

Supplementary data for

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

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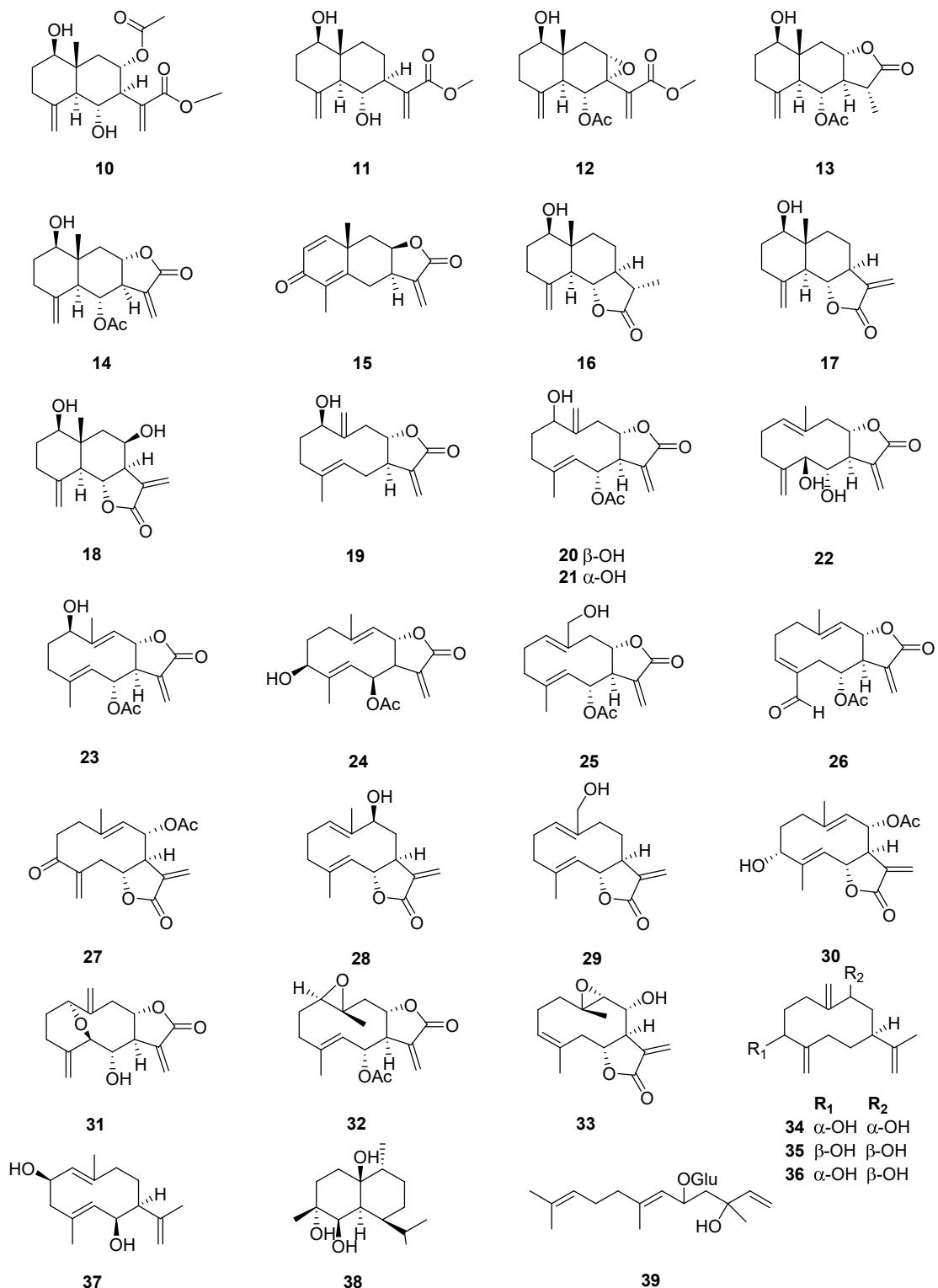


Figure S1 Structures of known compounds 10-39

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 ₆ Na
		375.1808	4.7	12.5	8.5	41.9	1.887	15.16	C ₂₁ H ₂₇ O ₆

YSQ

AD-B2G4C2E1-Pos 742 (5.423) Cm (741:743)

1: TOF MS ES+

3.62e+006

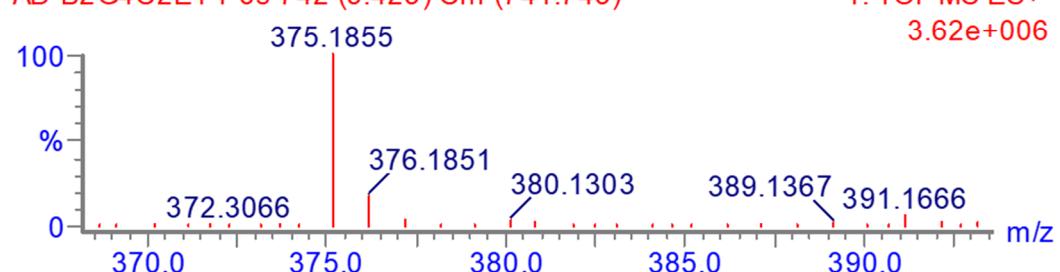


Figure S2 HR-ESIMS spectrum of compound 1

D3-AD-B2G4C2E1.1, fid
D3-AD-B2G4C2E1 CDCl₃ 1H

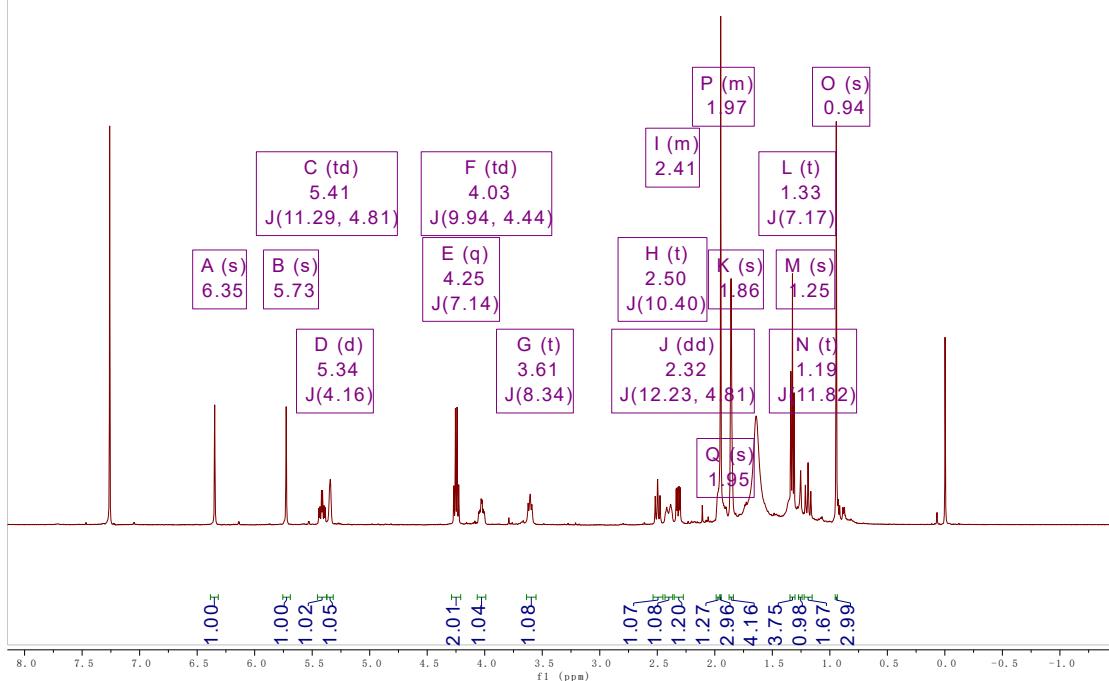


Figure S3 ¹H NMR spectrum of compound 1

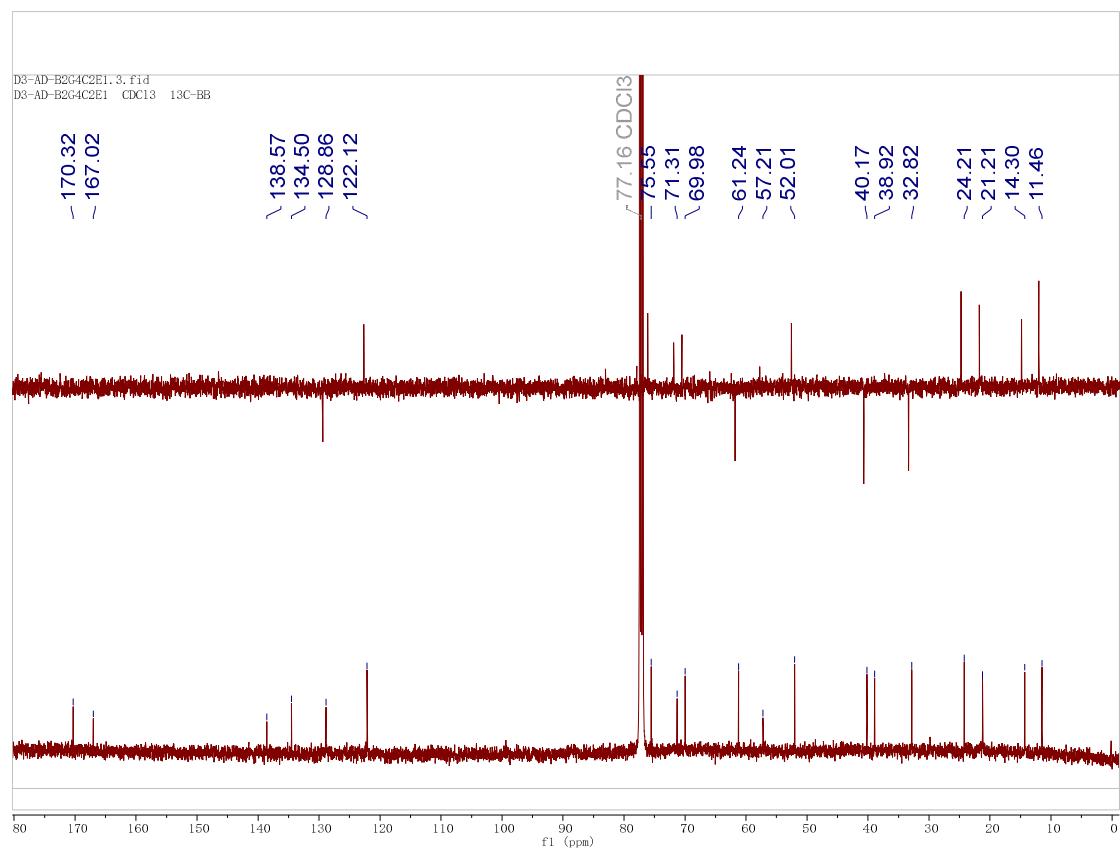


Figure S4 ^{13}C NMR spectrum of compound **1**

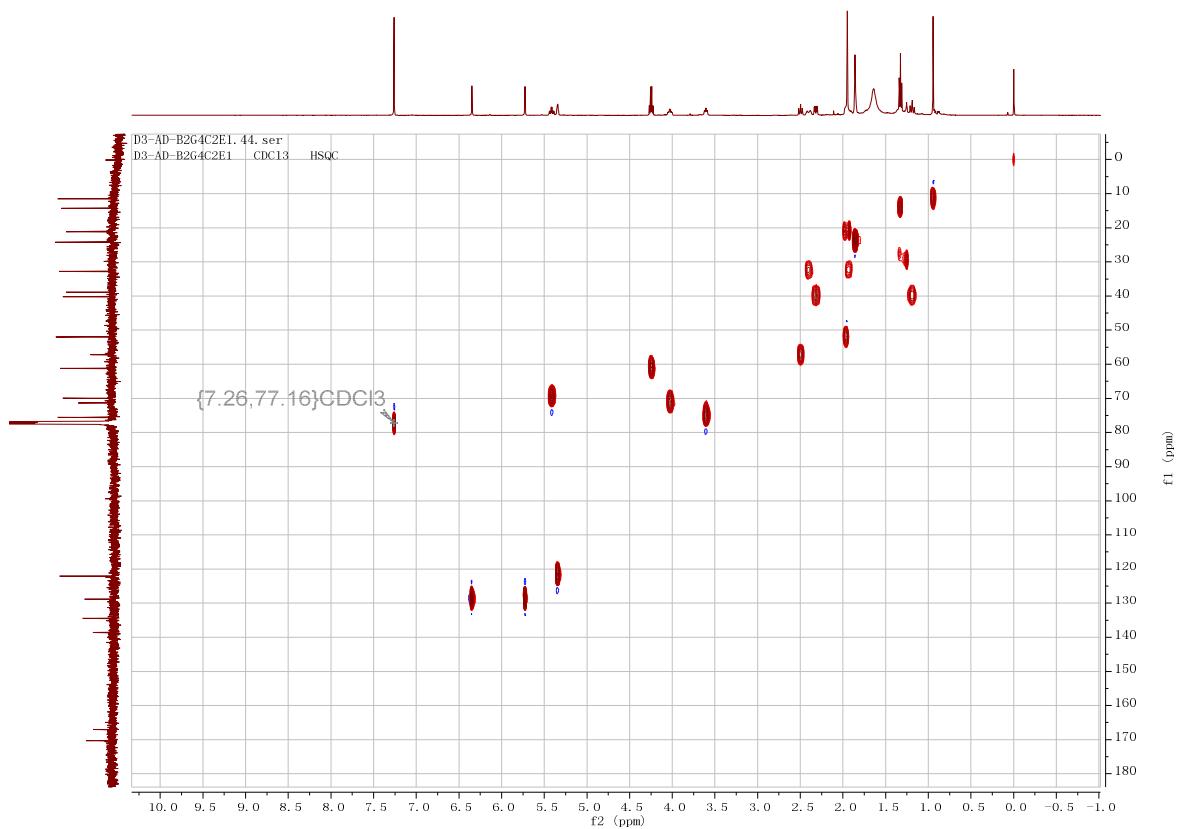


Figure S5 HSQC spectrum of compound **1**

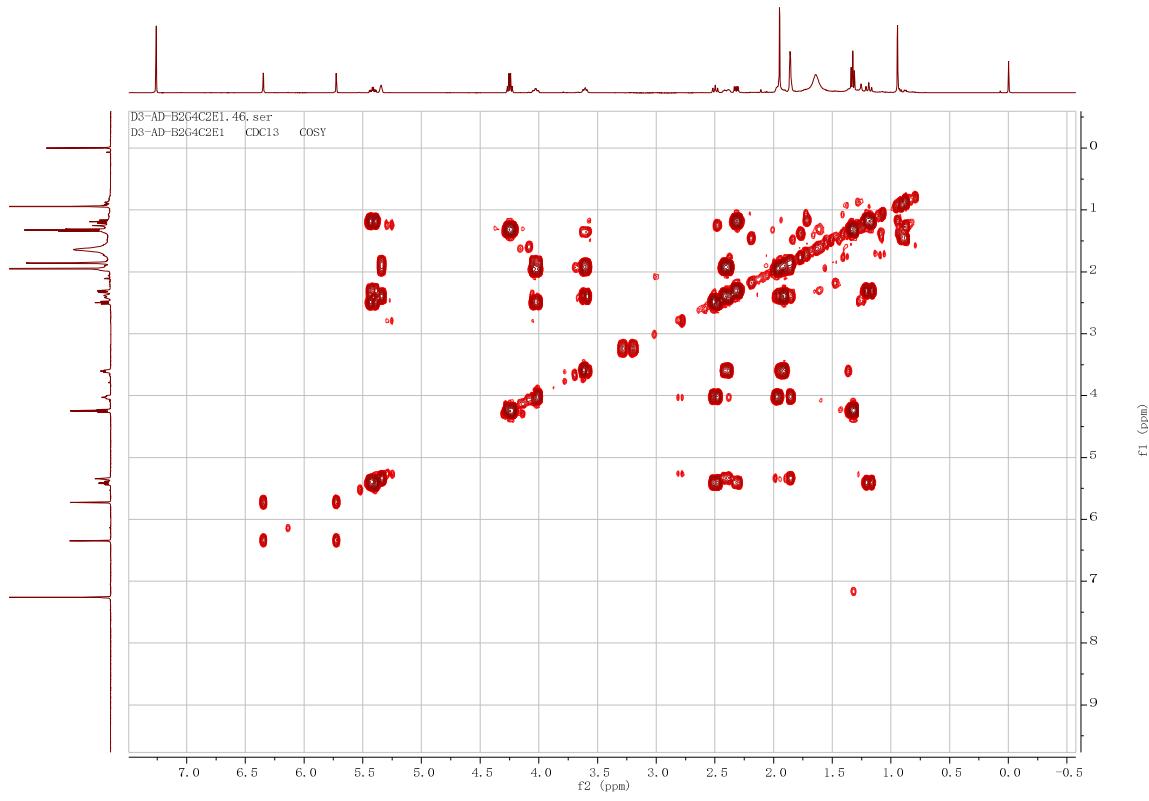


Figure S6 ¹H-¹H COSY spectrum of compound **1**

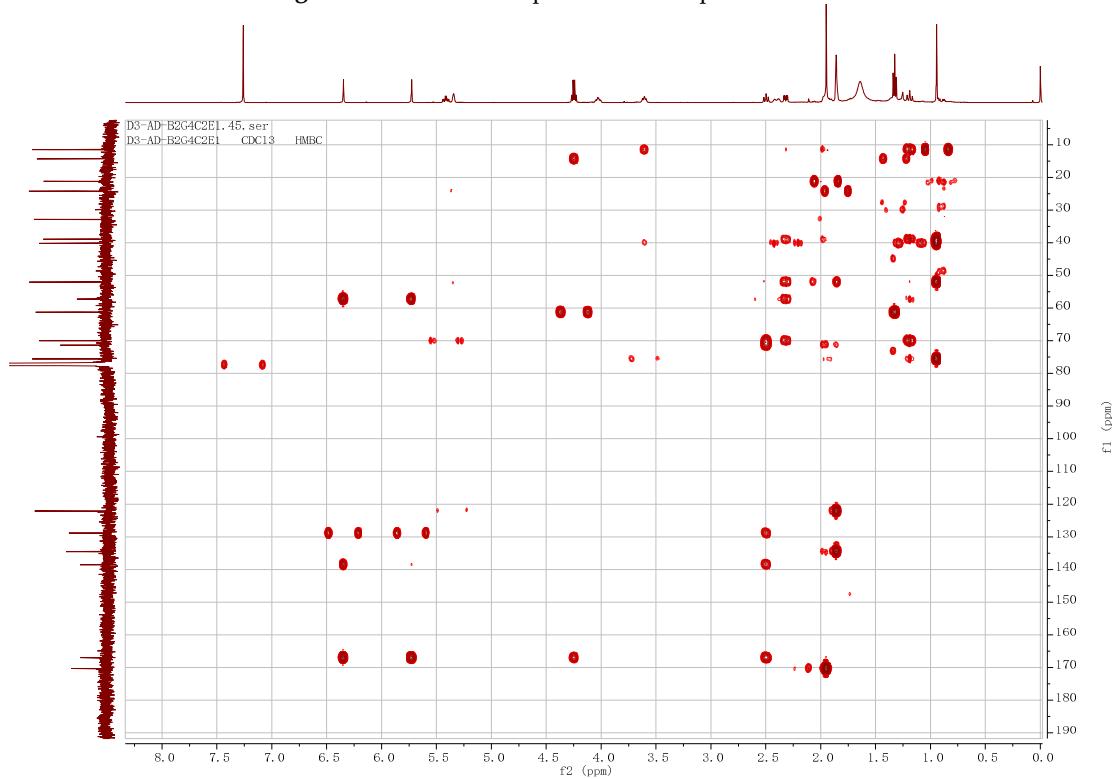


Figure S7 HMBC spectrum of compound **1**

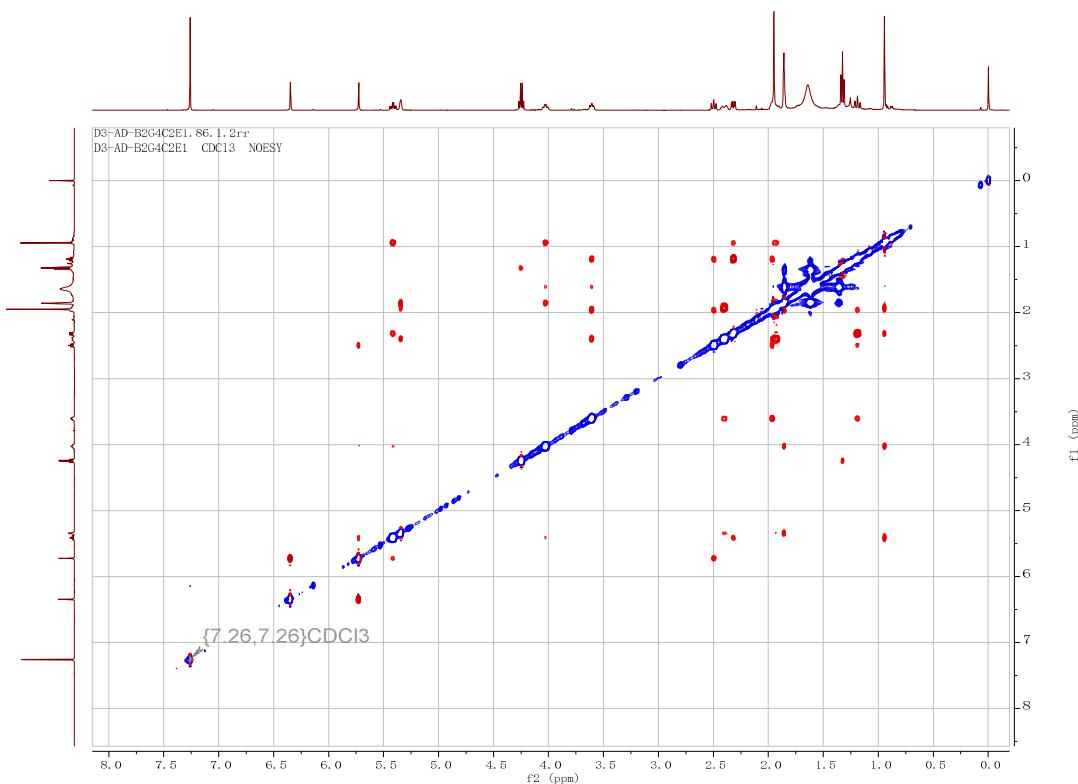


Figure S8 NOESY spectrum of compound **1**

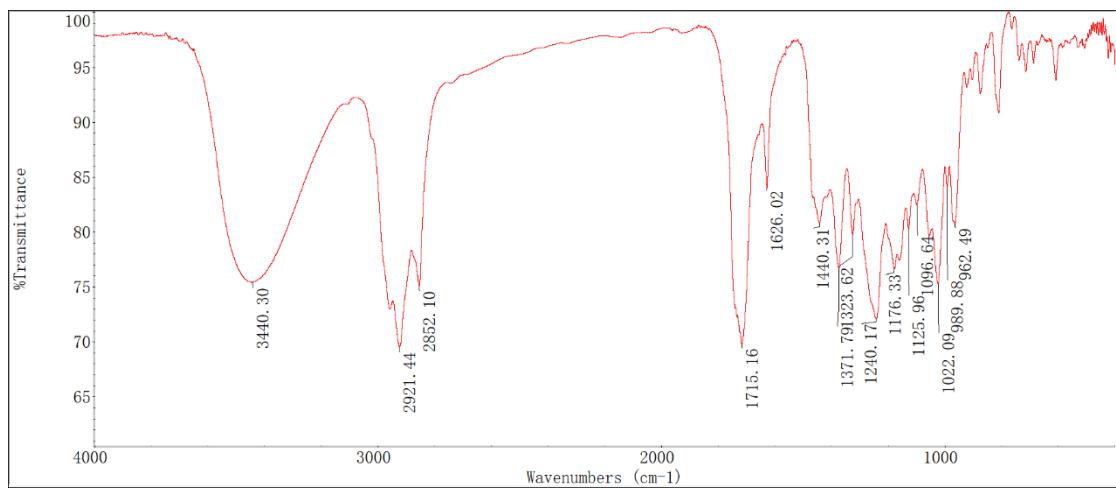


Figure S9 IR spectrum of compound **1**

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	$C_{19}H_{28}O_6Na$

YSQ

AD-B2G4C2E2-Pos 768 (5.609)

1: TOF MS ES+

1.27e+006

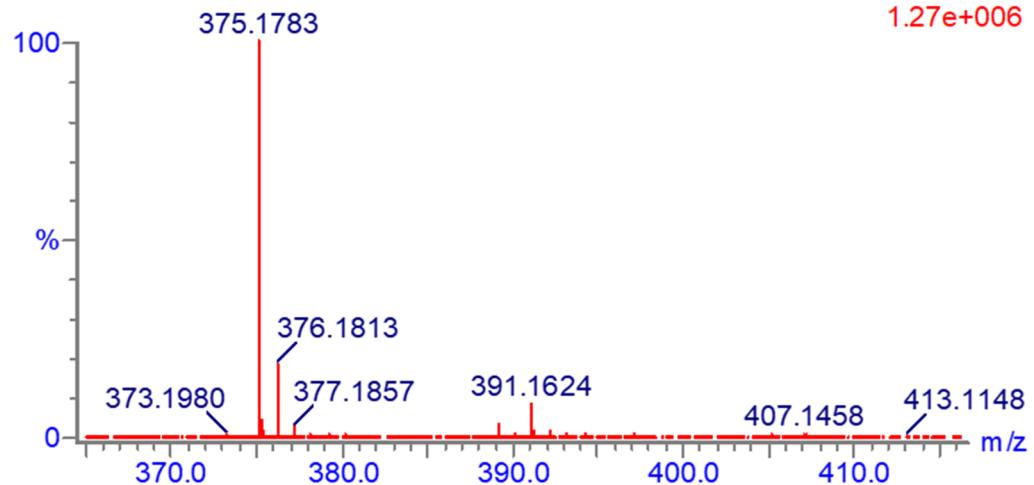


Figure S10 HR-ESIMS spectrum of compound 2

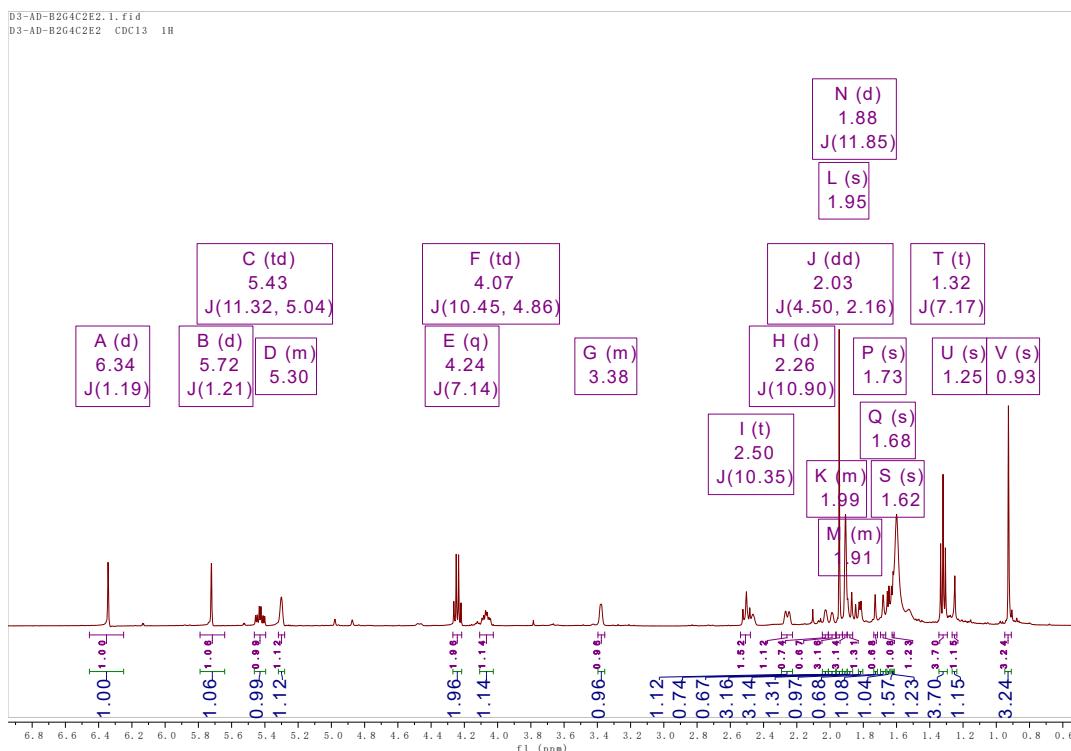


Figure S11 ¹H NMR spectrum of compound 2

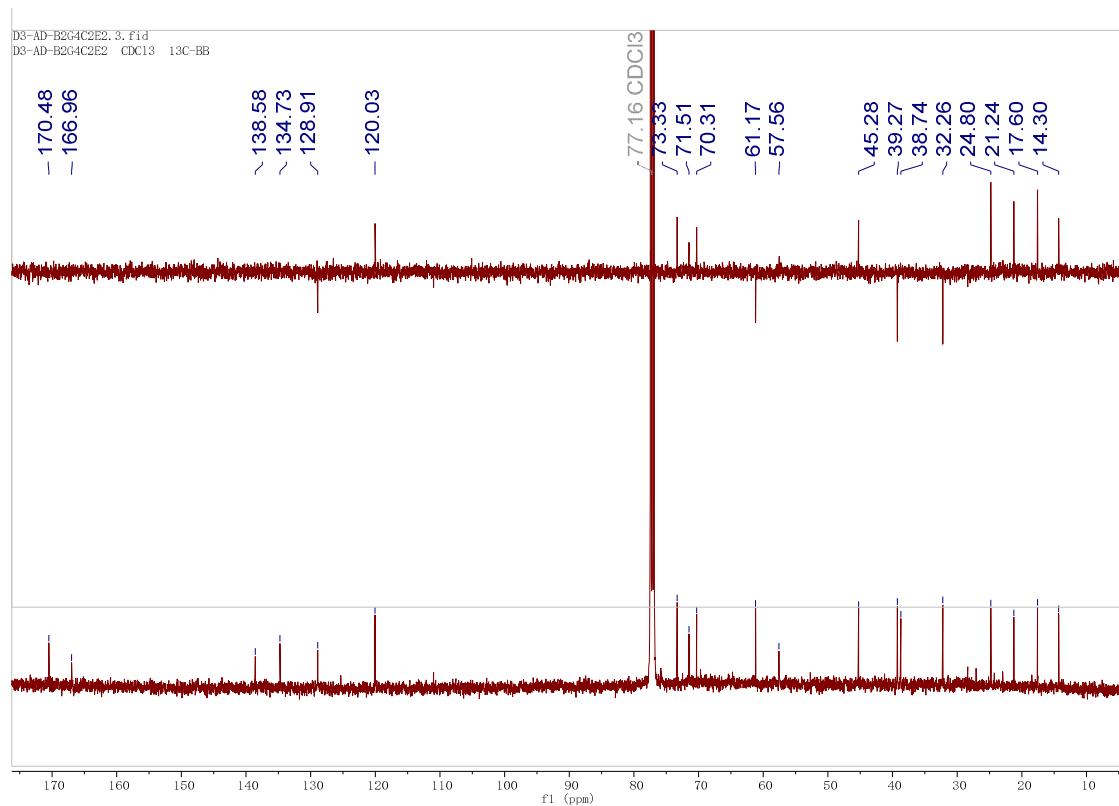


Figure S12 ^{13}C NMR spectrum of compound 2

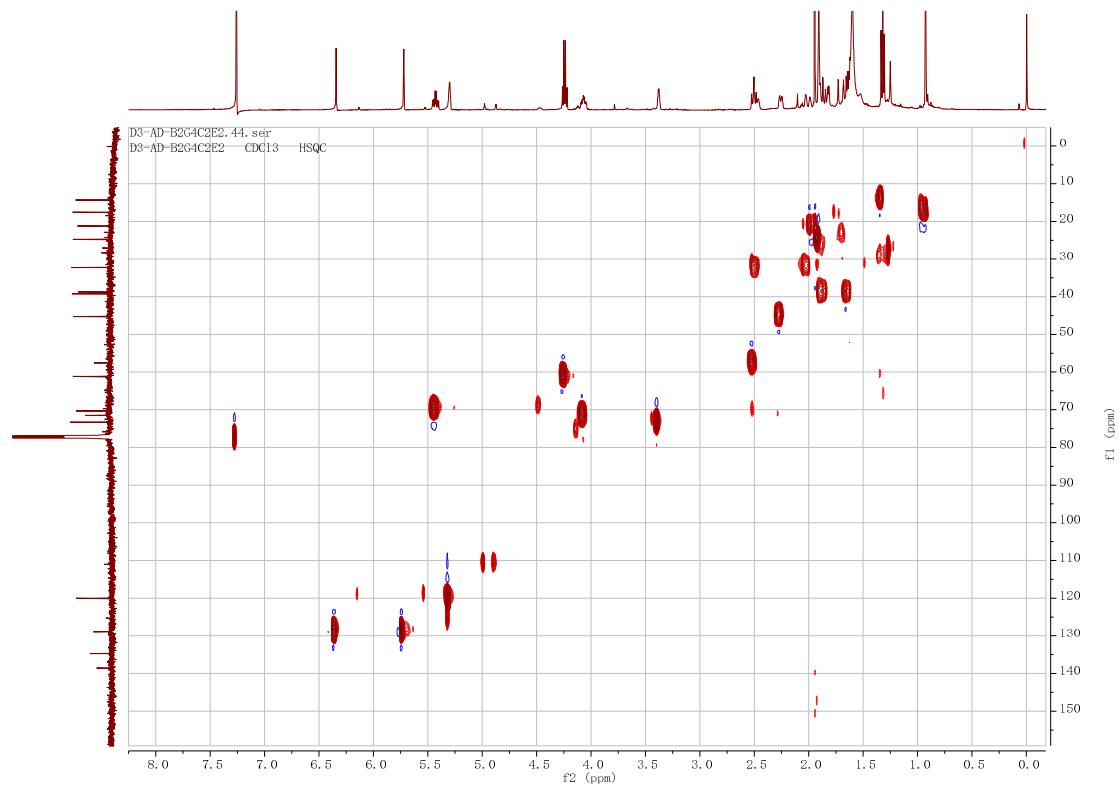


Figure S13 HSQC spectrum of compound 2

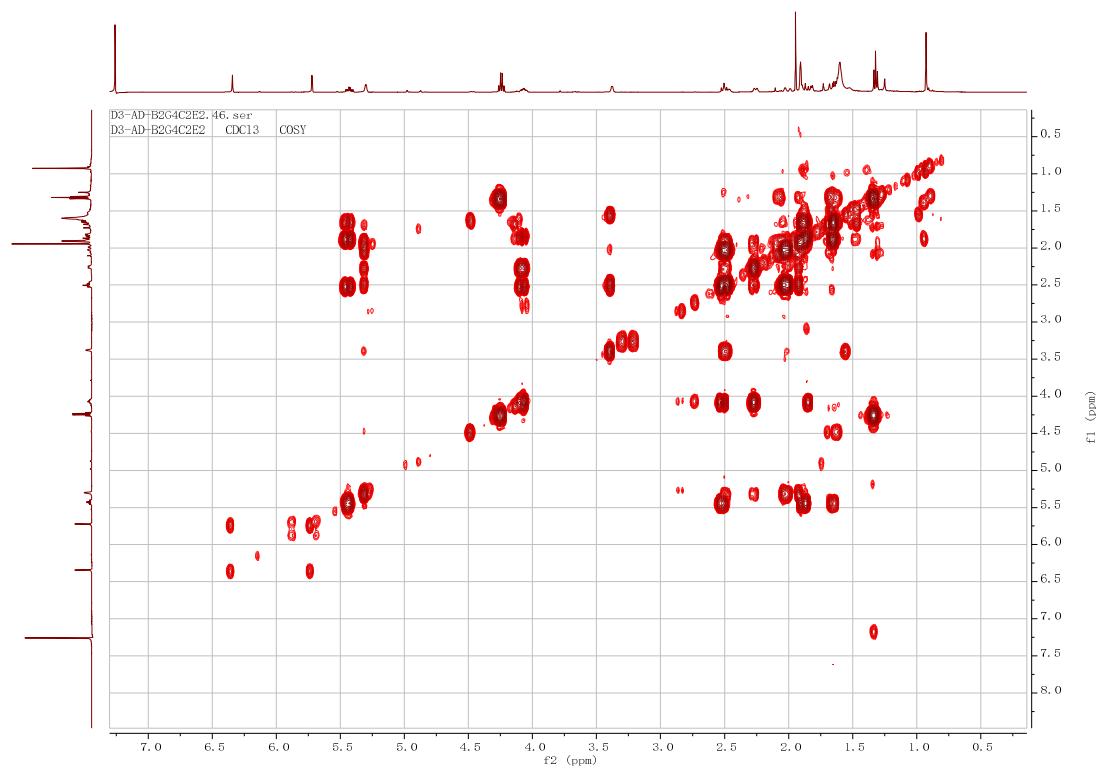


Figure S14 ^1H - ^1H COSY spectrum of compound 2

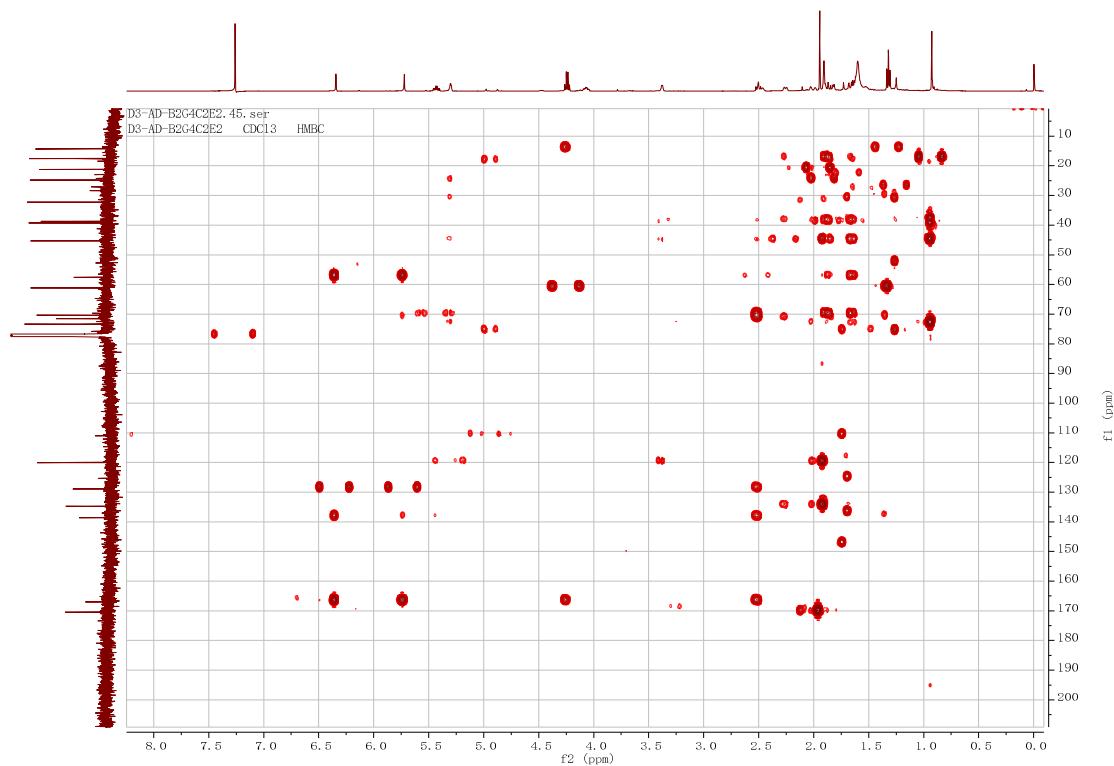


Figure S15 HMBC spectrum of compound 2

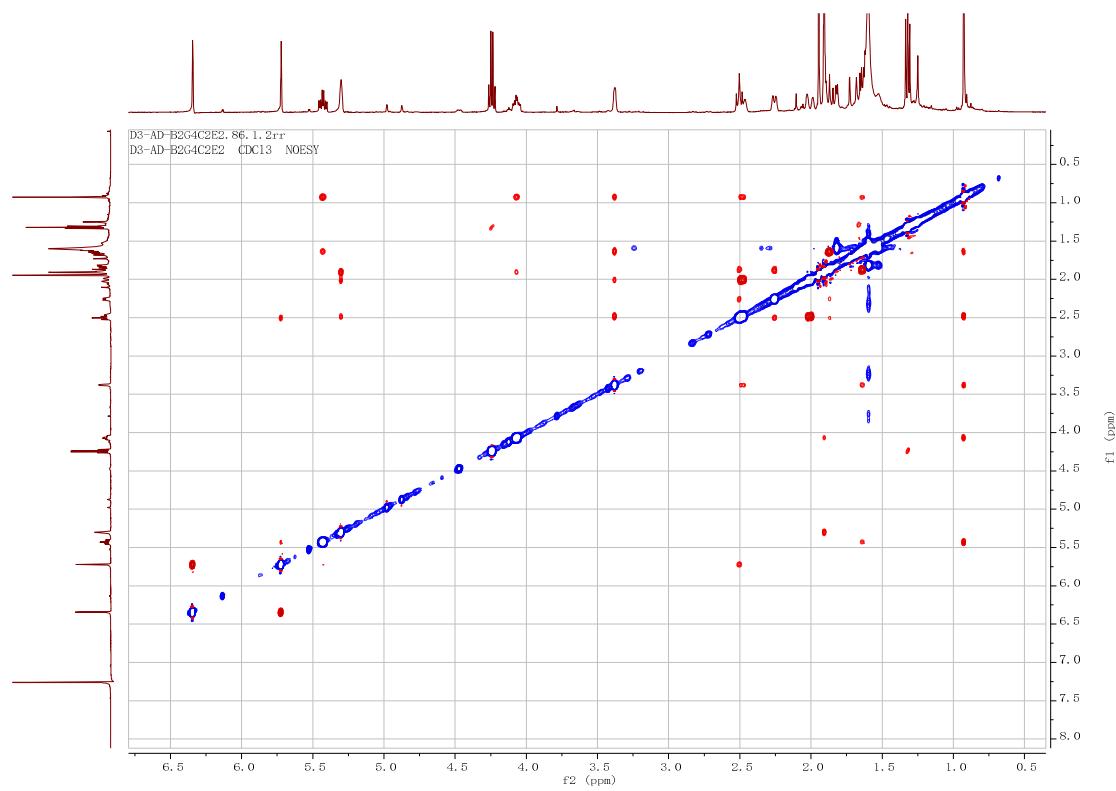


Figure S16 NOESY spectrum of compound 2

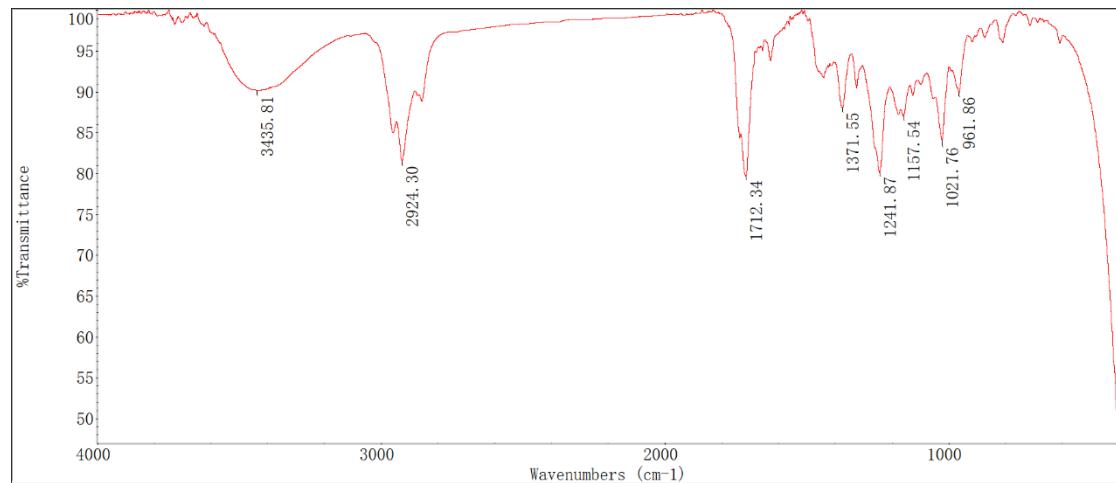


Figure S17 IR spectrum of compound 2

truncated structures used for DFT calculation

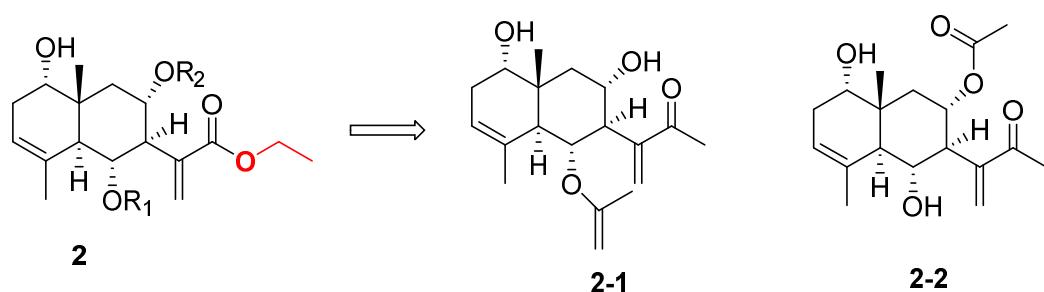
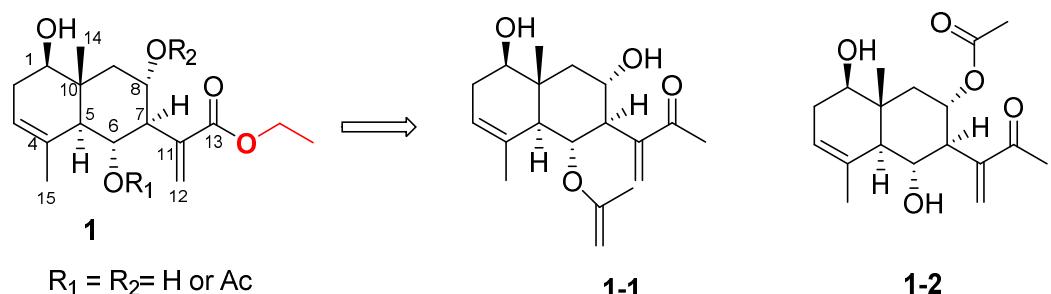


Figure S18 Possible isomers of compound 1 and 2

Functional	Solvent?	Basis Set	
mPW1PW91	PCM	6-311G(d, p)	
	Isomer 1	Isomer 2	Isomer 3
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
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	$\text{C}_{19}\text{H}_{28}\text{O}_6\text{Na}$

YSQ

AD-B2G4B2C-Pos 691 (5.053)

1: TOF MS ES+

9.90e+005

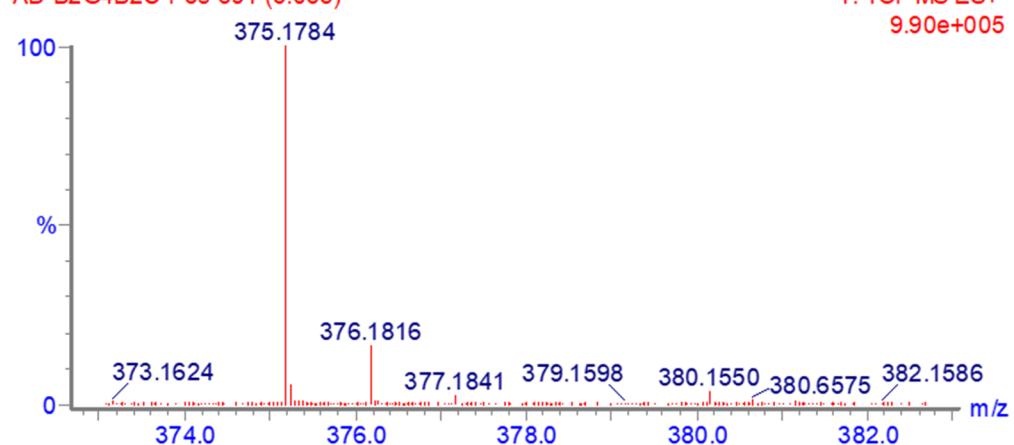


Figure S21 HR-ESIMS spectrum of compound 3

D3-AD-B2G4B2C.1.fid
D3-AD-B2G4B2C CDCl₃ 1H

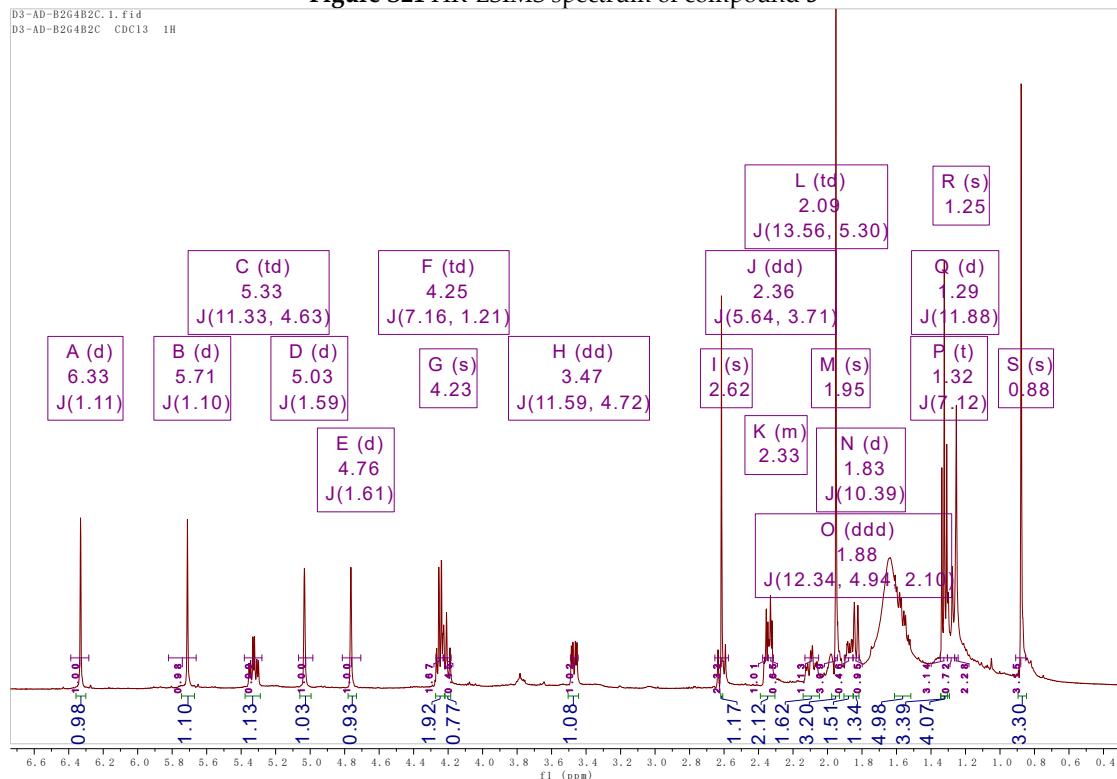


Figure S22 ¹H NMR spectrum of compound 3

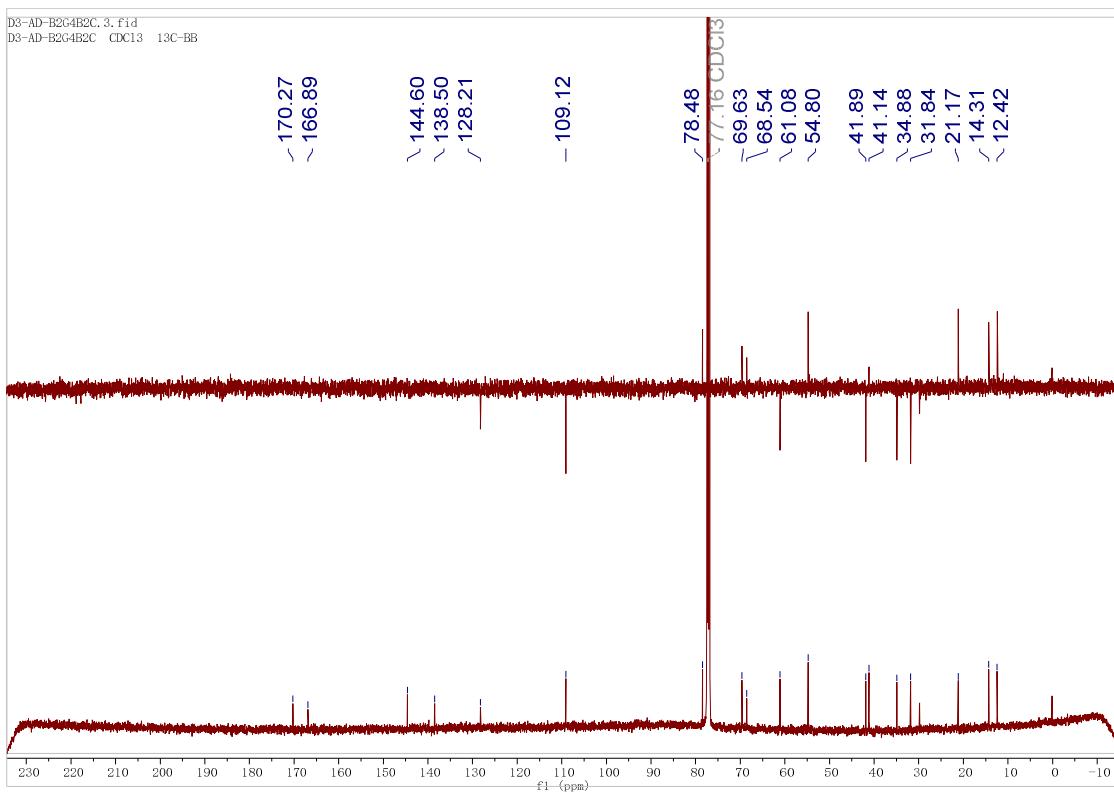


Figure S23 ^{13}C NMR spectrum of compound 3

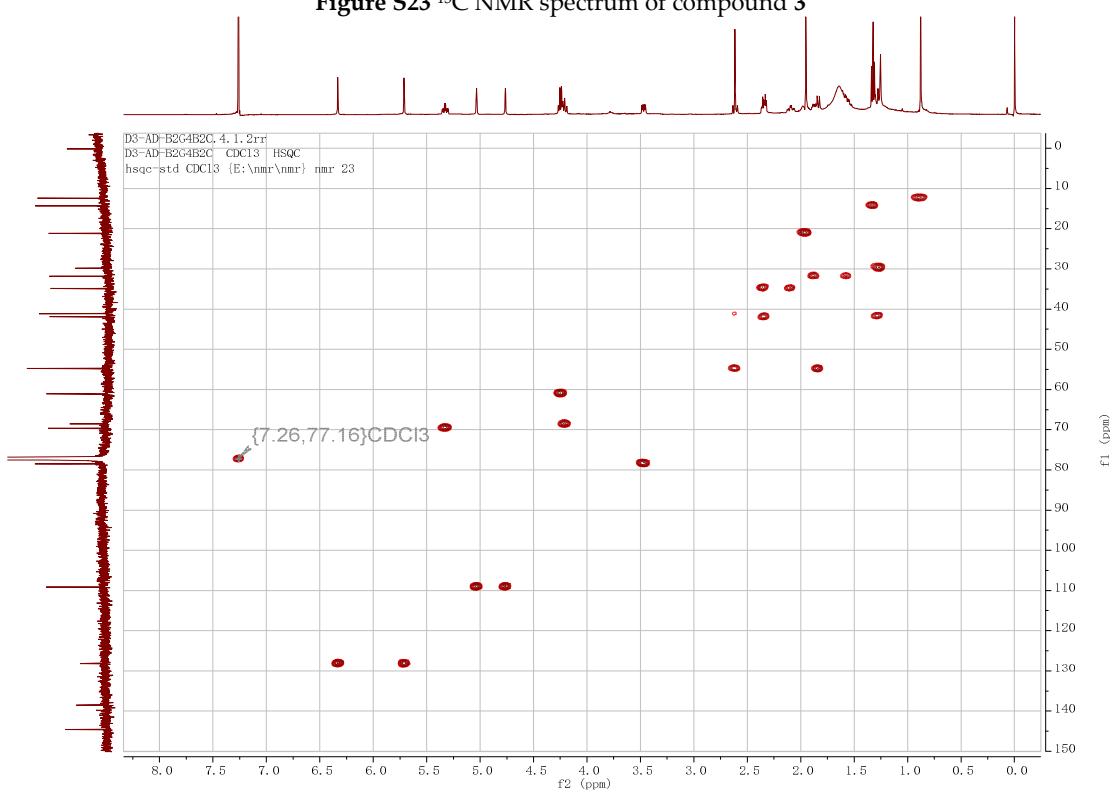


Figure S24 HSQC NMR spectrum of compound 3

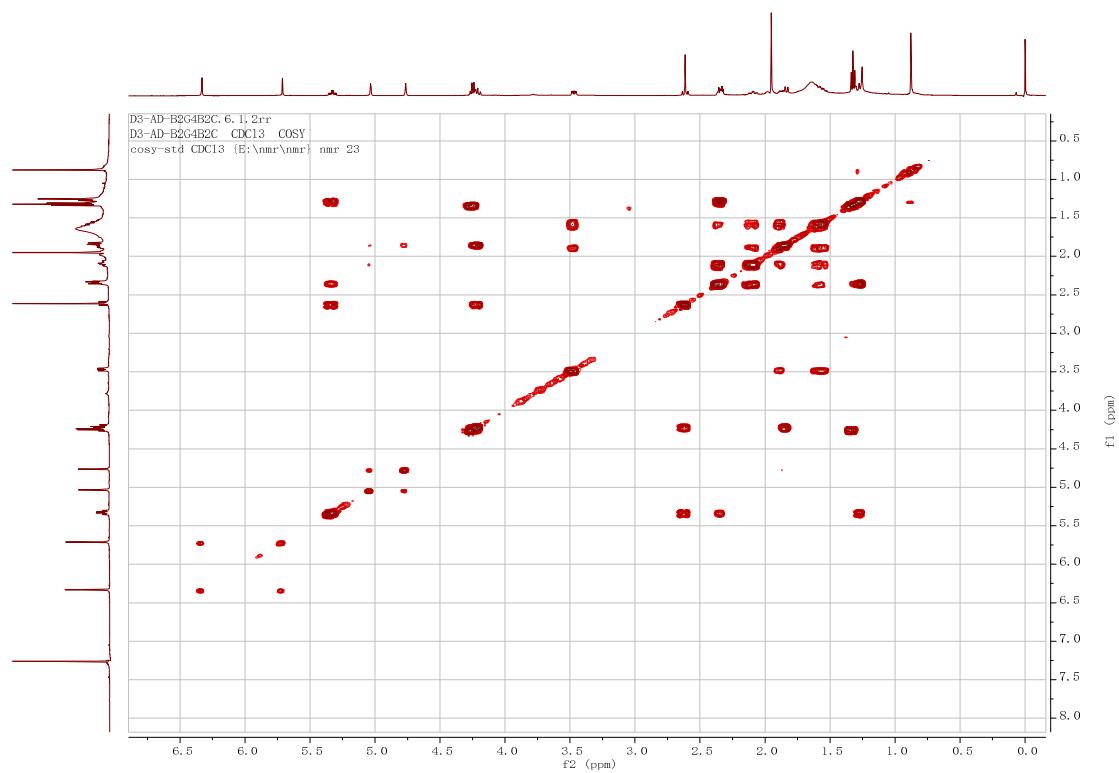


Figure S25 ^1H - ^1H COSY spectrum of compound 3

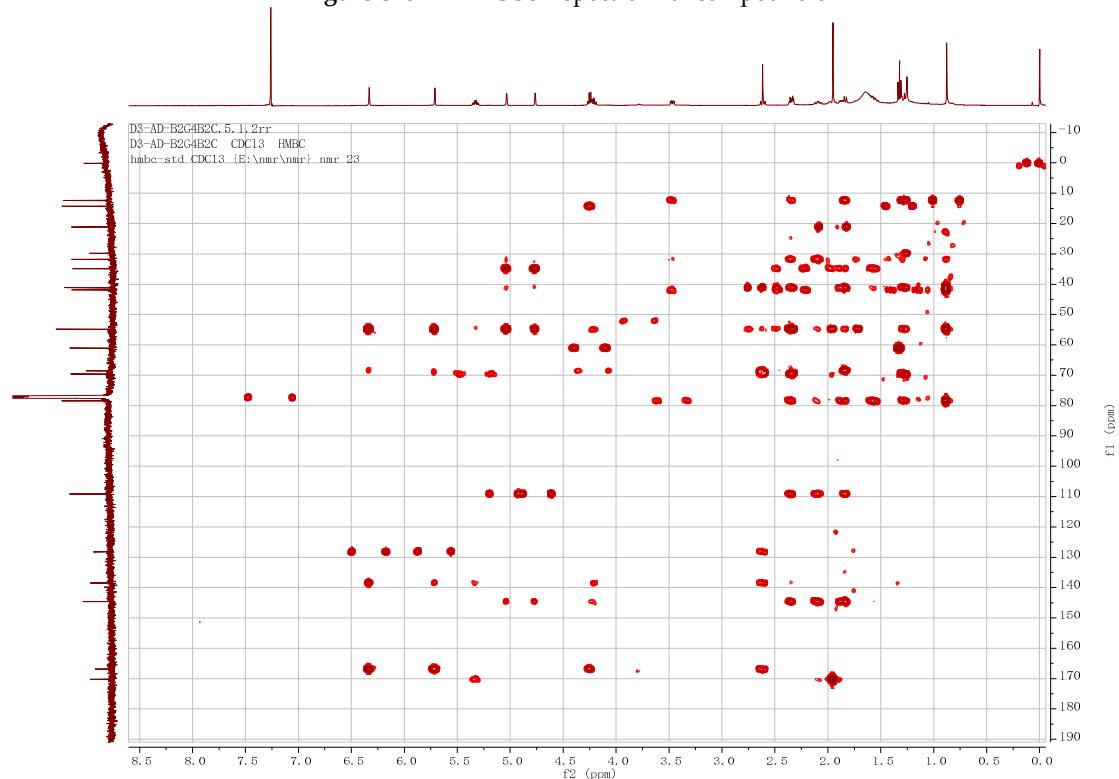


Figure S26 HMBC spectrum of compound 3

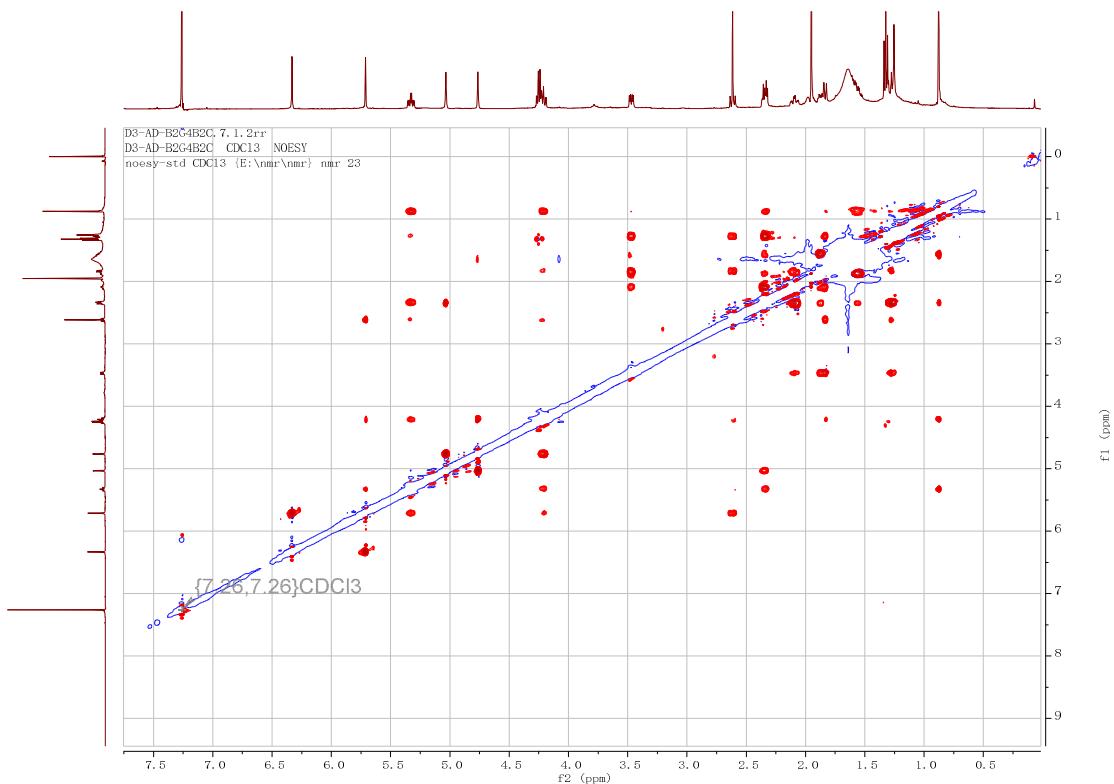


Figure S27 NOESY spectrum of compound 3

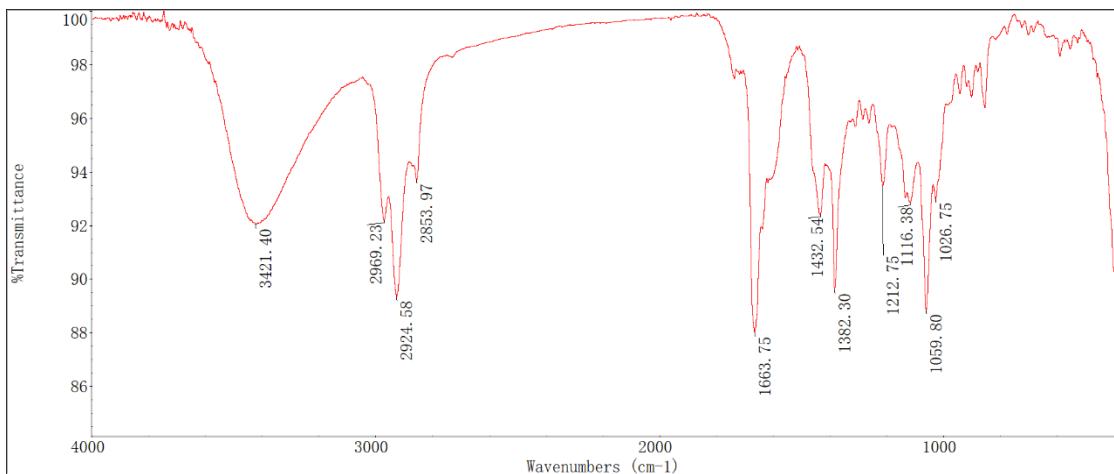
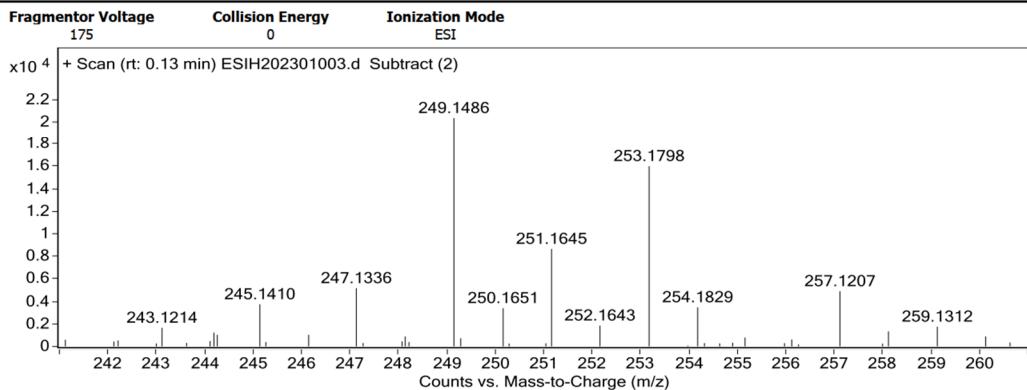


Figure S28 IR spectrum of compound 3

Qualitative Analysis Report

Data Filename	ESIH202301003.d	Sample Name	D3-D3-AD-B2G7C2B2B
Sample ID		Position	P1-A3
Instrument Name	Agilent G6520 Q-TOF	Acq Method	20160322_MS_ESIH_POS_1min.m
Acquired Time	2/17/2023 10:25:17	IRM Calibration Status	Success
DA Method	small molecular data analysis method.m	Comment	ESIH by fangsu

User Spectra



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
249.1486	249.1485	-0.07	-0.29	C15 H21 O3	(M+H)+

Figure S29 HR-ESIMS spectrum of compound 4

D3-AD-B2G7C2B2B.91.fid

D3-AD-B2G7C2B2B CDCl3 1H

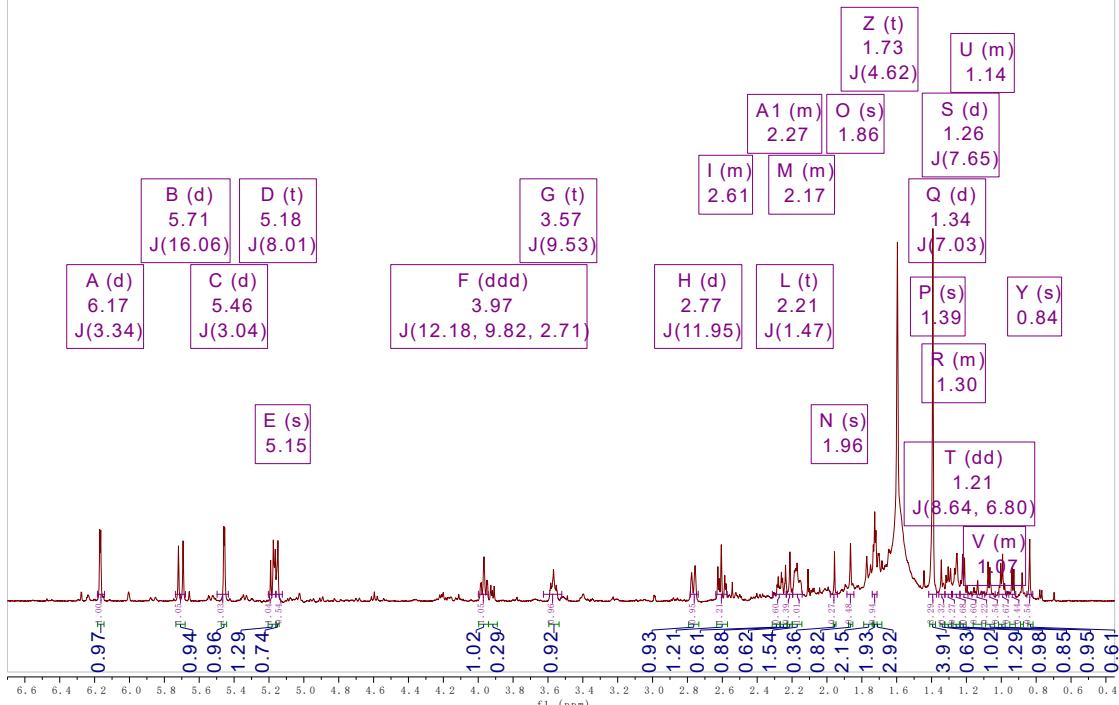


Figure S30 ^1H NMR spectrum of compound 4

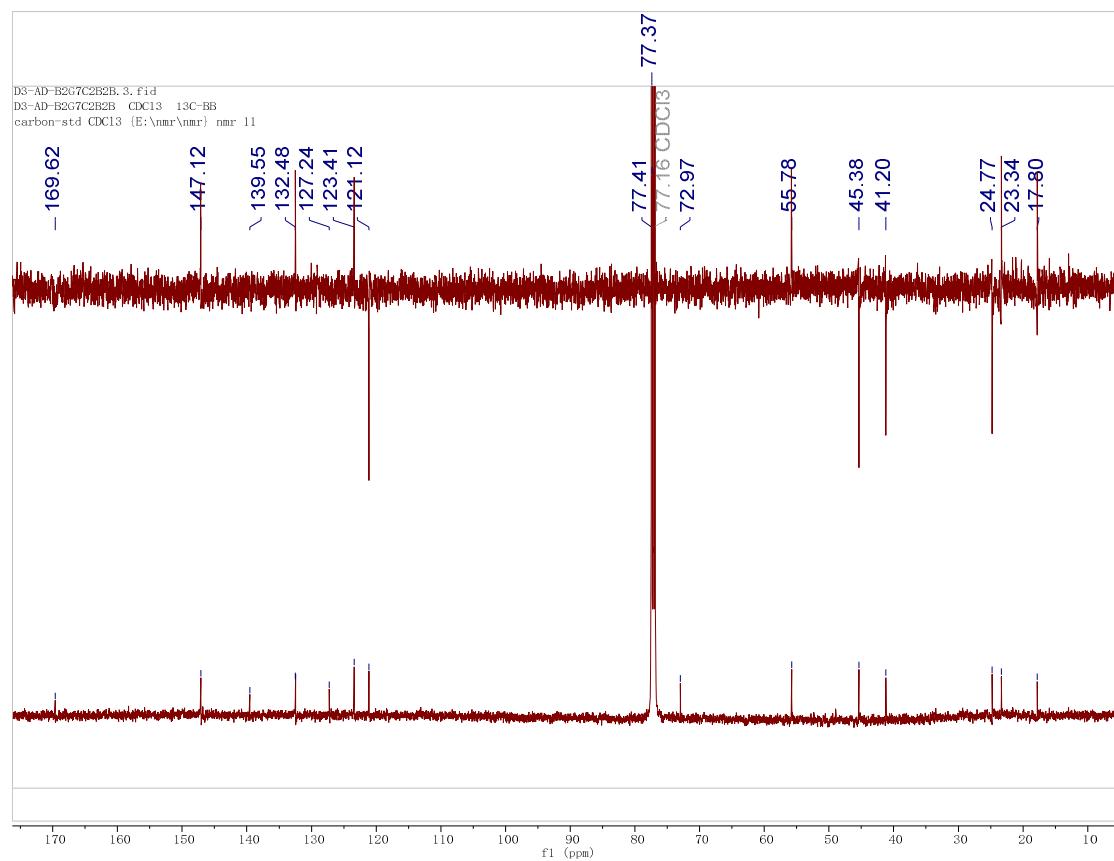


Figure S31 ^{13}C NMR spectrum of compound 4



Figure S32 HSQC spectrum of compound 4

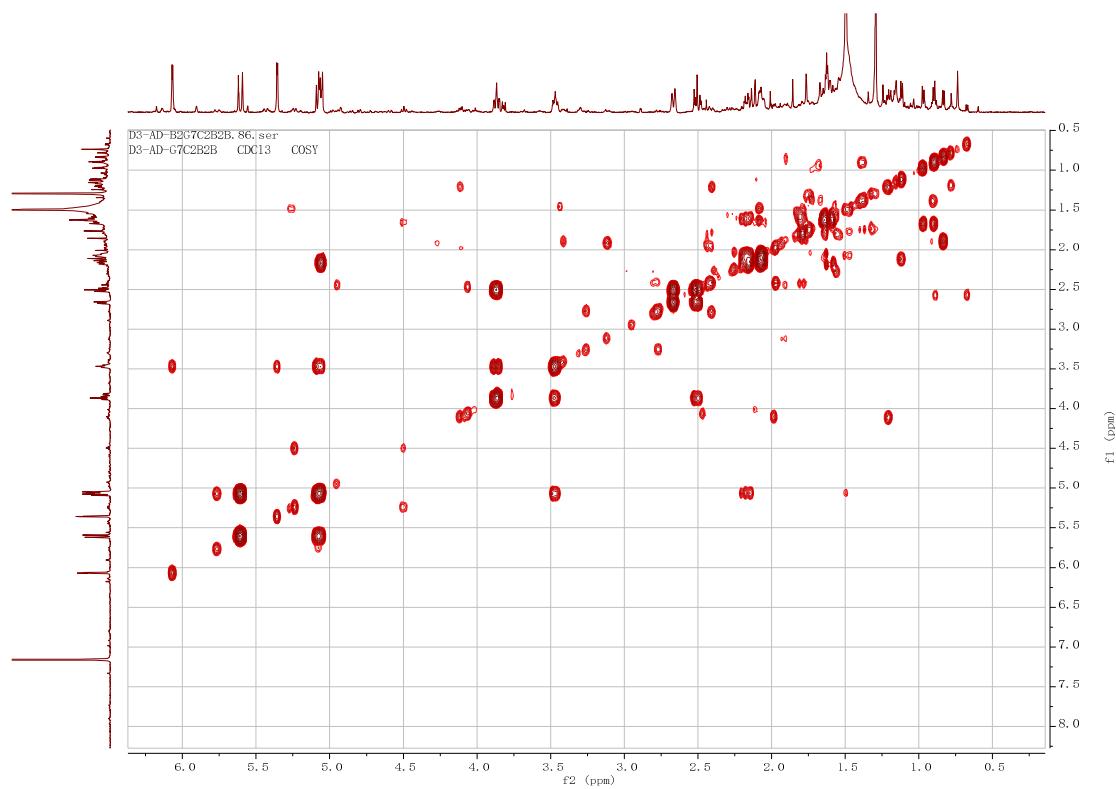


Figure S33 ¹H-¹H COSY spectrum of compound 4

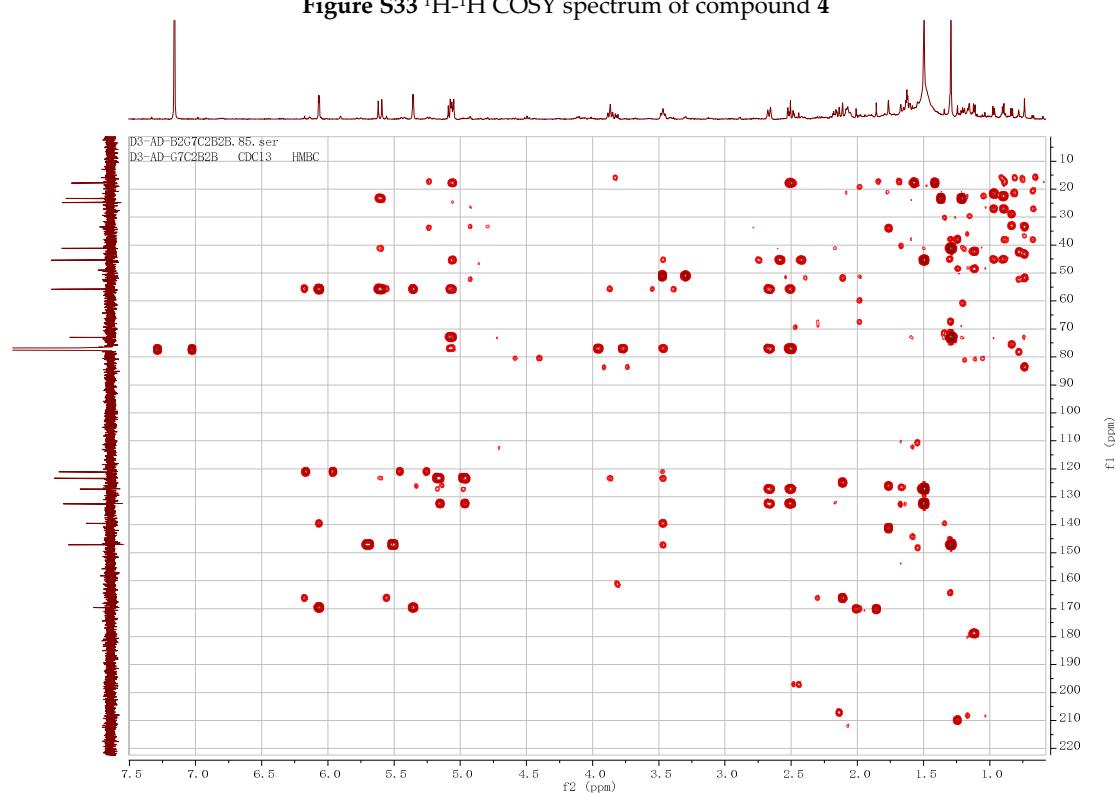


Figure S34 HMBC spectrum of compound 4

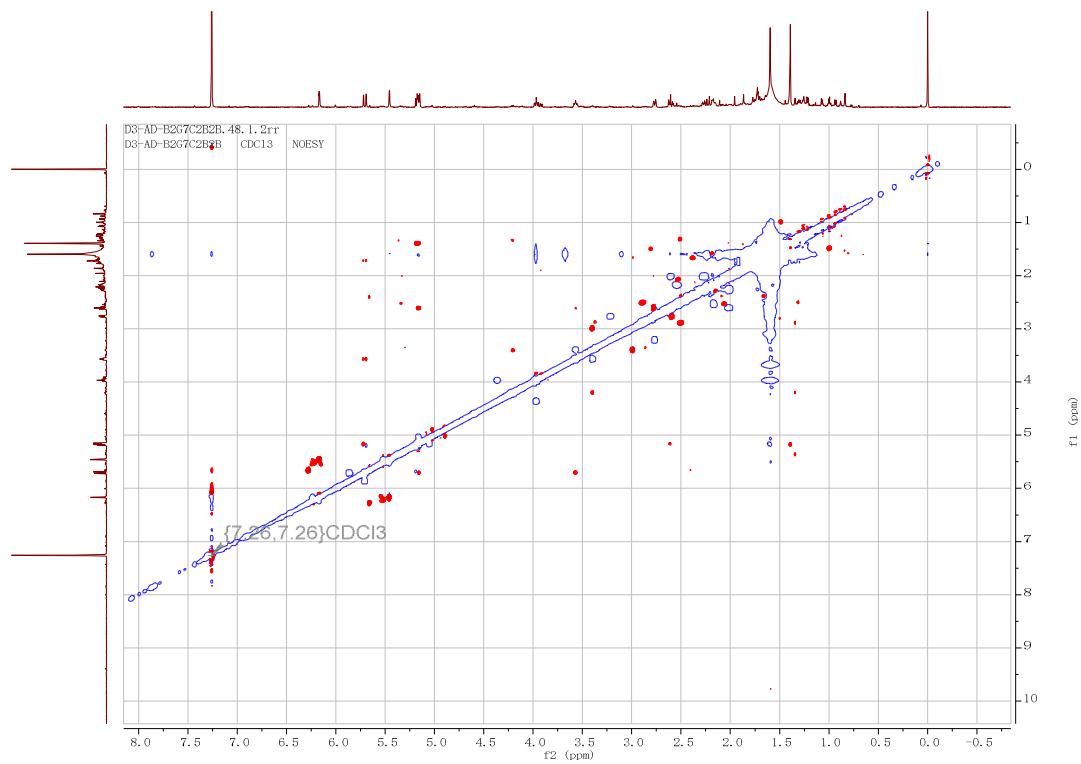


Figure S35 NOESY spectrum of compound 4

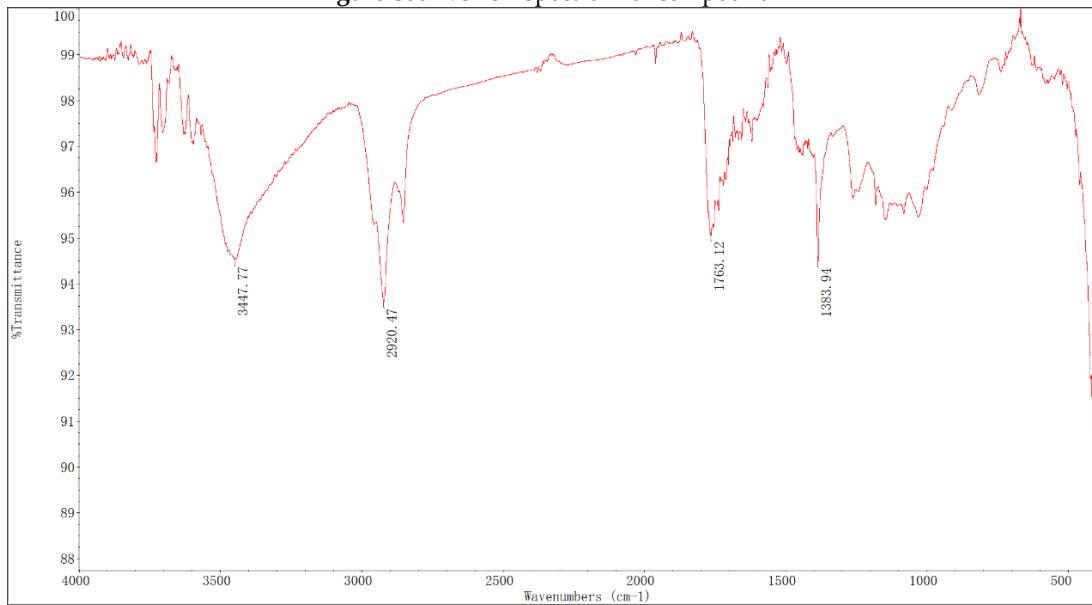


Figure S36 IR spectrum of compound 4

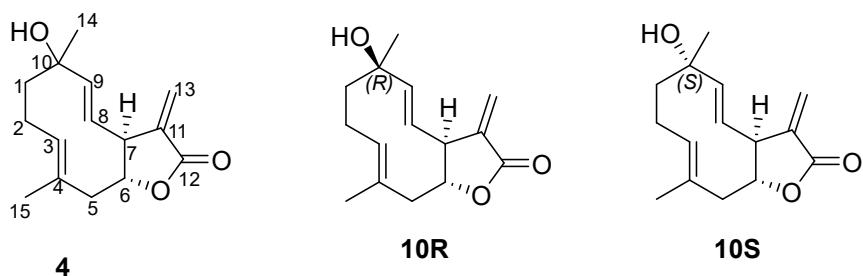


Figure S37 Possible isomers of compound 4

Functional	Solvent?	Basis Set	
mPW1PW91	PCM	6-311G(d,p)	
	Isomer 1	Isomer 2	Isomer 3
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%	–

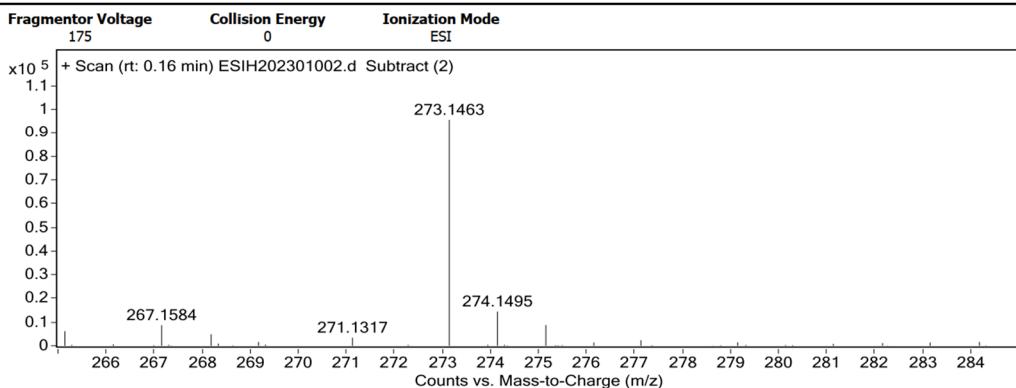
Figure S38 DP4+ probability statistics of compound 4

Qualitative Analysis Report

Data Filename ESIH202301002.d
Sample ID
Instrument Name Agilent G6520 Q-TOF
Acquired Time 2/17/2023 10:24:00
DA Method small molecular data analysis method.m

Sample Name D3-D3-AD-B2G6C2A1
Position P1-A2
Acq Method 20160322_MS_ESIH_POS_1min.m
IRM Calibration Status Success
Comment ESIH by fangsu

User Spectra



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
273.1463	273.1461	-0.17	-0.62	C15 H22 Na O3	(M+Na)+

Figure S39 HR-ESIMS spectrum of compound 5

D3-AD-B2G6C2A-20220923_91.fid
D3-AD-B2G6C2A CDC13 1H

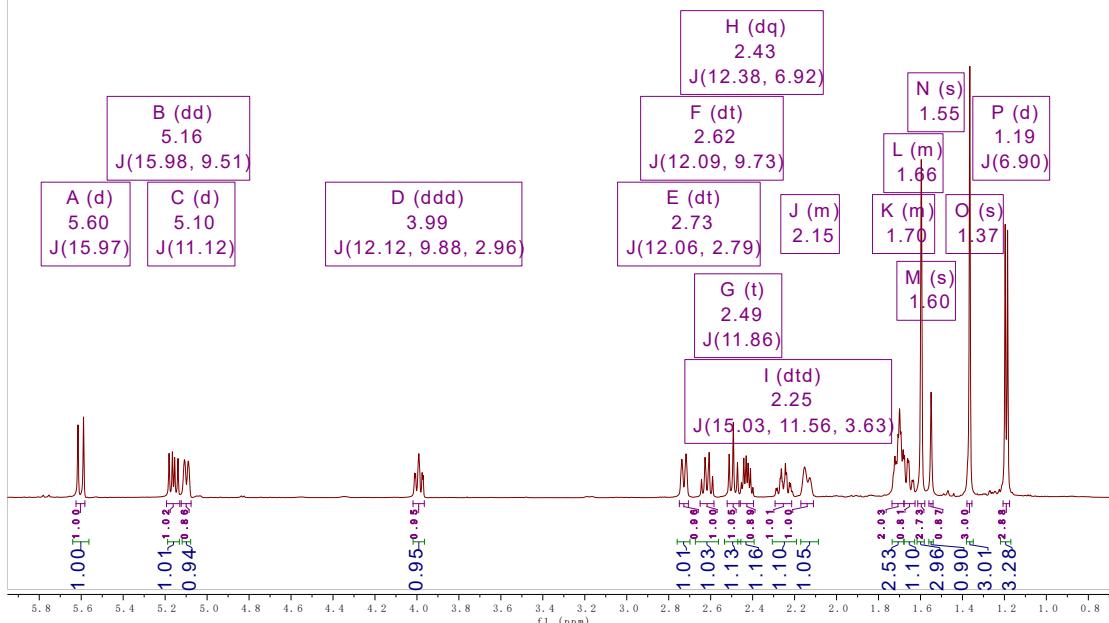


Figure S40 ¹H NMR spectrum of compound 5

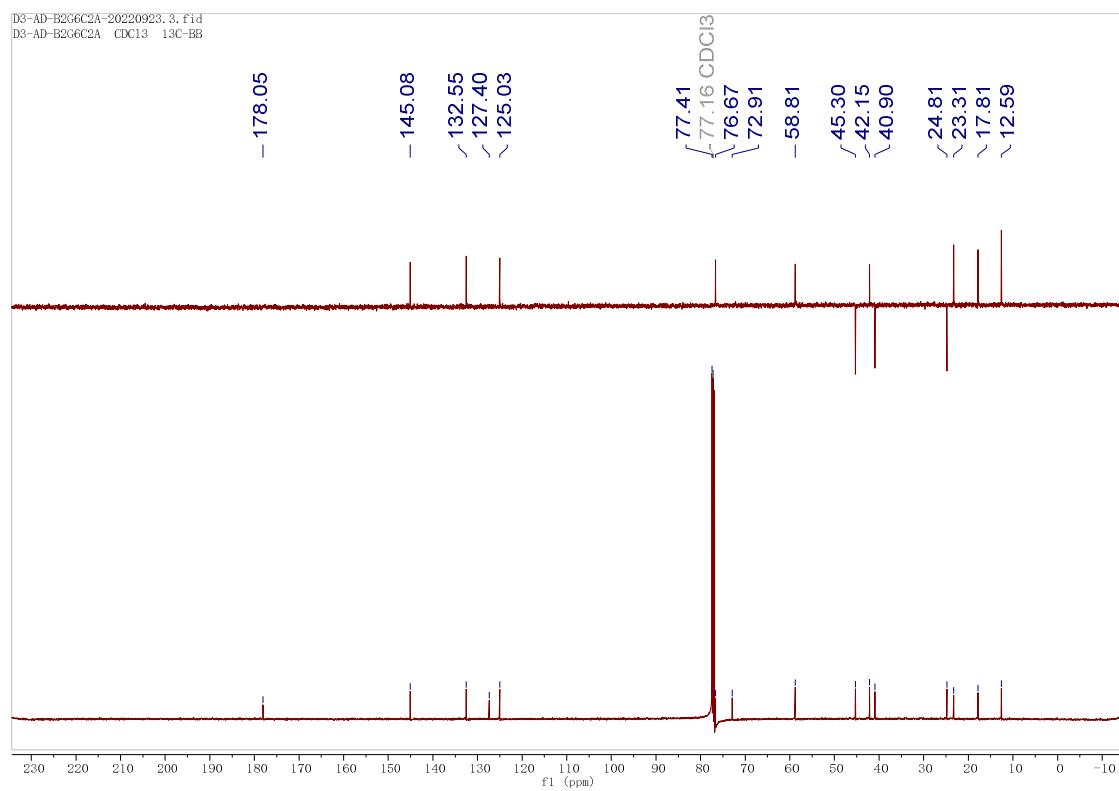


Figure S41 ^{13}C NMR spectrum of compound 5

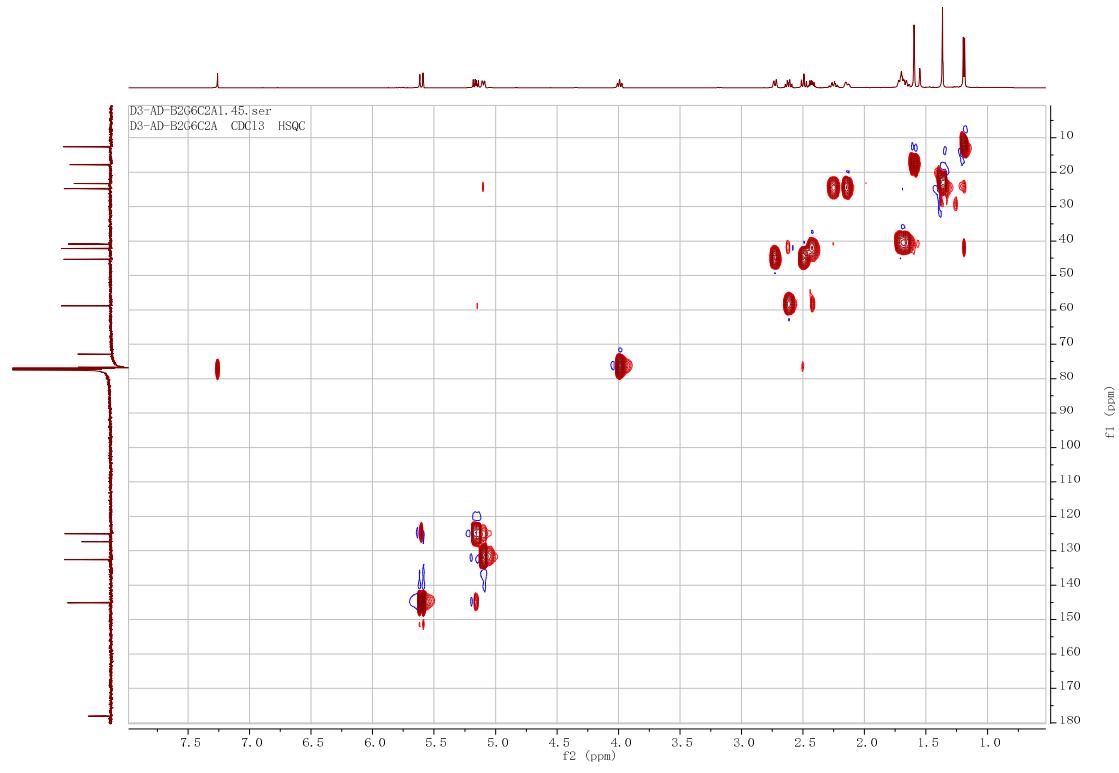


Figure S42 HSQC spectrum of compound 5

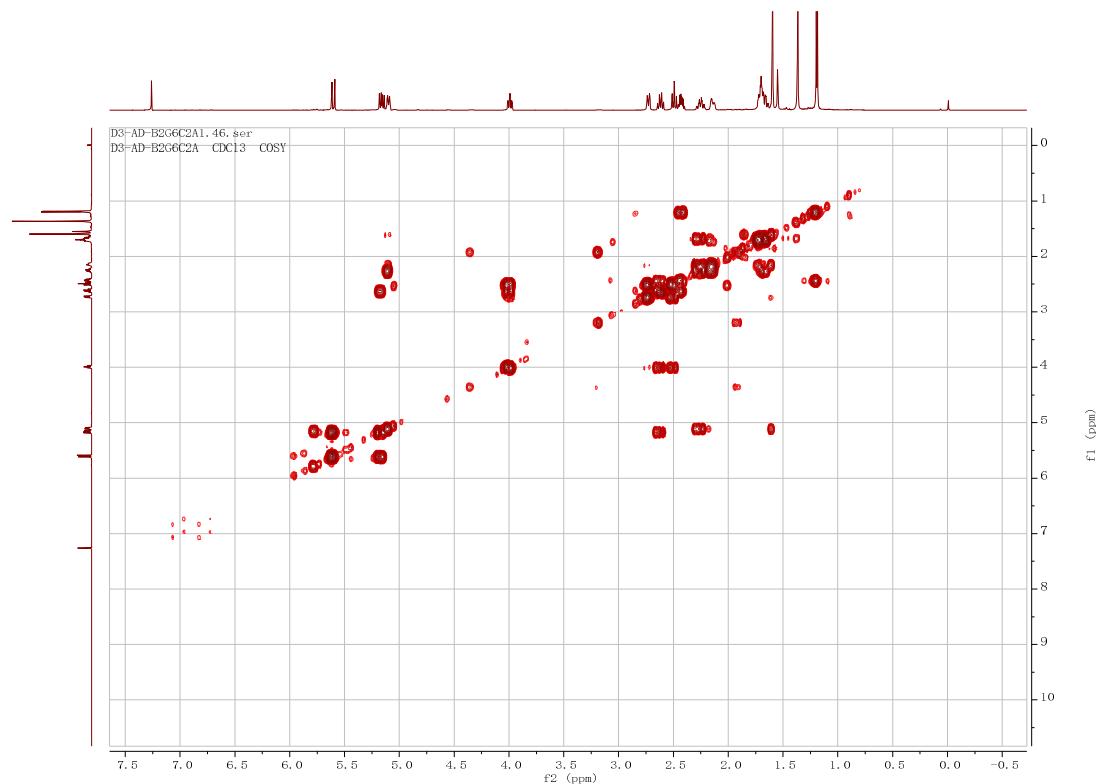


Figure S43 ^1H - ^1H COSY spectrum of compound 5

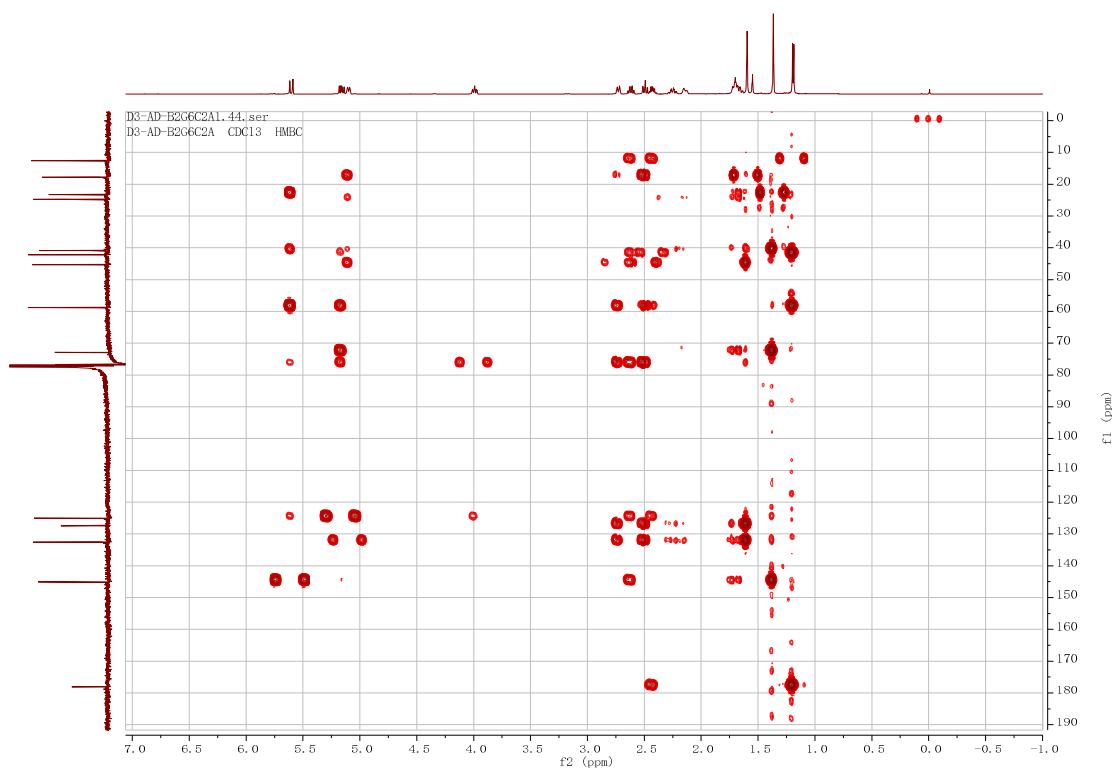


Figure S44 HMBC spectrum of compound 5

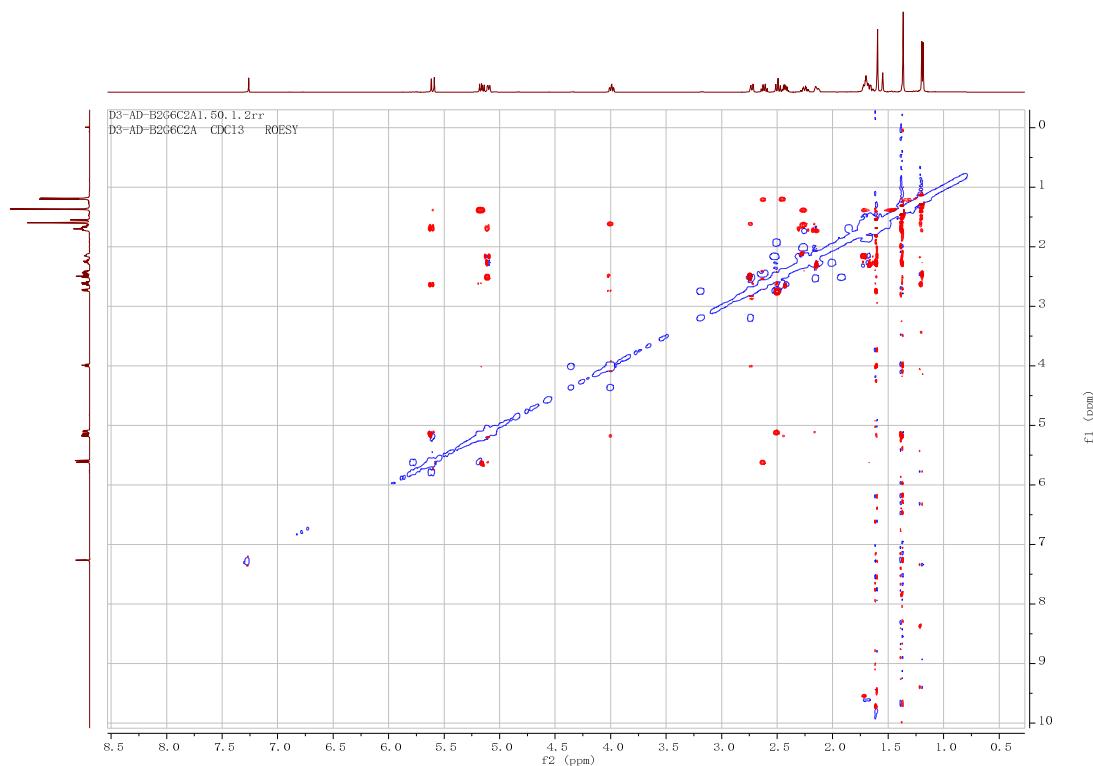


Figure S45 NOESY spectrum of compound 5

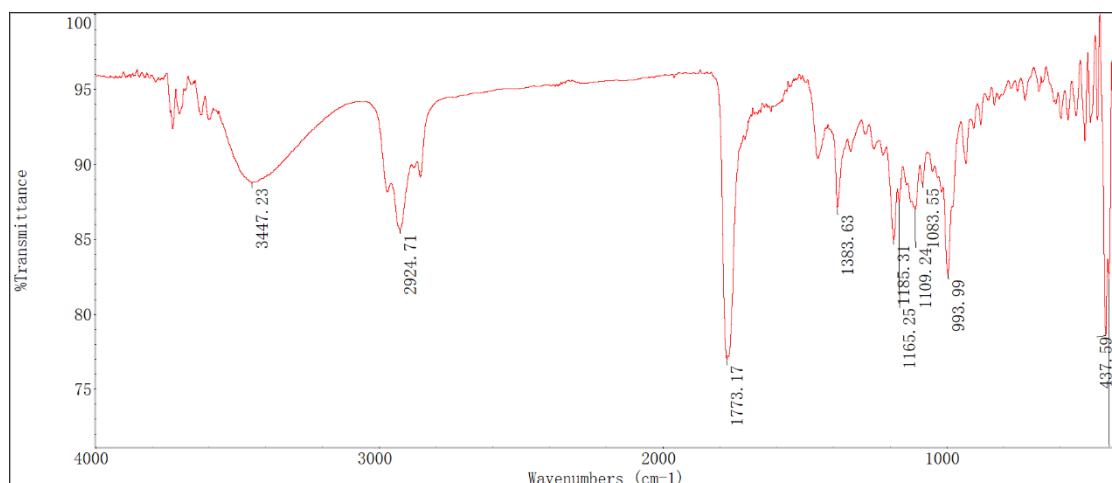


Figure S46 IR spectrum of compound 5

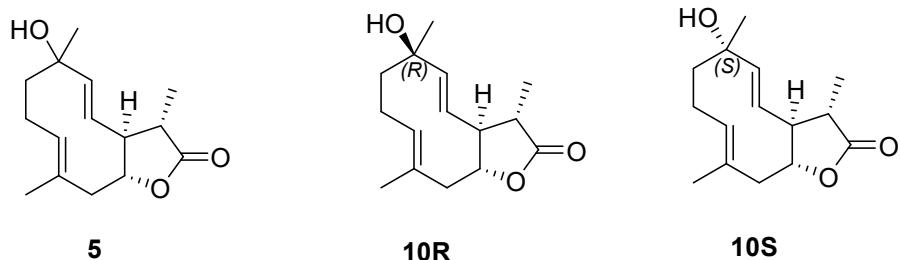


Figure S47 Possible isomers of compound 5

Functional	Solvent?	Basis Set
mPW1PW91	PCM	6-311G(d, p)
	Isomer 1	Isomer 2
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	$C_{15}H_{23}O$

YSQ

20230203_S025 735 (5.367)

1: TOF MS ES+

5.18e+005

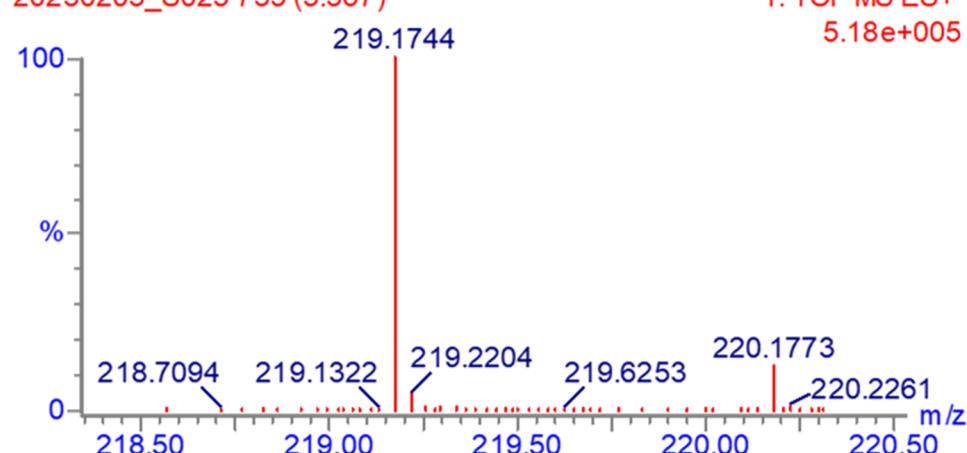


Figure S49 HR-ESIMS spectrum of compound 6

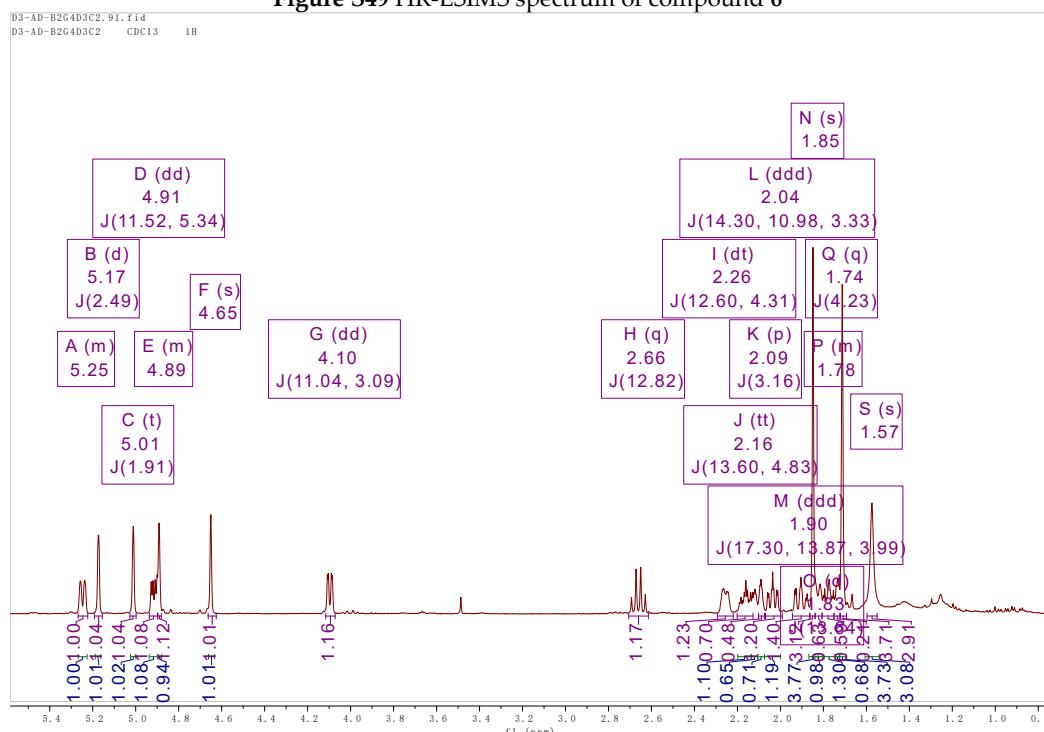


Figure S50 1H NMR spectrum of compound 6

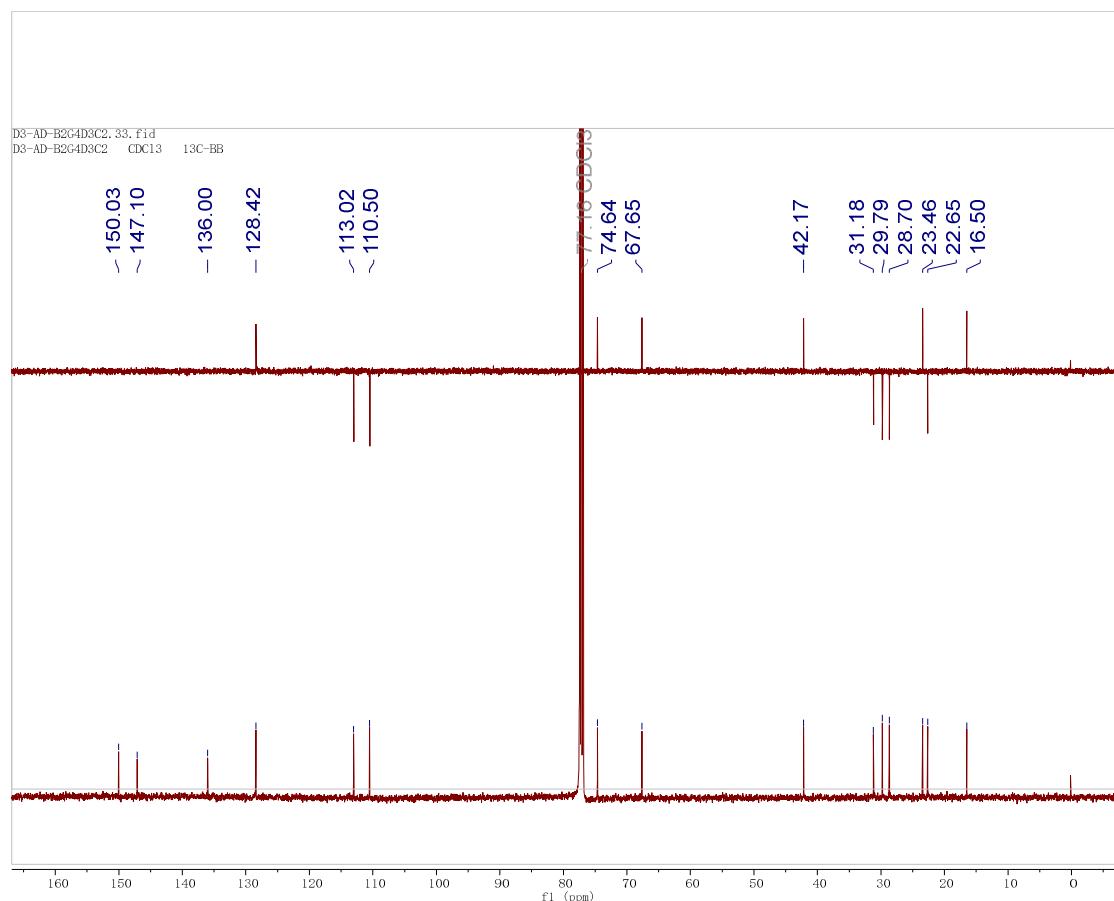


Figure S51 ^{13}C NMR spectrum of compound 6

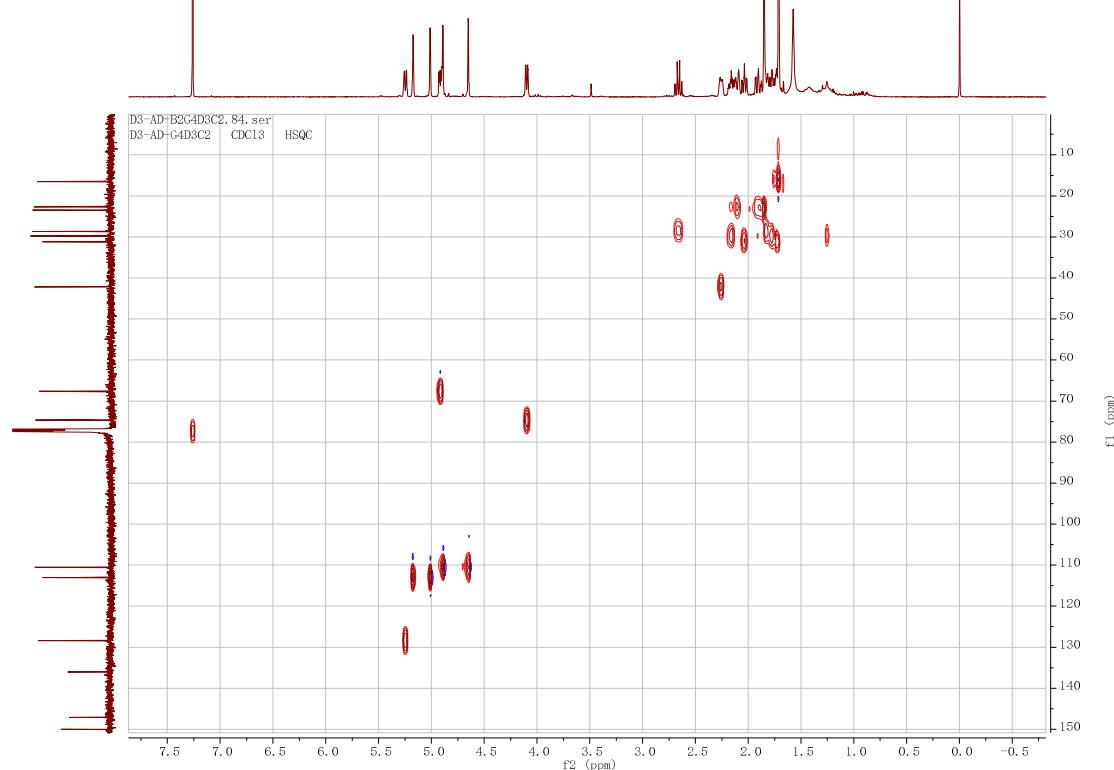


Figure S52 HSQC spectrum of compound 6

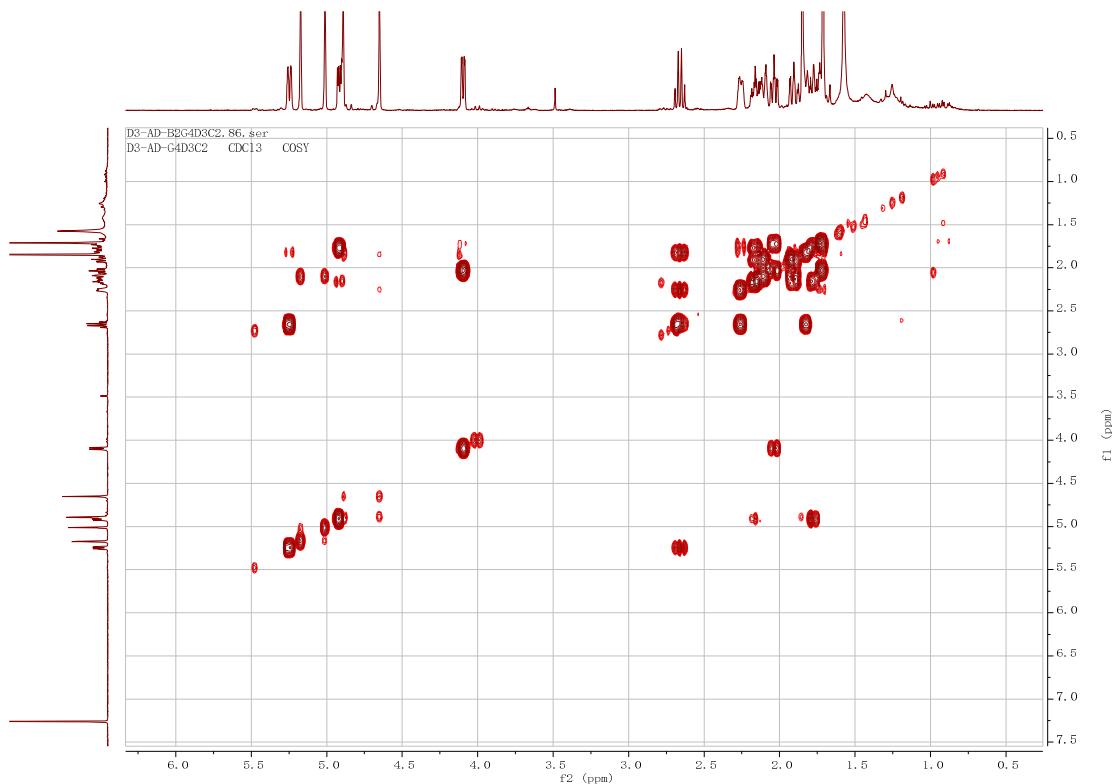


Figure S53 ¹H-¹H COSY spectrum of compound 6

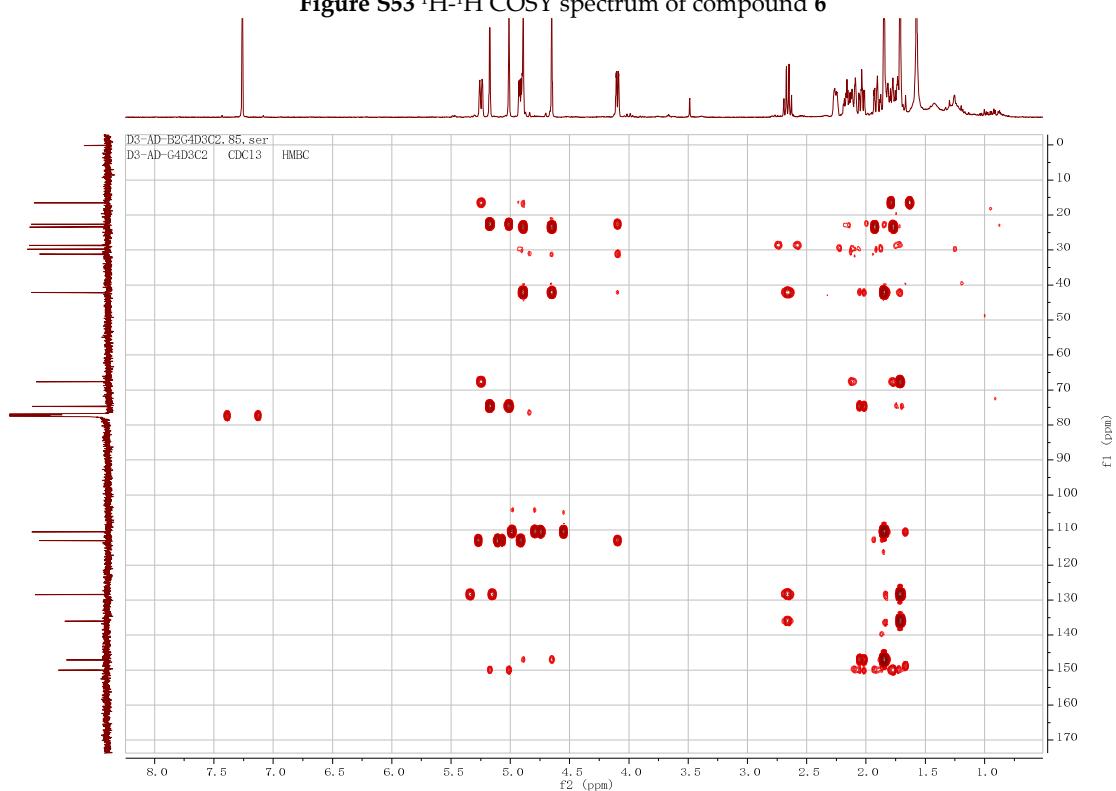


Figure S54 HMBC spectrum of compound 6

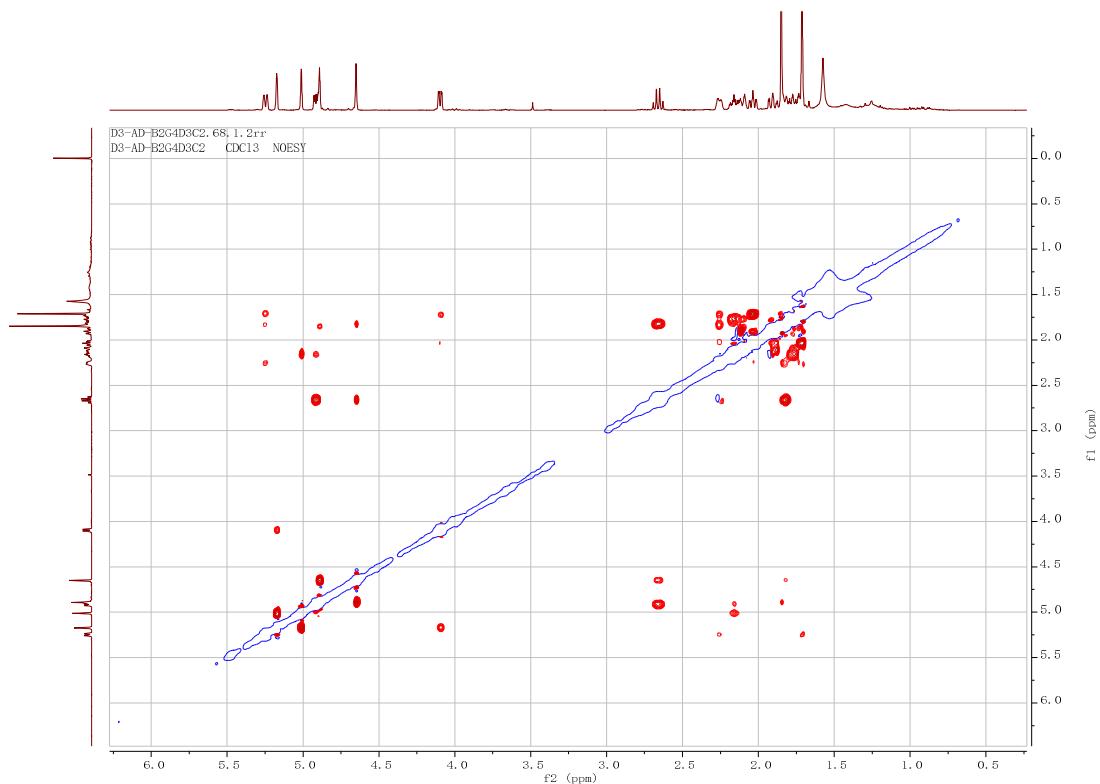


Figure S55 NOESY spectrum of compound 6

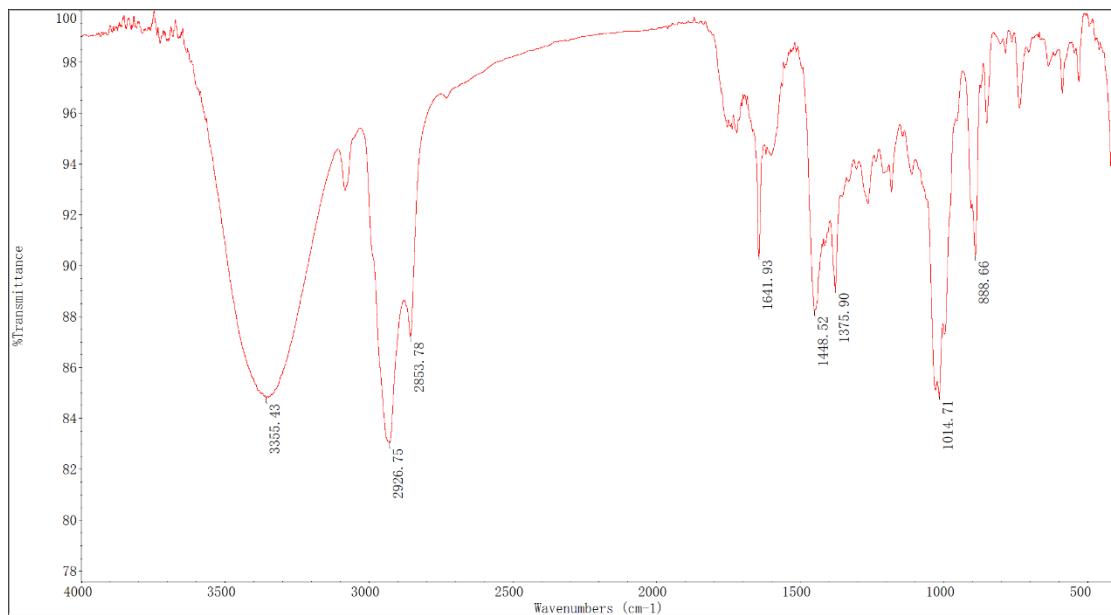


Figure S56 IR spectrum of compound 6

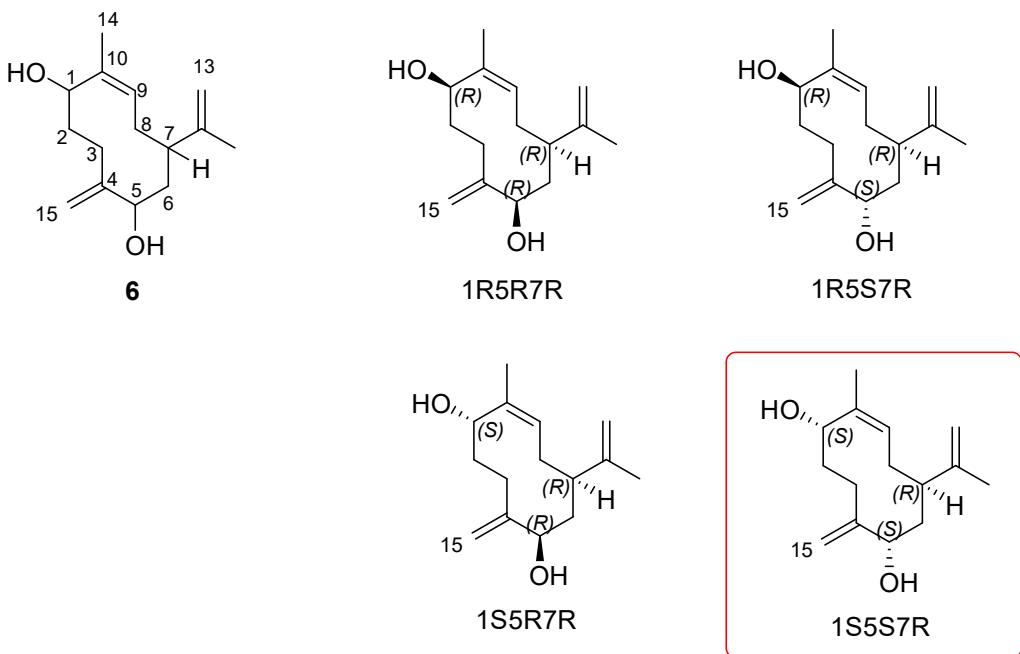


Figure S57 Possible isomers of compound 6

Functional	Solvent?	Basis Set	
mPW1PW91	PCM	6-311G (d, p)	
		Isomer 1	Isomer 2
sDP4+ (H data)		1. 36%	0. 58%
sDP4+ (C data)		0. 03%	0. 00%
sDP4+ (all data)		0. 00%	0. 00%
uDP4+ (H data)		2. 31%	0. 00%
uDP4+ (C data)		0. 04%	0. 00%
uDP4+ (all data)		0. 00%	0. 00%
DP4+ (H data)		0. 03%	0. 00%
DP4+ (C data)		0. 00%	0. 00%
DP4+ (all data)		0. 00%	0. 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 Maximum: 100.00
 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 C₁₅H₂₃O

YSQ

20230203_S030 799 (5.837)

1: TOF MS ES+
 3.17e+005

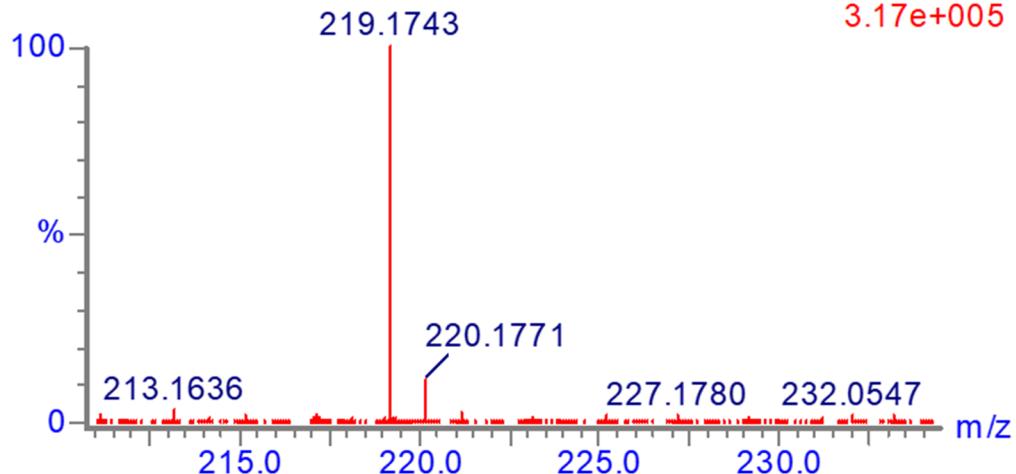


Figure S59 HR-ESIMS spectrum of compound 7

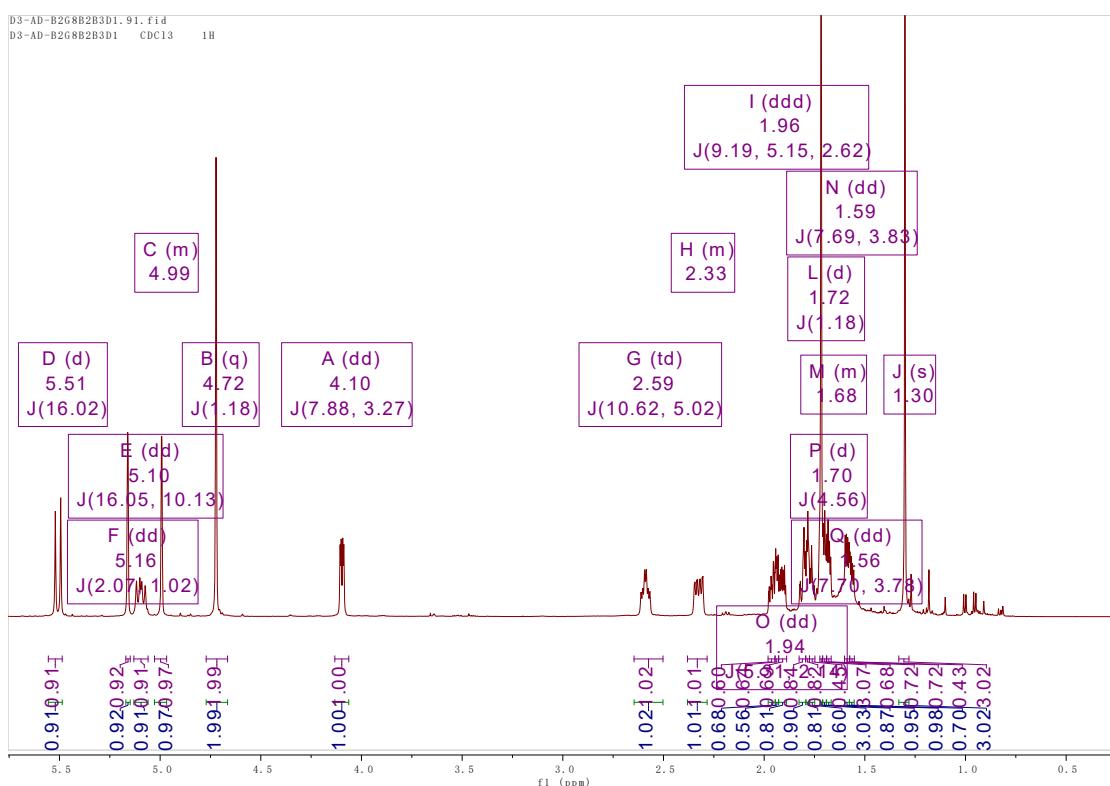


Figure S60 ¹H NMR spectrum of compound 7



Figure S61 ¹³C NMR spectrum of compound 7

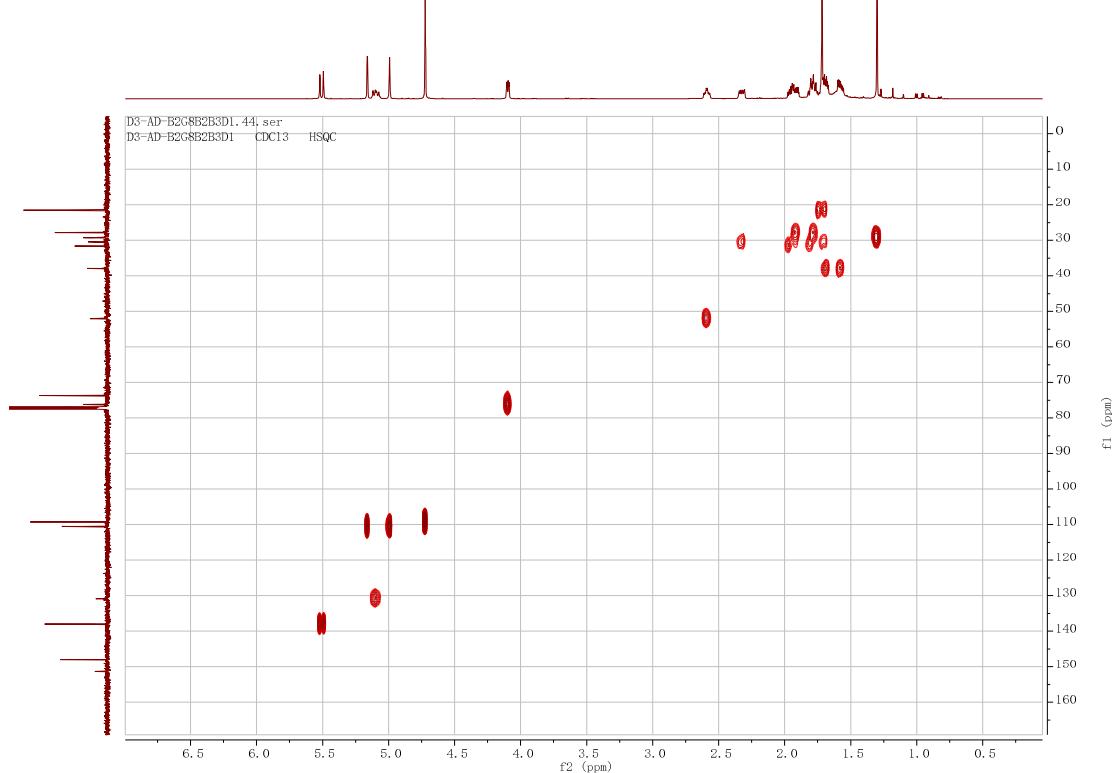


Figure S62 HSQC spectrum of compound 7

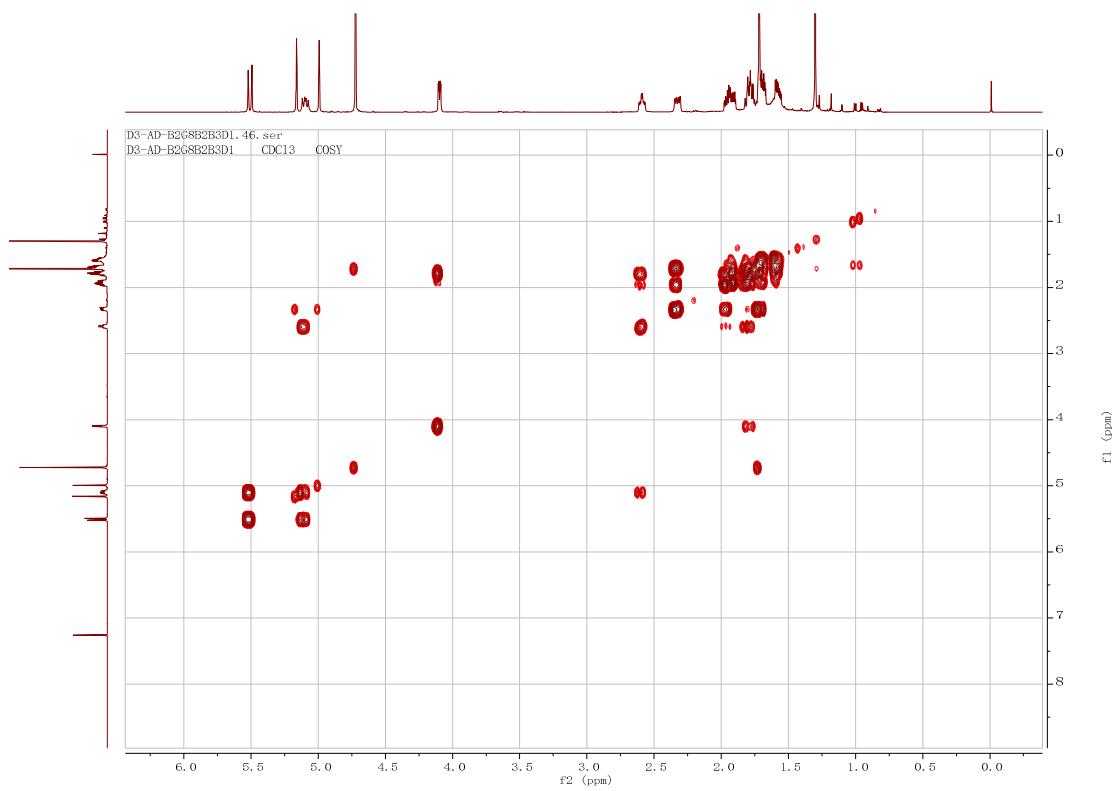


Figure S63 ^1H - ^1H COSY spectrum of compound 7

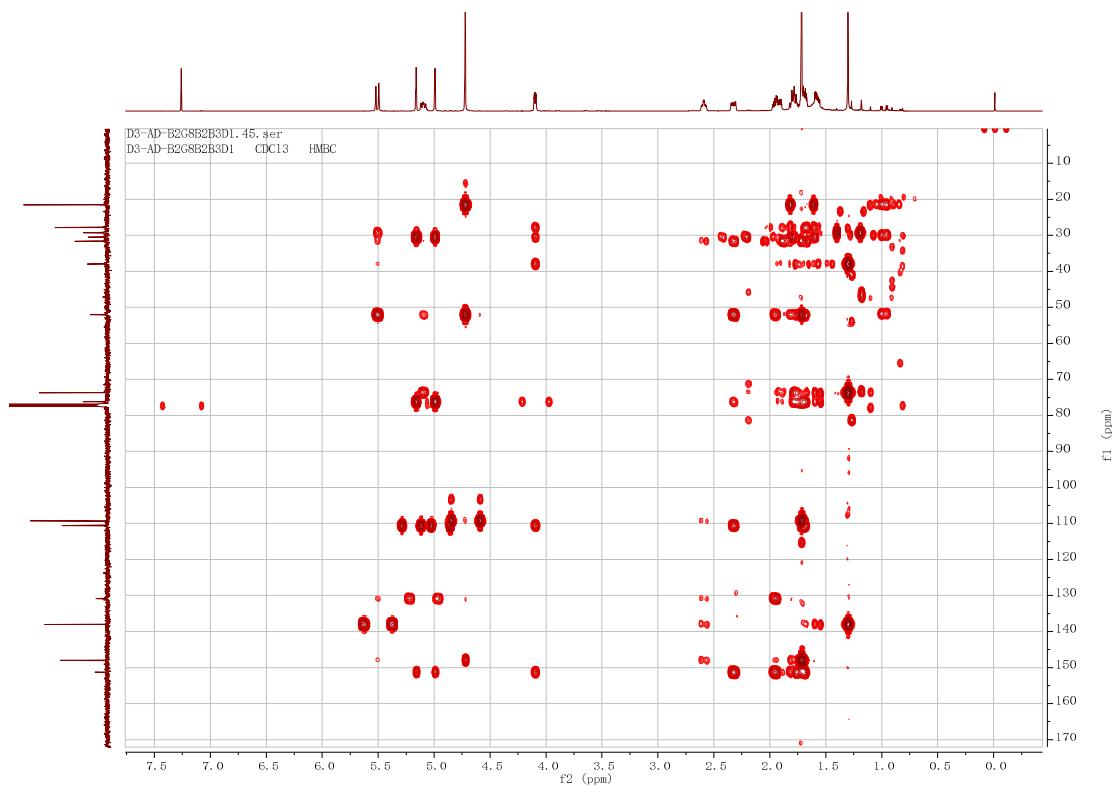


Figure S64 HMBC spectrum of compound 7

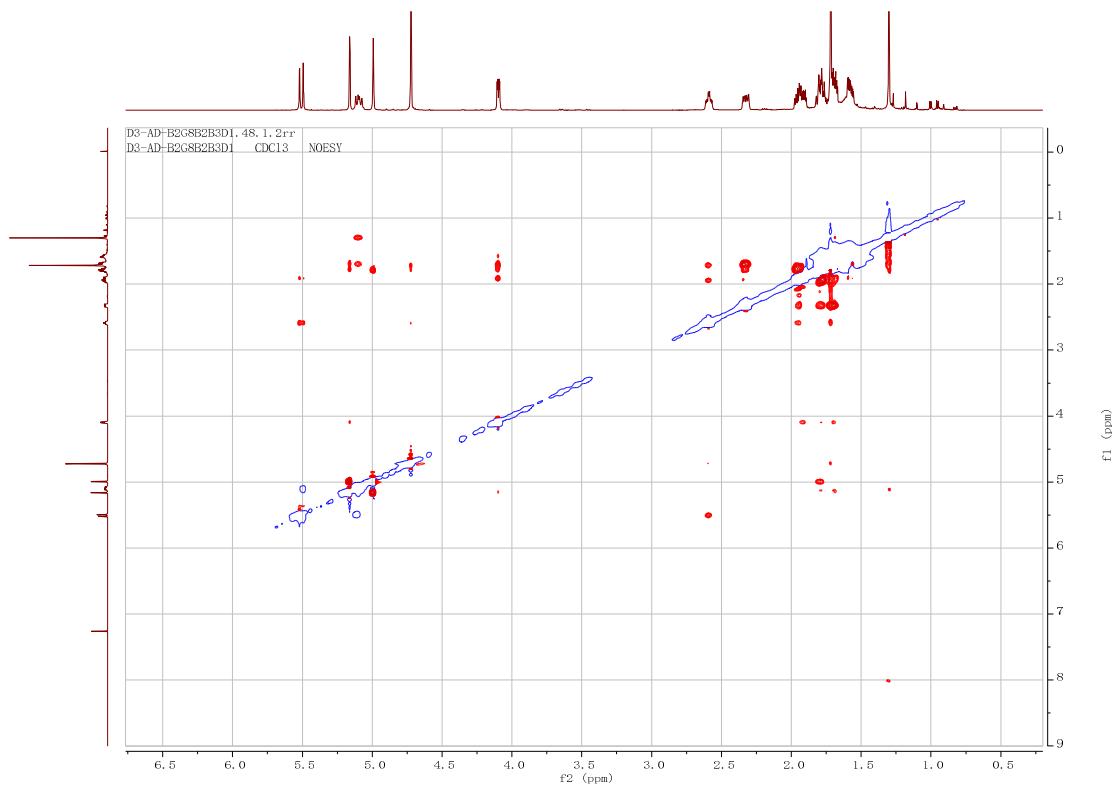


Figure S65 NOESY spectrum of compound 7

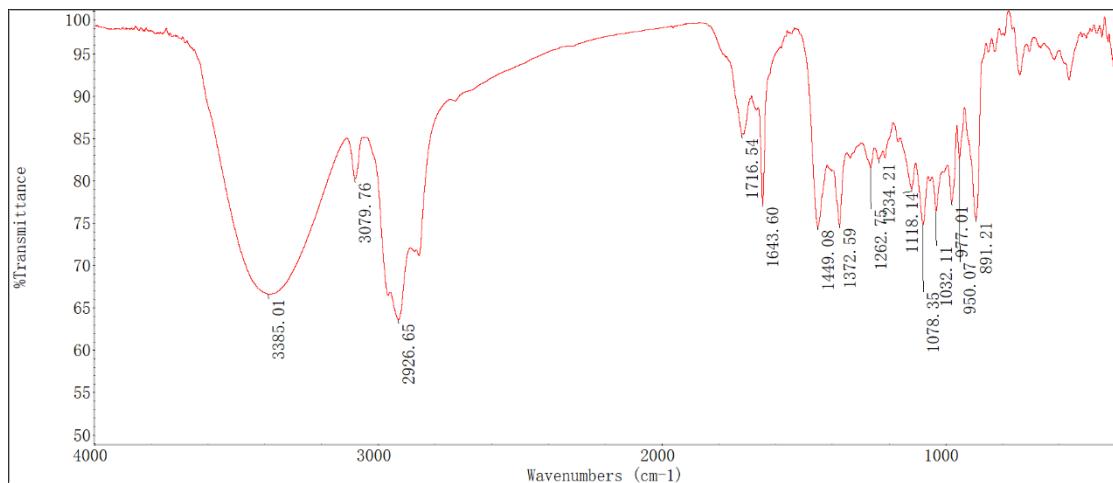


Figure S66 IR spectrum of compound 7

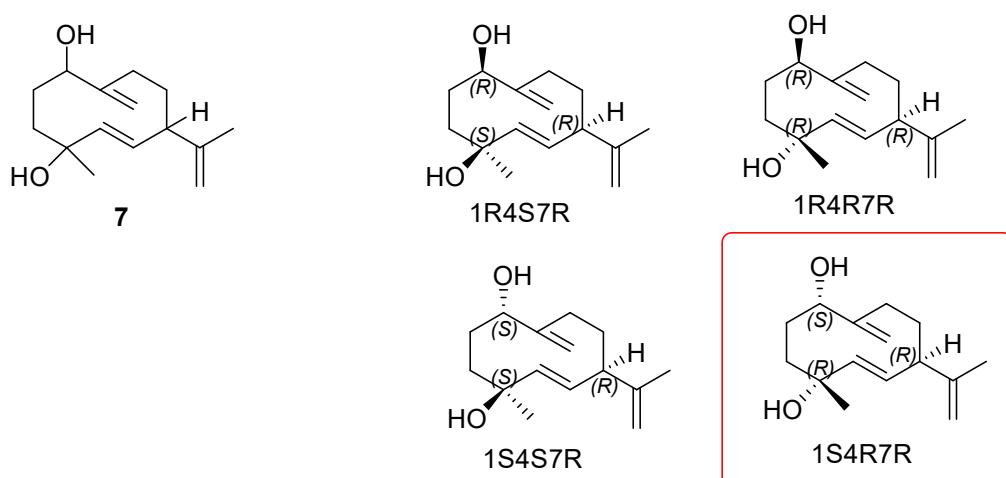


Figure S67 Possible isomers of compound 7

Functional	Solvent?	Basis Set		
mPW1PW91	PCM	6-311G (d, p)		
		Isomer 1	Isomer 2	Isomer 3
sDP4+ (H data)		56. 38%	3. 53%	39. 68%
sDP4+ (C data)		0. 01%	0. 00%	99. 95%
sDP4+ (all data)		0. 01%	0. 00%	99. 99%
uDP4+ (H data)		73. 73%	0. 16%	15. 74%
uDP4+ (C data)		0. 01%	0. 00%	99. 99%
uDP4+ (all data)		0. 04%	0. 00%	99. 96%
DP4+ (H data)		86. 85%	0. 01%	13. 05%
DP4+ (C data)		0. 00%	0. 00%	100. 00%
DP4+ (all data)		0. 00%	0. 00%	100. 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 Maximum: 100.00 -1.5
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

YSQ

20230203_S029 798 (5.830)

1: TOF MS ES+

2.34e+005

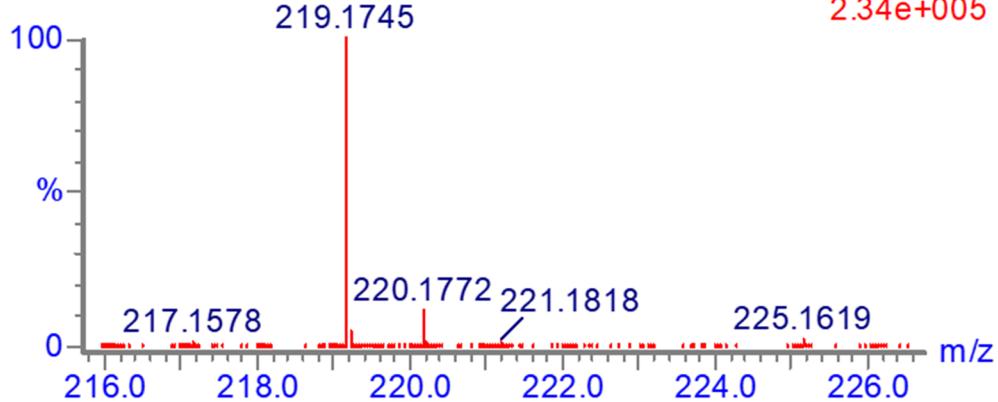


Figure S69 HR-ESIMS spectrum of compound 8

Figure S70 ¹H NMR spectrum of compound 8

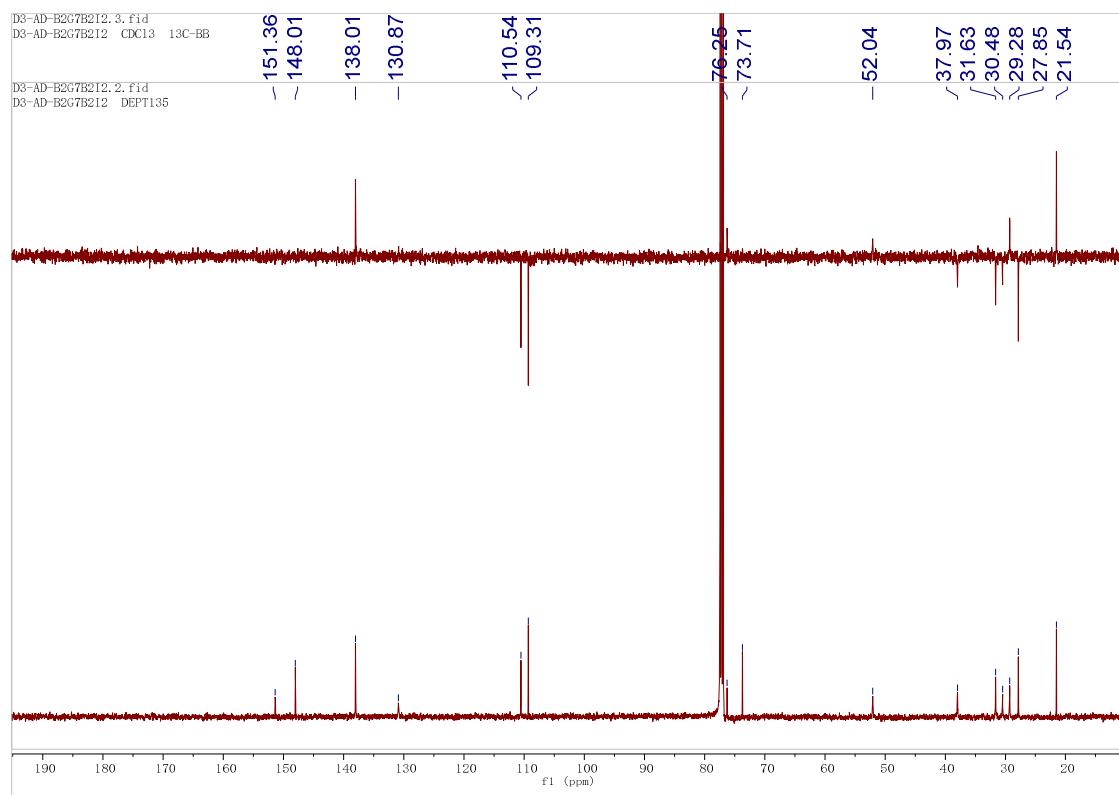


Figure S71 ^{13}C NMR spectrum of compound 8

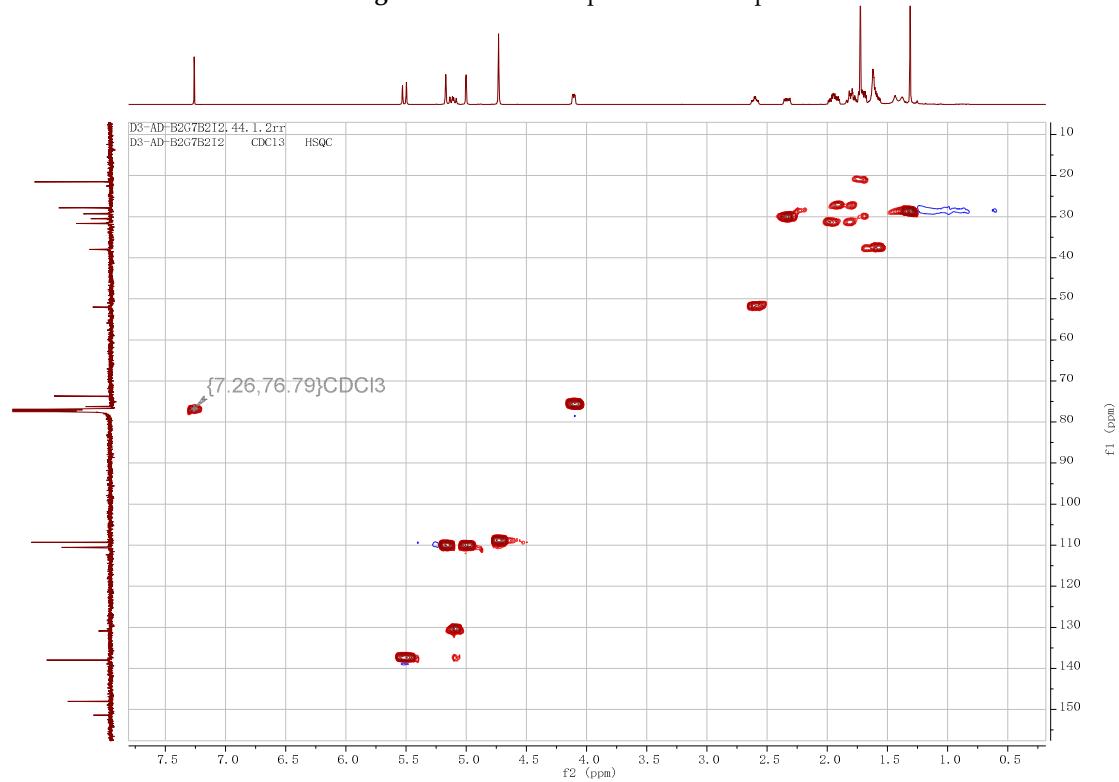


Figure S72 HSQC spectrum of compound 8

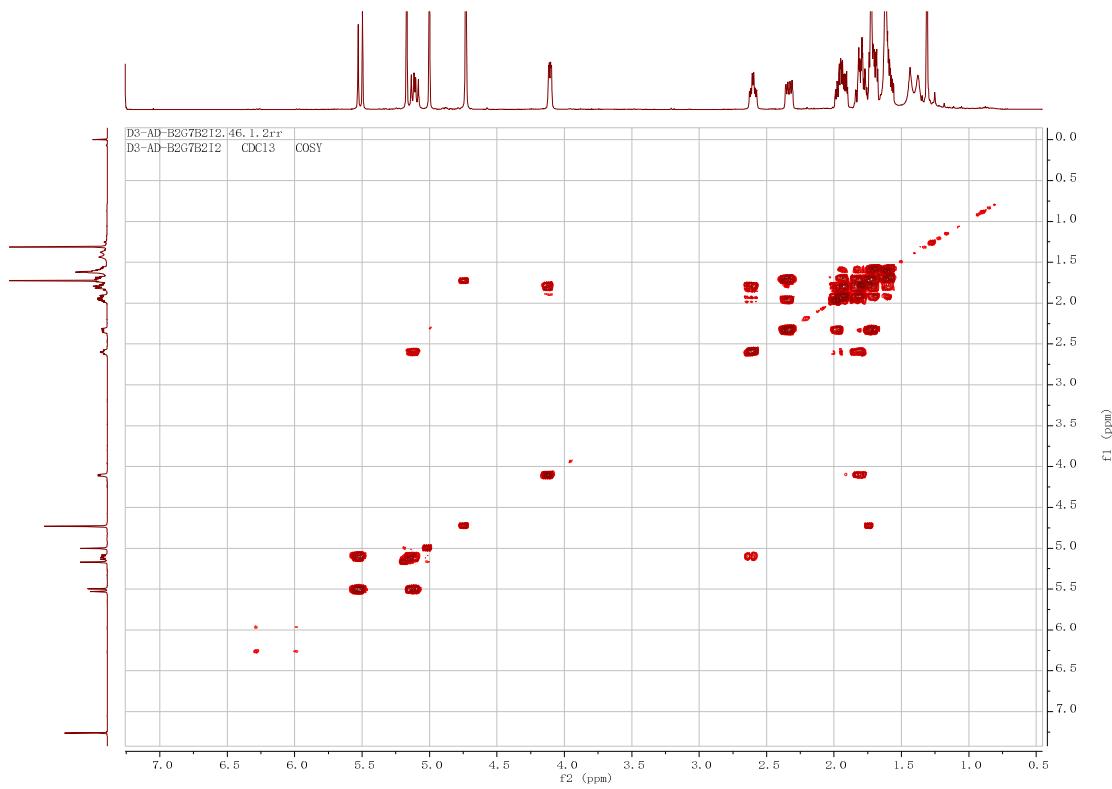


Figure S73 ^1H - ^1H COSY spectrum of compound 8

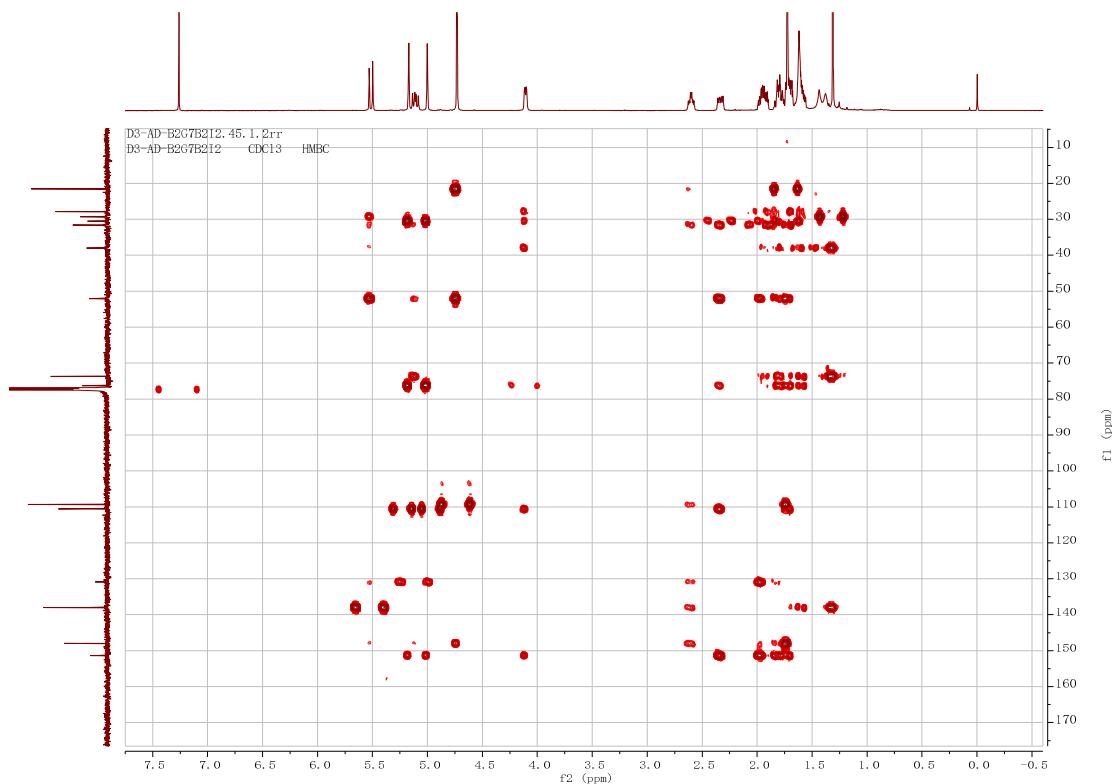


Figure S74 HMBC spectrum of compound 8

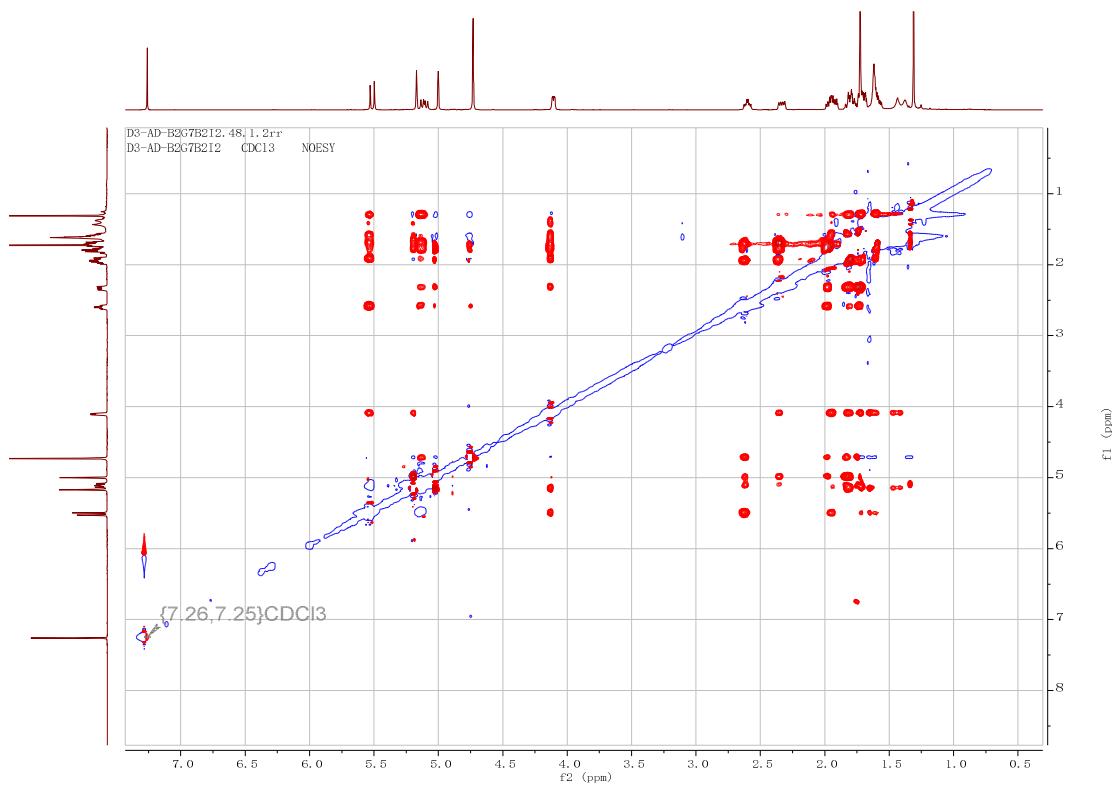


Figure S75 NOESY spectrum of compound 8

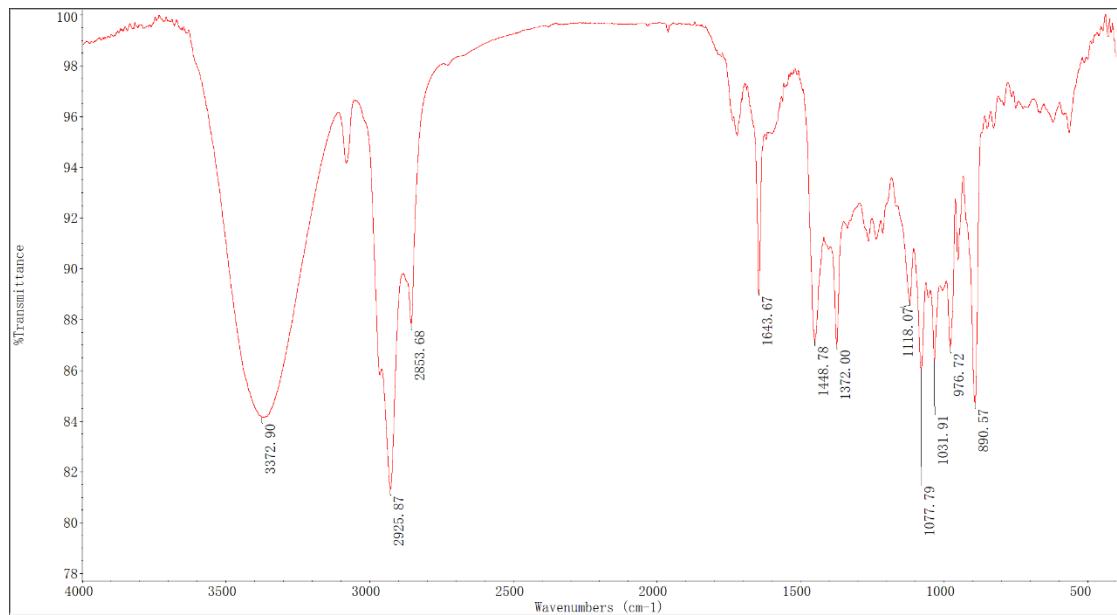


Figure S76 IR spectrum of compound 8

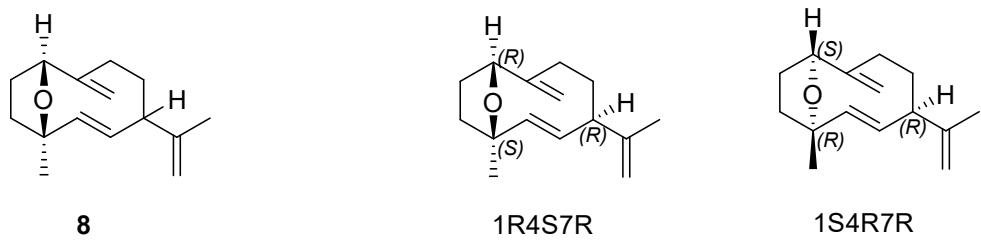


Figure S77 Possible isomers of compound 8

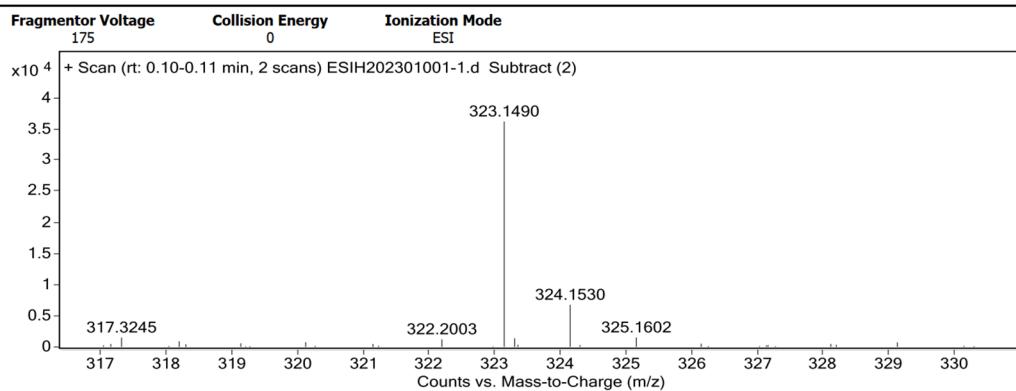
Functional mPW1PW91	Solvent? PCM	Basis Set 6-311G(d, p)		
		Isomer 1	Isomer 2	Isomer 3
sDP4+ (H data)	99. 96%	0. 04%	–	–
sDP4+ (C data)	98. 89%	1. 11%	–	–
sDP4+ (all data)	100. 00%	0. 00%	–	–
uDPP4+ (H data)	96. 93%	3. 07%	–	–
uDPP4+ (C data)	58. 19%	41. 81%	–	–
uDPP4+ (all data)	97. 77%	2. 23%	–	–
DP4+ (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



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

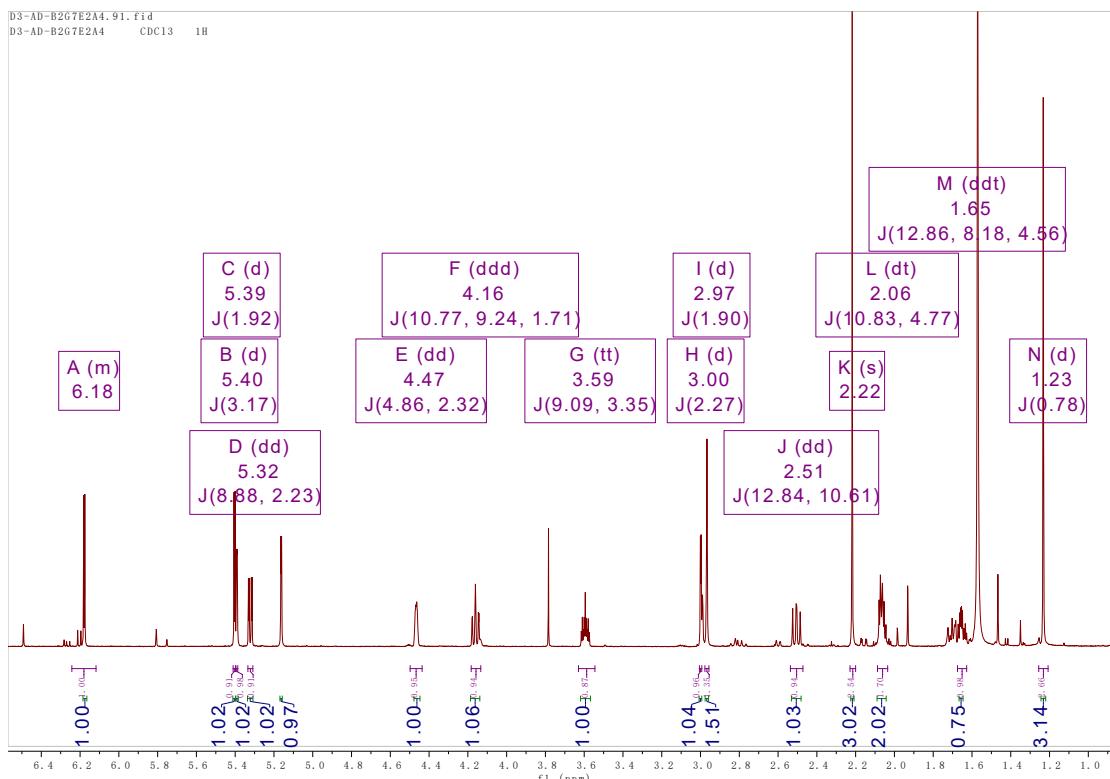


Figure S80 ¹H NMR spectrum of compound 9

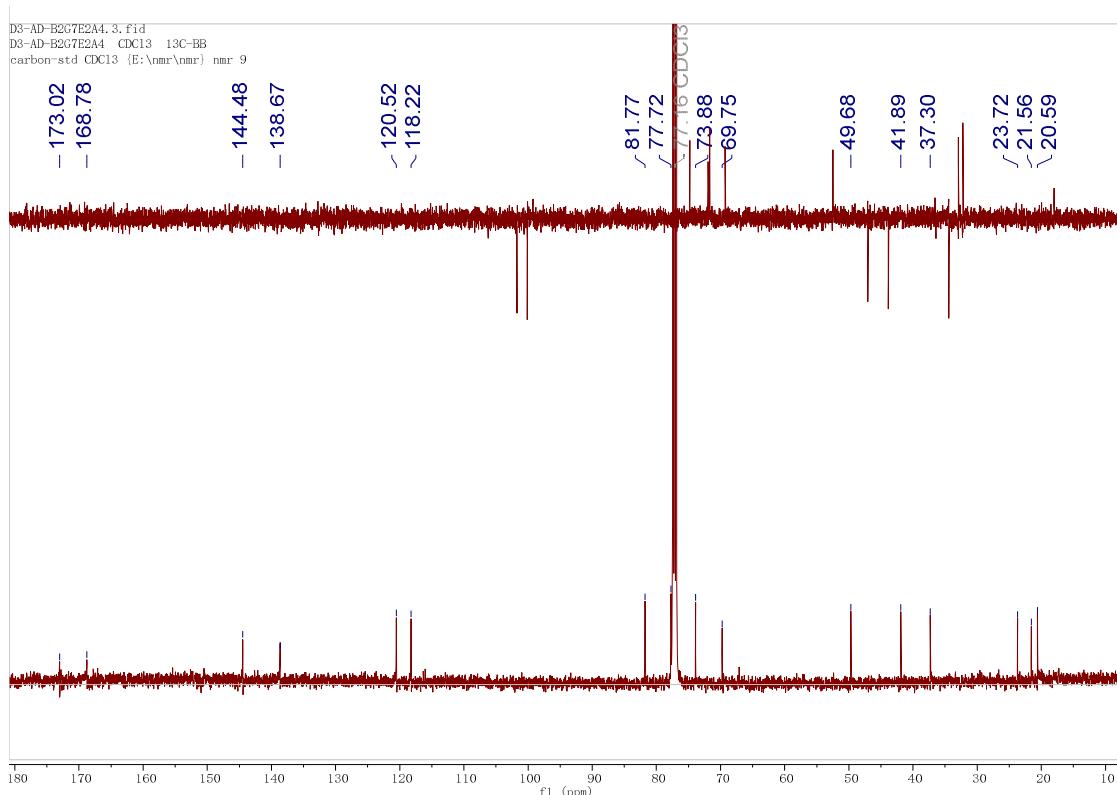


Figure S81 ^{13}C NMR spectrum of compound **9**

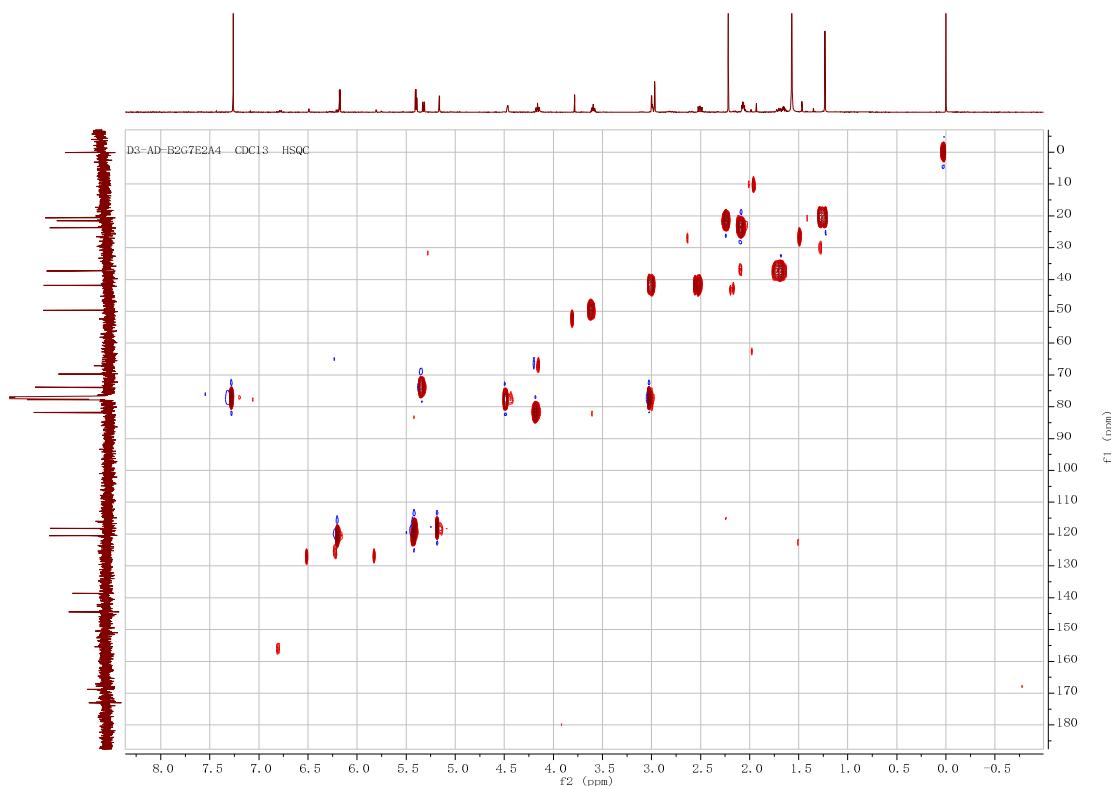


Figure S82 HSQC spectrum of compound **9**

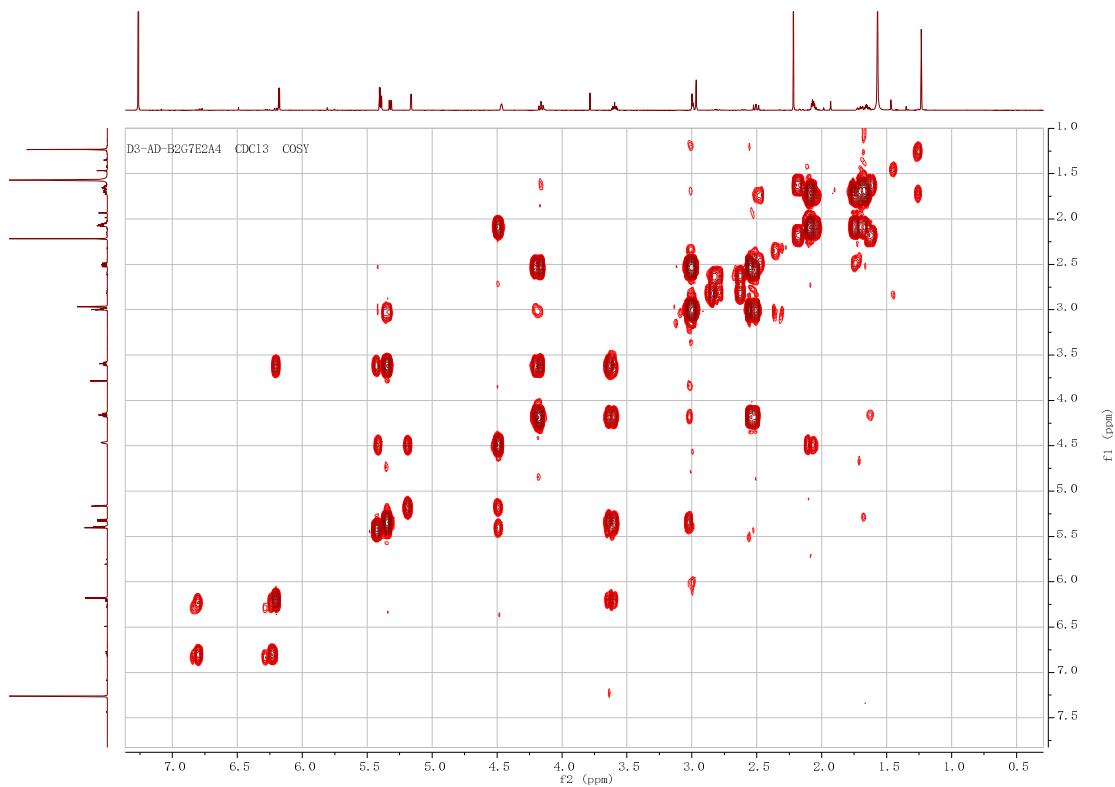


Figure S83 ^1H - ^1H COSY spectrum of compound 9

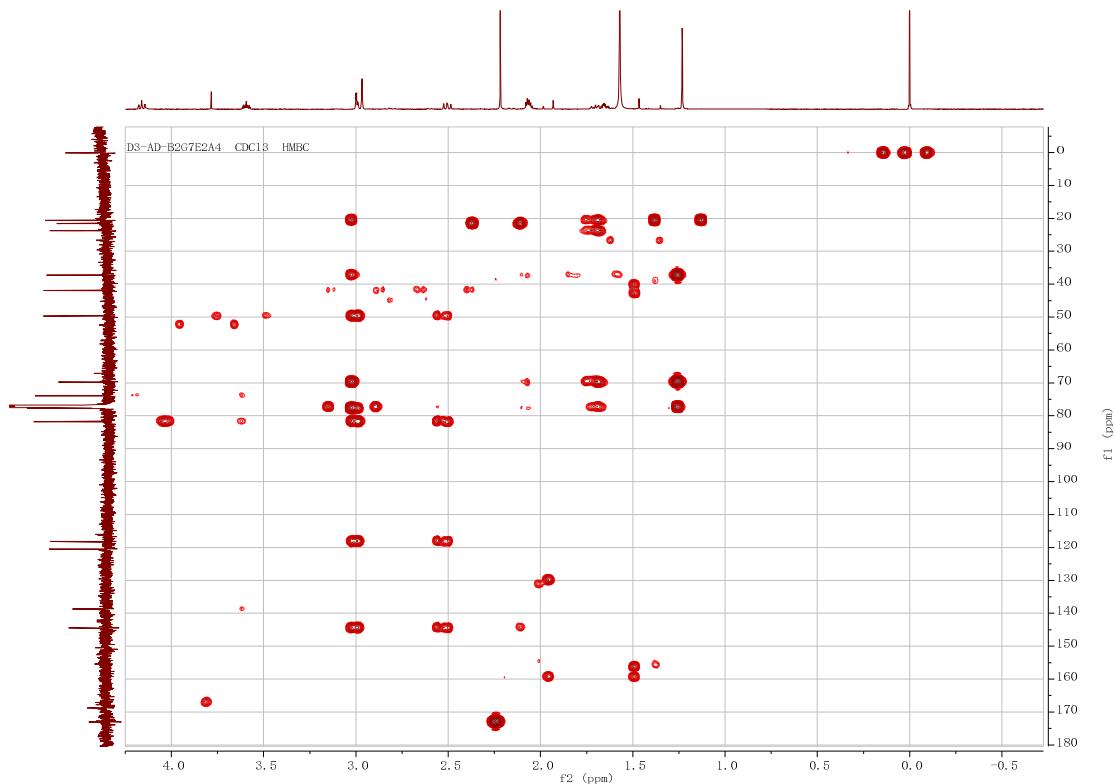


Figure S84 HMBC spectrum of compound 9

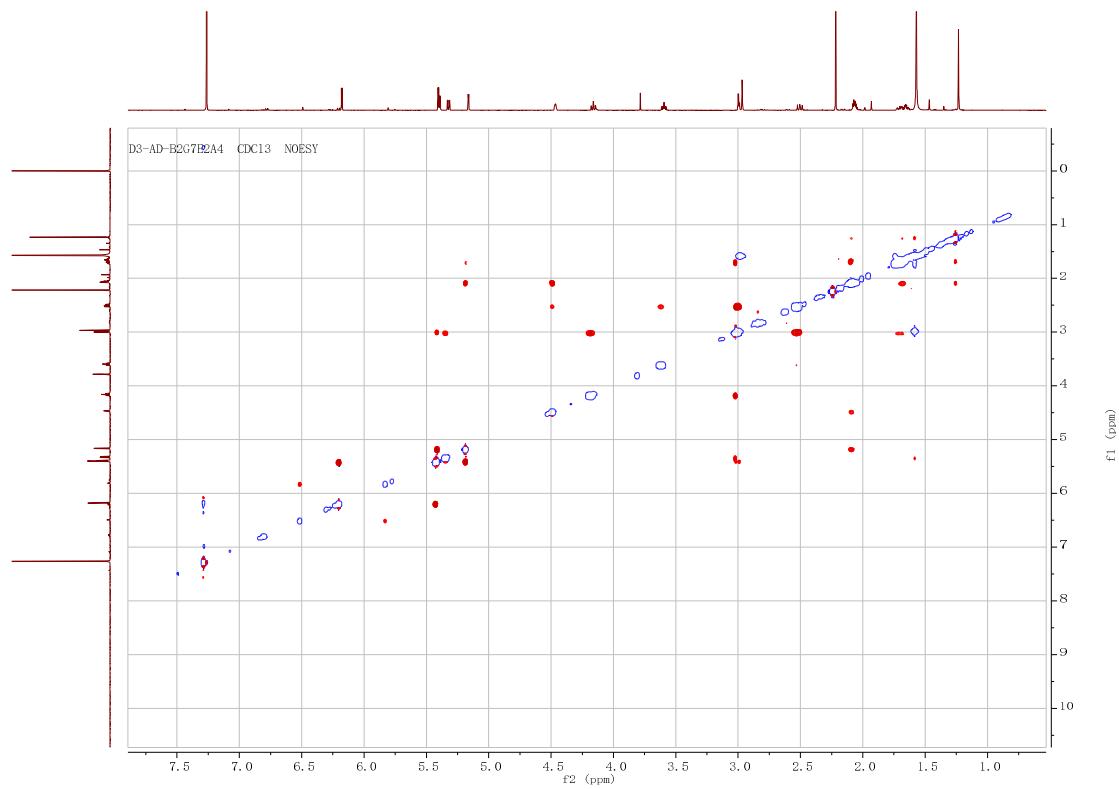


Figure S85 NOESY spectrum of compound **9**

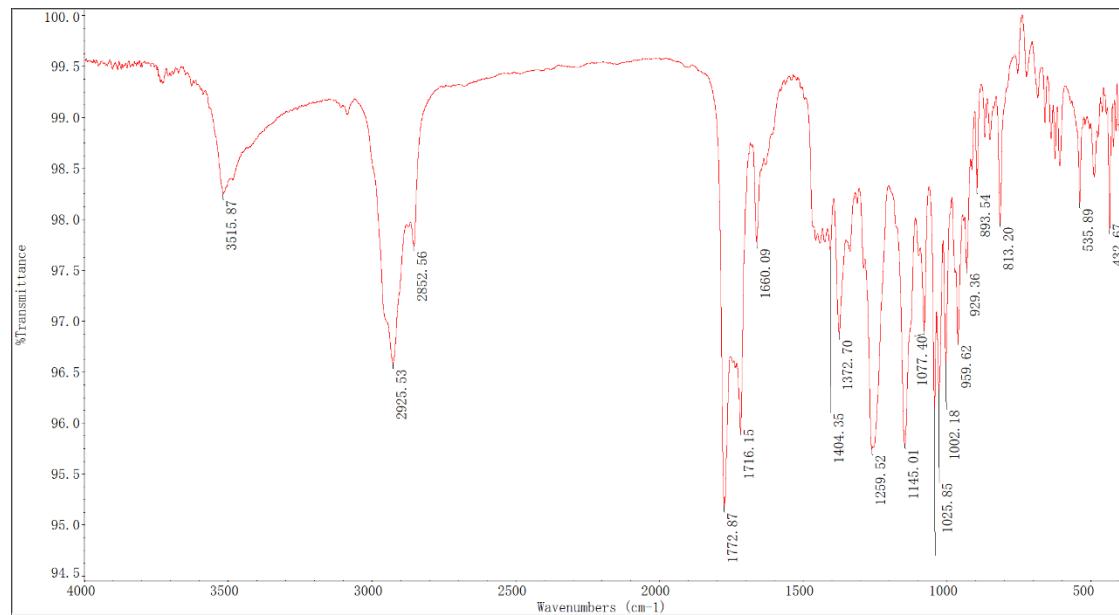


Figure S86 IR spectrum of compound **9**

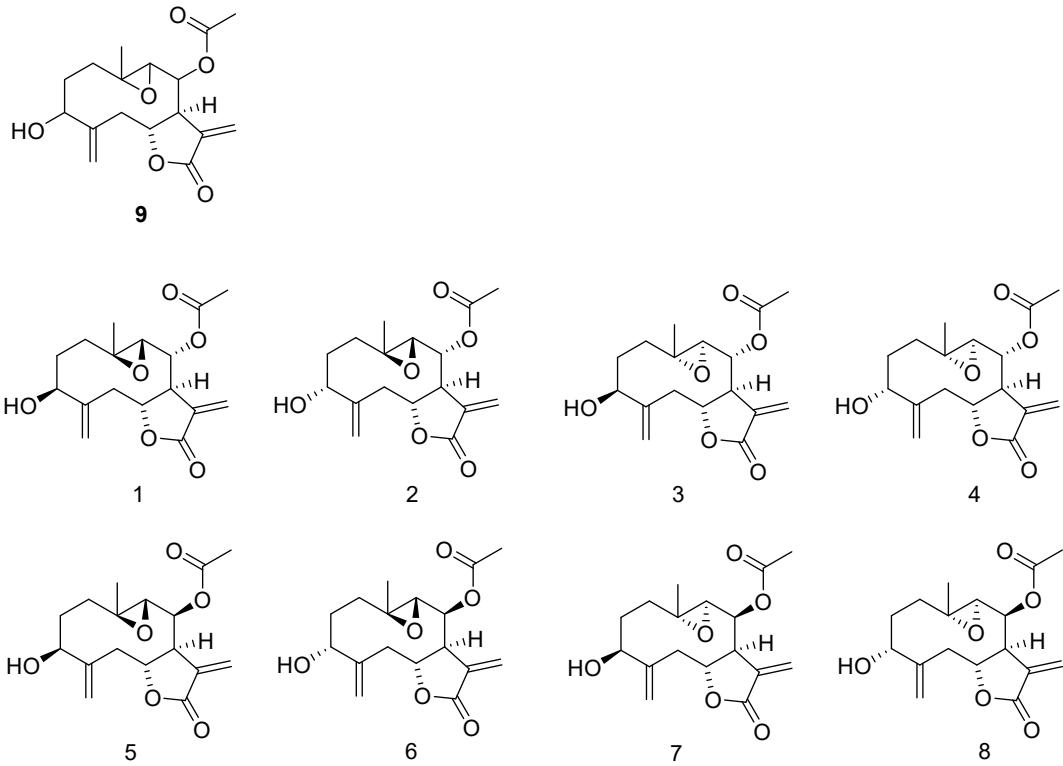


Figure S87 Possible isomers of compound 9

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