Supporting information

New Drimane Sesquiterpenes and Polyketides from Marine-Derived Fungus *Penicillium sp*. TW58-16 and their Anti-Inflammatory and α-Glucosidase Inhibitory Effects

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[†] These authors contributed equally to this work.

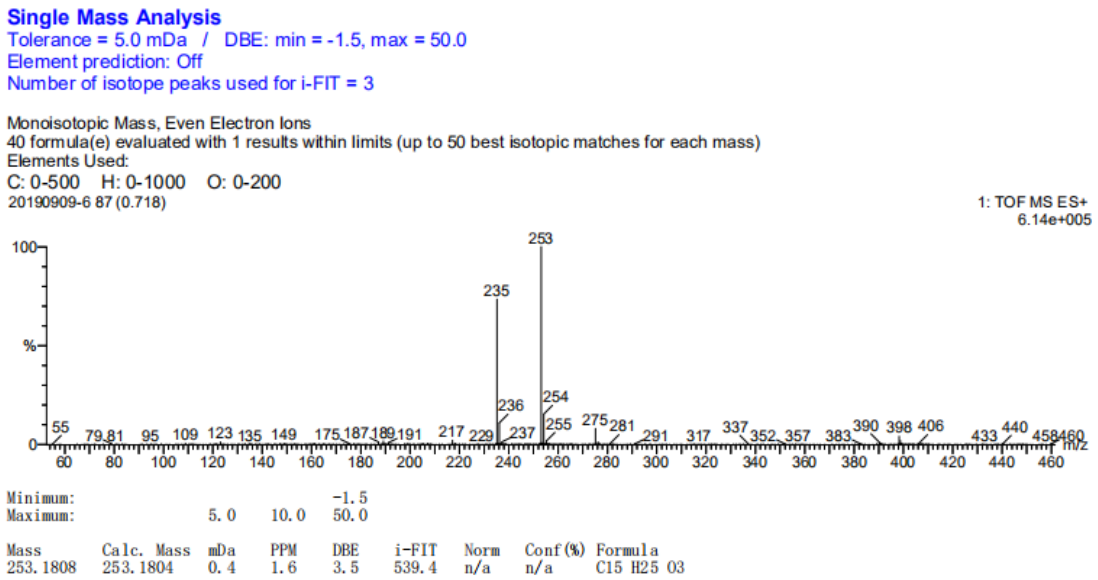


Figure S1 HR-ESI-MS spectrum of compound **1**

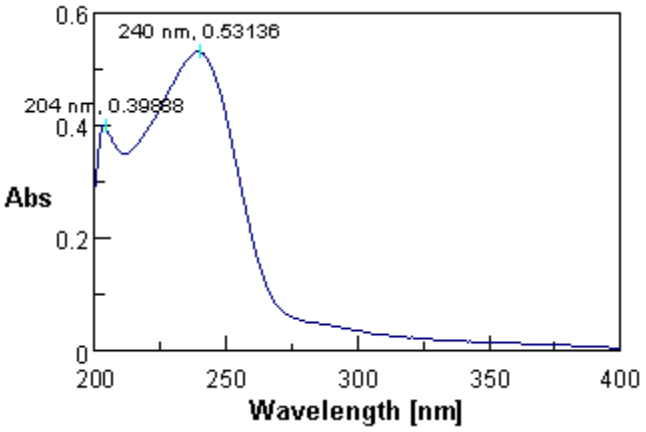


Figure S2 UV spectrum of compound **1**

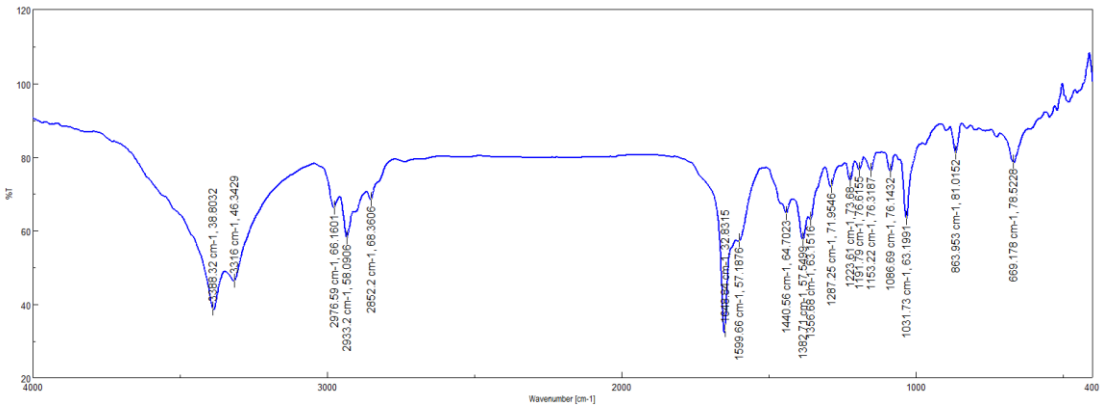


Figure S3 IR spectrum of compound **1**

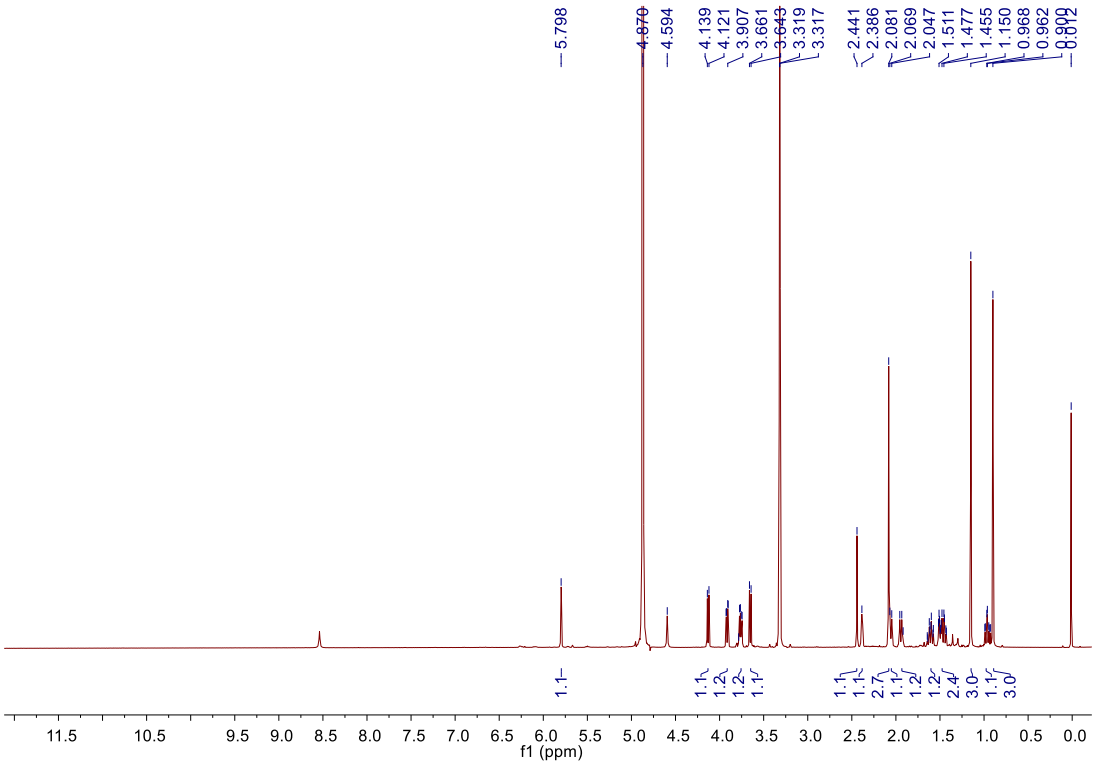


Figure S4 ^{1}H-NMR spectrum of compound **1** (in CD_3OD)

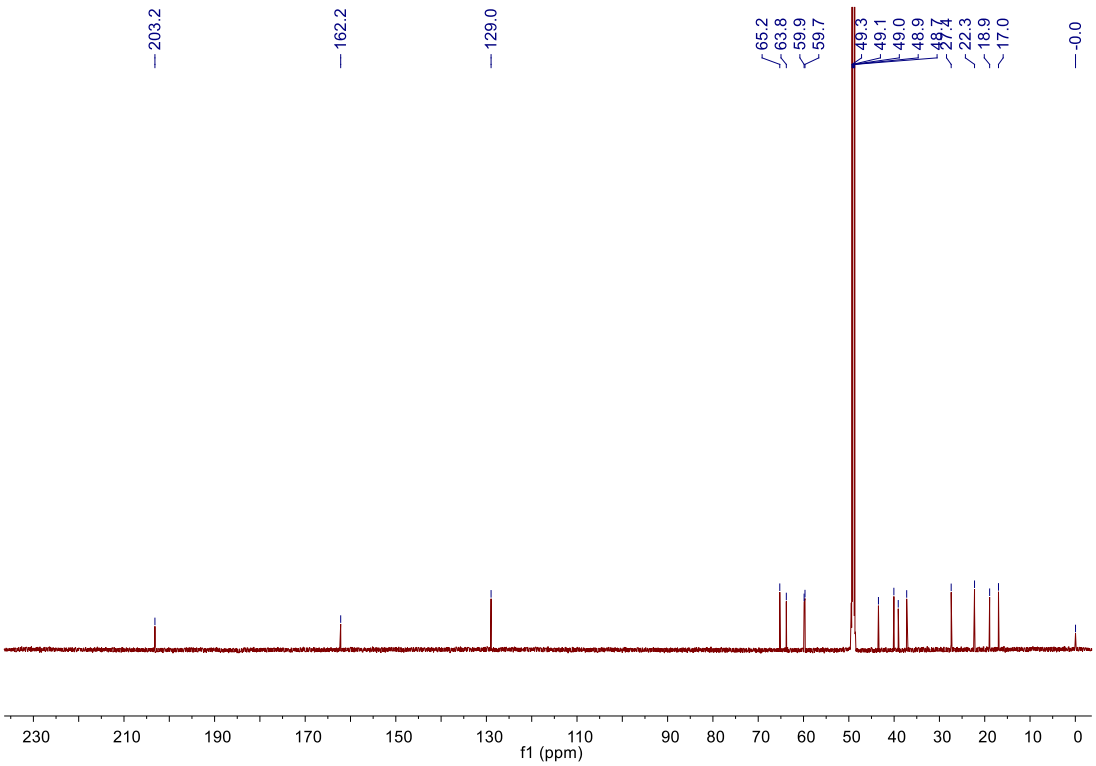


Figure S5 ^{13}C-NMR spectrum of compound **1** (in CD_3OD)

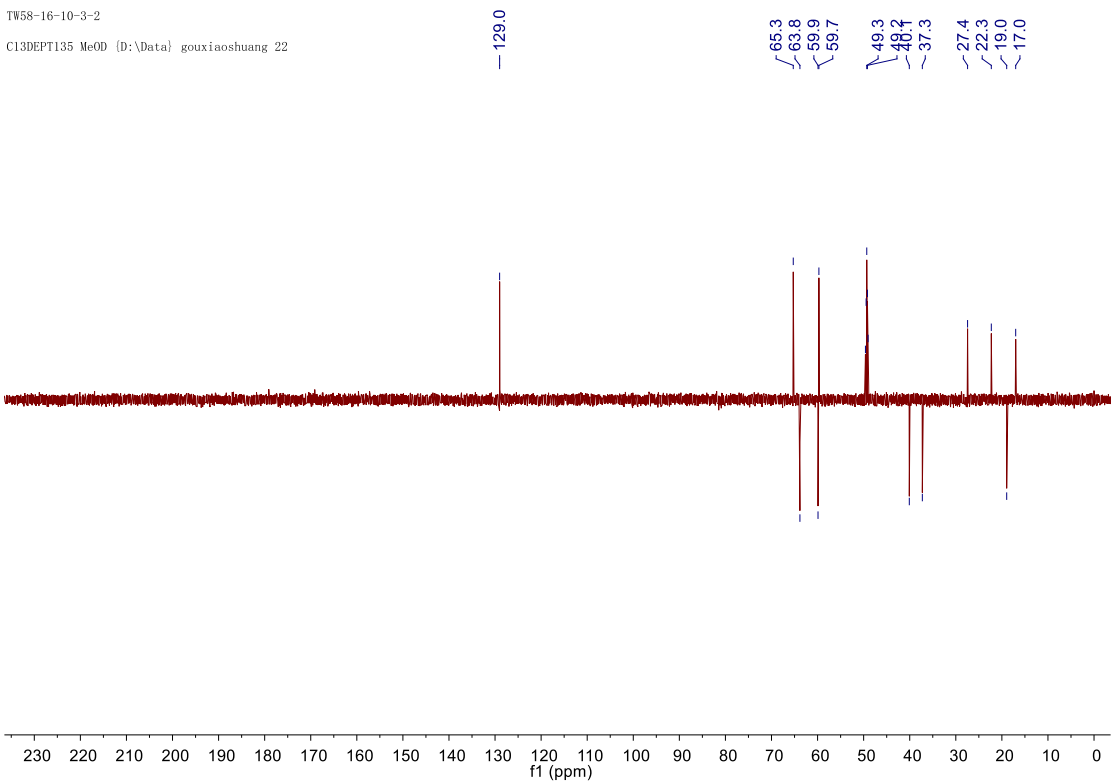


Figure S6 The DEPT135 spectrum of compound **1** (in CD_3OD)

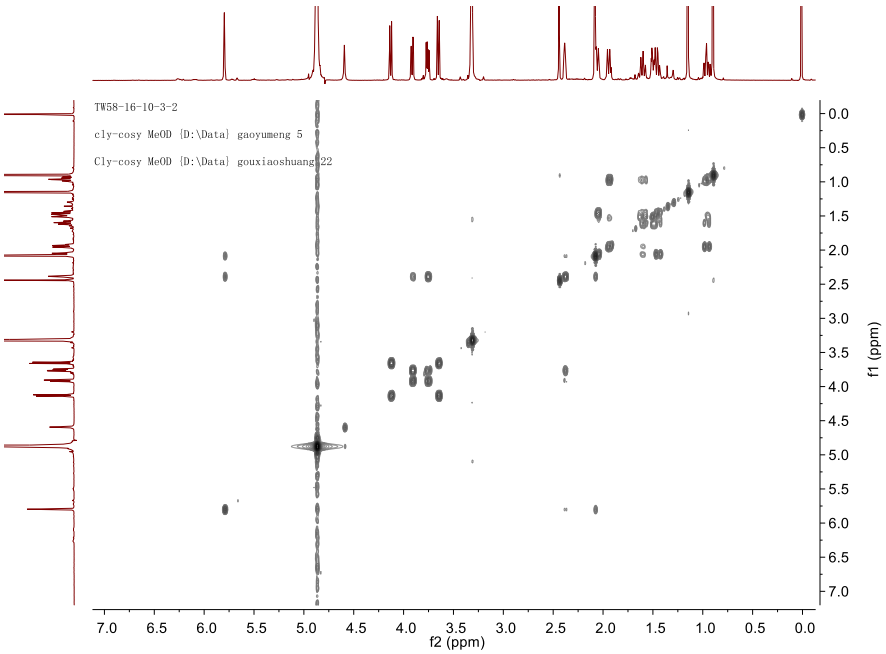


Figure S7 ^{1}H-^{1}H COSY spectrum of compound **1** (in CD_3OD)

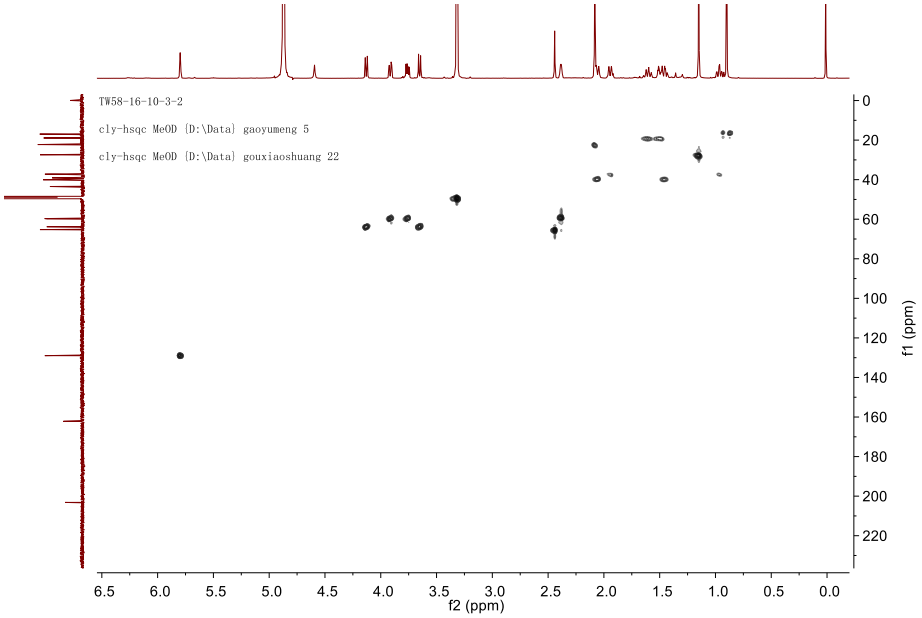


Figure S8 HSQC spectrum of compound **1** (in CD_3OD)

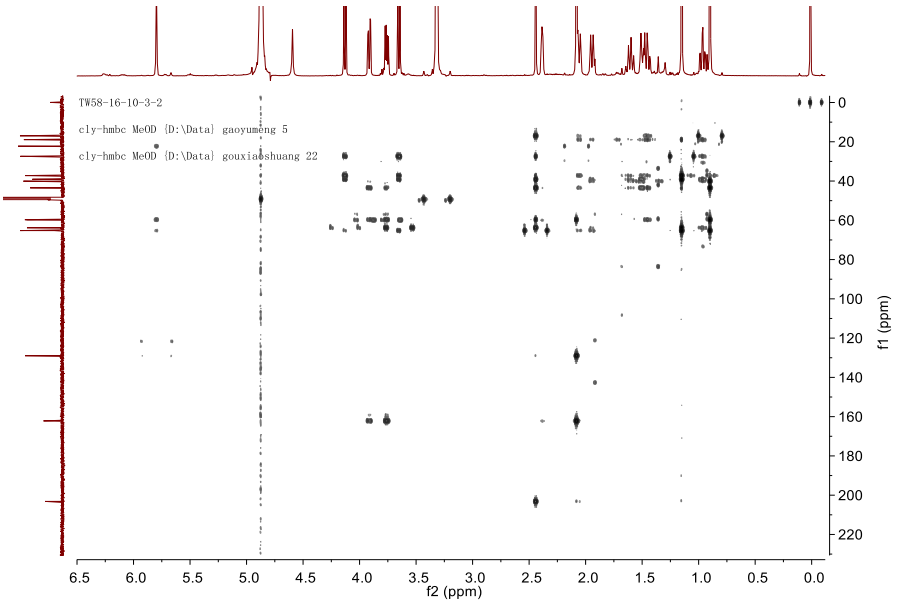


Figure S9 HMBC spectrum of compound **1** (in CD_3OD)

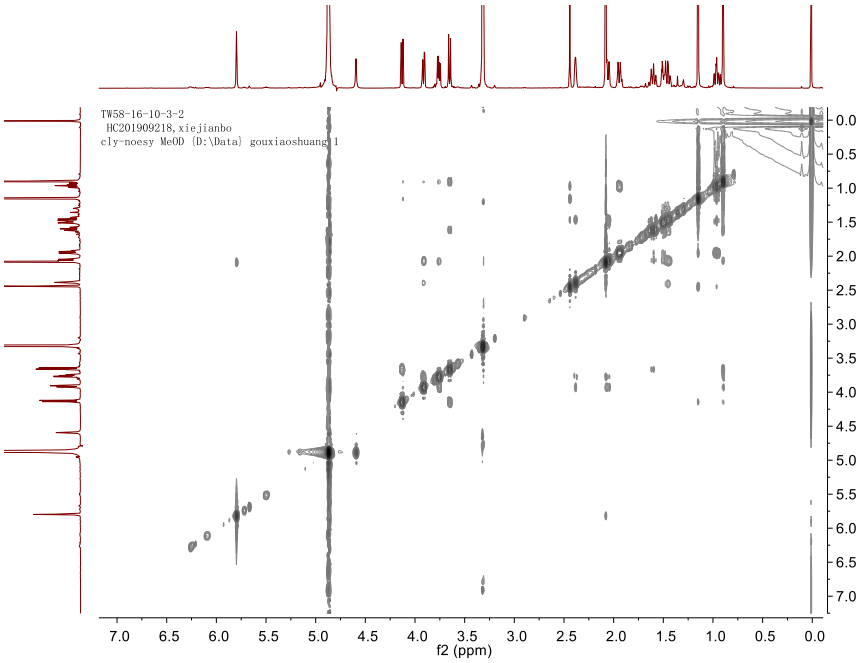


Figure S10 The NOESY spectrum of compound **1** (in CD_3OD)

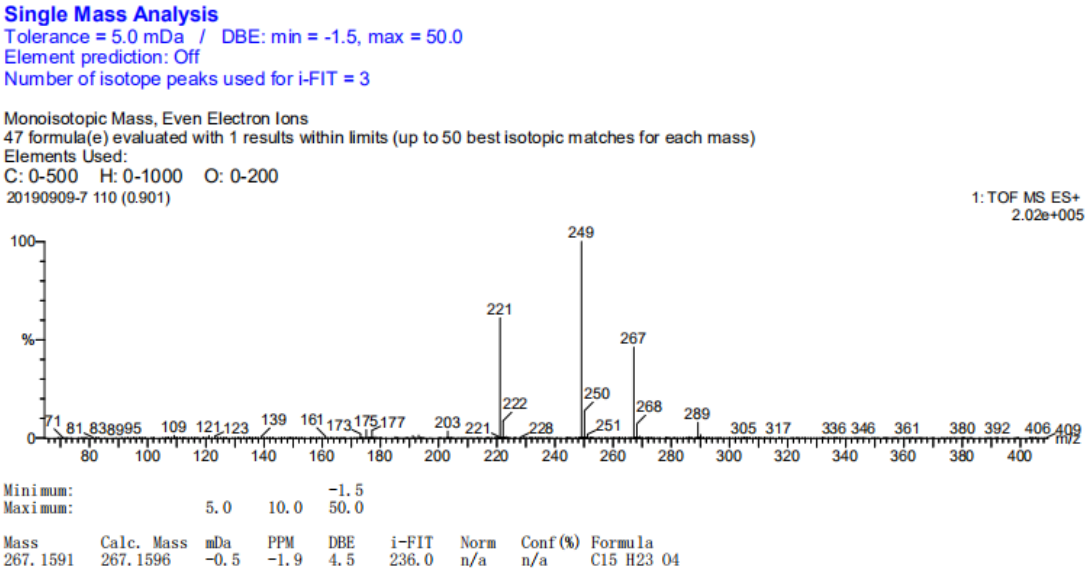


Figure S11 HR-ESI-MS spectrum of compound **2**

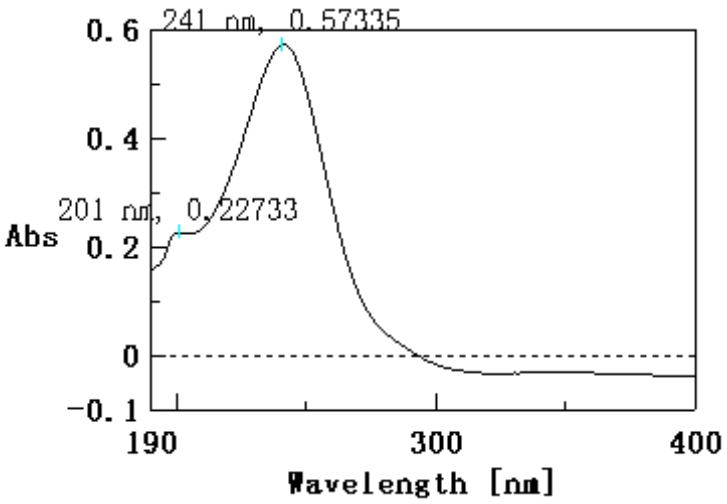


Figure S12 UV spectrum of compound **2**

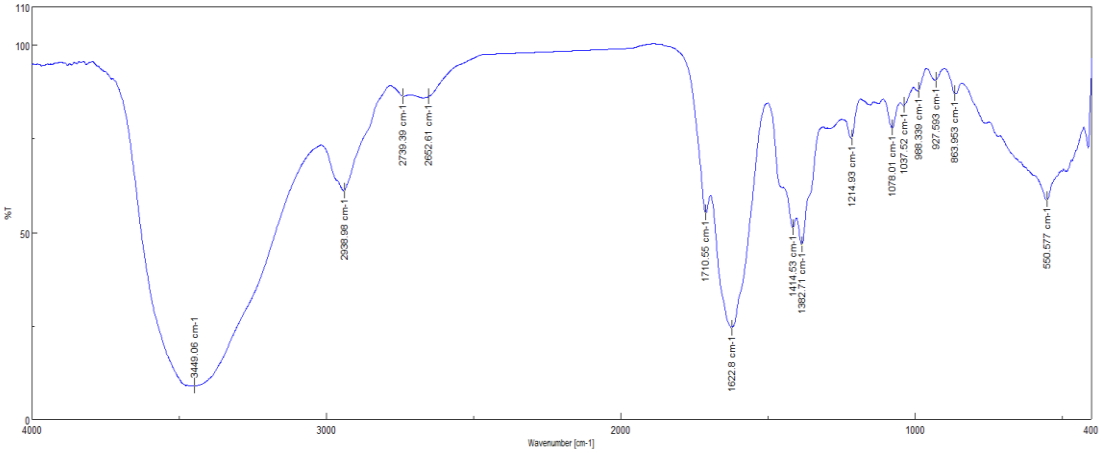


Figure S13 IR spectrum of compound **2**

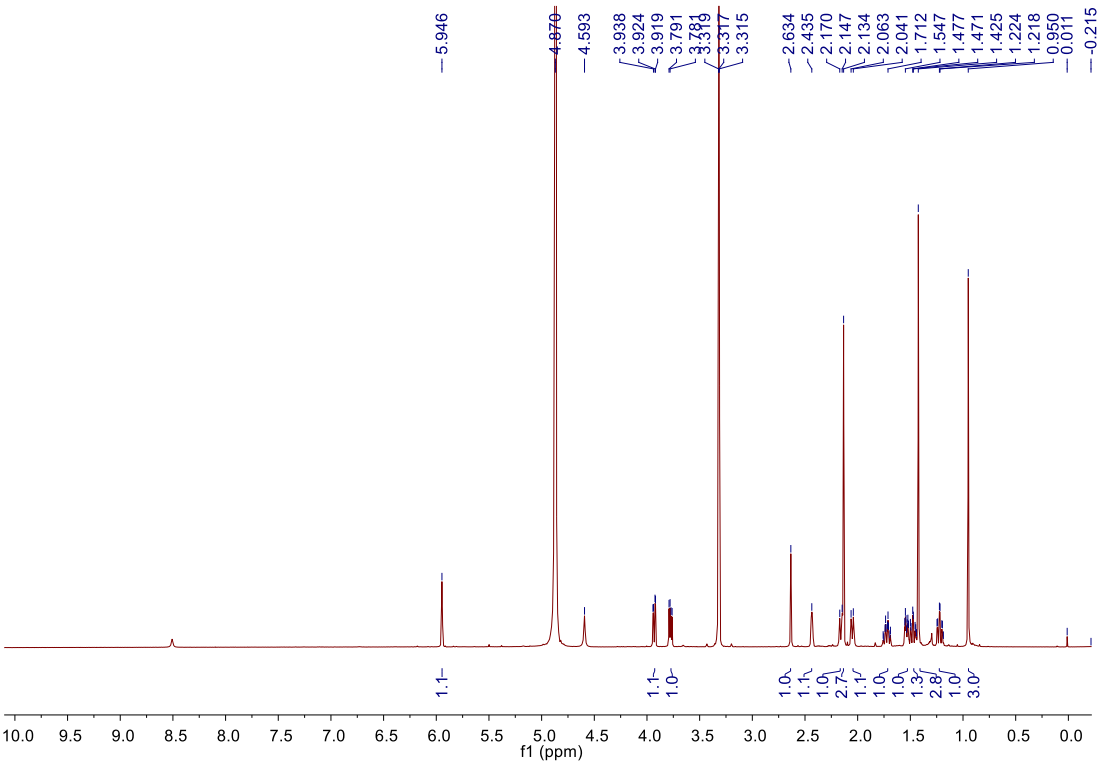


Figure S14 ^{1}H-NMR spectrum of compound **2** (in CD_3OD)

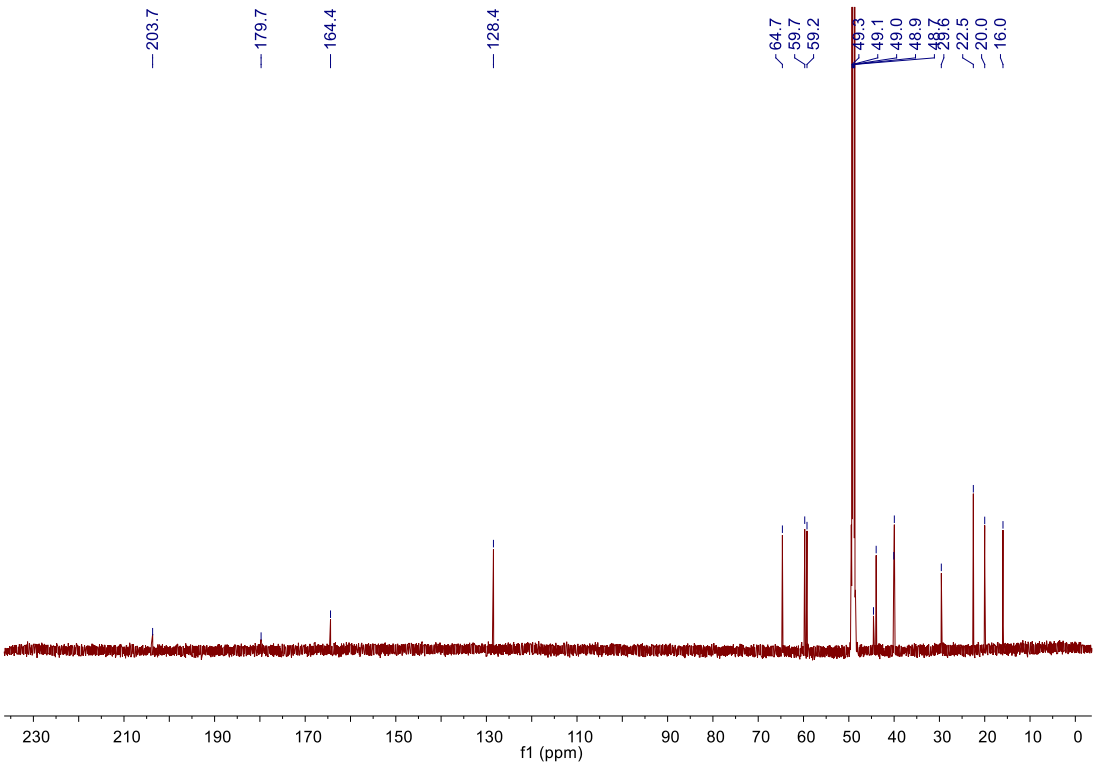


Figure S15 ^{13}C-NMR spectrum of compound **2** (in CD_3OD)

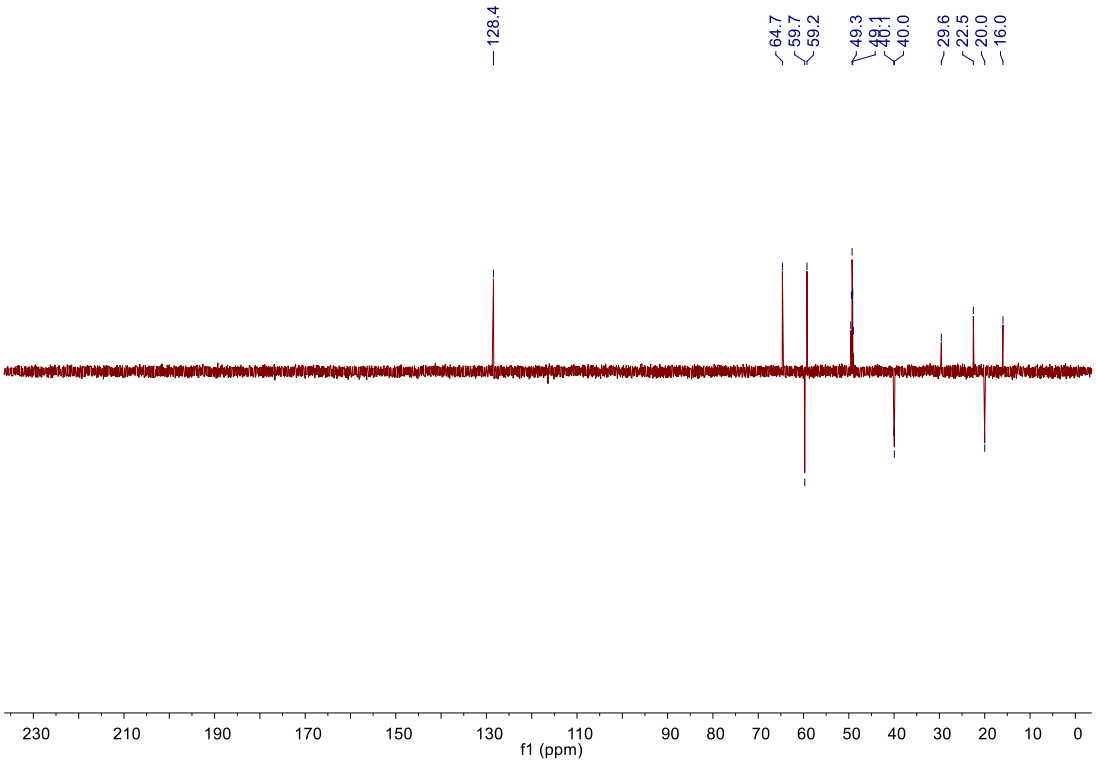


Figure S16 The DEPT135 spectrum of compound **2** (in CD_3OD)

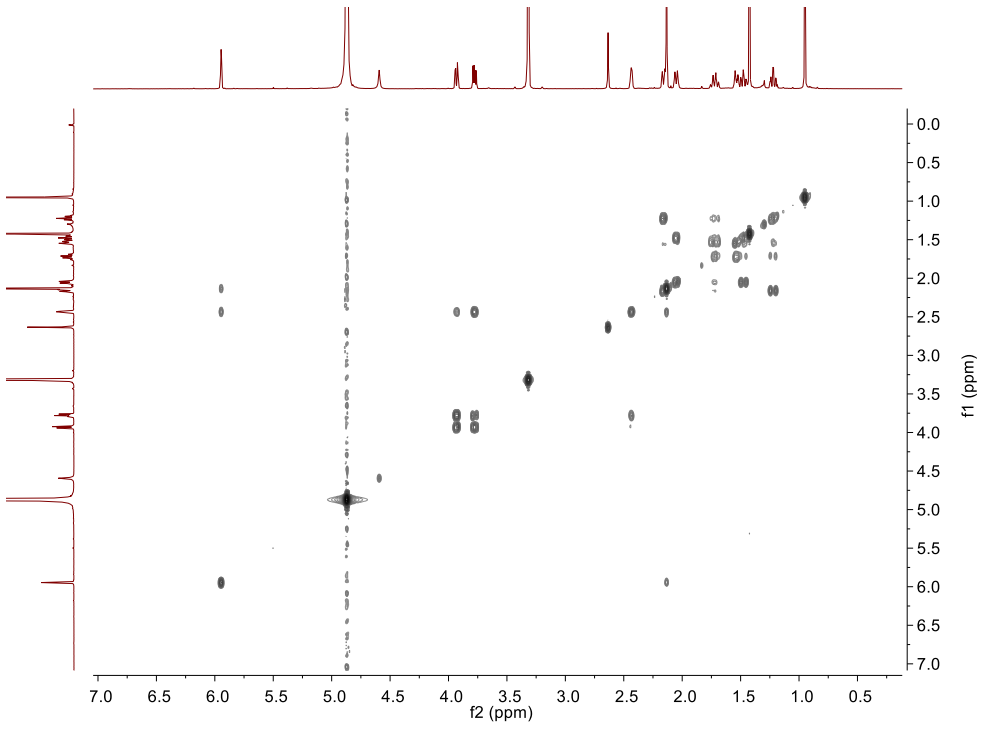


Figure S17 ^1H-^1H COSY spectrum of compound **2** (in CD_3OD)

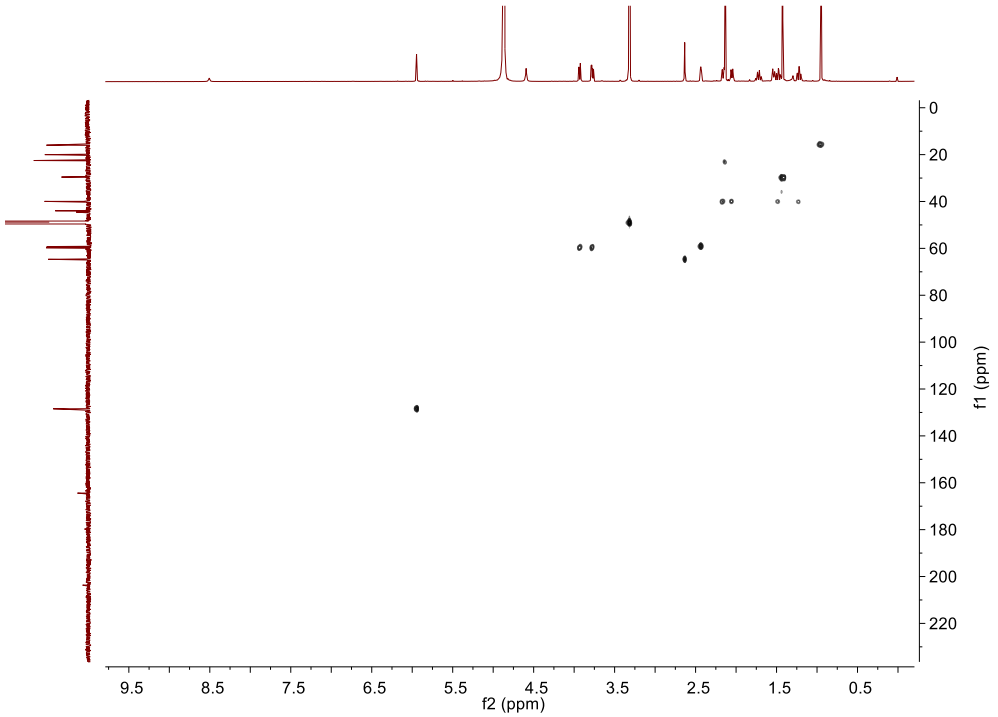


Figure S18 HSQC spectrum of compound **2** (in CD_3OD)

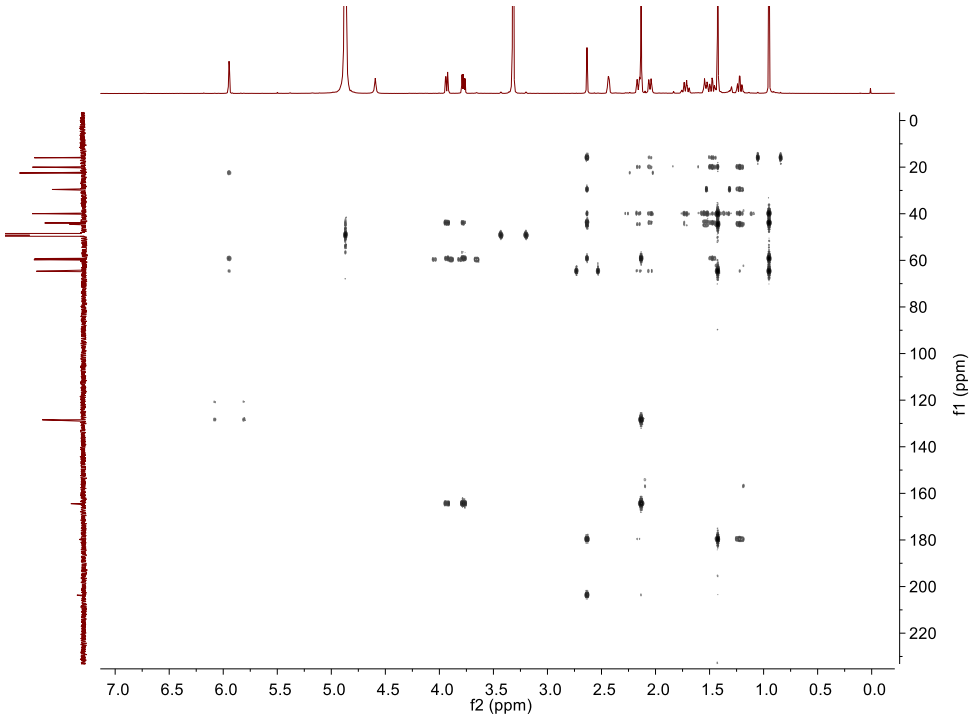


Figure S19 HMBC spectrum of compound **2** (in CD_3OD)

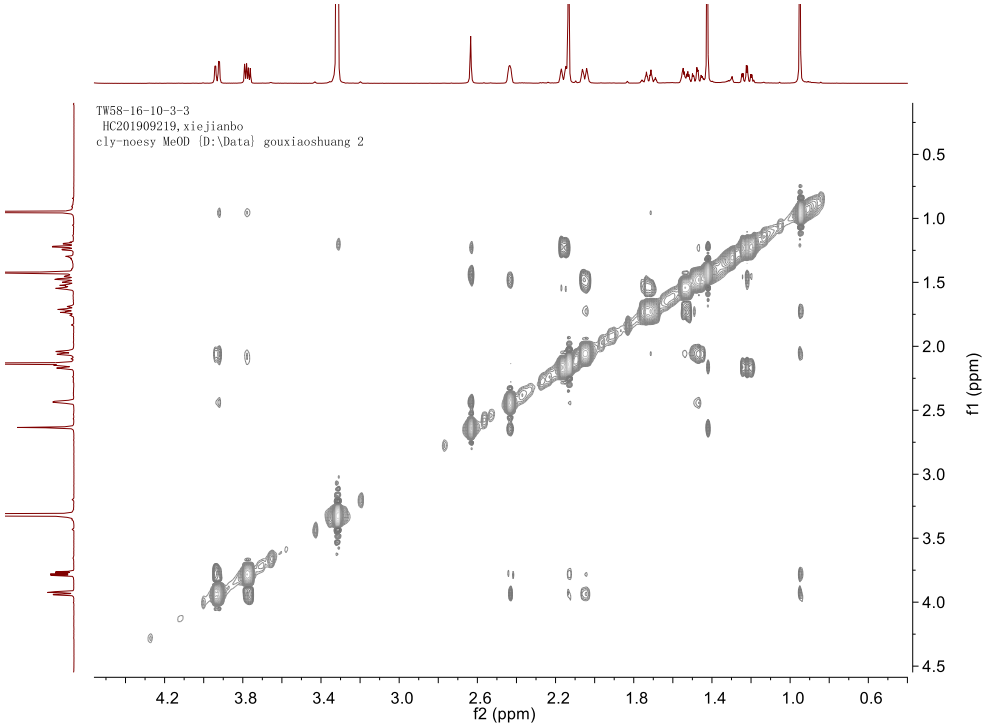
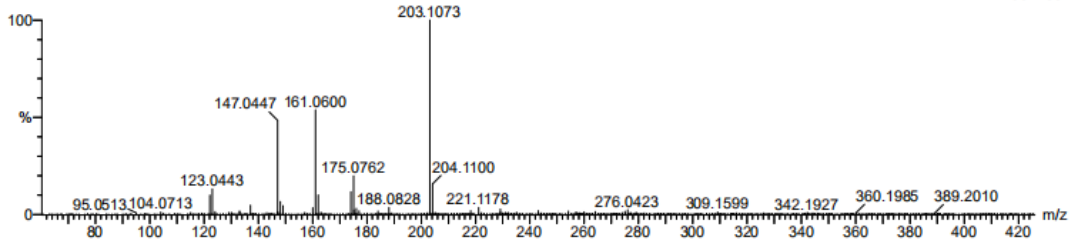


Figure S20 The NOESY spectrum of compound **2** (in CD_3OD)

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
287 formula(e) evaluated with 4 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200
20190909-9 99 (0.808)

1: TOF MS ES+
2.90e+004



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
221.1178	221.1178	0.0	0.0	5.5	78.2	0.345	70.81	C13 H17 O3
	221.1151	2.7	12.2	6.5	79.6	1.784	16.79	C9 H13 N6 O
	221.1137	4.1	18.5	1.5	80.2	2.329	9.74	C8 H17 N2 O5
	221.1223	-4.5	-20.4	2.5	81.5	3.627	2.66	C3 H13 N10 O2

Figure S21 HR-ESI-MS spectrum of compound **3**

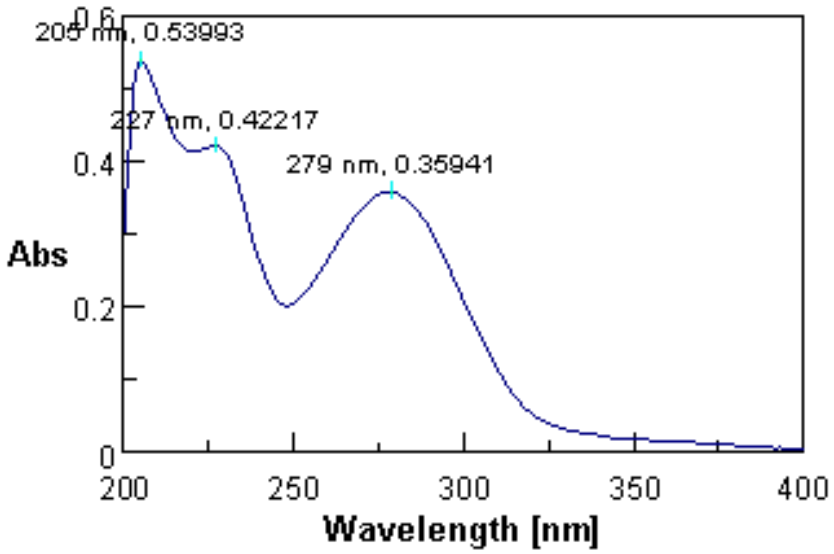


Figure S22 UV spectrum of compound **3**

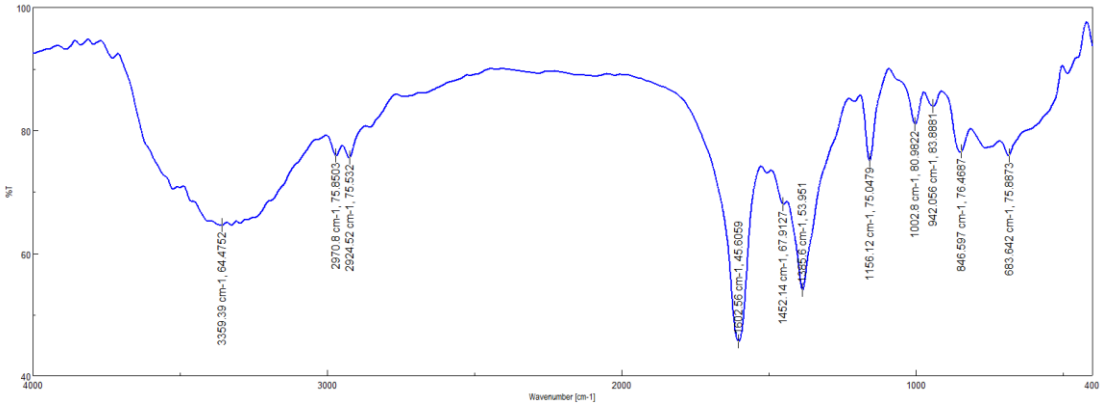


Figure S23 IR spectrum of compound **3**

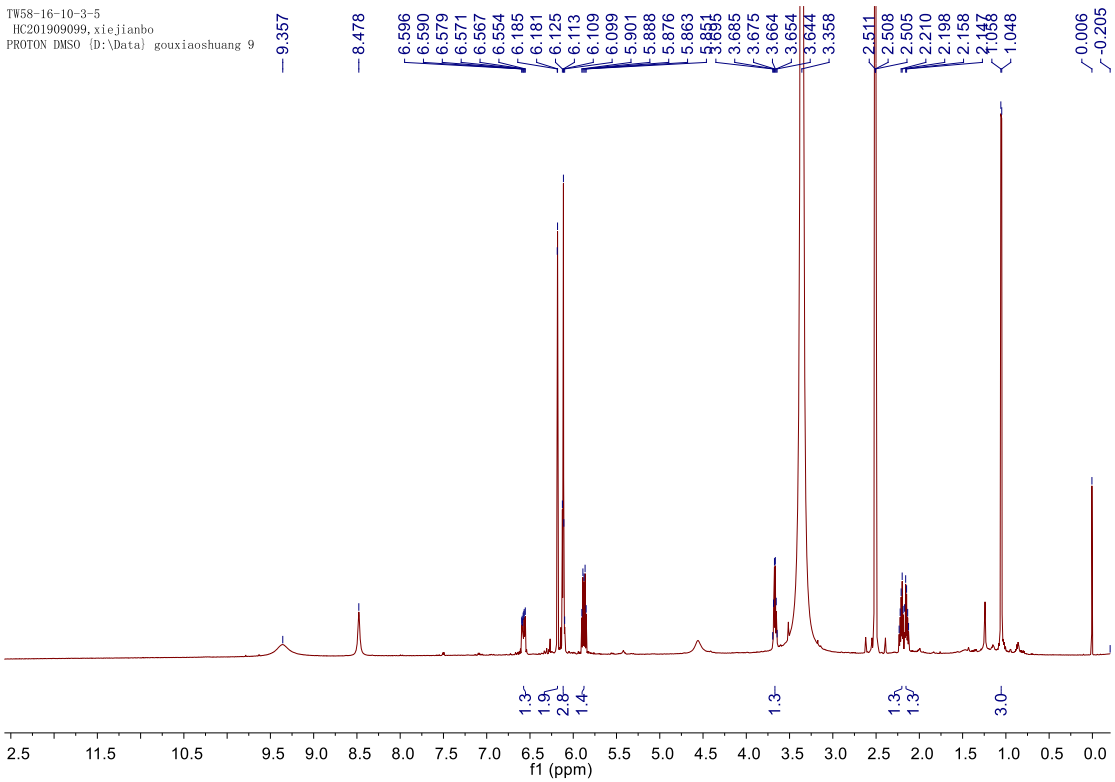


Figure S24 ^{1}H-NMR spectrum of compound **3** (in DMSO-d_6)

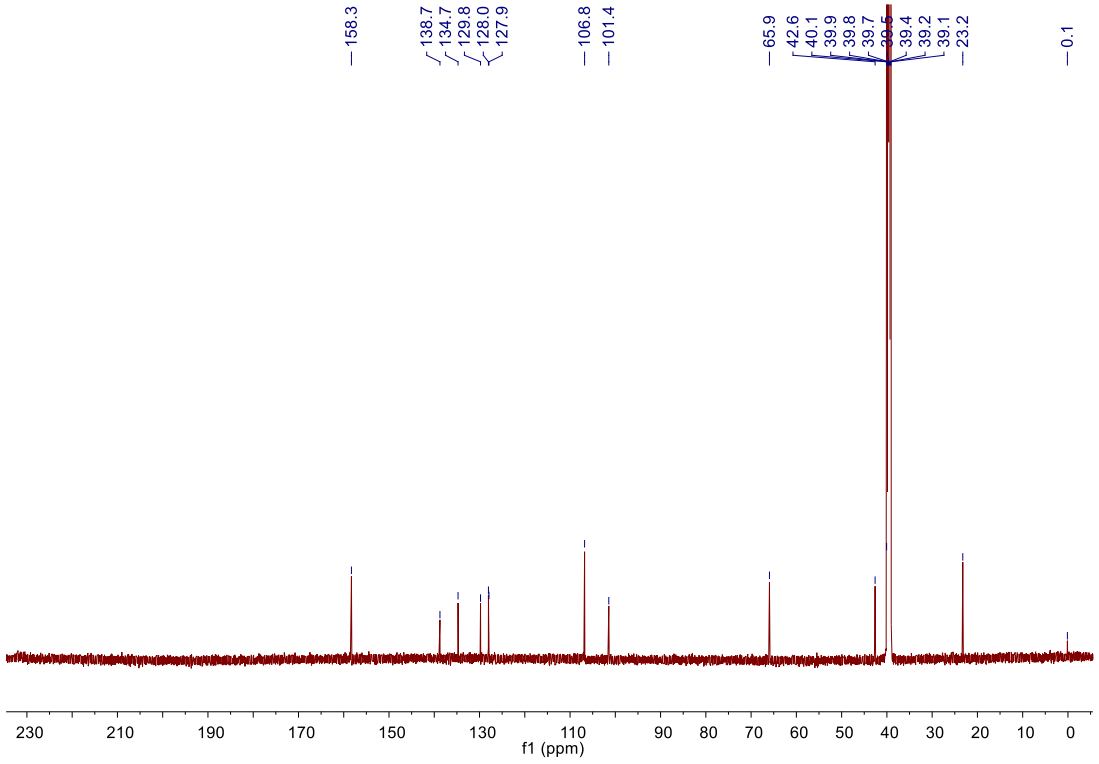


Figure S25 ^{13}C-NMR spectrum of compound **3** (in DMSO-d_6)

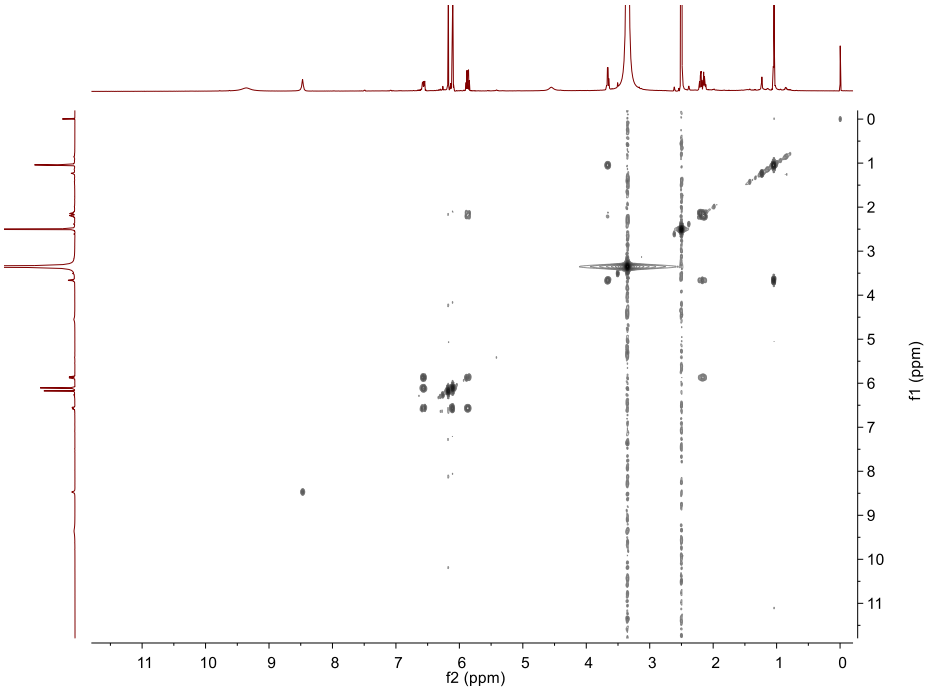


Figure S26 ^{1}H-^{1}H COSY spectrum of compound **3** (in DMSO-d_6)

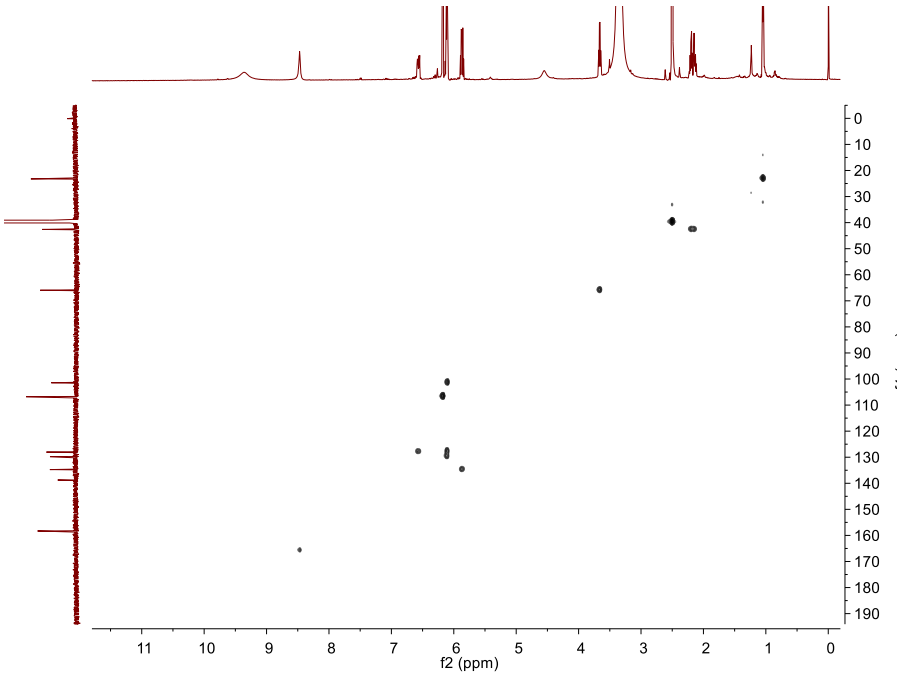


Figure S27 HSQC spectrum of compound **3** (in DMSO-d_6)

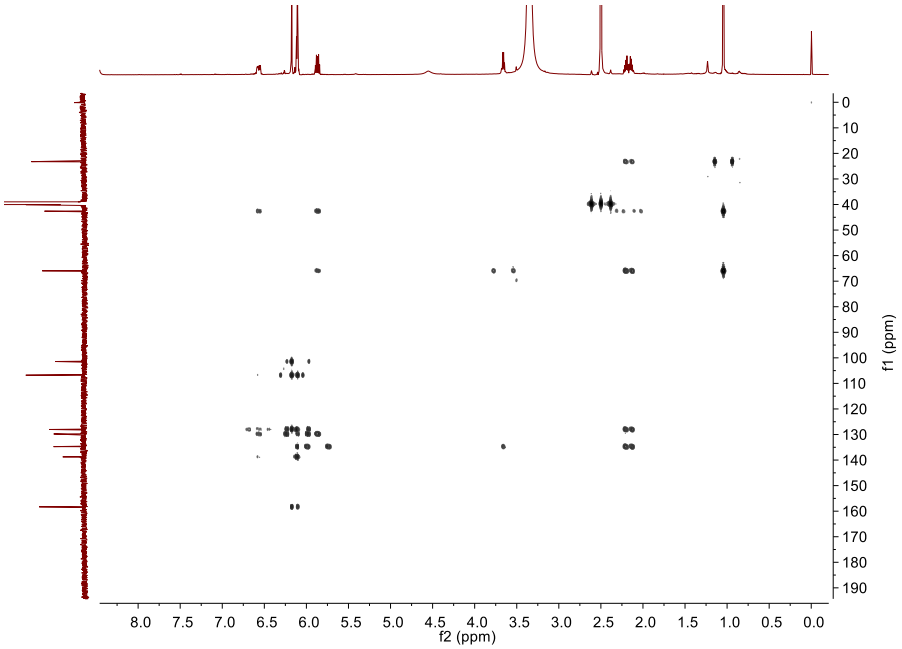
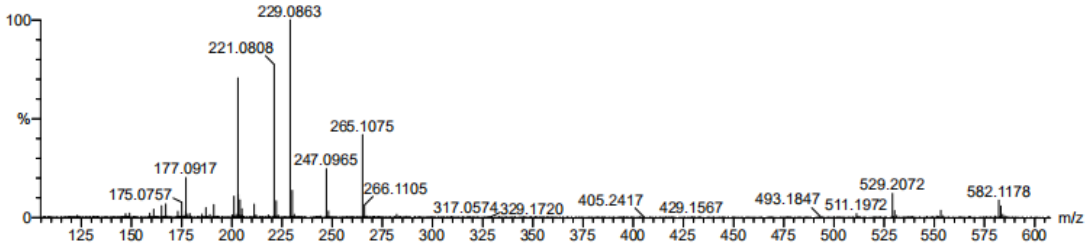


Figure S28 HMBC spectrum of compound **3** (in DMSO-d_6)

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
445 formula(e) evaluated with 7 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200
20190923011 95 (0.778)

1: TOF MS ES+
6.56e+004



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
265.1075	265.1076	-0.1	-0.4	6.5	186.5	0.112	89.45	C14 H17 O5
	265.1049	2.6	9.8	7.5	189.0	2.629	7.22	C10 H13 N6 O3
	265.1089	-1.4	-5.3	11.5	189.9	3.472	3.11	C15 H13 N4 O
	265.1036	3.9	14.7	2.5	192.5	6.064	0.23	C9 H17 N2 O7
	265.1121	-4.6	-17.4	3.5	198.5	12.118	0.00	C4 H13 N10 O4
	265.1108	-3.3	-12.4	-1.5	198.5	12.137	0.00	C3 H17 N6 O8
	265.1094	-1.9	-7.2	4.5	203.2	16.810	0.00	H9 N16 O2

Figure S29 HR-ESI-MS spectrum of compound **4**

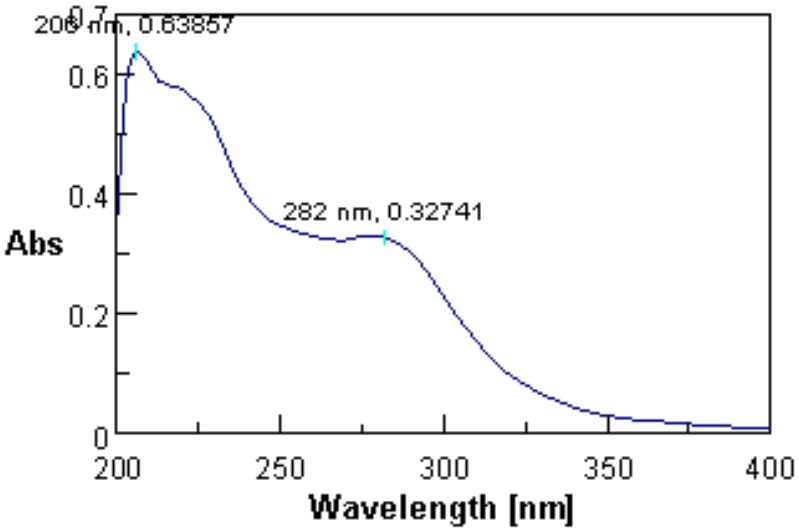


Figure S30 UV spectrum of compound **4**

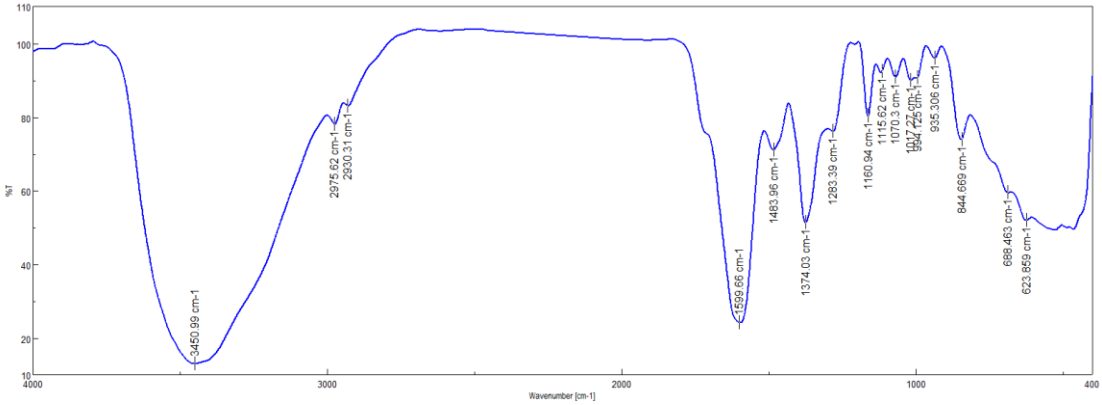


Figure S31 IR spectrum of compound **4**

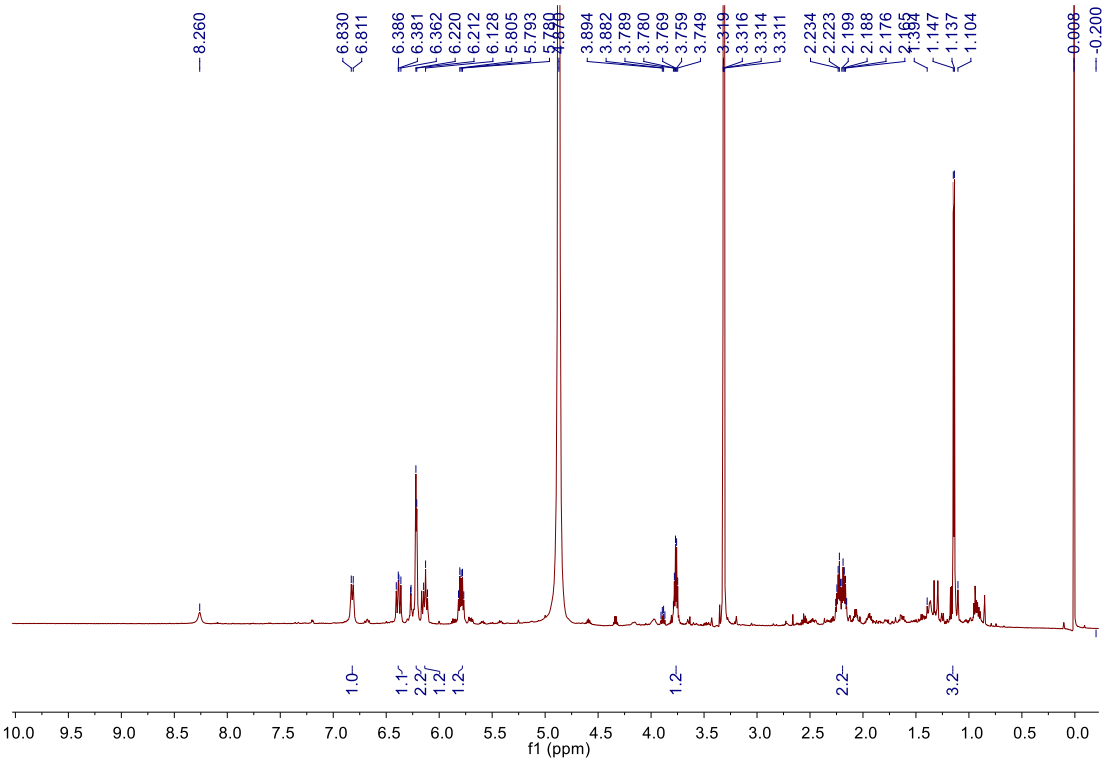


Figure S32 ^{1}H-NMR spectrum of compound **4** (in CD_3OD)

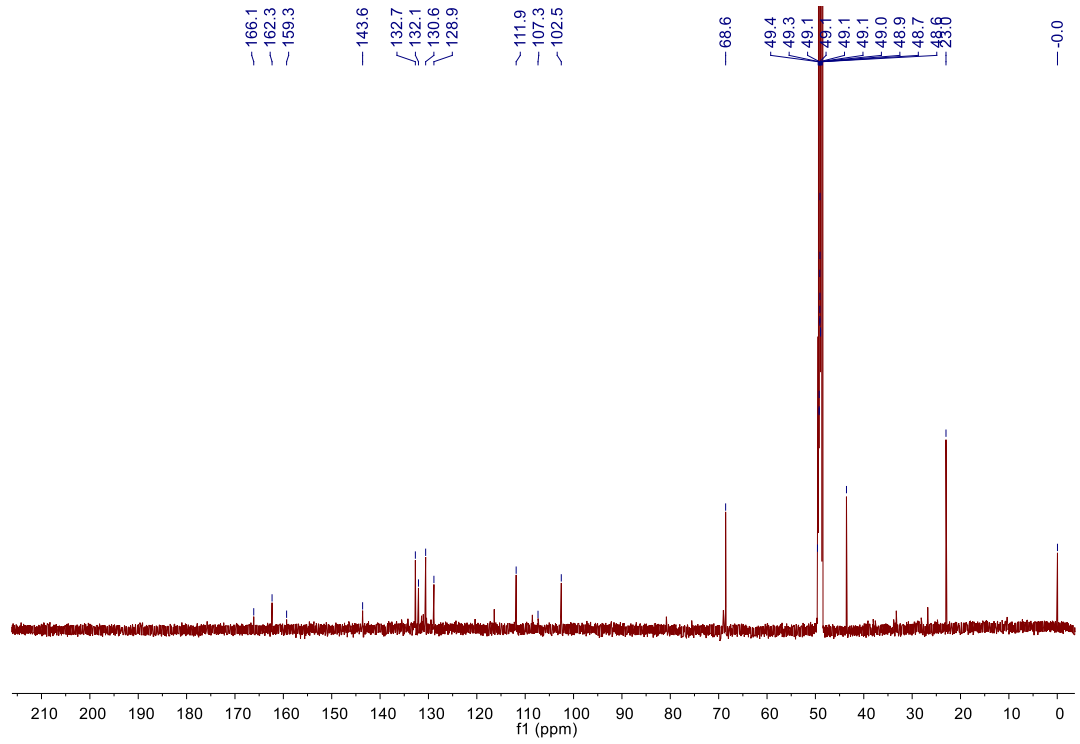


Figure S33 ^{13}C-NMR spectrum of compound **4** (in CD_3OD)

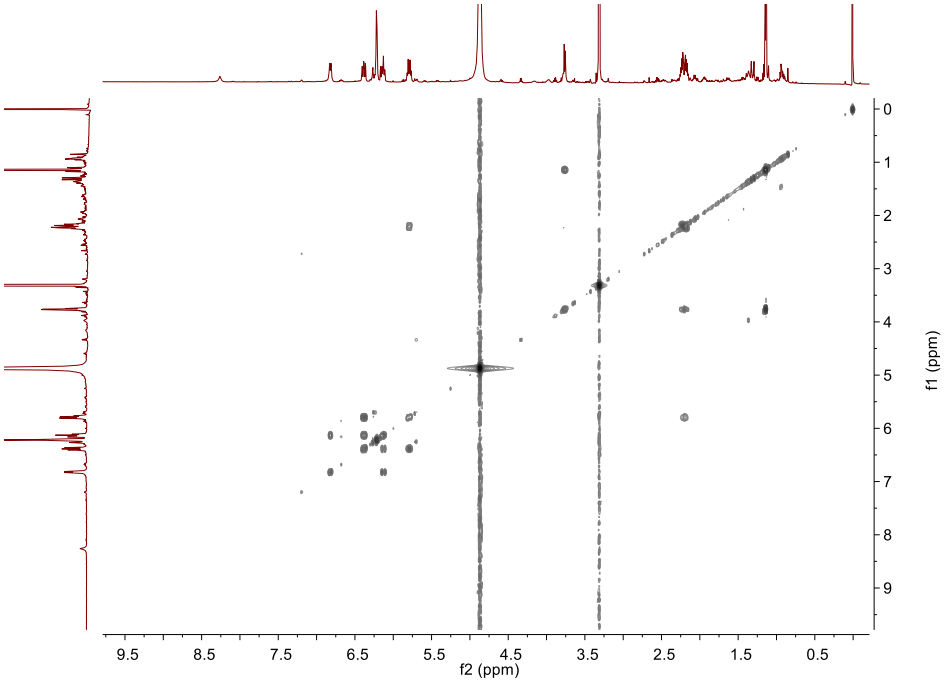


Figure S34 ^{1}H-^{1}H COSY spectrum of compound **4** (in CD_3OD)

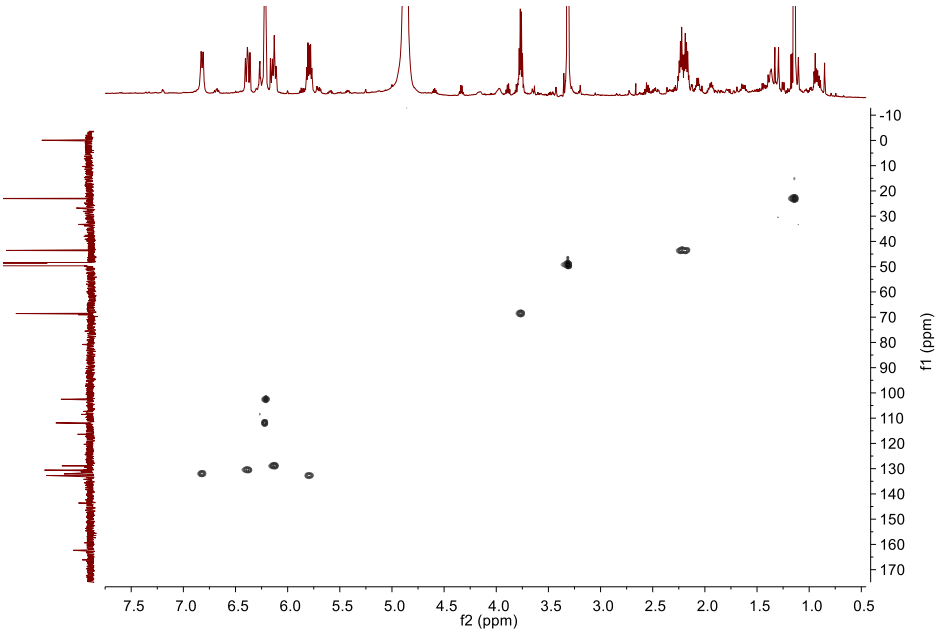


Figure S35 HSQC spectrum of compound **4** (in CD_3OD)

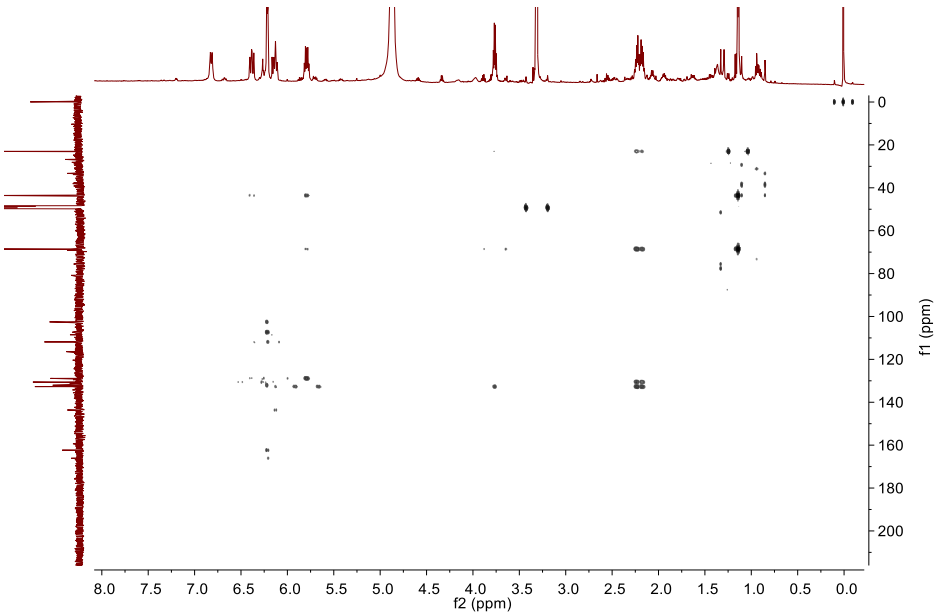


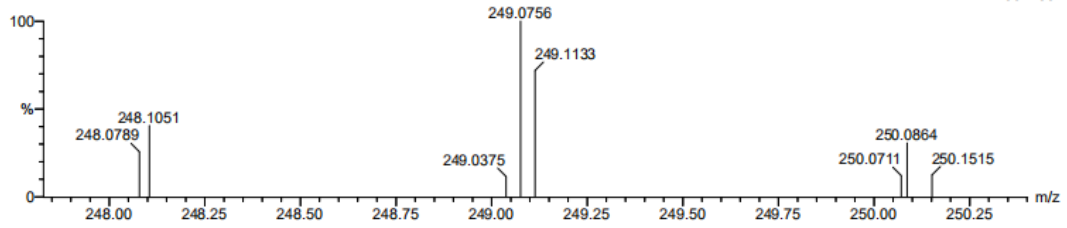
Figure S36 HMBC spectrum of compound **4** (in CD_3OD)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = 0.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
35 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-50 H: 0-100 O: 0-50
TW58-16-78-8-1
20200803044 81 (0.662)

1: TOF MS ES-
1.06e+002



Minimum:				0.0				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
249.1133	249.1127	0.6	2.4	6.5	27.1	n/a	n/a	C14 H17 O4

Figure S37 HR-ESI-MS spectrum of compound **5**

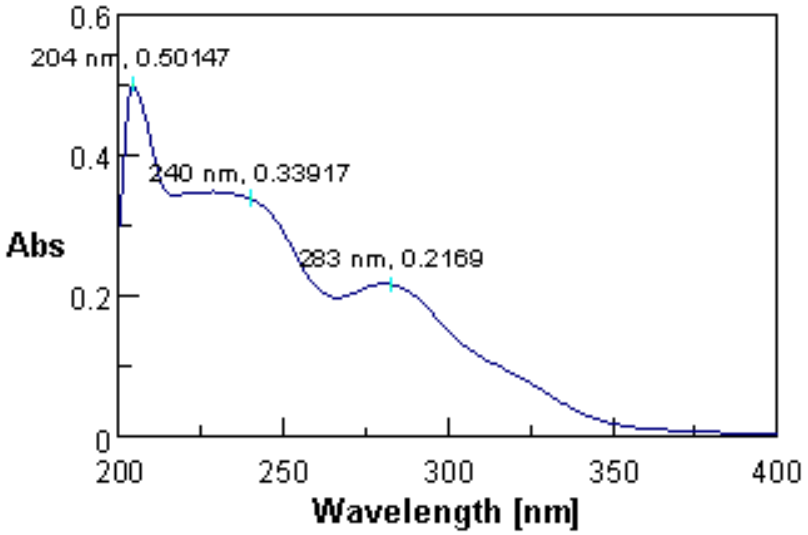


Figure S38 UV spectrum of compound **5**

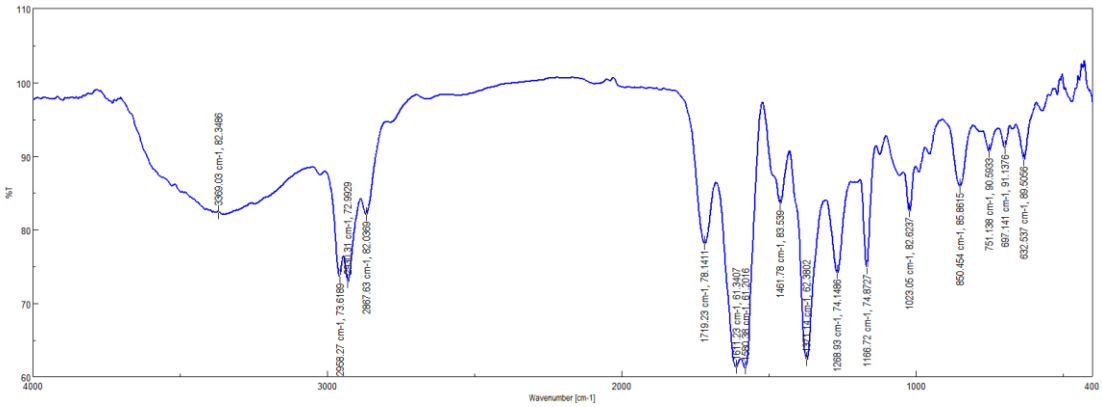


Figure S39 IR spectrum of compound **5**

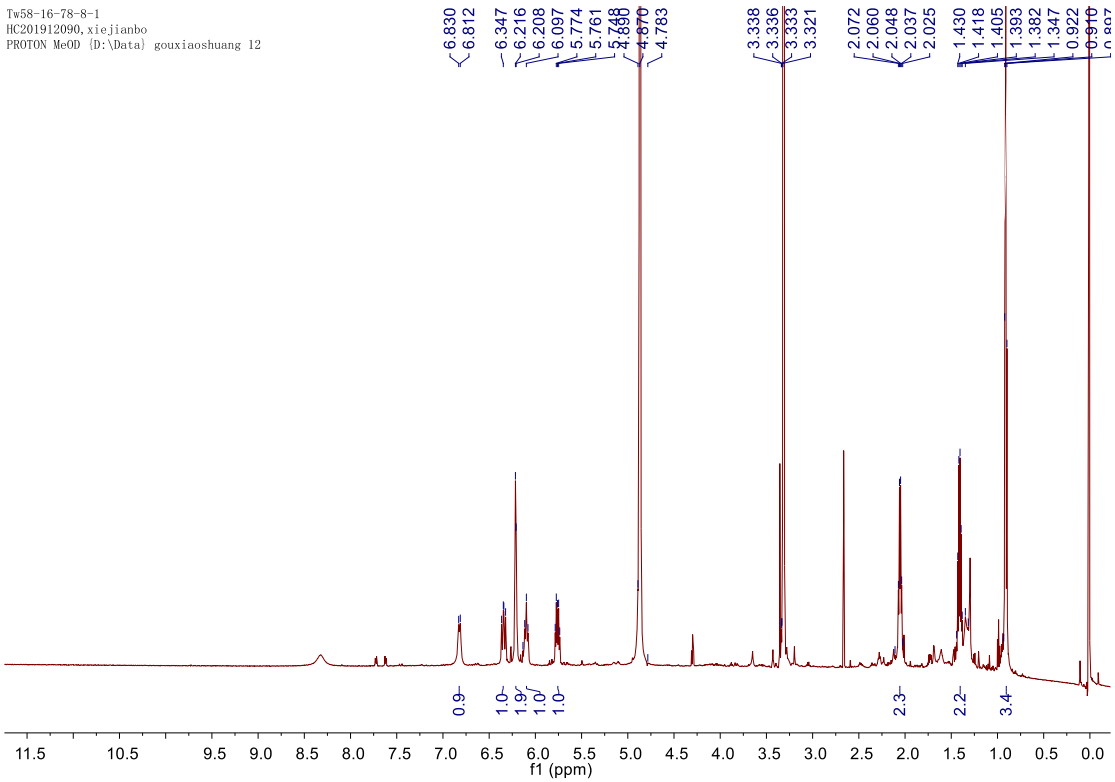


Figure S40 ^{1}H-NMR spectrum of compound **5** (in CD_3OD)

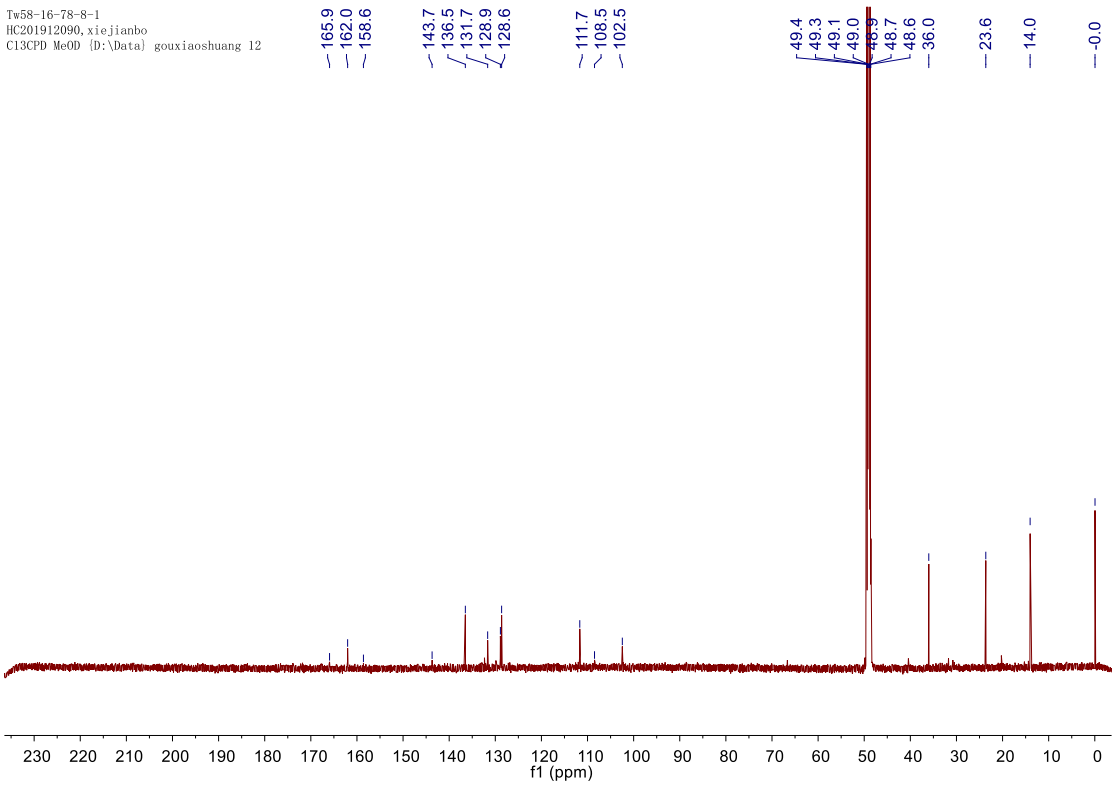


Figure S41 ^{13}C-NMR spectrum of compound **5** (in CD_3OD)

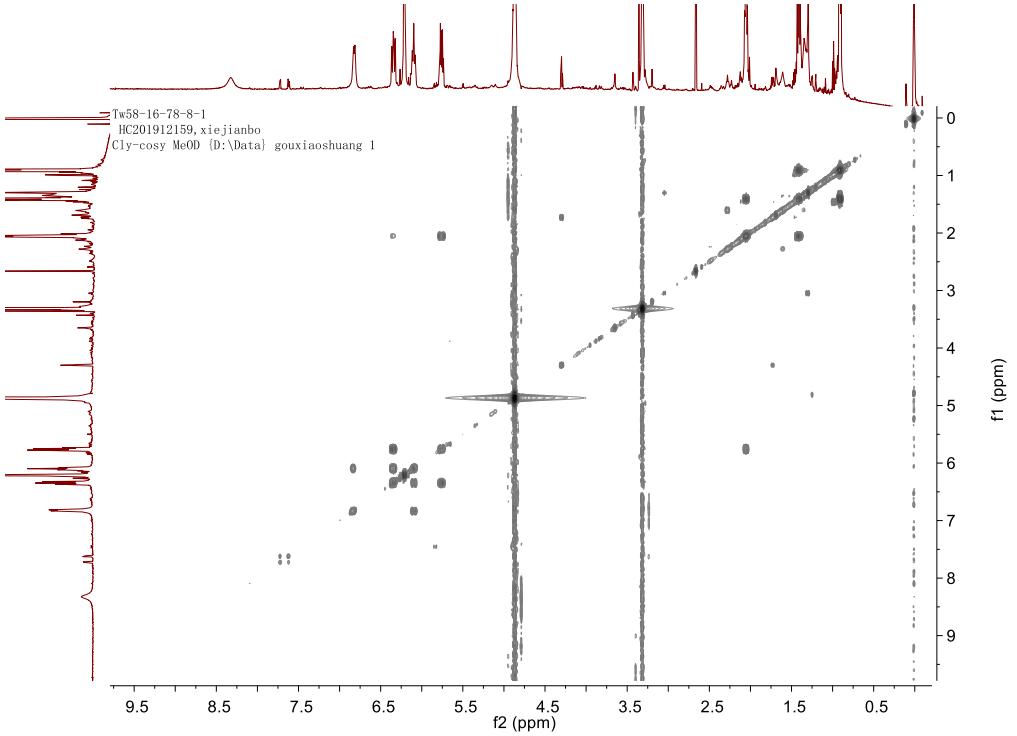


Figure S42 ^{1}H-^{1}H COSY spectrum of compound **5** (in CD_3OD)

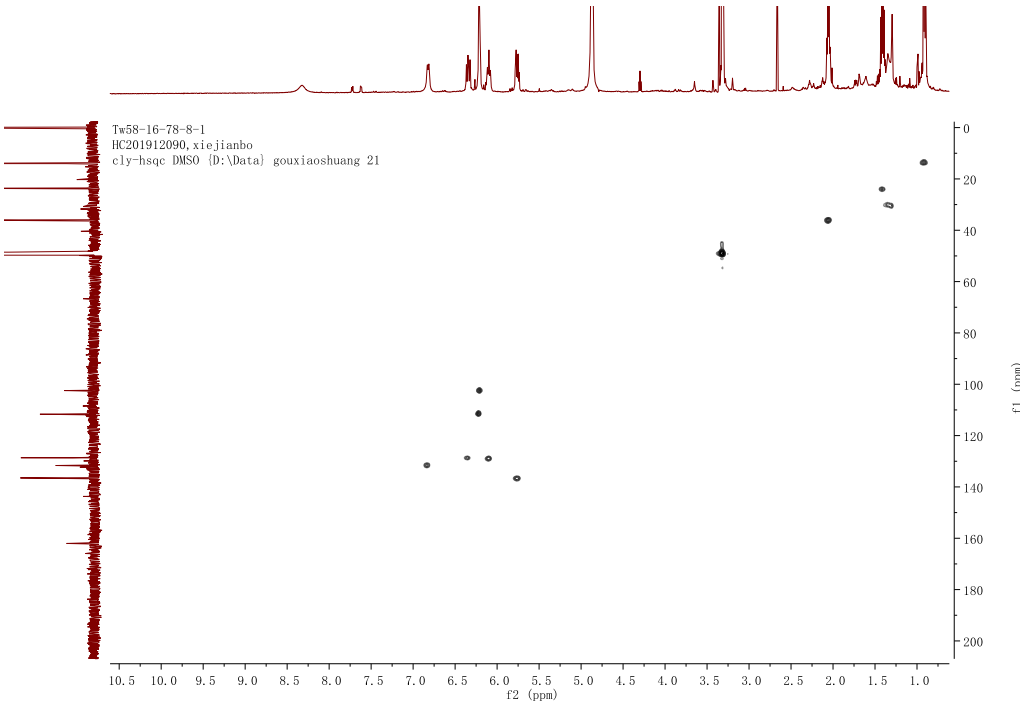


Figure S43 HSQC spectrum of compound **5** (in CD_3OD)

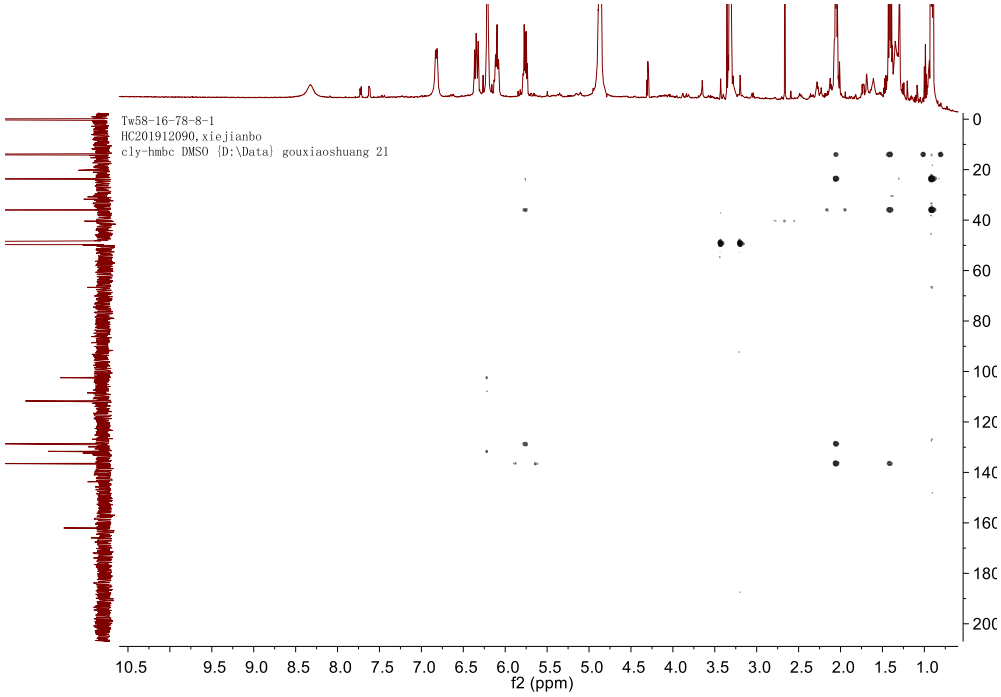
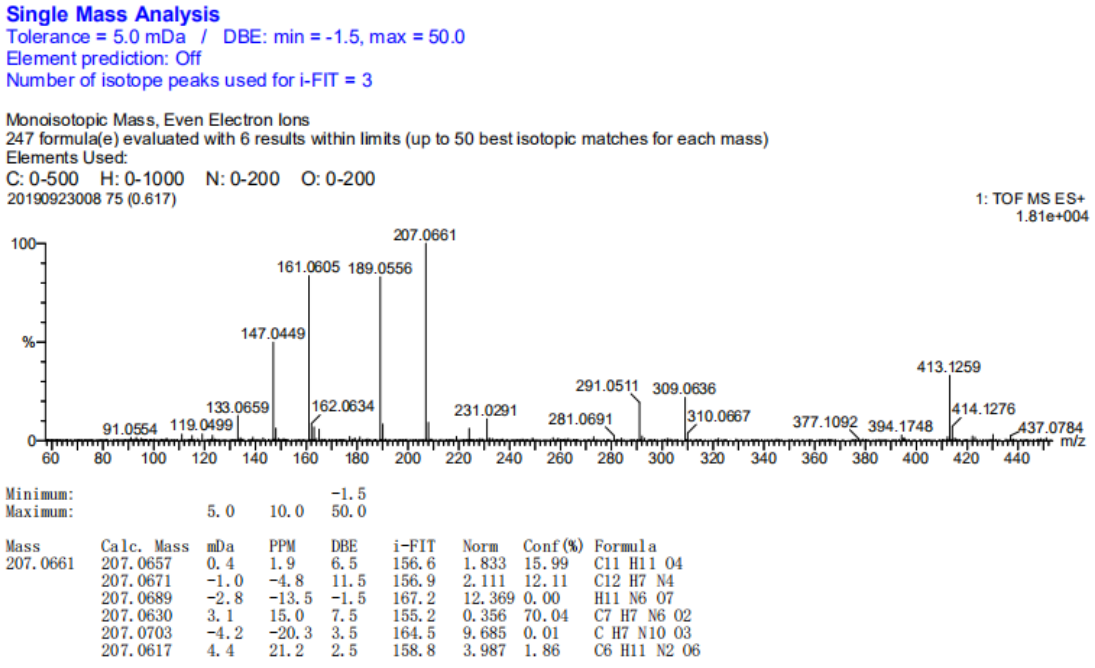


Figure S44 HMBC spectrum of compound **5** (in CD_3OD)



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
207.0661	207.0657	0.4	1.9	6.5	156.6	1.833	15.99	C11 H11 O4
	207.0671	-1.0	-4.8	11.5	156.9	2.111	12.11	C12 H7 N4
	207.0689	-2.8	-13.5	-1.5	167.2	12.369	0.00	H11 N6 O7
	207.0630	3.1	15.0	7.5	155.2	0.356	70.04	C7 H7 N6 O2
	207.0703	-4.2	-20.3	3.5	164.5	9.685	0.01	C H7 N10 O3
	207.0617	4.4	21.2	2.5	158.8	3.987	1.86	C6 H11 N2 O6

Figure S45 HR-ESI-MS spectrum of compound **6**

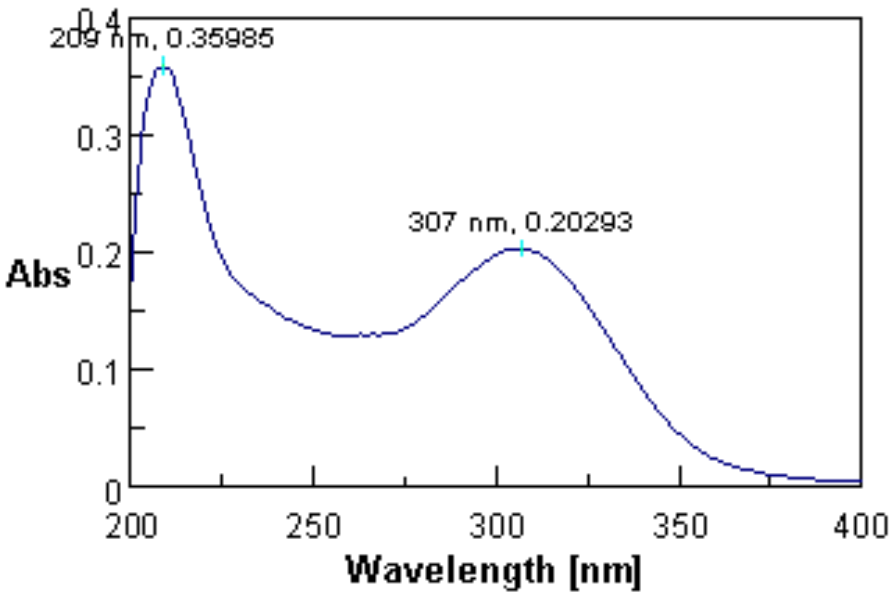


Figure S46 UV spectrum of compound **6**

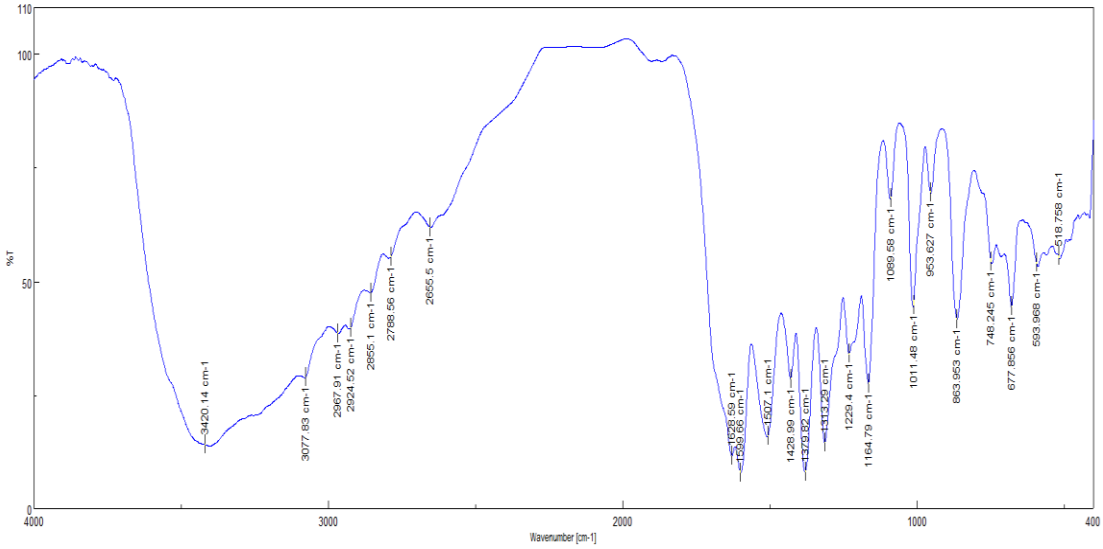


Figure S47 IR spectrum of compound **6**

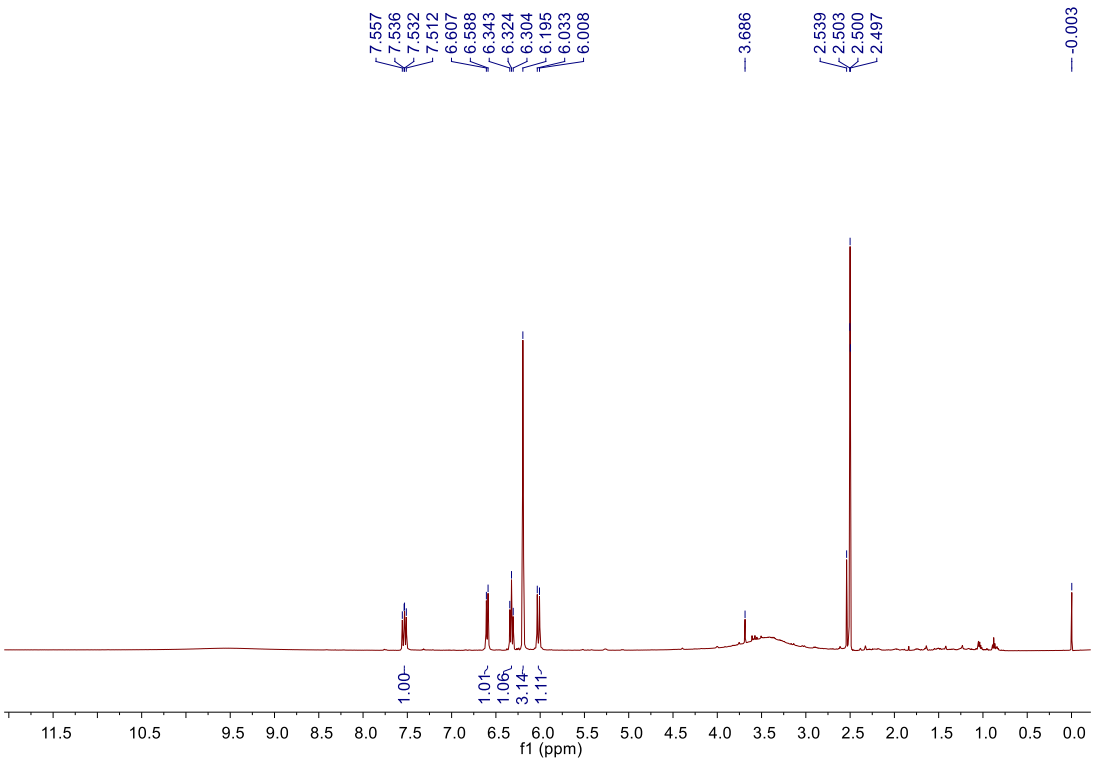


Figure S48 [1]H-NMR spectrum of compound **6** (in DMSO-d_6)

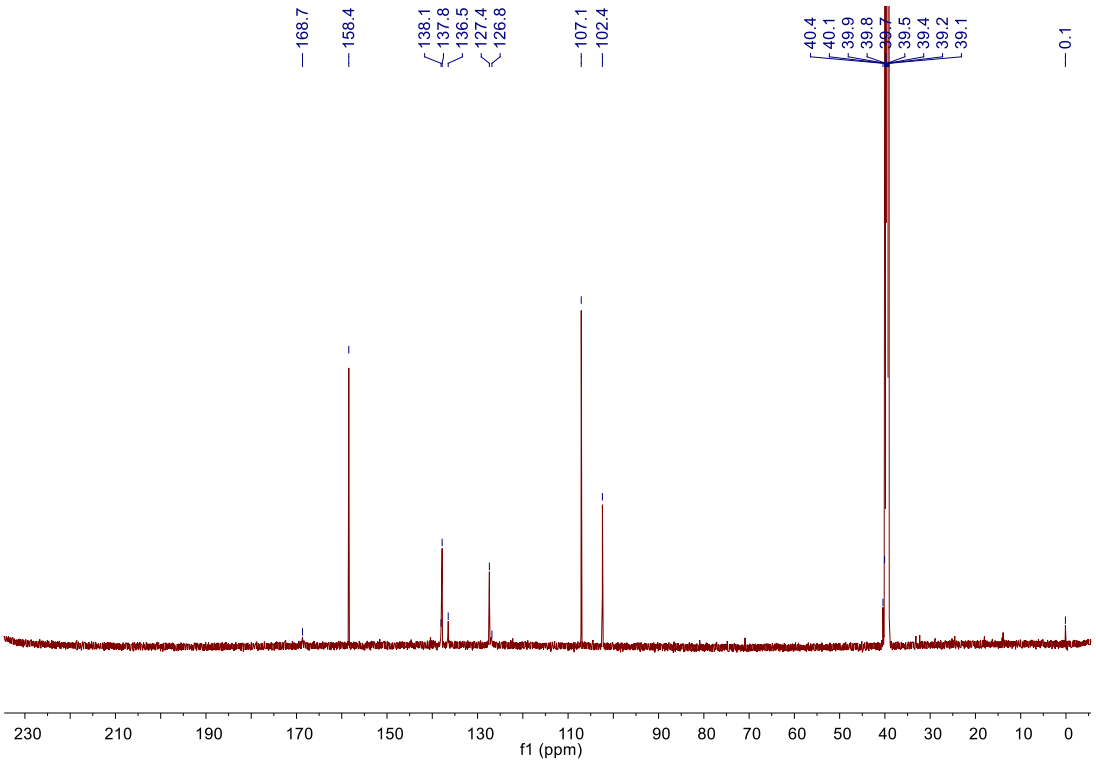


Figure S49[13]C-NMR spectrum of compound **6** (in DMSO-d_6)

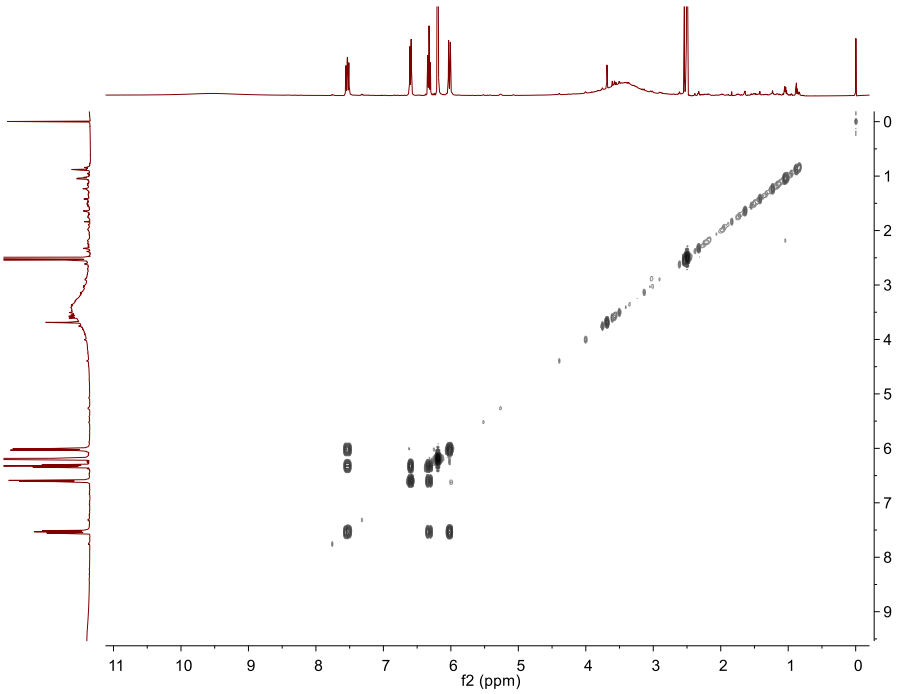


Figure S50 ^{1}H-^{1}H COSY spectrum of compound **6** (in DMSO-d_6)

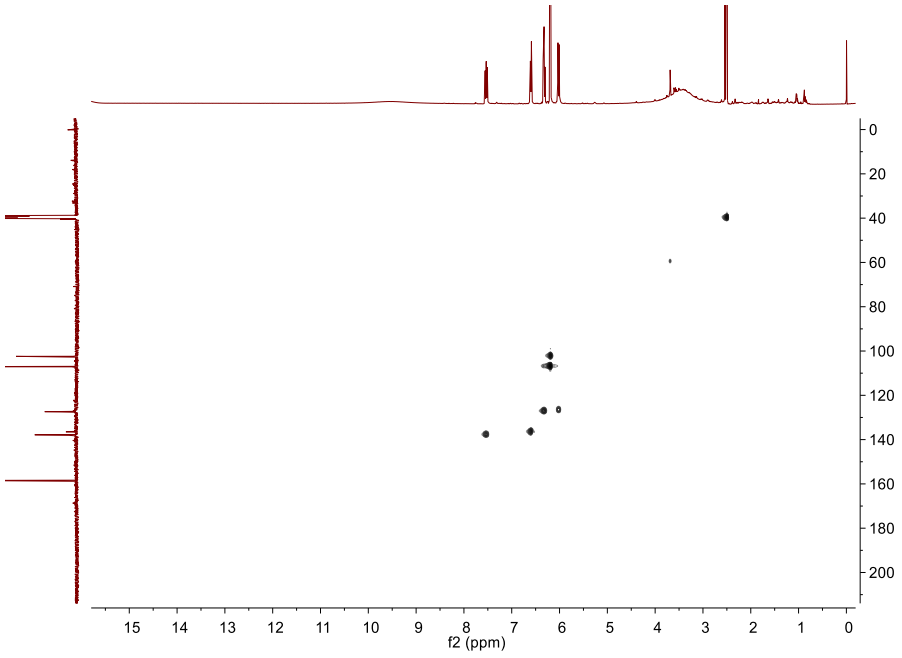


Figure S51 HSQC spectrum of compound **6** (in DMSO-d_6)

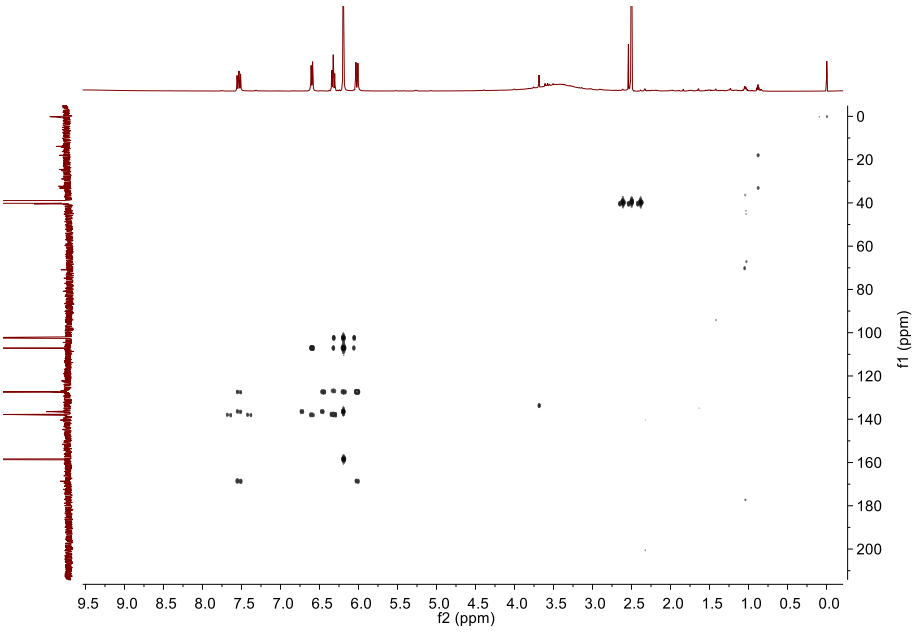


Figure S52 HMBC spectrum of compound **6** (in DMSO-d_6)

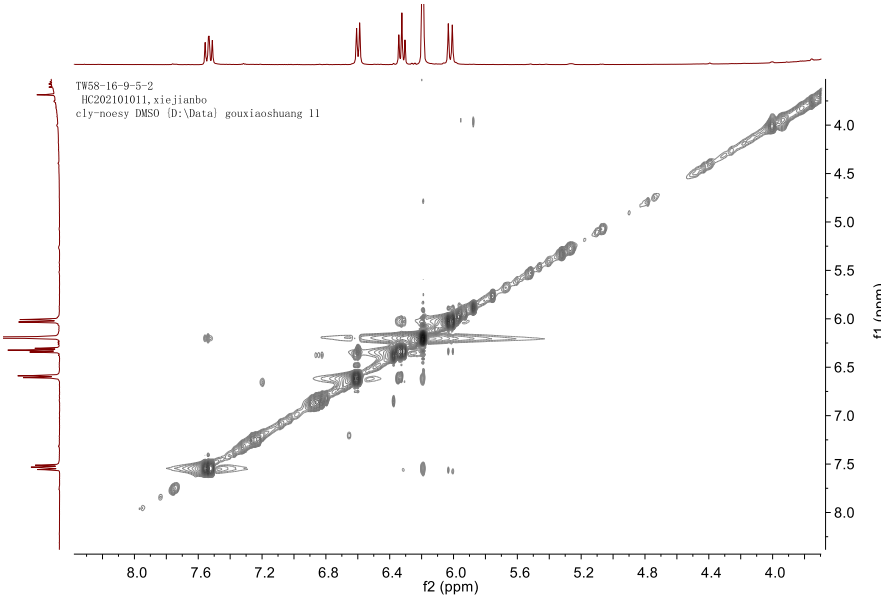


Figure S53 NOESY spectrum of compound **6** (in DMSO-d_6)

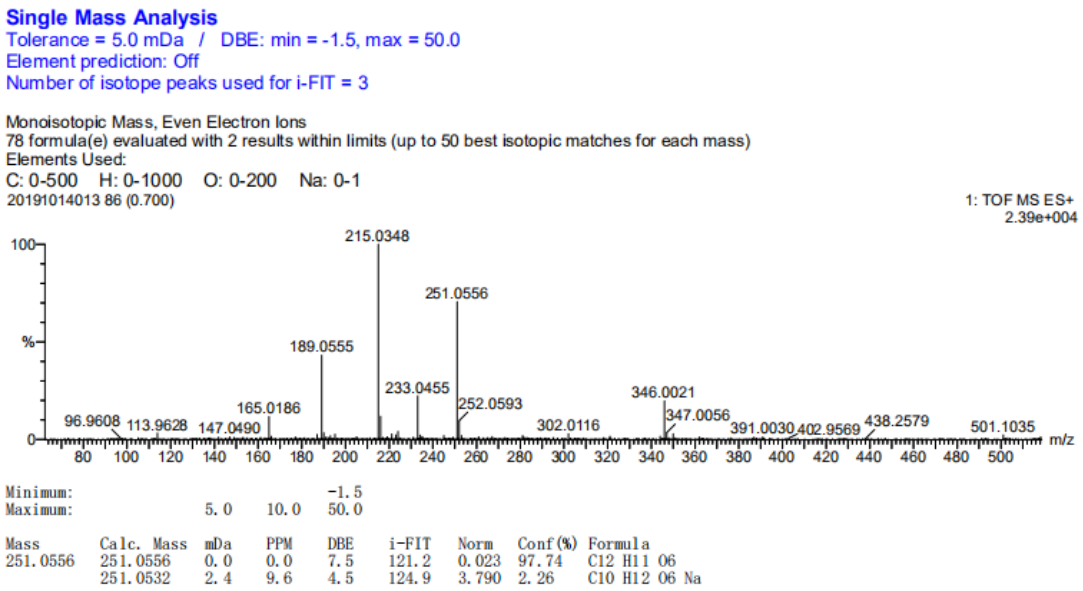


Figure S54 HR-ESI-MS spectrum of compound **7**

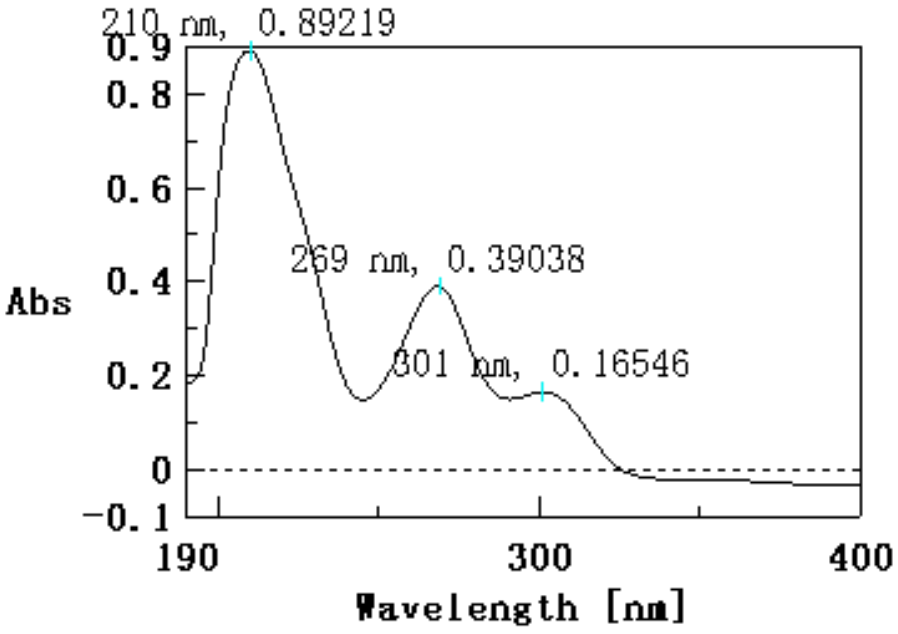


Figure S55 UV spectrum of compound **7**

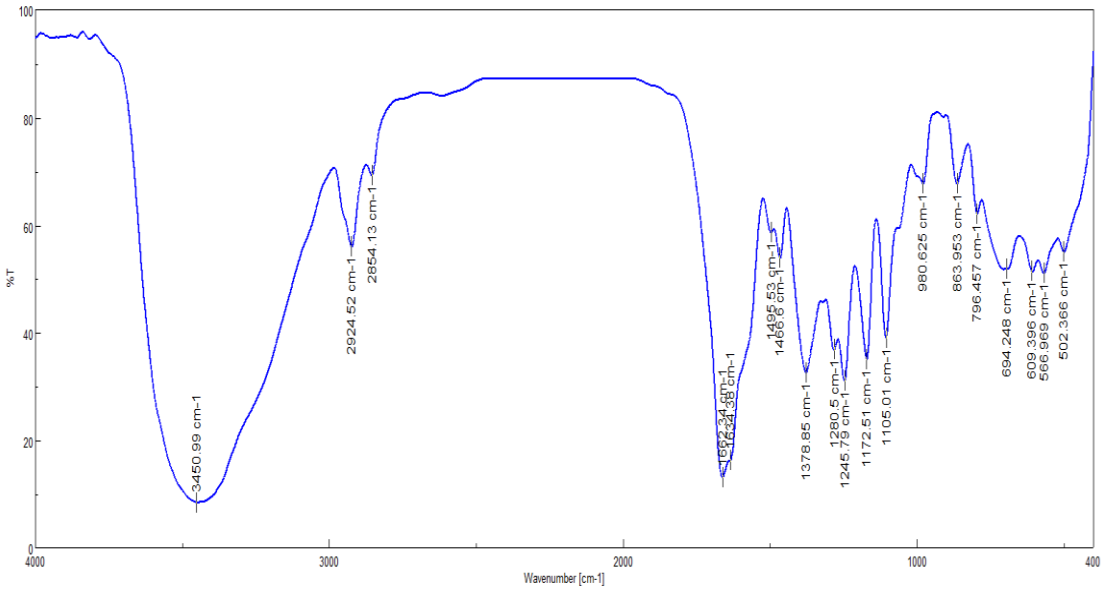


Figure S56 IR spectrum of compound **7**

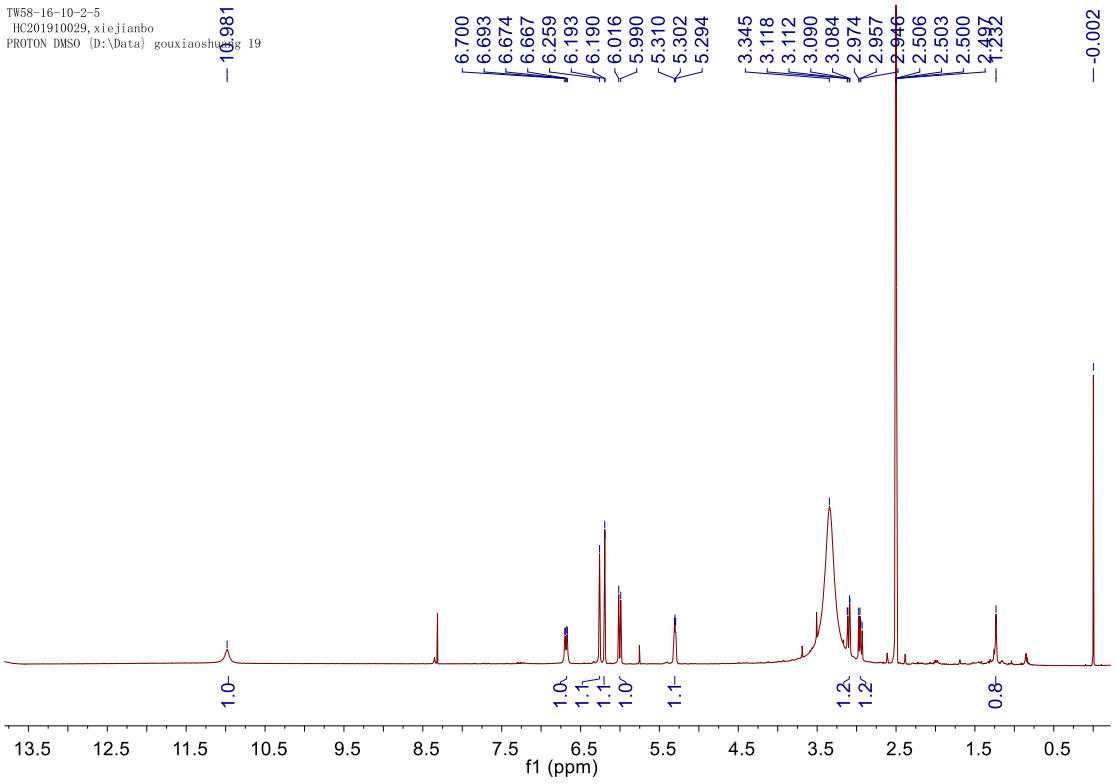


Figure S57 The ^{1}H-NMR spectrum of compound **7** (in DMSO-d_6)

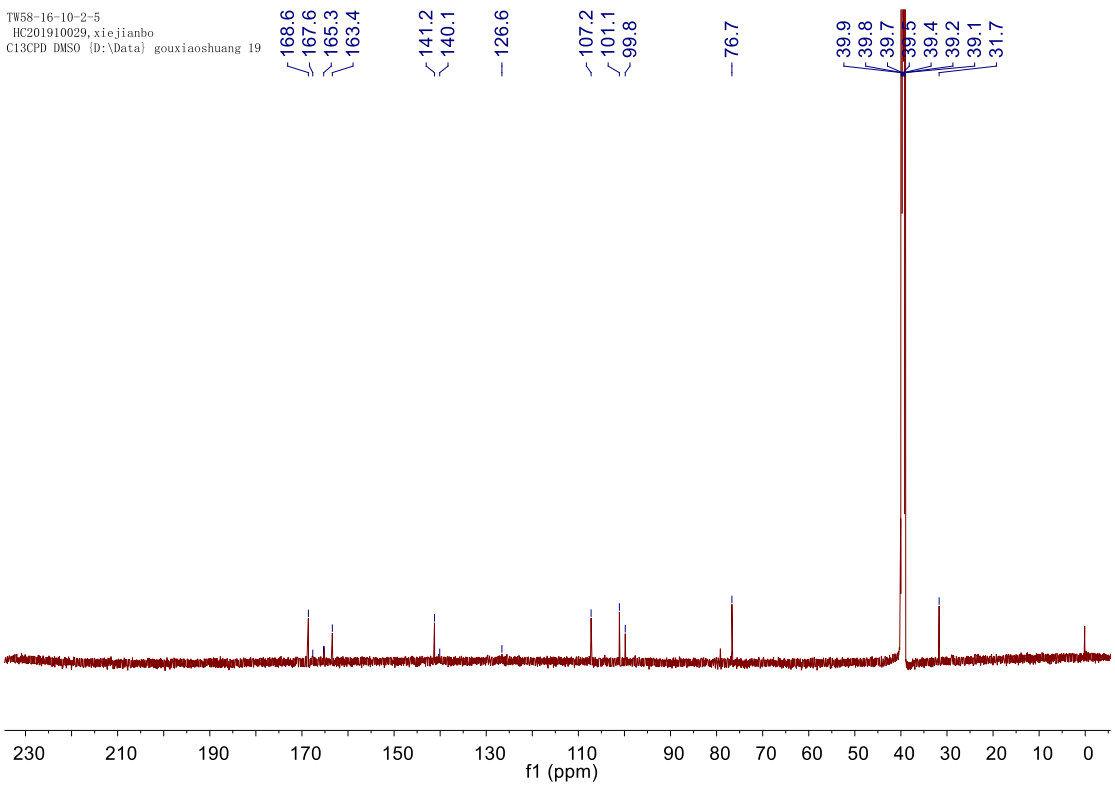


Figure S58 The ^{13}C-NMR spectrum of compound **7** (in DMSO-d_6)

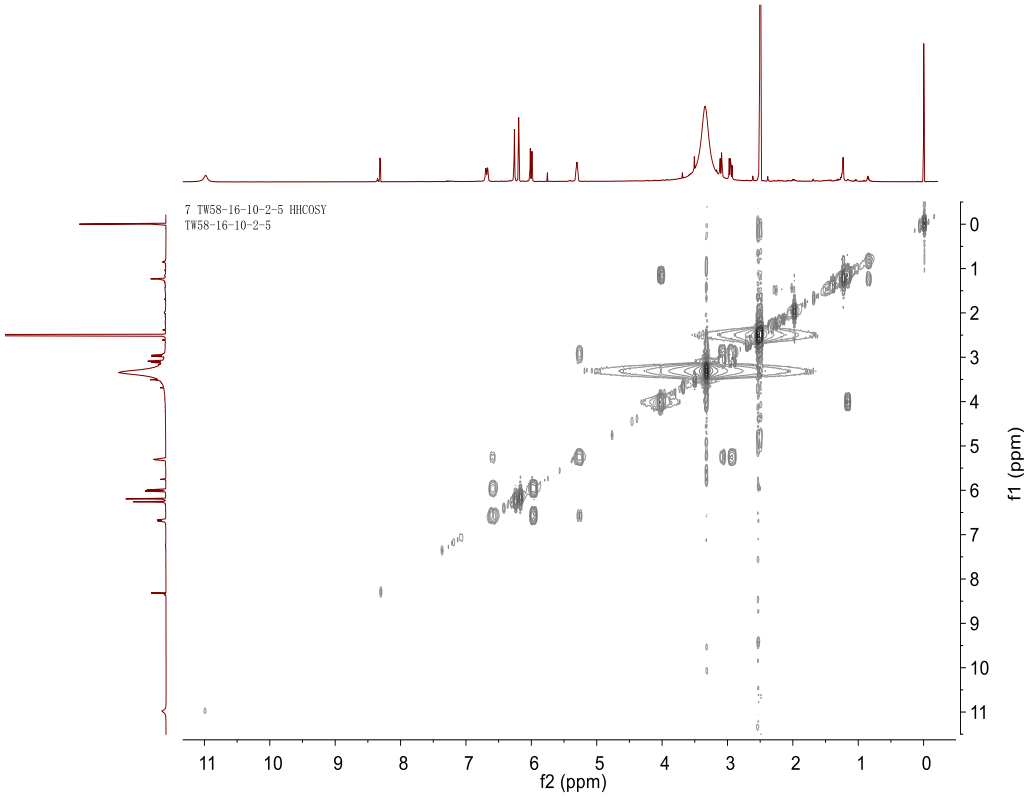


Figure S59 The ^{1}H-^{1}H COSY spectrum of compound **7** (in DMSO-d_6)

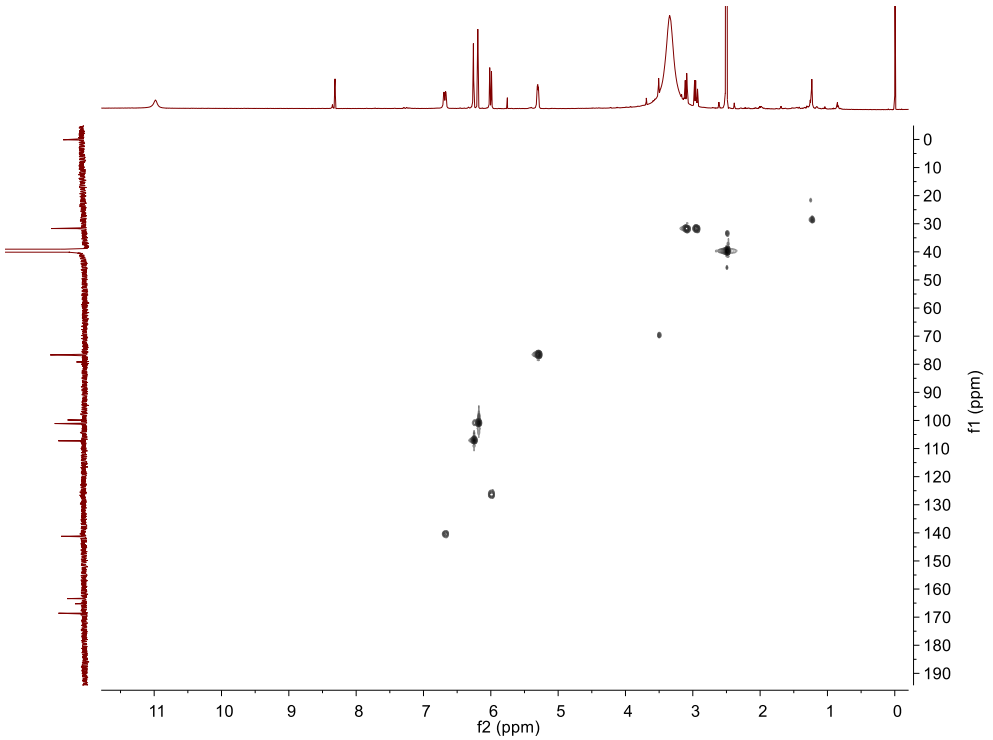


Figure S60 The HSQC spectrum of compound **7** (in DMSO-d_6)

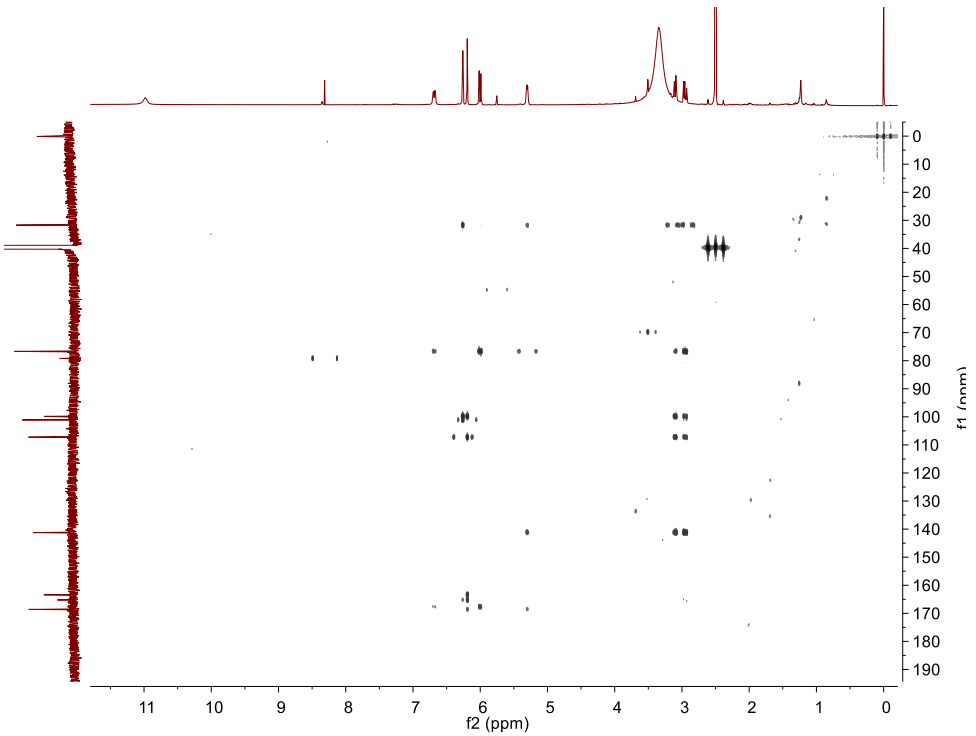


Figure S61 The HMBC spectrum of compound **7** (in DMSO-d_6)

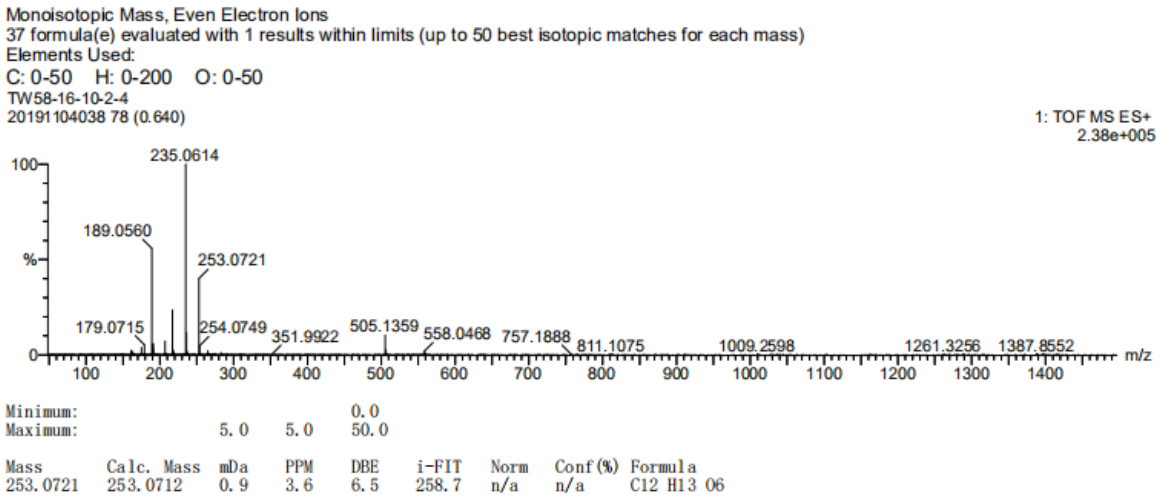


Figure S62 HR-ESI-MS spectrum of compound **8**

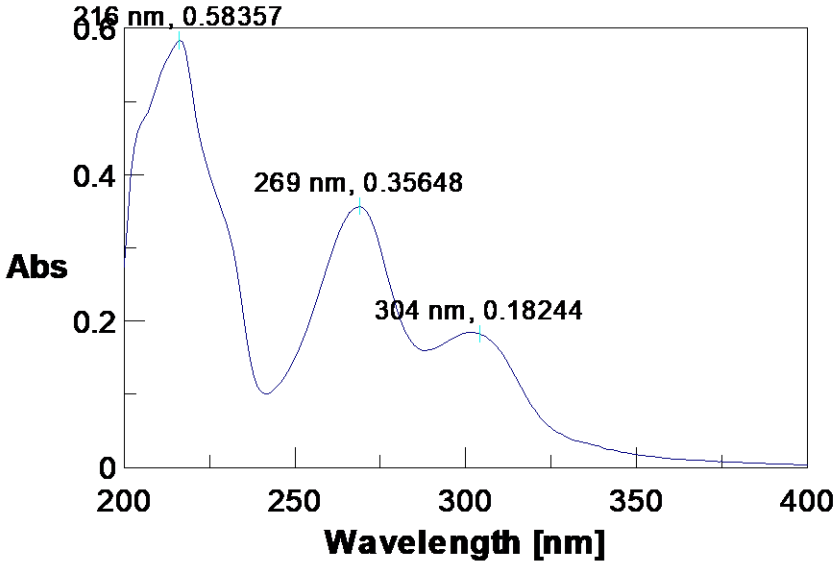


Figure S63 The UV spectrum of compound **8**

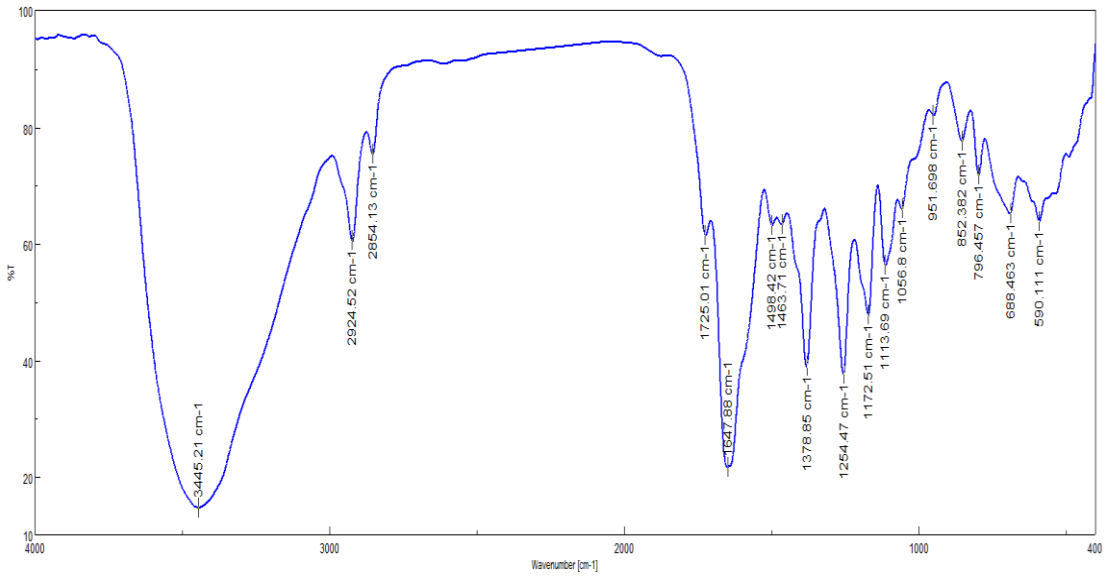


Figure S64 IR spectrum of compound **8**

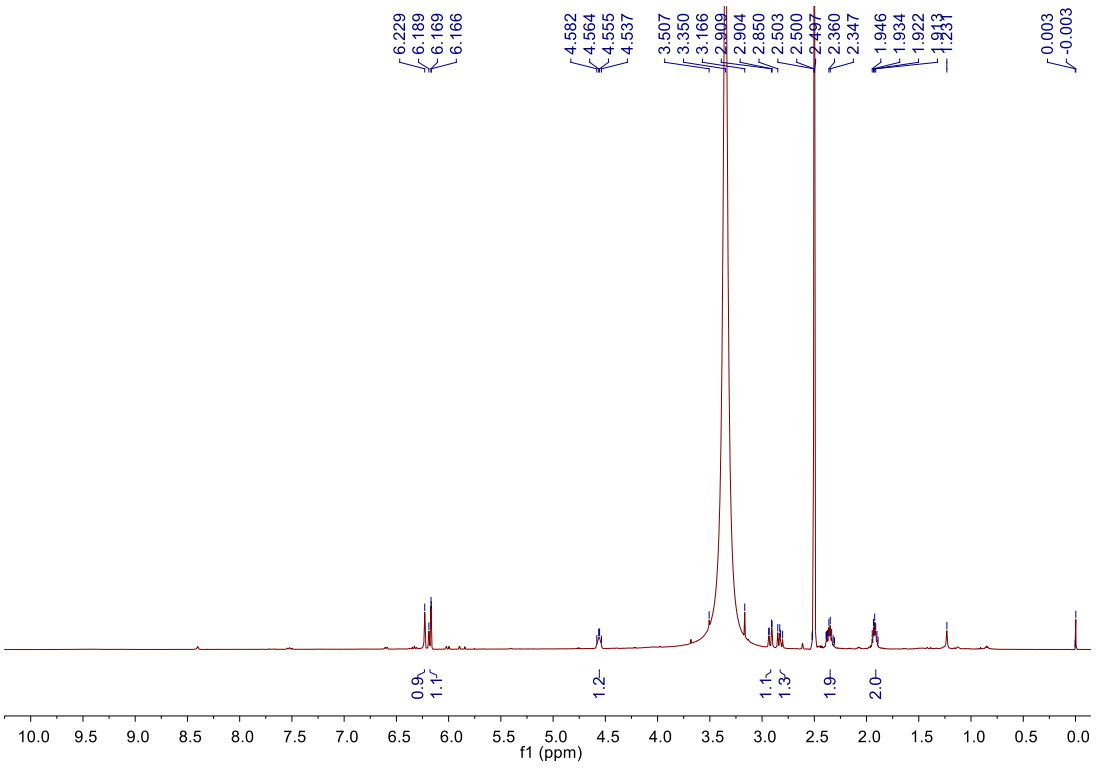


Figure S65 The ^{1}H-NMR spectrum of compound **8** (in DMSO-d_6)

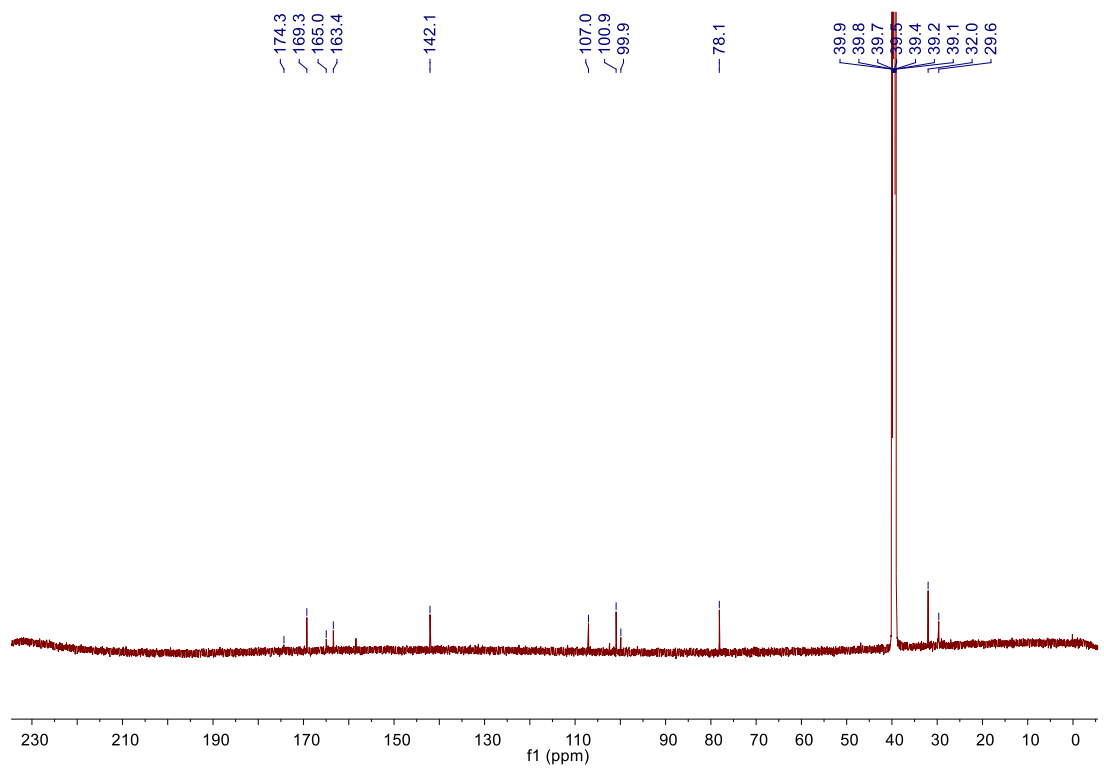


Figure S66 The ^{13}C-NMR spectrum of compound **8** (in DMSO-d_6)

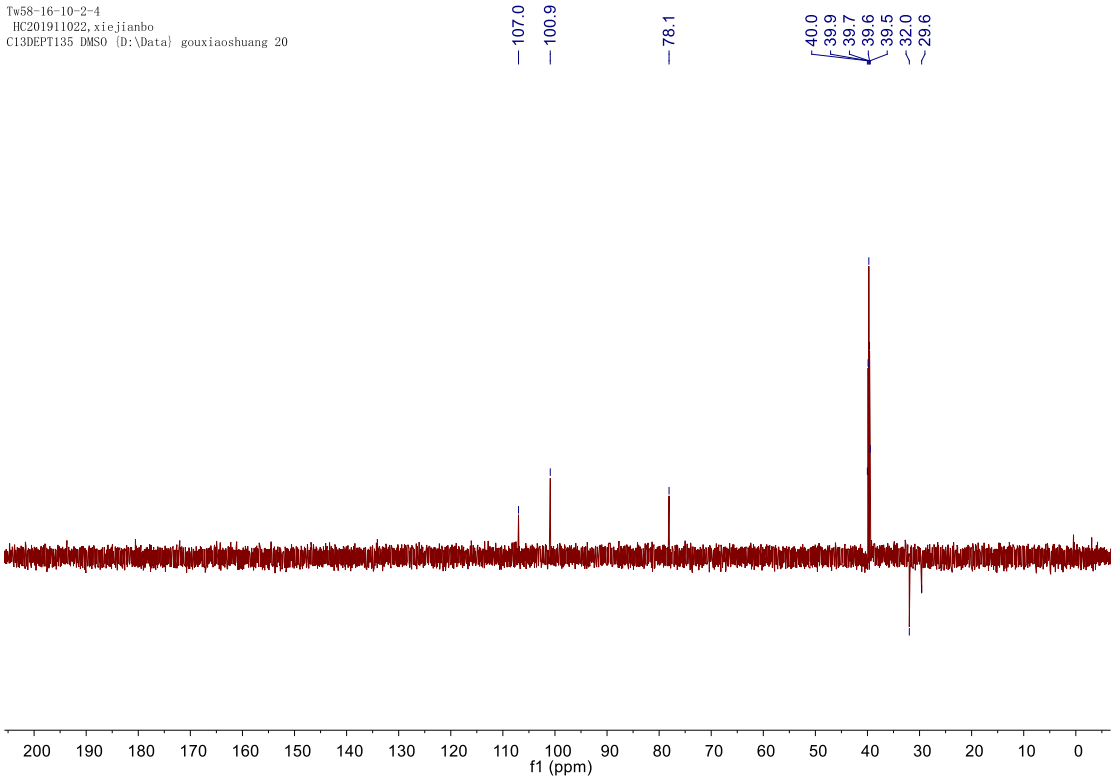


Figure S67 The DEPT135 spectrum of compound **8** (in DMSO-d_6)

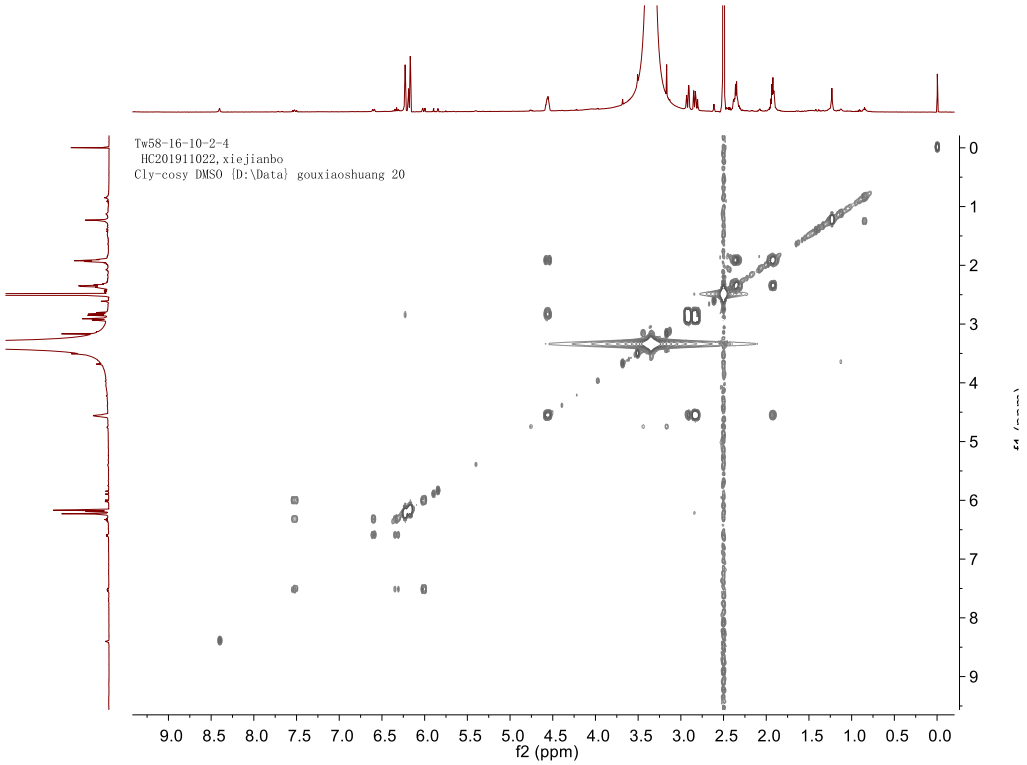


Figure S68 The ^{1}H-^{1}H COSY spectrum of compound **8** (in DMSO-d_6)

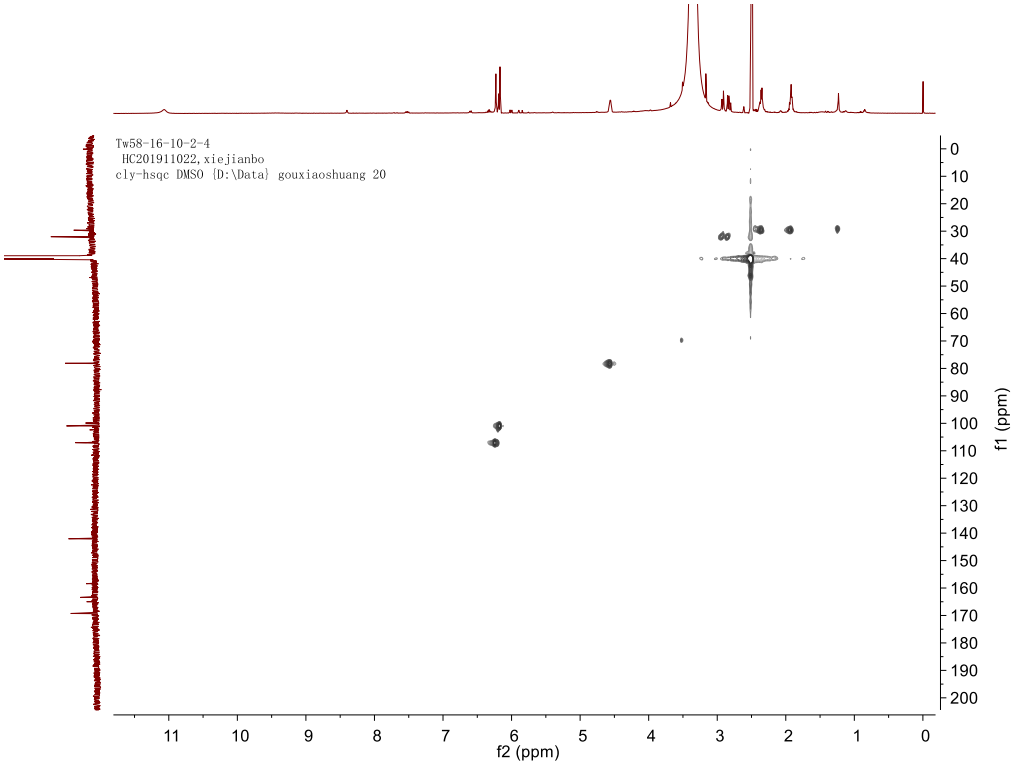


Figure S69 The HSQC spectrum of compound **8** (in DMSO-d_6)

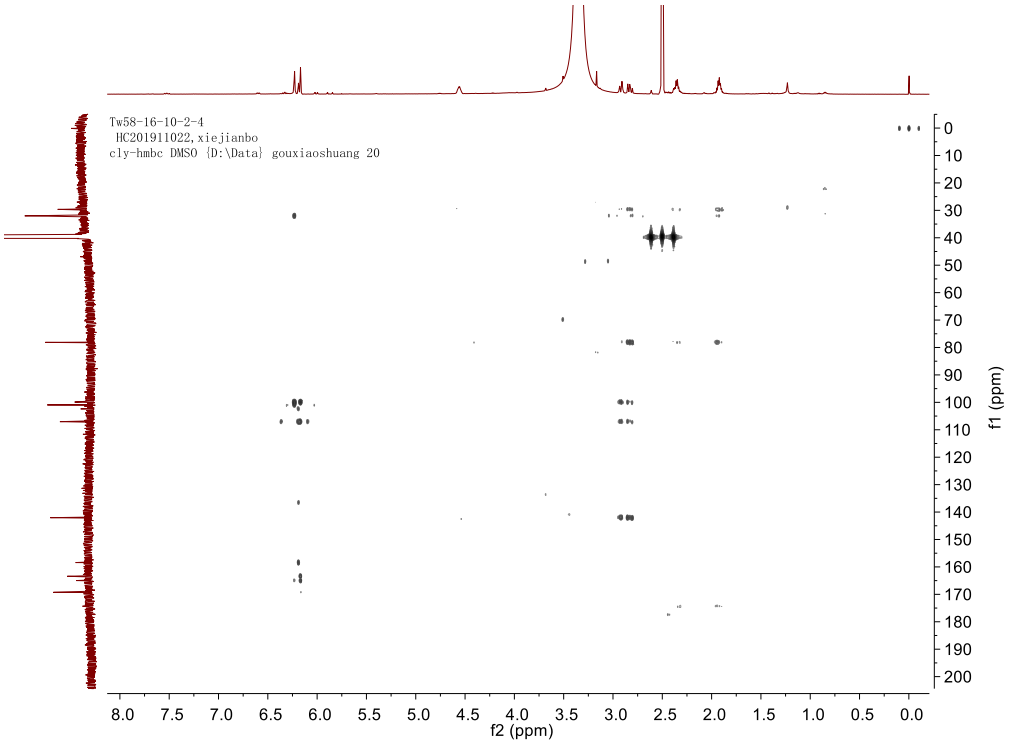


Figure S70 The HMBC spectrum of compound **8** (in DMSO-d_6)