

Electronic Supplementary Information (ESI) for New Journal of Chemistry

**Dihydroagarofuran Sesquiterpenoid Derivatives from the
Leaves of *Tripterygium wilfordii* with potential
neuroprotective effects against H₂O₂-induced SH-SY5Y cell
injury**

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Shenyang 110016, People's Republic of China*

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Fig. S3.8 Most stable conformers of **3** in solvated model calculations at the B3LYP/6-311++G (2d, p) level in ECD calculation

Fig. S3.9 ¹H NMR spectrum (600 MHz, DMSO) of compound **3**

Fig. S3.10 ¹H-¹H COSY spectrum (600 MHz, DMSO) of compound **3**

Fig. S4.1 HRESIMS spectrum of compound **4**

Fig. S4.2 UV spectrum of compound **4**

Fig. S4.3 ¹H NMR spectrum (600 MHz, CDCl₃) of compound **4**

Fig. S4.4 ¹³C NMR spectrum (150 MHz, CDCl₃) of compound **4**

Fig. S4.5 HSQC spectrum (600 MHz, CDCl₃) of compound **4**

Fig. S4.6 HMBC spectrum (600 MHz, CDCl₃) of compound **4**

Fig. S4.7 NOESY spectrum (600 MHz, CDCl₃) of compound **4**.

Fig. S4.8 Most stable conformers of **4** in solvated model calculations at the B3LYP/6-311++G (2d, p) level in ECD calculation

Fig. S4.9 ¹H NMR spectrum (600 MHz, DMSO) of compound **4**

Fig. S4.10 ¹H-¹H COSY spectrum (600 MHz, DMSO) of compound **4**

Fig. S5.1 HRESIMS spectrum of compound **5**

Fig. S5.2 UV spectrum of compound **5**

Fig. S5.3 ¹H NMR spectrum (600 MHz, CDCl₃) of compound **5**

Fig. S5.4 ¹³C NMR spectrum (150 MHz, CDCl₃) of compound **5**

Fig. S5.5 HSQC spectrum (600 MHz, CDCl₃) of compound **5**

Fig. S5.6 HMBC spectrum (600 MHz, CDCl₃) of compound **5**

Fig. S5.7 NOESY spectrum (600 MHz, CDCl₃) of compound **5**

Fig. S5.8 Most stable conformers of **5** in solvated model calculations at the B3LYP/6-311++G (2d, p) level in ECD calculation

Fig. S5.9 ¹H NMR spectrum (600 MHz, DMSO) of compound **5**

Fig. S5.10 ¹H-¹H COSY spectrum (600 MHz, DMSO) of compound **5**

Fig. S6.1 HRESIMS spectrum of compound **6**

Fig. S6.2 UV spectrum of compound **6**

Fig. S6.3 ¹H NMR spectrum (600 MHz, CDCl₃) of compound **6**

Fig. S6.4 ^{13}C NMR spectrum (150 MHz, CDCl_3) of compound **6**

Fig. S6.5 HSQC spectrum (600 MHz, CDCl_3) of compound **6**

Fig. S6.6 HMBC spectrum (600 MHz, CDCl_3) of compound **6**

Fig. S6.7 NOESY spectrum (600 MHz, CDCl_3) of compound **6**

Fig. S6.8 Most stable conformers of **6** in solvated model calculations at the B3LYP/6-311++G (2d, p) level in ECD calculation

Fig. S6.9 ^1H NMR spectrum (600 MHz, DMSO) of compound **6**

Fig. S6.10 ^1H - ^1H COSY spectrum (600 MHz, DMSO) of compound **6**

Fig. S7.1 HRESIMS spectrum of compound **7**

Fig. S7.2 UV spectrum of compound **7**

Fig. S7.3 ^1H NMR spectrum (600 MHz, CDCl_3) of compound **7**

Fig. S7.4 ^{13}C NMR spectrum (150 MHz, CDCl_3) of compound **7**

Fig. S7.5 HSQC spectrum (600 MHz, CDCl_3) of compound **7**

Fig. S7.6 HMBC spectrum (600 MHz, CDCl_3) of compound **7**

Fig. S7.7 NOESY spectrum (600 MHz, CDCl_3) of compound **7**

Fig. S7.8 Most stable conformers of **7** in solvated model calculations at the B3LYP/6-311++G (2d, p) level in ECD calculation

Fig. S7.9 ^1H NMR spectrum (600 MHz, DMSO) of compound **7**

Fig. S7.10 ^1H - ^1H COSY spectrum (600 MHz, DMSO) of compound **7**

Fig. S8.1 HRESIMS spectrum of compound **8**

Fig. S8.2 UV spectrum of compound **8**

Fig. S8.3 ^1H NMR spectrum (600 MHz, CDCl_3) of compound **8**

Fig. S8.4 ^{13}C NMR spectrum (150 MHz, CDCl_3) of compound **8**

Fig. S8.5 HSQC spectrum (600 MHz, CDCl_3) of compound **8**

Fig. S8.6 HMBC spectrum (600 MHz, CDCl_3) of compound **8**

Fig. S8.7 NOESY spectrum (600 MHz, CDCl_3) of compound **8**

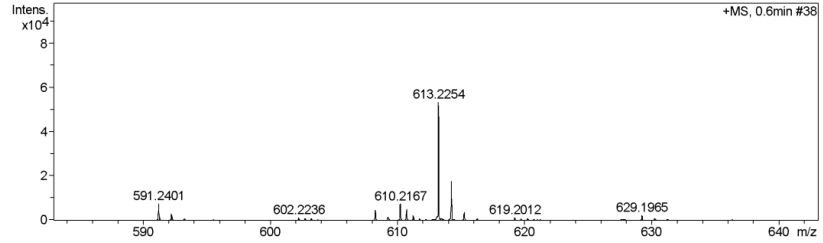
Fig. S8.8 Most stable conformers of **8** in solvated model calculations at the B3LYP/6-311++G (2d, p) level in ECD calculation

Fig. S8.9 ^1H NMR spectrum (600 MHz, DMSO) of compound **8**

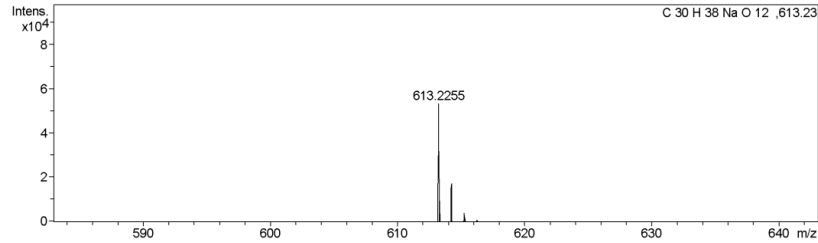
Fig. S8.10 ^1H - ^1H COSY spectrum (600 MHz, DMSO) of compound **8**

Analysis Info
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 Sample Name DLD-6
 Comment
 Acquisition Date 3/20/2019 1:08:35 PM
 Operator Bruker Customer
 Instrument / Ser# micrOTOF-Q 125

Acquisition Parameter
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 Scan End 3000 m/z Set Collision Cell RF 600.0 Vpp Set Divert Valve Waste



Meas. #	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e ⁻ Conf	mSigma	Std I	Std Mean	Std Var	Std No	Std m/z	Std Diff	Std Comb Dev
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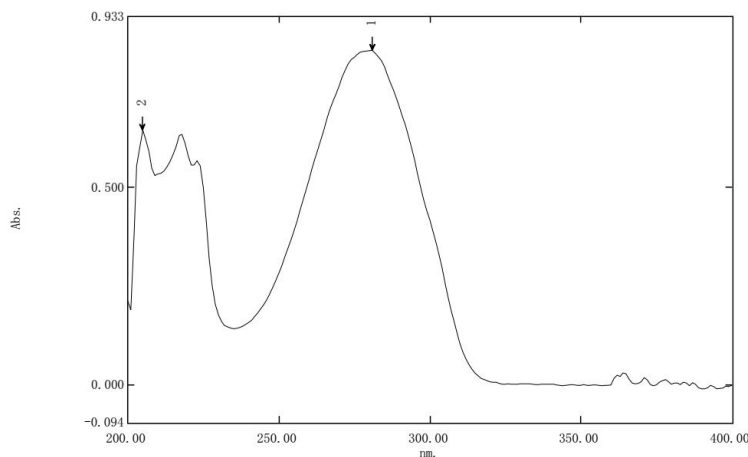
Meas. #	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e ⁻ Conf	mSigma	Std I	Std Mean	Std Var	Std No	Std m/z	Std Diff	Std Comb Dev
613.2255	C ₃₀ H ₃₈ NaO ₁₂	613.2255													

Fig. S1.1 HRESIMS spectrum of compound **1**

Spectrum Peak Pick Report

FIELD FIELD TEXT

Data Set: 没有



测定属性
 波长范围 (nm.): 200.00到400.00
 扫描速度: 中速
 采样间隔: 1.0
 自动采样间隔: 停用
 扫描模式: 单一的

No.	P/V	Wavelength	Abs.	描述
1	●	281.00	.847	
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3	●	235.00	.143	
4	●	209.00	.531	

Fig. S1.2 UV spectrum of compound **1**

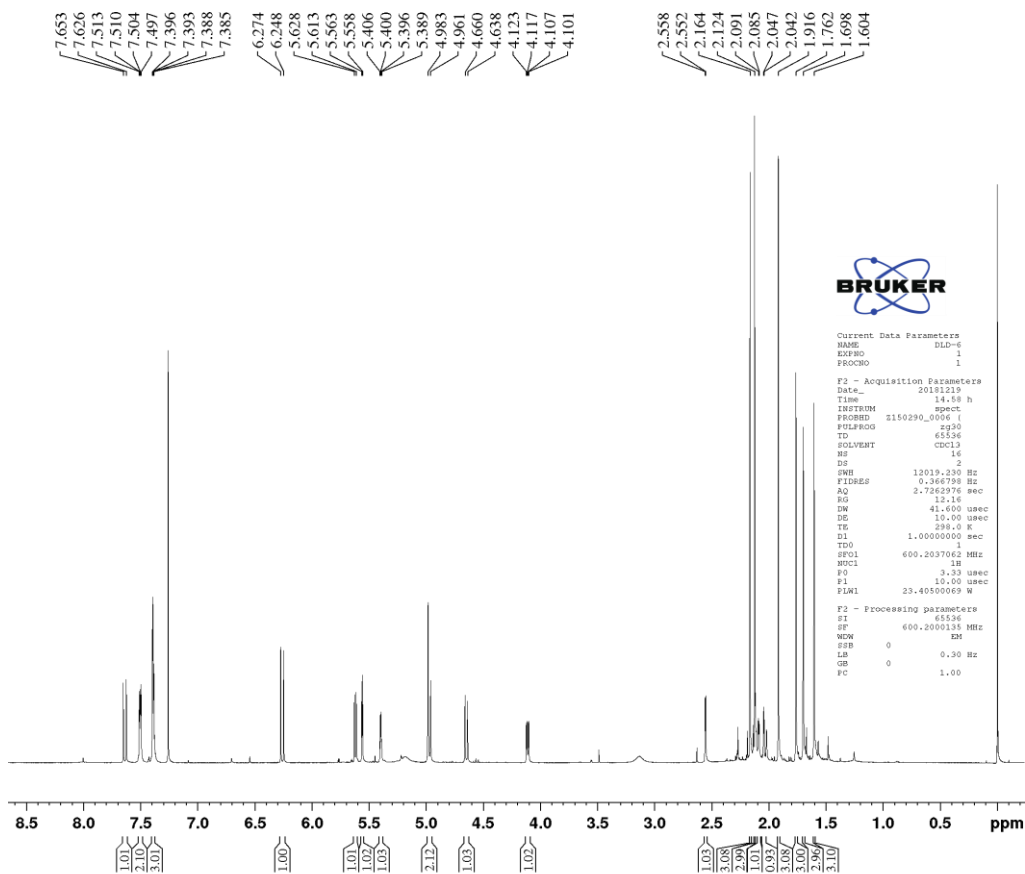


Fig. S1.3 ^1H NMR spectrum (600 MHz, CDCl_3) of compound 1

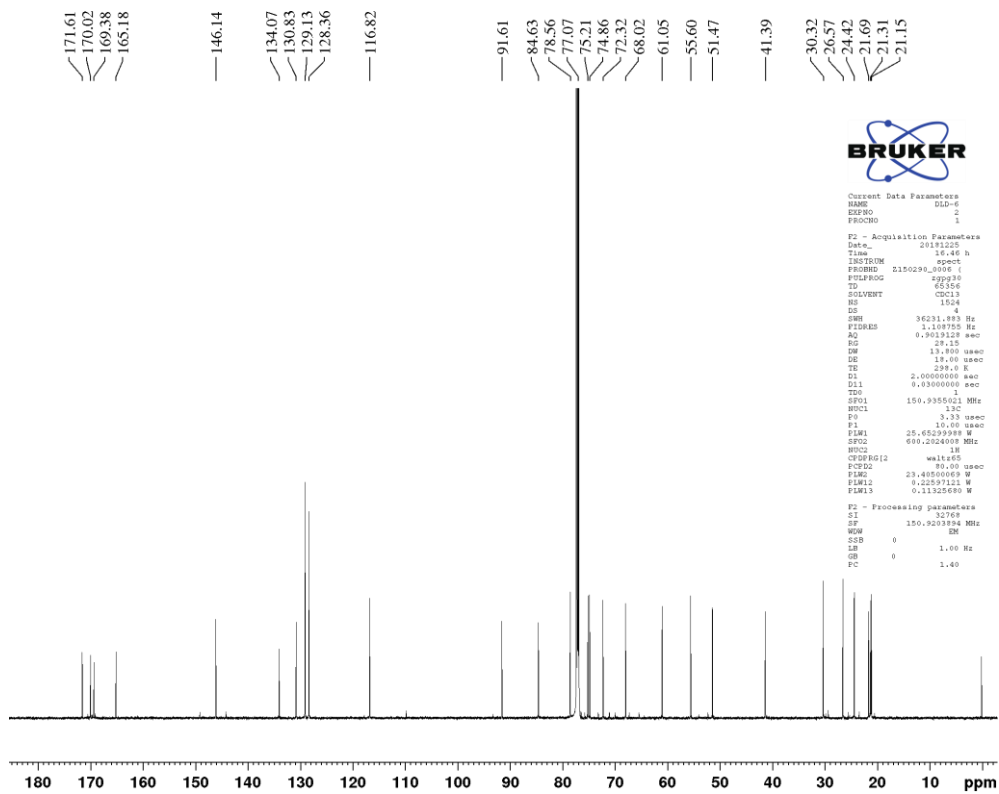


Fig. S1.4 ^{13}C NMR spectrum (150 MHz, CDCl_3) of compound 1

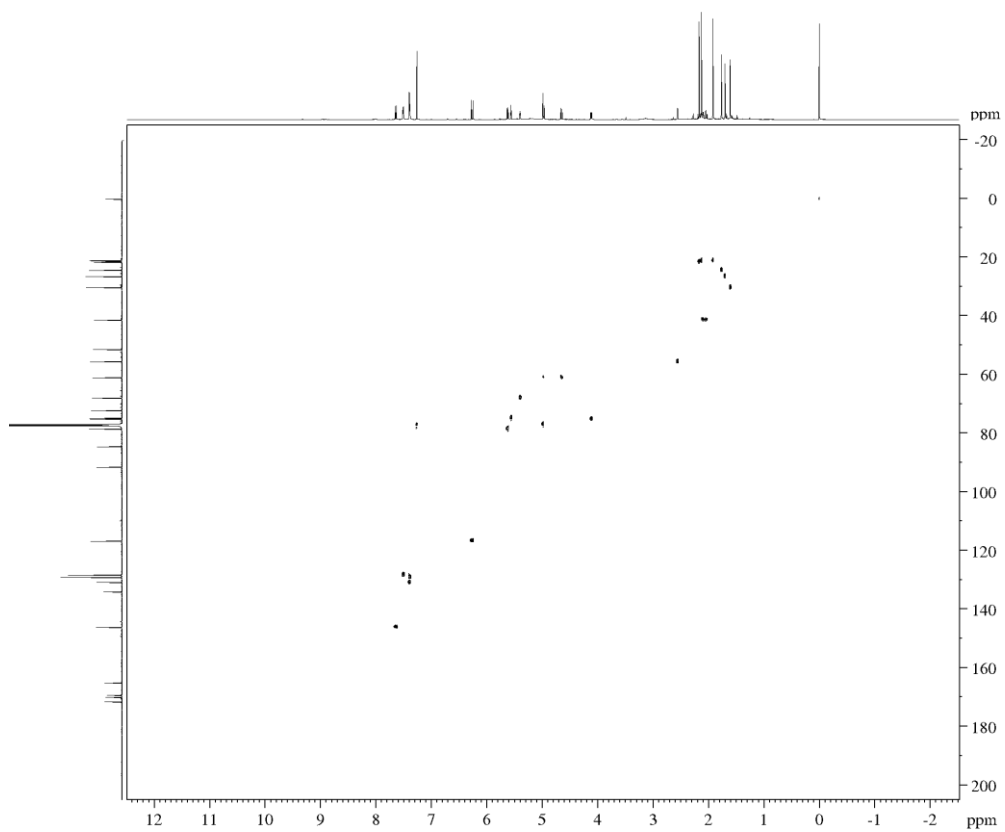


Fig. S1.5 HSQC spectrum (600 MHz, CDCl₃) of compound **1**

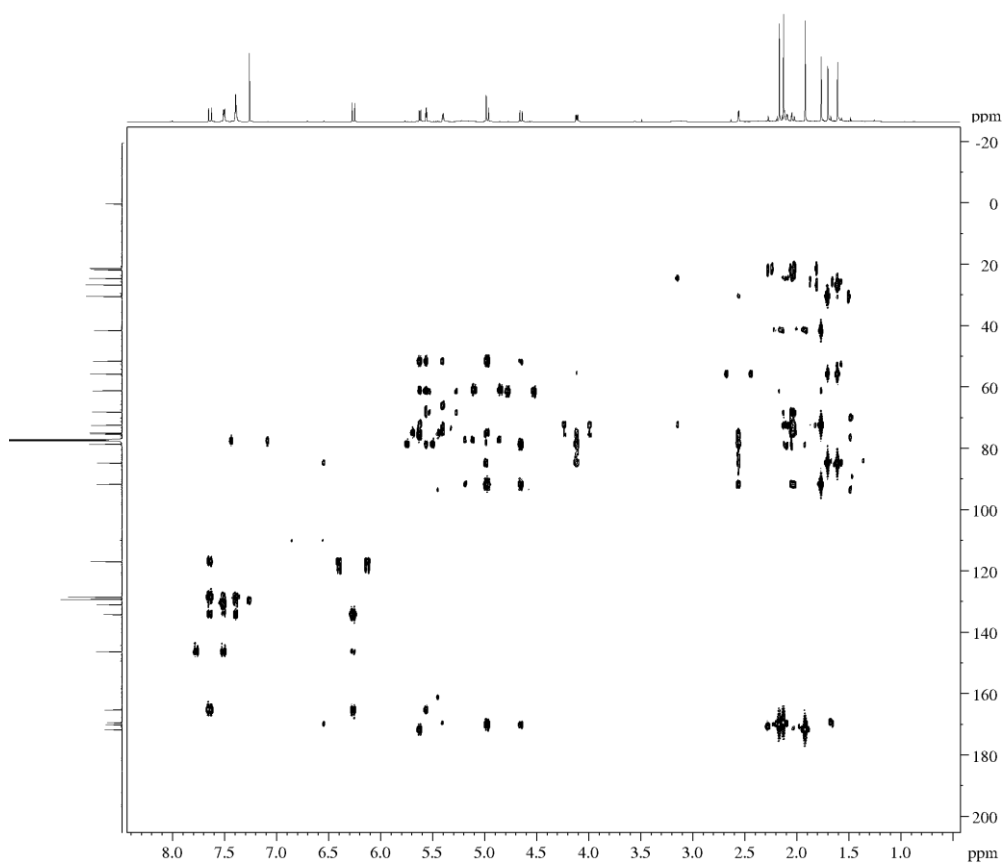


Fig. S1.6 HMBC spectrum (600 MHz, CDCl₃) of compound **1**

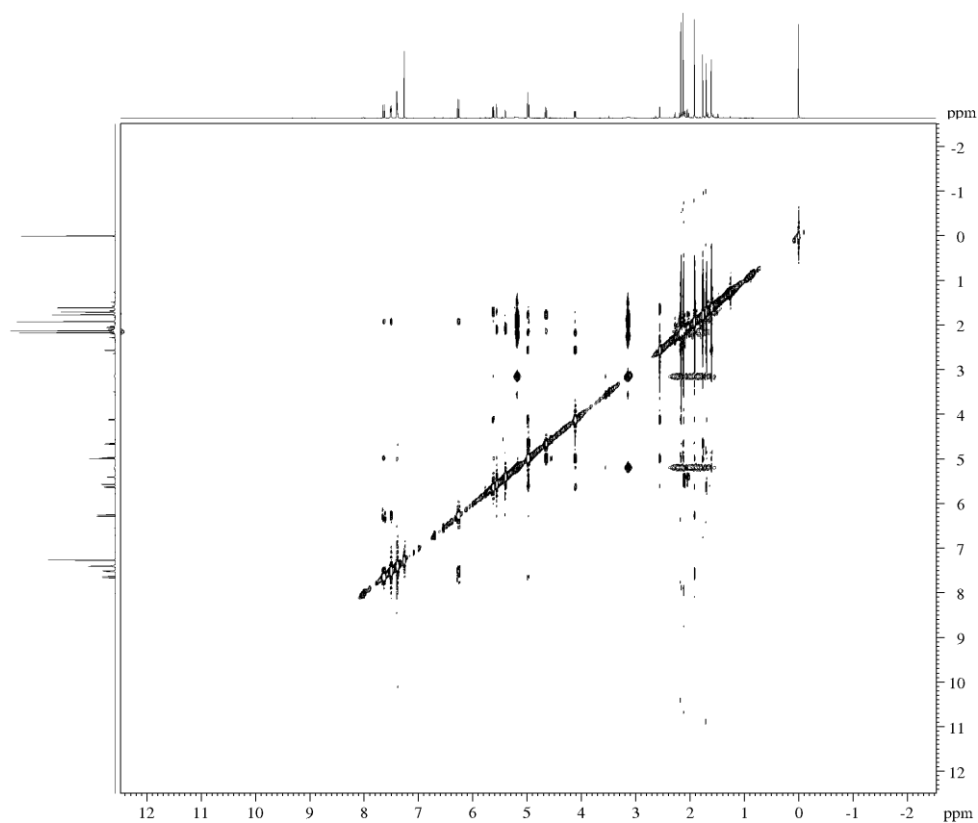


Fig. S1.7 NOESY spectrum (600 MHz, CDCl_3) of compound **1**

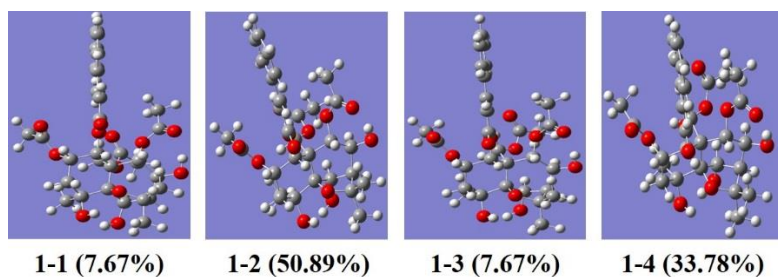


Fig. S1.8 Most stable conformers of **1** in solvated model calculations at the B3LYP/6-311++G (2d, p) level in ECD calculation

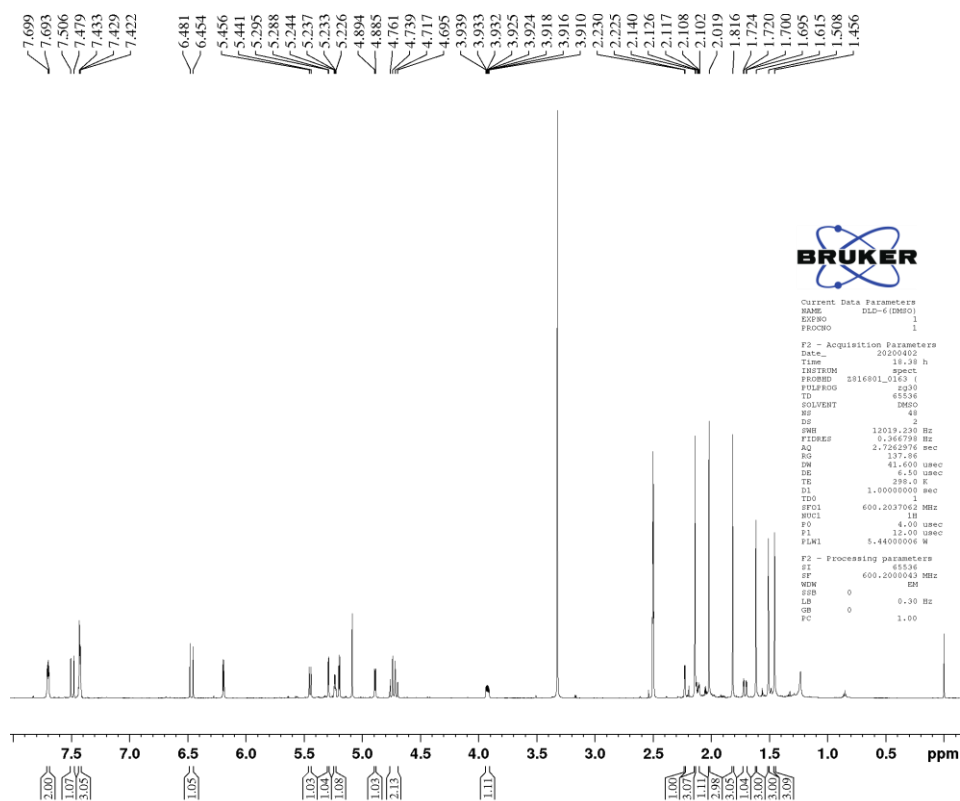


Fig. S1.9 ^1H NMR spectrum (600 MHz, DMSO) of compound 1

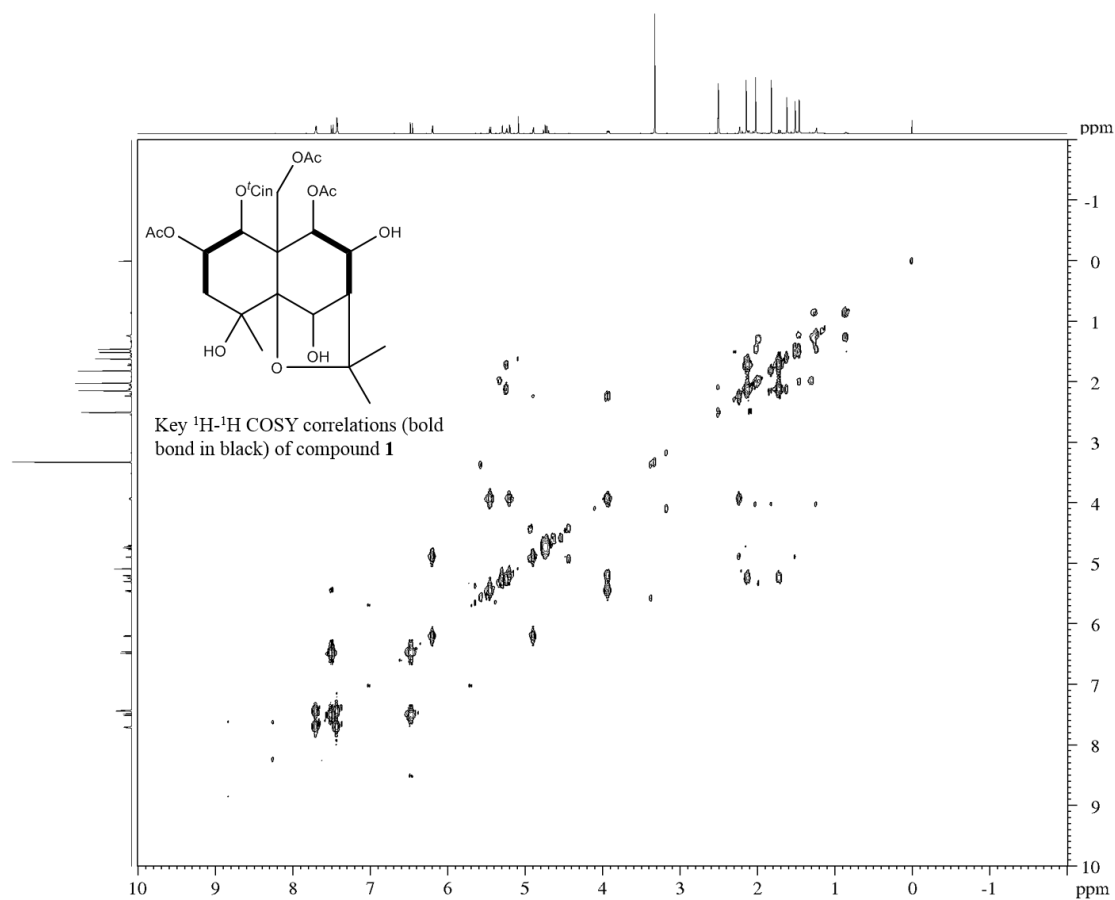
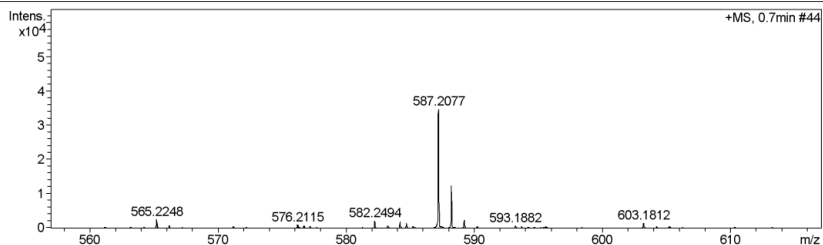


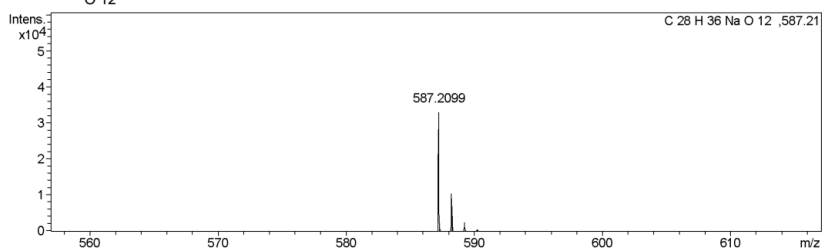
Fig. S1.10 ^1H - ^1H COSY spectrum (600 MHz, DMSO) of compound 1

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 Method 20180614yezhi.m Operator Bruker Customer
 Sample Name DLD-1 Instrument / Ser# microTOF-Q 125
 Comment

Acquisition Parameter
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 Scan Begin 50 m/z Set End Plate Offset -500 V Set Dry Gas 4.0 l/min
 Scan End 3000 m/z Set Collision Cell RF 600.0 Vpp Set Divert Valve Waste



Meas. #	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e ⁻ Conf	mSigma	Std I	Std Mean m/z	Std I VarNo	Std m/z Diff	Std Comb Dev
587.2077	1 C ₂₈ H ₃₆ NaO ₁₂	587.2099	3.8	4.8	10.5	ok	even	22.18	0.0323	0.0030	0.0106	0.0025	0.8427



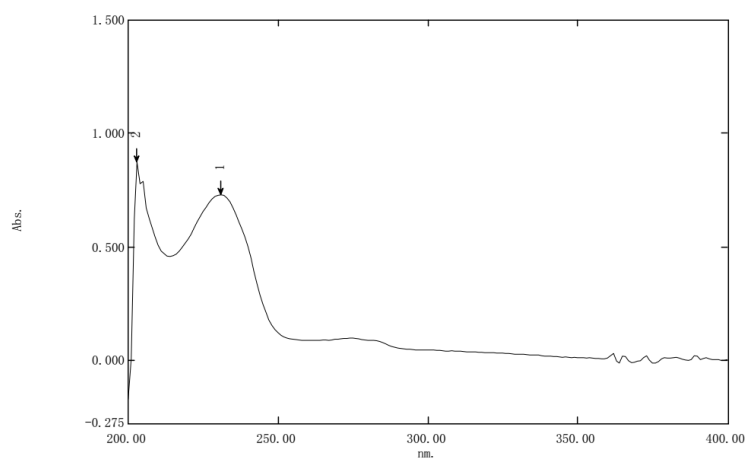
Meas. #	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e ⁻ Conf	mSigma	Std I	Std Mean m/z	Std I VarNo	Std m/z Diff	Std Comb Dev
587.2099	C ₂₈ H ₃₆ NaO ₁₂	587.2099											

Fig. S2.1 HRESIMS spectrum of compound 2

Spectrum Peak Pick Report

FIELD FIELD TEXT

Data Set: 没有



测定属性
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 扫描速度: 中速
 采样间隔: 1.0
 自动采样间隔: 停用
 扫描模式: 单一的

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Fig. S2.2 UV spectrum of compound 2

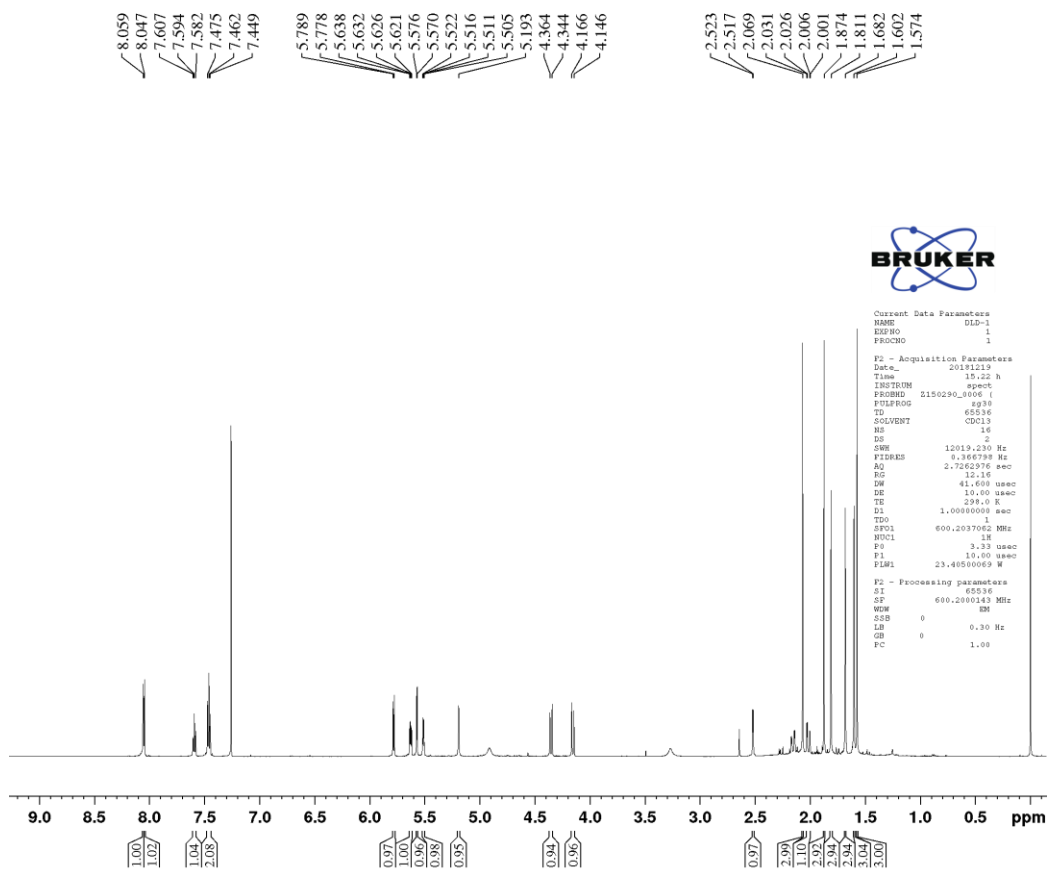


Fig. S2.3 ^1H NMR spectrum (600 MHz, CDCl_3) of compound 2

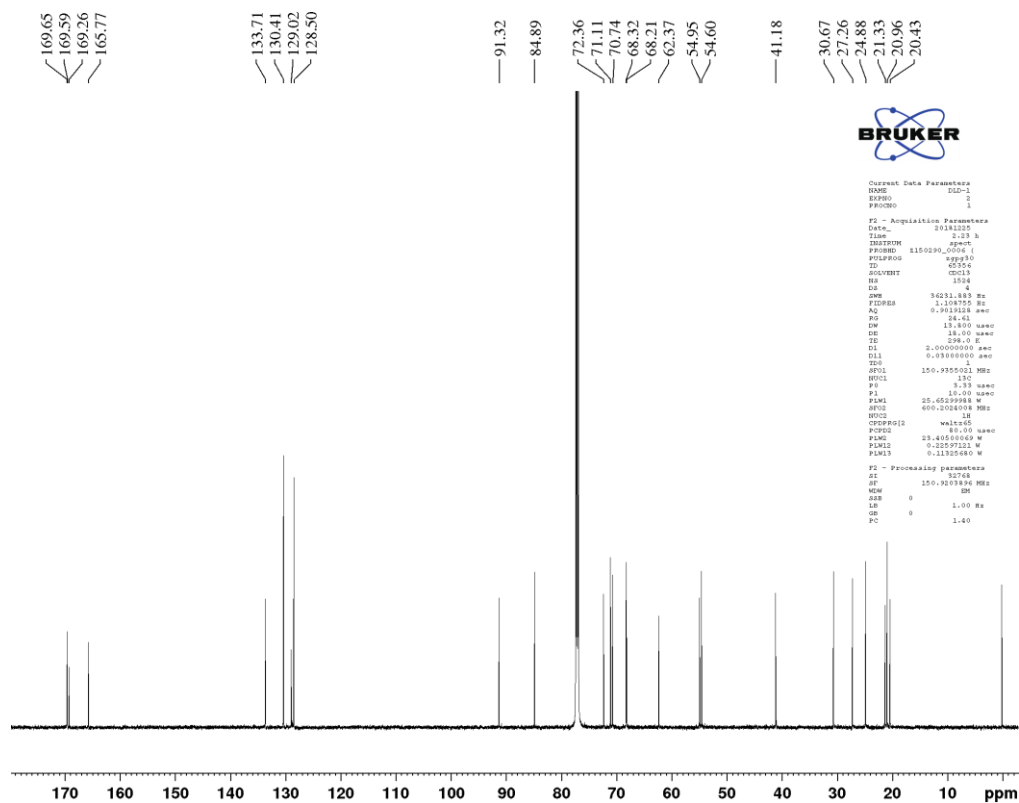


Fig. S2.4 ^{13}C NMR spectrum (150 MHz, CDCl_3) of compound 2

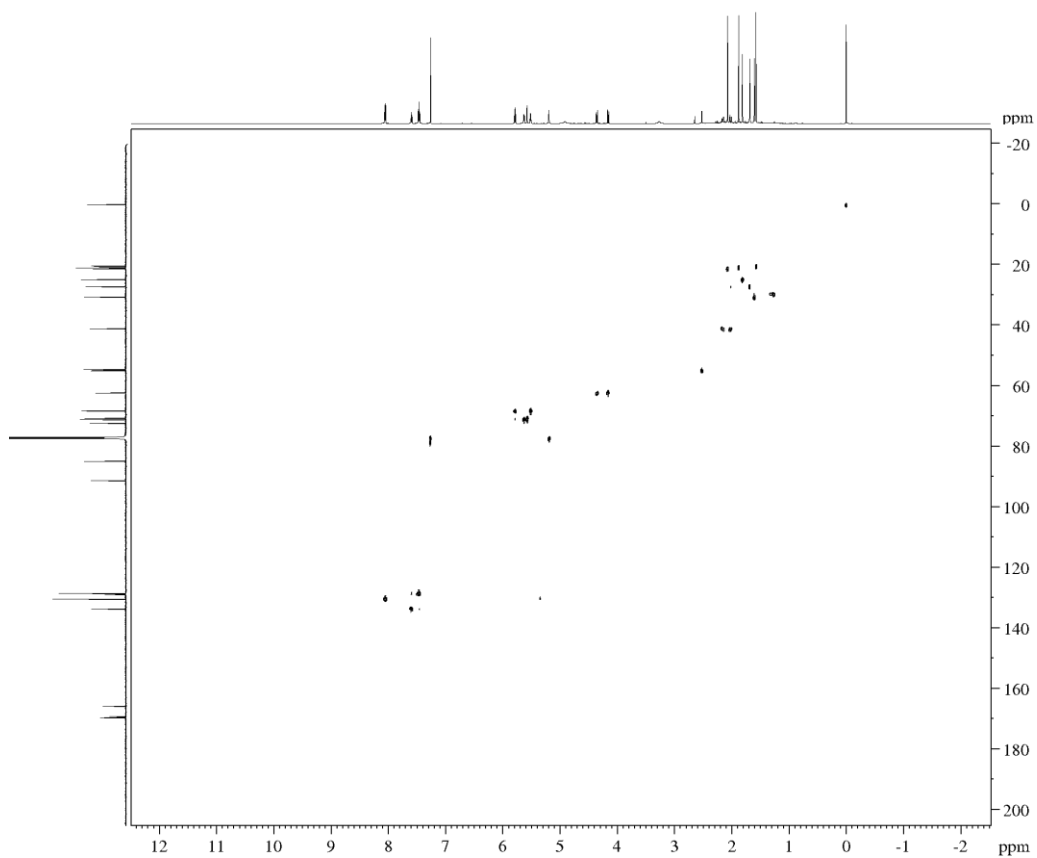


Fig. S2.5 HSQC spectrum (600 MHz, CDCl₃) of compound **2**

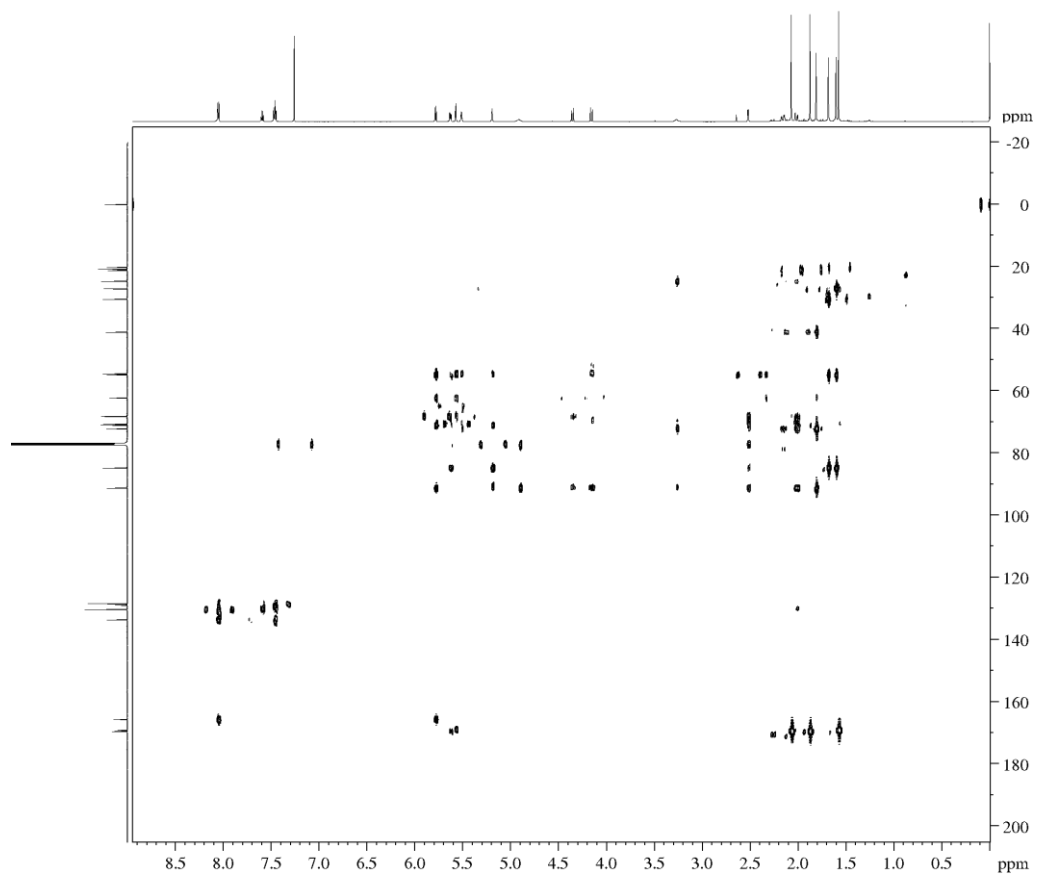


Fig. S2.6 HMBC spectrum (600 MHz, CDCl₃) of compound **2**

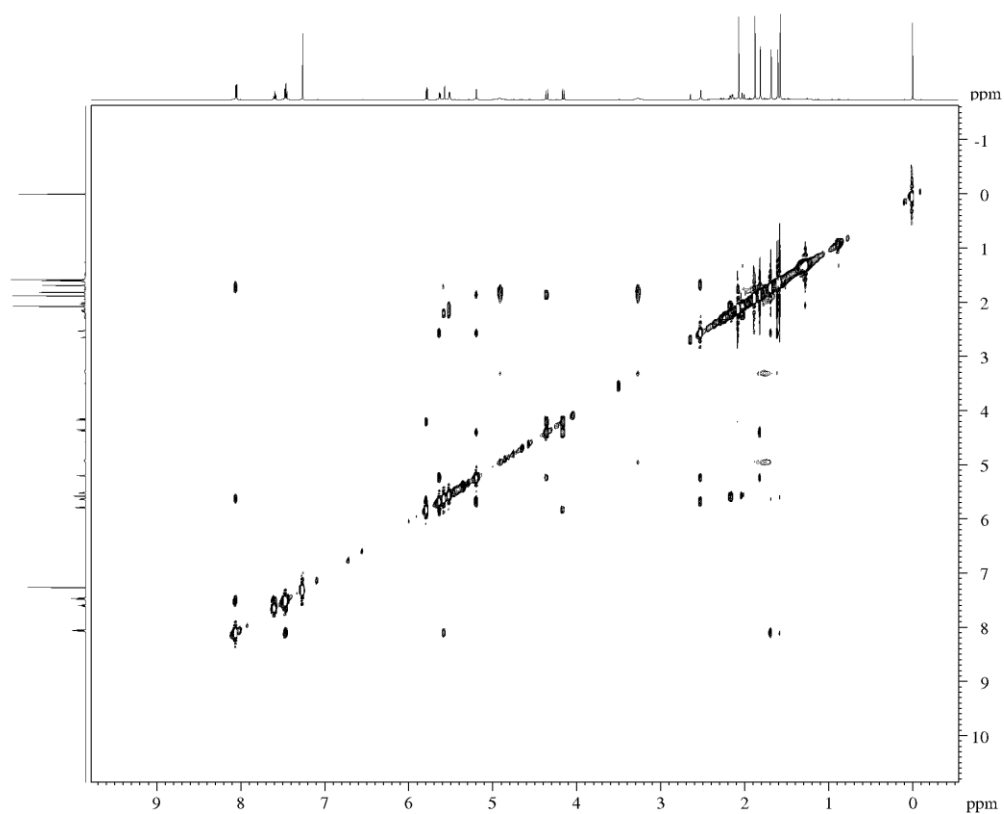


Fig. S2.7 NOESY spectrum (600 MHz, CDCl_3) of compound **2**

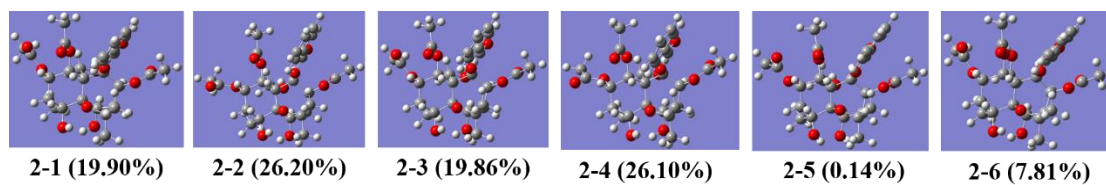


Fig. S2.8 Most stable conformers of **2** in solvated model calculations at the B3LYP/6-311++G (2d, p) level in ECD calculation

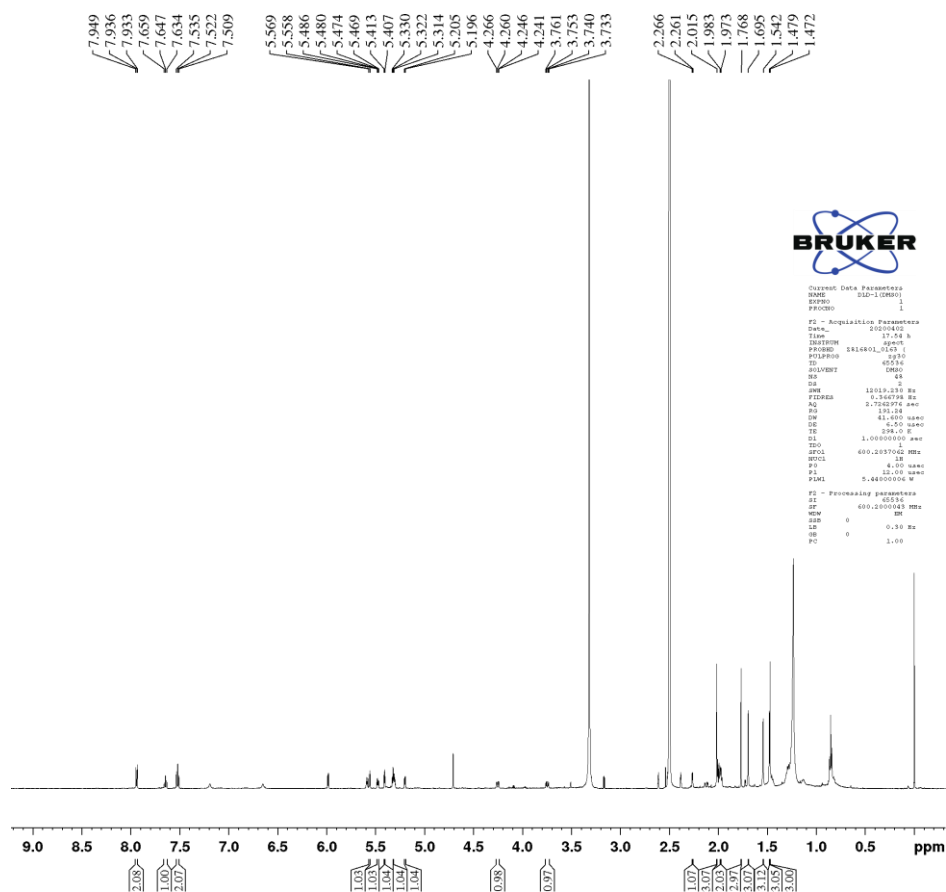


Fig. S2.9 ^1H NMR spectrum (600 MHz, DMSO) of compound **2**

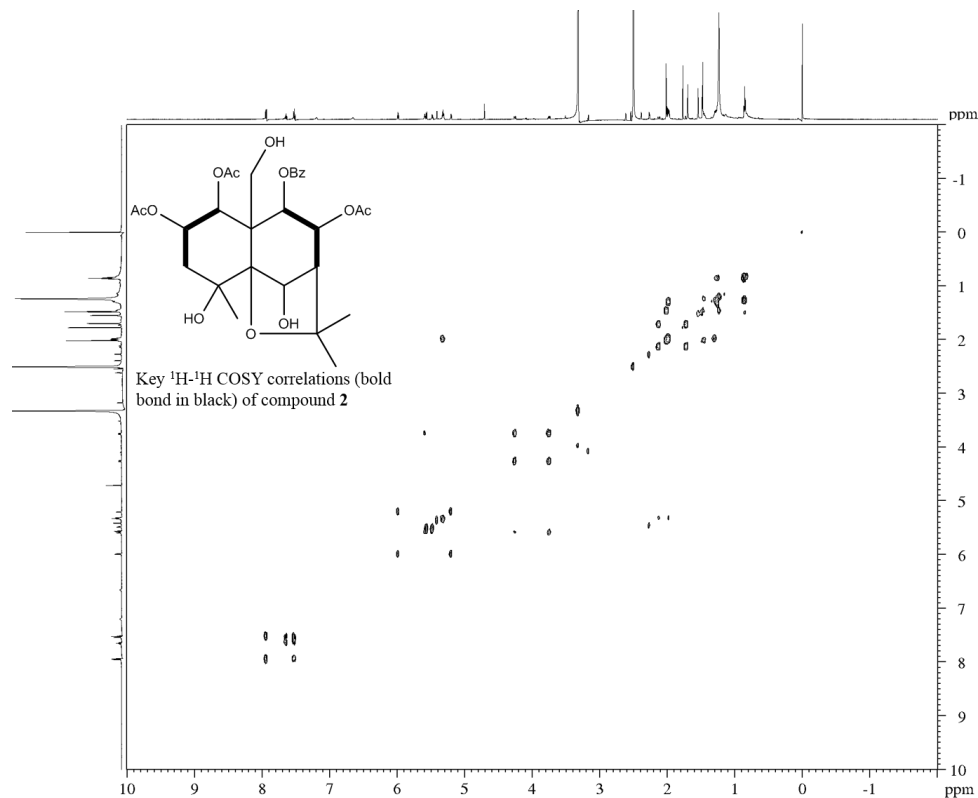


Fig. S2.10 ^1H - ^1H COSY spectrum (600 MHz, DMSO) of compound **2**

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 Acquisition Date: 3/21/2019 4:25:07 PM
 Operator: Bruker Customer
 Instrument / Ser#: micrOTOF-Q 125

Acquisition Parameter
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 Scan End: 1500 m/z
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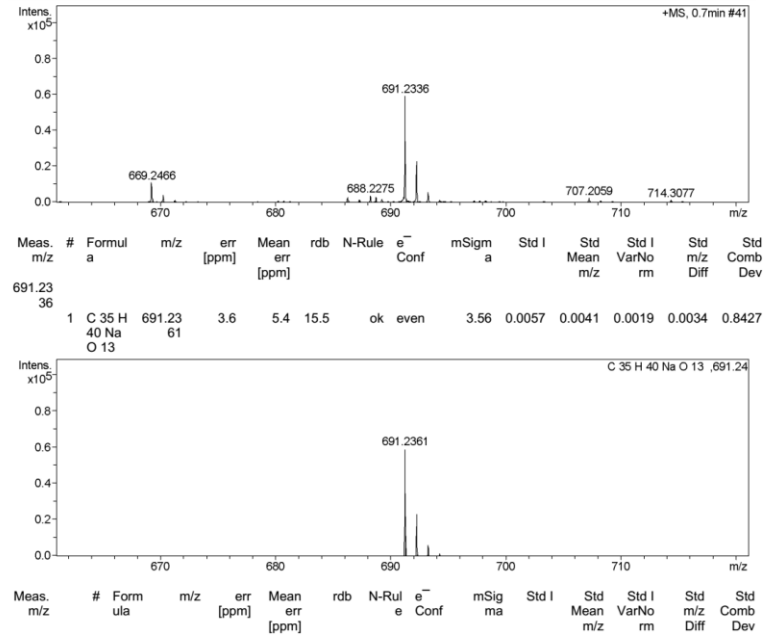
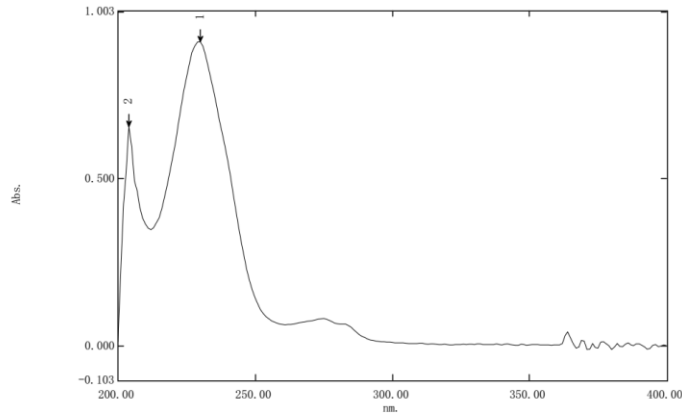


Fig. S3.1 HRESIMS spectrum of compound **3**

Spectrum Peak Pick Report

FIELD FIELD TEXT

Data Set: 没有



测定属性
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 扫描速度: 中速
 采样间隔: 1.0
 自动采样间隔: 停用
 扫描模式: 单一的

No.	P/V	Wavelength	Abs.	描述
1	●	230.00	.911	
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3	●	261.00	.064	
4	●	212.00	.349	

Fig. S3.2 UV spectrum of compound **3**

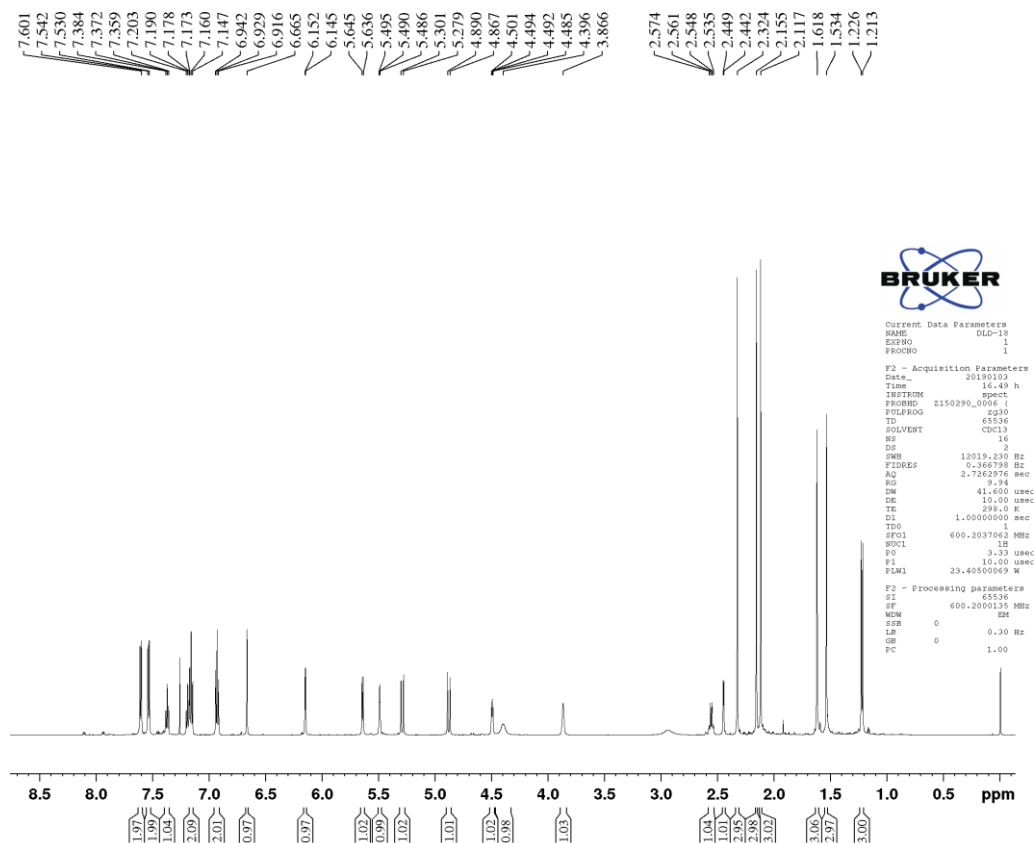


Fig. S3.3 ^1H NMR spectrum (600 MHz, CDCl_3) of compound **3**

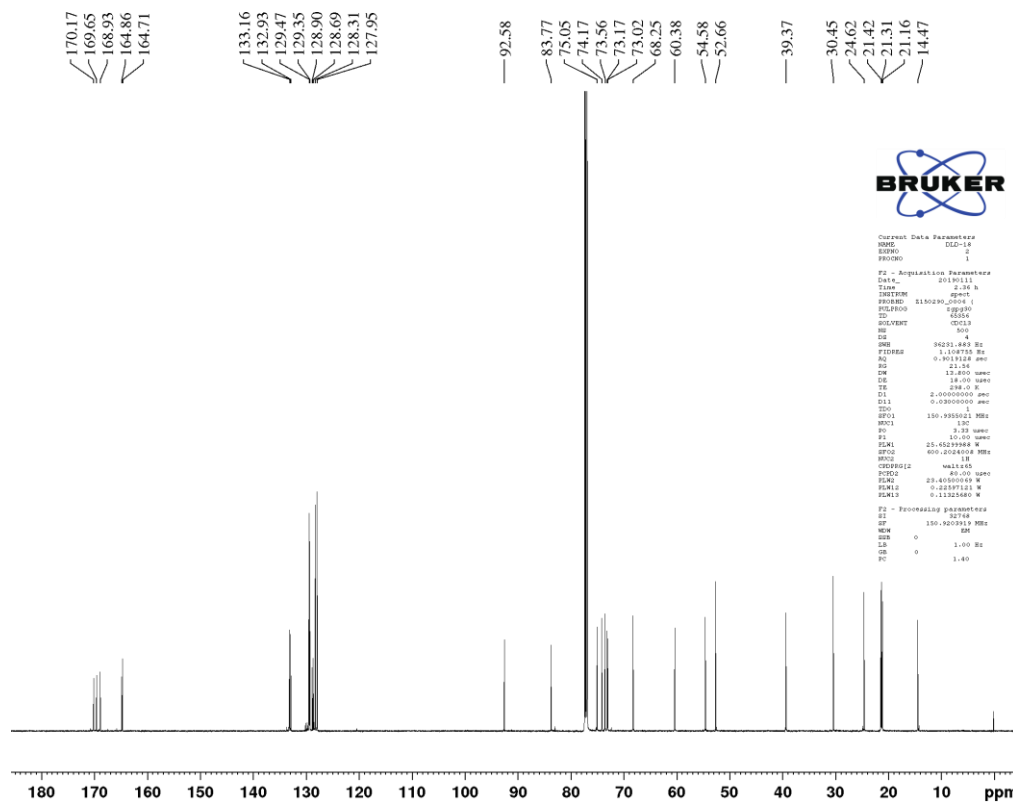


Fig. S3.4 ^{13}C NMR spectrum (150 MHz, CDCl_3) of compound **3**

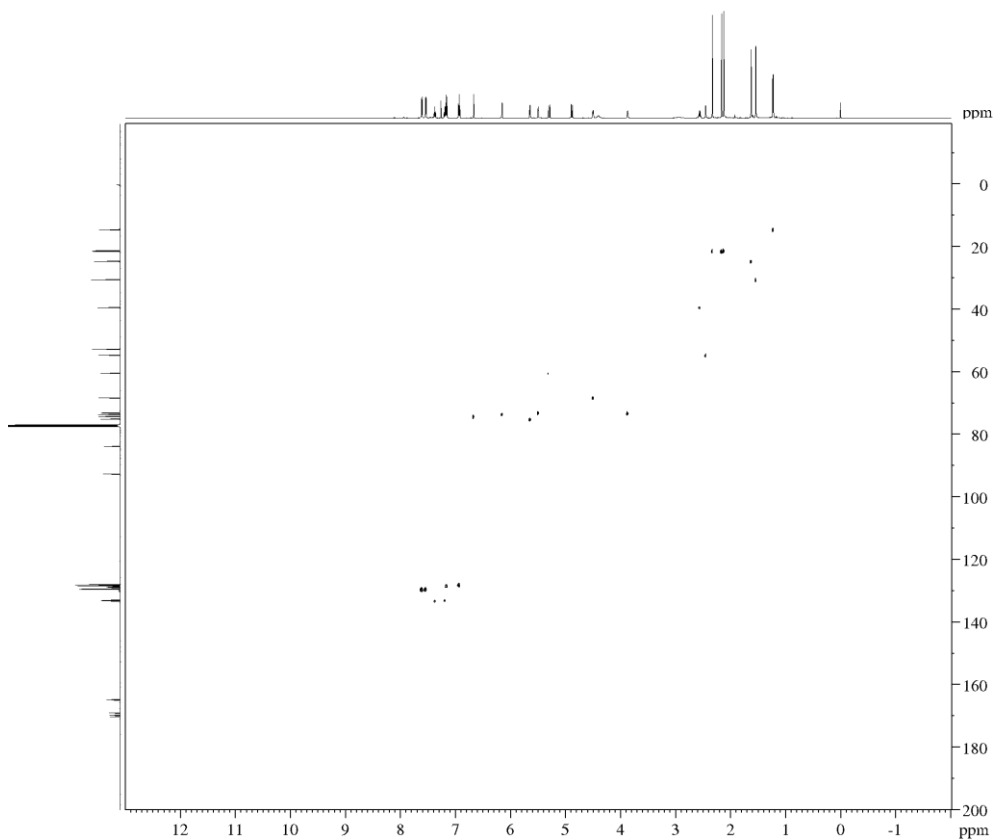


Fig. S3.5 HSQC spectrum (600 MHz, CDCl₃) of compound **3**

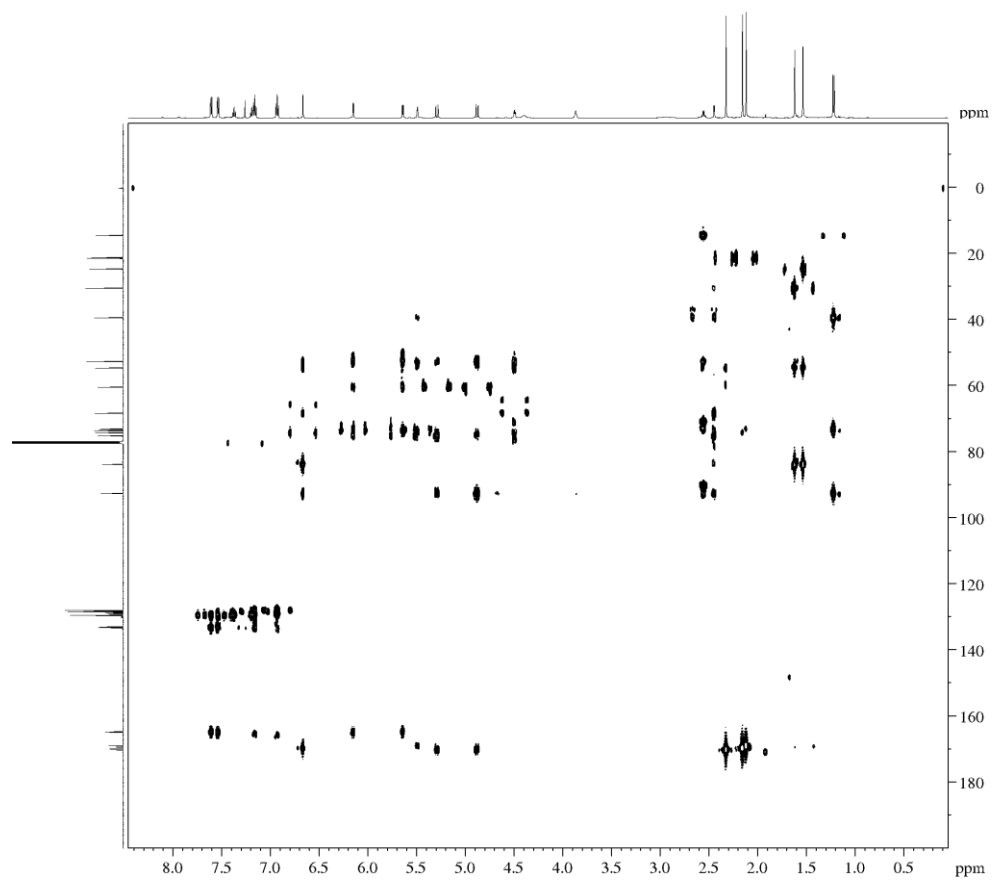


Fig. S3.6 HMBC spectrum (600 MHz, CDCl₃) of compound **3**

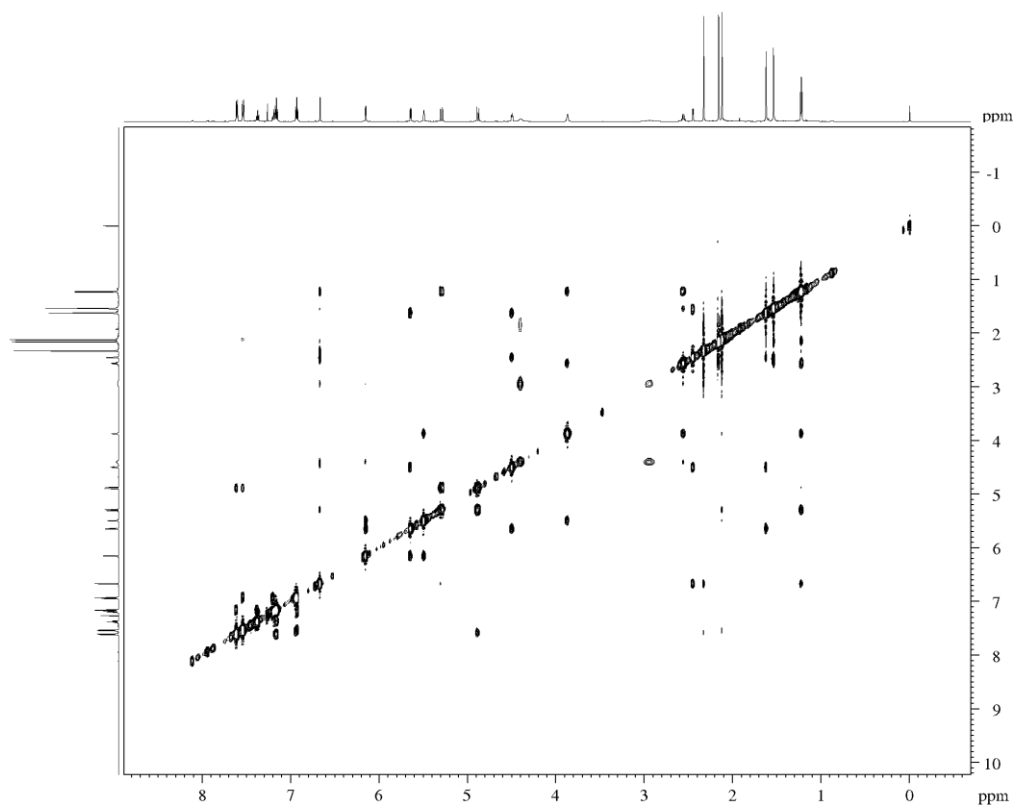


Fig. S3.7 NOESY spectrum (600 MHz, CDCl_3) of compound **3**

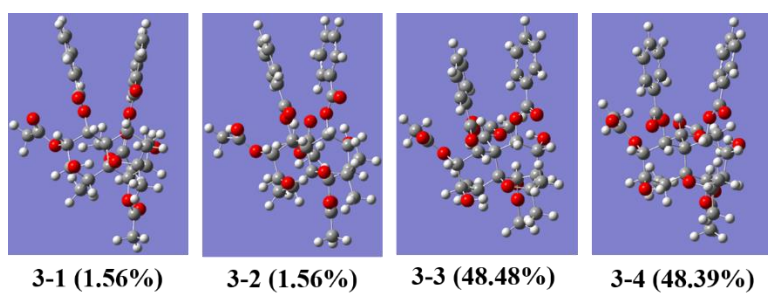


Fig. S3.8 Most stable conformers of **3** in solvated model calculations at the B3LYP/6-311++G (2d, p) level in ECD calculation

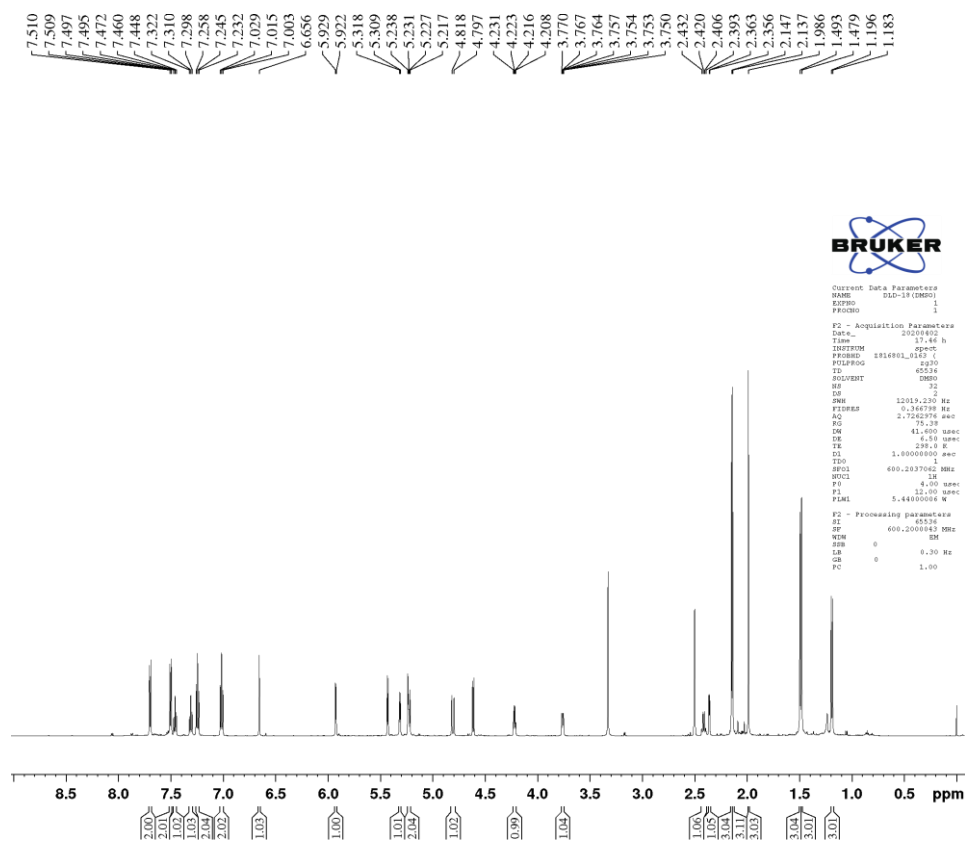


Fig. S3.9 ^1H NMR spectrum (600 MHz, DMSO) of compound 3

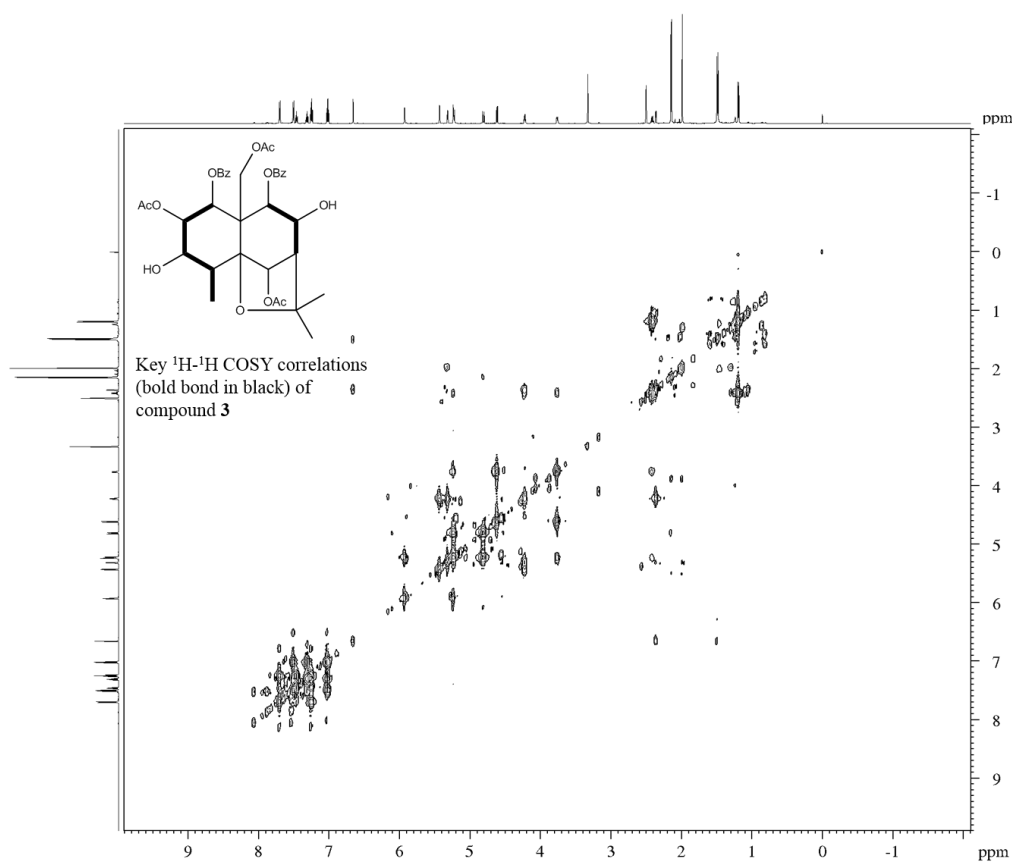


Fig. S3.10 ^1H - ^1H COSY spectrum (600 MHz, DMSO) of compound 3

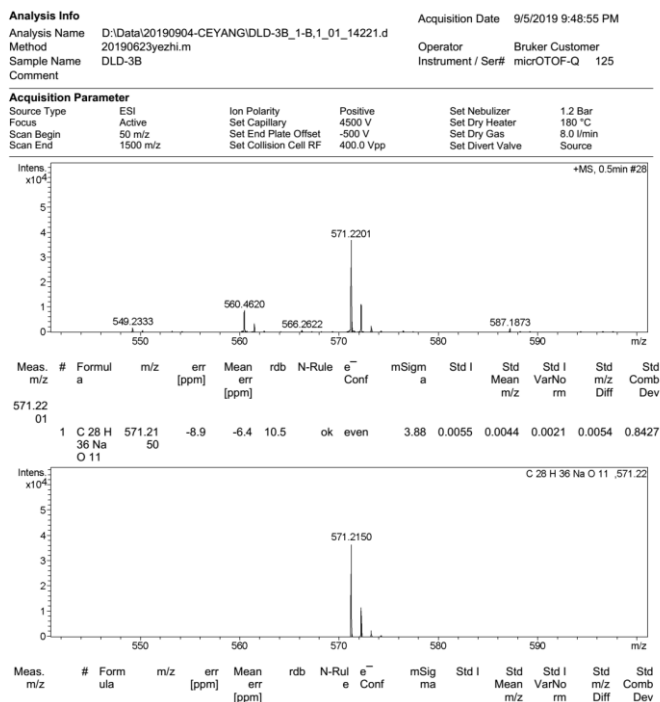
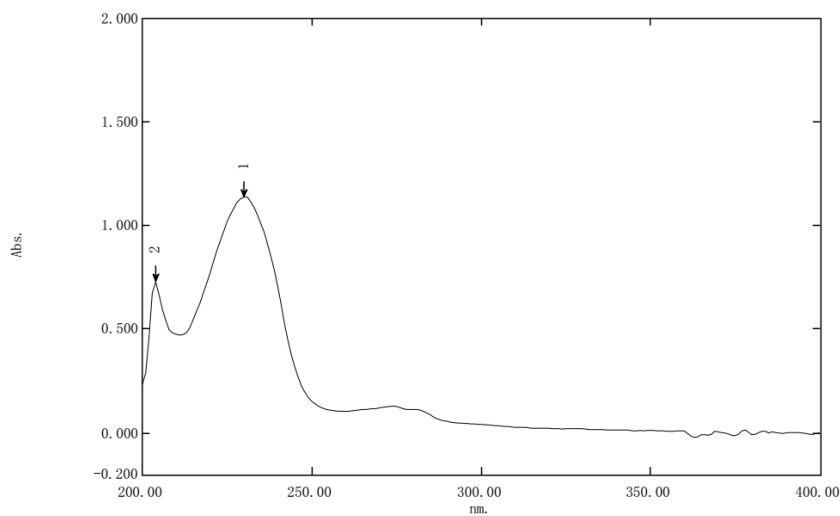


Fig. S4.1 HRESIMS spectrum of compound 4
Spectrum Peak Pick Report

FIELD FIELD TEXT

Data Set: 没有



测定属性
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 扫描速度: 中速
 采样间隔: 1.0
 自动采样间隔: 停用
 扫描模式: 单一的

No.	P/V	Wavelength	Abs.	描述
1	●	230.00	1.139	
2	●	204.00	.729	
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Fig. S4.2 UV spectrum of compound 4

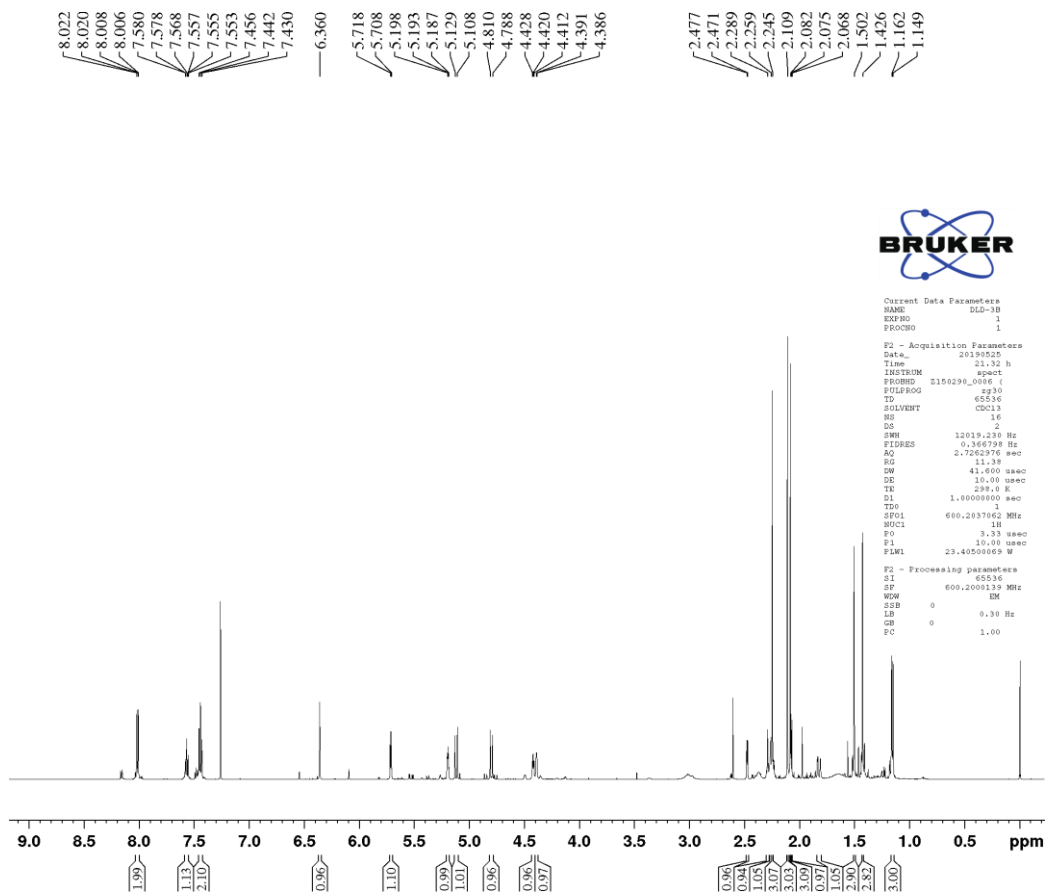


Fig. S4.3 ¹H NMR spectrum (600 MHz, CDCl₃) of compound 4

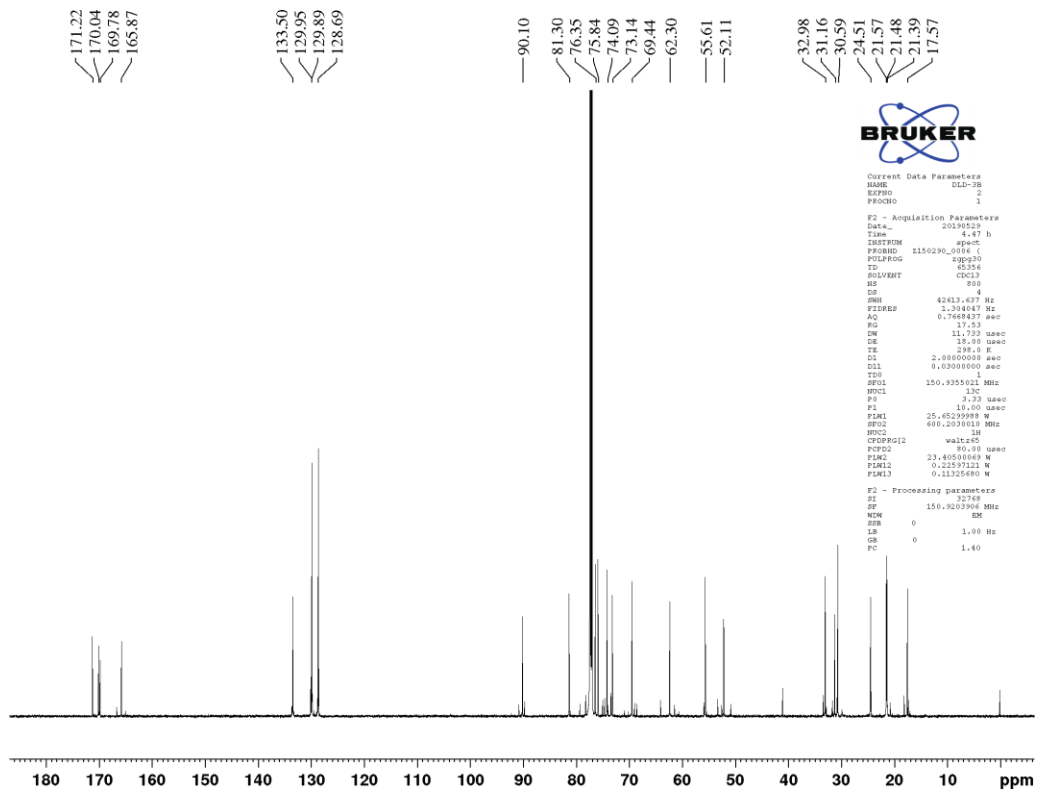


Fig. S4.4 ¹³C NMR spectrum (150 MHz, CDCl₃) of compound 4

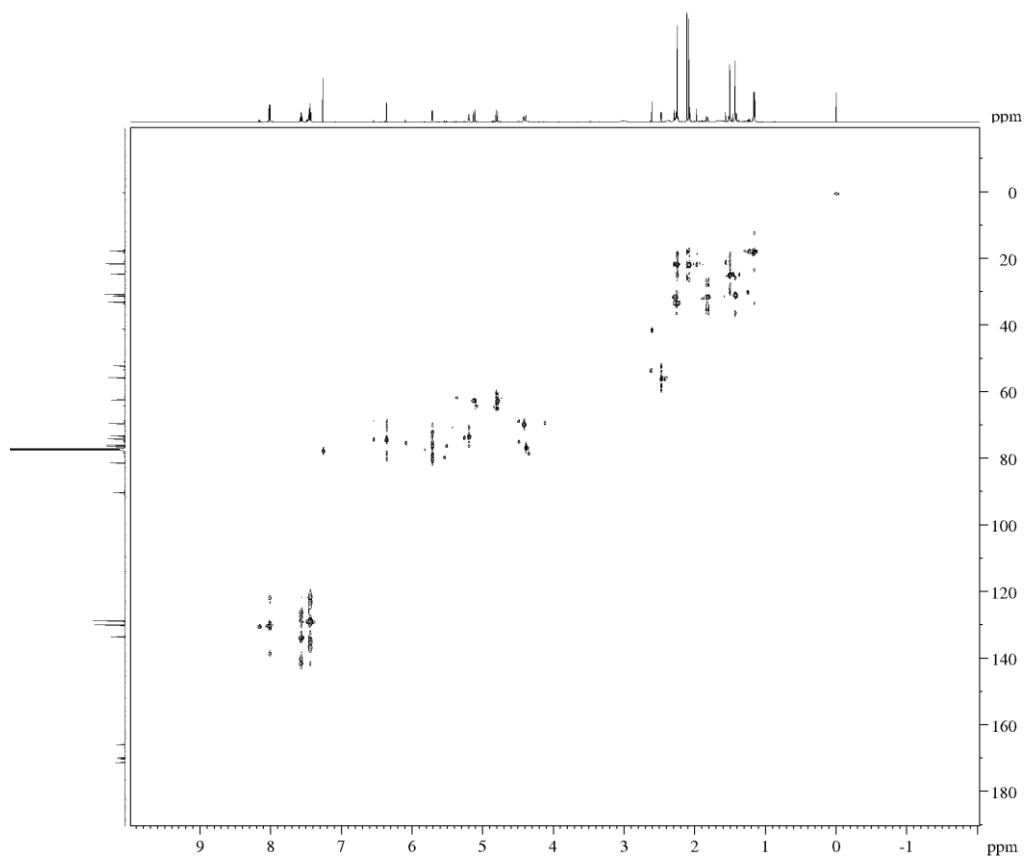


Fig. S4.5 HSQC spectrum (600 MHz, CDCl₃) of compound **4**

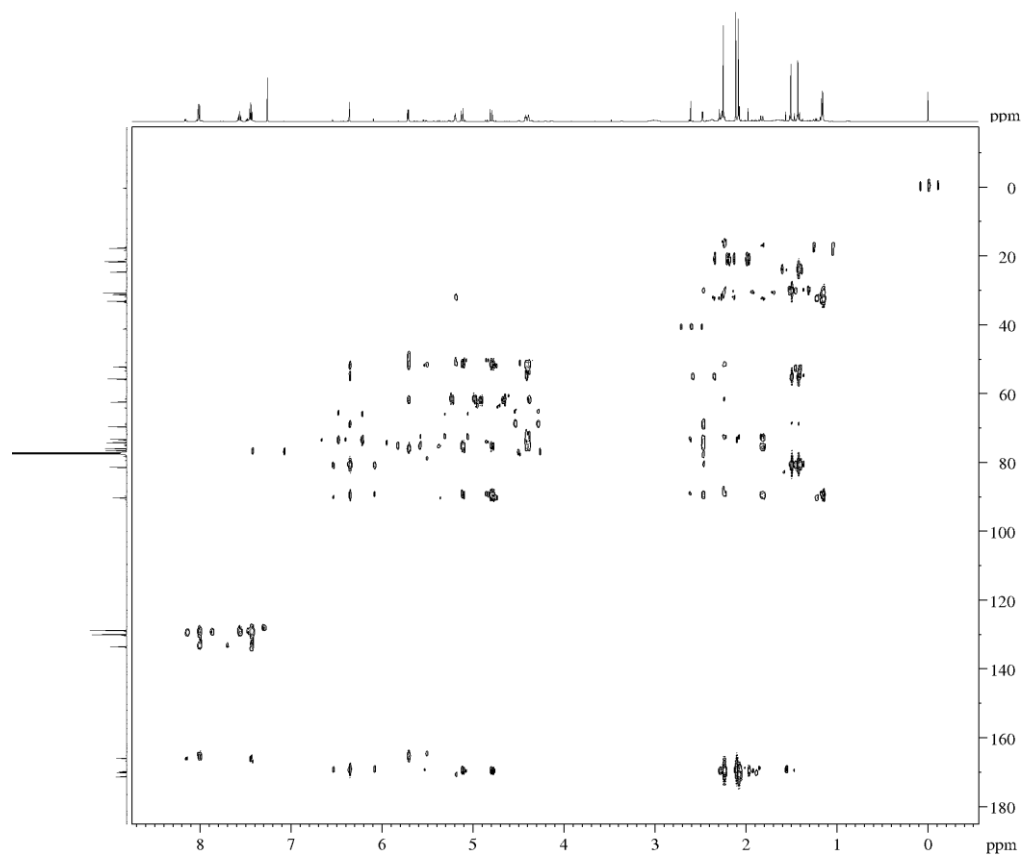


Fig. S4.6 HMBC spectrum (600 MHz, CDCl₃) of compound **4**

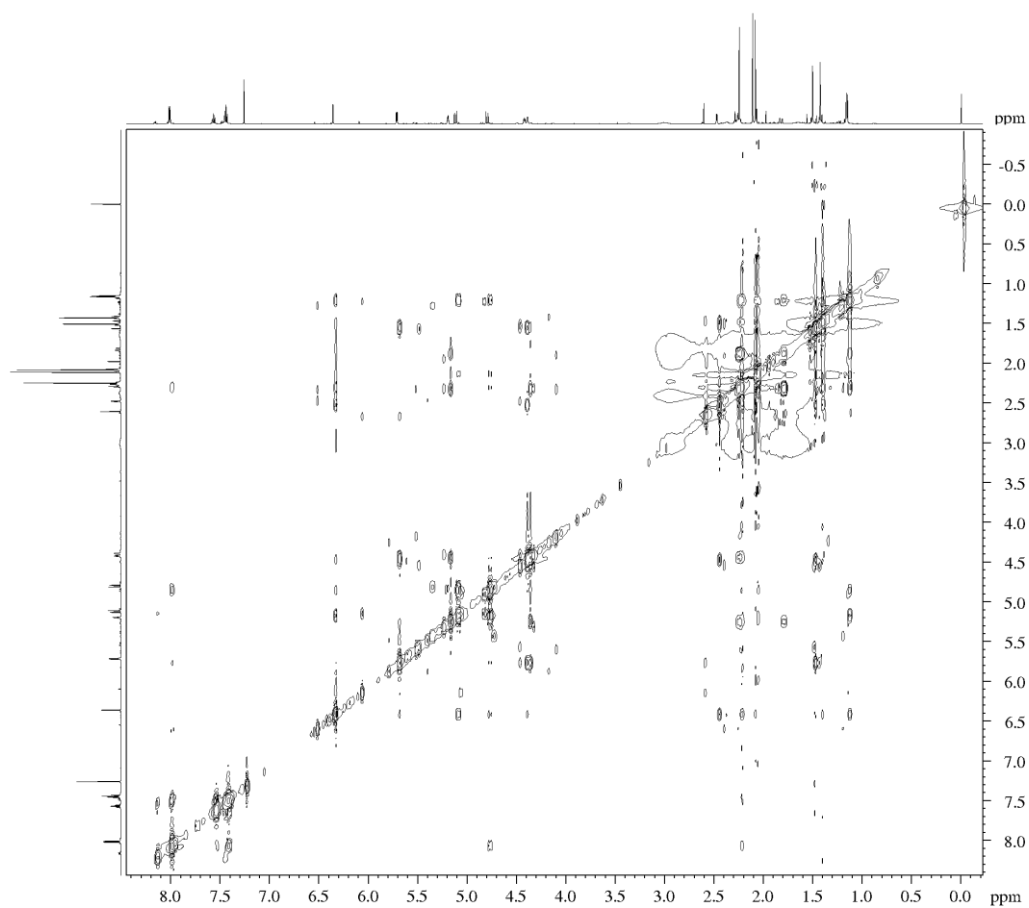


Fig. S4.7 NOESY spectrum (600 MHz, CDCl_3) of compound **4**

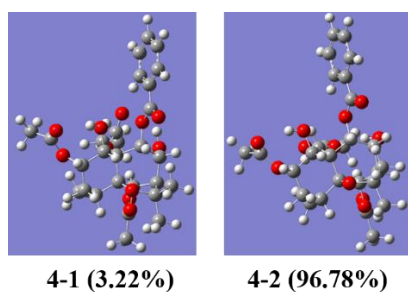


Fig. S4.8 Most stable conformers of **4** in solvated model calculations at the B3LYP/6-311++G (2d, p) level in ECD calculation

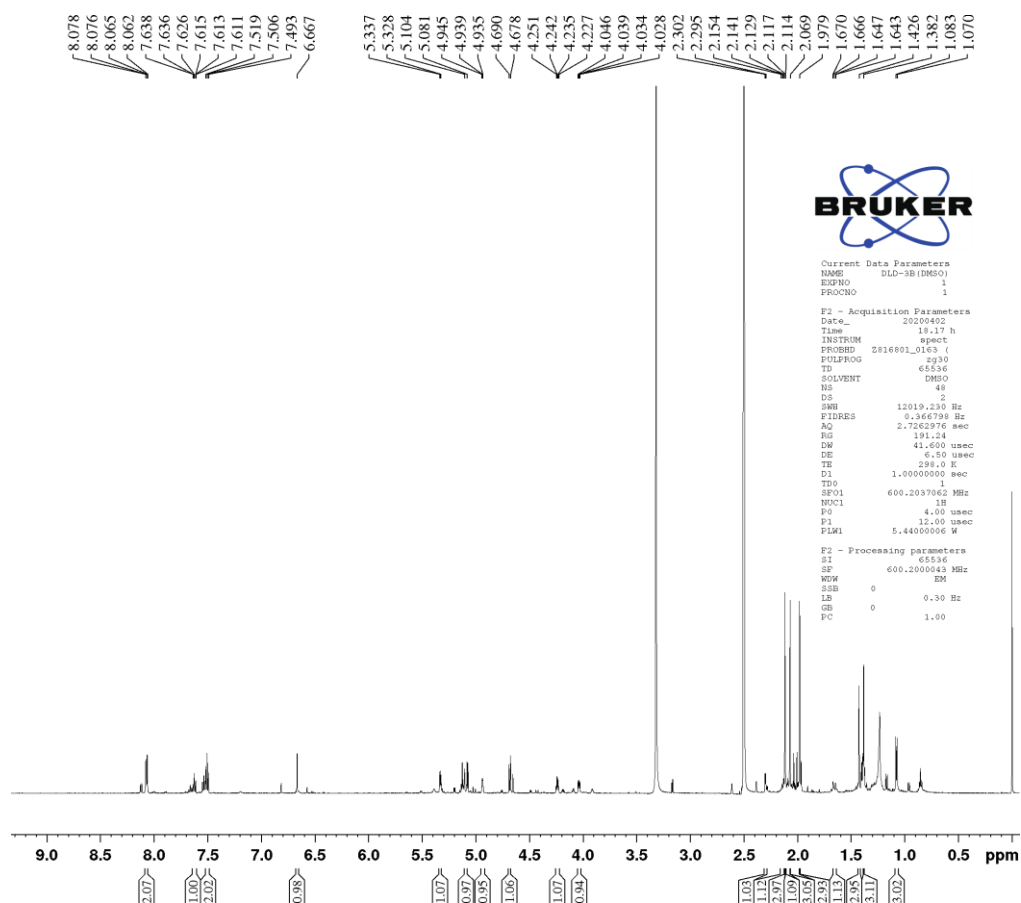


Fig. S4.9 ^1H NMR spectrum (600 MHz, DMSO) of compound **4**

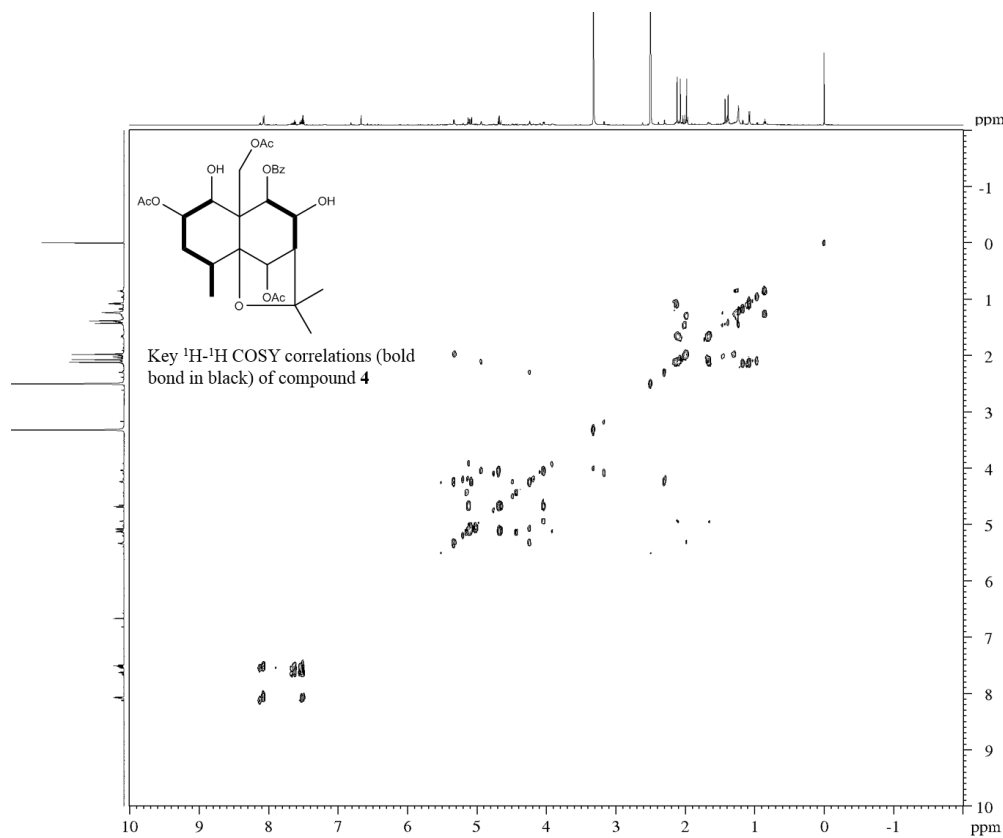
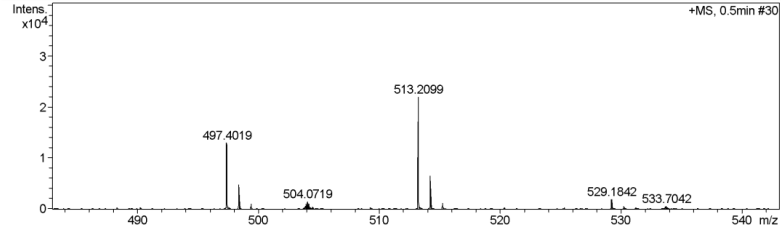


Fig. S4.10 ^1H - ^1H COSY spectrum (600 MHz, DMSO) of compound **4**

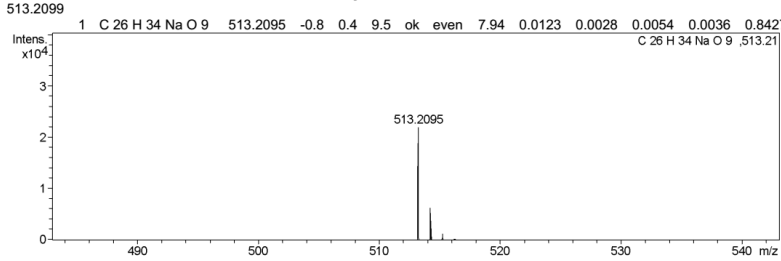
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 Comment:
 Acquisition Date: 11/13/2019 4:54:47 PM
 Operator: Bruker Customer
 Instrument / Ser#: micrOTOF-Q 125

Acquisition Parameter

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 Focus: Active
 Scan Begin: 50 m/z
 Scan End: 1500 m/z
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 Set End Plate Offset: -500 V
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 Set Nebulizer: 1.2 Bar
 Set Dry Heater: 180 °C
 Set Dry Gas: 8.0 l/min
 Set Divert Valve: Source



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e ⁻ Conf	mSigma	Std I	Std Mean m/z	Std VarNo	Std I m/z	Std m/z Diff	Std Comb Dev
513.2099	1	C ₂₆ H ₃₄ NaO ₉	513.2095	-0.8	0.4	9.5	ok	even	7.94	0.0123	0.0028	0.0054	0.0036	0.8427	



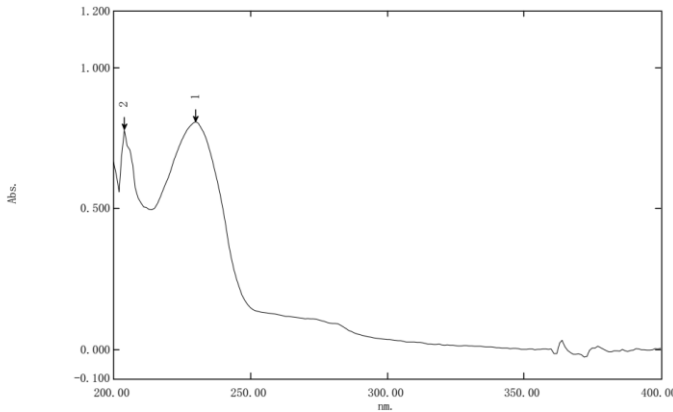
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513.2095		C ₂₆ H ₃₄ NaO ₉	513.21												

Fig. S5.1 HRESIMS spectrum of compound 5

Spectrum Peak Pick Report

FIELD FIELD TEXT

Data Set: 没有



测定属性
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 扫描速度: 中速
 采样间隔: 1.0
 自动采样间隔: 停用
 扫描模式: 单一的

No.	P/V	Wavelength	Abs.	描述
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3	●	214.00	.497	
4	●	202.00	.560	

Fig. S5.2 UV spectrum of compound 5

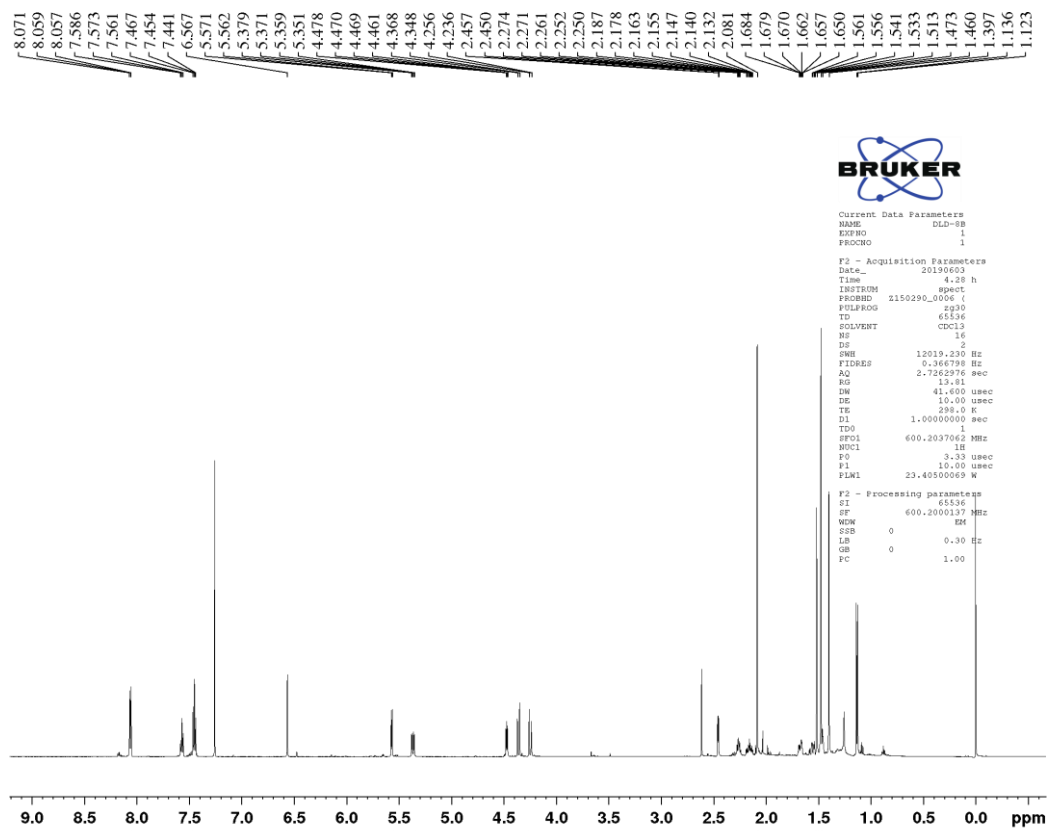


Fig. S5.3 ^1H NMR spectrum (600 MHz, CDCl_3) of compound **5**

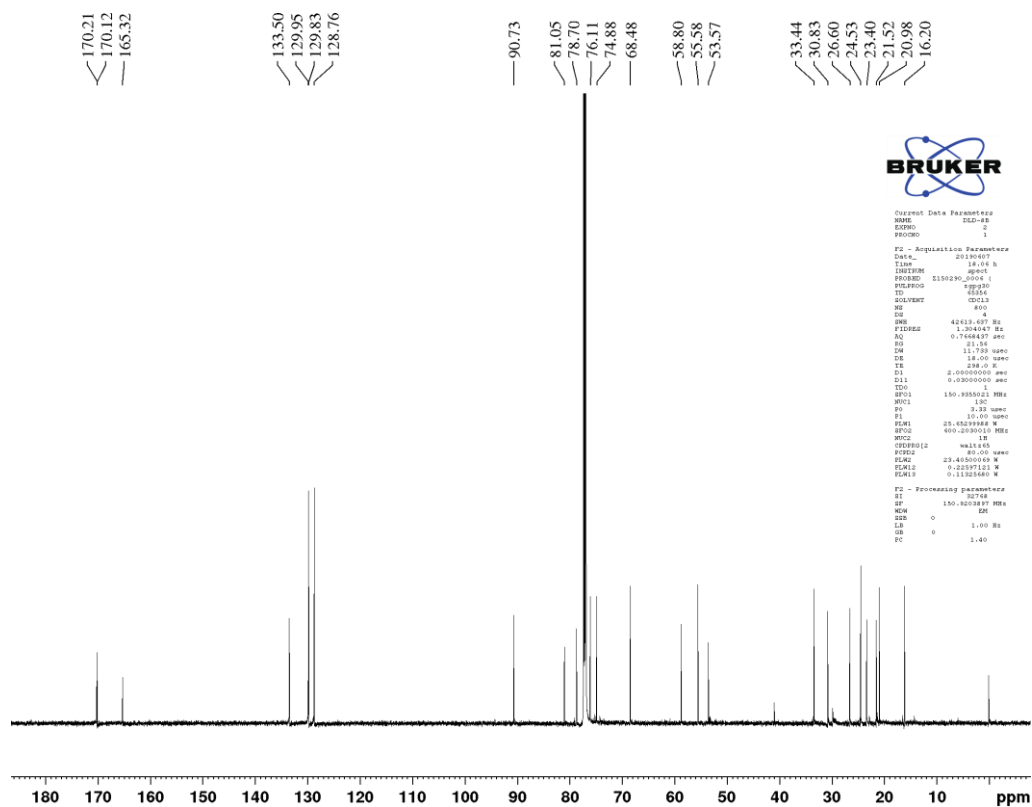


Fig. S5.4 ^{13}C NMR spectrum (150 MHz, CDCl_3) of compound **5**

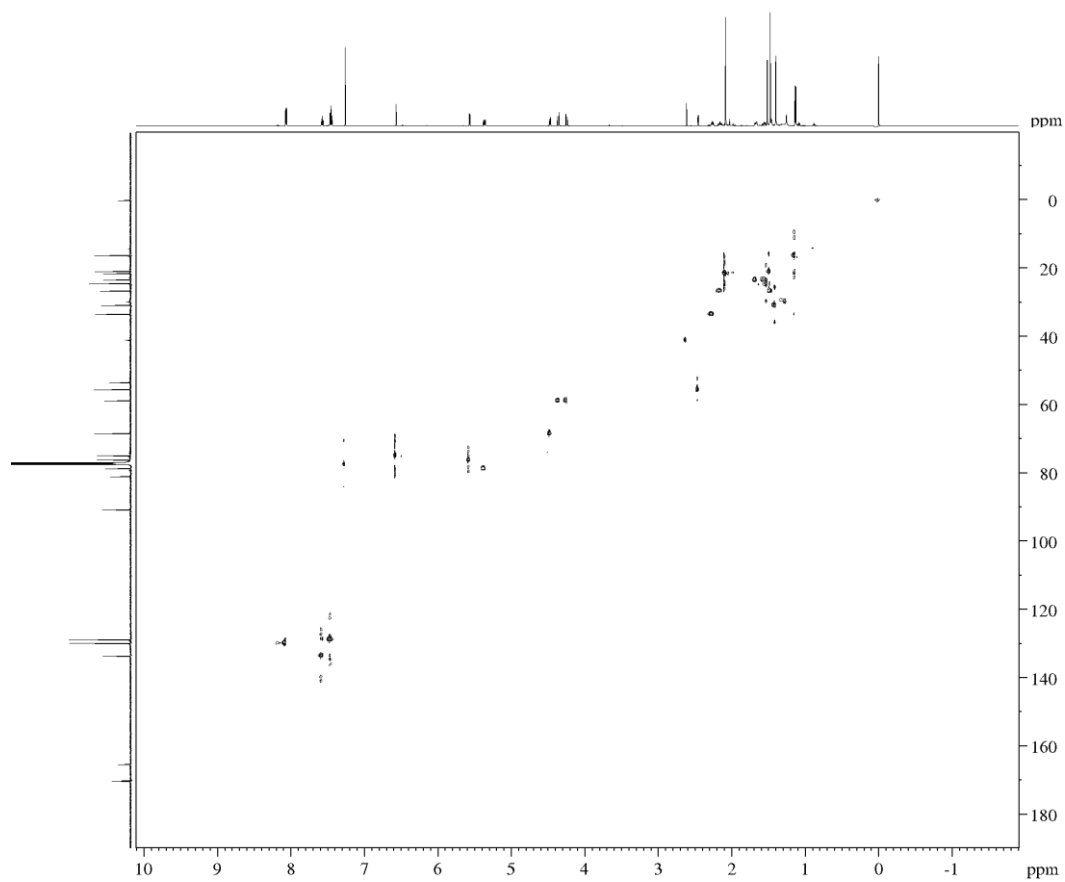


Fig. S5.5 HSQC spectrum (600 MHz, CDCl₃) of compound **5**

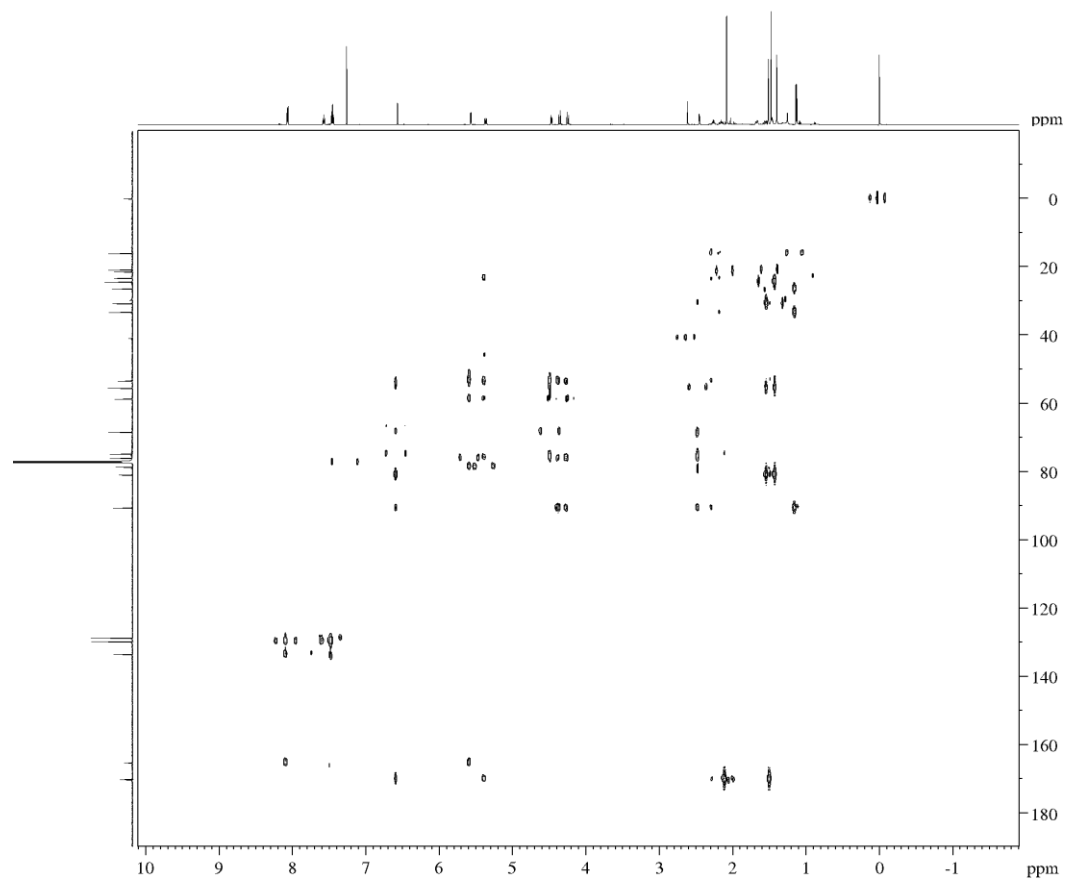


Fig. S5.6 HMBC spectrum (600 MHz, CDCl₃) of compound **5**

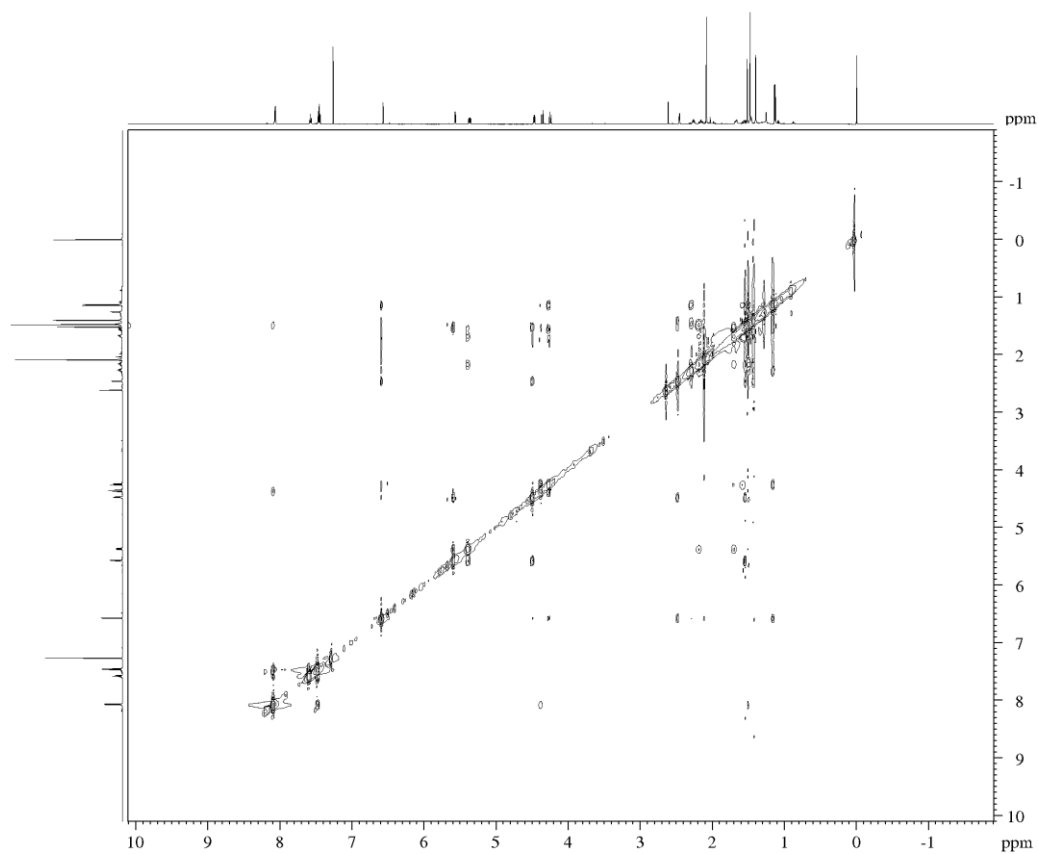


Fig. S5.7 NOESY spectrum (600 MHz, CDCl₃) of compound **5**

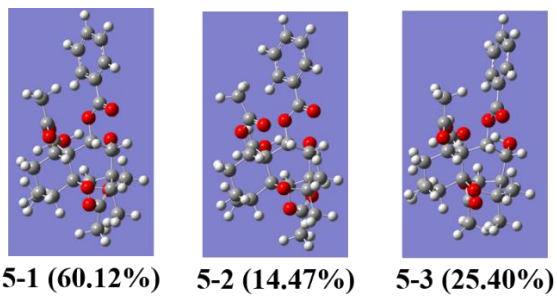


Fig. S5.8 Most stable conformers of **5** in solvated model calculations at the B3LYP/6-311++G (2d, p) level in ECD calculation

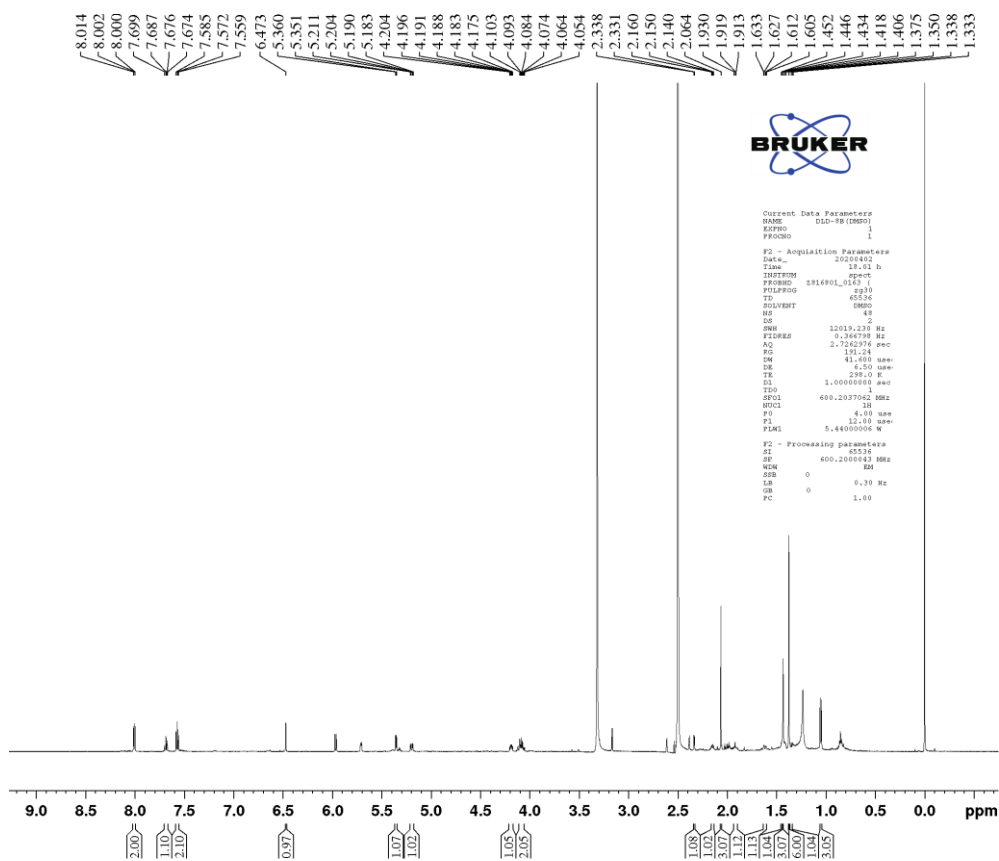


Fig. S5.9 ^1H NMR spectrum (600 MHz, DMSO) of compound **5**

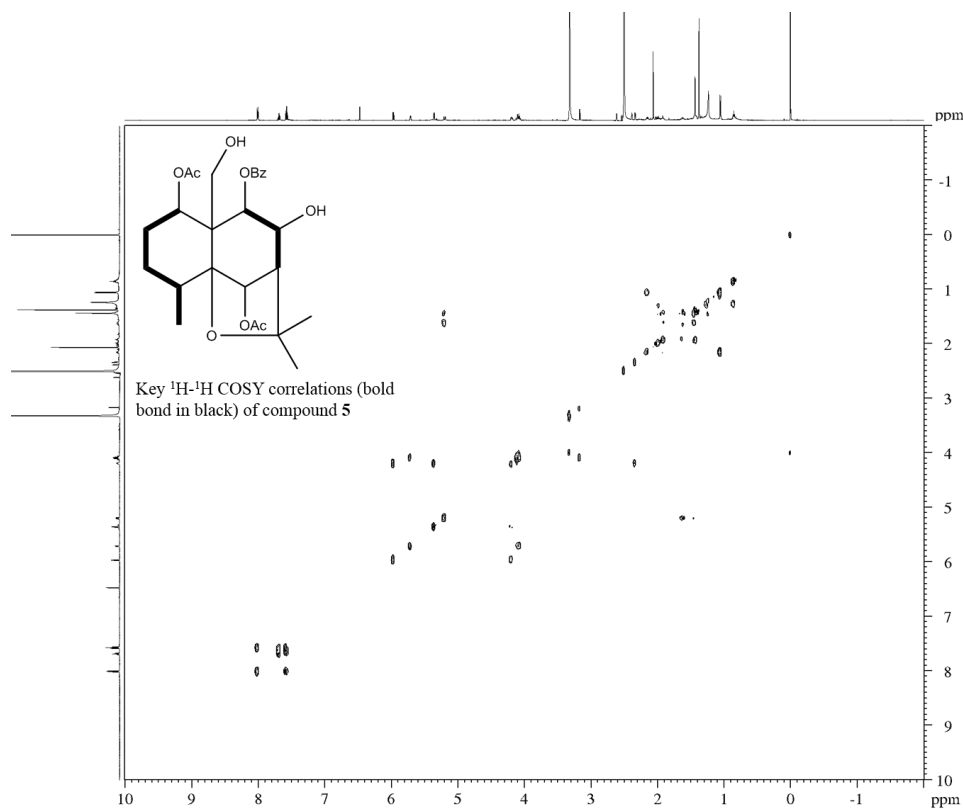
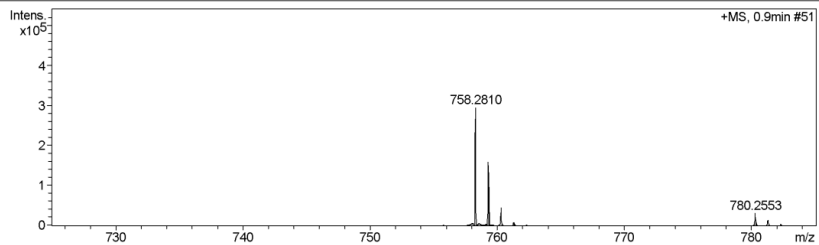


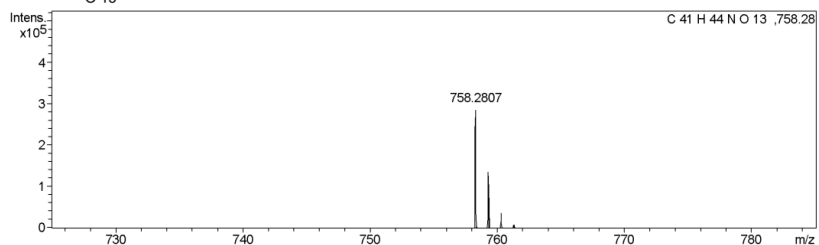
Fig. S5.10 ^1H - ^1H COSY spectrum (600 MHz, DMSO) of compound **5**

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 Sample Name DLD-4
 Comment
 Acquisition Date 7/10/2019 3:26:42 PM
 Operator Bruker Customer
 Instrument / Ser# micrOTOF-Q 125

Acquisition Parameter
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 Focus Active Set Capillary 4500 V Set Dry Heater 180 °C
 Scan Begin 50 m/z Set End Plate Offset -500 V Set Dry Gas 8.0 l/min
 Scan End 1500 m/z Set Collision Cell RF 400.0 Vpp Set Divert Valve Source



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e ⁻ Conf	mSigma	Std I	Std Mean m/z	Std I VarNo	Std I m/z Diff	Std Comb Dev
758.28	10	C ₄₁ H ₄₄ N ₄ O ₁₃	758.2807	-0.3	0.6	20.5	ok	even	43.26	0.0507	0.0022	0.0167	0.0045	0.8427



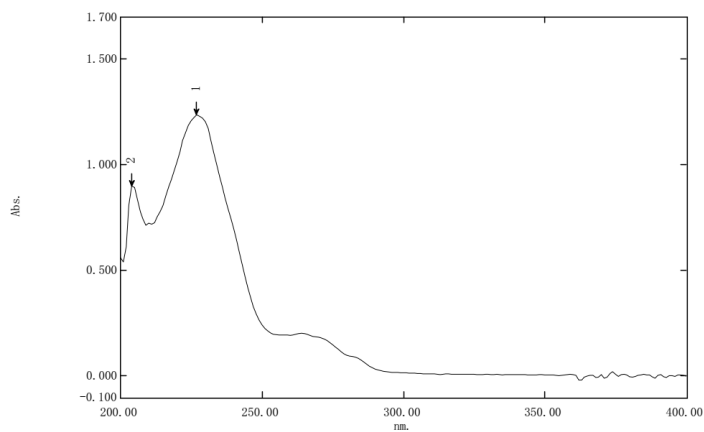
Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e ⁻ Conf	mSigma	Std I	Std Mean m/z	Std I VarNo	Std I m/z Diff	Std Comb Dev
758.28	10	C ₄₁ H ₄₄ N ₄ O ₁₃	758.2807	-0.3	0.6	20.5	ok	even	43.26	0.0507	0.0022	0.0167	0.0045	0.8427

Fig. S6.1 HRESIMS spectrum of compound **6**

Spectrum Peak Pick Report

FIELD FIELD TEXT

Data Set: 没有



测定属性
 波长范围 (nm.): 200.00到400.00
 扫描速度: 中速
 采样间隔: 1.0
 自动采样间隔: 停用
 扫描模式: 单一的

No.	P/V	Wavelength	Abs.	描述
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2	●	204.00	.900	
3	●	209.00	.714	

Fig. S6.2 UV spectrum of compound **6**

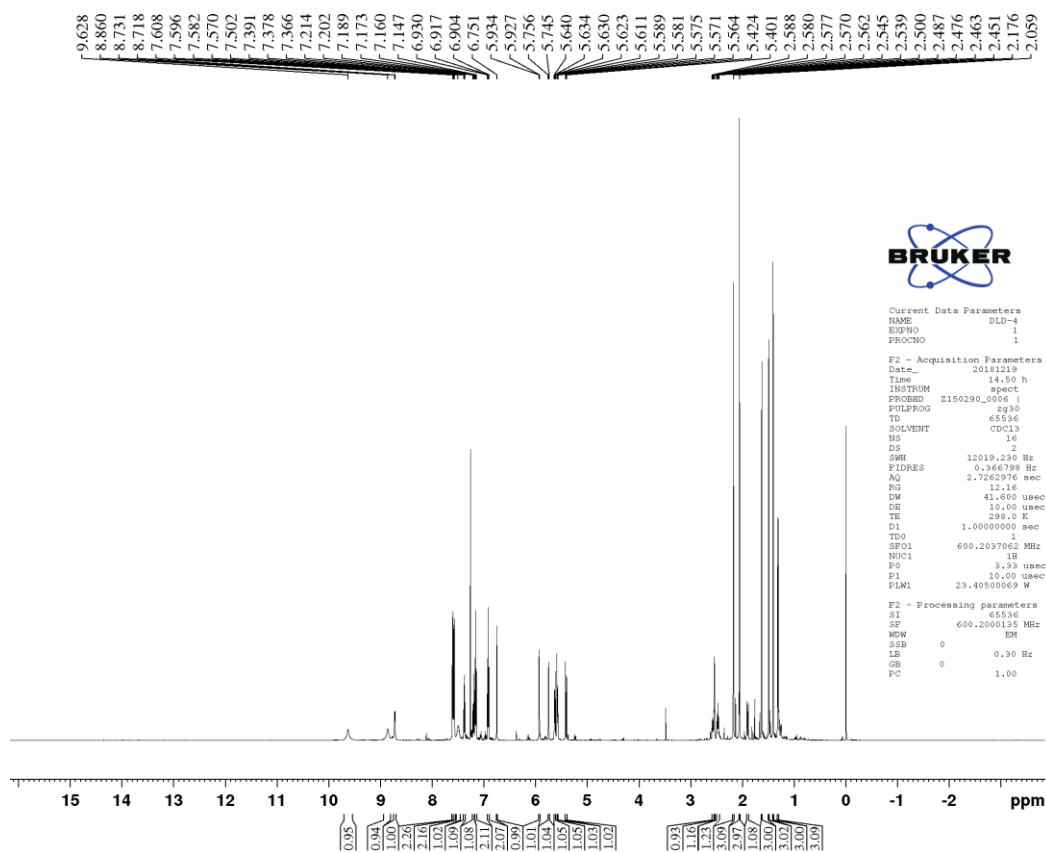


Fig. S6.3 ^1H NMR spectrum (600 MHz, CDCl_3) of compound 6

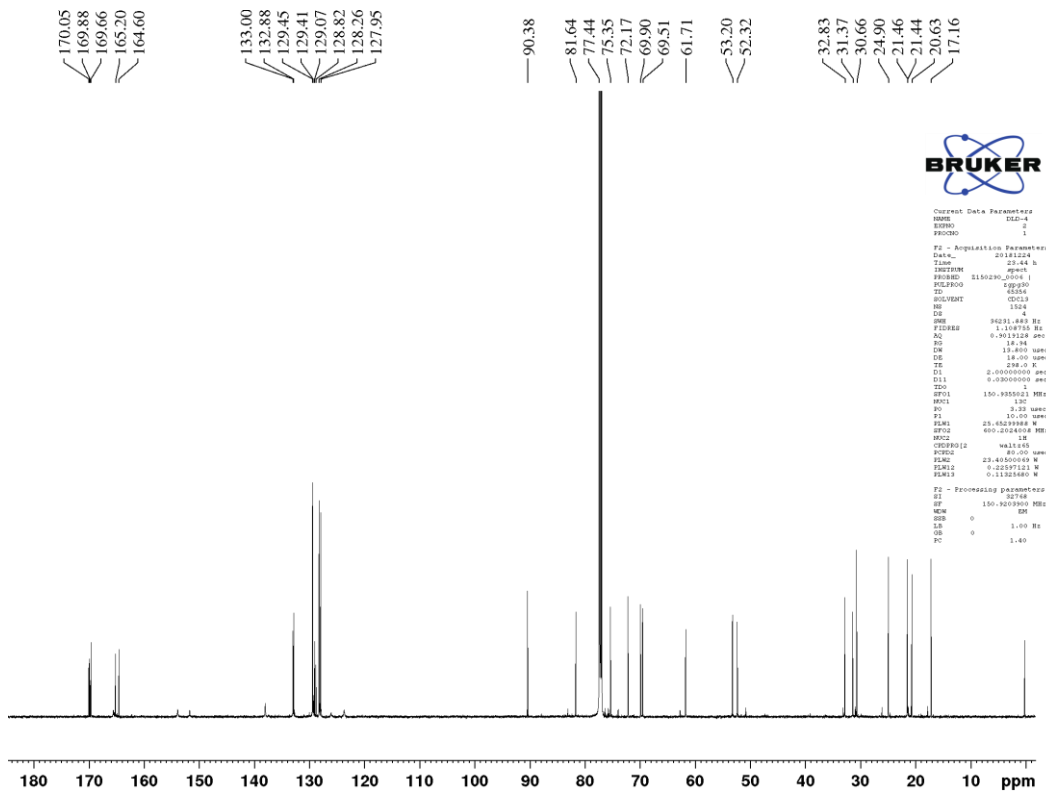


Fig. S6.4 ^{13}C NMR spectrum (150 MHz, CDCl_3) of compound 6

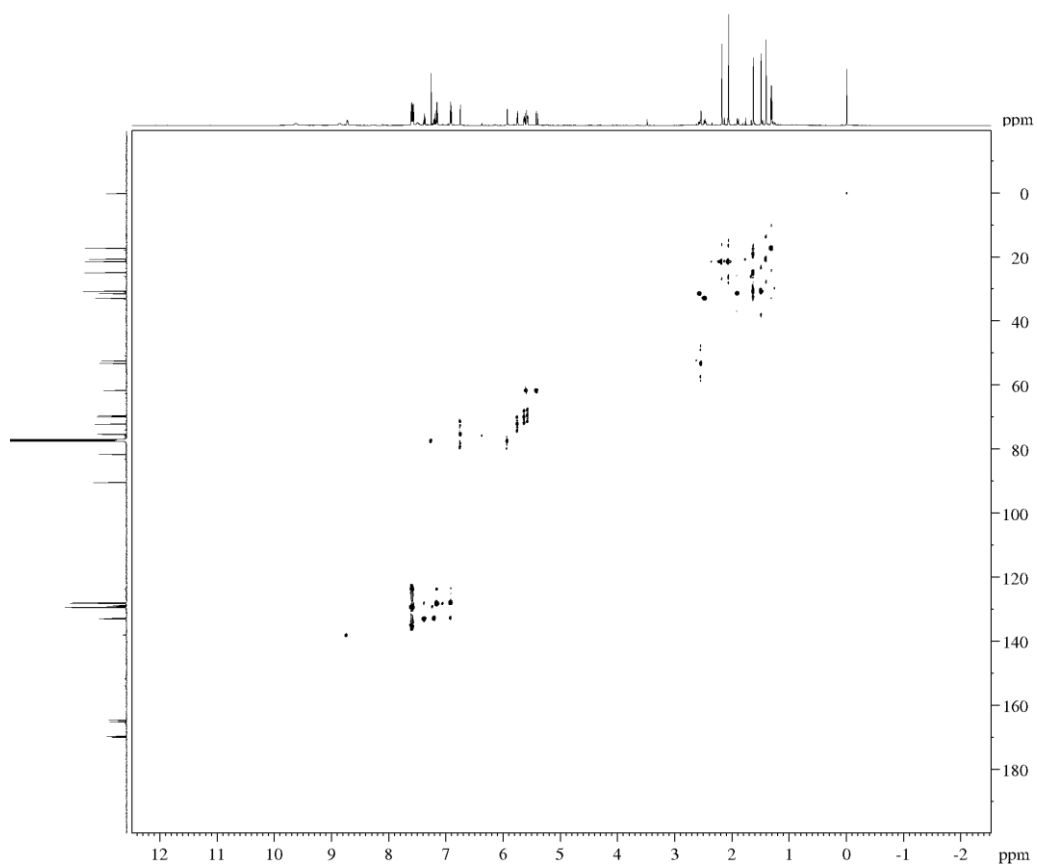


Fig. S6.5 HSQC spectrum (600 MHz, CDCl₃) of compound **6**

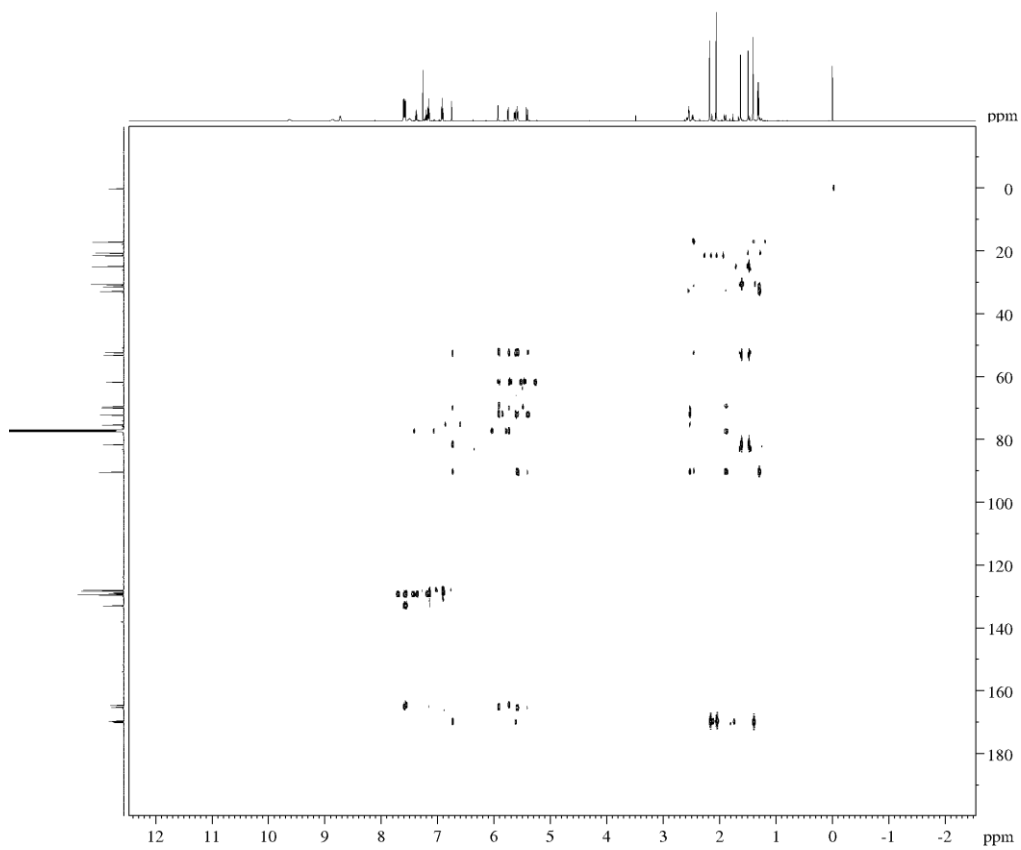


Fig. S6.6 HMBC spectrum (600 MHz, CDCl₃) of compound **6**

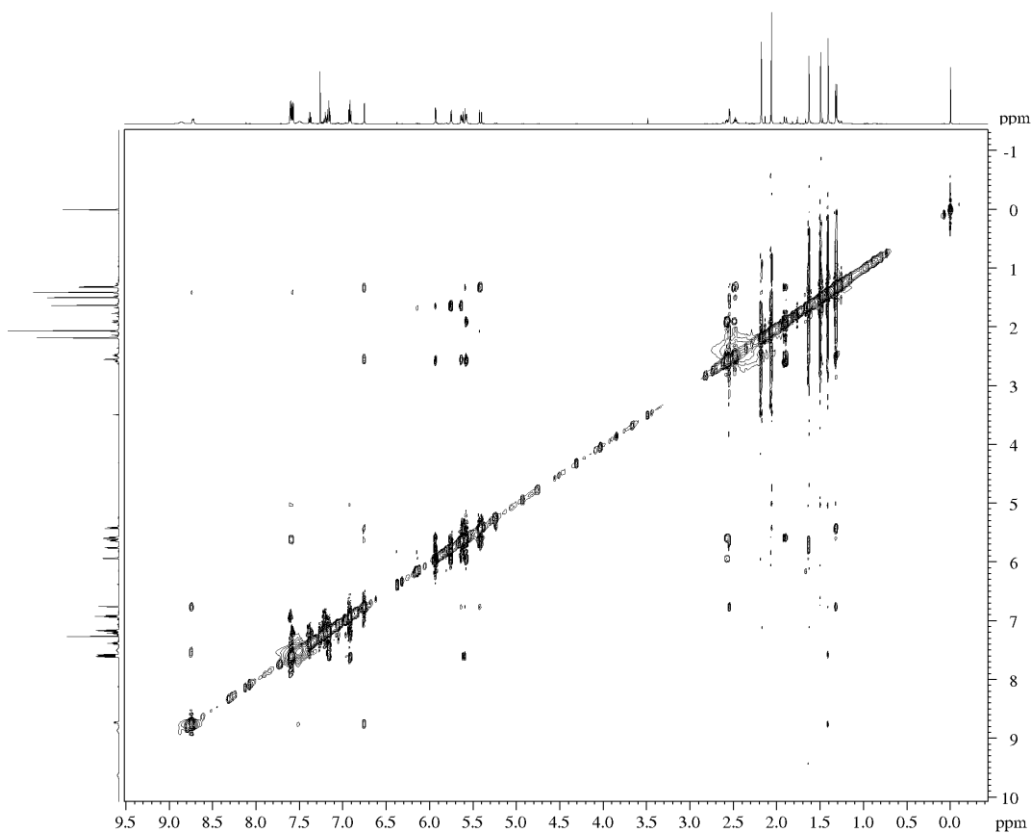


Fig. S6.7 NOESY spectrum (600 MHz, CDCl₃) of compound **6**

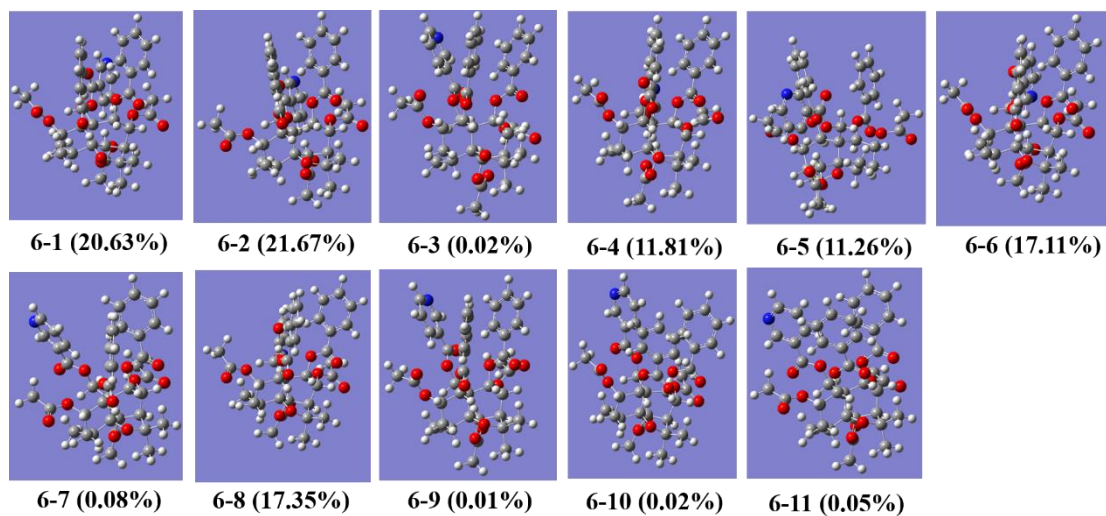


Fig. S6.8 Most stable conformers of **6** in solvated model calculations at the B3LYP/6-311++G (2d, p) level in ECD calculation

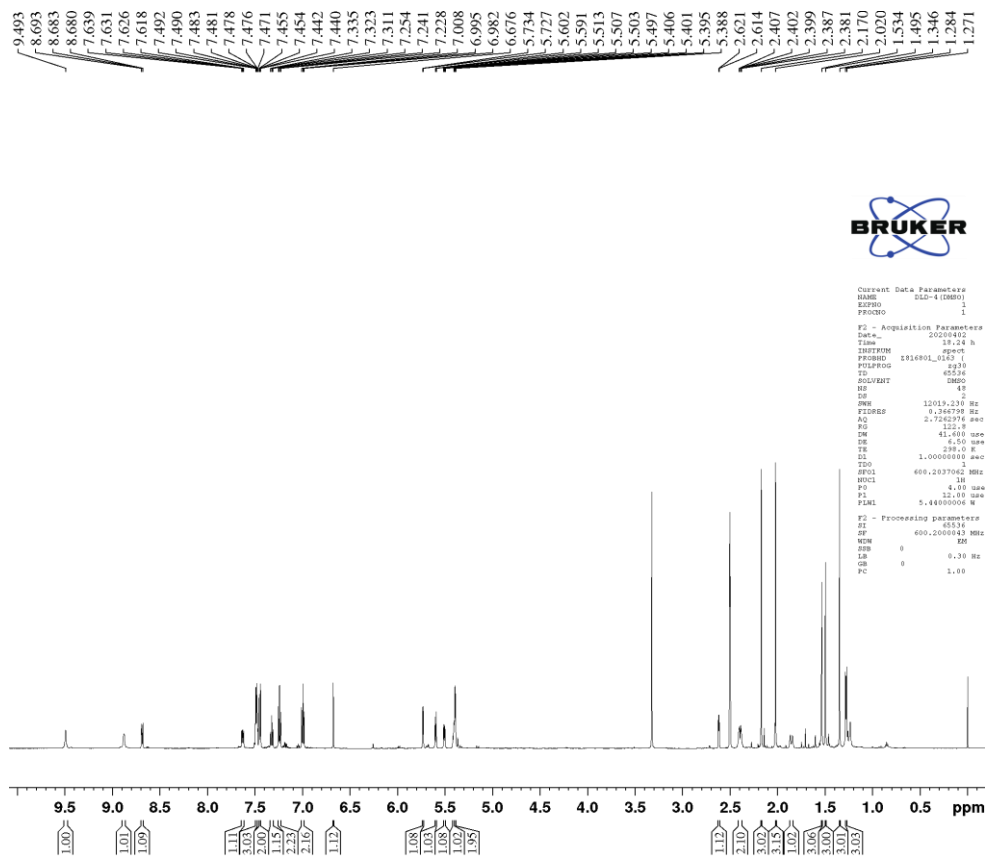


Fig. S6.9 ^1H NMR spectrum (600 MHz, DMSO) of compound **6**

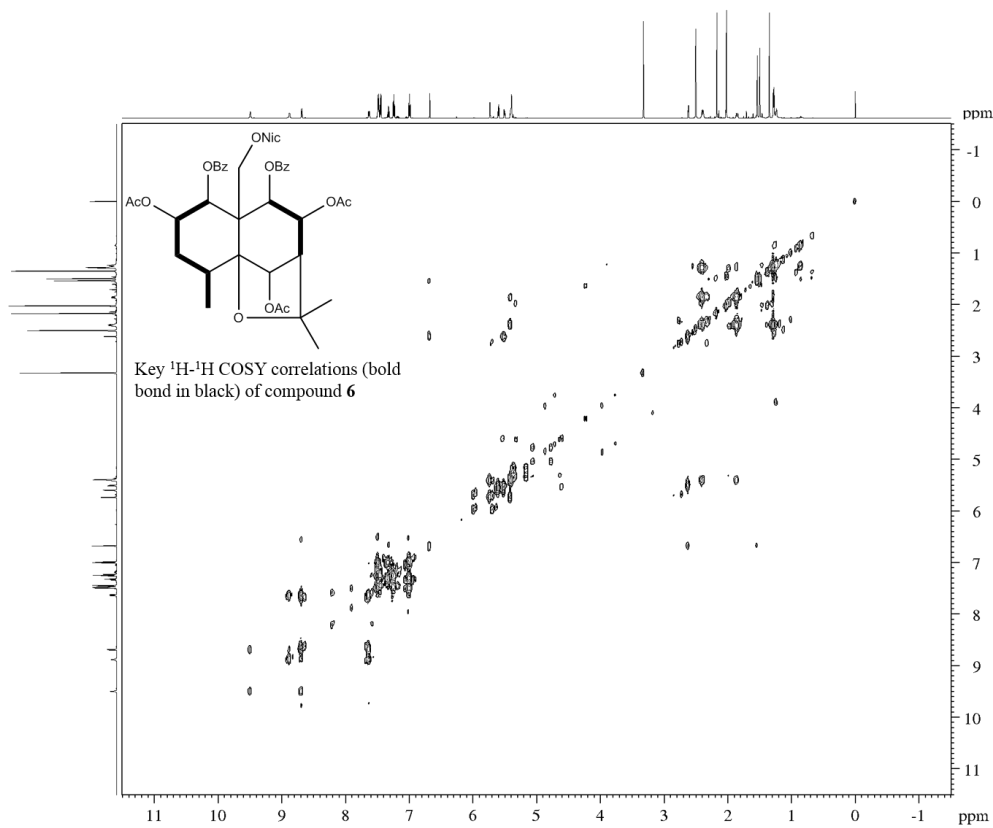


Fig. S6.10 ^1H - ^1H COSY spectrum (600 MHz, DMSO) of compound **6**

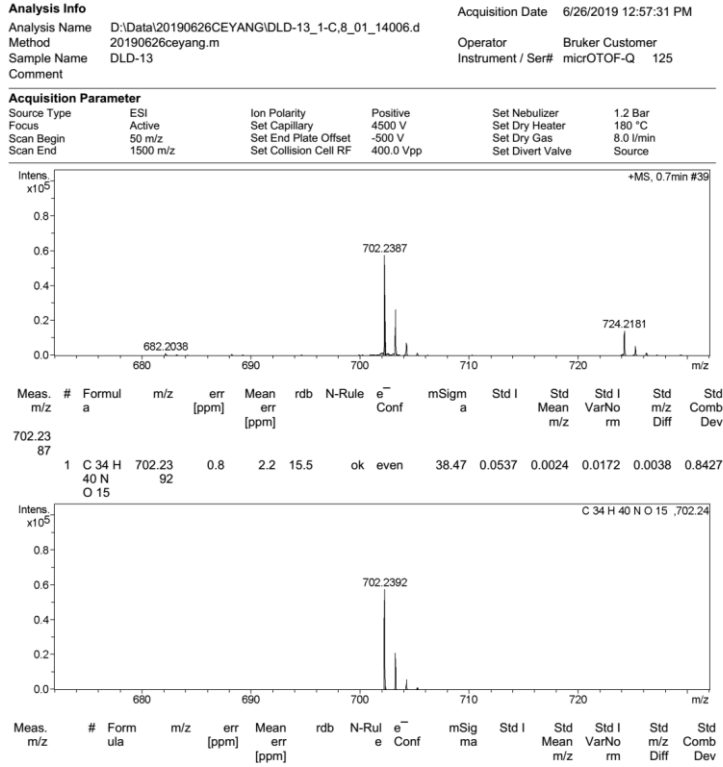
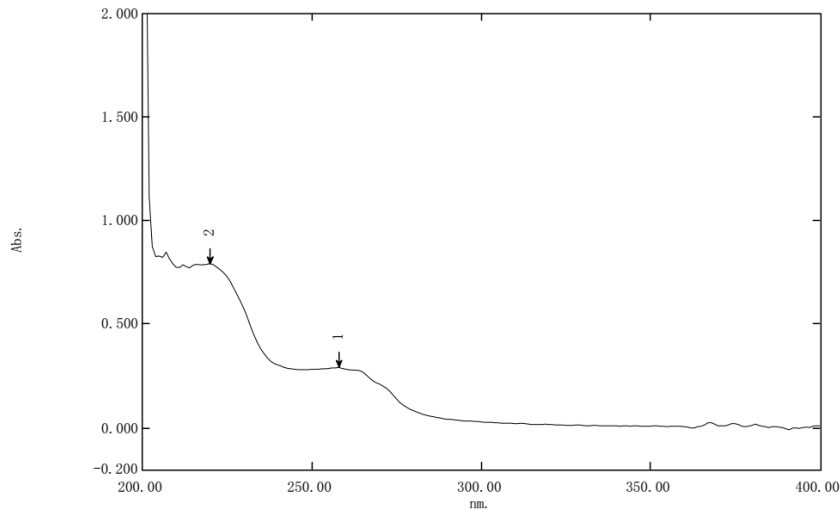


Fig. S7.1 HRESIMS spectrum of compound 7

Spectrum Peak Pick Report

FIELD FIELD TEXT

Data Set: 没有



测定属性
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 扫描速度: 中速
 采样间隔: 1.0
 自动采样间隔: 停用
 扫描模式: 单一的

No.	P/V	Wavelength	Abs.	描述
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4	●	210.00	.774	

Fig. S7.2 UV spectrum of compound 7

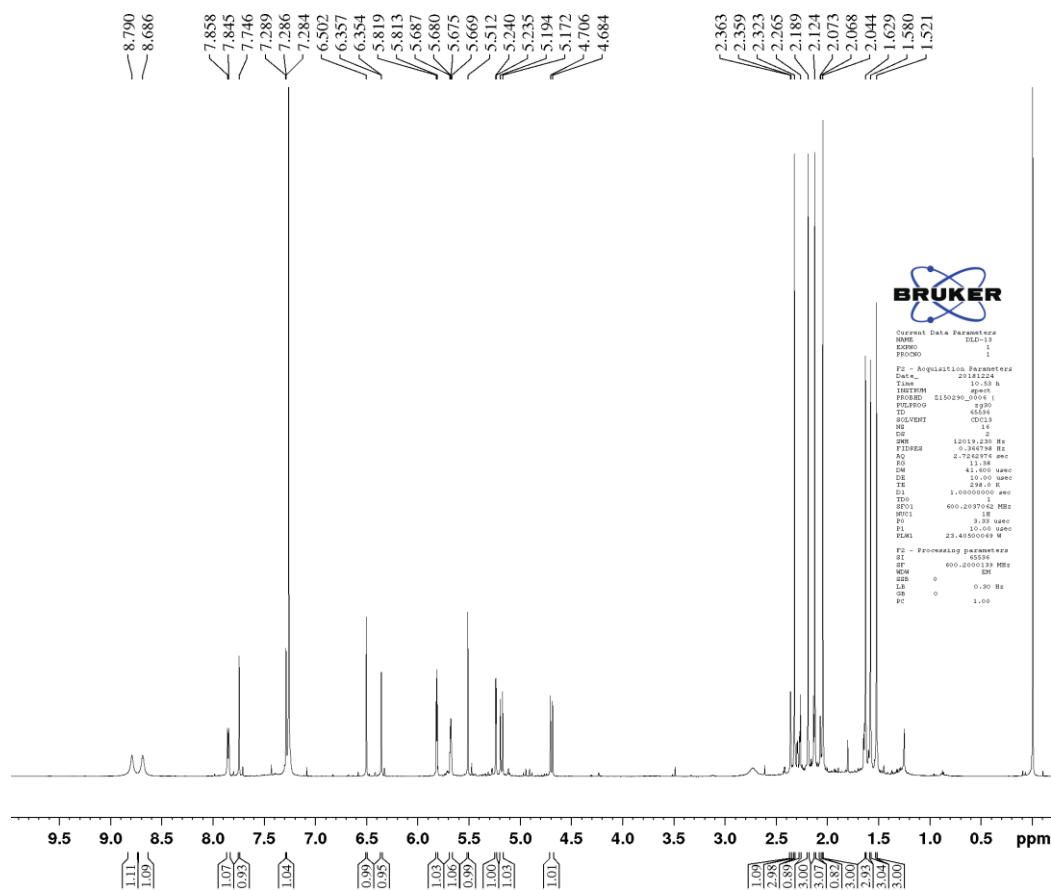


Fig. S7.3 ¹H NMR spectrum (600 MHz, CDCl₃) of compound 7

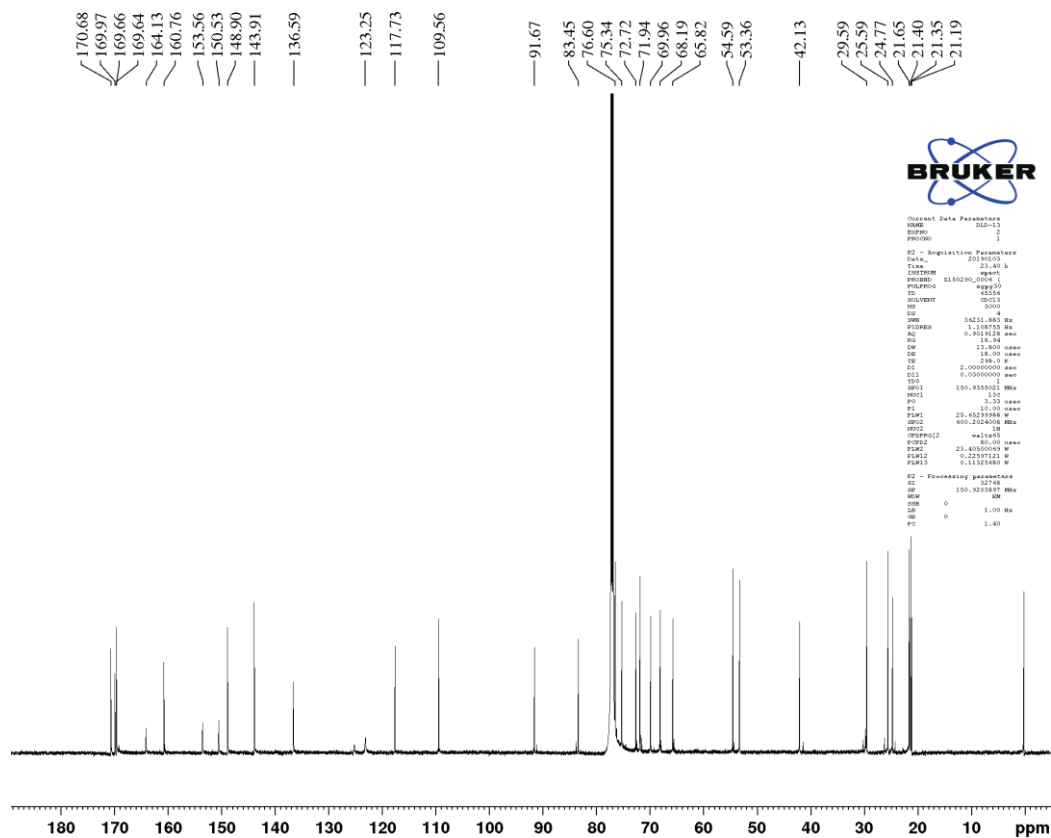


Fig. S7.4 ¹³C NMR spectrum (150 MHz, CDCl₃) of compound 7

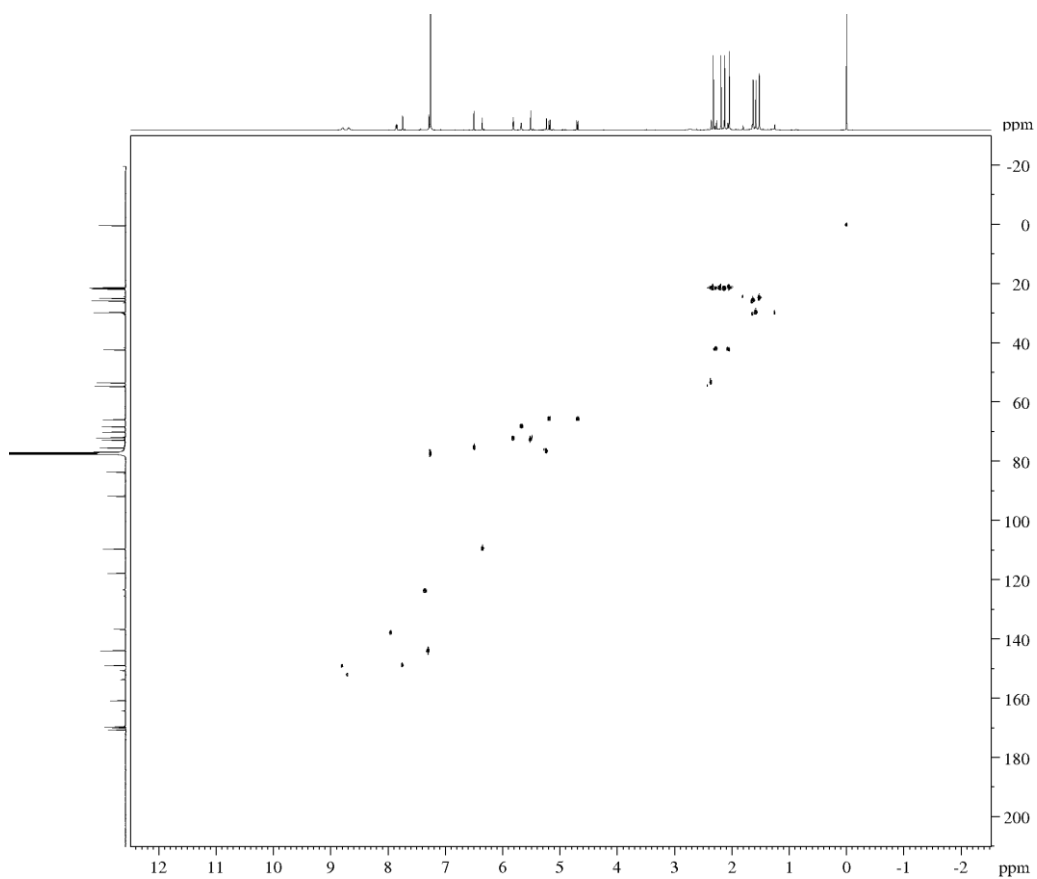


Fig. S7.5 HSQC spectrum (600 MHz, CDCl₃) of compound **7**

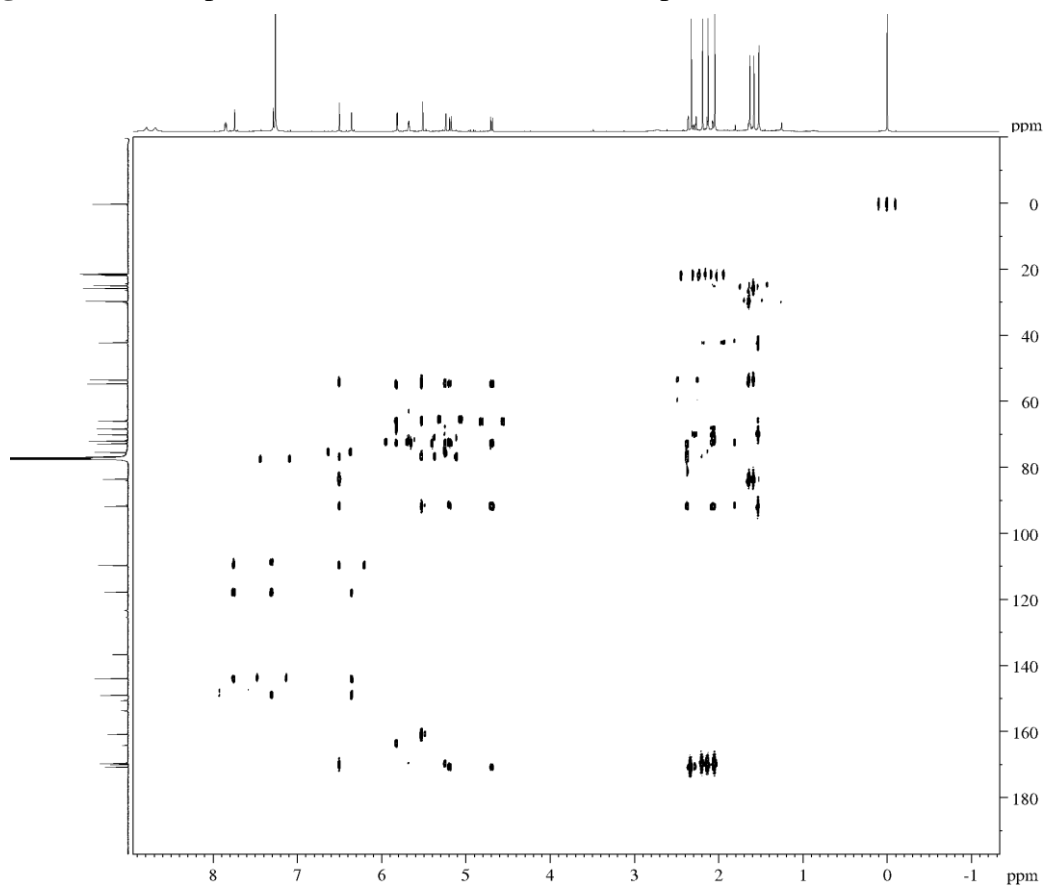


Fig. S7.6 HMBC spectrum (600 MHz, CDCl₃) of compound **7**

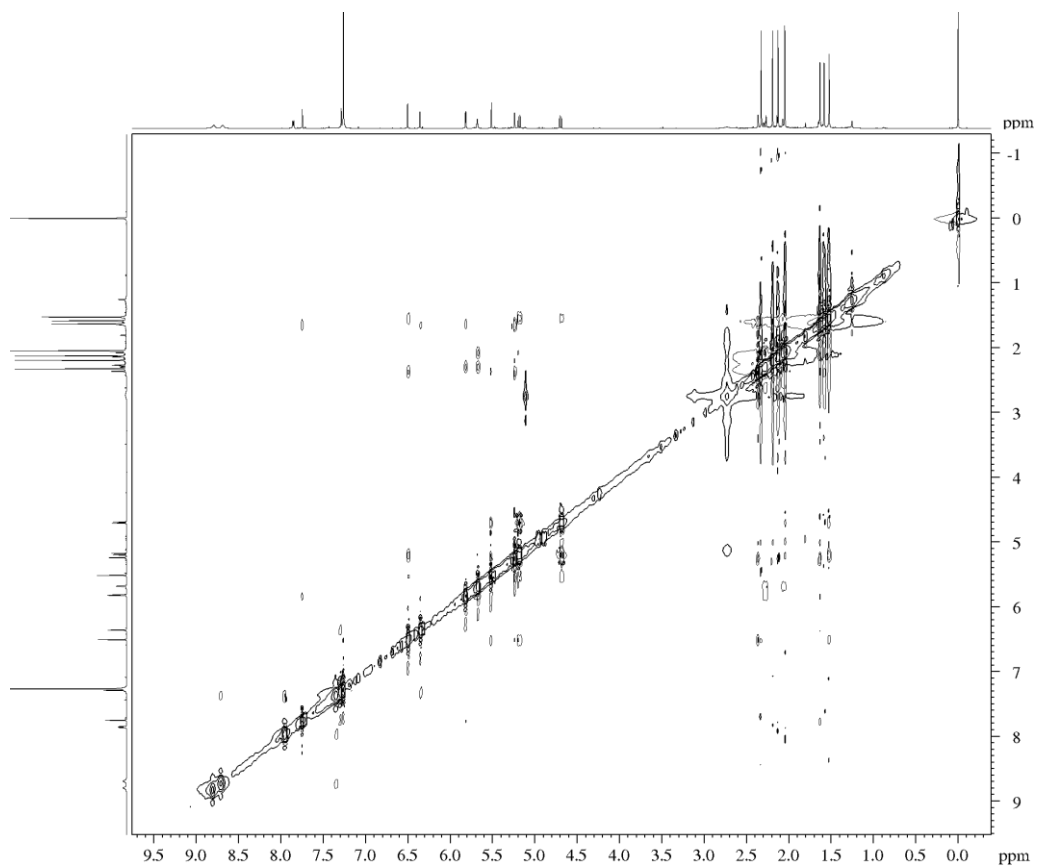


Fig. S7.7 NOESY spectrum (600 MHz, CDCl_3) of compound **7**

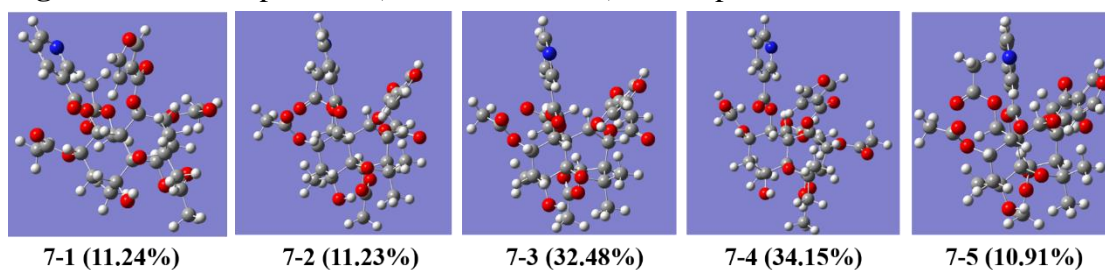


Fig. S7.8 Most stable conformers of **7** in solvated model calculations at the B3LYP/6-311++G (2d, p) level in ECD calculation

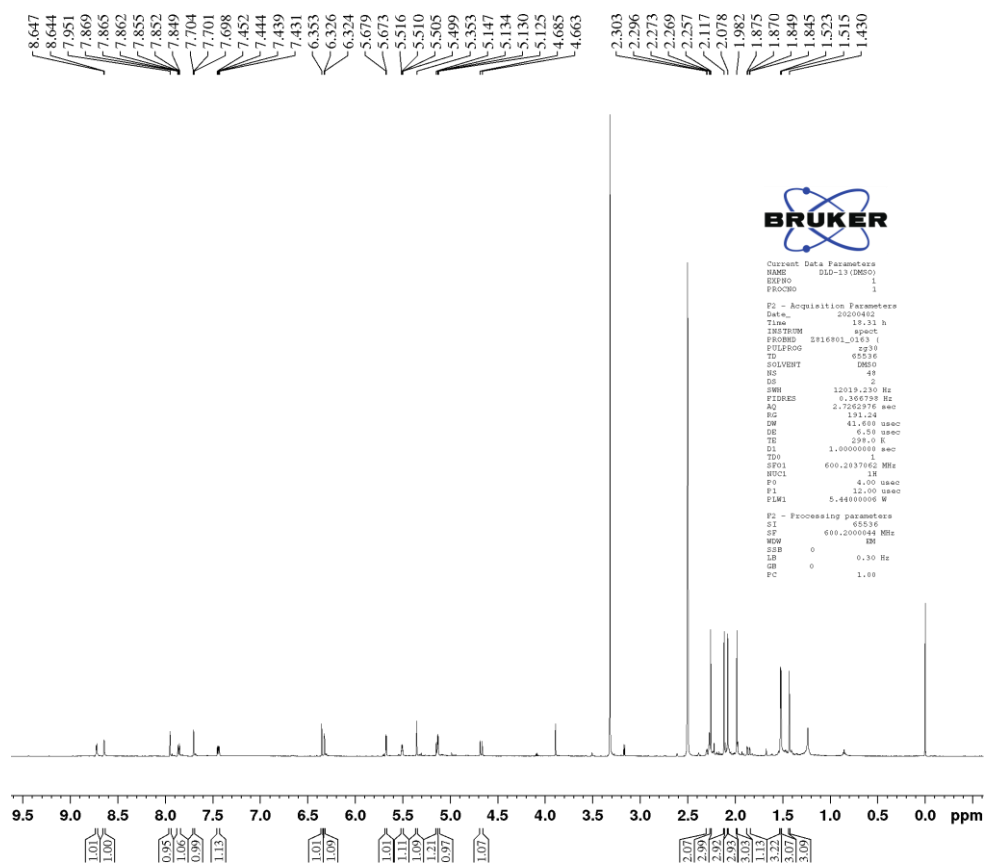


Fig. S7.9 ^1H NMR spectrum (600 MHz, DMSO) of compound **7**

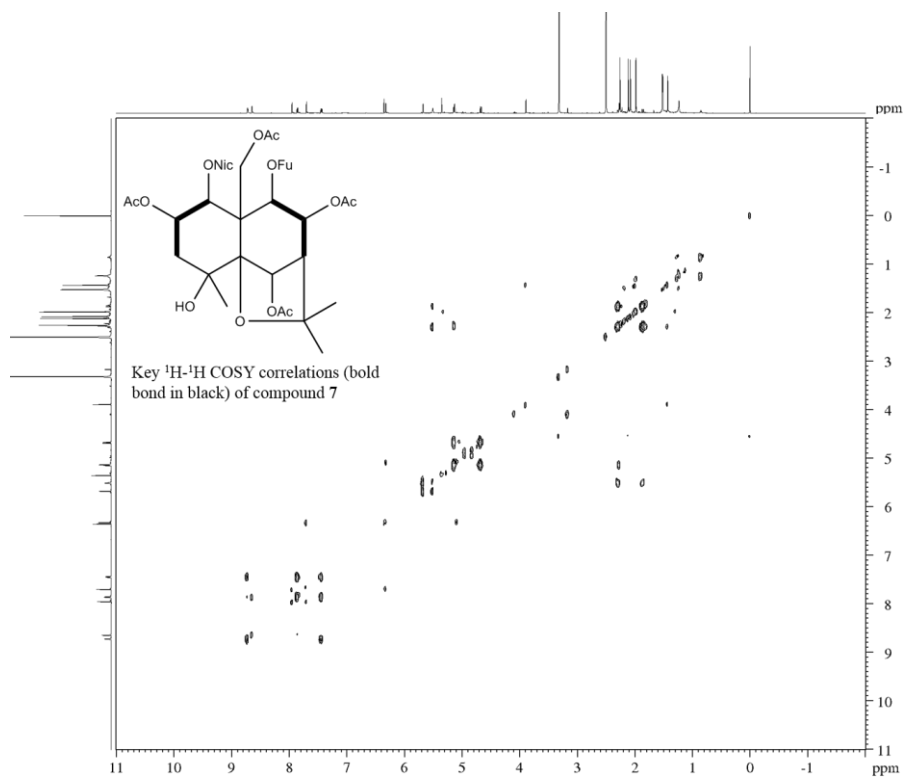
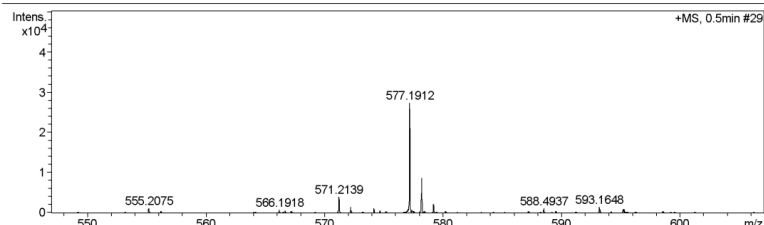


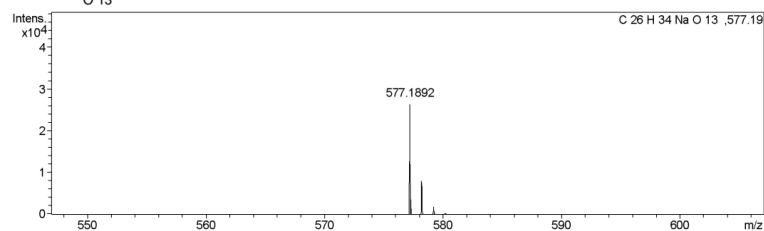
Fig. S7.10 ^1H - ^1H COSY spectrum (600 MHz, DMSO) of compound **7**

Analysis Info
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 Sample Name DLLD-12C
 Comment
 Acquisition Date 9/5/2019 9:56:21 PM
 Operator Bruker Customer
 Instrument / Ser# micrOTOF-Q 125

Acquisition Parameter
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 Focus Active Set Capillary 4500 V Set Dry Heater 180 °C
 Scan Begin 50 m/z Set End Plate Offset -500 V Set Dry Gas 8.0 l/min
 Scan End 1500 m/z Set Collision Cell RF 400.0 Vpp Set Divert Valve Source



Meas. #	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e ⁻ Conf	mSigma	Std I	Std Mean	Std Var	Std I Norm	Std m/z Diff	Std Comb Dev
577.1912	C ₂₆ H ₃₄ NaO ₁₃	577.1892	-3.6	-2.3	9.5	ok	even	14.42	0.0270	0.0020	0.0090	0.0038	0.8427	



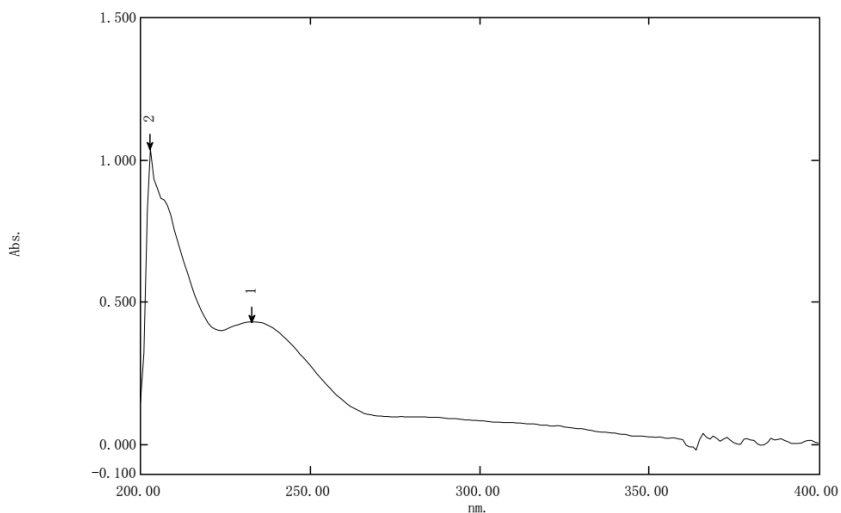
Meas. #	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e ⁻ Conf	mSigma	Std I	Std Mean	Std Var	Std I Norm	Std m/z Diff	Std Comb Dev
577.1912	C ₂₆ H ₃₄ NaO ₁₃	577.1892	-3.6	-2.3	9.5	ok	even	14.42	0.0270	0.0020	0.0090	0.0038	0.8427	

Fig. S8.1 HRESIMS spectrum of compound 8

Spectrum Peak Pick Report

FIELD FIELD TEXT

Data Set: 没有



测定属性
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 扫描速度: 中速
 采样间隔: 1.0
 自动采样间隔: 停用
 扫描模式: 单一的

No.	P/V	Wavelength	Abs.	描述
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2	●	203.00	1.038	
3	●	224.00	.401	

Fig. S8.2 UV spectrum of compound 8

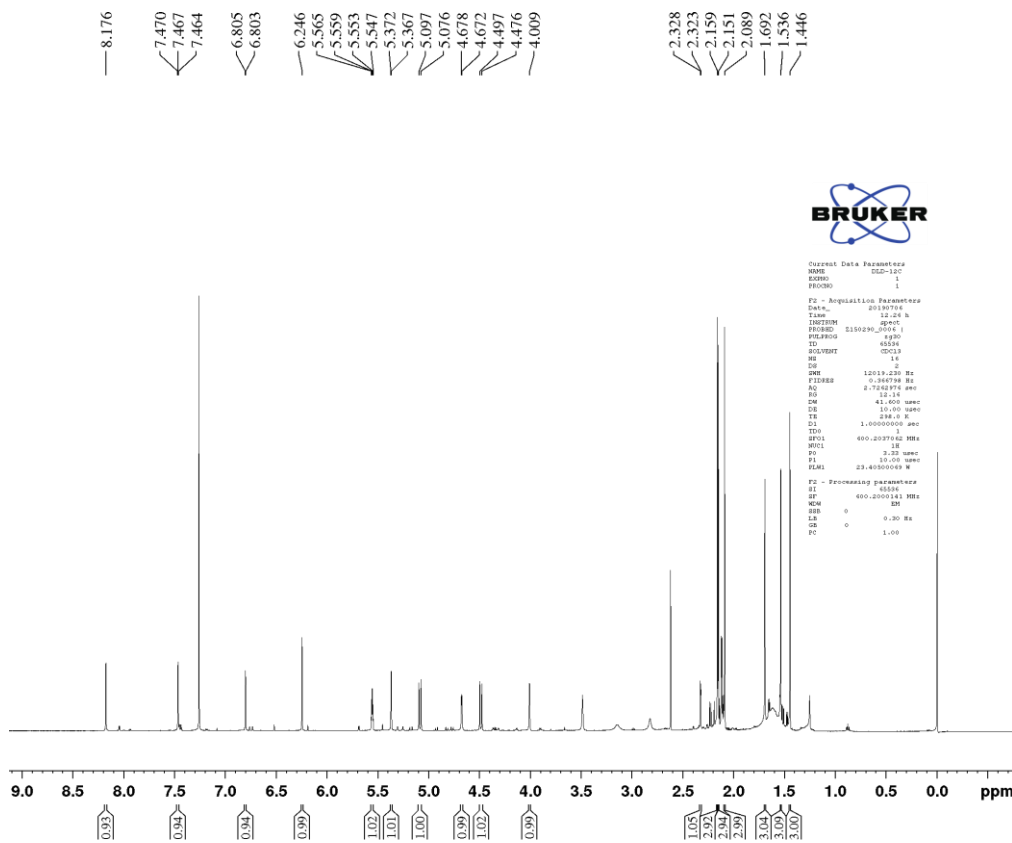


Fig. S8.3 ^1H NMR spectrum (600 MHz, CDCl_3) of compound **8**

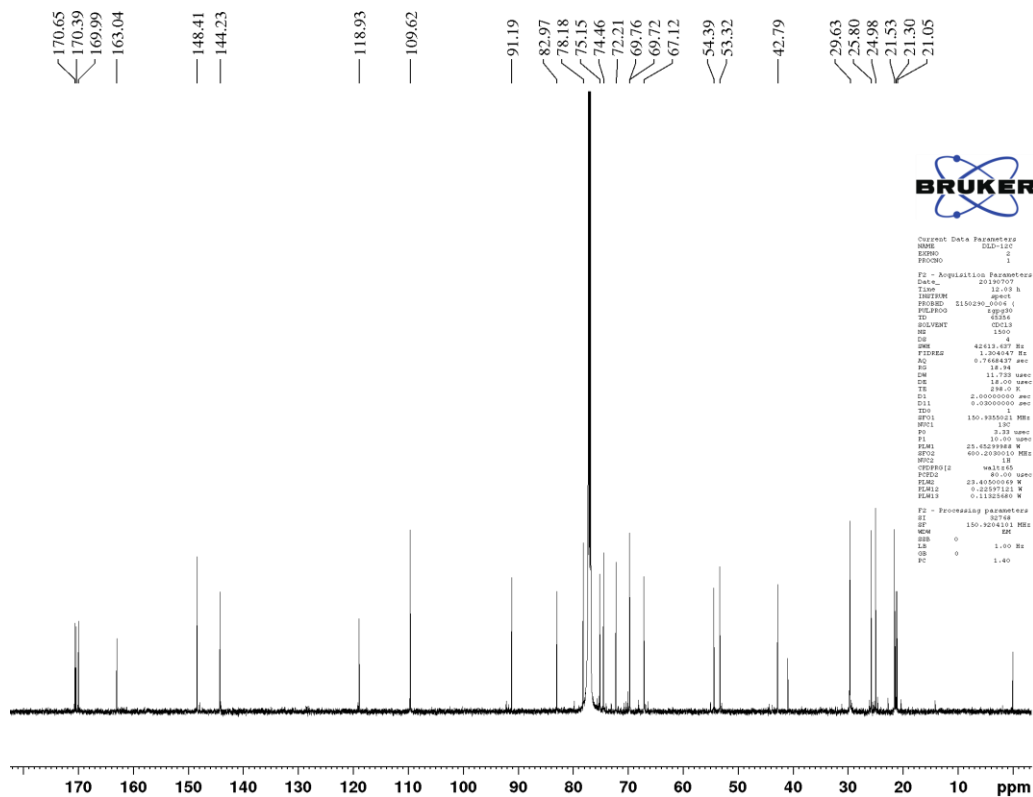


Fig. S8.4 ^{13}C NMR spectrum (150 MHz, CDCl_3) of compound **8**

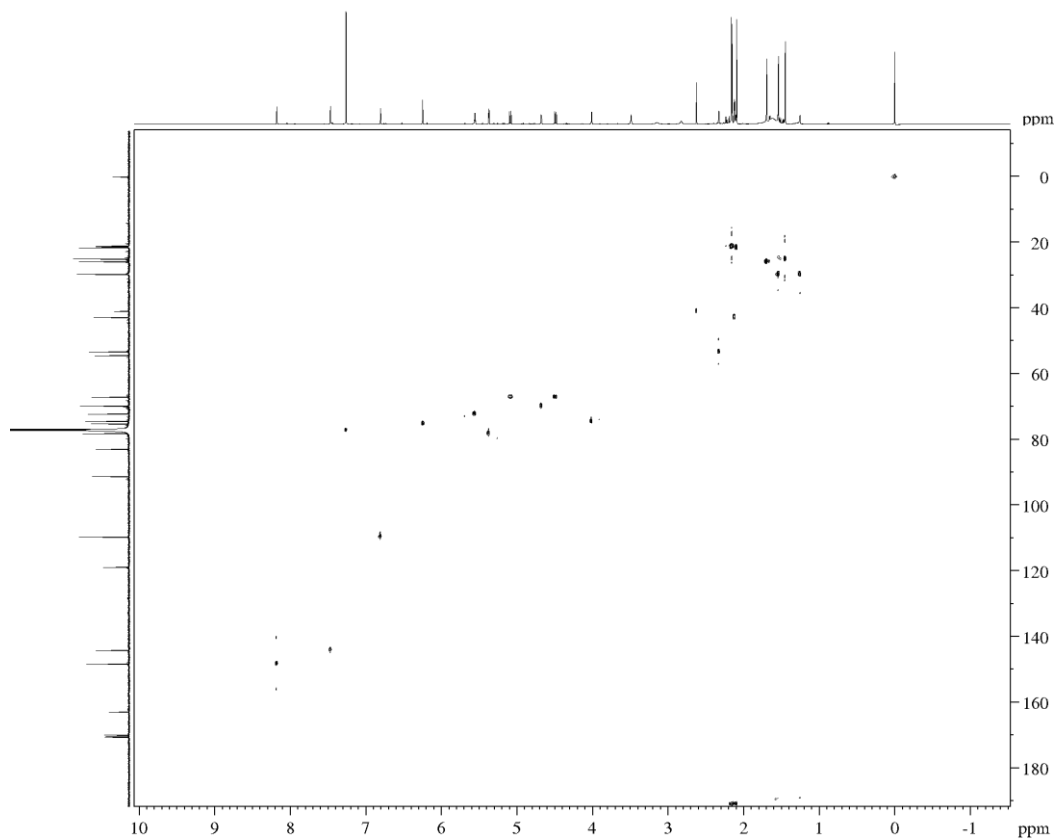


Fig. S8.5 HSQC spectrum (600 MHz, CDCl₃) of compound **8**

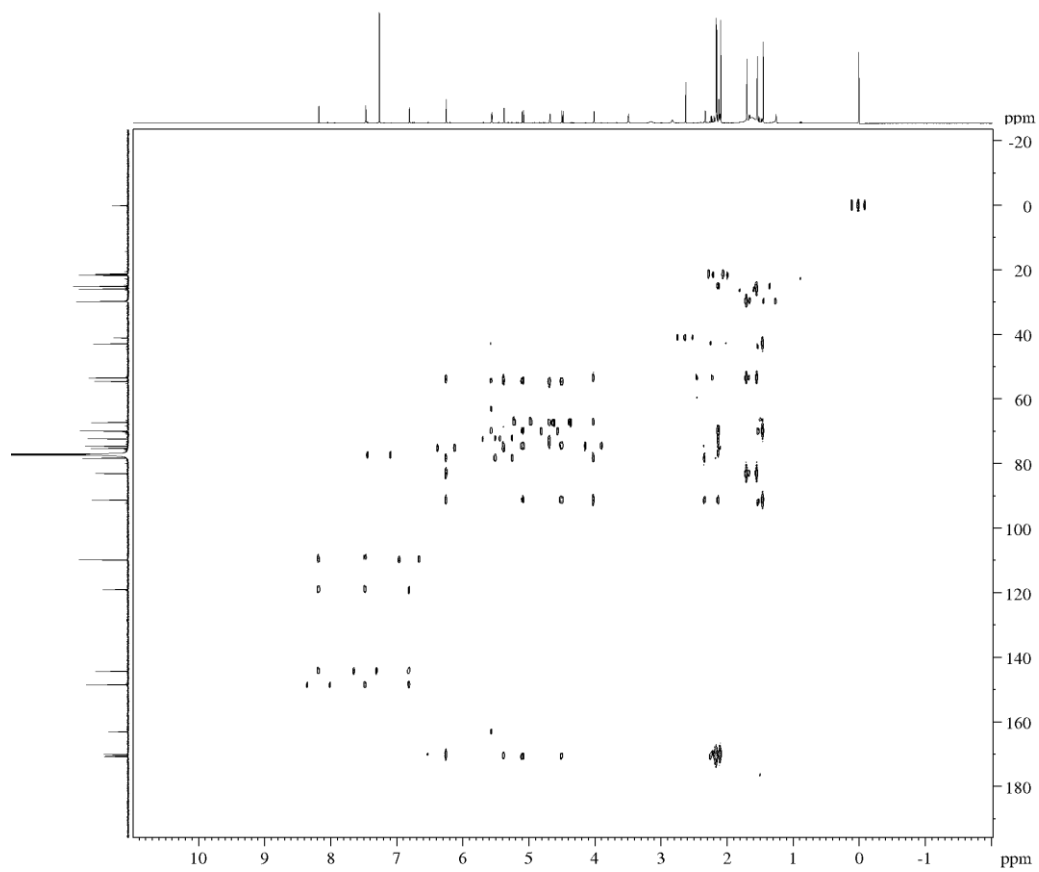


Fig. S8.6 HMBC spectrum (600 MHz, CDCl₃) of compound **1**

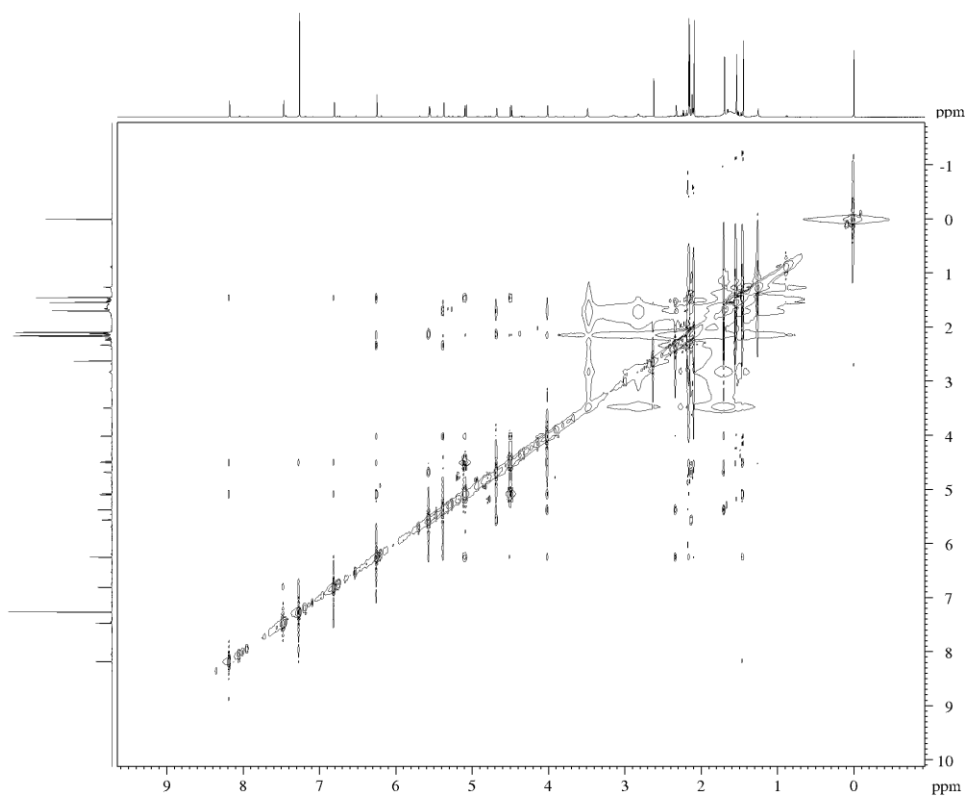


Fig. S8.7 NOESY spectrum (600 MHz, CDCl_3) of compound **8**

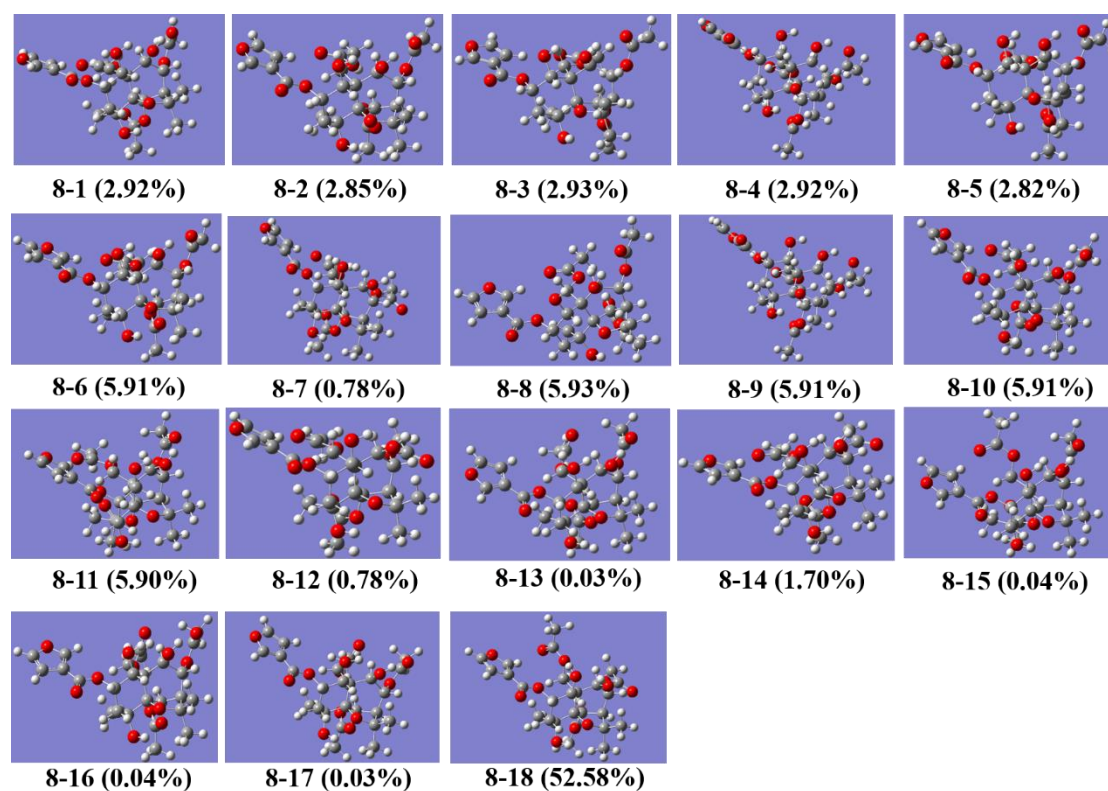


Fig. S8.8 Most stable conformers of **8** in solvated model calculations at the B3LYP/6-311++G (2d, p) level in ECD calculation

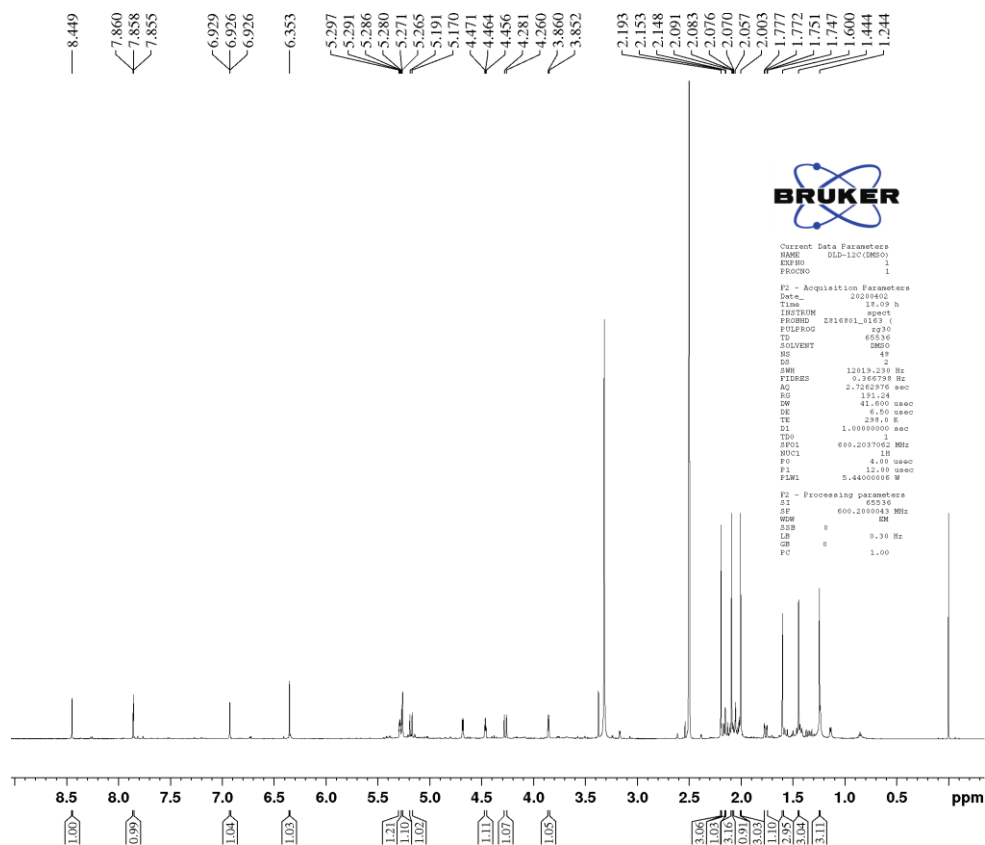


Fig. S8.9 ^1H NMR spectrum (600 MHz, DMSO) of compound **8**

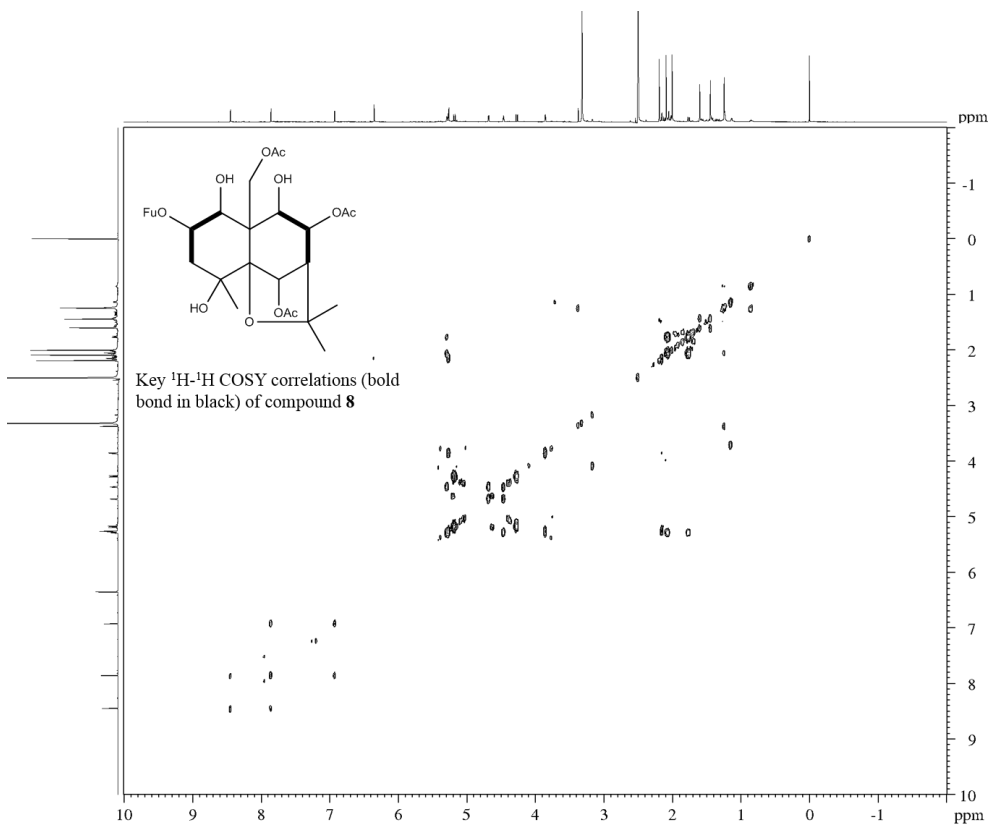


Fig. S8.10 ^1H - ^1H COSY spectrum (600 MHz, DMSO) of compound **8**