Electronic Supplementary Material (ESI) for RSC Advances.

Illiciumlignans G-O from the leaves of *Illicium dunnianum* and their anti-inflammatory activities

Sen-Ju Ma, [‡, a] Hai-Bo Li, [‡, b] Ting Li,[a] Zhen-zhen Su, [b] Zhen-Zhong Wang,[b] Xin-Sheng Yao*[,a] Wei Xiao, *[,b] and Yang Yu,*[, a]

[‡] These authors have contributed equally to this work

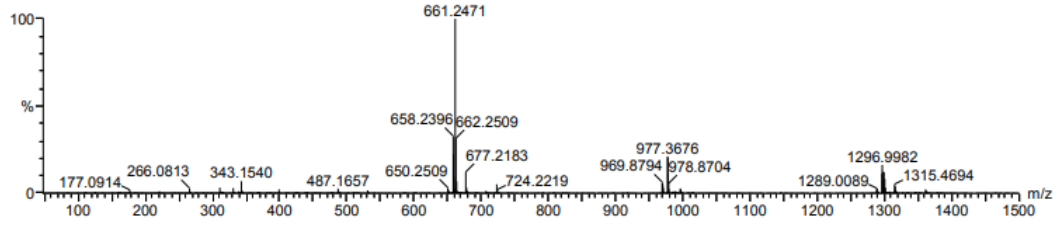
List of supporting information

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 3.0 PPM / DBE: min = -20.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
349 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-70 H: 0-100 O: 0-20 Na: 0-1
ID-3L4D
20200113003 37 (0.311)

1: TOF MS ES+
2.66e+005



Minimum:				-20.0	
Maximum:		5.0	3.0	50.0	

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Conf(%)	Formula
661.2471	661.2472	-0.1	-0.2	10.5	349.8	n/a	C31 H42 O14 Na

Fig. S1 HR-ESI-MS spectrum of compound 1

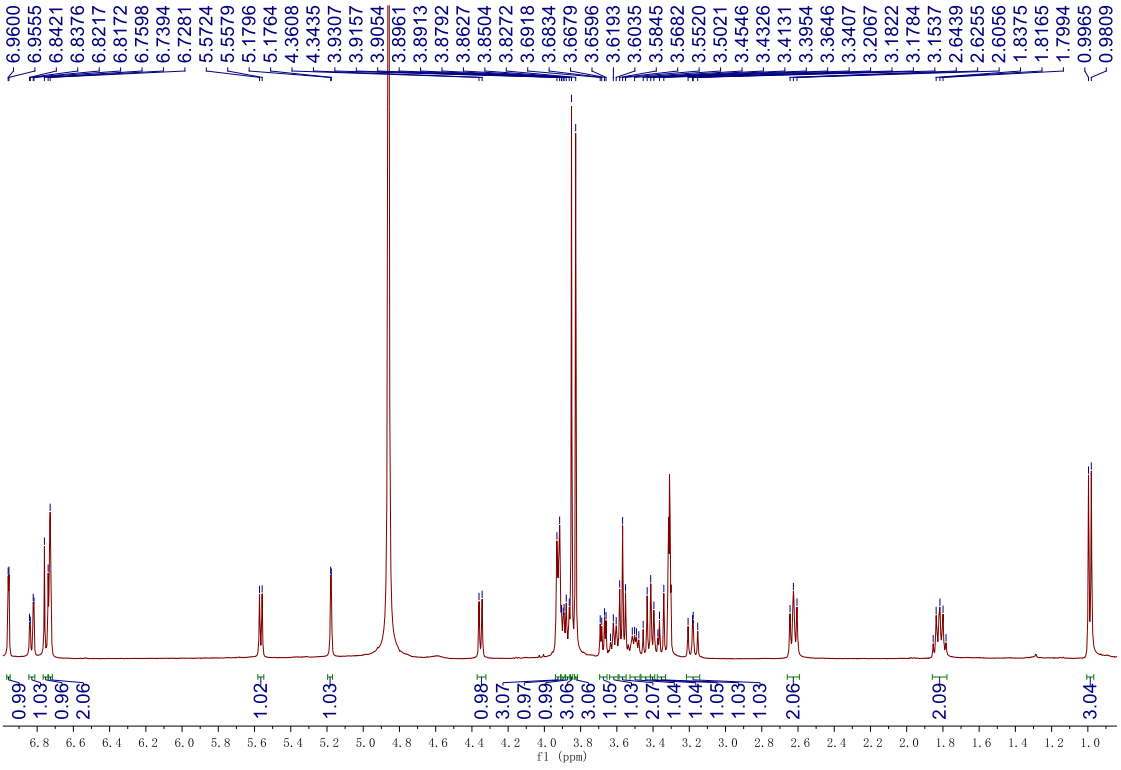


Fig. S2 ^{1}H NMR spectrum of compound 1

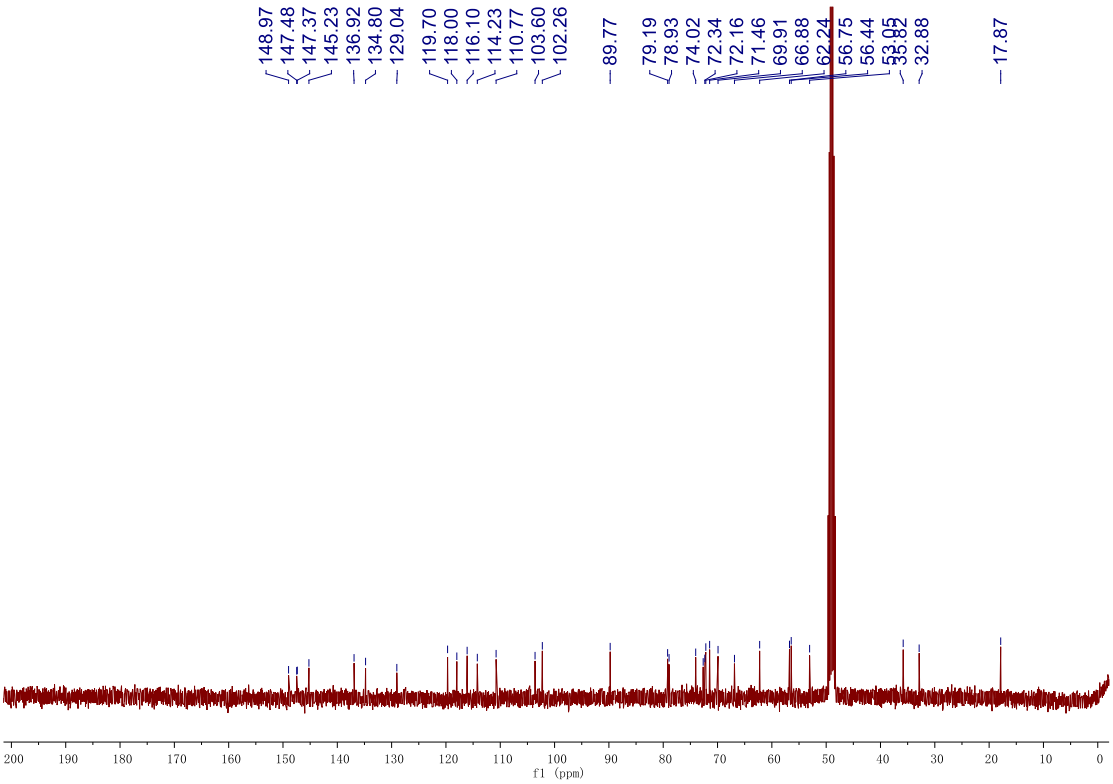


Fig. S3 ^{13}C NMR spectrum of compound 1

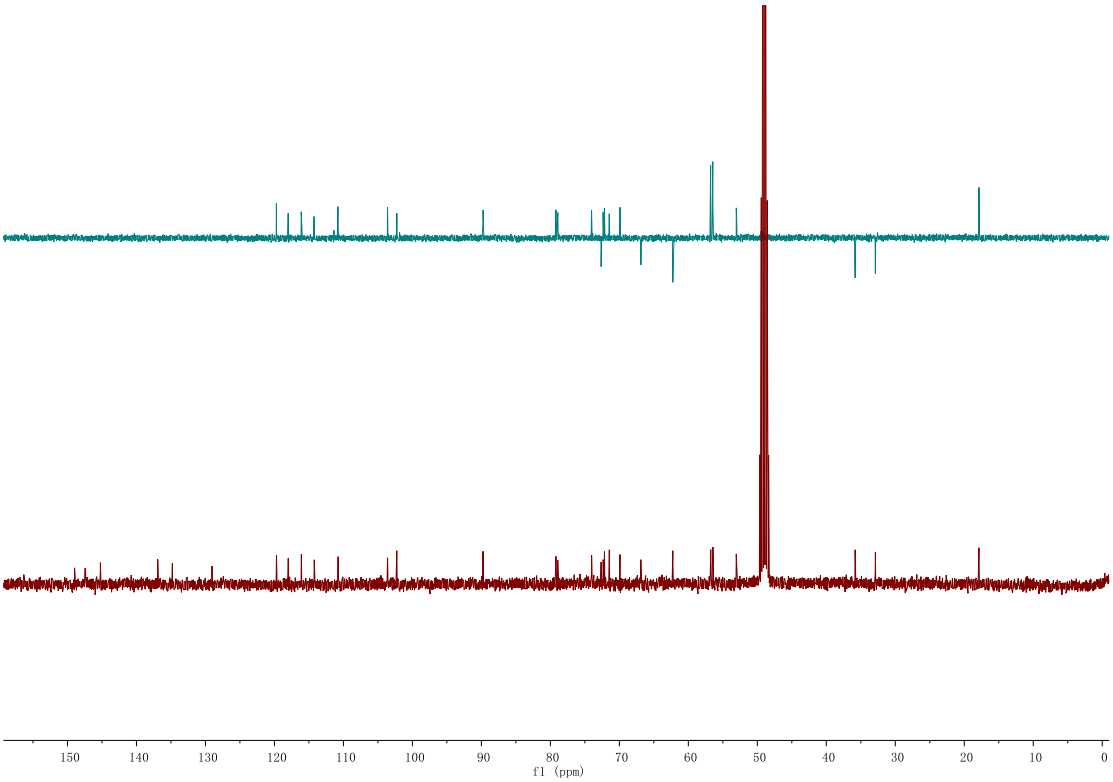


Fig. S4 ^{13}C-NMR and DEPT 135 spectra of compound 1

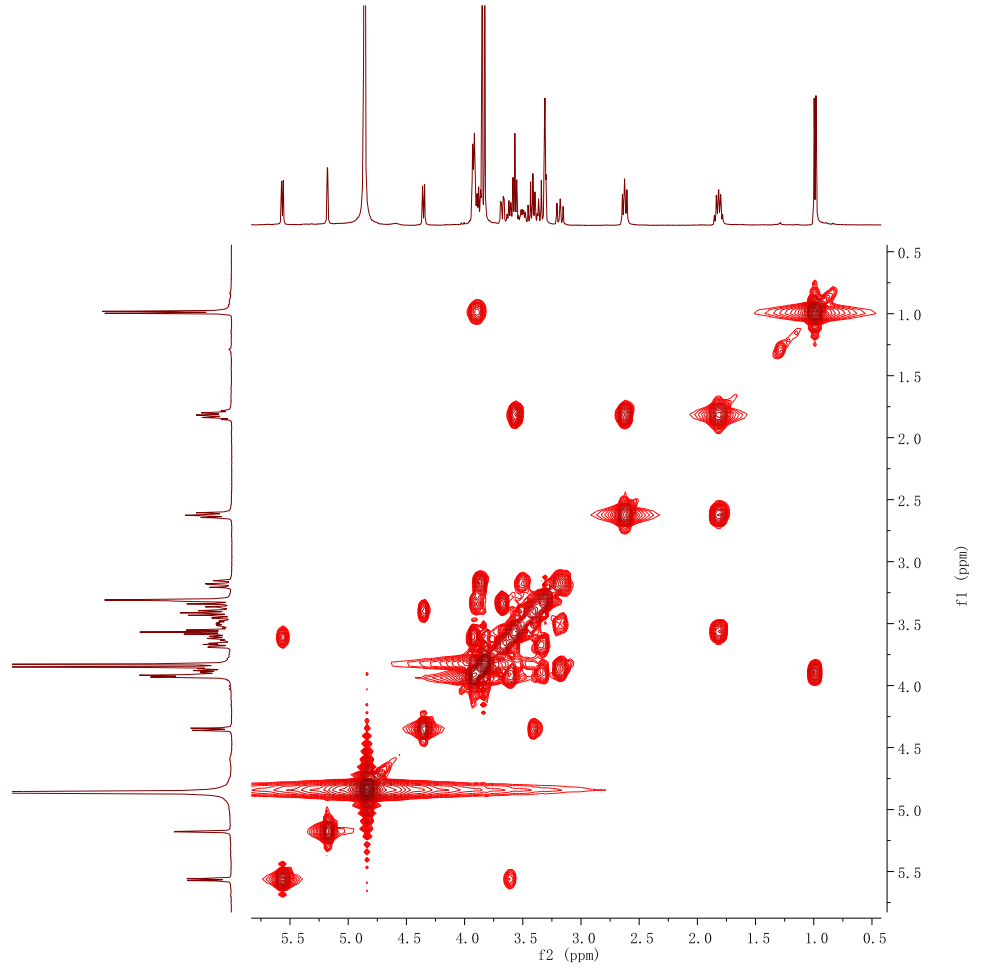


Fig. S5 ^{1}H-^{1}H COSY spectrum of compound 1

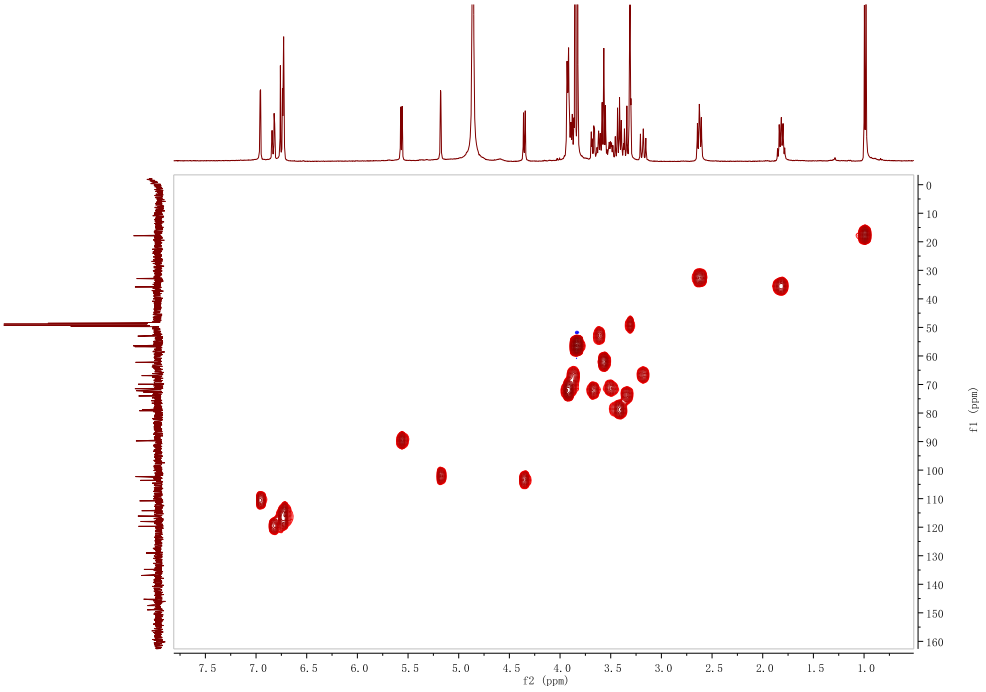


Fig. S6 HSQC spectrum of compound 1

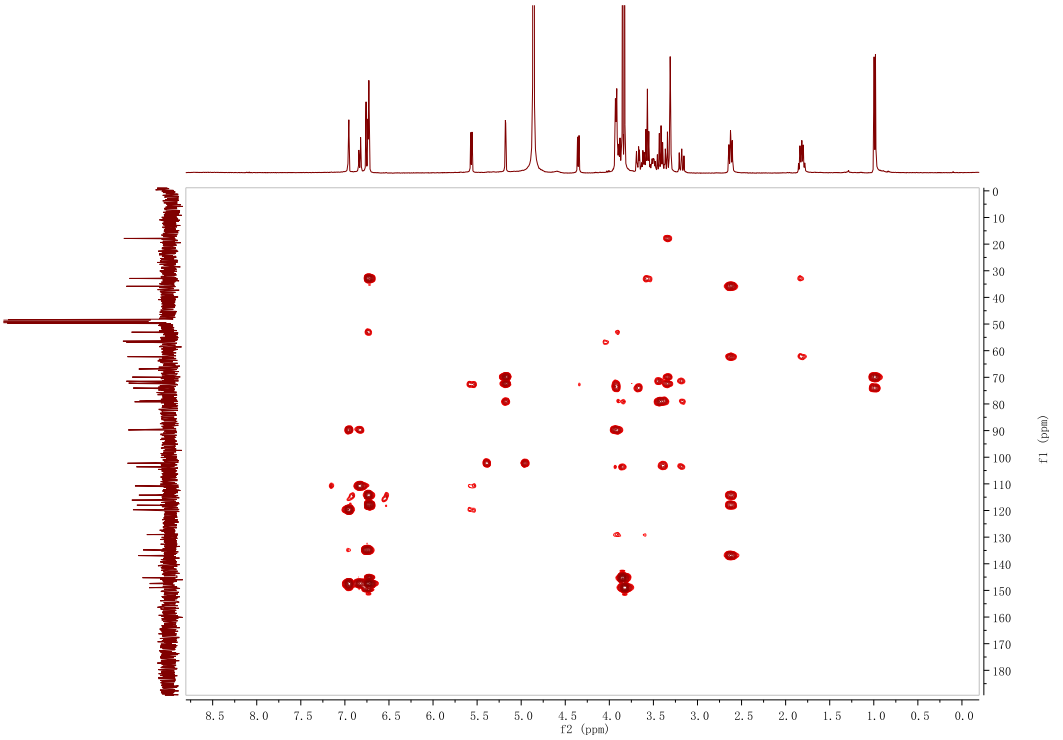


Fig. S7 HMBC spectrum of compound 1

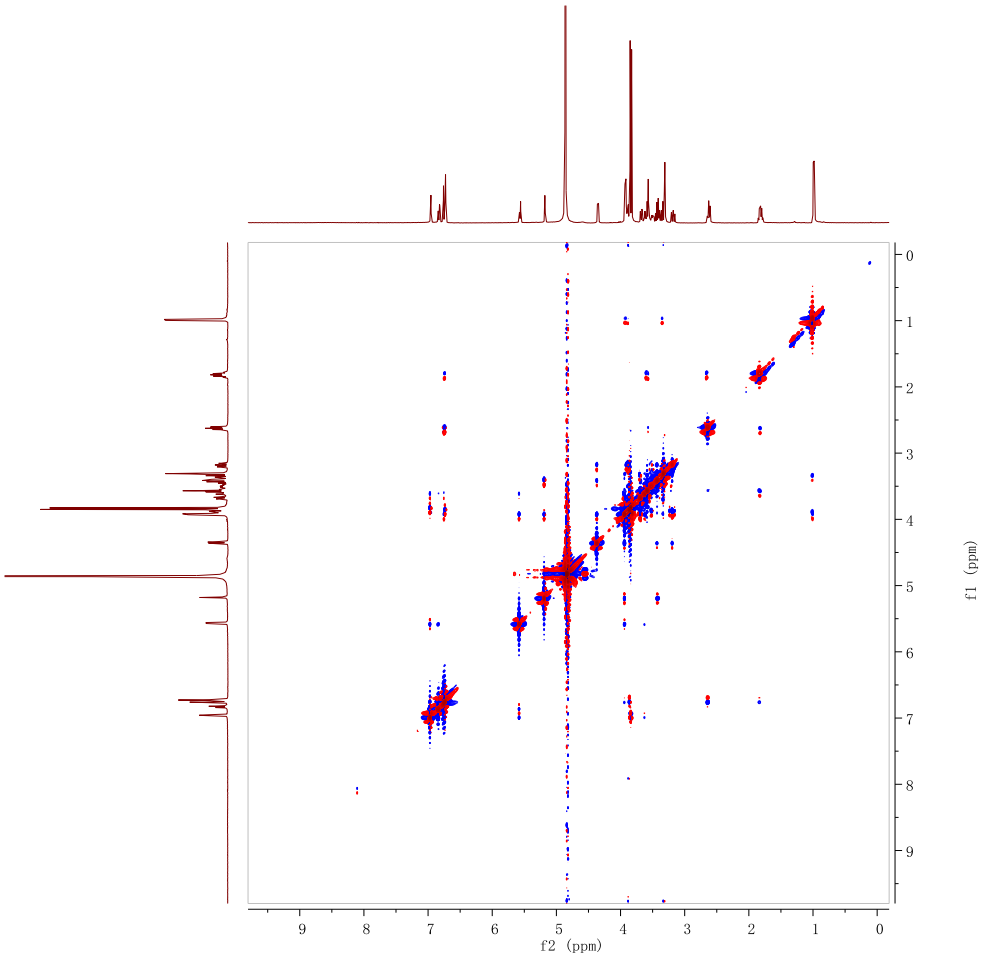


Fig. S8 NOESY spectrum of compound 1

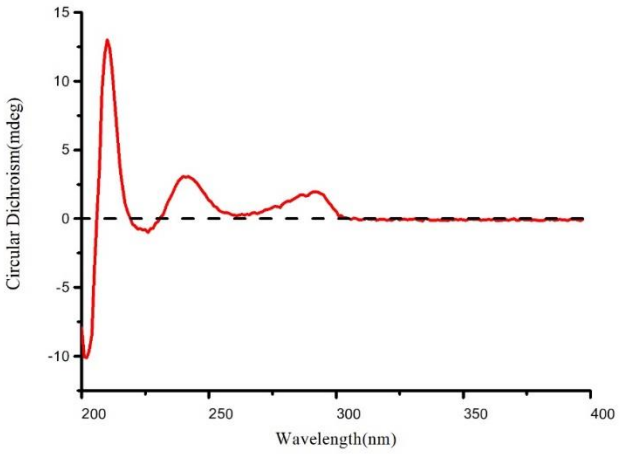


Fig. S9 Experimental CD spectrum of compound 1

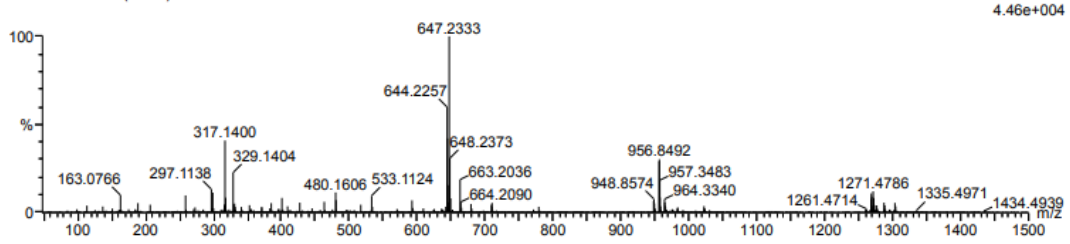
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
392 formula(e) evaluated with 3 results within limits (up to 60 closest results for each mass)
Elements Used:
C: 0-70 H: 0-200 O: 0-40 Na: 0-1

ID-3L4A1
20200824002 41 (0.341)

1: TOF MS ES+
4.46e+004



Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Conf(%)	Formula
647.2333	647.2340	-0.7	-1.1	13.5	264.8	12.91	C32 H39 O14
	647.2316	1.7	2.6	10.5	262.9	87.08	C30 H40 O14 Na
	647.2351	-1.8	-2.8	32.5	271.9	0.01	C48 H32 O Na

Fig. S10 HR-ESI-MS spectrum of compound 2

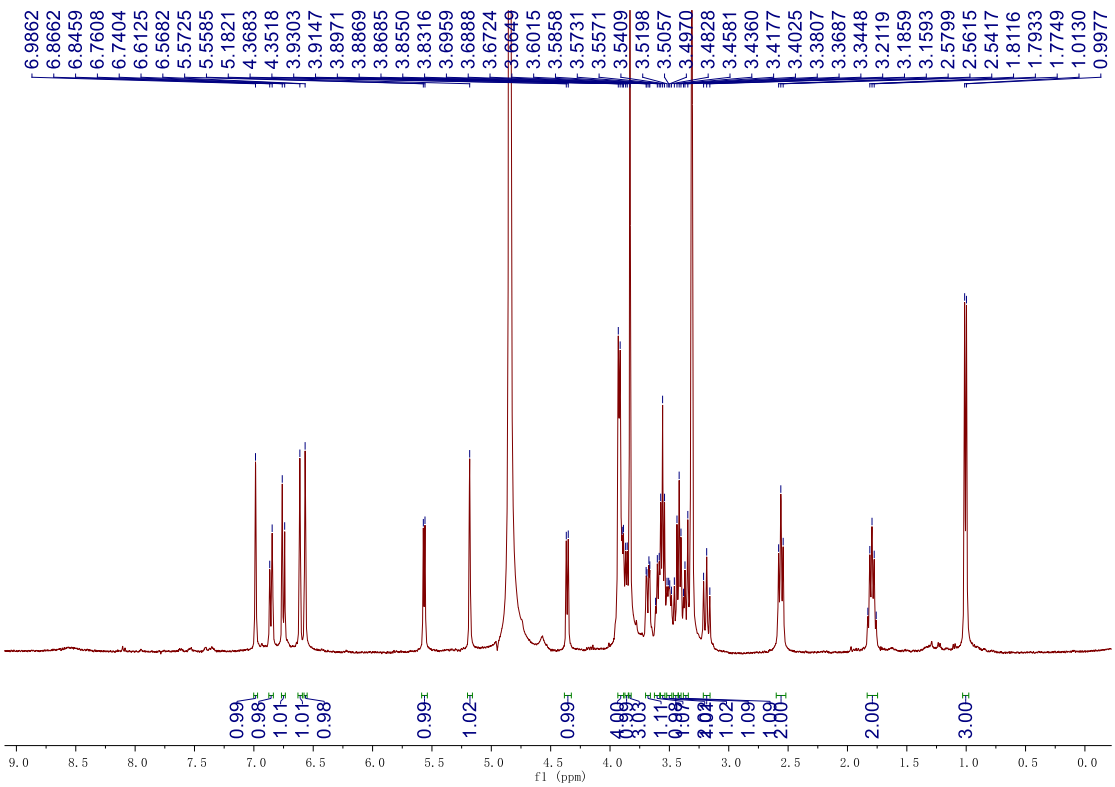


Fig. S11 ^{1}H NMR spectrum of compound 2

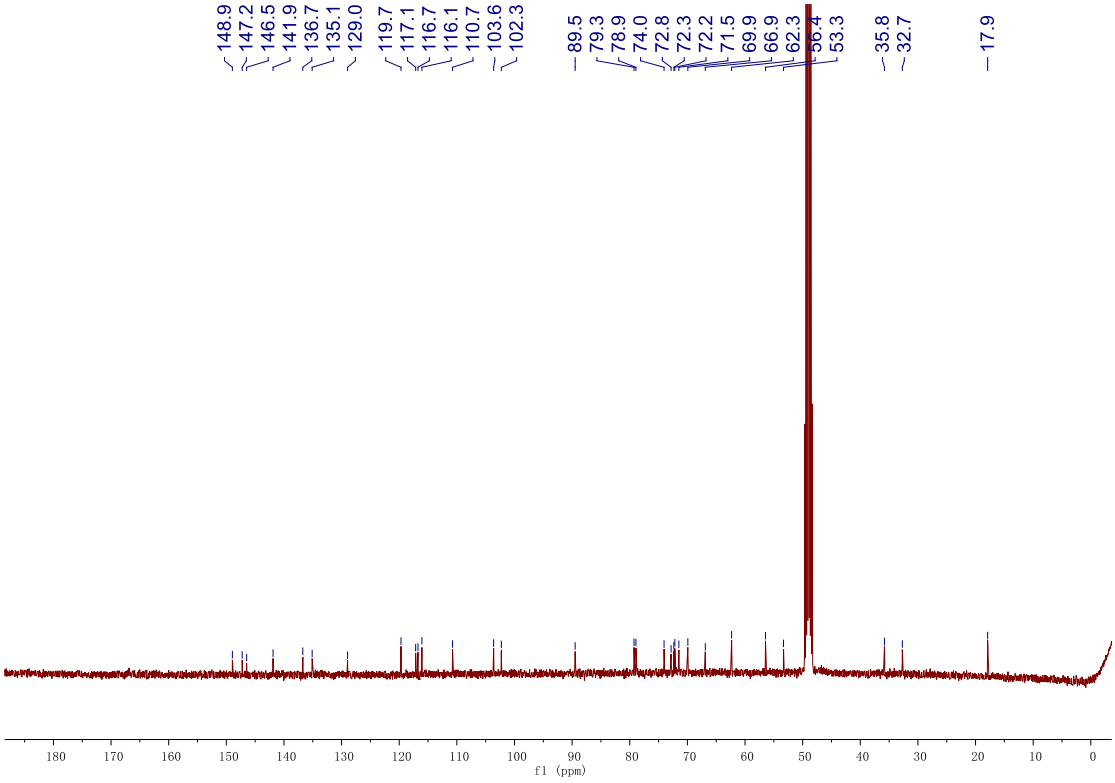


Fig. S12 ^{13}C NMR spectrum of compound 2

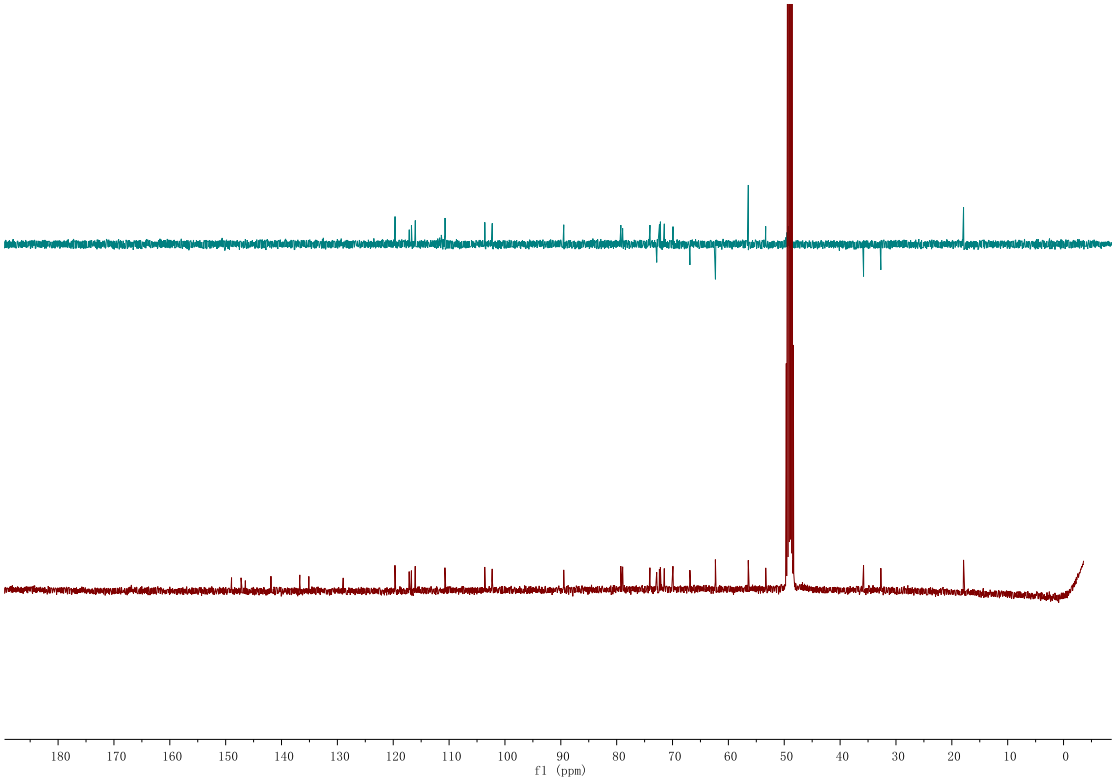


Fig. S13 ^{13}C-NMR and DEPT 135 spectra of compound 2

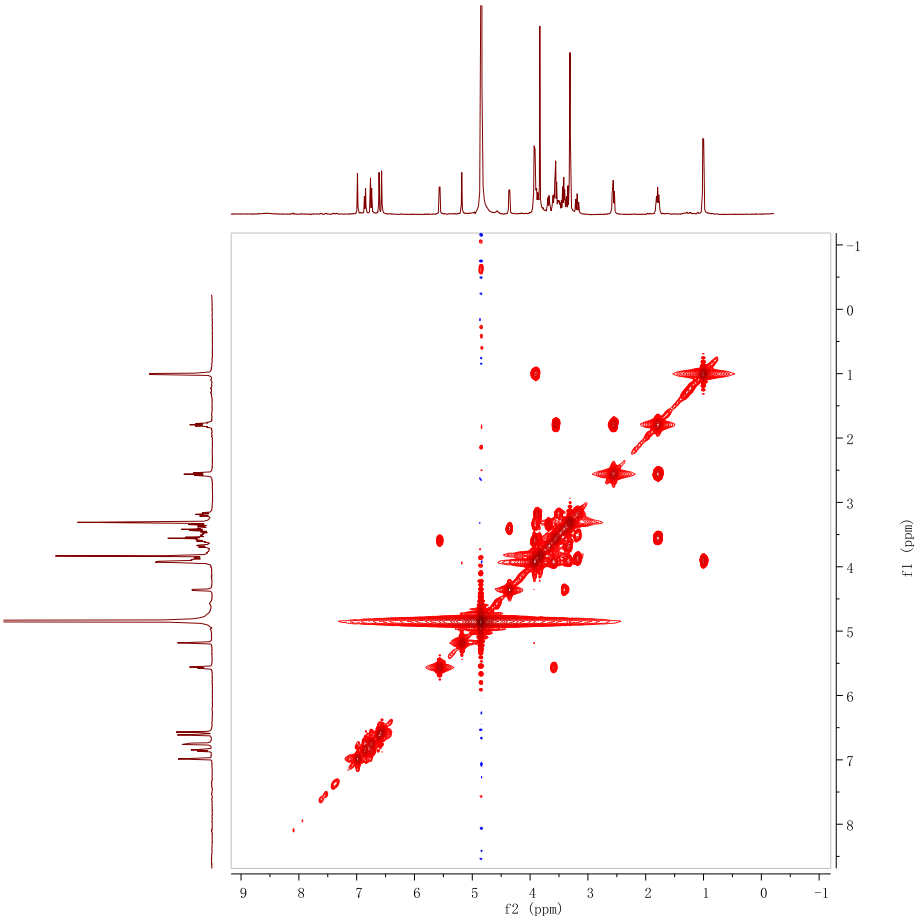


Fig. S14 ^{1}H-^{1}H COSY spectrum of compound 2

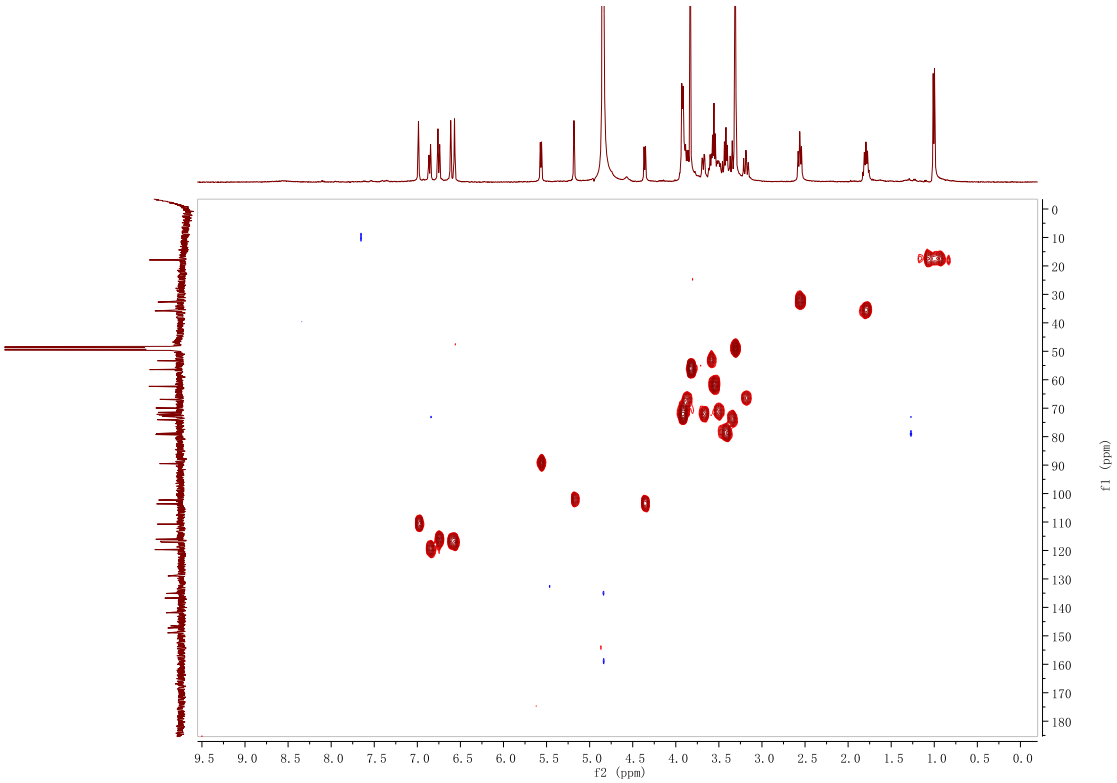


Fig. S15 HSQC spectrum of compound 2

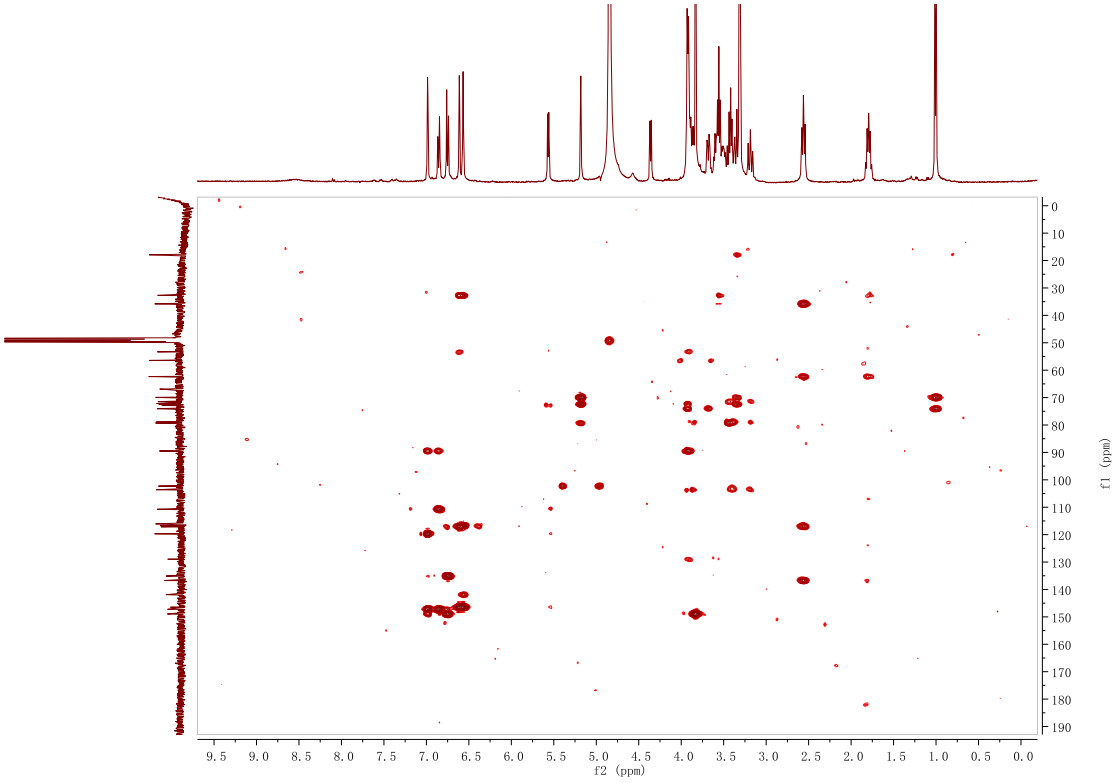


Fig. S16 HMBC spectrum of compound 2

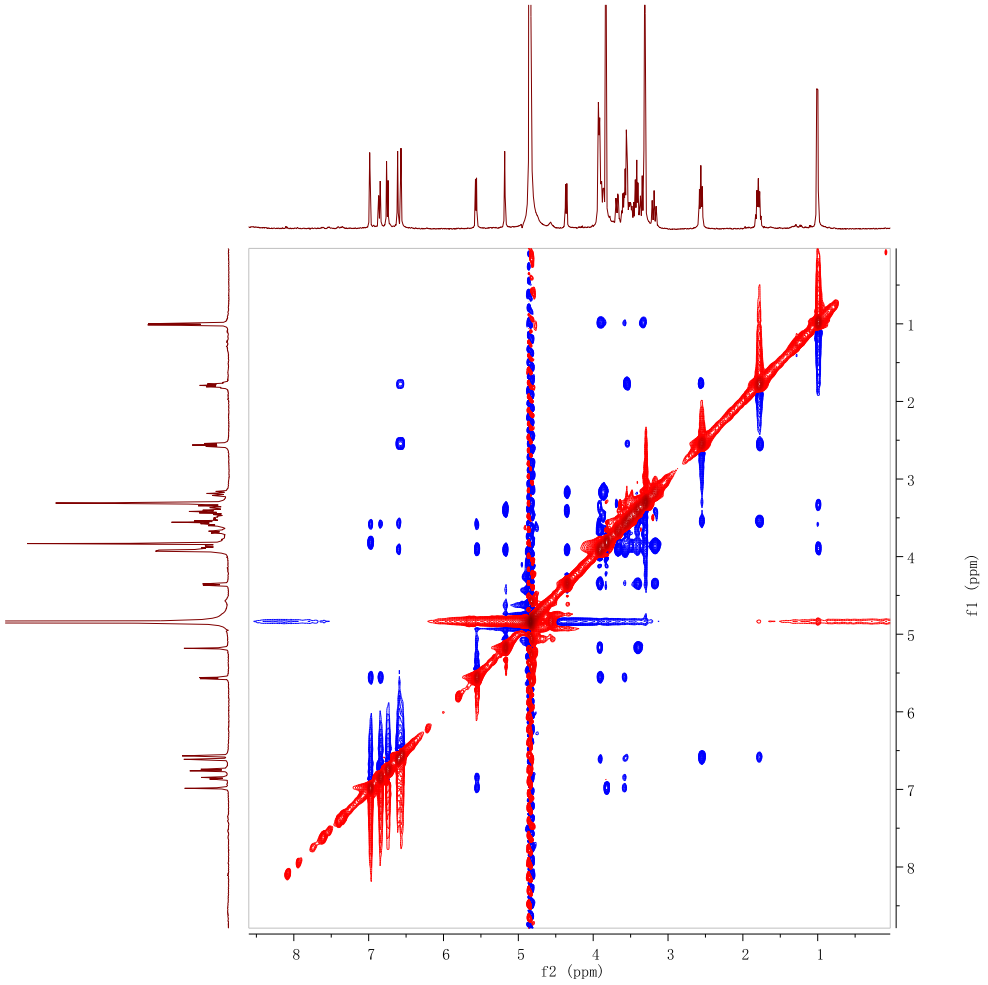


Fig. S17 NOESY spectrum of compound 2

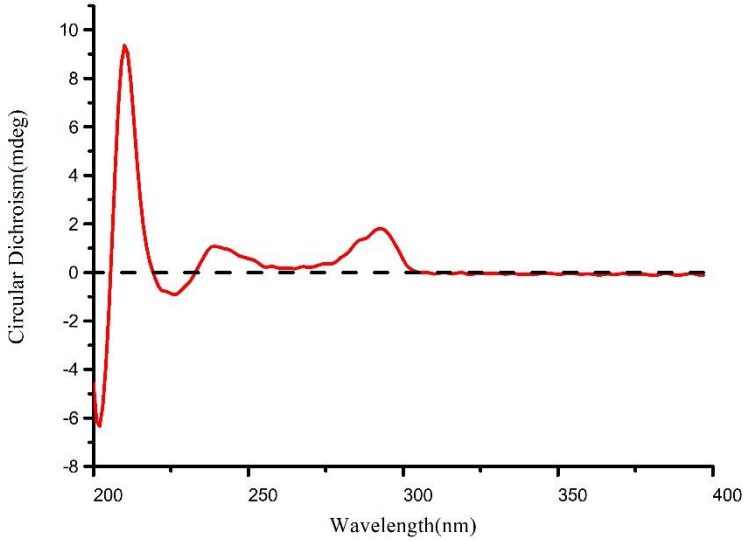
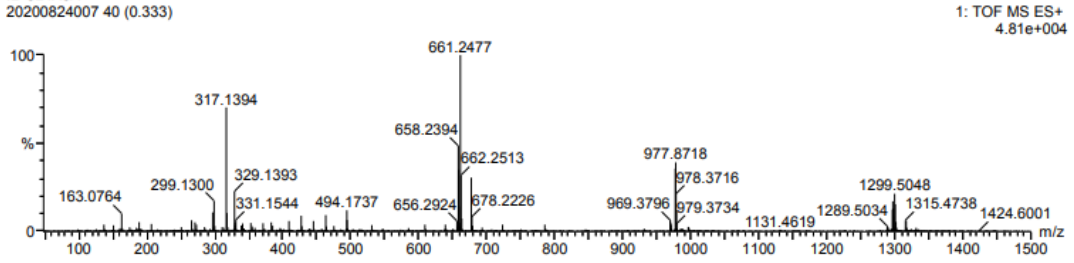


Fig. S18 Experimental CD spectrum of compound 2

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
392 formula(e) evaluated with 3 results within limits (up to 60 closest results for each mass)
Elements Used:
C: 0-70 H: 0-200 O: 0-40 Na: 0-1
ID-3L4A5A
20200824007 40 (0.333)



Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Conf(%)	Formula
661.2477	661.2472	0.5	0.8	10.5	251.3	93.36	C31 H42 O14 Na
	661.2496	-1.9	-2.9	13.5	254.0	6.62	C33 H41 O14
	661.2507	-3.0	-4.5	32.5	260.1	0.01	C49 H34 O Na

Fig. S19 HR-ESI-MS spectrum of compound 3

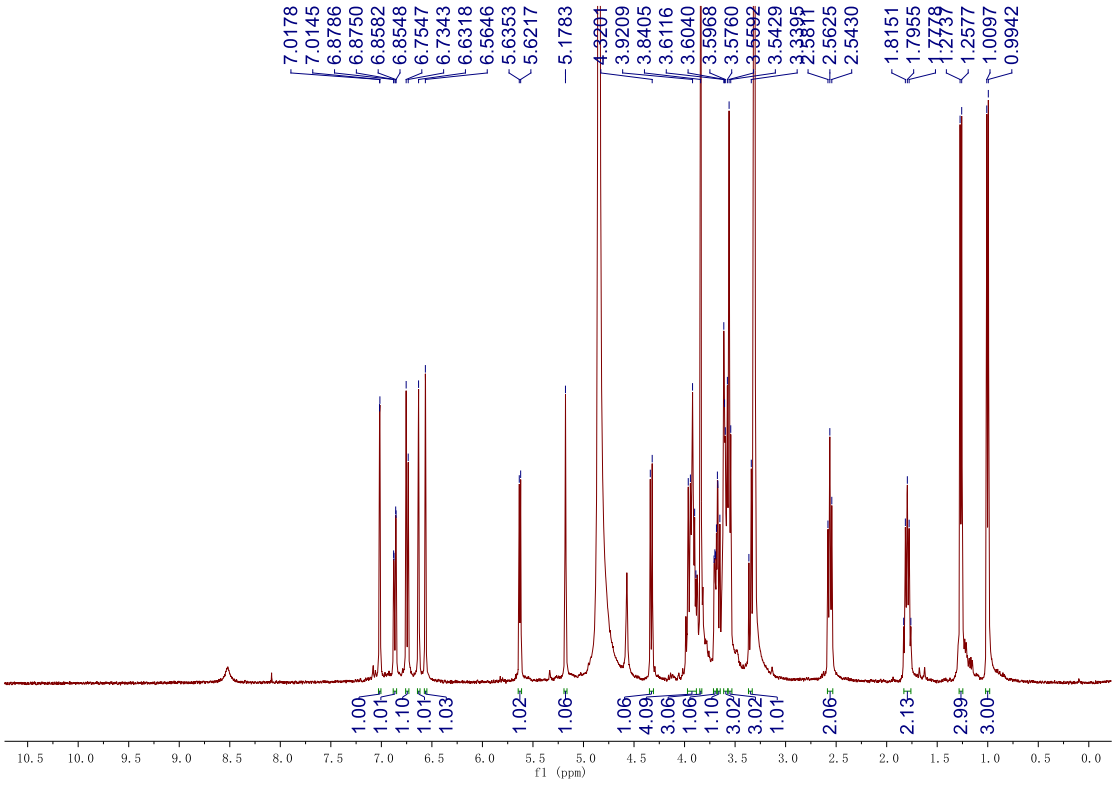


Fig. S20 ^{1}H NMR spectrum of compound 3

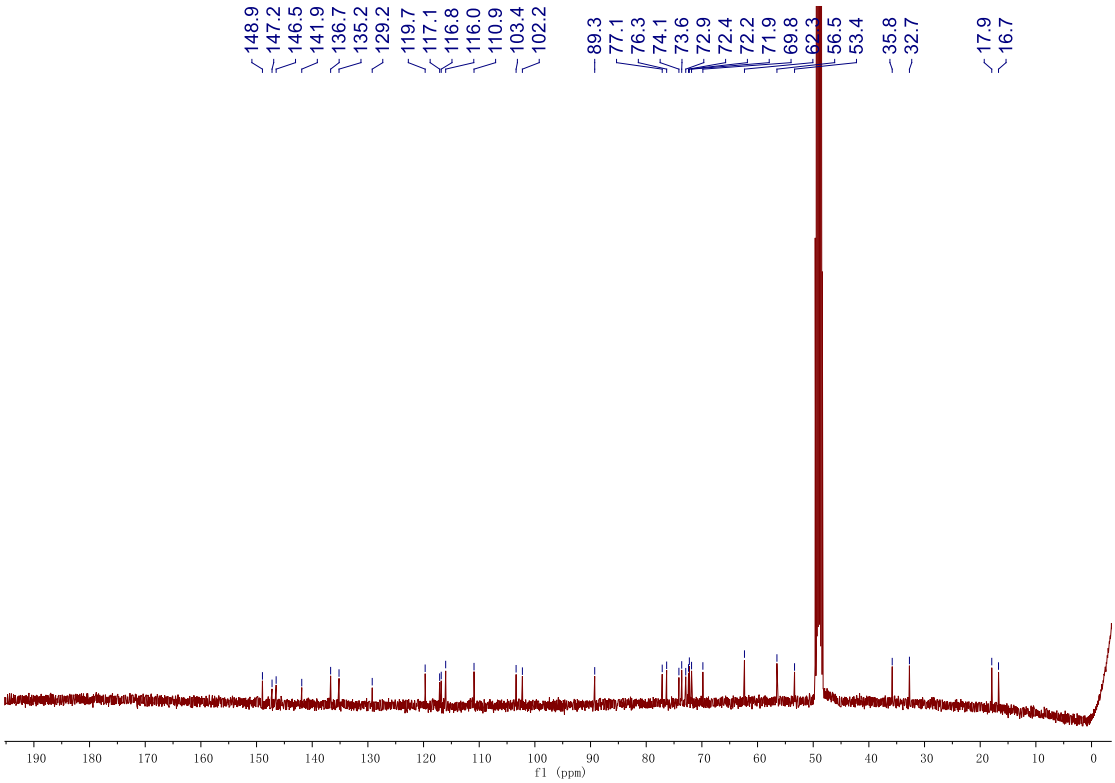


Fig. S21 ^{13}C NMR spectrum of compound 3

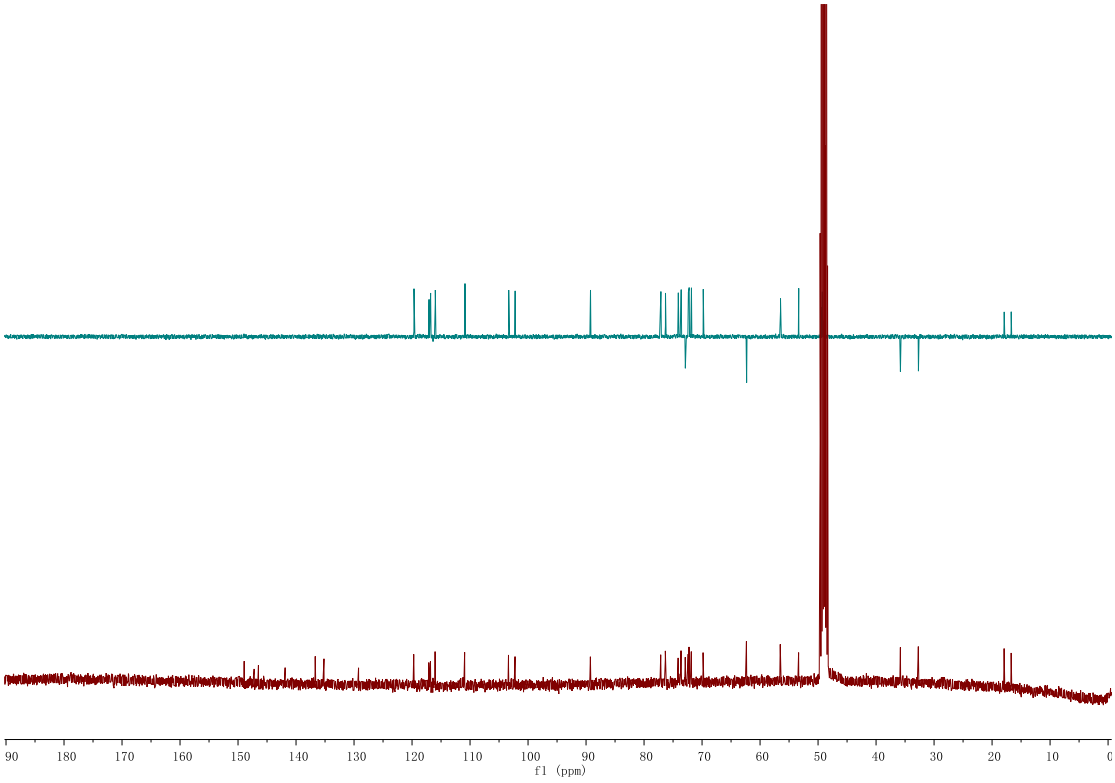


Fig. S22 ^{13}C-NMR and DEPT 135 spectra of compound 3

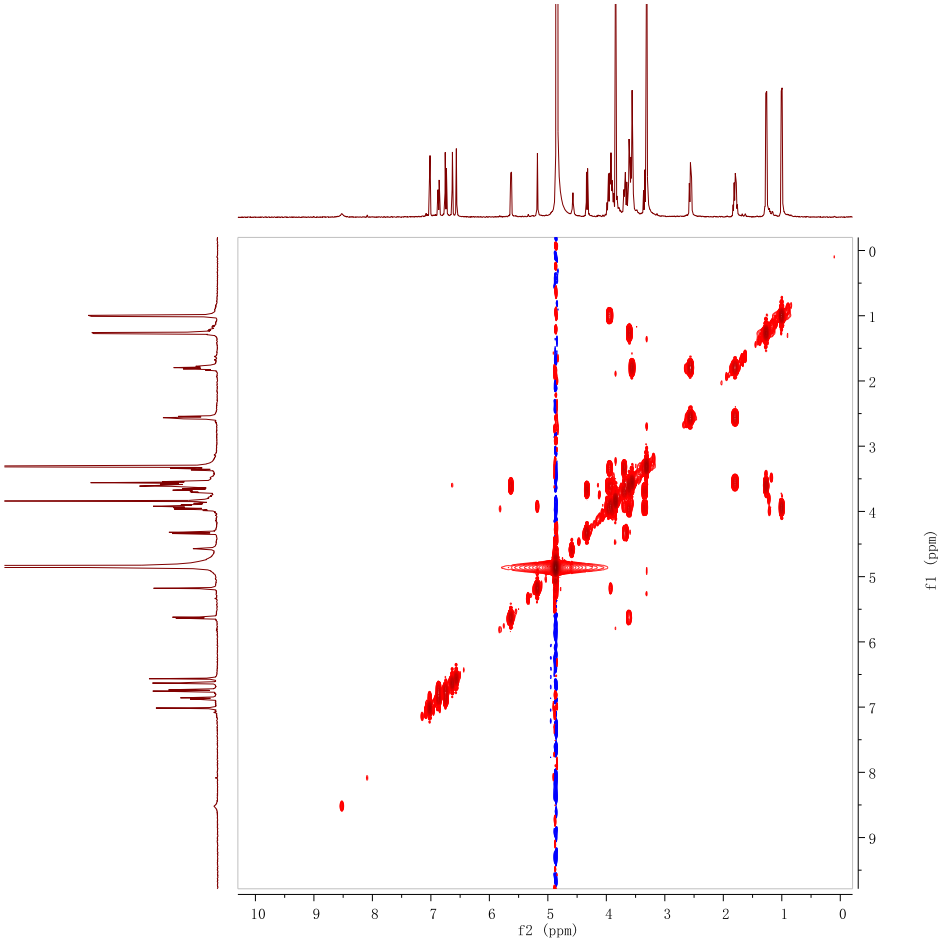


Fig. S23 ^{1}H-^{1}H COSY spectrum of compound 3

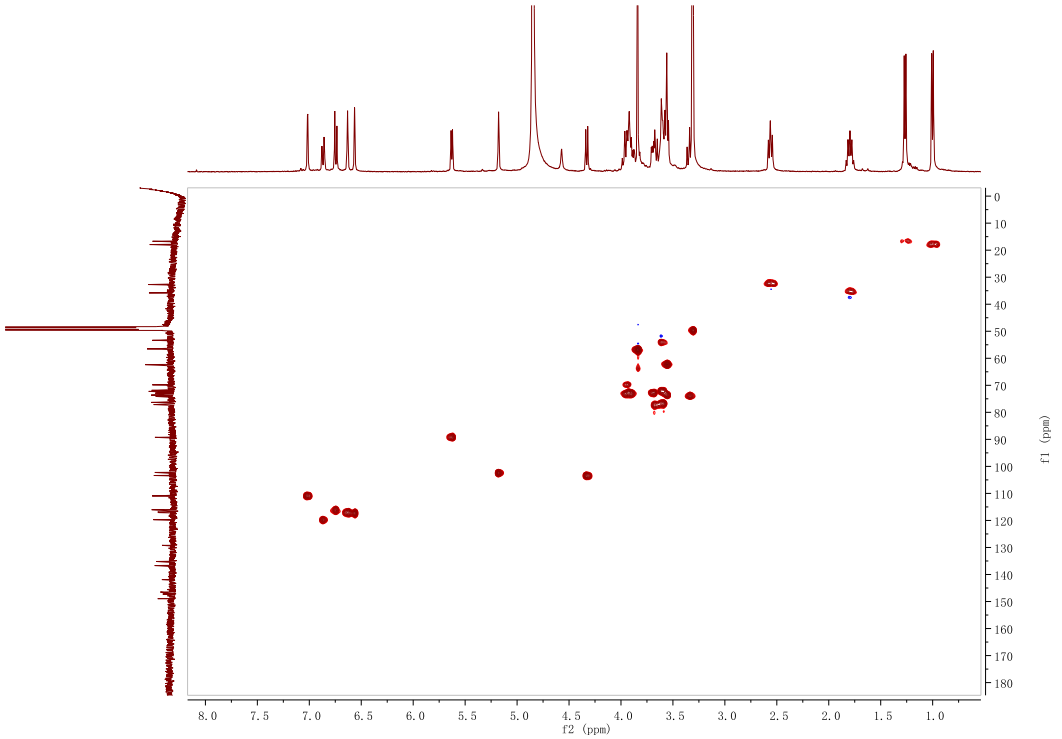


Fig. S24 HSQC spectrum of compound 3

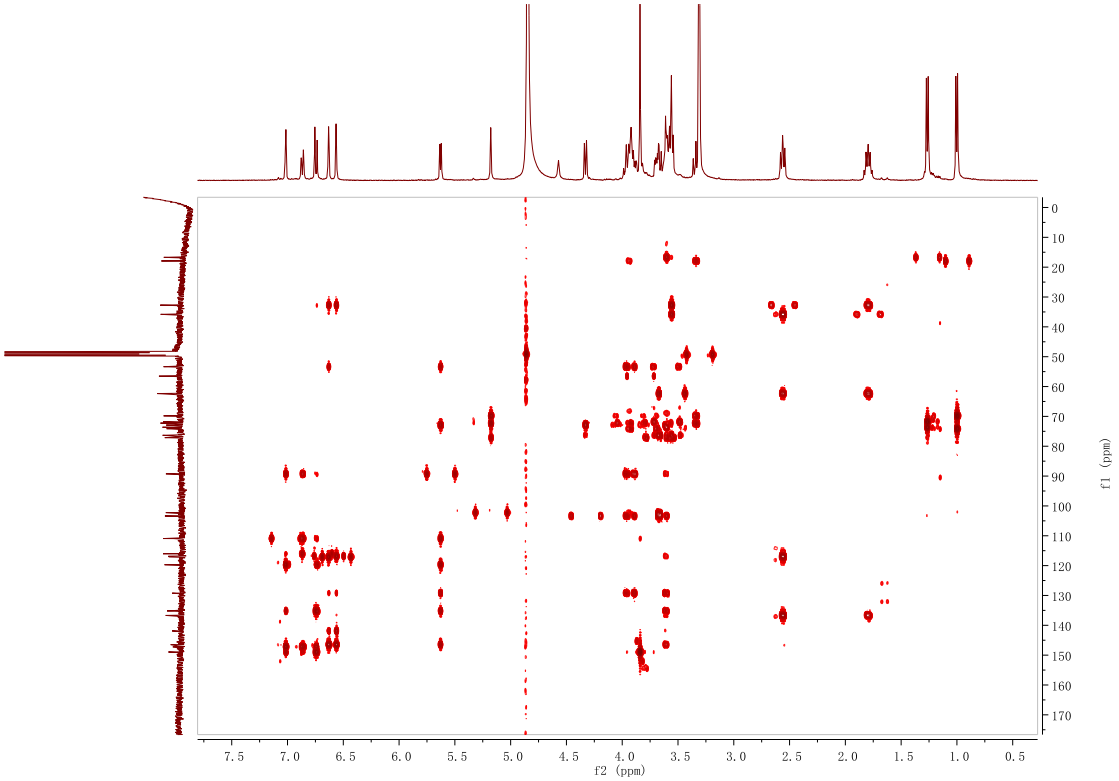


Fig. S25 HMBC spectrum of compound 3

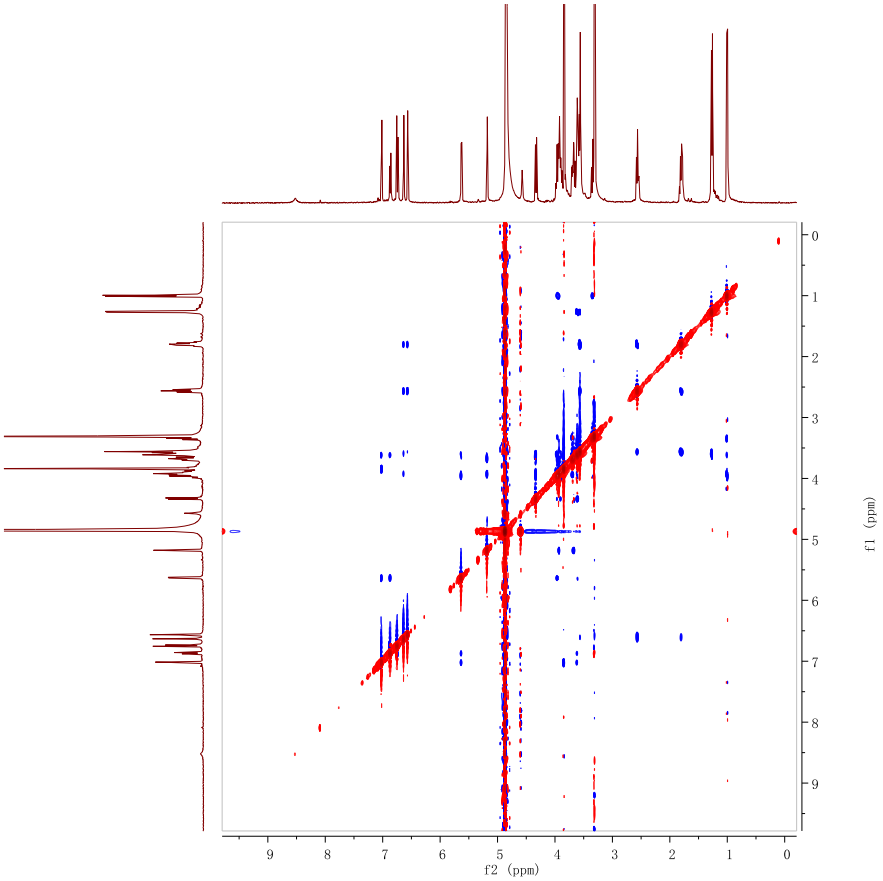


Fig. S26 NOESY spectrum of compound 3

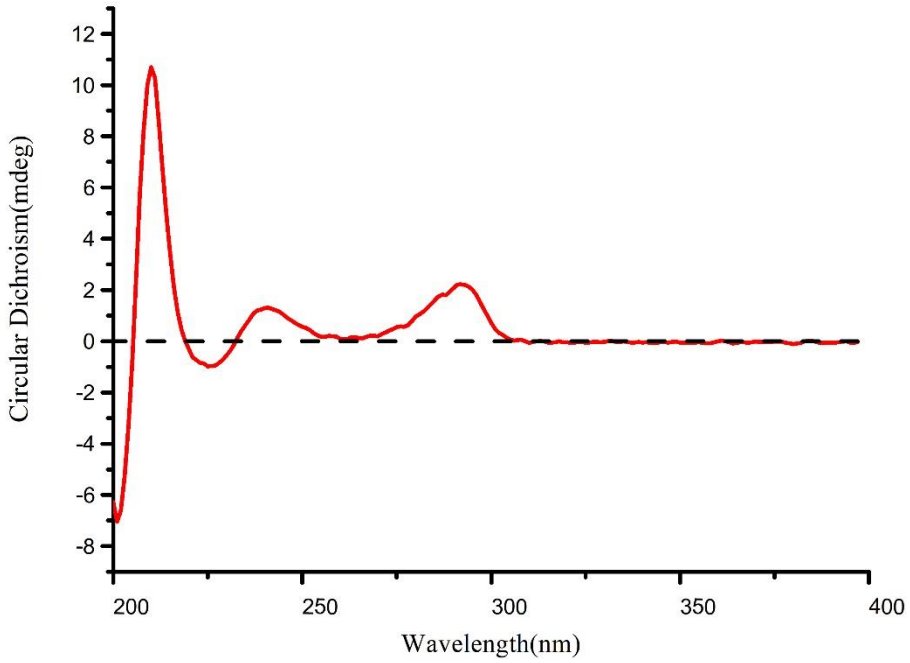


Fig. S27 Experimental CD spectrum of compound 3

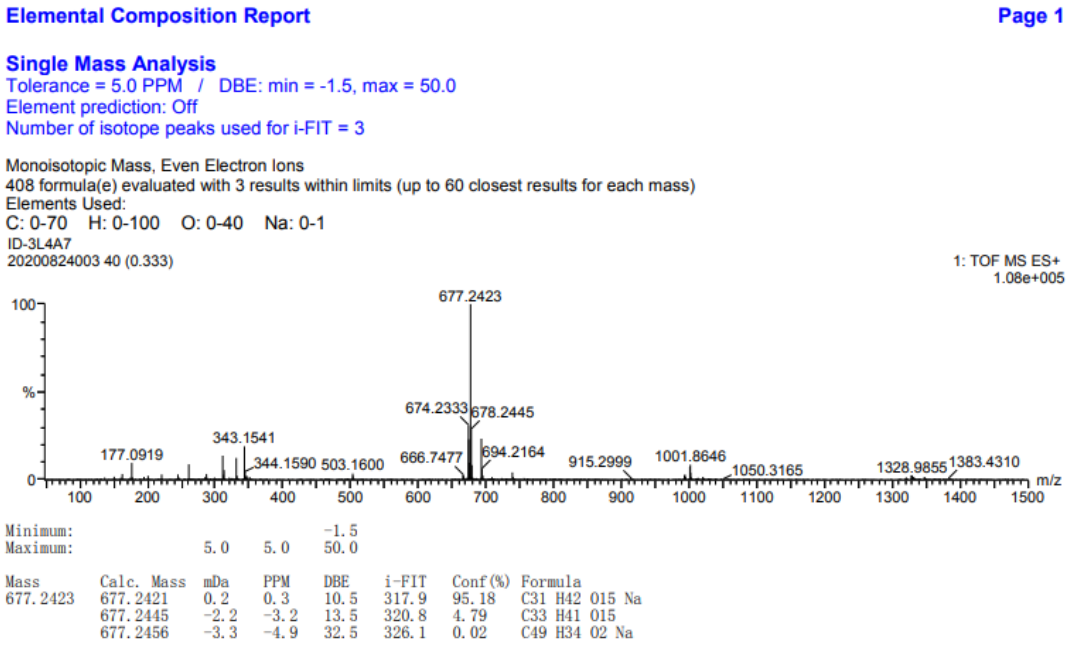


Fig. S28 HR-ESI-MS spectrum of compound 4

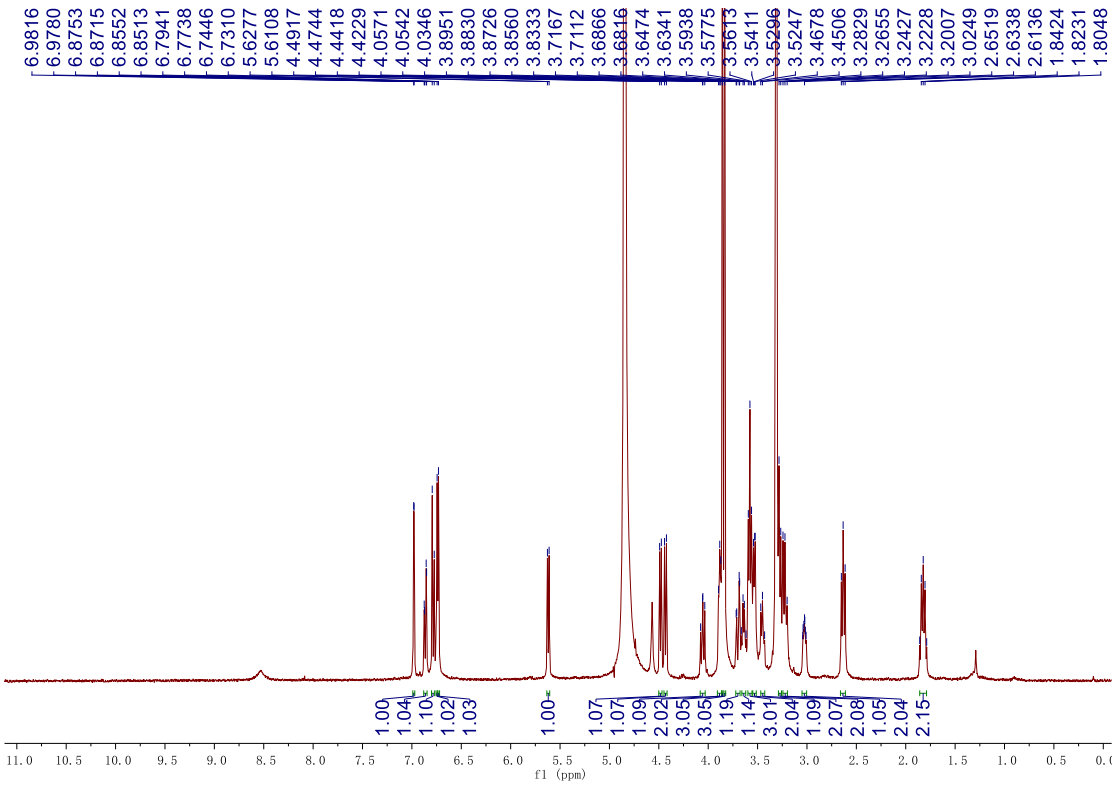


Fig. S29 ^{1}H NMR spectrum of compound 4

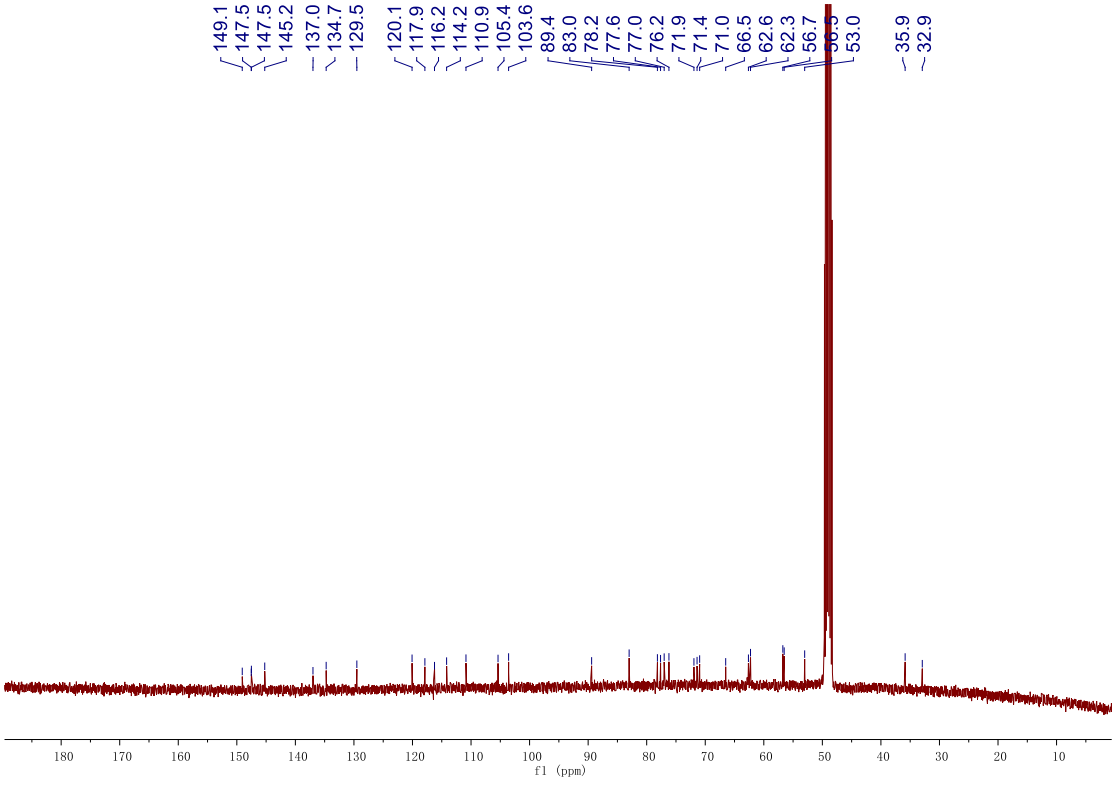


Fig. S30 ^{13}C NMR spectrum of compound 4

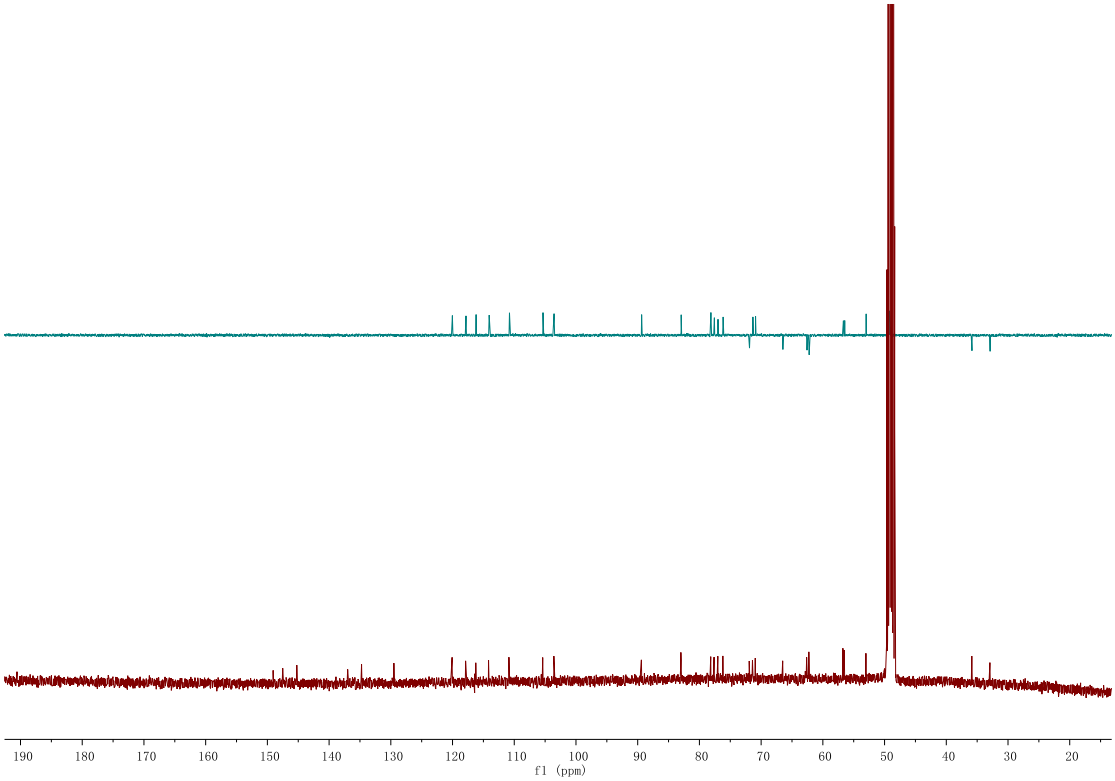


Fig. S31 ^{13}C-NMR and DEPT 135 spectra of compound 4

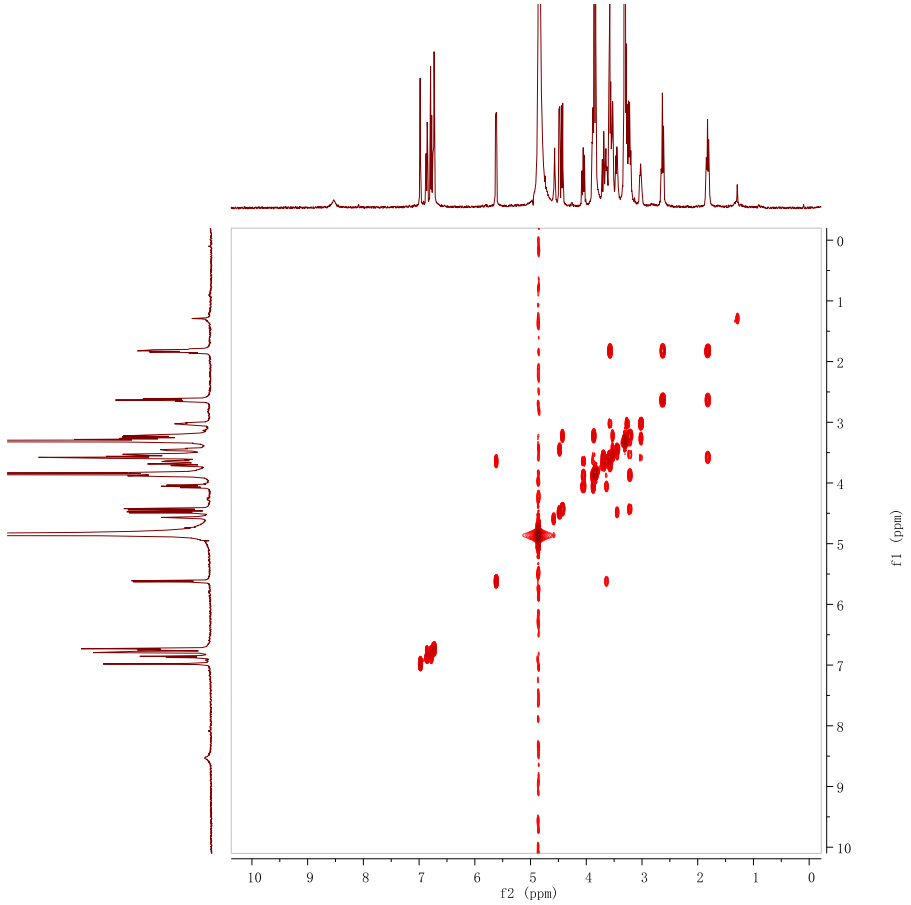


Fig. S32 ^{1}H-^{1}H COSY spectrum of compound 4

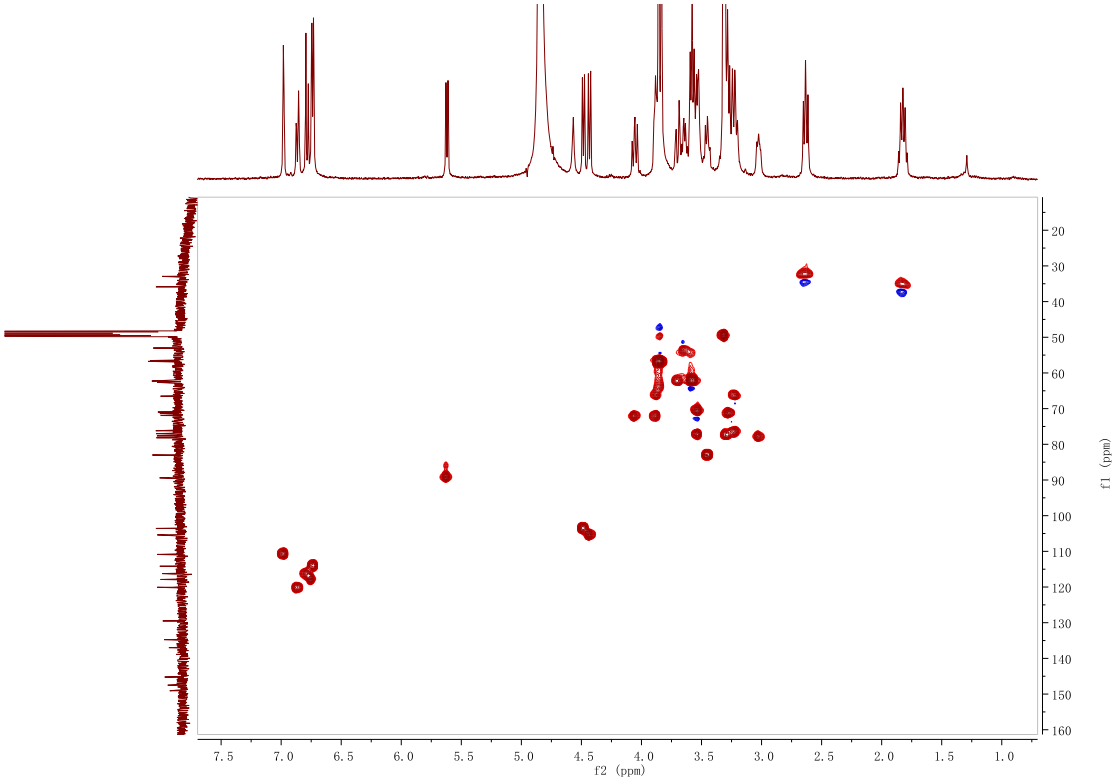


Fig. S33 HSQC spectrum of compound 4

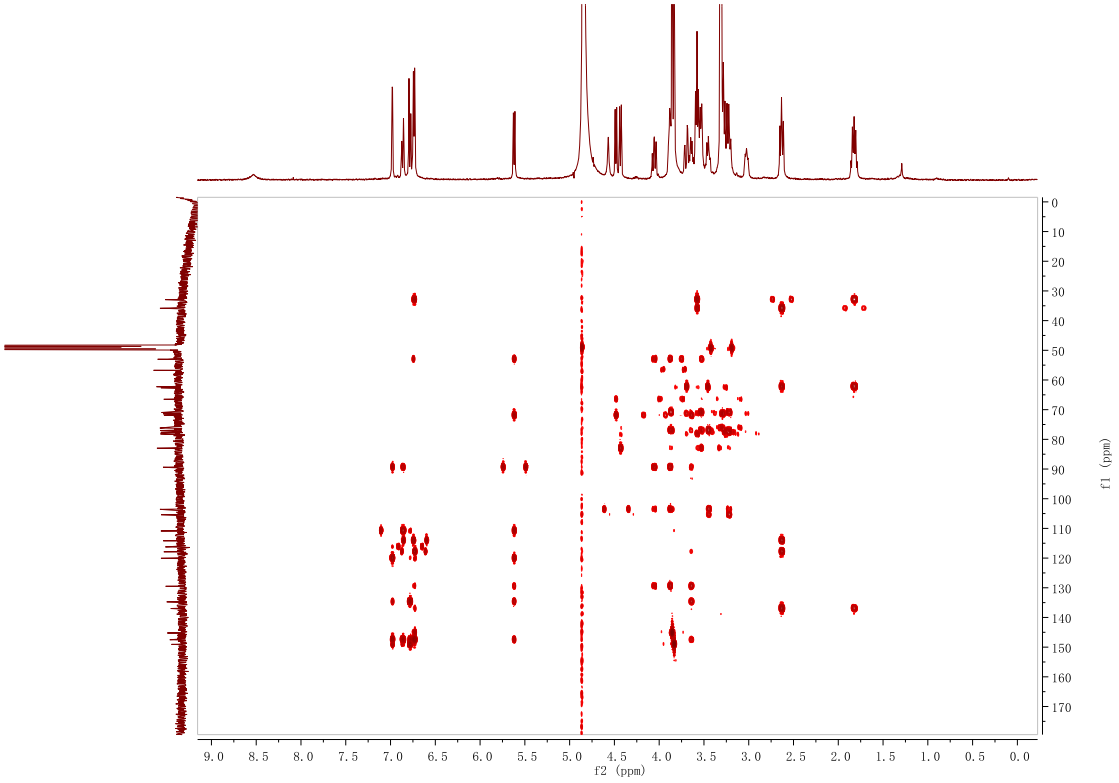


Fig. S34 HMBC spectrum of compound 4

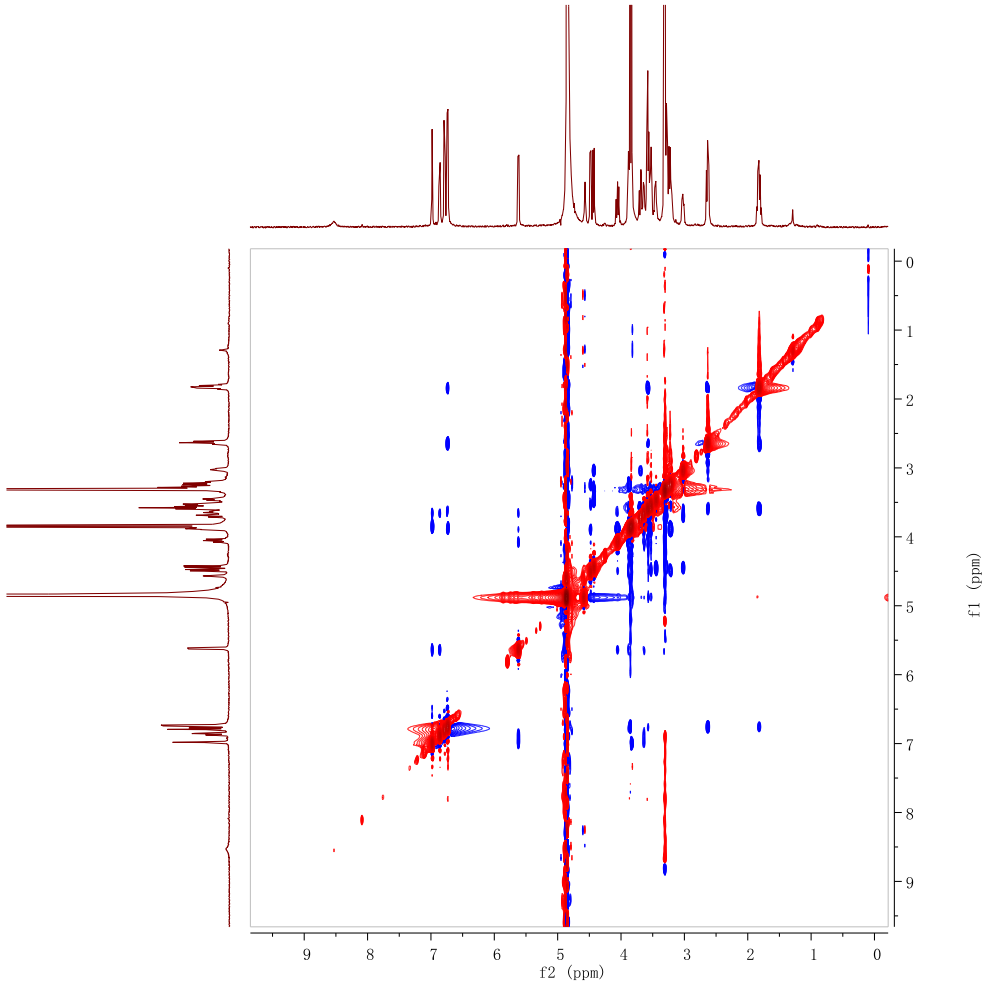


Fig. S35 NOESY spectrum of compound 4

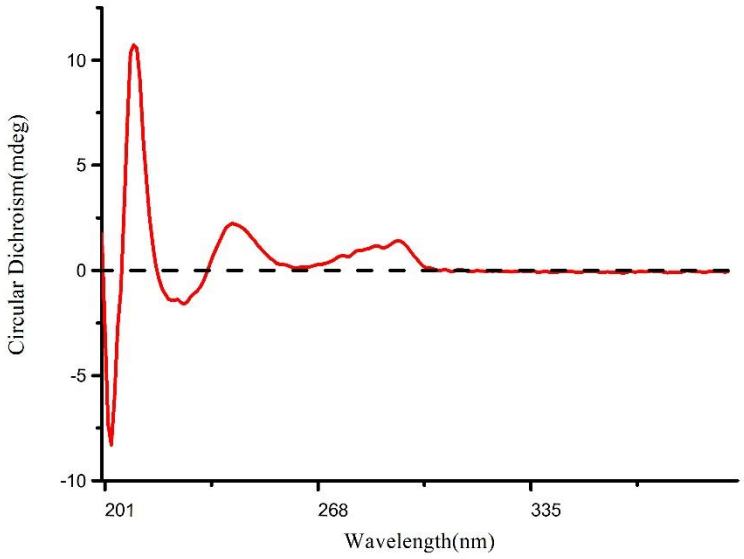


Fig. S36 Experimental CD spectrum of compound 4

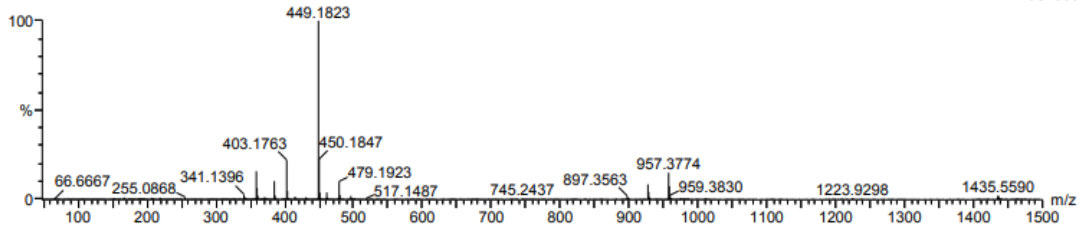
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
229 formula(e) evaluated with 1 results within limits (up to 60 closest results for each mass)
Elements Used:
C: 0-70 H: 0-200 O: 0-40 Na: 0-1

ID-3L4A8
2020081720 74 (0.610)

1: TOF MS ES+
1.19e+006



Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Conf(%)	Formula
479.1923	479.1917	0.6	1.3	9.5	386.4	n/a	C24 H31 O10

Fig. S37 HR-ESI-MS spectrum of compound 5

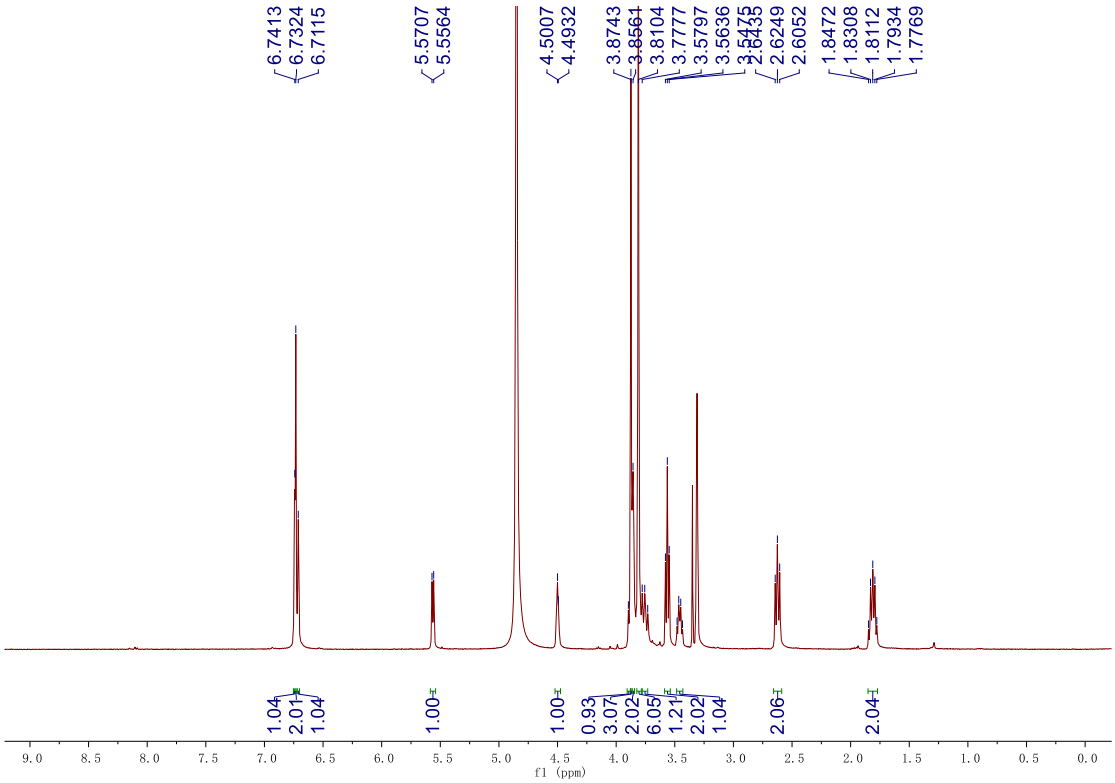


Fig. S38 ^{1}H NMR spectrum of compound 5

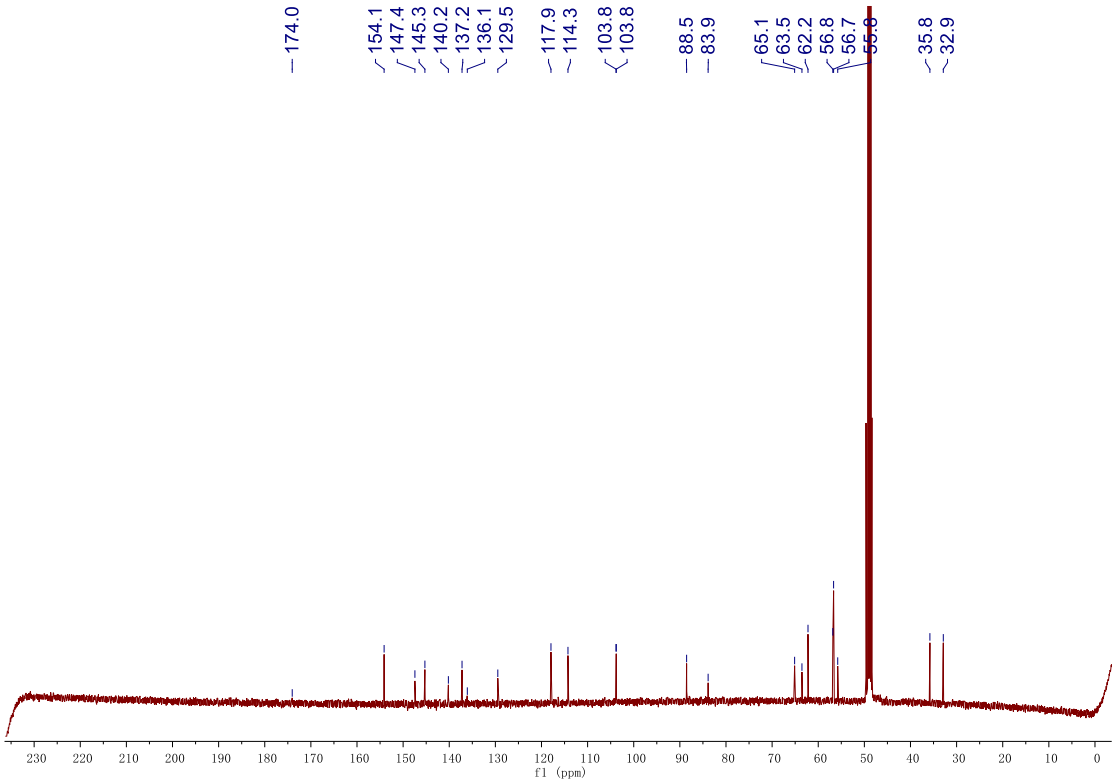


Fig. S39 ^{13}C NMR spectrum of compound 5

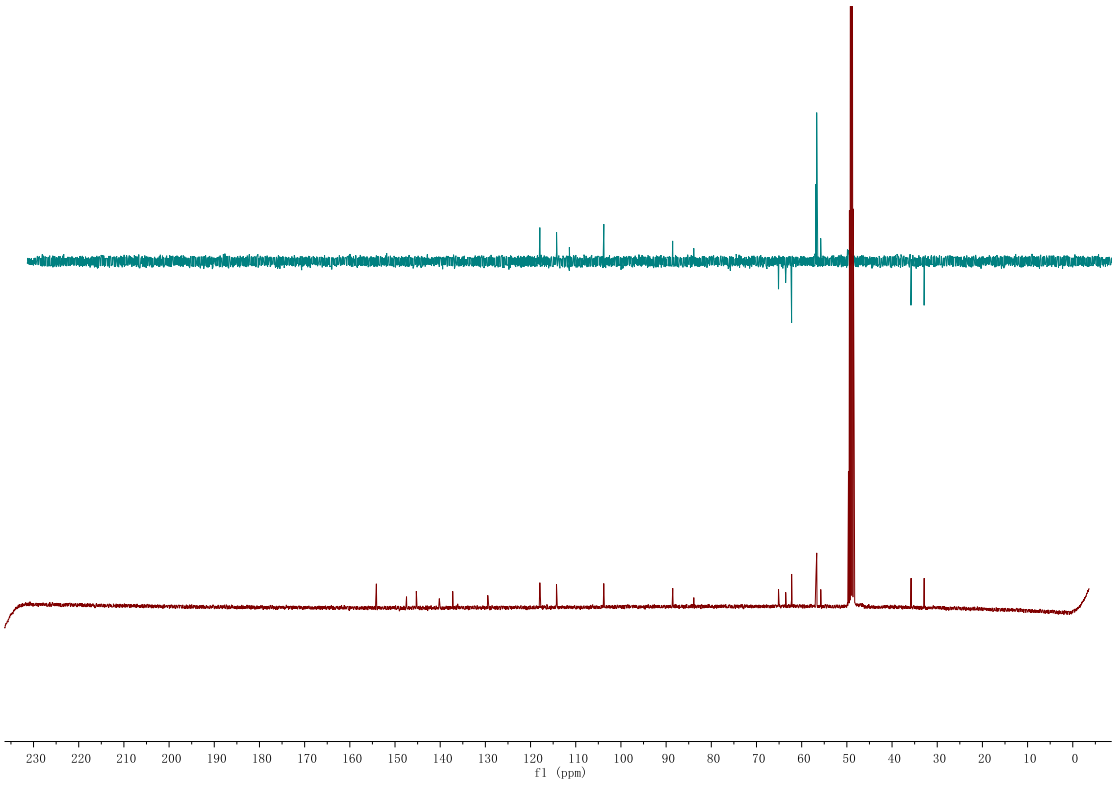


Fig. S40 ^{13}C-NMR and DEPT 135 spectra of compound 5

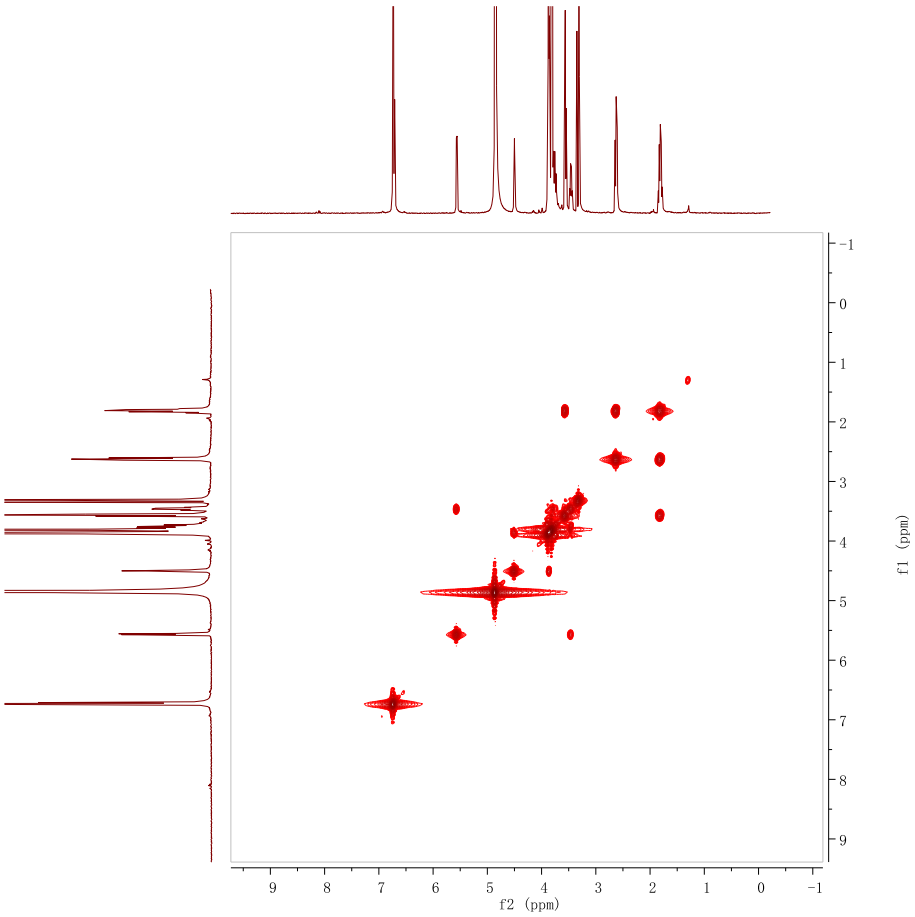


Fig. S41 ^{1}H-^{1}H COSY spectrum of compound 5

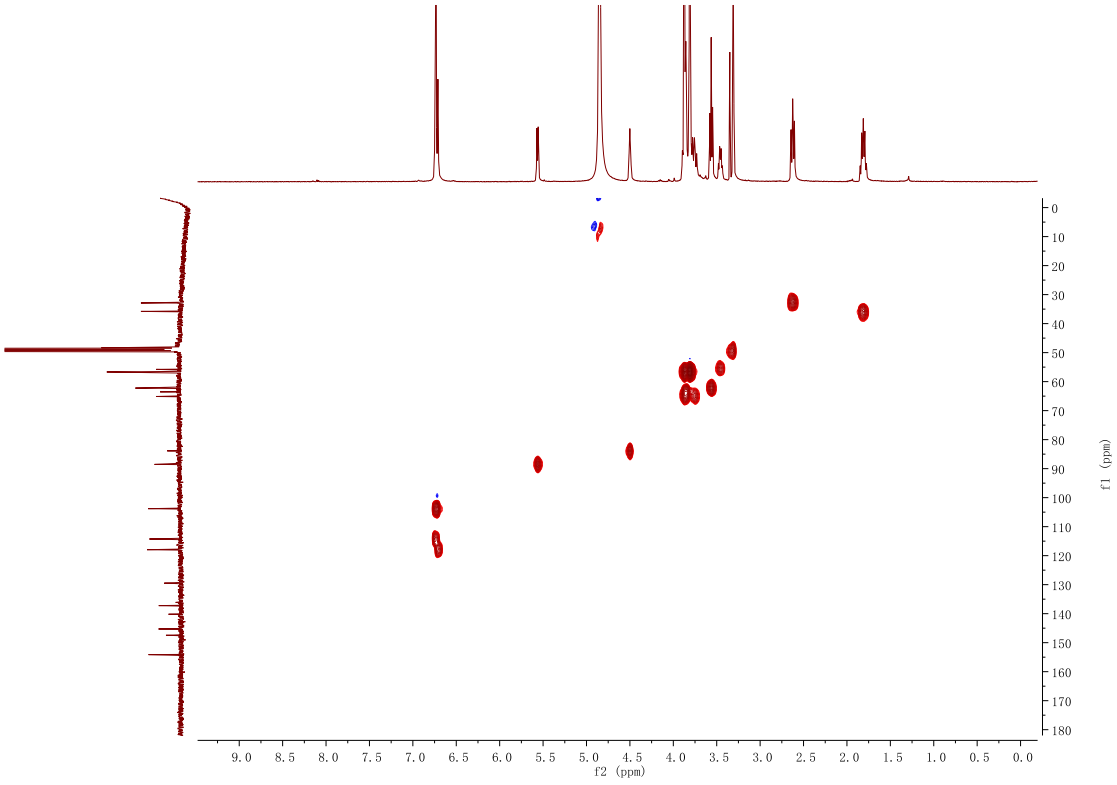


Fig. S42 HSQC spectrum of compound 5

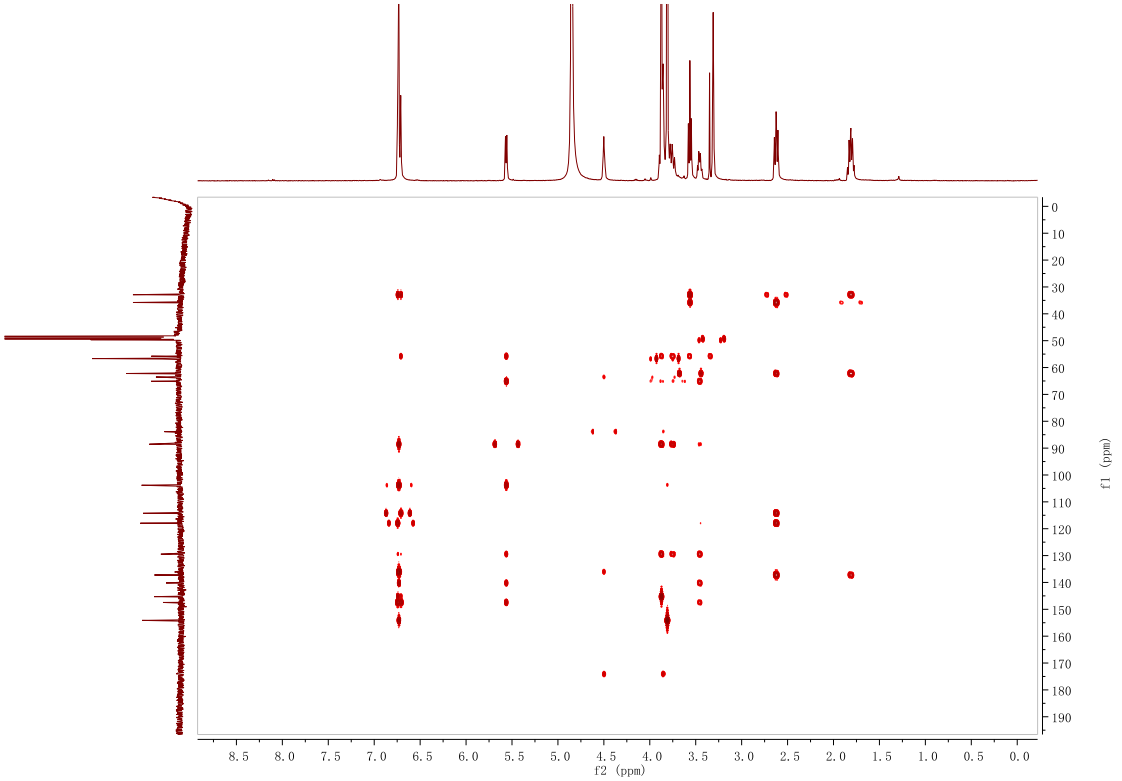


Fig. S43 HMBC spectrum of compound 5

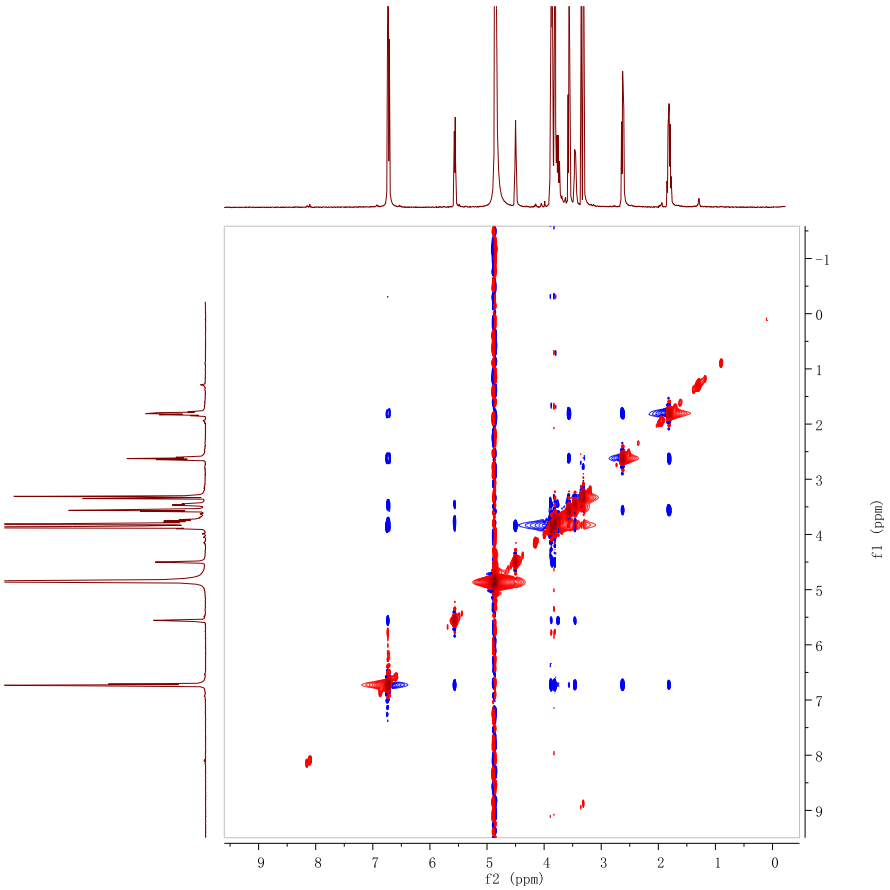
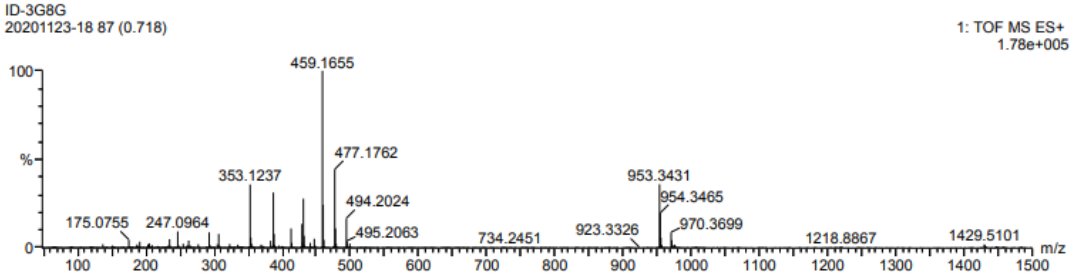


Fig. S44 NOESY spectrum of compound 5

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
217 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 O: 0-200 Na: 0-1
ID-3G8G
20201123-18 87 (0.718)



Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Conf(%)	Formula
477.1762	477.1761	0.1	0.2	10.5	352.5	n/a	C24 H29 O10

Fig. S45 HR-ESI-MS spectrum of compound 6

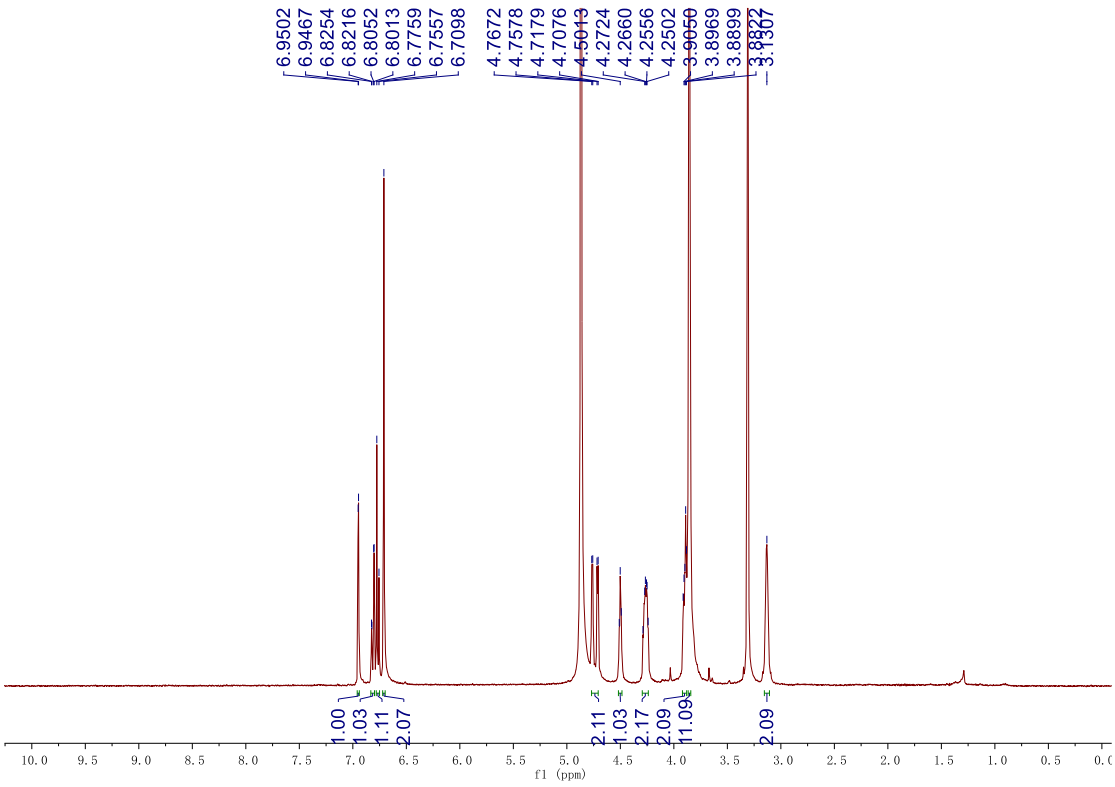


Fig. S46 ^{1}H NMR spectrum of compound 6

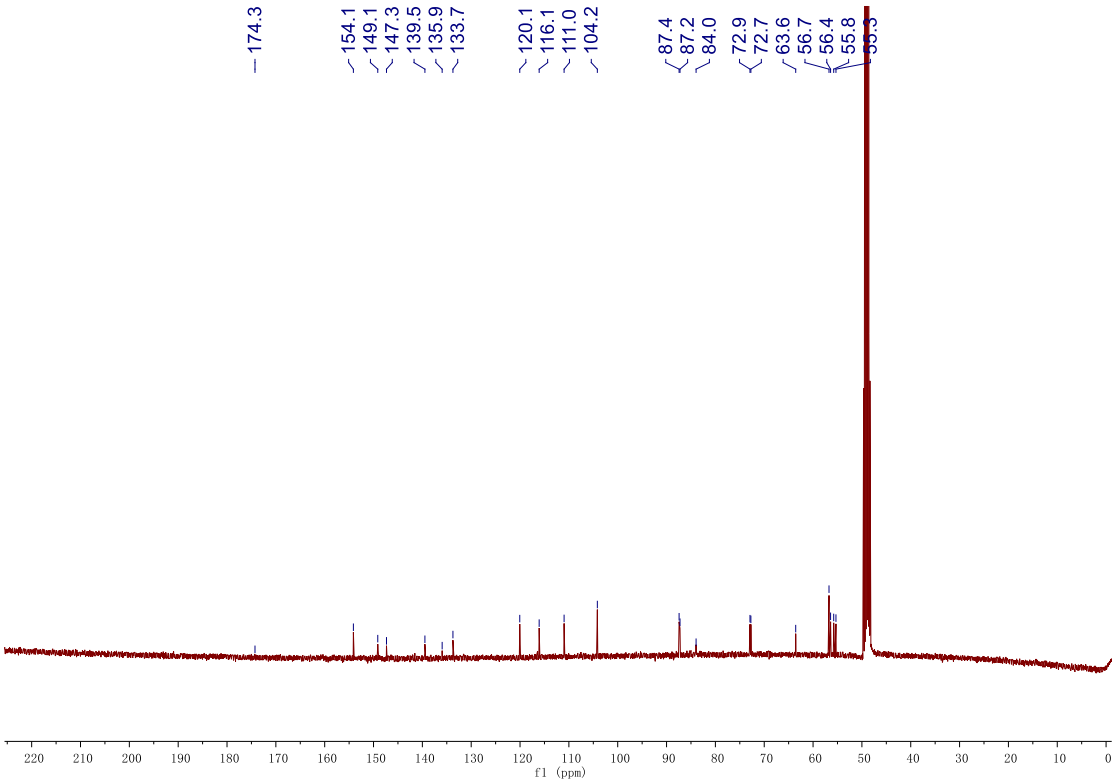


Fig. S47 ^{13}C NMR spectrum of compound 6

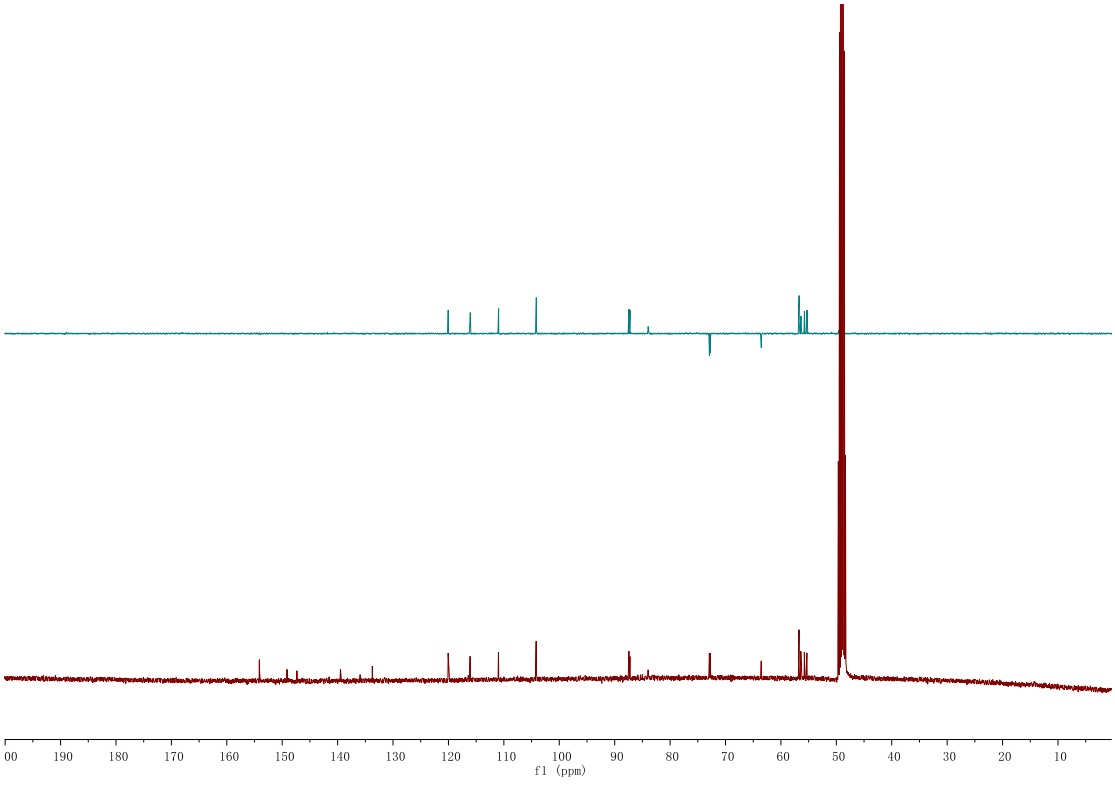


Fig. S48 ^{13}C-NMR and DEPT 135 spectra of compound 6

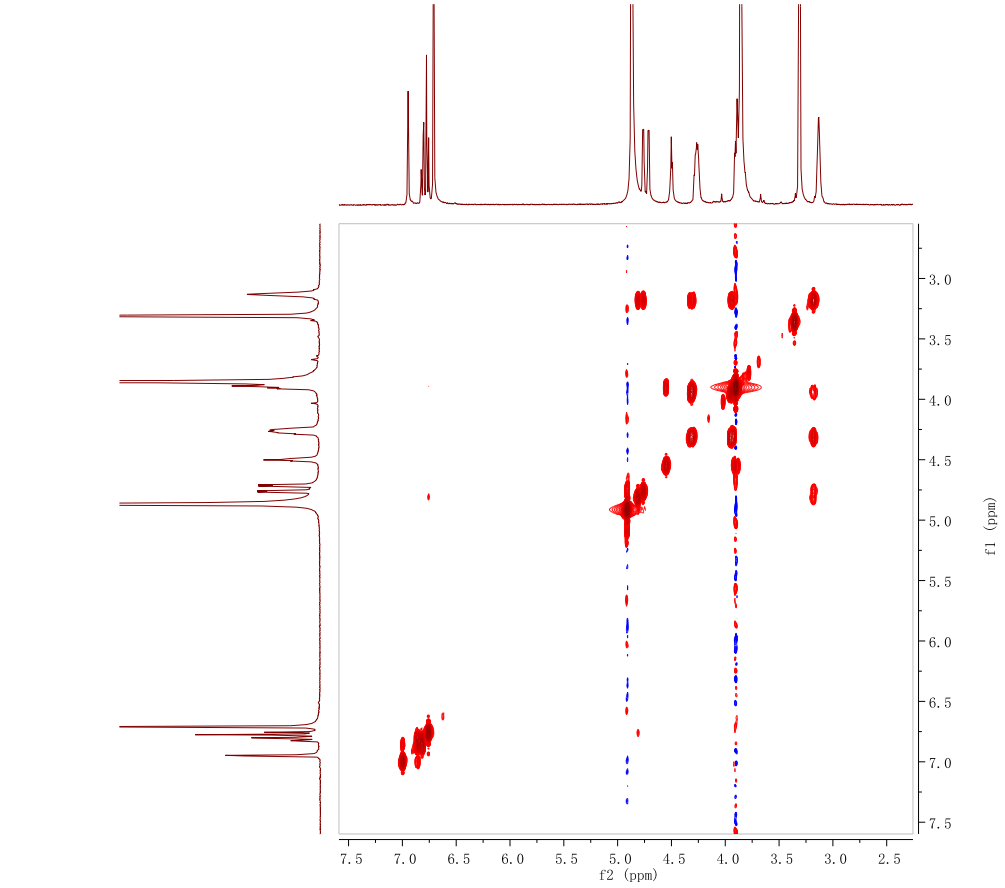


Fig. S49 ^{1}H-^{1}H COSY spectrum of compound 6

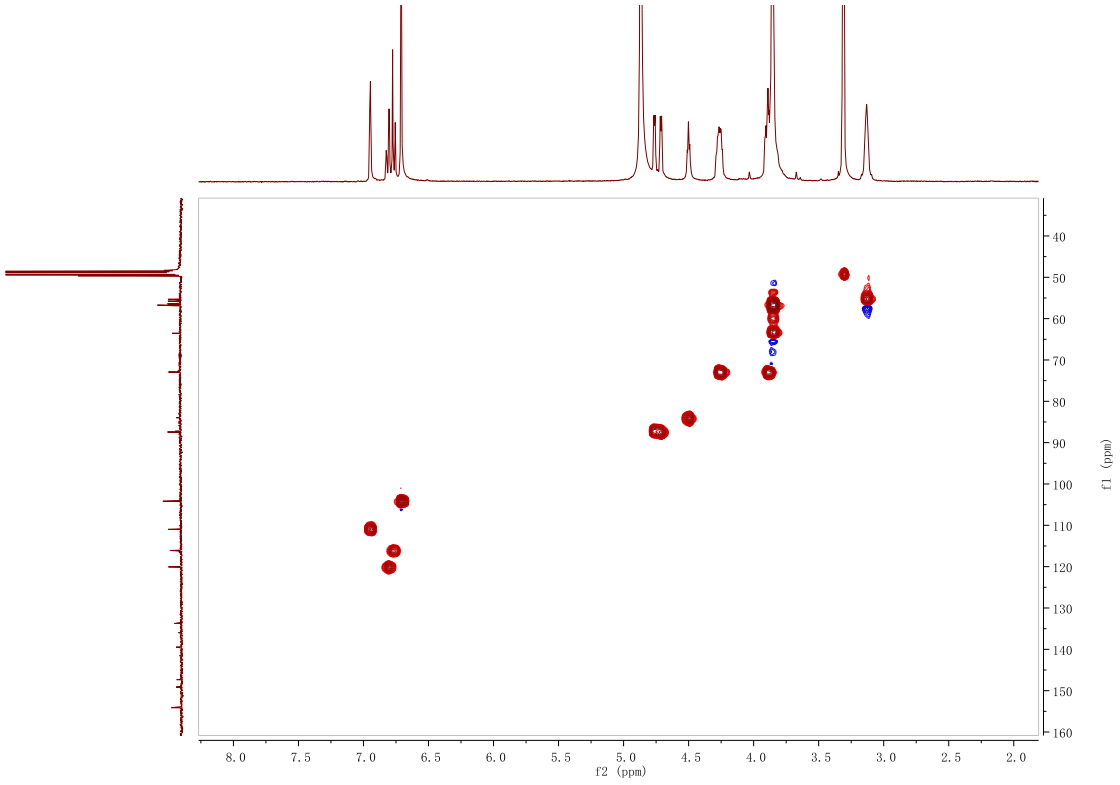


Fig. S50 HSQC spectrum of compound 6

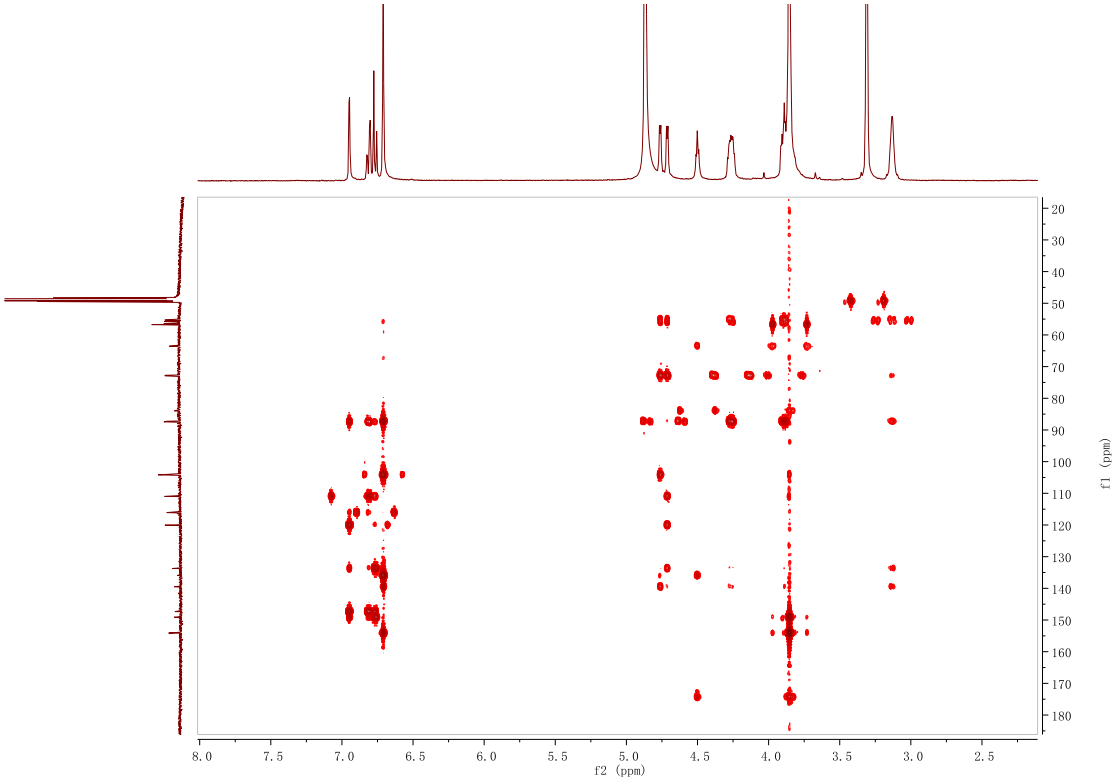


Fig. S51 HMBC spectrum of compound 6

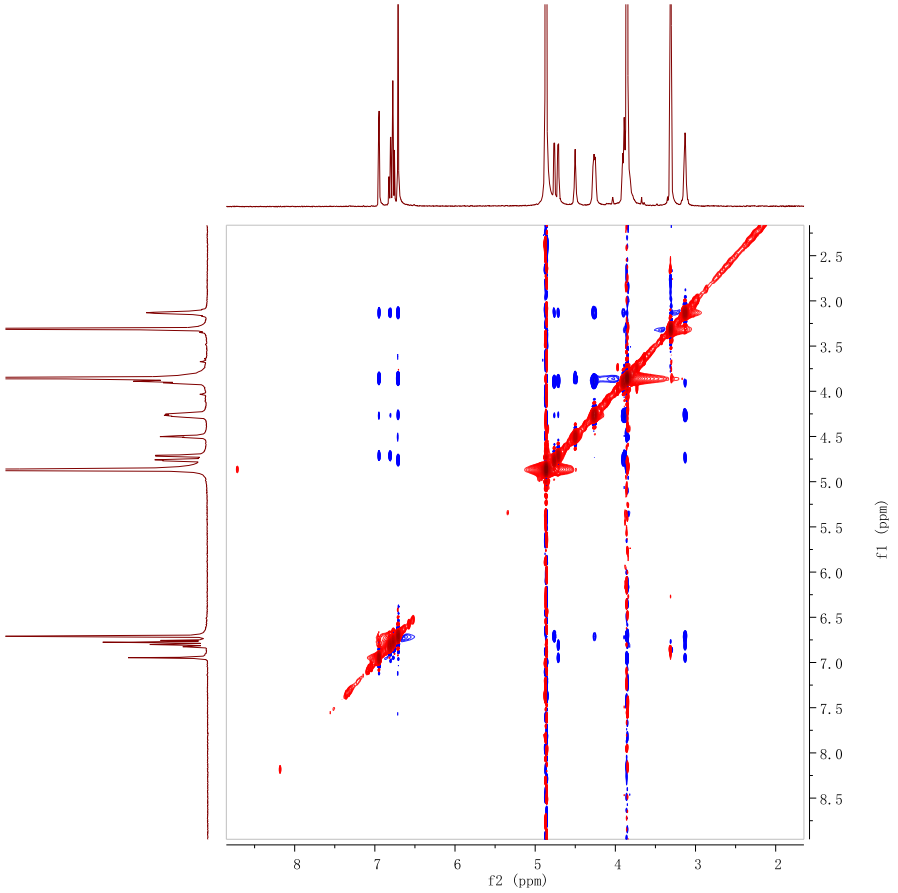
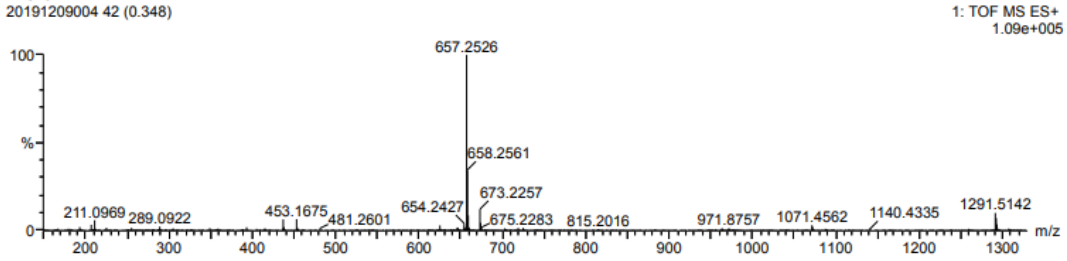


Fig. S52 NOESY spectrum of compound 6

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 1.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
388 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 O: 0-200 Na: 0-1
ID-3F9F1
20191209004 42 (0.348)



Minimum:				-1.5			
Maximum:		5.0	1.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Conf(%)	Formula
657.2526	657.2523	0.3	0.5	11.5	315.3	n/a	C32 H42 O13 Na

Fig. S53 HR-ESI-MS spectrum of compound 7

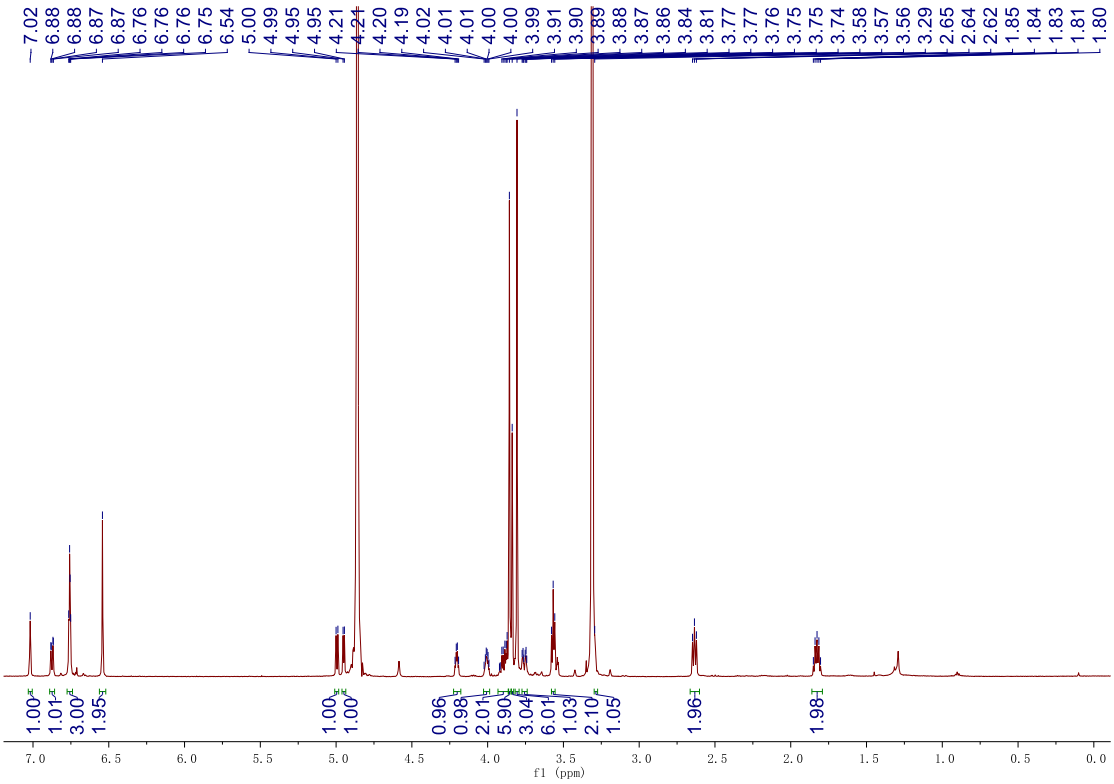


Fig. S54 ^{1}H NMR spectrum of compound 7

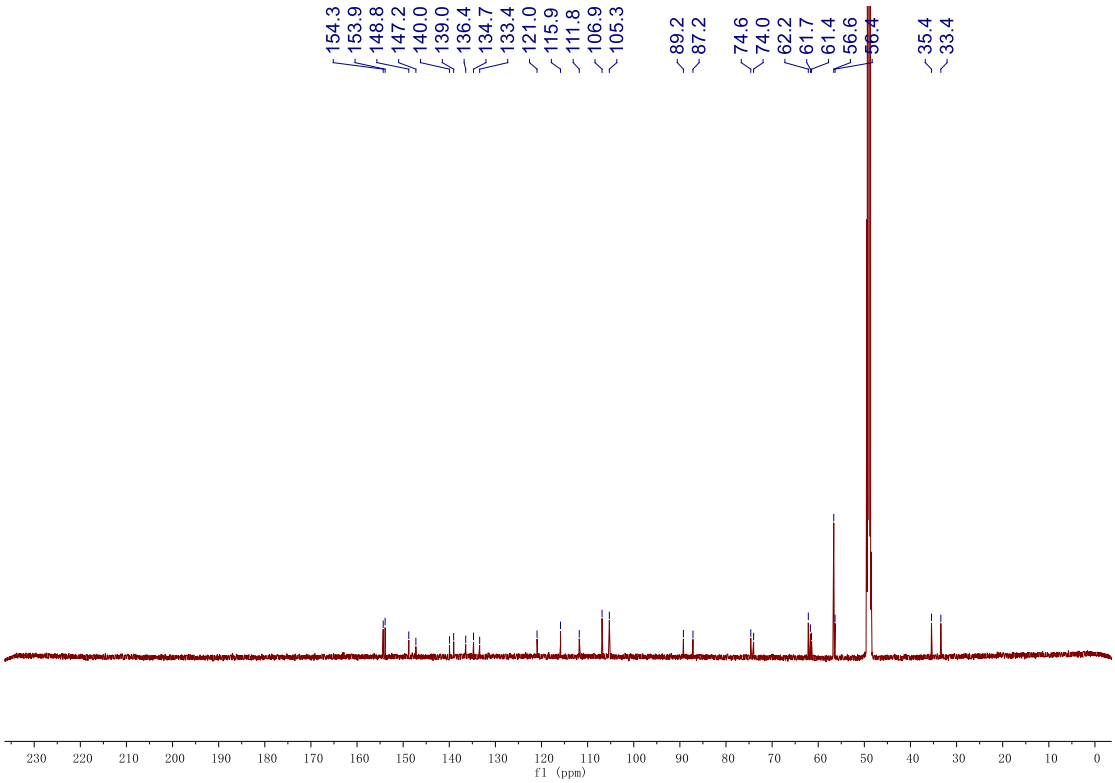


Fig. S55 ^{13}C NMR spectrum of compound 7

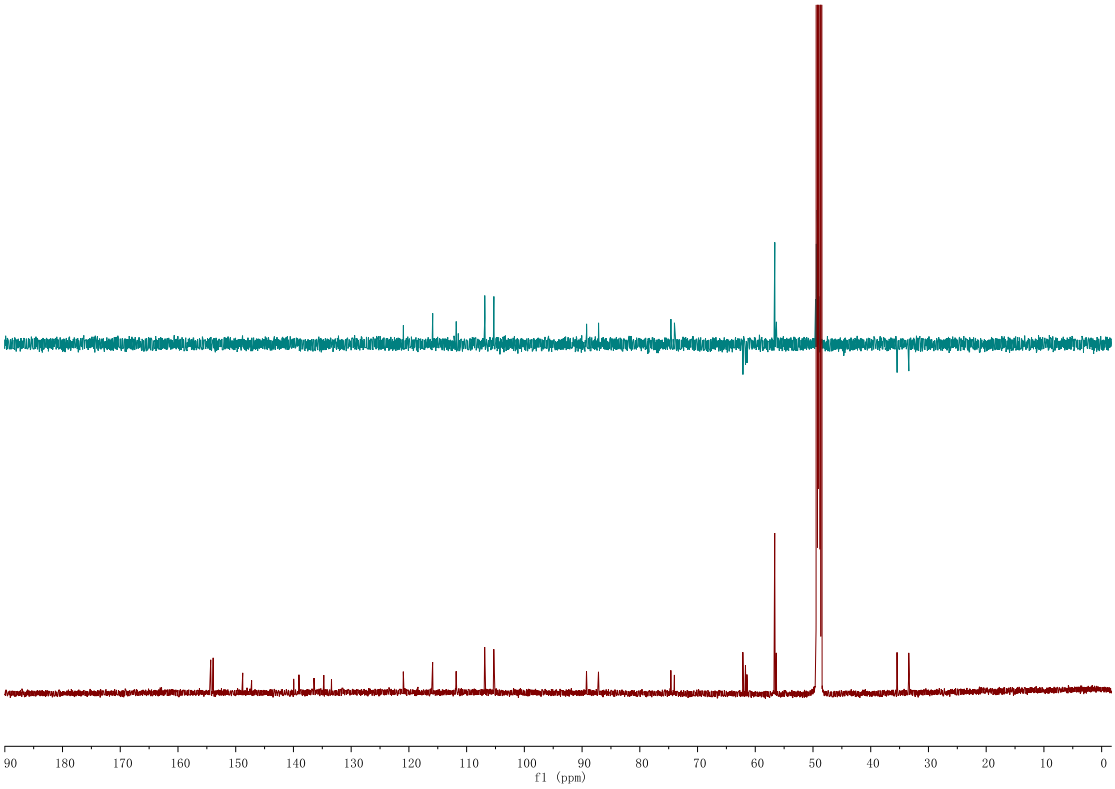


Fig. S56 ^{13}C-NMR and DEPT 135 spectra of compound 7

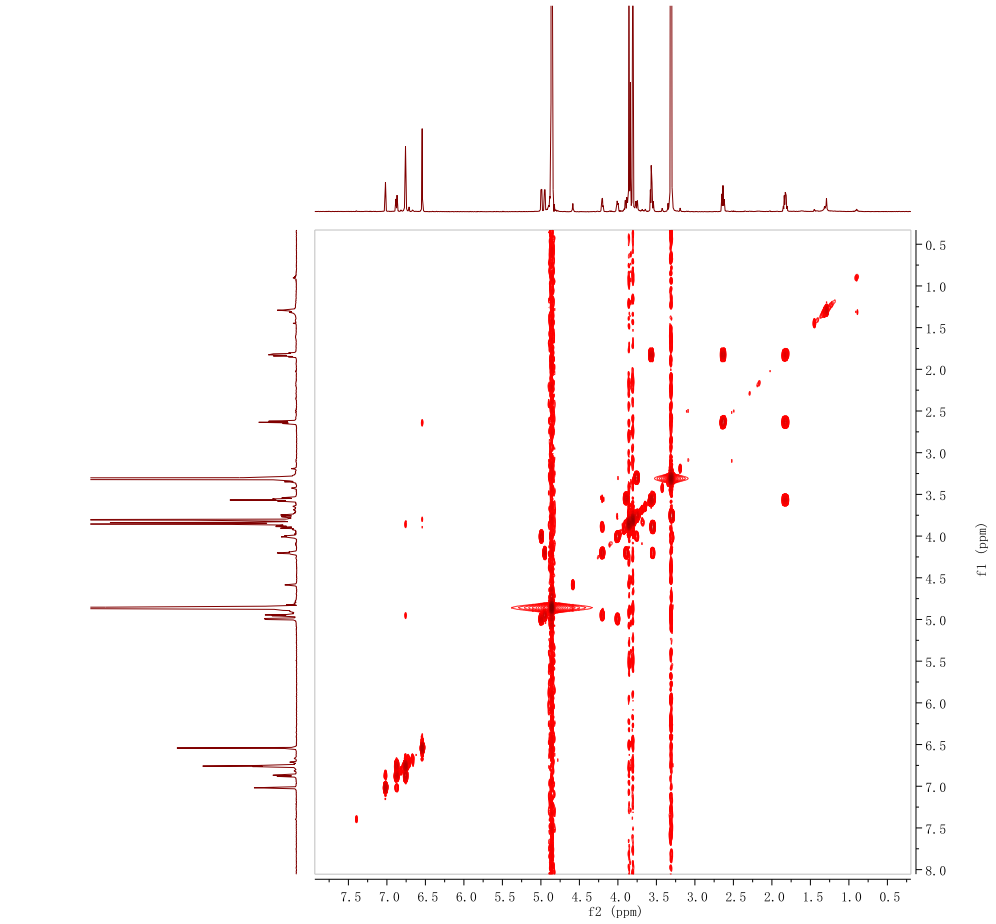


Fig. S57 ^{1}H-^{1}H COSY spectrum of compound 7

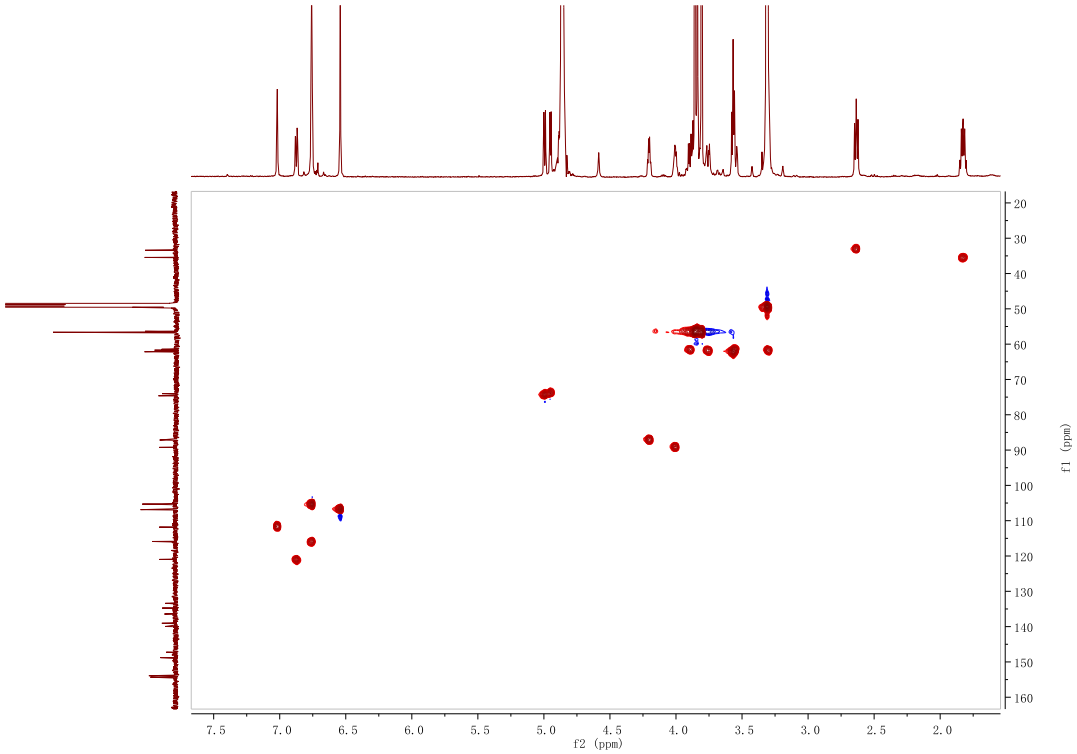


Fig. S58 HSQC spectrum of compound 7

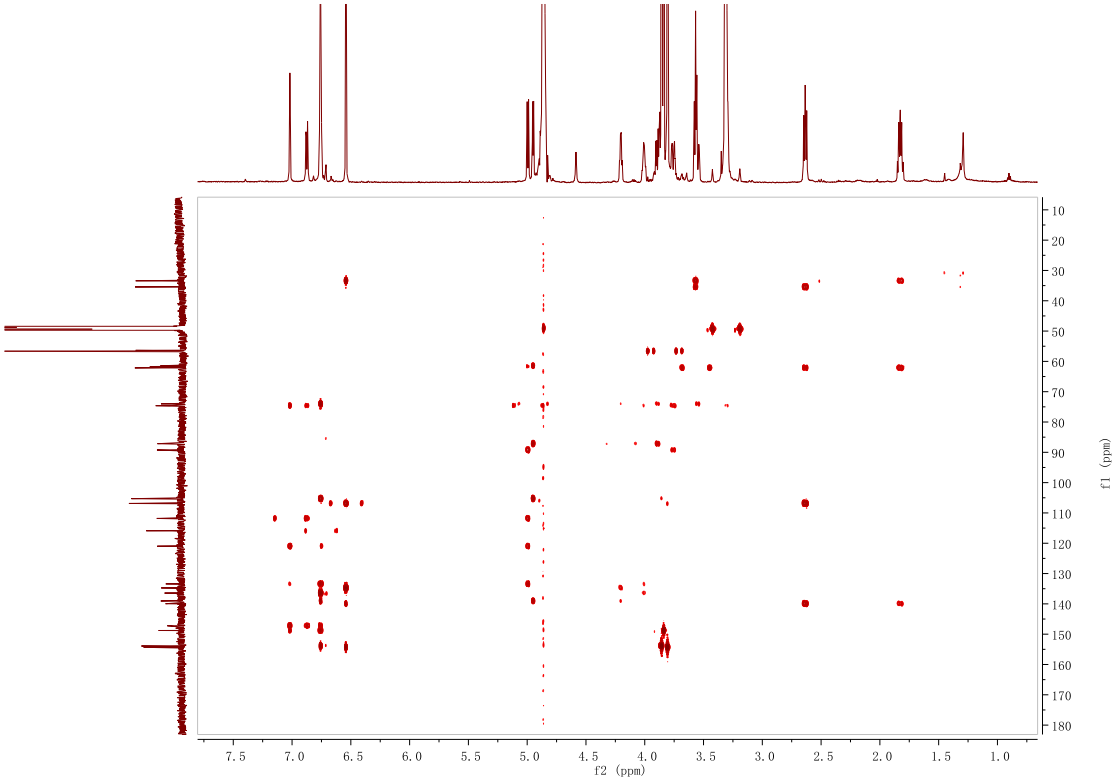


Fig. S59 HMBC spectrum of compound 7

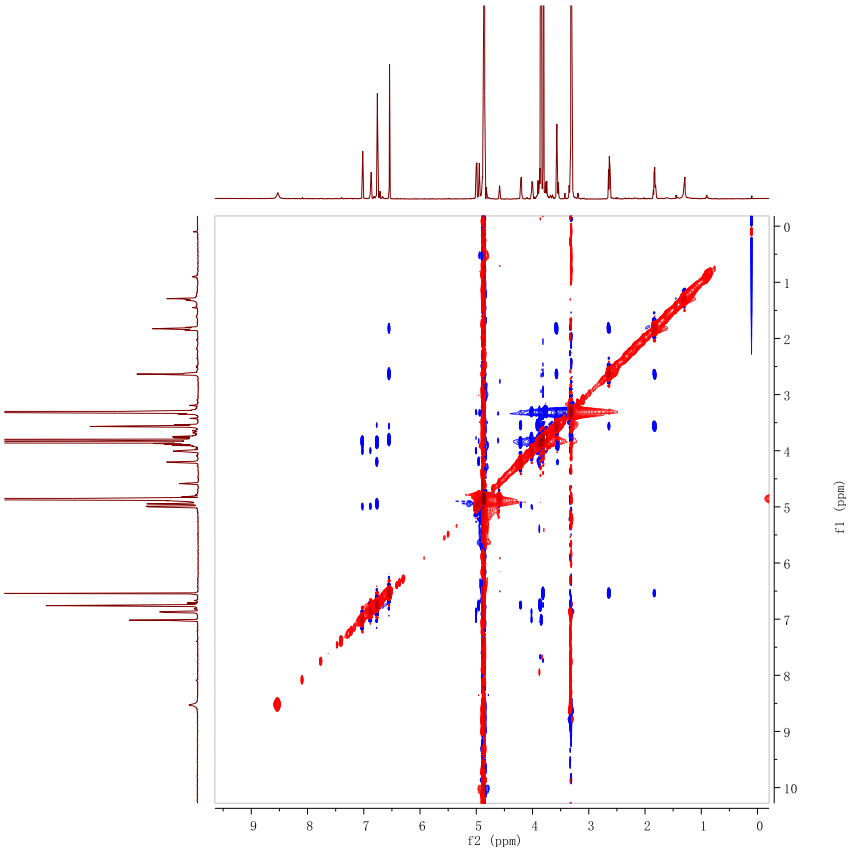
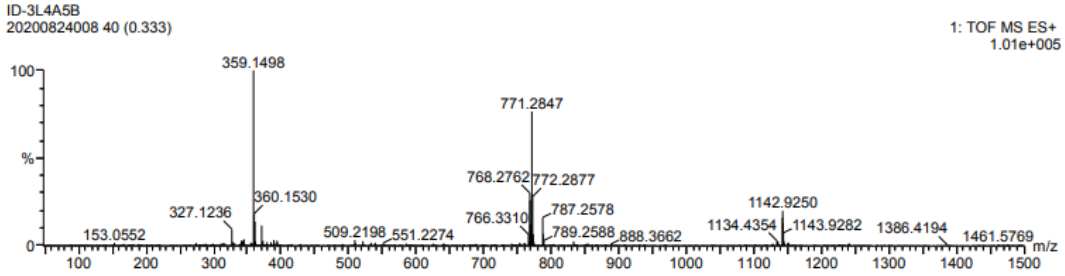


Fig. S60 NOESY spectrum of compound 7

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
514 formula(e) evaluated with 3 results within limits (up to 60 closest results for each mass)
Elements Used:
C: 0-70 H: 0-200 O: 0-40 Na: 0-1
ID-3L4A5B
20200824008 40 (0.333)



Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Conf(%)	Formula
771.2847	771.2840	0.7	0.9	13.5	291.7	83.35	C37 H48 O16 Na
	771.2864	-1.7	-2.2	16.5	293.3	16.47	C39 H47 O16
	771.2875	-2.8	-3.6	35.5	297.9	0.18	C55 H40 O3 Na

Fig. S61 HR-ESI-MS spectrum of compound 8

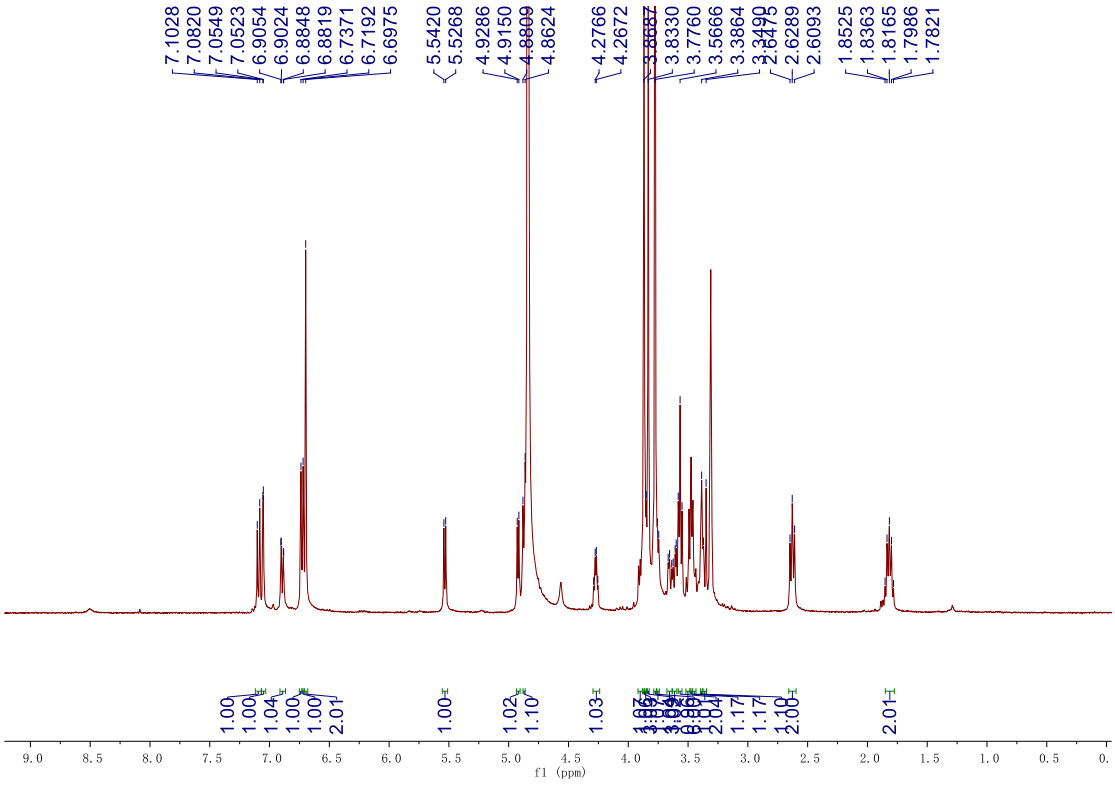


Fig. S62 ^{1}H NMR spectrum of compound 8

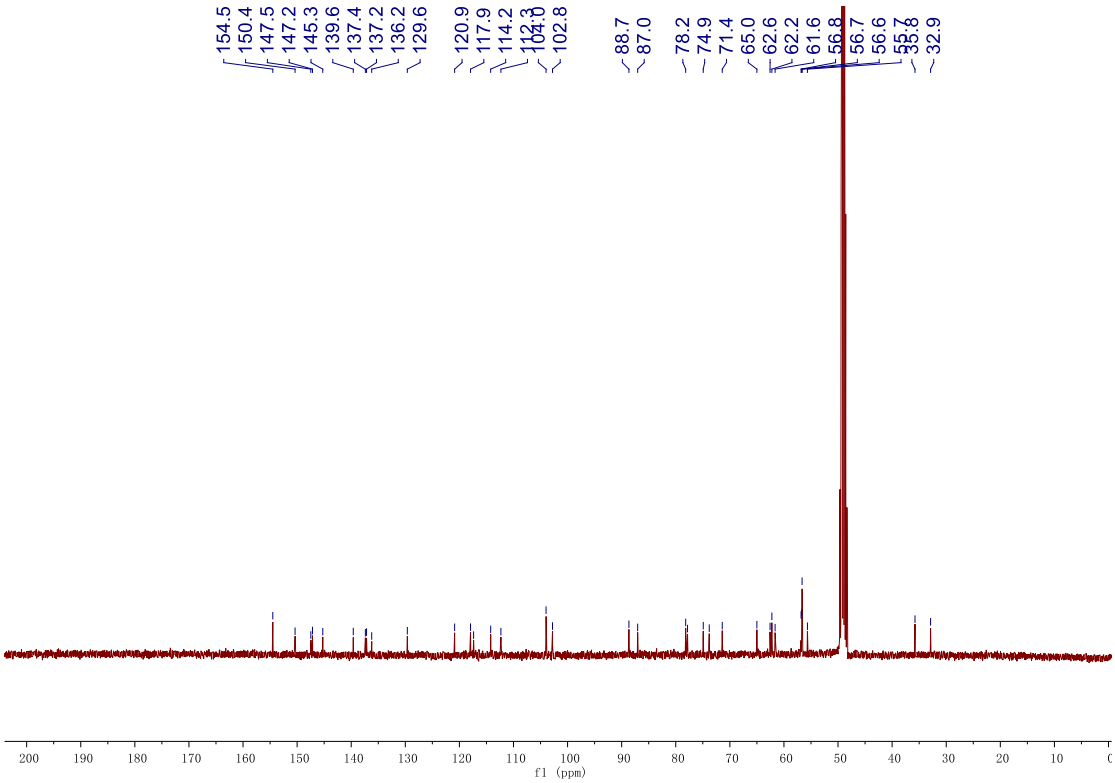


Fig. S63 ^{13}C NMR spectrum of compound 8

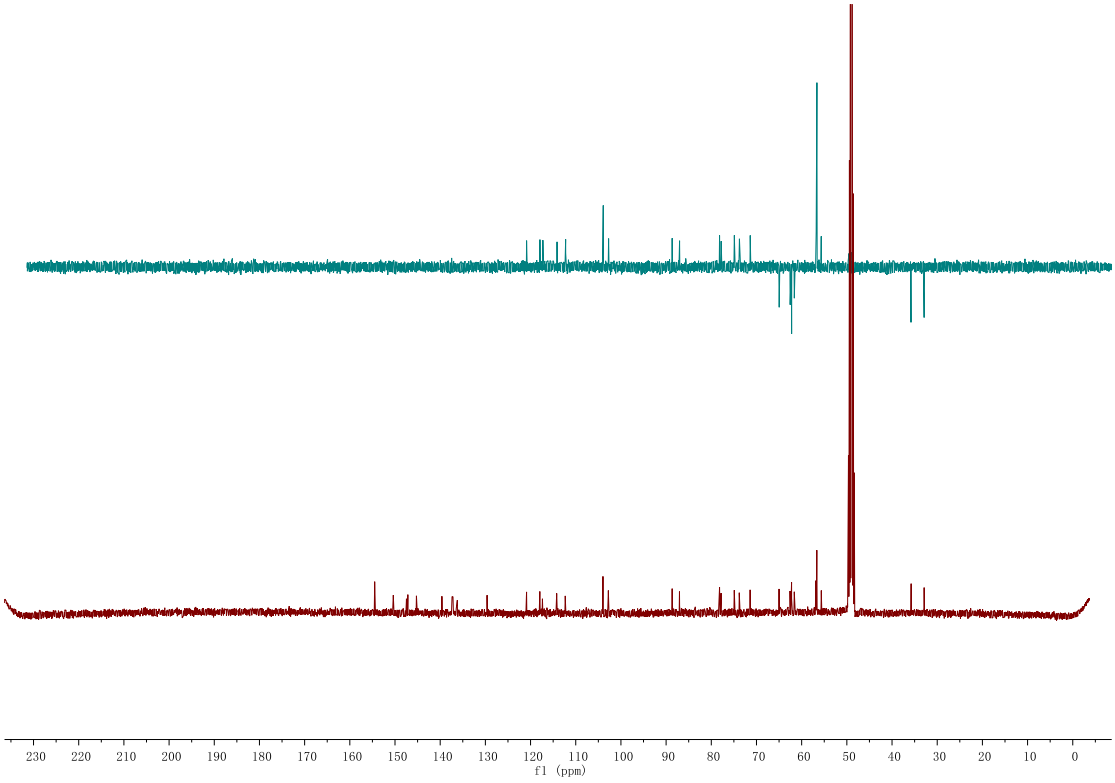


Fig. S64 ^{13}C-NMR and DEPT 135 spectra of compound 8

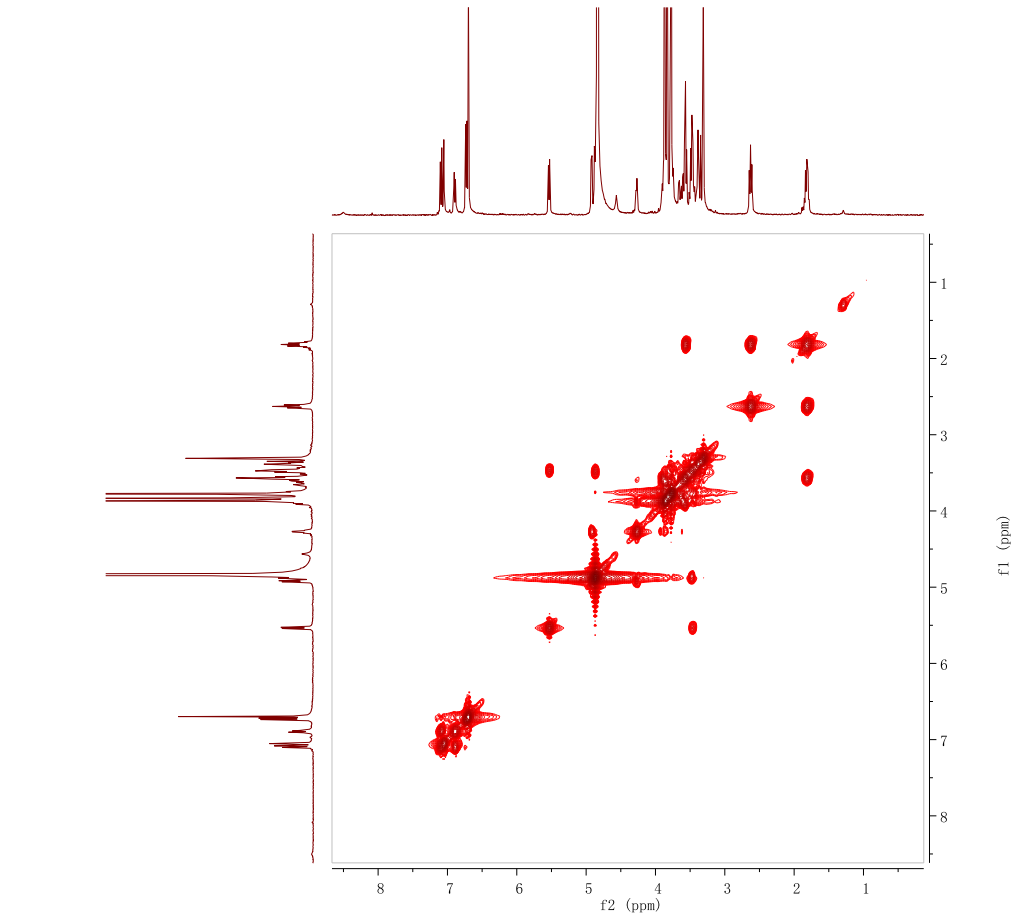


Fig. S65 ^{1}H-^{1}H COSY spectrum of compound 8

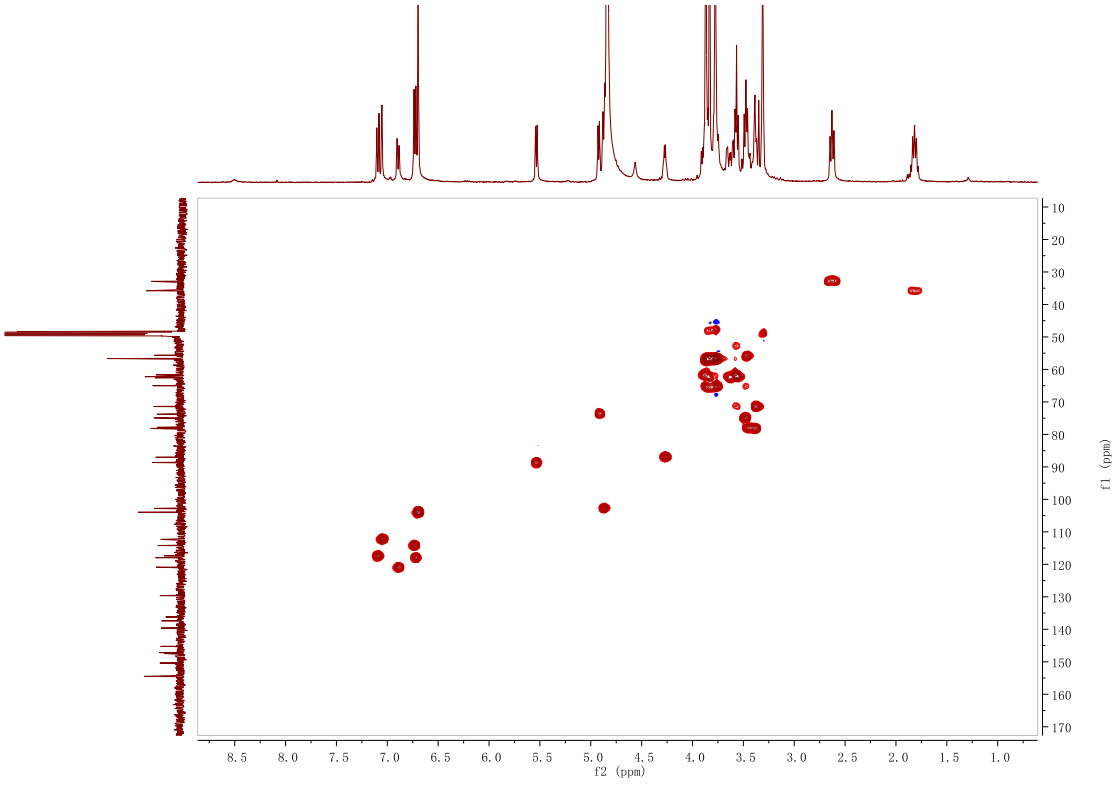


Fig. S66 HSQC spectrum of compound 8

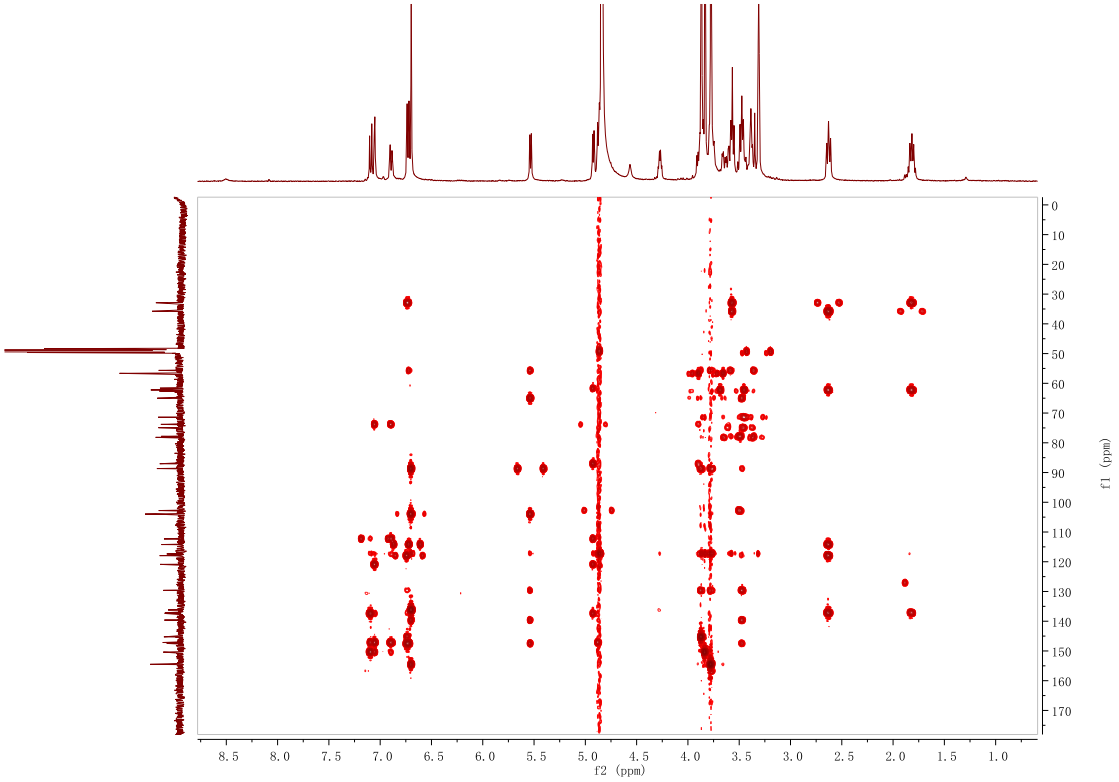


Fig. S67 HMBC spectrum of compound 8

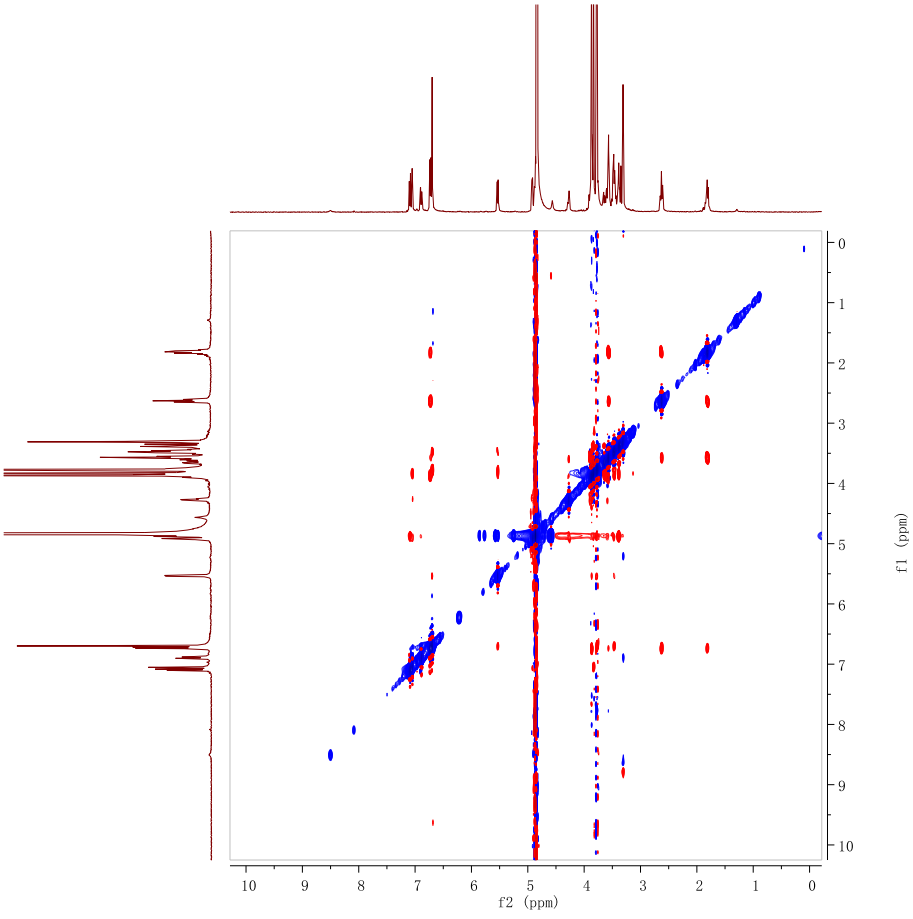


Fig. S68 NOESY spectrum of compound 8

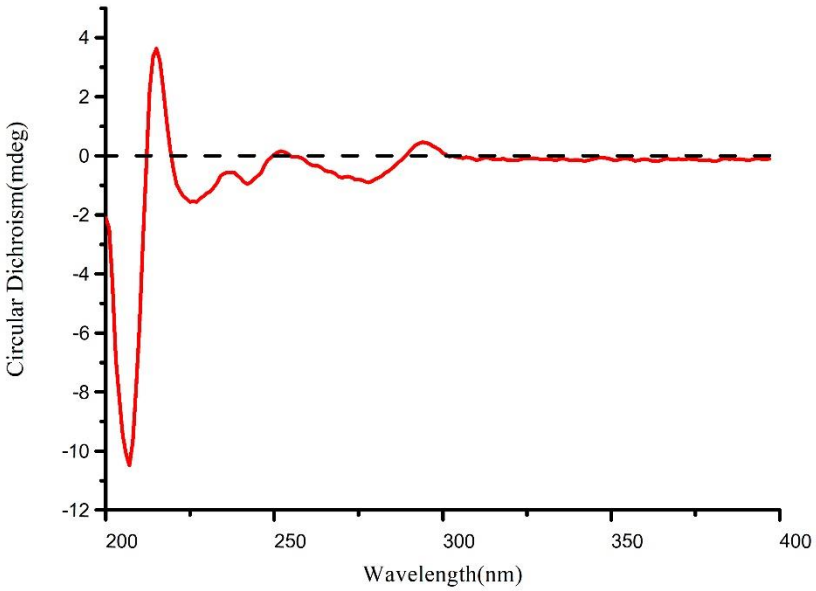
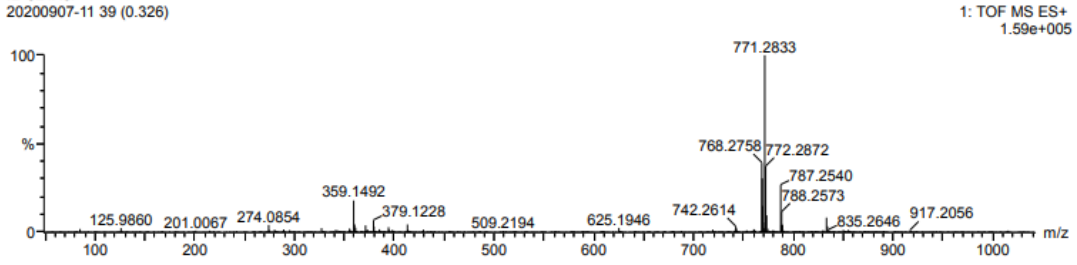


Fig. S69 Experimental CD spectrum of compound 8

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
378 formula(e) evaluated with 3 results within limits (up to 60 closest results for each mass)
Elements Used:
C: 0-60 H: 0-100 O: 0-25 Na: 0-1
ID-3L4A6F
20200907-11 39 (0.326)



Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Conf(%)	Formula
771.2833	771.2840	-0.7	-0.9	13.5	358.7	96.97	C37 H48 O16 Na
	771.2805	2.8	3.6	25.5	364.5	0.29	C46 H43 O11
	771.2864	-3.1	-4.0	16.5	362.2	2.74	C39 H47 O16

Fig. S70 HR-ESI-MS spectrum of compound 9

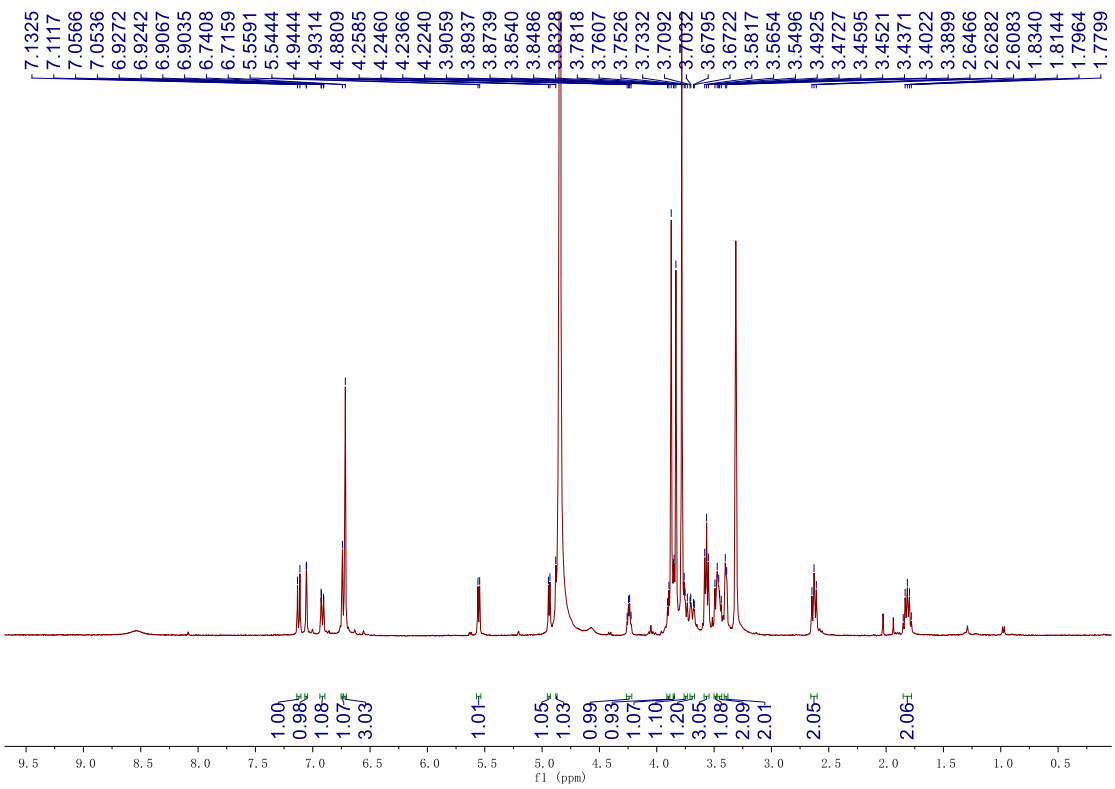


Fig. S71 ^{1}H NMR spectrum of compound 9

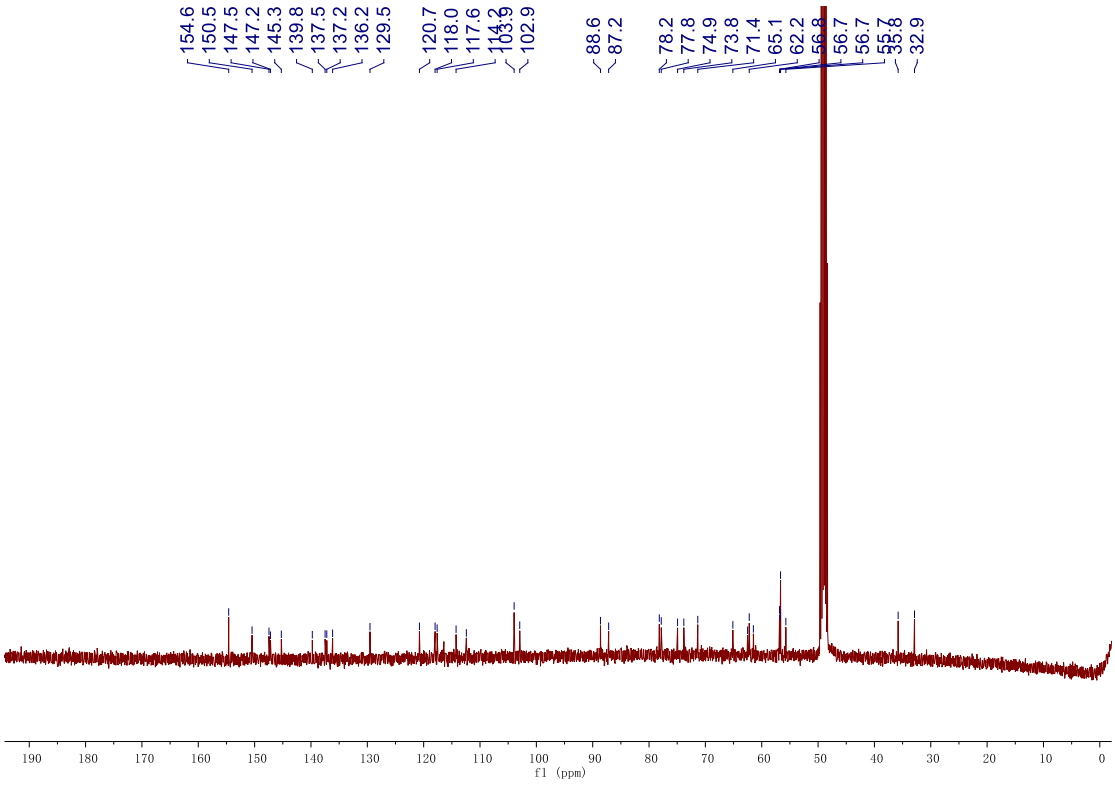


Fig. S72 ^{13}C NMR spectrum of compound 9

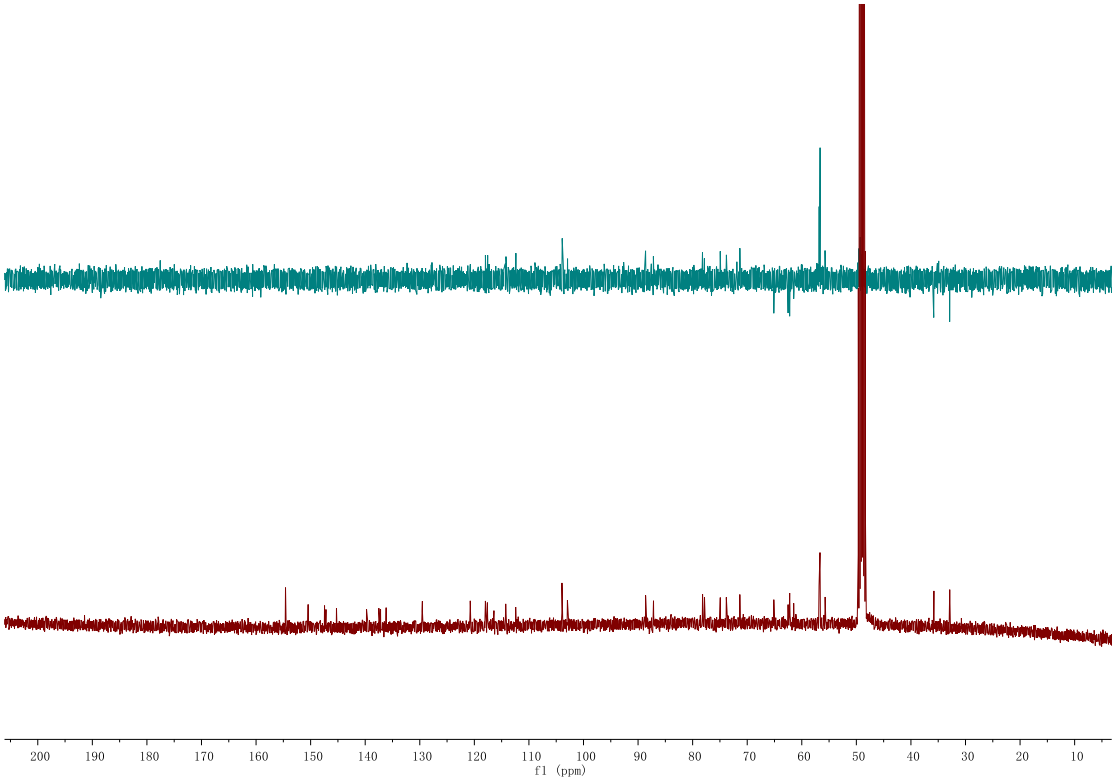


Fig. S73 ^{13}C-NMR and DEPT 135 spectra of compound 9

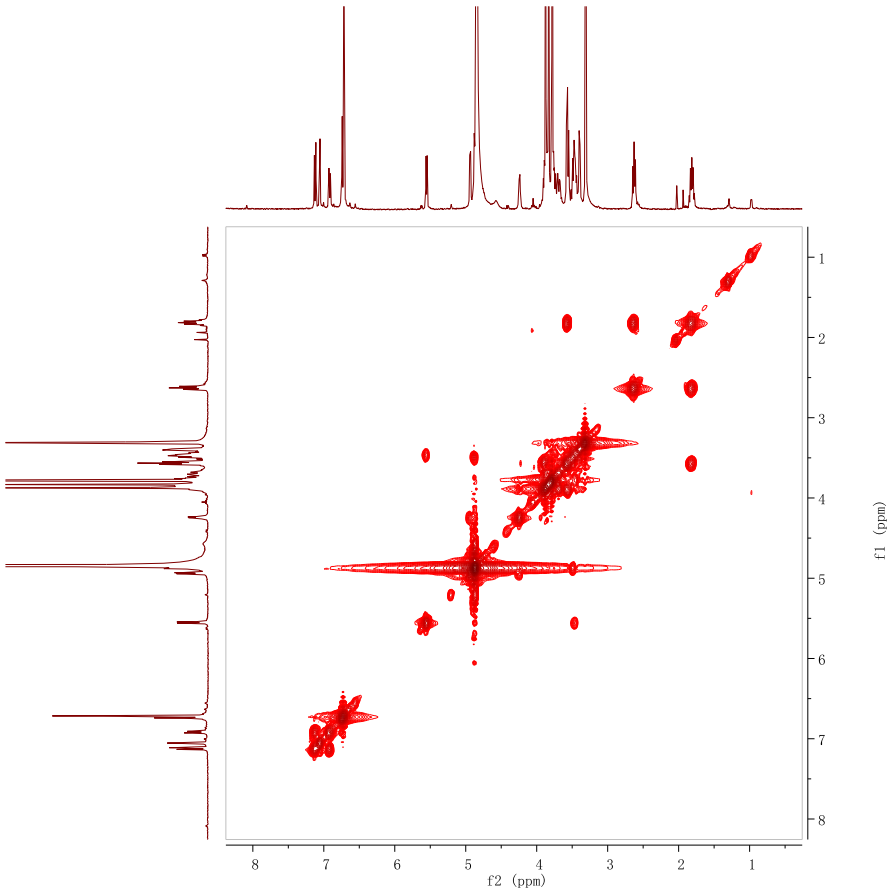


Fig. S74 ^{1}H-^{1}H COSY spectrum of compound 9

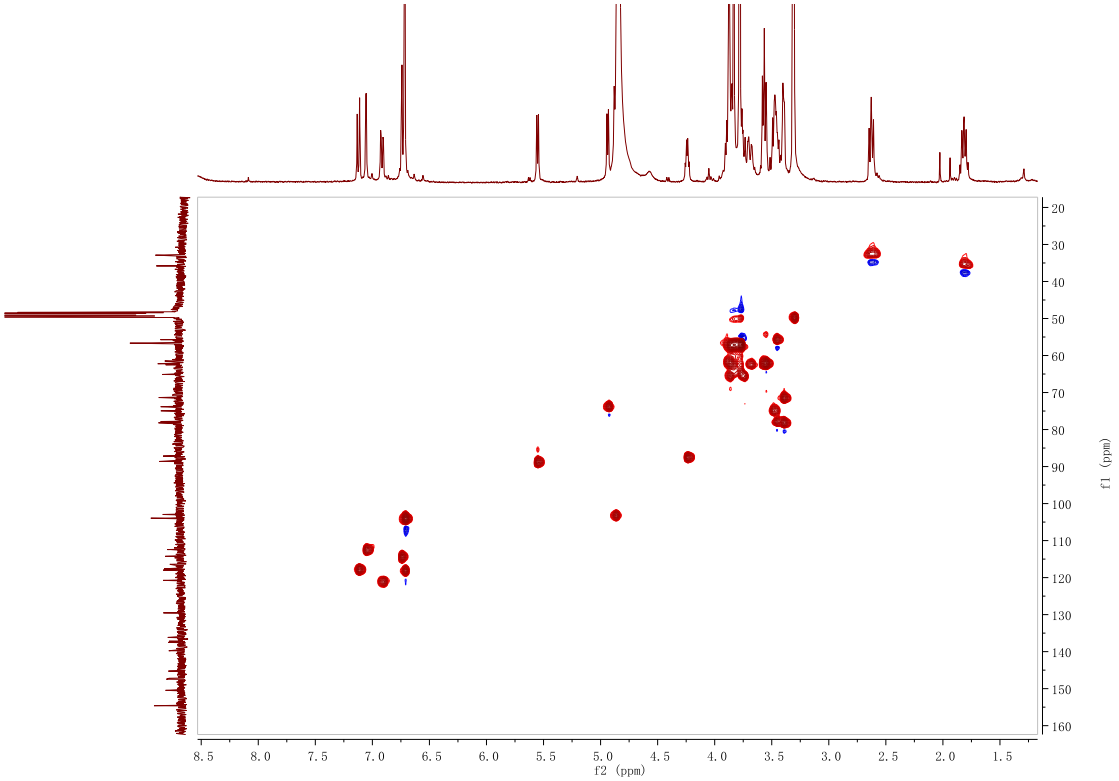


Fig. S75 HSQC spectrum of compound 9

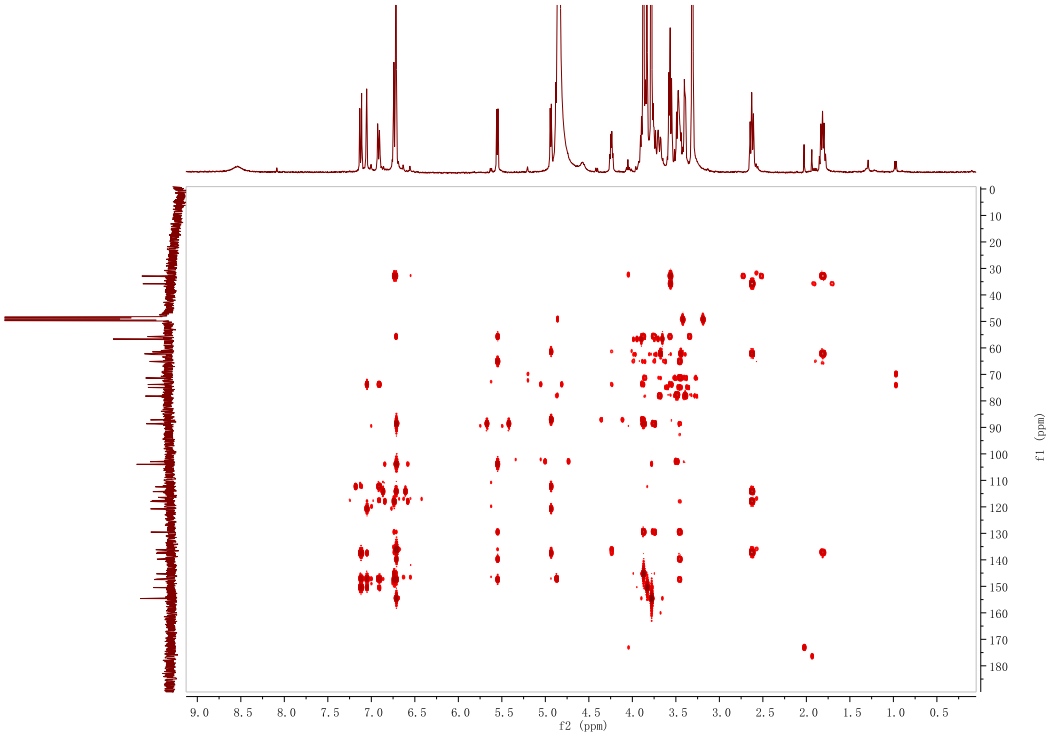


Fig. S76 HMBC spectrum of compound 9

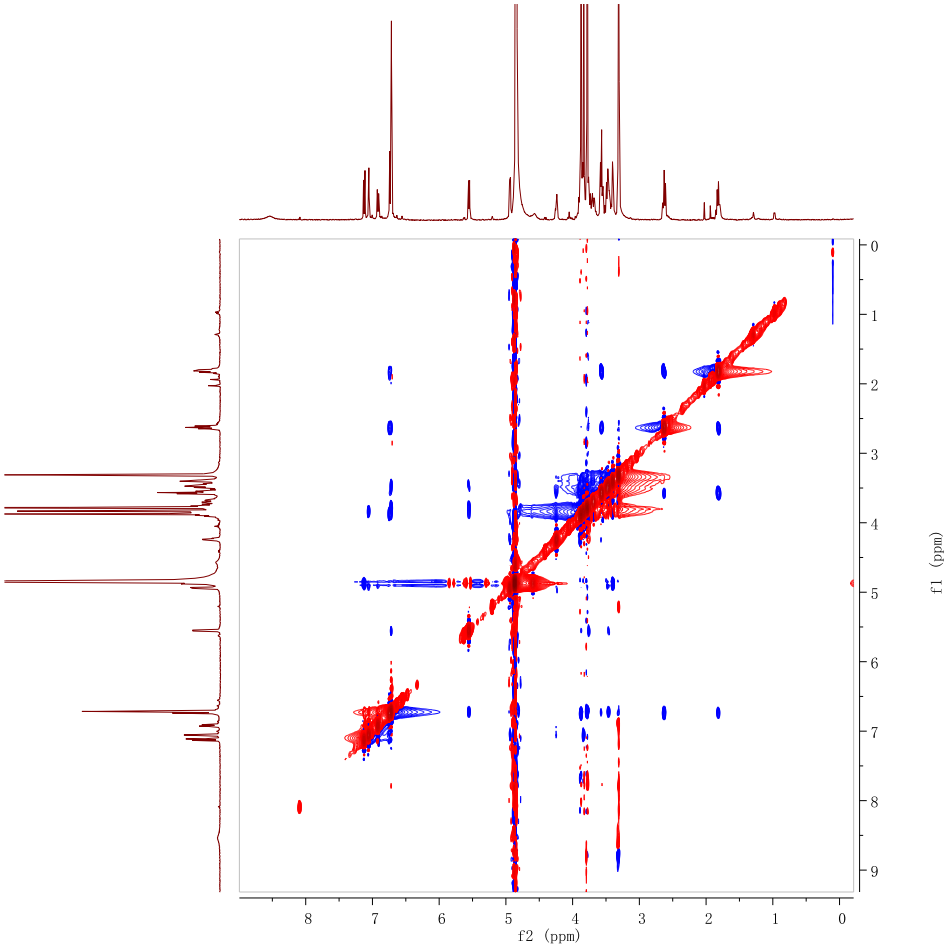


Fig. S77 NOESY spectrum of compound 9

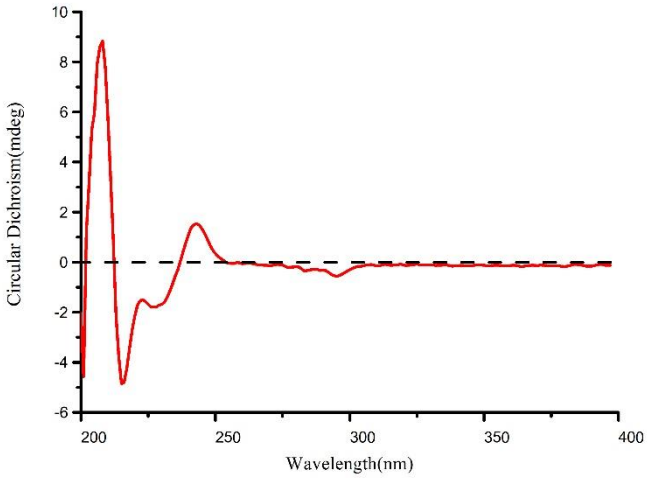


Fig. S78 Experimental CD spectrum of compound 9

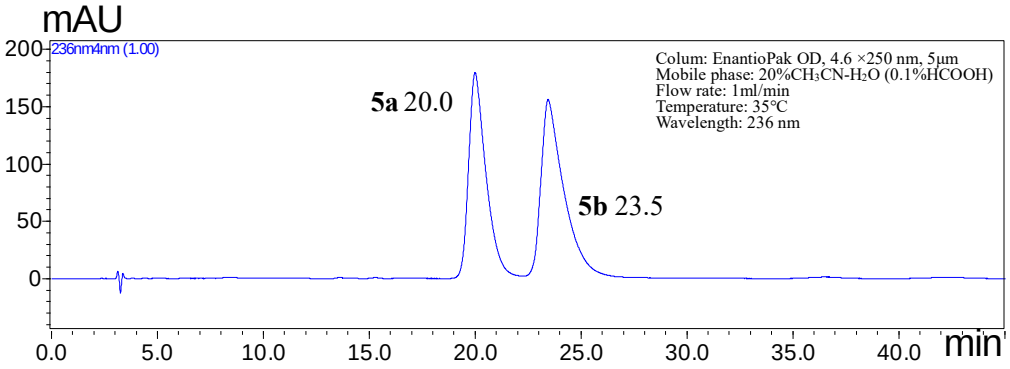


Fig. S79 Chiral-phase HPLC analytical chromatograms of compound 5

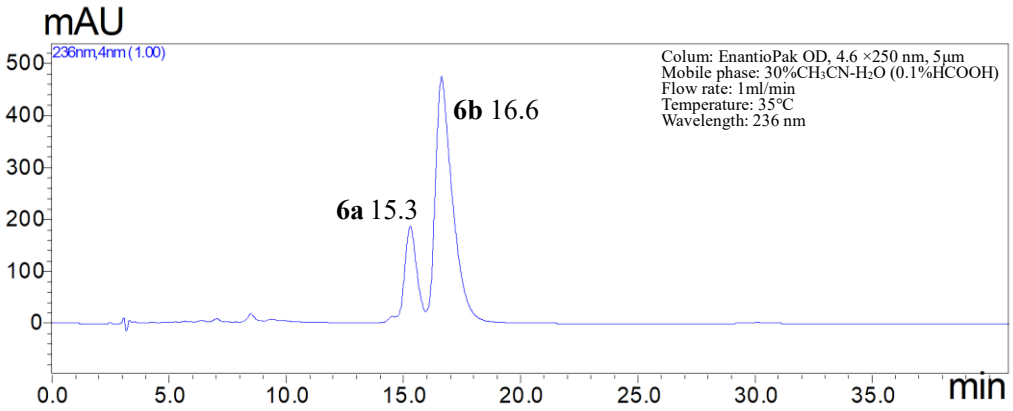


Fig. S80 Chiral-phase HPLC analytical chromatograms of compound 6

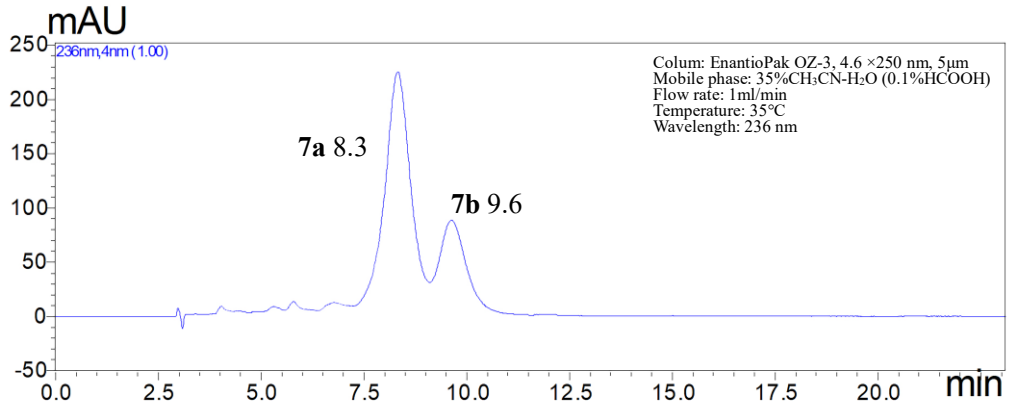


Fig. S81 Chiral-phase HPLC analytical chromatograms of compound 7

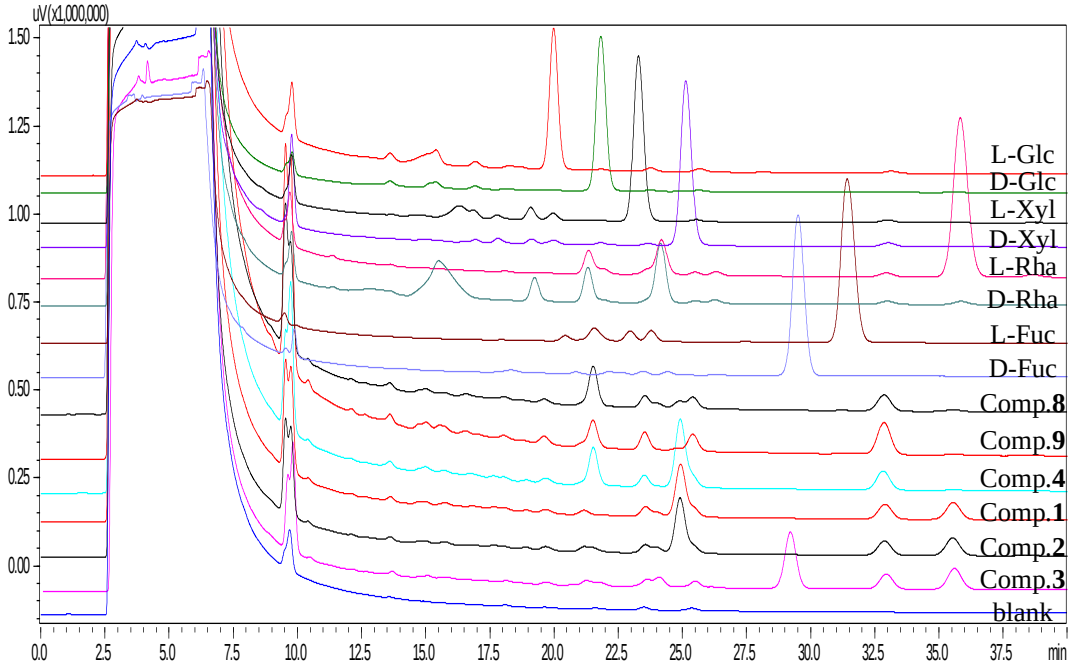


Fig. S82 HPLC chromatograph for the derivative of compound 1-4, 8-9

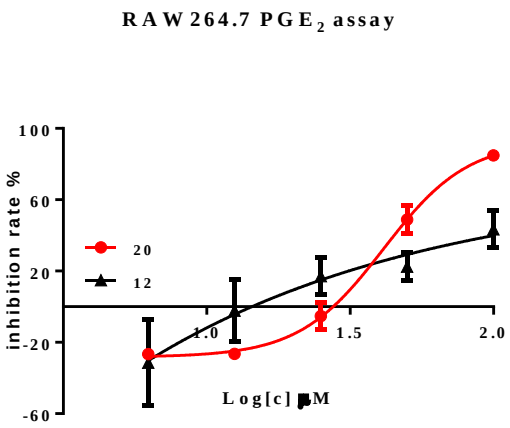


Fig. S83 Effect of compounds 12 and 20 on PGE2 production in LPS-stimulated RAW264.7 cells

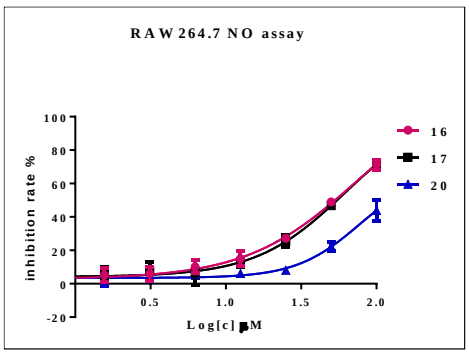


Fig. S84 Effect of compounds 16,17 and 20 on NO production in LPS-stimulated RAW264.7 cells