Support Information

Polyketide Derivatives from Mangrove Derived Endophytic Fungus *Pseudopestalotiopsis theae*

Xiaoqin Yu [1,2], Werner E. G. Müller [3], Dieter Meier [1], Rainer Kalscheuer [1], Zhiyong Guo [2], Kun Zou [2], Blessing O. Umeokoli [4], Zhen Liu [1,*] and Peter Proksch [1,2,*]

[1] Institute of Pharmaceutical Biology and Biotechnology, Heinrich-Heine-University Duesseldorf, 40225 Duesseldorf, Germany; xiyu101@hhu.de (X.Y.); dieter.meier@hhu.de (D.M.); Rainer.Kalscheuer@hhu.de (R.K.)

[2] Hubei Key Laboratory of Natural Products Research and Development, College of Biological and Pharmaceutical Sciences, China Three Gorges University, Yichang 443002, People's Republic of China; zhyguoctgu@foxmail.com (Z.G.); kzou@ctgu.edu.cn (K.Z.)

[3] Institute of Physiological Chemistry, Universitätsmedizin der Johannes Gutenberg-Universität Mainz, 55128 Mainz, Germany; wmueller@uni-mainz.de (W.E.G.M.)

[4] Department of Pharmaceutical and Medicinal Chemistry, Nnamdi Azikiwe University, Awka, Nigeria; blessingumeokoli@gmail.com (B.O.U.)

* Correspondence: zhenfeizi0@sina.com (Z.L.); proksch@uni-duesseldorf (P.P.); Tel.: +49-211-81-14163

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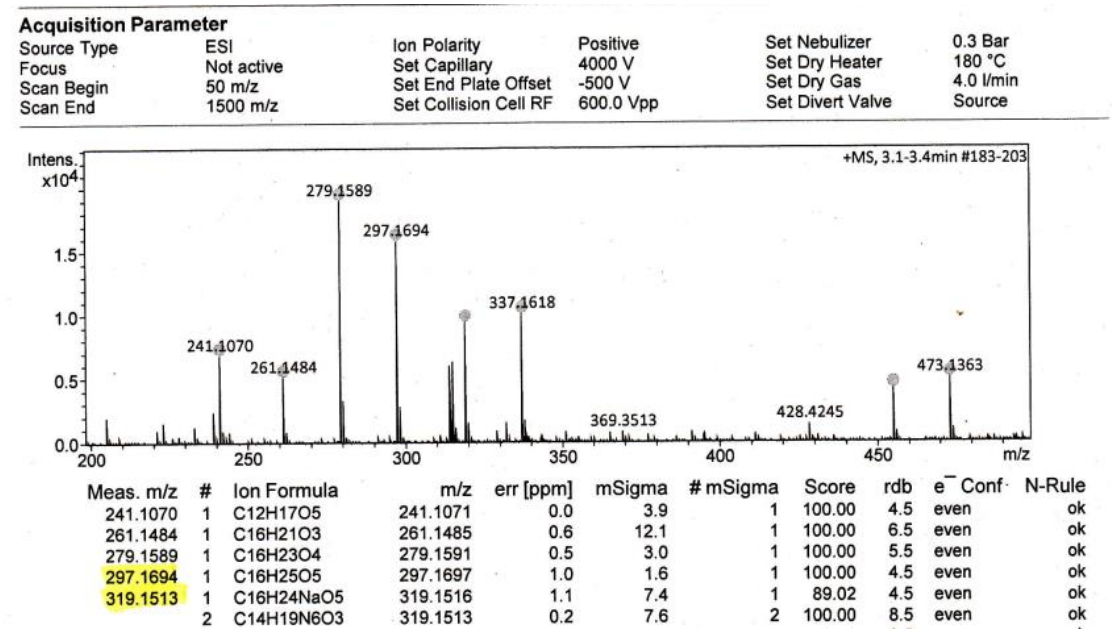


Figure S1. The HRESIMS of compound **1**.

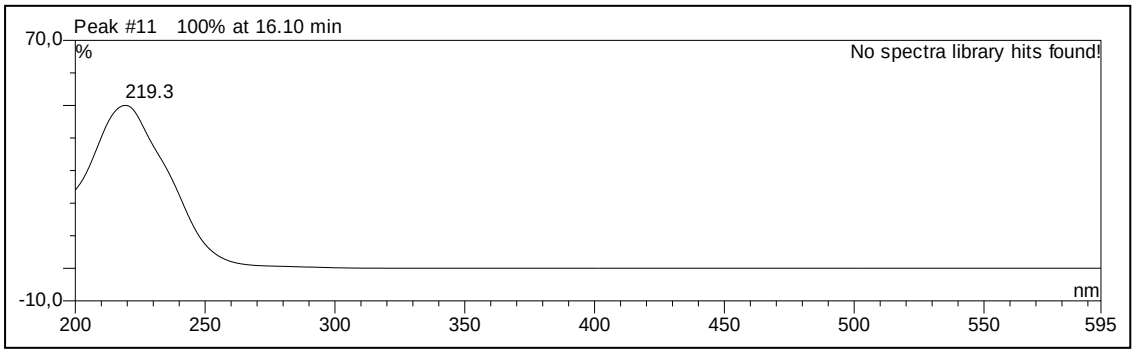


Figure S2. The UV spectrum of compound **1**.

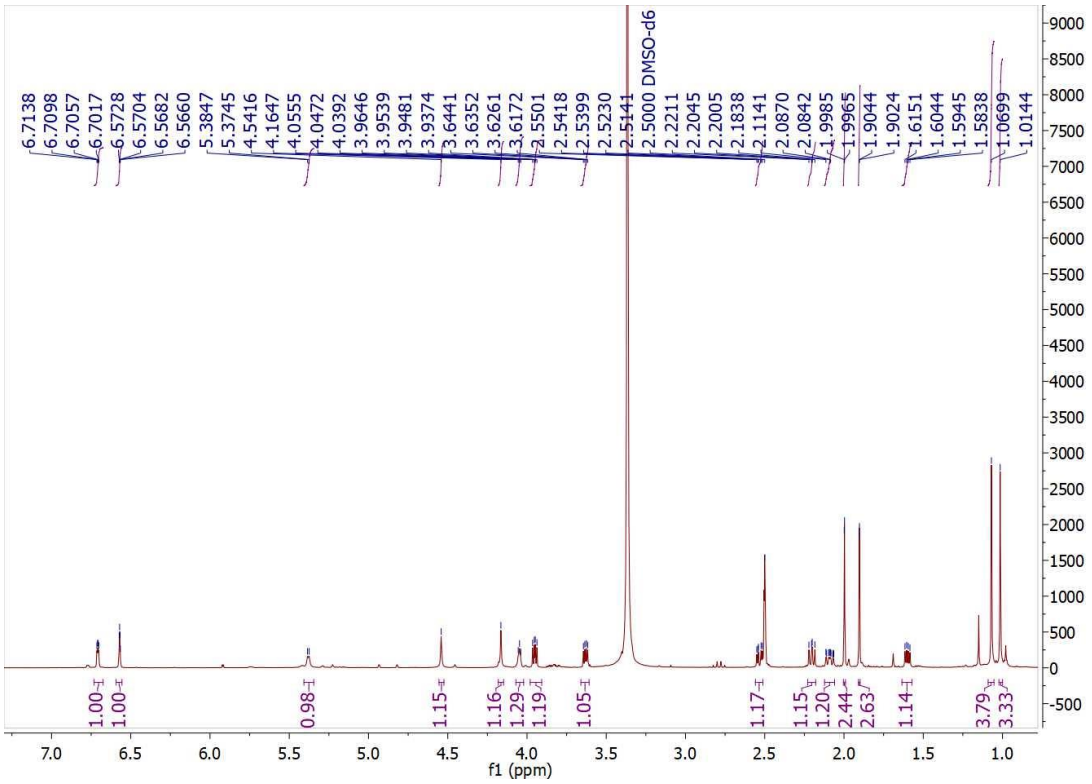


Figure S3. The ^{1}H-NMR (600 MHz, DMSO-d_6) spectrum of compound **1**.

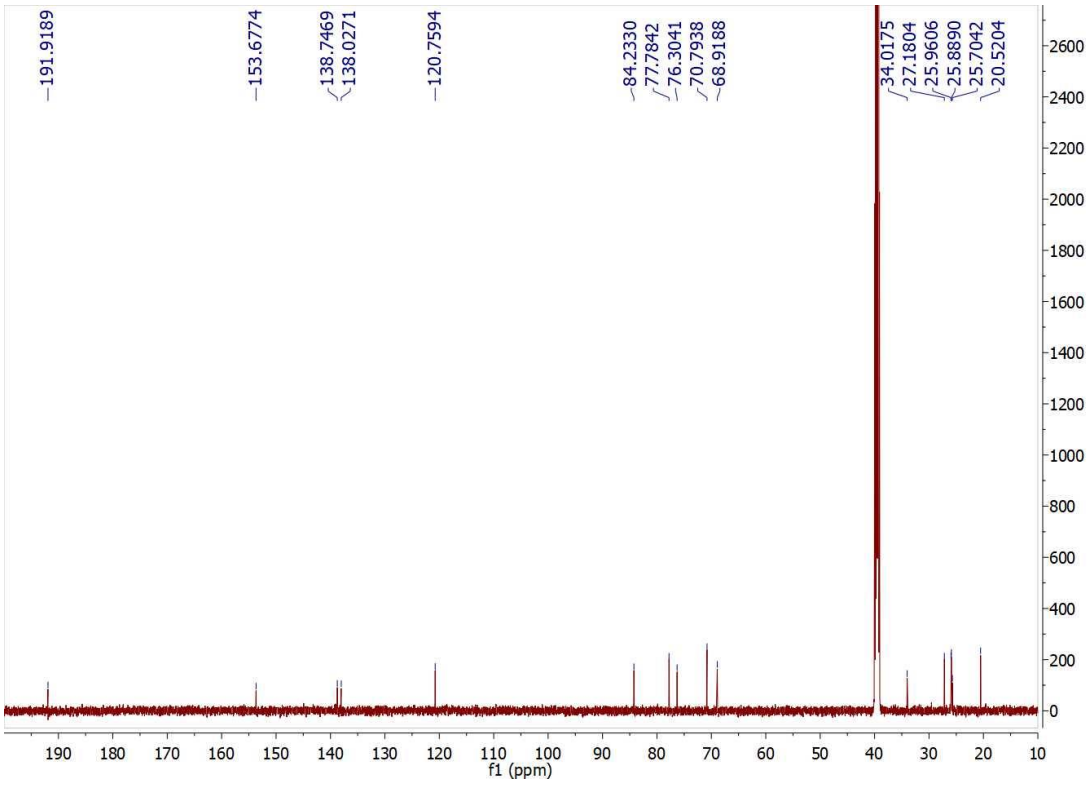


Figure S4. The ^{13}C-NMR (150 MHz, DMSO-d_6) spectrum of compound **1**.

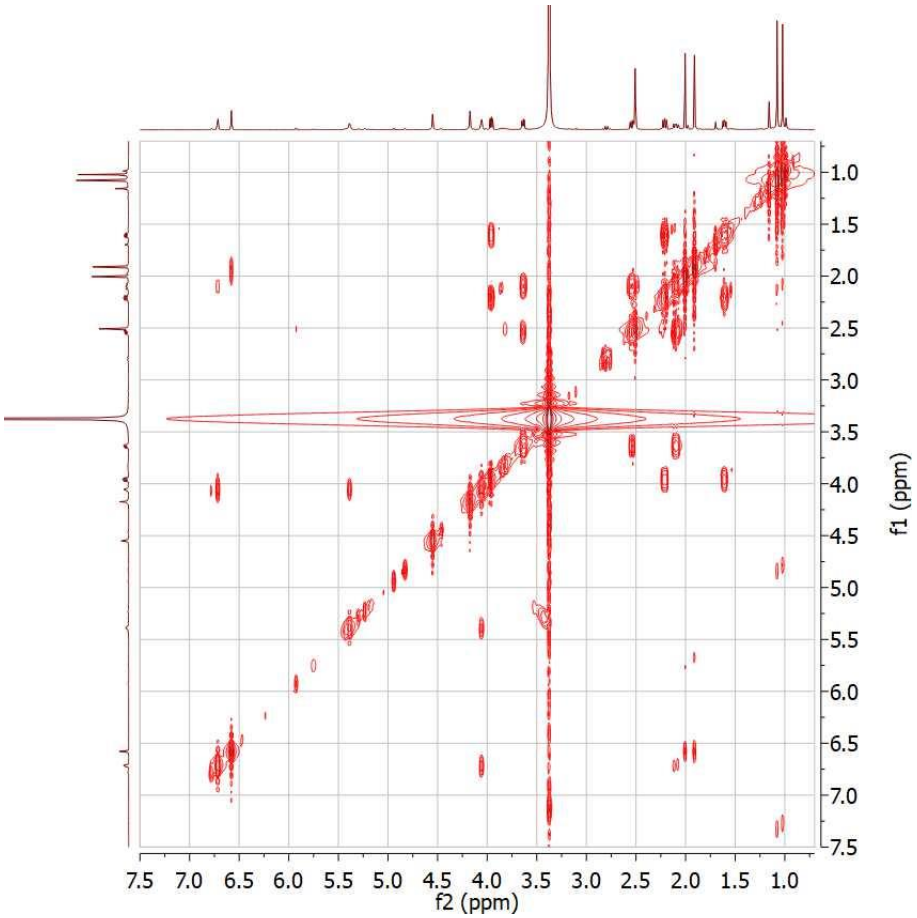


Figure S5. The ^{1}H-^{1}H COSY (600 MHz, DMSO-d_6) spectrum of compound **1**.

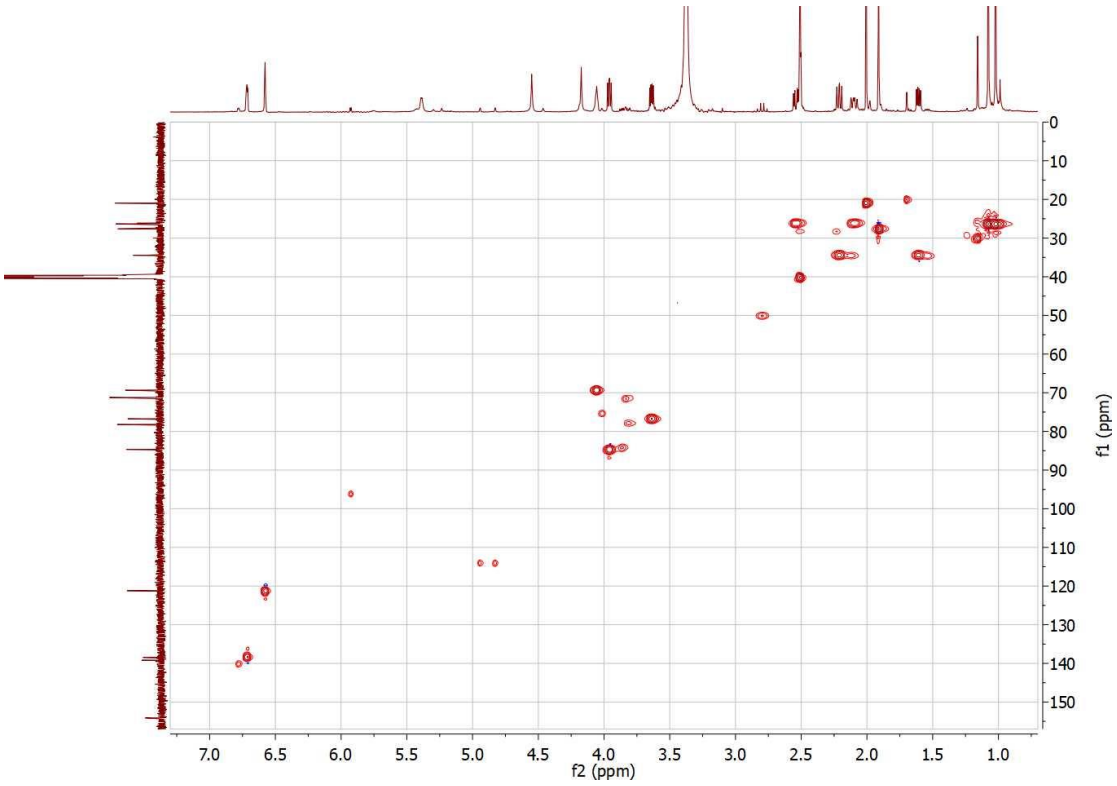


Figure S6. The HSQC (600 MHz, DMSO-d_6) spectrum of compound **1**.

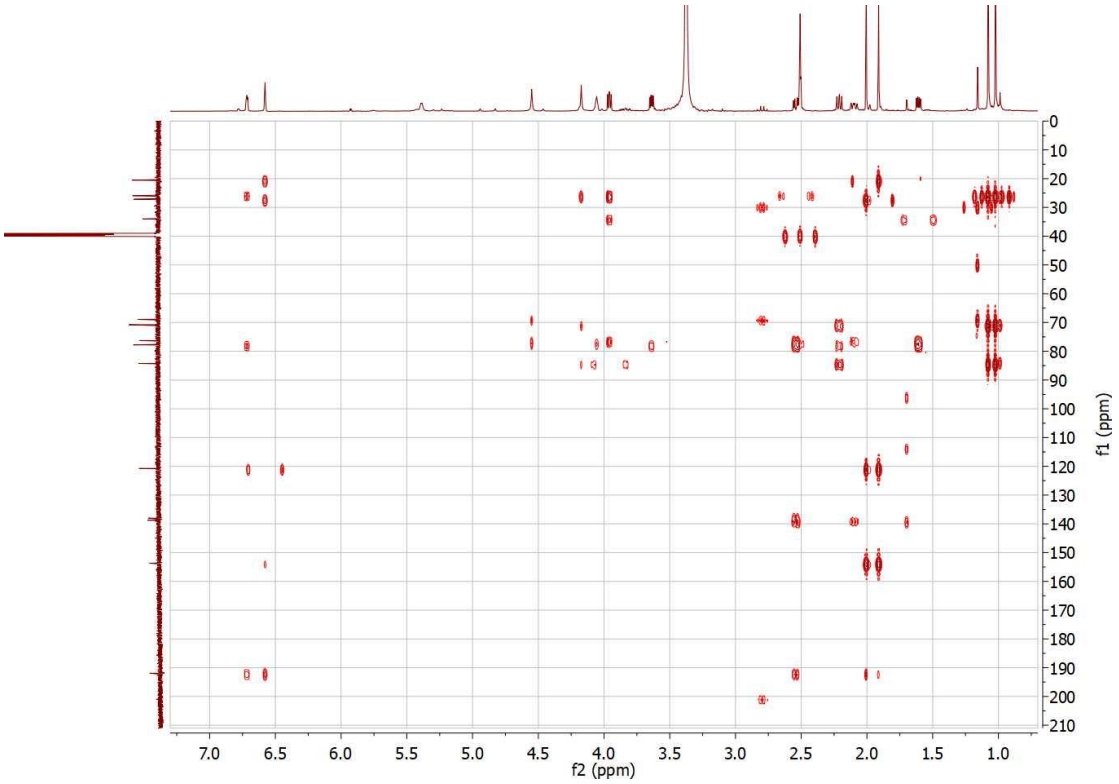


Figure S7. The HMBC (600 MHz, DMSO-d_6) spectrum of compound **1**.

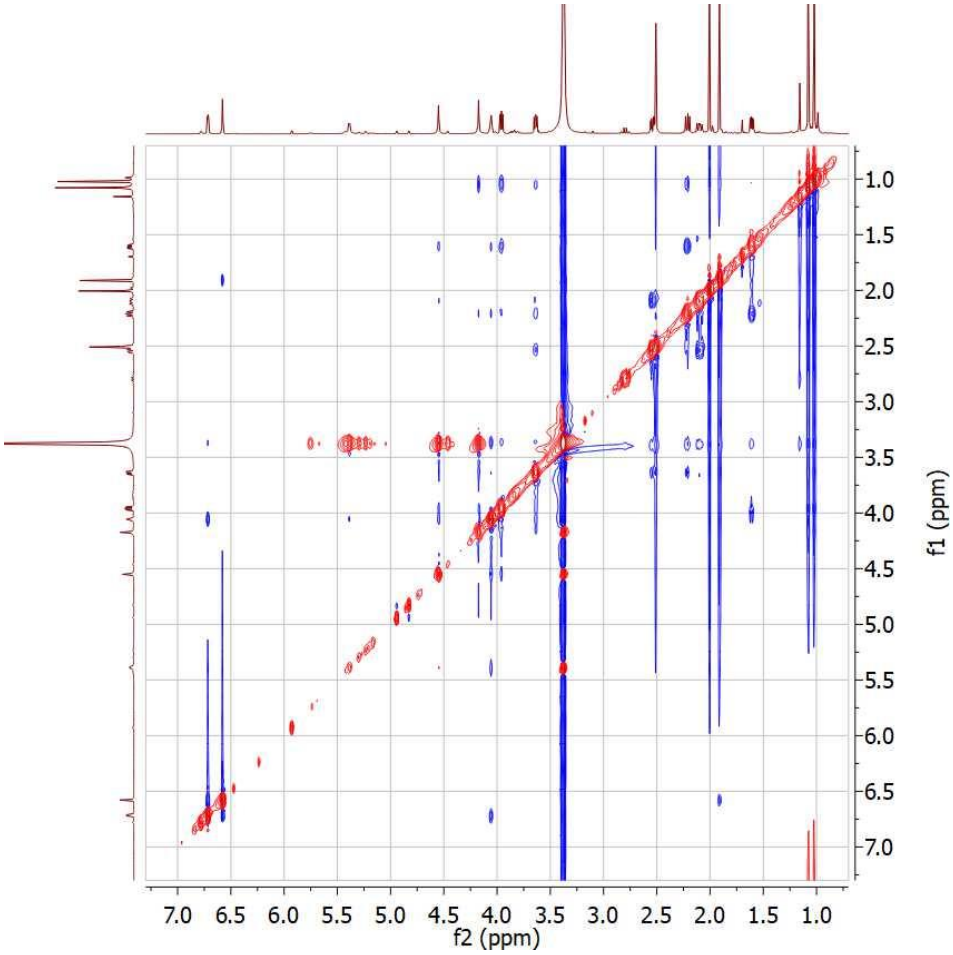


Figure S8. The ROESY (600 MHz, DMSO-d_6) spectrum of compound **1**.

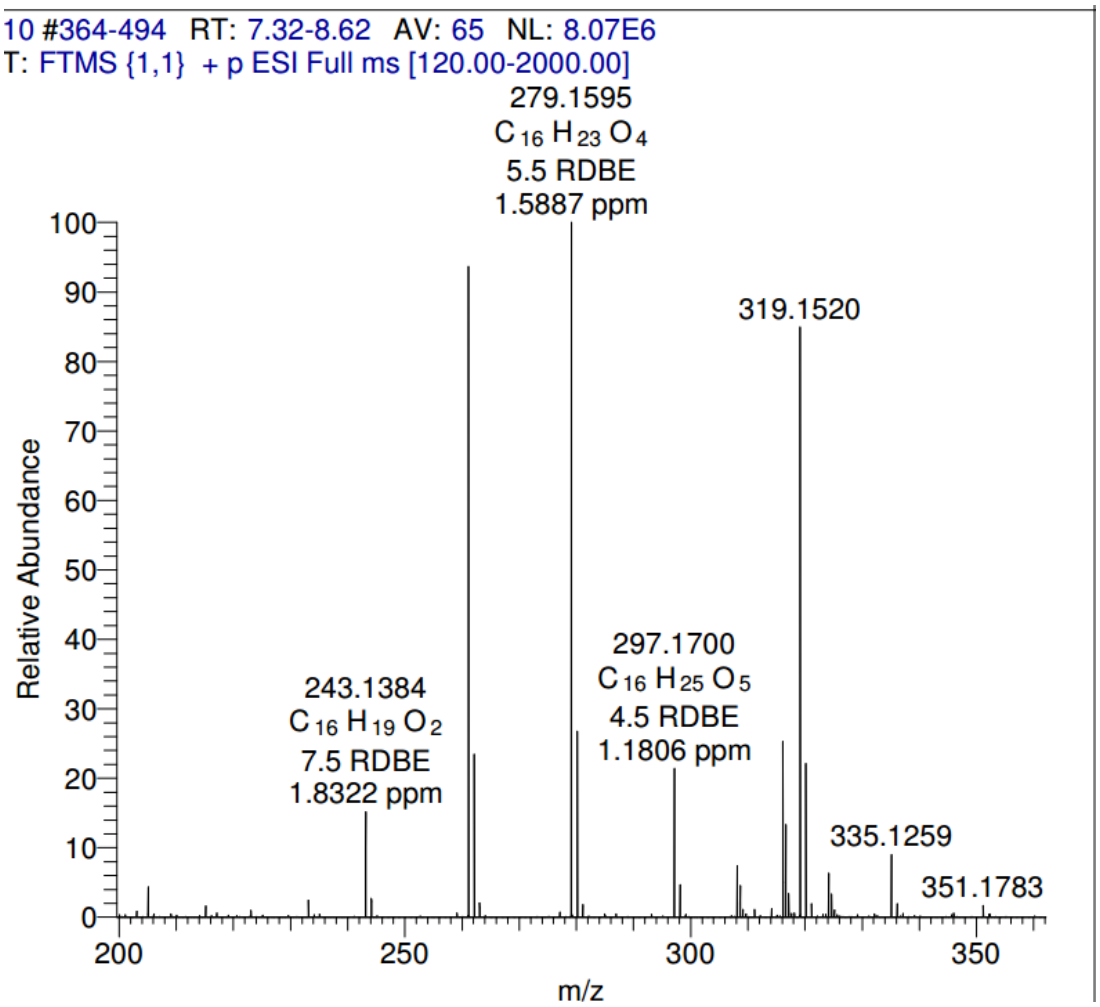


Figure S9. The HRESIMS of compound **2**.

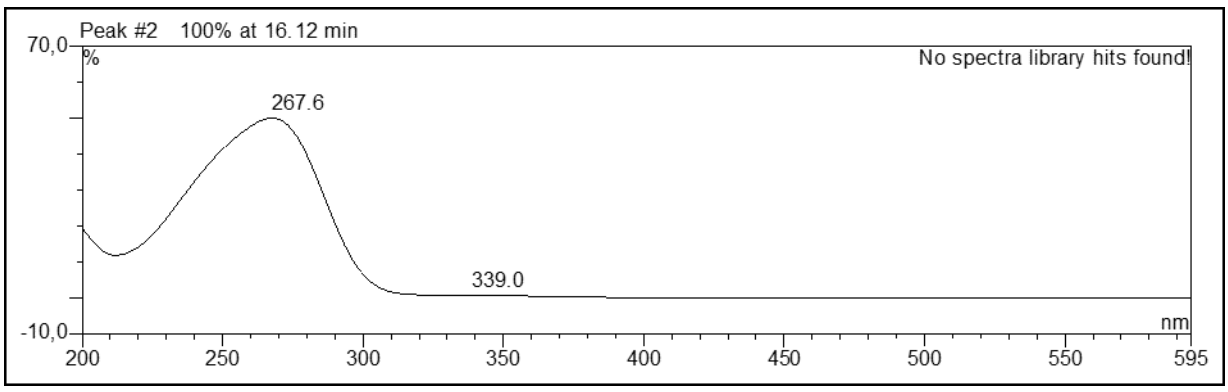


Figure S10. The UV spectrum of compound **2**.

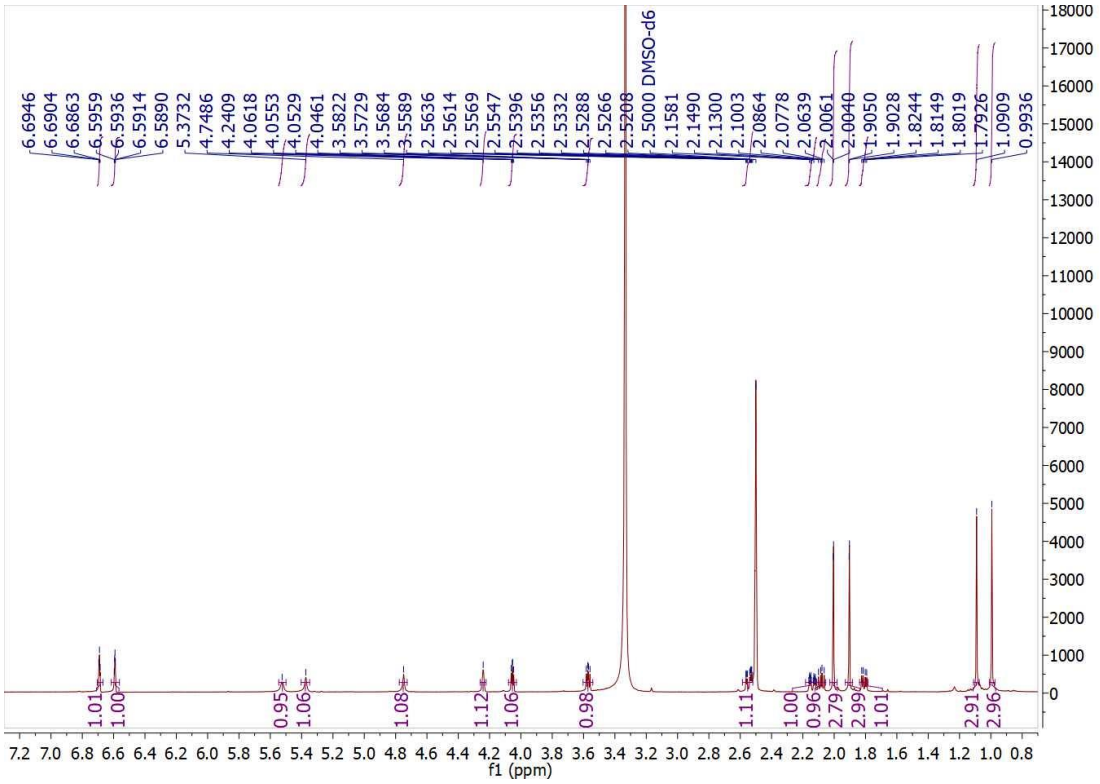


Figure S11. The ^{1}H-NMR (600 MHz, DMSO-d_6) spectrum of compound **2**.

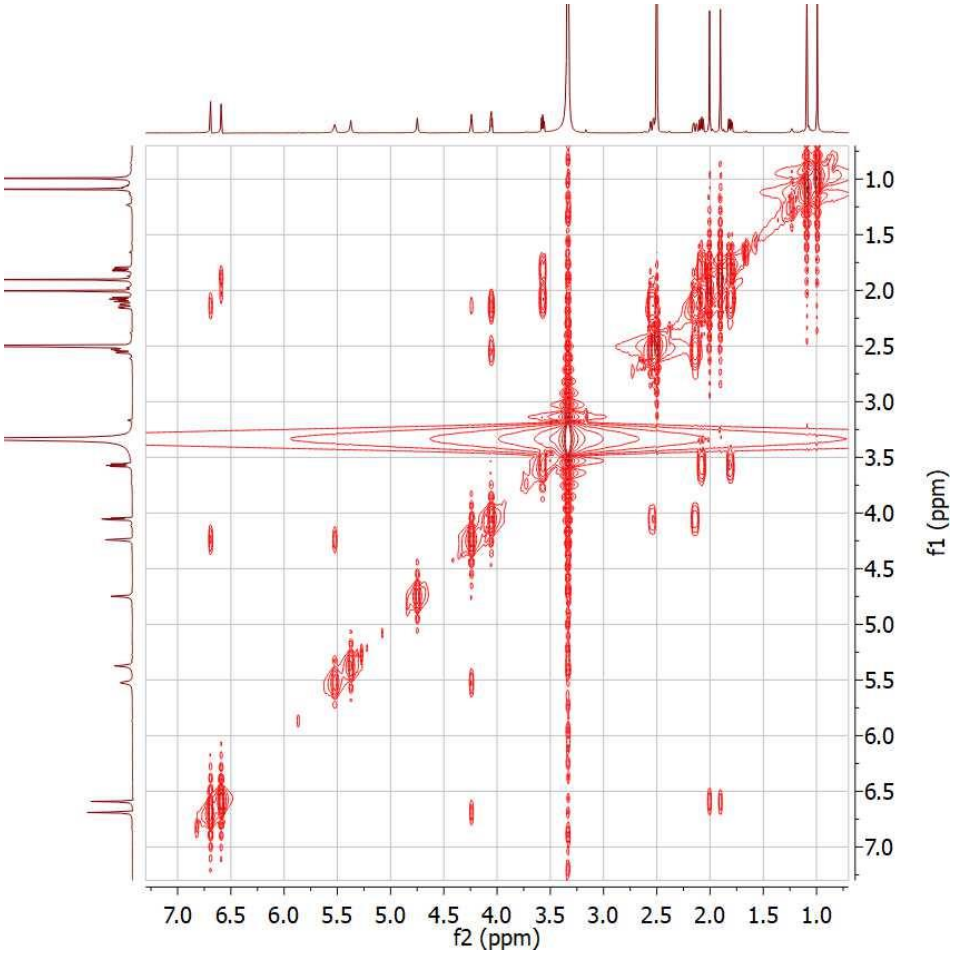


Figure S12. The ^{1}H-^{1}H COSY (600 MHz, DMSO-d_6) spectrum of compound **2**.

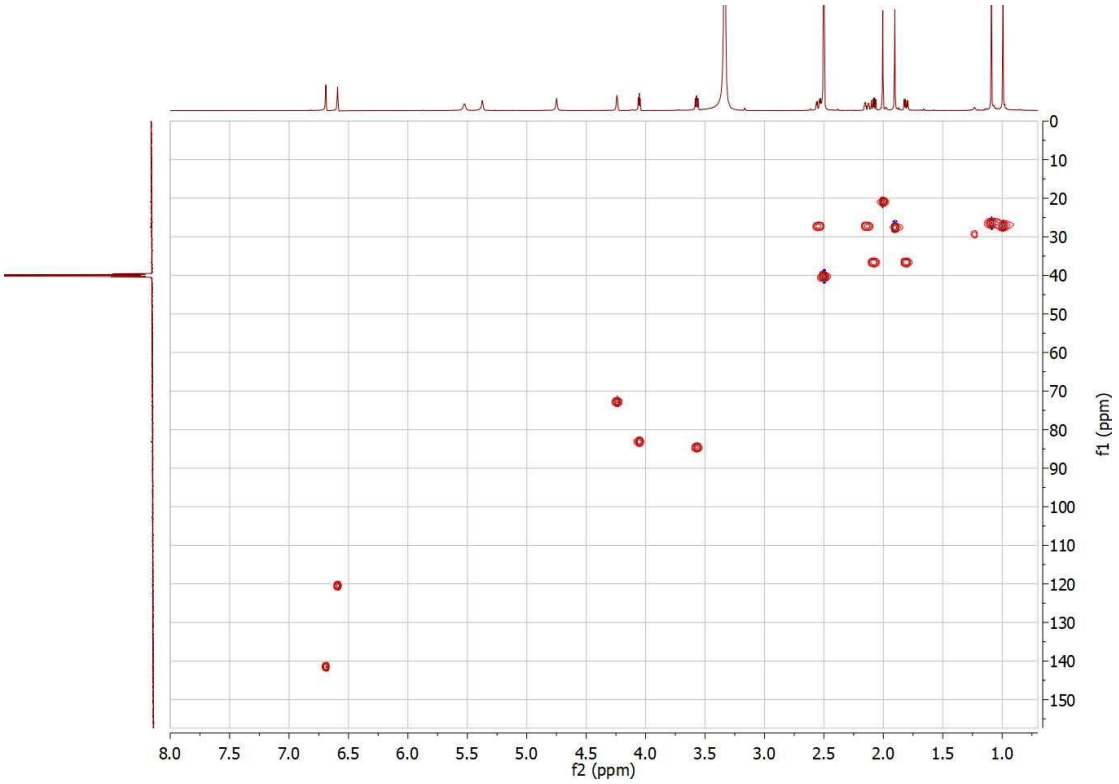


Figure S13. The HSQC (600 MHz, DMSO-d_6) spectrum of compound **2**.

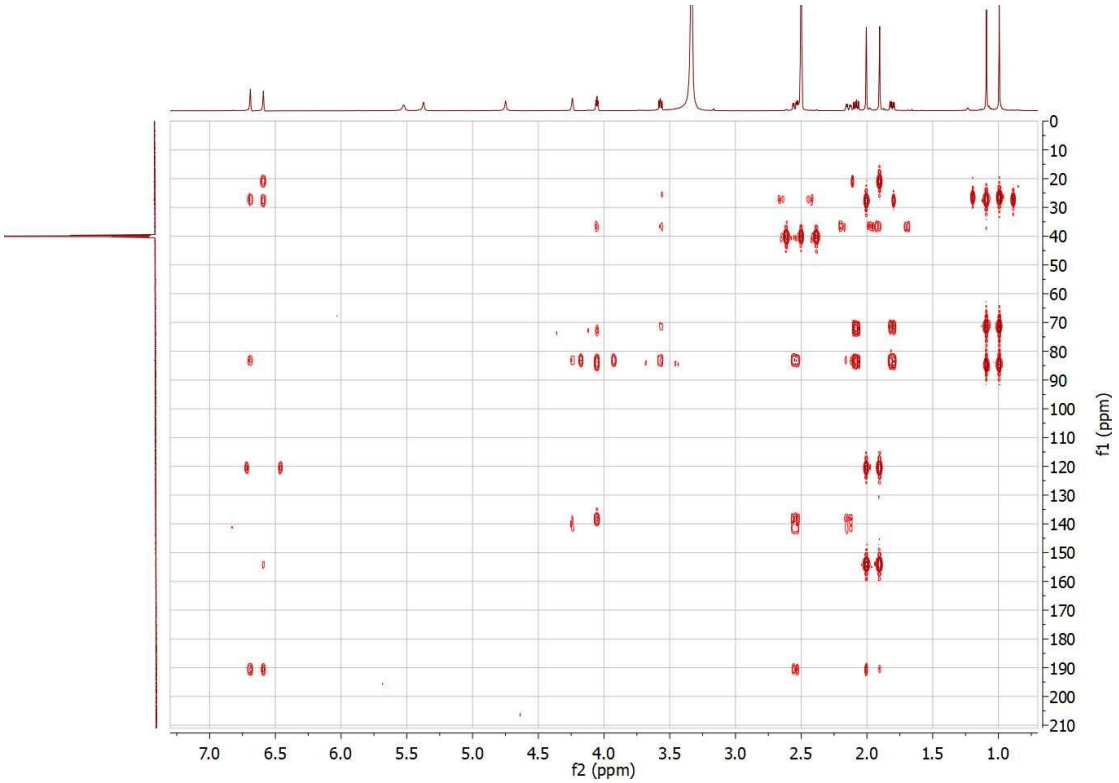


Figure S14. The HMBC (600 MHz, DMSO-d_6) spectrum of compound **2**.

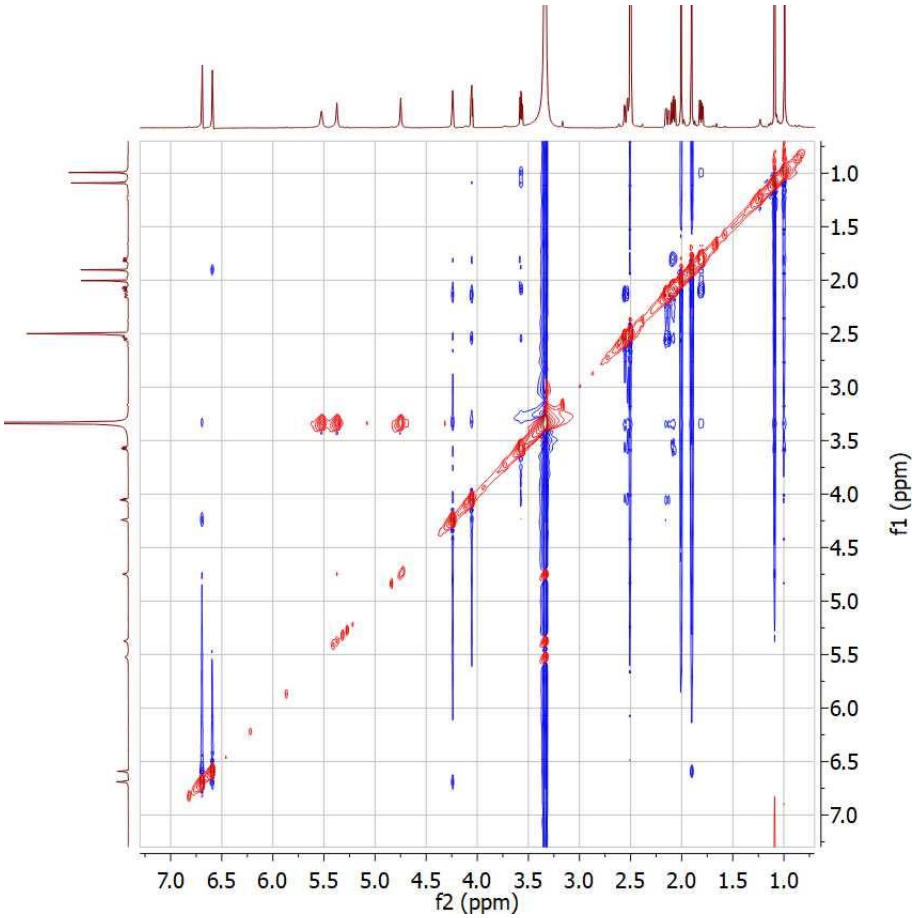


Figure S15. The ROESY (600 MHz, DMSO-d_6) spectrum of compound **2**.

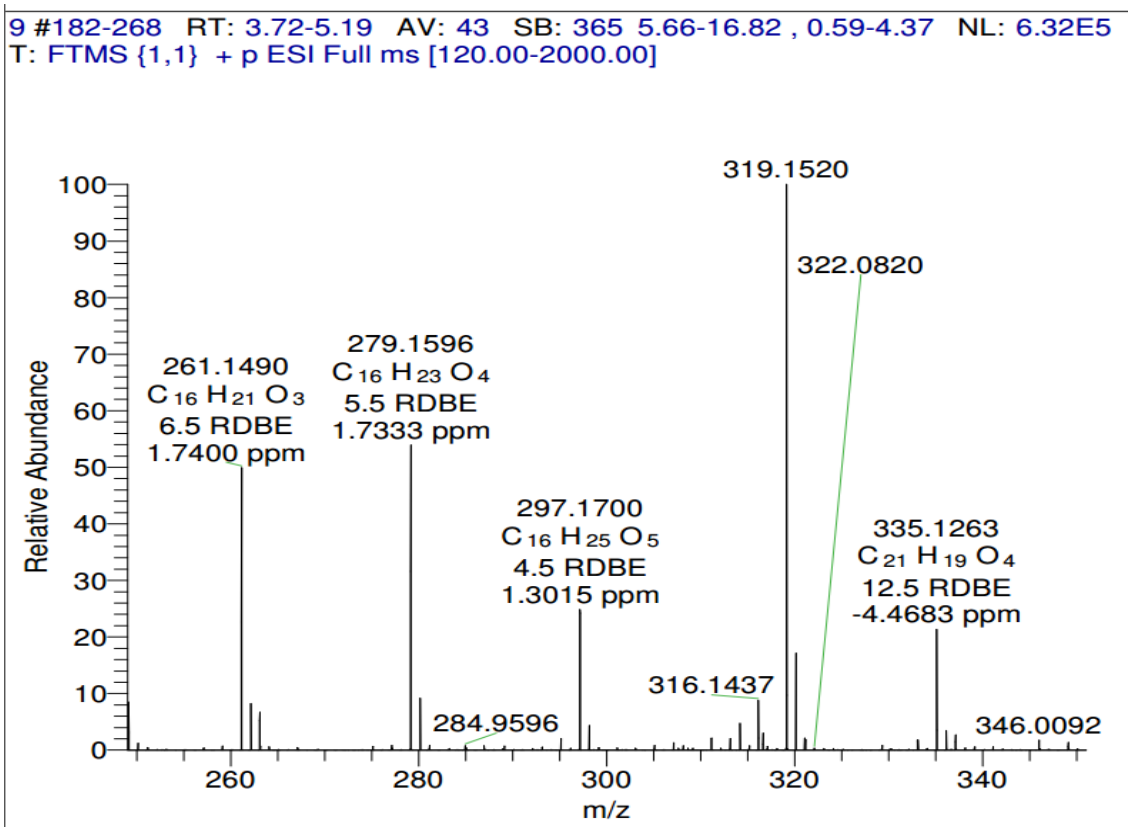


Figure S16. The HRESIMS of compound **3**.

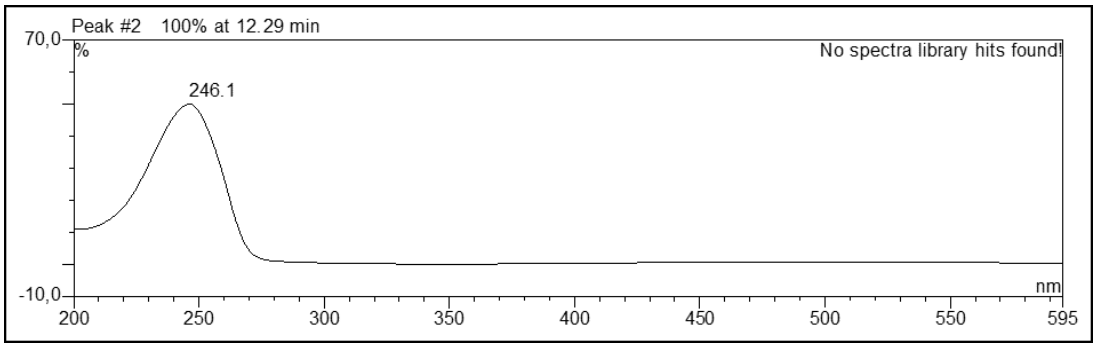


Figure S17. The UV spectrum of compound **3**.

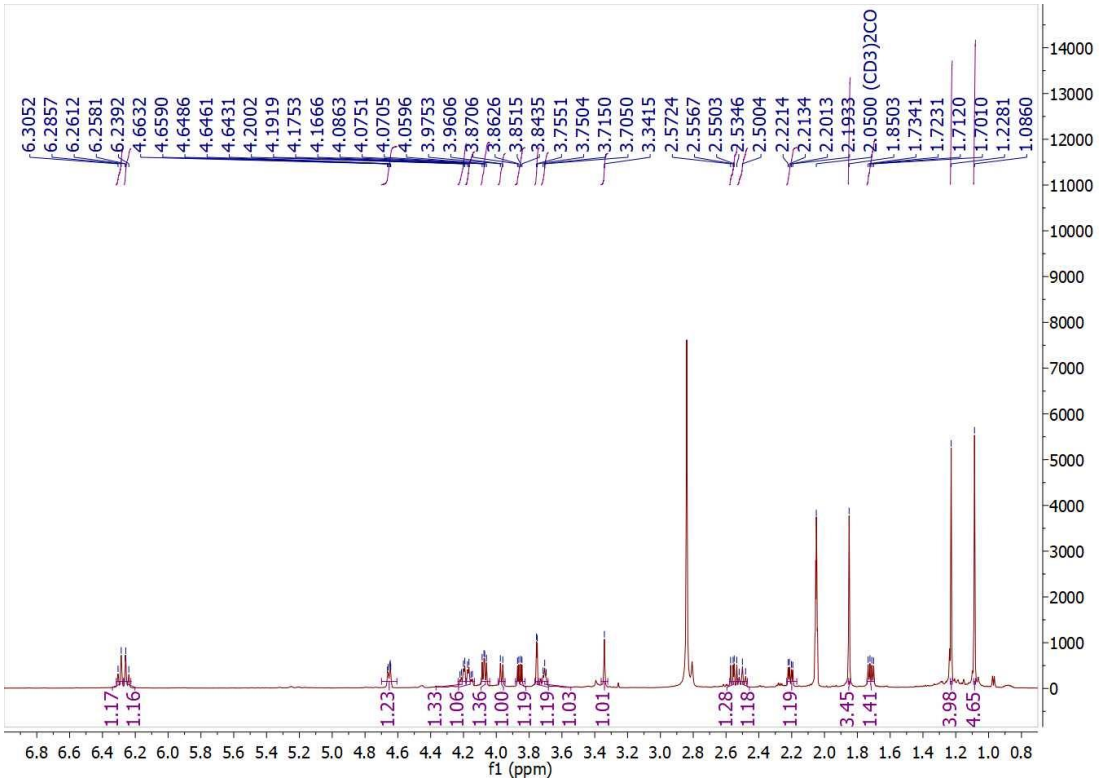


Figure S18. The ^{1}H-NMR (600 MHz, Acetone-d_6) spectrum of compound **3**.

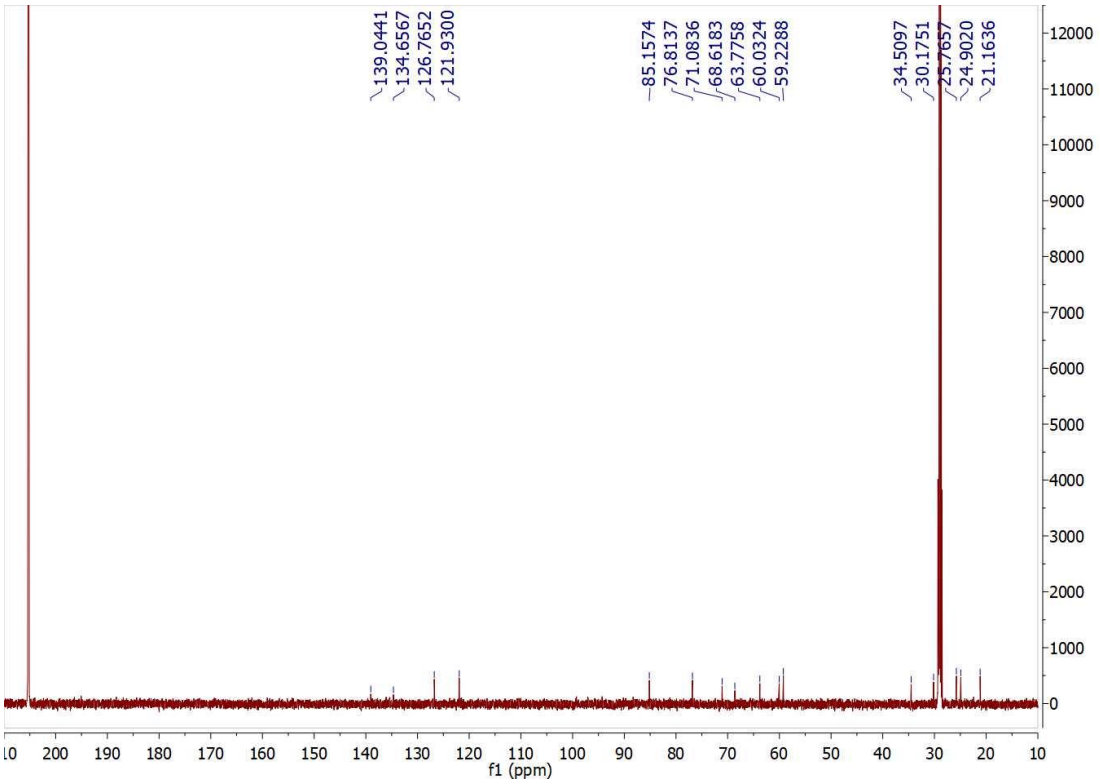


Figure S19. The ^{13}C-NMR (150 MHz, Acetone-d_6) spectrum of compound **3**.

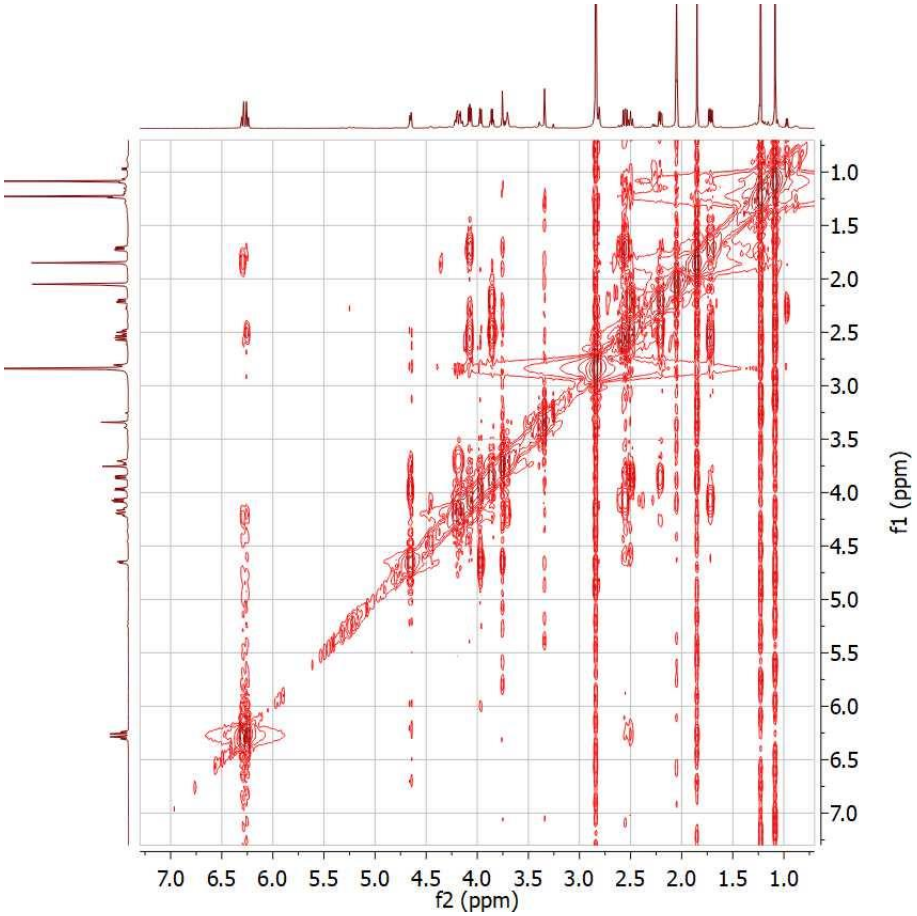


Figure S20. The ^{1}H-^{1}H COSY (600 MHz, Acetone-d_6) spectrum of compound **3**.

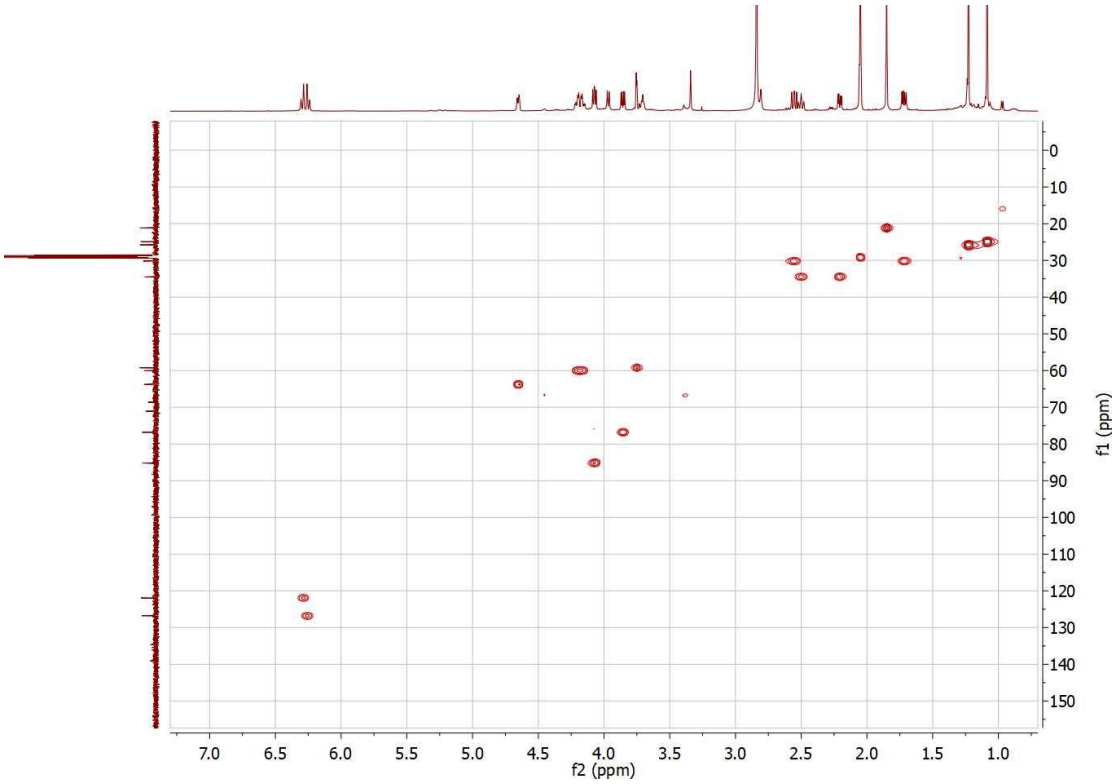


Figure S21. The HSQC (600 MHz, Acetone-d_6) spectrum of compound **3**.

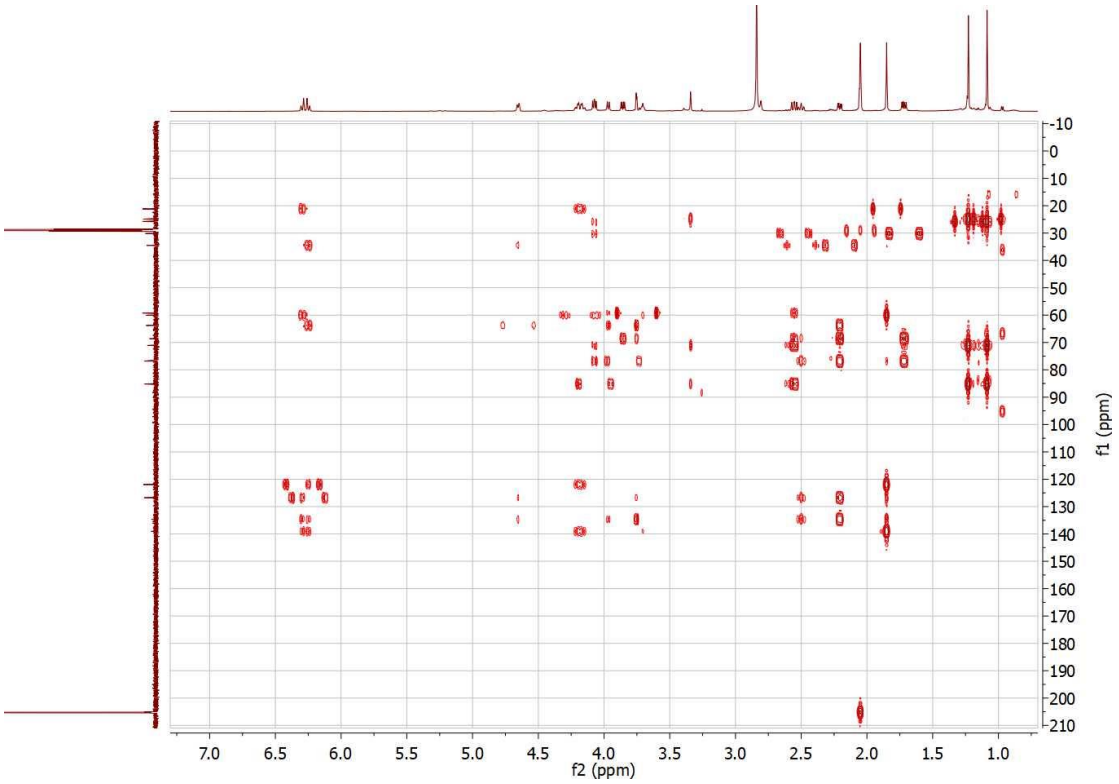


Figure S22. The HMBC (600 MHz, Acetone-d_6) spectrum of compound **3**.

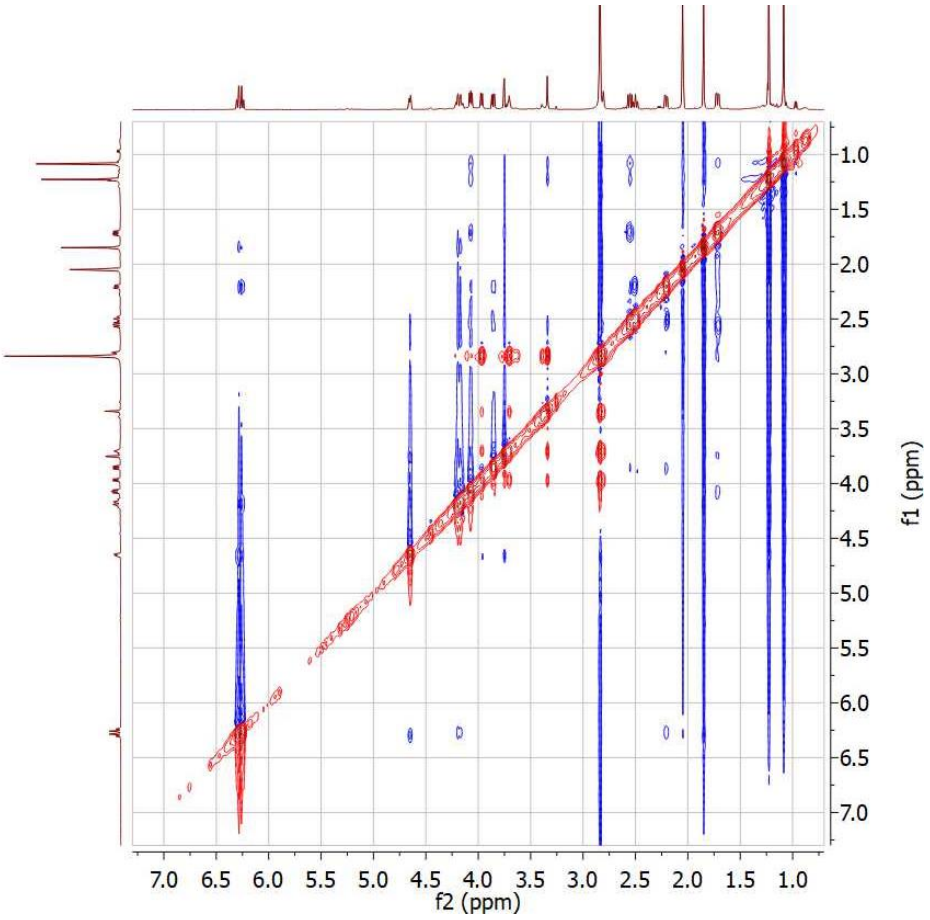
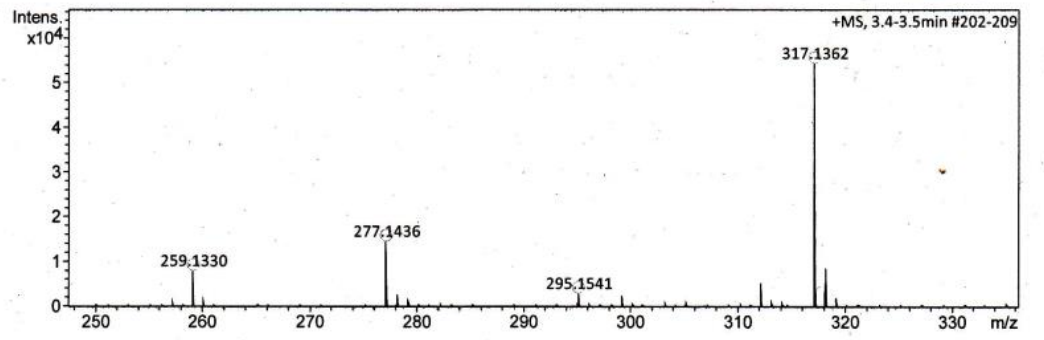


Figure S23. The ROESY (600 MHz, Acetone-d_6) spectrum of compound **3**.

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¯ Conf	N-Rule
259.1330	1	C16H19O3	259.1329	-0.4	18.4	1	100.00	7.5	even	ok
277.1436	1	C16H21O4	277.1434	-0.7	37.7	1	100.00	6.5	even	ok
295.1541	1	C16H23O5	295.1540	-0.4	55.0	1	100.00	5.5	even	ok
317.1362	1	C16H22NaO5	317.1359	-0.9	13.4	1	100.00	5.5	even	ok

Figure S24. The HRESIMS of compound **4**.

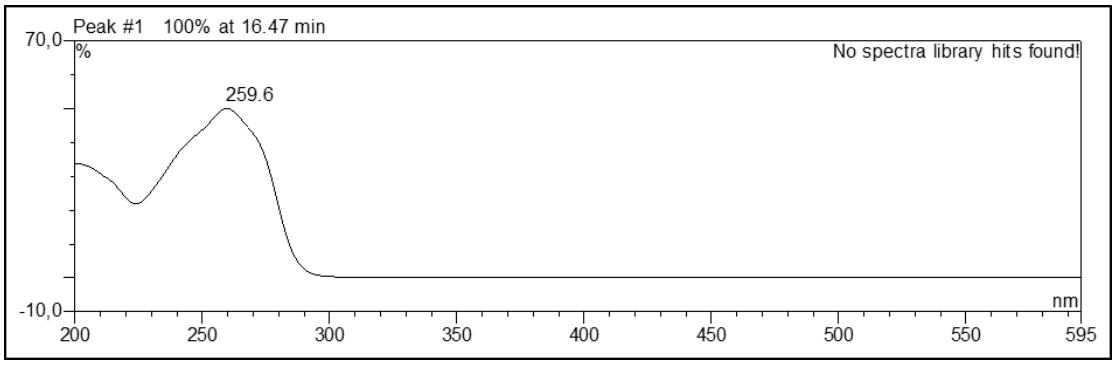


Figure S25. The UV spectrum of compound **4**.

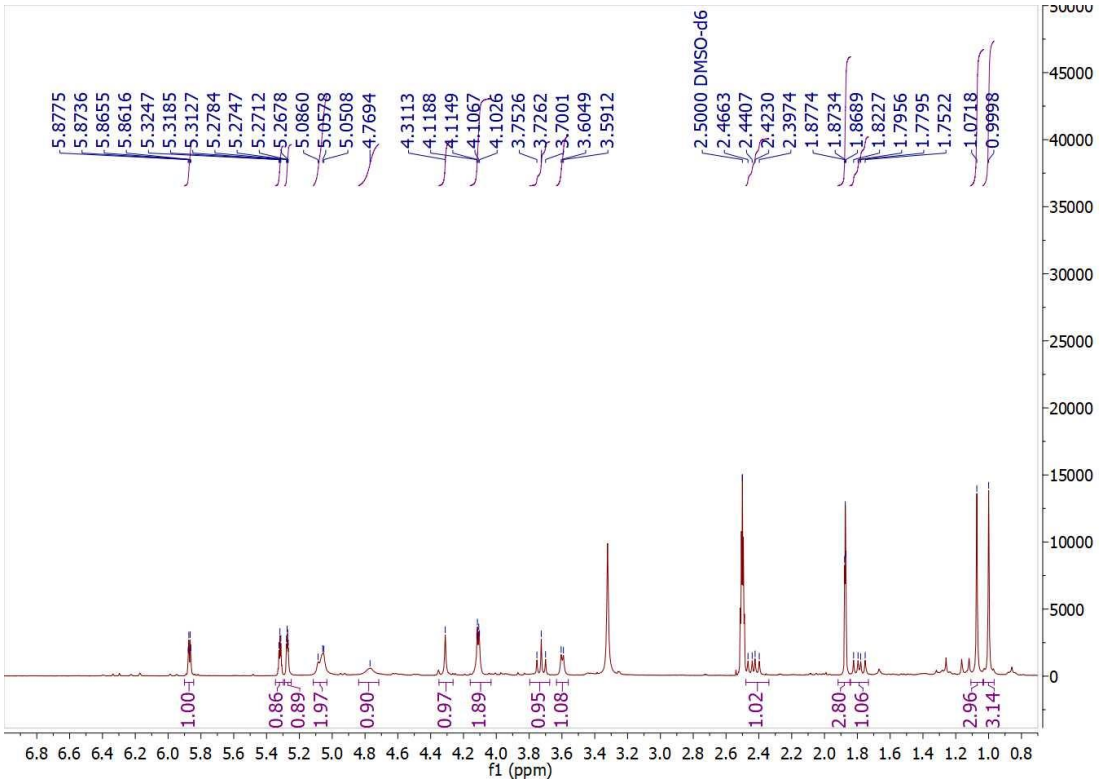


Figure S26. The ^{1}H-NMR (600 MHz, DMSO-d_6) spectrum of compound **4**.

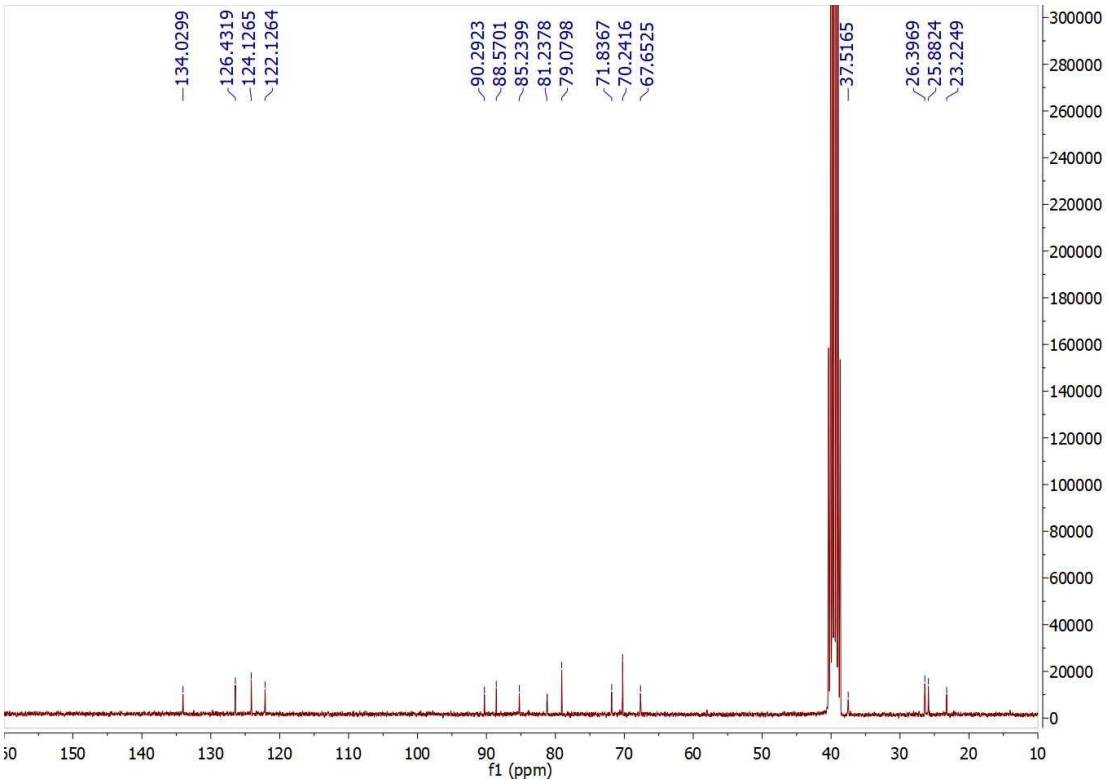


Figure S27. The ^{13}C-NMR (150 MHz, DMSO-d_6) spectrum of compound **4**.

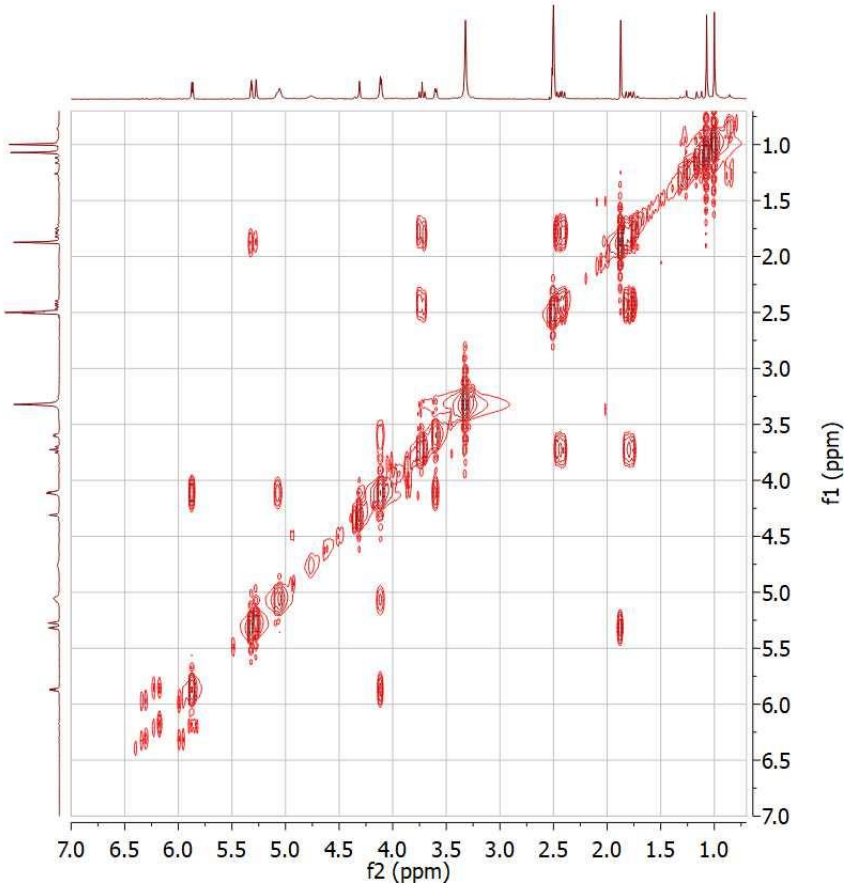


Figure S28. The ^{1}H-^{1}H COSY (600 MHz, DMSO-d_6) spectrum of compound **4**.

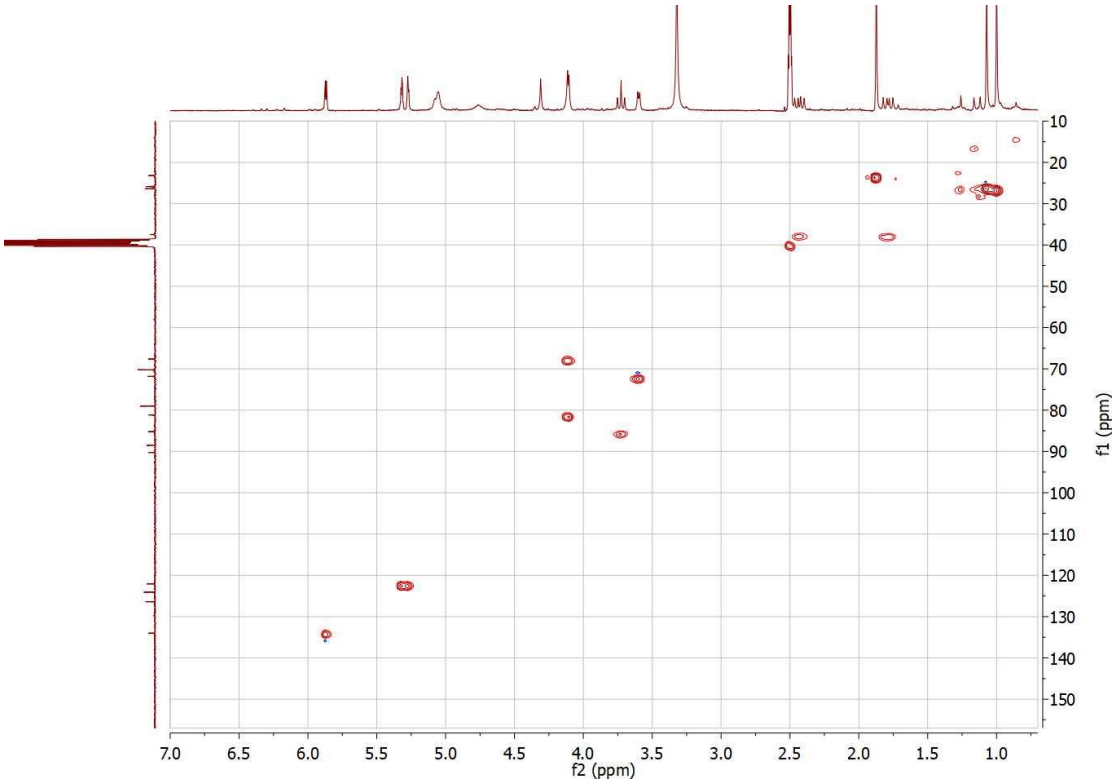


Figure S29. The HSQC (600 MHz, DMSO-d_6) spectrum of compound **4**.

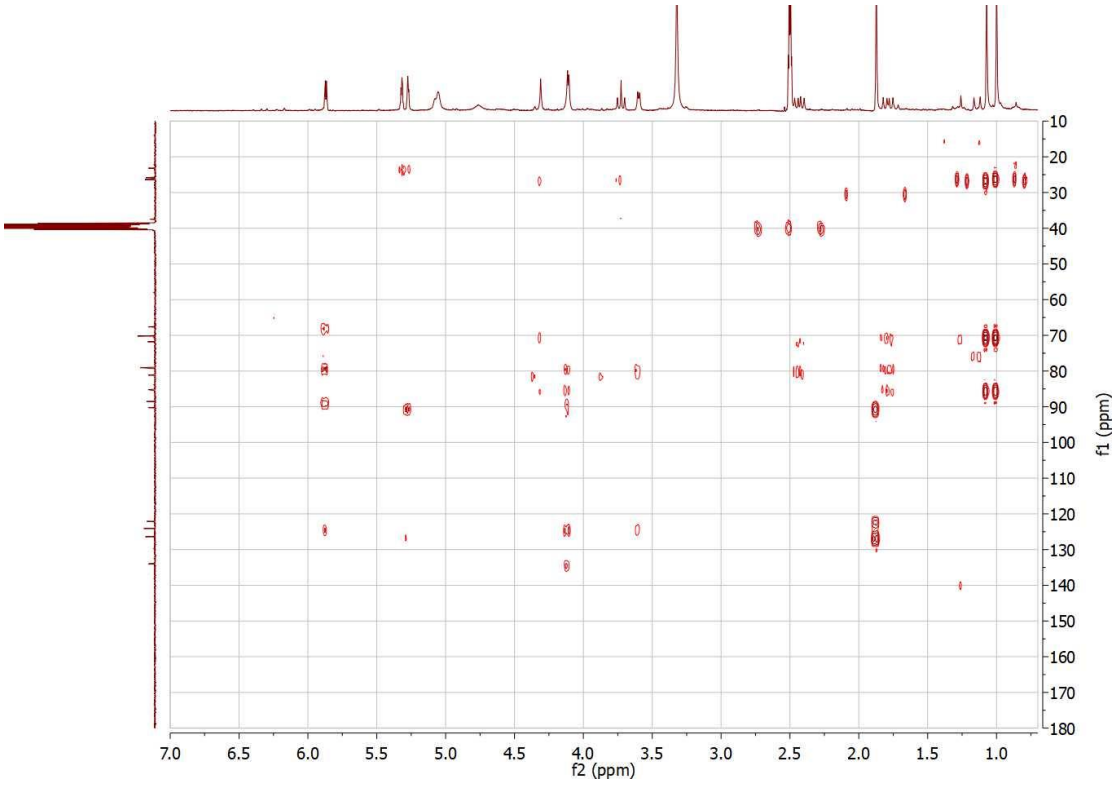


Figure S30. The HMBC (600MHz, DMSO-d_6) spectrum of compound **4**.

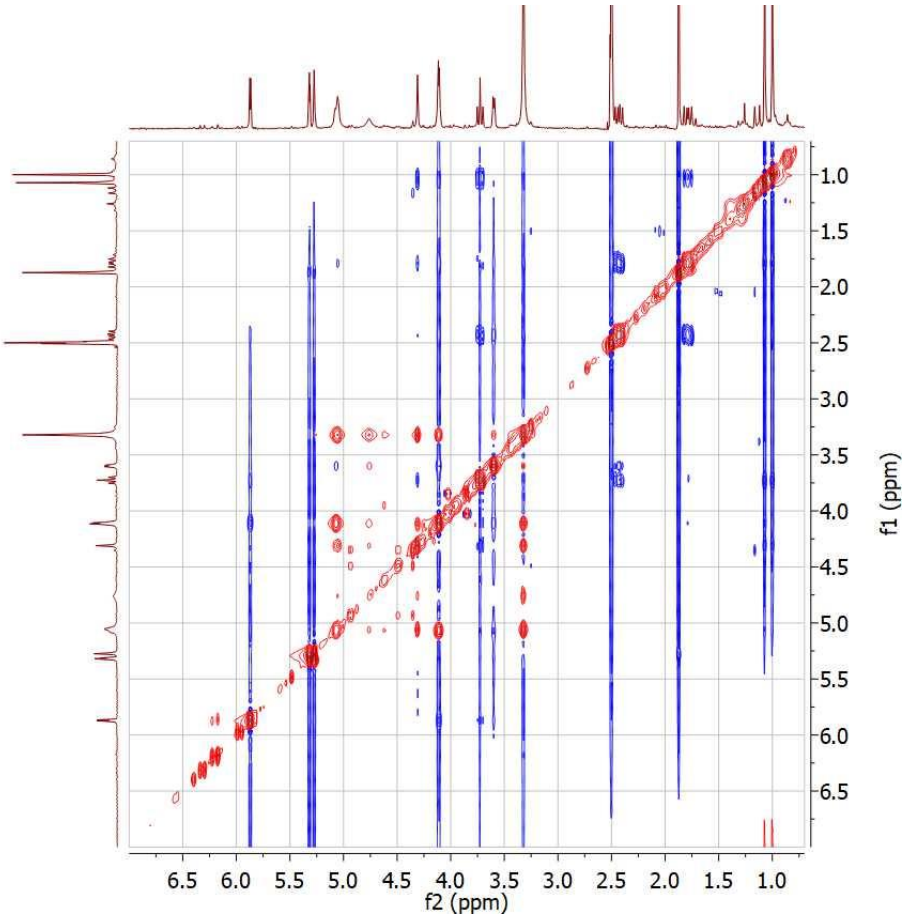


Figure S31. The ROESY (600 MHz, DMSO-d_6) spectrum of compound **4**.

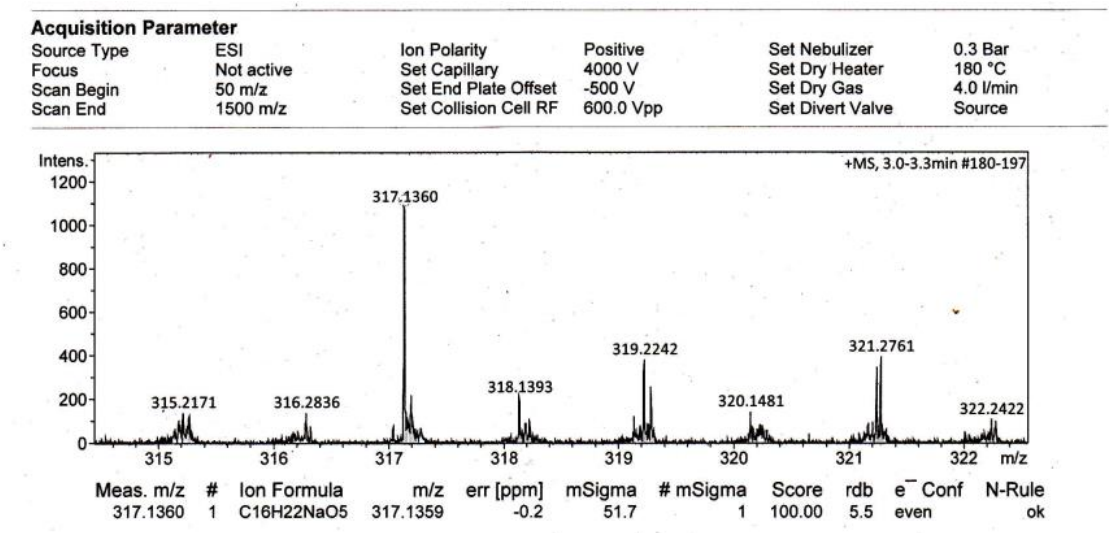


Figure S32. The HRESIMS of compound **5**.

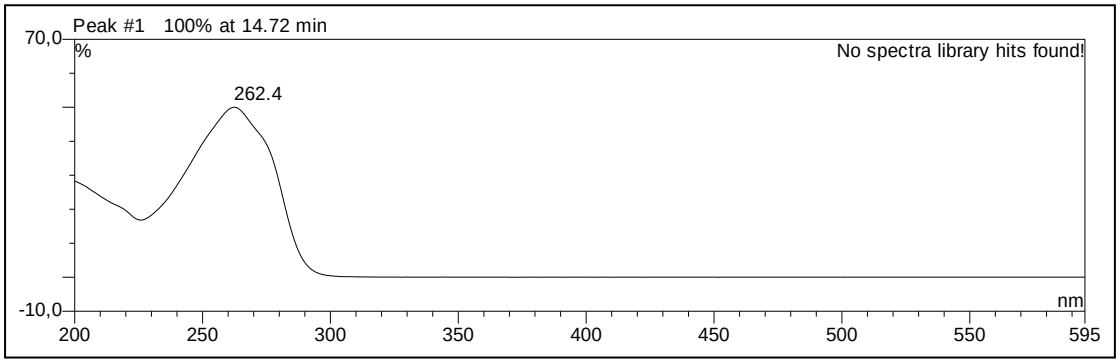


Figure S33. The UV spectrum of compound **5**.

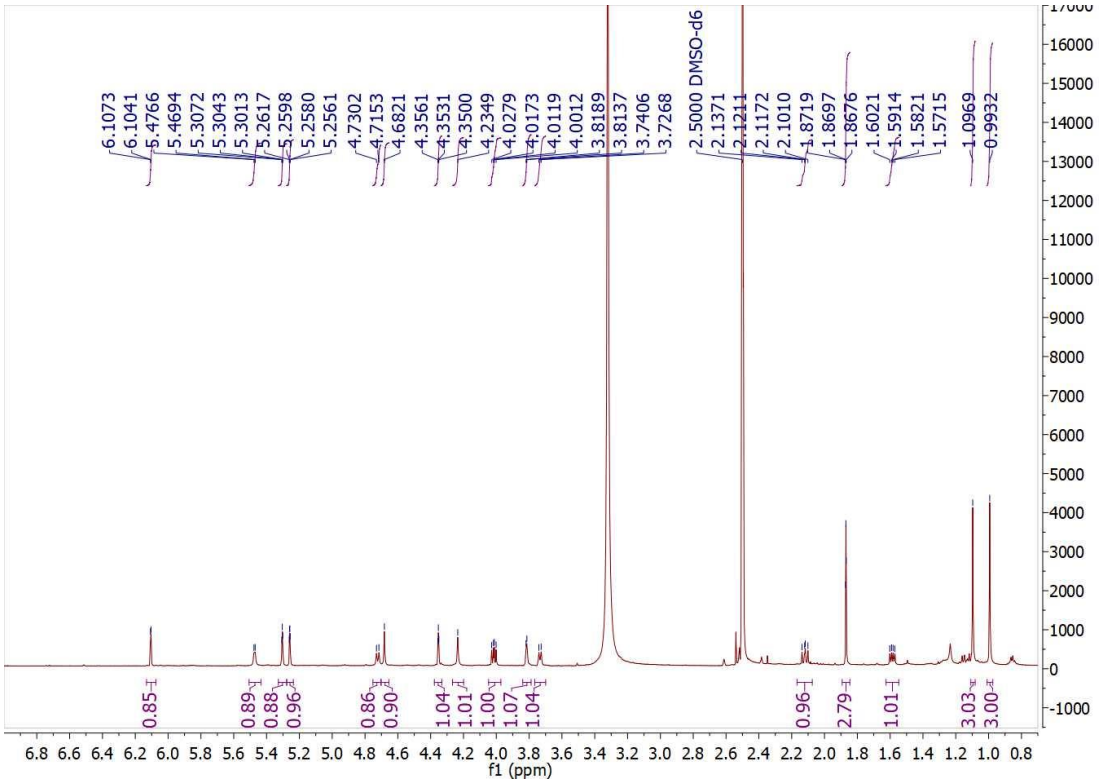


Figure S34. The ^{1}H-NMR (600 MHz, DMSO-d_6) spectrum of compound **5**.

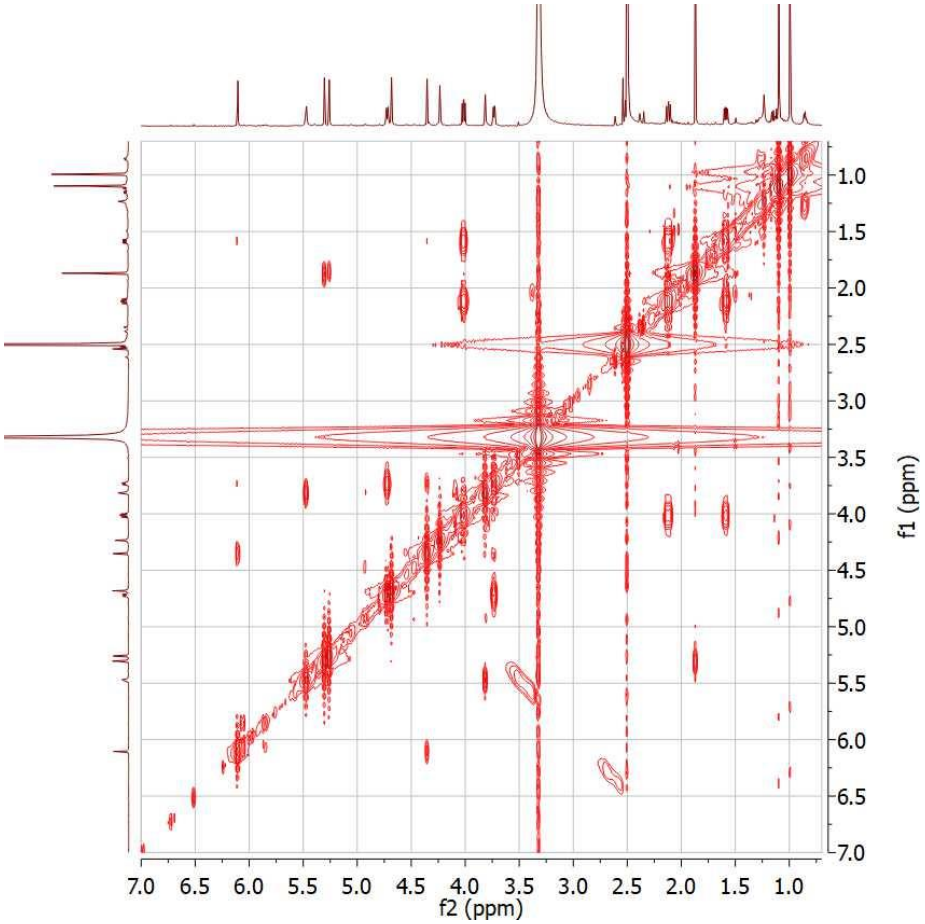


Figure S35. The ^{1}H-^{1}H COSY (600 MHz, DMSO-d_6) spectrum of compound **5**.

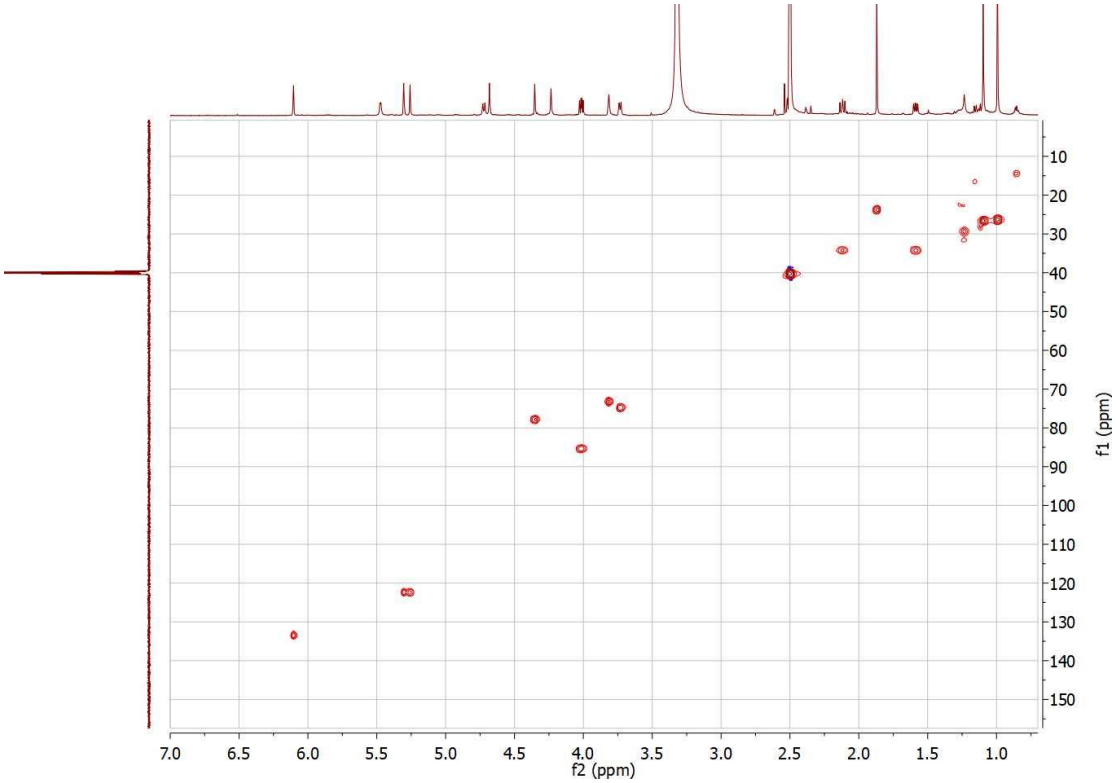


Figure S36. The HSQC (600 MHz, DMSO-d_6) spectrum of compound **5**.

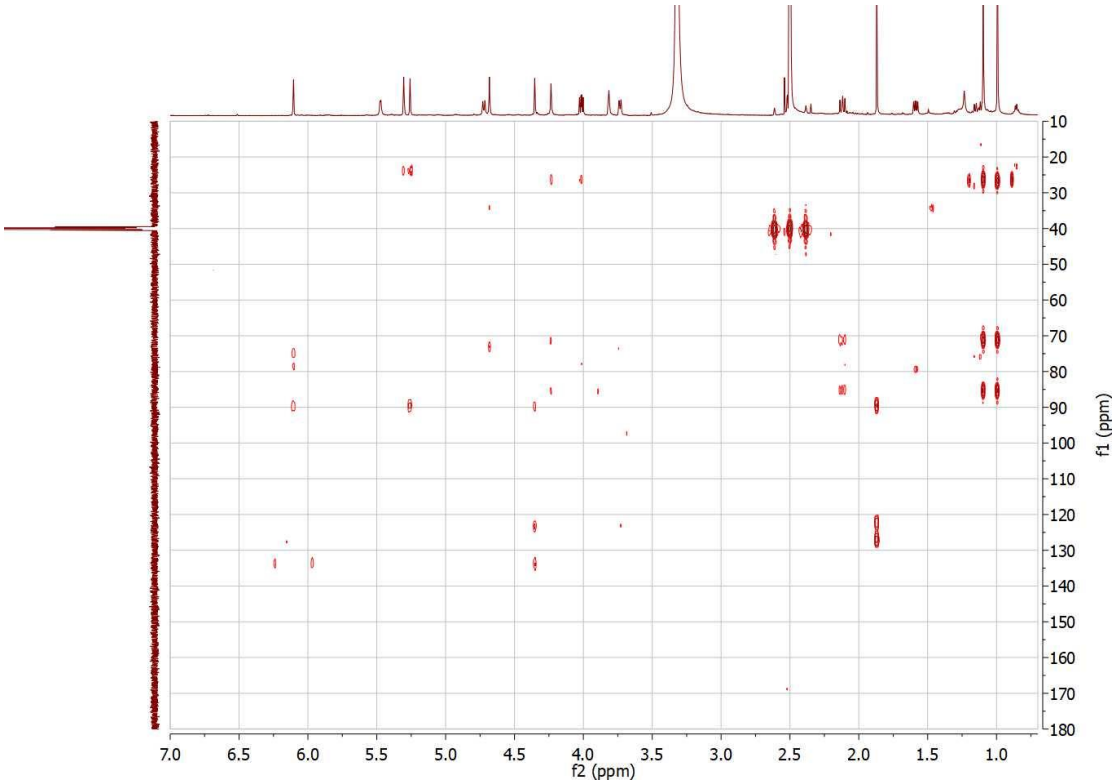


Figure S37. The HMBC (600MHz, DMSO-d_6) spectrum of compound **5**.

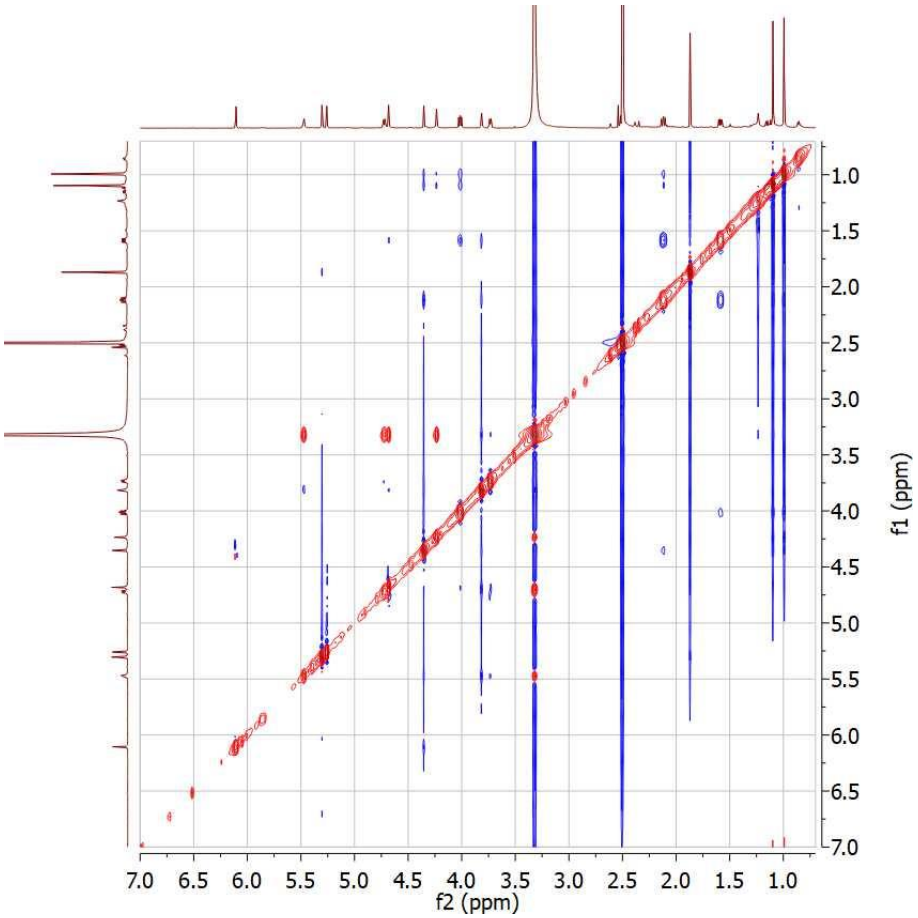
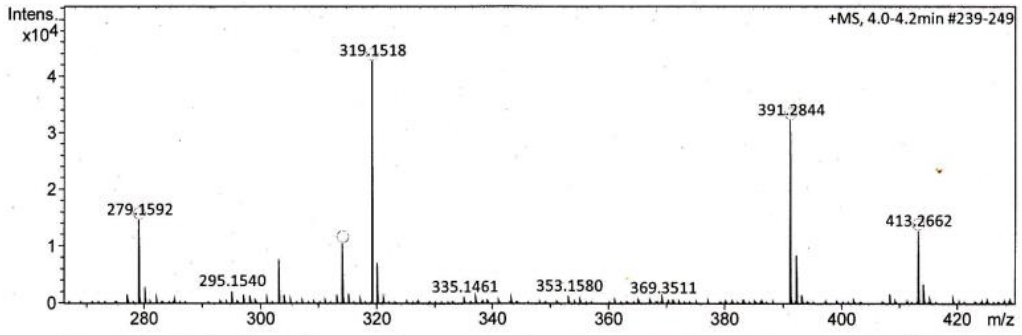


Figure S38. The ROESY (600 MHz, DMSO-d_6) spectrum of compound **5**.

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
279.1592	1	C17H19N4	279.1604	4.4	9.7	1	57.04	10.5	even	ok
	2	C16H23O4	279.1591	-0.4	10.4	2	100.00	5.5	even	ok
	3	C15H20N4Na	279.1580	-4.2	12.9	3	55.47	7.5	even	ok
314.1963	1	C16H28NO5	314.1962	-0.5	8.9	1	100.00	3.5	even	ok
	2	C15H25N5NaO	314.1951	-3.9	10.9	2	55.67	5.5	even	ok
	3	C17H24N5O	314.1975	3.8	22.6	3	44.40	8.5	even	ok
319.1518	1	C14H19N6O3	319.1513	-1.4	6.7	1	90.01	8.5	even	ok
	2	C13H23N2O7	319.1500	-5.6	7.5	2	40.26	3.5	even	ok
	3	C16H24NaO5	319.1516	-0.5	7.8	3	100.00	4.5	even	ok
	4	C17H20N4NaO	319.1529	3.7	20.8	4	45.83	9.5	even	ok

Figure S39. The HRESIMS of compound **6**.

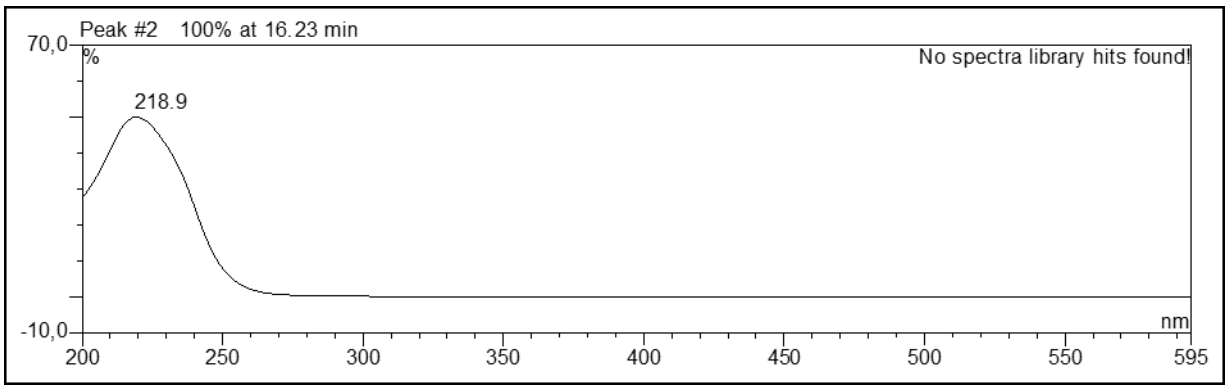


Figure S40. The UV spectrum of compound **6**.

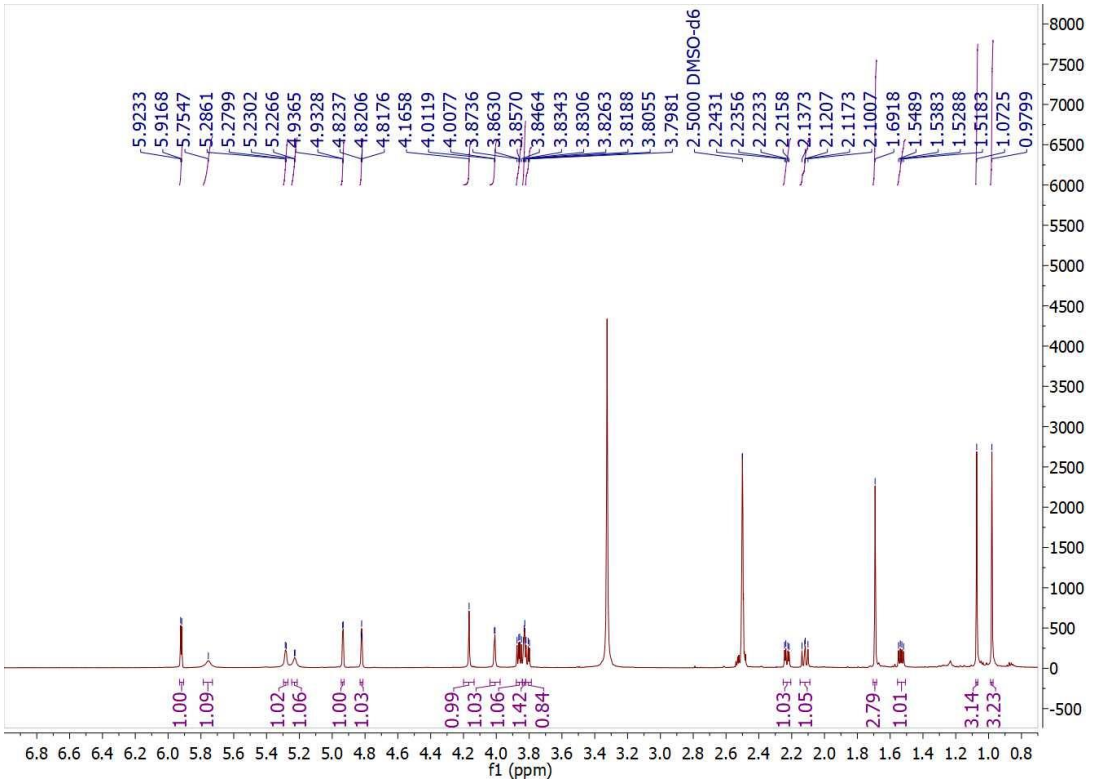


Figure S41. The ^{1}H-NMR (600 MHz, DMSO-d_6) spectrum of compound **6**.

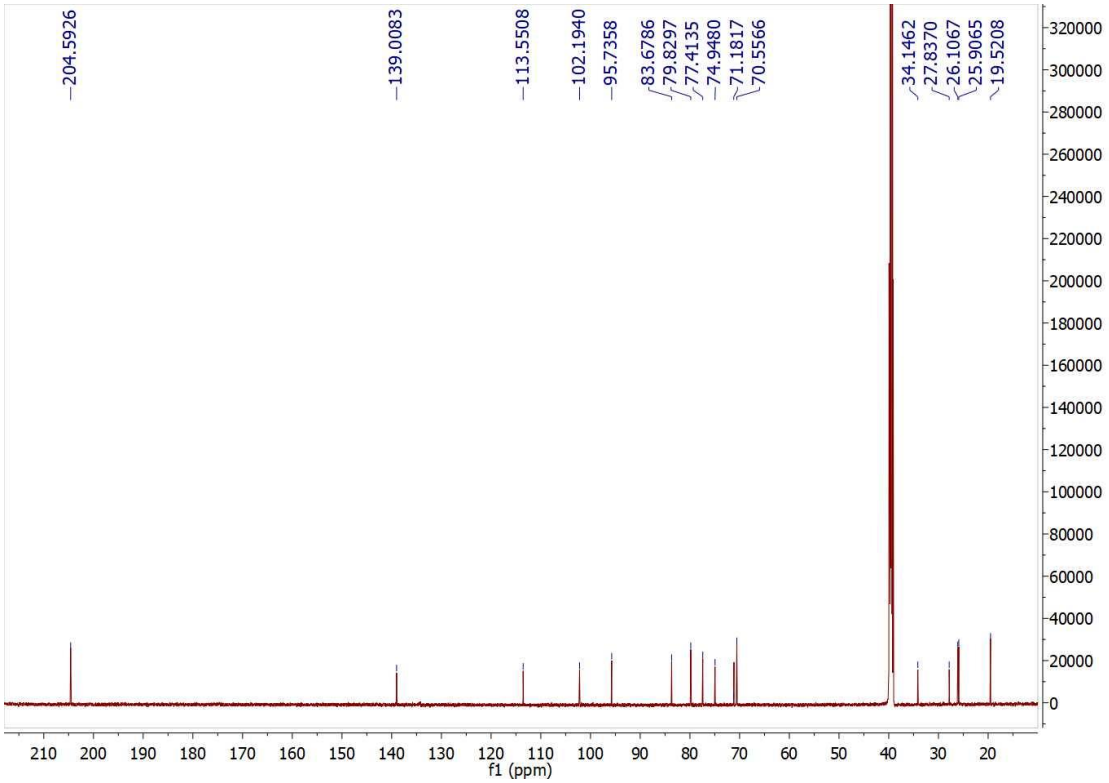


Figure S42. The ^{13}C-NMR (150 MHz, DMSO-d_6) spectrum of compound **6**.

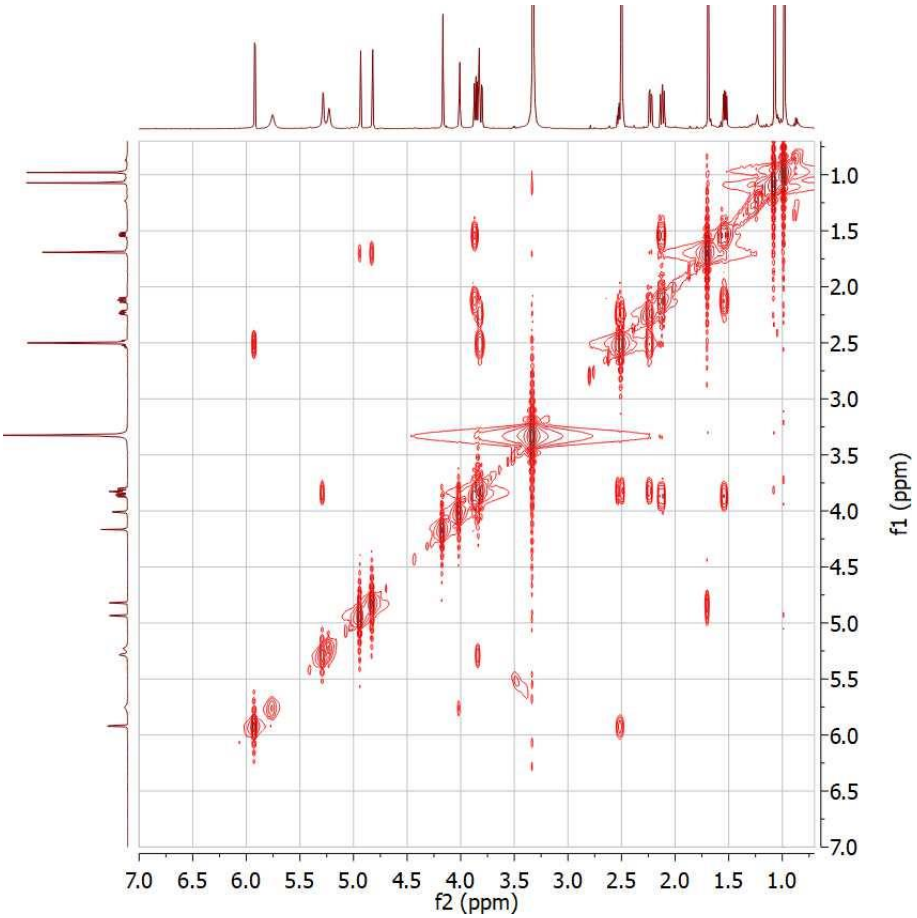


Figure S43. The ^{1}H-^{1}H COSY (600 MHz, DMSO-d_6) spectrum of compound **6**.

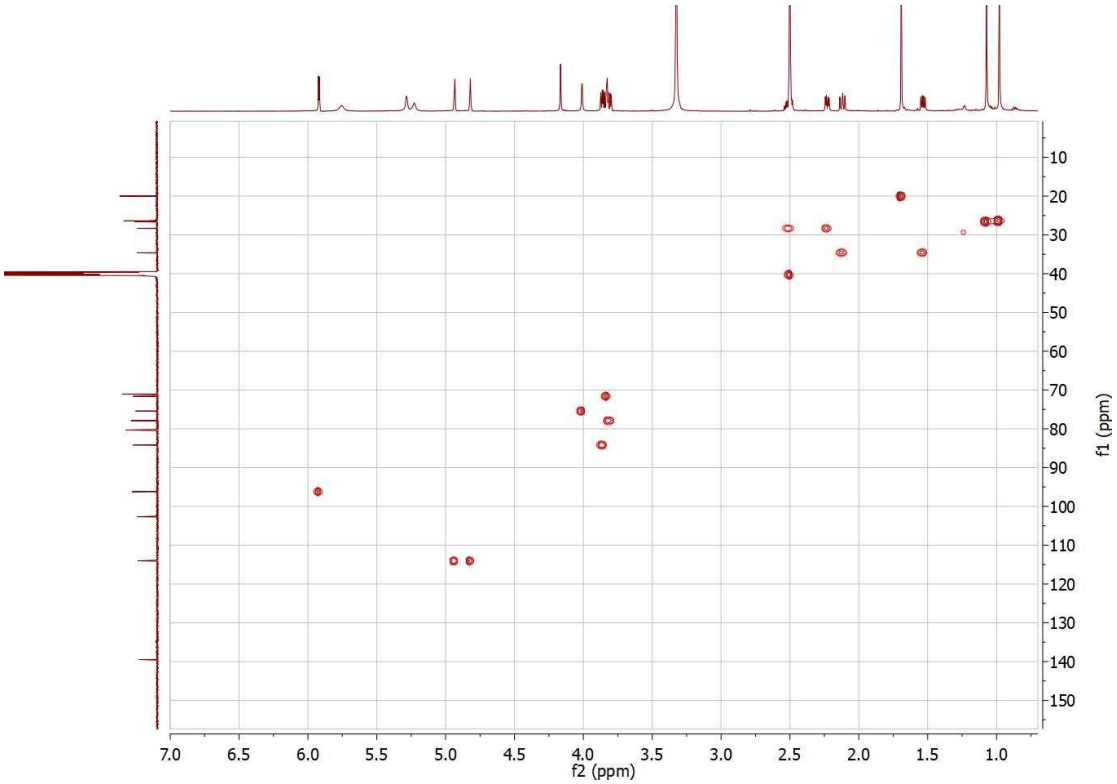


Figure S44. The HSQC (600 MHz, DMSO-d_6) spectrum of compound **6**.

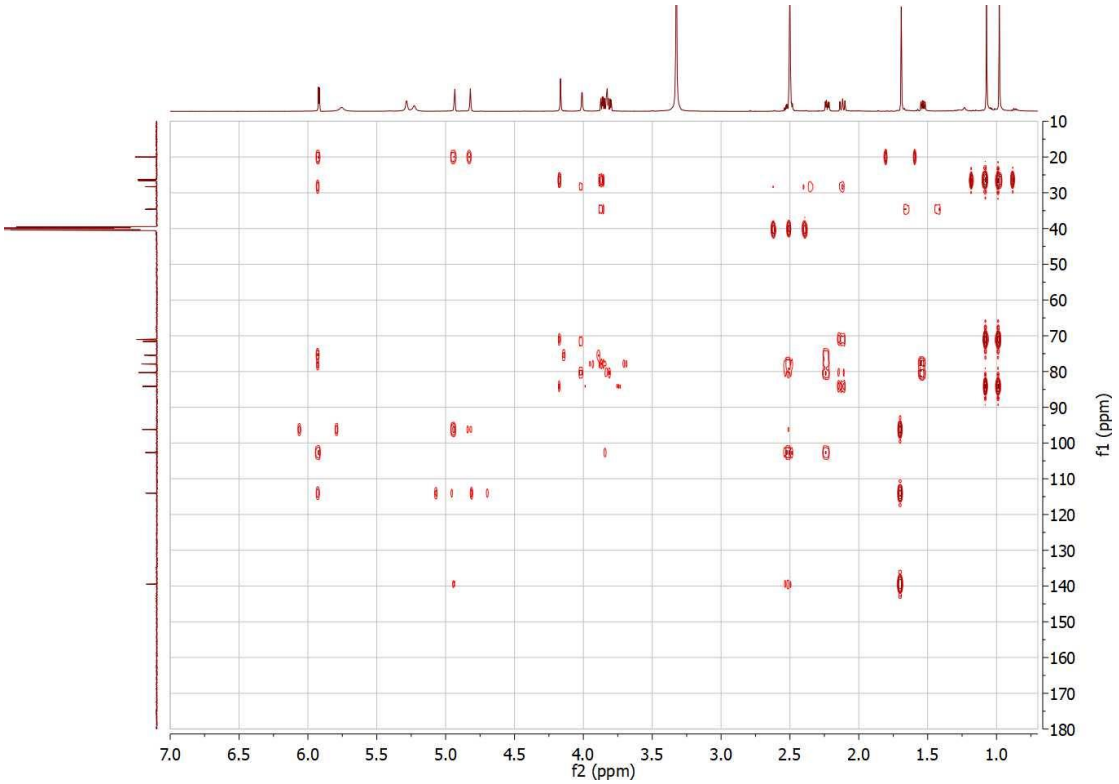


Figure S45. The HMBC (600 MHz, DMSO-d_6) spectrum of compound **6**.

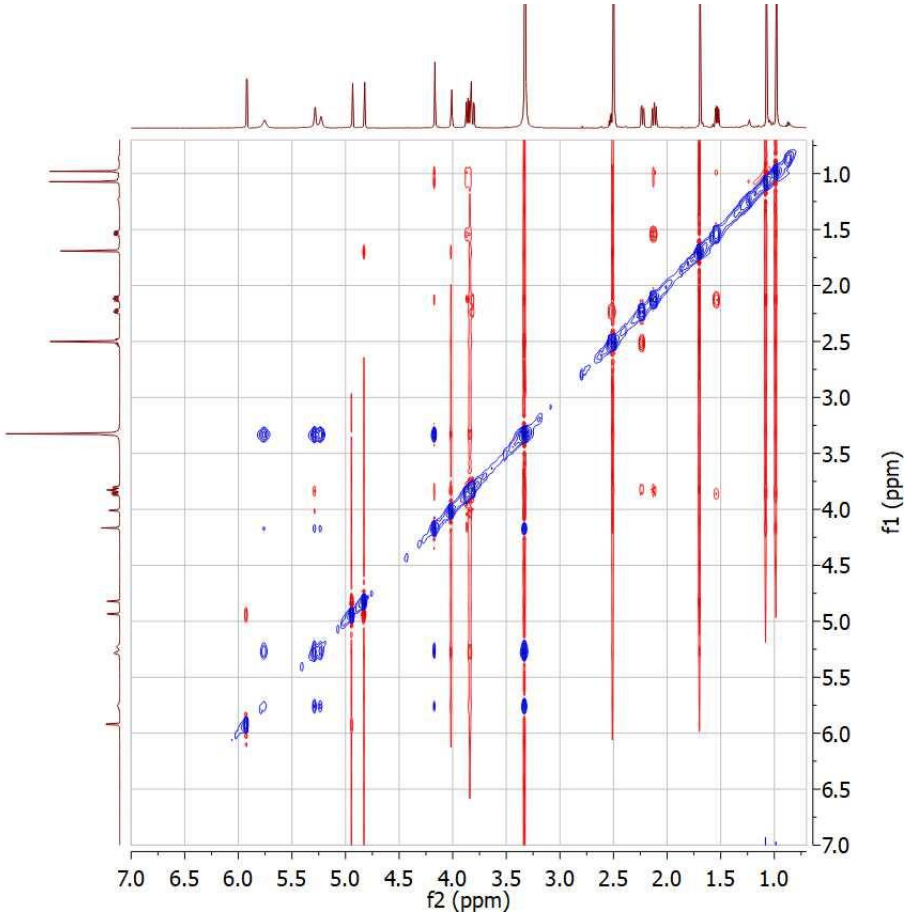


Figure S46. The ROESY (600 MHz, DMSO-d_6) spectrum of compound **6**.

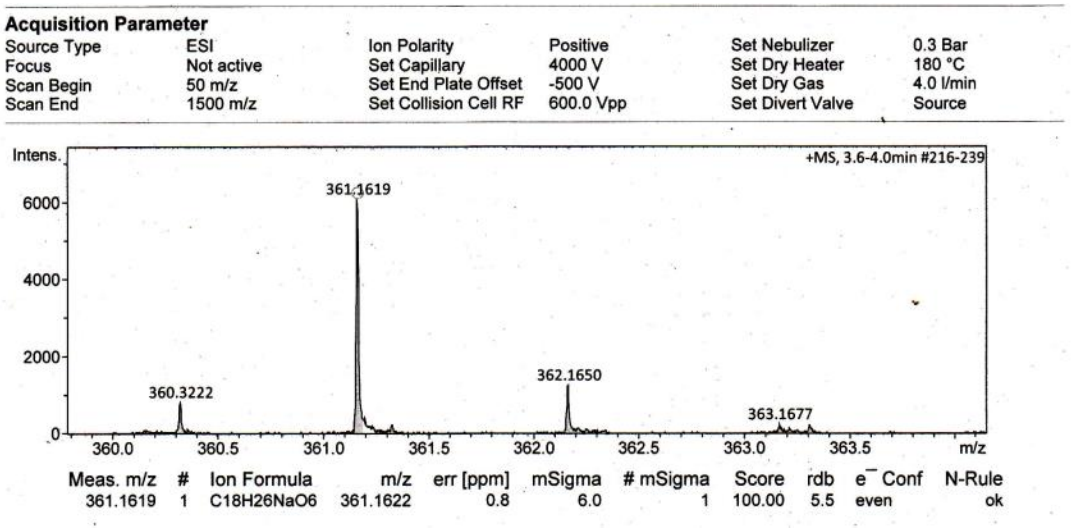


Figure S47. The HRESIMS of compound **7**.

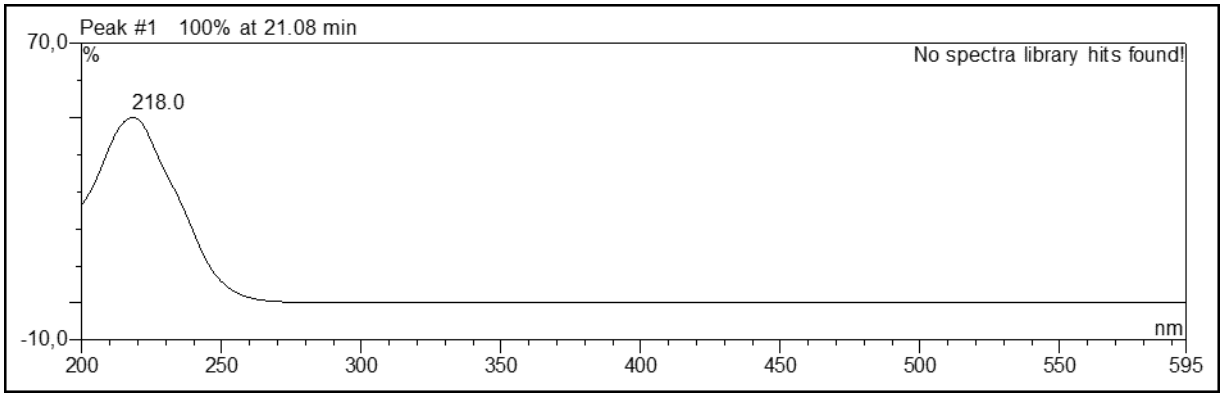


Figure S48. The UV spectrum of compound **7**.

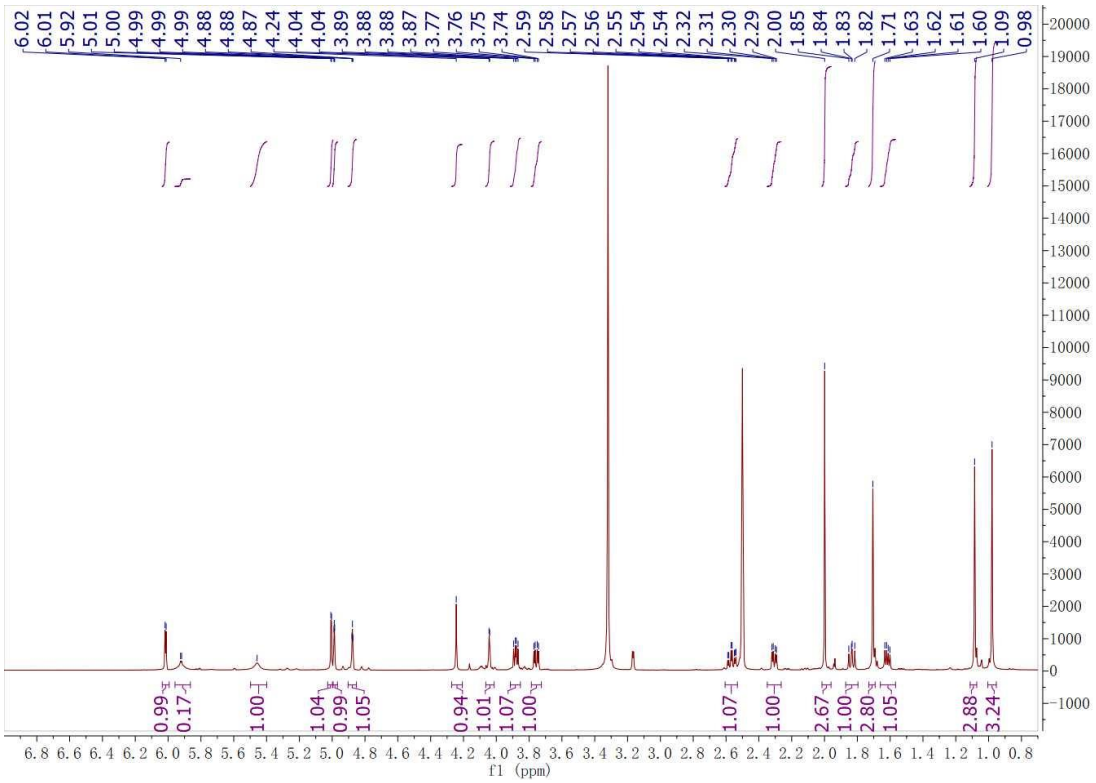


Figure S49. The ^{1}H-NMR (600 MHz, DMSO-d_6) spectrum of compound **7**.

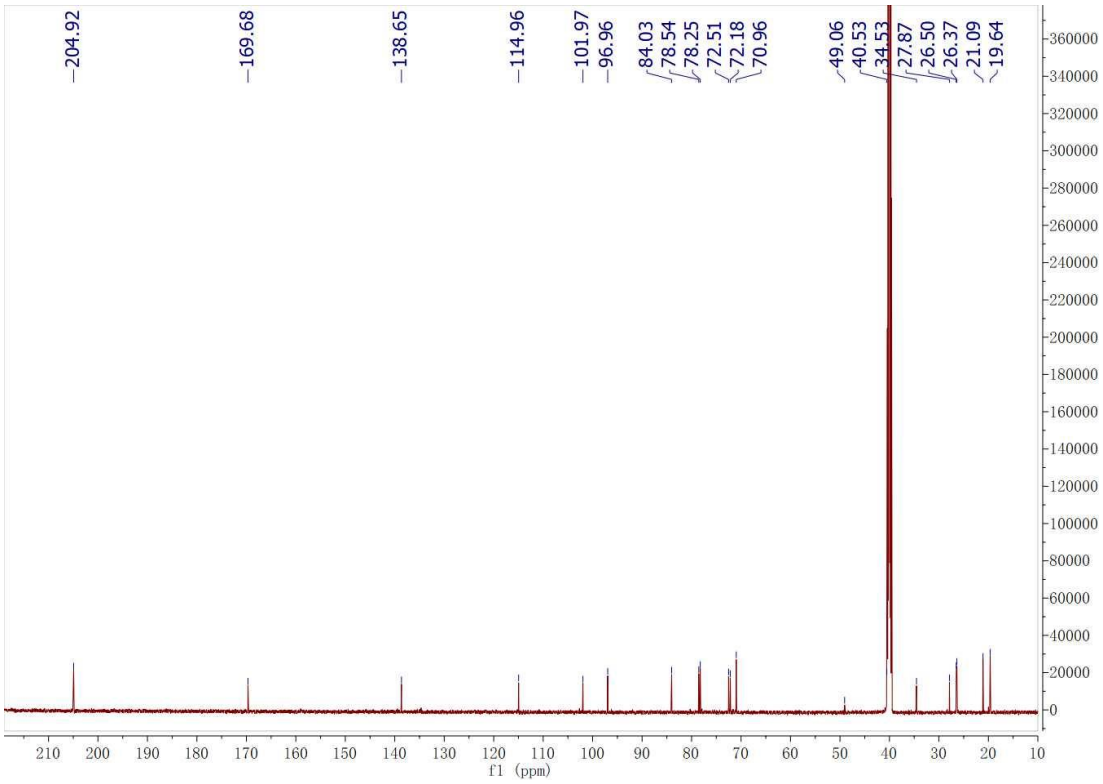


Figure S50. The ^{13}C-NMR (150 MHz, DMSO-d_6) spectrum of compound **7**.

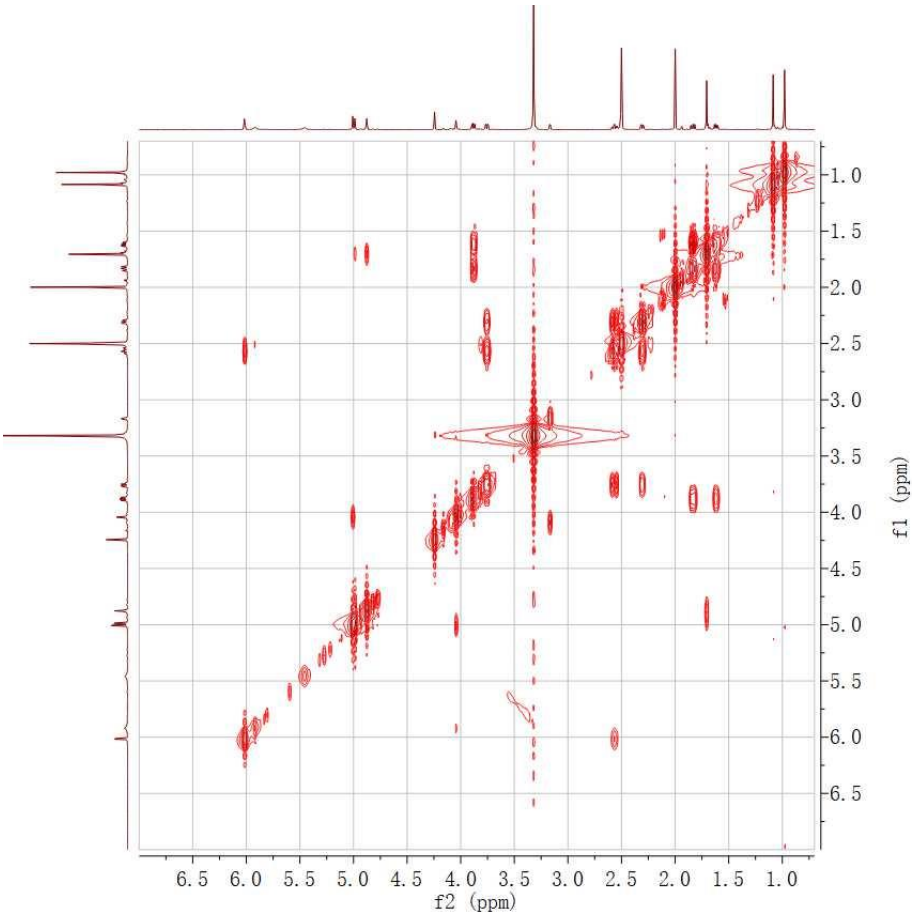


Figure S51. The ^{1}H-^{1}H COSY (600 MHz, DMSO-d_6) spectrum of compound **7**.

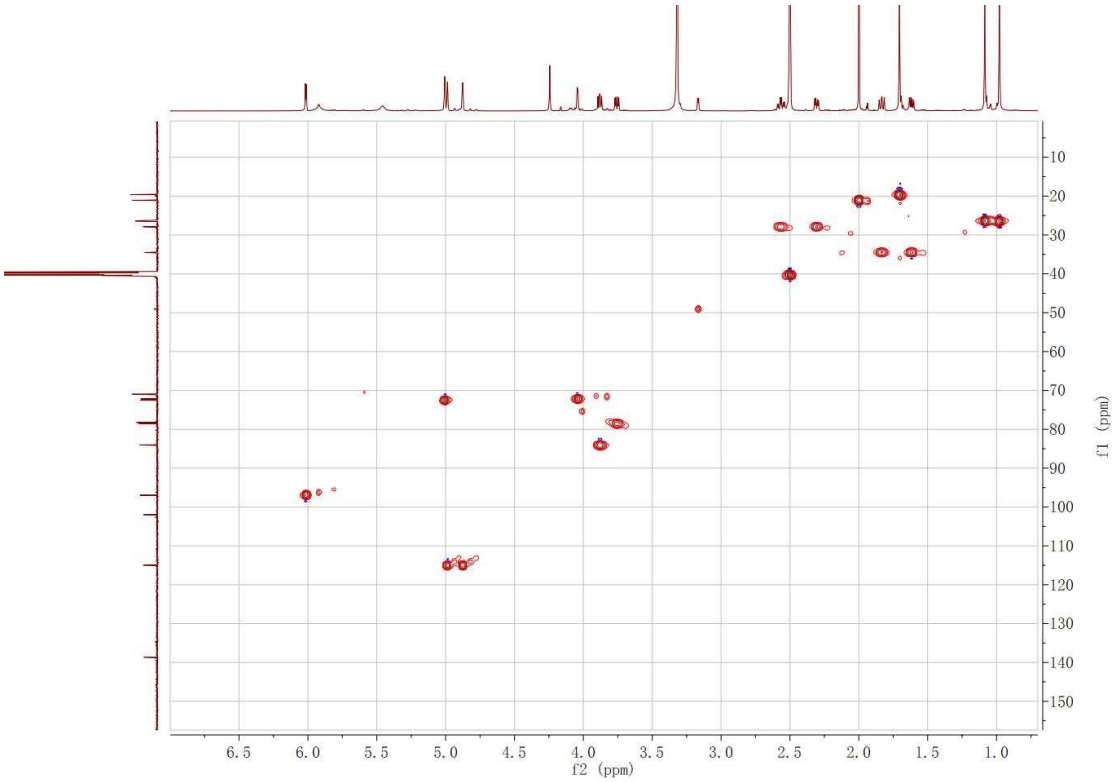


Figure S52. The HSQC (600 MHz, DMSO-d_6) spectrum of compound **7**.

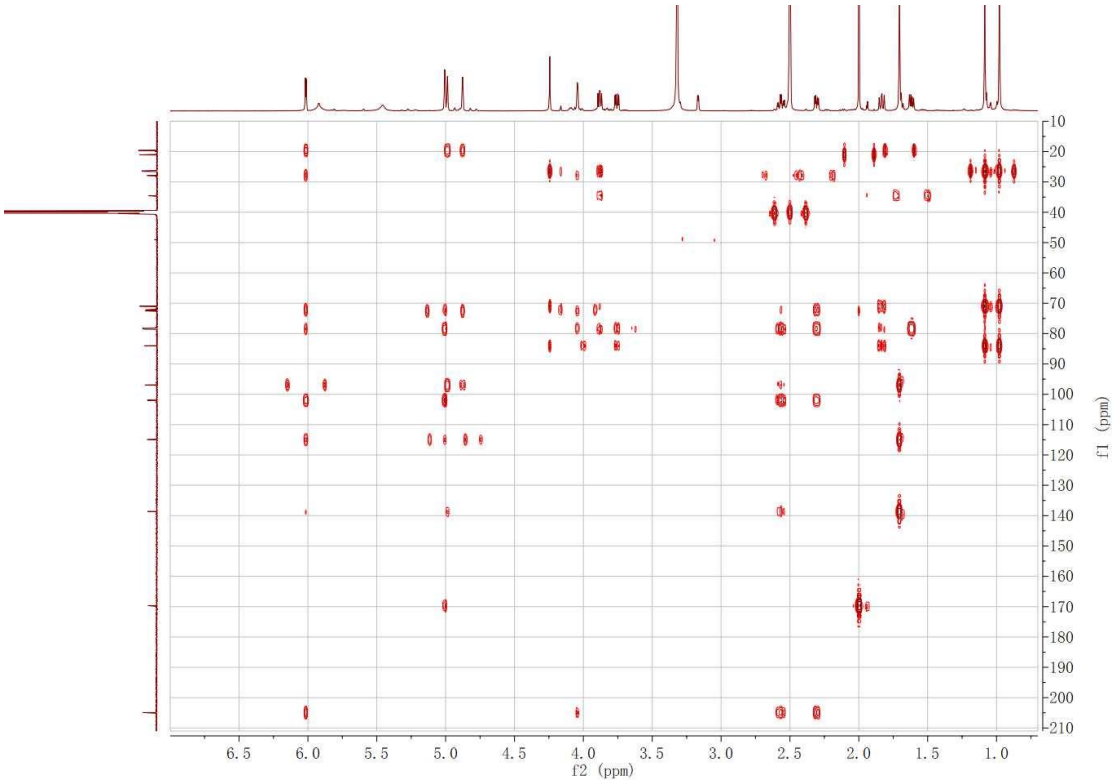


Figure S53. The HMBC (600 MHz, DMSO-d_6) spectrum of compound **7**.

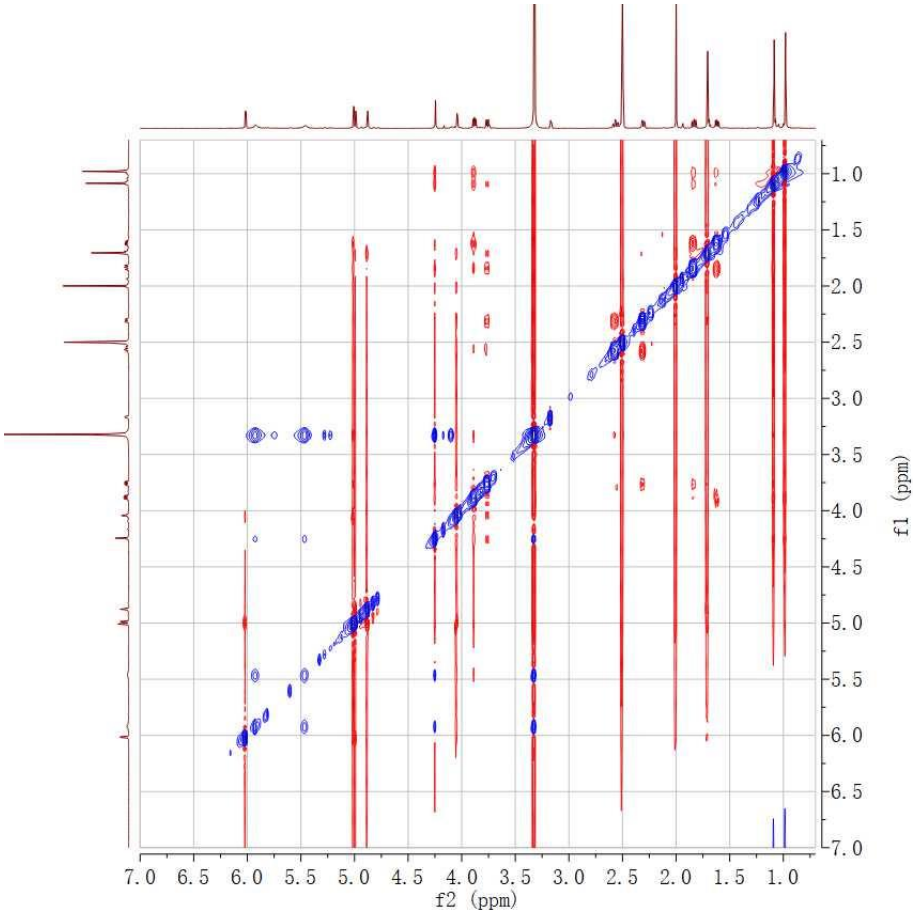


Figure S54. The ROESY (600 MHz, DMSO-d_6) spectrum of compound **7**.

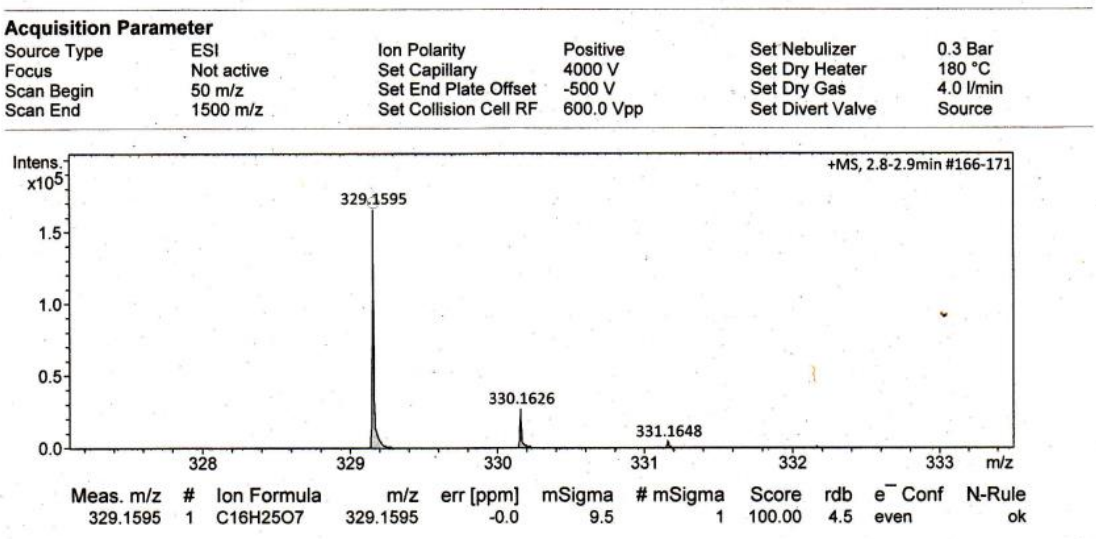


Figure S55. The HREISMS of compound **8**.

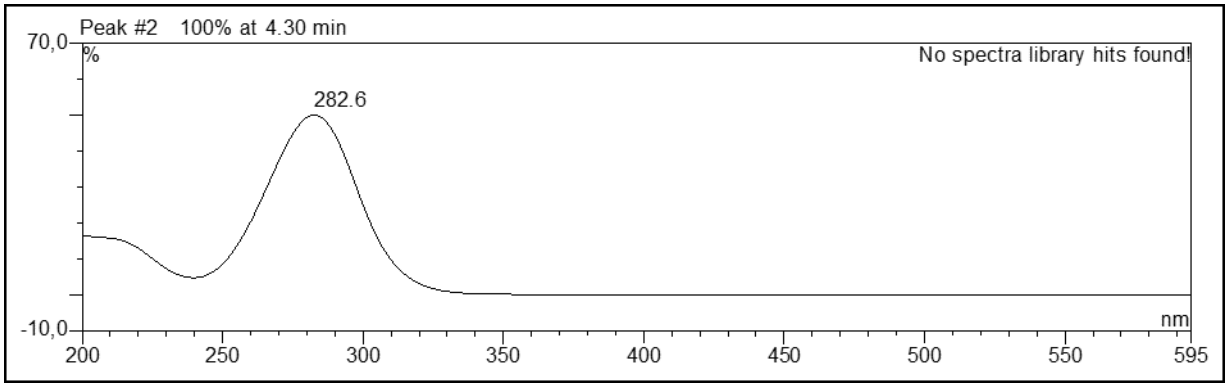


Figure S56. The UV spectrum of compound **8**.

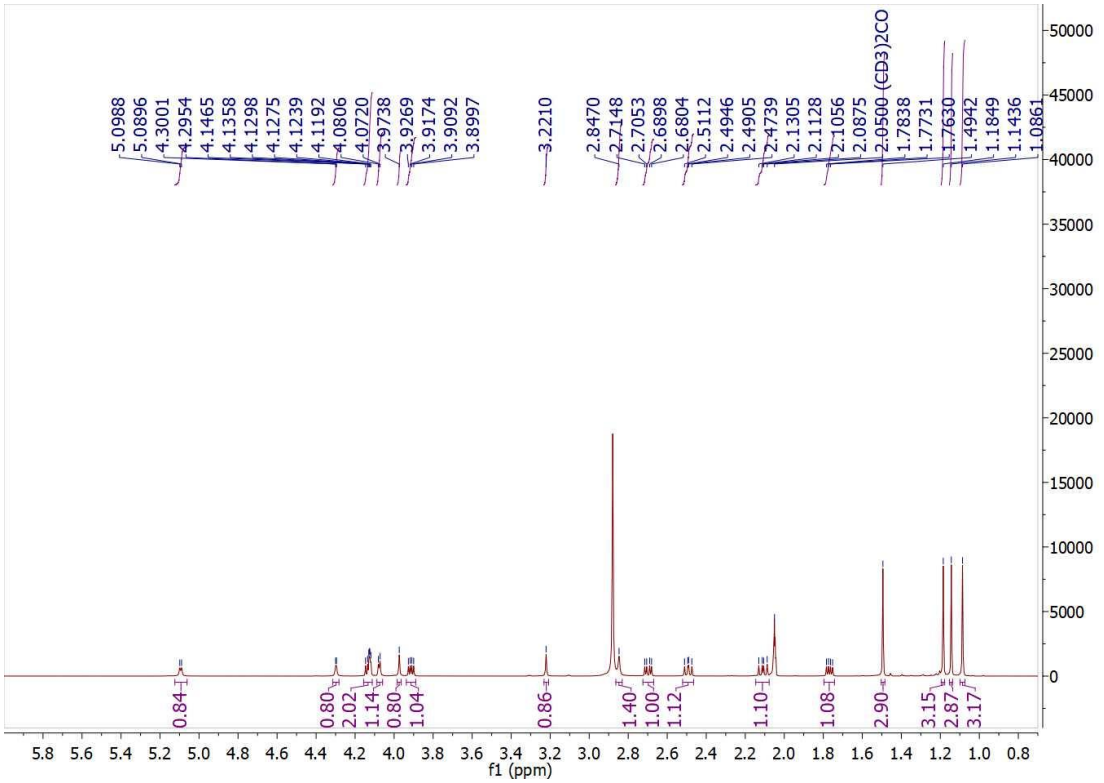


Figure S57. The ^{1}H-NMR (600 MHz, Acetone-d_6) spectrum of compound **8**.

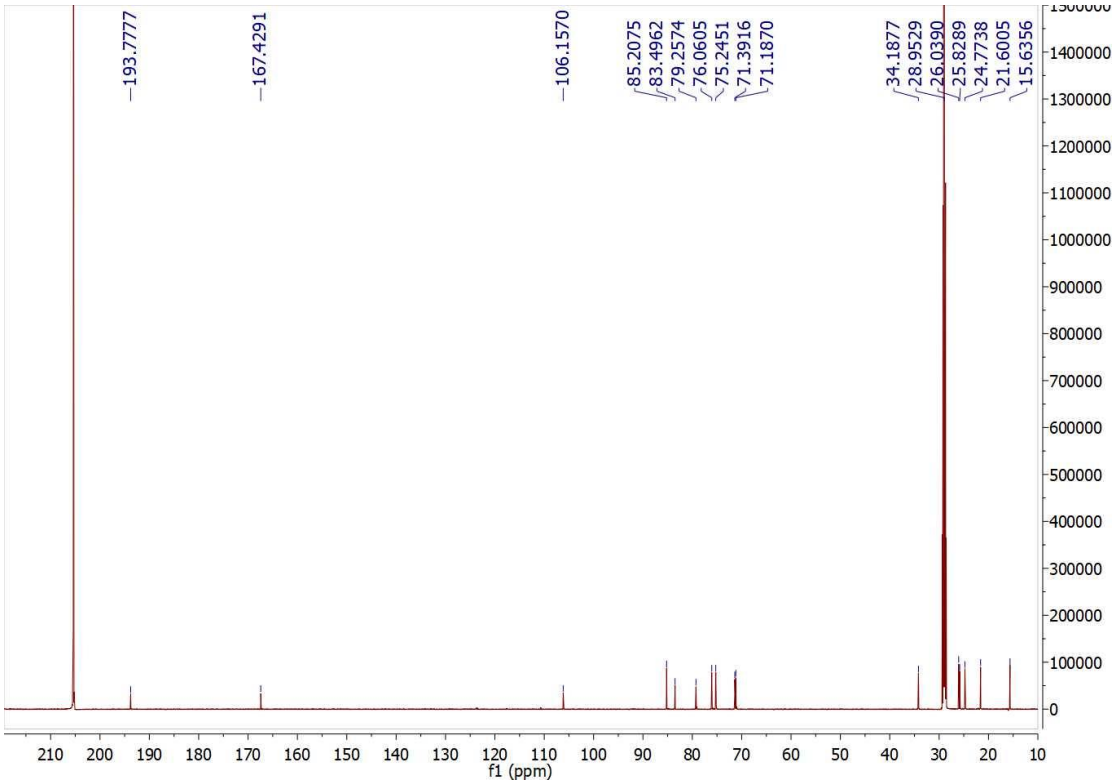


Figure S58. The ^{13}C-NMR (150 MHz, Acetone-d_6) spectrum of compound **8**.

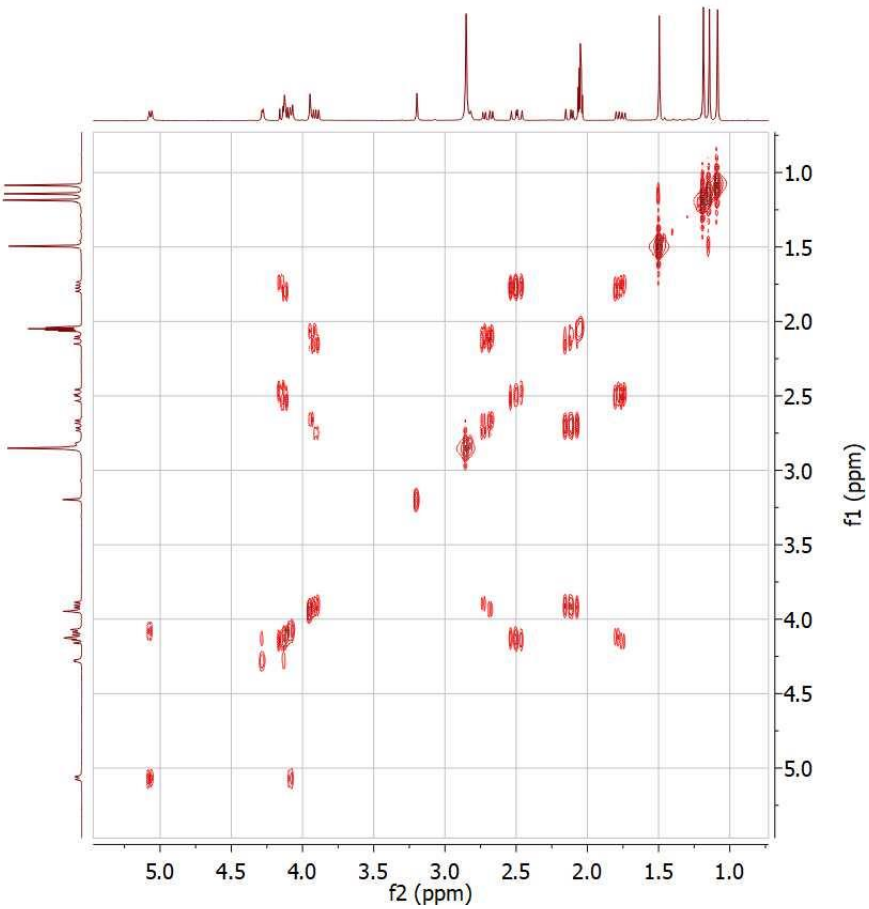


Figure S59. The ^{1}H-H COSY (600 MHz, Acetone-d_6) spectrum of compound **8**.

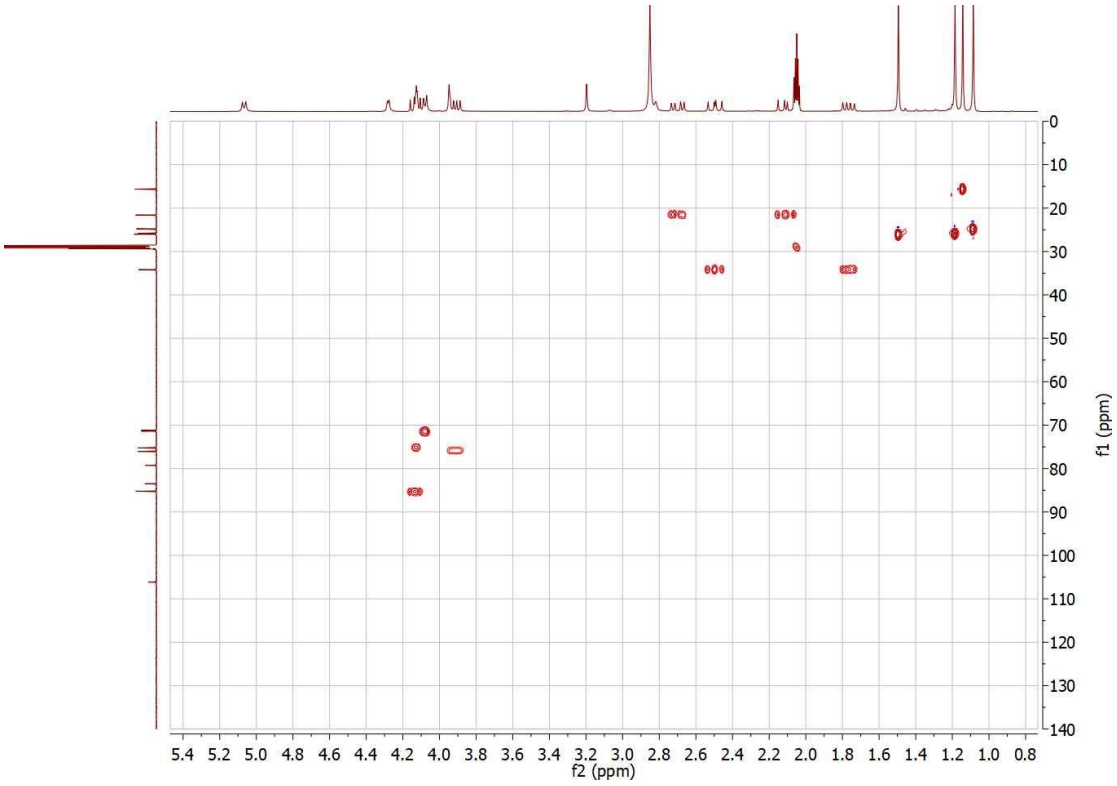


Figure S60. The HSQC (600 MHz, Acetone-d_6) spectrum of compound **8**.

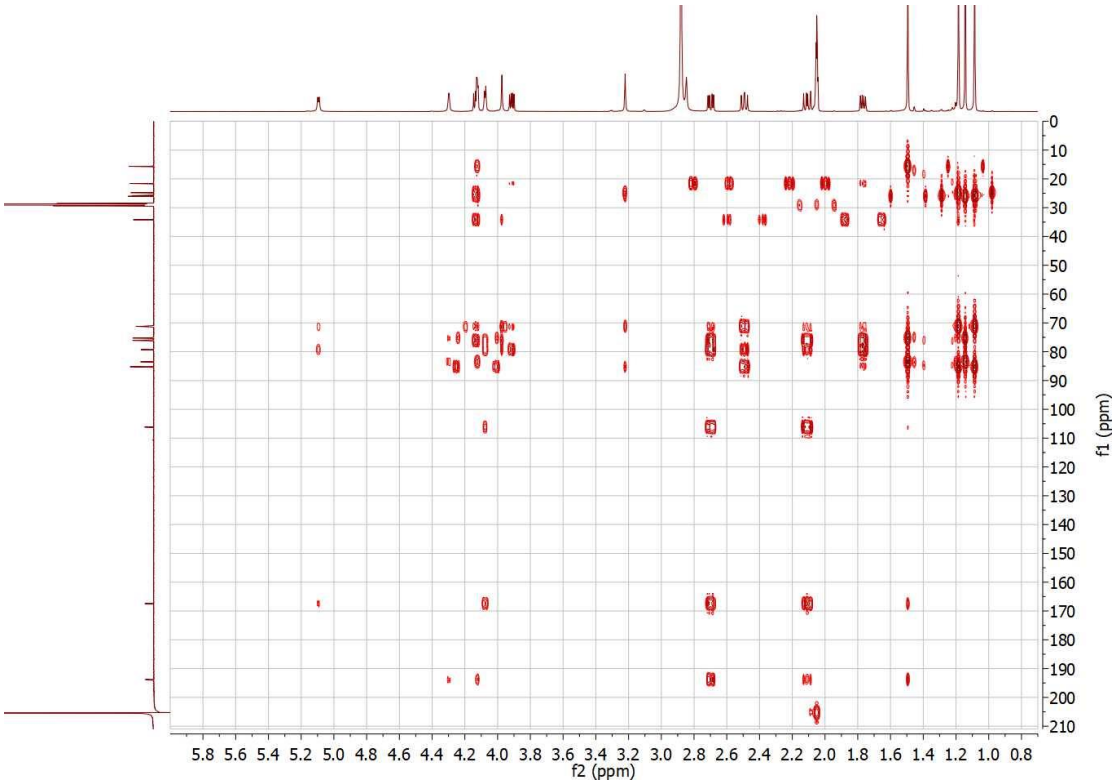


Figure S61. The HMBC (600 MHz, Acetone-d_6) spectrum of compound **8**.

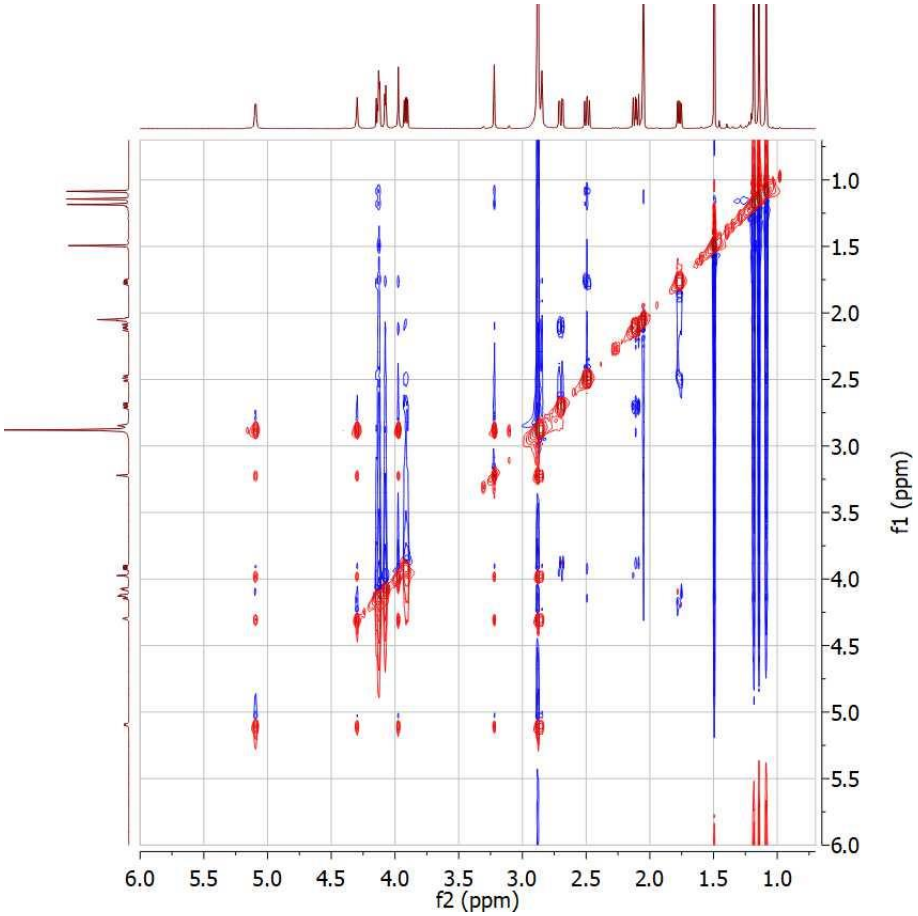


Figure S62. The ROESY (600 MHz, Acetone-d_6) spectrum of compound **8**.

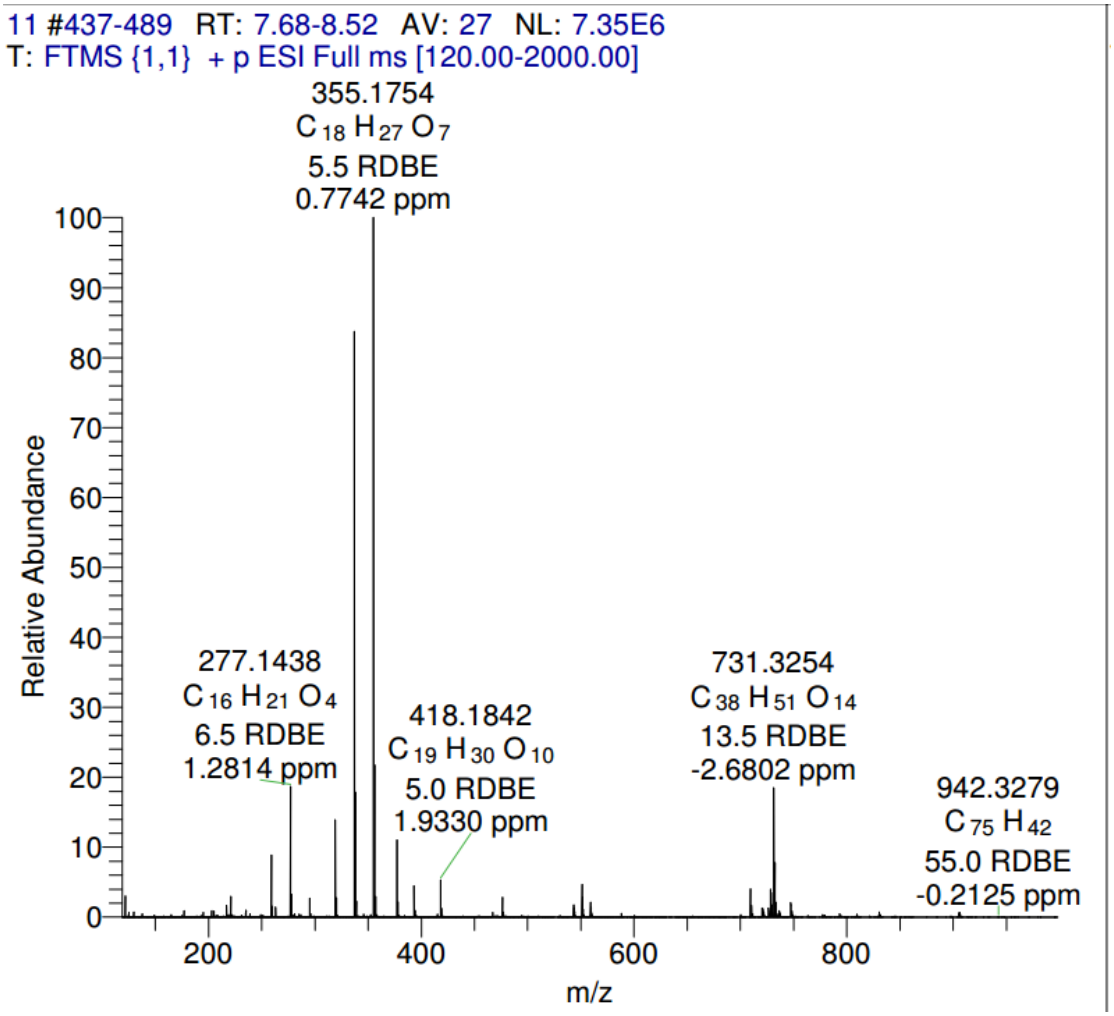


Figure S63. The HREISMS of compound **9**.

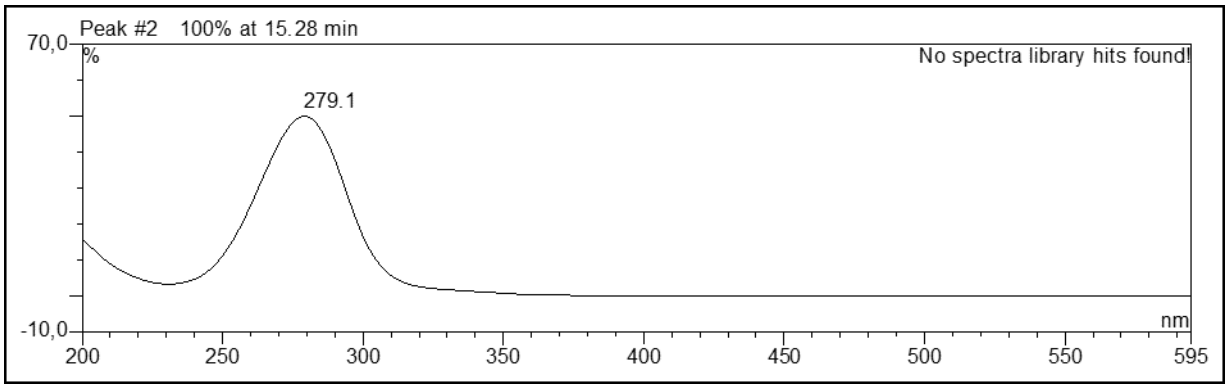


Figure S64. The UV spectrum of compound **9**.

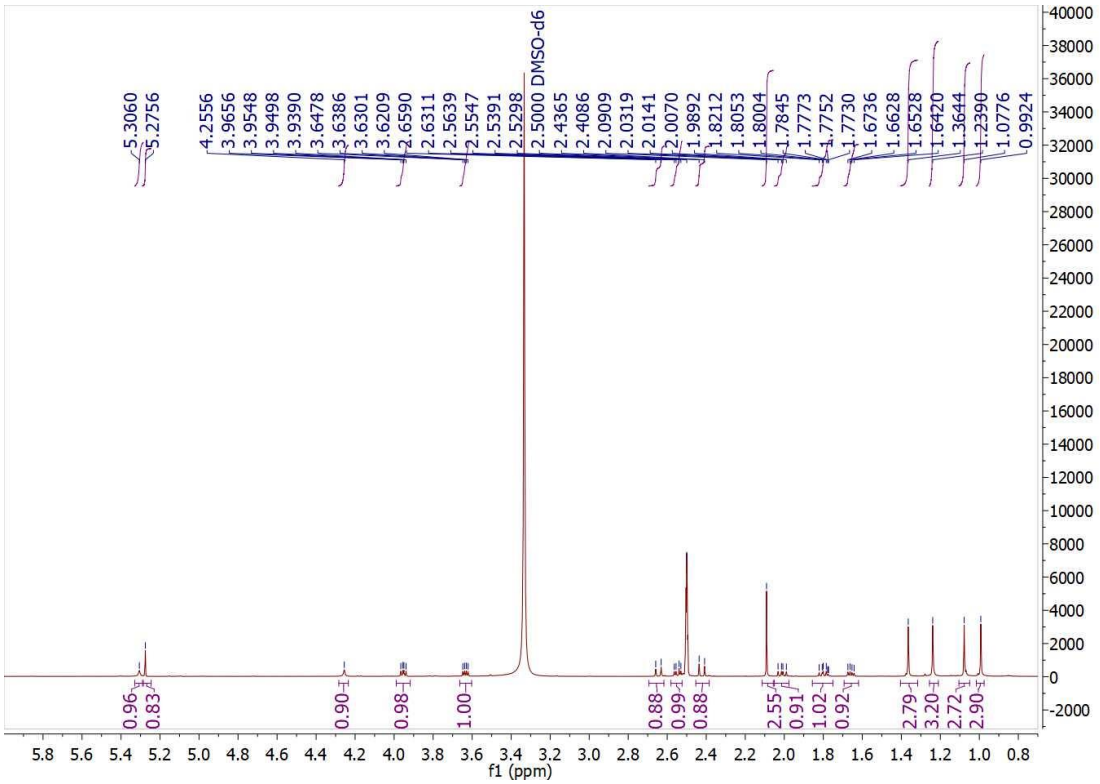


Figure S65. The ^{1}H-NMR (600 MHz, DMSO-d_6) spectrum of compound **9**.

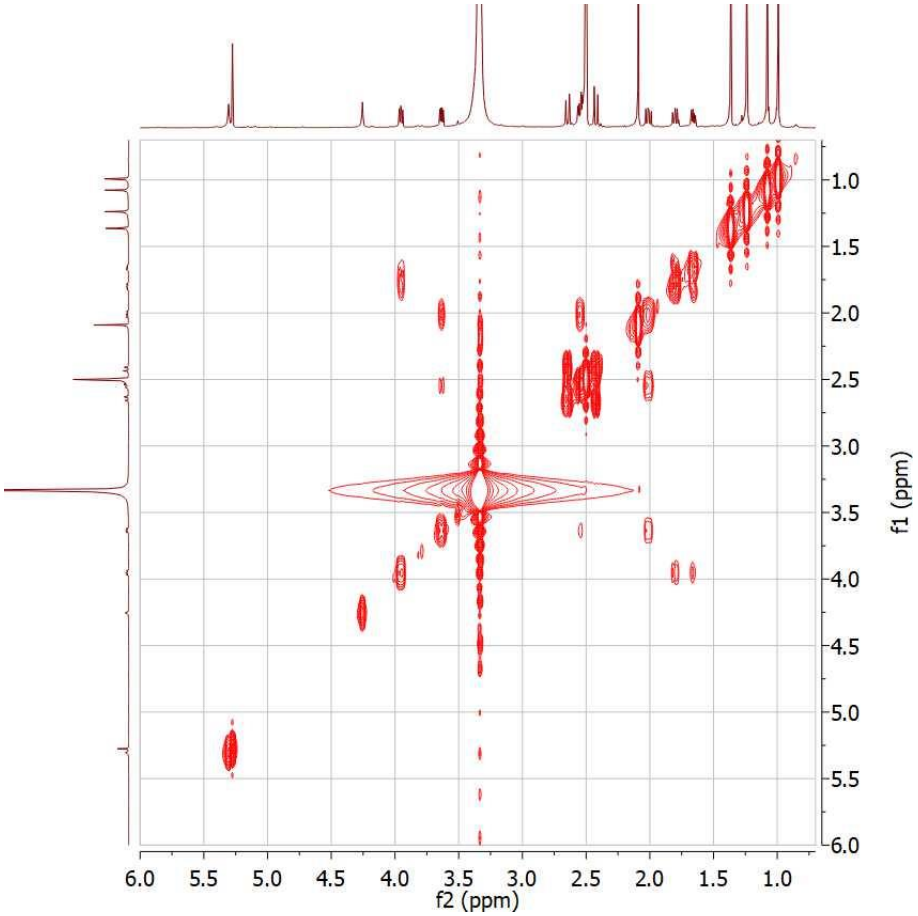


Figure S66. The ^{1}H-^{1}H COSY (600 MHz, DMSO-d_6) spectrum of compound **9**.

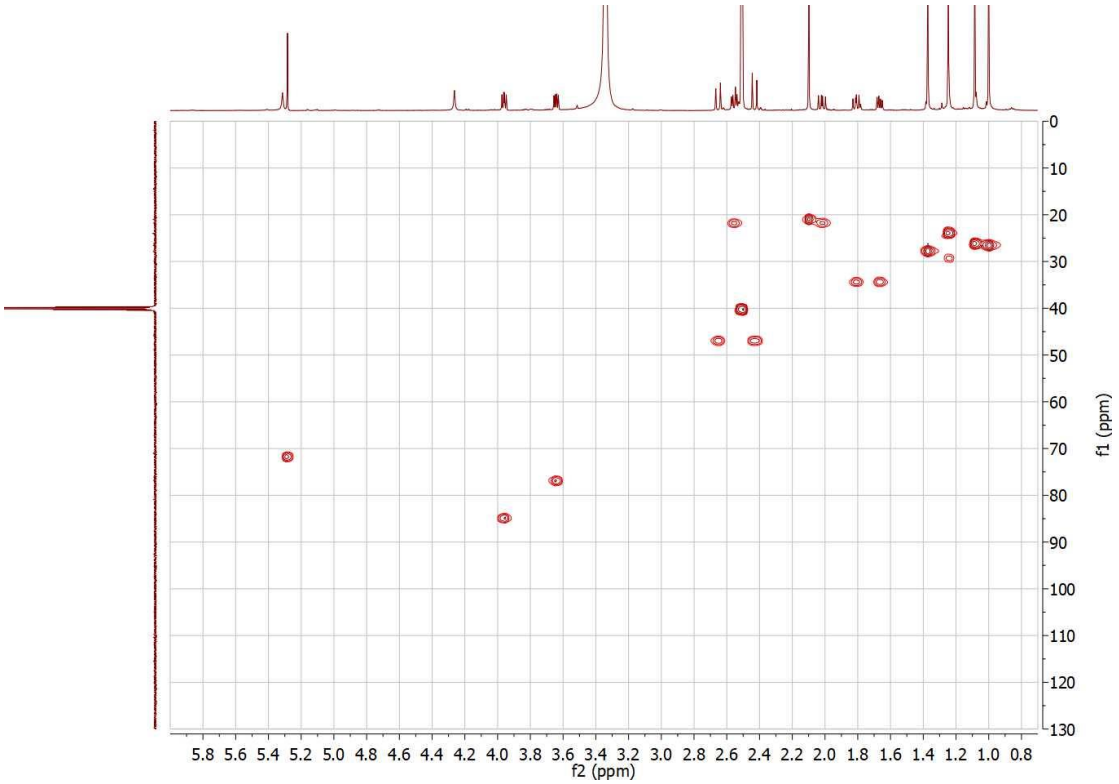


Figure S67. The HSQC (600 MHz, DMSO-d_6) spectrum of compound **9**.

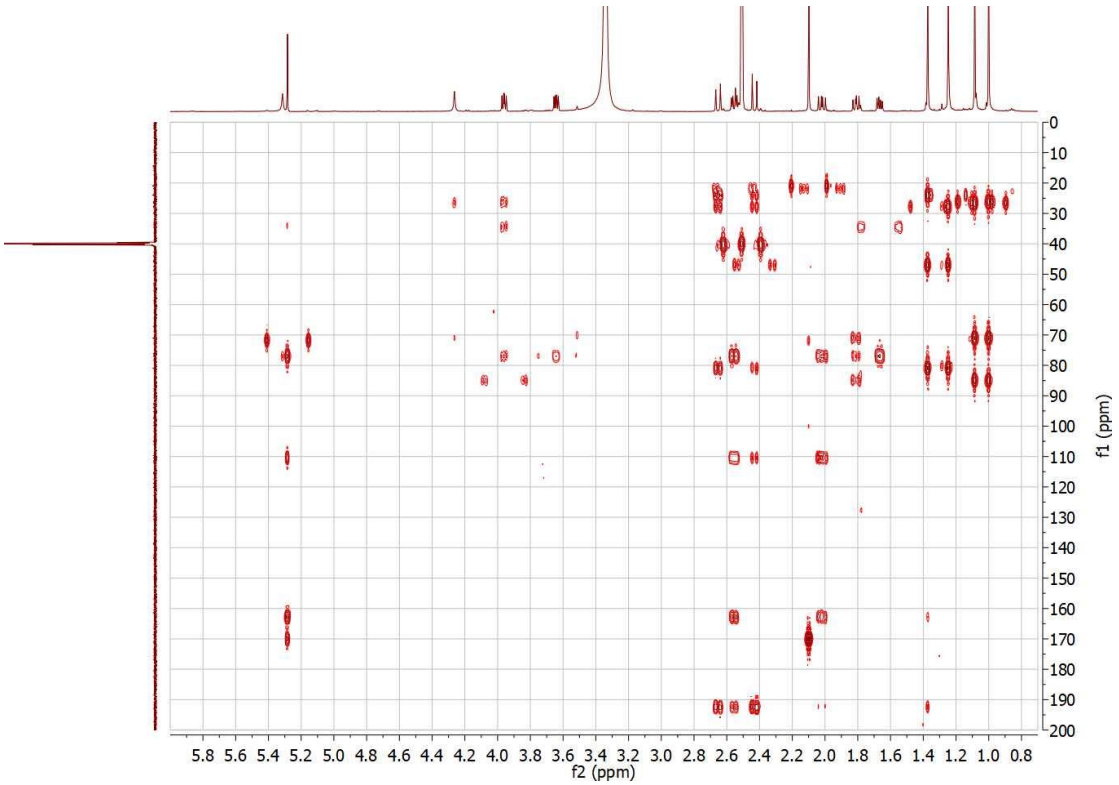


Figure S68. The HMBC (600 MHz, DMSO-d_6) spectrum of compound **9**.

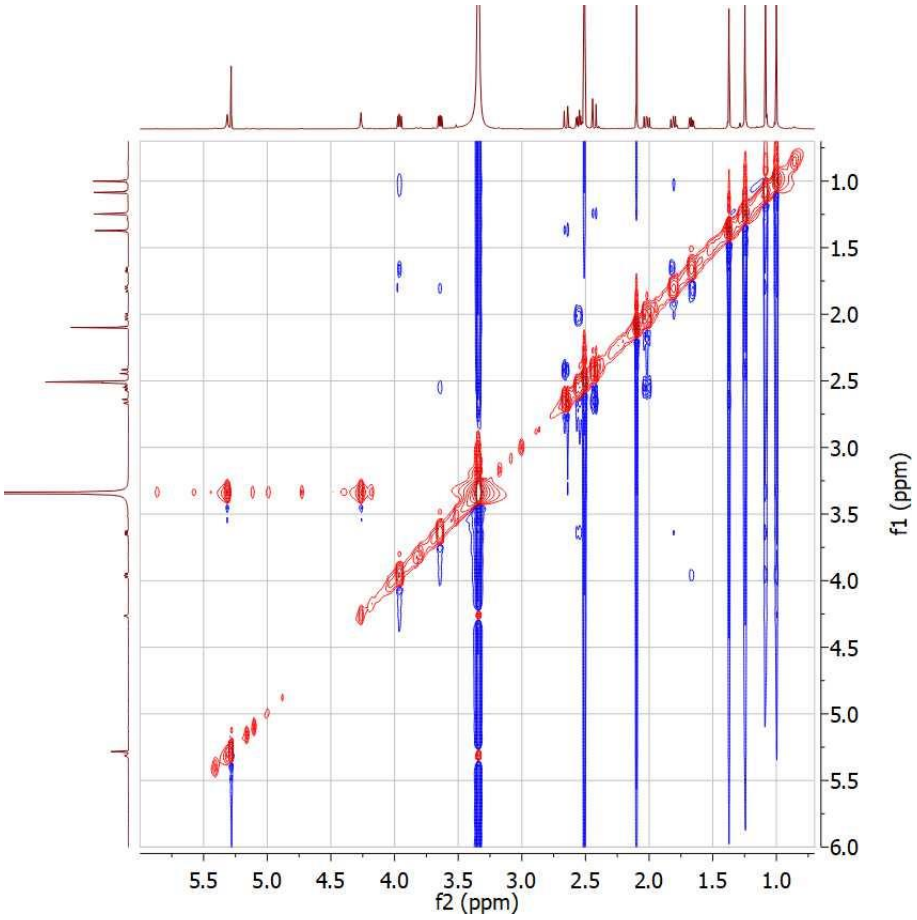
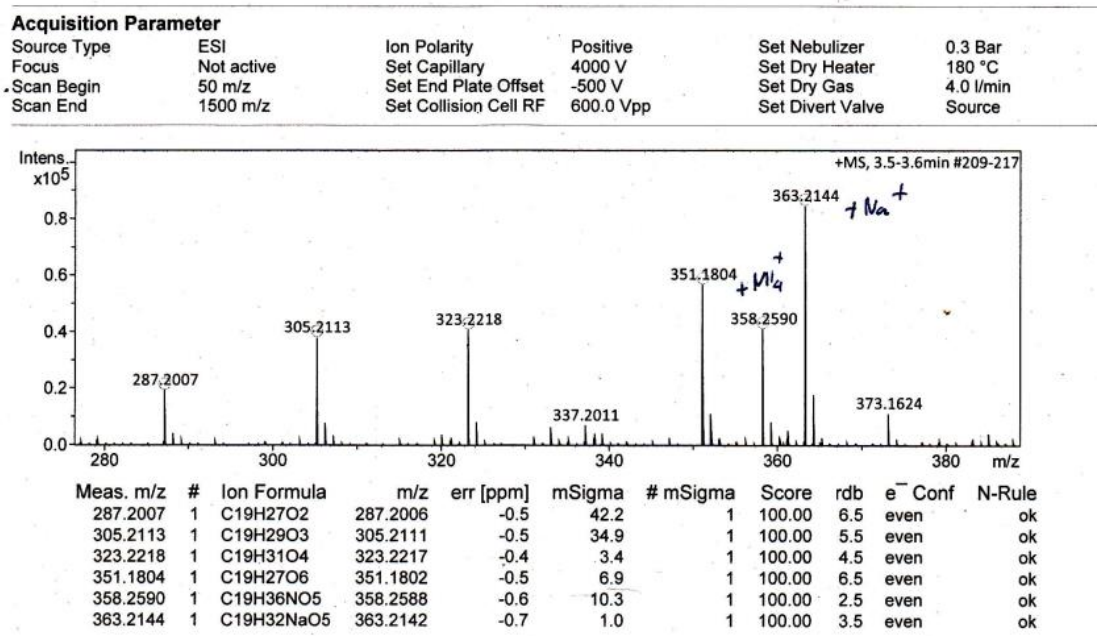


Figure S69. The ROESY (600 MHz, DMSO-d_6) spectrum of compound **9**.



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
287.2007	1	C19H27O2	287.2006	-0.5	42.2	1	100.00	6.5	even	ok
305.2113	1	C19H29O3	305.2111	-0.5	34.9	1	100.00	5.5	even	ok
323.2218	1	C19H31O4	323.2217	-0.4	3.4	1	100.00	4.5	even	ok
351.1804	1	C19H27O6	351.1802	-0.5	6.9	1	100.00	6.5	even	ok
358.2590	1	C19H36NO5	358.2588	-0.6	10.3	1	100.00	2.5	even	ok
363.2144	1	C19H32NaO5	363.2142	-0.7	1.0	1	100.00	3.5	even	ok

Figure S70. The HREISMS of compound **15**.

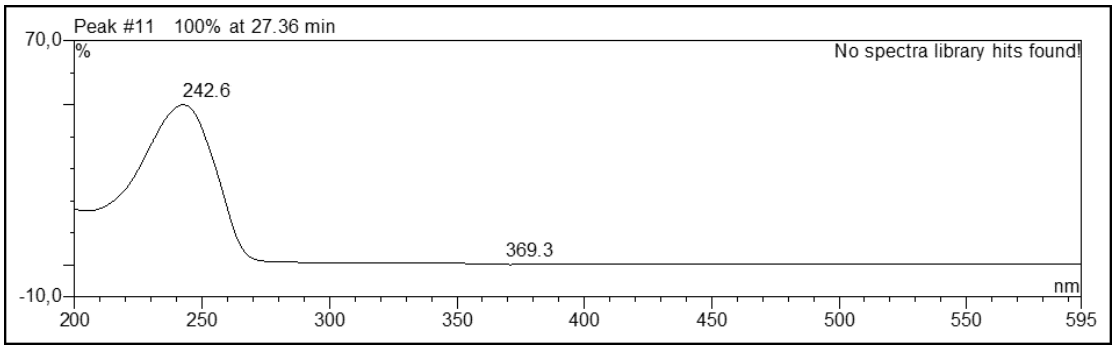


Figure S71. The UV spectrum of compound **15**.

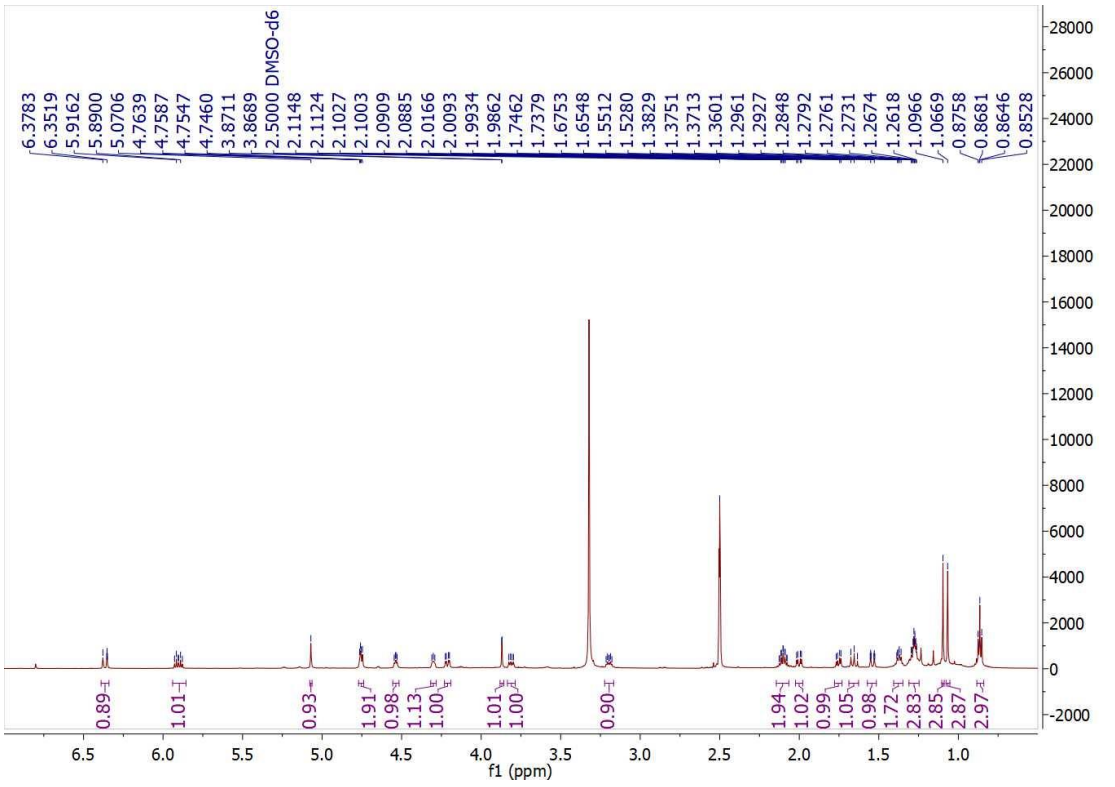


Figure S72. The ^{1}H-NMR (600 MHz, DMSO-d_6) spectrum of compound **15**.

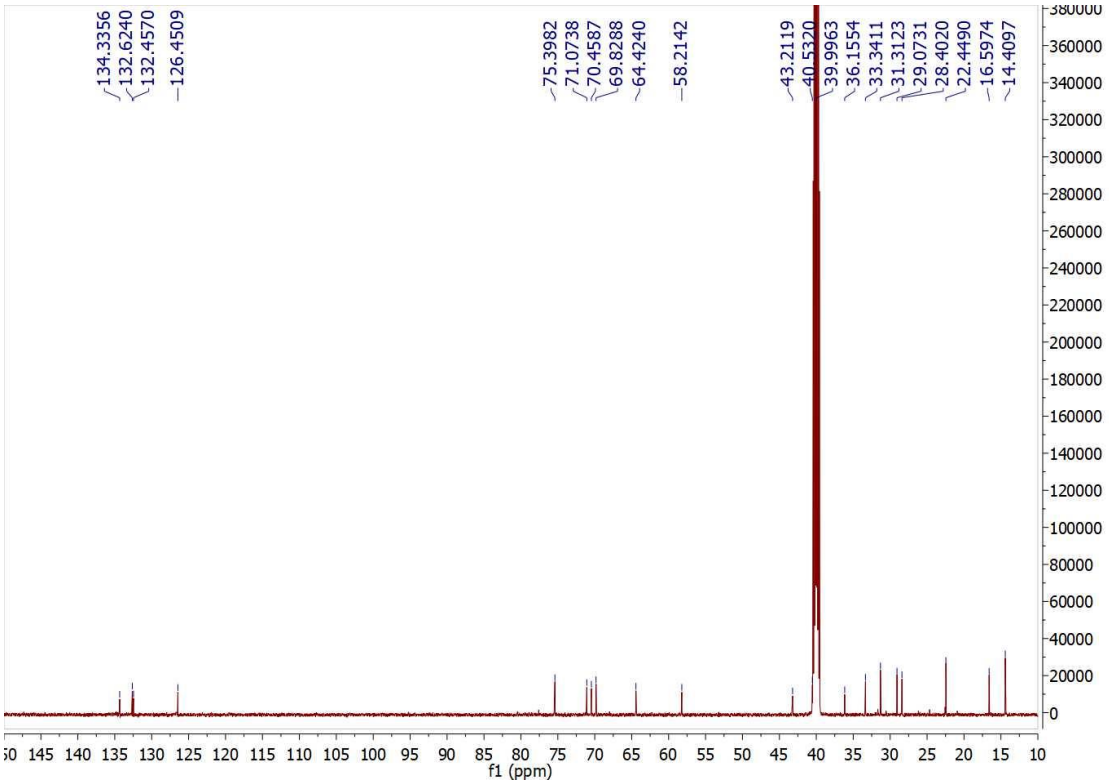


Figure S73. The ^{13}C-NMR (150 MHz, DMSO-d_6) spectrum of compound **15**.

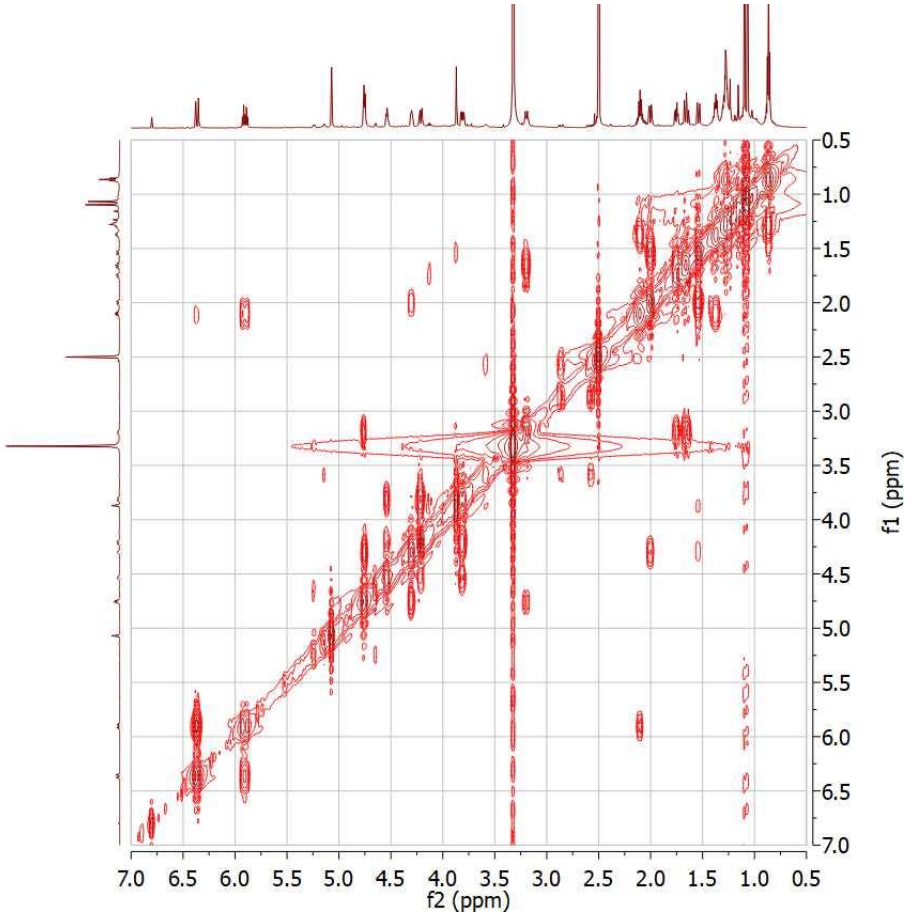


Figure S74. The ^{1}H-^{1}H COSY (600 MHz, DMSO-d_6) spectrum of compound **15**.

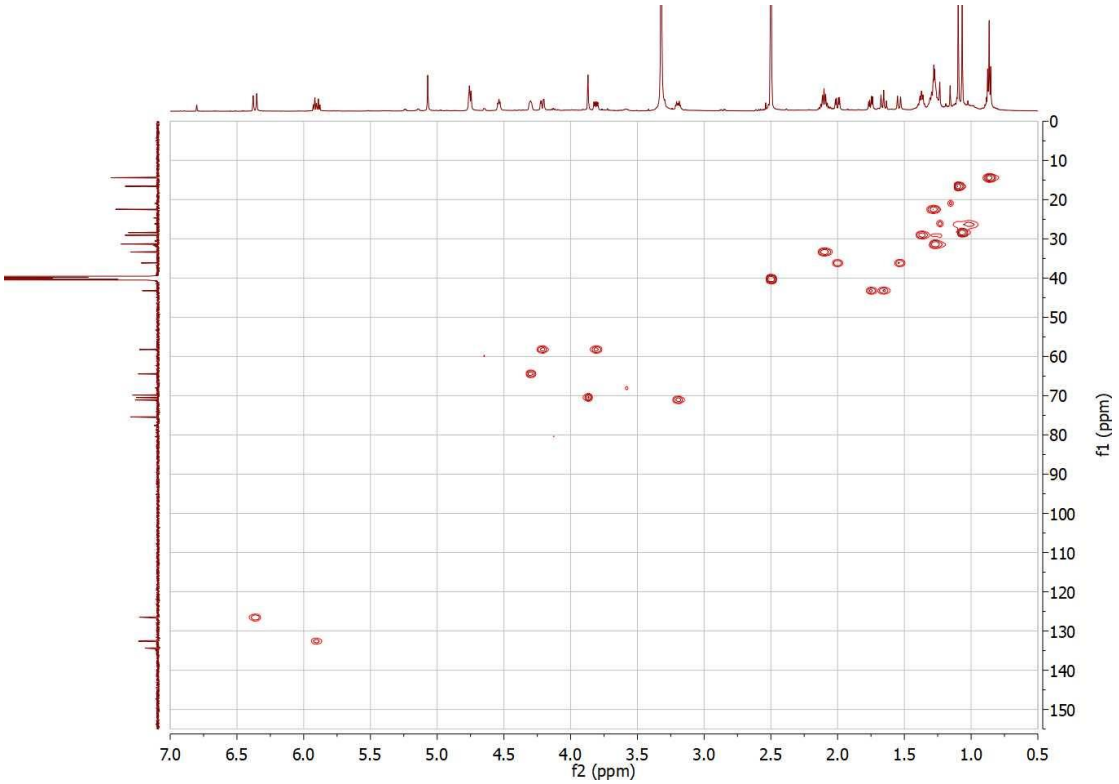


Figure S75. The HSQC (600 MHz, DMSO-d_6) spectrum of compound **15**.

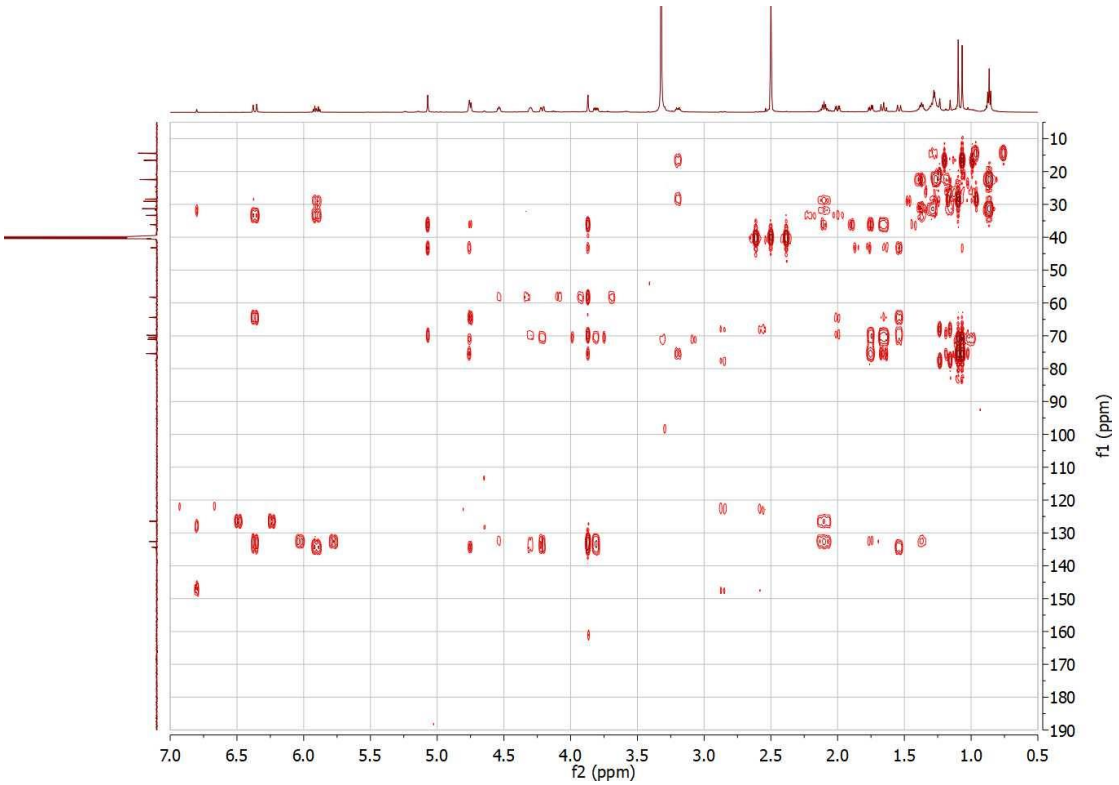


Figure S76. The HMBC (600 MHz, DMSO-d_6) spectrum of compound **15**.

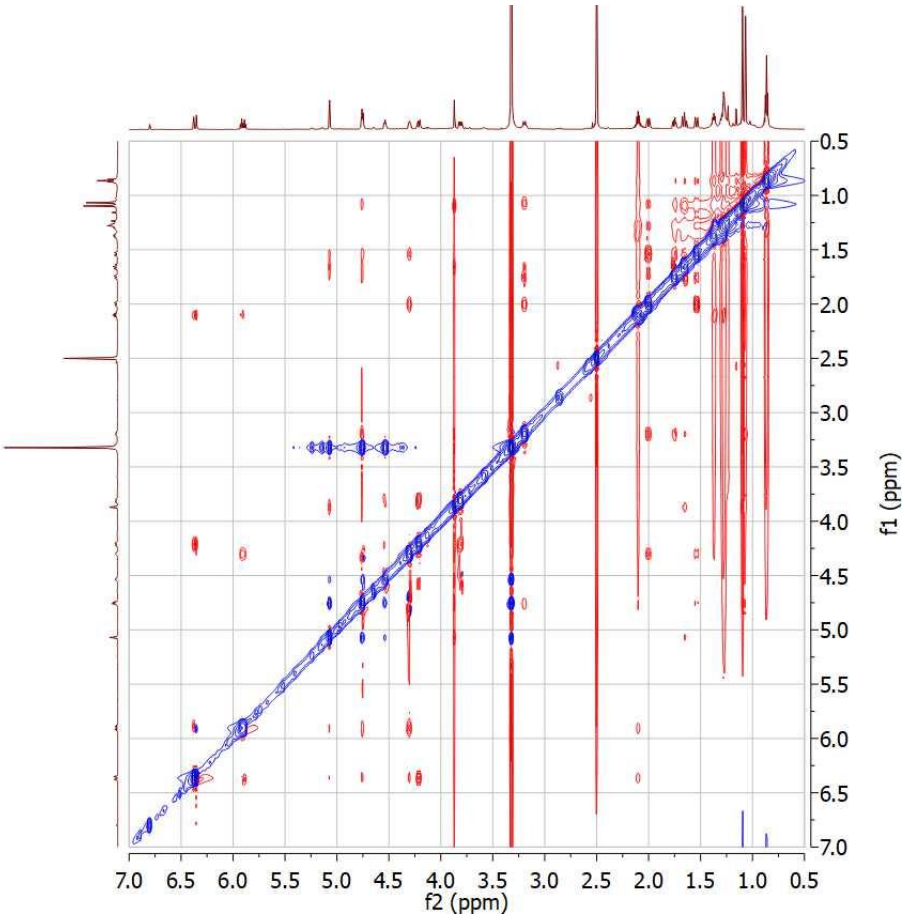


Figure S77. The ROESY (600 MHz, DMSO-d_6) spectrum of compound **15**.

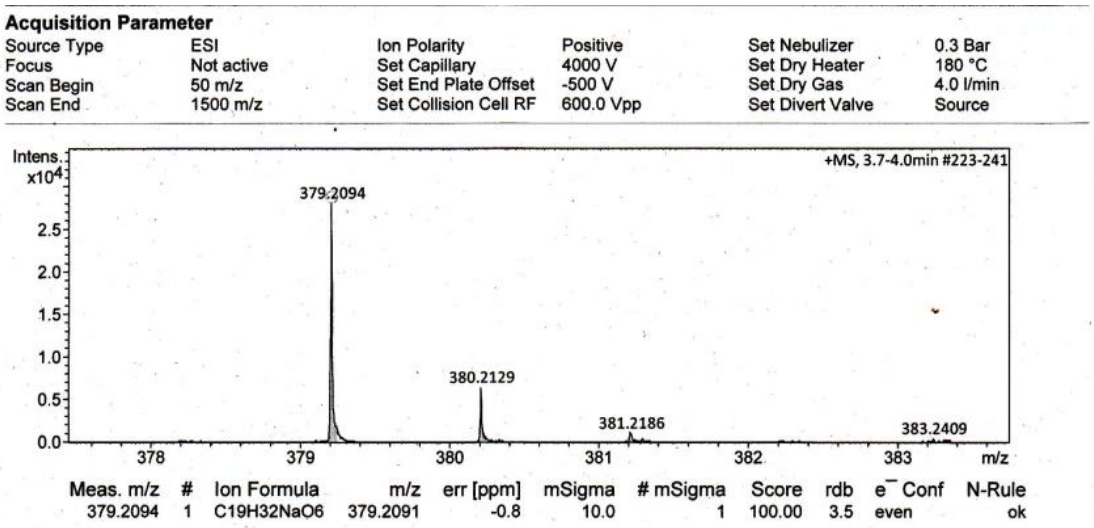


Figure S78. The HREISMS of compound **16**.

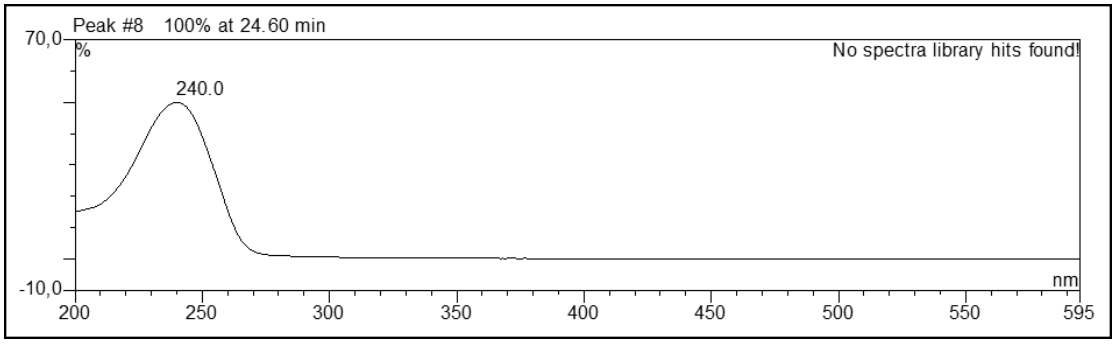


Figure S79. The UV spectrum of compound **16**.

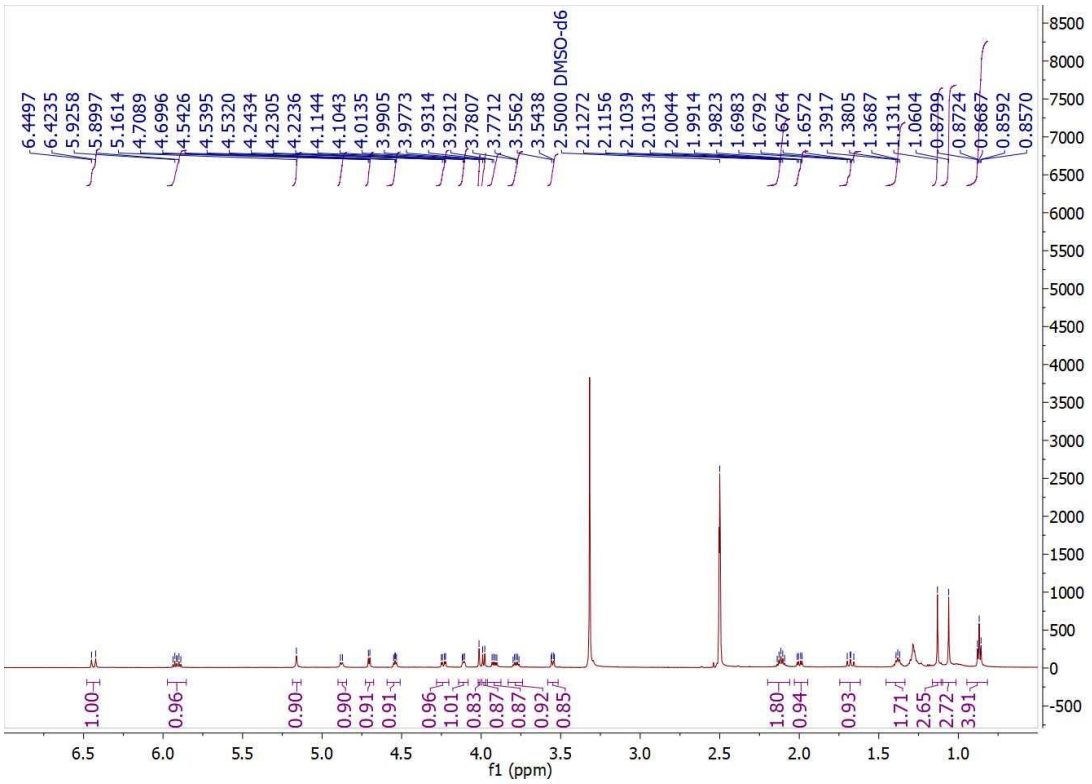


Figure S80. The ^{1}H-NMR (600 MHz, DMSO-d_6) spectrum of compound **16**.

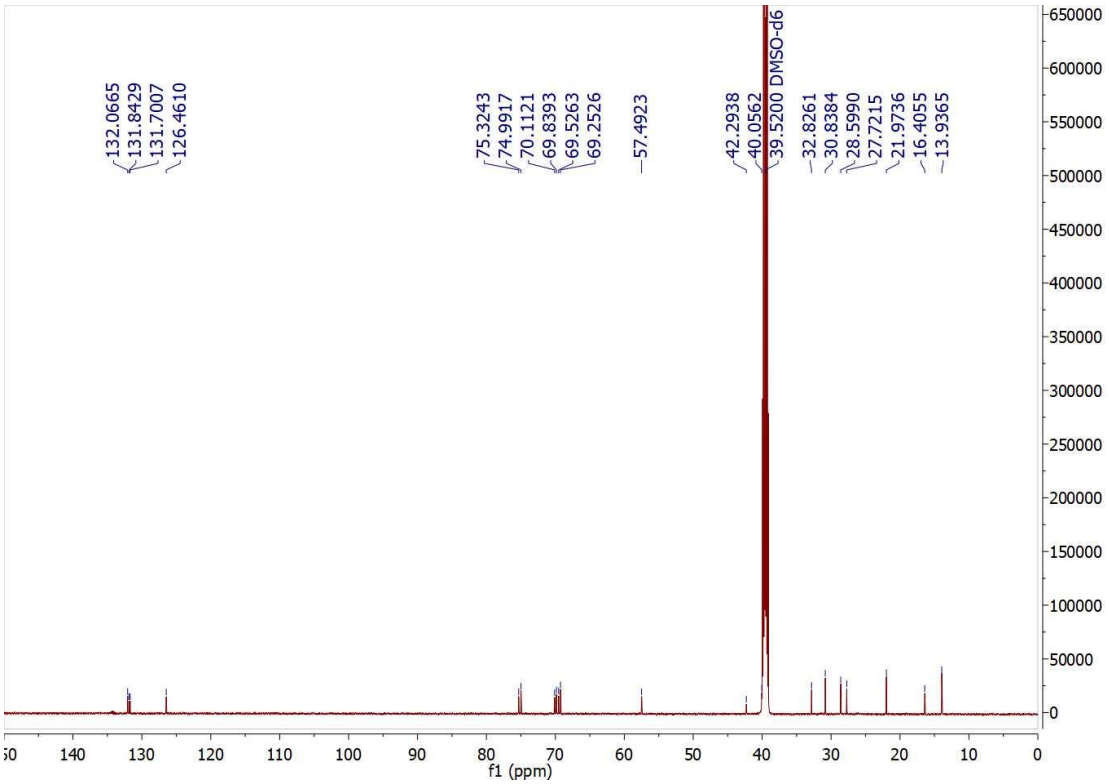


Figure S81. The ^{13}C-NMR (150 MHz, DMSO-d_6) spectrum of compound **16**.

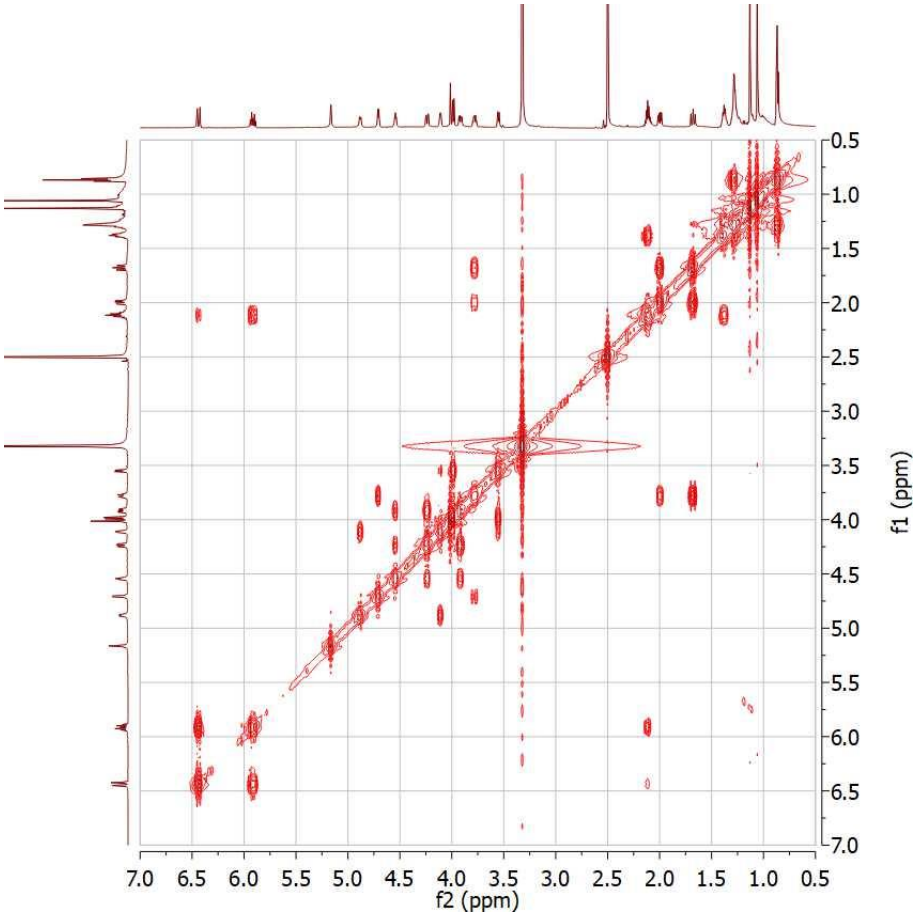


Figure S82. The ^{1}H-^{1}H COSY (600 MHz, DMSO-d_6) spectrum of compound **16**.

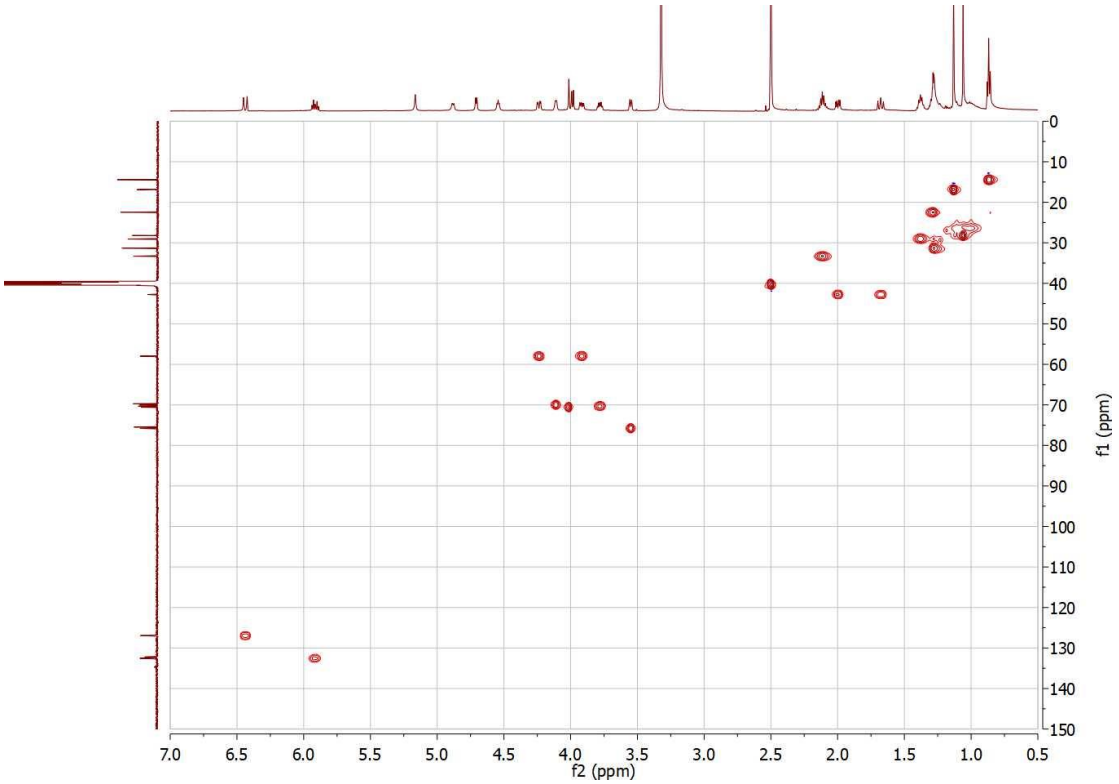


Figure S83. The HSQC (600 MHz, DMSO-d_6) spectrum of compound **16**.

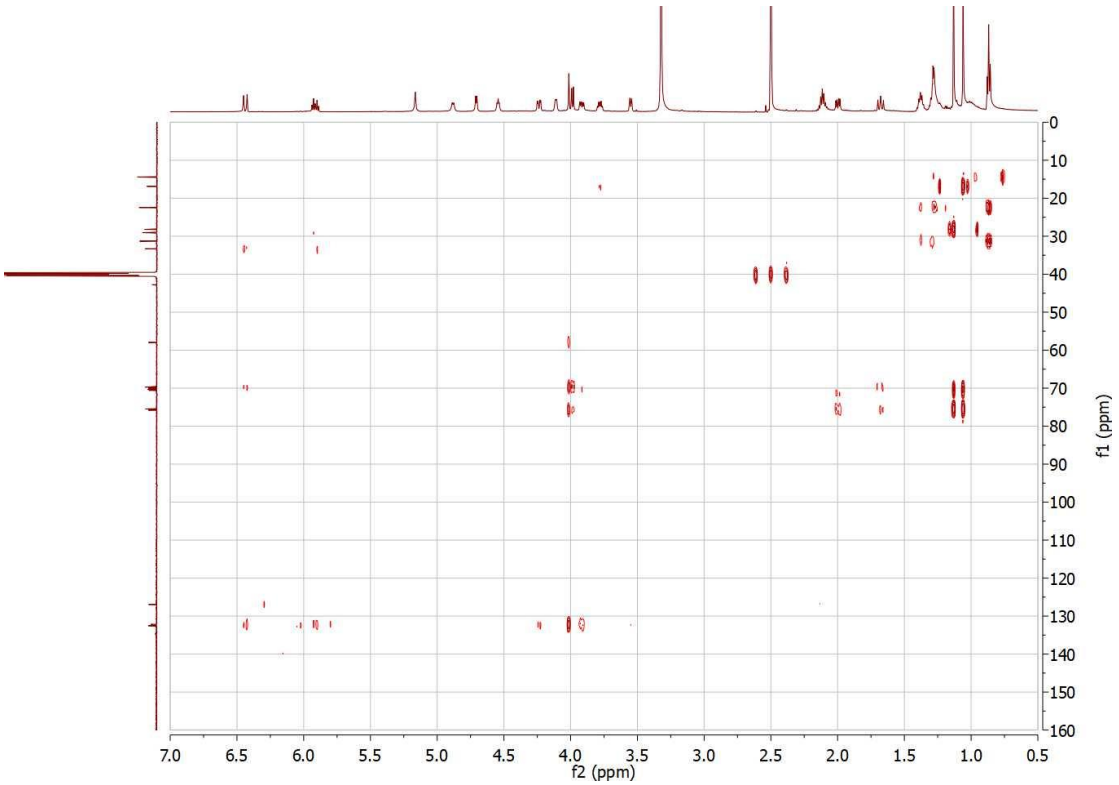


Figure S84. The HMBC (600 MHz, DMSO-d_6) spectrum of compound **16**.

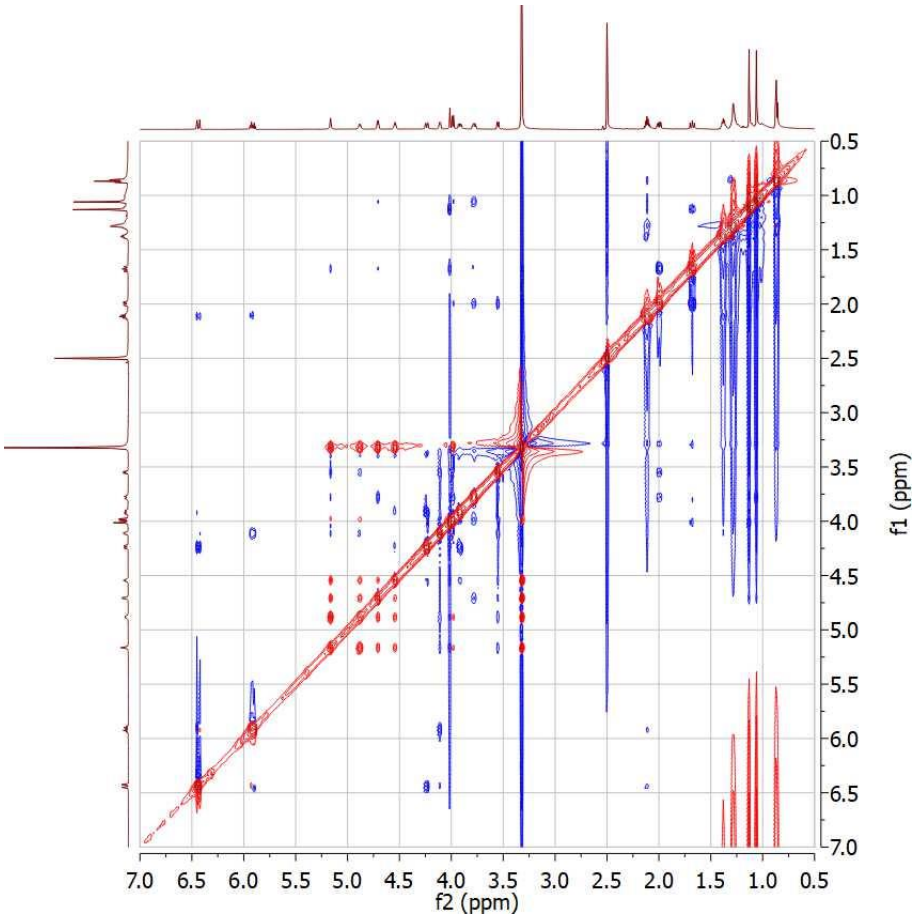
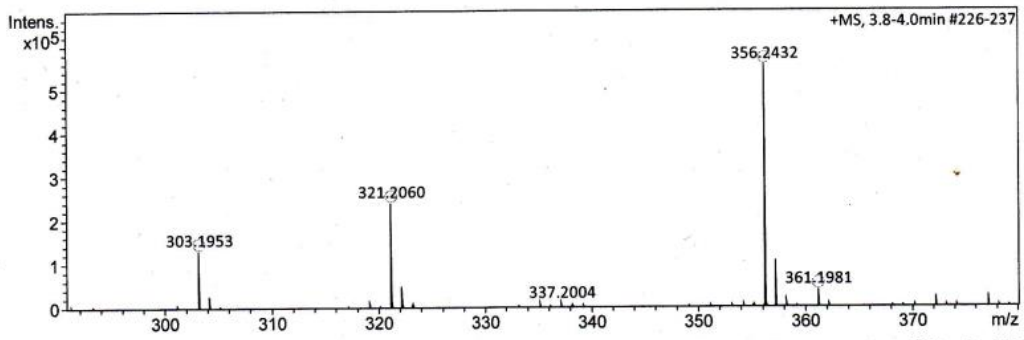


Figure S85. The ROESY (600 MHz, DMSO-d_6) spectrum of compound **16**.

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
303.1953	1	C19H27O3	303.1955	0.5	6.3	1	100.00	6.5	even	ok
321.2060	1	C19H29O4	321.2060	0.1	4.9	1	100.00	5.5	even	ok
	2	C18H26N4Na	321.2050	-3.3	7.5	2	57.53	7.5	even	ok
	3	C20H25N4	321.2074	4.2	18.5	3	38.70	10.5	even	ok
356.2432	1	C19H34NO5	356.2431	-0.2	13.3	1	100.00	3.5	even	ok
	2	C18H31N5NaO	356.2421	-3.2	14.5	2	57.33	5.5	even	ok

Figure S86. The HREISMS of compound **17**.

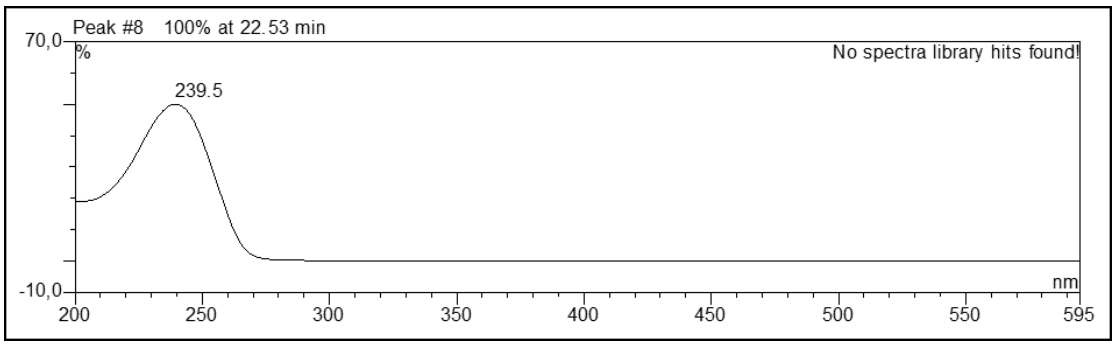


Figure S87. The UV spectrum of compound **17**.

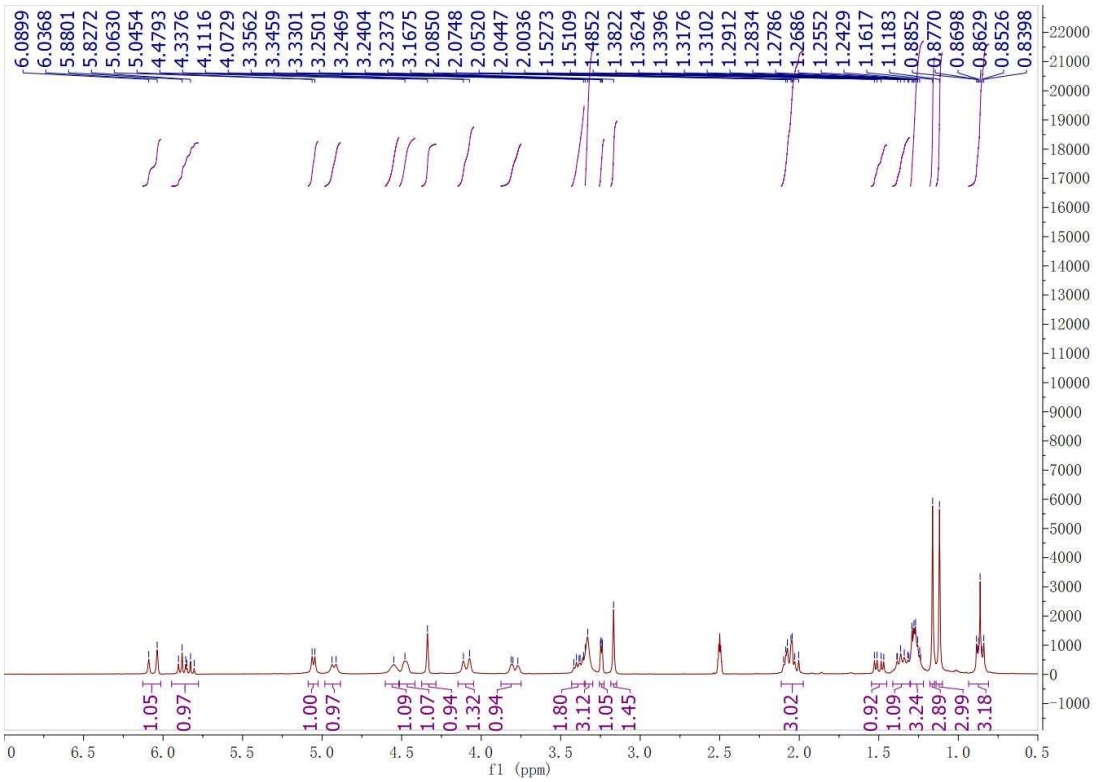


Figure S88. The ^{1}H-NMR (300 MHz, DMSO-d_6) spectrum of compound **17**.

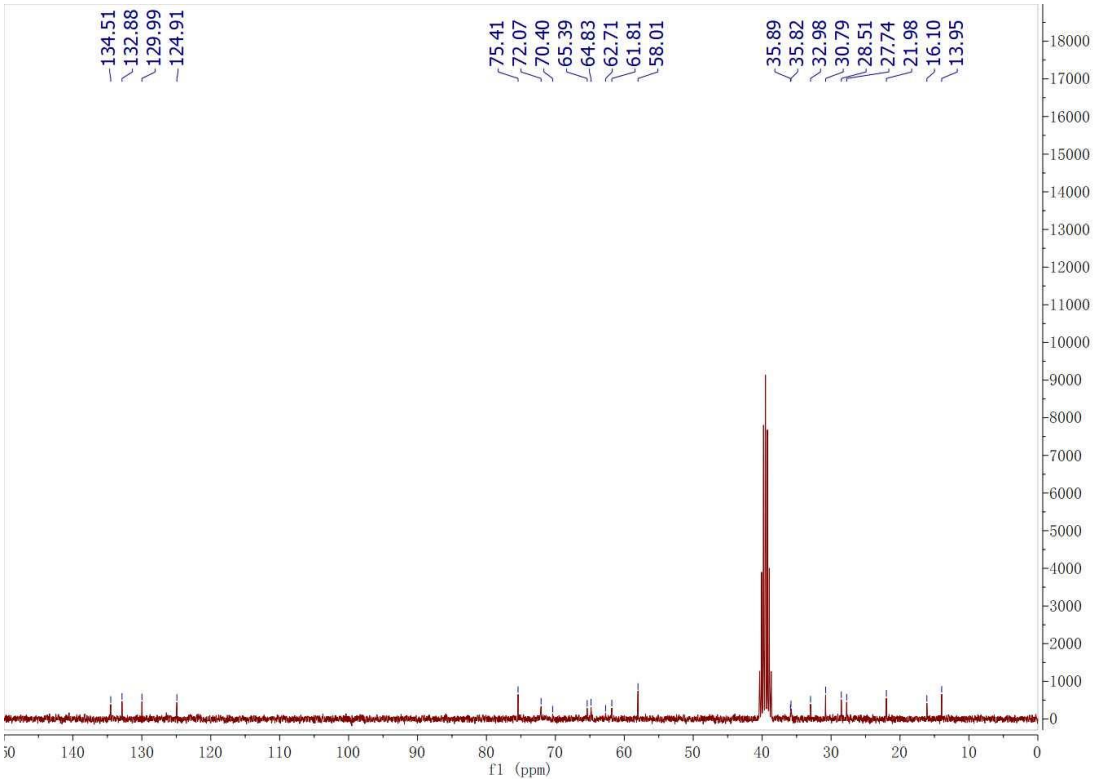


Figure S89. The ^{13}C-NMR (75 MHz, DMSO-d_6) spectrum of compound **17**.

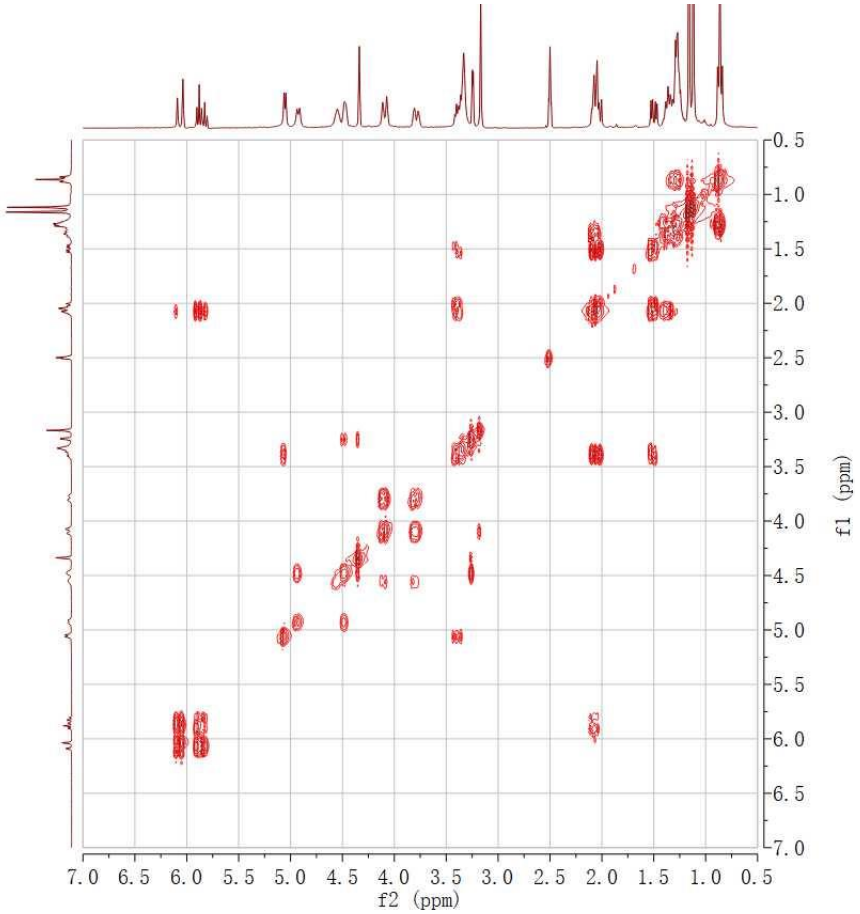


Figure S90. The ^{1}H-^{1}H COSY (300 MHz, DMSO-d_6) spectrum of compound **17**.

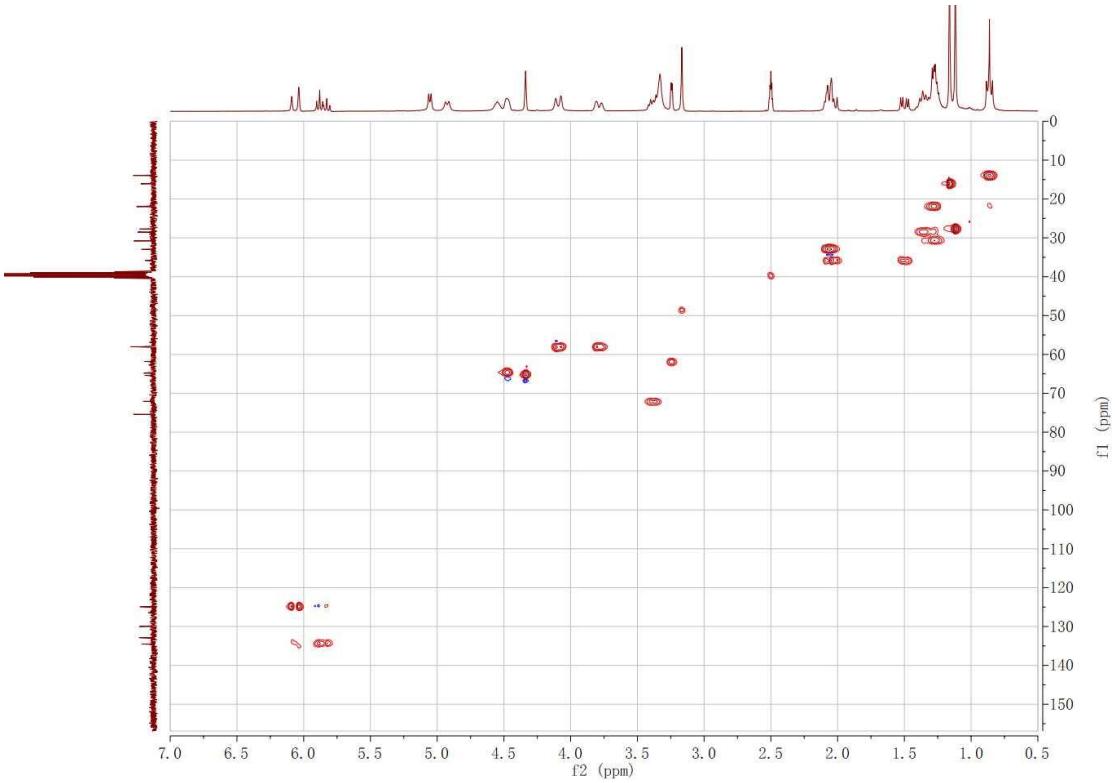


Figure S91. The HSQC (300 MHz, DMSO-d_6) spectrum of compound **17**.

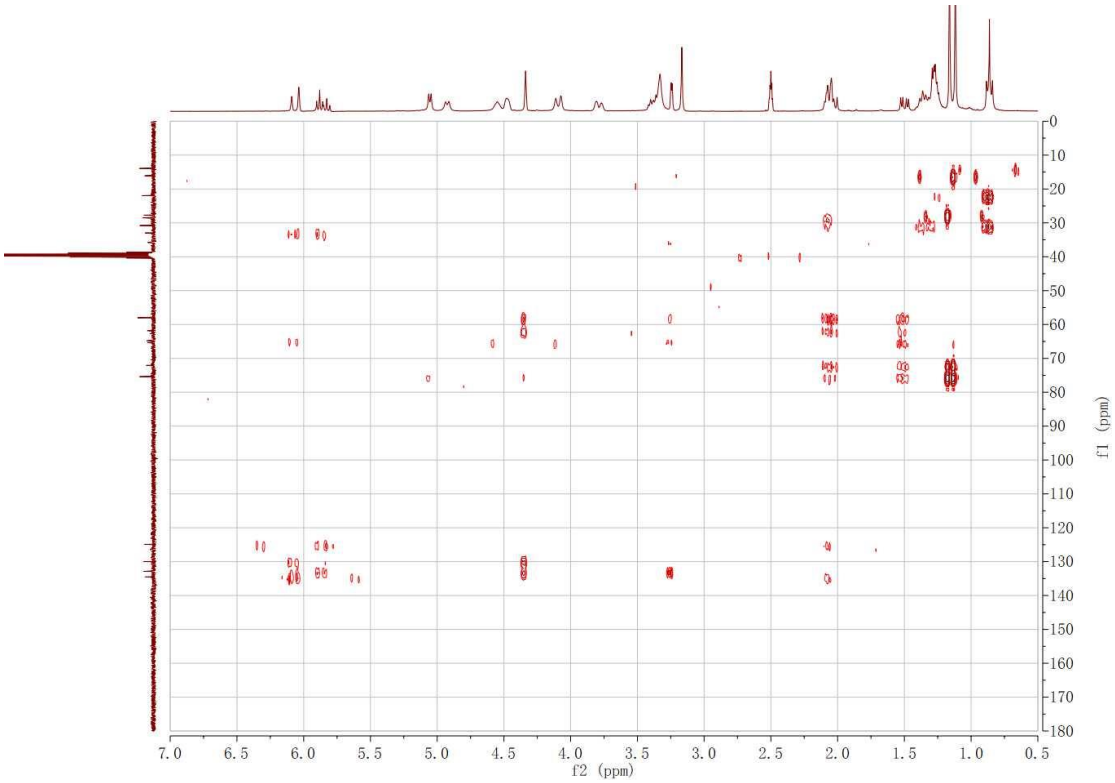


Figure S92. The HMBC (300 MHz, DMSO-d_6) spectrum of compound **17**.

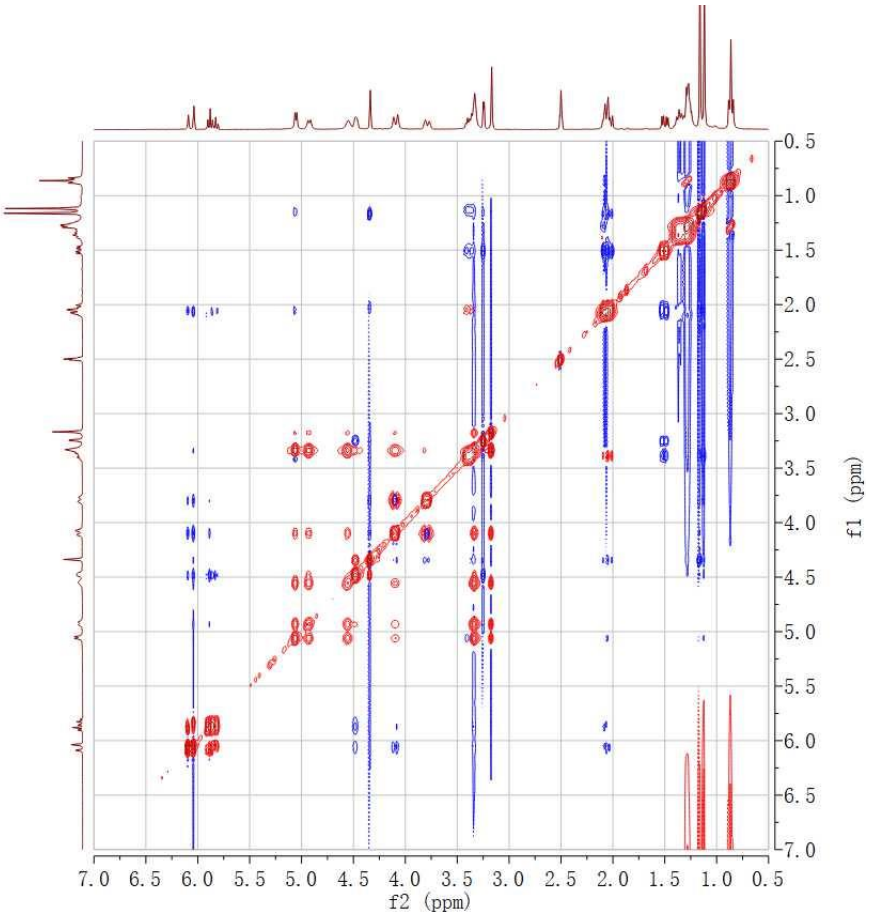


Figure S93. The ROESY (300 MHz, DMSO-d_6) spectrum of compound **17**.

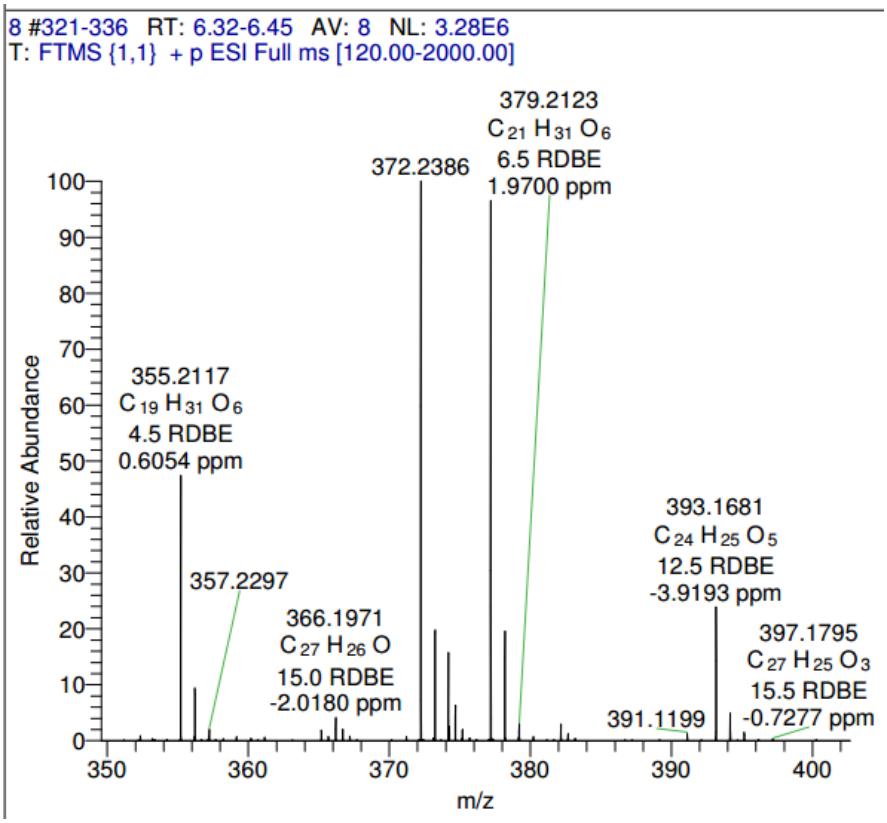


Figure S94. The HREISMS of compound **18**.

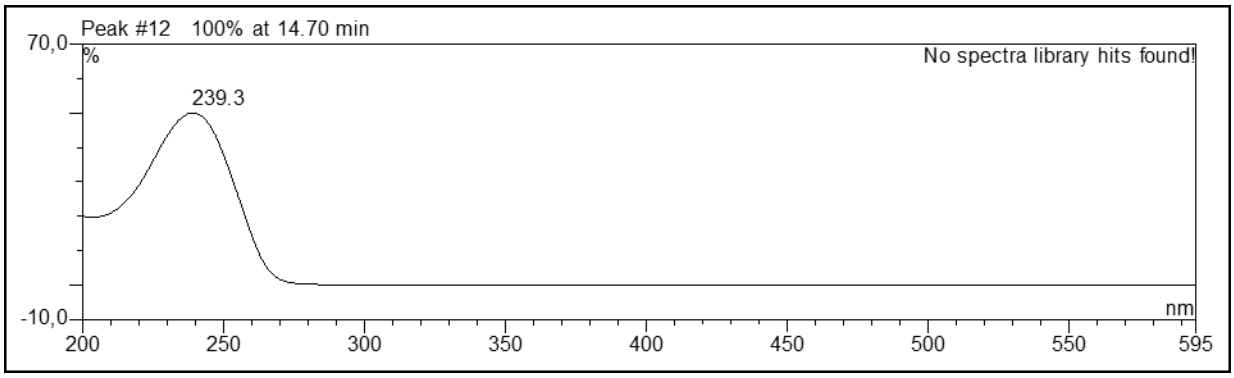


Figure S95. The UV spectrum of compound **18**.

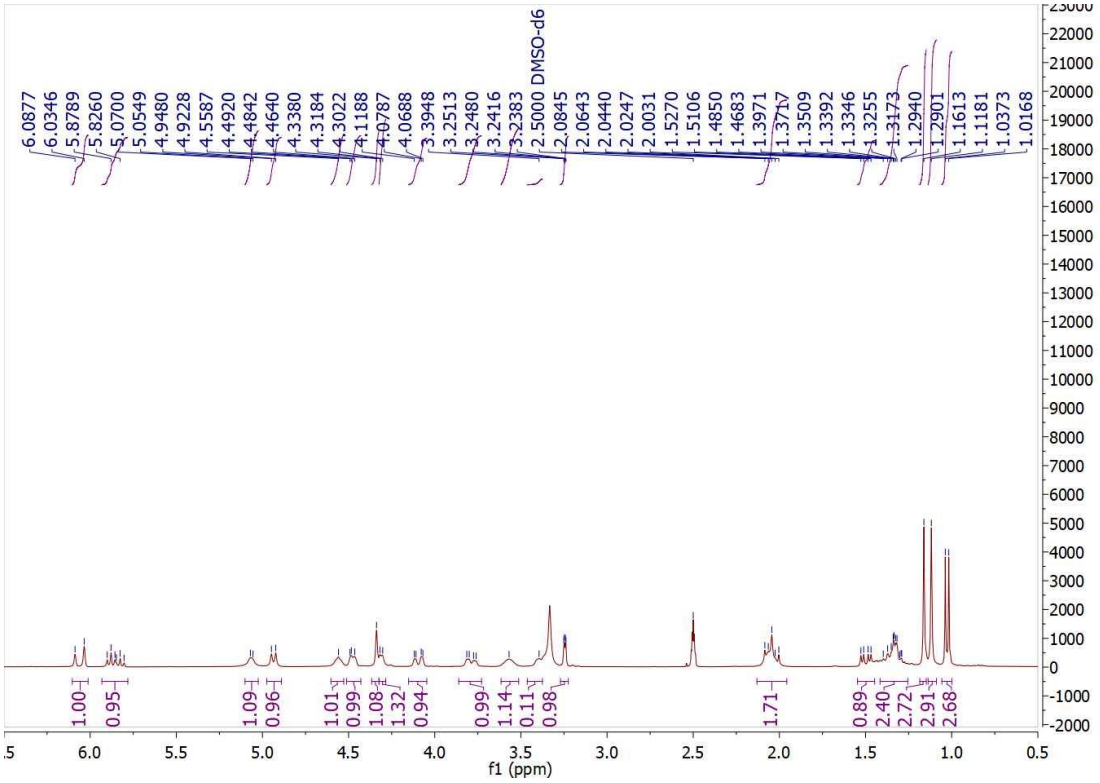


Figure S96. The ^{1}H-NMR (300 MHz, DMSO-d_6) spectrum of compound **18**.

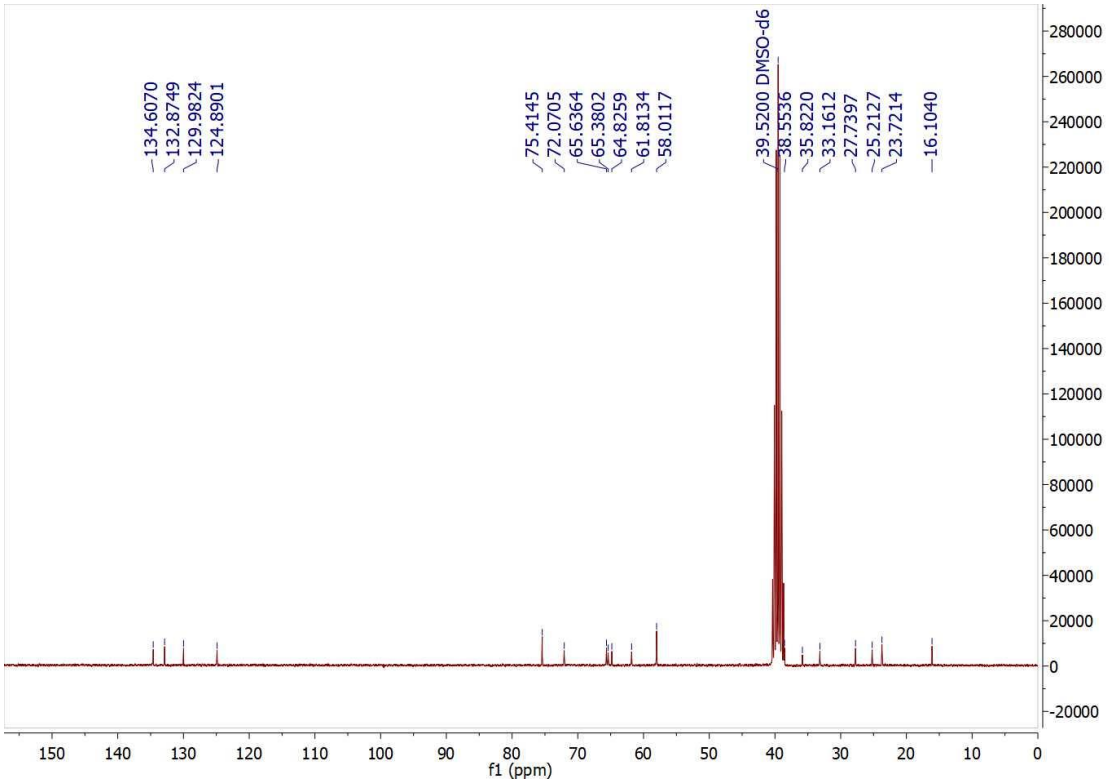


Figure S97. The ^{13}C-NMR (75 MHz, DMSO-d_6) spectrum of compound **18**.

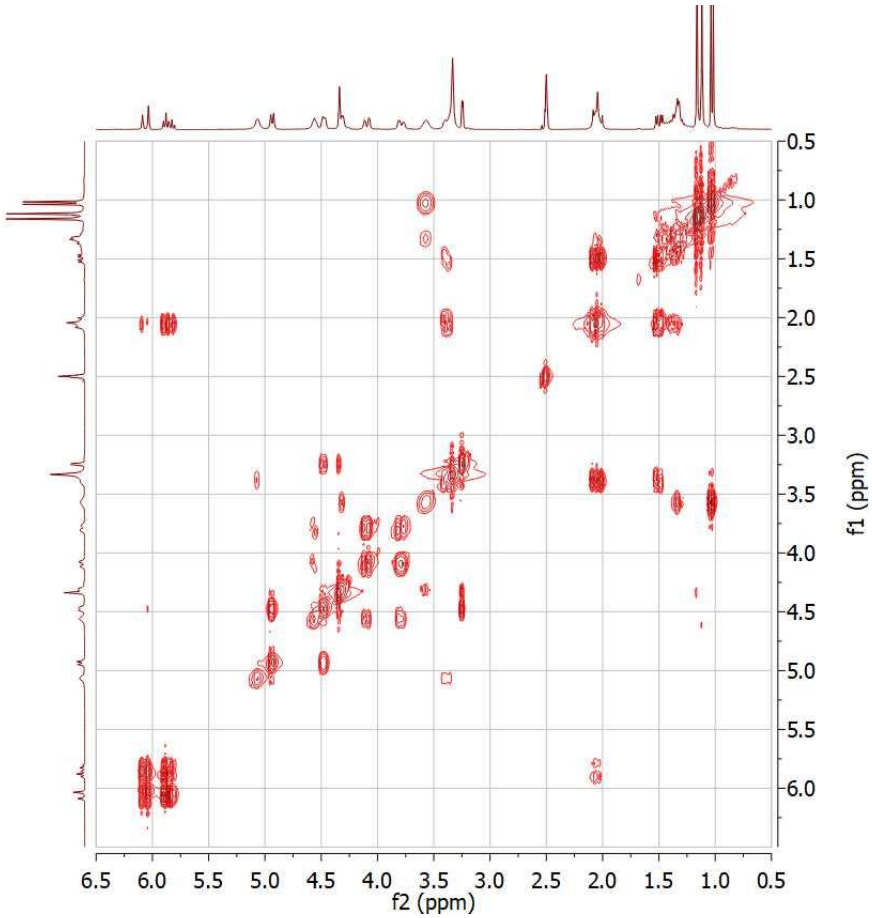


Figure S98. The ^{1}H-^{1}H COSY (300 MHz, DMSO-d_6) spectrum of compound **18**.

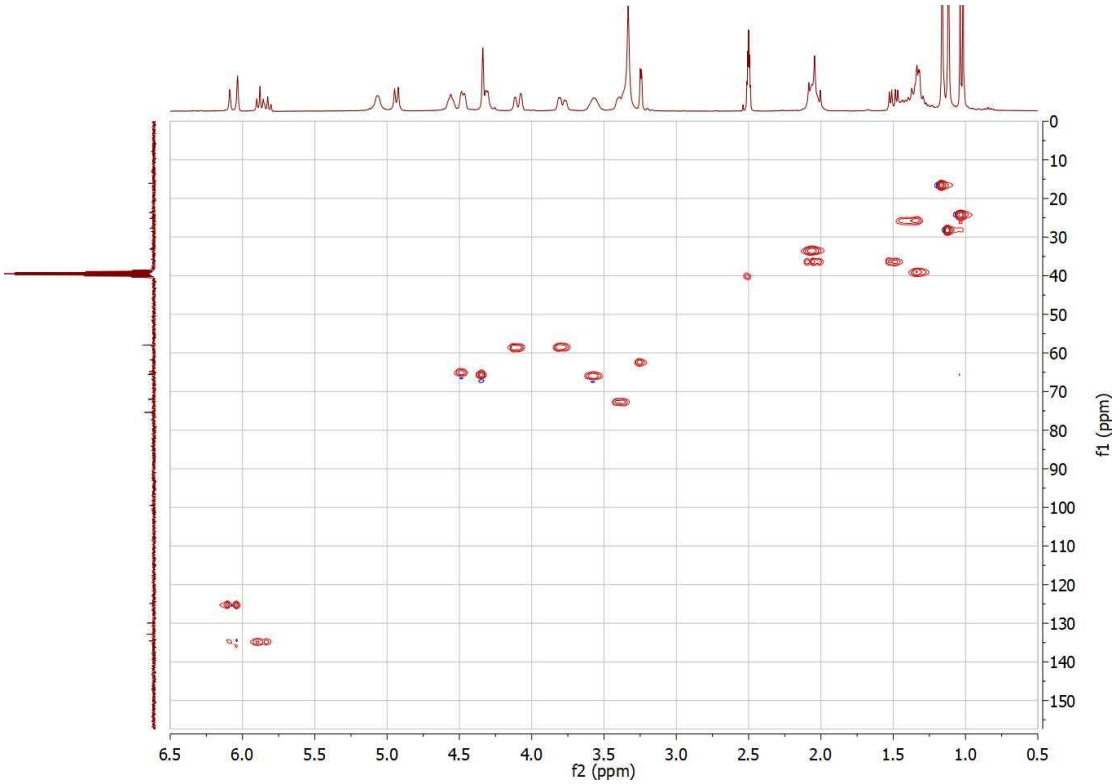


Figure S99. The HSQC (300 MHz, DMSO-d_6) spectrum of compound **18**.

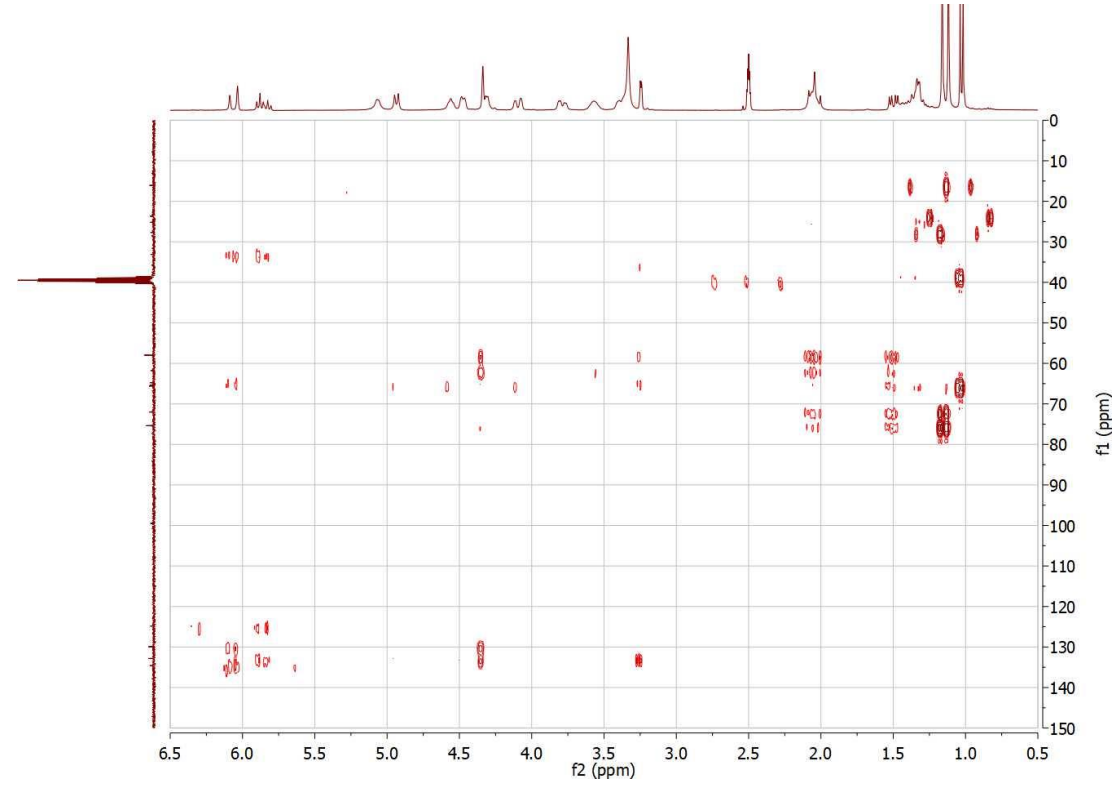


Figure S100. The HMBC (300 MHz, DMSO-d_6) spectrum of compound **18**.

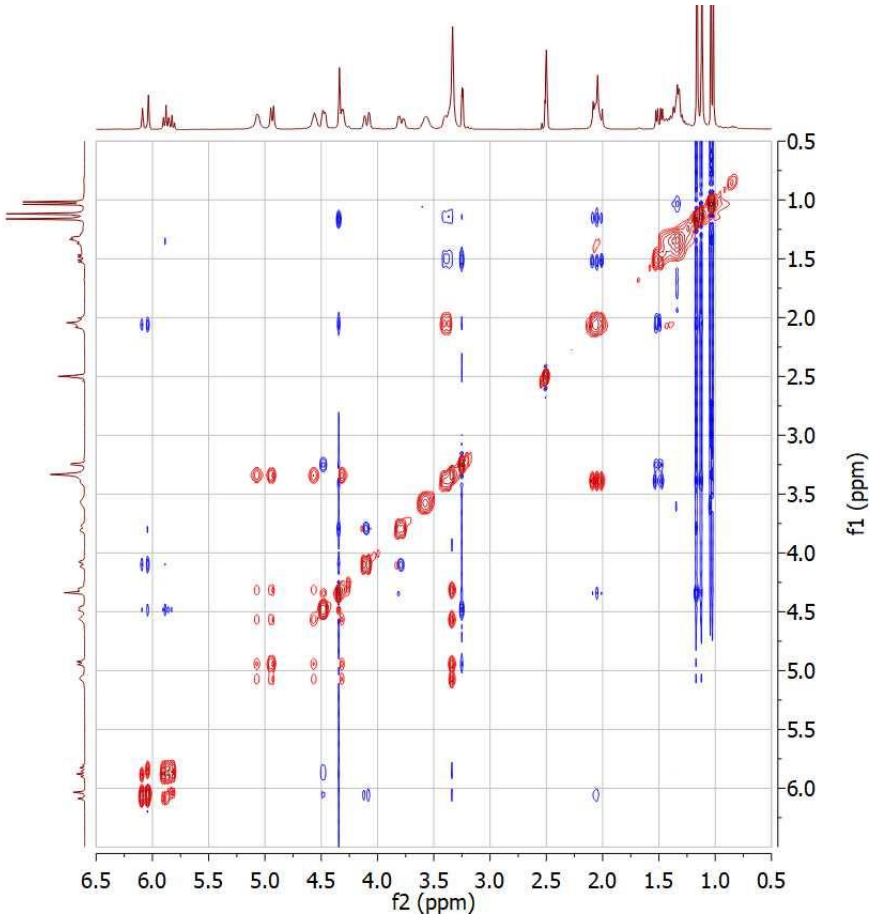


Figure S101. The ROESY (300 MHz, DMSO-d_6) spectrum of compound **18**.

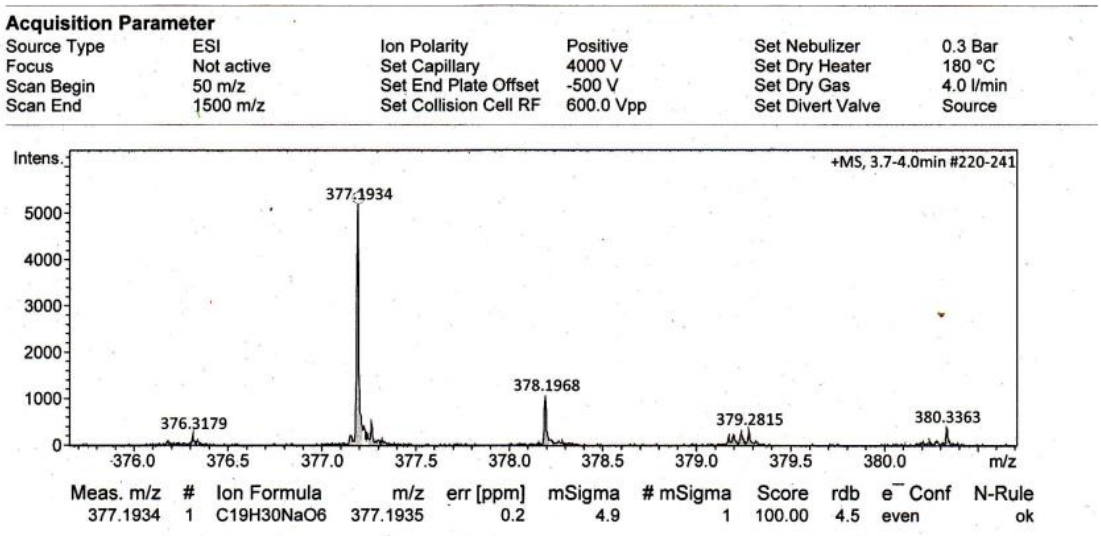


Figure S102. The HREISMS of compound **19**.

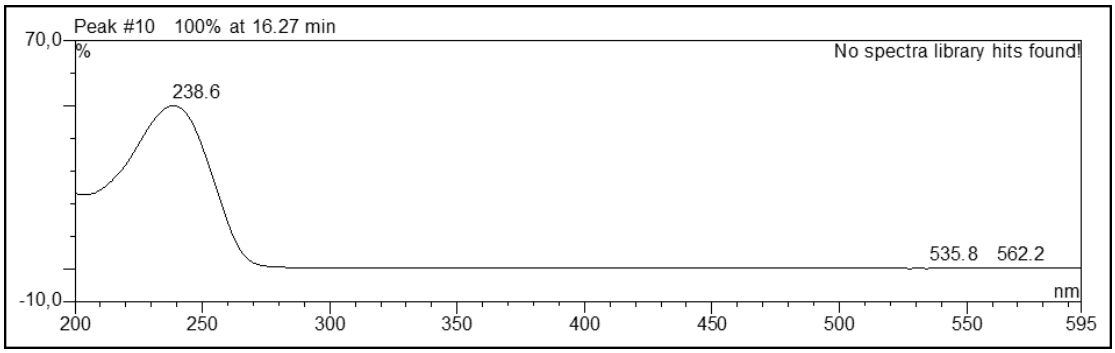


Figure S103. The UV spectrum of compound **19**.

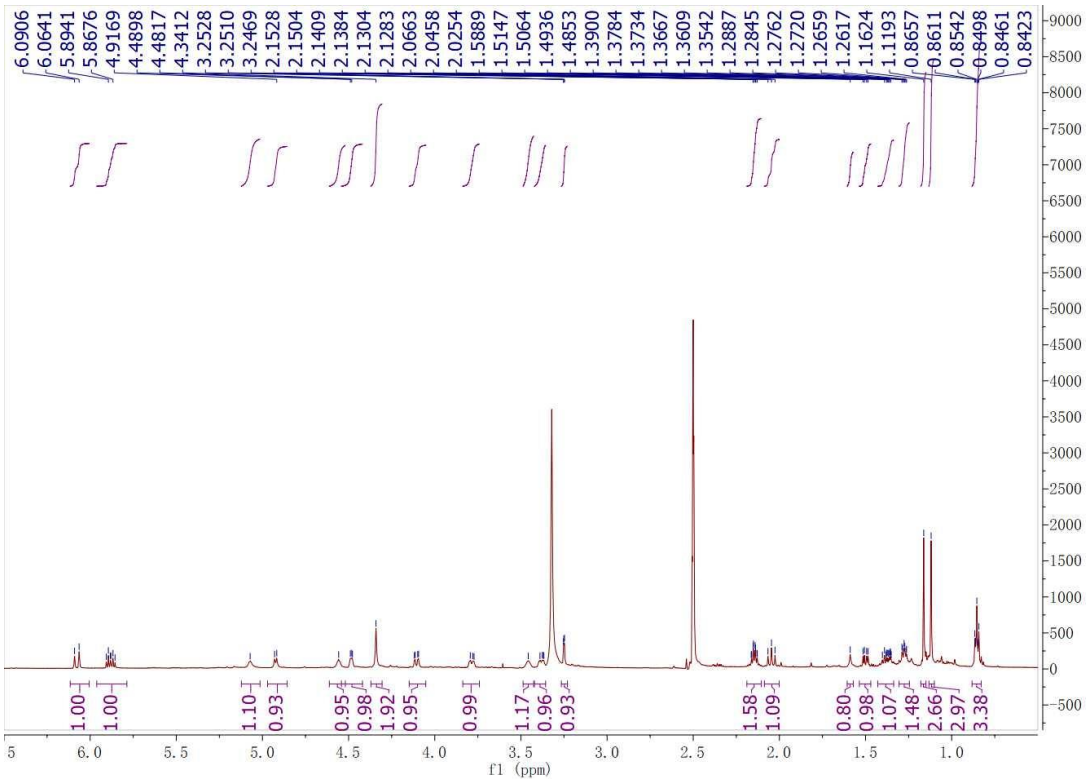


Figure S104. The ^{1}H-NMR (600 MHz, DMSO-d_6) spectrum of compound **19**.

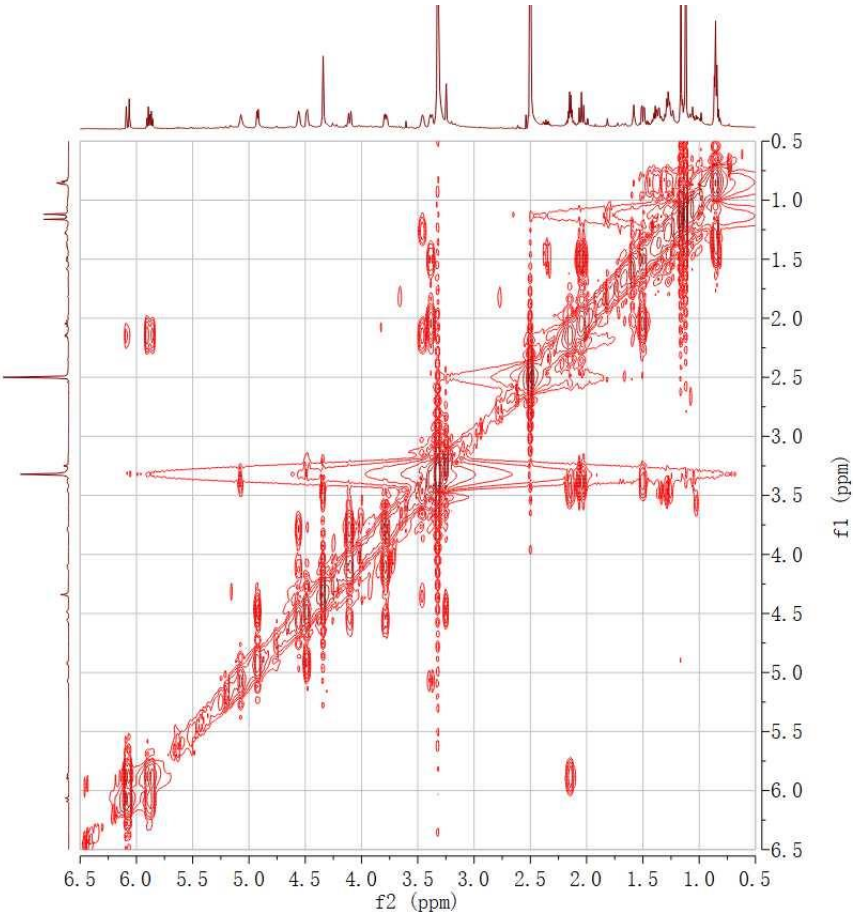


Figure S105. The ^{1}H-^{1}H COSY (600 MHz, DMSO-d_6) spectrum of compound **19**.

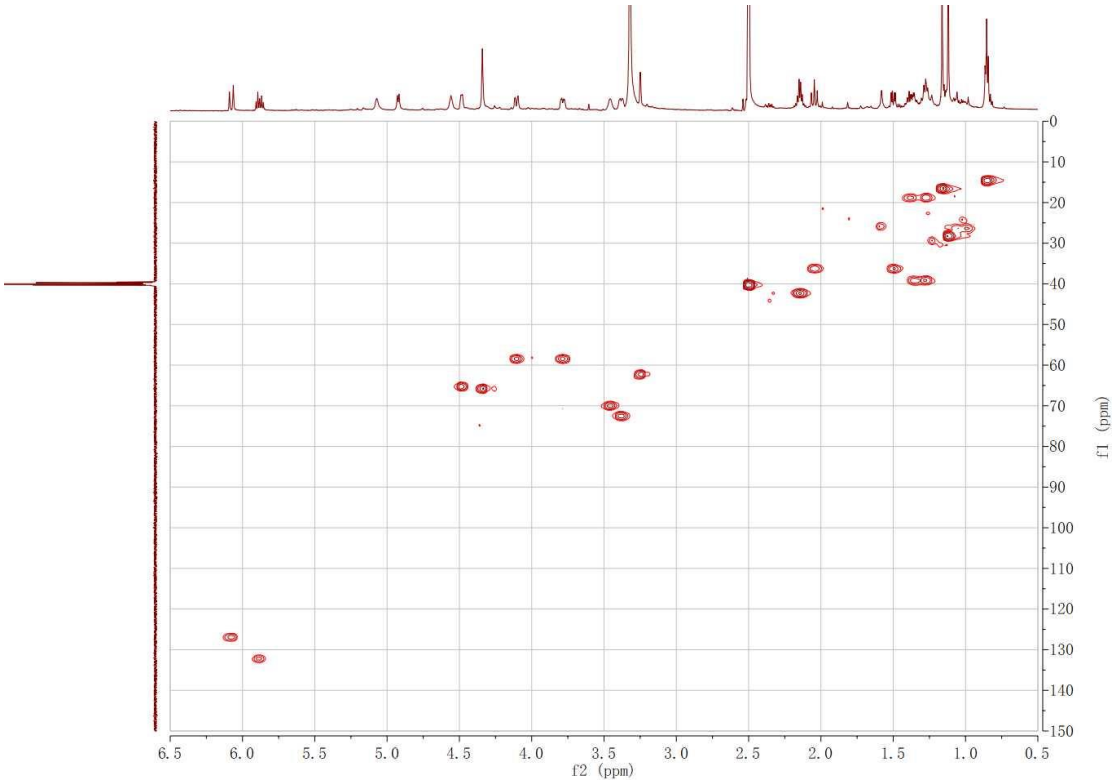


Figure S106. The HSQC (600MHz, DMSO-d_6) spectrum of compound **19**.

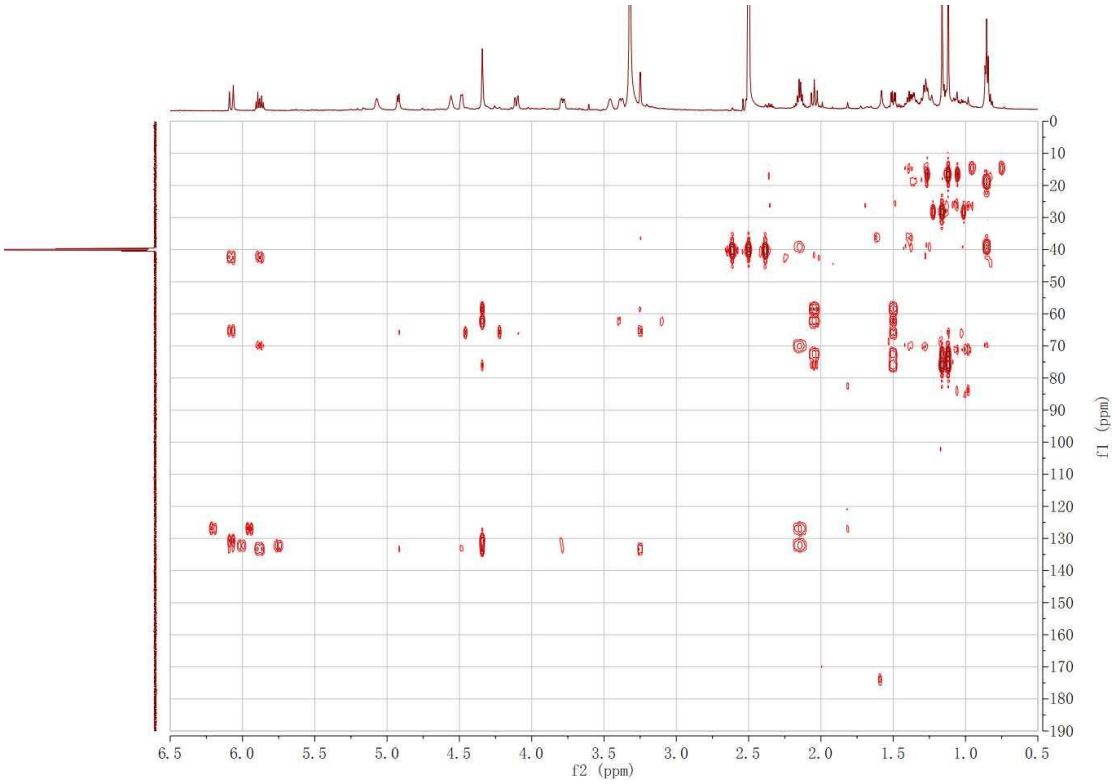


Figure S107. The HMBC (600MHz, DMSO-d_6) spectrum of compound **19**.

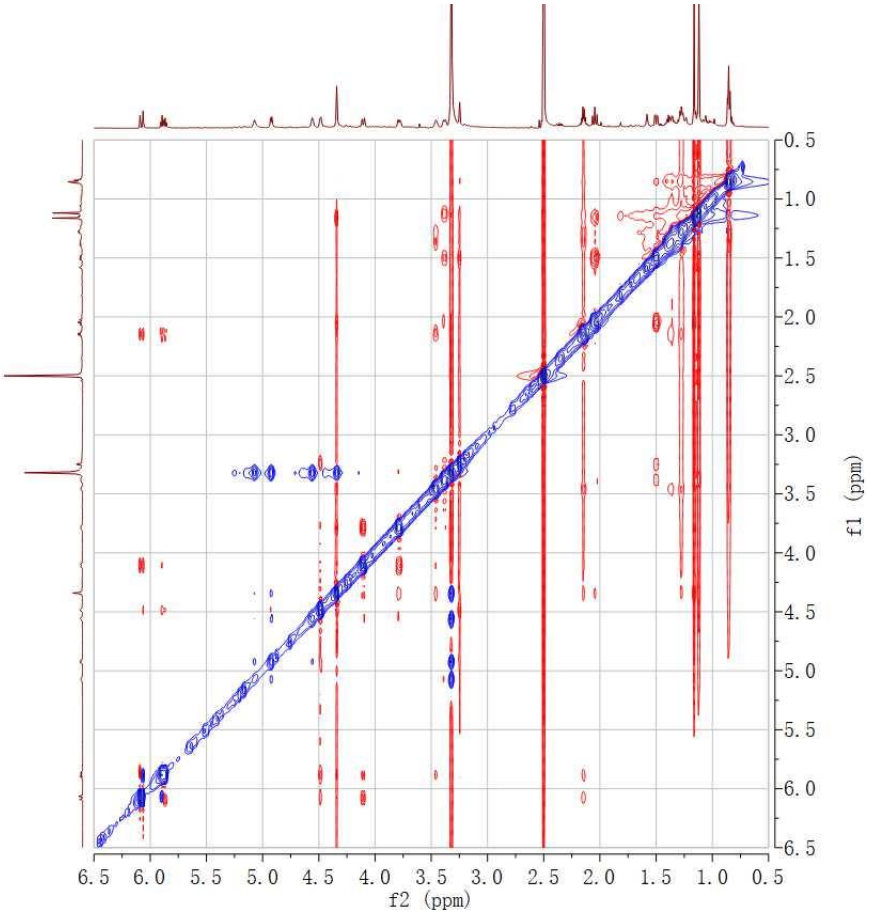


Figure S108. The ROESY (600 MHz, DMSO-d_6) spectrum of compound **19**.

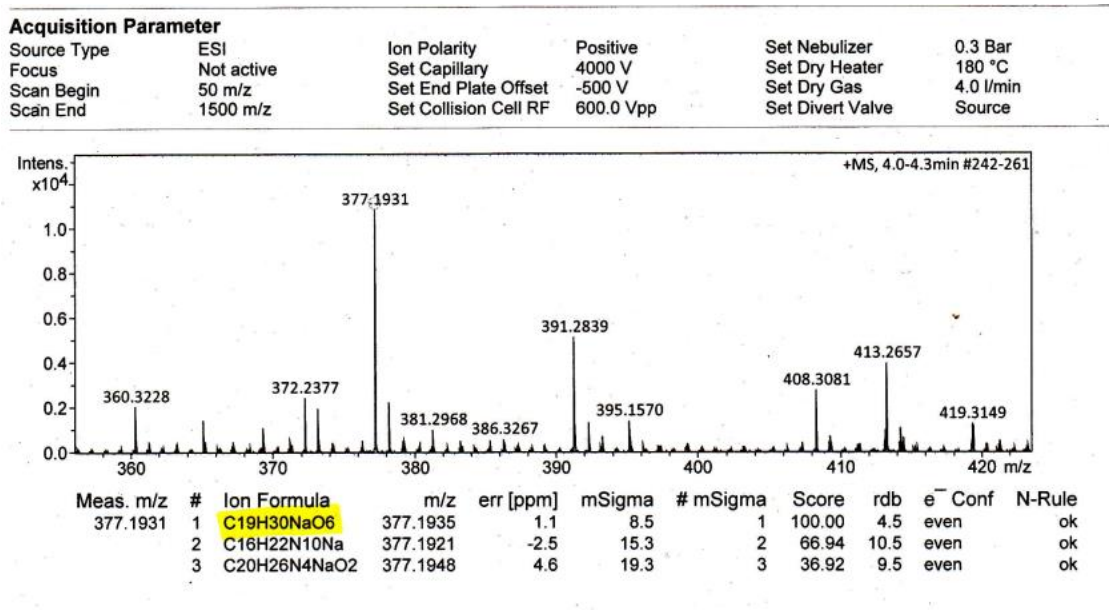


Figure S109. The HREISMS of compound **20**.

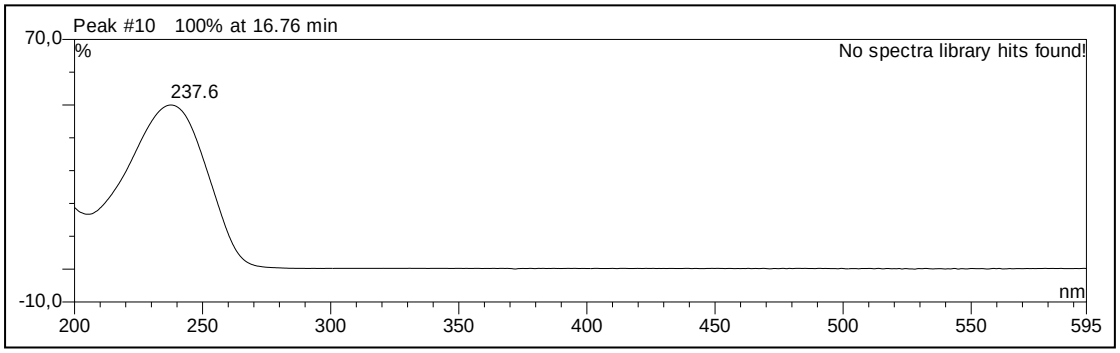


Figure S110. The UV spectrum of compound **20**.

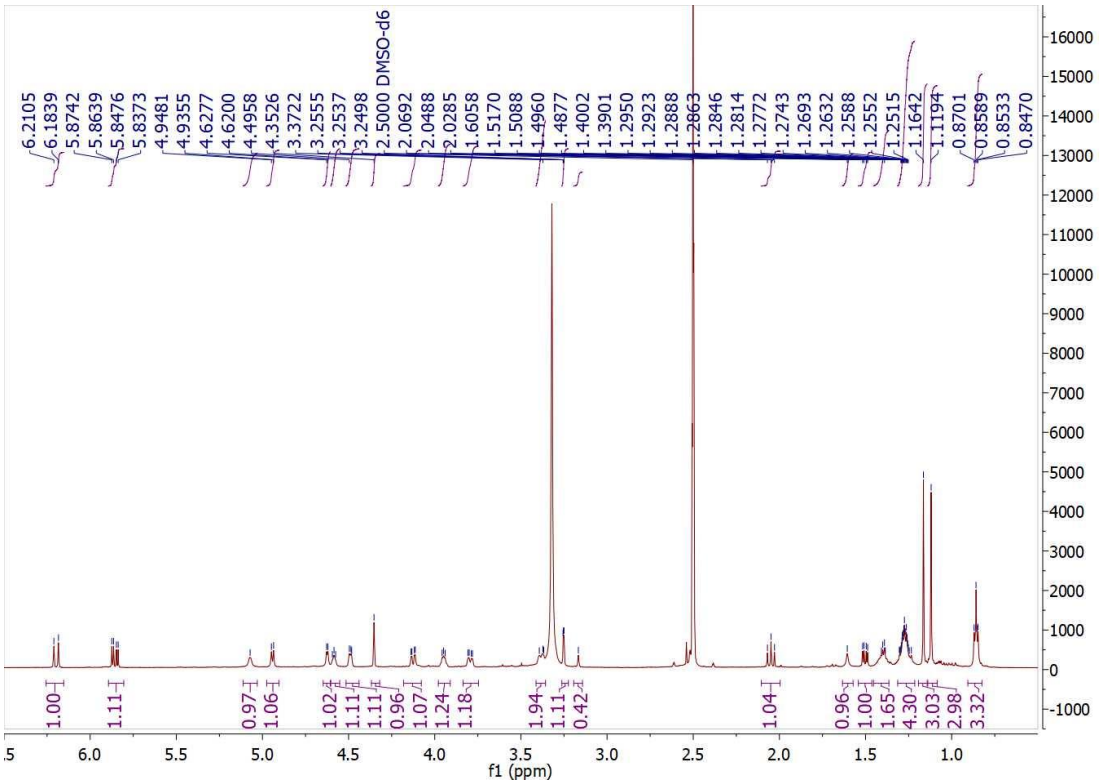


Figure S111. The ^{1}H-NMR (600 MHz, DMSO-d_6) spectrum of compound **20**.

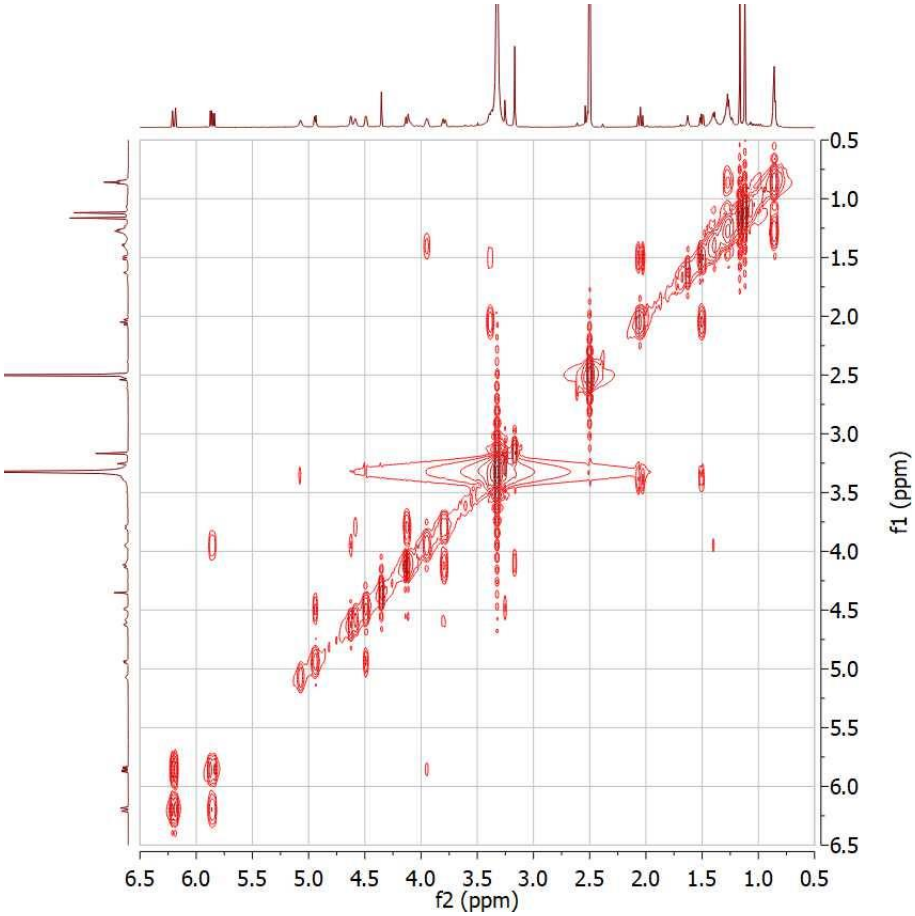


Figure S112. The ^{1}H-^{1}H COSY (600 MHz, DMSO-d_6) spectrum of compound **20**.

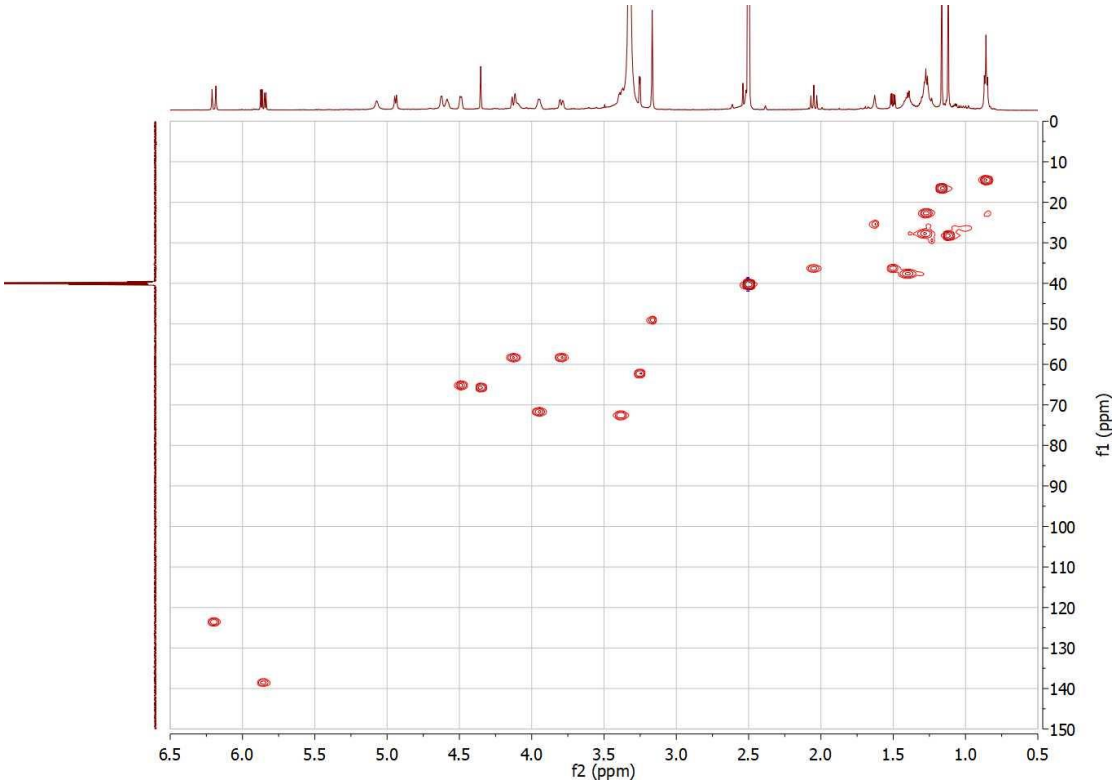


Figure S113. The HSQC (600 MHz, DMSO-d_6) spectrum of compound **20**.

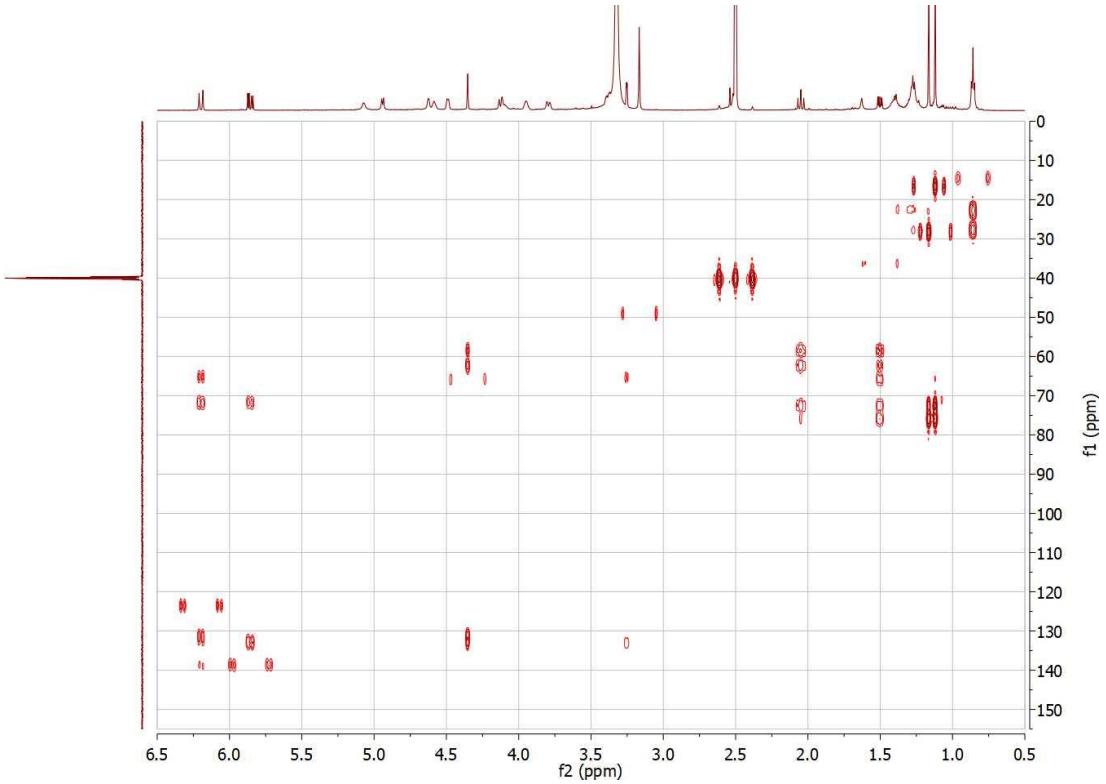


Figure S114. The HMBC (600 MHz, DMSO-d_6) spectrum of compound **20**.

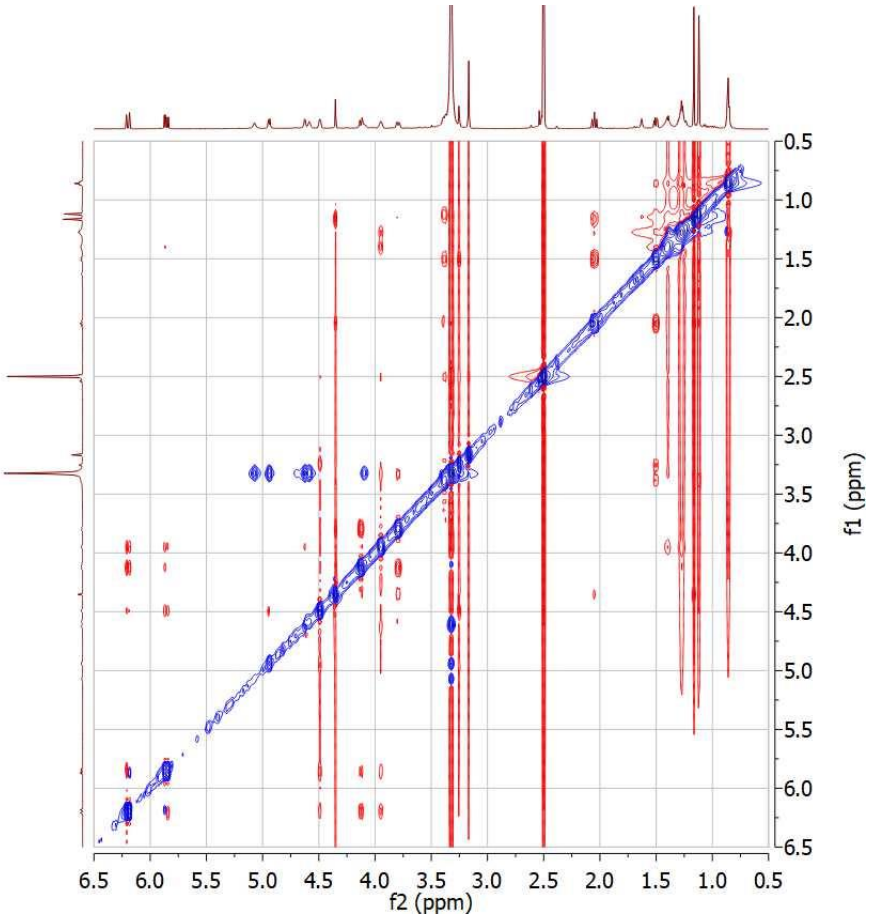
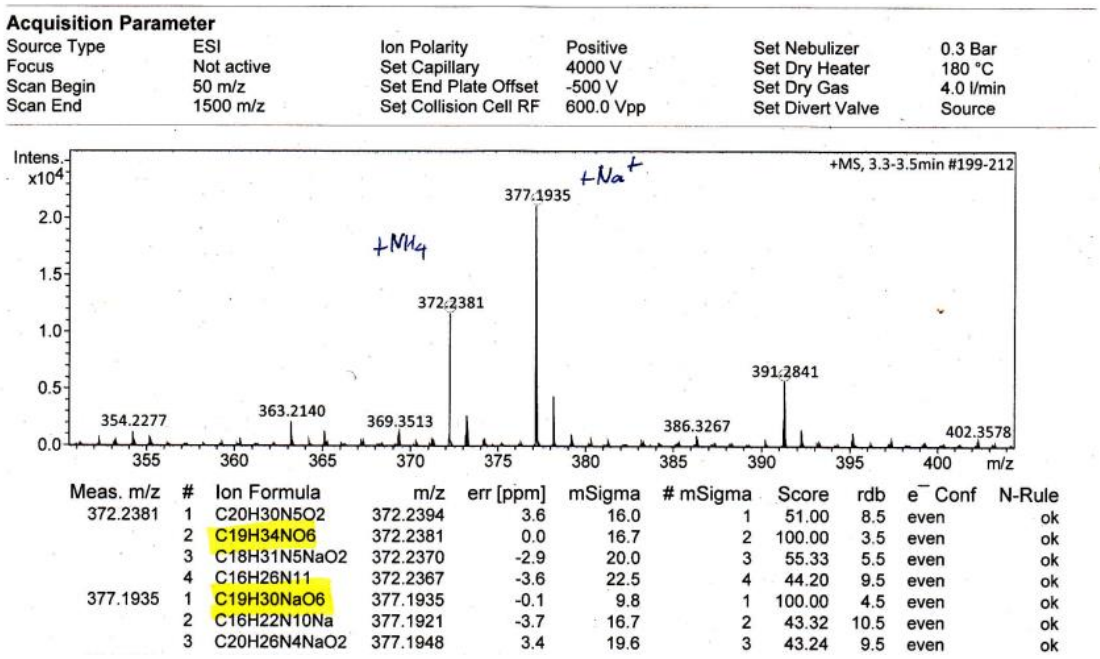


Figure S115. The ROESY ((600 MHz, DMSO-d_6) spectrum of compound **20**.



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
372.2381	1	C20H30N5O2	372.2394	3.6	16.0	1	51.00	8.5	even	ok
	2	C19H34NO6	372.2381	0.0	16.7	2	100.00	3.5	even	ok
	3	C18H31N5NaO2	372.2370	-2.9	20.0	3	55.33	5.5	even	ok
	4	C16H26N11	372.2367	-3.6	22.5	4	44.20	9.5	even	ok
377.1935	1	C19H30NaO6	377.1935	-0.1	9.8	1	100.00	4.5	even	ok
	2	C16H22N10Na	377.1921	-3.7	16.7	2	43.32	10.5	even	ok
	3	C20H26N4NaO2	377.1948	3.4	19.6	3	43.24	9.5	even	ok

Figure S116. The HREISMS of compound **21**.

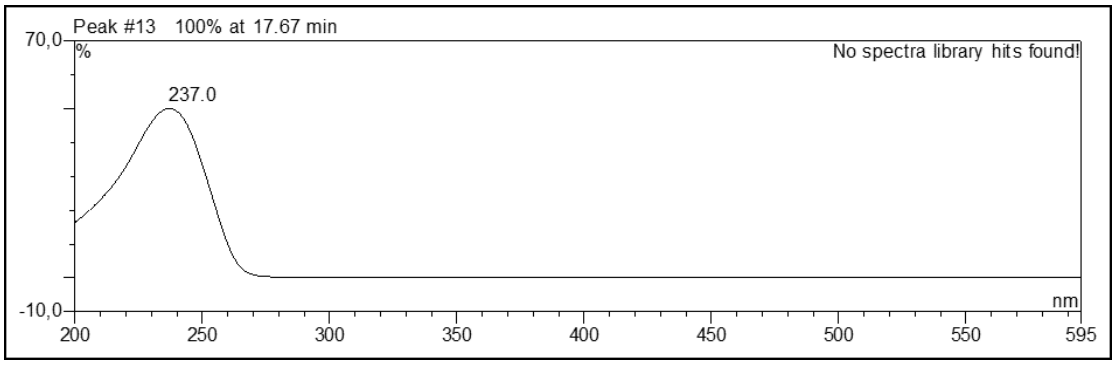


Figure S117. The UV spectrum of compound **21**.

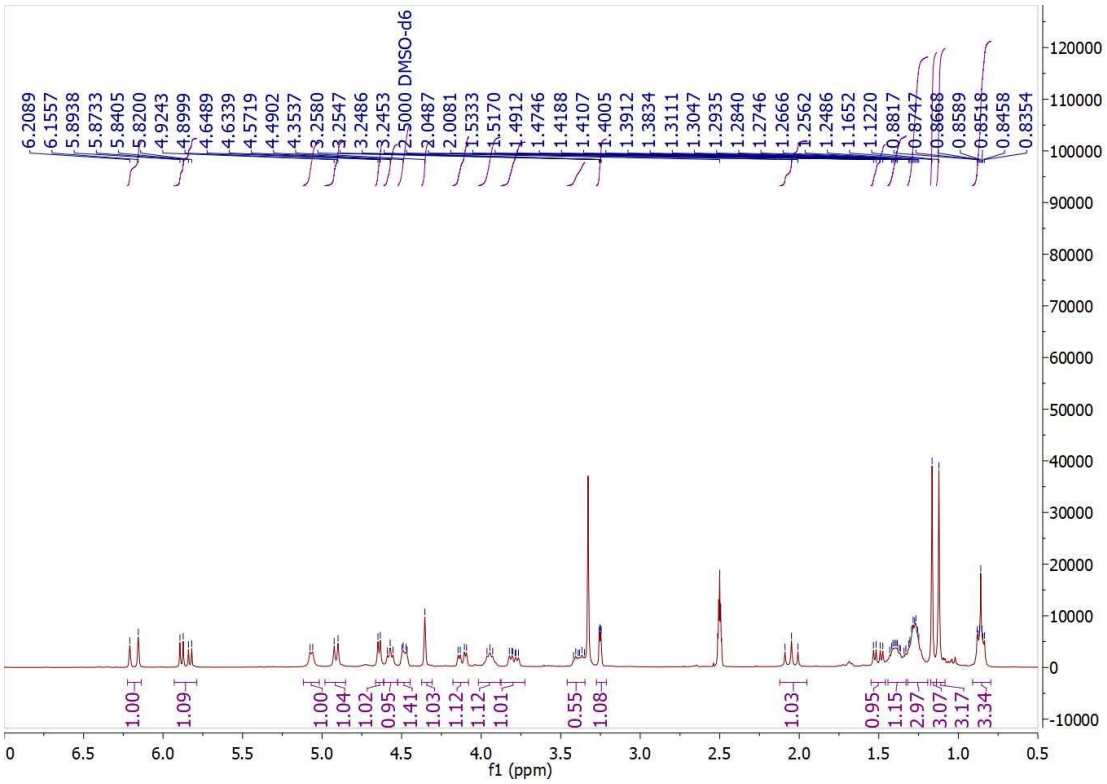


Figure S118. The ^{1}H-NMR (300 MHz, DMSO-d_6) spectrum of compound **21.**

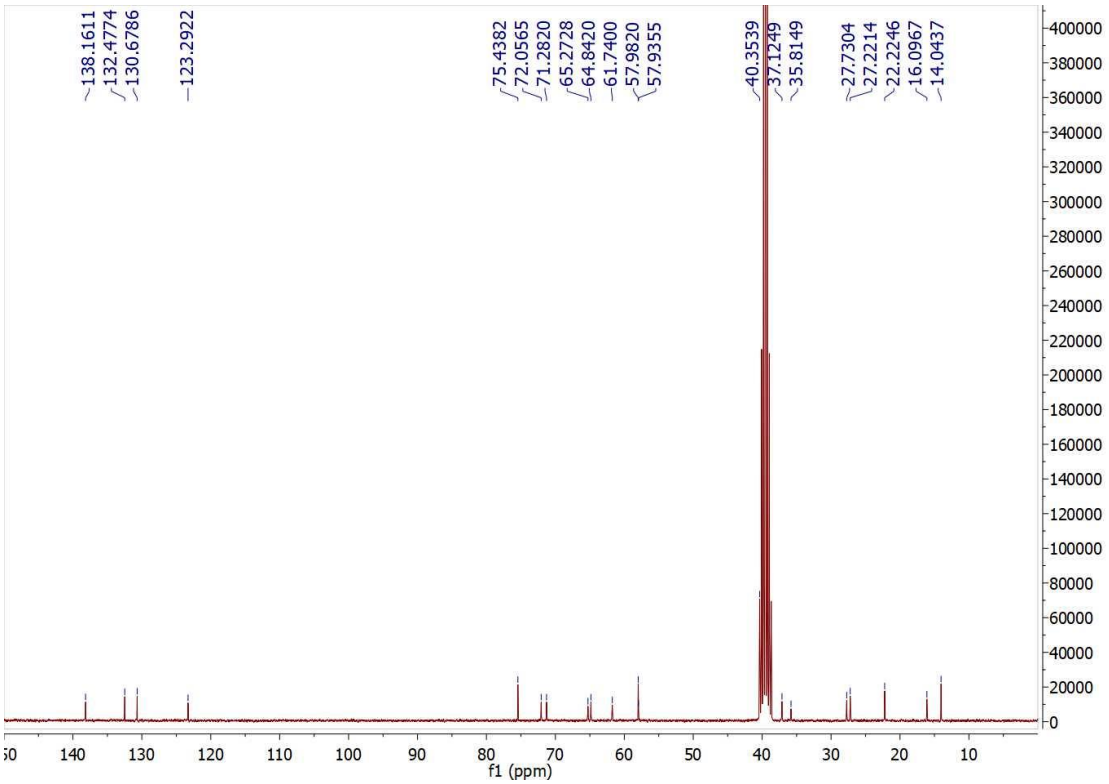


Figure S119. The ^{13}C-NMR (75 MHz, DMSO-d_6) spectrum of compound **21**.

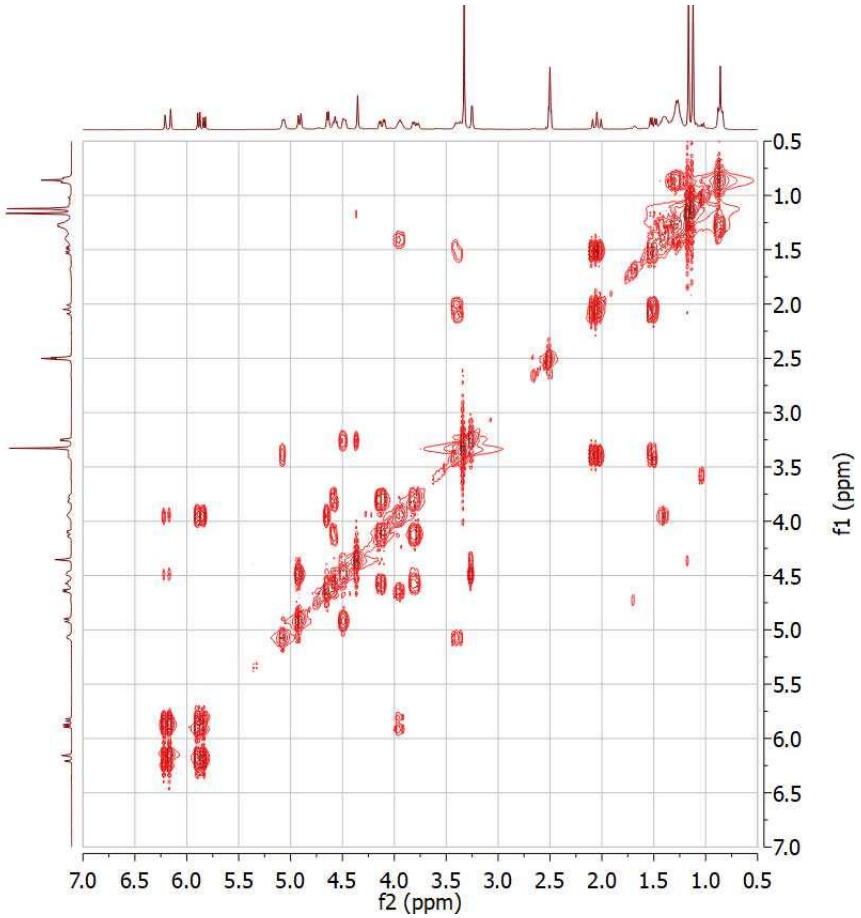


Figure S120. The ^{1}H-^{1}H COSY (300 MHz, DMSO-d_6) spectrum of compound **21**.

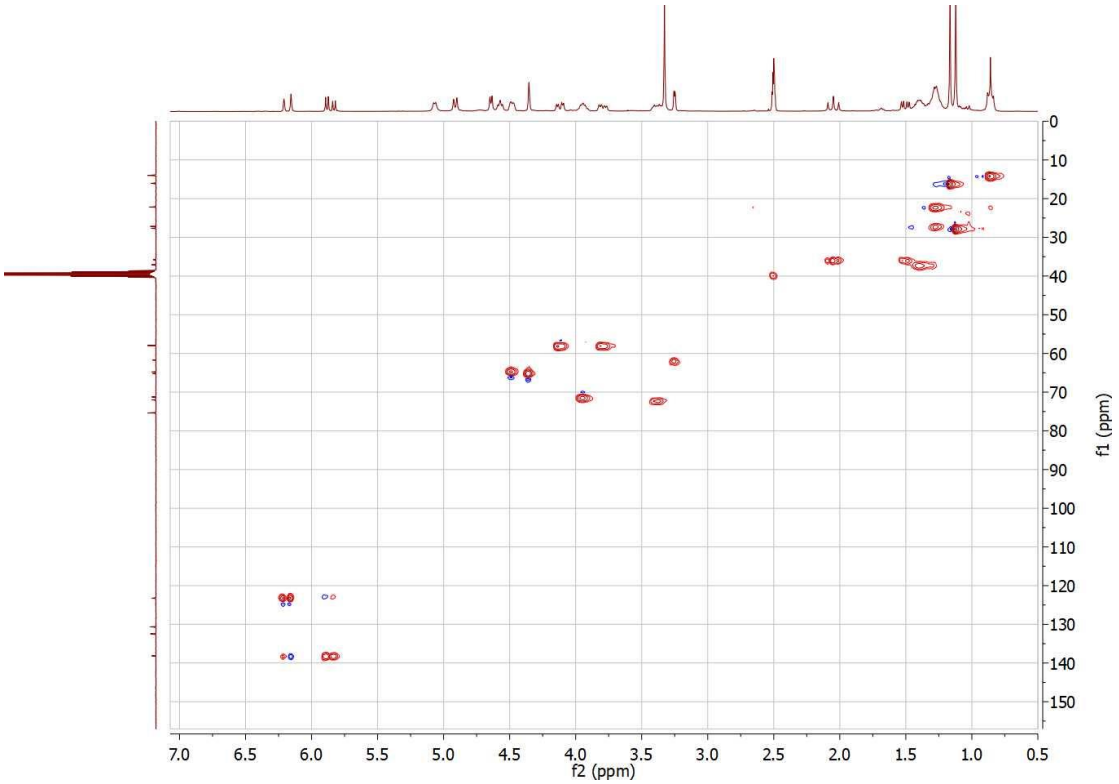


Figure S121. The HSQC (300 MHz, DMSO-d_6) spectrum of compound **21**.

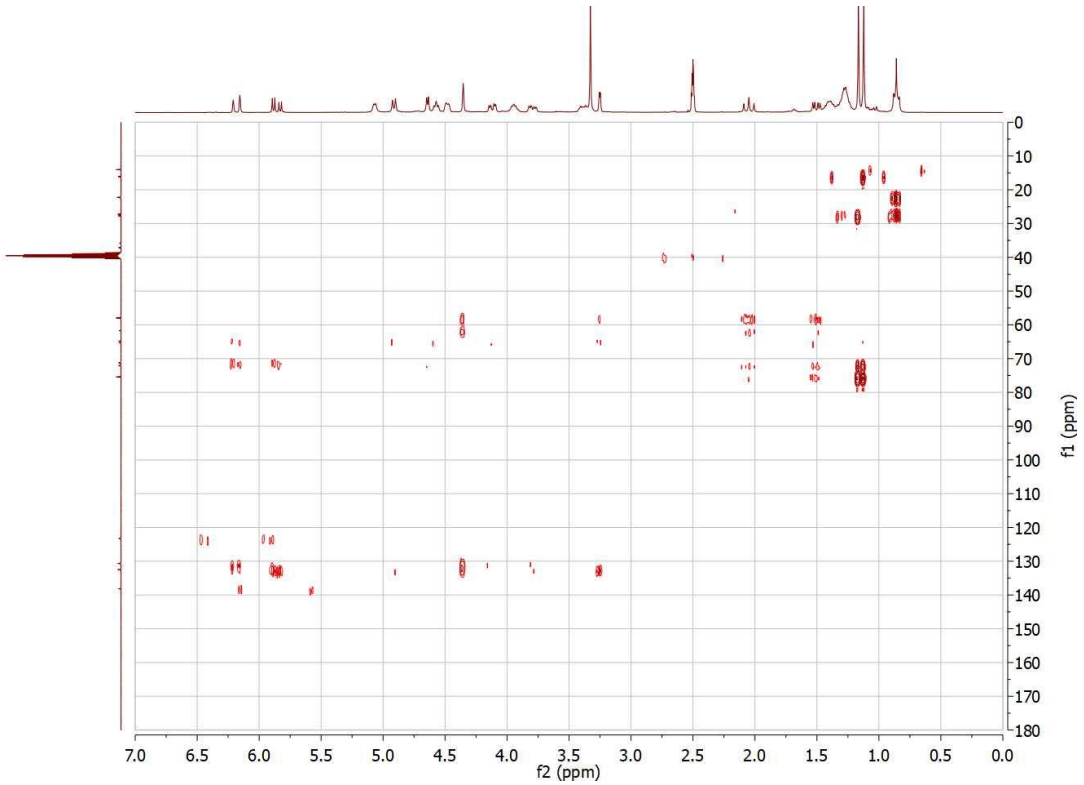


Figure S122. The HMBC (300 MHz, DMSO-d_6) spectrum of compound **21**.

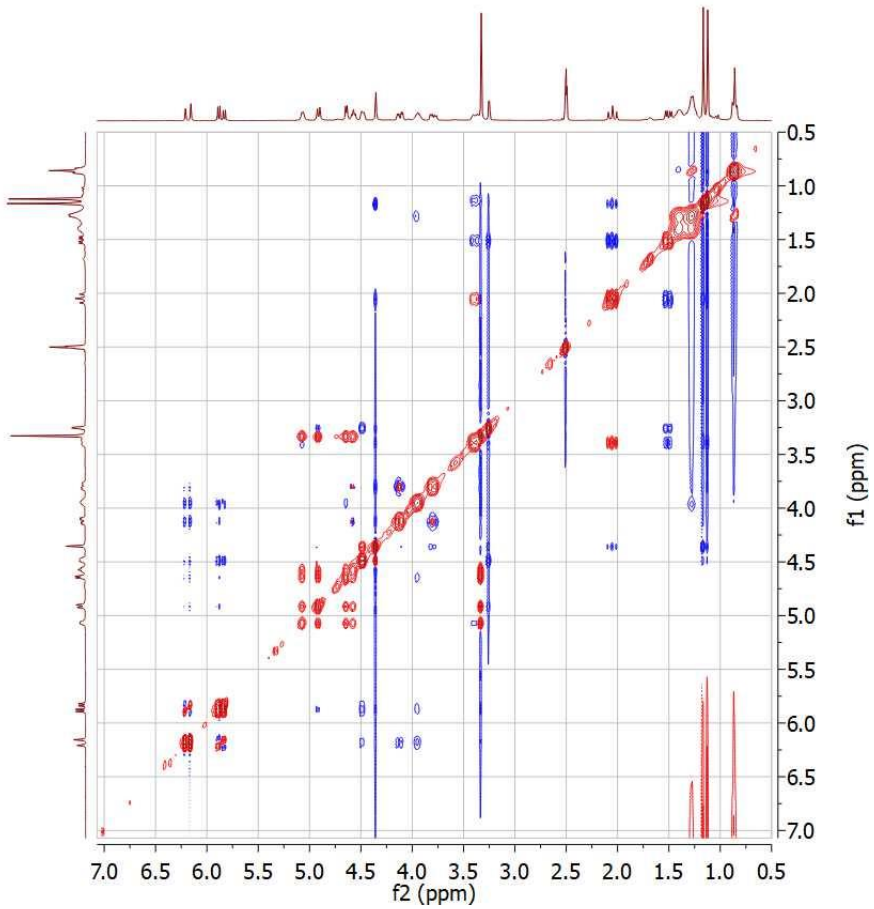


Figure S123. The ROESY (300 MHz, DMSO-d_6) spectrum of compound **21**.

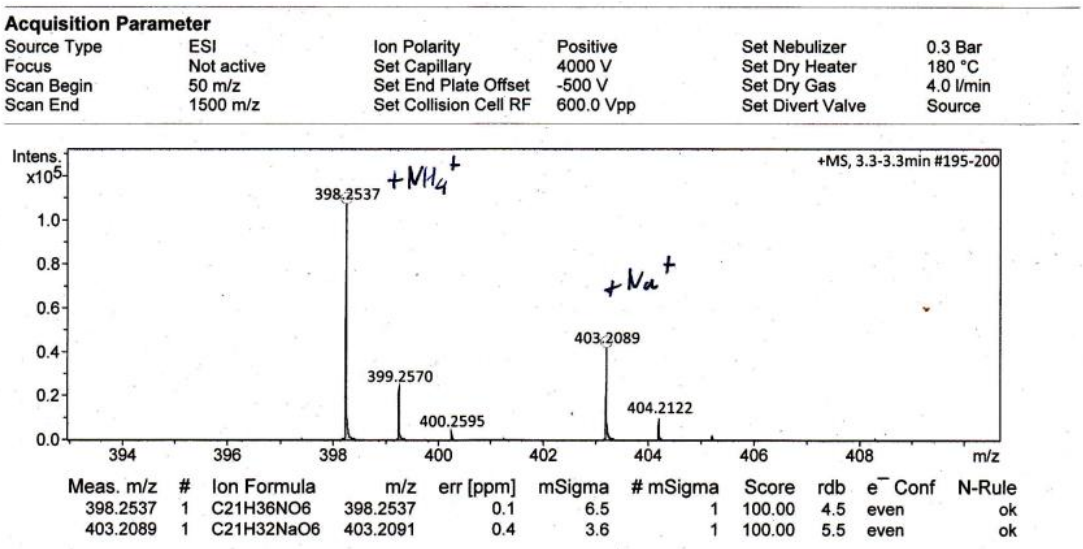


Figure S124. The HREISMS of compound **22**.

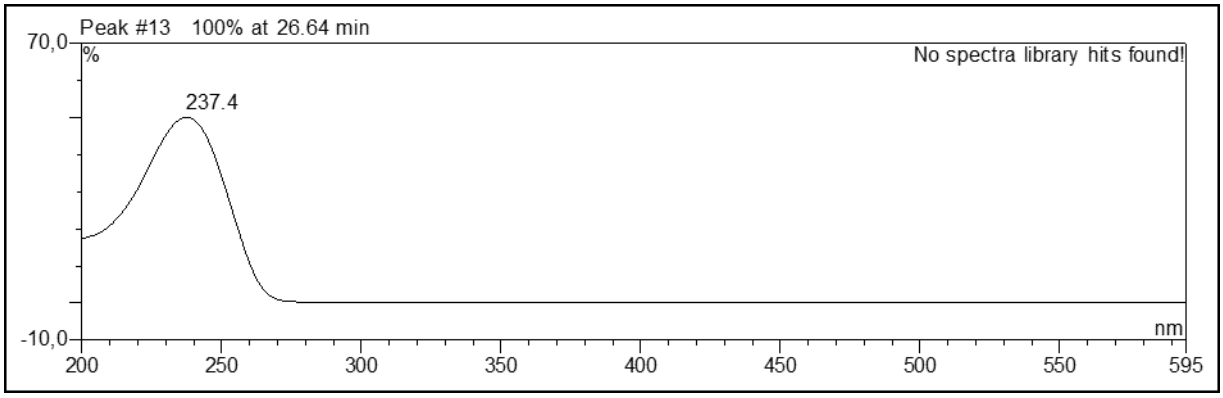


Figure S125. The UV spectrum of compound **22**.

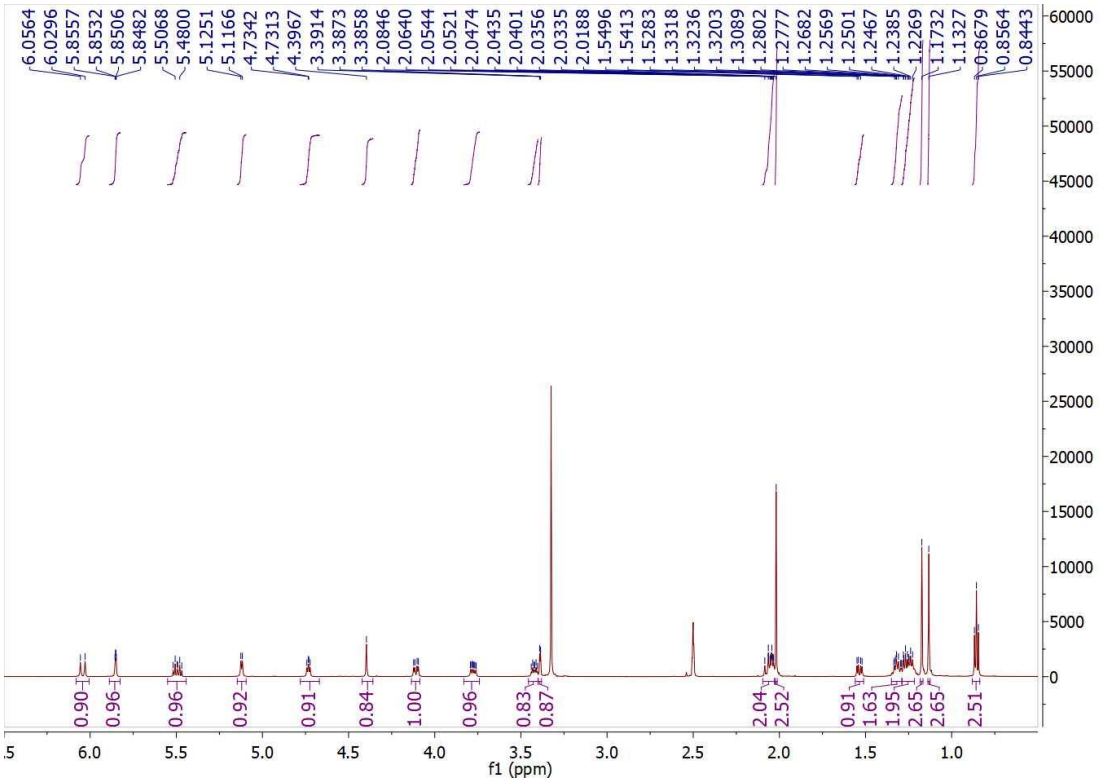


Figure S126. The ^{1}H-NMR (600 MHz, DMSO-d_6) spectrum of compound **22**.

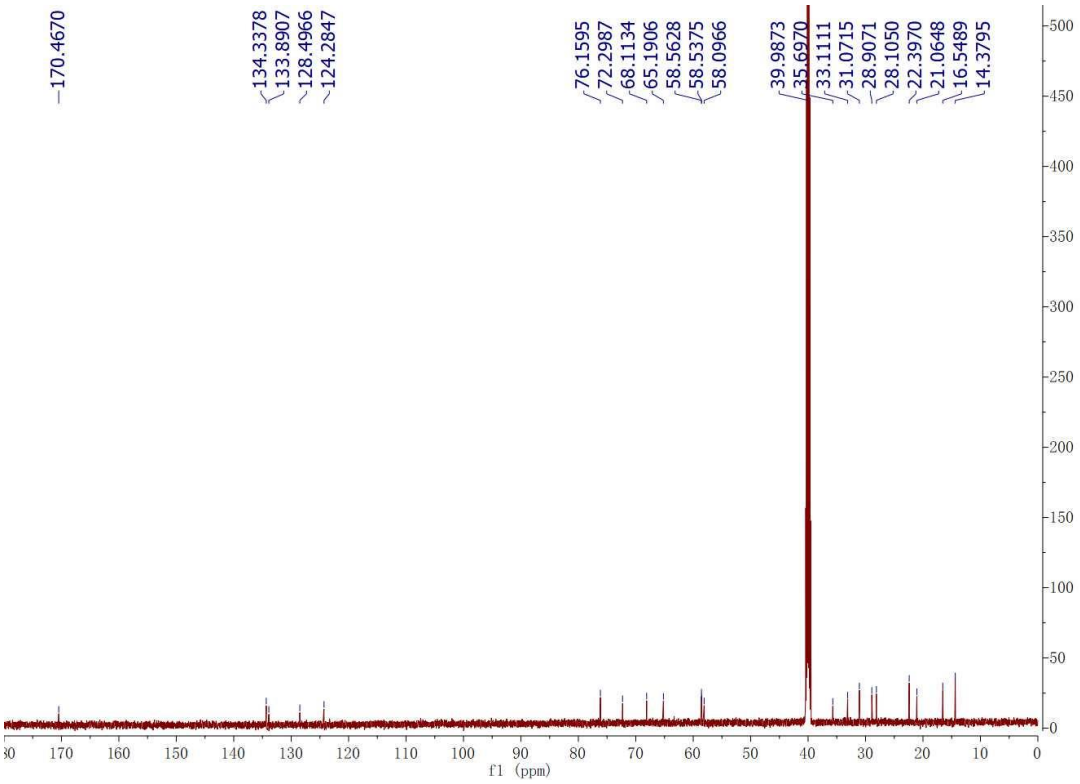


Figure S127. The ^{13}C-NMR (150 MHz, DMSO-d_6) spectrum of compound **22**.

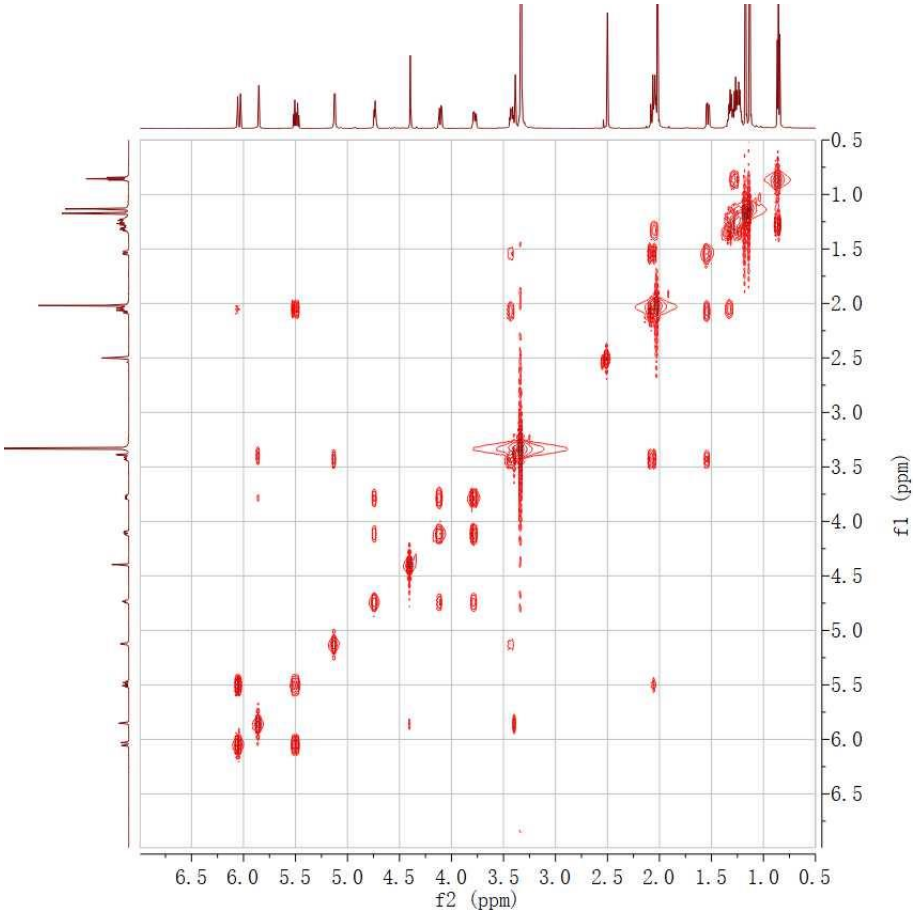


Figure S128. The ^{1}H-^{1}H COSY (600 MHz, DMSO-d_6) spectrum of compound **22**.

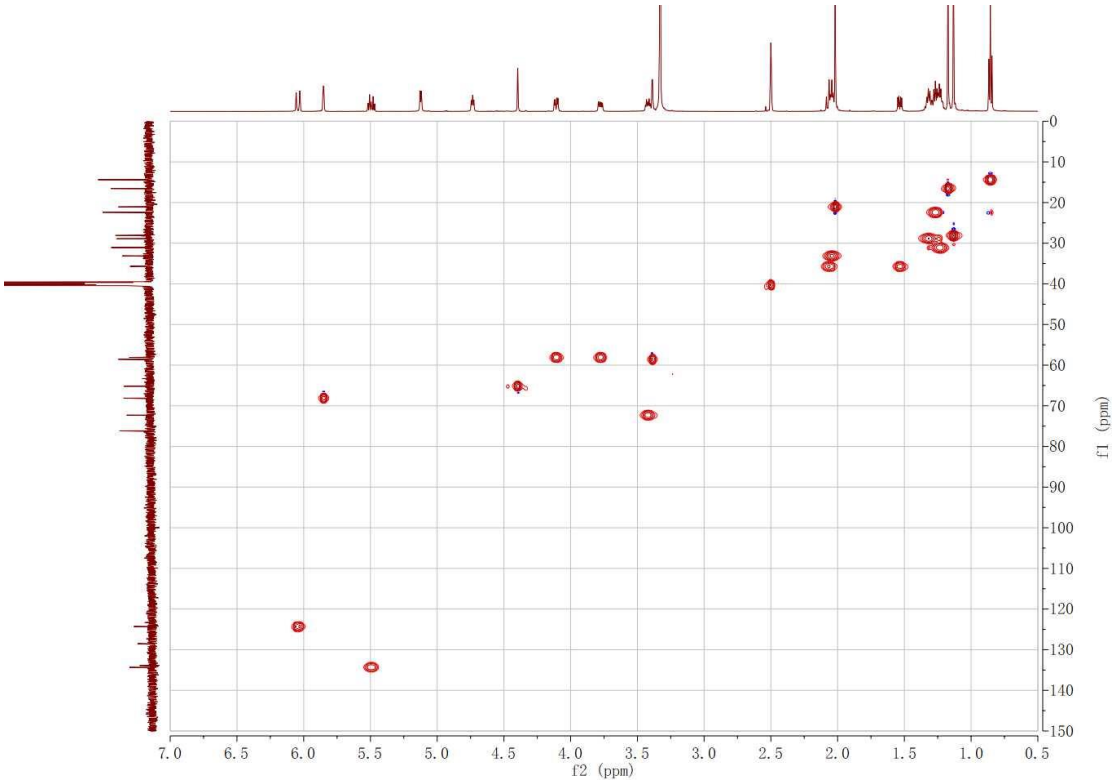


Figure S129. The HSQC (600 MHz, DMSO-d_6) spectrum of compound **22**.

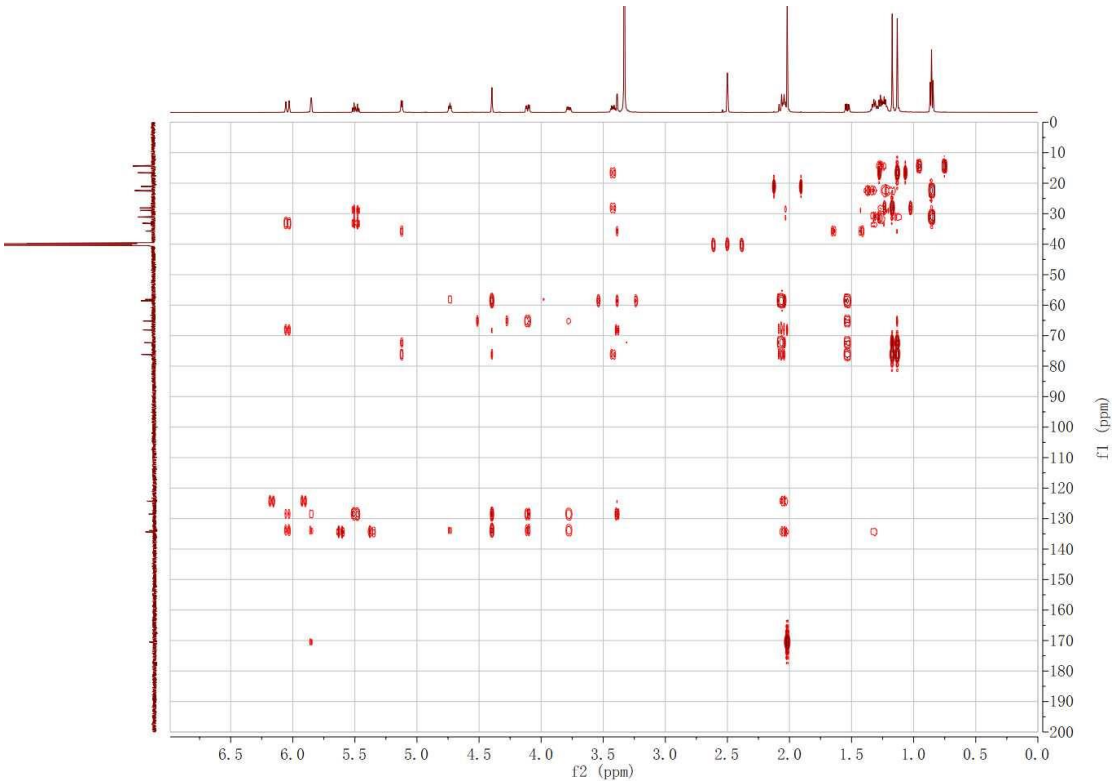


Figure S130. The HMBC (600 MHz, DMSO-d_6) spectrum of compound **22**.

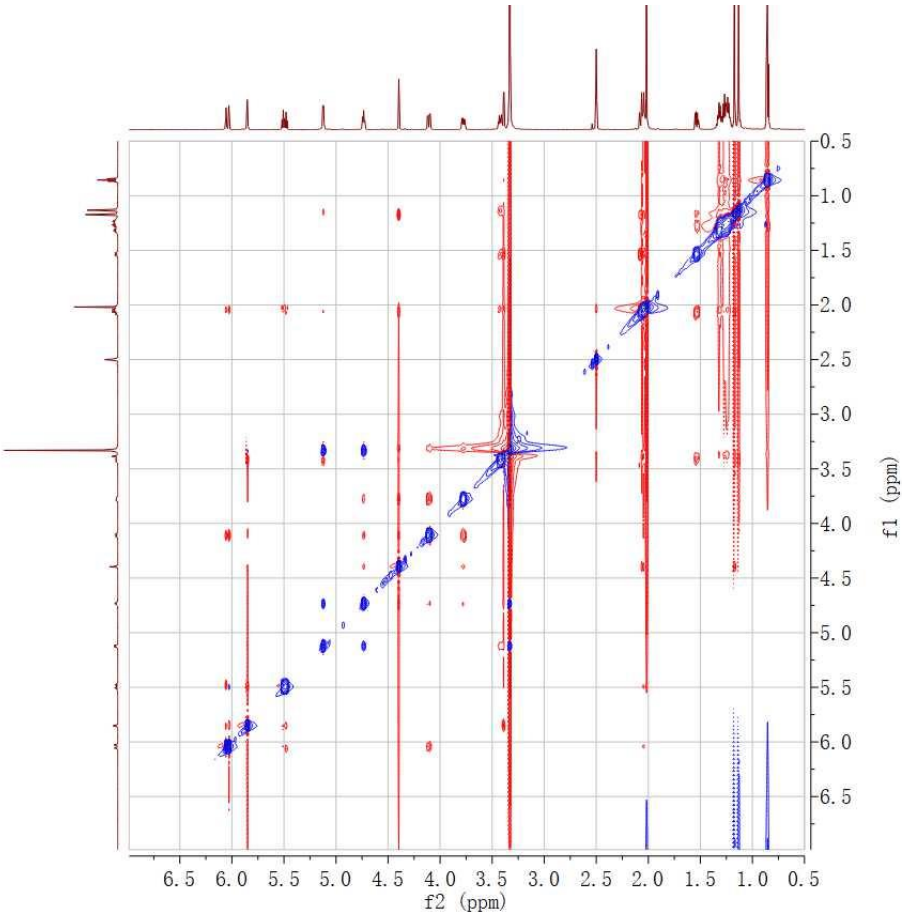


Figure S131. The ROESY (600 MHz, DMSO-d_6) spectrum of compound **22**.

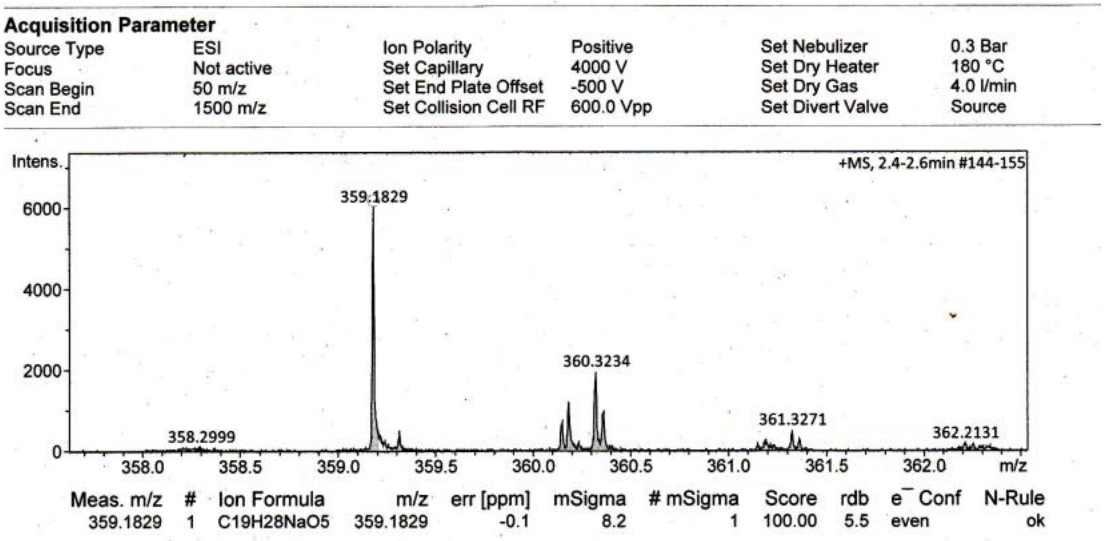


Figure S132. The HREISMS of compound **23**.

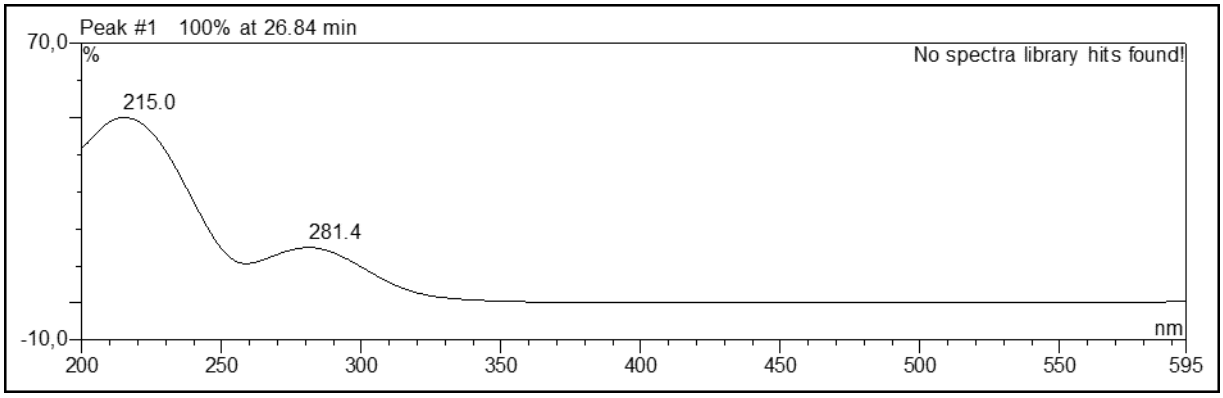


Figure S133. The UV spectrum of compound **23**.

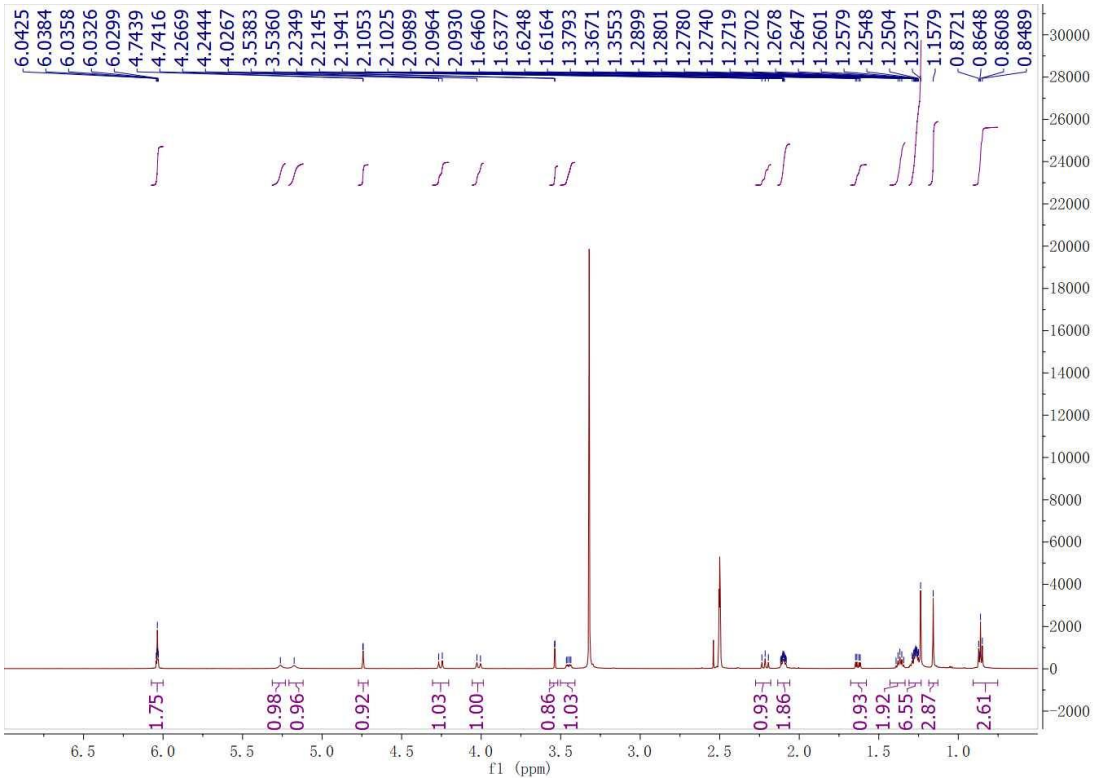


Figure S134. The ^{1}H-NMR (600 MHz, DMSO-d_6) spectrum of compound **23**.

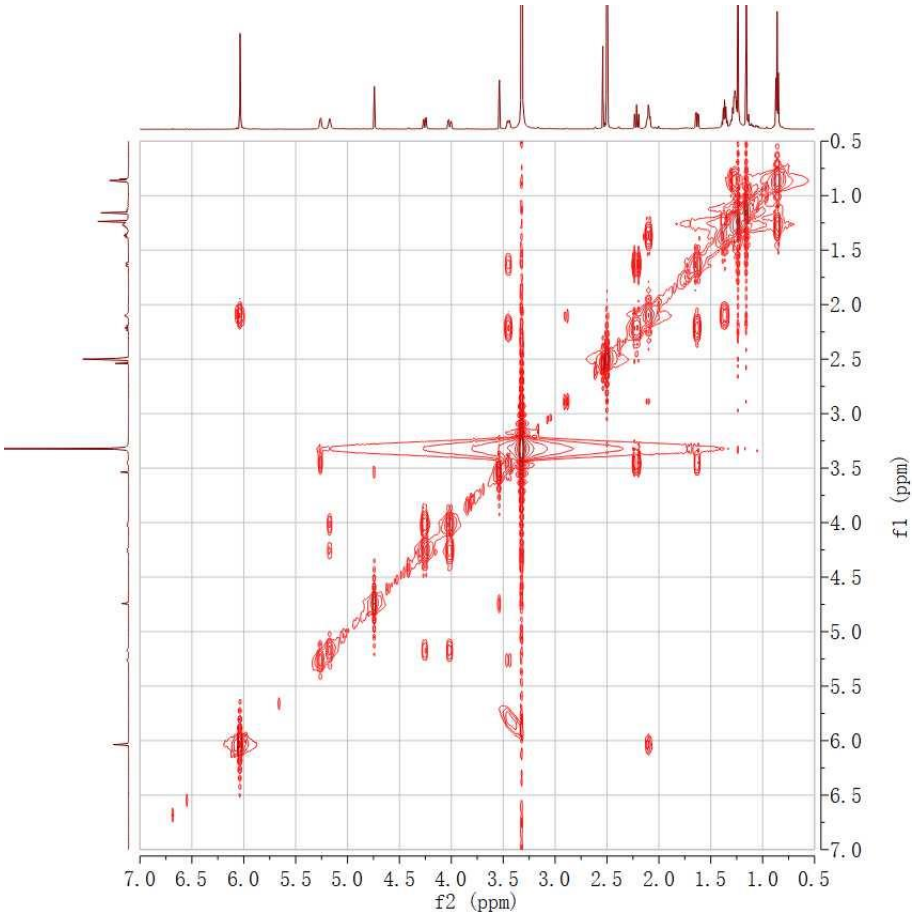


Figure S135. The ^{1}H-^{1}H COSY (600 MHz, DMSO-d_6) spectrum of compound **23**.

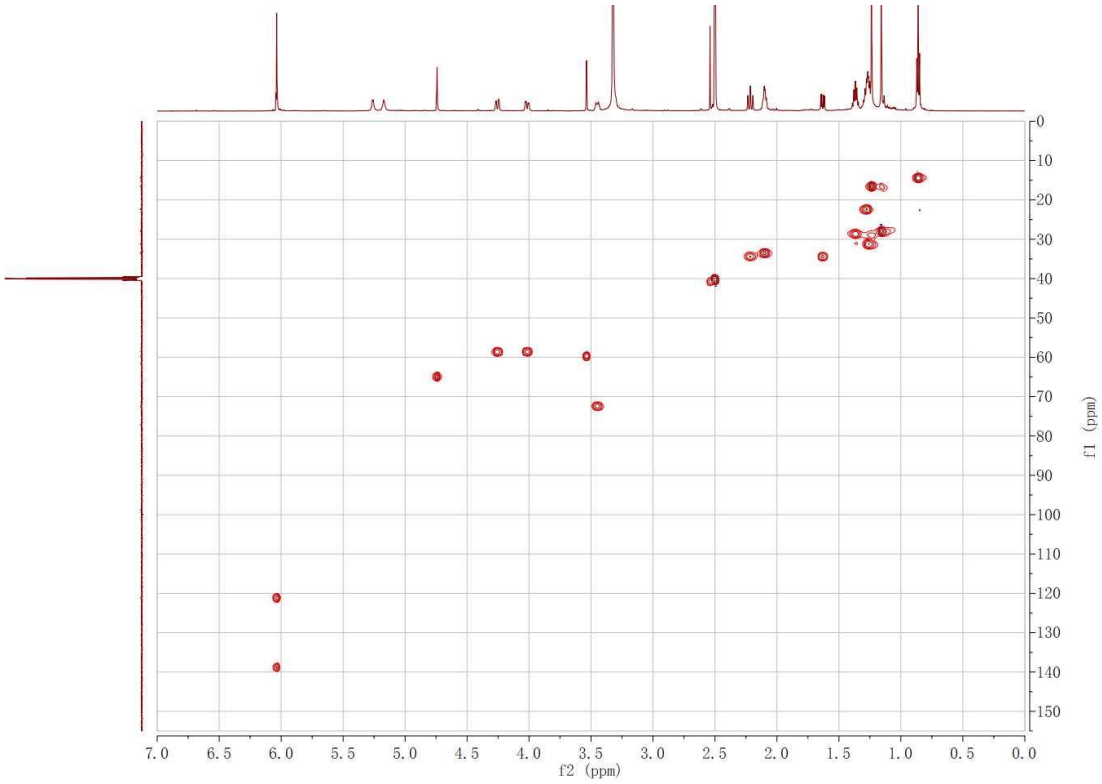


Figure S136. The HSQC (600 MHz, DMSO-d_6) spectrum of compound **23**.

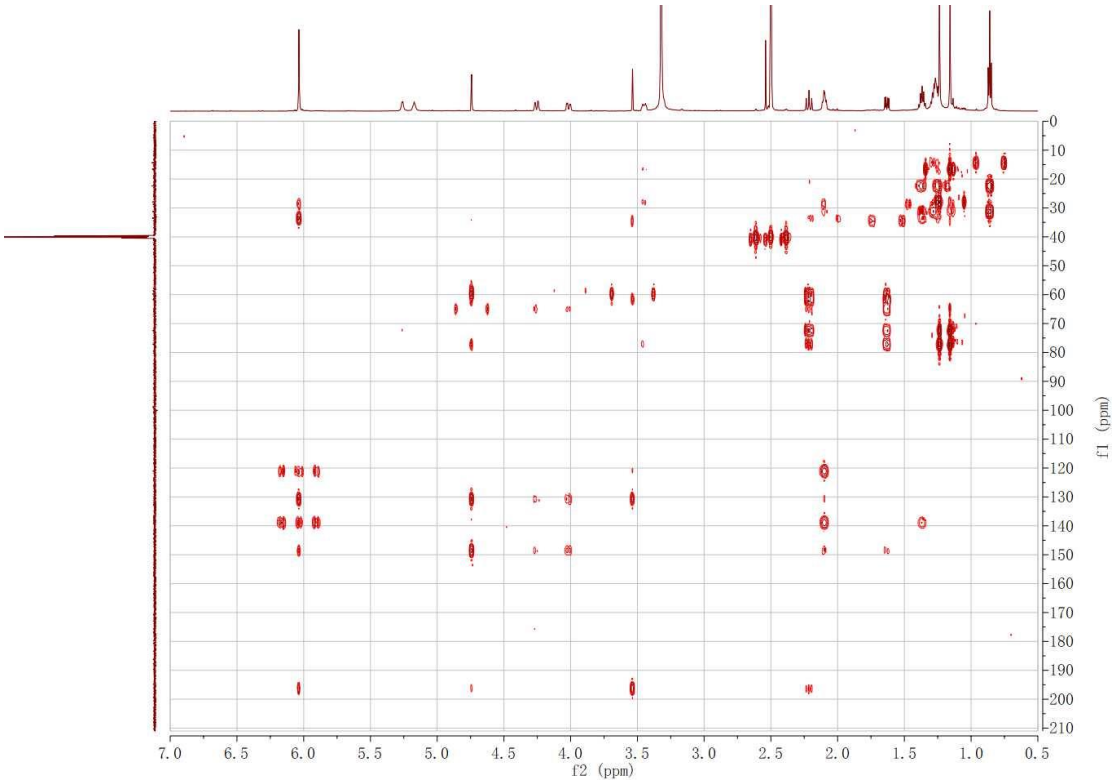


Figure S137. The HMBC (600 MHz, DMSO-d_6) spectrum of compound **23**.

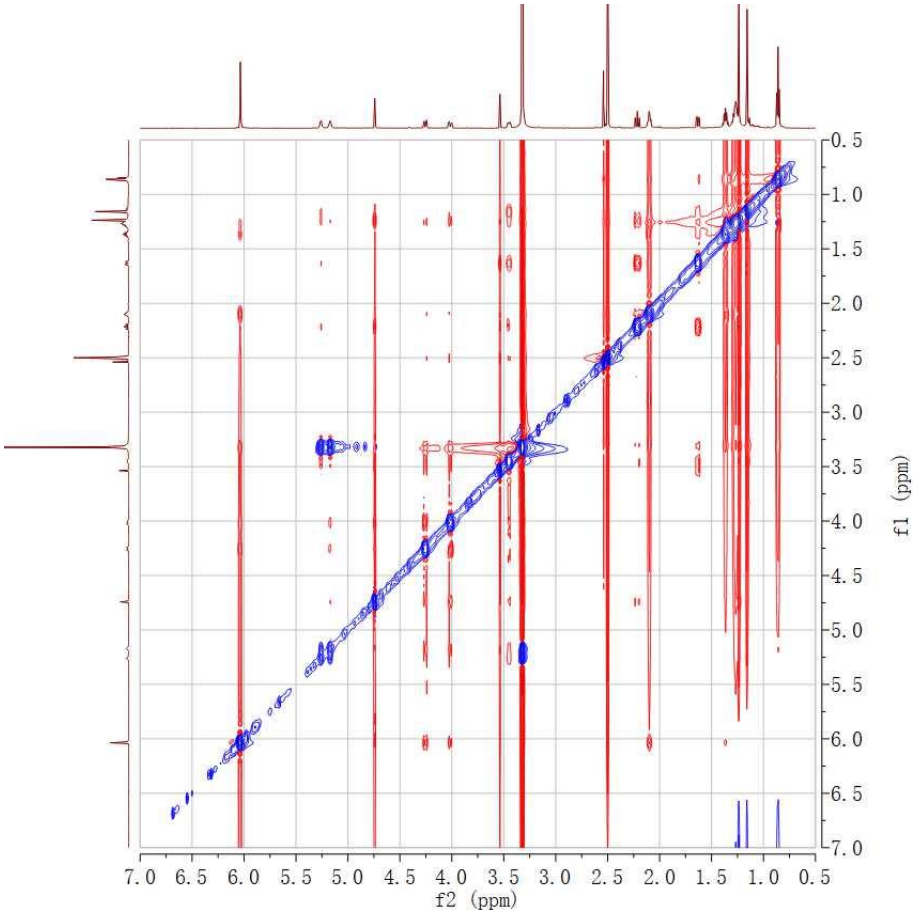


Figure S138. The ROESY (600 MHz, DMSO-d_6) spectrum of compound **23**.

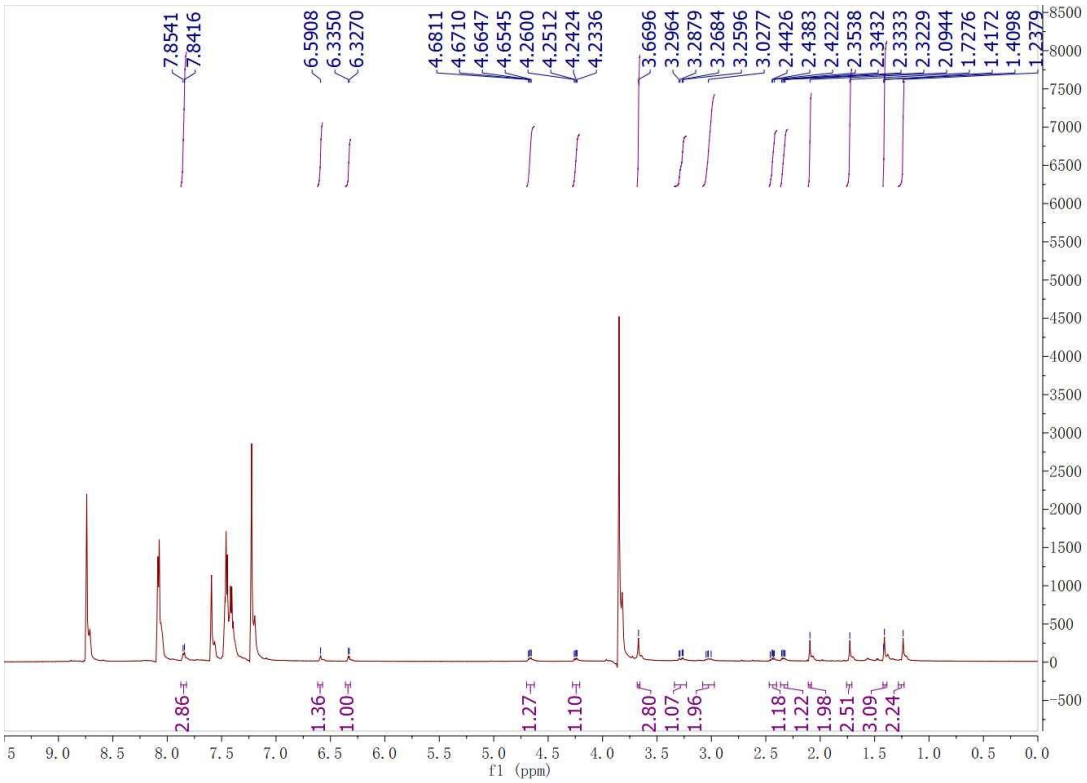


Figure S139. The ^{1}H-NMR (600 MHz, Prydine-d_5) spectrum of **1a**.

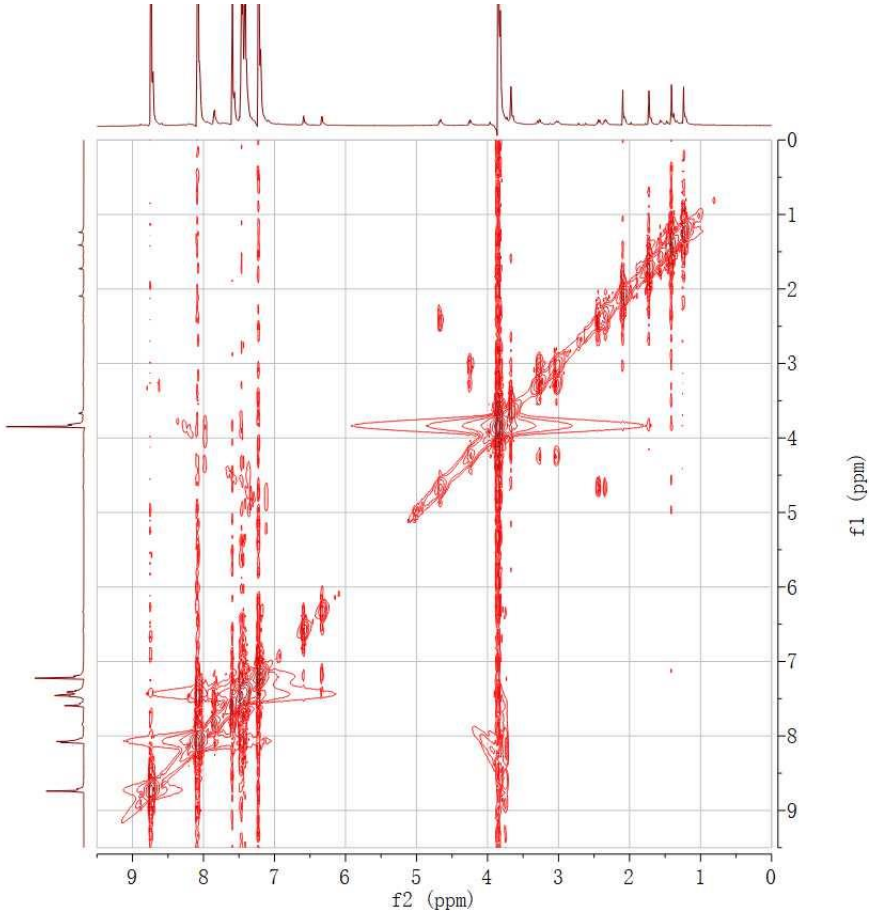


Figure S140. The ^{1}H-^{1}H COSY (600 MHz, Prydine-d_5) spectrum of **1a**.

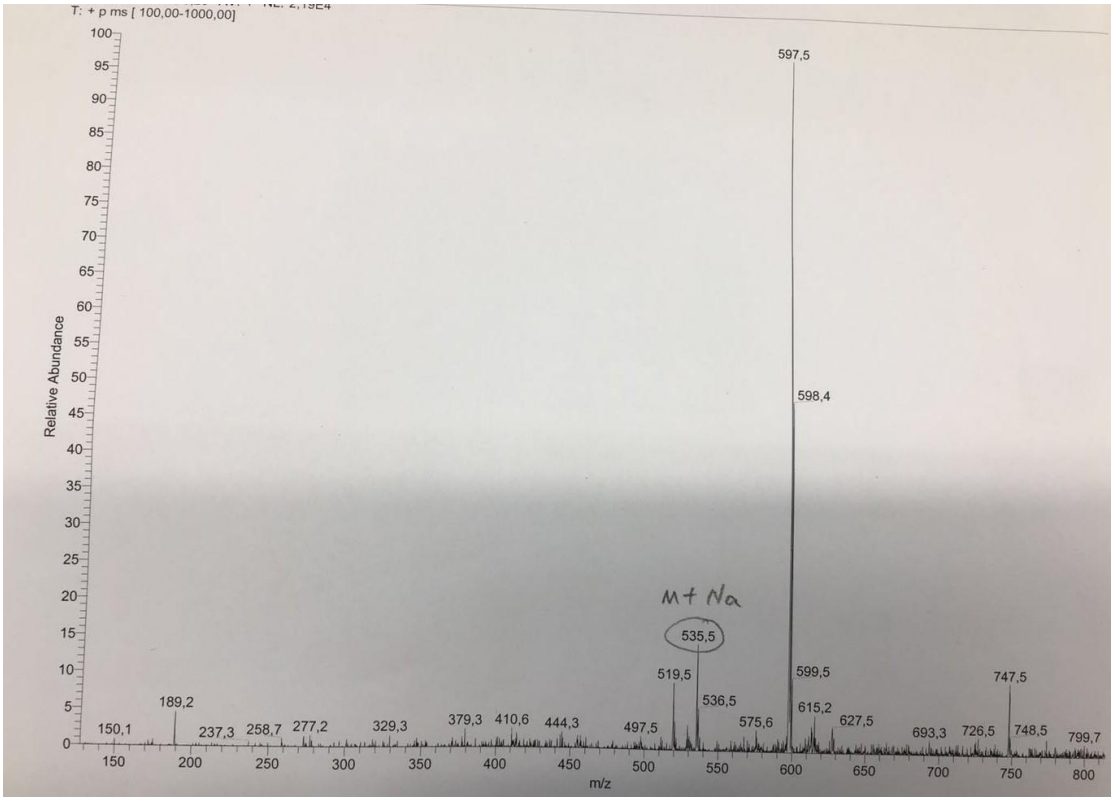


Figure S141. The ESIMS of **1a**.

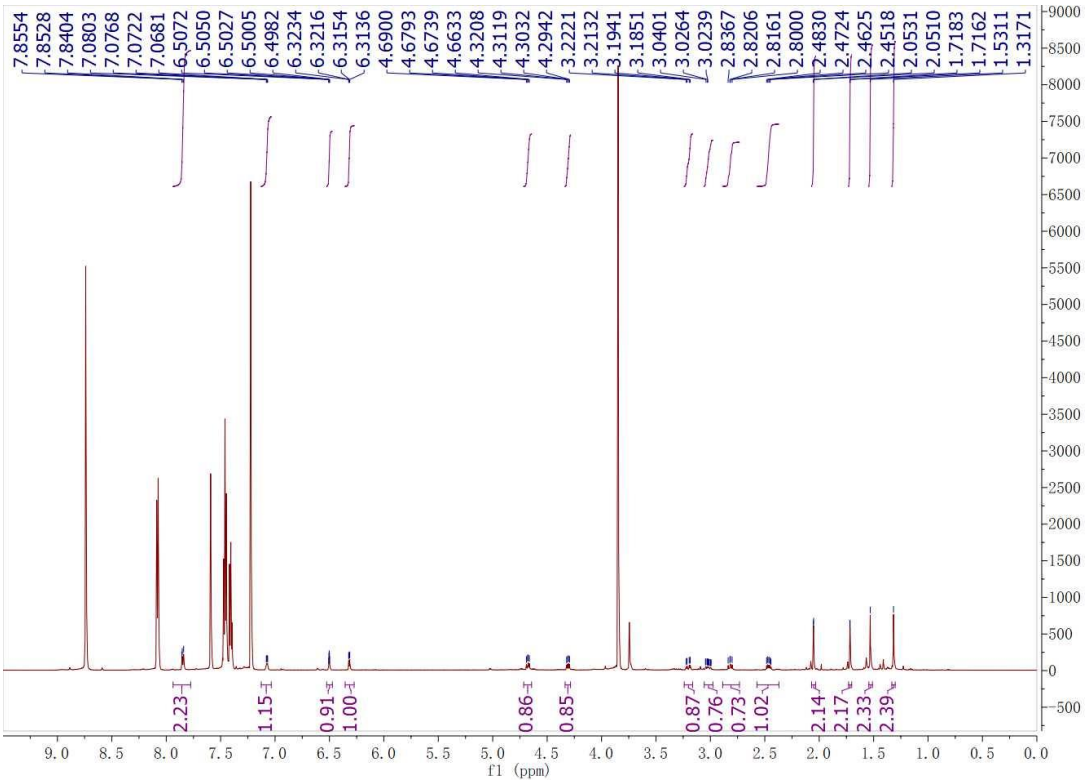


Figure S142. The ^{1}H-NMR (600 MHz, Prydine-d_5) spectrum of **1b**.

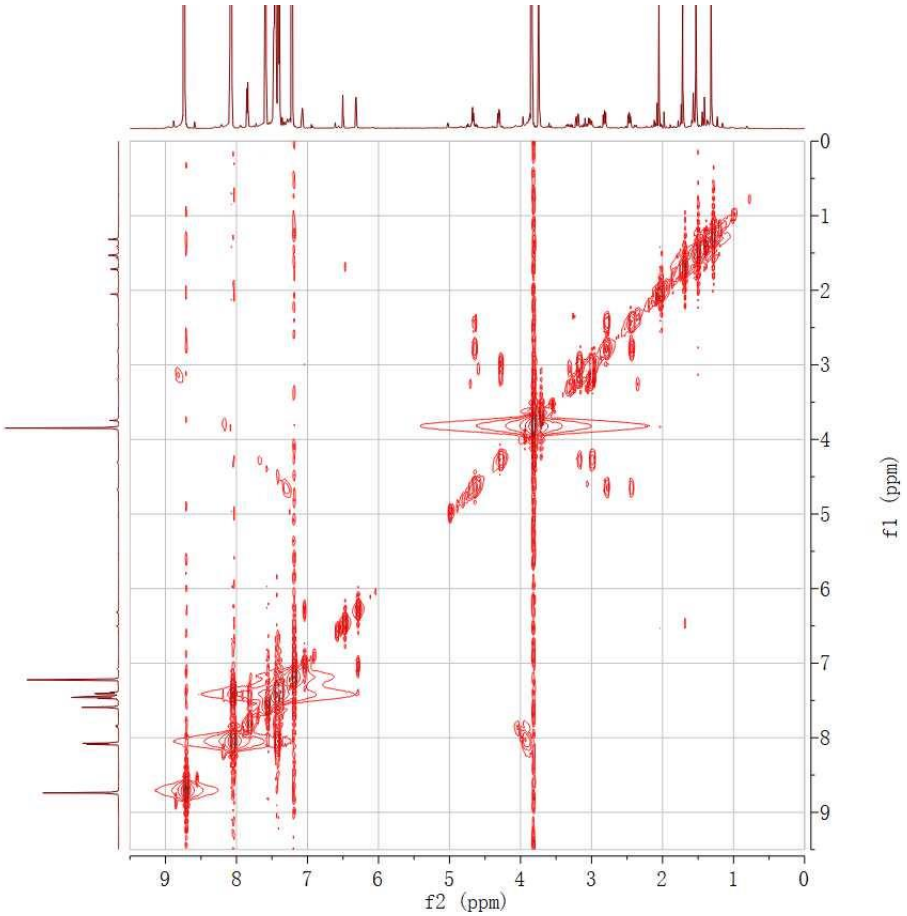


Figure S143. The ^{1}H-^{1}H COSY (600 MHz, Prydine-d_5) spectrum of **1b**.

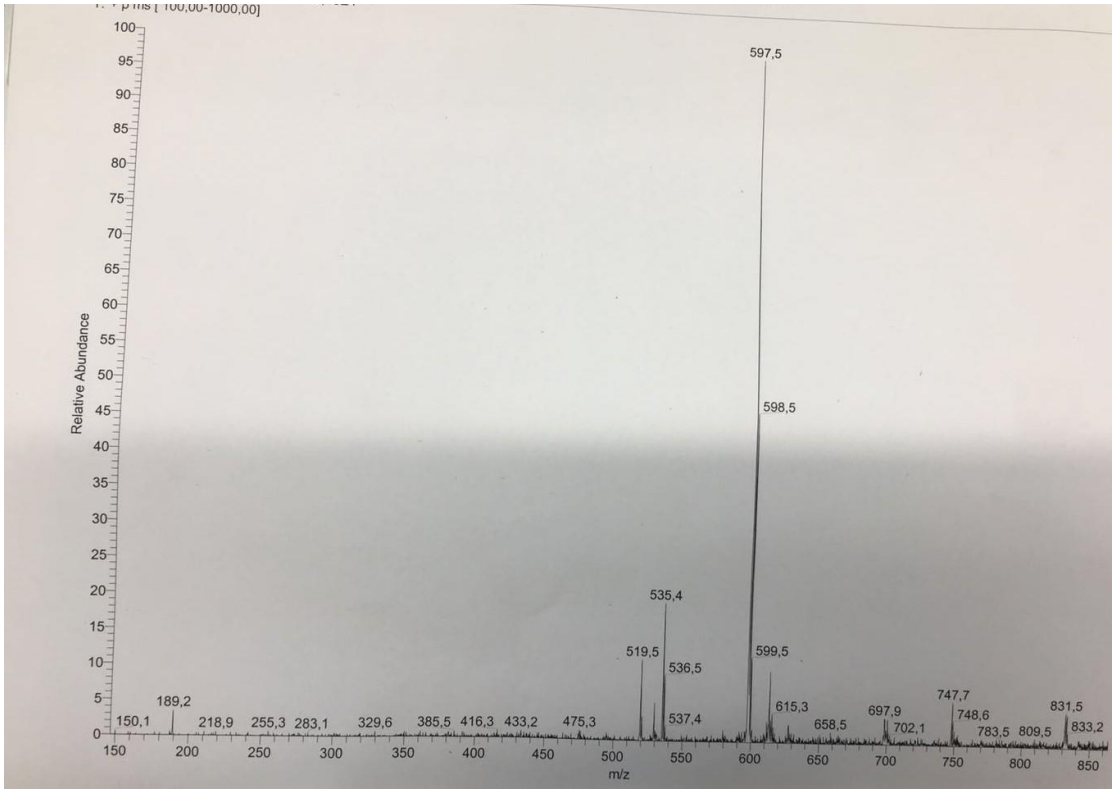


Figure S144. The ESIMS of **1b**.

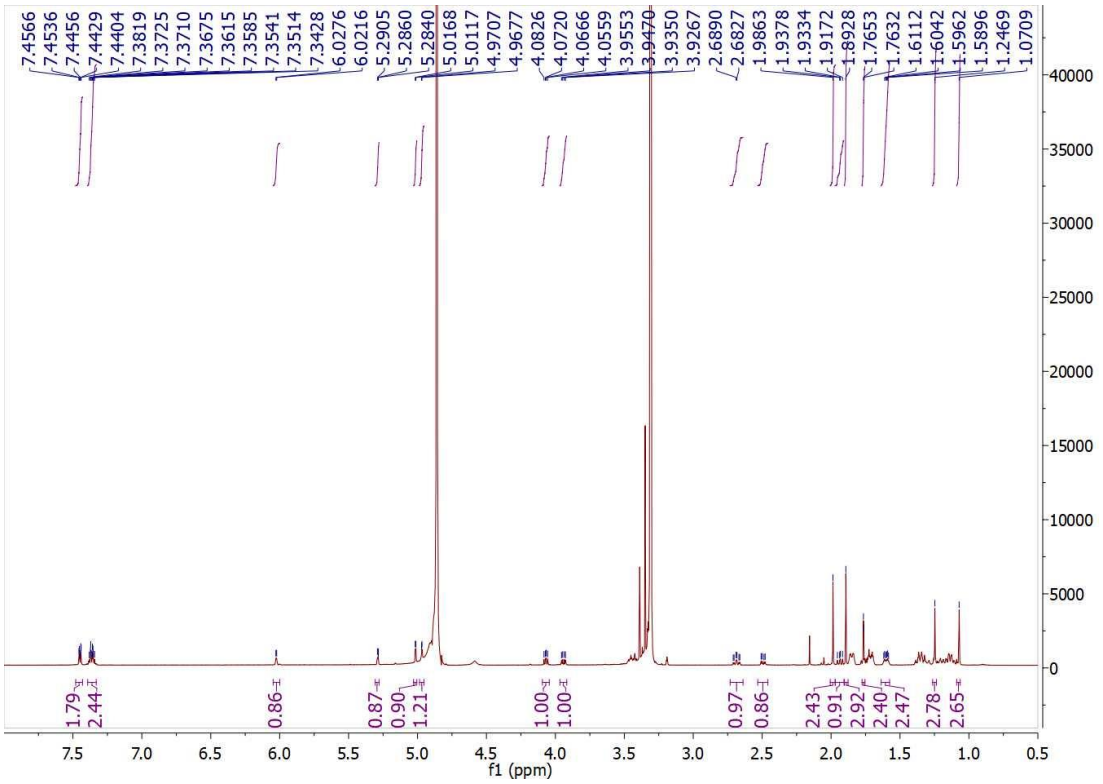


Figure S145. The ^{1}H-NMR (600 MHz, CD_3OD) spectrum of **7a**.

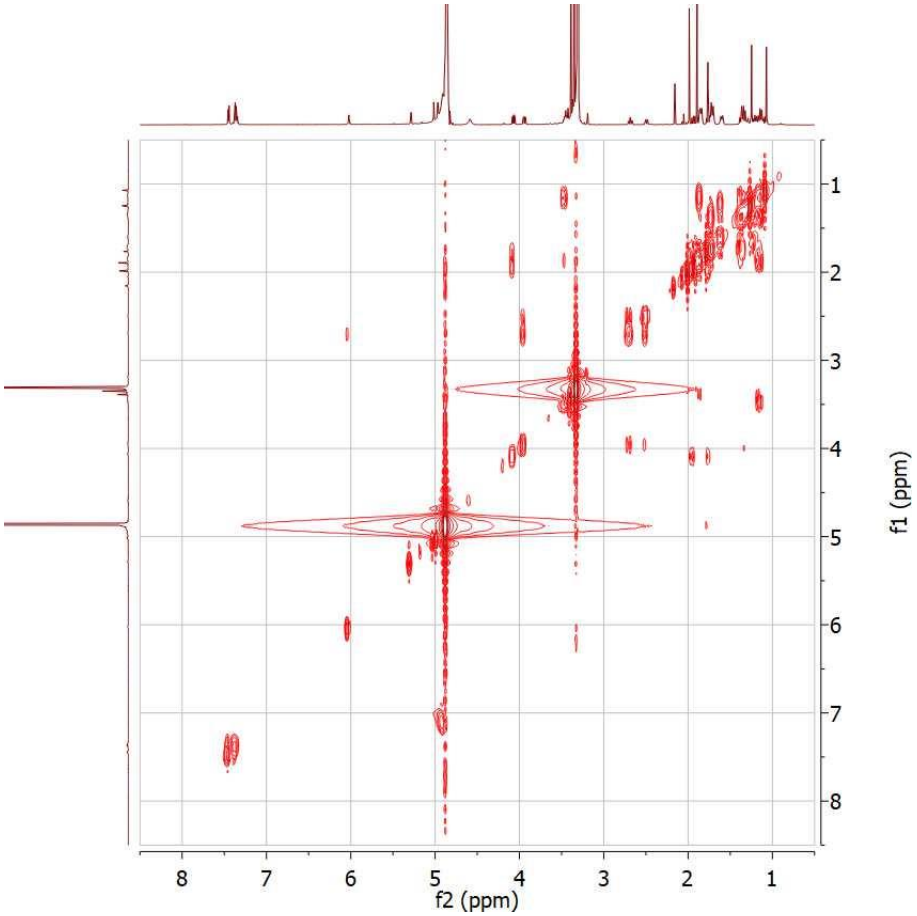


Figure S146. The ^{1}H-^{1}H COSY (600 MHz, CD_3OD) spectrum of **7a**.

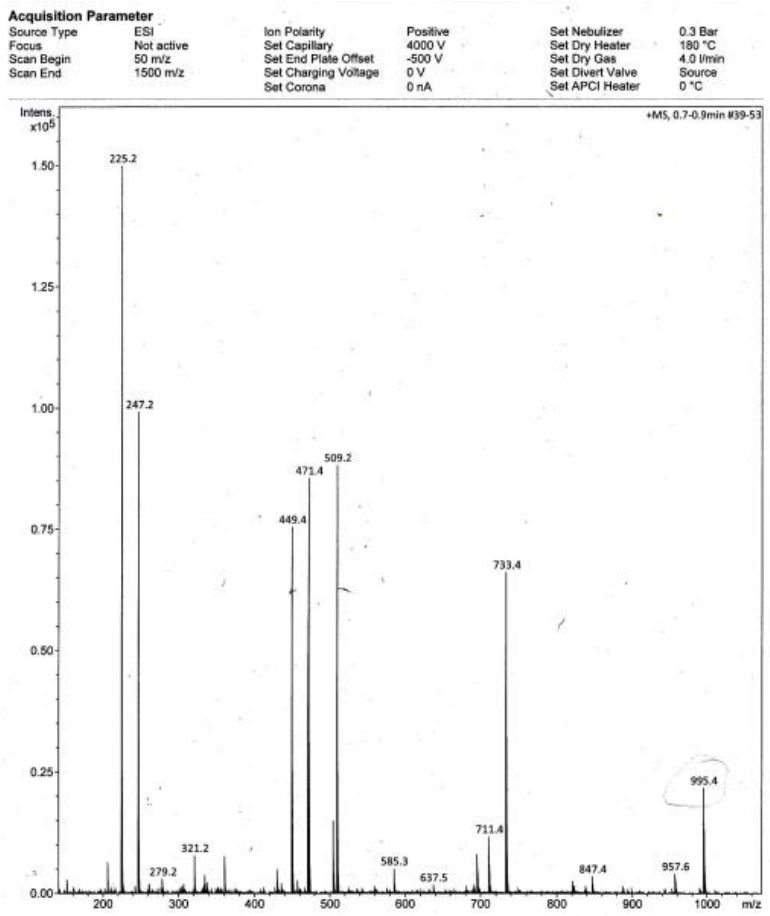


Figure S147. The ESIMS of **7a**.

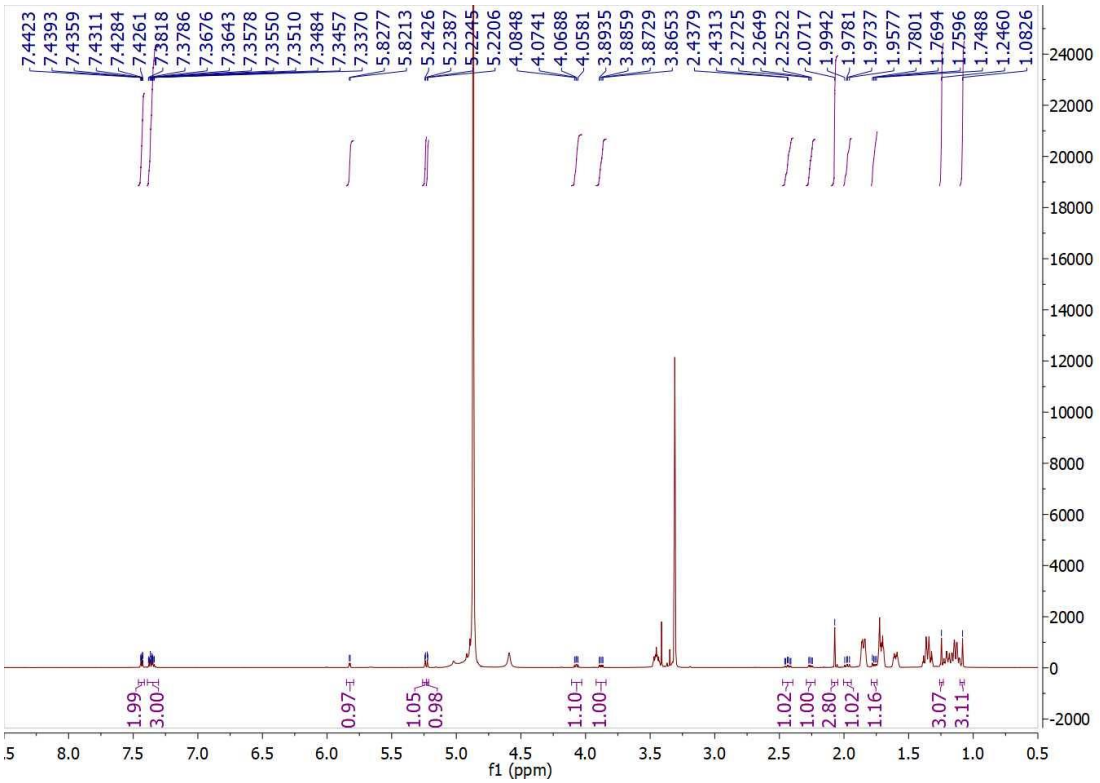


Figure S148. The ^{1}H-NMR (600 MHz, CD_3OD) spectrum of **7b**.

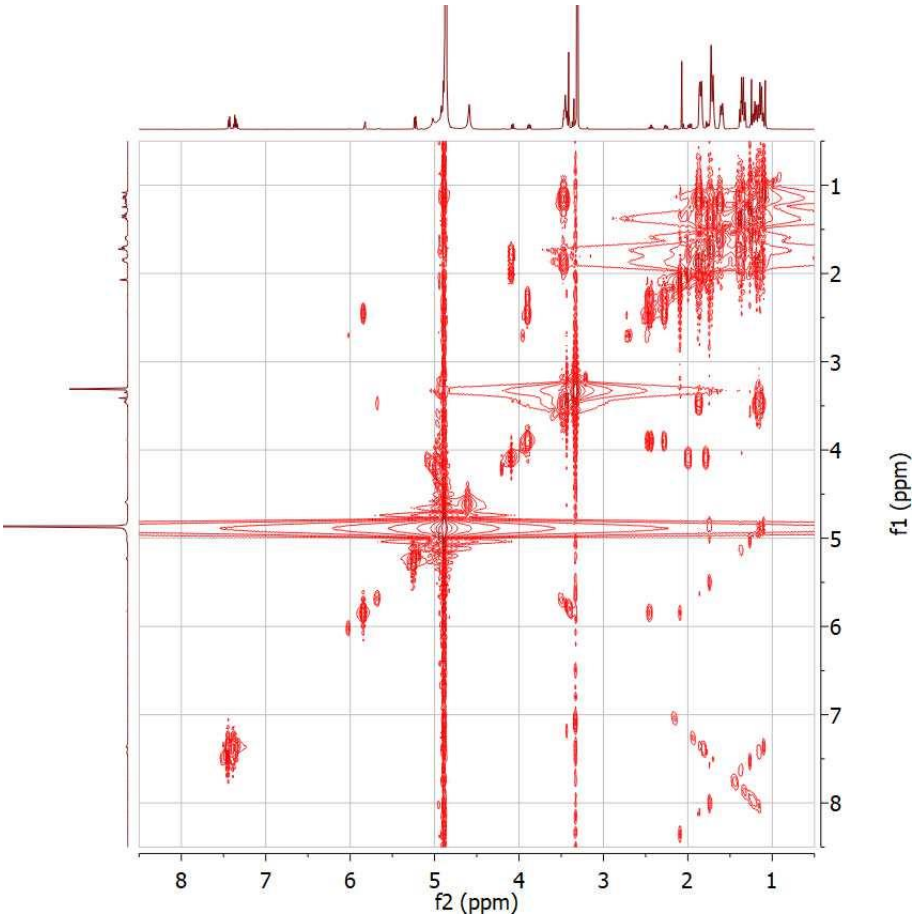


Figure S149. The ^{1}H-^{1}H COSY (600 MHz, CD_3OD) spectrum of **7b**.

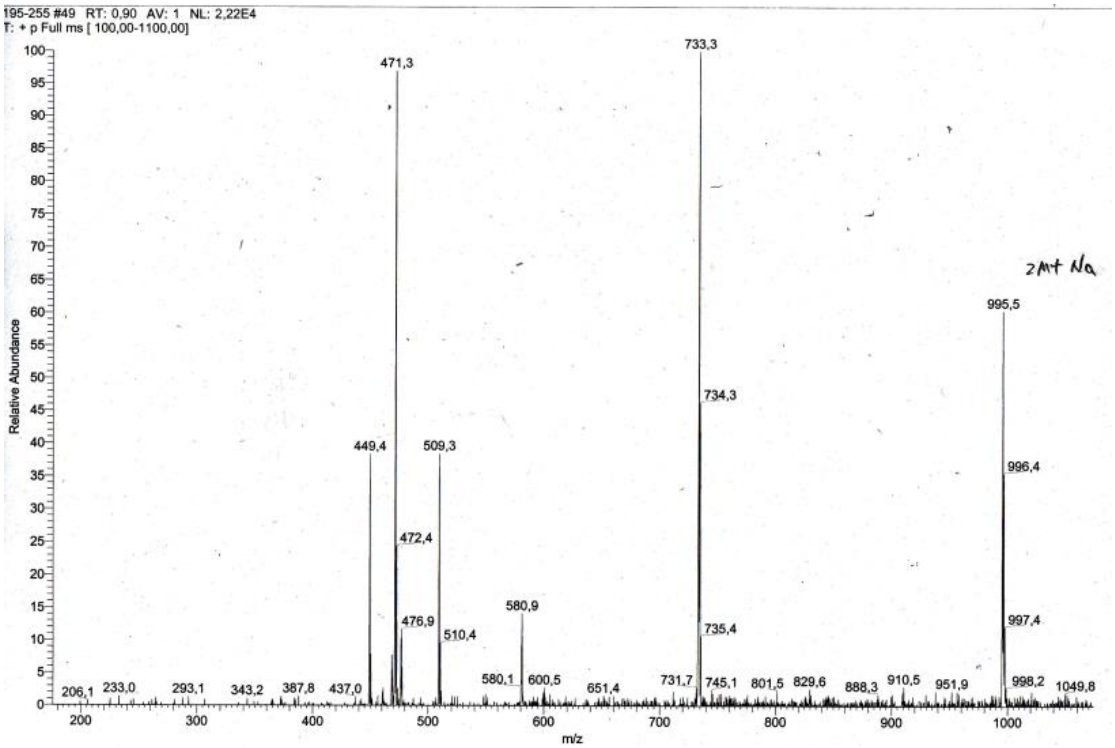


Figure S150. The ESIMS of **7b**.

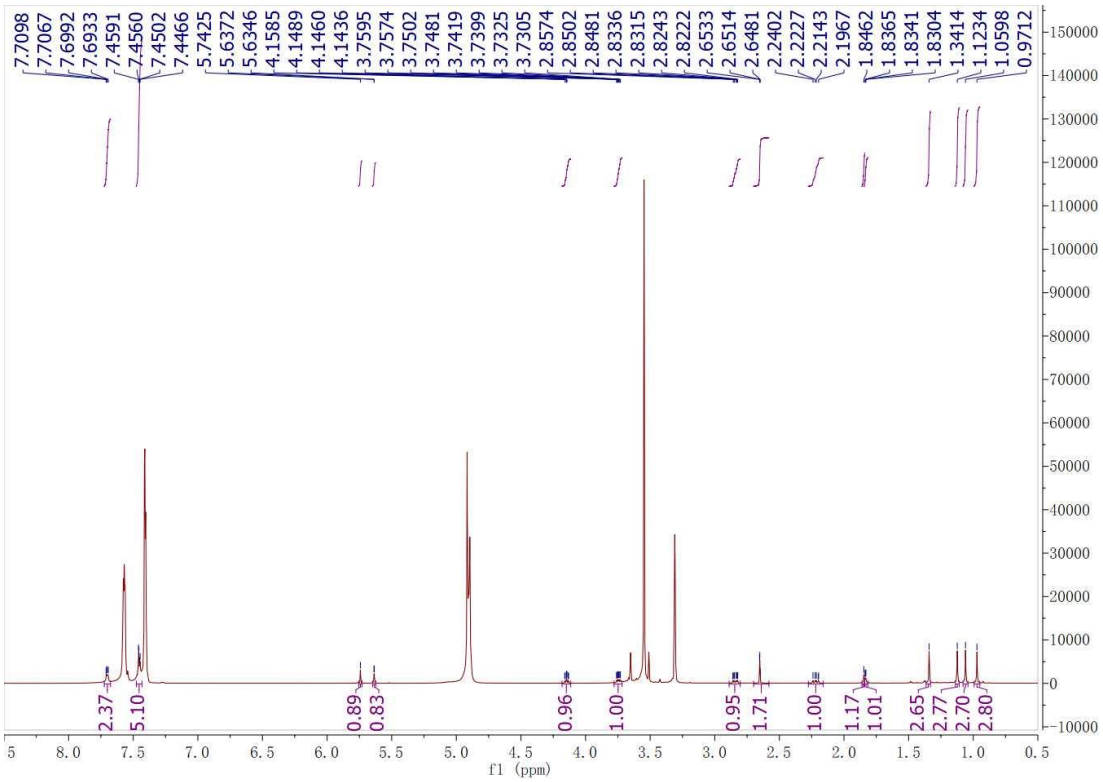


Figure S151. The ^{1}H-NMR (600 MHz, CD_3OD) spectrum of **8a**.

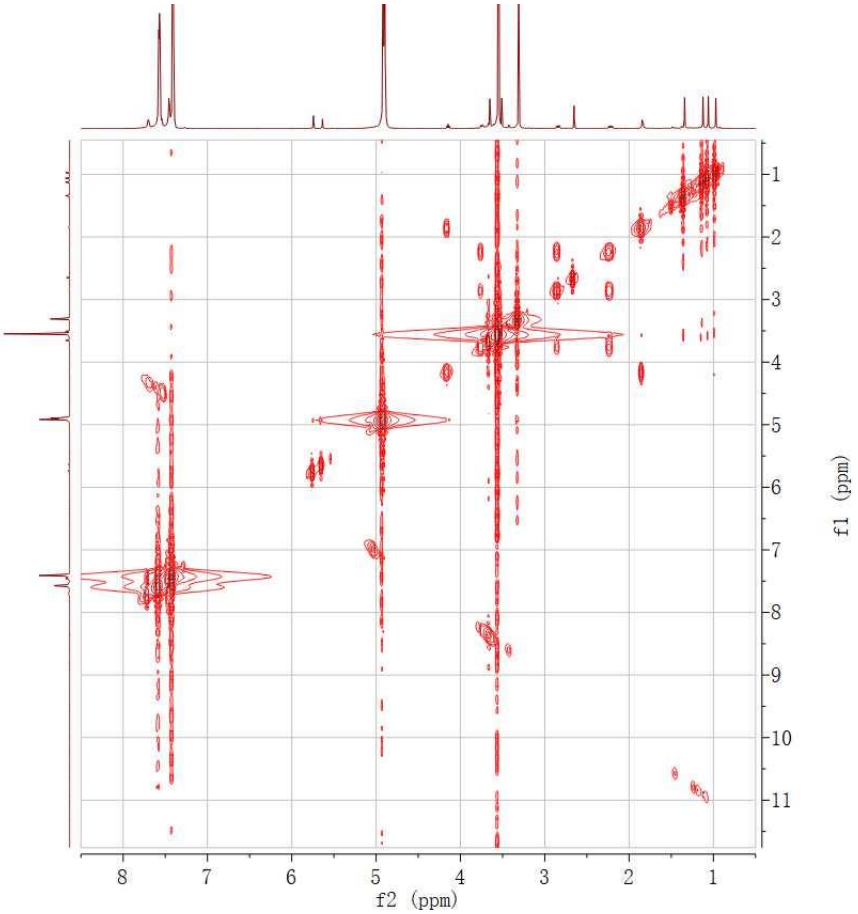


Figure S152. The ^{1}H-^{1}H COSY (600 MHz, CD_3OD) spectrum of **8a**.

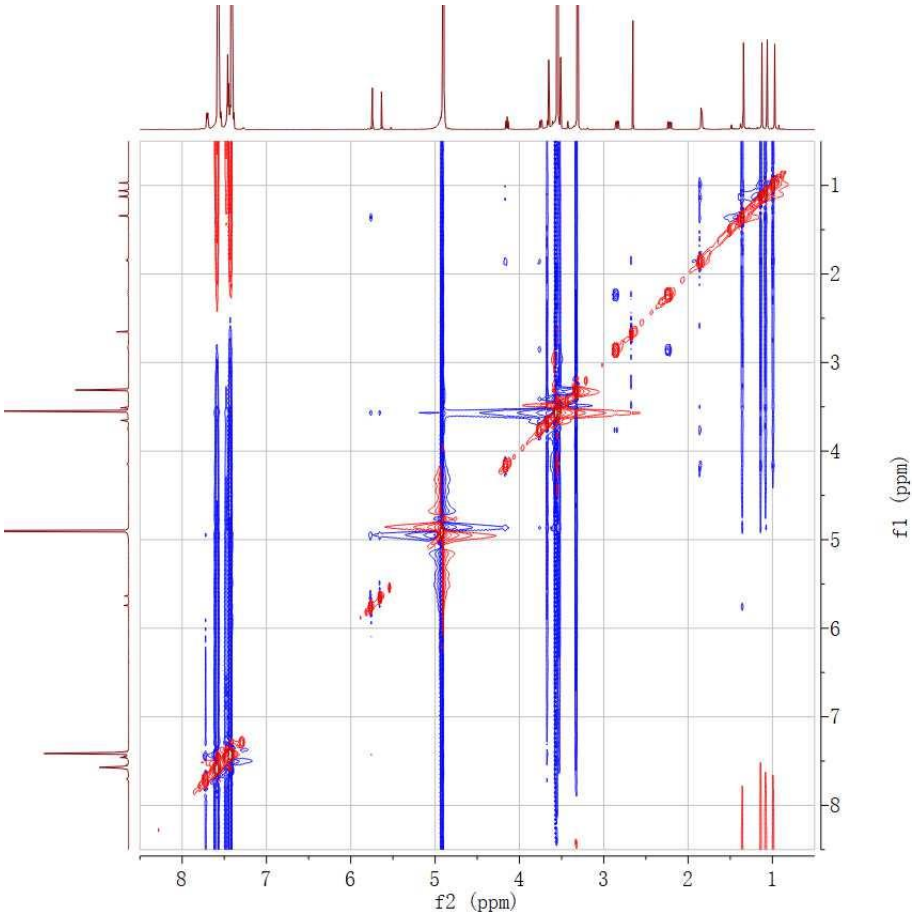


Figure S153. The ROESY (600 MHz, CD_3OD) spectrum of **8a.**

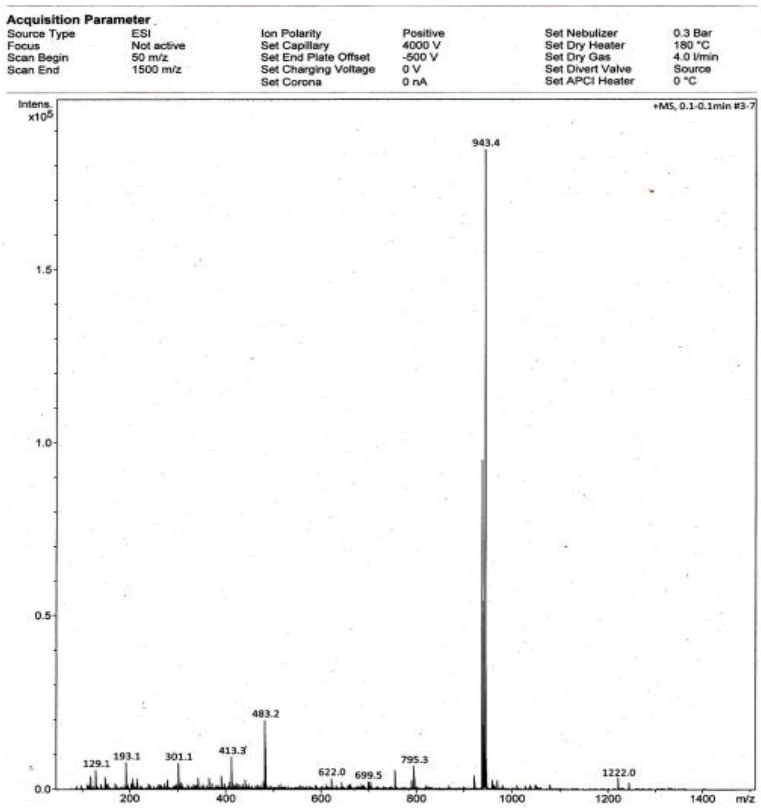


Figure S154. The ESIMS of **8a**.

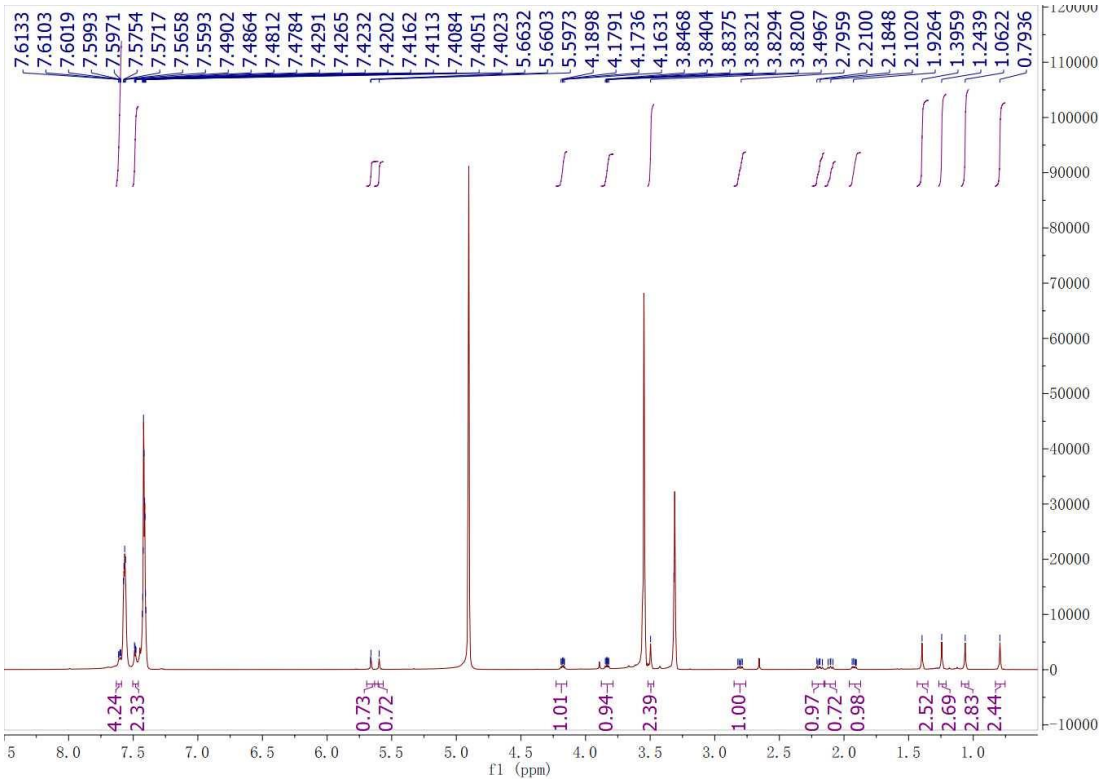


Figure S155. The ^{1}H-NMR (600 MHz, CD_3OD) spectrum of **8b**.

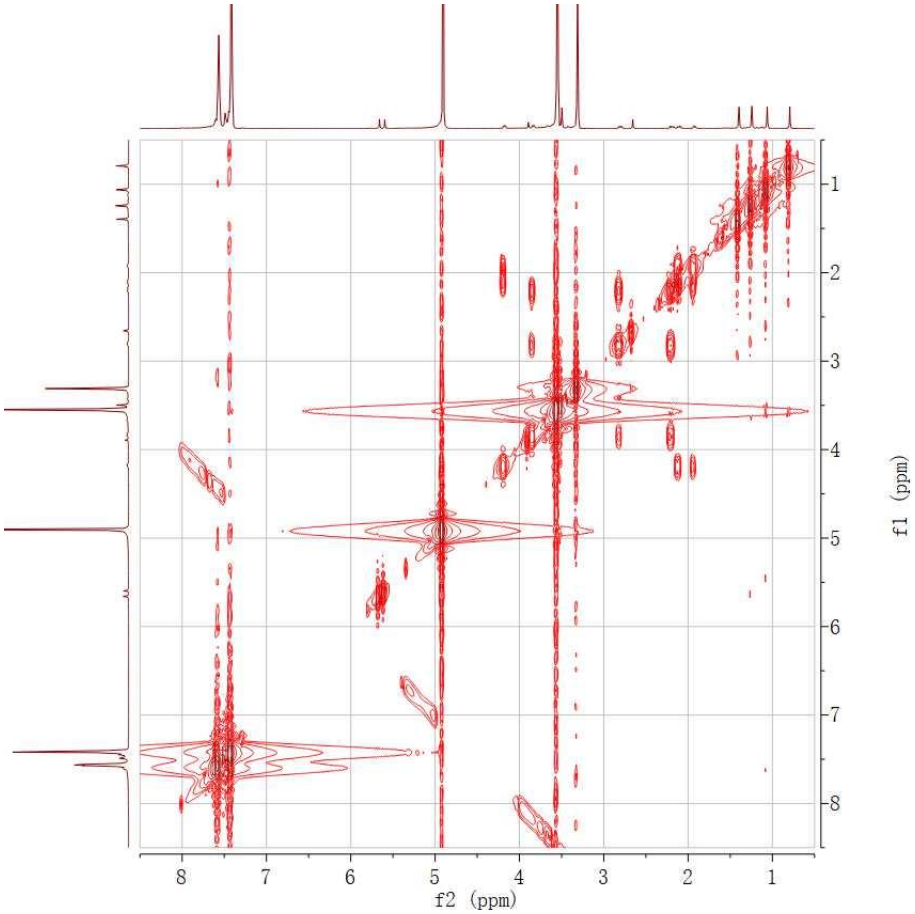


Figure S156. The ^{1}H-^{1}H COSY (600 MHz, CD_3OD) spectrum of **8b**.

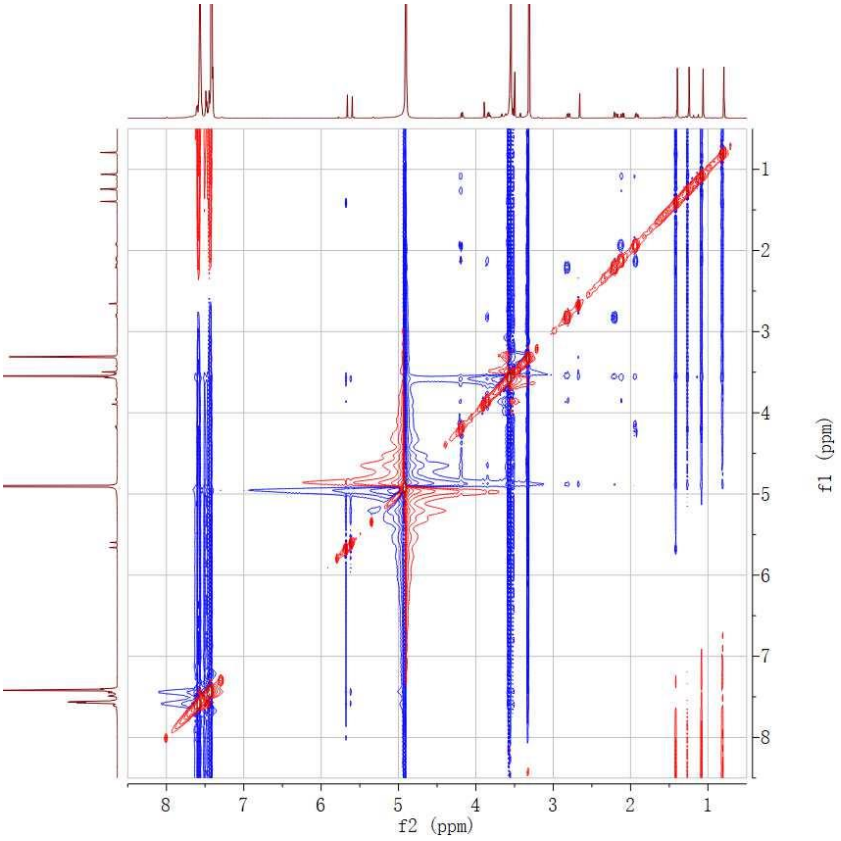


Figure S157. The ROESY (600 MHz, CD_3OD) spectrum of **8b.**

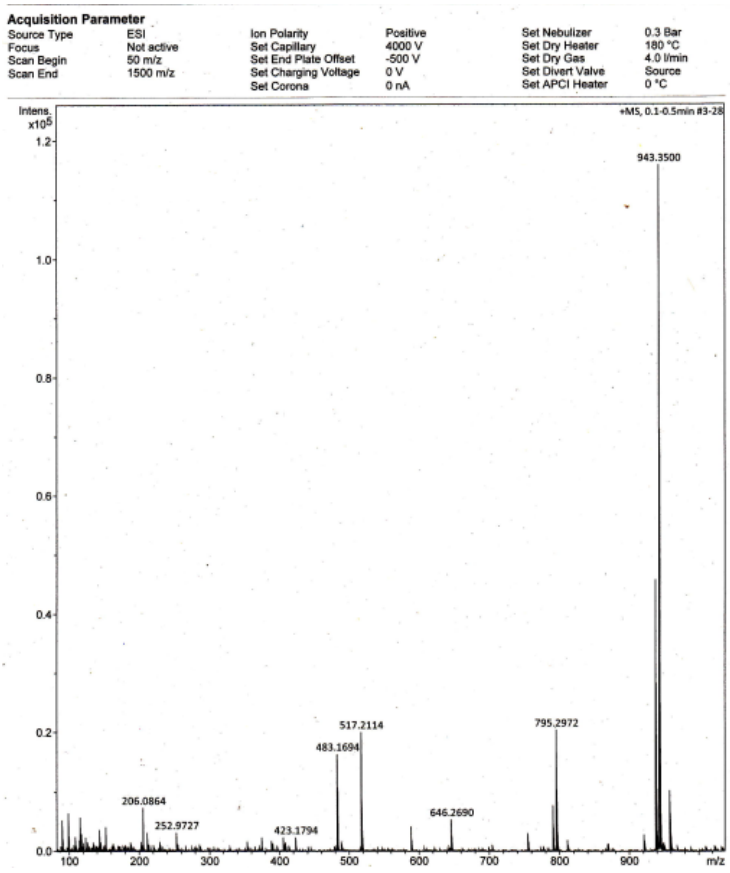


Figure S158. The ESIMS of **8b**.

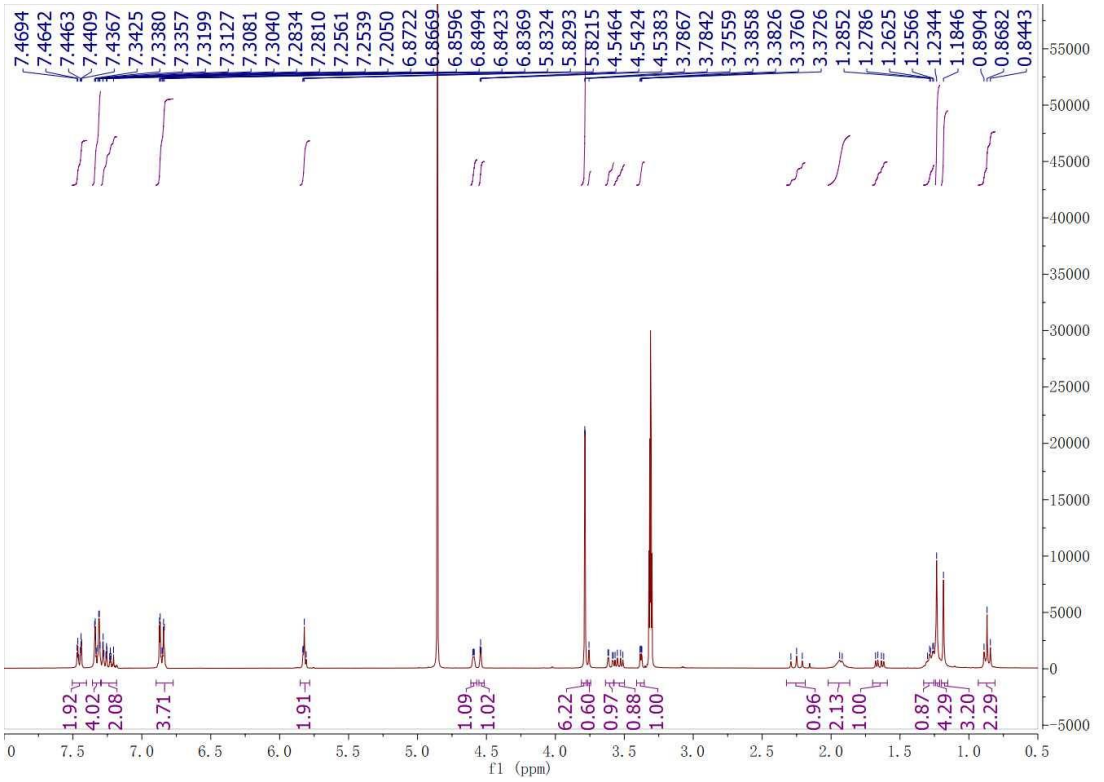


Figure S159. The ^{1}H-NMR (600 MHz, CD_3OD) spectrum of 1**7a**.

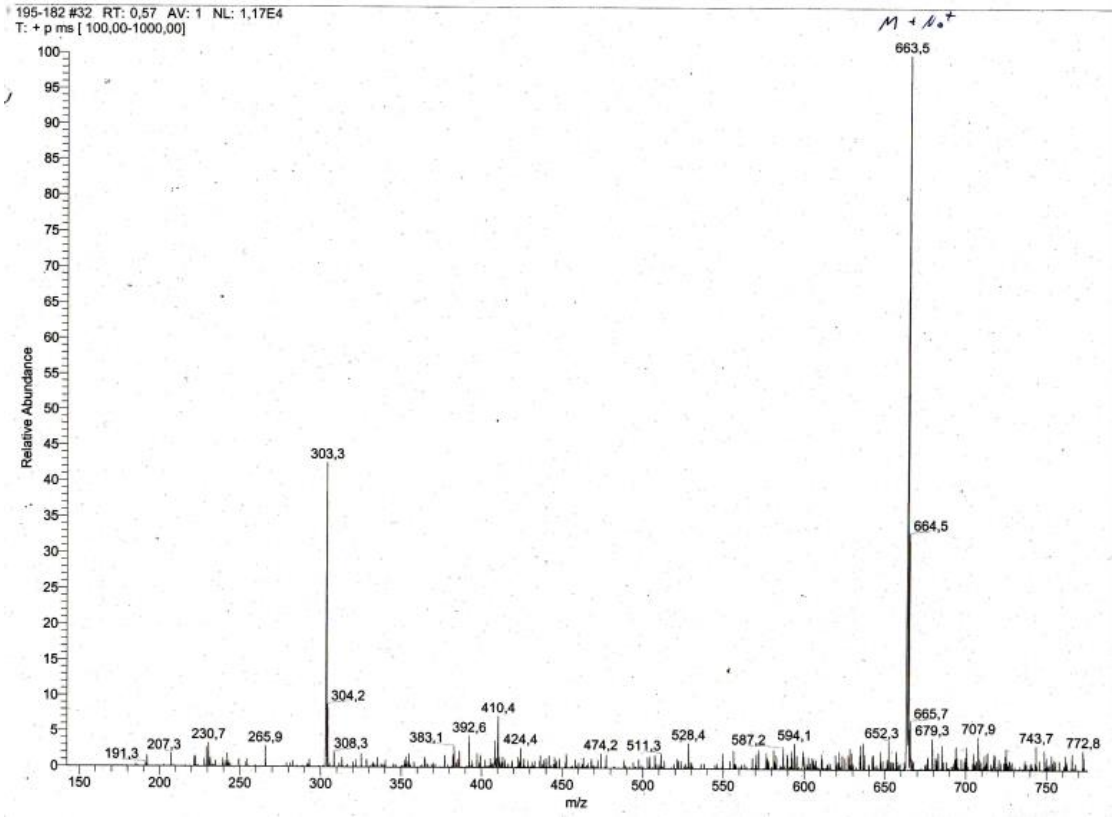


Figure S160. The ESIMS of 1**7a**.

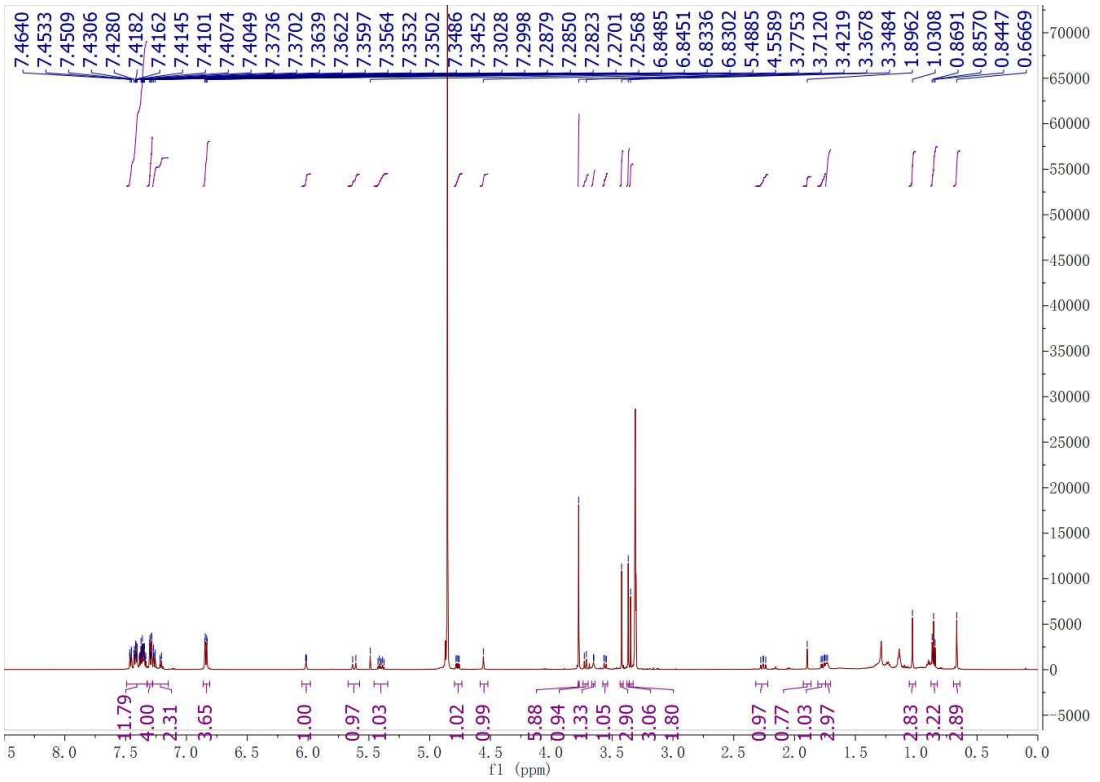


Figure S161. The ^{1}H-NMR (600 MHz, CD_3OD) spectrum of 1**7b**.

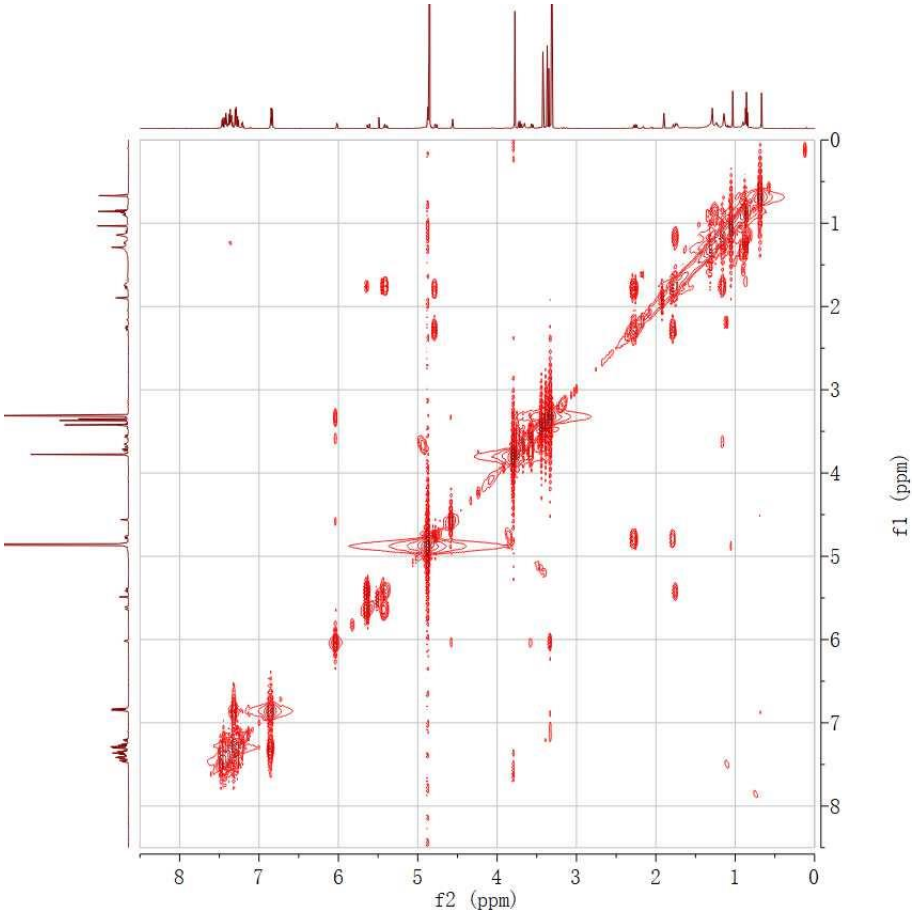


Figure S162. The ^{1}H-^{1}H COSY (600 MHz, CD_3OD) spectrum of 1**7b**.

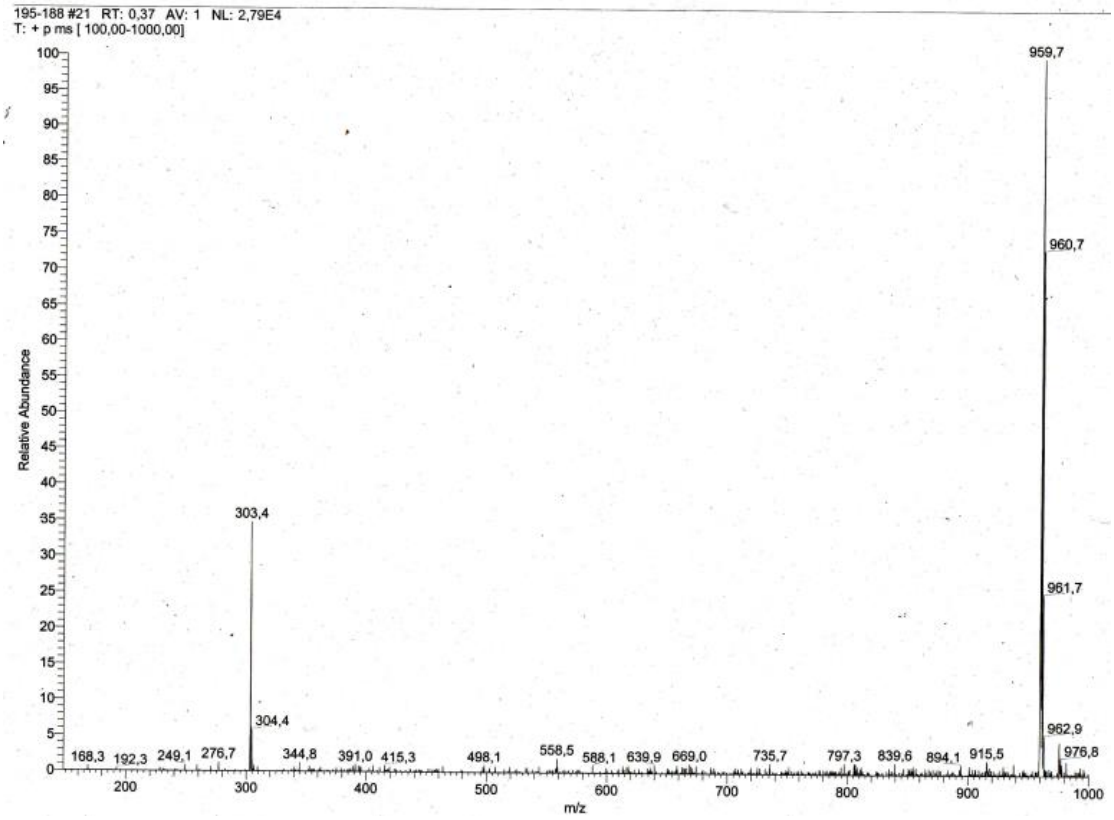


Figure S163. The ESIMS of 1**7b**.

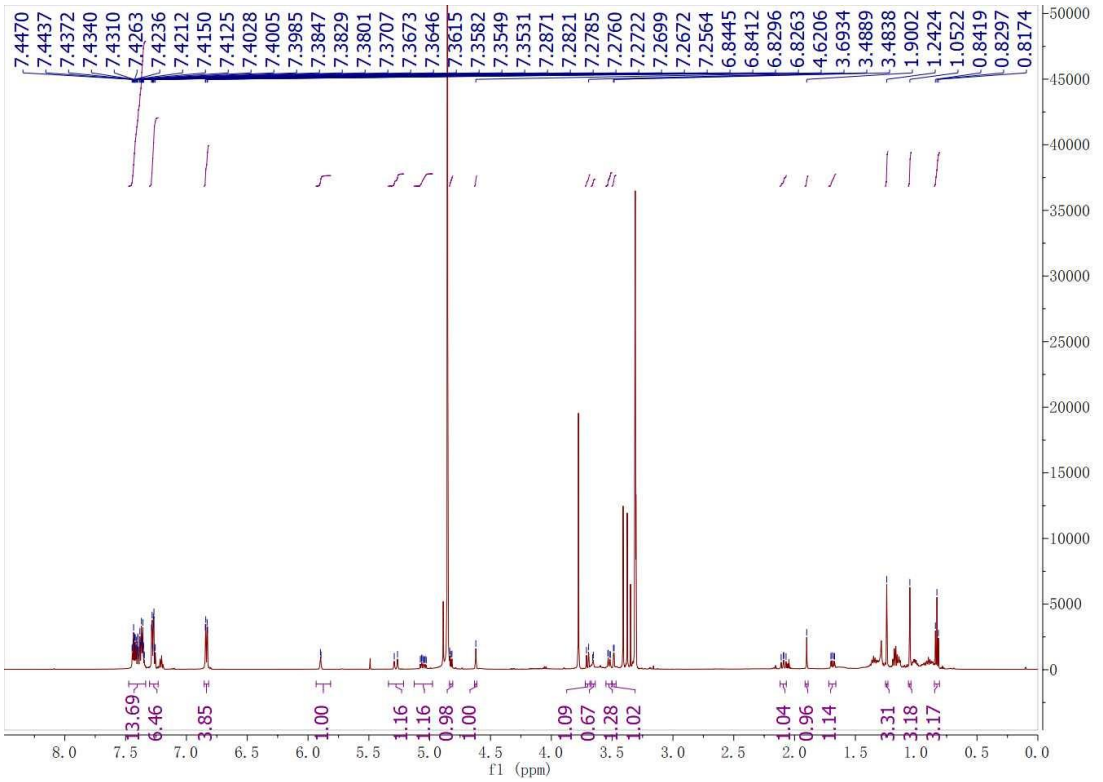


Figure S164. The ^{1}H-NMR (600 MHz, CD_3OD) spectrum of **17c**.

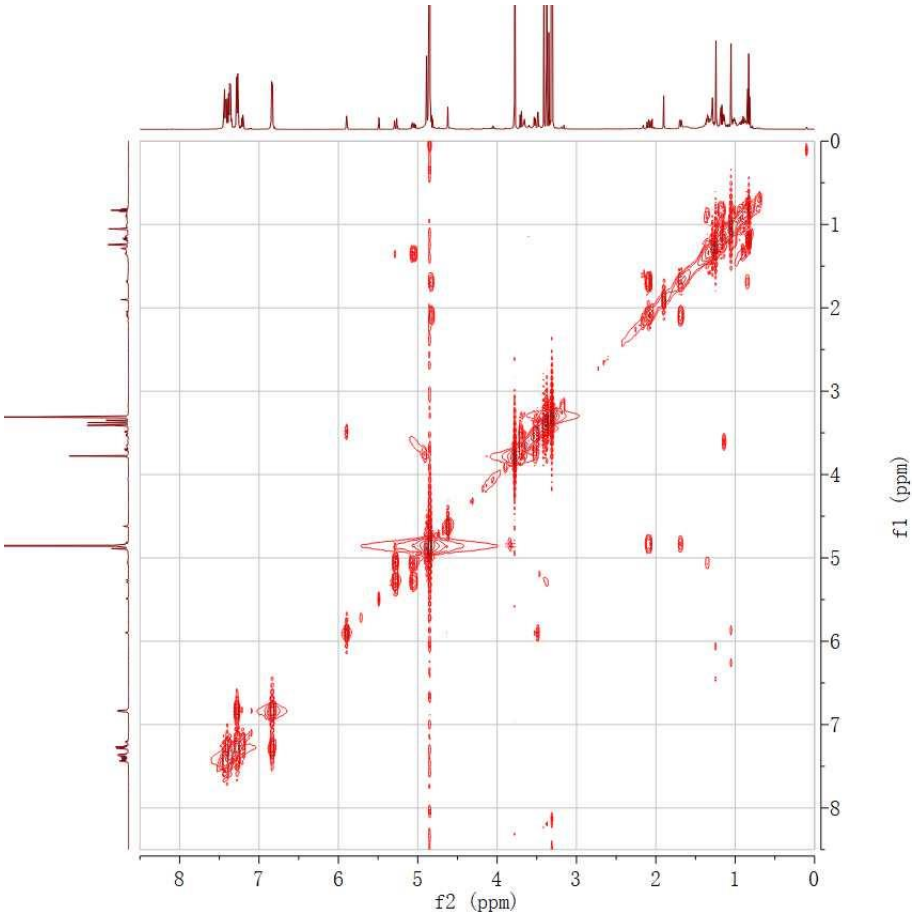


Figure S165. The ^{1}H-^{1}H COSY (600 MHz, CD_3OD) spectrum of 1**7c.**

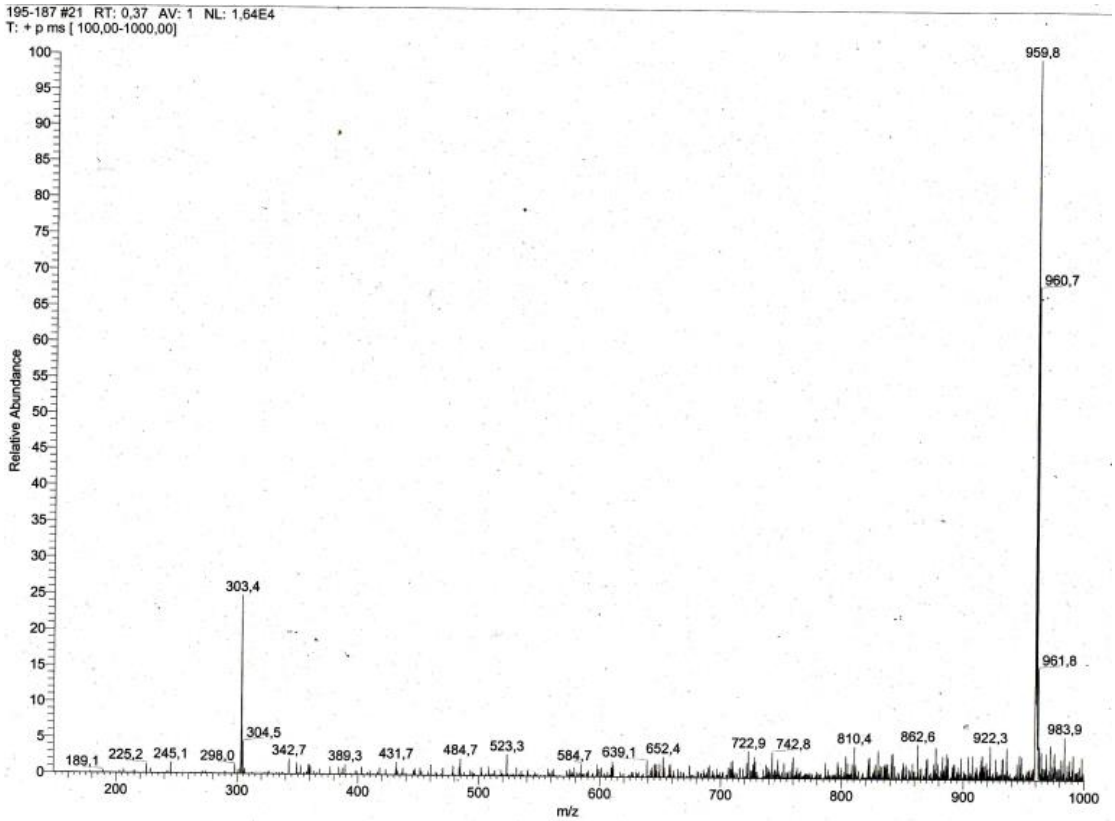


Figure S166. The ESIMS of 1**7c**.

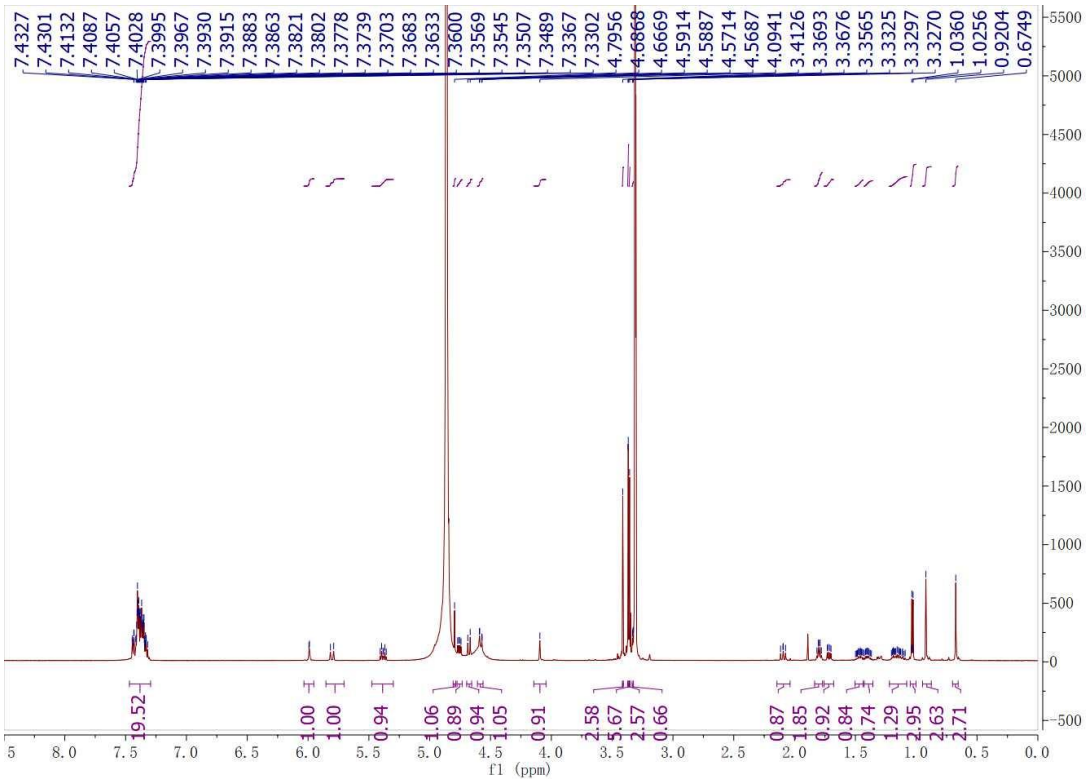


Figure S167. The ^{1}H-NMR (600 MHz, CD_3OD) spectrum of **18a**.

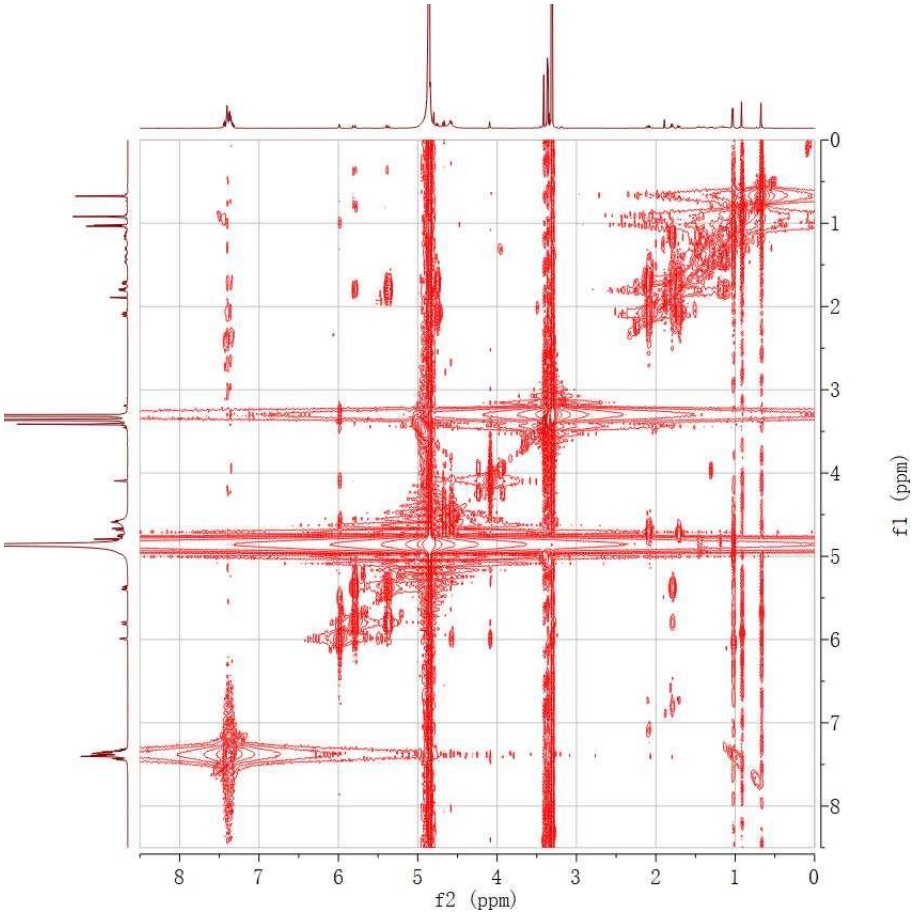


Figure S168. The ^{1}H-^{1}H COSY (600 MHz, CD3OD) spectrum of 1**8a.**

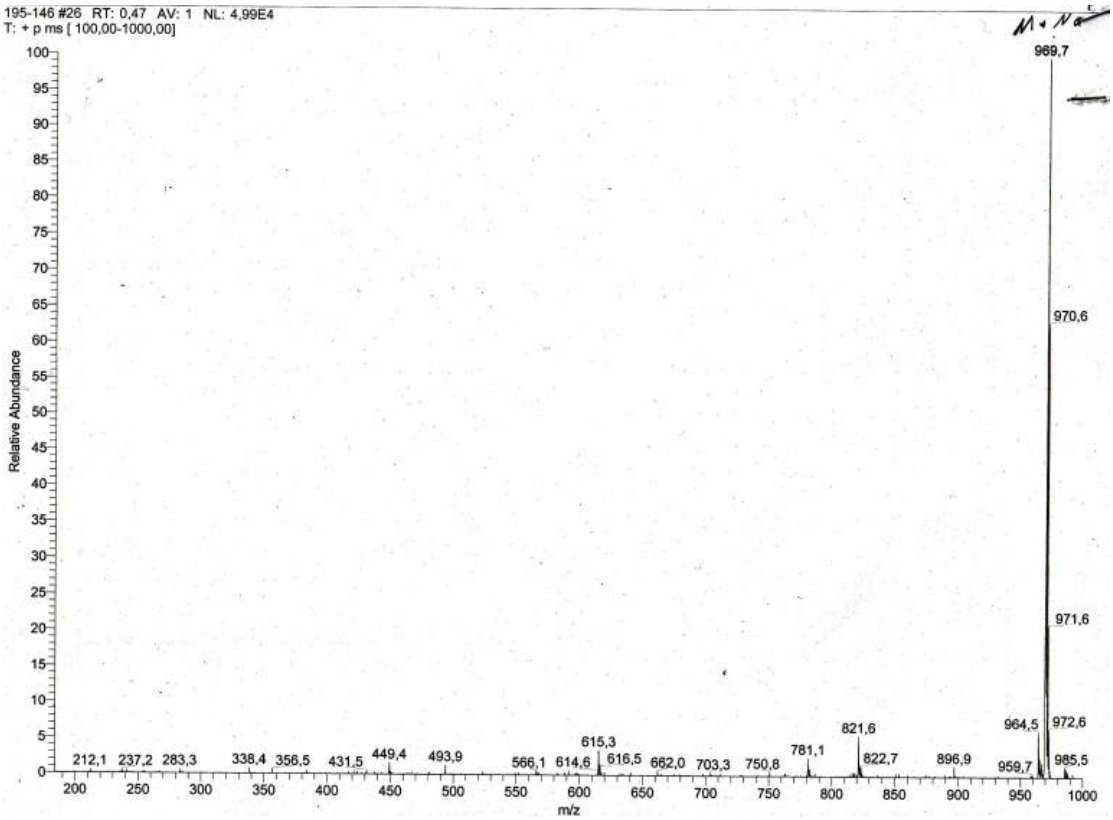


Figure S169. The ESIMS of 1**8a**.

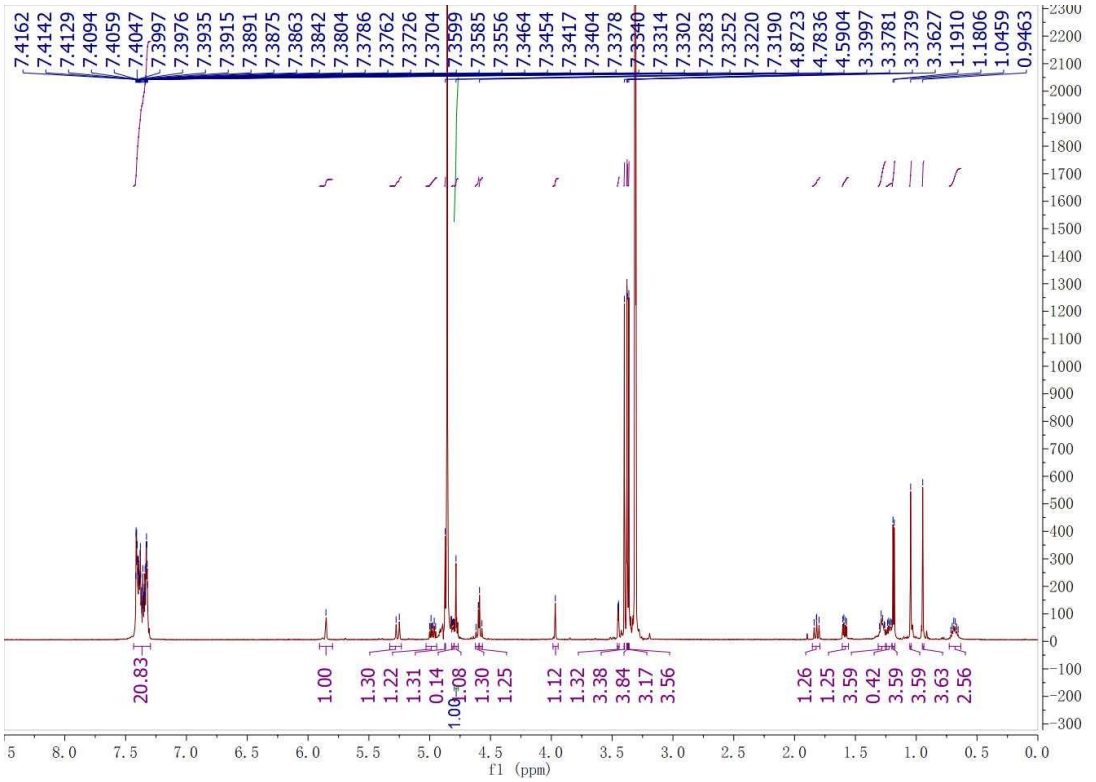


Figure S170. The ^{1}H-NMR (600 MHz, CD_3OD) spectrum of **18b**.

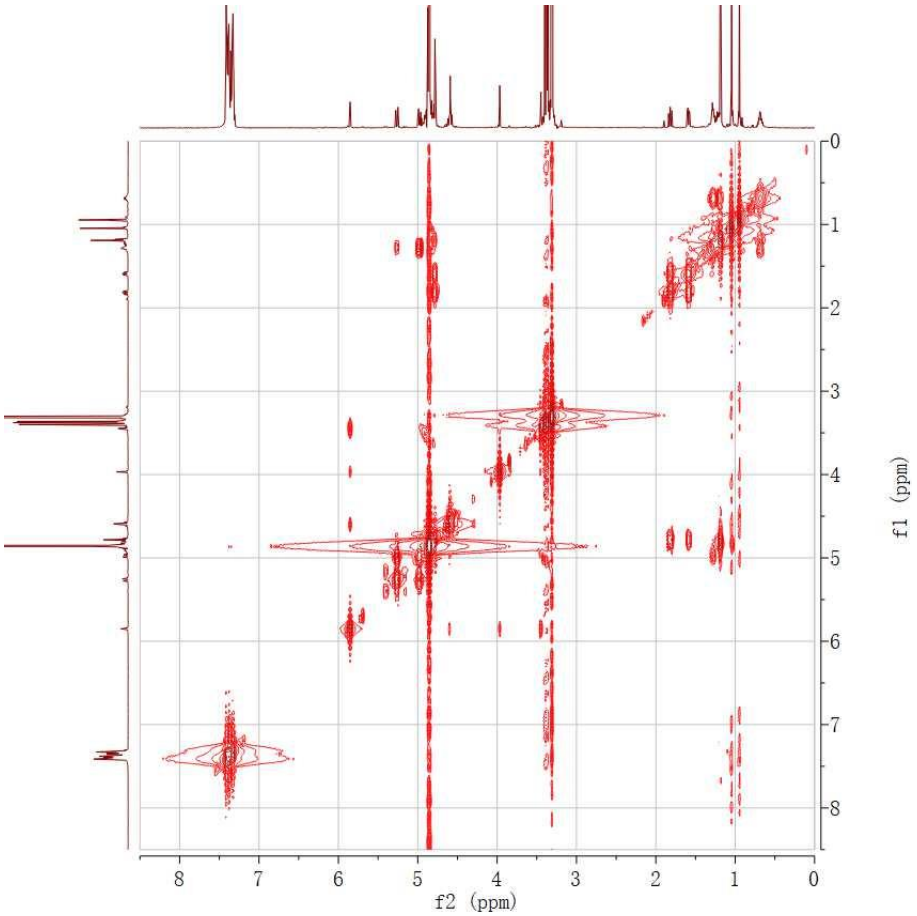


Figure S171. The ^{1}H-^{1}H COSY (600 MHz, CD_3OD) spectrum of 1**8b**.

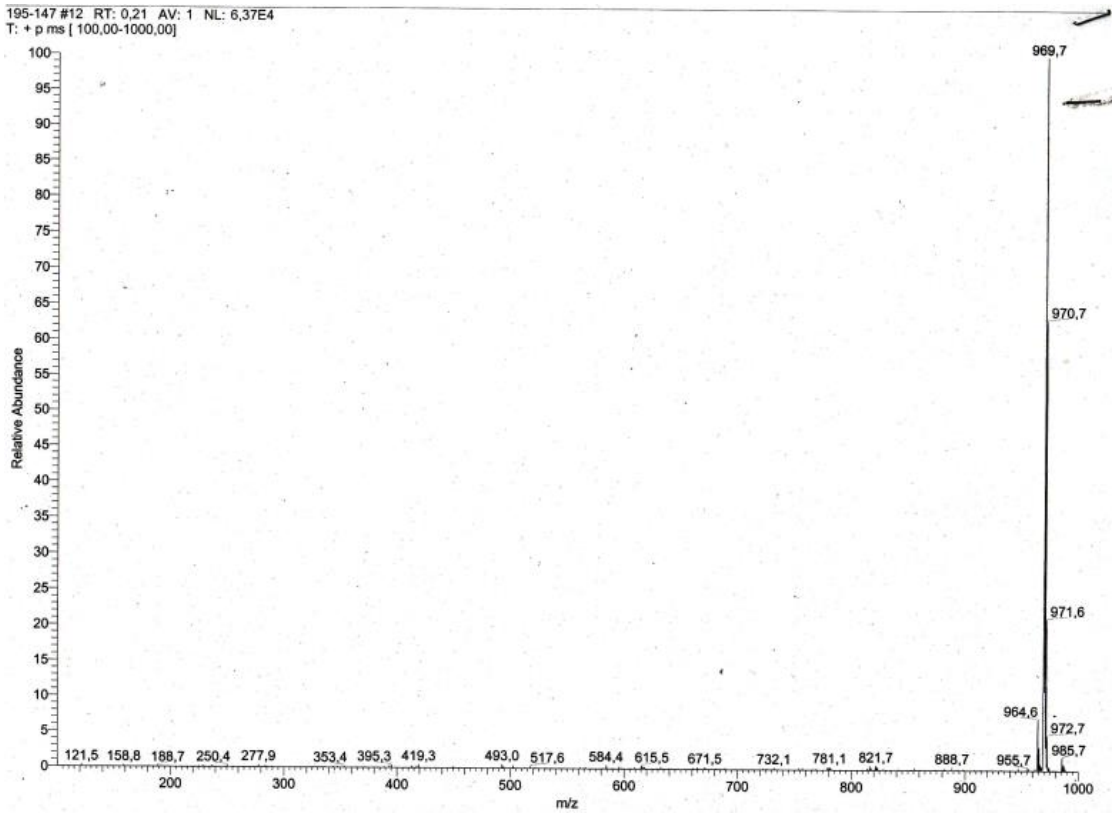


Figure S172. The ESIMS of 1**8b**.

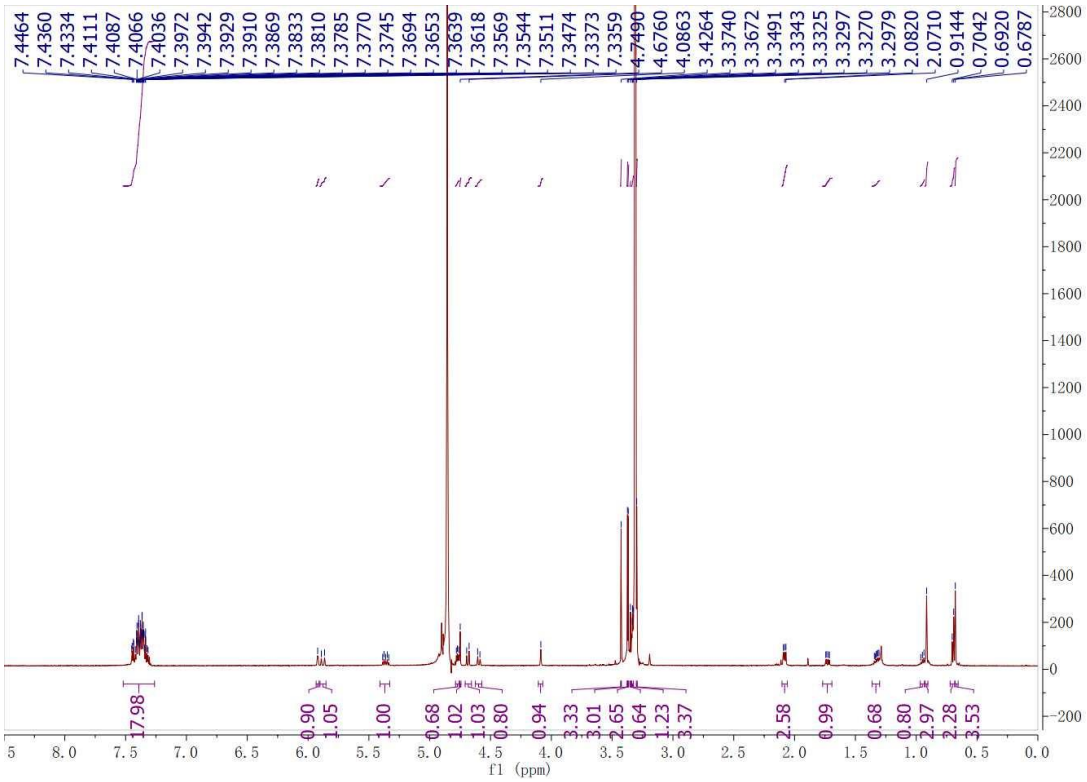


Figure S173. The ^{1}H-NMR (600 MHz, CD_3OD) spectrum of **25a**.

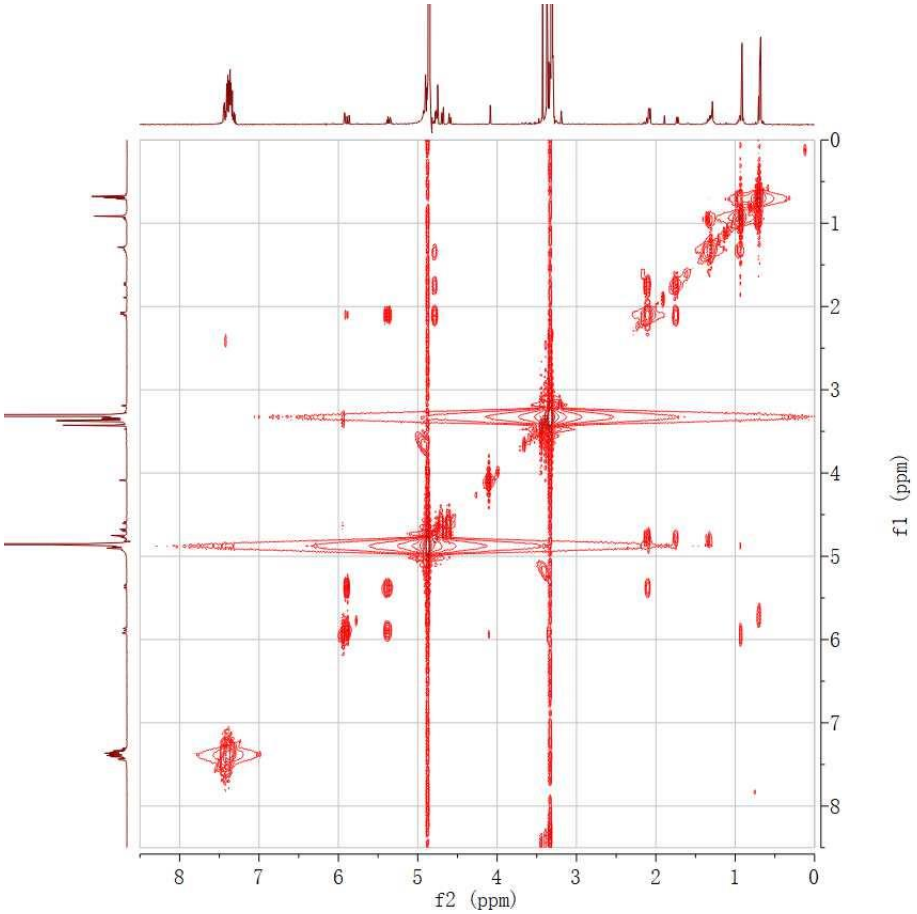


Figure S174. The ^{1}H-^{1}H COSY (600 MHz, CD_3OD) spectrum of **25a**.

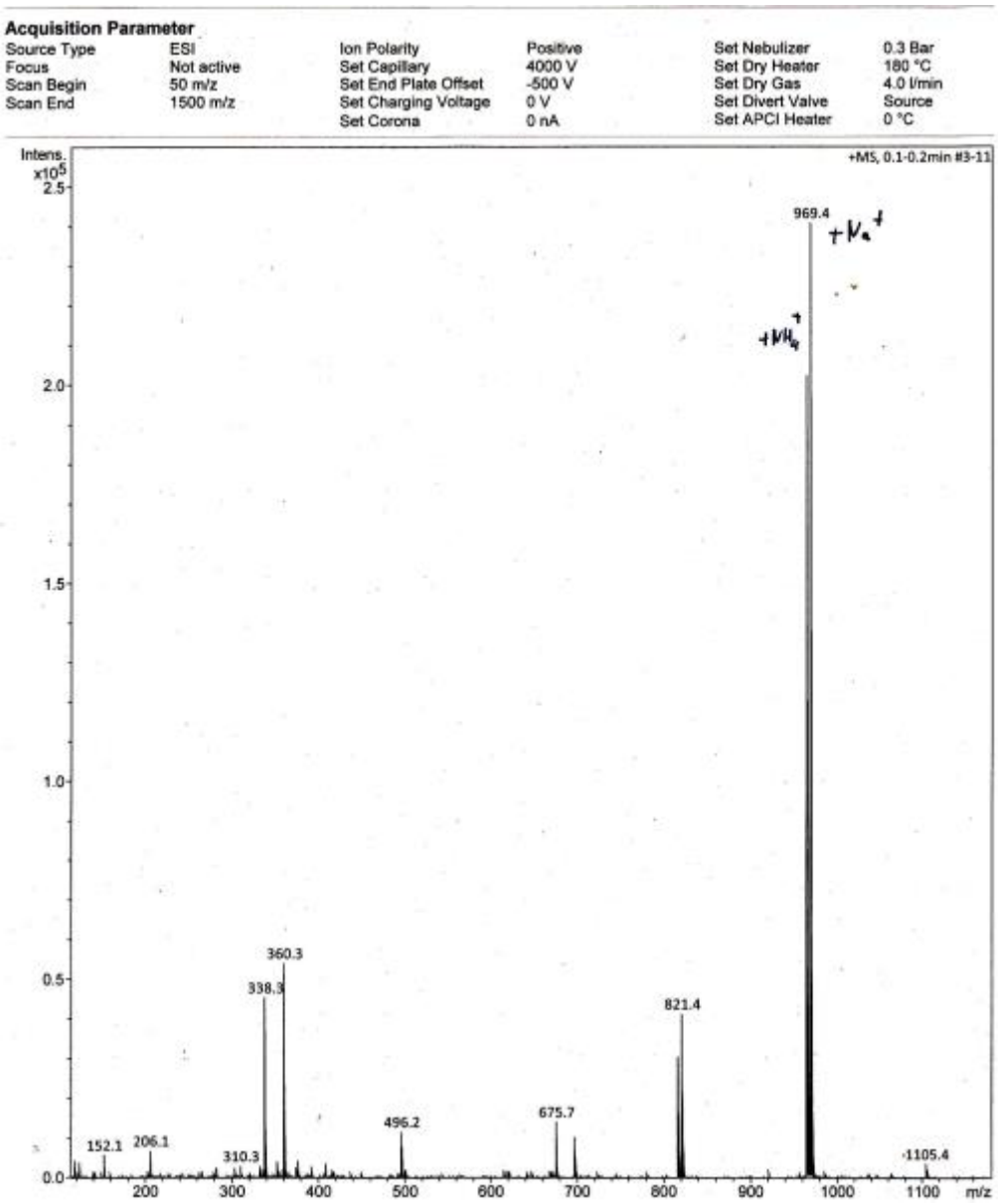


Figure S175. The ESIMS of **25a**.

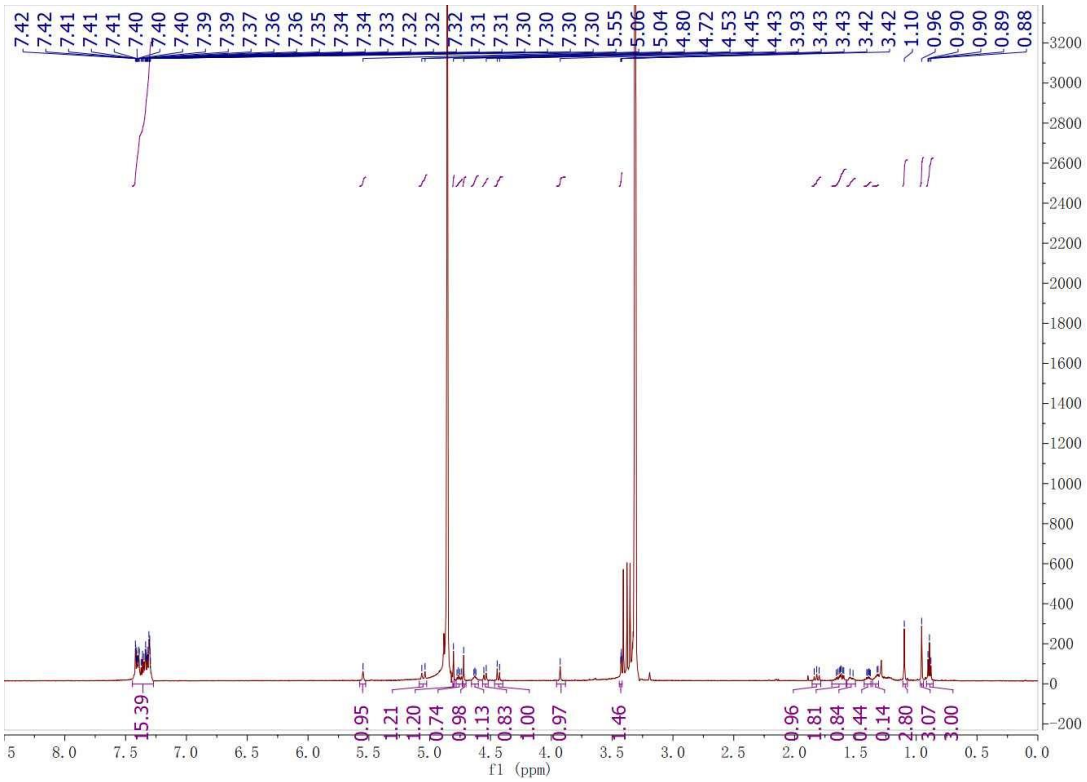


Figure S176. The ^{1}H-NMR (600 MHz, CD_3OD) spectrum of **25b**.

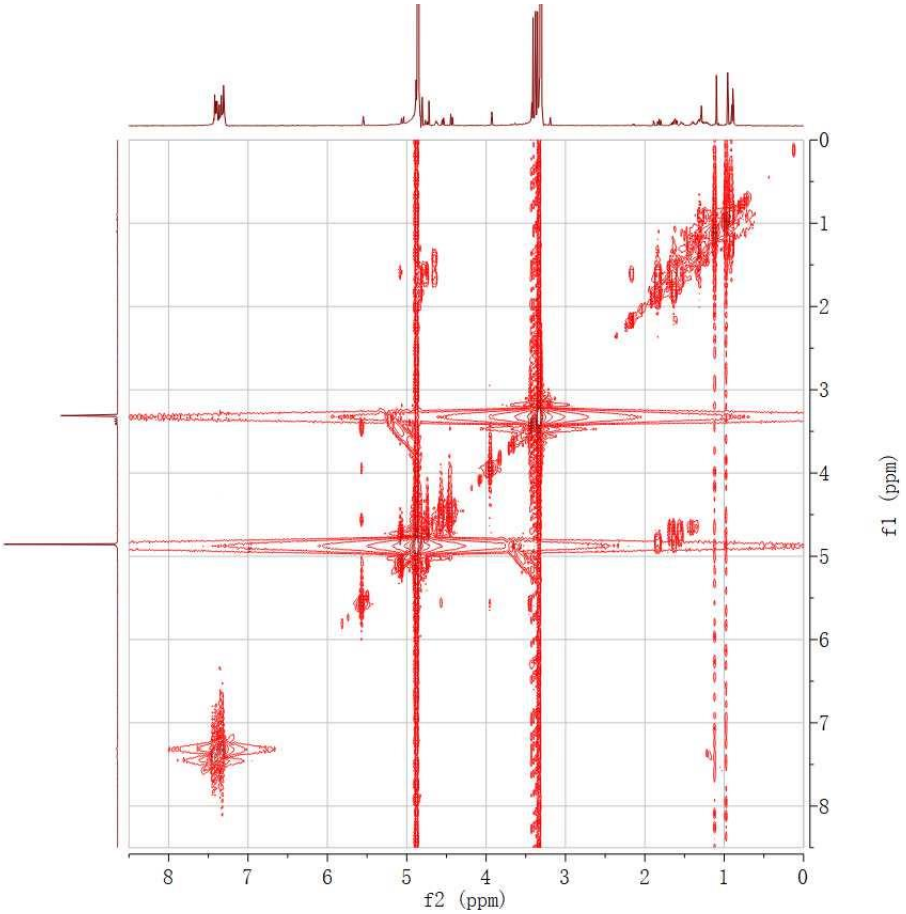


Figure S177. The ^{1}H-^{1}H COSY (600 MHz, CD_3OD) spectrum of **25b**.

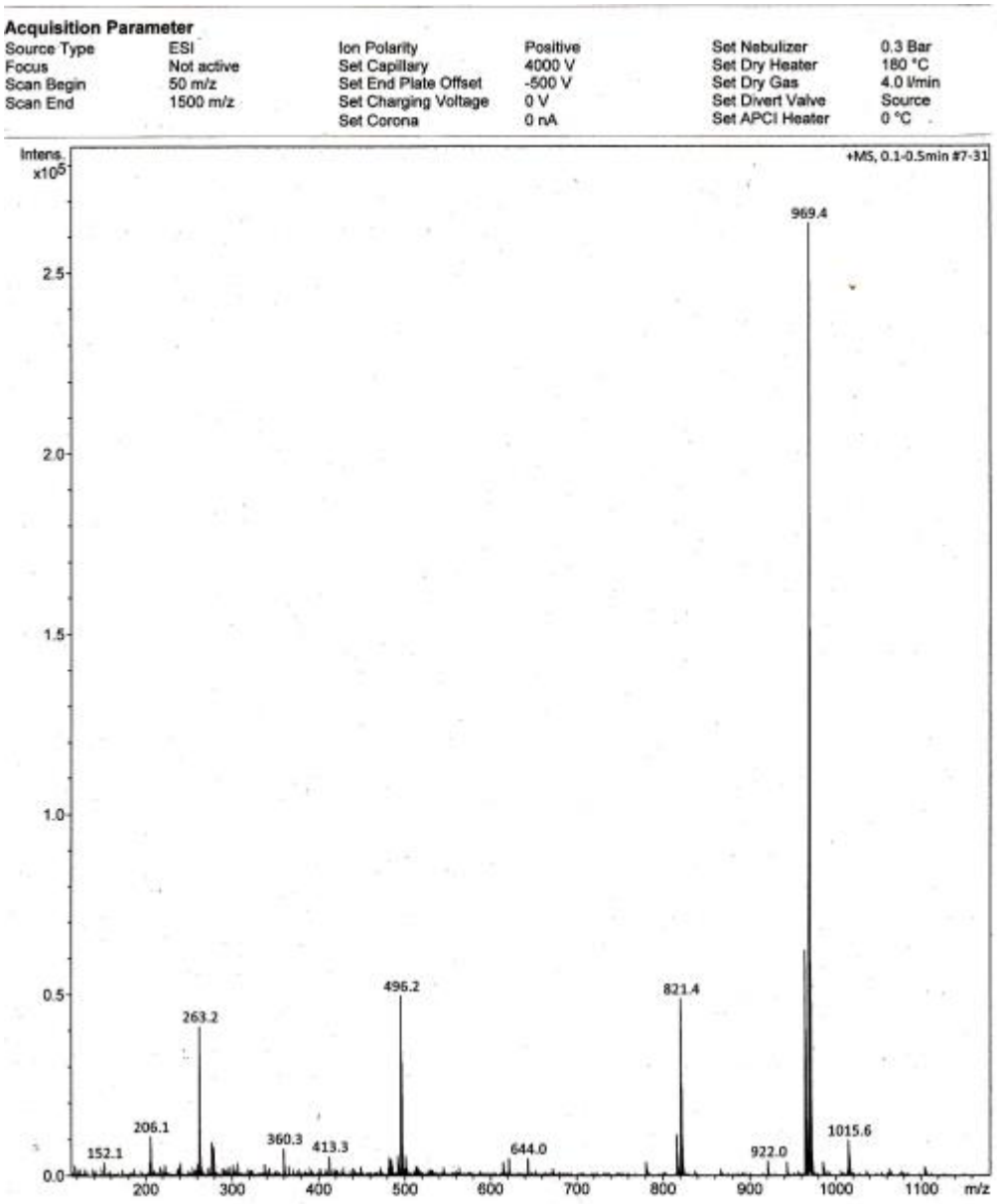


Figure S178. The ESIMS of **25b**.

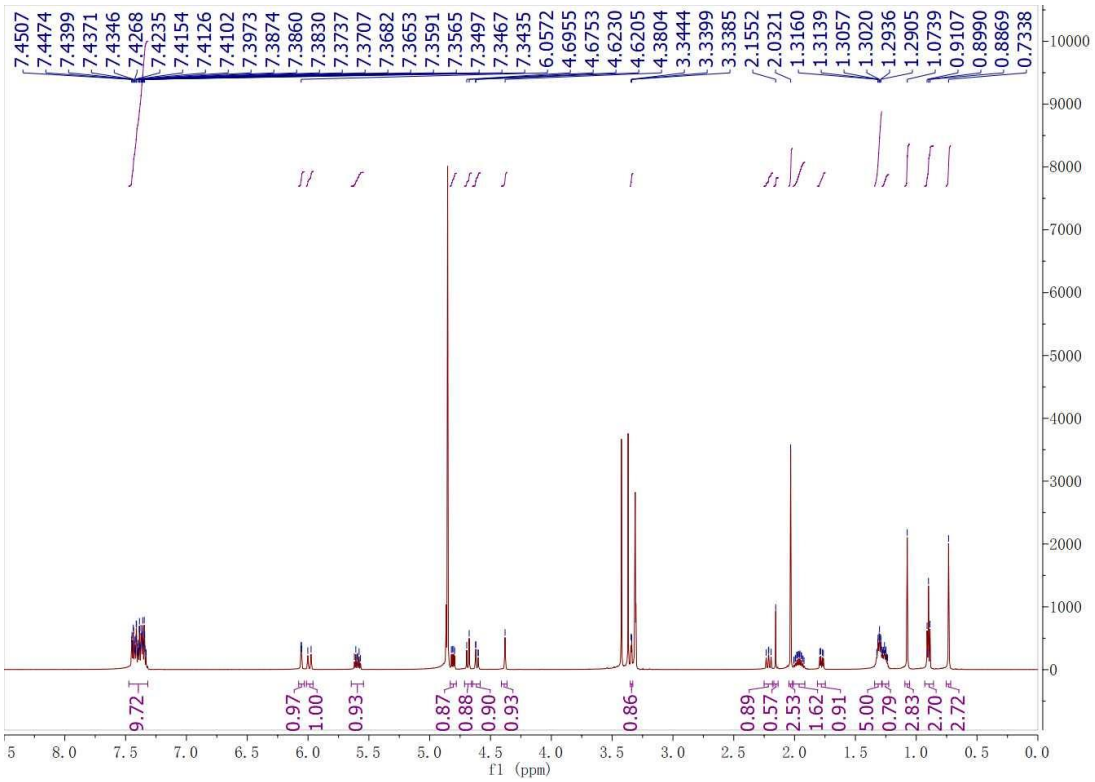


Figure S179. The ^{1}H-NMR (600 MHz, CD_3OD) spectrum of **26a**.

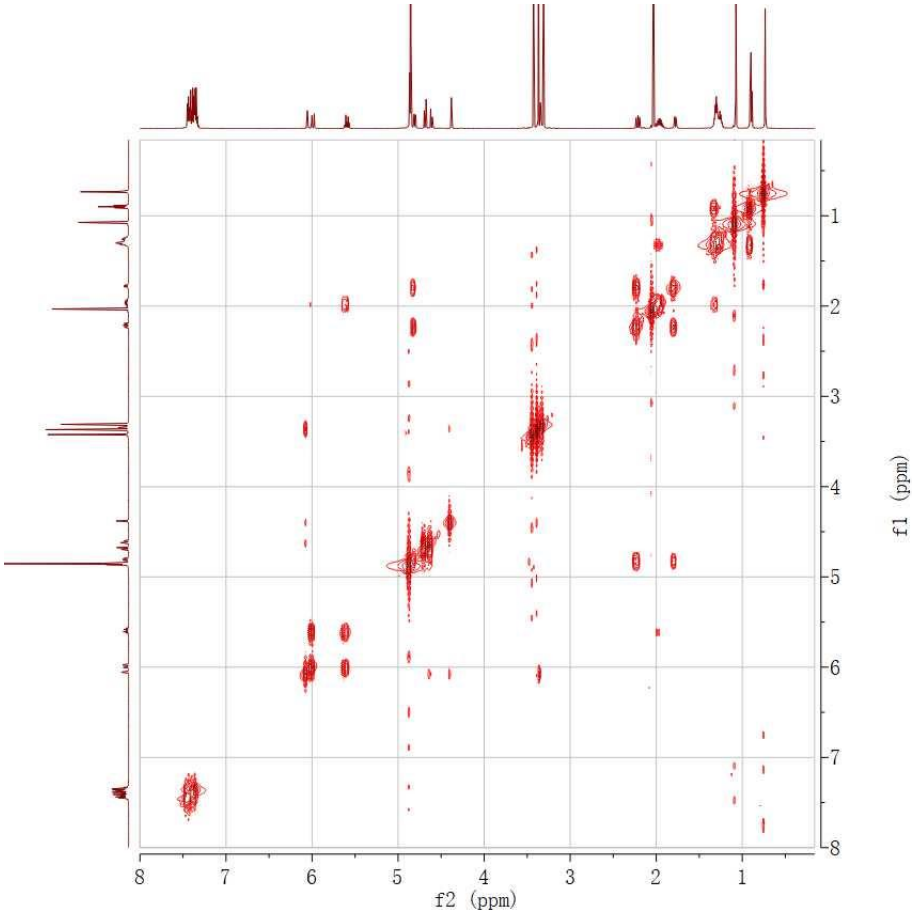


Figure S180. The ^{1}H-^{1}H COSY (600 MHz, CD_3OD) spectrum of **26a**.

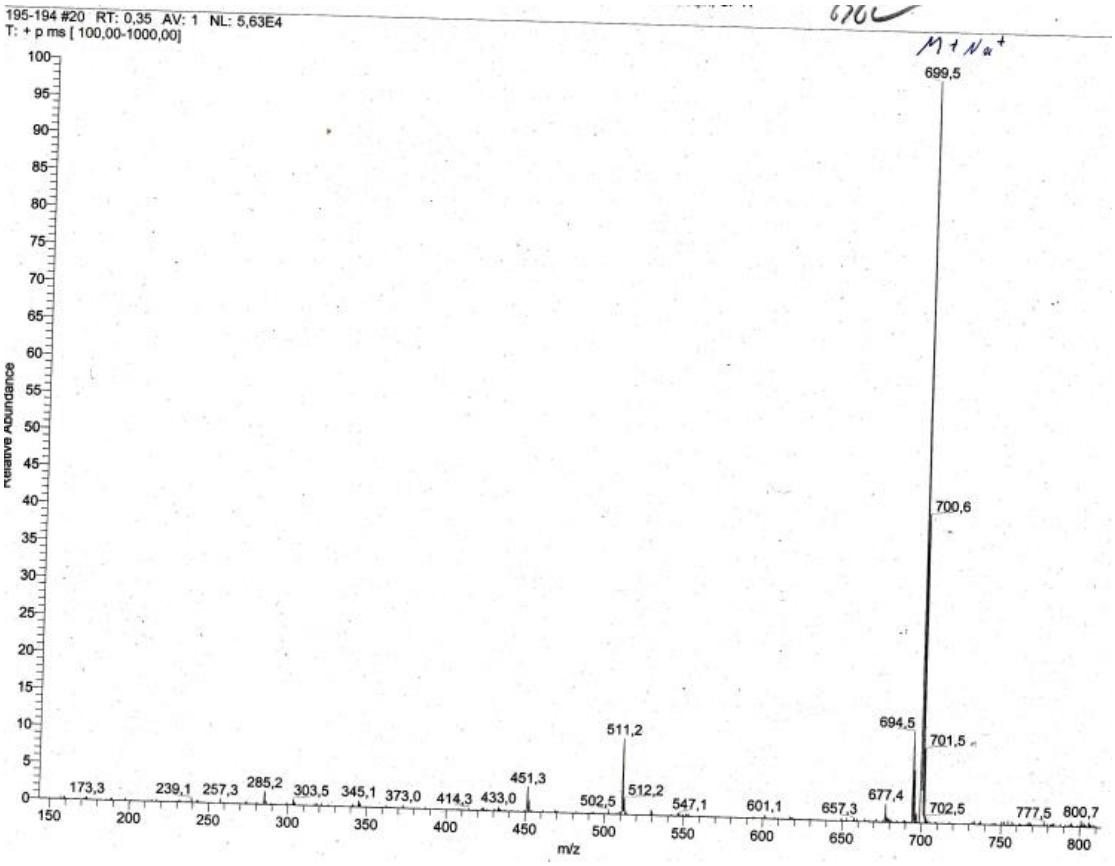


Figure S181. The ESIMS of **26a**.

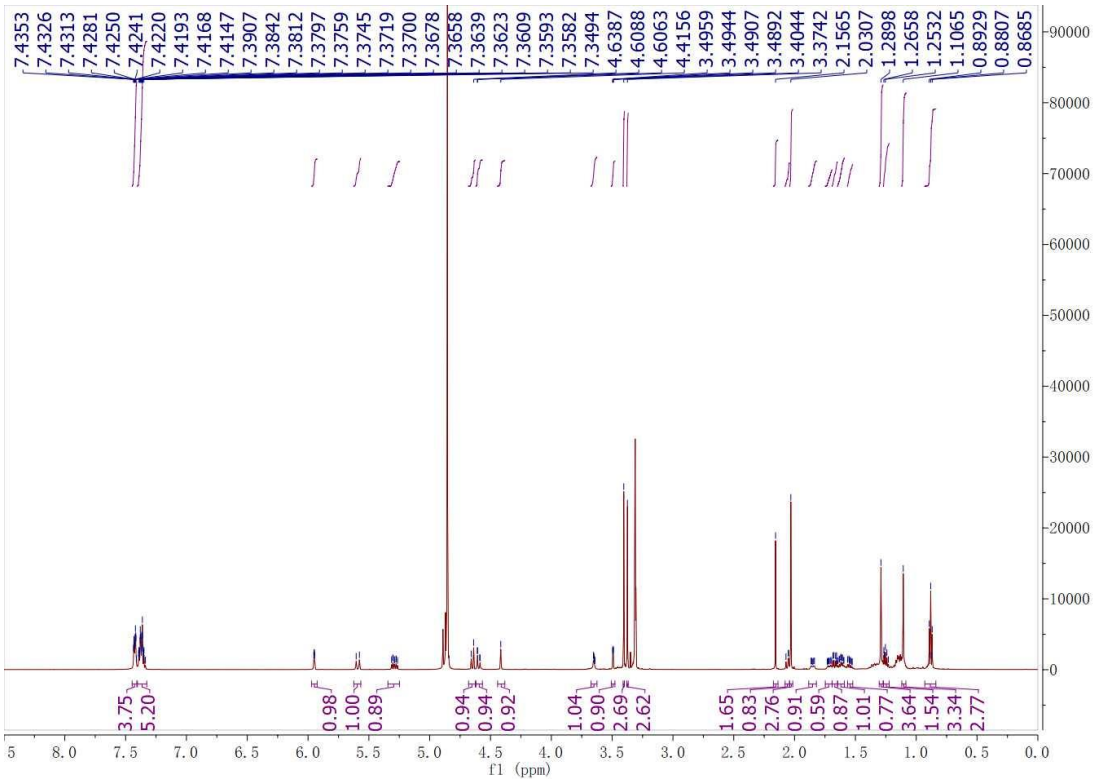


Figure S182. The ^{1}H-NMR (600 MHz, CD_3OD) spectrum of **26b**.

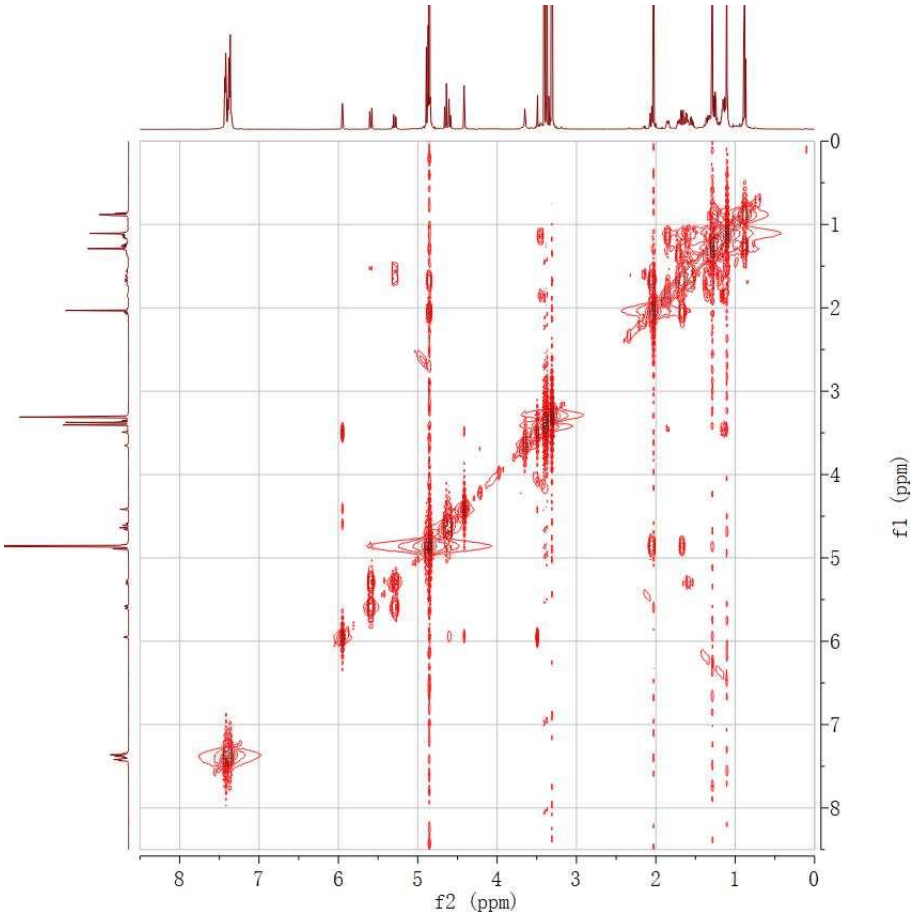


Figure S183. The ^{1}H-^{1}H COSY (600 MHz, CD_3OD) spectrum of **26b**.

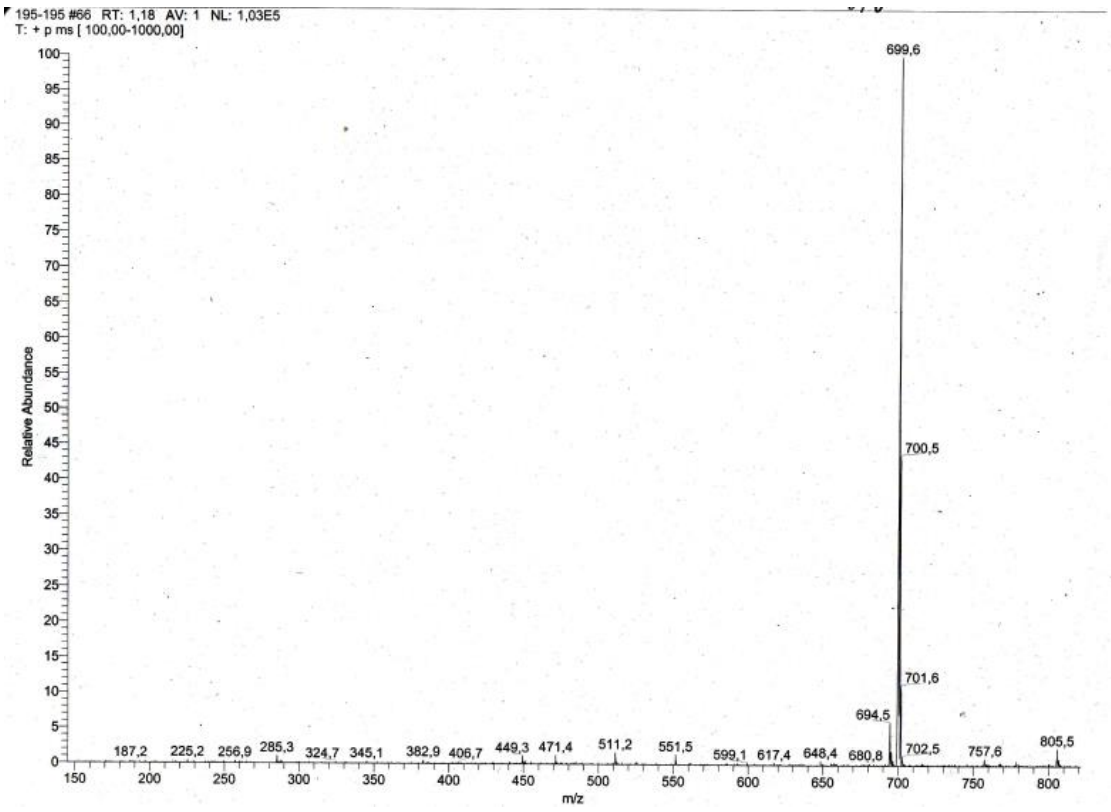


Figure S184. The ESIMS of **26b**.

Table S1. SMILES table of compounds **1**–**26**.

No.	**SMILES**
1	CC(C)(O)[C@H](O1)C[C@]2([R1])[C@]1([H])CC(C(/C=C(C)/C)=O)=C[C@@H]2[R2]
2	CC(C)(O)[C@H](O1)C[C@@]2([R1])[C@]1([H])CC(C(/C=C(C)/C)=O)=C[C@H]2[R2]
3	CC(C)(O)[C@H](O1)C[C@]23[C@]1([H])C/C([C@@H](O)[C@H]2O3)=C/C=C(CO)/C
4	CC(C)(O)[C@H](O1)C[C@@]2(O)[C@]1([H])C=C(C#CC(C)=C)[C@@H](O)[C@H]2O
5	CC(C)(O)C(O1)C[C@]2(O)[C@]1([H])C=C(C#CC(C)=C)[C@@H](O)[C@@H]2O
6	CC(C)(O)[C@H](O1)C[C@]2(O)[C@]1([H])CC([C@@H](O)[C@@H]2O)=[C@]=CC(C)=C
7	CC(C)(O)[C@H](O1)C[C@]2(O)[C@]1([H])CC([C@@H](O)[C@@H]2OC(C)=O)=[C@]=CC(C)=C
8	CC(C)(O)[C@H](O1)C[C@]2(O)[C@]1([H])CC(C([C@H](O)C(C)(C)O3)=O)=C3[C@@H]2O
9	CC(C)(O)[C@H](O1)C[C@]2(O)[C@]1([H])CC(C(C([H])C(C)(C)O3)=O)=C3[C@@H]2OC(C)=O
10	C=C(C)C#C[C@H]1C[C@@](OC(C)(C)[C@@H](O)C2)([H])[C@]2(O3)[C@H]3[C@@H]1O
11	CC(C)(O)[C@H](O1)C[C@]23[C@]1([H])CC([C@@H](O)[C@H]2O3)=[C@]=CC(C)=C
12	CC(C)(O)[C@H](O1)C[C@]2(O)[C@]1([H])CC([C@@H](O)[C@@H]2Cl)=[C@]=CC(C)=C
13	CC(C)(O)[C@H](O1)C[C@]2(O)[C@]1([H])CC(C(C([H])C(C)(C)O3)=O)=C3[C@@H]2O
14	CC1(C)CC(C2=C(O1)C=C(C[C@H](C(C)(O)C)O3)C3=C2)=O
15	O[C@@H]1C(/C=C/CCCCC)=C(CO)[C@@]2([H])OC(C)(C)[C@H](O)C[C@@]2(O)C1[H]
16	O[C@@H]1C(/C=C/CCCCC)=C(CO)[C@@]2([H])OC(C)(C)[C@H](O)C[C@@]2(O)[C@H]1O
17	O[C@@H]1C(/C=C/CCCCC)=C(CO)[C@@]2([H])OC(C)(C)[C@H](O)C[C@@]23[C@@H]1O3
18	O[C@@H]1C(/C=C/CCC([H])[C@@H](O)C)=C(CO)[C@@]2([H])OC(C)(C)[C@H](O)C[C@@]23[C@@H]1O3
19	O[C@@H]1C(/C=C/C[C@H](O)CCC)=C(CO)[C@@]2([H])OC(C)(C)[C@H](O)C[C@@]23[C@@H]1O3
20	O[C@@H]1C(/C=C/[C@@H](O)CCCC)=C(CO)[C@@]2([H])OC(C)(C)[C@H](O)C[C@@]23[C@@H]1O3 or O[C@@H]1C(/C=C/[C@H](O)CCCC)=C(CO)[C@@]2([H])OC(C)(C)[C@H](O)C[C@@]23[C@@H]1O3
21	O[C@@H]1C(/C=C/[C@@H](O)CCCC)=C(CO)[C@@]2([H])OC(C)(C)[C@H](O)C[C@@]23[C@@H]1O3 or O[C@@H]1C(/C=C/[C@H](O)CCCC)=C(CO)[C@@]2([H])OC(C)(C)[C@H](O)C[C@@]23[C@@H]1O3
22	CCCCC/C=C/C1=C(CO)[C@@]2([H])OC(C)(C)[C@H](O)C[C@@]23[C@H](O3)[C@]1([H])OC(C)=O
23	CCCCC/C=C/C1=C(CO)[C@@]2([H])OC(C)(C)[C@H](O)C[C@@]23[C@H](O3)C1=O
24	O[C@@H]1C(/C=C/CCC(O)C([H])C)=C(CO)[C@@]2([H])OC(C)(C)[C@H](O)C[C@@]23[C@@H]1O3
25	O[C@@H]1C(/C=C/C[C@@H](O)CCC)=C(CO)[C@@]2([H])OC(C)(C)[C@H](O)C[C@@]23[C@@H]1O3
26	O[C@@H]1C(/C=C/CCCCC)=C(COC(C)=O)[C@@]2([H])OC(C)(C)[C@H](O)C[C@@]23[C@@H]1O3

Table S2. Results of cytotoxicity and antibacterial activity assay of compounds **1**−**26**.

No.	Antibacterial activity (MIC, μM)					Cell growth (%) at 10 μg/mL	Cytotoxity (IC_{50}, μM)
	A. baumannii (BAA1605)	*A.baumannii* (BAA1605) + colistin (0.1 μM)	*P. aeruginosa* (27853)	*S. aureus* (29213)	*M. tuberculosis* (H37Rv)	Mouse lymphoma cell line L5178Y	
1	>100	>100	>100	>100	>100	58.5	>20
2	>100	>100	>100	>100	>100	65.4	>20
3	>100	>100	>100	>100	>100	64.8	>20
4	>100	>100	>100	>100	>100	77.4	>20
5	>100	>100	>100	>100	>100	64.3	>20
6	>100	>100	>100	>100	>100	68.3	>20
7	>100	>100	>100	>100	>100	67.1	>20
8	>100	>100	>100	>100	>100	77.8	>20
9	>100	>100	>100	>100	>100	53.0	>20
10	>100	>100	>100	>100	>100	56.1	>20
11	>100	>100	>100	>100	>100	76.5	>20
12	>100	>100	>100	>100	>100	66.7	>20
13	>100	>100	>100	>100	>100	77.5	>20
14	>100	>100	>100	>100	>100	67.2	>20
15	>100	>100	>100	>100	>100	54.4	>20
16	>100	>100	>100	>100	>100	53.2	>20
17	>100	>100	>100	>100	>100	70.5	>20
18	>100	>100	>100	>100	>100	64.8	>20
19	>100	>100	>100	>100	>100	78.1	>20
20	>100	>100	>100	>100	>100	70.1	>20
21	>100	>100	>100	>100	>100	63.6	>20
22	>100	50	>100	>100	>100	44.2	>20
23	>100	100	>100	>100	>100	1.90	3.0
24	>100	>100	>100	>100	>100	80.0	>20
25	>100	>100	>100	>100	>100	77.4	>20
26	>100	>100	>100	>100	>100	65.7	>20