

Supplementary Information

New polyketides from a hydrothermal vent sediment fungus *Trichoderma* sp. JWM29-10-1 and their antimicrobial effects

Changrong Lai ^{a, 1}, Jiayi Chen ^{a, 1}, Jing Liu ^{b, 1}, Danmei Tian ^a, Donghe Lan ^c, Tongzheng Liu ^a, Bin Wu ^{c, *}, Hongkai Bi ^{b, *} and Jinshan Tang ^{a, *}

^a *Institute of Traditional Chinese Medicine and Natural Products, College of Pharmacy/Guangdong Province Key Laboratory of Pharmacodynamic Constituents of Traditional Chinese Medicine and New Drug Research/International Cooperative Laboratory of Traditional Chinese Medicine Modernization and Innovative Drug Development of Ministry of Education (MOE) of China, Jinan University, Guangzhou 510632, China*

^b *Department of Pathogen Biology, Jiangsu Key Laboratory of Pathogen Biology, Helicobacter pylori Research Centre, Nanjing Medical University, Nanjing 211166, China*

^c *Ocean College, Zhejiang University, Zhoushan Campus, Zhoushan 316021, China*

¹ These authors contributed equally to this work.

Corresponding authors

Email address: jstang0615@jnu.edu.cn (J. Tang); hkbi@njmu.edu.cn (H. Bi); wubin@zju.edu.cn (B.W.)

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Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

46 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-30 H: 0-50 O: 0-10

JWM29-7-11-2

20220411-24 162 (1.313)

1: TOF MS ES+
1.11e+005

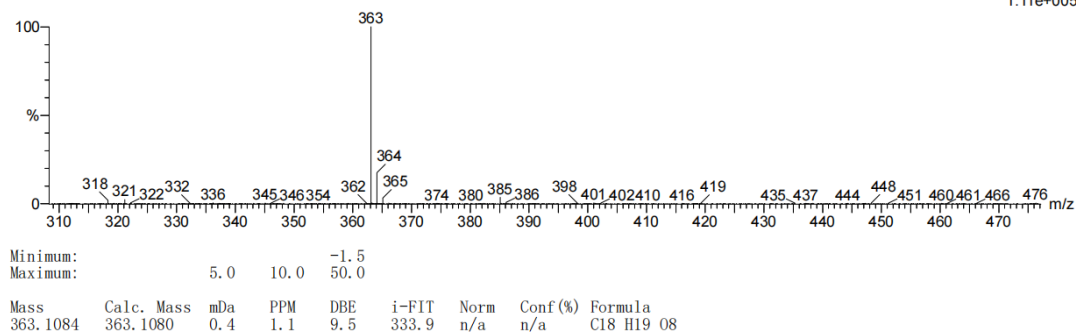


Figure S1 HR-ESI-MS spectrum of compound **1**

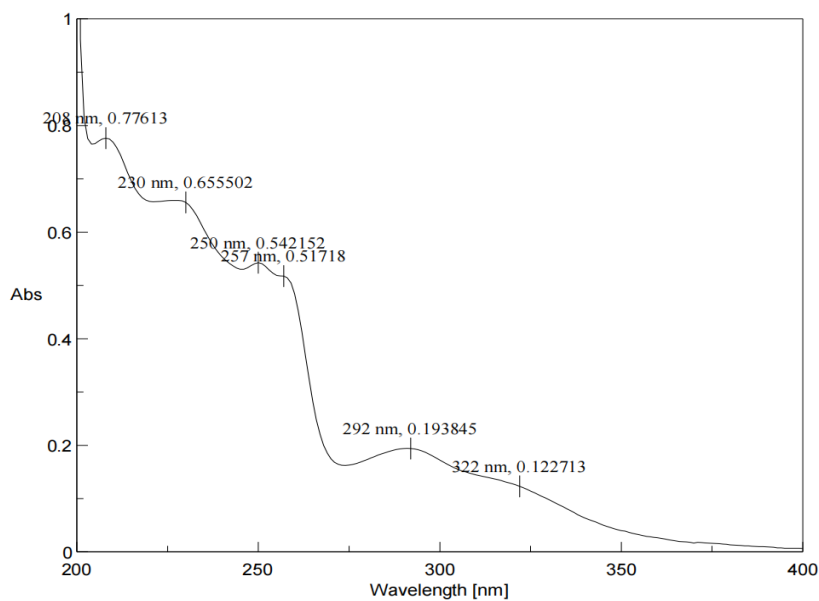


Figure S2 UV spectrum of compound **1**

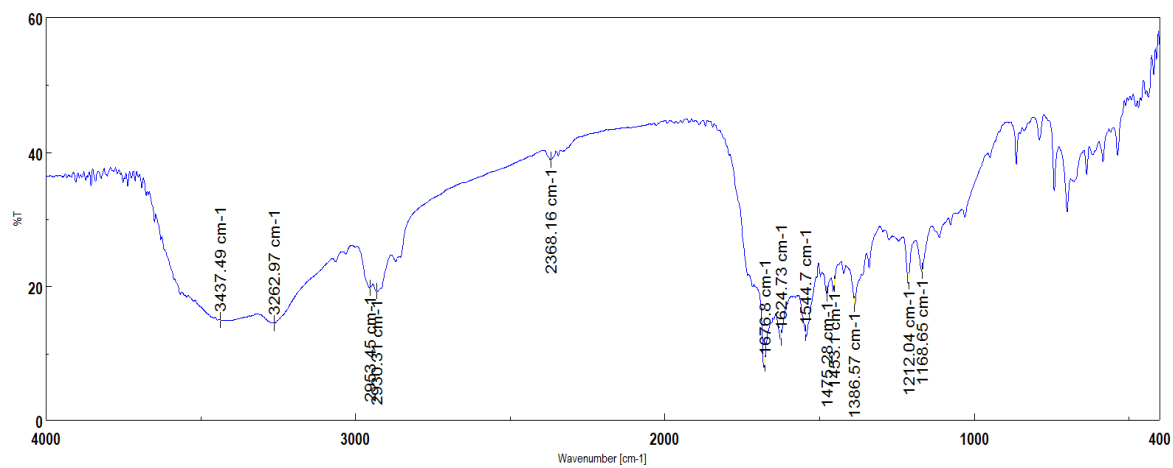


Figure S3 IR spectrum of compound **1**

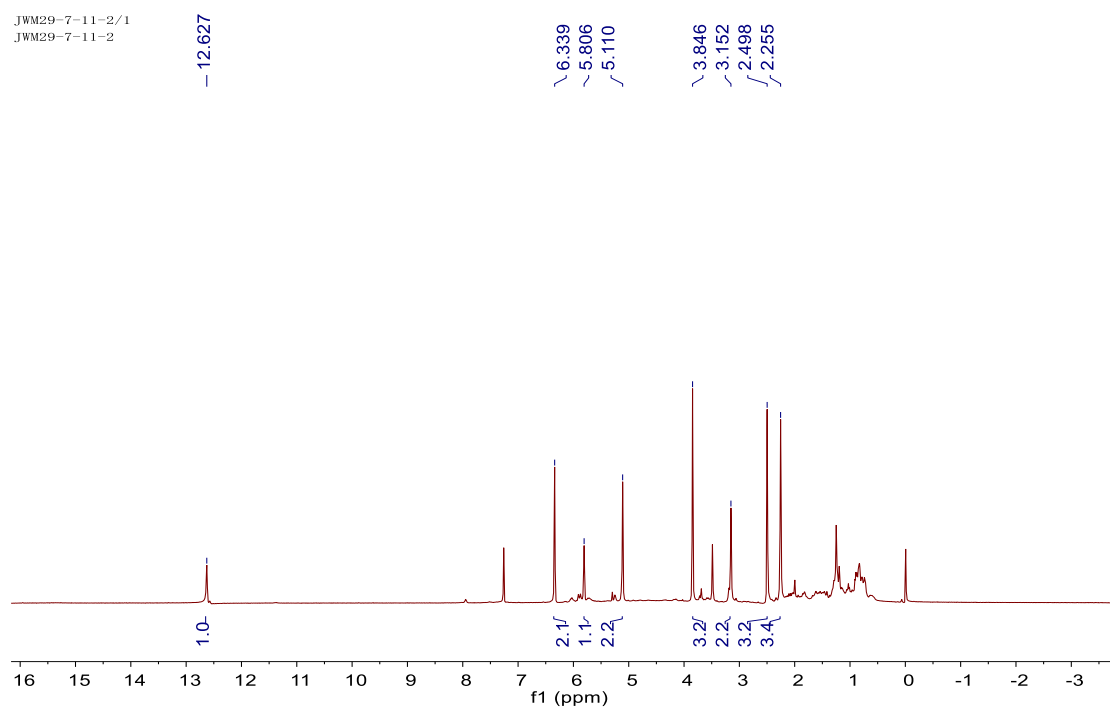


Figure S4 ¹H-NMR spectrum of compound **1** (in CDCl₃)

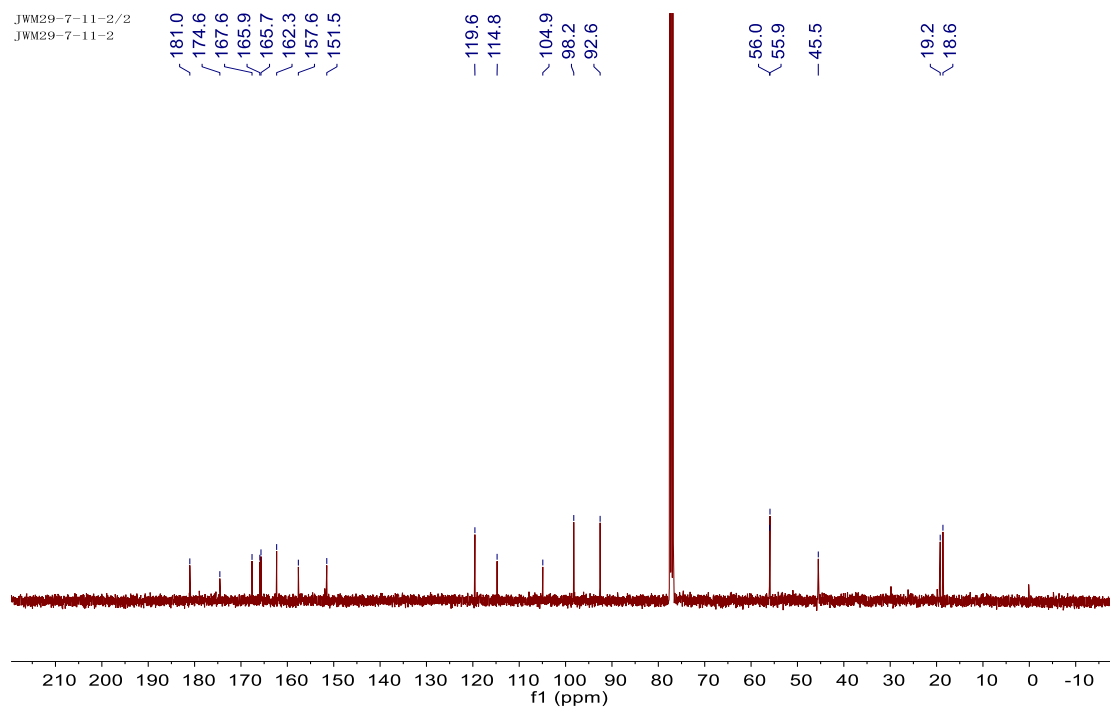


Figure S5 ^{13}C -NMR spectrum of compound **1** (in CDCl_3)

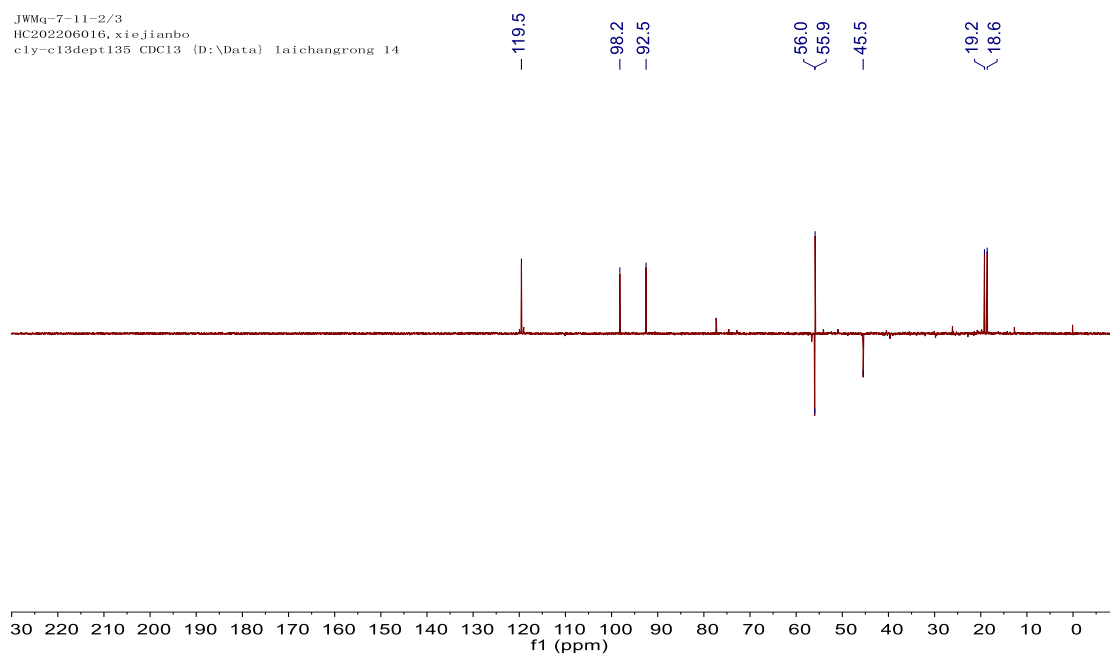


Figure S6 DEPT135 spectrum of compound **1** (in CDCl_3)

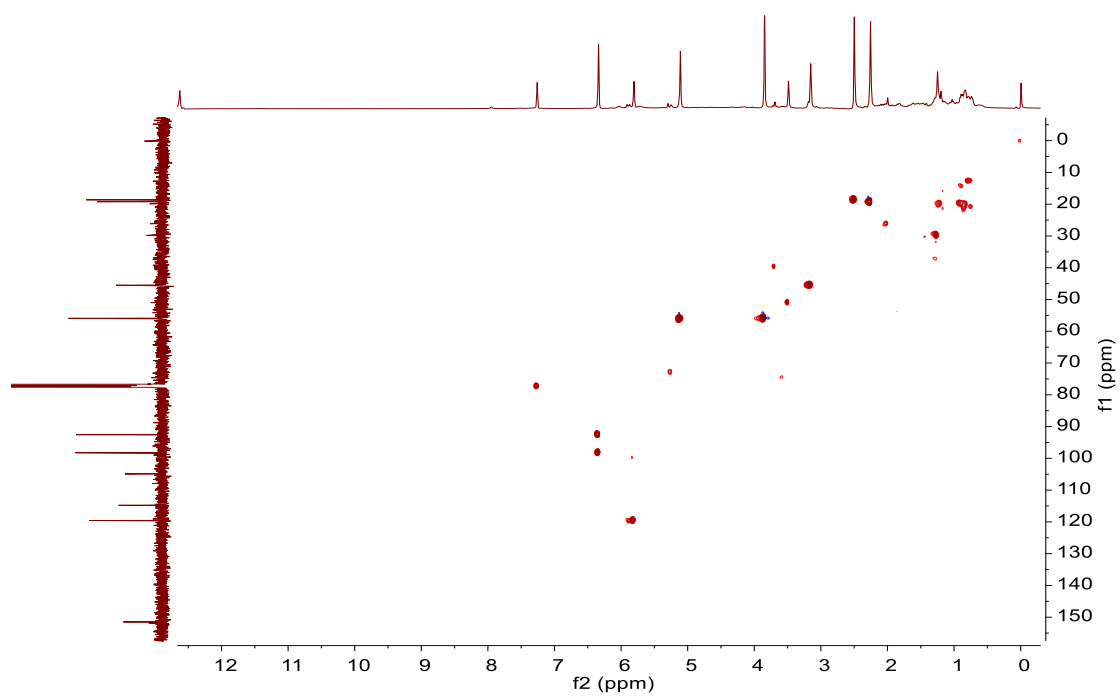


Figure S7 HSQC spectrum of compound **1** (in CDCl₃)

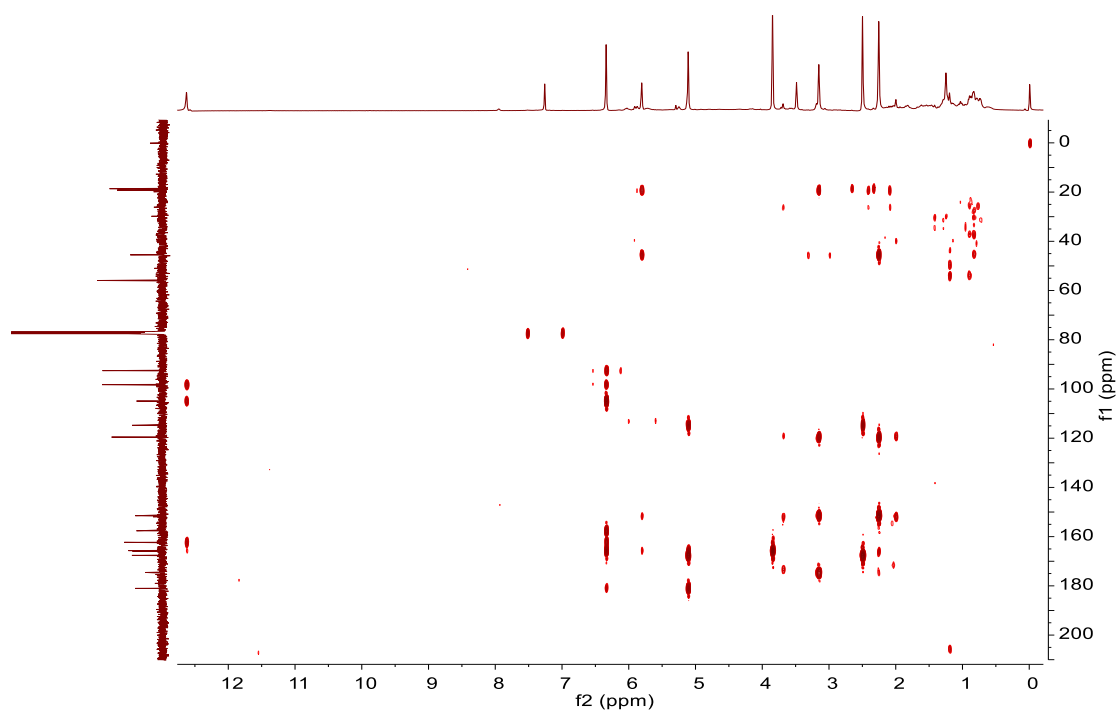


Figure S8 HMBC spectrum of compound **1** (in CDCl₃)

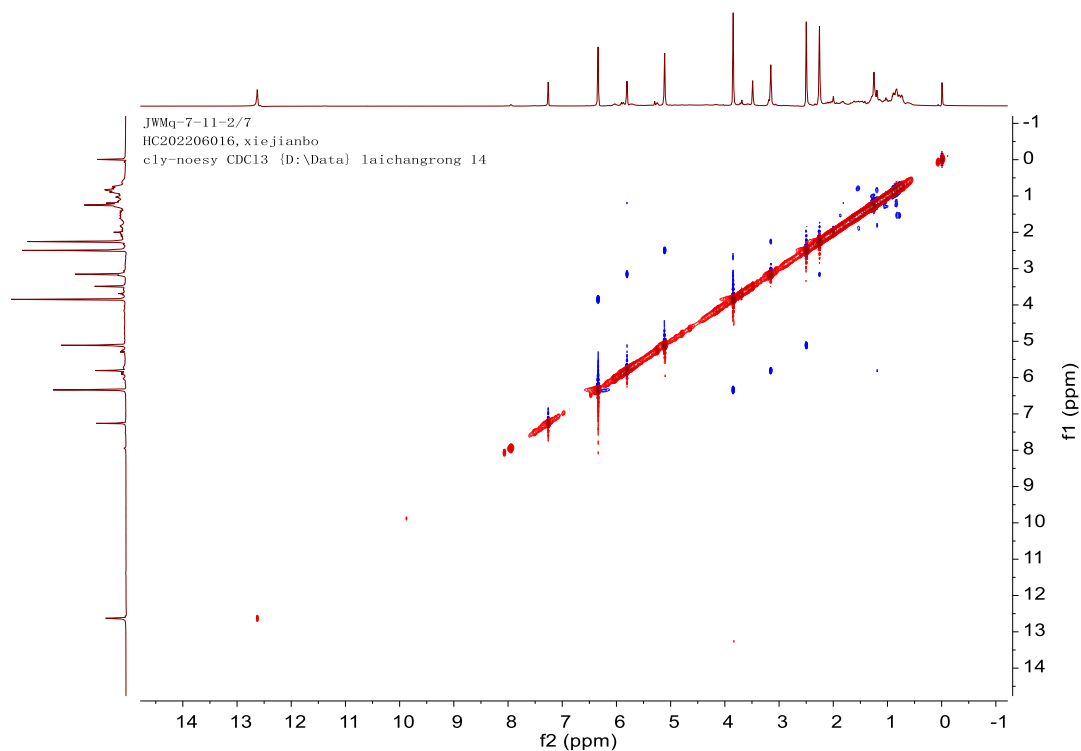


Figure S9 NOESY spectrum of compound **1** (in CDCl₃)

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

33 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-30 H: 0-50 O: 0-10

JWM29-3-5-4

20220322008 129 (1.044)

1: TOF MS ES+
1.46e+005

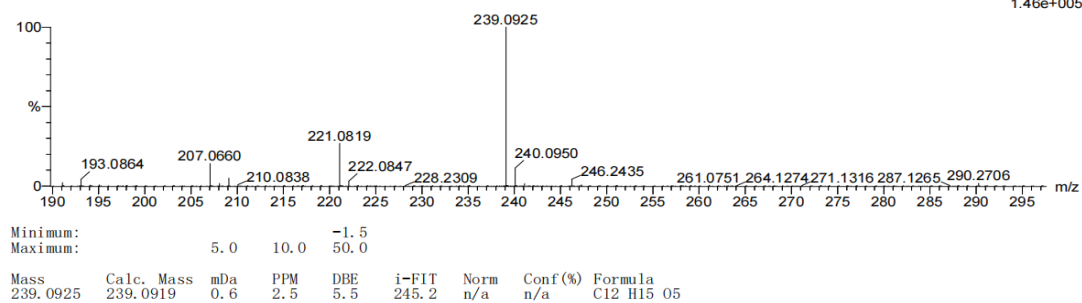


Figure S10 HR-ESI-MS spectrum of compound **2**

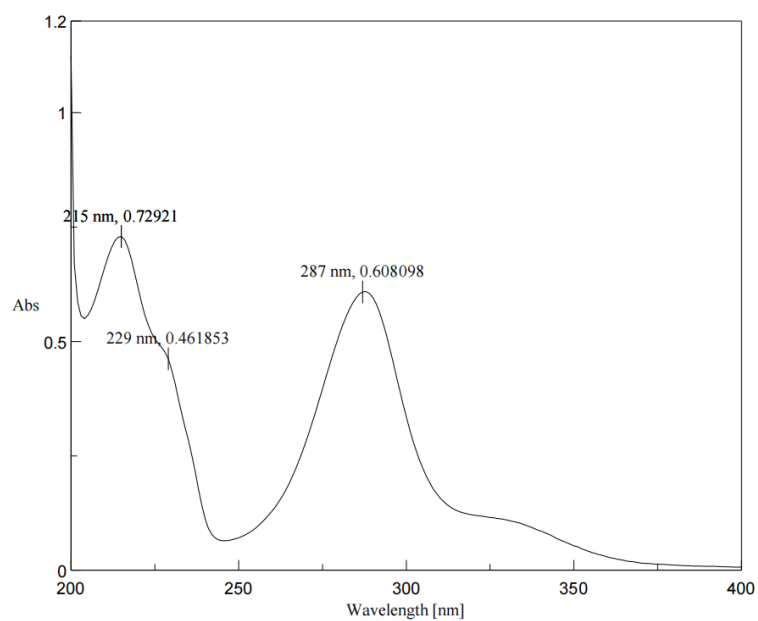


Figure S11 UV spectrum of compound **2**

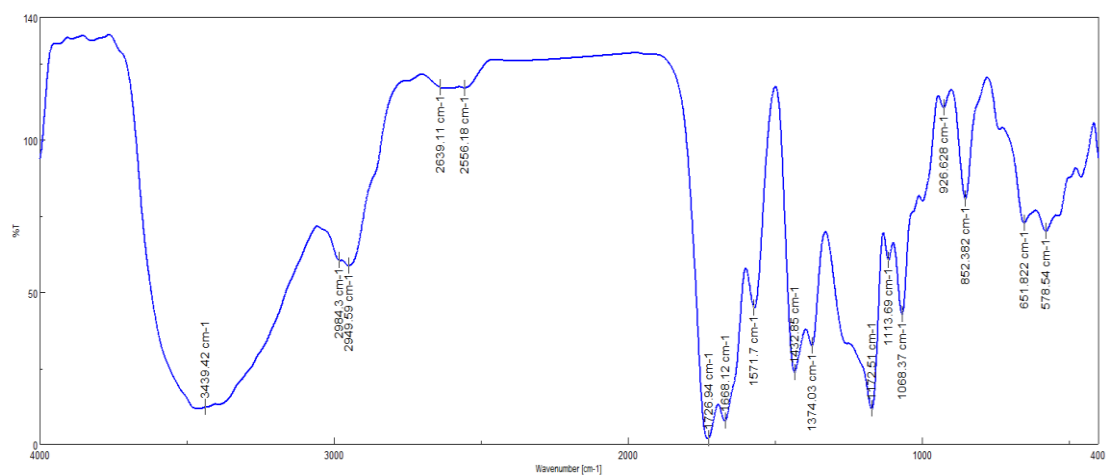


Figure S12 IR spectrum of compound **2**

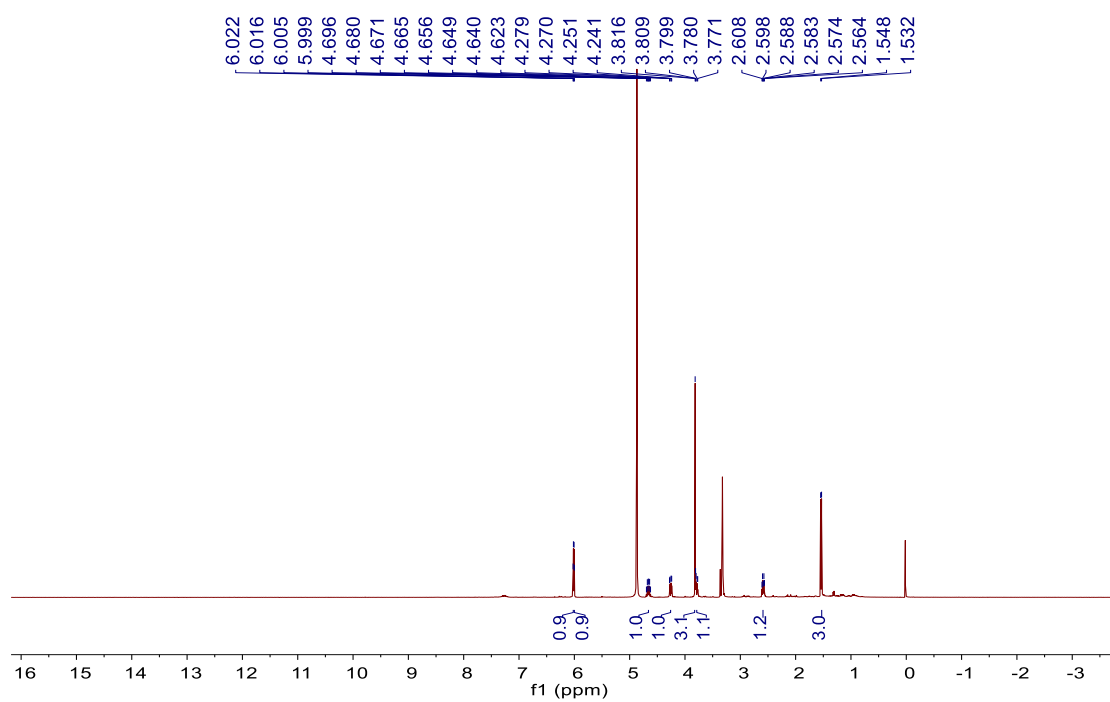


Figure S13 ¹H-NMR spectrum of compound **2** (in CD₃OD)

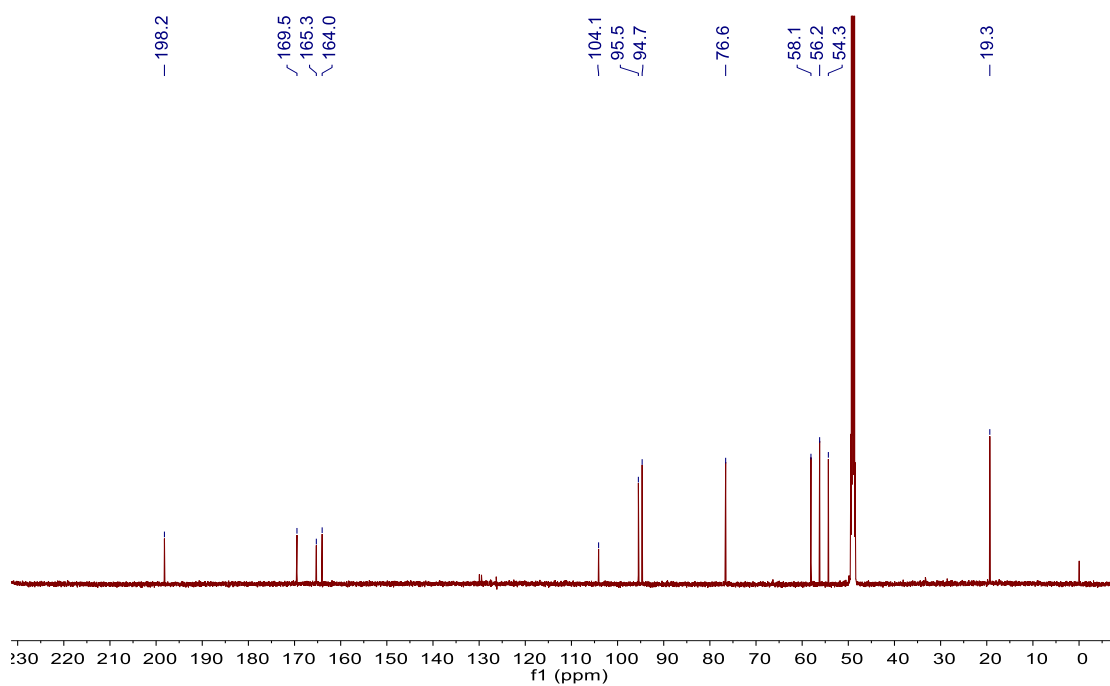


Figure S14 ¹³C-NMR spectrum of compound **2** (in CD₃OD)

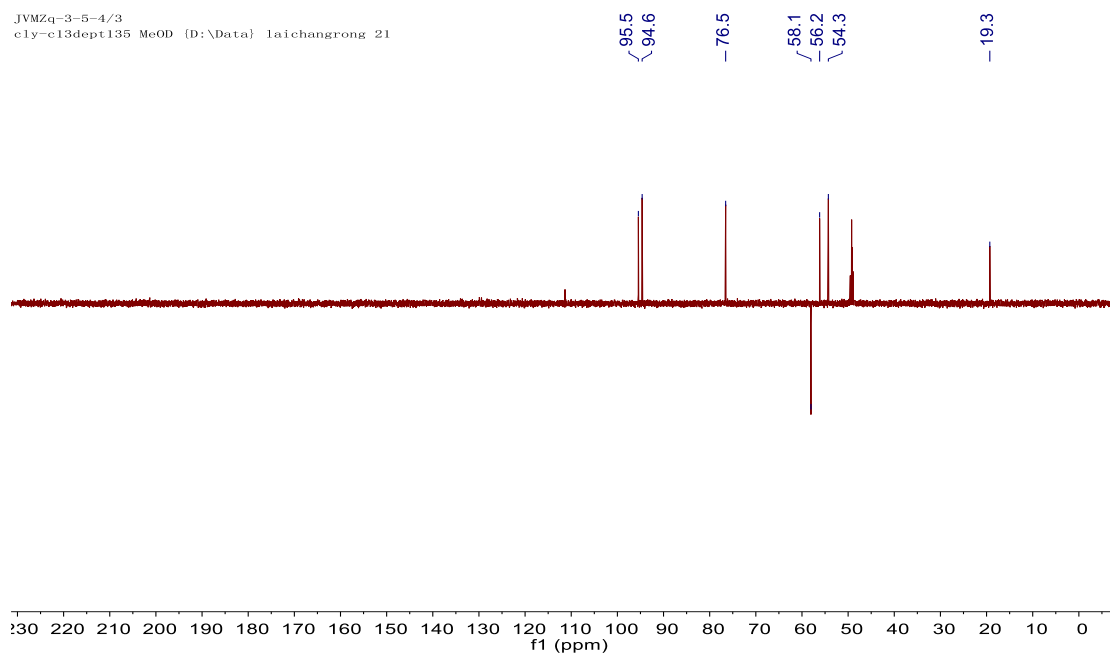


Figure S15 DEPT135 spectrum of compound **2** (in CD₃OD)

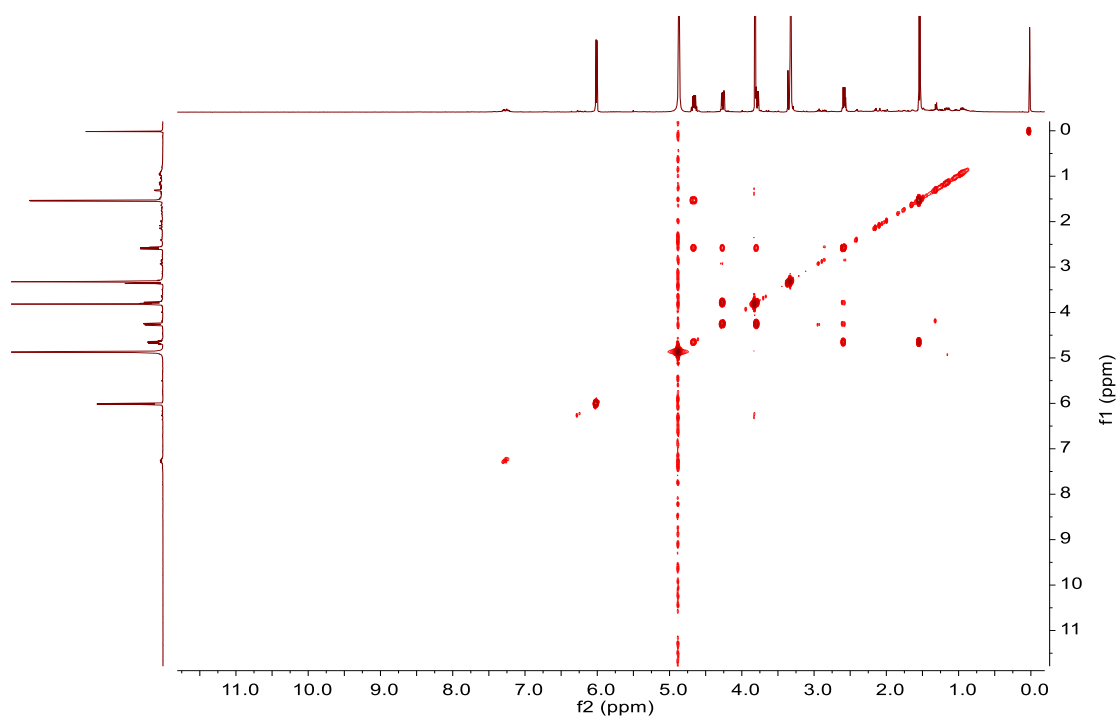


Figure S16 ¹H-¹H COSY spectrum of compound **2** (in CD₃OD)

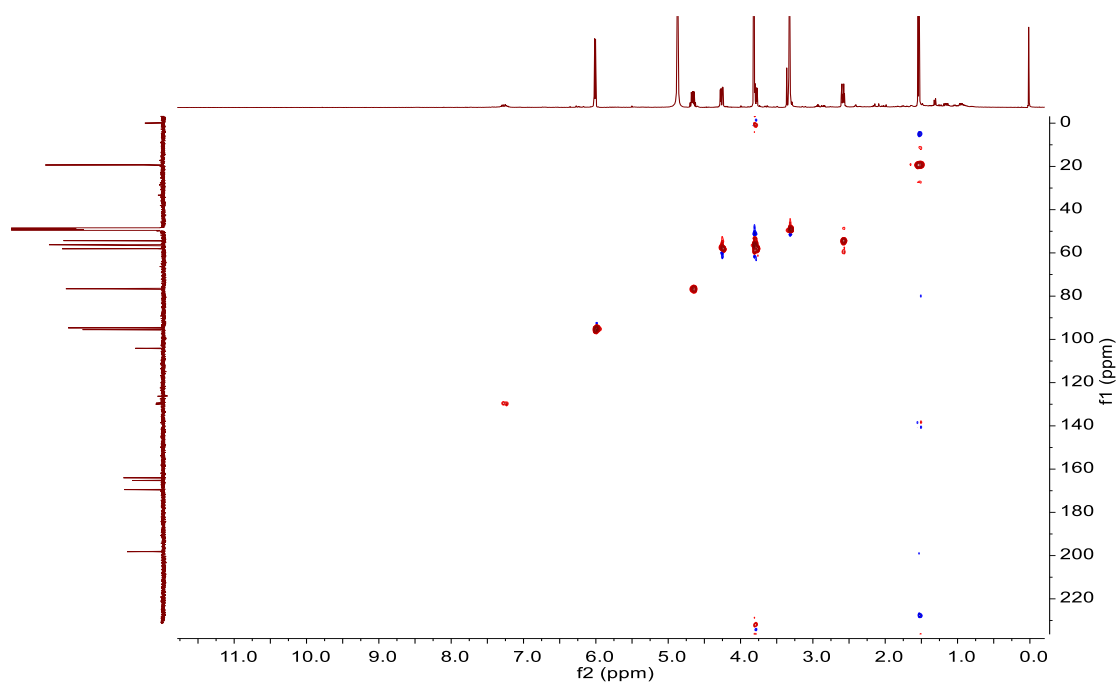


Figure S17 HSQC spectrum of compound **2** (in CD₃OD)

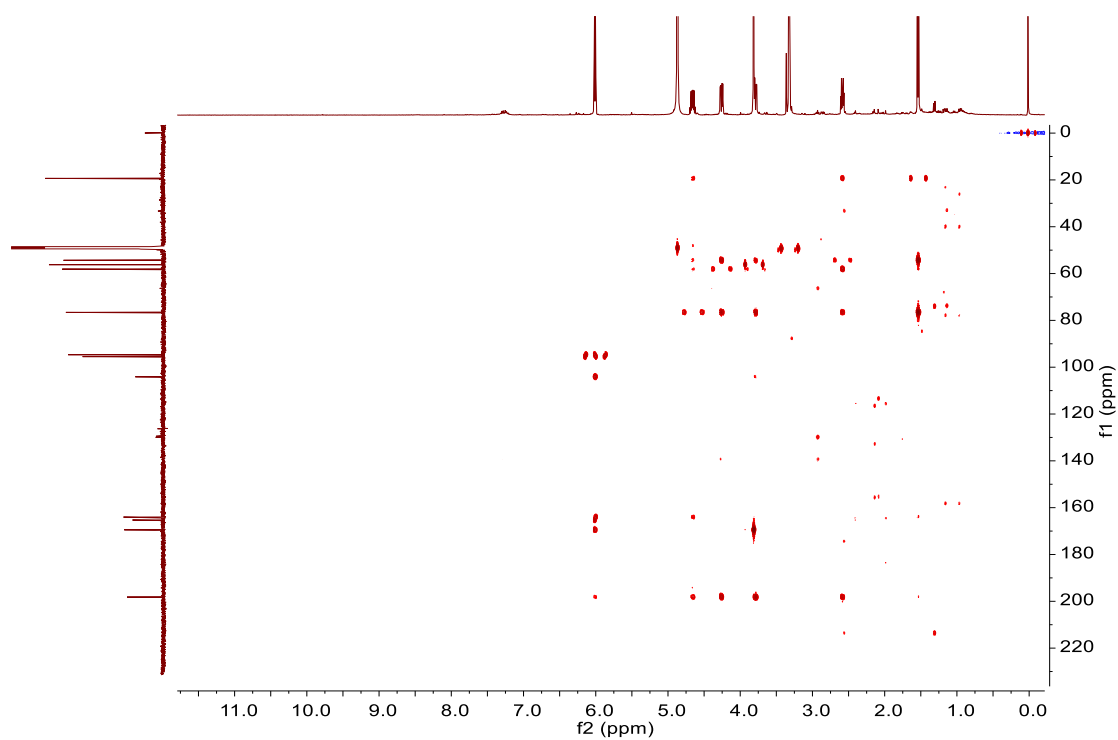


Figure S18 HMBC spectrum of compound **2** (in CD₃OD)

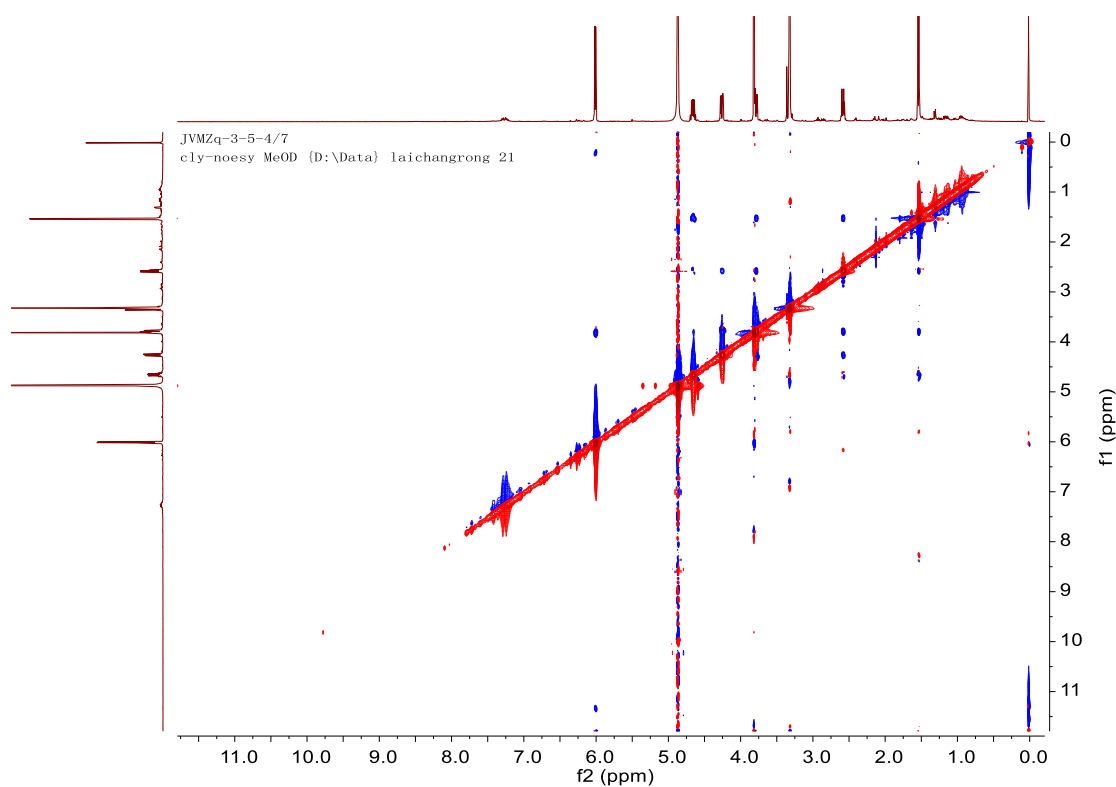


Figure S19 NOESY spectrum of compound **2** (in CD₃OD)

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

30 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-30 H: 0-50 O: 0-10

JVM29-9-9-1

20220613033 131 (1.070)

1: TOF MS ES+
9.00e+004



Minimum: -1.5
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
451.2707	451.2696	1.1	2.4	6.5	130.0	n/a	n/a	C25 H39 O7

Figure S20 HR-ESI-MS spectrum of compound **6**

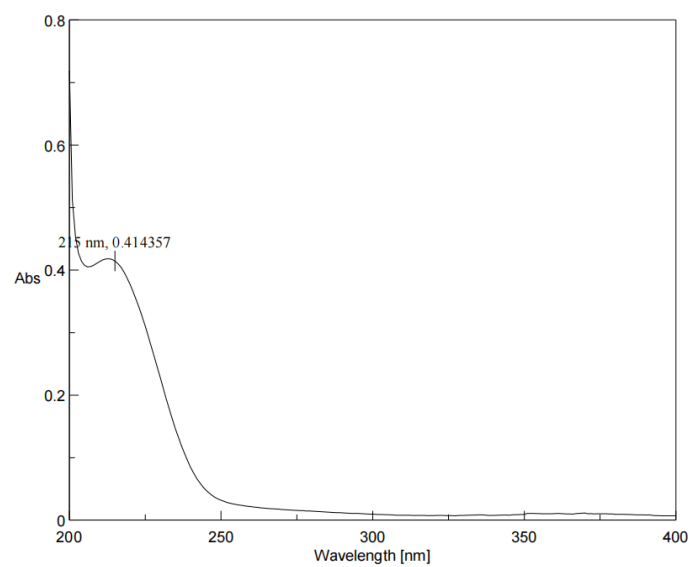


Figure S21 UV spectrum of compound **6**

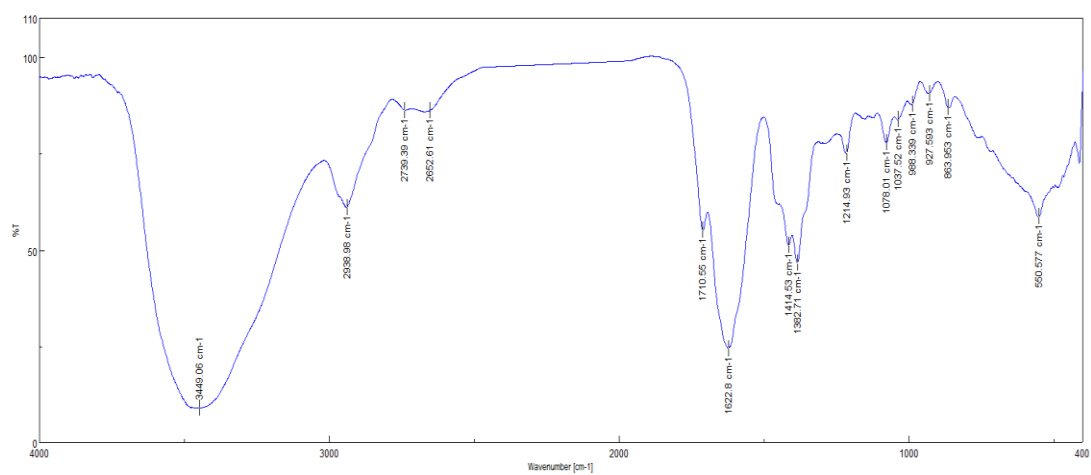


Figure S22 IR spectrum of compound **6**

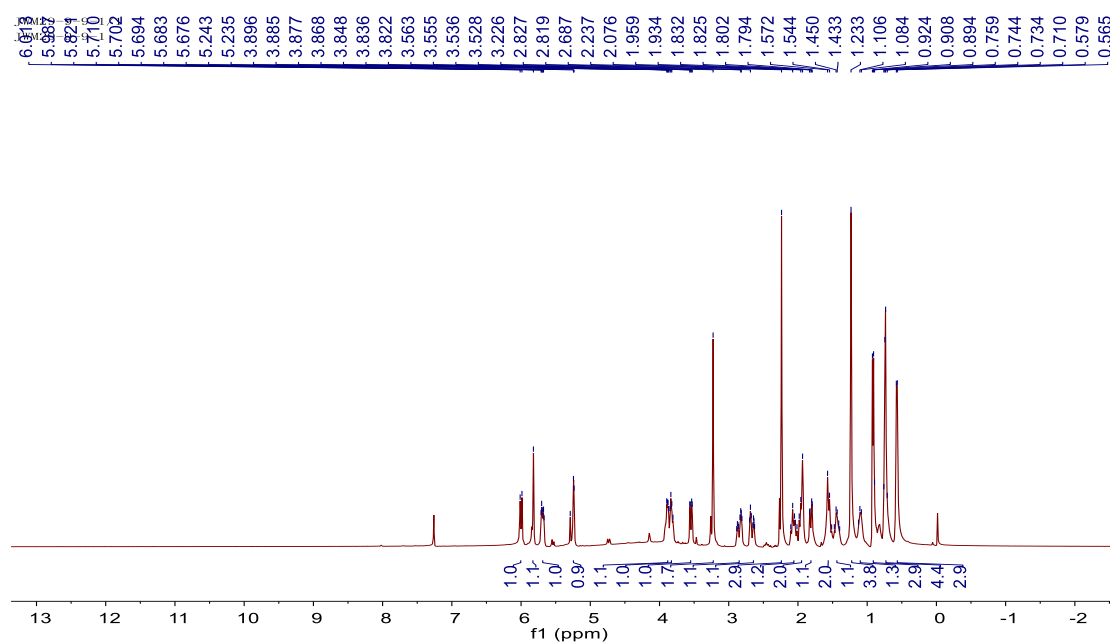


Figure S23 ¹H-NMR spectrum of compound **6** (in CDCl₃)

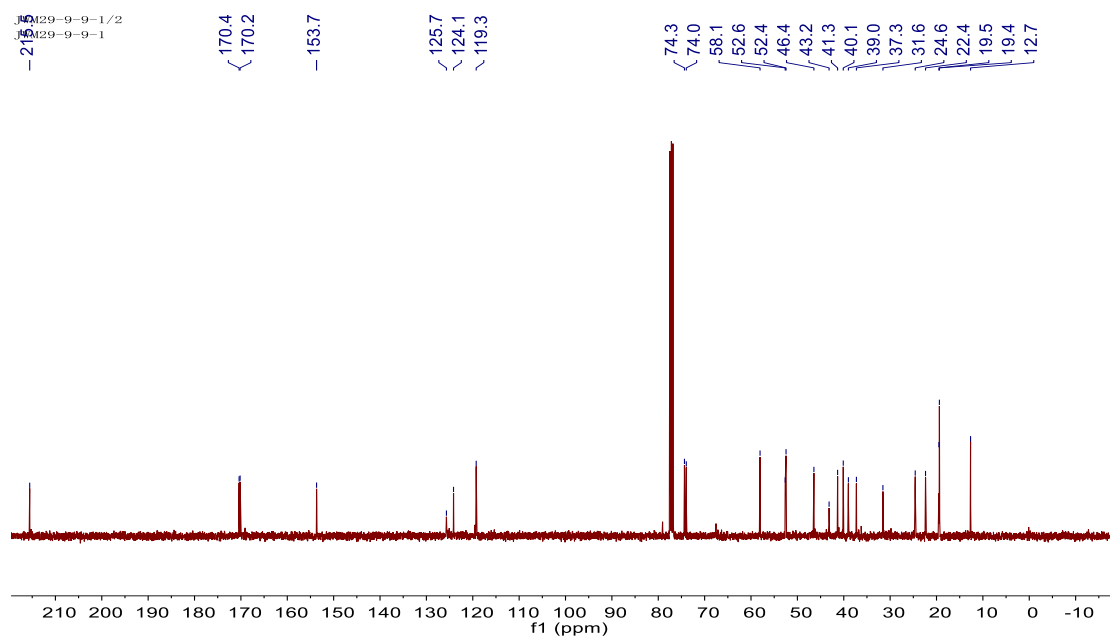


Figure S24 ¹³C-NMR spectrum of compound **6** (in CDCl₃)

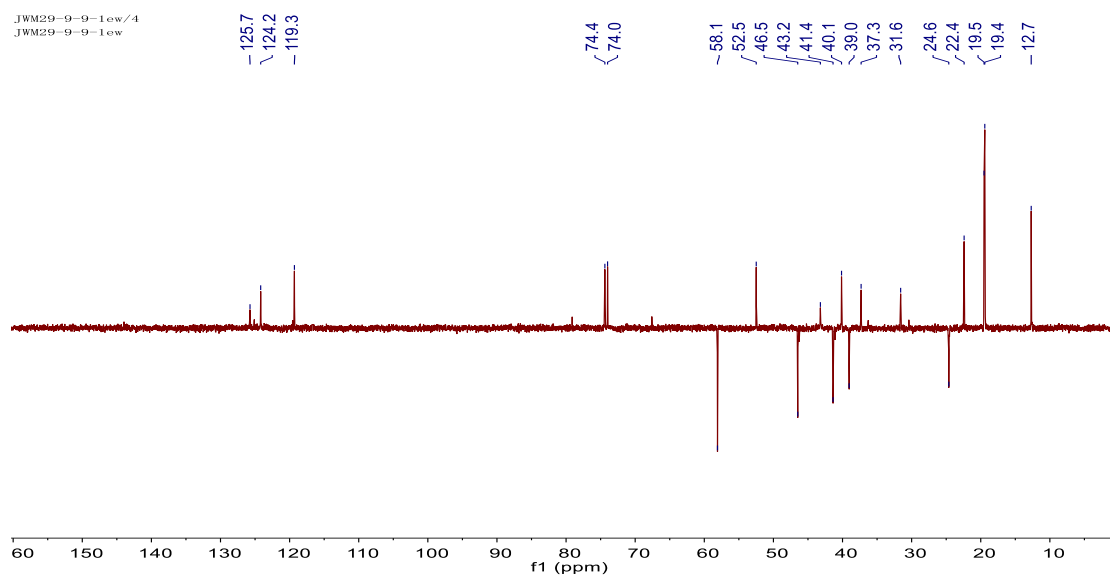


Figure S25 DEPT135 spectrum of compound **6** (in CDCl₃)

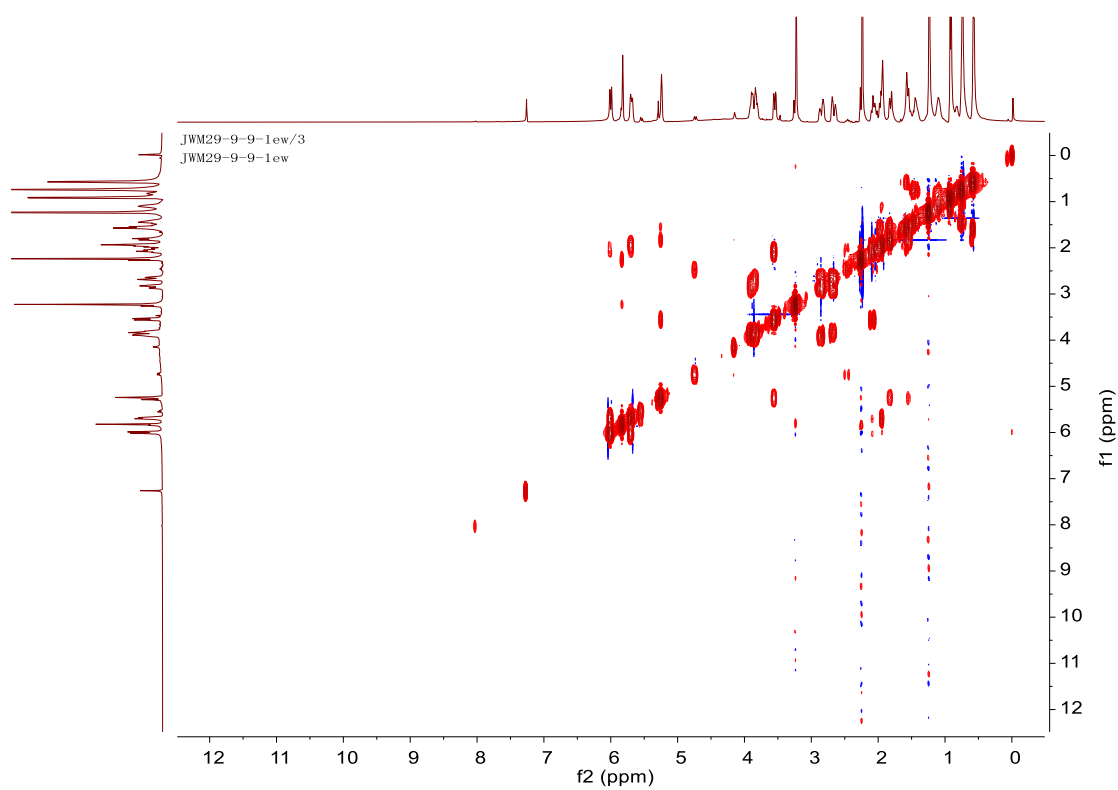


Figure S26 ¹H-¹H COSY spectrum of compound **6** (in CDCl₃)

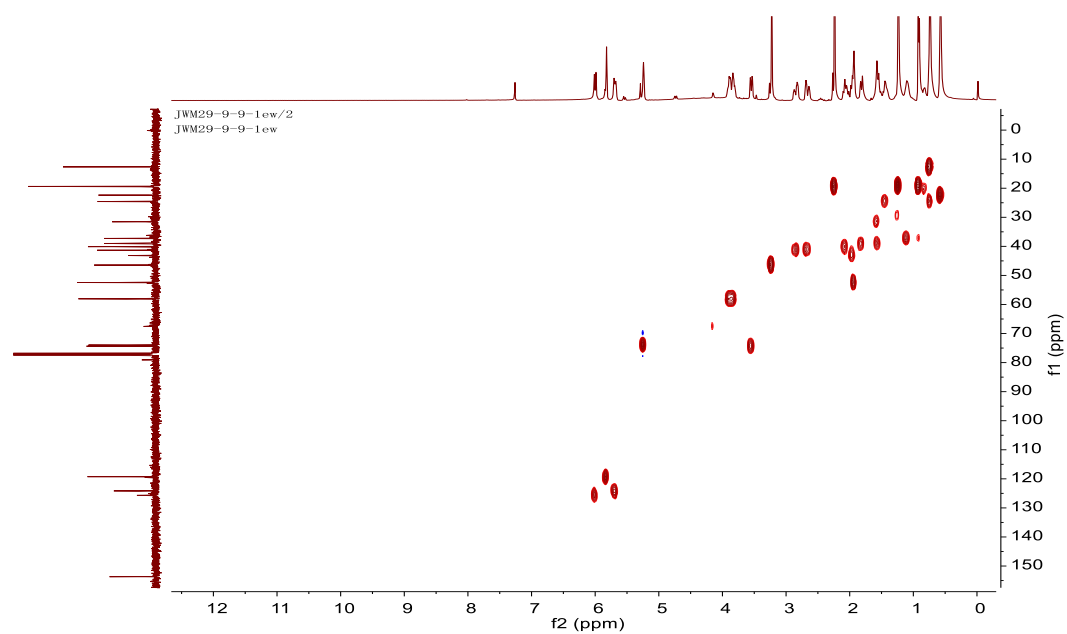


Figure S27 HSQC spectrum of compound **6** (in CDCl_3)

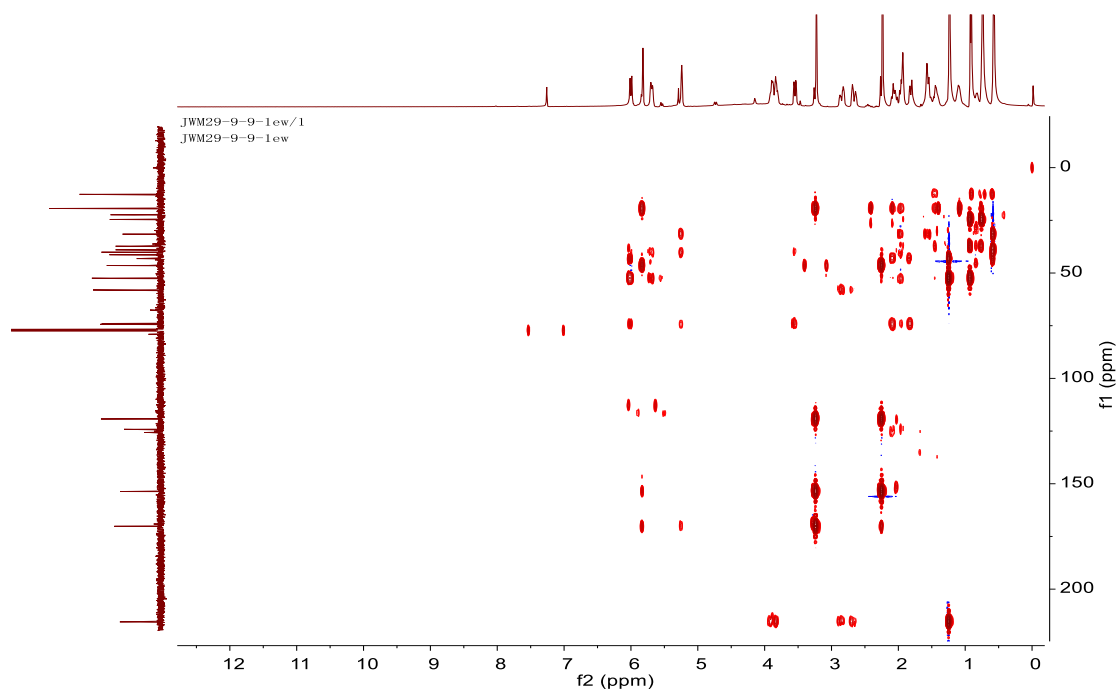


Figure S28 HMBC spectrum of compound **6** (in CDCl_3)

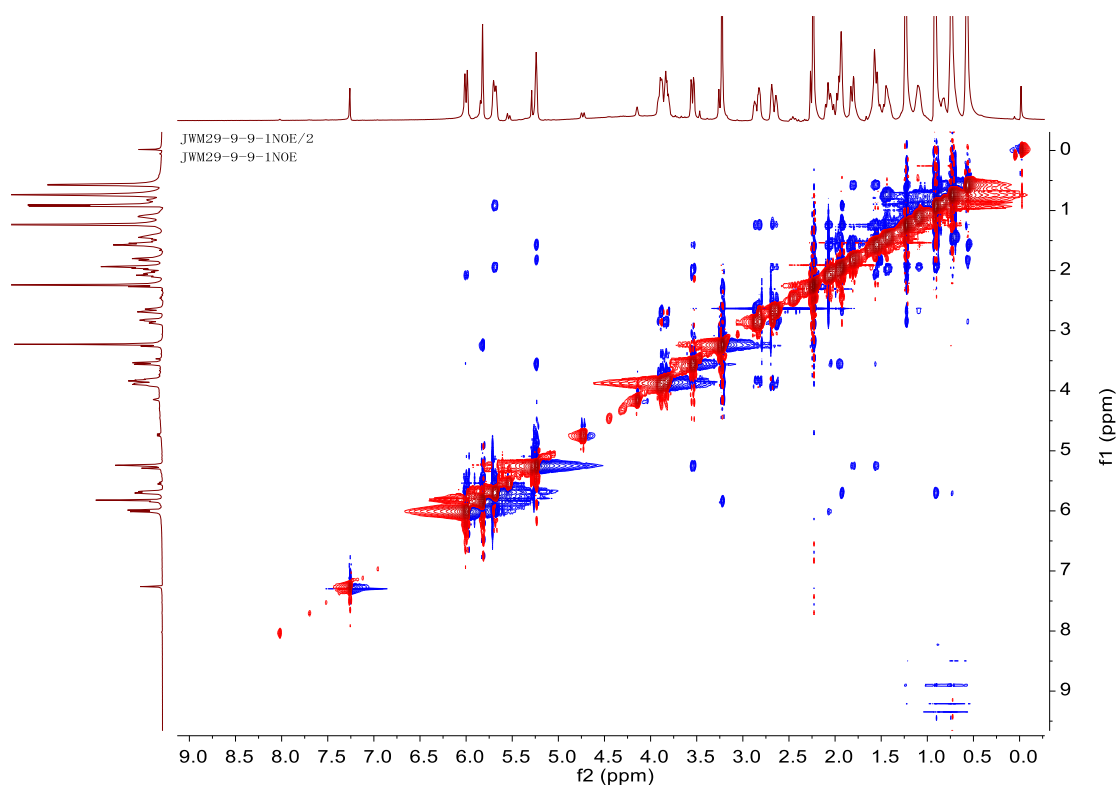


Figure S29 NOESY spectrum of compound **6** (in CDCl_3)

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

30 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

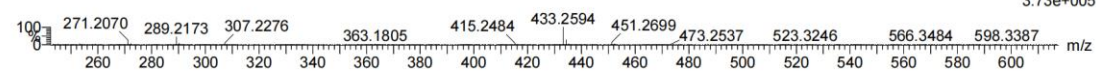
Elements Used:

C: 0-30 H: 0-50 O: 0-10

JWM29-9-9-2

20220613034 132 (1.077)

1: TOF MS ES+
3.73e+005



Minimum: -1.5
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
451.2699	451.2696	0.3	0.7	6.5	229.4	n/a	n/a	C25 H39 O7

Figure S30 HR-ESI-MS spectrum of compound **7**

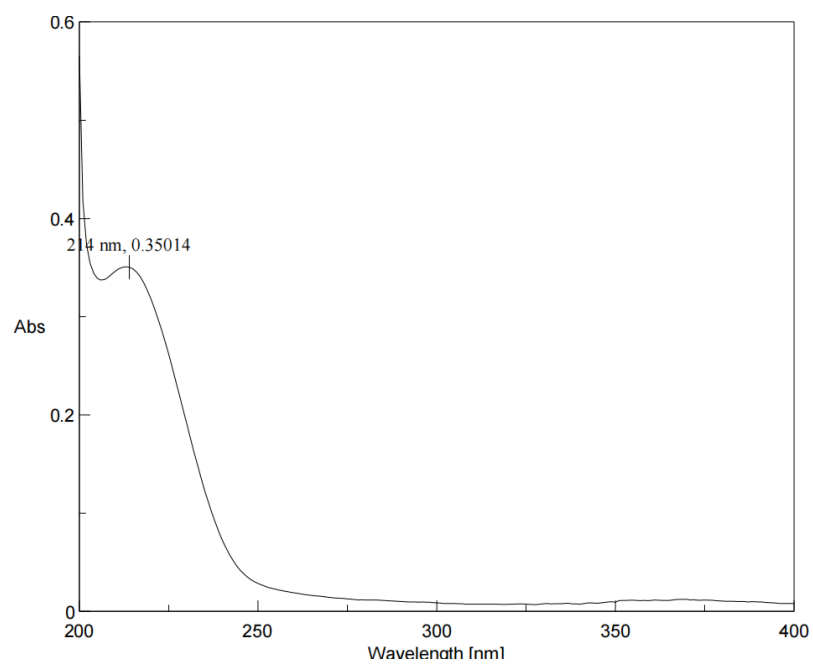


Figure S31 UV spectrum of compound **7**

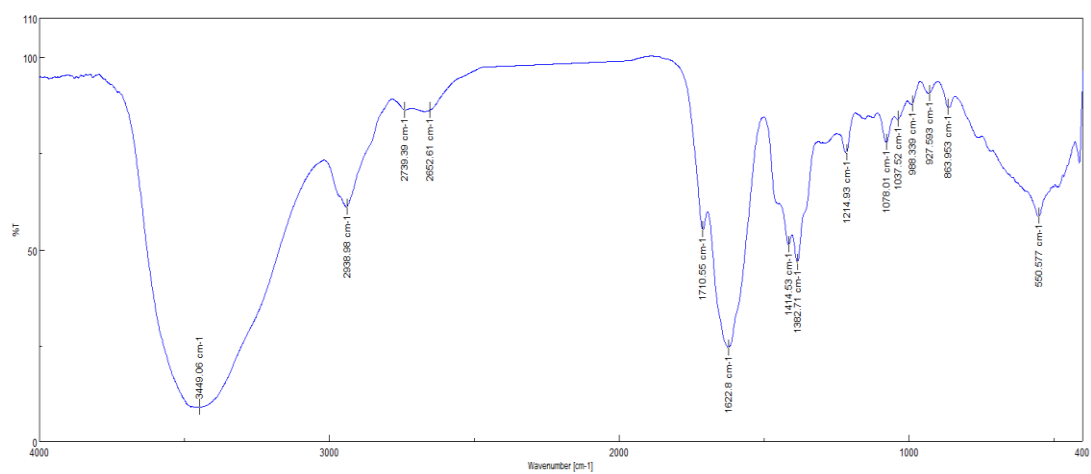


Figure S32 IR spectrum of compound **7**

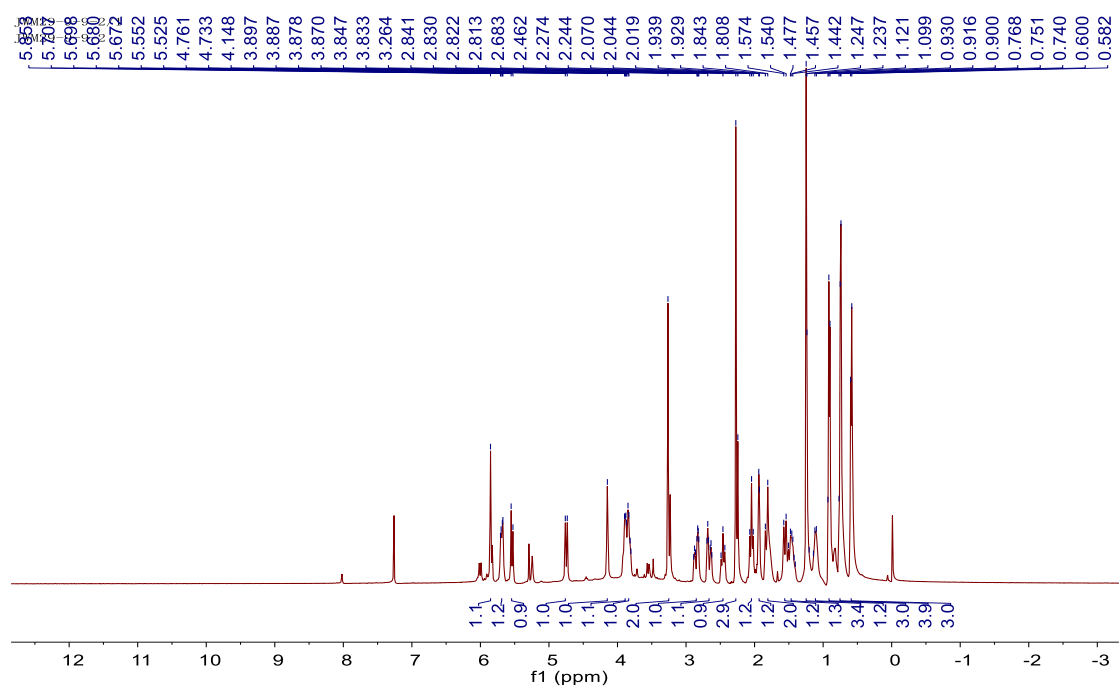


Figure S33 ^1H -NMR spectrum of compound **7** (in CDCl_3)

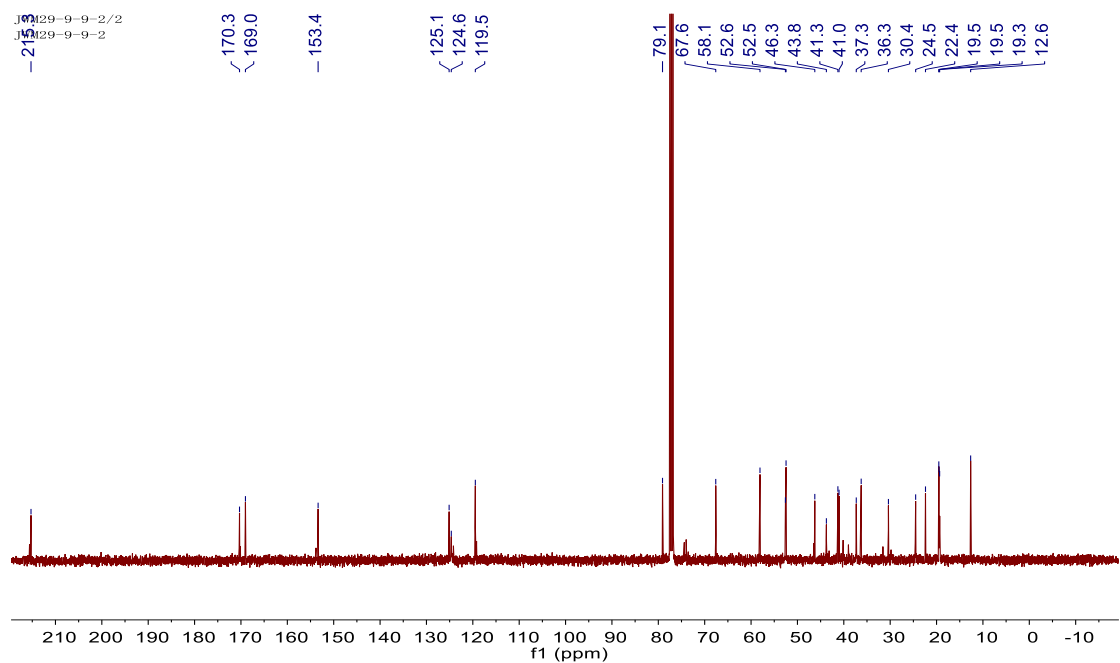


Figure S34 ^{13}C -NMR spectrum of compound **7** (in CDCl_3)

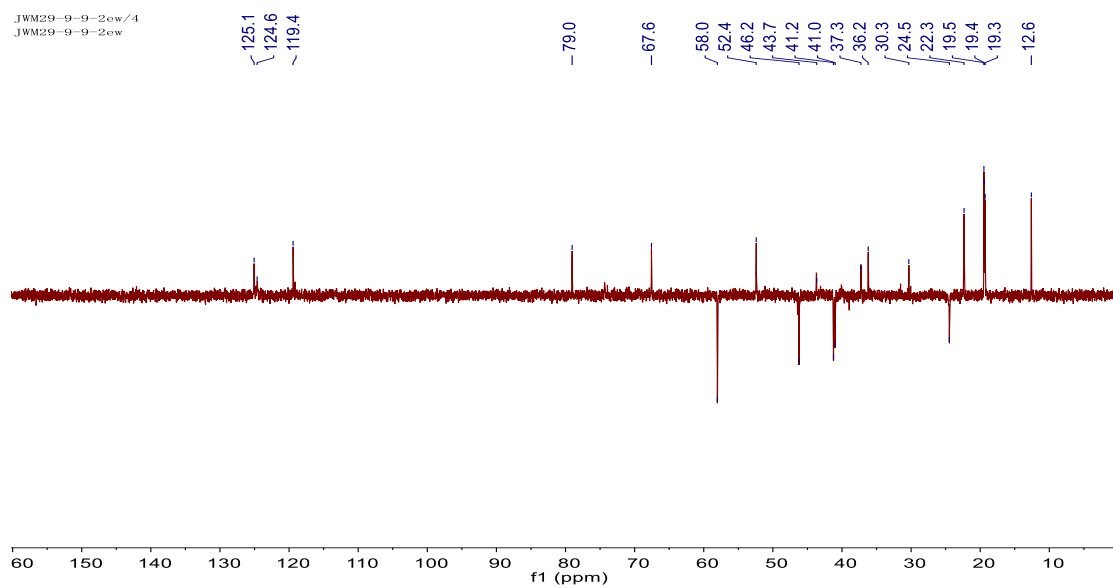


Figure S35 DEPT135 spectrum of compound **7** (in CDCl₃)

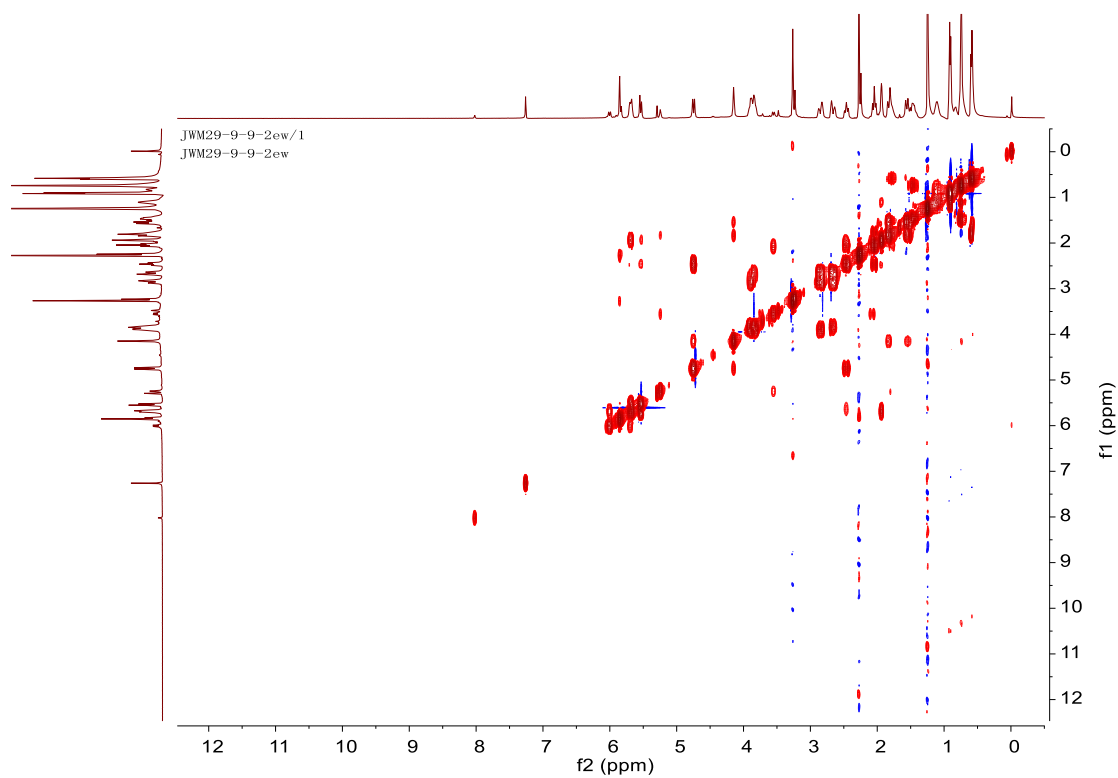


Figure S36 ¹H-¹H COSY spectrum of compound **7** (in CDCl₃)

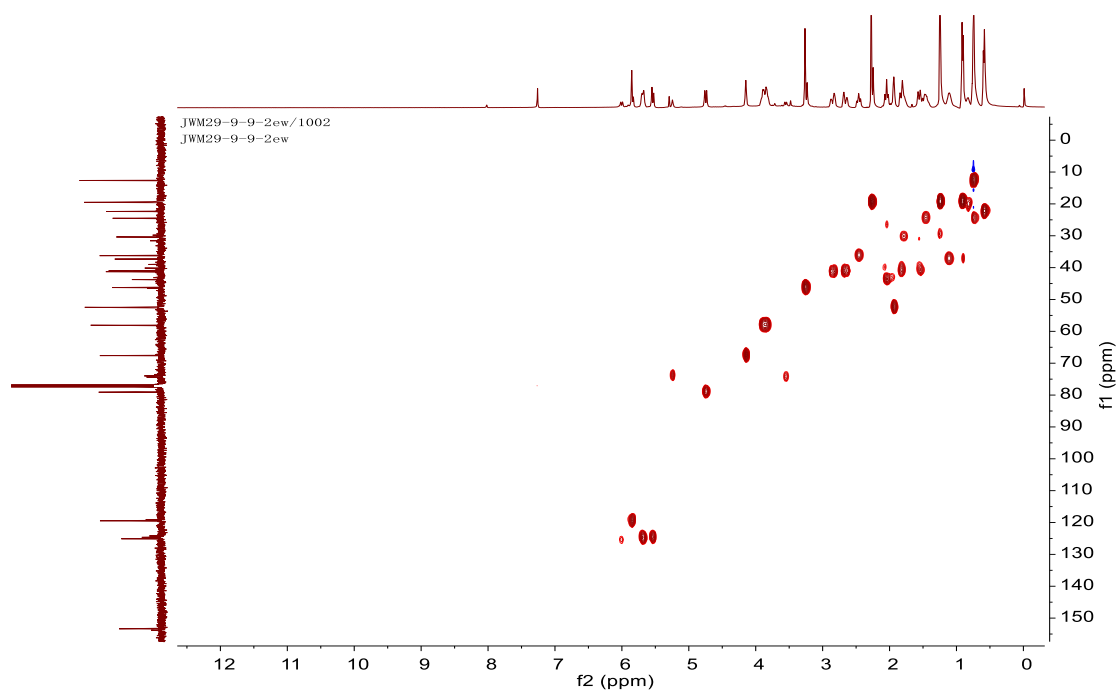


Figure S37 HSQC spectrum of compound **7** (in CDCl₃)

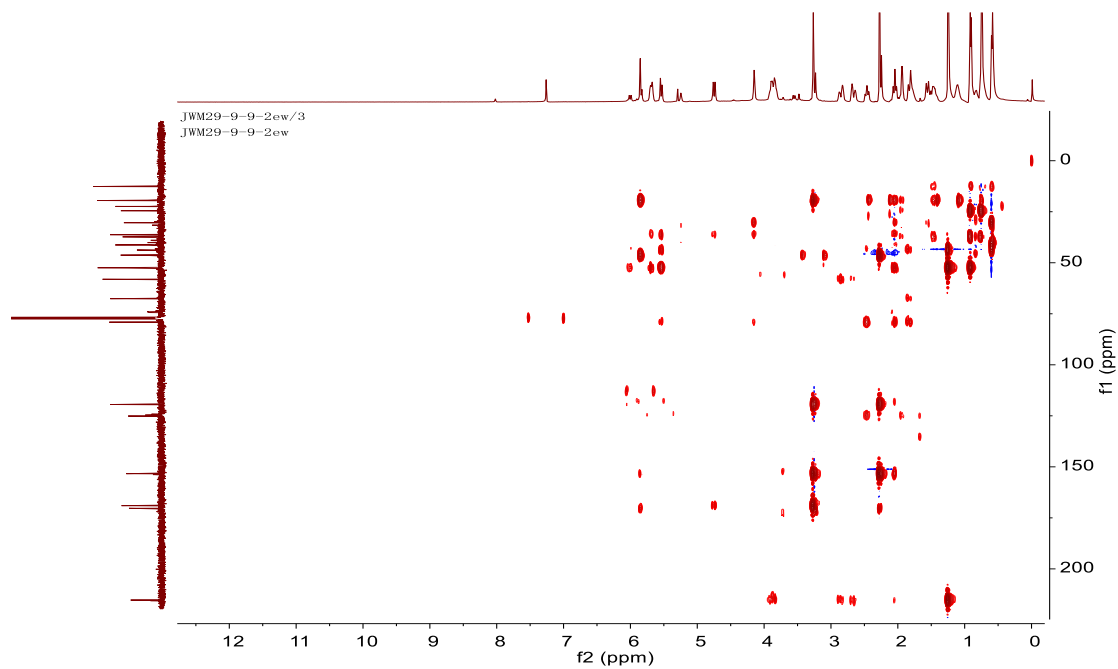


Figure S38 HMBC spectrum of compound **7** (in CDCl₃)

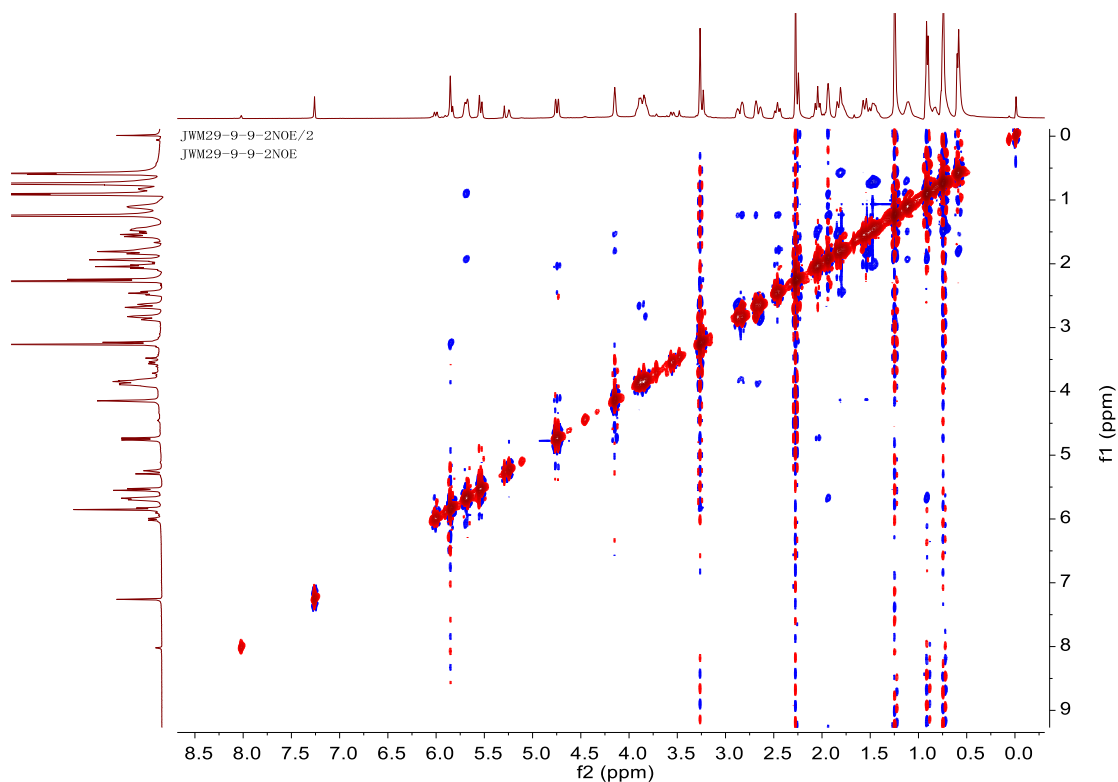


Figure S39 NOESY spectrum of compound **7** (in CDCl₃)

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

30 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

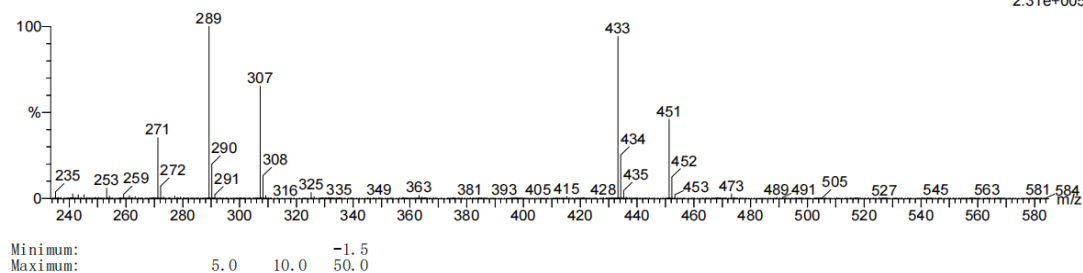
Elements Used:

C: 0-30 H: 0-50 O: 0-10

JWM29-9-9-4

20220613037 142 (1.152)

1: TOF MS ES+
2.31e+005



Minimum: -1.5
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
451.2697	451.2696	0.1	0.2	6.5	275.9	n/a	n/a	C ₂₅ H ₃₉ O ₇

Figure S40 HR-ESI-MS spectrum of compound **8**

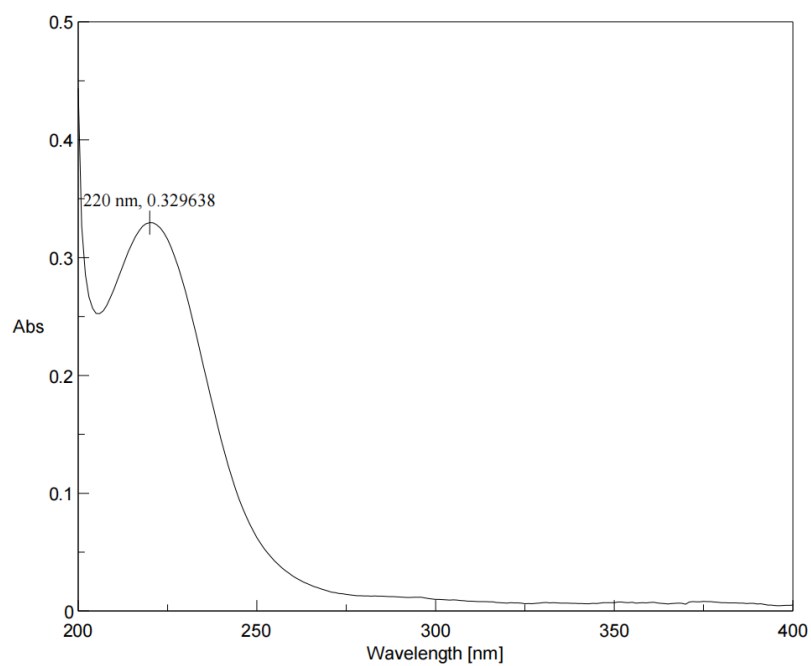


Figure S41 UV spectrum of compound **8**

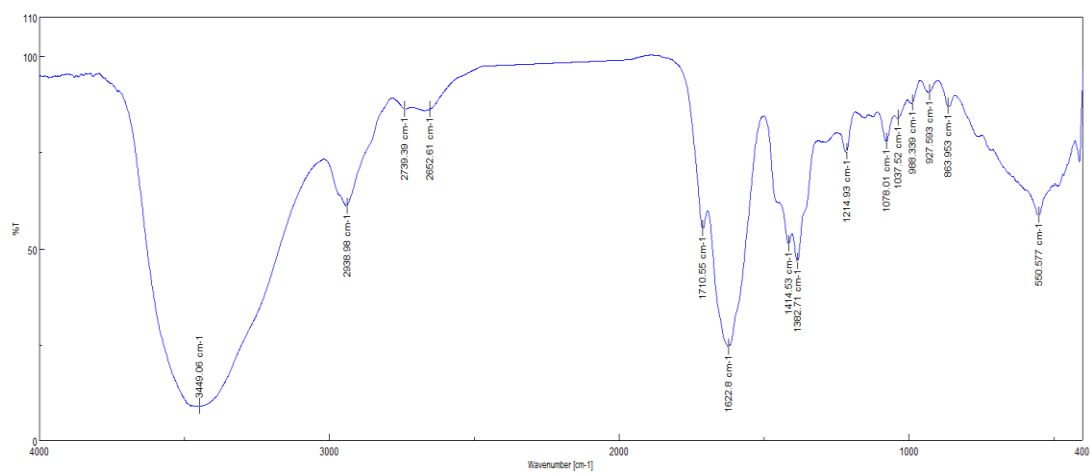


Figure S42 IR spectrum of compound **8**

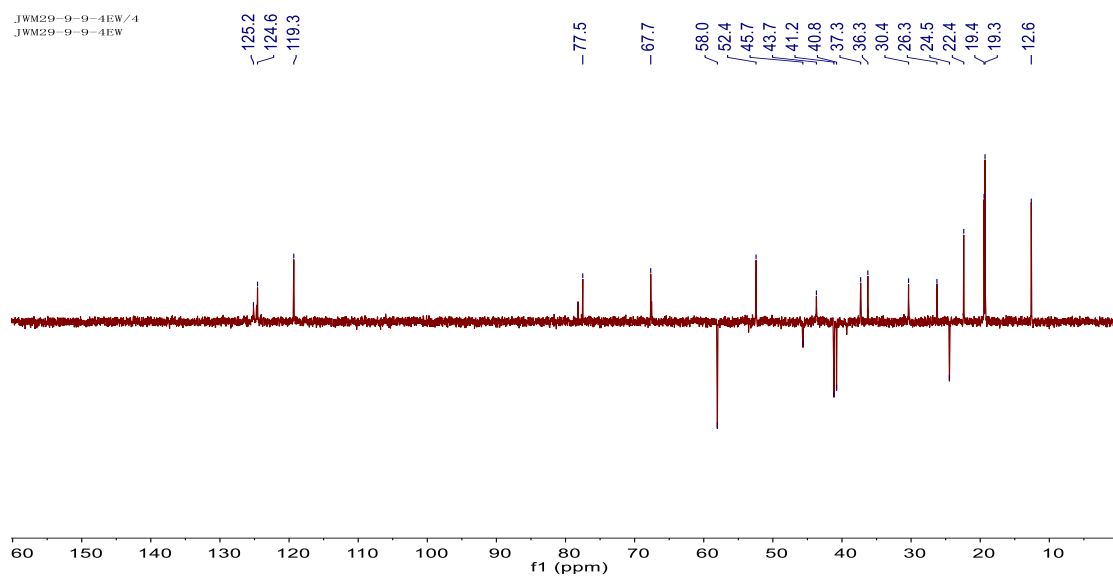


Figure S45 DEPT135 spectrum of compound **8** (in CDCl₃)

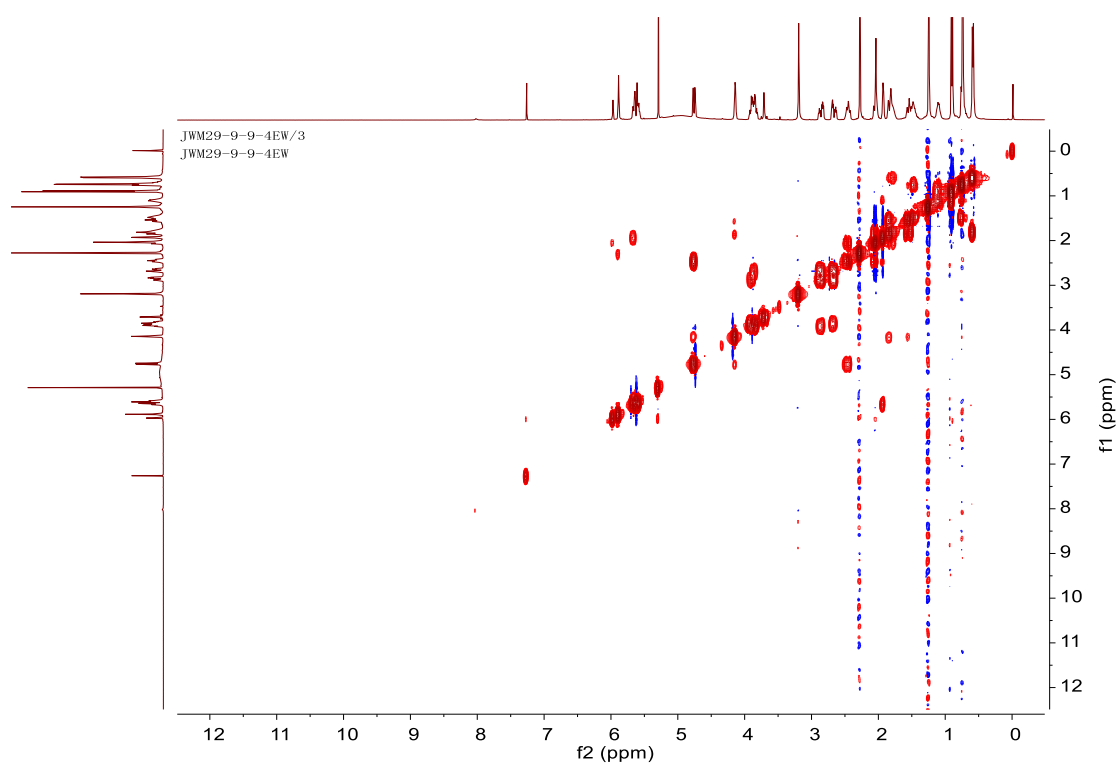


Figure S46 ¹H-¹H COSY spectrum of compound **8** (in CDCl₃)

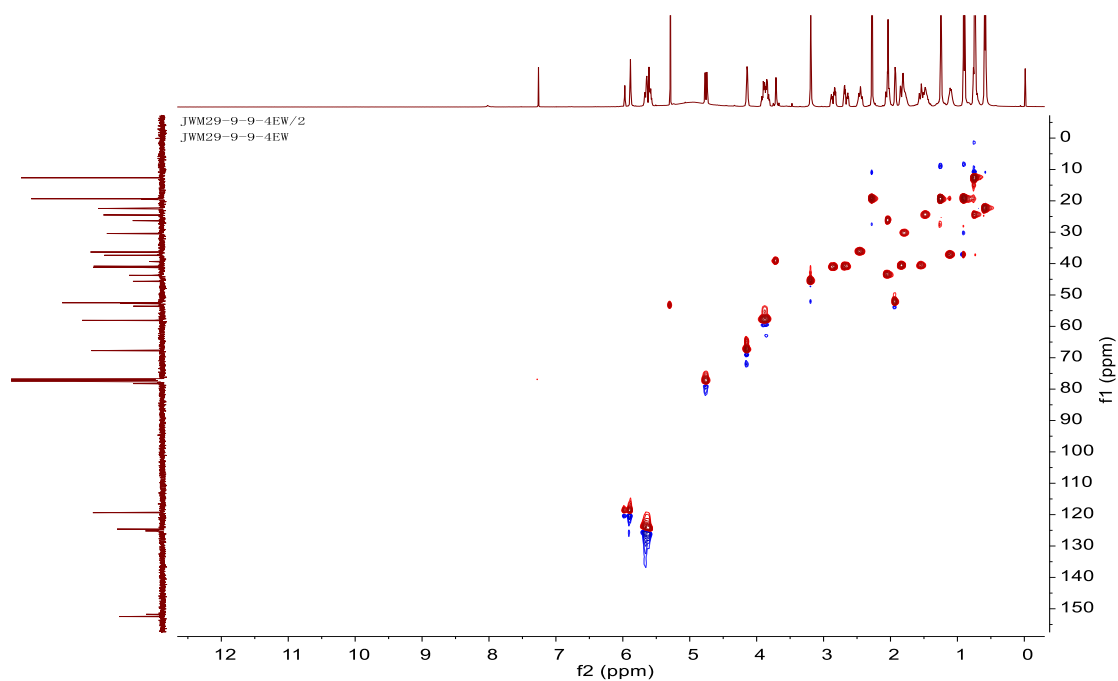


Figure S47 HSQC spectrum of compound **8** (in CDCl₃)

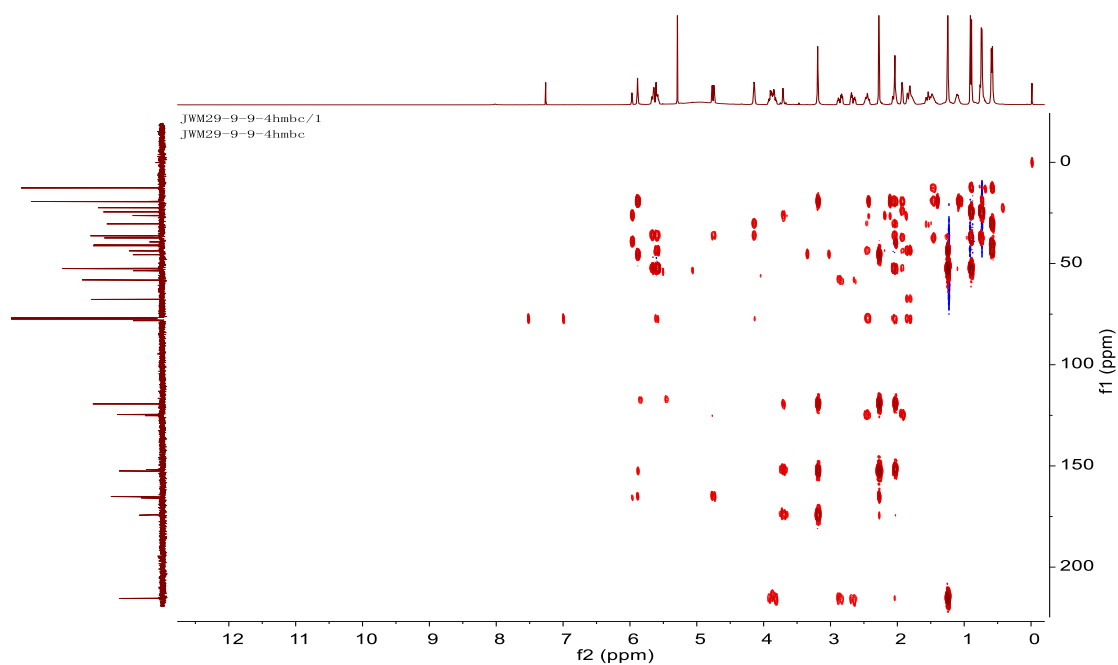


Figure S48 HMBC spectrum of compound **8** (in CDCl₃)

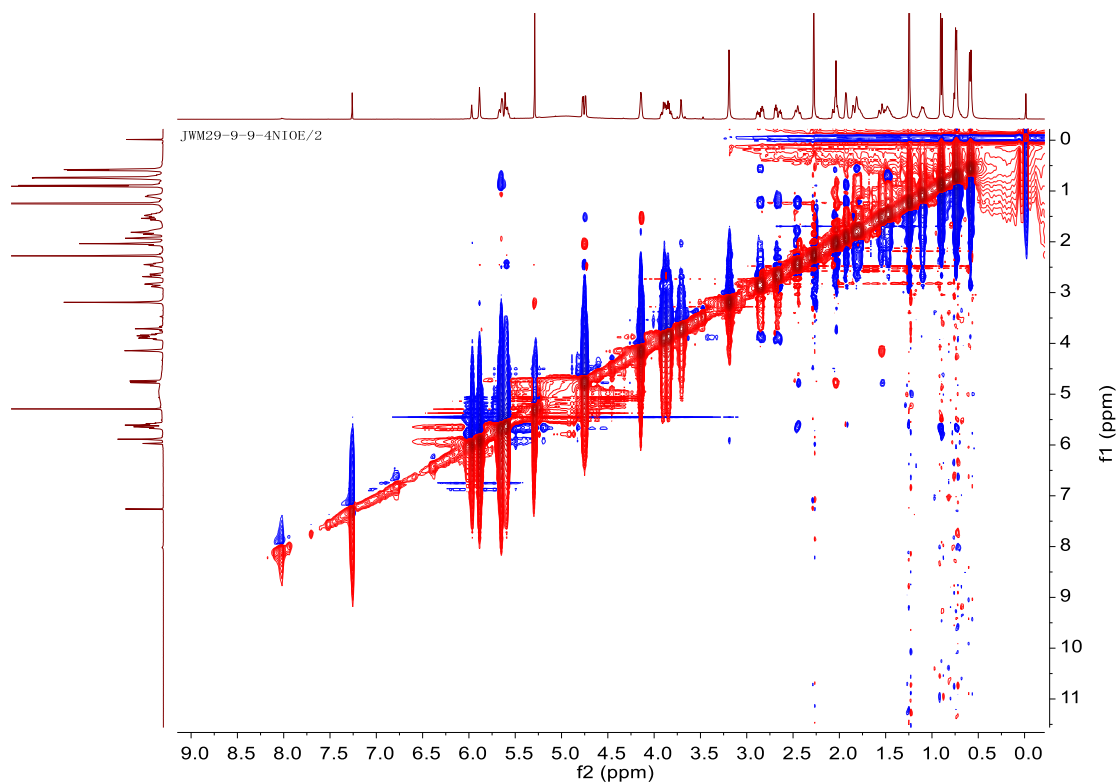


Figure S49 NOESY spectrum of compound **8** (in CDCl₃)

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

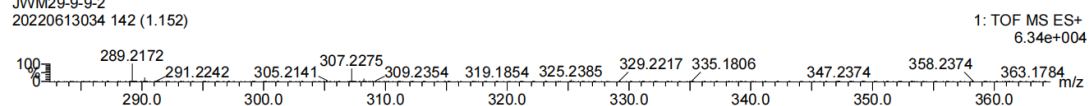
42 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-30 H: 0-50 O: 0-10

JWM29-9-9-2

20220613034 142 (1.152)



Minimum:

Maximum: 5.0 10.0 -1.5 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
325.2385	325.2379	0.6	1.8	3.5	102.5	n/a	n/a	C19 H33 O4

Figure S50 HR-ESI-MS spectrum of compound **6A**

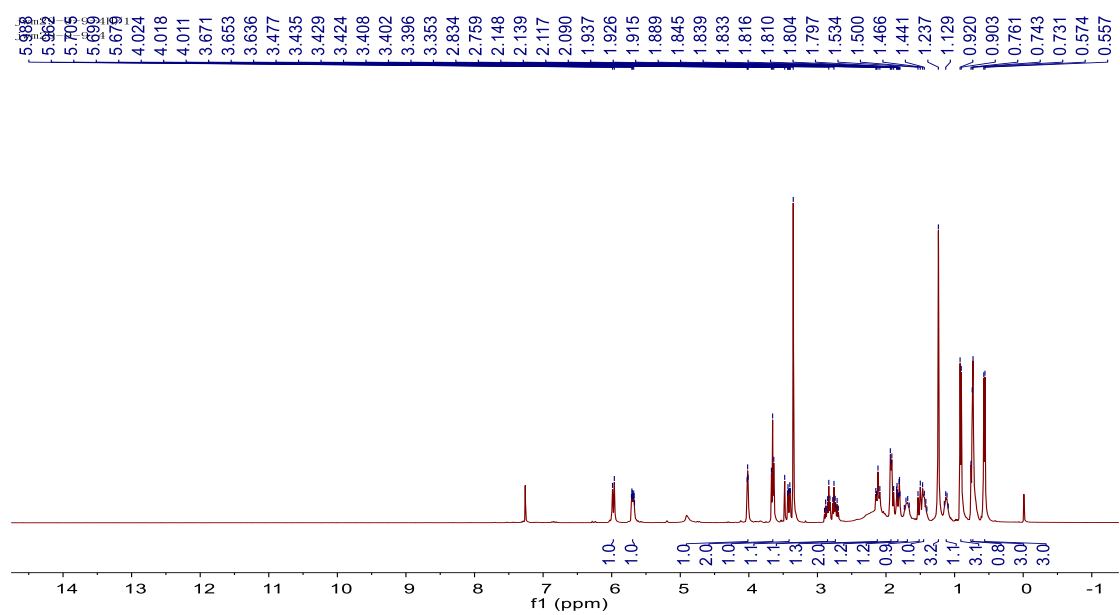


Figure S51 ¹H-NMR spectrum of compound **6A** (in CDCl₃)

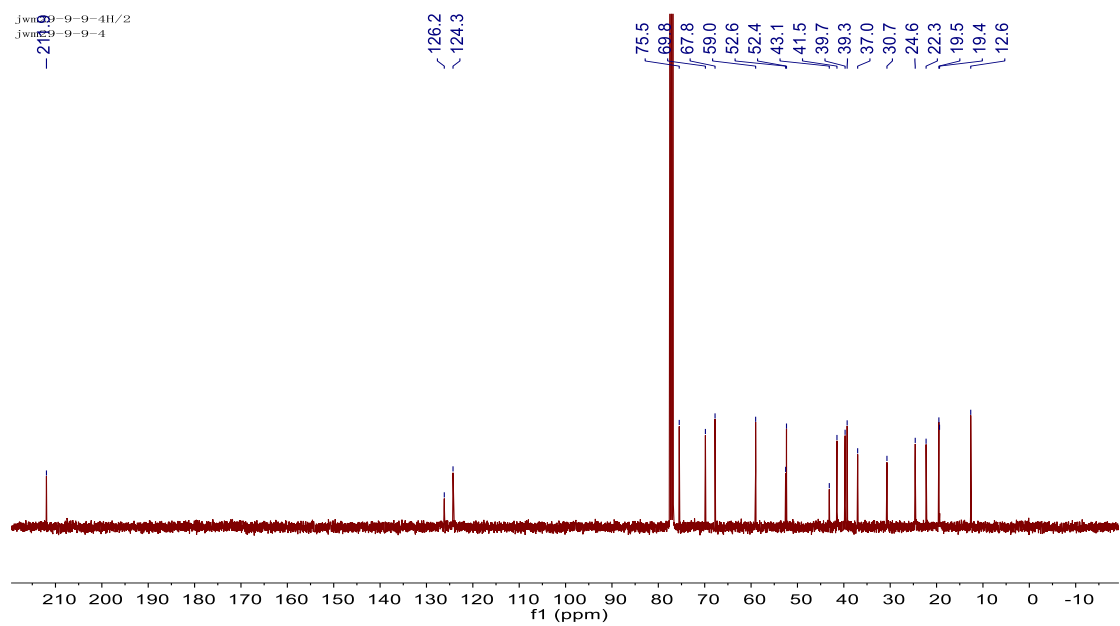


Figure S52 ¹³C-NMR spectrum of compound **6A** (in CDCl₃)