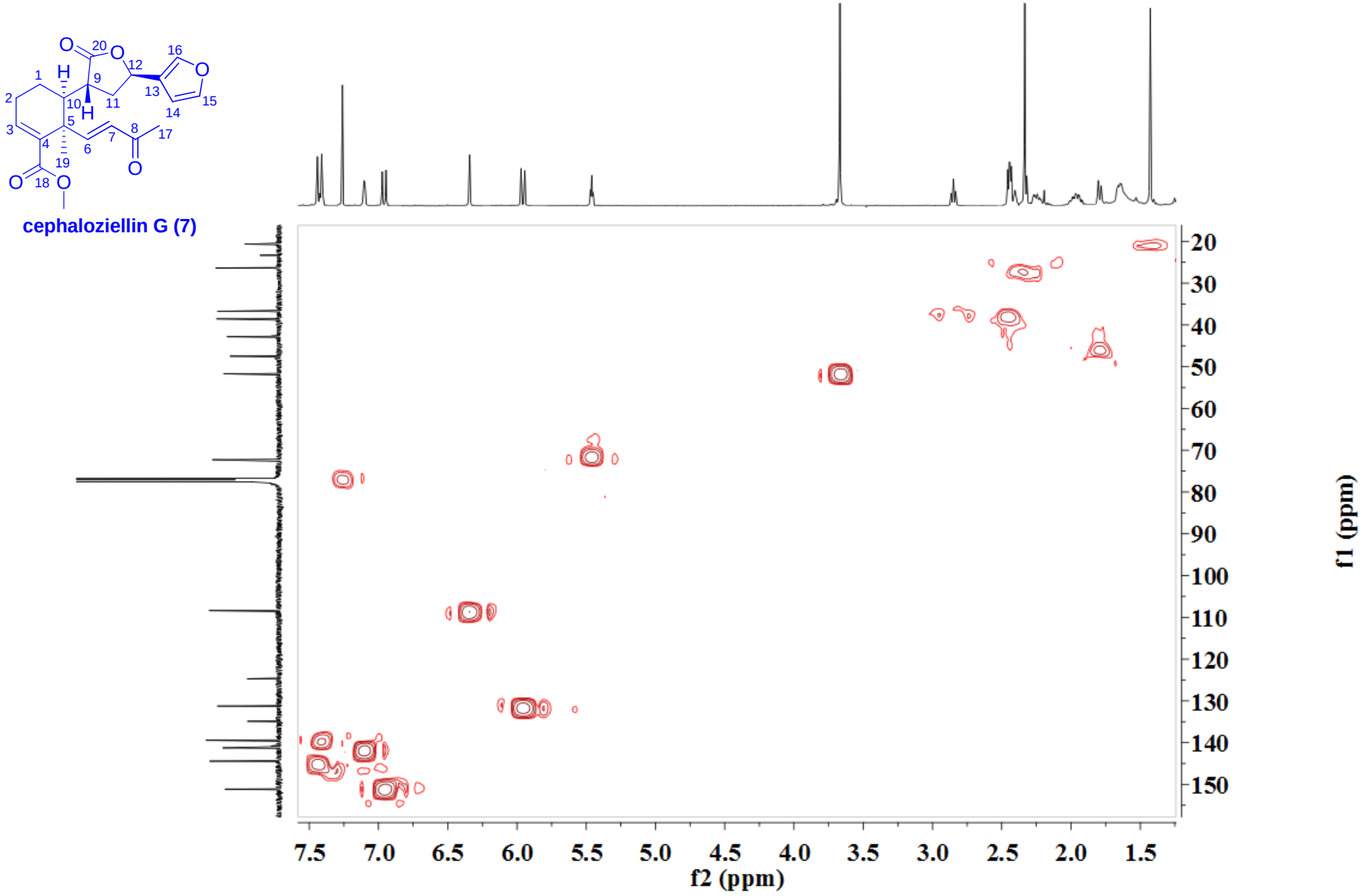
S73 ^{1}H NMR spectrum (600 MHz) of cephaloziellin G (**7**) in $CDCl_3$.



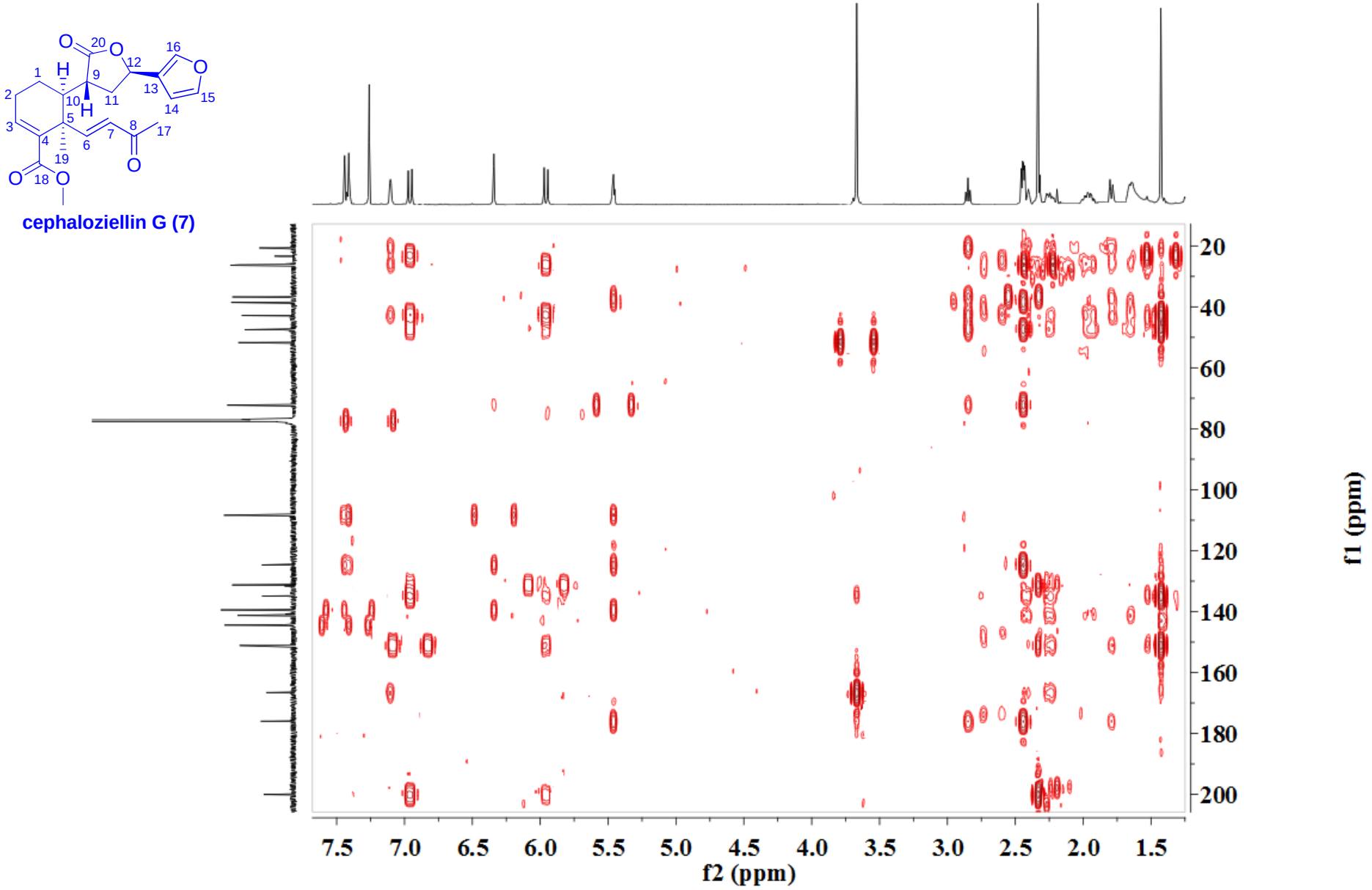
S74. ^{13}C NMR spectrum (150 MHz) of cephaloziellin G (**7**) in $CDCl_3$.



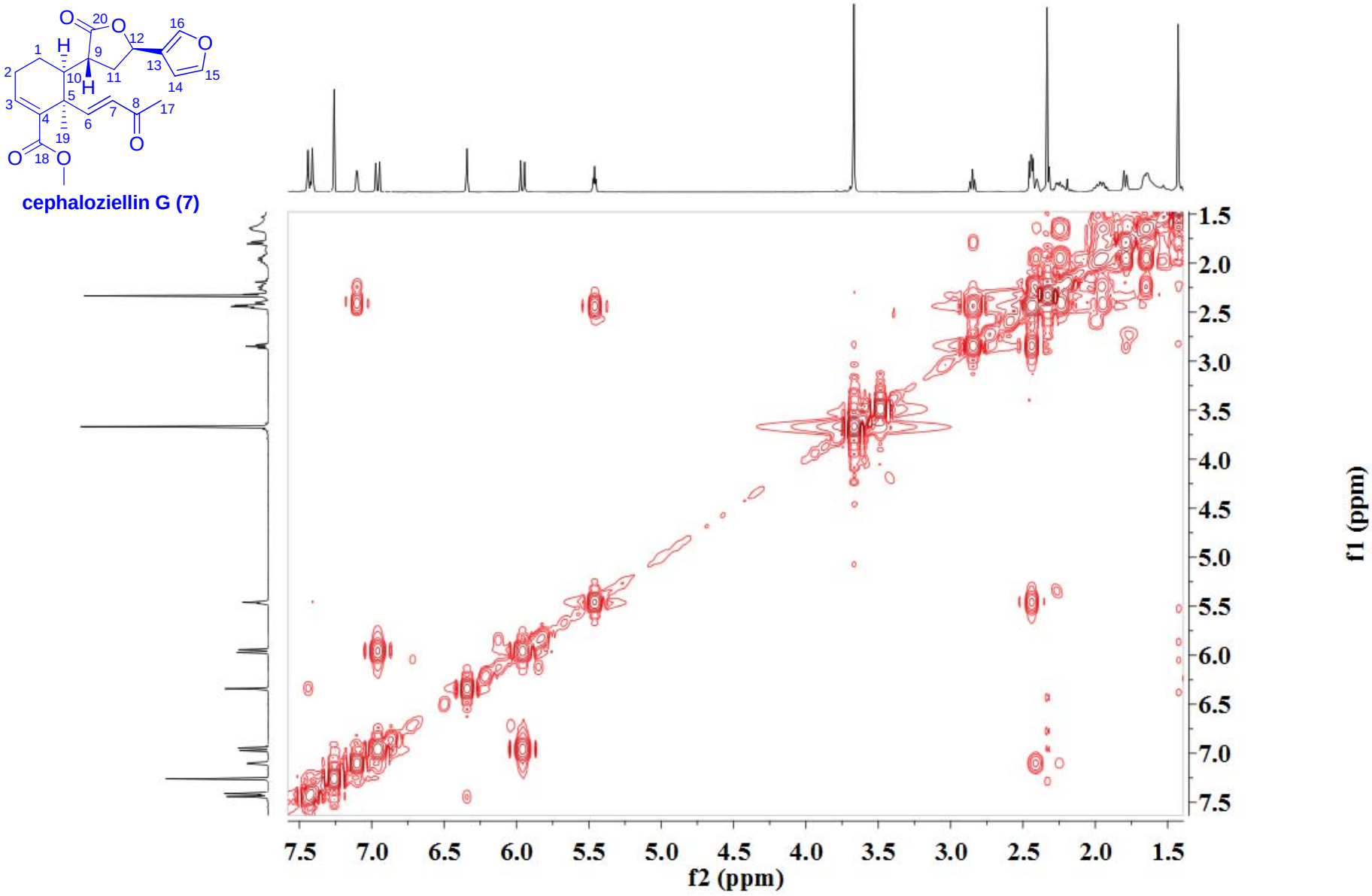
S75. HSQC spectrum (600 MHz) of cephaloziellin G (**7**) in $CDCl_3$.



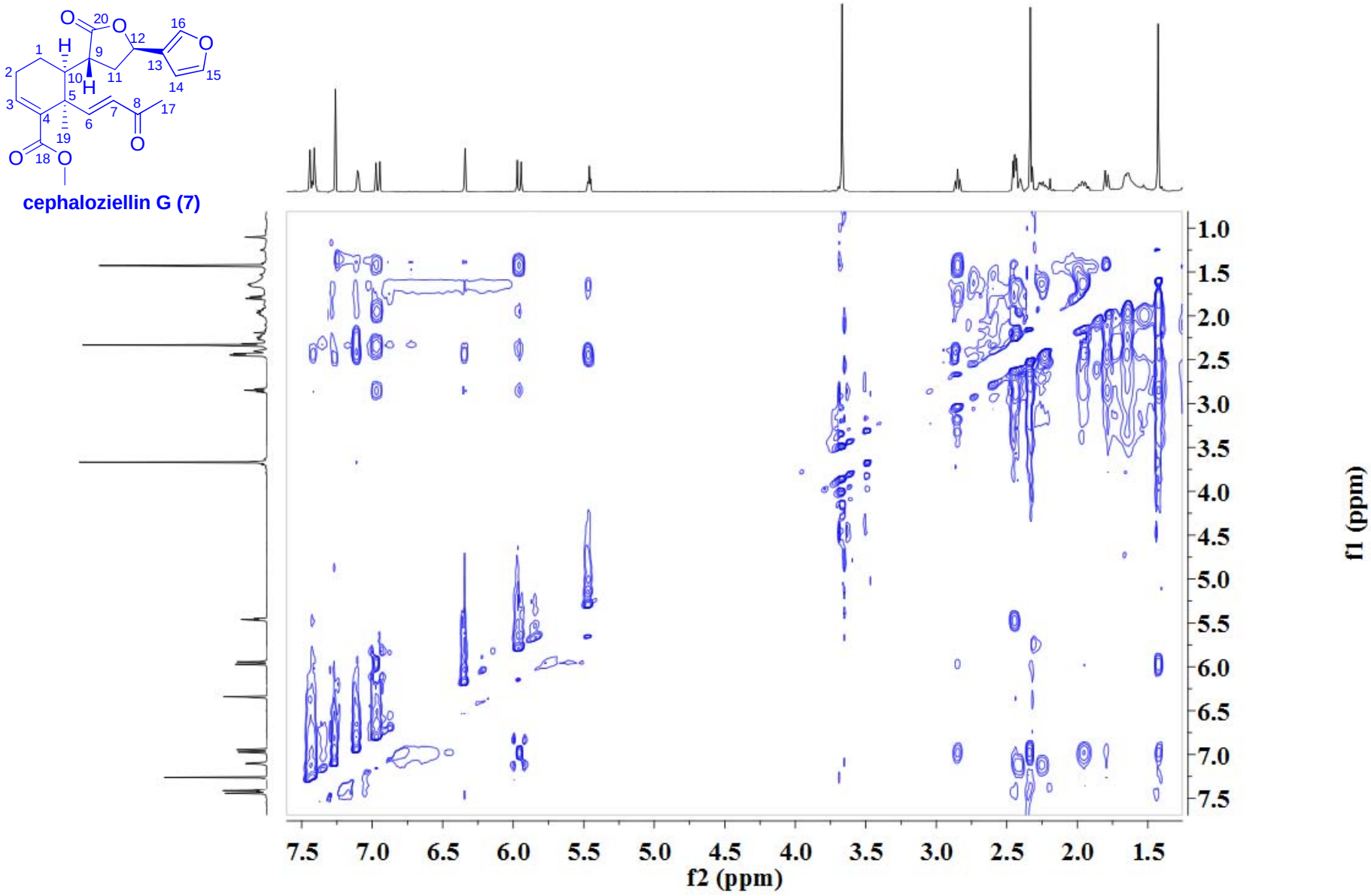
S76. HMBC spectrum (600 MHz) of cephaloziellin G (**7**) in $CDCl_3$.



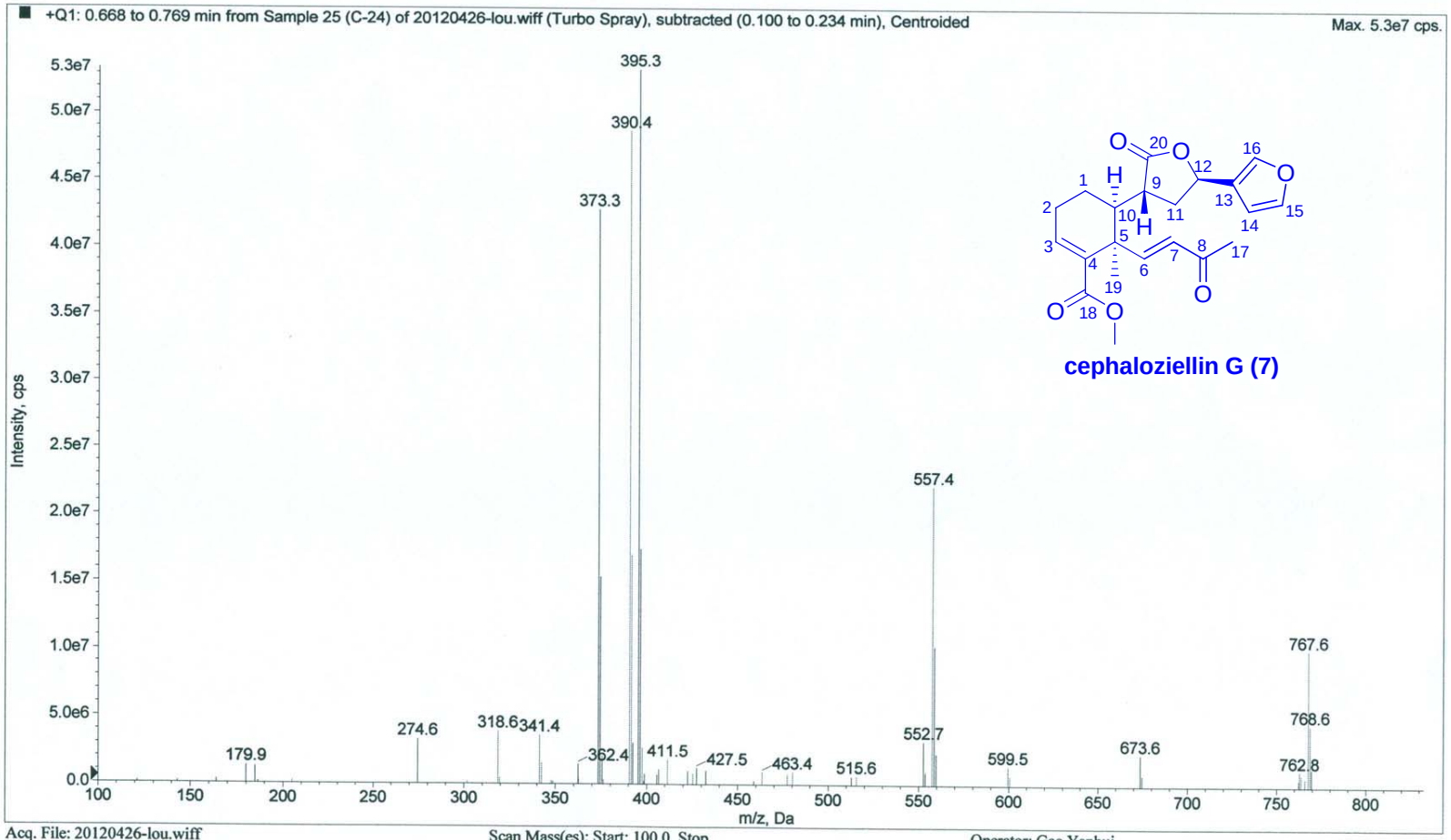
S77. ^{1}H-^{1}H COSY spectrum (600 MHz) of cephaloziellin G (**7**) in $CDCl_3$.



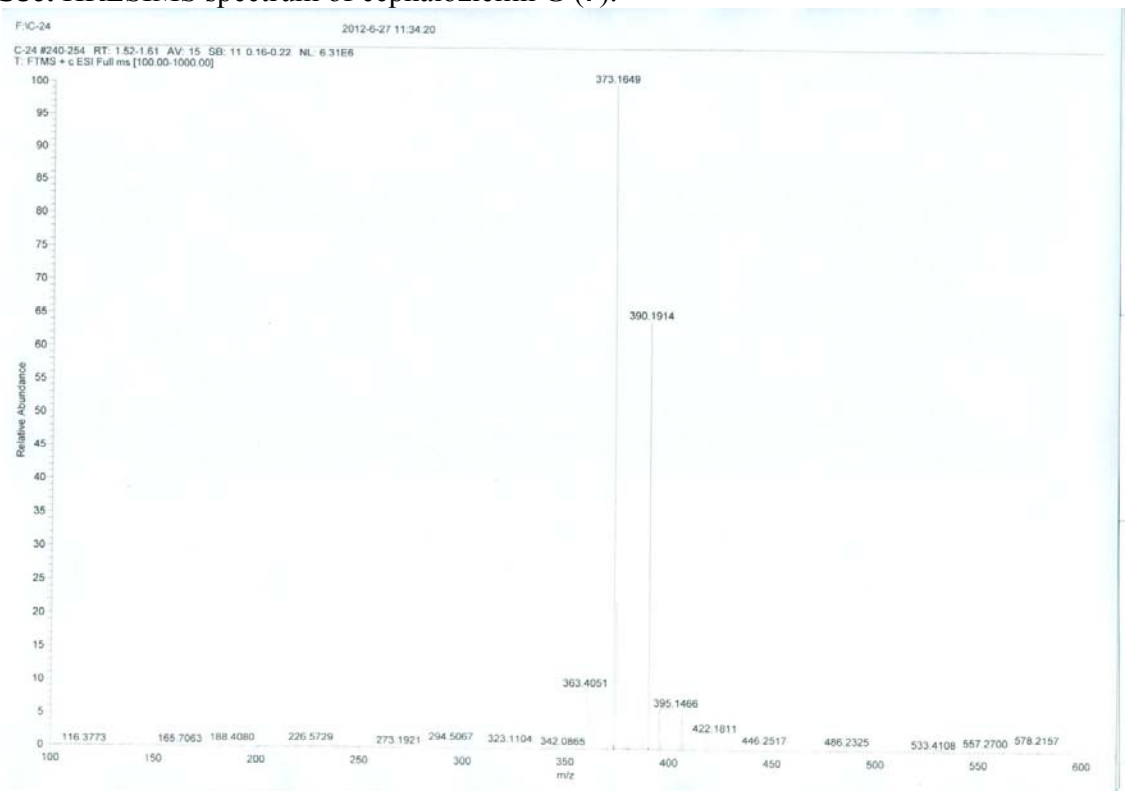
S78. NOESY spectrum (600 MHz) of cephaloziellin G (**7**) in $CDCl_3$.

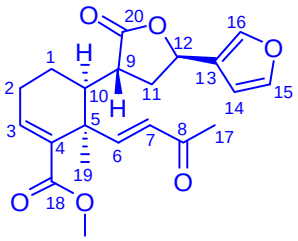


S79. ESIMS spectrum of cephaloziellin G (**7**).



S80. HRESIMS spectrum of cephaloziellin G (**7**).



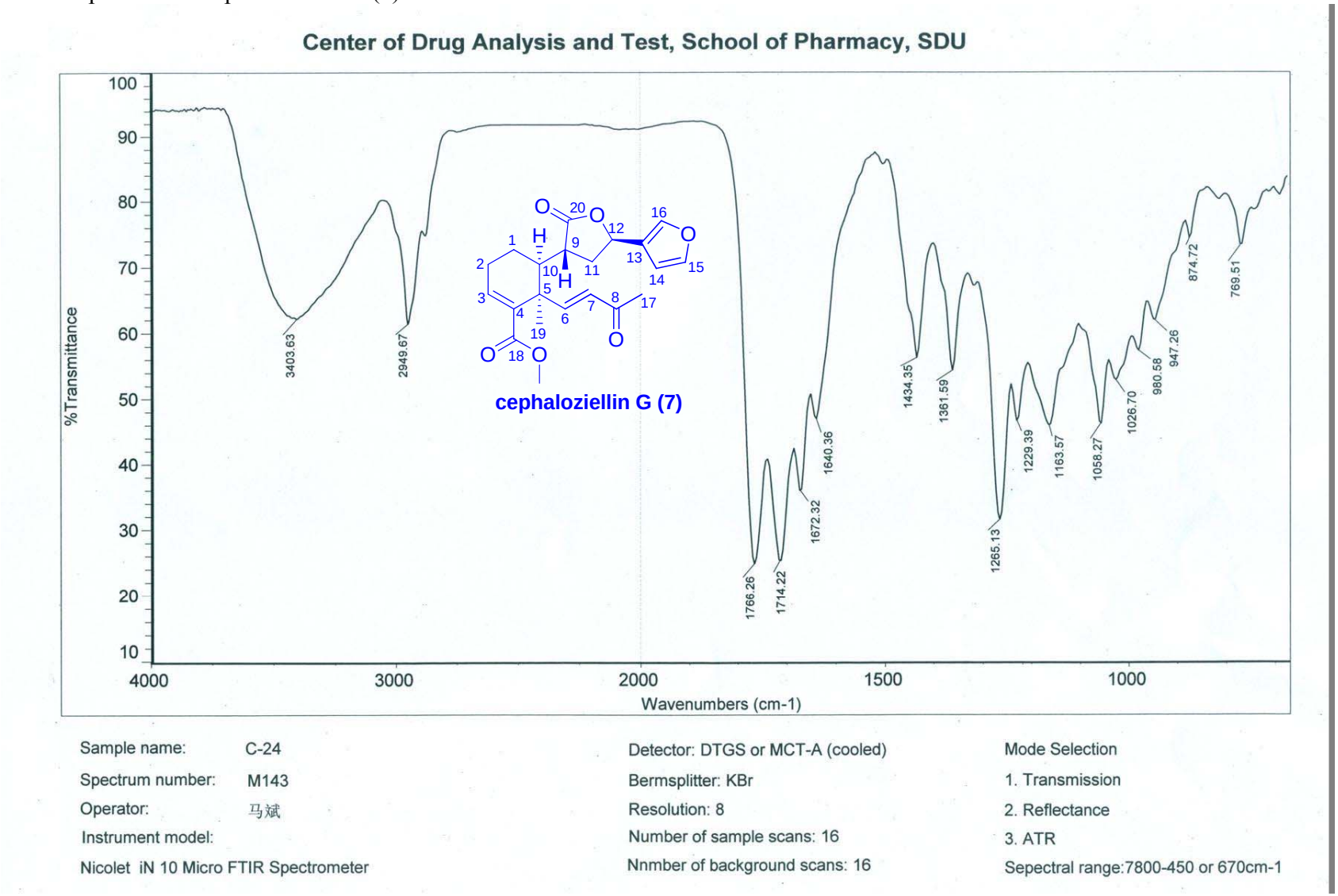


cephaloziellin G (7)

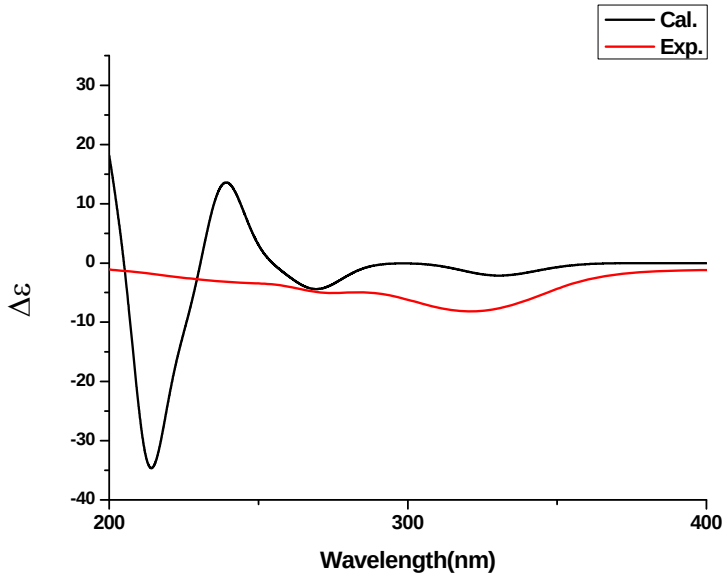
SPECTRUM - simulation :

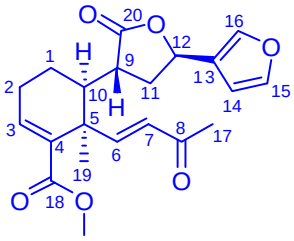
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
373.1649	373.1646	1.01	9.5	$^{12}C_{21}H_{25}O_6$

S81. IR spectrum of cephaloziellin G (**7**).

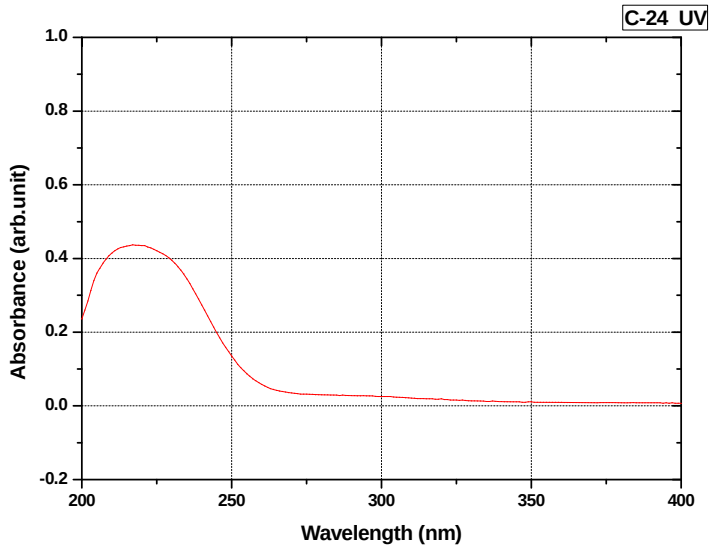


S82. Experimental ECD and calculated ECD, and UV spectra of cephaloziellin G (**7**).

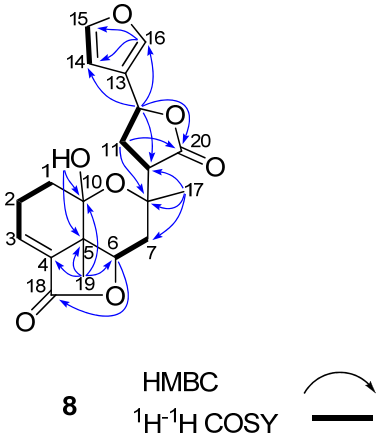




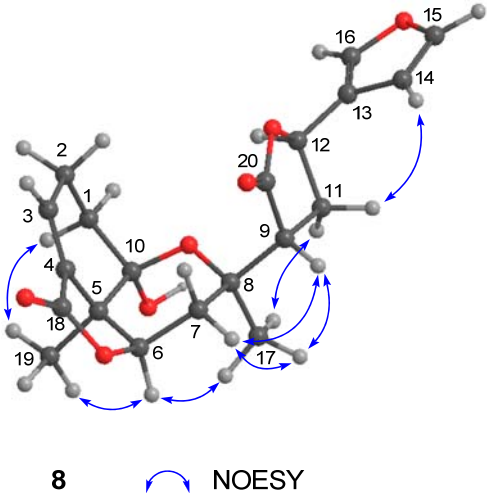
cephaloziellin G (7)



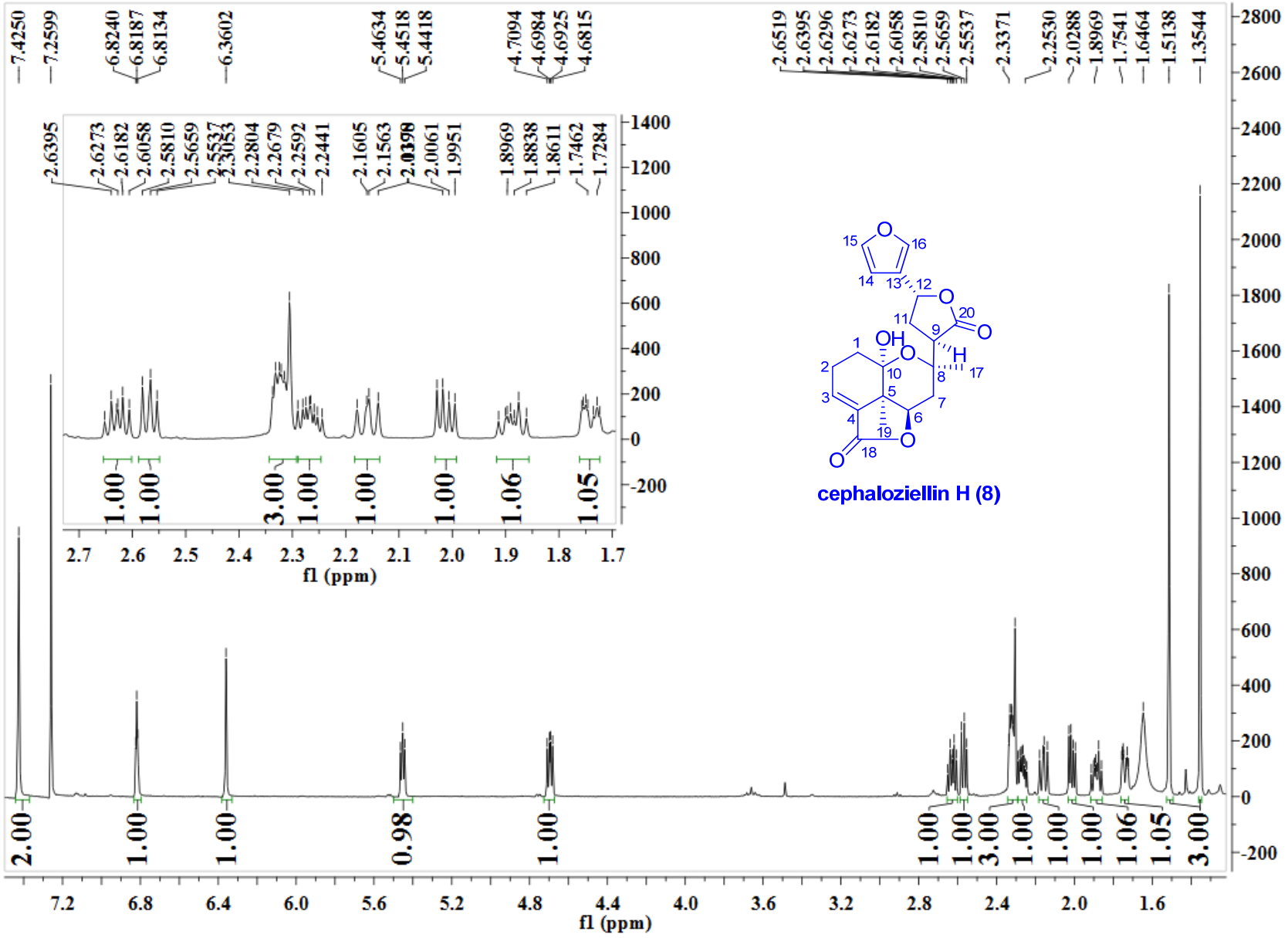
S83. Key HMBC and ^{1}H-^{1}H COSY correlations (in figure) of cephaloziellin H (**8**).



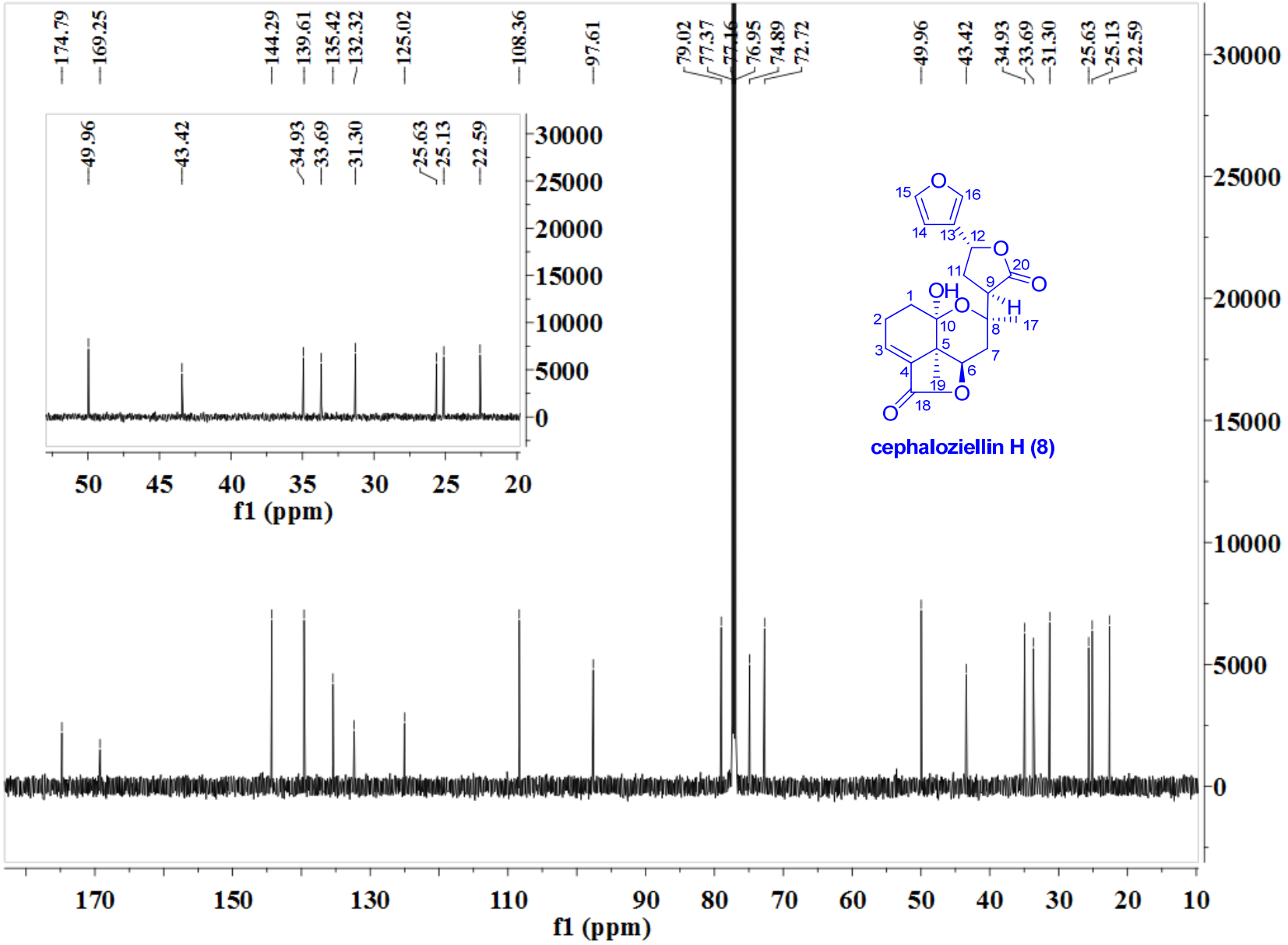
S84. Key NOESY correlations (in figure) of cephaloziellin H (**8**).



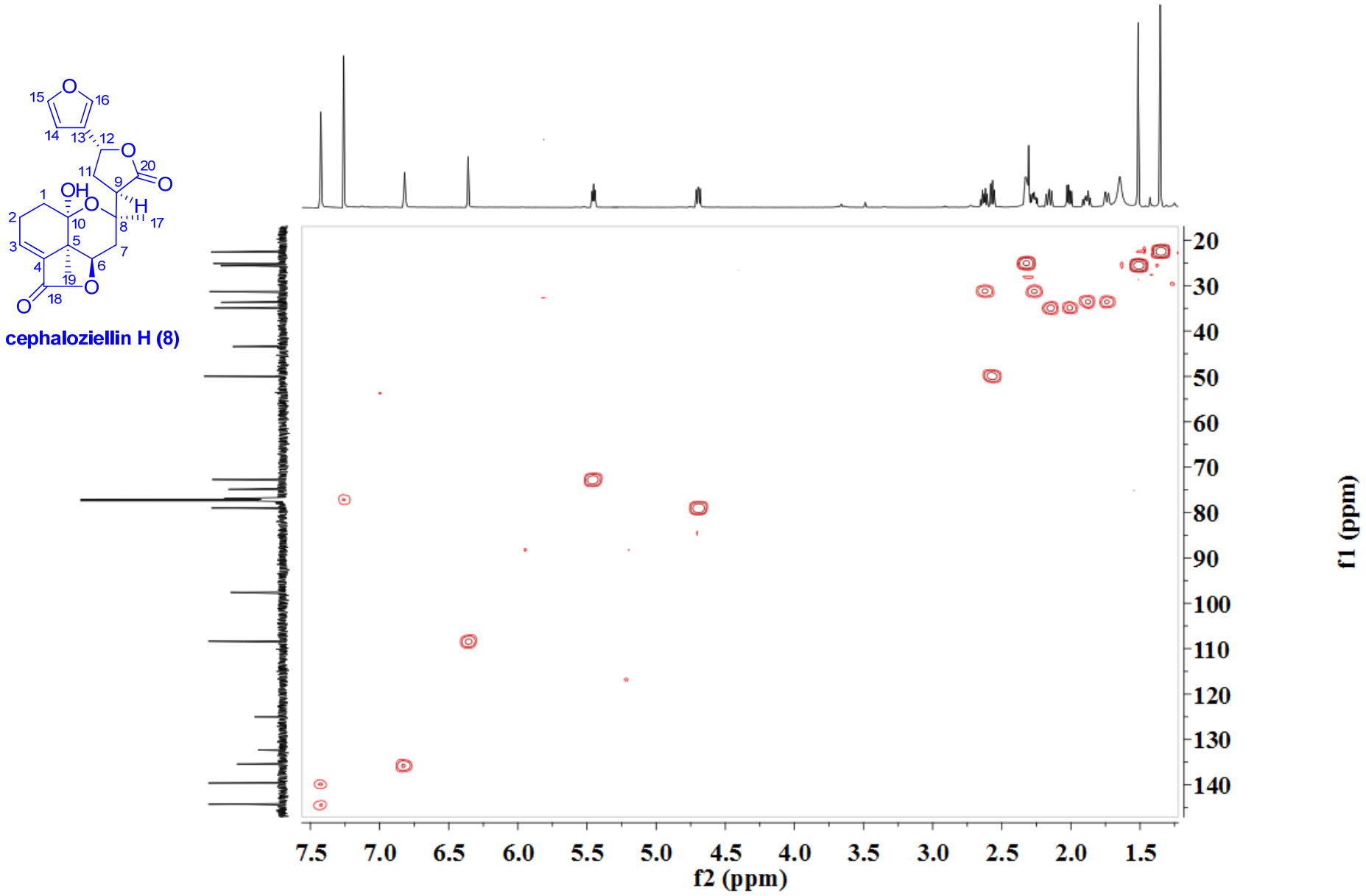
S85. ^{1}H NMR spectrum (600 MHz) of cephaloziellin H (**8**) in $CDCl_3$.



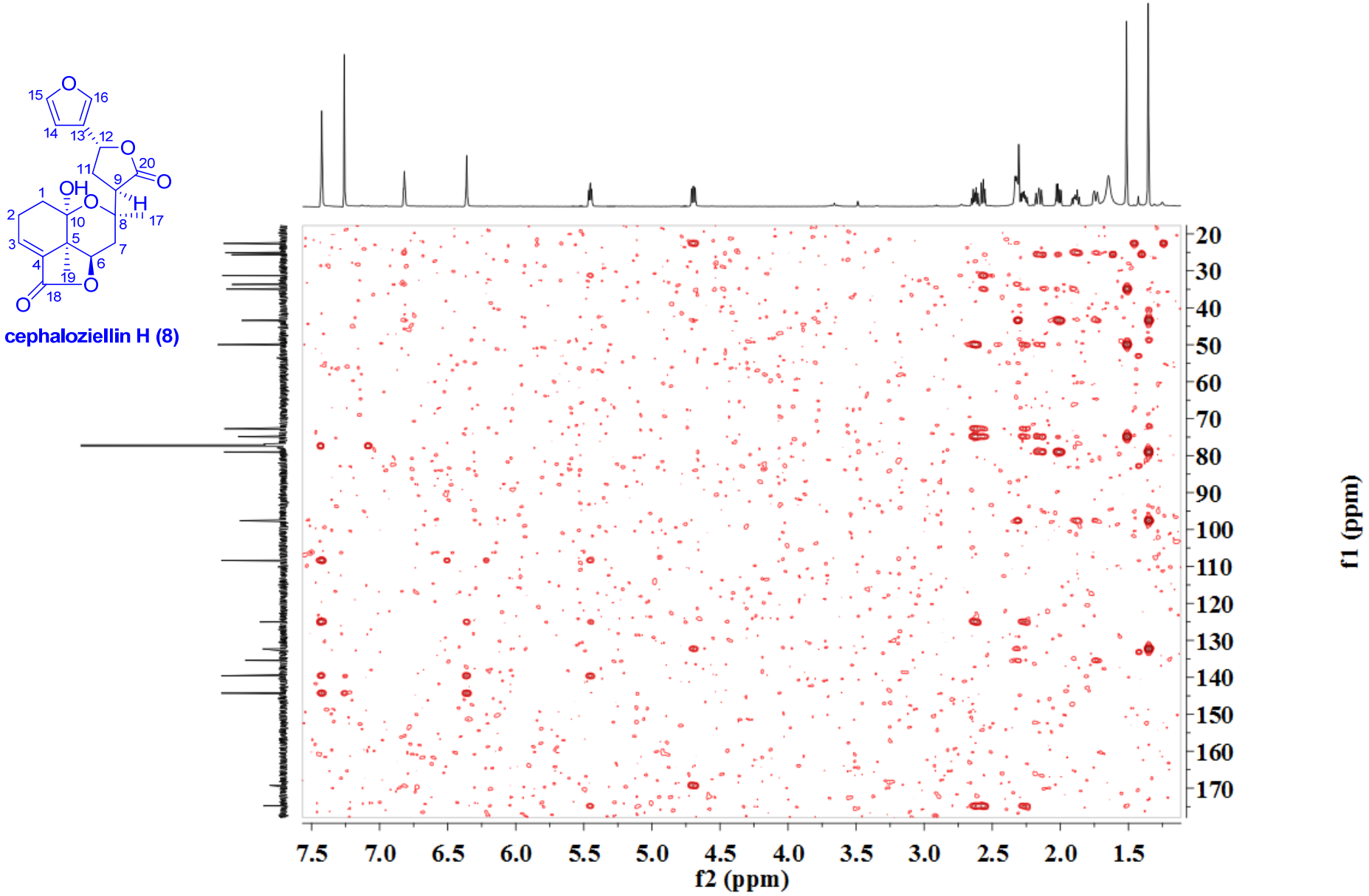
S86. ^{13}C NMR spectrum (150 MHz) of cephaloziellin H (**8**) in $CDCl_3$.



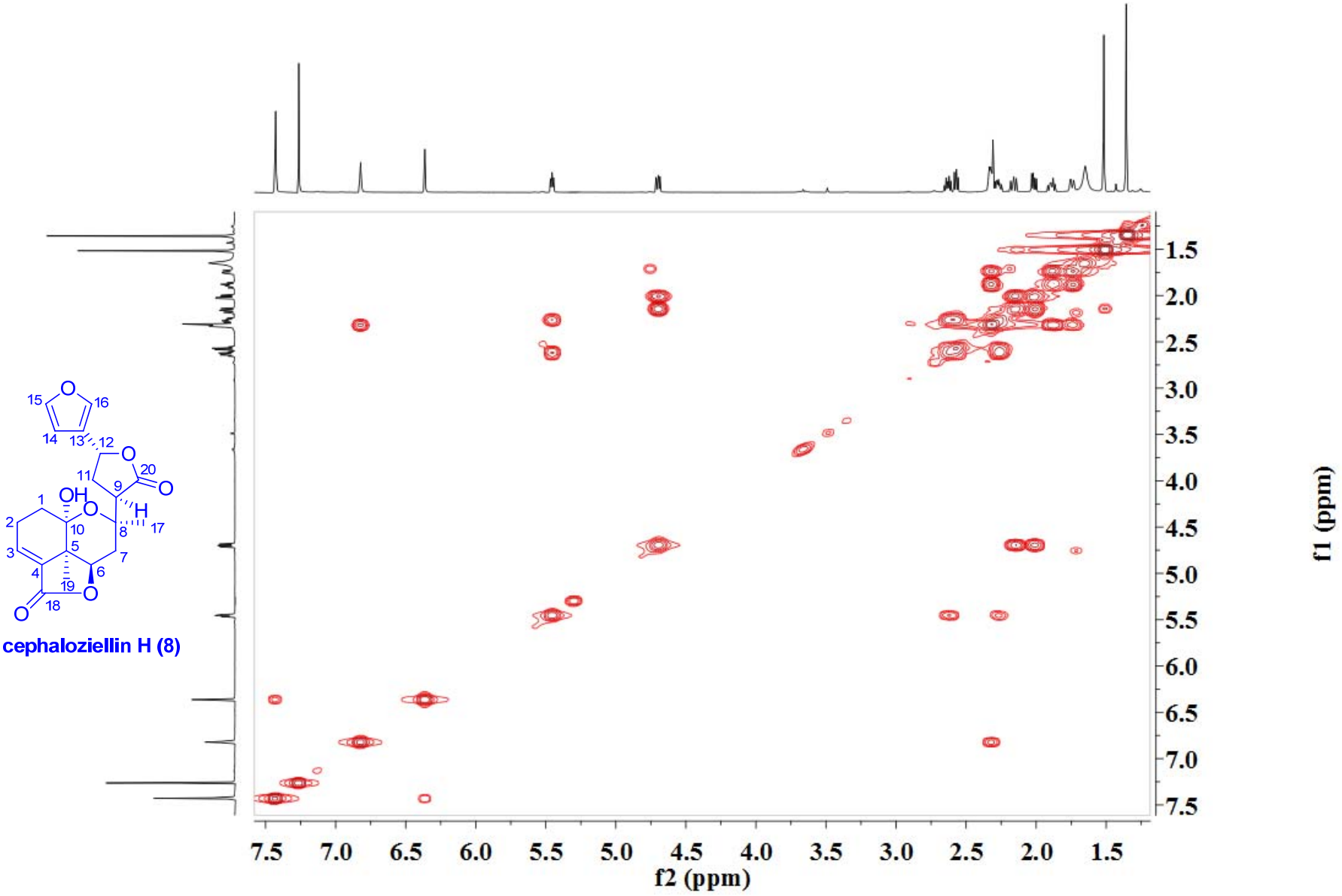
S87. HSQC spectrum (600 MHz) of cephaloziellin H (**8**) in $CDCl_3$.



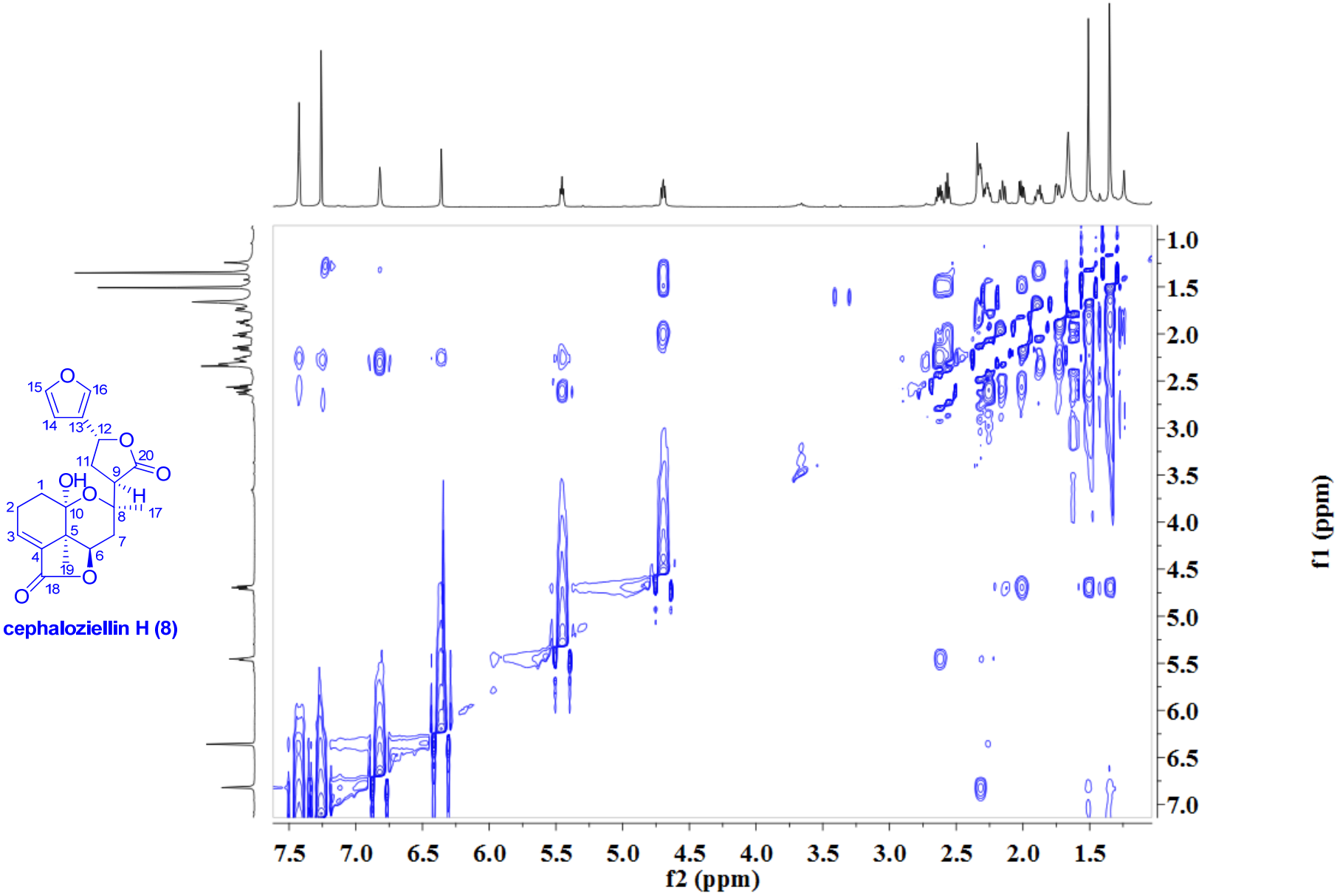
S88. HMBC spectrum (600 MHz) of cephaloziellin H (**8**) in $CDCl_3$.



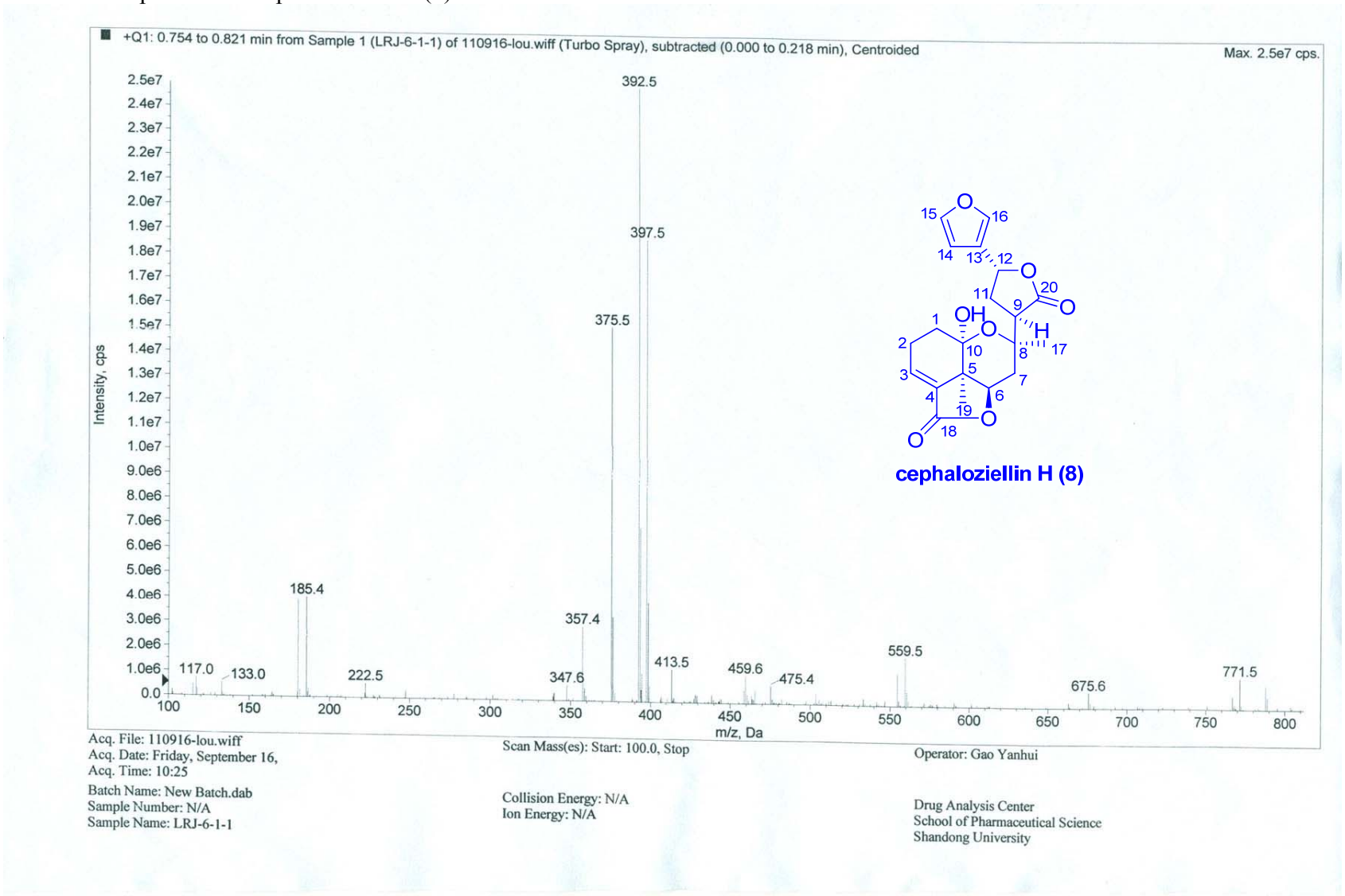
S89. ^{1}H-^{1}H COSY spectrum (600 MHz) of cephaloziellin H (**8**) in $CDCl_3$.



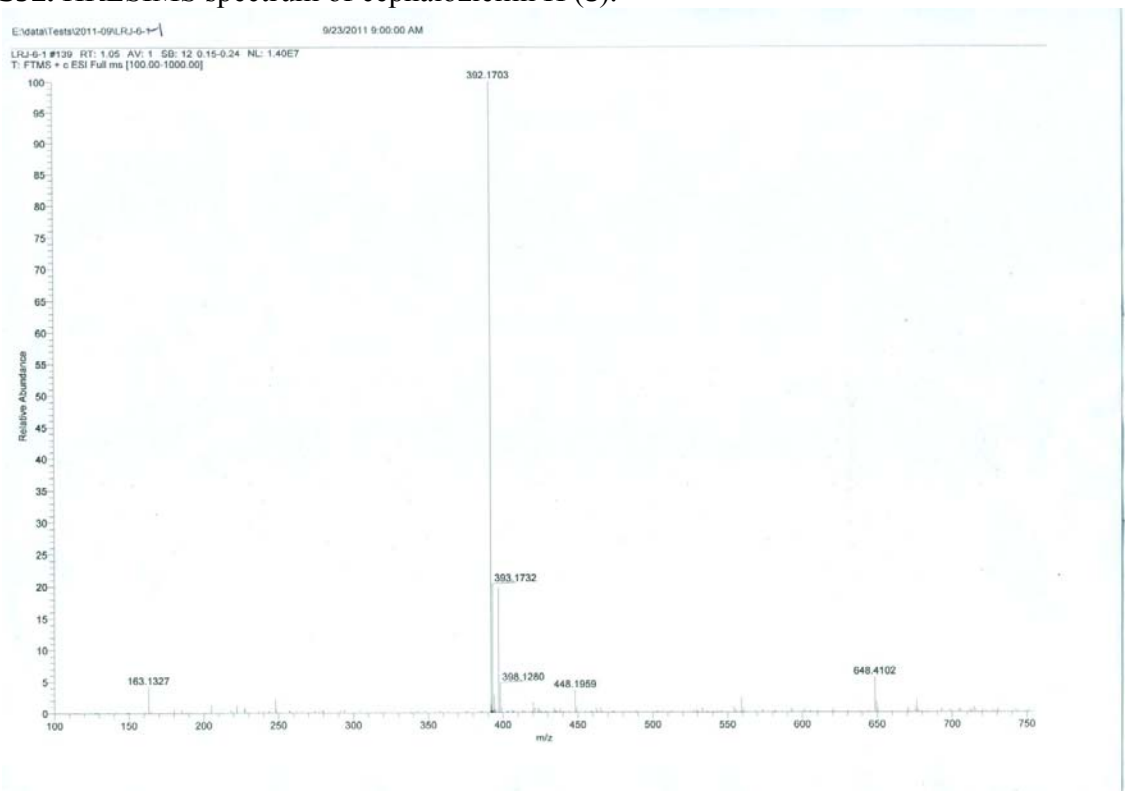
S90. NOESY spectrum (600 MHz) of cephaloziellin H (**8**) in $CDCl_3$.

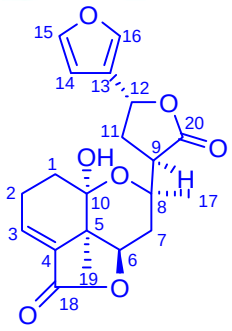


S91. ESIMS spectrum of cephaloziellin H (**8**).



S92. HRESIMS spectrum of cephaloziellin H (**8**).



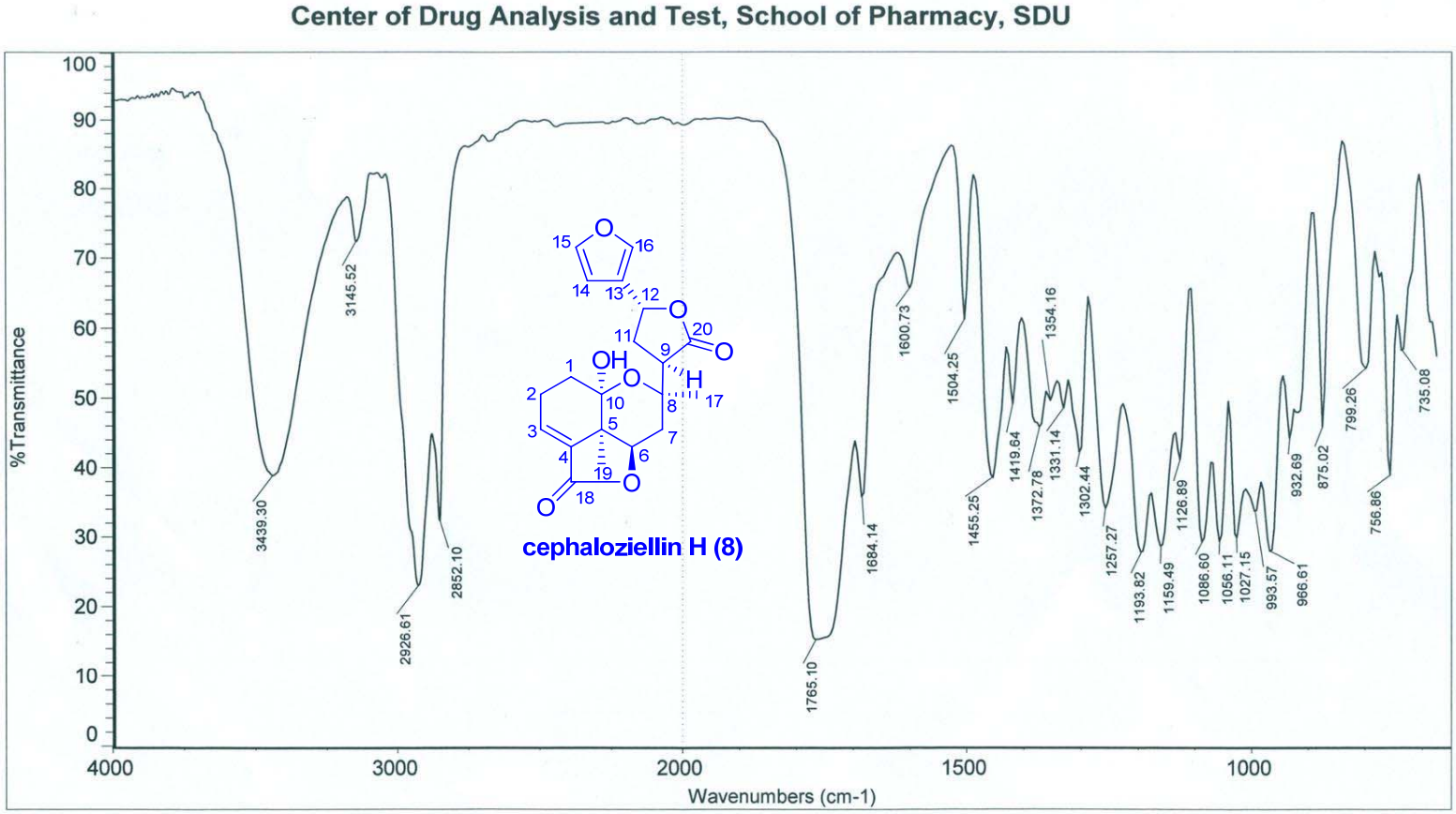


cephaloziellin H (8)

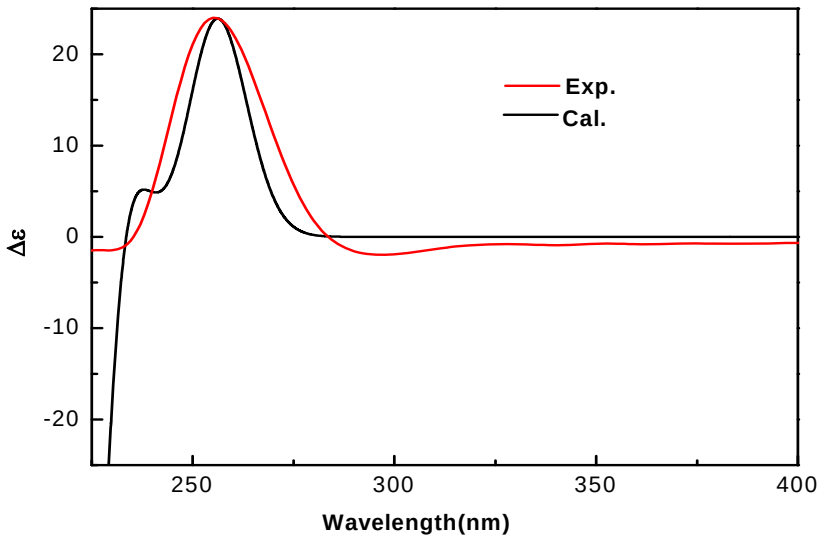
SPECTRUM - simulation :

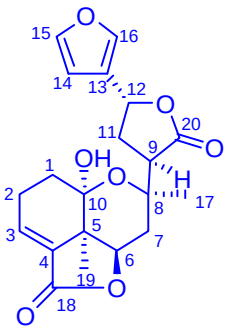
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
392.1703	392.1704	−0.10	8.5	$^{12}C_{20}H_{26}O_7N_1$

S93. IR spectrum of cephaloziellin H (**8**).

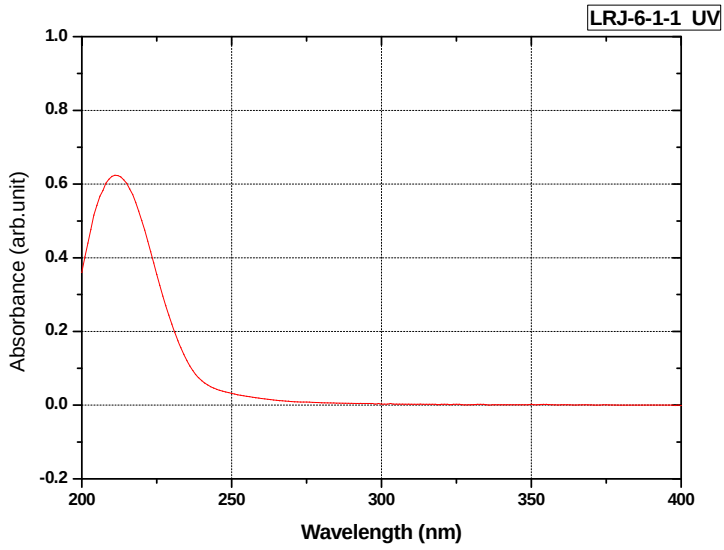


S94. Experimental ECD and calculated ECD, and UV spectra of cephaloziellin H (**8**).

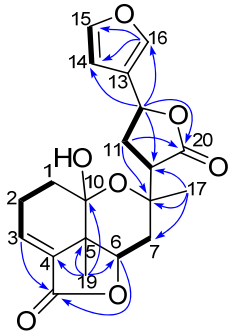




cephaloziellin H (8)



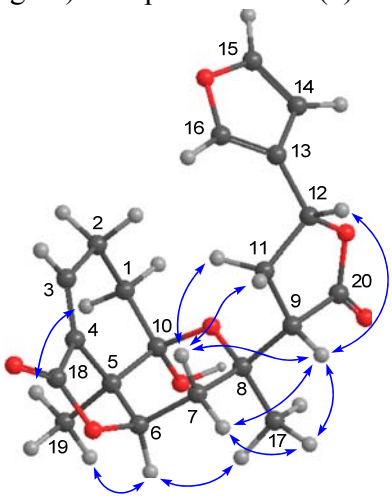
S95 Key HMBC and ^{1}H-^{1}H COSY correlations (in figure) of cephaloziellin I (**9**).



9 HMBC

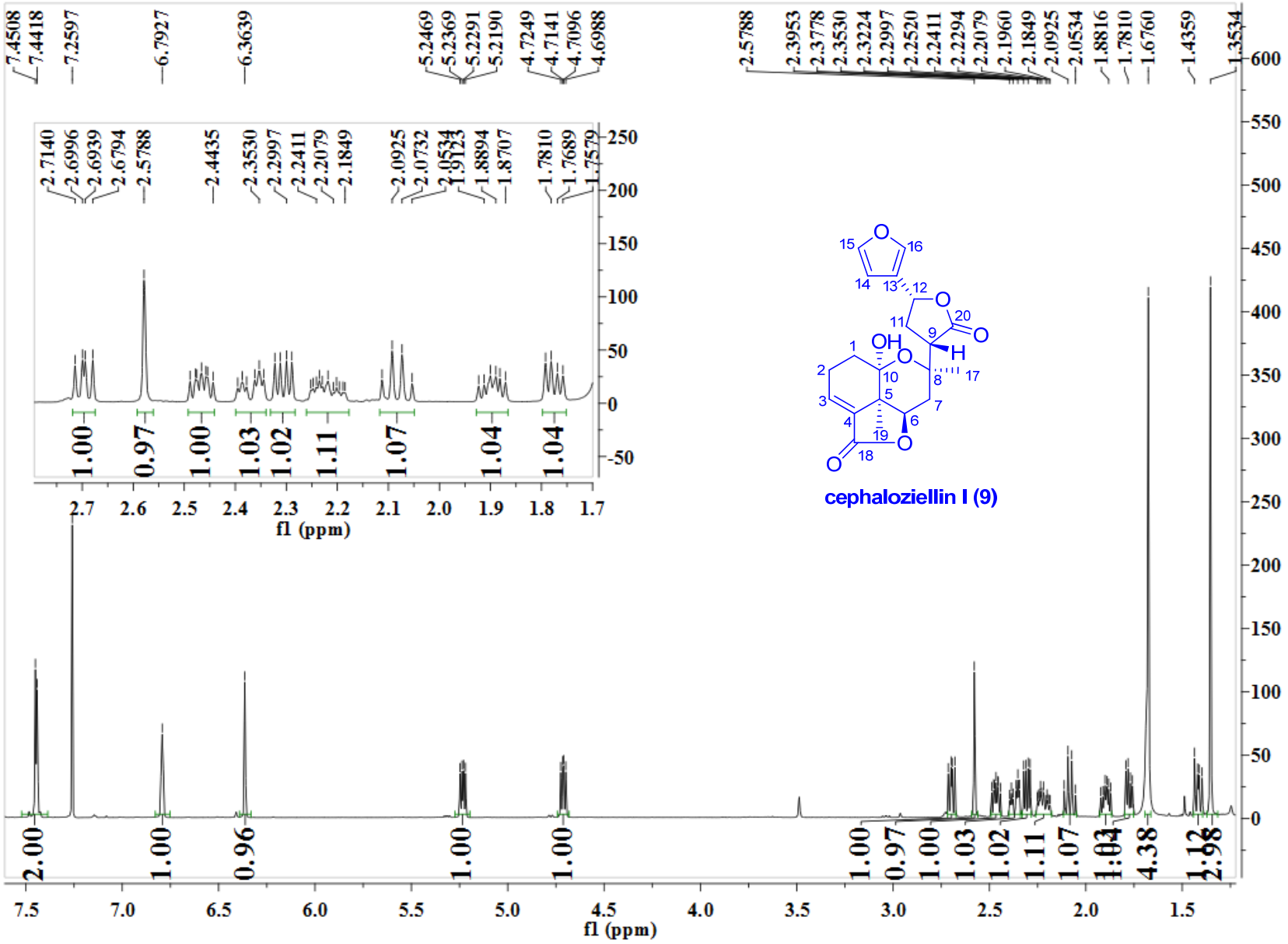
^{1}H-^{1}H COSY

S96. Key NOESY correlations (in figure) of cephaloziellin I (**9**).

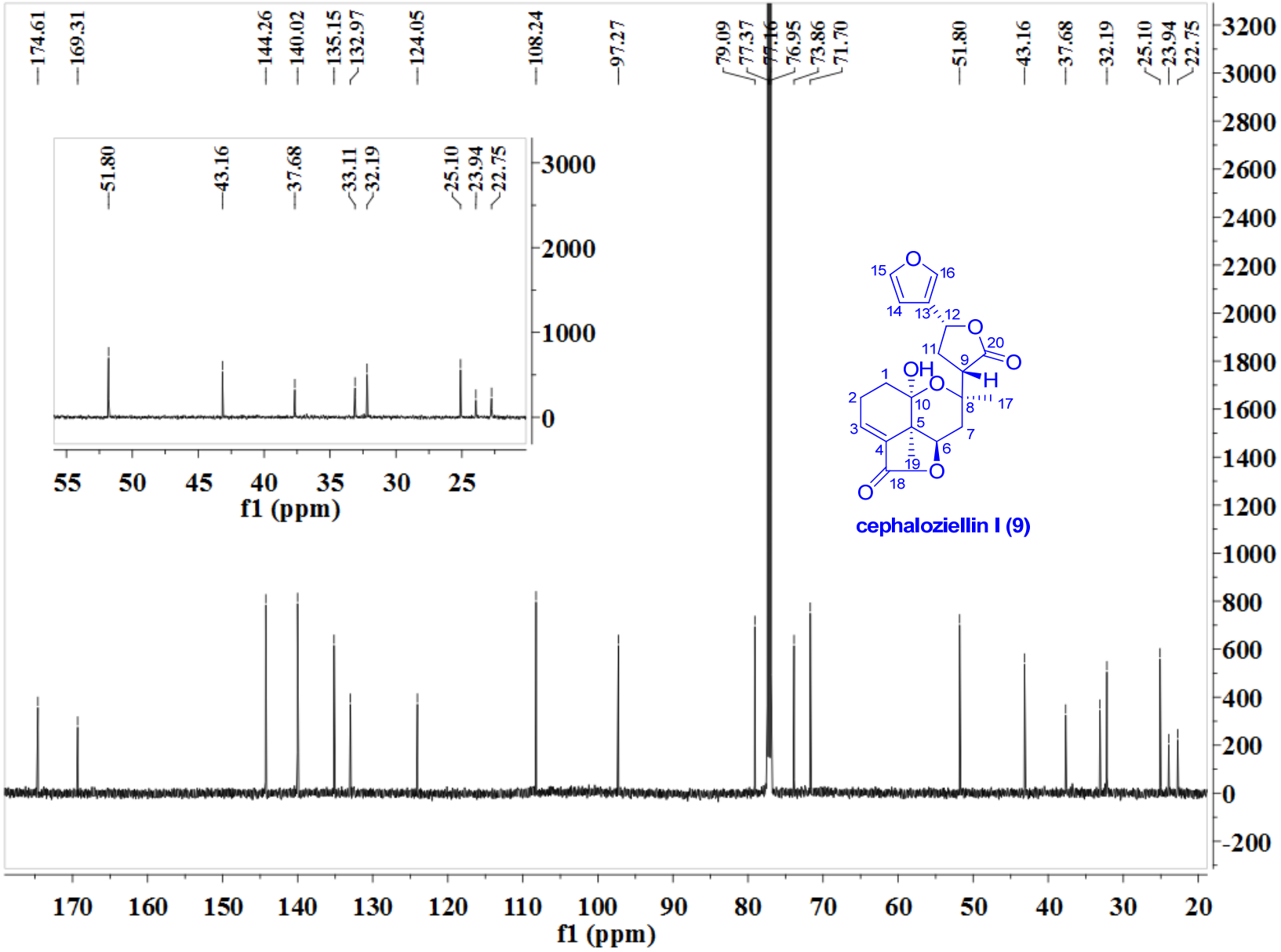


9 NOESY

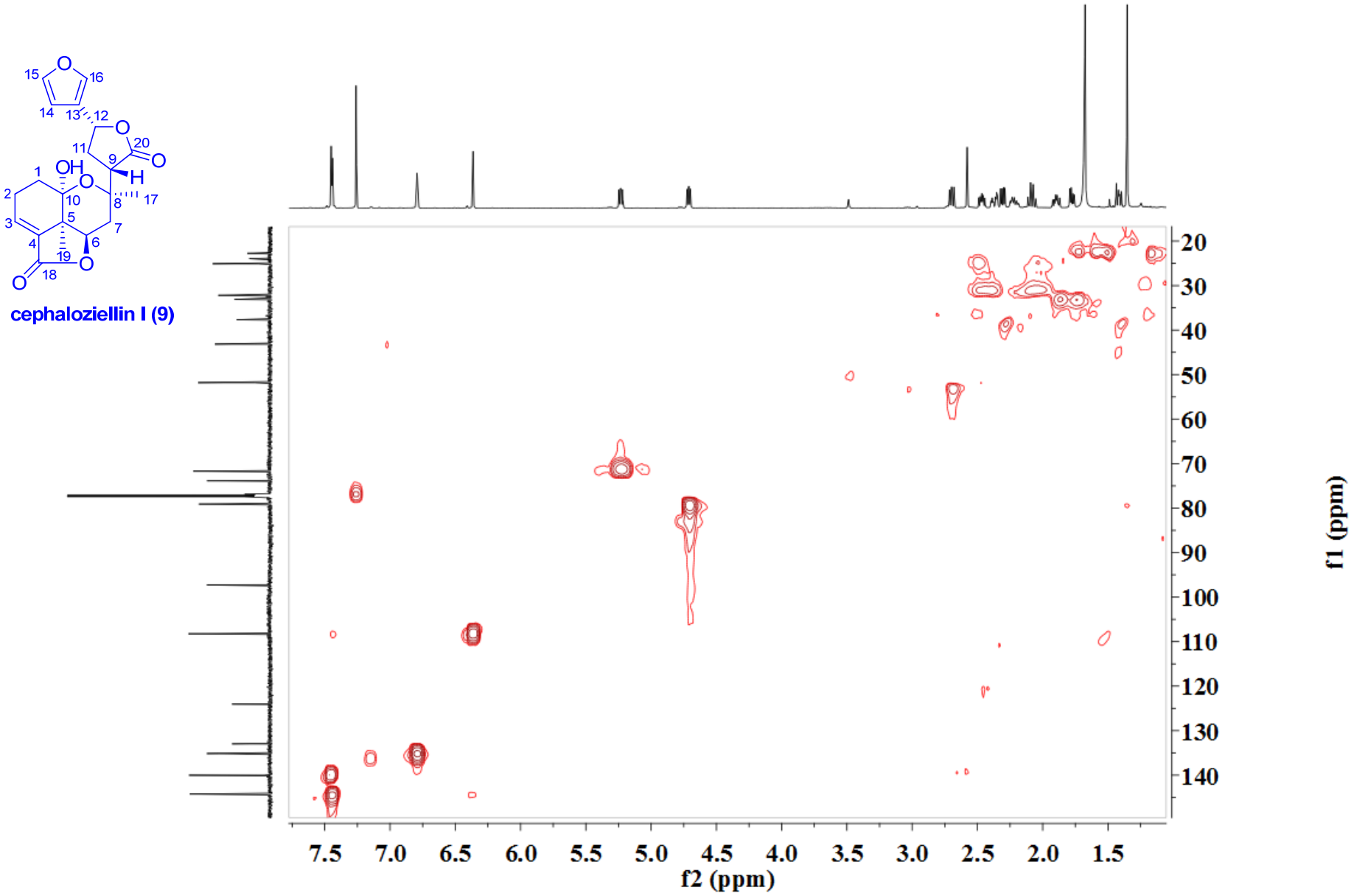
S97. ^{1}H NMR spectrum (600 MHz) of cephaloziellin I (**9**) in $CDCl_3$.



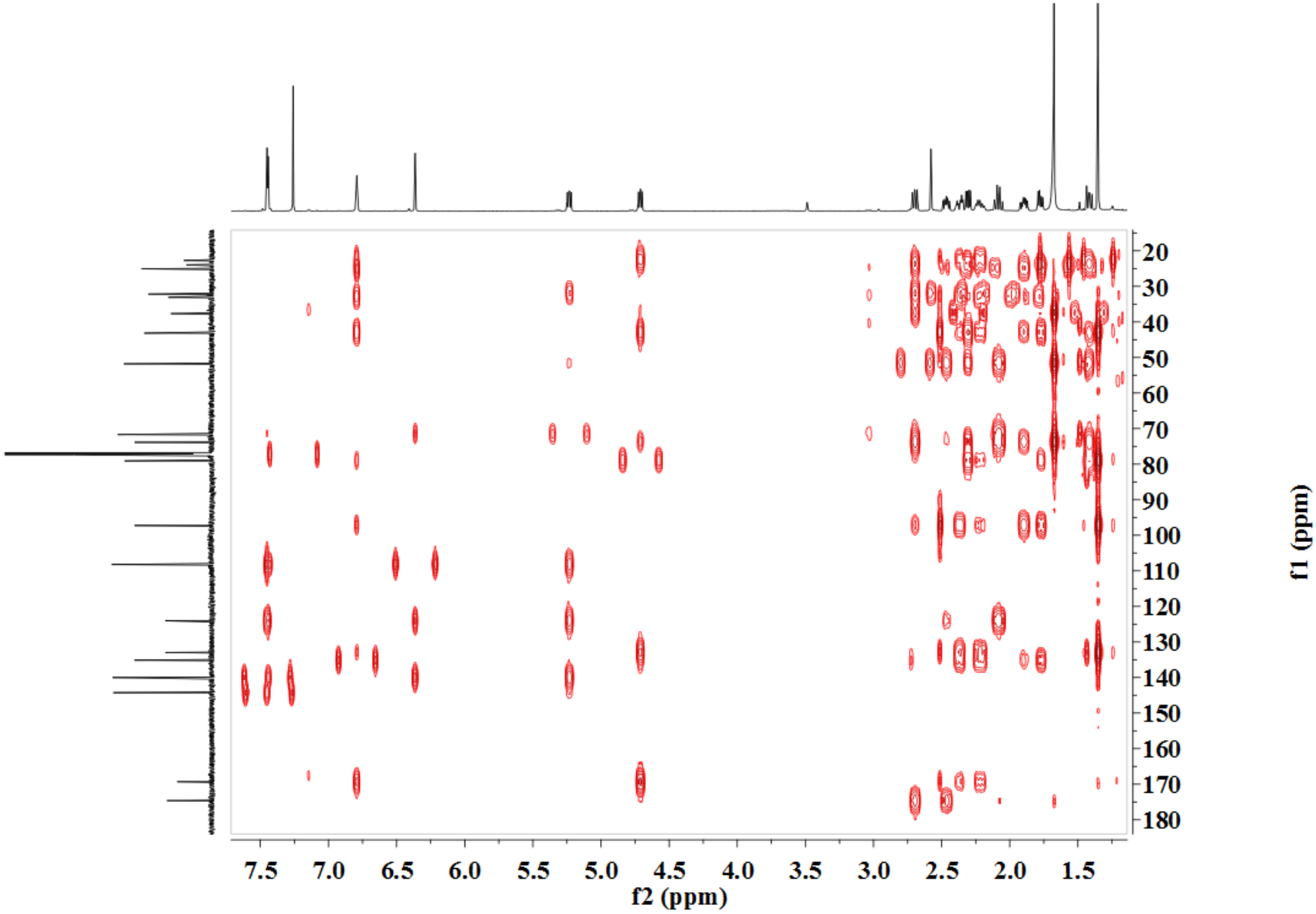
S98. ^{13}C NMR spectrum (150 MHz) of cephaloziellin I (**9**) in $CDCl_3$.



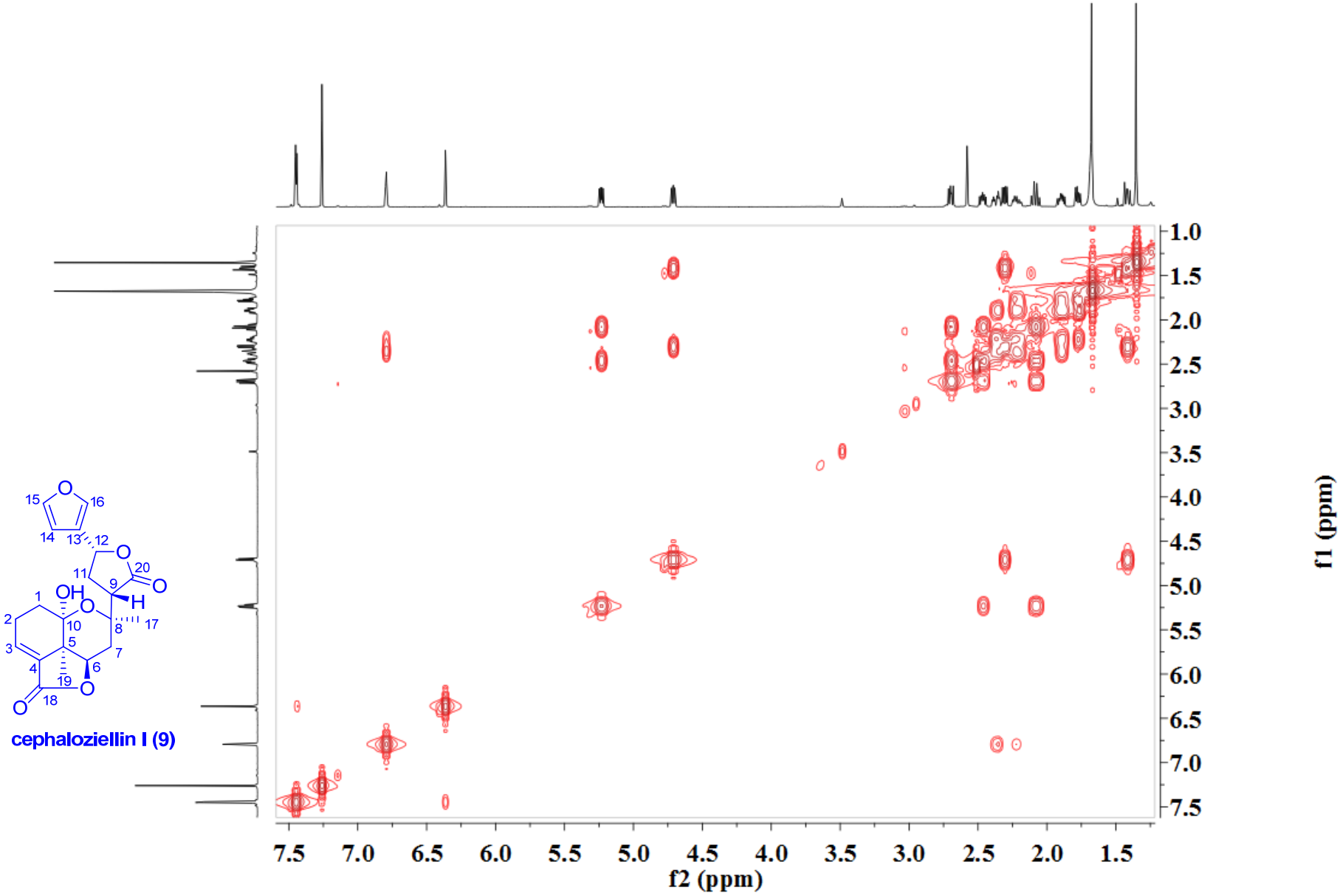
S99. HSQC spectrum (600 MHz) of cephaloziellin I (**9**) in $CDCl_3$.



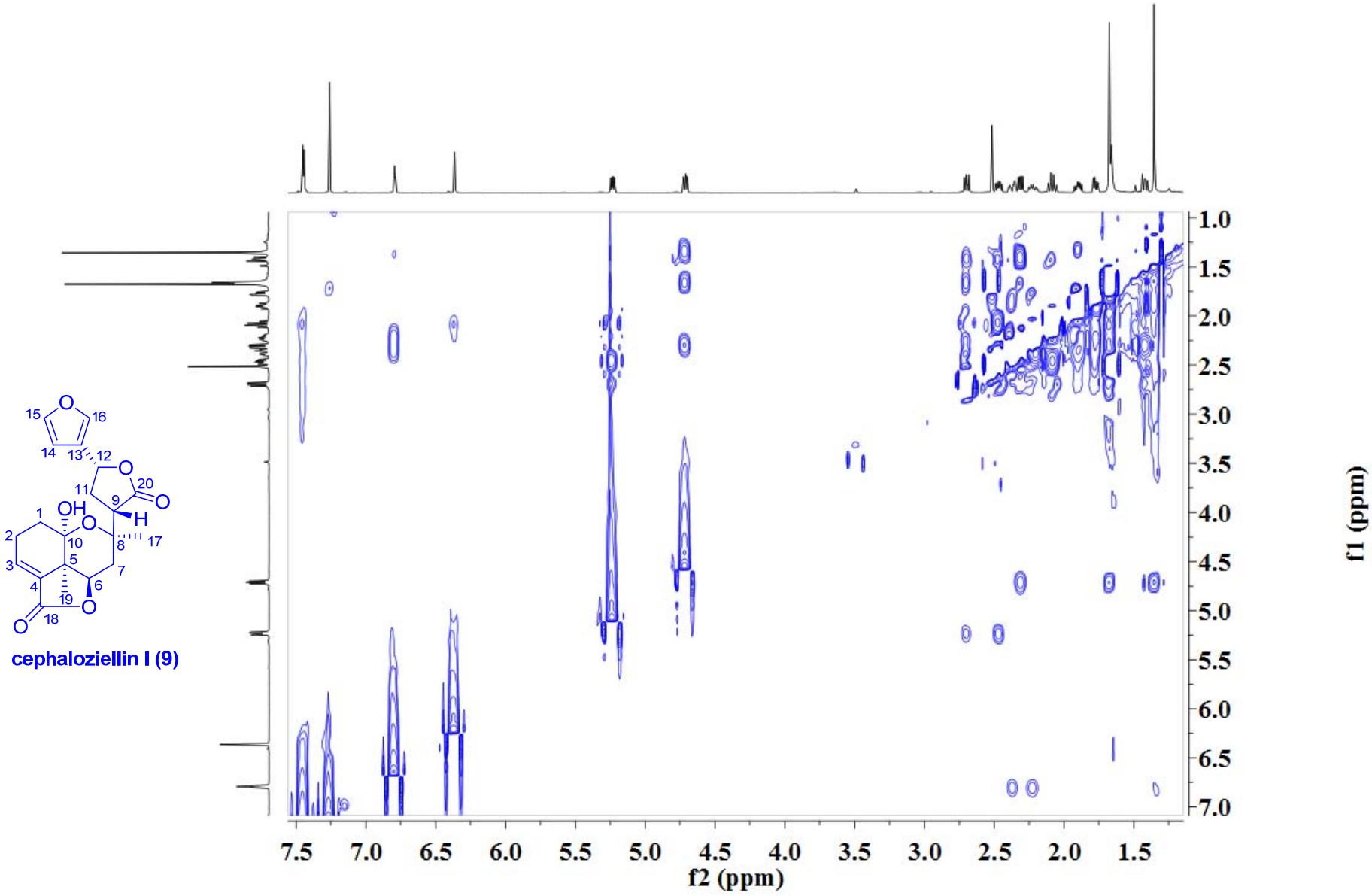
S100. HMBC spectrum (600 MHz) of cephaloziellin I (**9**) in $CDCl_3$.



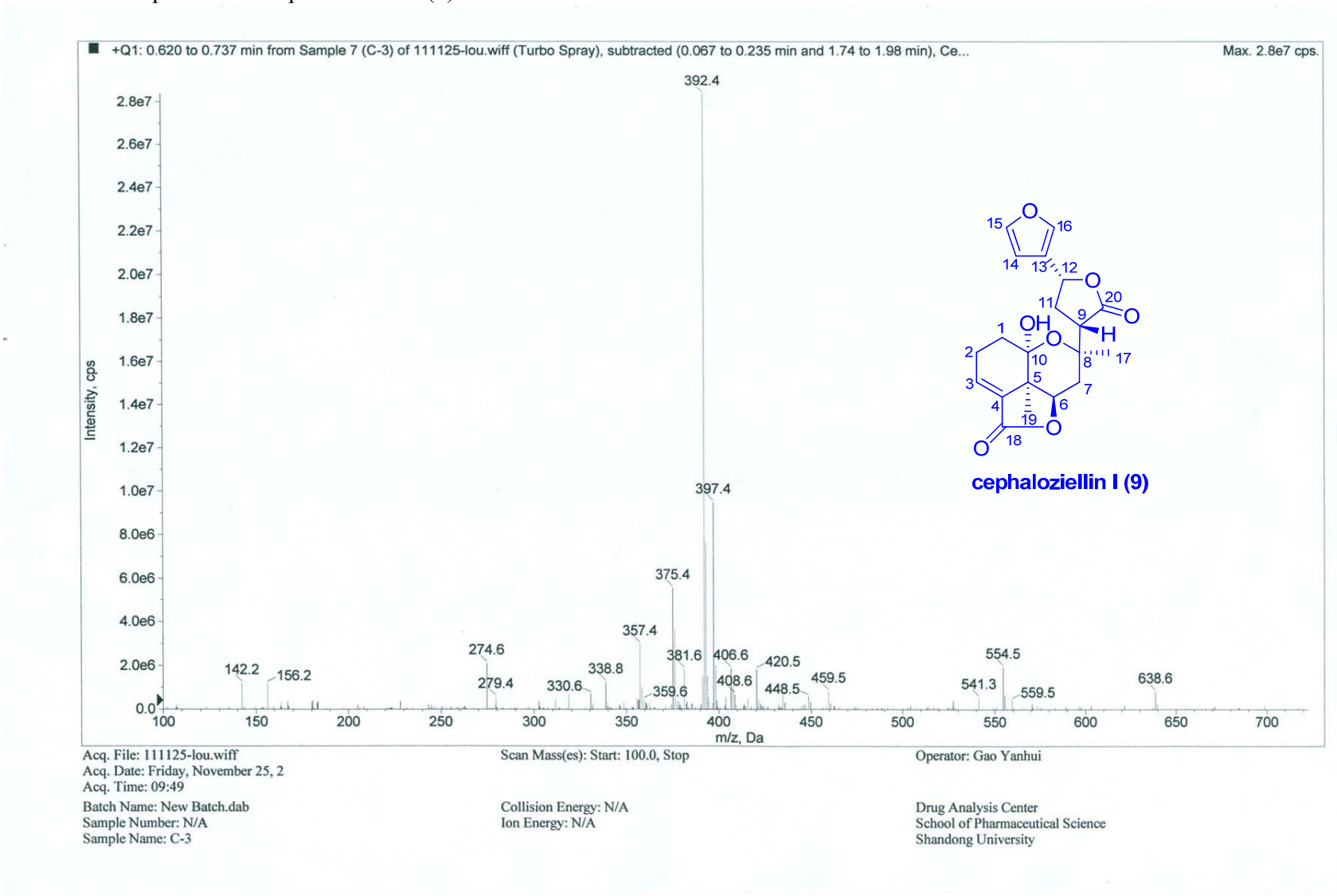
S101. ^{1}H-^{1}H COSY spectrum (600 MHz) of cephaloziellin I (**9**) in $CDCl_3$.



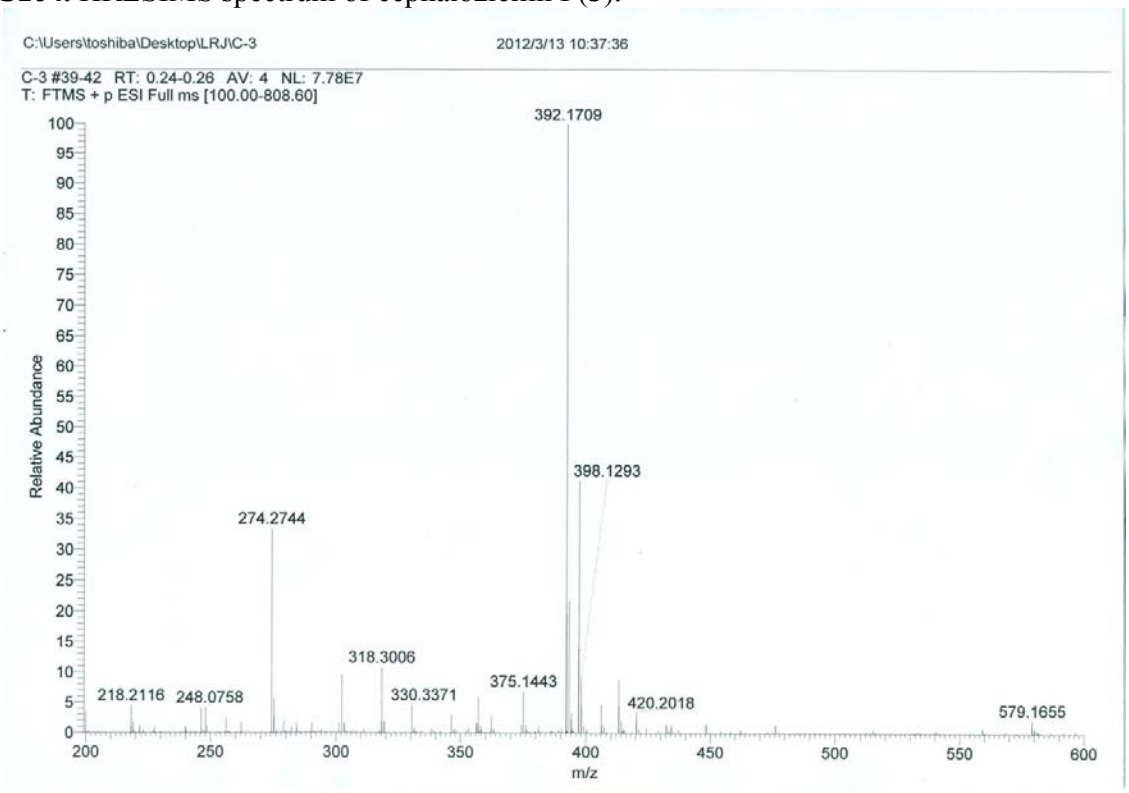
S102. NOESY spectrum (600 MHz) of cephaloziellin I (**9**) in $CDCl_3$.

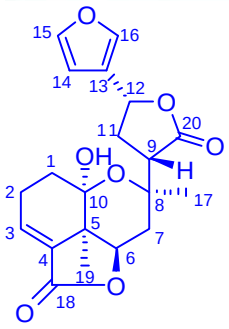


S103. ESIMS spectrum of cephaloziellin I (**9**).



S104. HRESIMS spectrum of cephaloziellin I (**9**).



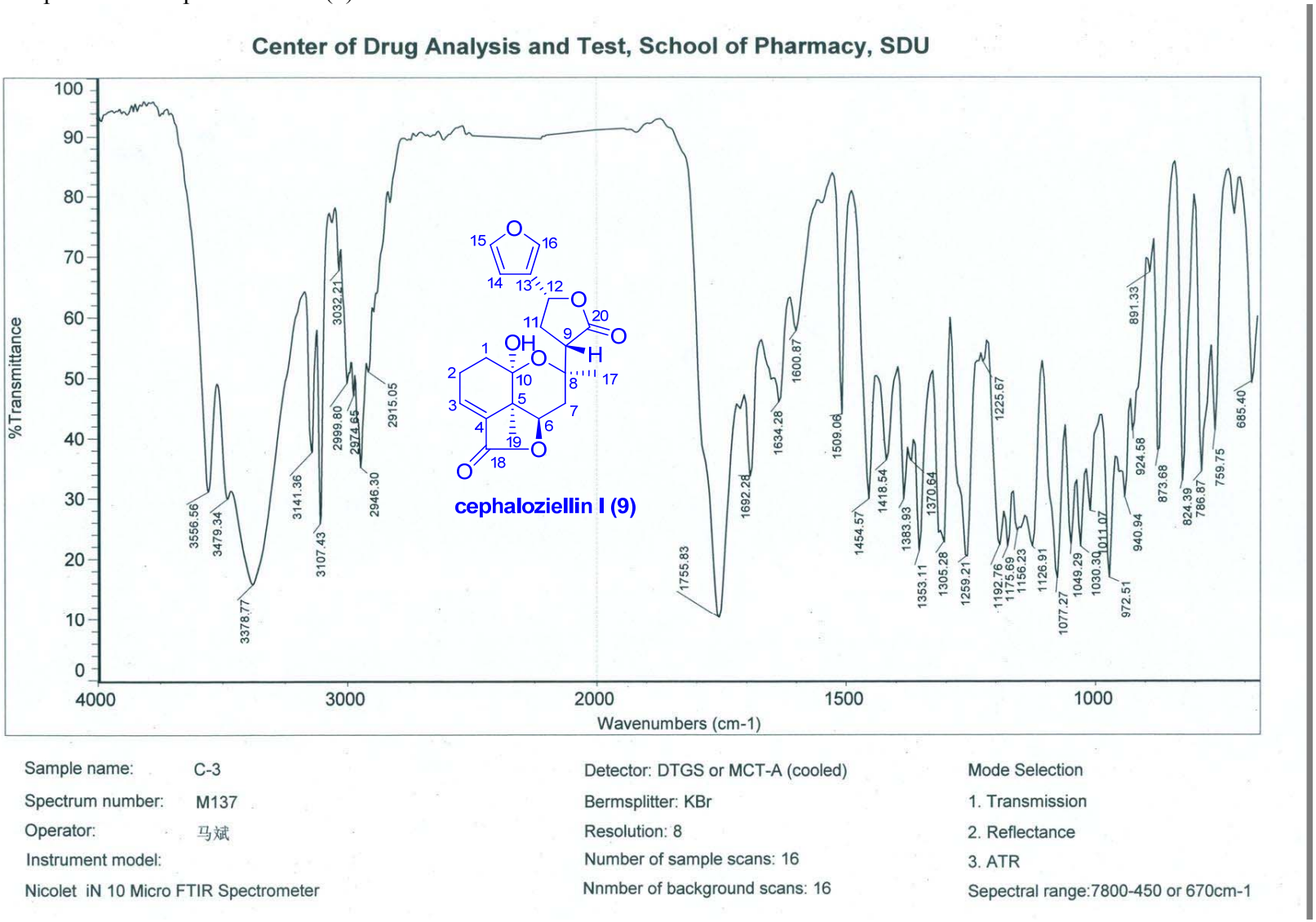


cephaloziellin I (9)

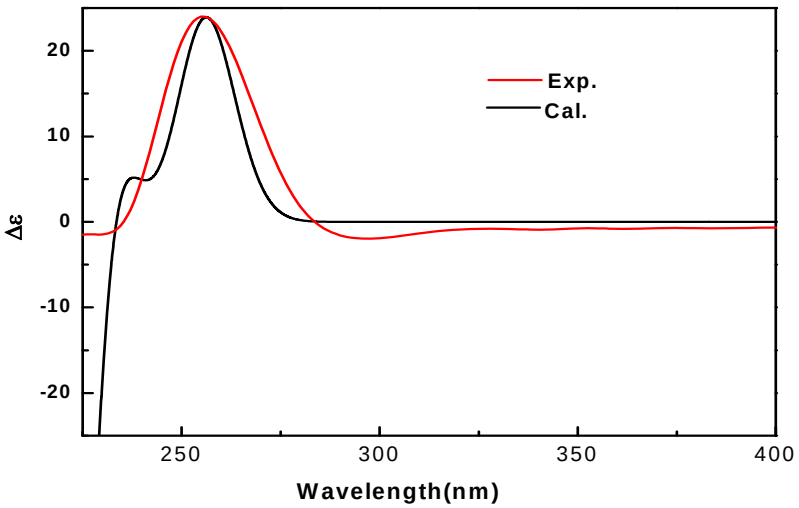
SPECTRUM - simulation :

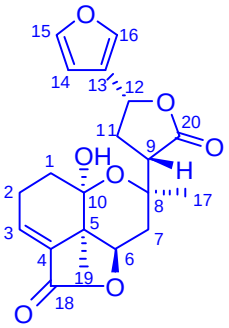
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
392.1709	392.1704	1.38	8.5	$^{12}C_{20}H_{26}O_7N_1$

S105. IR spectrum of cephaloziellin I (**9**).

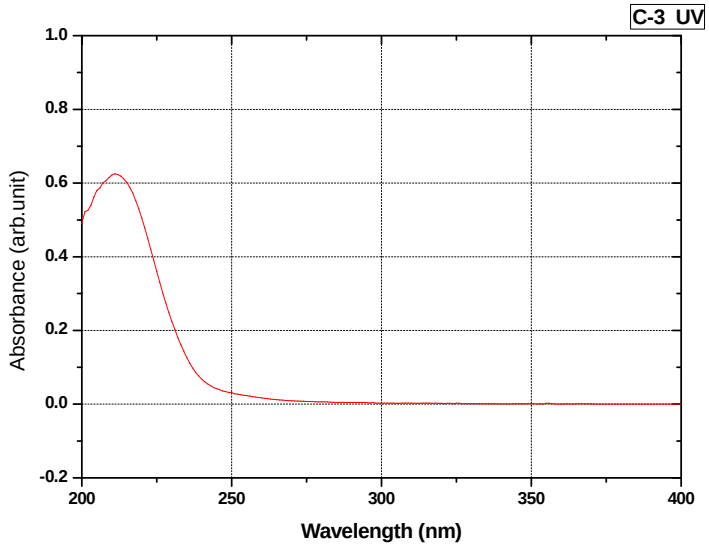


S106. Experimental ECD and calculated ECD, and UV spectra of cephaloziellin I (**9**).

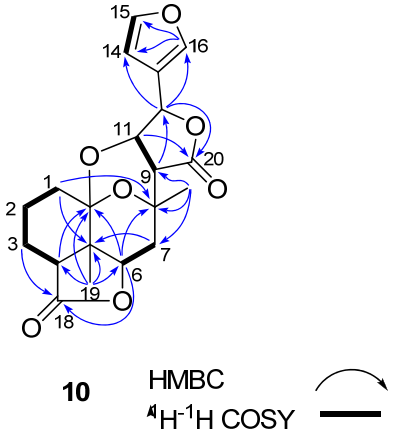




cephaloziellin I (9)

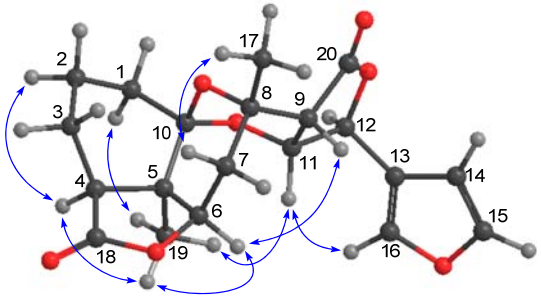


S107. Key HMBC and ^{1}H-^{1}H COSY correlations (in figure) of cephaloziellin J (**10**).



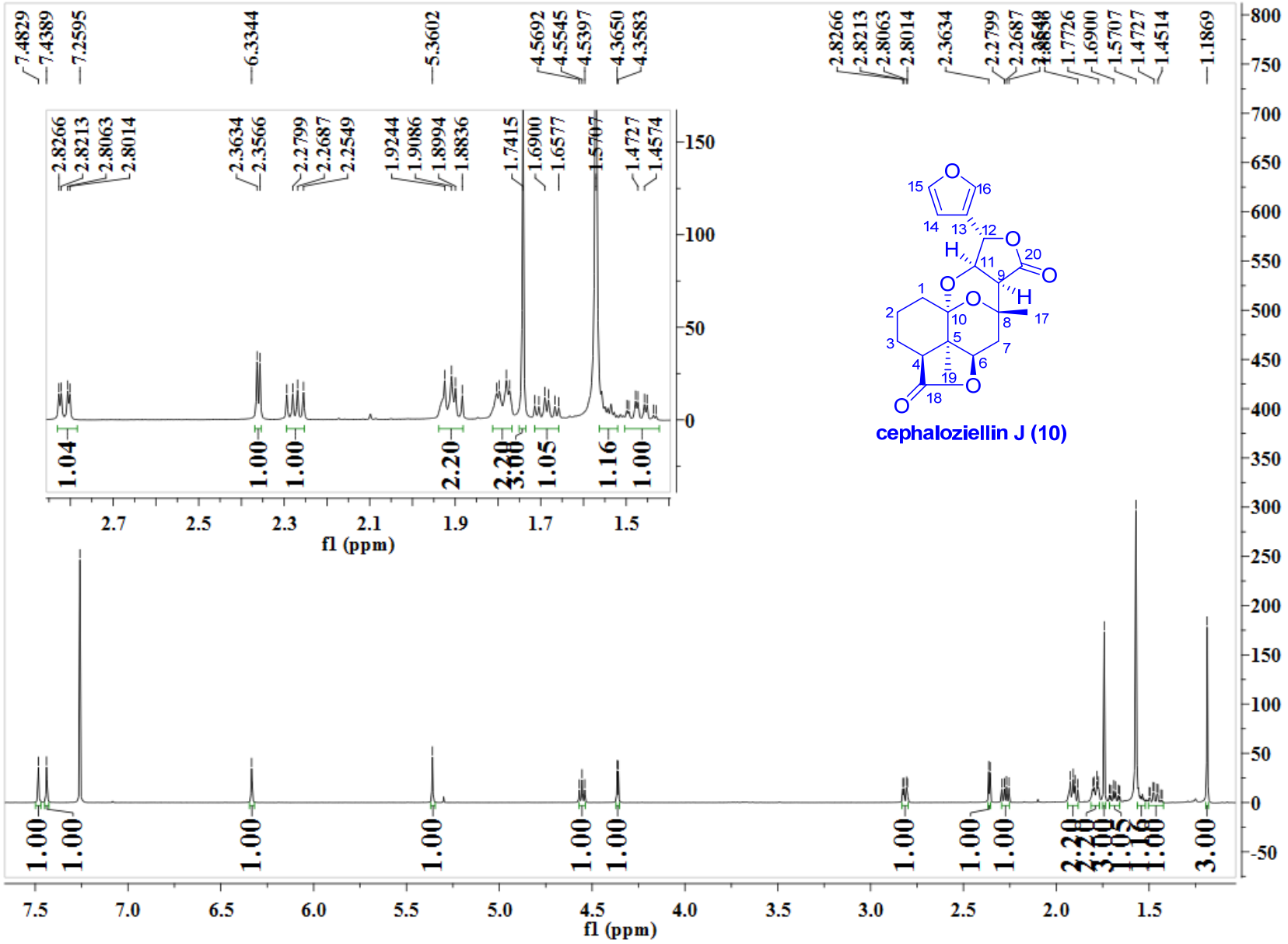
10 HMBC, ^{1}H-^{1}H COSY

S108. Key NOESY correlations (in figure) of cephaloziellin J (**10**).

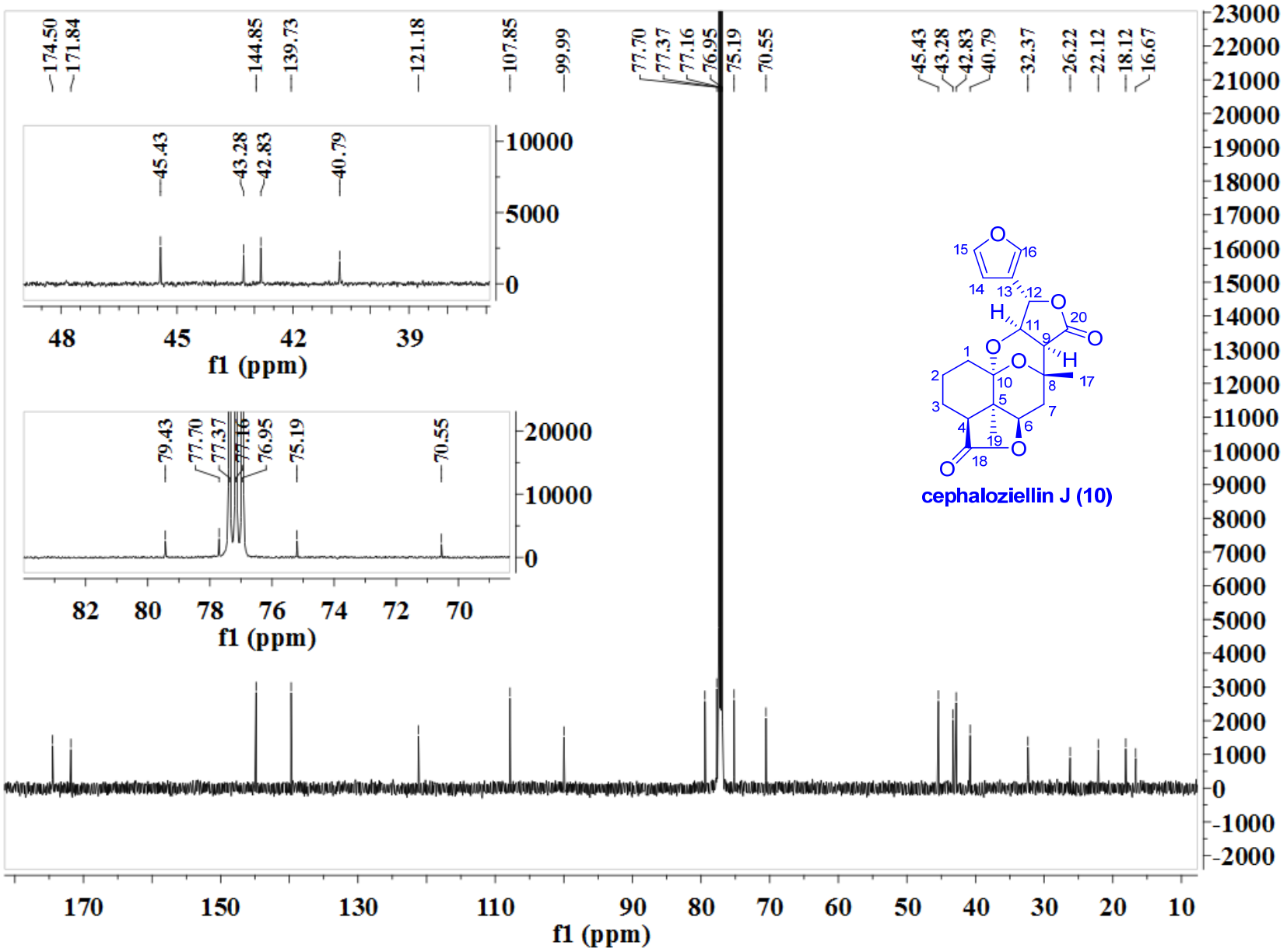


10 NOESY

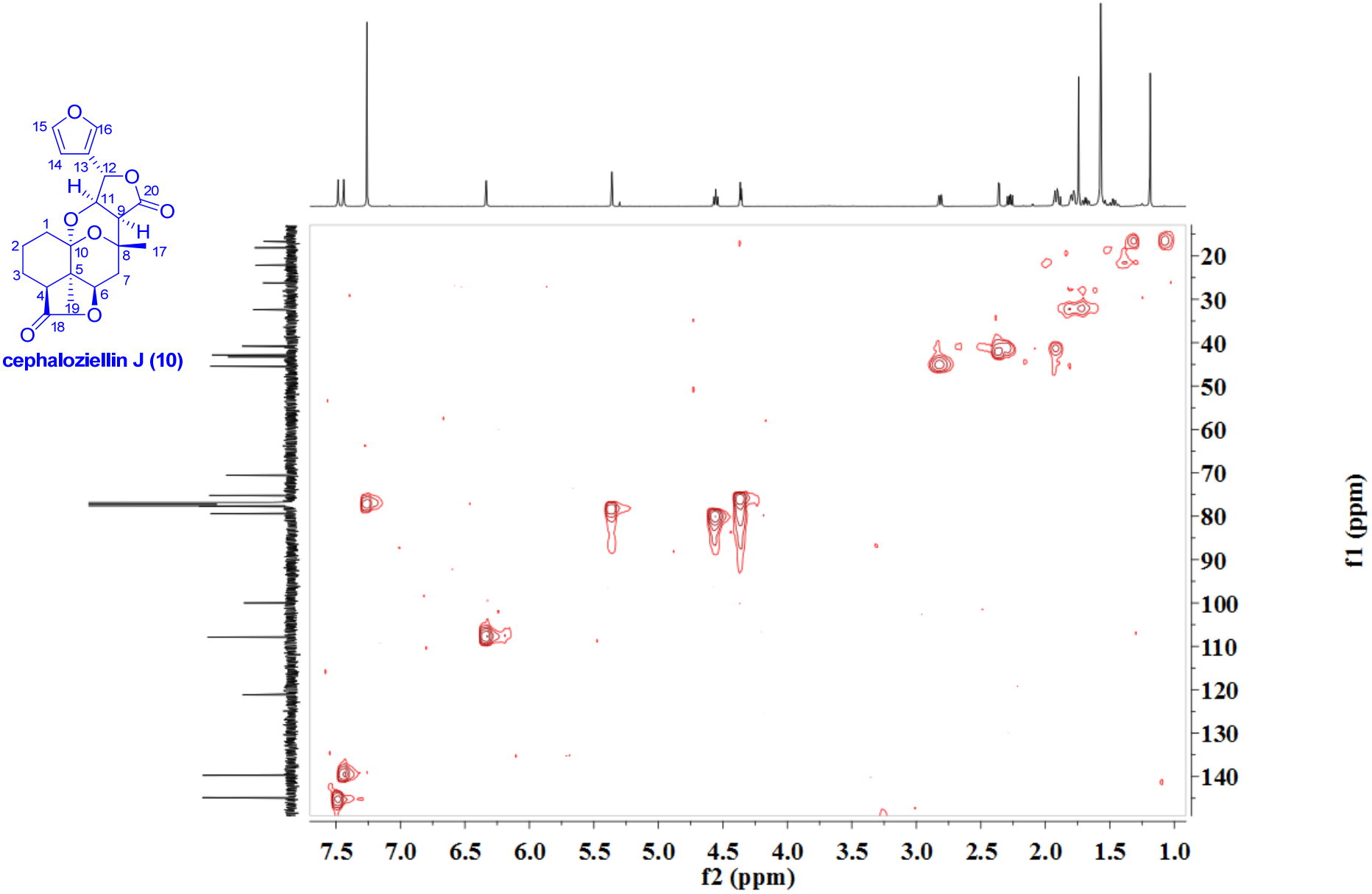
S109. ^{1}H NMR spectrum (600 MHz) of cephaloziellin J (**10**) in $CDCl_3$.



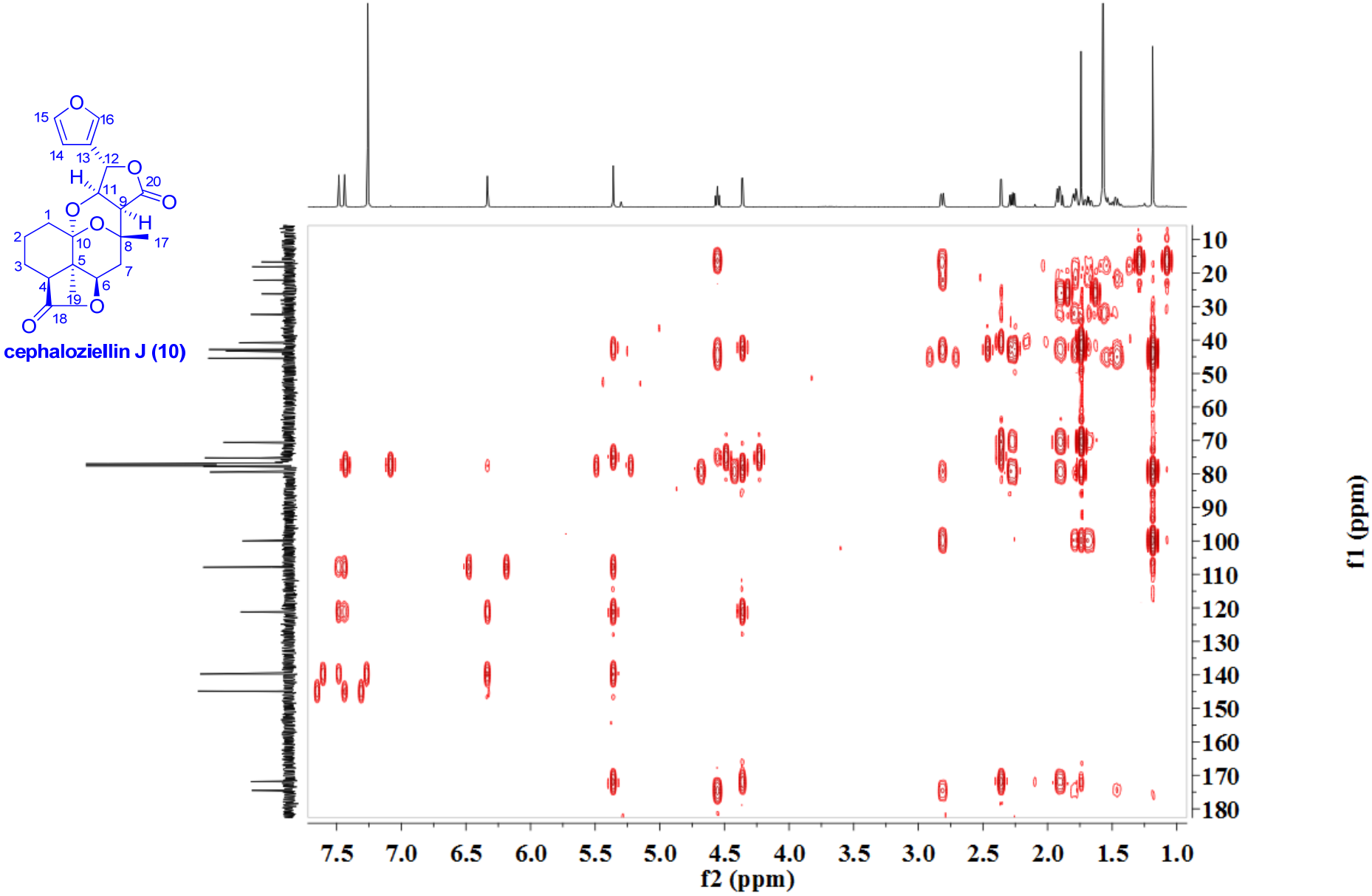
S110. ^{13}C NMR spectrum (150 MHz) of cephaloziellin J (**10**) in $CDCl_3$.



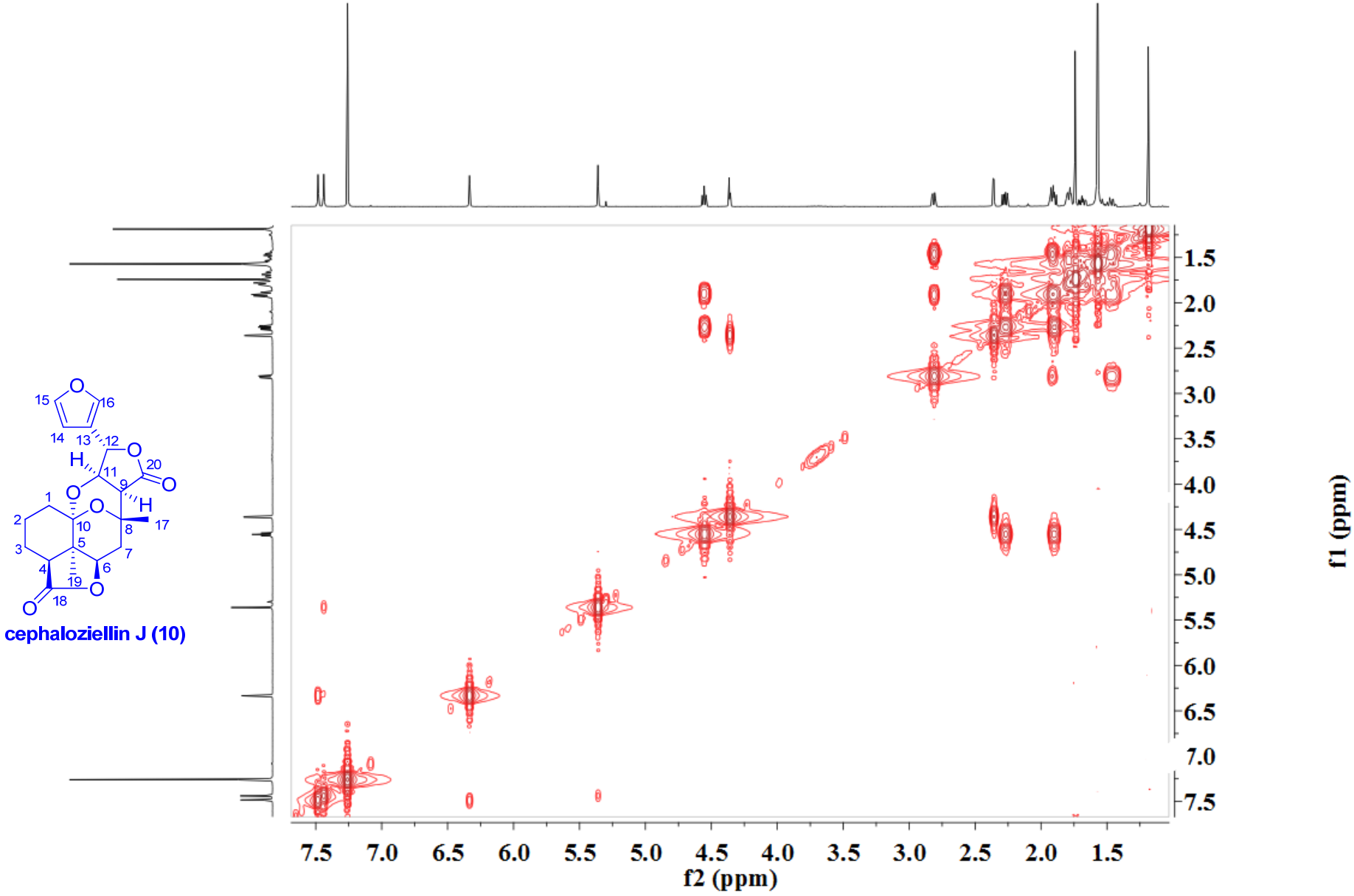
S111. HSQC spectrum (600 MHz) of cephaloziellin J (**10**) in $CDCl_3$.



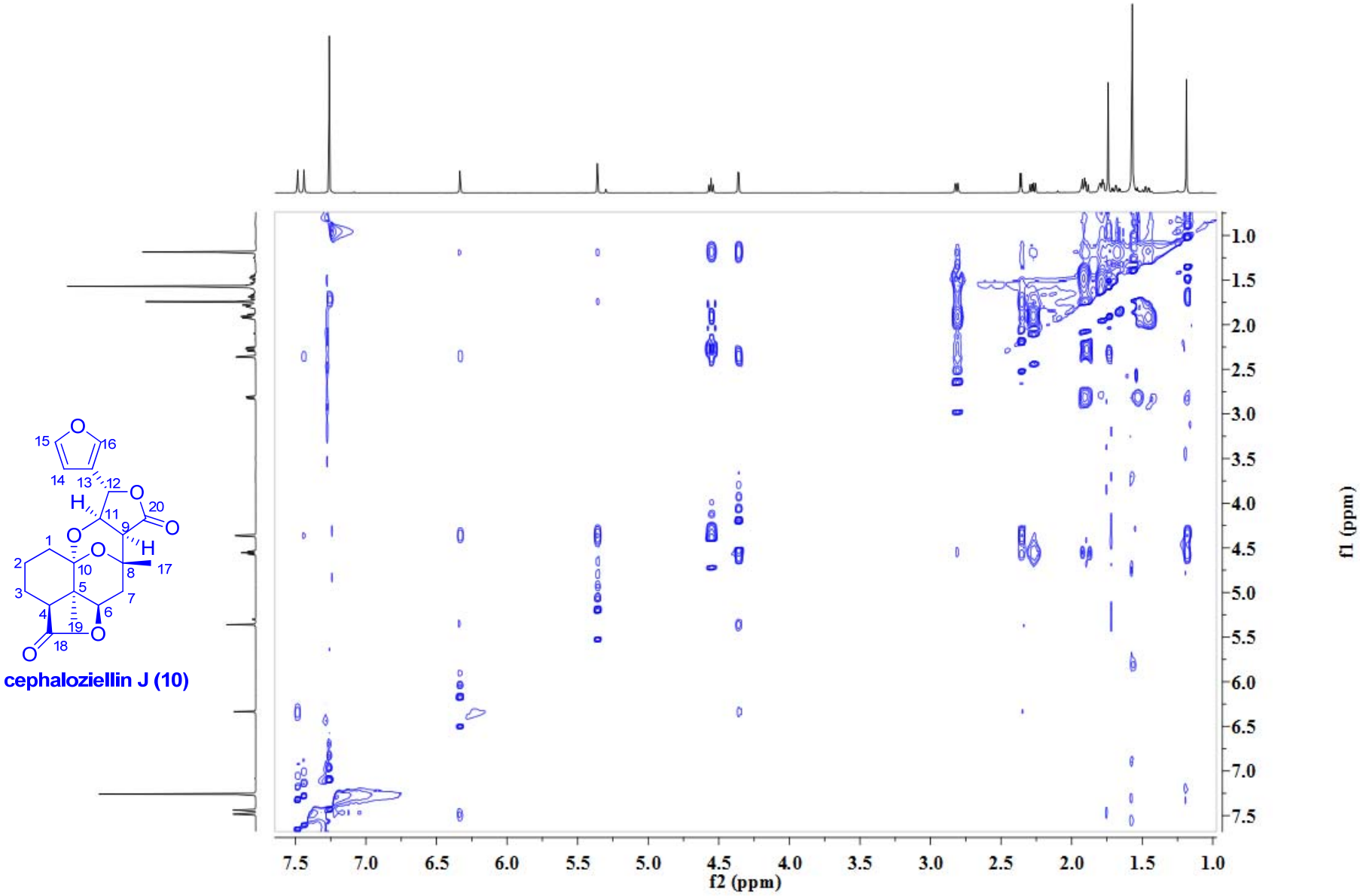
S112. HMBC spectrum (600 MHz) of cephaloziellin J (**10**) in $CDCl_3$.



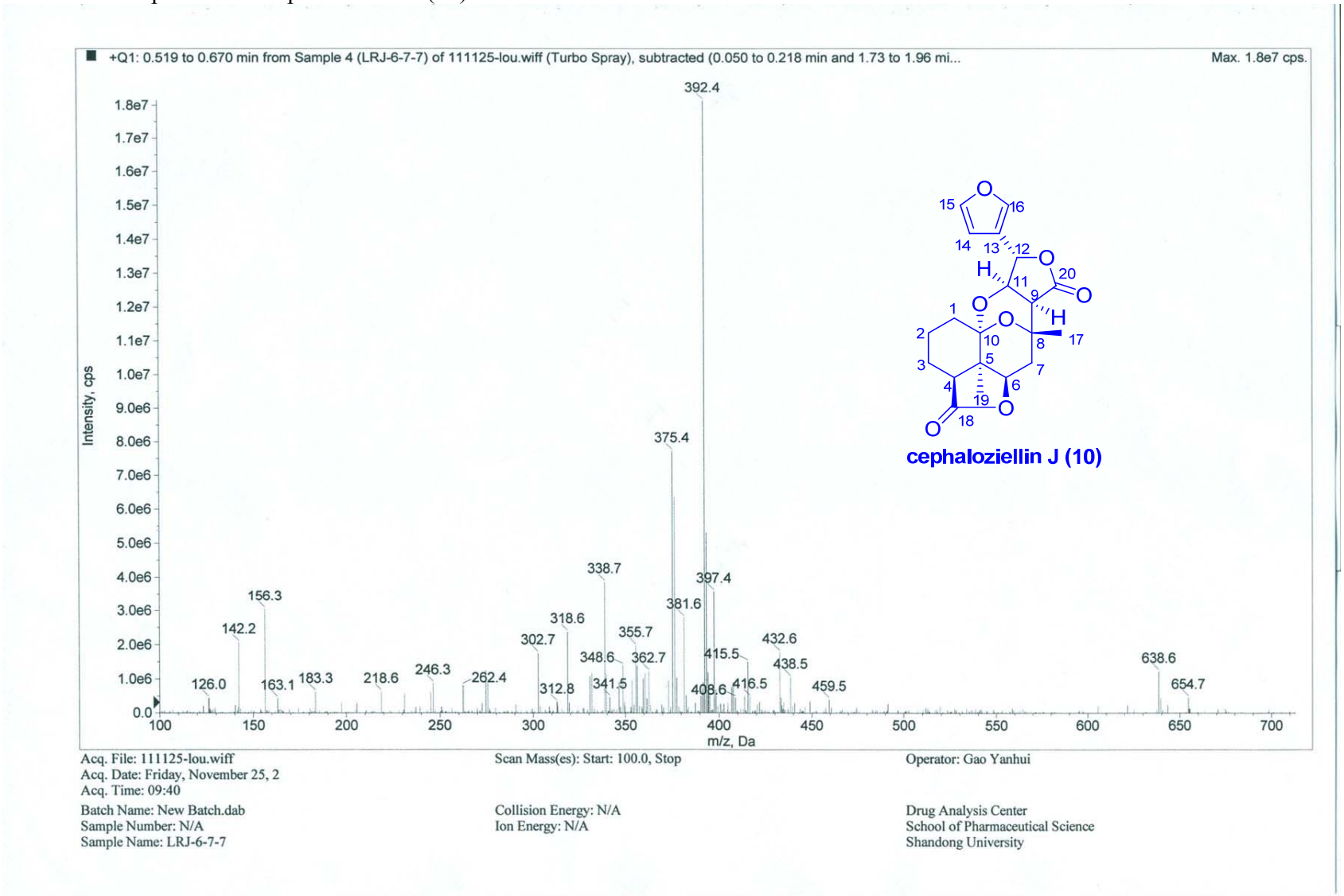
S113. ^{1}H-^{1}H COSY spectrum (600 MHz) of cephaloziellin J (**10**) in $CDCl_3$.



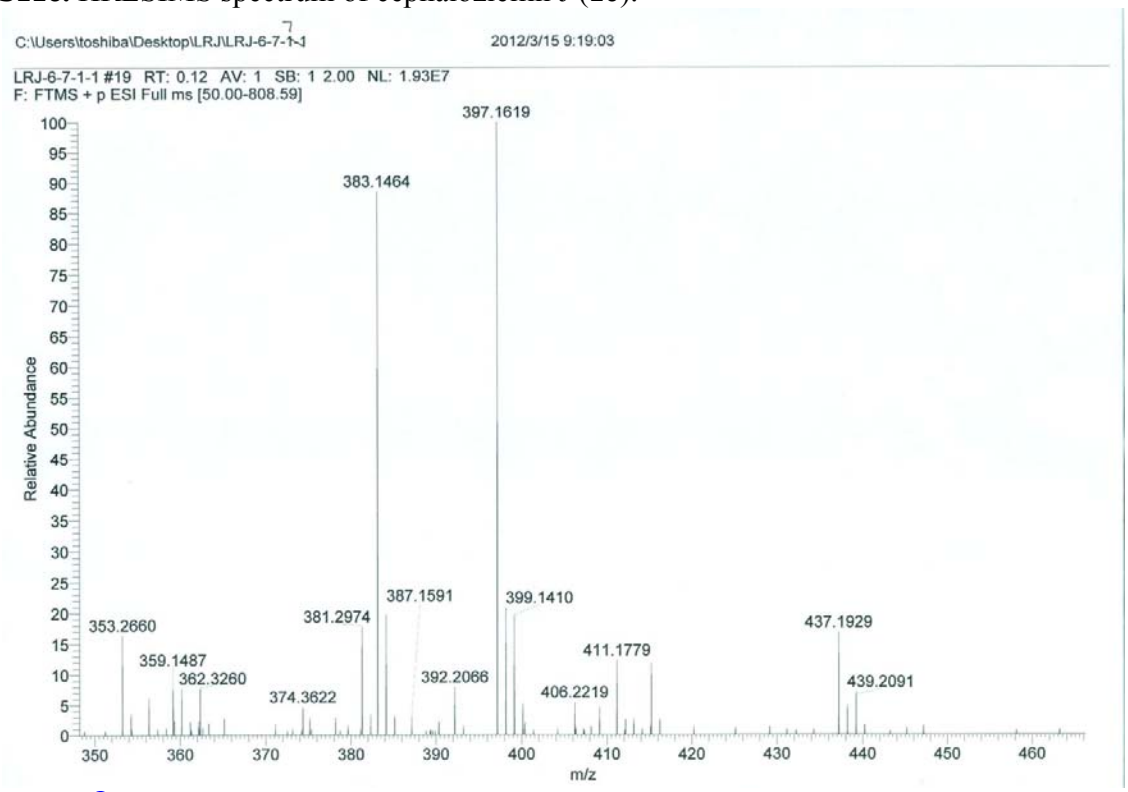
S114. NOESY spectrum (600 MHz) of cephaloziellin J (**10**) in $CDCl_3$.

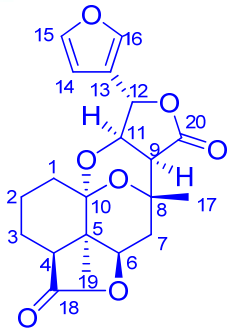


S115. ESIMS spectrum of cephaloziellin J (**10**).



S116. HRESIMS spectrum of cephaloziellin J (**10**).



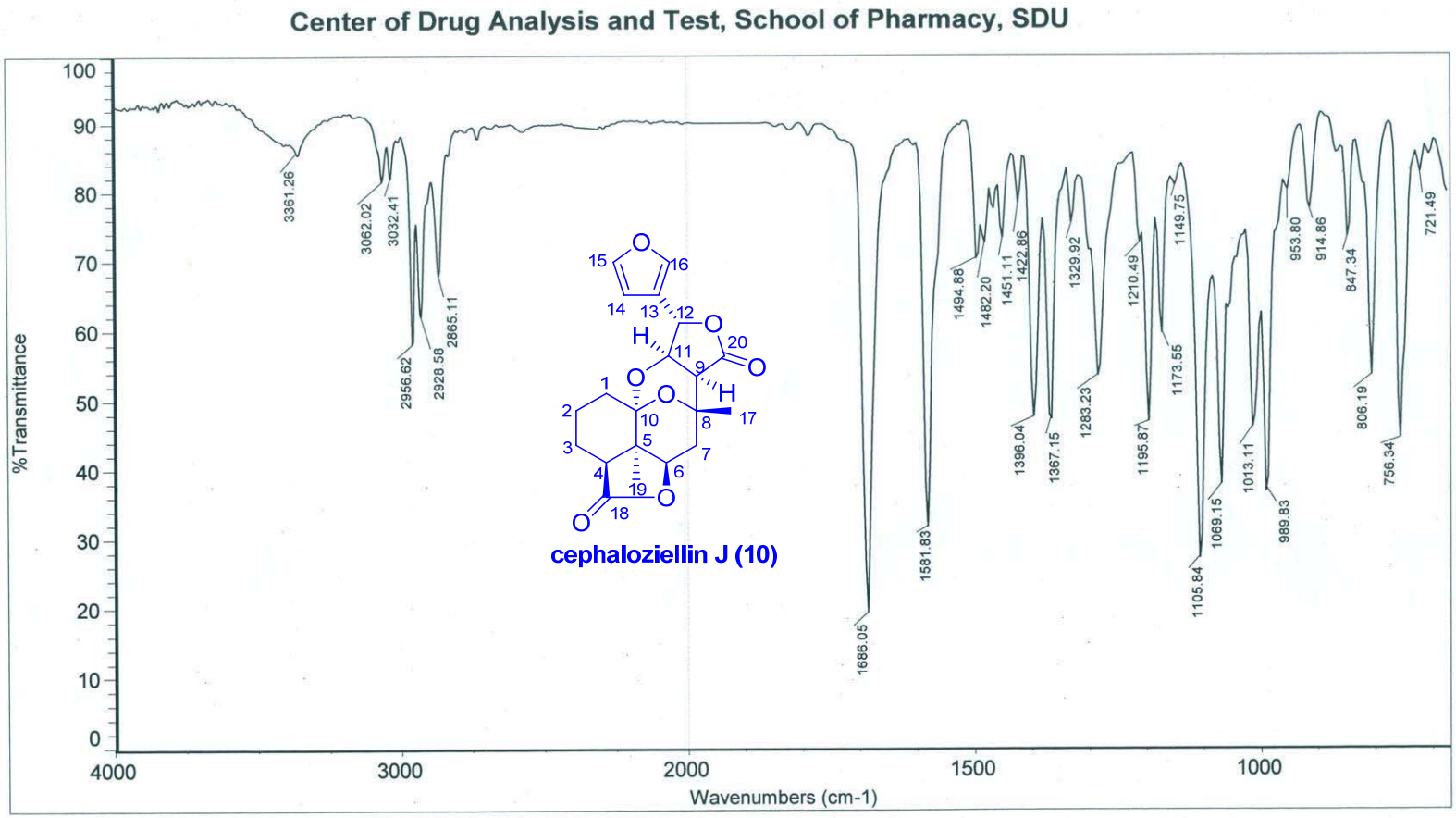


cephaloziellin J (10)

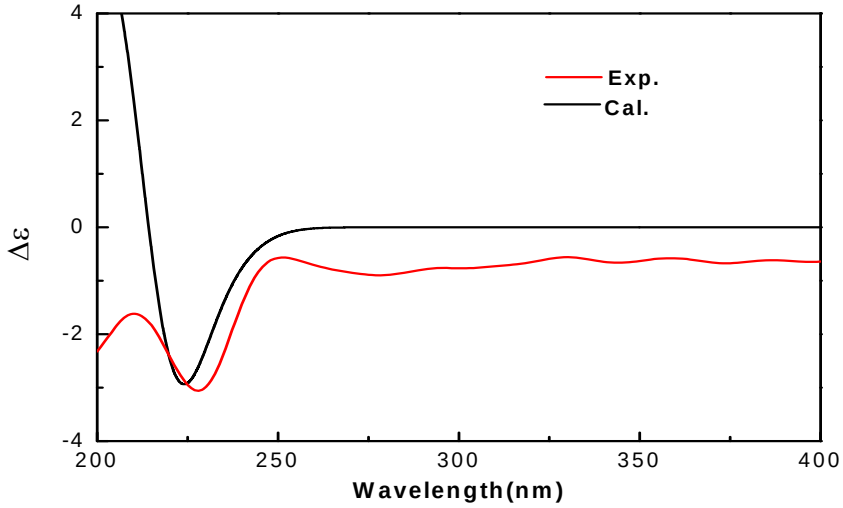
SPECTRUM - simulation :

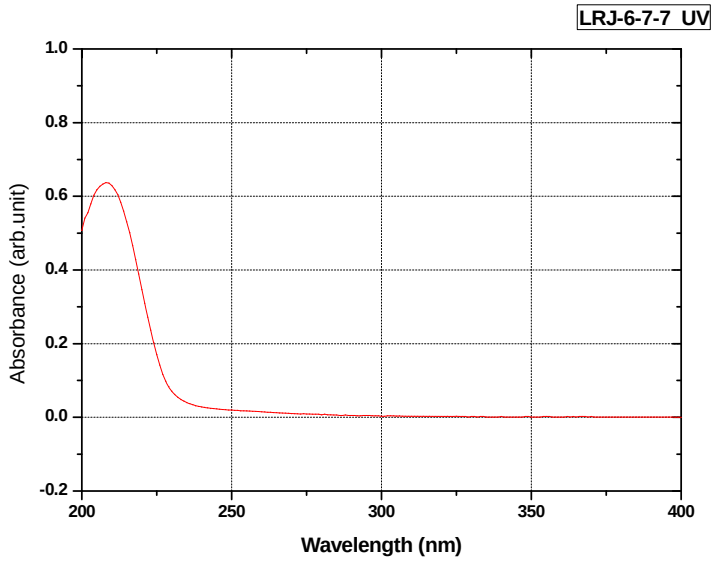
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
397.1619	397.1622	−0.65	8.5	$^{12}C_{20}H_{22}O_7Na$

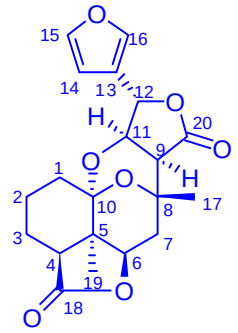
S117. IR spectrum of cephaloziellin J (**10**).



S118. Experimental ECD and calculated ECD, and UV spectra of cephaloziellin J (**10**).

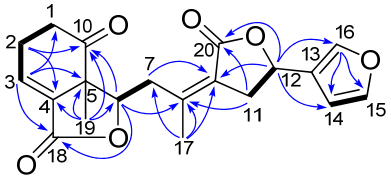






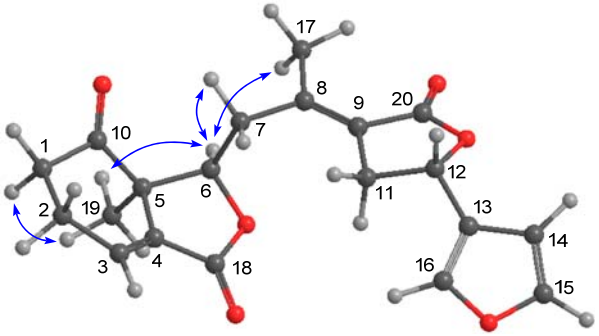
cephaloziellin J (10)

S119. Key HMBC and ^{1}H-^{1}H COSY correlations (in figure) of cephaloziellin K (**11**).



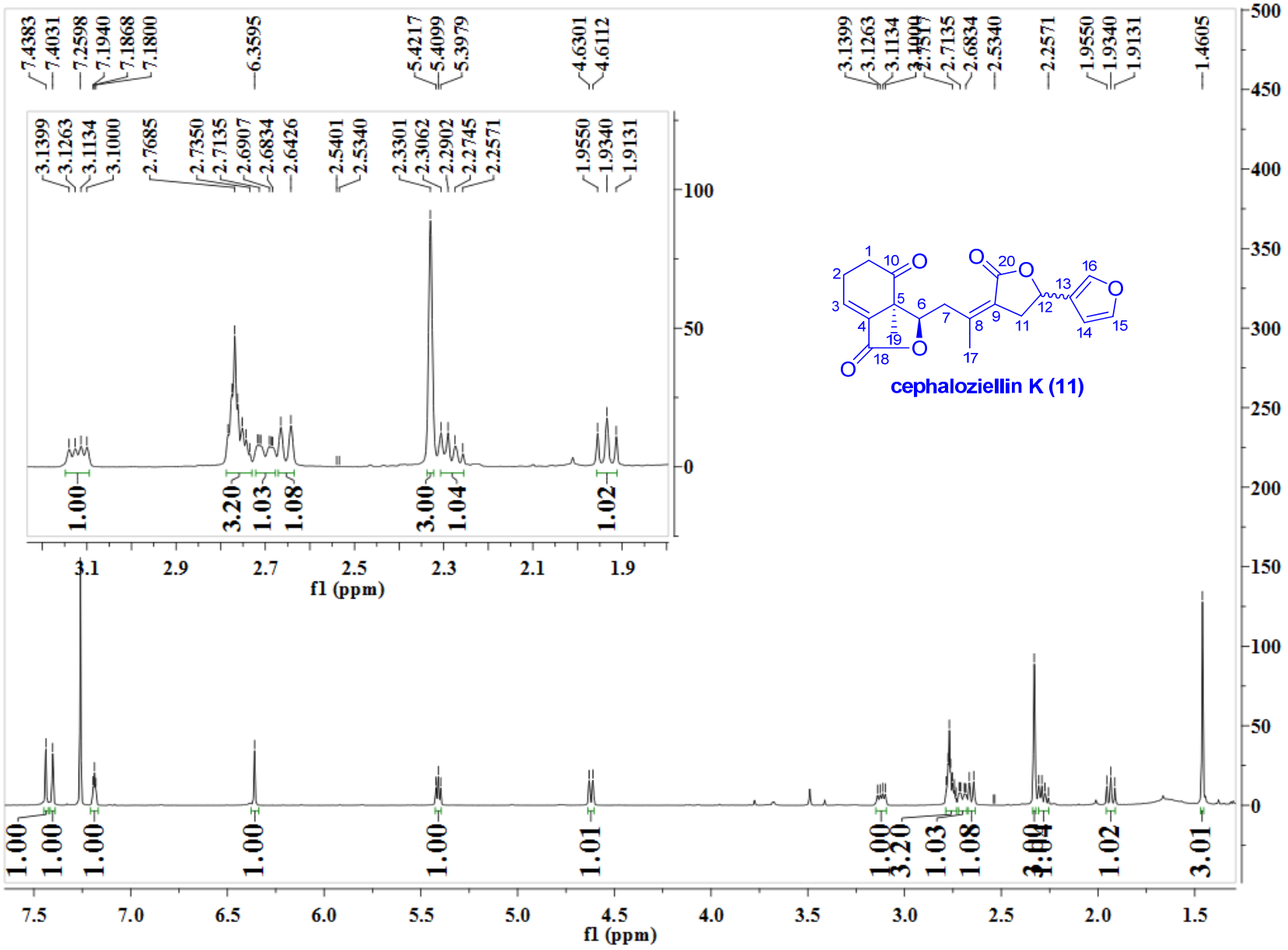
11 HMBC ^{1}H-^{1}H COSY

S120. Key NOESY correlations (in figure) of cephaloziellin K (**11**).

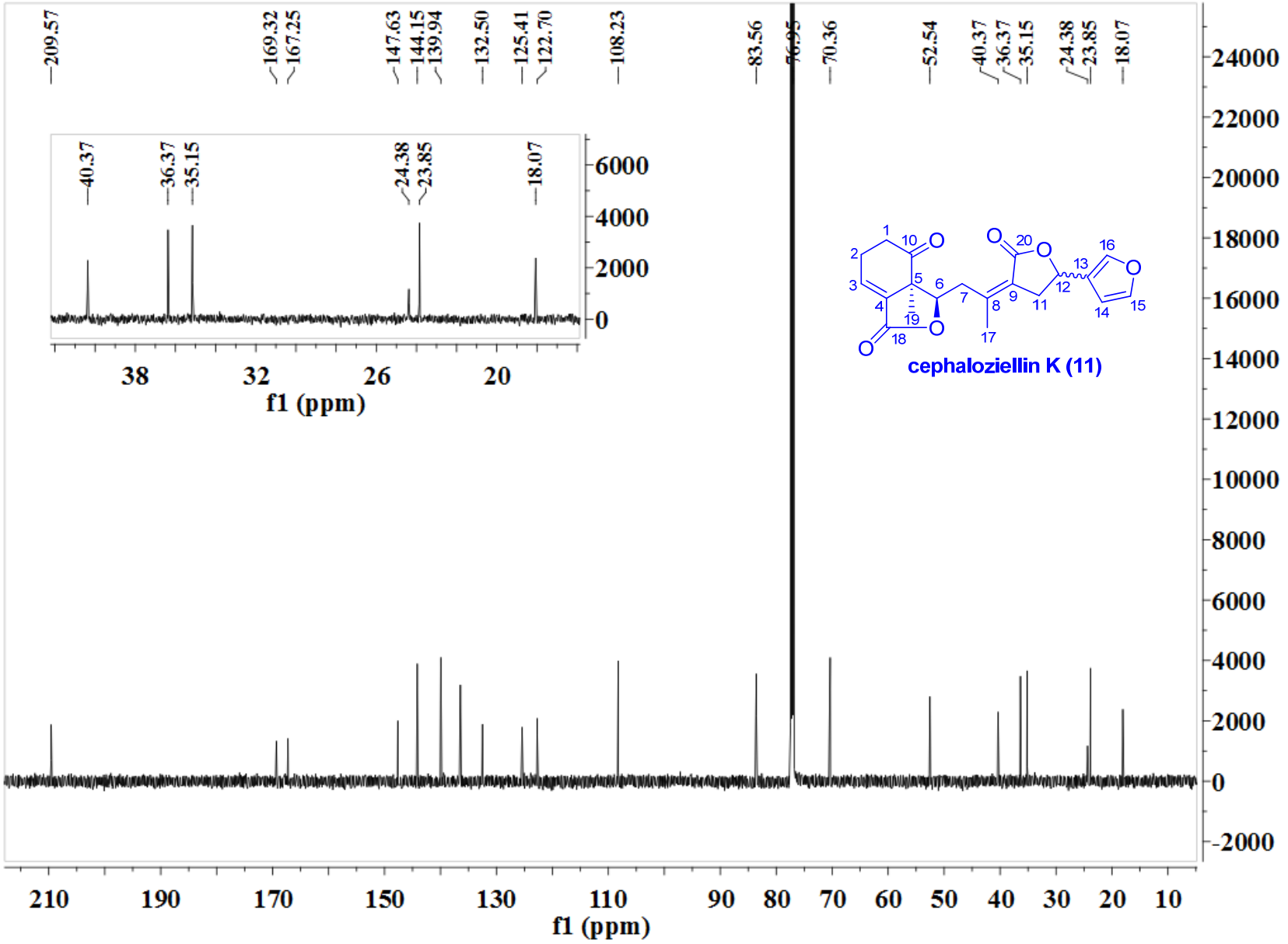


11 NOESY

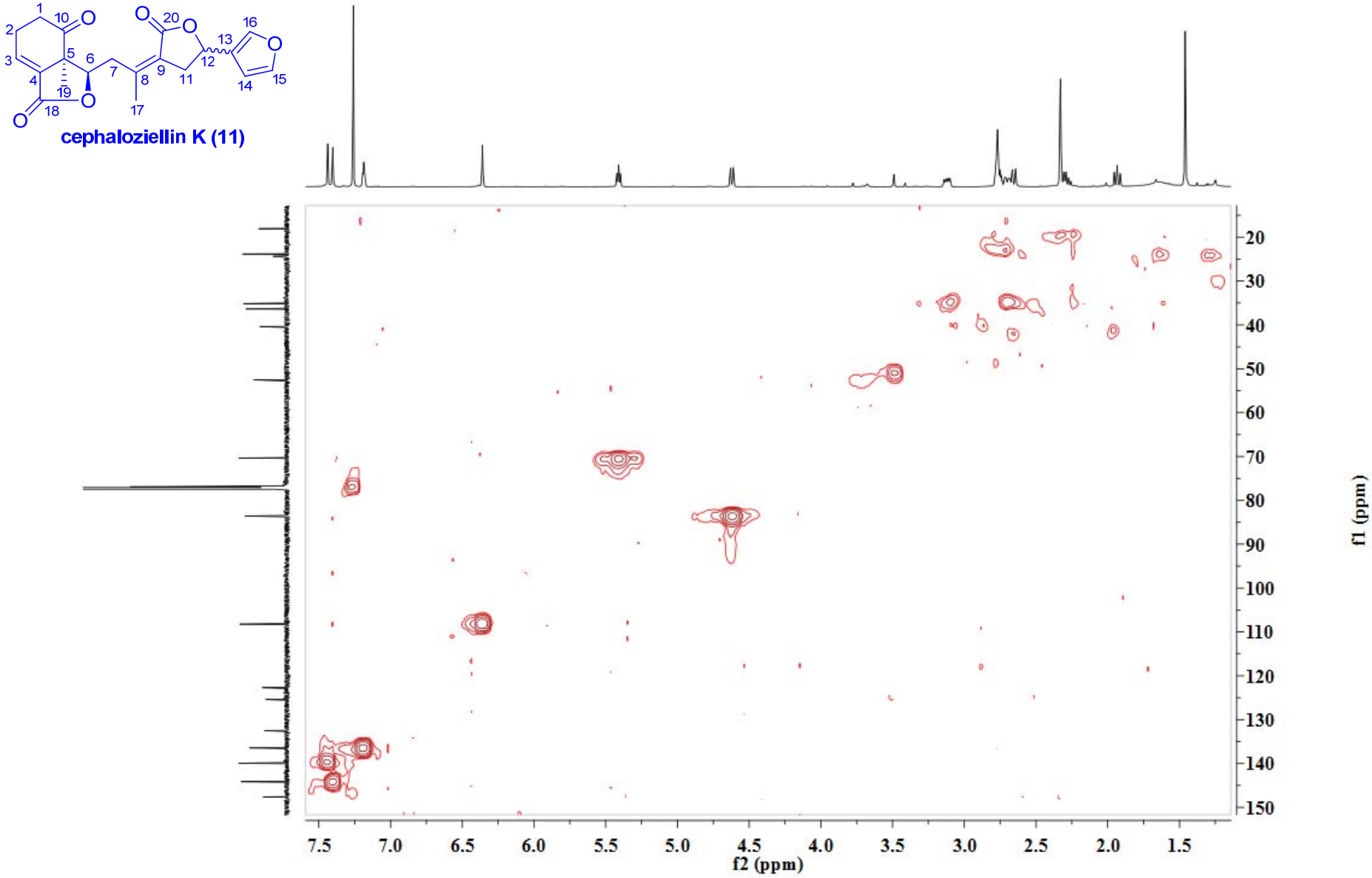
S121. ^{1}H NMR spectrum (600 MHz) of cephaloziellin K (**11**) in $CDCl_3$.



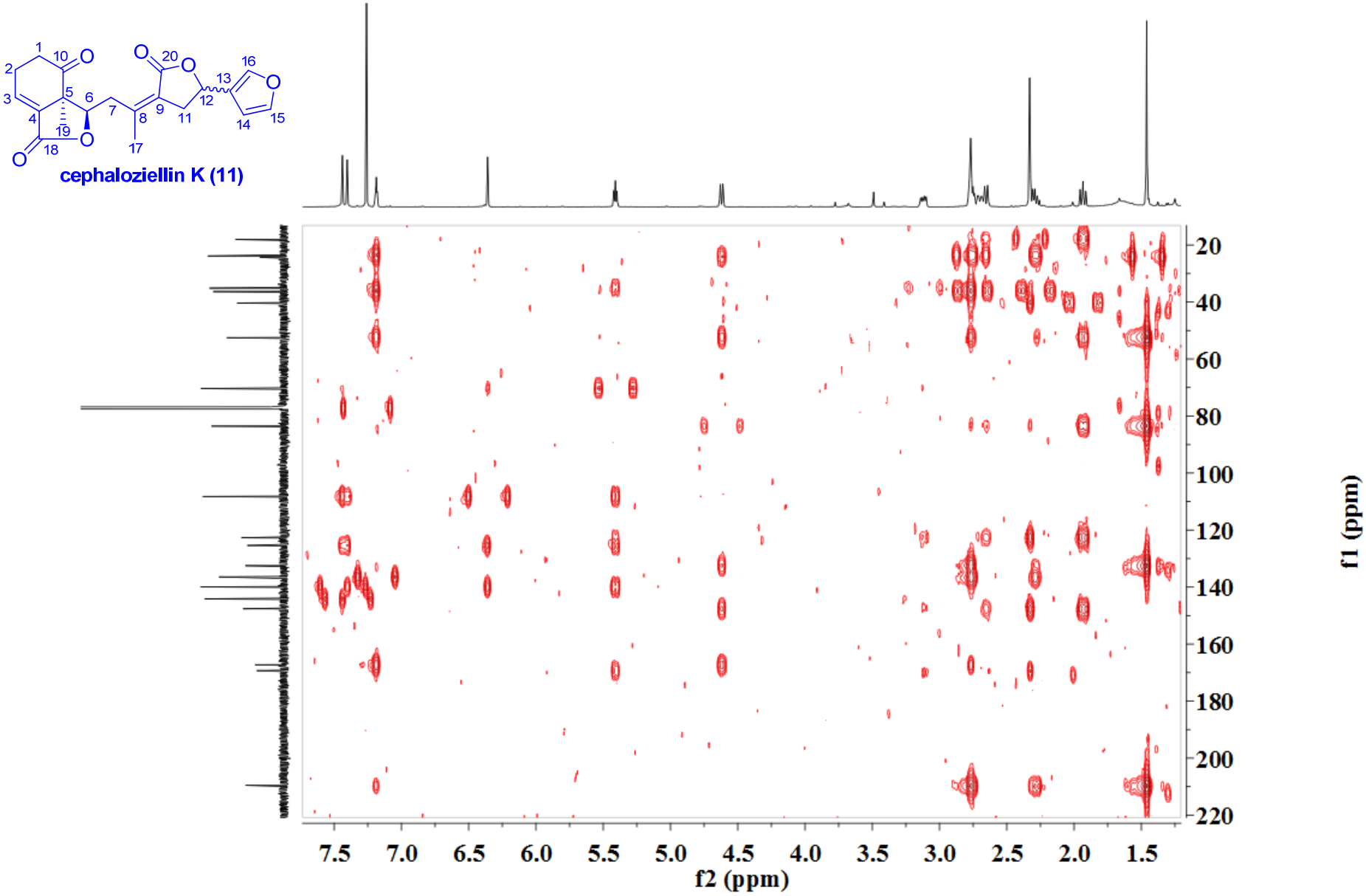
S122. ^{13}C NMR spectrum (150 MHz) of cephaloziellin K (**11**) in $CDCl_3$.



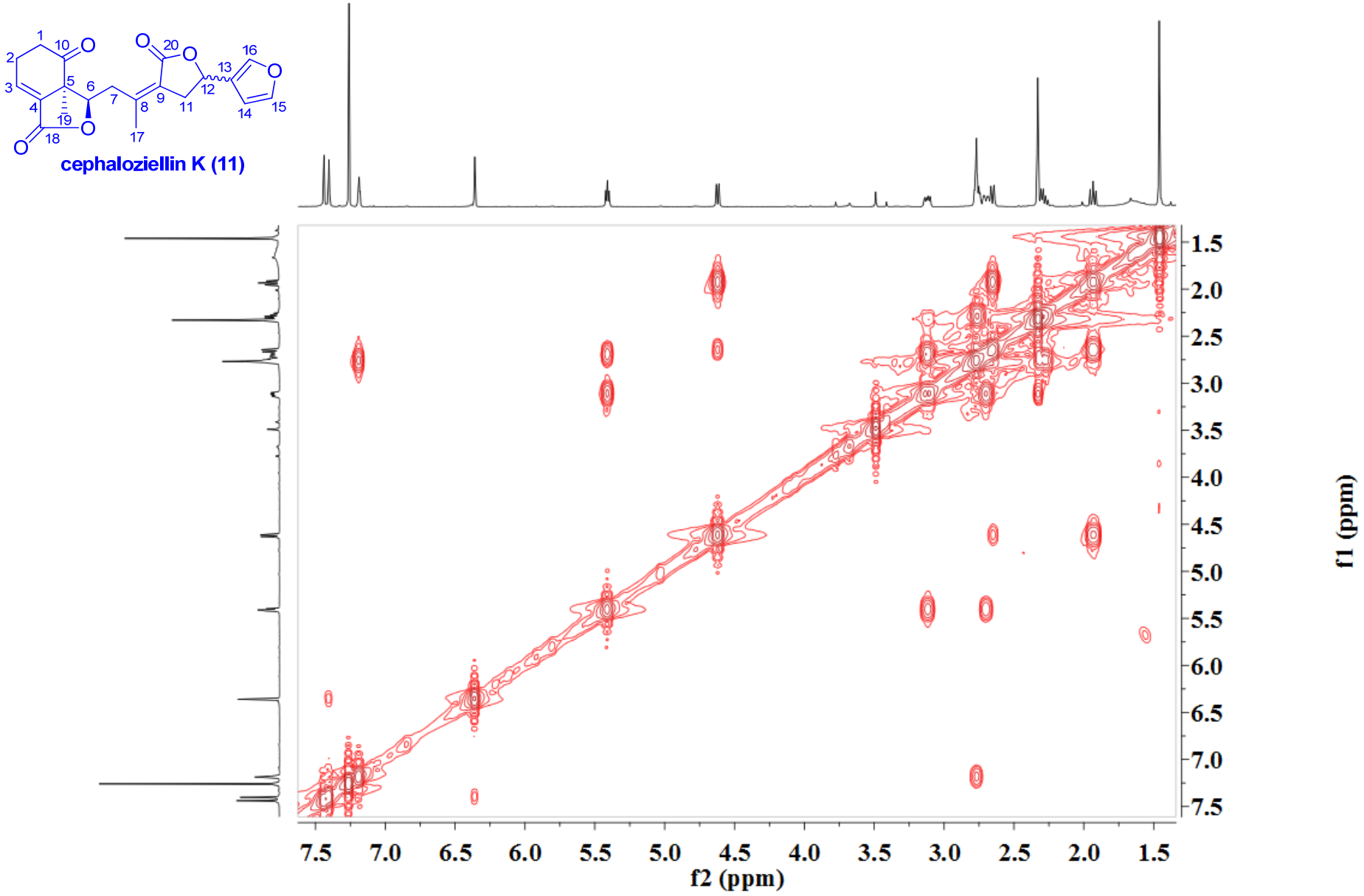
S123. HSQC spectrum (600 MHz) of cephaloziellin K (**11**) in $CDCl_3$.



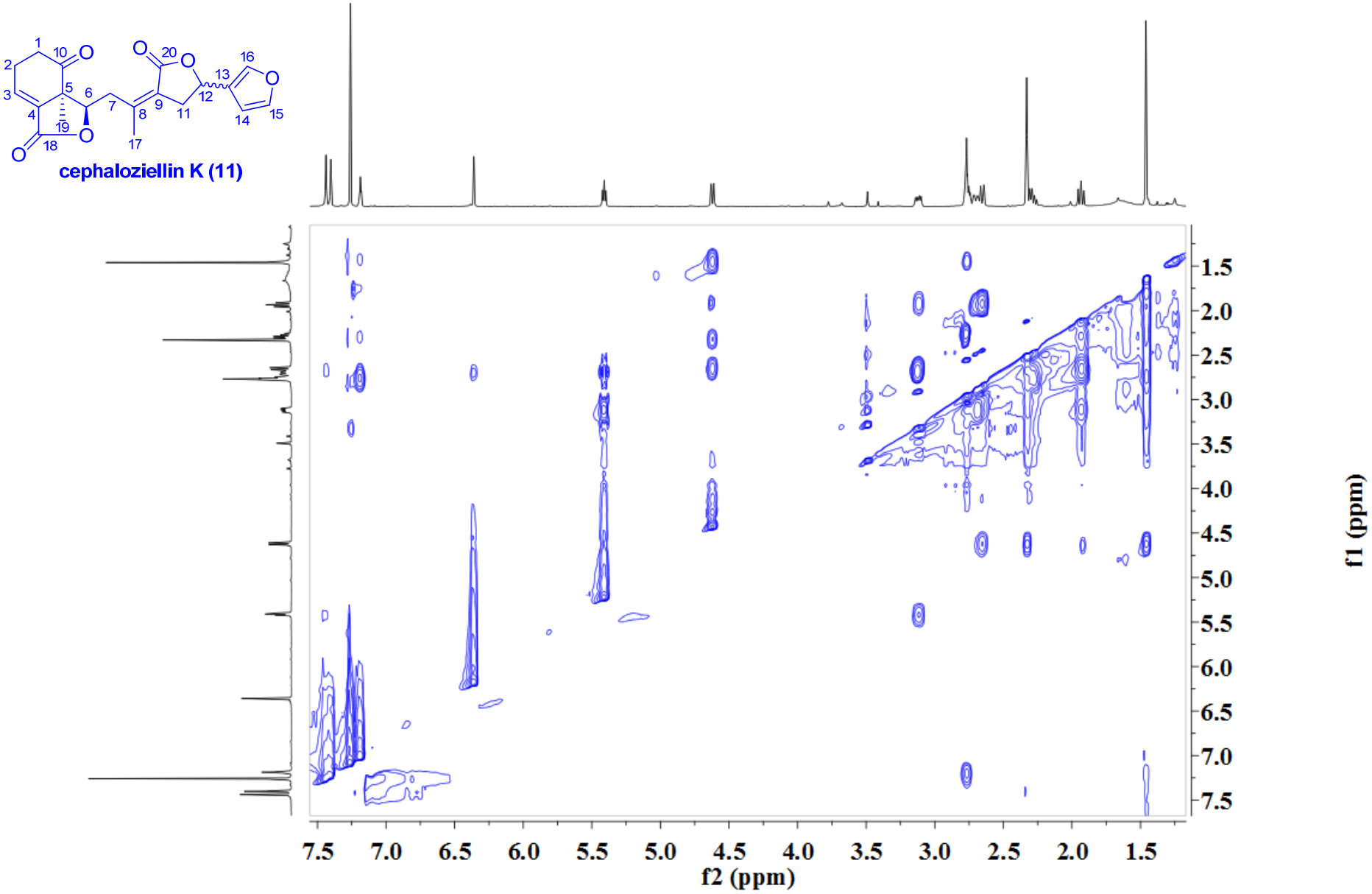
S124. HMBC spectrum (600 MHz) of cephaloziellin K (**11**) in $CDCl_3$.



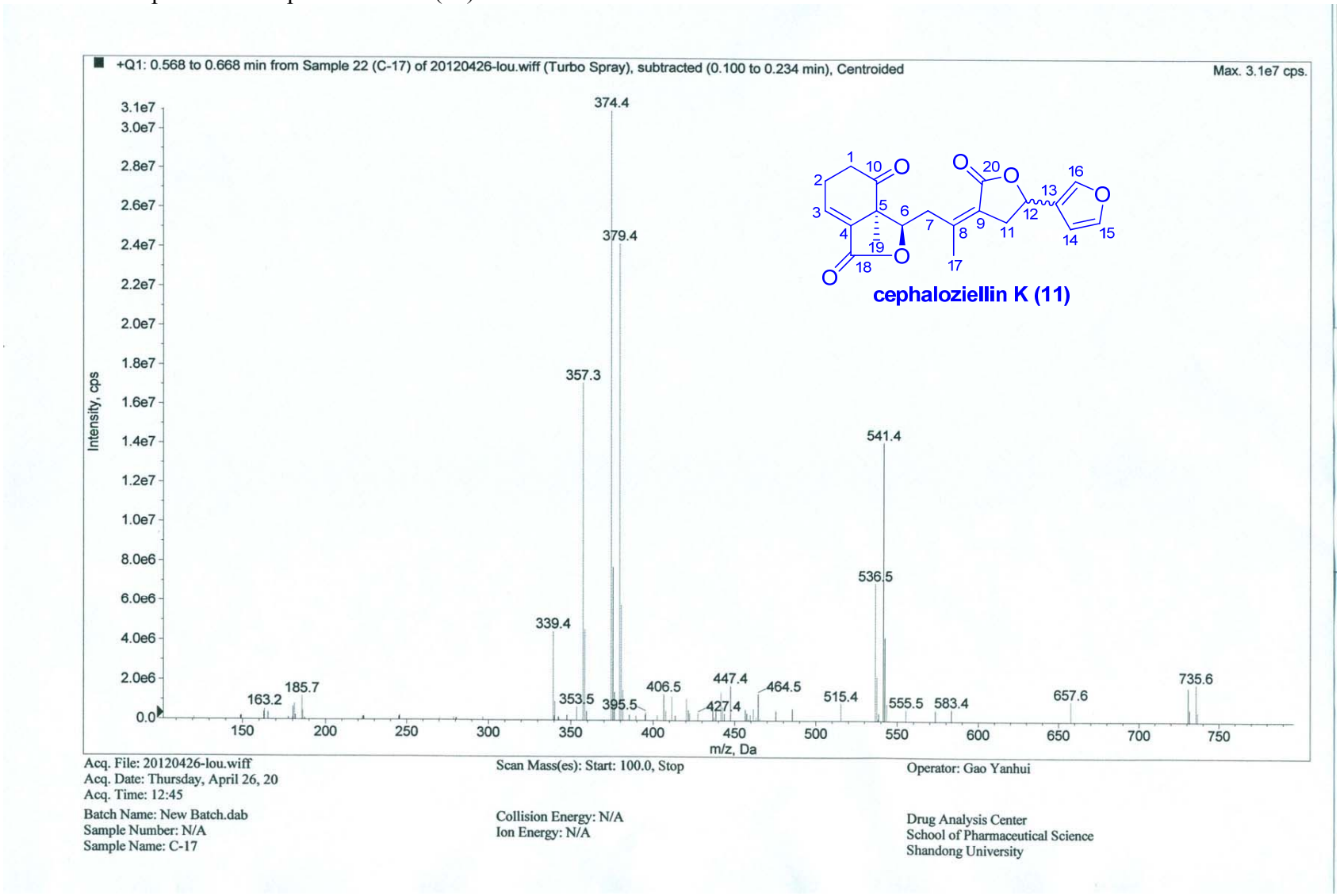
S125. ^{1}H-^{1}H COSY spectrum (600 MHz) of cephaloziellin K (**11**) in $CDCl_3$.



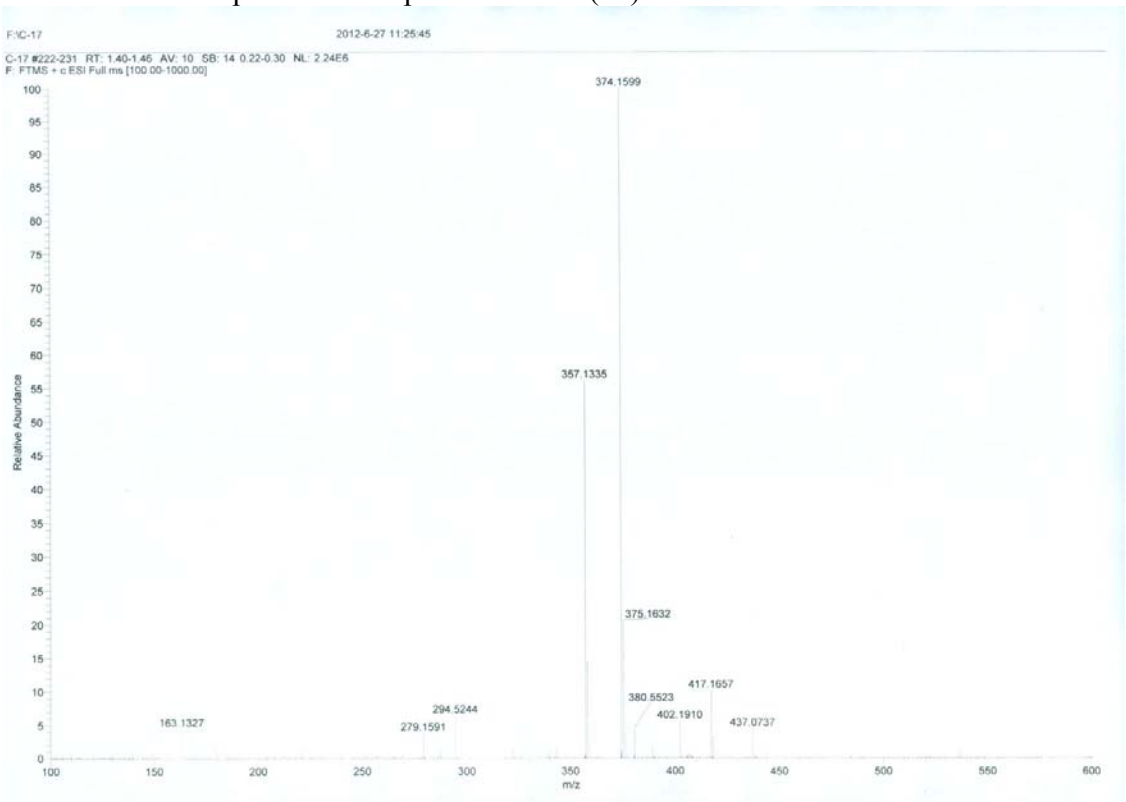
S126. NOESY spectrum (600 MHz) of cephaloziellin K (**11**) in $CDCl_3$.

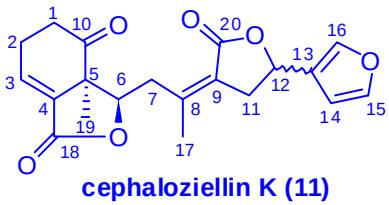


S127. ESIMS spectrum of cephaloziellin K (**11**).



S128. HRESIMS spectrum of cephaloziellin K (**11**).



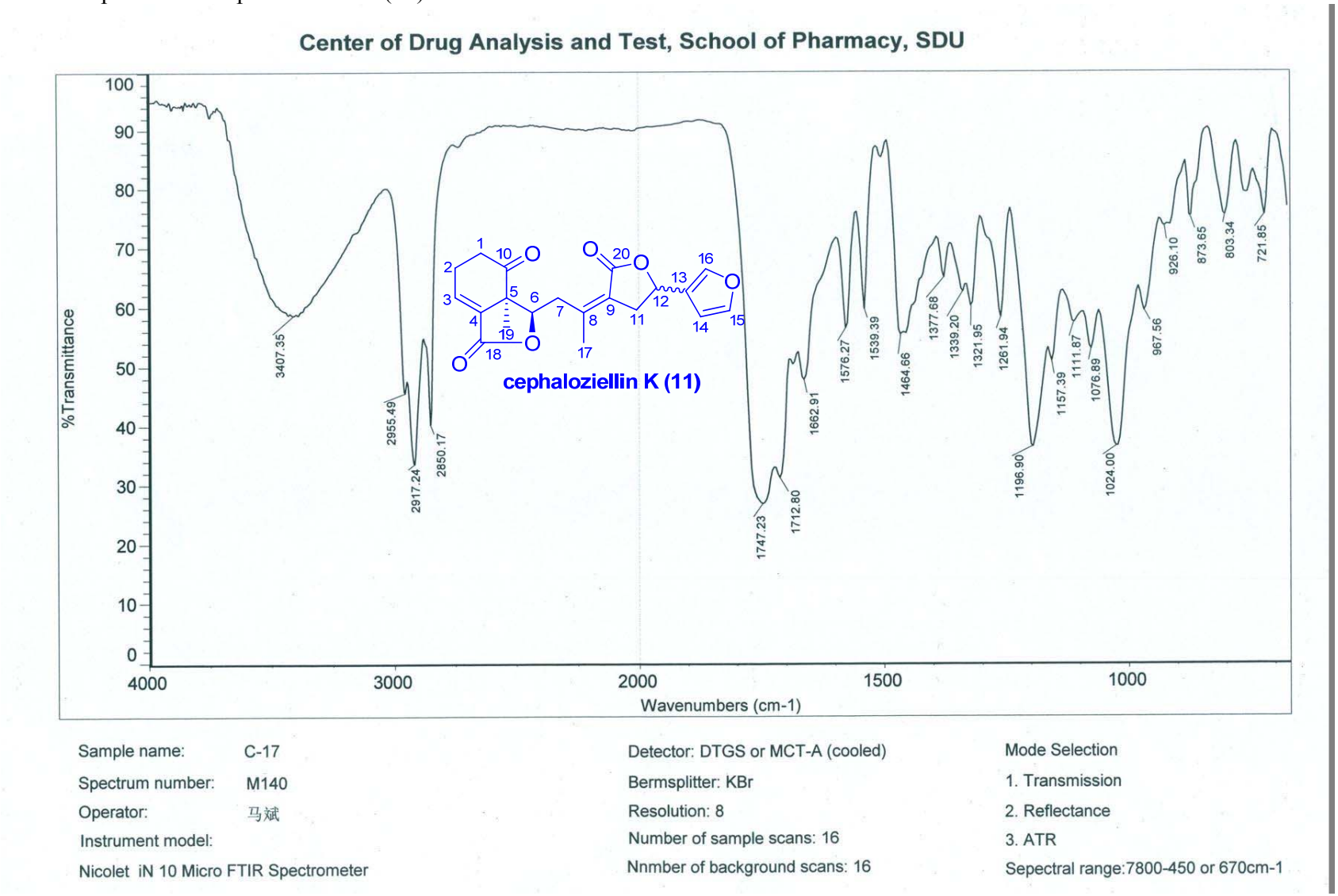


cephaloziellin K (11)

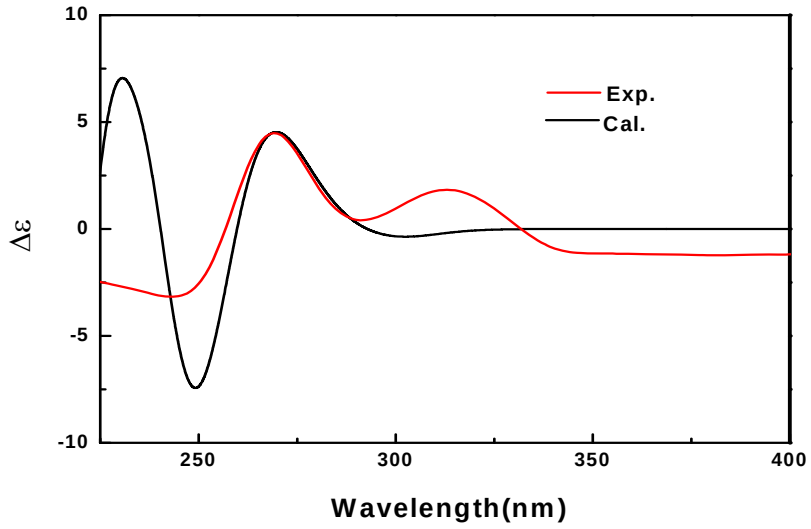
SPECTRUM - simulation :

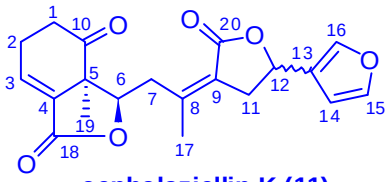
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
357.1335	357.1333	0.57	10.5	$^{12}C_{20}H_{21}O_6$

S129. IR spectrum of cephaloziellin K (**11**).

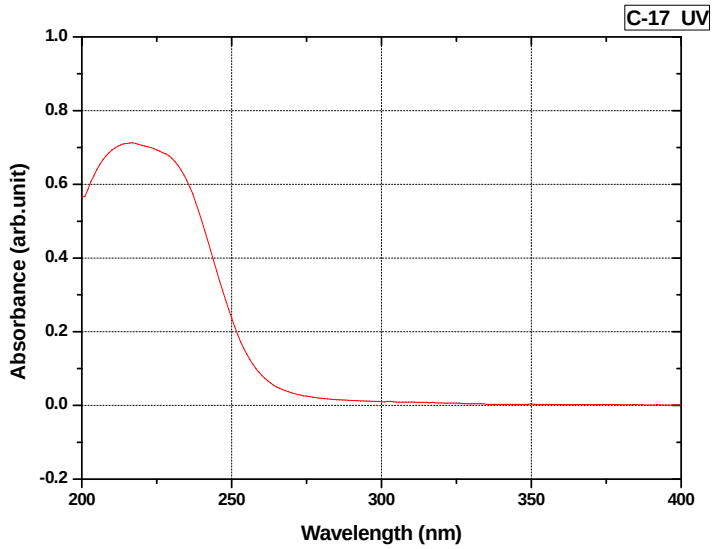


S130. Experimental ECD and calculated ECD, and UV spectra of cephaloziellin K (**11**).

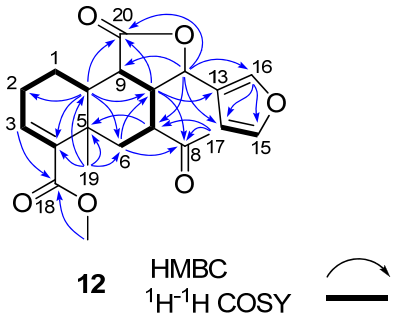




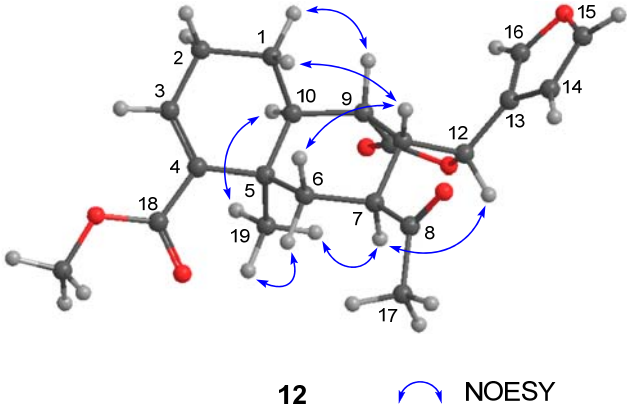
cephaloziellin K (11)



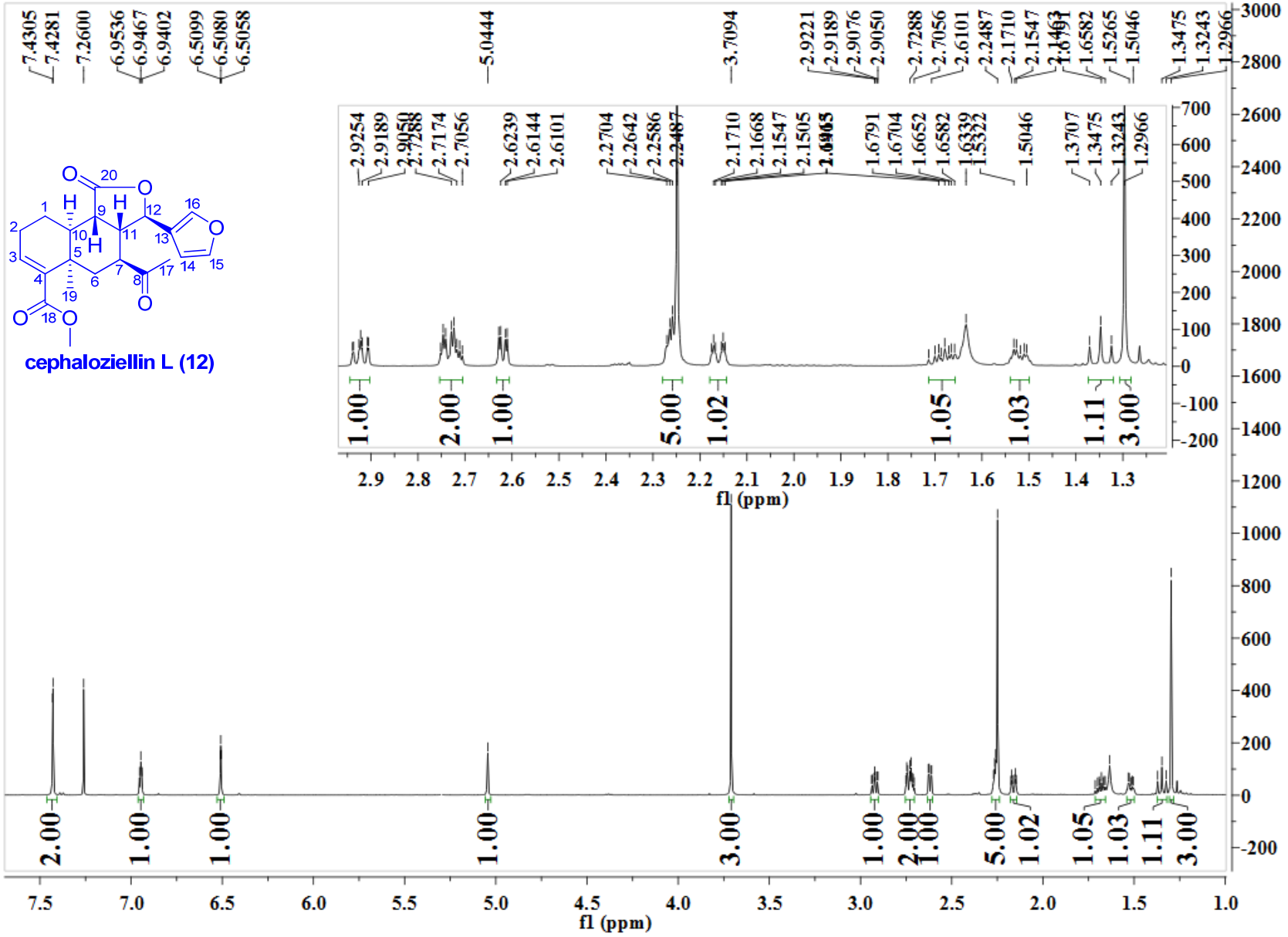
S131. Key HMBC and ^{1}H-^{1}H COSY correlations (in figure) cephaloziellin L (**12**).



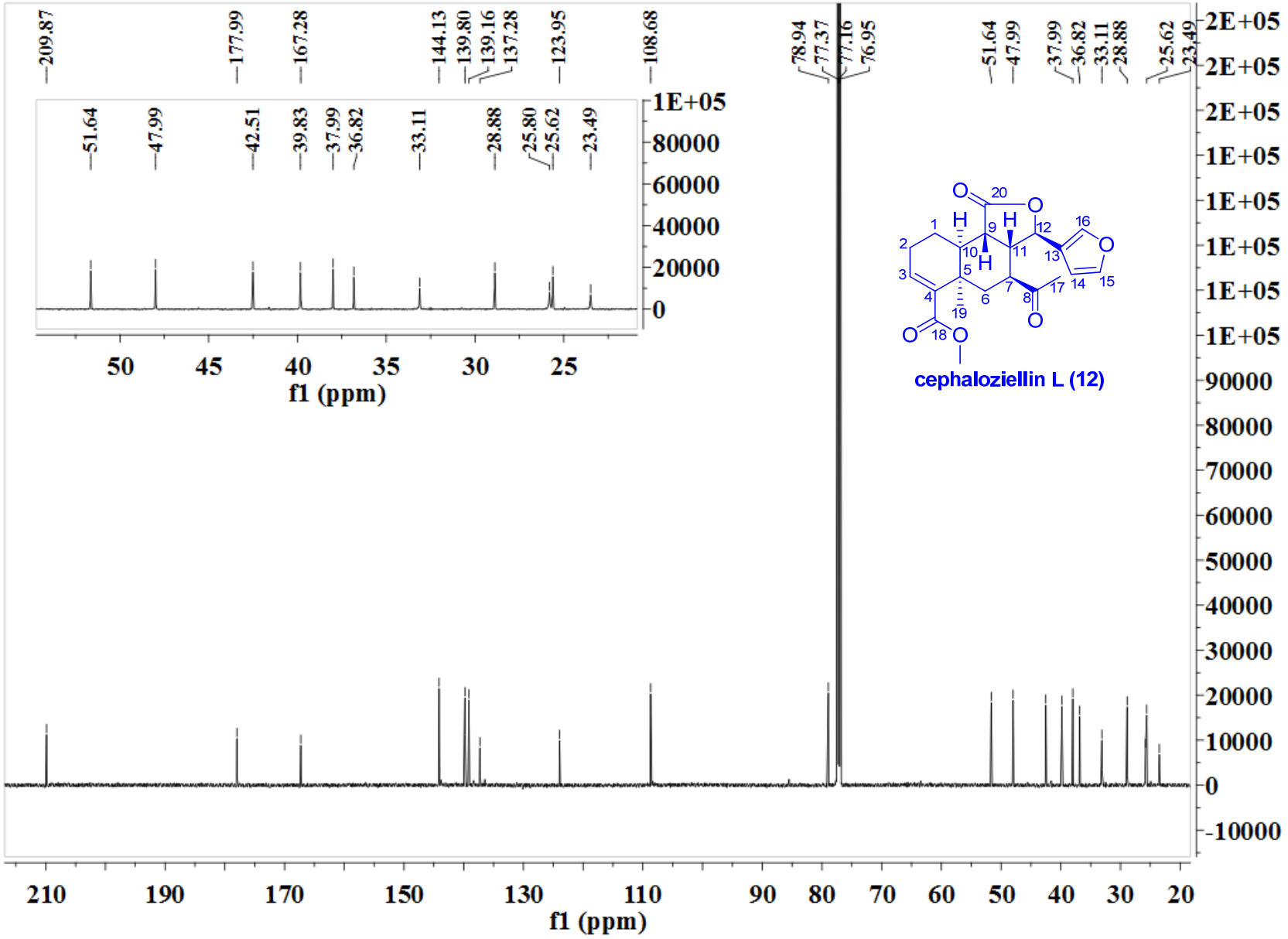
S132. Key NOESY correlations (in figure) of cephaloziellin L (**12**).



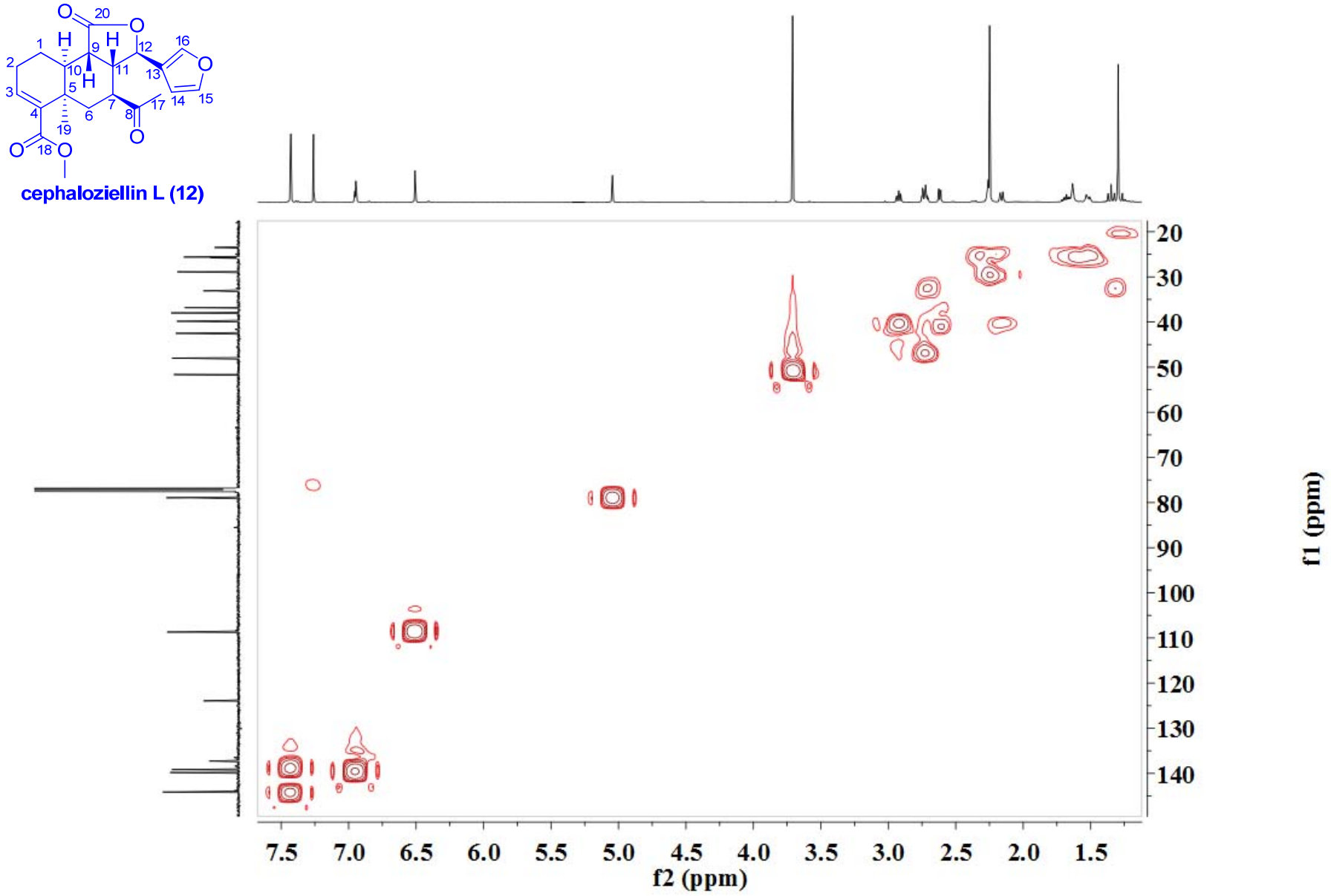
S133. ^{1}H NMR spectrum (600 MHz) of cephaloziellin L (**12**) in $CDCl_3$.



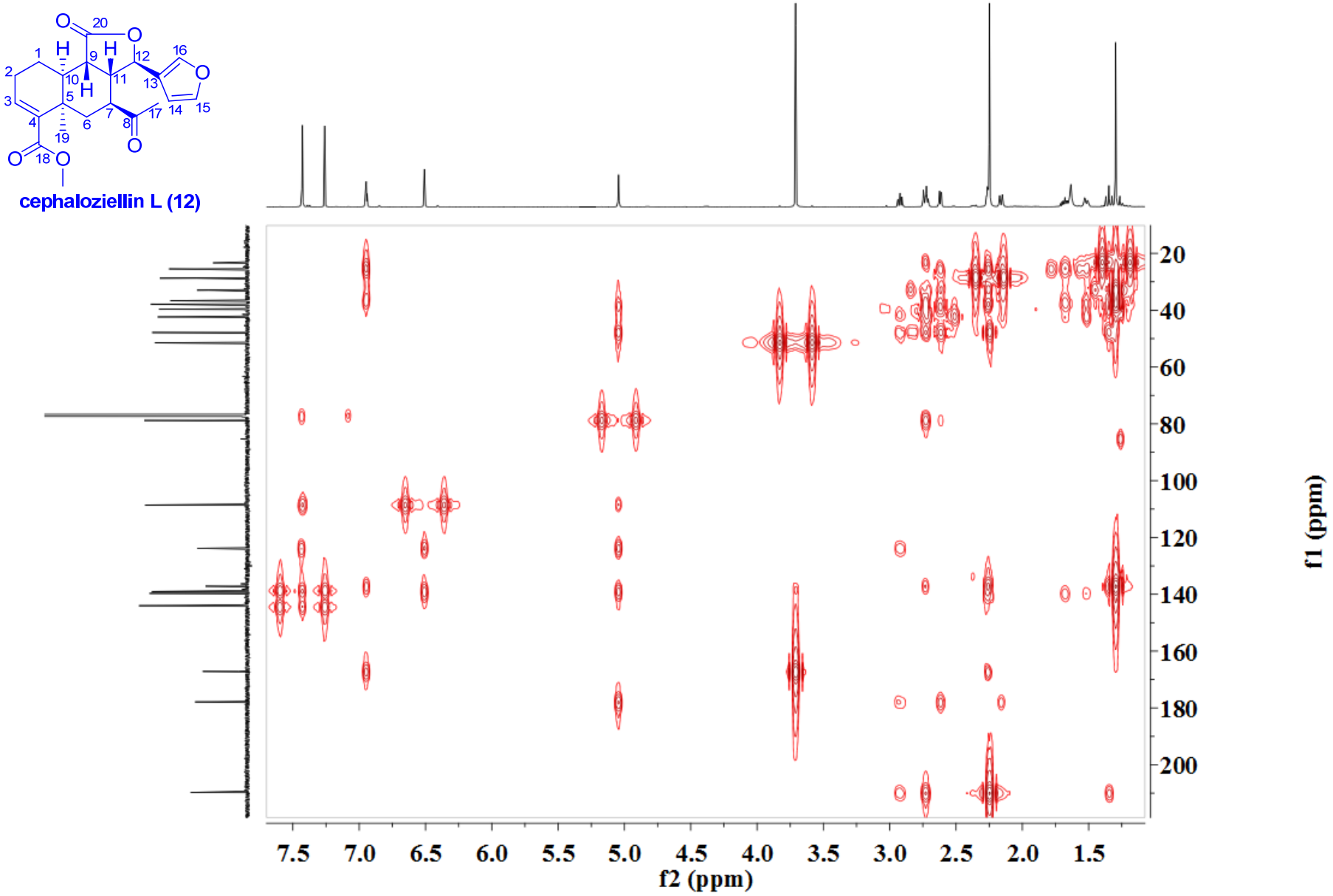
S134. ^{13}C NMR spectrum (150 MHz) of cephaloziellin L (**12**) in $CDCl_3$.



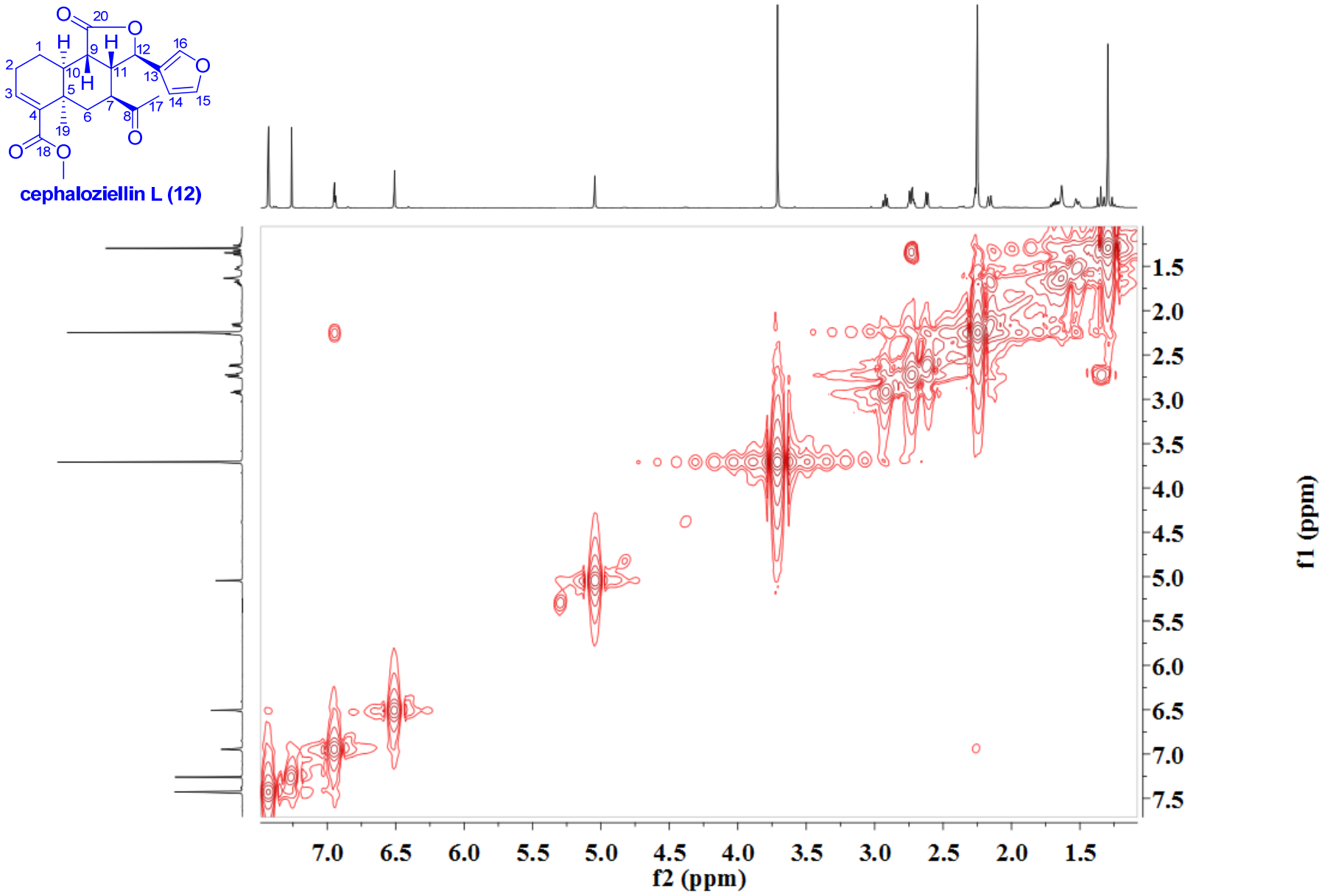
S135. HSQC spectrum (600 MHz) of cephaloziellin L (**12**) in $CDCl_3$.



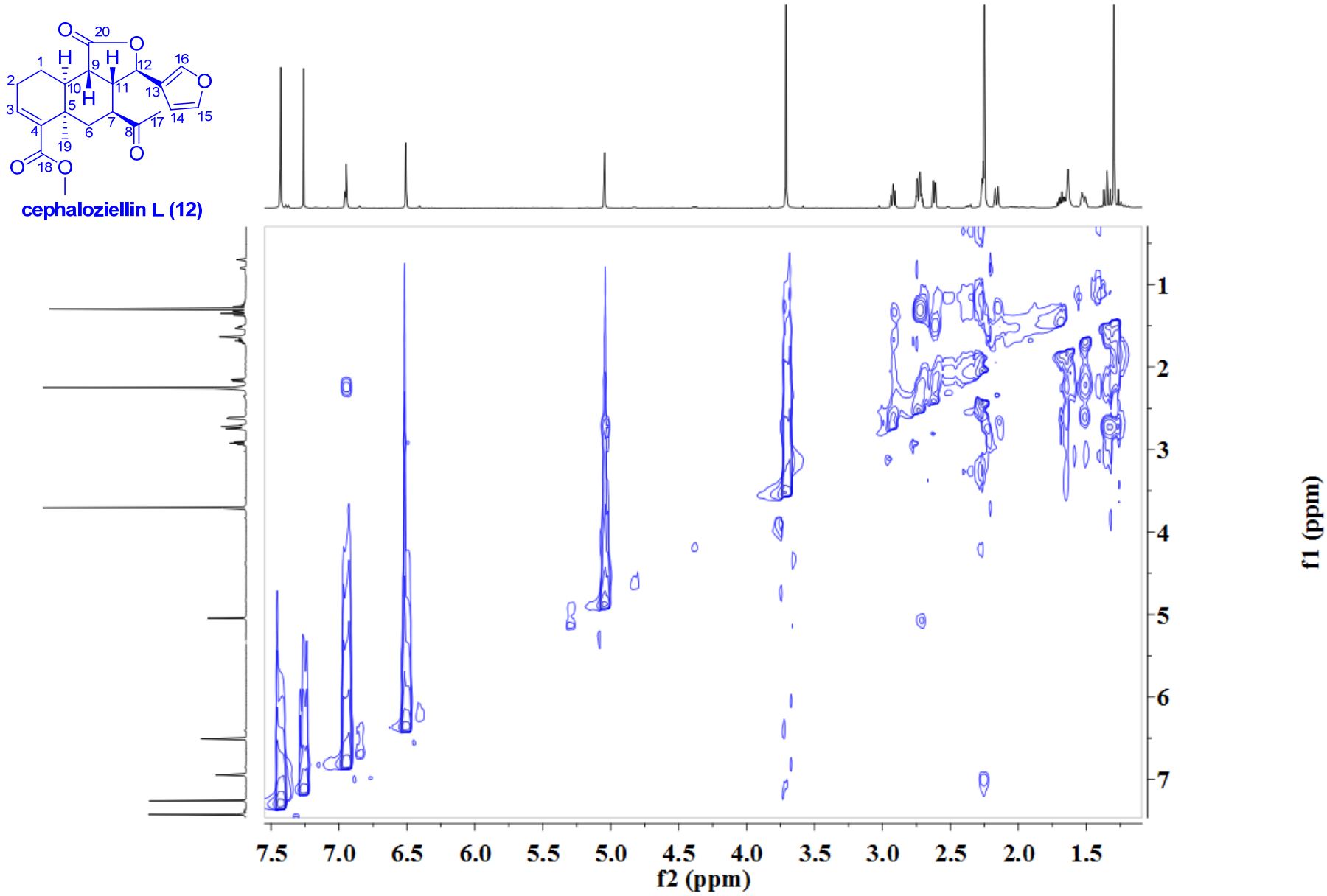
S136. HMBC spectrum (600 MHz) of cephaloziellin L (**12**) in $CDCl_3$.



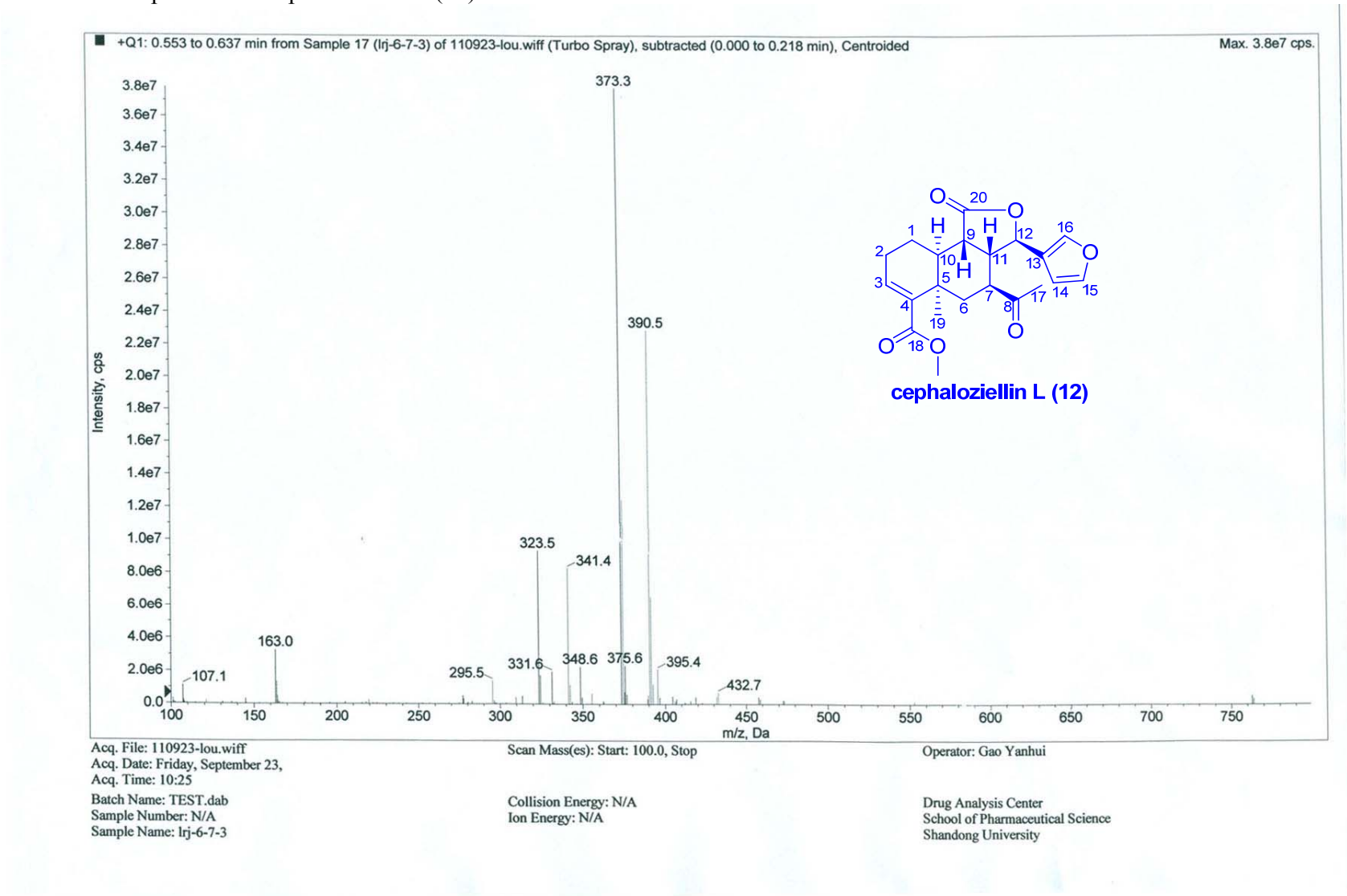
S137. ^{1}H-^{1}H COSY spectrum (600 MHz) of cephaloziellin L (**12**) in $CDCl_3$.



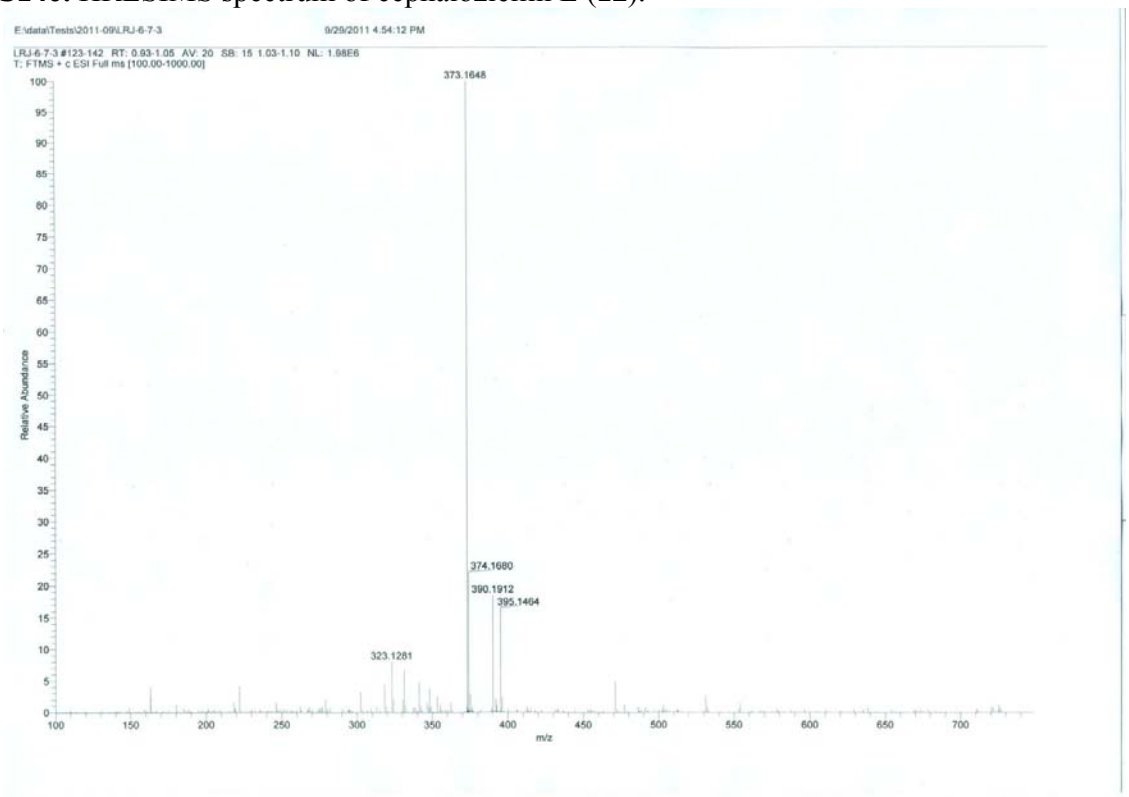
S138. NOESY spectrum (600 MHz) of cephaloziellin L (**12**) in $CDCl_3$.

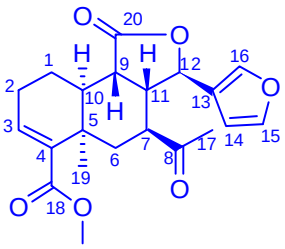


S139. ESIMS spectrum of cephaloziellin L (**12**).



S140. HRESIMS spectrum of cephaloziellin L (**12**).



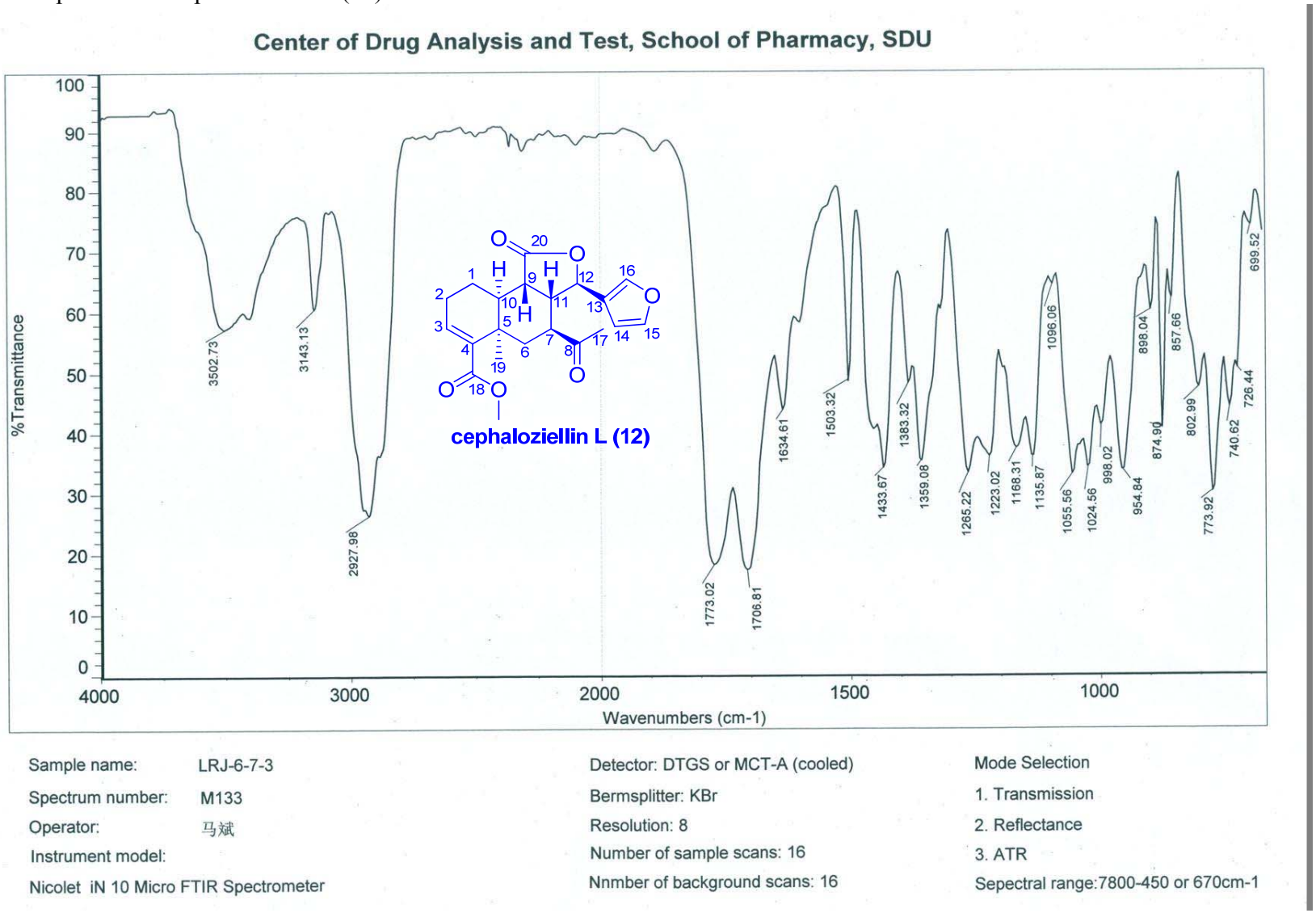


cephaloziellin L (12)

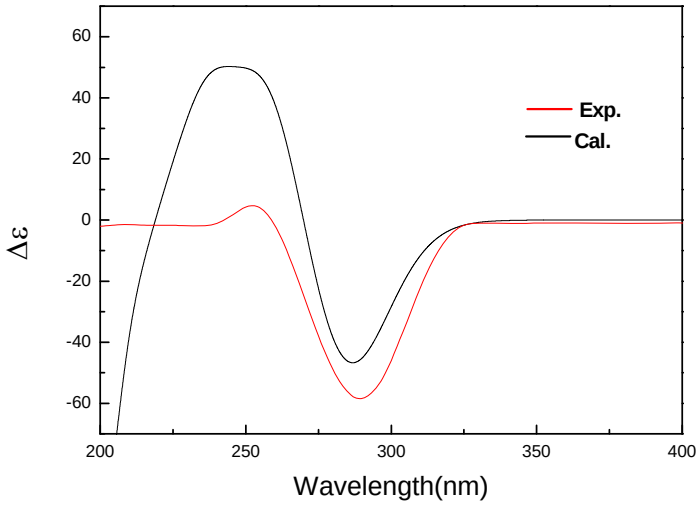
SPECTRUM - simulation :

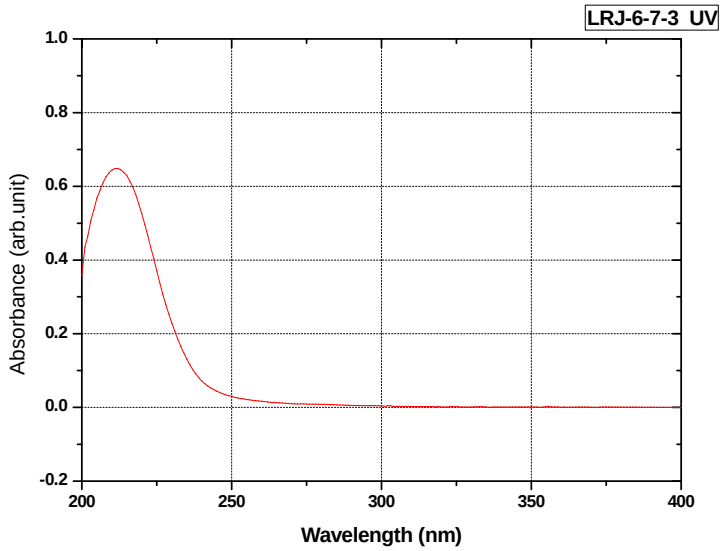
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
373.1648	373.1646	0.58	9.5	$^{12}C_{21}H_{25}O_6$

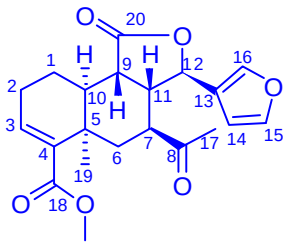
S141. IR spectrum of cephaloziellin L (**12**).



S142. Experimental ECD and calculated ECD, and UV spectra of cephaloziellin L (**12**).

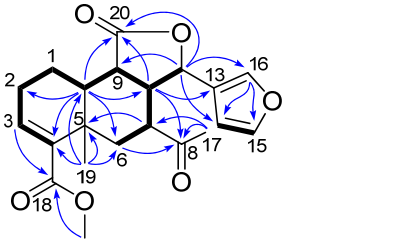






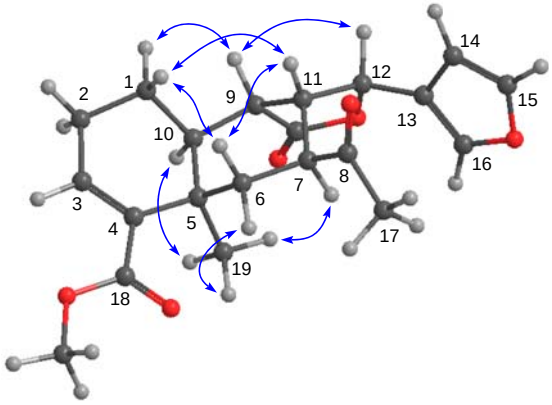
cephaloziellin L (12)

S143. Key HMBC and ^{1}H-^{1}H COSY correlations (in figure) of cephaloziellin M (**13**).



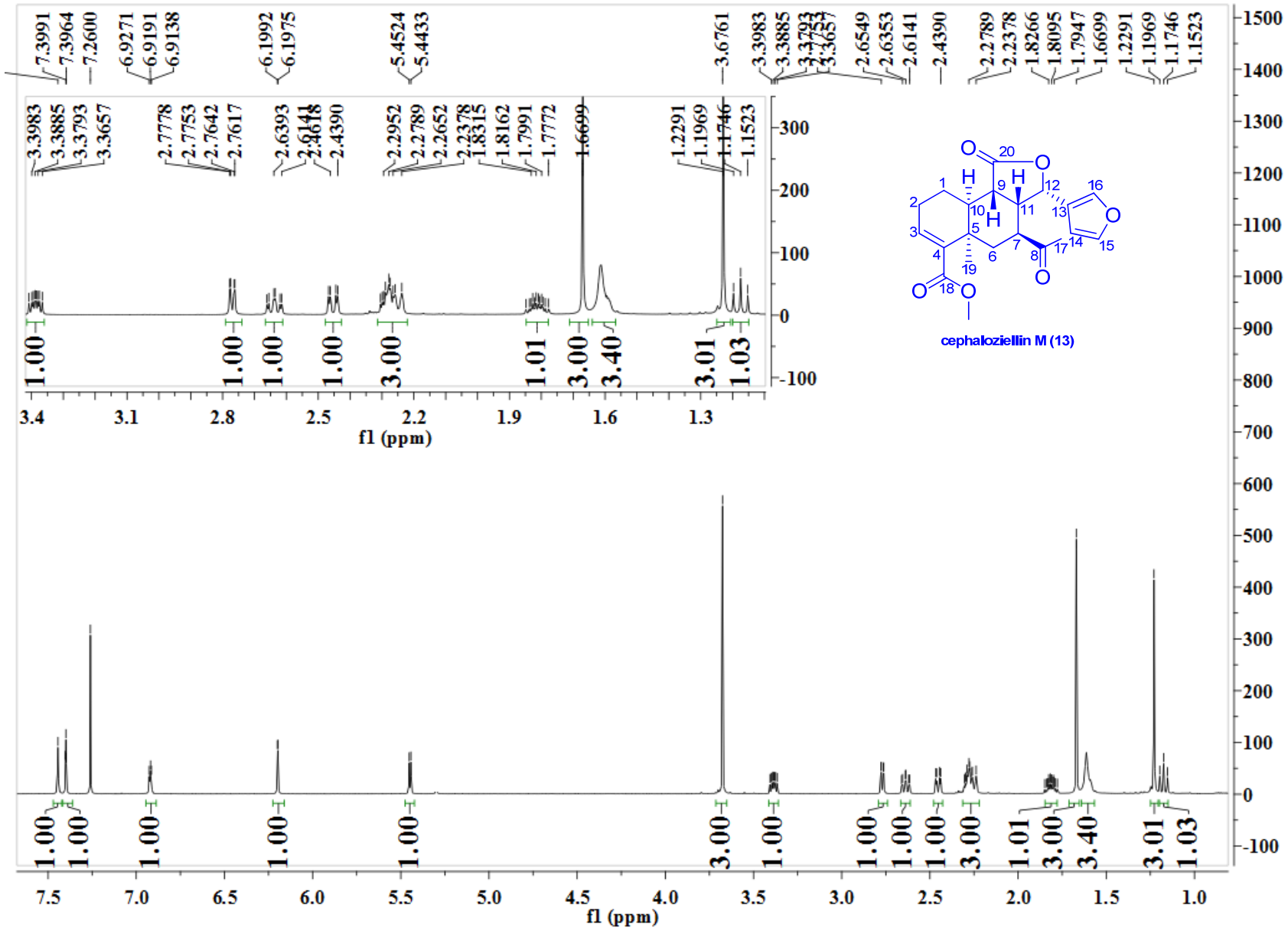
13 HMBC ^{1}H-^{1}H COSY

S144. Key NOESY correlations (in figure) of cephaloziellin M (**13**).

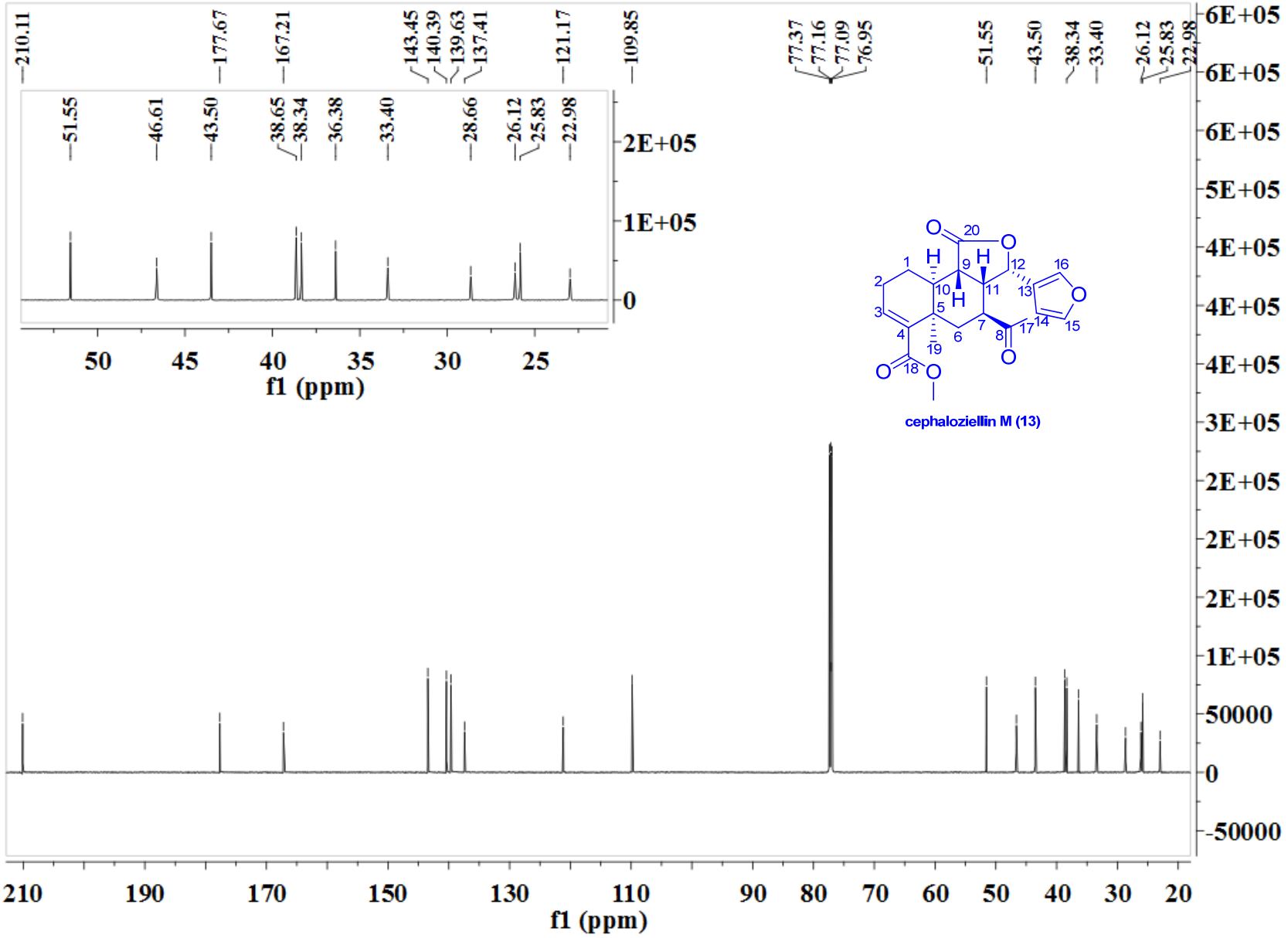


13 NOESY

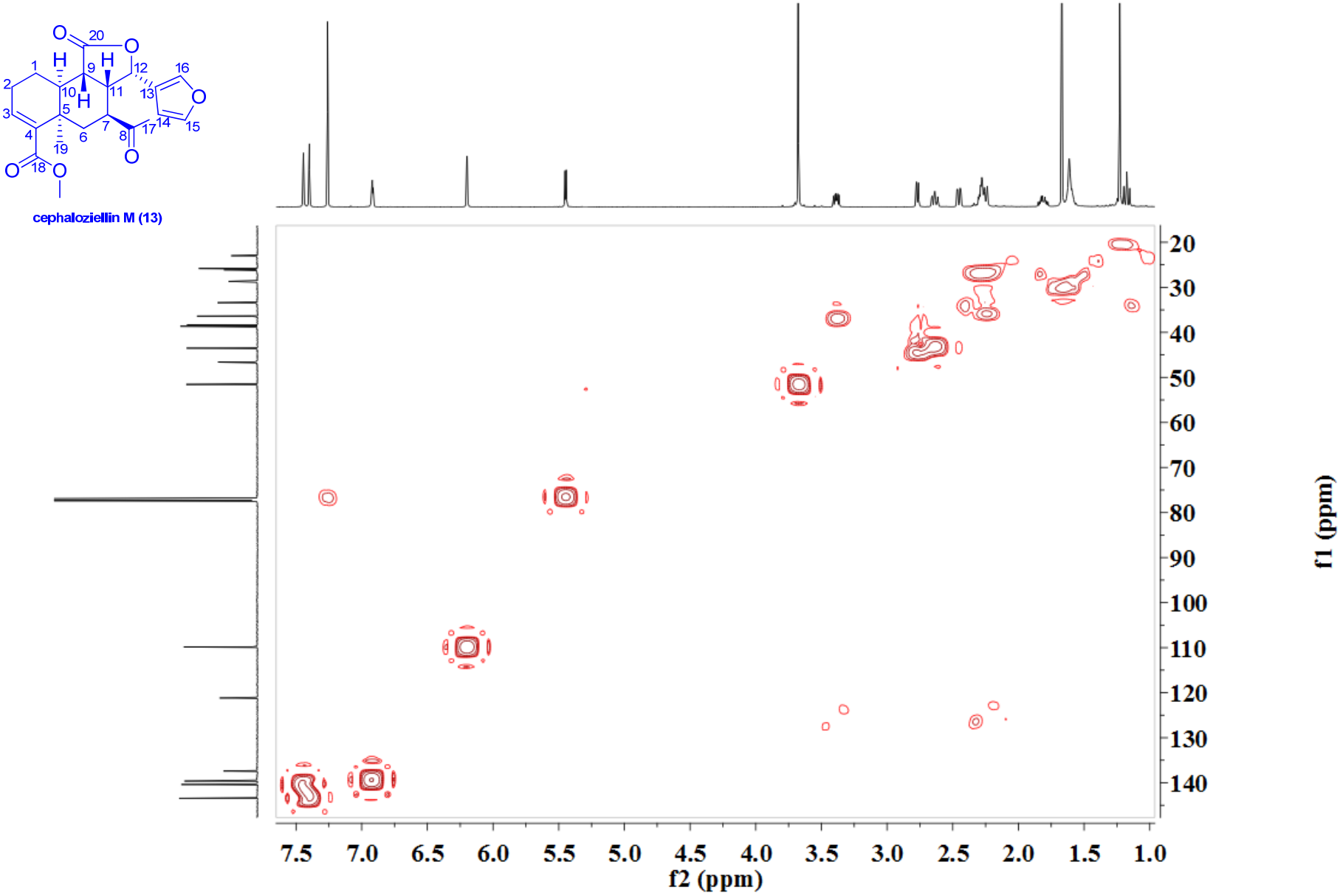
S145. ^{1}H NMR spectrum (600 MHz) of cephaloziellin M (**13**) in $CDCl_3$.



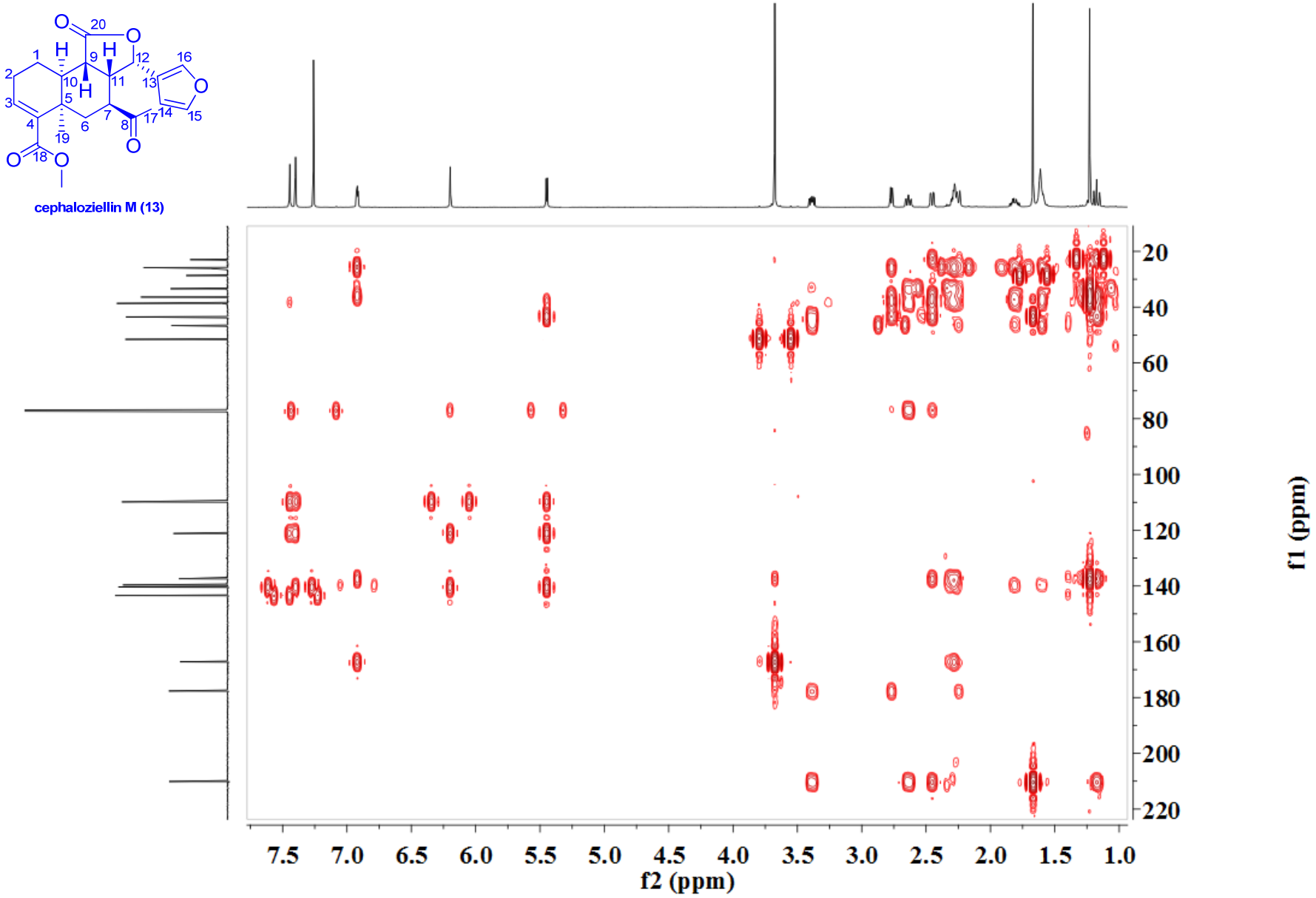
S146. ^{13}C NMR spectrum (150 MHz) of cephaloziellin M (**13**) in $CDCl_3$.



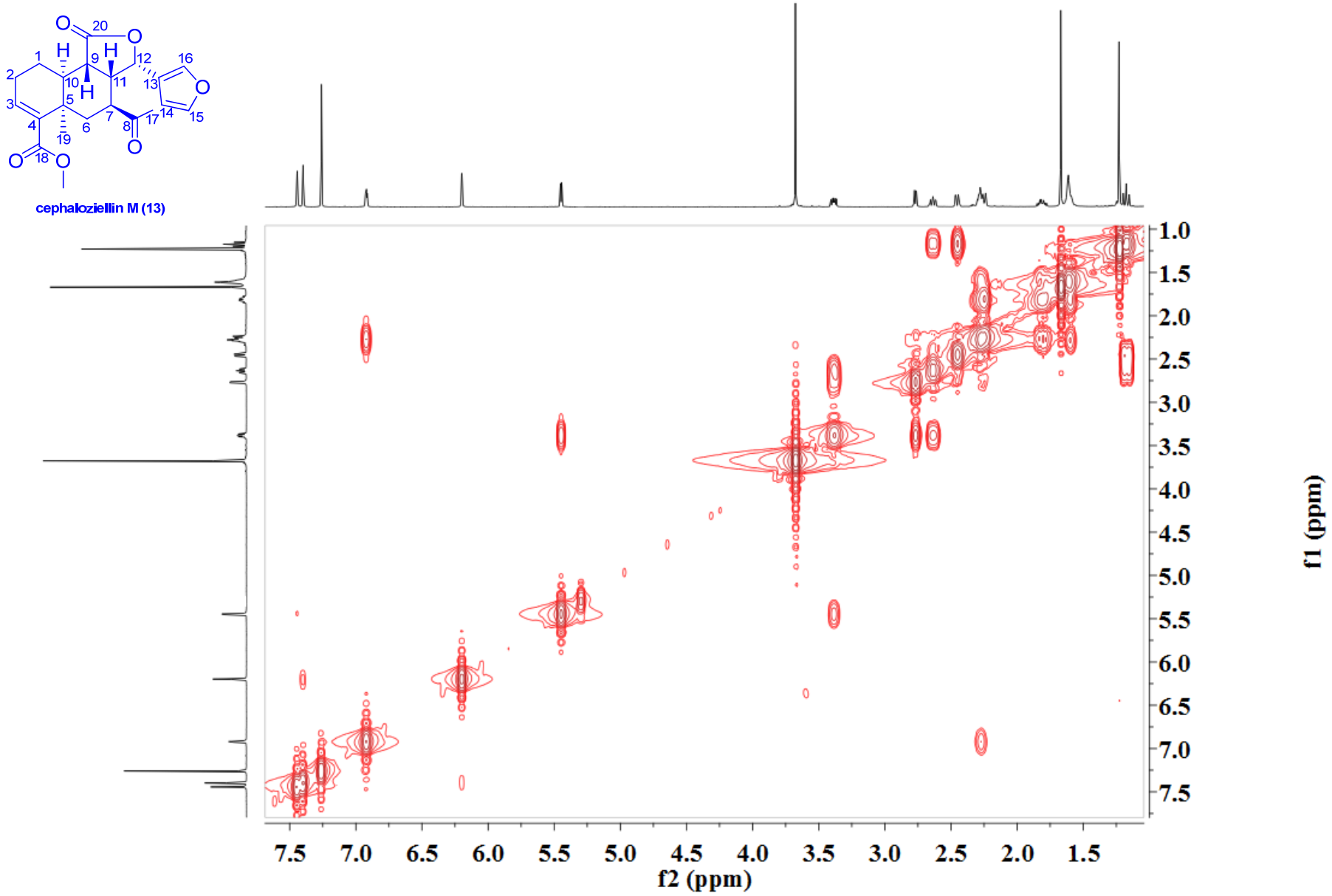
S147. HSQC spectrum (600 MHz) of cephaloziellin M (**13**) in $CDCl_3$.



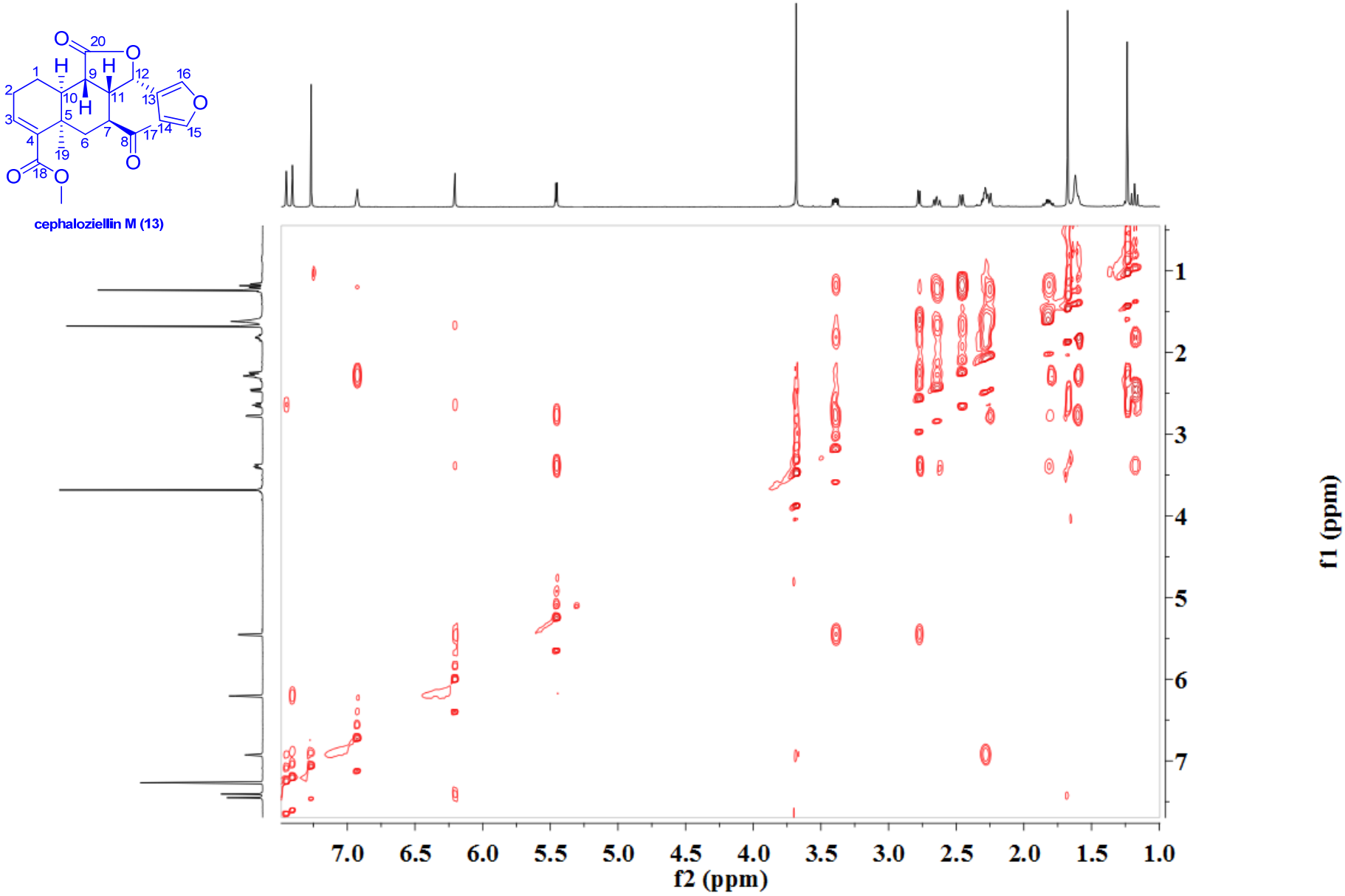
S148. HMBC spectrum (600 MHz) of cephaloziellin M (**13**) in $CDCl_3$.



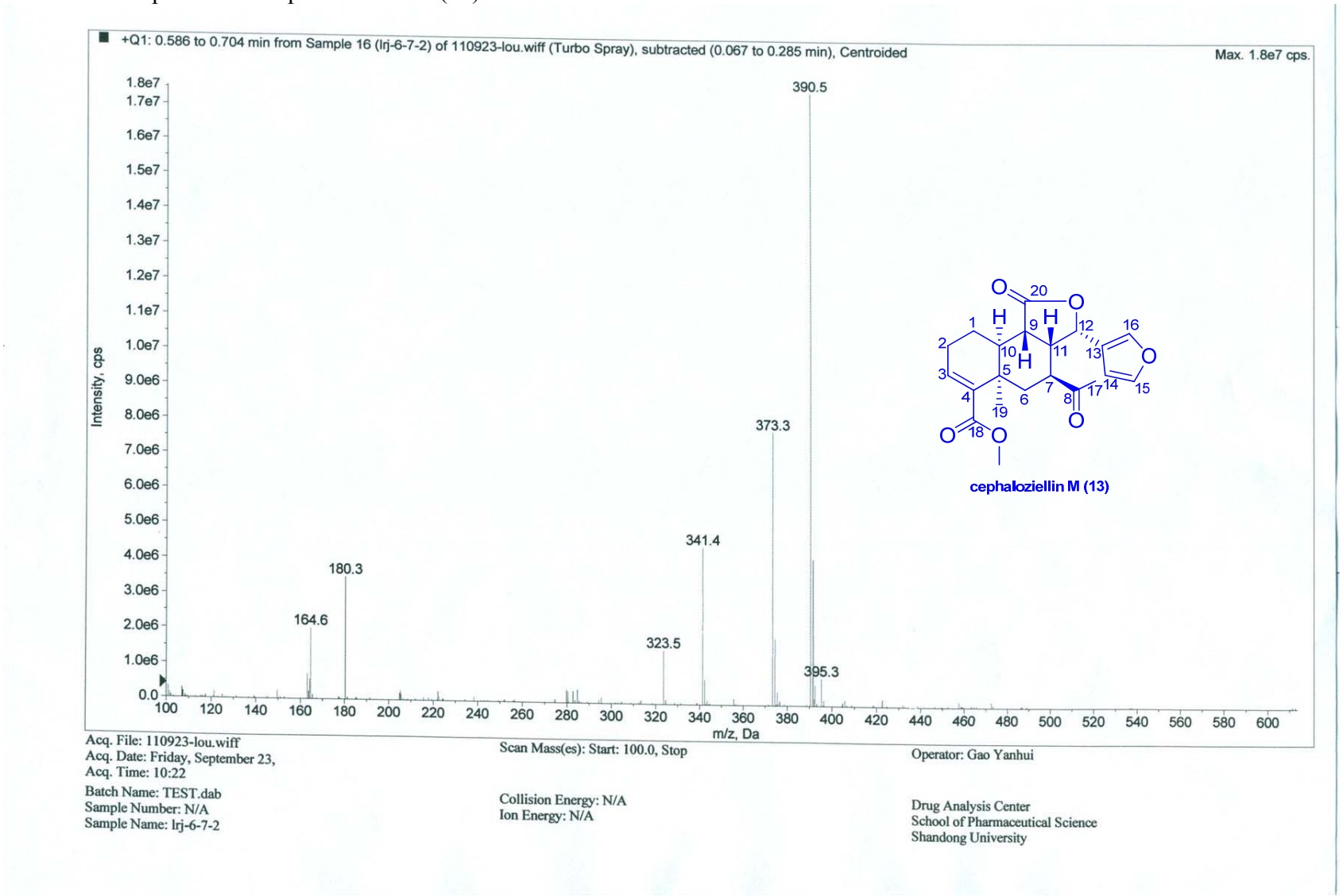
S149. ^{1}H-^{1}H COSY spectrum (600 MHz) of cephaloziellin M (**13**) in $CDCl_3$.



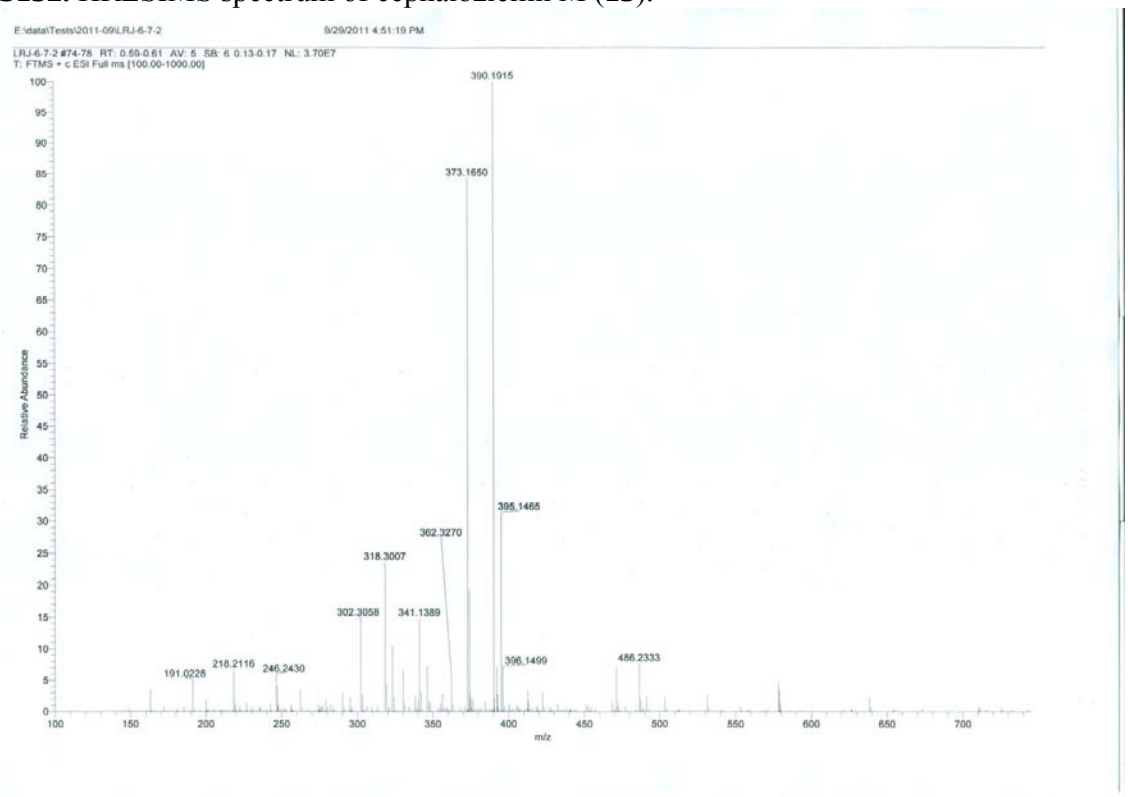
S150. NOESY spectrum (600 MHz) of cephaloziellin M (**13**) in $CDCl_3$.

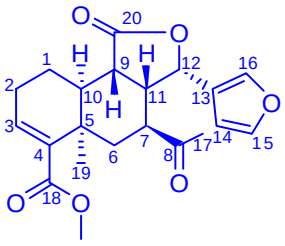


S151. ESIMS spectrum of cephaloziellin M (**13**).



S152. HRESIMS spectrum of cephaloziellin M (**13**).



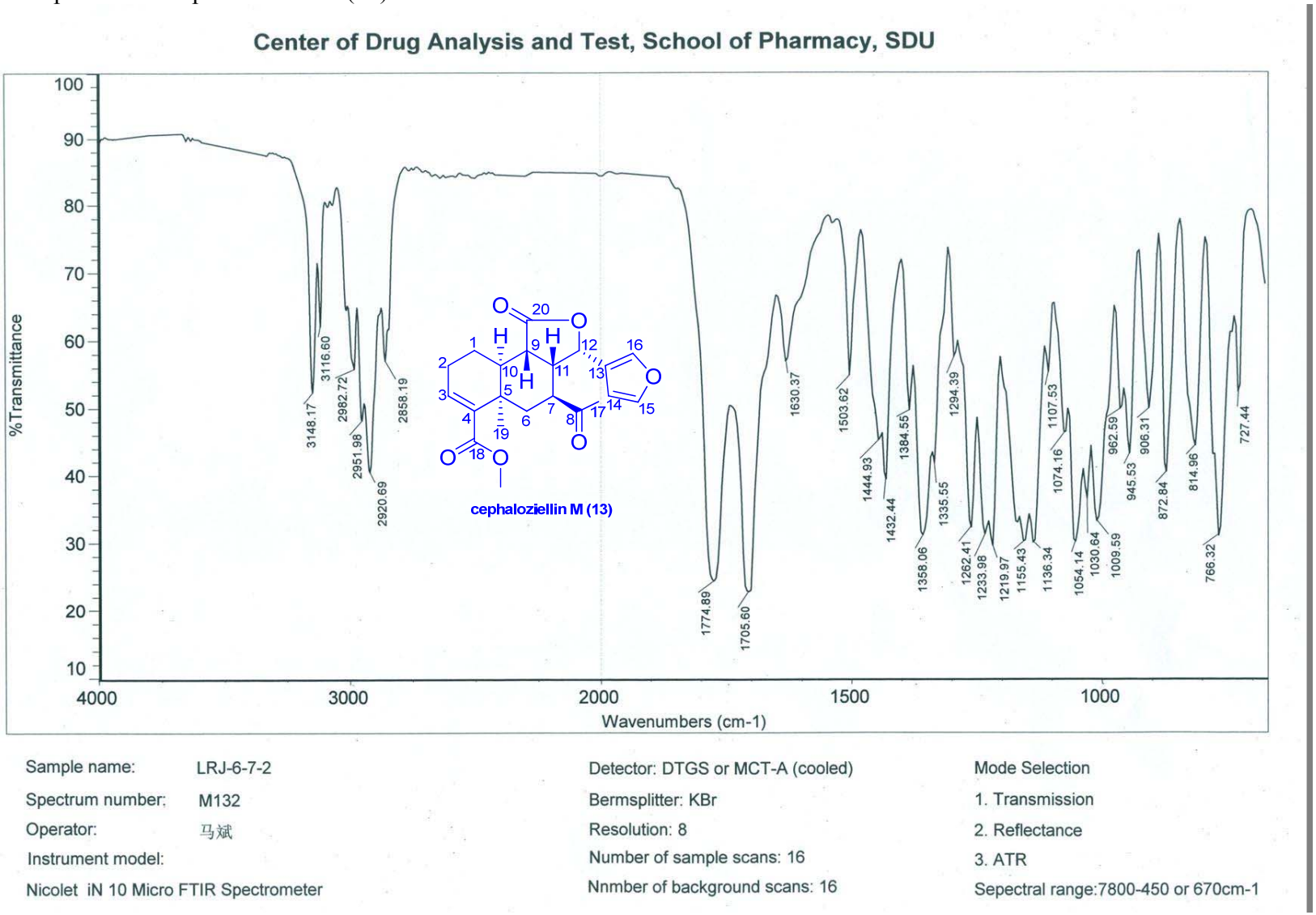


cephaloziellin M (13)

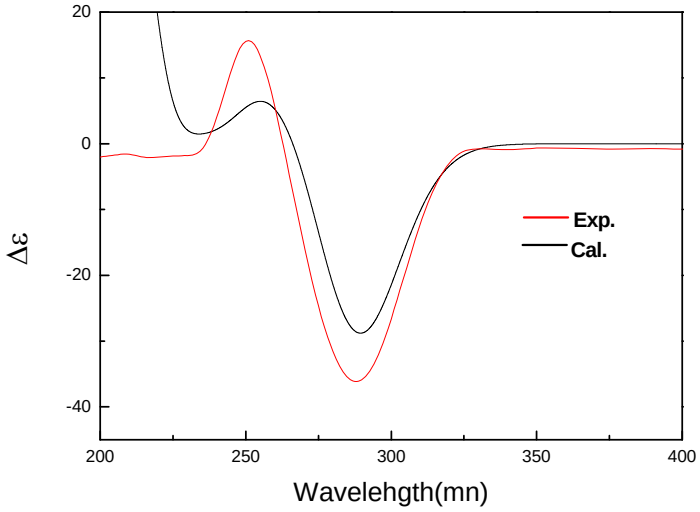
SPECTRUM - simulation :

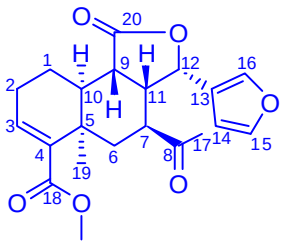
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
390.1915	390.1911	1.09	8.5	$^{12}C_{21}H_{28}O_6N_1$

S153. IR spectrum of cephaloziellin M (**13**).

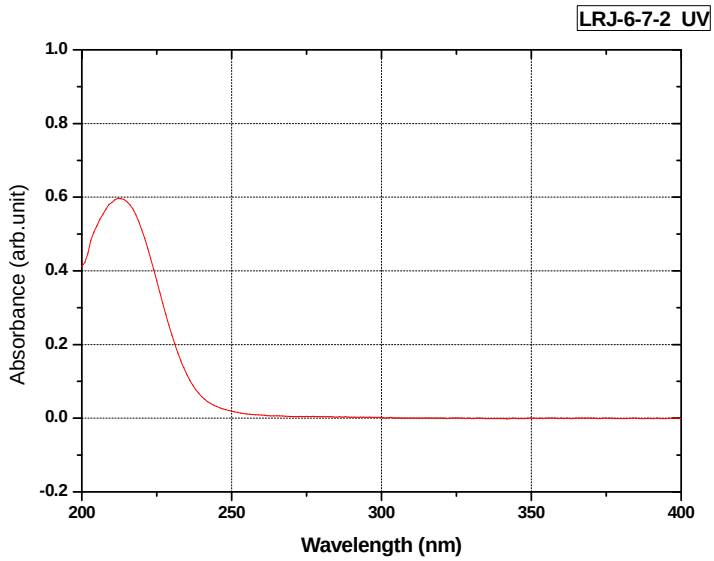


S154. Experimental ECD and calculated ECD and UV spectra of cephaloziellin M (**13**).

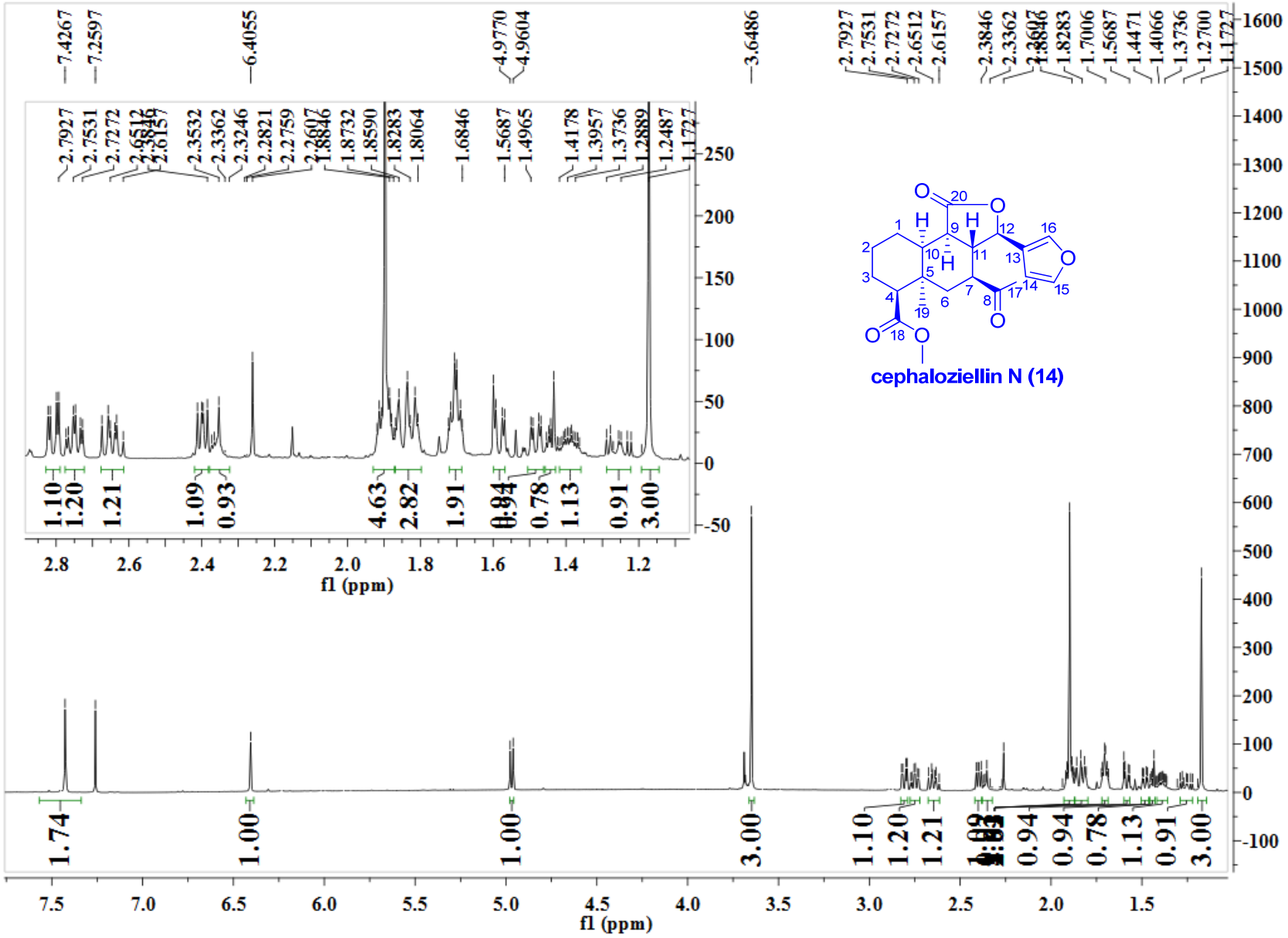




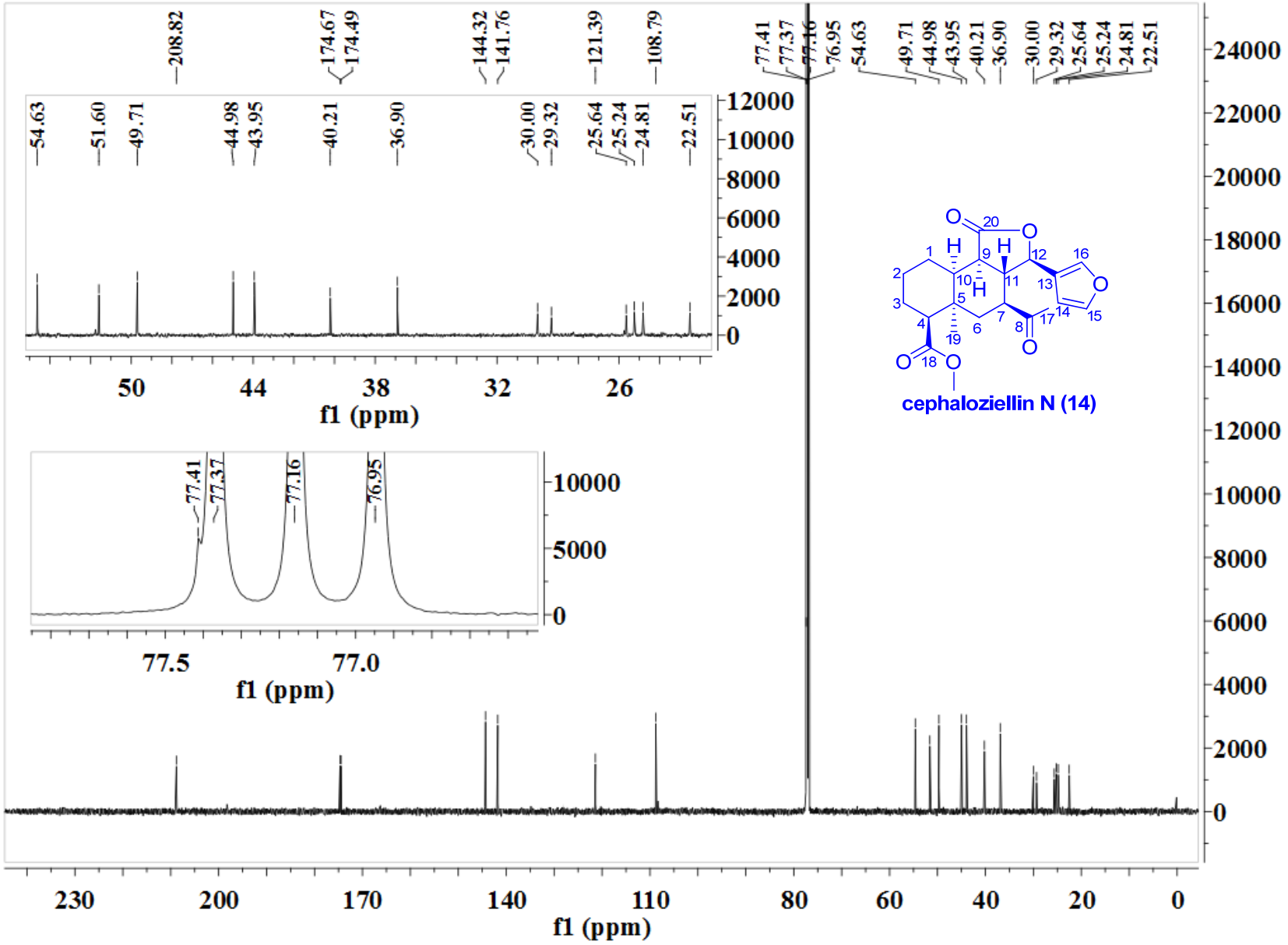
cephaloziellin M (13)



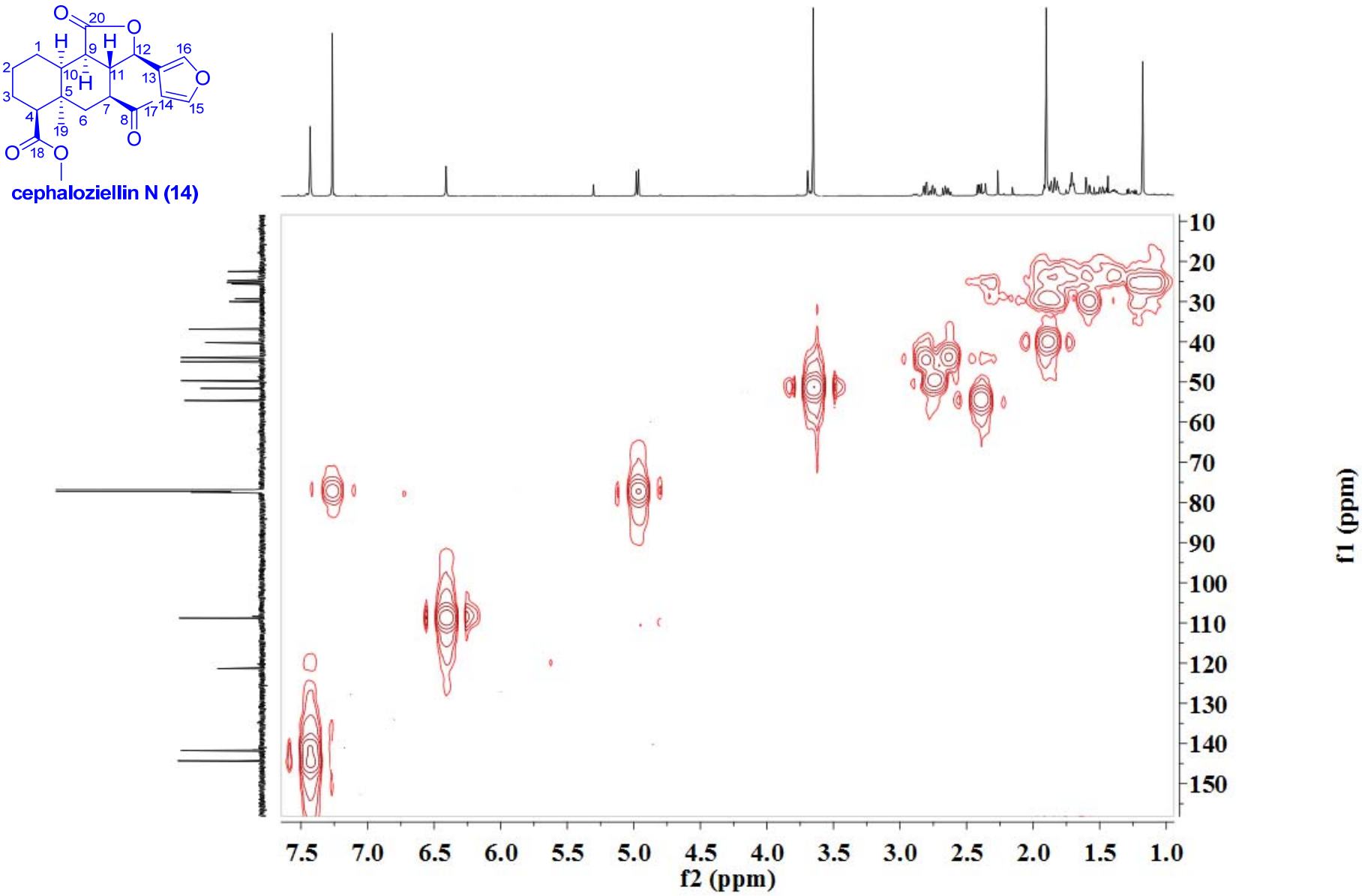
S155. ^{1}H NMR spectrum (600 MHz) of cephaloziellin N (**14**) in $CDCl_3$.



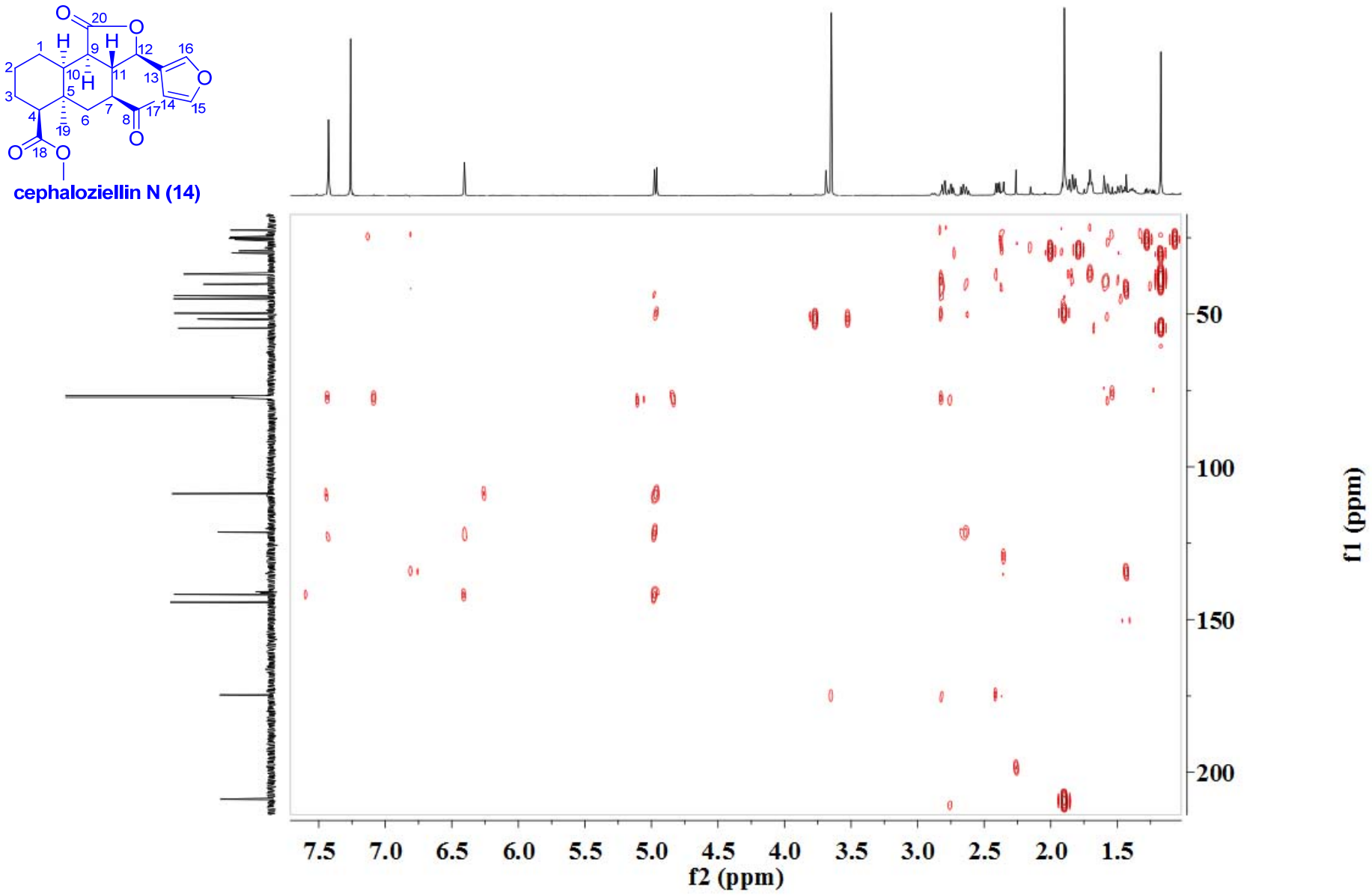
S156. ^{13}C NMR spectrum (150 MHz) of cephaloziellin N (**14**) in $CDCl_3$.



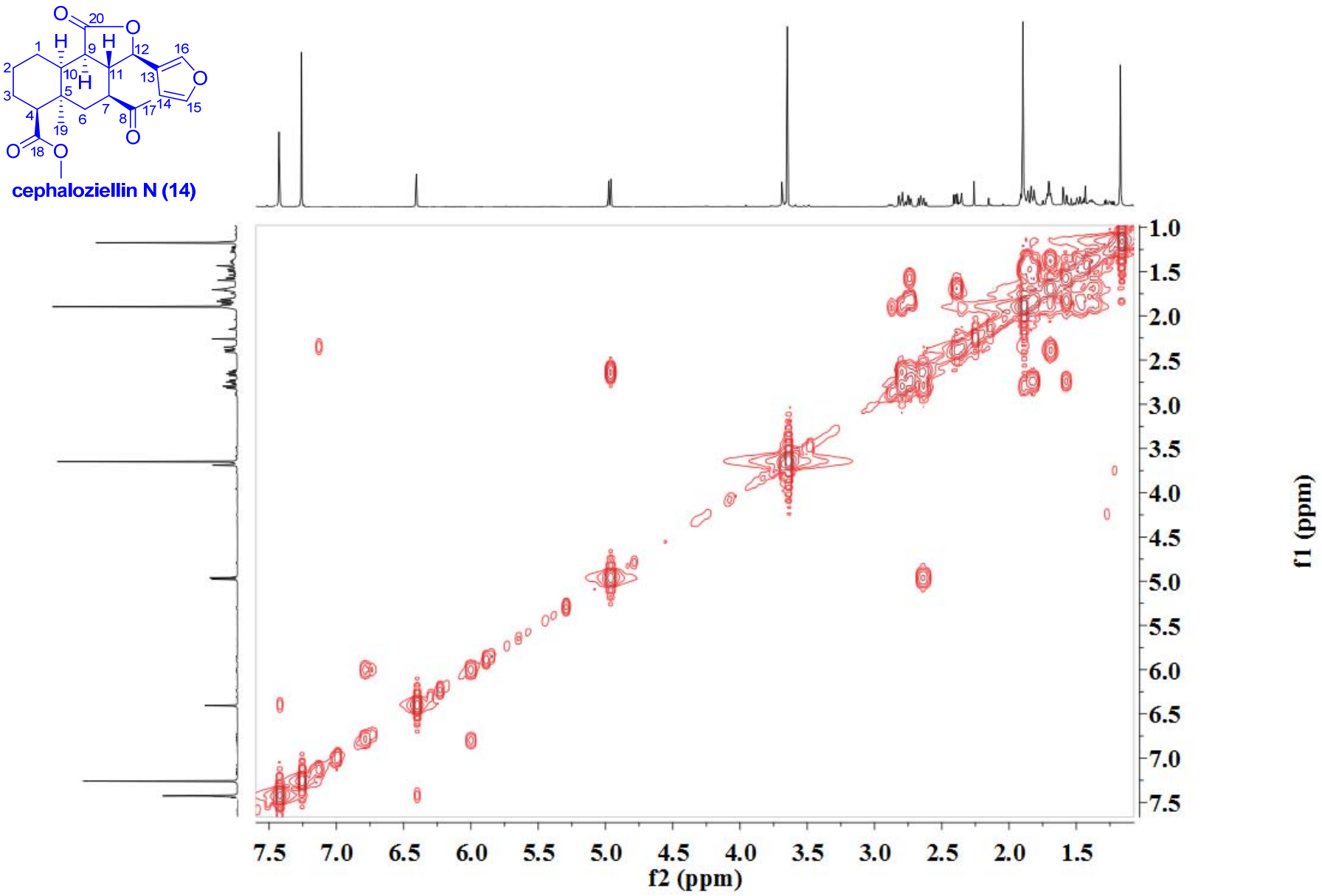
S157. HSQC spectrum (600 MHz) of cephaloziellin N (**14**) in $CDCl_3$.



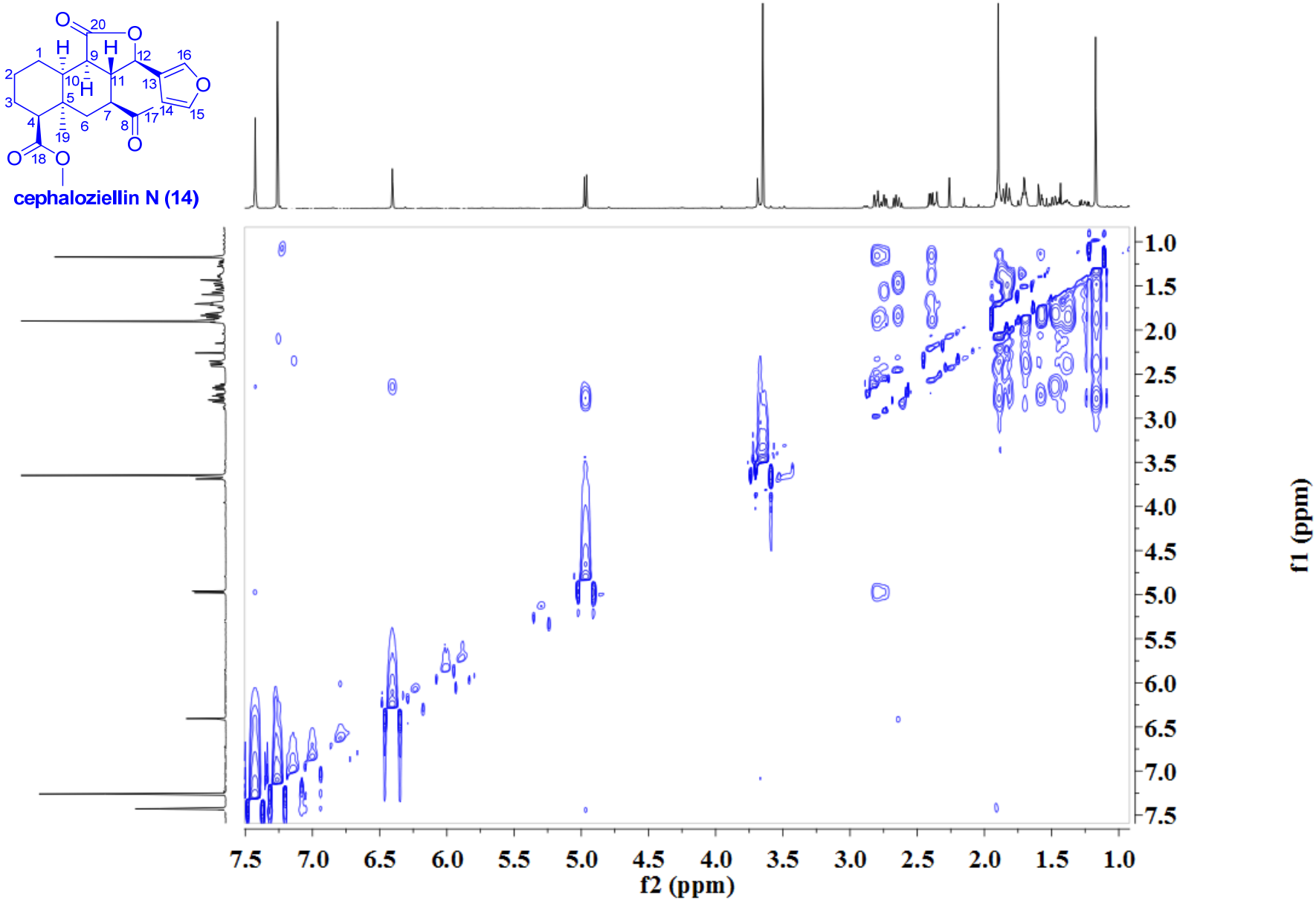
S158. HMBC spectrum (600 MHz) of cephaloziellin N (**14**) in $CDCl_3$.



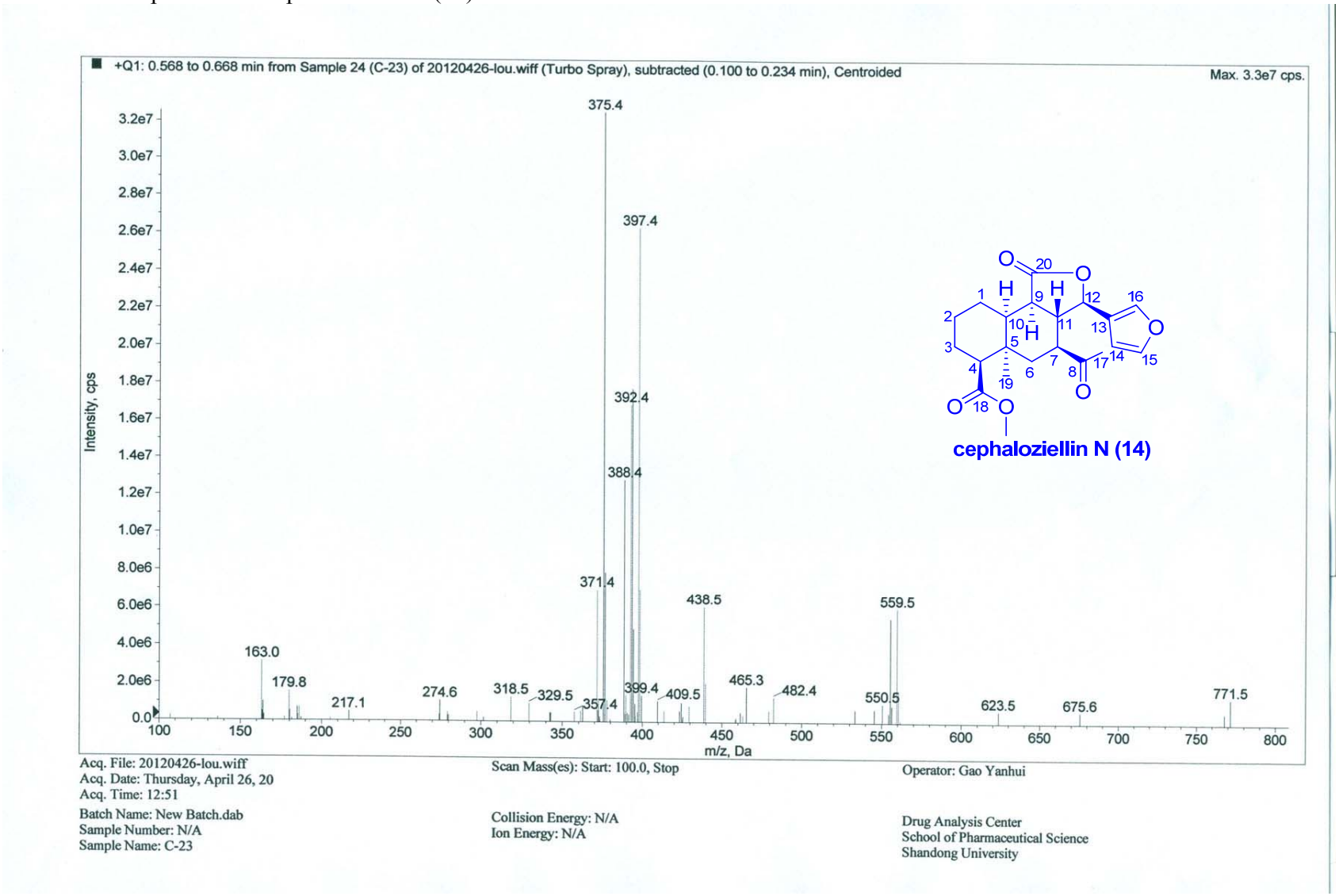
S159. ^{1}H-^{1}H COSY spectrum (600 MHz) of cephaloziellin N (**14**) in $CDCl_3$.



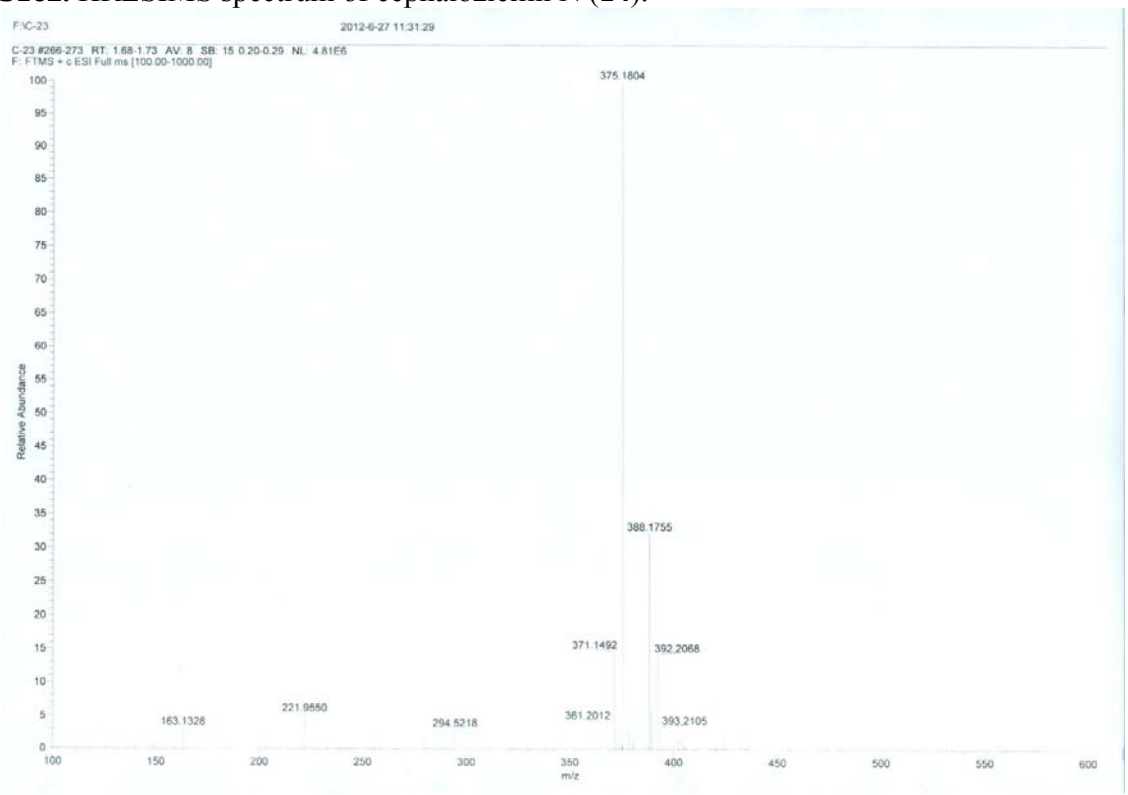
S160. NOESY spectrum (600 MHz) of cephaloziellin N (**14**) in $CDCl_3$.

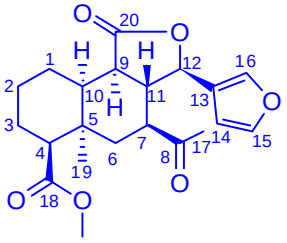


S161. ESIMS spectrum of cephaloziellin N (**14**).



S162. HRESIMS spectrum of cephaloziellin N (**14**).



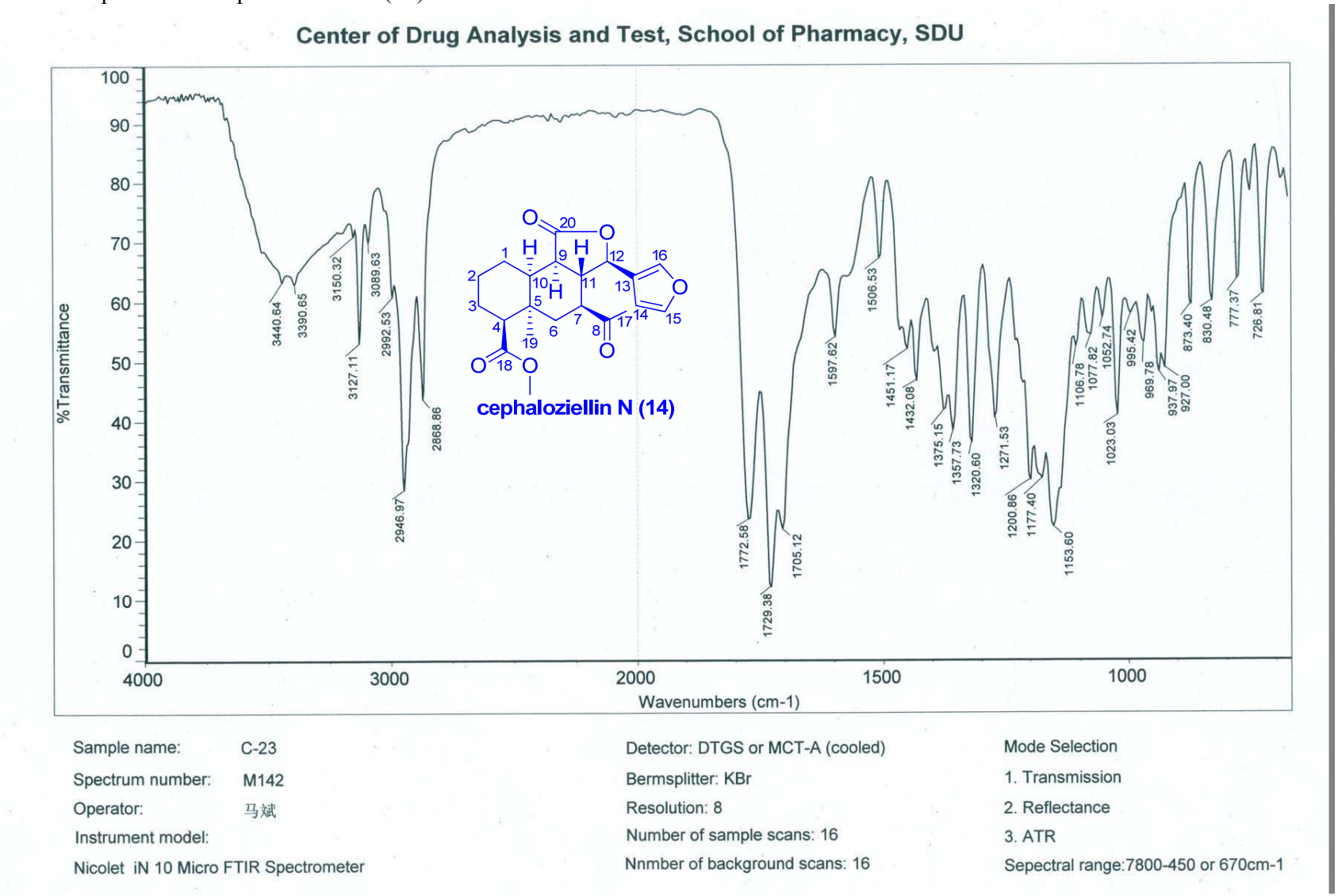


cephaloziellin N (14)

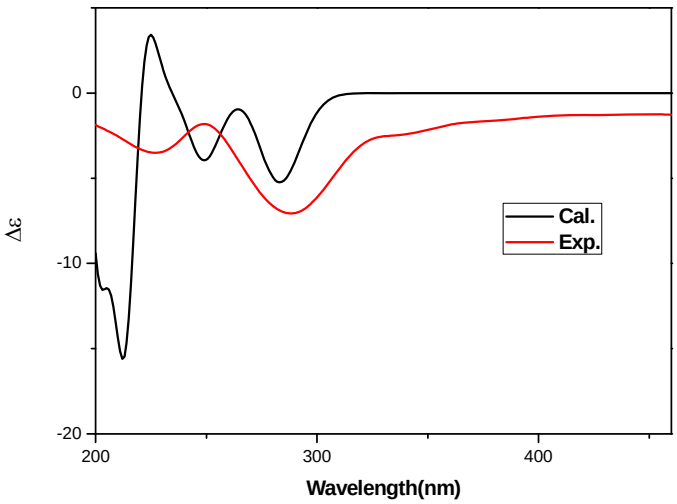
SPECTRUM - simulation :

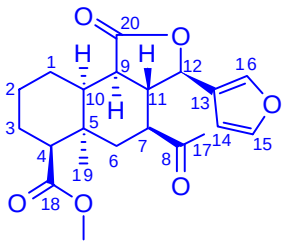
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
375.1804	375.1802	0.41	8.5	$^{12}C_{21}H_{27}O_6$

S163. IR spectrum of cephaloziellin N (**14**).

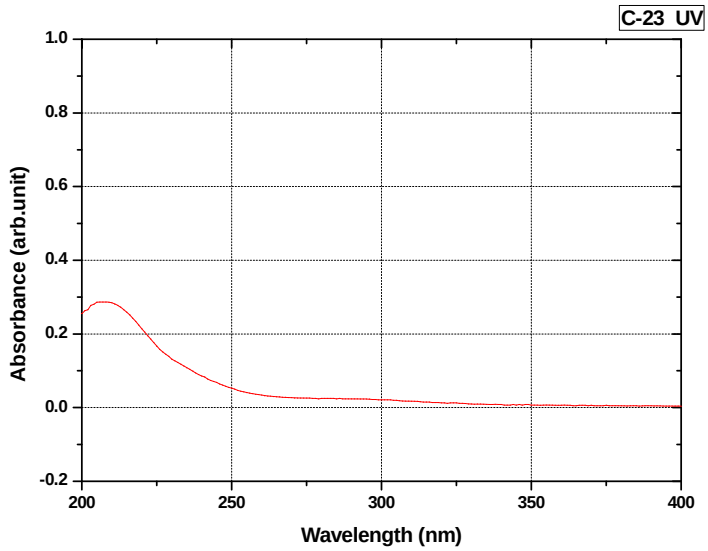


S164. Experimental ECD and calculated ECD, and UV spectra of cephaloziellin N (**14**).

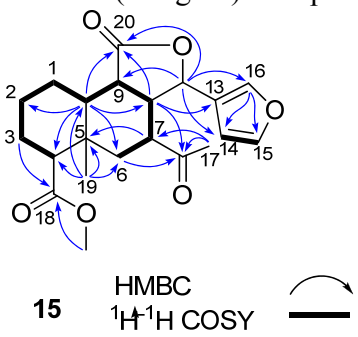




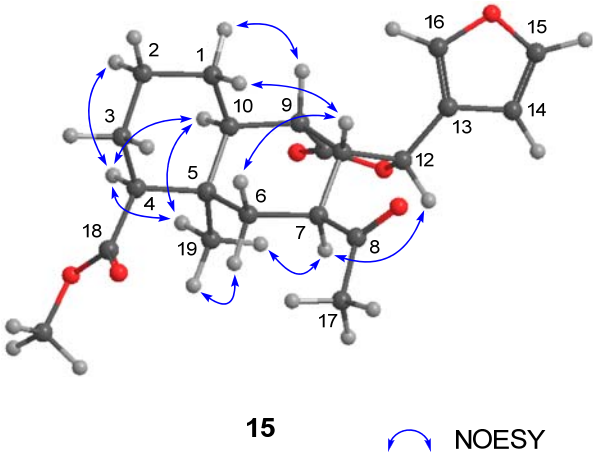
cephaloziellin N (14)



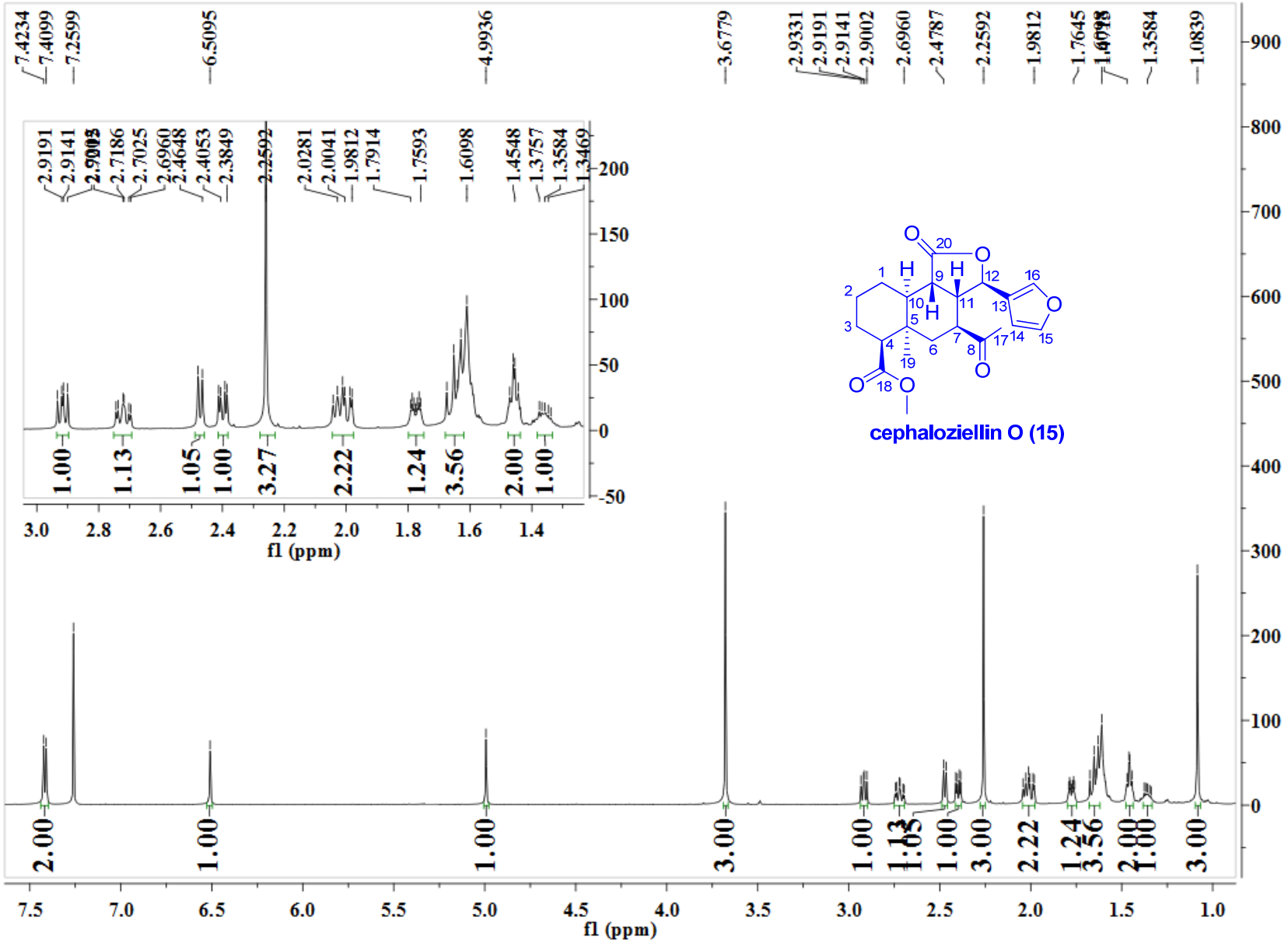
S165. Key HMBC and ^{1}H-^{1}H COSY correlations (in figure) of cephaloziellin O (**15**).



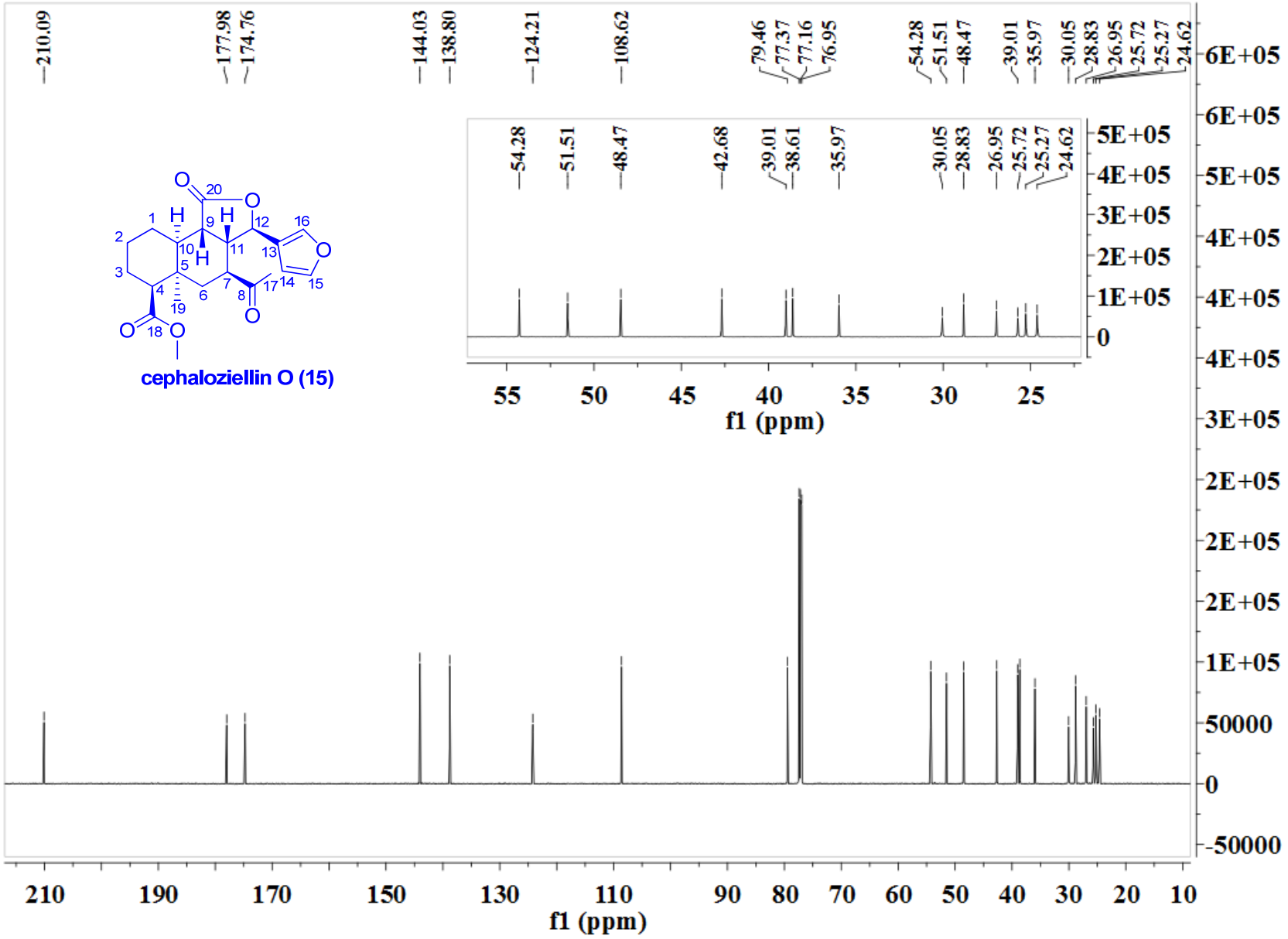
S166. Key NOESY correlations (in figure) of cephaloziellin O (**15**).



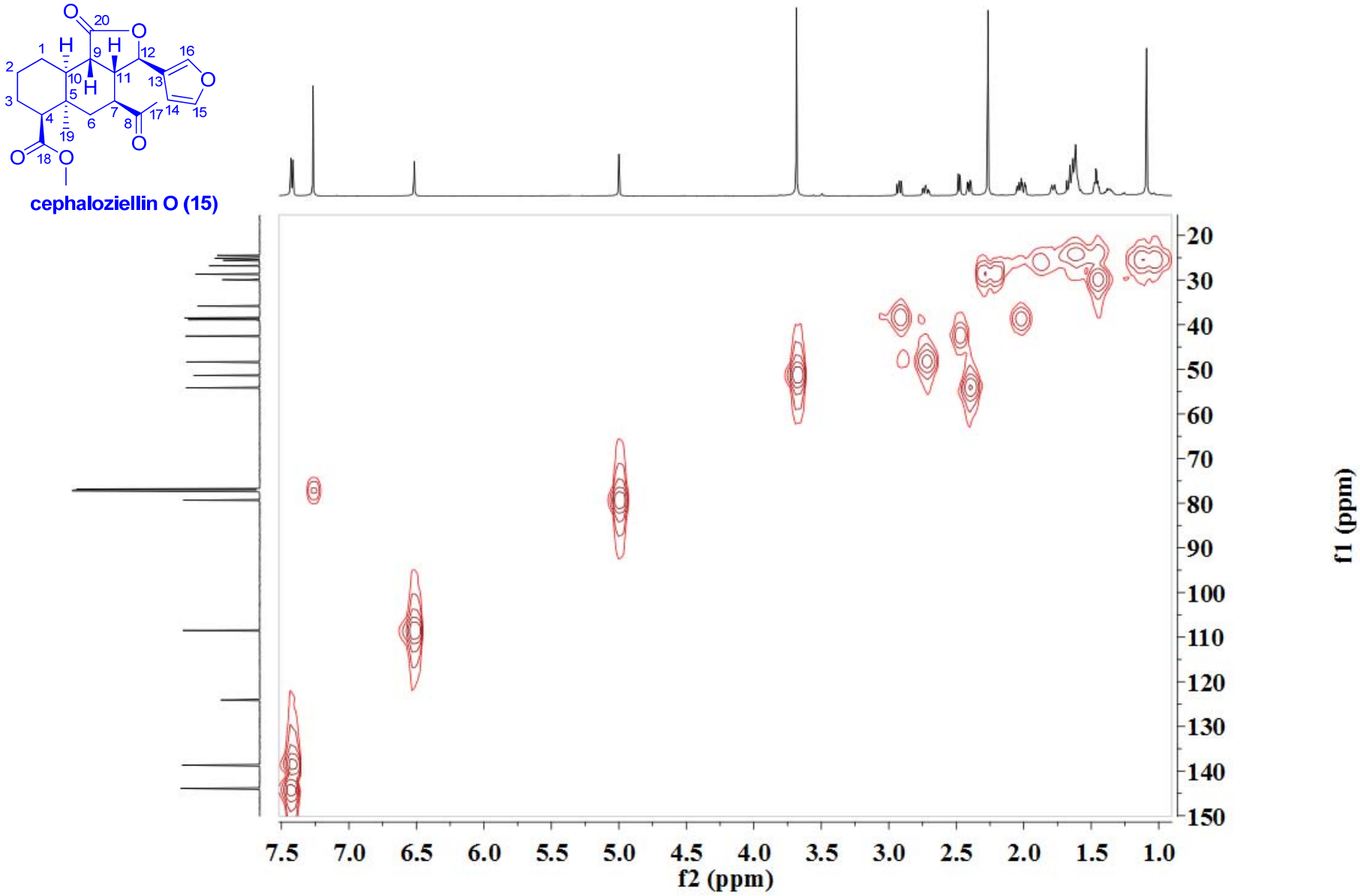
S167. ^{1}H NMR spectrum (600 MHz) of cephaloziellin O (**15**) in $CDCl_3$.



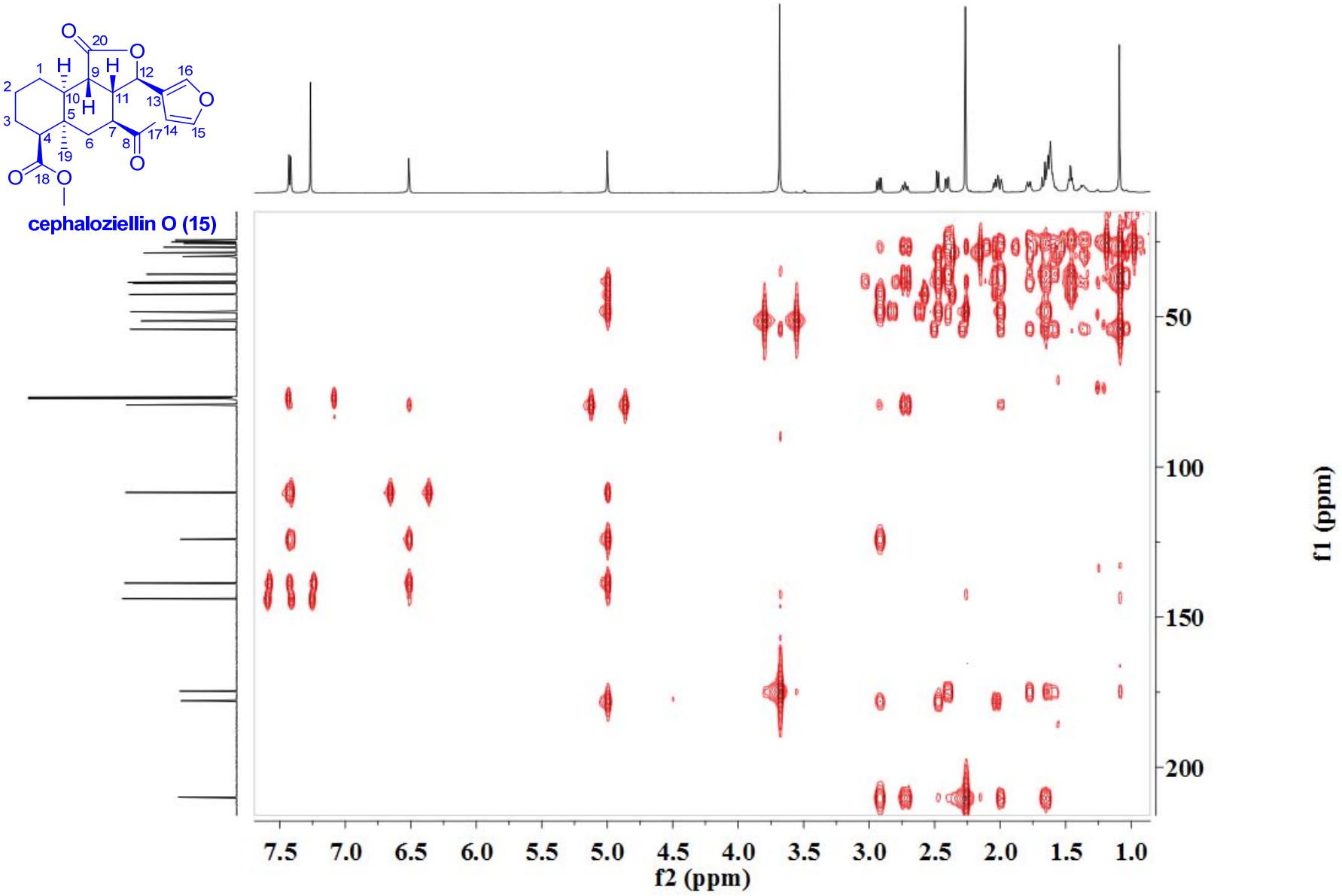
S168. ^{13}C NMR spectrum (150 MHz) of cephaloziellin O (**15**) in $CDCl_3$.



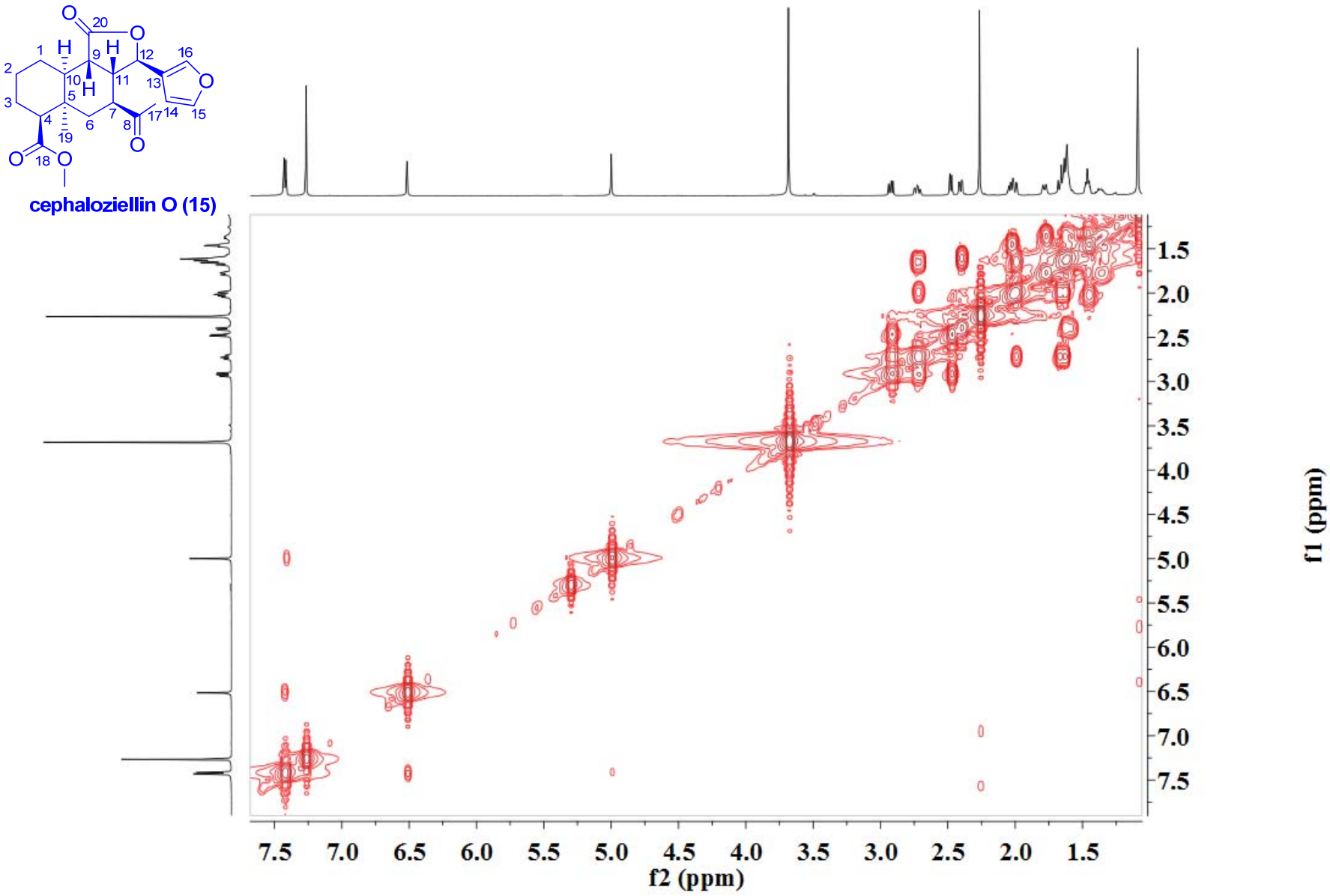
S169. HSQC spectrum (600 MHz) of cephaloziellin O (**15**) in $CDCl_3$.



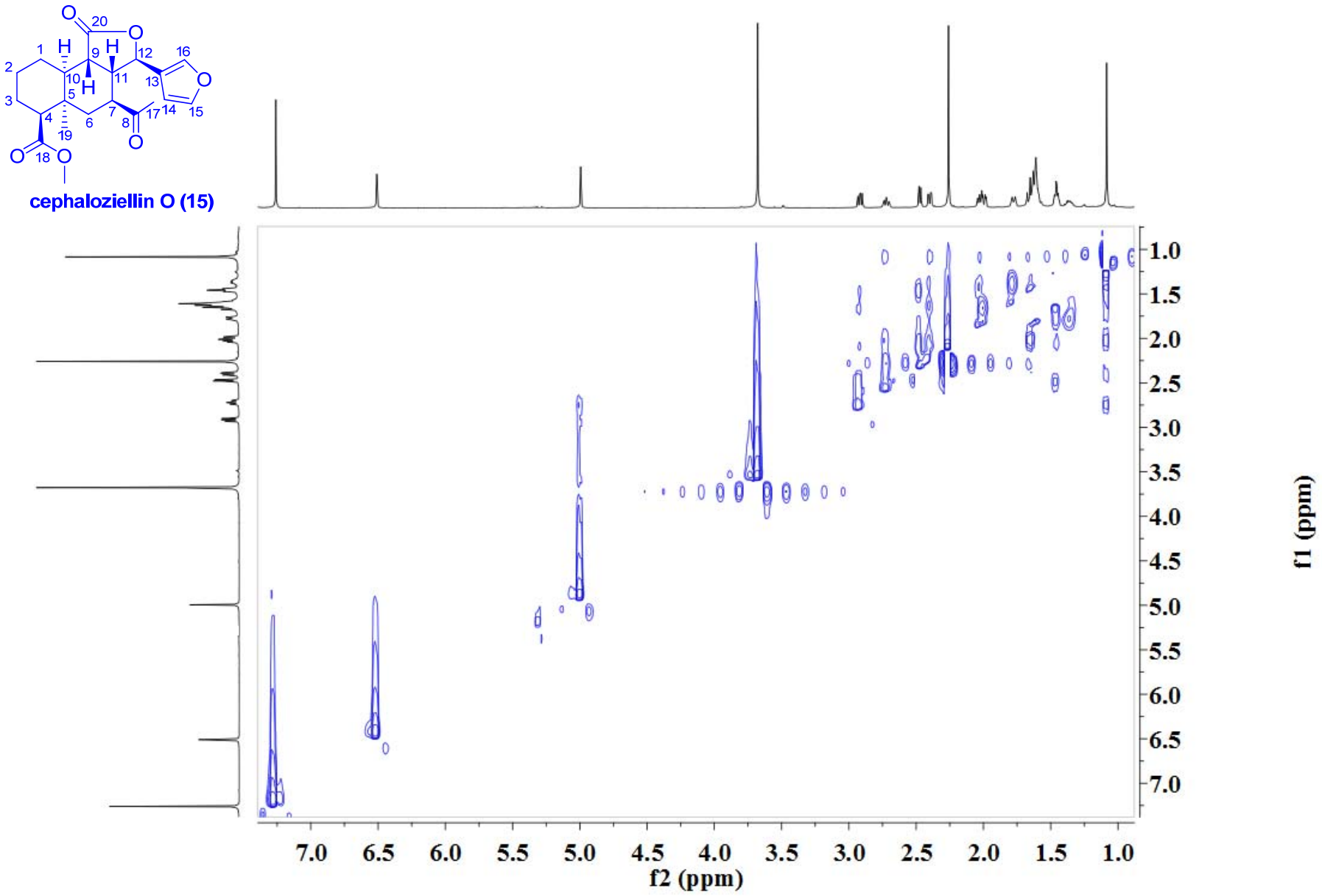
S170. HMBC spectrum (600 MHz) of cephaloziellin O (**15**) in $CDCl_3$.



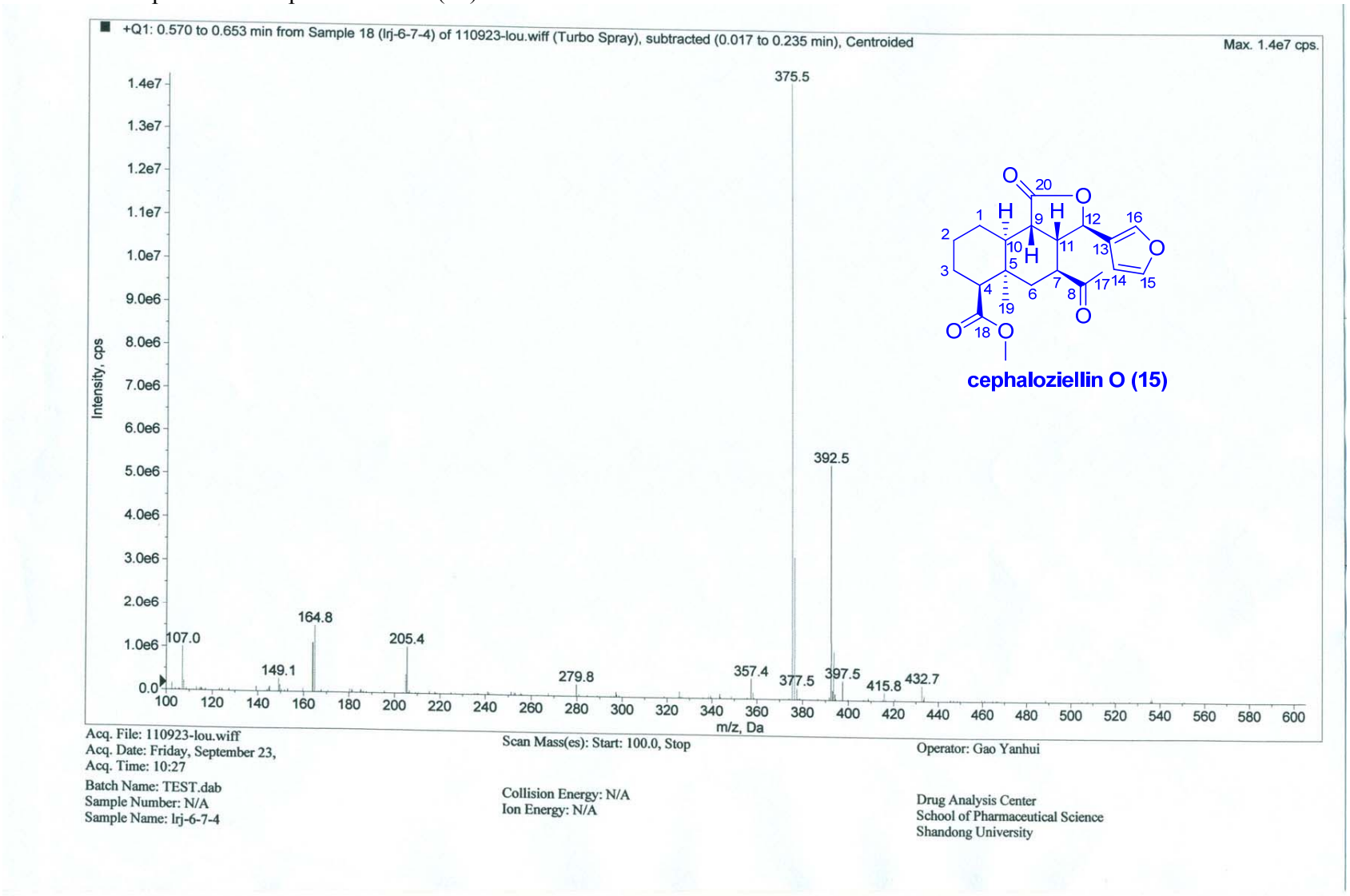
S171. ^{1}H-^{1}H COSY spectrum (600 MHz) of cephaloziellin O (**15**) in $CDCl_3$.



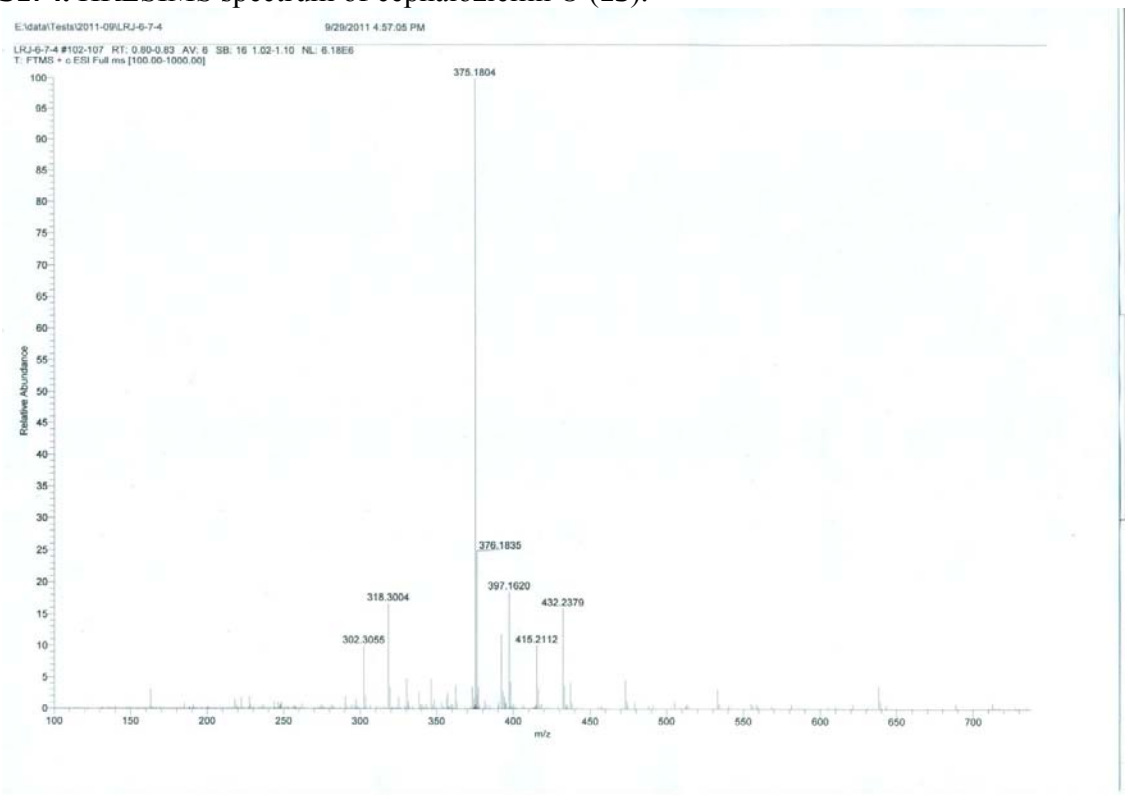
S172. NOESY spectrum (600 MHz) of cephaloziellin O (**15**) in $CDCl_3$.

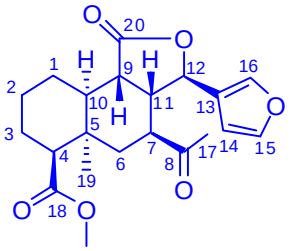


S173. ESIMS spectrum of cephaloziellin O (**15**).



S174. HRESIMS spectrum of cephaloziellin O (**15**).



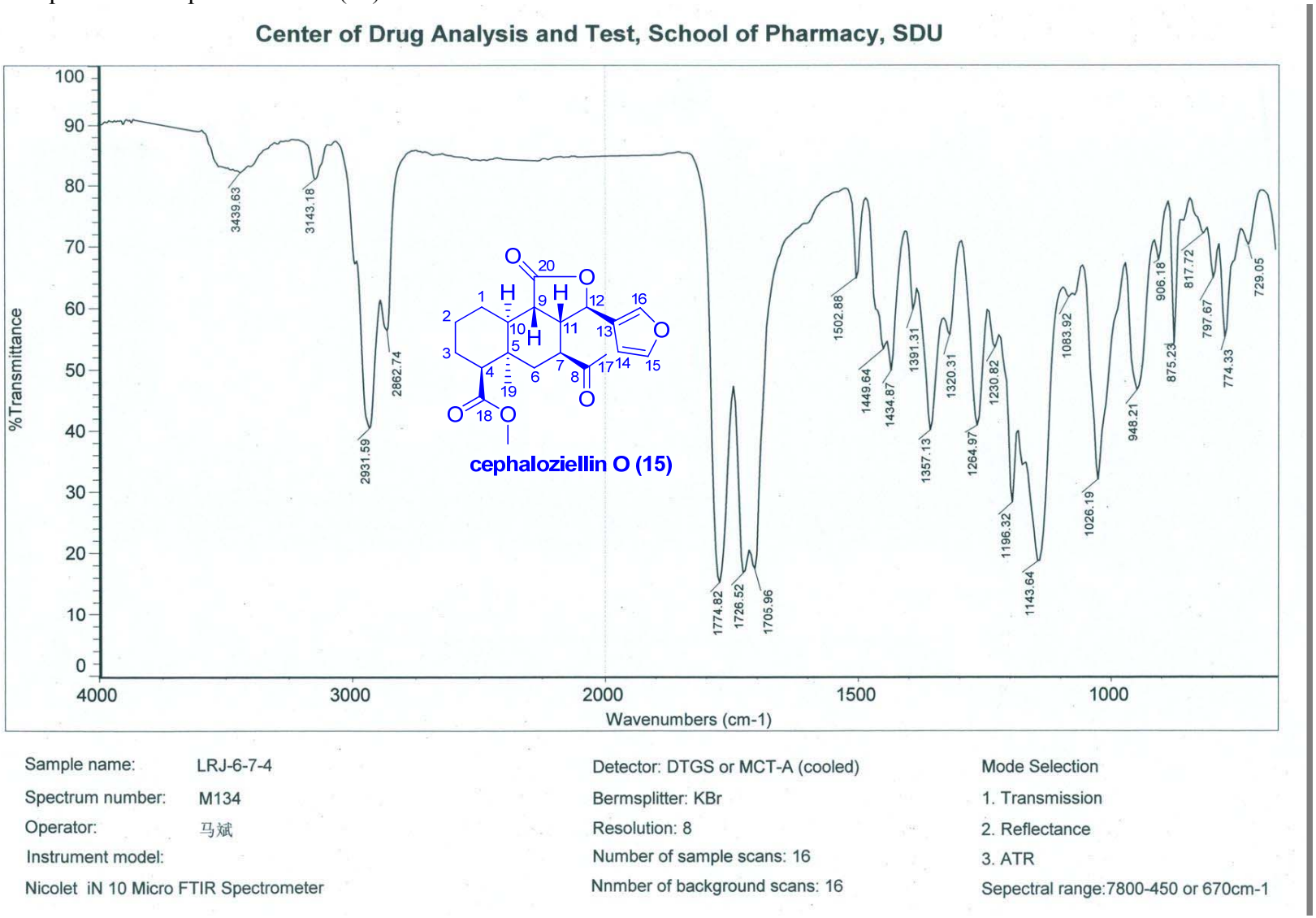


cephaloziellin O (15)

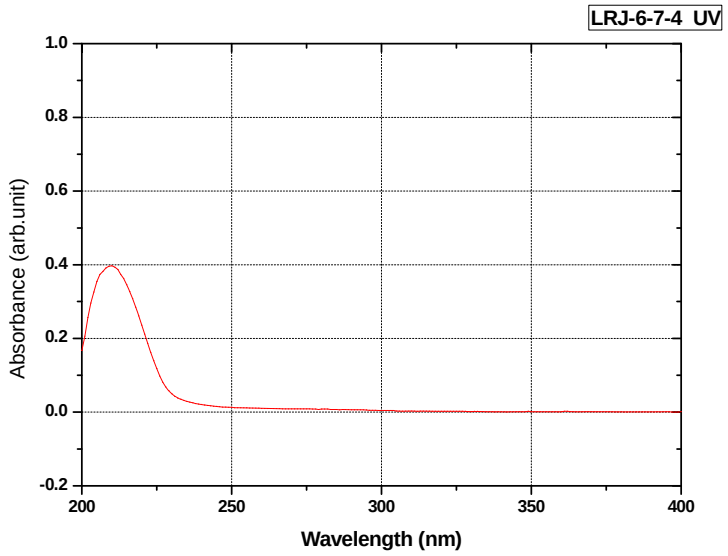
SPECTRUM - simulation :

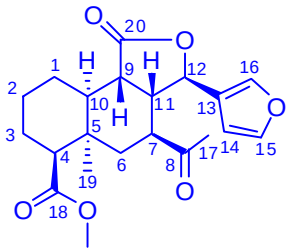
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
375.1804	375.1802	0.52	8.5	$^{12}C_{21}H_{27}O_6$

S175. IR spectrum of cephaloziellin O (**15**).



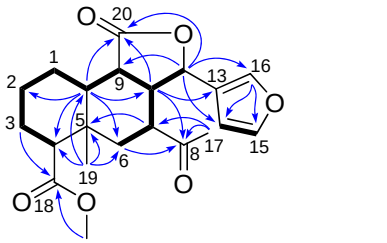
S176. UV spectra of cephaloziellin O (**15**).





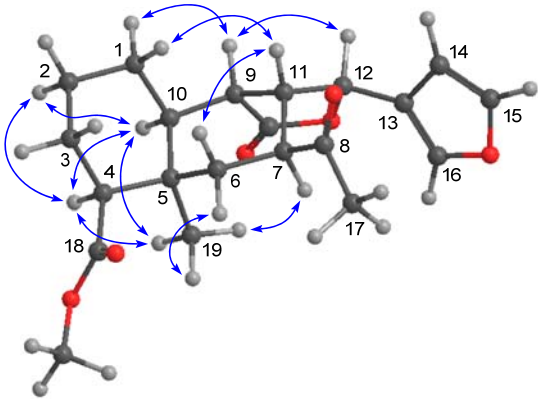
cephaloziellin O (15)

S177. Key HMBC and ^{1}H-^{1}H COSY correlations (in figure) of cephaloziellin P (**16**).



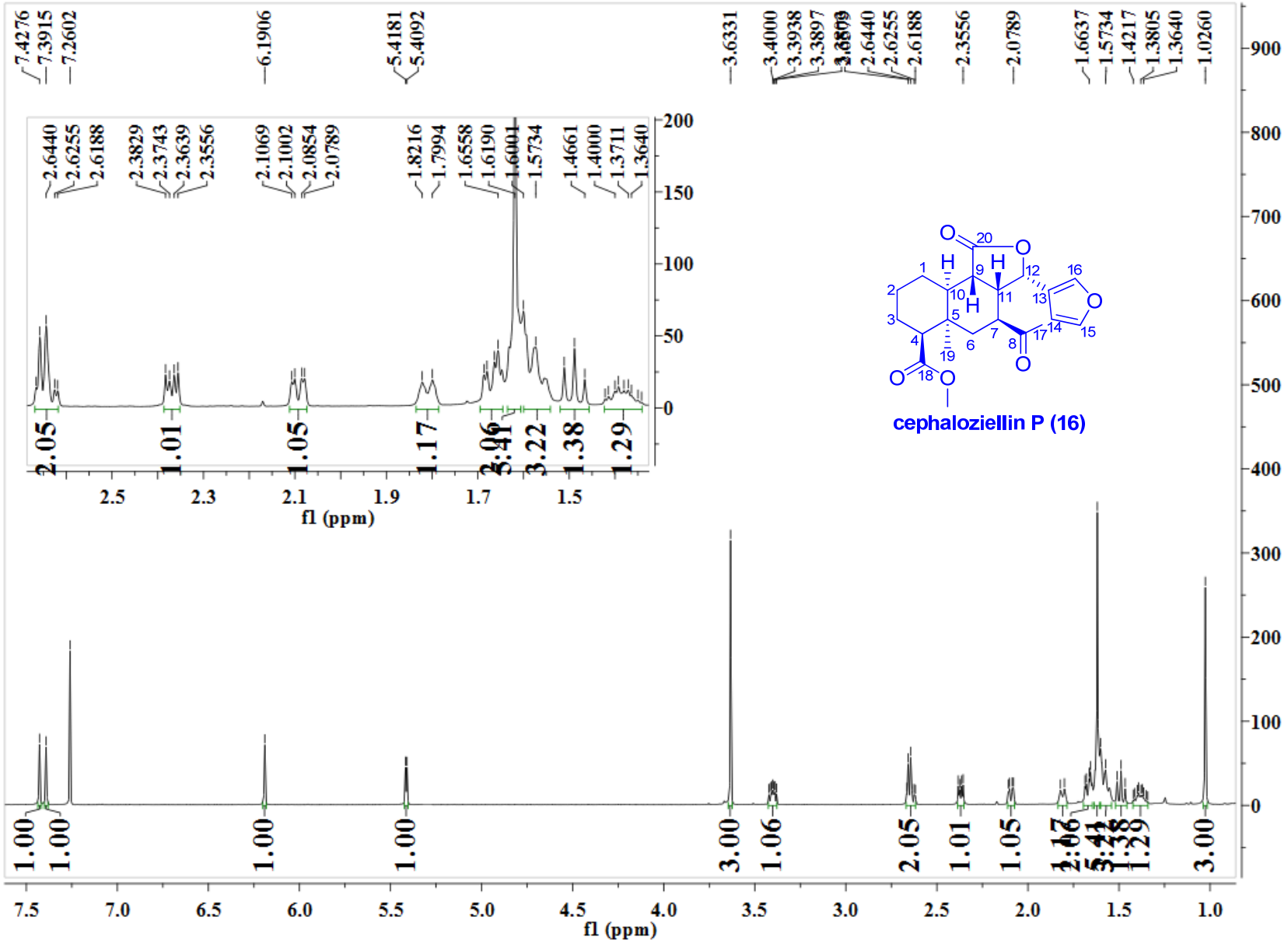
16 HMBC ^{1}H-^{1}H COSY

S178. Key NOESY correlations (in figure) of cephaloziellin P (**16**).

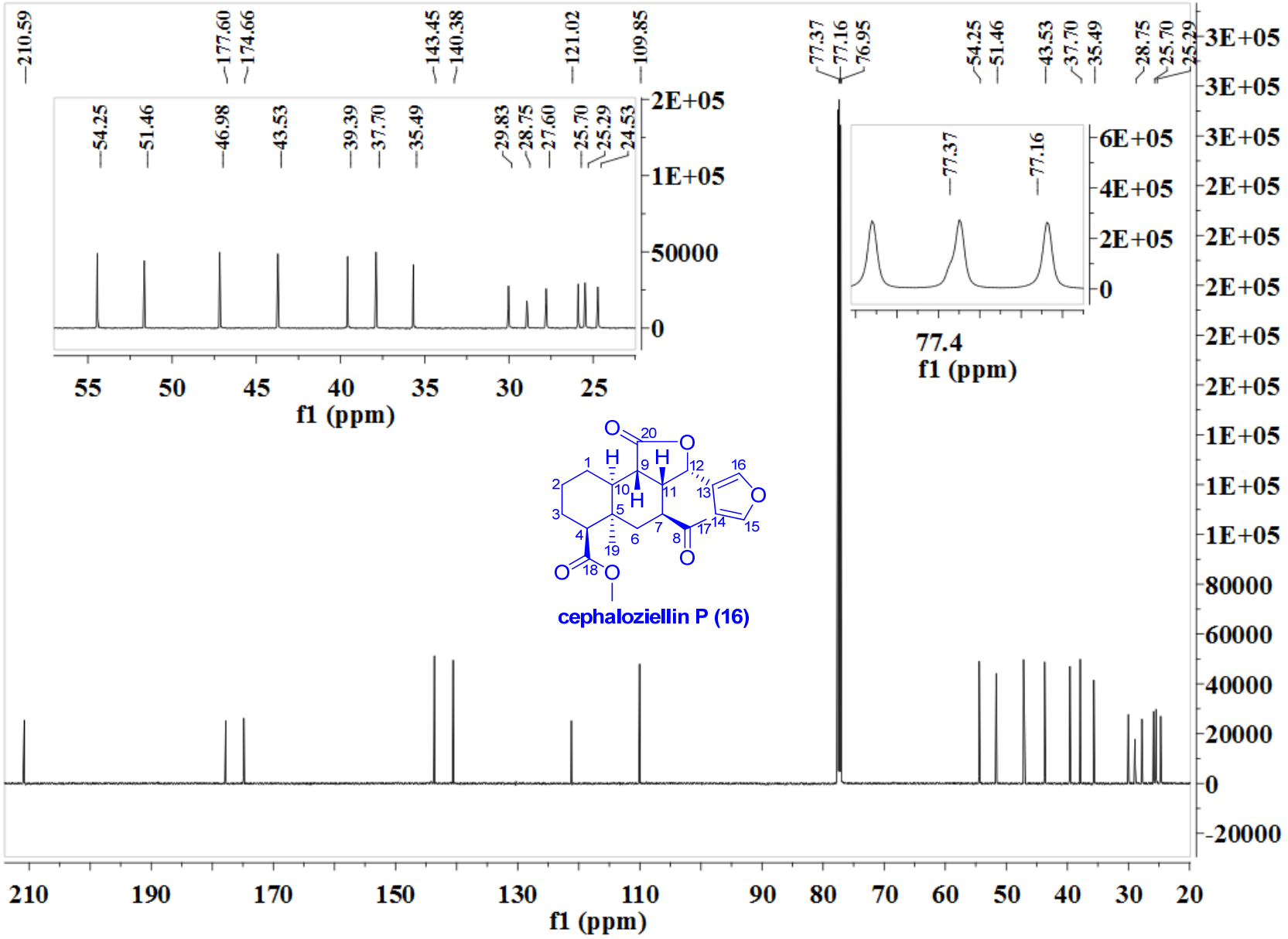


16 NOESY

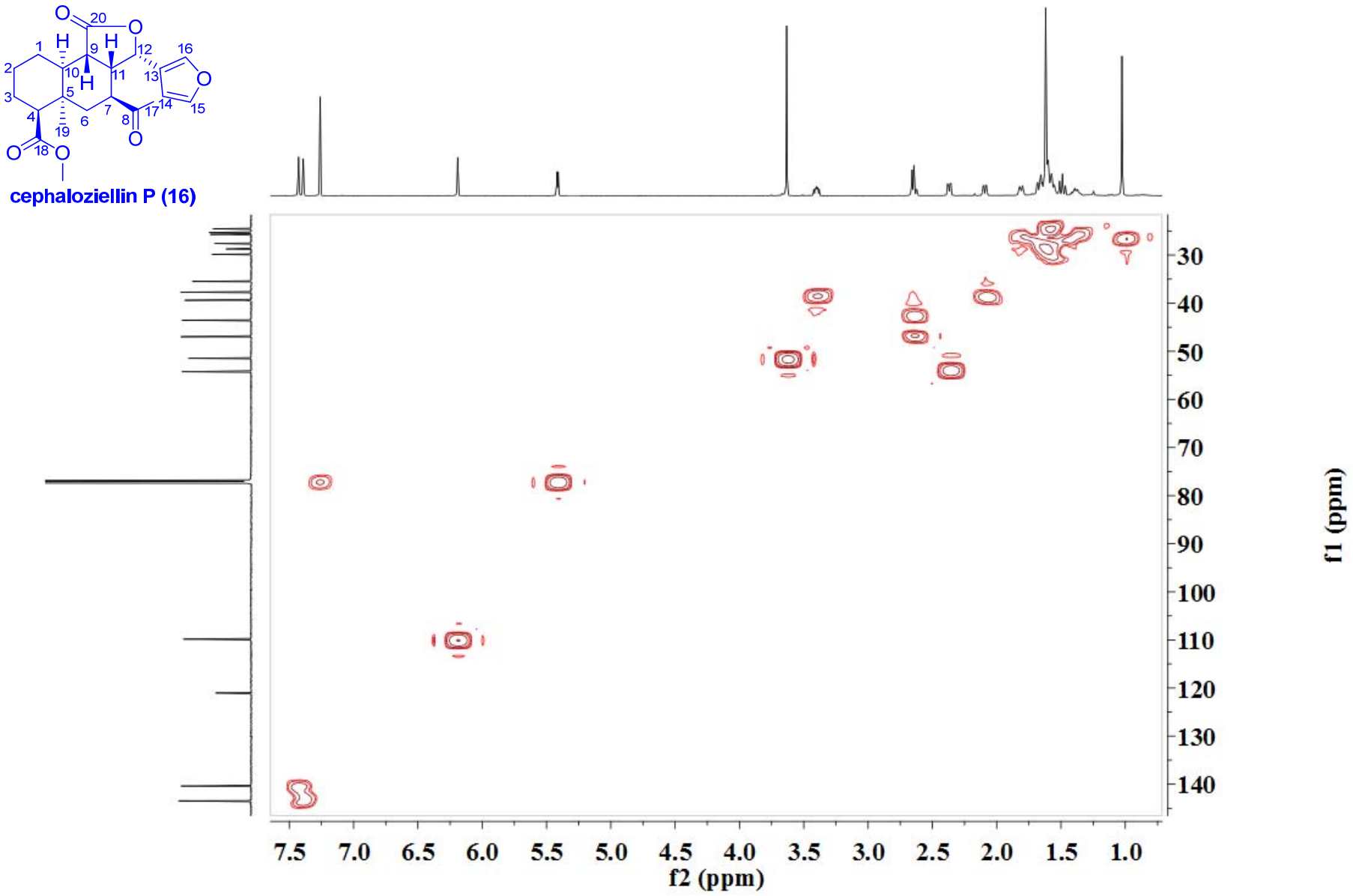
S179. ^{1}H NMR spectrum (600 MHz) of cephaloziellin P (**16**) in $CDCl_3$.



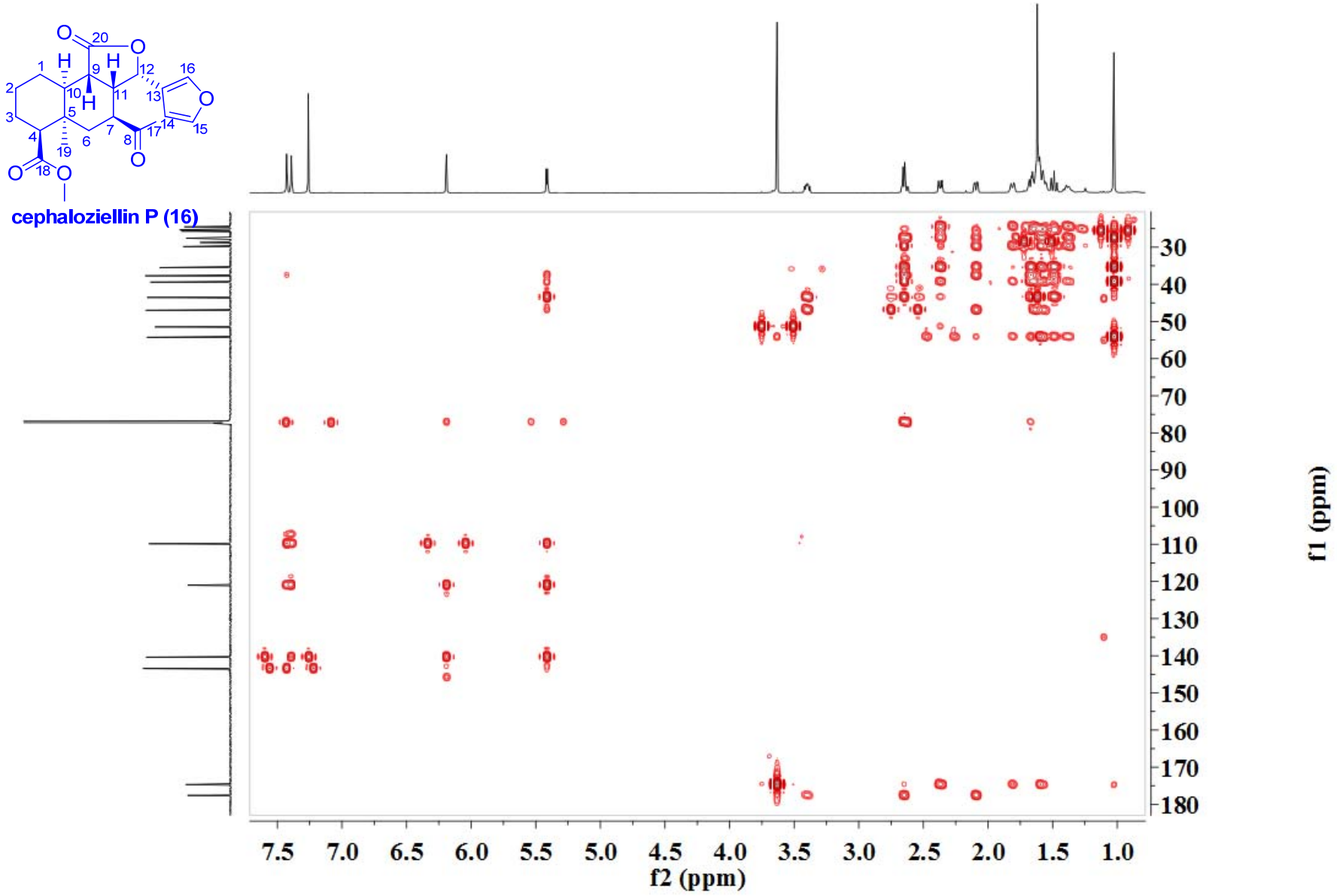
S180. ^{13}C NMR spectrum (150 MHz) of cephaloziellin P (**16**) in $CDCl_3$.



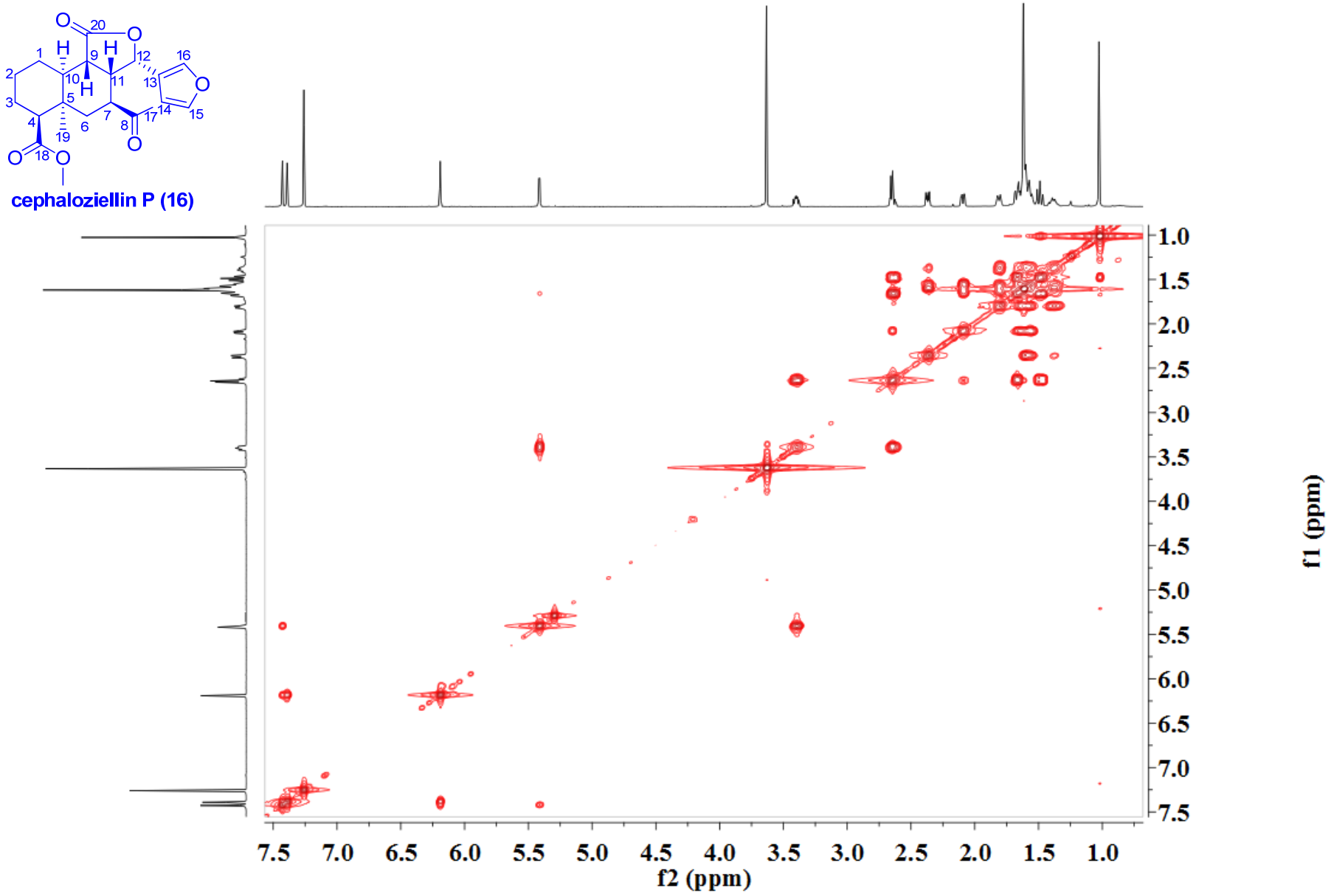
S181. HSQC spectrum (600 MHz) of cephaloziellin P (**16**) in $CDCl_3$.



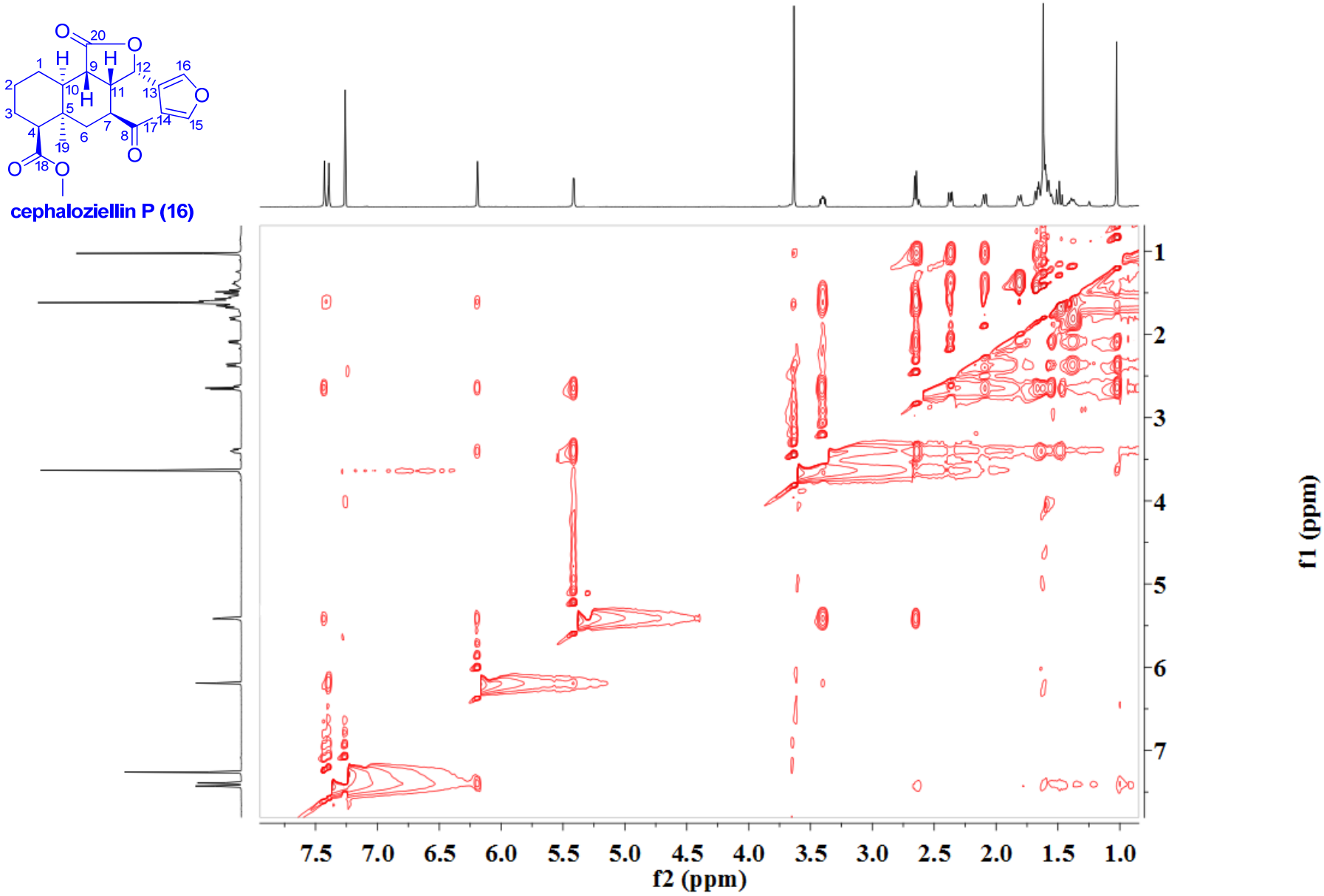
S182. HMBC spectrum (600 MHz) of cephaloziellin P (**16**) in $CDCl_3$.



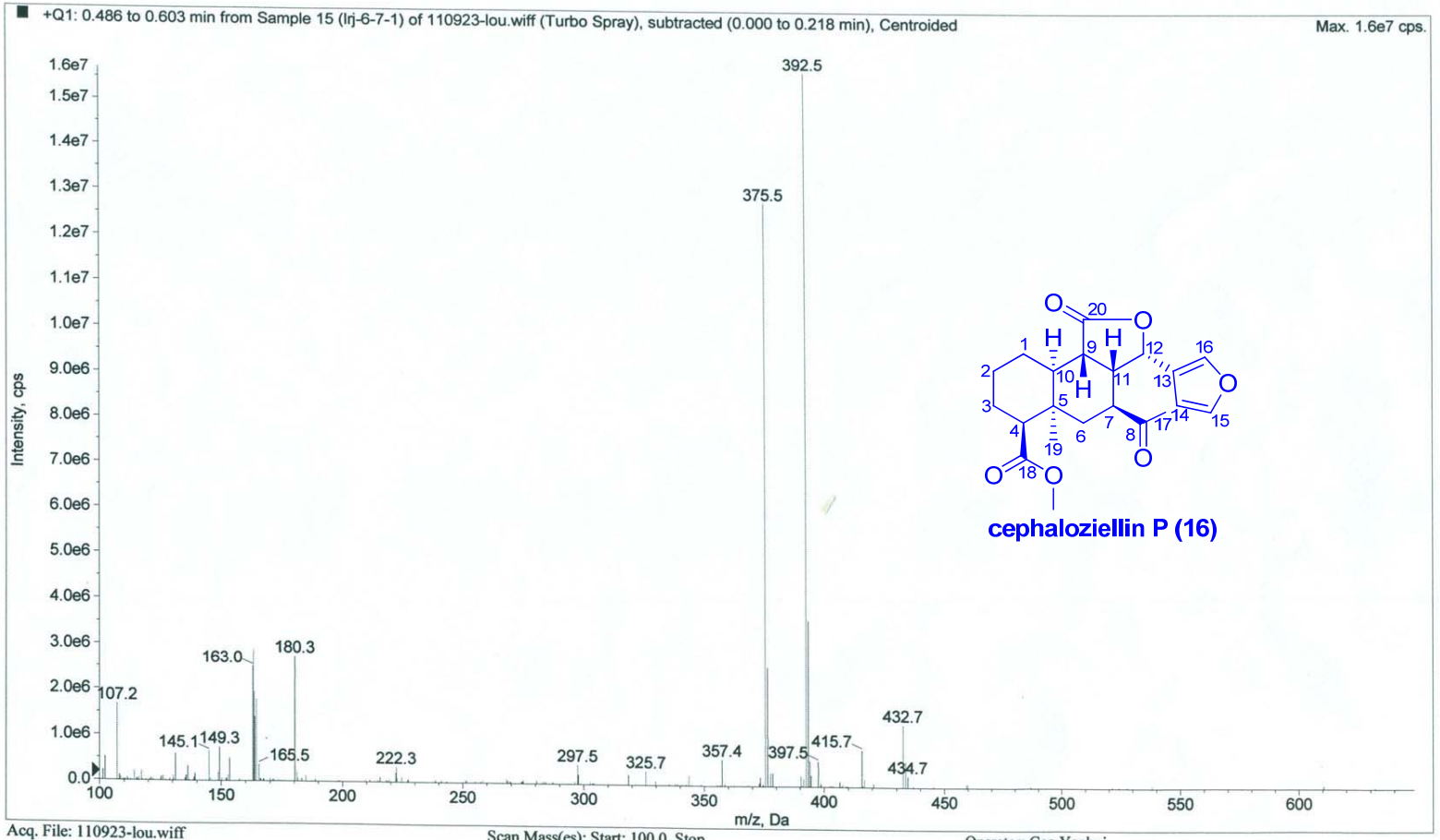
S183. ^{1}H-^{1}H COSY spectrum (600 MHz) of cephaloziellin P (**16**) in $CDCl_3$.



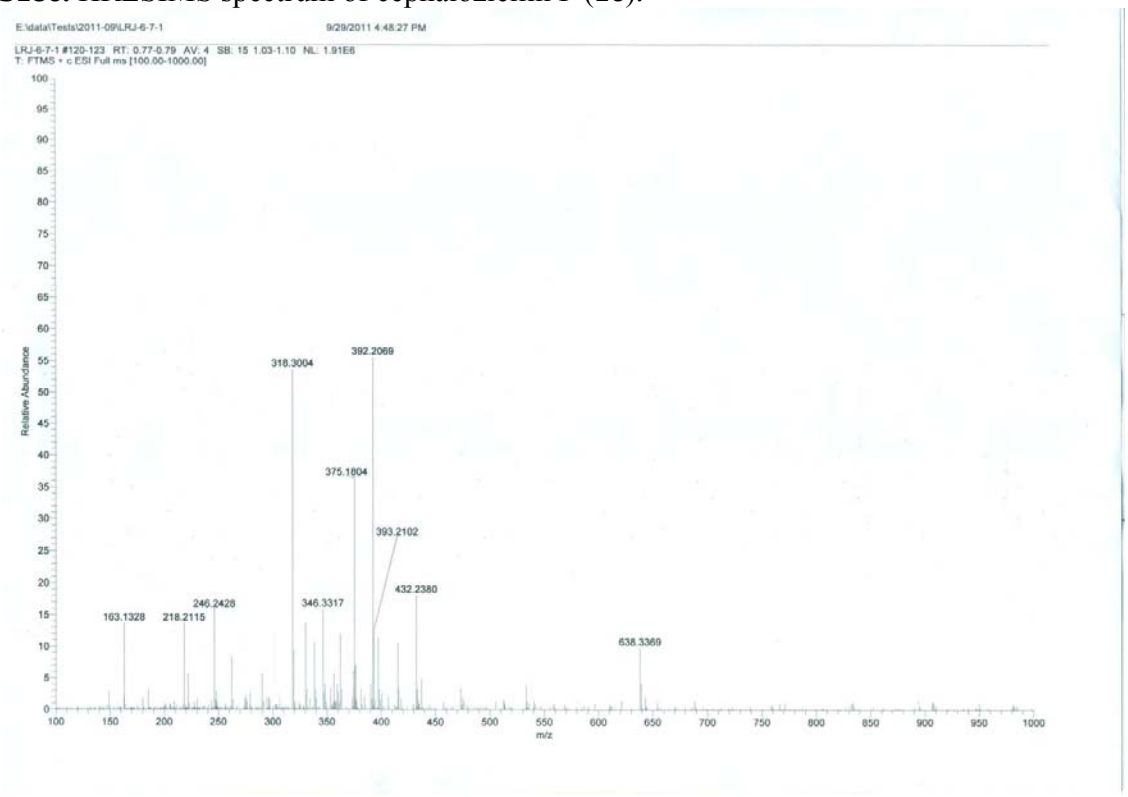
S184. NOESY spectrum (600 MHz) of cephaloziellin P (**16**) in $CDCl_3$.

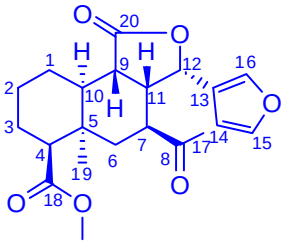


S185. ESIMS spectrum of cephaloziellin P (**16**).



S186. HRESIMS spectrum of cephaloziellin P (**16**).



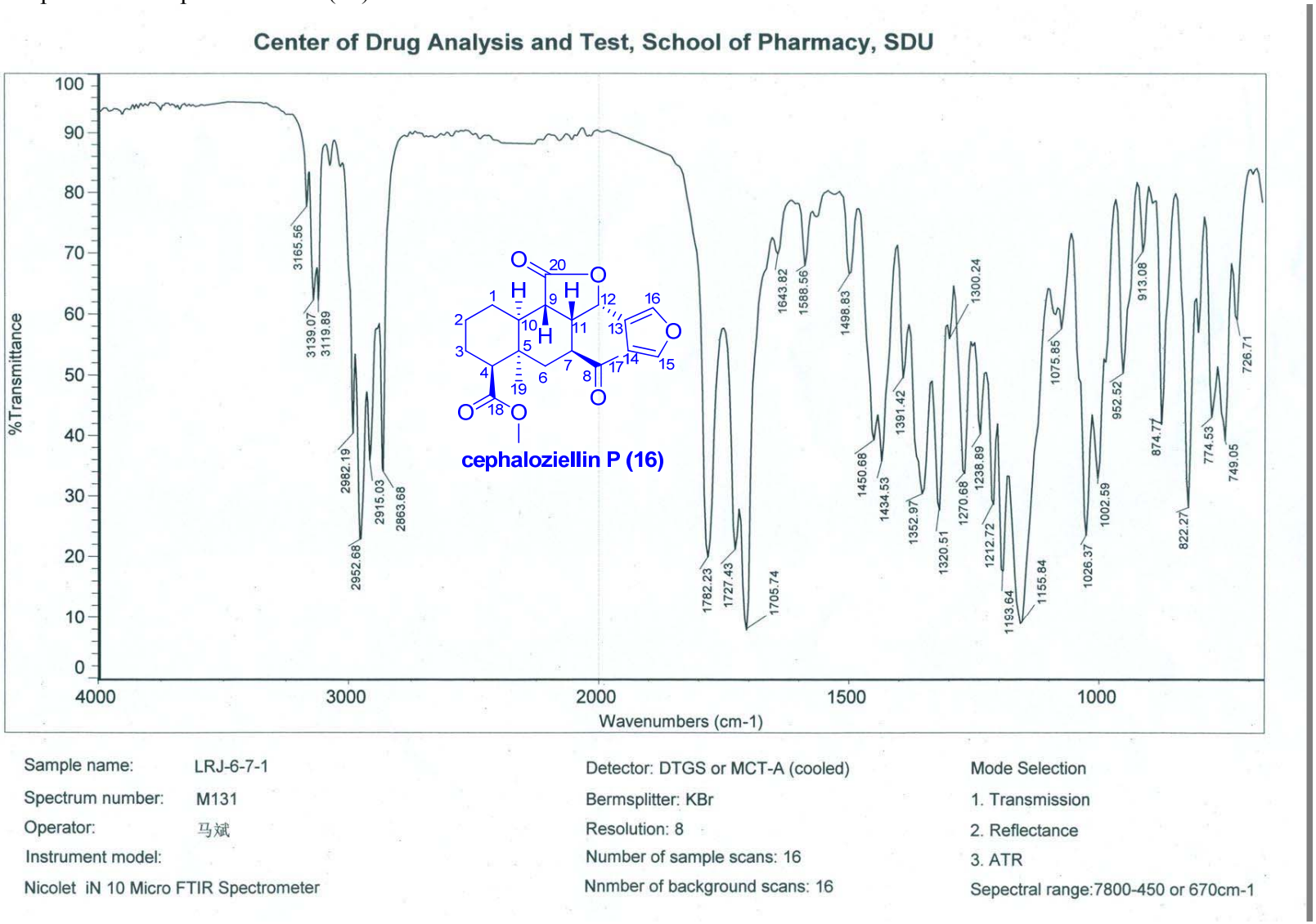


cephaloziellin P (16)

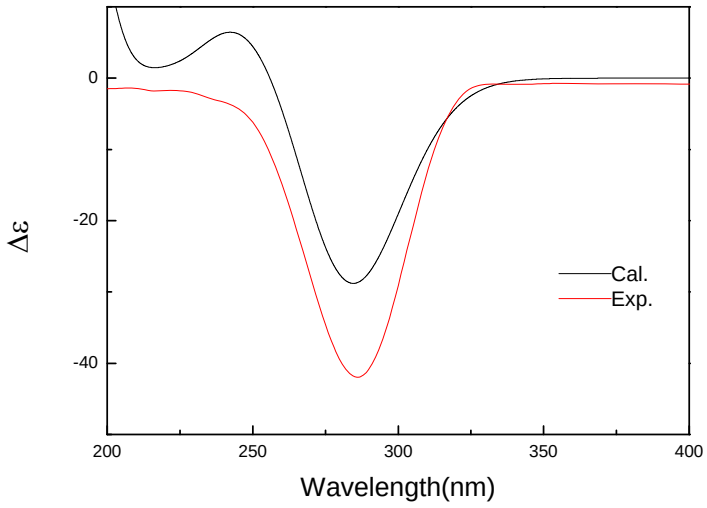
SPECTRUM - simulation :

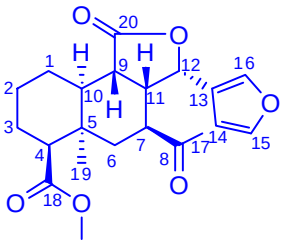
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
392.2069	392.2068	0.37	7.5	$^{12}C_{21}H_{30}O_6N_1$

S187. IR spectrum of cephaloziellin P (**16**).

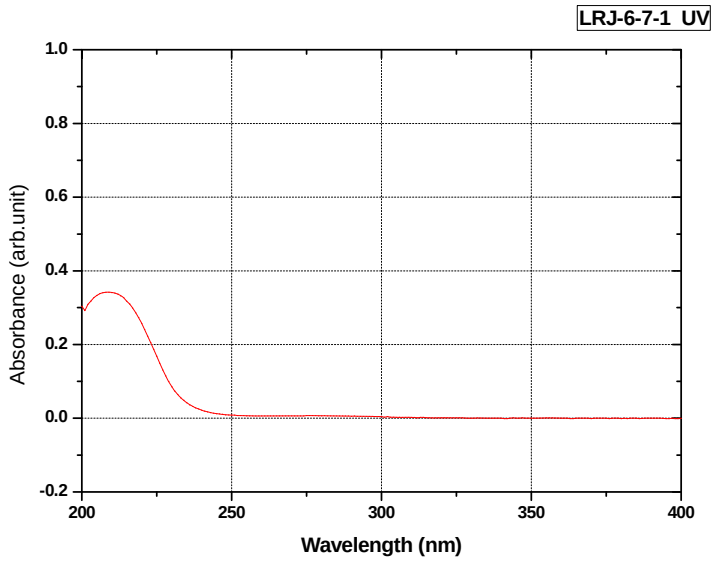


S188. Experimental ECD and calculated ECD, and UV spectra of cephaloziellin P (**16**).

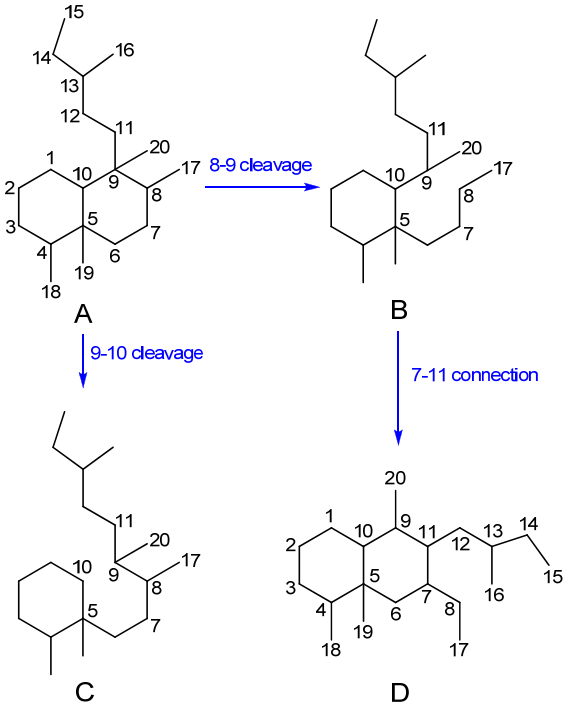




cephaloziellin P (16)



S189. Plausible routes for the biogenesis of *seco*-clerodanes and modified clerodanes.



These clerodane diterpenoids could be divided into four types based on plausible routes for their biogenesis: Type A: clerodanes (compounds **1**−**4** and **17**); Type B: *seco*-clerodanes cleaved between C8-C9 (compounds **5**−**7**); Type C: *seco*-clerodanes cleaved between C9-C10 (compounds **8**−**11**); and Type D; modified clerodanes cleaved between C8-C9 with C-7 subsequently bound to C-11 (compounds **12**−**16** and **18**).

S190. Comparison of the 1D NMR data between **3** and **17**.

positio	δ_H		δ_C	
	17	**3**	**17**	**3**
1	1.95 m	1.95 m; 1.89 m	17.9 t	17.9 t
2	2.39 m	2.39 m	24.7 t	24.8 t
3	6.87 t (3.6)	6.87 t (3.6)	136.2 d	136.3 d
4	—	—	133.5 s	133.6 s
5	—	—	39.6 s	39.7 s
6	4.33 dd (10.8, 7.2)	4.34 dd (10.8, 7.2)	85.0 d	85.2 d
7	1.88 m	1.90 m	34.9 t	34.9 t
	1.25 m	1.29 m		
8	1.47 m	1.46 m	32.3 d	32.3 d
9	—	—	39.3 s	39.3 s
10	1.72 m	1.74 m	41.7 d	41.6 d
11	1.53 m	1.54 m	35.3 t	34.8 t
	1.76 m	1.76 m		
12	2.29 dt (12.0, 4.2)	2.24 m; 2.39 m	22.3 t	21.3 t
13	—	—	170.0 s	169.0 s
14	5.87 m	5.89 br s	**115.6 d**	**117.8 d**
15	—	—	**173.8 s**	**170.6 s**
16	**4.76 d (2.4)**	**6.03 d (4.8)**	**73.1 t**	**98.7 d**
17	0.85 d (6.6)	0.85 dd (6.6, 2.4)	15.4 q	15.4 q
18	—	—	169.7 s	169.9 s
19	1.27 s	1.27 s	30.8 q	30.8 q
20	0.77 s	0.77 s	16.5 q	16.5 q

S191. X-ray data of compound **5**.

Table 1. Crystal data and structure refinement for yxy_liruijuanc20.

Identification code	yxy_liruijuanc20
Empirical formula	C20 H22 O6
Formula weight	358.38
Temperature	293(2) K
Wavelength	0.71069 A
Crystal system, space group	Monoclinic, P2(1)
Unit cell dimensions	a = 8.783(2) A alpha = 90 deg. b = 11.166(3) A beta = 104.489(3) deg. c = 9.402(2) A gamma = 90 deg.
Volume	892.7(4) A^3
Z, Calculated density	2, 1.333 Mg/m^3
Absorption coefficient	0.098 mm^-1
F(000)	380
Crystal size	0.48 x 0.14 x 0.04 mm
Theta range for data collection	2.24 to 27.49 deg.
Limiting indices	-11<=h<=11, -14<=k<=14, -12<=l<=12
Reflections collected / unique	10496 / 4066 [R(int) = 0.0358]
Completeness to theta = 27.49	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9961 and 0.9543
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4066 / 1 / 238
Goodness-of-fit on F^2	0.986
Final R indices [I>2sigma(I)]	R1 = 0.0424, wR2 = 0.0806
R indices (all data)	R1 = 0.0769, wR2 = 0.0913
Extinction coefficient	0.017(3)
Largest diff. peak and hole	0.155 and -0.126 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for yxy_liruijuanc20. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	-3024(3)	5637(2)	7351(2)	57(1)
C(2)	-3892(3)	4534(3)	7684(3)	67(1)
C(3)	-3757(2)	3480(2)	6774(3)	58(1)
C(4)	-2831(2)	3483(2)	5859(2)	44(1)
C(5)	-1835(2)	4517(2)	5604(2)	39(1)
C(6)	-456(2)	3808(2)	5259(2)	40(1)
C(7)	431(2)	4368(2)	4252(2)	46(1)
C(8)	1976(3)	3786(2)	4312(3)	53(1)
C(9)	-175(2)	4838(2)	8271(2)	45(1)
C(10)	-1455(2)	5350(2)	6967(2)	42(1)
C(11)	1494(2)	5164(2)	8176(2)	47(1)
C(12)	1740(2)	6387(2)	8907(2)	51(1)

C(13)	3397(3)	6739(2)	9552(2)	49(1)
C(14)	4595(3)	6130(2)	10600(2)	57(1)
C(15)	5894(3)	6777(2)	10790(3)	61(1)
C(16)	4087(3)	7717(3)	9212(3)	79(1)
C(17)	2742(3)	4065(3)	3101(3)	85(1)
C(18)	-2504(3)	2458(2)	5012(3)	51(1)
C(19)	-2712(2)	5222(2)	4235(2)	50(1)
C(20)	-196(3)	5403(2)	9730(2)	57(1)
O(1)	5635(2)	7771(2)	9946(2)	78(1)
O(2)	886(2)	6294(2)	10060(2)	64(1)
O(3)	-976(2)	5143(2)	10562(2)	84(1)
O(4)	-3193(2)	1518(2)	4699(2)	70(1)
O(5)	-1189(2)	2699(1)	4551(2)	50(1)
O(6)	2593(2)	3133(2)	5307(2)	77(1)

Table 3. Bond lengths [A] and angles [deg] for yxy_liruijuanc20.

C(1)-C(2)	1.523(3)
C(1)-C(10)	1.544(3)
C(1)-H(1A)	0.9700
C(1)-H(1B)	0.9700
C(2)-C(3)	1.477(3)
C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700
C(3)-C(4)	1.323(3)
C(3)-H(3)	0.9300
C(4)-C(18)	1.464(3)
C(4)-C(5)	1.503(3)
C(5)-C(19)	1.541(3)
C(5)-C(6)	1.548(3)
C(5)-C(10)	1.550(3)
C(6)-O(5)	1.475(2)
C(6)-C(7)	1.505(2)
C(6)-H(6)	0.9800
C(7)-C(8)	1.492(3)
C(7)-H(7A)	0.9700
C(7)-H(7B)	0.9700
C(8)-O(6)	1.202(3)
C(8)-C(17)	1.494(3)
C(9)-C(20)	1.514(3)
C(9)-C(11)	1.535(3)
C(9)-C(10)	1.550(3)
C(9)-H(9)	0.9800
C(10)-H(10)	0.9800
C(11)-C(12)	1.520(3)
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(12)-O(2)	1.467(2)
C(12)-C(13)	1.483(3)
C(12)-H(12)	0.9800

C(13)-C(16)	1.326(3)
C(13)-C(14)	1.422(3)
C(14)-C(15)	1.324(3)
C(14)-H(14)	0.9300
C(15)-O(1)	1.350(3)
C(15)-H(15)	0.9300
C(16)-O(1)	1.364(3)
C(16)-H(16)	0.9300
C(17)-H(17A)	0.9600
C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600
C(18)-O(4)	1.211(3)
C(18)-O(5)	1.358(2)
C(19)-H(19A)	0.9600
C(19)-H(19B)	0.9600
C(19)-H(19C)	0.9600
C(20)-O(3)	1.197(3)
C(20)-O(2)	1.356(3)

C(2)-C(1)-C(10)	113.72(18)
C(2)-C(1)-H(1A)	108.8
C(10)-C(1)-H(1A)	108.8
C(2)-C(1)-H(1B)	108.8
C(10)-C(1)-H(1B)	108.8
H(1A)-C(1)-H(1B)	107.7
C(3)-C(2)-C(1)	114.09(17)
C(3)-C(2)-H(2A)	108.7
C(1)-C(2)-H(2A)	108.7
C(3)-C(2)-H(2B)	108.7
C(1)-C(2)-H(2B)	108.7
H(2A)-C(2)-H(2B)	107.6
C(4)-C(3)-C(2)	121.7(2)
C(4)-C(3)-H(3)	119.1
C(2)-C(3)-H(3)	119.1
C(3)-C(4)-C(18)	126.0(2)
C(3)-C(4)-C(5)	125.6(2)
C(18)-C(4)-C(5)	108.18(17)
C(4)-C(5)-C(19)	109.67(15)
C(4)-C(5)-C(6)	99.08(15)
C(19)-C(5)-C(6)	109.89(15)
C(4)-C(5)-C(10)	110.02(15)
C(19)-C(5)-C(10)	110.06(16)
C(6)-C(5)-C(10)	117.51(15)
O(5)-C(6)-C(7)	107.54(15)
O(5)-C(6)-C(5)	104.37(14)
C(7)-C(6)-C(5)	118.36(17)
O(5)-C(6)-H(6)	108.7
C(7)-C(6)-H(6)	108.7
C(5)-C(6)-H(6)	108.7
C(8)-C(7)-C(6)	113.84(18)
C(8)-C(7)-H(7A)	108.8

C(6)-C(7)-H(7A)	108.8
C(8)-C(7)-H(7B)	108.8
C(6)-C(7)-H(7B)	108.8
H(7A)-C(7)-H(7B)	107.7
O(6)-C(8)-C(7)	121.5(2)
O(6)-C(8)-C(17)	121.2(2)
C(7)-C(8)-C(17)	117.3(2)
C(20)-C(9)-C(11)	100.52(17)
C(20)-C(9)-C(10)	113.11(17)
C(11)-C(9)-C(10)	112.35(17)
C(20)-C(9)-H(9)	110.2
C(11)-C(9)-H(9)	110.2
C(10)-C(9)-H(9)	110.2
C(1)-C(10)-C(5)	107.31(16)
C(1)-C(10)-C(9)	113.87(16)
C(5)-C(10)-C(9)	113.37(17)
C(1)-C(10)-H(10)	107.3
C(5)-C(10)-H(10)	107.3
C(9)-C(10)-H(10)	107.3
C(12)-C(11)-C(9)	102.48(17)
C(12)-C(11)-H(11A)	111.3
C(9)-C(11)-H(11A)	111.3
C(12)-C(11)-H(11B)	111.3
C(9)-C(11)-H(11B)	111.3
H(11A)-C(11)-H(11B)	109.2
O(2)-C(12)-C(13)	110.34(16)
O(2)-C(12)-C(11)	103.25(17)
C(13)-C(12)-C(11)	115.89(18)
O(2)-C(12)-H(12)	109.0
C(13)-C(12)-H(12)	109.0
C(11)-C(12)-H(12)	109.0
C(16)-C(13)-C(14)	104.9(2)
C(16)-C(13)-C(12)	125.5(2)
C(14)-C(13)-C(12)	129.6(2)
C(15)-C(14)-C(13)	107.2(2)
C(15)-C(14)-H(14)	126.4
C(13)-C(14)-H(14)	126.4
C(14)-C(15)-O(1)	110.9(2)
C(14)-C(15)-H(15)	124.6
O(1)-C(15)-H(15)	124.6
C(13)-C(16)-O(1)	111.9(2)
C(13)-C(16)-H(16)	124.1
O(1)-C(16)-H(16)	124.1
C(8)-C(17)-H(17A)	109.5
C(8)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(8)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
O(4)-C(18)-O(5)	120.5(2)
O(4)-C(18)-C(4)	131.0(2)

O(5)-C(18)-C(4)	108.54(19)
C(5)-C(19)-H(19A)	109.5
C(5)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(5)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
O(3)-C(20)-O(2)	120.8(2)
O(3)-C(20)-C(9)	129.0(2)
O(2)-C(20)-C(9)	110.21(19)
C(15)-O(1)-C(16)	105.1(2)
C(20)-O(2)-C(12)	109.99(16)
C(18)-O(5)-C(6)	109.36(15)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for yxy_liruijuanc20. The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	49(1)	75(2)	47(1)	-2(1)	11(1)	17(1)
C(2)	45(1)	102(2)	58(1)	-3(2)	20(1)	3(1)
C(3)	40(1)	70(2)	63(2)	10(1)	11(1)	-1(1)
C(4)	31(1)	48(1)	49(1)	8(1)	4(1)	3(1)
C(5)	35(1)	44(1)	37(1)	2(1)	7(1)	2(1)
C(6)	40(1)	41(1)	37(1)	-3(1)	7(1)	-2(1)
C(7)	48(1)	50(1)	44(1)	-4(1)	16(1)	-7(1)
C(8)	52(1)	51(1)	61(1)	-3(1)	20(1)	-7(1)
C(9)	41(1)	56(1)	37(1)	4(1)	6(1)	6(1)
C(10)	39(1)	49(1)	36(1)	2(1)	6(1)	4(1)
C(11)	43(1)	58(1)	39(1)	-4(1)	7(1)	1(1)
C(12)	54(1)	58(2)	38(1)	-2(1)	5(1)	7(1)
C(13)	55(1)	49(1)	37(1)	-4(1)	4(1)	1(1)
C(14)	49(1)	62(2)	56(1)	6(1)	8(1)	3(1)
C(15)	51(2)	77(2)	50(1)	3(1)	5(1)	2(1)
C(16)	85(2)	66(2)	65(2)	13(1)	-19(1)	-15(2)
C(17)	79(2)	102(2)	91(2)	0(2)	54(2)	-1(2)
C(18)	43(1)	48(1)	60(1)	5(1)	6(1)	-3(1)
C(19)	53(1)	52(1)	40(1)	3(1)	2(1)	4(1)
C(20)	43(1)	86(2)	38(1)	3(1)	5(1)	10(1)
O(1)	77(1)	76(1)	71(1)	7(1)	-2(1)	-24(1)
O(2)	62(1)	85(1)	43(1)	-16(1)	12(1)	9(1)
O(3)	62(1)	152(2)	43(1)	7(1)	21(1)	6(1)
O(4)	55(1)	51(1)	99(1)	-6(1)	13(1)	-13(1)
O(5)	47(1)	45(1)	58(1)	-7(1)	15(1)	-7(1)
O(6)	51(1)	81(1)	102(1)	17(1)	28(1)	11(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for yxy_liruijuanc20.

	x	y	z	U(eq)
H(1A)	-2816	6164	8198	68
H(1B)	-3700	6065	6534	68
H(2A)	-3484	4324	8711	80
H(2B)	-4996	4731	7538	80
H(3)	-4339	2797	6845	70
H(6)	292	3598	6186	48
H(7A)	-214	4328	3252	56
H(7B)	610	5206	4508	56
H(9)	-284	3967	8324	54
H(10)	-1049	6102	6670	51
H(11A)	2258	4589	8701	57
H(11B)	1561	5208	7163	57
H(12)	1234	6997	8195	61
H(14)	4486	5411	11066	68
H(15)	6855	6573	11420	73
H(16)	3576	8296	8553	94
H(17A)	3802	3768	3354	127
H(17B)	2753	4916	2960	127
H(17C)	2165	3689	2210	127
H(19A)	-2919	4705	3393	75
H(19B)	-2076	5884	4078	75
H(19C)	-3688	5518	4382	75

Table 6. Torsion angles [deg] for yxy_liruijuanc20.

C(10)-C(1)-C(2)-C(3)	-36.6(3)
C(1)-C(2)-C(3)-C(4)	6.3(3)
C(2)-C(3)-C(4)-C(18)	174.1(2)
C(2)-C(3)-C(4)-C(5)	-0.8(3)
C(3)-C(4)-C(5)-C(19)	-96.6(2)
C(18)-C(4)-C(5)-C(19)	87.77(19)
C(3)-C(4)-C(5)-C(6)	148.4(2)
C(18)-C(4)-C(5)-C(6)	-27.3(2)
C(3)-C(4)-C(5)-C(10)	24.6(3)
C(18)-C(4)-C(5)-C(10)	-151.04(16)
C(4)-C(5)-C(6)-O(5)	31.32(18)
C(19)-C(5)-C(6)-O(5)	-83.54(19)
C(10)-C(5)-C(6)-O(5)	149.62(16)
C(4)-C(5)-C(6)-C(7)	150.78(17)
C(19)-C(5)-C(6)-C(7)	35.9(2)
C(10)-C(5)-C(6)-C(7)	-90.9(2)
O(5)-C(6)-C(7)-C(8)	-78.1(2)
C(5)-C(6)-C(7)-C(8)	164.14(19)
C(6)-C(7)-C(8)-O(6)	-16.4(3)
C(6)-C(7)-C(8)-C(17)	164.8(2)

C(2)-C(1)-C(10)-C(5)	59.0(2)
C(2)-C(1)-C(10)-C(9)	-67.3(2)
C(4)-C(5)-C(10)-C(1)	-50.7(2)
C(19)-C(5)-C(10)-C(1)	70.3(2)
C(6)-C(5)-C(10)-C(1)	-162.93(17)
C(4)-C(5)-C(10)-C(9)	76.0(2)
C(19)-C(5)-C(10)-C(9)	-163.08(16)
C(6)-C(5)-C(10)-C(9)	-36.3(2)
C(20)-C(9)-C(10)-C(1)	-37.0(3)
C(11)-C(9)-C(10)-C(1)	-150.00(18)
C(20)-C(9)-C(10)-C(5)	-160.11(17)
C(11)-C(9)-C(10)-C(5)	86.9(2)
C(20)-C(9)-C(11)-C(12)	-34.5(2)
C(10)-C(9)-C(11)-C(12)	86.04(19)
C(9)-C(11)-C(12)-O(2)	34.68(19)
C(9)-C(11)-C(12)-C(13)	155.42(18)
O(2)-C(12)-C(13)-C(16)	-120.1(3)
C(11)-C(12)-C(13)-C(16)	123.0(3)
O(2)-C(12)-C(13)-C(14)	61.8(3)
C(11)-C(12)-C(13)-C(14)	-55.0(3)
C(16)-C(13)-C(14)-C(15)	-0.7(3)
C(12)-C(13)-C(14)-C(15)	177.7(2)
C(13)-C(14)-C(15)-O(1)	0.3(3)
C(14)-C(13)-C(16)-O(1)	0.9(3)
C(12)-C(13)-C(16)-O(1)	-177.6(2)
C(3)-C(4)-C(18)-O(4)	17.7(4)
C(5)-C(4)-C(18)-O(4)	-166.7(2)
C(3)-C(4)-C(18)-O(5)	-162.4(2)
C(5)-C(4)-C(18)-O(5)	13.2(2)
C(11)-C(9)-C(20)-O(3)	-154.9(2)
C(10)-C(9)-C(20)-O(3)	85.1(3)
C(11)-C(9)-C(20)-O(2)	23.1(2)
C(10)-C(9)-C(20)-O(2)	-96.9(2)
C(14)-C(15)-O(1)-C(16)	0.3(3)
C(13)-C(16)-O(1)-C(15)	-0.7(3)
O(3)-C(20)-O(2)-C(12)	176.8(2)
C(9)-C(20)-O(2)-C(12)	-1.4(2)
C(13)-C(12)-O(2)-C(20)	-145.79(19)
C(11)-C(12)-O(2)-C(20)	-21.3(2)
O(4)-C(18)-O(5)-C(6)	-171.60(19)
C(4)-C(18)-O(5)-C(6)	8.5(2)
C(7)-C(6)-O(5)-C(18)	-152.60(16)
C(5)-C(6)-O(5)-C(18)	-26.08(19)

Symmetry transformations used to generate equivalent atoms:

S192. X-ray data of compound **9**.

Table 1. Crystal data and structure refinement for c3.

Identification code	c3
Empirical formula	C20 H22 O7
Formula weight	374.38
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 8.237(7) A alpha = 90 deg. b = 23.983(19) A beta = 90 deg. c = 9.258(7) A gamma = 90 deg.
Volume	1829(3) A^3
Z, Calculated density	4, 1.360 Mg/m^3
Absorption coefficient	0.103 mm^-1
F(000)	792
Crystal size	0.35 x 0.32 x 0.03 mm
Theta range for data collection	2.36 to 26.97 deg.
Limiting indices	-10<=h<=10, -30<=k<=30, -11<=l<=7
Reflections collected / unique	10553 / 3904 [R(int) = 0.1215]
Completeness to theta = 26.97	99.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9969 and 0.9648
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3904 / 4 / 248
Goodness-of-fit on F^2	0.979
Final R indices [I>2sigma(I)]	R1 = 0.1052, wR2 = 0.2603
R indices (all data)	R1 = 0.2108, wR2 = 0.3173
Extinction coefficient	0.058(9)
Largest diff. peak and hole	0.454 and -0.375 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for c3.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	6427(8)	571(3)	5870(9)	62(2)
C(2)	5197(9)	892(4)	4985(10)	65(2)
C(3)	3486(9)	793(4)	5547(9)	64(2)
C(4)	3249(8)	536(3)	6792(9)	54(2)
C(5)	4476(8)	321(3)	7820(8)	48(2)
C(6)	3711(8)	539(4)	9234(9)	60(2)
C(7)	3956(9)	1136(4)	9476(10)	67(2)
C(8)	5722(9)	1306(3)	9297(8)	53(2)
C(9)	5860(10)	1935(4)	9278(9)	65(2)
C(10)	6168(8)	579(3)	7521(8)	48(2)
C(11)	4899(10)	2226(4)	8092(9)	63(2)
C(12)	5816(12)	2764(4)	7790(10)	73(3)

C(13)	5663(13)	2953(4)	6280(12)	79(3)
C(14)	4499(13)	3294(4)	5594(16)	91(3)
C(15)	4716(15)	3333(5)	4283(15)	90(3)
C(16)	6575(17)	2818(5)	5168(12)	109(4)
C(17)	6719(12)	1061(4)	10512(10)	82(3)
C(18)	1668(10)	484(4)	7502(10)	65(2)
C(19)	4520(10)	-304(3)	7791(11)	71(3)
C(20)	7587(12)	2153(4)	8845(10)	70(2)
O(1)	6067(15)	3036(4)	3898(9)	130(3)
O(2)	7494(7)	2608(3)	8082(8)	80(2)
O(3)	8866(8)	1968(3)	9256(8)	86(2)
O(4)	6260(5)	1143(2)	7874(5)	48(1)
O(5)	7296(6)	252(3)	8166(7)	68(2)
O(6)	1920(6)	448(2)	8899(6)	64(2)
O(7)	323(6)	457(3)	6981(9)	87(2)

Table 3. Bond lengths [A] and angles [deg] for c3.

C(1)-C(2)	1.513(11)
C(1)-C(10)	1.543(11)
C(1)-H(1A)	0.9700
C(1)-H(1B)	0.9700
C(2)-C(3)	1.521(10)
C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700
C(3)-C(4)	1.321(11)
C(3)-H(3)	0.9300
C(4)-C(18)	1.464(11)
C(4)-C(5)	1.481(11)
C(5)-C(19)	1.500(11)
C(5)-C(6)	1.544(11)
C(5)-C(10)	1.549(10)
C(6)-C(7)	1.465(11)
C(6)-O(6)	1.523(9)
C(6)-H(6)	0.9800
C(7)-C(8)	1.519(11)
C(7)-H(7A)	0.9700
C(7)-H(7B)	0.9700
C(8)-O(4)	1.443(9)
C(8)-C(17)	1.512(11)
C(8)-C(9)	1.514(12)
C(9)-C(11)	1.523(11)
C(9)-C(20)	1.567(12)
C(9)-H(9)	0.9800
C(10)-O(5)	1.354(8)
C(10)-O(4)	1.394(9)
C(11)-C(12)	1.522(13)
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(12)-O(2)	1.457(11)

C(12)-C(13)	1.474(14)
C(12)-H(12)	0.9800
C(13)-C(16)	1.316(14)
C(13)-C(14)	1.412(14)
C(14)-C(15)	1.231(16)
C(14)-H(14)	0.9300
C(15)-O(1)	1.367(15)
C(15)-H(15)	0.9300
C(16)-O(1)	1.353(14)
C(16)-H(16)	0.9300
C(17)-H(17A)	0.9600
C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600
C(18)-O(7)	1.210(10)
C(18)-O(6)	1.313(10)
C(19)-H(19A)	0.9600
C(19)-H(19B)	0.9600
C(19)-H(19C)	0.9600
C(20)-O(3)	1.205(11)
C(20)-O(2)	1.302(11)
O(5)-H(5)	0.8200

C(2)-C(1)-C(10)	115.9(6)
C(2)-C(1)-H(1A)	108.3
C(10)-C(1)-H(1A)	108.3
C(2)-C(1)-H(1B)	108.3
C(10)-C(1)-H(1B)	108.3
H(1A)-C(1)-H(1B)	107.4
C(1)-C(2)-C(3)	110.9(7)
C(1)-C(2)-H(2A)	109.5
C(3)-C(2)-H(2A)	109.5
C(1)-C(2)-H(2B)	109.5
C(3)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	108.1
C(4)-C(3)-C(2)	120.5(7)
C(4)-C(3)-H(3)	119.7
C(2)-C(3)-H(3)	119.7
C(3)-C(4)-C(18)	124.3(7)
C(3)-C(4)-C(5)	128.4(7)
C(18)-C(4)-C(5)	106.8(7)
C(4)-C(5)-C(19)	110.6(7)
C(4)-C(5)-C(6)	98.5(6)
C(19)-C(5)-C(6)	111.3(7)
C(4)-C(5)-C(10)	111.1(6)
C(19)-C(5)-C(10)	112.0(6)
C(6)-C(5)-C(10)	112.6(6)
C(7)-C(6)-O(6)	107.8(6)
C(7)-C(6)-C(5)	113.8(6)
O(6)-C(6)-C(5)	100.0(6)
C(7)-C(6)-H(6)	111.6
O(6)-C(6)-H(6)	111.6

C(5)-C(6)-H(6)	111.6
C(6)-C(7)-C(8)	112.2(7)
C(6)-C(7)-H(7A)	109.2
C(8)-C(7)-H(7A)	109.2
C(6)-C(7)-H(7B)	109.2
C(8)-C(7)-H(7B)	109.2
H(7A)-C(7)-H(7B)	107.9
O(4)-C(8)-C(17)	114.0(7)
O(4)-C(8)-C(9)	103.7(6)
C(17)-C(8)-C(9)	110.7(7)
O(4)-C(8)-C(7)	108.8(6)
C(17)-C(8)-C(7)	109.6(7)
C(9)-C(8)-C(7)	109.9(6)
C(8)-C(9)-C(11)	115.1(7)
C(8)-C(9)-C(20)	113.8(7)
C(11)-C(9)-C(20)	97.8(7)
C(8)-C(9)-H(9)	109.9
C(11)-C(9)-H(9)	109.9
C(20)-C(9)-H(9)	109.9
O(5)-C(10)-O(4)	114.9(6)
O(5)-C(10)-C(1)	109.5(6)
O(4)-C(10)-C(1)	103.7(6)
O(5)-C(10)-C(5)	107.9(6)
O(4)-C(10)-C(5)	113.2(5)
C(1)-C(10)-C(5)	107.2(6)
C(12)-C(11)-C(9)	105.2(7)
C(12)-C(11)-H(11A)	110.7
C(9)-C(11)-H(11A)	110.7
C(12)-C(11)-H(11B)	110.7
C(9)-C(11)-H(11B)	110.7
H(11A)-C(11)-H(11B)	108.8
O(2)-C(12)-C(13)	109.6(8)
O(2)-C(12)-C(11)	102.6(7)
C(13)-C(12)-C(11)	113.1(8)
O(2)-C(12)-H(12)	110.4
C(13)-C(12)-H(12)	110.4
C(11)-C(12)-H(12)	110.4
C(16)-C(13)-C(14)	100.3(11)
C(16)-C(13)-C(12)	128.1(10)
C(14)-C(13)-C(12)	131.5(10)
C(15)-C(14)-C(13)	112.9(12)
C(15)-C(14)-H(14)	123.6
C(13)-C(14)-H(14)	123.6
C(14)-C(15)-O(1)	109.6(11)
C(14)-C(15)-H(15)	125.2
O(1)-C(15)-H(15)	125.2
C(13)-C(16)-O(1)	114.1(11)
C(13)-C(16)-H(16)	123.0
O(1)-C(16)-H(16)	123.0
C(8)-C(17)-H(17A)	109.5
C(8)-C(17)-H(17B)	109.5

H(17A)-C(17)-H(17B)	109.5
C(8)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
O(7)-C(18)-O(6)	122.3(8)
O(7)-C(18)-C(4)	129.8(8)
O(6)-C(18)-C(4)	107.9(7)
C(5)-C(19)-H(19A)	109.5
C(5)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(5)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
O(3)-C(20)-O(2)	122.1(9)
O(3)-C(20)-C(9)	126.2(9)
O(2)-C(20)-C(9)	111.4(8)
C(16)-O(1)-C(15)	103.1(10)
C(20)-O(2)-C(12)	111.8(7)
C(10)-O(4)-C(8)	117.4(5)
C(10)-O(5)-H(5)	109.5
C(18)-O(6)-C(6)	110.2(6)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for c3.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	13(3)	84(6)	87(6)	-6(5)	0(4)	3(4)
C(2)	35(4)	106(7)	54(5)	4(5)	6(4)	-6(4)
C(3)	26(4)	106(7)	60(5)	-12(5)	-8(4)	1(4)
C(4)	28(4)	79(5)	54(5)	-2(4)	6(3)	5(3)
C(5)	32(4)	63(5)	49(5)	-1(4)	11(3)	-1(3)
C(6)	24(3)	82(6)	74(6)	19(5)	14(4)	0(4)
C(7)	30(4)	111(8)	59(5)	6(5)	20(4)	3(4)
C(8)	47(4)	73(6)	39(4)	1(4)	0(3)	1(4)
C(9)	45(5)	104(7)	46(5)	-6(5)	-5(4)	6(4)
C(10)	21(3)	70(5)	53(4)	7(4)	9(3)	6(3)
C(11)	53(5)	87(6)	48(5)	-7(4)	0(4)	6(4)
C(12)	75(7)	72(5)	71(7)	-12(5)	5(5)	-2(5)
C(13)	64(6)	79(7)	95(8)	-5(6)	11(5)	-7(5)
C(14)	60(6)	85(7)	127(11)	7(7)	-20(7)	1(5)
C(15)	74(7)	118(9)	77(8)	29(7)	-26(6)	-17(6)
C(16)	129(10)	142(10)	56(6)	12(6)	25(7)	43(8)
C(17)	61(6)	126(8)	59(6)	10(5)	-17(5)	1(5)
C(18)	43(5)	84(6)	68(6)	4(5)	7(4)	-4(4)
C(19)	41(5)	83(6)	88(7)	10(5)	18(4)	6(4)
C(20)	54(6)	95(7)	61(5)	-7(5)	-13(4)	-12(5)
O(1)	159(10)	158(8)	74(5)	17(5)	-16(6)	11(7)

O(2)	59(4)	89(4)	93(5)	2(4)	-6(4)	-13(3)
O(3)	52(4)	122(5)	82(4)	-1(4)	-21(3)	-13(4)
O(4)	35(3)	74(4)	36(3)	3(2)	3(2)	-1(2)
O(5)	31(3)	102(4)	72(4)	17(3)	7(3)	9(3)
O(6)	27(3)	105(4)	60(4)	5(3)	13(2)	0(3)
O(7)	23(3)	122(5)	117(5)	3(4)	0(3)	-6(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for c3.

	x	y	z	U(eq)
H(1A)	7497	720	5665	74
H(1B)	6419	186	5550	74
H(2A)	5263	775	3984	78
H(2B)	5446	1287	5029	78
H(3)	2600	914	5009	77
H(6)	4059	318	10070	72
H(7A)	3598	1231	10443	80
H(7B)	3295	1345	8797	80
H(9)	5552	2087	10223	78
H(11A)	4849	1995	7232	75
H(11B)	3801	2304	8412	75
H(12)	5465	3058	8454	87
H(14)	3657	3471	6082	109
H(15)	4062	3533	3650	108
H(16)	7489	2592	5246	131
H(17A)	7852	1118	10316	123
H(17B)	6502	669	10589	123
H(17C)	6438	1242	11403	123
H(19A)	4868	-428	6855	106
H(19B)	3454	-448	7988	106
H(19C)	5264	-437	8511	106
H(5)	8184	306	7789	102

Table 6. Torsion angles [deg] for c3.

C(10)-C(1)-C(2)-C(3)	-42.5(11)
C(1)-C(2)-C(3)-C(4)	10.7(12)
C(2)-C(3)-C(4)-C(18)	172.1(8)
C(2)-C(3)-C(4)-C(5)	1.2(14)
C(3)-C(4)-C(5)-C(19)	-108.0(10)
C(18)-C(4)-C(5)-C(19)	79.8(8)
C(3)-C(4)-C(5)-C(6)	135.3(9)
C(18)-C(4)-C(5)-C(6)	-36.8(8)
C(3)-C(4)-C(5)-C(10)	17.0(12)
C(18)-C(4)-C(5)-C(10)	-155.2(7)
C(4)-C(5)-C(6)-C(7)	-76.7(8)
C(19)-C(5)-C(6)-C(7)	167.2(7)

C(10)-C(5)-C(6)-C(7)	40.5(9)
C(4)-C(5)-C(6)-O(6)	37.9(7)
C(19)-C(5)-C(6)-O(6)	-78.2(7)
C(10)-C(5)-C(6)-O(6)	155.1(6)
O(6)-C(6)-C(7)-C(8)	-159.9(6)
C(5)-C(6)-C(7)-C(8)	-49.9(9)
C(6)-C(7)-C(8)-O(4)	56.6(9)
C(6)-C(7)-C(8)-C(17)	-68.7(10)
C(6)-C(7)-C(8)-C(9)	169.4(7)
O(4)-C(8)-C(9)-C(11)	57.3(8)
C(17)-C(8)-C(9)-C(11)	180.0(7)
C(7)-C(8)-C(9)-C(11)	-58.8(9)
O(4)-C(8)-C(9)-C(20)	-54.4(8)
C(17)-C(8)-C(9)-C(20)	68.3(9)
C(7)-C(8)-C(9)-C(20)	-170.5(7)
C(2)-C(1)-C(10)-O(5)	176.7(7)
C(2)-C(1)-C(10)-O(4)	-60.2(8)
C(2)-C(1)-C(10)-C(5)	59.8(9)
C(4)-C(5)-C(10)-O(5)	-161.6(6)
C(19)-C(5)-C(10)-O(5)	-37.3(8)
C(6)-C(5)-C(10)-O(5)	89.0(8)
C(4)-C(5)-C(10)-O(4)	70.1(8)
C(19)-C(5)-C(10)-O(4)	-165.6(6)
C(6)-C(5)-C(10)-O(4)	-39.4(8)
C(4)-C(5)-C(10)-C(1)	-43.7(8)
C(19)-C(5)-C(10)-C(1)	80.6(8)
C(6)-C(5)-C(10)-C(1)	-153.2(6)
C(8)-C(9)-C(11)-C(12)	-152.4(7)
C(20)-C(9)-C(11)-C(12)	-31.5(8)
C(9)-C(11)-C(12)-O(2)	31.6(9)
C(9)-C(11)-C(12)-C(13)	149.6(8)
O(2)-C(12)-C(13)-C(16)	25.7(15)
C(11)-C(12)-C(13)-C(16)	-88.1(14)
O(2)-C(12)-C(13)-C(14)	-158.0(10)
C(11)-C(12)-C(13)-C(14)	88.1(12)
C(16)-C(13)-C(14)-C(15)	1.3(13)
C(12)-C(13)-C(14)-C(15)	-175.7(11)
C(13)-C(14)-C(15)-O(1)	-1.3(14)
C(14)-C(13)-C(16)-O(1)	-0.7(14)
C(12)-C(13)-C(16)-O(1)	176.4(10)
C(3)-C(4)-C(18)-O(7)	30.2(15)
C(5)-C(4)-C(18)-O(7)	-157.2(10)
C(3)-C(4)-C(18)-O(6)	-151.9(8)
C(5)-C(4)-C(18)-O(6)	20.6(9)
C(8)-C(9)-C(20)-O(3)	-42.7(12)
C(11)-C(9)-C(20)-O(3)	-164.6(9)
C(8)-C(9)-C(20)-O(2)	144.1(7)
C(11)-C(9)-C(20)-O(2)	22.2(9)
C(13)-C(16)-O(1)-C(15)	0.0(15)
C(14)-C(15)-O(1)-C(16)	0.8(14)
O(3)-C(20)-O(2)-C(12)	-176.6(9)

C(9)-C(20)-O(2)-C(12)	-3.1(10)
C(13)-C(12)-O(2)-C(20)	-138.2(8)
C(11)-C(12)-O(2)-C(20)	-17.7(9)
O(5)-C(10)-O(4)-C(8)	-73.5(7)
C(1)-C(10)-O(4)-C(8)	167.0(5)
C(5)-C(10)-O(4)-C(8)	51.1(8)
C(17)-C(8)-O(4)-C(10)	63.7(9)
C(9)-C(8)-O(4)-C(10)	-175.8(5)
C(7)-C(8)-O(4)-C(10)	-59.0(8)
O(7)-C(18)-O(6)-C(6)	-175.7(8)
C(4)-C(18)-O(6)-C(6)	6.2(9)
C(7)-C(6)-O(6)-C(18)	90.2(8)
C(5)-C(6)-O(6)-C(18)	-29.0(8)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for c3 [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(5)-H(5)...O(7)#1	0.82	1.95	2.768(8)	177.0

Symmetry transformations used to generate equivalent atoms:
#1 x+1,y,z

S193. X-ray data of compound **15**.

Table 1. Crystal data and structure refinement for yy_liruijuan01.

Identification code	yy_liruijuan01
Empirical formula	C21 H26 O6
Formula weight	374.42
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)
Unit cell dimensions	a = 9.098(2) A alpha = 90 deg.
	b = 10.562(2) A beta = 104.753(3) deg.
	c = 10.531(2) A gamma = 90 deg.
Volume	978.6(4) A^3
Z, Calculated density	2, 1.271 Mg/m^3
Absorption coefficient	0.093 mm^-1
F(000)	400
Crystal size	0.48 x 0.15 x 0.13 mm
Theta range for data collection	2.00 to 27.42 deg.
Limiting indices	-11<=h<=11, -13<=k<=13, -13<=l<=11
Reflections collected / unique	6054 / 4231 [R(int) = 0.0142]
Completeness to theta = 27.42	98.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9881 and 0.9569
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4231 / 1 / 248
Goodness-of-fit on F^2	1.053
Final R indices [I>2sigma(I)]	R1 = 0.0381, wR2 = 0.0906
R indices (all data)	R1 = 0.0452, wR2 = 0.0956
Absolute structure parameter	0.1(10)
Extinction coefficient	0.007(2)
Largest diff. peak and hole	0.147 and -0.126 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for yy_liruijuan01. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	3916(2)	9561(2)	8763(2)	53(1)
C(2)	4978(2)	10422(2)	8263(2)	65(1)
C(3)	4313(2)	10720(2)	6825(2)	60(1)
C(4)	4019(2)	9505(2)	6017(2)	48(1)
C(5)	2945(2)	8543(2)	6470(2)	39(1)
C(6)	1301(2)	9044(2)	6144(2)	39(1)
C(7)	216(2)	8152(2)	6617(2)	38(1)
C(8)	-1397(2)	8668(2)	6208(2)	48(1)
C(9)	2418(2)	7585(2)	8555(2)	41(1)
C(10)	3537(2)	8339(2)	7978(2)	43(1)
C(11)	733(2)	7937(2)	8094(2)	39(1)

C(12)	-29(2)	6767(2)	8517(2)	48(1)
C(13)	-274(2)	6879(2)	9858(2)	54(1)
C(14)	-1361(4)	7697(2)	10192(3)	90(1)
C(15)	-1222(5)	7564(3)	11468(3)	111(1)
C(16)	445(3)	6312(2)	10972(2)	75(1)
C(17)	-2132(2)	8734(2)	4775(2)	66(1)
C(18)	3425(2)	9843(2)	4578(2)	50(1)
C(19)	2997(2)	7285(2)	5748(2)	55(1)
C(20)	2386(3)	6156(2)	8445(2)	53(1)
C(21)	3408(3)	9281(3)	2402(2)	88(1)
O(1)	3937(2)	9058(2)	3796(1)	69(1)
O(2)	2592(2)	10716(2)	4172(1)	73(1)
O(3)	3397(2)	5441(2)	8401(2)	73(1)
O(4)	989(2)	5725(1)	8455(1)	60(1)
O(5)	-112(3)	6716(2)	11991(2)	103(1)
O(6)	-2052(2)	9002(2)	7012(2)	78(1)

Table 3. Bond lengths [A] and angles [deg] for yy_liruijuan01.

C(1)-C(2)	1.515(3)
C(1)-C(10)	1.525(3)
C(1)-H(1A)	0.9700
C(1)-H(1B)	0.9700
C(2)-C(3)	1.514(3)
C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700
C(3)-C(4)	1.525(3)
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(4)-C(18)	1.516(2)
C(4)-C(5)	1.565(2)
C(4)-H(4)	0.9800
C(5)-C(19)	1.538(3)
C(5)-C(6)	1.541(2)
C(5)-C(10)	1.557(2)
C(6)-C(7)	1.537(2)
C(6)-H(6A)	0.9700
C(6)-H(6B)	0.9700
C(7)-C(8)	1.521(2)
C(7)-C(11)	1.523(2)
C(7)-H(7)	0.9800
C(8)-O(6)	1.205(2)
C(8)-C(17)	1.489(3)
C(9)-C(20)	1.514(3)
C(9)-C(11)	1.532(2)
C(9)-C(10)	1.534(2)
C(9)-H(9)	0.9800
C(10)-H(10)	0.9800
C(11)-C(12)	1.537(2)
C(11)-H(11)	0.9800

C(12)-O(4)	1.451(2)
C(12)-C(13)	1.489(3)
C(12)-H(12)	0.9800
C(13)-C(16)	1.331(3)
C(13)-C(14)	1.423(3)
C(14)-C(15)	1.324(4)
C(14)-H(14)	0.9300
C(15)-O(5)	1.356(4)
C(15)-H(15)	0.9300
C(16)-O(5)	1.367(3)
C(16)-H(16)	0.9300
C(17)-H(17A)	0.9600
C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600
C(18)-O(2)	1.201(2)
C(18)-O(1)	1.333(2)
C(19)-H(19A)	0.9600
C(19)-H(19B)	0.9600
C(19)-H(19C)	0.9600
C(20)-O(3)	1.199(2)
C(20)-O(4)	1.353(3)
C(21)-O(1)	1.443(3)
C(21)-H(21A)	0.9600
C(21)-H(21B)	0.9600
C(21)-H(21C)	0.9600

C(2)-C(1)-C(10)	113.31(16)
C(2)-C(1)-H(1A)	108.9
C(10)-C(1)-H(1A)	108.9
C(2)-C(1)-H(1B)	108.9
C(10)-C(1)-H(1B)	108.9
H(1A)-C(1)-H(1B)	107.7
C(3)-C(2)-C(1)	110.19(15)
C(3)-C(2)-H(2A)	109.6
C(1)-C(2)-H(2A)	109.6
C(3)-C(2)-H(2B)	109.6
C(1)-C(2)-H(2B)	109.6
H(2A)-C(2)-H(2B)	108.1
C(2)-C(3)-C(4)	110.59(18)
C(2)-C(3)-H(3A)	109.5
C(4)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3B)	109.5
C(4)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	108.1
C(18)-C(4)-C(3)	109.05(16)
C(18)-C(4)-C(5)	111.46(14)
C(3)-C(4)-C(5)	114.22(14)
C(18)-C(4)-H(4)	107.3
C(3)-C(4)-H(4)	107.3
C(5)-C(4)-H(4)	107.3
C(19)-C(5)-C(6)	109.69(14)

C(19)-C(5)-C(10)	109.76(14)
C(6)-C(5)-C(10)	109.78(12)
C(19)-C(5)-C(4)	108.07(14)
C(6)-C(5)-C(4)	110.82(13)
C(10)-C(5)-C(4)	108.69(13)
C(7)-C(6)-C(5)	112.63(13)
C(7)-C(6)-H(6A)	109.1
C(5)-C(6)-H(6A)	109.1
C(7)-C(6)-H(6B)	109.1
C(5)-C(6)-H(6B)	109.1
H(6A)-C(6)-H(6B)	107.8
C(8)-C(7)-C(11)	111.53(14)
C(8)-C(7)-C(6)	109.99(13)
C(11)-C(7)-C(6)	111.45(13)
C(8)-C(7)-H(7)	107.9
C(11)-C(7)-H(7)	107.9
C(6)-C(7)-H(7)	107.9
O(6)-C(8)-C(17)	121.55(17)
O(6)-C(8)-C(7)	121.35(17)
C(17)-C(8)-C(7)	117.10(16)
C(20)-C(9)-C(11)	102.68(15)
C(20)-C(9)-C(10)	119.25(16)
C(11)-C(9)-C(10)	117.41(13)
C(20)-C(9)-H(9)	105.4
C(11)-C(9)-H(9)	105.4
C(10)-C(9)-H(9)	105.4
C(1)-C(10)-C(9)	107.80(14)
C(1)-C(10)-C(5)	114.04(14)
C(9)-C(10)-C(5)	112.61(13)
C(1)-C(10)-H(10)	107.4
C(9)-C(10)-H(10)	107.4
C(5)-C(10)-H(10)	107.4
C(7)-C(11)-C(9)	112.55(13)
C(7)-C(11)-C(12)	111.78(13)
C(9)-C(11)-C(12)	101.68(13)
C(7)-C(11)-H(11)	110.2
C(9)-C(11)-H(11)	110.2
C(12)-C(11)-H(11)	110.2
O(4)-C(12)-C(13)	110.76(15)
O(4)-C(12)-C(11)	104.85(13)
C(13)-C(12)-C(11)	113.46(15)
O(4)-C(12)-H(12)	109.2
C(13)-C(12)-H(12)	109.2
C(11)-C(12)-H(12)	109.2
C(16)-C(13)-C(14)	105.8(2)
C(16)-C(13)-C(12)	129.9(2)
C(14)-C(13)-C(12)	124.29(19)
C(15)-C(14)-C(13)	107.0(3)
C(15)-C(14)-H(14)	126.5
C(13)-C(14)-H(14)	126.5
C(14)-C(15)-O(5)	110.6(2)

C(14)-C(15)-H(15)	124.7
O(5)-C(15)-H(15)	124.7
C(13)-C(16)-O(5)	110.7(2)
C(13)-C(16)-H(16)	124.6
O(5)-C(16)-H(16)	124.6
C(8)-C(17)-H(17A)	109.5
C(8)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(8)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
O(2)-C(18)-O(1)	123.00(17)
O(2)-C(18)-C(4)	124.71(18)
O(1)-C(18)-C(4)	112.29(17)
C(5)-C(19)-H(19A)	109.5
C(5)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(5)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
O(3)-C(20)-O(4)	121.31(19)
O(3)-C(20)-C(9)	129.1(2)
O(4)-C(20)-C(9)	109.56(16)
O(1)-C(21)-H(21A)	109.5
O(1)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
O(1)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(18)-O(1)-C(21)	116.66(18)
C(20)-O(4)-C(12)	110.92(14)
C(15)-O(5)-C(16)	105.8(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for yy_liruijuan01.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	50(1)	71(1)	34(1)	-3(1)	6(1)	-13(1)
C(2)	58(1)	84(2)	49(1)	-4(1)	6(1)	-26(1)
C(3)	56(1)	73(1)	48(1)	5(1)	11(1)	-21(1)
C(4)	37(1)	68(1)	39(1)	6(1)	12(1)	2(1)
C(5)	37(1)	50(1)	30(1)	2(1)	9(1)	7(1)
C(6)	36(1)	46(1)	33(1)	4(1)	7(1)	2(1)
C(7)	36(1)	42(1)	35(1)	-1(1)	7(1)	1(1)
C(8)	38(1)	53(1)	53(1)	0(1)	9(1)	-4(1)
C(9)	46(1)	46(1)	29(1)	2(1)	8(1)	4(1)
C(10)	36(1)	57(1)	34(1)	5(1)	6(1)	6(1)

C(11)	40(1)	41(1)	39(1)	-2(1)	11(1)	-2(1)
C(12)	52(1)	44(1)	47(1)	0(1)	13(1)	-5(1)
C(13)	66(1)	46(1)	55(1)	4(1)	27(1)	-11(1)
C(14)	127(2)	72(2)	94(2)	22(1)	70(2)	24(2)
C(15)	189(4)	72(2)	109(2)	5(2)	105(3)	2(2)
C(16)	92(2)	78(2)	61(1)	15(1)	33(1)	-3(1)
C(17)	47(1)	83(2)	61(1)	17(1)	-1(1)	4(1)
C(18)	44(1)	69(1)	39(1)	9(1)	14(1)	-1(1)
C(19)	63(1)	60(1)	45(1)	-2(1)	20(1)	12(1)
C(20)	66(1)	53(1)	39(1)	9(1)	13(1)	14(1)
C(21)	101(2)	126(2)	38(1)	5(1)	23(1)	16(2)
O(1)	69(1)	101(1)	40(1)	7(1)	20(1)	20(1)
O(2)	86(1)	81(1)	50(1)	18(1)	15(1)	22(1)
O(3)	87(1)	66(1)	70(1)	15(1)	26(1)	36(1)
O(4)	80(1)	39(1)	66(1)	0(1)	28(1)	0(1)
O(5)	160(2)	103(2)	61(1)	11(1)	56(1)	-19(2)
O(6)	45(1)	119(1)	69(1)	-15(1)	12(1)	17(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for yy_liruijuan01.

	x	y	z	U(eq)
H(1A)	2980	10014	8732	63
H(1B)	4382	9351	9674	63
H(2A)	5132	11201	8766	78
H(2B)	5956	10011	8376	78
H(3A)	5013	11253	6509	72
H(3B)	3368	11181	6720	72
H(4)	5002	9084	6116	57
H(6A)	1291	9867	6552	46
H(6B)	939	9155	5202	46
H(7)	226	7332	6183	46
H(9)	2710	7765	9499	49
H(10)	4476	7842	8127	51
H(11)	522	8689	8564	47
H(12)	-1009	6620	7883	57
H(14)	-2041	8225	9622	108
H(15)	-1804	7992	11939	133
H(16)	1221	5722	11046	89
H(17A)	-1720	9435	4398	99
H(17B)	-3208	8847	4640	99
H(17C)	-1942	7962	4362	99
H(19A)	2523	7392	4830	82
H(19B)	2465	6646	6103	82
H(19C)	4035	7031	5861	82
H(21A)	3601	10146	2215	131
H(21B)	2336	9116	2121	131
H(21C)	3935	8729	1943	131

Table 6. Torsion angles [deg] for yy_liruijuan01.

C(10)-C(1)-C(2)-C(3)	56.1(2)
C(1)-C(2)-C(3)-C(4)	-57.7(2)
C(2)-C(3)-C(4)-C(18)	-177.40(15)
C(2)-C(3)-C(4)-C(5)	57.2(2)
C(18)-C(4)-C(5)-C(19)	66.29(18)
C(3)-C(4)-C(5)-C(19)	-169.55(15)
C(18)-C(4)-C(5)-C(6)	-53.92(18)
C(3)-C(4)-C(5)-C(6)	70.24(18)
C(18)-C(4)-C(5)-C(10)	-174.64(15)
C(3)-C(4)-C(5)-C(10)	-50.49(19)
C(19)-C(5)-C(6)-C(7)	62.83(17)
C(10)-C(5)-C(6)-C(7)	-57.85(18)
C(4)-C(5)-C(6)-C(7)	-177.92(13)
C(5)-C(6)-C(7)-C(8)	-177.26(13)
C(5)-C(6)-C(7)-C(11)	58.51(17)
C(11)-C(7)-C(8)-O(6)	8.9(2)
C(6)-C(7)-C(8)-O(6)	-115.3(2)
C(11)-C(7)-C(8)-C(17)	-170.80(16)
C(6)-C(7)-C(8)-C(17)	65.0(2)
C(2)-C(1)-C(10)-C(9)	-178.03(16)
C(2)-C(1)-C(10)-C(5)	-52.2(2)
C(20)-C(9)-C(10)-C(1)	-152.06(16)
C(11)-C(9)-C(10)-C(1)	82.92(17)
C(20)-C(9)-C(10)-C(5)	81.27(19)
C(11)-C(9)-C(10)-C(5)	-43.7(2)
C(19)-C(5)-C(10)-C(1)	165.25(15)
C(6)-C(5)-C(10)-C(1)	-74.11(18)
C(4)-C(5)-C(10)-C(1)	47.25(18)
C(19)-C(5)-C(10)-C(9)	-71.50(17)
C(6)-C(5)-C(10)-C(9)	49.14(19)
C(4)-C(5)-C(10)-C(9)	170.50(13)
C(8)-C(7)-C(11)-C(9)	-172.45(14)
C(6)-C(7)-C(11)-C(9)	-49.10(18)
C(8)-C(7)-C(11)-C(12)	73.85(18)
C(6)-C(7)-C(11)-C(12)	-162.80(13)
C(20)-C(9)-C(11)-C(7)	-89.46(16)
C(10)-C(9)-C(11)-C(7)	43.45(19)
C(20)-C(9)-C(11)-C(12)	30.28(16)
C(10)-C(9)-C(11)-C(12)	163.19(14)
C(7)-C(11)-C(12)-O(4)	90.41(16)
C(9)-C(11)-C(12)-O(4)	-29.88(16)
C(7)-C(11)-C(12)-C(13)	-148.61(16)
C(9)-C(11)-C(12)-C(13)	91.10(17)
O(4)-C(12)-C(13)-C(16)	10.7(3)
C(11)-C(12)-C(13)-C(16)	-106.9(3)
O(4)-C(12)-C(13)-C(14)	-171.4(2)
C(11)-C(12)-C(13)-C(14)	71.0(3)
C(16)-C(13)-C(14)-C(15)	-0.1(3)

C(12)-C(13)-C(14)-C(15)	-178.4(2)
C(13)-C(14)-C(15)-O(5)	0.2(4)
C(14)-C(13)-C(16)-O(5)	0.0(3)
C(12)-C(13)-C(16)-O(5)	178.13(19)
C(3)-C(4)-C(18)-O(2)	-36.1(3)
C(5)-C(4)-C(18)-O(2)	90.9(2)
C(3)-C(4)-C(18)-O(1)	143.65(17)
C(5)-C(4)-C(18)-O(1)	-89.32(18)
C(11)-C(9)-C(20)-O(3)	161.31(19)
C(10)-C(9)-C(20)-O(3)	29.5(3)
C(11)-C(9)-C(20)-O(4)	-21.31(19)
C(10)-C(9)-C(20)-O(4)	-153.14(14)
O(2)-C(18)-O(1)-C(21)	-1.6(3)
C(4)-C(18)-O(1)-C(21)	178.59(19)
O(3)-C(20)-O(4)-C(12)	179.74(17)
C(9)-C(20)-O(4)-C(12)	2.1(2)
C(13)-C(12)-O(4)-C(20)	-104.67(17)
C(11)-C(12)-O(4)-C(20)	18.08(18)
C(14)-C(15)-O(5)-C(16)	-0.2(4)
C(13)-C(16)-O(5)-C(15)	0.2(3)

Symmetry transformations used to generate equivalent atoms: