

Cytochalasans from the Endophytic Fungus *Phomopsis* sp. shj2 and Their Antimigratory Activities

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1. NMR, HRESIMS, UV, ORD, and CD spectra of compound 1

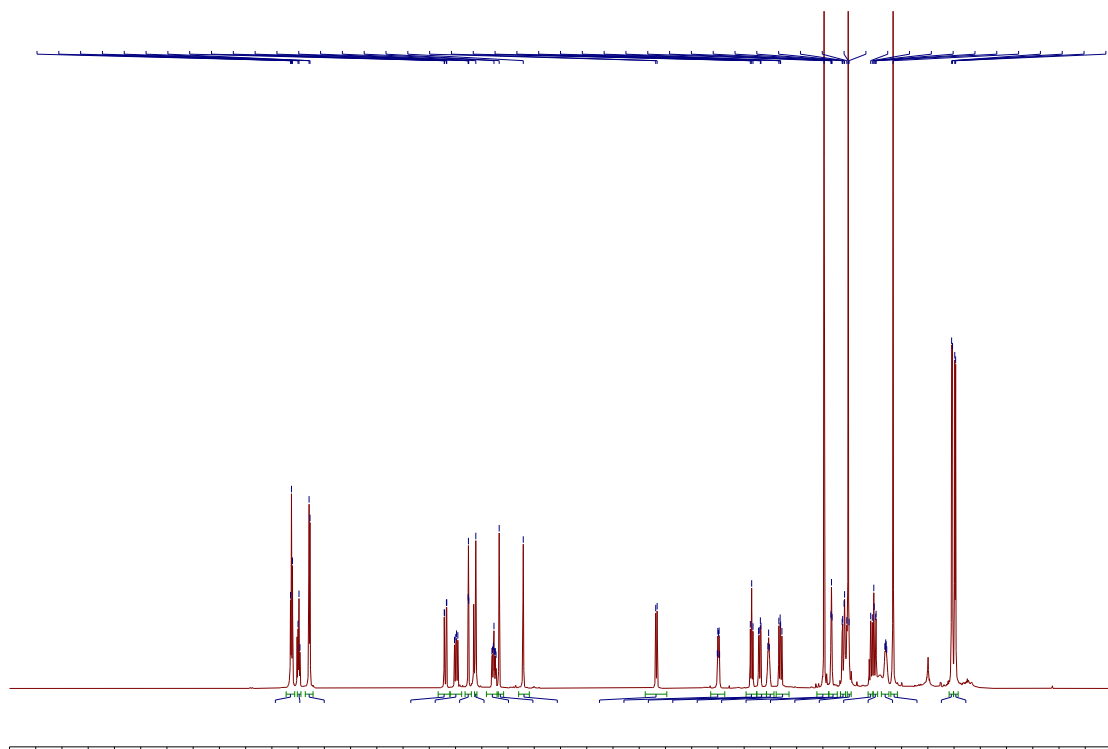


Figure S1. ^1H NMR spectrum of **1** (800 MHz, CDCl_3).

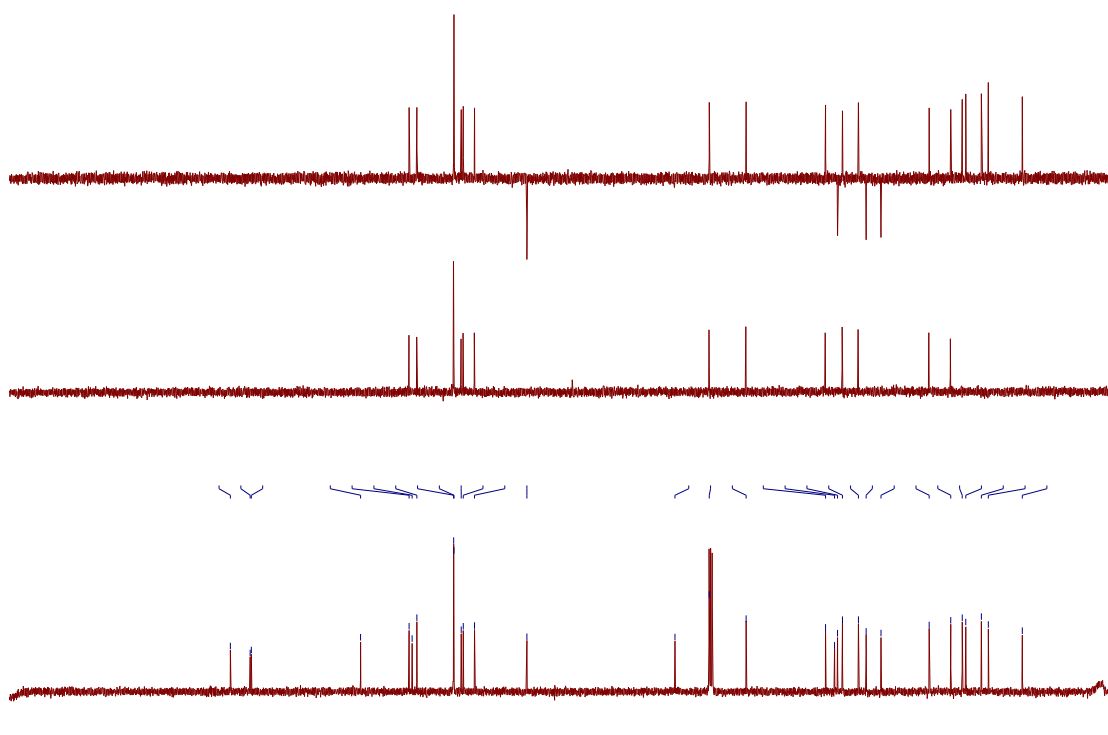


Figure S2. ^{13}C NMR, DEPT-90 and DEPT-135 spectra of **1** (100 MHz, CDCl_3).

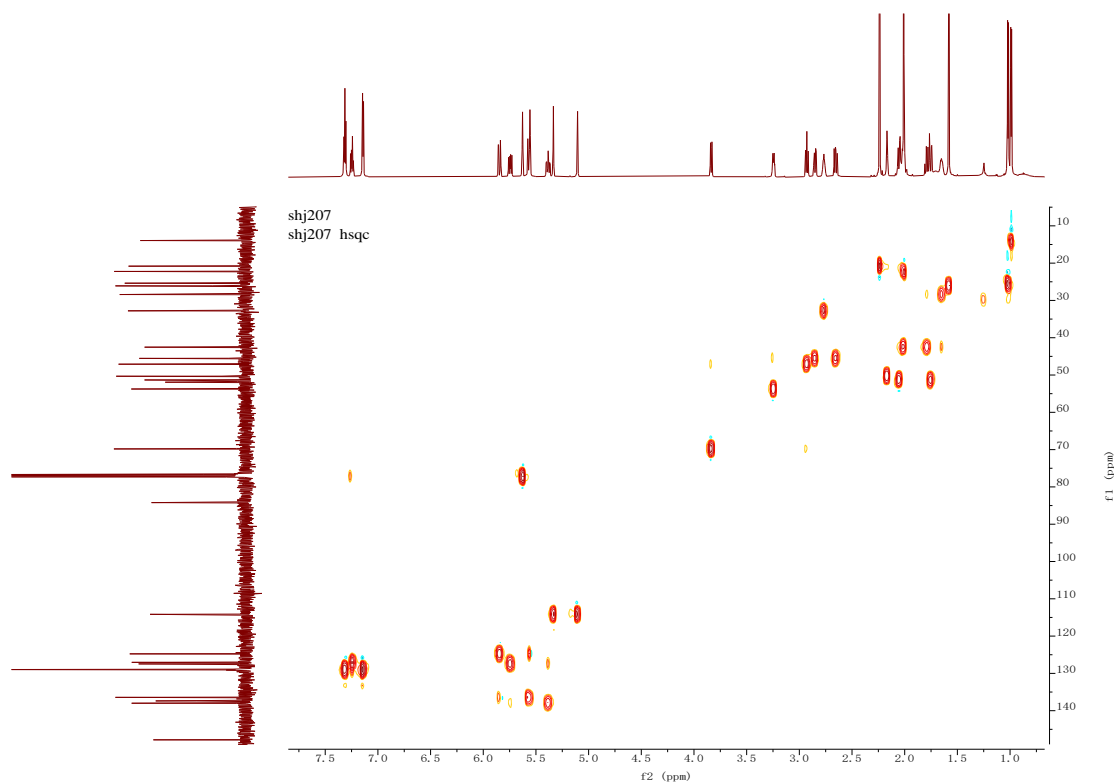


Figure S3. HSQC spectrum of **1** (400 MHz, CDCl₃).

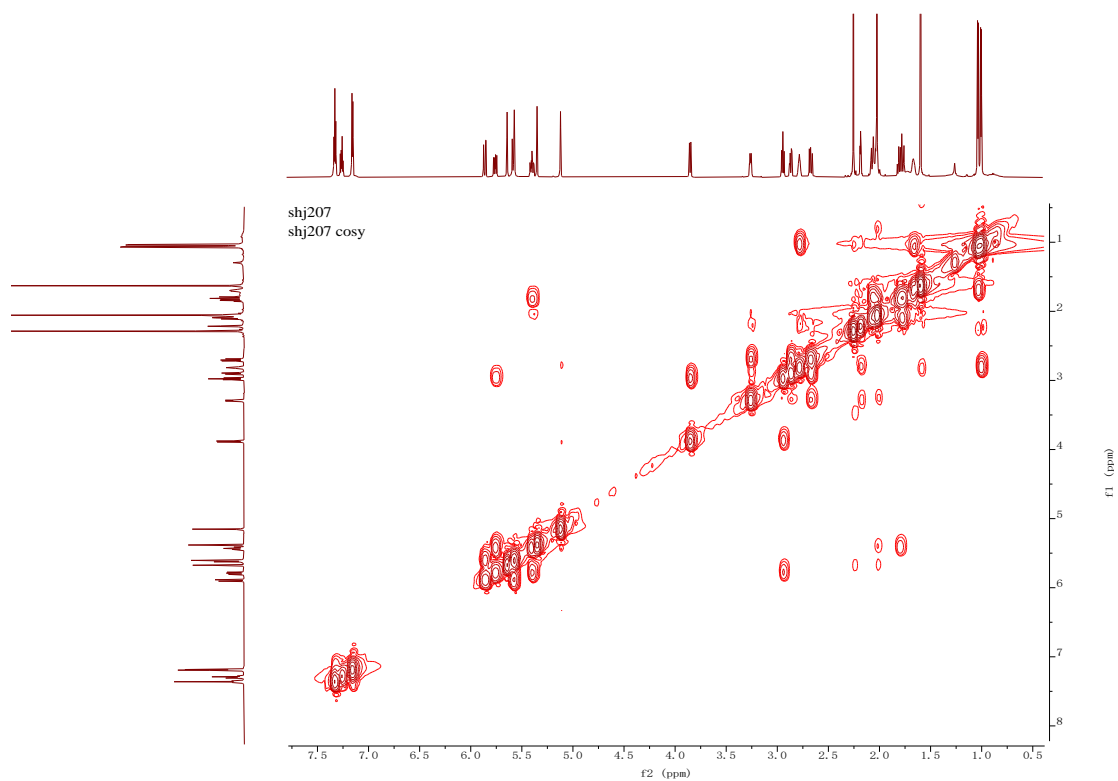


Figure S4. ¹H-¹H COSY spectrum of **1** (400 MHz, CDCl₃).

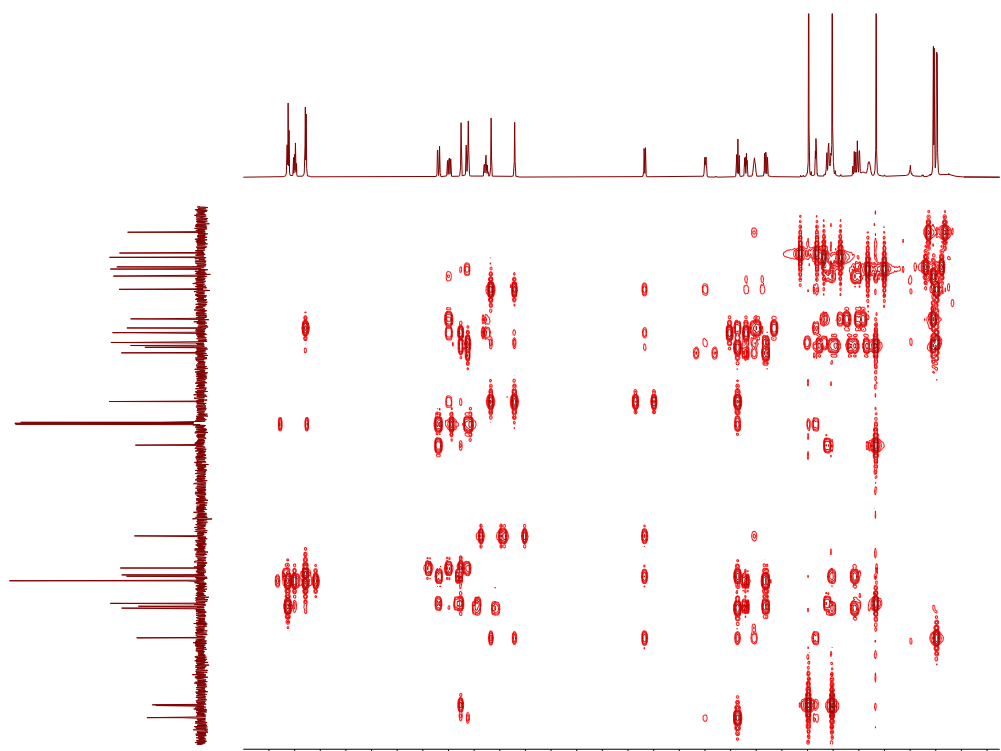


Figure S5. HMBC spectrum of **1** (400 MHz, CDCl₃).

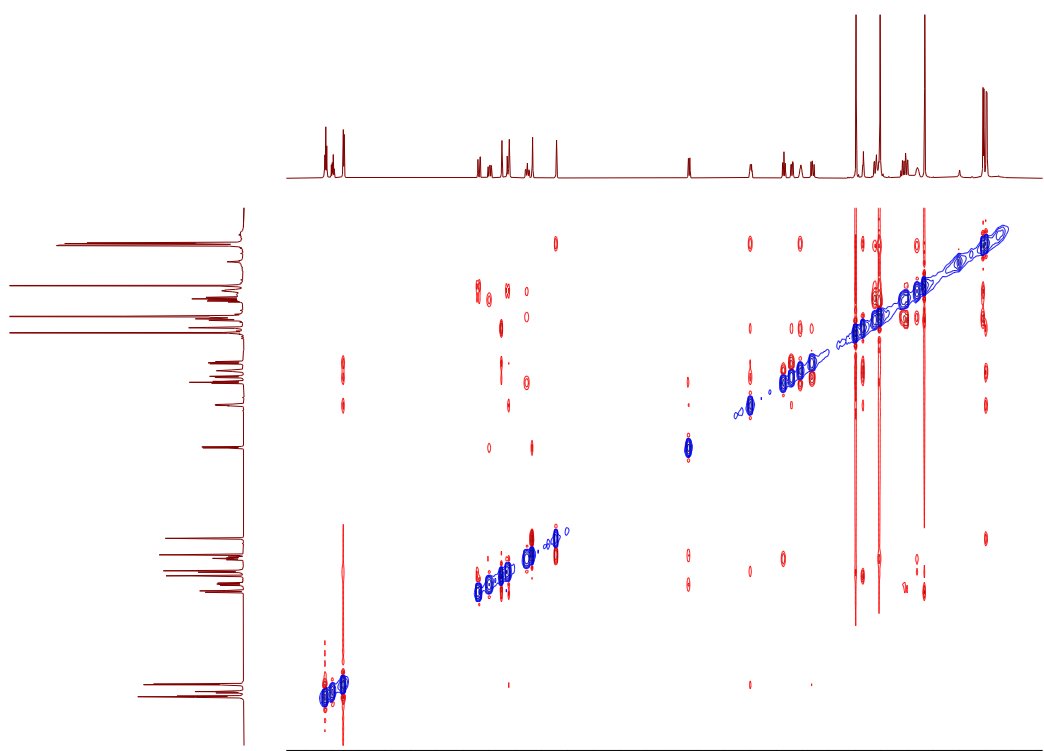


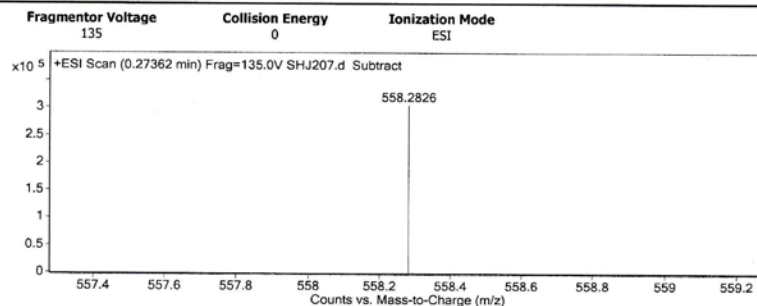
Figure S6. ROESY spectrum of **1** (400 MHz, CDCl₃).

Qualitative Analysis Report

Data Filename	SHJ207.d	Sample Name	SHJ207
Sample Type	Sample	Position	P1-A1
Instrument Name	Instrument 1	User Name	
Acq Method	SIBU.m	Acquired Time	12/23/2014 9:20:46 AM
IRM Calibration Status	Success	DA Method	Default.m
Comment			

Sample Group	Info.
Acquisition SW	6200 series TOF/6500 series
Version	Q-TOF B.05.01 (B5125.2)

User Spectra



Peak List

m/z	z	Abund	Formula	Ion
476.279	1	101074.23		
477.2823	1	33766.22		
536.3005	1	59321.33		
537.3039	1	20107.72		
558.2826	1	304737.38	C32 H41 N O6	(M+Na)+
559.2854	1	104583.77	C32 H41 N O6	(M+Na)+
560.2875	1	20597.91	C32 H41 N O6	(M+Na)+
574.2633	1	18297.42		
1093.5742	1	41656.8		
1094.5808	1	30091.71		

Formula Calculator Element Limits

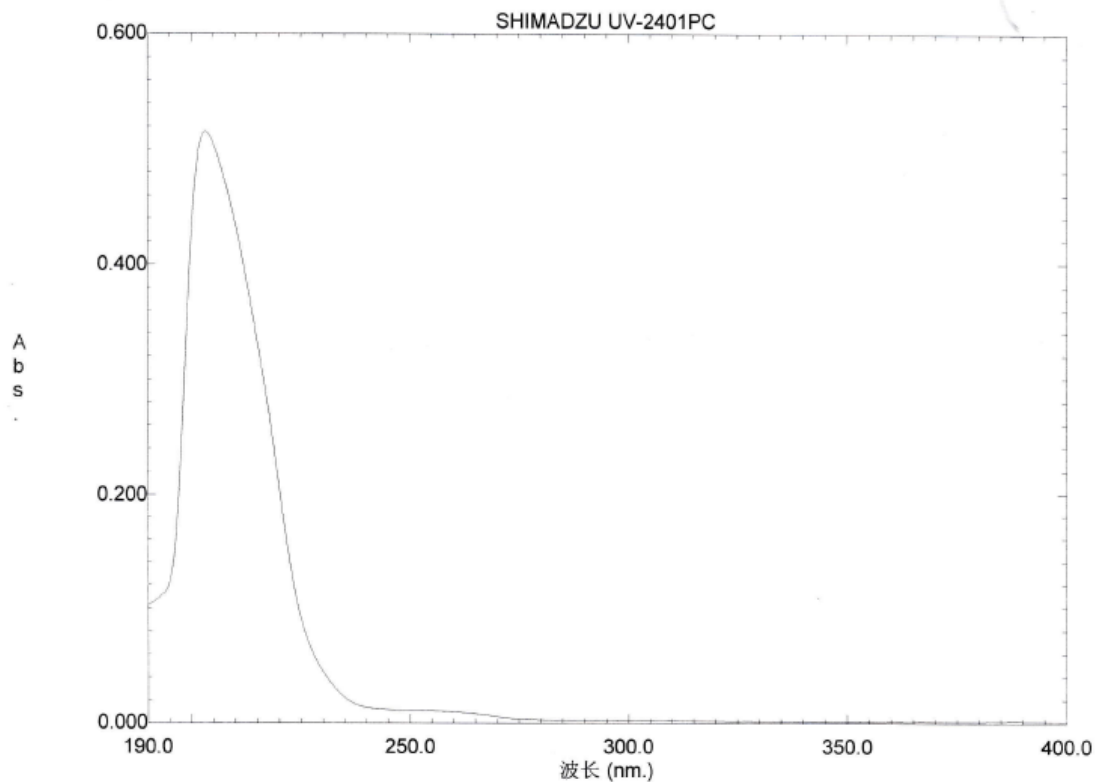
Element	Min	Max
C	3	60
H	0	120
O	0	10
N	0	3

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C32 H41 N O6	535.2934	558.2826	558.2826	0.2	0.4	13.0000

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Figure S7. HRESIMS spectrum of **1**.



文件名: SHJ207

SHJ207

创建于: 15:12 15-01-23

样品浓度: 0.0128毫克/毫升

数据: 原始

溶剂: 甲醇

测量模式: Abs.
扫描速度: 中速
狭缝: 5.0
采样间隔: 0.2

否.	波长 (nm.)	Abs.
1	203.20	0.5151

Figure S8. UV spectrum of **1**.

Optical rotation measurement

Model : P-1020 (A060460638)

No.	Sample	Mode	Data	Monitor Blank	Temp. Cell Temp Point	Date Comment Sample Name	Light Filter Operator	Cycle Time Integ Time
No.1	20 (1/3)	Sp.Rot	44.3860	0.0506 0.0000	19.6 50.00	Thu Jan 22 18:11:51 2015 0.00228g/mL MeOH SHJ207	Na 589nm	2 sec 10 sec
No.2	20 (2/3)	Sp.Rot	45.2630	0.0516 0.0000	19.6 50.00	Thu Jan 22 18:12:04 2015 0.00228g/mL MeOH SHJ207	Na 589nm	2 sec 10 sec
No.3	20 (3/3)	Sp.Rot	42.8070	0.0488 0.0000	19.6 50.00	Thu Jan 22 18:12:18 2015 0.00228g/mL MeOH SHJ207	Na 589nm	2 sec 10 sec

+44.150°

Figure S9. ORD spectrum of **1**.

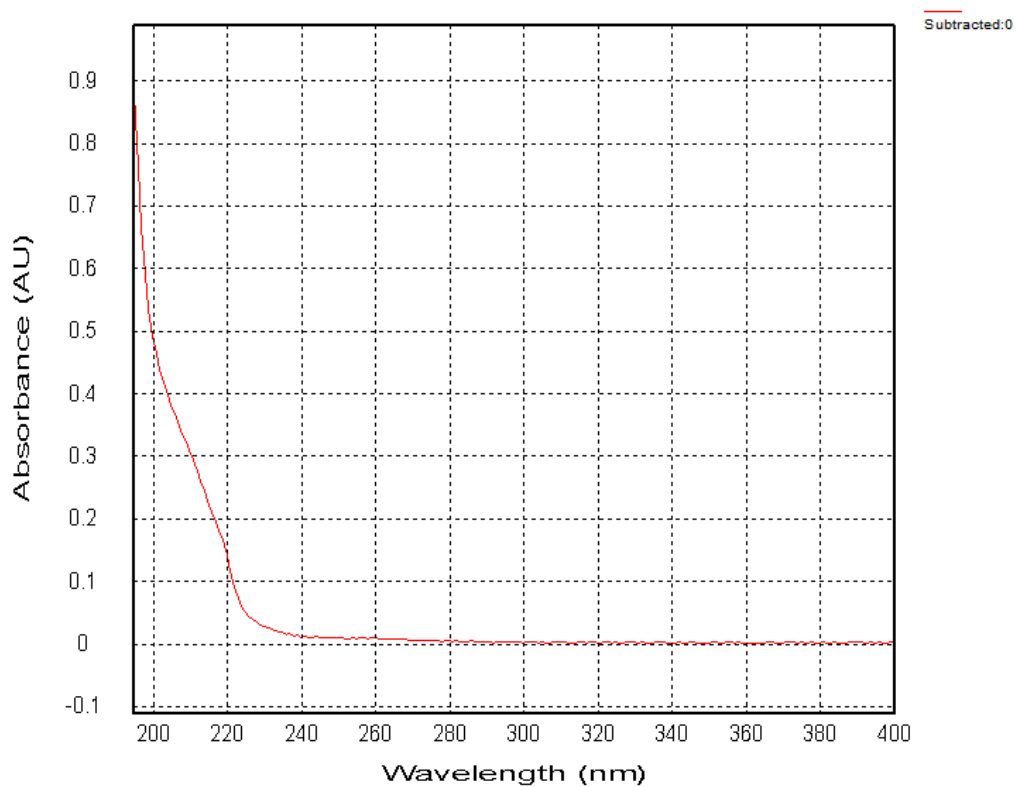
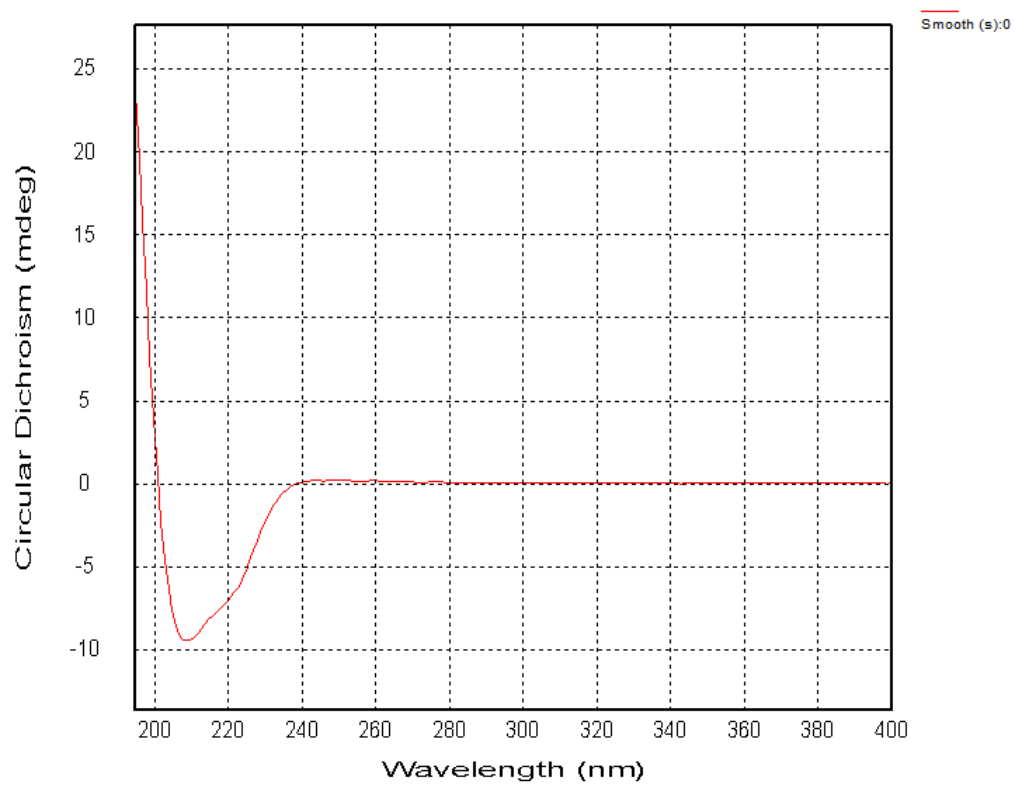


Figure S10. CD spectrum of **1**.

2. NMR, HRESIMS, UV, ORD, and CD spectra of compound 2

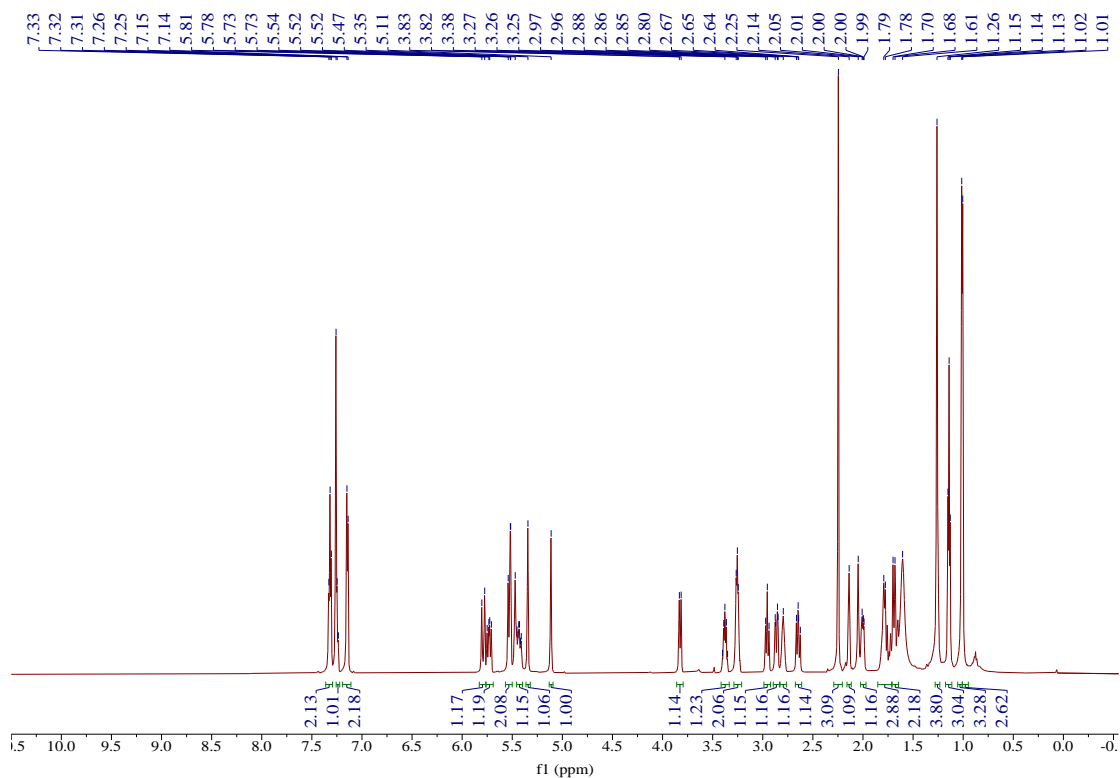


Figure S10. ¹H NMR spectrum of 2 (600 MHz, CDCl₃).

shj07

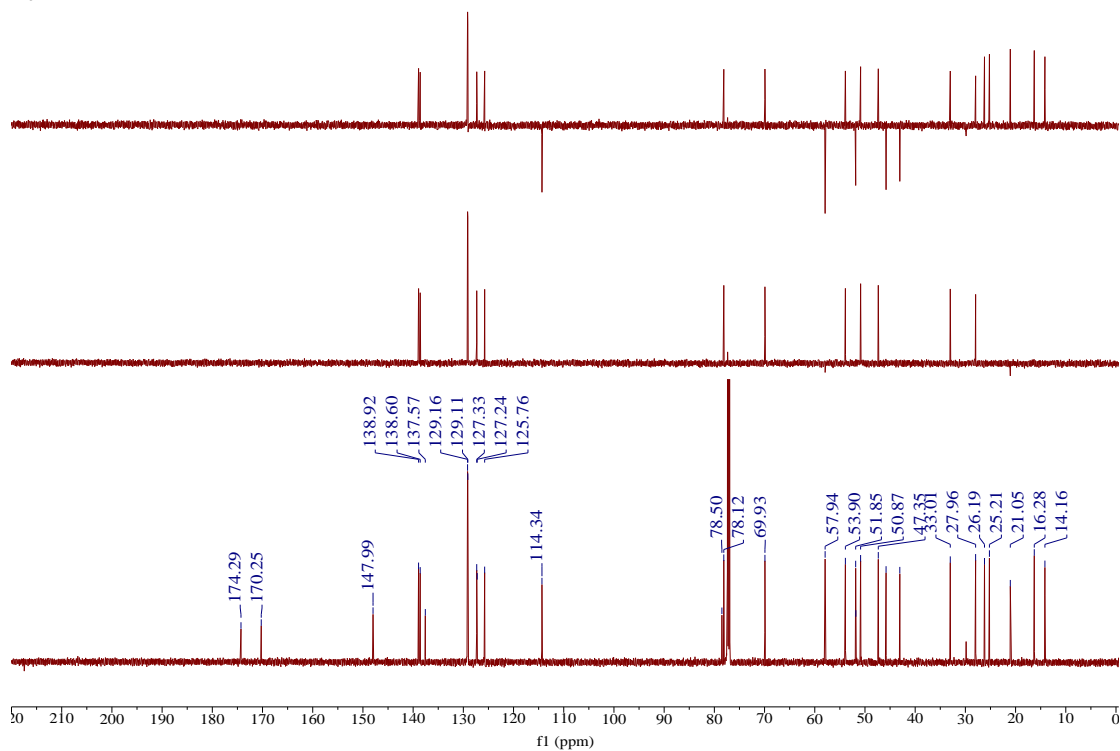


Figure S11. ¹³C NMR, DEPT-90 and DEPT-135 spectra of 2 (150 MHz, CDCl₃).

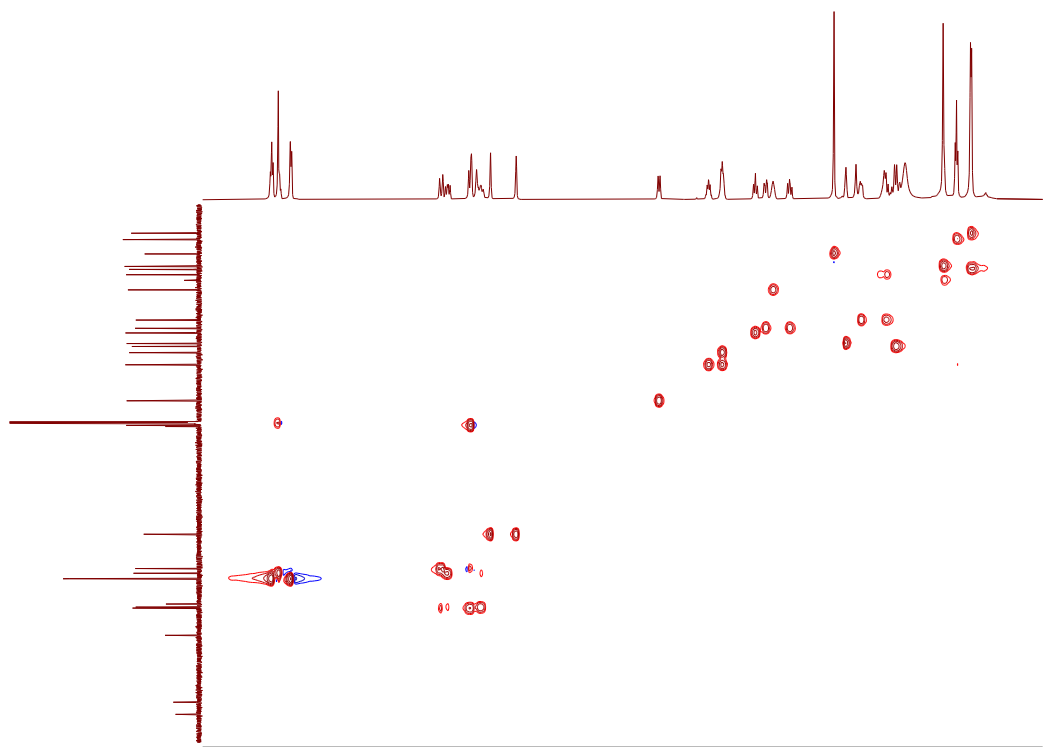


Figure S12. HSQC spectrum of **2** (600 MHz, CDCl_3).

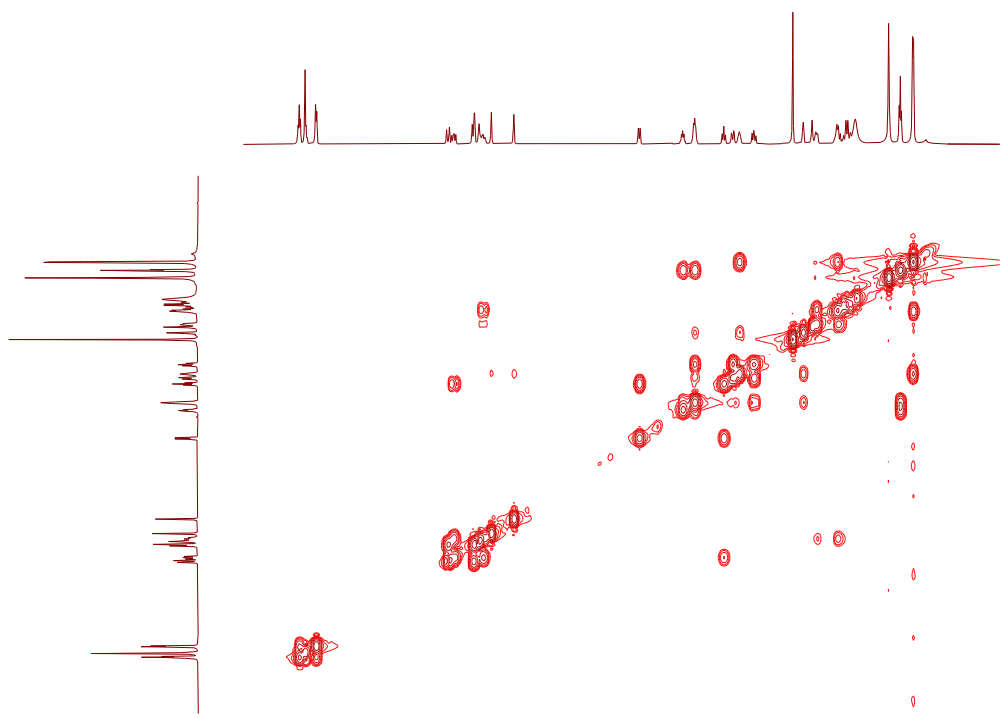


Figure S13. ^1H - ^1H COSY spectrum of **2** (600 MHz, CDCl_3).

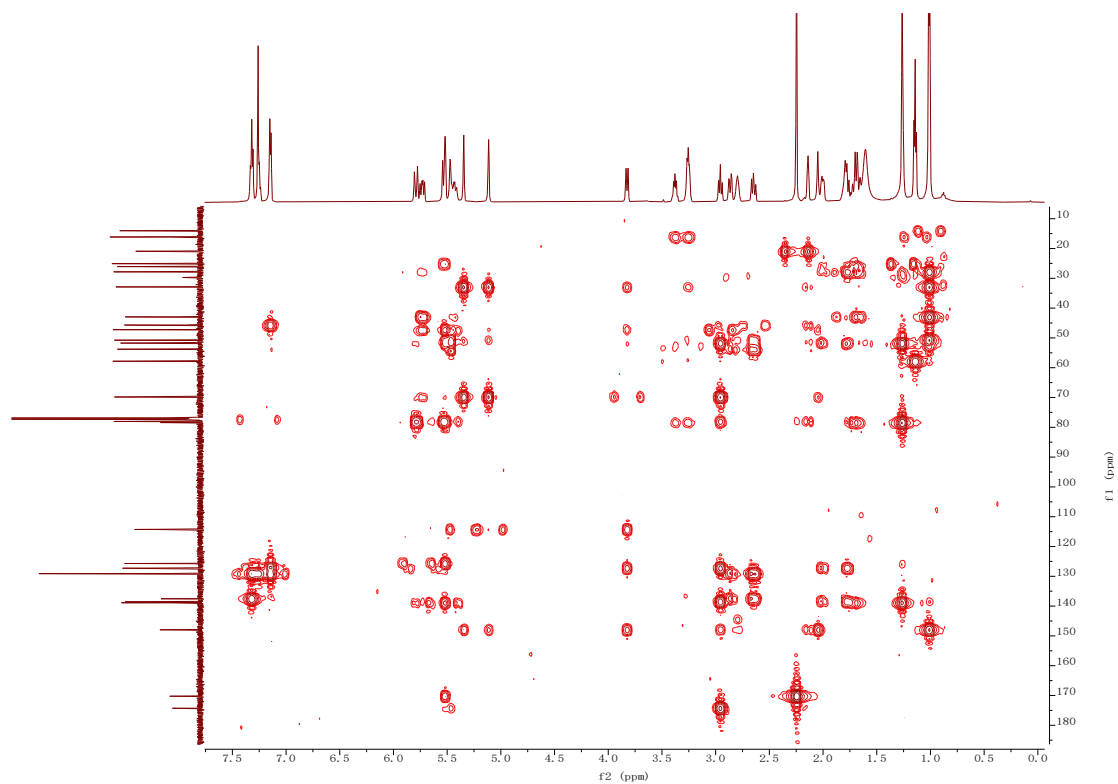


Figure S14. HMBC spectrum of **2** (600 MHz, CDCl₃).

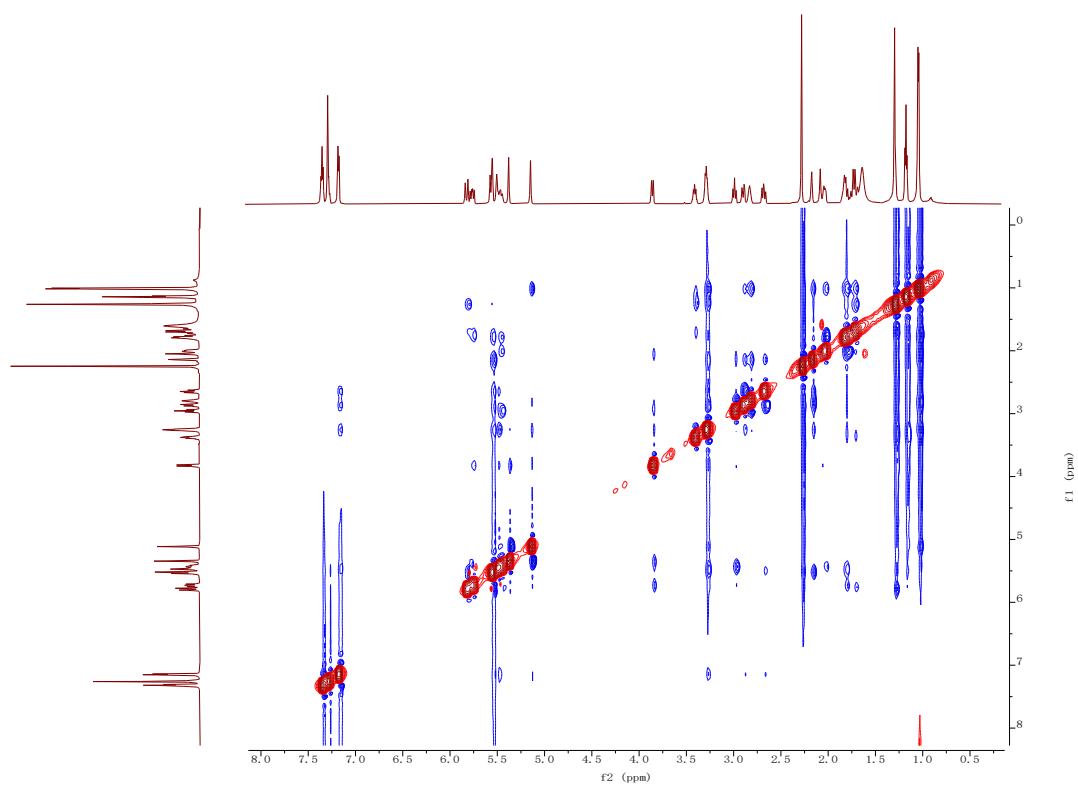


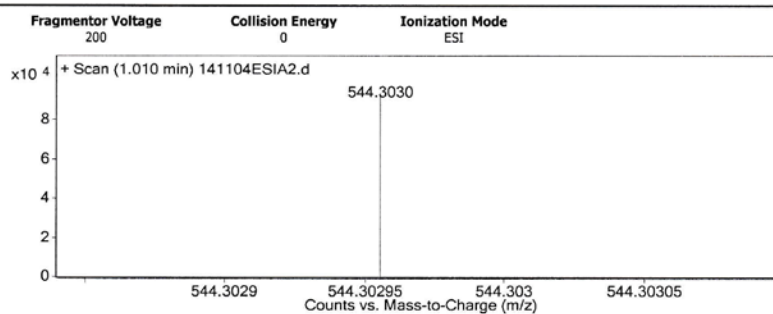
Figure S15. ROESY spectrum of **2** (600 MHz, CDCl₃).

Qualitative Analysis Report

Data Filename	141104ESIA2.d	Sample Name	SHJ07
Sample Type	Sample	Position	
Instrument Name	Agilent G6230 TOF MS	User Name	KIB
Acq Method	ESI.m	Acquired Time	11/4/2014 10:08:07 AM
IRM Calibration Status	Success	DA Method	demo.m
Comment			

Sample Group		Info.	
Acquisition SW	6200 series TOF/6500 series		
Version	Q-TOF B.05.01 (B5125.2)		

User Spectra



Peak List

m/z	z	Abund	Formula	Ion
544.303	1	93731.61	C32 H43 N Na O5	M+

Formula Calculator Element Limits

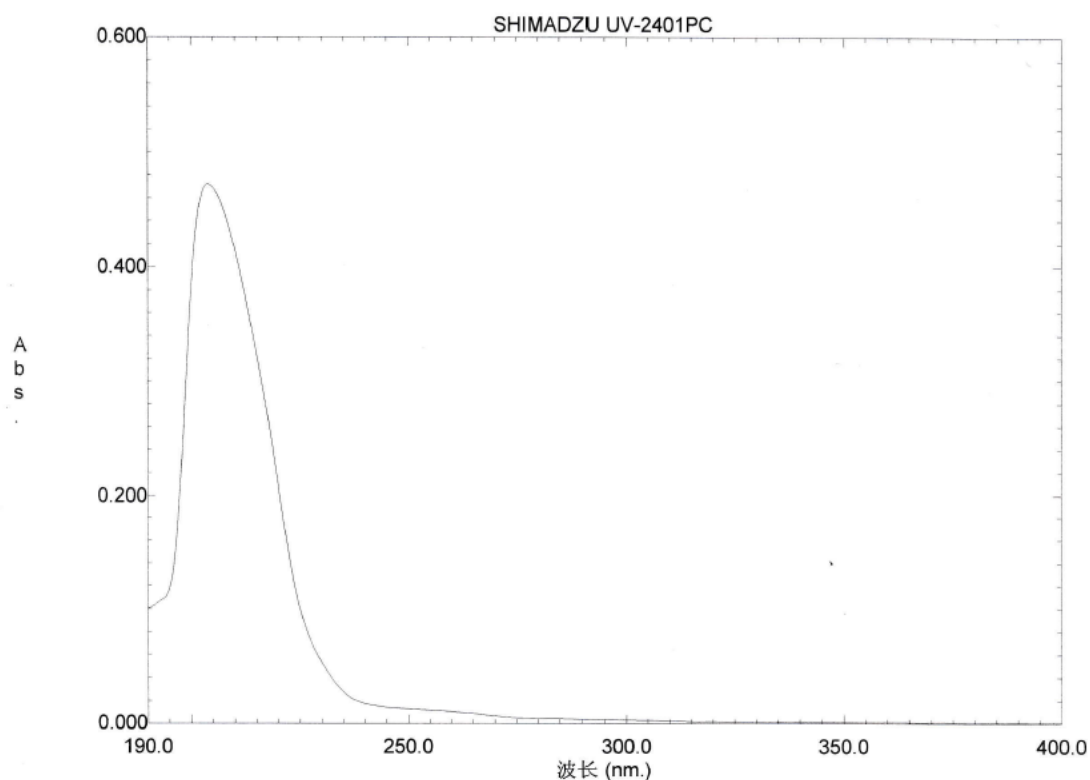
Element	Min	Max
C	0	200
H	0	400
O	1	8
Na	1	1
N	1	1

Formula Calculator Results

Formula	Calculated Mass	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C32 H43 N Na O5	544.3039	544.3030	0.9	1.6	11.5

--- End Of Report ---

Figure S16. HRESIMS spectrum of **2**.



文件名: SHJ07

SHJ07

创建于: 15:53 15-01-21

样品浓度: 0.0111毫克/毫升

数据: 原始

溶剂: 甲醇

测量模式: Abs.

扫描速度: 中速

狭缝: 5.0

采样间隔: 0.2

否	波长 (nm.)	Abs.
1	204.00	0.4717

Figure S17. UV spectrum of **2**.

Optical rotation measurement

Model: P-1020 (A060460638)

No.	Sample	Mode	Data	Monitor Blank	Temp. Cell Temp Point	Date Comment Sample Name	Light Filter Operator	Cycle Time Integ Time
No.1	17 (1/3)	Sp.Rot	38.5710	0.0297 0.0000	18.1 50.00 Cell	Tue Jan 20 20:57:47 2015 0.00154g/mL MeOH SHJ07	Na 589nm	2 sec 10 sec
No.2	17 (2/3)	Sp.Rot	39.3510	0.0303 0.0000	18.1 50.00 Cell	Tue Jan 20 20:58:00 2015 0.00154g/mL MeOH SHJ07	Na 589nm	2 sec 10 sec
No.3	17 (3/3)	Sp.Rot	38.9610	0.0300 0.0000	18.1 50.00 Cell	Tue Jan 20 20:58:13 2015 0.00154g/mL MeOH SHJ07	Na 589nm	2 sec 10 sec

+38.9610°

Figure S18. ORD spectrum of **2**.

SHJ07

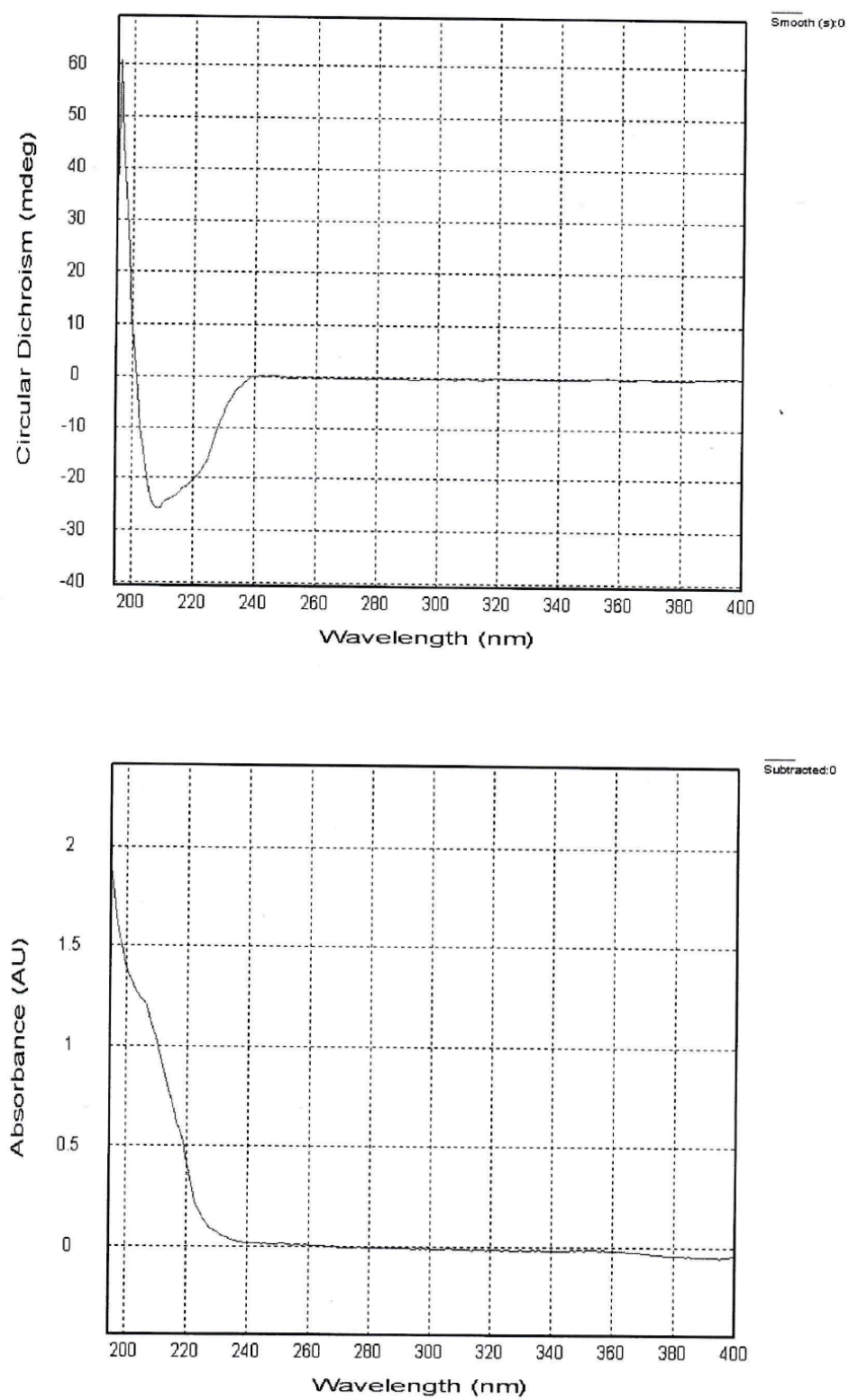


Figure S19. CD spectrum of **2**.

3. NMR, HRESIMS, UV, ORD, and CD spectra of compound **3**

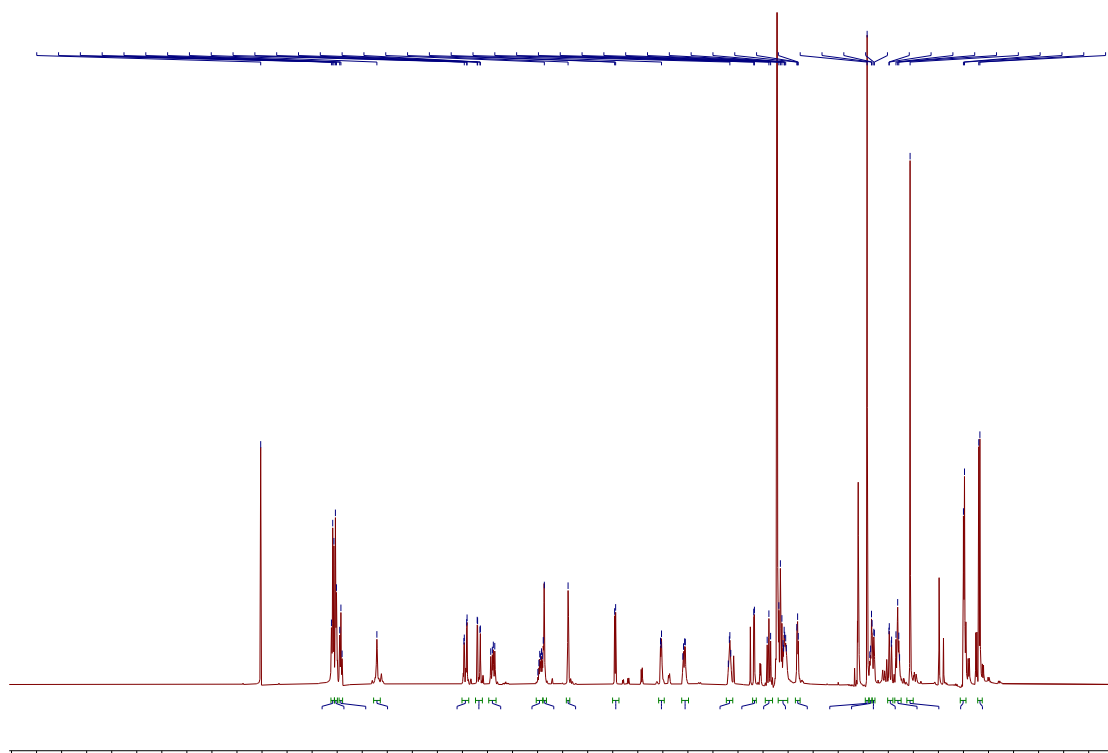


Figure S20. ^1H NMR spectrum of **3** (600 MHz, acetone- d_6).

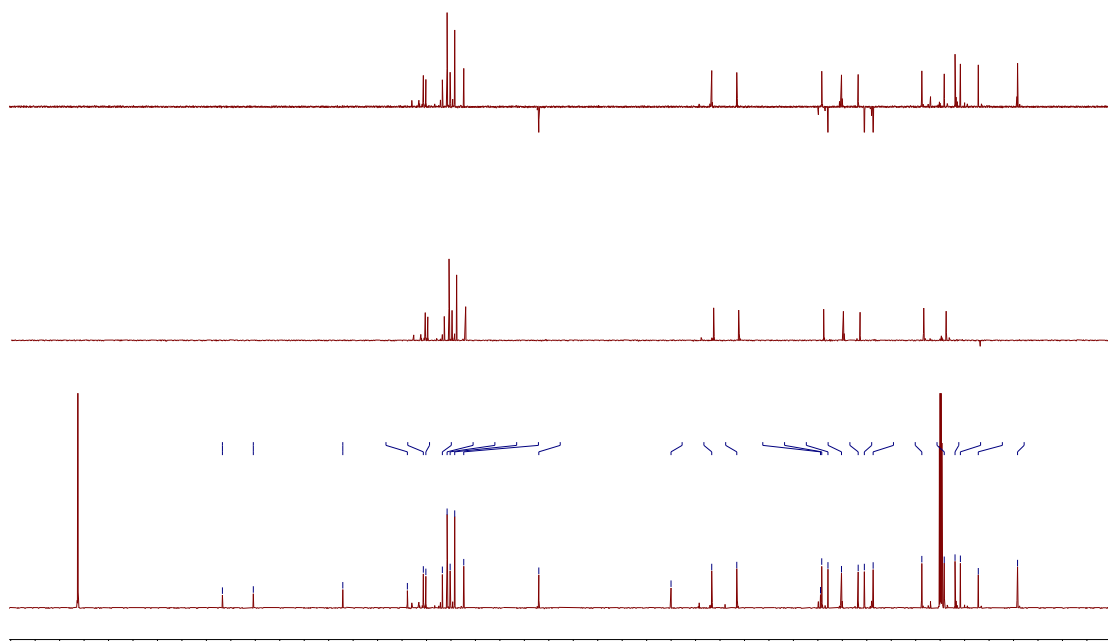


Figure S21. ^{13}C NMR, DEPT-90 and DEPT-135 spectra of **3** (150 MHz, acetone- d_6).

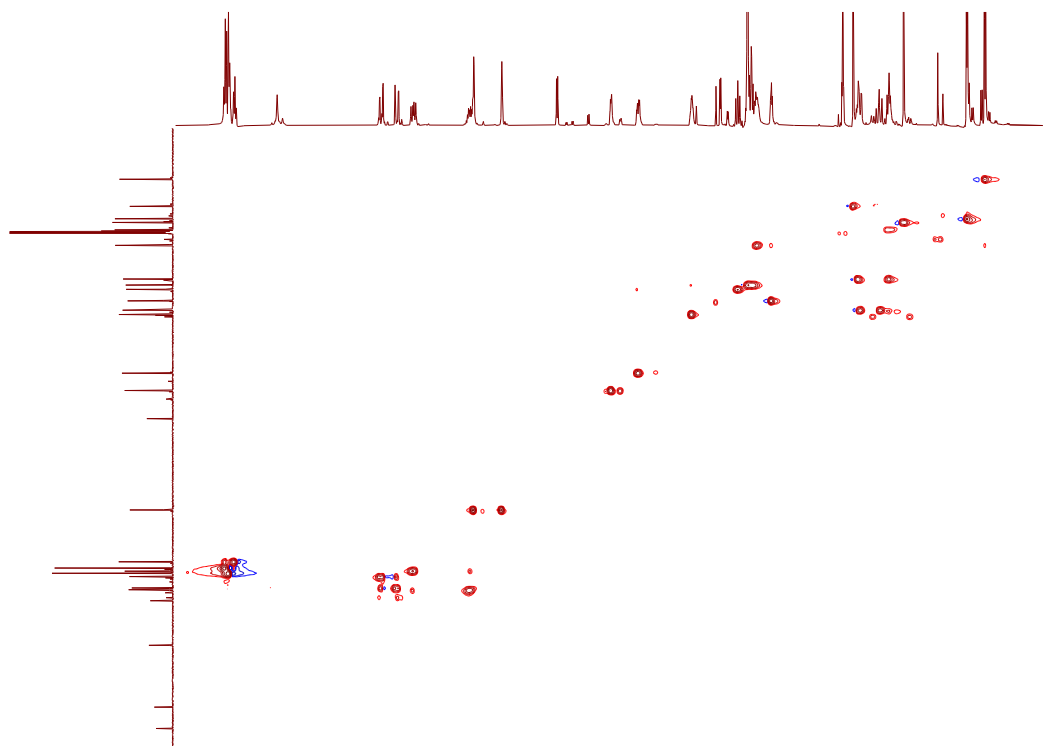


Figure S22. HSQC spectrum of **3** (600 MHz, acetone- d_6).

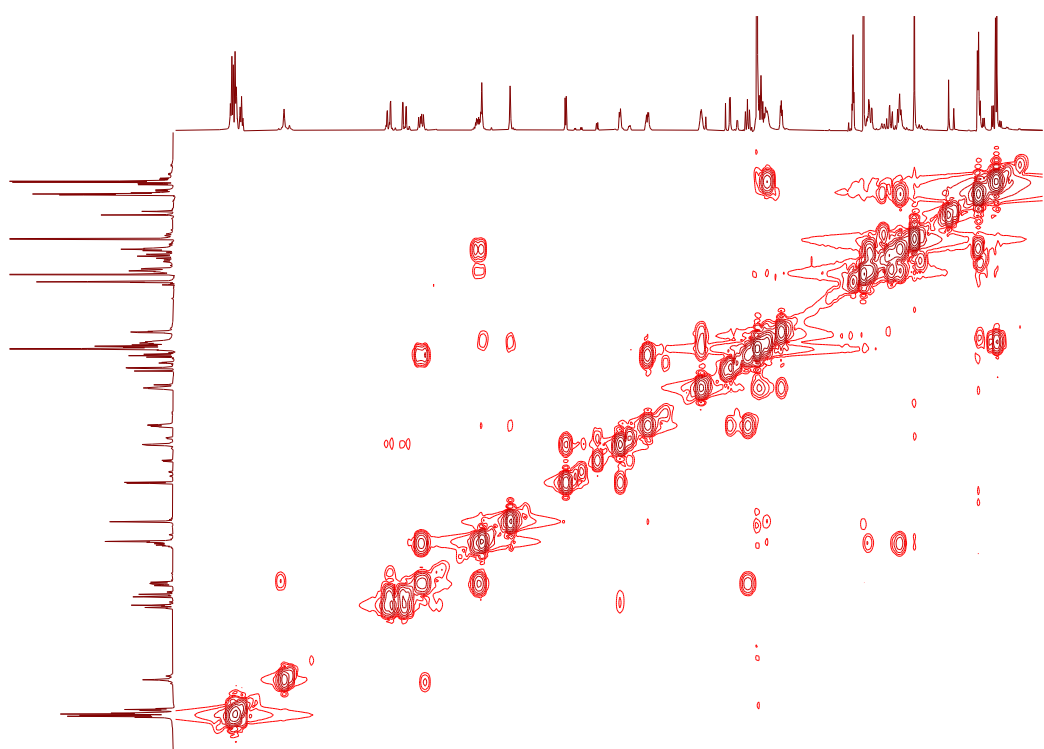


Figure S23. ^1H - ^1H COSY spectrum of **3** (600 MHz, acetone- d_6).

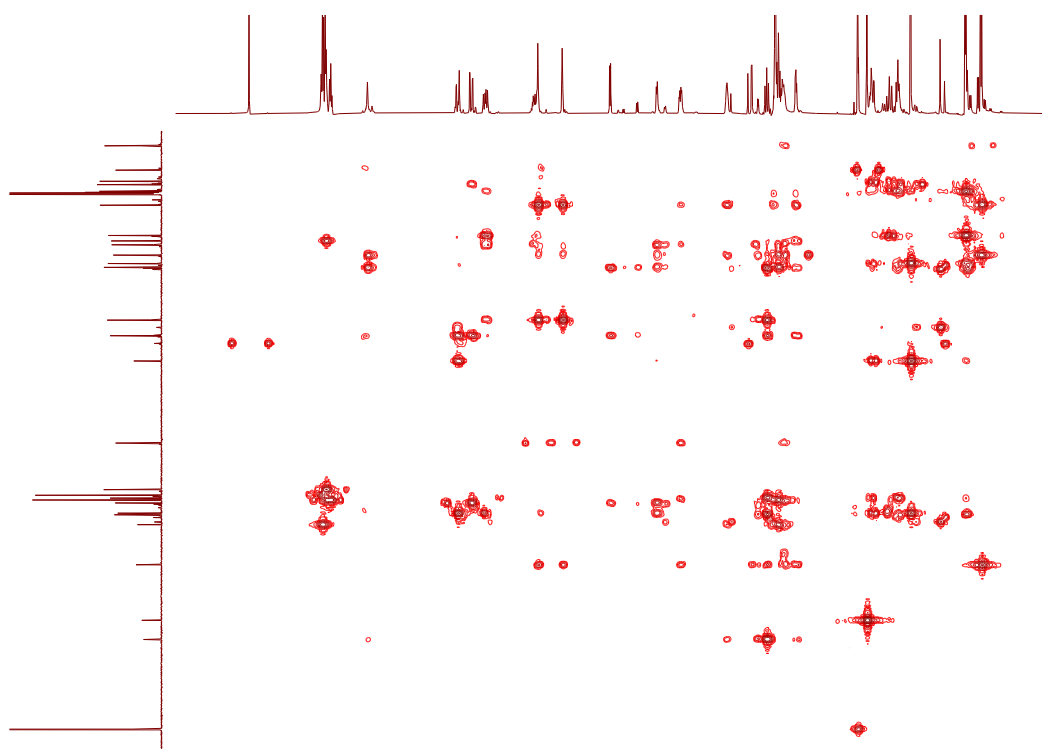


Figure S24. HMBC spectrum of **3** (600 MHz, acetone- d_6).

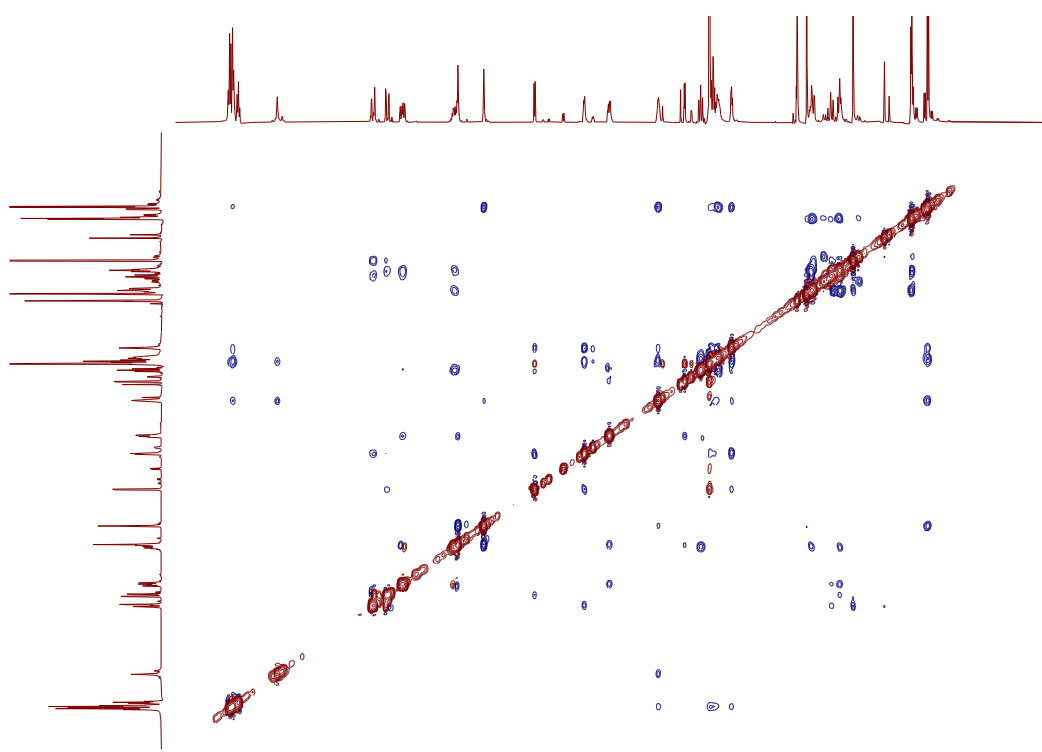


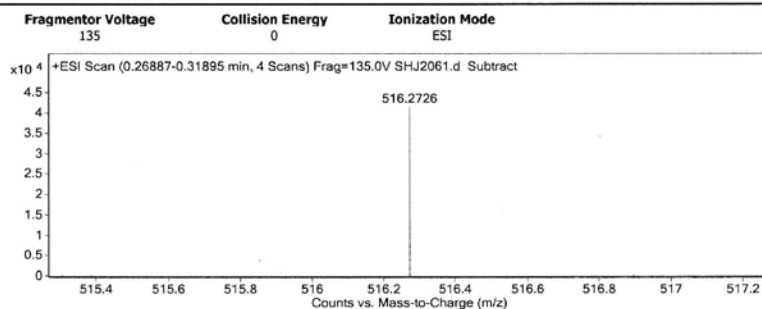
Figure S25. ROESY spectrum of **3** (600 MHz, acetone- d_6).

Qualitative Analysis Report

Data Filename	SHJ2061.d	Sample Name	SHJ2061
Sample Type	Sample	Position	P1-B1
Instrument Name	Instrument 1	User Name	
Acq Method	SIBU.m	Acquired Time	11/5/2014 10:04:48 AM
IRM Calibration Status	Success	DA Method	Default.m
Comment			

Sample Group	Info.
Acquisition SW	6200 series TOF/6500 series
Version	Q-TOF B.05.01 (B5125.2)

User Spectra



Peak List

m/z	z	Abund	Formula	Ion
301.1415	1	9981.23		
315.1566	1	6578.91		
416.2595	1	6534.67		
434.269	1	14929.77		
435.2731	1	5252.26		
494.2906	1	24097.41		
495.2942	1	8625.36		
516.2726	1	41536.34	C30 H39 N O5	(M+Na)+
517.2759	1	12547.21	C30 H39 N O5	(M+Na)+
652.2481	1	5529.75		

Formula Calculator Element Limits

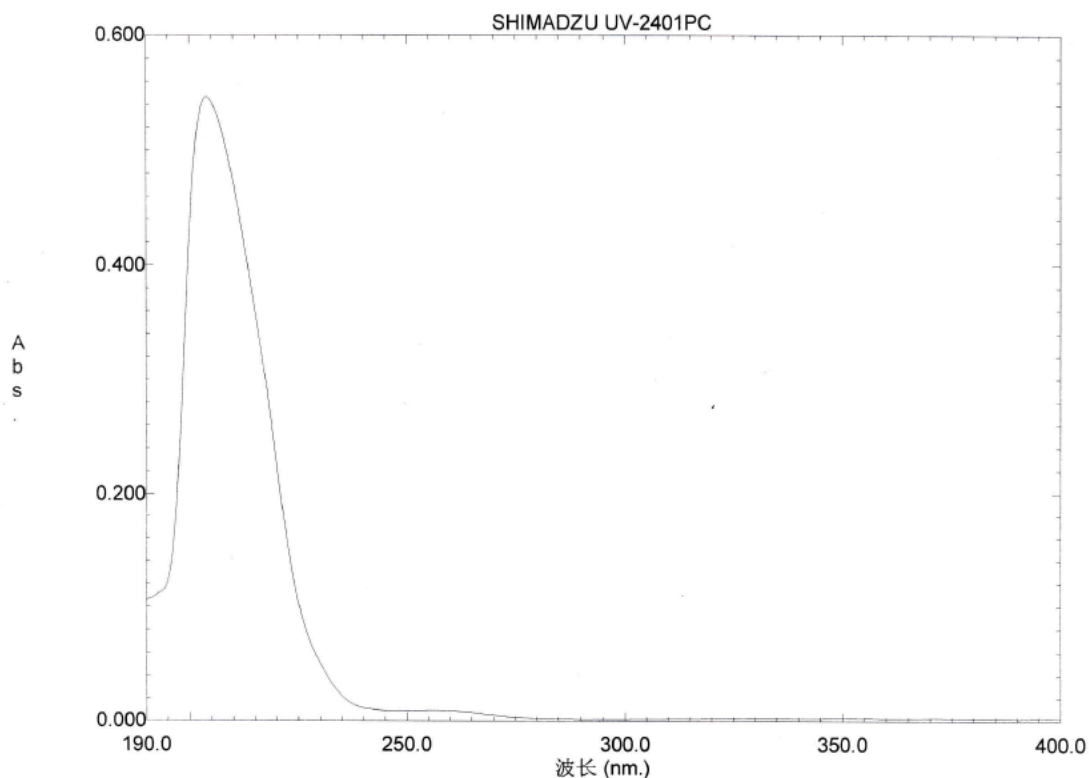
Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	5

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C30 H39 N O5	493.2828	516.2720	516.2726	-0.6	-1.2	12.0000

--- End Of Report ---

Figure S26. HRESIMS spectrum of 3.



文件名: 15012103
样品名称: SHJ2061

15012103

创建于: 16:39 15-01-21
数据: 原始

样品浓度: 0.0108毫克/毫升
溶剂: 甲醇

测量模式: Abs.
扫描速度: 中速
狭缝: 5.0
采样间隔: 0.2

否.	波长 (nm.)	Abs.
1	204.00	0.5467

Figure S27. UV spectrum of **3**.

Optical rotation measurement

Model: P-1020 (A060460638)

No.	Sample	Mode	Data	Monitor Blank	Temp. Cell Temp Point	Date Comment Sample Name	Light Filter Operator	Cycle Time Integ Time
No.1	8 (1/3)	Sp.Rot	22.4690	0.0273 0.0000	21.5 50.00 Cell	Wed Oct 29 20:34:44 2014 0.00243g/mL MeOH SHJ2061	Na 589nm	2 sec 10 sec
No.2	8 (2/3)	Sp.Rot	20.9880	0.0255 0.0000	21.5 50.00 Cell	Wed Oct 29 20:34:57 2014 0.00243g/mL MeOH SHJ2061	Na 589nm	2 sec 10 sec
No.3	8 (3/3)	Sp.Rot	22.5510	0.0274 0.0000	21.6 50.00 Cell	Wed Oct 29 20:35:10 2014 0.00243g/mL MeOH SHJ2061	Na 589nm	2 sec 10 sec

+22.0027°

Figure S28. ORD spectrum of **3**.

SHJ2061

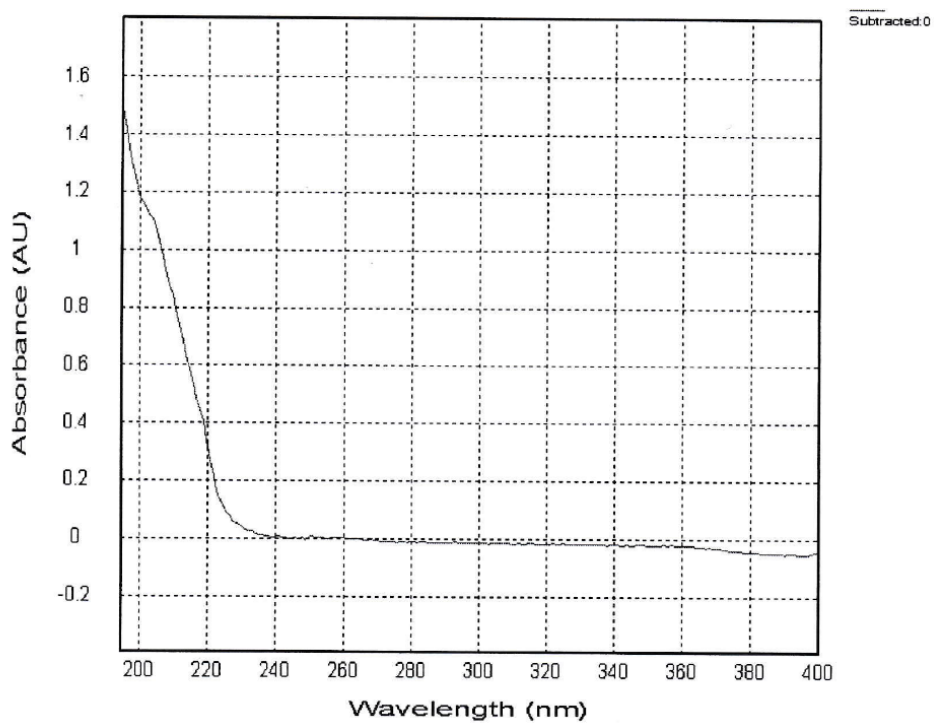
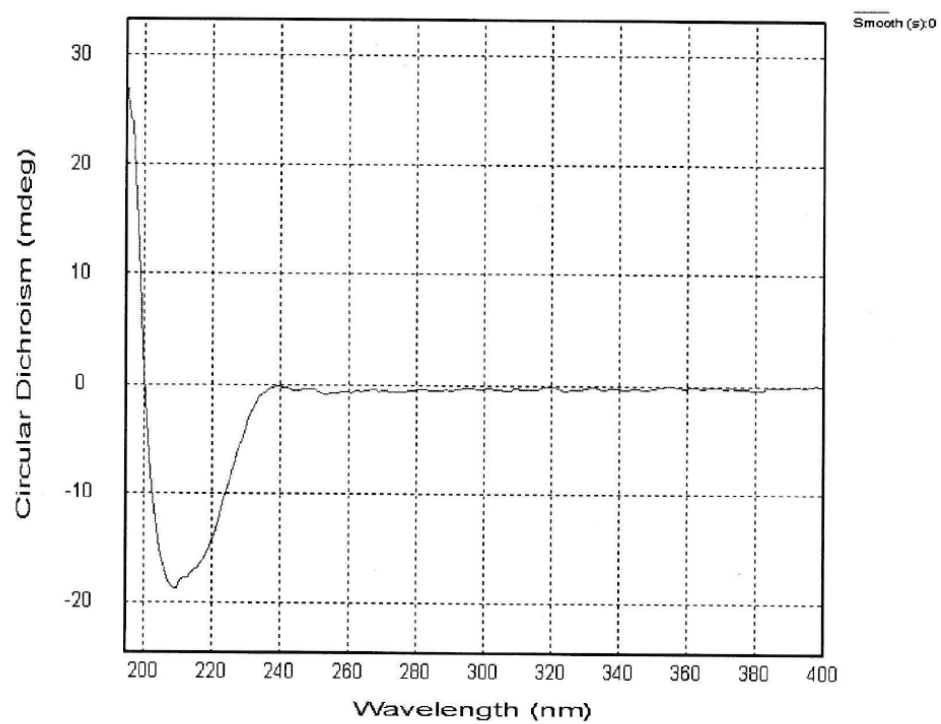


Figure S29. CD spectrum of **3**.

4. NMR, HRESIMS, UV, ORD, and CD spectra of compound **4**

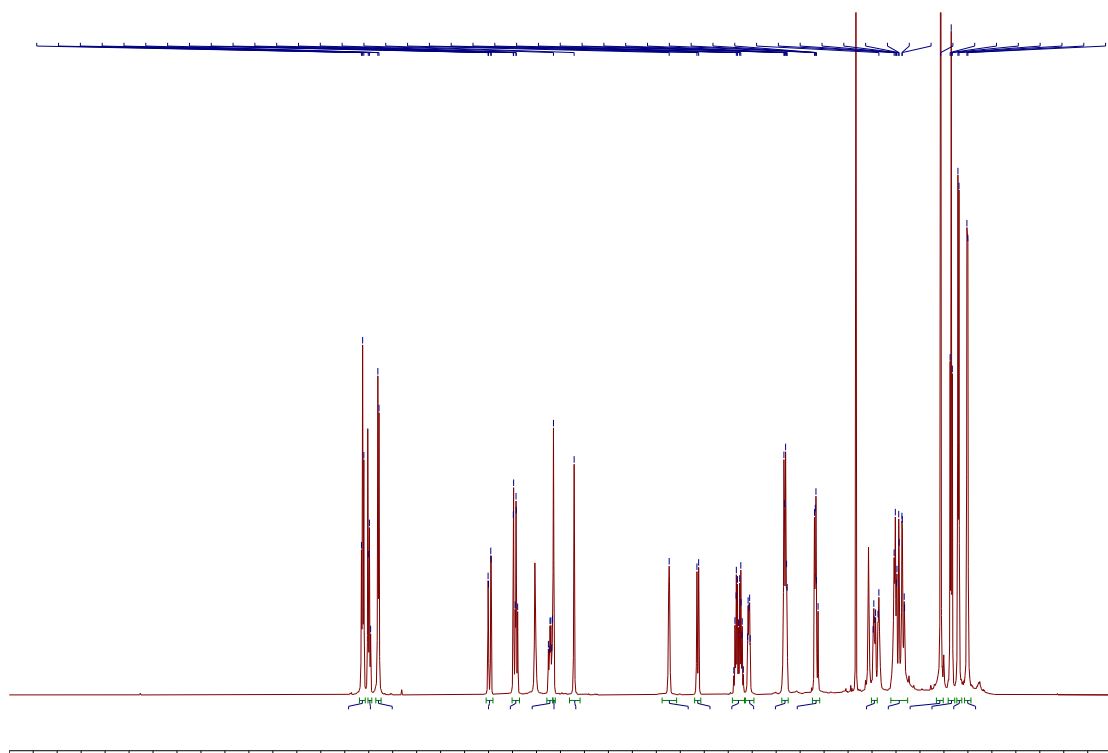


Figure S30. ^1H NMR spectrum of **4** (600 MHz, CDCl_3).

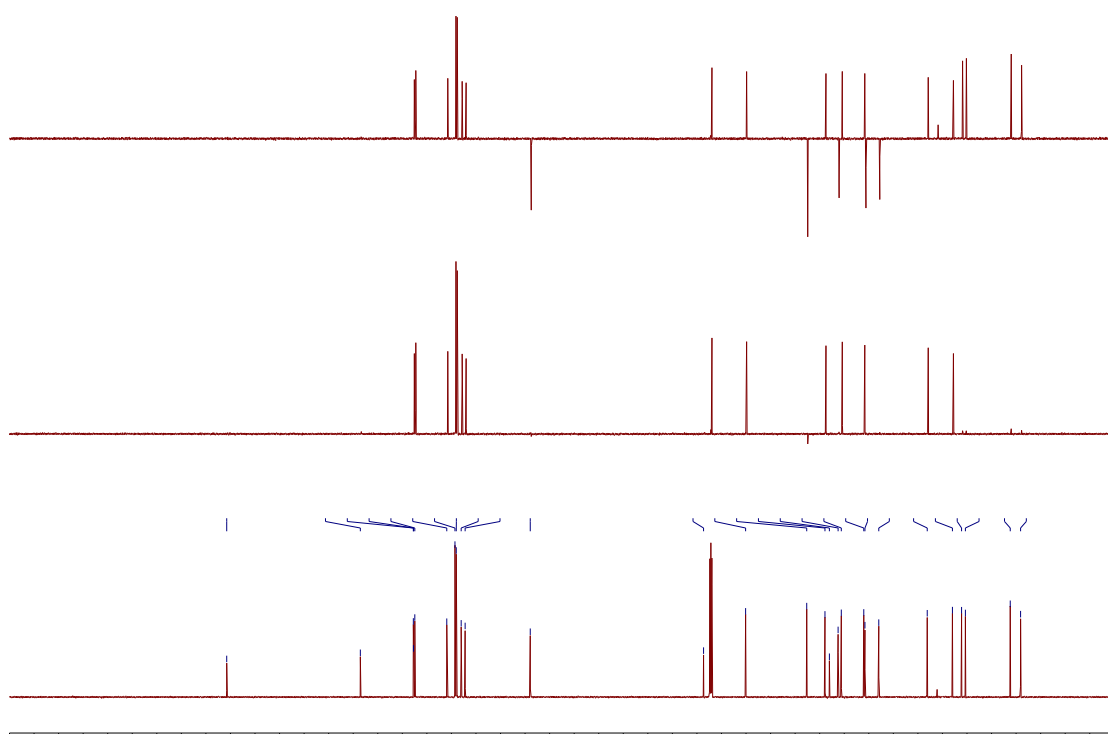


Figure S31. ^{13}C NMR, DEPT-90 and DEPT-135 spectra of **4** (150 MHz, CDCl_3).

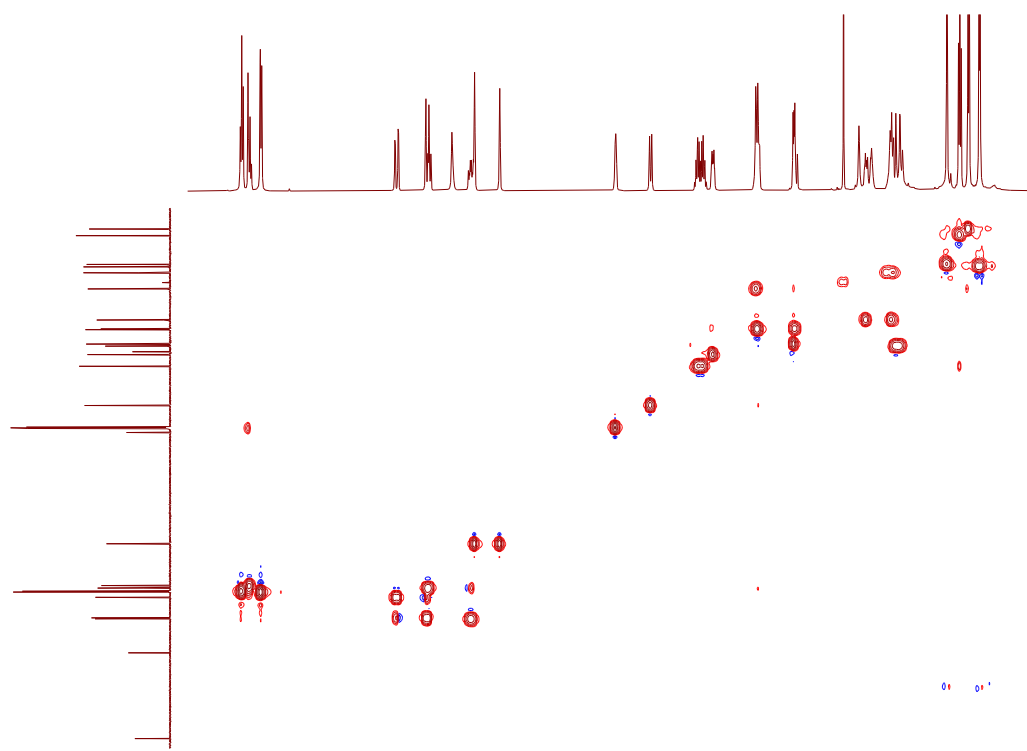


Figure S32. HSQC spectrum of **4** (600 MHz, CDCl₃).

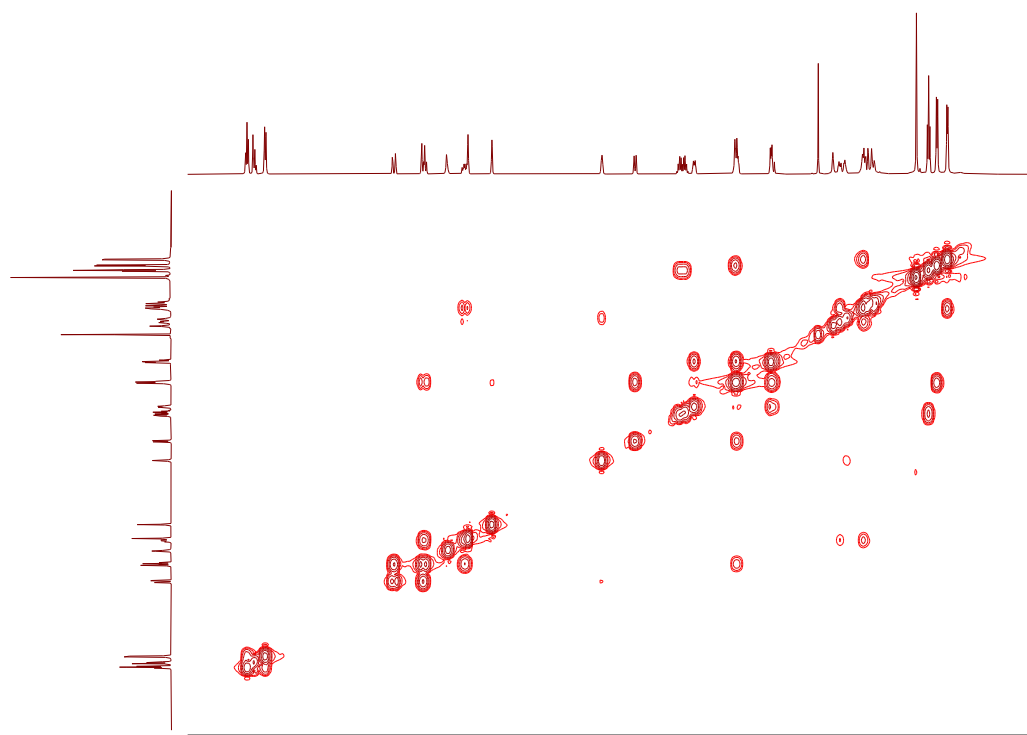


Figure S33. ¹H-¹H COSY spectrum of **4** (600 MHz, CDCl₃).

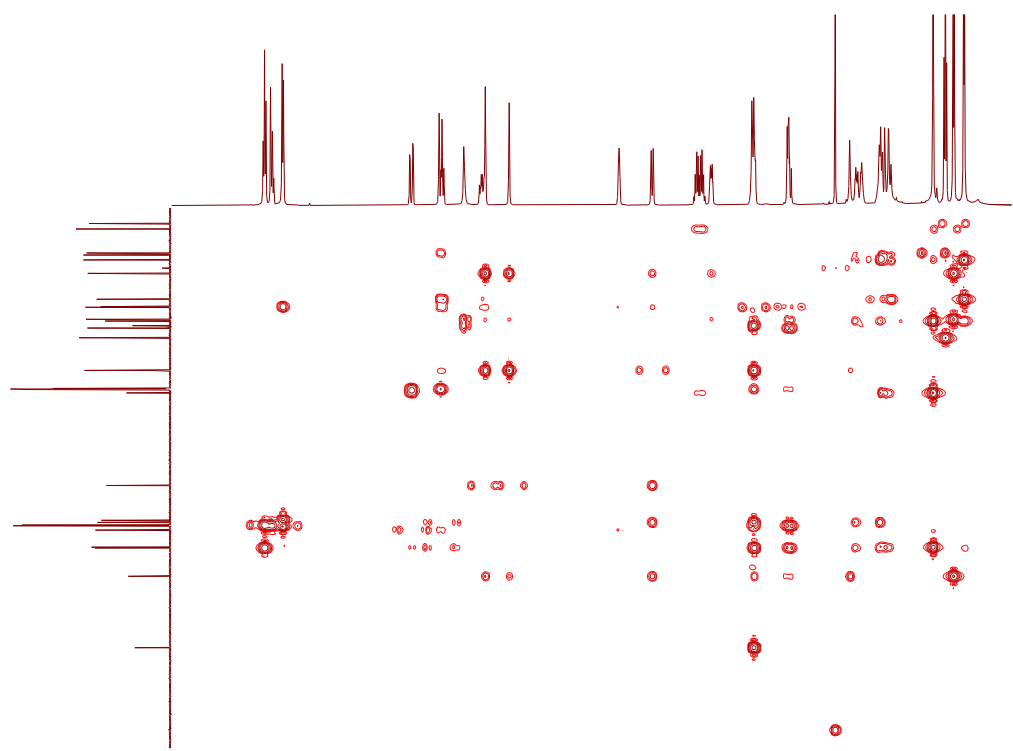


Figure S34. HMBC spectrum of **4** (600 MHz, CDCl_3).

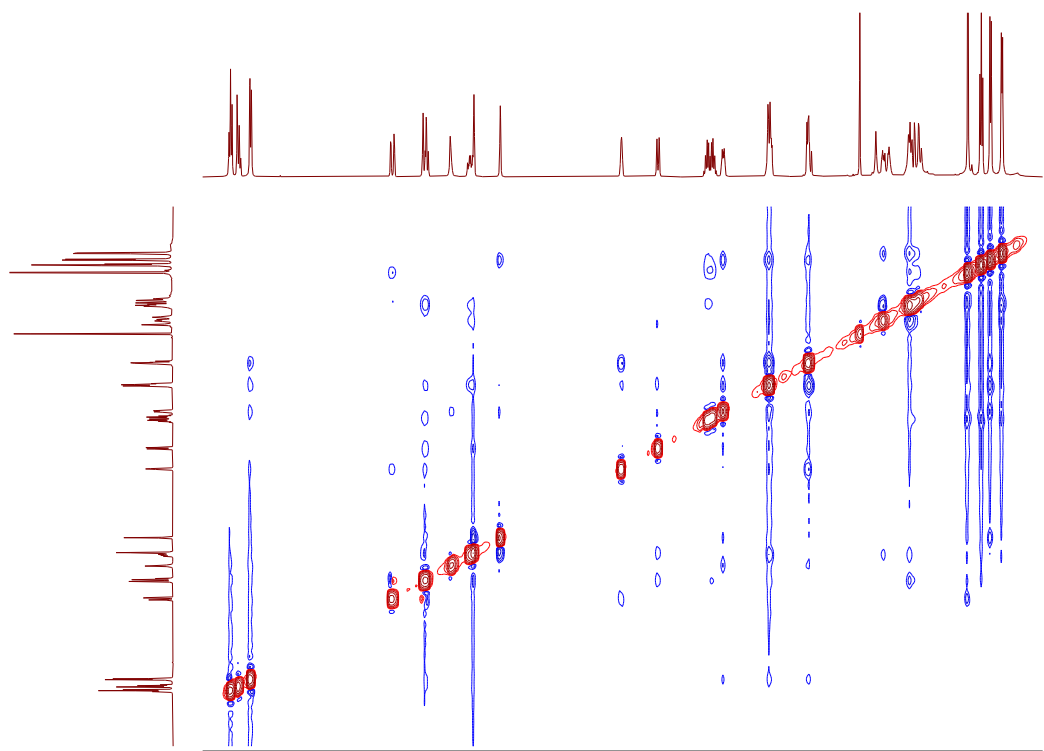


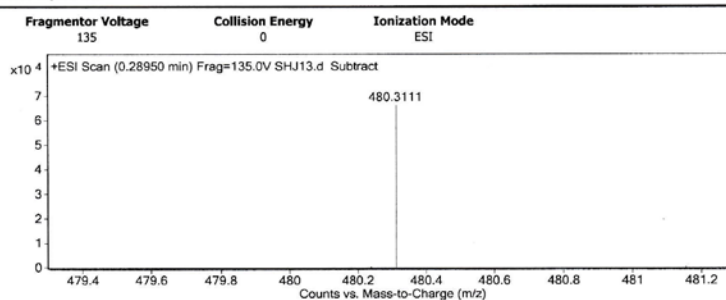
Figure S35. ROESY spectrum of **4** (600 MHz, CDCl_3).

Qualitative Analysis Report

Data Filename	SHJ13.d	Sample Name	SHJ13
Sample Type	Sample	Position	P1-A2
Instrument Name	Instrument 1	User Name	
Acq Method	SIBU.m	Acquired Time	12/25/2014 3:10:10 PM
IRM Calibration Status	Success	DA Method	Default.m
Comment			

Sample Group	Info.
Acquisition SW	6200 series TOF/6500 series
Version	Q-TOF B.05.01 (B5125.2)

User Spectra



Peak List

m/z	z	Abund	Formula	Ion
434.2692	1	20036.47		
480.3111	1	66189.3	C30 H41 N O4	(M+H)+
502.2929	1	45060.74		
981.5964	1	33772.45		
982.6006	1	21777.8		

Formula Calculator Element Limits

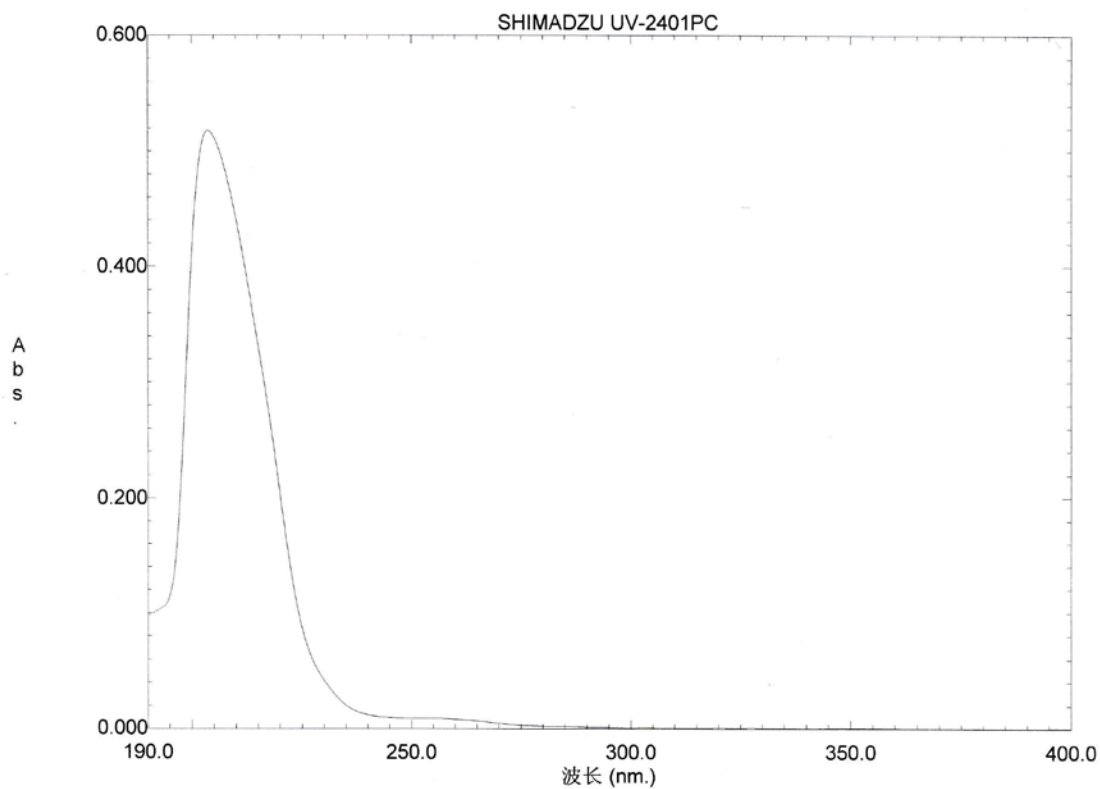
Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	5

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C30 H41 N O4	479.3036	480.3108	480.3111	-0.2	-0.5	11.0000

--- End Of Report ---

Figure S36. HRESIMS spectrum of **4**.



文件名: SHJ13

SHJ13

创建于: 16:09 15-01-21

样品浓度: 0.0086毫克/毫升

数据: 原始

溶剂: 甲醇

测量模式: Abs.
扫描速度: 中速
狭缝: 5.0
采样间隔: 0.2

否.	波长 (nm.)	Abs.
1	203.80	0.5179

Figure S37. UV spectrum of 4.

Optical rotation measurement

Model: P-1020 (A060460638)

No.	Sample	Mode	Data	Monitor Blank	Temp. Cell Temp Point	Date Comment Sample Name	Light Filter Operator	Cycle Time Integ Time
No.1	18 (1/3)	Sp.Rot	49.1100	0.0469 0.0000	18.2 50.00	Tue Jan 20 21:11:24 2015 0.00191g/mL MeOH SHJ13	Na 589nm	2 sec 10 sec
No.2	18 (2/3)	Sp.Rot	50.1570	0.0479 0.0000	18.2 50.00	Tue Jan 20 21:11:37 2015 0.00191g/mL MeOH SHJ13	Na 589nm	2 sec 10 sec
No.3	18 (3/3)	Sp.Rot	50.6810	0.0484 0.0000	18.2 50.00	Tue Jan 20 21:11:51 2015 0.00191g/mL MeOH SHJ13	Na 589nm	2 sec 10 sec

+49.985°

Figure S38. ORD spectrum of 4.

SHJ13

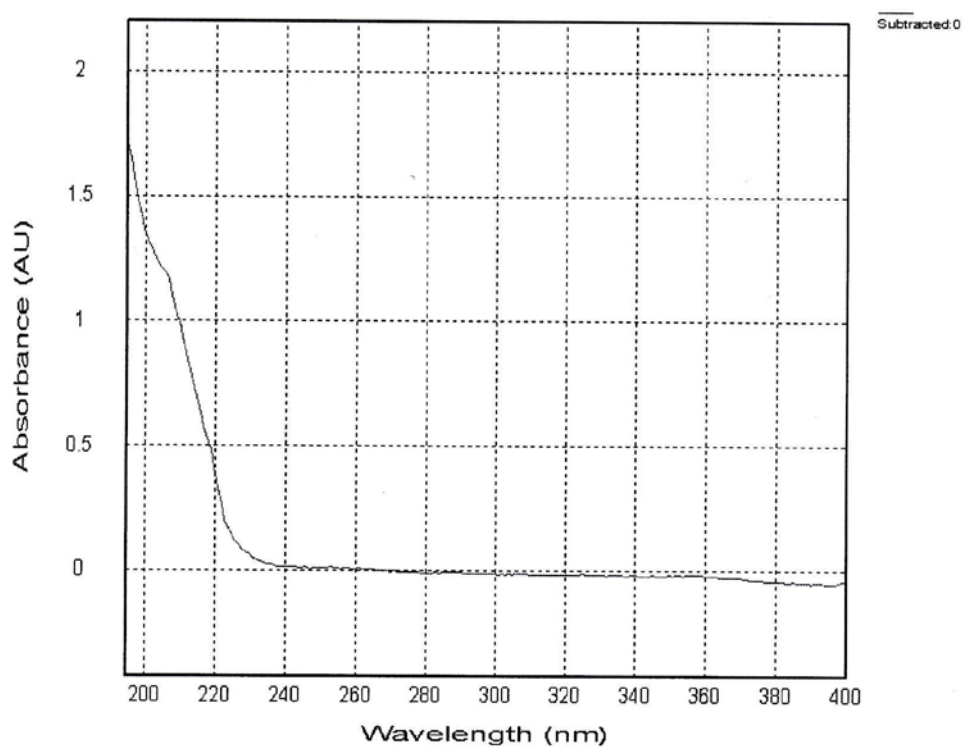
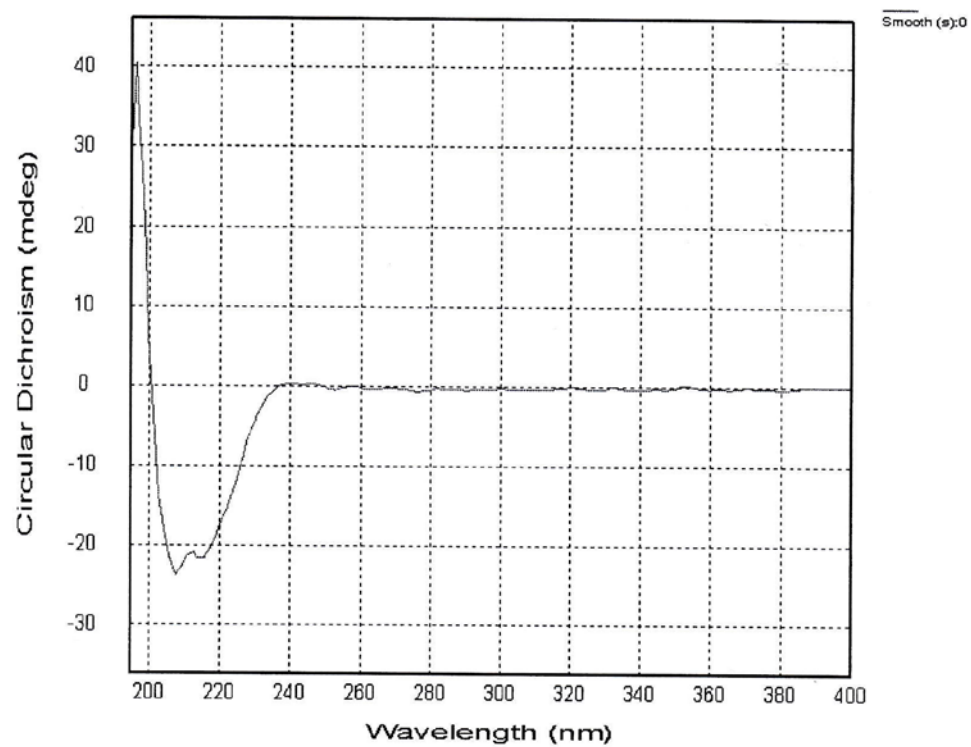


Figure S39. CD spectrum of **4**.

5. NMR, HRESIMS, UV, ORD, and CD spectra of compound **5**

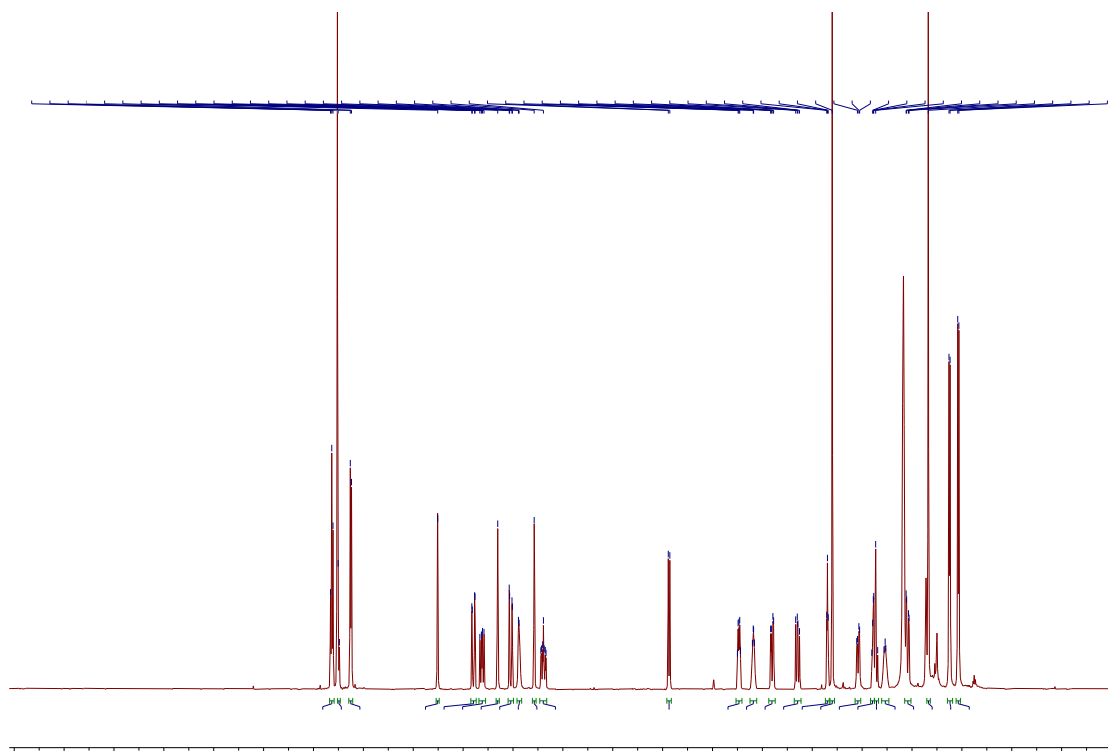


Figure S40. ^1H NMR spectrum of **5** (600 MHz, CDCl_3).

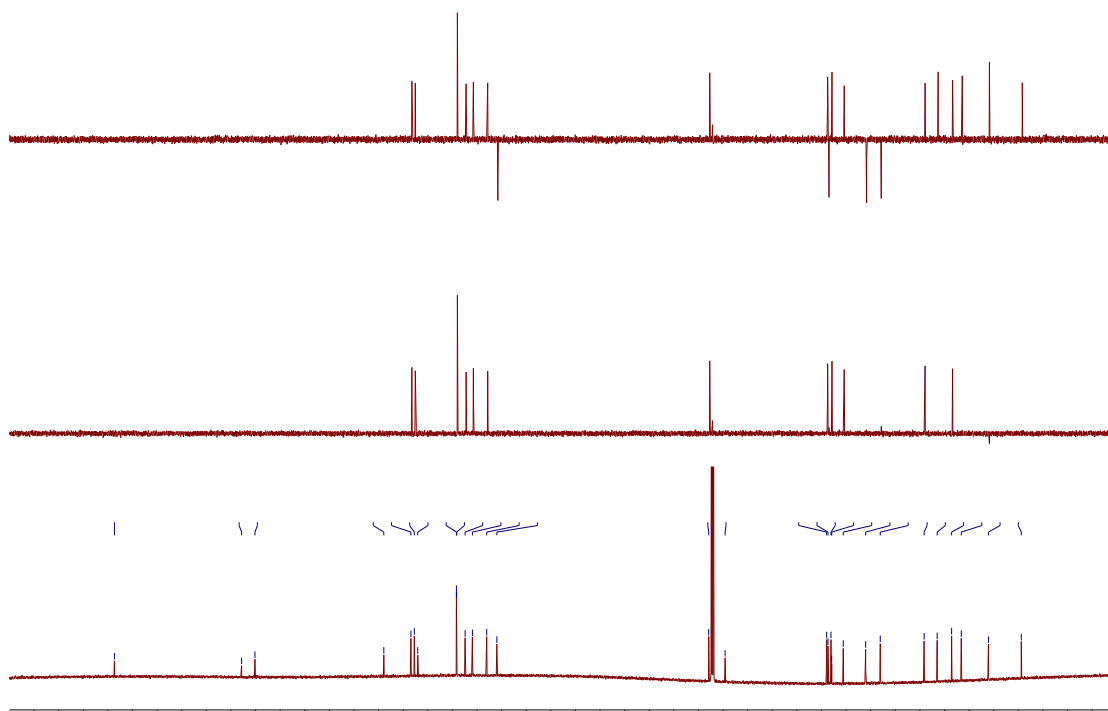


Figure S41. ^{13}C NMR, DEPT-90 and DEPT-135 spectra of **5** (150 MHz, CDCl_3).

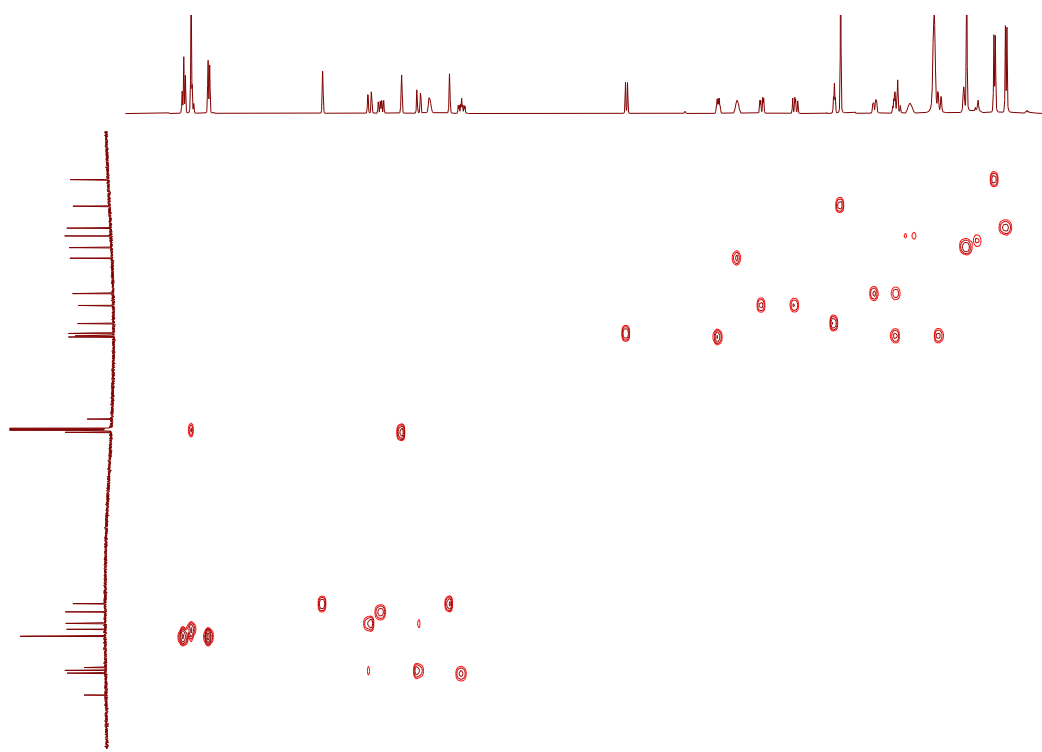


Figure S42. HSQC spectrum of **5** (600 MHz, CDCl₃).

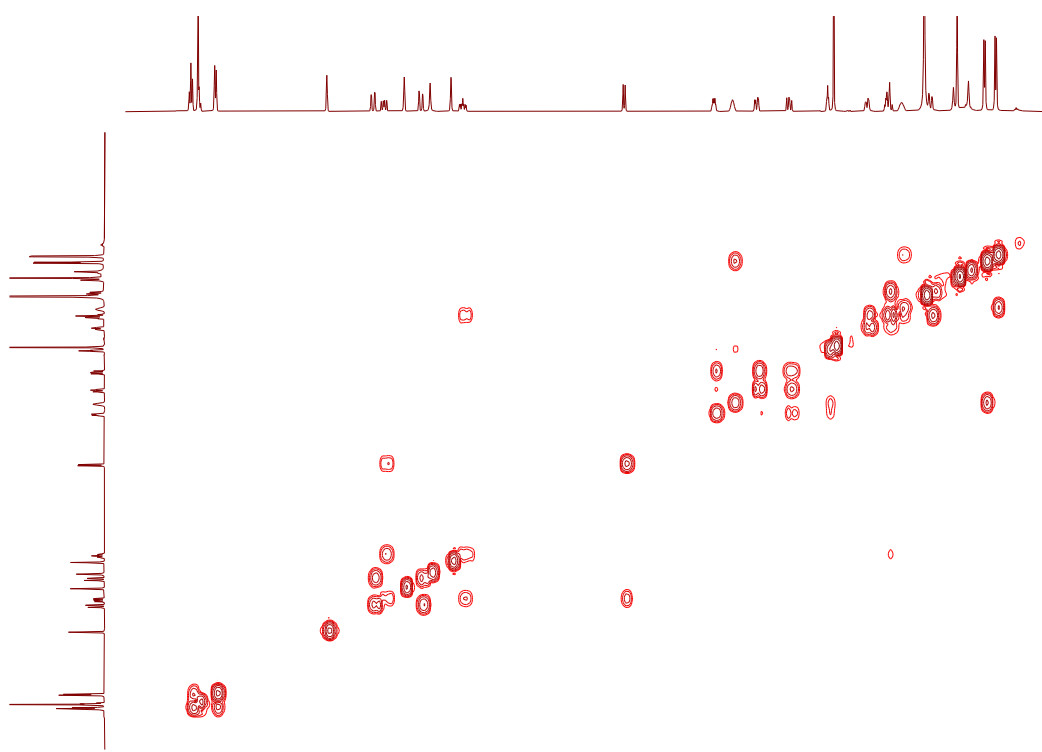


Figure S43. ¹H-¹H COSY spectrum of **5** (600 MHz, CDCl₃).

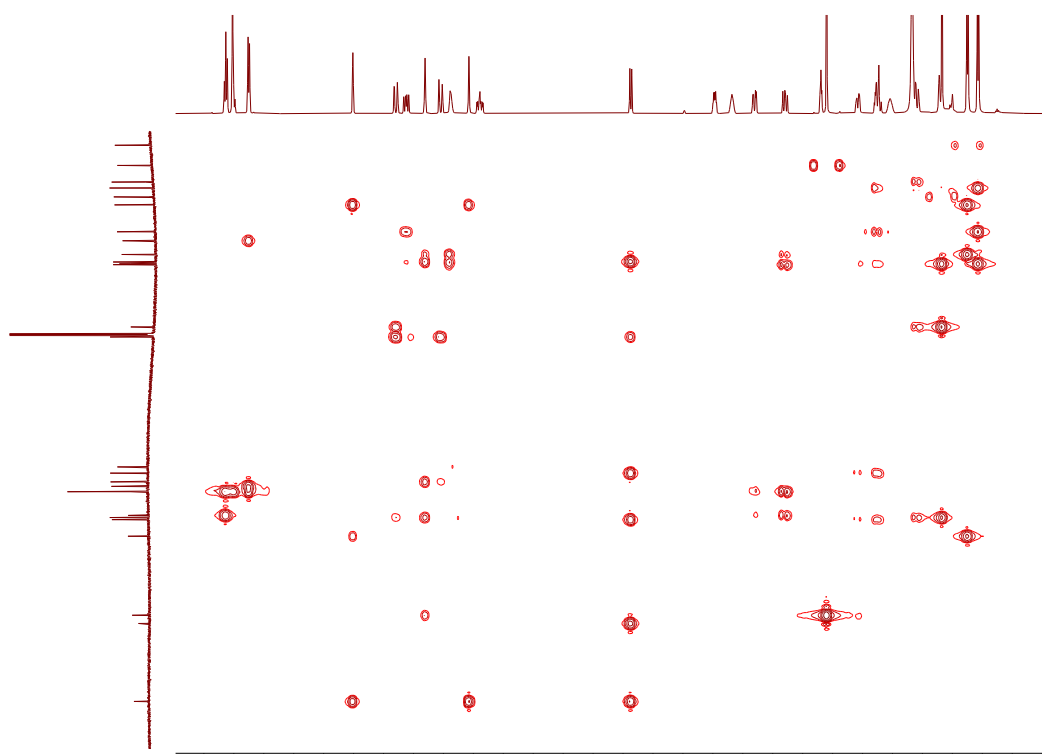


Figure S44. HMBC spectrum of **5** (600 MHz, CDCl_3).

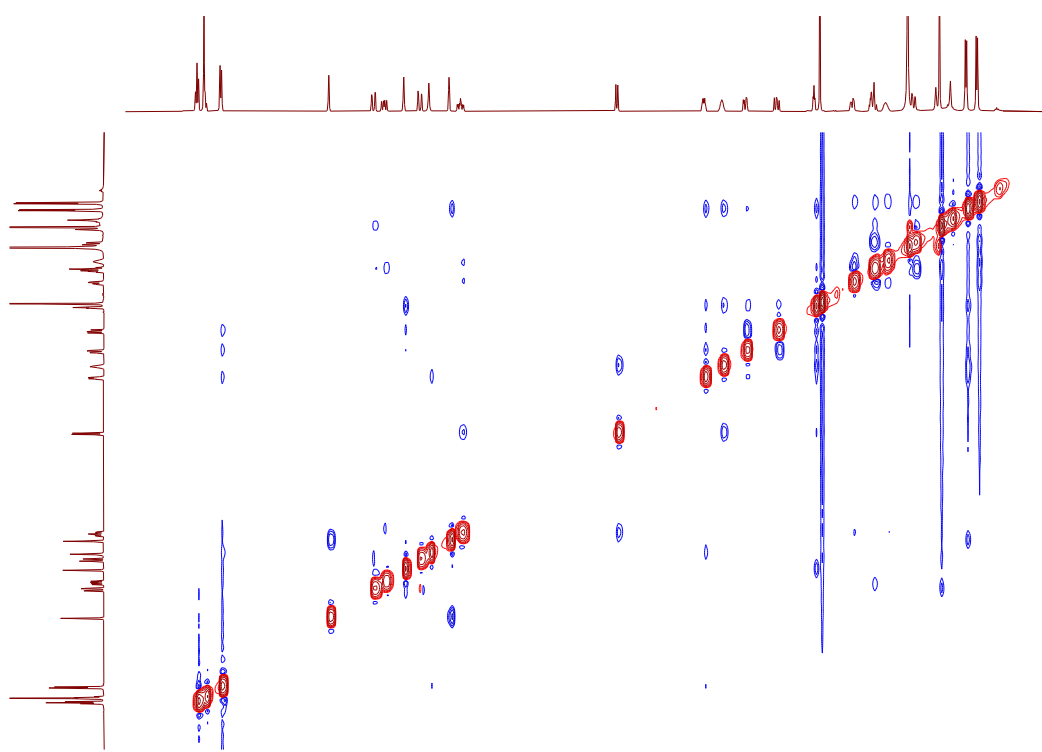


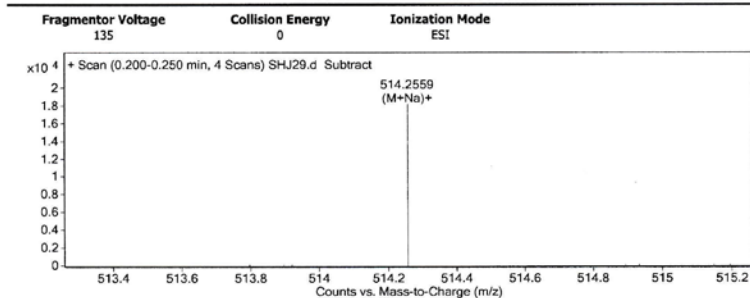
Figure S45. ROESY spectrum of **5** (600 MHz, CDCl_3).

Qualitative Analysis Report

Data Filename	SHJ29.d	Sample Name	SHJ29
Sample Type	Sample	Position	P1-A1
Instrument Name	Instrument 1	User Name	
Acq Method	SIBU.m	Acquired Time	7/16/2015 3:13:22 PM
IRM Calibration Status	Success	DA Method	Default.m
Comment			

Sample Group		Info.	
Acquisition SW	6200 series TOF/6500 series		
Version	Q-TOF B.05.01 (B5125.2)		

User Spectra



Peak List

m/z	z	Abund	Formula	Ion
102.128		2445.02		
306.6404	2	2378.82		
432.2536	1	3563.13		
492.2744	1	4787.3		
514.2559	1	18229.21	C30 H37 N O5	(M+Na)+
515.2594	1	5280.5	C30 H37 N O5	(M+Na)+
530.2295	1	7563.51		
531.2326	1	2451		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	10
N	0	5

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C30 H37 N O5	491.2672	514.2564	514.2559	0.4	0.9	13.0000

--- End Of Report ---

Figure S46. HRESIMS spectrum of 5.

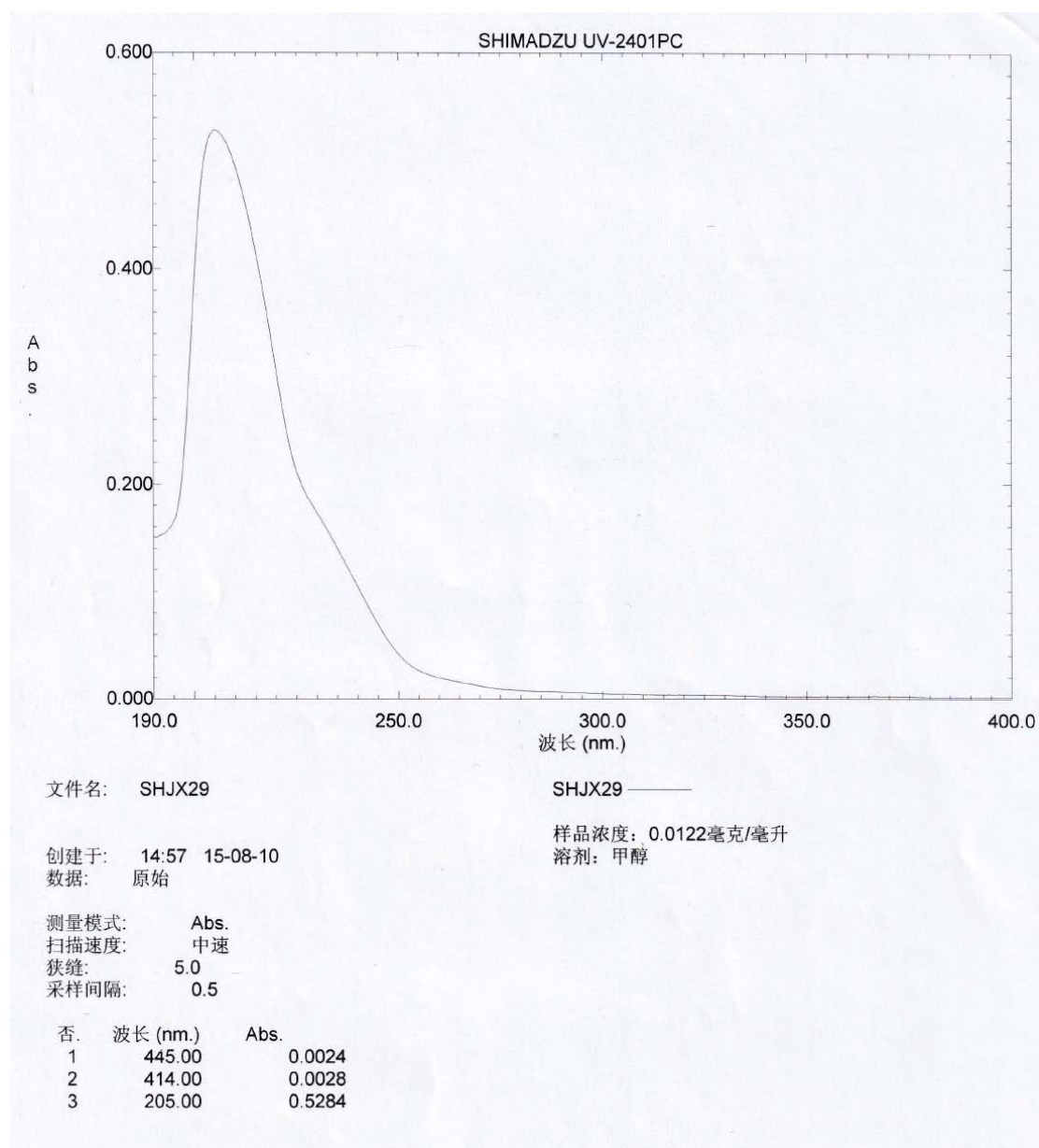


Figure S47. UV spectrum of **5**.

Optical rotation measurement

Model : P-1020 (A060460638)

No.	Sample	Mode	Data	Monitor Blank	Temp. Cell Temp Point	Date Comment Sample Name	Light Filter Operator	Cycle Time Integ Time
No.1	13 (1/3)	Sp.Rot	-11.6840	-0.0111 0.0000	23.6 50.00 Cell	Thu Aug 06 17:34:16 2015 0.00190g/mL MeOH SHJX29	Na 589nm	2 sec 10 sec
No.2	13 (2/3)	Sp.Rot	-12.9470	-0.0123 0.0000	23.5 50.00 Cell	Thu Aug 06 17:34:29 2015 0.00190g/mL MeOH SHJX29	Na 589nm	2 sec 10 sec
No.3	13 (3/3)	Sp.Rot	-12.2110	-0.0116 0.0000	23.4 50.00 Cell	Thu Aug 06 17:34:43 2015 0.00190g/mL MeOH SHJX29	Na 589nm	2 sec 10 sec

Figure S48. ORD spectrum of **5**.

SHJX29

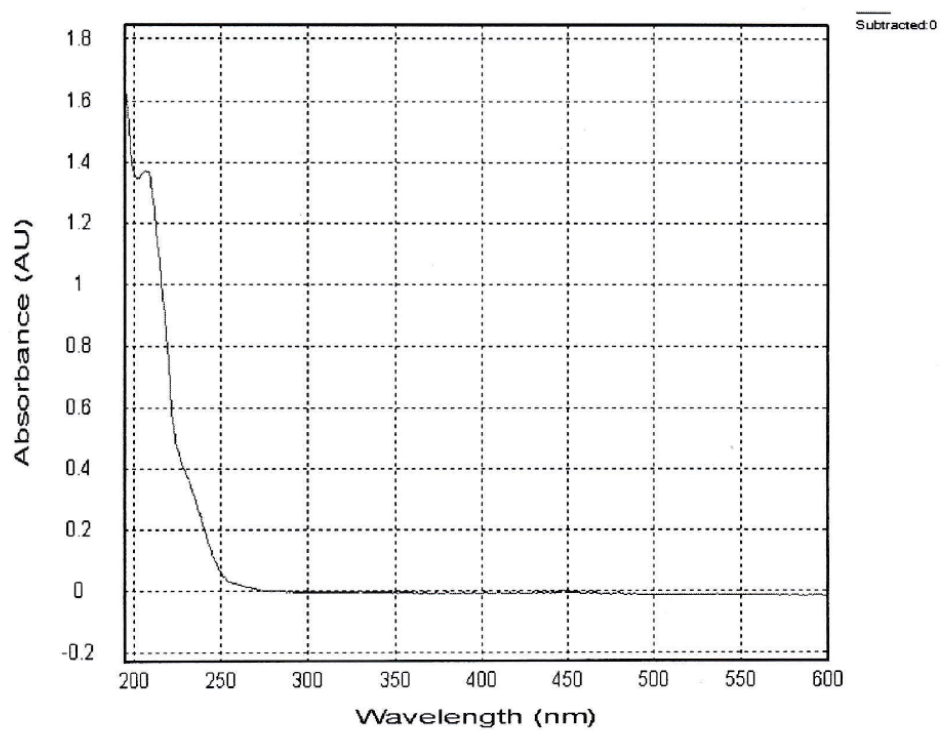
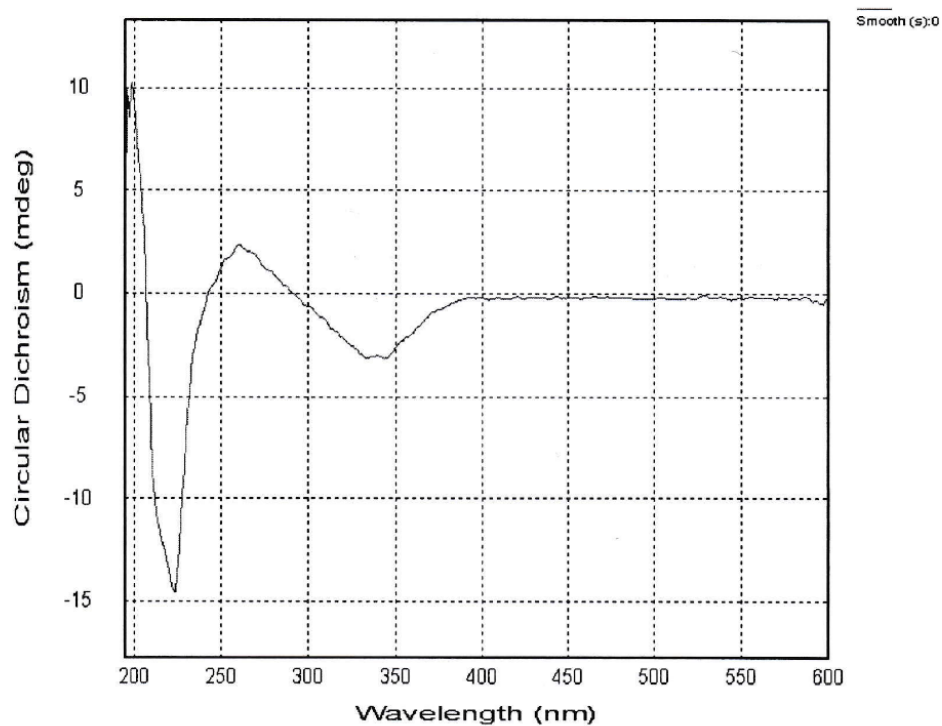


Figure S49. CD spectrum of **5**.

6. NMR, HRESIMS, UV, ORD, and CD spectra of compound 6

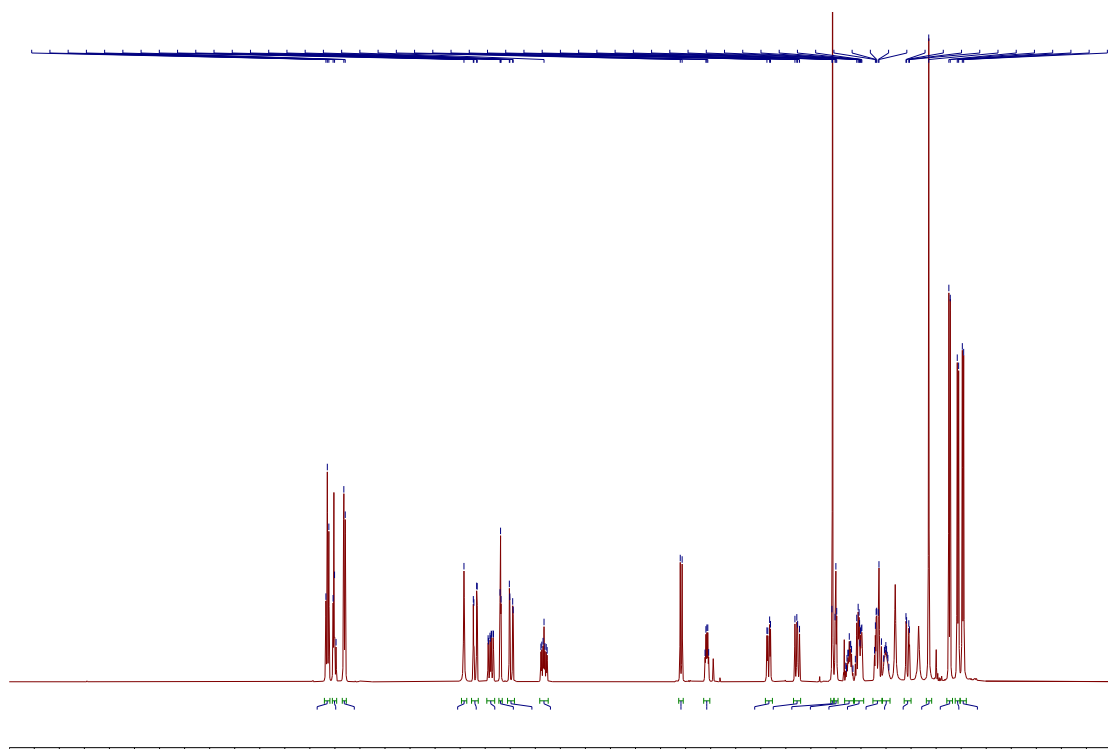


Figure S50. ^1H NMR spectrum of **6** (500 MHz, CDCl_3).

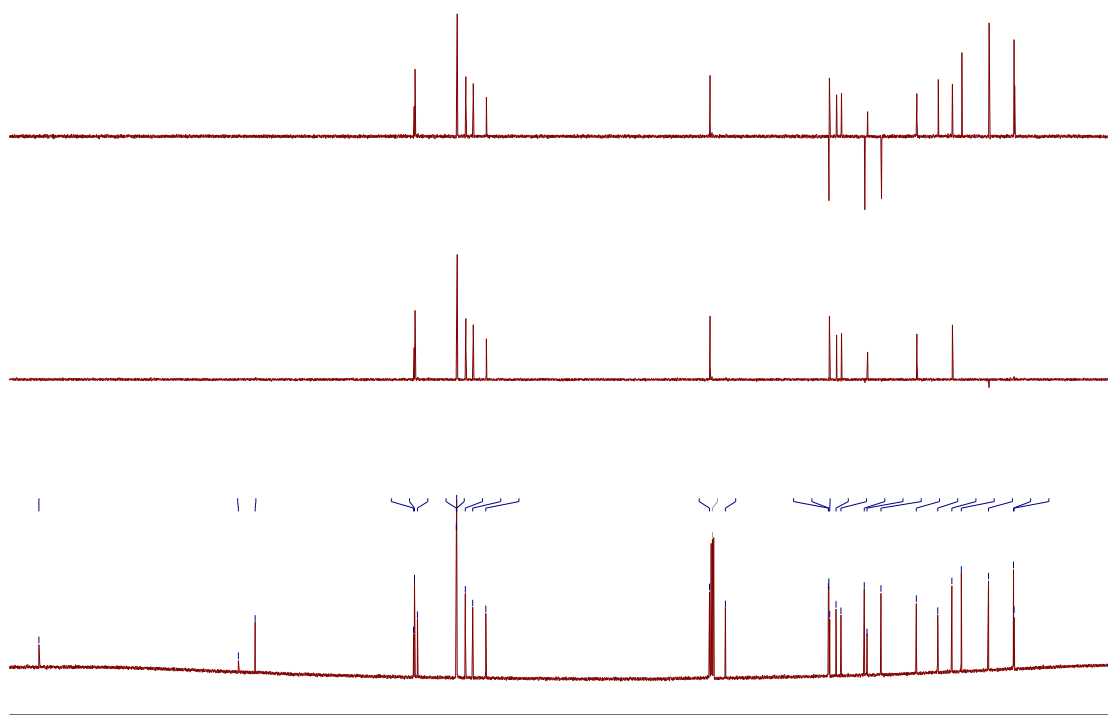


Figure S51. ^{13}C NMR, DEPT-90 and DEPT-135 spectra of **6** (125 MHz, CDCl_3).

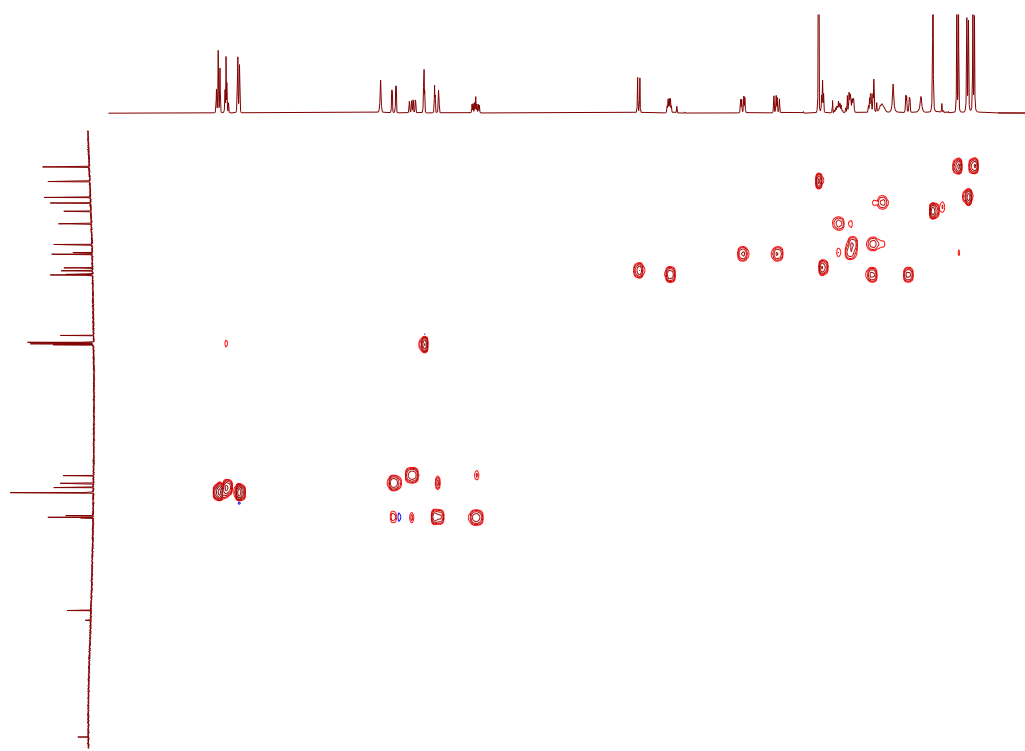


Figure S52. HSQC spectrum of **6** (500 MHz, CDCl₃).

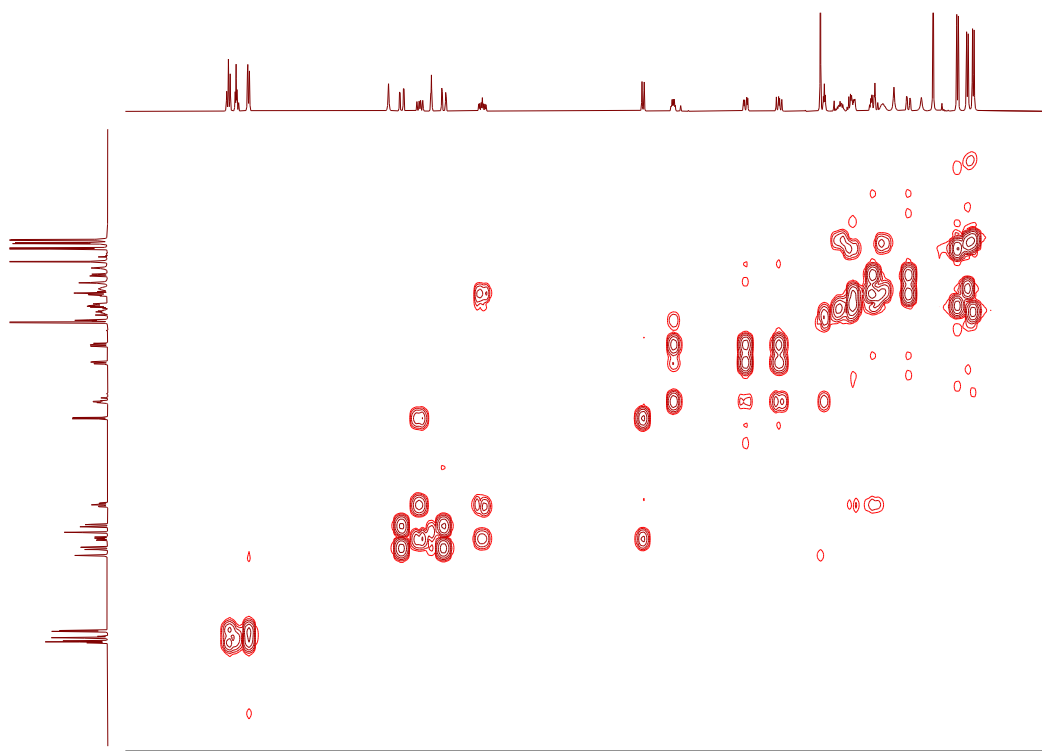


Figure S53. ¹H-¹H COSY spectrum of **6** (500 MHz, CDCl₃).

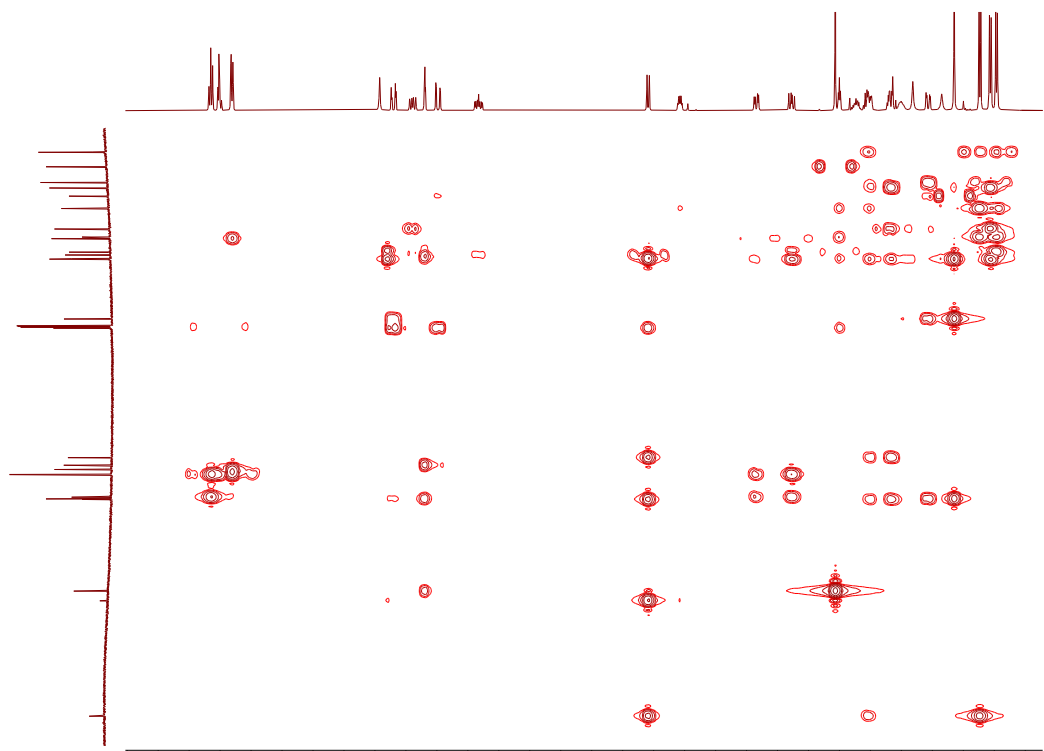


Figure S54. HMBC spectrum of **6** (500 MHz, CDCl₃).

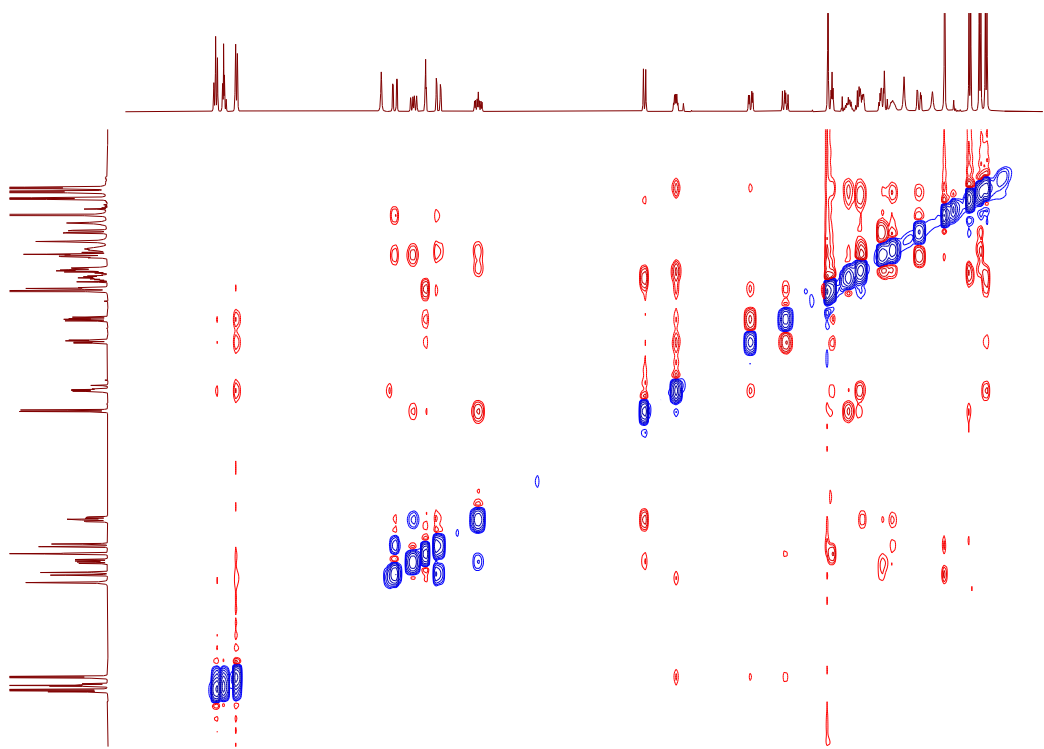


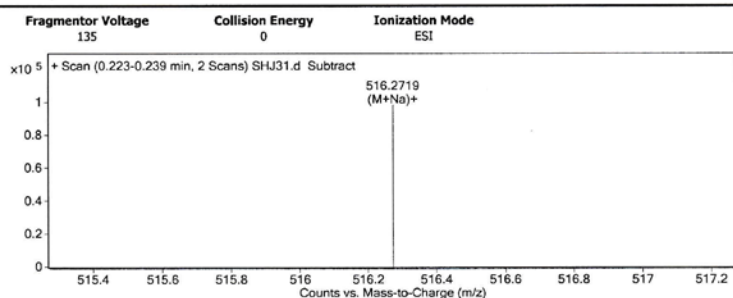
Figure S55. ROESY spectrum of **6** (500 MHz, CDCl₃).

Qualitative Analysis Report

Data Filename	SHJ31.d	Sample Name	SHJ31
Sample Type	Sample	Position	P1-A2
Instrument Name	Instrument 1	User Name	
Acq Method	SIBU.m	Acquired Time	7/16/2015 3:14:52 PM
IRM Calibration Status	Success	DA Method	Default.m
Comment			

Sample Group		Info.	
Acquisition SW	6200 series TOF/6500 series		
Version	Q-TOF B.05.01 (B5125.2)		

User Spectra



Peak List

m/z	z	Abund	Formula	Ion
494.2902	1	34874.45		
516.2719	1	98321.98	C30 H39 N O5	(M+Na)+
532.245	1	40913.93		
987.5729	1	45465.29		
1009.5546	1	49088.25		
1025.5275	1	37422.34		
1502.8366	1	59278.76		
1503.8395	1	61104.78		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	10
N	0	5

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C30 H39 N O5	493.2828	516.2720	516.2719	0.3	0.5	12.0000

--- End Of Report ---

Figure S56. HRESIMS spectrum of **6**.

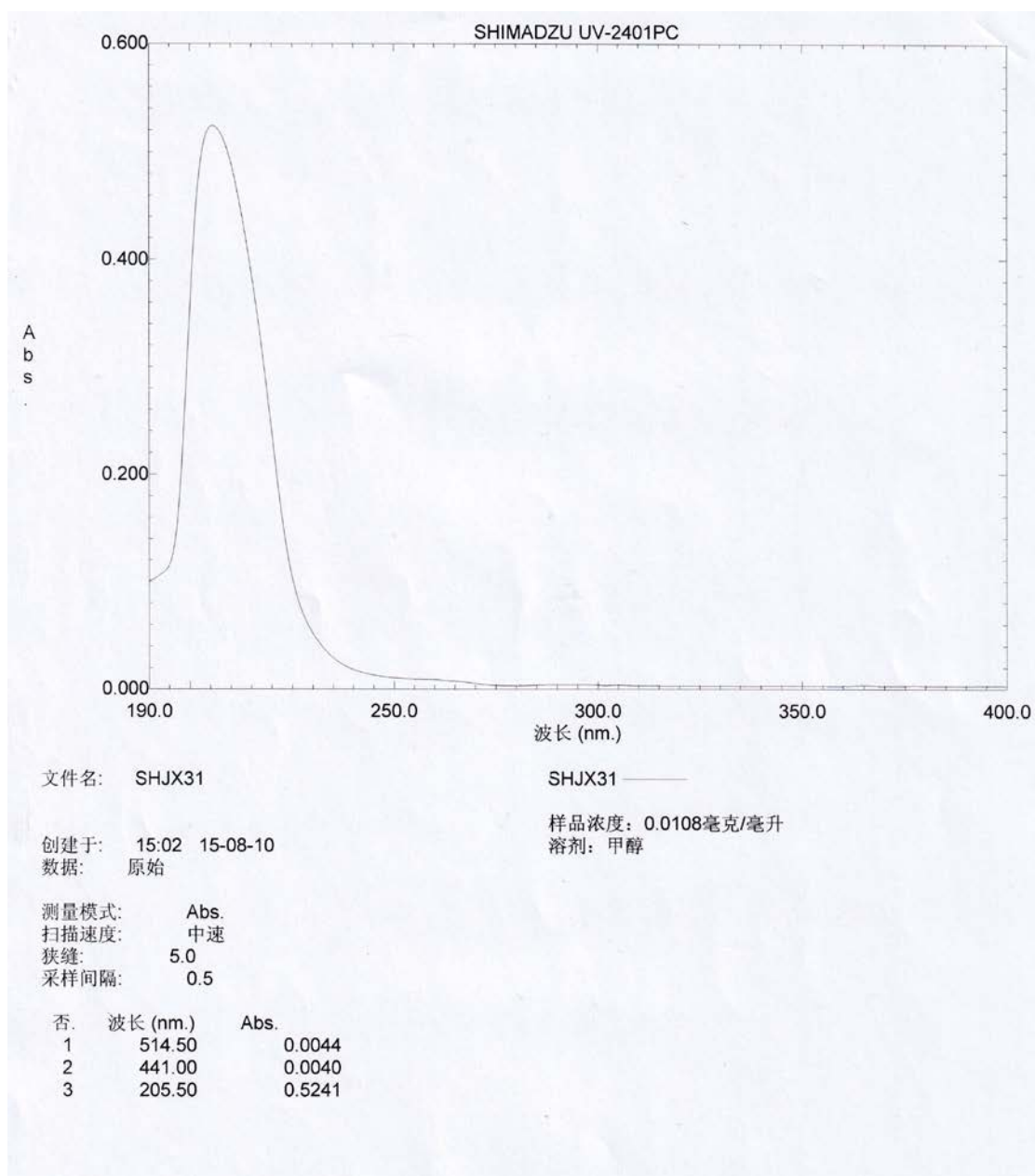


Figure S57. UV spectrum of **6**.

Optical rotation measurement

Model : P-1020 (A060460638)

No.	Sample	Mode	Data	Monitor Blank	Temp. Cell Temp Point	Date Comment Sample Name	Light Filter Operator	Cycle Time Integ Time
No.1	14 (1/3)	Sp.Rot	-64.2490	-0.0620 0.0000	23.6 50.00 Cell	Thu Aug 06 17:42:47 2015 0.00193g/mL MeOH SHJX31	Na 589nm	2 sec 10 sec
No.2	14 (2/3)	Sp.Rot	-63.1090	-0.0609 0.0000	23.6 50.00 Cell	Thu Aug 06 17:43:00 2015 0.00193g/mL MeOH SHJX31	Na 589nm	2 sec 10 sec
No.3	14 (3/3)	Sp.Rot	-62.1760	-0.0600 0.0000	23.6 50.00 Cell	Thu Aug 06 17:43:14 2015 0.00193g/mL MeOH SHJX31	Na 589nm	2 sec 10 sec

Figure S58. ORD spectrum of **6**.

SHJX31

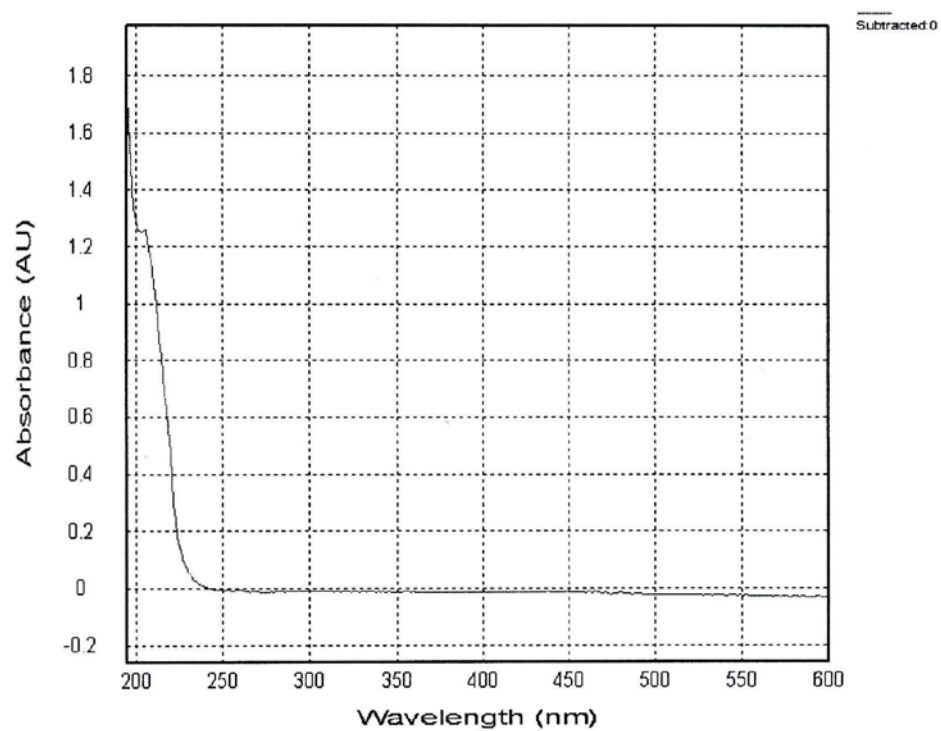
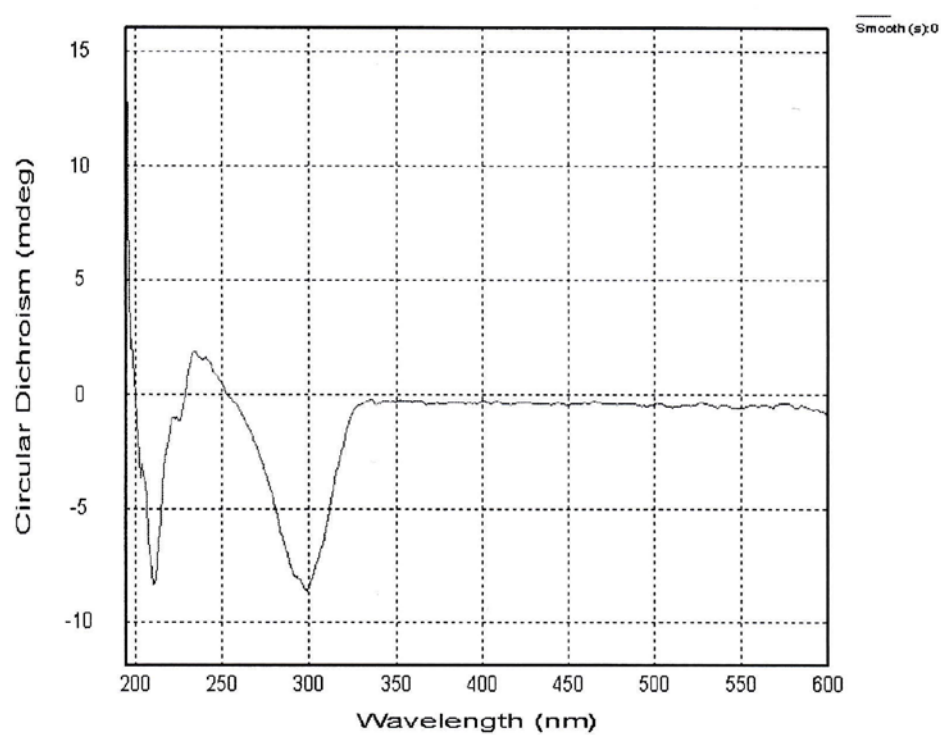


Figure S59. CD spectrum of **6**.

7. NMR, HRESIMS, UV, ORD, and CD spectra of compound 7

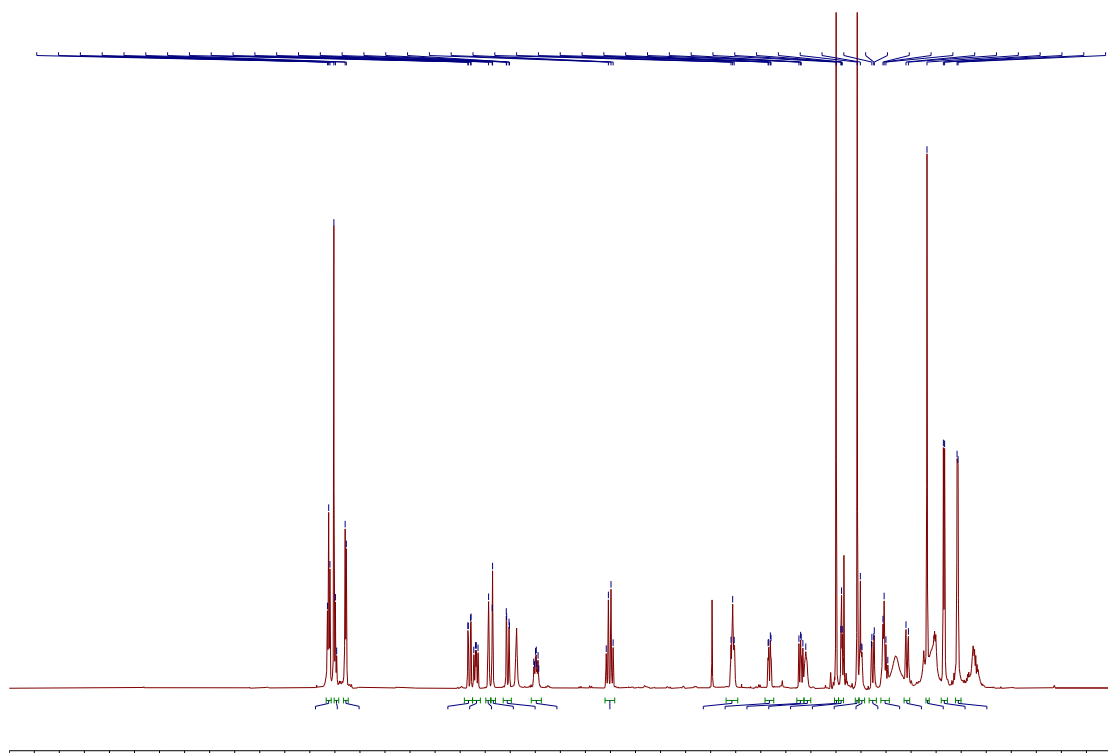


Figure S60. ^1H NMR spectrum of 7 (600 MHz, CDCl_3).

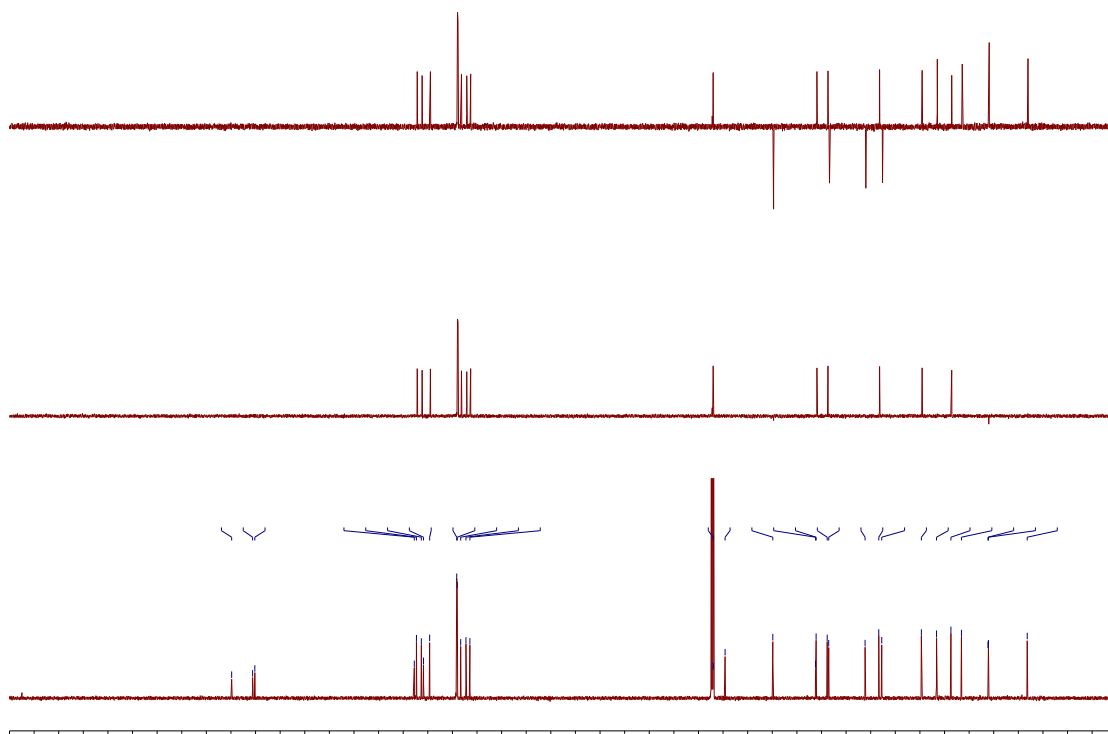


Figure S61. ^{13}C NMR, DEPT-90 and DEPT-135 spectra of **7** (150 MHz, CDCl_3).

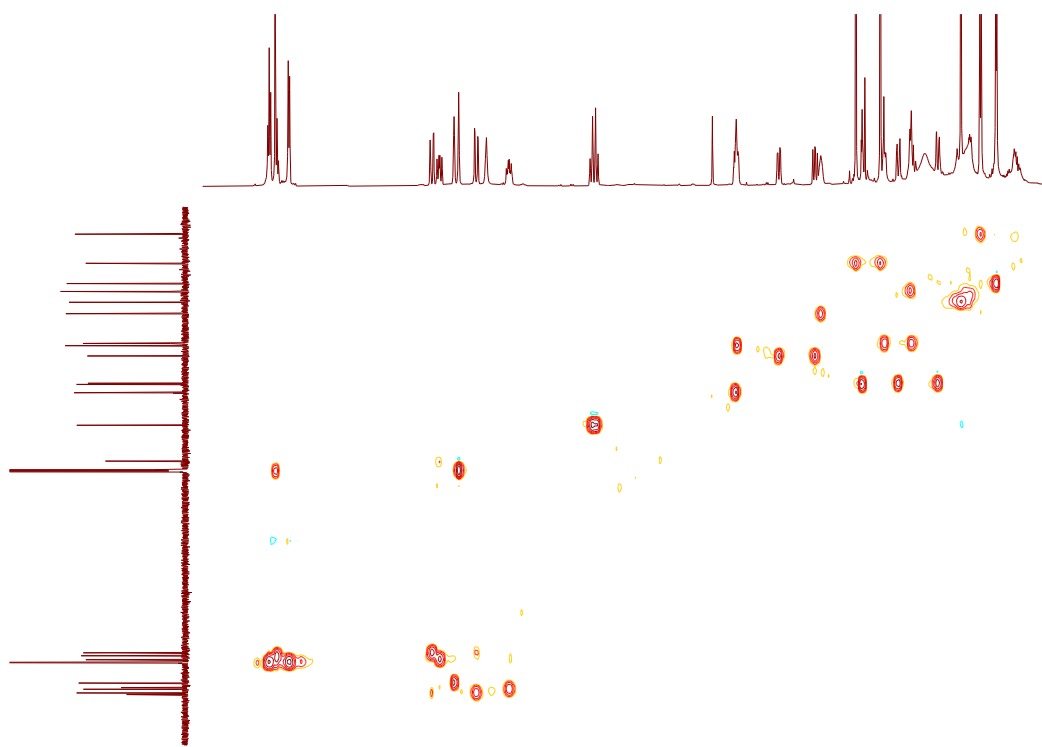


Figure S62. HSQC spectrum of **7** (600 MHz, CDCl_3).

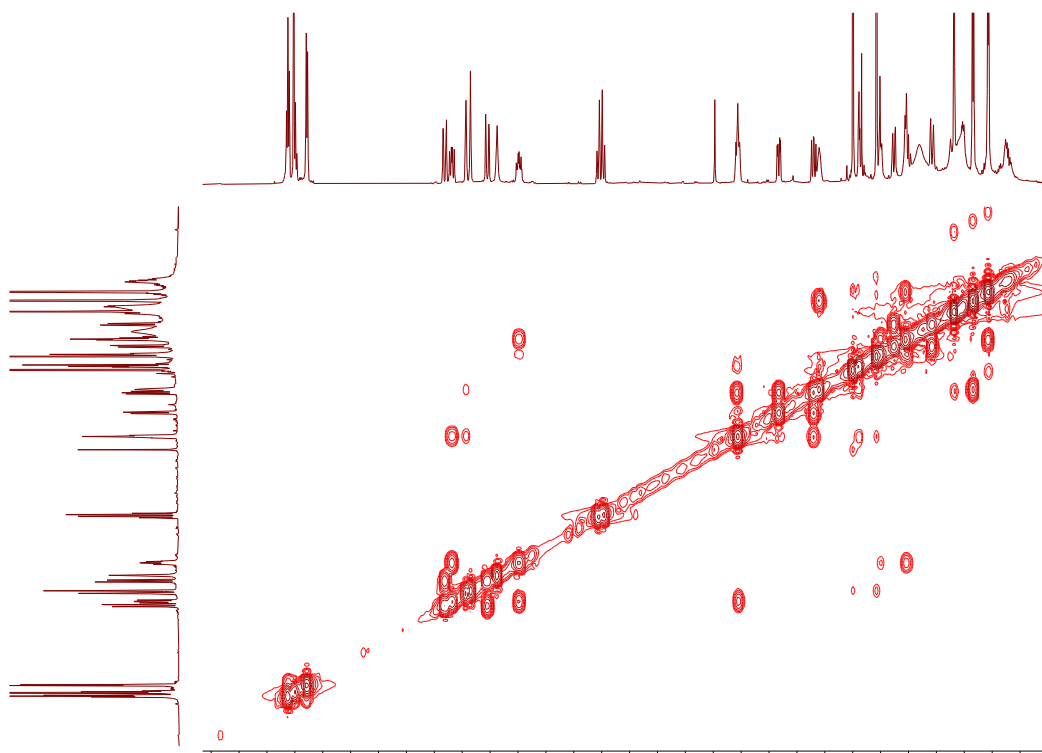


Figure S63. ^1H - ^1H COSY spectrum of **7** (600 MHz, CDCl_3).

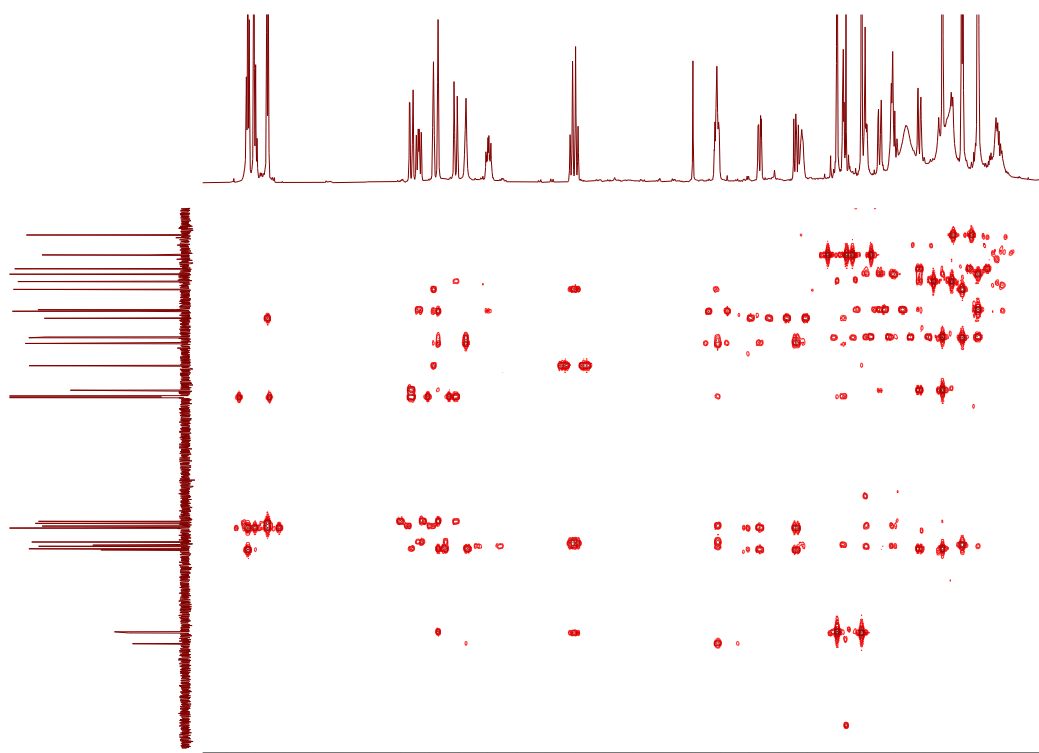


Figure S64. HMBC spectrum of **7** (600 MHz, CDCl_3).

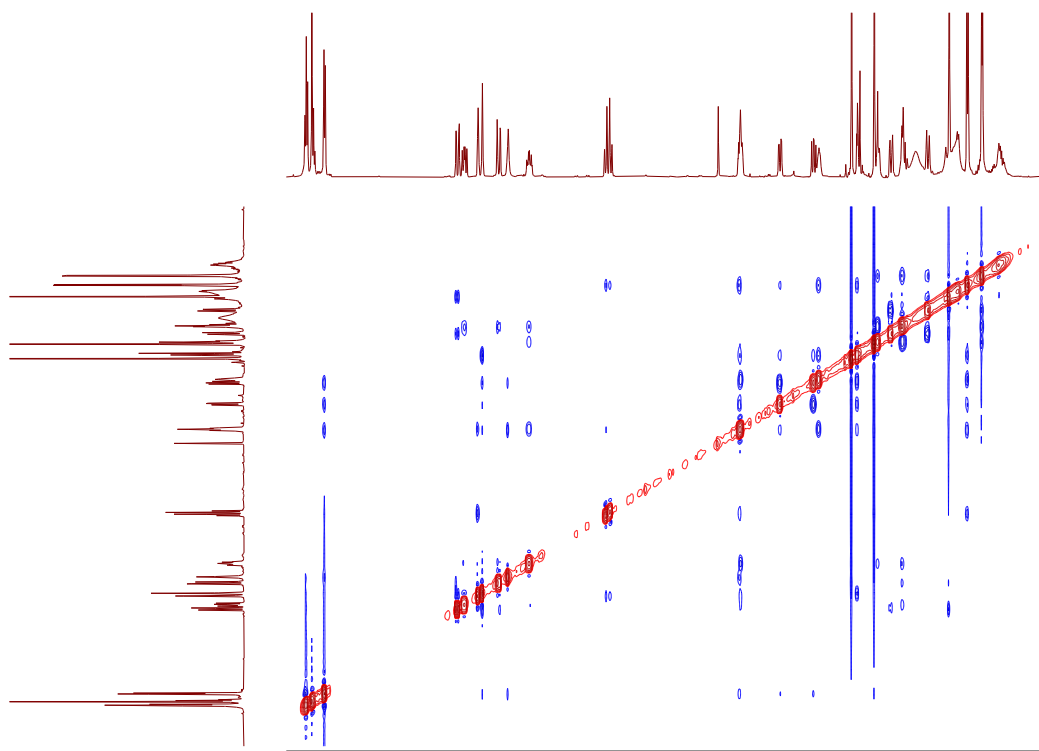


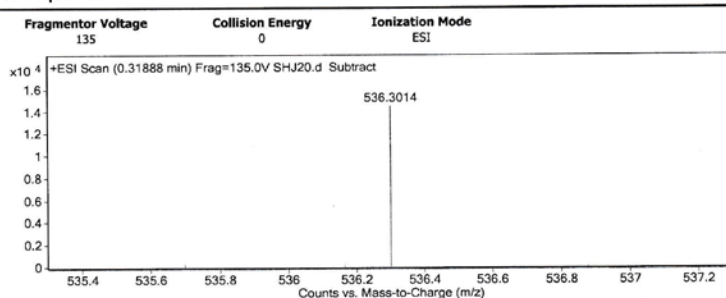
Figure S65. ROESY spectrum of **7** (600 MHz, CDCl_3).

Qualitative Analysis Report

Data Filename	SHJ20.d	Sample Name	SHJ20
Sample Type	Sample	Position	P1-A1
Instrument Name	Instrument 1	User Name	
Acq Method	SIBU.m	Acquired Time	12/30/2014 1:43:33 PM
IRM Calibration Status	Success	DA Method	Default.m
Comment			

Sample Group	Info.
Acquisition SW	6200 series TOF/6500 series
Version	Q-TOF B.05.01 (B5125.2)

User Spectra



Peak List

m/z	z	Abund	Formula	Ion
416.2584	1	18167.43		
476.2792	1	37347.07		
536.3014	1	14513.92	C32 H41 N O6	(M+H)+
558.2831	1	73034.31		
559.2863	1	29266.66		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	10
N	0	3

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C32 H41 N O6	535.2934	536.3007	536.3014	-0.4	-0.8	13.0000

--- End Of Report ---

Figure S66. HRESIMS spectrum of 7.

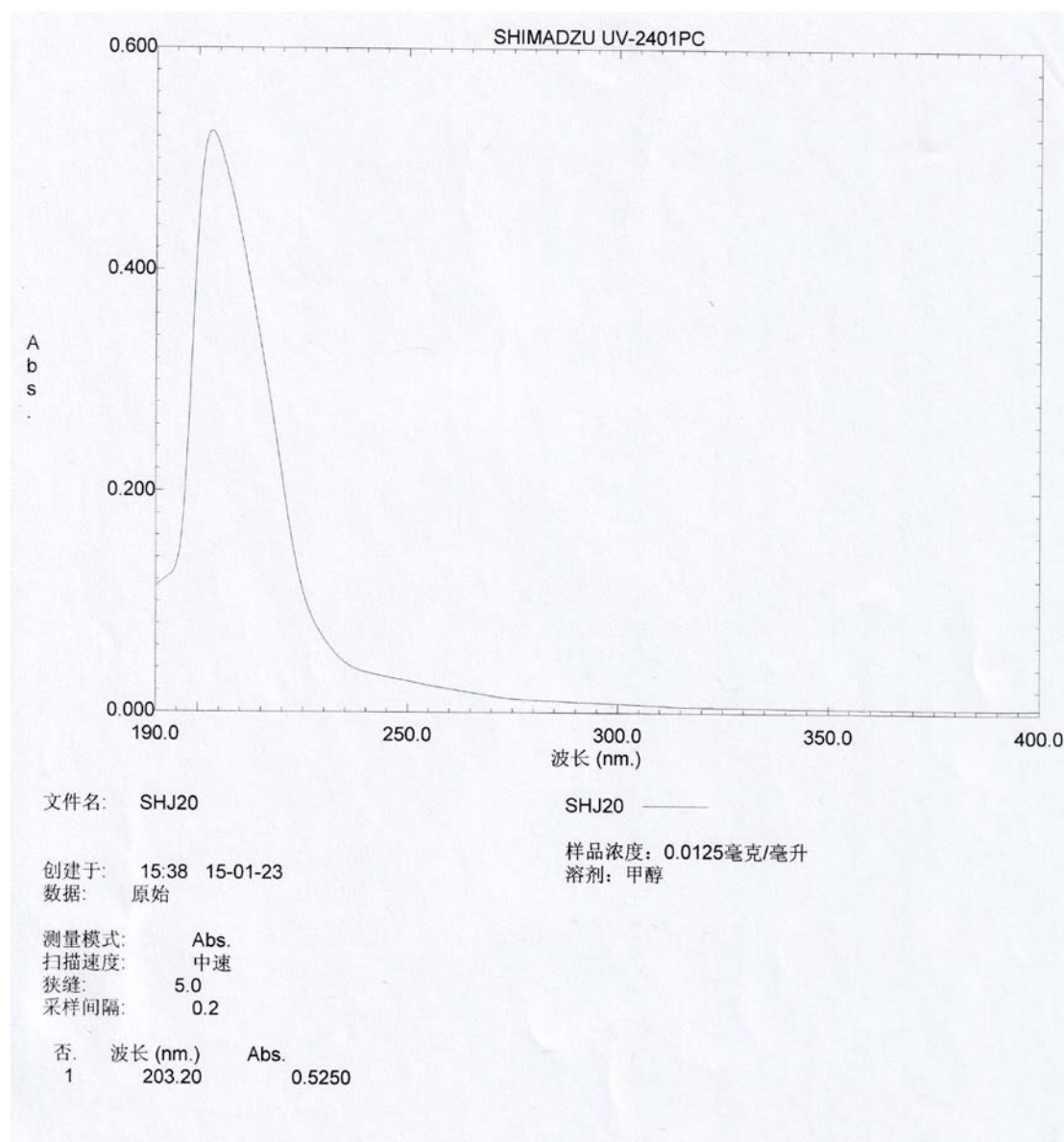


Figure S67. UV spectrum of **7**.

Optical rotation measurement

Model : P-1020 (A060460638)

No.	Sample	Mode	Data	Monitor Blank	Temp. Cell Temp Point	Date Comment Sample Name	Light Filter Operator	Cycle Time Integ Time
No.1	21 (1/3)	Sp.Rot	-28.5870	-0.0263 0.0000	19.6 50.00 Cell	Thu Jan 22 18:33:53 2015 0.00184g/mL MeOH SHJ20	Na 589nm	2 sec 10 sec
No.2	21 (2/3)	Sp.Rot	-29.4570	-0.0271 0.0000	19.6 50.00 Cell	Thu Jan 22 18:34:06 2015 0.00184g/mL MeOH SHJ20	Na 589nm	2 sec 10 sec
No.3	21 (3/3)	Sp.Rot	-27.1740	-0.0250 0.0000	19.6 50.00 Cell	Thu Jan 22 18:34:20 2015 0.00184g/mL MeOH SHJ20	Na 589nm	2 sec 10 sec

-28.4058°

Figure S68. ORD spectrum of **7**.

SHJ20

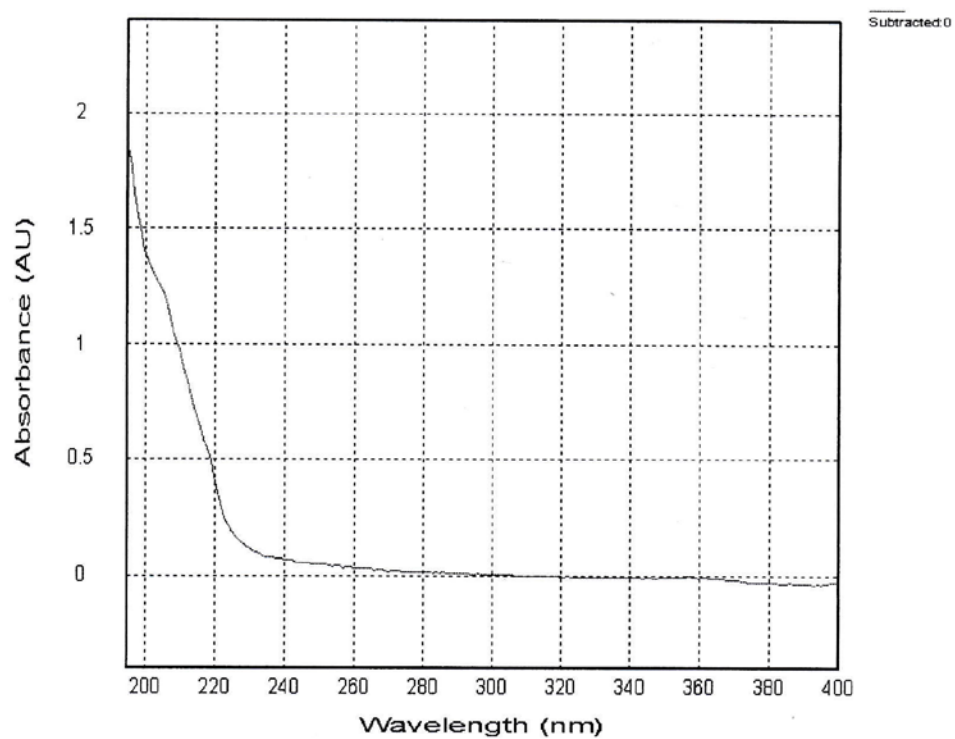
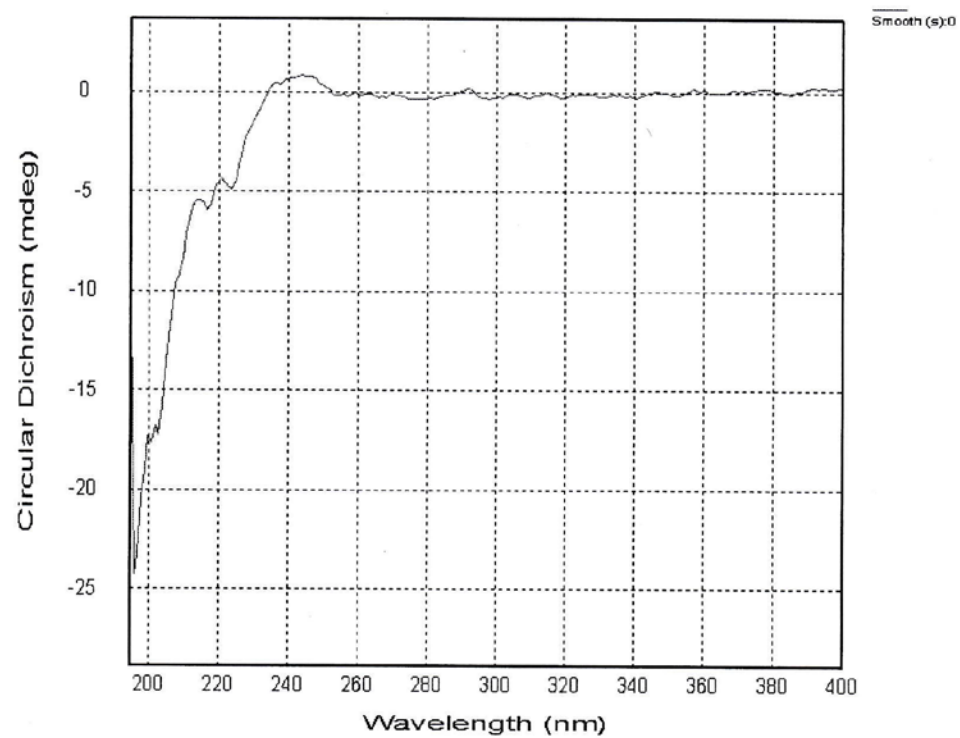


Figure S69. CD spectrum of **7**.