Supporting Information for

Original article

New guaiane-type sesquiterpenoid dimers from *Artemisia atrovirens* and their antihepatoma activity

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Contents

1. General experimental procedures

Melting points were obtained on an SGW® X-4B microscopic melting point apparatus (Shanghai Precision & Scientific Instrument Co., Ltd., Shanghai, China). Optical rotations were measured in MeOH with an Autopol VI (Serial #91058) polarimeter (Rudolph Research Analytical, Hackettstown, NJ, USA). The ECD spectra were recorded on a Chirascan CD spectrometer (Applied Photophysics Ltd., Leatherhead, UK). IR spectra were obtained on a Nicolet iS10 spectrometer (Thermo Fisher Scientific, Madison, WI, USA) using KBr pellets. 1D and 2D NMR experiments were carried out using Avance III HD 400 (Bruker, Bremerhaven, Germany) and Avance III 600 (Bruker, Faellanden, Switzerland) spectrometers with TMS as the internal standard. X-ray crystallographic analyses using Cu Kα radiation were performed on a Bruker D8 QUEST instrument (Bruker, Karlsruher, Germany). High resolution mass spectra were acquired on a Shimadzu LC/MS-IT-TOF mass spectrometer (Shimadzu, Kyoto, Japan). TLC detections were performed on silica gel HSGF254 plates (Yantai Jiangyou Silica Gel Development Co., Ltd., Yantai, China), and compounds were visualized by heating after spraying with 10% H_2SO_4 in ethanol. Silica gel (200–300 mesh, Qingdao Makall Group Co., Ltd., Qingdao, China) and Sephadex LH-20 (GE Healthcare Bio-Sciences AB, Uppsala, Sweden) were used for column chromatography. MPLC separations were achieved on a Dr-Flash II apparatus (Lisui, Suzhou, China) using an MCI gel CHP 20P column (75–150 μm, Mitsubishi Chemical Corporation, Tokyo, Japan). Preparative HPLC purification was performed on a Waters 2988 system (Waters, Milford, Massachusetts, USA) with the Waters XBridge® Prep OBD™ C18 column (5 μm, 19 × 250 mm, Waters, Ireland). Semipreparative HPLC purification was performed on a Shimadzu LC-CBM-20 system (Shimadzu, Kyoto, Japan) with an Agilent Eclipse XDB-C18 column (5 μm, 9.4 × 250 mm, Agilent Technologies, Santa Clara, CA, USA).

Cell cycle and apoptosis assays were performed on a flow cytometer (FACSCalibur, Becton Dickinson Co., Ltd., New Jersey, USA). Western blot assay was conducted on vertical electrophoresis apparatus (DYCZ-24DN, Liuyi Biotechnology Co., Ltd., Beijing, China) and a Semi-Dry Blotter (YRDIMES, wealtec Co., Ltd., Nevada, USA.), exposured by MultiSpectral imaging system (BioSpectrum, Analytik Jena Co., Ltd., Jena, Germany).

2. NMR, MS, IR, $[\alpha]_D$ and CD spectra of compound 1

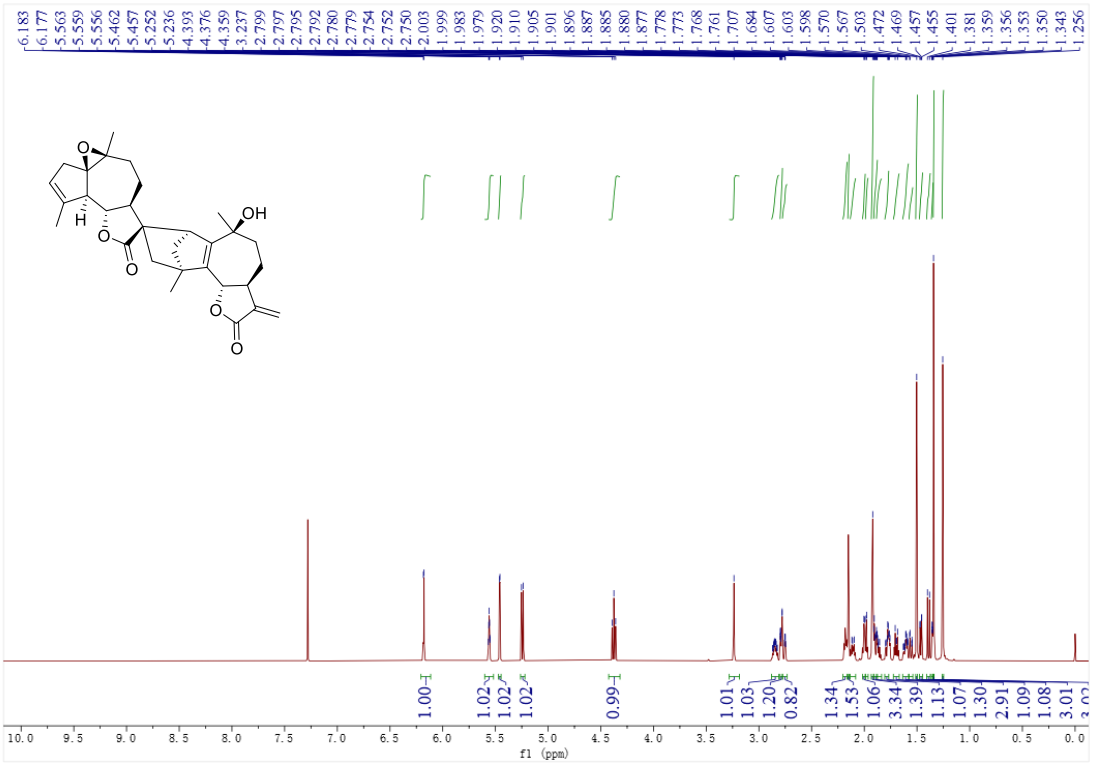


Figure S1 ^{1}H NMR spectrum (600 MHz) of artematrolide A (**1**) in $CDCl_3$.

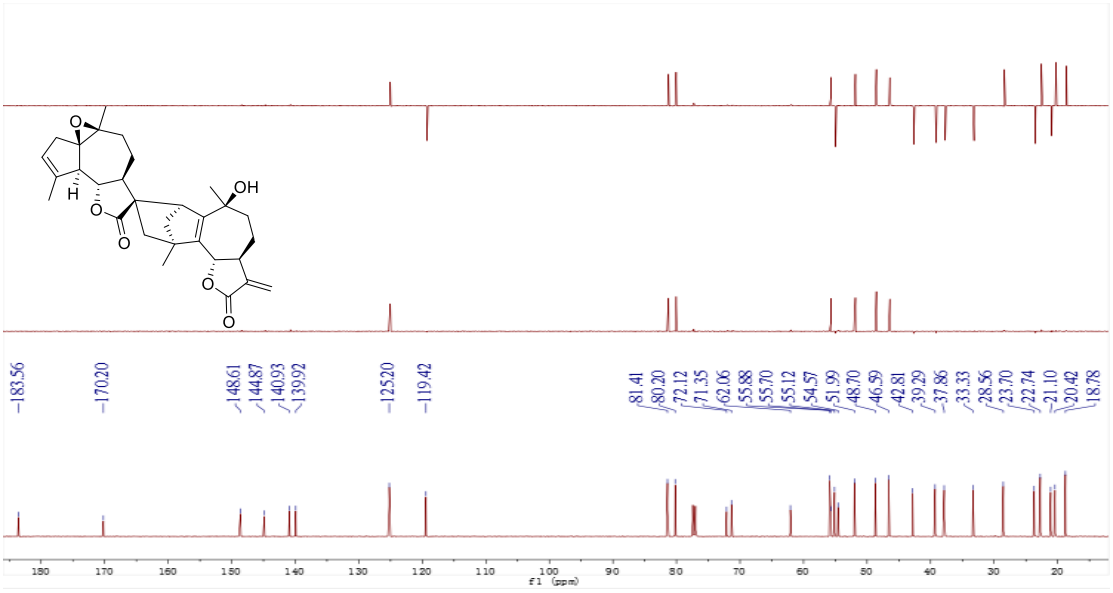


Figure S2 ^{13}C NMR spectra (150 MHz) of artematrolide A (**1**) in $CDCl_3$.

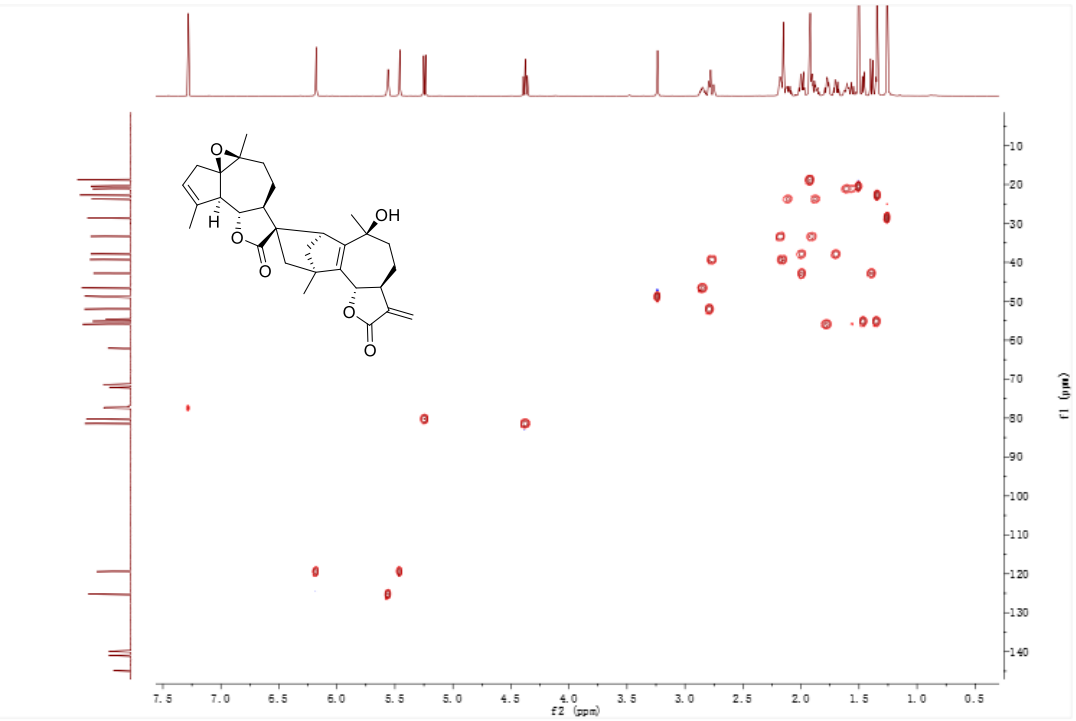


Figure S3 HSQC spectrum (600 MHz) of artematrolide A (**1**) in $CDCl_3$.

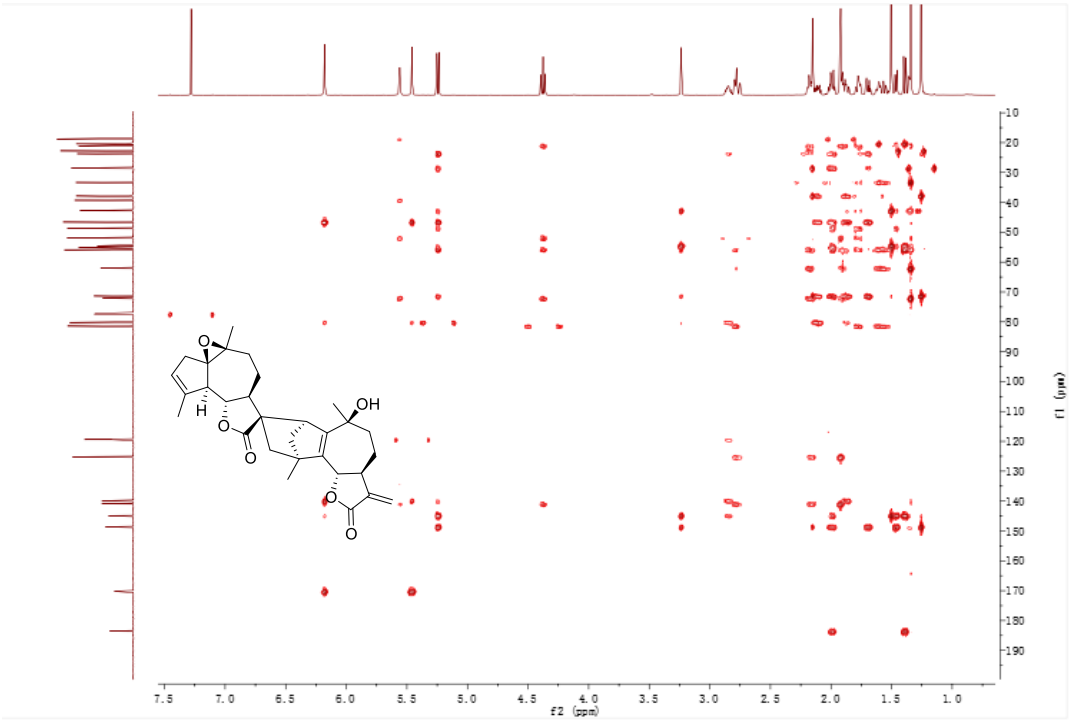


Figure S4 HMBC spectrum (600 MHz) of artematrolide A (**1**) in $CDCl_3$.

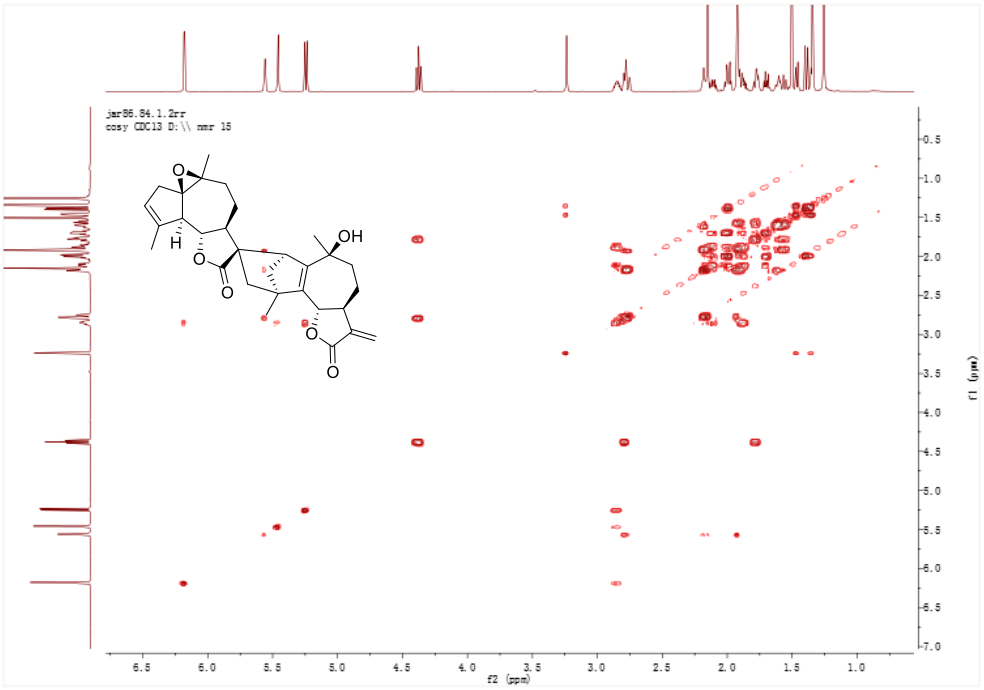


Figure S5 ^{1}H–^{1}H COSY spectrum (600 MHz) of artematrolide A (**1**) in $CDCl_3$.

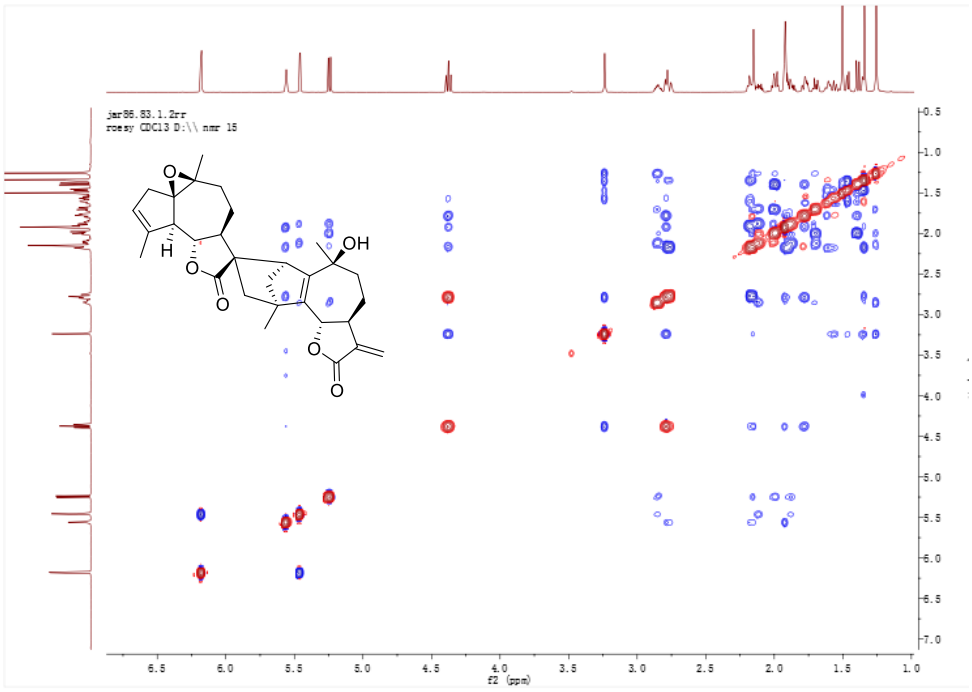


Figure S6 ROESY spectrum (600 MHz) of artematrolide A (**1**) in $CDCl_3$.

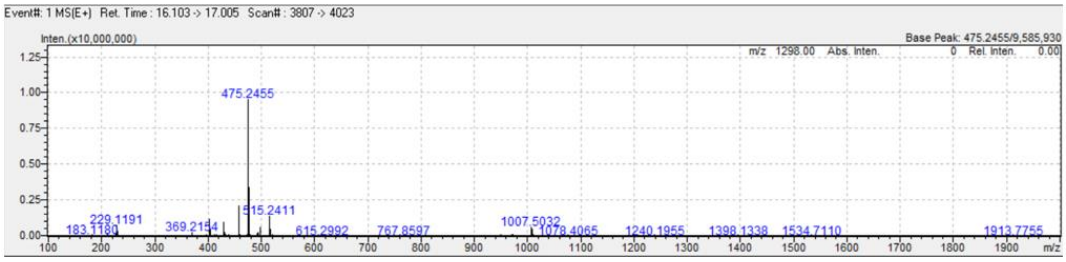


Figure S7 HRESIMS spectrum of artematrolide A (**1**).

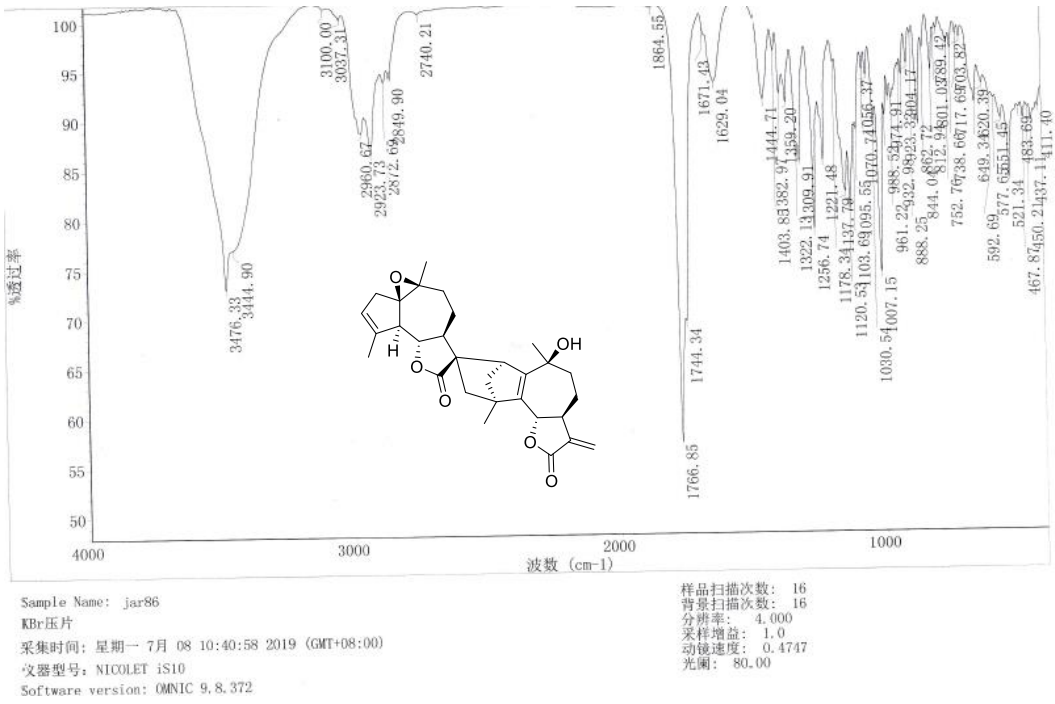


Figure S8 IR spectrum of artematrolide A (**1**).

Rudolph Research Analytical

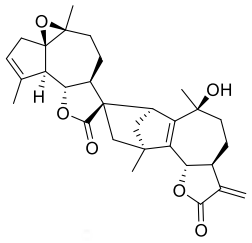
This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Monday, 08-JUL-2019

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled



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5	29.79	0.54	1.81	30.36	29.29

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	jar86	05:12:12 PM	29.29	SR	0.0082	589	100.00	0.028	24.6
2	jar86	05:12:20 PM	30.36	SR	0.0085	589	100.00	0.028	24.6
3	jar86	05:12:28 PM	29.29	SR	0.0082	589	100.00	0.028	24.5
4	jar86	05:12:36 PM	29.64	SR	0.0083	589	100.00	0.028	24.5
5	jar86	05:12:44 PM	30.36	SR	0.0085	589	100.00	0.028	24.5

Figure S9 Optical rotation spectrum of artematrolide A (**1**).

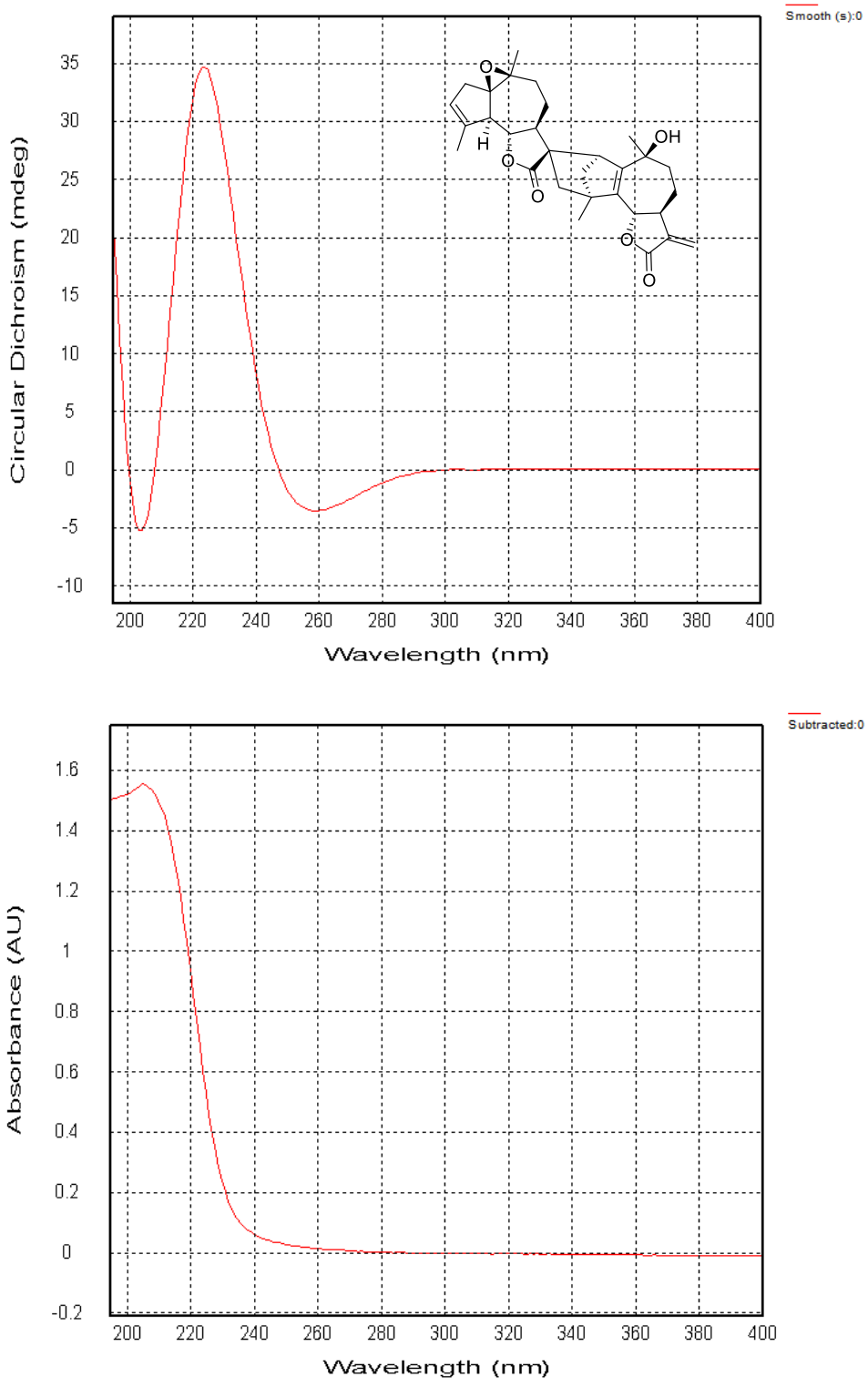


Figure S10 CD (top) and UV (bottom) spectra of artematrolide A (**1**).

3. NMR, MS, IR, $[\alpha]_D$ and CD spectra of compound 2

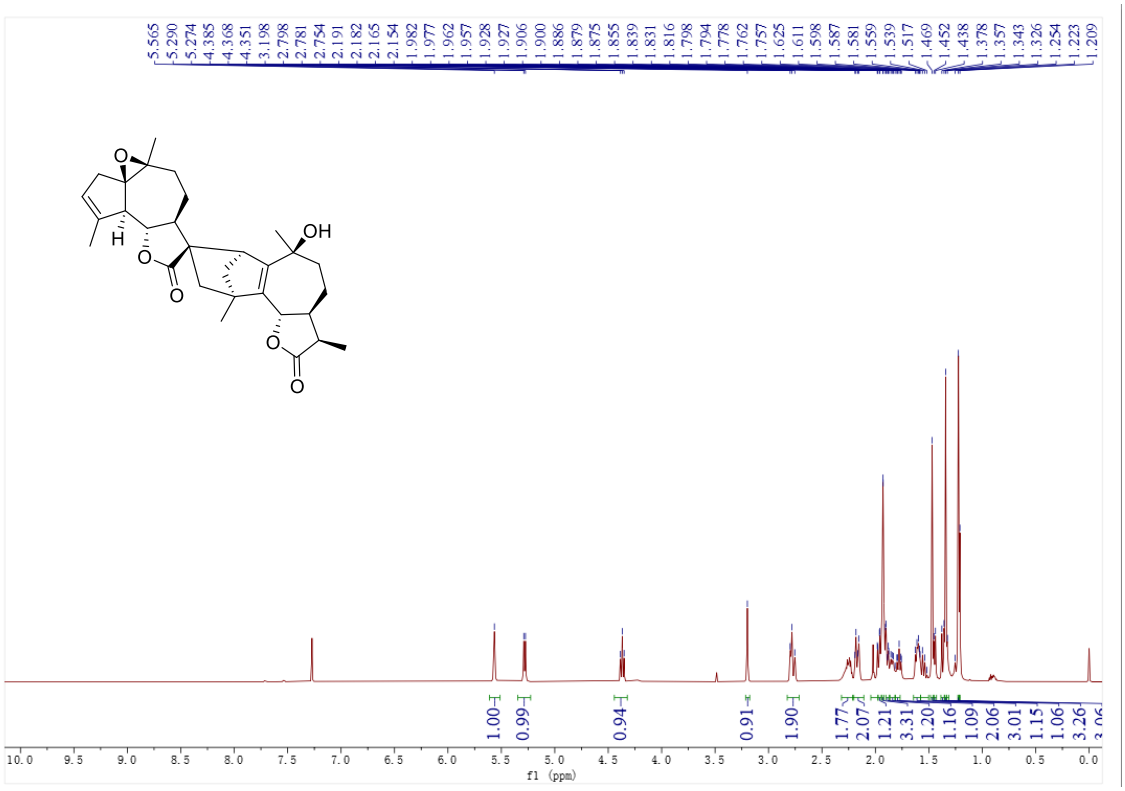


Figure S11 ^{1}H NMR spectrum (600 MHz) of artematrolide B (**2**) in $CDCl_3$.

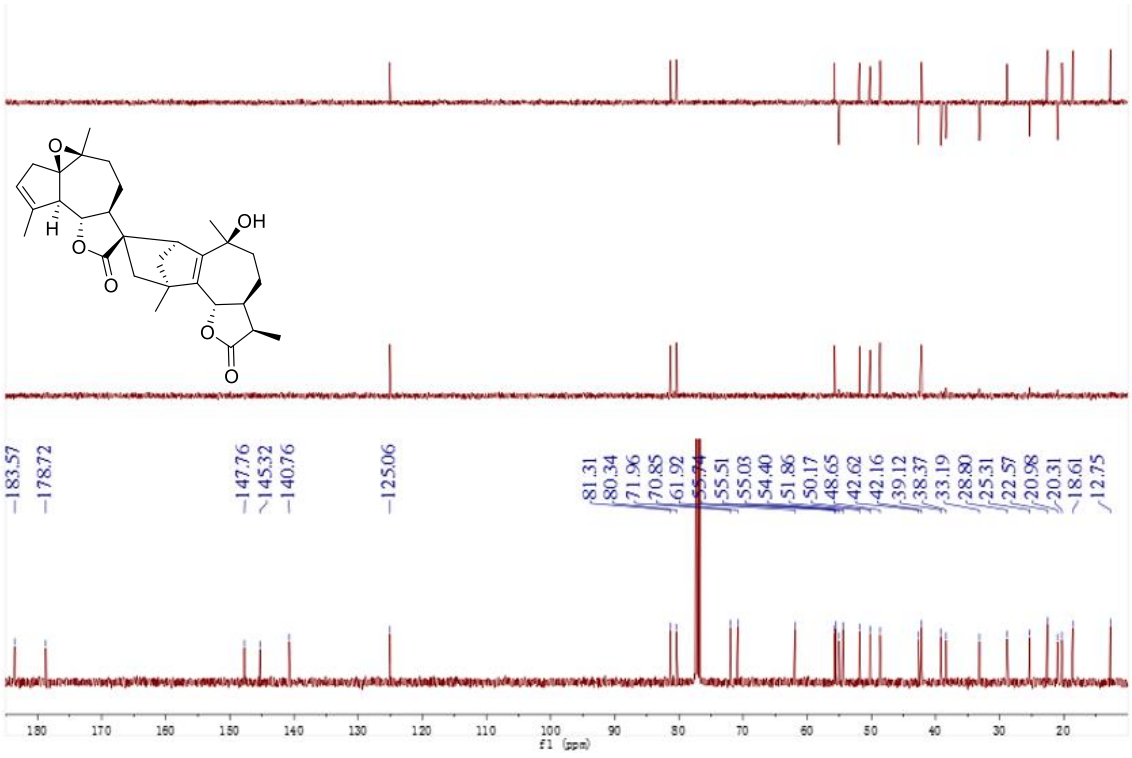


Figure S12 ^{13}C NMR spectra (150 MHz) of artematrolide B (**2**) in $CDCl_3$.

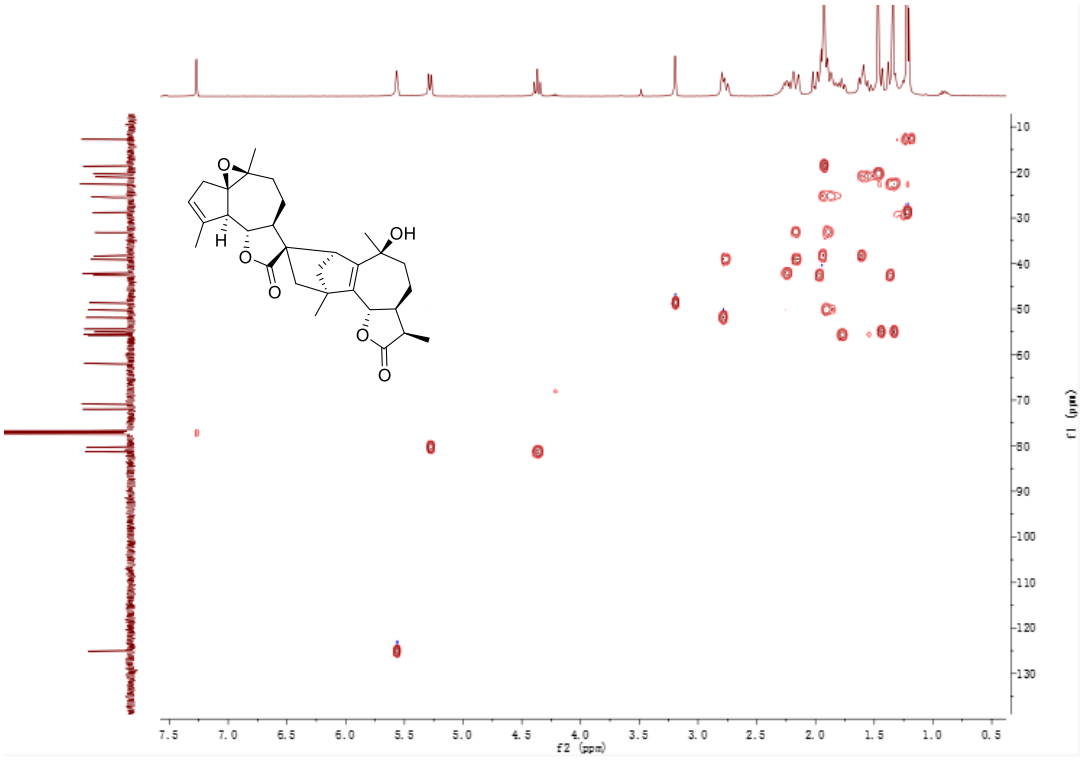


Figure S13 HSQC spectrum (600 MHz) of artematrolide B (**2**) in $CDCl_3$.

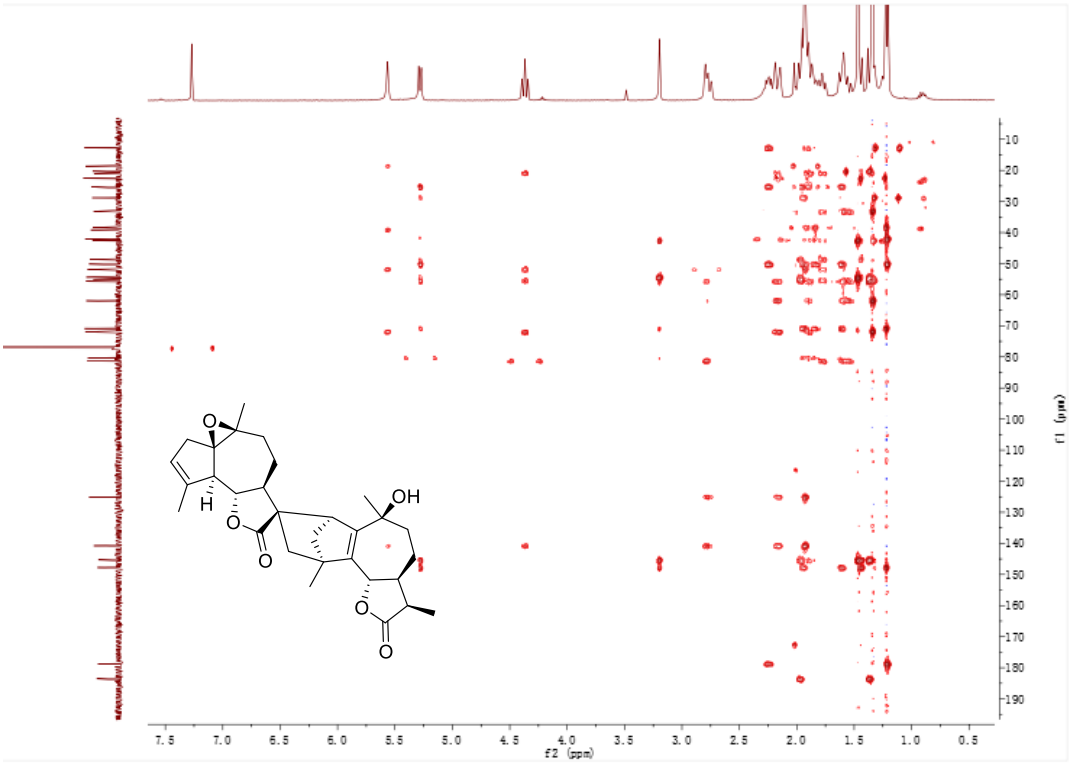


Figure S14 HMBC spectrum (600 MHz) of artematrolide B (**2**) in $CDCl_3$.

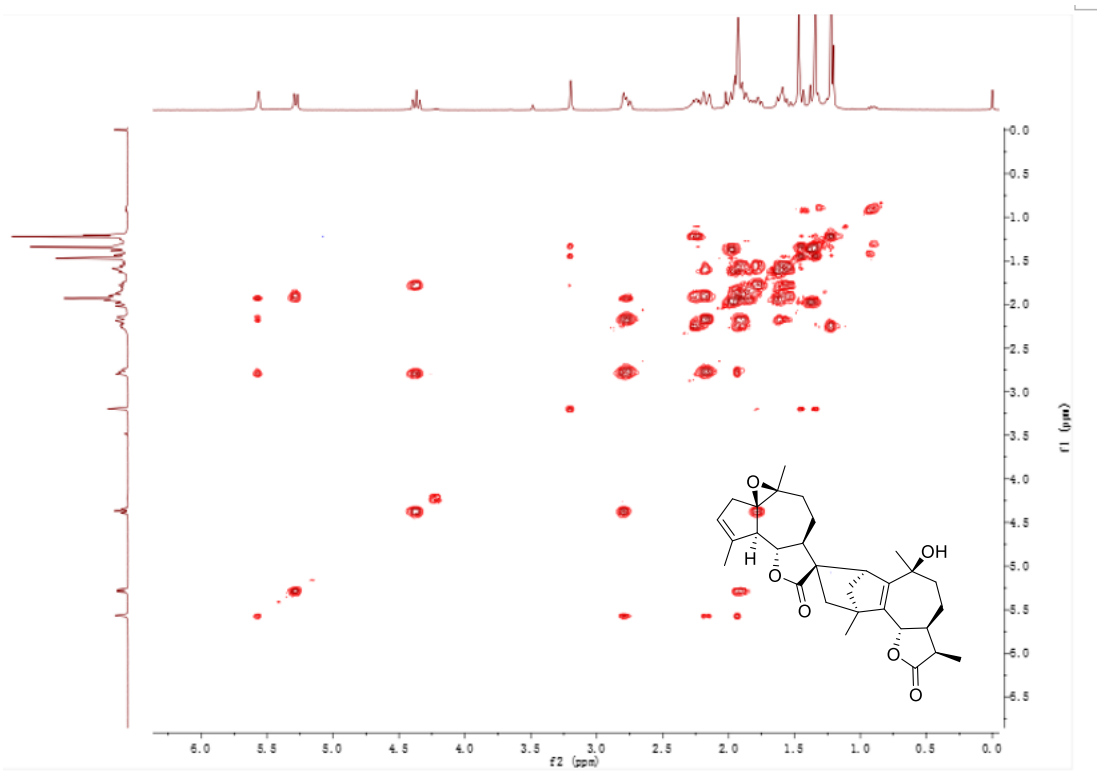


Figure S15 ^{1}H–^{1}H COSY spectrum (600 MHz) of artematrolide B (**2**) in $CDCl_3$.

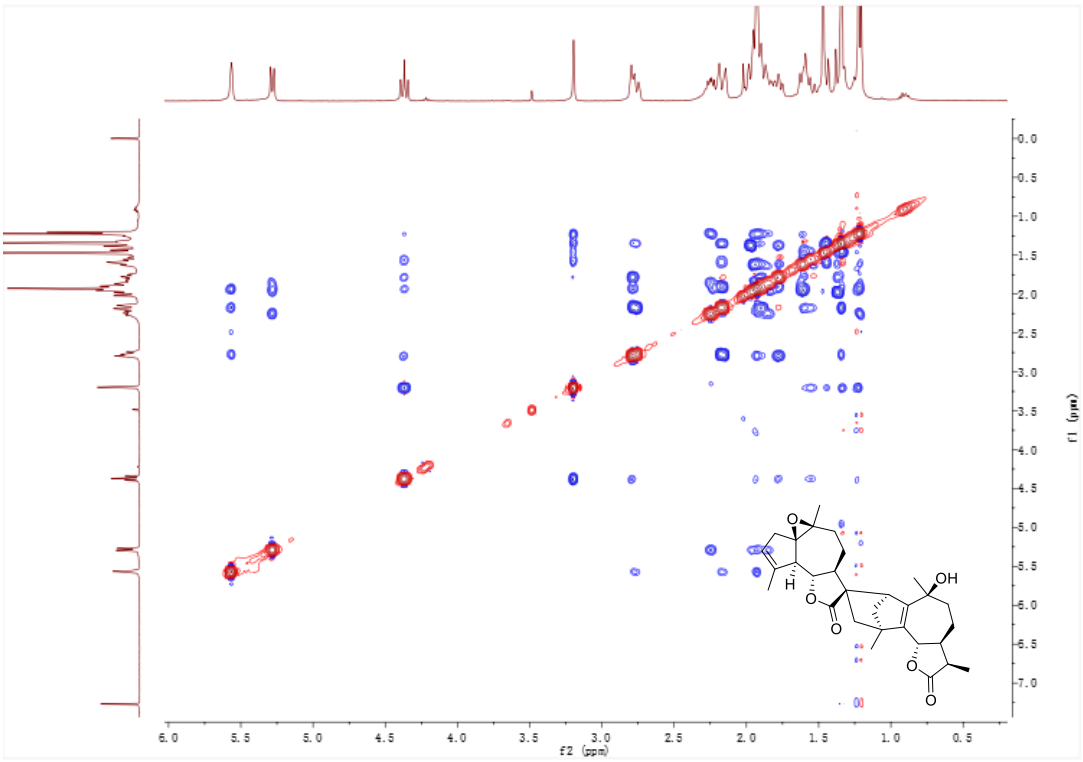


Figure S16 ROESY spectrum (600 MHz) of artematrolide B (**2**) in $CDCl_3$.

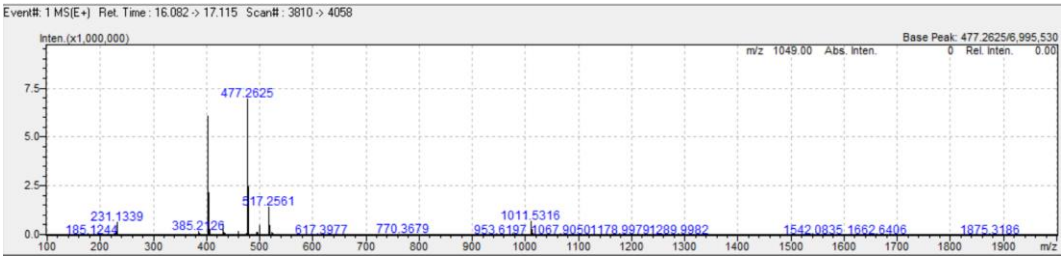


Figure S17 HRESIMS spectrum of artematrolide B (**2**).

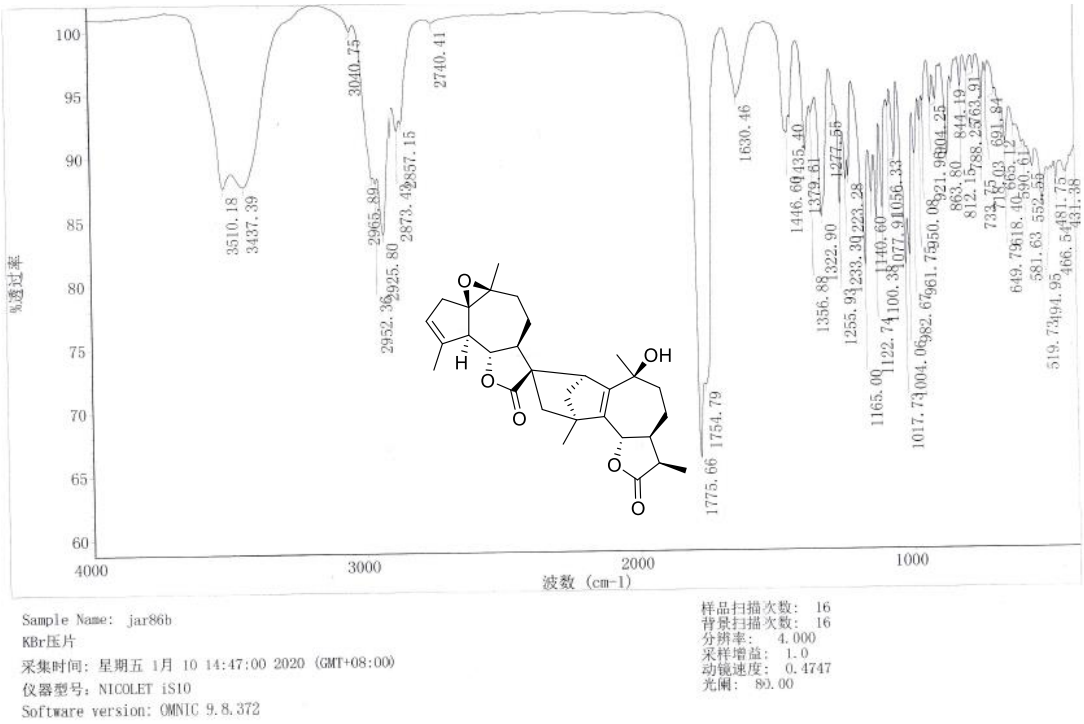


Figure S18 IR spectrum of artematrolide B (**2**).

Rudolph Research Analytical

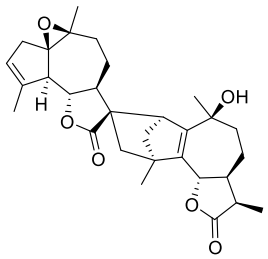
This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Saturday, 04-JAN-2020

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled



n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	121.76	0.55	0.45	122.20	120.80

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	jar86b	12:38:31 PM	122.00	SR	0.0610	589	100.00	0.050	21.6
2	jar86b	12:38:39 PM	122.20	SR	0.0611	589	100.00	0.050	21.6
3	jar86b	12:38:47 PM	122.00	SR	0.0610	589	100.00	0.050	21.6
4	jar86b	12:38:56 PM	121.80	SR	0.0609	589	100.00	0.050	21.6
5	jar86b	12:39:04 PM	120.80	SR	0.0604	589	100.00	0.050	21.6

Figure S19 Optical rotation spectrum of artematrolide B (**2**).

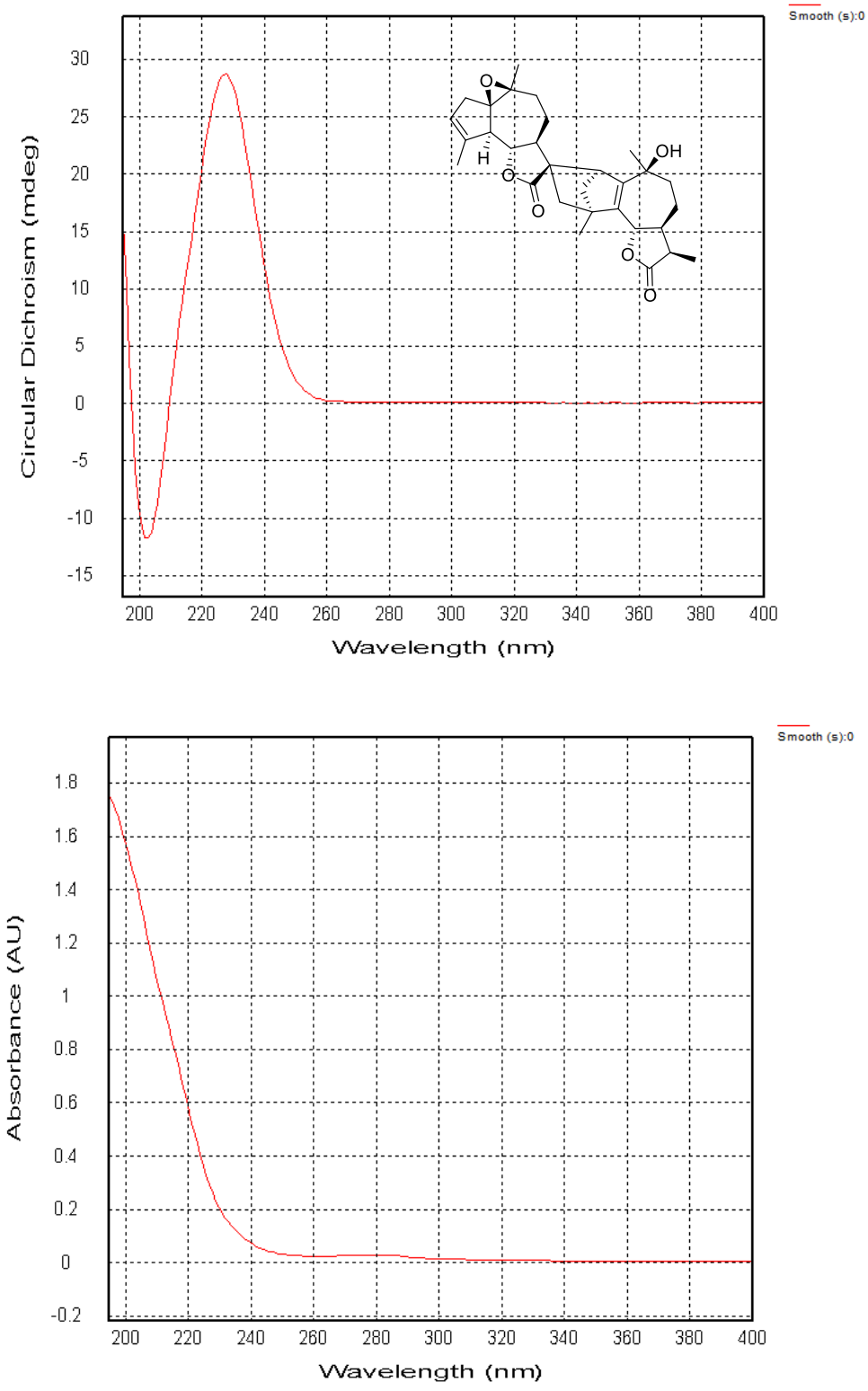


Figure S20 CD (top) and UV (bottom) spectra of artematrolide B (**2**).

4. NMR, MS, IR, $[\alpha]_D$ and CD spectra of compound 3

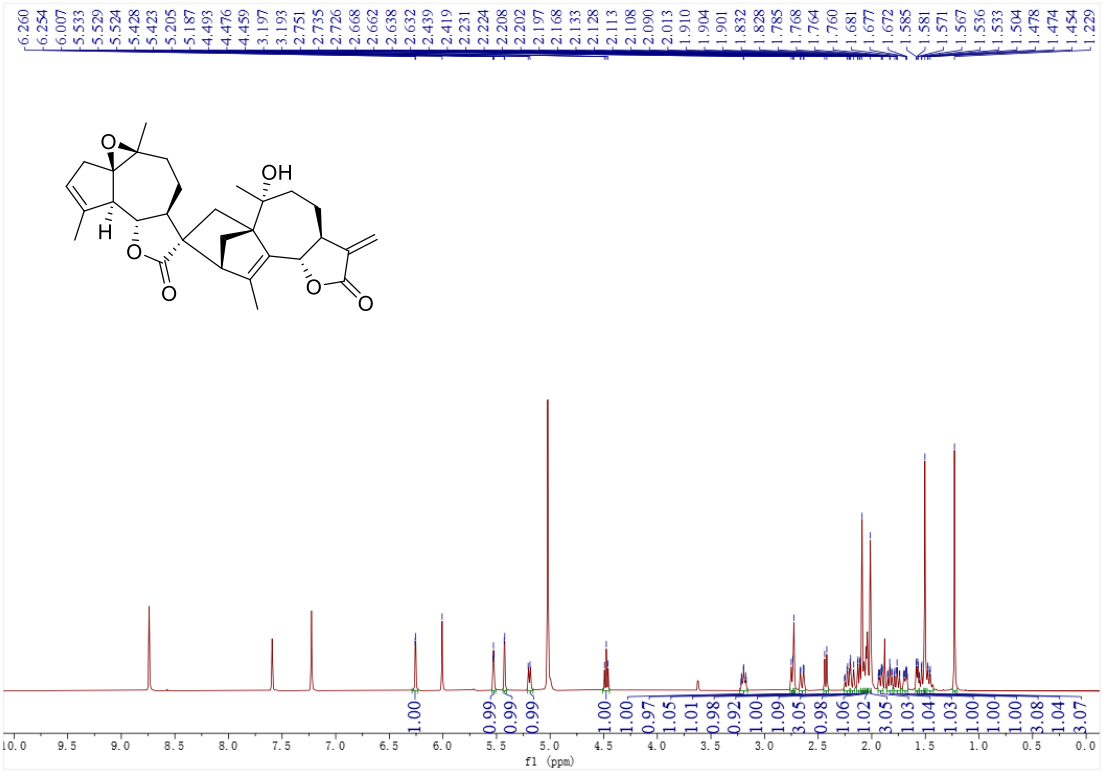


Figure S21 ^{1}H NMR spectrum (600 MHz) of lavandiolide A (**3**) in pyridine-d_5.

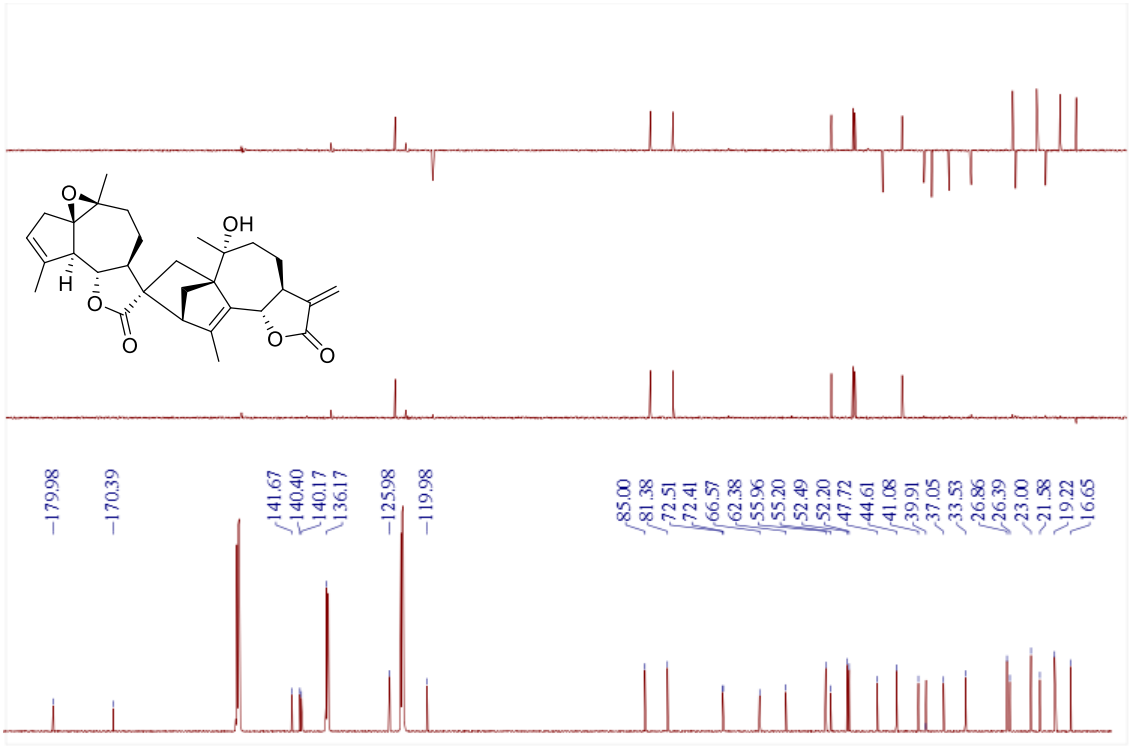


Figure S22 ^{13}C NMR spectrum (150 MHz) of lavandiolide A (**3**) in pyridine-d_5.

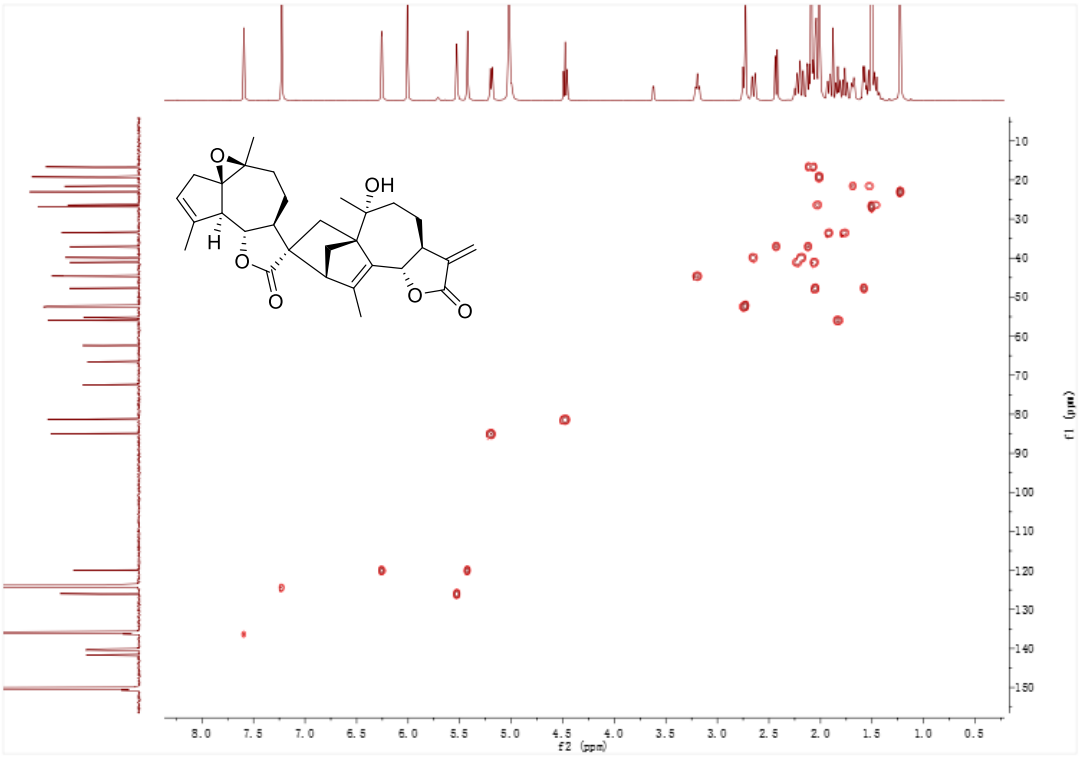


Figure S23 HSQC spectrum (600 MHz) of lavandiolide A (**3**) in pyridine-d_5.

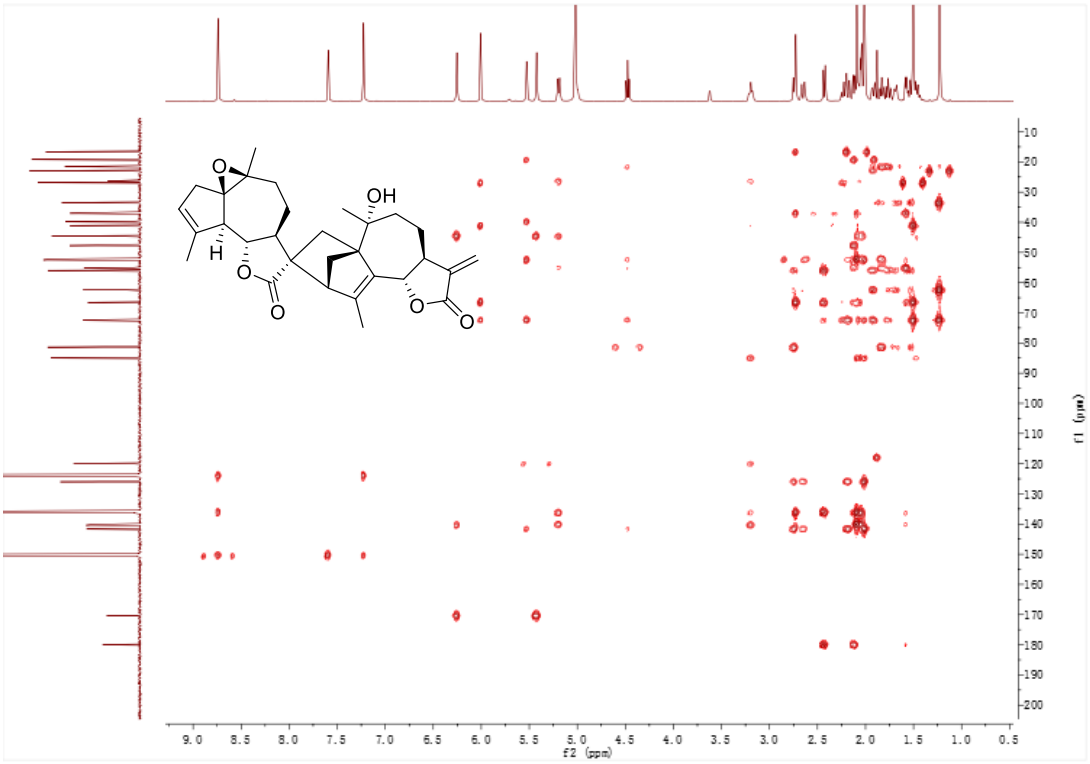


Figure S24 HMBC spectrum (600 MHz) of lavandiolide A (**3**) in pyridine-d_5.

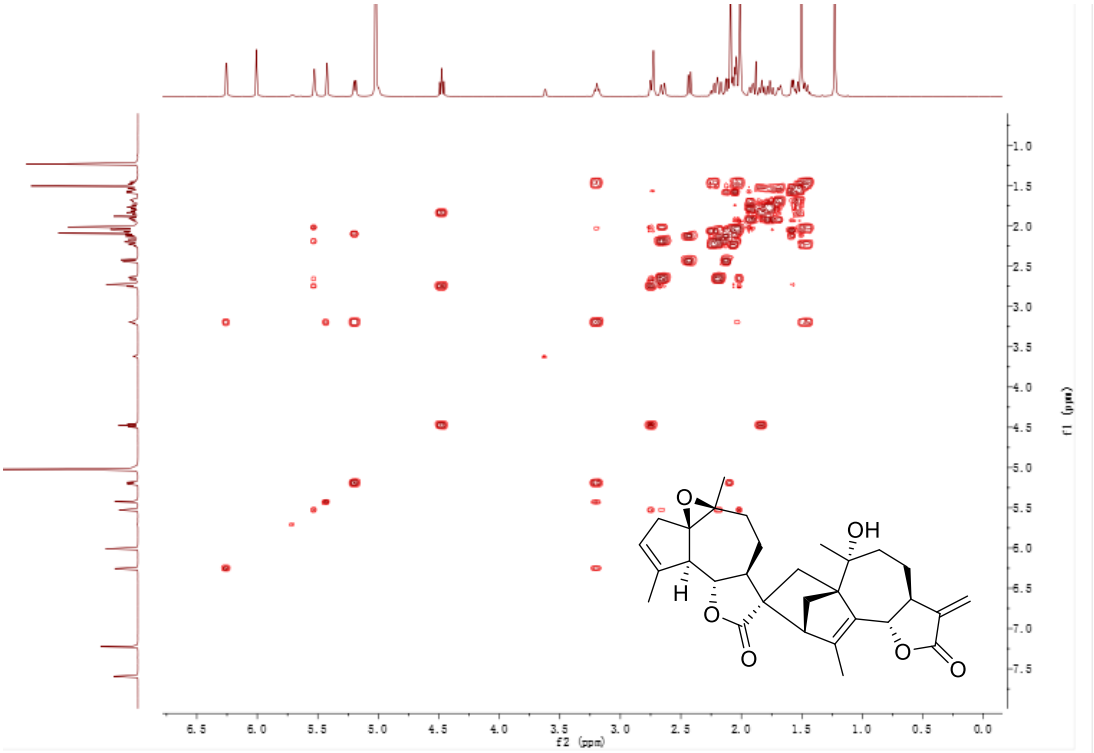


Figure S25 ^{1}H–^{1}H COSY spectrum (600 MHz) of lavandiolide A (**3**) in pyridine-d_5.

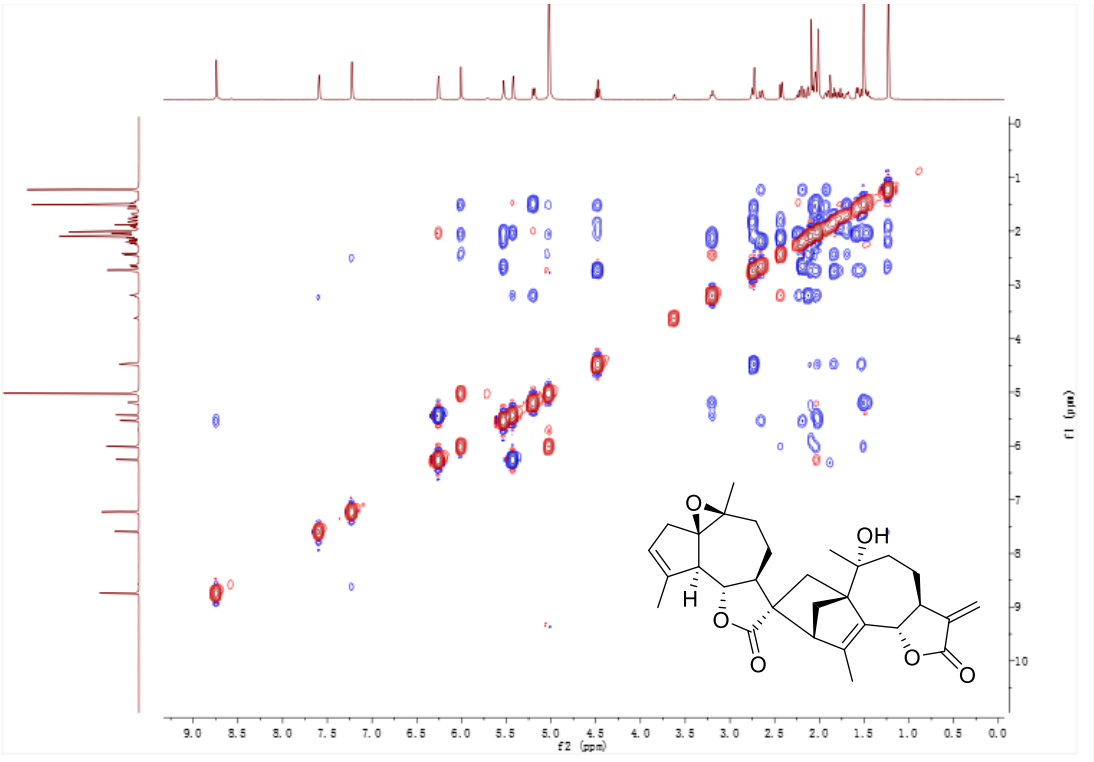


Figure S26 ROESY spectrum of (600 MHz) lavandiolide A (**3**) in pyridine-d_5.

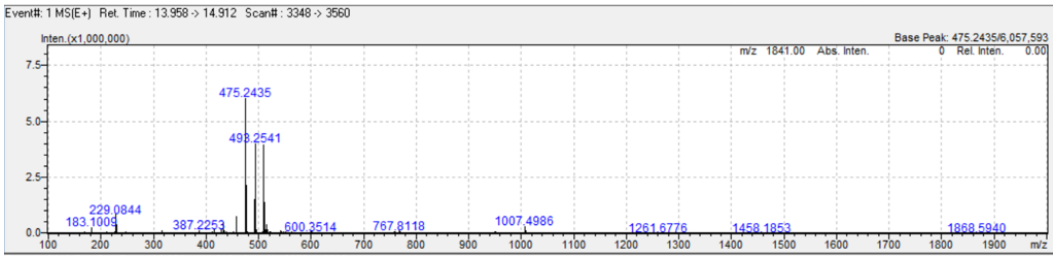


Figure S27 HRESIMS spectrum of lavandiolide A (**3**).

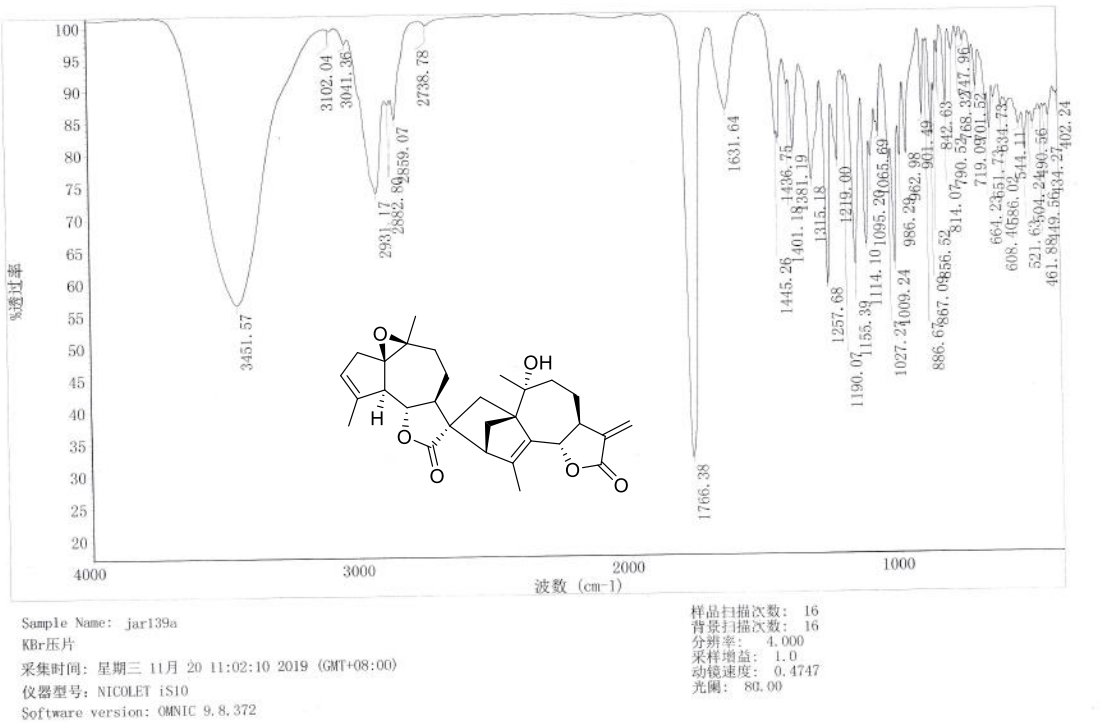


Figure S28 IR spectrum of lavandiolide A (**3**).

Rudolph Research Analytical

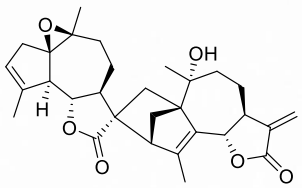
This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Monday, 07-SEP-2020

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled



n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	29.80	0.36	1.20	30.13	29.25

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
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2	JAR139A	05:00:13 PM	30.13	SR	0.0241	589	100.00	0.080	24.9
3	JAR139A	05:00:21 PM	29.75	SR	0.0238	589	100.00	0.080	24.9
4	JAR139A	05:00:29 PM	29.75	SR	0.0238	589	100.00	0.080	24.9
5	JAR139A	05:00:37 PM	29.25	SR	0.0234	589	100.00	0.080	25.0

Figure S29 Optical rotation spectrum of lavandiolide A (**3**).

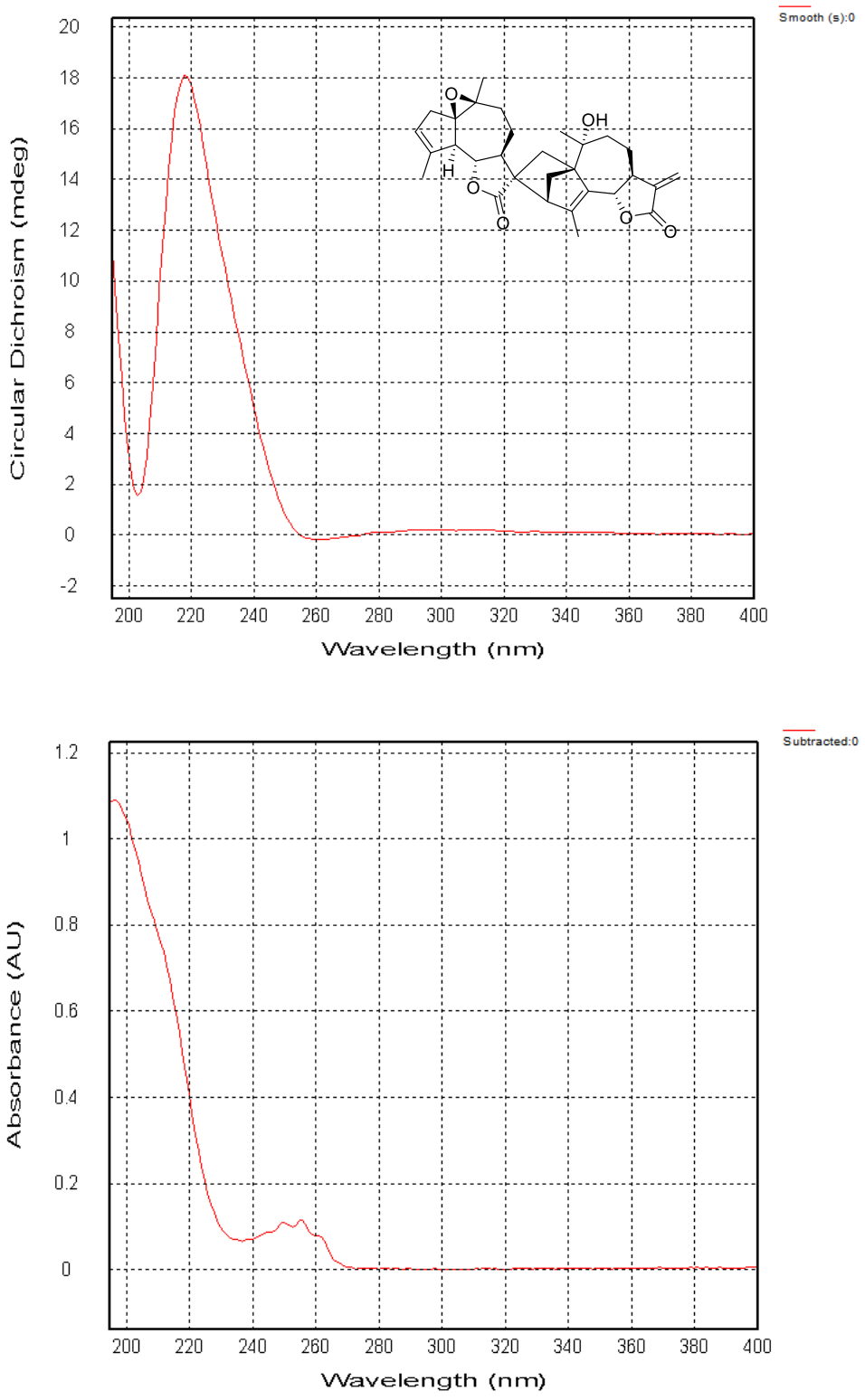


Figure S30 CD (top) and UV (bottom) spectra of lavandiolide A (**3**).

5. NMR, MS, IR, $[\alpha]_D$ and CD spectra of compound 4

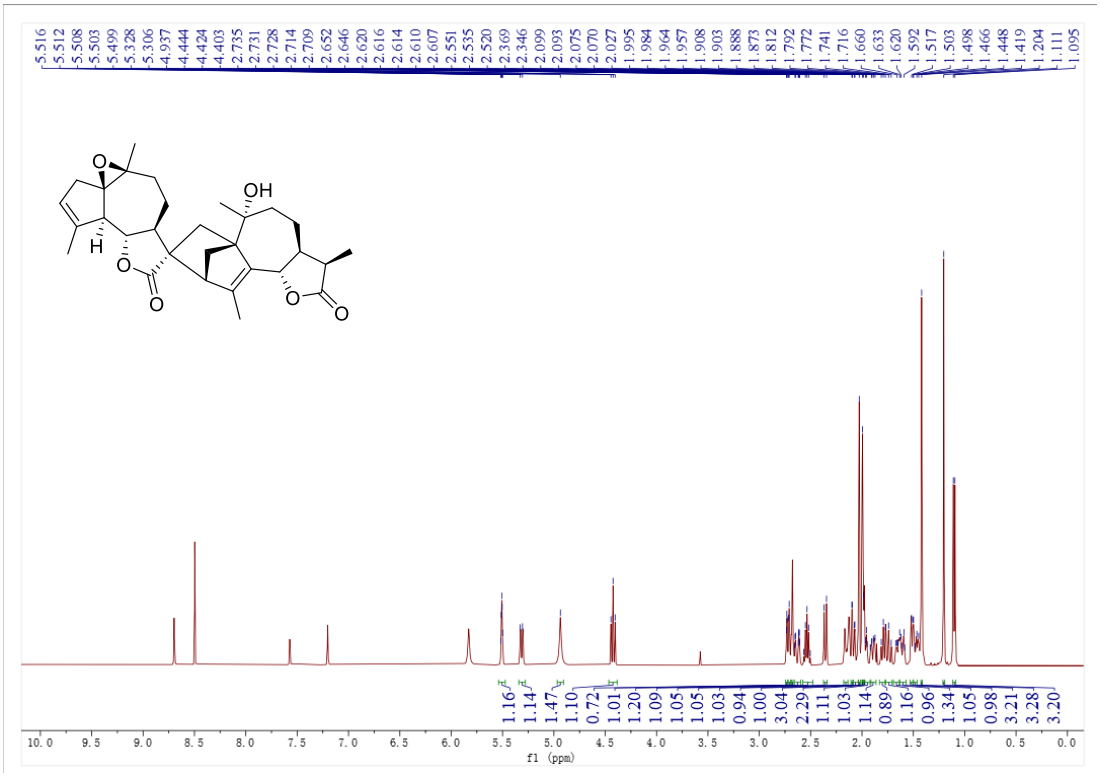


Figure S31 ^{1}H NMR spectrum (600 MHz) of lavandiolide B (**4**) in pyridine-d_5.

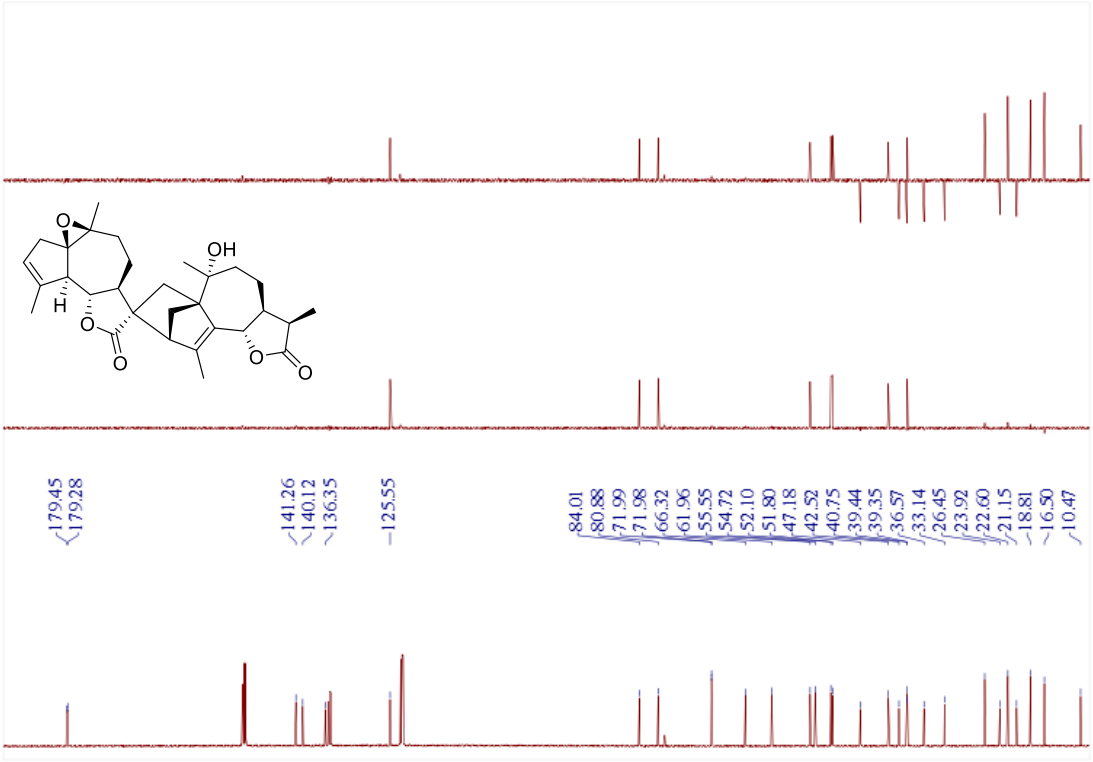


Figure S32 ^{13}C NMR spectrum (150 MHz) of lavandiolide B (**4**) in pyridine-d_5.

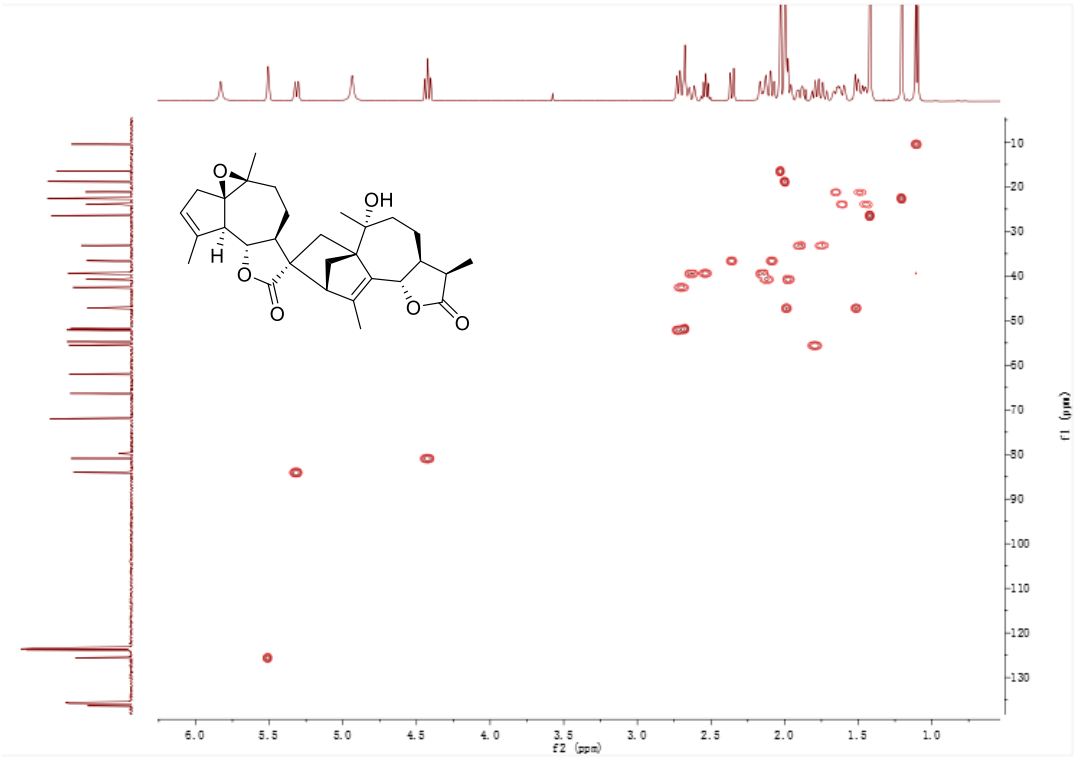


Figure S33 HSQC spectrum (600 MHz) of lavandiolide B (**4**) in pyridine-d_5.

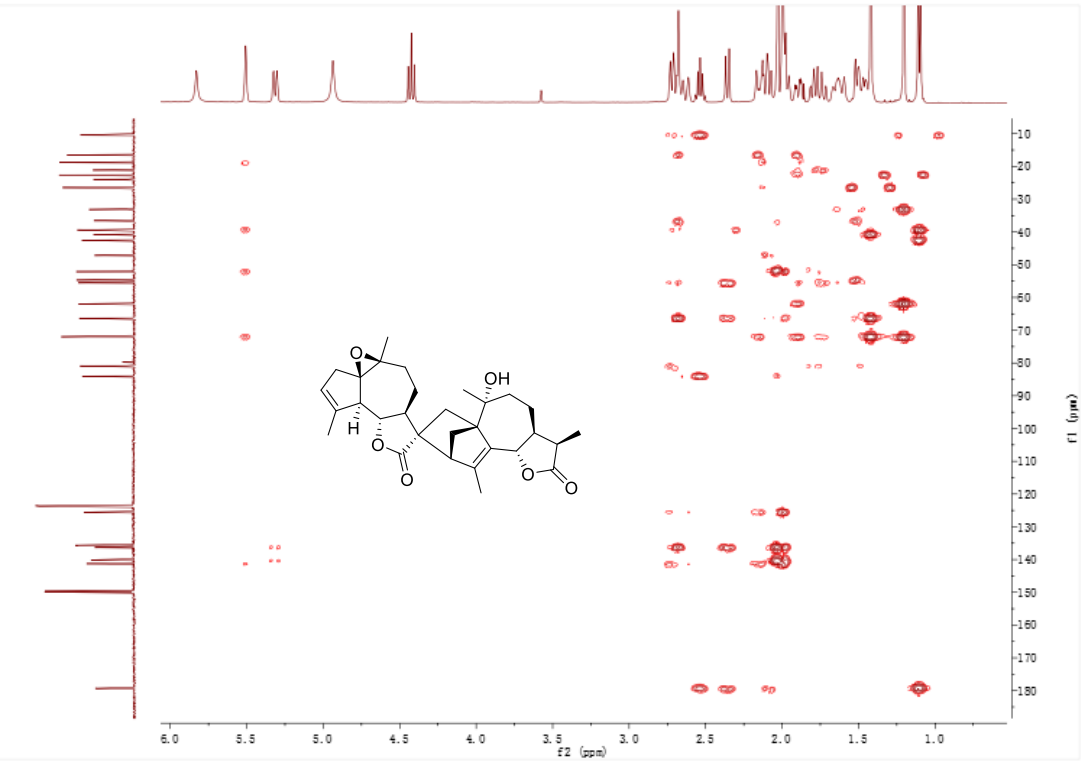


Figure S34 HMBC spectrum (600 MHz) of lavandiolide B (**4**) in pyridine-d_5.

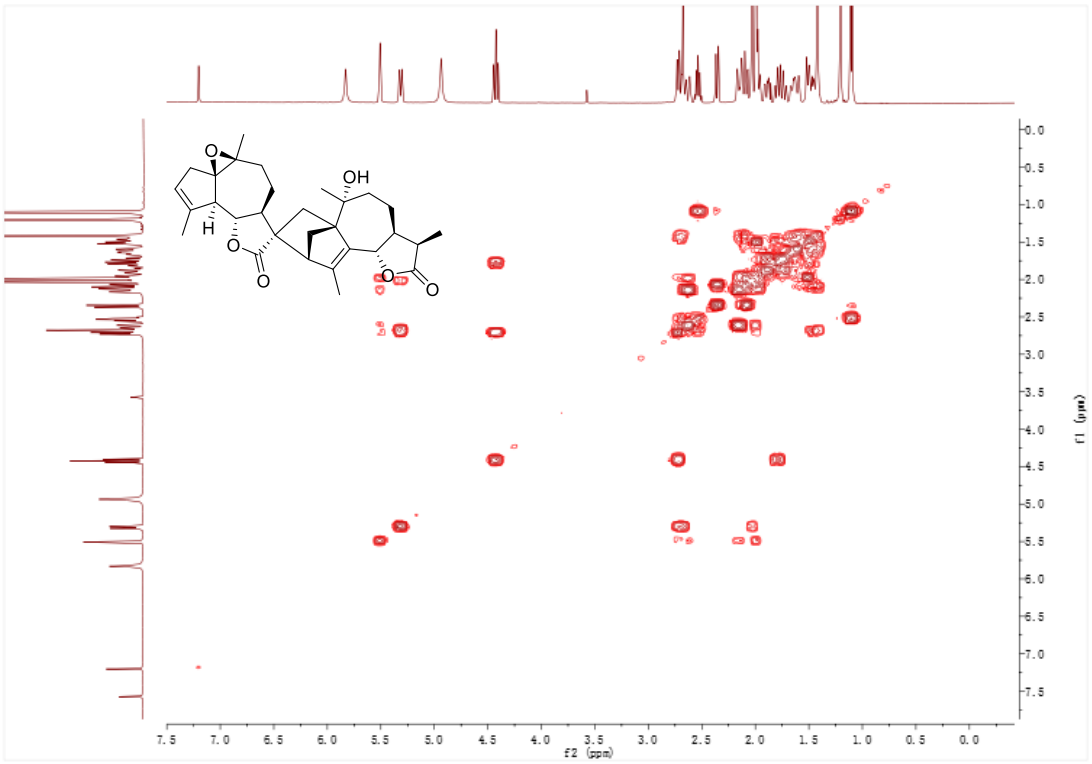


Figure S35 ^{1}H–^{1}H COSY spectrum (600 MHz) of lavandiolide B (**4**) in pyridine-d_5.

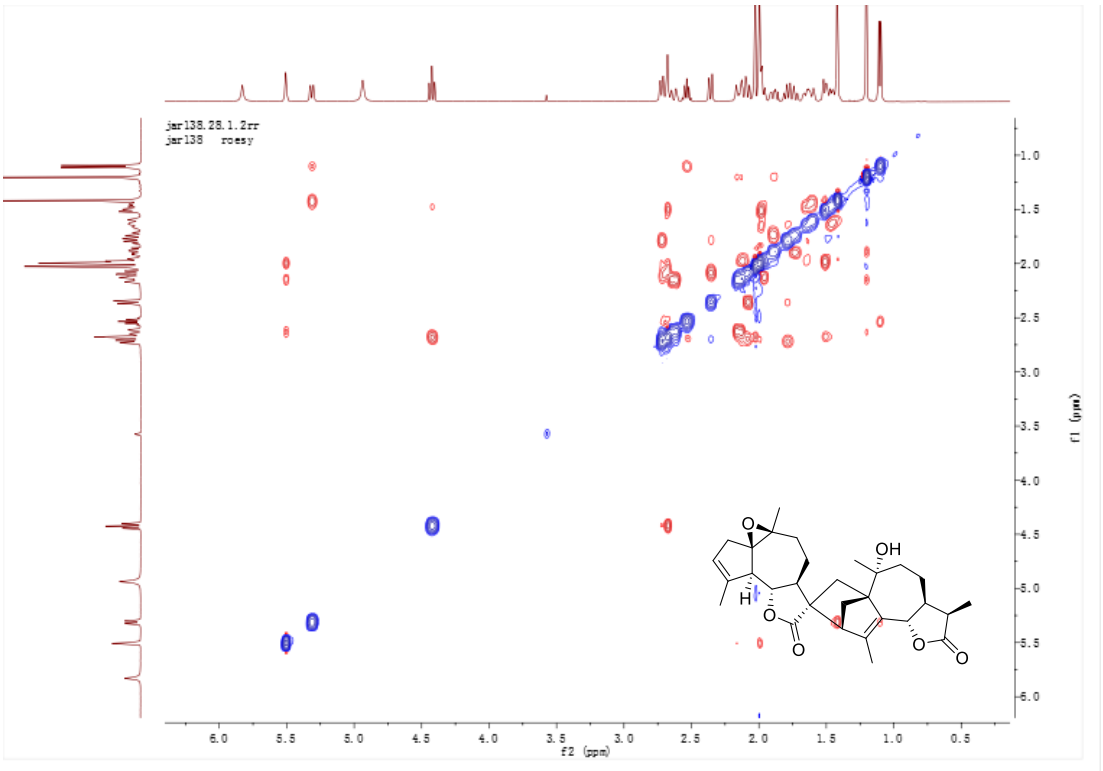


Figure S36 ROESY spectrum (600 MHz) of lavandiolide B (**4**) in pyridine-d_5.

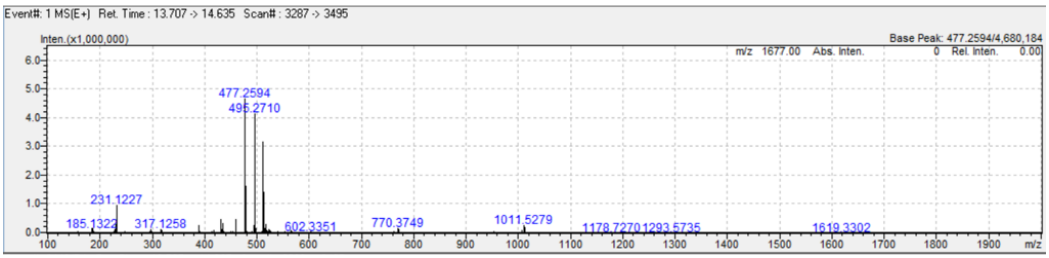


Figure S37 HRESIMS spectrum of lavandiolide B (**4**).

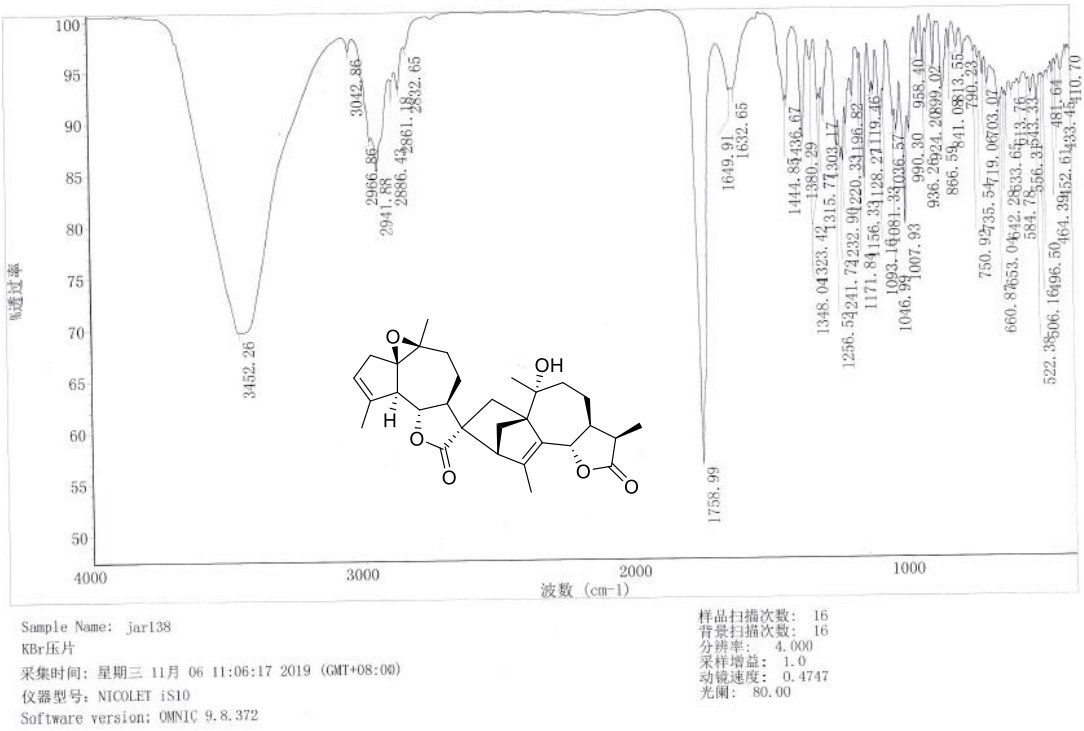


Figure S38 IR spectrum of lavandiolide B (**4**).

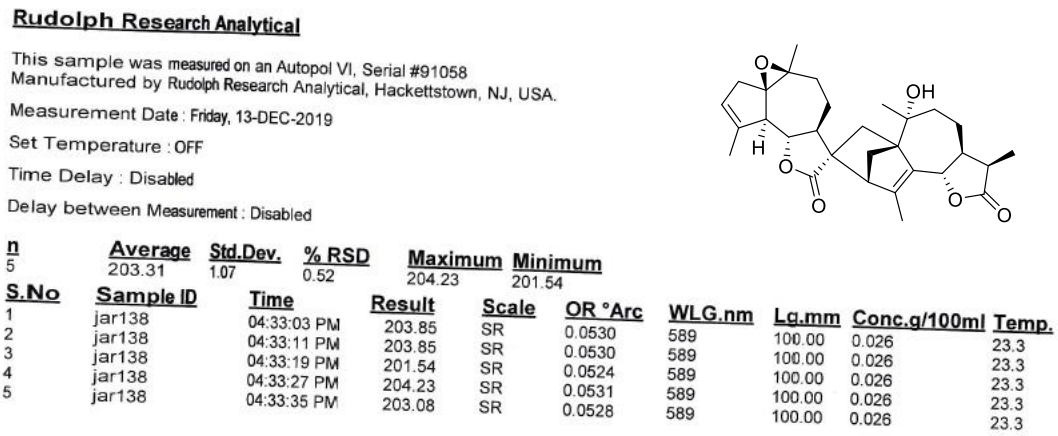


Figure S39 Optical rotation spectrum of lavandiolide B (**4**).

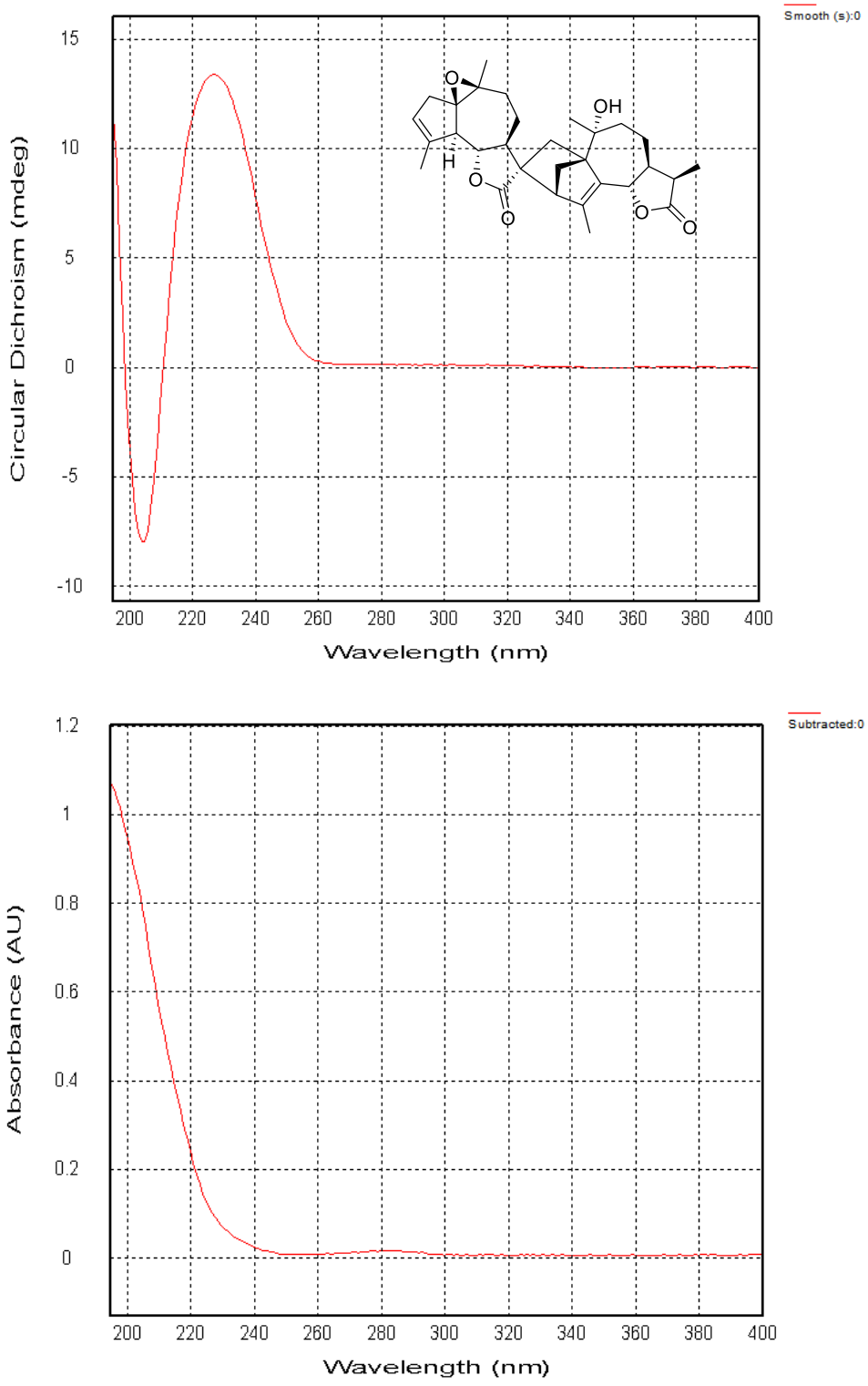


Figure S40 CD (top) and UV (bottom) spectra of lavandiolide B (**4**).

6. NMR, MS, IR, $[\alpha]_D$ and CD spectra of compound 5

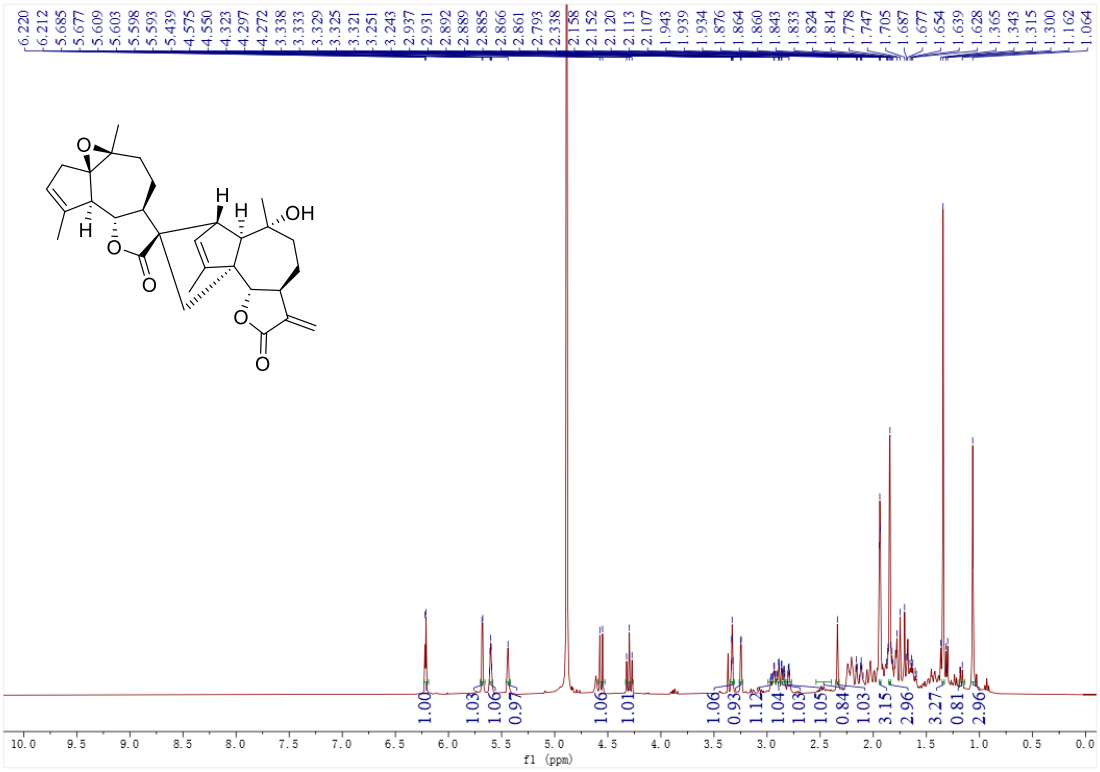


Figure S41 ^{1}H NMR spectrum (400 MHz) of artematrolide C (**5**) in CD_3OD.

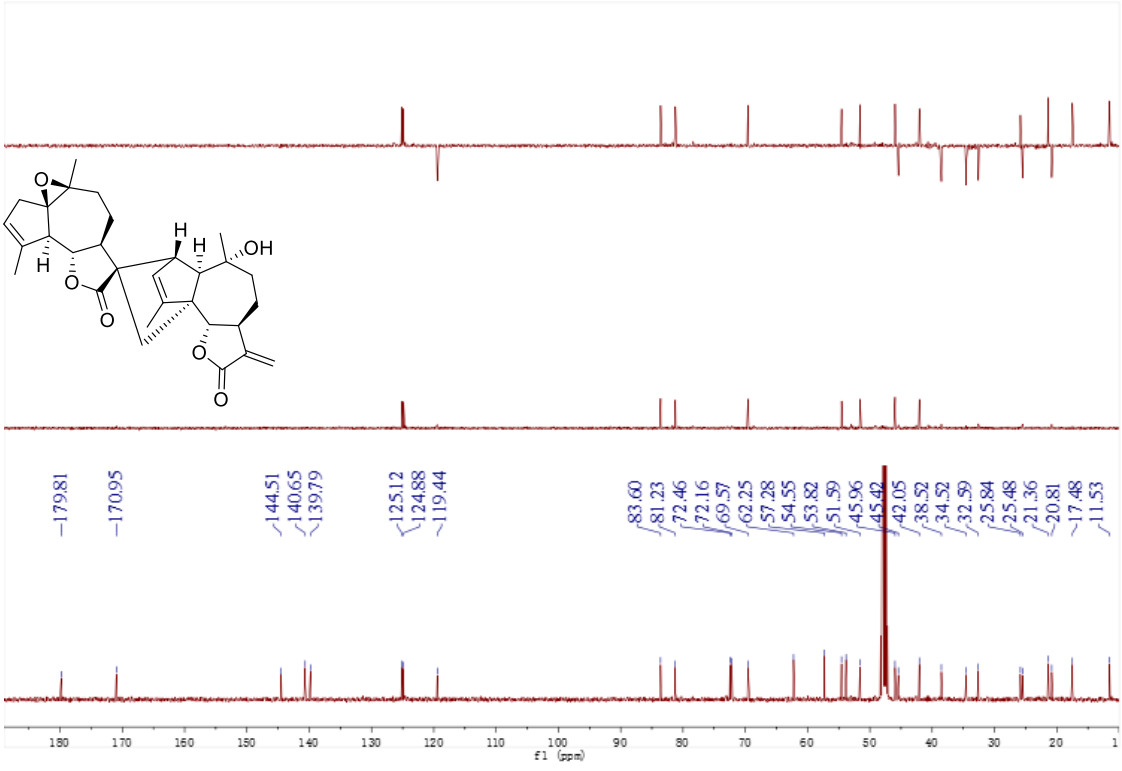


Figure S42 ^{13}C NMR spectrum (100 MHz) of artematrolide C (**5**) in CD_3OD.

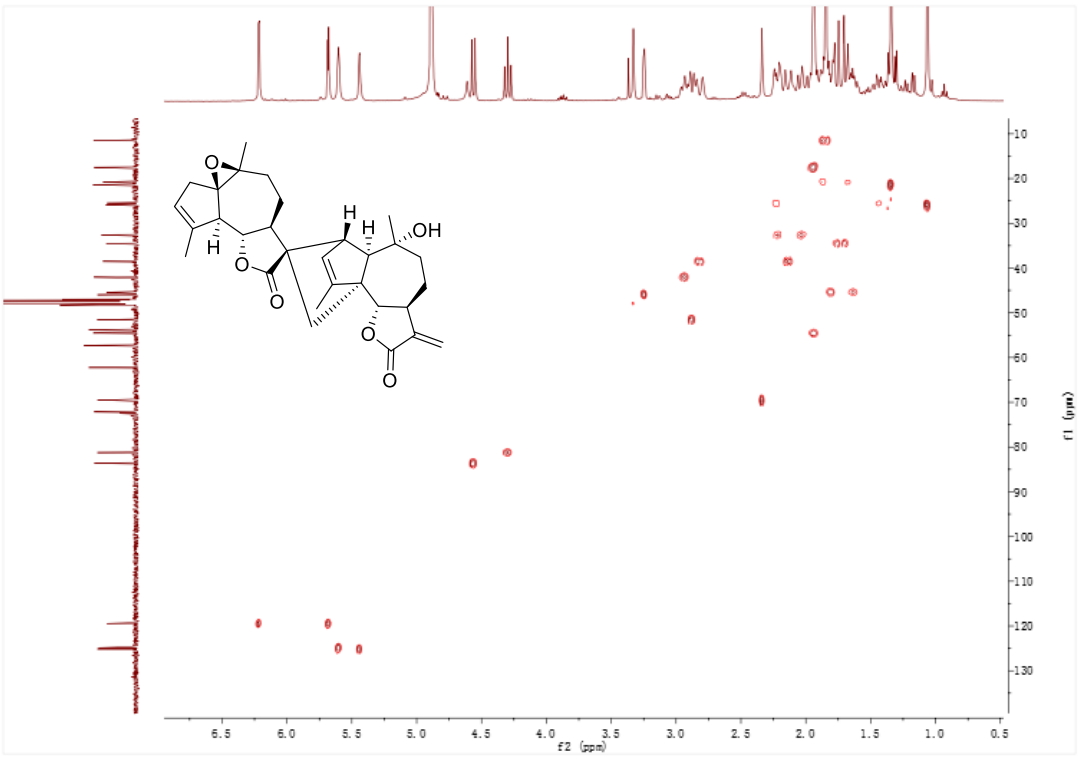


Figure S43 HSQC spectrum (600 MHz) of artematrolide C (**5**) in CD_3OD.

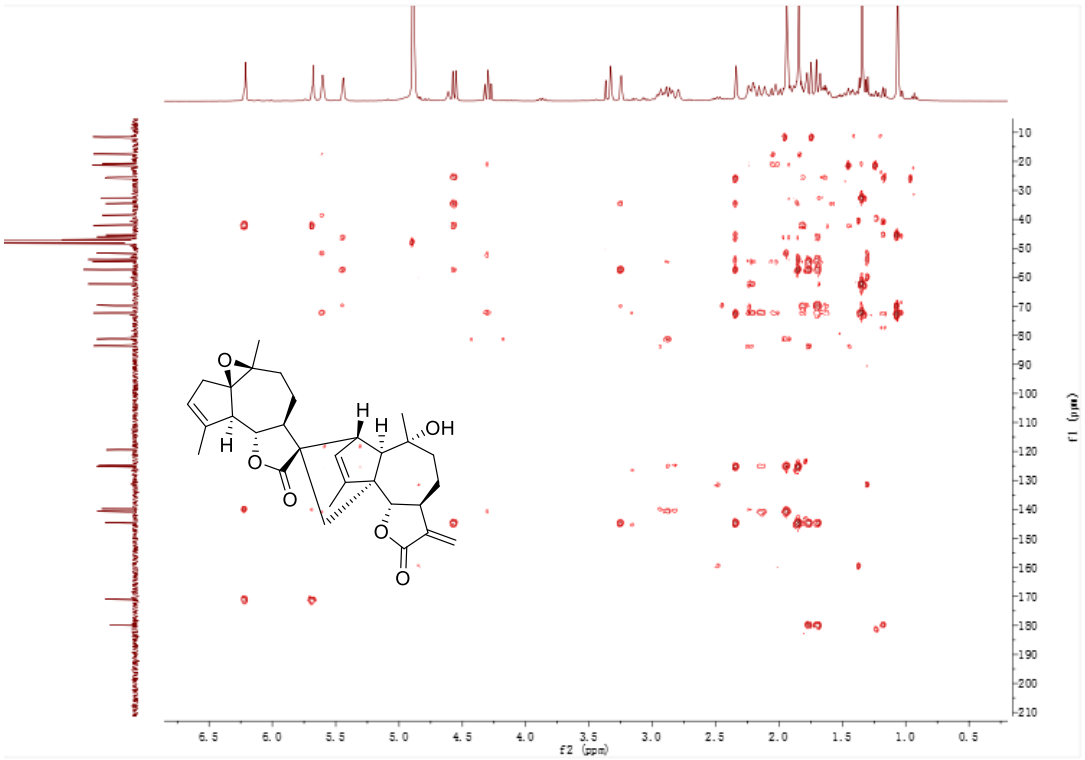


Figure S44 HMBC spectrum (600 MHz) of artematrolide C (**5**) in CD_3OD.

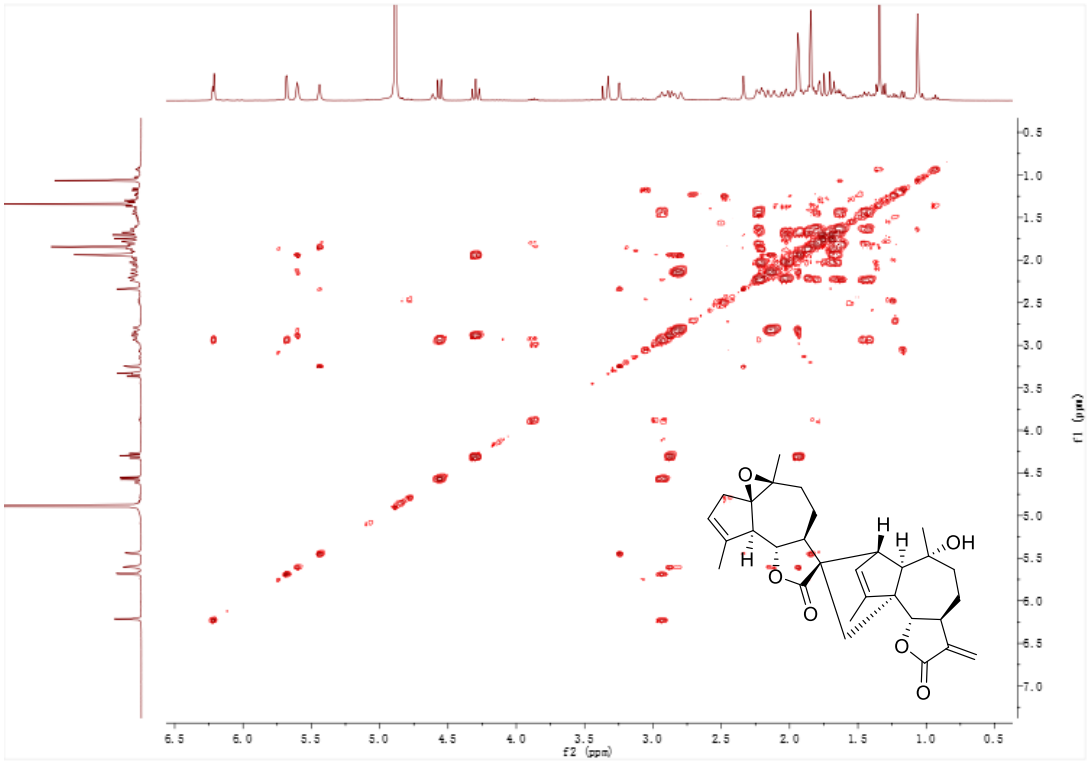


Figure S45 ^{1}H–^{1}H COSY spectrum (600 MHz) of artematrolide C (**5**) in CD_3OD.

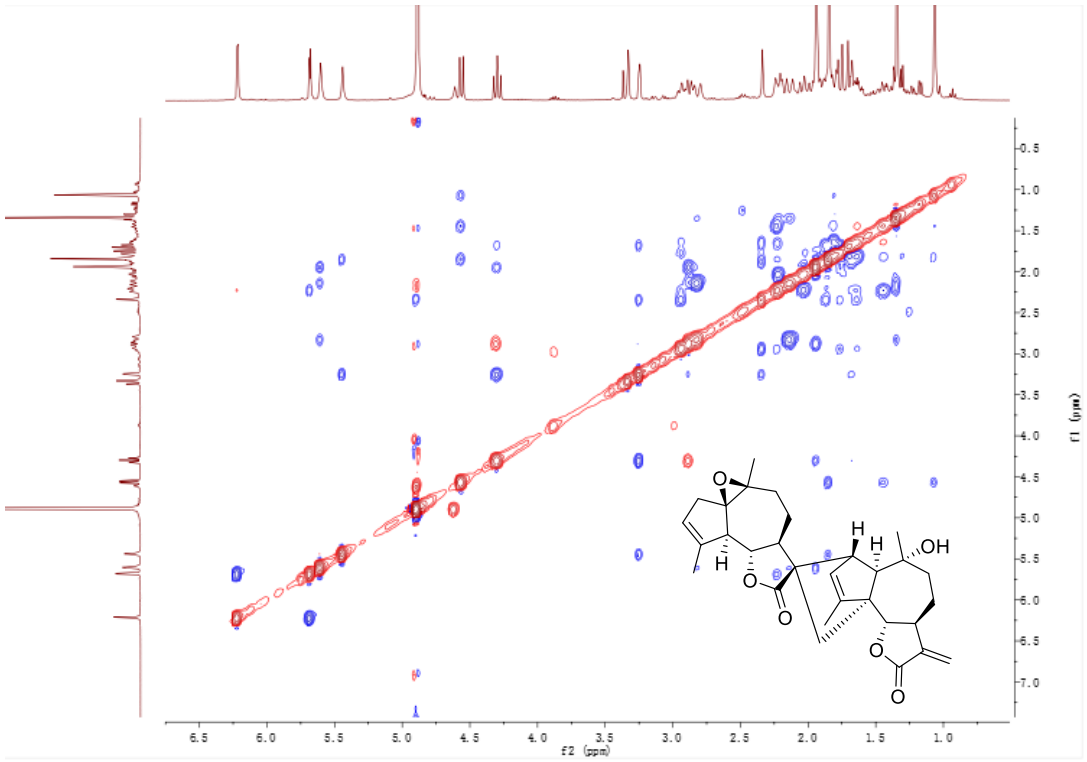


Figure S46 ROESY spectrum (600 MHz) of artematrolide C (**5**) in CD_3OD.

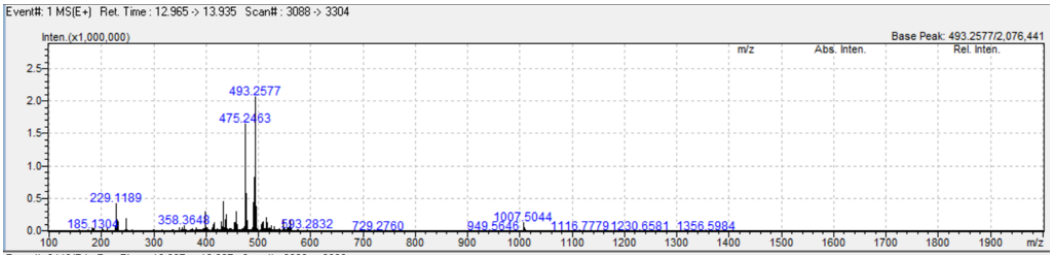


Figure S47 HRESIMS spectrum of artematrolide C (**5**).

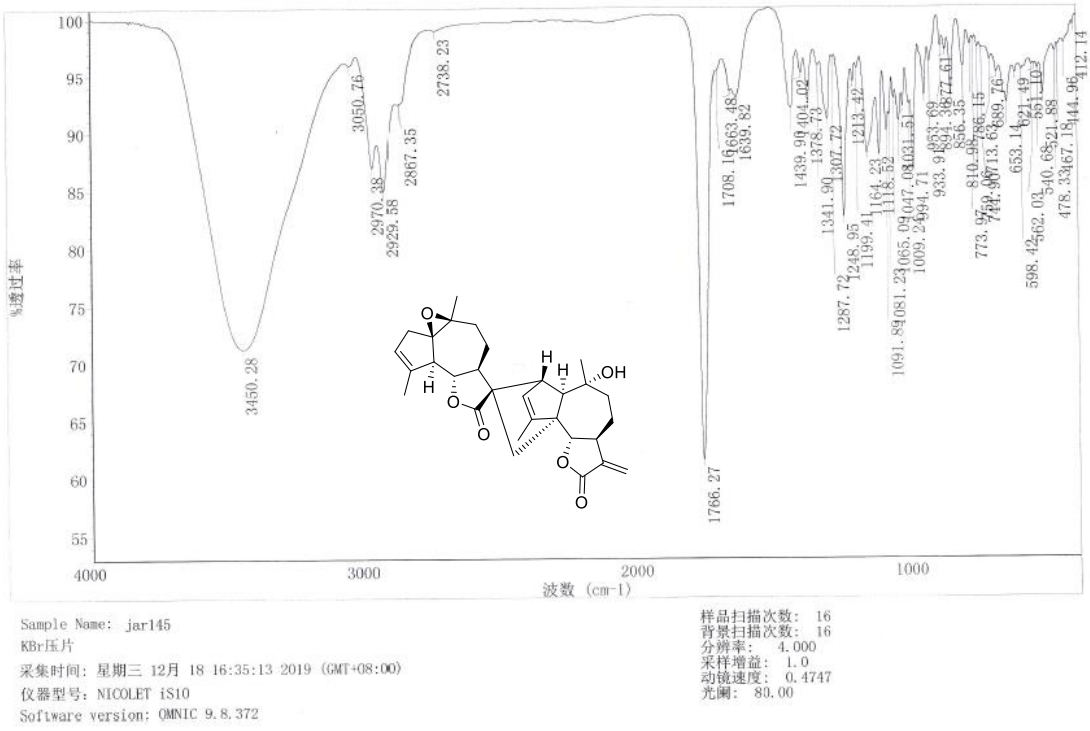


Figure S48 IR spectrum of artematrolide C (**5**).

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Friday, 13-DEC-2019

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	54.98	0.12	0.21	55.11	54.89

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	jar145	05:06:37 PM	54.89	SR	0.0247	589	100.00	0.045	23.5
2	jar145	05:06:45 PM	54.89	SR	0.0247	589	100.00	0.045	23.5
3	jar145	05:06:53 PM	54.89	SR	0.0247	589	100.00	0.045	23.4
4	jar145	05:07:01 PM	55.11	SR	0.0248	589	100.00	0.045	23.4
5	jar145	05:07:09 PM	55.11	SR	0.0248	589	100.00	0.045	23.4

Figure S49 Optical rotation spectrum of artematrolide C (**5**).

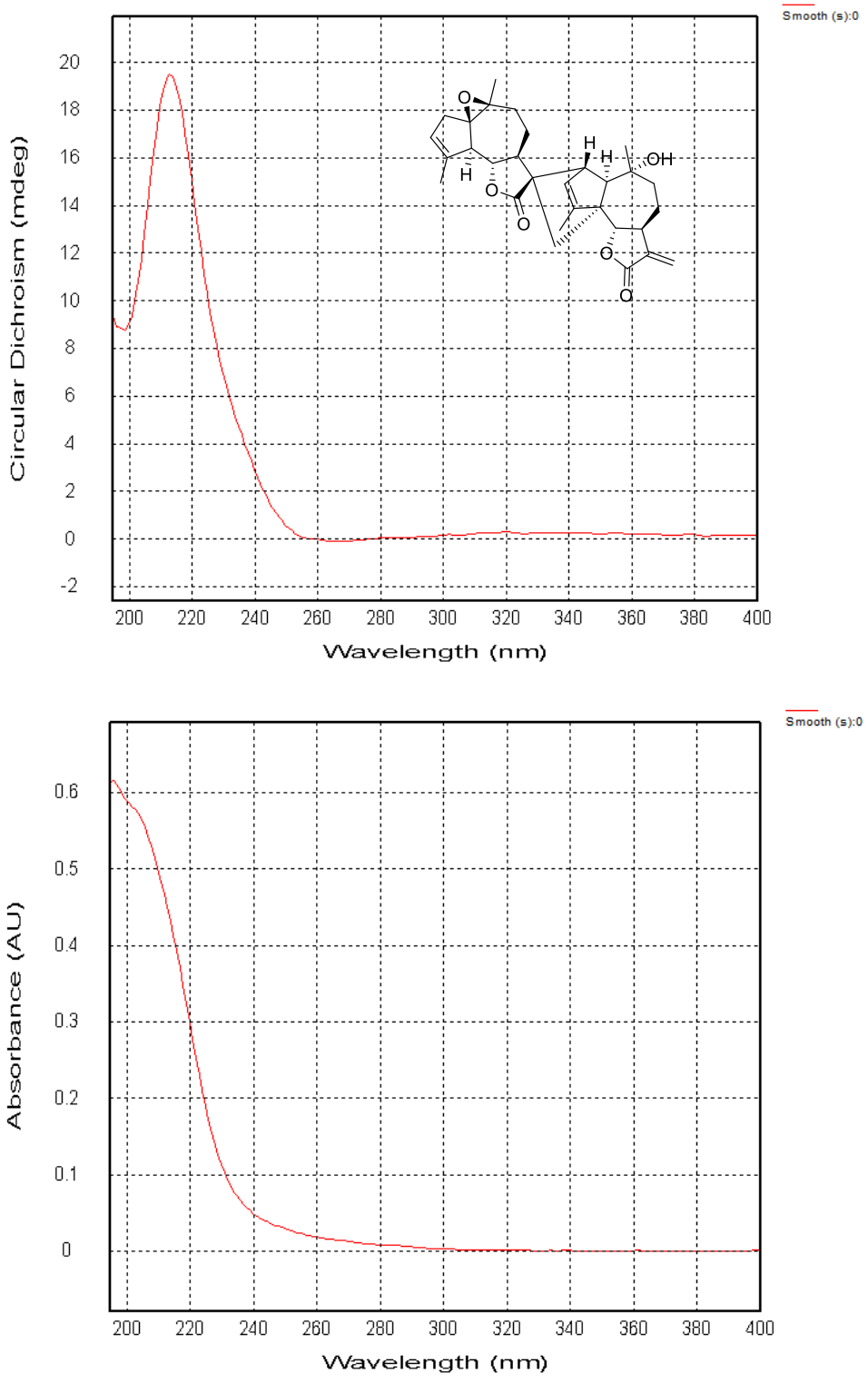


Figure S50 CD (top) and UV (bottom) spectra of artematrolide C (**5**).

7. NMR, MS, IR, $[\alpha]_D$ and CD spectra of compound 6

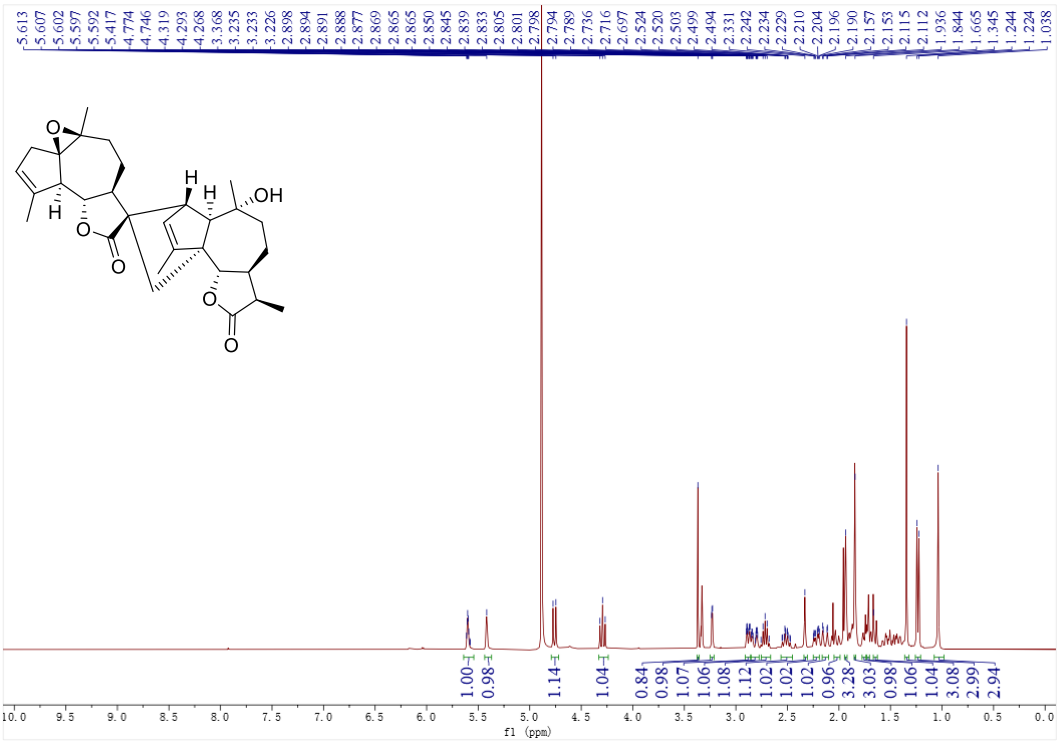


Figure S51 ^{1}H NMR spectrum (400 MHz) of artematrolide D (**6**) in CD_3OD.

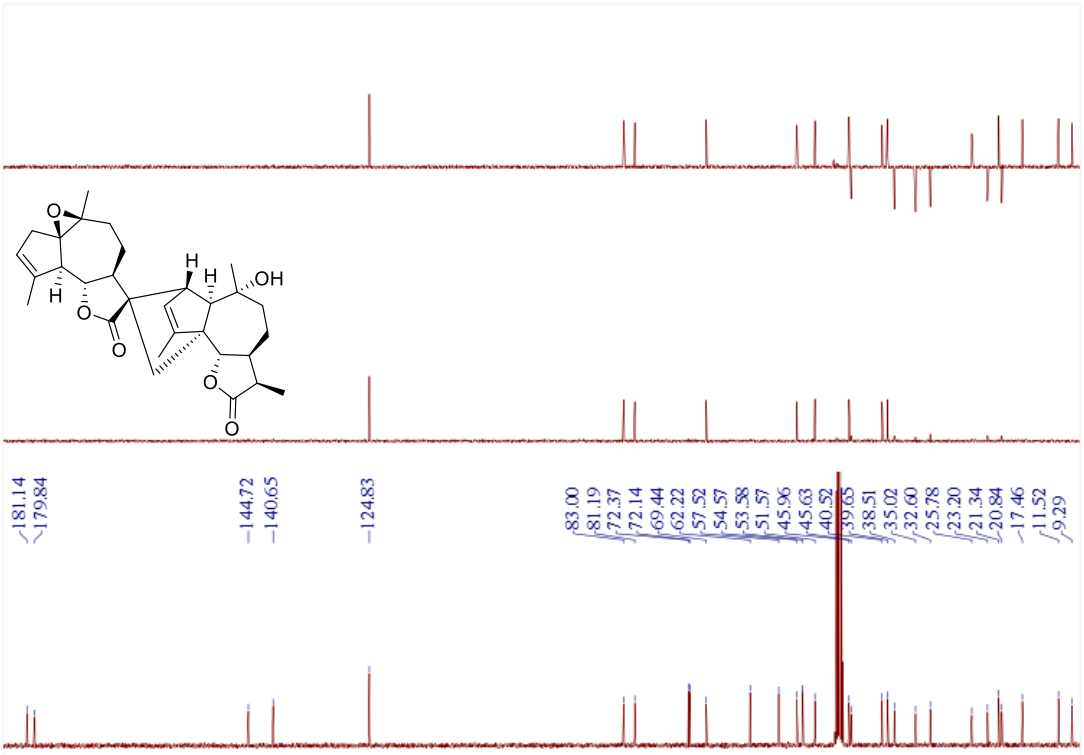


Figure S52 ^{13}C NMR spectrum (100 MHz) of artematrolide D (**6**) in CD_3OD.

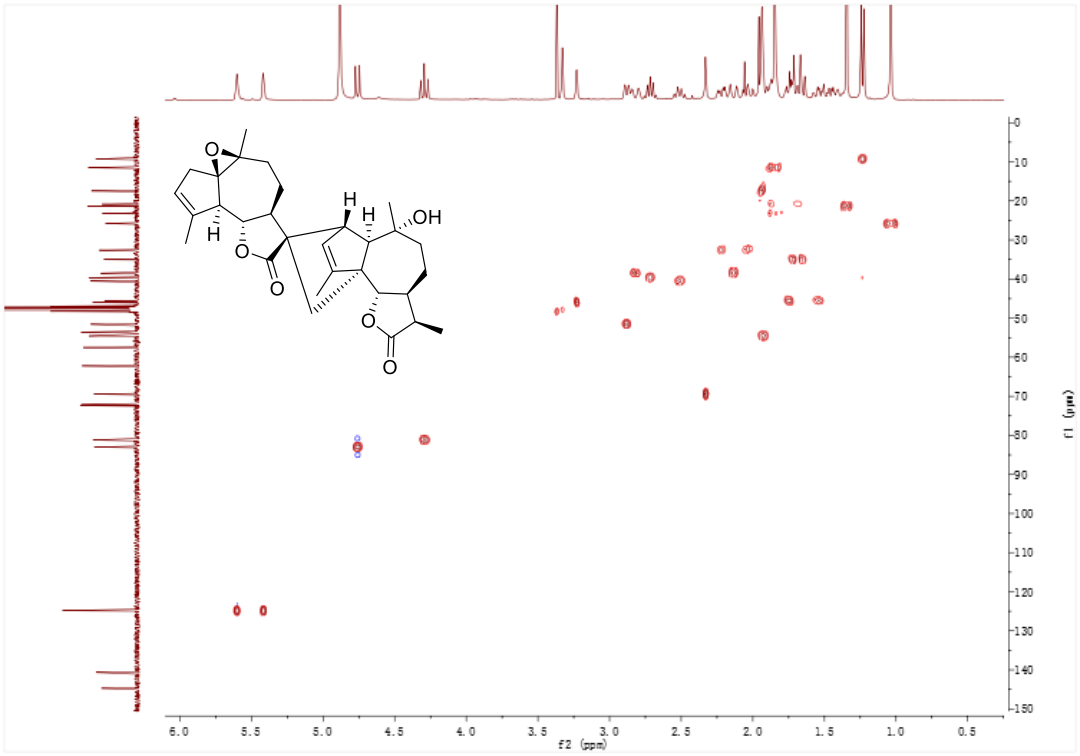


Figure S53 HSQC spectrum (600 MHz) of artematrolide D (**6**) in CD_3OD.

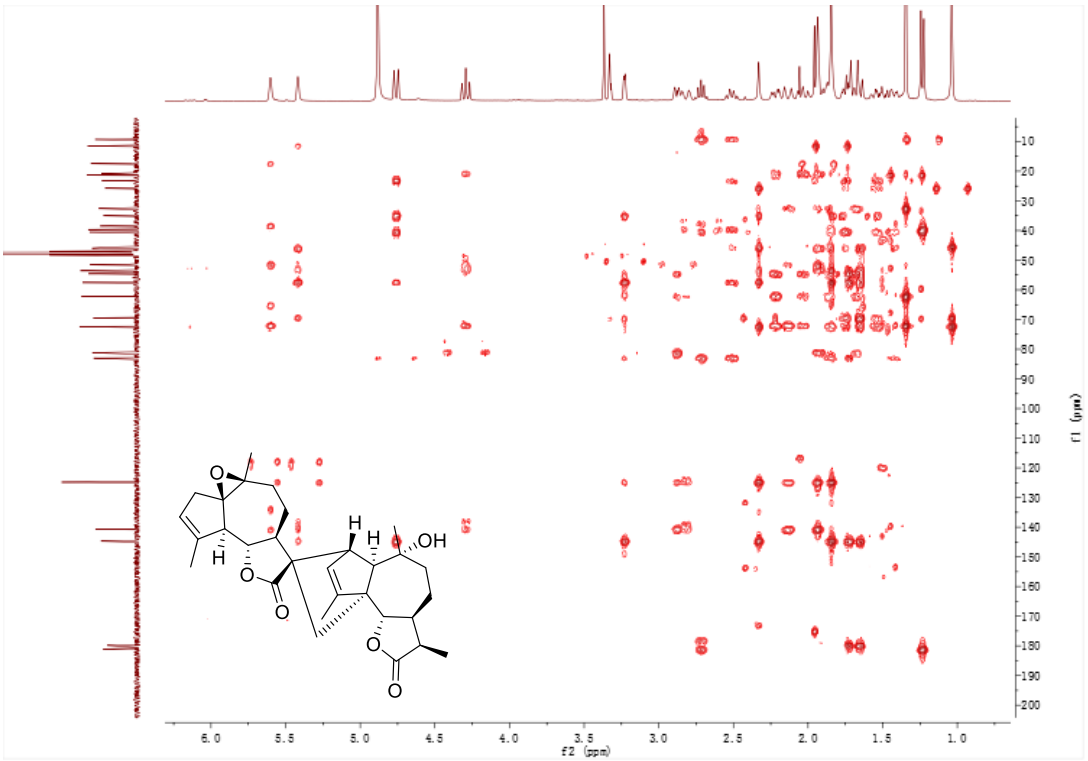


Figure S54 HMBC spectrum (600 MHz) of artematrolide D (**6**) in CD_3OD.

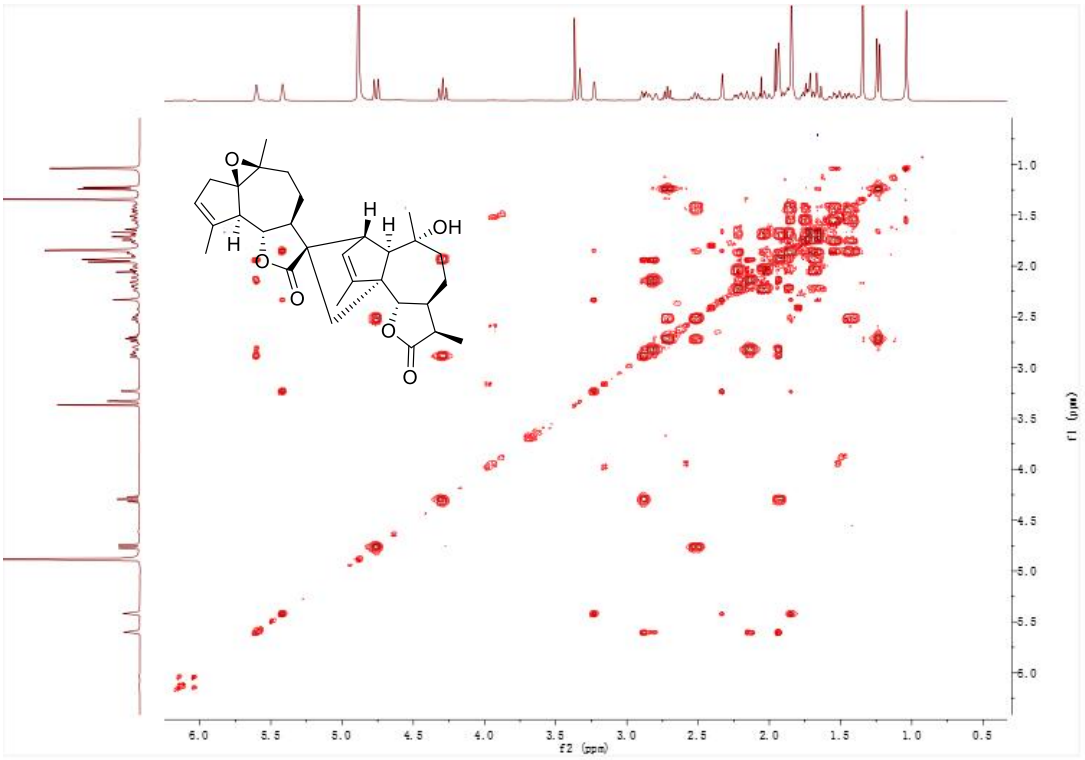


Figure S55 ^{1}H–^{1}H COSY spectrum (600 MHz) of artematrolide D (**6**) in CD_3OD.

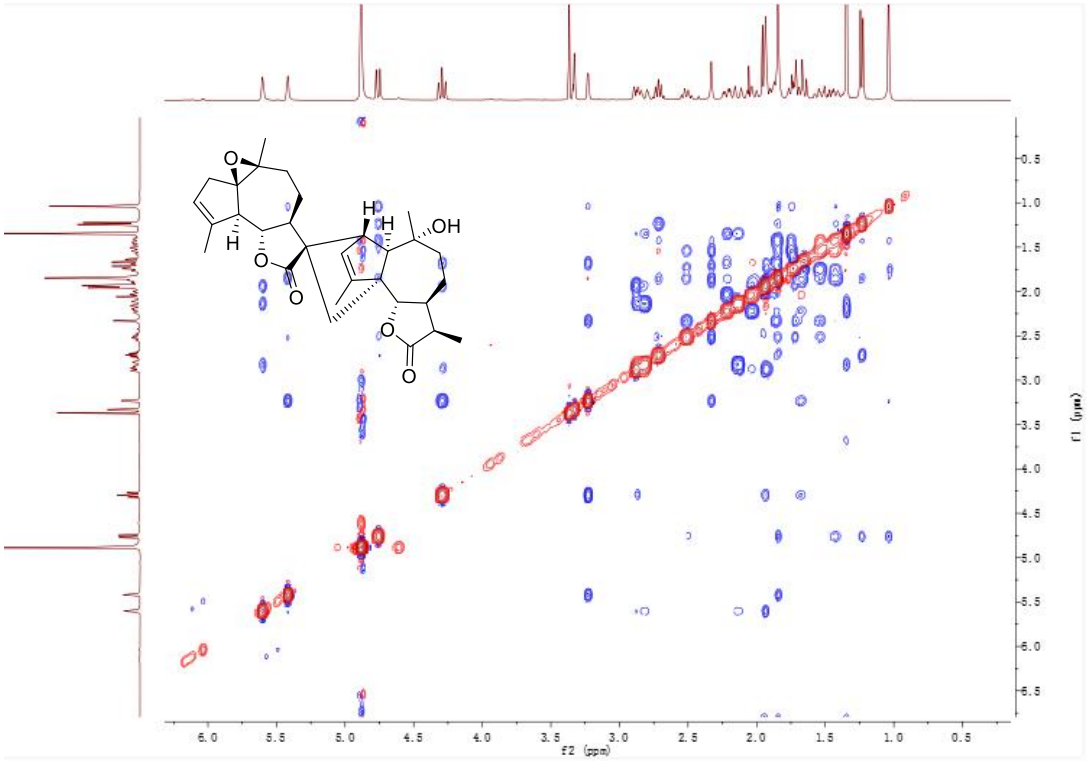


Figure S56 ROESY spectrum (600 MHz) of artematrolide D (**6**) in CD_3OD.

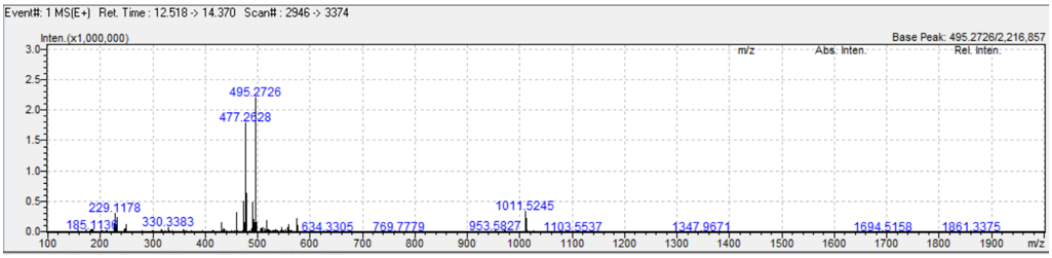


Figure S57 HRESIMS spectrum of artematrolide D (**6**).

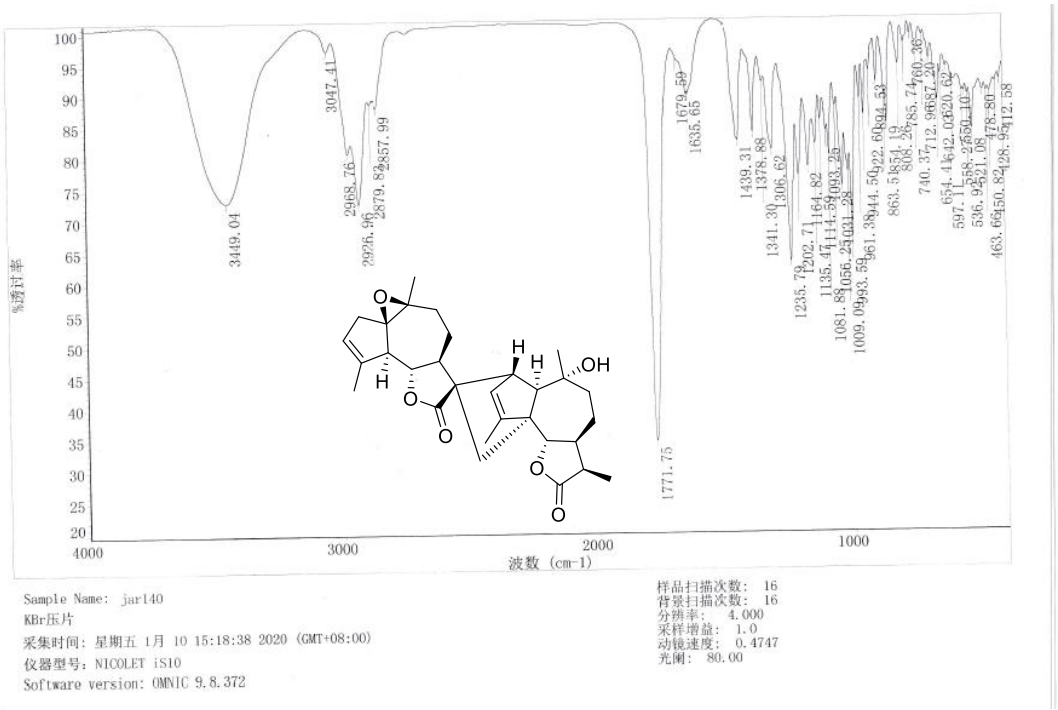


Figure S58 IR spectrum of artematrolide D (**6**).

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Saturday, 04-JAN-2020

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	180.04	0.51	0.28	180.52	179.31

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	jar140	01:53:45 PM	180.00	SR	0.1044	589	100.00	0.058	22.6
2	jar140	01:53:53 PM	179.83	SR	0.1043	589	100.00	0.058	22.6
3	jar140	01:54:01 PM	180.52	SR	0.1047	589	100.00	0.058	22.6
4	jar140	01:54:09 PM	179.31	SR	0.1040	589	100.00	0.058	22.6
5	jar140	01:54:17 PM	180.52	SR	0.1047	589	100.00	0.058	22.6

Figure S59 Optical rotation spectrum of artematrolide D (**6**).

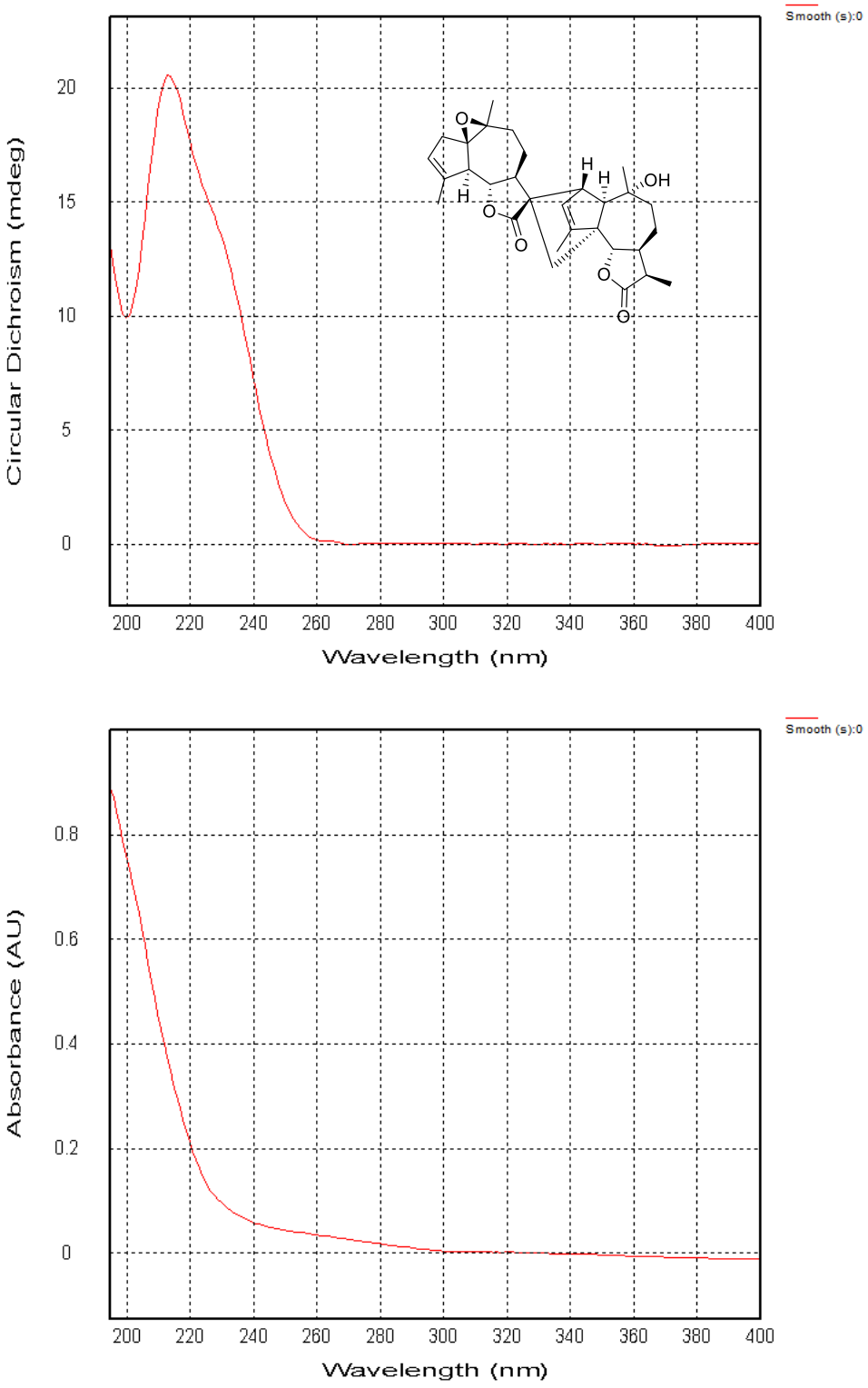


Figure S60 CD (top) and UV (bottom) spectra of artematrolide D (**6**).

8. NMR, MS, IR, $[\alpha]_D$ and CD spectra of compound 7

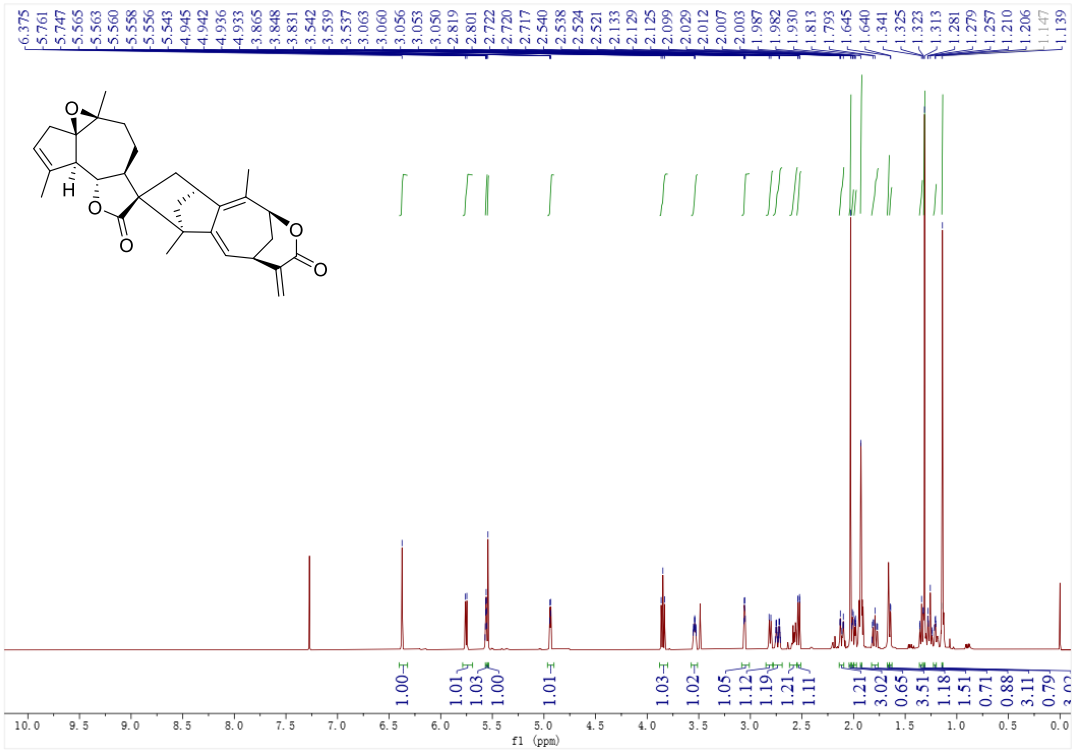


Figure S61 ^{1}H NMR spectrum (600 MHz) of artematrolide E (**7**) in $CDCl_3$.

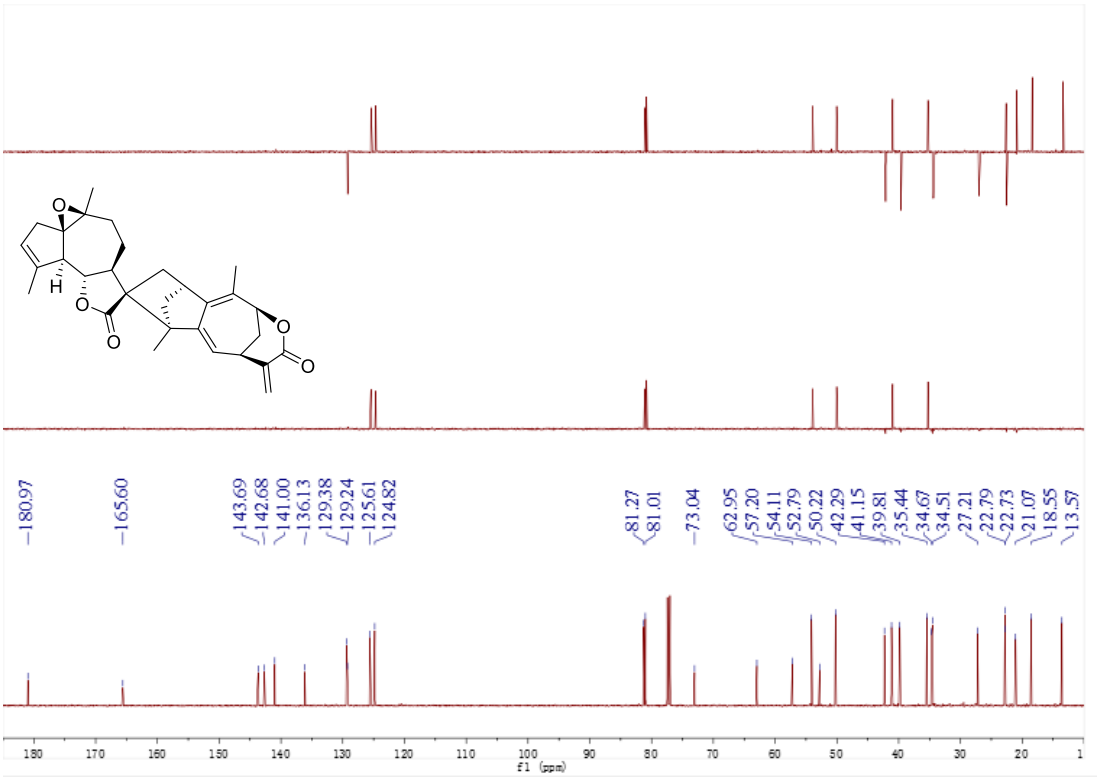


Figure S62 ^{13}C NMR spectrum (150 MHz) of artematrolide E (**7**) in $CDCl_3$.

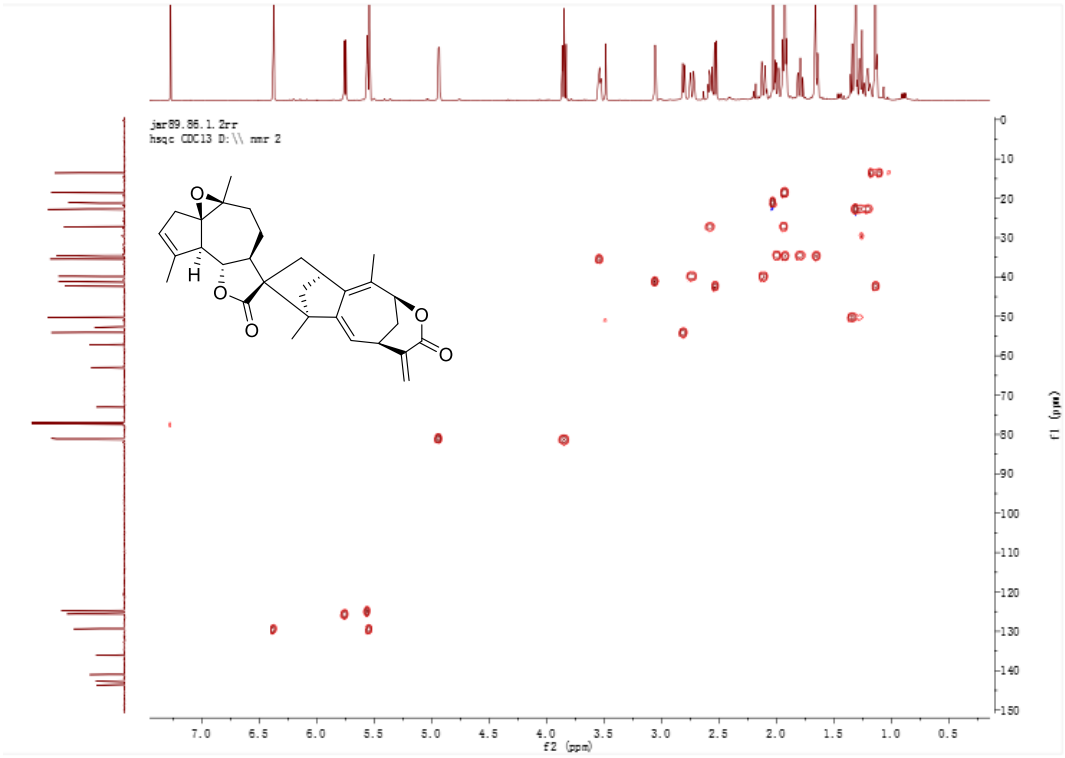


Figure S63 HSQC spectrum (600 MHz) of artematrolide E (**7**) in $CDCl_3$.

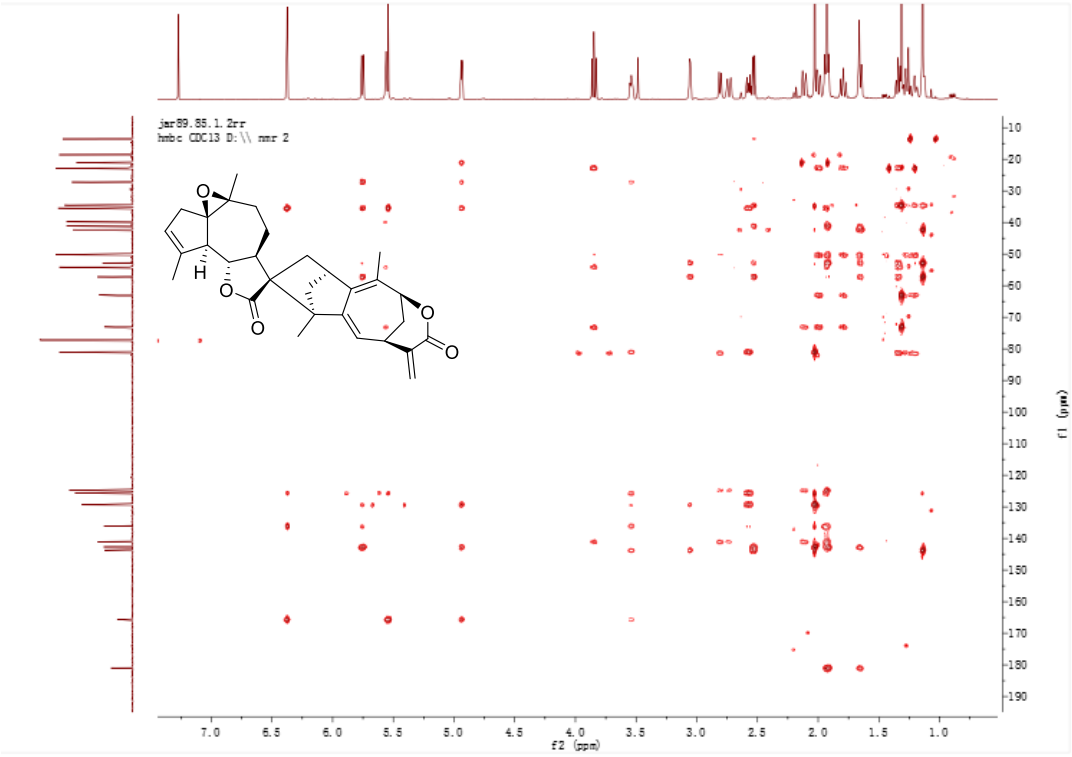


Figure S64 HMBC spectrum (600 MHz) of artematrolide E (**7**) in $CDCl_3$.

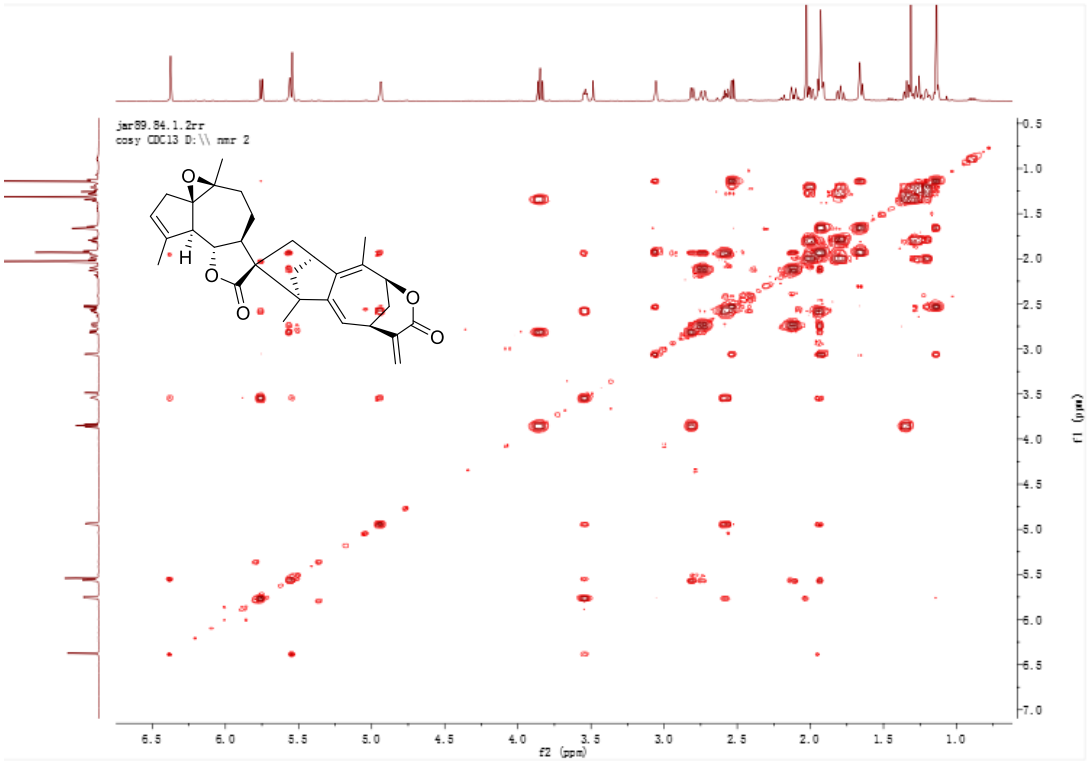


Figure S65 ^{1}H–^{1}H COSY spectrum (600 MHz) of artematrolide E (**7**) in $CDCl_3$.

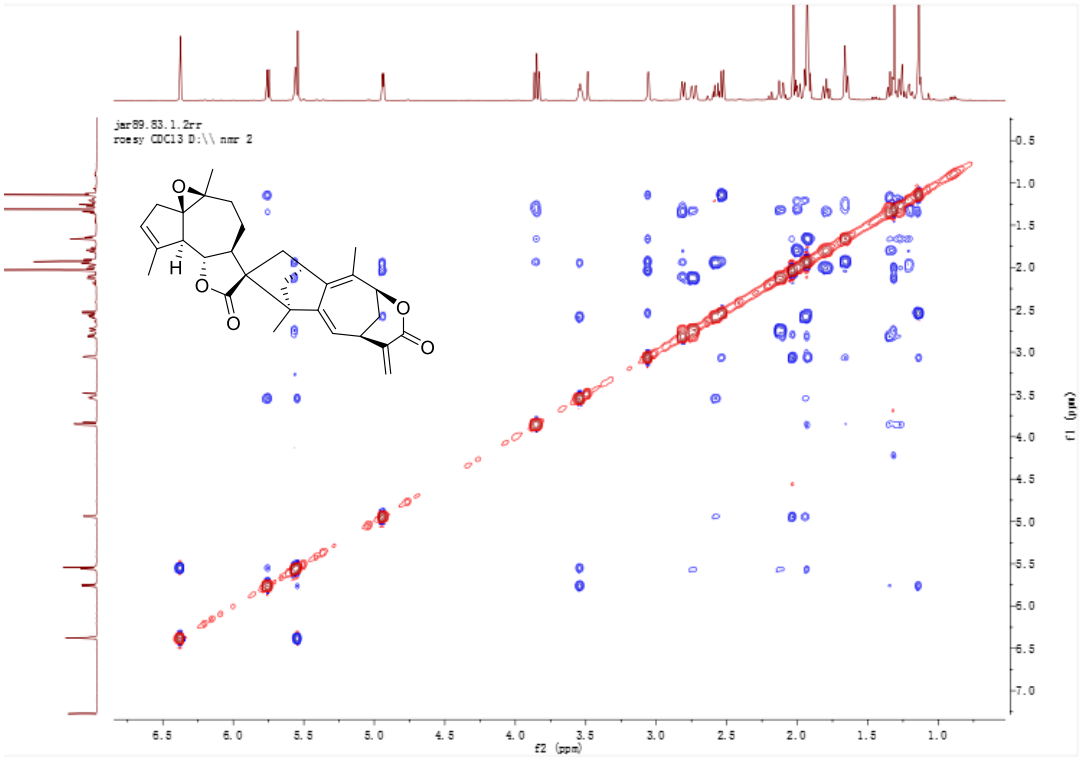


Figure S66 ROESY spectrum (600 MHz) of artematrolide E (**7**) in $CDCl_3$.

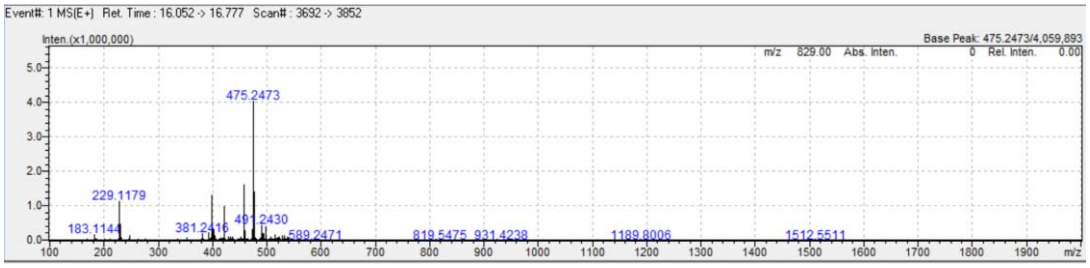


Figure S67 HRESIMS spectrum of artematrolide E (**7**).

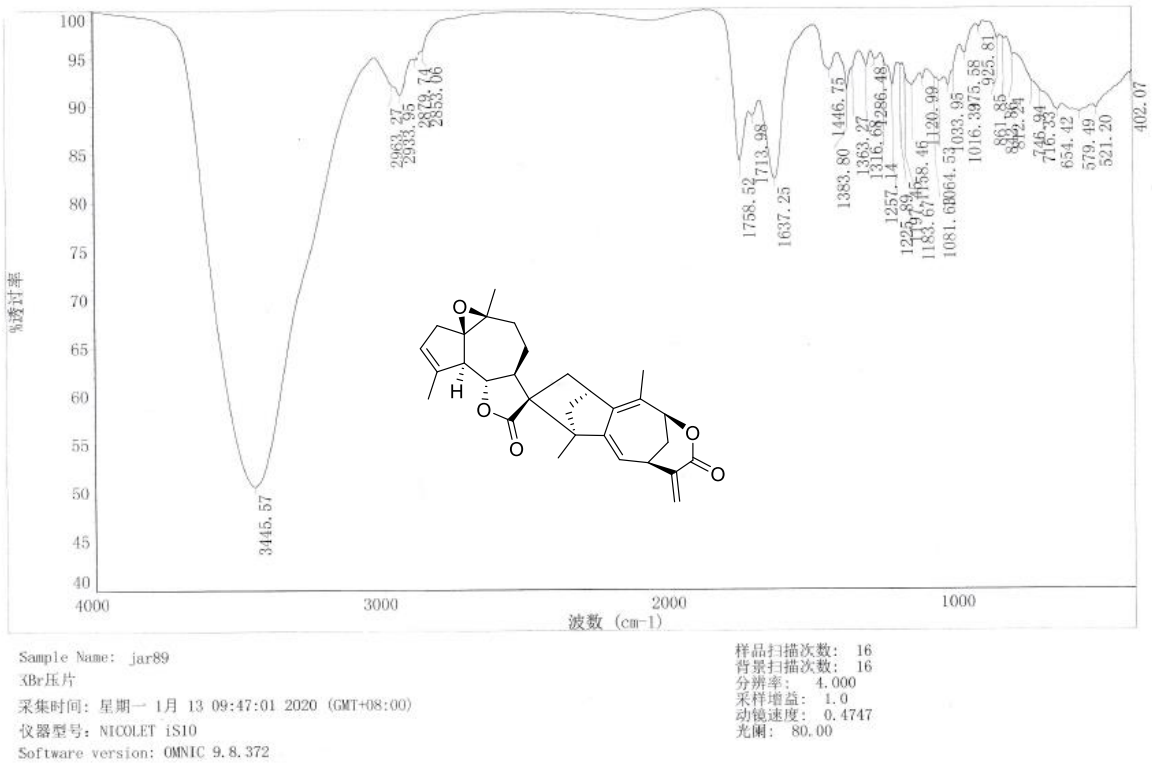


Figure S68 IR spectrum of artematrolide E (**7**).

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Saturday, 04-JAN-2020

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	48.41	0.46	0.95	49.04	47.83

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	jar89	12:49:01 PM	48.19	SR	0.0400	589	100.00	0.083	21.8
2	jar89	12:49:10 PM	47.83	SR	0.0397	589	100.00	0.083	21.8
3	jar89	12:49:18 PM	48.67	SR	0.0404	589	100.00	0.083	21.8
4	jar89	12:49:26 PM	49.04	SR	0.0407	589	100.00	0.083	21.8
5	jar89	12:49:35 PM	48.31	SR	0.0401	589	100.00	0.083	21.8

Figure S69 Optical rotation spectrum of artematrolide E (**7**).

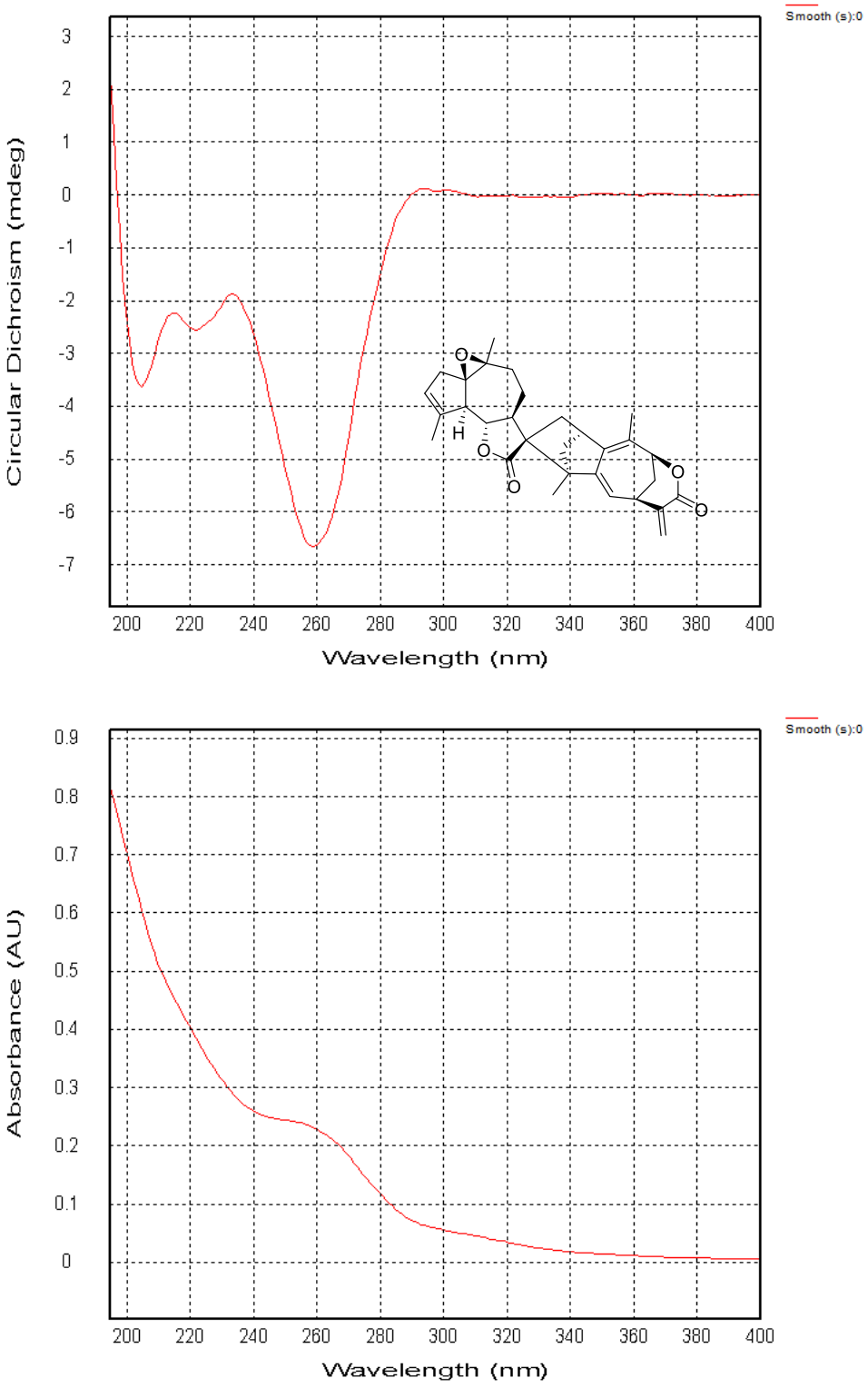


Figure S70 CD (top) and UV (bottom) spectra of artematrolide E (**7**).

9. NMR, MS, IR, $[\alpha]_D$ and CD spectra of compound 8

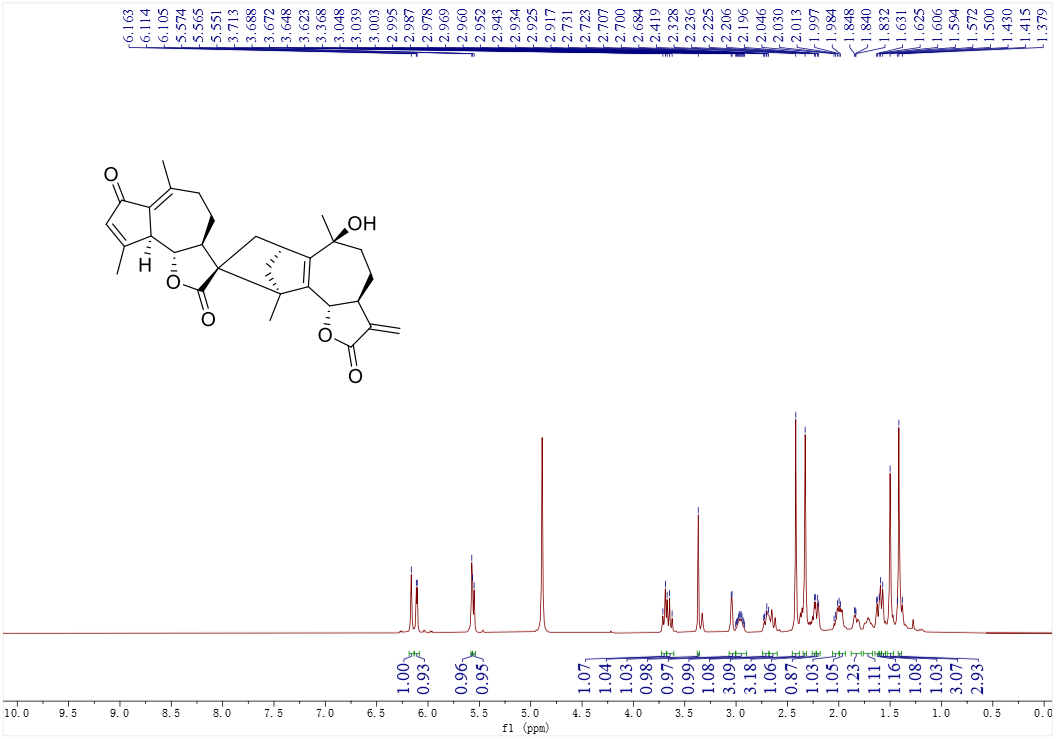


Figure S71 ^{1}H NMR spectrum (400 MHz) of artematrolide F (**8**) in CD_3OD.

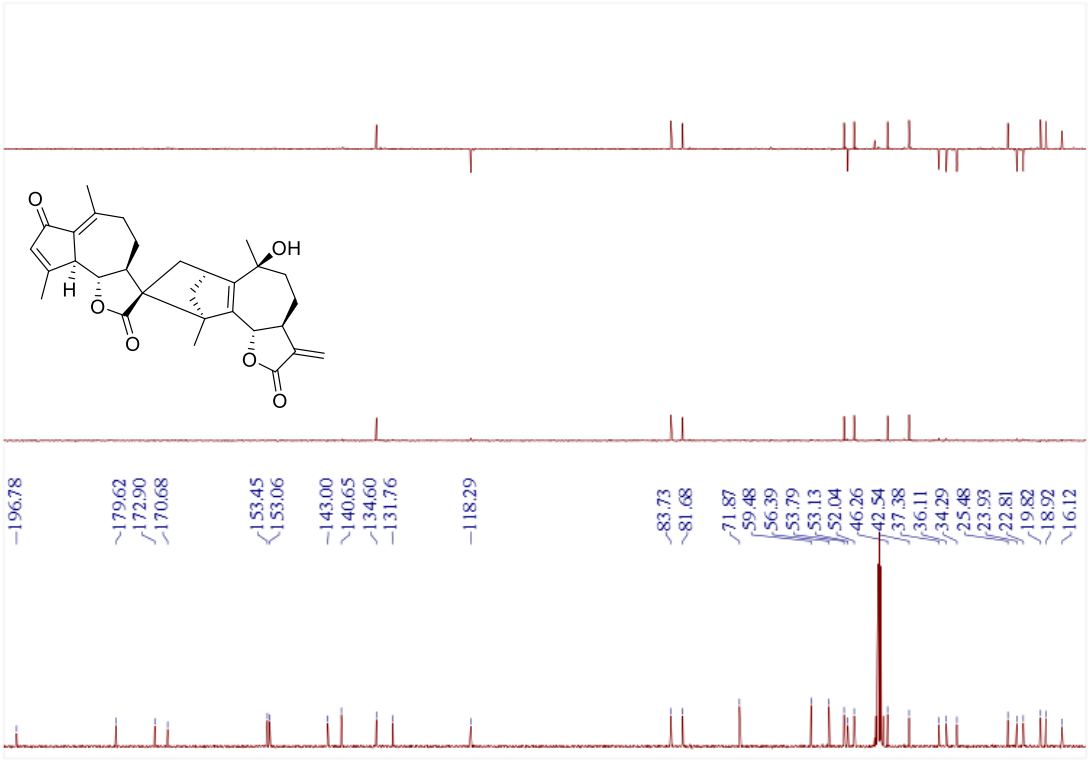


Figure S72 ^{13}C NMR spectrum (100 MHz) of artematrolide F (**8**) in CD_3OD.

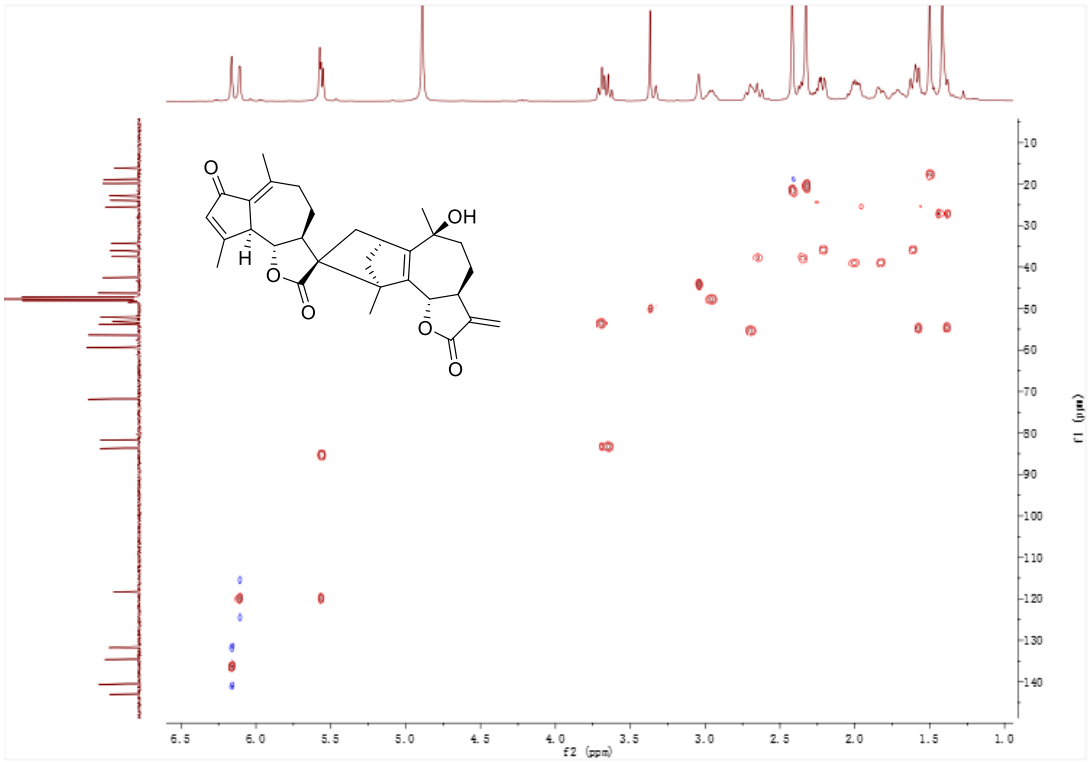


Figure S73 HSQC spectrum (600 MHz) of artematrolide F (**8**) in CD_3OD.

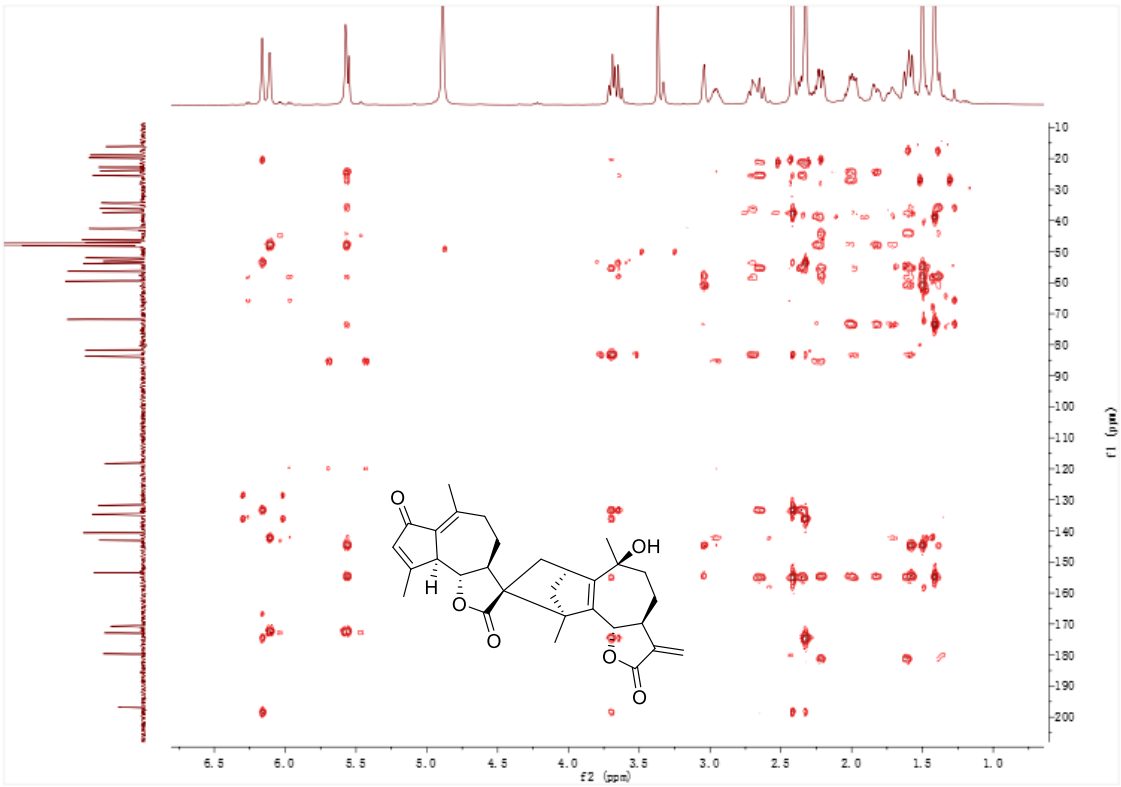


Figure S74 HMBC spectrum (600 MHz) of artematrolide F (**8**) in CD_3OD.

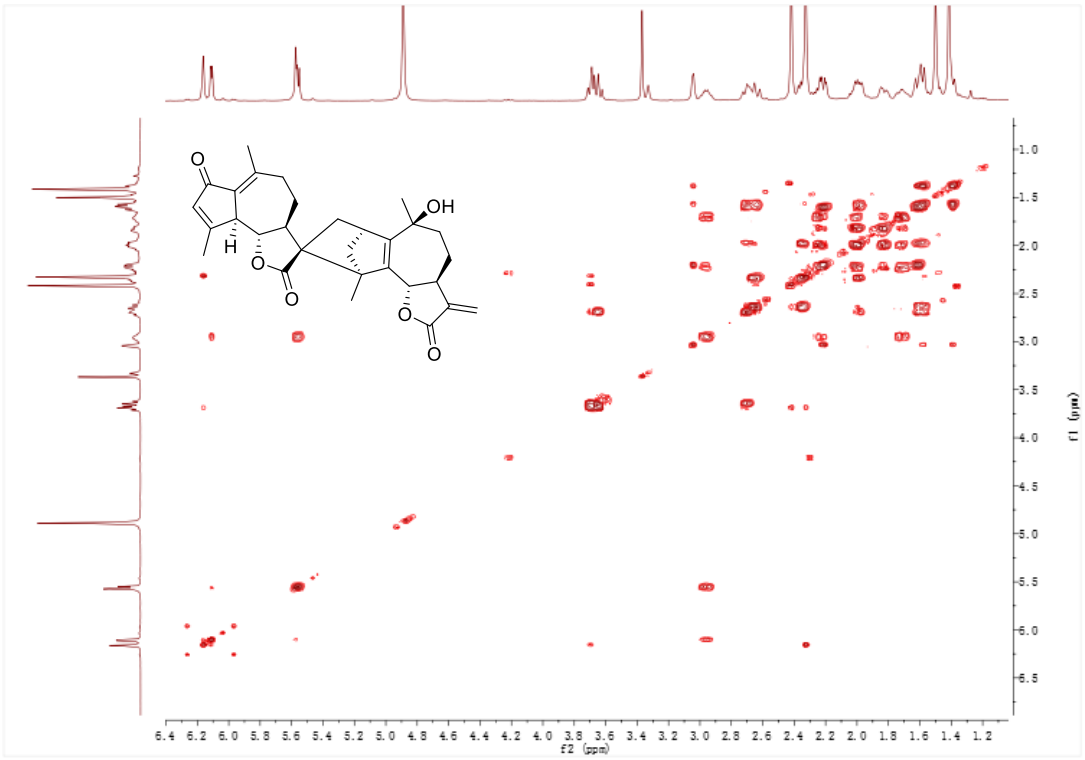


Figure S75 ^{1}H–^{1}H COSY spectrum (600 MHz) of artematrolide F (**8**) in CD_3OD.

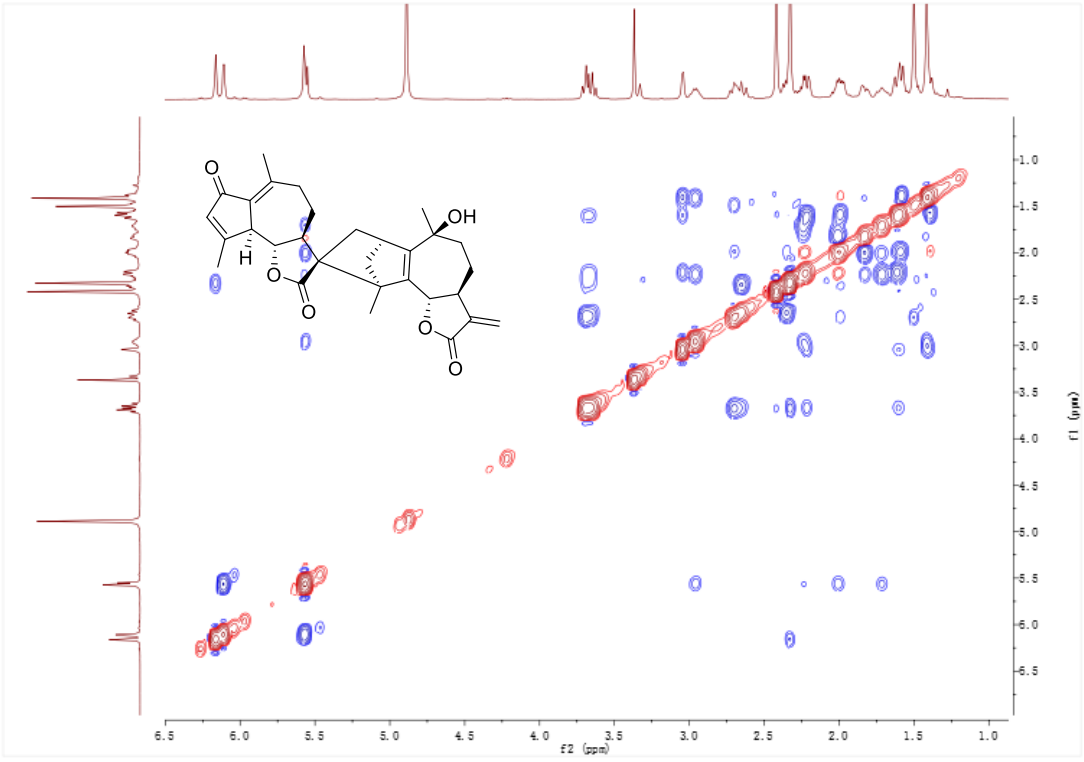


Figure S76 ROESY spectrum (600 MHz) of artematrolide F (**8**) in CD_3OD.

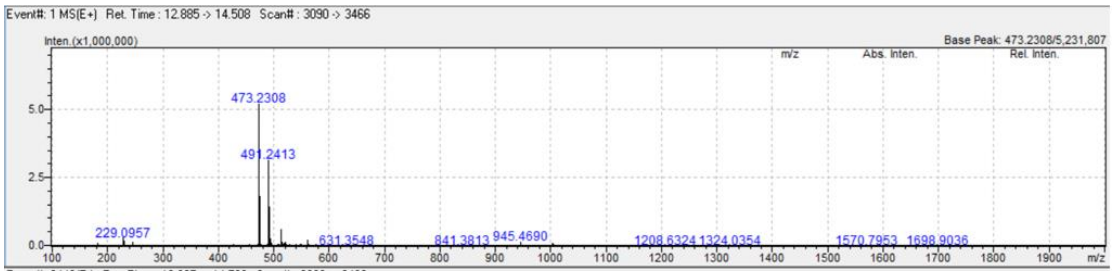


Figure S77 HRESIMS spectrum of artematrolide F (**8**).

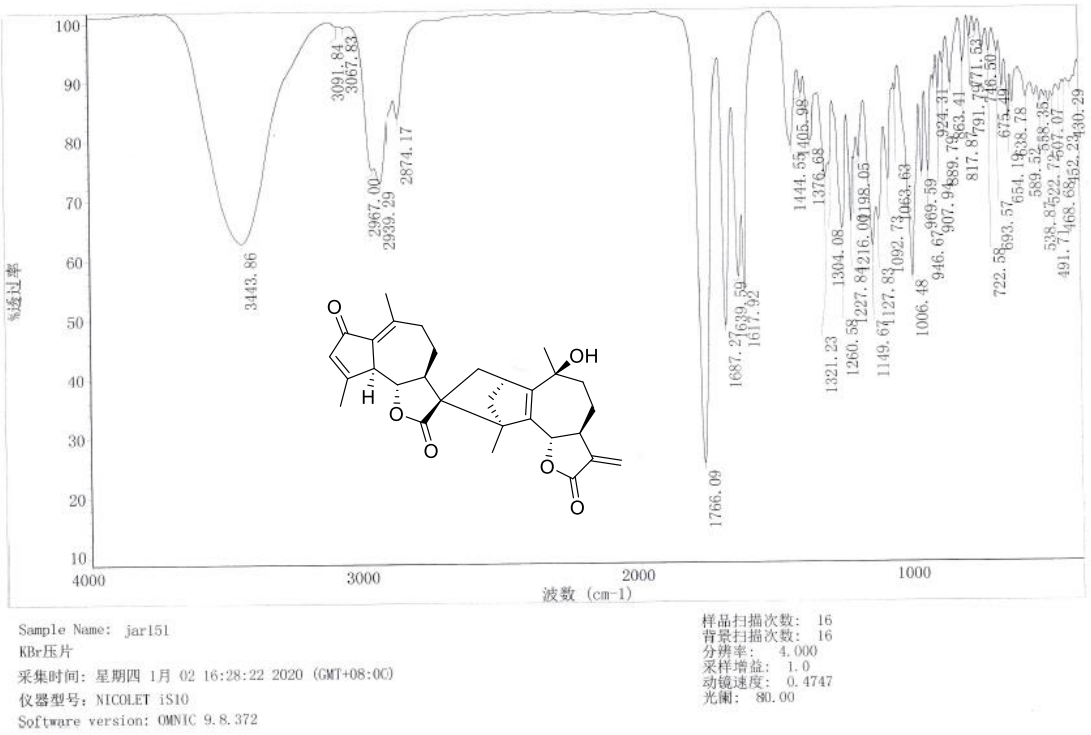


Figure S78 IR spectrum of artematrolide F (**8**).

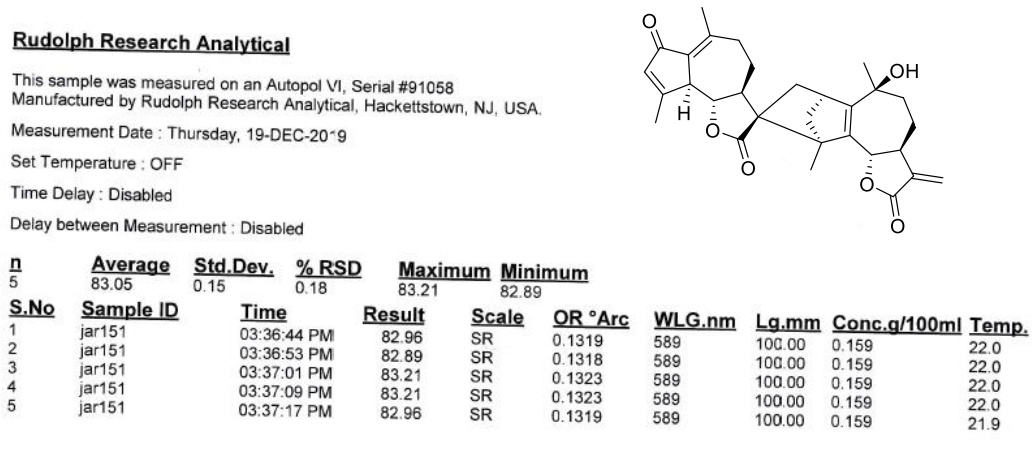


Figure S79 Optical rotation spectrum of artematrolide F (**8**).

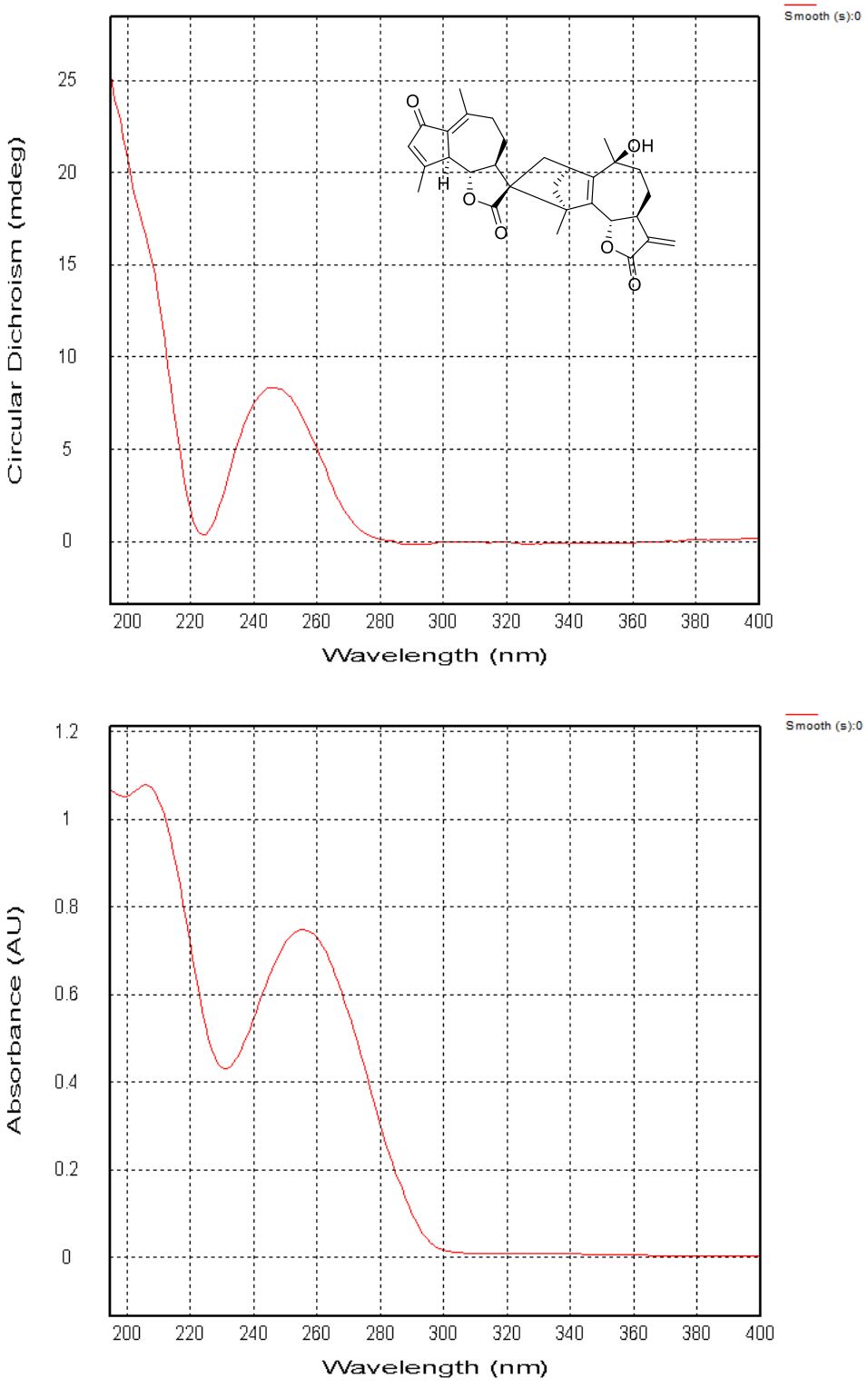


Figure S80 CD (top) and UV (bottom) spectra of artematrolide F (**8**).

10. NMR, MS, IR, $[\alpha]_D$ and CD spectra of compound 9

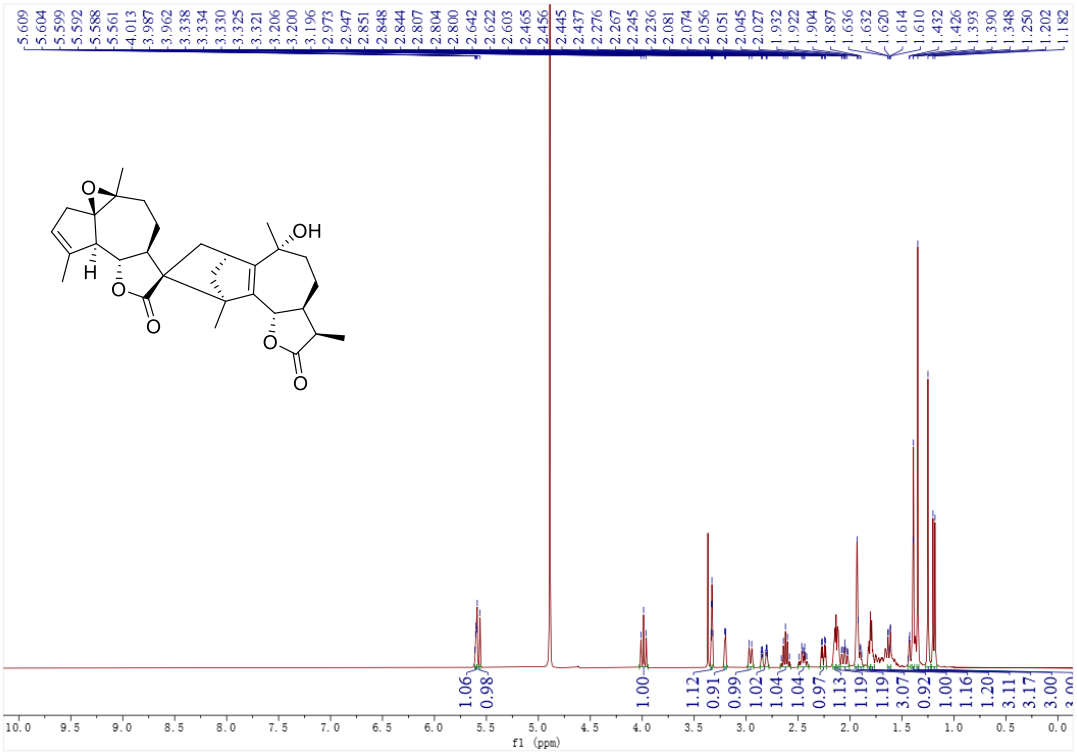


Figure S81 ^{1}H NMR spectrum (400 MHz) of lavandiolide J (**9**) in CD_3OD.

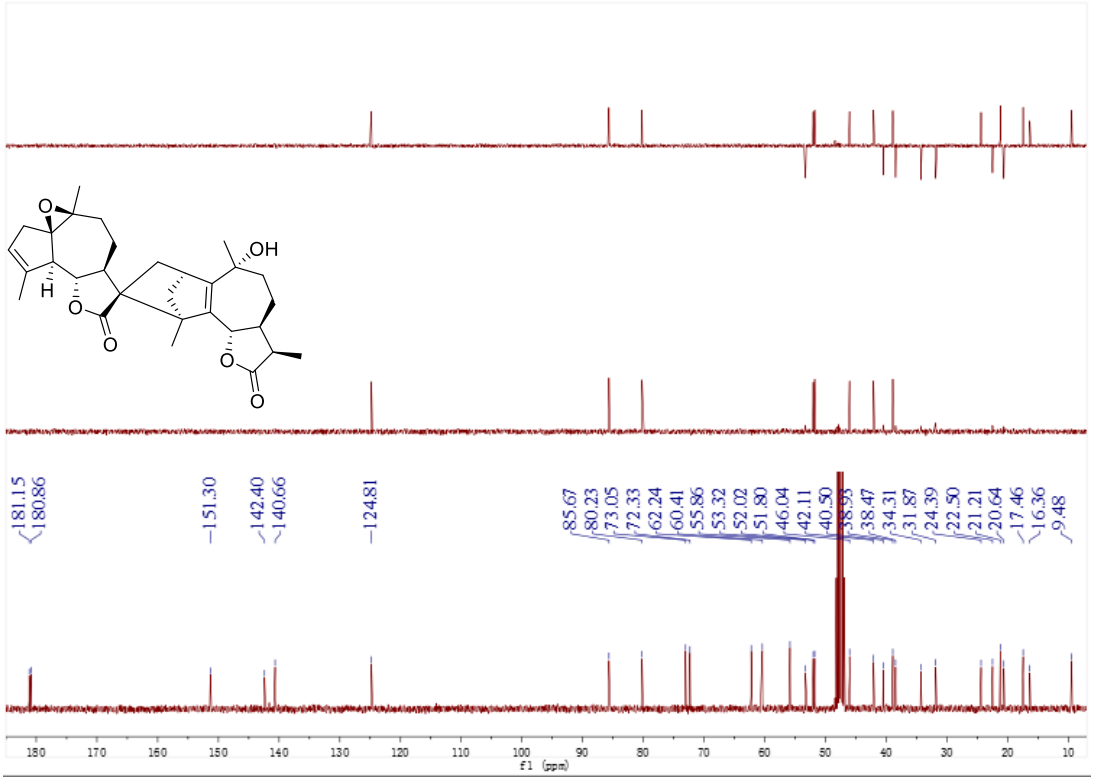


Figure S82 ^{13}C NMR spectrum (100 MHz) of lavandiolide J (**9**) in CD_3OD.

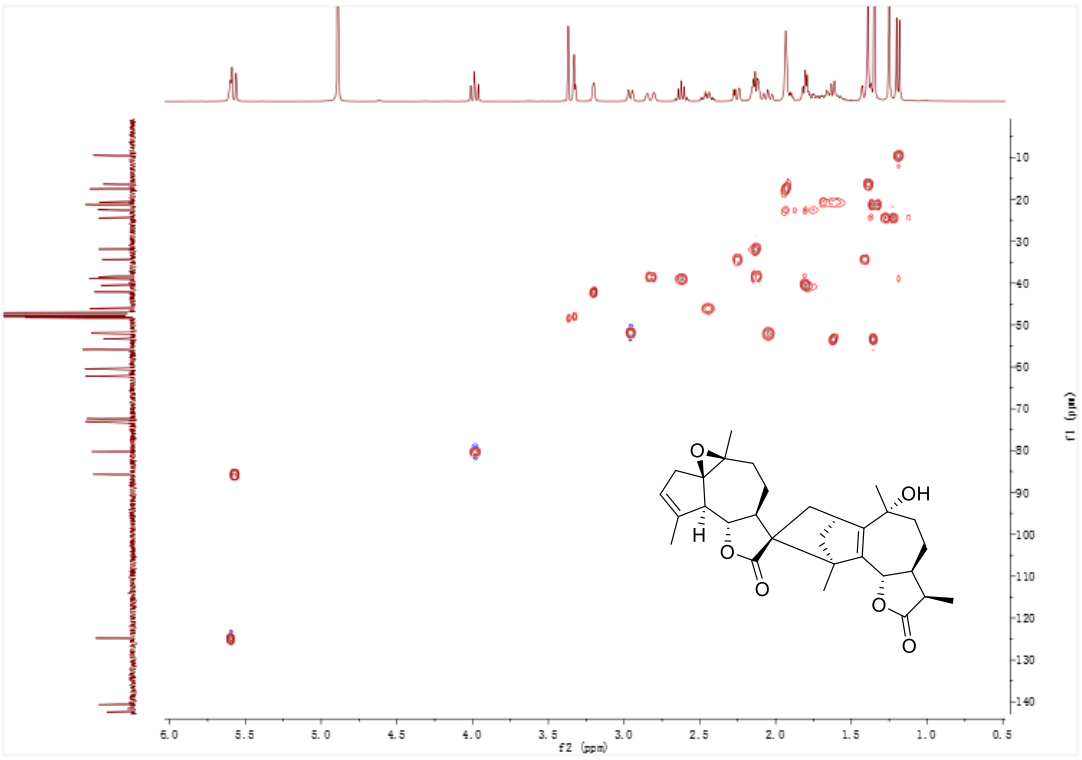


Figure S83 HSQC spectrum (600 MHz) of lavandiolide J (**9**) in CD_3OD.

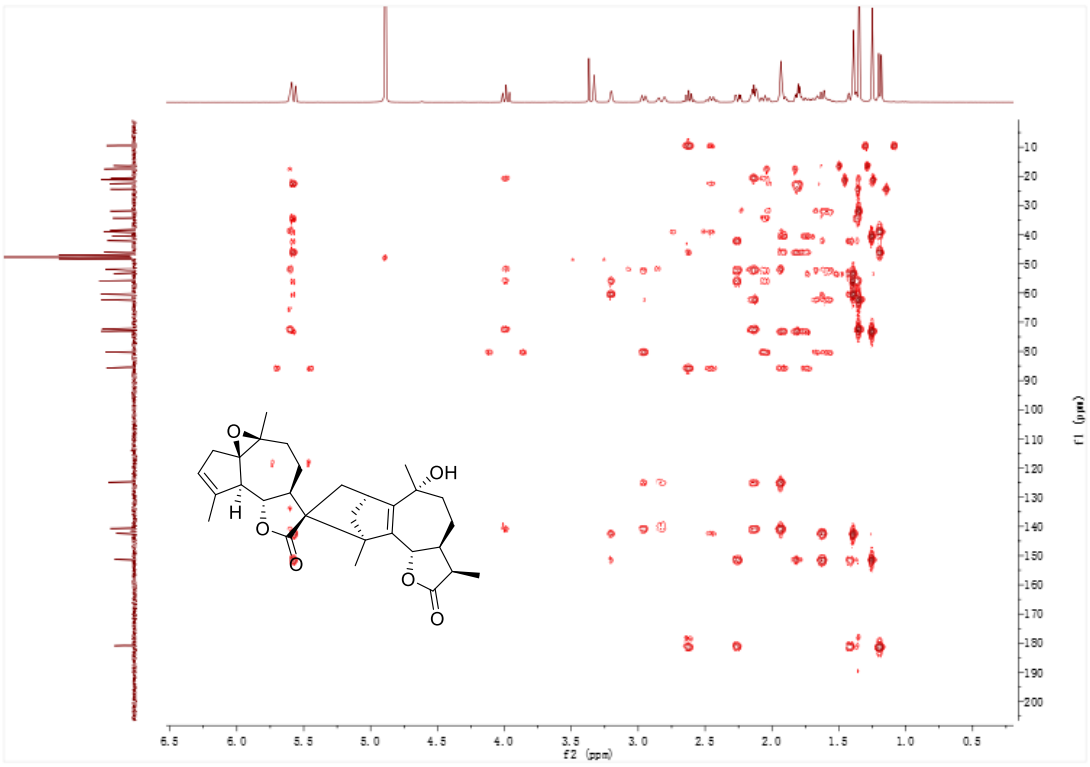


Figure S84 HMBC spectrum (600 MHz) of lavandiolide J (**9**) in CD_3OD.

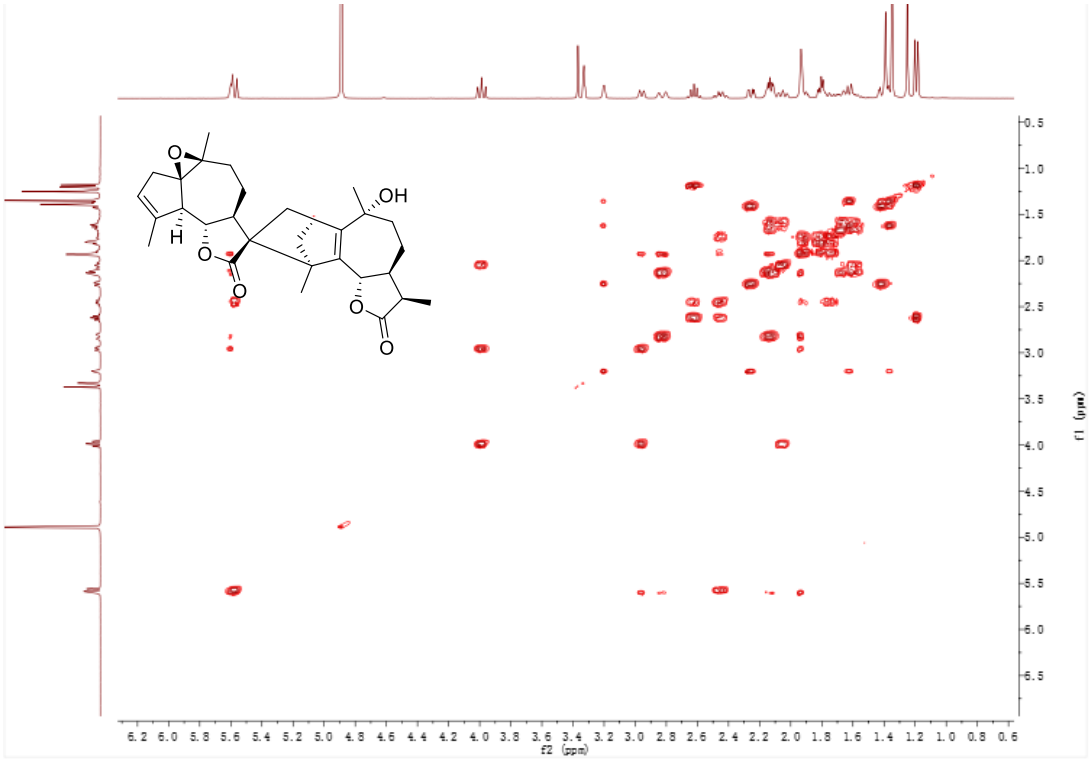


Figure S85 ^{1}H–^{1}H COSY spectrum (600 MHz) of lavandiolide J (**9**) in CD_3OD.

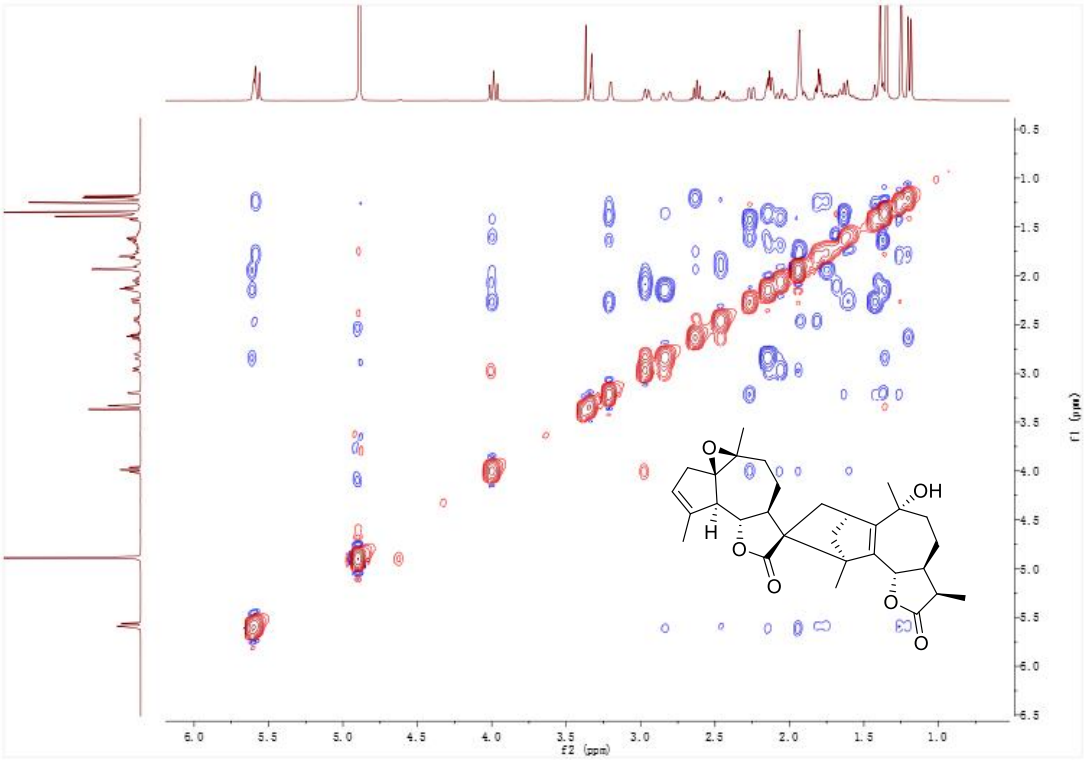


Figure S86 ROESY spectrum (600 MHz) of lavandiolide J (**9**) in CD_3OD.

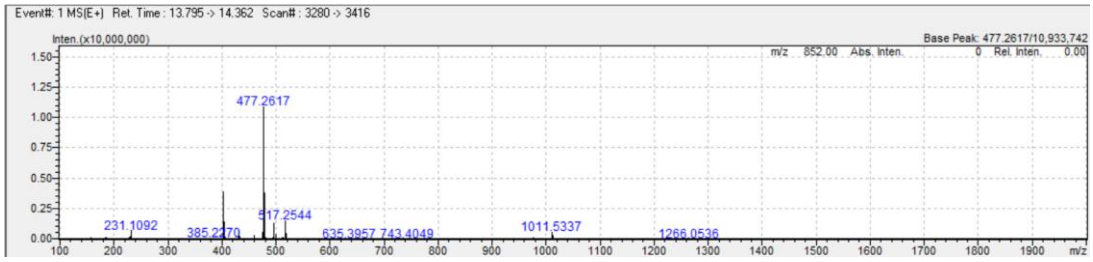


Figure S87 HRESIMS spectrum of lavandiolide J (**9**).

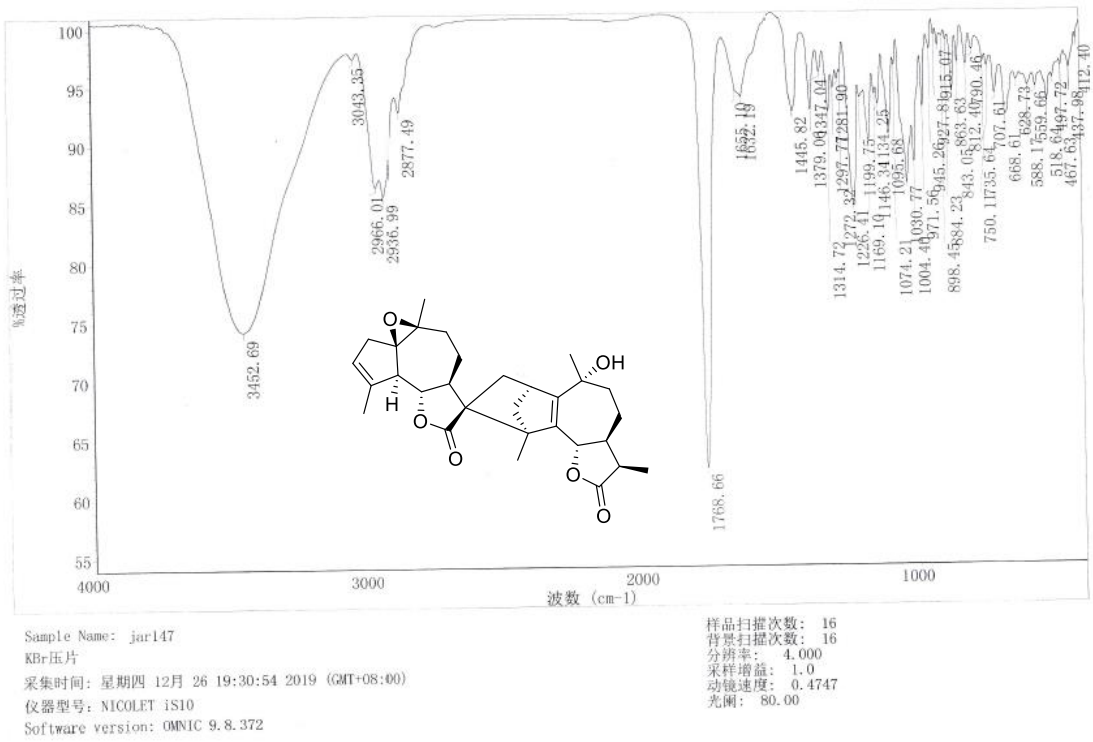


Figure S88 IR spectrum of lavandiolide J (**9**).

Rudolph Research Analytical

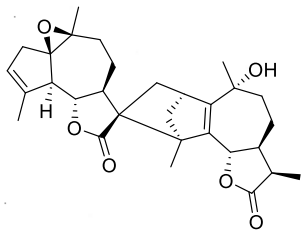
This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Friday, 13-DEC-2019

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled



n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	69.45	0.16	0.23	69.61	69.22

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	jar147	05:20:42 PM	69.41	SR	0.0354	589	100.00	0.051	23.2
2	jar147	05:20:51 PM	69.61	SR	0.0355	589	100.00	0.051	23.2
3	jar147	05:20:59 PM	69.61	SR	0.0355	589	100.00	0.051	23.2
4	jar147	05:21:07 PM	69.41	SR	0.0354	589	100.00	0.051	23.1
5	jar147	05:21:15 PM	69.22	SR	0.0353	589	100.00	0.051	23.1

Figure S89 Optical rotation spectrum of lavandiolide J (**9**).

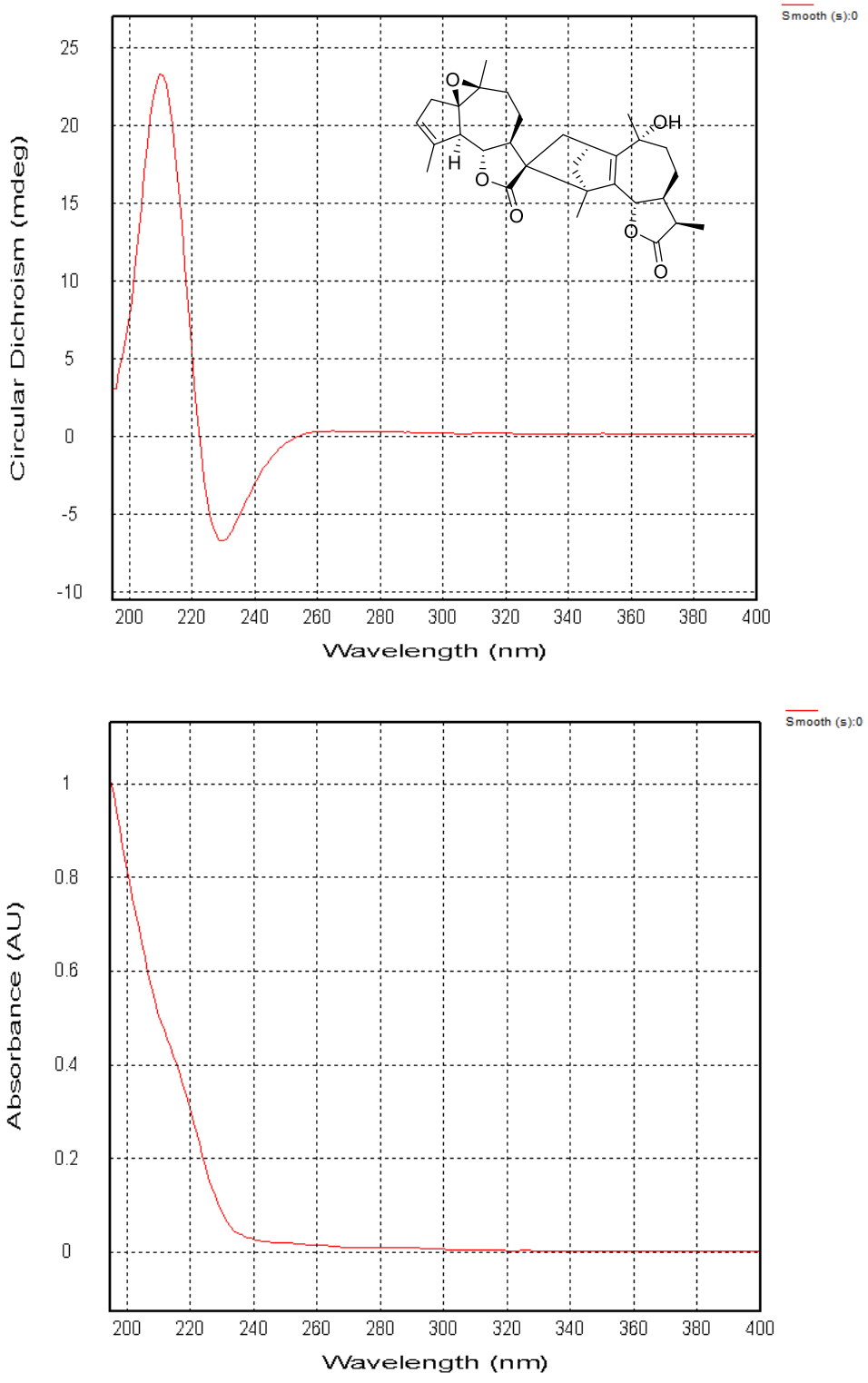


Figure S90 CD (top) and UV (bottom) spectra of lavandiolide J (**9**).

11. NMR, MS, IR, $[\alpha]_D$ and CD spectra of compound 10

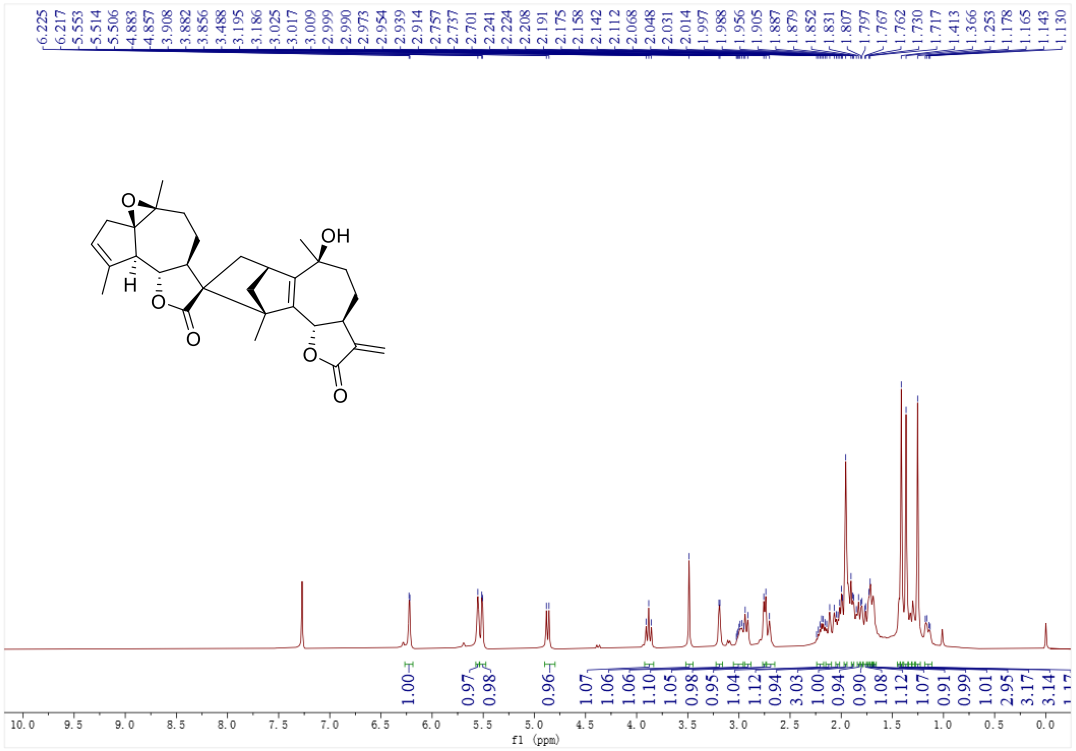


Figure S91 ^{1}H NMR spectrum (400 MHz) of artematrolide G (**10**) in $CDCl_3$.

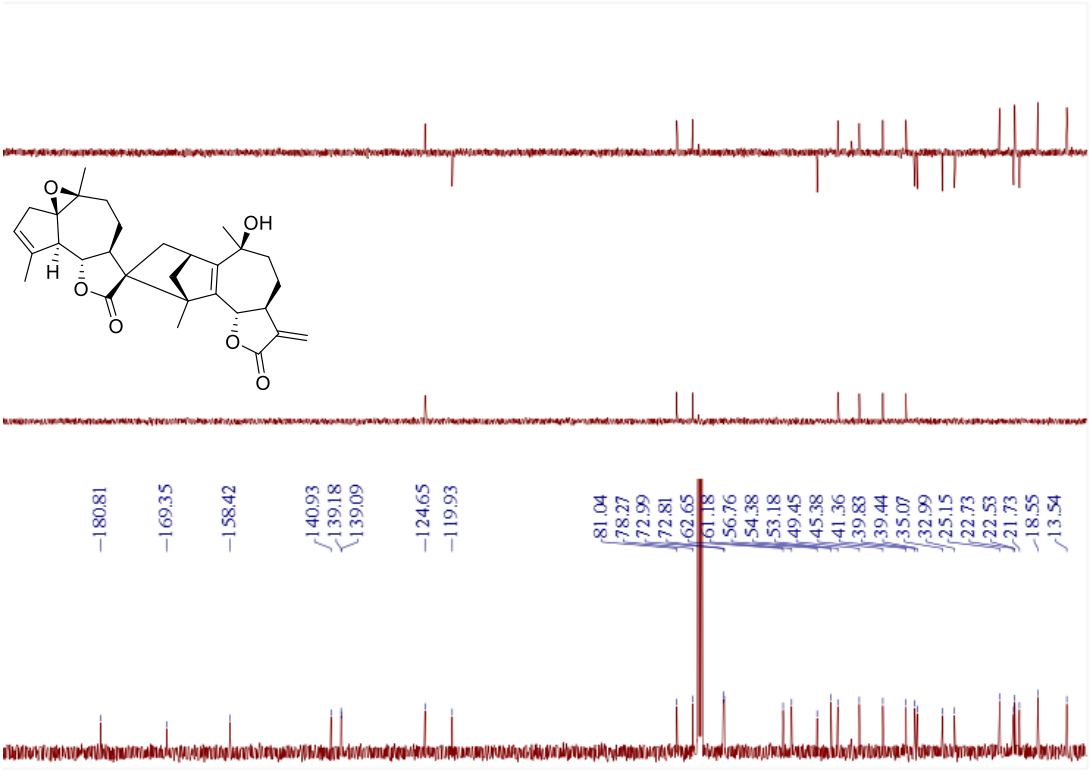


Figure S92 ^{13}C NMR spectrum (100 MHz) of artematrolide G (**10**) in $CDCl_3$.

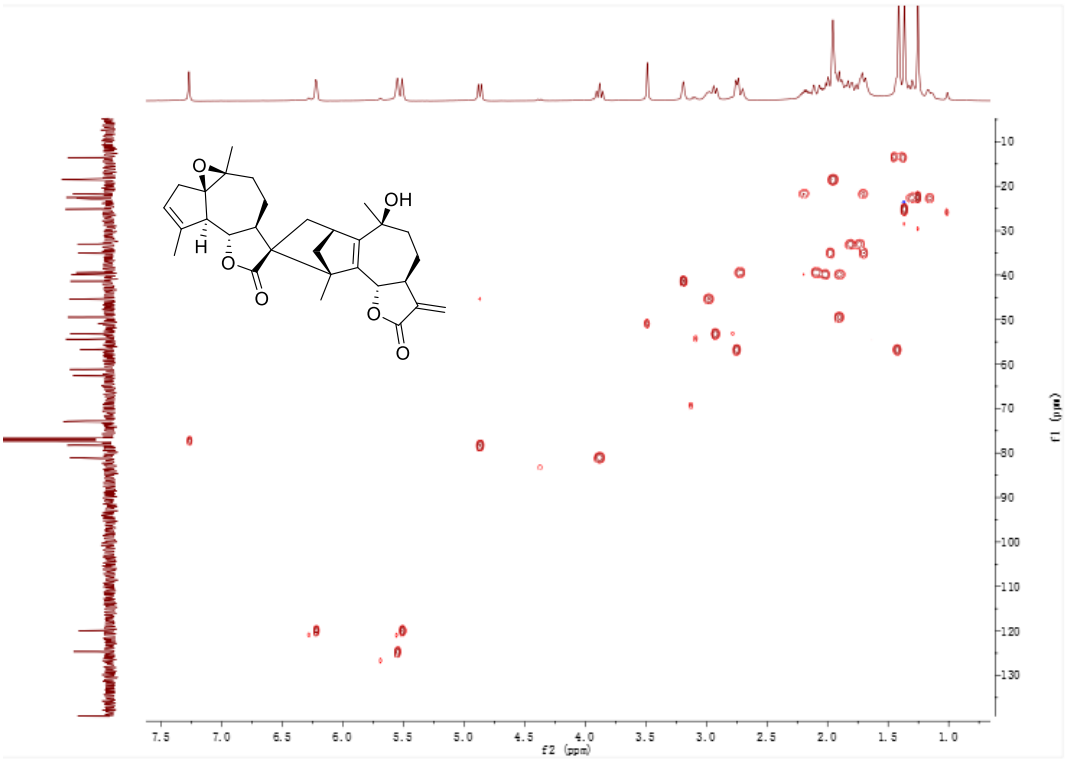


Figure S93 HSQC spectrum (600 MHz) of artematrolide G (**10**) in $CDCl_3$.

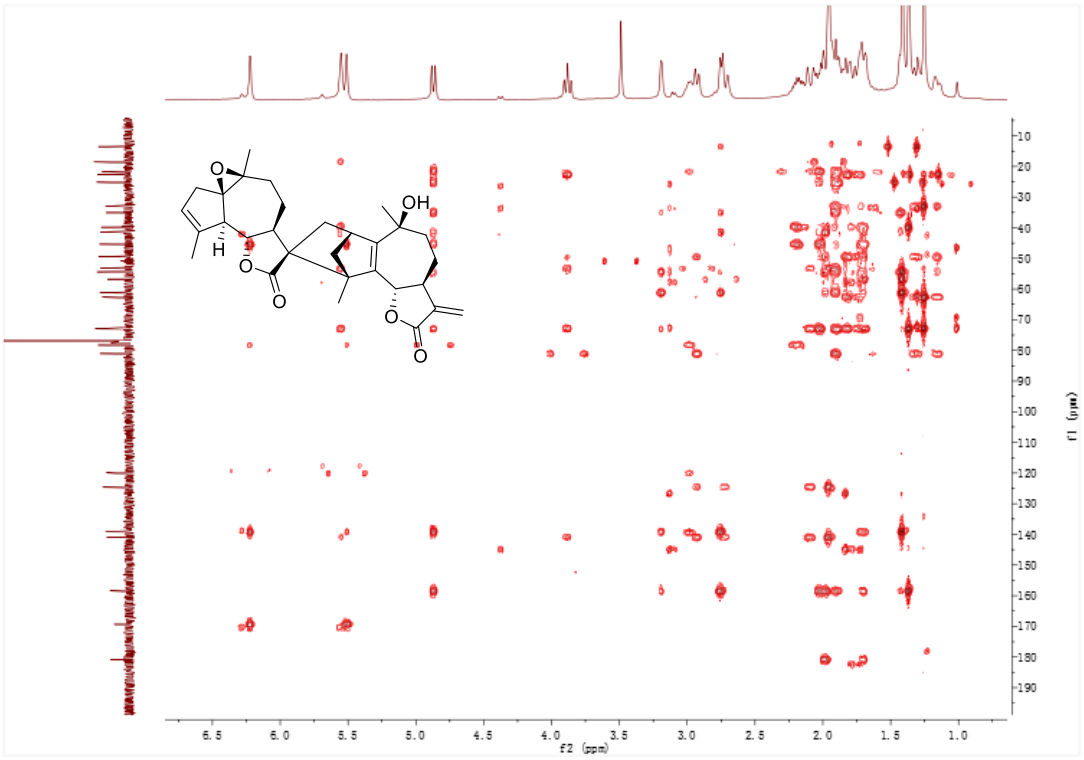


Figure S94 HMBC spectrum (600 MHz) of artematrolide G (**10**) in $CDCl_3$.

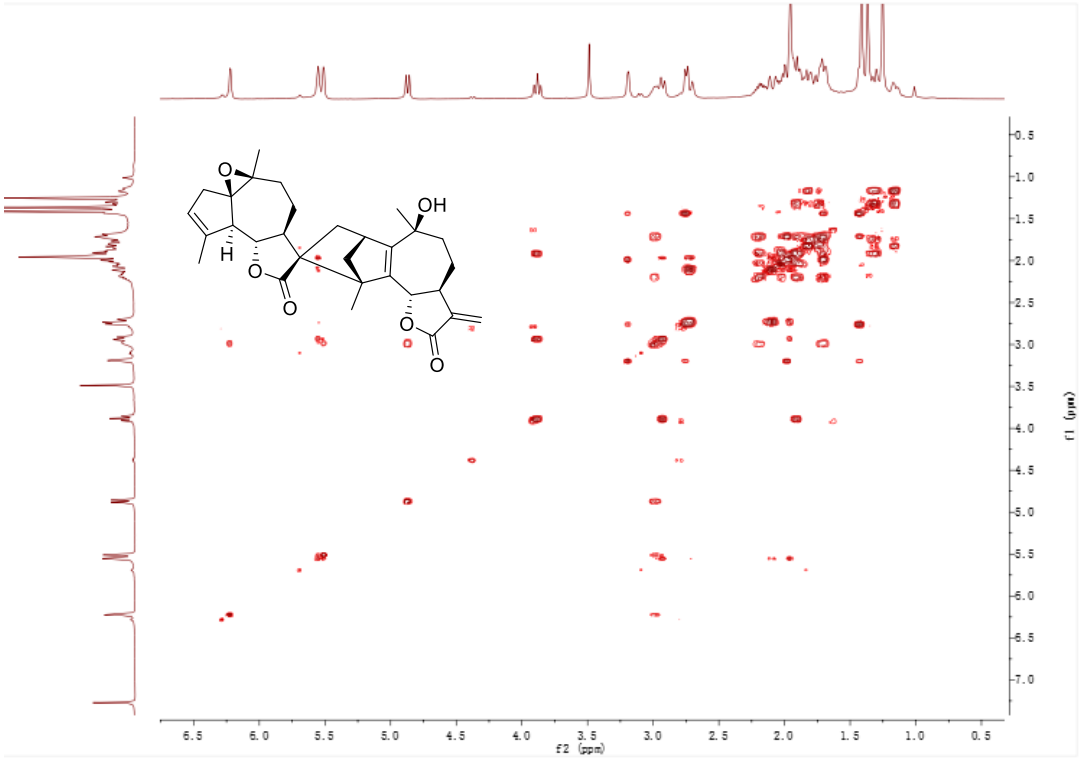


Figure S95 ^{1}H–^{1}H COSY spectrum (600 MHz) of artematrolide G (**10**) in $CDCl_3$.

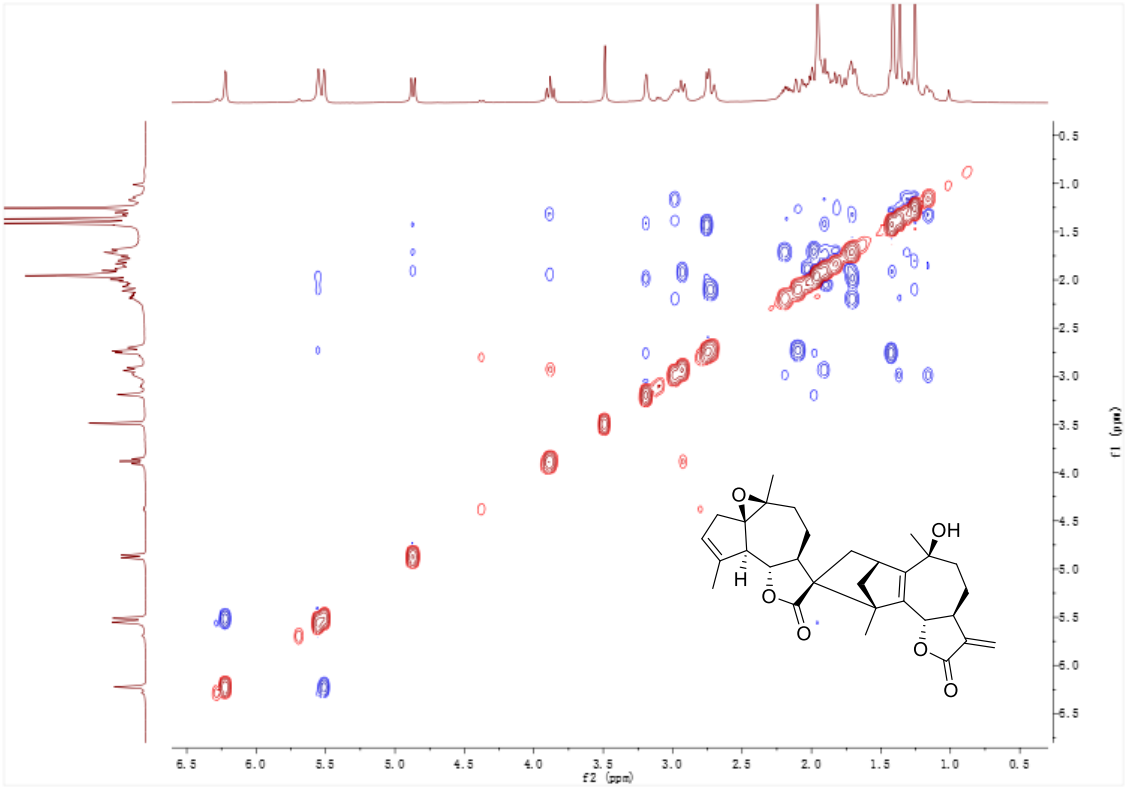


Figure S96 ROESY spectrum (600 MHz) of artematrolide G (**10**) in $CDCl_3$.

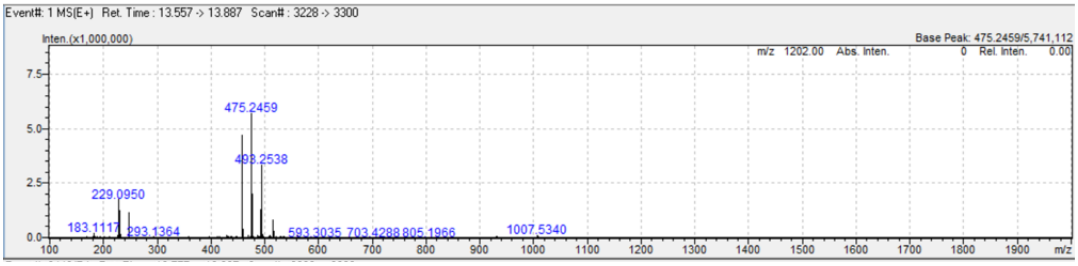


Figure S97 HRESIMS spectrum of artematrolide G (**10**).

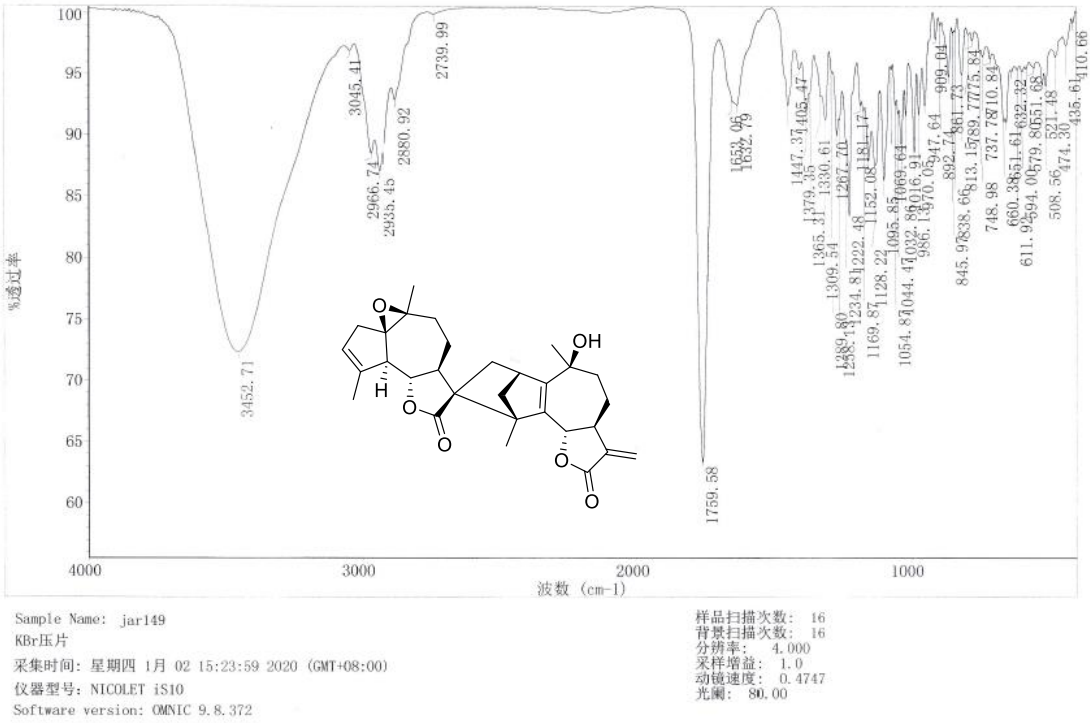


Figure S98 IR spectrum of artematrolide G (**10**).

Rudolph Research Analytical

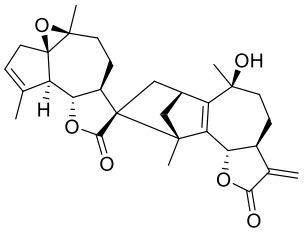
This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Thursday, 19-DEC-2019

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled



n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	77.23	0.75	0.97	77.87	75.96

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	jar149	03:17:14 PM	75.96	SR	0.0357	589	100.00	0.047	20.9
2	jar149	03:17:22 PM	77.45	SR	0.0364	589	100.00	0.047	20.9
3	jar149	03:17:30 PM	77.87	SR	0.0366	589	100.00	0.047	20.9
4	jar149	03:17:39 PM	77.23	SR	0.0363	589	100.00	0.047	20.9
5	jar149	03:17:47 PM	77.66	SR	0.0365	589	100.00	0.047	20.9

Figure S99 Optical rotation spectrum of artematrolide G (**10**).

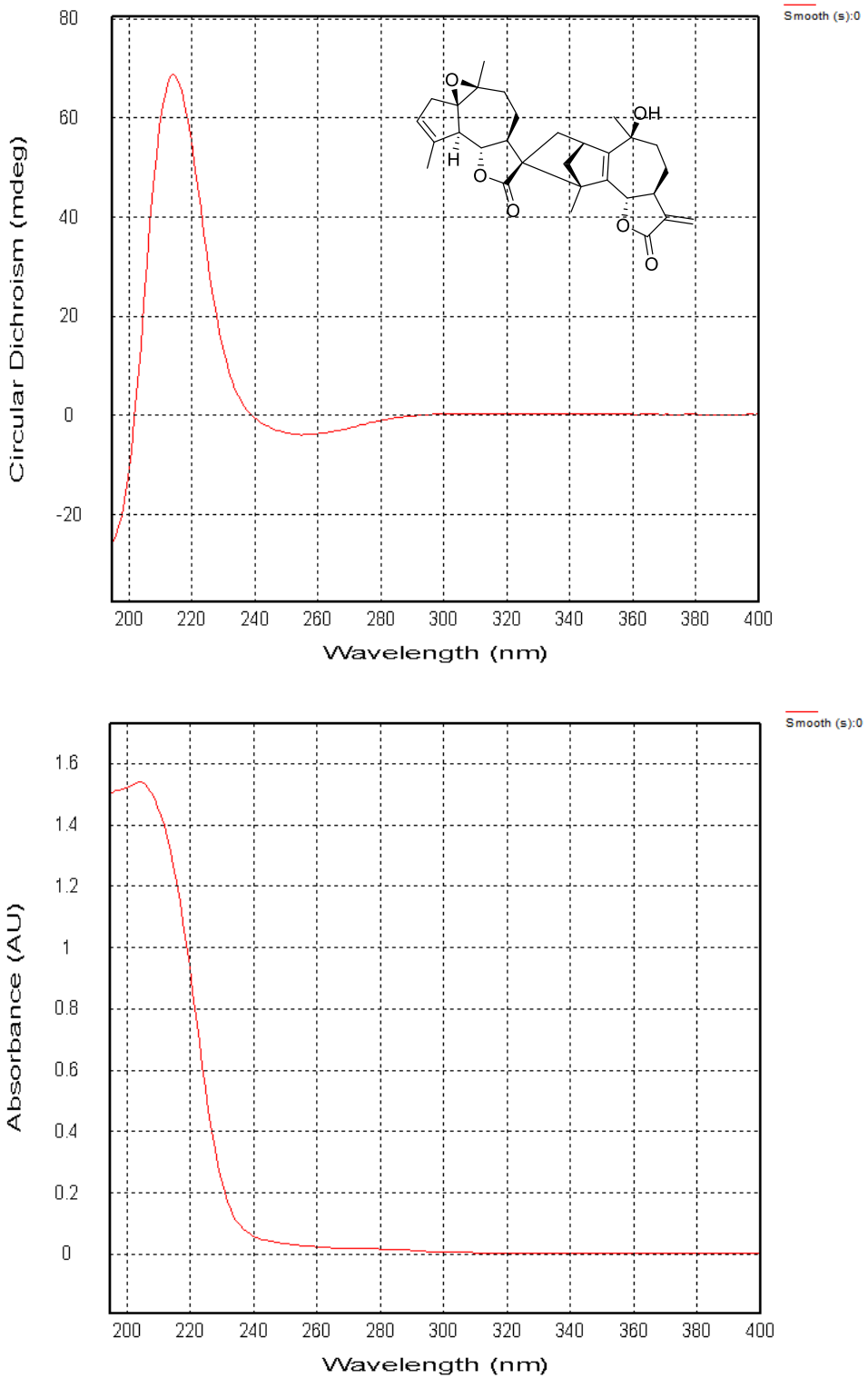


Figure S100 CD (top) and UV (bottom) spectra of artematrolide G (**10**).

12. NMR, MS, IR, $[\alpha]_D$ and CD spectra of compound 11

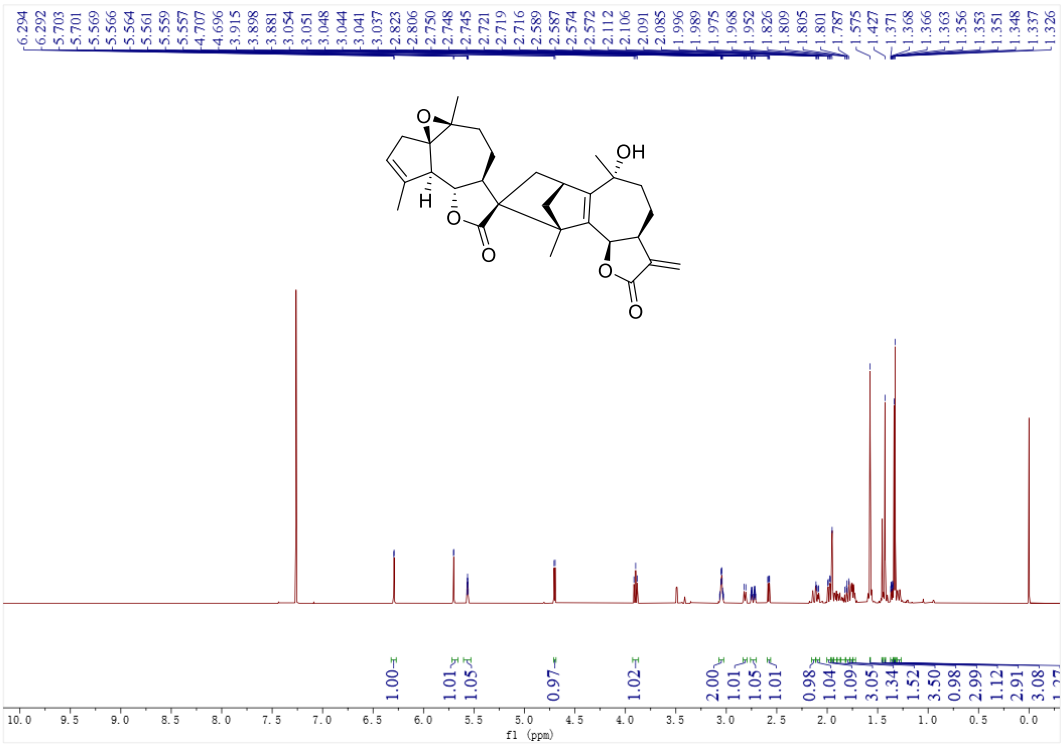


Figure S101 ^{1}H NMR spectrum (600 MHz) of artematrolide H (**11**) in $CDCl_3$.

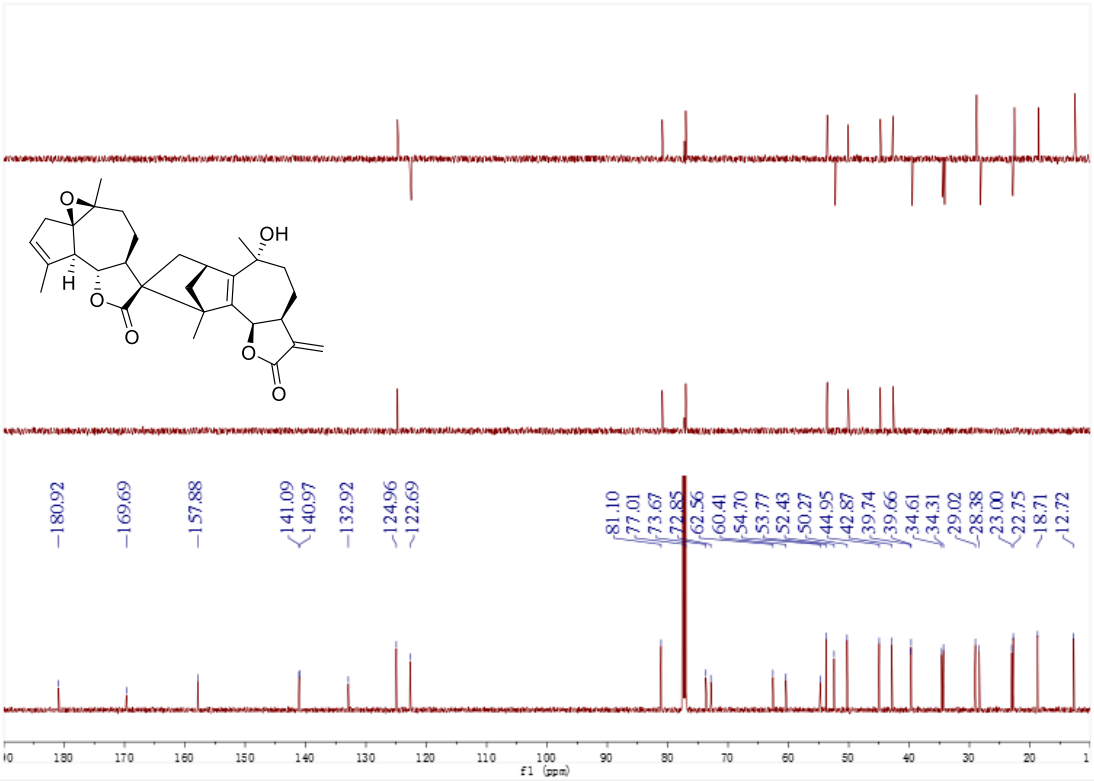


Figure S102 ^{13}C NMR spectrum (150 MHz) of artematrolide H (**11**) in $CDCl_3$.

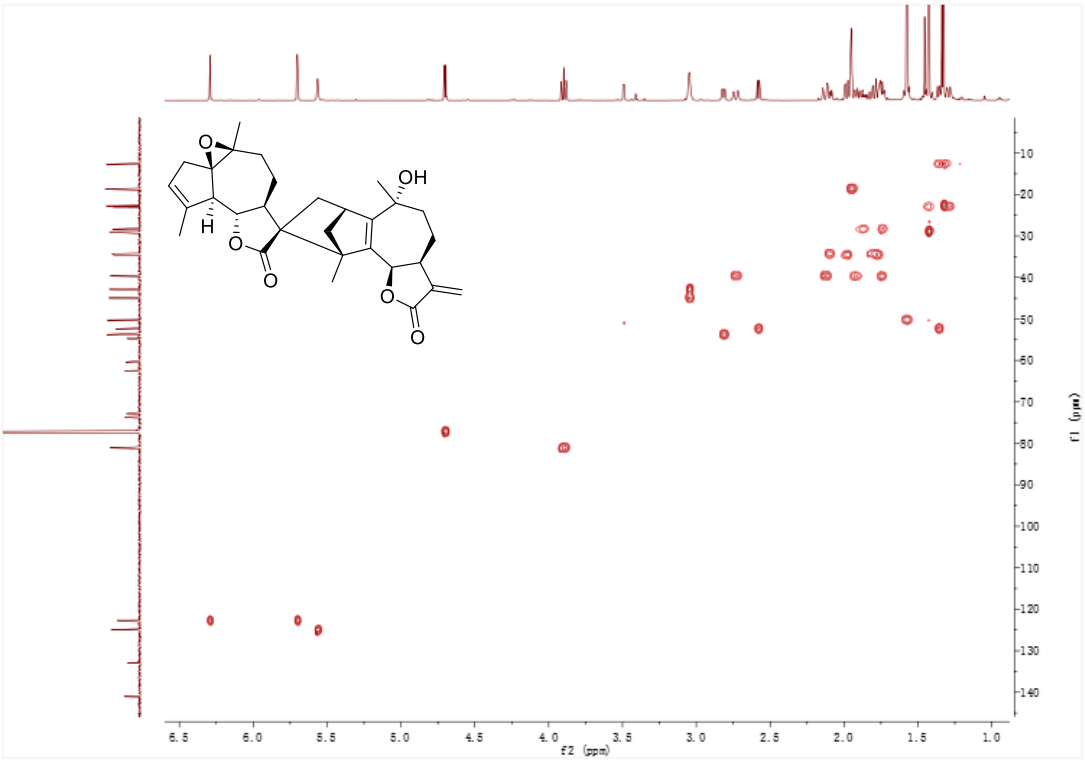


Figure S103 HSQC spectrum (600 MHz) of artematrolide H (**11**) in $CDCl_3$.

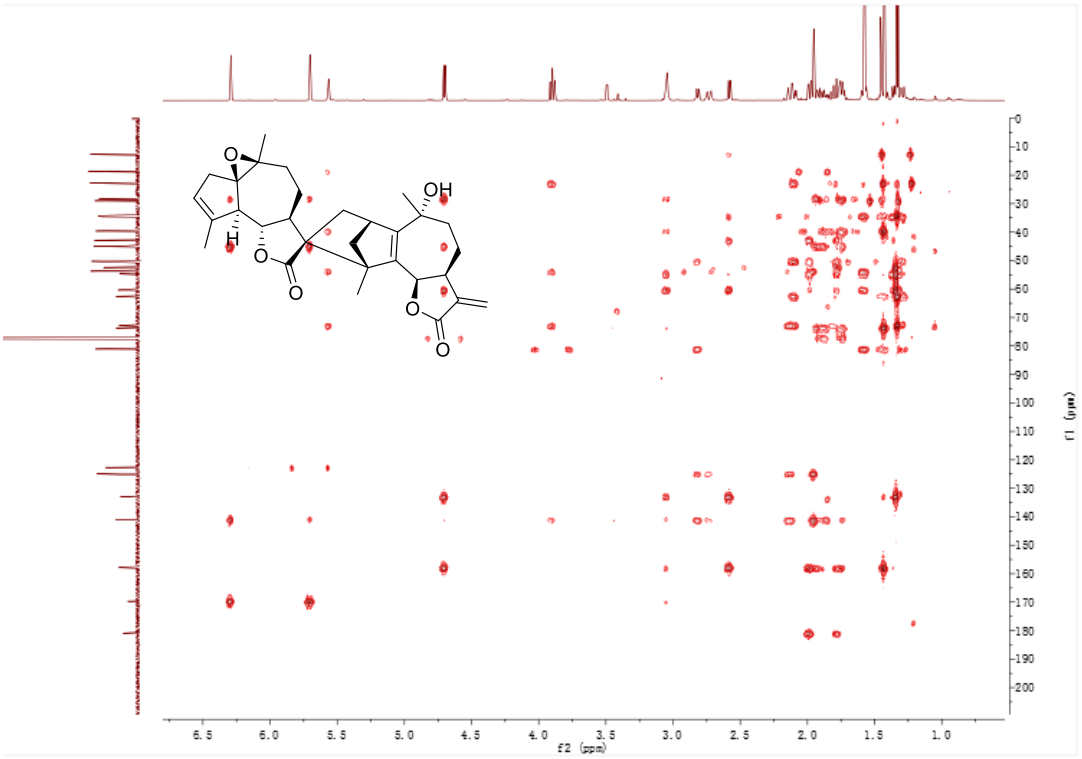


Figure S104 HMBC spectrum (600 MHz) of artematrolide H (**11**) in $CDCl_3$.

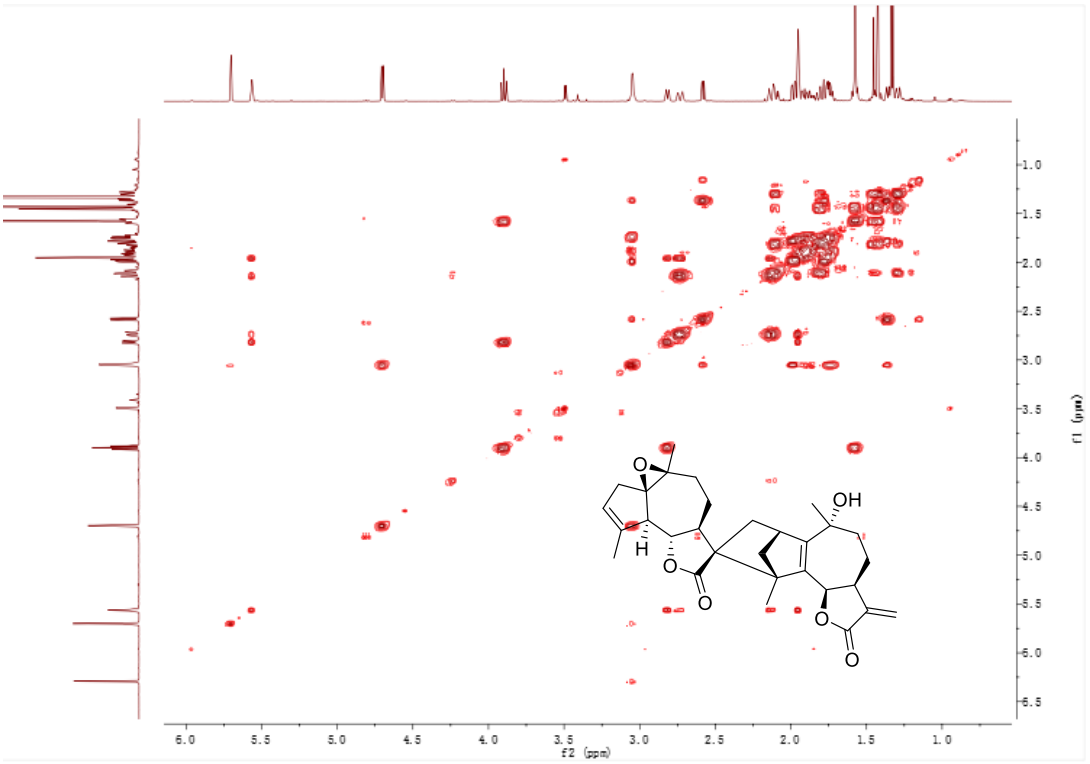


Figure S105 ^{1}H–^{1}H COSY spectrum (600 MHz) of artematrolide H (**11**) in $CDCl_3$.

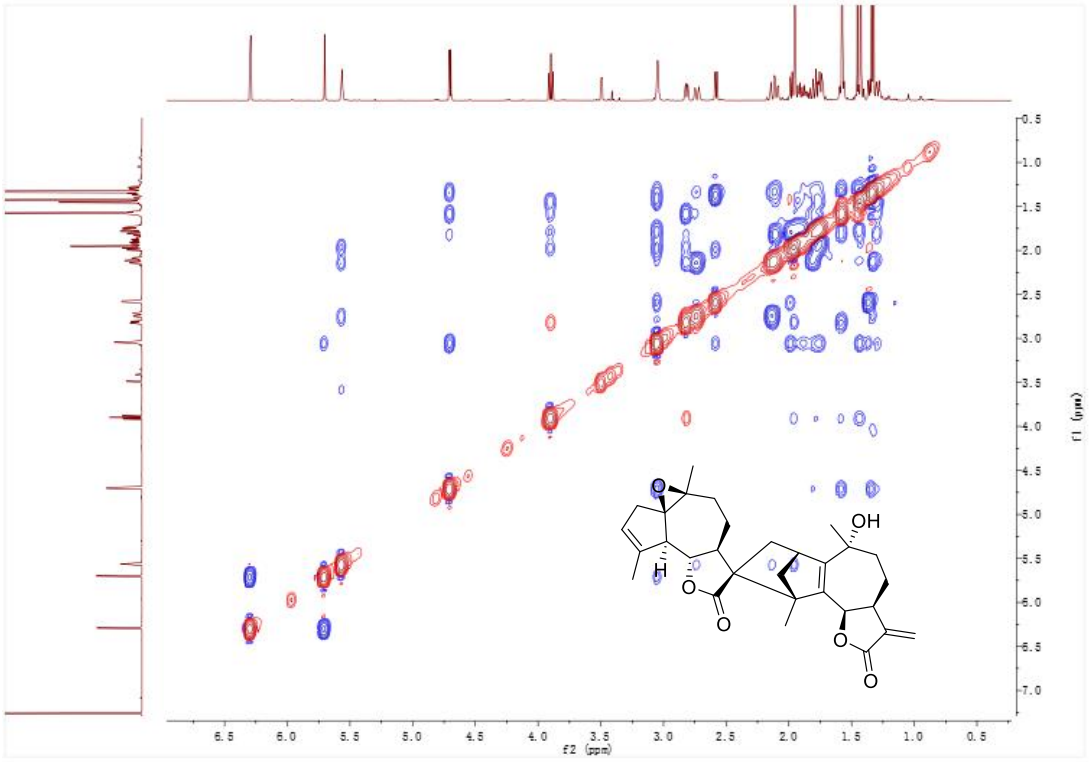


Figure S106 ROESY spectrum (600 MHz) of artematrolide H (**11**) in $CDCl_3$.

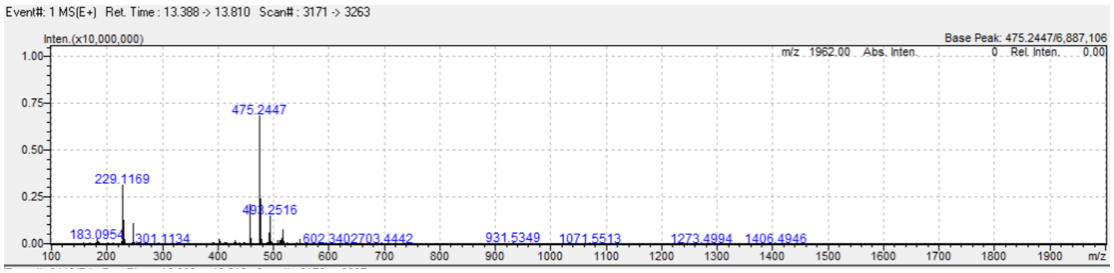


Figure S107 HRESIMS spectrum of artematrolide H (**11**).

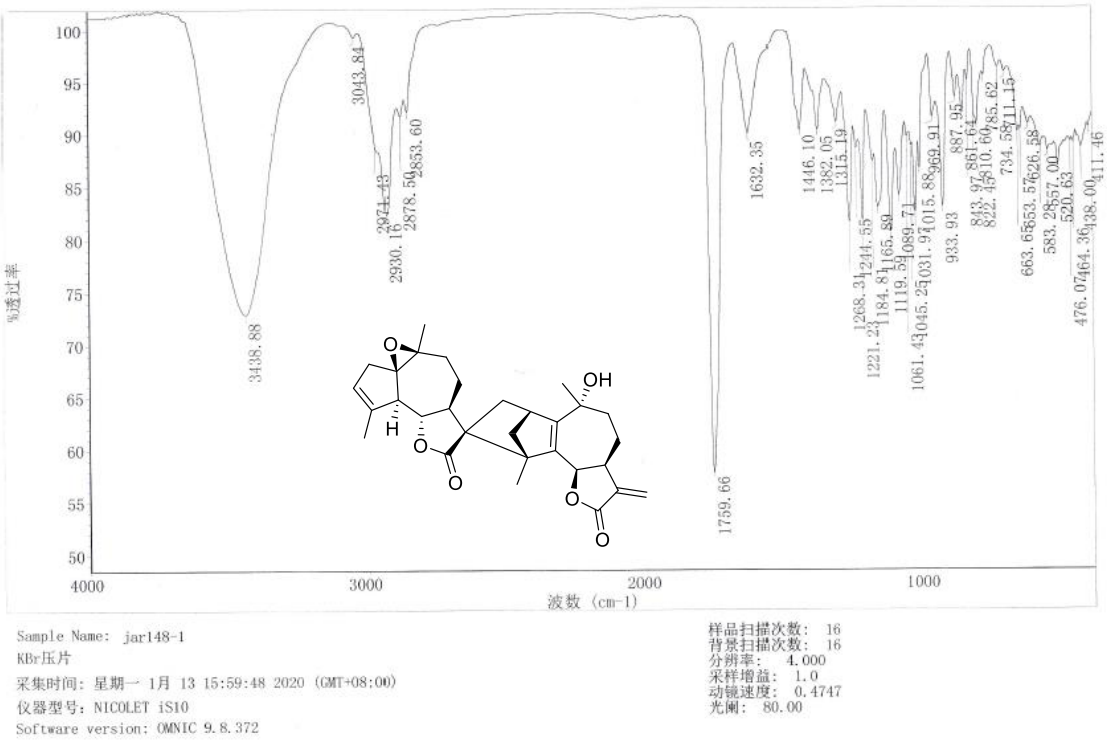


Figure S108 IR spectrum of artematrolide H (**11**).

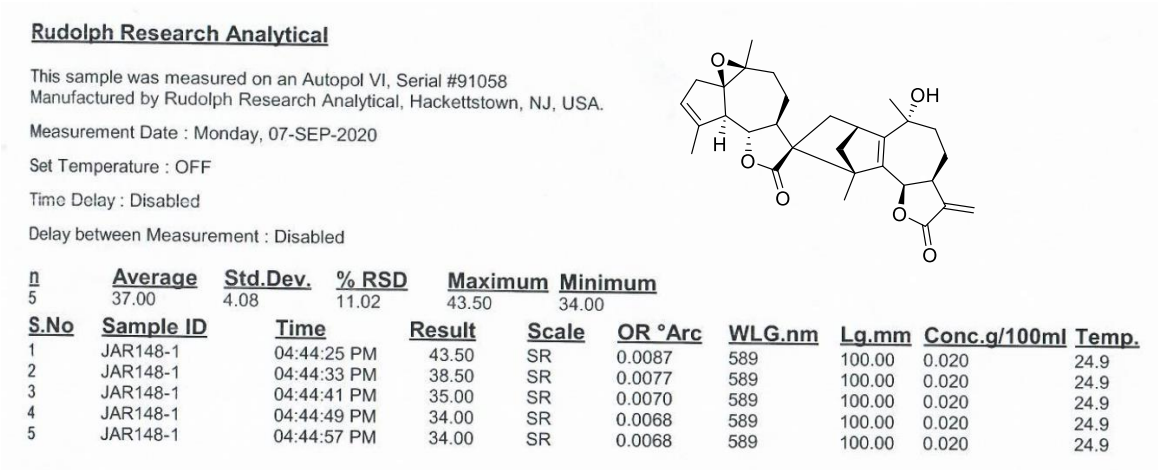


Figure S109 Optical rotation spectrum of artematrolide H (**11**).

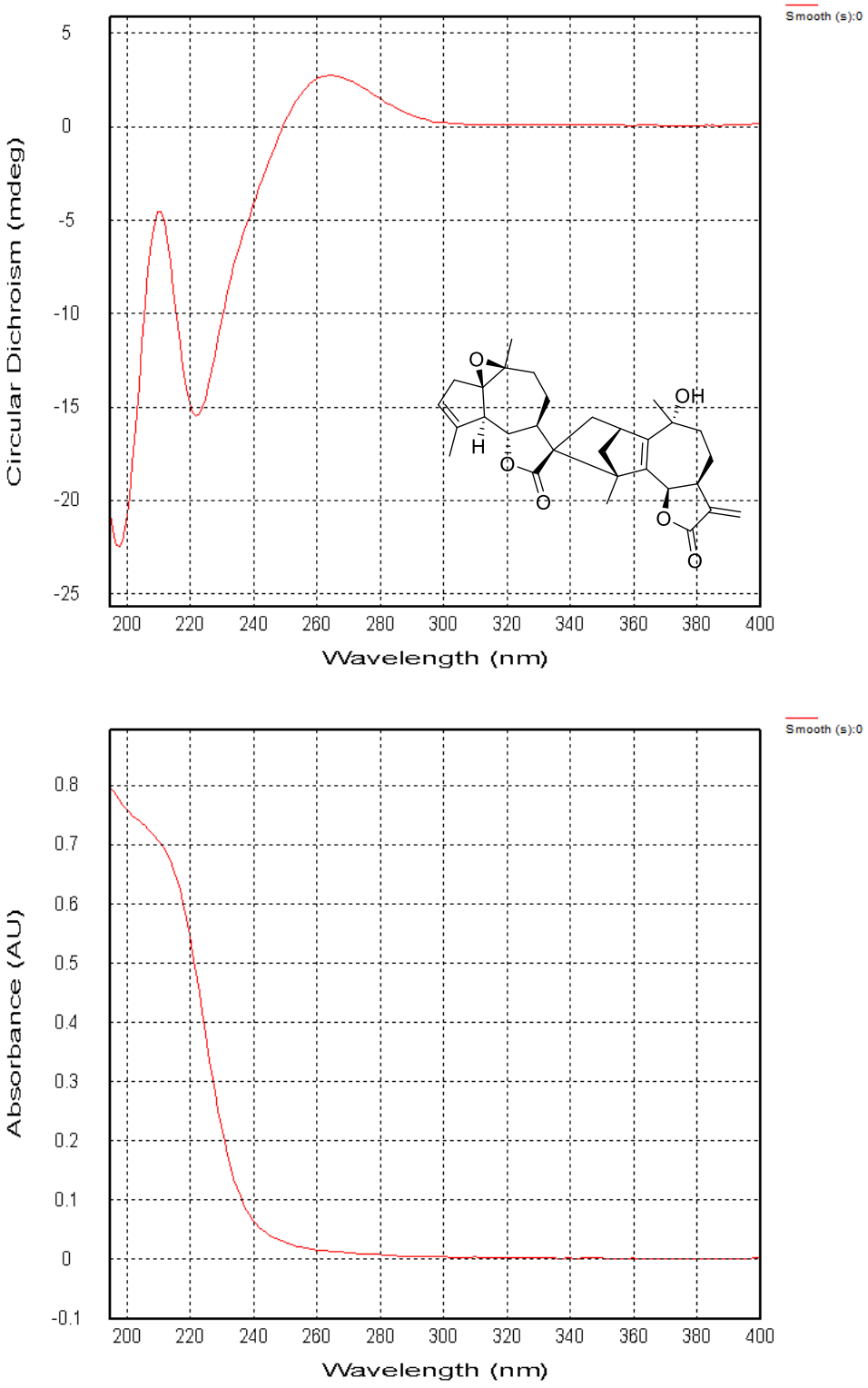


Figure S110 CD (top) and UV (bottom) spectra of artematrolide H (**11**).

13. NMR, MS, IR, $[\alpha]_D$ and CD spectra of compound 12

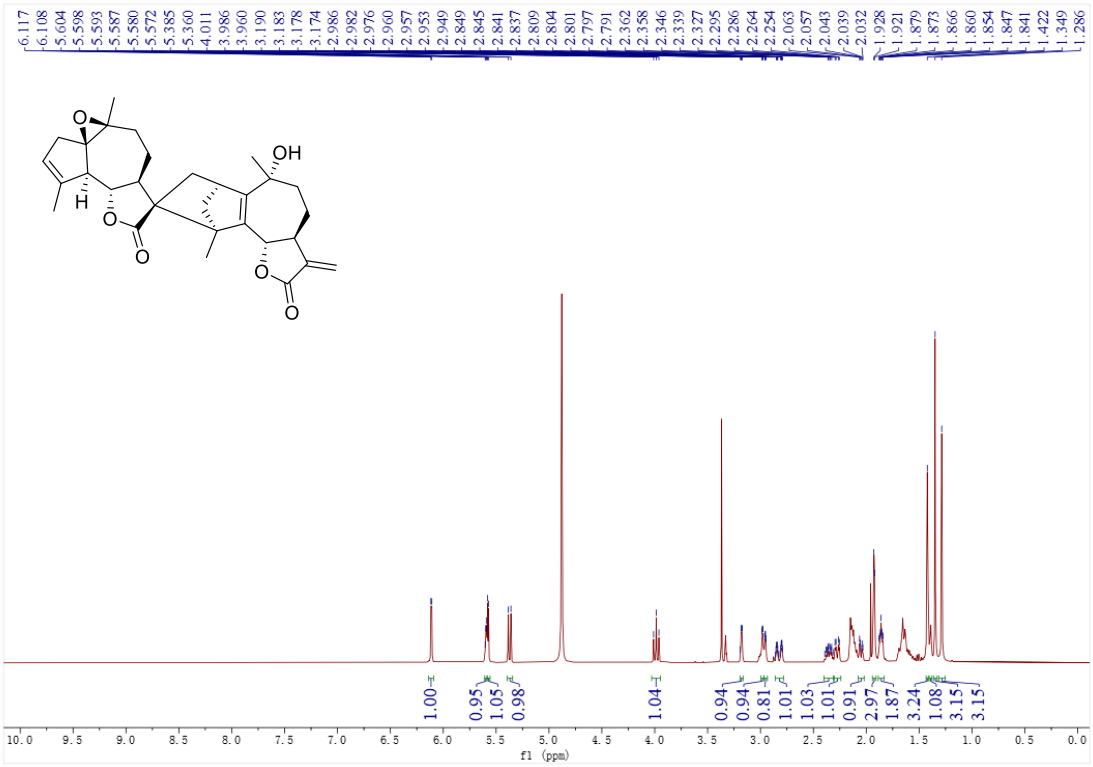


Figure S111 ^{1}H NMR spectrum (400 MHz) of lavandiolide H (**12**) in CD_3OD.

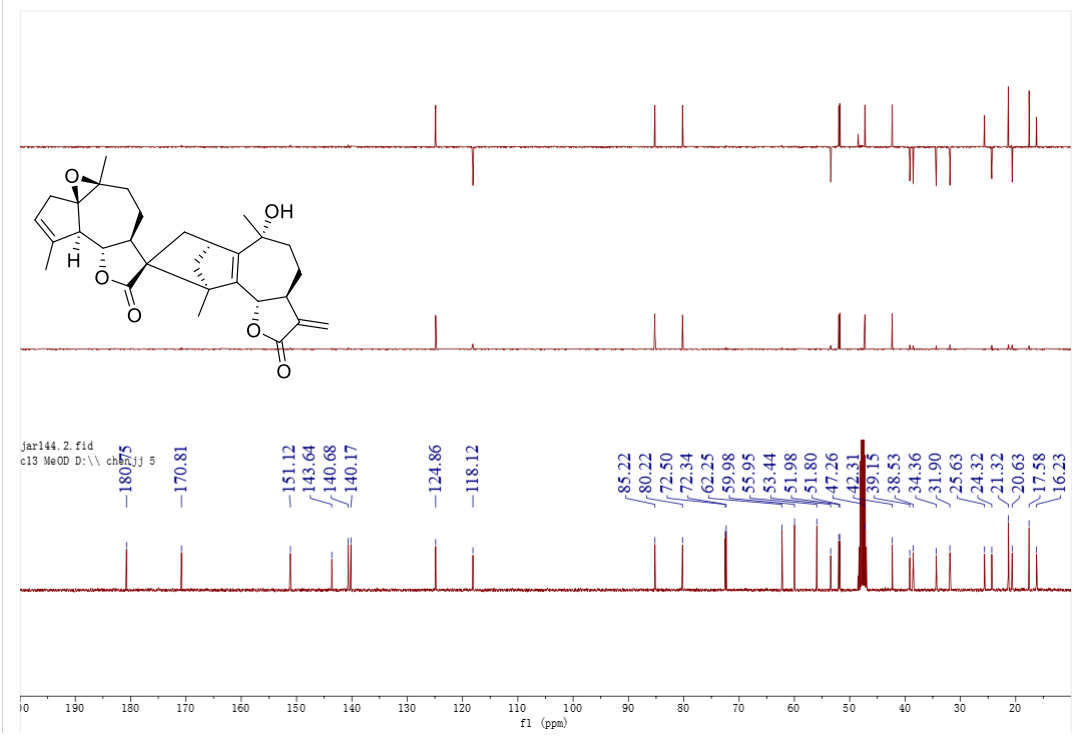


Figure S112 ^{13}C NMR spectrum (100 MHz) of lavandiolide H (**12**) in CD_3OD.

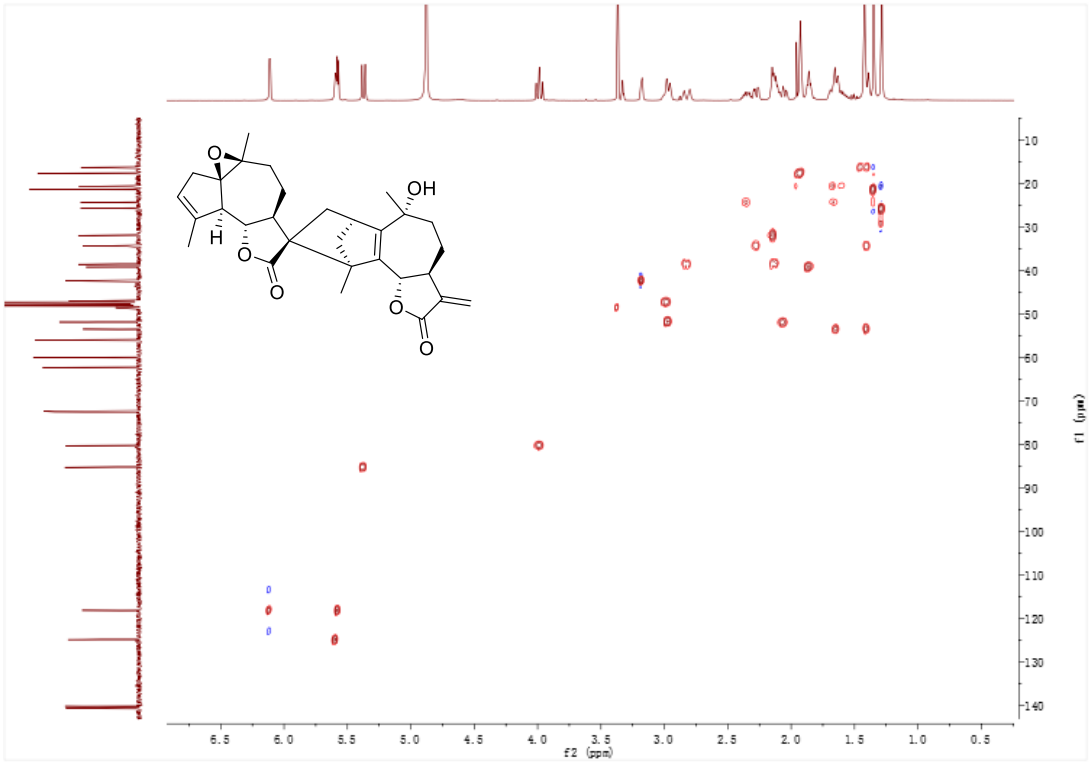


Figure S113 HSQC spectrum (600 MHz) of lavandiolide H (**12**) in CD_3OD.

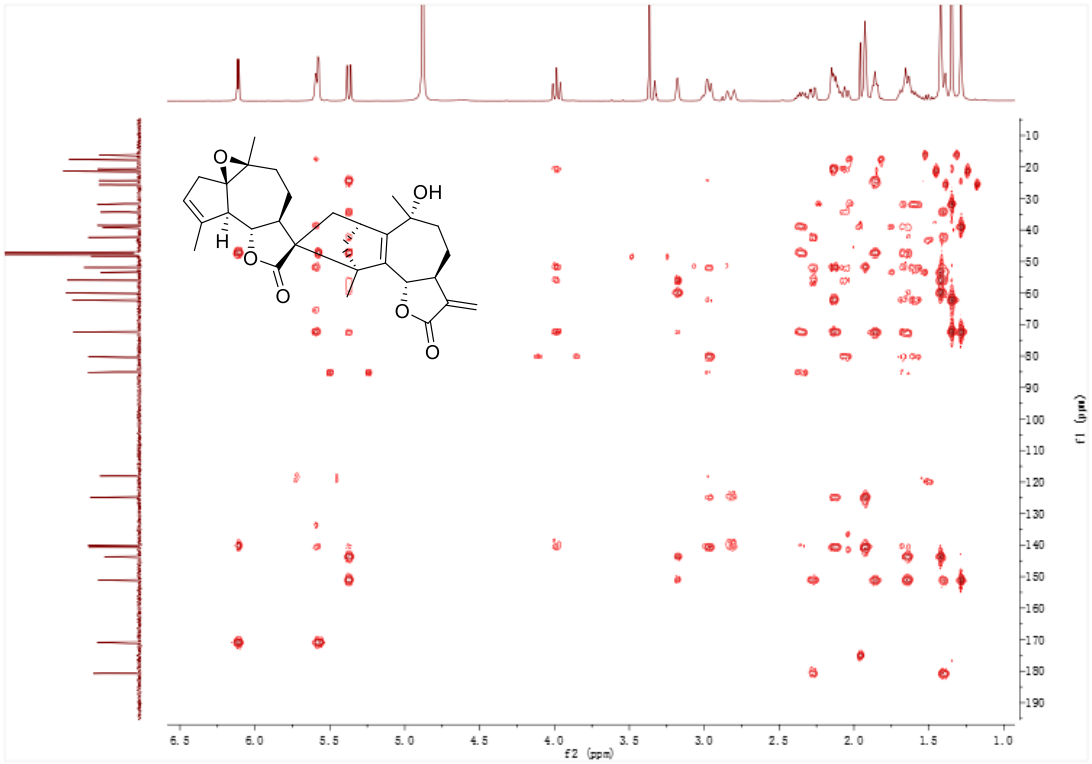


Figure S114 HMBC spectrum (600 MHz) of lavandiolide H (**12**) in CD_3OD.

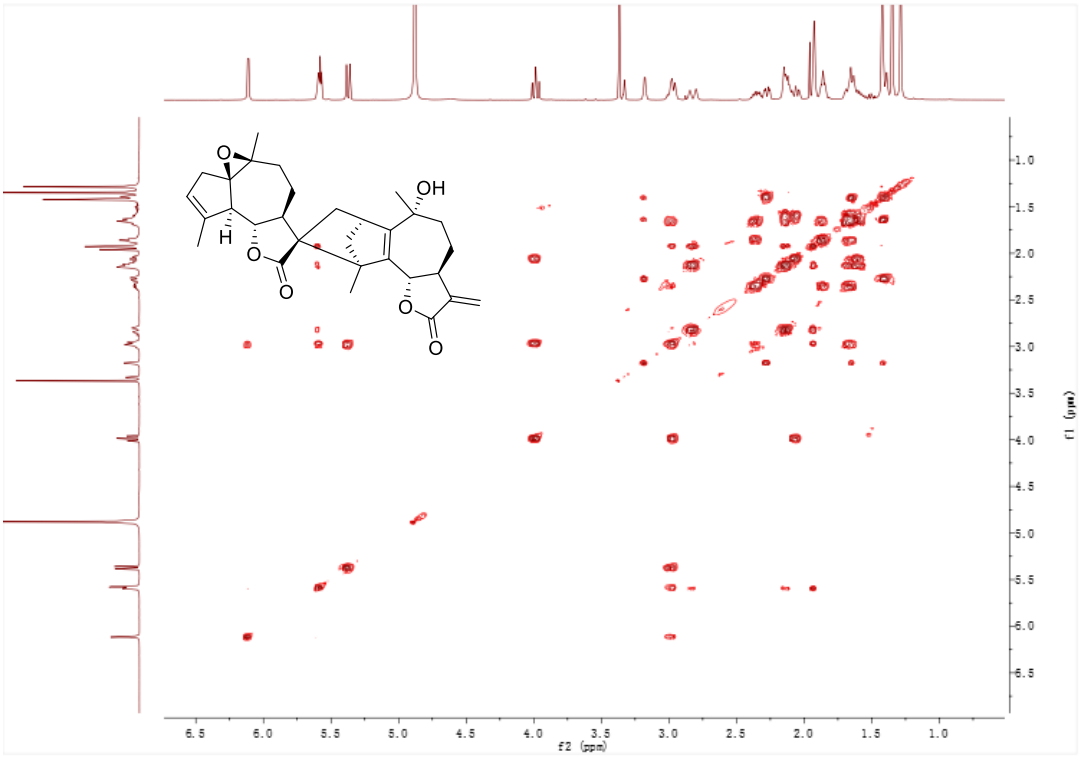


Figure S115 ^{1}H–^{1}H COSY spectrum (600 MHz) of lavandiolide H (**12**) in CD_3OD.

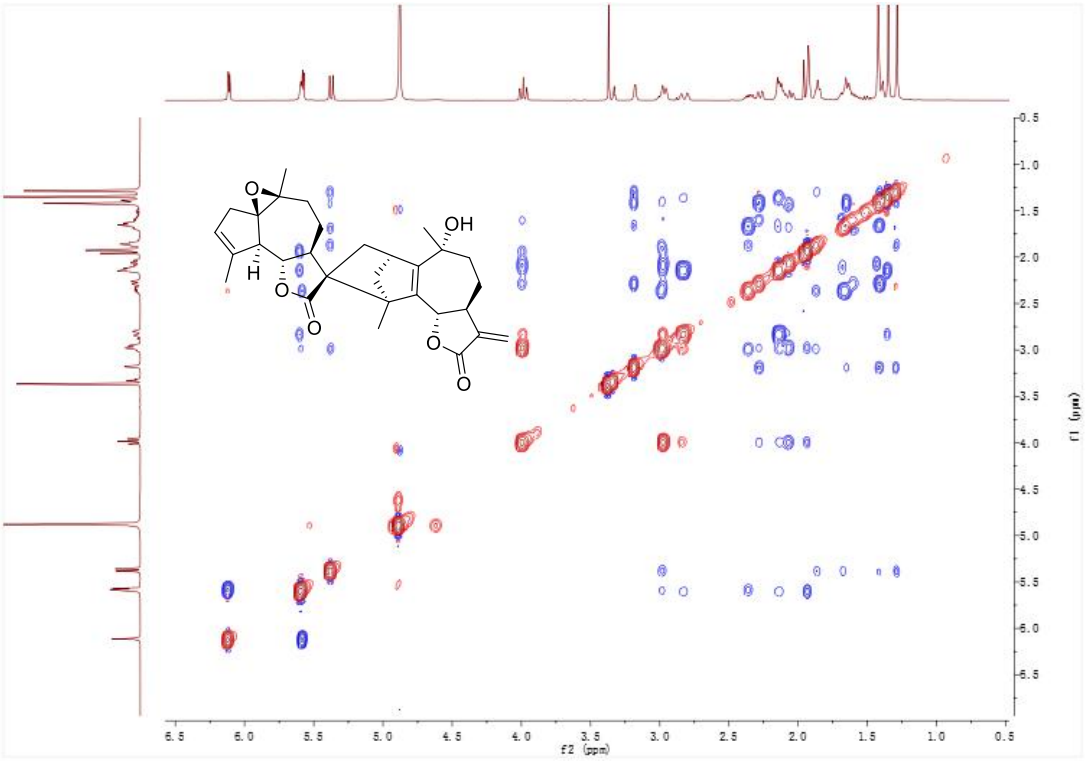


Figure S116 ROESY spectrum (600 MHz) of lavandiolide H (**12**) in CD_3OD.

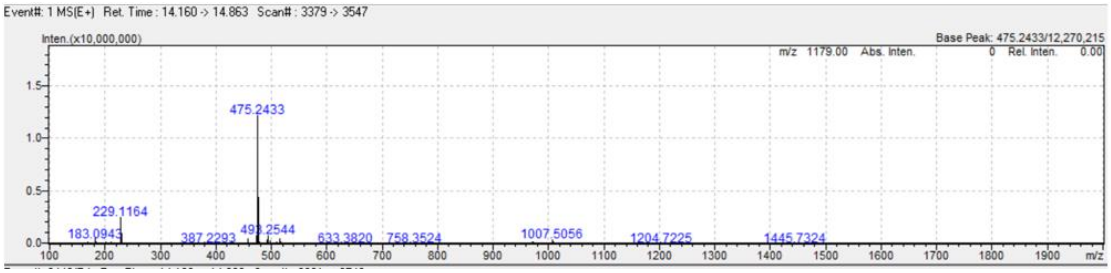


Figure S117 HRESIMS spectrum of lavandiolide H (**12**).

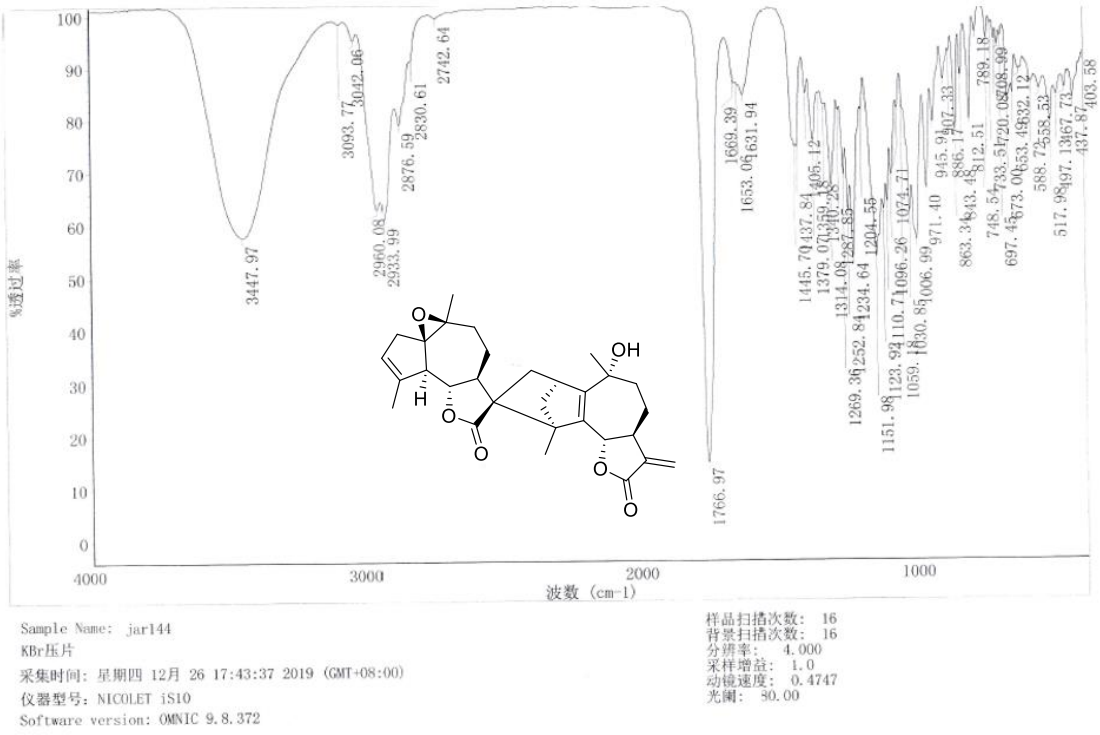


Figure S118 IR spectrum of lavandiolide H (**12**).

Rudolph Research Analytical

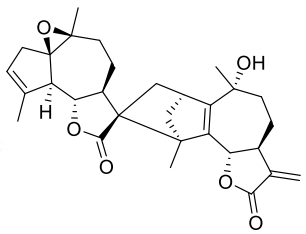
This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Friday, 13-DEC-2019

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled



n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	74.53	0.35	0.46	74.94	74.13

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	jar144	04:50:04 PM	74.13	SR	0.1186	589	100.00	0.160	23.5
2	jar144	04:50:13 PM	74.19	SR	0.1187	589	100.00	0.160	23.5
3	jar144	04:50:21 PM	74.69	SR	0.1195	589	100.00	0.160	23.5
4	jar144	04:50:29 PM	74.69	SR	0.1195	589	100.00	0.160	23.5
5	jar144	04:50:37 PM	74.94	SR	0.1199	589	100.00	0.160	23.5

Figure S119 Optical rotation spectrum of lavandiolide H (**12**).

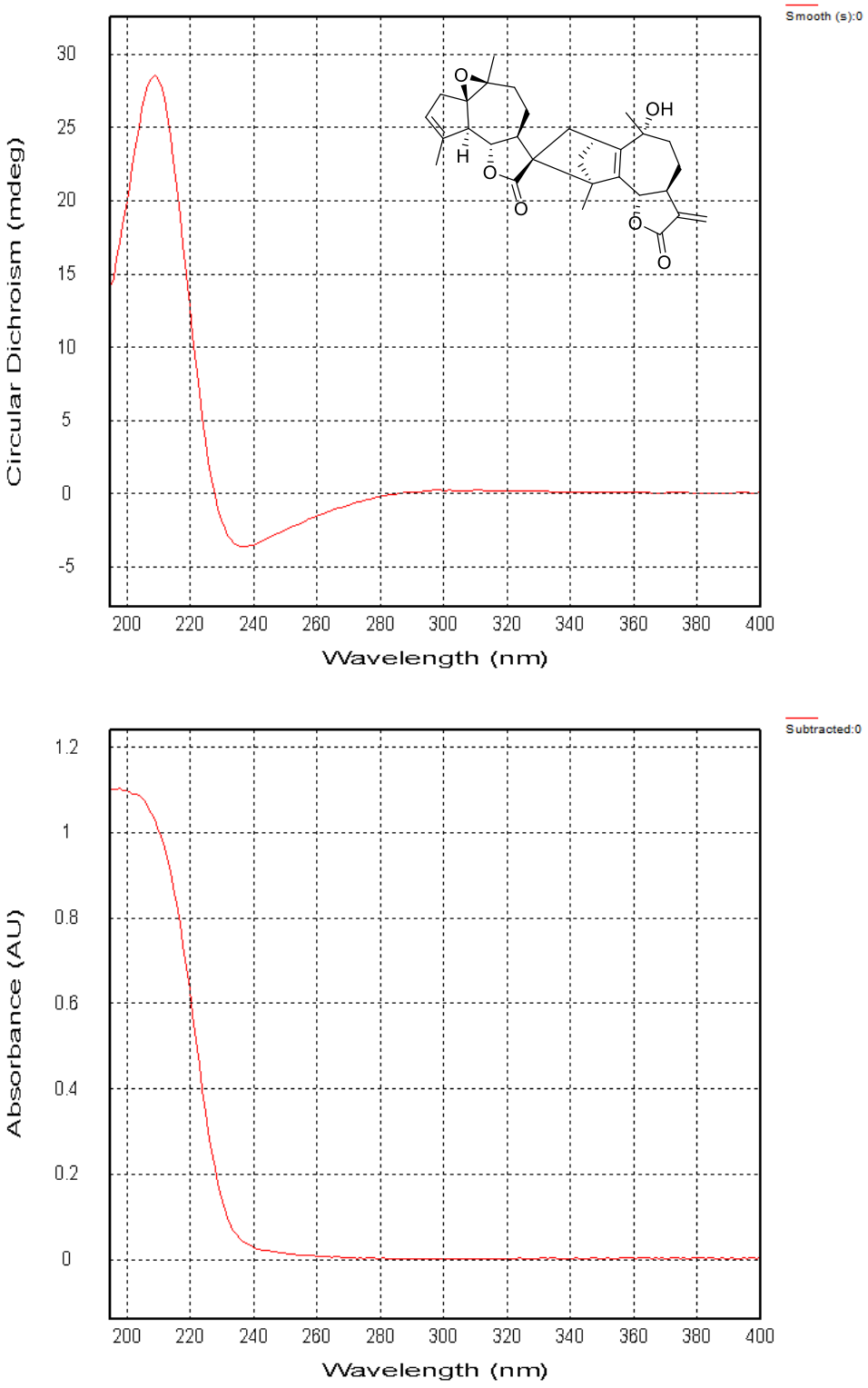


Figure S120 CD (top) and UV (bottom) spectra of lavandiolide H (**12**).

14. NMR, MS, IR, $[\alpha]_D$ and CD spectra of compound 13

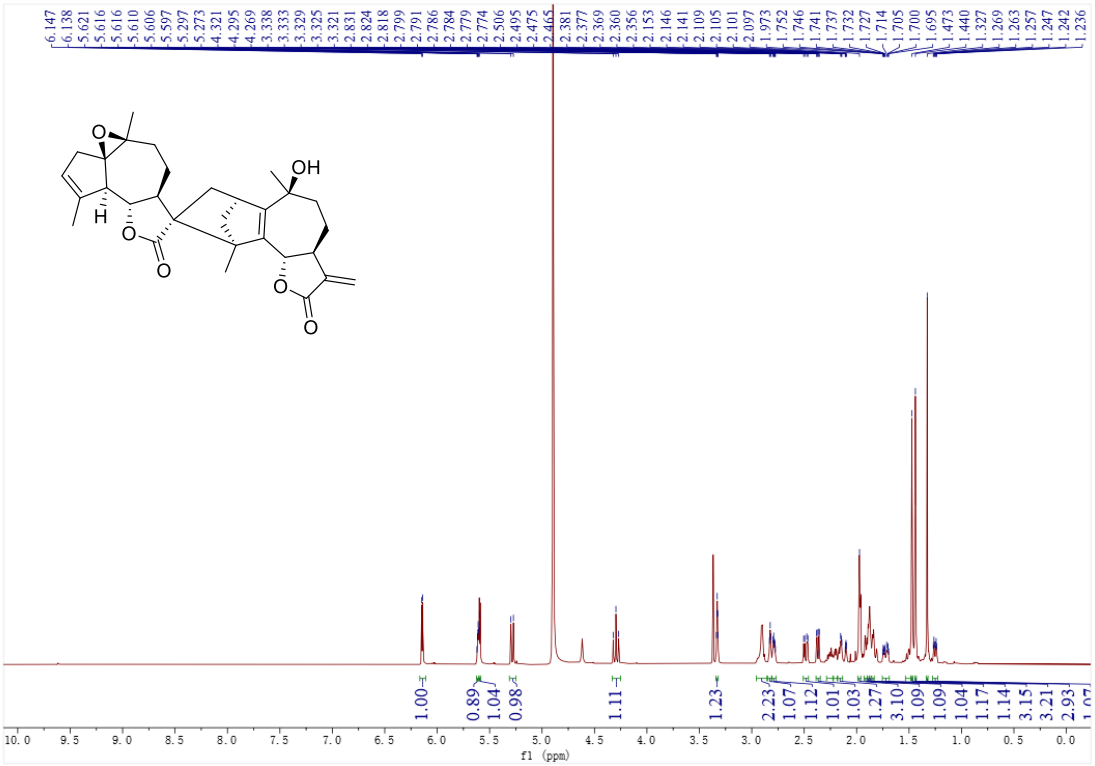


Figure S121 ^{1}H NMR spectrum (400 MHz) of artematrolide I (**13**) in CD_3OD.

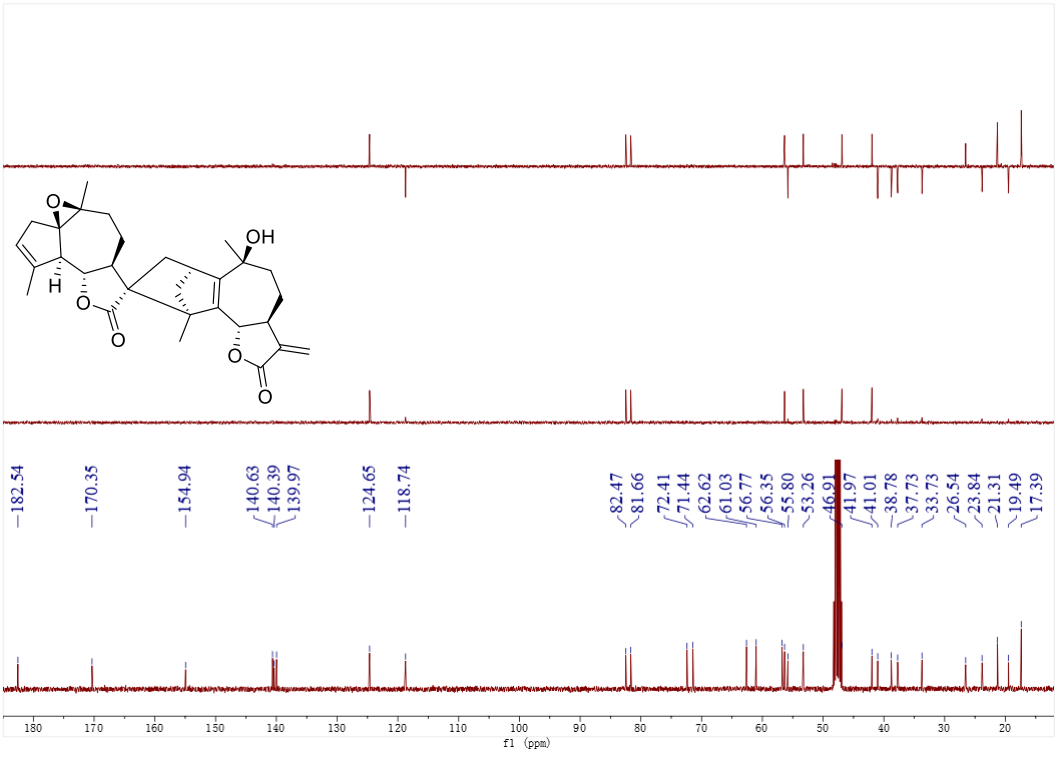


Figure S122 ^{13}C NMR NMR spectrum (100 MHz) of artematrolide I (**13**) in CD_3OD.

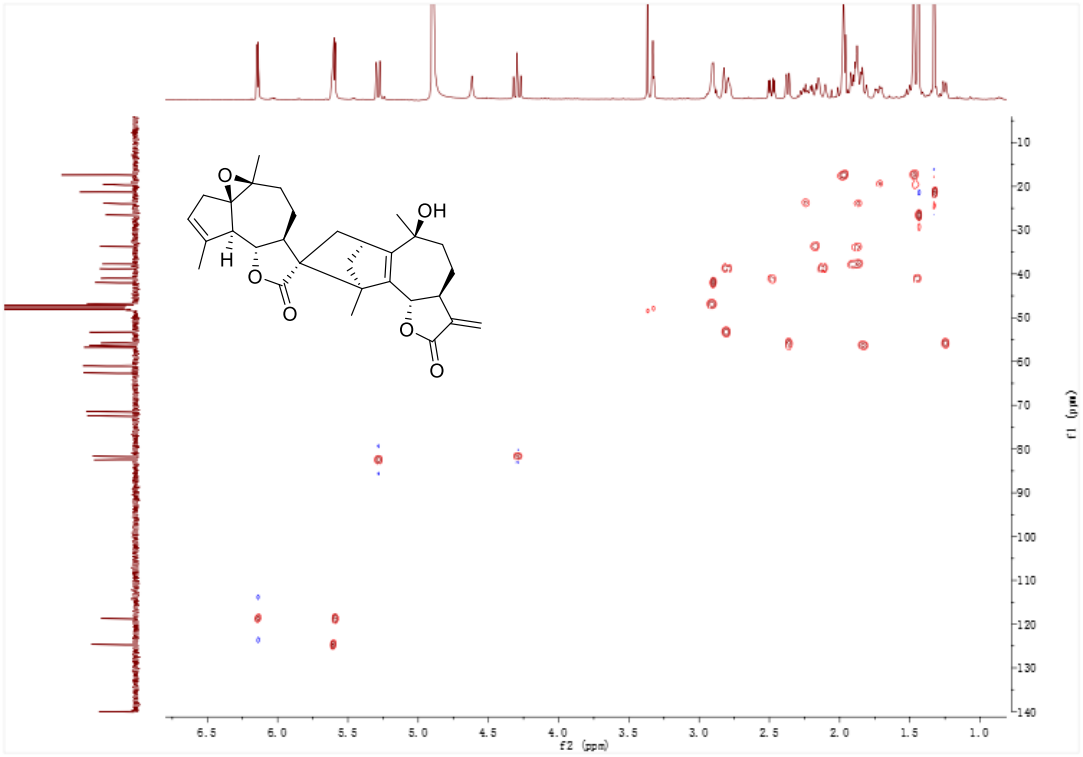


Figure S123 HSQC spectrum (600 MHz) of artematrolide I (**13**) in CD_3OD.

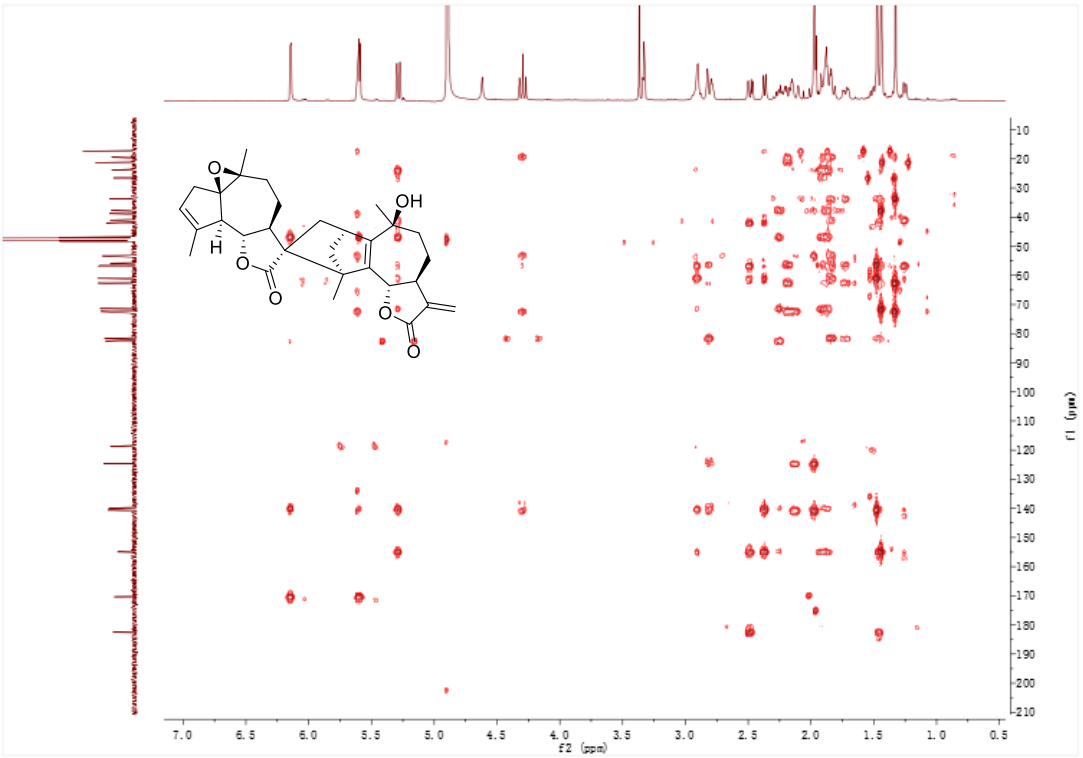


Figure S124 HMBC spectrum (600 MHz) of artematrolide I (**13**) in CD_3OD.

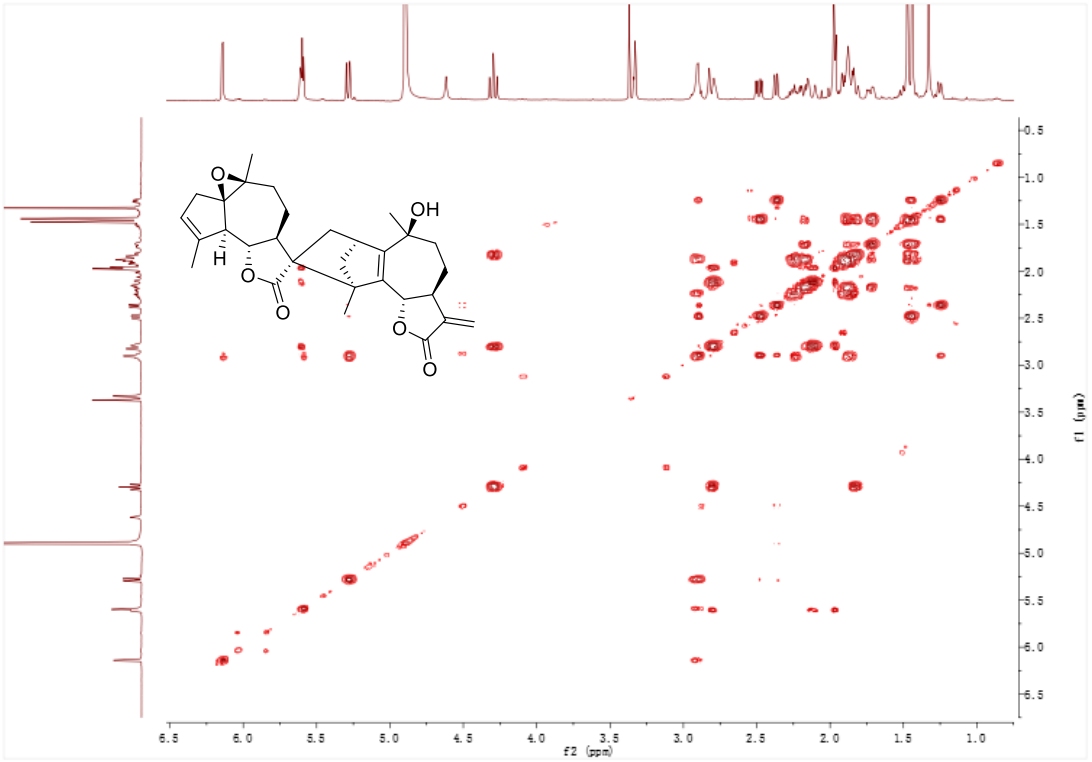


Figure S125 ^{1}H–^{1}H COSY spectrum (600 MHz) of artematrolide I (**13**) in CD_3OD.

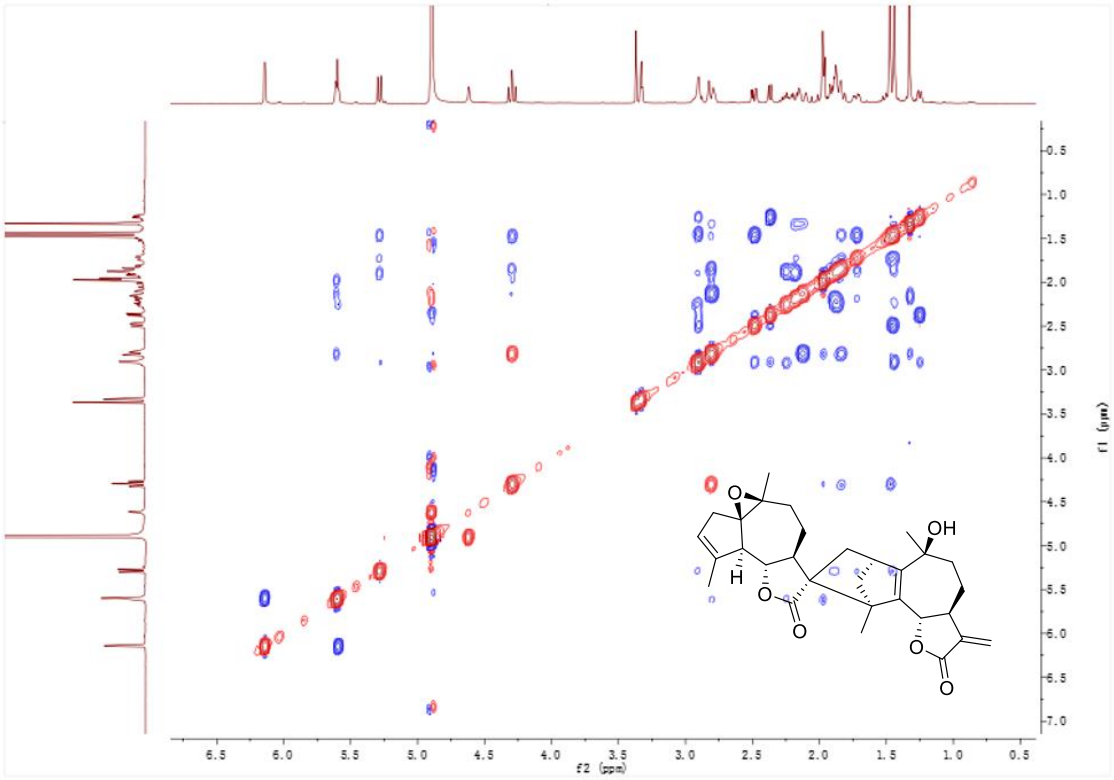


Figure S126 ROESY spectrum (600 MHz) of artematrolide I (**13**) in CD_3OD.

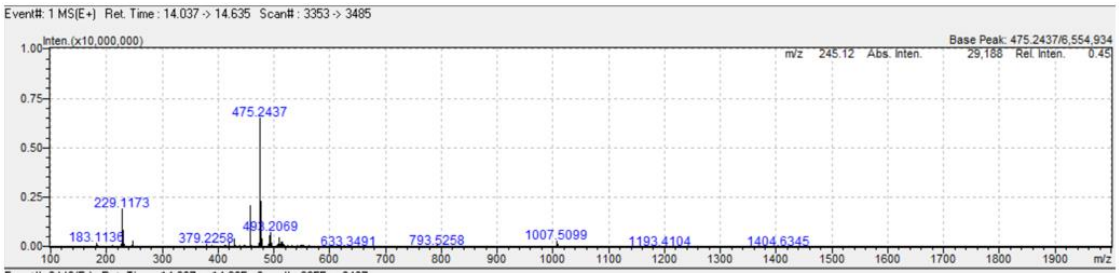


Figure S127 HRESIMS spectrum of artematrolide I (**13**).

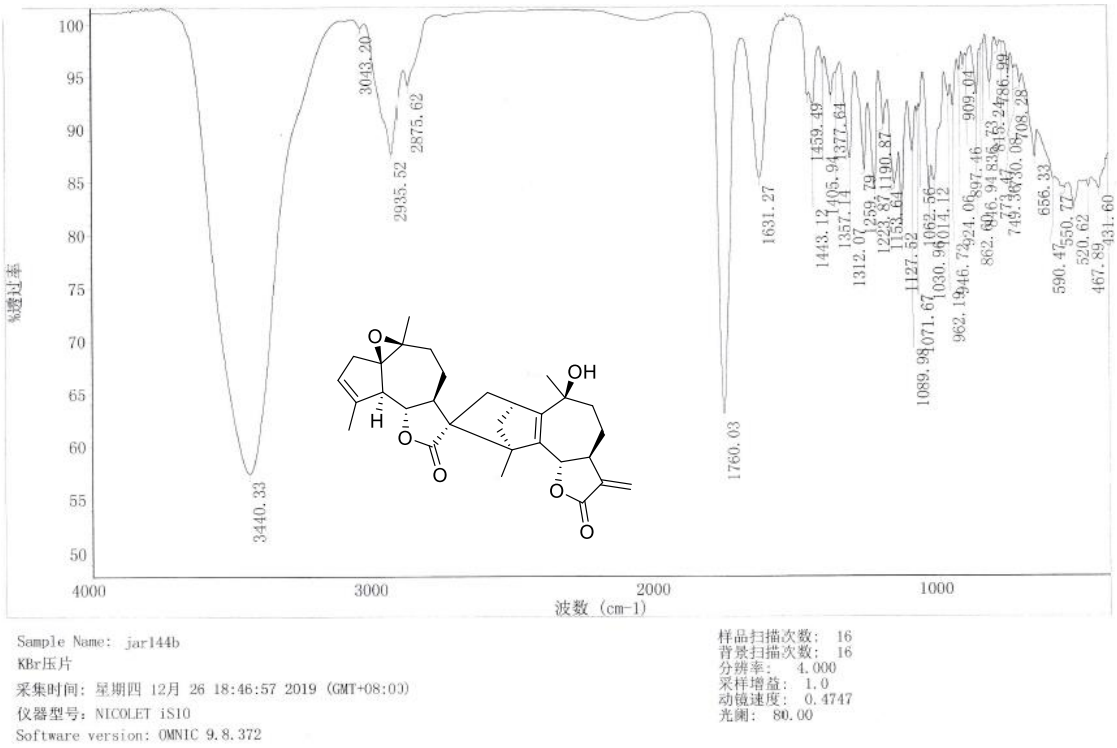
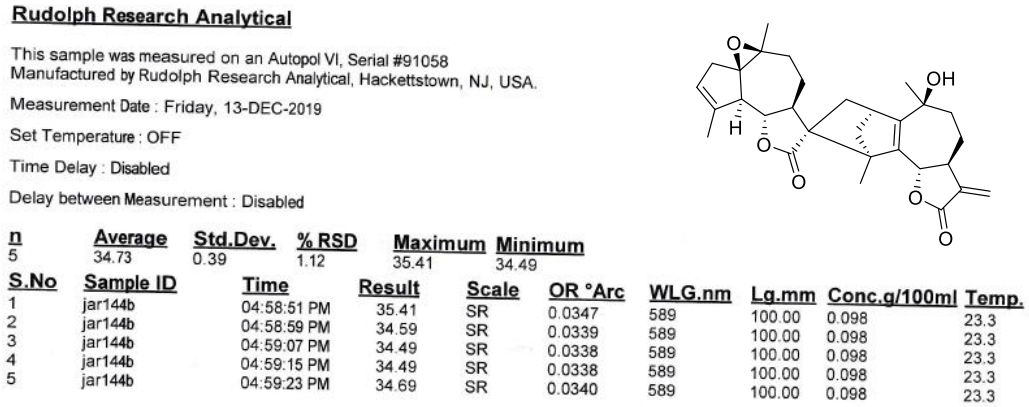


Figure S128 IR spectrum of artematrolide I (**13**).



Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Friday, 13-DEC-2019

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	34.73	0.39	1.12	35.41	34.49

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	jar144b	04:58:51 PM	35.41	SR	0.0347	589	100.00	0.098	23.3
2	jar144b	04:58:59 PM	34.59	SR	0.0339	589	100.00	0.098	23.3
3	jar144b	04:59:07 PM	34.49	SR	0.0338	589	100.00	0.098	23.3
4	jar144b	04:59:15 PM	34.49	SR	0.0338	589	100.00	0.098	23.3
5	jar144b	04:59:23 PM	34.69	SR	0.0340	589	100.00	0.098	23.3

Figure S129 Optical rotation spectrum of artematrolide I (**13**).

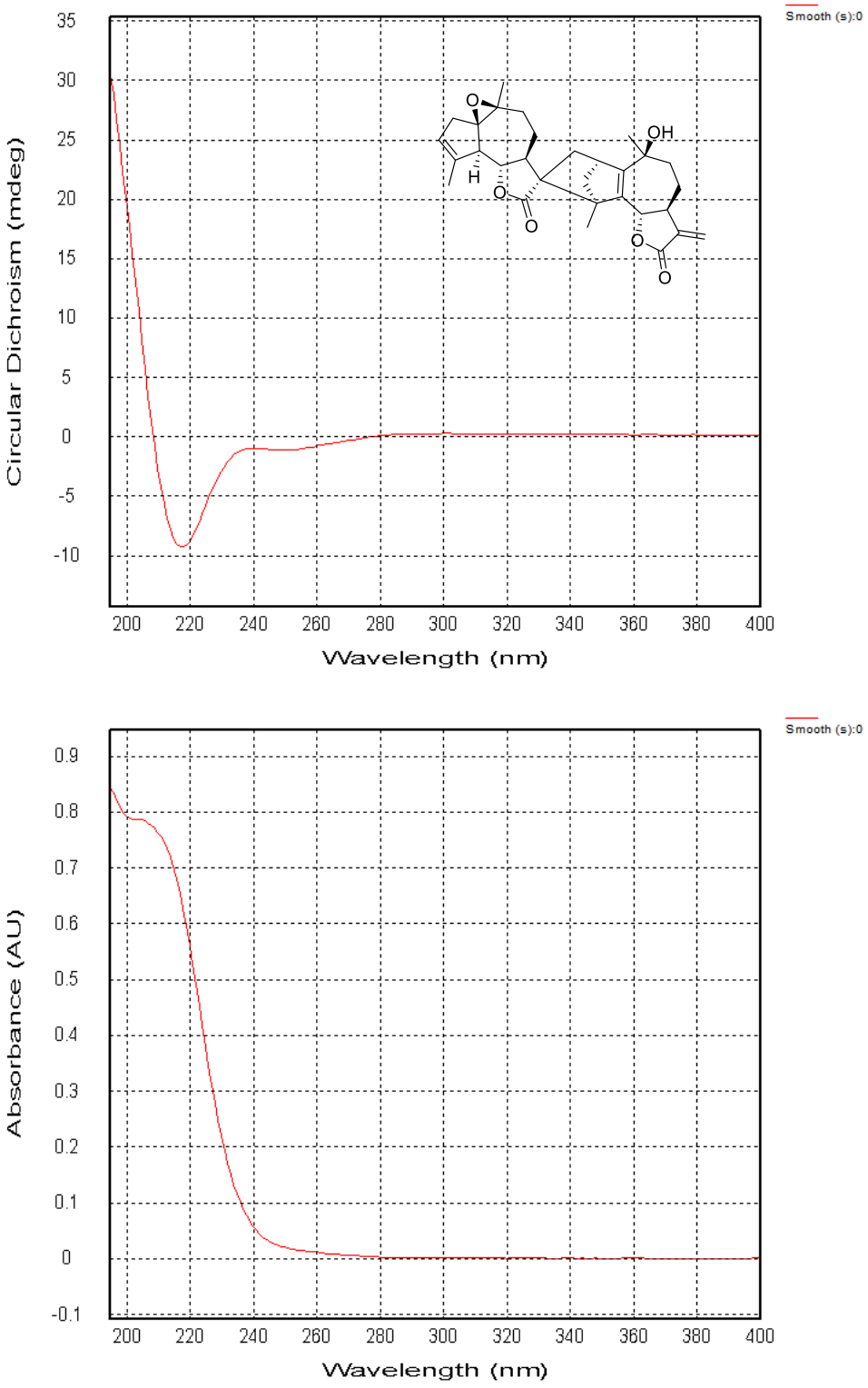


Figure S130 CD (top) and UV (bottom) spectra of artematrolide I (**13**).

15. NMR, MS, IR, $[\alpha]_D$ and CD spectra of compound 14

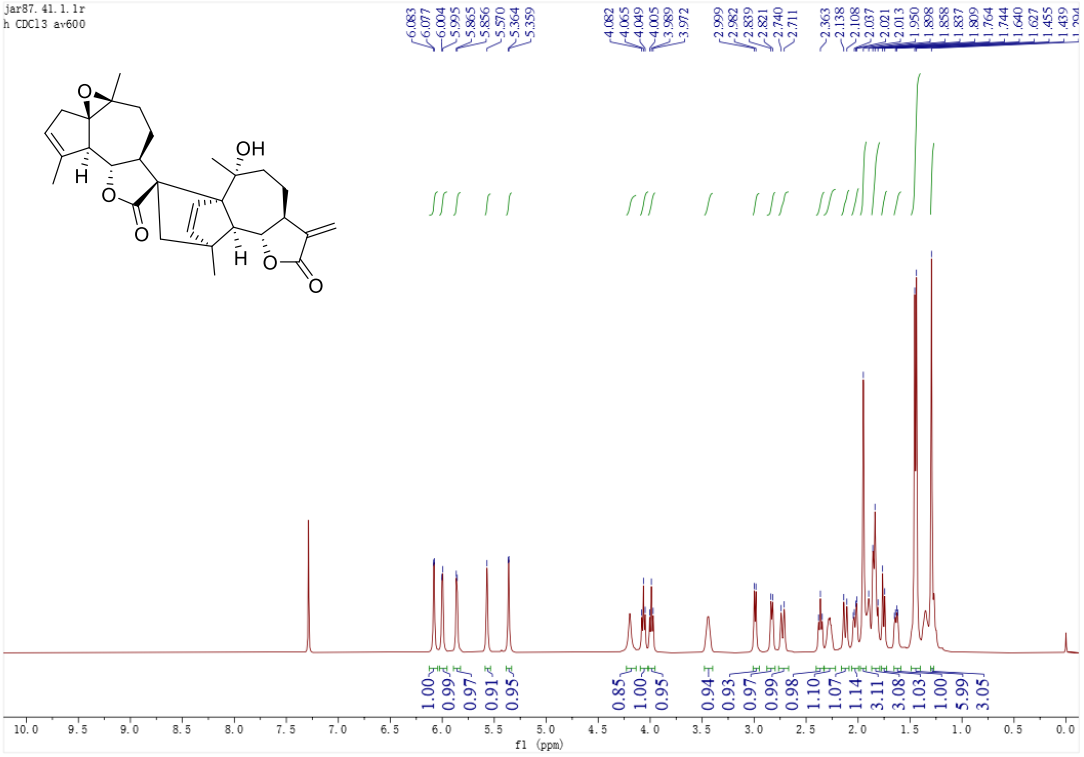


Figure S131 ^{1}H NMR spectrum (600 MHz) of artematrolide J (**14**) in $CDCl_3$.

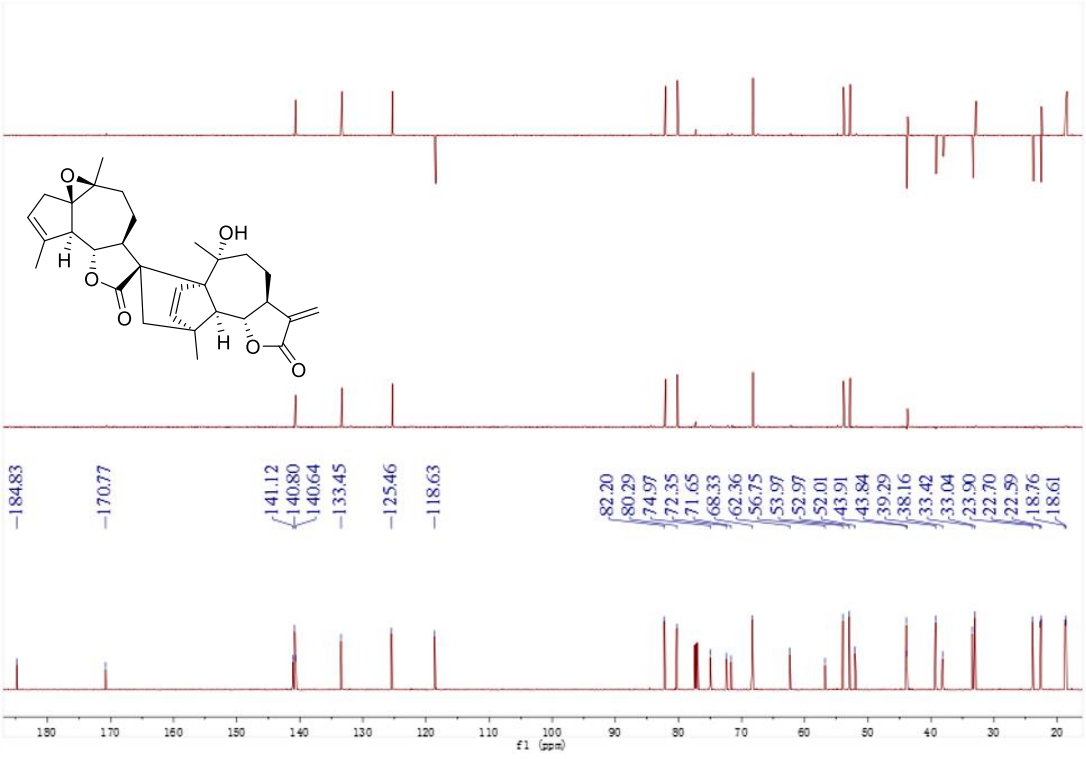


Figure S132 ^{13}C NMR spectrum (150 MHz) of artematrolide J (**14**) in $CDCl_3$.

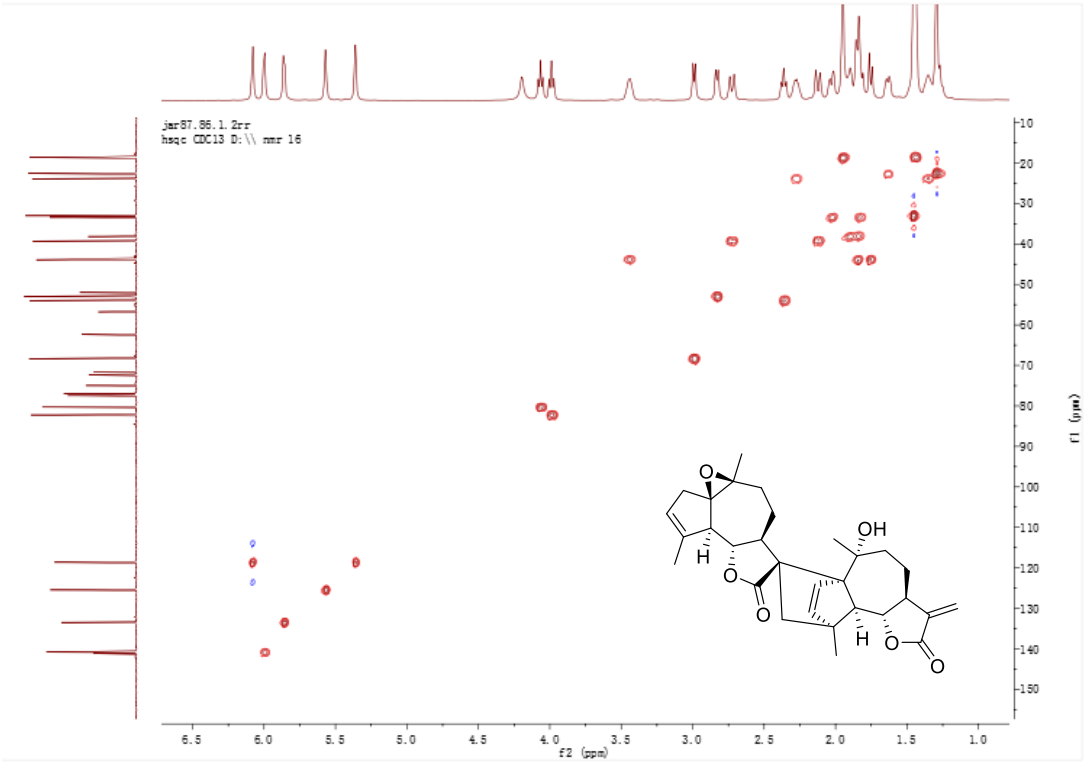


Figure S133 HSQC spectrum (600 MHz) of artematrolide J (**14**) in $CDCl_3$.

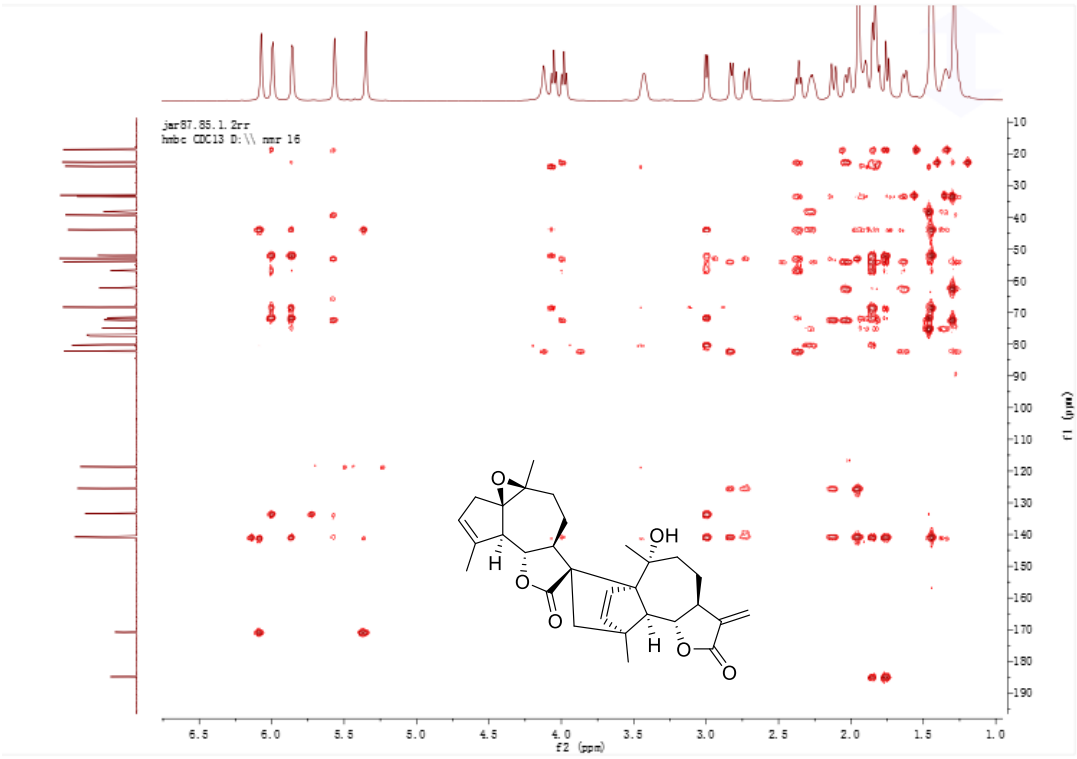


Figure S134 HMBC spectrum (600 MHz) of artematrolide J (**14**) in $CDCl_3$.

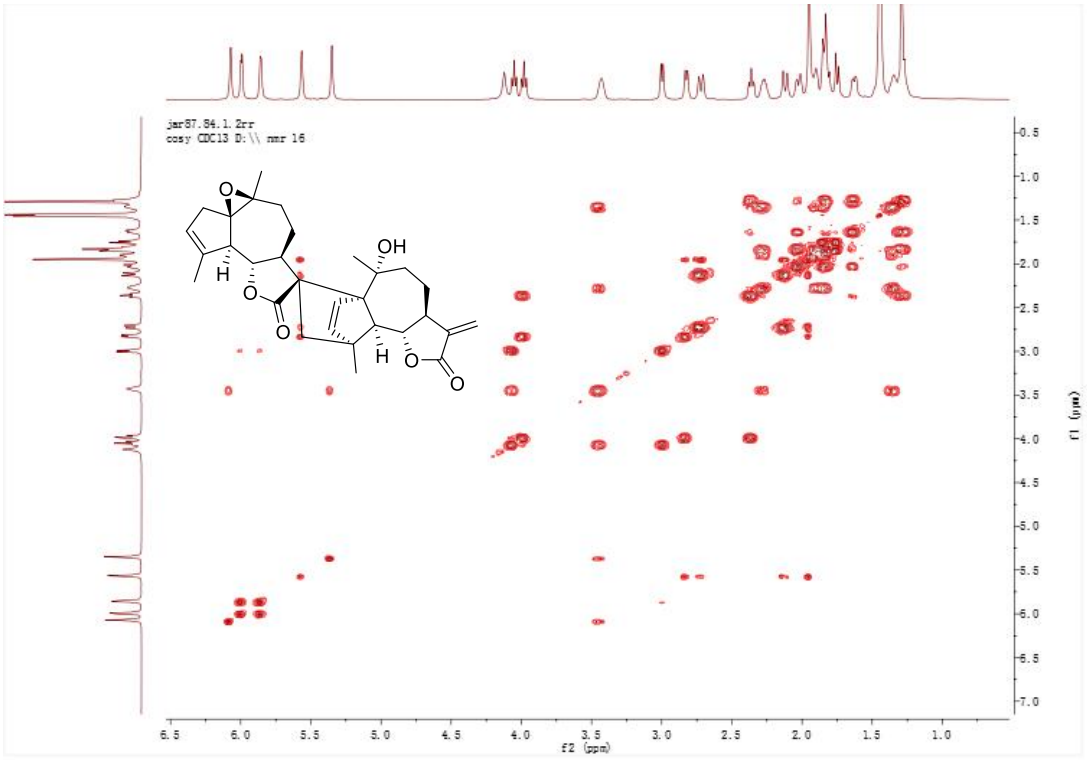


Figure S135 ^{1}H–^{1}H COSY spectrum (600 MHz) of artematrolide J (**14**) in $CDCl_3$.

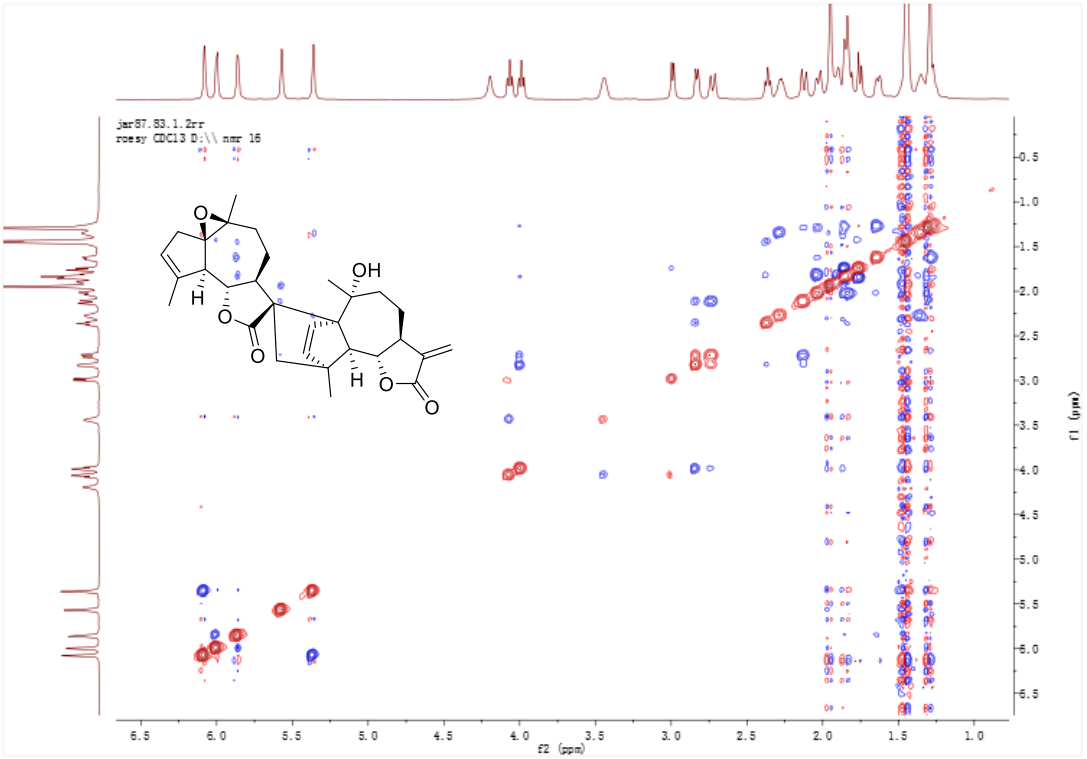


Figure S136 ROESY spectrum (600 MHz) of artematrolide J (**14**) in $CDCl_3$.

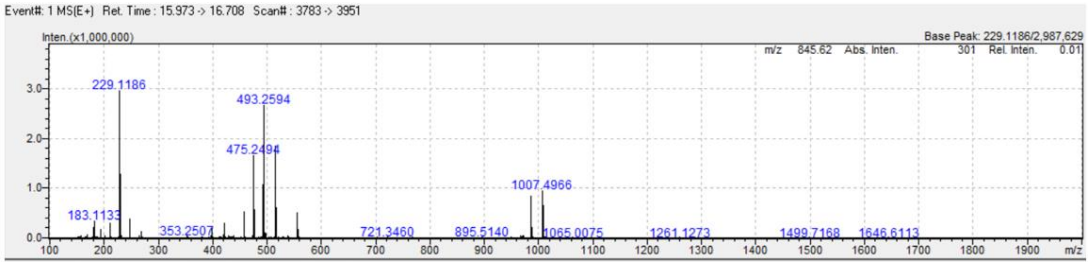


Figure S137 HRESIMS spectrum of artematrolide J (**14**).

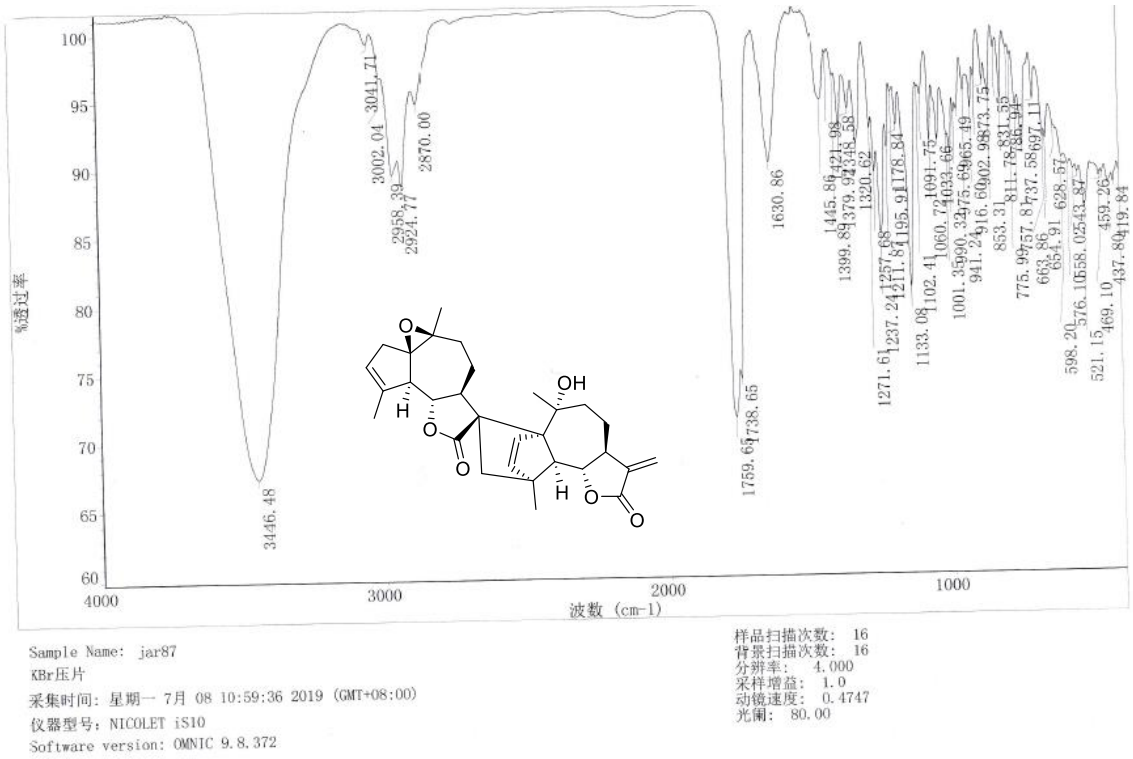


Figure S138 IR spectrum of artematrolide J (**14**).

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Monday, 08-JUL-2019

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	49.43	0.57	1.15	50.00	48.57

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	jar87	05:23:13 PM	49.71	SR	0.0174	589	100.00	0.035	24.3
2	jar87	05:23:22 PM	49.71	SR	0.0174	589	100.00	0.035	24.3
3	jar87	05:23:30 PM	49.14	SR	0.0172	589	100.00	0.035	24.3
4	jar87	05:23:37 PM	48.57	SR	0.0170	589	100.00	0.035	24.3
5	jar87	05:23:45 PM	50.00	SR	0.0175	589	100.00	0.035	24.3

Figure S139 Optical rotation spectrum of artematrolide J (**14**).

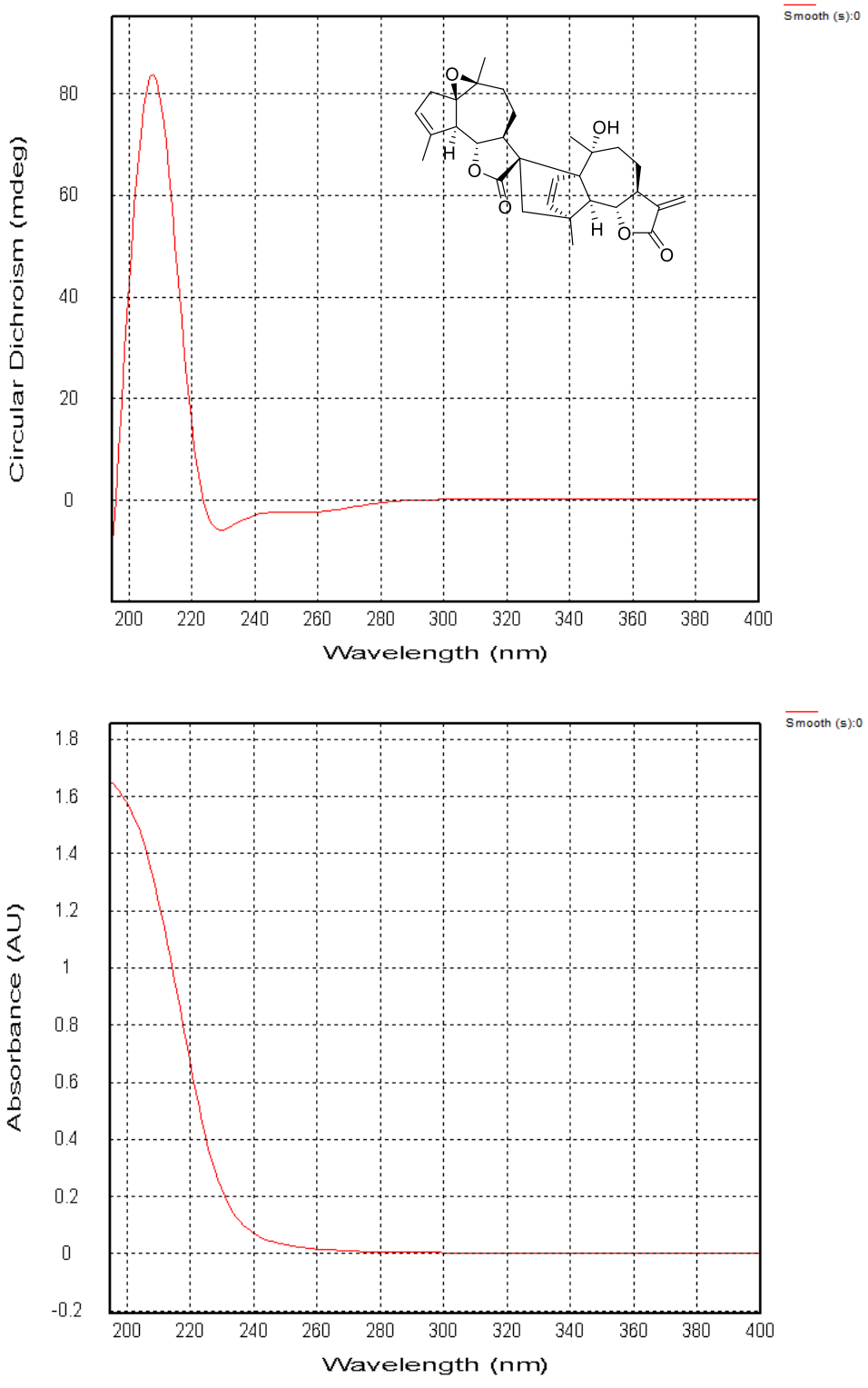


Figure S140 CD (top) and UV (bottom) spectra of artematrolide J (**14**).

16. NMR, MS, IR, $[\alpha]_D$ and CD spectra of compound 15

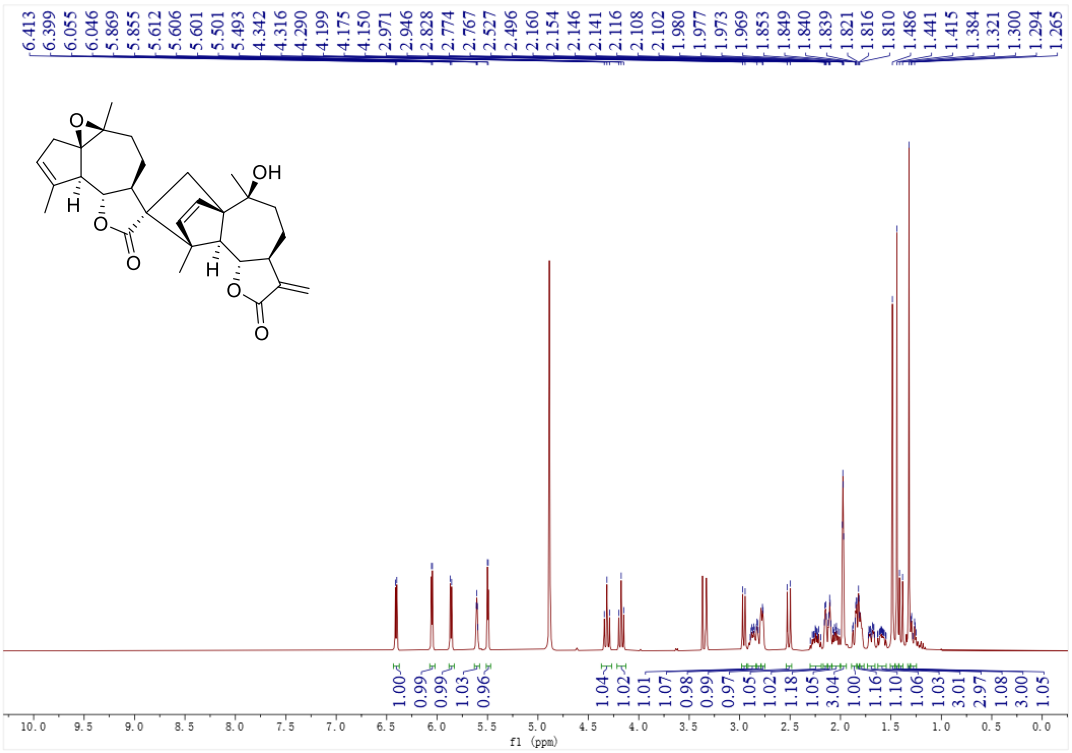


Figure S141 ^{1}H NMR spectrum (400 MHz) of artematrolide K (**15**) in CD_3OD.

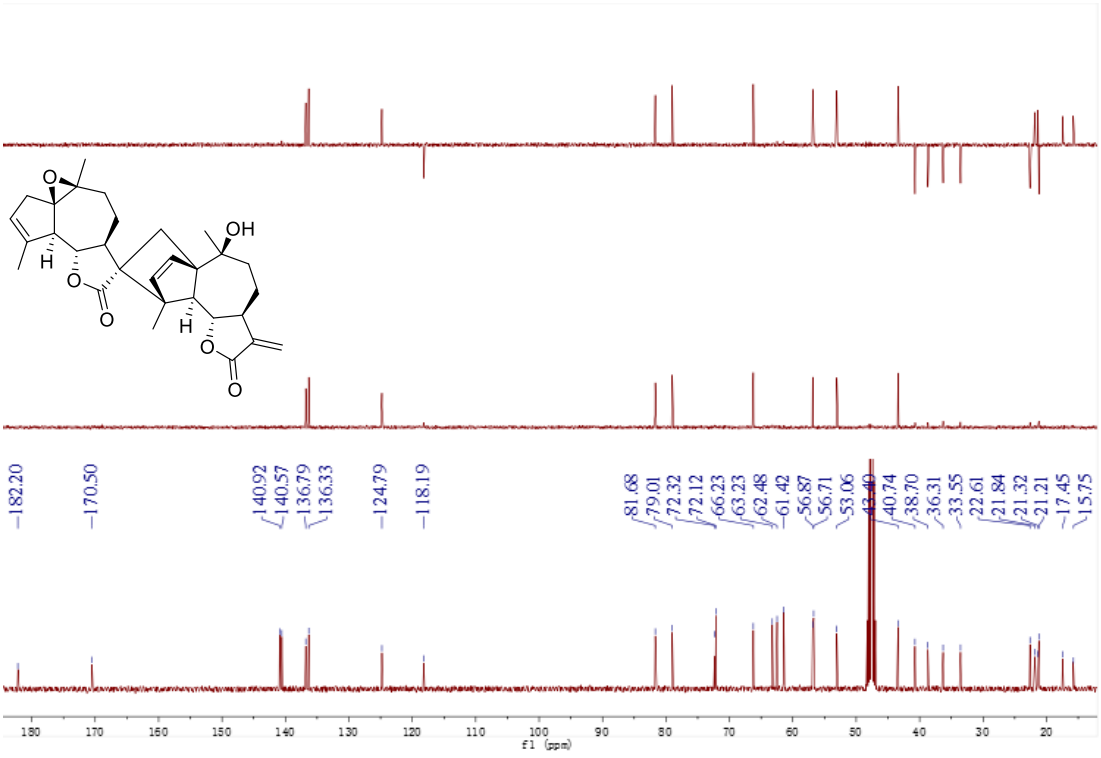


Figure S142 ^{13}C NMR spectrum (100 MHz) of artematrolide K (**15**) in CD_3OD.

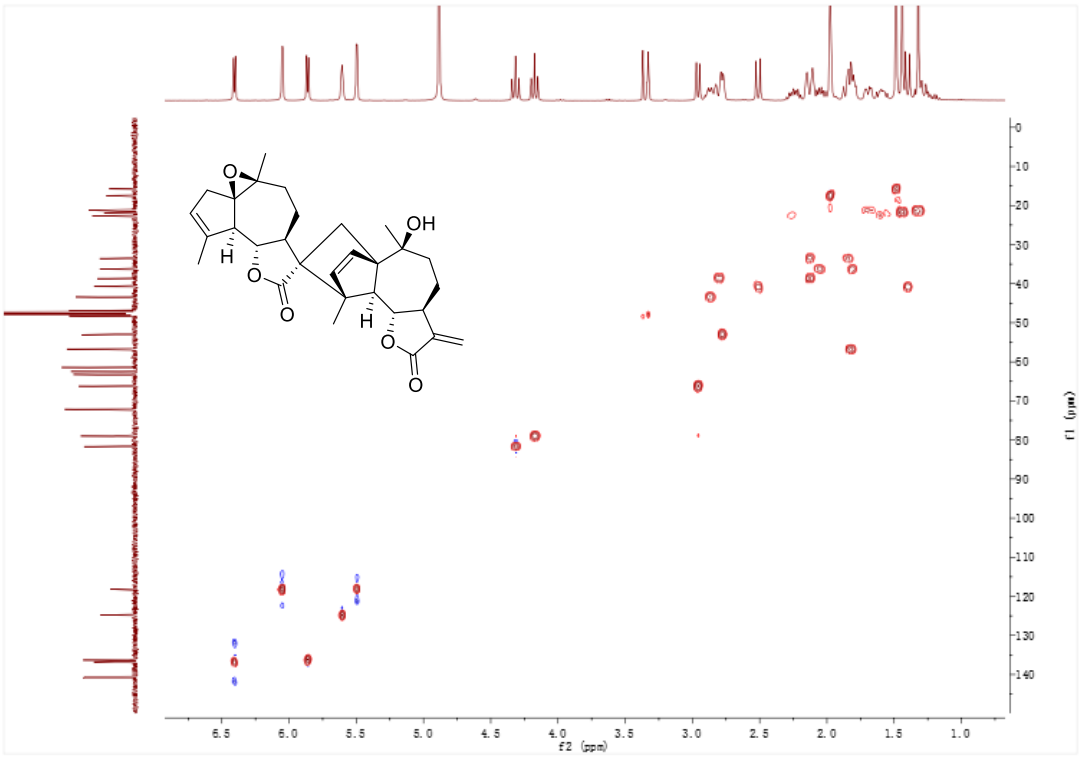


Figure S143 HSQC spectrum (600 MHz) of artematrolide K (**15**) in CD_3OD.

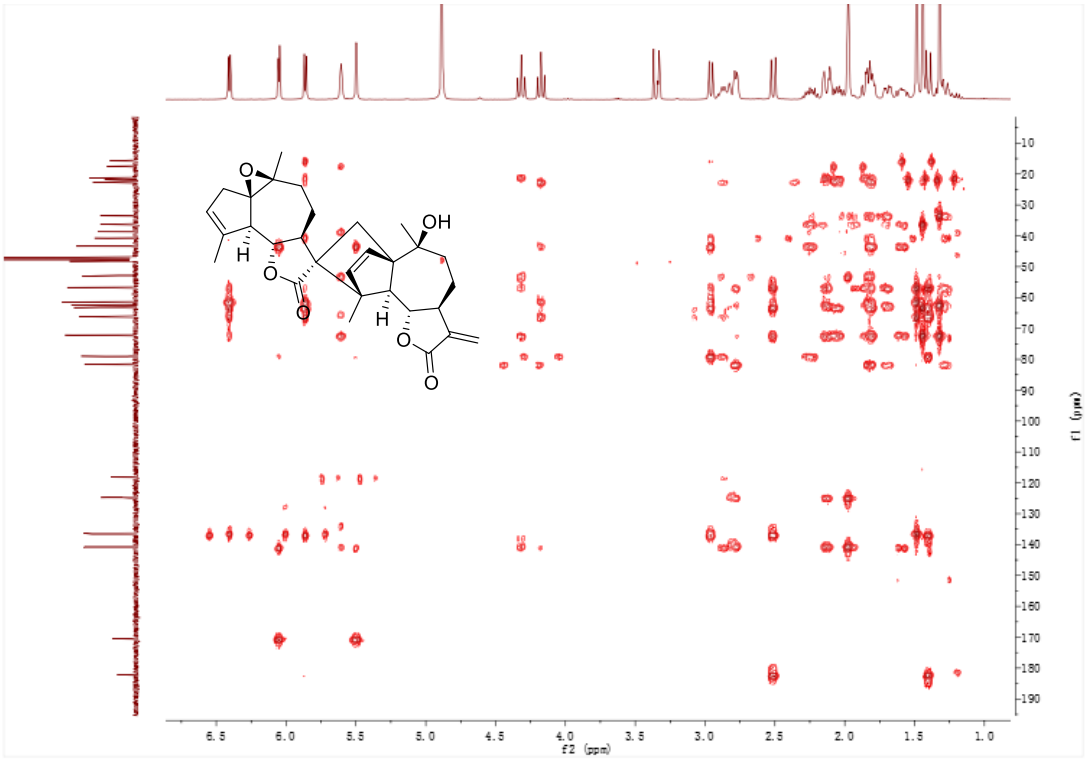


Figure S144 HMBC spectrum (600 MHz) of artematrolide K (**15**) in CD_3OD.

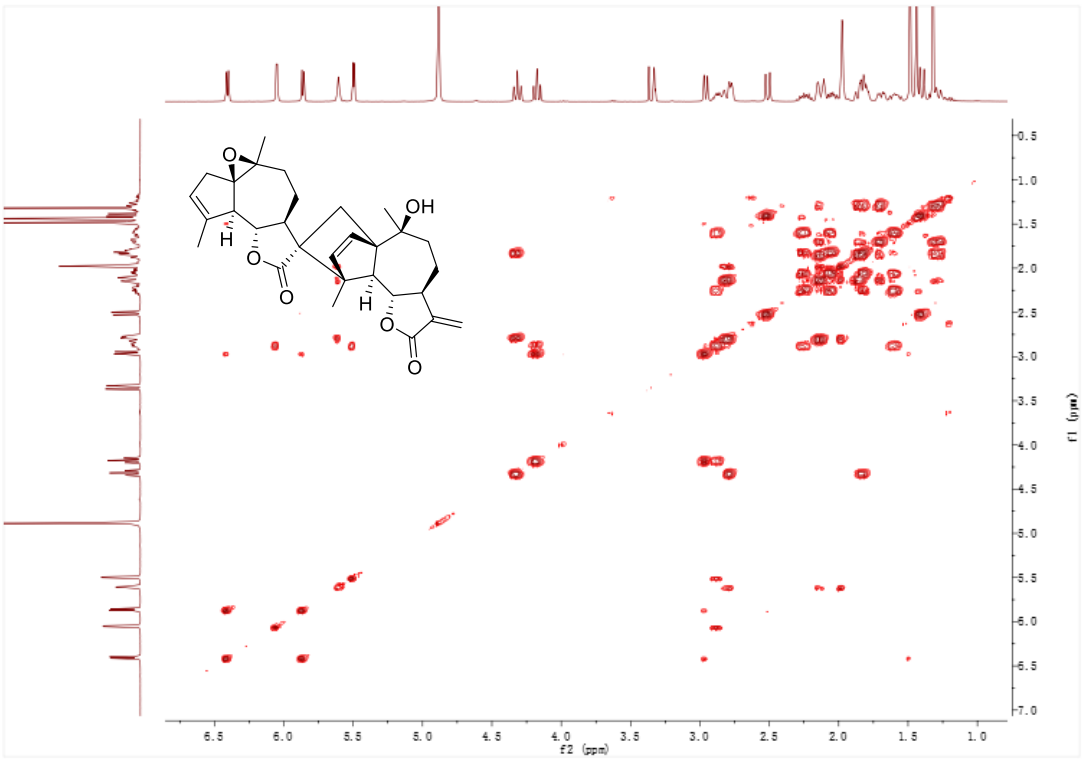


Figure S145 ^{1}H–^{1}H COSY spectrum (600 MHz) of artematrolide K (**15**) in CD_3OD.

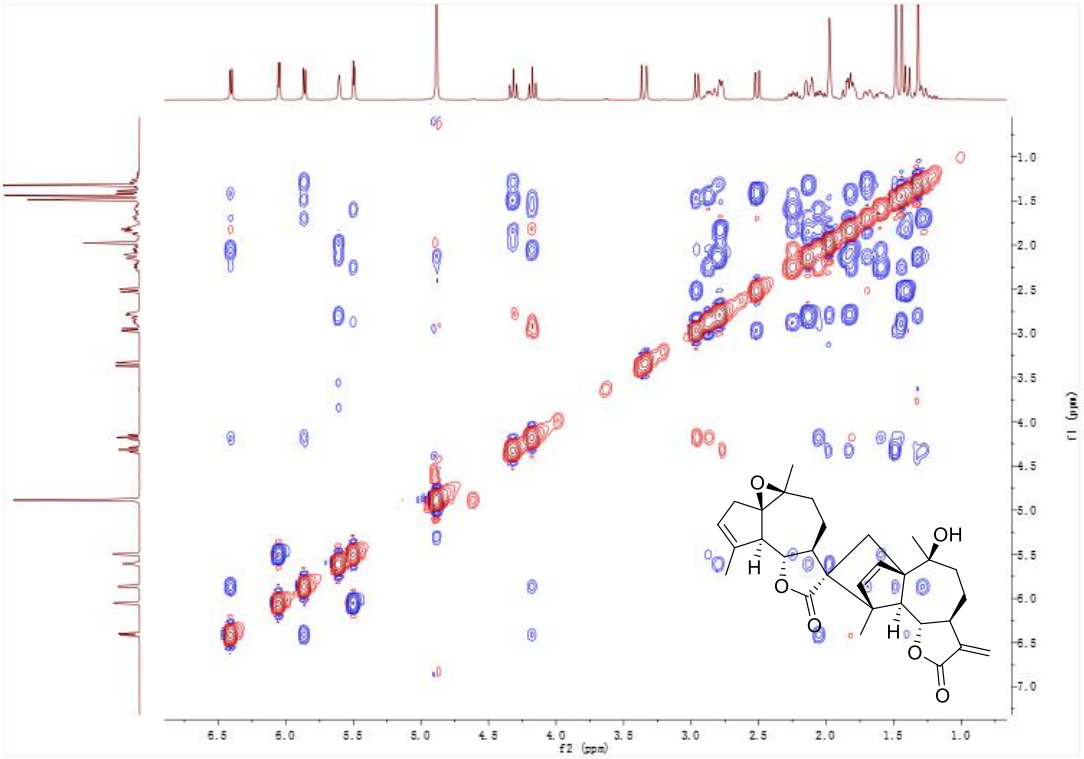


Figure S146 ROESY spectrum (600 MHz) of artematrolide K (**15**) in CD_3OD.

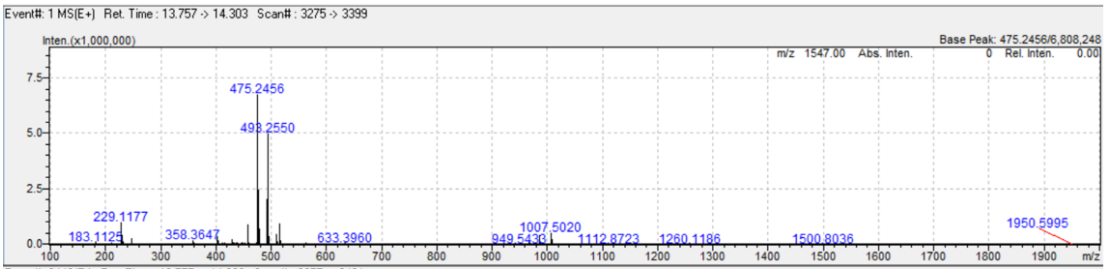


Figure S147 HRESIMS spectrum of artematrolide K (**15**).

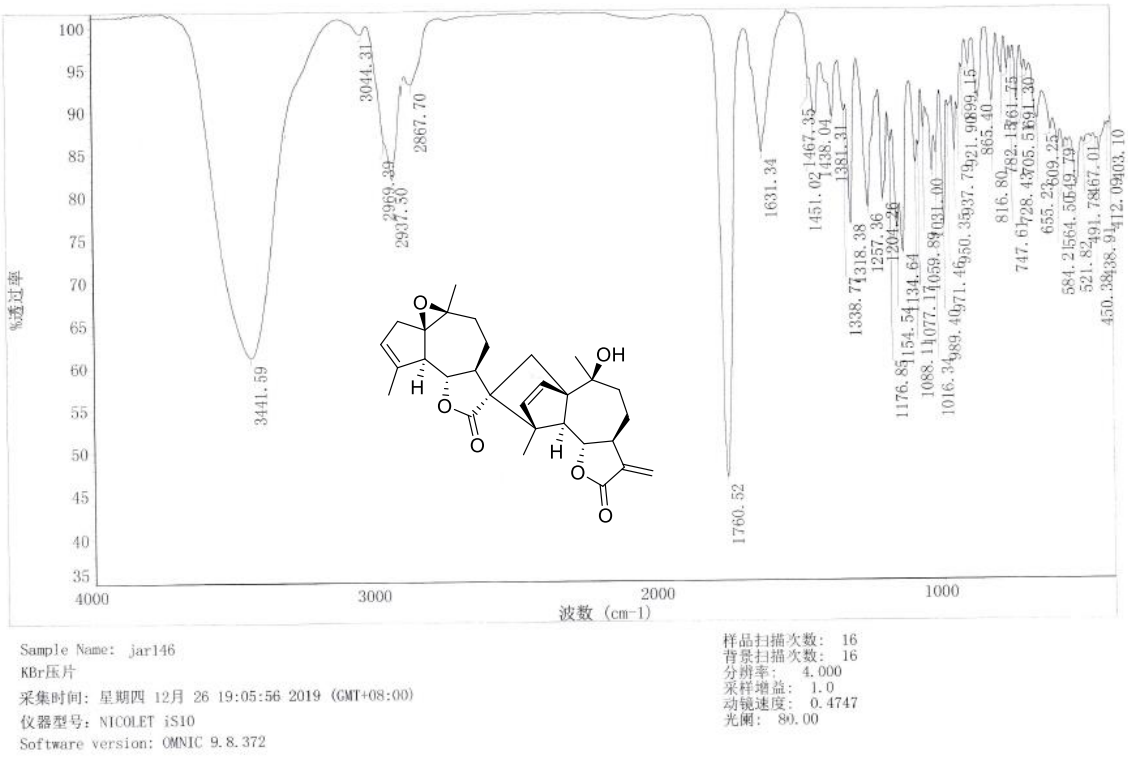


Figure S148 IR spectrum of artematrolide K (**15**).

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Friday, 13-DEC-2019

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	17.39	0.35	2.01	17.95	17.05

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	jar146	05:13:39 PM	17.05	SR	0.0133	589	100.00	0.078	23.4
2	jar146	05:13:48 PM	17.95	SR	0.0140	589	100.00	0.078	23.4
3	jar146	05:13:56 PM	17.18	SR	0.0134	589	100.00	0.078	23.4
4	jar146	05:14:04 PM	17.31	SR	0.0135	589	100.00	0.078	23.4
5	jar146	05:14:12 PM	17.44	SR	0.0136	589	100.00	0.078	23.3

Figure S149 Optical rotation spectrum of artematrolide K (**15**).

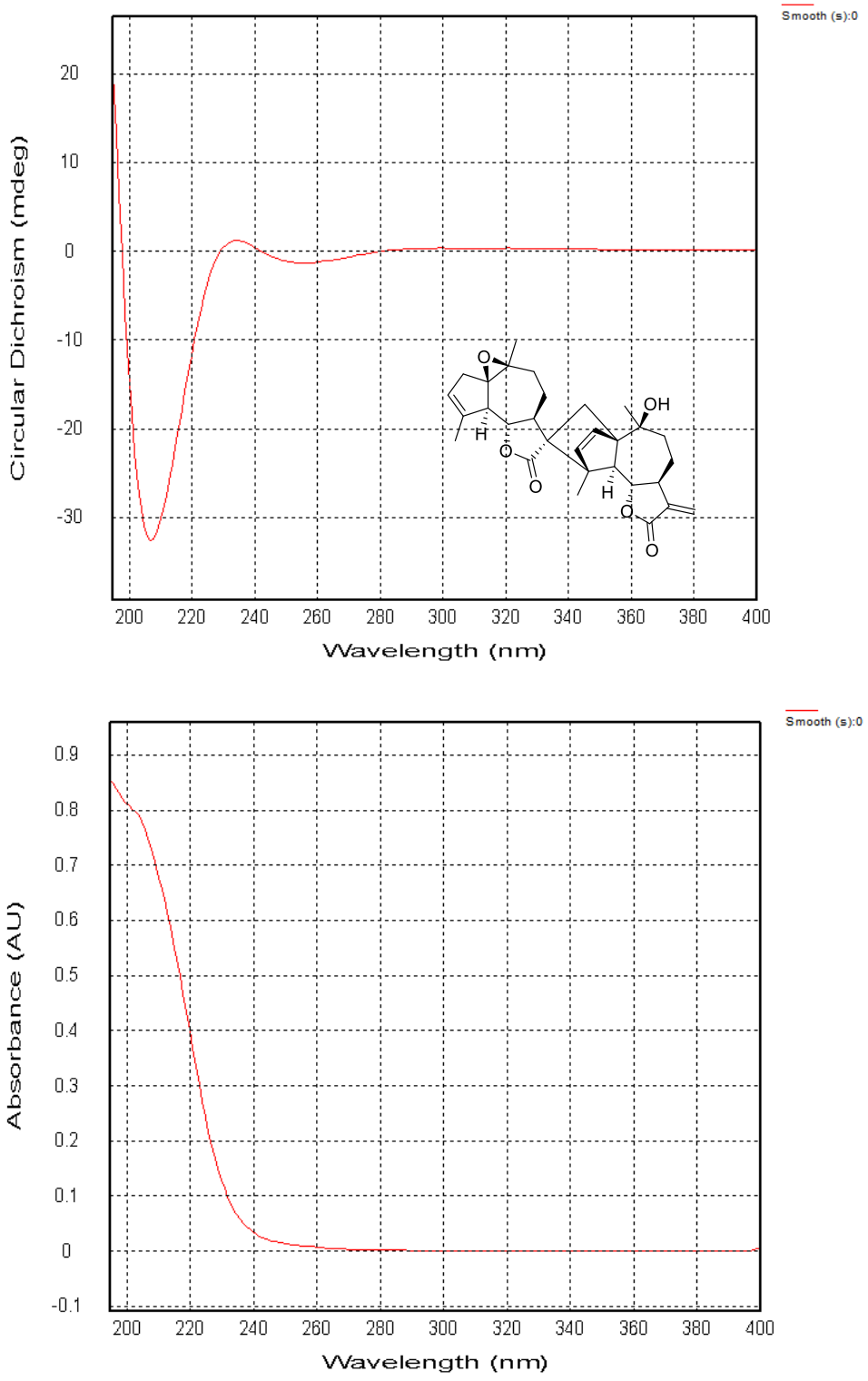


Figure S150 CD (top) and UV (bottom) spectra of artematrolide K (**15**).

17. NMR, MS, IR, $[\alpha]_D$ and CD spectra of compound 16

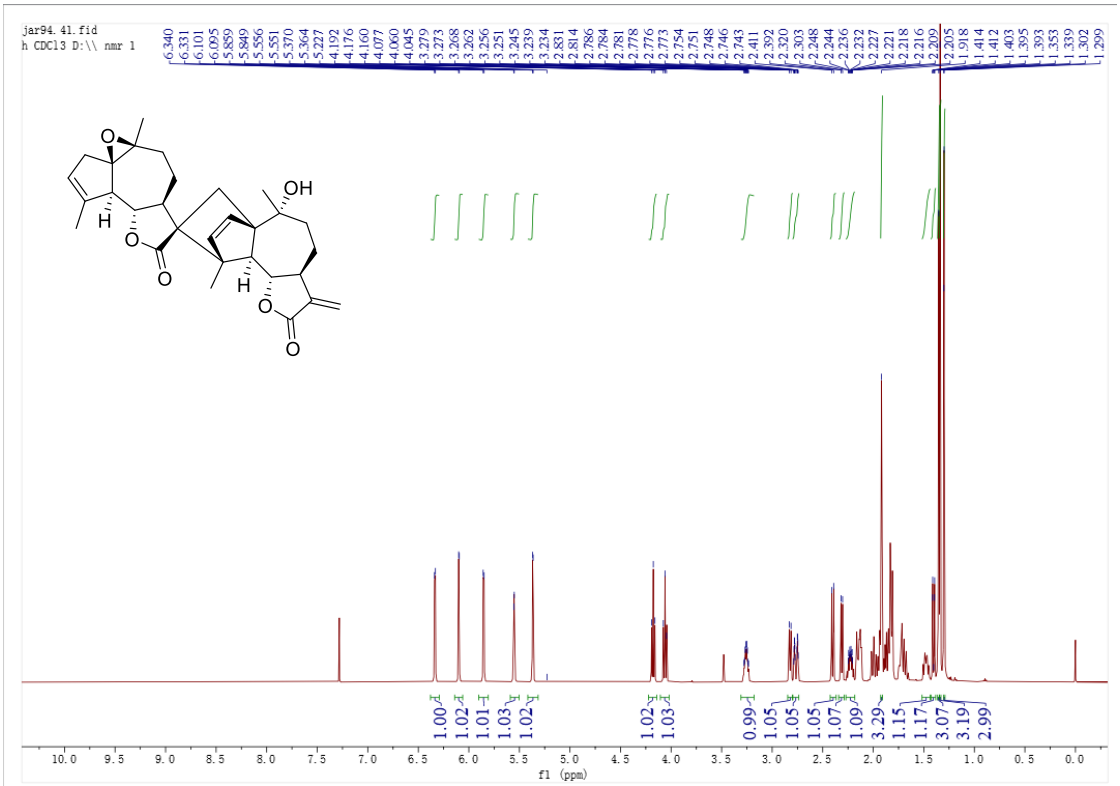


Figure S151 ^{1}H NMR spectrum (600 MHz) of artematrolide L (**16**) in $CDCl_3$.

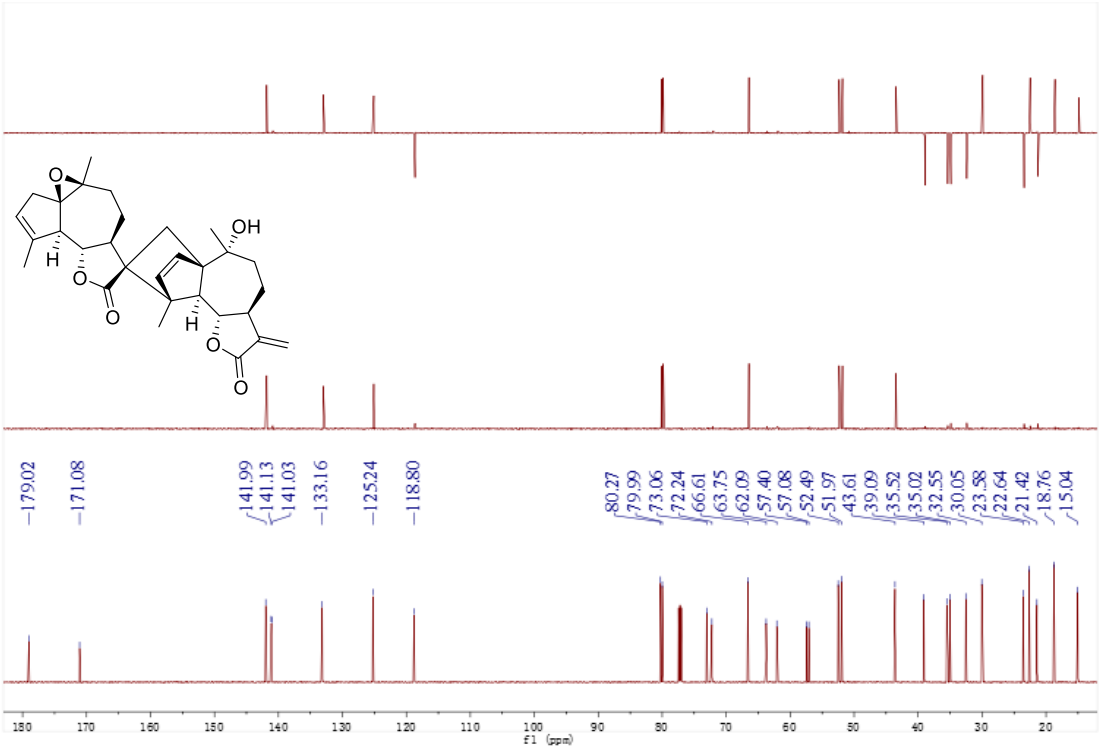


Figure S152 ^{13}C NMR spectrum (150 MHz) of artematrolide L (**16**) in $CDCl_3$.

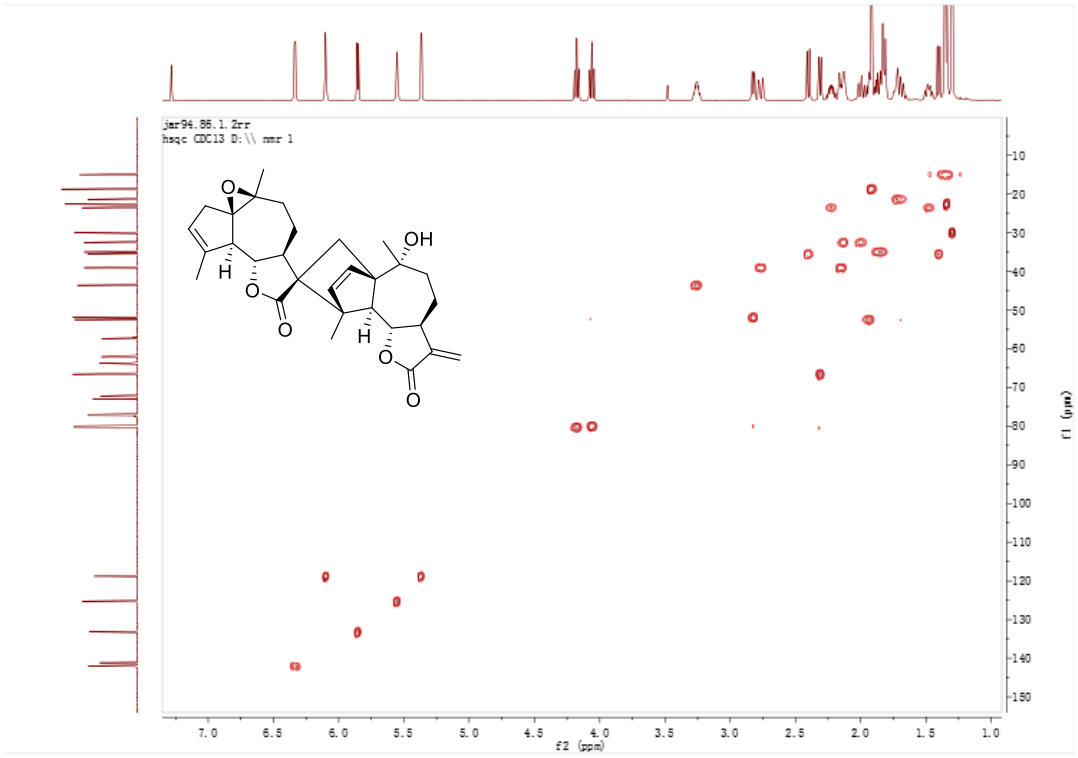


Figure S153 HSQC spectrum (600 MHz) of artematrolide L (**16**) in $CDCl_3$.

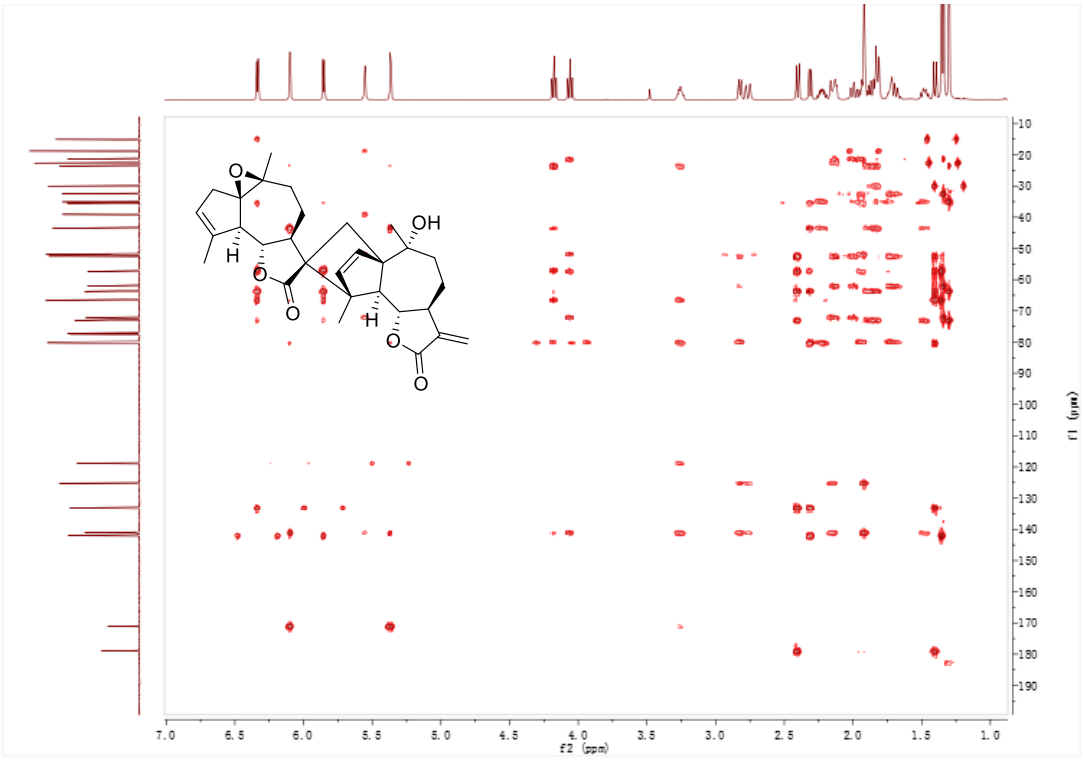


Figure S154 HMBC spectrum (600 MHz) of artematrolide L (**16**) in $CDCl_3$.

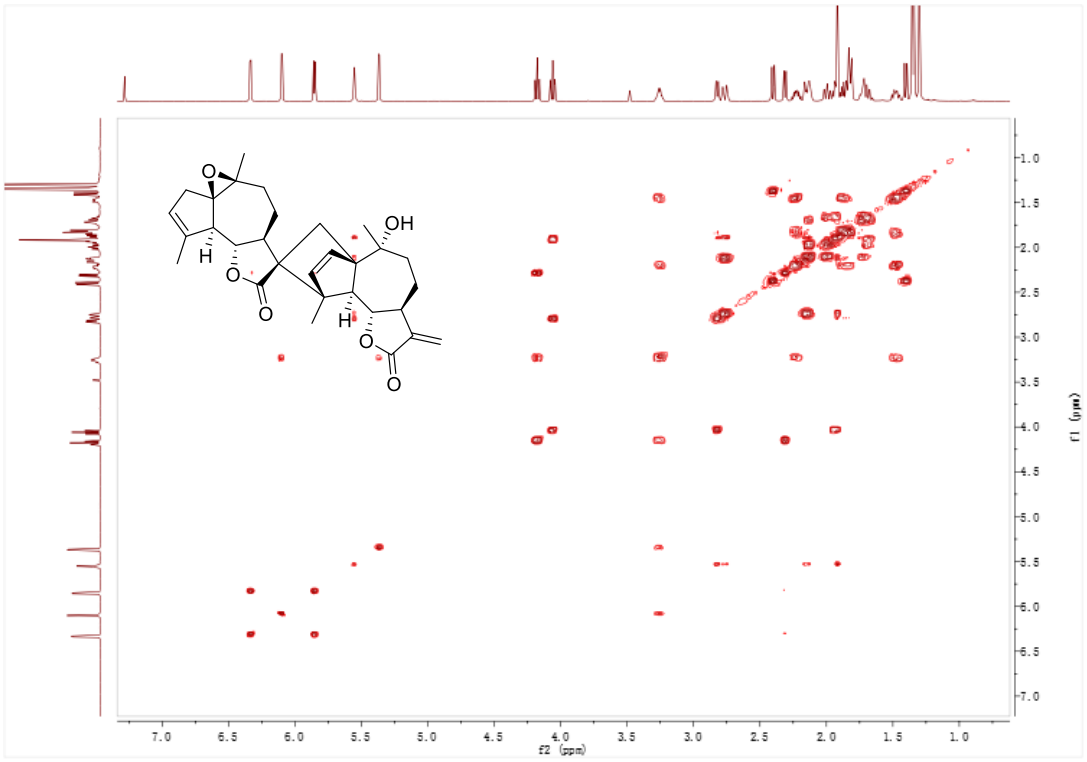


Figure S155 ^{1}H–^{1}H COSY spectrum (600 MHz) of artematrolide L (**16**) in $CDCl_3$.

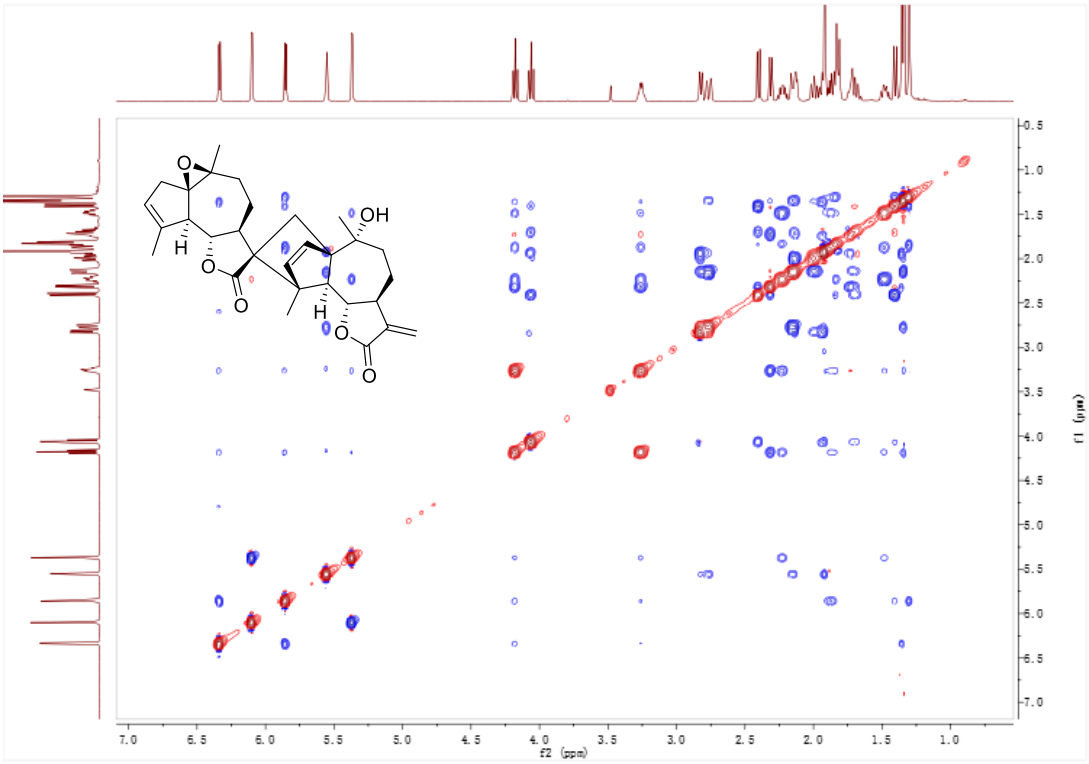


Figure S156 ROESY spectrum (600 MHz) of artematrolide L (**16**) in $CDCl_3$.

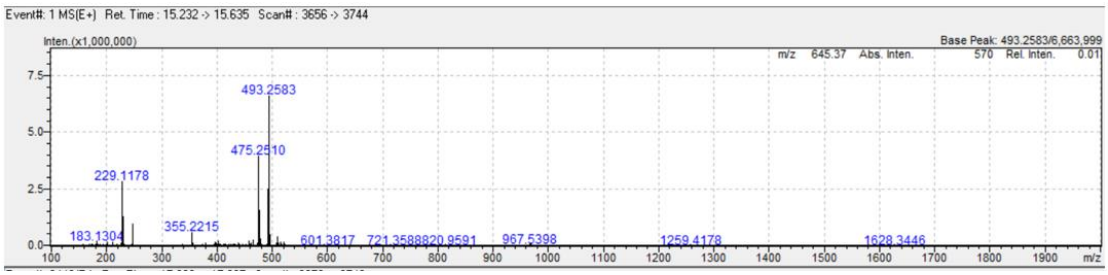


Figure S157 HRESIMS spectrum of artematrolide L (**16**).

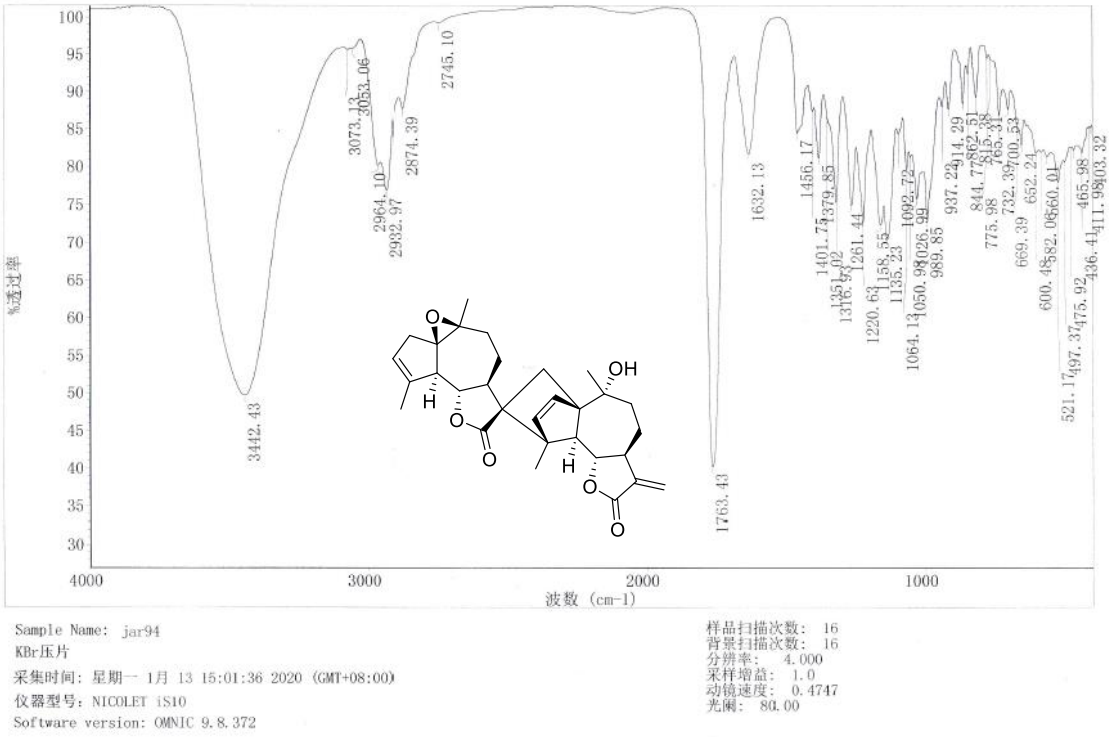


Figure S158 IR spectrum of artematrolide L (**16**).

Rudolph Research Analytical

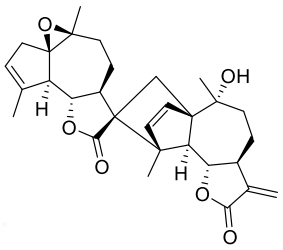
This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Saturday, 04-JAN-2020

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled



n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	11.97	2.98	24.89	16.51	9.05

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	jar94	01:36:47 PM	9.68	SR	0.0061	589	100.00	0.063	22.9
2	jar94	01:36:55 PM	9.05	SR	0.0057	589	100.00	0.063	22.9
3	jar94	01:37:03 PM	11.59	SR	0.0073	589	100.00	0.063	22.9
4	jar94	01:37:11 PM	13.02	SR	0.0082	589	100.00	0.063	22.8
5	jar94	01:37:28 PM	16.51	SR	0.0104	589	100.00	0.063	22.8

Figure S159 Optical rotation spectrum of artematrolide L (**16**).

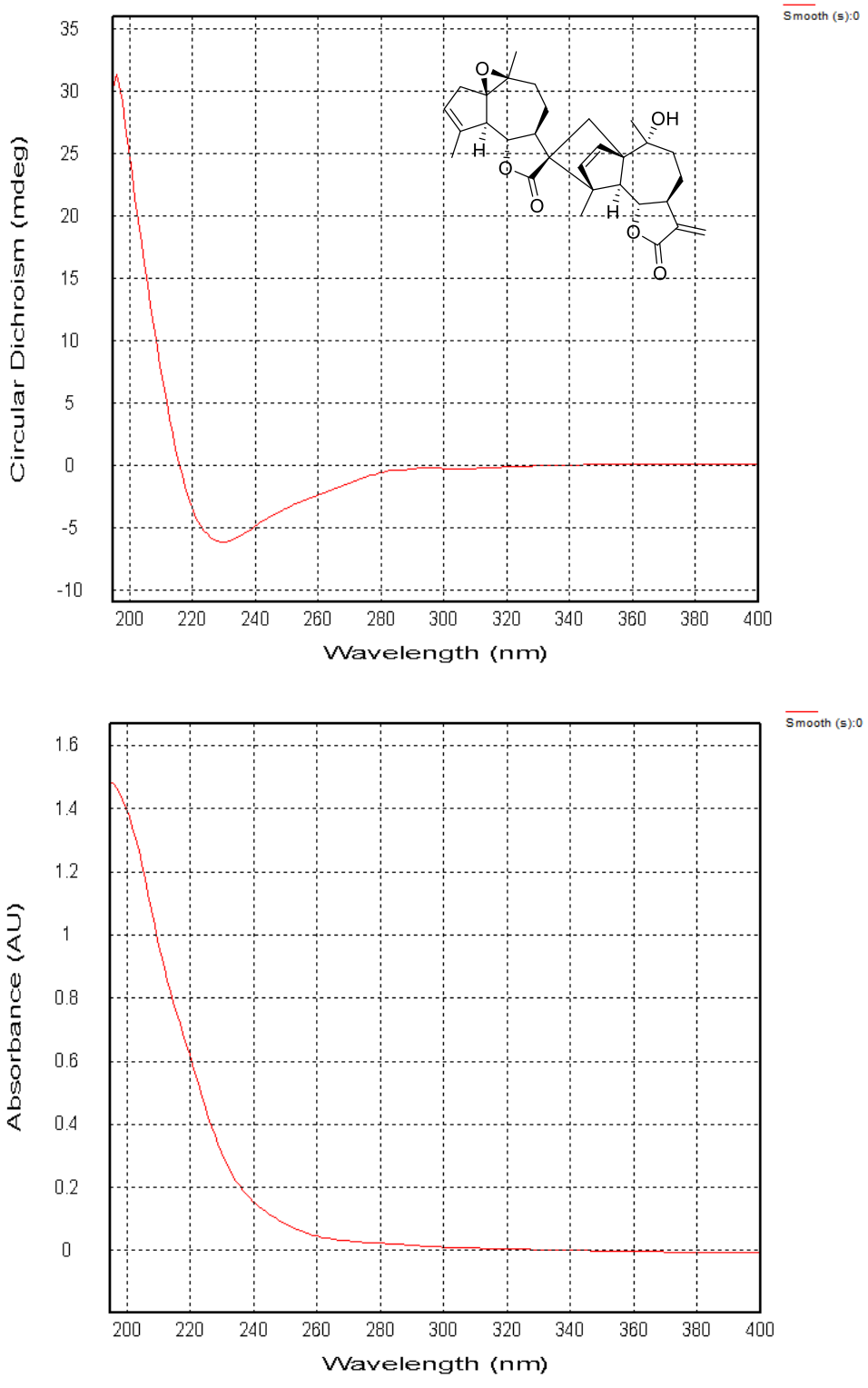


Figure S160 CD (top) and UV (bottom) spectra of artematrolide L (**16**).

18. NMR, MS, IR, $[\alpha]_D$ and CD spectra of compound 17

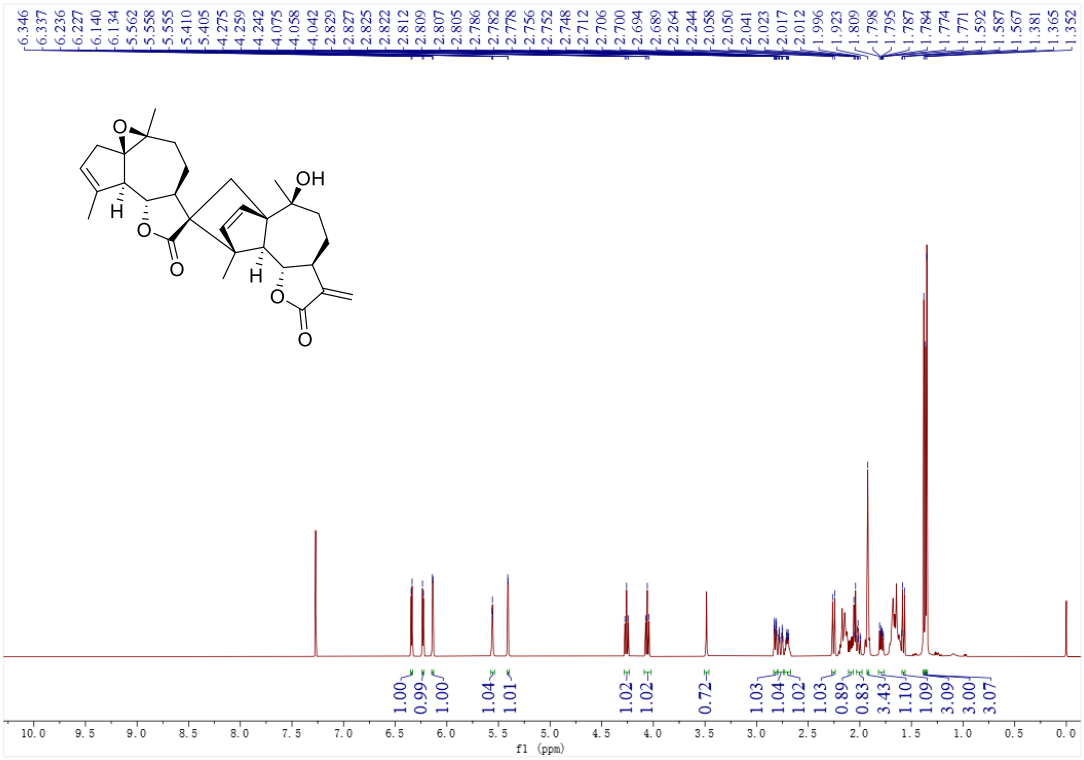


Figure S161 ^{1}H NMR spectrum (600 MHz) of artematrolide M (**17**) in $CDCl_3$.

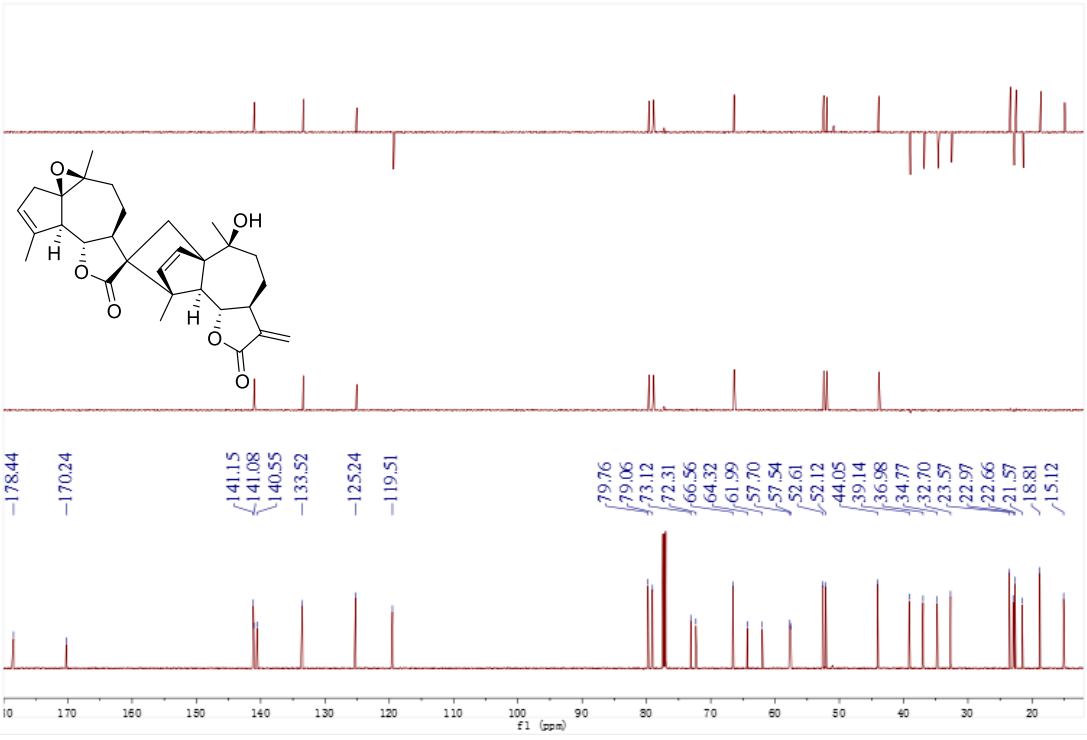


Figure S162 ^{13}C NMR spectrum (150 MHz) of artematrolide M (**17**) in $CDCl_3$.

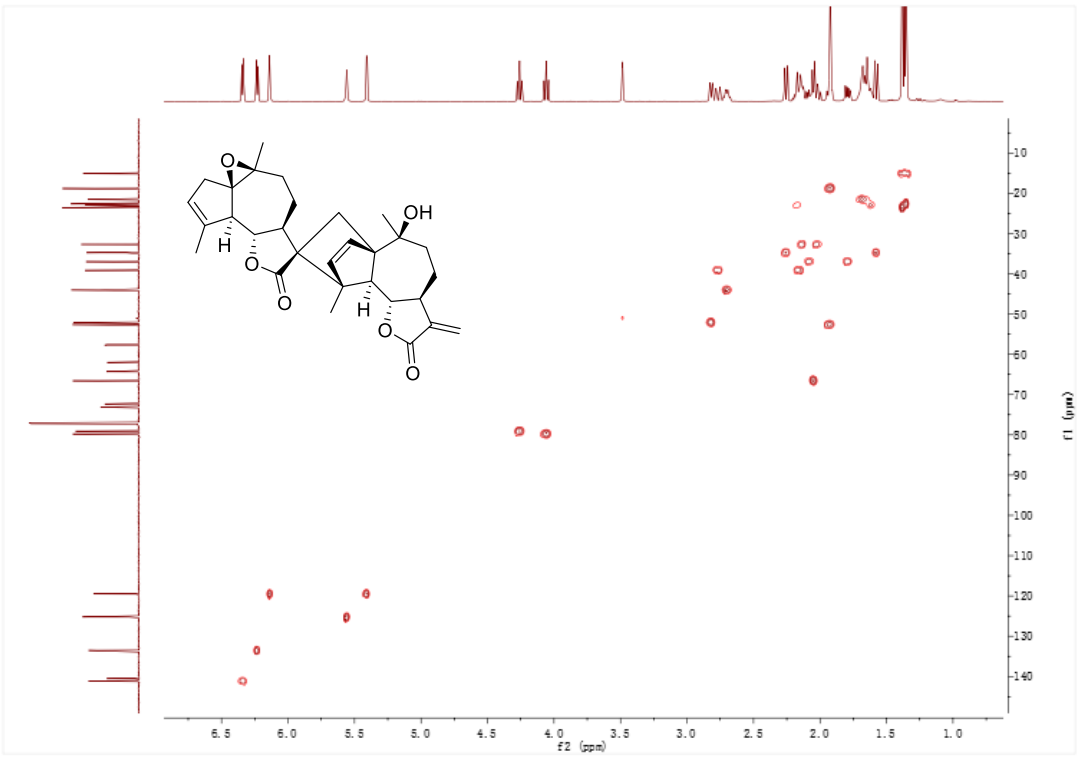


Figure S163 HSQC spectrum (600 MHz) of artematrolide M (**17**) in $CDCl_3$.

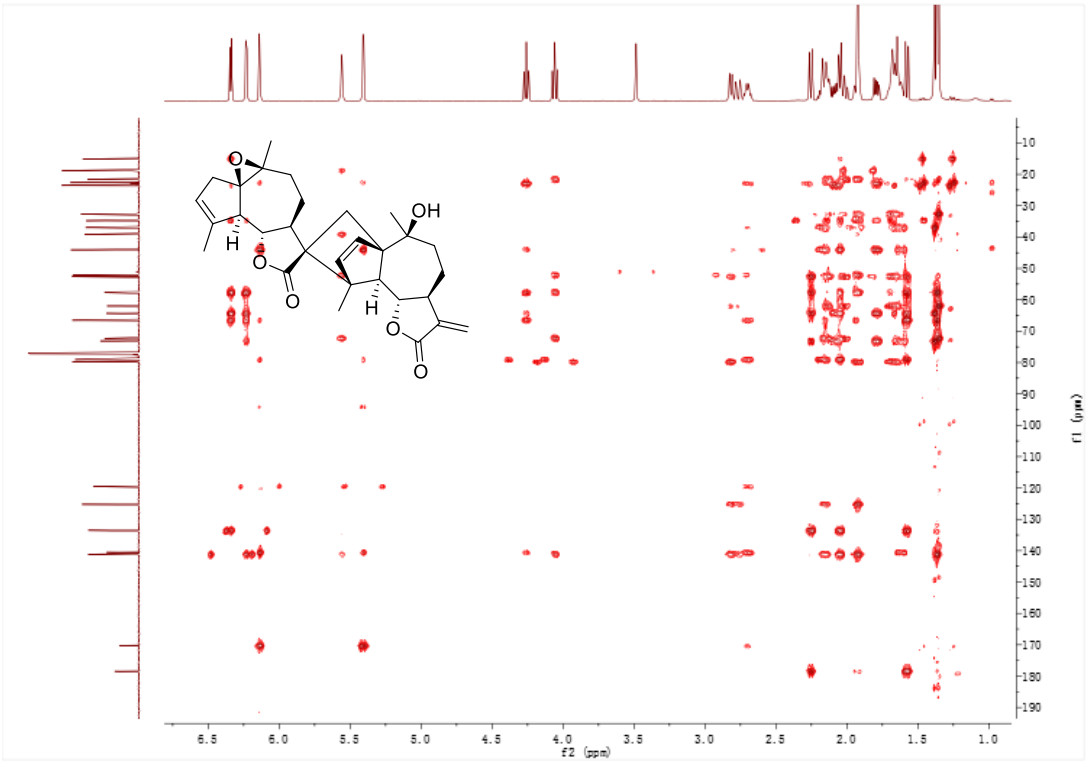


Figure S164 HMBC spectrum (600 MHz) of artematrolide M (**17**) in $CDCl_3$.

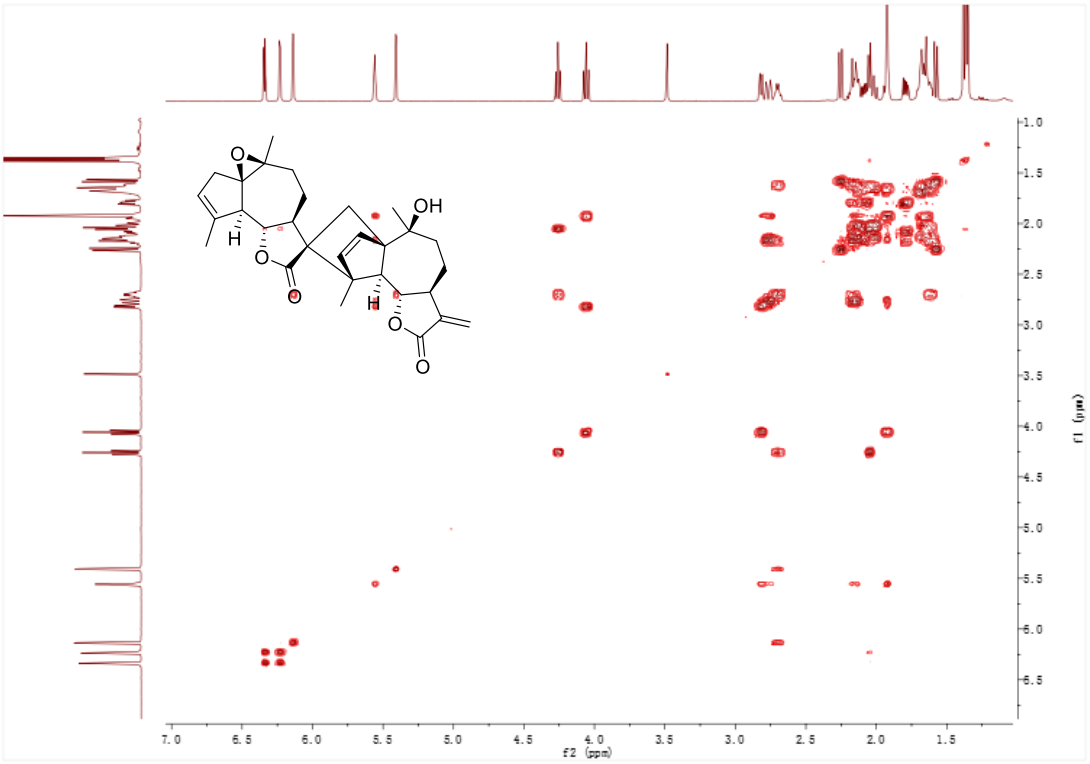


Figure S165 ^{1}H–^{1}H COSY spectrum (600 MHz) of artematrolide M (**17**) in $CDCl_3$.

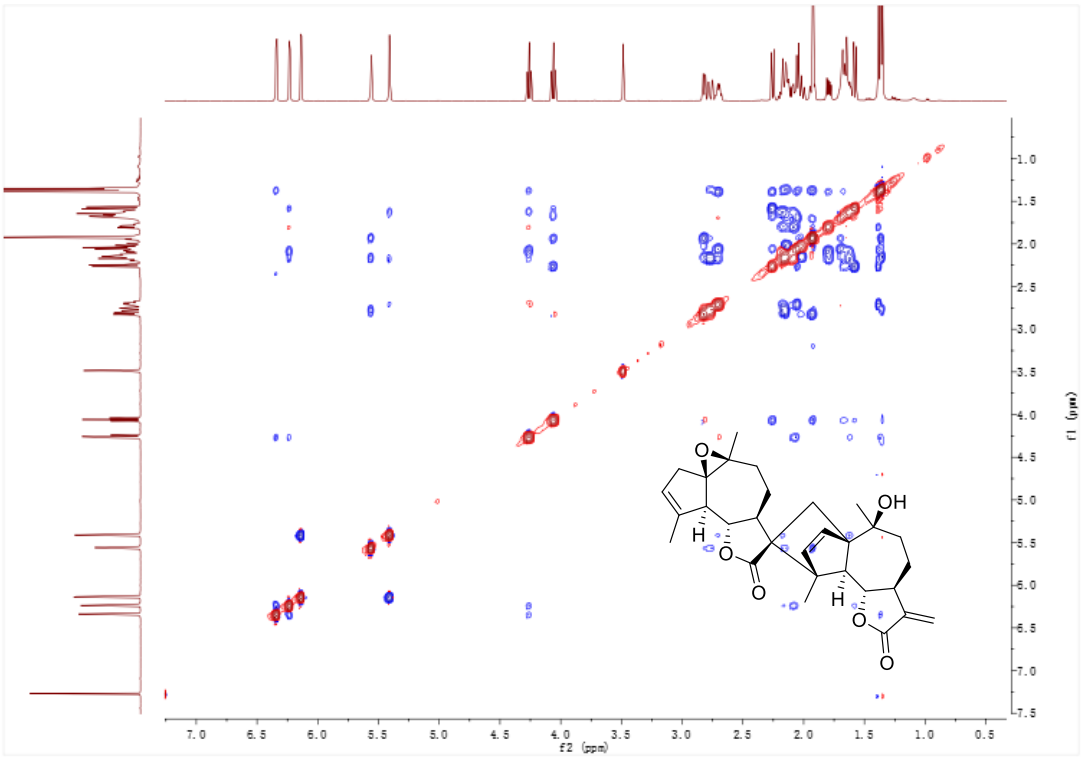


Figure S166 ROESY spectrum (600 MHz) of artematrolide M (**17**) in $CDCl_3$.

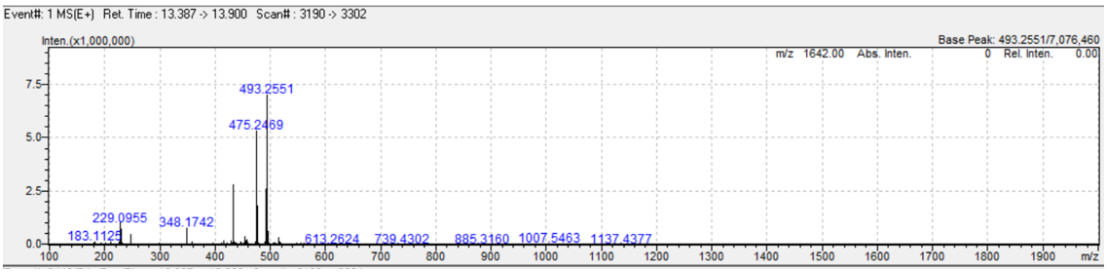


Figure S167 HRESIMS spectrum of artematrolide M (**17**).

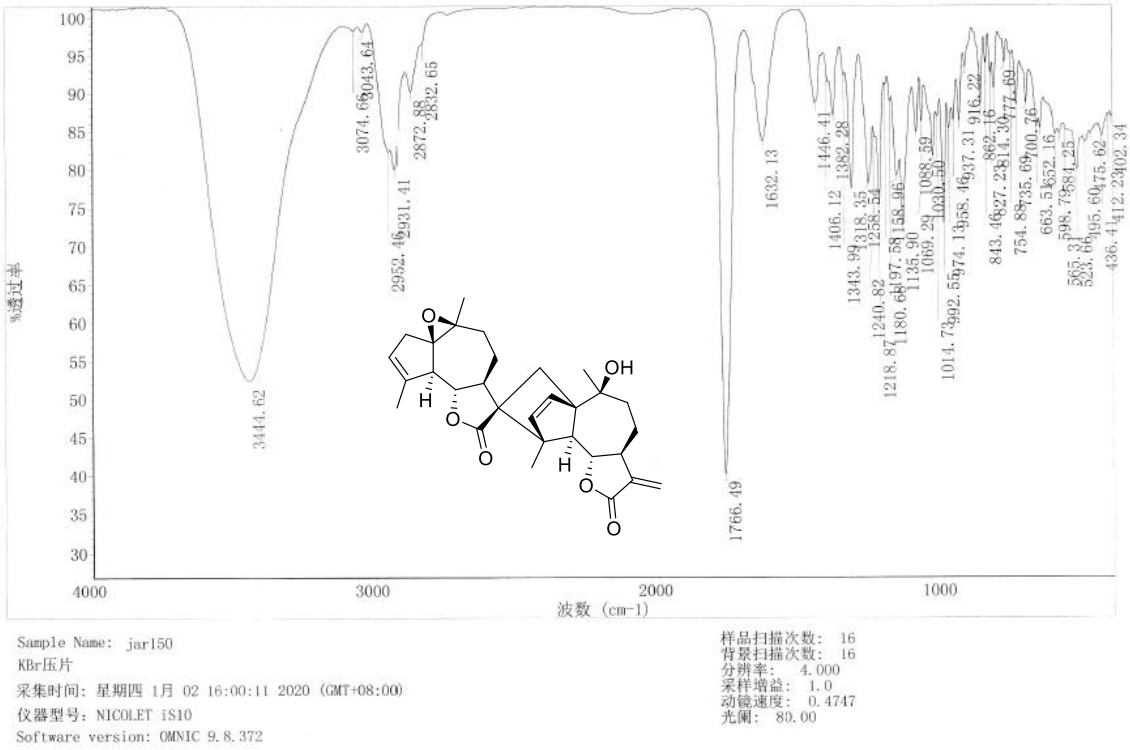


Figure S168 IR spectrum of artematrolide M (**17**).

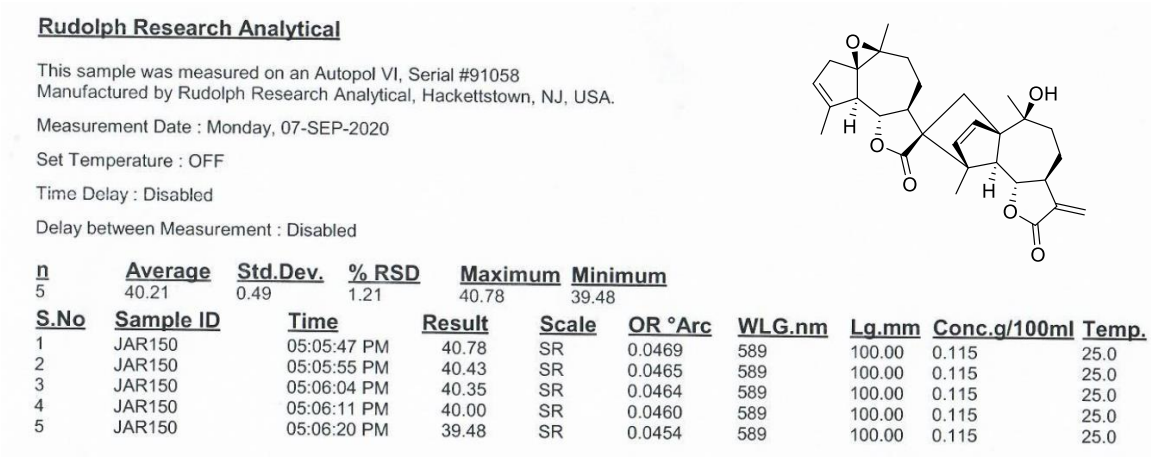


Figure S169 Optical rotation spectrum of artematrolide M (**17**).

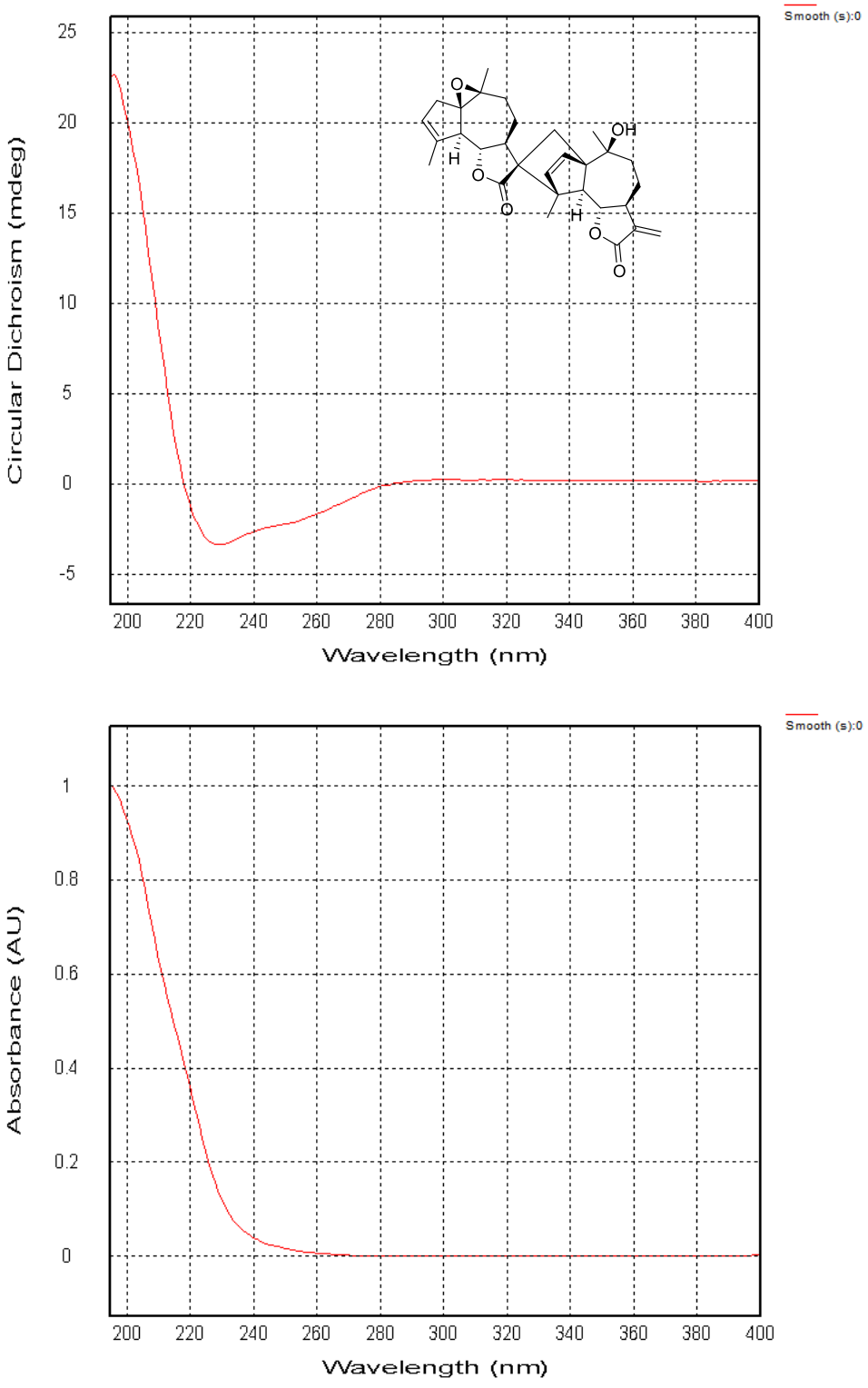


Figure S170 CD (top) and UV (bottom) spectra of artematrolide M (**17**).

19. NMR, MS, IR, $[\alpha]_D$ and CD spectra of compound 18

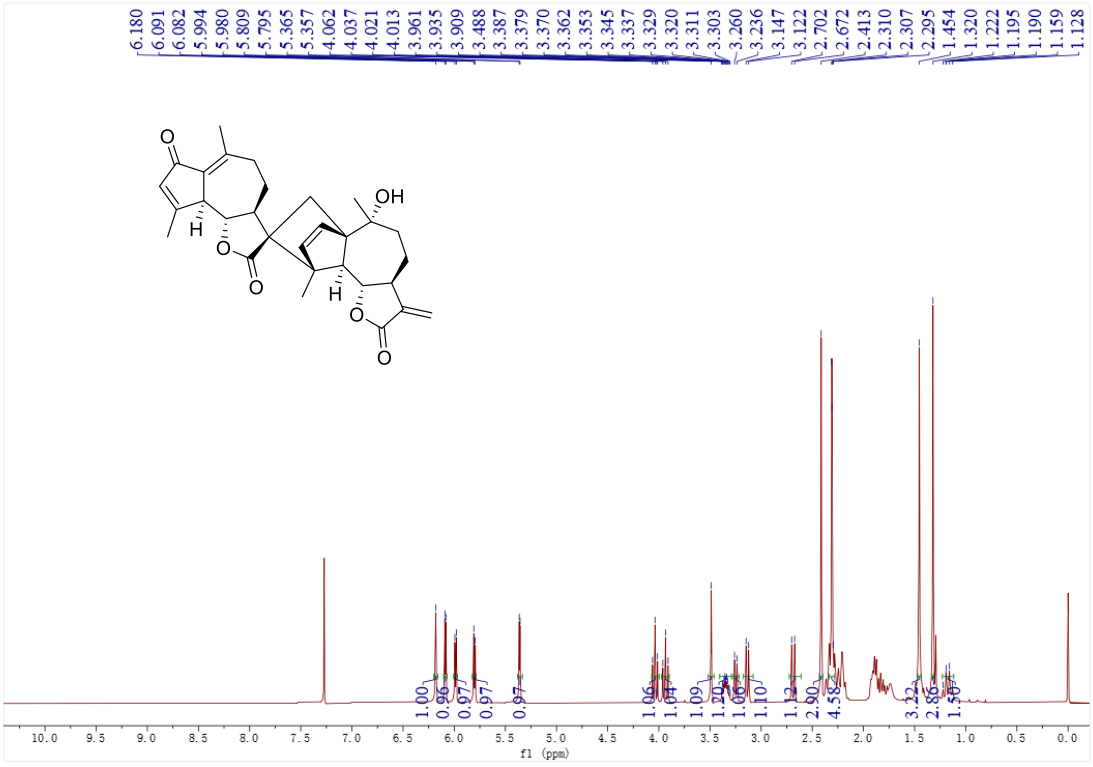


Figure S171 ^{1}H NMR spectrum (400 MHz) of artematrolide N (**18**) in $CDCl_3$.

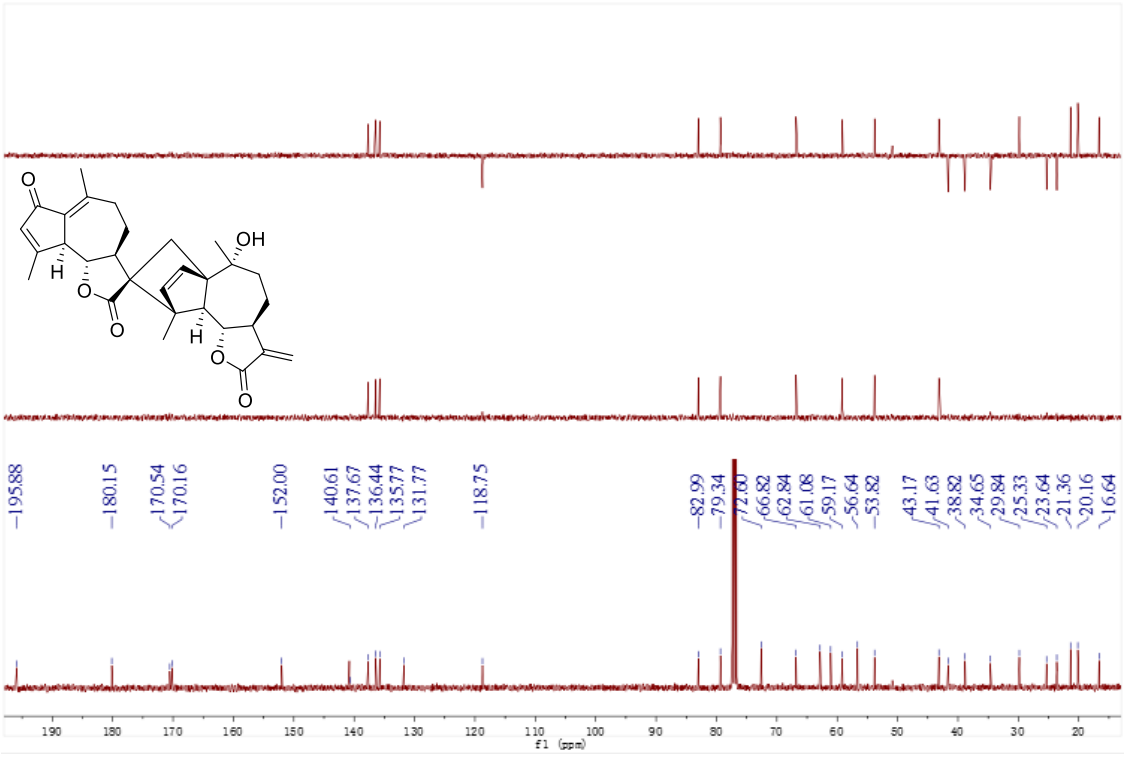


Figure S172 ^{13}C NMR spectrum (100 MHz) of artematrolide N (**18**) in $CDCl_3$.

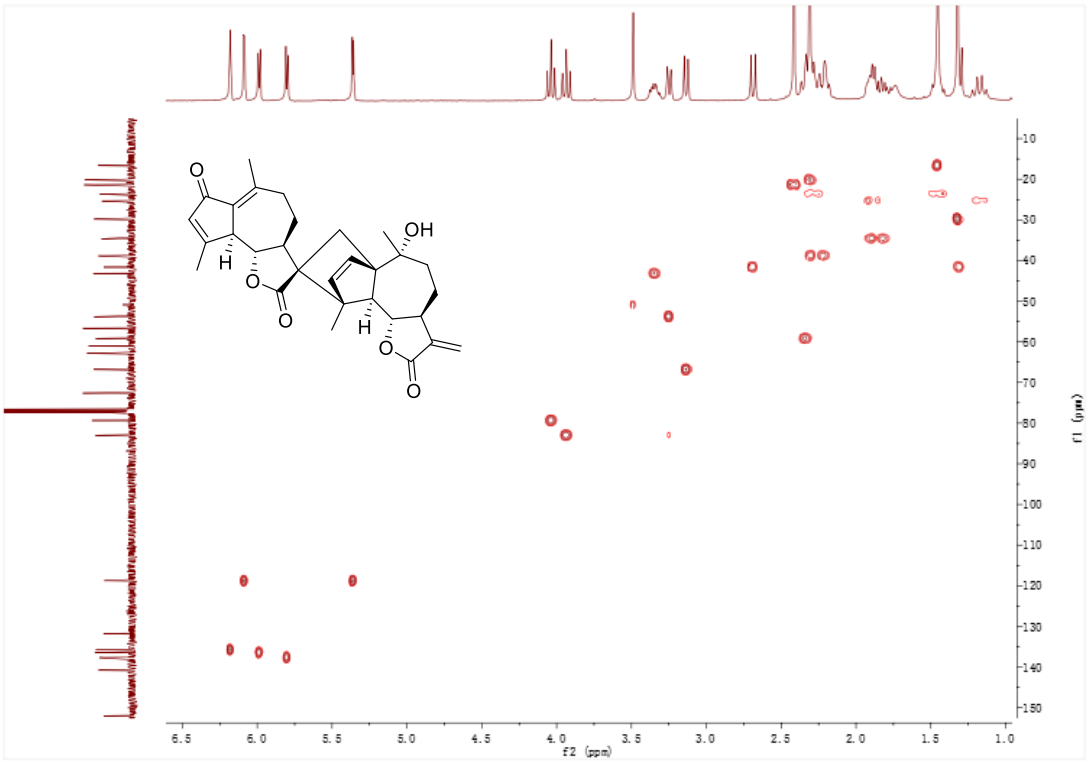


Figure S173 HSQC spectrum (600 MHz) of artematrolide N (**18**) in $CDCl_3$.

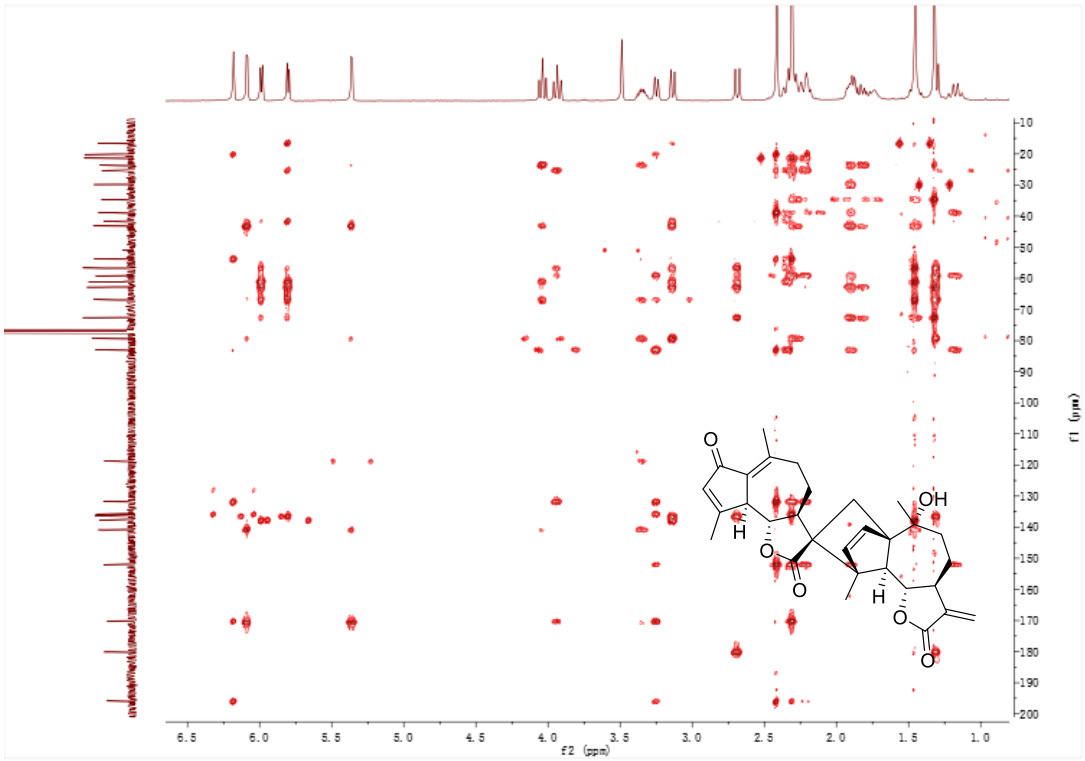


Figure S174 HMBC spectrum (600 MHz) of artematrolide N (**18**) in $CDCl_3$.

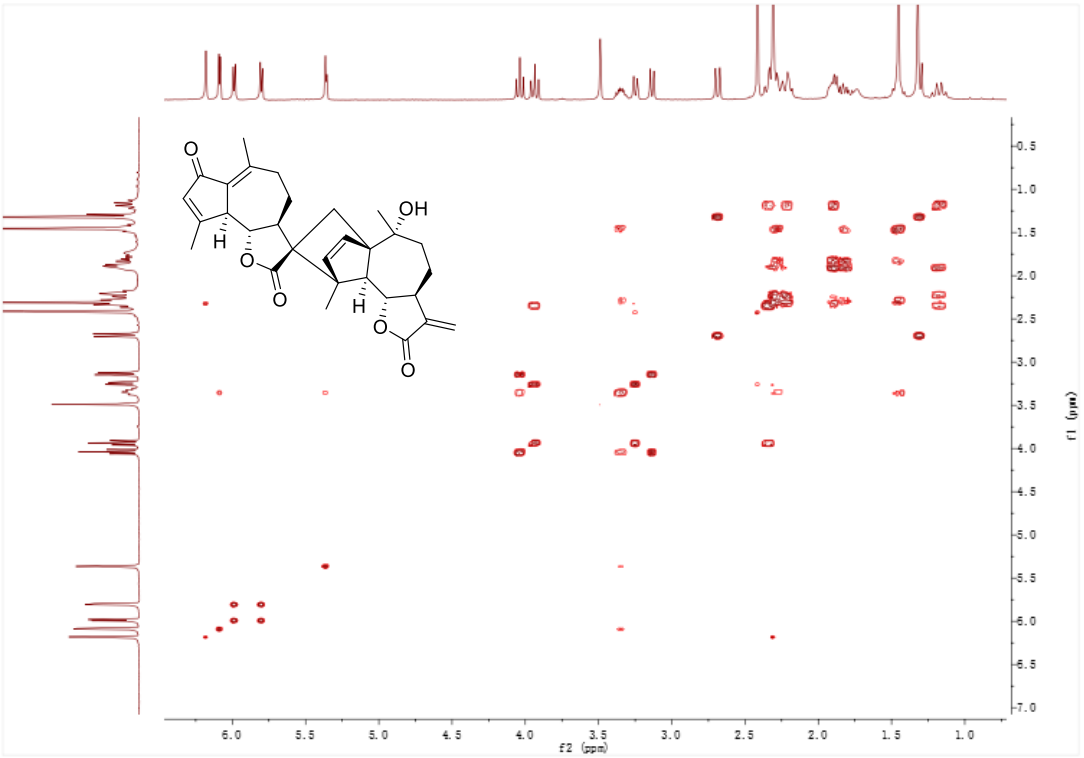


Figure S175 ^{1}H–^{1}H COSY spectrum (600 MHz) of artematrolide N (**18**) in $CDCl_3$.

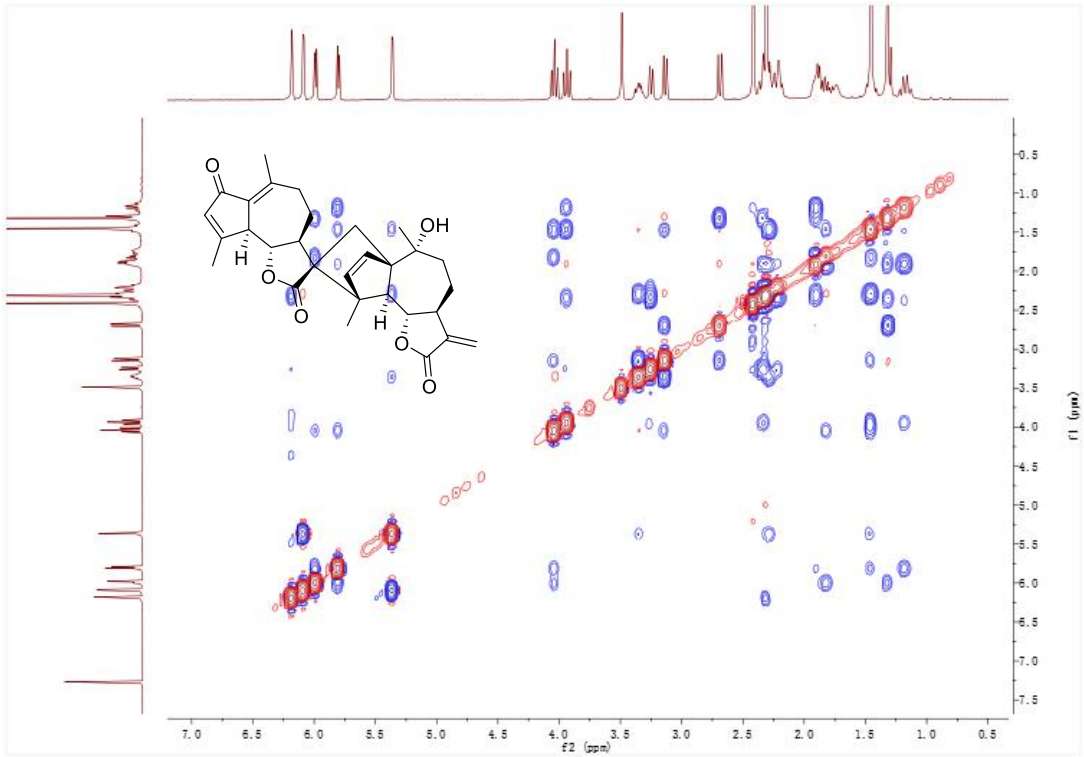


Figure S176 ROESY spectrum (600 MHz) of artematrolide N (**18**) in $CDCl_3$.

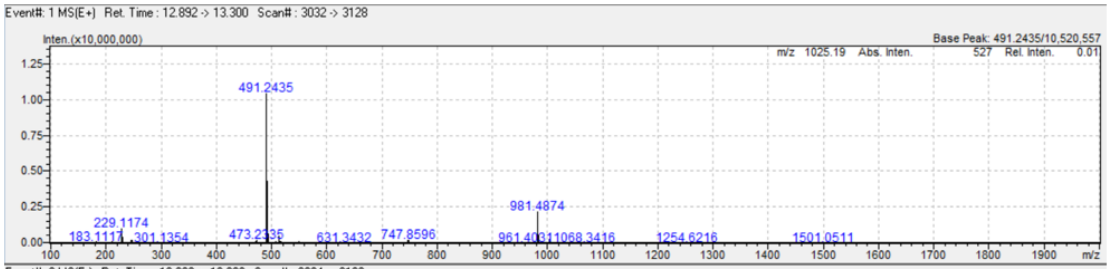


Figure S177 HRESIMS spectrum of artematrolide N (**18**).

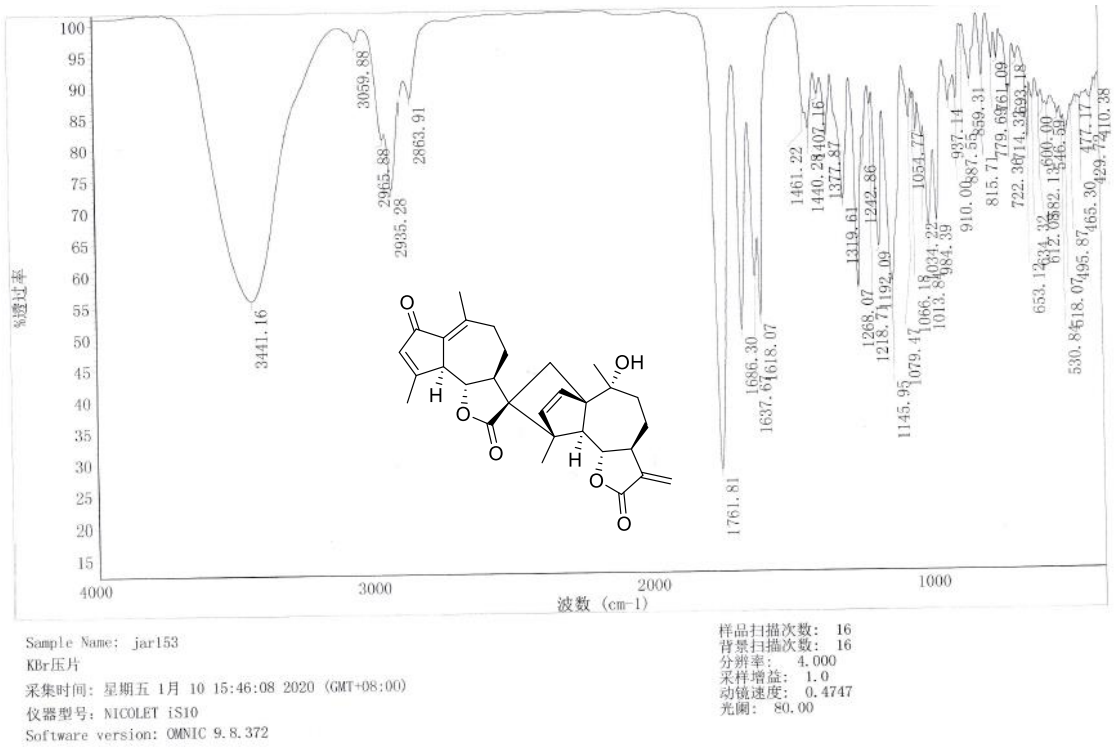


Figure S178 IR spectrum of artematrolide N (**18**).

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Saturday, 04-JAN-2020

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	38.38	0.25	0.65	38.67	38.07

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	jar153	02:11:18 PM	38.67	SR	0.0321	589	100.00	0.083	23.0
2	jar153	02:11:27 PM	38.07	SR	0.0316	589	100.00	0.083	23.0
3	jar153	02:11:34 PM	38.55	SR	0.0320	589	100.00	0.083	22.9
4	jar153	02:11:43 PM	38.19	SR	0.0317	589	100.00	0.083	22.9
5	jar153	02:11:51 PM	38.43	SR	0.0319	589	100.00	0.083	22.9

Figure S179 Optical rotation spectrum of artematrolide N (**18**).

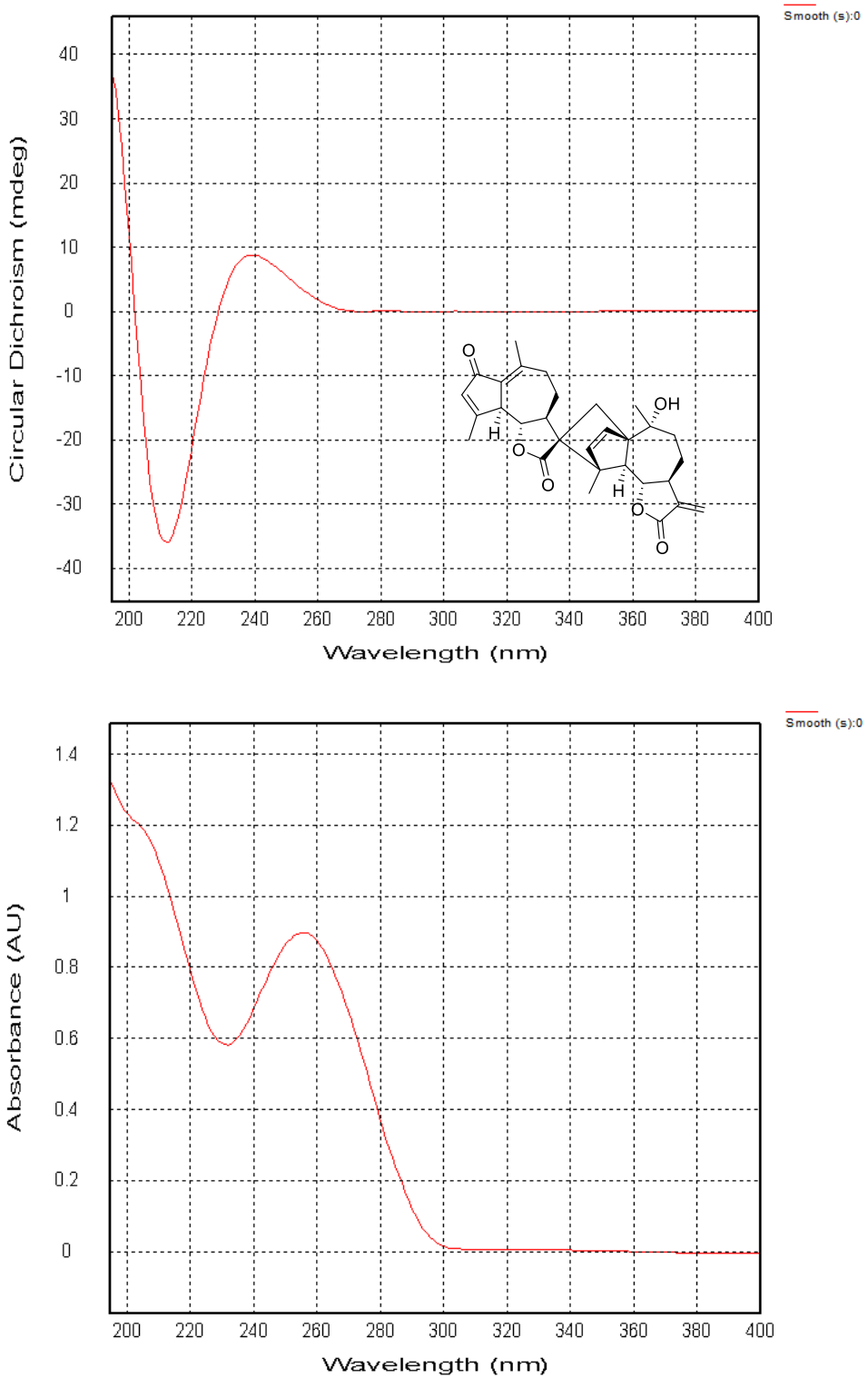


Figure S180 CD (top) and UV (bottom) spectra of artematrolide N (**18**).

20. NMR, MS, IR, $[\alpha]_D$ and CD spectra of compound 19

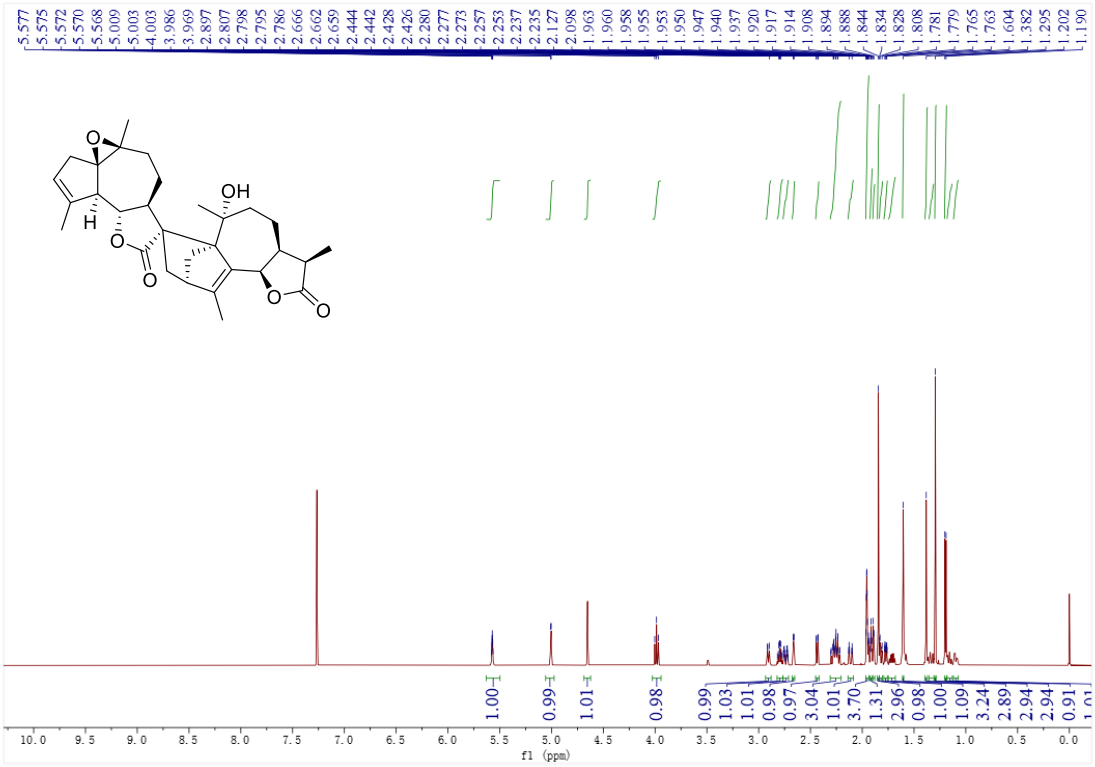


Figure S181 ^{1}H NMR spectrum (600 MHz) of artematrolide O (**19**) in $CDCl_3$.

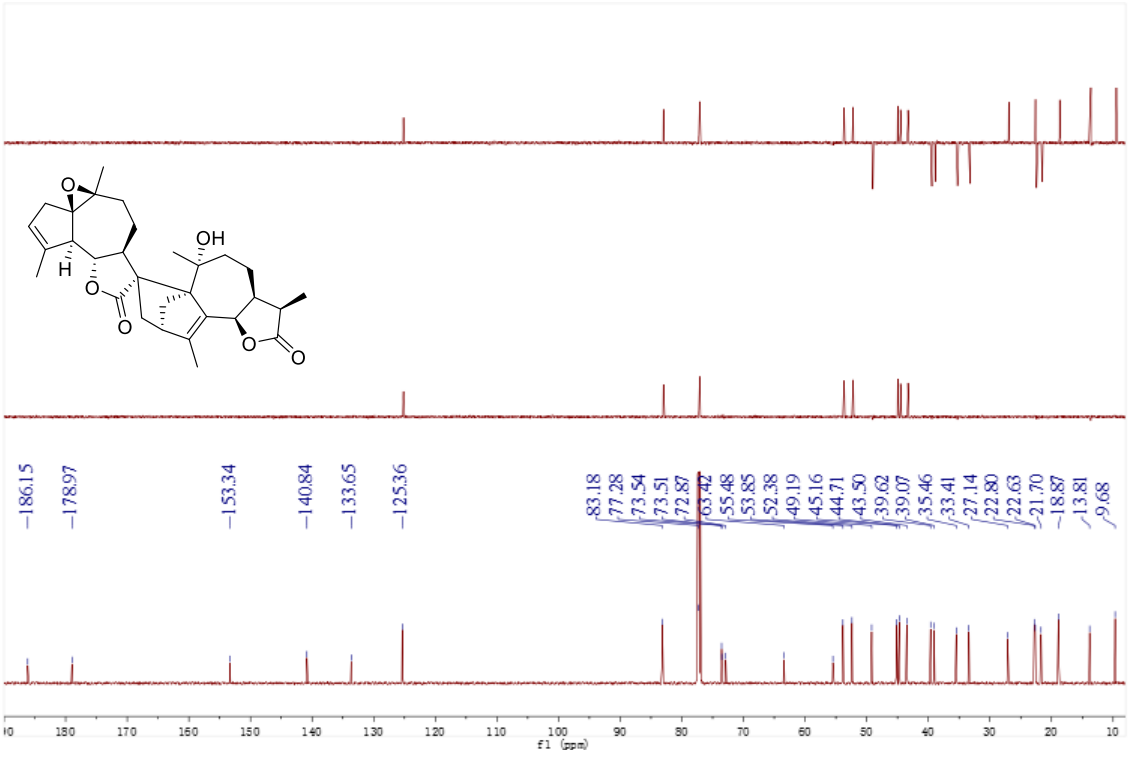


Figure S182 ^{13}C NMR spectrum (150 MHz) of artematrolide O (**19**) in $CDCl_3$.

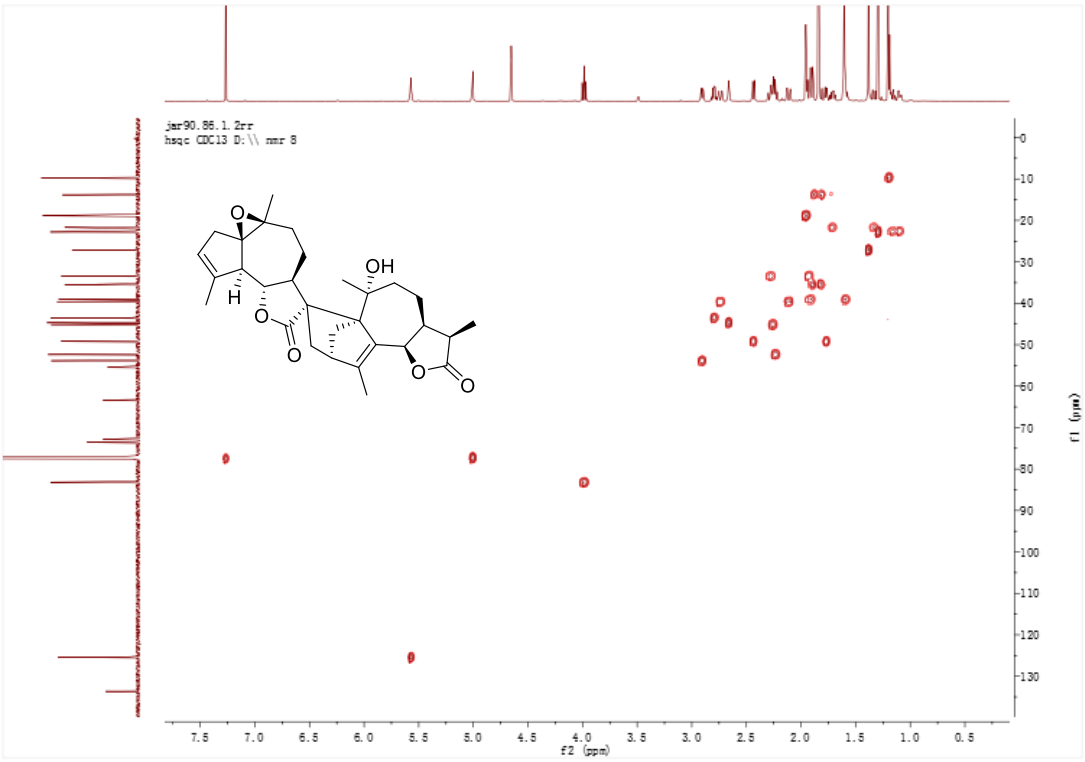


Figure S183 HSQC spectrum (600 MHz) of artematrolide O (**19**) in $CDCl_3$.

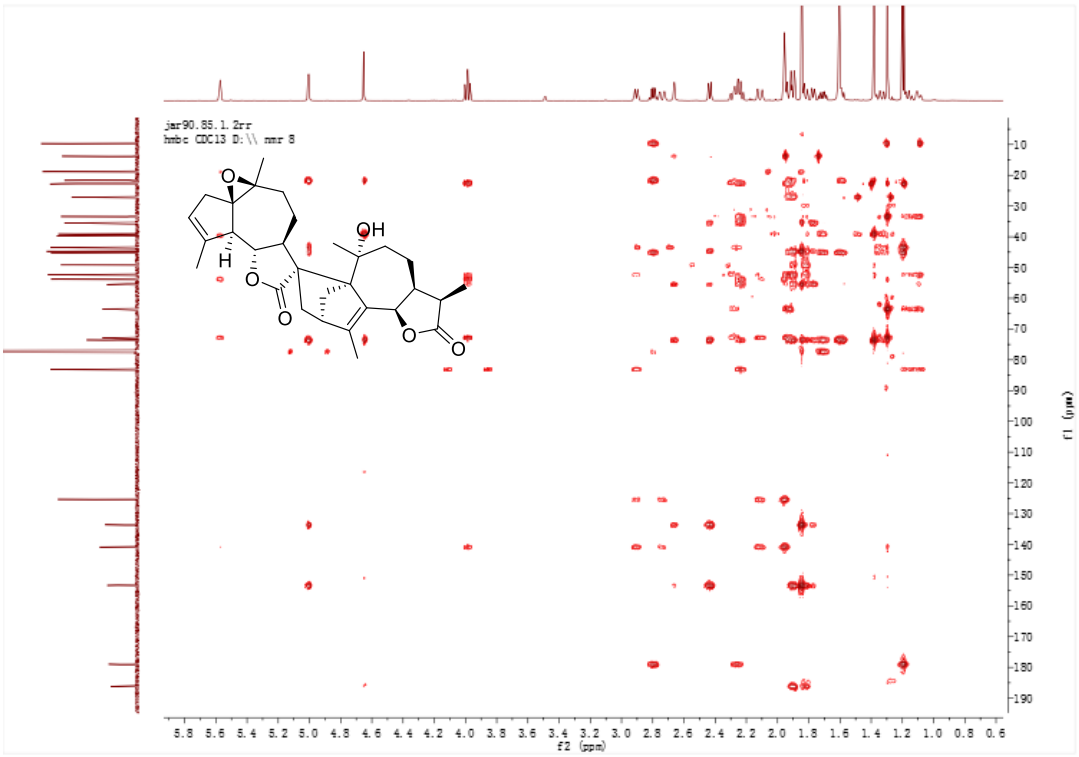


Figure S184 HMBC spectrum (600 MHz) of artematrolide O (**19**) in $CDCl_3$.

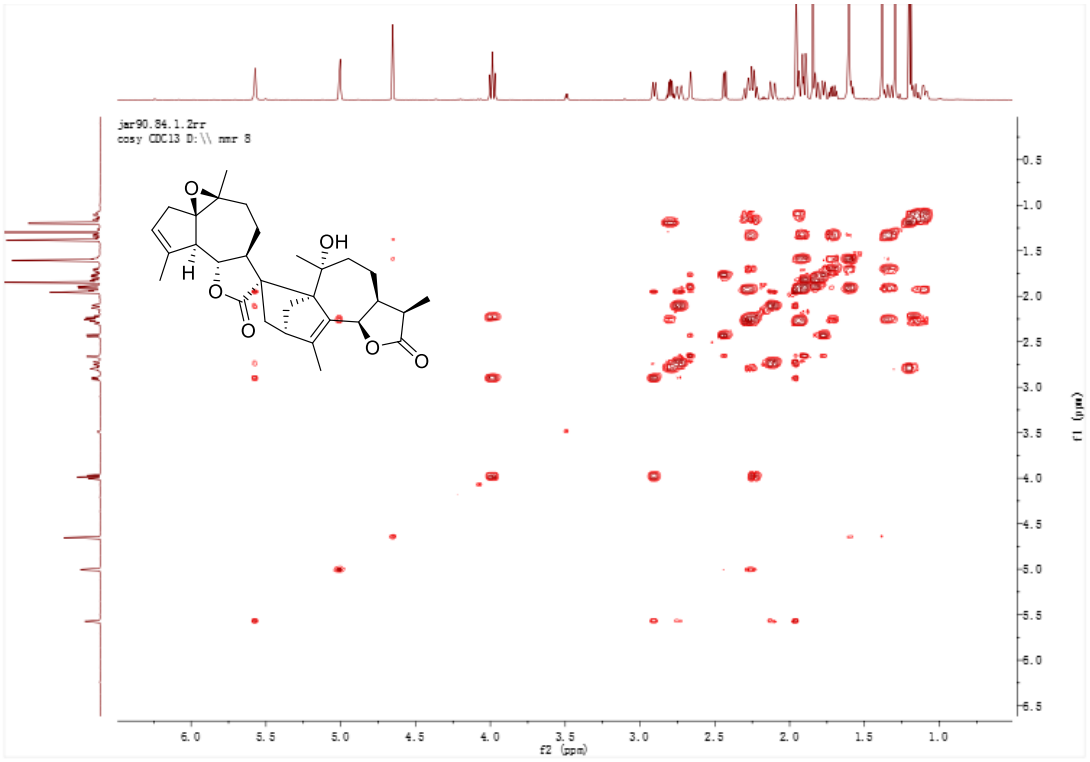


Figure S185 ^{1}H–^{1}H COSY spectrum (600 MHz) of artematrolide O (**19**) in $CDCl_3$.

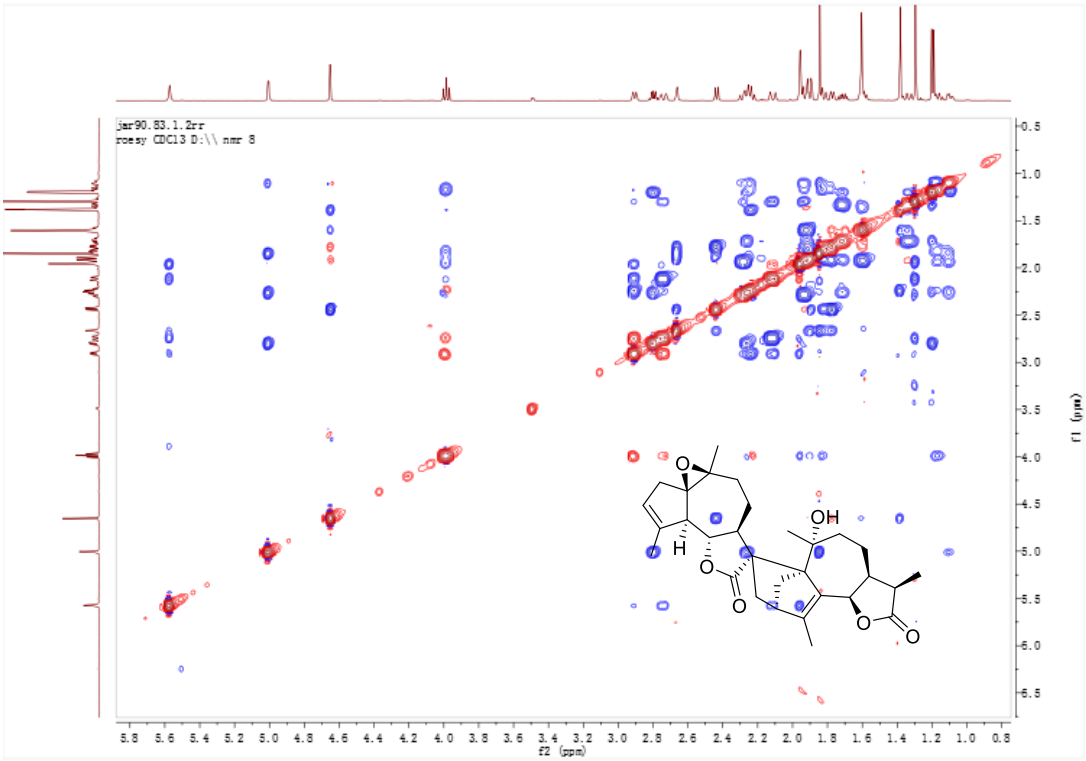


Figure S186 ROESY spectrum (600 MHz) of artematrolide O (**19**) in $CDCl_3$.

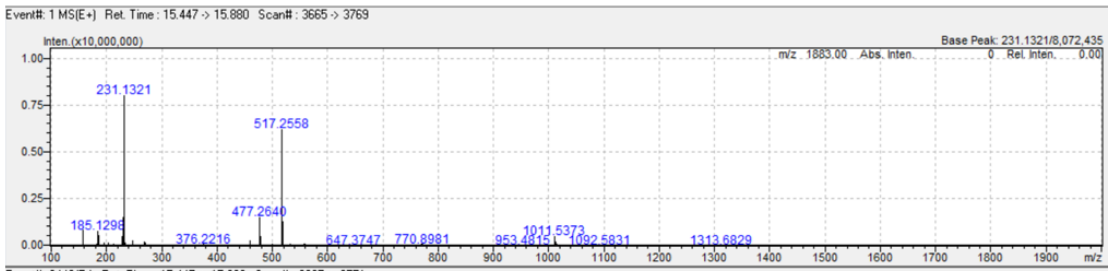


Figure S187 HRESIMS spectrum of artematrolide O (**19**).

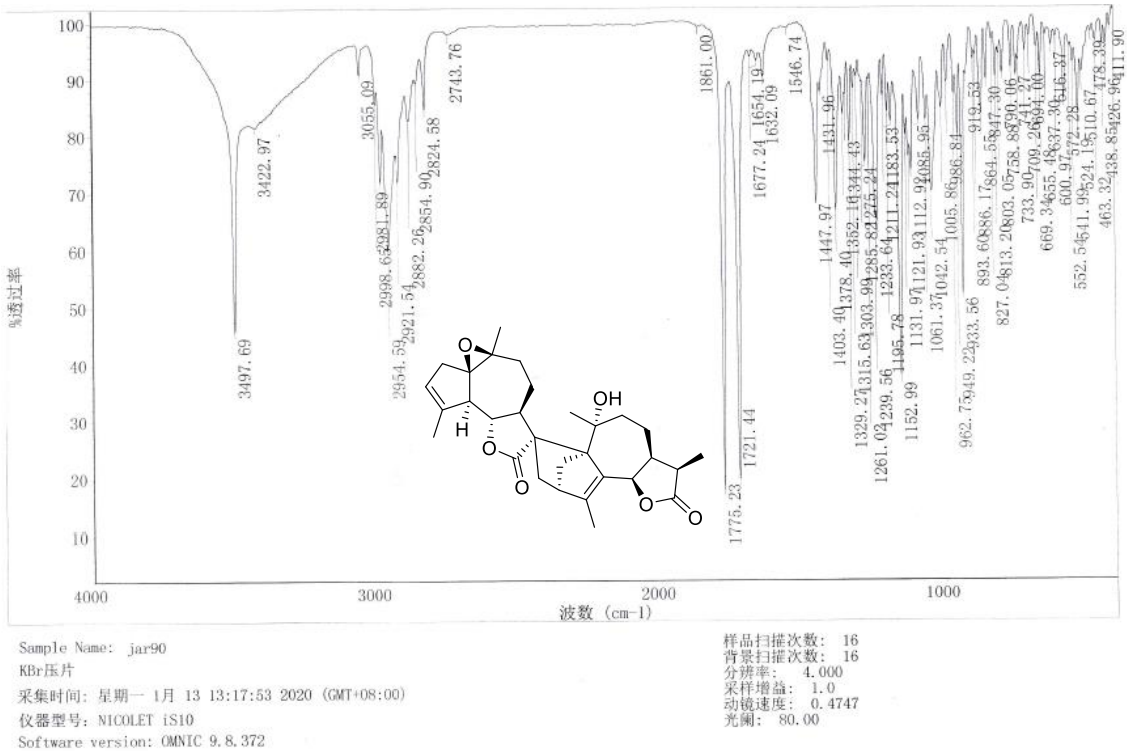


Figure S188 IR spectrum of artematrolide O (**19**).

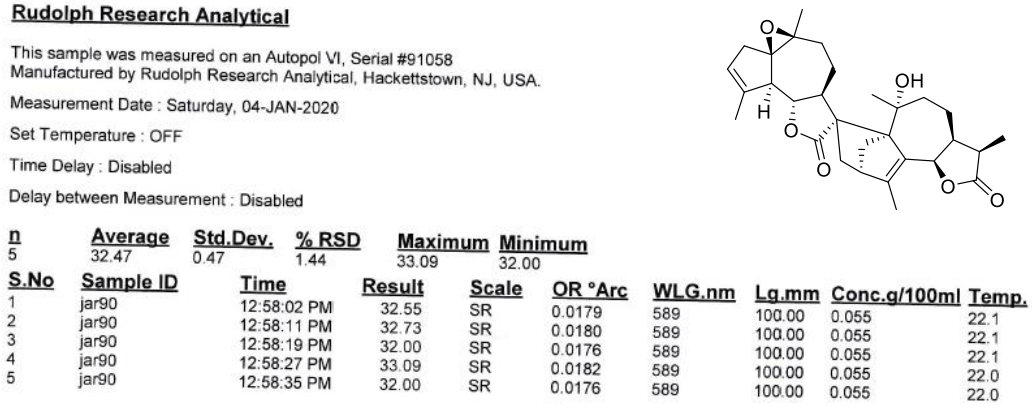


Figure S189 Optical rotation spectrum of artematrolide O (**19**).

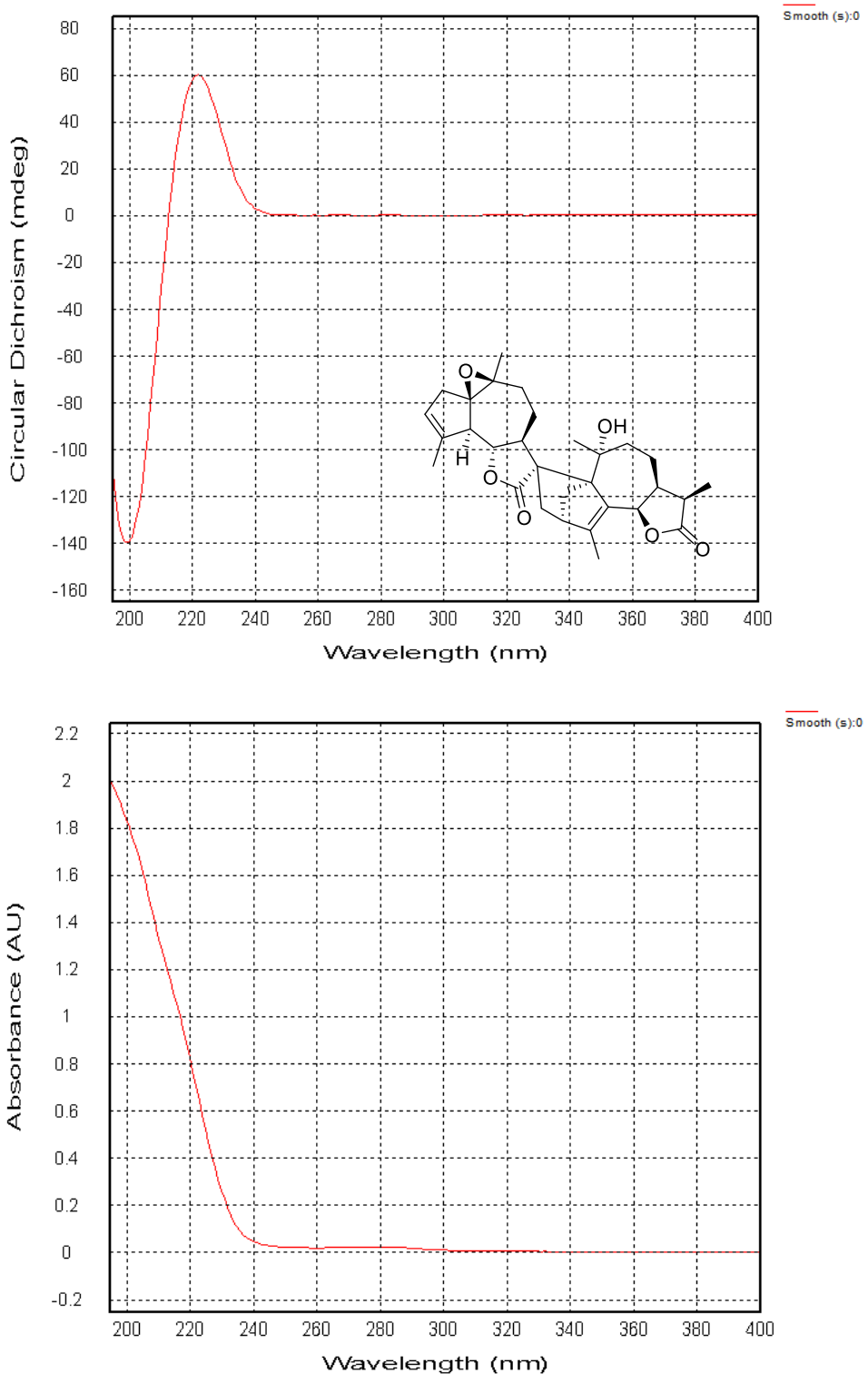


Figure S190 CD (top) and UV (bottom) spectra of artematrolide O (**19**).

21. NMR, MS, IR, $[\alpha]_D$ and CD spectra of compound 20

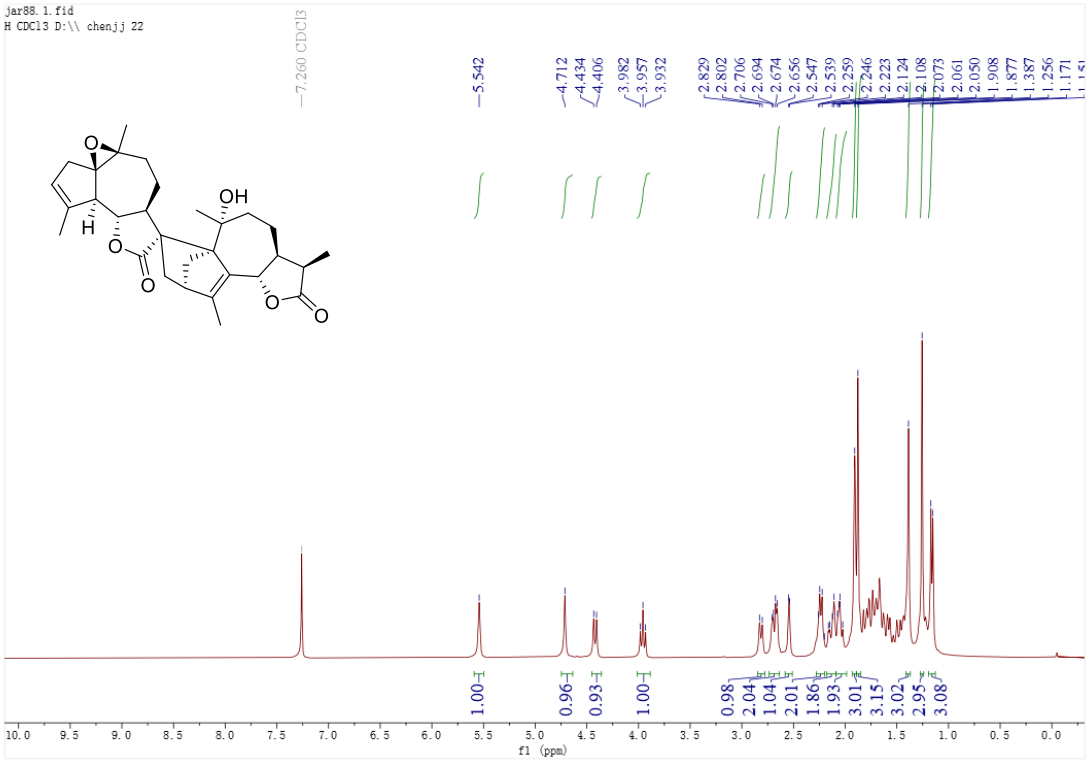


Figure S191 ^{1}H NMR spectrum (400 MHz) of artematrolide P (**20**) in $CDCl_3$.

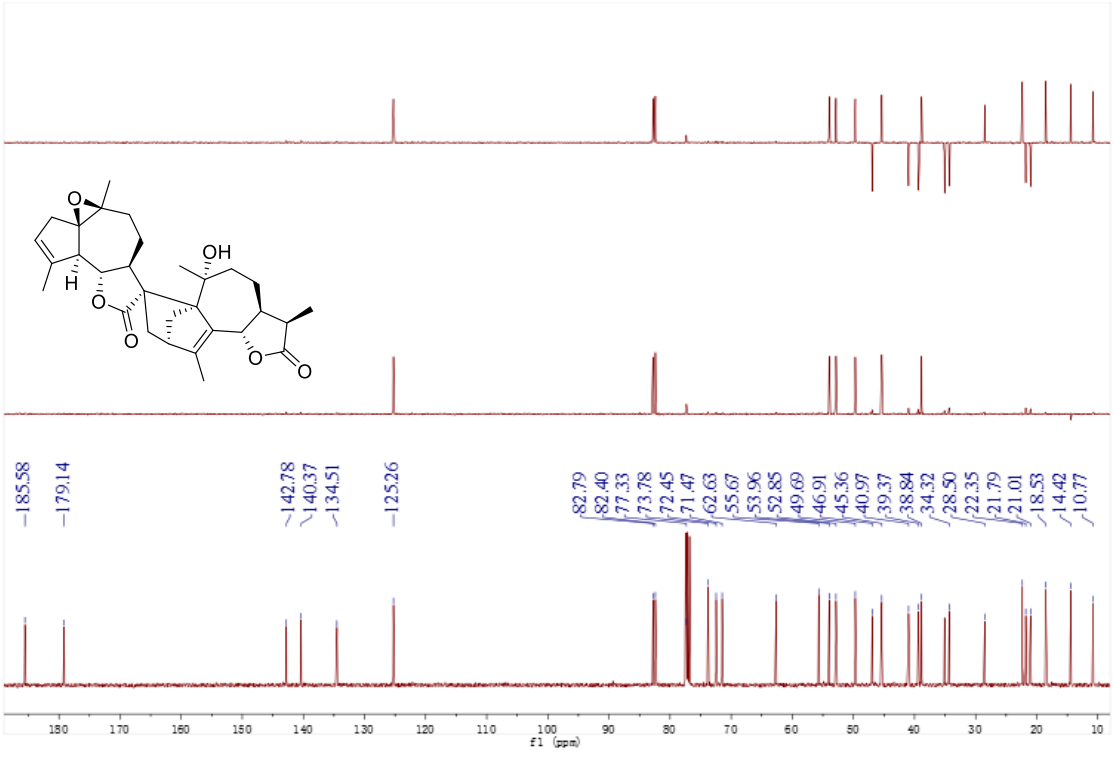


Figure S192 ^{13}C NMR spectrum (100 MHz) of artematrolide P (**20**) in $CDCl_3$.

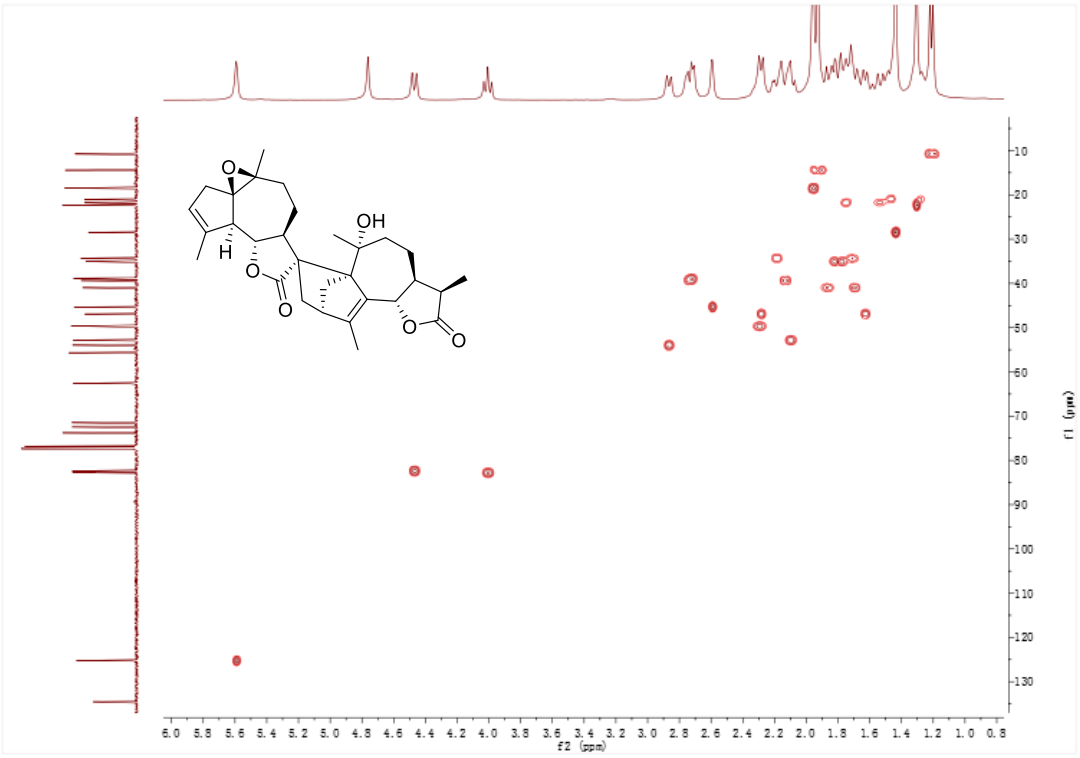


Figure S193 HSQC spectrum (600 MHz) of artematrolide P (**20**) in $CDCl_3$.

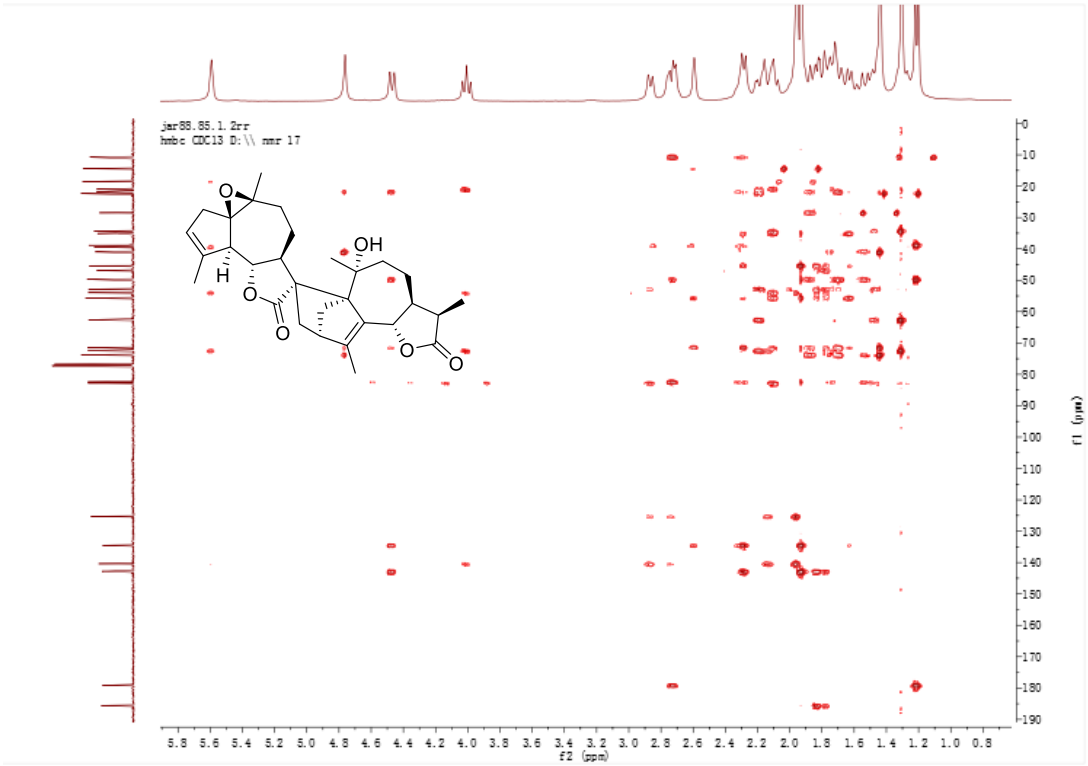


Figure S194 HMBC spectrum (600 MHz) of artematrolide P (**20**) in $CDCl_3$.

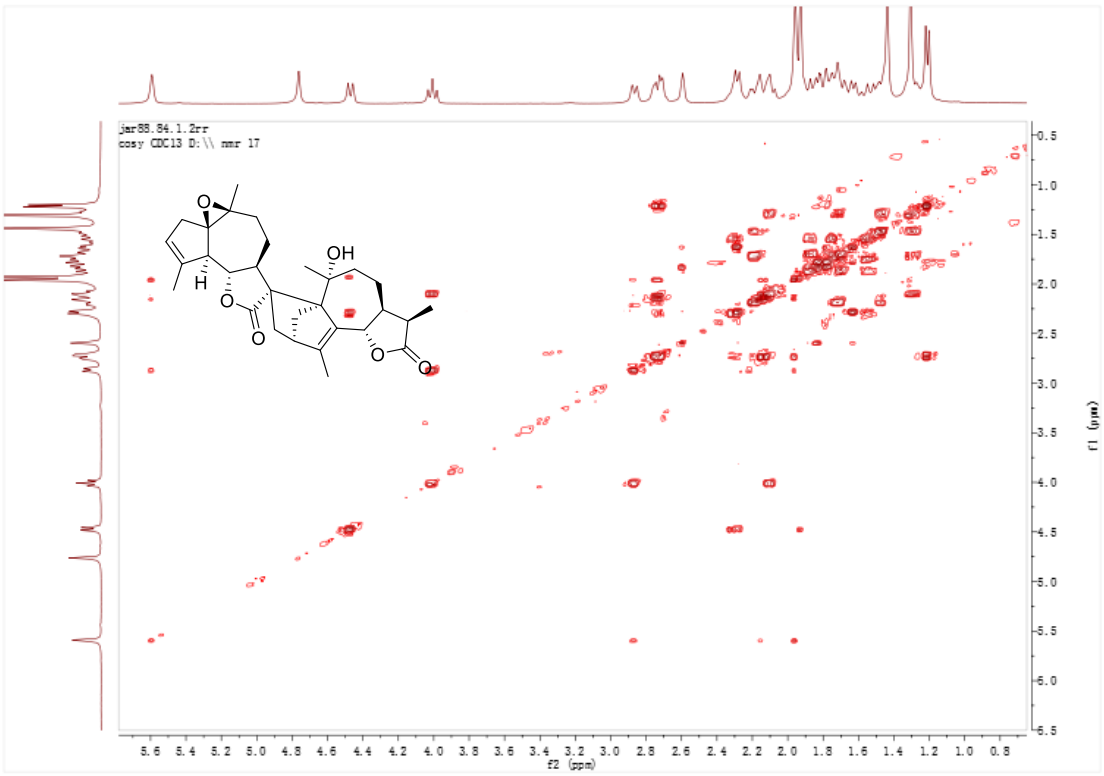


Figure S195 ^{1}H–^{1}H COSY spectrum (600 MHz) of artematrolide P (**20**) in $CDCl_3$.

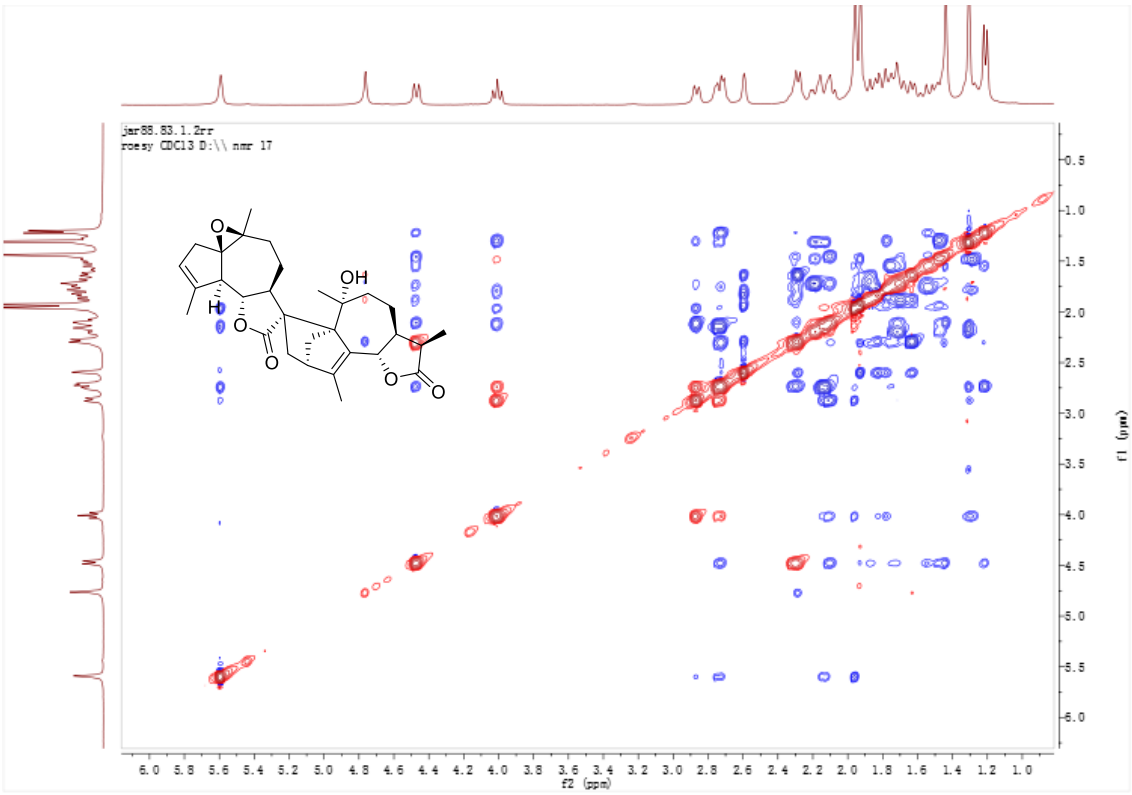


Figure S196 ROESY spectrum (600 MHz) of artematrolide P (**20**) in $CDCl_3$.

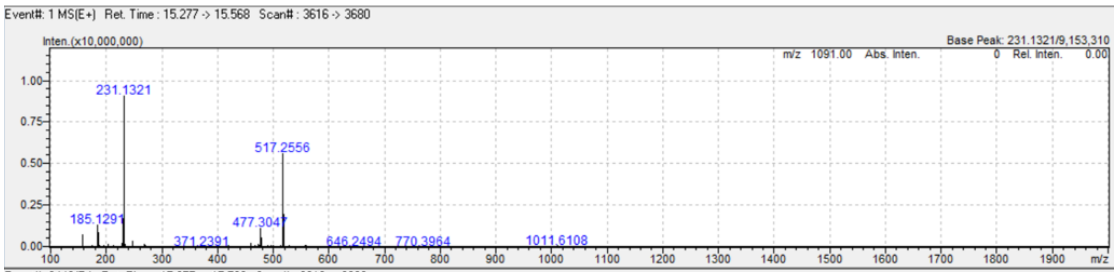


Figure S197 HRESIMS spectrum of artematrolide P (**20**).

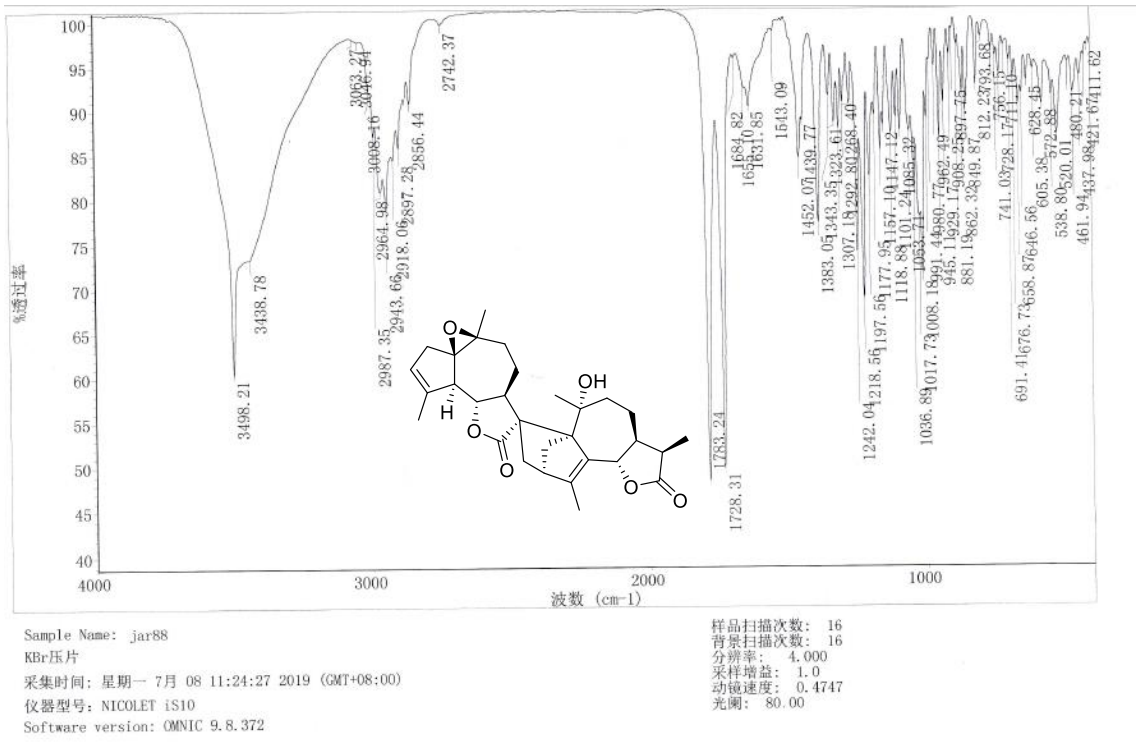


Figure S198 IR spectrum of artematrolide P (**20**).

Rudolph Research Analytical

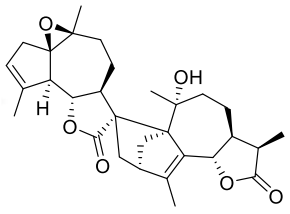
This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Monday, 08-JUL-2019

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled



n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	88.67	1.13	1.27	90.00	87.33

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	jar88	05:31:15 PM	89.33	SR	0.0268	589	100.00	0.030	24.4
2	jar88	05:31:24 PM	90.00	SR	0.0270	589	100.00	0.030	24.4
3	jar88	05:31:32 PM	89.00	SR	0.0267	589	100.00	0.030	24.4
4	jar88	05:31:40 PM	87.67	SR	0.0263	589	100.00	0.030	24.4
5	jar88	05:31:48 PM	87.33	SR	0.0262	589	100.00	0.030	24.4

Figure S199 Optical rotation spectrum of artematrolide P (**20**).

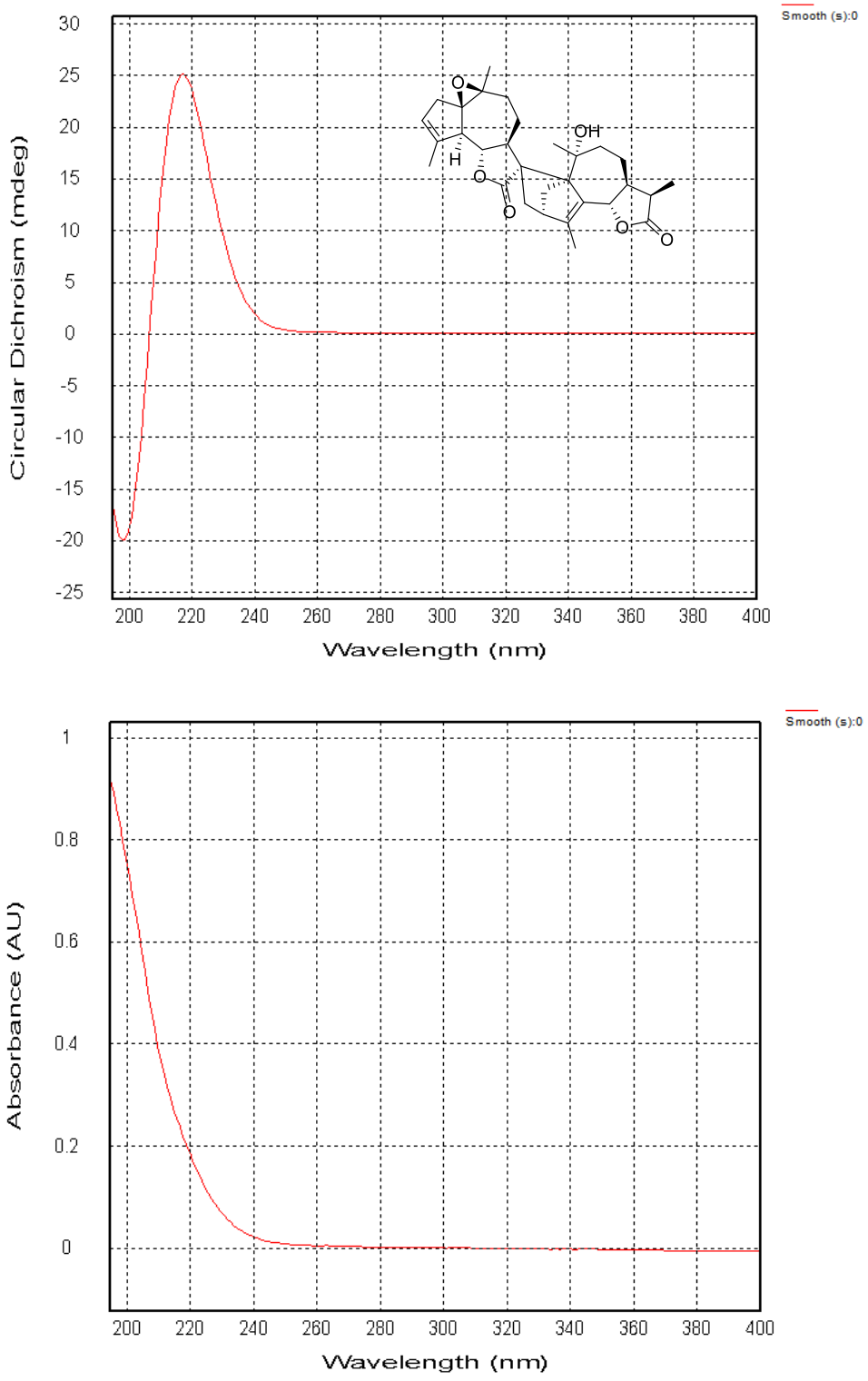


Figure S200 CD (top) and UV (bottom) spectra of artematrolide P (**20**).

22. NMR, MS, IR, $[\alpha]_D$ and CD spectra of compound 21

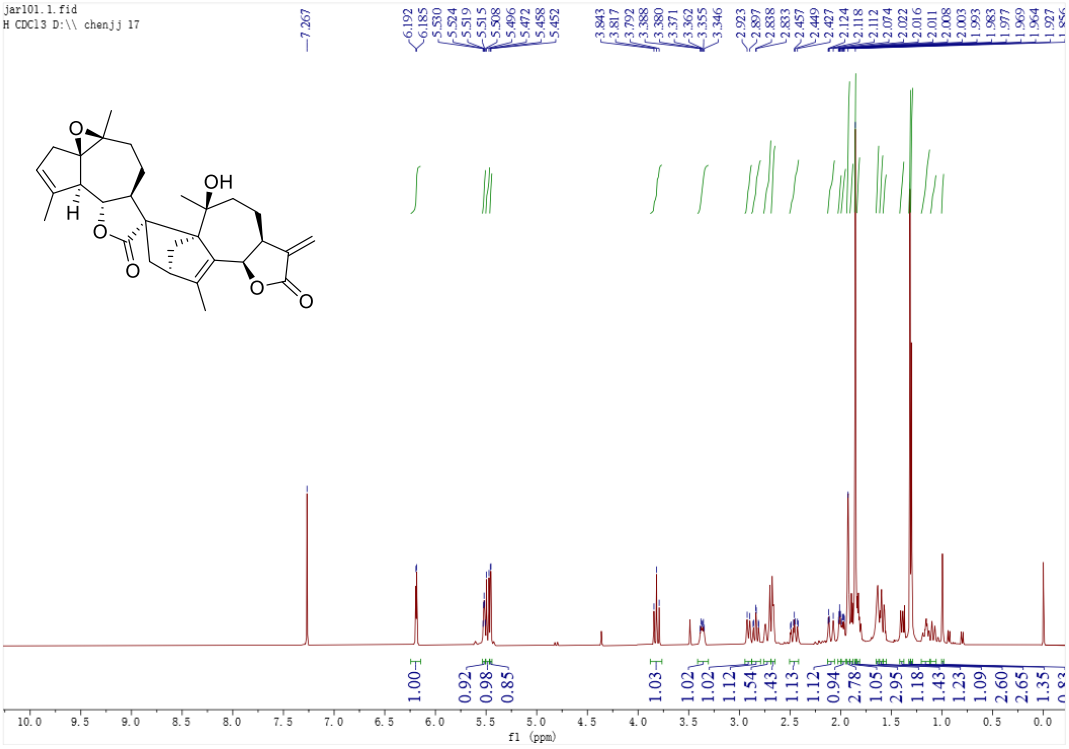


Figure S201 ^{1}H NMR spectrum (400 MHz) of artematrolide Q (**21**) in $CDCl_3$.

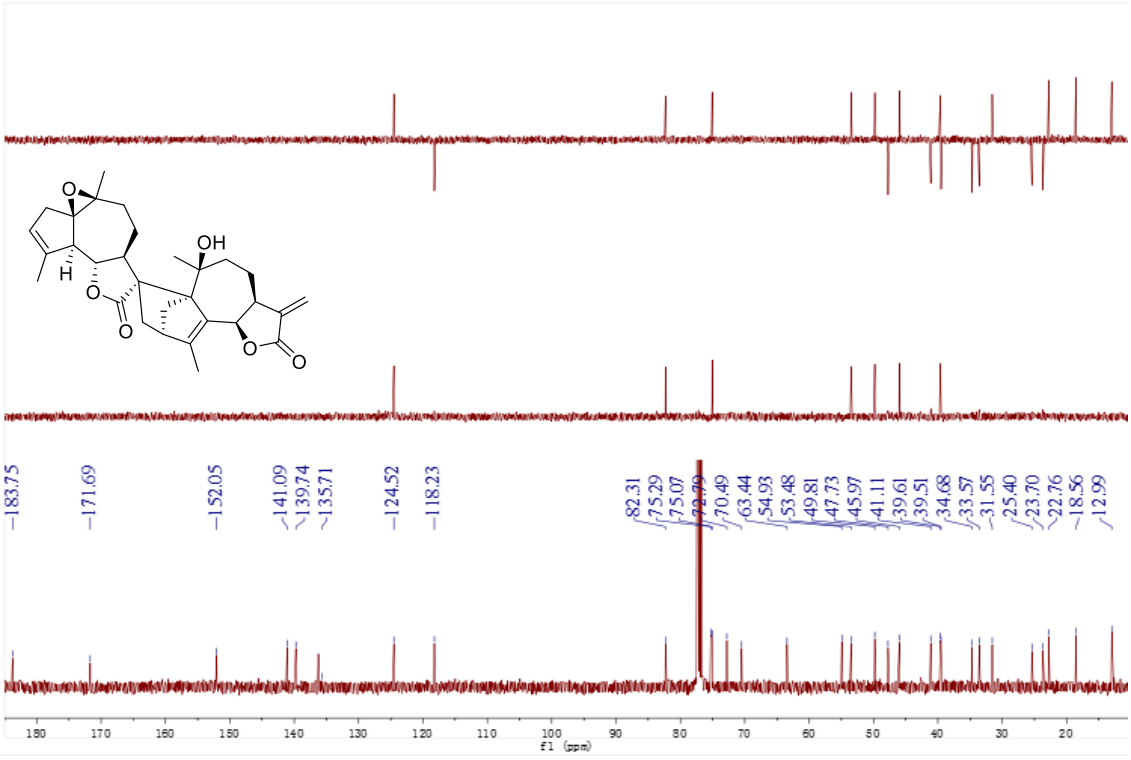


Figure S202 ^{13}C NMR spectrum (100 MHz) of artematrolide Q (**21**) in $CDCl_3$.

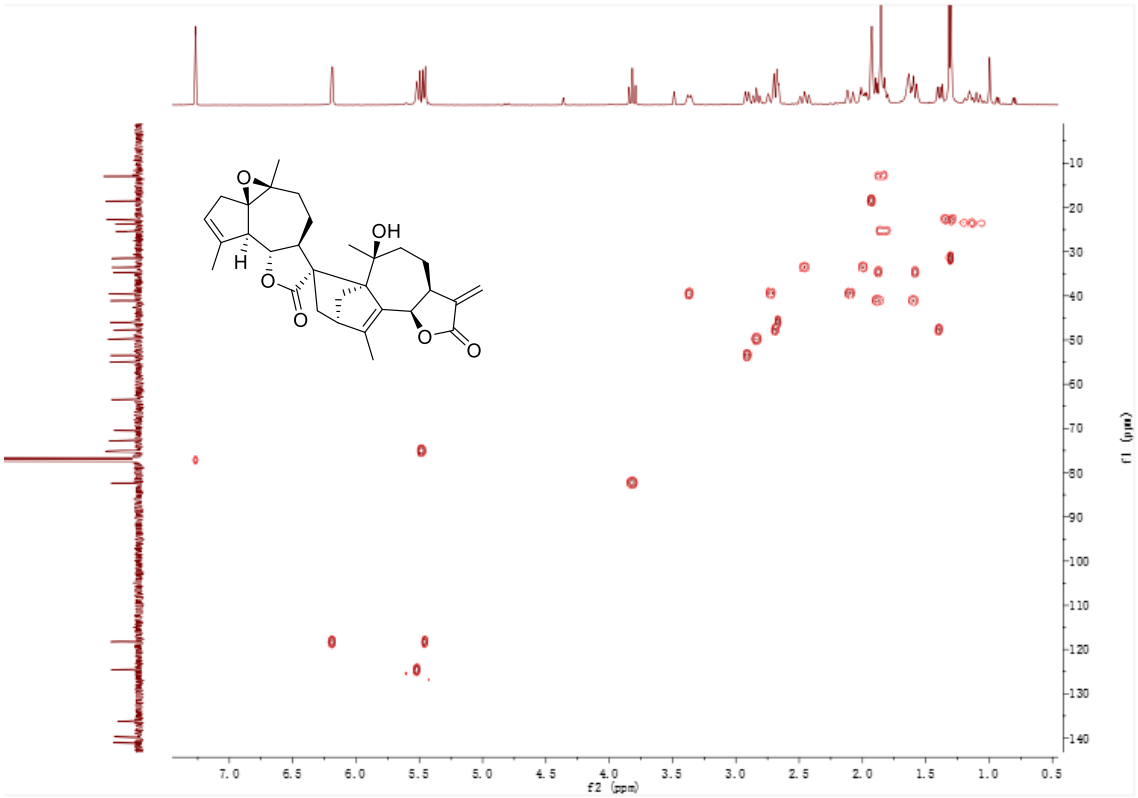


Figure S203 HSQC spectrum (600 MHz) of artematrolide Q (**21**) in $CDCl_3$.

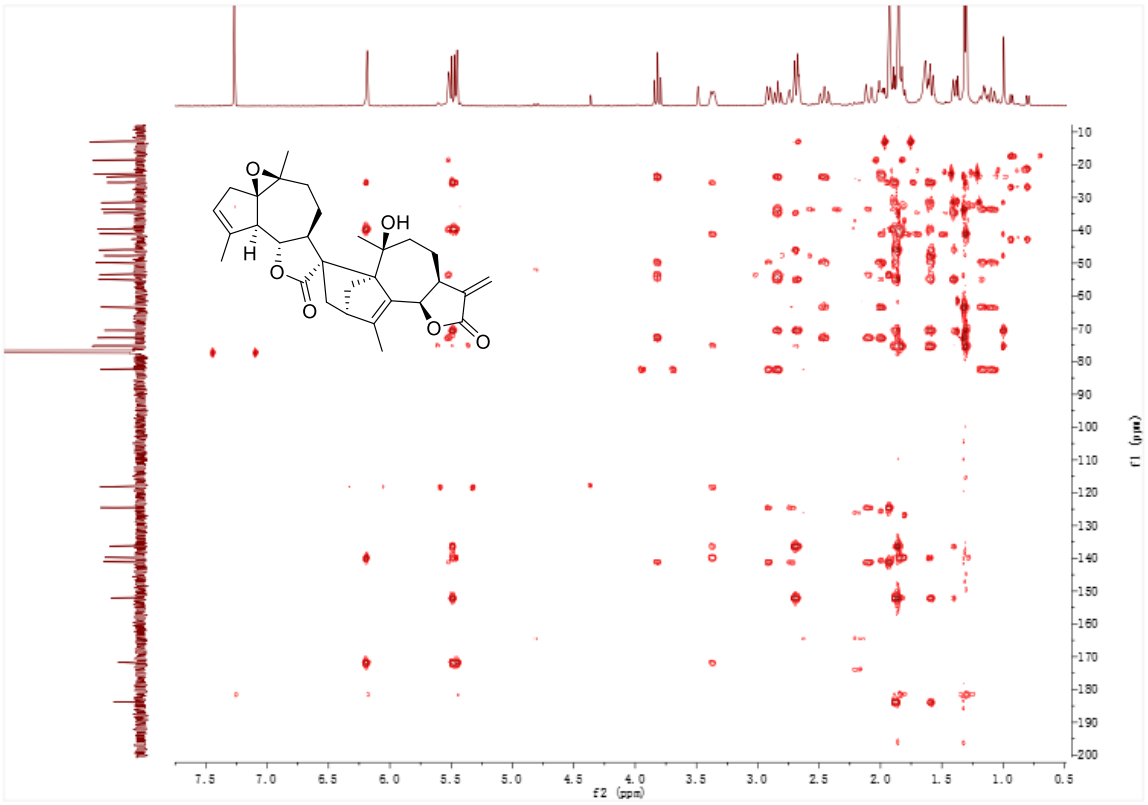


Figure S204 HMBC spectrum (600 MHz) of artematrolide Q (**21**) in $CDCl_3$.

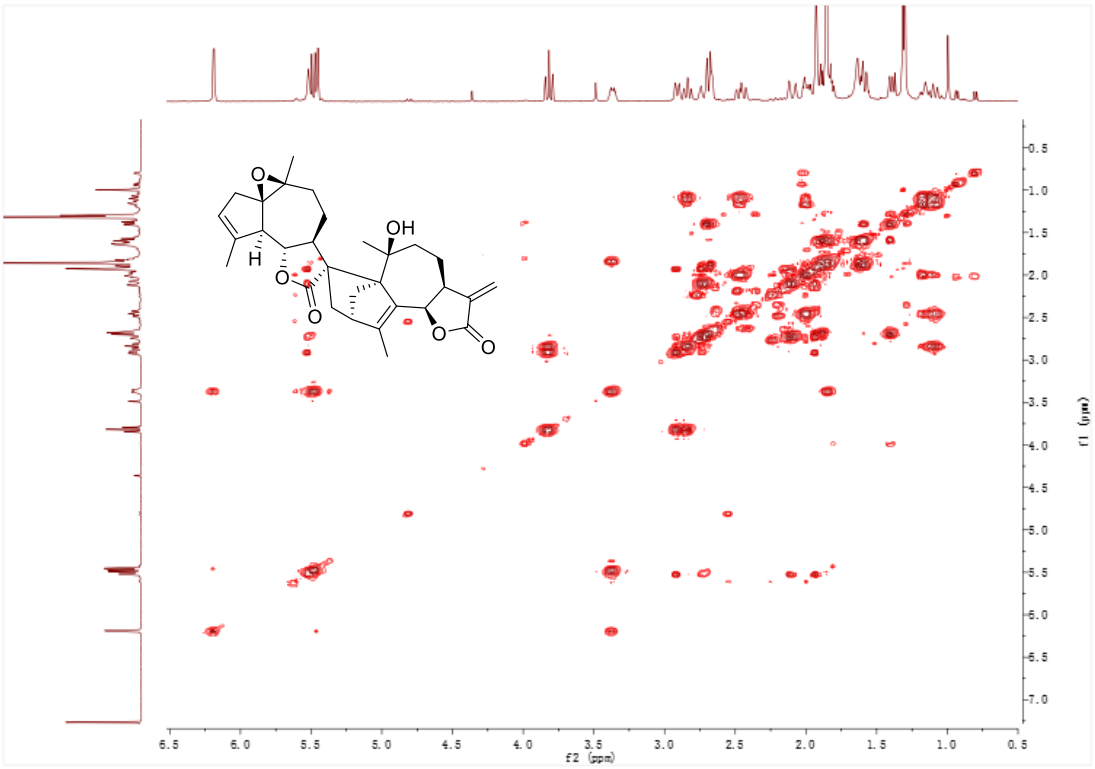


Figure S205 ^{1}H–^{1}H COSY spectrum (600 MHz) of artematrolide Q (**21**) in $CDCl_3$.

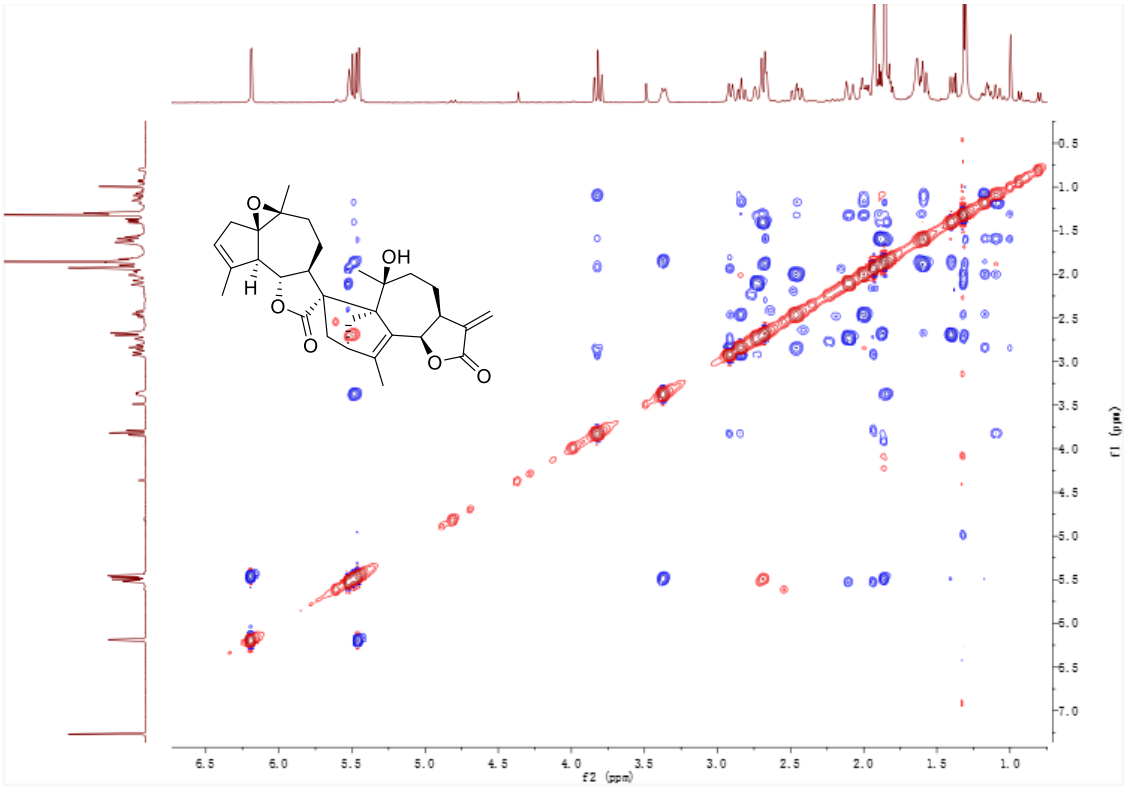


Figure S206 ROESY spectrum (600 MHz) of artematrolide Q (**21**) in $CDCl_3$.

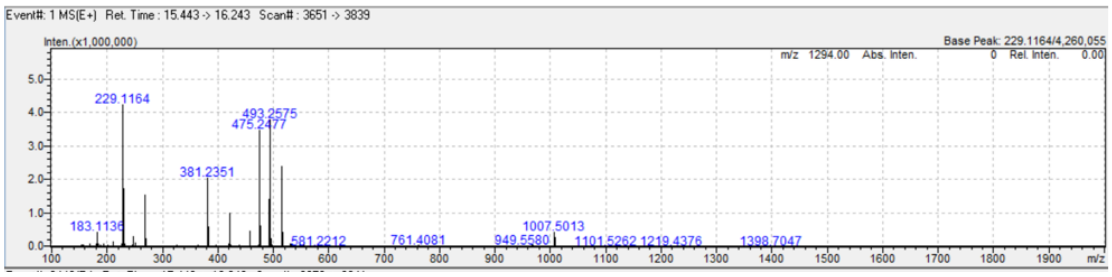


Figure S207 HRESIMS spectrum of artematrolide Q (**21**).

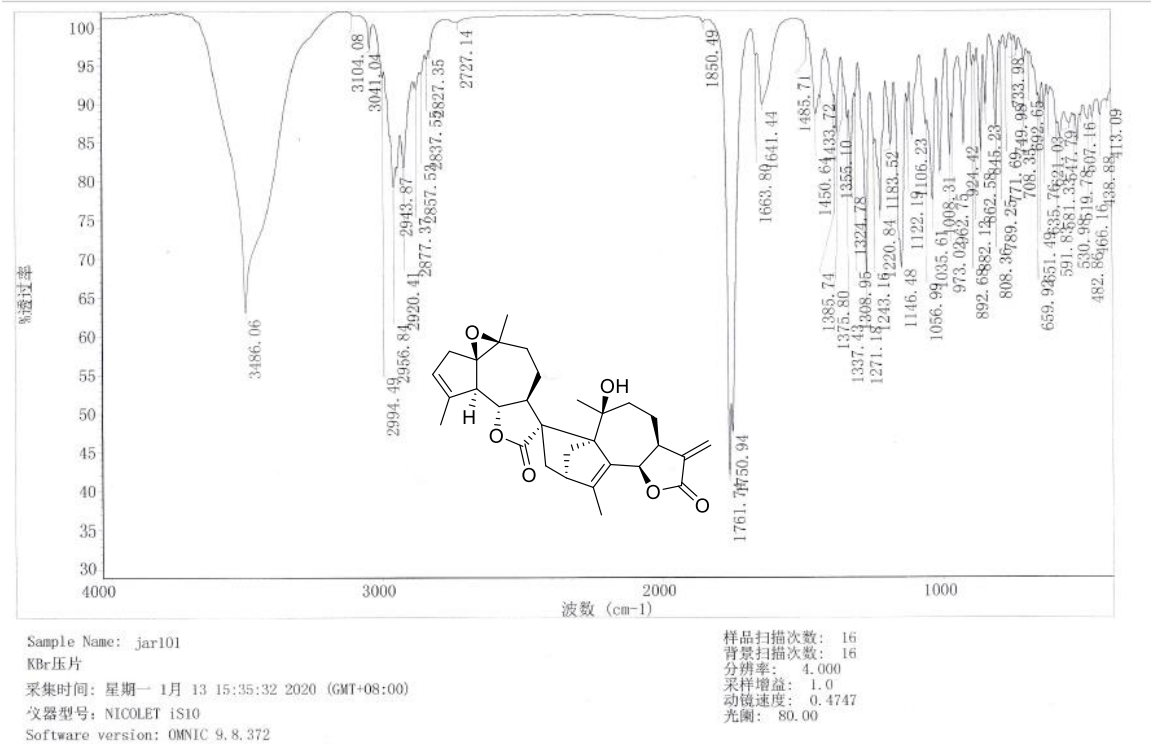
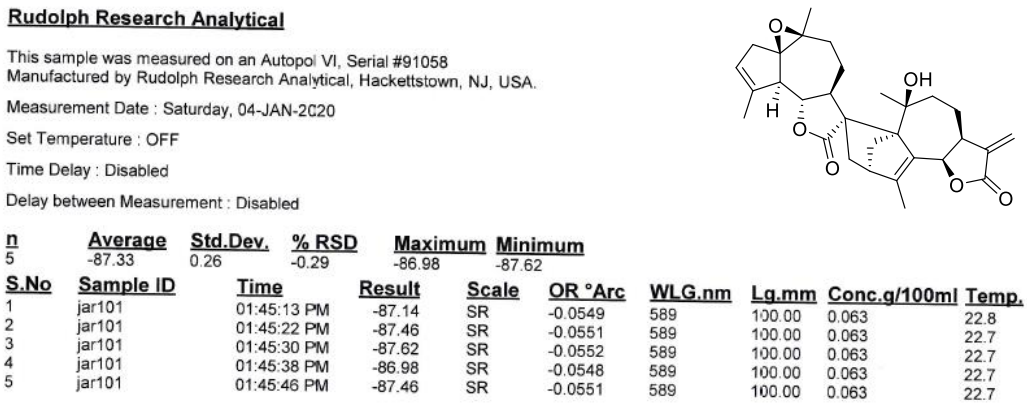


Figure S208 IR spectrum of artematrolide Q (**21**).



Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Saturday, 04-JAN-2020

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	-87.33	0.26	-0.29	-86.98	-87.62

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	jar101	01:45:13 PM	-87.14	SR	-0.0549	589	100.00	0.063	22.8
2	jar101	01:45:22 PM	-87.46	SR	-0.0551	589	100.00	0.063	22.7
3	jar101	01:45:30 PM	-87.62	SR	-0.0552	589	100.00	0.063	22.7
4	jar101	01:45:38 PM	-86.98	SR	-0.0548	589	100.00	0.063	22.7
5	jar101	01:45:46 PM	-87.46	SR	-0.0551	589	100.00	0.063	22.7

Figure S209 Optical rotation spectrum of artematrolide Q (**21**).

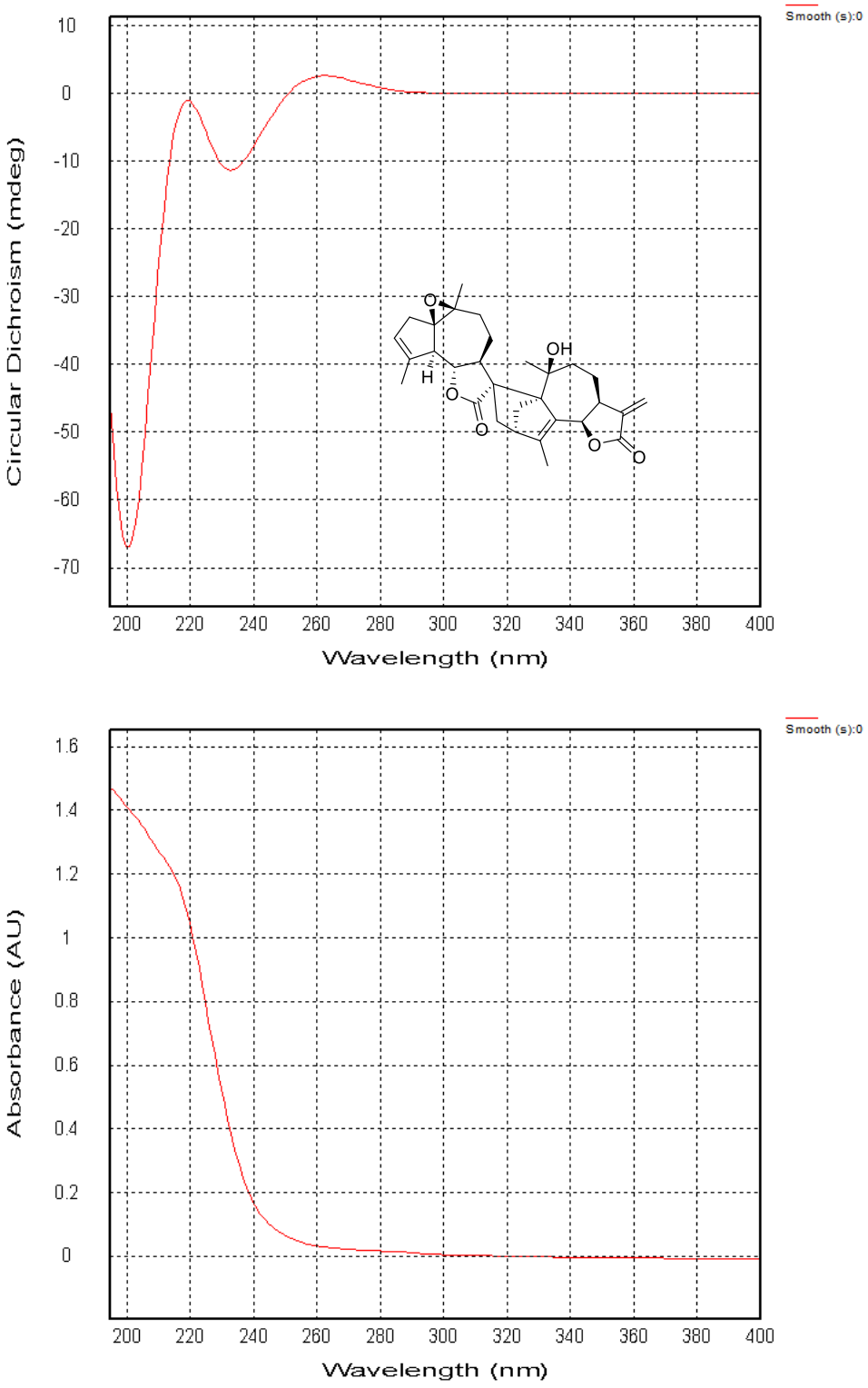


Figure S210 CD (top) and UV (bottom) spectra of artematrolide Q (**21**).

23. NMR, MS, IR, $[\alpha]_D$ and CD spectra of compound 22

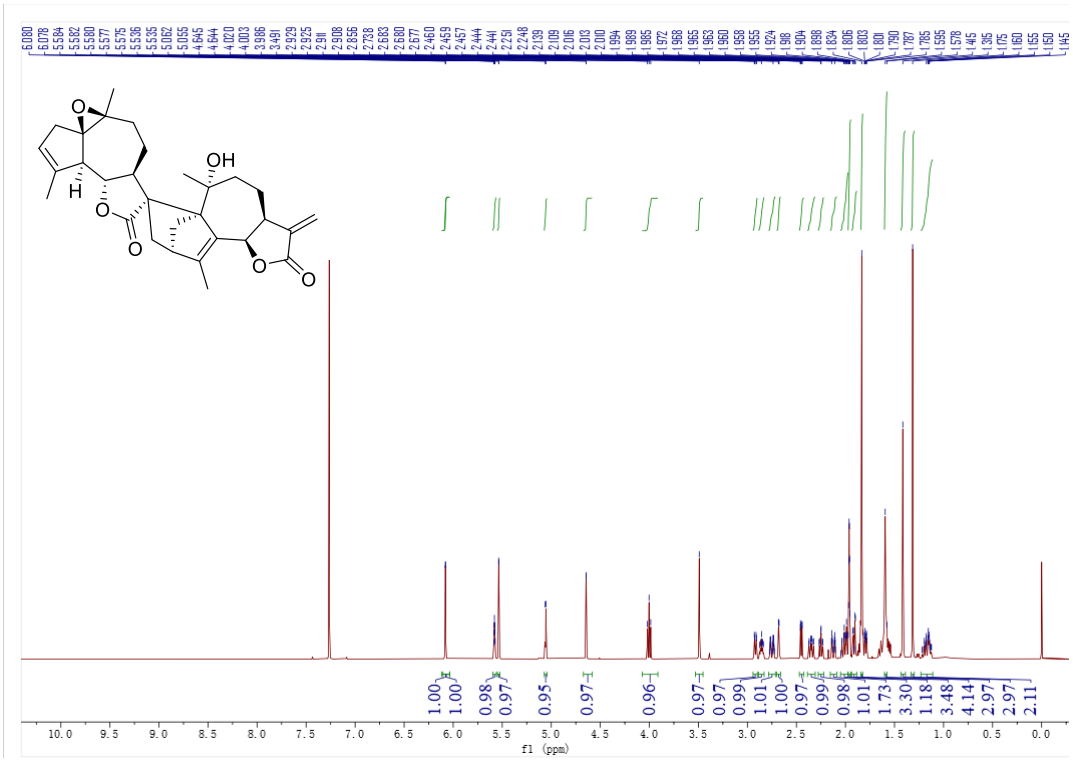


Figure S211 ^{1}H spectrum (600 MHz) of artematrolide R (**22**) in $CDCl_3$.

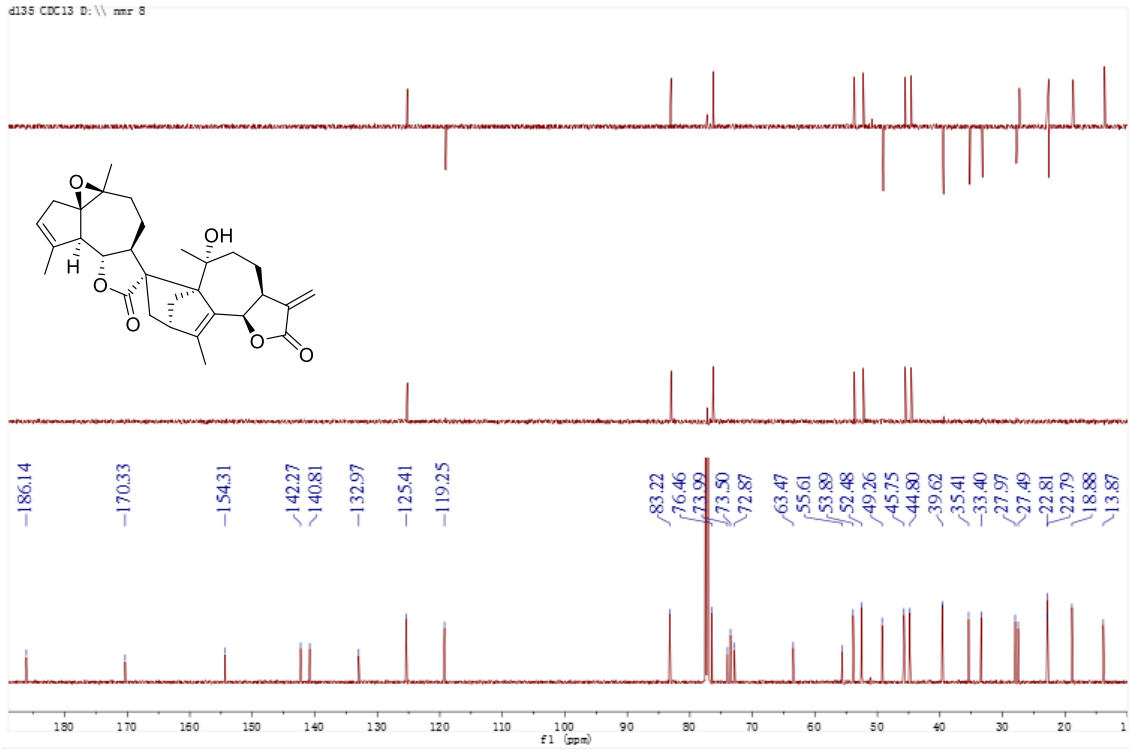


Figure S212 ^{13}C NMR spectrum (150 MHz) of artematrolide R (**22**) in $CDCl_3$.

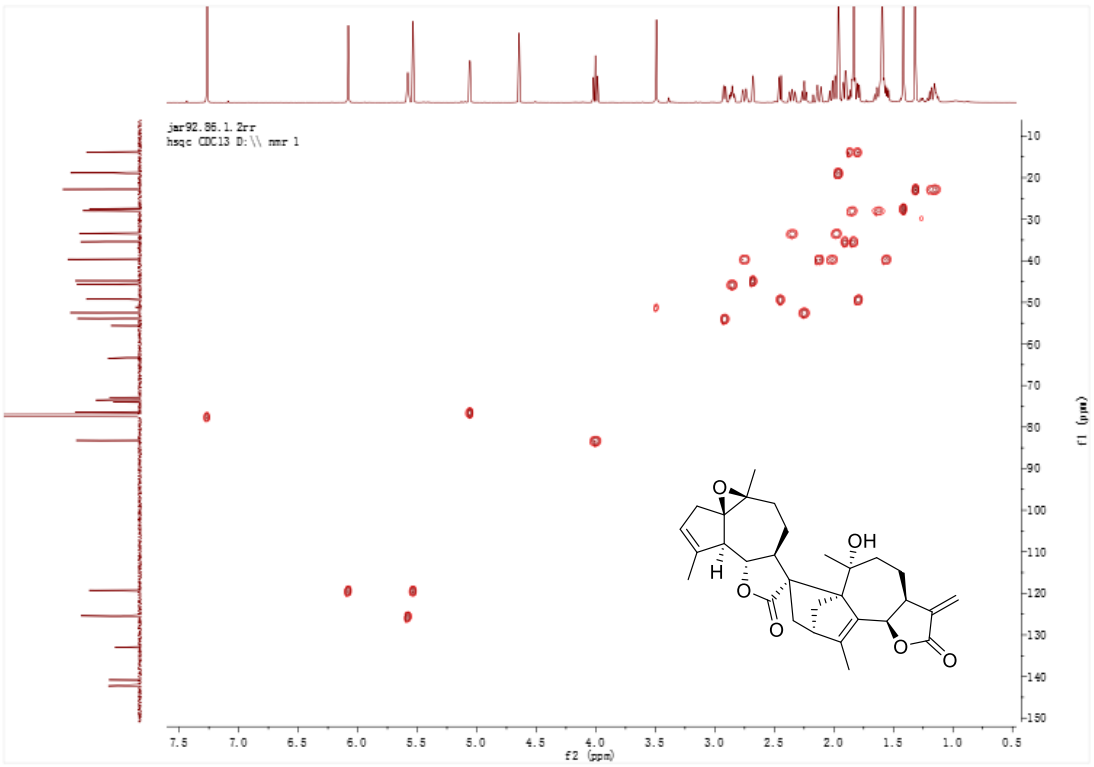


Figure S213 HSQC spectrum (600 MHz) of artematrolide R (**22**) in $CDCl_3$.

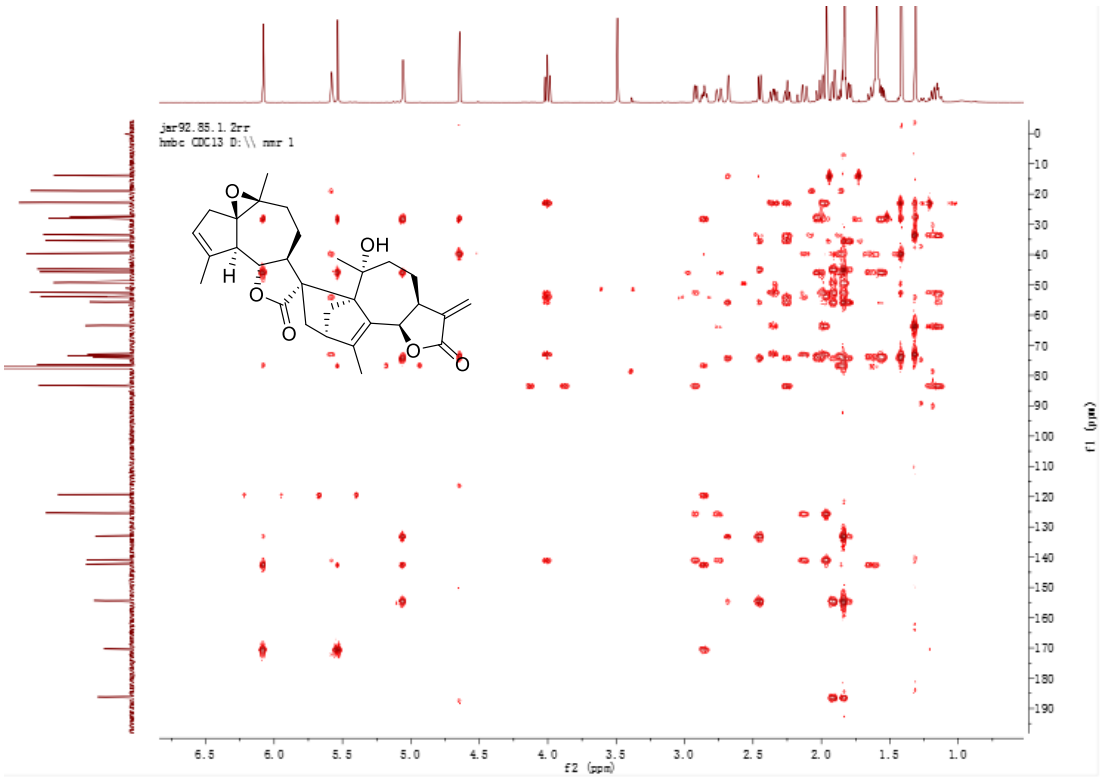


Figure S214 HMBC spectrum (600 MHz) of artematrolide R (**22**) in $CDCl_3$.

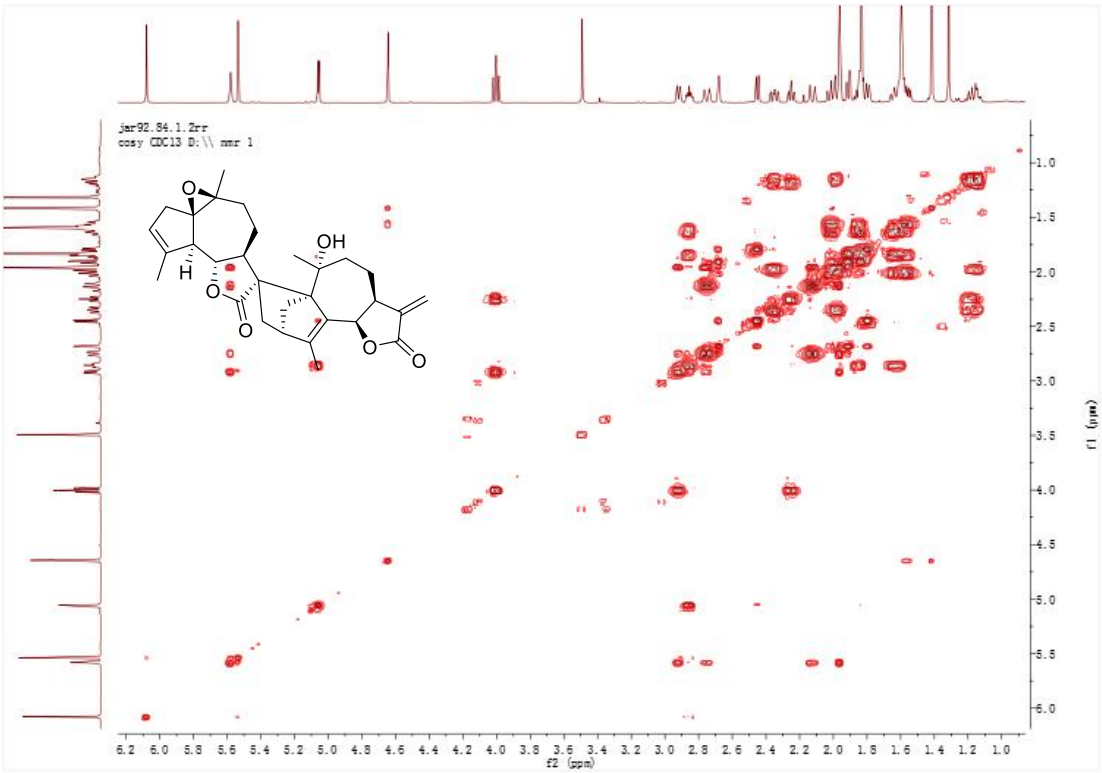


Figure S215 ^{1}H–^{1}H COSY spectrum (600 MHz) of artematrolide R (**22**) in $CDCl_3$.

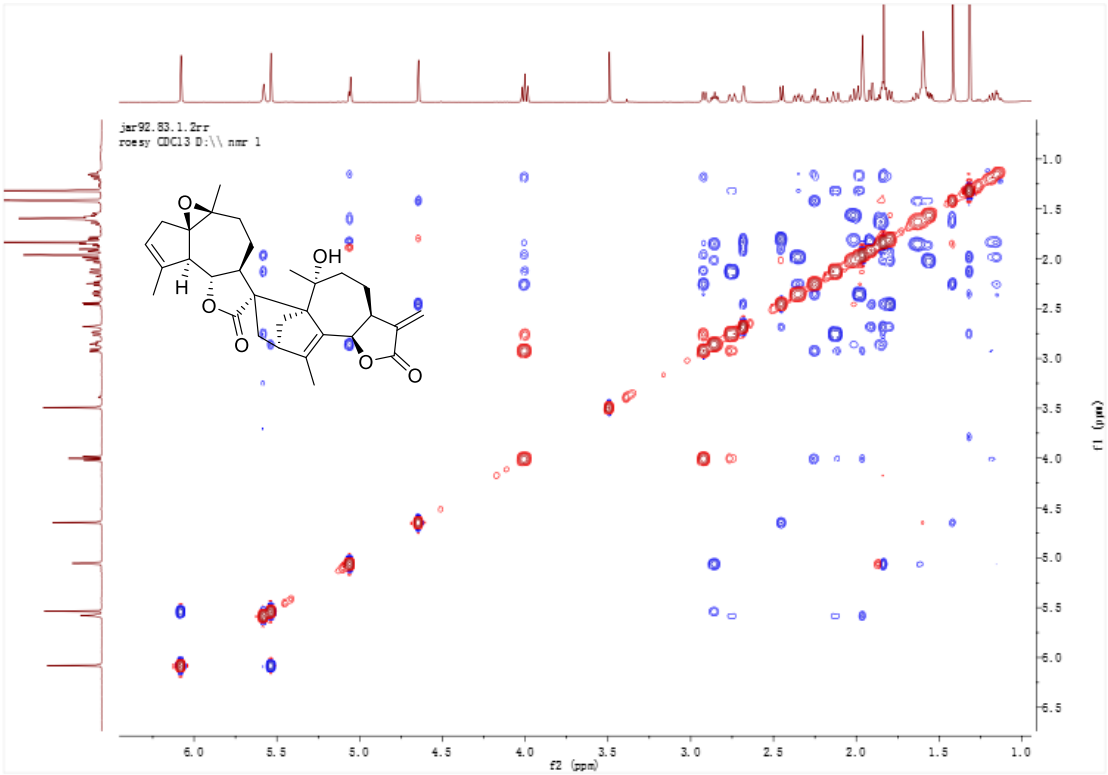


Figure S216 ROESY spectrum (600 MHz) of artematrolide R (**22**) in $CDCl_3$.

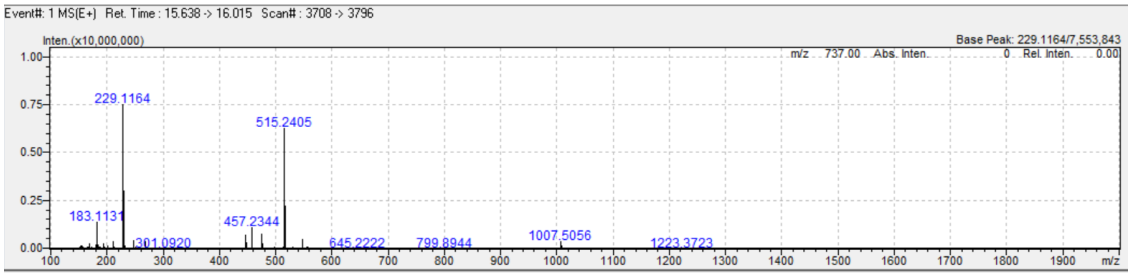


Figure S217 HRESIMS spectrum of artematrolide R (**22**).

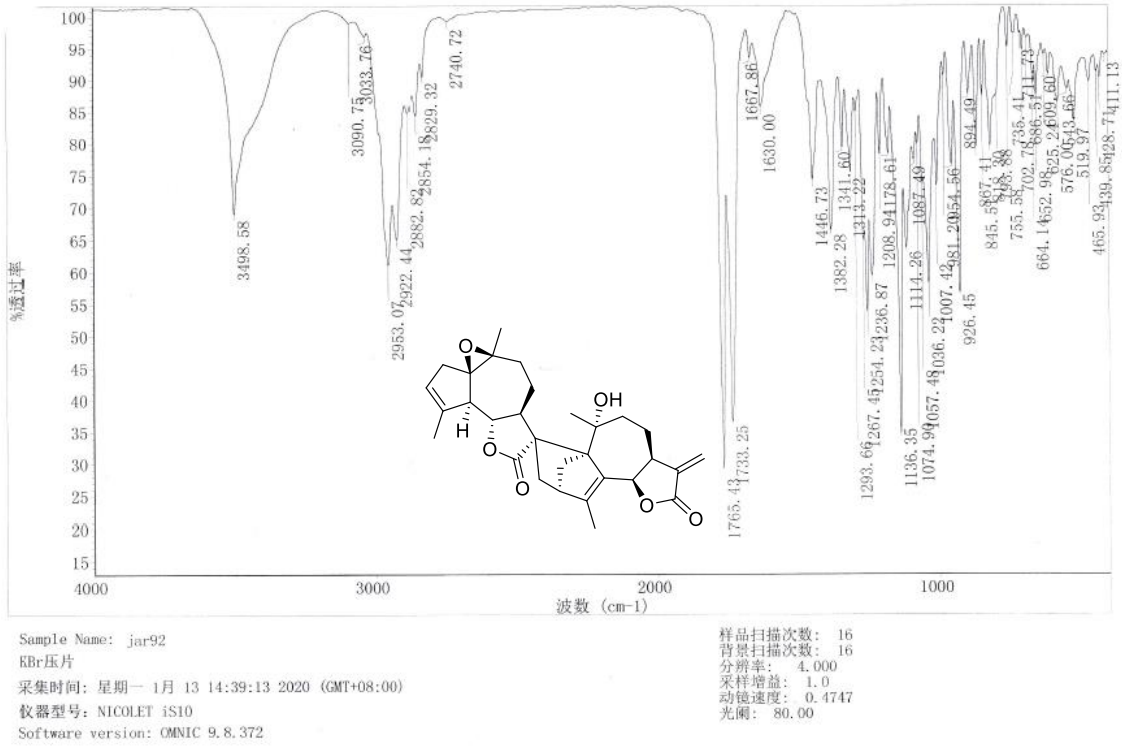


Figure S218 IR spectrum of artematrolide R (**22**).

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Saturday, 04-JAN-2020

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	17.90	0.23	1.28	18.31	17.80

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	jar92	01:07:47 PM	17.80	SR	0.0105	589	100.00	0.059	22.2
2	jar92	01:07:56 PM	18.31	SR	0.0108	589	100.00	0.059	22.2
3	jar92	01:08:03 PM	17.80	SR	0.0105	589	100.00	0.059	22.2
4	jar92	01:08:12 PM	17.80	SR	0.0105	589	100.00	0.059	22.2
5	jar92	01:08:19 PM	17.80	SR	0.0105	589	100.00	0.059	22.2

Figure S219 Optical rotation spectrum of artematrolide R (**22**).

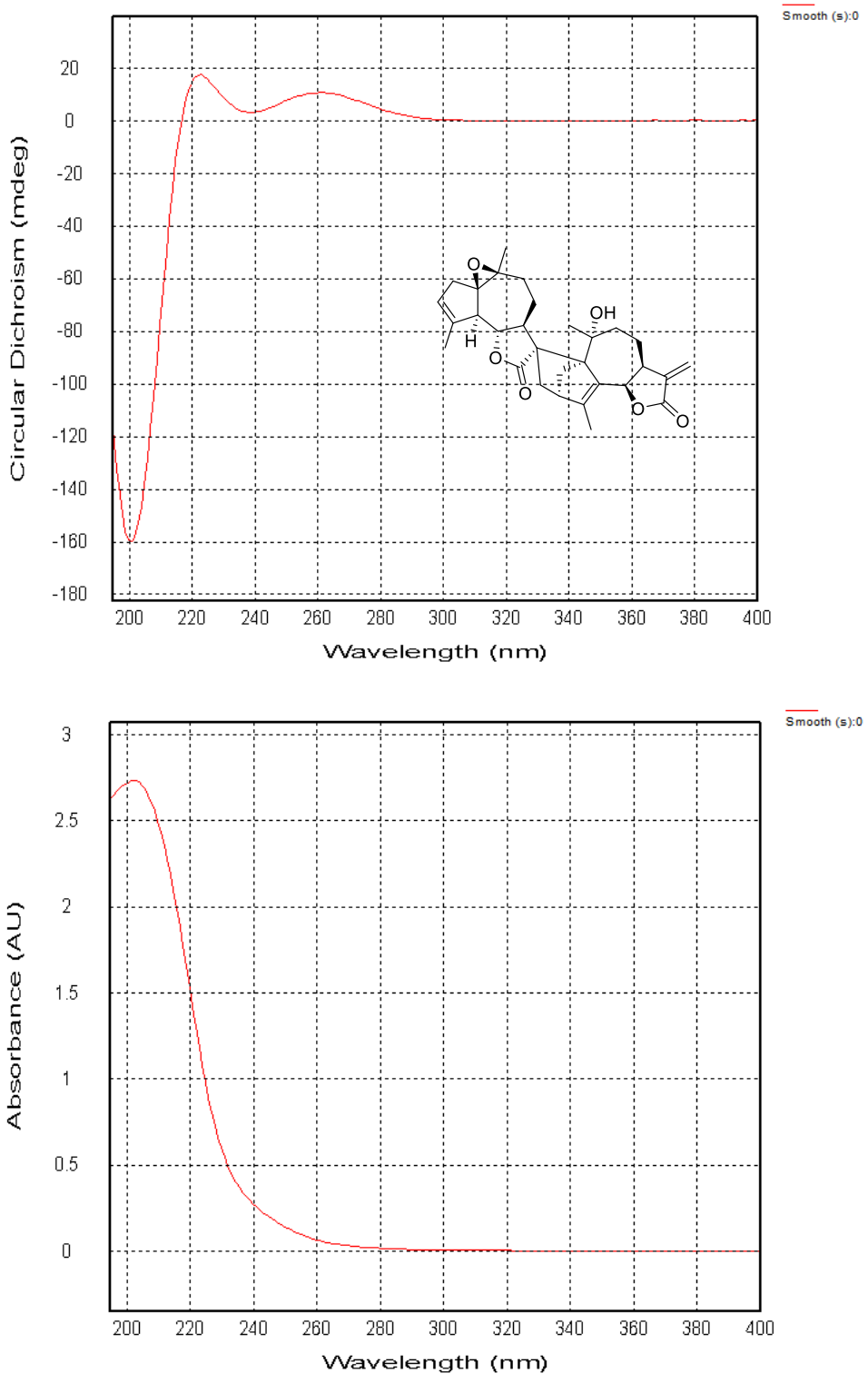


Figure S220 CD (top) and UV (bottom) spectra of artematrolide R (**22**).

24. NMR, MS, IR, $[\alpha]_D$ and CD spectra of compound 23

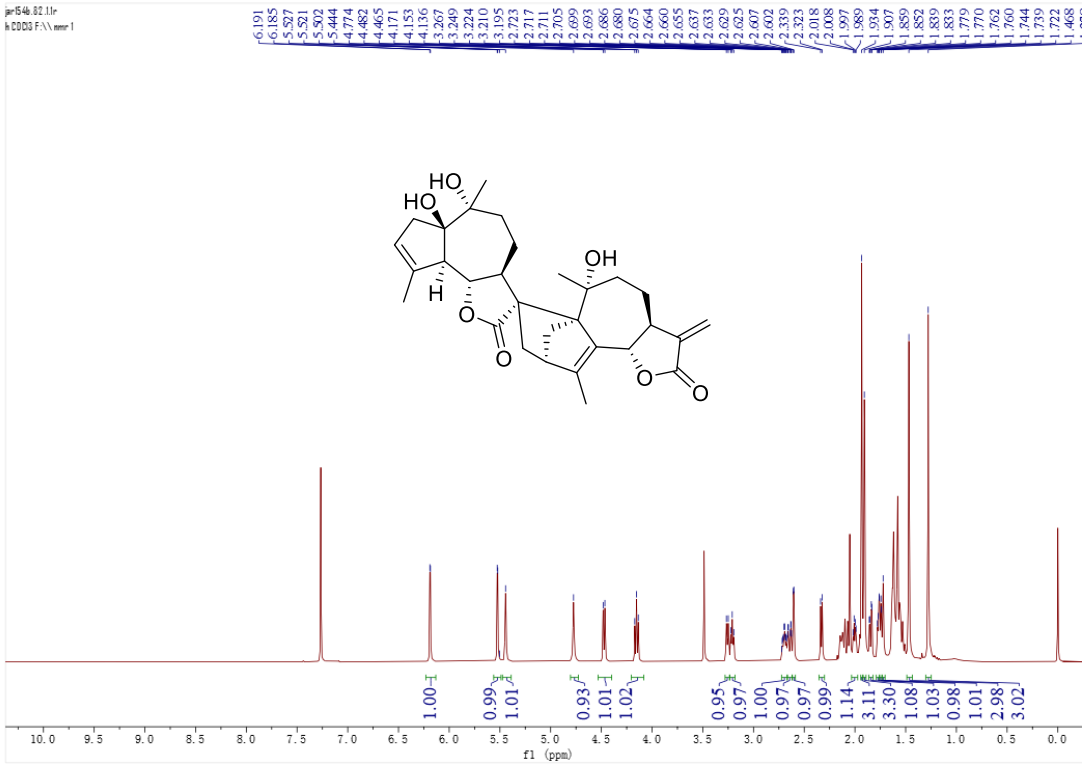


Figure S221 ^{1}H NMR spectrum (600 MHz) of lavandiolide C (**23**) in $CDCl_3$.

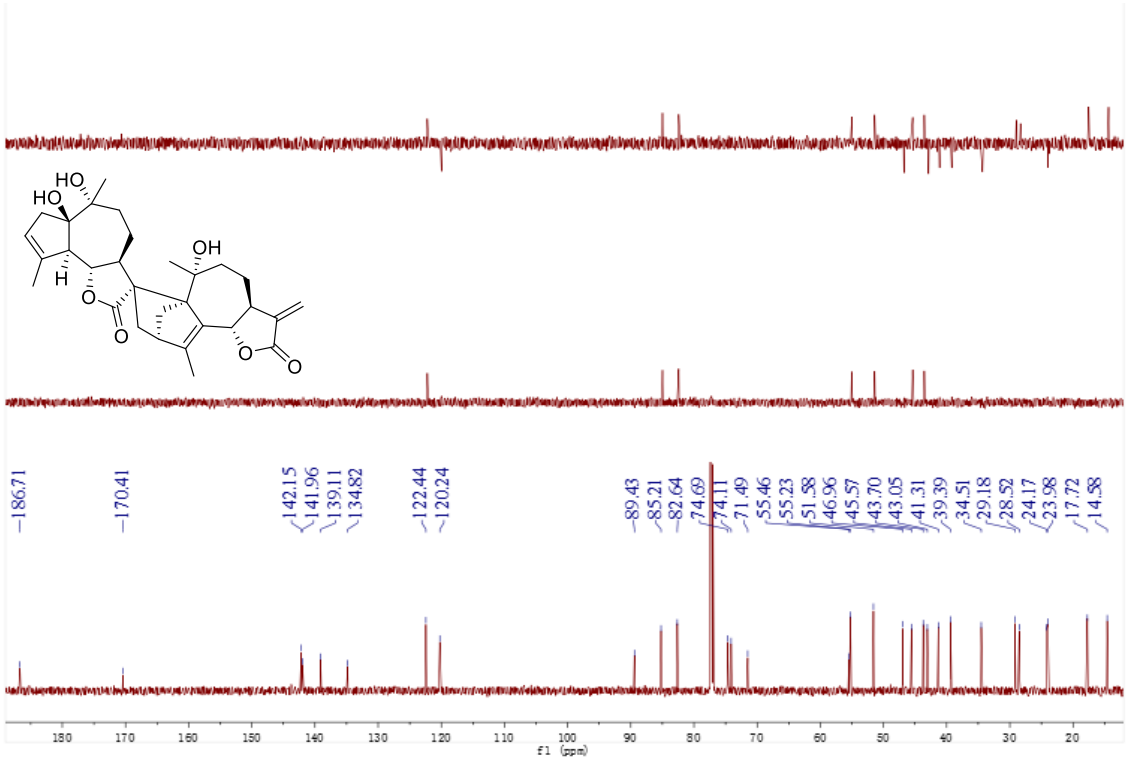


Figure S222 ^{13}C NMR spectrum (150 MHz) of lavandiolide C (**23**) in $CDCl_3$.

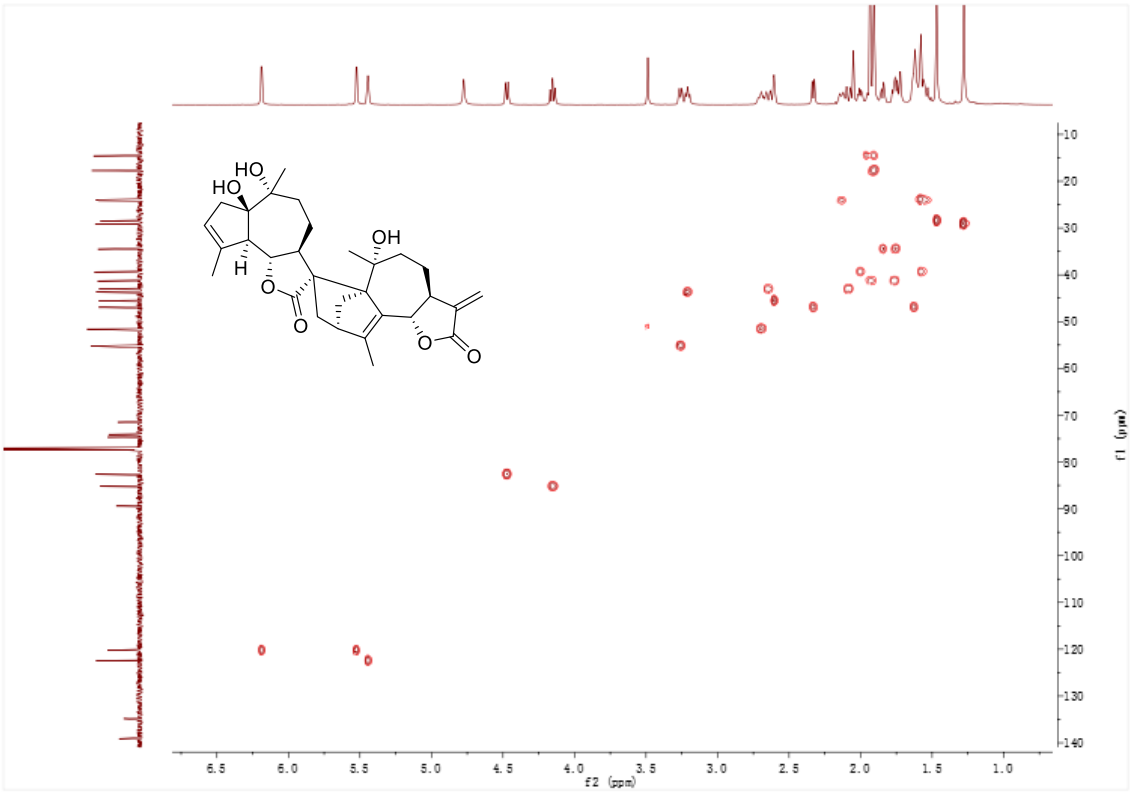


Figure S223 HSQC spectrum (600 MHz) of lavandiolide C (**23**) in $CDCl_3$.

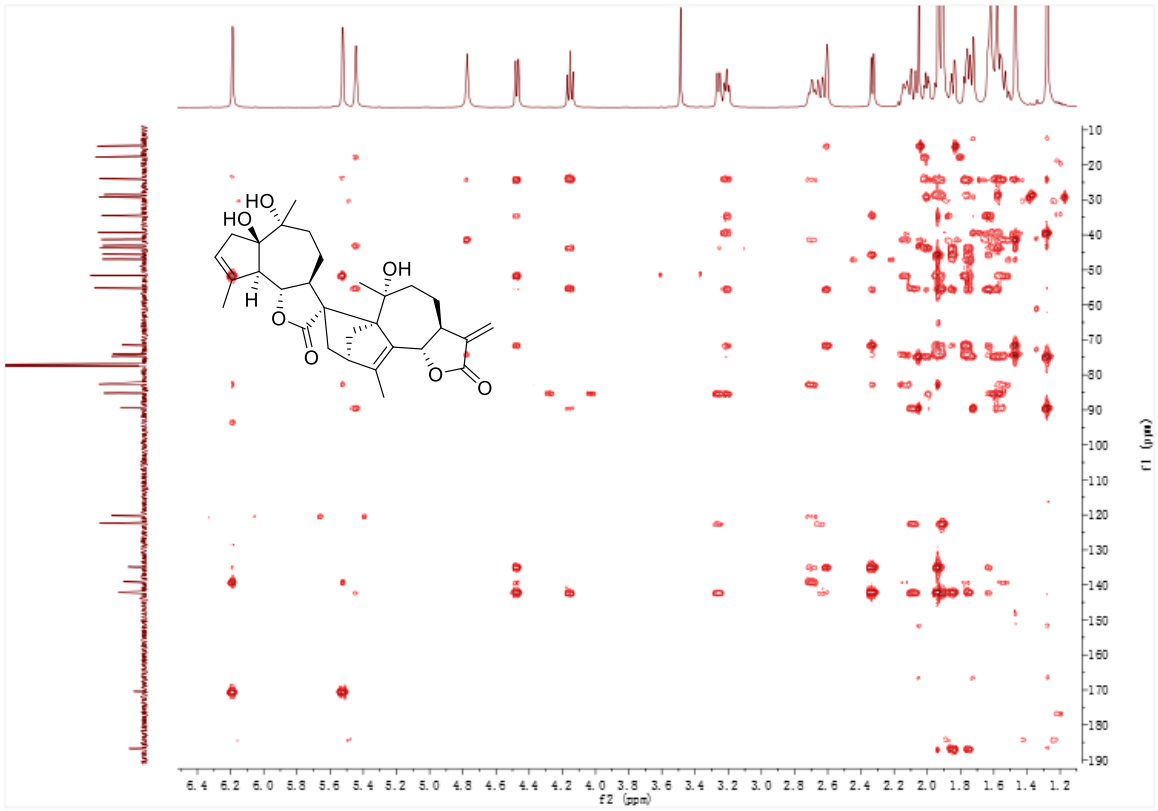


Figure S224 HMBC spectrum (600 MHz) of lavandiolide C (**23**) in $CDCl_3$.

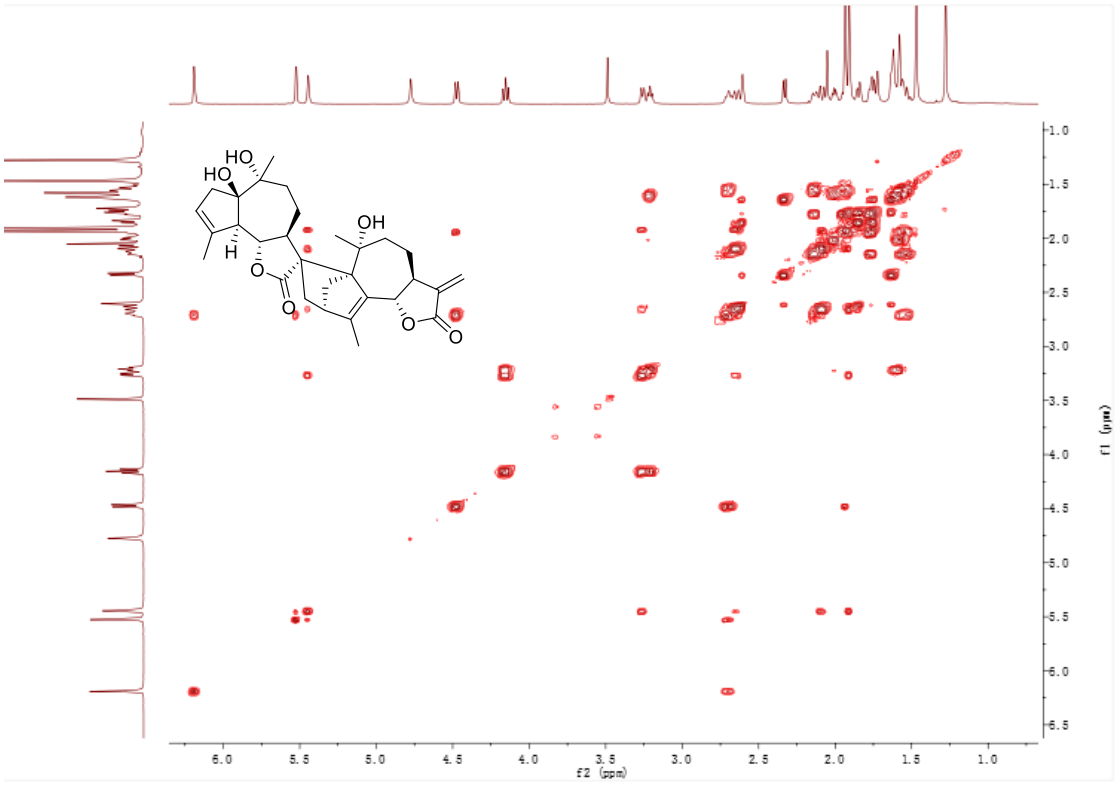


Figure S225 ^{1}H–^{1}H COSY spectrum (600 MHz) of lavandiolide C (**23**) in $CDCl_3$.

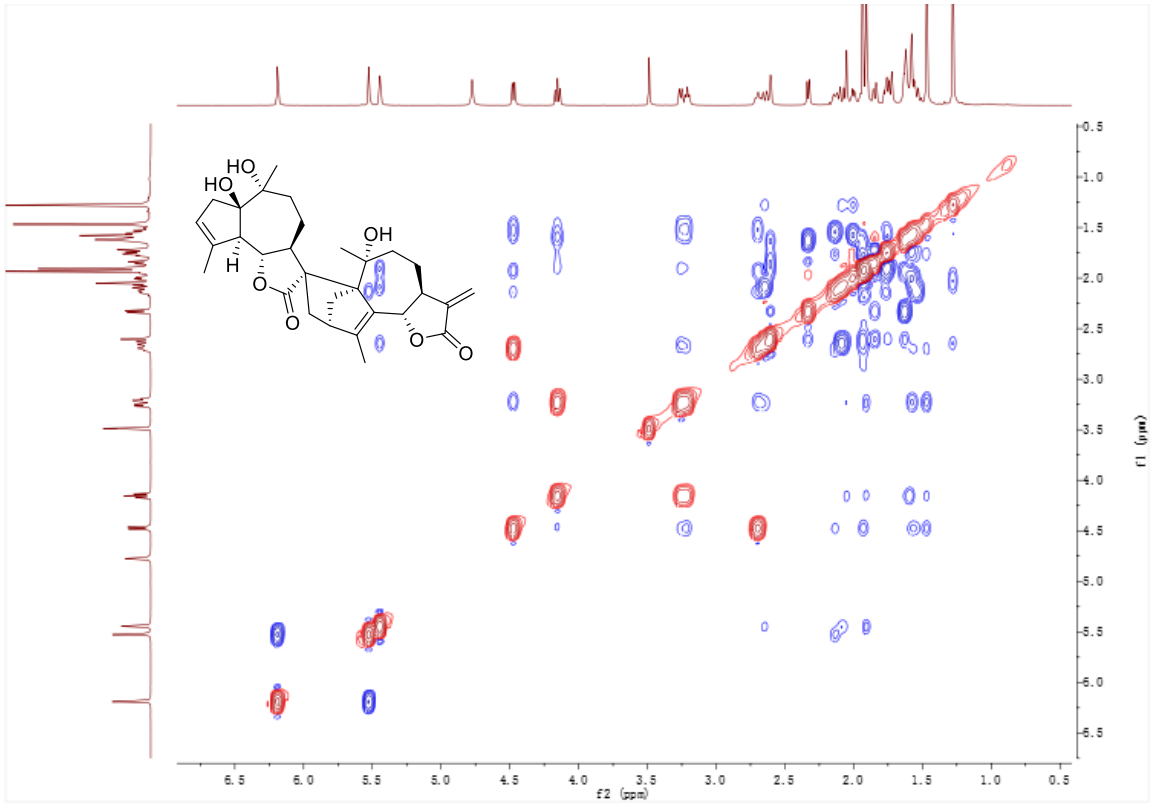


Figure S226 ROESY spectrum (600 MHz) of lavandiolide C (**23**) in $CDCl_3$.

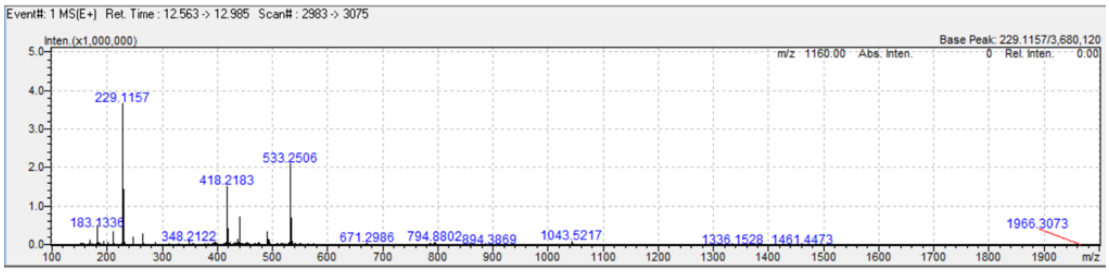


Figure S227 HRESIMS spectrum of lavandiolide C (**23**).

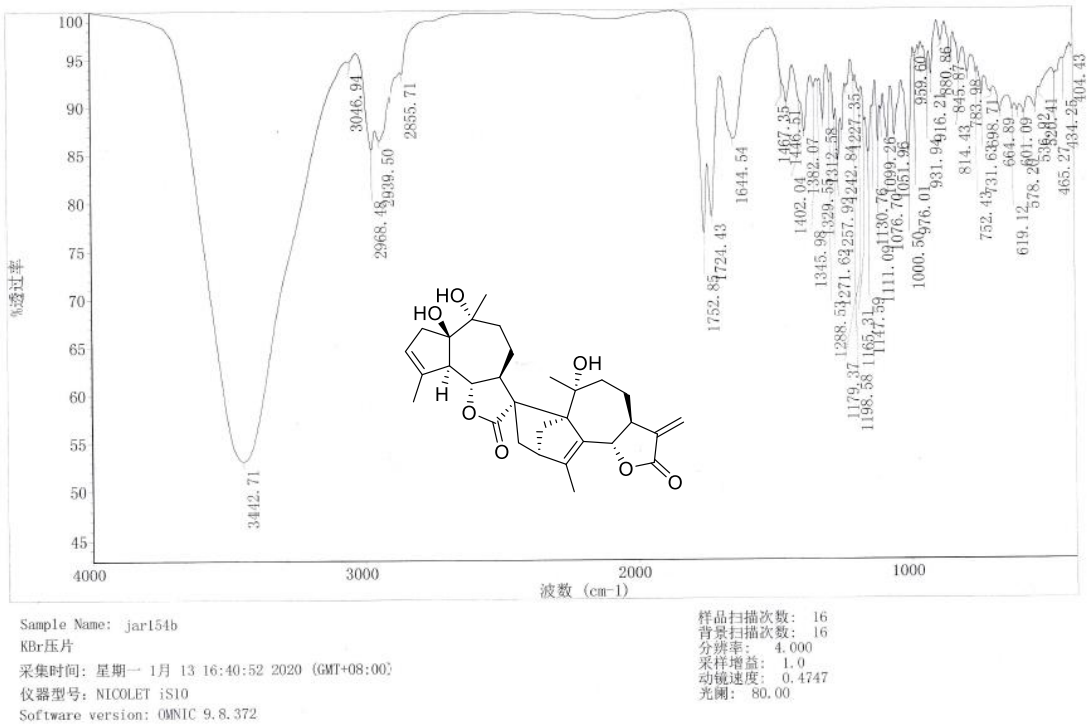


Figure S228 IR spectrum of lavandiolide C (**23**).

Rudolph Research Analytical

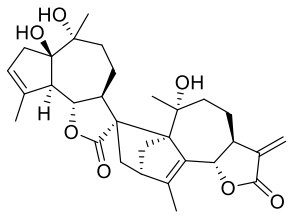
This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Monday, 13-JAN-2020

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled



n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	102.27	0.15	0.14	102.43	102.16

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	JAR154B	02:53:44 PM	102.16	SR	0.0378	589	100.00	0.037	21.2
2	JAR154B	02:53:52 PM	102.16	SR	0.0378	589	100.00	0.037	21.2
3	JAR154B	02:54:00 PM	102.16	SR	0.0378	589	100.00	0.037	21.2
4	JAR154B	02:54:09 PM	102.43	SR	0.0379	589	100.00	0.037	21.2
5	JAR154B	02:54:16 PM	102.43	SR	0.0379	589	100.00	0.037	21.2

Figure S229 Optical rotation spectrum of lavandiolide C (**23**).

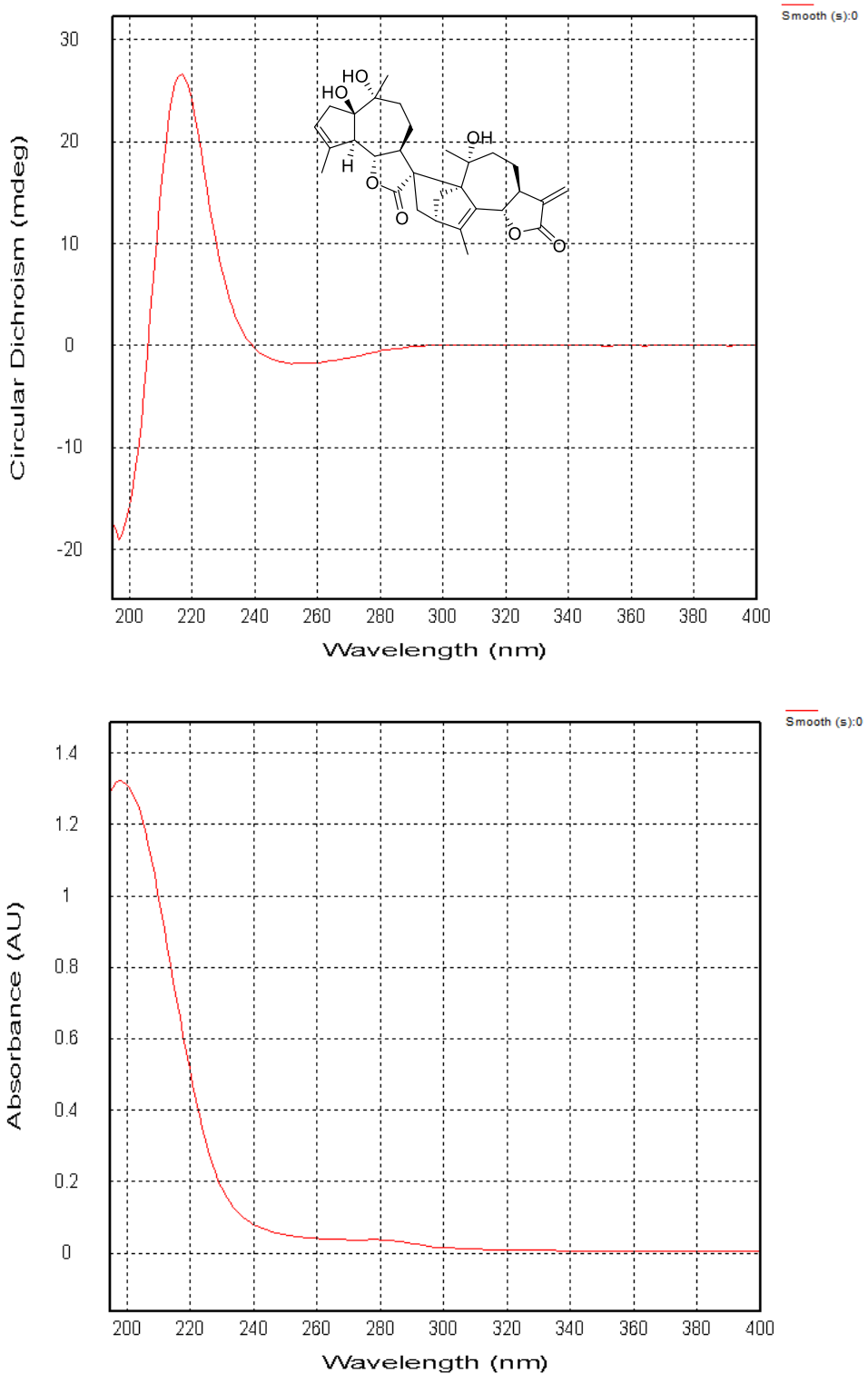


Figure S230 CD (top) and UV (bottom) spectra of lavandiolide C (**23**).

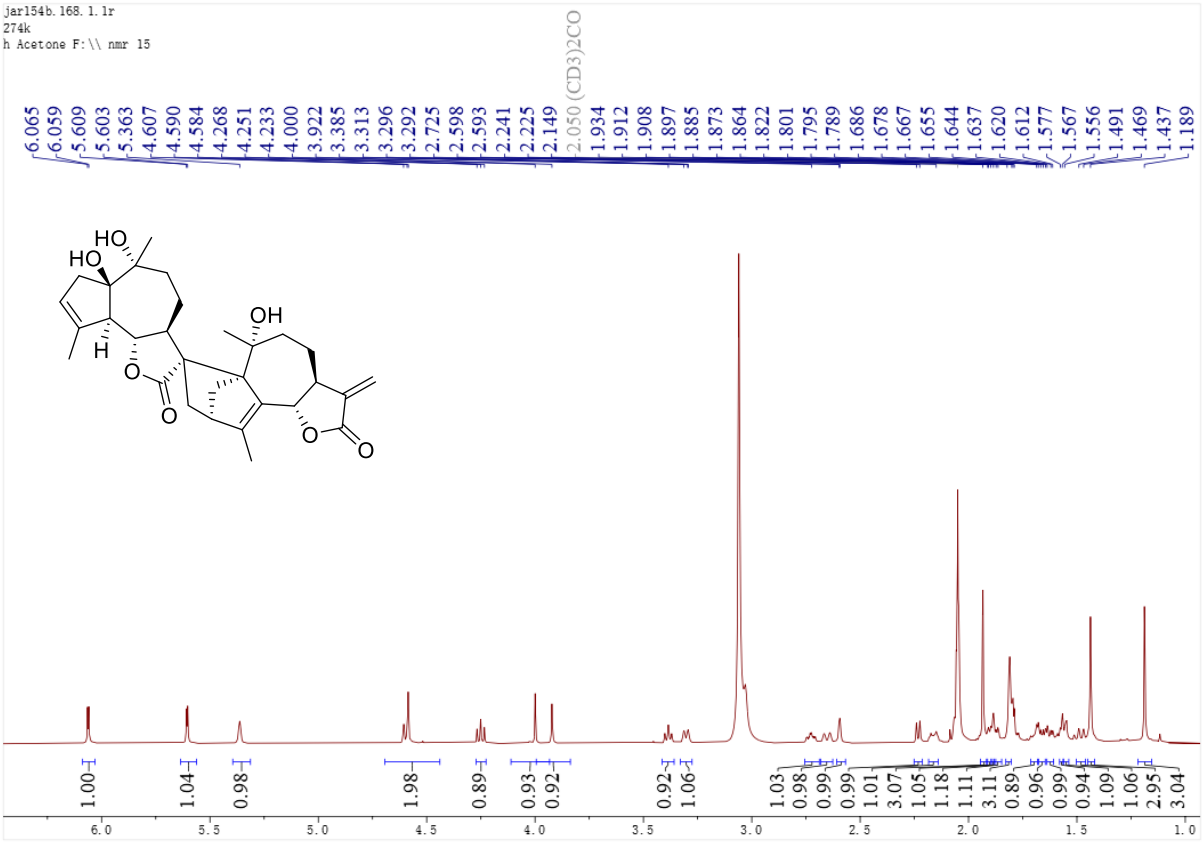


Figure S231 ^{1}H NMR spectrum (600 MHz) of lavandiolide C (**23**) in acetone-d_6.

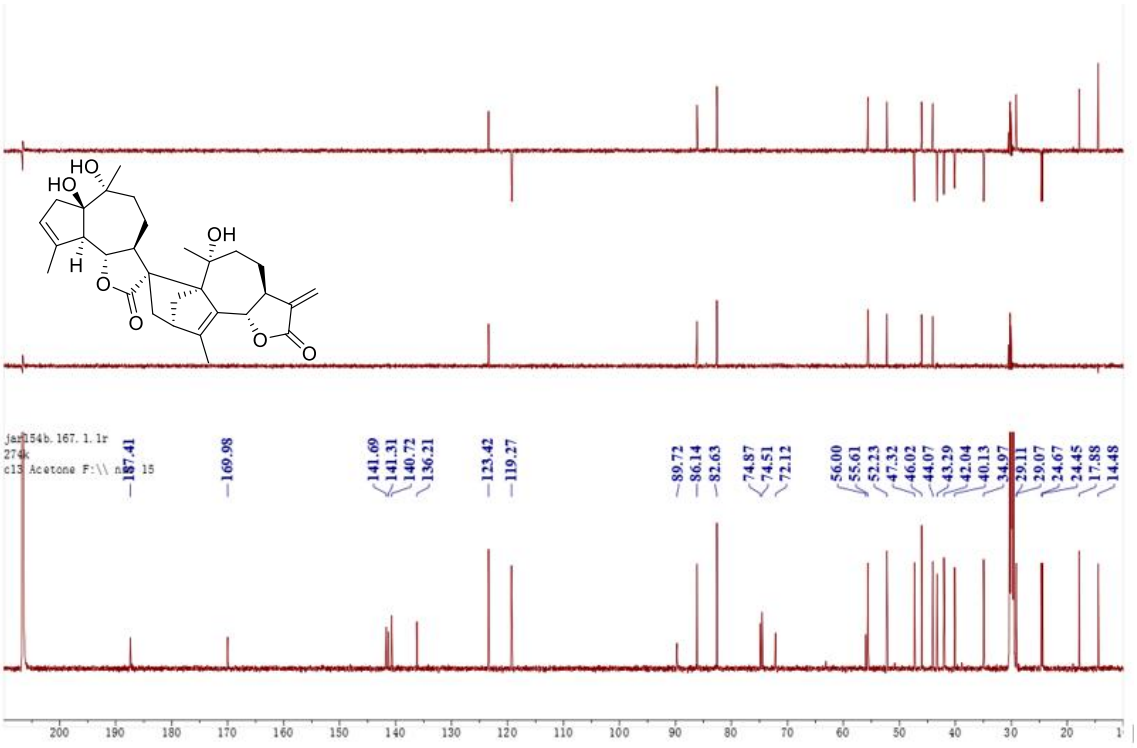


Figure S232 ^{13}C NMR spectrum (150 MHz) of lavandiolide C (**23**) in acetone-d_6.

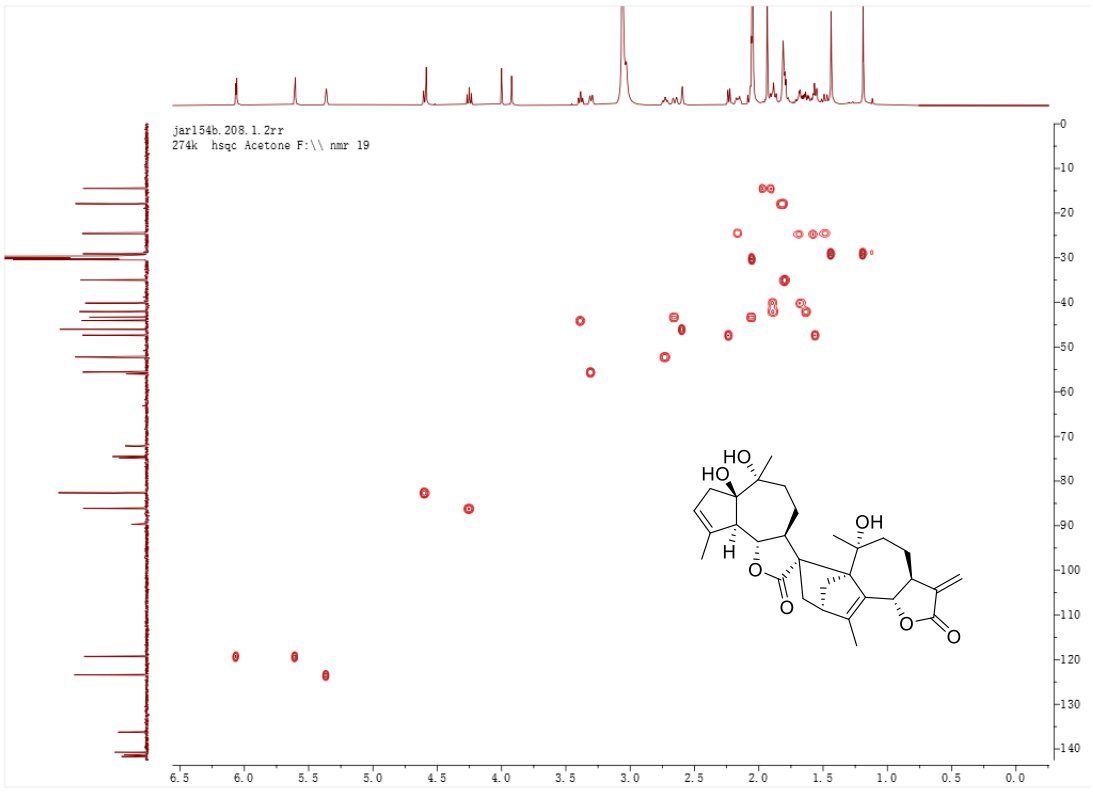


Figure S233 HSQC spectrum (600 MHz) of lavandiolide C (**23**) in acetone-d_6.

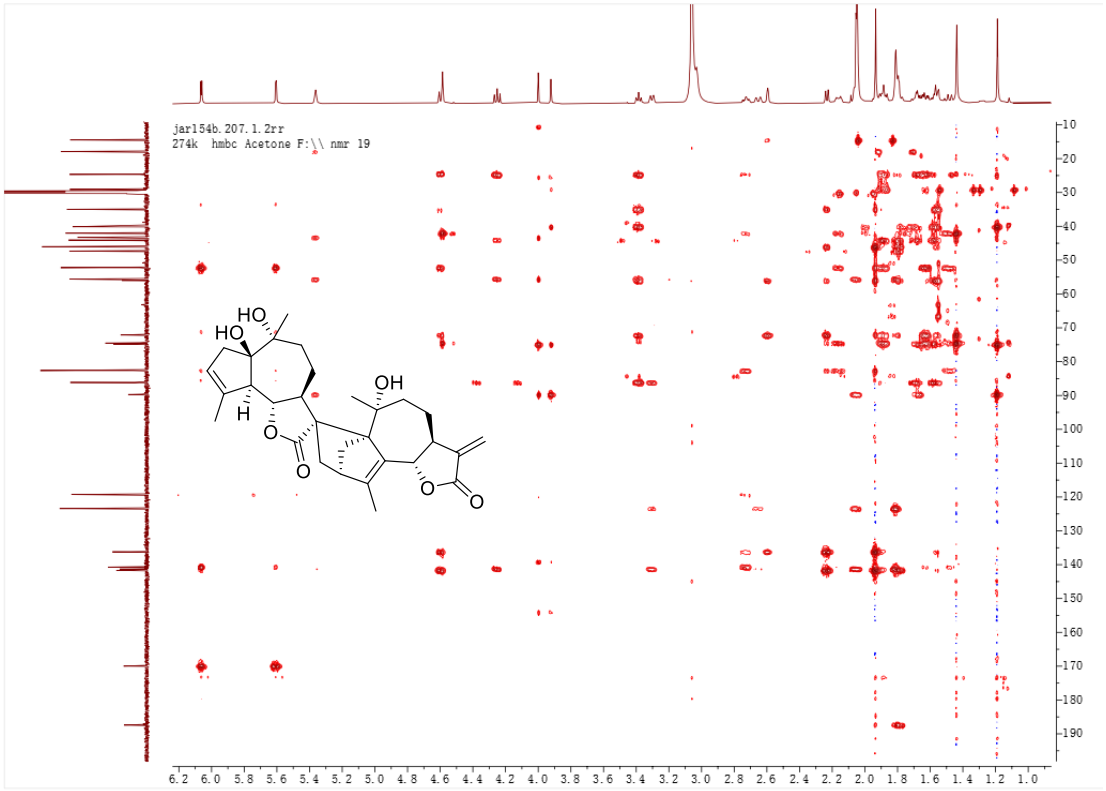


Figure S234 HMBC spectrum (600 MHz) of lavandiolide C (**23**) in acetone-d_6.

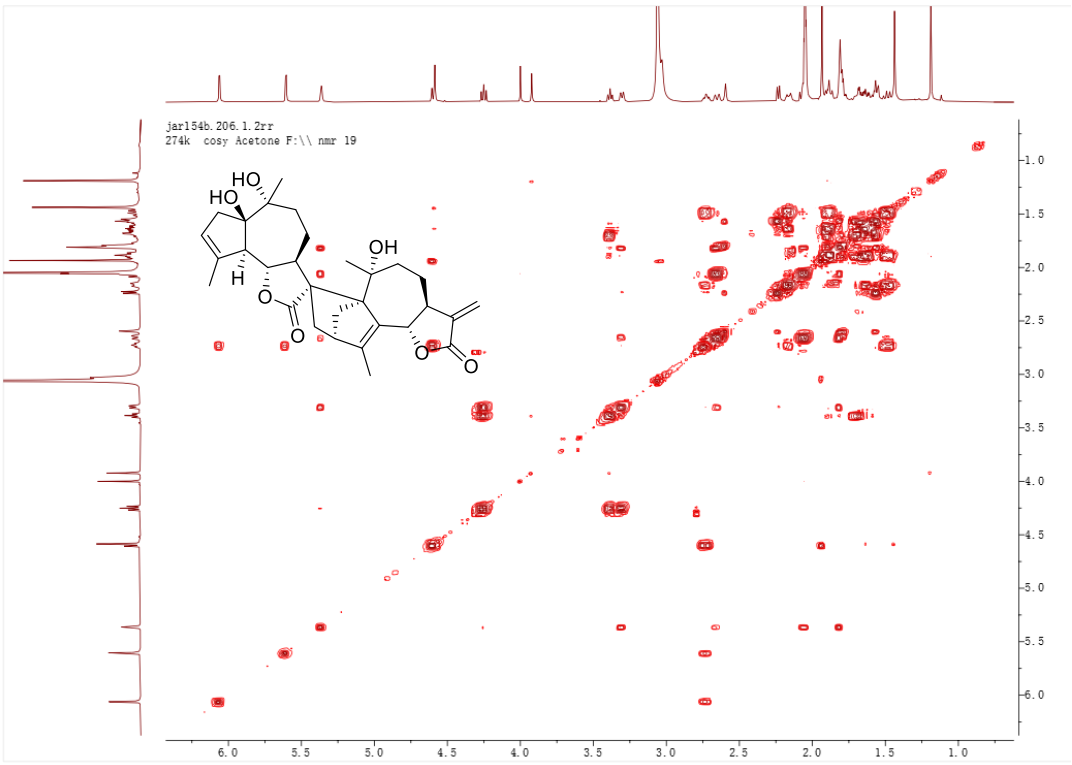


Figure S235 ^{1}H–^{1}H COSY spectrum (600 MHz) of lavandiolide C (**23**) in acetone-d_6.

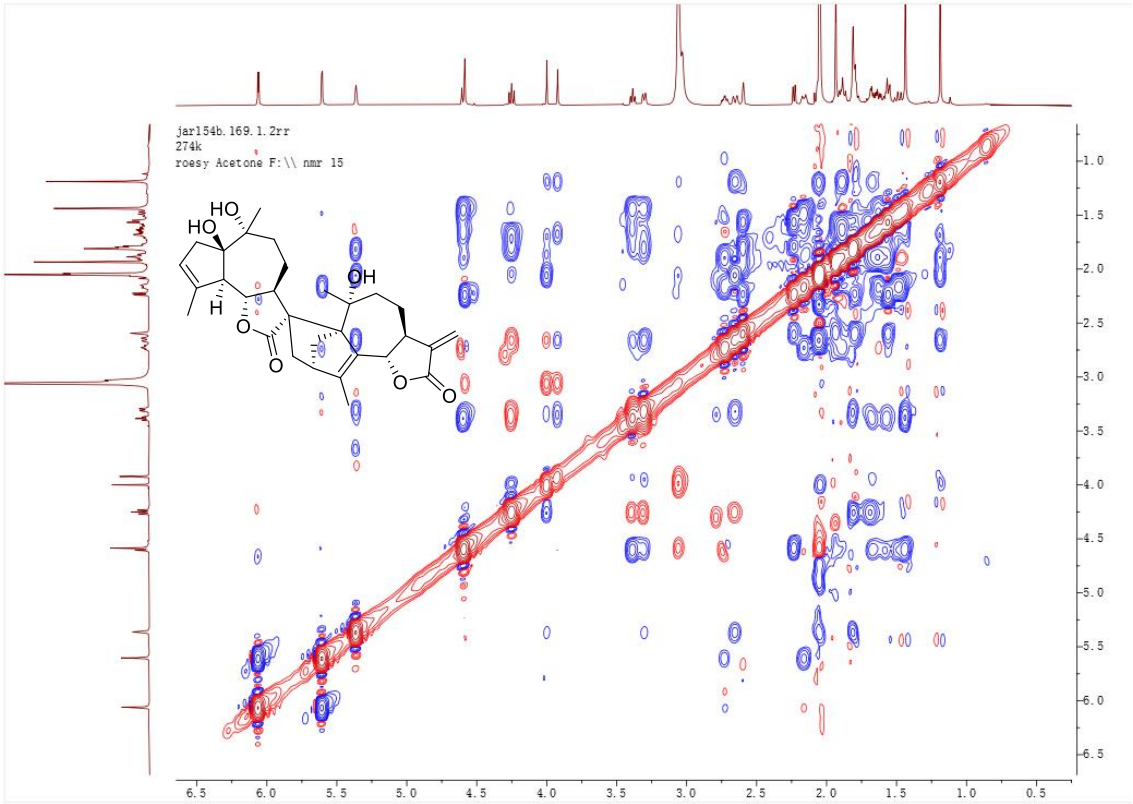


Figure S236 ROESY spectrum (600 MHz) of lavandiolide C (**23**) in acetone-d_6.

25. Cytotoxicity assays

24.1. Cell lines and cell culture

HepG2 cell line was obtained as a gift from Service Center for Bioactivity Screening (Kunming Institute of Botany, Chinese Academy of Sciences, Kunming, China). SMMC-7721 and Huh7 cell lines were purchased from the Shanghai Jining Biotechnology Co., Ltd. (Shanghai, China). HepG2 and Huh7 cells were cultured in Dulbecco′s Modified Eagle′s Medium (DMEM; Gibco, Thermo Fisher Scientific Co., Ltd., Suzhou, China) supplemented with 10% heat-inactivated fetal bovine serum (FBS; Gibco, Life Technologies, NY, USA). While the SMMC-7721 cells were cultured in RPMI-1640 (Gibco, Thermo Fisher Biochemical Products Co., Ltd., Beijing, China) with 10% heat-inactivated fetal bovine serum (FBS), at 37 °C in an atmosphere of 5% CO_2, 95% air and > 95% humidity.

24.2. MTT assay

The cytotoxicity of the compounds **1**–**23** was tested by the MTT assay[1–4]. Briefly, cells in a density of 3×10^4 cells/well were seeded into 96-well plates and incubated at 37 °C with 5% CO_2 for 24 h. The culture medium was replaced with fresh medium containing different concentrations of guaianolide dimers, and cells were incubated for additional 48 h. After removal of the medium, 100 μL of MTT reagent (1 mg/mL) was added into each well, and the plates were kept in incubator for 4 h. After that, 100 μL of dimethyl sulfoxide (DMSO) was added into each well, and the plates were measured at 490 nm using microplate reader (BIO-RAD, USA). The inhibitory ratio was calculated as $[(A_{490\ \text{control}} - A_{490}\ \text{treated})/A_{490}\ \text{control}] \times 100\%$. The cytotoxicity of compounds was expressed as IC_{50} values calculated by GraphPad Prism 5 (GraphPad Software, California, USA).

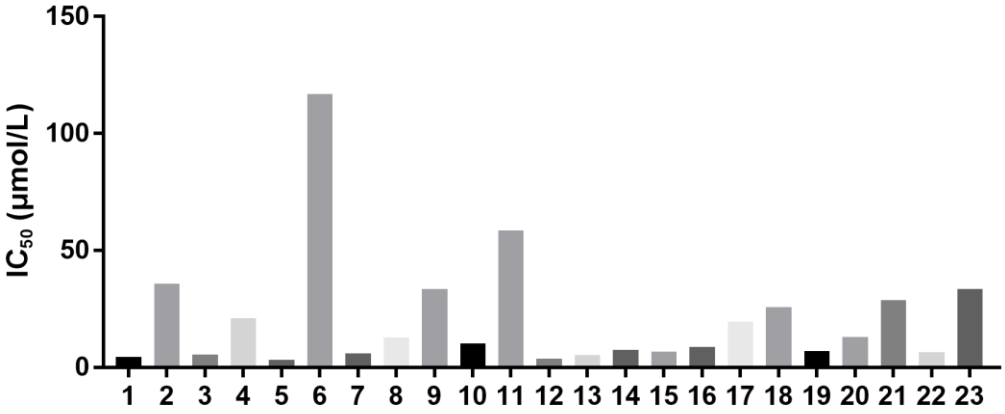


Figure S237 Cytotoxicity of **1**–**23** from *A. atrovirens* against HepG2 cells. Sorafenib was used as the positive control (IC_{50}: 7.7 μmol/L).

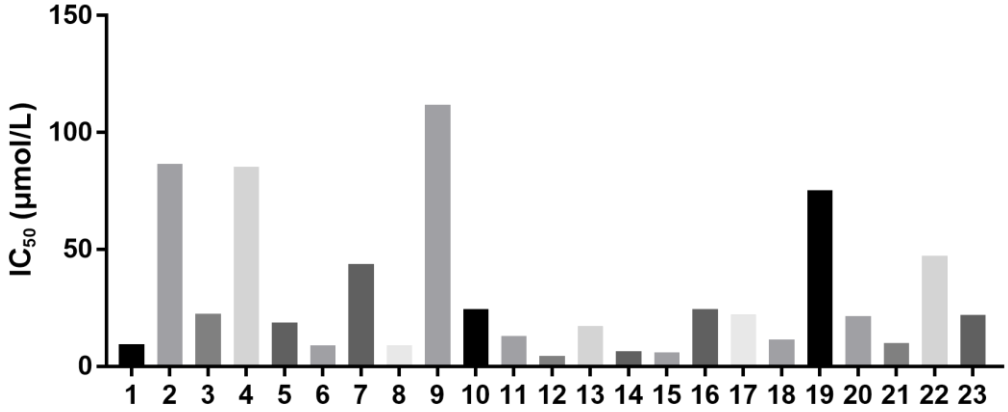


Figure S238 Cytotoxicity of **1**–**23** from *A. atrovirens* against SMMC-7721 cells. Sorafenib was used as the positive control (IC_{50}: 9.9 μmol/L).

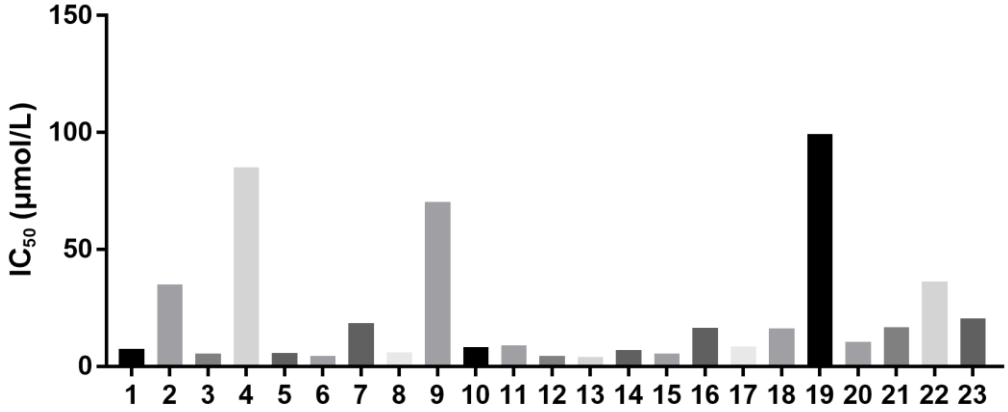


Figure S239 Cytotoxicity of **1**–**23** from *A. atrovirens* against Huh7 cells. Sorafenib was used as the positive control (IC_{50}: 8.3 μmol/L).

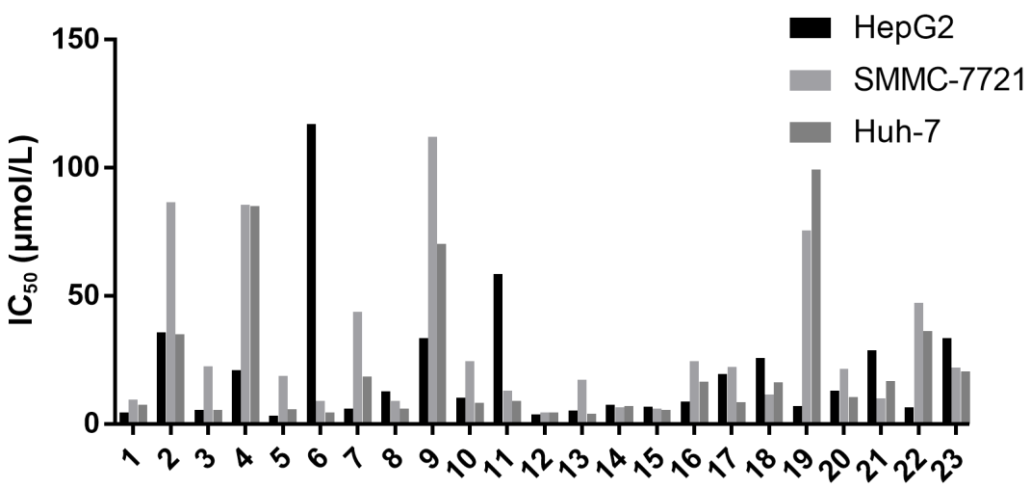


Figure S240 Cytotoxicity of **1**–**23** from *A. atrovirens* against HepG2, SMMC-7721 and Huh7 cell lines. Sorafenib was used as the positive control (IC_{50}: 7.7, 9.9, 8.3 μmol/L).

References

1. Ma L, Meng YY, Tu CH, Cao XQ, Wang HY, Li YY, et al. A cardiac glycoside HTF-1 isolated from *Helleborus thibetanus* Franch displays potent in *vitro* anti-cancer activity *via* caspase-9, MAPK and PI3K-Akt-mTOR pathways. *Eur J Med Chem* 2018;**158**:743–52.
2. Su LH, Geng CA, Li TZ, Huang XY, Ma YB, Zhang XM, et al. Spiroseoflosterol, a rearranged ergostane-steroid from the fruiting bodies of *Butyriboletus roseoflavus*. *J Nat Prod* 2020;**83**:1706–10.
3. Xue R, Han N, Ye C, Wang LH, Yang JY, Wang Y, et al. The cytotoxic activities of cardiac glycosides from *streptocaulon juventas* and the structure−activity relationships. *Fitoterapia* 2014;**98**:228–33.
4. Xue R, Han N, Sakurai H, Saiki I, Ye C, Yin J. Cytotoxic cardiac glycosides from the roots of *Streptocaulon juventas*. *Planta Med* 2013;**79**:157–62.

26. Computational data of compounds 2, 5–8, 11, 14–18, and 22

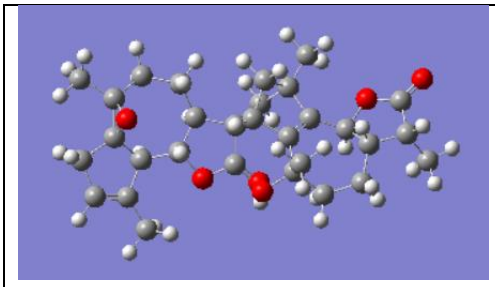
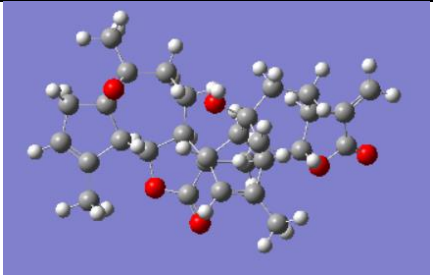
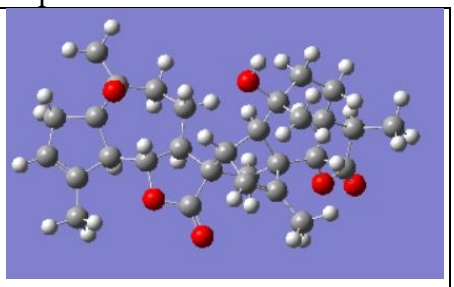
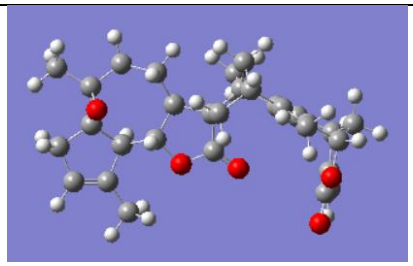
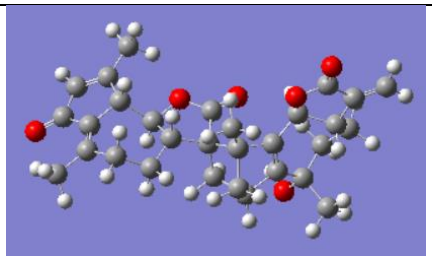
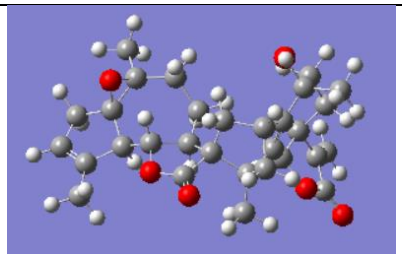
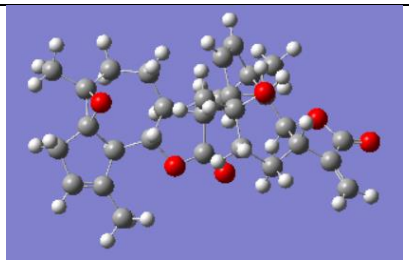
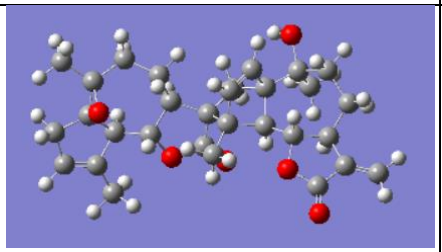
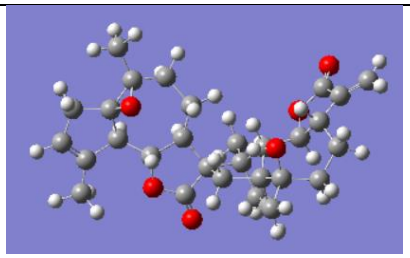
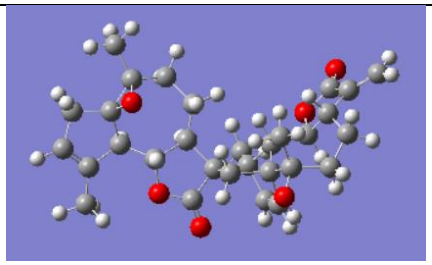
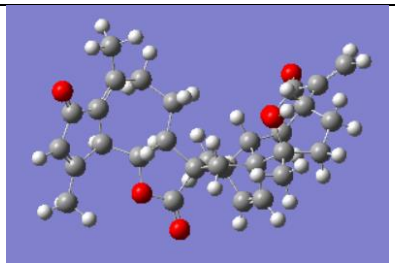
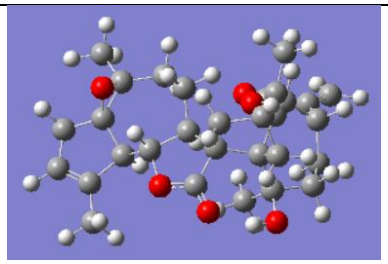
The ECD calculations for compounds **2**, **5**–**8**, **11**, **14**–**18**, and **22** were performed with the Gaussian 09 program package. Their relative configurations were generated by

referring to the related compounds that were confirmed by X-ray diffraction. The conformation search was performed by Spartan 14 software using molecular mechanics MMFF94s force field. The lowest-energy conformer was confirmed by the ROESY experiment, which was pre-optimized with MM2 method and further optimized by the DFT calculation at the b3lyp/6-31G(d,p) level in the gas phase. Frequency calculation was performed at the same level to exclude imaginary frequencies. ECD calculation was performed using the TD-DFT methodology at the b3lyp/6-311+g(d,p) level in methanol. Solvent effects were taken into consideration using the SCRF method with the IEFPCM model. The calculated ECD spectra were simulated by the SpecDis program with σ = ~0.3 eV.[5–6]

References

5. Frisch M J, Trucks GW, Schlegel HB, Scuseria GE, Robb MA, Cheeseman JR, et al. *Gaussian 09*, Revision C.01; Gaussian, Inc., Wallingford CT: **2010**.
6. Willoughby PH, Jansma MJ, Hoye TR. *Nat Protoc* 2014; **9**:643–60.

The lowest-energy conformers of the calculated compounds

 **2**	 **5**	 **6**
 **7**	 **8**	 **11**
 **14**	 **15**	 **16**
 **17**	 **18**	 **22**

Cartesian coordinates of the lowest-energy formers optimized at the b3lyp/6-311+g(d,p) level

Standard orientation of **2**

Center number	Atomic number	Atomic type	Coordinates (Angstroms) *X*	*Y*	*Z*
1	6	0	6.034827	−0.230228	0.241017
2	6	0	−4.091139	−0.552002	−0.769377
3	6	0	−5.075871	0.175400	0.177658
4	6	0	−6.359010	−0.660982	0.231739
5	6	0	5.860907	1.169662	−0.345315
6	6	0	4.248791	−2.117461	0.659869
7	6	0	2.763975	−2.475014	0.475372
8	6	0	1.704653	−1.669909	1.259543
9	6	0	1.544928	−0.236980	0.755515
10	6	0	−2.470732	2.118542	0.262352
11	6	0	−3.925785	2.534308	−0.014497
12	6	0	4.581515	−0.622116	0.588567
13	6	0	−5.016000	1.608171	0.529214
14	6	0	−0.546968	−0.831892	−1.173391
15	6	0	−4.685021	−1.962435	−0.847885
16	6	0	−4.018153	−3.117976	−1.534521
17	6	0	−5.915126	−1.985473	−0.320173
18	6	0	−6.280553	2.339444	0.938079
19	6	0	0.216457	0.505769	0.898310
20	6	0	0.738148	1.948125	1.023367
21	6	0	2.370943	3.151868	−0.601270
22	6	0	1.959339	−1.683382	2.774006
23	6	0	3.749748	0.190173	−0.433265
24	6	0	6.778278	−1.112980	−0.777558
25	6	0	2.381968	0.570532	0.067788
26	6	0	1.612779	1.876985	−0.249392
27	6	0	0.513584	1.499633	−1.308367
28	6	0	−0.464083	0.558373	−0.551216
29	6	0	−1.974223	0.940842	−0.576148
30	6	0	−2.641082	−0.416969	−0.298188
31	1	0	−7.162284	−0.218693	−0.376415
32	1	0	−3.115165	−3.439611	−1.008695
33	1	0	−4.704734	−3.966795	−1.602586
34	1	0	−3.698973	−2.848208	−2.547987
35	1	0	−6.729527	−0.716241	1.261325
36	1	0	−6.558065	−2.860835	−0.321041
37	1	0	−6.688678	2.901500	0.090279
38	1	0	−6.055086	3.056470	1.734807
39	1	0	−7.049260	1.656875	1.302403
40	1	0	−2.353022	1.911854	1.330267
41	1	0	−2.201368	1.177602	−1.628972
42	1	0	3.665013	−0.344948	−1.391102
43	1	0	−0.444178	0.123977	1.676522
44	1	0	1.331796	2.094002	1.930389
45	1	0	−0.028612	2.724251	0.968726
46	1	0	3.109811	3.406051	0.162241
47	1	0	2.903449	3.068750	−1.550788
48	1	0	1.659258	3.982484	−0.679954
49	1	0	1.136837	−1.188152	3.297604
50	1	0	2.888733	−1.170977	3.034276

51	1	0	2.009697	−2.717703	3.127756
52	1	0	2.499890	−2.396759	−0.585899
53	1	0	−0.004901	2.406609	−1.641512
54	1	0	2.625245	−3.525751	0.754127
55	1	0	4.610525	−2.505542	1.619400
56	1	0	4.803604	−2.659645	−0.112961
57	1	0	4.357960	−0.169909	1.562068
58	1	0	7.007608	−2.095422	−0.356373
59	1	0	7.720063	−0.631428	−1.053754
60	1	0	0.359300	−2.588230	0.171122
61	1	0	0.942319	1.016436	−2.189823
62	1	0	−1.848163	2.989453	0.031612
63	1	0	−4.079878	2.675064	−1.093739
64	1	0	−4.078028	3.522005	0.437233
65	1	0	−4.150316	−0.102489	−1.774902
66	1	0	−2.572714	−0.685479	0.760090
67	8	0	0.446436	−2.357731	1.108438
68	8	0	6.707516	2.006523	−0.528416
69	8	0	4.558991	1.368610	−0.695005
70	8	0	−1.793236	−1.341584	−1.038526
71	8	0	0.329788	−1.467686	−1.720114
72	8	0	−4.567219	0.598404	1.464616
73	1	0	6.654591	−0.142159	1.138544
74	1	0	6.196502	−1.262874	−1.693217

Rotational constants (GHZ): 0.2656443 0.0623354 0.0560255

Standard orientation of **5**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) *X*	*Y*	*Z*
1	6	0	−4.804981	−1.133956	−1.610604
2	6	0	3.999081	0.390562	−0.704547
3	6	0	4.531793	−1.018104	−0.347914
4	6	0	6.059319	−0.922383	−0.268568
5	6	0	−4.708040	0.205124	−2.275507
6	6	0	−4.087533	−1.944902	0.751278
7	6	0	−2.894049	−2.217352	1.686984
8	6	0	−2.076150	−1.020341	2.249154
9	6	0	−1.383167	−0.281882	1.076752
10	6	0	1.313563	−1.488577	−0.435609
11	6	0	2.391497	−2.314765	−1.159084
12	6	0	−3.748749	−1.173225	−0.532041
13	6	0	3.799322	−2.282167	−0.560755
14	6	0	1.019925	2.305244	−0.219507
15	6	0	5.194046	1.291910	−0.375698
16	6	0	5.150917	2.791226	−0.414447
17	6	0	6.293702	0.557697	−0.165564
18	6	0	4.566377	−3.576824	−0.753170
19	6	0	−0.215249	0.693173	1.371710
20	6	0	−0.960147	1.946066	1.786484
21	6	0	−3.061506	3.147247	0.971538
22	6	0	−2.918187	−0.179611	3.216819
23	6	0	−3.527269	0.335120	−0.289478

24	6	0	−5.706949	−2.039713	−1.987128
25	6	0	−2.145818	0.752250	0.196831
26	6	0	−2.093788	2.012612	1.075752
27	6	0	−1.052680	0.960457	−0.917355
28	6	0	0.292087	0.959624	−0.127761
29	6	0	1.428710	0.023812	−0.632916
30	6	0	2.667713	0.692445	−0.009284
31	1	0	6.543040	−1.346923	−1.161185
32	1	0	4.516832	3.203207	0.374936
33	1	0	6.158709	3.203103	−0.307558
34	1	0	4.727009	3.151414	−1.358937
35	1	0	6.428294	−1.487054	0.594904
36	1	0	7.277367	0.979606	0.019203
37	1	0	4.640612	−3.823021	−1.818630
38	1	0	4.039678	−4.399522	−0.257535
39	1	0	5.574556	−3.521048	−0.340641
40	1	0	1.309195	−1.746005	0.627913
41	1	0	1.501619	0.203431	−1.718434
42	1	0	−4.279914	0.665899	0.438595
43	1	0	0.553256	0.327683	2.051412
44	1	0	−0.551891	2.728471	2.416559
45	1	0	−5.796611	−3.009753	−1.508213
46	1	0	−2.770529	3.969353	1.630349
47	1	0	−3.099708	3.530512	−0.055174
48	1	0	−4.085053	2.849613	1.233145
49	1	0	−2.306941	0.579843	3.703776
50	1	0	−3.342713	−0.835180	3.988523
51	1	0	−3.751966	0.325625	2.722084
52	1	0	−2.178712	−2.870215	1.172025
53	1	0	−1.081545	0.141880	−1.645457
54	1	0	−3.268263	−2.792866	2.545331
55	1	0	−4.509851	−2.918601	0.476217
56	1	0	−4.885979	−1.413113	1.284254
57	1	0	−2.835074	−1.596942	−0.976528
58	1	0	−6.384988	−1.812046	−2.803922
59	1	0	−1.318877	−2.099506	3.706377
60	1	0	−1.204409	1.895797	−1.457424
61	1	0	0.351233	−1.814155	−0.847051
62	1	0	2.446334	−2.020276	−2.216618
63	1	0	2.059398	−3.360115	−1.159823
64	1	0	3.820253	0.450445	−1.791363
65	1	0	2.753001	0.446203	1.053806
66	8	0	−0.961268	−1.581777	2.971752
67	8	0	−5.245412	0.588610	−3.284018
68	8	0	−3.862480	0.991517	−1.542240
69	8	0	2.364907	2.108544	−0.119622
70	8	0	0.553351	3.406695	−0.366842
71	8	0	3.904224	−1.703626	0.761661
72	1	0	−1.016701	−1.090047	0.441372

Rotational constants (GHZ): 0.1991333 0.0701674 0.0653589

Standard orientation of **6**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) *X*	*Y*	*Z*

1	6	0	−4.803815	−1.121967	−1.706739
2	6	0	4.053774	0.430047	−0.663309
3	6	0	4.592546	−0.992071	−0.376127
4	6	0	6.119347	−0.893157	−0.289218
5	6	0	−4.507664	0.207189	−2.405243
6	6	0	−4.049219	−1.981148	0.656005
7	6	0	−2.853138	−2.304208	1.570795
8	6	0	−2.038139	−1.135814	2.187812
9	6	0	−1.341211	−0.349603	1.050292
10	6	0	1.377197	−1.474569	−0.495299
11	6	0	2.460780	−2.259025	−1.255601
12	6	0	−3.718004	−1.172671	−0.607063
13	6	0	3.867103	−2.247774	−0.653071
14	6	0	1.062602	2.303398	−0.106369
15	6	0	5.243303	1.319440	−0.285685
16	6	0	5.192355	2.818504	−0.247367
17	6	0	6.346286	0.580986	−0.110603
18	6	0	4.641551	−3.527367	−0.907429
19	6	0	−0.181294	0.617501	1.397974
20	6	0	−0.937784	1.847886	1.856869
21	6	0	−3.035789	3.072928	1.072382
22	6	0	−2.884192	−0.336509	3.186434
23	6	0	−3.476520	0.323617	−0.332764
24	6	0	−6.267706	−1.123820	−1.228205
25	6	0	−2.101578	0.715737	0.205621
26	6	0	−2.064985	1.937913	1.138453
27	6	0	−0.994668	0.978914	−0.884581
28	6	0	0.340829	0.951736	−0.082145
29	6	0	1.486130	0.045633	−0.620231
30	6	0	2.718113	0.690631	0.040606
31	1	0	6.606253	−1.269444	−1.201537
32	1	0	4.551391	3.185928	0.558276
33	1	0	6.197269	3.229525	−0.113246
34	1	0	4.772043	3.224895	−1.174590
35	1	0	6.489979	−1.499057	0.545100
36	1	0	7.327405	0.997721	0.097973
37	1	0	4.717363	−3.721344	−1.983548
38	1	0	4.119163	−4.375977	−0.452594
39	1	0	5.649332	−3.486176	−0.492259
40	1	0	1.372231	−1.782390	0.554583
41	1	0	1.564785	0.275972	−1.695788
42	1	0	−4.248250	0.673920	0.365744
43	1	0	0.581509	0.227416	2.070521
44	1	0	−0.540286	2.605958	2.522594
45	1	0	−2.747319	3.873236	1.758568
46	1	0	−3.074171	3.490771	0.059113
47	1	0	−4.058874	2.764768	1.324185
48	1	0	−2.274828	0.400496	3.709005
49	1	0	−3.312923	−1.024346	3.927225
50	1	0	−3.714963	0.191148	2.710088
51	1	0	−3.224881	−2.921659	2.400842
52	1	0	−1.011058	0.191884	−1.646707
53	1	0	−2.140177	−2.931313	1.021714
54	1	0	−4.830960	−1.463250	1.225480
55	1	0	−4.488621	−2.939345	0.352287
56	1	0	−2.811175	−1.589280	−1.066136

57	1	0	−6.528433	−2.078559	−0.763324
58	1	0	−6.929874	−0.966111	−2.083418
59	1	0	−1.287416	−2.282712	3.595838
60	1	0	−1.146521	1.935065	−1.386651
61	1	0	0.417150	−1.784006	−0.923927
62	1	0	2.515966	−1.912736	−2.297403
63	1	0	2.134700	−3.304970	−1.308045
64	1	0	3.878545	0.543530	−1.746441
65	1	0	2.800545	0.394461	1.091087
66	8	0	−0.926011	−1.726898	2.891503
67	8	0	−4.891375	0.576487	−3.484720
68	8	0	−3.735315	0.990074	−1.597099
69	8	0	2.407899	2.108716	−0.003910
70	8	0	0.592176	3.408458	−0.207127
71	8	0	3.966001	−1.734793	0.696625
72	1	0	−4.678187	−1.925445	−2.438765
73	1	0	−6.464824	−0.327966	−0.502406
74	1	0	−0.966151	−1.131090	0.387234

Rotational constants (GHZ): 0.2027094 0.0690285 0.0646955

Standard orientation of **7**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) *X*	*Y*	*Z*
1	6	0	−4.810149	0.287026	−0.173678
2	6	0	−3.579971	1.134827	0.226139
3	6	0	−2.268668	0.533670	−0.290417
4	6	0	−1.735240	−0.676276	0.495328
5	6	0	−2.535683	−1.972695	0.343660
6	6	0	−3.951115	−1.929085	0.946741
7	6	0	−5.000628	−1.136946	0.163834
8	6	0	−5.962052	1.255999	−0.460087
9	6	0	−5.256187	2.572698	−0.615297
10	6	0	−3.962518	2.533128	−0.272482
11	6	0	−3.037771	3.714561	−0.253322
12	8	0	−4.612007	−0.741357	−1.173406
13	6	0	−6.400912	−1.708500	0.278518
14	8	0	−1.200989	1.501638	−0.150129
15	6	0	−0.005281	0.881122	0.072124
16	6	0	−0.219515	−0.643778	0.118046
17	8	0	1.009962	1.519901	0.167193
18	6	0	0.768403	−1.446666	1.070303
19	6	0	2.220567	−1.012201	0.767675
20	6	0	2.504420	−1.502894	−0.604776
21	6	0	1.246218	−2.271185	−0.999227
22	6	0	0.802521	−2.829354	0.362839
23	6	0	2.996950	−0.354627	1.639913
24	6	0	4.431149	0.092457	1.474527
25	6	0	5.256822	−0.752988	0.506933
26	6	0	4.829872	−0.565203	−0.945340
27	6	0	3.578745	−1.299632	−1.393388
28	1	0	−3.506117	1.177575	1.326002
29	6	0	0.391875	−1.449101	2.546495
30	6	0	0.117346	−1.251010	−1.300170

31	6	0	3.647088	−1.742678	−2.834758
32	6	0	4.480690	1.547016	1.025900
33	8	0	4.717696	0.839120	−1.322440
34	6	0	4.506497	1.857441	−0.443754
35	8	0	4.414827	2.979598	−0.887980
36	6	0	4.517167	2.578397	1.874797
37	1	0	−2.374935	0.296184	−1.354380
38	1	0	−1.791983	−0.383810	1.554474
39	1	0	−2.002279	−2.775026	0.861052
40	1	0	−2.612636	−2.264279	−0.707801
41	1	0	−4.308513	−2.963160	1.022920
42	1	0	−3.912720	−1.551459	1.978343
43	1	0	−6.506358	0.940458	−1.357204
44	1	0	−6.689548	1.281431	0.365155
45	1	0	−5.769991	3.474015	−0.936650
46	1	0	−2.210931	3.599290	−0.958851
47	1	0	−3.585256	4.629273	−0.498593
48	1	0	−2.575479	3.840500	0.732537
49	1	0	−7.132782	−1.111528	−0.267144
50	1	0	−6.422417	−2.726938	−0.124235
51	1	0	−6.708938	−1.759604	1.329159
52	1	0	1.387024	−3.004816	−1.793439
53	1	0	−0.161059	−3.341917	0.325506
54	1	0	1.541632	−3.498077	0.815352
55	1	0	2.543962	−0.028046	2.572570
56	1	0	4.902487	0.036581	2.463990
57	1	0	6.308126	−0.456599	0.599102
58	1	0	5.191869	−1.815647	0.760981
59	1	0	5.648704	−0.921723	−1.580605
60	1	0	1.145313	−1.988104	3.128314
61	1	0	0.322821	−0.433650	2.952171
62	1	0	−0.570812	−1.939963	2.715410
63	1	0	−0.753545	−1.758301	−1.725669
64	1	0	0.439654	−0.490643	−2.016336
65	1	0	3.905571	−0.884271	−3.467262
66	1	0	4.435320	−2.493013	−2.986657
67	1	0	2.710213	−2.158682	−3.206418
68	1	0	4.526385	3.595325	1.499379
69	1	0	4.527472	2.426286	2.950467

Rotational constants (GHZ): 0.2508610 0.0719881 0.0643598

Standard orientation of **8**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) *X*	*Y*	*Z*
1	1	0	6.280304	−0.971629	−2.861925
2	1	0	−6.920490	−2.974378	0.178733
3	1	0	−7.250059	−1.353822	−0.674072
4	8	0	−2.355623	3.235531	−1.609345
5	1	0	−1.827268	2.713855	−2.230011
6	8	0	−0.604395	−0.670426	−1.754689
7	8	0	1.601864	−0.680102	−1.446236
8	8	0	−3.131892	−1.951688	0.869160
9	8	0	−4.601706	−3.551484	1.481913

10	6	0	3.694691	−2.243891	−2.821890
11	1	0	4.342505	−2.493533	−3.665816
12	1	0	2.789688	−1.757031	−3.194387
13	1	0	3.366051	−3.176255	−2.346585
14	6	0	4.412108	−1.376450	−1.836690
15	6	0	3.837016	−1.022138	−0.464497
16	1	0	3.585243	−1.952343	0.068197
17	6	0	2.570572	−0.147438	−0.508142
18	1	0	2.853531	0.852474	−0.862669
19	6	0	1.771069	−0.068842	0.800668
20	1	0	1.658707	−1.109672	1.135623
21	6	0	0.364482	0.370989	0.288550
22	6	0	−0.874591	0.083825	1.270165
23	6	0	−2.165936	0.261045	0.427179
24	6	0	−3.105156	−0.815670	−0.045829
25	1	0	−2.771086	−1.209750	−1.011565
26	6	0	−4.578135	−0.344758	−0.115719
27	1	0	−4.721235	0.320372	0.747947
28	6	0	−5.322571	−1.620266	0.173277
29	6	0	−6.565662	−1.995149	−0.127689
30	6	0	−2.264117	1.570824	0.110963
31	6	0	−3.177126	2.308014	−0.863354
32	6	0	−4.182757	3.205856	−0.132490
33	1	0	−4.761362	3.780327	−0.862219
34	1	0	−4.869340	2.621658	0.485014
35	1	0	−3.657044	3.913115	0.514475
36	6	0	−3.854256	1.375119	−1.893301
37	1	0	−4.277498	2.019485	−2.671590
38	1	0	−3.057375	0.787731	−2.367954
39	6	0	−4.947723	0.415367	−1.392671
40	1	0	−5.879512	0.965801	−1.218869
41	1	0	−5.159620	−0.304767	−2.191679
42	6	0	−1.093522	2.289211	0.773395
43	1	0	−1.218026	3.365827	0.895463
44	6	0	0.207133	1.912477	0.000704
45	1	0	1.061330	2.473796	0.390608
46	1	0	0.127470	2.145688	−1.063014
47	6	0	−0.736151	−1.162142	2.138731
48	1	0	−1.614423	−1.284150	2.774628
49	1	0	0.139932	−1.081122	2.790082
50	1	0	−0.645399	−2.076781	1.547400
51	6	0	−0.928908	1.434124	2.036026
52	1	0	−1.794192	1.479935	2.703017
53	1	0	−0.023521	1.659162	2.607136
54	6	0	0.333935	−0.382456	−1.050576
55	6	0	4.977001	−0.265486	0.214642
56	6	0	4.969187	0.206799	1.479152
57	6	0	6.124087	0.954426	2.091466
58	1	0	6.474583	0.421533	2.985495
59	1	0	5.784388	1.939831	2.438180
60	1	0	6.950595	1.080402	1.396000
61	6	0	3.775630	0.009501	2.398671
62	1	0	4.033185	0.399836	3.388251
63	1	0	3.586772	−1.064731	2.536148
64	6	0	2.464384	0.687685	1.936090
65	1	0	1.793821	0.725396	2.799514
66	1	0	2.674157	1.726141	1.654690

67	6	0	6.088955	−0.132278	−0.788194
68	8	0	7.164246	0.442070	−0.658390
69	6	0	5.644853	−0.858991	−1.990837
70	6	0	−4.377620	−2.511572	0.913275

Rotational constants (GHZ): 0.2278833 0.0616838 0.0594514

Standard orientation of **11**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) *X*	*Y*	*Z*
1	6	0	3.151954	−2.196678	0.978997
2	6	0	4.002120	−1.450513	0.017980
3	6	0	−3.263378	−1.502090	1.853713
4	6	0	3.450194	−3.656893	1.269107
5	6	0	−3.821526	−1.903172	−1.979967
6	6	0	−3.038757	−1.656653	−0.711126
7	6	0	−2.382505	−0.297316	−1.054973
8	6	0	−4.104519	−0.569684	−2.593122
9	6	0	−1.951769	0.686772	−0.010006
10	6	0	−3.978165	−1.664569	0.509900
11	6	0	−4.277694	0.659978	2.706618
12	6	0	2.627041	0.675919	0.011286
13	6	0	−2.977561	−0.064376	2.307914
14	6	0	3.588812	−0.199145	−0.786140
15	6	0	5.256995	−1.977075	−0.682557
16	6	0	5.832797	−0.700046	−1.246889
17	1	0	6.848877	−0.632662	−1.623768
18	6	0	4.952287	0.309824	−1.268376
19	1	0	−4.823003	−3.020254	−3.442666
20	6	0	5.192404	1.682938	−1.817665
21	1	0	−4.031793	−4.012417	−2.081280
22	6	0	1.442309	2.636802	−0.103775
23	6	0	−1.014621	1.863370	−0.397145
24	6	0	−1.544682	2.935360	0.585775
25	6	0	−0.966430	2.259658	−1.869205
26	6	0	−2.205191	0.785479	1.313340
27	6	0	−4.244499	−3.043984	−2.524137
28	6	0	−1.445627	2.015028	1.810350
29	6	0	0.072720	1.647086	1.804912
30	6	0	0.407042	1.549836	0.274094
31	6	0	1.160628	0.279592	−0.202664
32	6	0	0.801393	−1.132244	0.324432
33	6	0	1.723449	−1.774490	1.379198
34	1	0	−2.308889	−2.041885	1.837449
35	1	0	0.654368	2.435497	2.292080
36	1	0	0.257923	0.712636	2.338959
37	1	0	3.051636	−0.538312	−1.688428
38	1	0	4.486738	−3.914569	1.048009
39	1	0	3.263344	−3.873760	2.326679
40	1	0	1.206281	−2.671437	1.738041
41	1	0	0.747672	−1.814340	−0.533103
42	1	0	−0.204783	−1.107884	0.748772
43	1	0	1.820978	−1.121632	2.253732
44	1	0	5.920608	−2.479077	0.027218

45	1	0	5.011806	−2.698813	−1.477268
46	1	0	2.796061	−4.305627	0.675532
47	1	0	2.908434	0.629495	1.067694
48	1	0	5.055039	2.453122	−1.053491
49	1	0	6.206010	1.762738	−2.221029
50	1	0	4.481587	1.921136	−2.618056
51	1	0	1.030805	0.260139	−1.293970
52	1	0	−2.574621	3.219395	0.350519
53	1	0	−0.908257	3.820476	0.635595
54	1	0	−0.530169	1.476261	−2.499786
55	1	0	−2.259442	−2.411298	−0.557752
56	1	0	−0.366721	3.163560	−1.995500
57	1	0	−1.972535	2.451409	−2.247112
58	1	0	−1.783771	2.428033	2.764783
59	1	0	−1.515513	−0.511307	−1.694662
60	1	0	−2.130689	0.584382	3.966130
61	1	0	−3.858252	−1.966198	2.647653
62	1	0	−4.501260	−2.627155	0.500586
63	1	0	−4.756123	−0.902913	0.380978
64	1	0	−4.780875	0.100851	3.501633
65	1	0	−4.067504	1.669629	3.075971
66	1	0	−4.960426	0.761978	1.858994
67	8	0	−3.360746	0.366173	−1.933201
68	8	0	4.172549	−1.274294	1.436051
69	8	0	2.653540	2.072980	−0.366473
70	8	0	−4.852300	−0.293110	−3.498340
71	8	0	−2.159870	−0.252523	3.483862
72	8	0	1.286217	3.831839	−0.172942

Rotational constants (GHZ): 0.1720780 0.0768173 0.0740032

Standard orientation of **14**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) *X*	*Y*	*Z*
1	6	0	−4.930597	1.498055	0.253955
2	6	0	3.450688	0.936986	−0.820010
3	6	0	4.567758	0.217074	−0.027528
4	6	0	5.765873	1.168900	0.048290
5	6	0	−5.502354	0.428076	−0.624121
6	6	0	−2.531190	2.000089	1.102409
7	6	0	−1.244521	1.474210	1.811818
8	6	0	−0.971356	−0.039802	1.996522
9	6	0	−0.971581	−0.923593	0.698501
10	6	0	2.165416	−1.974103	−0.011741
11	6	0	3.625406	−2.196815	−0.445165
12	6	0	−3.610195	0.973207	0.758698
13	6	0	4.665659	−1.244669	0.148121
14	6	0	−0.095219	0.925623	−1.067153
15	6	0	3.907478	2.399430	−0.787657
16	6	0	3.097386	3.545351	−1.319508
17	6	0	5.163650	2.490706	−0.333128
18	6	0	6.016689	−1.889859	0.388358
19	6	0	−0.630881	−2.399102	0.965258
20	6	0	−1.170747	−3.147530	−0.002216

21	6	0	−2.927624	−2.902539	−1.874181
22	6	0	0.316585	−0.187308	2.833899
23	6	0	−3.238173	0.002841	−0.381785
24	6	0	−5.563958	2.651075	0.466073
25	6	0	−2.401864	−1.178108	0.074631
26	6	0	−1.909883	−2.229107	−0.961883
27	6	0	−0.798378	−1.429778	−1.712664
28	6	0	−0.068430	−0.558780	−0.635393
29	6	0	1.493855	−0.758789	−0.656135
30	6	0	2.059889	0.614114	−0.257141
31	1	0	6.566417	0.875033	−0.646916
32	1	0	2.204264	3.732206	−0.717632
33	1	0	3.700545	4.457473	−1.344011
34	1	0	2.739311	3.340389	−2.335201
35	1	0	6.196271	1.155101	1.055861
36	1	0	5.722814	3.420493	−0.283860
37	1	0	6.418147	−2.296142	−0.547021
38	1	0	5.913498	−2.720797	1.094502
39	1	0	6.740203	−1.183556	0.797385
40	1	0	2.128296	−1.911493	1.078847
41	1	0	1.710463	−0.838196	−1.733826
42	1	0	−2.786604	0.550624	−1.207967
43	1	0	−1.051600	−4.216955	−0.148005
44	1	0	0.026412	−2.746688	1.752006
45	1	0	−3.694067	−3.420566	−1.290151
46	1	0	−3.438213	−2.177009	−2.511058
47	1	0	−2.435050	−3.641012	−2.517745
48	1	0	0.214399	0.412978	3.741362
49	1	0	0.467207	−1.223494	3.150065
50	1	0	1.221241	0.131993	2.317148
51	1	0	−0.368383	1.916685	1.328825
52	1	0	−0.101632	−2.103028	−2.222053
53	1	0	−1.242415	1.866382	2.833408
54	1	0	−2.980457	2.749262	1.763356
55	1	0	−2.253538	2.527914	0.186267
56	1	0	−3.815743	0.364883	1.648511
57	1	0	−5.149465	3.436703	1.089838
58	1	0	−6.530940	2.825850	0.004391
59	1	0	−1.915266	−1.454822	2.988017
60	1	0	−1.249640	−0.784744	−2.472459
61	1	0	1.604353	−2.866005	−0.299068
62	1	0	3.704169	−2.177100	−1.541448
63	1	0	3.903137	−3.215118	−0.147374
64	1	0	3.466919	0.599727	−1.870083
65	1	0	2.082728	0.760237	0.822767
66	8	0	−2.048623	−0.507950	2.837485
67	8	0	−6.617534	0.328678	−1.074611
68	8	0	−4.527221	−0.500932	−0.858521
69	8	0	1.086079	1.536386	−0.804040
70	8	0	−0.972441	1.538212	−1.630339
71	8	0	4.193141	−0.400916	1.227158
72	1	0	−3.001269	−1.690148	0.831526

Rotational constants (GHZ): 0.2357324 0.0755597 0.0685804

Standard orientation of **15**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) *X*	*Y*	*Z*
1	6	0	4.934459	−0.013061	−0.386443
2	6	0	4.022210	−0.509452	0.761988
3	6	0	2.556921	−0.614369	0.327406
4	6	0	1.808991	0.727279	0.234131
5	6	0	2.178080	1.608493	−0.959406
6	6	0	3.594414	2.203772	−0.887930
7	6	0	4.755058	1.240069	−1.147903
8	6	0	6.283517	−0.724197	−0.231173
9	6	0	5.949836	−1.872063	0.678067
10	6	0	4.724715	−1.794798	1.212149
11	6	0	4.155628	−2.760234	2.210014
12	8	0	4.387896	−0.035702	−1.726156
13	8	0	1.797375	−1.349281	1.324870
14	6	0	0.542889	−0.851262	1.454332
15	6	0	0.326953	0.328575	0.490347
16	8	0	−0.237113	−1.320128	2.250038
17	6	0	−0.611768	−0.148257	−0.737986
18	6	0	−1.996611	−0.092401	0.004402
19	6	0	−1.891004	1.434656	0.335353
20	6	0	−1.497442	1.982861	−1.035589
21	6	0	−0.753005	1.061615	−1.654273
22	6	0	−3.241499	−0.488049	−0.781289
23	6	0	−4.532300	−0.428413	0.069886
24	6	0	−5.237514	0.936000	0.136980
25	6	0	−4.333653	2.184536	0.109599
26	6	0	−3.068484	2.203802	0.997758
27	1	0	4.063490	0.209477	1.597698
28	6	0	−0.205439	−1.448508	−1.426909
29	8	0	−3.141890	−1.878352	−1.203221
30	6	0	−4.360919	−2.495291	−1.162096
31	6	0	−5.331008	−1.574285	−0.495364
32	8	0	−2.714114	3.604926	1.016044
33	6	0	−3.379154	1.768051	2.437874
34	8	0	−4.546056	−3.600051	−1.608381
35	6	0	−6.640917	−1.819984	−0.475237
36	6	0	−0.550256	1.429044	1.156279
37	6	0	5.956174	1.910065	−1.789075
38	1	0	−1.966328	−0.704069	0.910498
39	1	0	2.500445	−1.172242	−0.609785
40	1	0	2.098920	1.287916	1.138690
41	1	0	1.472428	2.443020	−1.005336
42	1	0	2.074649	1.054007	−1.896486
43	1	0	3.657520	3.000183	−1.639326
44	1	0	3.749902	2.697590	0.081842
45	1	0	6.660526	−1.036584	−1.211199
46	1	0	7.045002	−0.065263	0.212618
47	1	0	6.660325	−2.661962	0.903687
48	1	0	4.905142	−3.508605	2.483114
49	1	0	3.831416	−2.245366	3.121920
50	1	0	3.271139	−3.274262	1.824398
51	1	0	−1.713040	2.994587	−1.357483
52	1	0	−0.254021	1.156621	−2.612141
53	1	0	−3.344101	0.112240	−1.691592

54	1	0	−4.236797	−0.723451	1.087098
55	1	0	−5.860600	0.952241	1.038393
56	1	0	−5.930304	1.016635	−0.708735
57	1	0	−4.021619	2.387450	−0.920154
58	1	0	−4.934268	3.047640	0.415024
59	1	0	−0.131192	−2.280957	−0.721280
60	1	0	−0.945589	−1.730885	−2.176705
61	1	0	0.759028	−1.337669	−1.932677
62	1	0	−1.968823	3.710100	1.622922
63	1	0	−4.254134	2.313675	2.802875
64	1	0	−3.574636	0.696804	2.527213
65	1	0	−2.545276	1.999133	3.108343
66	1	0	−7.351866	−1.151251	−0.000353
67	1	0	−7.024389	−2.720217	−0.945590
68	1	0	−0.056552	2.405682	1.116285
69	1	0	−0.726651	1.172814	2.203792
70	1	0	6.312427	2.735355	−1.162008
71	1	0	6.781250	1.214190	−1.945300
72	1	0	5.674532	2.328958	−2.761183

Rotational constants (GHZ): 0.2264118 0.0658249 0.0600325

Standard orientation of **16**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) *X*	*Y*	*Z*
1	6	0	−4.316008	1.286555	0.531675
2	6	0	−4.018922	0.111245	−0.430185
3	6	0	−2.695020	−0.584606	−0.095334
4	6	0	−1.417529	0.150889	−0.543301
5	6	0	−1.085742	1.440814	0.210587
6	6	0	−2.095402	2.584411	0.008181
7	6	0	−3.433295	2.450247	0.737353
8	6	0	−5.828686	1.309112	0.775931
9	6	0	−6.262650	−0.045833	0.294897
10	6	0	−5.300557	−0.724437	−0.342539
11	6	0	−5.478215	−2.062369	−0.998375
12	8	0	−3.501348	1.391168	1.724015
13	8	0	−2.610119	−1.840224	−0.818170
14	6	0	−1.318645	−2.122533	−1.145315
15	6	0	−0.394029	−1.030781	−0.580701
16	8	0	−1.043215	−3.104851	−1.787762
17	6	0	0.939905	−0.834900	−1.427160
18	6	0	1.858553	−0.224743	−0.314487
19	6	0	1.731402	−1.456624	0.639738
20	6	0	2.025593	−2.587328	−0.343819
21	6	0	1.562908	−2.226021	−1.543392
22	6	0	3.277654	0.175043	−0.690636
23	6	0	4.057295	0.790846	0.494089
24	6	0	4.803578	−0.202791	1.391948
25	6	0	4.073646	−1.528646	1.694270
26	6	0	2.548542	−1.472776	1.963477
27	1	0	−3.933290	0.492819	−1.461495
28	6	0	0.762076	−0.095558	−2.748751
29	8	0	3.228726	1.230799	−1.695166

30	6	0	4.221808	2.148332	−1.493297
31	6	0	4.890613	1.840007	−0.192849
32	8	0	2.314401	−0.269496	2.717699
33	6	0	2.157092	−2.684588	2.827673
34	8	0	4.454162	3.034887	−2.277818
35	6	0	6.019330	2.442977	0.181248
36	6	0	0.166725	−1.462036	0.826033
37	6	0	−4.017962	3.776711	1.182805
38	1	0	1.402812	0.655935	0.143703
39	1	0	−2.665945	−0.807031	0.976537
40	1	0	−1.592538	0.431046	−1.592804
41	1	0	−0.124654	1.815873	−0.151604
42	1	0	−0.976726	1.253845	1.283148
43	1	0	−1.619089	3.507511	0.359102
44	1	0	−2.283216	2.737509	−1.063742
45	1	0	−6.036609	1.486916	1.836943
46	1	0	−6.322606	2.114569	0.212113
47	1	0	−7.278284	−0.409810	0.420204
48	1	0	−6.523525	−2.379124	−0.938097
49	1	0	−5.186949	−2.027778	−2.054557
50	1	0	−4.851099	−2.830960	−0.539105
51	1	0	2.428691	−3.556580	−0.071514
52	1	0	1.523693	−2.830592	−2.439893
53	1	0	3.824002	−0.662988	−1.136608
54	1	0	3.316609	1.304018	1.121103
55	1	0	5.769692	−0.449381	0.935012
56	1	0	5.025877	0.303482	2.336296
57	1	0	4.236991	−2.233896	0.872819
58	1	0	4.558699	−1.971746	2.570976
59	1	0	1.703825	−0.053520	−3.298912
60	1	0	0.025365	−0.612819	−3.373876
61	1	0	0.431802	0.936781	−2.606606
62	1	0	1.435526	−0.330117	3.114291
63	1	0	2.710972	−2.652128	3.770064
64	1	0	1.087358	−2.684877	3.062514
65	1	0	2.384949	−3.631546	2.329522
66	1	0	6.514604	2.217054	1.120311
67	1	0	6.469377	3.190101	−0.465271
68	1	0	−0.138655	−0.744761	1.595223
69	1	0	−0.194842	−2.446753	1.130066
70	1	0	−4.156613	4.440813	0.322110
71	1	0	−4.979319	3.653292	1.683131
72	1	0	−3.332101	4.272886	1.877921

Rotational constants (GHZ): 0.1960840 0.0725629 0.0660643

Standard orientation of **17**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) *X*	*Y*	*Z*
1	1	0	−7.299762	−0.457800	0.353688
2	1	0	6.616581	3.057669	−0.532105
3	1	0	6.626870	2.116168	1.072687
4	8	0	2.179662	−2.741282	2.626028
5	1	0	2.535806	−3.464357	2.092807

6	8	0	−1.012503	−3.065184	−1.808649
7	8	0	−2.600042	−1.831043	−0.835360
8	8	0	−3.564029	1.370979	1.724158
9	8	0	3.264054	1.243349	−1.688120
10	8	0	4.566608	2.977429	−2.318393
11	6	0	−5.460463	−2.088629	−1.040279
12	1	0	−6.503249	−2.416393	−0.997346
13	1	0	−4.833025	−2.851181	−0.571395
14	1	0	−5.151979	−2.049678	−2.091354
15	6	0	−5.307524	−0.749950	−0.379934
16	6	0	−4.033801	0.099962	−0.446323
17	1	0	−3.939888	0.488246	−1.474517
18	6	0	−2.706656	−0.584279	−0.100480
19	1	0	−2.686666	−0.817282	0.969198
20	6	0	−1.433033	0.170557	−0.526811
21	1	0	−1.601560	0.465628	−1.573321
22	6	0	−0.395982	−0.999072	−0.570368
23	6	0	0.939427	−0.779354	−1.411268
24	6	0	1.860648	−0.176158	−0.293299
25	6	0	3.287543	0.197066	−0.673326
26	1	0	3.815984	−0.657523	−1.107786
27	6	0	4.089440	0.809817	0.497799
28	1	0	3.368586	1.400531	1.081993
29	6	0	4.971125	1.800908	−0.217634
30	6	0	6.133990	2.349236	0.134138
31	1	0	1.532791	−2.764187	−2.439171
32	1	0	1.410243	0.714827	0.153405
33	1	0	2.424153	−3.509439	−0.085031
34	6	0	1.722136	−1.411352	0.657138
35	6	0	2.525841	−1.495647	1.985409
36	6	0	2.132763	−0.443255	3.028714
37	1	0	2.816599	−0.496409	3.880732
38	1	0	1.127748	−0.645957	3.404281
39	1	0	2.154251	0.573465	2.630536
40	6	0	4.055178	−1.508489	1.729624
41	1	0	4.508308	−1.954154	2.622072
42	1	0	4.251791	−2.206208	0.905930
43	6	0	4.788321	−0.179732	1.442424
44	1	0	4.984684	0.339262	2.387360
45	1	0	5.771564	−0.428967	1.026658
46	6	0	2.027081	−2.532202	−0.340196
47	6	0	0.160799	−1.433833	0.835632
48	1	0	−0.155235	−0.727626	1.606740
49	1	0	−0.173077	−2.425049	1.146819
50	6	0	0.758562	−0.026613	−2.724833
51	1	0	1.699069	0.027146	−3.275951
52	1	0	0.420474	1.001604	−2.570665
53	1	0	0.023977	−0.541482	−3.354227
54	6	0	1.569203	−2.165446	−1.538975
55	6	0	−1.303524	−2.094231	−1.155225
56	6	0	−4.356320	1.266723	0.516991
57	6	0	−3.488461	2.437157	0.746953
58	6	0	−4.094471	3.755023	1.190094
59	1	0	−4.220319	4.424935	0.331895
60	1	0	−3.428332	4.251204	1.904132
61	1	0	−5.065320	3.619397	1.668375
62	6	0	−2.137174	2.591208	0.046291

63	1	0	−1.675287	3.512633	0.420564
64	1	0	−2.304718	2.759027	−1.026825
65	6	0	−1.123790	1.451354	0.252377
66	1	0	−0.158369	1.838342	−0.085919
67	1	0	−1.035403	1.248204	1.323780
68	6	0	−5.873233	1.274875	0.735425
69	1	0	−6.100847	1.447965	1.793151
70	1	0	−6.364729	2.077227	0.164982
71	6	0	−6.286264	−0.082955	0.244175
72	6	0	4.301685	2.116684	−1.516482

Rotational constants (GHZ): 0.1961734 0.0715228 0.0654377

Standard orientation of **18**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) *X*	*Y*	*Z*
1	1	0	−7.022227	−0.495150	0.783598
2	1	0	6.519152	3.103750	−0.596709
3	1	0	6.476395	2.323554	1.091704
4	8	0	2.044349	0.034510	2.687203
5	1	0	2.361004	0.078773	3.599605
6	8	0	−1.014038	−3.249929	−1.557579
7	8	0	−2.592155	−1.857347	−0.799570
8	8	0	3.324852	1.028121	−1.753268
9	8	0	4.596353	2.747314	−2.478058
10	6	0	−5.515692	−1.912828	−1.222297
11	1	0	−6.528970	−2.275557	−1.032690
12	1	0	−4.798672	−2.702230	−0.982562
13	1	0	−5.409225	−1.720988	−2.297084
14	6	0	−5.237633	−0.670175	−0.437264
15	6	0	−3.976266	0.172464	−0.629720
16	1	0	−3.887915	0.448081	−1.691930
17	6	0	−2.671019	−0.532454	−0.215265
18	1	0	−2.675161	−0.648911	0.876445
19	6	0	−1.366039	0.126570	−0.695879
20	1	0	−1.501577	0.284857	−1.776096
21	6	0	−0.368593	−1.067407	−0.558001
22	6	0	1.002304	−0.981048	−1.362182
23	6	0	1.874079	−0.252461	−0.283452
24	6	0	3.313364	0.096470	−0.632752
25	1	0	3.875076	−0.789268	−0.948393
26	6	0	4.035946	0.844628	0.511355
27	1	0	3.265976	1.430314	1.030070
28	6	0	4.914696	1.802688	−0.248690
29	6	0	6.029697	2.439817	0.109204
30	1	0	1.606267	−3.083136	−2.114257
31	1	0	1.401548	0.674259	0.048510
32	1	0	2.407494	−3.537023	0.357015
33	6	0	1.690672	−1.370257	0.793525
34	6	0	2.434904	−1.242466	2.145992
35	6	0	1.989160	−2.349497	3.118042
36	1	0	2.495423	−2.224380	4.082800
37	1	0	0.912165	−2.311590	3.295031
38	1	0	2.244829	−3.346366	2.746590

39	6	0	3.977317	−1.325877	1.965766
40	1	0	4.419327	−1.675535	2.907383
41	1	0	4.185057	−2.116626	1.236878
42	6	0	4.724607	−0.037819	1.559838
43	1	0	4.895134	0.576812	2.450695
44	1	0	5.717883	−0.327317	1.196428
45	6	0	2.025616	−2.603389	−0.041048
46	6	0	0.121389	−1.349014	0.910582
47	1	0	−0.188864	−0.559352	1.598858
48	1	0	−0.257940	−2.298971	1.293861
49	6	0	0.892681	−0.394858	−2.765392
50	1	0	1.858148	−0.424546	−3.273697
51	1	0	0.571429	0.650010	−2.756410
52	1	0	0.177060	−0.973449	−3.360485
53	6	0	1.614787	−2.379674	−1.292092
54	6	0	−1.291374	−2.197805	−1.040026
55	6	0	−4.223517	1.388384	0.260675
56	6	0	−3.409131	2.458810	0.372843
57	6	0	−3.694486	3.627694	1.277582
58	1	0	−3.751231	4.549184	0.682788
59	1	0	−2.857789	3.767217	1.975535
60	1	0	−4.617421	3.499661	1.838557
61	6	0	−2.122992	2.561891	−0.427194
62	1	0	−1.686432	3.551589	−0.260106
63	1	0	−2.348626	2.507575	−1.501658
64	6	0	−1.051933	1.497540	−0.092689
65	1	0	−0.104906	1.854148	−0.508734
66	1	0	−0.917955	1.440777	0.993774
67	6	0	−5.518288	1.160445	0.987511
68	8	0	−6.052209	1.873540	1.830200
69	6	0	−6.058340	−0.109848	0.470763
70	6	0	4.315468	1.959502	−1.609190

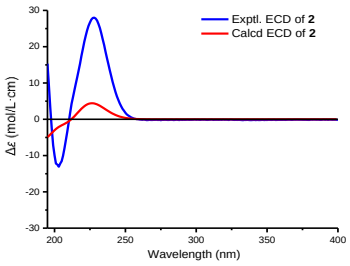
Rotational constants (GHZ): 0.1952390 0.0700479 0.0651915

Standard orientation of **22**

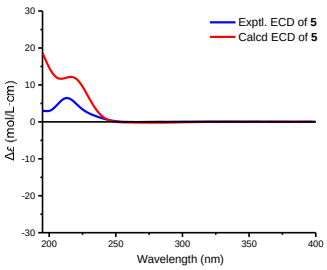
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) *X*	*Y*	*Z*
1	6	0	−3.761560	1.113056	0.061102
2	6	0	−3.126092	−0.091471	−0.676619
3	6	0	−2.202553	−0.903383	0.235074
4	6	0	−0.817600	−0.269989	0.473651
5	6	0	−0.881916	0.843496	1.529635
6	6	0	−1.521972	2.148149	1.027256
7	6	0	−3.038266	2.147051	0.830250
8	6	0	−5.142243	1.335019	−0.567483
9	6	0	−5.416663	0.017227	−1.234191
10	6	0	−4.349393	−0.789368	−1.283055
11	6	0	−4.310320	−2.128393	−1.959432
12	8	0	−3.759365	1.084553	1.507007
13	6	0	−3.649335	3.528667	0.981863
14	8	0	−1.912339	−2.198124	−0.360574
15	6	0	−0.671029	−2.604787	−0.043573
16	6	0	0.100145	−1.515034	0.711577

17	8	0	−0.291757	−3.718994	−0.351971
18	6	0	2.298954	−0.556159	2.314588
19	6	0	2.247296	−0.234609	0.999376
20	6	0	1.663980	−1.454495	0.250080
21	6	0	2.242058	−2.590151	1.146368
22	6	0	1.773486	−1.971856	2.462856
23	6	0	2.657290	1.102061	0.467891
24	6	0	3.802984	1.243600	−0.564491
25	6	0	3.758906	0.297552	−1.788215
26	6	0	3.508508	−1.189891	−1.526556
27	6	0	2.050352	−1.652185	−1.260512
28	1	0	−2.510386	0.285484	−1.510068
29	6	0	0.233632	−1.941437	2.223894
30	6	0	2.683963	0.251652	3.514662
31	8	0	1.542790	1.824478	−0.164657
32	6	0	2.050219	2.853994	−0.912710
33	6	0	3.530580	2.655916	−1.030424
34	8	0	2.131039	−3.050448	−1.558094
35	6	0	1.079728	−1.002163	−2.263653
36	8	0	1.351267	3.724992	−1.370215
37	6	0	4.347951	3.604581	−1.486600
38	1	0	−2.712540	−1.100931	1.183144
39	1	0	−0.500192	0.191056	−0.466042
40	1	0	0.128554	1.087321	1.856366
41	1	0	−1.436977	0.502406	2.409591
42	1	0	−1.301243	2.924352	1.770981
43	1	0	−1.030800	2.480883	0.105056
44	1	0	−5.872771	1.595433	0.205740
45	1	0	−5.131444	2.160802	−1.294850
46	1	0	−6.381417	−0.227145	−1.669334
47	1	0	−5.264789	−2.331400	−2.453802
48	1	0	−3.515437	−2.170110	−2.713440
49	1	0	−4.101876	−2.938972	−1.255868
50	1	0	−3.191630	4.225422	0.270770
51	1	0	−4.727788	3.525851	0.819199
52	1	0	−3.457530	3.910133	1.990499
53	1	0	3.329454	−2.653685	1.064270
54	1	0	1.804652	−3.565848	0.936230
55	1	0	2.056554	−2.478073	3.389538
56	1	0	2.949486	1.711626	1.329869
57	1	0	4.763125	1.137640	−0.049500
58	1	0	4.725784	0.407514	−2.293331
59	1	0	3.022342	0.670574	−2.506669
60	1	0	4.154041	−1.554250	−0.719397
61	1	0	3.807478	−1.743750	−2.422295
62	1	0	−0.177908	−2.941120	2.393452
63	1	0	−0.284900	−1.253384	2.893409
64	1	0	2.967090	1.281304	3.284571
65	1	0	1.852054	0.285985	4.229819
66	1	0	3.524723	−0.217707	4.040815
67	1	0	1.305315	−3.476209	−1.268921
68	1	0	1.466299	−1.149042	−3.276710
69	1	0	0.097825	−1.481016	−2.225806
70	1	0	0.939925	0.068126	−2.095178
71	1	0	5.420918	3.456418	−1.559950
72	1	0	3.944387	4.562745	−1.799791

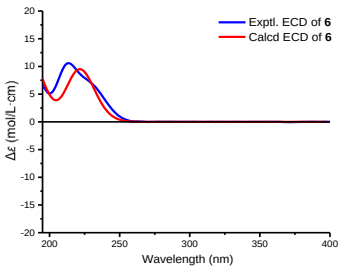
Rotational constants (GHZ): 0.1650413 0.1001960 0.0830411



UV shift: –20 nm



UV shift: –21 nm



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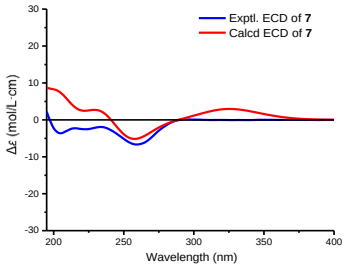
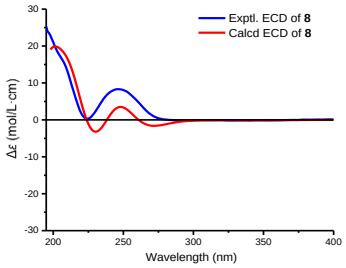
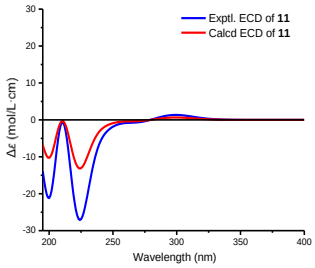


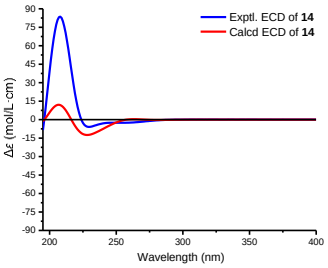
UV shift: –22 nm



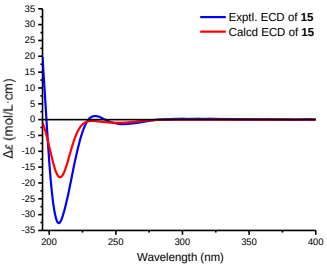
UV shift: –8 nm



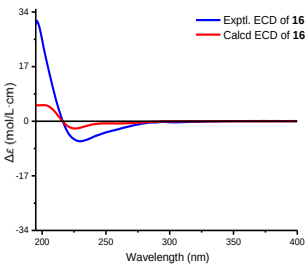
UV shift: +11 nm



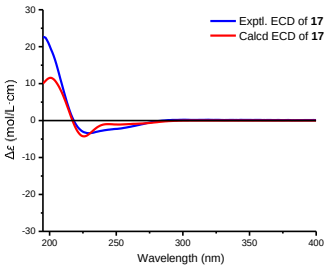
UV shift: +5 nm



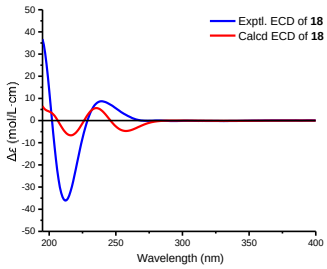
UV shift: –16 nm



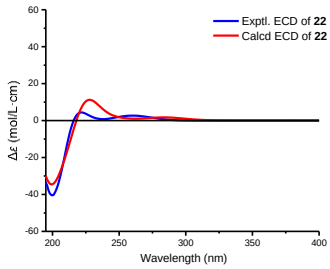
UV shift: –13 nm



UV shift: –9 nm



UV shift: –15 nm



UV shift: –14 nm

Experimental and calculated ECD spectra of compounds **2**, **5**–**8**, **11**, **14**–**18**, and **22**.

Rotatory strengths (R) in cgs (10**−40 erg−esu−cm/Gauss) of **2**.

State	*XX*	*YY*	*ZZ*	*R* (length)	*R* (au)
1	133.1744	−4.7022	−2.6571	41.9384	0.089
2	−44.7385	−4.6028	−8.3463	−19.2292	−0.0408
3	−12.6163	3.7286	−0.4505	−3.1127	−0.0066
4	90.9666	108.3398	−29.3177	56.6629	0.1202
5	8.1266	−3.7588	17.6508	7.3395	0.0156
6	−131.2087	34.9946	−124.1076	−73.4405	−0.1558
7	−11.0473	26.189	−63.6176	−16.1586	−0.0343
8	−5.7362	10.0705	−3.1343	0.4	0.0008
9	0.2111	−7.4160	−9.2398	−5.4816	−0.0116
10	−0.6132	11.1866	−29.7190	−6.3819	−0.0135
11	0.9813	−4.1206	−1.5223	−1.5539	−0.0033
12	0.9118	2.3854	−2.8811	0.1387	0.0003
13	1.6696	4.3161	9.2506	5.0787	0.0108
14	2.3152	0.3219	−9.8309	−2.3979	−0.0051
15	93.7993	−8.4584	26.4069	37.2492	0.079
16	17.7508	−18.9752	−9.0330	−3.4191	−0.0073
17	−1.1431	−33.9663	−22.7699	−19.2931	−0.0409
18	342.6336	−14.7336	−202.0599	41.9467	0.089
19	−1.4178	−4.1031	1.2475	−1.4245	−0.0030
20	−13.6109	−2.6106	−21.2928	−12.5048	−0.0265
21	18.8034	26.9587	1.1054	15.6225	0.0331
22	18.3259	−27.7308	3.2755	−2.0431	−0.0043
23	140.0256	25.5552	−121.6159	14.655	0.0311
24	−4.0388	−8.4621	−20.3339	−10.9450	−0.0232
25	7.4968	39.3862	−20.4974	8.7952	0.0187
26	29.2979	14.5095	−3.6208	13.3955	0.0284
27	−0.2347	−40.6111	16.4953	−8.1169	−0.0172
28	−0.2568	−5.2275	13.4376	2.6511	0.0056
29	5.8681	34.6987	−11.2362	9.7769	0.0207
30	36.2426	−15.7213	13.7183	11.4132	0.0242

1/2[<0|del|b>*<b|r|0> + (<0|r|b>*<b|del|0>)*] (Au)

State	*X*	*Y*	*Z*	Dip. S.	Osc.(frdel)
1	−0.0603	−0.0080	−0.0016	0.0699	0.0466
2	−0.0081	−0.0023	−0.0035	0.0139	0.0093
3	−0.0012	−0.0002	0.0000	0.0015	0.0010
4	−0.0302	−0.0059	−0.0076	0.0436	0.0291
5	−0.0001	−0.0002	−0.0008	0.0011	0.0007
6	−0.1102	−0.0624	−0.0159	0.1886	0.1257
7	−0.0076	−0.0016	−0.0263	0.0354	0.0236
8	−0.0023	−0.0006	−0.0008	0.0037	0.0025
9	−0.0173	−0.0005	−0.0007	0.0185	0.0123
10	0.0000	−0.0019	−0.0133	0.0152	0.0102
11	−0.0001	0.0000	−0.0003	0.0004	0.0002
12	−0.0043	−0.0017	−0.0038	0.0098	0.0065
13	−0.0010	−0.0040	−0.0004	0.0054	0.0036

14	−0.0002	−0.0054	−0.0004	0.0059	0.0040
15	−0.0249	−0.0026	−0.0051	0.0326	0.0217
16	−0.0036	−0.0006	−0.0036	0.0078	0.0052
17	−0.0086	−0.0020	−0.0038	0.0144	0.0096
18	−0.1450	−0.0001	−0.0337	0.1788	0.1192
19	−0.0007	−0.0005	0.0000	0.0013	0.0009
20	−0.0134	−0.0001	−0.0036	0.0171	0.0114
21	−0.0105	−0.0034	−0.0026	0.0165	0.0110
22	−0.0093	−0.0011	−0.0020	0.0124	0.0083
23	−0.1347	−0.0006	−0.0049	0.1402	0.0934
24	−0.0149	−0.0108	−0.0013	0.0271	0.0180
5	−0.0196	−0.0040	−0.0009	0.0245	0.0163
26	−0.0098	−0.0050	−0.0001	0.0149	0.0099
27	0.0000	−0.0056	−0.0040	0.0097	0.0064
28	0.0000	−0.0008	−0.0012	0.0019	0.0013
29	−0.0018	−0.0134	−0.0006	0.0158	0.0106
30	−0.0180	−0.0070	−0.0006	0.0256	0.0171

Ground to Excited state transition densities written to RWF 633

Excitation energies and oscillator strengths of **2**

Excited state 1: Singlet−A 5.0782 eV 244.15 nm *f*=0.0466 <S**2>=0.000
133 −> 134 0.60169
133 −> 135 0.30588
133 −> 136 −0.12588
This state for optimization and/or second−order correction.
Copying the Excited state density for this state as the 1−particle RhoCI density.

Excited state 2: Singlet−A 5.3760 eV 230.63 nm *f*=0.0093 <S**2>=0.000
129 −> 135 0.10977
133 −> 134 −0.28725
133 −> 135 0.61381
133 −> 136 0.11315

Excited state 3: Singlet−A 5.5226 eV 224.50 nm *f*=0.0011 <S**2>=0.000
128 −> 134 −0.13914
130 −> 134 −0.10952
132 −> 134 0.60053
132 −> 135 0.26902

Excited state 4: Singlet−A 5.7169 eV 216.87 nm *f*=0.0289 <S**2>=0.000
128 −> 135 −0.22197
129 −> 134 −0.26780
129 −> 135 0.43172
129 −> 136 0.19829
130 −> 135 −0.10783
133 −> 134 0.14960
133 −> 135 −0.10650
133 −> 136 0.14598

Excited state 5:	Singlet−A	5.7173 eV	216.86 nm	*f*=0.0008	<S**2>=0.000
128 −> 134	0.37320				
128 −> 135	0.15022				
128 −> 136	−0.11738				
129 −> 135	0.23592				
130 −> 134	0.28553				
130 −> 135	0.13642				
131 −> 134	0.18169				
131 −> 135	0.10585				
132 −> 134	0.22739				
133 −> 135	−0.11249				
Excited state 6:	Singlet−A	5.7763 eV	214.64 nm	*f*=0.1271	<S**2>=0.000
129 −> 135	−0.18236				
133 −> 134	0.12359				
133 −> 136	0.57220				
133 −> 137	−0.25041				
133 −> 138	−0.12430				
Excited state 7:	Singlet−A	5.8608 eV	211.55 nm	*f*=0.0238	<S**2>=0.000
133 −> 136	0.28790				
133 −> 137	0.54810				
133 −> 138	0.27860				
Excited state 8:	Singlet−A	5.8933 eV	210.38 nm	*f*=0.0025	<S**2>=0.000
132 −> 134	−0.27334				
132 −> 135	0.59479				
132 −> 136	−0.21935				
Excited state 9:	Singlet−A	5.9390 eV	208.76 nm	*f*=0.0127	<S**2>=0.000
132 −> 136	0.11233				
132 −> 137	0.54440				
132 −> 138	−0.19413				
132 −> 140	0.29509				
132 −> 142	−0.13912				
132 −> 143	0.14287				
Excited state 10:	Singlet−A	6.0709 eV	204.23 nm	*f*=0.0099	<S**2>=0.000
133 −> 137	−0.27469				
133 −> 138	0.52395				
133 −> 141	−0.35490				
Excited state 11:	Singlet−A	6.0988 eV	203.29 nm	*f*=0.0003	<S**2>=0.000
132 −> 135	0.23468				
132 −> 136	0.63664				
Excited state 12:	Singlet−A	6.1210 eV	202.56 nm	*f*=0.0065	<S**2>=0.000
133 −> 139	0.60438				
133 −> 140	−0.31549				
133 −> 143	0.12872				
Excited state 13:	Singlet−A	6.1636 eV	201.16 nm	*f*=0.0035	<S**2>=0.000
133 −> 137	−0.15601				
133 −> 138	0.27180				
133 −> 139	−0.12026				
133 −> 140	−0.12377				

133 −> 141	0.57927				
Excited state 14:	Singlet−A	6.2370 eV	198.79 nm	*f*=0.0040	<S**2>=0.000
130 −> 134	−0.10148				
133 −> 138	0.18136				
133 −> 139	0.26233				
133 −> 140	0.50690				
133 −> 141	0.12870				
133 −> 142	0.28924				
Excited state 15:	Singlet−A	6.2851 eV	197.27 nm	*f*=0.0216	<S**2>=0.000
128 −> 134	−0.35613				
128 −> 135	−0.10678				
130 −> 134	0.49125				
130 −> 136	0.14737				
131 −> 134	0.17895				
133 −> 140	0.12784				
Excited state 16:	Singlet−A	6.3310 eV	195.84 nm	*f*=0.0052	<S**2>=0.000
132 −> 137	0.40131				
132 −> 138	0.24921				
132 −> 139	0.27337				
132 −> 140	−0.28737				
132 −> 142	0.19016				
132 −> 143	−0.18865				
132 −> 144	0.13019				
Excited state 17:	Singlet−A	6.3427 eV	195.47 nm	*f*=0.0098	<S**2>=0.000
132 −> 136	−0.10986				
132 −> 138	−0.37435				
132 −> 139	0.45236				
132 −> 142	−0.28124				
132 −> 143	−0.10267				
Excited state 18:	Singlet−A	6.3508 eV	195.23 nm	*f*=0.1206	<S**2>=0.000
132 −> 138	0.38841				
132 −> 139	0.28599				
132 −> 140	0.34398				
132 −> 141	−0.20480				
132 −> 142	−0.12748				
132 −> 144	−0.19213				
Excited state 19:	Singlet−A	6.4238 eV	193.01 nm	*f*=0.0009	<S**2>=0.000
131 −> 134	0.15538				
133 −> 140	−0.29236				
133 −> 142	0.51284				
133 −> 143	−0.22241				
133 −> 144	−0.14866				
Excited state 20:	Singlet−A	6.4292 eV	192.85 nm	*f*=0.0118	<S**2>=0.000
130 −> 134	−0.18598				
131 −> 134	0.43699				
131 −> 135	0.21520				
133 −> 142	−0.26007				
133 −> 143	−0.30472				
Excited state 21:	Singlet−A	6.4412 eV	192.48 nm	*f*=0.0111	<S**2>=0.000

130 −> 134 −0.18104
130 −> 135 −0.15336
131 −> 134 0.35146
131 −> 135 0.10171
133 −> 142 0.10308
133 −> 143 0.49840

Excited state 22: Singlet−A 6.4824 eV 191.26 nm *f*=0.0082 <S**2>=0.000
128 −> 134 −0.13808
128 −> 135 −0.11502
129 −> 134 −0.13842
130 −> 135 0.39375
130 −> 136 −0.36631
131 −> 135 0.16236
131 −> 136 −0.15987
133 −> 143 0.17837
133 −> 144 0.13139

Excited state 23: Singlet−A 6.5740 eV 188.60 nm *f*=0.0948 <S**2>=0.000
131 −> 137 0.10560
132 −> 138 0.19392
132 −> 141 0.55701
132 −> 142 −0.25522
132 −> 143 0.11047
132 −> 144 0.13267

Excited state 24: Singlet−A 6.5971 eV 187.94 nm *f*=0.0183 <S**2>=0.000
129 −> 134 0.10174
132 −> 140 −0.13410
132 −> 142 −0.14615
133 −> 142 0.14030
133 −> 143 −0.10183
133 −> 144 0.57603
133 −> 146 0.13340

Excited state 25: Singlet−A 6.6099 eV 187.57 nm *f*=0.0164 <S**2>=0.000
132 −> 138 −0.15934
132 −> 139 0.22788
132 −> 140 0.30677
132 −> 141 0.23664
132 −> 142 0.39897
132 −> 145 0.10028
132 −> 146 −0.12548
133 −> 144 0.18801

Excited state 26: Singlet−A 6.6293 eV 187.02 nm *f*=0.0099 <S**2>=0.000
126 −> 134 0.15076
128 −> 135 −0.23013
128 −> 136 0.17011
129 −> 134 0.46198
129 −> 136 0.30156
130 −> 135 0.12249
130 −> 136 −0.10528
133 −> 144 −0.11676

Excited state 27: Singlet−A 6.6657 eV 186.00 nm *f*=0.0065 <S**2>=0.000
132 −> 139 0.22674

132 −> 140 −0.19676
132 −> 142 0.11069
132 −> 143 0.47711
132 −> 144 −0.19337
132 −> 145 0.22011
132 −> 146 0.10137
132 −> 147 −0.11438
133 −> 145 −0.13168

Excited state 28: Singlet−A 6.6755 eV 185.73 nm *f*=0.0013 <S**2>=0.000
128 −> 134 −0.22836
128 −> 135 0.18219
128 −> 136 −0.25668
129 −> 134 0.24361
129 −> 135 0.13653
131 −> 134 −0.17217
131 −> 135 0.38177
131 −> 136 −0.20658

Excited state 29: Singlet−A 6.6927 eV 185.25 nm *f*=0.0109 <S**2>=0.000
132 −> 143 0.11645
133 −> 144 −0.14867
133 −> 145 0.47017
133 −> 146 0.33434
133 −> 147 0.23033
133 −> 148 −0.15113
133 −> 150 −0.10721

Excited state 30: Singlet−A 6.7327 eV 184.15 nm *f*=0.0171 <S**2>=0.000
128 −> 134 −0.11920
128 −> 135 0.11587
128 −> 136 −0.14658
130 −> 135 0.10828
131 −> 136 0.20762
131 −> 137 0.43667
131 −> 138 −0.27286
132 −> 141 −0.17305
132 −> 144 0.17787
132 −> 149 −0.10757
SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 LETran= 520.

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Rotatory strengths (R) in cgs (10**−40 erg−esu−cm/Gauss) of **5**.

State	*X*	*Y*	*Z*	Dip. S.	Osc.(frdel)
1	−0.0603	−0.0080	−0.0016	0.0699	0.0466
2	−0.0081	−0.0023	−0.0035	0.0139	0.0093
3	−0.0012	−0.0002	0.0000	0.0015	0.0010
4	−0.0302	−0.0059	−0.0076	0.0436	0.0291
5	−0.0001	−0.0002	−0.0008	0.0011	0.0007
6	−0.1102	−0.0624	−0.0159	0.1886	0.1257
7	−0.0076	−0.0016	−0.0263	0.0354	0.0236
8	−0.0023	−0.0006	−0.0008	0.0037	0.0025
9	−0.0173	−0.0005	−0.0007	0.0185	0.0123

10	0.0000	−0.0019	−0.0133	0.0152	0.0102
11	−0.0001	0.0000	−0.0003	0.0004	0.0002
12	−0.0043	−0.0017	−0.0038	0.0098	0.0065
13	−0.0010	−0.0040	−0.0004	0.0054	0.0036
14	−0.0002	−0.0054	−0.0004	0.0059	0.0040
15	−0.0249	−0.0026	−0.0051	0.0326	0.0217
16	−0.0036	−0.0006	−0.0036	0.0078	0.0052
17	−0.0086	−0.0020	−0.0038	0.0144	0.0096
18	−0.1450	−0.0001	−0.0337	0.1788	0.1192
19	−0.0007	−0.0005	0.0000	0.0013	0.0009
20	−0.0134	−0.0001	−0.0036	0.0171	0.0114
21	−0.0105	−0.0034	−0.0026	0.0165	0.0110
22	−0.0093	−0.0011	−0.0020	0.0124	0.0083
23	−0.1347	−0.0006	−0.0049	0.1402	0.0934
24	−0.0149	−0.0108	−0.0013	0.0271	0.0180
25	−0.0196	−0.0040	−0.0009	0.0245	0.0163
26	−0.0098	−0.0050	−0.0001	0.0149	0.0099
27	0.0000	−0.0056	−0.0040	0.0097	0.0064
28	0.0000	−0.0008	−0.0012	0.0019	0.0013
29	−0.0018	−0.0134	−0.0006	0.0158	0.0106
30	−0.0180	−0.0070	−0.0006	0.0256	0.0171

1/2[<0|del|b>*<b|r|0> + (<0|r|b>*<b|del|0>)*] (Au)

State	*X*	*Y*	*Z*	Dip. S.	Osc.(frdel)
1	−0.0023	−0.0011	−0.0008	0.0042	0.0028
2	0.0000	0.0000	0.0000	0.0000	0.0000
3	−0.0014	−0.0016	−0.0002	0.0031	0.0021
4	−0.0331	−0.0003	−0.0039	0.0373	0.0249
5	−0.0102	−0.0045	−0.0037	0.0184	0.0123
6	−0.0024	−0.0017	−0.0012	0.0053	0.0035
7	−0.0141	−0.0114	−0.0046	0.0301	0.0201
8	−0.1599	−0.1263	−0.0447	0.3309	0.2206
9	−0.0020	−0.0006	−0.0004	0.0030	0.0020
10	−0.0202	−0.0097	−0.0111	0.0410	0.0273
11	−0.0044	−0.0049	−0.0002	0.0096	0.0064
12	0.0000	−0.0002	−0.0002	0.0003	0.0002
13	−0.0738	−0.0029	−0.0017	0.0785	0.0523
14	−0.0153	−0.0818	−0.0098	0.1068	0.0712
15	−0.0117	−0.0055	−0.0007	0.0178	0.0119
16	−0.0230	−0.0015	−0.0094	0.0338	0.0226
17	−0.0136	−0.0024	−0.0007	0.0167	0.0111
18	−0.0004	0.0000	−0.0014	0.0018	0.0012
19	−0.0004	−0.0006	−0.0009	0.0019	0.0013
20	−0.0481	−0.0045	−0.0103	0.0628	0.0419

21	−0.0001	−0.0001	−0.0018	0.0019	0.0013
22	−0.0075	−0.0005	−0.0184	0.0264	0.0176
23	−0.0576	−0.0187	−0.0065	0.0828	0.0552
24	0.0000	0.0000	−0.0017	0.0018	0.0012
25	−0.0426	−0.0233	−0.0027	0.0686	0.0457
26	−0.0178	−0.0016	−0.0056	0.0250	0.0167
27	−0.0113	−0.0005	−0.0006	0.0124	0.0083
28	−0.0002	−0.0034	−0.0017	0.0053	0.0036
29	−0.0147	0.0000	−0.0127	0.0275	0.0183
30	−0.0038	−0.0015	−0.0007	0.0061	0.0041

Ground to Excited state transition densities written to RWF 633

Excitation energies and oscillator strengths:

Excited state 1: Singlet−A 4.1082 eV 301.79 nm *f*=0.0028 <S**2>=0.000
132 −>133 0.70653
This state for optimization and/or second−order correction.
Copying the Excited state density for this state as the 1−particle RhoCI density.

Excited state 2: Singlet−A 4.5506 eV 272.46 nm *f*=0.0000 <S**2>=0.000
131 −>133 0.70668

Excited state 3: Singlet−A 4.7689 eV 259.99 nm *f*=0.0020 <S**2>=0.000
123 −>133 0.12061
125 −>133 0.59778
127 −>133 −0.19304
128 −>133 −0.17695
129 −>133 −0.20324

Excited state 4: Singlet−A 5.1428 eV 241.08 nm *f*=0.0250 <S**2>=0.000
128 −>134 −0.13121
132 −>134 0.68505

Excited state 5: Singlet−A 5.2871 eV 234.50 nm *f*=0.0125 <S**2>=0.000
125 −>133 0.14327
127 −>133 −0.13219
129 −>133 0.51840
130 −>133 0.42824

Excited state 6: Singlet−A 5.3719 eV 230.80 nm *f*=0.0035 <S**2>=0.000
125 −>133 −0.11103
127 −>133 0.12162
128 −>133 −0.10860
129 −>133 −0.39294
130 −>133 0.55115

Excited state 7: Singlet−A 5.4932 eV 225.71 nm *f*=0.0204 <S**2>=0.000
127 −>133 −0.29445
128 −>133 0.61302
129 −>133 −0.11516
130 −>133 0.10529

Excited state 8: Singlet−A 5.5882 eV 221.87 nm *f*=0.2233 <S**2>=0.000
123 −>133 −0.16923

124 −>133	0.10093				
125 −>133	0.30067				
127 −>133	0.52811				
128 −>133	0.26729				
Excited state 9:	Singlet−A	5.6405 eV	219.81 nm	*f*=0.0020	<S**2>=0.000
128 −>134	0.32459				
129 −>134	−0.14241				
130 −>134	−0.15408				
131 −>134	0.56686				
132 −>134	0.10261				
Excited state 10:	Singlet−A	5.7472 eV	215.73 nm	*f*=0.0275	<S**2>=0.000
132 −>135	0.60051				
132 −>136	0.15748				
132 −>137	−0.25159				
132 −>138	−0.15460				
Excited state 11:	Singlet−A	5.7835 eV	214.38 nm	*f*=0.0064	<S**2>=0.000
126 −>133	0.70189				
Excited state 12:	Singlet−A	5.7993 eV	213.79 nm	*f*=0.0002	<S**2>=0.000
128 −>134	0.44197				
129 −>134	−0.19369				
130 −>134	−0.21285				
131 −>134	−0.41052				
132 −>134	0.12279				
Excited state 13:	Singlet−A	5.8723 eV	211.13 nm	*f*=0.0523	<S**2>=0.000
132 −>135	0.34110				
132 −>136	−0.30925				
132 −>137	0.38265				
132 −>138	0.31300				
132 −>140	−0.12867				
Excited state 14:	Singlet−A	5.9248 eV	209.26 nm	*f*=0.0708	<S**2>=0.000
123 −>133	0.52417				
124 −>133	−0.36783				
127 −>133	0.21854				
129 −>133	0.12457				
Excited state 15:	Singlet−A	5.9298 eV	209.09 nm	*f*=0.0122	<S**2>=0.000
131 −>135	0.35207				
131 −>136	0.45144				
131 −>137	0.18782				
131 −>140	0.28608				
131 −>141	−0.12346				
131 −>142	−0.11481				
Excited state 16:	Singlet−A	6.0067 eV	206.41 nm	*f*=0.0225	<S**2>=0.000
132 −>136	0.53450				
132 −>137	0.39179				
132 −>139	0.14566				
132 −>141	0.11349				
Excited state 17:	Singlet−A	6.0433 eV	205.16 nm	*f*=0.0110	<S**2>=0.000
132 −>136	0.19151				
132 −>137	−0.19946				

132 −>138	0.48046				
132 −>139	−0.39919				
Excited state 18:	Singlet−A	6.0777 eV	204.00 nm	*f*=0.0013	<S**2>=0.000
131 −>135	0.57469				
131 −>136	−0.32911				
131 −>140	−0.14476				
131 −>142	0.13642				
Excited state 19:	Singlet−A	6.0925 eV	203.50 nm	*f*=0.0013	<S**2>=0.000
122 −>133	−0.15521				
123 −>133	0.36903				
124 −>133	0.57861				
Excited state 20:	Singlet−A	6.1610 eV	201.24 nm	*f*=0.0421	<S**2>=0.000
132 −>137	−0.28432				
132 −>138	0.30756				
132 −>139	0.49775				
132 −>140	−0.21737				
Excited state 21:	Singlet−A	6.2256 eV	199.15 nm	*f*=0.0013	<S**2>=0.000
132 −>136	−0.13036				
132 −>138	0.11207				
132 −>139	0.20687				
132 −>140	0.50354				
132 −>141	0.32460				
132 −>142	−0.14917				
132 −>143	−0.10799				
132 −>144	0.10146				
Excited state 22:	Singlet−A	6.2573 eV	198.14 nm	*f*=0.0179	<S**2>=0.000
113 −>133	−0.11096				
119 −>133	−0.22398				
120 −>133	0.50072				
121 −>133	−0.32117				
122 −>133	0.20778				
Excited state 23:	Singlet−A	6.3201 eV	196.17 nm	*f*=0.0560	<S**2>=0.000
131 −>135	−0.12247				
131 −>137	0.59517				
131 −>138	−0.17984				
131 −>140	−0.15999				
131 −>143	0.18413				
Excited state 24:	Singlet−A	6.3325 eV	195.79 nm	*f*=0.0012	<S**2>=0.000
120 −>133	−0.11032				
121 −>133	0.22496				
122 −>133	0.63392				
123 −>133	0.13699				
Excited state 25:	Singlet−A	6.3438 eV	195.44 nm	*f*=0.0462	<S**2>=0.000
131 −>136	−0.24705				
131 −>137	0.13042				
131 −>138	0.38708				
131 −>140	0.29722				
131 −>141	−0.31615				
131 −>142	0.12471				

131 ->143 -0.11413
131 ->146 0.11333

Excited state 26: Singlet-A 6.3682 eV 194.69 nm *f*=0.0170 <S**2>=0.000
131 ->136 0.30032
131 ->138 0.40660
131 ->140 -0.32998
131 ->142 0.30333
131 ->145 0.10806

Excited state 27: Singlet-A 6.3960 eV 193.85 nm *f*=0.0083 <S**2>=0.000
132 ->138 -0.12189
132 ->140 -0.39327
132 ->141 0.46795
132 ->142 -0.21144
132 ->143 -0.11146
132 ->146 0.11266

Excited state 28: Singlet-A 6.4373 eV 192.60 nm *f*=0.0036 <S**2>=0.000
132 ->141 0.29178
132 ->142 0.60981
132 ->145 -0.11262

Excited state 29: Singlet-A 6.4813 eV 191.29 nm *f*=0.0185 <S**2>=0.000
119 ->133 0.48801
120 ->133 0.42128
121 ->133 0.22189

Excited state 30: Singlet-A 6.5136 eV 190.35 nm *f*=0.0041 <S**2>=0.000
132 ->143 0.50653
132 ->144 0.43652
132 ->146 0.12375
SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 LETran= 520.

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Rotatory strengths (R) in cgs (10**-40 erg-esu-cm/Gauss) of **6**.

State	*XX*	*YY*	*ZZ*	*R* (length)	*R* (au)
1	61.9263	-6.0644	11.2607	22.3742	0.0475
2	-0.3340	2.1565	0.1289	0.6505	0.0014
3	-5.1453	-0.3589	-1.2409	-2.2483	-0.0048
4	18.1441	-0.5436	-15.8431	0.5858	0.0012
5	143.1945	-52.4799	-83.5875	2.3757	0.0050
6	5.5952	5.5298	-1.0662	3.3529	0.0071
7	93.0600	-36.0326	-23.8204	11.0690	0.0235
8	-0.6222	-0.2492	-0.2871	-0.3862	-0.0008
9	-11.8283	-0.9271	-7.9217	-6.8924	-0.0146
10	128.4627	-26.9986	-128.0593	-8.8651	-0.0188
11	-8.6919	13.4795	36.2785	13.6887	0.0290
12	0.0399	1.0178	-13.4273	-4.1232	-0.0087
13	186.8732	-42.0537	-79.2831	21.8455	0.0463
14	31.0577	-7.1806	-21.4940	0.7944	0.0017

15	103.6131	116.4600	−195.5100	8.1877	0.0174
16	30.4493	10.6933	−10.6367	10.1686	0.0216
17	3.9076	−0.5164	18.6239	7.3384	0.0156
18	8.9034	23.2970	−61.0778	−9.6258	−0.0204
19	0.3119	−8.8786	3.6702	−1.6322	−0.0035
20	−25.0679	−5.2705	6.7871	−7.8504	−0.0167
21	1.8112	25.1542	−23.0182	1.3157	0.0028
22	−0.7354	4.0843	2.5659	1.9716	0.0042
23	−5.7119	4.4497	−15.2864	−5.5162	−0.0117
24	−15.0062	−4.3154	−7.6858	−9.0025	−0.0191
25	11.2771	−4.1600	17.4434	8.1868	0.0174
26	5.7852	−18.8080	7.7710	−1.7506	−0.0037
27	3.7937	−13.8979	82.3483	24.0813	0.0511
28	21.9607	5.4270	−25.1064	0.7605	0.0016
29	2.4884	−2.1023	18.7883	6.3915	0.0136
30	23.5433	−60.2972	22.7585	−4.6651	−0.0099

1/2[<0|del|b>*<b|r|0> + (<0|r|b>*<b|del|0>)*] (Au)

State	*X*	*Y*	*Z*	Dip. S.	Osc.(frdel)
1	−0.0328	−0.0004	−0.0036	0.0368	0.0245
2	0.0000	−0.0007	−0.0001	0.0007	0.0005
3	−0.0002	0.0000	−0.0001	0.0002	0.0002
4	−0.0024	0.0000	−0.0001	0.0026	0.0017
5	−0.0247	−0.0066	−0.0123	0.0436	0.0290
6	−0.0002	−0.0001	−0.0001	0.0003	0.0002
7	−0.0552	−0.0015	−0.0009	0.0576	0.0384
8	−0.0001	0.0000	0.0000	0.0001	0.0001
9	−0.0143	−0.0026	−0.0002	0.0170	0.0114
10	−0.0453	−0.0017	−0.0130	0.0599	0.0400
11	−0.0079	−0.0032	−0.0022	0.0132	0.0088
12	−0.0006	0.0000	−0.0024	0.0030	0.0020
13	−0.0609	−0.0027	−0.0070	0.0705	0.0470
14	−0.0039	−0.0002	−0.0035	0.0076	0.0051
15	−0.0892	−0.0327	−0.0082	0.1302	0.0868
16	−0.0044	−0.0066	−0.0005	0.0115	0.0077
17	−0.0139	−0.0023	−0.0008	0.0170	0.0113
18	−0.0179	−0.0018	−0.0043	0.0240	0.0160
19	0.0000	−0.0038	−0.0018	0.0056	0.0037
20	−0.0044	−0.0024	−0.0003	0.0071	0.0048
21	−0.0757	−0.0305	−0.0001	0.1063	0.0709
22	−0.0001	−0.0001	−0.0038	0.0039	0.0026
23	−0.0010	−0.0001	−0.0034	0.0045	0.0030
24	−0.0330	−0.0115	−0.0001	0.0446	0.0297
25	−0.0010	−0.0001	−0.0050	0.0061	0.0041

26	−0.0060	−0.0024	−0.0003	0.0087	0.0058
27	−0.0027	−0.0060	−0.0085	0.0173	0.0115
28	−0.0007	−0.0007	−0.0018	0.0031	0.0021
29	−0.0008	−0.0005	−0.0011	0.0024	0.0016
30	−0.0135	−0.0135	−0.0006	0.0276	0.0184

Ground to Excited state transition densities written to RWF 633
Excitation energies and oscillator strengths:

Excited state 1: Singlet−A 5.1273 eV 241.81 nm *f*=0.0246 <S**2>=0.000
129 −> 135 0.12000
133 −> 134 −0.16691
133 −> 135 0.66569
This state for optimization and/or second−order correction.
Copying the Excited state density for this state as the 1−particle RhoCI density.

Excited state 2: Singlet−A 5.4142 eV 229.00 nm *f*=0.0005 <S**2>=0.000
133 −> 134 0.68439
133 −> 135 0.16679

Excited state 3: Singlet−A 5.6422 eV 219.75 nm *f*=0.0002 <S**2>=0.000
128 −> 135 0.10145
129 −> 135 0.32511
130 −> 135 −0.13308
131 −> 135 −0.16608
132 −> 134 −0.13776
132 −> 135 0.53533
133 −> 135 −0.10840

Excited state 4: Singlet−A 5.6839 eV 218.13 nm *f*=0.0014 <S**2>=0.000
128 −> 134 0.58094
129 −> 134 −0.25737
130 −> 134 −0.17058

Excited state 5: Singlet−A 5.7304 eV 216.36 nm *f*=0.0292 <S**2>=0.000
133 −> 136 0.61146
133 −> 137 0.10411
133 −> 138 −0.28342
133 −> 139 −0.10489

Excited state 6: Singlet−A 5.7994 eV 213.79 nm *f*=0.0002 <S**2>=0.000
128 −> 135 0.12565
129 −> 135 0.40804
130 −> 135 −0.16607
131 −> 135 −0.21126
132 −> 134 0.15630
132 −> 135 −0.40401
133 −> 135 −0.11420

Excited state 7: Singlet−A 5.8461 eV 212.08 nm *f*=0.0385 <S**2>=0.000
133 −> 136 0.32399
133 −> 137 −0.21462
133 −> 138 0.46996
133 −> 139 0.29800

Excited state 8: Singlet−A 5.9049 eV 209.97 nm *f*=0.0001 <S**2>=0.000

132 −> 134	0.66031				
132 −> 135	0.20141				
Excited state 9:	Singlet−A	5.9306 eV	209.06 nm	*f*=0.0117	<S**2>=0.000
132 −> 134	−0.13765				
132 −> 136	0.35617				
132 −> 137	0.45474				
132 −> 141	0.30012				
132 −> 143	−0.14435				
Excited state 10:	Singlet−A	5.9794 eV	207.35 nm	*f*=0.0399	<S**2>=0.000
133 −> 137	0.60554				
133 −> 138	0.25806				
133 −> 140	−0.14777				
133 −> 142	0.13303				
Excited state 11:	Singlet−A	6.0129 eV	206.20 nm	*f*=0.0088	<S**2>=0.000
133 −> 137	0.13674				
133 −> 138	−0.16818				
133 −> 139	0.37068				
133 −> 140	0.53140				
133 −> 142	0.10685				
Excited state 12:	Singlet−A	6.0850 eV	203.75 nm	*f*=0.0021	<S**2>=0.000
132 −> 136	0.56475				
132 −> 137	−0.32757				
132 −> 141	−0.14485				
132 −> 143	0.13654				
Excited state 13:	Singlet−A	6.1138 eV	202.79 nm	*f*=0.0471	<S**2>=0.000
132 −> 136	0.10316				
133 −> 138	−0.27907				
133 −> 139	0.46994				
133 −> 140	−0.40732				
Excited state 14:	Singlet−A	6.2092 eV	199.68 nm	*f*=0.0051	<S**2>=0.000
133 −> 137	−0.13743				
133 −> 141	0.49959				
133 −> 142	0.40829				
133 −> 144	0.11451				
133 −> 147	−0.11466				
Excited state 15:	Singlet−A	6.3289 eV	195.90 nm	*f*=0.0880	<S**2>=0.000
132 −> 138	0.47810				
132 −> 139	−0.34643				
132 −> 140	−0.13273				
132 −> 141	−0.20888				
132 −> 144	−0.22509				
Excited state 16:	Singlet−A	6.3419 eV	195.50 nm	*f*=0.0077	<S**2>=0.000
132 −> 136	−0.12000				
132 −> 137	−0.16793				
132 −> 138	0.34256				
132 −> 139	0.22596				
132 −> 141	0.21330				
132 −> 142	−0.31373				
132 −> 146	0.12893				

133 −> 141	0.21661				
133 −> 142	−0.22385				
Excited state 17:	Singlet−A	6.3549 eV	195.10 nm	*f*=0.0114	<S**2>=0.000
132 −> 138	−0.15197				
132 −> 139	−0.15499				
132 −> 141	−0.13044				
132 −> 142	0.16903				
133 −> 141	0.41687				
133 −> 142	−0.40680				
133 −> 144	−0.11847				
133 −> 147	0.11091				
Excited state 18:	Singlet−A	6.3672 eV	194.72 nm	*f*=0.0162	<S**2>=0.000
132 −> 137	0.32938				
132 −> 139	0.41873				
132 −> 140	−0.11734				
132 −> 141	−0.31213				
132 −> 142	−0.13316				
132 −> 143	0.24130				
Excited state 19:	Singlet−A	6.4364 eV	192.63 nm	*f*=0.0037	<S**2>=0.000
133 −> 143	0.66117				
133 −> 146	0.12665				
Excited state 20:	Singlet−A	6.4791 eV	191.36 nm	*f*=0.0048	<S**2>=0.000
133 −> 142	−0.14884				
133 −> 144	0.65759				
133 −> 147	0.11009				
Excited state 21:	Singlet−A	6.4954 eV	190.88 nm	*f*=0.0718	<S**2>=0.000
132 −> 140	0.64767				
132 −> 141	−0.19442				
Excited state 22:	Singlet−A	6.5105 eV	190.44 nm	*f*=0.0027	<S**2>=0.000
133 −> 142	0.10339				
133 −> 143	0.13737				
133 −> 145	0.65179				
Excited state 23:	Singlet−A	6.5488 eV	189.32 nm	*f*=0.0031	<S**2>=0.000
132 −> 138	0.27590				
132 −> 139	0.29770				
132 −> 142	0.49697				
132 −> 143	−0.19365				
132 −> 147	0.15350				
Excited state 24:	Singlet−A	6.5794 eV	188.44 nm	*f*=0.0304	<S**2>=0.000
129 −> 135	0.23158				
130 −> 135	−0.14694				
131 −> 134	−0.23610				
131 −> 135	0.59103				
Excited state 25:	Singlet−A	6.6087 eV	187.61 nm	*f*=0.0042	<S**2>=0.000
128 −> 134	0.12743				
130 −> 134	0.55404				
131 −> 134	0.33400				
131 −> 135	0.16004				

Excited state 26:	Singlet−A	6.6664 eV	185.98 nm	*f*=0.0058	<S**2>=0.000
131 −> 136	−0.11199				
132 −> 138	0.11828				
132 −> 141	0.30481				
132 −> 142	0.16621				
132 −> 143	0.44888				
132 −> 144	0.10204				
132 −> 146	−0.29244				
132 −> 147	−0.14318				
Excited state 27:	Singlet−A	6.6791 eV	185.63 nm	*f*=0.0118	<S**2>=0.000
130 −> 135	0.16219				
130 −> 136	0.20659				
130 −> 137	−0.11502				
131 −> 136	0.46129				
131 −> 137	0.16549				
131 −> 138	0.13187				
132 −> 144	−0.16731				
132 −> 146	−0.10694				
133 −> 148	−0.10840				
Excited state 28:	Singlet−A	6.6929 eV	185.25 nm	*f*=0.0021	<S**2>=0.000
128 −> 135	0.11114				
129 −> 135	0.17459				
130 −> 135	0.50202				
130 −> 136	0.17253				
130 −> 138	−0.15233				
130 −> 140	0.13451				
131 −> 136	−0.11860				
131 −> 137	−0.12812				
131 −> 138	−0.11277				
132 −> 144	0.15024				
Excited state 29:	Singlet−A	6.7086 eV	184.81 nm	*f*=0.0016	<S**2>=0.000
129 −> 134	−0.13229				
129 −> 136	0.11610				
130 −> 134	−0.23763				
130 −> 135	0.15967				
130 −> 136	−0.27255				
131 −> 134	0.37505				
131 −> 135	0.13019				
131 −> 137	0.19934				
132 −> 144	−0.15430				
133 −> 148	0.14029				
Excited state 30:	Singlet−A	6.7178 eV	184.56 nm	*f*=0.0189	<S**2>=0.000
129 −> 136	−0.13676				
130 −> 134	−0.22289				
130 −> 135	−0.10654				
130 −> 136	0.13310				
130 −> 138	0.10762				
131 −> 134	0.38211				
131 −> 135	0.11779				
131 −> 137	−0.20990				
132 −> 144	0.24331				
133 −> 147	−0.10108				

133 −> 148 −0.14412
SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 LETran= 520.
****
Rotatory strengths (R) in cgs (10**−40 erg−esu−cm/Gauss) of **7**.

State	*XX*	*YY*	*ZZ*	*R* (length)	*R* (au)
1	4.5008	−67.8890	121.9460	19.5193	0.0414
2	198.3666	−22.6075	−270.4566	−31.5658	−0.0670
3	0.2782	−0.0991	1.3428	0.5073	0.0011
4	2.0743	21.3842	16.0678	13.1754	0.0279
5	2.3082	0.4976	18.8028	7.2029	0.0153
6	−0.2094	−13.9189	2.0193	−4.0363	−0.0086
7	0.7786	−2.7082	0.1326	−0.5990	−0.0013
8	1.5279	7.3163	0.9328	3.2590	0.0069
9	−11.0054	0.1824	18.5027	2.5599	0.0054
10	−2.1788	−268.5521	301.7788	10.3493	0.0220
11	−2.9809	−43.7806	44.4208	−0.7802	−0.0017
12	0.1443	−0.3887	1.0308	0.2621	0.0006
13	16.6473	−1.3523	1.2602	5.5184	0.0117
14	71.7036	−10.4982	24.4515	28.5523	0.0606
15	−8.0571	−7.5421	8.1673	−2.4773	−0.0053
16	7.0193	121.0127	−208.4207	−26.7962	−0.0568
17	−2.1284	1.3719	0.0171	−0.2465	−0.0005
18	24.5759	−4.5554	−1.4090	6.2038	0.0132
19	33.6442	−29.9875	20.2297	7.9621	0.0169
20	16.5469	−454.0823	377.6848	−19.9502	−0.0423
21	15.9955	−227.1936	387.7458	58.8492	0.1248
22	0.1746	−3.0036	12.1381	3.1031	0.0066
23	−19.2954	2.7057	−16.3325	−10.9741	−0.0233
24	−7.8285	−57.3774	55.1326	−3.3578	−0.0071
25	−17.2157	−11.1442	23.4262	−1.6446	−0.0035
26	−27.5071	−18.7227	22.6259	−7.8680	−0.0167
27	9.6333	−18.4609	42.7754	11.3160	0.0240
28	−4.8699	−22.9664	21.9604	−1.9586	−0.0042
29	6.4970	−2.6580	−13.1495	−3.1035	−0.0066
30	29.6411	26.3539	10.0943	22.0298	0.0467

1/2[<0|del|b>*<b|r|0> + (<0|r|b>*<b|del|0>)*] (Au)

State	*X*	*Y*	*Z*	Dip. S.	Osc.(frdel)
1	−0.0115	−0.0246	−0.0098	0.0459	0.0306
2	−0.0106	−0.0151	−0.2277	0.2535	0.1690
3	−0.0008	−0.0001	−0.0003	0.0012	0.0008
4	−0.0010	−0.0059	−0.0038	0.0106	0.0071
5	−0.0031	−0.0035	−0.0079	0.0144	0.0096
6	−0.0001	−0.0019	−0.0047	0.0067	0.0044
7	−0.0019	−0.0004	0.0000	0.0023	0.0015

8	−0.0001	−0.0020	−0.0018	0.0038	0.0025
9	−0.0028	−0.0008	−0.0104	0.0140	0.0093
10	−0.0387	−0.0221	−0.0668	0.1276	0.0851
11	−0.0064	−0.0032	−0.0141	0.0237	0.0158
12	−0.0002	−0.0001	−0.0014	0.0017	0.0011
13	−0.0005	−0.0002	−0.0016	0.0023	0.0016
14	−0.0066	−0.0022	−0.0038	0.0126	0.0084
15	−0.0021	−0.0043	−0.0009	0.0074	0.0049
16	−0.0571	−0.0184	−0.0189	0.0944	0.0629
17	−0.0003	−0.0001	0.0000	0.0003	0.0002
18	−0.0033	−0.0001	−0.0008	0.0042	0.0028
19	−0.0178	−0.0069	−0.0007	0.0255	0.0170
20	−0.0004	−0.0514	−0.0703	0.1221	0.0814
21	−0.0035	−0.0508	−0.0343	0.0886	0.0591
22	−0.0014	−0.0014	−0.0007	0.0036	0.0024
23	−0.0246	−0.0002	−0.0035	0.0283	0.0188
24	−0.0014	−0.0171	−0.0050	0.0235	0.0156
25	−0.0045	−0.0007	−0.0062	0.0114	0.0076
26	−0.0065	−0.0009	−0.0074	0.0148	0.0099
27	−0.0741	−0.0011	−0.0076	0.0828	0.0552
28	−0.0007	−0.0027	−0.0062	0.0096	0.0064
29	−0.0275	0.0000	−0.0134	0.0410	0.0273
30	−0.0066	−0.0099	−0.0004	0.0169	0.0113

Ground to Excited state transition densities written to RWF 633

Excitation energies and oscillator strengths:

Excited state 1: Singlet−A 3.5692 eV 347.37 nm *f*=0.0310 <S**2>=0.000
127 −>128 0.70116
This state for optimization and/or second−order correction.
Copying the Excited state density for this state as the 1−particle RhoCI density.

Excited state 2: Singlet−A 4.4773 eV 276.92 nm *f*=0.1696 <S**2>=0.000
127 −>129 0.69391

Excited state 3: Singlet−A 4.6265 eV 267.99 nm *f*=0.0008 <S**2>=0.000
126 −>128 0.70570

Excited state 4: Singlet−A 4.8100 eV 257.76 nm *f*=0.0069 <S**2>=0.000
119 −>128 0.14340
120 −>128 0.12595
122 −>128 0.60232
123 −>128 −0.20976
124 −>128 −0.10125
125 −>128 −0.10469

Excited state 5: Singlet−A 4.9274 eV 251.62 nm *f*=0.0099 <S**2>=0.000
125 −>130 0.11992
127 −>130 0.68289

Excited state 6:	Singlet−A	5.0534 eV	245.35 nm	*f*=0.0046	<S**2>=0.000
123 −>128	−0.15471				
124 −>128	0.16258				
125 −>128	0.65604				
Excited state 7:	Singlet−A	5.1452 eV	240.97 nm	*f*=0.0015	<S**2>=0.000
126 −>129	0.69903				
Excited state 8:	Singlet−A	5.2897 eV	234.39 nm	*f*=0.0025	<S**2>=0.000
127 −>131	0.56690				
127 −>132	0.40048				
Excited state 9:	Singlet−A	5.4550 eV	227.29 nm	*f*=0.0096	<S**2>=0.000
119 −>128	−0.10535				
122 −>128	0.11202				
123 −>128	0.24893				
123 −>129	0.12137				
124 −>129	0.18633				
125 −>129	0.54489				
125 −>130	−0.15500				
Excited state 10:	Singlet−A	5.5013 eV	225.37 nm	*f*=0.0847	<S**2>=0.000
119 −>128	−0.11928				
122 −>128	0.21476				
123 −>128	0.52903				
124 −>128	−0.15255				
125 −>128	0.15896				
125 −>129	−0.24651				
Excited state 11:	Singlet−A	5.5164 eV	224.76 nm	*f*=0.0157	<S**2>=0.000
120 −>128	0.11101				
122 −>128	0.10481				
124 −>128	0.65018				
125 −>128	−0.15077				
Excited state 12:	Singlet−A	5.5408 eV	223.76 nm	*f*=0.0011	<S**2>=0.000
127 −>131	−0.24521				
127 −>132	0.42938				
127 −>133	0.27780				
127 −>134	−0.37195				
Excited state 13:	Singlet−A	5.5930 eV	221.68 nm	*f*=0.0014	<S**2>=0.000
120 −>128	−0.17857				
125 −>130	−0.26783				
126 −>130	−0.15718				
127 −>131	0.26217				
127 −>132	−0.27405				
127 −>133	0.31172				
127 −>134	−0.19834				
127 −>136	−0.13598				
Excited state 14:	Singlet−A	5.6103 eV	221.00 nm	*f*=0.0086	<S**2>=0.000
120 −>128	0.18910				
123 −>129	0.25153				
125 −>129	0.14018				
125 −>130	0.30009				

126 −>130	0.19706				
127 −>131	0.17978				
127 −>132	−0.18370				
127 −>133	0.25664				
127 −>134	−0.20216				
Excited state 15:	Singlet−A	5.6564 eV	219.19 nm	*f*=0.0050	<S**2>=0.000
120 −>128	0.53416				
121 −>128	0.14496				
122 −>128	−0.14797				
123 −>129	0.13168				
125 −>130	−0.24205				
126 −>130	−0.20551				
Excited state 16:	Singlet−A	5.7210 eV	216.72 nm	*f*=0.0633	<S**2>=0.000
120 −>128	−0.24849				
123 −>129	0.58093				
125 −>129	−0.16624				
126 −>130	−0.11650				
Excited state 17:	Singlet−A	5.7467 eV	215.75 nm	*f*=0.0002	<S**2>=0.000
127 −>133	0.36968				
127 −>134	0.46216				
127 −>135	−0.31251				
127 −>137	0.15747				
Excited state 18:	Singlet−A	5.8178 eV	213.11 nm	*f*=0.0028	<S**2>=0.000
125 −>130	−0.27618				
126 −>130	0.59415				
127 −>135	0.10288				
Excited state 19:	Singlet−A	5.8388 eV	212.35 nm	*f*=0.0172	<S**2>=0.000
119 −>128	−0.11546				
126 −>130	−0.12332				
127 −>132	0.15195				
127 −>133	0.22183				
127 −>134	0.15134				
127 −>135	0.44560				
127 −>136	−0.34084				
127 −>137	−0.13968				
Excited state 20:	Singlet−A	5.8548 eV	211.76 nm	*f*=0.0827	<S**2>=0.000
118 −>128	0.21532				
119 −>128	0.40459				
119 −>129	0.12110				
120 −>129	−0.23907				
122 −>128	−0.11003				
122 −>129	−0.29720				
123 −>128	0.19164				
127 −>135	0.12509				
127 −>136	−0.12810				
Excited state 21:	Singlet−A	5.9135 eV	209.66 nm	*f*=0.0601	<S**2>=0.000
118 −>128	0.11638				
119 −>128	0.36252				
119 −>129	−0.12311				
120 −>129	0.14077				

121 −>128	0.17318				
122 −>129	0.47493				
Excited state 22:	Singlet−A	5.9184 eV	209.49 nm	*f*=0.0024	<S**2>=0.000
118 −>128	−0.15863				
120 −>128	−0.15227				
121 −>128	0.64560				
122 −>129	−0.14892				
Excited state 23:	Singlet−A	5.9223 eV	209.35 nm	*f*=0.0192	<S**2>=0.000
126 −>131	0.53396				
126 −>132	−0.25277				
126 −>133	0.11166				
126 −>134	−0.10790				
126 −>135	0.30359				
126 −>137	0.11519				
Excited state 24:	Singlet−A	5.9509 eV	208.34 nm	*f*=0.0156	<S**2>=0.000
119 −>128	0.10897				
127 −>133	0.21756				
127 −>134	0.12251				
127 −>135	0.28697				
127 −>136	0.49539				
127 −>137	−0.10236				
127 −>138	−0.13293				
127 −>139	−0.15105				
127 −>141	−0.10262				
Excited state 25:	Singlet−A	5.9948 eV	206.82 nm	*f*=0.0077	<S**2>=0.000
119 −>129	−0.18018				
120 −>129	0.23686				
123 −>129	−0.14118				
124 −>129	0.53808				
125 −>129	−0.16318				
127 −>137	0.14007				
127 −>141	0.12263				
Excited state 26:	Singlet−A	6.0134 eV	206.18 nm	*f*=0.0099	<S**2>=0.000
119 −>129	0.18223				
120 −>129	−0.31881				
122 −>129	0.27255				
124 −>129	0.36682				
125 −>129	−0.10676				
127 −>135	−0.11807				
127 −>137	−0.22140				
127 −>138	0.10107				
127 −>141	−0.15543				
Excited state 27:	Singlet−A	6.0772 eV	204.02 nm	*f*=0.0559	<S**2>=0.000
118 −>128	−0.20475				
119 −>129	0.22637				
120 −>129	−0.17410				
122 −>129	0.14714				
127 −>135	0.10353				
127 −>137	0.41367				
127 −>138	−0.29775				
127 −>141	0.14711				

Excited state 28: Singlet−A 6.0846 eV 203.77 nm *f*=0.0064 <S**2>=0.000
127 −>134 −0.11401
127 −>135 0.16594
127 −>136 0.13354
127 −>137 0.28381
127 −>138 0.55678
127 −>142 0.13053

Excited state 29: Singlet−A 6.0951 eV 203.42 nm *f*=0.0274 <S**2>=0.000
118 −>128 0.55340
119 −>128 −0.30450
121 −>128 0.12195
127 −>137 0.17436

Excited state 30: Singlet−A 6.1624 eV 201.19 nm *f*=0.0113 <S**2>=0.000
119 −>129 −0.22649
127 −>137 0.14957
127 −>138 −0.12861
127 −>139 0.50776
127 −>140 −0.14431
127 −>141 −0.24571
127 −>143 0.11619
SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 LETran= 520.

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Rotatory strengths (R) in cgs (10**−40 erg−esu−cm/Gauss) of **8**.

State	*XX*	*YY*	*ZZ*	*R* (length)	*R* (au)
1	−4.5026	1.8332	0.5960	−0.6911	−0.0015
2	−2.4428	−2.1580	0.1126	−1.4961	−0.0032
3	1.4539	−1.1364	3.0233	1.1136	0.0024
4	24.9651	−877.6675	820.8856	−10.6056	−0.0225
5	−11.1564	15.9800	−11.3387	−2.1717	−0.0046
6	−0.1132	−0.1010	−0.0044	−0.0728	−0.0002
7	227.0204	−568.7667	437.295	31.8499	0.0676
8	−1.3148	−0.2237	0.0549	−0.4945	−0.0010
9	−41.7647	−18.0052	14.4603	−15.1032	−0.0320
10	68.5227	−121.4929	24.0376	−9.6442	−0.0205
11	−13.7356	7.1928	−0.1327	−2.2252	−0.0047
12	0.0223	−5.2164	0.1337	−1.6868	−0.0036
13	−1.7717	2.5832	−1.8136	−0.3341	−0.0007
14	−211.2143	165.1495	4.3660	−13.8996	−0.0295
15	12.9652	−0.9040	5.0419	5.7011	0.0121
16	−0.4762	−22.0677	−5.4390	−9.3276	−0.0198
17	−28.1435	−54.2934	142.5854	20.0495	0.0425
18	128.6624	−194.5182	89.5400	7.8947	0.0167
19	5.0810	0.6173	7.9972	4.5652	0.0097
20	−128.4304	47.5907	128.1460	15.7688	0.0334
21	13.1186	−3.2054	24.7372	11.5501	0.0245

22	5.6141	3.9084	17.6710	9.0645	0.0192
23	−2.7064	−55.5401	55.9640	−0.7608	−0.0016
24	−5.8739	6.3858	6.7593	2.4237	0.0051
25	−15.8145	−5.1305	−14.7363	−11.8938	−0.0252
26	2.4483	7.1062	128.6206	46.0584	0.0977
27	2.0109	−170.2329	54.2552	−37.9889	−0.0806
28	4.0143	4.3094	41.4152	16.5796	0.0352
29	−0.1568	−69.9865	144.2730	24.7099	0.0524
30	0.0024	15.5842	33.4897	16.3587	0.0347

1/2[<0|del|b>*<b|r|0> + (<0|r|b>*<b|del|0>)*] (Au)

State	*X*	*Y*	*Z*	Dip. S.	Osc.(frdel)
1	0.0000	0.0000	0.0000	0.0001	0.0000
2	−0.0025	−0.0011	0.0000	0.0036	0.0024
3	−0.0018	0.0000	−0.0003	0.0021	0.0014
4	−0.0197	−0.0356	−0.2854	0.3407	0.2271
5	−0.0059	−0.0004	−0.0004	0.0067	0.0045
6	−0.0001	0.0000	0.0000	0.0001	0.0001
7	−0.2042	−0.0466	−0.0305	0.2813	0.1875
8	−0.0009	−0.0002	0.0000	0.0011	0.0007
9	−0.0074	−0.0015	−0.0005	0.0095	0.0063
10	−0.0445	−0.0138	−0.0004	0.0586	0.0391
11	−0.0194	−0.0036	0.0000	0.0230	0.0154
12	0.0000	−0.0005	0.0000	0.0006	0.0004
13	−0.0084	−0.0003	−0.0007	0.0095	0.0063
14	−0.1830	−0.0969	−0.0005	0.2804	0.1869
15	−0.0090	−0.0006	−0.0001	0.0096	0.0064
16	0.0000	−0.0020	−0.0003	0.0023	0.0015
17	−0.0046	−0.0406	−0.0151	0.0604	0.0403
18	−0.0216	−0.0425	−0.0079	0.0721	0.0480
19	−0.0046	−0.0009	−0.0008	0.0064	0.0042
20	−0.2110	−0.0022	−0.0183	0.2315	0.1543
21	−0.0047	−0.0010	−0.0025	0.0083	0.0055
22	−0.0128	−0.0003	−0.0030	0.0161	0.0107
23	−0.0003	−0.0121	−0.0077	0.0201	0.0134
24	−0.0077	−0.0013	−0.0007	0.0097	0.0065
25	−0.0433	−0.0931	−0.0001	0.1366	0.0910
26	−0.0001	−0.0025	−0.0248	0.0274	0.0183
27	−0.0004	−0.0084	−0.0133	0.0221	0.0147
28	−0.0001	0.0000	−0.0059	0.0060	0.0040
29	−0.0023	−0.0015	−0.0450	0.0487	0.0325
30	0.0000	−0.0017	−0.0101	0.0118	0.0078

Ground to Excited state transition densities written to RWF 633

Excitation energies and oscillator strengths:

Excited state 1: Singlet−A 3.5564 eV 348.62 nm *f*=0.0000 <S**2>=0.000
130 −>132 0.70000
This state for optimization and/or second−order correction.
Copying the Excited state density for this state as the 1−particle RhoCI density.

Excited state 2: Singlet−A 4.1487 eV 298.85 nm *f*=0.0024 <S**2>=0.000
131 −>133 0.70311

Excited state 3: Singlet−A 4.2009 eV 295.13 nm *f*=0.0014 <S**2>=0.000
131 −>132 0.70645

Excited state 4: Singlet−A 4.5780 eV 270.83 nm *f*=0.2278 <S**2>=0.000
128 −>132 0.11292
129 −>132 0.68474

Excited state 5: Singlet−A 4.7912 eV 258.77 nm *f*=0.0044 <S**2>=0.000
123 −>133 0.15628
124 −>133 0.56372
126 −>133 0.11178
127 −>133 0.31422

Excited state 6: Singlet−A 4.9116 eV 252.43 nm *f*=0.0001 <S**2>=0.000
130 −>133 0.70671

Excited state 7: Singlet−A 4.9580 eV 250.07 nm *f*=0.1929 <S**2>=0.000
128 −>132 0.68027
129 −>132 −0.10621

Excited state 8: Singlet−A 4.9995 eV 247.99 nm *f*=0.0007 <S**2>=0.000
129 −>133 0.69645

Excited state 9: Singlet−A 5.1590 eV 240.32 nm *f*=0.0063 <S**2>=0.000
125 −>134 0.12000
131 −>134 0.65568
131 −>135 −0.12373

Excited state 10: Singlet−A 5.2895 eV 234.40 nm *f*=0.0404 <S**2>=0.000
125 −>132 0.22031
126 −>132 −0.34055
127 −>132 0.56345

Excited state 11: Singlet−A 5.3139 eV 233.32 nm *f*=0.0156 <S**2>=0.000
124 −>133 −0.10688
126 −>133 −0.20271
127 −>133 0.13339
128 −>133 0.64603

Excited state 12: Singlet−A 5.4520 eV 227.41 nm *f*=0.0004 <S**2>=0.000
126 −>132 0.60138
127 −>132 0.35298

Excited state 13: Singlet−A 5.4963 eV 225.58 nm *f*=0.0064 <S**2>=0.000
125 −>133 0.11396
126 −>133 0.55653
127 −>133 −0.33582

128 ->133	0.24500				
Excited state 14:	Singlet-A	5.5287 eV	224.25 nm	*f*=0.1892	<S**2>=0.000
124 ->133	-0.31810				
125 ->133	0.20480				
126 ->133	0.25438				
127 ->133	0.41607				
131 ->135	0.28415				
Excited state 15:	Singlet-A	5.5546 eV	223.21 nm	*f*=0.0066	<S**2>=0.000
124 ->132	-0.17545				
125 ->132	0.63053				
127 ->132	-0.22888				
Excited state 16:	Singlet-A	5.5692 eV	222.62 nm	*f*=0.0018	<S**2>=0.000
130 ->135	0.29969				
130 ->136	0.61883				
Excited state 17:	Singlet-A	5.6088 eV	221.05 nm	*f*=0.0411	<S**2>=0.000
124 ->133	0.11611				
125 ->133	-0.18698				
125 ->134	0.19924				
126 ->134	-0.10815				
127 ->133	-0.13307				
127 ->134	0.13192				
128 ->134	0.15090				
129 ->134	-0.19263				
131 ->135	0.50311				
Excited state 18:	Singlet-A	5.6336 eV	220.08 nm	*f*=0.0478	<S**2>=0.000
125 ->134	-0.26549				
126 ->134	0.16644				
127 ->134	-0.19218				
128 ->134	-0.21607				
129 ->134	0.28914				
131 ->134	0.23129				
131 ->135	0.29509				
Excited state 19:	Singlet-A	5.6869 eV	218.02 nm	*f*=0.0043	<S**2>=0.000
122 ->132	-0.11399				
123 ->132	-0.29634				
124 ->132	0.58933				
125 ->132	0.17725				
Excited state 20:	Singlet-A	5.7213 eV	216.70 nm	*f*=0.1562	<S**2>=0.000
125 ->133	0.61781				
126 ->133	-0.21205				
127 ->133	-0.18300				
Excited state 21:	Singlet-A	5.7912 eV	214.09 nm	*f*=0.0056	<S**2>=0.000
121 ->132	0.18201				
122 ->132	0.24985				
123 ->132	0.51498				
124 ->132	0.34004				
Excited state 22:	Singlet-A	5.8416 eV	212.24 nm	*f*=0.0108	<S**2>=0.000
131 ->135	0.14554				

131 −>136	0.68291				
Excited state 23:	Singlet−A	5.9796 eV	207.35 nm	*f*=0.0135	<S**2>=0.000
121 −>133	−0.29456				
123 −>133	0.56890				
124 −>133	−0.14839				
130 −>134	−0.14402				
Excited state 24:	Singlet−A	5.9817 eV	207.27 nm	*f*=0.0065	<S**2>=0.000
123 −>133	0.12792				
129 −>134	0.13848				
130 −>134	0.65748				
130 −>136	0.11813				
Excited state 25:	Singlet−A	6.0243 eV	205.81 nm	*f*=0.0910	<S**2>=0.000
122 −>133	−0.14325				
131 −>135	0.11310				
131 −>137	0.50767				
131 −>138	−0.37711				
131 −>140	−0.12993				
Excited state 26:	Singlet−A	6.0742 eV	204.11 nm	*f*=0.0184	<S**2>=0.000
120 −>133	0.11660				
121 −>132	−0.14822				
121 −>133	−0.31788				
122 −>133	0.50596				
123 −>133	−0.11761				
127 −>133	0.10510				
131 −>138	−0.11011				
Excited state 27:	Singlet−A	6.0802 eV	203.91 nm	*f*=0.0151	<S**2>=0.000
116 −>132	0.16599				
118 −>132	−0.21380				
120 −>132	−0.13325				
121 −>132	0.50048				
122 −>132	0.10667				
122 −>133	0.15192				
123 −>132	−0.14465				
129 −>135	0.15991				
129 −>136	0.17027				
Excited state 28:	Singlet−A	6.0948 eV	203.43 nm	*f*=0.0040	<S**2>=0.000
121 −>132	0.14385				
125 −>134	0.16603				
126 −>134	−0.11223				
127 −>134	0.14124				
128 −>134	0.21548				
129 −>134	0.50320				
129 −>135	−0.23186				
130 −>134	−0.11955				
Excited state 29:	Singlet−A	6.1271 eV	202.35 nm	*f*=0.0328	<S**2>=0.000
121 −>132	−0.13155				
126 −>135	0.10752				
128 −>135	−0.15056				
129 −>134	0.27727				
129 −>135	0.47745				

129 −>136 0.26901

Excited state 30: Singlet−A 6.1426 eV 201.84 nm *f*=0.0078 <S**2>=0.000
131 −>137 −0.25510
131 −>138 −0.40013
131 −>139 0.47367
131 −>140 0.11540
SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 LETran= 520.

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Rotatory strengths (R) in cgs (10**−40 erg−esu−cm/Gauss) of **11**.

State	*XX*	*YY*	*ZZ*	*R* (length)	*R* (au)
1	17.7353	11.3644	−17.7552	3.7815	0.0080
2	0.3493	0.0676	0.2441	0.2203	0.0005
3	−14.7864	36.1357	−27.1233	−1.9246	−0.0041
4	1.4528	−0.1245	−1.7599	−0.1439	−0.0003
5	3.2828	4.7088	−8.9594	−0.3226	−0.0007
6	1.0591	−2.8369	−14.0010	−5.2596	−0.0112
7	−68.7493	71.4656	−93.6148	−30.2995	−0.0643
8	−5.0958	55.2534	16.1525	22.1034	0.0469
9	318.3316	501.4355	−761.8752	19.2973	0.0409
10	−0.6961	−0.0738	−5.0513	−1.9404	−0.0041
11	−15.4272	−16.0463	−19.5112	−16.9949	−0.0360
12	−14.6802	−11.0076	2.0878	−7.8667	−0.0167
13	−1.7377	−99.9648	98.0964	−1.2020	−0.0025
14	−78.8341	−36.1953	30.7585	−28.0903	−0.0596
15	−17.9870	−10.7889	−20.2772	−16.3510	−0.0347
16	−20.1039	−15.3715	40.0187	1.5144	0.0032
17	12.3821	−2.9989	30.6819	13.3551	0.0283
18	−18.8581	25.9828	−11.8967	−1.5907	−0.0034
19	5.2086	8.2546	−37.8755	−8.1374	−0.0173
20	−22.8007	9.0565	−59.0127	−24.2523	−0.0514
21	−11.5824	43.5986	5.9296	12.6486	0.0268
22	−13.8811	39.4704	53.2760	26.2884	0.0558
23	−9.4082	135.3819	−41.9519	28.0073	0.0594
24	−1.9073	1.2132	5.8834	1.7297	0.0037
25	−0.2540	8.5163	−15.6758	−2.4712	−0.0052
26	−100.3348	59.3953	41.3783	0.1463	0.0003
27	15.8835	6.8690	−4.5016	6.0836	0.0129
28	−12.7013	42.9019	13.2268	14.4758	0.0307
29	−76.4229	40.6022	−23.3717	−19.7308	−0.0419
30	−82.3761	32.2764	−147.4097	−65.8365	−0.1396

1/2[<0|del|b>*<b|r|0> + (<0|r|b>*<b|del|0>)*] (Au)

State	*X*	*Y*	*Z*	Dip. S.	Osc.(frdel)
1	−0.0041	−0.0047	−0.0094	0.0181	0.0121

2	0.0000	−0.0001	−0.0002	0.0003	0.0002
3	−0.0008	−0.0036	−0.0013	0.0057	0.0038
4	−0.0003	−0.0005	−0.0002	0.0009	0.0006
5	−0.0011	−0.0027	−0.0010	0.0049	0.0033
6	−0.0004	0.0000	−0.0089	0.0093	0.0062
7	−0.0077	−0.0281	−0.1326	0.1684	0.1123
8	−0.0038	−0.0050	−0.0155	0.0242	0.0162
9	−0.1144	−0.2541	−0.0649	0.4334	0.2889
10	0.0000	−0.0027	−0.0003	0.0030	0.0020
11	−0.0046	−0.0015	−0.0097	0.0157	0.0105
12	−0.0032	−0.0034	−0.0022	0.0088	0.0059
13	−0.0001	−0.0075	−0.0876	0.0951	0.0634
14	−0.0078	−0.0479	−0.0008	0.0566	0.0377
15	−0.0240	−0.0097	−0.0009	0.0345	0.0230
16	−0.0029	−0.0026	−0.0015	0.0070	0.0047
17	−0.0142	0.0000	−0.0074	0.0217	0.0145
18	−0.0036	−0.0066	−0.0044	0.0145	0.0097
19	−0.0002	−0.0072	−0.0042	0.0116	0.0077
20	−0.0039	−0.0005	−0.0284	0.0328	0.0219
21	−0.0273	−0.0022	−0.0136	0.0431	0.0287
22	−0.0073	−0.0108	−0.0041	0.0223	0.0148
23	−0.0331	−0.0478	−0.0005	0.0814	0.0543
24	−0.0012	−0.0027	−0.0007	0.0045	0.0030
25	−0.0002	−0.0009	−0.0024	0.0035	0.0023
26	−0.0140	−0.0203	−0.0010	0.0354	0.0236
27	−0.0121	−0.0043	−0.0023	0.0188	0.0125
28	−0.0021	−0.0086	−0.0003	0.0111	0.0074
29	−0.0294	−0.0115	−0.0004	0.0413	0.0275
30	−0.0514	−0.0343	−0.0048	0.0906	0.0604

Ground to Excited state transition densities written to RWF 633

Excitation energies and oscillator strengths:

Excited state 1: Singlet−A 4.3130 eV 287.47 nm *f*=0.0123 <S**2>=0.000
125 −> 133 −0.12029
131 −> 133 0.65430
132 −> 133 0.22532
This state for optimization and/or second−order correction.
Copying the Excited state density for this state as the 1−particle RhoCI density.

Excited state 2: Singlet−A 4.5058 eV 275.16 nm *f*=0.0002 <S**2>=0.000
131 −> 133 −0.22038
132 −> 133 0.67012

Excited state 3: Singlet−A 4.7974 eV 258.44 nm *f*=0.0037 <S**2>=0.000
125 −> 133 0.62681
128 −> 133 −0.14390

129 −> 133	−0.16260				
131 −> 133	0.14529				
Excited state 4:	Singlet−A	5.2234 eV	237.36 nm	*f*=0.0006	<S**2>=0.000
125 −> 133	−0.13078				
129 −> 133	−0.19282				
130 −> 133	0.66124				
Excited state 5:	Singlet−A	5.3573 eV	231.43 nm	*f*=0.0033	<S**2>=0.000
125 −> 133	0.11214				
129 −> 133	0.64578				
130 −> 133	0.22754				
Excited state 6:	Singlet−A	5.4329 eV	228.21 nm	*f*=0.0059	<S**2>=0.000
126 −> 135	−0.10966				
129 −> 134	−0.23433				
129 −> 135	−0.22035				
130 −> 134	0.16356				
130 −> 135	0.14484				
131 −> 134	0.12968				
132 −> 134	0.46699				
132 −> 135	0.23726				
Excited state 7:	Singlet−A	5.5527 eV	223.29 nm	*f*=0.1140	<S**2>=0.000
128 −> 133	−0.21286				
129 −> 134	0.16525				
129 −> 135	0.20183				
130 −> 134	−0.12675				
130 −> 135	−0.14259				
131 −> 134	0.49175				
131 −> 135	0.15889				
132 −> 134	0.16581				
Excited state 8:	Singlet−A	5.5620 eV	222.91 nm	*f*=0.0161	<S**2>=0.000
129 −> 134	0.20331				
129 −> 135	0.19260				
130 −> 134	−0.13247				
130 −> 135	−0.12699				
131 −> 134	−0.31926				
131 −> 135	−0.18966				
132 −> 134	0.44811				
Excited state 9:	Singlet−A	5.6073 eV	221.11 nm	*f*=0.2918	<S**2>=0.000
124 −> 133	−0.18257				
125 −> 133	0.17024				
128 −> 133	0.55132				
131 −> 134	0.15475				
131 −> 135	0.24890				
Excited state 10:	Singlet−A	5.6657 eV	218.83 nm	*f*=0.0020	<S**2>=0.000
126 −> 133	0.50378				
127 −> 133	−0.46708				
128 −> 133	−0.11142				
Excited state 11:	Singlet−A	5.7431 eV	215.88 nm	*f*=0.0104	<S**2>=0.000
126 −> 133	0.30819				
127 −> 133	0.33840				

131 −> 135	0.14689				
132 −> 134	−0.14219				
132 −> 135	0.45752				
Excited state 12:	Singlet−A	5.7492 eV	215.66 nm	*f*=0.0059	<S**2>=0.000
126 −> 133	−0.35732				
127 −> 133	−0.38418				
132 −> 134	−0.13479				
132 −> 135	0.41676				
Excited state 13:	Singlet−A	5.8217 eV	212.97 nm	*f*=0.0641	<S**2>=0.000
128 −> 133	−0.16537				
131 −> 134	−0.27243				
131 −> 135	0.55697				
132 −> 135	−0.16305				
132 −> 136	−0.10948				
Excited state 14:	Singlet−A	5.8571 eV	211.68 nm	*f*=0.0373	<S**2>=0.000
122 −> 133	0.10147				
123 −> 133	−0.27239				
124 −> 133	0.56720				
128 −> 133	0.19990				
131 −> 135	0.11707				
Excited state 15:	Singlet−A	5.9089 eV	209.83 nm	*f*=0.0235	<S**2>=0.000
132 −> 135	−0.13404				
132 −> 136	0.58891				
132 −> 139	0.13226				
132 −> 140	−0.22386				
132 −> 143	−0.11536				
Excited state 16:	Singlet−A	6.1062 eV	203.05 nm	*f*=0.0048	<S**2>=0.000
126 −> 134	−0.26656				
127 −> 134	0.15619				
129 −> 134	0.36350				
129 −> 135	−0.28565				
130 −> 134	−0.28454				
130 −> 135	0.18304				
131 −> 136	−0.14995				
131 −> 137	−0.10753				
Excited state 17:	Singlet−A	6.1536 eV	201.48 nm	*f*=0.0145	<S**2>=0.000
121 −> 133	0.18273				
123 −> 133	−0.34833				
124 −> 133	−0.16215				
131 −> 136	0.45741				
131 −> 138	0.16397				
132 −> 136	0.10833				
132 −> 138	0.12054				
Excited state 18:	Singlet−A	6.1581 eV	201.34 nm	*f*=0.0097	<S**2>=0.000
121 −> 133	−0.25283				
122 −> 133	0.10248				
123 −> 133	0.44824				
124 −> 133	0.15665				
131 −> 136	0.35365				
131 −> 138	0.12705				

Excited state 19:	Singlet−A	6.2065 eV	199.77 nm	*f*=0.0078	<S**2>=0.000
121 −> 133	−0.31102				
122 −> 133	0.46899				
123 −> 133	−0.20287				
124 −> 133	−0.22973				
131 −> 137	0.17353				
Excited state 20:	Singlet−A	6.2250 eV	199.17 nm	*f*=0.0223	<S**2>=0.000
122 −> 133	0.11486				
131 −> 136	−0.26664				
131 −> 137	−0.18913				
132 −> 136	0.17998				
132 −> 137	−0.21181				
132 −> 138	0.32265				
132 −> 140	0.29323				
132 −> 141	0.22503				
Excited state 21:	Singlet−A	6.2337 eV	198.89 nm	*f*=0.0288	<S**2>=0.000
122 −> 133	−0.10148				
131 −> 137	0.52875				
131 −> 138	−0.17833				
132 −> 136	0.14115				
132 −> 137	0.15560				
132 −> 138	0.13272				
132 −> 140	0.19902				
132 −> 141	0.14697				
Excited state 22:	Singlet−A	6.2859 eV	197.24 nm	*f*=0.0152	<S**2>=0.000
129 −> 134	0.35940				
130 −> 134	0.56303				
130 −> 135	0.11489				
Excited state 23:	Singlet−A	6.3129 eV	196.40 nm	*f*=0.0548	<S**2>=0.000
132 −> 137	0.31429				
132 −> 138	0.24228				
132 −> 139	0.48475				
132 −> 140	0.10081				
132 −> 141	−0.11515				
132 −> 142	−0.19429				
Excited state 24:	Singlet−A	6.3299 eV	195.87 nm	*f*=0.0030	<S**2>=0.000
121 −> 133	0.49160				
122 −> 133	0.44421				
123 −> 133	0.17897				
Excited state 25:	Singlet−A	6.3729 eV	194.55 nm	*f*=0.0024	<S**2>=0.000
131 −> 137	−0.23217				
132 −> 136	0.15833				
132 −> 137	0.50704				
132 −> 138	−0.14231				
132 −> 139	−0.16588				
132 −> 141	0.15595				
132 −> 142	0.20689				
132 −> 143	0.14967				
Excited state 26:	Singlet−A	6.4034 eV	193.62 nm	*f*=0.0241	<S**2>=0.000

130 −> 136 −0.10877
131 −> 136 −0.15435
131 −> 137 0.11567
131 −> 138 0.40650
132 −> 137 0.10969
132 −> 138 0.32874
132 −> 139 −0.19834
132 −> 140 −0.25857
132 −> 142 0.10332

Excited state 27: Singlet−A 6.4429 eV 192.43 nm *f*=0.0126 <S**2>=0.000
117 −> 133 −0.11714
119 −> 133 −0.19570
120 −> 133 0.62101
131 −> 139 0.11294

Excited state 28: Singlet−A 6.4490 eV 192.25 nm *f*=0.0074 <S**2>=0.000
120 −> 133 −0.13789
126 −> 134 0.11099
130 −> 135 0.20544
131 −> 137 0.14935
131 −> 138 0.34492
131 −> 139 0.34877
131 −> 140 0.22755
132 −> 138 −0.16883
132 −> 140 0.16297

Excited state 29: Singlet−A 6.4686 eV 191.67 nm *f*=0.0278 <S**2>=0.000
126 −> 134 −0.17265
127 −> 134 0.12258
130 −> 135 −0.20743
131 −> 138 −0.22056
131 −> 139 0.47921
131 −> 140 0.11175
132 −> 138 0.15498
132 −> 140 −0.15681
132 −> 142 0.12801

Excited state 30: Singlet−A 6.4764 eV 191.44 nm *f*=0.0611 <S**2>=0.000
126 −> 134 0.26973
127 −> 134 −0.14444
128 −> 134 −0.15209
130 −> 134 −0.10094
130 −> 135 0.42383
131 −> 138 −0.20422
132 −> 138 0.22032
132 −> 140 −0.20085
SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 LETran= 520.

****
Rotatory strengths (R) in cgs (10**−40 erg−esu−cm/Gauss) of **14**.

State	*XX*	*YY*	*ZZ*	*R* (length)	*R* (au)
1	−3.7890	−8.7037	−0.6177	−4.3701	−0.0093
2	−0.4444	−0.7678	−0.2287	−0.4803	−0.0010
3	49.0167	−11.8450	−11.5202	8.5505	0.0181

4	13.8838	−45.1736	−2.7332	−11.3410	−0.0241
5	−29.2295	−22.0724	−2.6756	−17.9925	−0.0382
6	−21.3679	117.1941	−91.8441	1.3274	0.0028
7	−16.7036	100.0740	−47.1634	12.0690	0.0256
8	−50.2189	68.9861	−49.2302	−10.1543	−0.0215
9	−179.6241	11.9726	3.3050	−54.7822	−0.1162
10	6.8228	105.2055	−108.7470	1.0937	0.0023
11	−16.8394	−5.4489	−8.0922	−10.1268	−0.0215
12	−2.7436	377.8682	−348.1261	8.9995	0.0191
13	−0.1644	0.3011	−1.6083	−0.4905	−0.0010
14	−31.4071	−15.5775	−19.2783	−22.0876	−0.0469
15	−30.9979	0.3044	−11.6507	−14.1147	−0.0299
16	138.7762	17.3384	108.0297	88.0481	0.1868
17	−23.0891	−0.1774	−14.2701	−12.5122	−0.0265
18	75.8096	8.6533	−6.9828	25.8267	0.0548
19	7.3789	3.3244	−28.2647	−5.8538	−0.0124
20	174.8455	−109.5494	−156.2146	−30.3062	−0.0643
21	−3.1789	0.8810	3.6401	0.4474	0.0009
22	151.8022	−5.3529	−52.0145	31.4783	0.0668
23	−154.5132	124.5858	79.5457	16.5394	0.0351
24	39.2753	−21.1836	−15.0977	0.9980	0.0021
25	−2.6703	24.3286	4.2849	8.6478	0.0183
26	−49.5469	−11.7376	−27.4282	−29.5709	−0.0627
27	30.7319	13.4410	−6.1768	12.6653	0.0269
28	0.5579	40.1930	−26.2287	4.8407	0.0103
29	121.8552	−3.3926	−46.7986	23.8880	0.0507
30	−90.0580	−12.2916	−66.3371	−56.2289	−0.1193

1/2[<0|del|b>*<b|r|0> + (<0|r|b>*<b|del|0>)*] (Au)

State	*X*	*Y*	*Z*	Dip. S.	Osc.(frdel)
1	−0.0001	−0.0009	0.0000	0.0010	0.0007
2	0.0000	−0.0001	0.0000	0.0001	0.0001
3	−0.0045	−0.0037	−0.0003	0.0085	0.0057
4	−0.0097	−0.0104	0.0000	0.0201	0.0134
5	−0.0358	−0.0027	0.0000	0.0385	0.0256
6	−0.0548	−0.1211	−0.0024	0.1783	0.1189
7	−0.0315	−0.0338	−0.0016	0.0669	0.0446
8	−0.0283	−0.0245	−0.0017	0.0544	0.0363
9	−0.0192	−0.0128	−0.0010	0.0329	0.0220
10	−0.0005	−0.0500	−0.0069	0.0574	0.0383
11	−0.0185	−0.0003	−0.0011	0.0199	0.0133
12	−0.0001	−0.1120	−0.0276	0.1397	0.0931
13	−0.0001	−0.0002	−0.0001	0.0004	0.0003
14	−0.0009	−0.0046	−0.0097	0.0152	0.0102

15	−0.0042	−0.0005	−0.0012	0.0059	0.0039
16	−0.0068	−0.0006	−0.0373	0.0447	0.0298
17	−0.0068	0.0000	−0.0046	0.0114	0.0076
18	−0.0206	−0.0014	−0.0011	0.0231	0.0154
19	−0.0318	−0.0010	−0.0053	0.0380	0.0253
20	−0.0747	−0.0063	−0.0264	0.1074	0.0716
21	−0.0036	−0.0010	−0.0002	0.0047	0.0031
22	−0.0690	−0.0004	−0.0059	0.0753	0.0502
23	−0.0192	−0.0427	−0.0033	0.0652	0.0434
24	−0.0198	−0.0020	−0.0059	0.0277	0.0185
25	−0.0196	−0.0058	−0.0004	0.0258	0.0172
26	−0.0052	−0.0024	−0.0093	0.0169	0.0112
27	−0.0061	−0.0054	−0.0001	0.0116	0.0077
28	−0.0001	−0.0042	−0.0019	0.0062	0.0041
29	−0.1337	0.0000	−0.0013	0.1350	0.0900
30	−0.0351	−0.0017	−0.0119	0.0487	0.0325

Ground to Excited state transition densities written to RWF 633
Excitation energies and oscillator strengths:

Excited state 1: Singlet−A 4.6710 eV 265.43 nm *f*=0.0006 <S**2>=0.000
124 −> 133 0.10073
125 −> 133 0.15091
126 −> 133 −0.22361
128 −> 133 −0.20139
131 −> 133 0.56944
132 −> 133 −0.19190
This state for optimization and/or second−order correction.
Copying the Excited state density for this state as the 1−particle RhoCI density.

Excited state 2: Singlet−A 4.7089 eV 263.30 nm *f*=0.0001 <S**2>=0.000
131 −> 133 0.13894
132 −> 133 0.67922

Excited state 3: Singlet−A 4.8693 eV 254.62 nm *f*=0.0057 <S**2>=0.000
124 −> 133 −0.15321
125 −> 133 −0.23452
126 −> 133 0.33367
127 −> 133 0.11755
128 −> 133 0.29345
130 −> 133 0.20901
131 −> 133 0.39141

Excited state 4: Singlet−A 5.2477 eV 236.26 nm *f*=0.0134 <S**2>=0.000
127 −> 134 −0.24146
127 −> 135 0.10704
131 −> 134 −0.33016
132 −> 134 0.52059

Excited state 5: Singlet−A 5.3378 eV 232.28 nm *f*=0.0258 <S**2>=0.000
127 −> 134 0.16995
130 −> 133 0.15417
131 −> 134 0.44174

131 −> 135	−0.10489				
132 −> 134	0.44853				
Excited state 6:	Singlet−A	5.3549 eV	231.53 nm	*f*=0.1208	<S**2>=0.000
128 −> 133	−0.29688				
130 −> 133	0.58739				
131 −> 134	−0.14961				
Excited state 7:	Singlet−A	5.5368 eV	223.93 nm	*f*=0.0453	<S**2>=0.000
124 −> 133	−0.12790				
125 −> 133	0.26216				
126 −> 133	−0.33200				
127 −> 133	0.14755				
128 −> 133	0.43194				
129 −> 133	−0.27819				
Excited state 8:	Singlet−A	5.5419 eV	223.72 nm	*f*=0.0367	<S**2>=0.000
124 −> 133	−0.14192				
125 −> 133	0.11405				
126 −> 133	−0.15490				
127 −> 133	−0.17683				
128 −> 133	0.19283				
129 −> 133	0.59581				
Excited state 9:	Singlet−A	5.6324 eV	220.13 nm	*f*=0.0222	<S**2>=0.000
127 −> 133	0.18332				
127 −> 134	0.41494				
127 −> 135	−0.14995				
129 −> 133	0.15323				
129 −> 134	−0.15017				
130 −> 134	0.20133				
131 −> 134	−0.35721				
Excited state 10:	Singlet−A	5.6860 eV	218.05 nm	*f*=0.0386	<S**2>=0.000
124 −> 133	0.11490				
127 −> 133	0.60695				
127 −> 134	−0.15698				
129 −> 133	0.20191				
131 −> 134	0.10995				
Excited state 11:	Singlet−A	5.8944 eV	210.34 nm	*f*=0.0136	<S**2>=0.000
132 −> 135	0.56124				
132 −> 136	0.33270				
132 −> 139	−0.13255				
132 −> 140	0.16303				
Excited state 12:	Singlet−A	5.8994 eV	210.17 nm	*f*=0.0932	<S**2>=0.000
124 −> 133	0.61647				
128 −> 133	0.21208				
130 −> 133	0.19048				
Excited state 13:	Singlet−A	5.9876 eV	207.07 nm	*f*=0.0003	<S**2>=0.000
125 −> 133	0.55911				
126 −> 133	0.42033				
Excited state 14:	Singlet−A	5.9962 eV	206.77 nm	*f*=0.0102	<S**2>=0.000
128 −> 134	−0.28461				

130 −> 134	0.34780				
131 −> 135	0.41173				
132 −> 135	−0.15726				
132 −> 136	0.21641				
Excited state 15:	Singlet−A	6.0121 eV	206.22 nm	*f*=0.0040	<S**2>=0.000
128 −> 134	0.14632				
130 −> 134	−0.17607				
131 −> 135	−0.17368				
132 −> 135	−0.37432				
132 −> 136	0.43137				
132 −> 137	−0.10536				
132 −> 139	−0.13827				
132 −> 140	0.15241				
132 −> 142	−0.11003				
Excited state 16:	Singlet−A	6.0608 eV	204.57 nm	*f*=0.0299	<S**2>=0.000
127 −> 134	0.13138				
128 −> 134	0.18423				
129 −> 134	−0.14829				
130 −> 134	−0.38899				
131 −> 135	0.46914				
131 −> 137	−0.10309				
Excited state 17:	Singlet−A	6.1572 eV	201.36 nm	*f*=0.0076	<S**2>=0.000
125 −> 134	0.10058				
126 −> 134	−0.10170				
128 −> 134	0.33273				
129 −> 134	0.57302				
Excited state 18:	Singlet−A	6.2038 eV	199.85 nm	*f*=0.0156	<S**2>=0.000
124 −> 134	−0.11431				
126 −> 134	−0.14692				
127 −> 134	−0.29781				
128 −> 134	0.40083				
129 −> 134	−0.31554				
130 −> 134	0.30849				
Excited state 19:	Singlet−A	6.2466 eV	198.48 nm	*f*=0.0259	<S**2>=0.000
122 −> 133	0.56099				
123 −> 133	0.37734				
Excited state 20:	Singlet−A	6.2669 eV	197.84 nm	*f*=0.0726	<S**2>=0.000
132 −> 136	0.20113				
132 −> 137	0.53591				
132 −> 138	0.17871				
132 −> 139	0.26740				
132 −> 141	0.10062				
132 −> 142	0.10109				
132 −> 143	−0.12098				
Excited state 21:	Singlet−A	6.3133 eV	196.39 nm	*f*=0.0032	<S**2>=0.000
120 −> 133	0.11431				
122 −> 133	−0.35311				
123 −> 133	0.57633				
Excited state 22:	Singlet−A	6.3315 eV	195.82 nm	*f*=0.0508	<S**2>=0.000

132 −> 137	−0.15840				
132 −> 138	0.61125				
132 −> 141	0.22989				
132 −> 142	−0.12127				
Excited state 23:	Singlet−A	6.3858 eV	194.15 nm	*f*=0.0434	<S**2>=0.000
131 −> 135	0.15891				
131 −> 136	−0.30632				
131 −> 137	0.45710				
131 −> 138	−0.12065				
131 −> 139	−0.14071				
131 −> 140	0.22696				
Excited state 24:	Singlet−A	6.4249 eV	192.97 nm	*f*=0.0186	<S**2>=0.000
132 −> 136	−0.25999				
132 −> 137	0.28360				
132 −> 139	−0.27111				
132 −> 140	0.36613				
132 −> 142	−0.27515				
132 −> 145	−0.12383				
Excited state 25:	Singlet−A	6.4484 eV	192.27 nm	*f*=0.0175	<S**2>=0.000
124 −> 134	0.27644				
125 −> 134	−0.17967				
126 −> 134	0.40402				
127 −> 135	0.11543				
128 −> 134	0.21140				
130 −> 134	0.11862				
131 −> 136	0.21405				
131 −> 137	0.21295				
131 −> 140	0.10549				
Excited state 26:	Singlet−A	6.4594 eV	191.94 nm	*f*=0.0112	<S**2>=0.000
124 −> 134	−0.15377				
126 −> 134	−0.18593				
128 −> 134	−0.15239				
131 −> 136	0.50347				
131 −> 137	0.28794				
131 −> 140	0.12219				
Excited state 27:	Singlet−A	6.5253 eV	190.00 nm	*f*=0.0078	<S**2>=0.000
128 −> 135	0.10081				
130 −> 135	−0.13273				
131 −> 136	−0.22236				
131 −> 137	0.13487				
131 −> 138	0.56333				
131 −> 139	0.10638				
131 −> 143	0.11378				
Excited state 28:	Singlet−A	6.5277 eV	189.94 nm	*f*=0.0042	<S**2>=0.000
119 −> 133	−0.19337				
120 −> 133	−0.16952				
121 −> 133	0.62670				
Excited state 29:	Singlet−A	6.5479 eV	189.35 nm	*f*=0.0913	<S**2>=0.000
131 −> 136	0.12313				
131 −> 139	−0.29194				

132 −> 137 −0.18277
132 −> 139 0.38271
132 −> 140 0.39496

Excited state 30: Singlet−A 6.5598 eV 189.00 nm *f*=0.0330 <S**2>=0.000
125 −> 134 −0.22916
126 −> 134 −0.13920
128 −> 135 −0.26720
130 −> 135 0.41273
131 −> 138 0.21214
131 −> 139 −0.19206
131 −> 140 −0.11438
SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 LETran= 520.

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Rotatory strengths (R) in cgs (10**−40 erg−esu−cm/Gauss) of **15**.

State	*XX*	*YY*	*ZZ*	*R* (length)	*R* (au)
1	2.8430	−9.5712	−0.8418	−2.5233	−0.0054
2	0.0151	−0.1159	−0.0036	−0.0348	−0.0001
3	−13.3064	7.9829	−1.6074	−2.3103	−0.0049
4	24.4099	−6.4020	−2.5318	5.1587	0.0109
5	11.2471	−10.7994	−25.4771	−8.3431	−0.0177
6	−23.2427	−9.1119	0.8609	−10.4979	−0.0223
7	−44.1163	6.0620	−10.9820	−16.3454	−0.0347
8	−2.9270	−12.4780	−1.6259	−5.6770	−0.0120
9	−213.7178	35.7325	0.7670	−59.0728	−0.1253
10	265.7660	−111.9885	−40.3502	37.8091	0.0802
11	0.0087	0.2076	−0.0117	0.0682	0.0001
12	1.1923	−16.5143	−19.9958	−11.7726	−0.0250
13	0.6248	65.0055	−35.1358	10.1648	0.0216
14	−51.6301	62.3845	12.9848	7.9130	0.0168
15	8.4566	−10.2445	3.8068	0.6730	0.0014
16	−2.4327	130.0975	−116.9603	3.5682	0.0076
17	3.5117	25.1009	−41.5366	−4.3080	−0.0091
18	−151.4549	43.9407	32.7853	−24.9096	−0.0528
19	28.0674	14.5281	0.2433	14.2796	0.0303
20	56.9856	−134.3967	−43.2843	−40.2318	−0.0853
21	40.6841	17.3950	−22.3128	11.9221	0.0253
22	259.7159	−0.6134	−108.9843	50.0394	0.1061
23	−4.9450	−31.1539	4.6234	−10.4918	−0.0223
24	−3.0882	−0.7926	3.6331	−0.0826	−0.0002
25	3.4386	5.4487	−9.0694	−0.0607	−0.0001
26	−2.3438	3.7507	−0.0417	0.4551	0.0010
27	−109.5913	96.4775	94.7524	27.2129	0.0577
28	170.9741	2.3000	−101.8779	23.7987	0.0505
29	1.9975	−0.6553	−3.9666	−0.8748	−0.0019

30	3.6837	−2.8388	−2.2631	−0.4727	−0.0010

1/2[<0|del|b>*<b|r|0> + (<0|r|b>*<b|del|0>)*] (Au)

State	*X*	*Y*	*Z*	Dip. S.	Osc.(frdel)
1	−0.0062	−0.0016	−0.0001	0.0078	0.0052
2	0.0000	0.0000	0.0000	0.0000	0.0000
3	−0.0052	−0.0001	0.0000	0.0053	0.0035
4	−0.0566	−0.0018	−0.0004	0.0589	0.0393
5	−0.0139	−0.0122	−0.0018	0.0278	0.0185
6	−0.0808	−0.0010	−0.0001	0.0820	0.0546
7	−0.0143	−0.0222	−0.0011	0.0376	0.0251
8	−0.0266	−0.0028	−0.0001	0.0295	0.0196
9	−0.0399	−0.0112	0.0000	0.0511	0.0341
10	−0.3017	−0.0139	−0.0019	0.3175	0.2117
11	0.0000	0.0000	0.0000	0.0000	0.0000
12	−0.0217	−0.0020	−0.0026	0.0263	0.0175
13	−0.0244	−0.0086	−0.0036	0.0366	0.0244
14	−0.0015	−0.0135	−0.0207	0.0356	0.0238
15	−0.0007	−0.0004	−0.0002	0.0013	0.0009
16	−0.0004	−0.0454	−0.0095	0.0553	0.0369
17	−0.0025	−0.0040	−0.0026	0.0090	0.0060
18	−0.1010	−0.0072	−0.0025	0.1106	0.0737
19	−0.0082	−0.0024	−0.0001	0.0107	0.0071
20	−0.0206	−0.0080	−0.0116	0.0402	0.0268
21	−0.0091	−0.0003	−0.0031	0.0124	0.0083
22	−0.0850	0.0000	−0.0170	0.1020	0.0680
23	−0.0002	−0.0028	−0.0025	0.0055	0.0036
24	−0.0003	0.0000	−0.0003	0.0006	0.0004
25	−0.0001	−0.0016	−0.0020	0.0037	0.0025
26	−0.0001	−0.0038	−0.0021	0.0060	0.0040
27	−0.0141	−0.0118	−0.0192	0.0451	0.0301
28	−0.0871	0.0000	−0.0087	0.0958	0.0639
29	−0.0012	0.0000	−0.0003	0.0015	0.0010
30	−0.0073	−0.0007	0.0000	0.0081	0.0054

Ground to Excited state transition densities written to RWF 633

Excitation energies and oscillator strengths:

Excited state 1: Singlet−A 4.5151 eV 274.60 nm *f*=0.0054 <S**2>=0.000
131 −> 133 0.69268
132 −> 133 0.11166
This state for optimization and/or second−order correction.
Copying the Excited state density for this state as the 1−particle RhoCI density.

Excited state 2: Singlet−A 4.6121 eV 268.82 nm *f*=0.0000 <S**2>=0.000
131 −> 133 −0.10960

132 −> 133	0.69799				
Excited state 3:	Singlet−A	4.7812 eV	259.31 nm	*f*=0.0035	<S**2>=0.000
125 −> 133	0.55957				
127 −> 133	0.26665				
128 −> 133	−0.17095				
129 −> 133	0.22384				
Excited state 4:	Singlet−A	5.3846 eV	230.26 nm	*f*=0.0397	<S**2>=0.000
127 −> 133	−0.10794				
128 −> 133	0.30784				
128 −> 134	−0.10198				
129 −> 133	0.29189				
130 −> 133	0.50114				
131 −> 134	−0.10857				
132 −> 134	−0.13192				
Excited state 5:	Singlet−A	5.4026 eV	229.49 nm	*f*=0.0186	<S**2>=0.000
128 −> 134	0.28219				
128 −> 135	0.10142				
129 −> 134	0.10185				
130 −> 133	0.18299				
130 −> 134	0.10388				
131 −> 134	0.31857				
132 −> 134	0.45372				
Excited state 6:	Singlet−A	5.4834 eV	226.11 nm	*f*=0.0554	<S**2>=0.000
127 −> 133	0.22127				
128 −> 133	−0.20685				
129 −> 133	−0.39056				
130 −> 133	0.41555				
131 −> 134	0.17624				
132 −> 134	−0.19610				
Excited state 7:	Singlet−A	5.4910 eV	225.80 nm	*f*=0.0254	<S**2>=0.000
128 −> 133	0.11776				
129 −> 133	0.15677				
130 −> 133	−0.16364				
131 −> 134	0.47176				
132 −> 134	−0.41897				
Excited state 8:	Singlet−A	5.5067 eV	225.15 nm	*f*=0.0199	<S**2>=0.000
127 −> 133	0.50585				
128 −> 133	0.46383				
130 −> 133	−0.11444				
Excited state 9:	Singlet−A	5.6369 eV	219.95 nm	*f*=0.0346	<S**2>=0.000
128 −> 134	0.45083				
128 −> 135	0.14441				
129 −> 134	0.18481				
130 −> 134	0.18732				
131 −> 134	−0.31579				
132 −> 134	−0.22645				
Excited state 10:	Singlet−A	5.6535 eV	219.30 nm	*f*=0.2141	<S**2>=0.000
124 −> 133	−0.10876				
125 −> 133	0.38816				

127 −> 133	−0.31083				
128 −> 133	0.30231				
129 −> 133	−0.34678				
Excited state 11:	Singlet−A	5.8801 eV	210.85 nm	*f*=0.0000	<S**2>=0.000
126 −> 133	0.70182				
Excited state 12:	Singlet−A	5.9209 eV	209.40 nm	*f*=0.0180	<S**2>=0.000
132 −> 135	0.49490				
132 −> 136	0.36753				
132 −> 138	0.18112				
132 −> 140	−0.21217				
132 −> 142	0.12262				
Excited state 13:	Singlet−A	5.9232 eV	209.32 nm	*f*=0.0240	<S**2>=0.000
123 −> 133	−0.10690				
124 −> 133	0.65175				
129 −> 133	−0.16817				
Excited state 14:	Singlet−A	6.0229 eV	205.86 nm	*f*=0.0239	<S**2>=0.000
131 −> 135	0.65775				
Excited state 15:	Singlet−A	6.1059 eV	203.06 nm	*f*=0.0009	<S**2>=0.000
132 −> 135	0.47158				
132 −> 136	−0.40651				
132 −> 138	−0.15746				
132 −> 140	0.17680				
132 −> 142	−0.11537				
Excited state 16:	Singlet−A	6.1124 eV	202.84 nm	*f*=0.0372	<S**2>=0.000
120 −> 133	0.11811				
121 −> 133	−0.25188				
122 −> 133	0.52083				
123 −> 133	−0.32421				
Excited state 17:	Singlet−A	6.1856 eV	200.44 nm	*f*=0.0060	<S**2>=0.000
121 −> 133	0.21402				
122 −> 133	0.42765				
123 −> 133	0.49193				
124 −> 133	0.12333				
Excited state 18:	Singlet−A	6.2854 eV	197.26 nm	*f*=0.0740	<S**2>=0.000
127 −> 134	0.20153				
130 −> 134	−0.19548				
131 −> 136	0.22885				
131 −> 137	0.41992				
131 −> 138	0.22314				
131 −> 140	0.24410				
131 −> 141	−0.11012				
Excited state 19:	Singlet−A	6.3091 eV	196.52 nm	*f*=0.0073	<S**2>=0.000
119 −> 133	0.10637				
121 −> 133	0.56492				
122 −> 133	0.10828				
123 −> 133	−0.33965				
Excited state 20:	Singlet−A	6.3107 eV	196.47 nm	*f*=0.0272	<S**2>=0.000

121 −> 133	−0.12507				
130 −> 134	−0.16518				
132 −> 136	0.23440				
132 −> 137	−0.31866				
132 −> 138	−0.13632				
132 −> 139	0.40966				
132 −> 140	0.11481				
132 −> 141	0.15855				
132 −> 143	0.14366				
Excited state 21:	Singlet−A	6.3217 eV	196.13 nm	*f*=0.0085	<S**2>=0.000
128 −> 134	−0.18700				
130 −> 134	0.59221				
131 −> 137	0.15913				
131 −> 138	0.12036				
131 −> 140	0.11786				
132 −> 139	0.13770				
Excited state 22:	Singlet−A	6.3374 eV	195.64 nm	*f*=0.0689	<S**2>=0.000
132 −> 136	−0.18632				
132 −> 138	0.54843				
132 −> 139	0.21172				
132 −> 141	0.21470				
132 −> 143	−0.14480				
132 −> 144	0.14725				
Excited state 23:	Singlet−A	6.3750 eV	194.49 nm	*f*=0.0037	<S**2>=0.000
127 −> 134	0.51732				
129 −> 134	−0.23501				
130 −> 134	0.12761				
131 −> 136	0.14797				
131 −> 138	−0.19542				
131 −> 139	0.14782				
131 −> 140	−0.16247				
Excited state 24:	Singlet−A	6.4039 eV	193.61 nm	*f*=0.0004	<S**2>=0.000
131 −> 138	−0.10908				
132 −> 136	0.19217				
132 −> 137	0.50018				
132 −> 139	0.25703				
132 −> 140	0.18986				
132 −> 141	−0.15831				
132 −> 142	−0.18458				
Excited state 25:	Singlet−A	6.4230 eV	193.03 nm	*f*=0.0025	<S**2>=0.000
127 −> 134	−0.14866				
131 −> 135	0.10764				
131 −> 136	0.58653				
131 −> 137	−0.13188				
131 −> 139	−0.26212				
Excited state 26:	Singlet−A	6.4280 eV	192.88 nm	*f*=0.0039	<S**2>=0.000
127 −> 134	−0.12974				
131 −> 137	0.44986				
131 −> 138	−0.43886				
131 −> 140	−0.20432				

Excited state 27: Singlet−A 6.4623 eV 191.86 nm *f*=0.0303 <S**2>=0.000
127 −> 134 −0.17737
131 −> 136 0.21527
131 −> 137 −0.10651
131 −> 139 0.59537

Excited state 28: Singlet−A 6.5093 eV 190.47 nm *f*=0.0649 <S**2>=0.000
132 −> 136 0.15399
132 −> 137 −0.24433
132 −> 138 0.21091
132 −> 139 −0.27812
132 −> 140 0.42301
132 −> 141 −0.18926
132 −> 142 −0.12884
132 −> 146 −0.11968

Excited state 29: Singlet−A 6.5415 eV 189.53 nm *f*=0.0010 <S**2>=0.000
127 −> 134 0.26897
128 −> 134 −0.15947
129 −> 134 0.59129

Excited state 30: Singlet−A 6.5874 eV 188.21 nm *f*=0.0056 <S**2>=0.000
118 −> 133 −0.21749
119 −> 133 0.17698
120 −> 133 0.59756
121 −> 133 0.13125
SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 LETran= 520.
****

Rotatory strengths (R) in cgs (10**−40 erg−esu−cm/Gauss) of **16**.

State	*XX*	*YY*	*ZZ*	*R* (length)	*R* (au)
1	5.7878	−14.6333	−0.5648	−3.1368	−0.0067
2	0.0624	−0.1431	0.0044	−0.0254	−0.0001
3	−6.2754	15.4267	−14.5071	−1.7852	−0.0038
4	−55.0869	−0.2328	16.0691	−13.0835	−0.0278
5	65.2885	−72.3769	6.2120	−0.2921	−0.0006
6	−0.2272	−0.2885	−0.7764	−0.4307	−0.0009
7	155.2248	−181.3953	25.7289	−0.1472	−0.0003
8	41.2654	−42.1506	4.4640	1.1929	0.0025
9	300.8506	−335.2584	72.3766	12.6563	0.0268
10	69.3230	1.7813	11.6594	27.5879	0.0585
11	1.8397	−0.1552	−0.6566	0.3426	0.0007
12	33.7732	−1.0755	−97.5870	−21.6298	−0.0459
13	−9.6735	45.5646	−4.5563	10.4449	0.0222
14	−147.1432	114.8334	12.9005	−6.4697	−0.0137
15	20.4669	7.5480	−45.8584	−5.9479	−0.0126
16	7.4888	125.1397	−124.2278	2.8002	0.0059
17	−493.7197	168.1205	332.0665	2.1558	0.0046
18	23.4392	4.4214	13.8220	13.8942	0.0295
19	−5.3631	37.4931	−31.1358	0.3314	0.0007
20	2.0610	57.0252	−75.9359	−5.6166	−0.0119

21	125.8299	4.5157	−117.1171	4.4095	0.0094
22	4.5930	−1.5023	−0.5088	0.8607	0.0018
23	97.4744	192.9955	−187.1117	34.4527	0.0731
24	−28.1289	8.6809	13.3374	−2.0369	−0.0043
25	31.1693	−30.3985	2.2331	1.0013	0.0021
26	6.7832	−19.0731	0.5410	−3.9163	−0.0083
27	−9.4232	1.2643	−0.4275	−2.8621	−0.0061
28	69.5069	71.6651	−184.0546	−14.2942	−0.0303
29	−14.5080	290.7437	−299.9237	−7.8960	−0.0167
30	−35.9754	−28.9008	−86.3345	−50.4035	−0.1069

1/2[<0|del|b>*<b|r|0> + (<0|r|b>*<b|del|0>)*] (Au)

State	*X*	*Y*	*Z*	Dip. S.	Osc.(frdel)
1	−0.0049	−0.0035	0.0000	0.0084	0.0056
2	0.0000	0.0000	0.0000	0.0001	0.0000
3	−0.0040	−0.0010	−0.0005	0.0055	0.0037
4	−0.0180	0.0000	−0.0003	0.0183	0.0122
5	−0.0433	−0.0171	−0.0022	0.0626	0.0417
6	−0.0001	0.0000	0.0000	0.0001	0.0001
7	−0.0842	−0.0330	−0.0057	0.1229	0.0820
8	−0.0386	−0.0031	−0.0048	0.0465	0.0310
9	−0.1595	−0.0482	−0.0222	0.2299	0.1533
10	−0.0127	−0.0001	−0.0028	0.0156	0.0104
11	−0.0013	0.0000	−0.0009	0.0021	0.0014
12	−0.0054	0.0000	−0.0147	0.0201	0.0134
13	−0.0125	−0.0024	−0.0197	0.0347	0.0231
14	−0.0130	−0.0144	−0.0267	0.0541	0.0361
15	−0.0139	−0.0012	−0.0087	0.0238	0.0159
16	−0.0012	−0.0125	−0.0297	0.0434	0.0289
17	−0.0832	−0.0073	−0.0384	0.1290	0.0860
18	−0.0015	−0.0020	−0.0043	0.0078	0.0052
19	−0.0020	−0.0013	−0.0156	0.0188	0.0125
20	−0.0017	−0.0095	−0.0125	0.0238	0.0158
21	−0.0478	0.0000	−0.0098	0.0576	0.0384
22	−0.0021	−0.0003	−0.0002	0.0026	0.0017
23	−0.0290	−0.0272	−0.0270	0.0833	0.0555
24	−0.0050	−0.0004	−0.0016	0.0070	0.0047
25	−0.0055	−0.0043	−0.0005	0.0103	0.0069
26	−0.0019	−0.0029	−0.0001	0.0048	0.0032
27	−0.0075	−0.0007	0.0000	0.0082	0.0055
28	−0.0262	−0.0250	−0.0335	0.0846	0.0564
29	−0.0940	−0.0322	−0.0118	0.1379	0.0920
30	−0.0039	−0.0045	−0.0188	0.0273	0.0182

Ground to Excited state transition densities written to RWF 633

Excitation energies and oscillator strengths:

Excited state 1: Singlet−A 4.4549 eV 278.31 nm *f*=0.0058 <S**2>=0.000
131 −> 133 0.62922
132 −> 133 −0.31472
This state for optimization and/or second−order correction.
Copying the Excited state density for this state as the 1−particle RhoCI density.

Excited state 2: Singlet−A 4.6551 eV 266.34 nm *f*=0.0000 <S**2>=0.000
131 −> 133 0.31587
132 −> 133 0.63243

Excited state 3: Singlet−A 4.7826 eV 259.24 nm *f*=0.0036 <S**2>=0.000
125 −> 133 0.56867
127 −> 133 0.11917
128 −> 133 0.29900
129 −> 133 −0.20285

Excited state 4: Singlet−A 5.2616 eV 235.64 nm *f*=0.0123 <S**2>=0.000
127 −> 134 0.13551
128 −> 134 −0.19300
129 −> 134 −0.11673
130 −> 134 −0.10171
131 −> 134 0.60422
132 −> 134 −0.14675

Excited state 5: Singlet−A 5.4161 eV 228.92 nm *f*=0.0424 <S**2>=0.000
128 −> 133 0.34709
129 −> 133 0.33687
130 −> 133 0.49057

Excited state 6: Singlet−A 5.4492 eV 227.53 nm *f*=0.0001 <S**2>=0.000
125 −> 133 0.17161
127 −> 133 −0.36877
128 −> 133 −0.30859
129 −> 133 −0.19958
130 −> 133 0.44279

Excited state 7: Singlet−A 5.5267 eV 224.34 nm *f*=0.0832 <S**2>=0.000
123 −> 133 −0.13104
125 −> 133 0.23037
127 −> 133 −0.42134
129 −> 133 0.42796
130 −> 133 −0.24107

Excited state 8: Singlet−A 5.6174 eV 220.71 nm *f*=0.0312 <S**2>=0.000
127 −> 133 −0.11900
128 −> 133 0.13123
128 −> 134 −0.11266
132 −> 134 0.64035

Excited state 9: Singlet−A 5.6260 eV 220.38 nm *f*=0.1548 <S**2>=0.000
125 −> 133 −0.24369
127 −> 133 −0.36922
128 −> 133 0.41144
129 −> 133 −0.26614

132 −> 134	−0.20561				
Excited state 10:	Singlet−A	5.8686 eV	211.27 nm	*f*=0.0104	<S**2>=0.000
127 −> 134	−0.27509				
128 −> 134	0.35703				
129 −> 134	0.18950				
130 −> 134	0.20725				
131 −> 134	0.30586				
131 −> 135	0.24142				
132 −> 134	0.13450				
132 −> 135	−0.10481				
Excited state 11:	Singlet−A	5.8774 eV	210.95 nm	*f*=0.0014	<S**2>=0.000
126 −> 133	0.69694				
Excited state 12:	Singlet−A	5.9218 eV	209.37 nm	*f*=0.0134	<S**2>=0.000
132 −> 135	0.36838				
132 −> 136	0.42599				
132 −> 137	−0.12895				
132 −> 138	−0.10547				
132 −> 139	0.24922				
132 −> 140	0.15192				
Excited state 13:	Singlet−A	5.9452 eV	208.54 nm	*f*=0.0229	<S**2>=0.000
123 −> 133	0.55787				
124 −> 133	−0.32879				
129 −> 133	0.14099				
Excited state 14:	Singlet−A	5.9495 eV	208.40 nm	*f*=0.0362	<S**2>=0.000
127 −> 134	0.10107				
128 −> 134	−0.12660				
131 −> 134	−0.11294				
131 −> 135	0.52479				
131 −> 136	0.14985				
131 −> 137	0.12306				
132 −> 135	−0.15343				
132 −> 136	0.14790				
132 −> 137	−0.13857				
132 −> 139	0.11242				
Excited state 15:	Singlet−A	6.0481 eV	205.00 nm	*f*=0.0161	<S**2>=0.000
131 −> 135	0.27333				
132 −> 135	0.55329				
132 −> 136	−0.28350				
Excited state 16:	Singlet−A	6.0544 eV	204.78 nm	*f*=0.0291	<S**2>=0.000
121 −> 133	0.17586				
122 −> 133	0.28345				
123 −> 133	0.32709				
124 −> 133	0.50046				
129 −> 133	0.10401				
Excited state 17:	Singlet−A	6.1637 eV	201.15 nm	*f*=0.0860	<S**2>=0.000
131 −> 135	−0.20656				
131 −> 136	0.46038				
131 −> 137	0.28950				
131 −> 139	−0.11340				

131 −> 140	0.15121				
132 −> 136	−0.19021				
132 −> 137	−0.12731				
132 −> 139	0.10332				
Excited state 18:	Singlet−A	6.2187 eV	199.37 nm	*f*=0.0053	<S**2>=0.000
131 −> 136	−0.33055				
131 −> 137	0.47388				
131 −> 138	−0.12260				
132 −> 136	0.13742				
132 −> 137	−0.24009				
132 −> 138	0.14982				
132 −> 139	−0.10485				
Excited state 19:	Singlet−A	6.2600 eV	198.06 nm	*f*=0.0128	<S**2>=0.000
131 −> 136	0.17028				
131 −> 137	−0.12752				
131 −> 139	−0.11234				
132 −> 136	0.26751				
132 −> 138	0.43242				
132 −> 139	−0.15415				
132 −> 140	−0.27282				
132 −> 142	0.19526				
Excited state 20:	Singlet−A	6.2869 eV	197.21 nm	*f*=0.0161	<S**2>=0.000
121 −> 133	0.38630				
122 −> 133	0.44883				
124 −> 133	−0.35085				
Excited state 21:	Singlet−A	6.2968 eV	196.90 nm	*f*=0.0385	<S**2>=0.000
131 −> 136	−0.24518				
131 −> 138	−0.33954				
131 −> 139	−0.13057				
131 −> 140	0.36390				
131 −> 142	0.11343				
132 −> 137	0.18734				
132 −> 139	0.24199				
132 −> 142	−0.10641				
Excited state 22:	Singlet−A	6.3277 eV	195.94 nm	*f*=0.0018	<S**2>=0.000
131 −> 136	0.10063				
131 −> 137	0.28858				
132 −> 136	0.21289				
132 −> 137	0.53503				
132 −> 138	−0.11303				
132 −> 141	−0.15692				
Excited state 23:	Singlet−A	6.3448 eV	195.41 nm	*f*=0.0564	<S**2>=0.000
131 −> 138	0.18625				
131 −> 139	0.19109				
131 −> 140	−0.16338				
132 −> 136	−0.11290				
132 −> 137	0.11425				
132 −> 138	0.30559				
132 −> 139	0.38731				
132 −> 141	0.21202				
132 −> 142	0.14127				

132 −> 143 0.15531

Excited state 24: Singlet−A 6.3764 eV 194.44 nm *f*=0.0047 <S**2>=0.000
131 −> 136 −0.14955
131 −> 137 0.10297
131 −> 138 0.48441
131 −> 139 −0.33181
131 −> 140 0.14096
131 −> 142 0.10035
132 −> 138 −0.14579
132 −> 139 0.11964
132 −> 140 −0.13103
Excited state 25: Singlet−A 6.3859 eV 194.15 nm *f*=0.0071 <S**2>=0.000
118 −> 133 0.14977
120 −> 133 0.29262
121 −> 133 0.45681
122 −> 133 −0.40201

Excited state 26: Singlet−A 6.4923 eV 190.97 nm *f*=0.0033 <S**2>=0.000
117 −> 133 −0.11972
118 −> 133 0.26930
119 −> 133 −0.26645
120 −> 133 0.46646
121 −> 133 −0.26226
122 −> 133 0.18147

Excited state 27: Singlet−A 6.5095 eV 190.47 nm *f*=0.0057 <S**2>=0.000
128 −> 134 −0.20281
129 −> 134 −0.16175
130 −> 134 0.58607
131 −> 139 −0.11609
132 −> 140 0.17292

Excited state 28: Singlet−A 6.5243 eV 190.04 nm *f*=0.0573 <S**2>=0.000
130 −> 134 0.21388
131 −> 139 0.34889
131 −> 140 0.25665
131 −> 141 −0.13780
132 −> 138 −0.19288
132 −> 140 −0.34120
132 −> 141 0.14255

Excited state 29: Singlet−A 6.5369 eV 189.67 nm *f*=0.0932 <S**2>=0.000
131 −> 138 0.21585
131 −> 139 0.14565
131 −> 140 0.37314
131 −> 141 −0.13486
132 −> 138 0.22335
132 −> 139 −0.14266
132 −> 140 0.37581

Excited state 30: Singlet−A 6.5915 eV 188.10 nm *f*=0.0185 <S**2>=0.000
128 −> 135 0.50718
128 −> 136 −0.14493
129 −> 135 0.26445
130 −> 135 0.24721
SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 LETran= 520.

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Rotatory strengths (R) in cgs (10**−40 erg−esu−cm/Gauss) of **17**.

State	*XX*	*YY*	*ZZ*	*R* (length)	*R* (au)
1	4.1574	−11.3274	−0.1800	−2.4500	−0.0052
2	0.0744	−0.1512	0.0081	−0.0229	0.0000
3	−5.2782	11.4009	−16.1027	−3.3267	−0.0071
4	−59.7257	0.7700	20.5982	−12.7858	−0.0271
5	16.1287	−18.5451	0.2087	−0.7359	−0.0016
6	−1.4991	1.3527	−1.8422	−0.6628	−0.0014
7	142.6095	−164.6987	19.4156	−0.8912	−0.0019
8	0.2139	−1.3627	−2.5416	−1.2301	−0.0026
9	397.0452	−388.9912	42.3392	16.7977	0.0356
10	2.6361	−1.8247	−0.2586	0.1843	0.0004
11	52.7309	10.8216	1.6186	21.7237	0.0461
12	12.7720	1.6006	−66.2246	−17.2840	−0.0367
13	7.9062	40.1619	−16.5679	10.5001	0.0223
14	−113.1082	128.9081	19.7496	11.8498	0.0251
15	−0.8101	73.6886	−115.6543	−14.2586	−0.0302
16	27.1269	27.8119	−6.4804	16.1528	0.0343
17	−500.3329	150.6064	335.7579	−4.6562	−0.0099
18	0.5998	−1.7329	5.1479	1.3383	0.0028
19	0.8323	64.4873	−39.8331	8.4955	0.0180
20	−0.8107	17.6170	−47.7919	−10.3285	−0.0219
21	152.5761	19.6784	−153.7494	6.1684	0.0131
22	24.4250	−11.8657	−1.7142	3.6150	0.0077
23	71.1283	164.5692	−149.6147	28.6943	0.0609
24	−0.4017	4.9305	−18.3952	−4.6222	−0.0098
25	−15.9984	11.3079	12.1851	2.4982	0.0053
26	3.1114	−11.0571	−6.4140	−4.7866	−0.0102
27	−1.5249	17.9420	−30.3905	−4.6578	−0.0099
28	83.6212	296.1333	−436.4442	−18.8966	−0.0401
29	11.8564	36.7654	−26.8597	7.2540	0.0154
30	−132.6326	−6.9115	33.4040	−35.3801	−0.0750

1/2[<0|del|b>*<b|r|0> + (<0|r|b>*<b|del|0>)*] (Au)

State	*X*	*Y*	*Z*	Dip. S.	Osc.(frdel)
1	−0.0046	−0.0028	0.0000	0.0074	0.0049
2	0.0000	0.0000	0.0000	0.0001	0.0001
3	−0.0034	−0.0005	−0.0005	0.0044	0.0029
4	−0.0172	0.0000	−0.0006	0.0178	0.0119
5	−0.0085	−0.0034	−0.0004	0.0122	0.0081
6	−0.0021	−0.0010	−0.0001	0.0032	0.0021
7	−0.1119	−0.0393	−0.0028	0.1540	0.1026

8	−0.0119	0.0000	−0.0017	0.0136	0.0091
9	−0.2131	−0.0437	−0.0302	0.2870	0.1913
10	−0.0019	−0.0001	−0.0007	0.0027	0.0018
11	−0.0227	−0.0009	0.0000	0.0237	0.0158
12	−0.0086	−0.0009	−0.0065	0.0160	0.0107
13	−0.0167	−0.0016	−0.0229	0.0412	0.0275
14	−0.0048	−0.0149	−0.0365	0.0562	0.0375
15	0.0000	−0.0070	−0.0287	0.0358	0.0238
16	−0.0156	−0.0038	−0.0012	0.0205	0.0137
17	−0.0939	−0.0060	−0.0345	0.1344	0.0896
18	−0.0014	0.0000	−0.0034	0.0047	0.0032
19	−0.0001	−0.0072	−0.0097	0.0169	0.0113
20	−0.0049	−0.0004	−0.0127	0.0180	0.0120
21	−0.0535	−0.0005	−0.0170	0.0710	0.0473
22	−0.0043	−0.0038	−0.0001	0.0082	0.0055
23	−0.0203	−0.0253	−0.0231	0.0686	0.0457
24	−0.0001	−0.0001	−0.0032	0.0035	0.0023
25	−0.0025	−0.0006	−0.0026	0.0056	0.0038
26	−0.0026	−0.0042	−0.0006	0.0074	0.0049
27	−0.0025	−0.0059	−0.0036	0.0120	0.0080
28	−0.1068	−0.0549	−0.0322	0.1940	0.1293
29	−0.0119	−0.0012	−0.0003	0.0133	0.0089
30	−0.0151	−0.0007	−0.0260	0.0418	0.0279

Ground to Excited state transition densities written to RWF 633

Excitation energies and oscillator strengths:

Excited state 1: Singlet−A 4.4348 eV 279.57 nm *f*=0.0051 <S**2>=0.000
131 −> 133 0.65477
132 −> 133 −0.26155
This state for optimization and/or second−order correction.
Copying the Excited state density for this state as the 1−particle RhoCI density.

Excited state 2: Singlet−A 4.6036 eV 269.32 nm *f*=0.0001 <S**2>=0.000
131 −> 133 0.26229
132 −> 133 0.65650

Excited state 3: Singlet−A 4.7764 eV 259.58 nm *f*=0.0028 <S**2>=0.000
125 −> 133 0.53993
127 −> 133 0.28753
128 −> 133 0.25808
129 −> 133 −0.18814

Excited state 4: Singlet−A 5.2924 eV 234.27 nm *f*=0.0120 <S**2>=0.000
127 −> 134 −0.12393
129 −> 134 −0.22440
130 −> 134 −0.10618
131 −> 134 0.59435
131 −> 135 0.15110

Excited state 5:	Singlet−A	5.3784 eV	230.52 nm	*f*=0.0083	<S**2>=0.000
128 −> 133	0.10264				
129 −> 133	0.29687				
130 −> 133	0.62402				
Excited state 6:	Singlet−A	5.4405 eV	227.89 nm	*f*=0.0022	<S**2>=0.000
125 −> 133	0.13443				
127 −> 133	−0.20064				
128 −> 133	0.28845				
129 −> 133	0.51916				
130 −> 133	−0.29544				
Excited state 7:	Singlet−A	5.5038 eV	225.27 nm	*f*=0.1043	<S**2>=0.000
123 −> 133	−0.11959				
127 −> 133	0.54999				
128 −> 133	−0.25792				
129 −> 133	0.28763				
130 −> 133	−0.14440				
Excited state 8:	Singlet−A	5.6454 eV	219.62 nm	*f*=0.0091	<S**2>=0.000
129 −> 134	−0.10997				
132 −> 134	0.67129				
132 −> 135	0.12085				
Excited state 9:	Singlet−A	5.6759 eV	218.44 nm	*f*=0.1931	<S**2>=0.000
125 −> 133	−0.40508				
127 −> 133	0.25786				
128 −> 133	0.48559				
Excited state 10:	Singlet−A	5.8288 eV	212.71 nm	*f*=0.0018	<S**2>=0.000
126 −> 133	0.70290				
Excited state 11:	Singlet−A	5.9099 eV	209.79 nm	*f*=0.0158	<S**2>=0.000
127 −> 134	0.24116				
128 −> 134	0.18735				
129 −> 134	0.39609				
130 −> 134	0.21578				
131 −> 134	0.29219				
131 −> 135	0.16154				
132 −> 134	0.16121				
Excited state 12:	Singlet−A	5.9280 eV	209.15 nm	*f*=0.0109	<S**2>=0.000
132 −> 135	0.26071				
132 −> 136	0.46316				
132 −> 137	0.21937				
132 −> 139	0.28408				
132 −> 140	−0.13888				
132 −> 141	0.14559				
Excited state 13:	Singlet−A	5.9556 eV	208.18 nm	*f*=0.0273	<S**2>=0.000
120 −> 133	0.10614				
123 −> 133	0.57040				
124 −> 133	−0.33085				
128 −> 133	−0.11056				
129 −> 133	0.10593				

Excited state 14:	Singlet−A	5.9817 eV	207.27 nm	*f*=0.0375	<S**2>=0.000
131 −> 134	−0.16307				
131 −> 135	0.54489				
131 −> 136	0.12695				
131 −> 137	−0.12901				
131 −> 138	−0.21530				
132 −> 135	−0.18479				
Excited state 15:	Singlet−A	6.0559 eV	204.73 nm	*f*=0.0240	<S**2>=0.000
121 −> 133	0.15054				
122 −> 133	0.28330				
123 −> 133	0.28672				
124 −> 133	0.51512				
132 −> 135	0.12716				
Excited state 16:	Singlet−A	6.0576 eV	204.68 nm	*f*=0.0137	<S**2>=0.000
124 −> 133	−0.11487				
131 −> 135	0.21377				
132 −> 134	−0.10213				
132 −> 135	0.58438				
132 −> 136	−0.23206				
Excited state 17:	Singlet−A	6.1691 eV	200.98 nm	*f*=0.0893	<S**2>=0.000
131 −> 134	0.13305				
131 −> 135	−0.24383				
131 −> 136	0.39930				
131 −> 137	−0.26794				
131 −> 138	−0.27628				
131 −> 140	−0.15066				
132 −> 136	−0.12606				
Excited state 18:	Singlet−A	6.2322 eV	198.94 nm	*f*=0.0032	<S**2>=0.000
131 −> 136	0.37247				
131 −> 137	0.21561				
131 −> 138	0.27609				
131 −> 142	−0.10467				
132 −> 136	−0.25310				
132 −> 138	−0.28614				
132 −> 139	0.17298				
132 −> 141	0.10088				
Excited state 19:	Singlet−A	6.2560 eV	198.19 nm	*f*=0.0114	<S**2>=0.000
121 −> 133	0.37025				
122 −> 133	0.46947				
123 −> 133	−0.14475				
124 −> 133	−0.31198				
Excited state 20:	Singlet−A	6.2611 eV	198.02 nm	*f*=0.0122	<S**2>=0.000
131 −> 136	0.35266				
131 −> 137	0.16169				
131 −> 138	0.17218				
132 −> 136	0.25581				
132 −> 137	−0.16511				
132 −> 138	0.27653				
132 −> 139	−0.19985				
132 −> 140	0.12134				
132 −> 141	−0.18627				

132 −> 142	0.15064				
Excited state 21:	Singlet−A	6.3118 eV	196.43 nm	*f*=0.0475	<S**2>=0.000
131 −> 137	0.38005				
131 −> 138	−0.27002				
131 −> 140	−0.23951				
132 −> 137	−0.30282				
132 −> 138	0.12654				
132 −> 139	0.26020				
Excited state 22:	Singlet−A	6.3317 eV	195.81 nm	*f*=0.0057	<S**2>=0.000
120 −> 133	−0.36927				
121 −> 133	0.40113				
122 −> 133	−0.39152				
123 −> 133	0.12810				
Excited state 23:	Singlet−A	6.3431 eV	195.46 nm	*f*=0.0465	<S**2>=0.000
131 −> 137	−0.21792				
131 −> 138	0.24453				
131 −> 140	0.13007				
132 −> 136	−0.10063				
132 −> 138	0.34313				
132 −> 139	0.32265				
132 −> 142	0.26116				
132 −> 143	0.12226				
Excited state 24:	Singlet−A	6.3597 eV	194.95 nm	*f*=0.0024	<S**2>=0.000
131 −> 137	0.28506				
132 −> 136	−0.19557				
132 −> 137	0.49472				
132 −> 138	0.22266				
132 −> 142	0.18971				
Excited state 25:	Singlet−A	6.4178 eV	193.19 nm	*f*=0.0038	<S**2>=0.000
131 −> 136	0.14791				
131 −> 137	0.15673				
131 −> 138	−0.23416				
131 −> 139	0.44653				
131 −> 140	0.32466				
131 −> 142	−0.11122				
131 −> 145	0.10525				
132 −> 139	−0.10252				
132 −> 140	−0.15249				
Excited state 26:	Singlet−A	6.4541 eV	192.10 nm	*f*=0.0050	<S**2>=0.000
118 −> 133	−0.26235				
119 −> 133	−0.21195				
120 −> 133	0.45551				
121 −> 133	0.34815				
122 −> 133	−0.16917				
Excited state 27:	Singlet−A	6.5391 eV	189.60 nm	*f*=0.0080	<S**2>=0.000
129 −> 134	−0.11917				
129 −> 135	−0.17294				
130 −> 134	0.44101				
131 −> 139	−0.19892				
131 −> 140	0.10061				

132 −> 138 0.11005
132 −> 140 −0.35213
132 −> 142 −0.11173

Excited state 28: Singlet−A 6.5512 eV 189.25 nm *f*=0.1315 <S**2>=0.000
129 −> 134 −0.17327
130 −> 134 0.43169
131 −> 139 0.12075
132 −> 138 −0.13713
132 −> 140 0.43351
132 −> 142 0.11461

Excited state 29: Singlet−A 6.5576 eV 189.07 nm *f*=0.0089 <S**2>=0.000
129 −> 134 0.14209
129 −> 135 −0.15851
130 −> 134 −0.14373
130 −> 135 −0.14528
131 −> 138 −0.16542
131 −> 139 −0.22186
131 −> 140 0.41945
131 −> 141 0.11996
131 −> 142 0.17978
132 −> 139 0.13419
132 −> 140 0.20375

Excited state 30: Singlet−A 6.5801 eV 188.42 nm *f*=0.0280 <S**2>=0.000
127 −> 134 0.18909
128 −> 135 0.17690
129 −> 134 −0.23923
129 −> 135 0.41532
129 −> 136 −0.12035
130 −> 135 0.19187
131 −> 139 −0.16483
131 −> 140 0.19932
132 −> 142 −0.10380
SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 LETran= 520.

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Rotatory strengths (R) in cgs (10**−40 erg−esu−cm/Gauss) of **18**.

State	*XX*	*YY*	*ZZ*	*R* (length)	*R* (au)
1	−5.0431	2.1170	0.5369	−0.7964	−0.0017
2	−0.0633	14.0081	−6.7088	2.4120	0.0051
3	5.8670	−13.9740	−0.6993	−2.9354	−0.0062
4	−187.4444	137.6408	−21.5089	−23.7708	−0.0504
5	−3.4476	11.4023	−16.0406	−2.6953	−0.0057
6	0.0147	−0.0025	−0.0356	−0.0078	0.0000
7	55.6499	1069.0352	−1023.1566	33.8428	0.0718
8	0.2123	1.2850	−0.4149	0.3608	0.0008
9	−56.0858	6.0394	20.7789	−9.7558	−0.0207
10	−1.4157	0.5506	−0.9853	−0.6168	−0.0013
11	25.4180	−52.8392	13.0409	−4.7934	−0.0102
12	19.0352	126.1661	−177.6048	−10.8012	−0.0229

13	9.5509	−11.3221	0.9239	−0.2824	−0.0006
14	0.3673	2.4816	−17.3444	−4.8318	−0.0102
15	299.5809	−368.3777	60.2210	−2.8586	−0.0061
16	−17.1272	1.9085	−4.7106	−6.6431	−0.0141
17	0.5845	−0.1832	0.0862	0.1625	0.0003
18	146.8085	−89.2414	−13.6808	14.6288	0.0310
19	42.8743	−86.2930	43.6193	0.0668	0.0001
20	−0.7795	89.6149	−27.5020	20.4444	0.0434
21	−169.0300	51.3756	−50.3915	−56.0153	−0.1188
22	5.5277	5.4648	−24.7772	−4.5949	−0.0097
23	32.8897	81.2979	−74.6557	13.1773	0.0280
24	26.5907	−5.9441	−2.0744	6.1907	0.0131
25	48.1958	0.0811	−29.7503	6.1755	0.0131
26	−13.2713	104.0023	11.8159	34.1823	0.0725
27	−5.9628	−4.2993	−17.8780	−9.3800	−0.0199
28	−24.9308	133.9419	−39.5912	23.1399	0.0491
29	10.1857	−22.8381	−6.9469	−6.5331	−0.0139
30	−315.2182	125.3965	356.7215	55.6333	0.1180

1/2[<0|del|b>*<b|r|0> + (<0|r|b>*<b|del|0>)*] (Au)

State	*X*	*Y*	*Z*	Dip. S.	Osc.(frdel)
1	−0.0001	0.0000	0.0000	0.0001	0.0001
2	0.0000	−0.0037	−0.0001	0.0038	0.0025
3	−0.0047	−0.0034	0.0000	0.0081	0.0054
4	−0.2123	−0.1439	0.0000	0.3562	0.2375
5	−0.0033	−0.0008	−0.0005	0.0046	0.0031
6	0.0000	0.0000	0.0000	0.0000	0.0000
7	−0.0358	−0.1485	−0.0877	0.2720	0.1813
8	−0.0005	−0.0008	−0.0001	0.0013	0.0009
9	−0.0151	−0.0002	−0.0011	0.0163	0.0109
10	−0.0006	−0.0001	−0.0003	0.0009	0.0006
11	−0.0686	−0.0273	−0.0005	0.0963	0.0642
12	−0.0059	−0.0127	−0.0219	0.0405	0.0270
13	−0.0060	−0.0031	−0.0002	0.0093	0.0062
14	0.0000	−0.0001	−0.0019	0.0020	0.0013
15	−0.1560	−0.0634	−0.0122	0.2316	0.1544
16	−0.0007	0.0000	−0.0004	0.0011	0.0007
17	0.0000	−0.0003	0.0000	0.0003	0.0002
18	−0.0809	−0.0040	−0.0164	0.1013	0.0675
19	−0.0118	−0.0117	−0.0060	0.0295	0.0197
20	0.0000	−0.0159	−0.0048	0.0208	0.0139
21	−0.0125	−0.0038	−0.0334	0.0496	0.0331
22	−0.0016	−0.0027	−0.0024	0.0067	0.0045

23	−0.0128	−0.0023	−0.0630	0.0781	0.0521
24	−0.0088	−0.0007	0.0000	0.0096	0.0064
25	−0.0173	−0.0001	−0.0052	0.0227	0.0151
26	−0.0079	−0.0271	−0.0001	0.0351	0.0234
27	−0.0024	−0.0002	−0.0022	0.0048	0.0032
28	−0.0302	−0.0744	−0.0002	0.1047	0.0698
29	−0.0115	−0.0072	−0.0001	0.0189	0.0126
30	−0.0267	−0.0062	−0.0535	0.0864	0.0576

Ground to Excited state transition densities written to RWF 633

Excitation energies and oscillator strengths:

Excited state 1: Singlet−A 3.5567 eV 348.59 nm *f*=0.0001 <S**2>=0.000
130 −>132 0.69533
This state for optimization and/or second−order correction.
Copying the Excited state density for this state as the 1−particle RhoCI density.

Excited state 2: Singlet−A 4.3807 eV 283.03 nm *f*=0.0026 <S**2>=0.000
131 −>132 0.70239

Excited state 3: Singlet−A 4.4851 eV 276.44 nm *f*=0.0056 <S**2>=0.000
131 −>133 0.70315

Excited state 4: Singlet−A 4.5761 eV 270.94 nm *f*=0.2384 <S**2>=0.000
128 −>132 0.11325
129 −>132 0.68161

Excited state 5: Singlet−A 4.7871 eV 258.99 nm *f*=0.0030 <S**2>=0.000
124 −>133 0.51817
125 −>133 0.30251
126 −>133 −0.30796
127 −>133 0.13784

Excited state 6: Singlet−A 4.9095 eV 252.54 nm *f*=0.0000 <S**2>=0.000
130 −>133 0.70257

Excited state 7: Singlet−A 4.9602 eV 249.96 nm *f*=0.1866 <S**2>=0.000
128 −>132 0.67972
129 −>132 −0.10643

Excited state 8: Singlet−A 4.9904 eV 248.44 nm *f*=0.0009 <S**2>=0.000
129 −>133 0.70146

Excited state 9: Singlet−A 5.2537 eV 235.99 nm *f*=0.0110 <S**2>=0.000
125 −>134 −0.21040
126 −>134 −0.11295
128 −>134 0.12273
129 −>134 −0.10114
131 −>134 0.61535

Excited state 10: Singlet−A 5.2631 eV 235.57 nm *f*=0.0006 <S**2>=0.000
126 −>132 0.13824
127 −>132 0.68860

Excited state 11:	Singlet−A	5.3174 eV	233.17 nm	*f*=0.0649	<S**2>=0.000
126 −>133	0.35378				
127 −>133	0.59981				
Excited state 12:	Singlet−A	5.3463 eV	231.90 nm	*f*=0.0280	<S**2>=0.000
125 −>132	0.51438				
126 −>132	0.45491				
Excited state 13:	Singlet−A	5.3789 eV	230.50 nm	*f*=0.0063	<S**2>=0.000
125 −>133	−0.10424				
128 −>133	0.68923				
Excited state 14:	Singlet−A	5.4564 eV	227.23 nm	*f*=0.0014	<S**2>=0.000
125 −>132	−0.43827				
126 −>132	0.51871				
127 −>132	−0.14167				
Excited state 15:	Singlet−A	5.5533 eV	223.26 nm	*f*=0.1568	<S**2>=0.000
123 −>133	−0.18991				
124 −>133	0.21238				
125 −>133	0.28814				
126 −>133	0.47505				
127 −>133	−0.27219				
128 −>133	0.14143				
Excited state 16:	Singlet−A	5.5700 eV	222.59 nm	*f*=0.0010	<S**2>=0.000
130 −>134	−0.15963				
130 −>135	0.63693				
130 −>136	0.20756				
Excited state 17:	Singlet−A	5.7231 eV	216.64 nm	*f*=0.0002	<S**2>=0.000
122 −>132	−0.13117				
124 −>132	0.67513				
125 −>132	0.14732				
Excited state 18:	Singlet−A	5.7510 eV	215.59 nm	*f*=0.0677	<S**2>=0.000
124 −>133	−0.26205				
125 −>133	0.36057				
125 −>134	−0.26619				
126 −>134	−0.12104				
128 −>134	0.17619				
129 −>134	−0.30022				
131 −>134	−0.22059				
Excited state 19:	Singlet−A	5.7606 eV	215.23 nm	*f*=0.0199	<S**2>=0.000
124 −>133	−0.30377				
125 −>133	0.41085				
125 −>134	0.23051				
126 −>134	0.10283				
127 −>133	0.11074				
128 −>134	−0.15407				
129 −>134	0.26587				
131 −>134	0.18887				
Excited state 20:	Singlet−A	5.7727 eV	214.78 nm	*f*=0.0141	<S**2>=0.000
122 −>132	0.66305				
124 −>132	0.15034				

Excited state 21:	Singlet−A	5.9664 eV	207.81 nm	*f*=0.0332	<S**2>=0.000
131 −>135	0.53448				
131 −>136	−0.36238				
131 −>137	−0.15845				
Excited state 22:	Singlet−A	5.9926 eV	206.89 nm	*f*=0.0045	<S**2>=0.000
130 −>134	0.67229				
130 −>135	0.13960				
Excited state 23:	Singlet−A	5.9994 eV	206.66 nm	*f*=0.0520	<S**2>=0.000
121 −>133	0.14708				
123 −>132	0.10879				
123 −>133	0.62321				
126 −>133	0.17679				
127 −>133	−0.11864				
Excited state 24:	Singlet−A	6.0072 eV	206.39 nm	*f*=0.0064	<S**2>=0.000
118 −>132	−0.10395				
120 −>132	0.15154				
121 −>132	−0.28764				
123 −>132	0.55475				
123 −>133	−0.11759				
131 −>136	−0.15388				
Excited state 25:	Singlet−A	6.0322 eV	205.54 nm	*f*=0.0151	<S**2>=0.000
123 −>132	0.13360				
131 −>135	0.44114				
131 −>136	0.47357				
131 −>137	0.14807				
131 −>140	−0.11208				
Excited state 26:	Singlet−A	6.1056 eV	203.07 nm	*f*=0.0237	<S**2>=0.000
120 −>132	−0.14418				
121 −>132	0.16613				
123 −>132	0.18238				
125 −>134	−0.21245				
126 −>134	−0.11114				
128 −>134	0.19448				
129 −>134	0.45104				
129 −>135	−0.26517				
Excited state 27:	Singlet−A	6.1144 eV	202.77 nm	*f*=0.0032	<S**2>=0.000
120 −>132	−0.29162				
121 −>132	0.37951				
123 −>132	0.33104				
125 −>134	0.12352				
128 −>134	−0.11967				
129 −>134	−0.26725				
Excited state 28:	Singlet−A	6.1545 eV	201.45 nm	*f*=0.0705	<S**2>=0.000
121 −>132	0.14831				
128 −>134	0.13914				
128 −>135	−0.13642				
129 −>134	0.17195				
129 −>135	0.59379				
129 −>136	0.10624				

Excited state 29: Singlet−A 6.1688 eV 200.99 nm *f*=0.0132 <S**2>=0.000
120 −>133 0.30294
121 −>133 0.51701
122 −>133 −0.29859

Excited state 30: Singlet−A 6.1794 eV 200.64 nm *f*=0.0572 <S**2>=0.000
121 −>133 0.11181
129 −>136 0.10640
131 −>134 0.10917
131 −>136 −0.24232
131 −>137 0.57160
131 −>138 −0.13793
131 −>140 −0.10325
SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 LETran= 520.

****

Rotatory strengths (R) in cgs (10**−40 erg−esu−cm/Gauss) of **22**.

State	*XX*	*YY*	*ZZ*	*R* (length)	*R* (au)
1	−12.0630	37.0323	−10.5883	4.7937	0.0102
2	−0.0830	0.1665	0.0302	0.0379	0.0001
3	41.8996	−15.5676	−17.9269	2.8017	0.0059
4	1.9714	1.1988	−5.7939	−0.8746	−0.0019
5	−59.9966	−17.0357	167.5572	30.1750	0.0640
6	−0.3573	0.5658	0.1732	0.1272	0.0003
7	−5.7456	2.5743	10.6124	2.4804	0.0053
8	−33.8246	40.7656	−9.6291	−0.8960	−0.0019
9	−43.0155	54.6420	−96.8375	−28.4037	−0.0602
10	−0.0345	33.0577	−31.7731	0.4167	0.0009
11	−12.7199	41.3153	−15.5412	4.3514	0.0092
12	−204.2058	59.9258	104.8919	−13.1294	−0.0278
13	−16.1599	242.8847	−349.3178	−40.8643	−0.0867
14	27.1865	74.5483	75.0539	58.9296	0.1250
15	−28.5483	7.5555	−184.4084	−68.4671	−0.1452
16	3.2470	77.4158	−81.9200	−0.4191	−0.0009
17	−4.0730	−0.5184	−0.3696	−1.6536	−0.0035
18	4.4840	4.6380	−4.0413	1.6936	0.0036
19	−1.3929	17.2933	−31.8956	−5.3317	−0.0113
20	0.5105	11.9722	10.2744	7.5857	0.0161
21	−4.7649	−21.1510	−1.9396	−9.2852	−0.0197
22	−37.4113	−6.7478	−61.6627	−35.2739	−0.0748
23	−0.8352	68.2991	1.3087	22.9242	0.0486
24	−0.6870	7.6762	−47.9755	−13.6621	−0.0290
25	−15.3618	190.6105	−49.6136	41.8784	0.0888
26	−15.4050	0.2823	−9.6479	−8.2569	−0.0175
27	−4.7049	18.9500	−14.7214	−0.1588	−0.0003
28	14.0616	23.7172	10.7092	16.1627	0.0343

29	−0.5161	5.5381	2.4651	2.4957	0.0053
30	−5.4941	−0.6741	0.8149	−1.7844	−0.0038

1/2[<0|del|b>*<b|r|0> + (<0|r|b>*<b|del|0>)*] (Au)

State	*X*	*Y*	*Z*	Dip. S.	Osc.(frdel)
1	−0.0027	−0.0088	−0.0070	0.0184	0.0123
2	−0.0001	−0.0001	0.0000	0.0002	0.0001
3	−0.0033	−0.0027	−0.0014	0.0074	0.0049
4	−0.0003	−0.0032	−0.0008	0.0043	0.0028
5	−0.0341	−0.0029	−0.0338	0.0708	0.0472
6	−0.0001	−0.0001	0.0000	0.0002	0.0001
7	−0.0021	−0.0001	−0.0008	0.0031	0.0021
8	−0.0056	−0.0029	−0.0005	0.0089	0.0059
9	−0.0967	−0.1325	−0.0413	0.2705	0.1803
10	−0.0086	−0.0181	−0.0042	0.0310	0.0206
11	−0.0305	−0.0280	−0.0096	0.0681	0.0454
12	−0.1555	−0.0380	−0.0212	0.2146	0.1431
13	−0.0005	−0.0229	−0.1289	0.1523	0.1016
14	−0.0263	−0.0089	−0.0286	0.0638	0.0425
15	−0.0027	0.0000	−0.0458	0.0485	0.0323
16	−0.0001	−0.0088	−0.0548	0.0636	0.0424
17	−0.0006	−0.0002	0.0000	0.0008	0.0005
18	−0.0015	−0.0096	−0.0009	0.0120	0.0080
19	−0.0006	−0.0040	−0.0027	0.0074	0.0049
20	−0.0184	−0.0099	−0.0002	0.0284	0.0189
21	−0.0056	−0.0036	−0.0001	0.0093	0.0062
22	−0.0227	−0.0002	−0.0098	0.0327	0.0218
23	−0.0040	−0.0162	−0.0103	0.0304	0.0203
24	−0.0069	−0.0003	−0.0067	0.0140	0.0093
25	−0.1146	−0.0366	−0.0007	0.1518	0.1012
26	−0.0014	0.0000	−0.0014	0.0028	0.0019
27	−0.0010	−0.0015	−0.0006	0.0031	0.0020
28	−0.0026	−0.0018	−0.0071	0.0114	0.0076
29	−0.0003	−0.0024	−0.0002	0.0029	0.0019
30	−0.0092	0.0000	0.0000	0.0092	0.0062

Ground to Excited state transition densities written to RWF 633

Excitation energies and oscillator strengths:

Excited state 1: Singlet−A 4.1888 eV 295.99 nm *f*=0.0124 <S**2>=0.000
131 −> 133 0.47543
132 −> 133 0.51394
This state for optimization and/or second−order correction.
Copying the Excited state density for this state as the 1−particle RhoCI density.

Excited state 2: Singlet−A 4.4961 eV 275.76 nm *f*=0.0001 <S**2>=0.000
131 −> 133 0.51800

132 −> 133	−0.48098				
Excited state 3:	Singlet−A	4.7796 eV	259.40 nm	*f*=0.0049	<S**2>=0.000
124 −> 133	0.26885				
125 −> 133	0.52472				
127 −> 133	0.18650				
128 −> 133	−0.29316				
Excited state 4:	Singlet−A	5.1718 eV	239.73 nm	*f*=0.0029	<S**2>=0.000
129 −> 133	0.56205				
130 −> 133	0.42352				
Excited state 5:	Singlet−A	5.2346 eV	236.86 nm	*f*=0.0477	<S**2>=0.000
131 −> 134	0.39865				
132 −> 134	0.56728				
Excited state 6:	Singlet−A	5.2627 eV	235.59 nm	*f*=0.0002	<S**2>=0.000
129 −> 133	−0.42364				
130 −> 133	0.55751				
Excited state 7:	Singlet−A	5.3355 eV	232.38 nm	*f*=0.0020	<S**2>=0.000
127 −> 134	−0.10320				
131 −> 134	0.55751				
132 −> 134	−0.38356				
Excited state 8:	Singlet−A	5.5320 eV	224.12 nm	*f*=0.0057	<S**2>=0.000
126 −> 134	0.30335				
127 −> 133	0.13990				
127 −> 134	0.35644				
129 −> 134	−0.29166				
130 −> 134	−0.27325				
131 −> 134	0.12834				
132 −> 134	−0.13595				
Excited state 9:	Singlet−A	5.5640 eV	222.83 nm	*f*=0.1827	<S**2>=0.000
124 −> 133	−0.22507				
125 −> 133	0.25152				
126 −> 133	0.18523				
127 −> 133	0.35346				
128 −> 133	0.42744				
Excited state 10:	Singlet−A	5.6032 eV	221.27 nm	*f*=0.0209	<S**2>=0.000
124 −> 133	0.12518				
125 −> 133	−0.36106				
127 −> 133	0.54749				
128 −> 133	−0.19315				
Excited state 11:	Singlet−A	5.6832 eV	218.16 nm	*f*=0.0458	<S**2>=0.000
124 −> 133	0.10543				
126 −> 133	0.67526				
127 −> 133	−0.10061				
128 −> 133	−0.11036				
Excited state 12:	Singlet−A	5.7897 eV	214.15 nm	*f*=0.1432	<S**2>=0.000
124 −> 133	0.57338				
128 −> 133	0.37284				

Excited state 13:	Singlet−A	5.8892 eV	210.53 nm	*f*=0.1026	<S**2>=0.000
131 −> 135	0.23479				
131 −> 136	−0.21703				
131 −> 137	0.14868				
132 −> 135	0.50009				
132 −> 136	−0.21333				
132 −> 137	0.16213				
Excited state 14:	Singlet−A	5.9112 eV	209.75 nm	*f*=0.0434	<S**2>=0.000
131 −> 137	−0.26285				
131 −> 139	0.16701				
132 −> 135	0.27341				
132 −> 136	0.52365				
132 −> 139	−0.12136				
Excited state 15:	Singlet−A	5.9305 eV	209.06 nm	*f*=0.0323	<S**2>=0.000
131 −> 135	0.11136				
131 −> 136	0.49098				
131 −> 139	−0.10197				
132 −> 135	0.24193				
132 −> 137	−0.30837				
132 −> 139	0.18456				
Excited state 16:	Singlet−A	5.9727 eV	207.59 nm	*f*=0.0430	<S**2>=0.000
131 −> 135	0.62132				
132 −> 135	−0.26584				
Excited state 17:	Singlet−A	5.9858 eV	207.13 nm	*f*=0.0005	<S**2>=0.000
126 −> 134	0.23845				
127 −> 134	0.29931				
129 −> 134	0.54207				
130 −> 134	0.16999				
Excited state 18:	Singlet−A	6.1169 eV	202.69 nm	*f*=0.0082	<S**2>=0.000
122 −> 133	−0.44881				
123 −> 133	0.51319				
Excited state 19:	Singlet−A	6.1744 eV	200.80 nm	*f*=0.0051	<S**2>=0.000
120 −> 133	−0.12747				
121 −> 133	0.17907				
122 −> 133	0.41898				
123 −> 133	0.39706				
131 −> 136	0.12710				
131 −> 137	0.14865				
132 −> 136	0.11056				
132 −> 137	0.15844				
Excited state 20:	Singlet−A	6.1778 eV	200.69 nm	*f*=0.0194	<S**2>=0.000
127 −> 134	0.13525				
129 −> 134	−0.30042				
130 −> 134	0.60248				
Excited state 21:	Singlet−A	6.1891 eV	200.33 nm	*f*=0.0062	<S**2>=0.000
122 −> 133	−0.23121				
123 −> 133	−0.15445				
131 −> 136	0.26900				
131 −> 137	0.34181				

131 −> 140	0.10623				
132 −> 136	0.22563				
132 −> 137	0.36160				
132 −> 140	0.11550				
Excited state 22:	Singlet−A	6.2833 eV	197.32 nm	*f*=0.0222	<S**2>=0.000
131 −> 136	0.25625				
131 −> 137	−0.16733				
131 −> 139	0.11960				
131 −> 141	0.18432				
132 −> 136	−0.25608				
132 −> 137	0.18168				
132 −> 138	0.42329				
132 −> 139	−0.11120				
132 −> 141	−0.15597				
Excited state 23:	Singlet−A	6.3027 eV	196.72 nm	*f*=0.0207	<S**2>=0.000
118 −> 133	0.11682				
120 −> 133	−0.20629				
121 −> 133	0.41068				
122 −> 133	−0.16058				
123 −> 133	−0.16417				
131 −> 136	0.11872				
131 −> 137	−0.12419				
131 −> 138	−0.25300				
132 −> 138	−0.23650				
Excited state 24:	Singlet−A	6.3110 eV	196.46 nm	*f*=0.0095	<S**2>=0.000
120 −> 133	−0.15785				
121 −> 133	0.33483				
123 −> 133	−0.12769				
131 −> 136	−0.12571				
131 −> 137	0.11670				
131 −> 138	0.27241				
132 −> 138	0.37112				
132 −> 141	0.10843				
Excited state 25:	Singlet−A	6.3172 eV	196.26 nm	*f*=0.1024	<S**2>=0.000
131 −> 137	−0.35874				
131 −> 139	−0.19714				
131 −> 141	−0.10231				
131 −> 143	−0.10381				
132 −> 137	0.30242				
132 −> 139	0.37141				
132 −> 140	0.11878				
132 −> 143	0.12635				
Excited state 26:	Singlet−A	6.3447 eV	195.41 nm	*f*=0.0018	<S**2>=0.000
131 −> 136	0.10944				
131 −> 137	−0.11476				
131 −> 138	0.48510				
131 −> 142	0.15238				
132 −> 136	−0.10374				
132 −> 137	0.15486				
132 −> 138	−0.19303				
132 −> 139	−0.23330				
132 −> 140	−0.13480				

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      132 -> 142        -0.17037

Excited state   27:      Singlet-A      6.3608 eV  194.92 nm  f=0.0021  <S**2>=0.000
      131 -> 139         0.38861
      131 -> 140         0.32862
      132 -> 139         0.19092
      132 -> 140         0.32662
      132 -> 141        -0.11012
      132 -> 142        -0.19097

Excited state   28:      Singlet-A      6.4273 eV  192.90 nm  f=0.0075  <S**2>=0.000
      121 -> 133         0.13260
      129 -> 135         0.53704
      130 -> 135         0.34454

Excited state   29:      Singlet-A      6.4596 eV  191.94 nm  f=0.0020  <S**2>=0.000
      119 -> 133         0.10856
      120 -> 133         0.46154
      121 -> 133         0.31838
      131 -> 139         0.15915
      131 -> 140        -0.14227
      132 -> 139         0.14835
      132 -> 140        -0.19417

Excited state   30:      Singlet-A      6.4659 eV  191.75 nm  f=0.0063  <S**2>=0.000
      120 -> 133         0.28291
      121 -> 133         0.16846
      131 -> 137        -0.11919
      131 -> 139        -0.29459
      131 -> 140         0.20851
      132 -> 137        -0.10629
      132 -> 139        -0.26583
      132 -> 140         0.31918
      132 -> 141         0.11145
SavETr:  write IOETrn=     770 NScale= 10 NData=   16 NLR=1 LETran=        520.

 ****************************************************************************
```

27. Table S1 Guaiane dimers from the *Artemisia* species.

Condensed pattern	Guaiane dimer	Sources
[4+2] Diels−Alder	Arteminolides B–D, artanomaloide-2, artanomaloide A, artanomaloide C, artemisians A–D, artemisianins A–D, argyinolide O	*A. argyi*
	Absinthin, isoabsinthin, absintholide, artenolide, absinthin A–E, isoanabsinthin, gnapholide	*A. absinthium*
	Artanomaloide-1, artanomalides A–D, artanomadimers A–F	*A. anomala*
	Artepestrins D–G, 6*a*-hydroxyartepestrin D, 2′*a*-hydroxyartepestrin F	*A. rupestris*
	11-Epiabsinthin, 10′,11′-epiabsinthin, 11,10′,11′-epiabsinthin, artesieversin	*A. sieversiana*
	Caruifolins B–D, anabsin, anabsinthin	*A. caruifolia*
	Artemyriantholides A–D	*A. myriantha*
	Arteminolide, 8-acetylarteminolide	*A. sylvatica*
	Artselenoide	*A. selengensis*
	Lavandiolides A–L	*A. lavandulifolia*
[2+2] Cycloaddition	Artelein	*A. leucodes*
	Artesin A	*A. sieversiana*
Ester linkage	Artemisianes A–D	*A. argyi*

28. Comparison of ^{1}H and ^{13}C NMR spectroscopic data for compounds 3, 4, 9, 12, and 23

Table S2 Comparison of ^{13}C NMR spectroscopic data for compounds **3**, **4**, **9**, **12**, and **23** (δ in ppm).

No.	**3**[b,d]	Lavandiolide A[a,f]	**4**[b,d]	Lavandiolide B[a,f]	**9**[c,e]	Lavandiolide J[a,f]	**12**[c,e]	Lavandiolide H[a,f]	**23**[a,d]	Lavandiolide C[a,f]
1	66.6	65.0	66.3	65.2	151.3	150.2	151.1	150.0	71.5	71.4
2	47.7	46.5	47.2	46.4	42.1	42.2	42.3	42.3	47.0	46.9
3	52.2	51.6	51.8	51.7	53.3	53.9	53.4	54.0	45.6	45.5
4	140.2	140.7	140.1	141.1	60.4	60.8	60.0	60.4	142.0	141.9
5	136.2	134.2	136.4	134.7	142.4	143.9	143.6	145.3	134.8	134.8
6	85.0	84.1	84.0	83.6	85.7	85.1	85.2	84.7	82.6	82.5
7	44.6	43.6	42.5	41.9	46.0	46.3	47.3	47.6	51.6	51.5
8	26.4	25.8	23.9	23.7	22.5	22.7	24.3	24.5	24.2	23.9
9	41.1	40.0	40.8	40.2	40.5	41.2	39.2	39.7	41.3	41.2
10	72.5	73.3	72.0	73.2	73.0	73.9	72.5	73.5	74.1	74.0
11	140.4	139.0	39.4	39.0	38.9	39.2	140.2	140.0	139.1	139.1
12	170.4	169.8	179.3	179.2	181.2	180.0	170.8	170.3	170.4	170.3
13	120.0	120.1	10.5	10.6	9.5	10.7	118.1	118.9	120.2	120.1
14	26.9	26.5	26.4	26.5	24.4	26.7	25.6	27.7	28.5	28.5
15	16.6	15.9	16.5	16.1	16.4	17.5	16.2	17.3	14.6	14.5
1′	72.4	72.2	72.0	72.2	72.3	72.2	72.3	72.2	89.4	89.4
2′	39.9	39.4	39.4	39.3	38.5	39.2	38.5	39.2	43.0	43.0
3′	126.0	125.1	125.6	125.0	124.8	125.2	124.9	125.2	122.4	122.4
4′	141.7	141.1	141.3	141.2	140.7	141.0	140.7	141.1	142.2	142.1
5′	52.5	52.2	52.1	52.2	51.8	52.6	51.8	52.6	55.2	55.2
6′	81.4	80.8	80.9	80.8	80.2	80.0	80.2	80.0	85.2	85.1
7′	56.0	55.5	55.6	55.5	52.0	52.4	52.0	52.4	43.7	43.7
8′	21.6	20.8	21.2	20.8	20.6	21.1	20.6	21.1	24.0	24.1
9′	33.5	33.4	33.1	33.4	31.9	32.9	31.9	32.9	39.4	39.3
10′	62.4	62.2	62.0	62.2	62.2	62.1	62.2	62.1	74.7	74.7
11′	55.2	54.4	54.7	54.4	55.9	55.8	56.0	55.9	55.5	55.4
12′	180.0	179.3	179.4	179.3	180.9	180.3	180.8	180.2	186.7	186.6
13′	37.0	36.2	36.6	36.2	34.3	34.7	34.4	34.7	34.5	34.5
14′	23.0	22.7	22.6	22.7	21.2	22.6	21.3	22.6	29.2	29.1
15′	19.2	18.7	18.8	18.7	17.5	18.6	17.6	18.6	17.7	17.6

[a]Recorded in $CDCl_3$. [b]Recorded in pyridine-d_5. [c]Recorded in CD_3OD. [d]Recorded at 150 MHz. [e]Recorded at 100 MHz. [f]Recorded at 126 MHz.

Table S3 Comparison of ^{1}H NMR spectroscopic data for compounds **3**, **4**, and **9** (δ in ppm, J in Hz).

No.	**3**[b,d]	Lavandiolide A[a,d]	**4**[b,d]	Lavandiolide B[a,d]	**9**[c,e]	Lavandiolide J[a,d]
1						
2	2.05 (overlapped)	1.69 m	1.99 (overlapped)	1.67 d (8.5)	3.20 m	3.17 dd (3.4, 1.8)
	1.58 m	1.48 d (2.3)	1.51 m	1.46 d (8.3)	1.62 m	1.53 dd (8.9, 1.6)
3	2.73 (overlapped)	2.73 m	2.68 m	2.72 m	1.36 m	1.36 (overlapped)
6	5.20 d (10.8)	4.93 dt (10.5, 2.3)	5.32 d (11.0)	5.10 d (9.0)	5.57 d (10.8)	5.57 d (10.9)
7	3.20 m	3.02 td (12.2, 2.7)	2.70 m	2.59 d (10.3)	2.45 m	2.42 tdd (11.6, 8.1, 3.7)
8	2.03 (overlapped)	2.18 d (11.7)	1.61 m	1.82 m	1.91 m	1.89 m
	1.46 m	1.50 q (2.5, 2.1)	1.45 m	1.52 s	1.75 m	1.69 tdd (8.9, 7.6, 4.8)
9	2.22 m	2.02 td (13.8, 4.2)	2.12 m	1.93 s	1.80 m	1.82 d (4.4)
	2.06 (overlapped)	1.83 m	1.97 m	1.77 d (13.6)	1.79 m	1.79 m
11	2.54 m		2.54 m	2.64 m	2.62 m	2.58 t (7.8)
13	6.26 d (3.3)	6.24 d (3.4)	1.10 d (8.0)	1.18 d (7.6)	1.19 d (8.0)	1.18 d (7.7)
	5.43 d (3.3)	5.49 d (3.1)				
14	1.50 s	1.32 s	1.42 s	1.29 s	1.25 s	1.29 s
15	2.09 s	1.87 d (2.3)	2.03 s	1.84 d (1.8)	1.39 s	1.40 m
2′	2.65 m	2.75 d (13.3)	2.63 m	2.75 d (10.5)	2.82 m	2.75 m
	2.19 (overlapped)	2.16 d (14.1)	2.15 m	2.18 m	2.13 (overlapped)	2.16 d (3.4)
3′	5.53 m	5.56 d (2.6)	5.51 m	5.56 s	5.60 m	5.55 m
5′	2.74 (overlapped)	2.77 s	2.73 m	2.77 s	2.96 d (10.4)	2.81 m
6′	4.48 dd (10.2, 10.2)	4.30 t (10.2)	4.42 dd (10.5, 10.0)	4.29 t (10.2)	3.99 dd (10.4, 10.0)	3.99 t (10.2)
7′	1.83 m	1.72 m	1.79 m	1.73 m	2.05 m	1.93 m
8′	1.69 m	1.53 dt (13.9, 3.7)	1.65 m	1.54 m	1.68 m	1.58 m
	1.52 m	1.62 dt (10.7, 3.0)	1.49 m	1.61 m	1.61 m	1.53 (overlapped)
9′	1.92 m	2.02 td (13.8, 4.2)	1.90 m	1.87 d (9.1)	2.14 m	2.12 m
	1.76 m	1.87 m	1.75 m	2.15 s	2.13 (overlapped)	2.09 dd (5.0, 3.1)
13′	2.43 d (12.0)	1.97 d (11.8)	2.36 d (11.5)	1.87 ddd (11.8, 2.8, 5.6)	2.26 dd (12.4, 3.6)	2.18 m
	2.12 br d	1.85 dt (5.6, 2.6)	2.10 br d	1.93 s	1.41 m	1.39 m
14′	1.23 s	1.33 s	1.20 s	1.33 s	1.35 s	1.33 s
15′	2.01 s	1.95 dt (3.1, 1.4)	2.00 s	1.95 d (3.3)	1.93 s	1.92 dt (3.2, 1.6)

[a]Recorded in $CDCl_3$. [b]Recorded in pyridine-d_5. [c]Recorded in CD_3OD. [d]Recorded at 600 MHz. [e]Recorded at 400 MHz.

Table S4 Comparison of ^{1}H NMR spectroscopic data for compounds **12** and **23** (δ in ppm, J in Hz).

No.	**12**[b,d]	Lavandiolide H[a,c]	**23**[a,c]	Lavandiolide C[a,c]
2	3.18 m	3.14 m	2.33 m	2.33 dd (9.6, 1.5)
			1.63 m	1.62 dt (9.7, 2.5)
3	1.65 m	1.56 m	2.60 m	2.60 m
	1.41 m	1.37 d (1.6)		
5				
6	5.37 d (10.0)	5.40 d (10.2)	4.47 d (10.2)	4.46 dd (10.5, 1.5)
7	2.99 m	2.93 td (10.7, 4.8)	2.70 m	2.70 tt (11.0, 3.5)
8	2.35 m	2.30 m	2.13 m	2.13 m
	1.66 m	1.65 m	1.56 m	1.57 t (2.9)
9	1.86 m	1.89 m	1.93 (overlapped)	1.93 (overlapped)
	1.85 m	1.87 m	1.76 m	1.75 m
11				
13	6.11 d (3.4)	6.15 d (3.5)	6.19 d (3.6)	6.20 d (3.4)
	5.58 d (3.4)	5.44 d (3.2)	5.52 d (3.6)	5.52 d (3.1)
14	1.29 s	1.32 s	1.47 s	1.46 s
15	1.42 s	1.43 s	1.93 s	1.93 s
2′	2.83 m	2.76 m	2.75 m	2.64 m
	2.14 (overlapped)	2.13 d (3.4)	2.03 m	2.08 ddd (15.9, 3.0, 1.6)
3′	5.60 m	5.56 dt (4.0, 2.6)	5.58 m	5.44 tt (3.0, 1.6)
5′	2.98 m	2.82 d (10.2)	2.92 d (10.2)	3.25 m
6′	3.99 dd (10.4, 10.0)	4.00 t (10.1)	4.00 dd (10.2, 10.2)	4.15 dd (11.0, 9.8)
7′	2.07 m	1.95 m	2.25 m	3.19 dd (9.7, 7.7)
8′	1.67 m	1.59 m	1.18 m	1.58 (overlapped)
	1.60 m		1.15 m	
9′	2.14 (overlapped)	2.11 dt (5.3, 2.8)	2.35 m	2.00 td (6.8, 4.5)
	2.13 m	2.02 m	1.98 m	1.54 m
13′	2.27 dd (12.4, 3.6)	2.19 dd (12.3, 3.7)	1.91 dd (12.0, 3.8)	1.75 ddd (11.7, 8.8, 4.2)
	1.41 m	1.39 dd (5.4, 2.4)	1.84 m	1.84 dd (11.9, 3.7)
14′	1.35 s	1.34 s	1.31 s	1.27 s
15′	1.93 s	1.92 dp (3.2, 1.9)	1.96 s	1.90 m

[a]Recorded in $CDCl_3$. [b]Recorded in CD_3OD. [c]Recorded at 600 MHz. [d]Recorded at 400 MHz.

Table S5 ^{1}H NMR and ^{13}C NMR data for compound **23** in acetone-d_6 (600 MHz, δ in ppm, J in Hz).

No.	δ_H	δ_C	No.	δ_H	δ_C
1		72.1, C	1′		89.7, C
2	2.23 (m)	47.3, CH_2	2′	2.65 (m)	43.3, CH_2
	1.56 (overlapped)			2.03 (m)	
3	2.60 (m)	46.0, CH	3′	5.36 (br s)	123.4, CH
4		136.2, C	4′		141.3, C
5		141.7, C	5′	3.30 (m)	55.6, CH
6	4.60 (d, 10.2)	82.6, CH	6′	4.25 (dd, 10.2, 10.2)	86.1, CH
7	2.73 (m)	52.2, CH	7′	3.39 (m)	44.1, CH
8	2.16 (m)	24.7, CH_2	8′	1.67 (m)	24.4, CH_2
	1.49 (m)			1.56 (overlapped)	
9	1.89 (m)	42.0, CH_2	9′	1.87 (m)	40.1, CH
	1.63 (m)			1.65 (m)	
10		74.5, C	10′		74.9, CH_2
11		140.7, C	11′		56.0, C
12		170.0, C	12′		187.4, C
13	6.06 (d, 3.6)	119.3, CH_2	13′	1.79 (m)	35.0, CH_2
	5.61 (d, 3.6)			1.78 (m)	
14	1.44 (s)	29.1, CH_3	14′	1.19 (s)	29.1, CH_3
15	1.93 (s)	14.5, CH_3	15′	1.80 (s)	17.9, CH_3
OH-10	4.58 (s)		OH-1′	4.00 (s)	
			OH-10′	3.92 (s)	