Xishaeleganins A–D, Sesquiterpenoid Hydroquinones from Xisha Marine Sponge *Dactylospongia elegans*

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Contents

Qualitative Analysis Report

Data Filename	ESIH202103582.d	**Sample Name**	A8-A8-3JCA31
Sample ID		**Position**	P1-C5
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	7/23/2021 16:24:06	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
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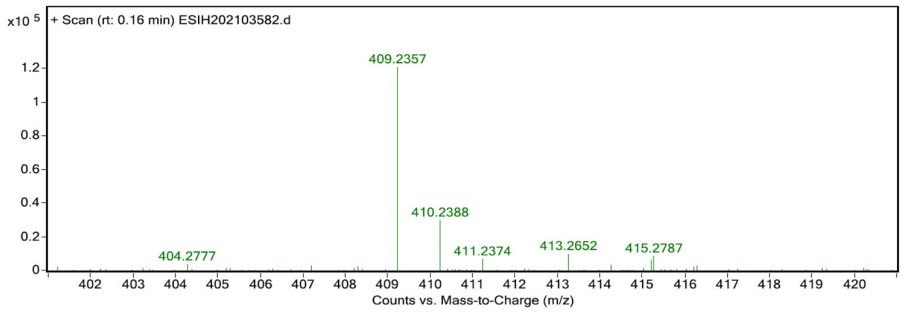

Formula Calculator Results

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409.2357	409.2349	-0.76	-1.86	C24 H34 Na O4	(M+Na)+

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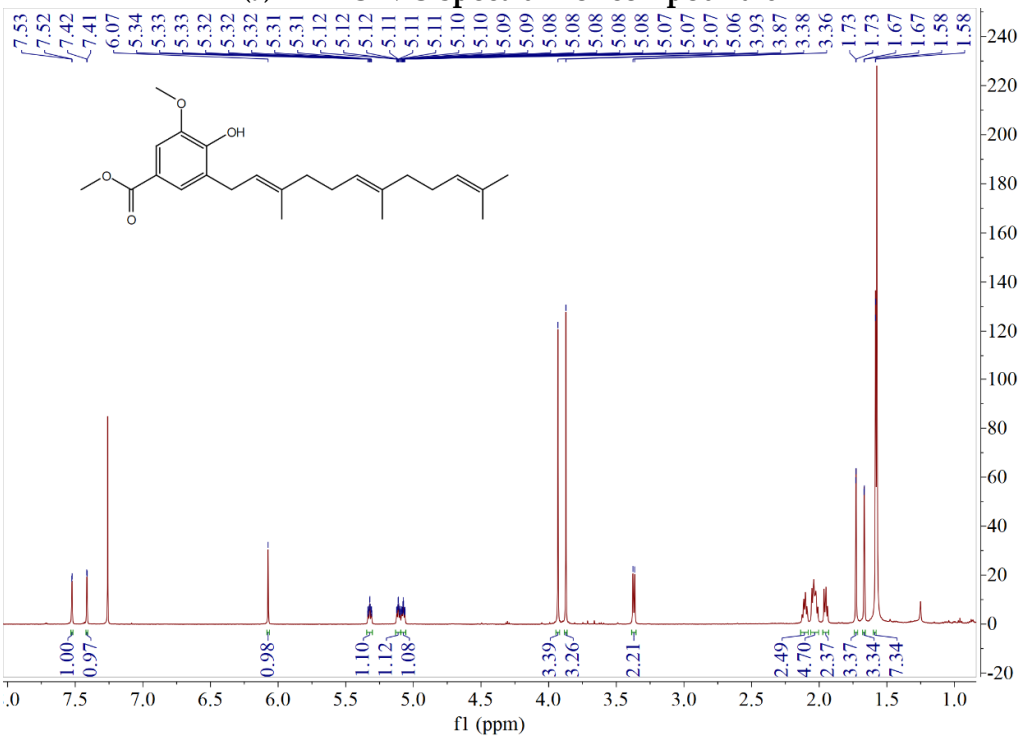
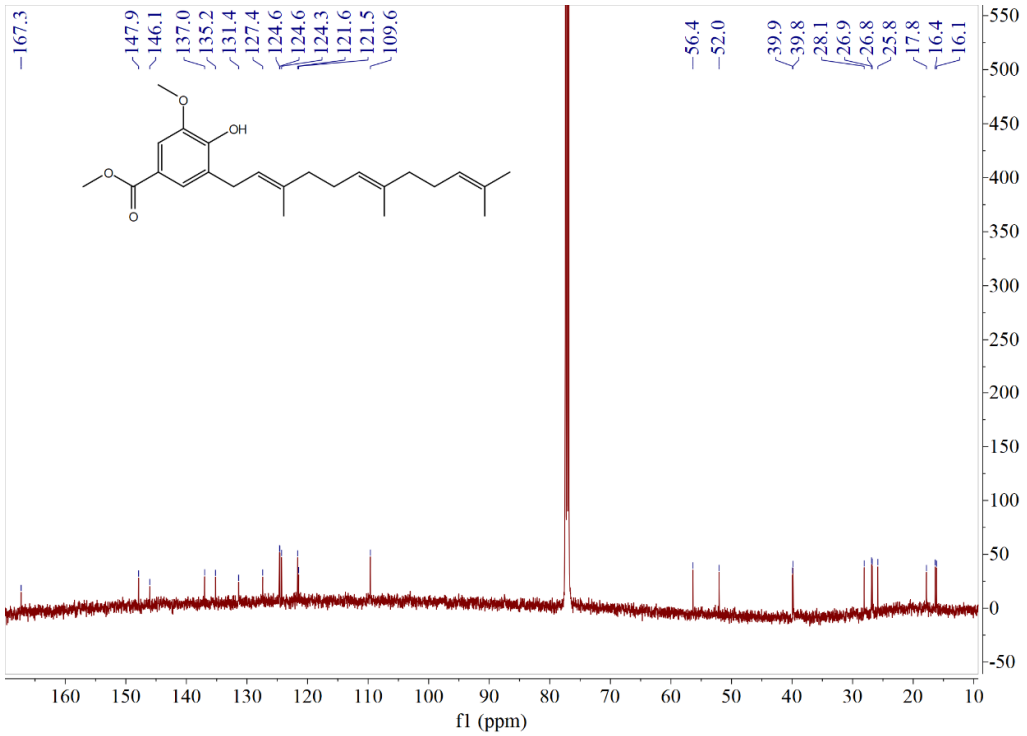
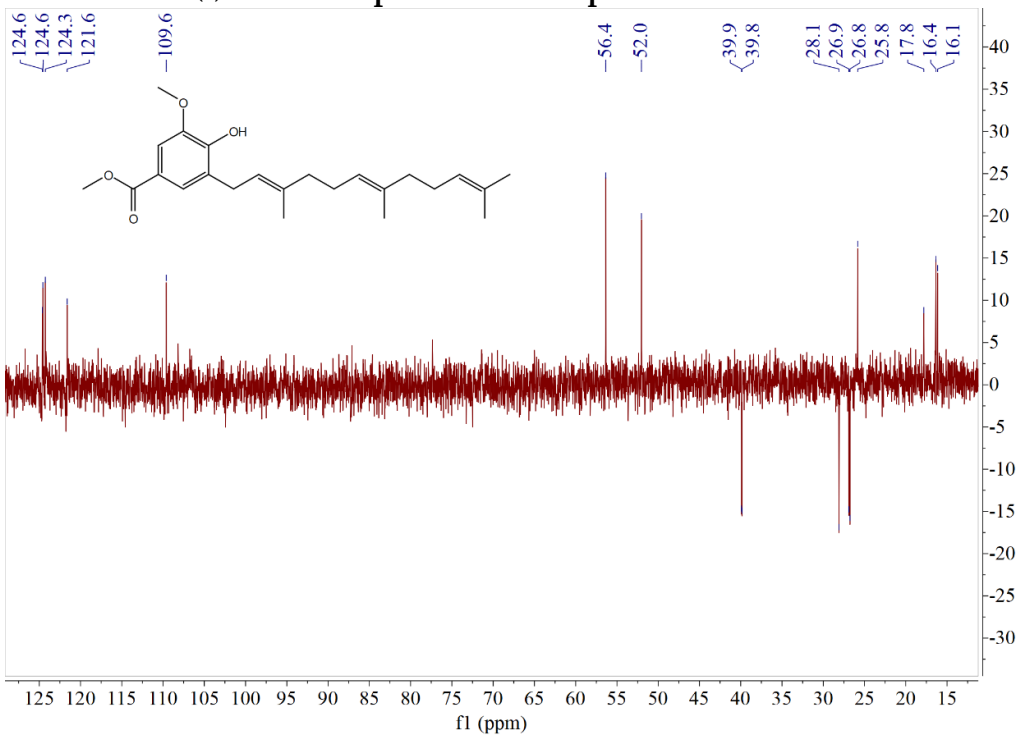
(a) HRESIMS spectrum of compound 6



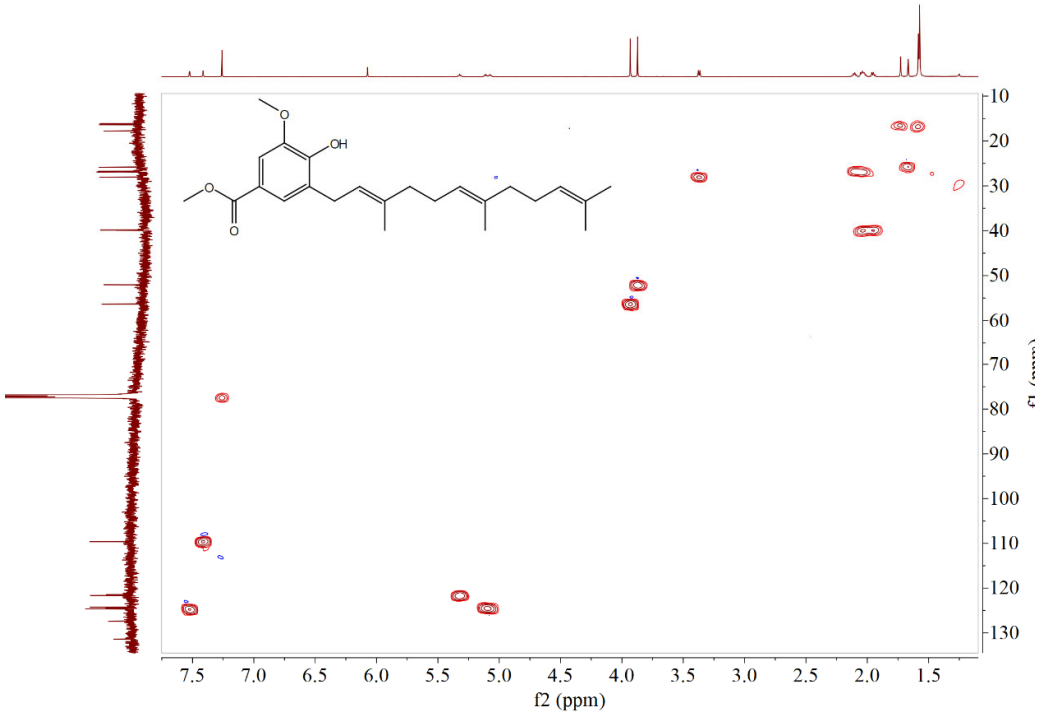
(b) ^{1}H NMR spectrum of compound 6 in $CDCl_3$



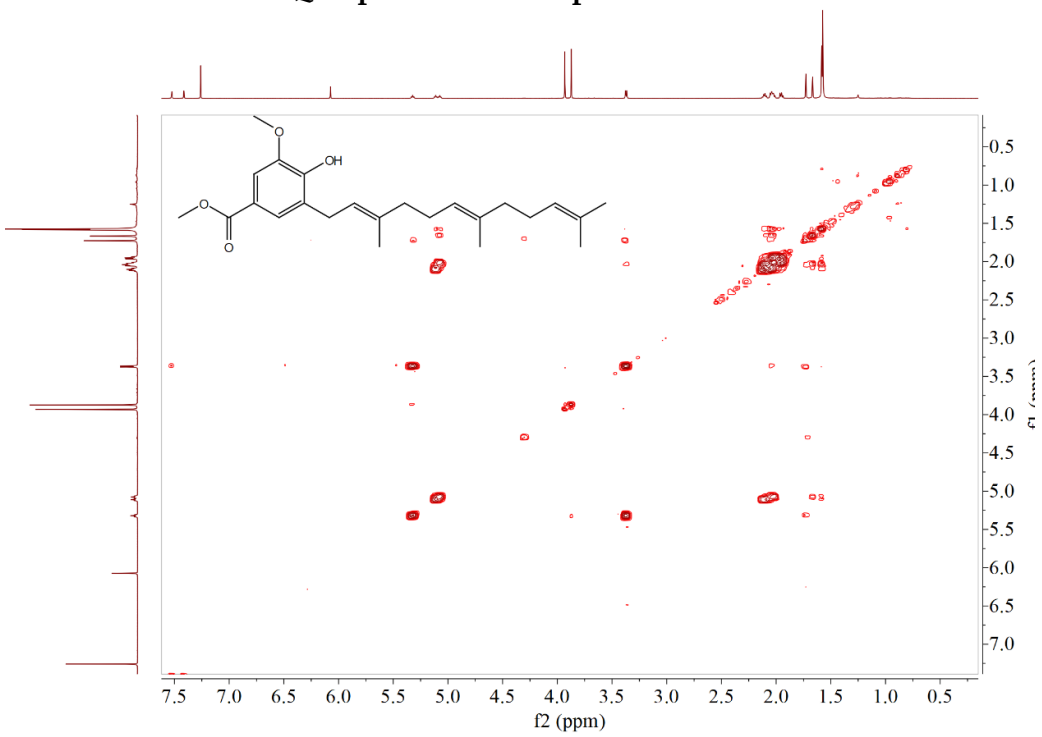
(c) ^{13}C NMR spectrum of compound 6 in $CDCl_3$



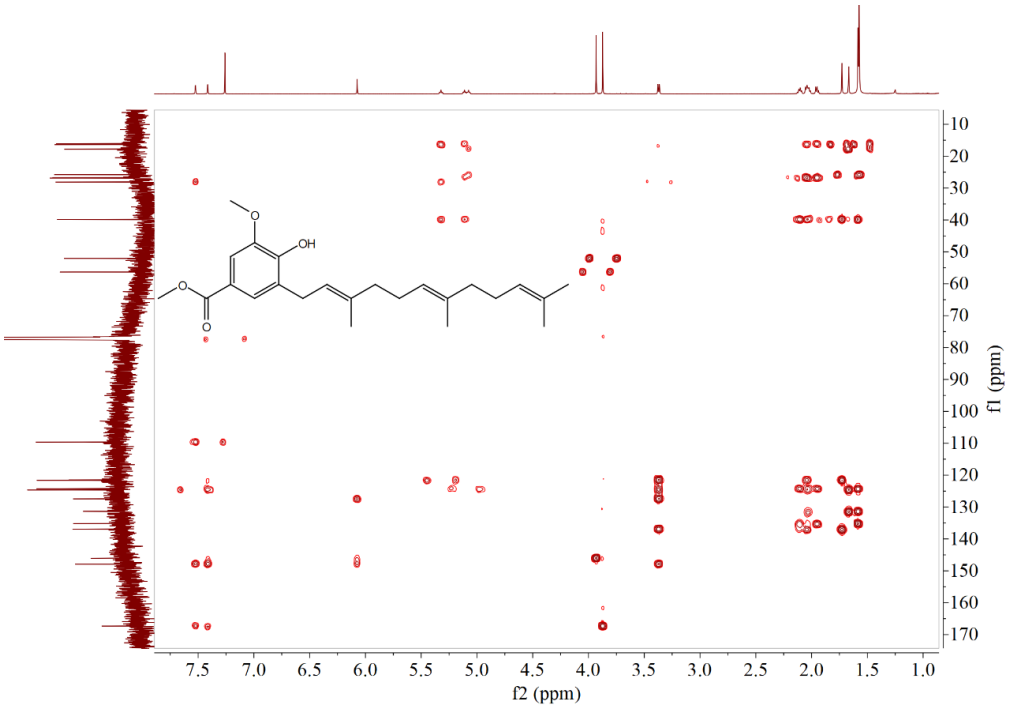
(d) DEPT spectrum of compound 6 in $CDCl_3$



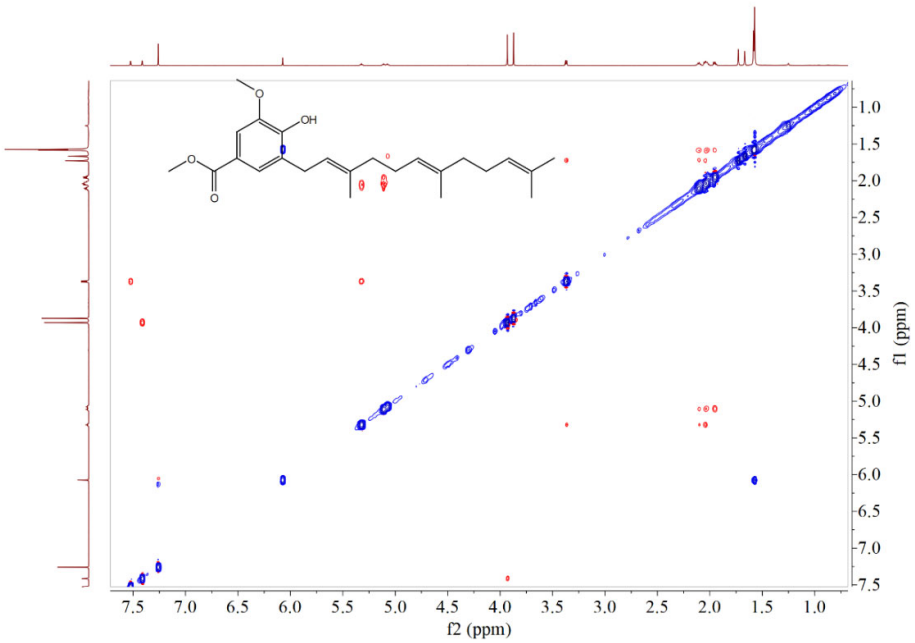
(e) HSQC spectrum of compound 6 in $CDCl_3$



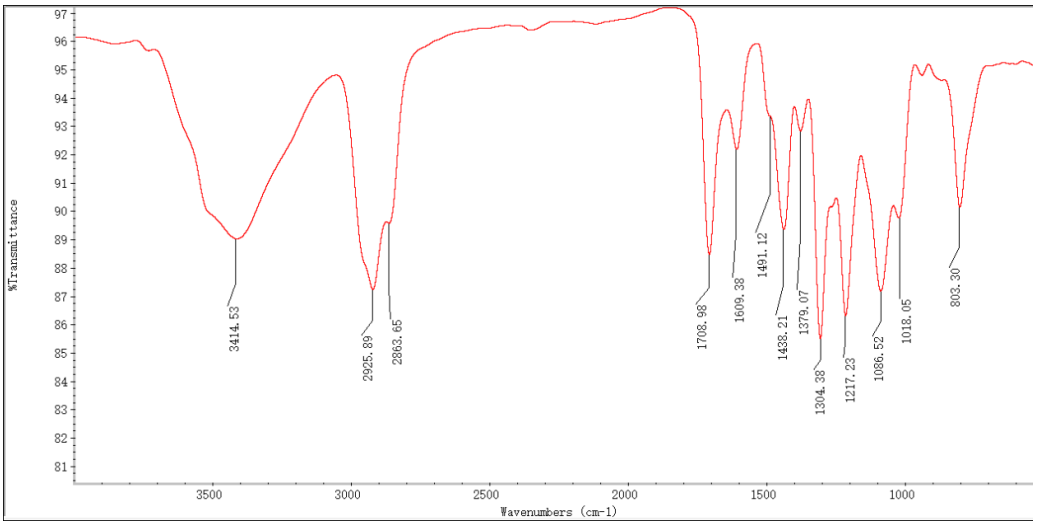
(f) ^1H-^1H COSY spectrum of compound 6 in $CDCl_3$



(g) HMBC spectrum of compound 6 in $CDCl_3$

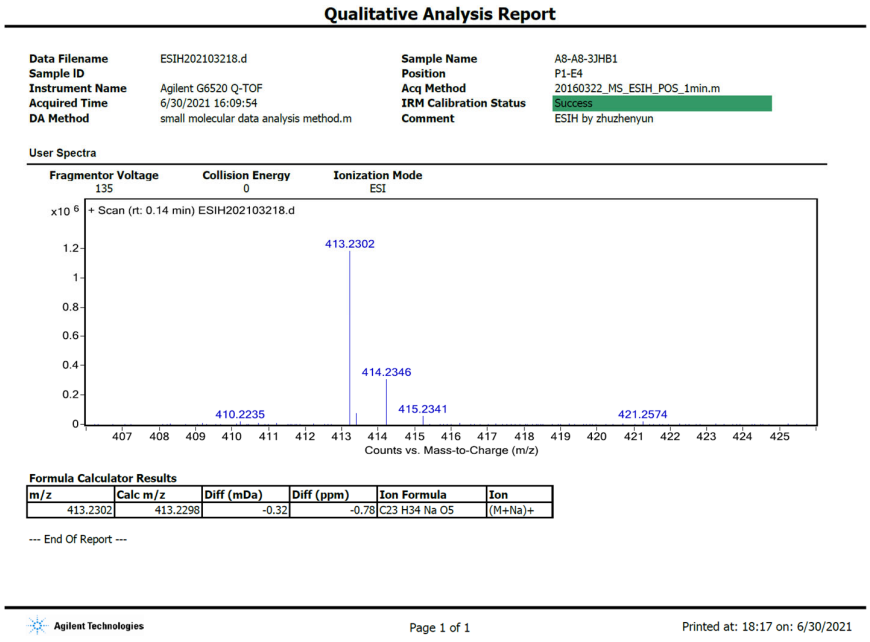


(h) NOESY spectrum of compound 6 in $CDCl_3$



(i) FT-IR spectrum of compound 6

Figure S1. 1D, 2D NMR, MS and IR spectra of Compound 6.



Qualitative Analysis Report

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Sample ID		**Position**	P1-E4
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	6/30/2021 16:09:54	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI

Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
413.2302	413.2298	-0.32	-0.78	C23 H34 Na O5	(M+Na)+

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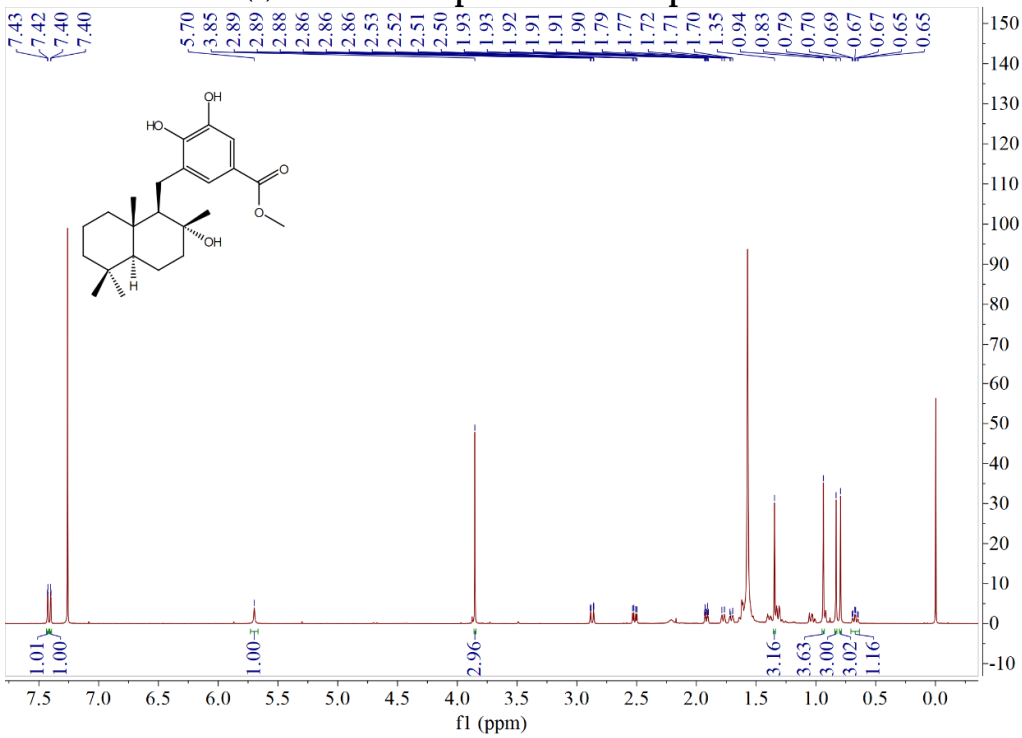
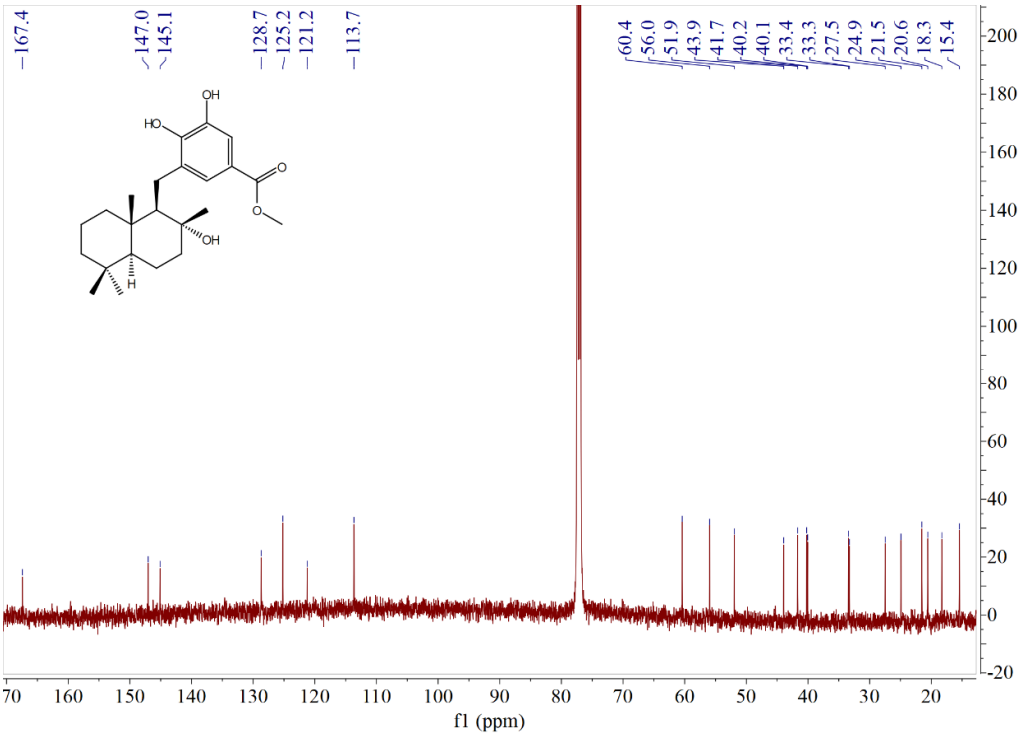
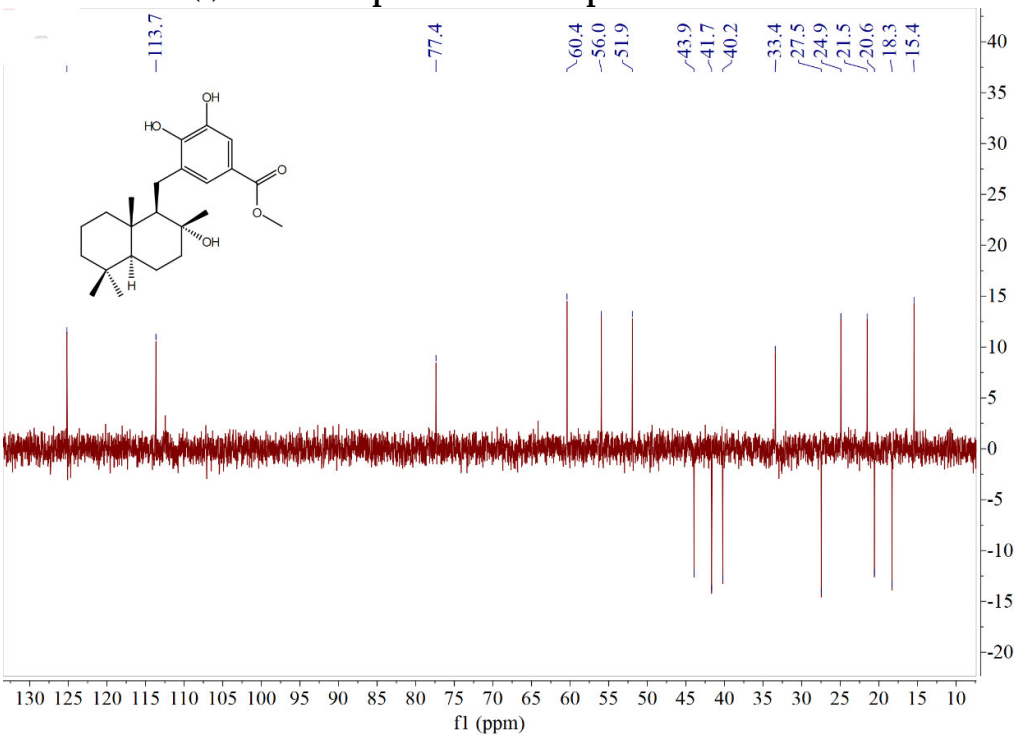
(a) HRESIMS spectrum of compound 7



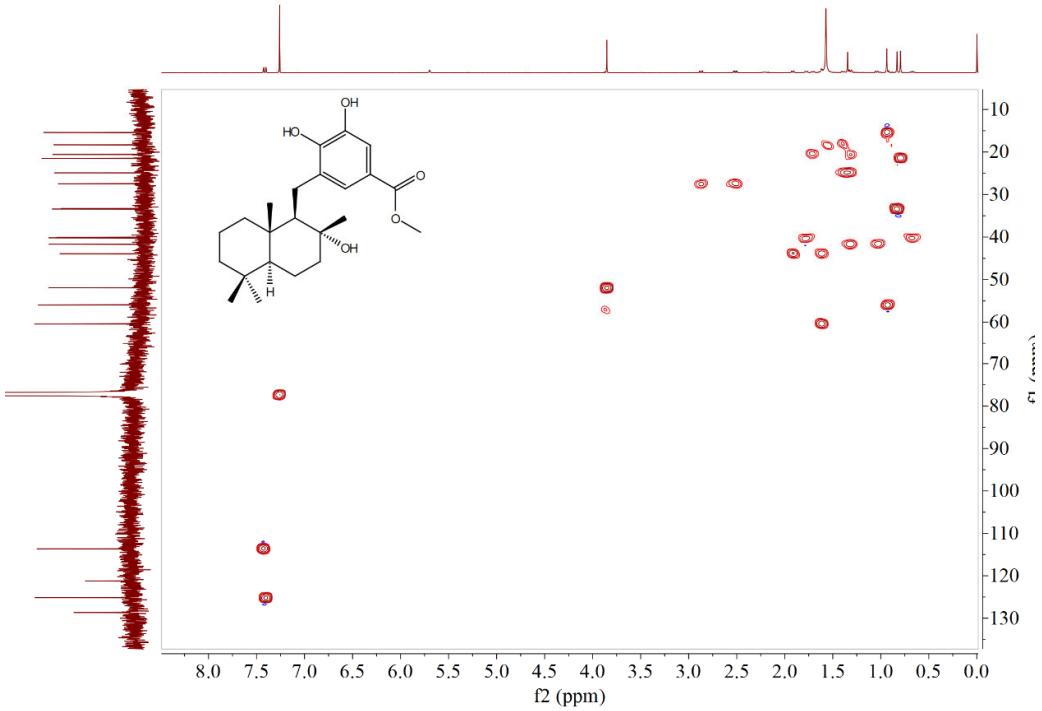
(b) ^{1}H NMR spectrum of compound 7 in $CDCl_3$



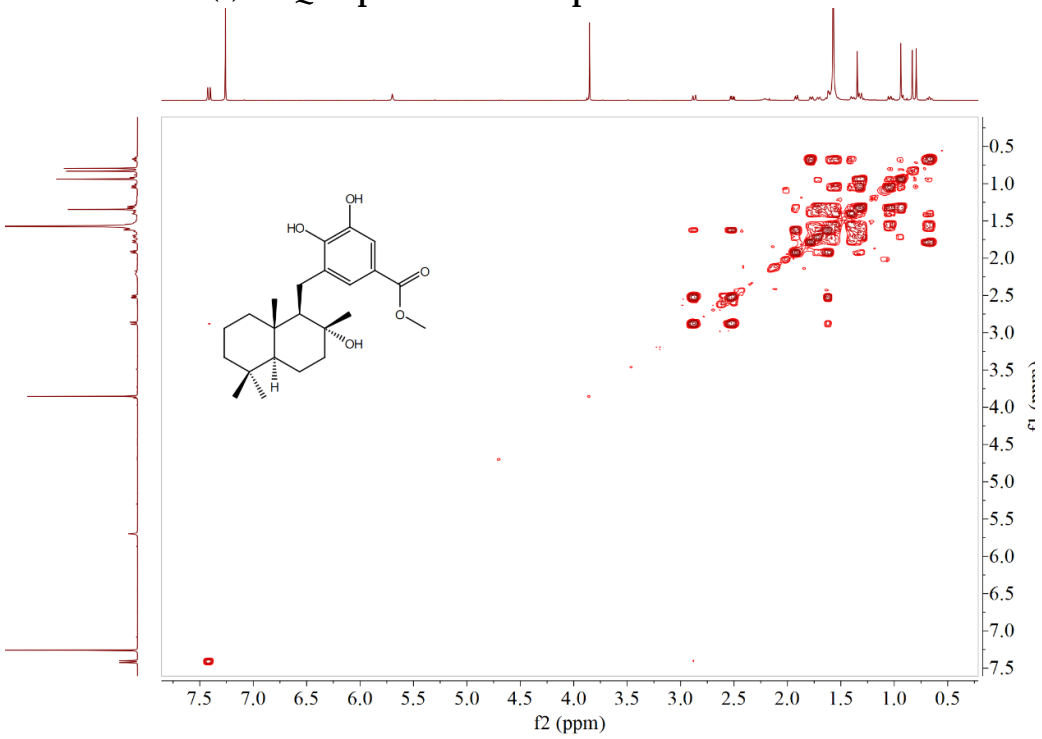
(c) ^{13}C NMR spectrum of compound 7 in $CDCl_3$



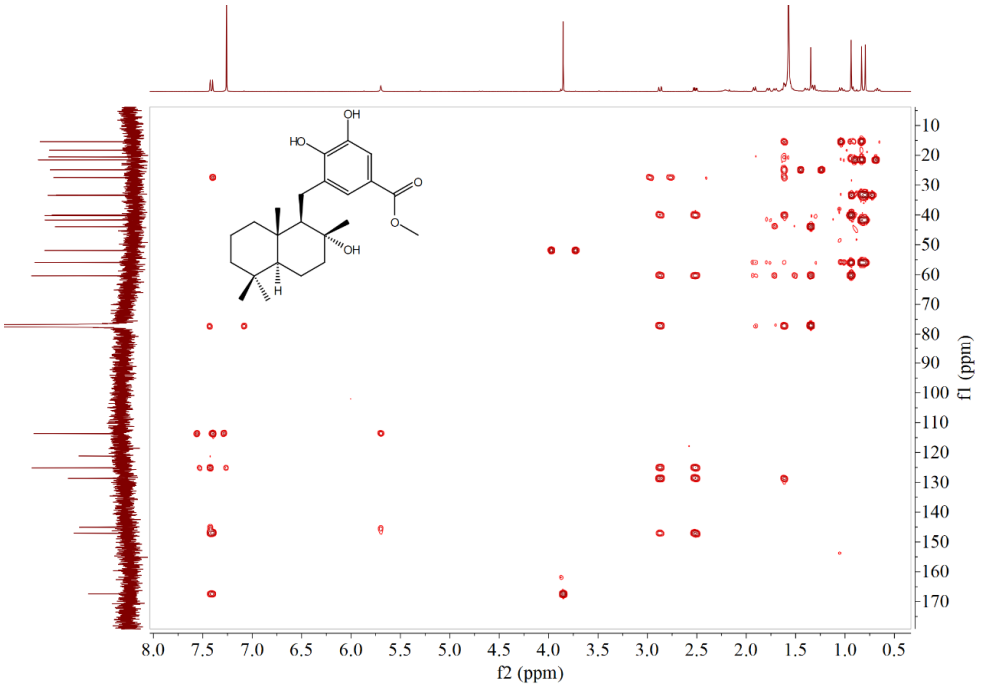
(d) DEPT spectrum of compound 7 in $CDCl_3$



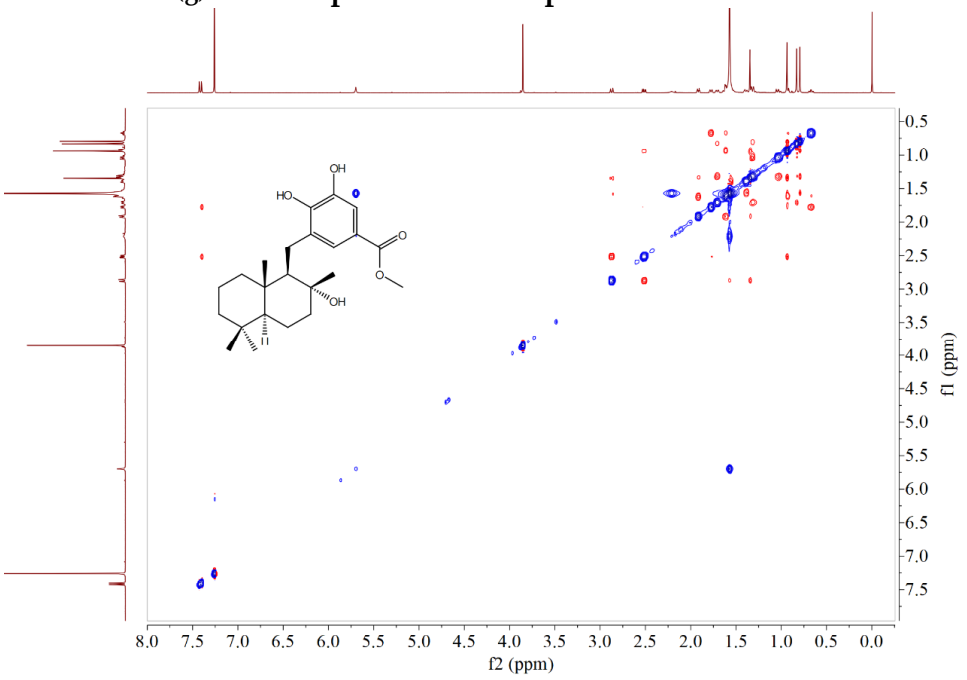
(e) HSQC spectrum of compound 7 in $CDCl_3$



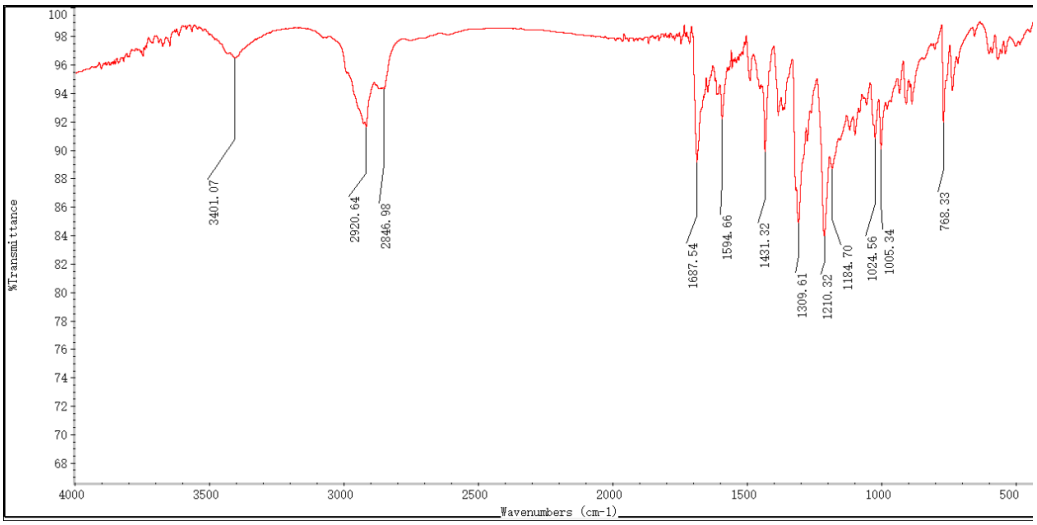
(f) ^1H-^1H COSY spectrum of compound 7 in $CDCl_3$



(g) HMBC spectrum of compound 7 in $CDCl_3$

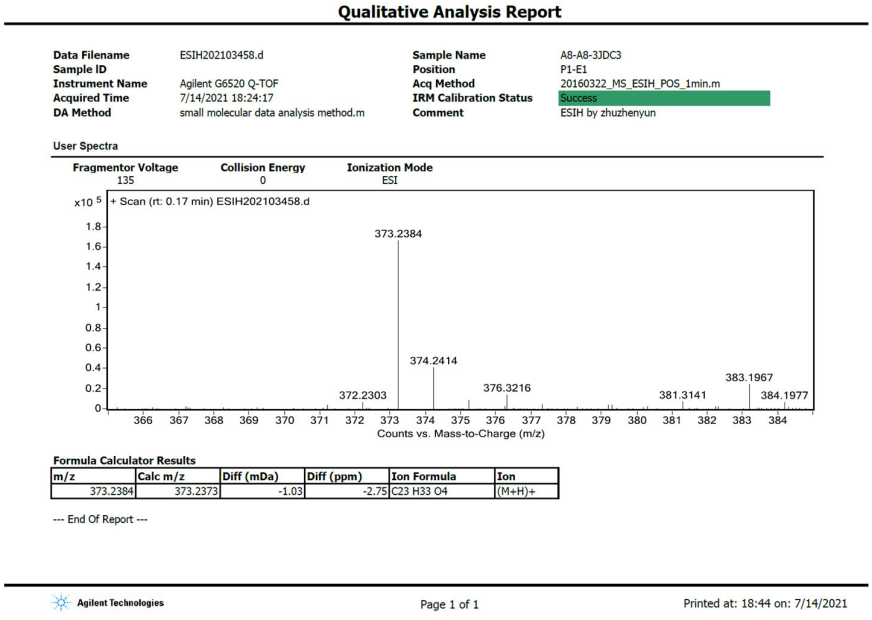


(h) NOESY spectrum of compound 7 in $CDCl_3$



(i) FT-IR spectrum of compound 7

Figure S2 1D, 2D NMR, MS and IR spectra of Compound 7



Qualitative Analysis Report

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Sample ID		**Position**	P1-E1
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	7/14/2021 18:24:17	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI

Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
373.2384	373.2373	-1.03	-2.75	C23 H33 O4	(M+H)+

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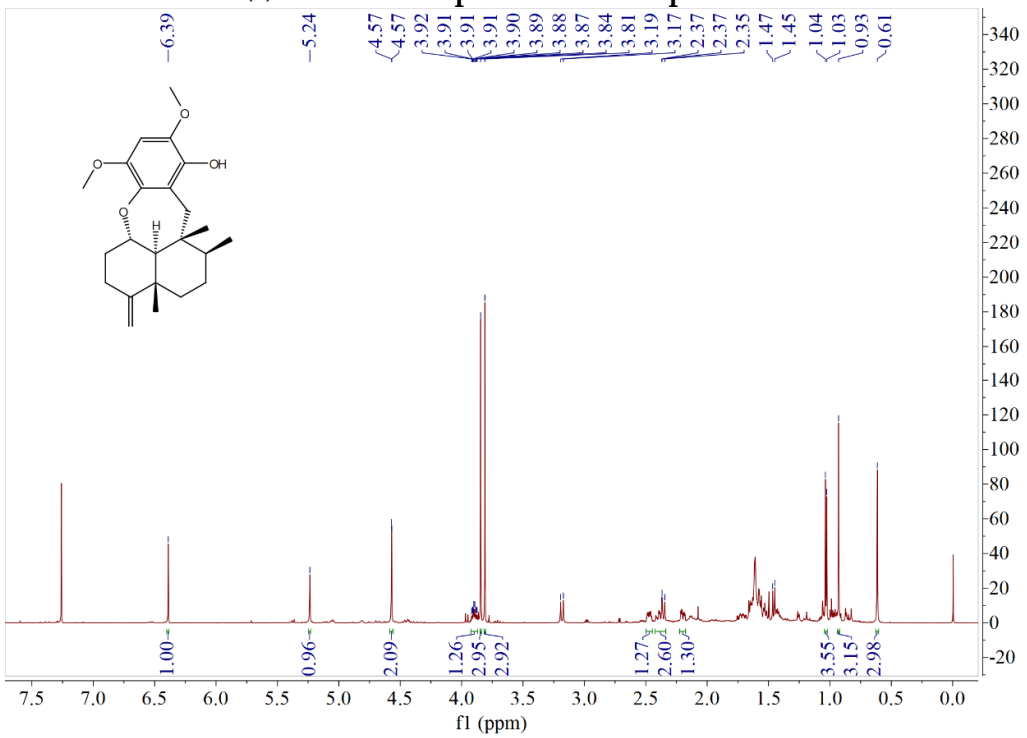
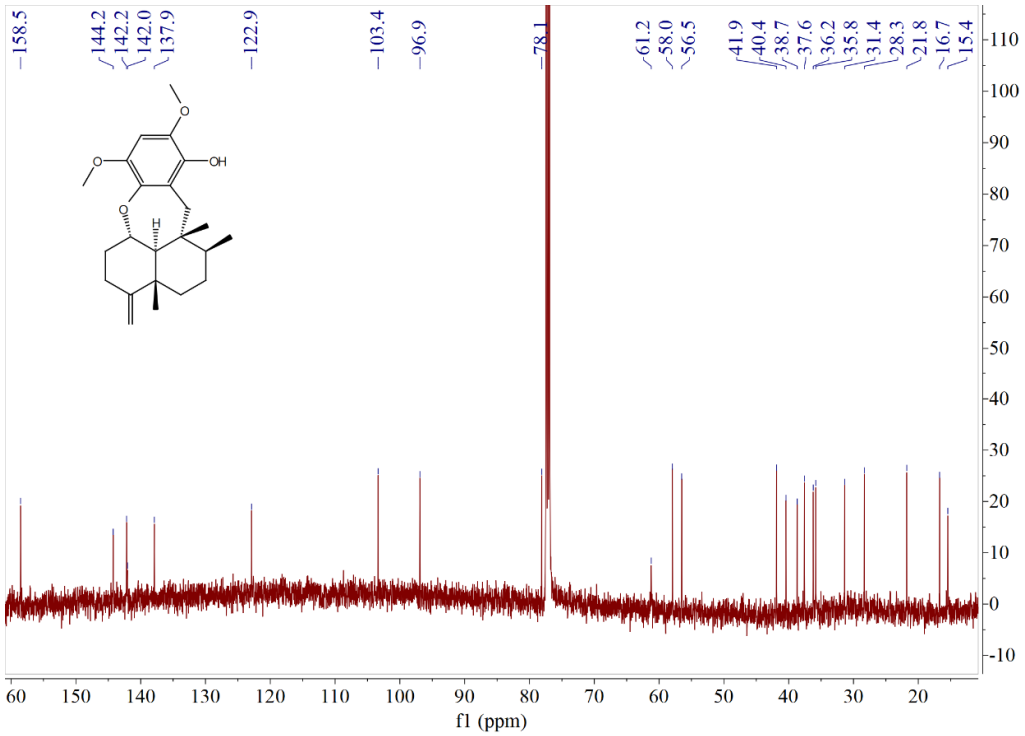
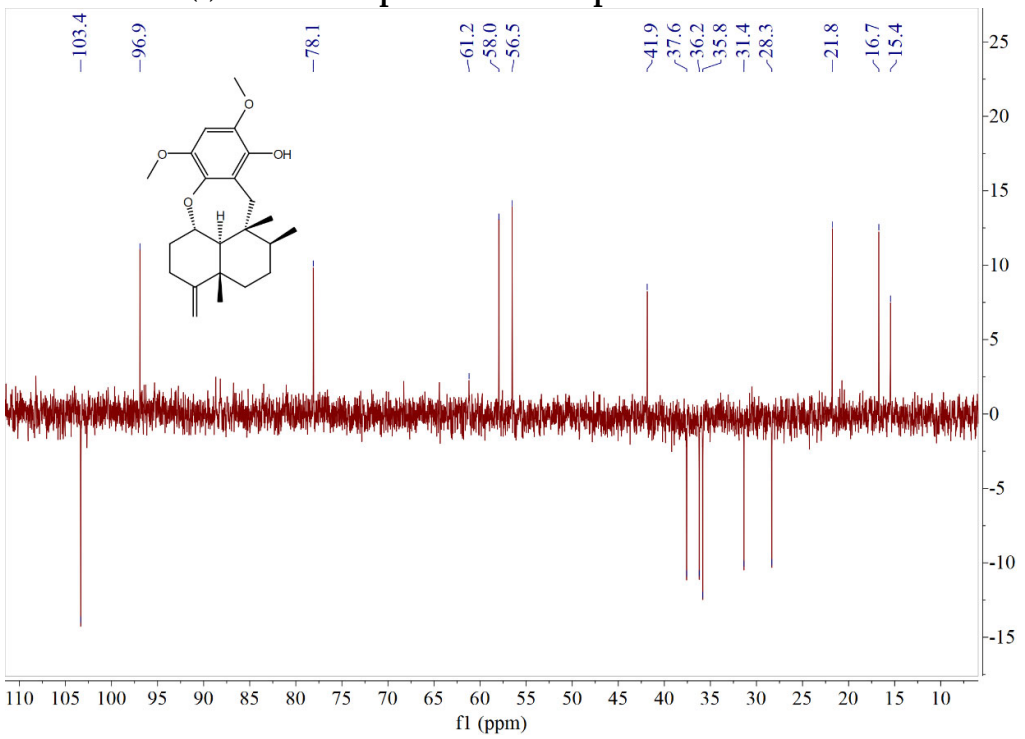
(a) HRESIMS spectrum of compound 8



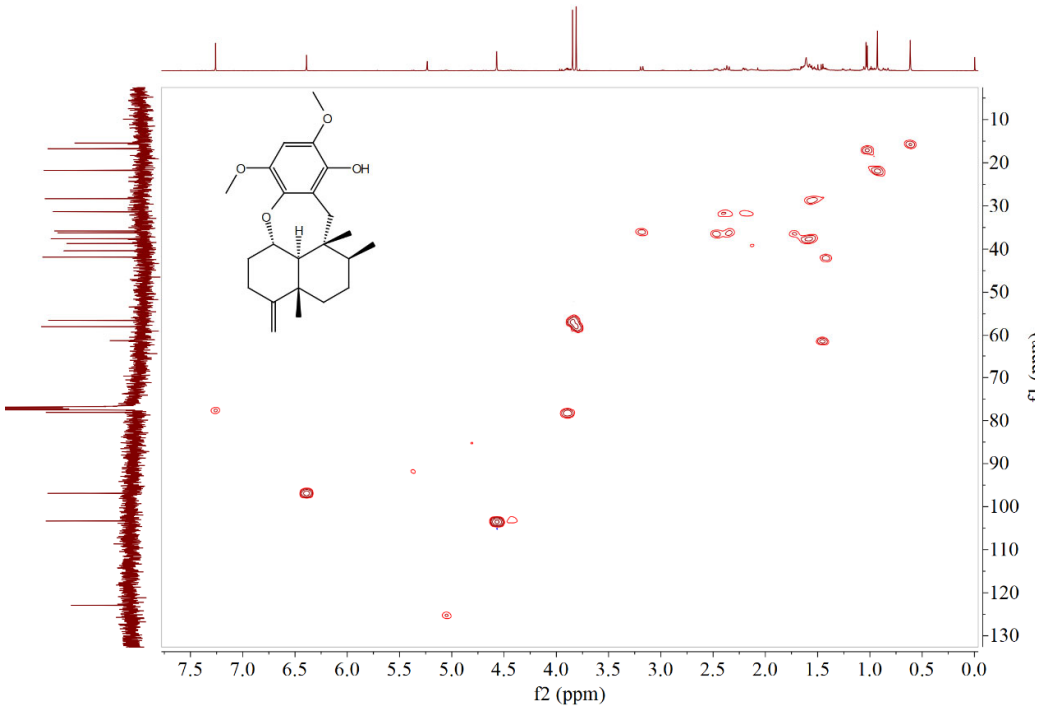
(b) ^{1}H NMR spectrum of compound 8 in $CDCl_3$



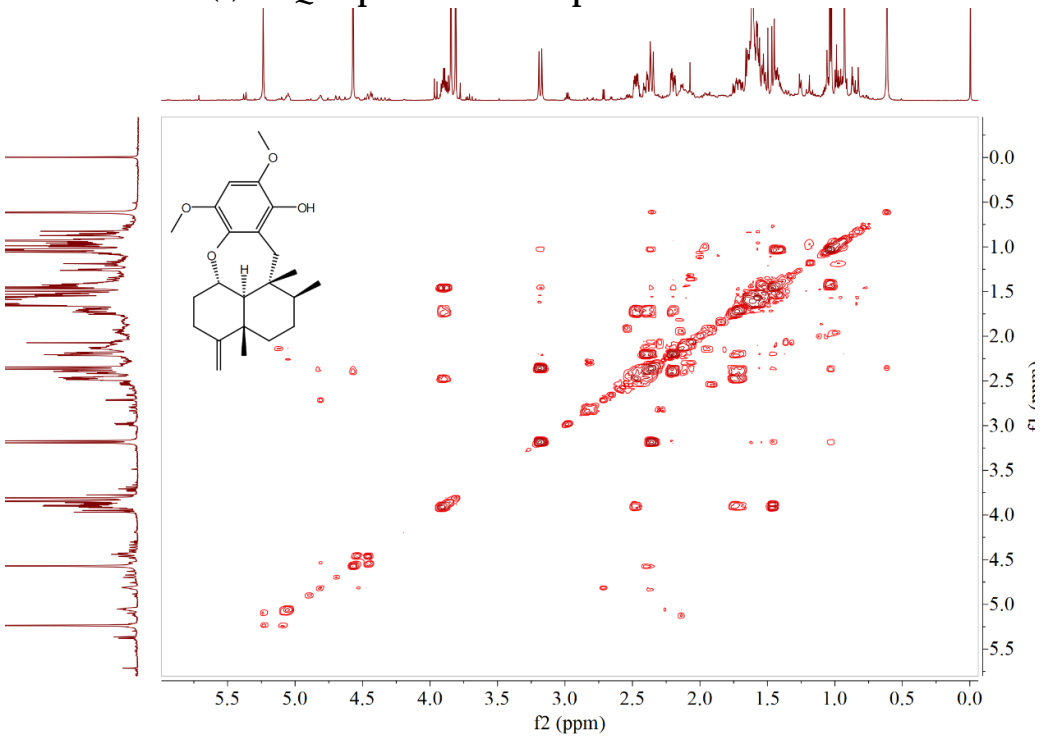
(c) ^{13}C NMR spectrum of compound 8 in $CDCl_3$



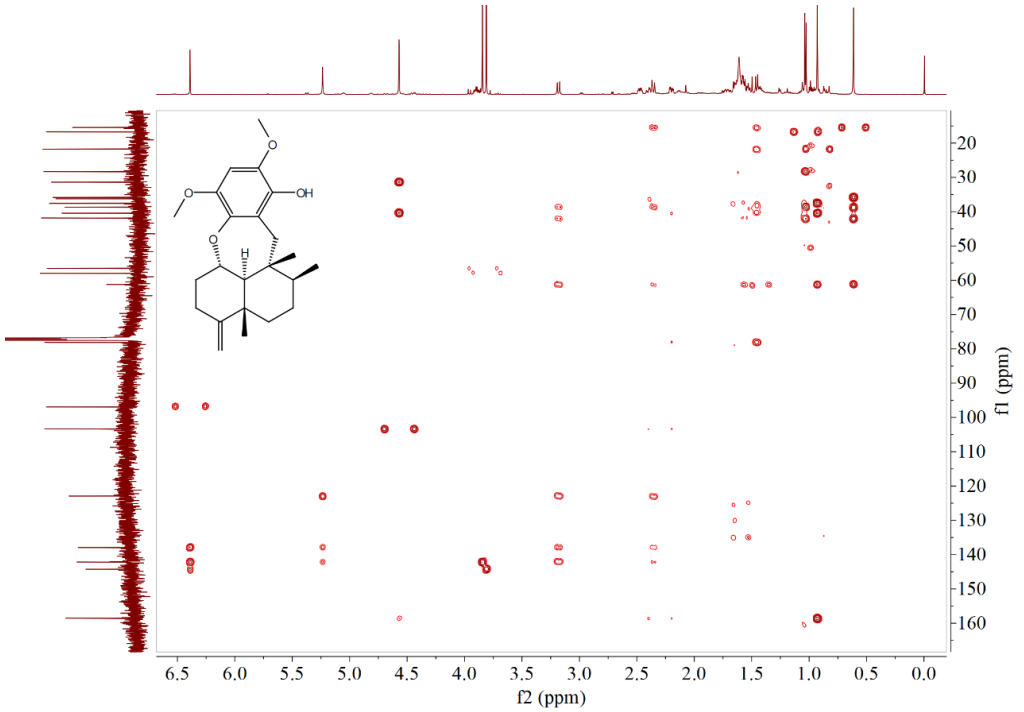
(d) DEPT spectrum of compound 8 in $CDCl_3$



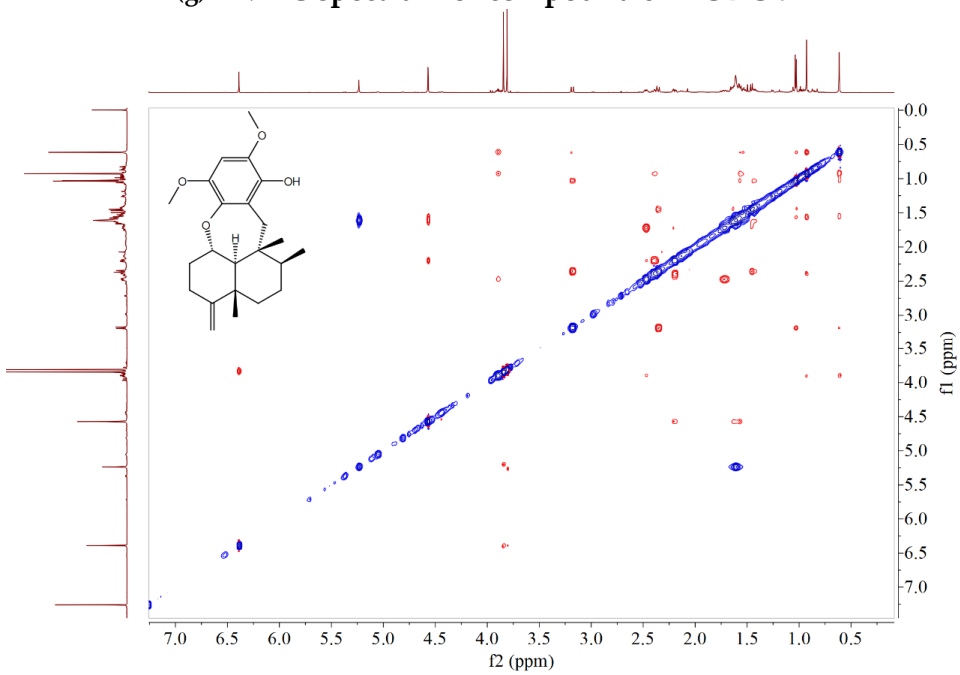
(e) HSQC spectrum of compound 8 in $CDCl_3$



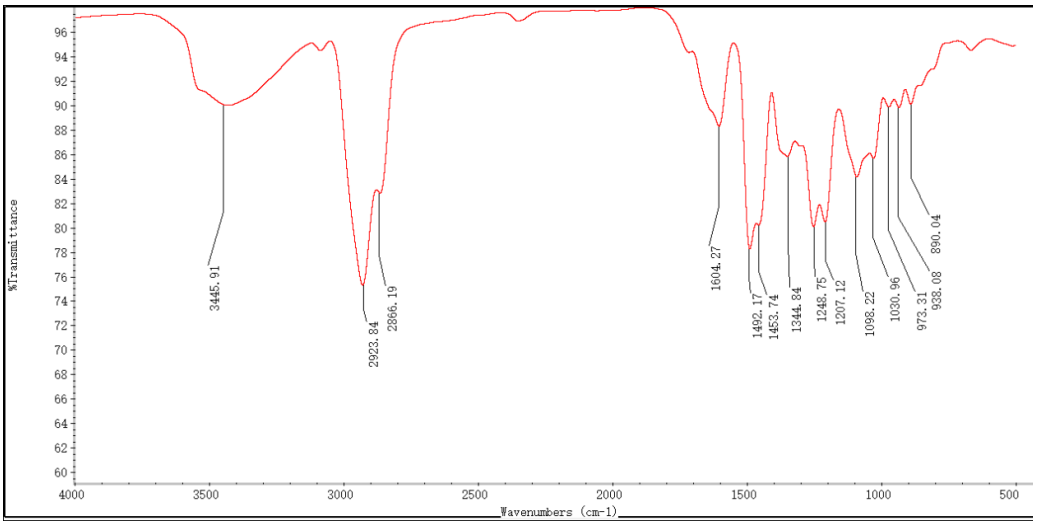
(f) ^1H-^1H COSY spectrum of compound 8 in $CDCl_3$



(g) HMBC spectrum of compound 8 in $CDCl_3$



(h) NOESY spectrum of compound 8 in $CDCl_3$



(i) FT-IR spectrum of compound 8

Figure S3 1D, 2D NMR, MS and IR spectra of Compound 8

D:\data\2021\EI202101307_A8-A8-2JGC4 -c1 6/15/2021 8:54:37 AM

EI202101307_A8-A8-2JGC4 -c1#7 RT: 1.24
T: + c EI Full ms [49.50-800.50]
m/z= 48-803

m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	RDB equiv.	Composition
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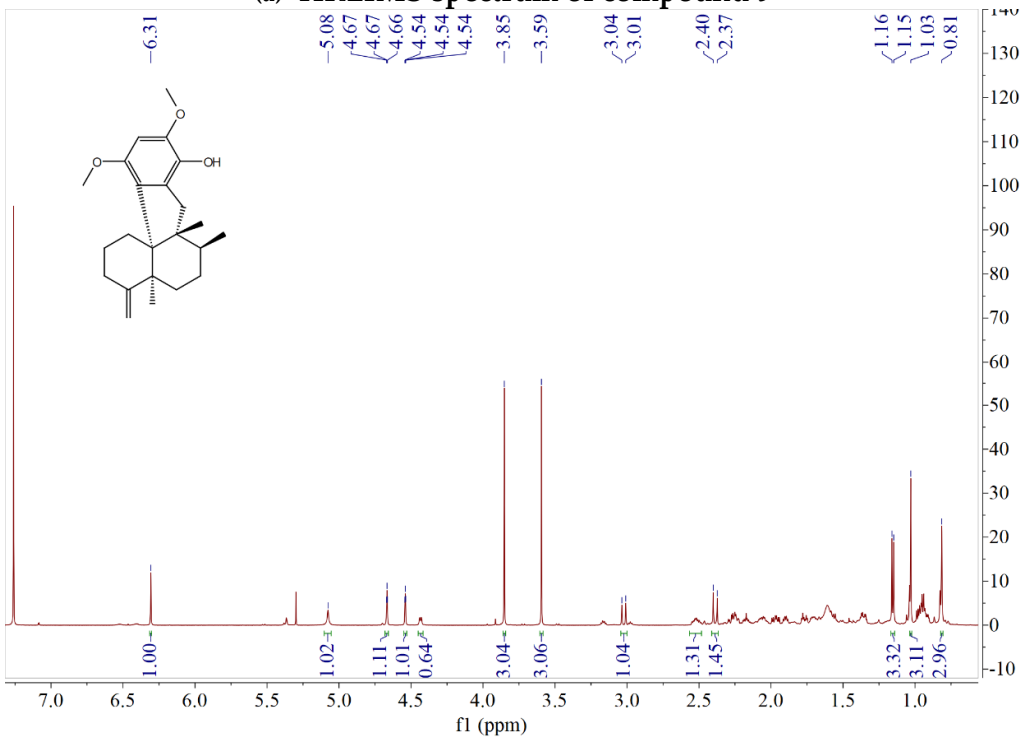
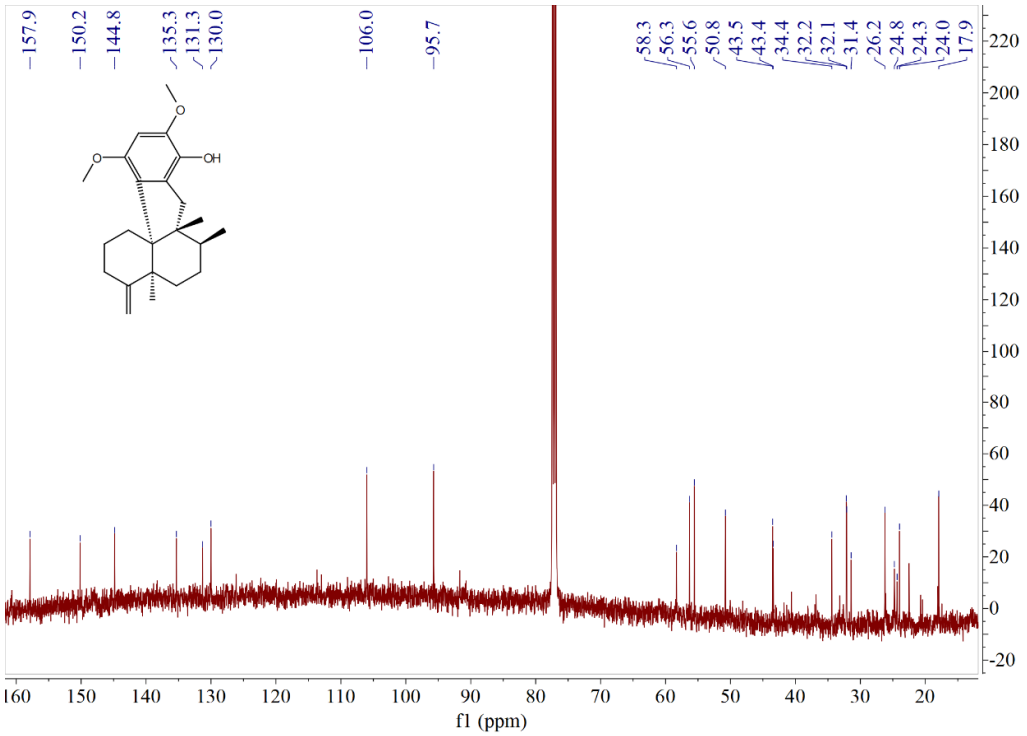
217.0858	228612.0	6.84	217.0859	-0.16	7.5	$C_{13}H_{13}O_3$
218.0939	311565.0	9.33	218.0937	0.11	7.0	$C_{13}H_{14}O_3$
219.1013	236693.0	7.09	219.1016	-0.30	6.5	$C_{13}H_{15}O_3$
220.1097	1258839.0	37.69	220.1094	0.35	6.0	$C_{13}H_{16}O_3$
231.1013	262170.0	7.85	231.1016	-0.27	7.5	$C_{14}H_{15}O_3$
232.1090	509735.0	15.26	232.1094	-0.40	7.0	$C_{14}H_{16}O_3$
233.1167	465511.0	13.94	233.1172	-0.56	6.5	$C_{14}H_{17}O_3$
356.2346	1504553.0	45.04	356.2346	0.00	8.0	$C_{23}H_{32}O_3$

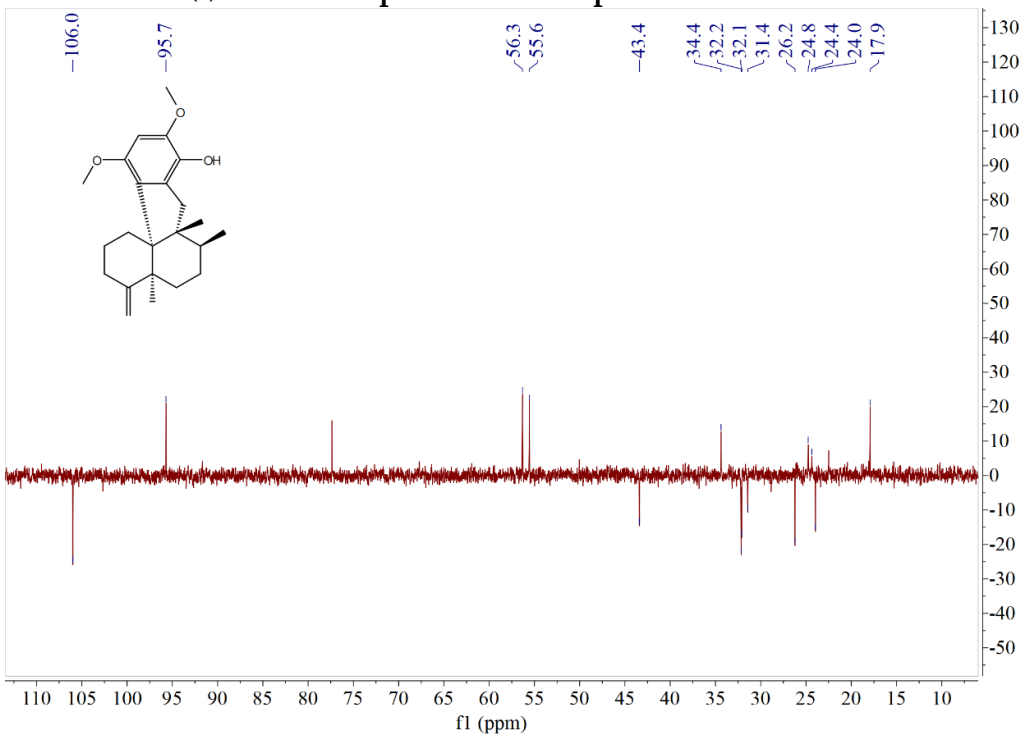
(a) HREIMS spectrum of compound 9



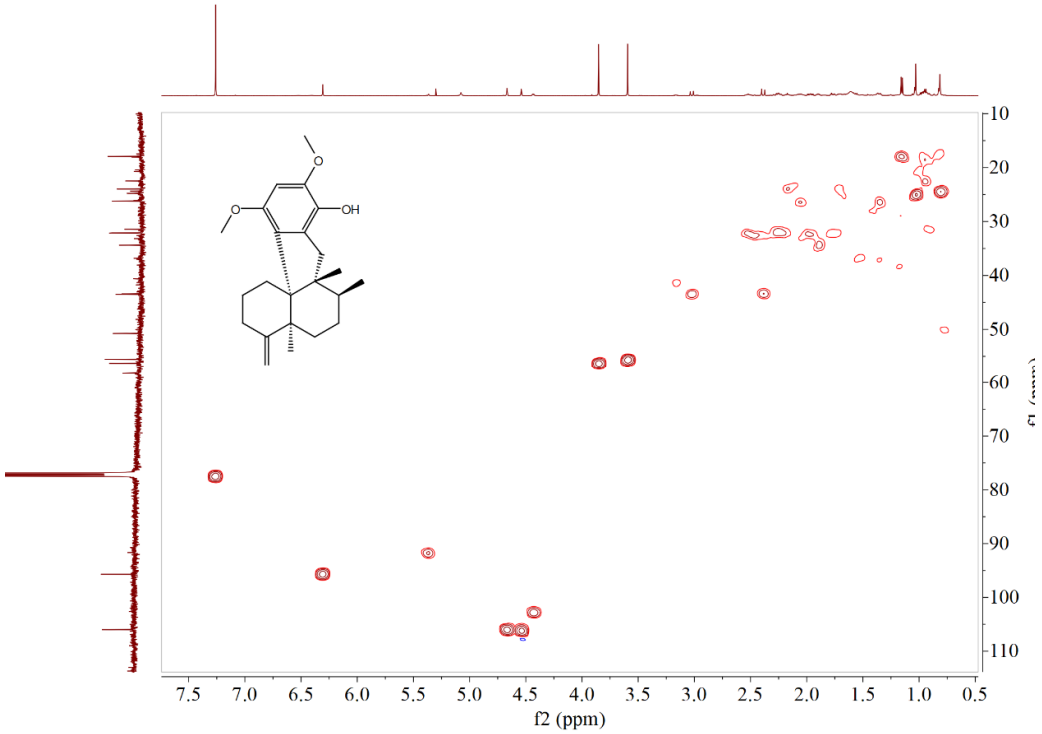
(b) ^{1}H NMR spectrum of compound 9 in $CDCl_3$



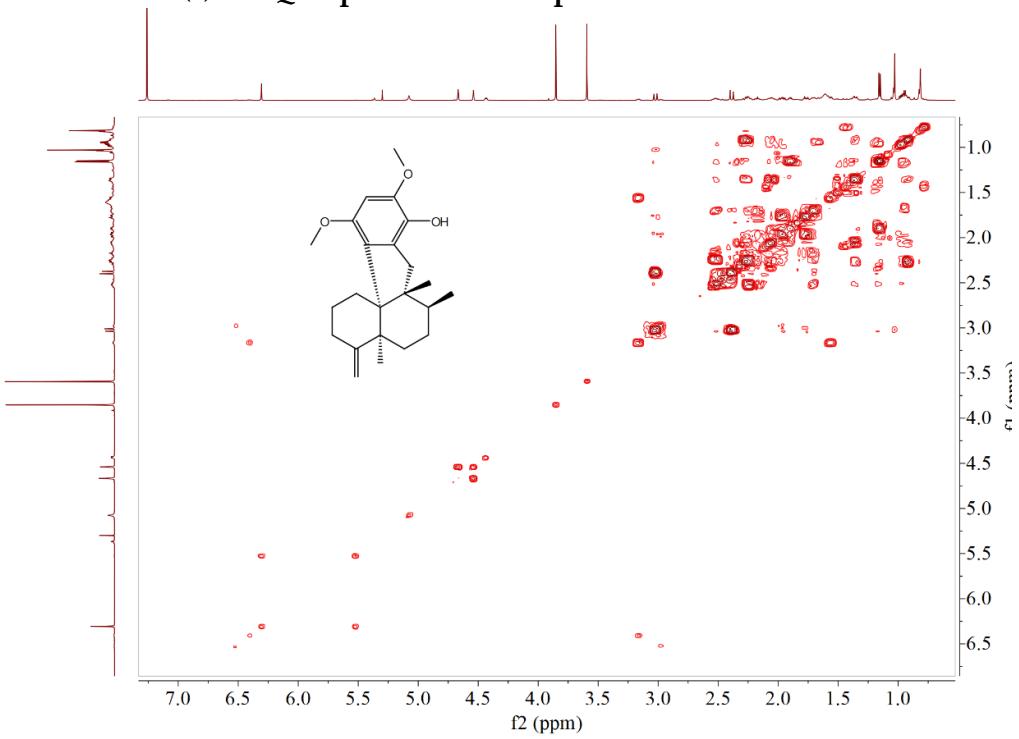
(c) ^{13}C NMR spectrum of compound 9 in $CDCl_3$



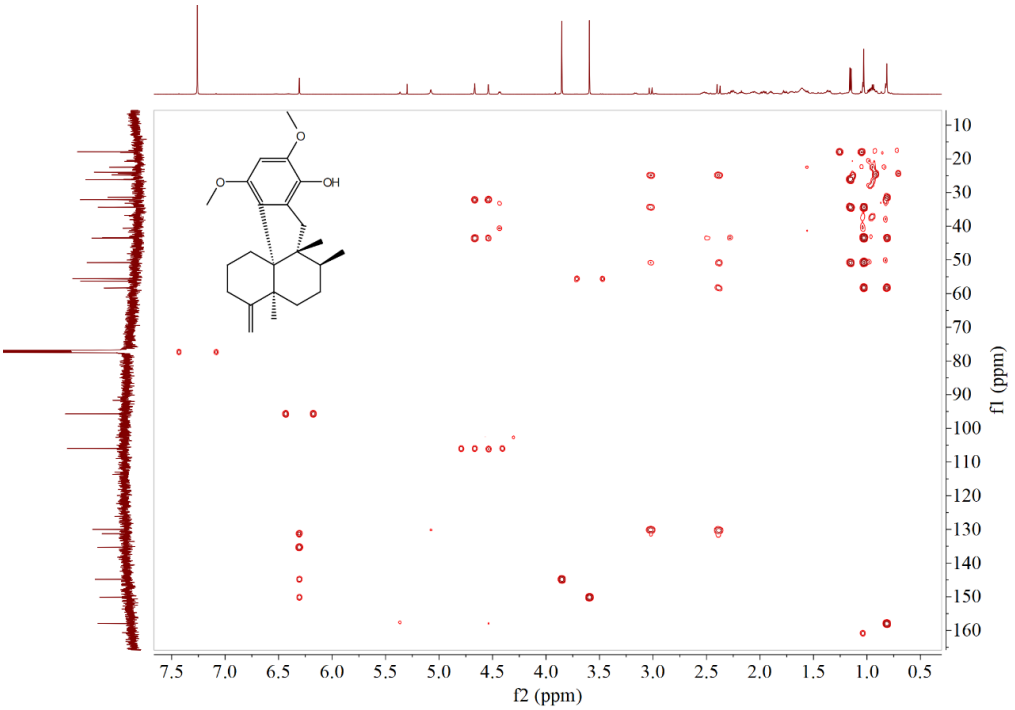
(d) DEPT spectrum of compound 9 in $CDCl_3$



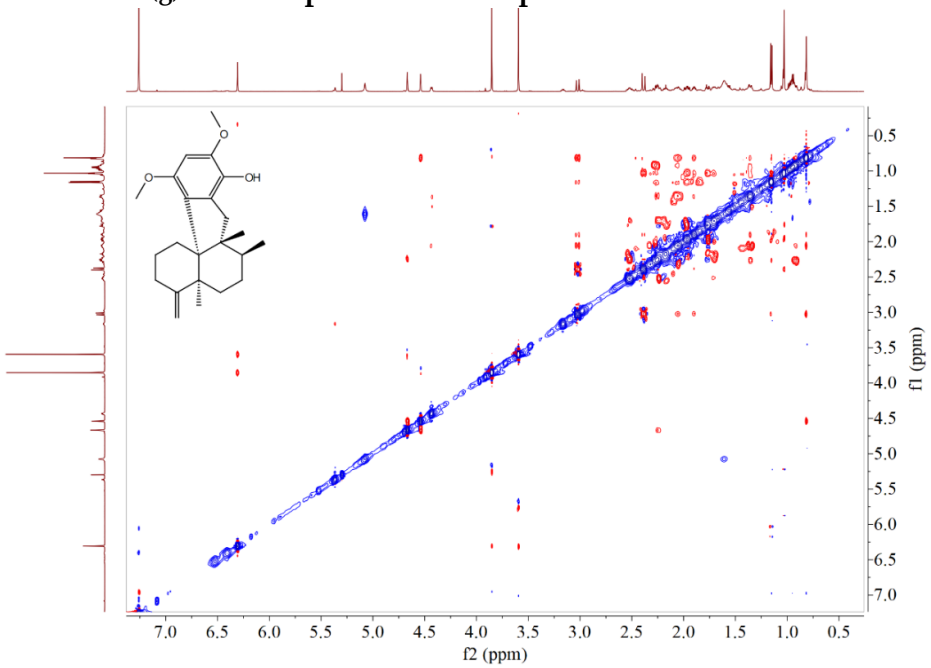
(e) HSQC spectrum of compound 9 in $CDCl_3$



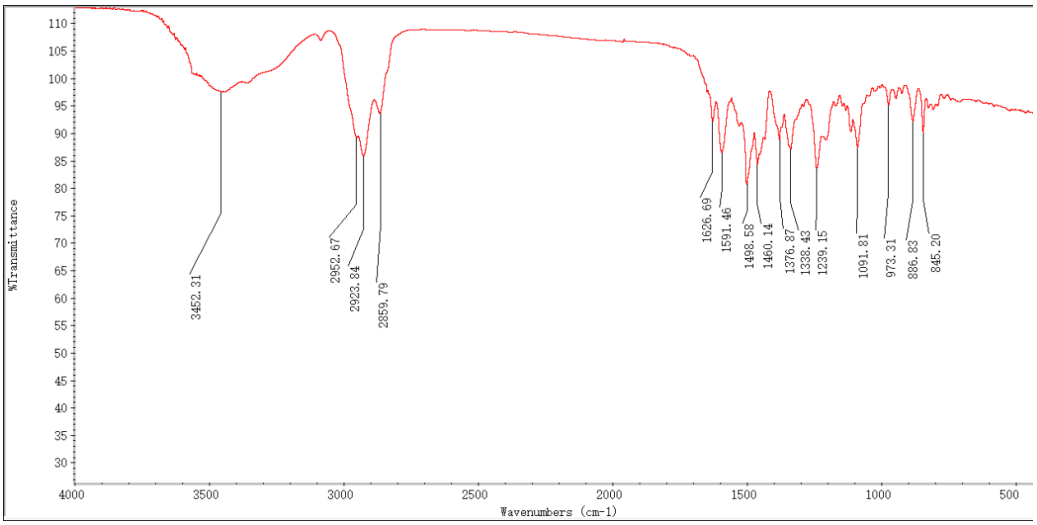
(f) ^1H-^1H COSY spectrum of compound 9 in $CDCl_3$



(g) HMBC spectrum of compound 9 in $CDCl_3$

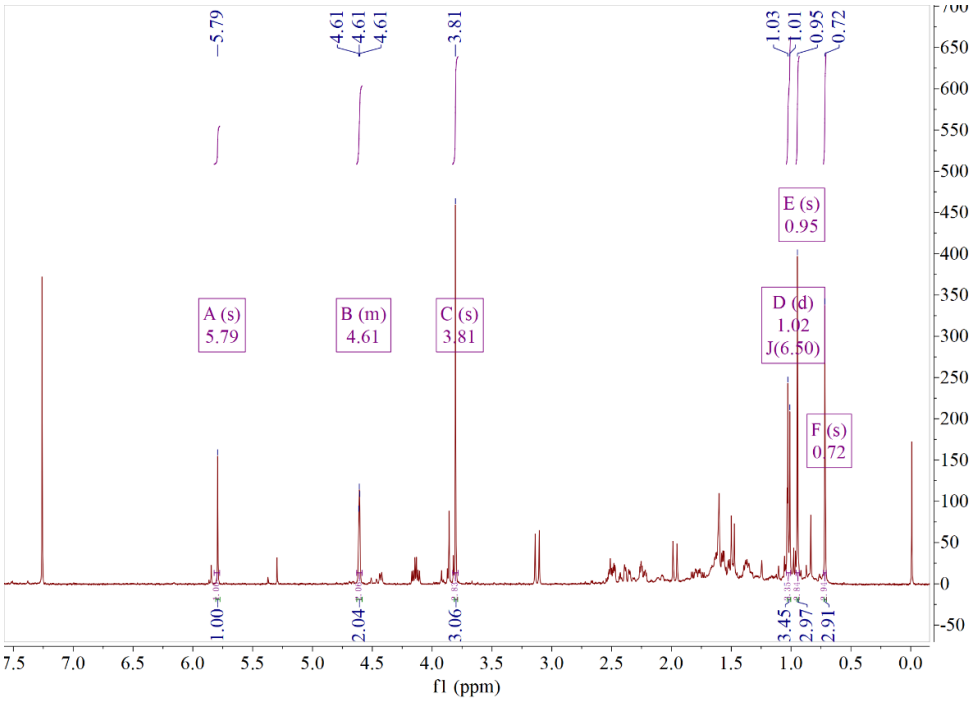


(h) NOESY spectrum of compound 9 in $CDCl_3$

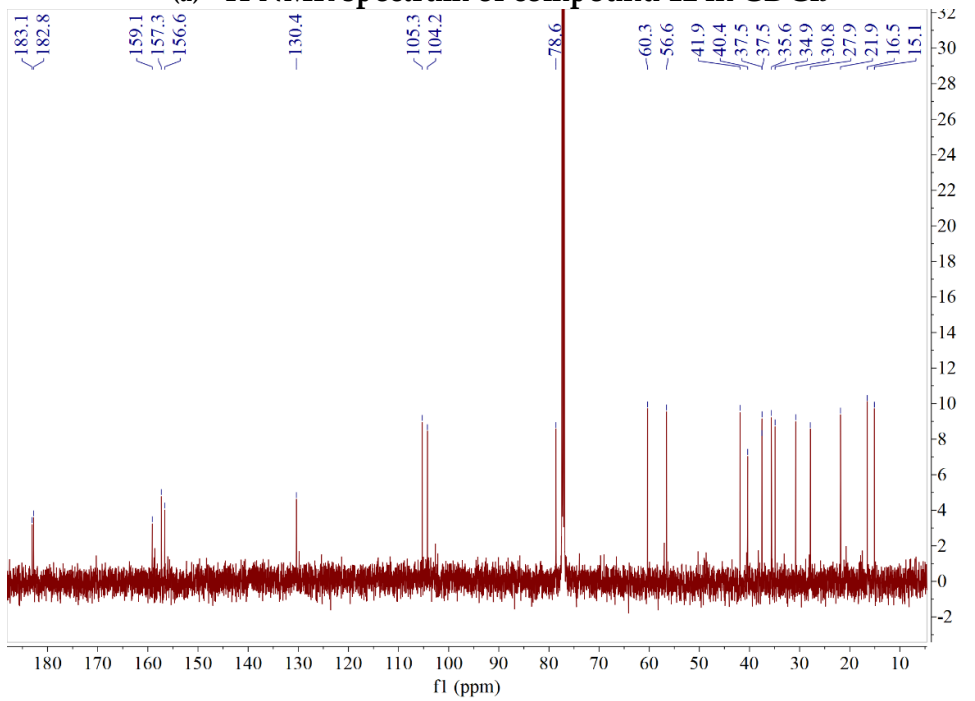


(i) FT-IR spectrum of compound 9

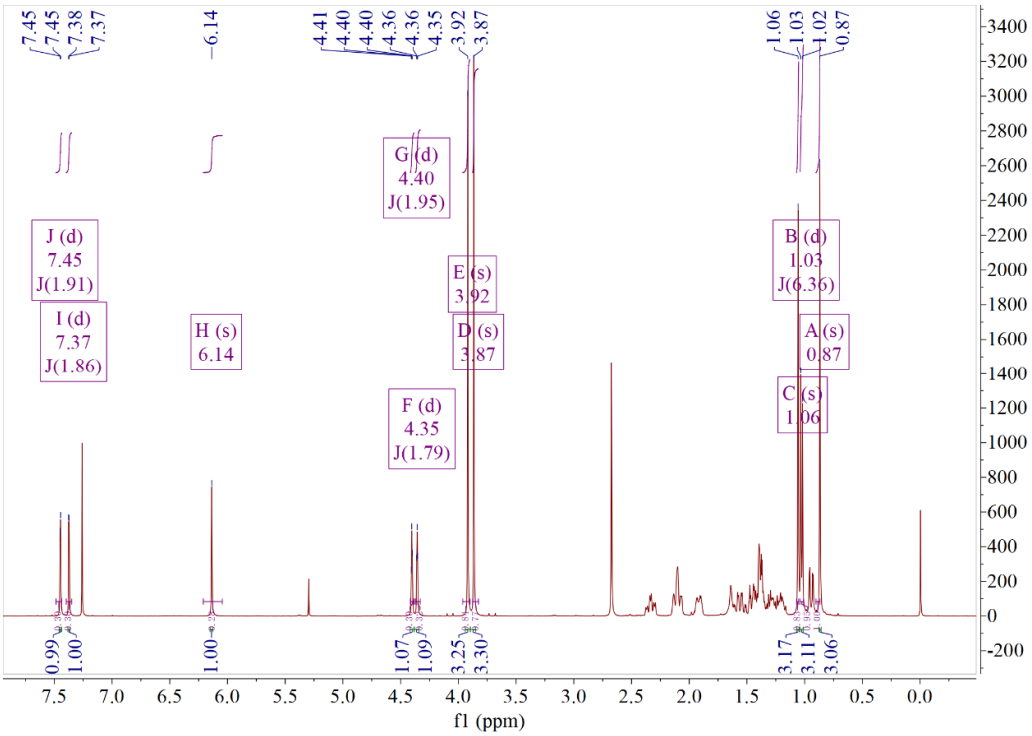
Figure S4 1D, 2D NMR, MS and IR spectra of Compound 9



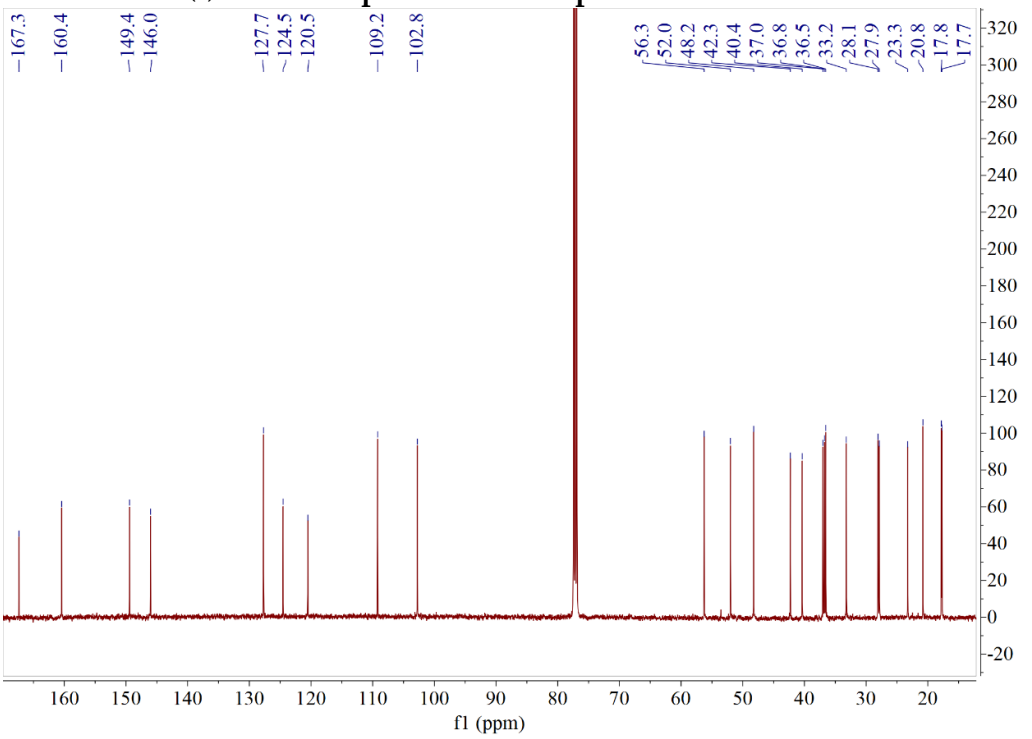
(a) ^{1}H NMR spectrum of compound 12 in $CDCl_3$



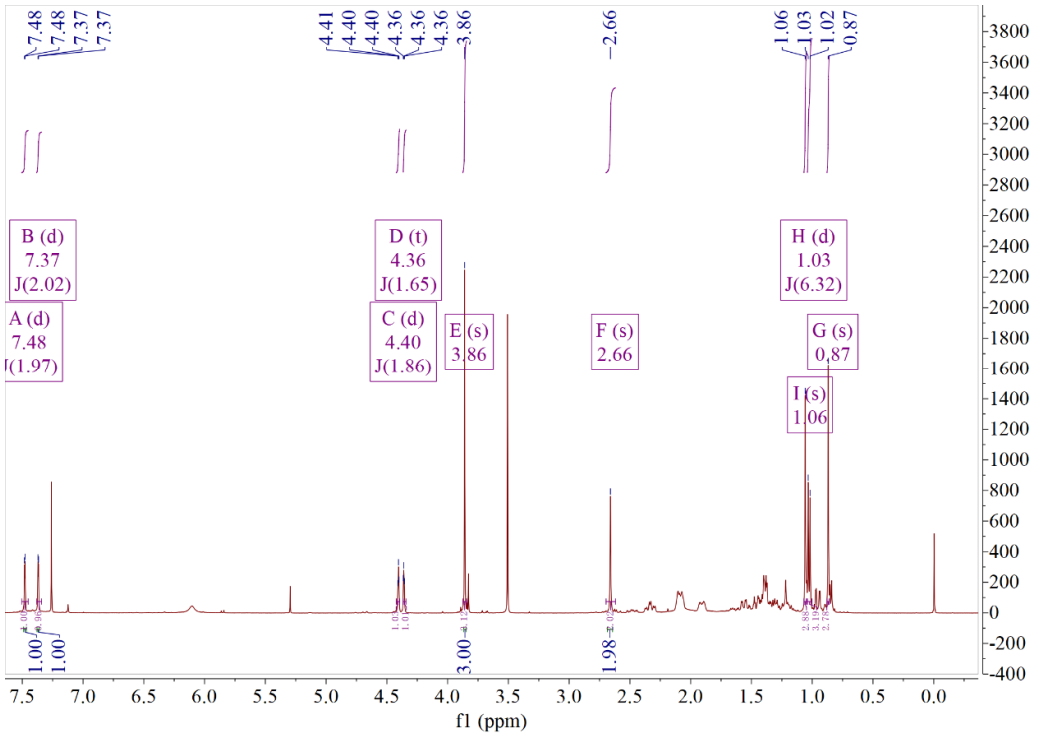
(b) ^{13}C NMR spectrum of compound 12 in $CDCl_3$



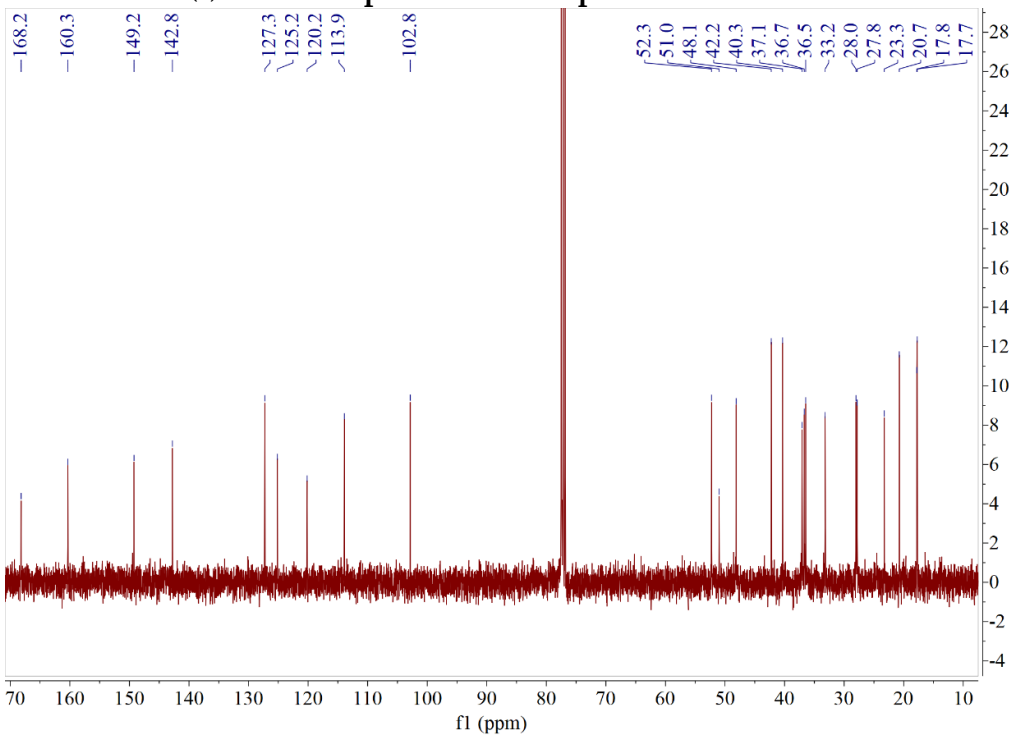
(c) ^{1}H NMR spectrum of compound 14 in $CDCl_3$



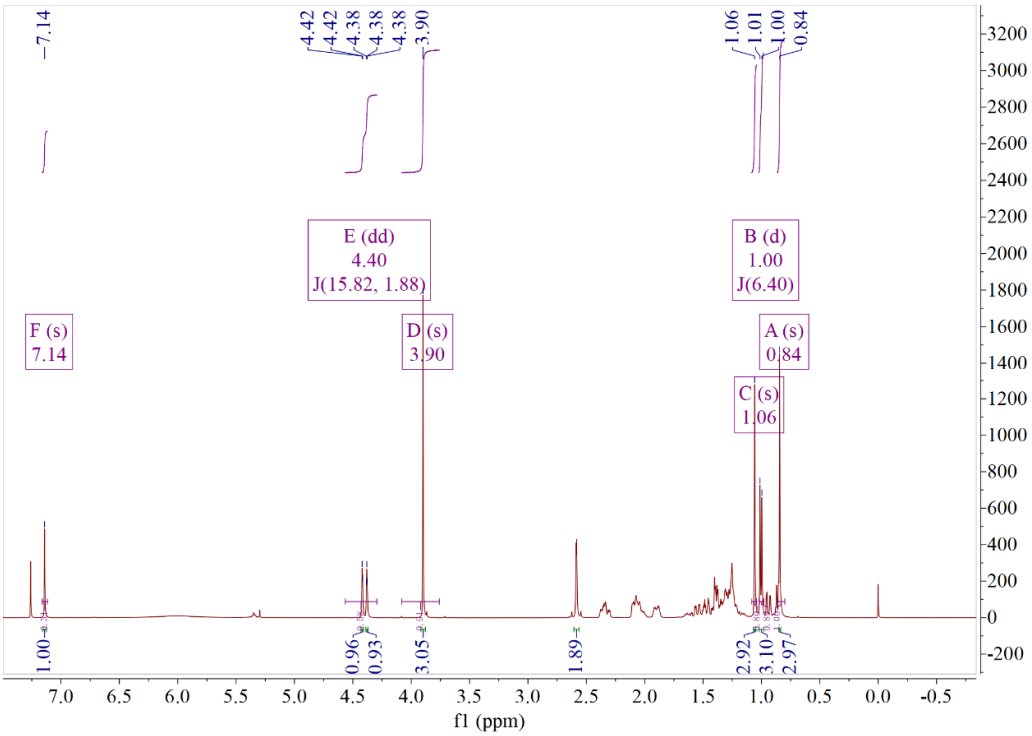
(d) ^{13}C NMR spectrum of compound 14 in $CDCl_3$



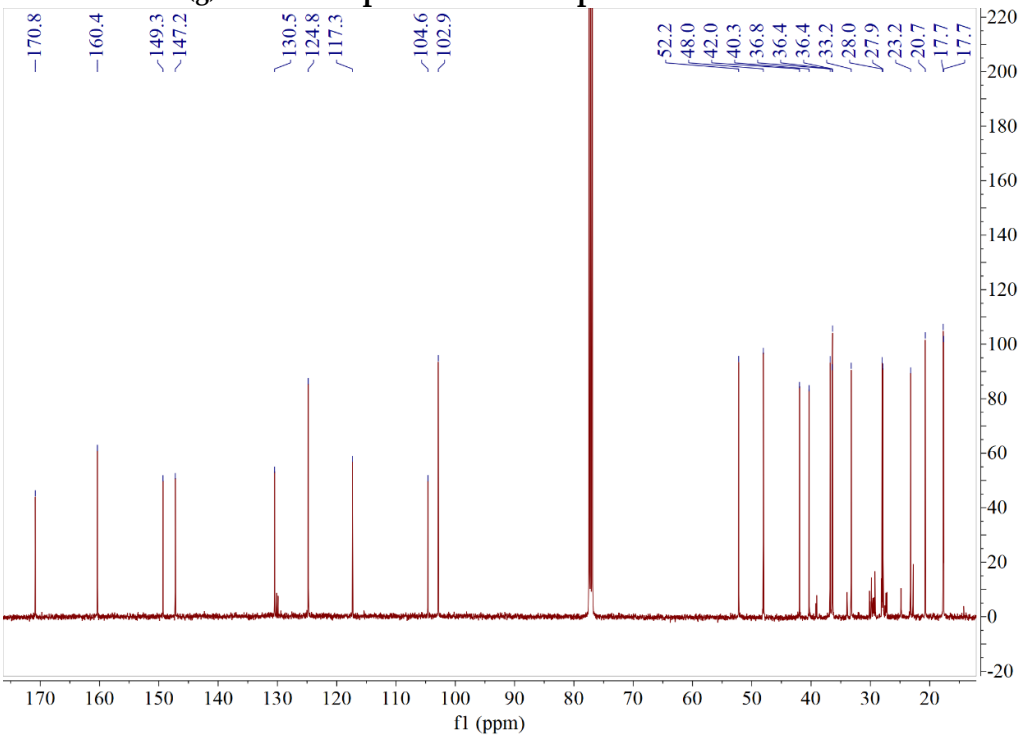
(e) ^{1}H NMR spectrum of compound 15 in $CDCl_3$



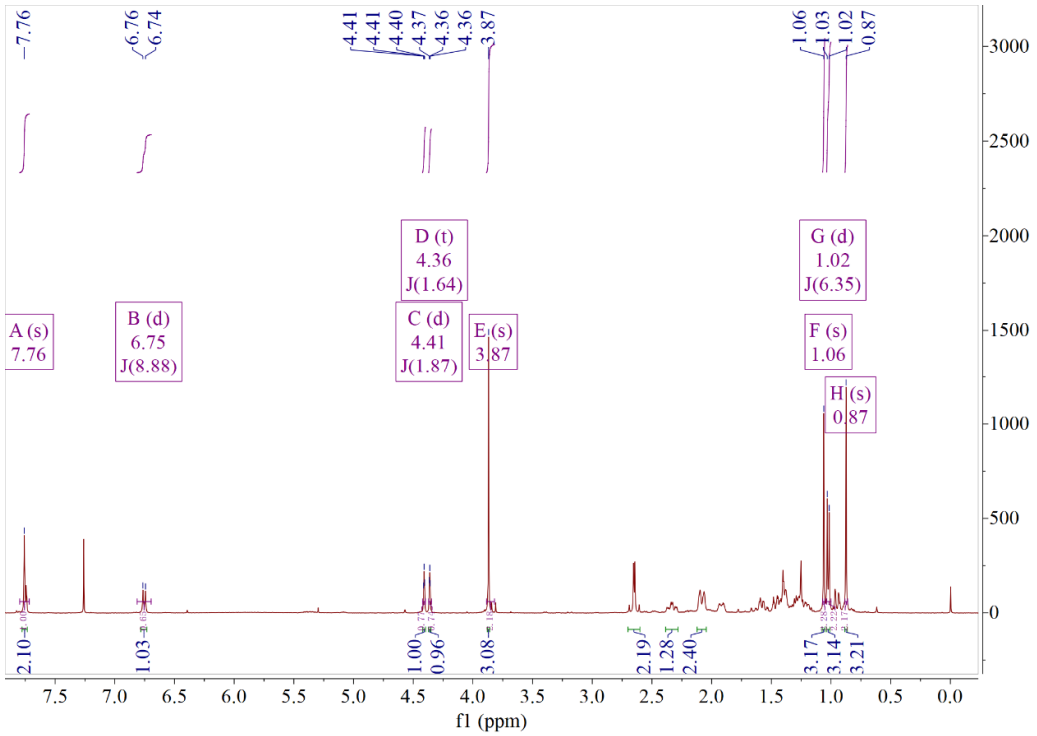
(f) ^{13}C NMR spectrum of compound 15 in $CDCl_3$



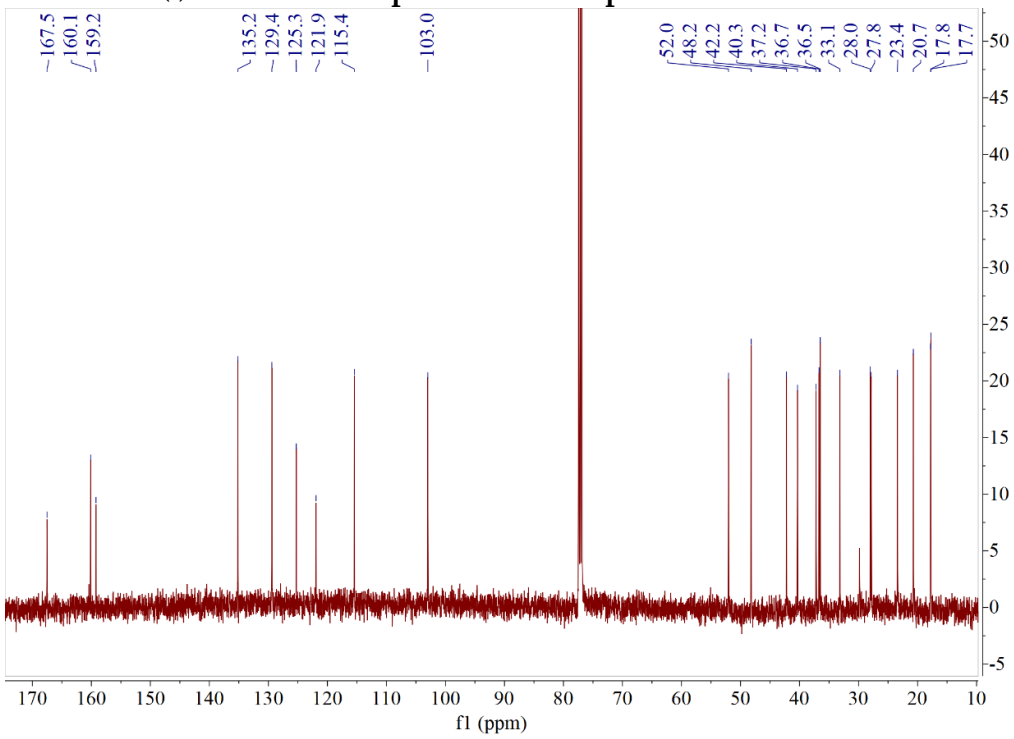
(g) ^{1}H NMR spectrum of compound 16 in $CDCl_3$



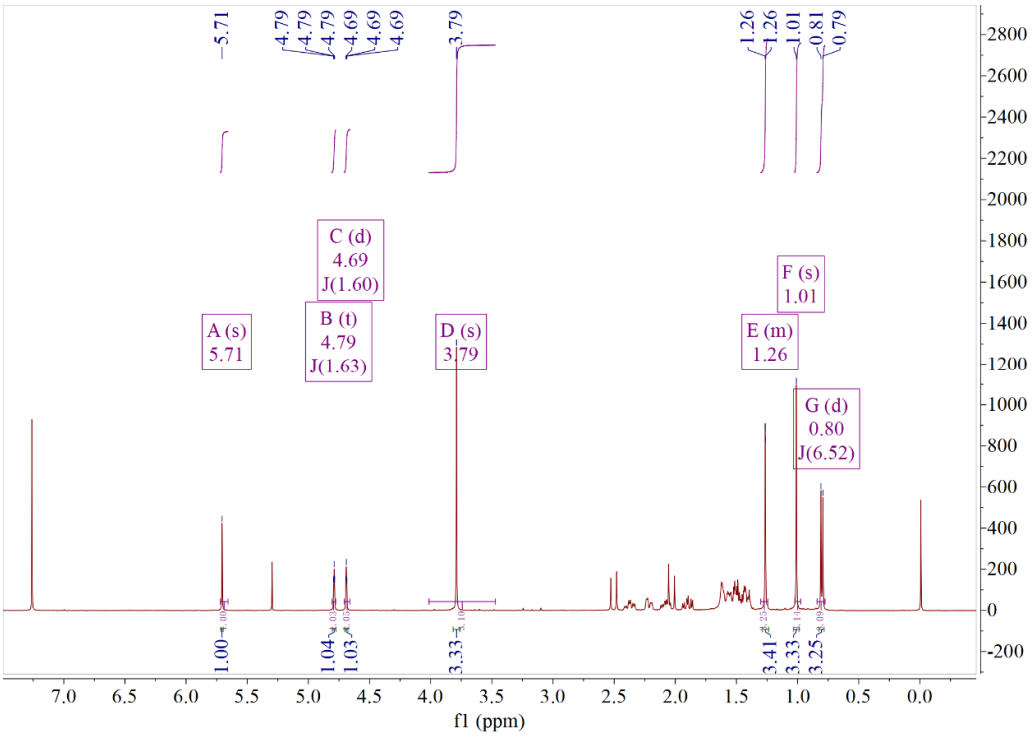
(h) ^{13}C NMR spectrum of compound 16 in $CDCl_3$



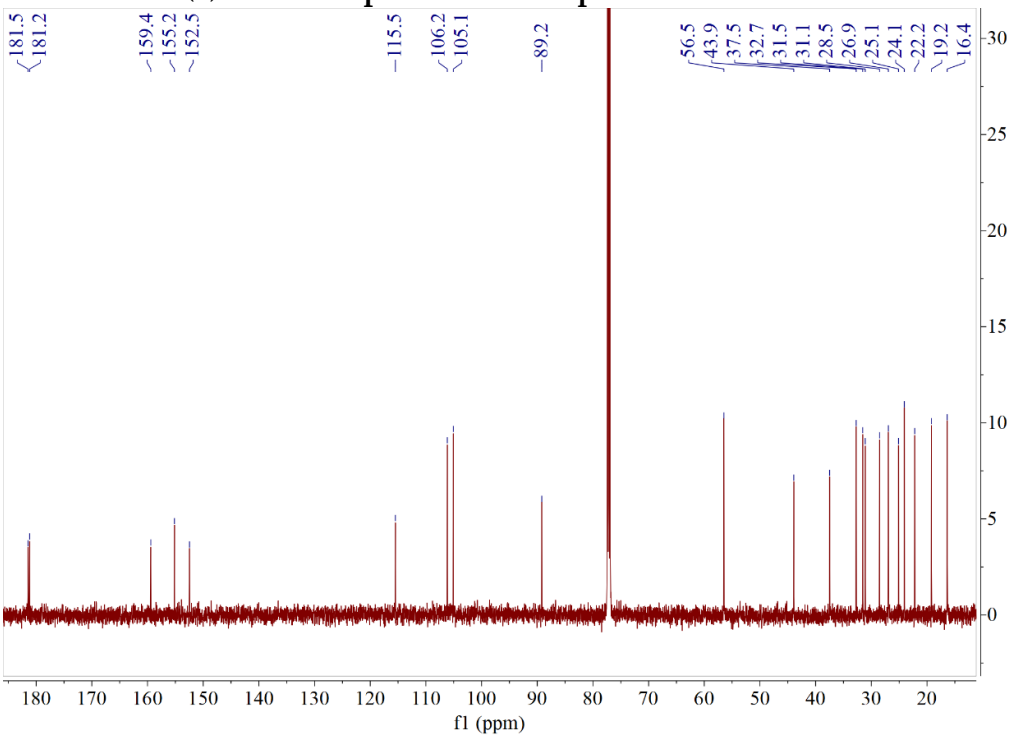
(i) ^{1}H NMR spectrum of compound 17 in $CDCl_3$



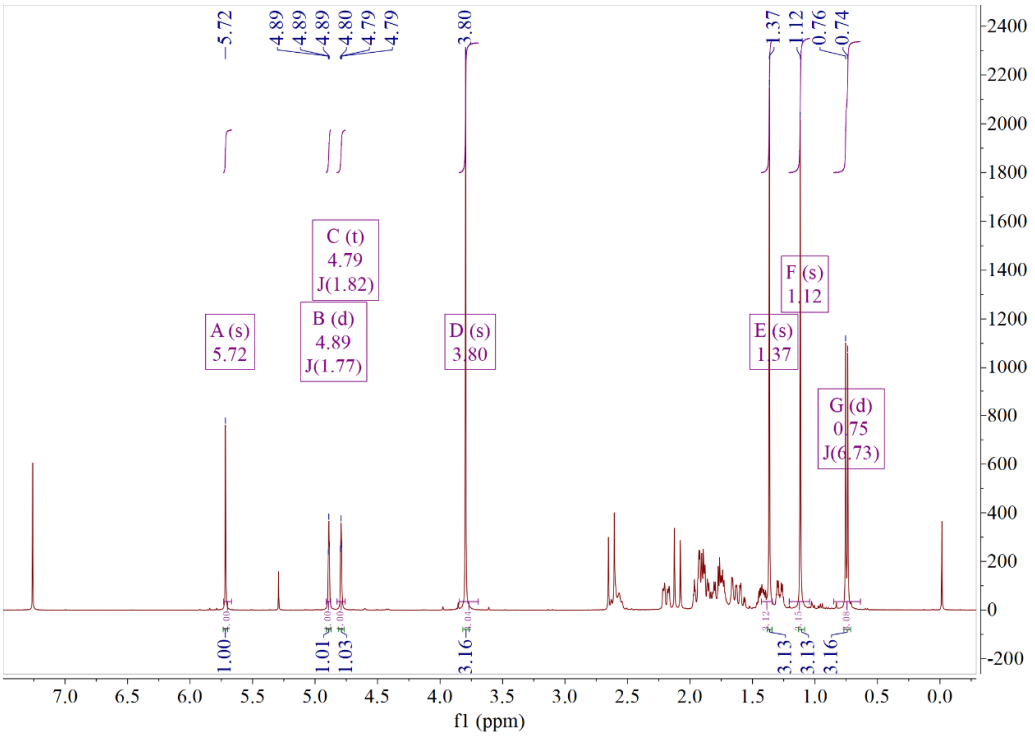
(j) ^{13}C NMR spectrum of compound 17 in $CDCl_3$



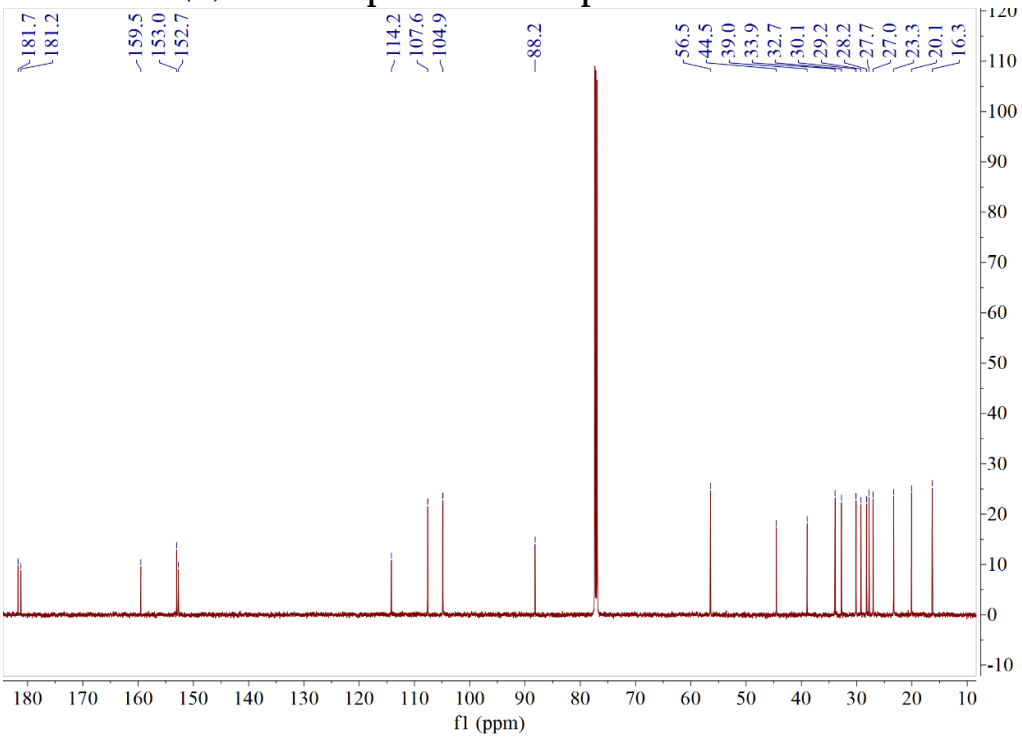
(k) ^{1}H NMR spectrum of compound 18 in $CDCl_3$



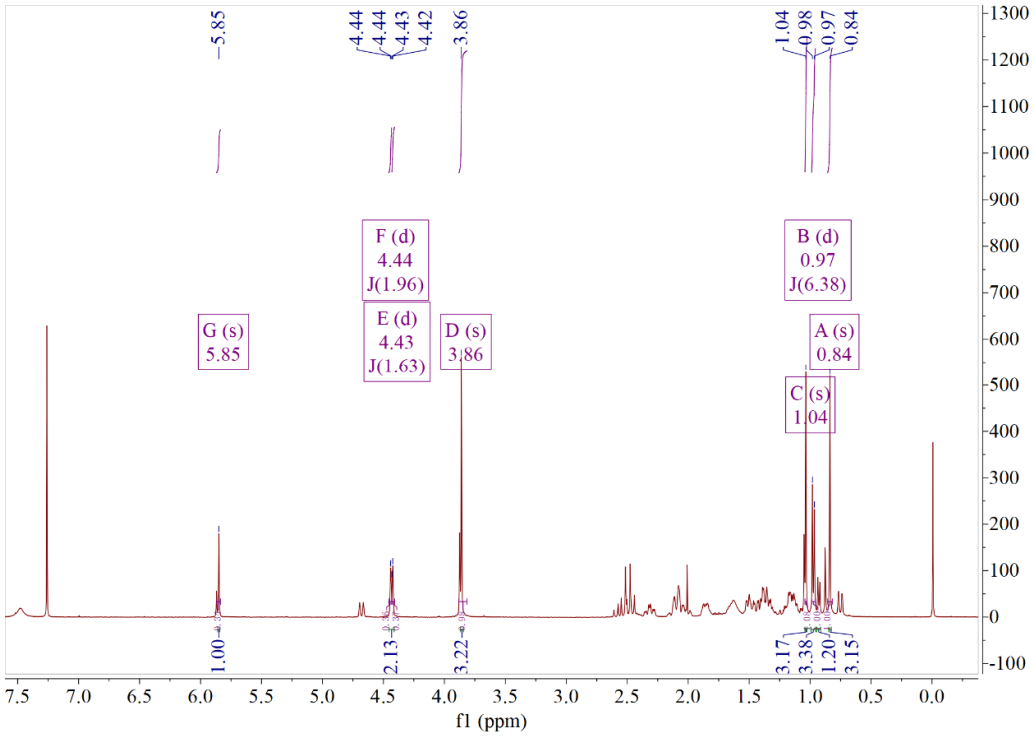
(l) ^{13}C NMR spectrum of compound 18 in $CDCl_3$



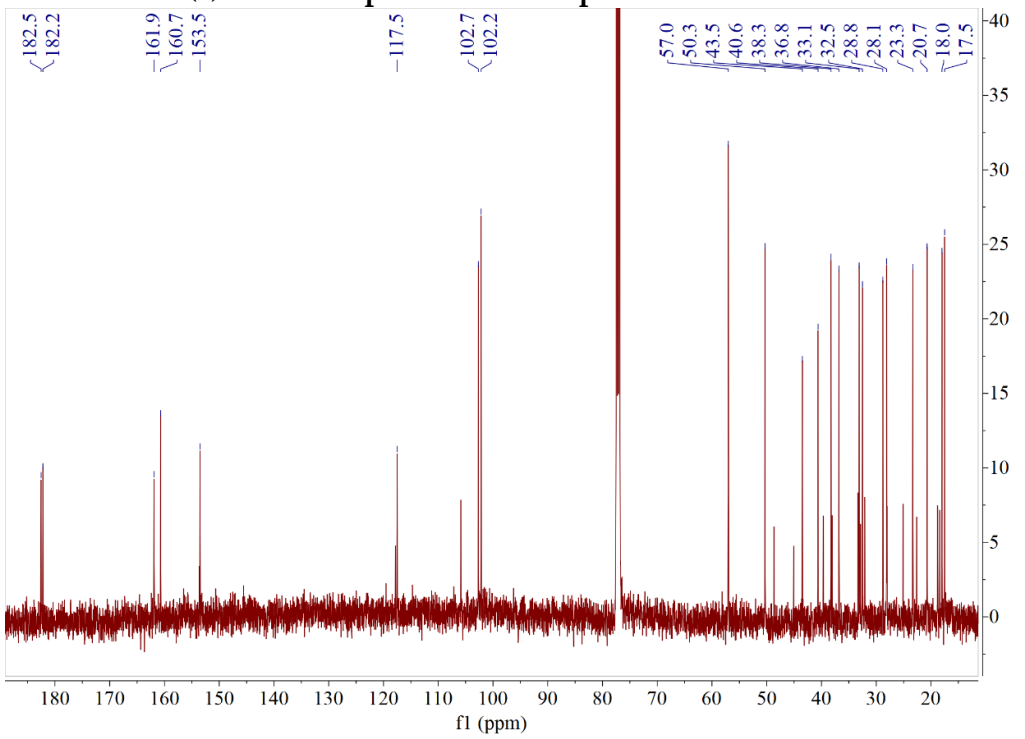
(m) ^{1}H NMR spectrum of compound 19 in $CDCl_3$



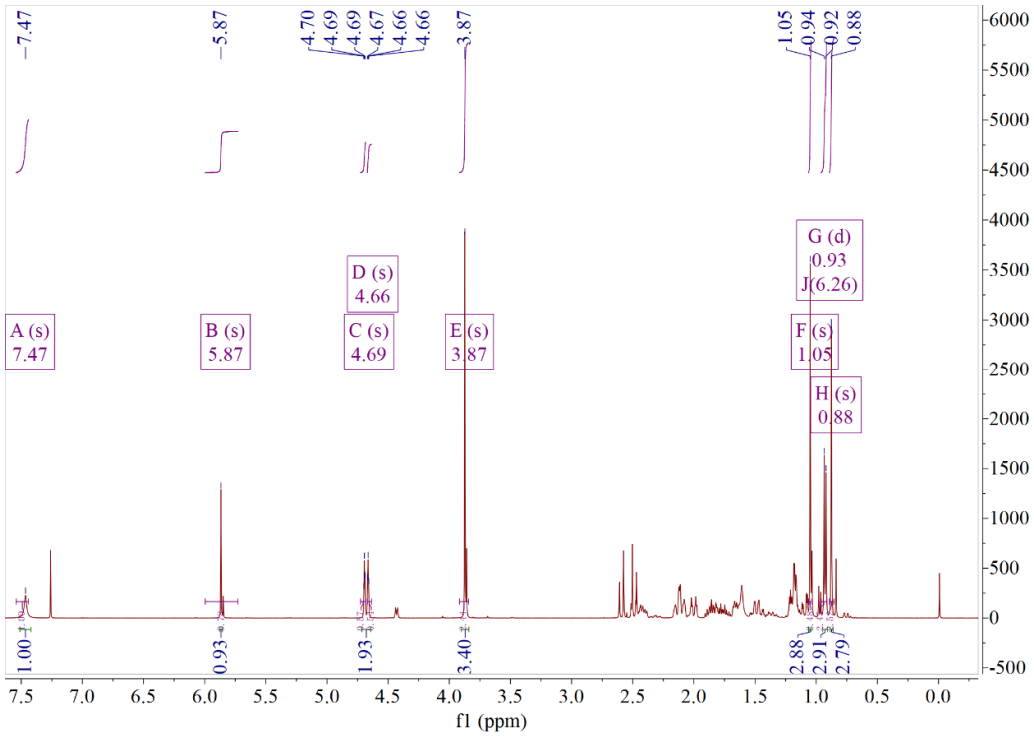
(n) ^{13}C NMR spectrum of compound 19 in $CDCl_3$



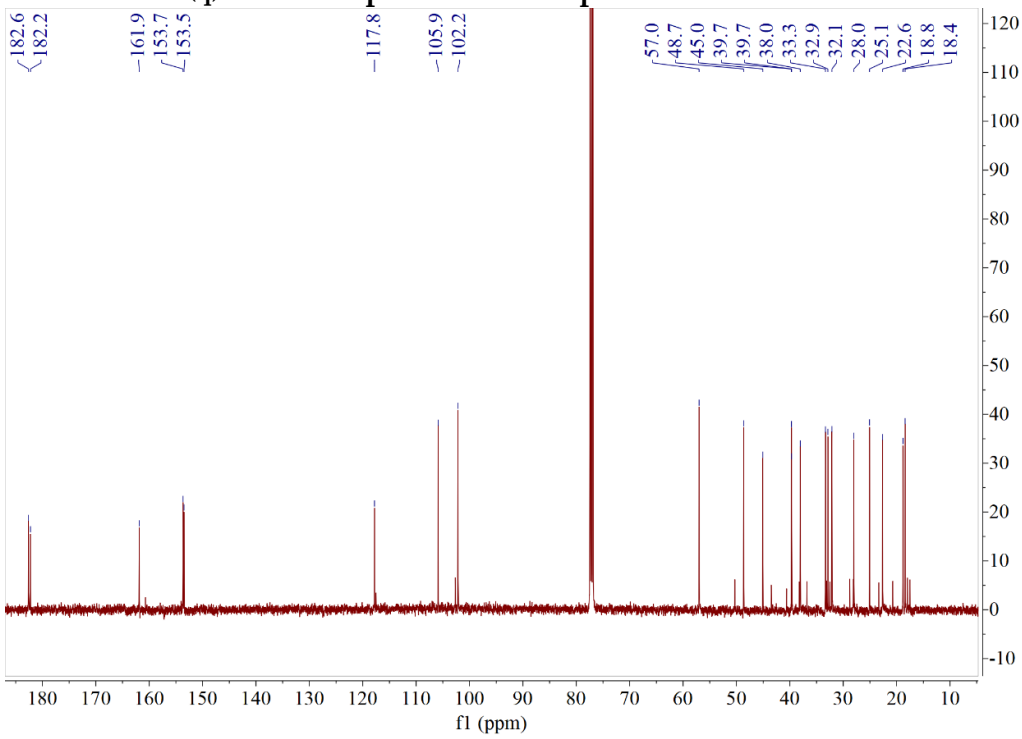
(o) ^{1}H NMR spectrum of compound 20 in $CDCl_3$



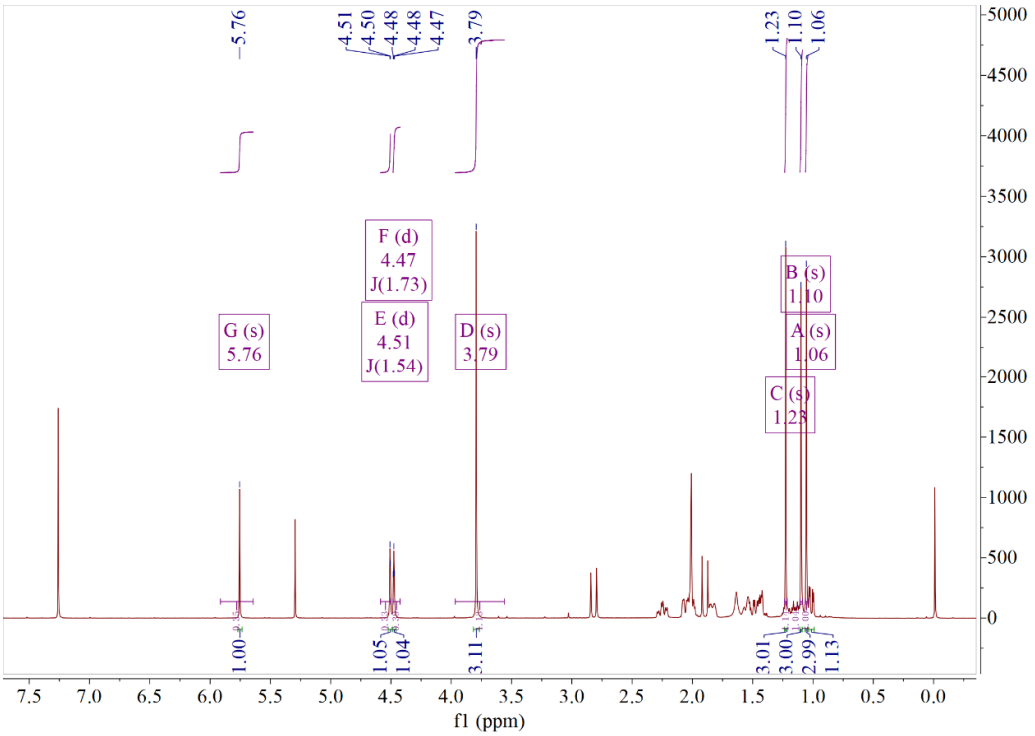
(p) ^{13}C NMR spectrum of compound 20 in $CDCl_3$



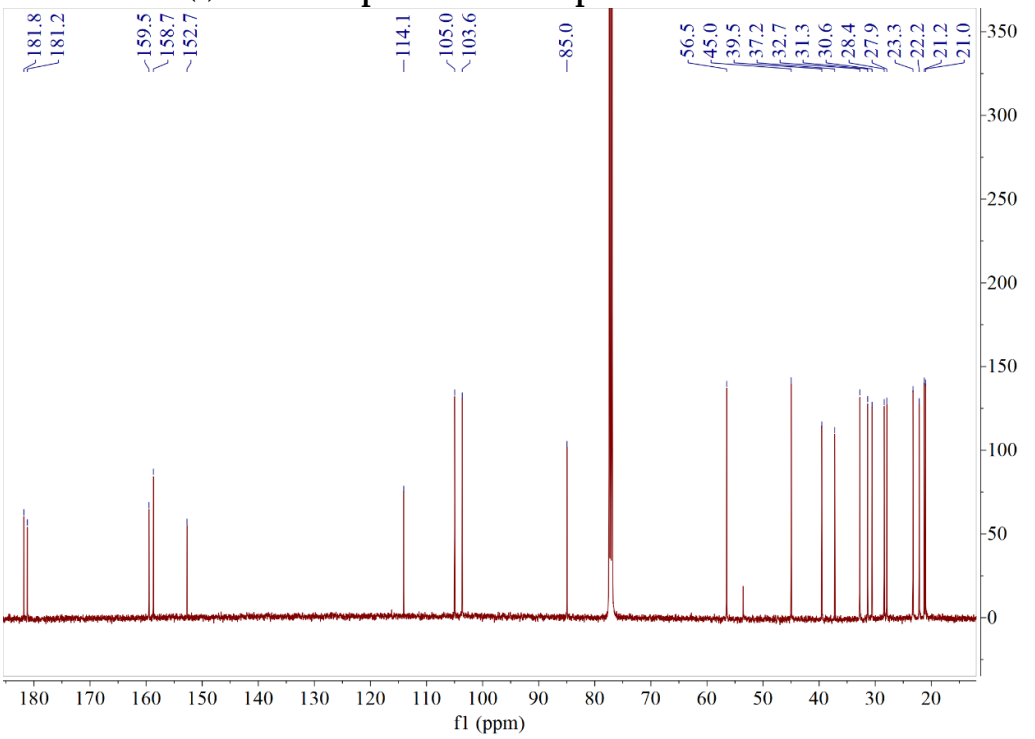
(q) ^{1}H NMR spectrum of compound 21 in $CDCl_3$



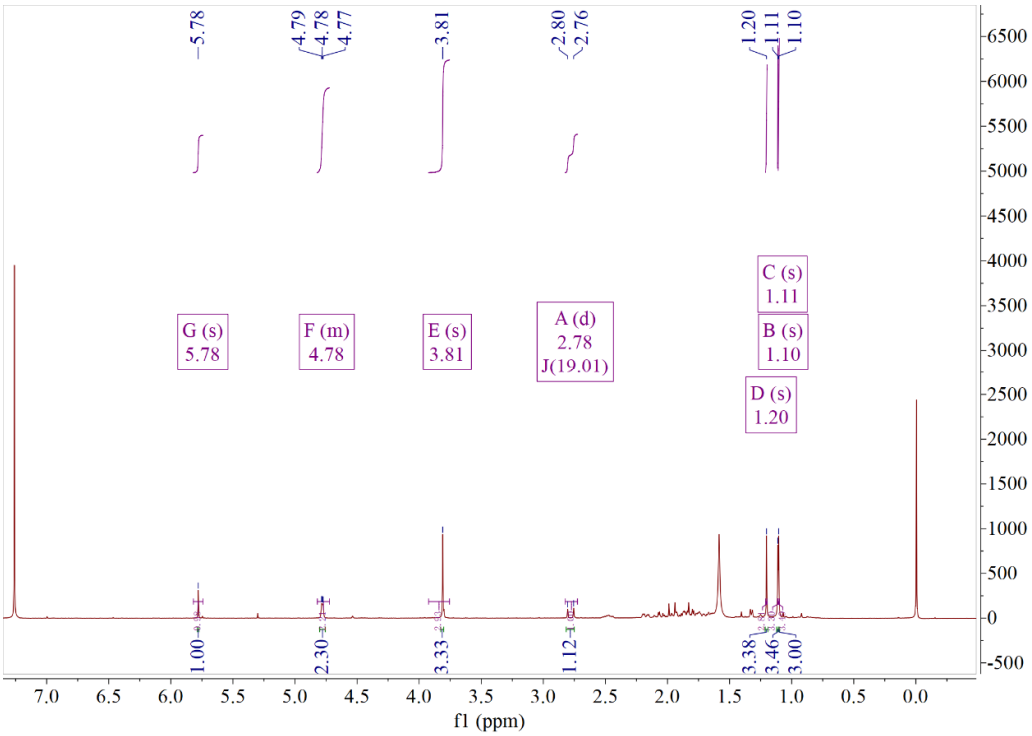
(r) ^{13}C NMR spectrum of compound 21 in $CDCl_3$



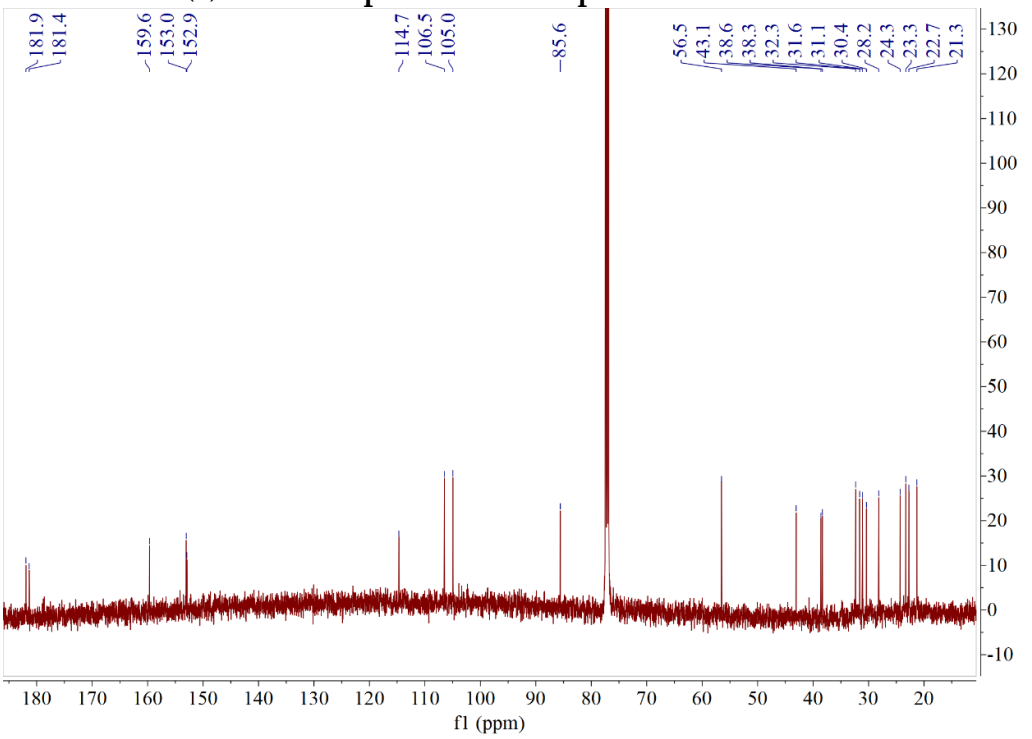
(s) ^{1}H NMR spectrum of compound 22 in $CDCl_3$



(t) ^{13}C NMR spectrum of compound 22 in $CDCl_3$



(u) ^{1}H NMR spectrum of compound 23 in $CDCl_3$



(v) ^{13}C NMR spectrum of compound 23 in $CDCl_3$

Figure S5 ^{1}H and ^{13}C NMR spectra of Compound 12 and 14–23