Supplementary Materials

Cyclonerane Derivatives from the Algicolous Endophytic Fungus *Trichoderma asperellum* A-YMD-9-2

Yin-Ping Song [1,2,3], Feng-Ping Miao [1,3], Xiang-Hong Liu [1,2,3], Xiu-Li Yin [1,3] and Nai-Yun Ji [1,3,*]

[1] Yantai Institute of Coastal Zone Research, Chinese Academy of Sciences, Yantai 264003, People's Republic of China; ypsong@yic.ac.cn (Y.-P.S.); fpmiao@yic.ac.cn (F.-P.M.); xianghongliu@yic.ac.cn (X.-H.L.); xlyin@yic.ac.cn@yic.ac.cn (X.-L.Y.)

[2] University of Chinese Academy of Sciences, Beijing 100049, People's Republic of China

[3] Center for Ocean Mega-Science, Chinese Academy of Sciences, Qingdao 266071, People's Republic of China

* Correspondence: nyji@yic.ac.cn; Tel.: +86-535-210-9176

Contents

Figure S33. COSY spectrum of compound **5** in $CDCl_3$.

Figure S34. NOESY spectrum of compound **5** in $CDCl_3$.

Figure S35. HREIMS spectrum of compound **5**.

Figure S36. ^{1}H NMR spectrum of compound **6** in $CDCl_3$.

Figure S37. ^{13}C NMR and DEPT spectra of compound **6** in $CDCl_3$.

Figure S38. HSQC spectrum of compound **6** in $CDCl_3$.

Figure S39. HMBC spectrum of compound **6** in $CDCl_3$.

Figure S40. COSY spectrum of compound **6** in $CDCl_3$.

Figure S41. NOESY spectrum of compound **6** in $CDCl_3$.

Figure S42. HREIMS spectrum of compound **6**.

Figure S43. ^{1}H NMR spectrum of compound **7** in $CDCl_3$.

Figure S44. ^{13}C NMR and DEPT spectra of compound **7** in $CDCl_3$.

Figure S45. HSQC spectrum of compound **7** in $CDCl_3$.

Figure S46. HMBC spectrum of compound **7** in $CDCl_3$.

Figure S47. COSY spectrum of compound **7** in $CDCl_3$.

Figure S48. NOESY spectrum of compound **7** in $CDCl_3$.

Figure S49. HREIMS spectrum of compound **7**.

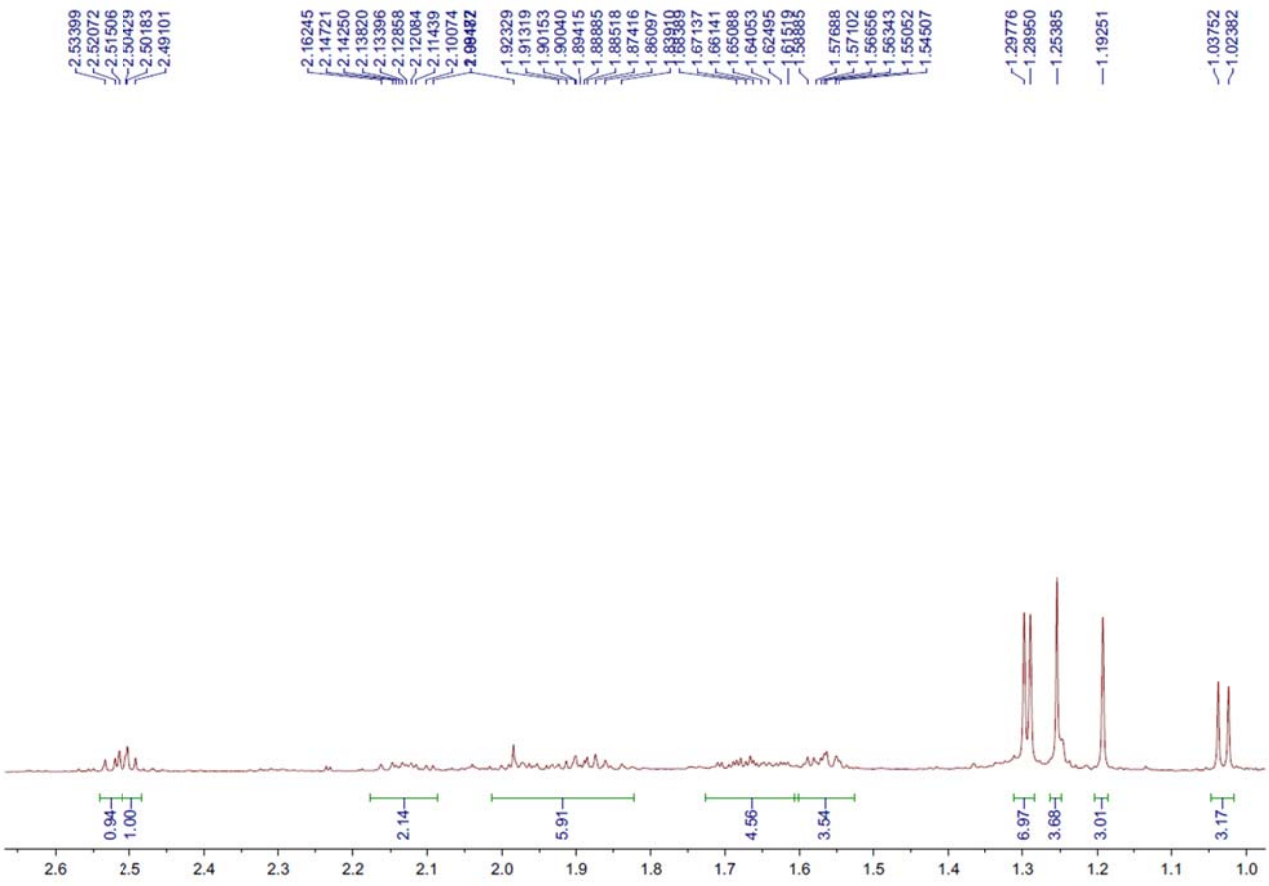


Figure S1. ^{1}H NMR spectrum of compound **1** in $CDCl_3$.

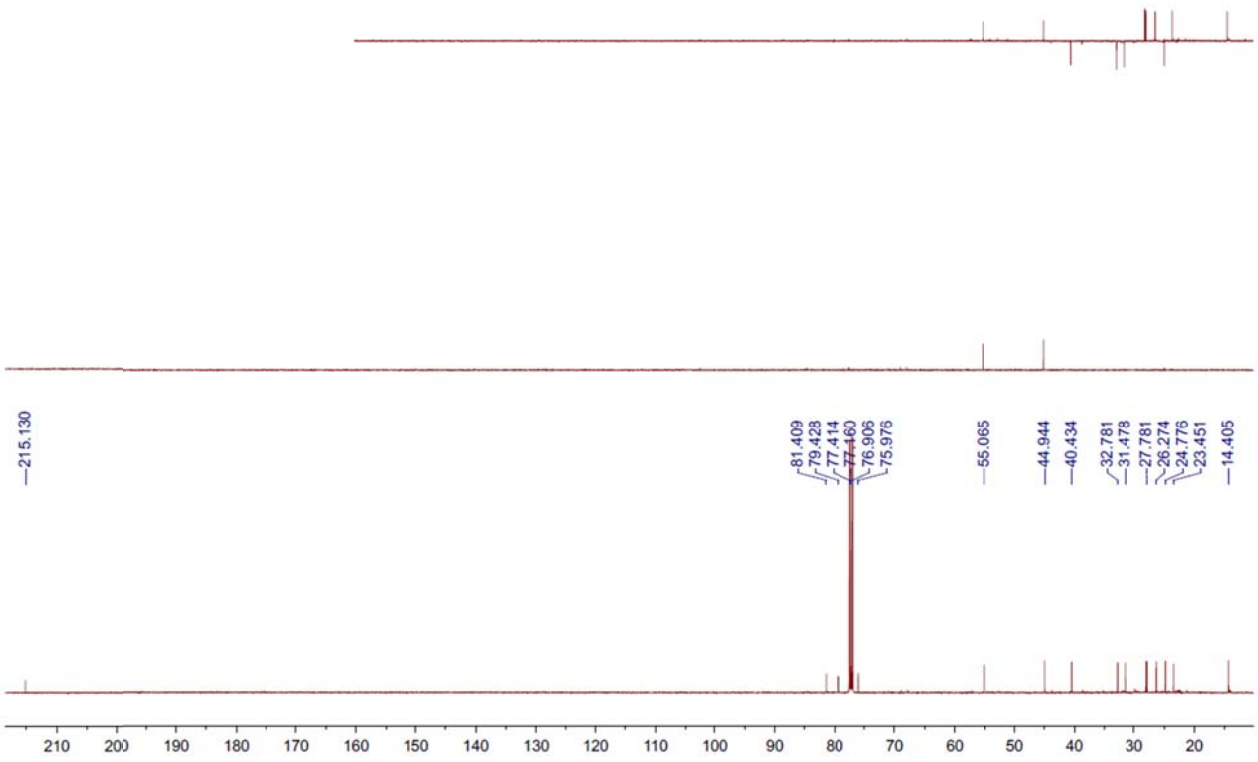


Figure S2. ^{13}C NMR and DEPT spectra of compound **1** in $CDCl_3$.

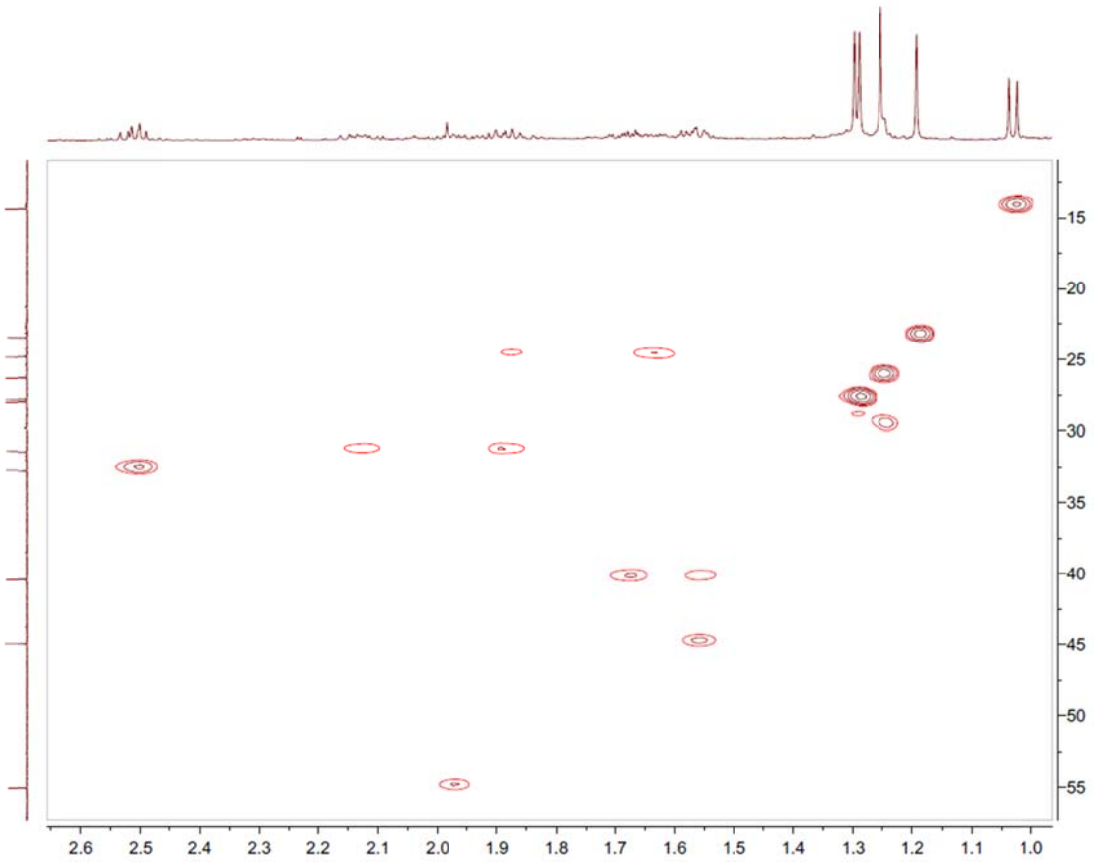


Figure S3. HSQC spectrum of compound **1** in $CDCl_3$.

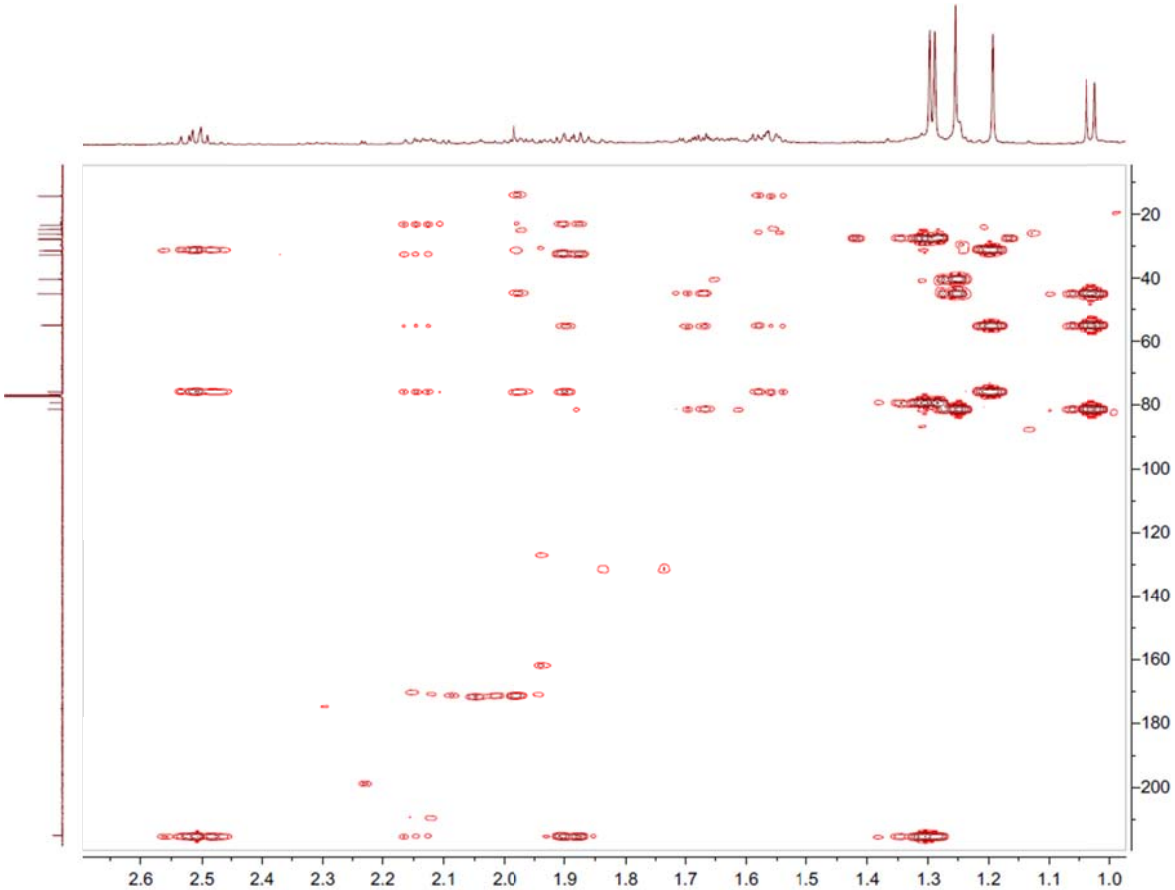


Figure S4. HMBC spectrum of compound **1** in $CDCl_3$.

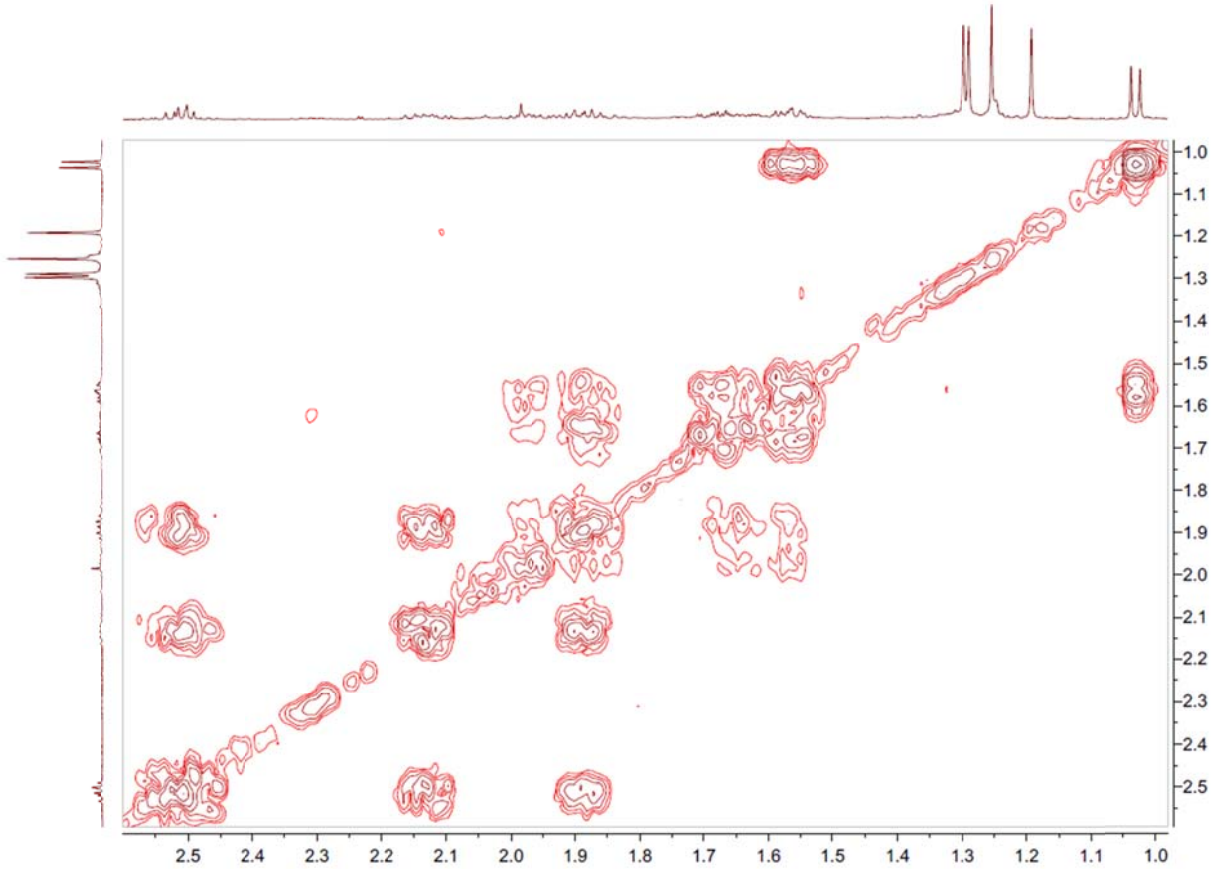


Figure S5. COSY spectrum of compound **1** in $CDCl_3$.

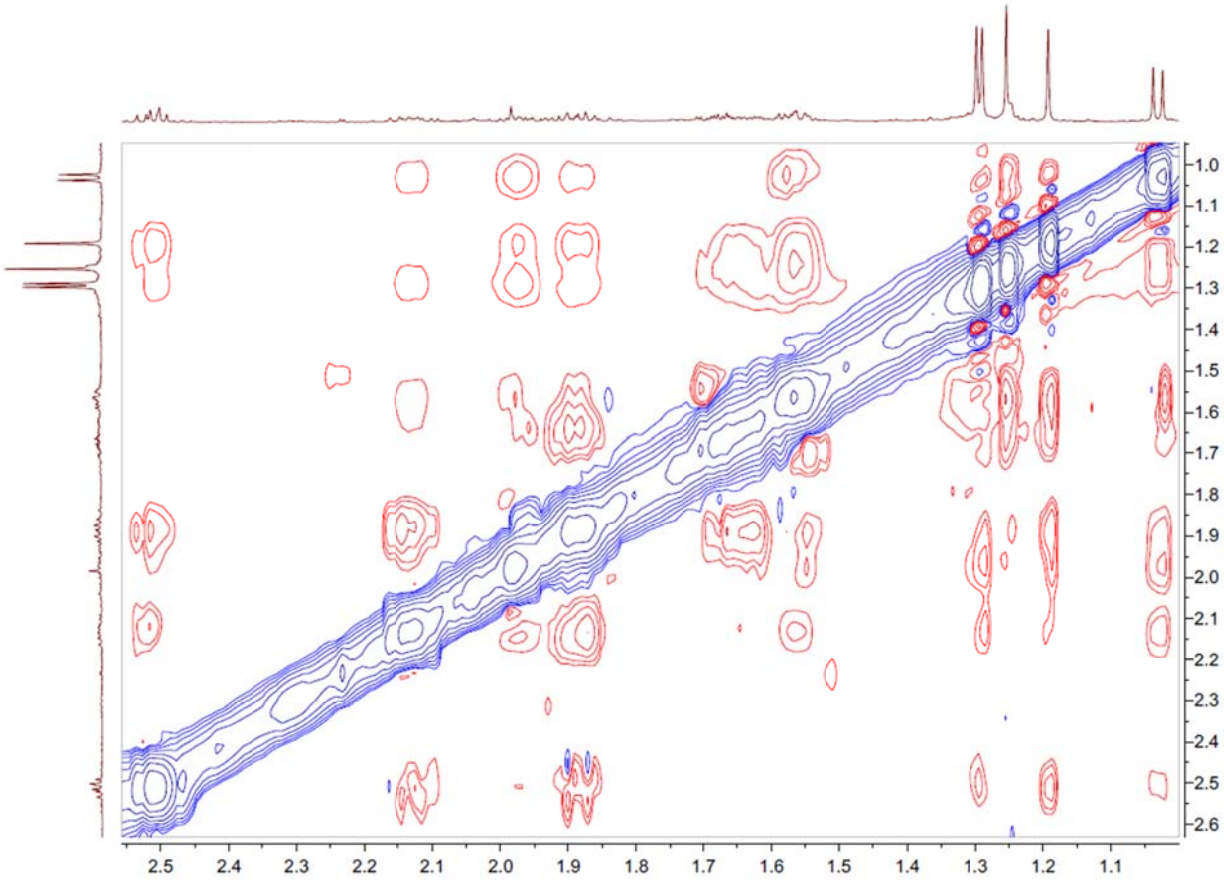


Figure S6. NOESY spectrum of compound **1** in $CDCl_3$**.**

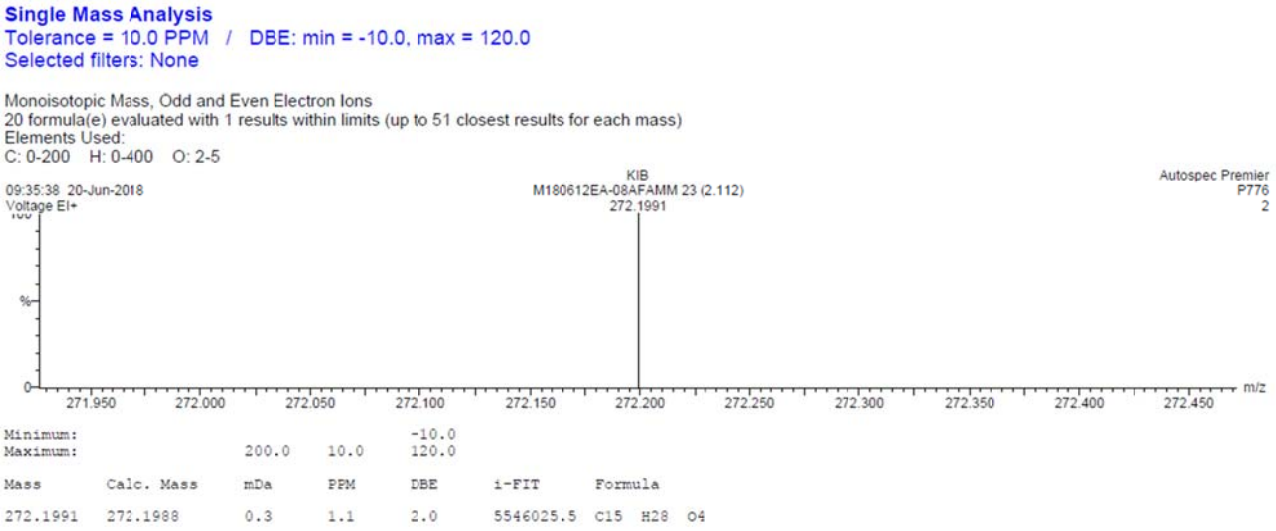


Figure S7. HREIMS spectrum of compound **1**.

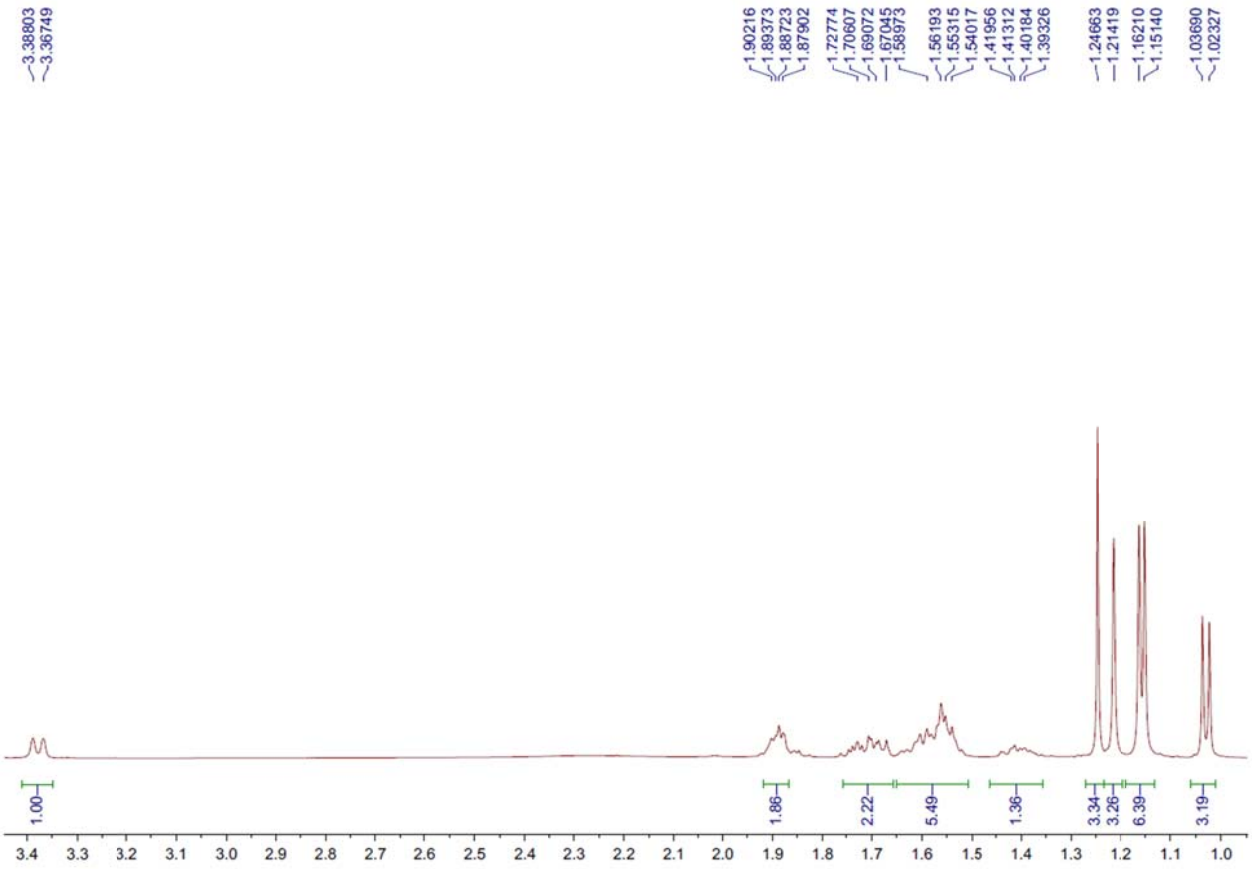


Figure S8. ^{1}H NMR spectrum of compound **2** in $CDCl_3$.

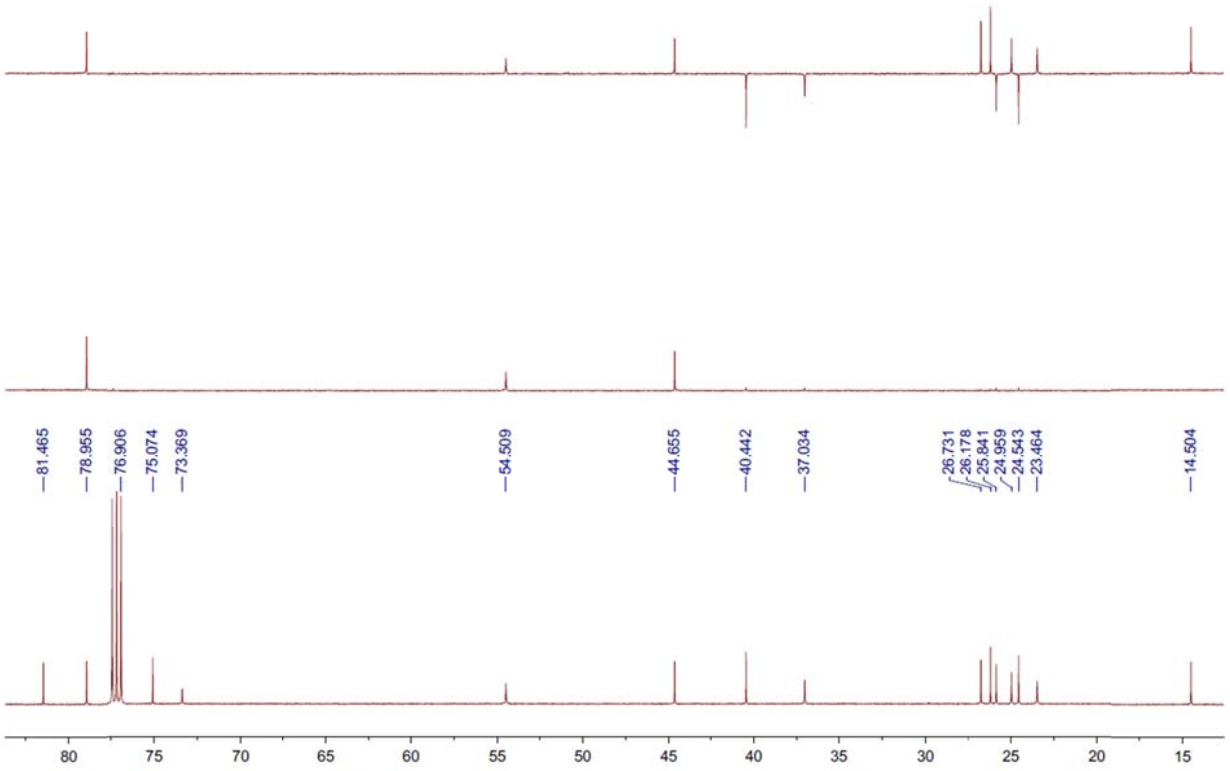


Figure S9. ^{13}C NMR and DEPT spectra of compound **2** in $CDCl_3$.

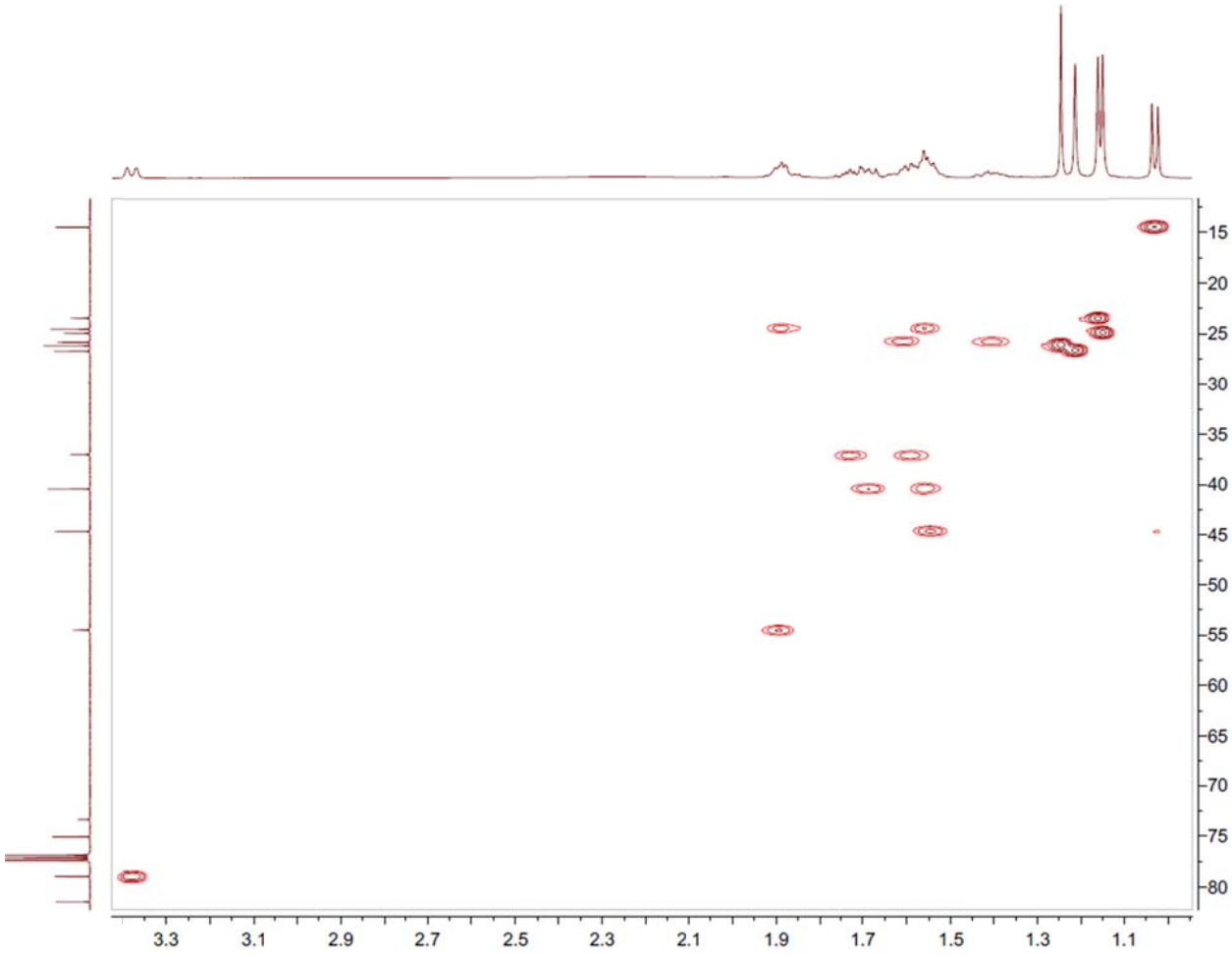


Figure S10. HSQC spectrum of compound **2** in $CDCl_3$.

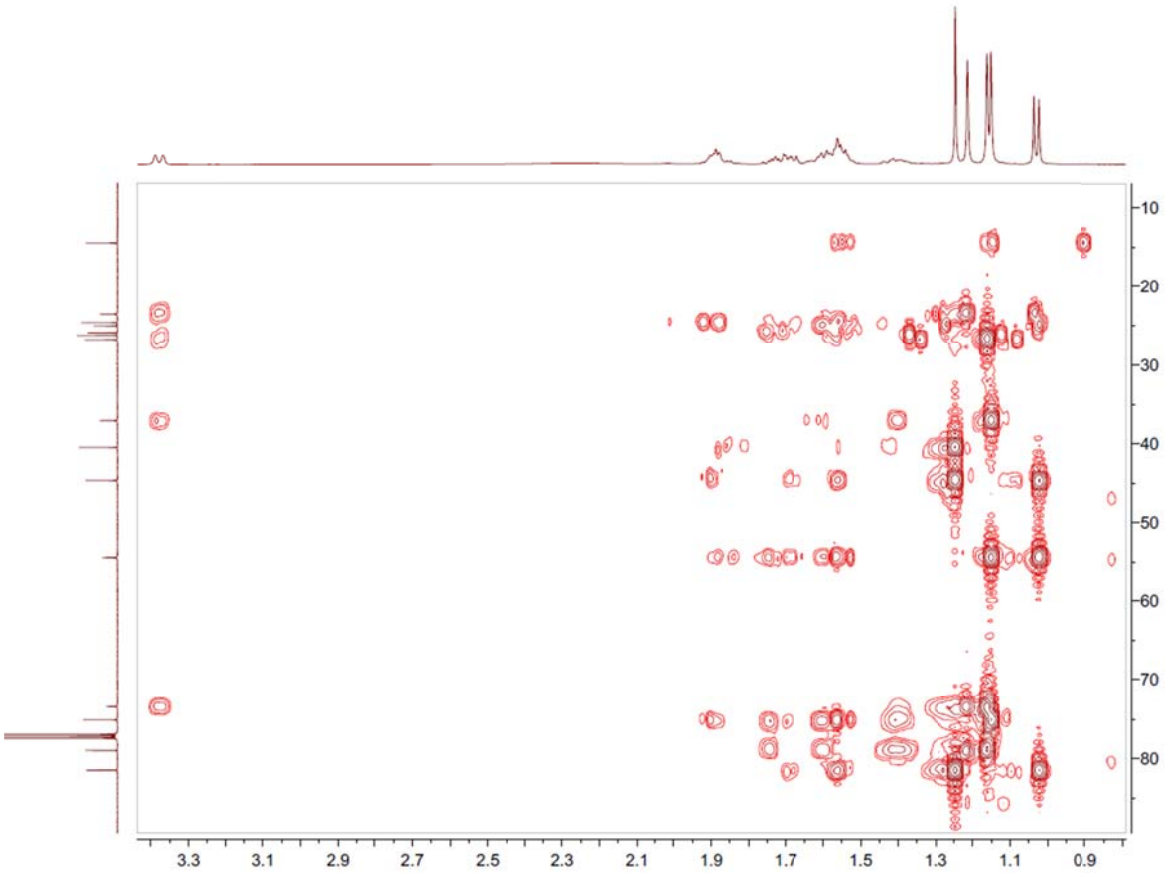


Figure S11. HMBC spectrum of compound **2** in $CDCl_3$.

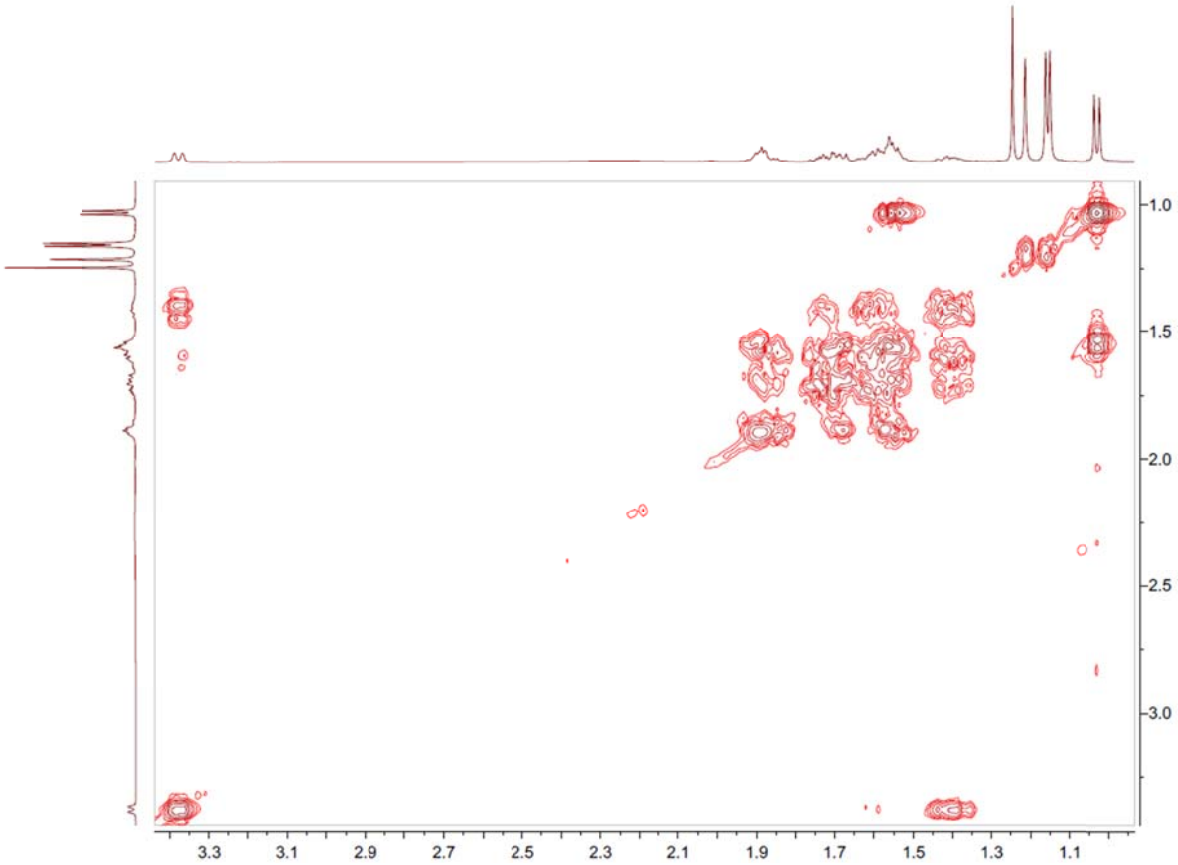


Figure S12. COSY spectrum of compound **2** in $CDCl_3$.

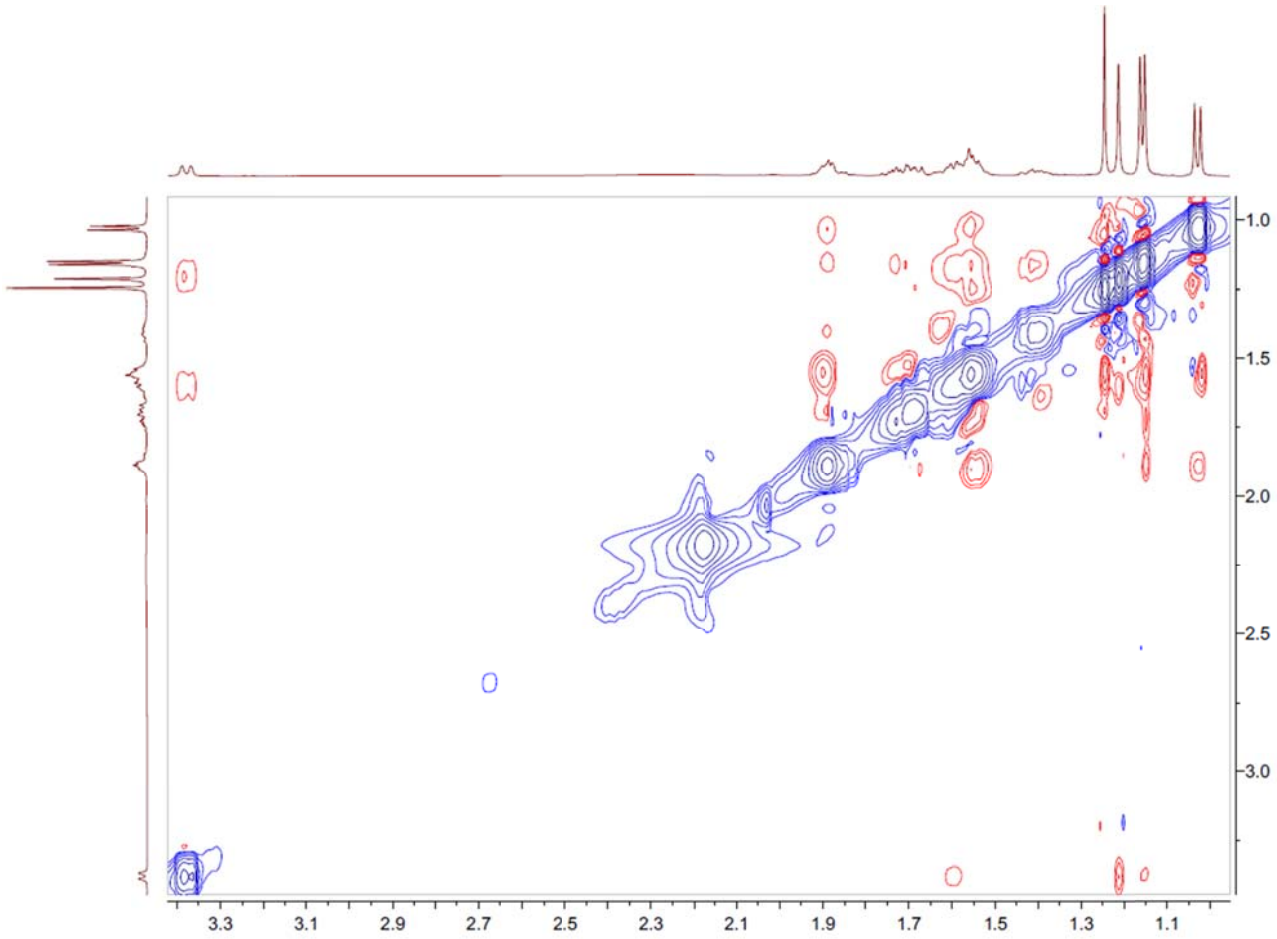


Figure S13. NOESY spectrum of compound **2** in $CDCl_3$.

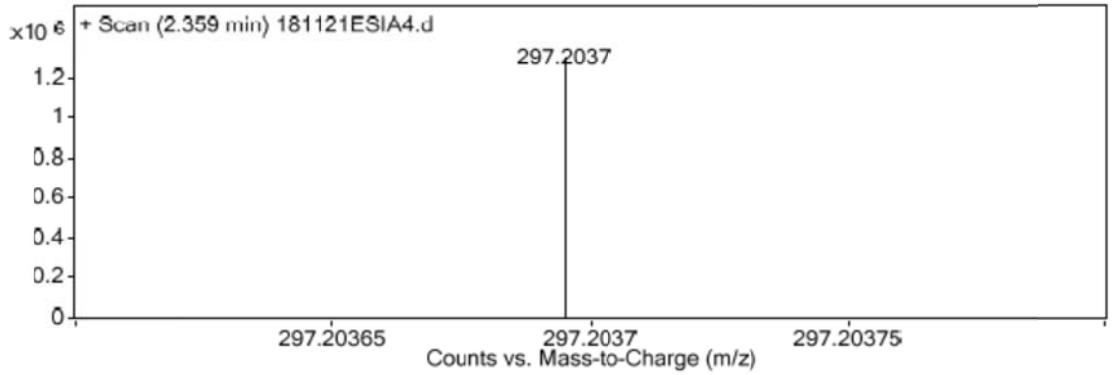
Qualitative Analysis Report

Data Filename	181121ESIA4.d	**Sample Name**	compound **2**
Sample Type	Sample	**Position**	
Instrument Name	Agilent G6230 TOF MS	**User Name**	KIB
Acq Method	ESI.m	**Acquired Time**	11/21/2018 9:39:20 AM
IRM Calibration Status	Success	**DA Method**	ESI.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
297.2037	1	1295062.75	C15 H30 Na O4	M+
298.2073	1	196830.22	C15 H30 Na O4	M+
310.1265	1	172631.41		
322.1268	1	651617.13		
338.2304	1	159140.7		
344.1088	1	166444.25		
571.4188	1	1124473.88		
572.4223	1	360450.06		
575.356	1	156204.05		
687.4812	1	189309.59		

Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	0	10
Na	1	1

Formula Calculator Results

Formula	CalculatedMass	Mz	Diff.(mDa)	Diff. (ppm)	DBE
C15 H30 Na O4	297.2042	297.2037	0.5	1.6	0.5

--- End Of Report ---

Figure S14. HRESI^{+}MS spectrum of compound **2**.

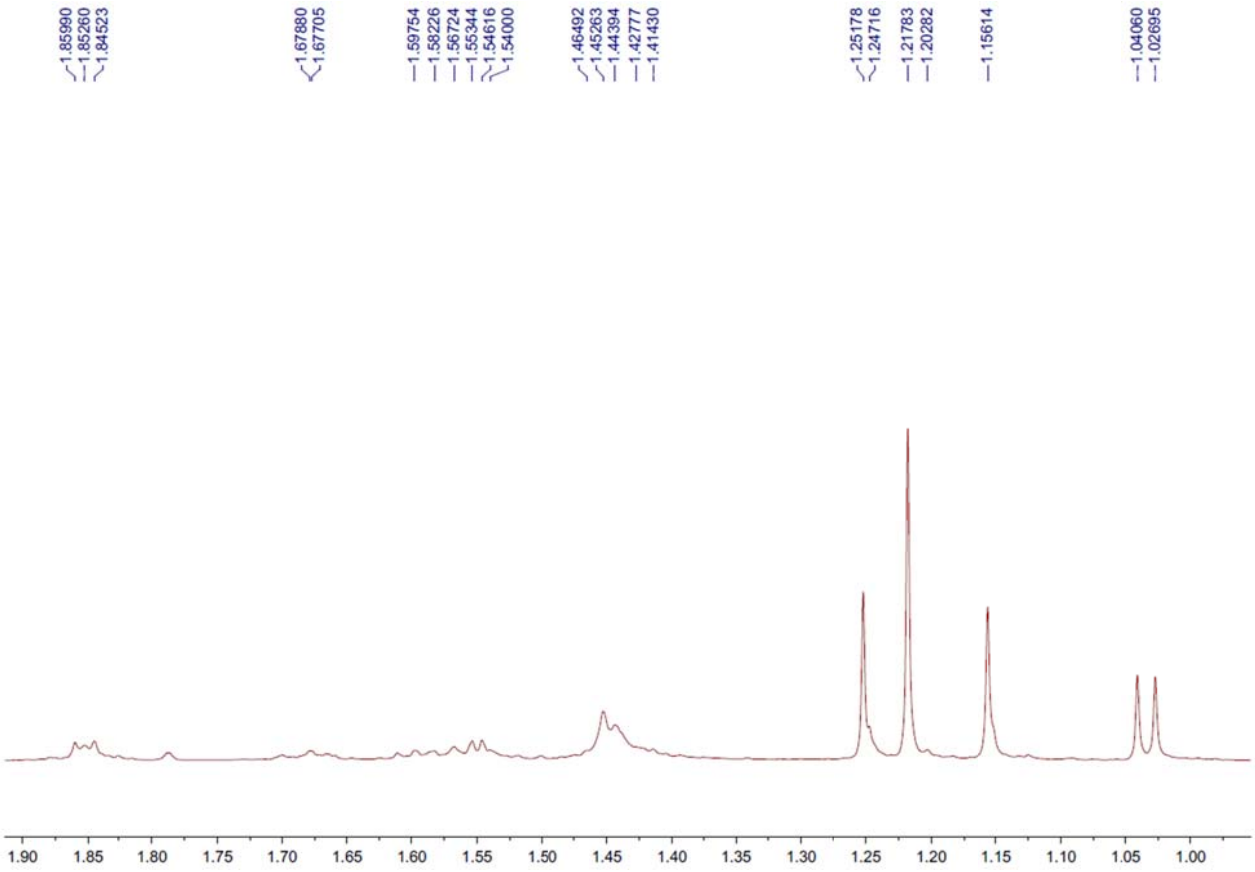


Figure S15. ^{1}H NMR spectrum of compound **3** in $CDCl_3$.

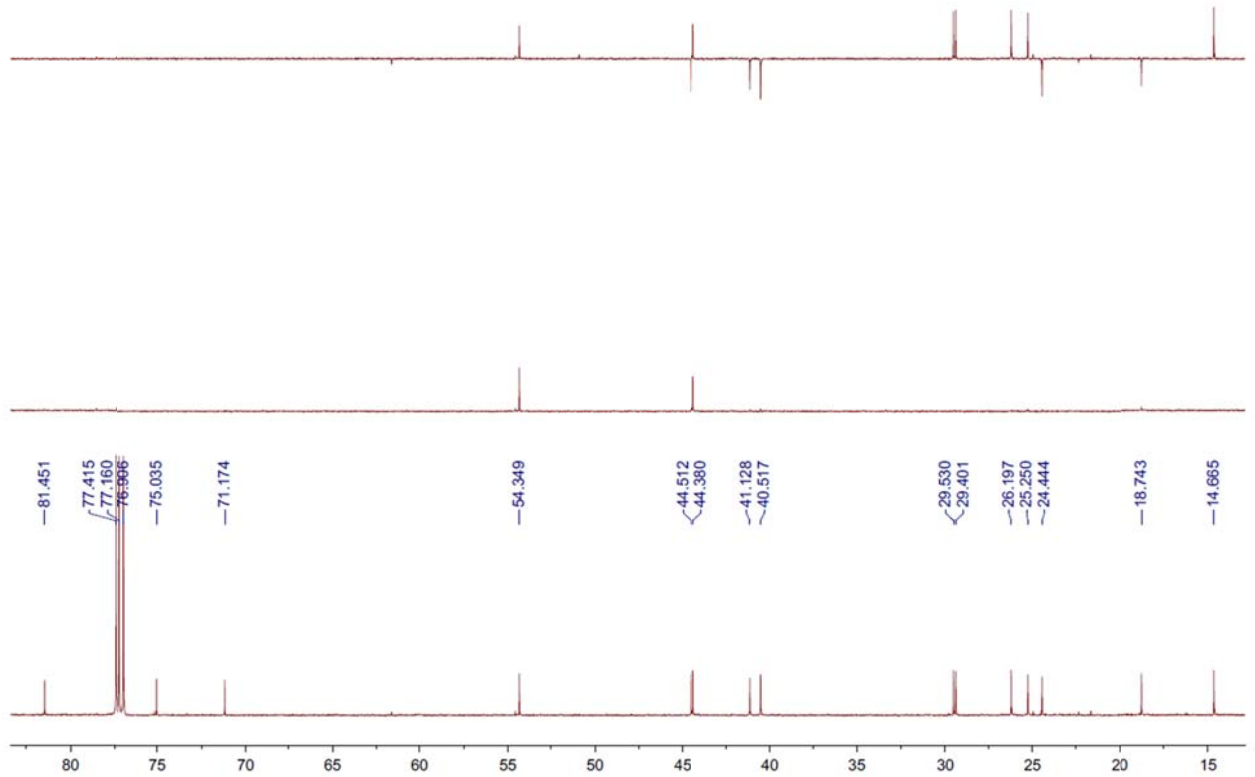


Figure S16. ^{13}C NMR and DEPT spectra of compound **3** in $CDCl_3$.

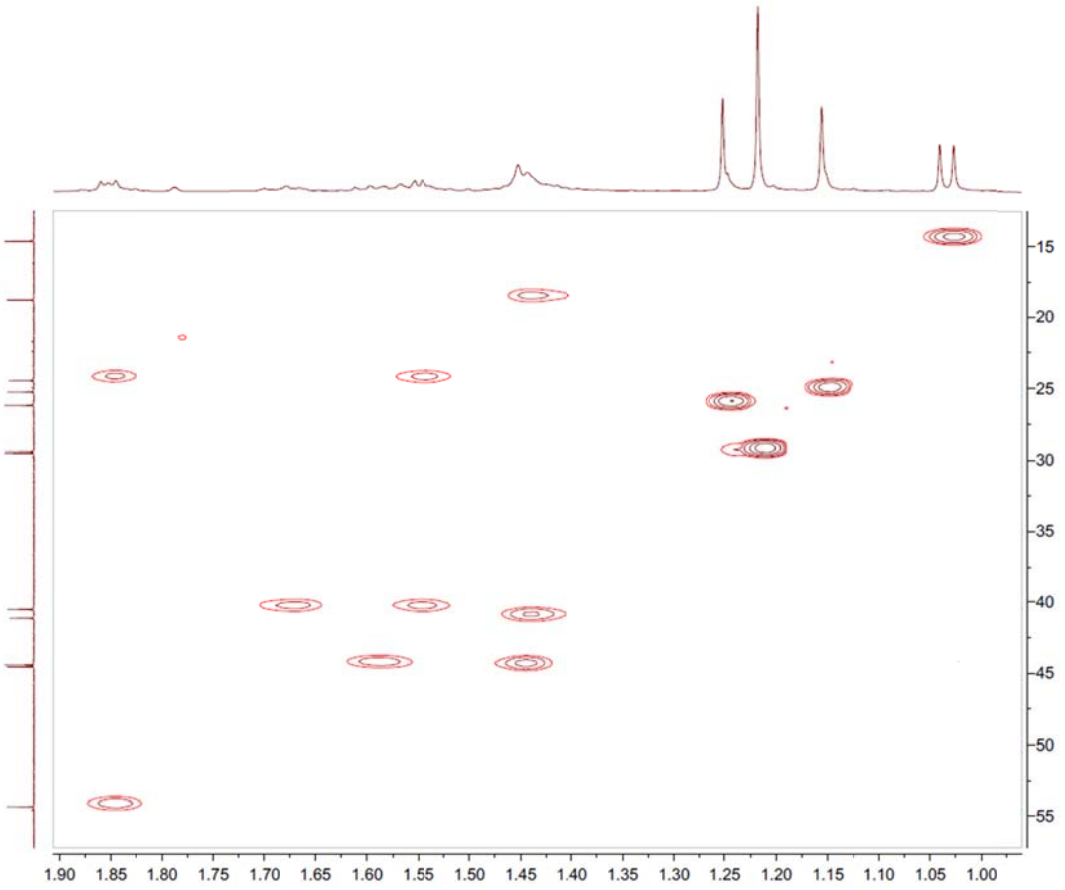


Figure S17. HSQC spectrum of compound **3** in $CDCl_3$.

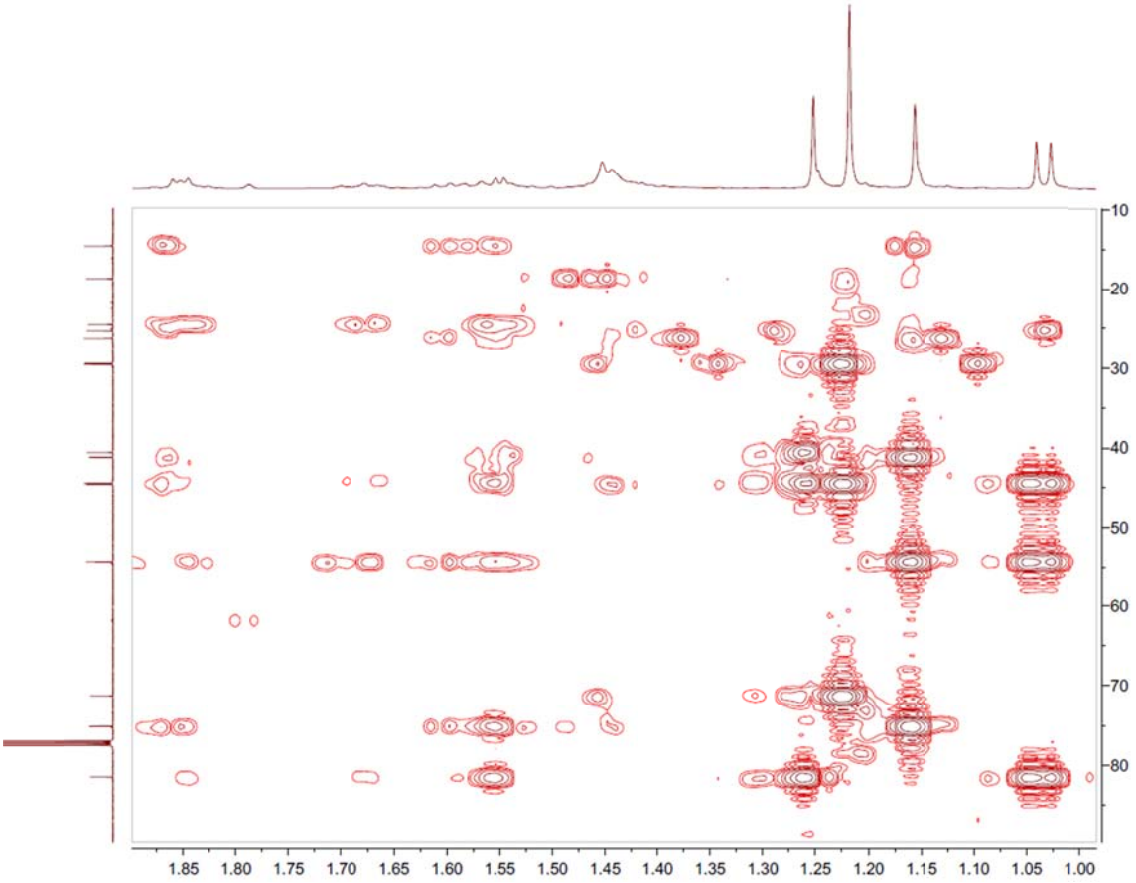


Figure S18. HMBC spectrum of compound **3** in $CDCl_3$.

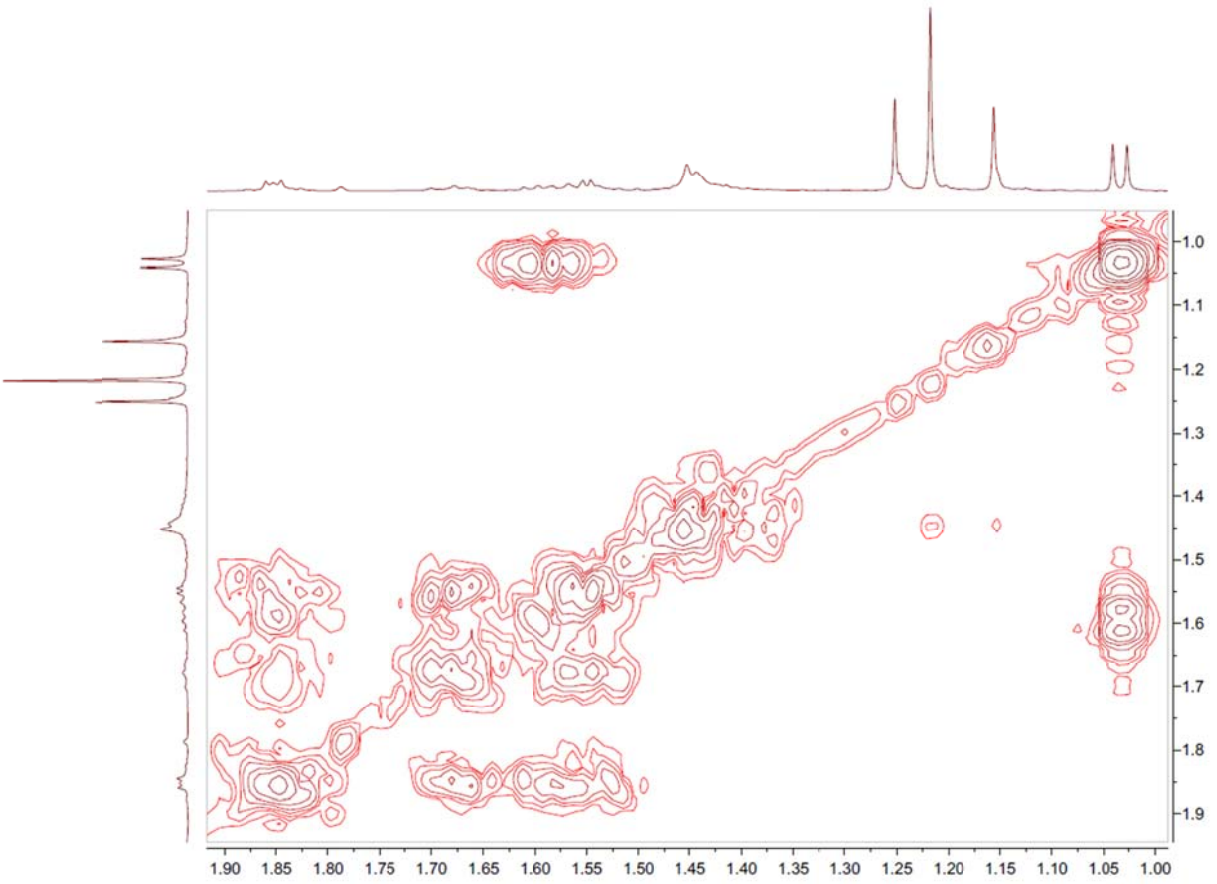


Figure S19. COSY spectrum of compound **3** in $CDCl_3$.

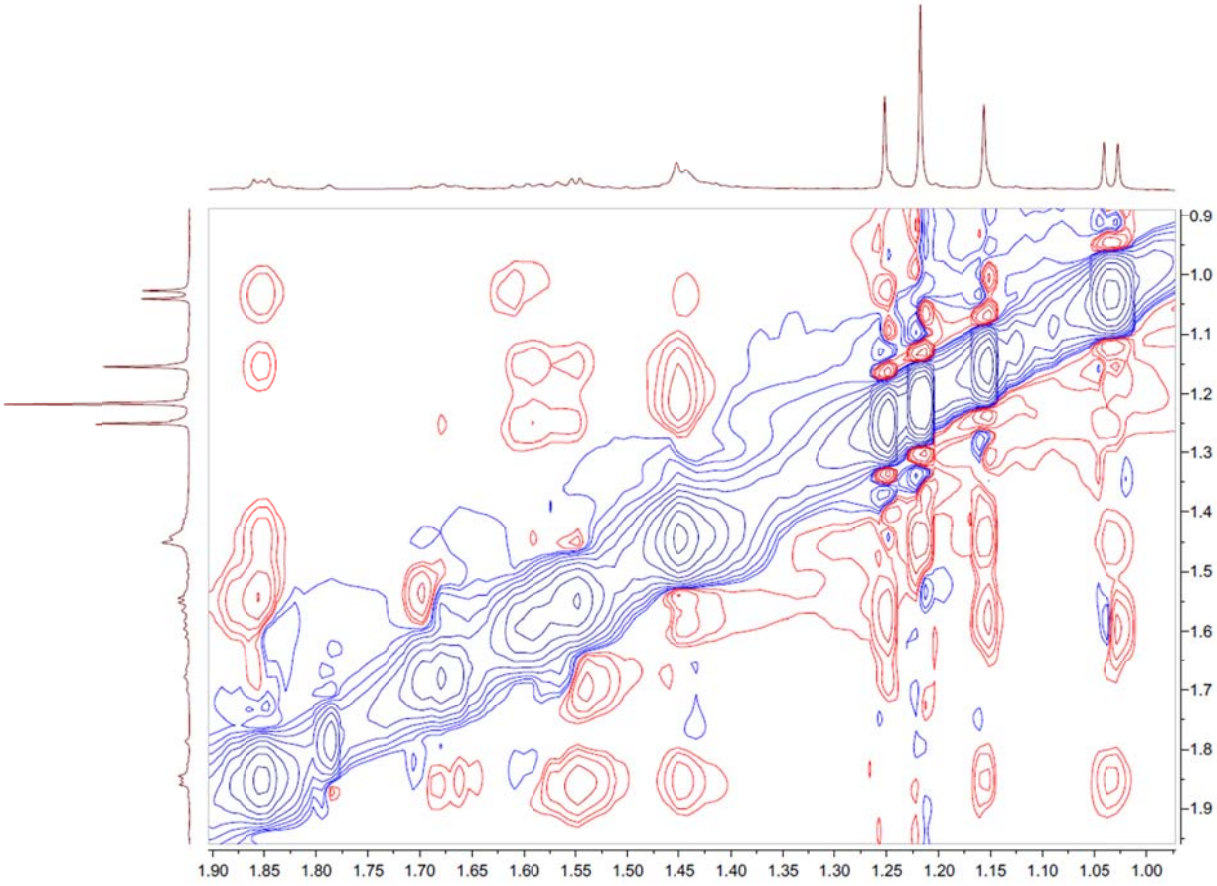


Figure S20. NOESY spectrum of compound **3** in $CDCl_3$.

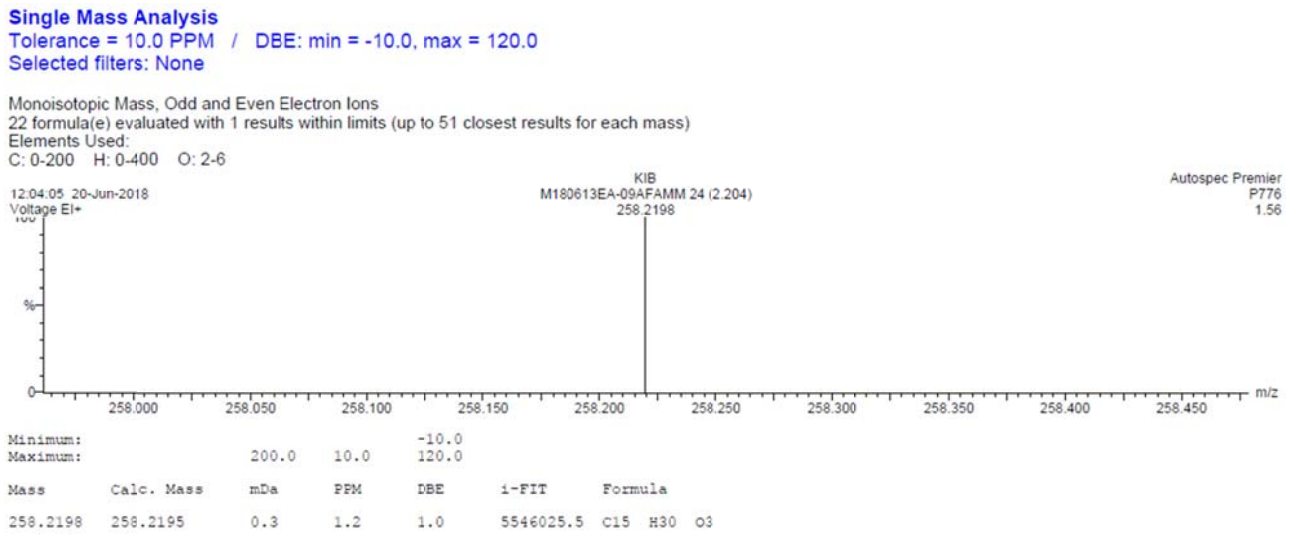


Figure S21. HREIMS spectrum of compound **3**.

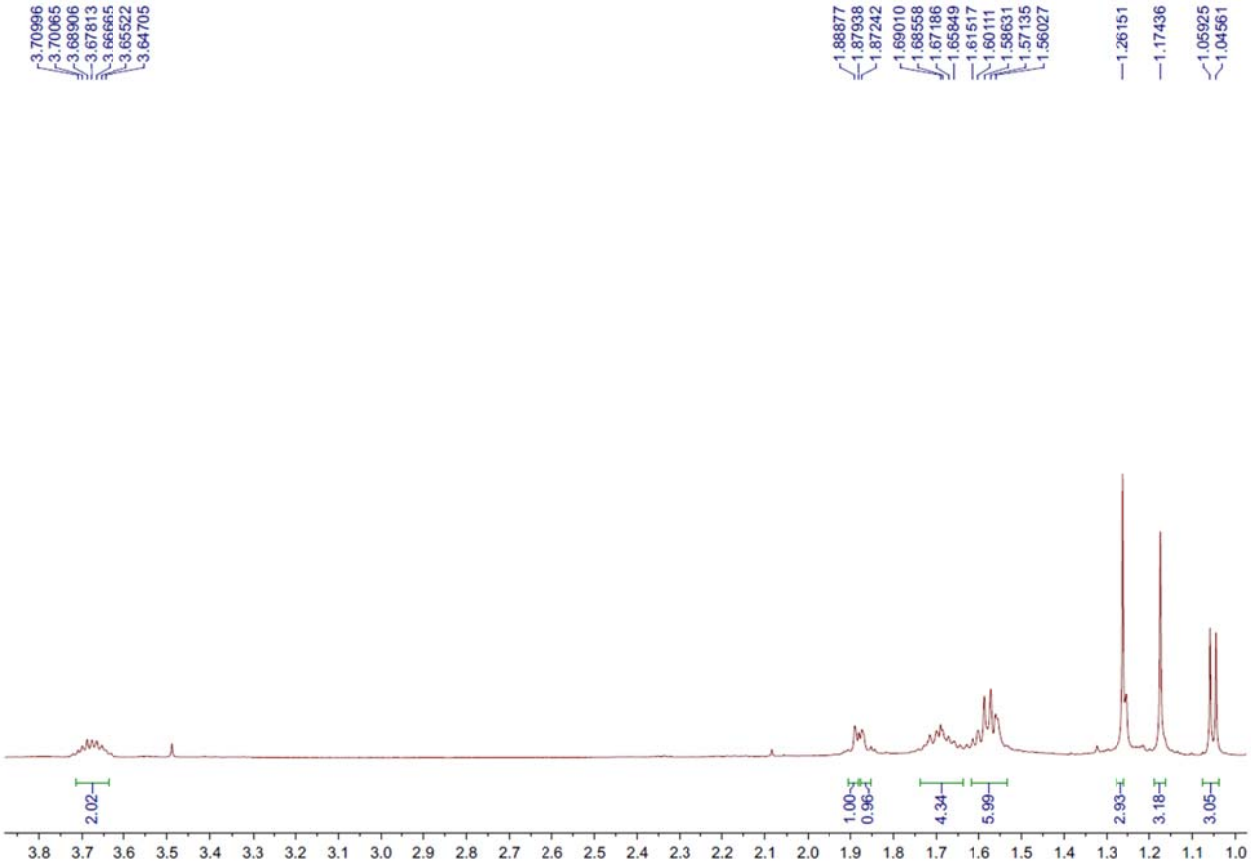


Figure S22. ^{1}H NMR spectrum of compound **4** in $CDCl_3$.

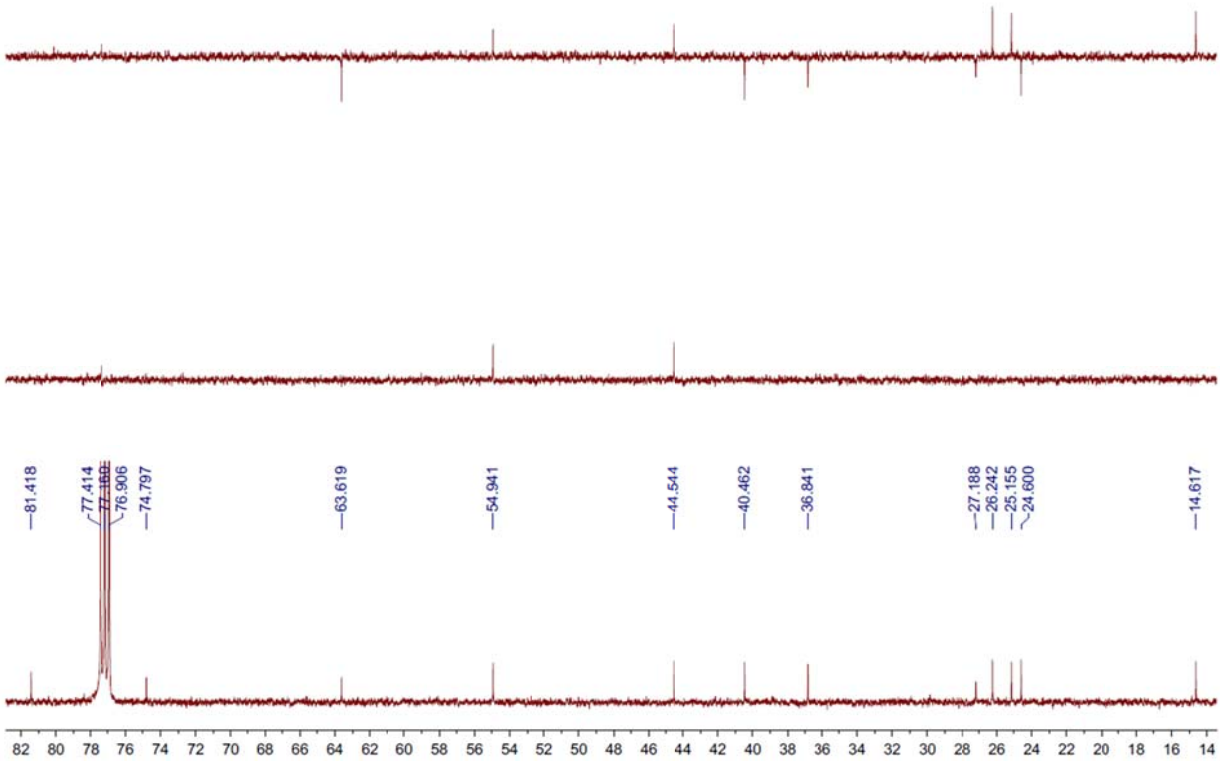


Figure S23. ^{13}C NMR and DEPT spectra of compound **4** in $CDCl_3$.

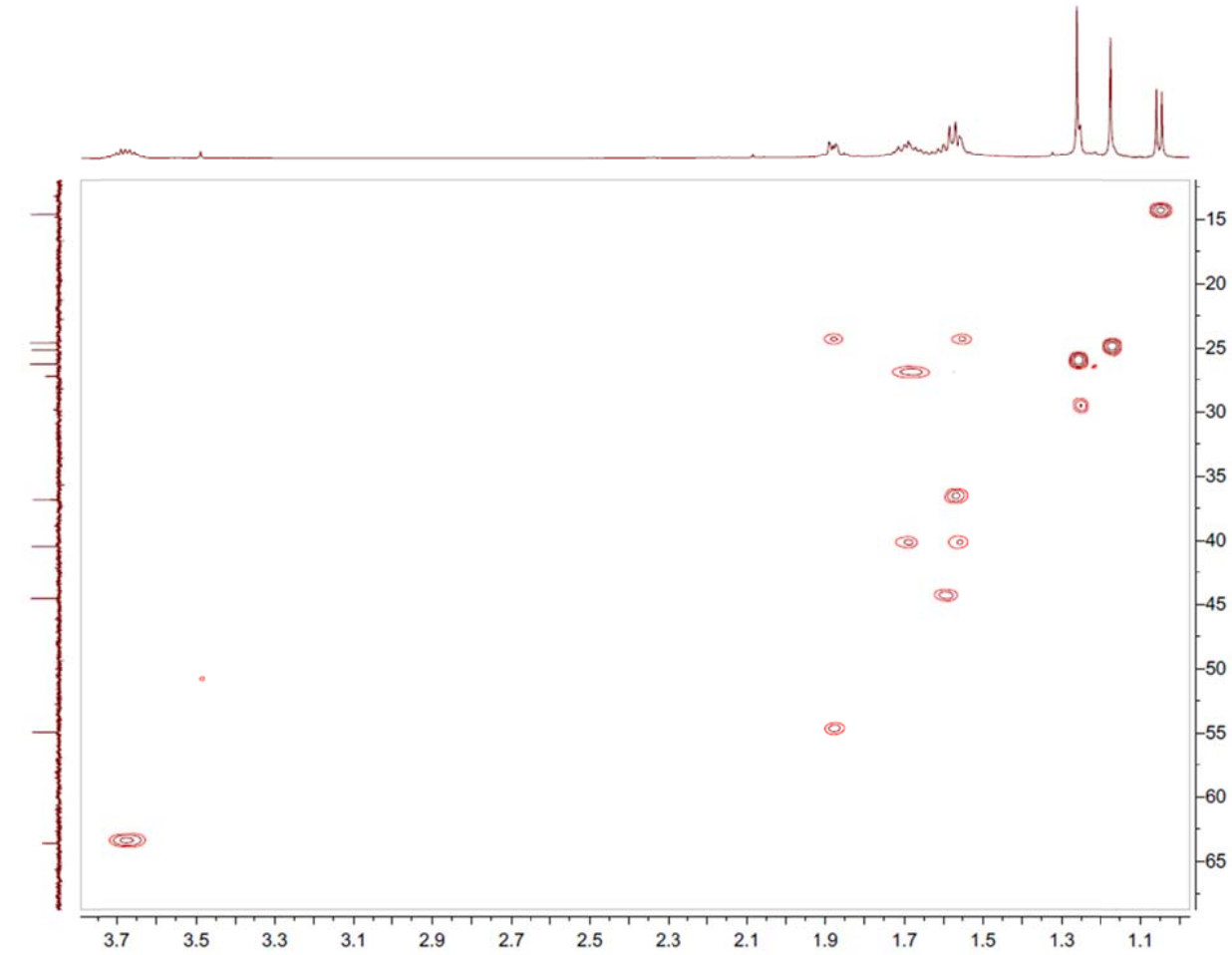


Figure S24. HSQC spectrum of compound **4** in $CDCl_3$.

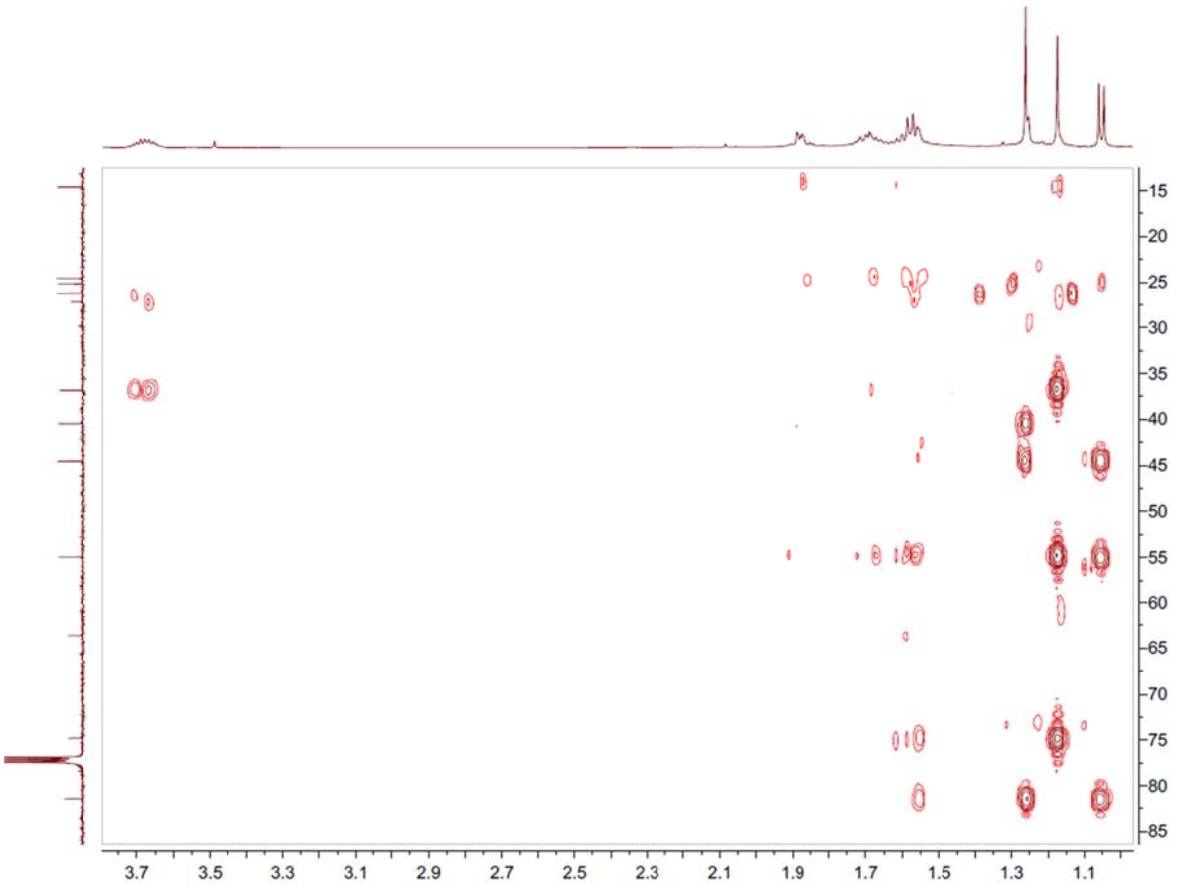


Figure S25. HMBC spectrum of compound **4** in $CDCl_3$.

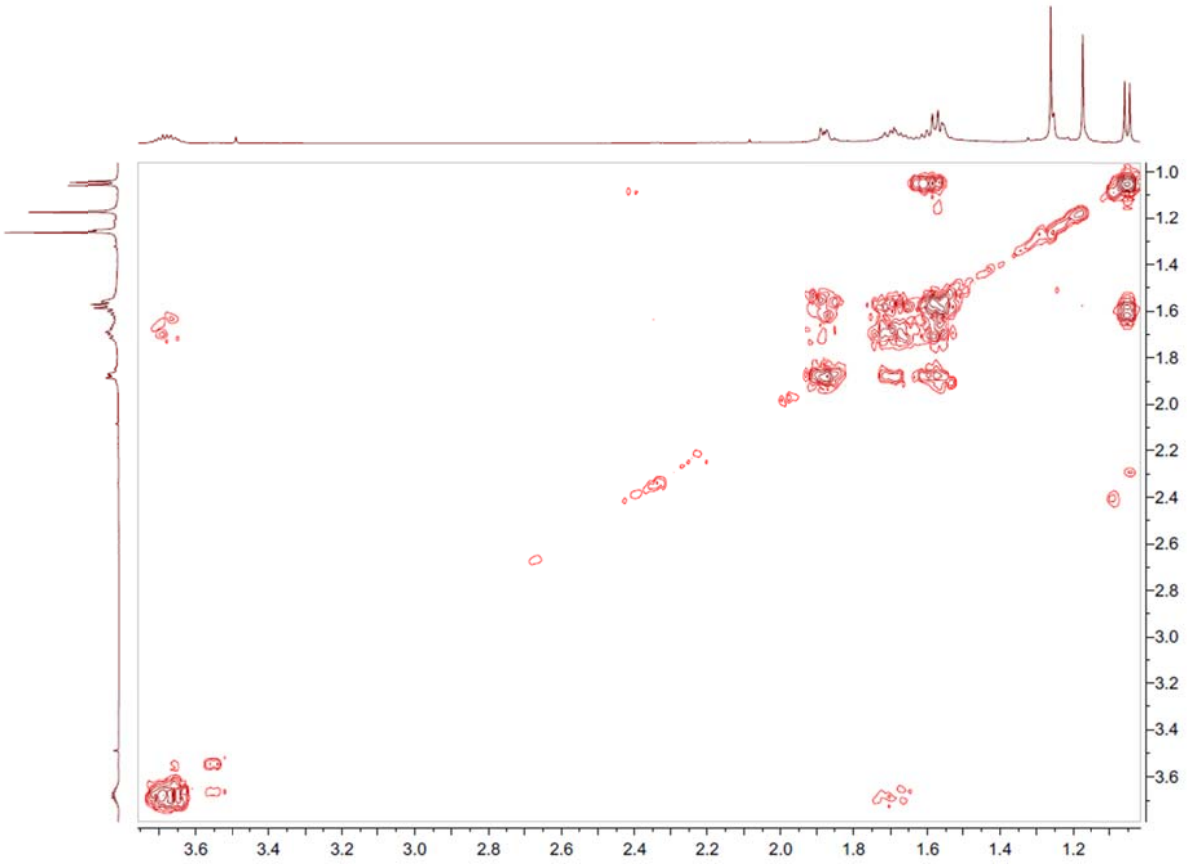


Figure S26. COSY spectrum of compound **4** in $CDCl_3$.

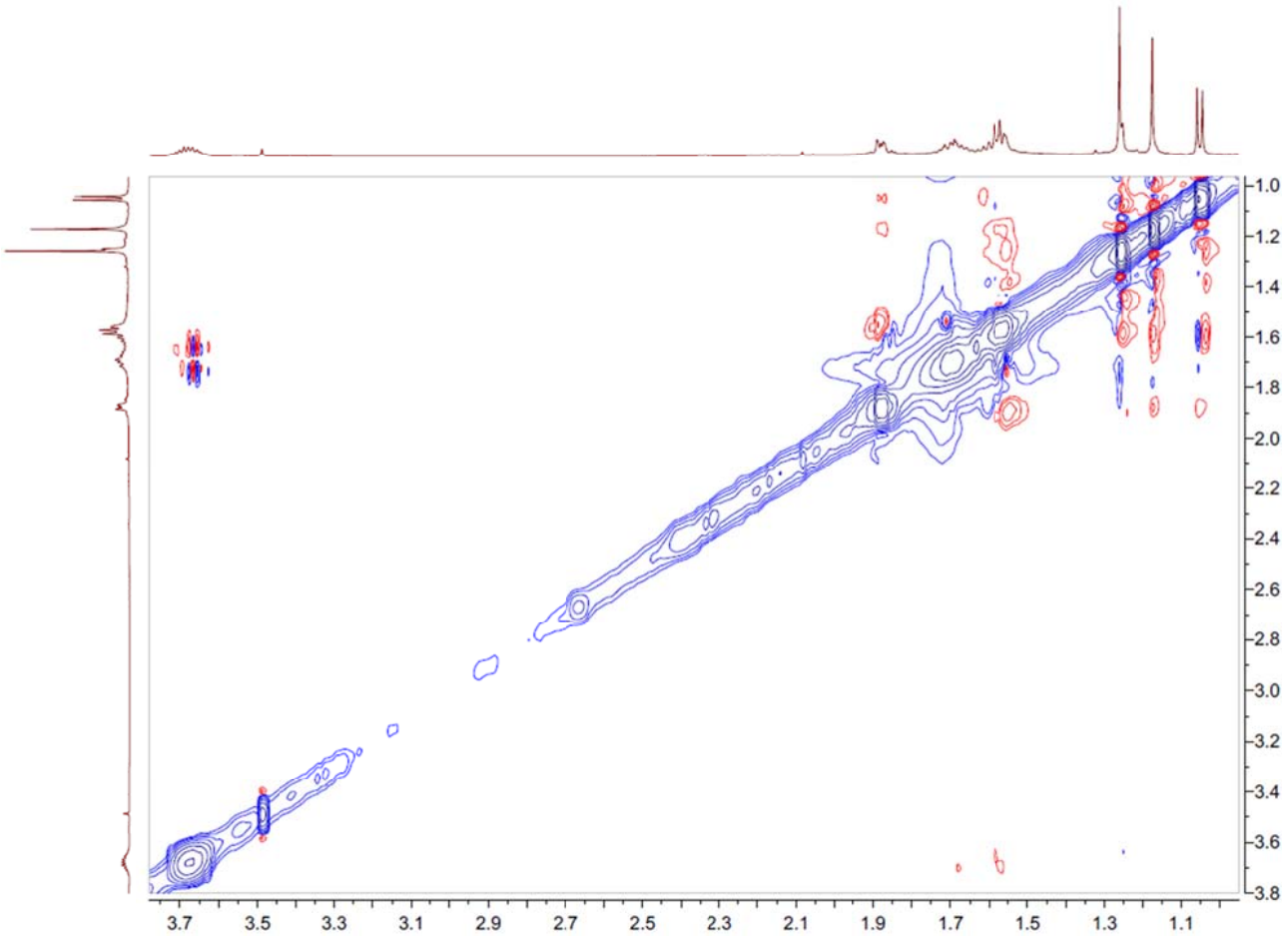


Figure S27. NOESY spectrum of compound **4** in $CDCl_3$.

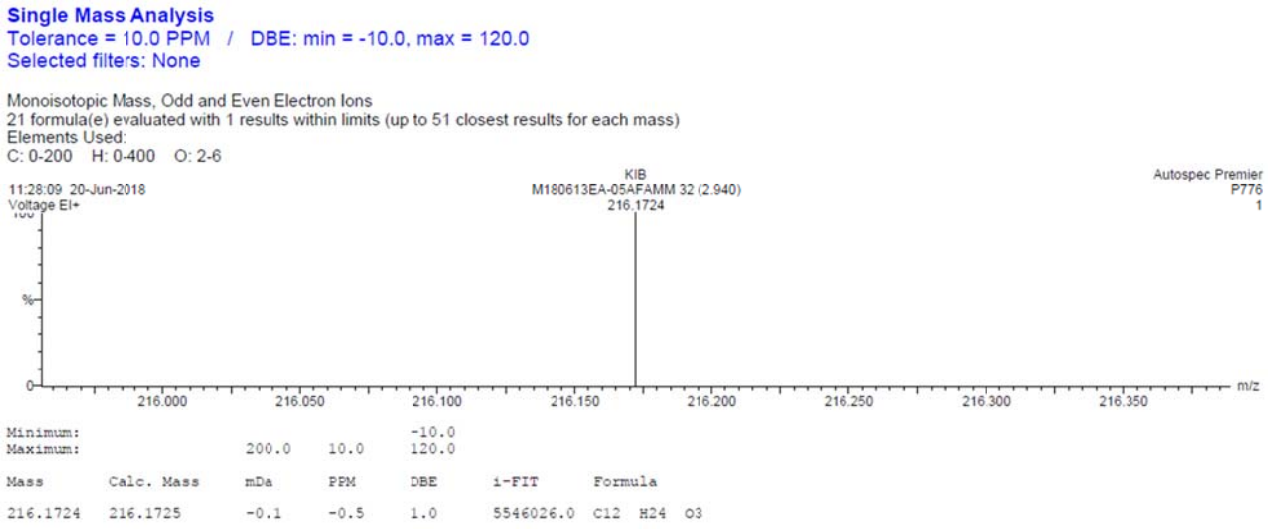


Figure S28. HREIMS spectrum of compound **4**.

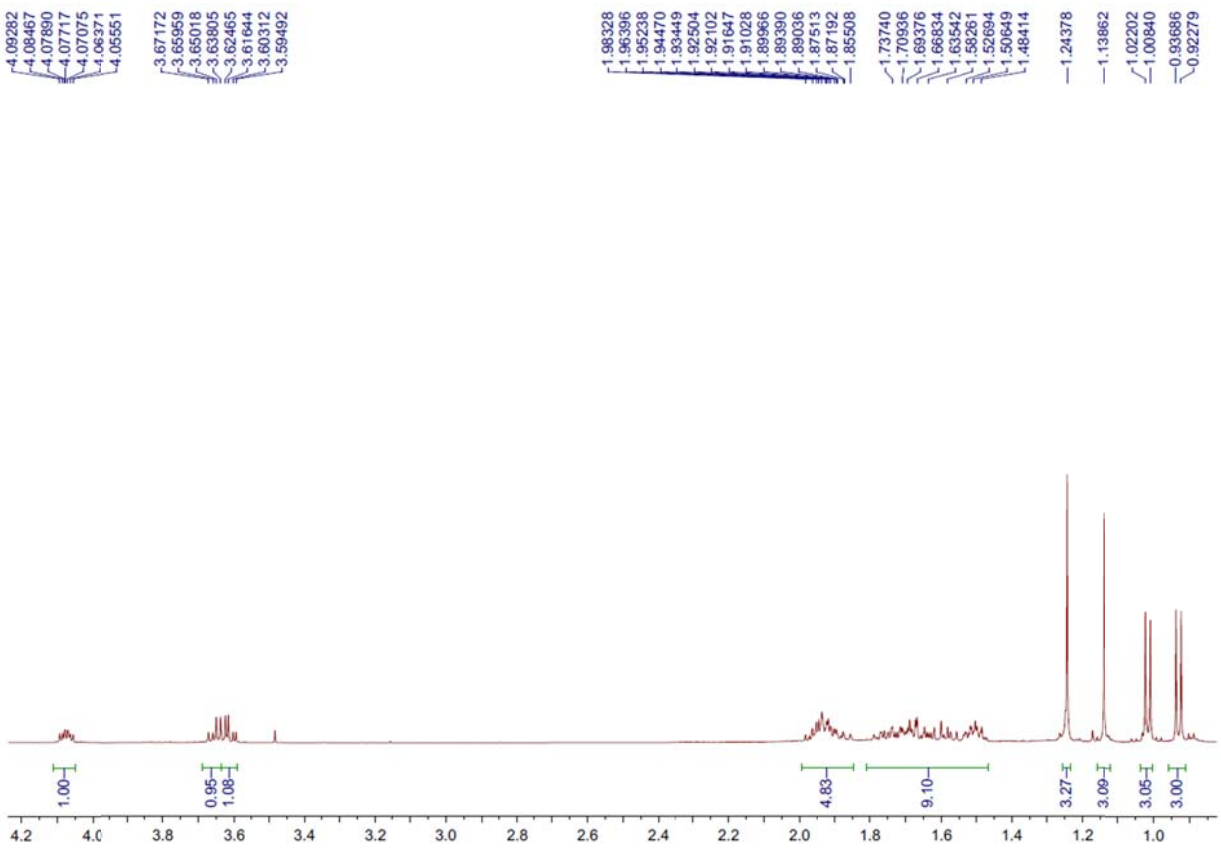


Figure S29. ^{1}H NMR spectrum of compound **5** in $CDCl_3$.

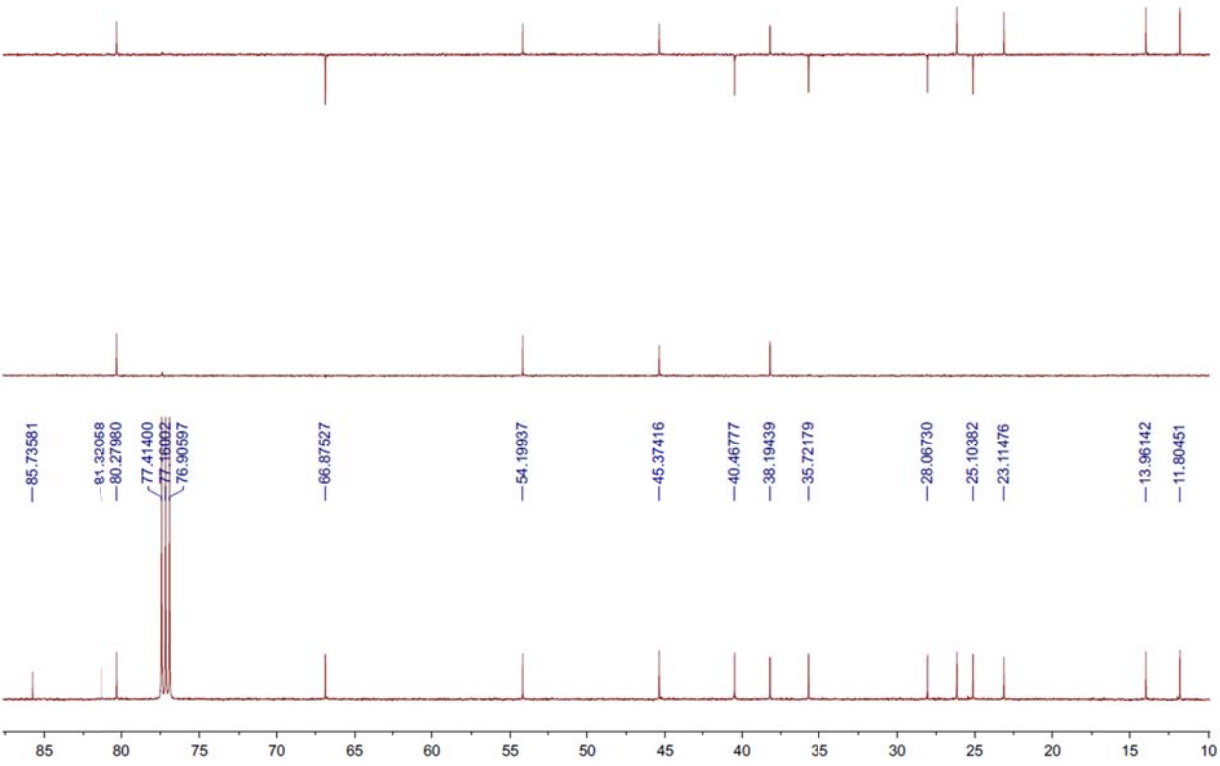


Figure S30. ^{13}C NMR and DEPT spectra of compound **5** in $CDCl_3$.

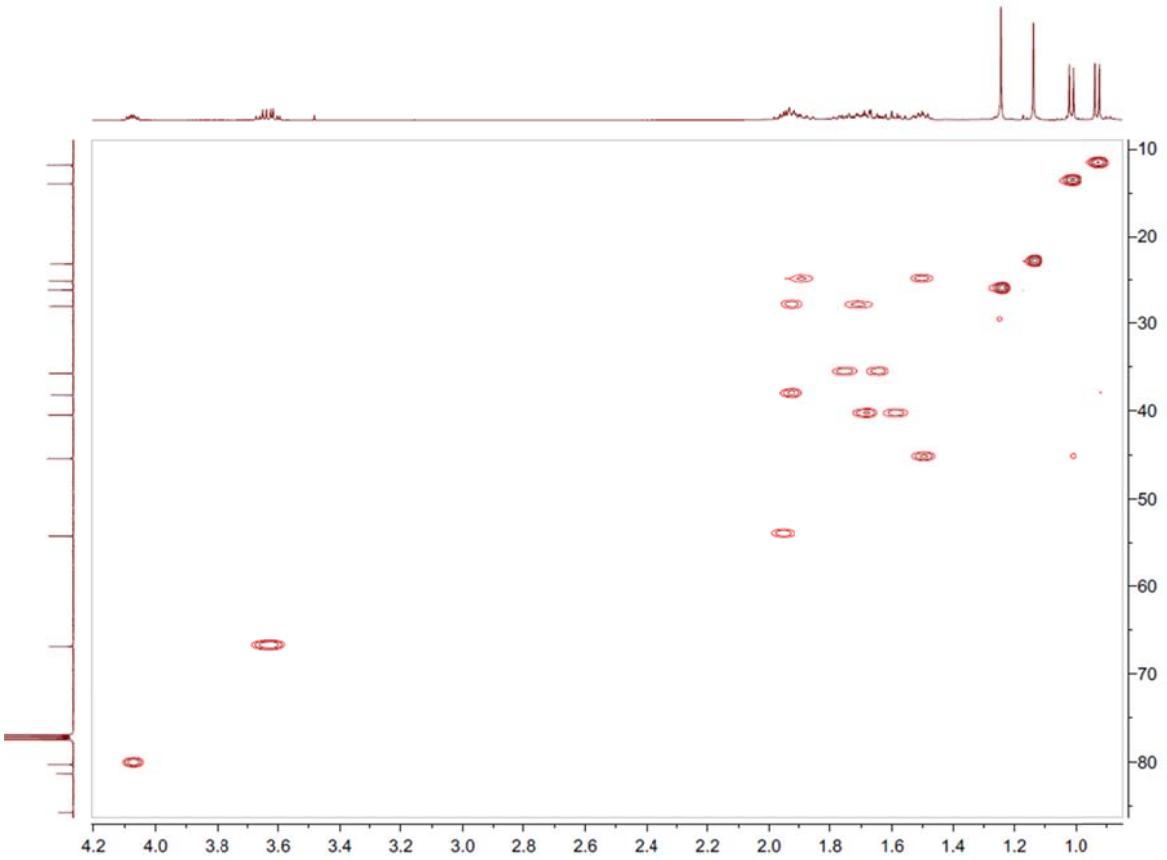


Figure S31. HSQC spectrum of compound **5** in $CDCl_3$.

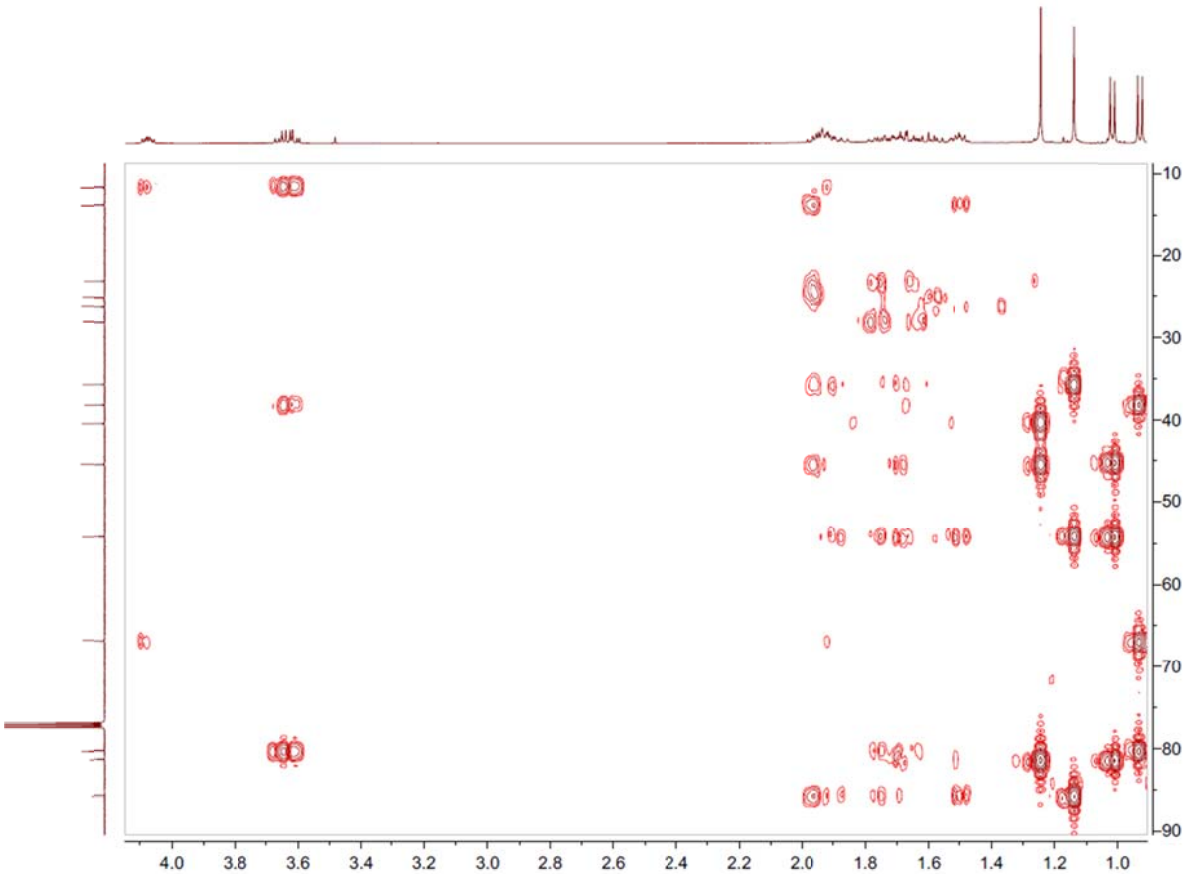


Figure S32. HMBC spectrum of compound **5** in $CDCl_3$.

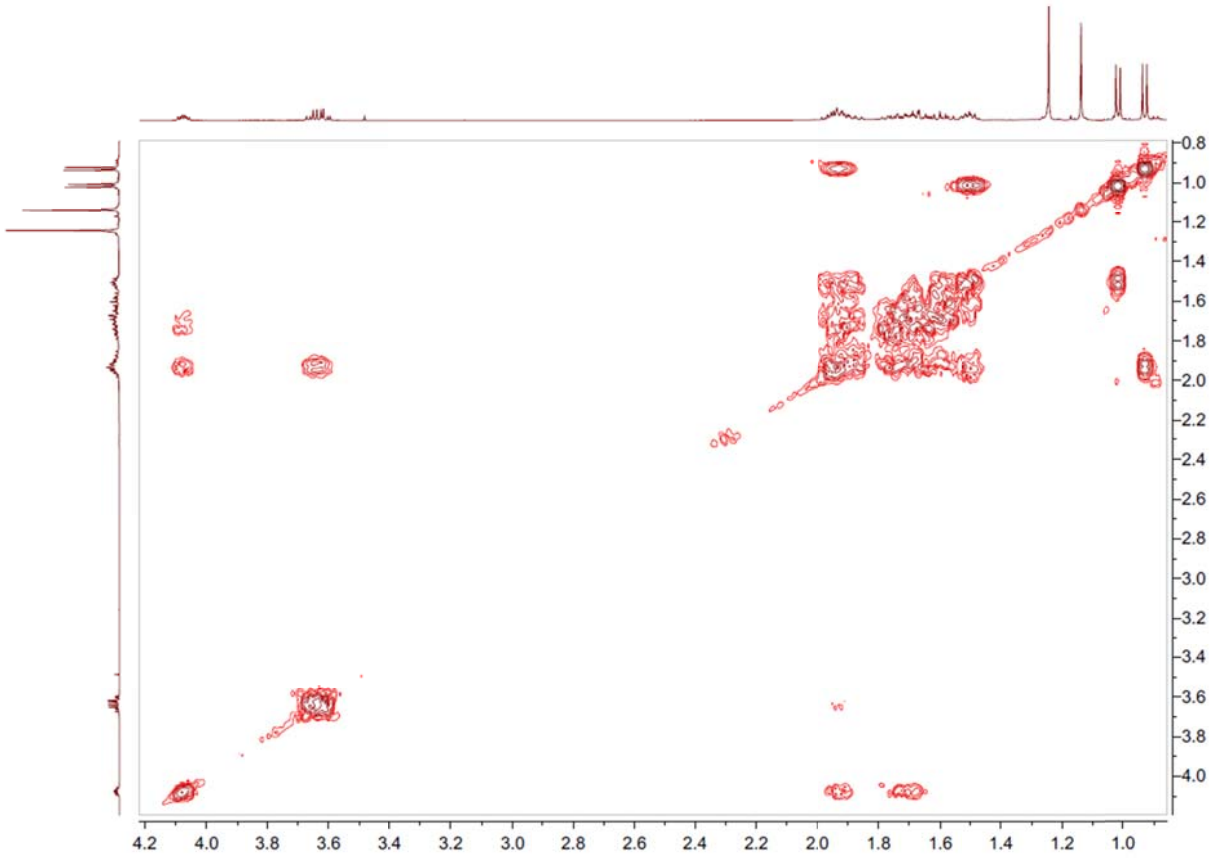


Figure S33. COSY spectrum of compound **5** in $CDCl_3$.

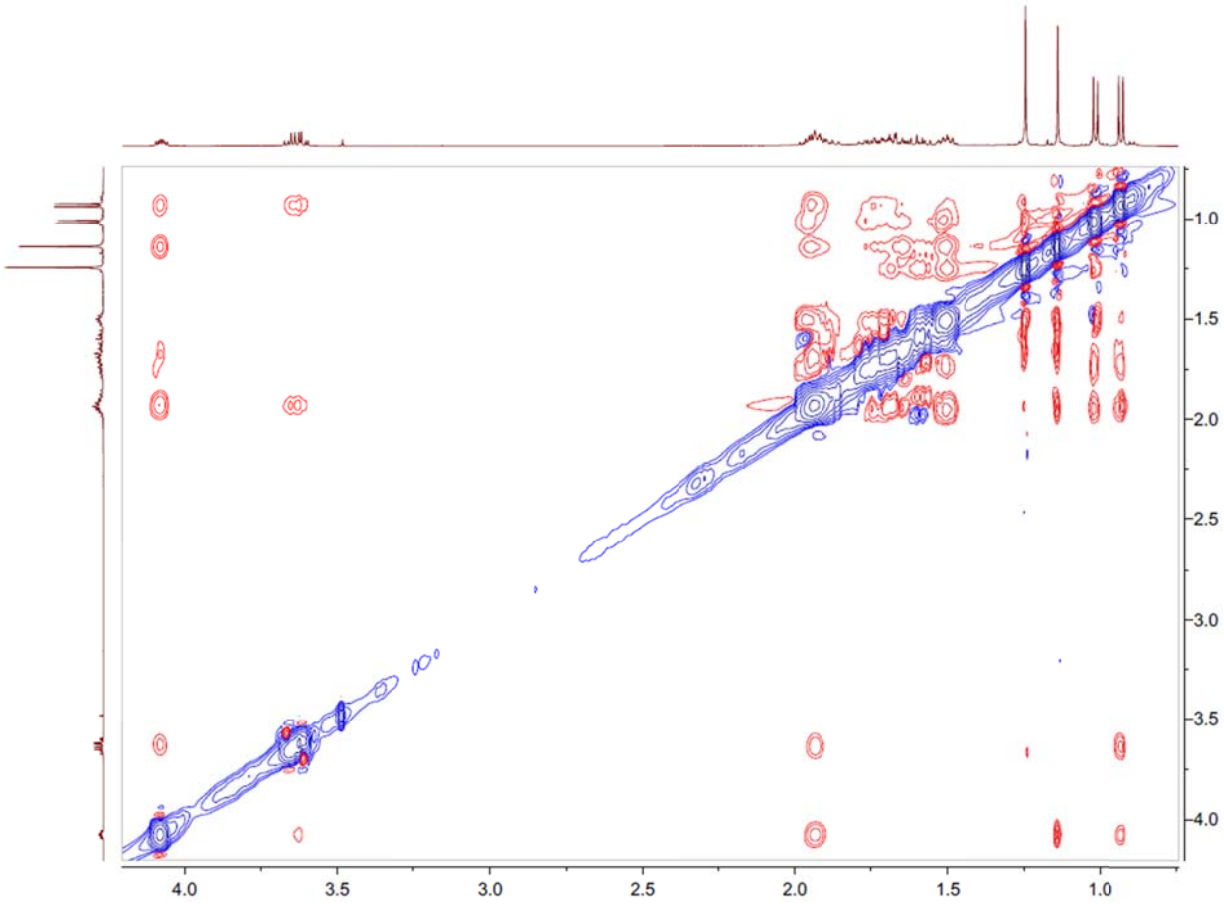


Figure S34. NOESY spectrum of compound **5** in $CDCl_3$.

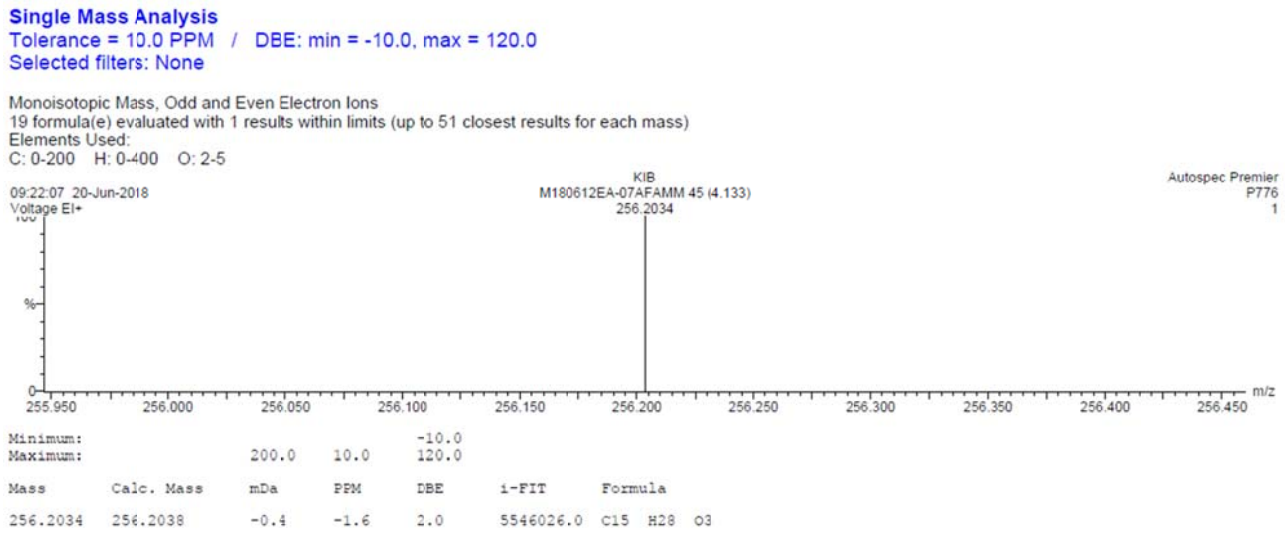


Figure S35. HREIMS spectrum of compound **5**.

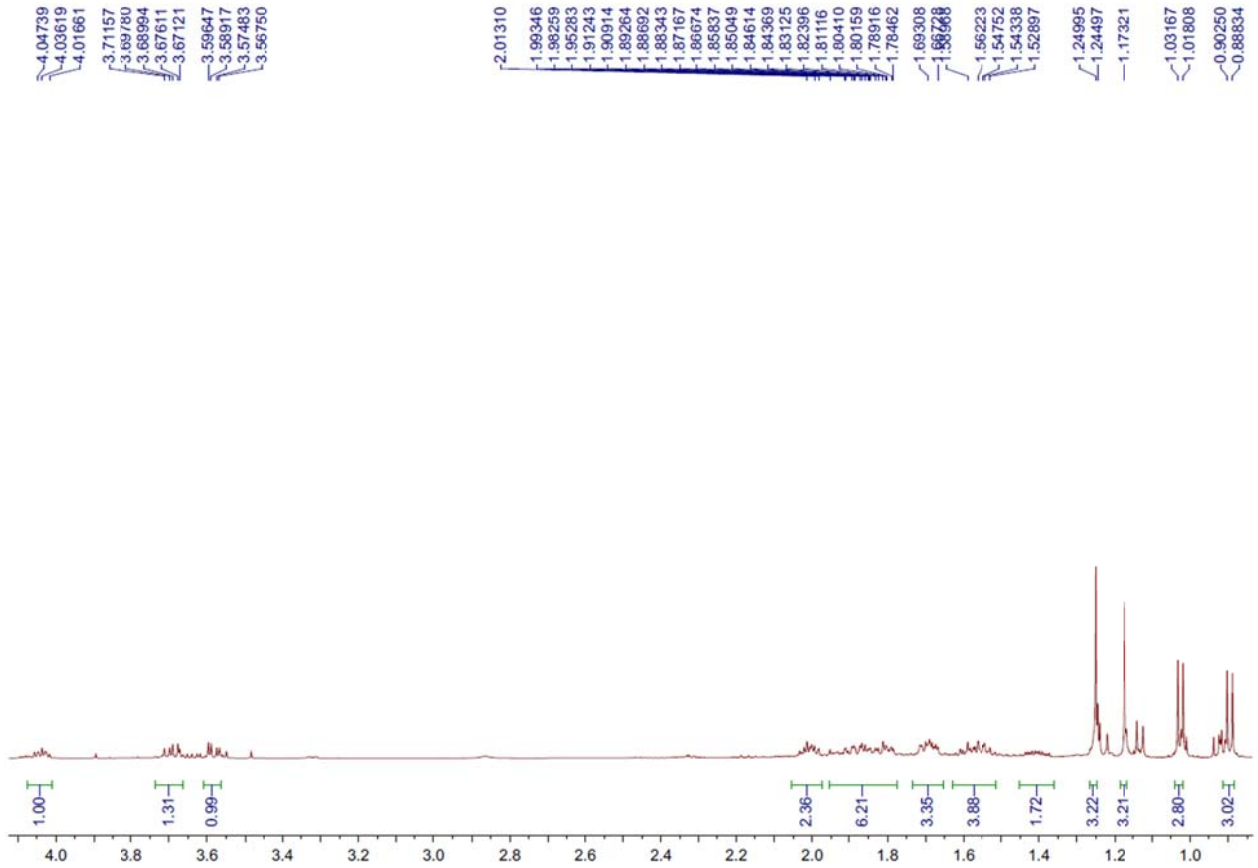


Figure S36. ^{1}H NMR spectrum of compound **6** in $CDCl_3$.

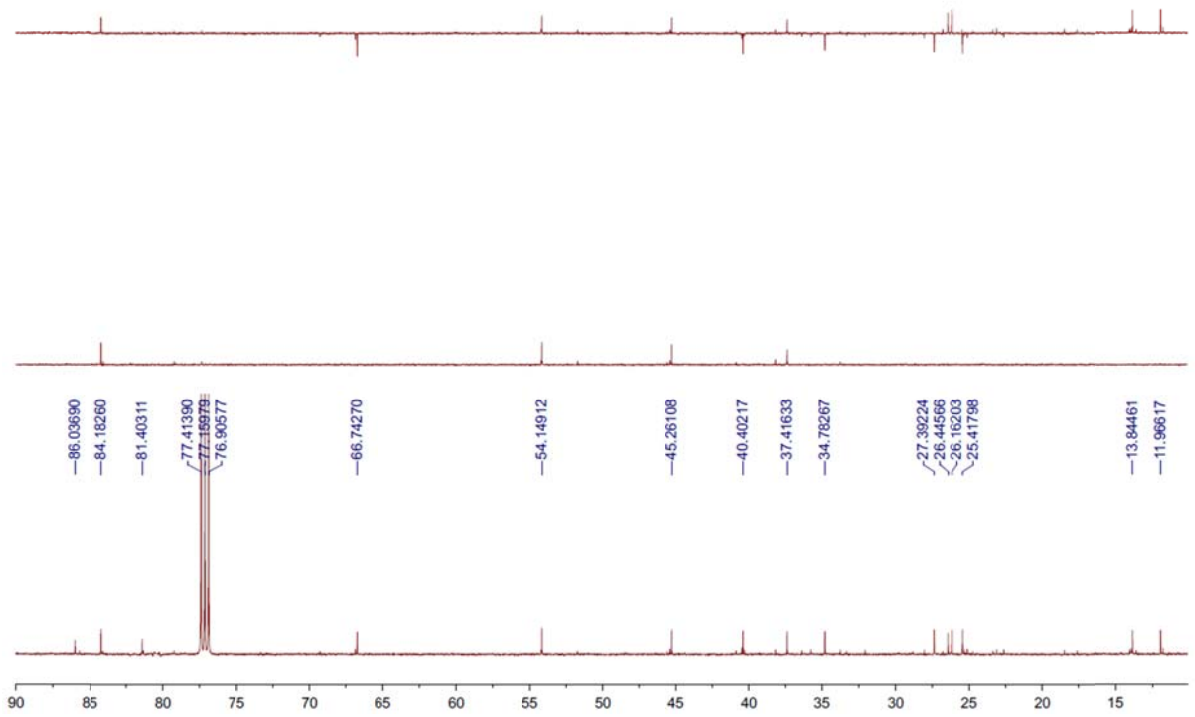


Figure S37. ^{13}C NMR and DEPT spectra of compound **6** in $CDCl_3$.

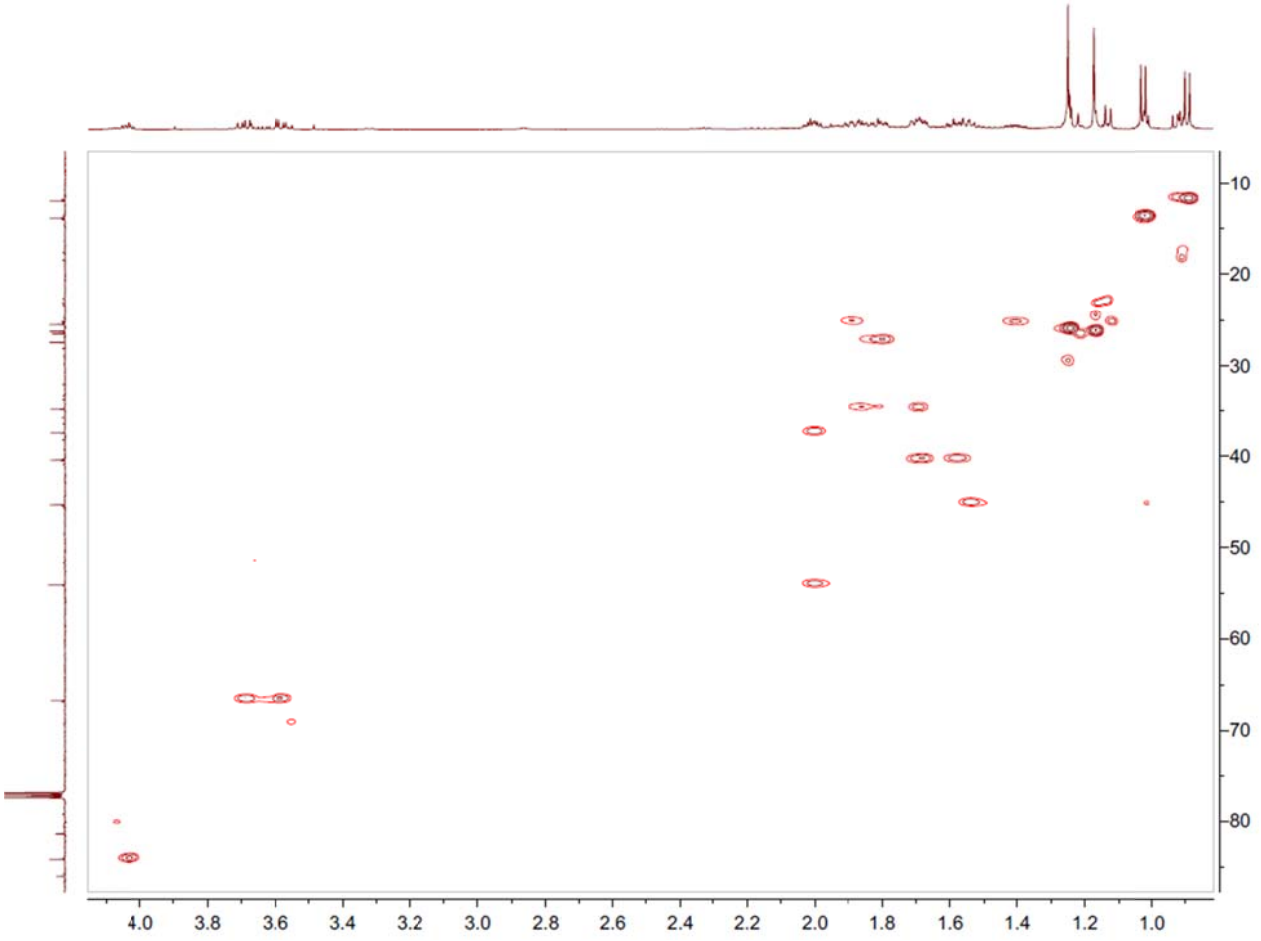


Figure S38. HSQC spectrum of compound **6** in $CDCl_3$.

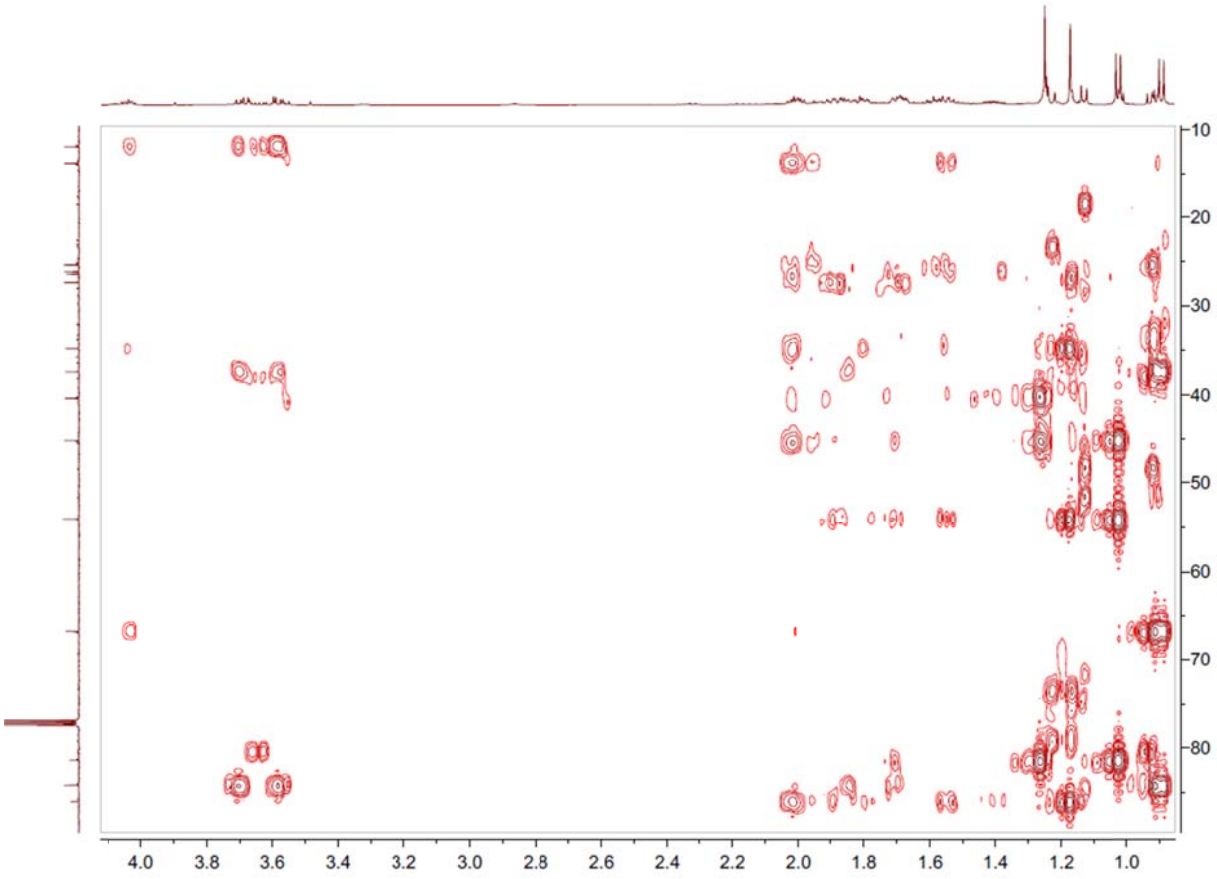


Figure S39. HMBC spectrum of compound **6** in $CDCl_3$.

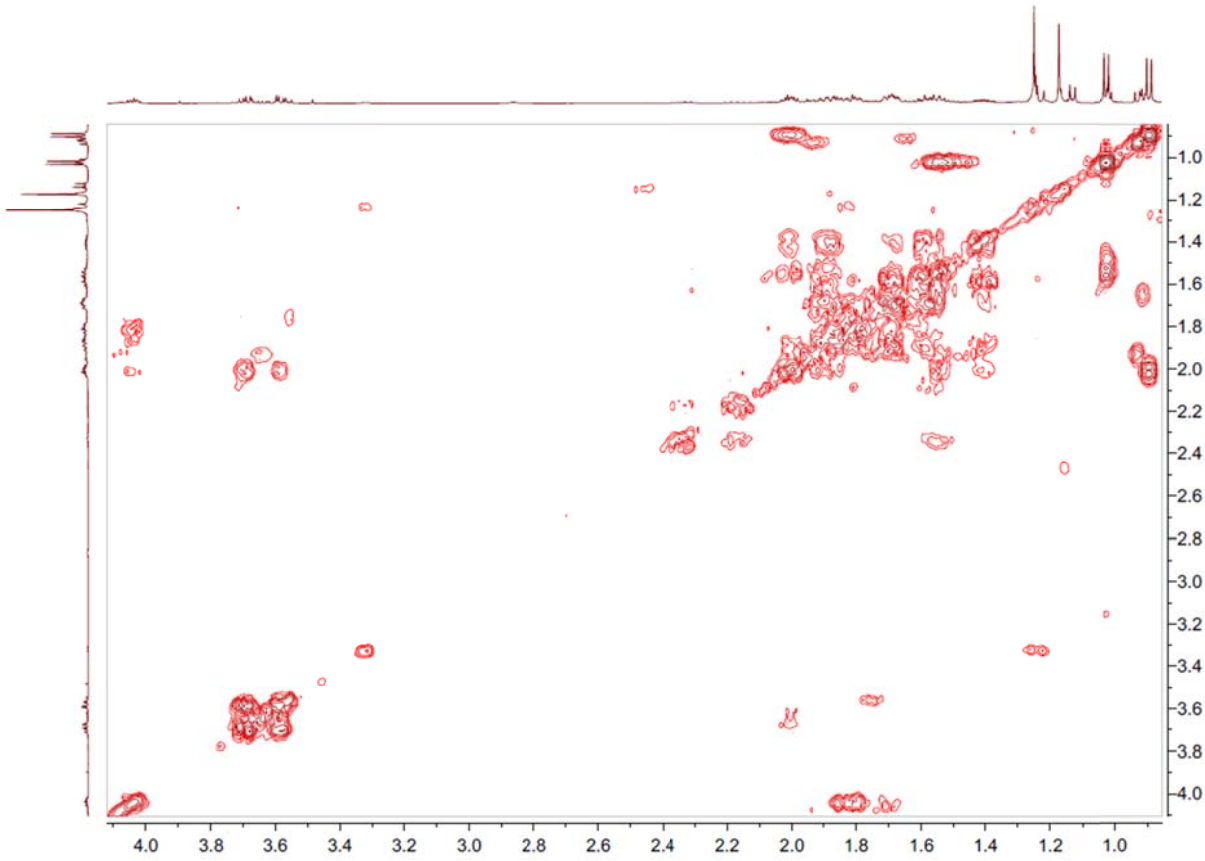


Figure S40. COSY spectrum of compound **6** in $CDCl_3$.

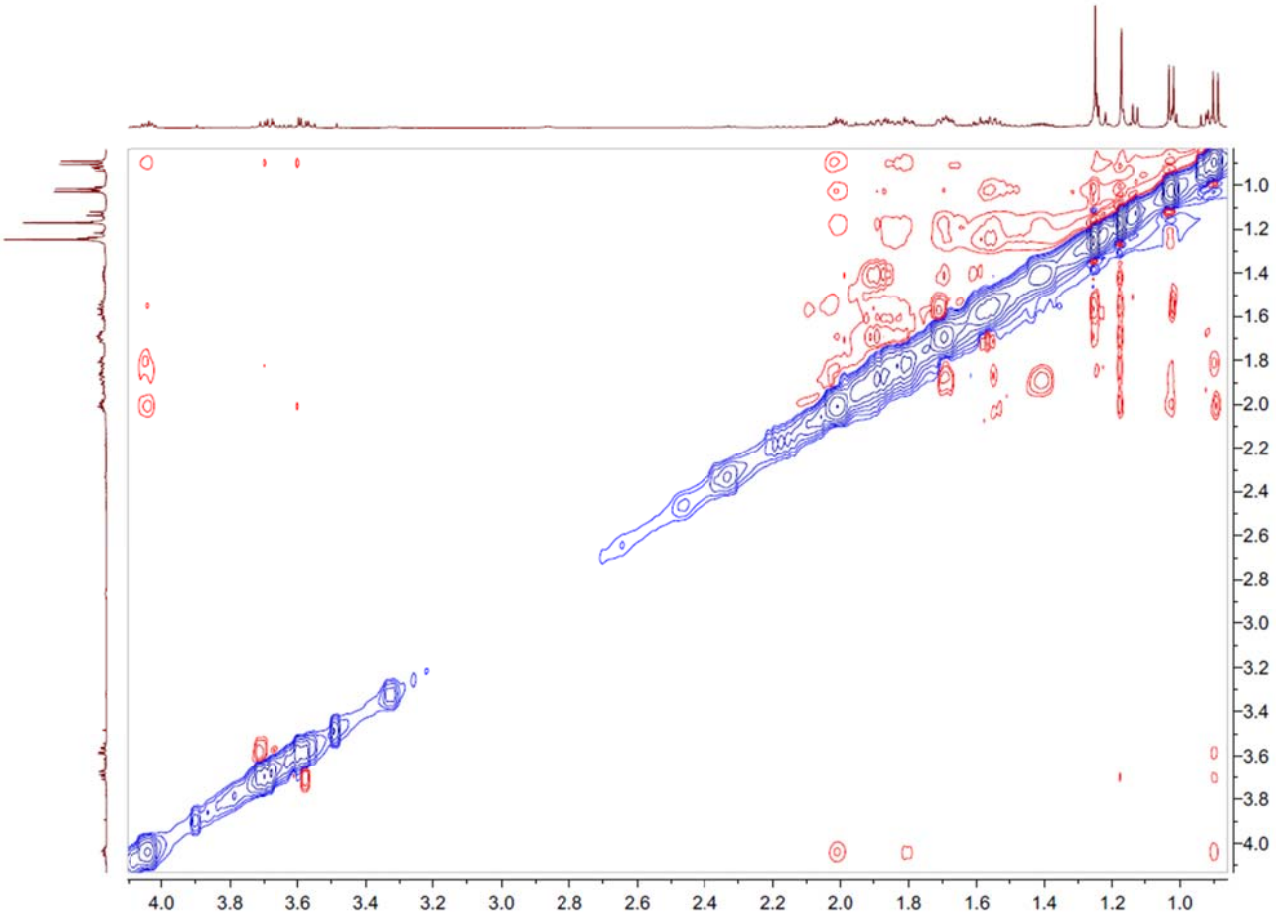


Figure S41. NOESY spectrum of compound **6** in $CDCl_3$.

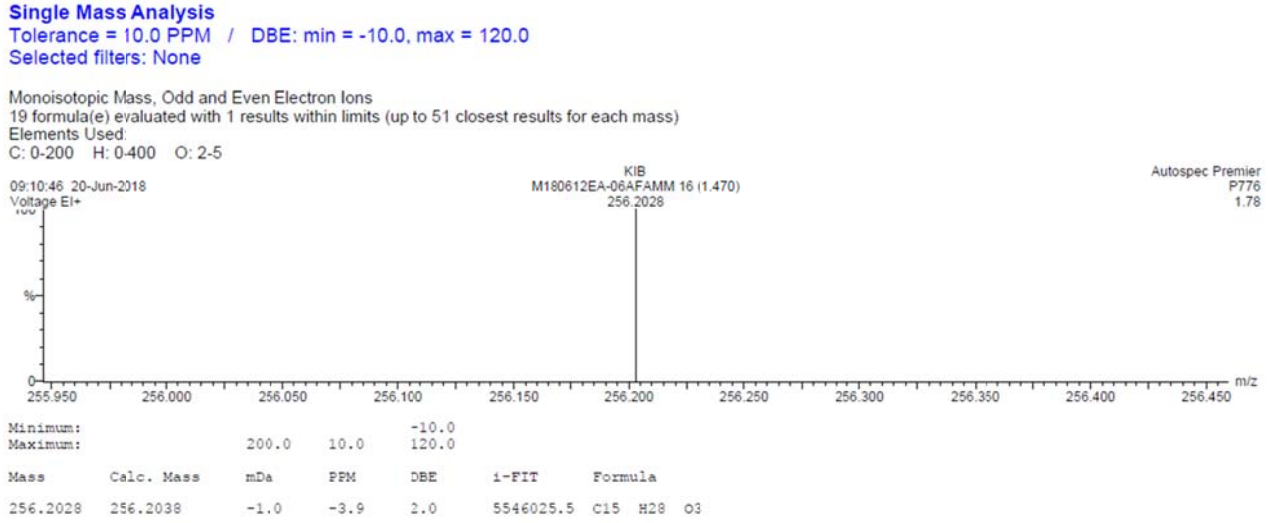


Figure S42. HREIMS spectrum of compound **6**.

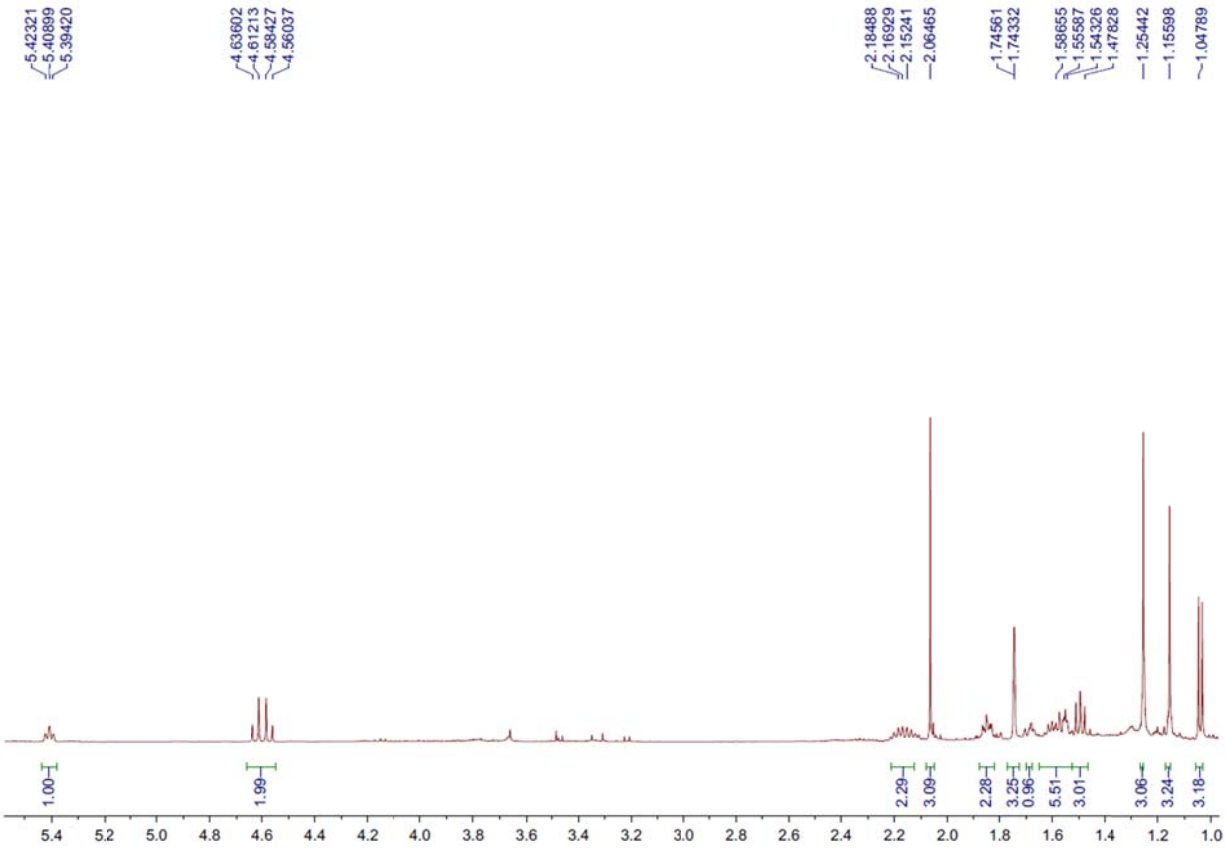


Figure S43. ^{1}H NMR spectrum of compound **7** in $CDCl_3$.

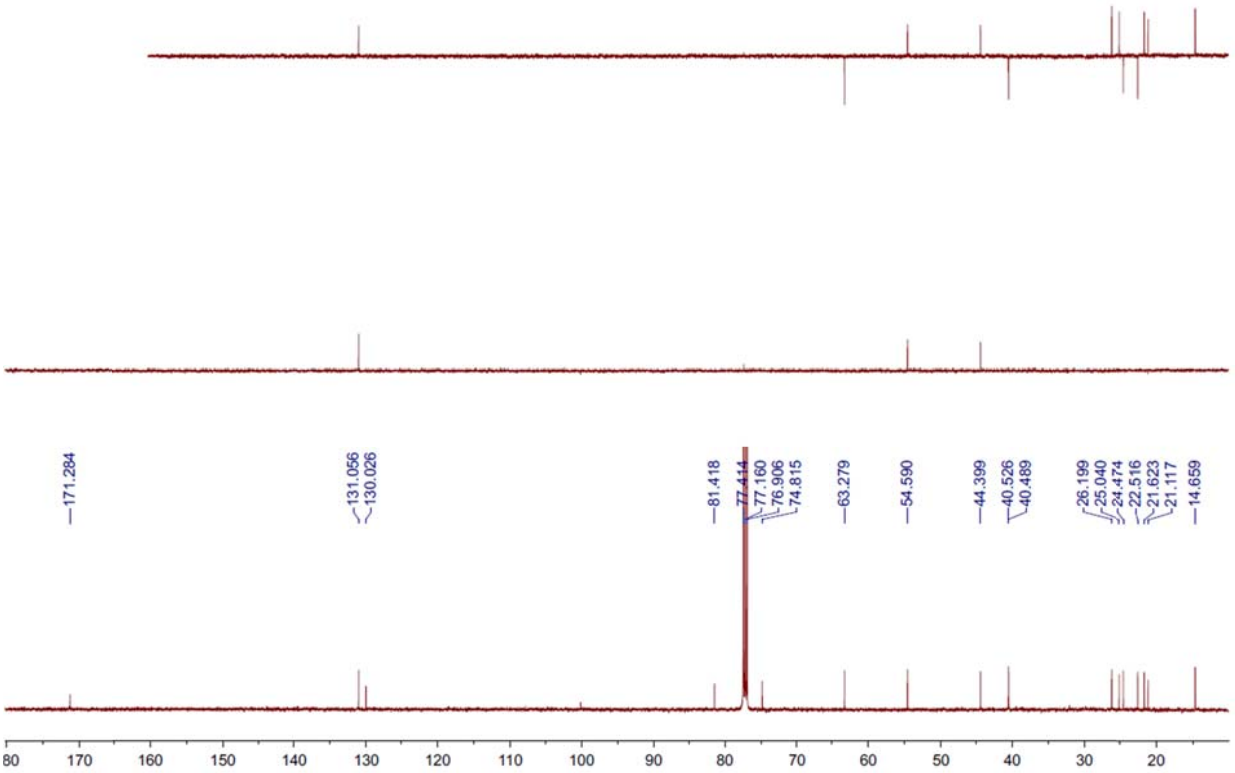


Figure S44. ^{13}C NMR and DEPT spectra of compound **7** in $CDCl_3$.

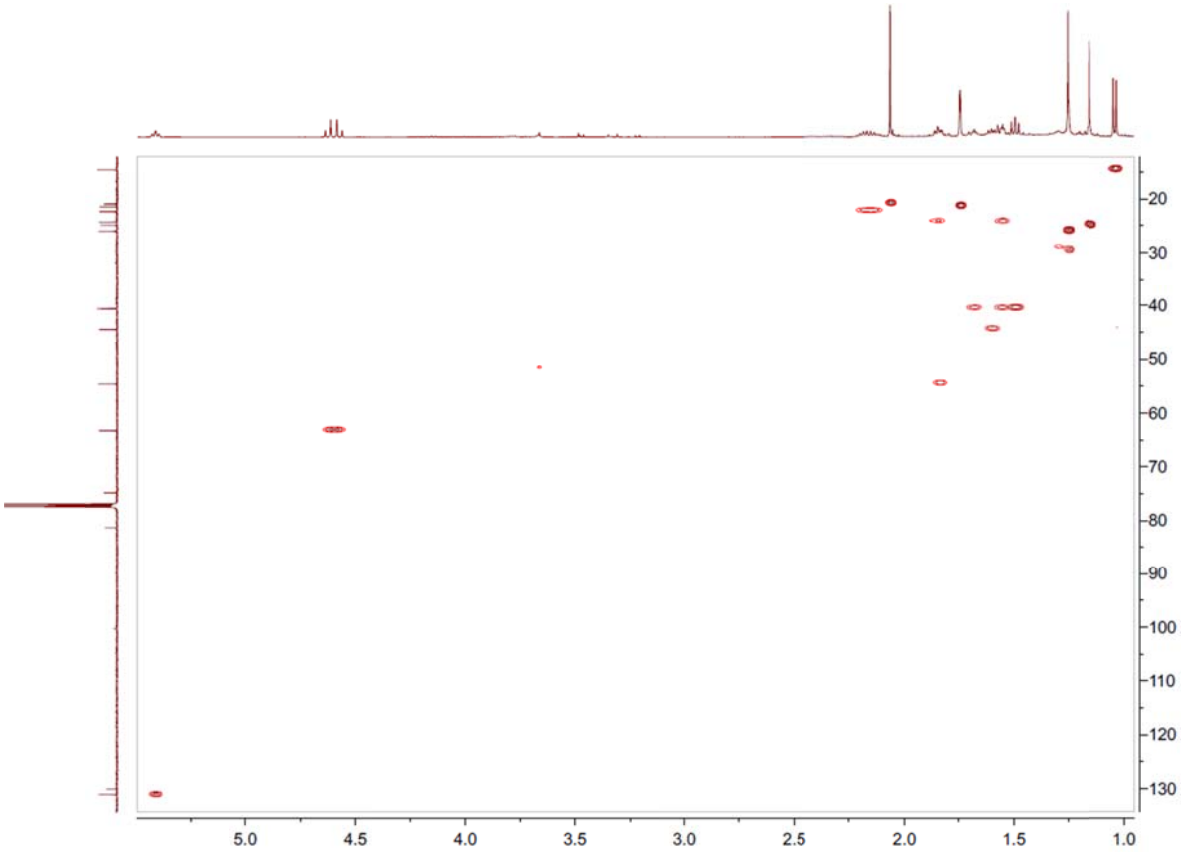


Figure S45. HSQC spectrum of compound **7** in $CDCl_3$.

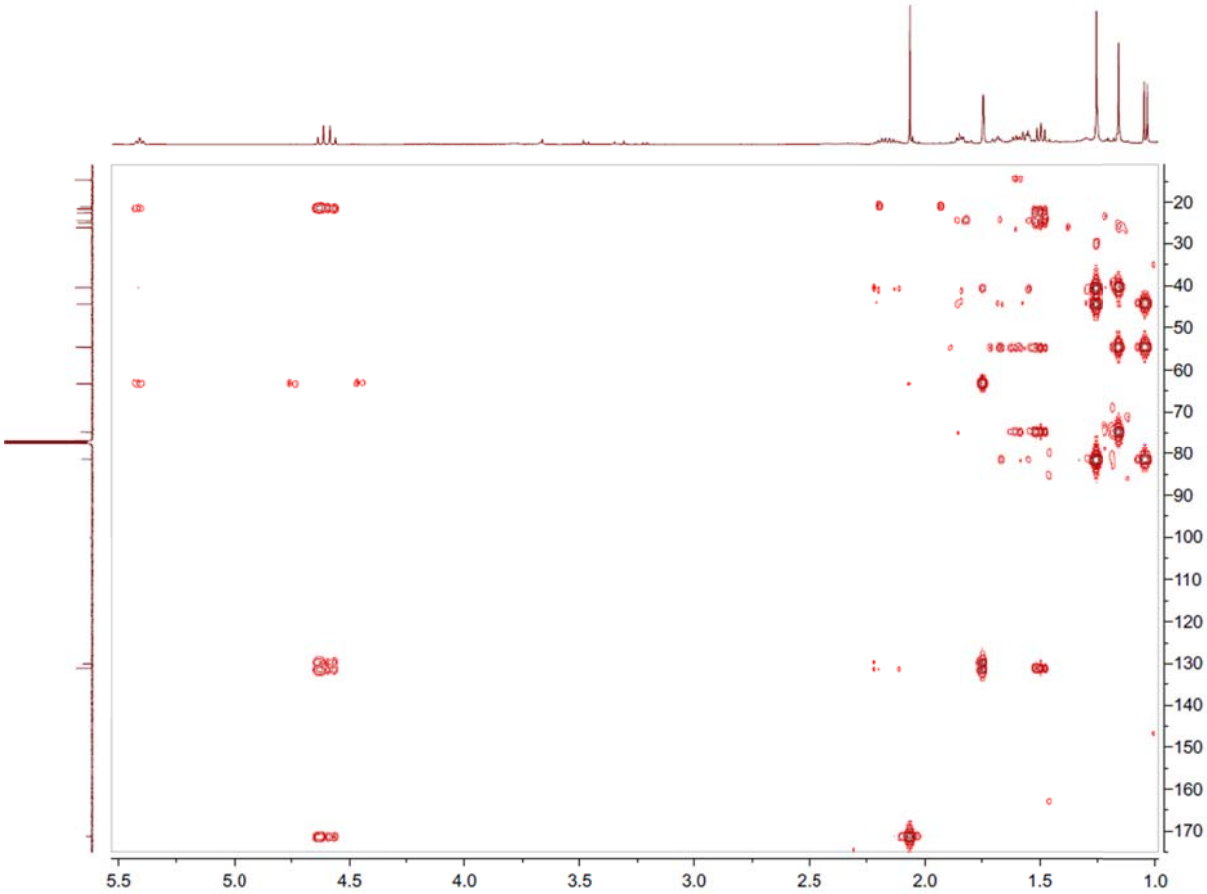


Figure S46. HMBC spectrum of compound **7** in $CDCl_3$.

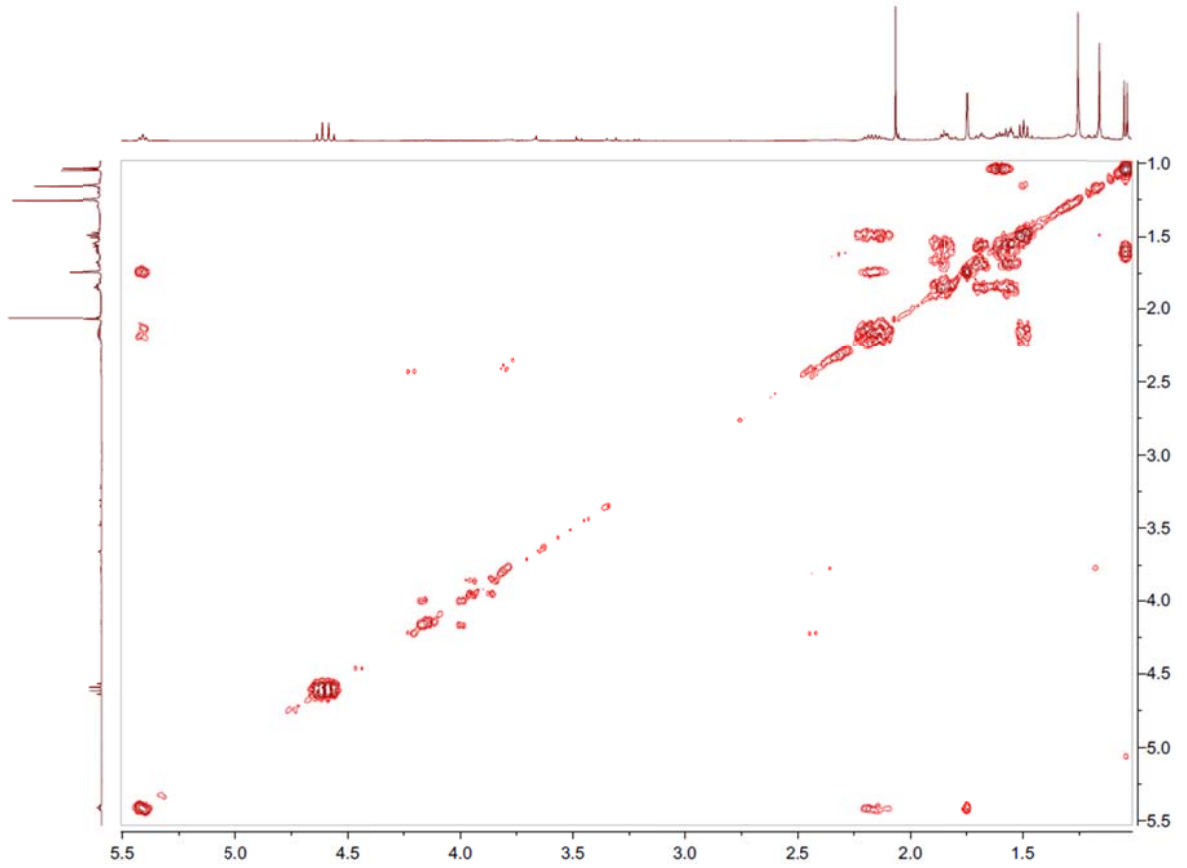


Figure S47. COSY spectrum of compound **7** in $CDCl_3$.

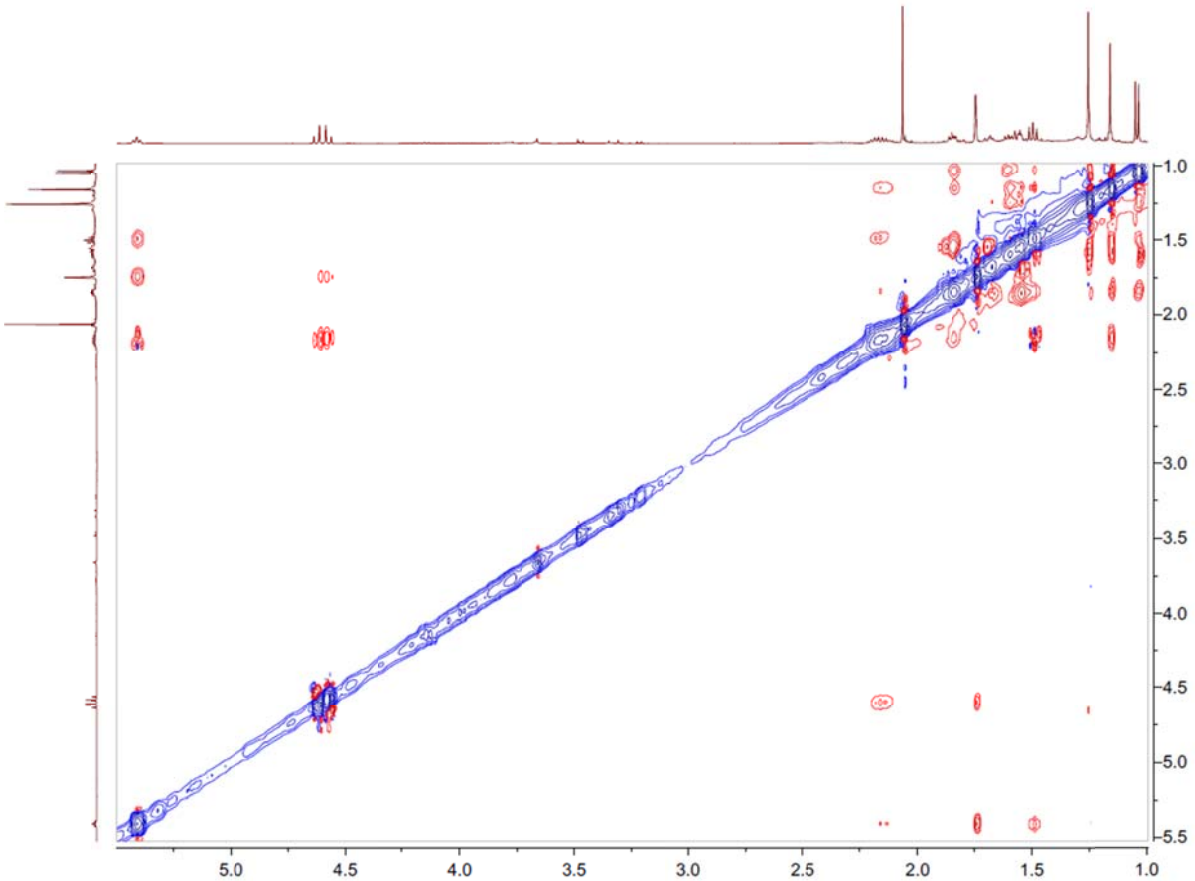
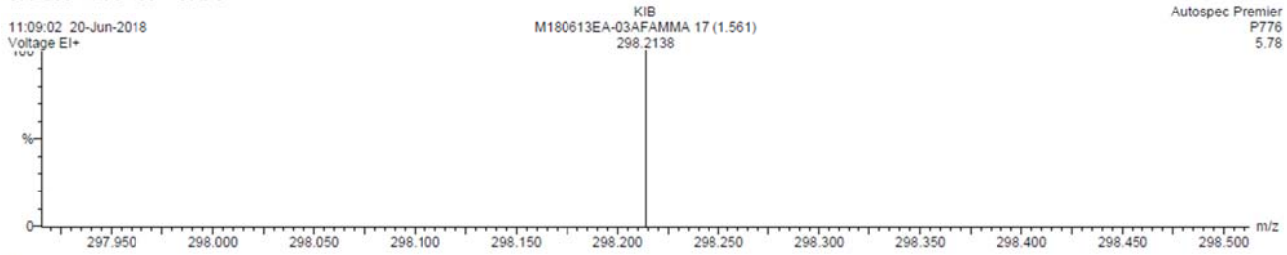


Figure S48. NOESY spectrum of compound **7** in $CDCl_3$.

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
25 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)
Elements Used:
C: 0-200 H: 0-400 O: 2-6



Minimum:				-10.0		
Maximum:		200.0	10.0	120.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
298.2138	298.2144	-0.6	-2.0	3.0	5546025.5	C17 H30 O4

Figure S49. HREIMS spectrum of compound **7**.