Supplementary data for

The first phytochemical investigation of *Artemisia divaricate*: sesquiterpenes and their anti-inflammatory activity

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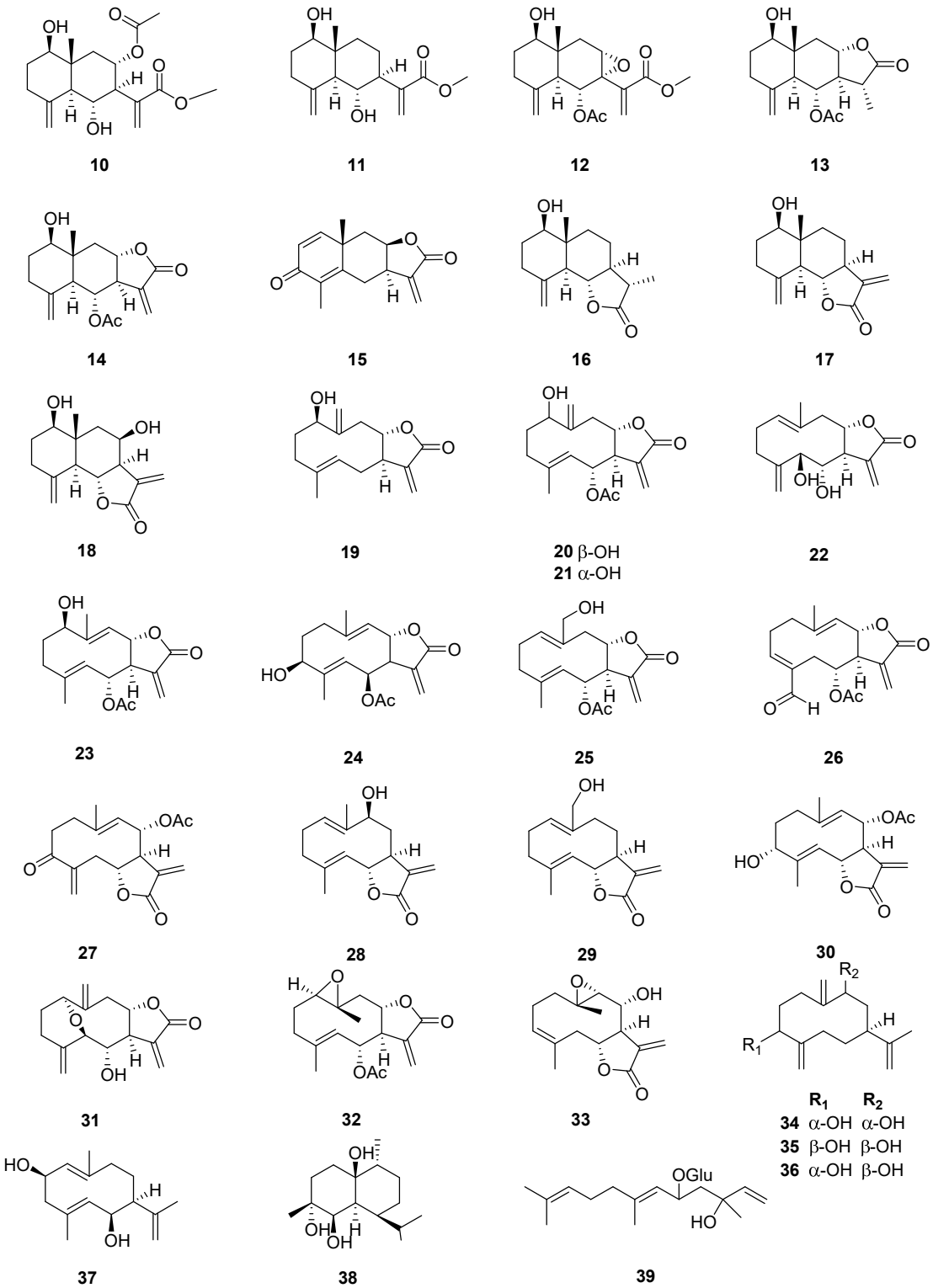


Figure S1 Structures of known compounds **10**-**39**

Elemental Composition Report
Tolerance = 20.0 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
66 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-200 H: 0-60 O: 0-6 Na: 0-1

Minimum:	80.00						-1.5		
Maximum:	100.00			2.0	20.0		50.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
375.1855	100.00	375.1784	7.1	18.9	5.5	40.1	0.164	84.84	$C_{19}H_{28}O_6Na$
		375.1808	4.7	12.5	8.5	41.9	1.887	15.16	$C_{21}H_{27}O_6$

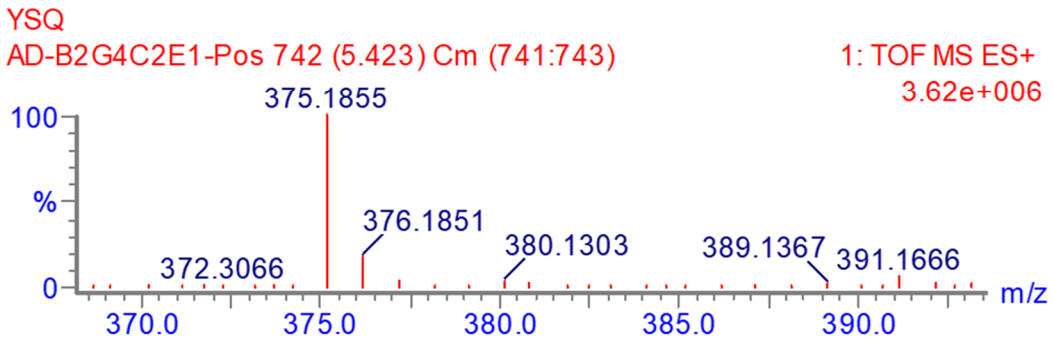


Figure S2 HR-ESIMS spectrum of compound **1**

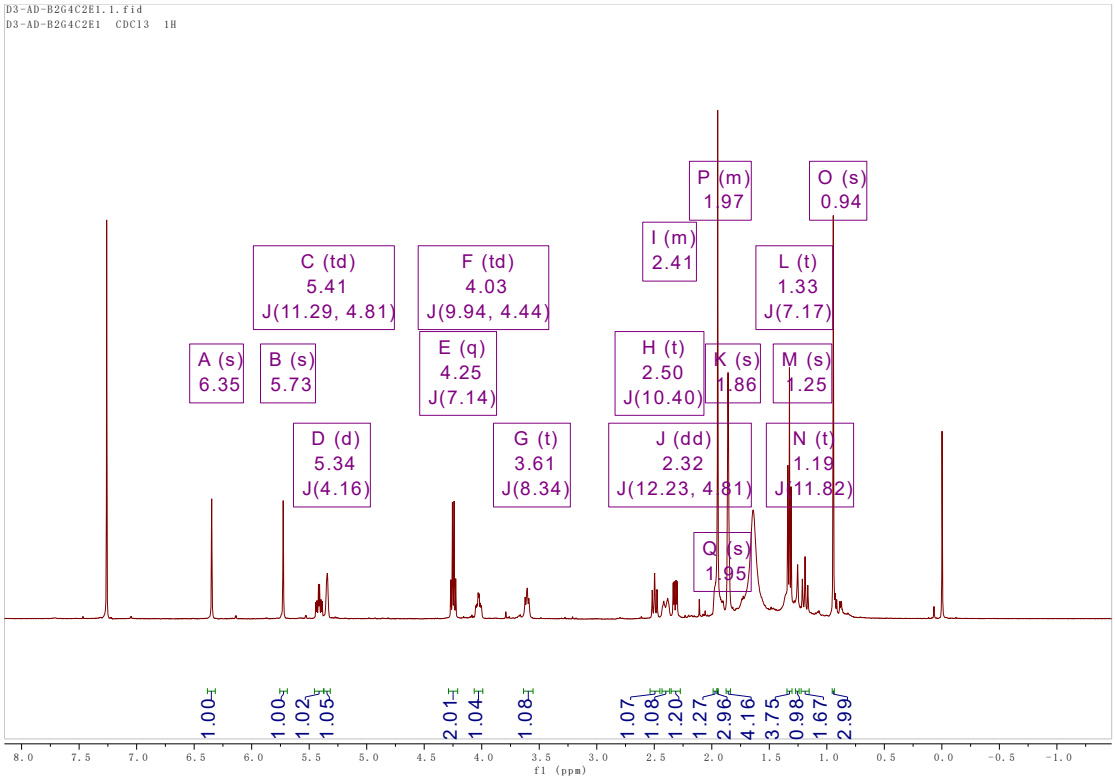


Figure S3 ^{1}H NMR spectrum of compound **1**

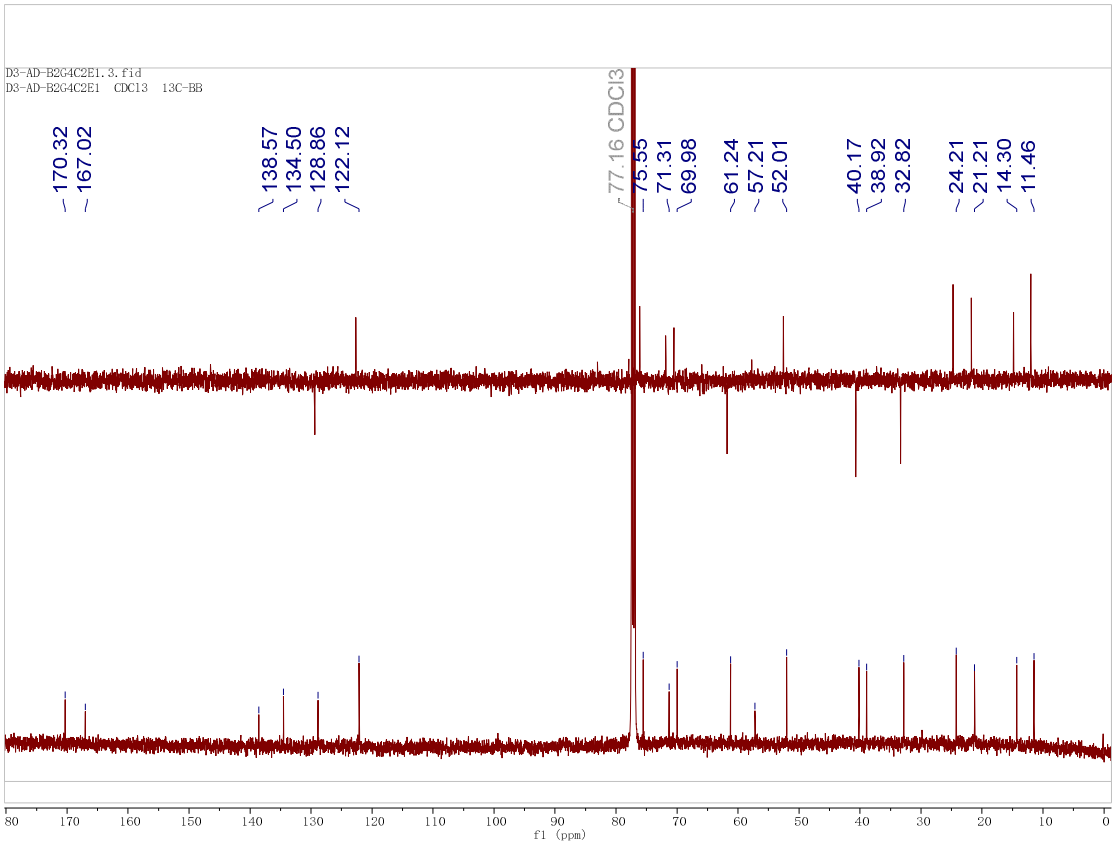


Figure S4 ^{13}C NMR spectrum of compound **1**

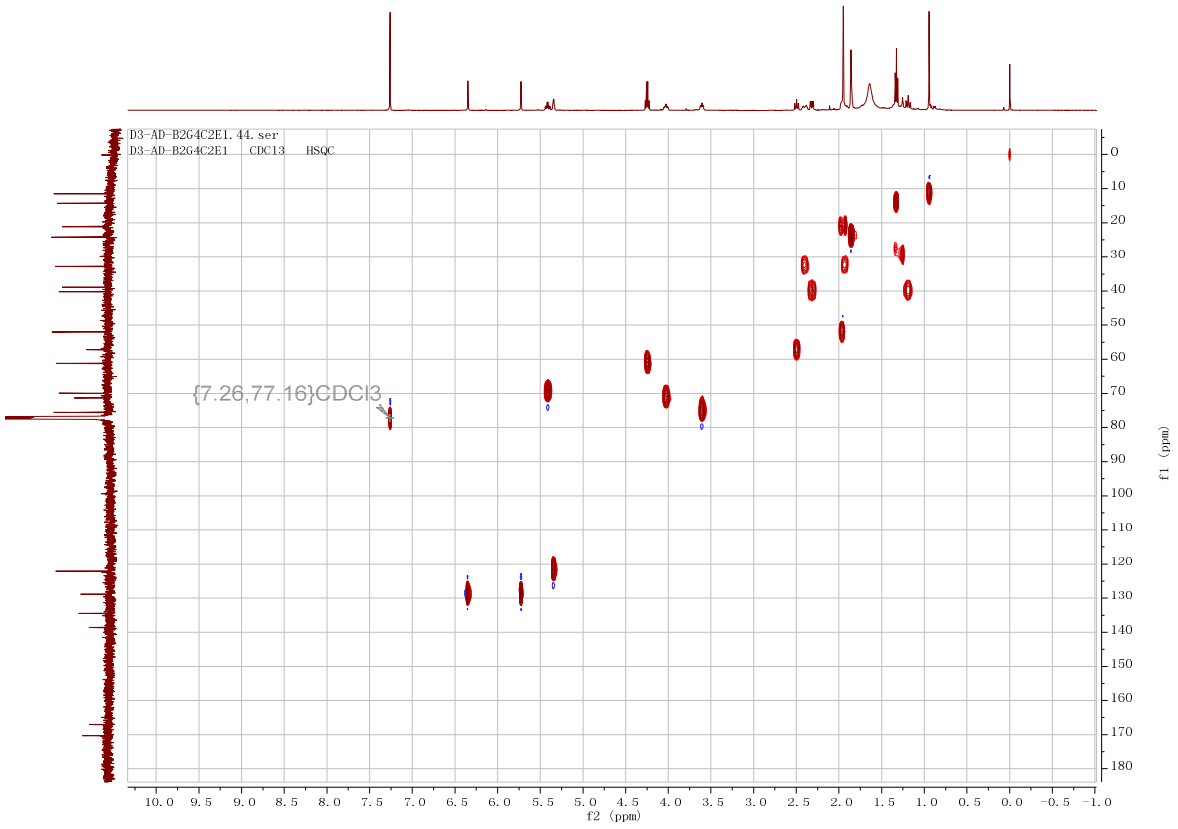


Figure S5 HSQC spectrum of compound **1**

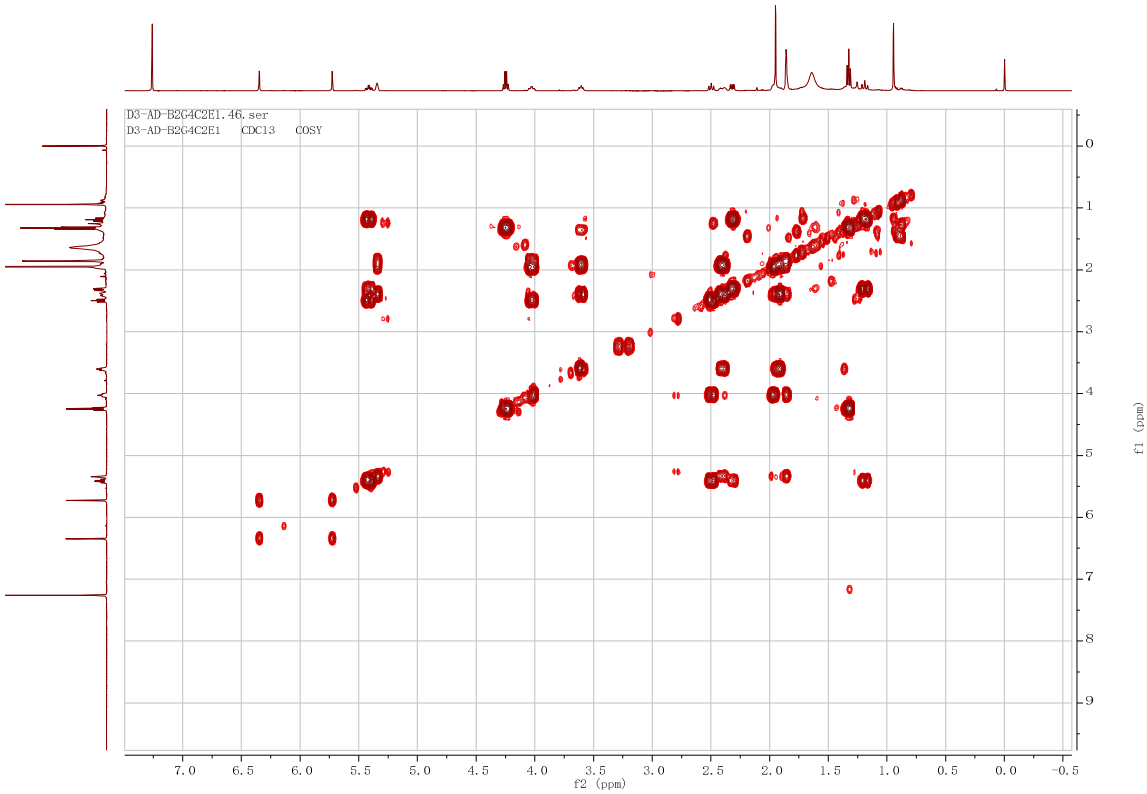


Figure S6 ^{1}H-^{1}H COSY spectrum of compound **1**

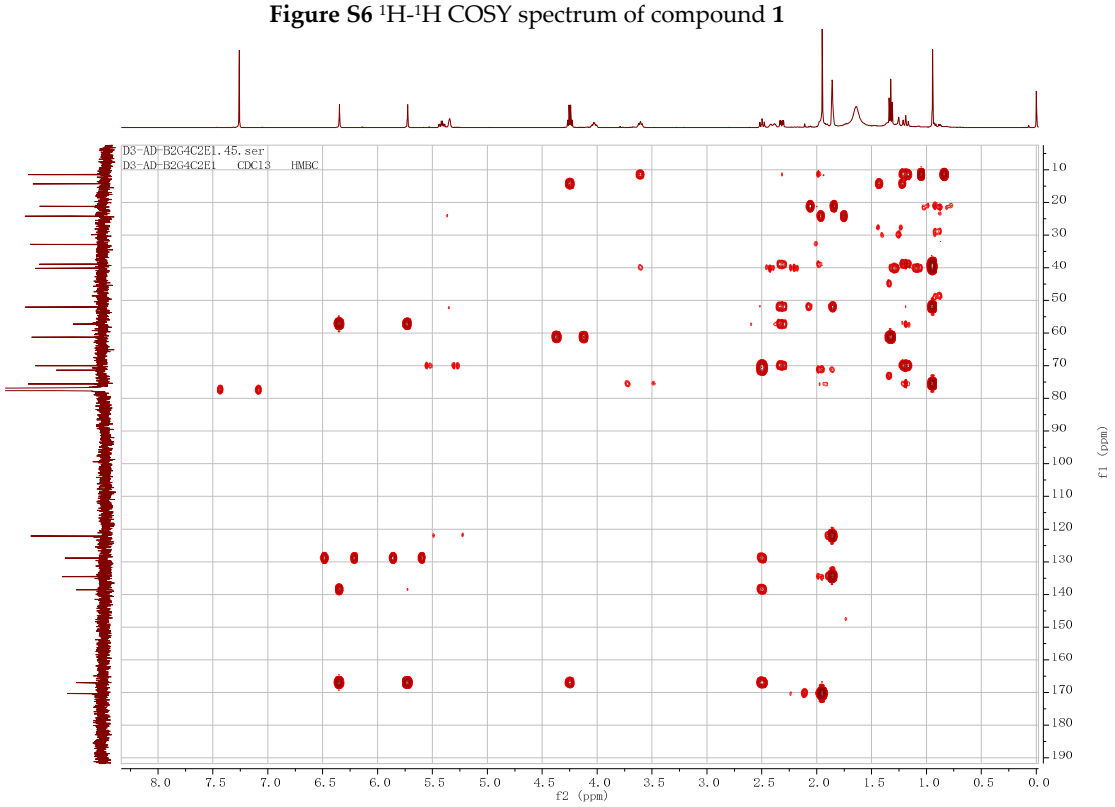


Figure S7 HMBC spectrum of compound **1**

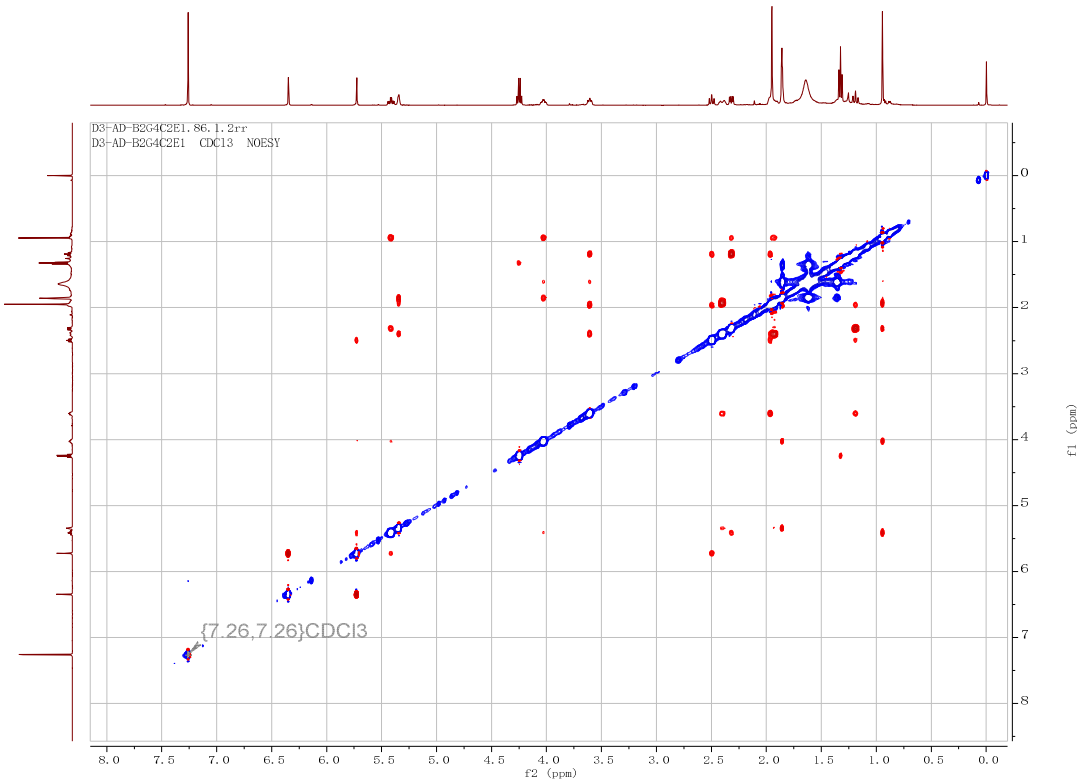


Figure S8 NOESY spectrum of compound **1**

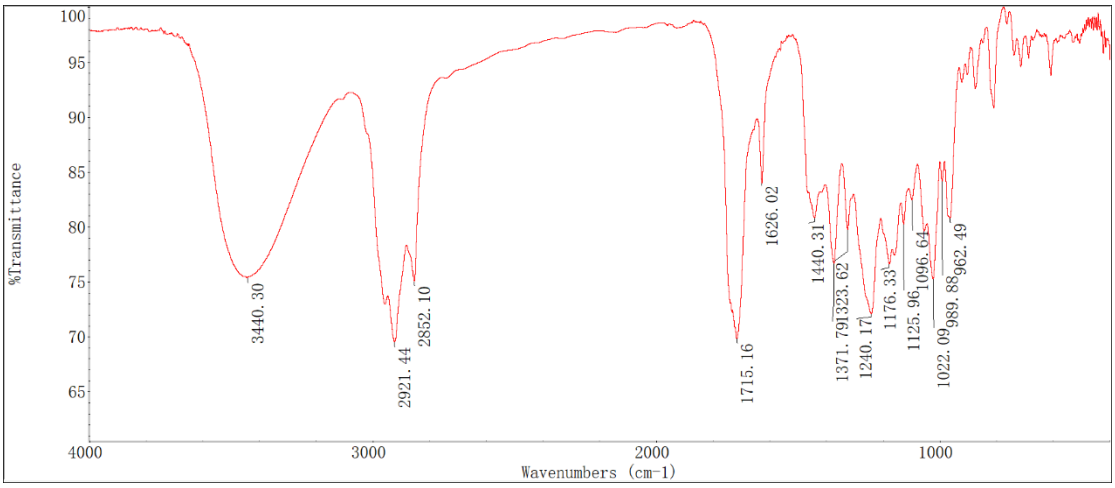


Figure S9 IR spectrum of compound **1**

Elemental Composition Report
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
66 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-200 H: 0-60 O: 0-6 Na: 0-1

Minimum:		80.00					-1.5		
Maximum:		100.00			2.0	5.0	50.0		
Mass	RA	CalcMass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
375.1783	100.0	375.1784	-0.1	-0.3	5.5	794.7	n/a	n/a	$C_{19}H_{28}O_6Na$

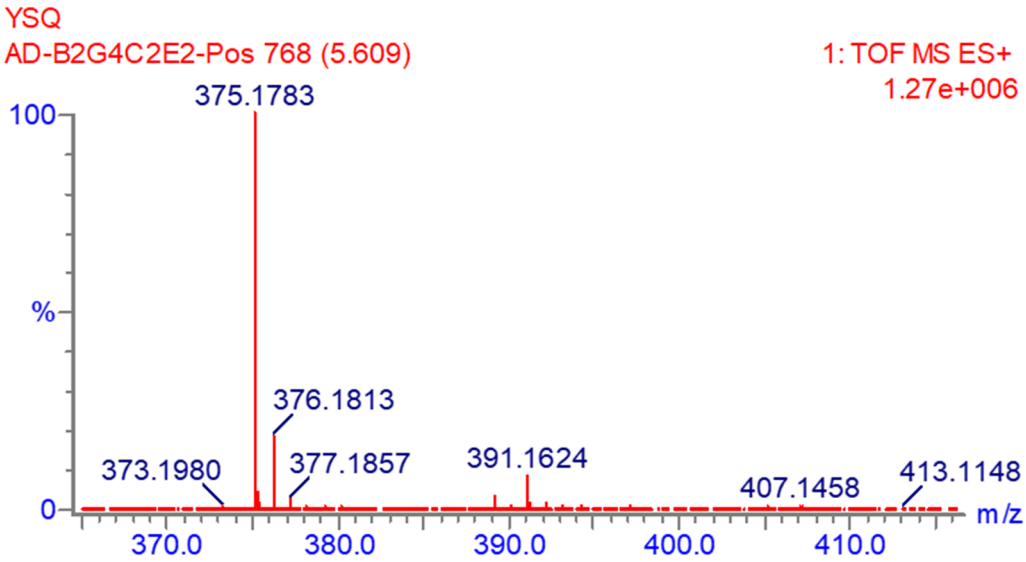


Figure S10 HR-ESIMS spectrum of compound **2**

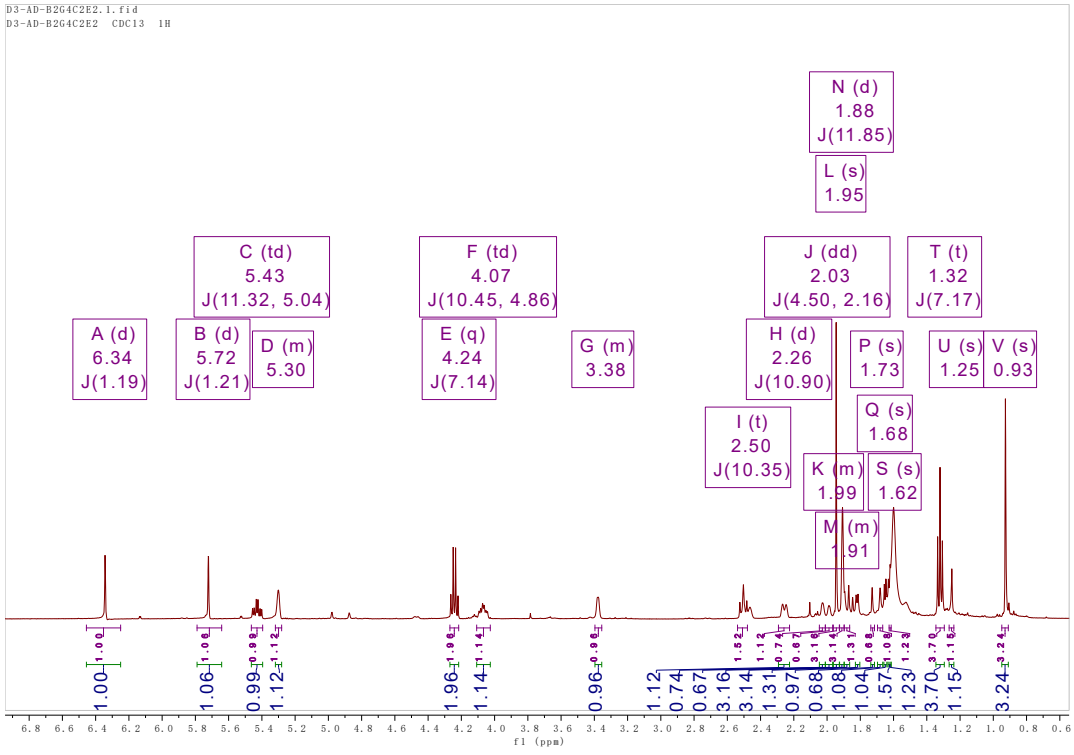


Figure S11 ^{1}H NMR spectrum of compound **2**

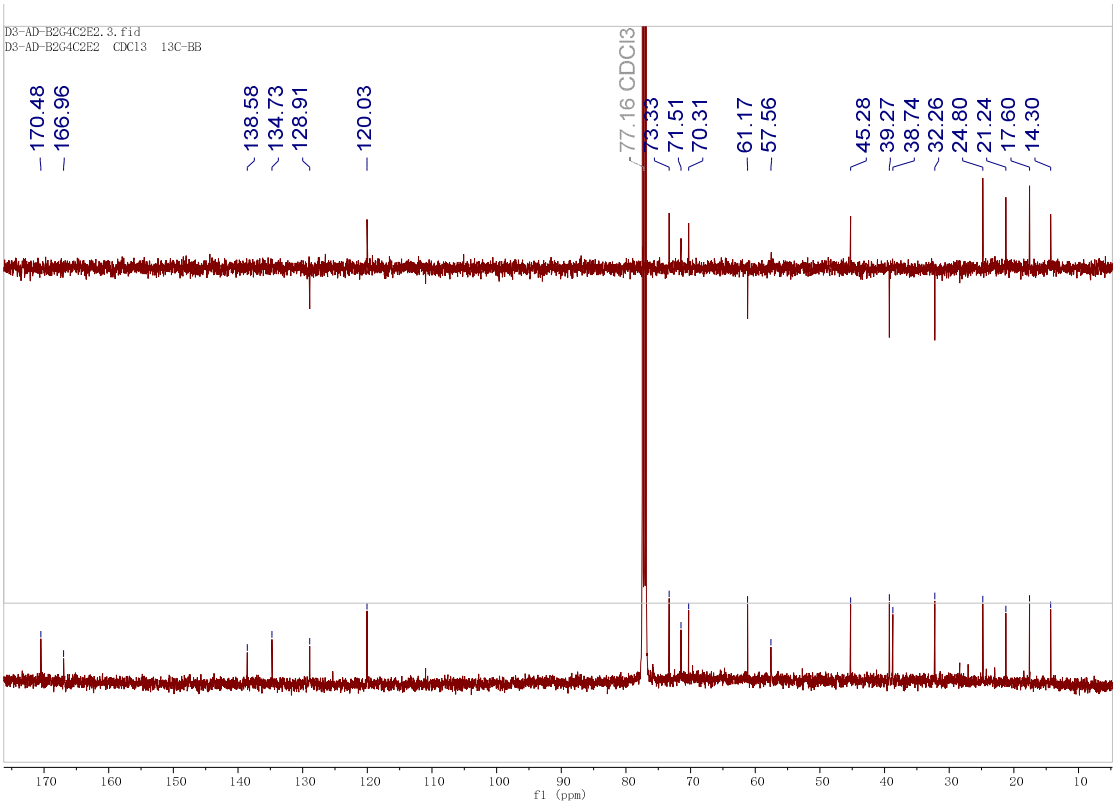


Figure S12 ^{13}C NMR spectrum of compound **2**

Figure S13 HSQC spectrum of compound **2**

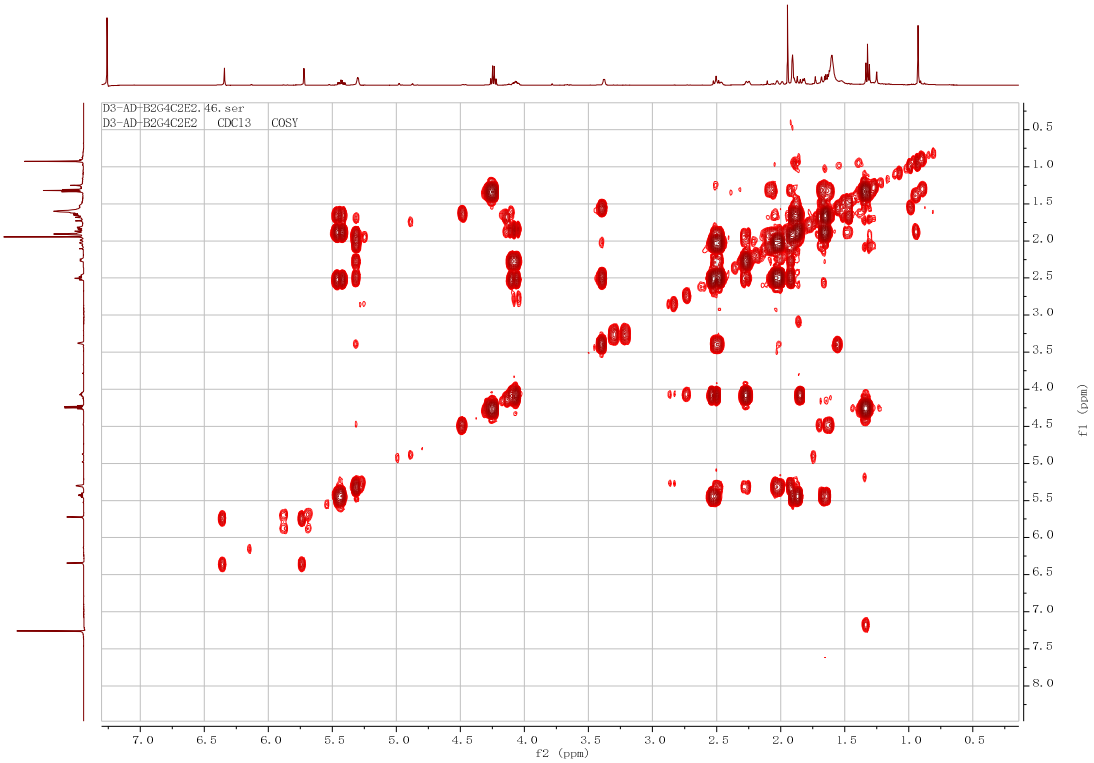


Figure S14 ^{1}H-^{1}H COSY spectrum of compound **2**

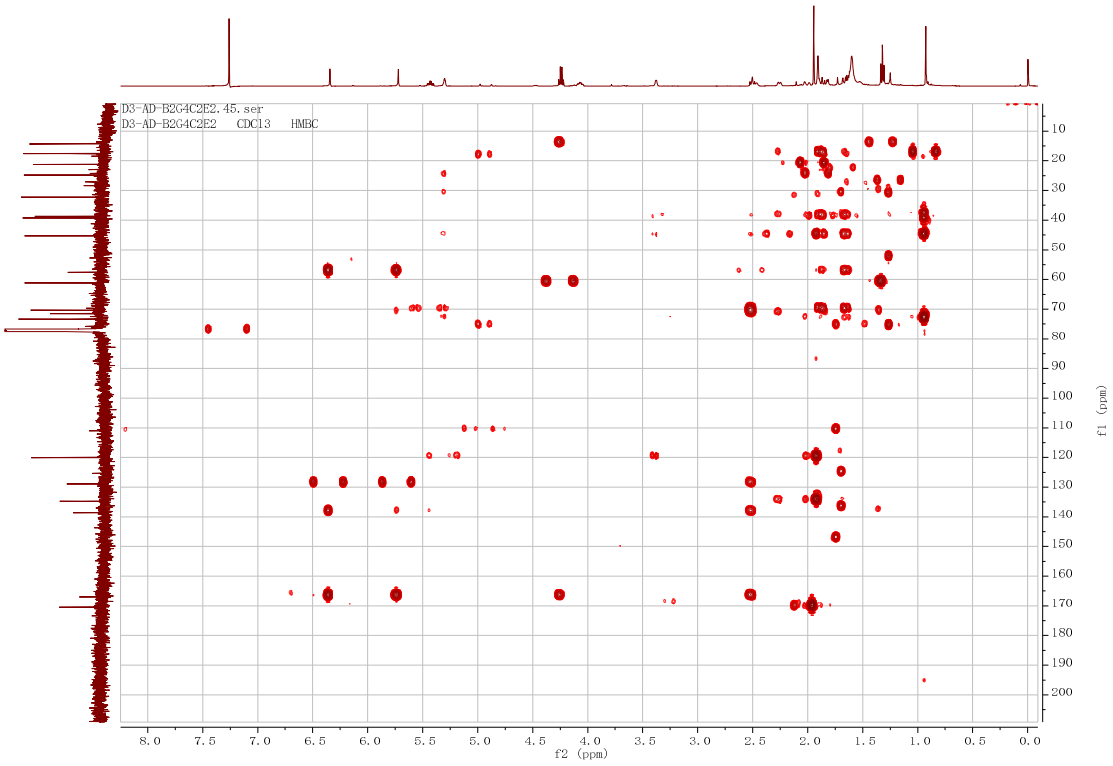


Figure S15 HMBC spectrum of compound **2**

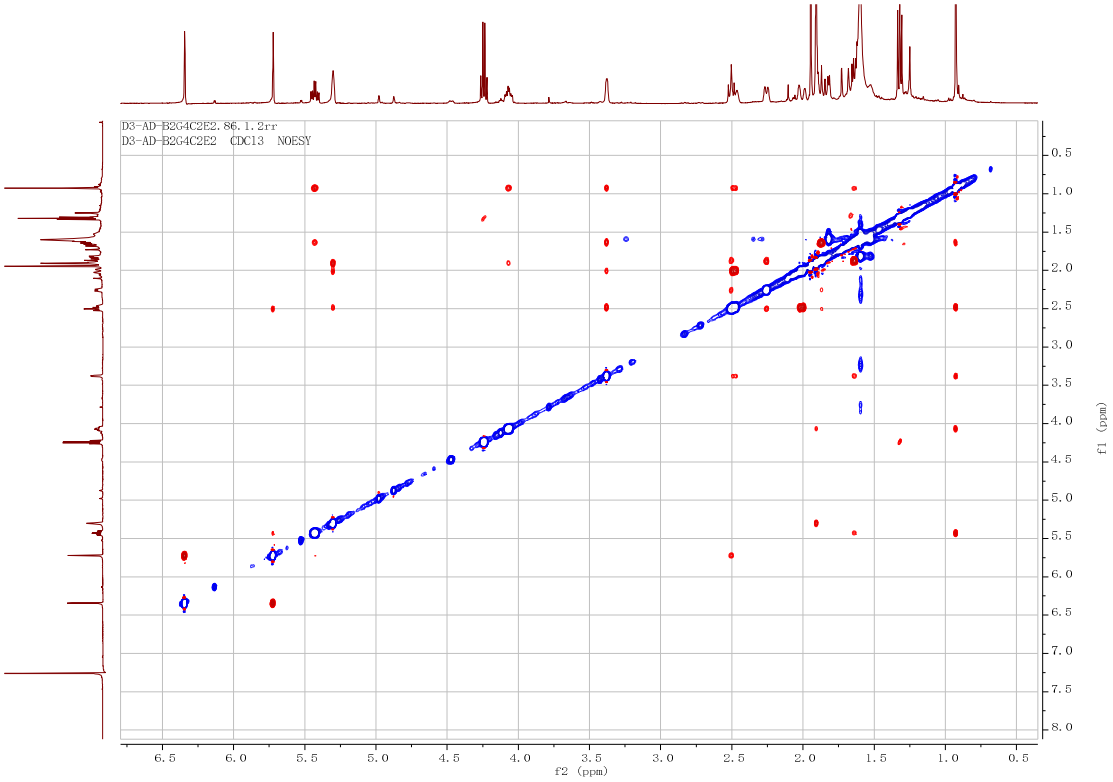


Figure S16 NOESY spectrum of compound **2**

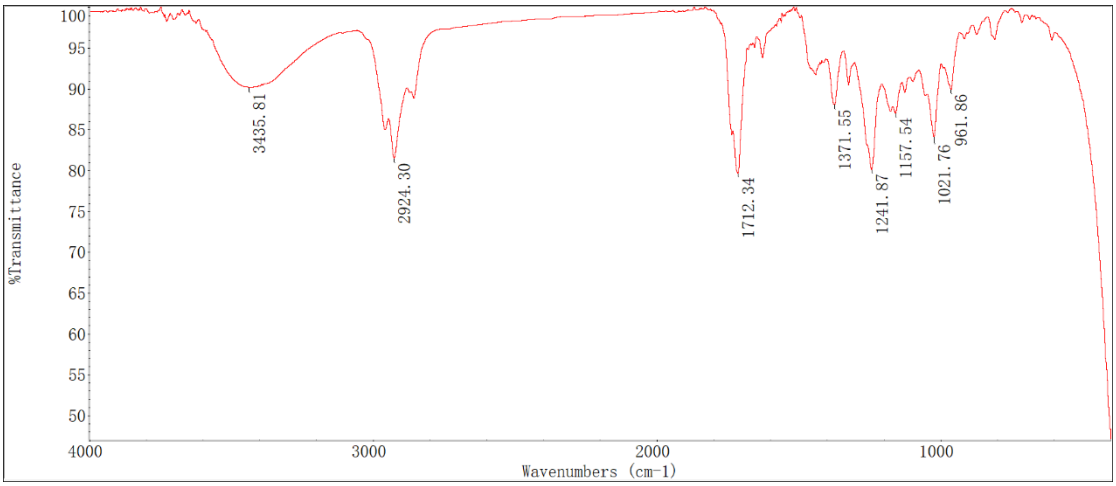


Figure S17 IR spectrum of compound **2**

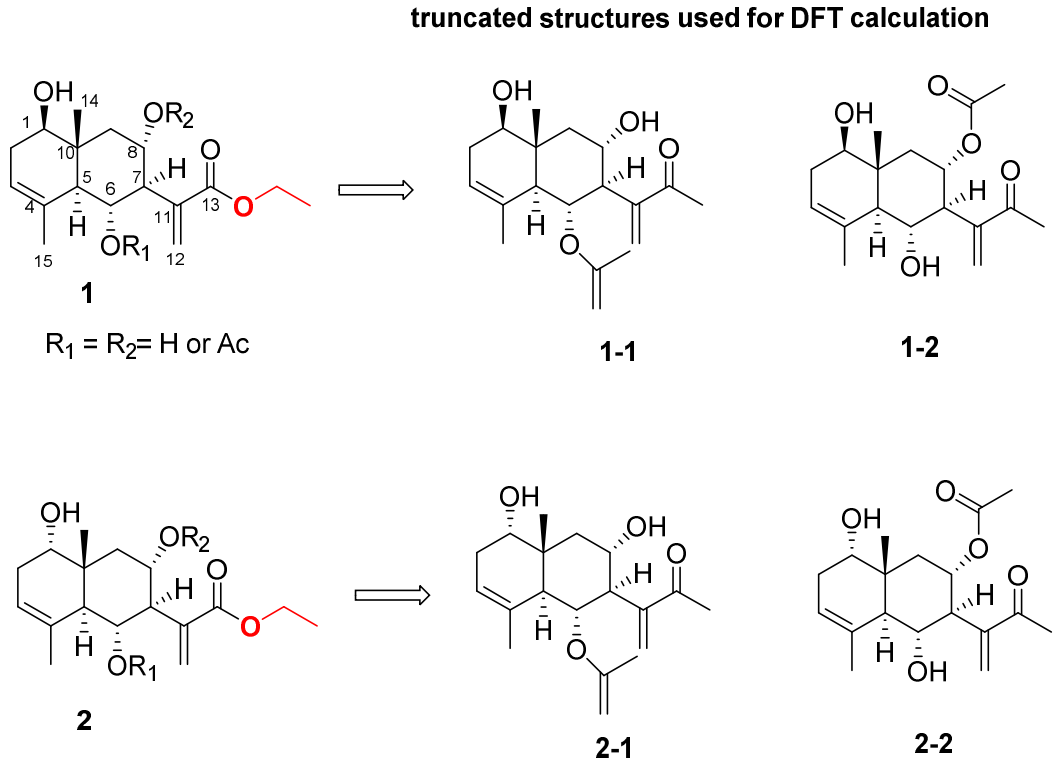


Figure S18 Possible isomers of compound **1** and **2**

Functional	Solvent?		Basis Set	
mPW1PW91	PCM		6-311G(d,p	
	Isomer 1	Isomer 2	Isomer 3	Isom
sDP4+ (H data)	0.00%	100.00%	–	
sDP4+ (C data)	73.05%	26.95%	–	
sDP4+ (all data)	0.00%	100.00%	–	
uDP4+ (H data)	0.00%	100.00%	–	
uDP4+ (C data)	91.34%	8.66%	–	
uDP4+ (all data)	0.00%	100.00%	–	
DP4+ (H data)	0.00%	100.00%	–	
DP4+ (C data)	96.62%	3.38%	–	
DP4+ (all data)	0.00%	100.00%	–	

Figure S19 DP4+ probability statistics of compound **1**

Functional	Solvent?		Basis Set	
mPW1PW91	PCM		6-311G(d,p	
	Isomer 1	Isomer 2	Isomer 3	Isom
sDP4+ (H data)	0.00%	100.00%	–	
sDP4+ (C data)	73.05%	26.95%	–	
sDP4+ (all data)	0.00%	100.00%	–	
uDP4+ (H data)	0.00%	100.00%	–	
uDP4+ (C data)	91.34%	8.66%	–	
uDP4+ (all data)	0.00%	100.00%	–	
DP4+ (H data)	0.00%	100.00%	–	
DP4+ (C data)	96.62%	3.38%	–	
DP4+ (all data)	0.00%	100.00%	–	

Figure S20 DP4+ probability statistics of compound **2**

Elemental Composition Report
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
66 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-200 H: 0-60 O: 0-6 Na: 0-1

Minimum:	80.00						-1.5		
Maximum:	100.00			2.0	5.0		50.0		
Mass	RA	Calc.Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
375.1784	100.00	375.1784	0.0	0.0	5.5	745.9	n/a	n/a	$C_{19}H_{28}O_6Na$

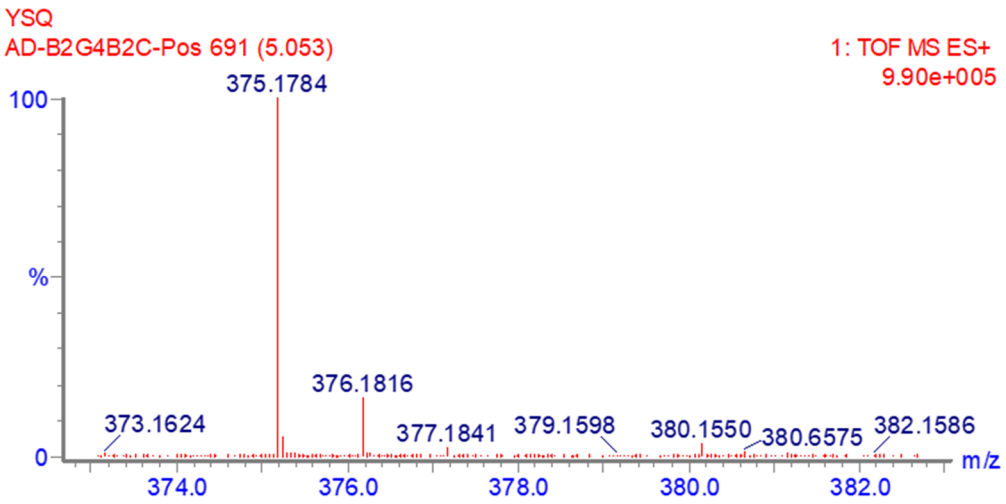


Figure S21 HR-ESIMS spectrum of compound **3**

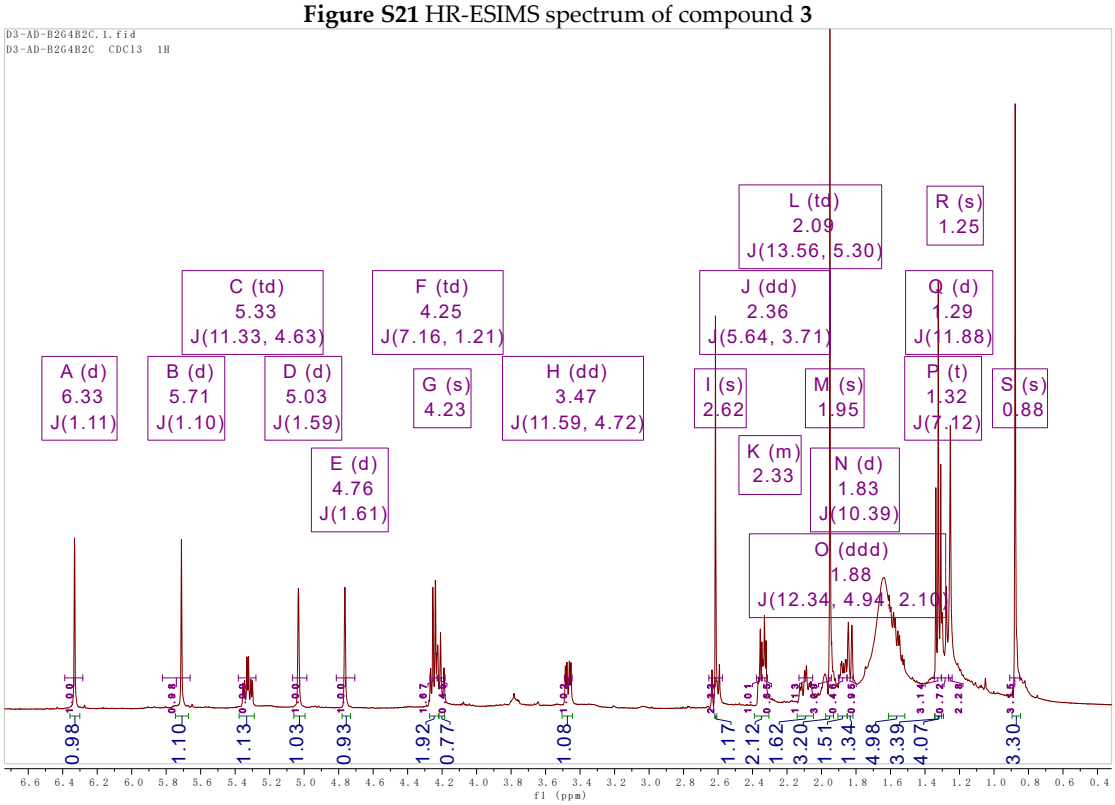


Figure S22 ^{1}H NMR spectrum of compound **3**

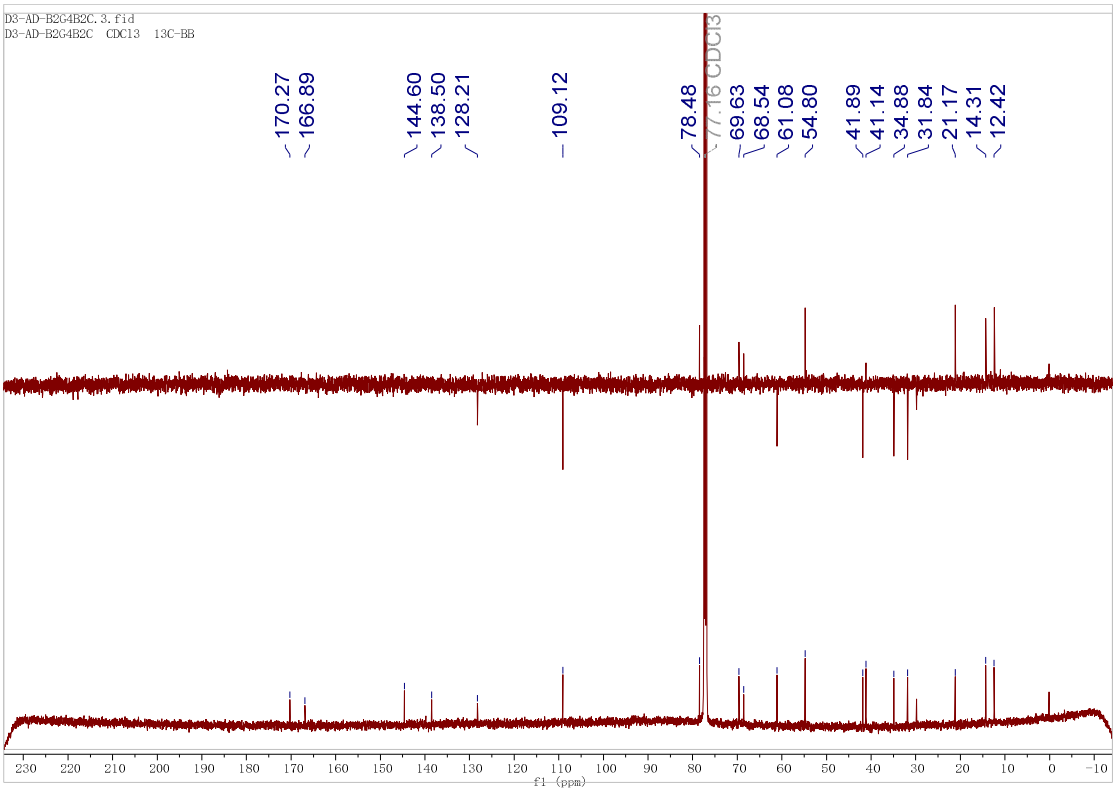


Figure S23 ^{13}C NMR spectrum of compound **3**

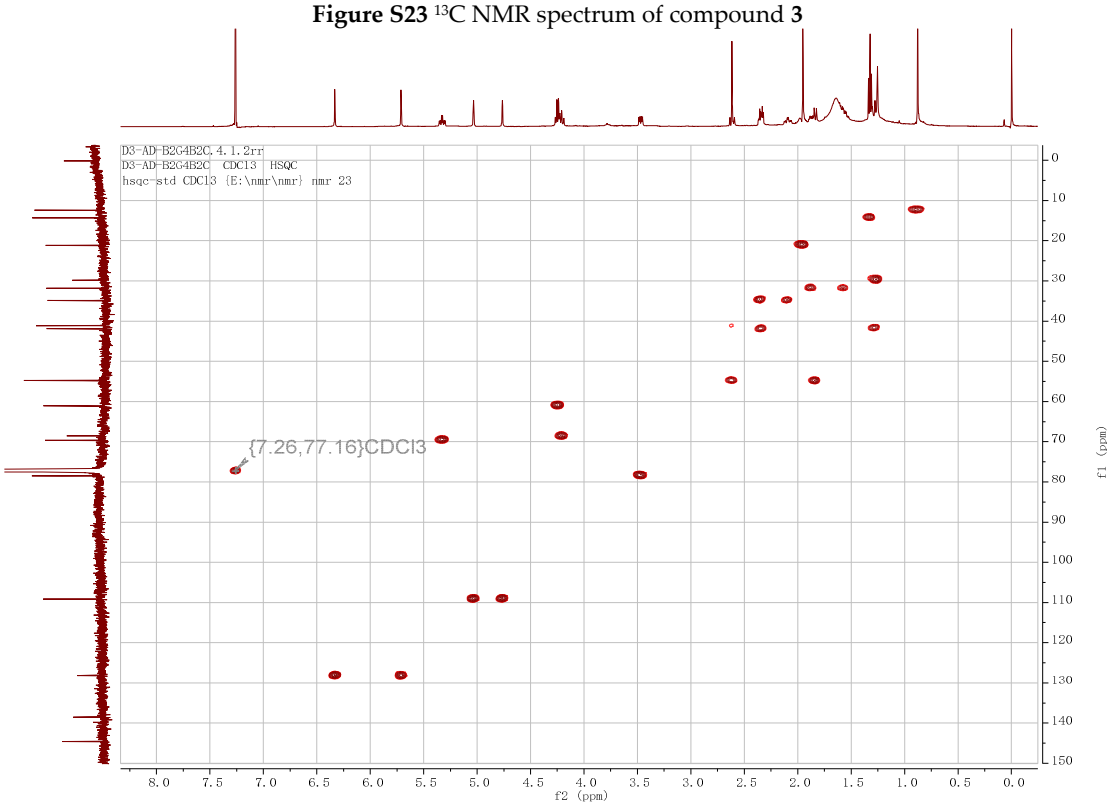


Figure S24 HSQC NMR spectrum of compound **3**

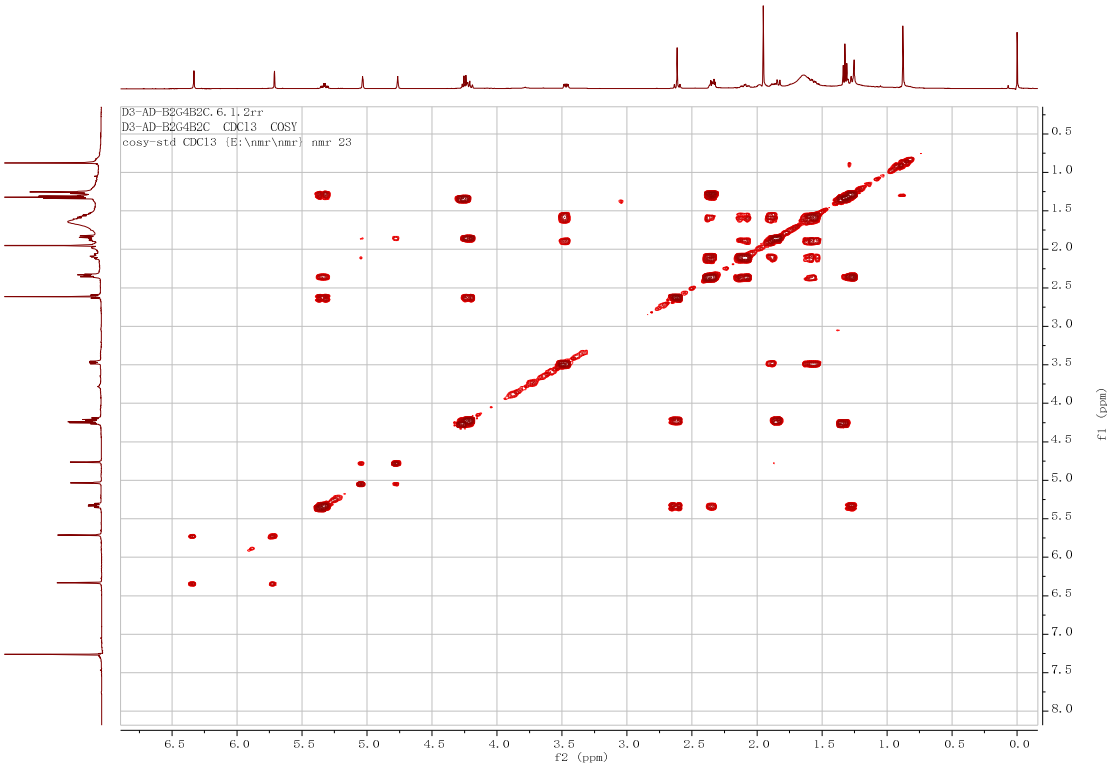


Figure S25 ^{1}H-^{1}H COSY spectrum of compound **3**

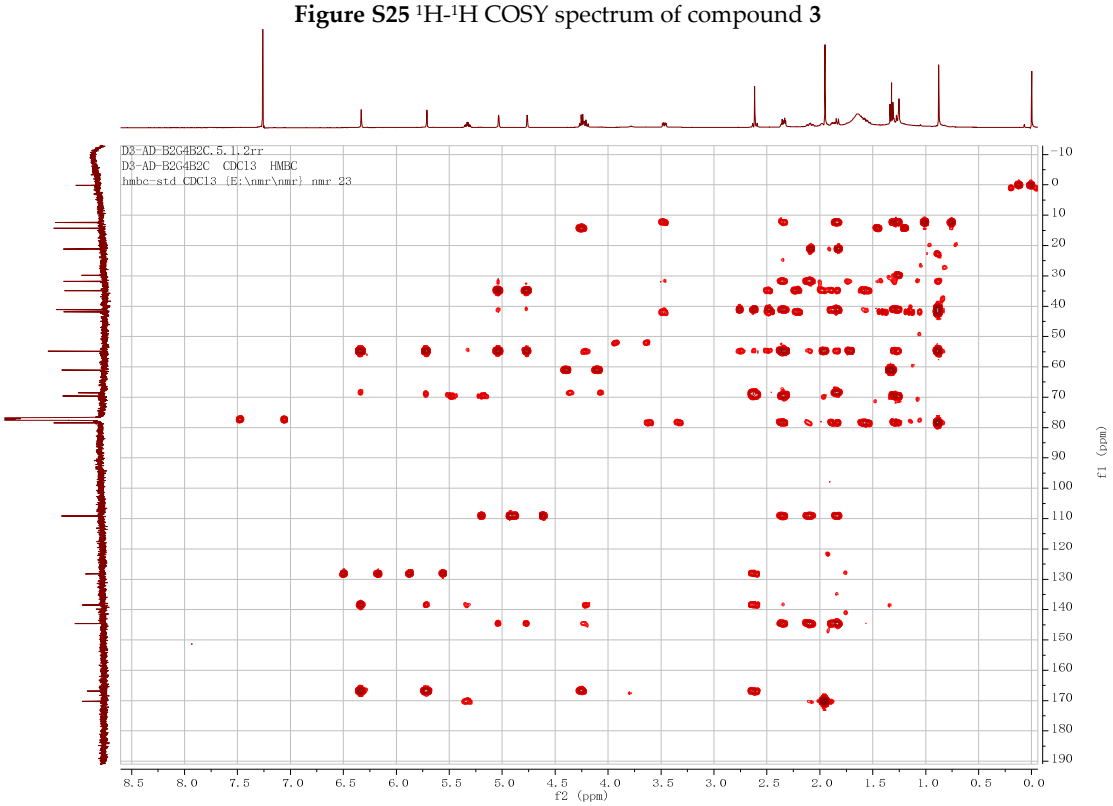


Figure S26 HMBC spectrum of compound **3**

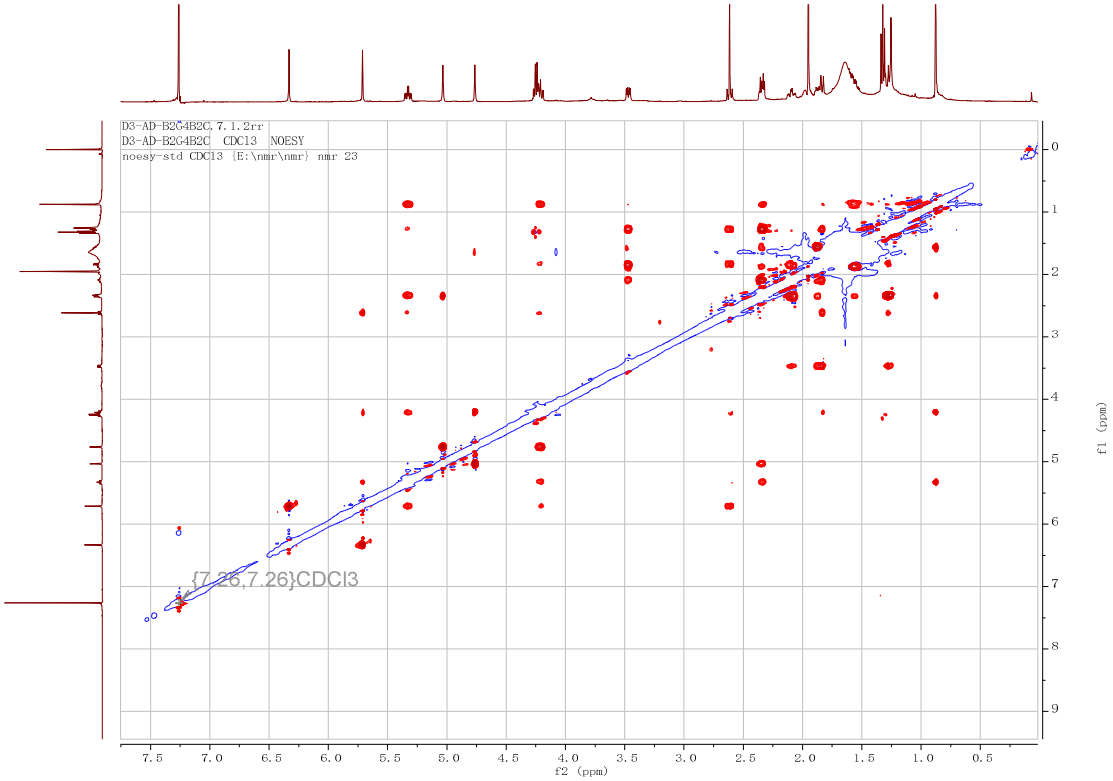


Figure S27 NOESY spectrum of compound **3**

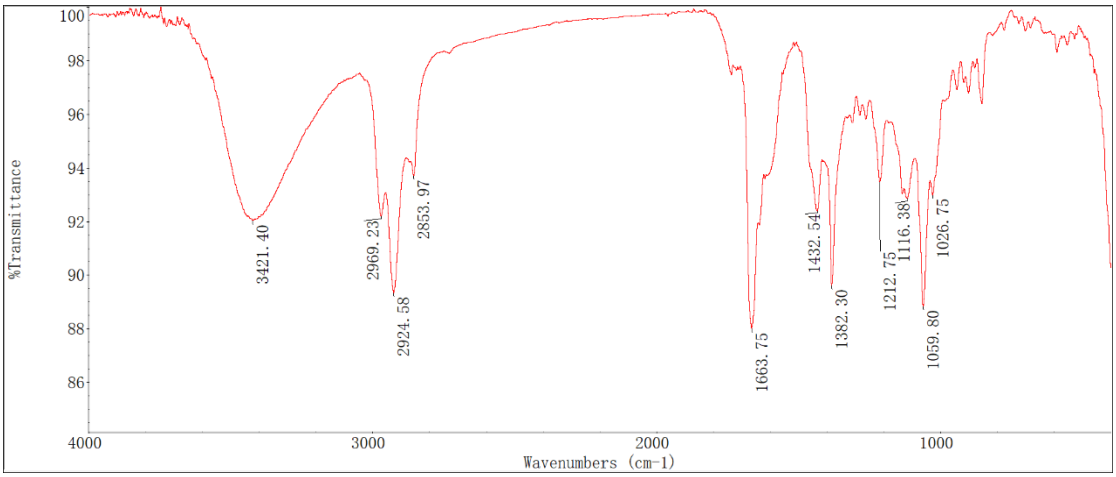


Figure S28 IR spectrum of compound **3**

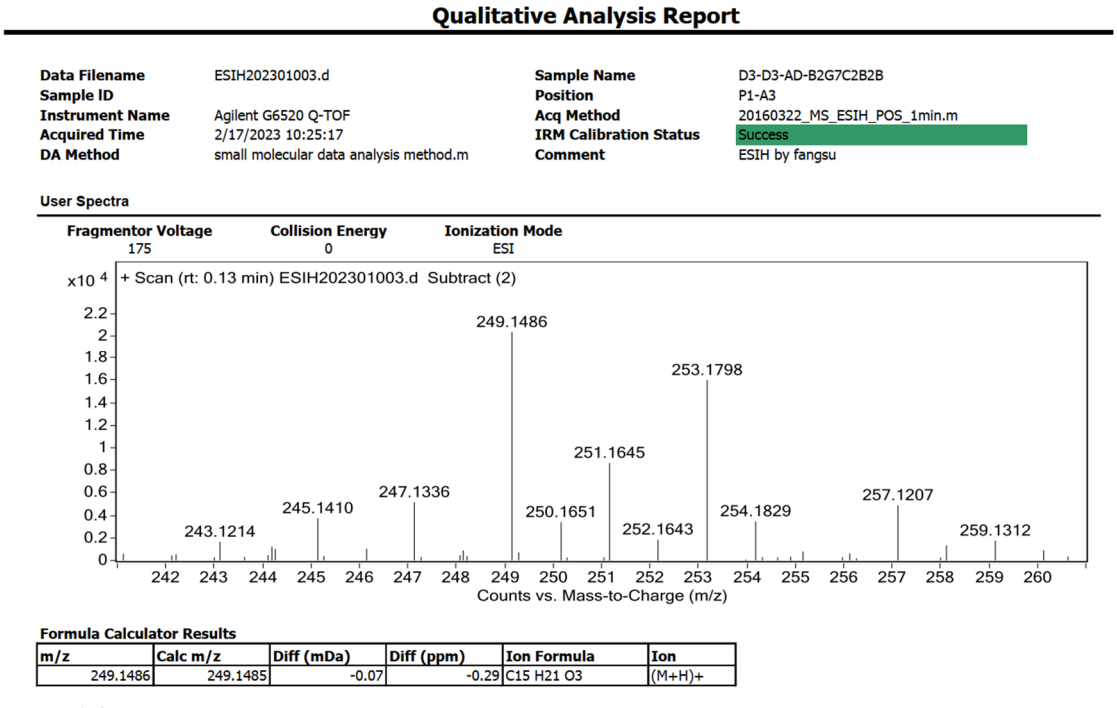


Figure S29 HR-ESIMS spectrum of compound **4**

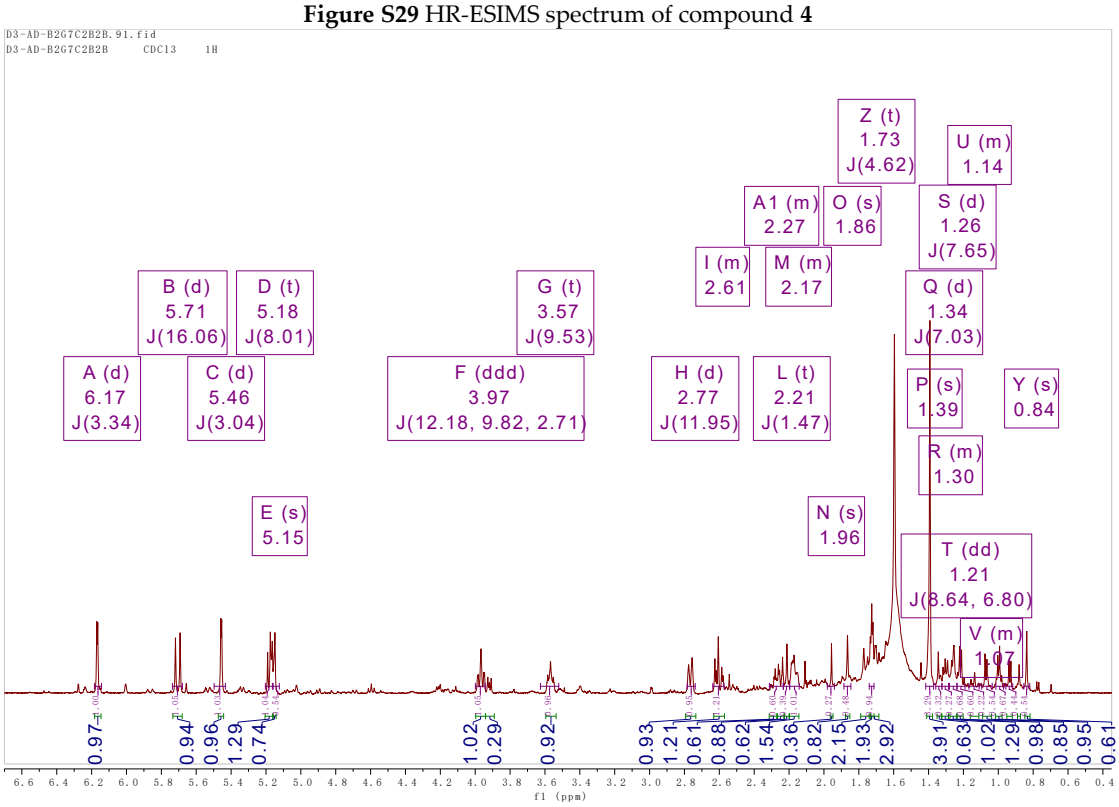


Figure S30 ^{1}H NMR spectrum of compound **4**

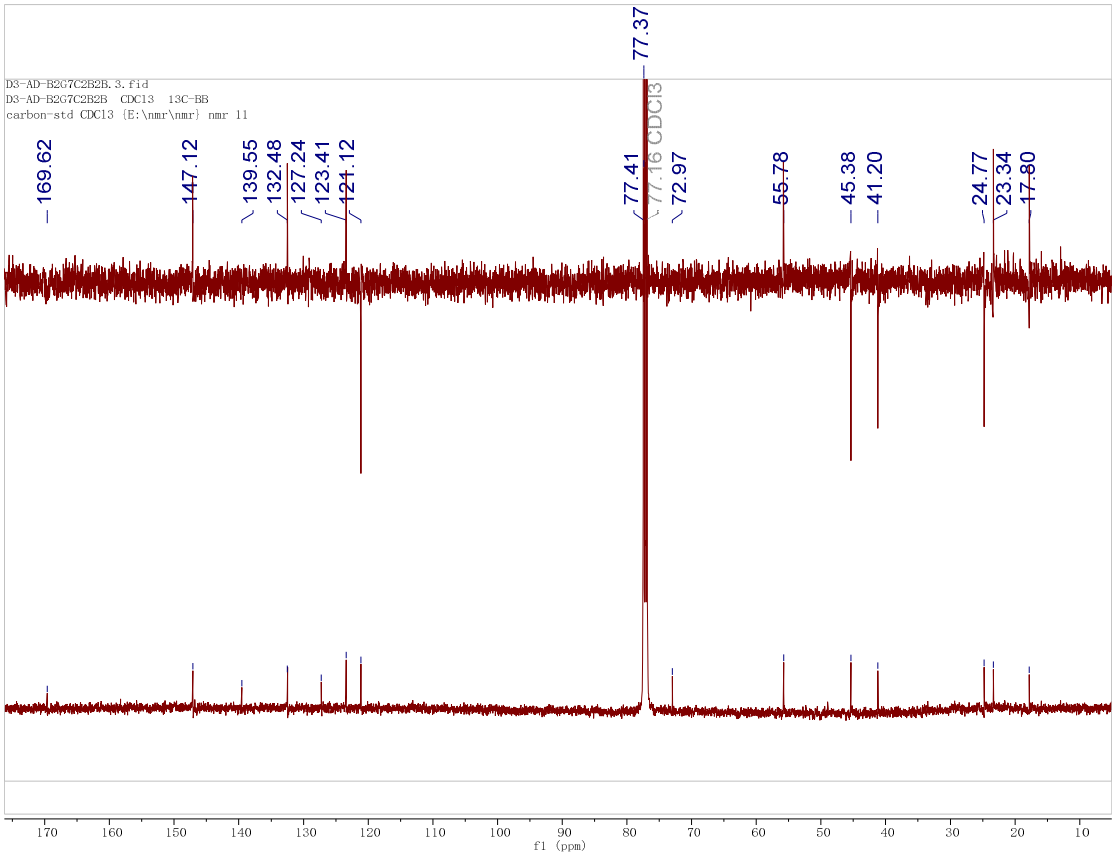


Figure S31 ^{13}C NMR spectrum of compound **4**

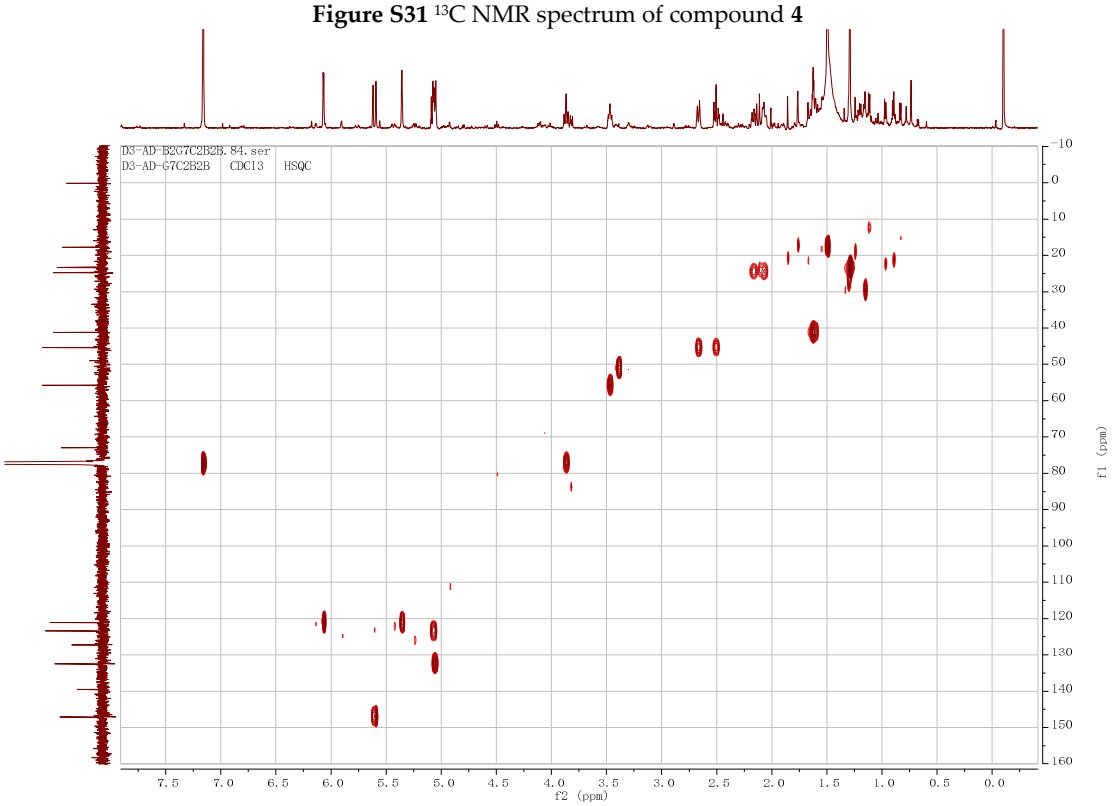


Figure S32 HSQC spectrum of compound **4**

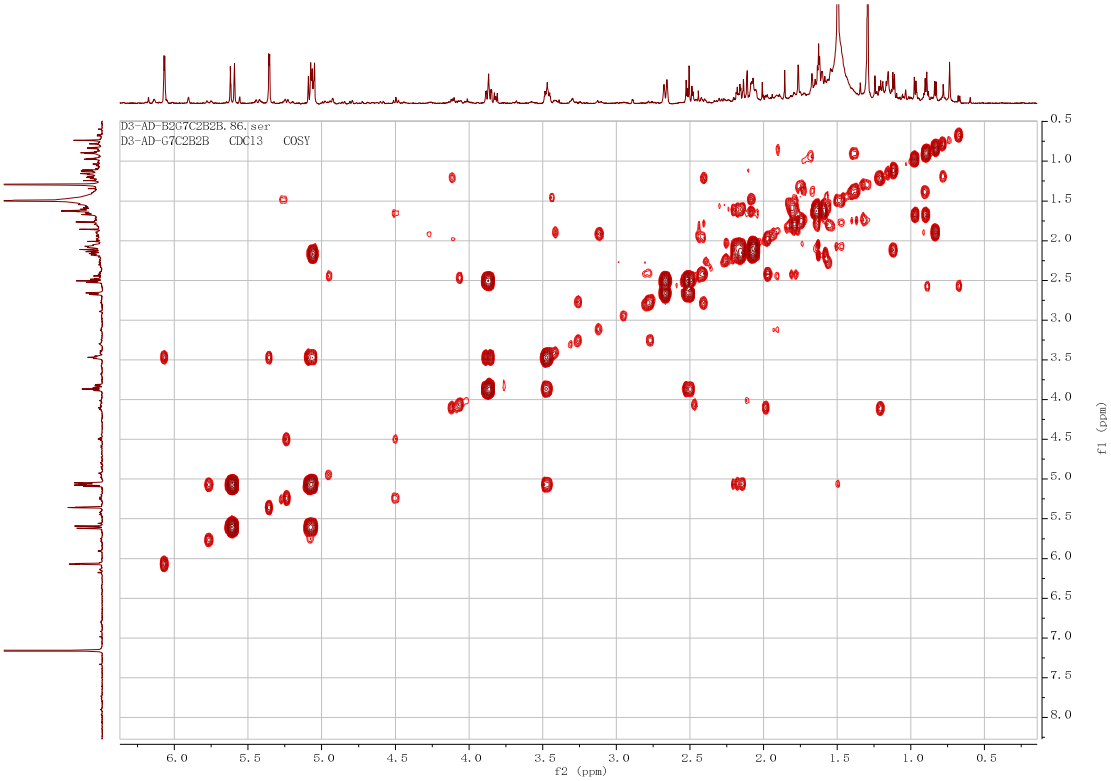


Figure S33 ^{1}H-^{1}H COSY spectrum of compound **4**

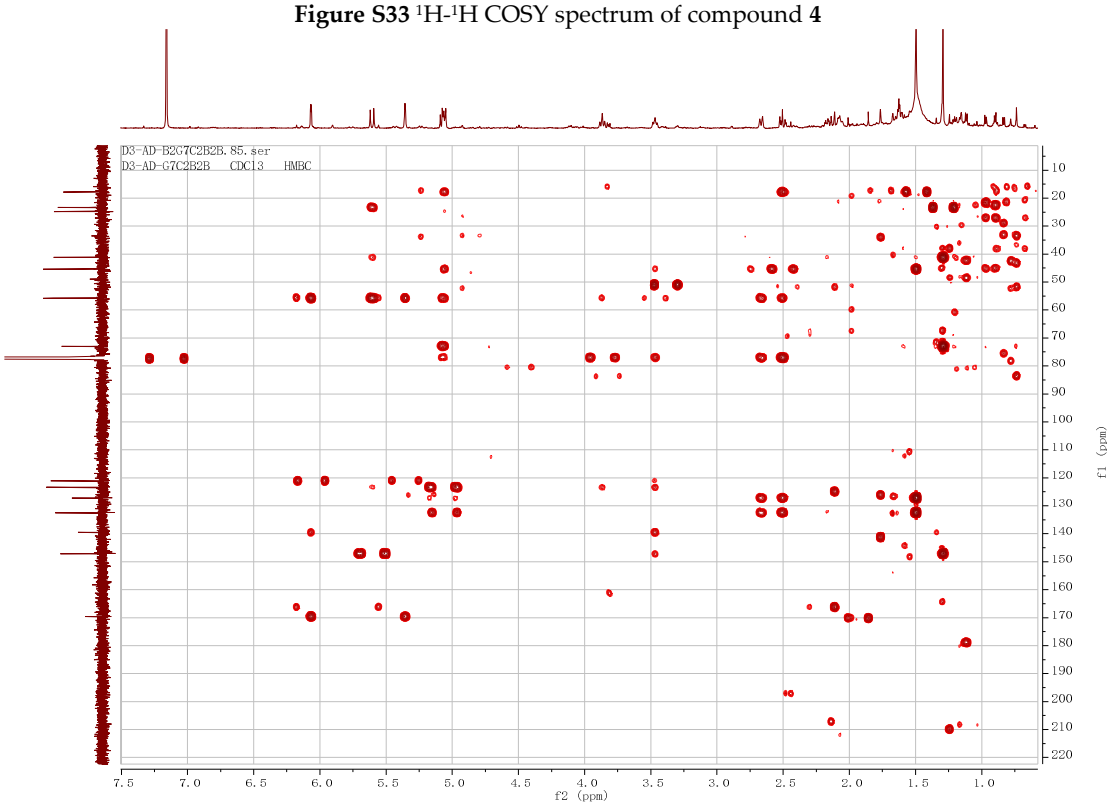


Figure S34 HMBC spectrum of compound **4**

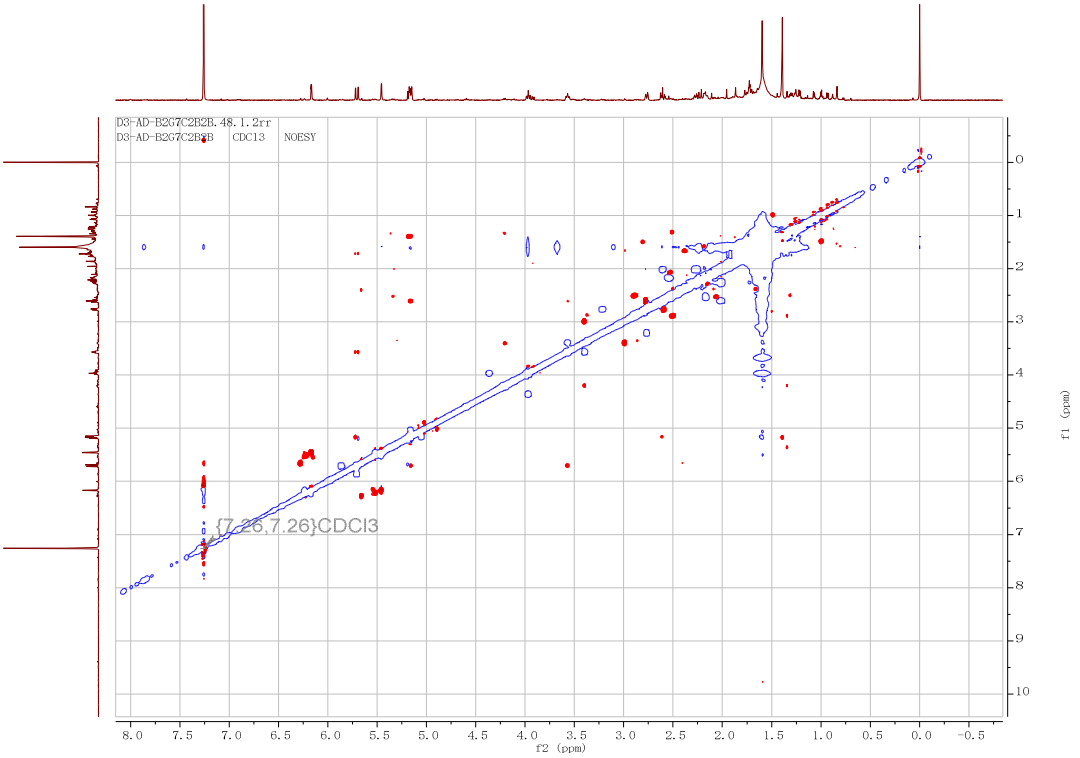


Figure S35 NOESY spectrum of compound **4**

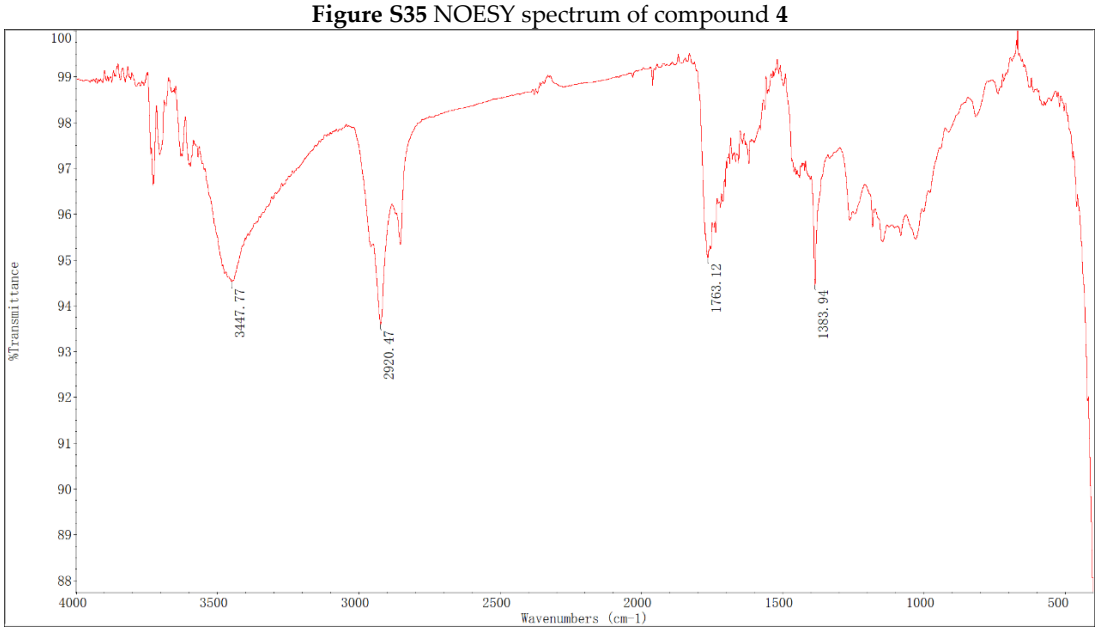
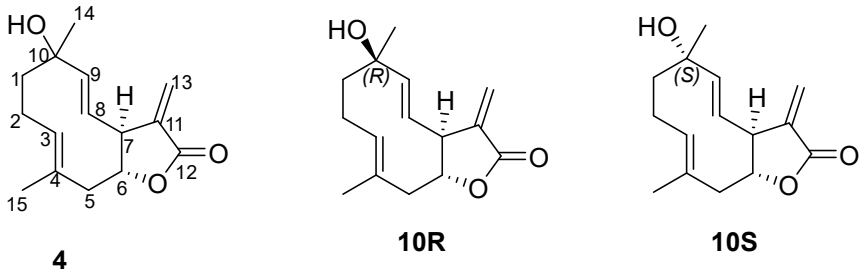


Figure S36 IR spectrum of compound **4**



4 **10R** **10S**

Figure S37 Possible isomers of compound **4**

Functional	Solvent?	Basis Set
mPW1PW91	PCM	6-311G(d,p)

	Isomer 1	Isomer 2	Isomer 3	Isom
sDP4+ (H data)	1.67%	98.33%	–	–
sDP4+ (C data)	0.02%	99.98%	–	–
sDP4+ (all data)	0.00%	100.00%	–	–
uDP4+ (H data)	9.94%	90.06%	–	–
uDP4+ (C data)	0.08%	99.92%	–	–
uDP4+ (all data)	0.01%	99.99%	–	–
DP4+ (H data)	0.19%	99.81%	–	–
DP4+ (C data)	0.00%	100.00%	–	–
DP4+ (all data)	0.00%	100.00%	–	–

Figure S38 DP4+ probability statistics of compound **4**

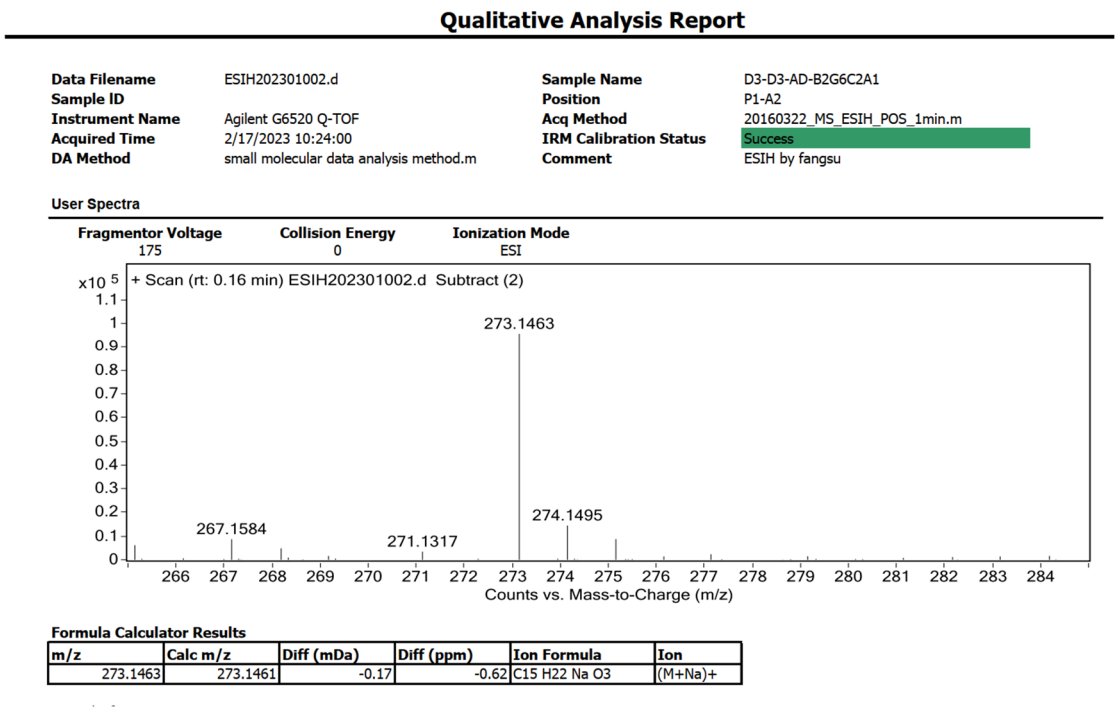


Figure S39 HR-ESIMS spectrum of compound **5**

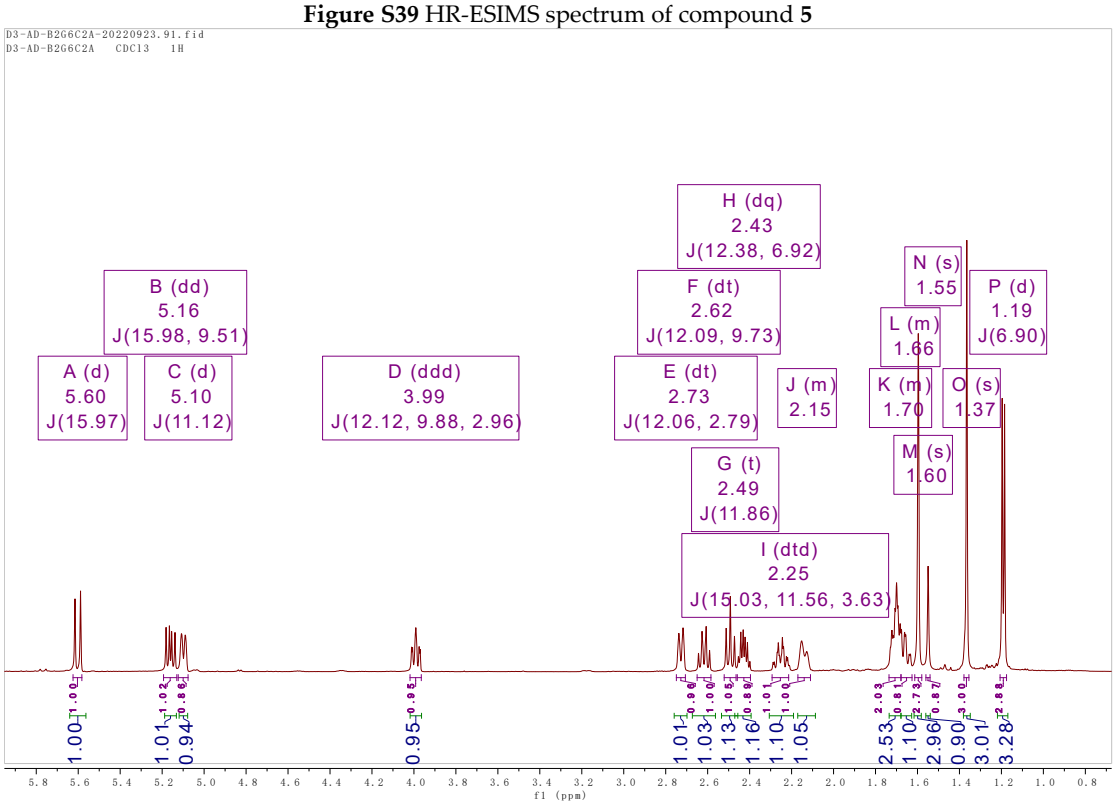


Figure S40 ^{1}H NMR spectrum of compound **5**

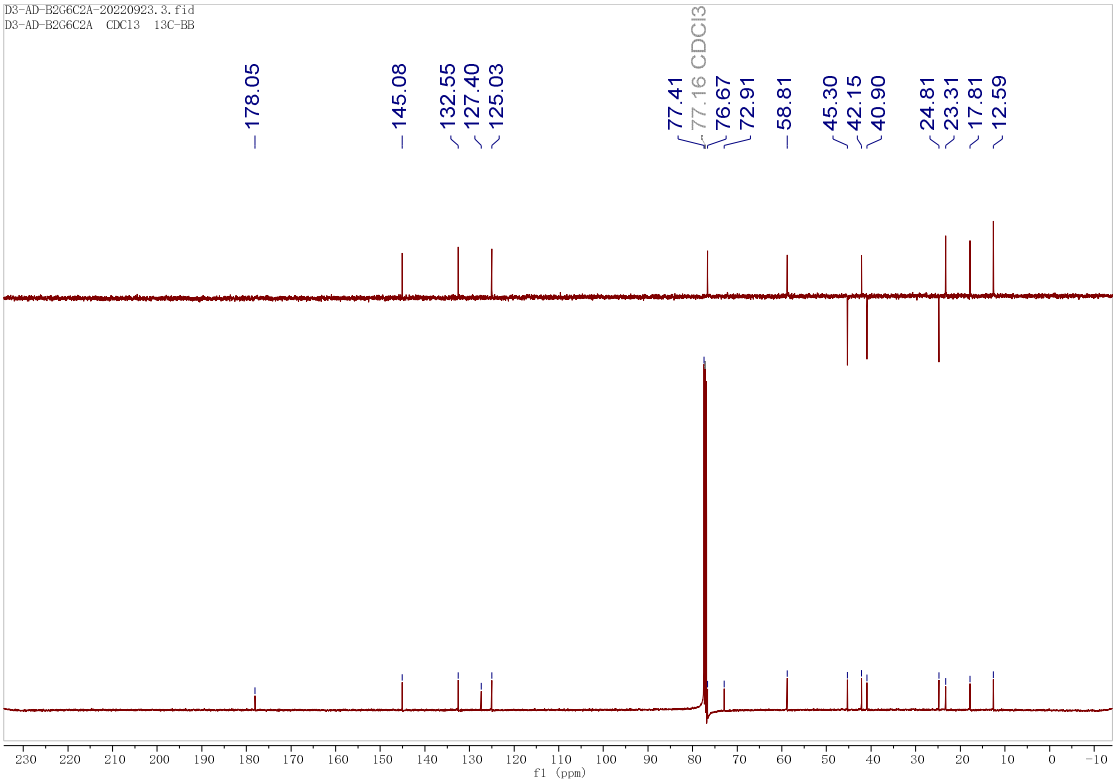


Figure S41 ^{13}C NMR spectrum of compound **5**

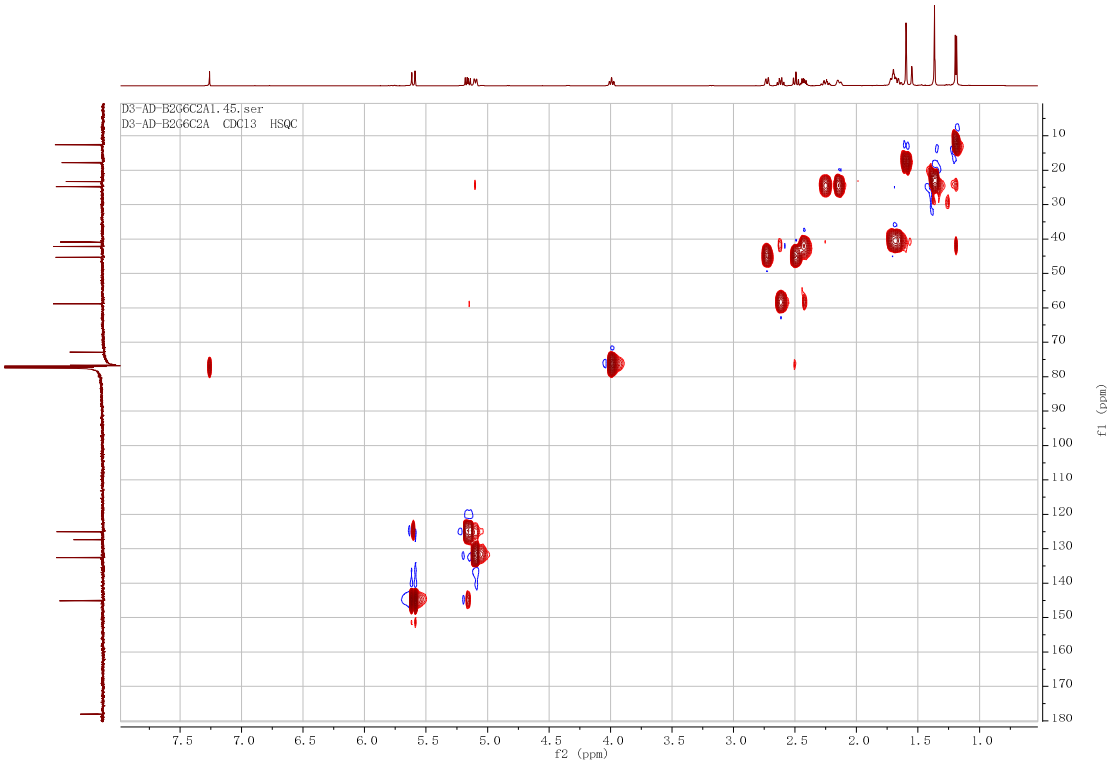


Figure S42 HSQC spectrum of compound **5**

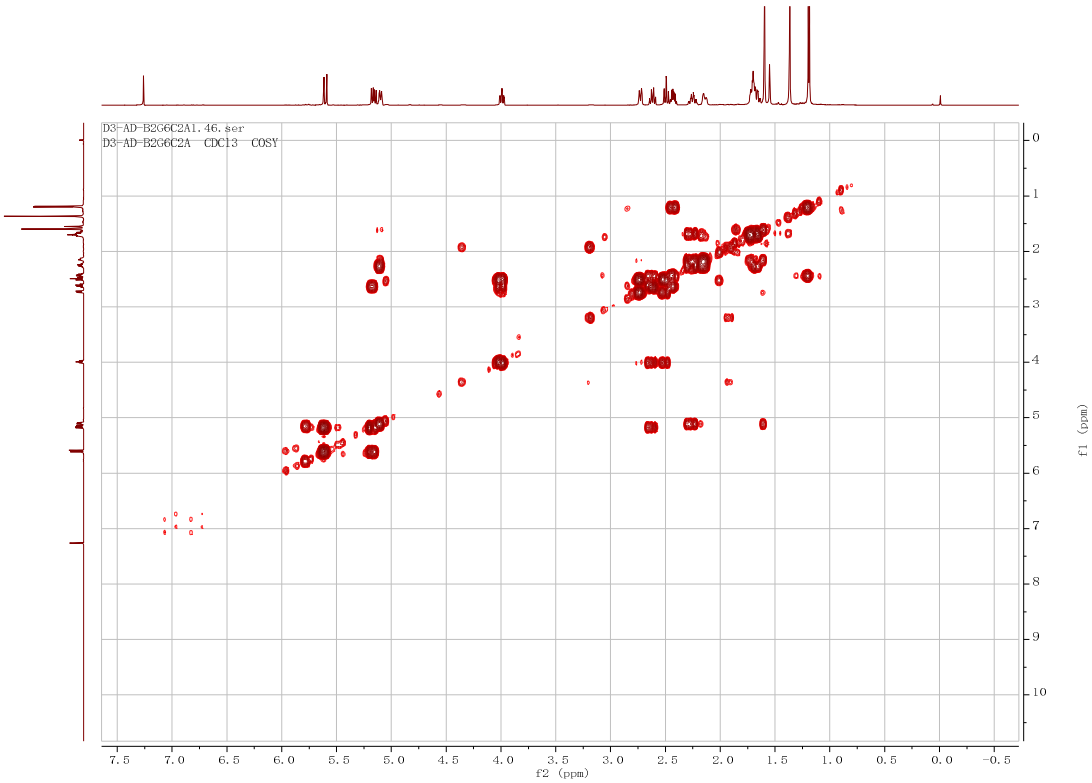


Figure S43 ^{1}H-^{1}H COSY spectrum of compound **5**

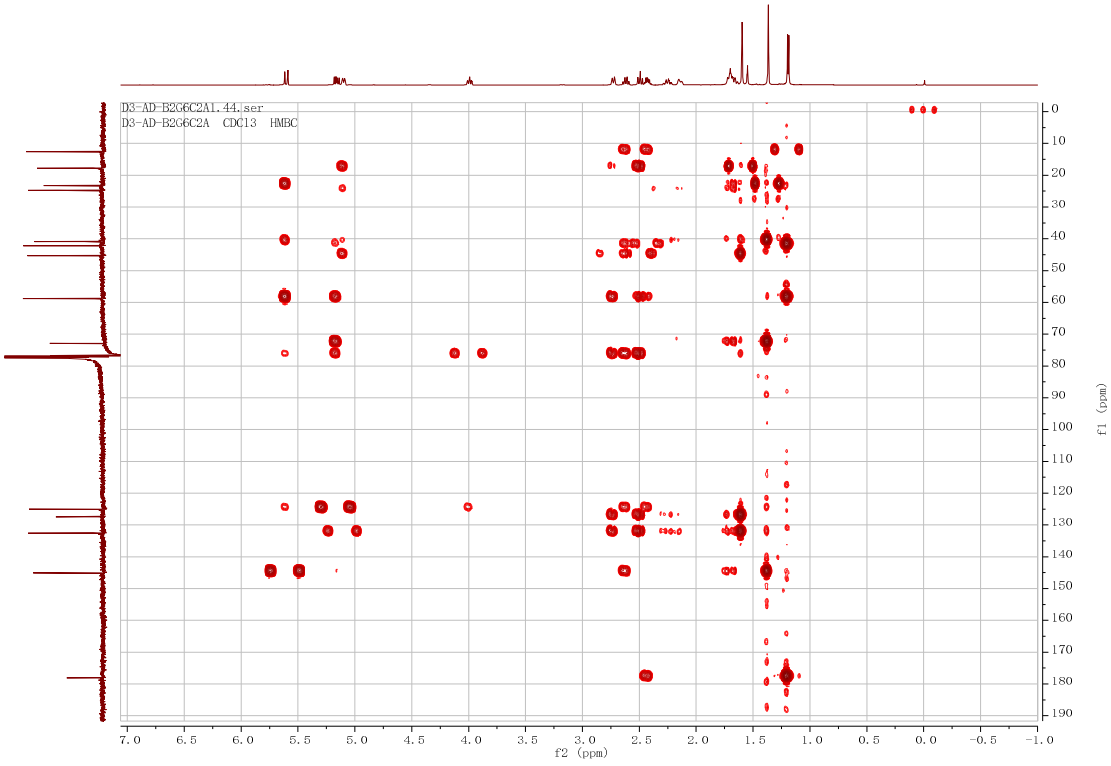


Figure S44 HMBC spectrum of compound **5**

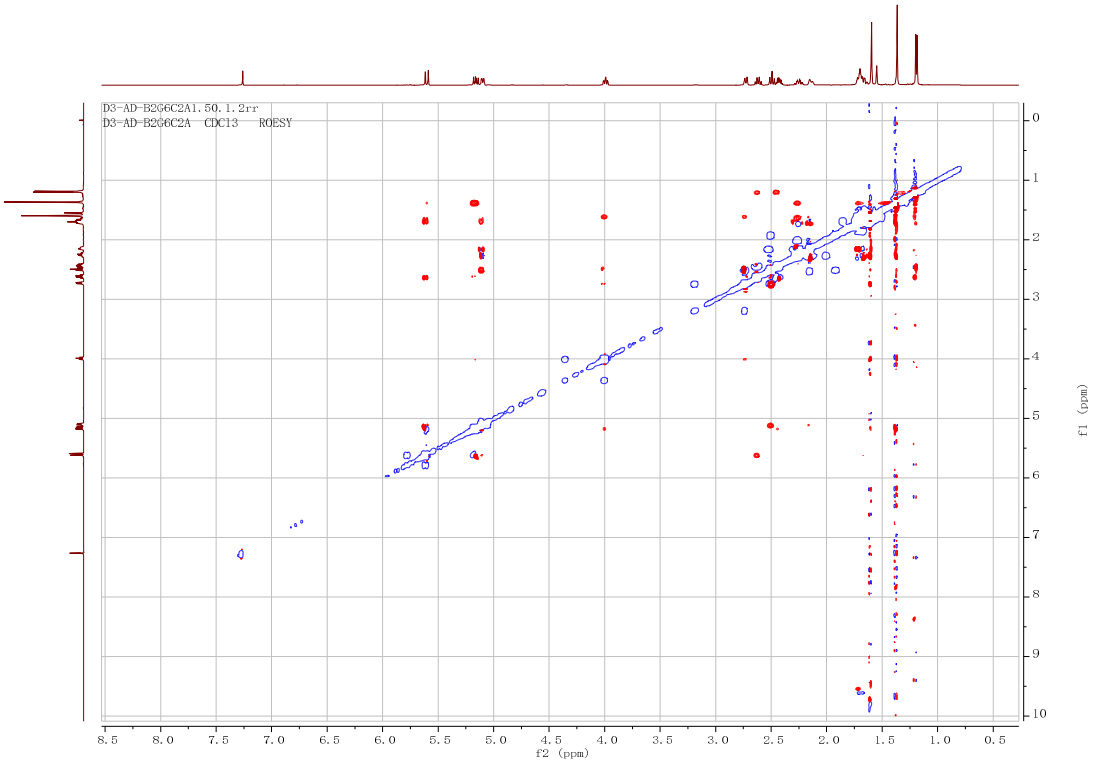


Figure S45 NOESY spectrum of compound **5**

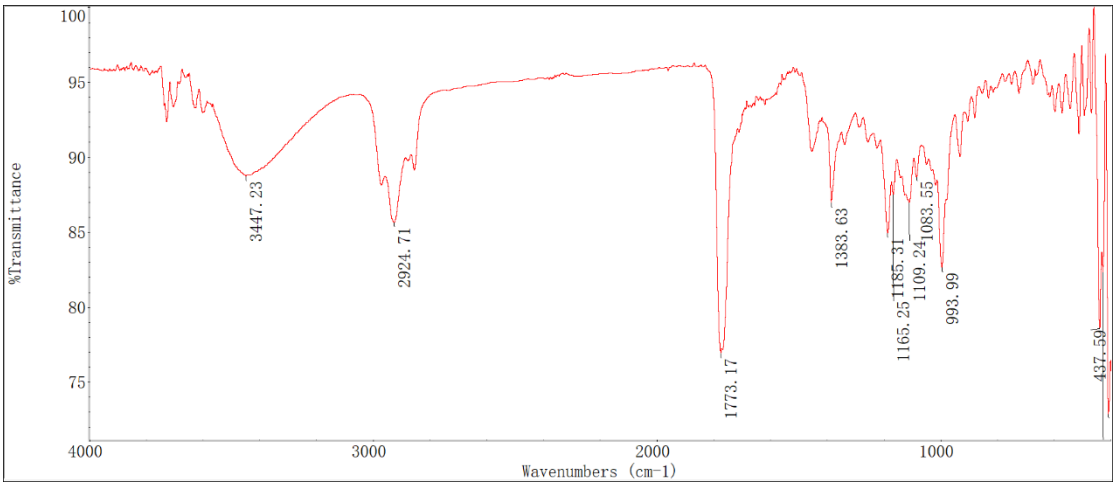


Figure S46 IR spectrum of compound **5**

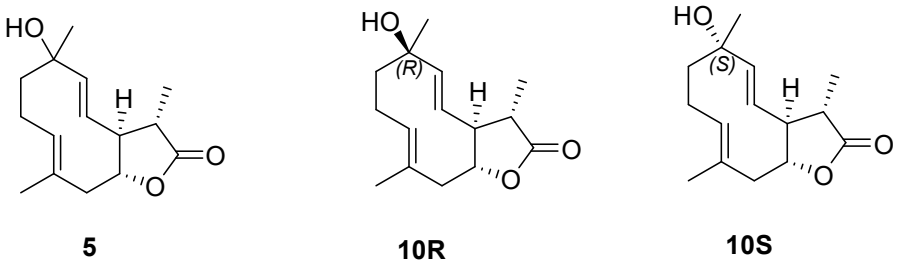


Figure S47 Possible isomers of compound **5**

Functional	Solvent?		Basis Set	
mPW1PW91	PCM		6-311G(d,p)	
	Isomer 1	Isomer 2	Isomer 3	Isom
sDP4+ (H data)	0.85%	99.15%	–	-
sDP4+ (C data)	3.75%	96.25%	–	-
sDP4+ (all data)	0.03%	99.97%	–	-
uDP4+ (H data)	0.20%	99.80%	–	-
uDP4+ (C data)	18.59%	81.41%	–	-
uDP4+ (all data)	0.05%	99.95%	–	-
DP4+ (H data)	0.00%	100.00%	–	-
DP4+ (C data)	0.88%	99.12%	–	-
DP4+ (all data)	0.00%	100.00%	–	-

Figure S48 DP4+ probability statistics of compound **5**

Elemental Composition Report
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
41 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-200 H: 0-60 O: 0-6 Na: 0-1

Minimum:		80.00					-1.5		
Maximum:		100.00			2.0	5.0	50.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
219.1744	00.00	219.1749	-0.5	-2.3	4.5	424.1	n/a	n/a	$C_{15}H_{23}O$

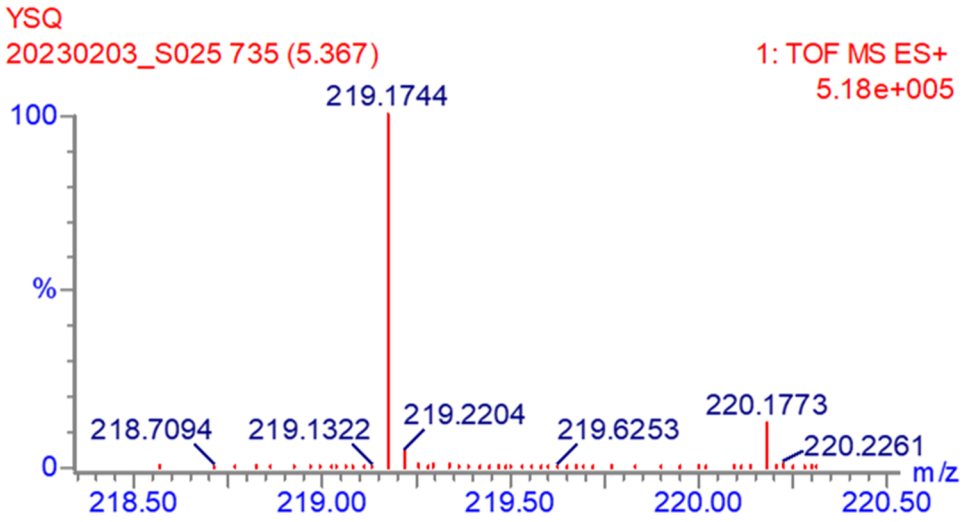


Figure S49 HR-ESIMS spectrum of compound **6**

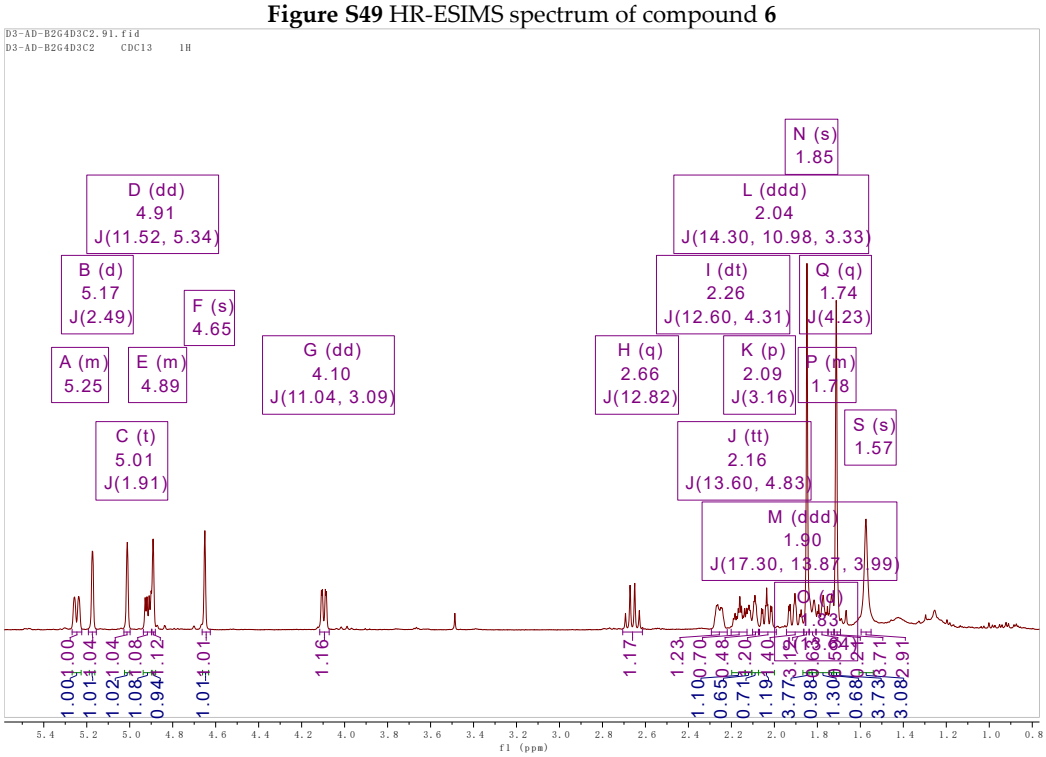


Figure S50 ^{1}H NMR spectrum of compound **6**

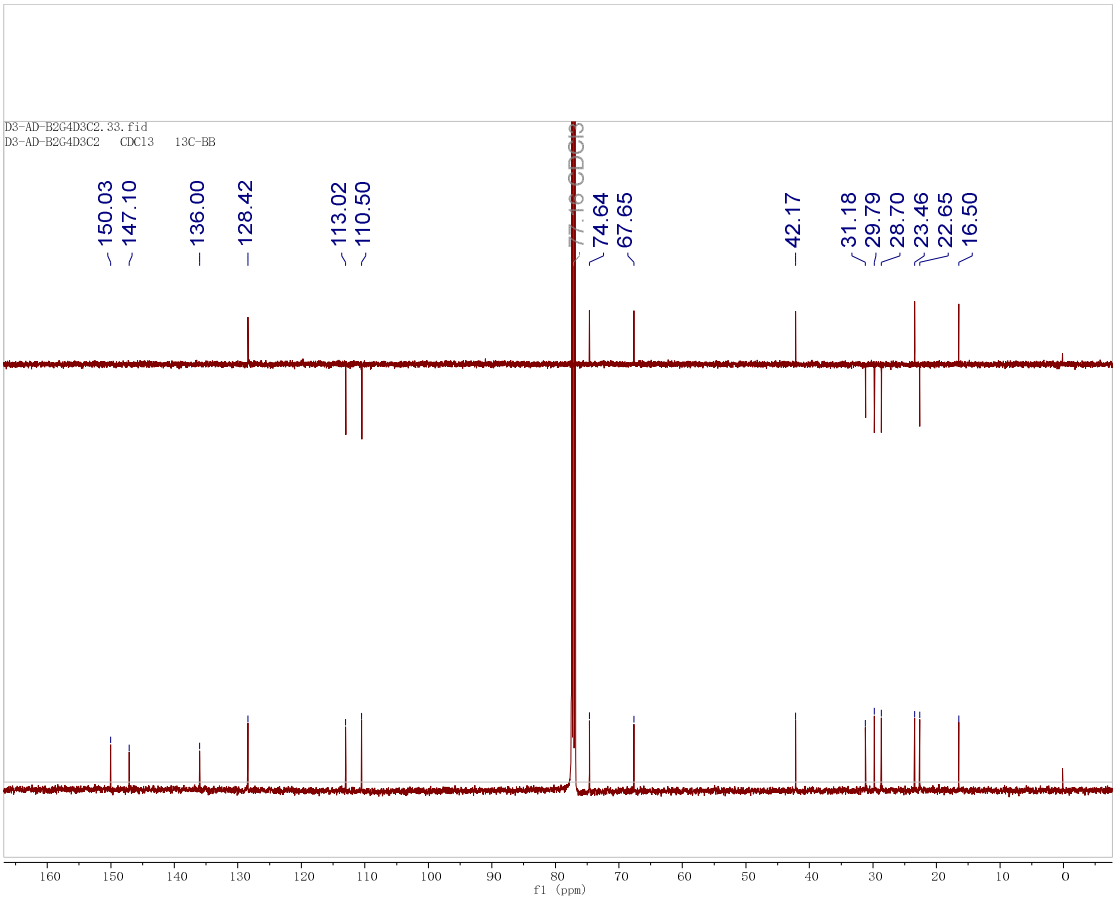


Figure S51 ^{13}C NMR spectrum of compound **6**

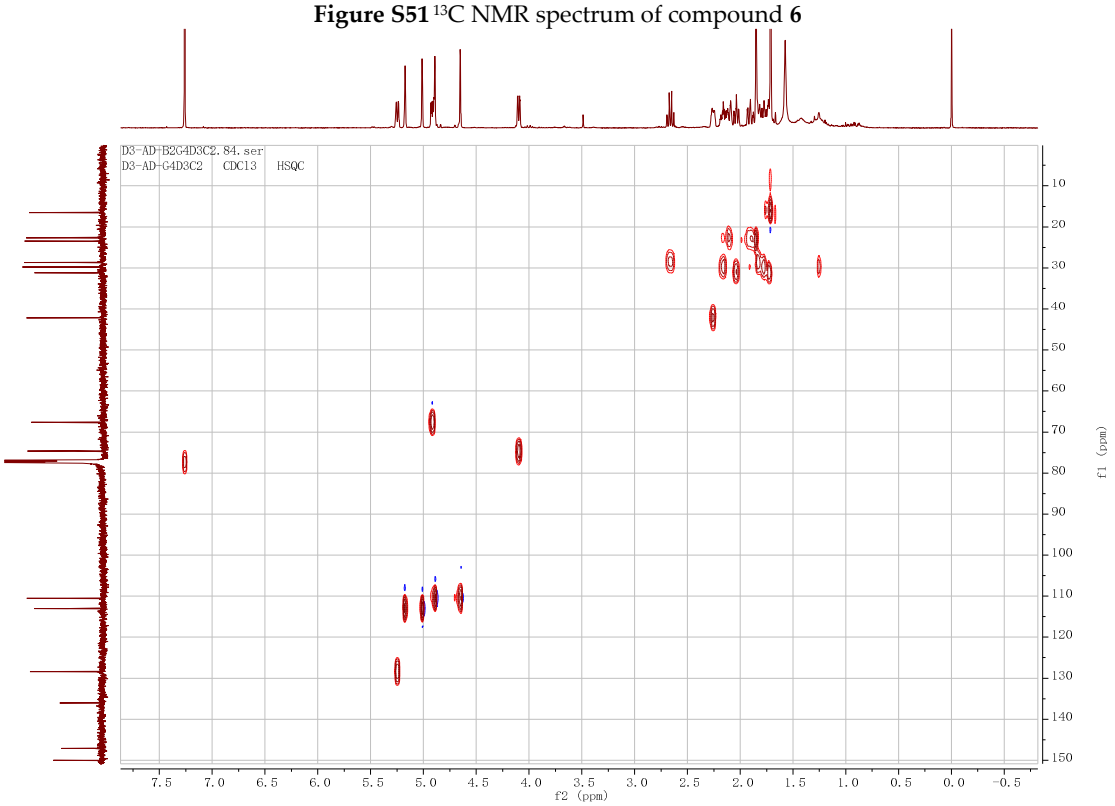


Figure S52 HSQC spectrum of compound **6**

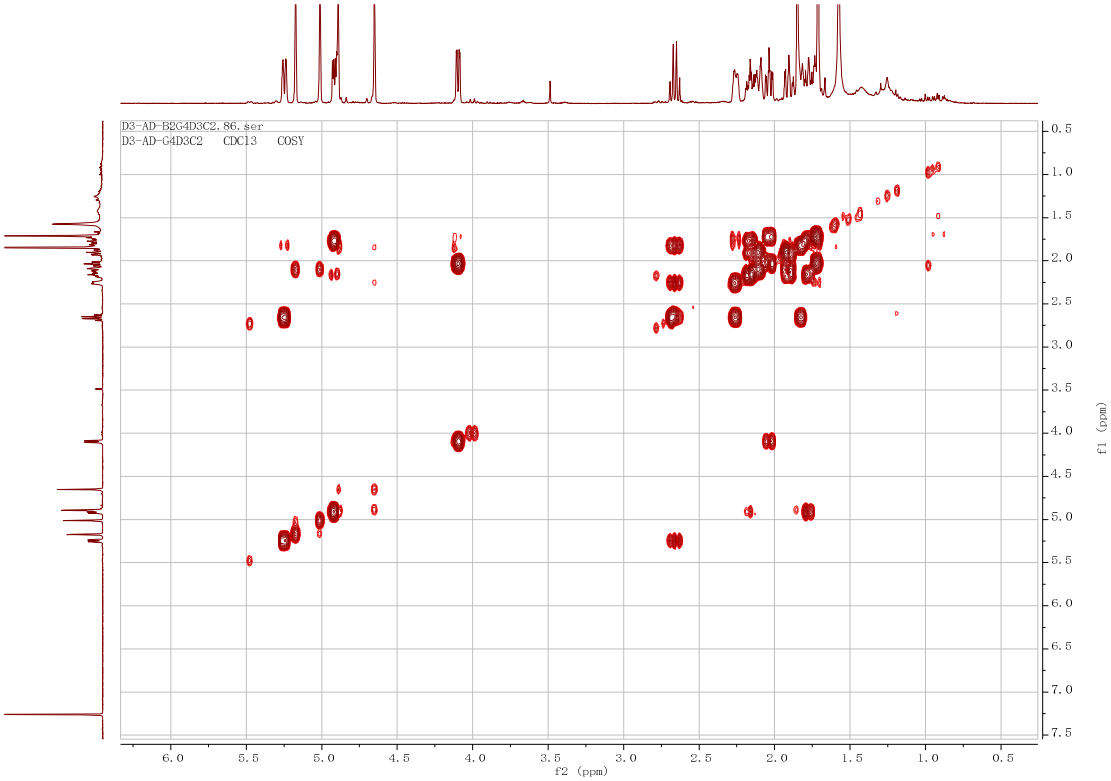


Figure S53 ^{1}H-^{1}H COSY spectrum of compound **6**

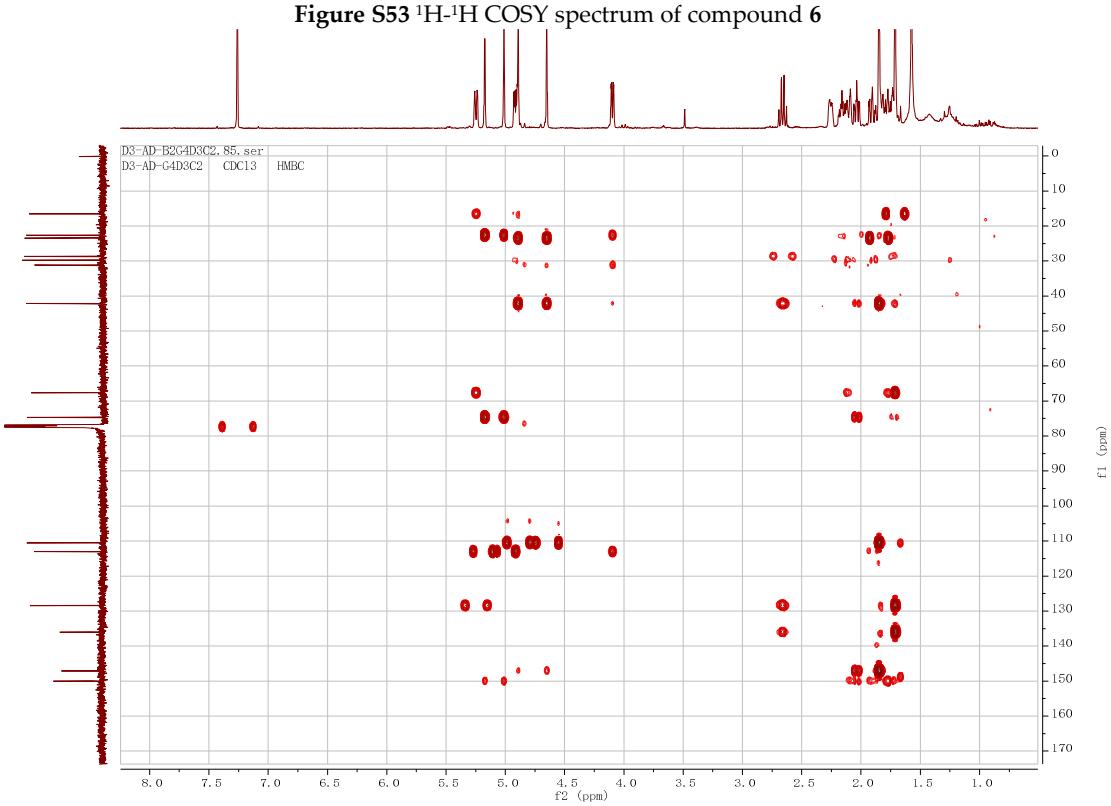


Figure S54 HMBC spectrum of compound **6**

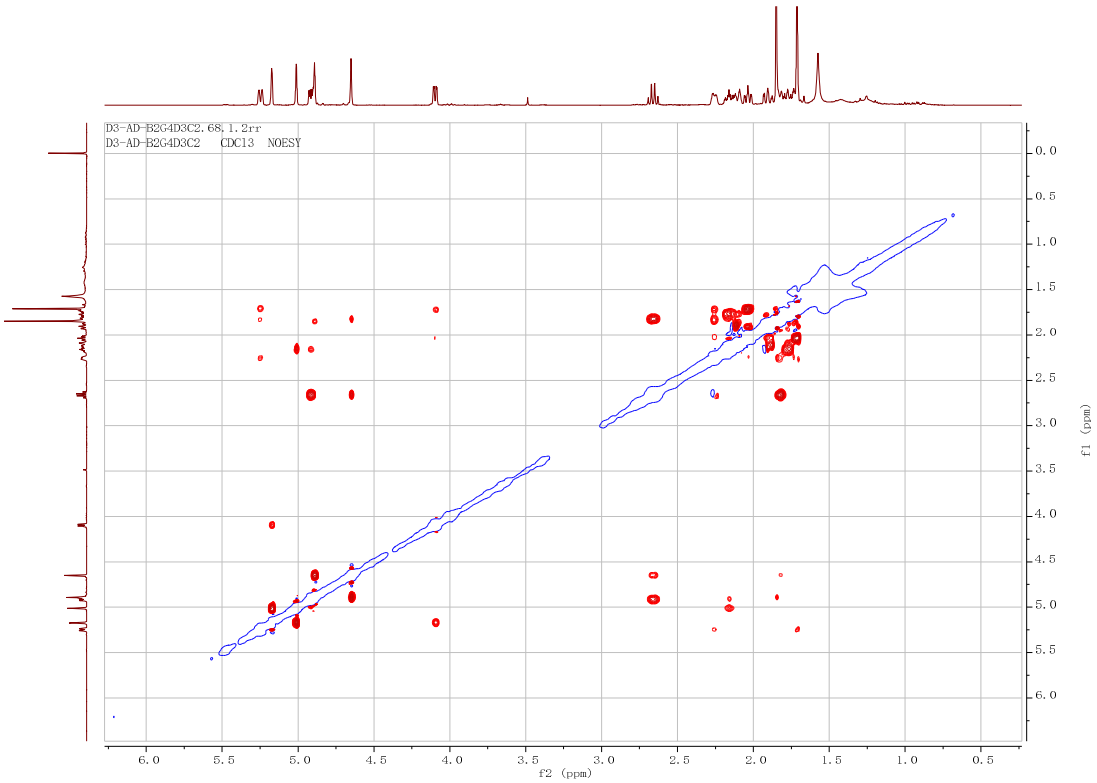


Figure S55 NOESY spectrum of compound **6**

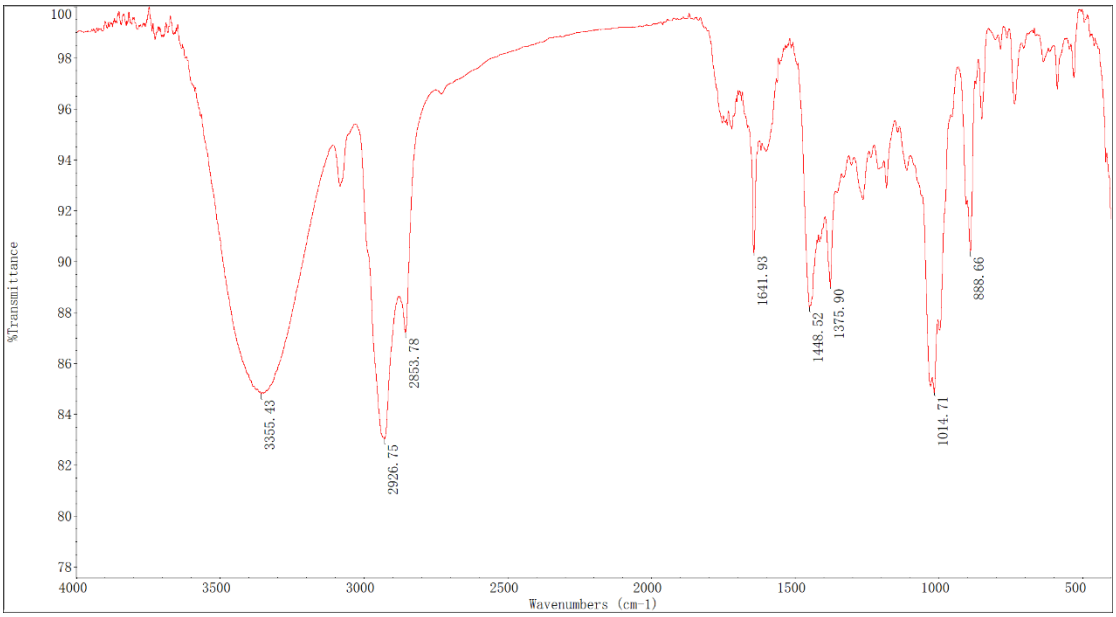


Figure S56 IR spectrum of compound **6**

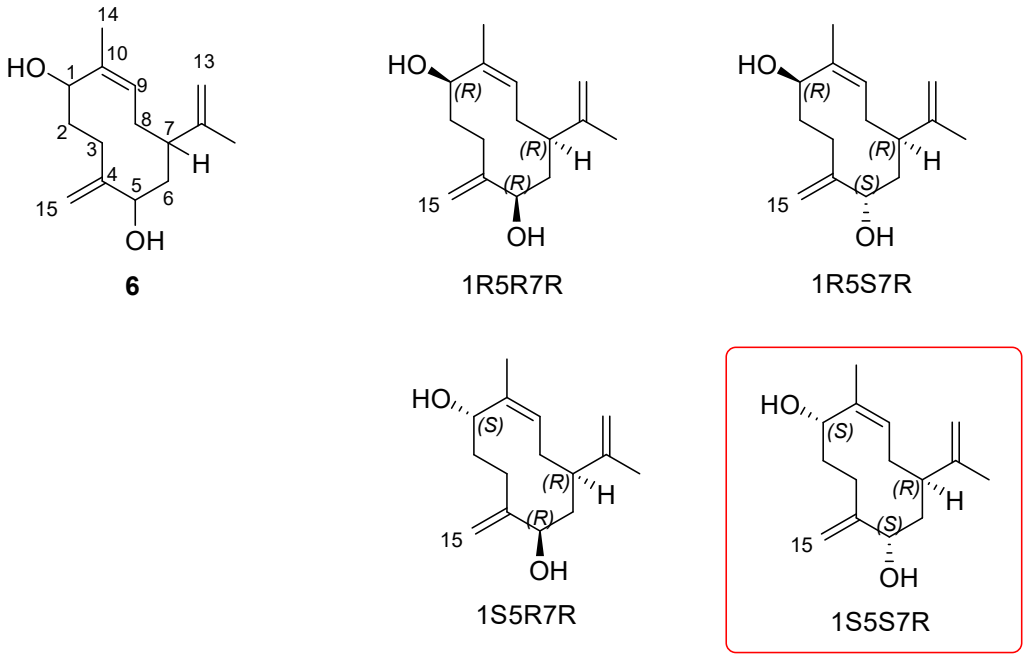


Figure S57 Possible isomers of compound **6**

Functional	Solvent?	Basis Set		
mPW1PW91	PCM	6-311G(d,p)		
	Isomer 1	Isomer 2	Isomer 3	Isomer 4
sDP4+ (H data)	1.36%	0.58%	0.00%	98.06%
sDP4+ (C data)	0.03%	0.00%	0.00%	99.97%
sDP4+ (all data)	0.00%	0.00%	0.00%	100.00%
uDP4+ (H data)	2.31%	0.00%	0.00%	97.69%
uDP4+ (C data)	0.04%	0.00%	0.00%	99.95%
uDP4+ (all data)	0.00%	0.00%	0.00%	100.00%
DP4+ (H data)	0.03%	0.00%	0.00%	99.97%
DP4+ (C data)	0.00%	0.00%	0.00%	100.00%
DP4+ (all data)	0.00%	0.00%	0.00%	100.00%

Figure S58 DP4+ probability statistics of compound **6**

Elemental Composition Report
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
22 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-200 H: 0-60 O: 0-6

Minimum:	80.00					-1.5			
Maximum:	100.00			2.0	5.0	50.0			
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
219.1743	100.00	219.1749	-0.6	-2.7	4.5	695.9	n/a	n/a	$C_{15}H_{23}O$

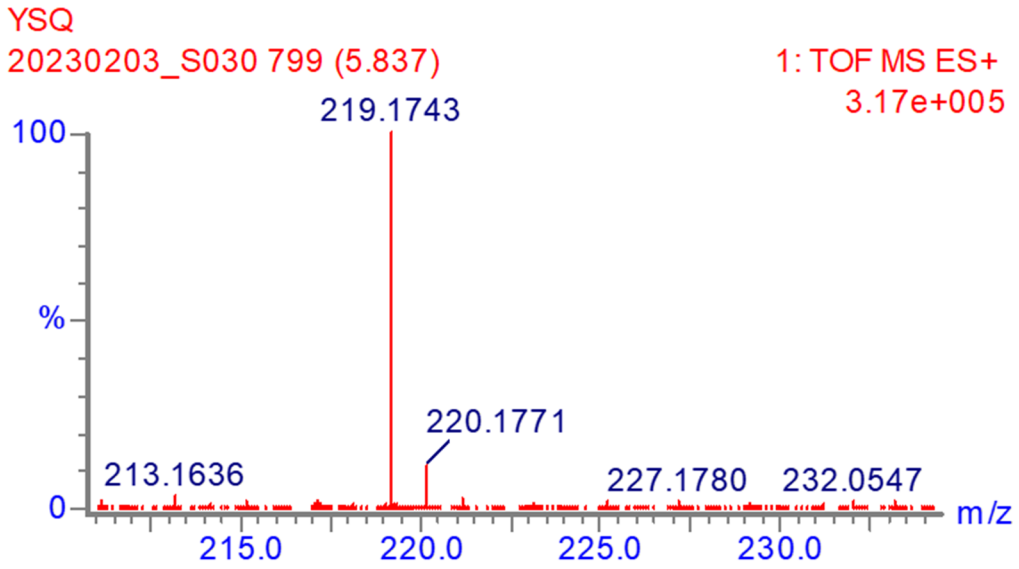


Figure S59 HR-ESIMS spectrum of compound **7**

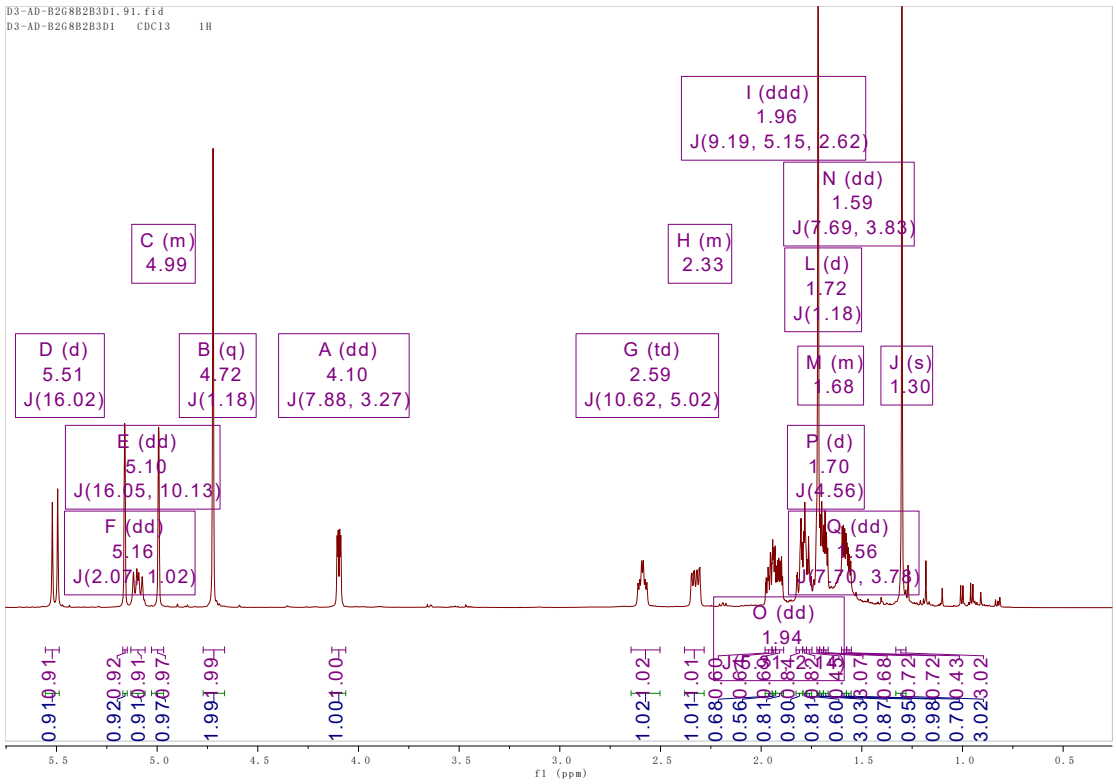


Figure S60 ^{1}H NMR spectrum of compound **7**

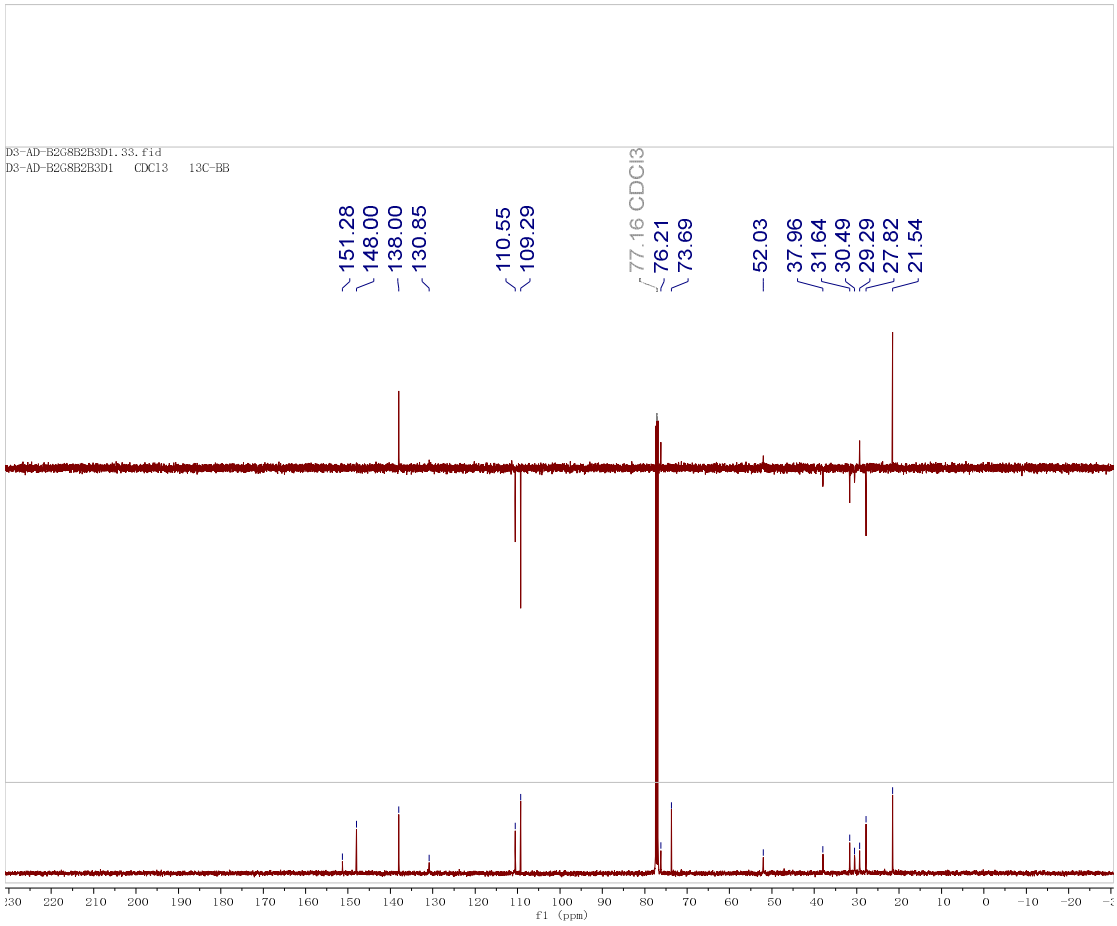


Figure S61 ^{13}C NMR spectrum of compound **7**

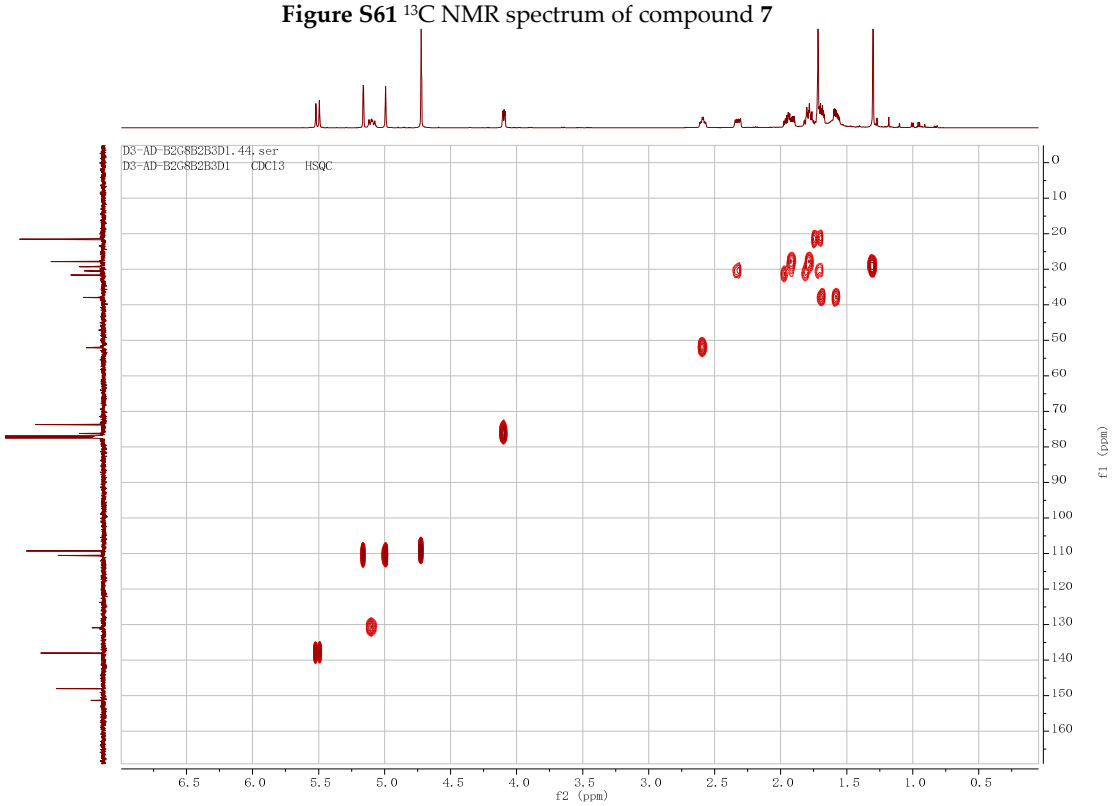


Figure S62 HSQC spectrum of compound **7**

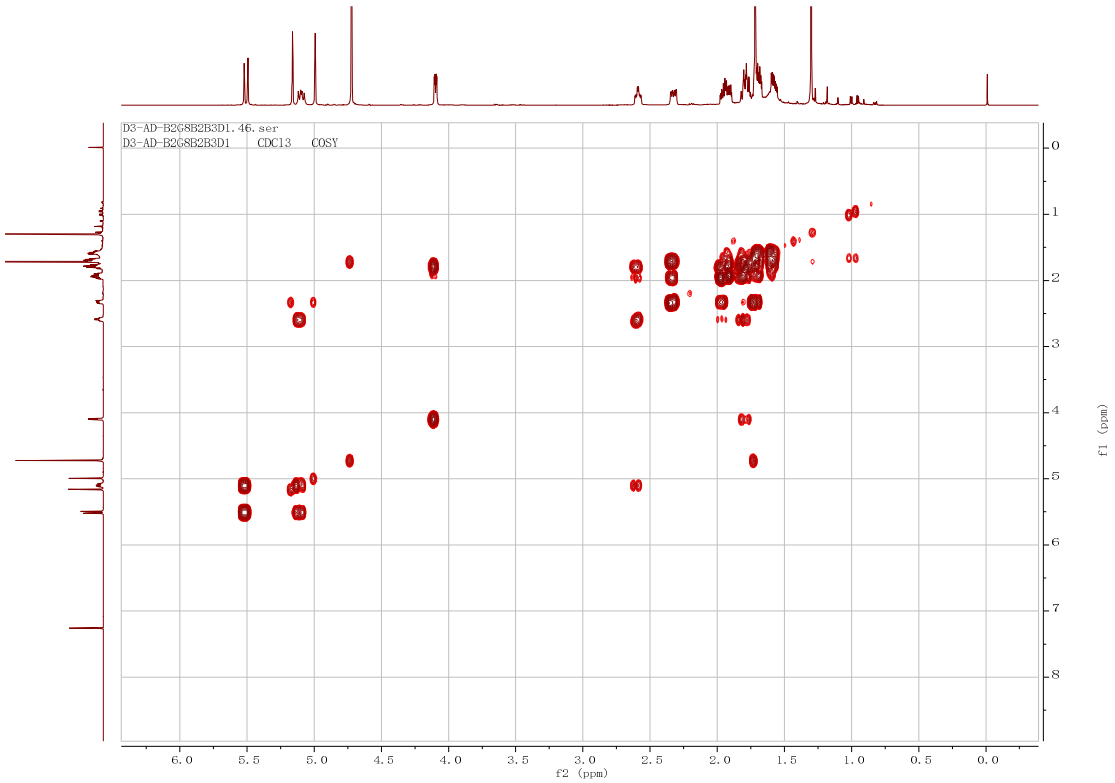


Figure S63 ^{1}H-^{1}H COSY spectrum of compound **7**

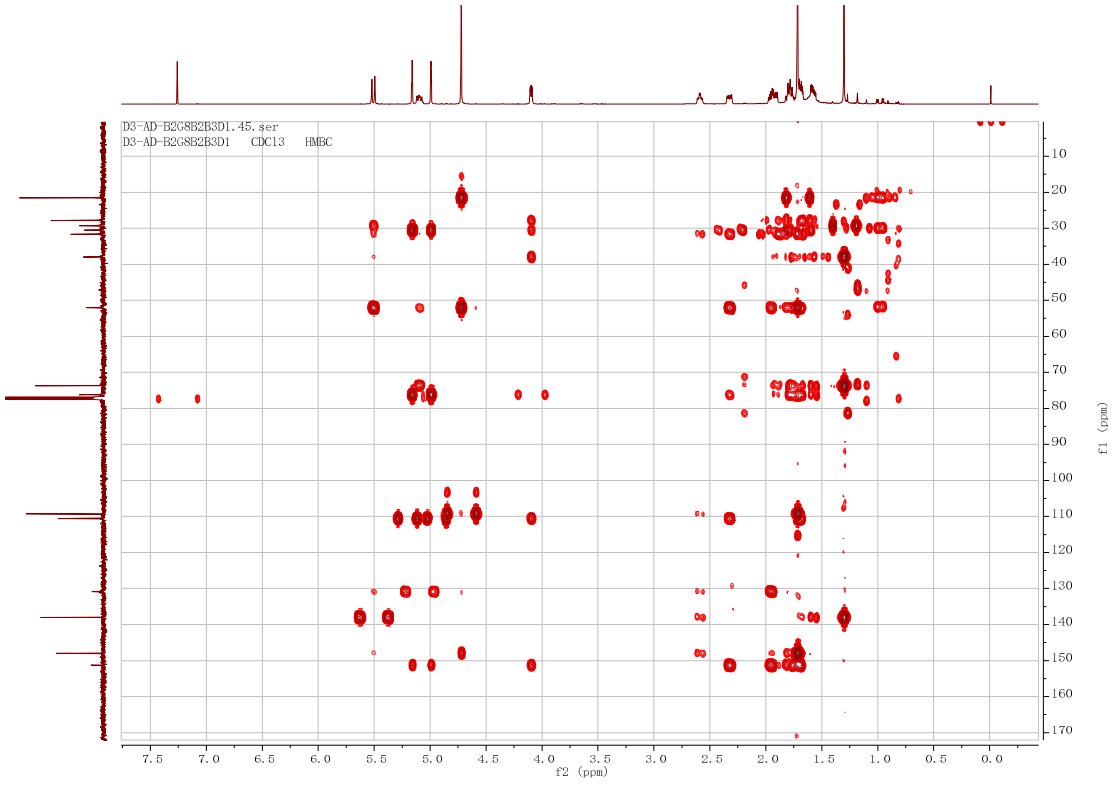


Figure S64 HMBC spectrum of compound **7**

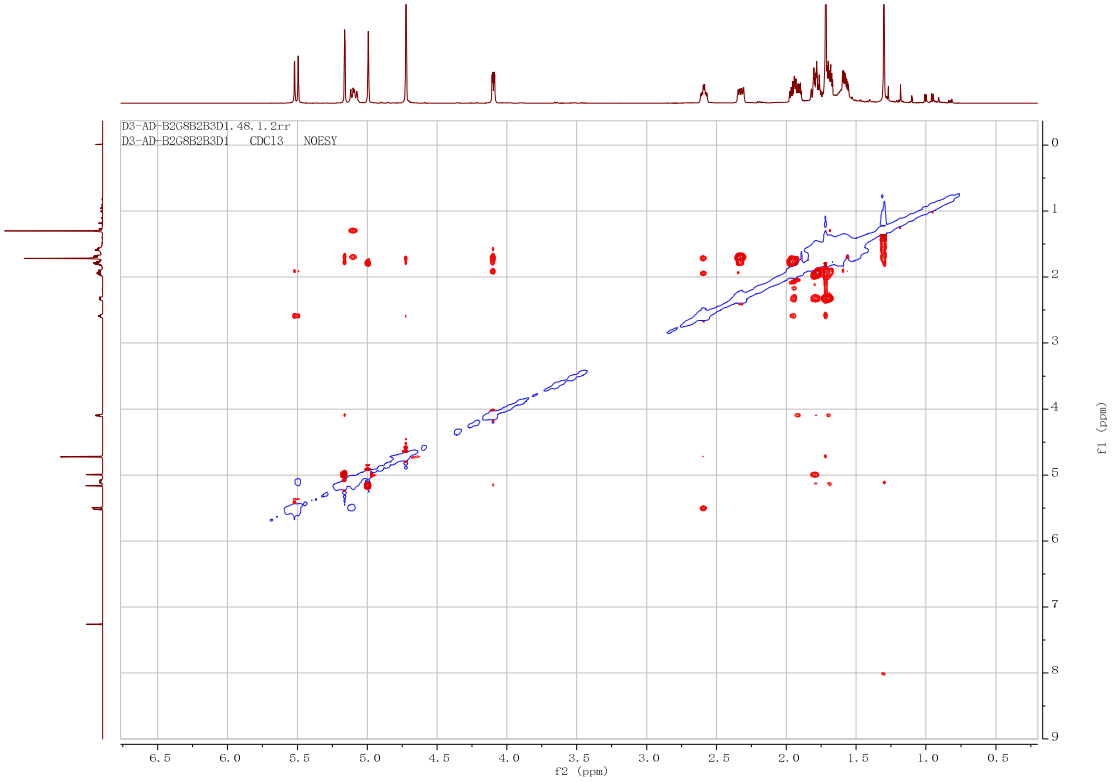


Figure S65 NOESY spectrum of compound **7**

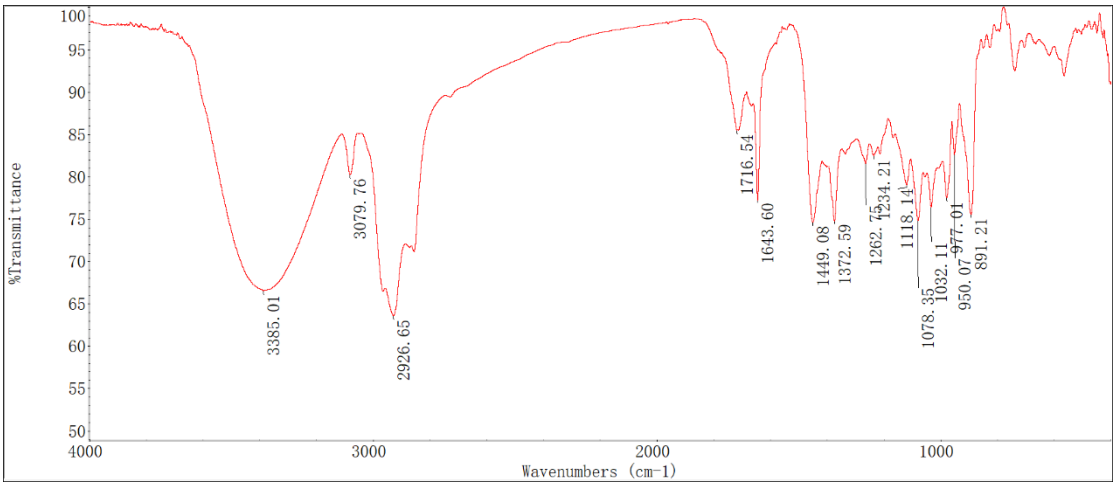


Figure S66 IR spectrum of compound **7**

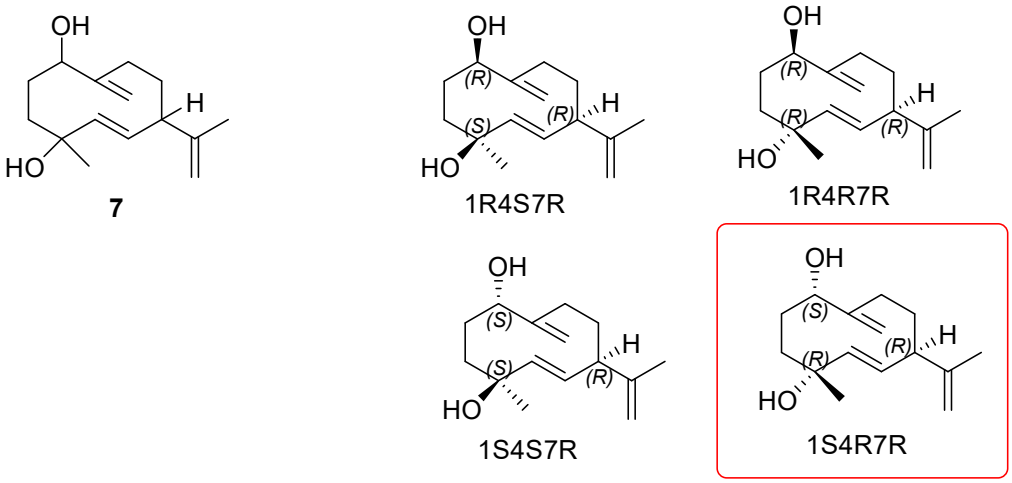


Figure S67 Possible isomers of compound **7**

Functional	Solvent?	Basis Set			
mPW1PW91	PCM	6-311G(d,p)			
	Isomer 1	Isomer 2	Isomer 3	Isomer 4
sDP4+ (H data)	56.38%	3.53%	39.68%	0.41%
sDP4+ (C data)	0.01%	0.00%	99.95%	0.05%
sDP4+ (all data)	0.01%	0.00%	99.99%	0.00%
uDP4+ (H data)	73.73%	0.16%	15.74%	10.38%
uDP4+ (C data)	0.01%	0.00%	99.99%	0.00%
uDP4+ (all data)	0.04%	0.00%	99.96%	0.00%
DP4+ (H data)	86.85%	0.01%	13.05%	0.09%
DP4+ (C data)	0.00%	0.00%	100.00%	0.00%
DP4+ (all data)	0.00%	0.00%	100.00%	0.00%

Figure S68 DP4+ probability statistics of compound **7**

Elemental Composition Report
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
22 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-200 H: 0-60 O: 0-6

Minimum:		80.00					-1.5		
Maximum:		100.00			2.0	5.0	50.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
219.1745	100.00	219.1749	-0.4	-1.8	4.5	582.0	n/a	n/a	$C_{15}H_{23}O$

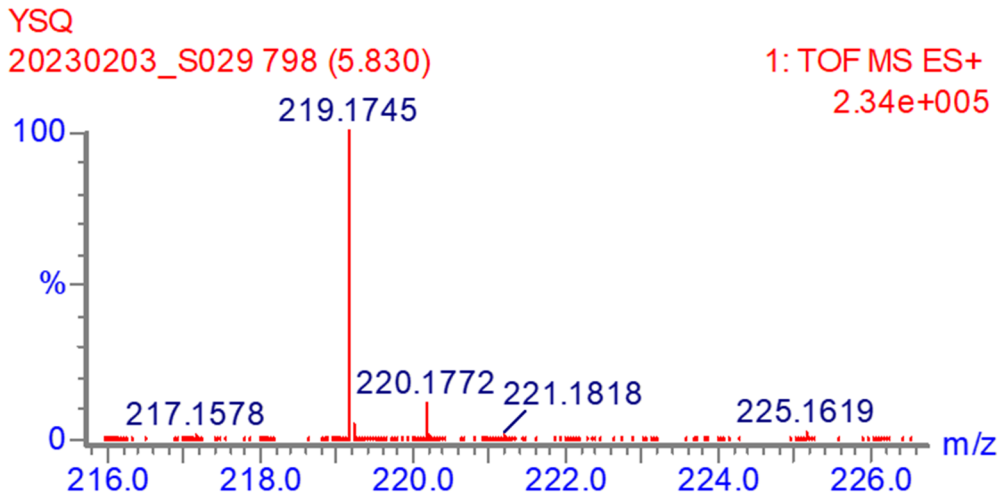


Figure S69 HR-ESIMS spectrum of compound **8**

Figure S70 ^{1}H NMR spectrum of compound **8**

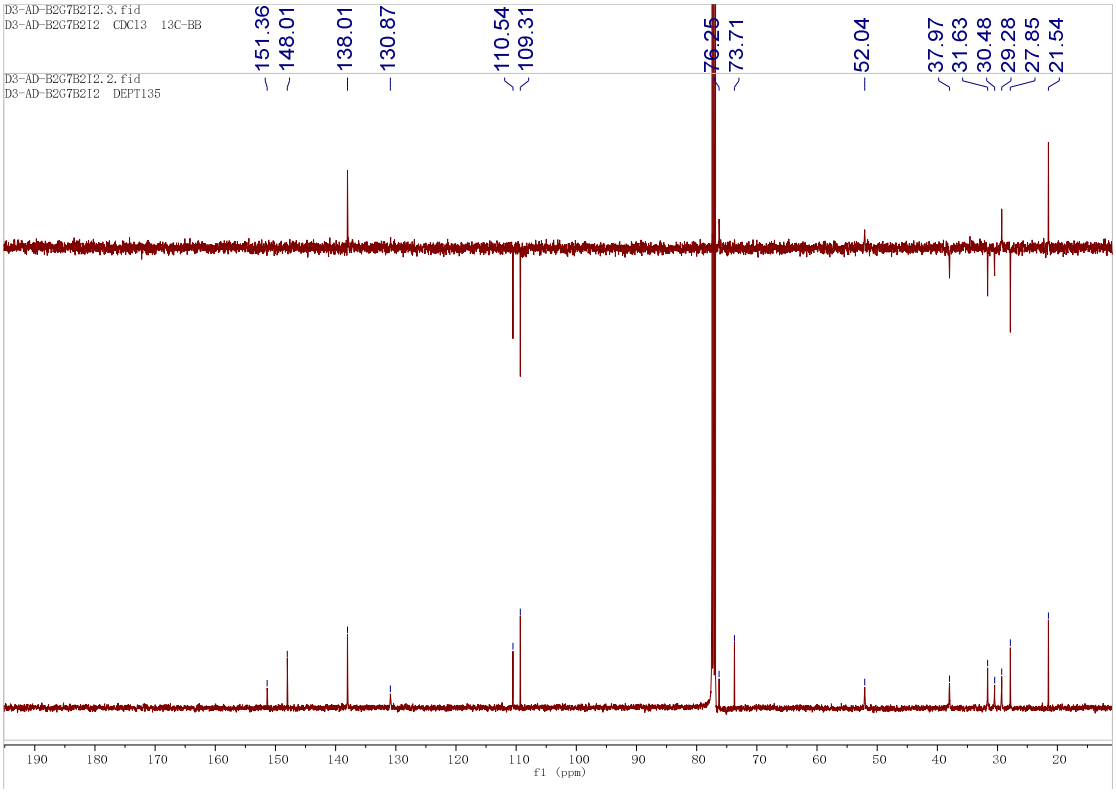


Figure S71 ^{13}C NMR spectrum of compound **8**

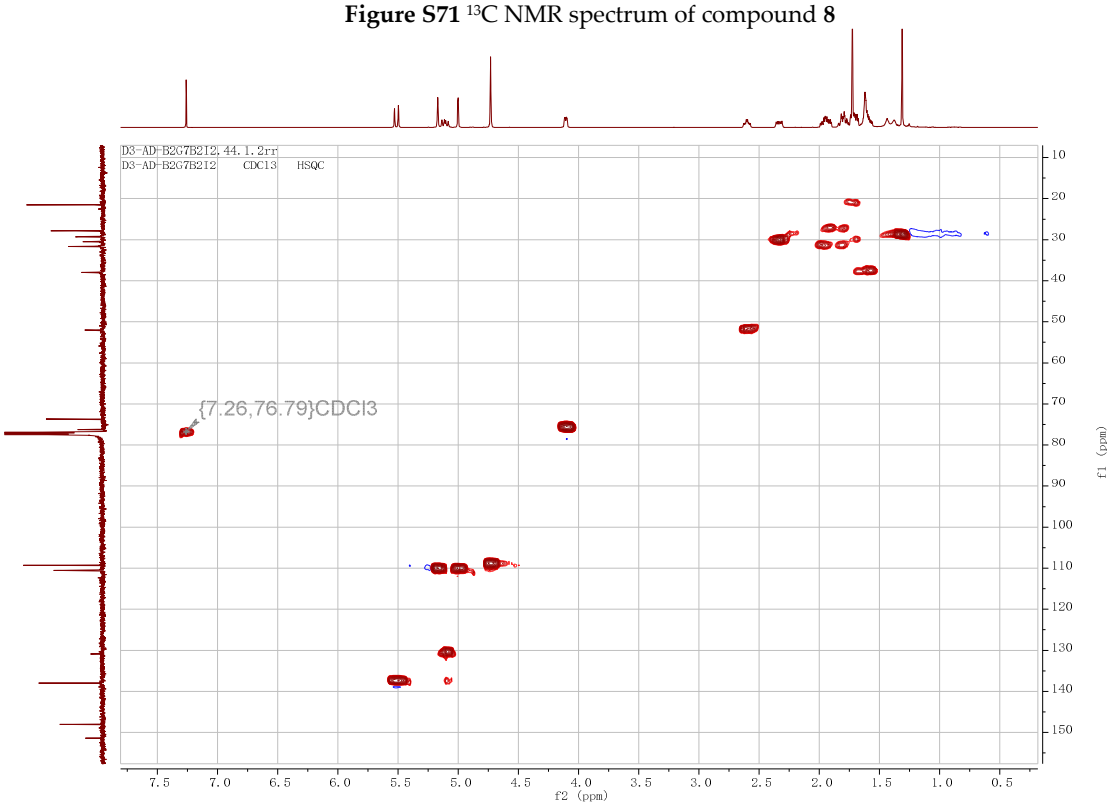


Figure S72 HSQC spectrum of compound **8**

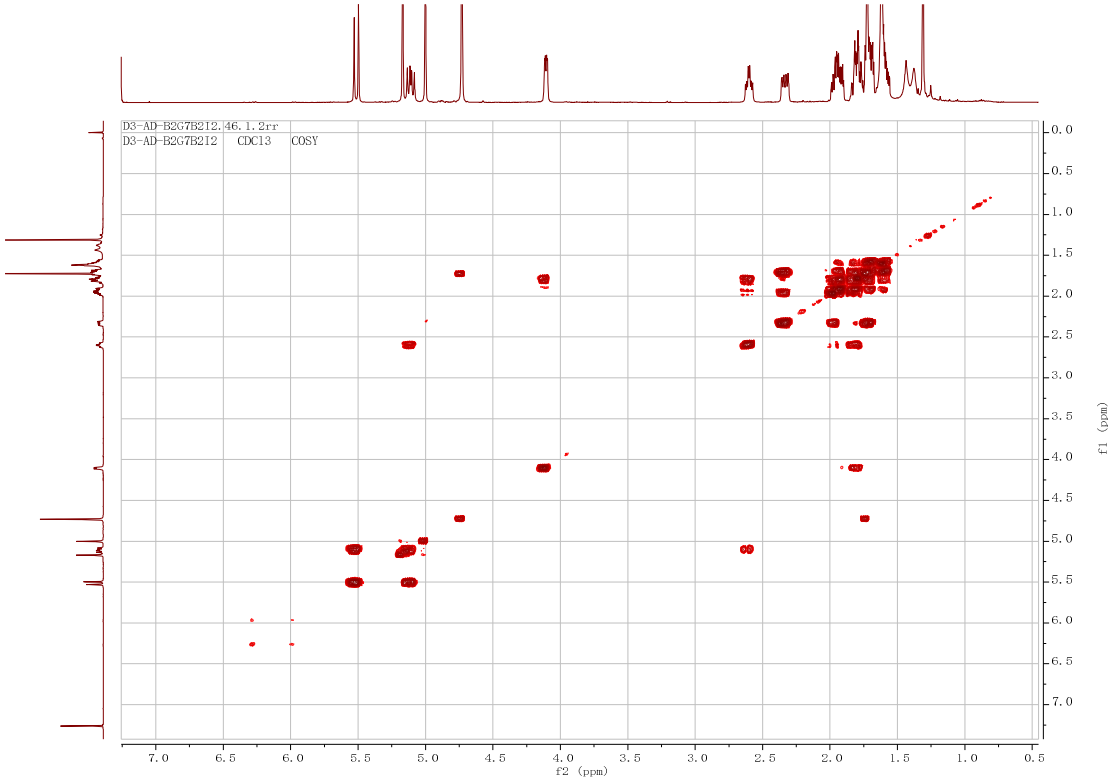


Figure S73 ^{1}H-^{1}H COSY spectrum of compound **8**

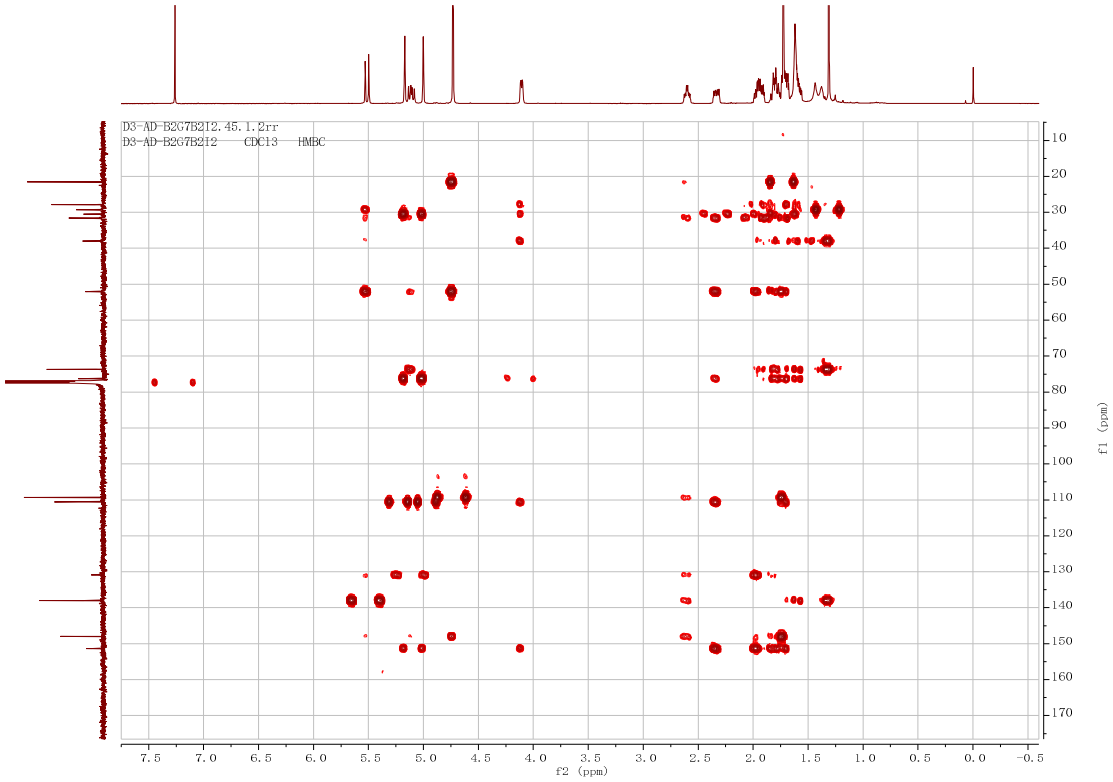


Figure S74 HMBC spectrum of compound **8**

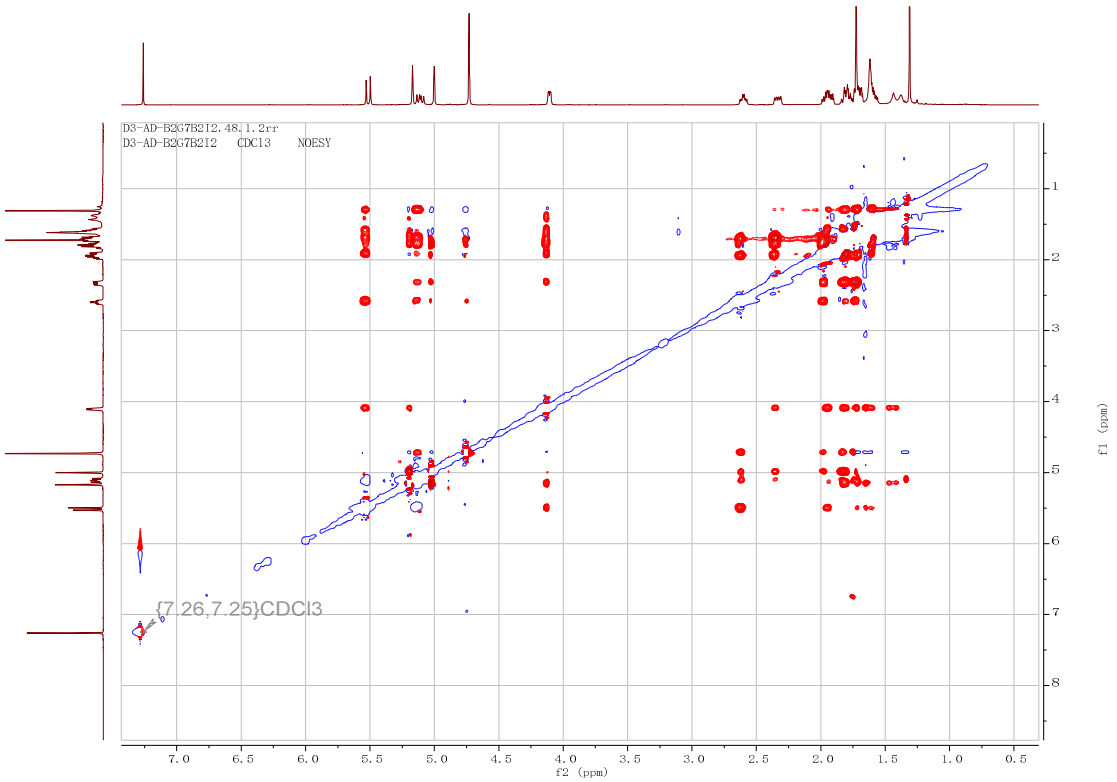


Figure S75 NOESY spectrum of compound **8**

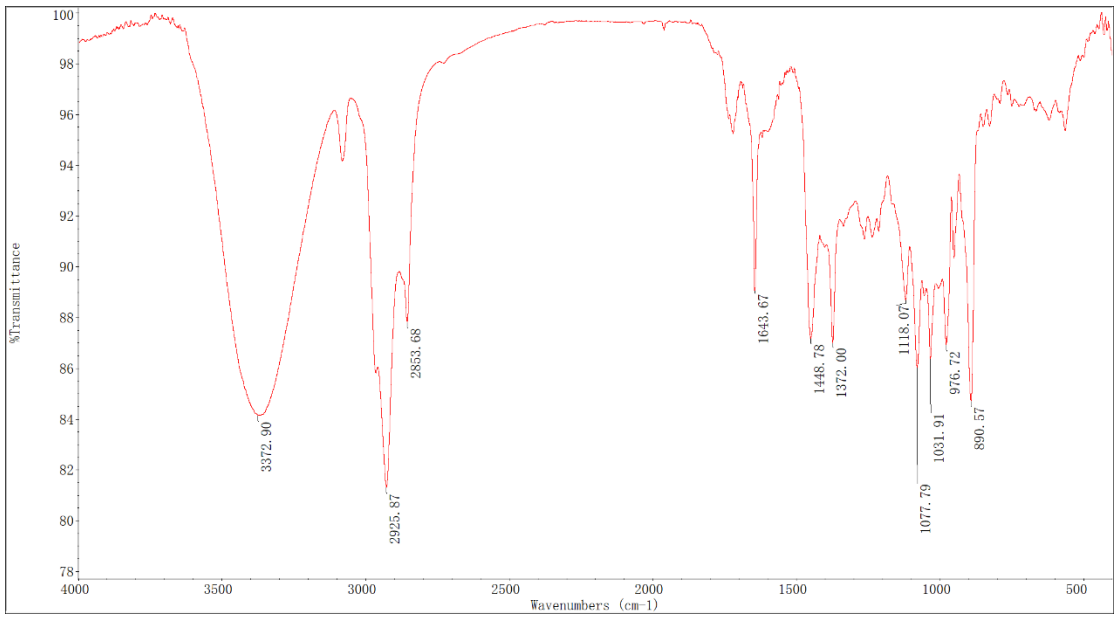
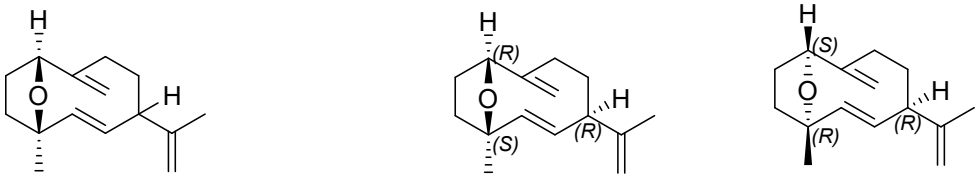


Figure S76 IR spectrum of compound **8**



8 1R4S7R 1S4R7R

Figure S77 Possible isomers of compound **8**

Functional	Solvent?	Basis Set		
mPW1PW91	PCM	6-311G(d,p)		
	Isomer 1	Isomer 2	Isomer 3	Isome
sDP4+ (H data)	99.96%	0.04%	–	–
sDP4+ (C data)	98.89%	1.11%	–	–
sDP4+ (all data)	100.00%	0.00%	–	–
uDP4+ (H data)	96.93%	3.07%	–	–
uDP4+ (C data)	58.19%	41.81%	–	–
uDP4+ (all data)	97.77%	2.23%	–	–
DP4+ (H data)	100.00%	0.00%	–	–
DP4+ (C data)	99.20%	0.80%	–	–
DP4+ (all data)	100.00%	0.00%	–	–

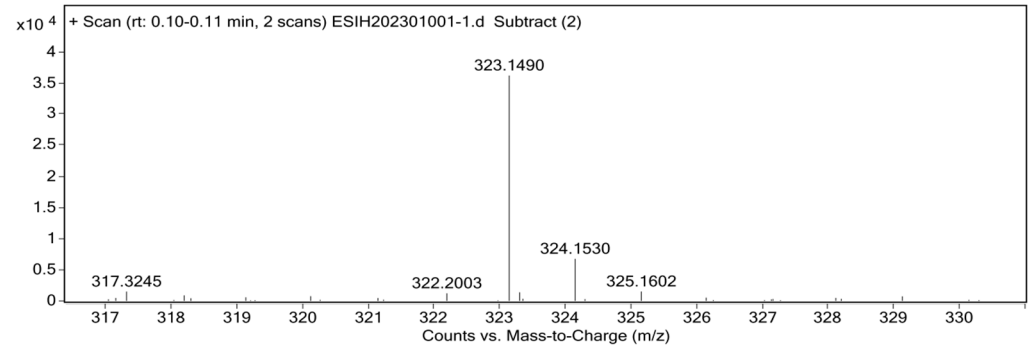
Figure S78 DP4+ probability statistics of compound **8**

Qualitative Analysis Report

Data Filename	ESIH202301001-1.d	**Sample Name**	D3-D3-AD-B2G7E2A4
Sample ID		**Position**	P1-A1
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	2/17/2023 10:47:37	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by fangsu

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
323.149	323.1489	-0.07	-0.22	C17 H23 O6	(M+H)+

Figure S79 HR-ESIMS spectrum of compound **9**

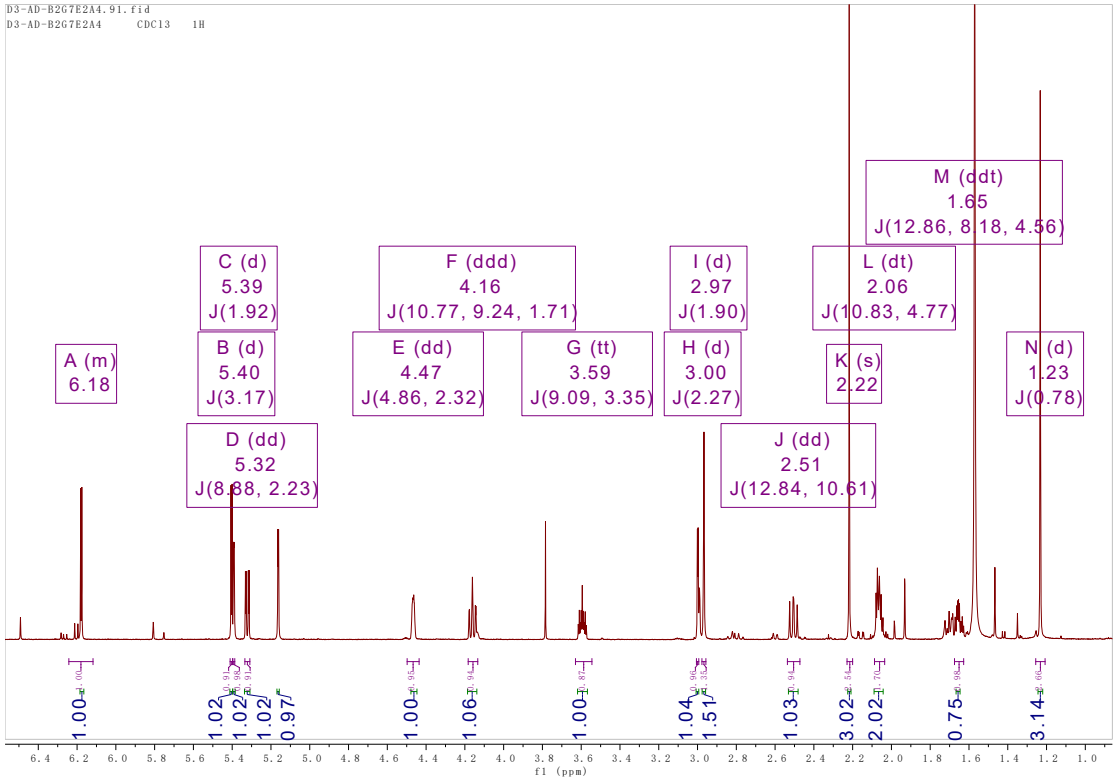


Figure S80 ^{1}H NMR spectrum of compound **9**

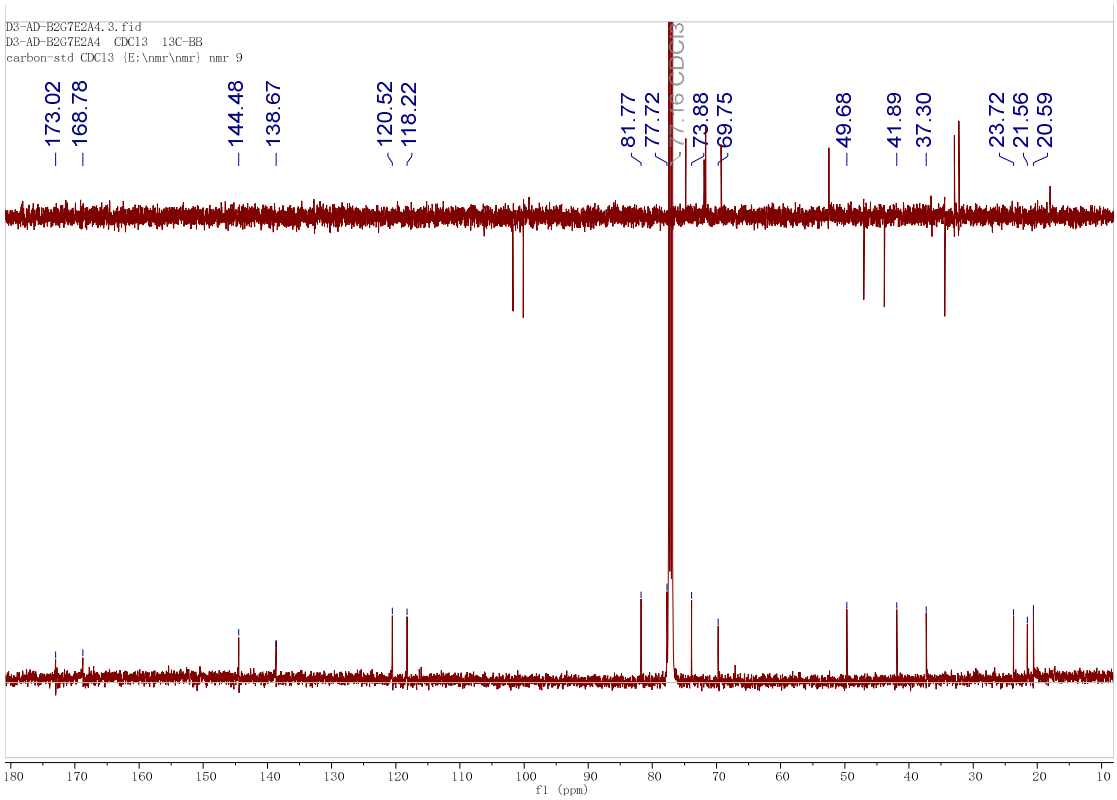


Figure S81 ^{13}C NMR spectrum of compound **9**

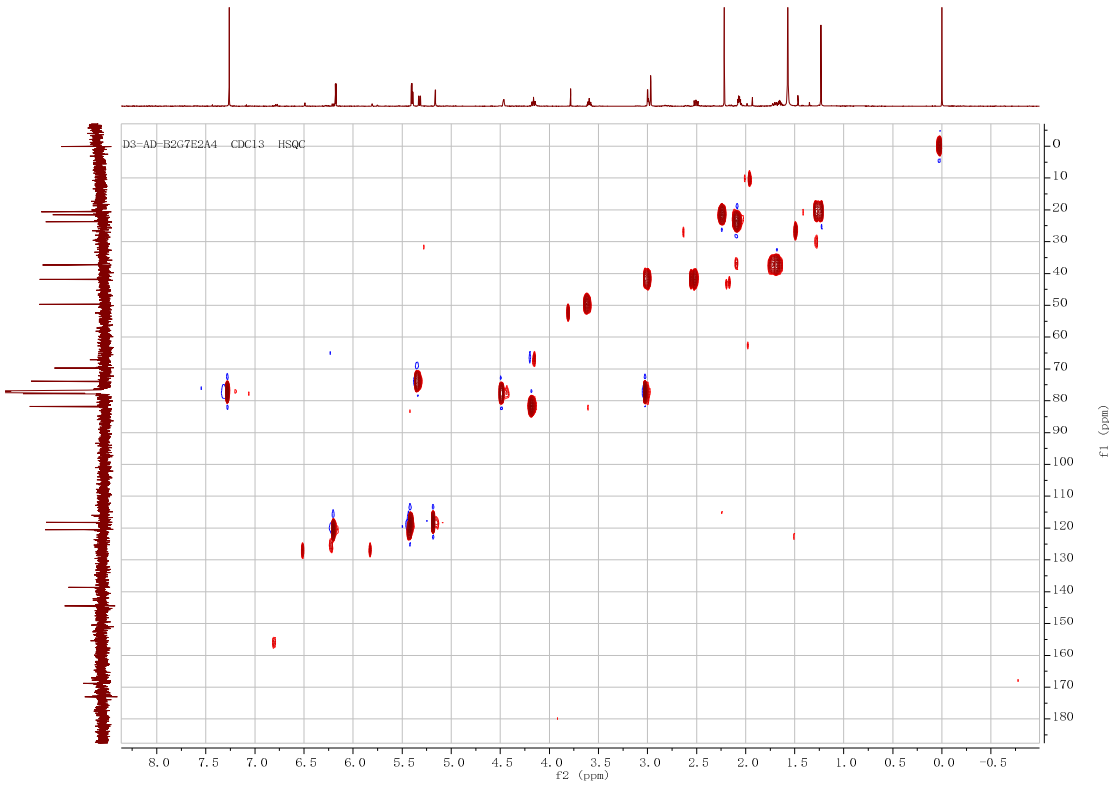


Figure S82 HSQC spectrum of compound **9**

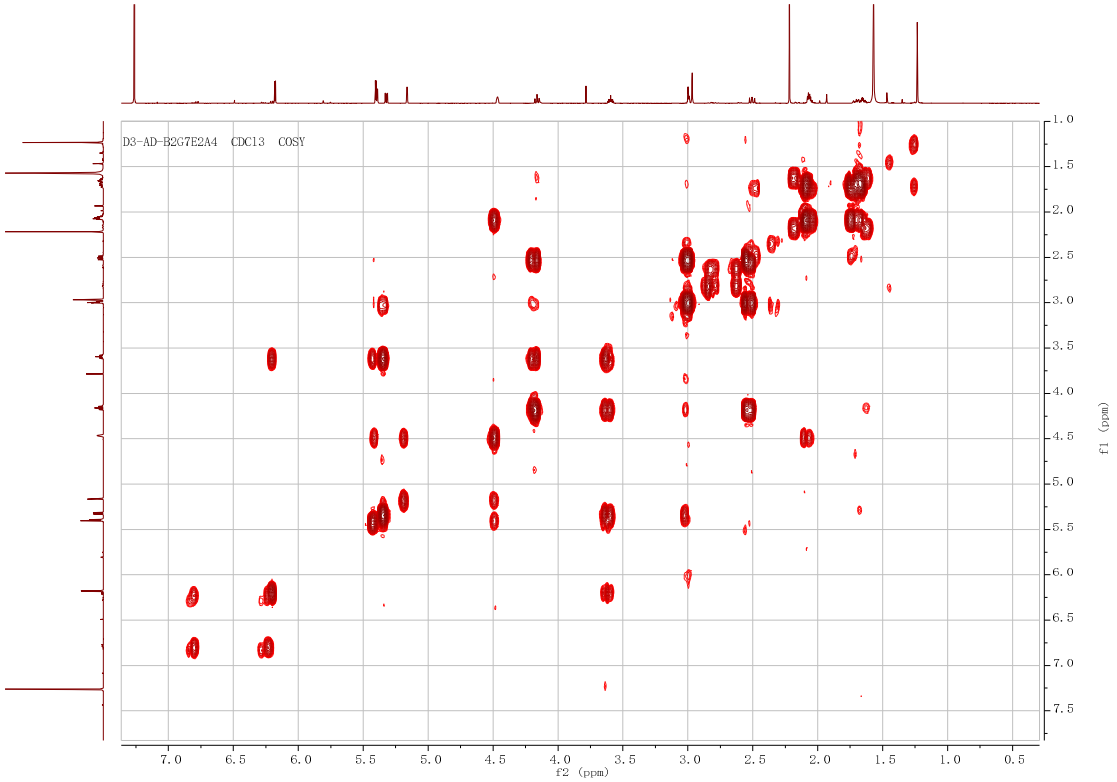


Figure S83 ^{1}H-^{1}H COSY spectrum of compound **9**

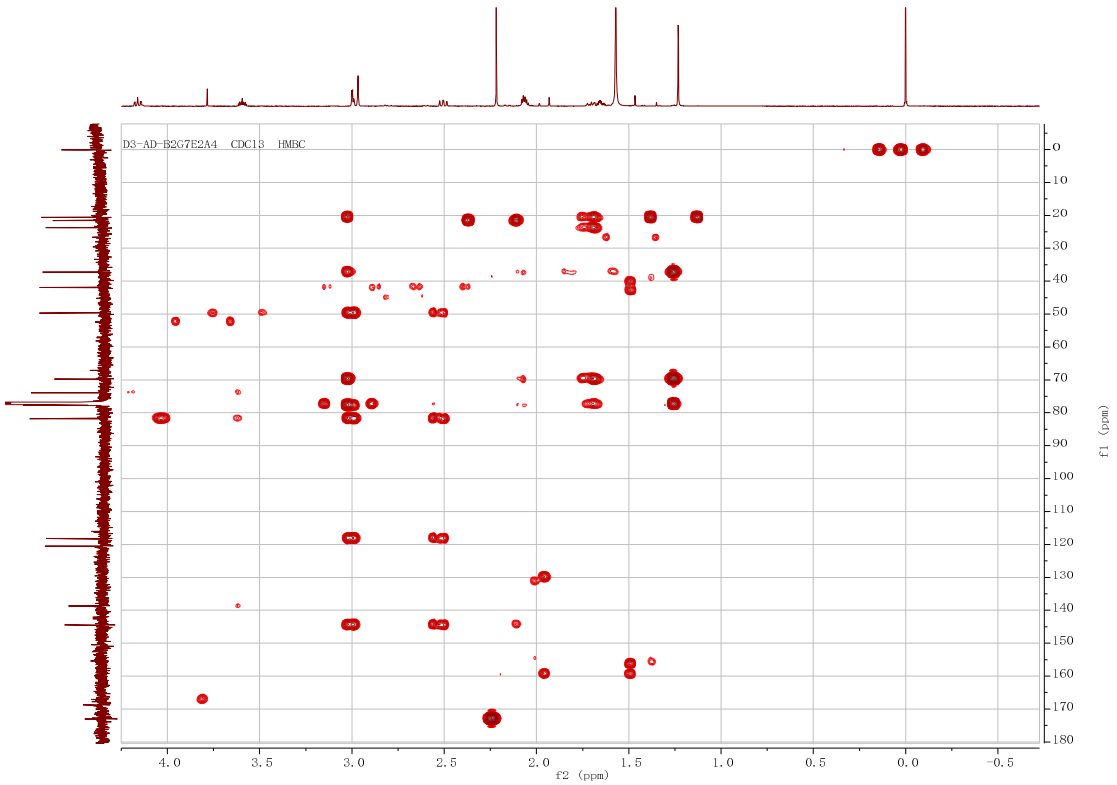


Figure S84 HMBC spectrum of compound **9**

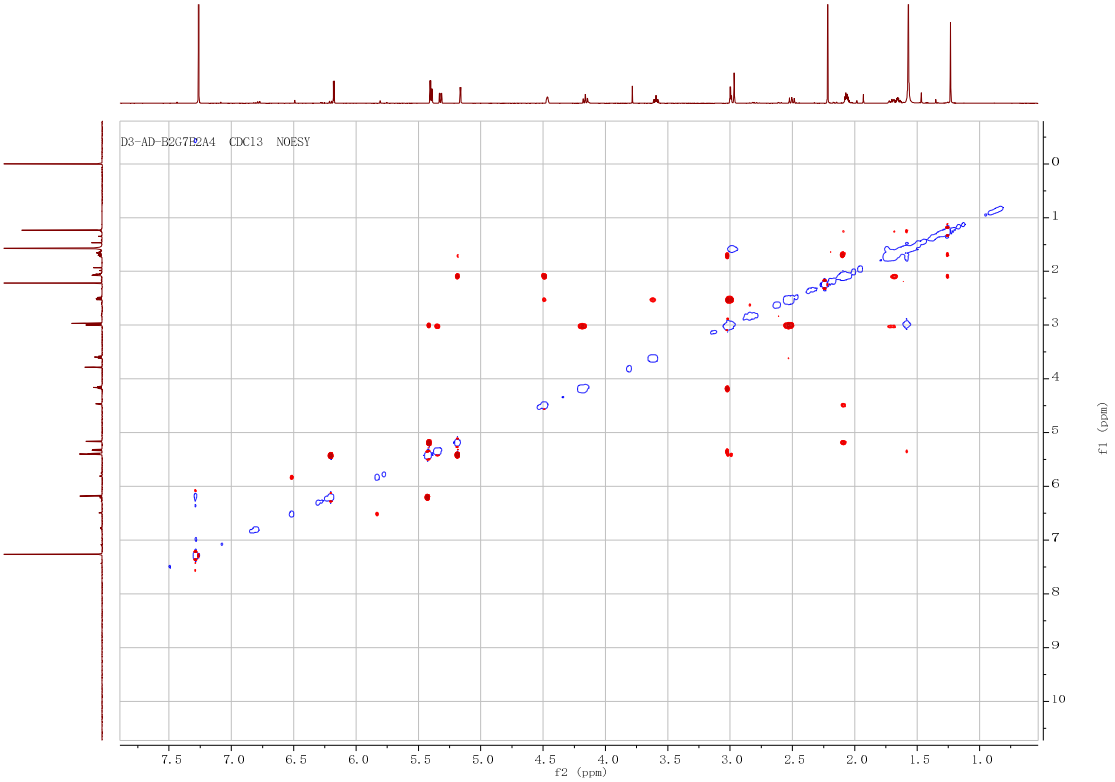


Figure S85 NOESY spectrum of compound **9**

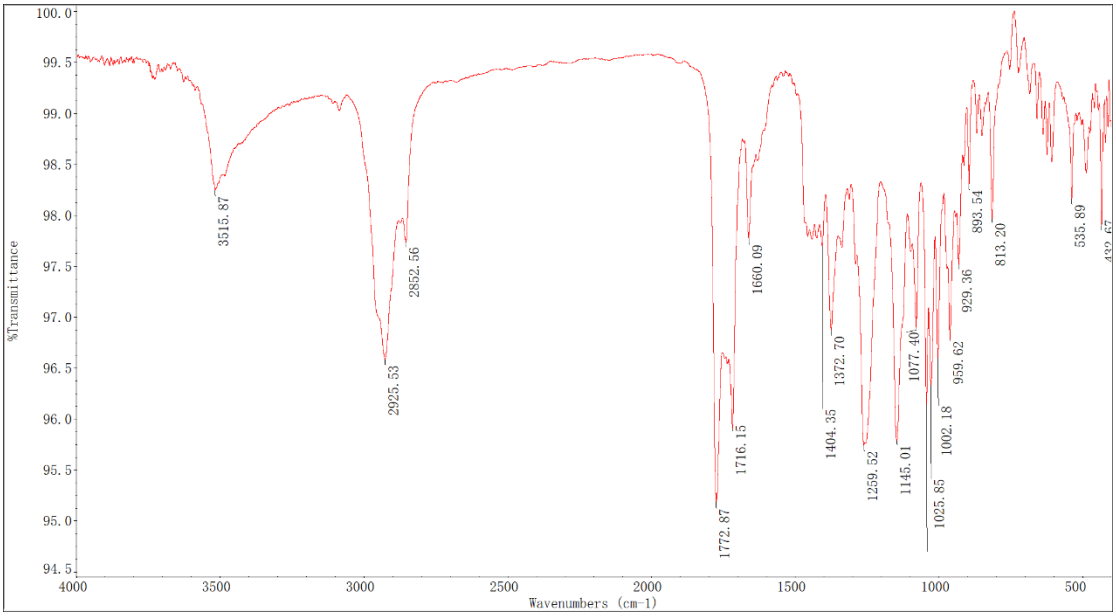


Figure S86 IR spectrum of compound **9**

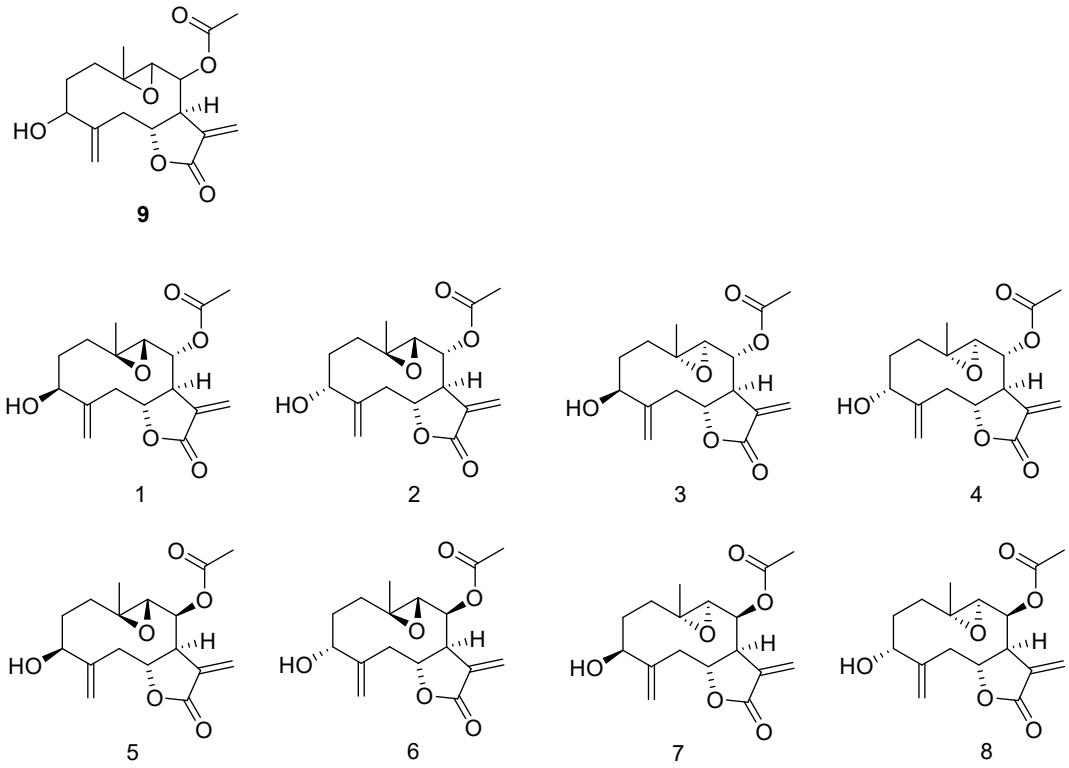


Figure S87 Possible isomers of compound **9**

Functional	Solvent?	Basis Set	Type of Data
mPW1PW91	PCM	6-311G(d,p)	Shielding Tensors

	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6	Isomer 7	Isomer 8
sDP4+ (H data)	0.02%	16.99%	0.00%	0.01%	0.00%	82.37%	0.57%	0.04%
sDP4+ (C data)	0.07%	44.23%	0.02%	6.19%	0.11%	0.01%	49.37%	0.00%
sDP4+ (all data)	0.00%	96.29%	0.00%	0.01%	0.00%	0.10%	3.60%	0.00%
uDP4+ (H data)	0.05%	96.23%	0.00%	0.00%	0.00%	3.58%	0.13%	0.02%
uDP4+ (C data)	1.04%	9.56%	0.31%	2.18%	19.70%	38.83%	28.27%	0.11%
uDP4+ (all data)	0.00%	86.59%	0.00%	0.00%	0.00%	13.07%	0.34%	0.00%
DP4+ (H data)	0.00%	84.73%	0.00%	0.00%	0.00%	15.26%	0.00%	0.00%
DP4+ (C data)	0.00%	23.05%	0.00%	0.74%	0.11%	0.02%	76.07%	0.00%
DP4+ (all data)	0.00%	99.97%	0.00%	0.00%	0.00%	0.02%	0.01%	0.00%

Figure S88 DP4+ probability statistics of compound **9**