

Supplementary Materials

Figure S1. $^1\text{H-NMR}$ spectrum of compound **1**.

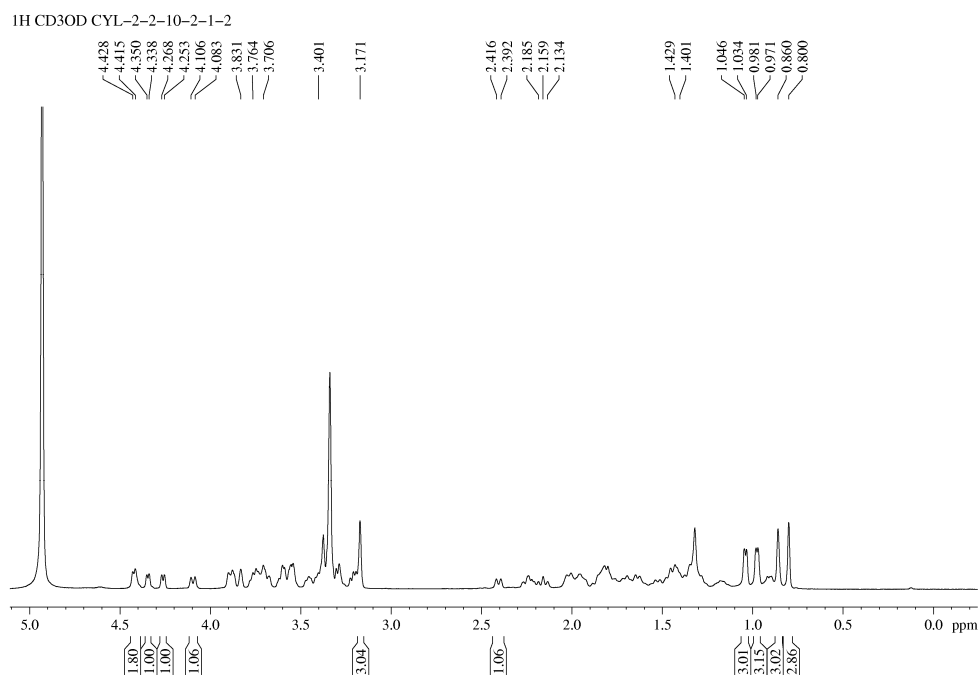


Figure S2. $^{13}\text{C-NMR}$ spectrum of compound **1**.

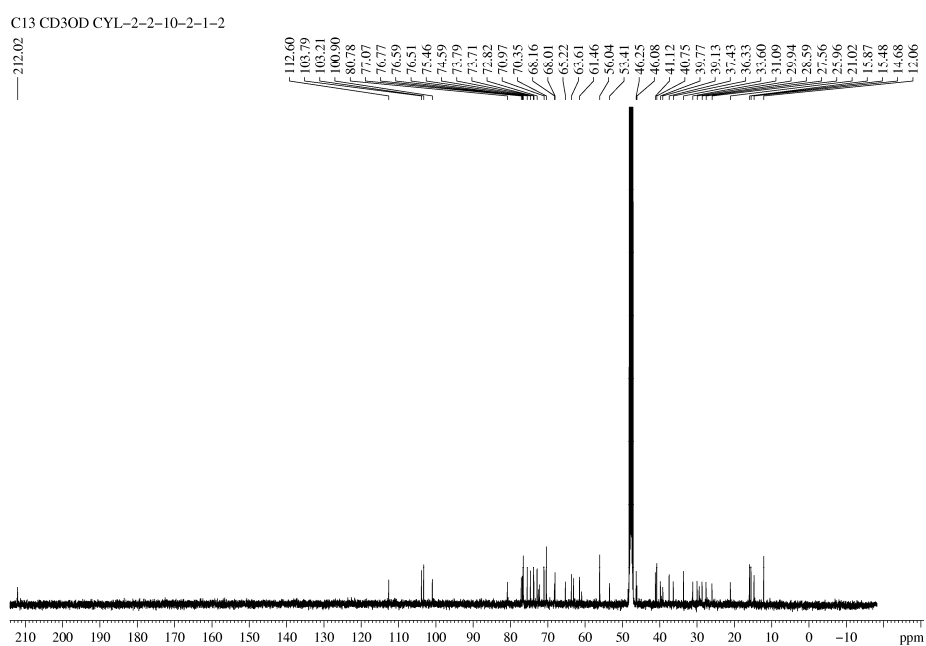


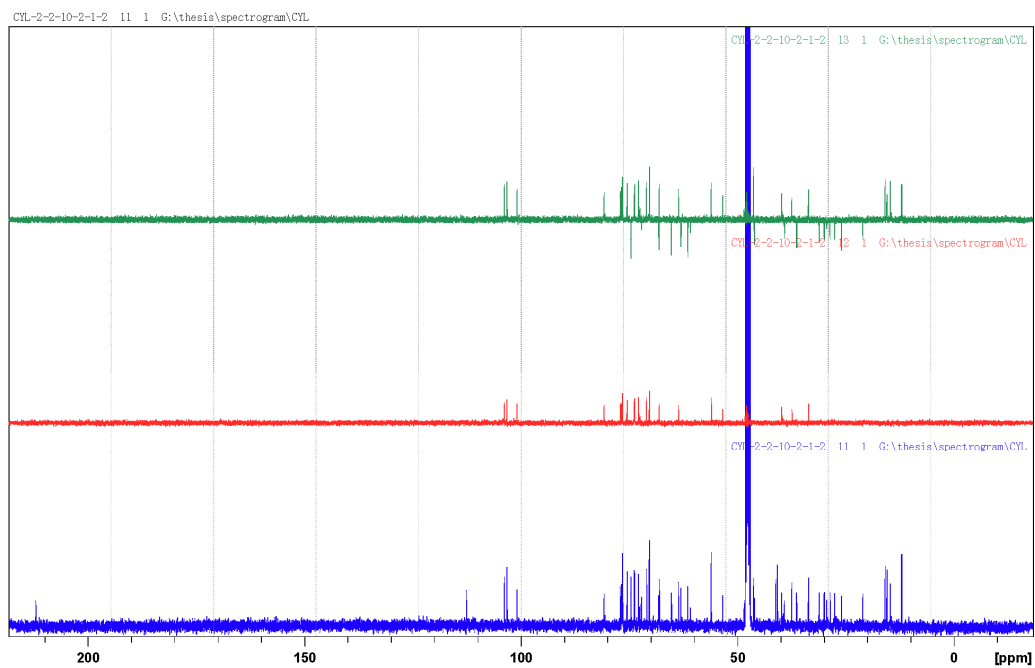
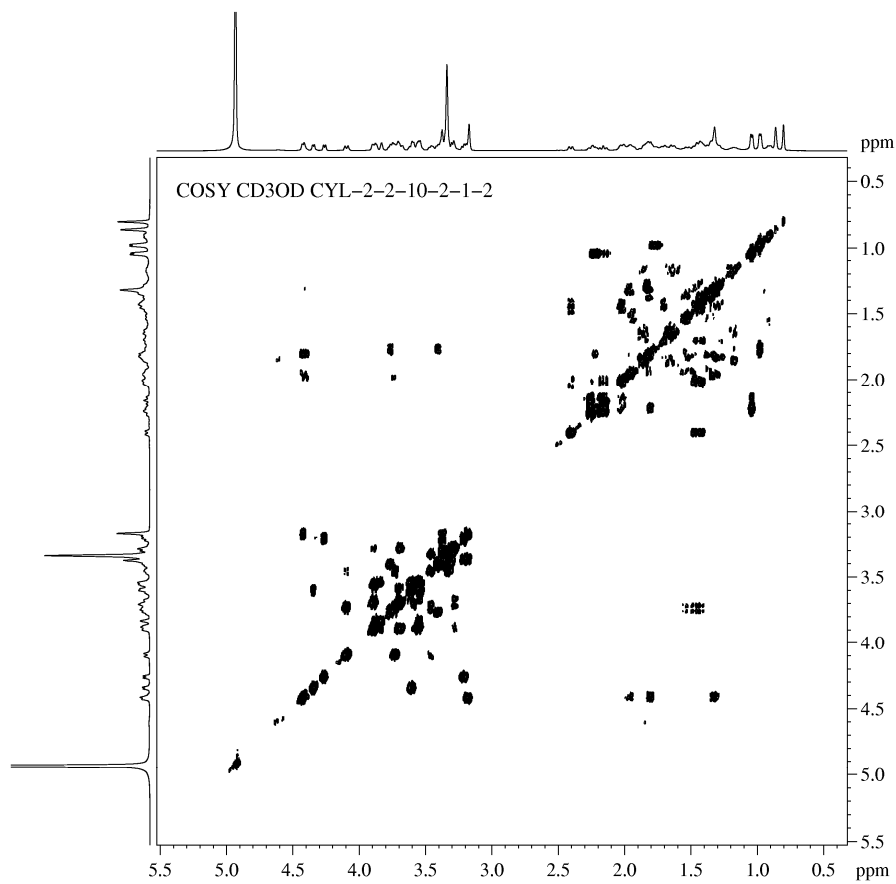
Figure S3. DEPT spectrum of compound 1.**Figure S4.** COSY spectrum of compound 1.

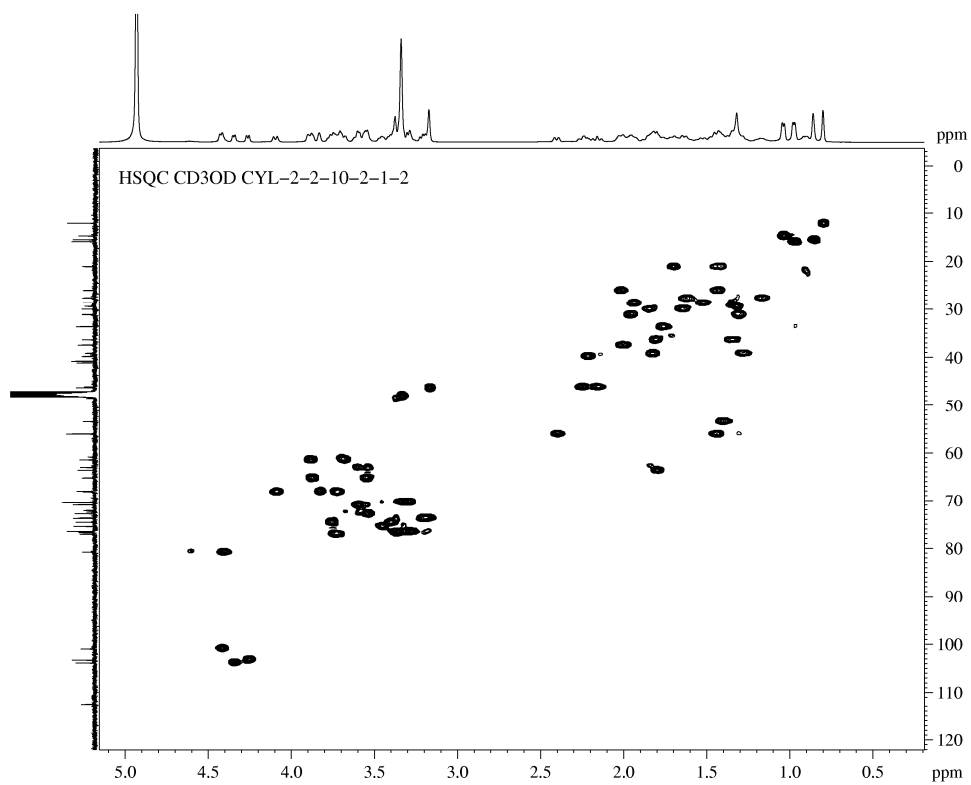
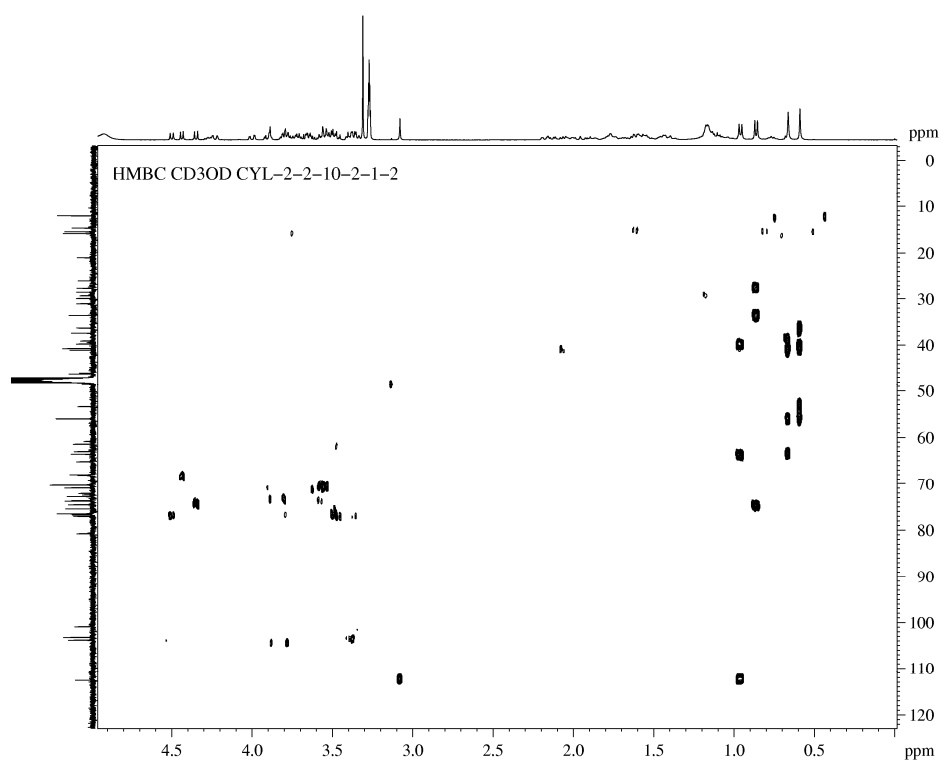
Figure S5. HSQC spectrum of compound **1**.**Figure S6.** HMBC spectrum of compound **1**.

Figure S7. NOESY spectrum of compound 1.

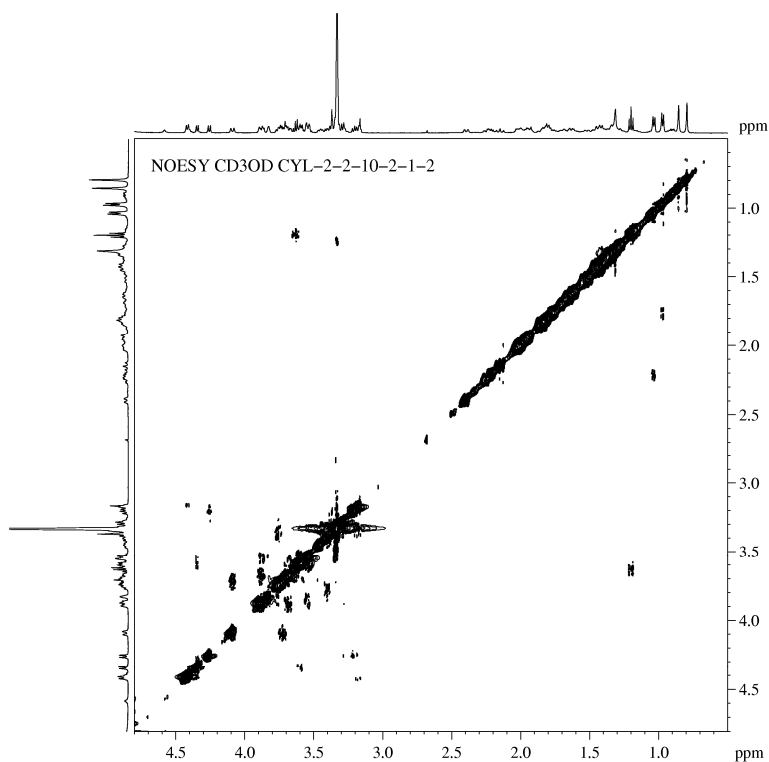
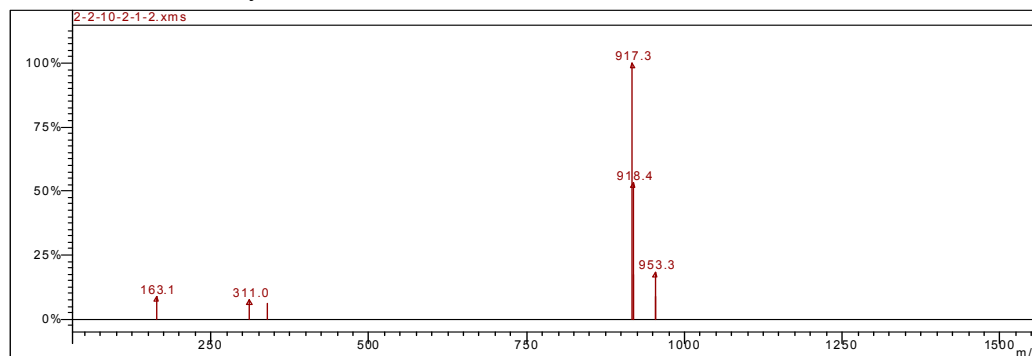


Figure S8. ESI-MS spectrum of compound 1.

Scan 186 from e:\szj\2-2-10-2-1-2\2-2-10-2-1-2.xml



Spectrum from e:\szj\2-2-10-2-1-2\2-2-10-2-1-2.xml
 Scan No: 186, Time: 3.347 minutes
 3 points averaged. Background corrected.
 Comment: 3.347 min. Scans: 183-187 100.0:1500.0>(-) RIC: 1.135e+8
 Pair Count: 8 MW: 0 Formula: None
 CAS No: None Acquired Range: 100.0 - 1500.0 m/z

Method Description: ESI

Scan 1 Channel Description: 100.0:1500.0> ESI;CID 175.0;Det 1100;W1Q1

Scan 2 Channel Description: 100.0:1500.0>(-) ESI;CID -165.0;Det 1100;W

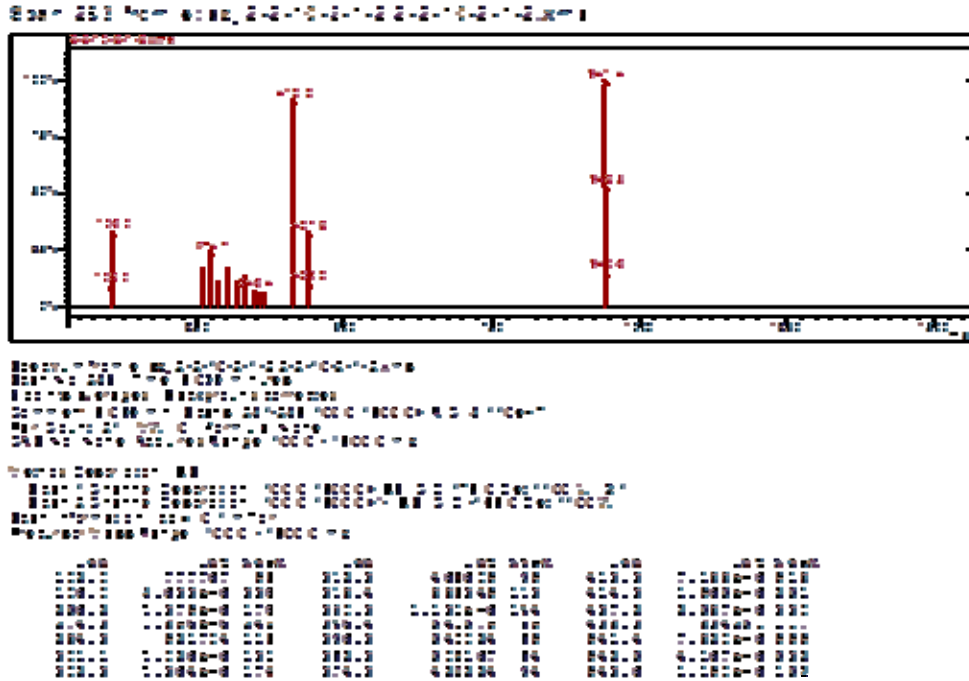
Scan Information: cp = 0.1 mTorr

Precursor Mass Range: 100.0 - 1500.0 m/z

Ion	Int	Norm	Ion	Int	Norm	Ion	Int	Norm
163.1	1.317e+6	90	917.3	1.460e+7	999	953.3	2.695e+6	184
311.0	1.118e+6	77	918.4	7.761e+6	531	954.6	1.265e+6	87
339.3	904857	62	919.5	2.523e+6	173			

(-) ESI

Figure S8. Cont.



(+) ESI

Figure S9. HR-ESI-MS spectrum of compound 1.

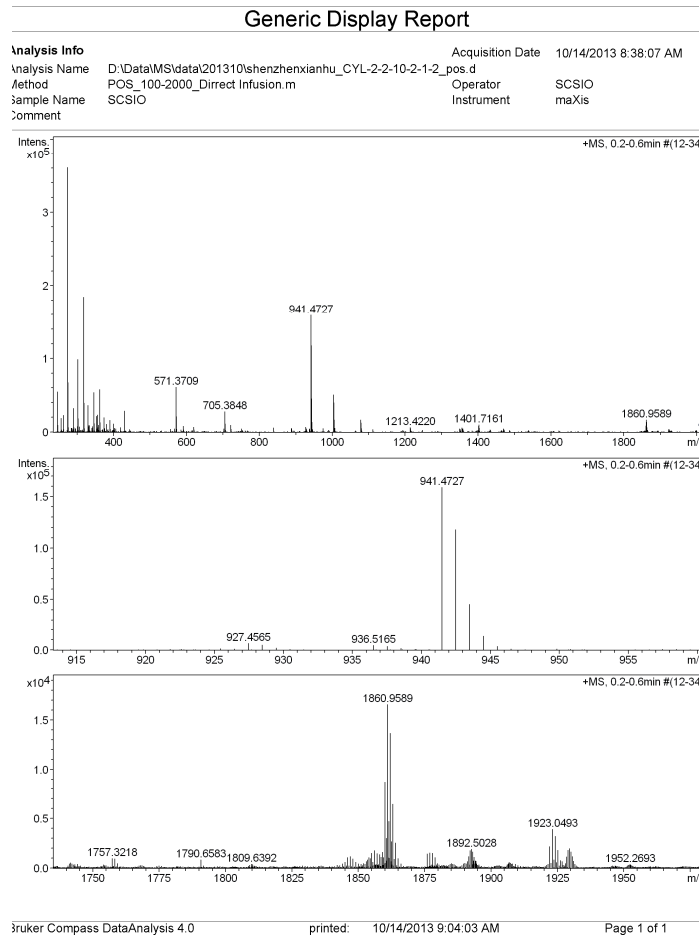


Figure S9. Cont.

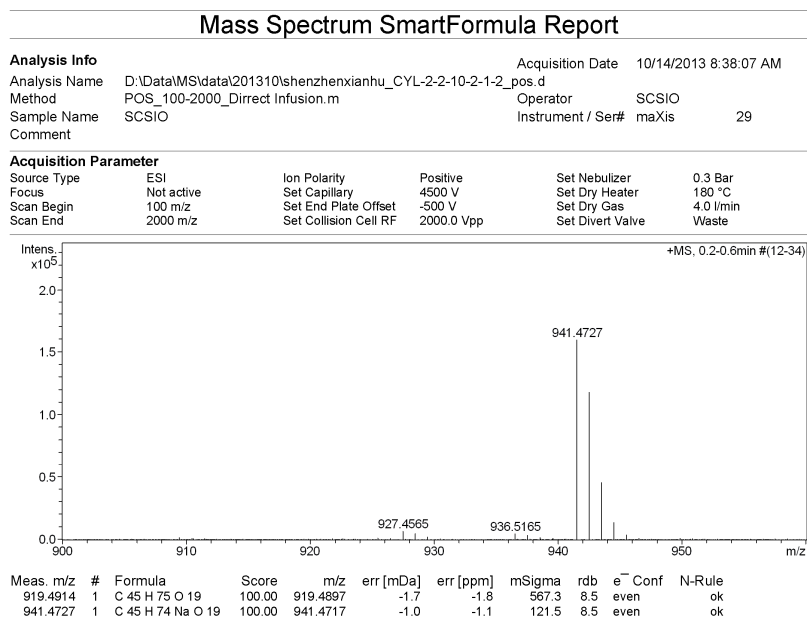


Figure S10. IR spectrum of compound 1.

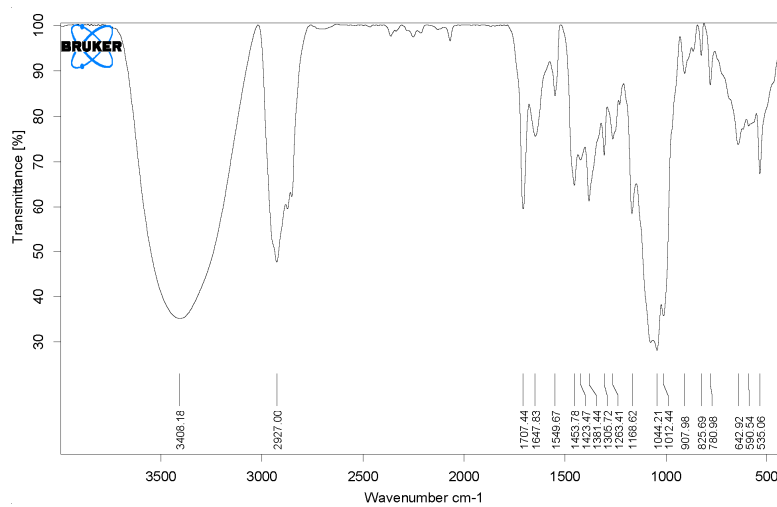


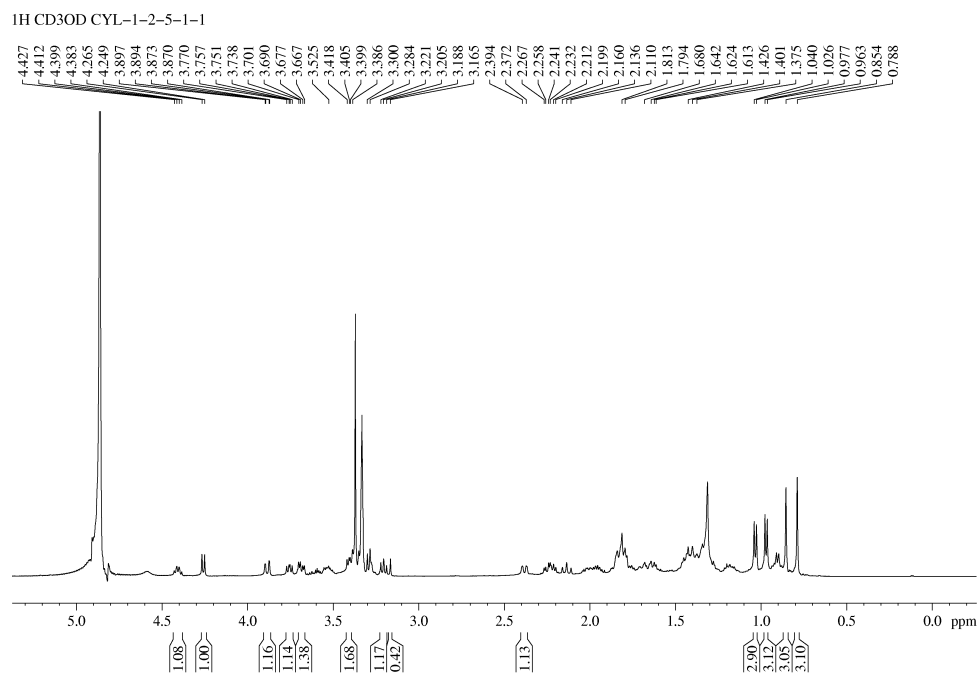
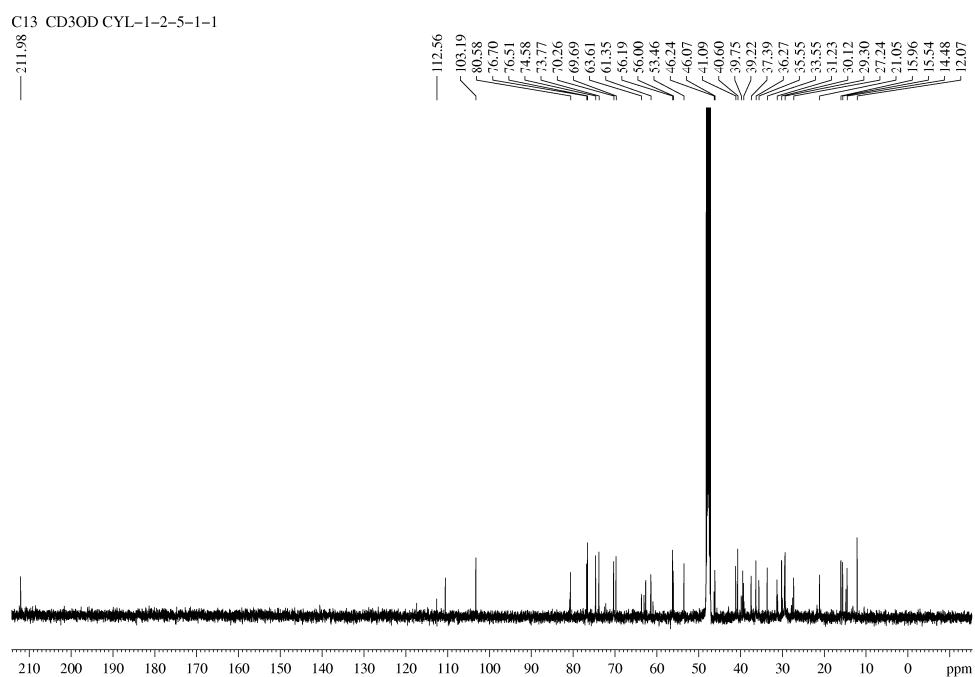
Figure S11. $^1\text{H-NMR}$ spectrum of compound 2.Figure S12. $^{13}\text{C-NMR}$ spectrum of compound 2.

Figure S13. DEPT spectrum of compound 2.

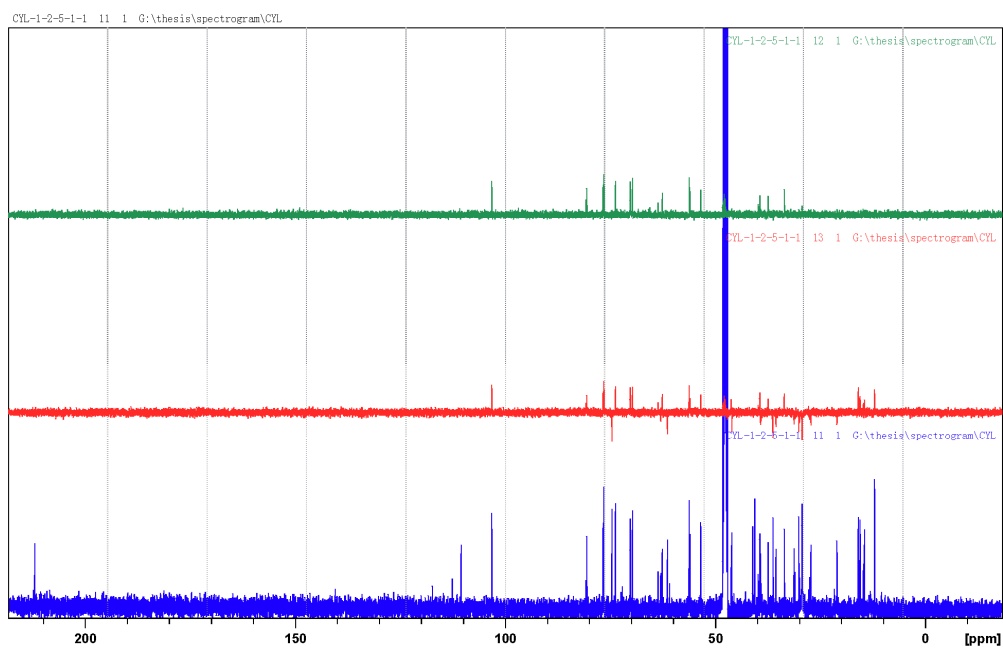


Figure S14. COSY spectrum of compound 2.

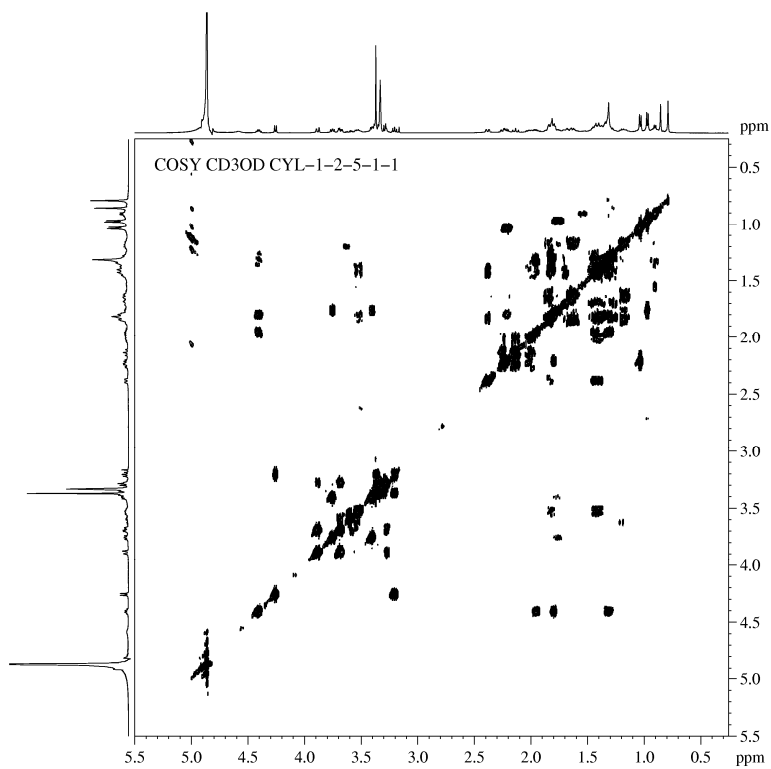


Figure S15. HSQC spectrum of compound 2.

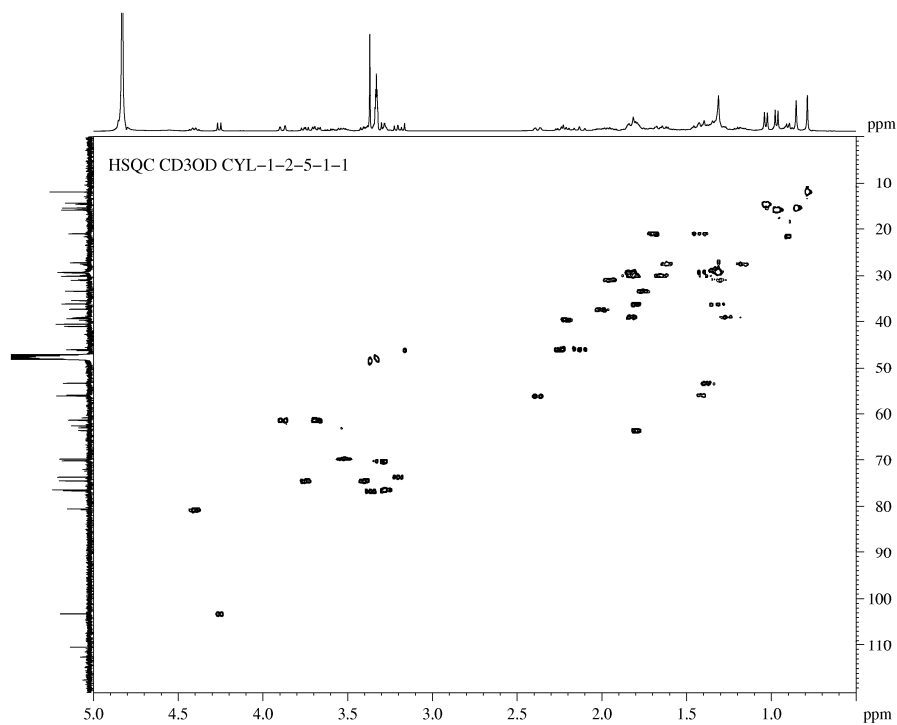


Figure S16. HMBC spectrum of compound 2.

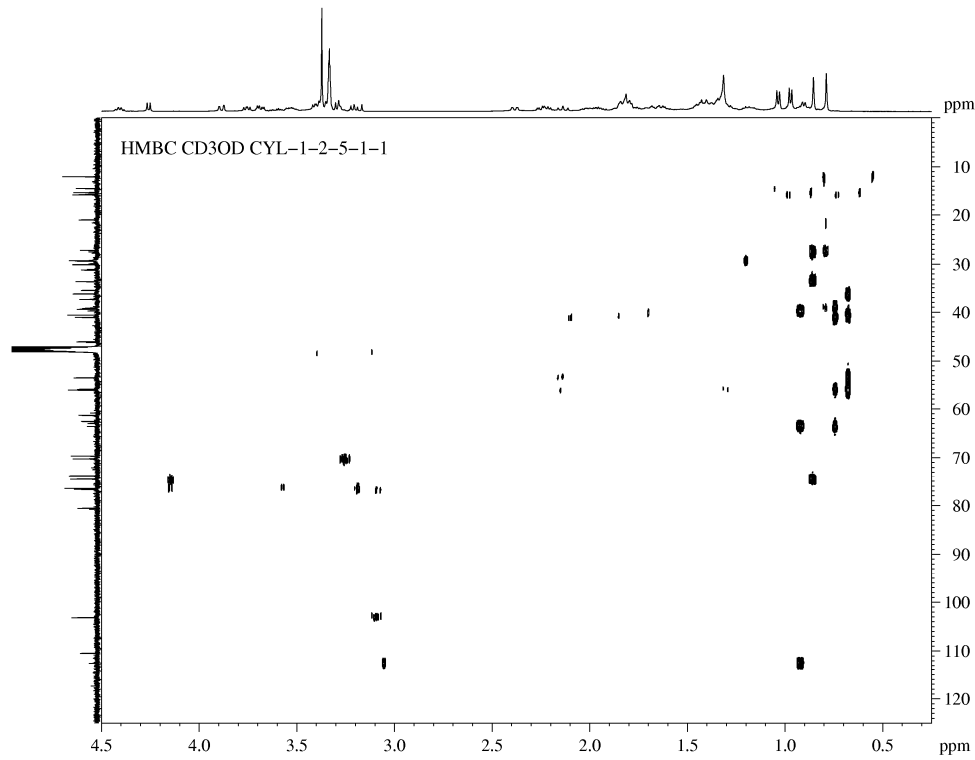


Figure S17. NOESY spectrum of compound 2.

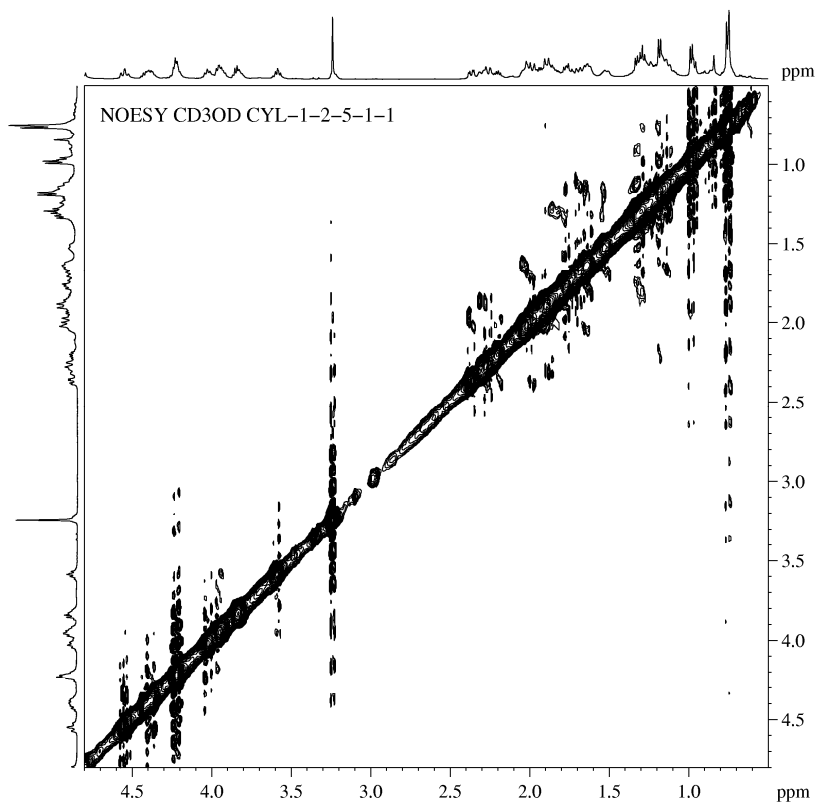
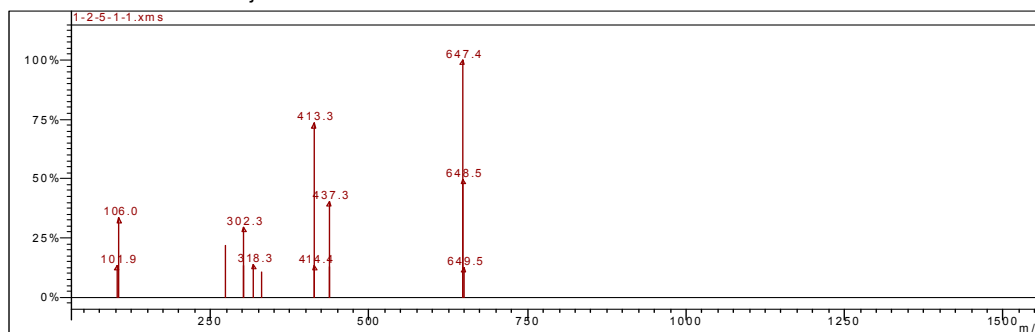


Figure S18. ESI-MS spectrum of compound 2.

Scan 267 from e:\szj\1-2-5-1-1\1-2-5-1-1.xms



Spectrum from e:\szj\1-2-5-1-1\1-2-5-1-1.xms
 Scan No: 267, Time: 4.808 minutes
 3 points averaged. Background corrected.
 Comment: 4.808 min. Scans: 265-269 100.0:1500.0> RIC: 1.411e+8
 Pair Count: 14 MW: 0 Formula: None
 CAS No: None Acquired Range: 100.0 - 1500.0 m/z

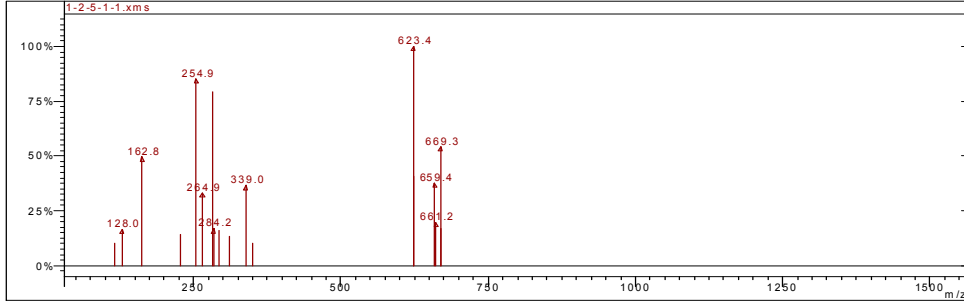
Method Description: ESI
 Scan 1 Channel Description: 100.0:1500.0> ESI;CID 175.0;Det 1150;W IQ 1
 Scan 2 Channel Description: 100.0:1500.0>(-) ESI;CID -140.0;Det 1150;W
 Scan Information: cp = 0.1 mTorr
 Precursor Mass Range: 100.0 - 1500.0 m/z

Ion	Int	Norm	Ion	Int	Norm	Ion	Int	Norm
101.9	1.514e+6	133	318.3	1.580e+6	139	438.4	1.450e+6	127
106.0	3.794e+6	333	330.4	1.191e+6	105	647.4	1.138e+7	999
274.3	2.498e+6	219	413.3	8.340e+6	732	648.5	5.645e+6	496
301.2	1.524e+6	134	414.4	1.506e+6	132	649.5	1.401e+6	123
302.3	3.353e+6	294	437.3	4.605e+6	404			

(+ ESI

Figure S18. Cont.

Scan 146 from e:\szj\1-2-5-1-1\1-2-5-1-1.xms



Spectrum from e:\szj\1-2-5-1-1\1-2-5-1-1.xms
 Scan No: 146, Time: 2.613 minutes
 3 points averaged, Background corrected
 Comment: 2.613 min. Scans: 143-147 100.0:1500.0>(-) RIC: 2.227e+8
 Pair Count: 18 MW: 0 Formula: None
 CAS No: None Acquired Range: 100.0 - 1500.0 m/z

Method Description: ESI
 Scan 1 Channel Description: 100.0:1500.0> ESI;CID 175.0;Det 1150;W IQ 1
 Scan 2 Channel Description: 100.0:1500.0>(-) ESI;CID -140.0;Det 1150;W
 Scan Information: cp = 0.1 mTorr
 Precursor Mass Range: 100.0 - 1500.0 m/z

Ion	Int	Norm	Ion	Int	Norm	Ion	Int	Norm
115.0	1.058e+6	104	283.1	8.052e+6	792	623.4	1.016e+7	999
128.0	1.676e+6	165	284.2	1.703e+6	167	624.4	4.158e+6	409
162.8	5.032e+6	495	292.8	1.648e+6	162	659.4	3.819e+6	375
226.8	1.425e+6	140	311.1	1.348e+6	133	661.2	2.008e+6	197
254.9	8.642e+6	850	339.0	3.706e+6	364	669.3	5.506e+6	541
264.9	3.382e+6	333	351.2	1.024e+6	101	670.4	1.711e+6	168

(-) ESI

Figure S19. HR-ESI-MS spectrum of compound 2.

Generic Display Report

Analysis Info
 Analysis Name: D:\Data\MS\data\201310\shenzhenxianhu_CYL-1-2-5-1-1_pos.d
 Method: POS_100-2000_Direct Infusion.m
 Sample Name: SCSIO
 Comment:
 Acquisition Date: 10/14/2013 8:31:04 AM
 Operator: SCSIO
 Instrument: maXis

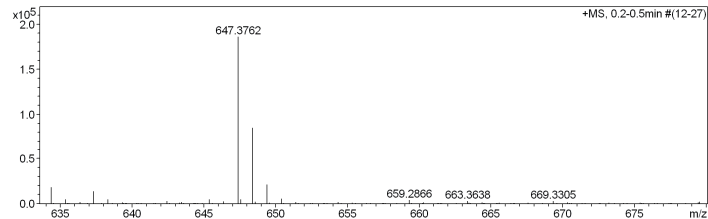
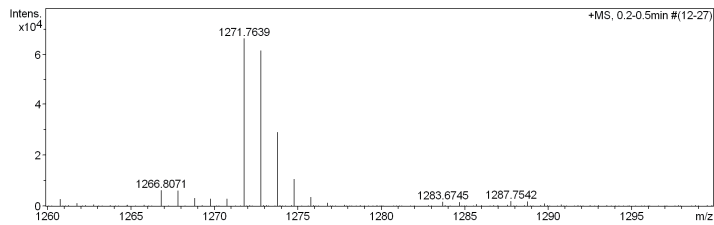
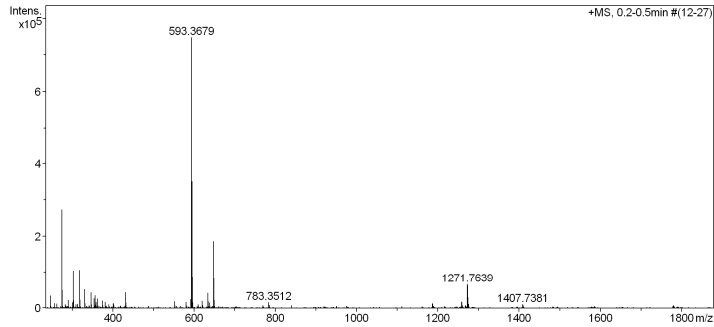
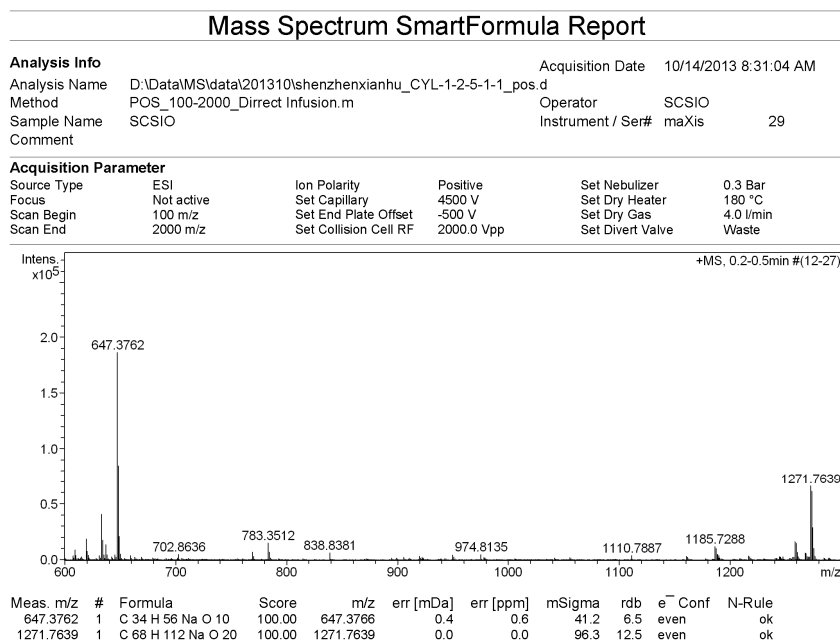


Figure S19. Cont.

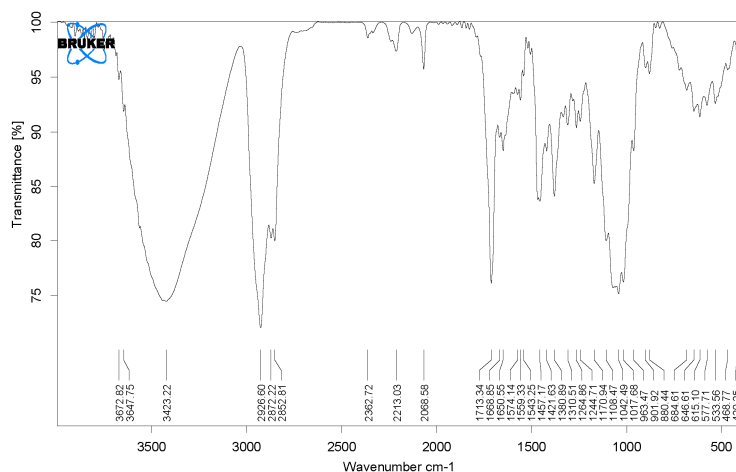


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Figure S20. IR spectrum of compound 2.



E:\DATABASE\MEAS\ 112511.0 12511 Instrument type and / or accessory

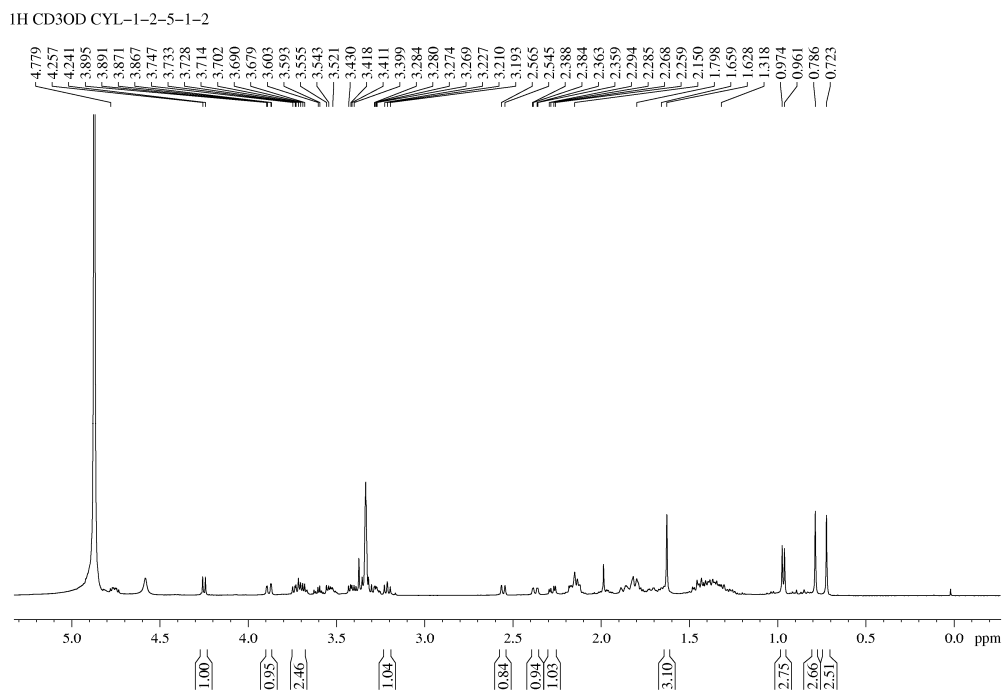
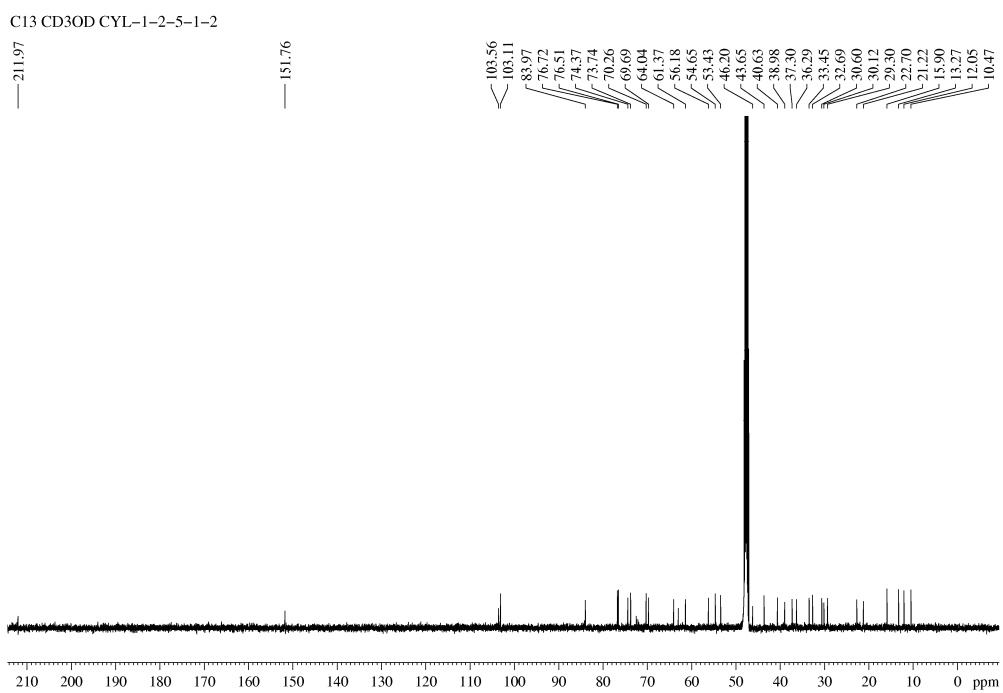
Figure S21. ^1H -NMR spectrum of compound 3.Figure S22. ^{13}C -NMR spectrum of compound 3.

Figure S23. DEPT spectrum of compound 3.

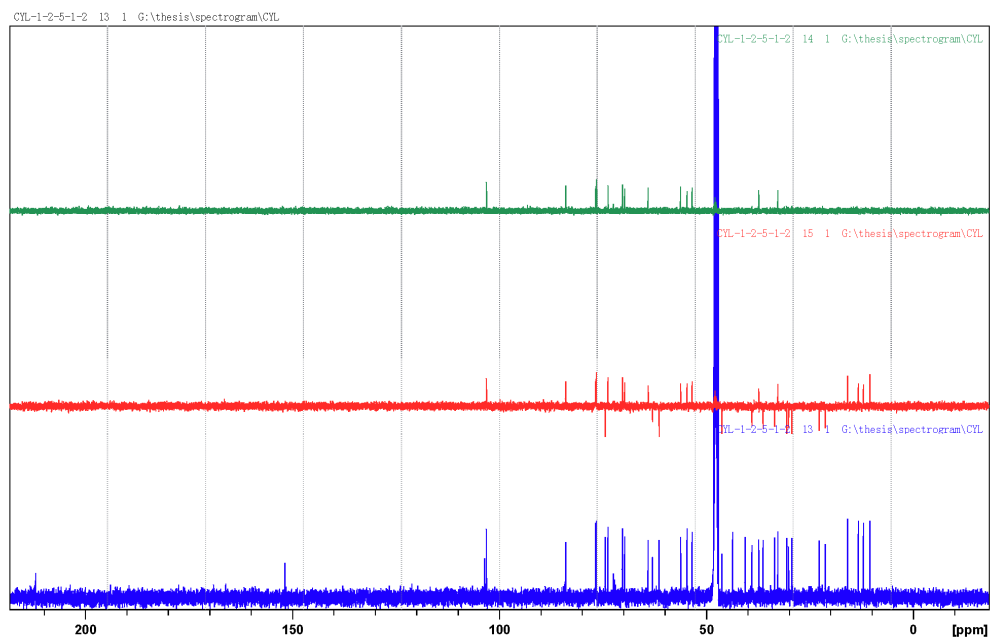


Figure S24. COSY spectrum of compound 3.

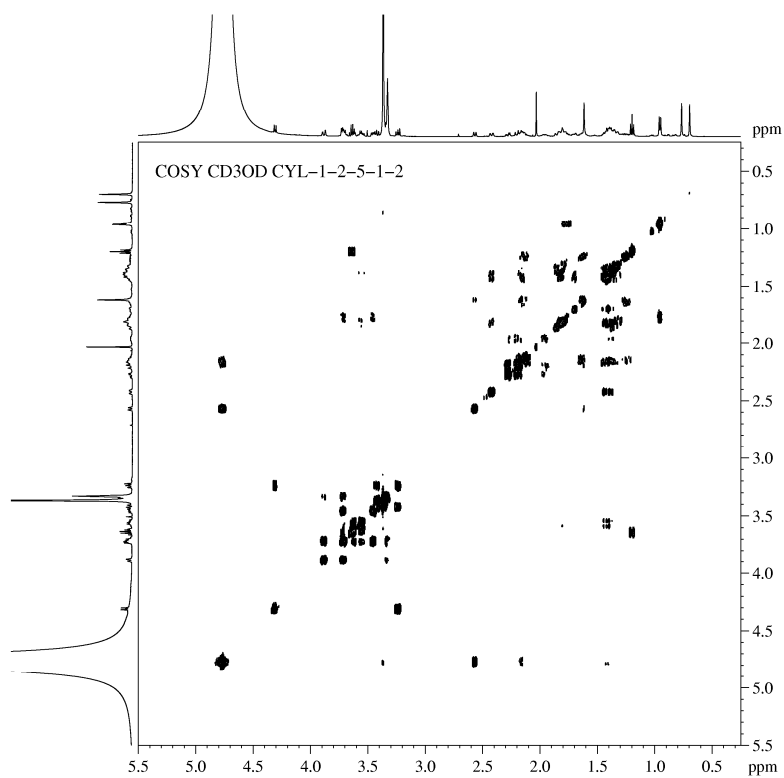


Figure S25. HSQC spectrum of compound 3.

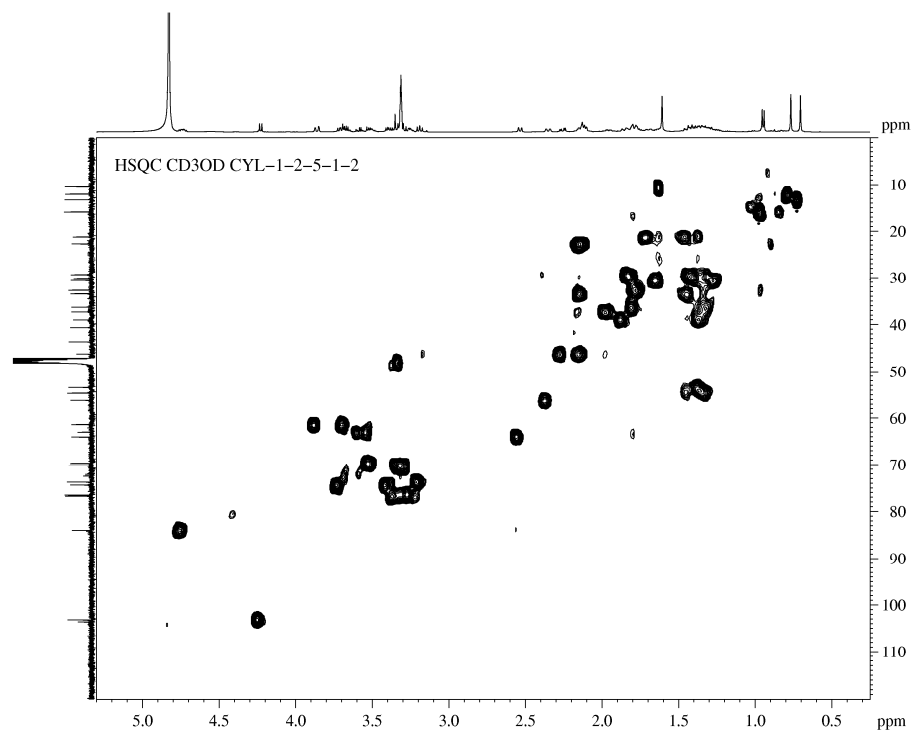


Figure S26. HMBC spectrum of compound 3.

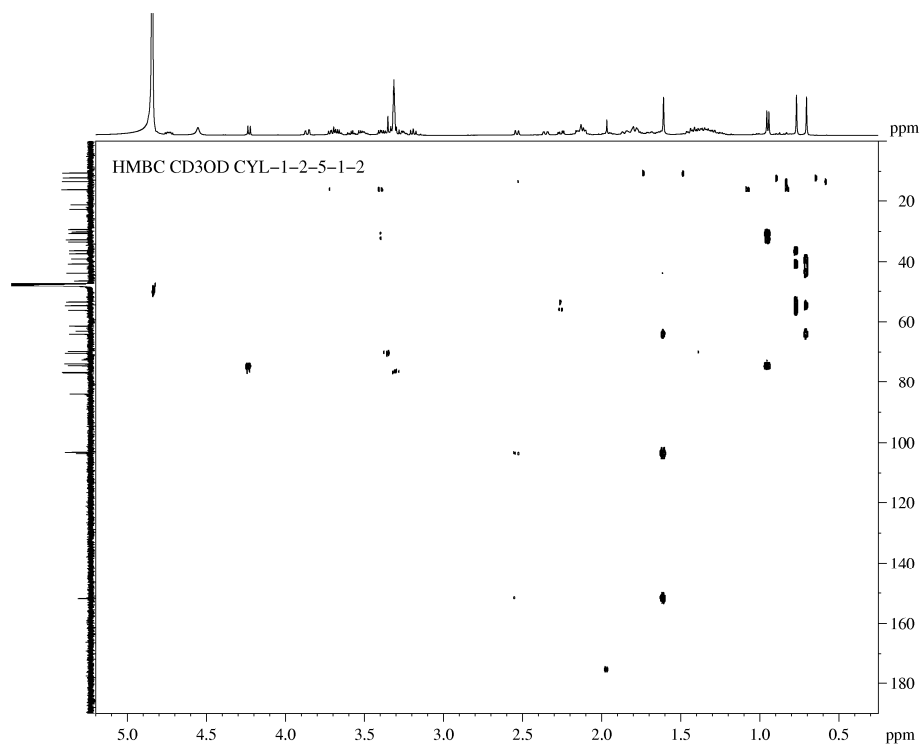


Figure S27. NOESY spectrum of compound 3.

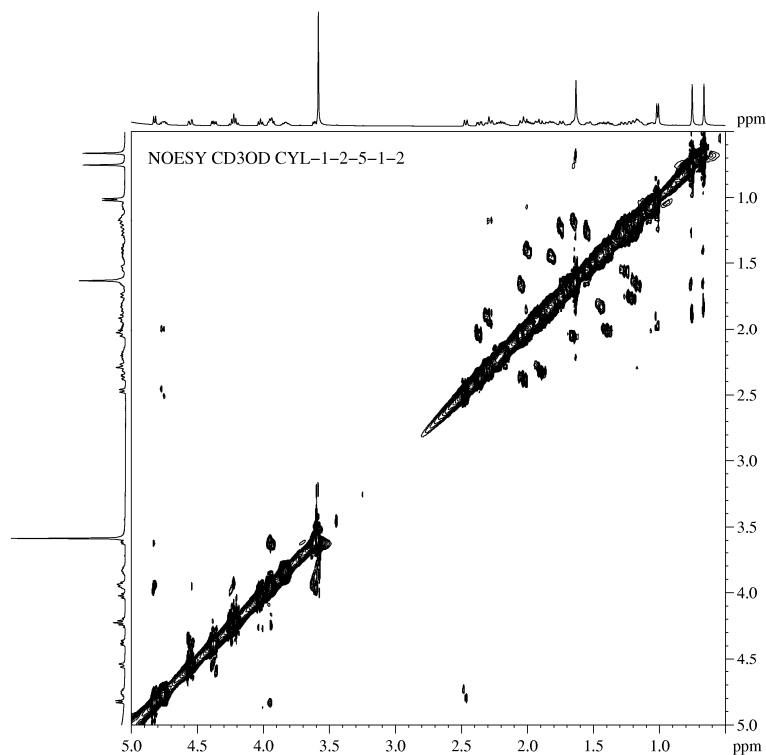
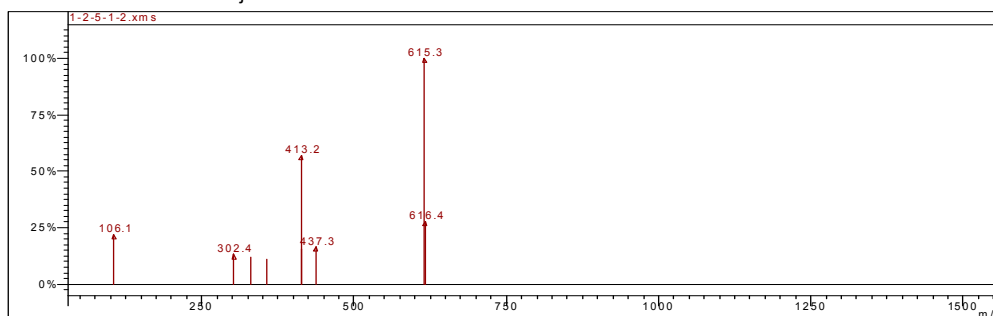


Figure S28. ESI-MS spectrum of compound 3.

Scan 301 from e:\szj\1-2-5-1-2\1-2-5-1-2.xms



Spectrum from e:\szj\1-2-5-1-2\1-2-5-1-2.xms
 Scan No: 301, Time: 5.427 minutes
 No averaging. Background corrected.
 Comment: 5.427 min. Scan: 301 100.0:1500.0> RIC: 6.624e+7
 Pair Count: 9 MW: 0 Formula: None
 CAS No: None Acquired Range: 100.0 - 1500.0 m/z

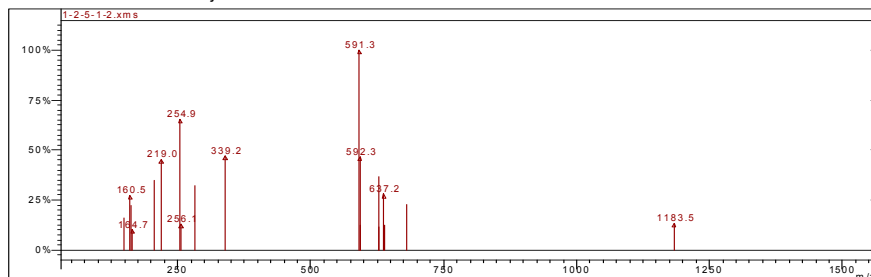
Method Description: ESI
 Scan 1 Channel Description: 100.0:1500.0> ESI;CID 175.0;Det 1100;WIQ 1
 Scan 2 Channel Description: 100.0:1500.0>(-) ESI;CID -120.0;Det 1100;W
 Scan Information: cp = 0.1 mTorr
 Precursor Mass Range: 100.0 - 1500.0 m/z

Ion	Int	Norm	Ion	Int	Norm	Ion	Int	Norm
106.1	1.573e+6	219	356.3	7.98325	111	437.3	1.171e+6	163
302.4	942496	132	413.2	4.066e+6	567	615.3	7.160e+6	999
330.2	850787	119	414.3	1.125e+6	157	616.4	1.993e+6	278

(+ ESI

Figure S28. Cont.

Scan 306 from e:\szj\1-2-5-1-2\1-2-5-1-2.xms



Spectrum from e:\szj\1-2-5-1-2\1-2-5-1-2.xms
 Scan No: 306, Time: 5.518 minutes
 3 points averaged. Background corrected.
 Comment: 5.518 min. Scans: 303-307 100.0:1500.0>(-) RIC: 1.179e+8
 Pair Count: 19 MW: 0 Formula: None
 CAS No: None Acquired Range: 100.0 - 1500.0 m/z

Method Description: ESI
 Scan 1 Channel Description: 100.0:1500.0> ESI:CID 175.0:Det 1100;W1Q1
 Scan 2 Channel Description: 100.0:1500.0>(-) ESI:CID -120.0:Det 1100;W
 Scan Information: cp = 0.1 mTorr
 Precursor Mass Range: 100.0 - 1500.0 m/z

Ion	Int	Norm	Ion	Int	Norm	Ion	Int	Norm
149.1	839841	160	256.1	677556	129	627.3	1.916e+6	365
160.5	1.424e+6	272	292.9	1.687e+6	322	628.3	609348	116
162.5	1.172e+6	224	339.2	2.468e+6	471	637.2	1.466e+6	279
164.7	543761	104	591.3	5.240e+6	999	638.4	655153	125
204.9	1.826e+6	348	592.3	2.447e+6	466	681.2	1.188e+6	227
219.0	2.378e+6	453	593.4	652343	124	1183.5	698558	133
254.9	3.431e+6	654						

(-) ESI

Figure S29. HR-ESI-MS spectrum of compound 3.

Generic Display Report

Analysis Info
 Analysis Name: D:\Data\MS\data\201310\shenzhenxianhu_CYL-1-2-5-1-2_pos.d
 Method: POS_100-2000_Direct Infusion.m
 Sample Name: SCSIO
 Comment:
 Acquisition Date: 10/14/2013 8:33:54 AM
 Operator: SCSIO
 Instrument: maXis

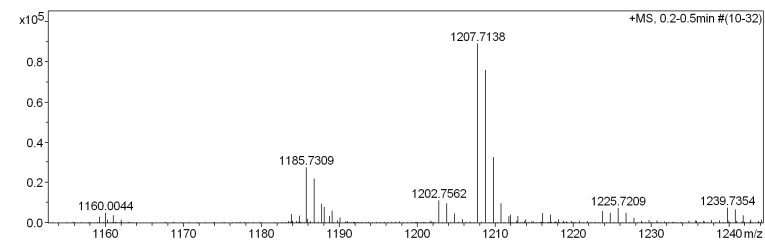
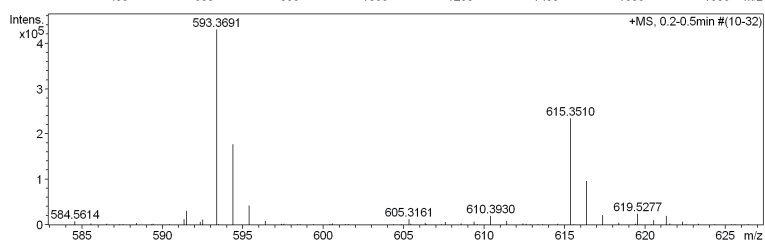
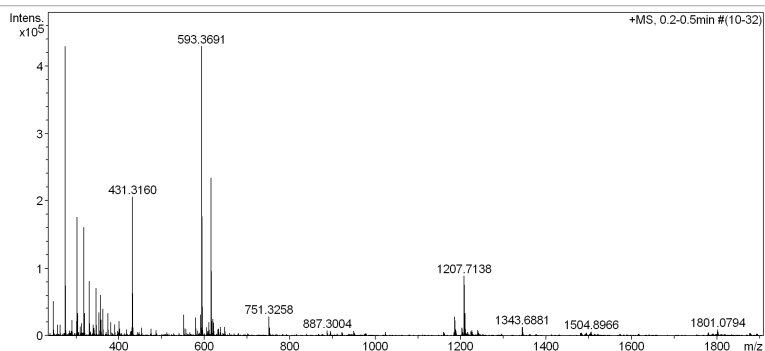


Figure S29. Cont.

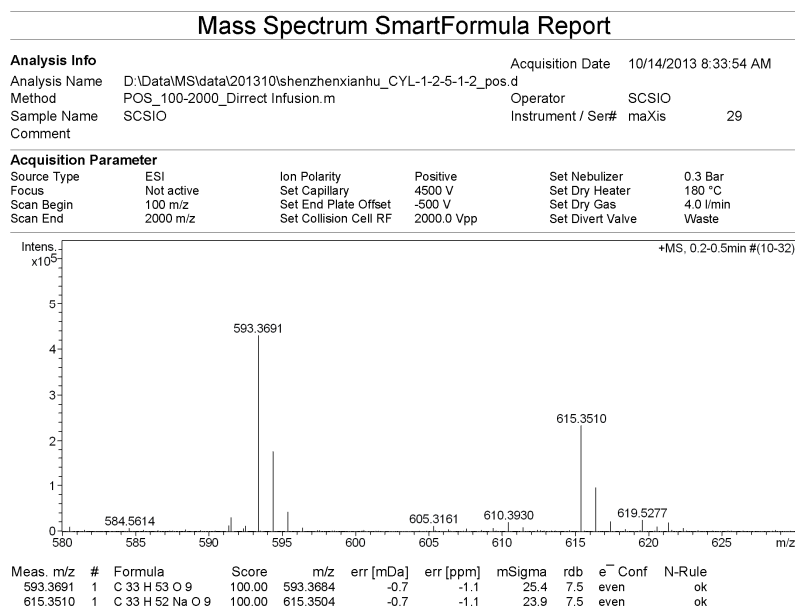


Figure S30. IR spectrum of compound 3.

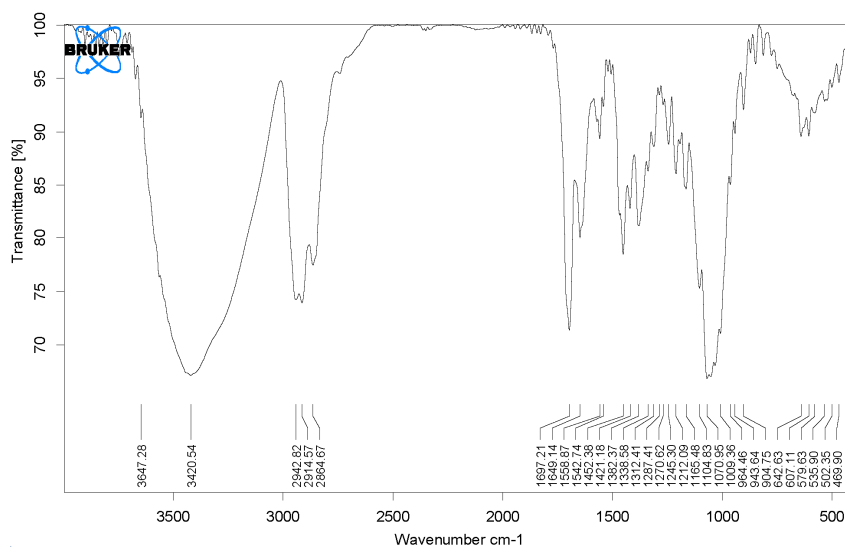


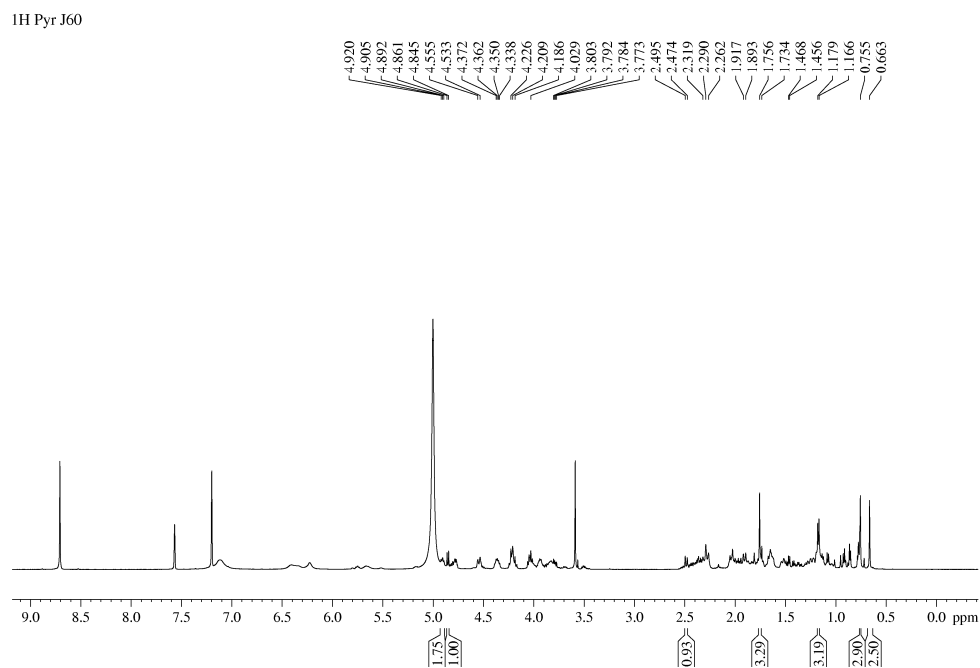
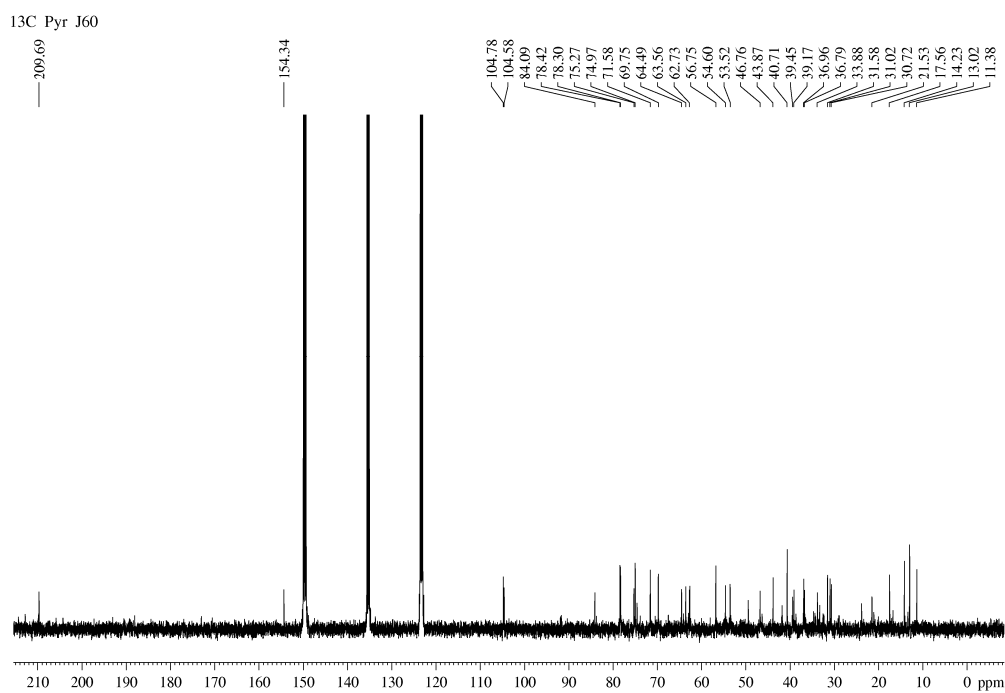
Figure S31. $^1\text{H-NMR}$ spectrum of compound 4.Figure S32. $^{13}\text{C-NMR}$ spectrum of compound 4.

Figure S33. DEPT spectrum of compound 4.

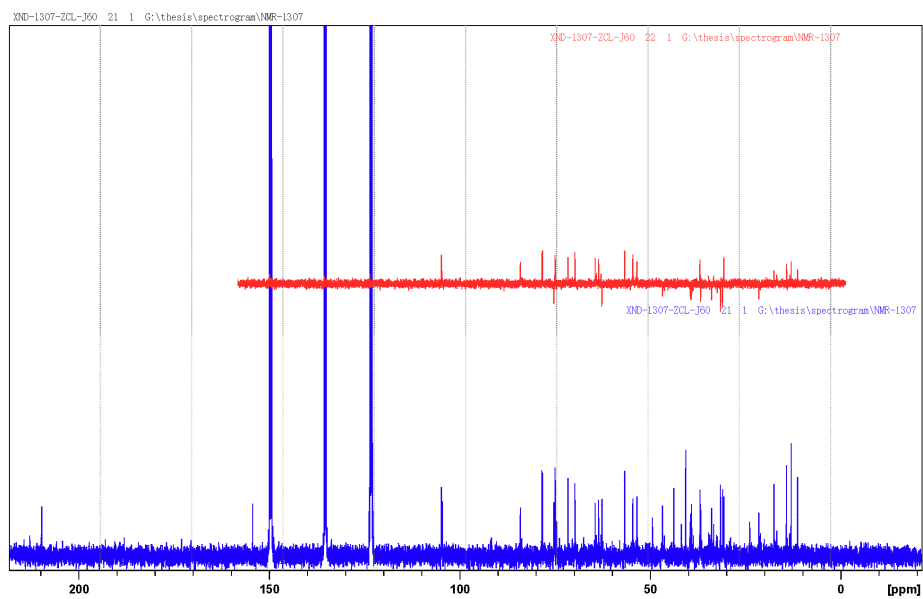


Figure S34. COSY spectrum of compound 4.

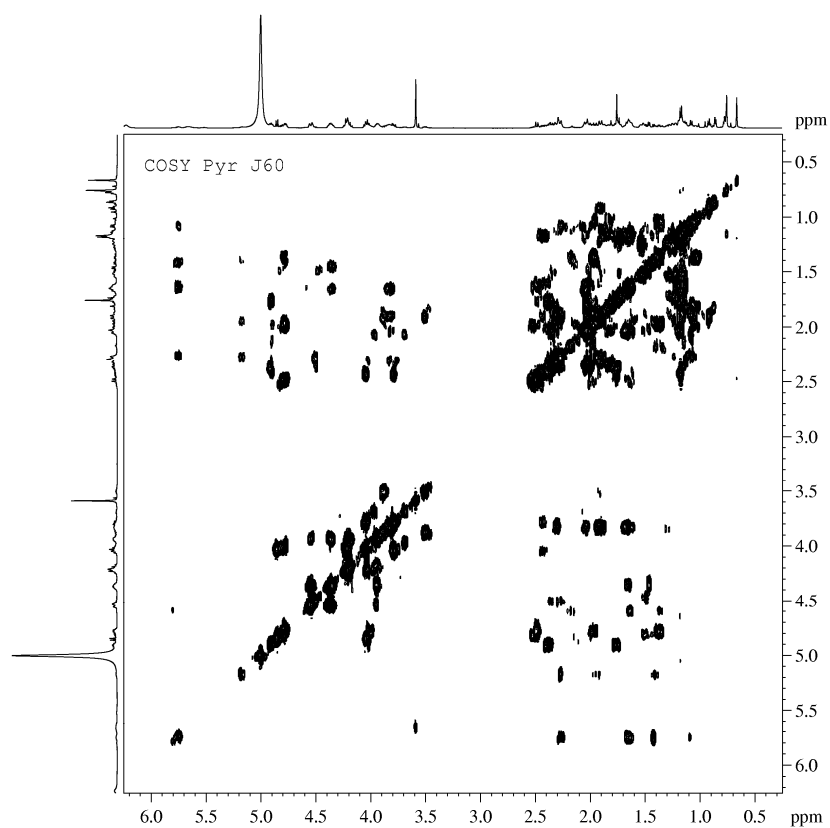


Figure S35. HSQC spectrum of compound 4.

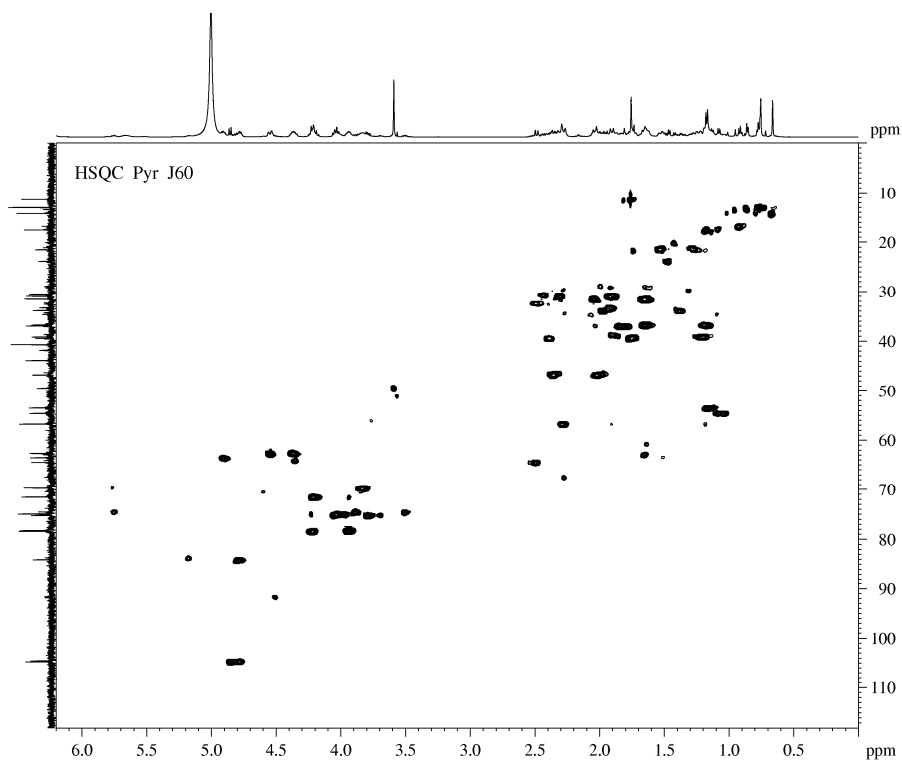


Figure S36. HMBC spectrum of compound 4.

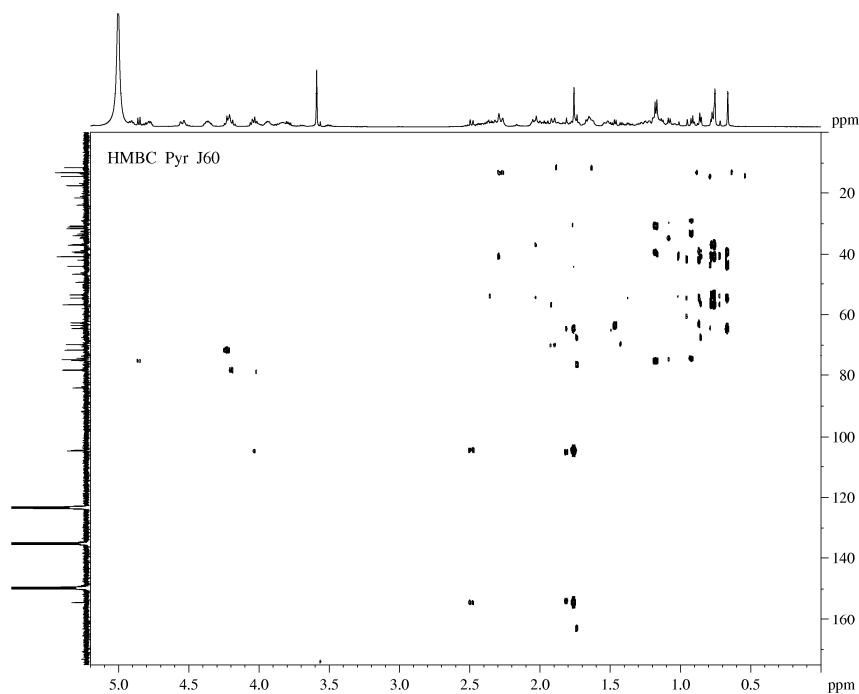
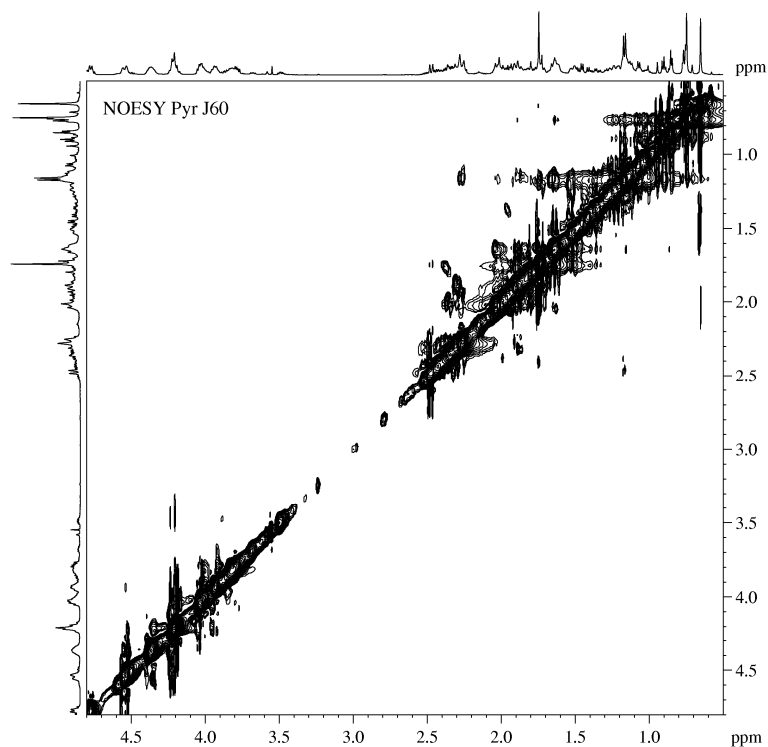


Figure S37. NOESY spectrum of compound 4.**Figure S38.** ESI-MS spectrum of compound 4.

Jie60 #20-25 RT: 0.08-0.10 AV: 6 NL: 5.47E3
T: ITMS + c ESI Full ms [50.00-2000.00]

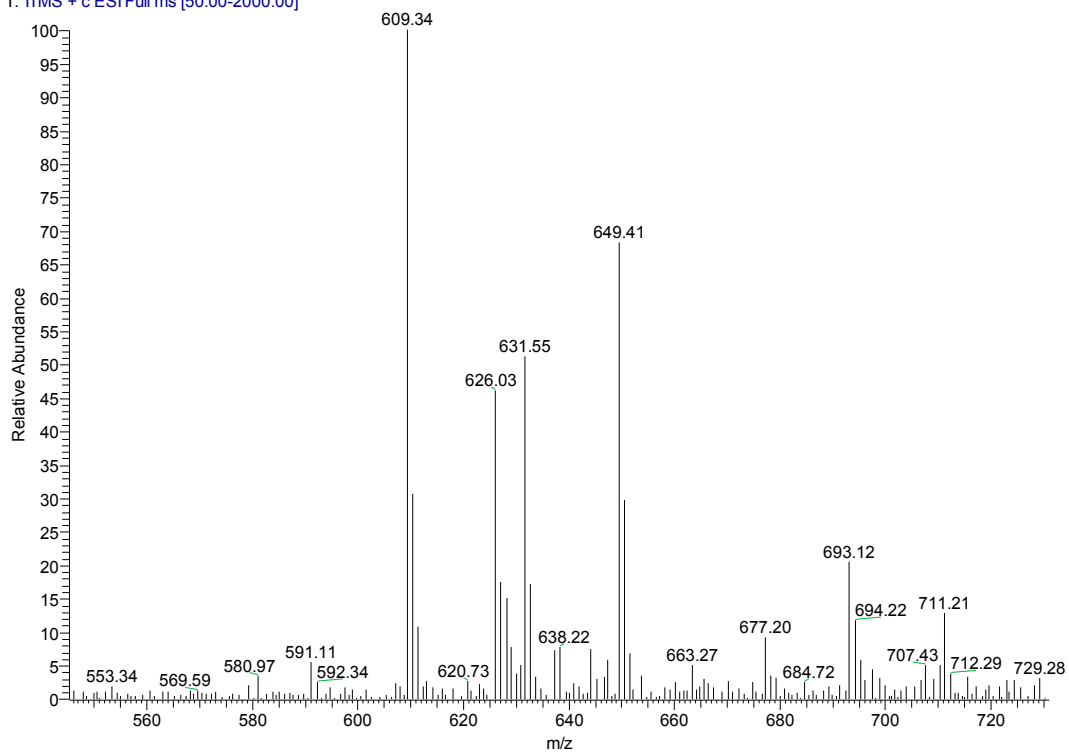
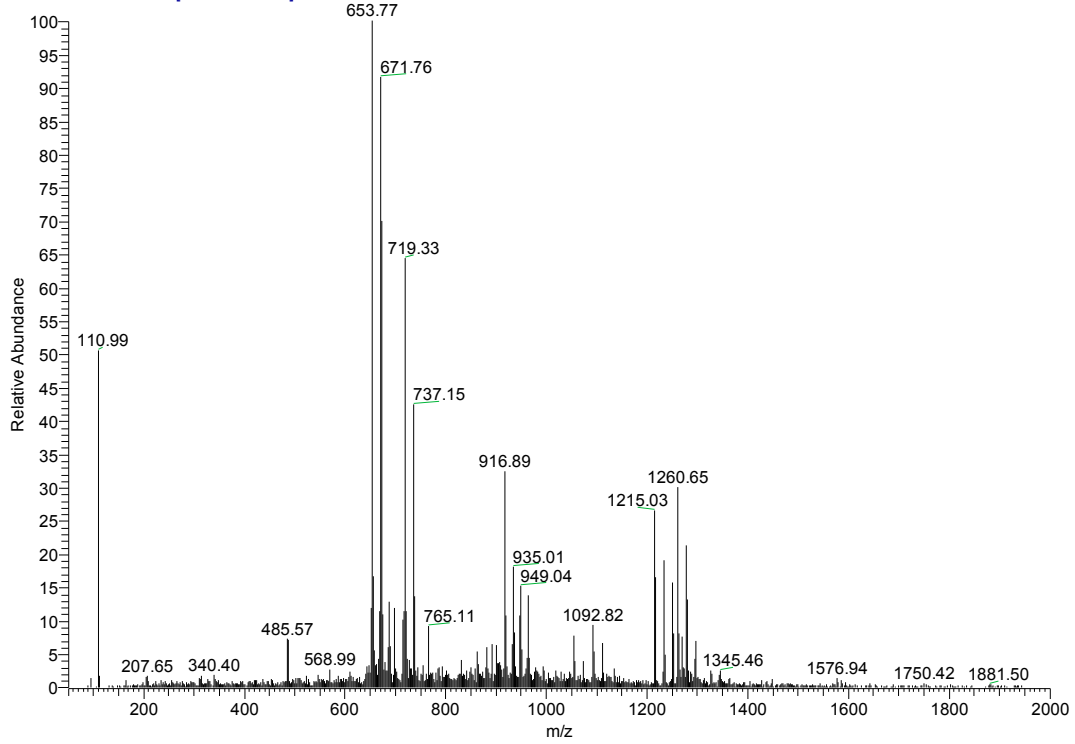


Figure S38. Cont.

Jie60 #52-55 RT: 0.42-0.47 AV: 4 NL: 2.38E2
 T: ITMS - c ESI Full ms [50.00-2000.00]



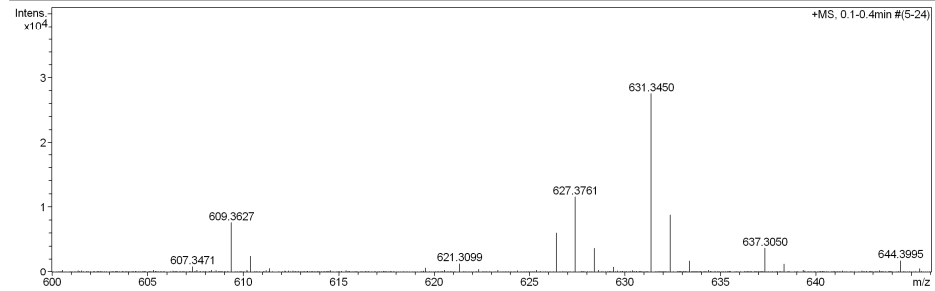
(-) ESI

Figure S39. HR-ESI-MS spectrum of compound 4.

Mass Spectrum SmartFormula Report

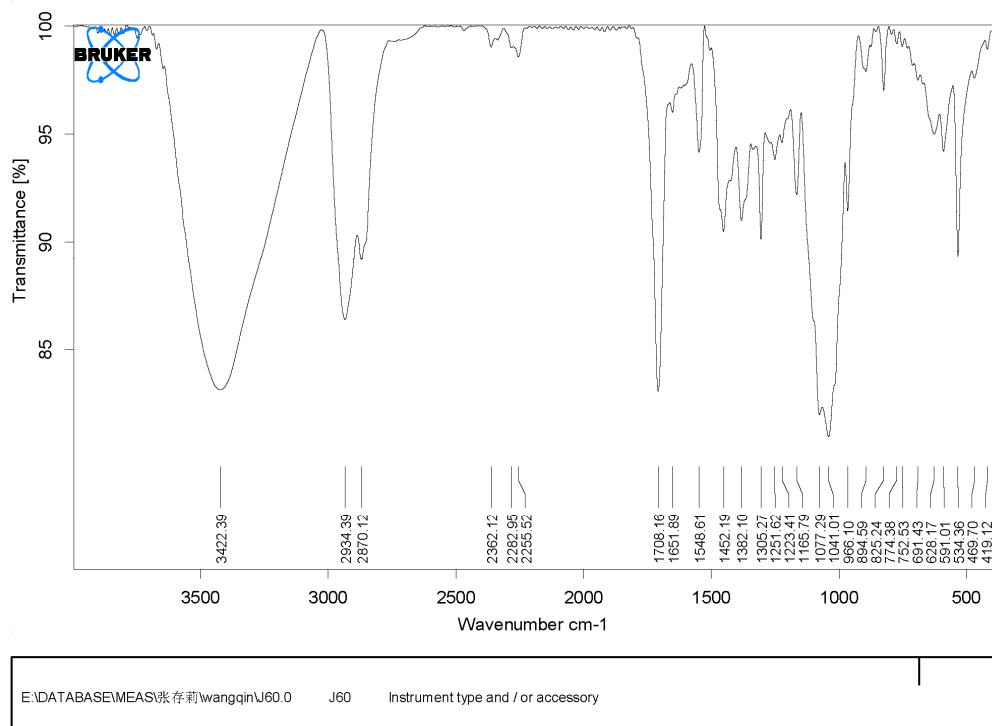
Analysis Info		Acquisition Date	
Analysis Name	D:\Data\MS\data\201312\shenzhenxianhu_J60_pos.d	12/23/2013 9:52:52 AM	
Method	POS_100-2000_Direct Infusion.m	Operator	SCSIO
Sample Name	SCSIO	Instrument / Ser#	maXis 29
Comment			

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Not active	Set Capillary	4800 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	2000.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e- Conf	N-Rule
609.3627	1	C 33 H 53 O 10	100.00	609.3633	0.7	1.1	19.1	7.5	even	ok
631.3450	1	C 33 H 52 Na O 10	100.00	631.3453	0.3	0.4	26.2	7.5	even	ok

Figure S40. IR spectrum of compound 4.



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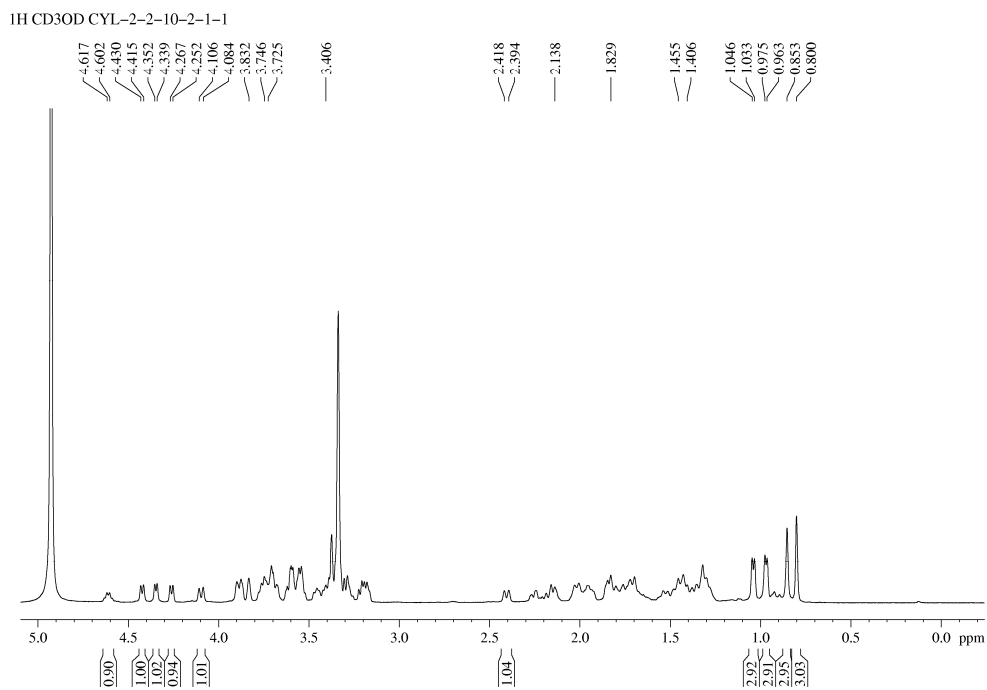
Figure S41. ¹H-NMR spectrum of compound 5.

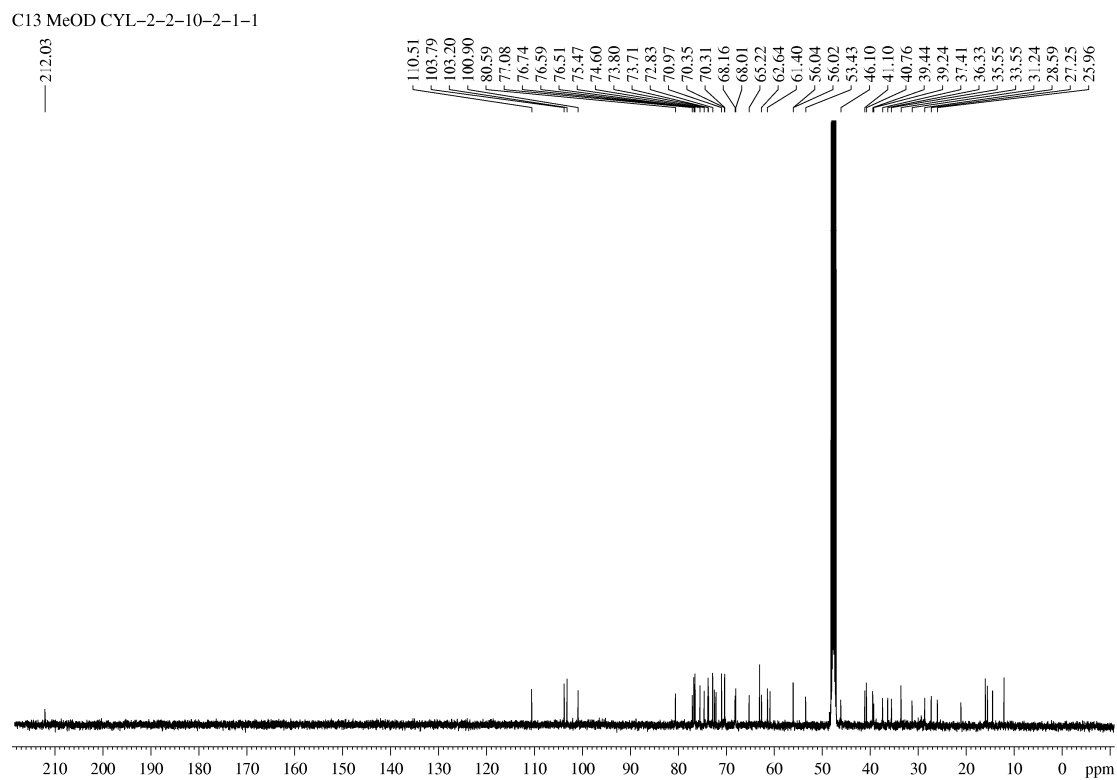
Figure S42. ^{13}C -NMR spectrum of compound 5.

Figure S43. DEPT spectrum of compound 5.

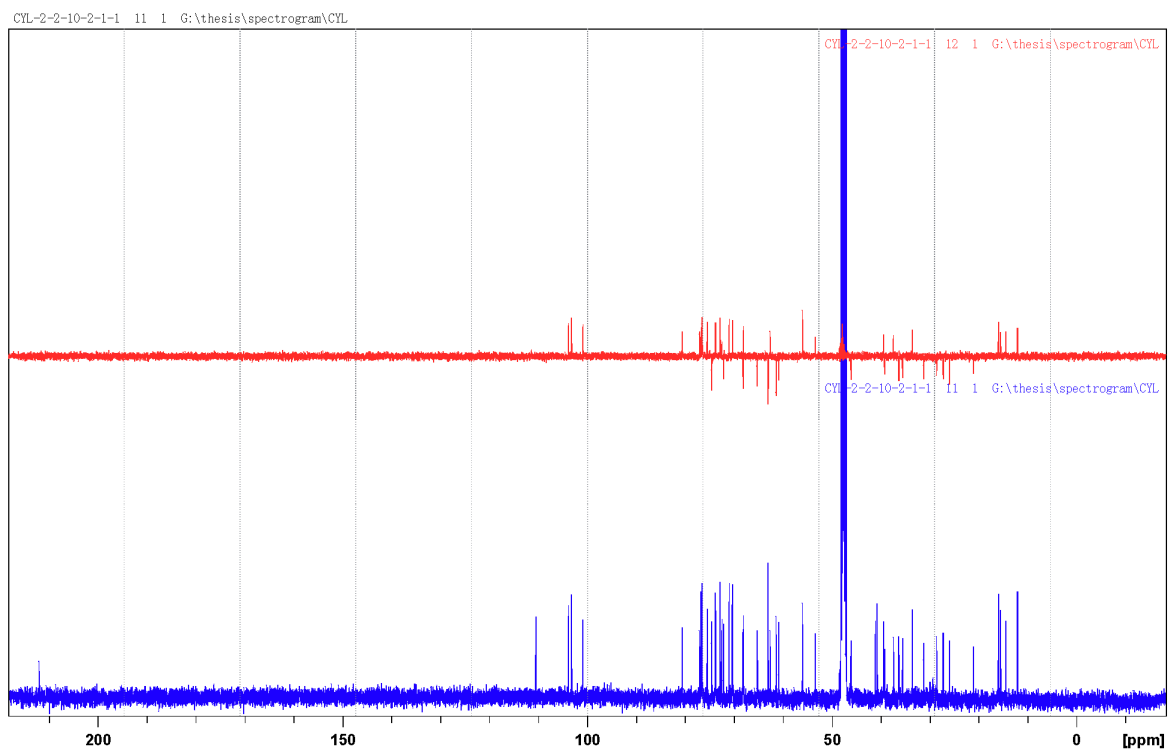


Figure S44. COSY spectrum of compound 5.

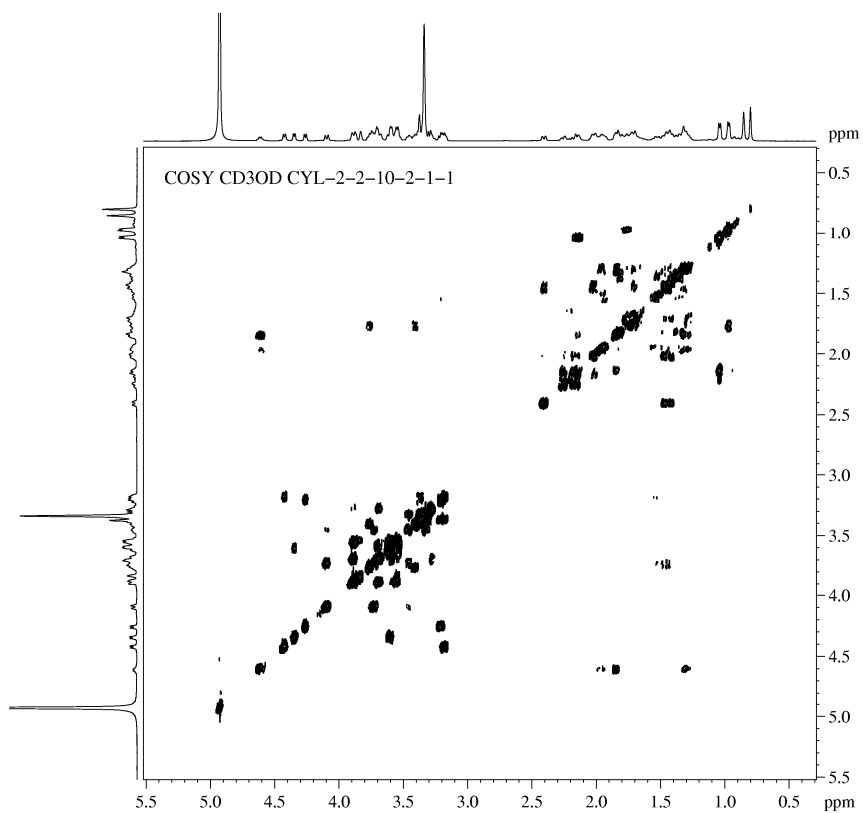


Figure S45. HSQC spectrum of compound 5.

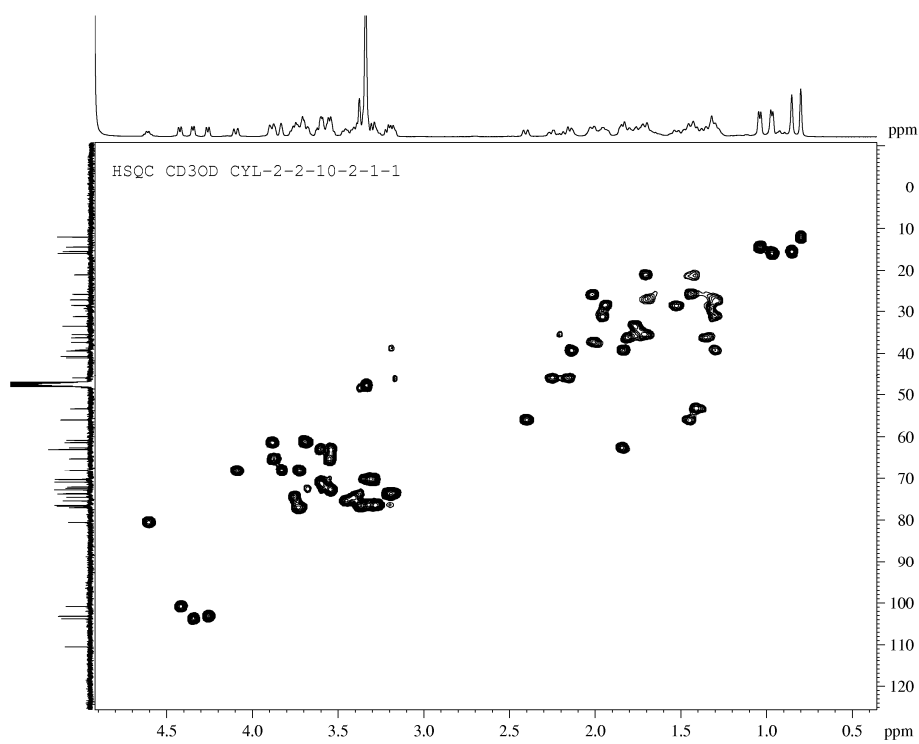
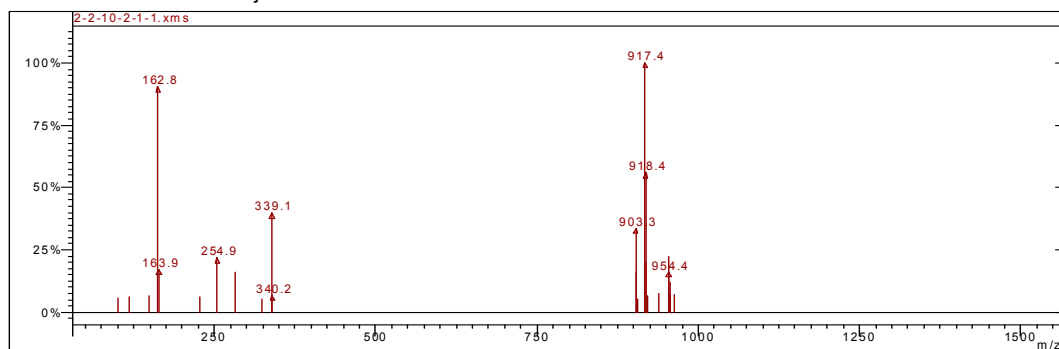


Figure S46. ESI-MS spectrum of compound 5.

Scan 250 from e:\szj\2-2-10-2-1-1\2-2-10-2-1-1.xms



Spectrum from e:\szj\2-2-10-2-1-1\2-2-10-2-1-1.xms
 Scan No: 250, Time: 4.505 minutes
 5 points averaged. Background corrected.
 Comment: 4.505 min. Scans: 245-253 100.0>(-) RIC: 2.285e+8
 Pair Count: 24 MW: 0 Formula: None
 CAS No: None Acquired Range: 100.0 - 1500.0 m/z

Method Description: ESI

Scan 1 Channel Description: 100.0:1500.0> ESI;CID 175.0;Det 1100;W IQ 1

Scan 2 Channel Description: 100.0:1500.0>(-) ESI;CID -165.0;Det 1100;W

Scan Information: cp = 0.1 mTorr

Precursor Mass Range: 100.0 - 1500.0 m/z

Ion	Int	Norm	Ion	Int	Norm	Ion	Int	Norm
100.7	964382	56	325.0	916719	54	919.5	3.446e+6	202
119.1	1.061e+6	62	339.1	6.775e+6	396	920.7	1.135e+6	66
148.8	1.108e+6	65	340.2	1.145e+6	67	939.2	1.278e+6	75
162.8	1.543e+7	903	903.3	5.736e+6	335	953.3	3.824e+6	224
163.9	2.884e+6	169	904.4	2.750e+6	161	954.4	2.766e+6	162
226.9	1.022e+6	60	905.4	894434	52	955.4	2.078e+6	122
254.9	3.699e+6	216	917.4	1.708e+7	999	956.3	1.176e+6	69
283.0	2.731e+6	160	918.4	9.534e+6	558	963.3	1.230e+6	72

Figure S47. ¹H-NMR spectrum of compound 6.

1H MeOD CYL-2-2-11-5-7

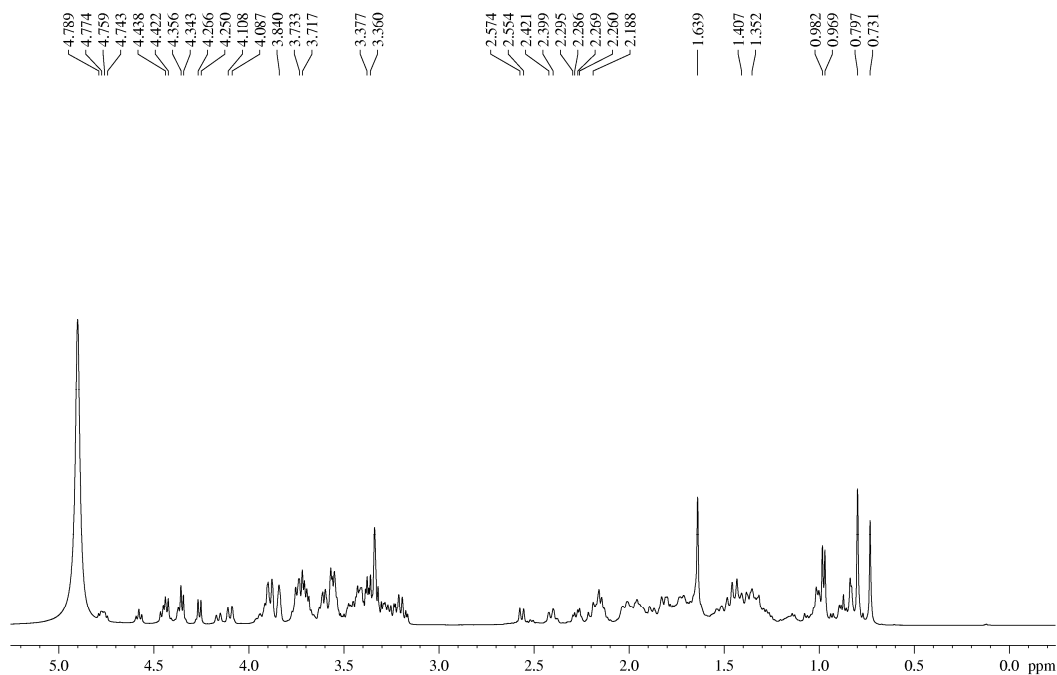


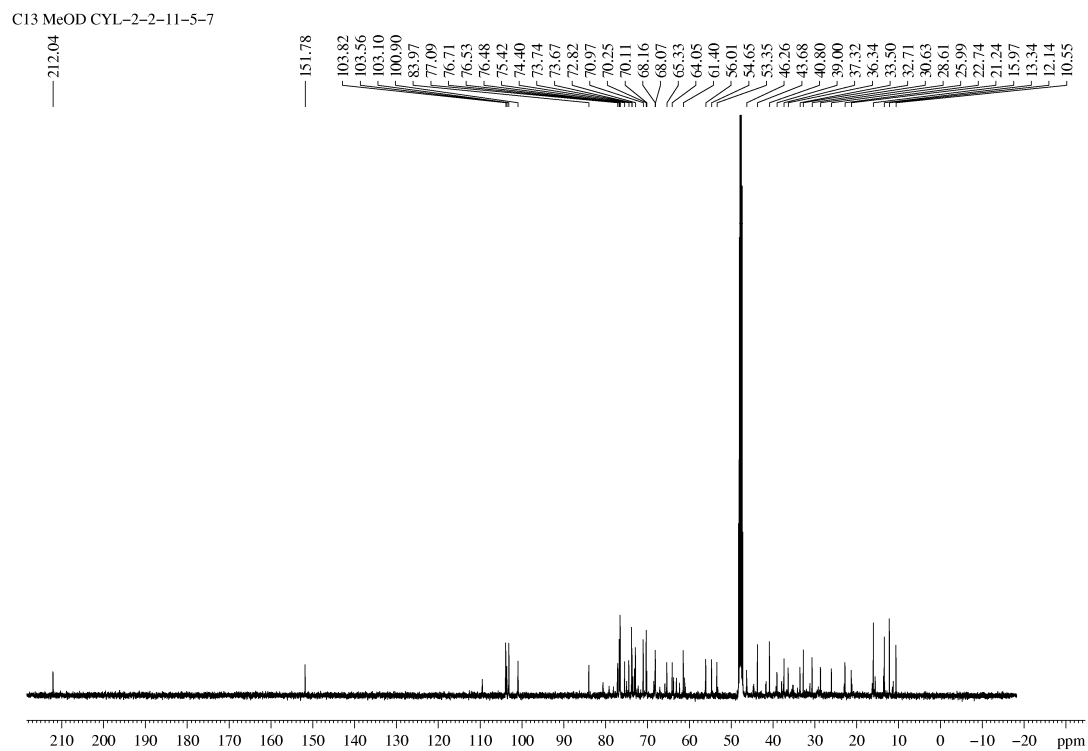
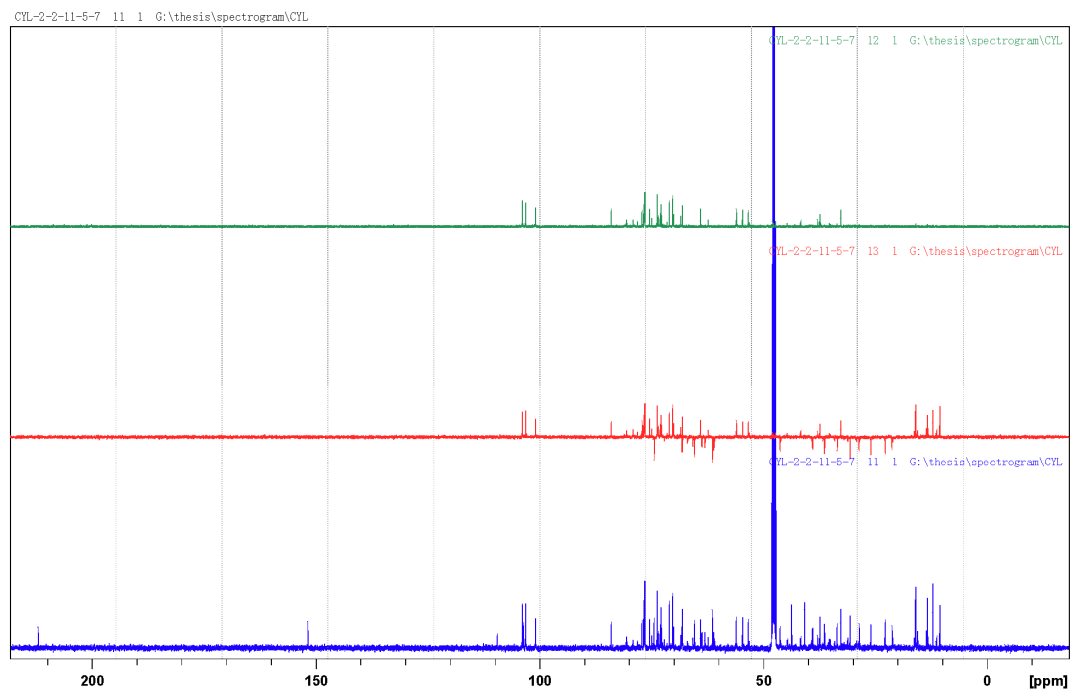
Figure S48. ^{13}C -NMR spectrum of compound **6**.**Figure S49.** DEPT spectrum of compound **6**.

Figure S50. HSQC spectrum of compound 6.

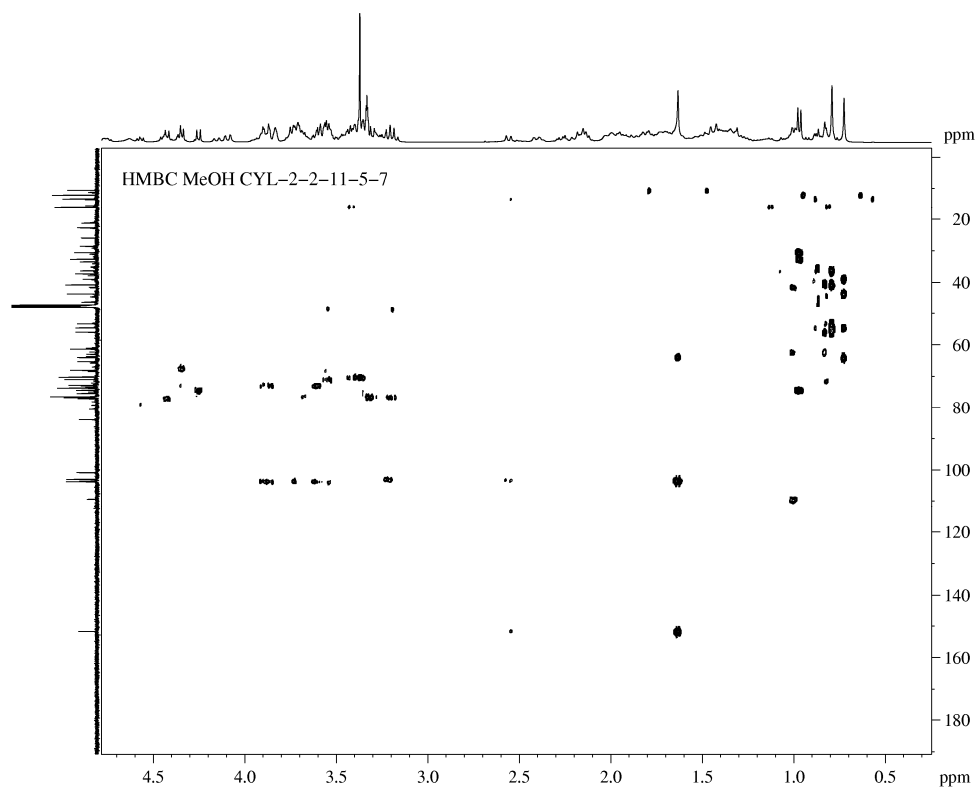


Figure S51. HMBC spectrum of compound 6.

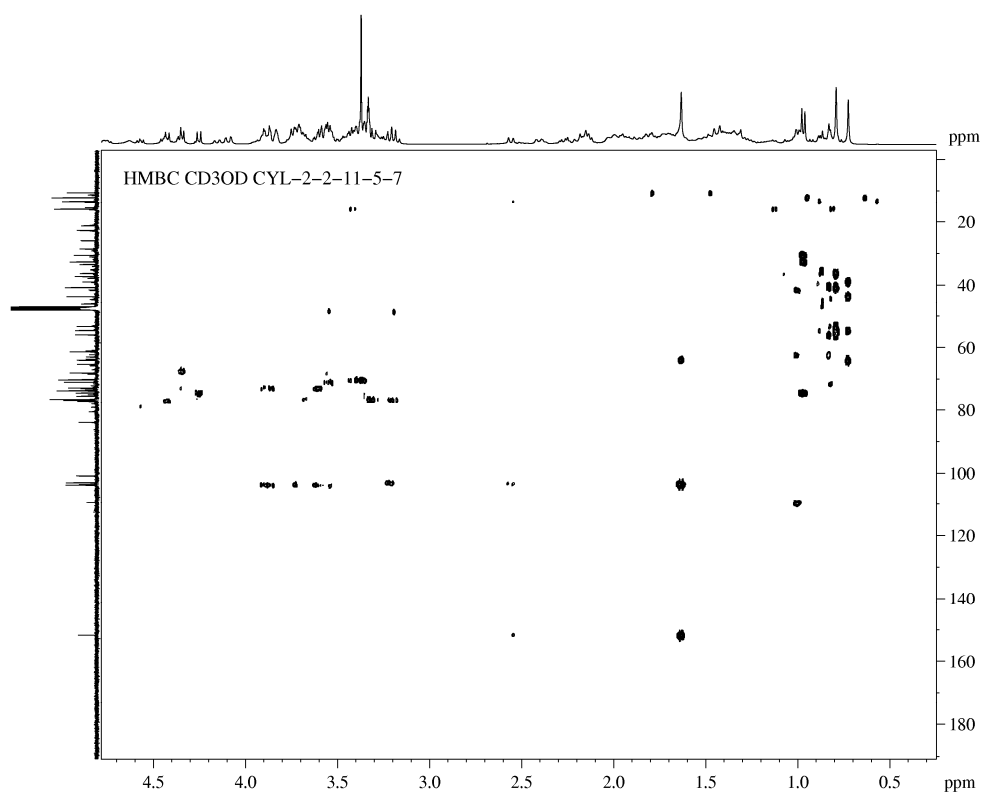


Figure S52. ESI-MS spectrum of compound 6.

Zhang CunLi CYL-2-2-11-5-7 #2-3 RT: 0.01-0.03 AV: 2 NL: 1.17E4
T: ITMS - c ESI Full ms [200.00-2000.00]

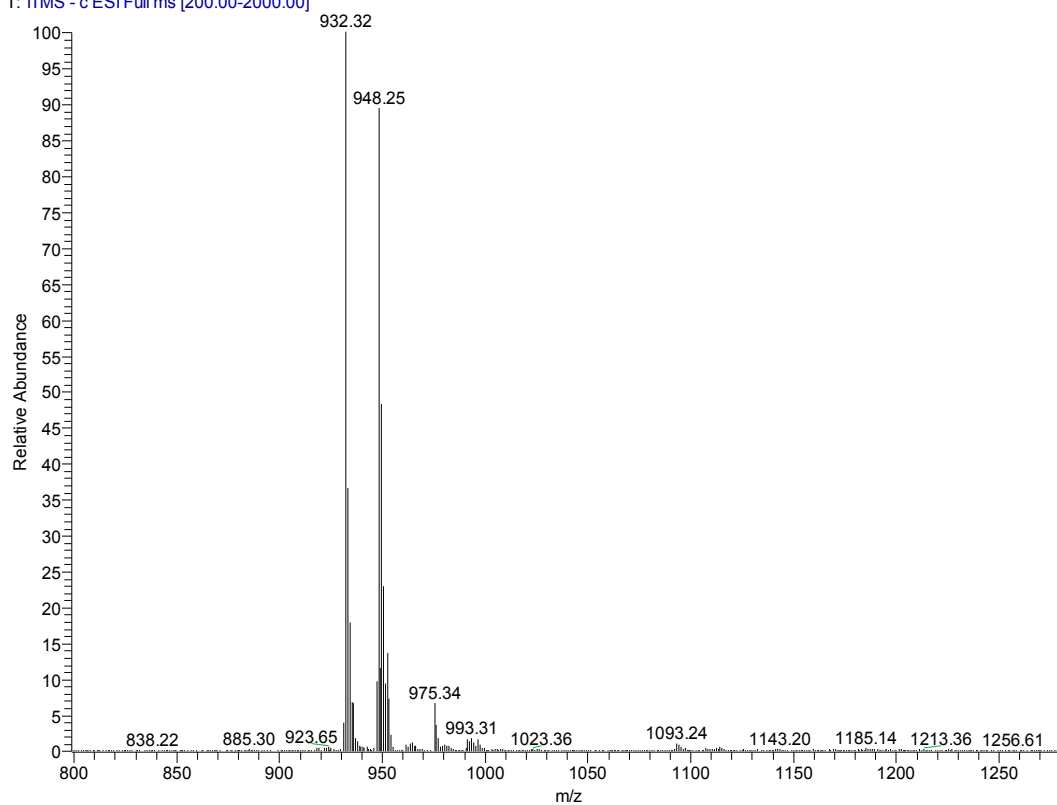
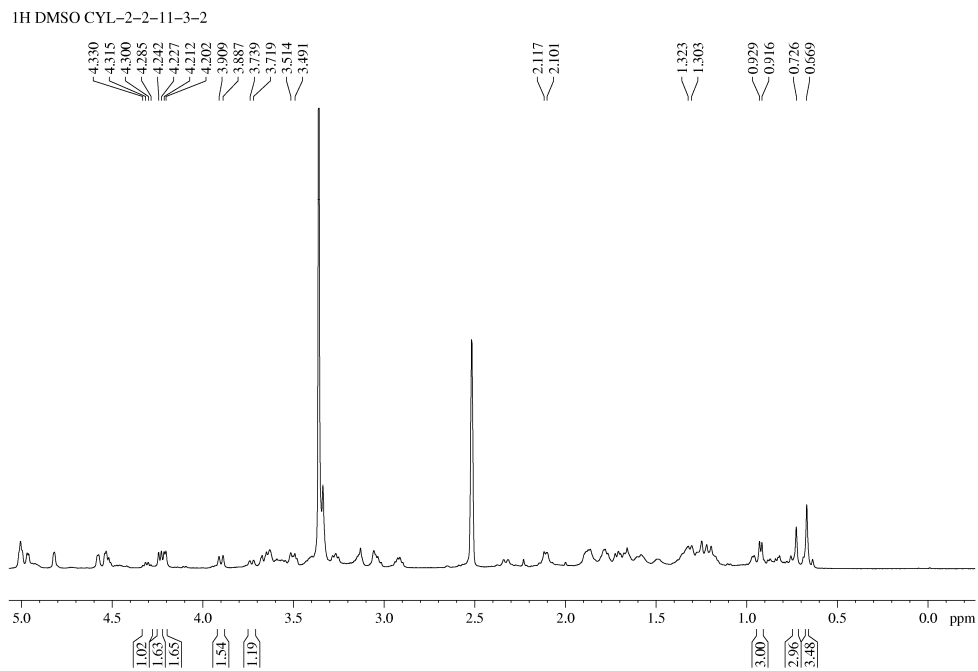
Figure S53. ¹H-NMR spectrum of compound 7.

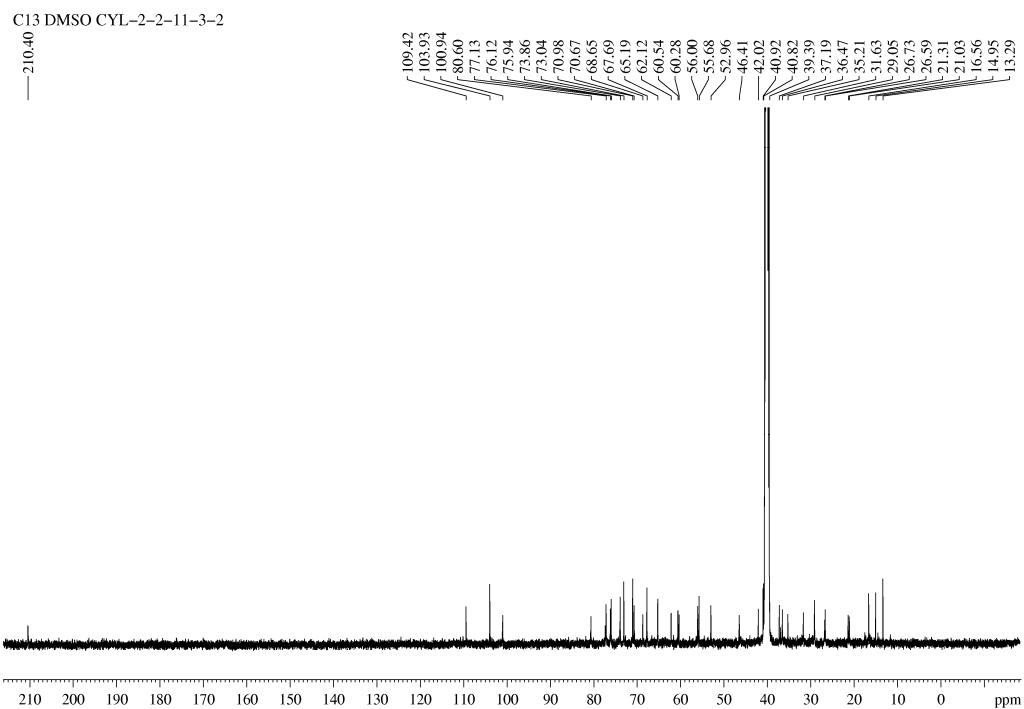
Figure S54. ^{13}C -NMR spectrum of compound 7.

Figure S55. DEPT spectrum of compound 7.

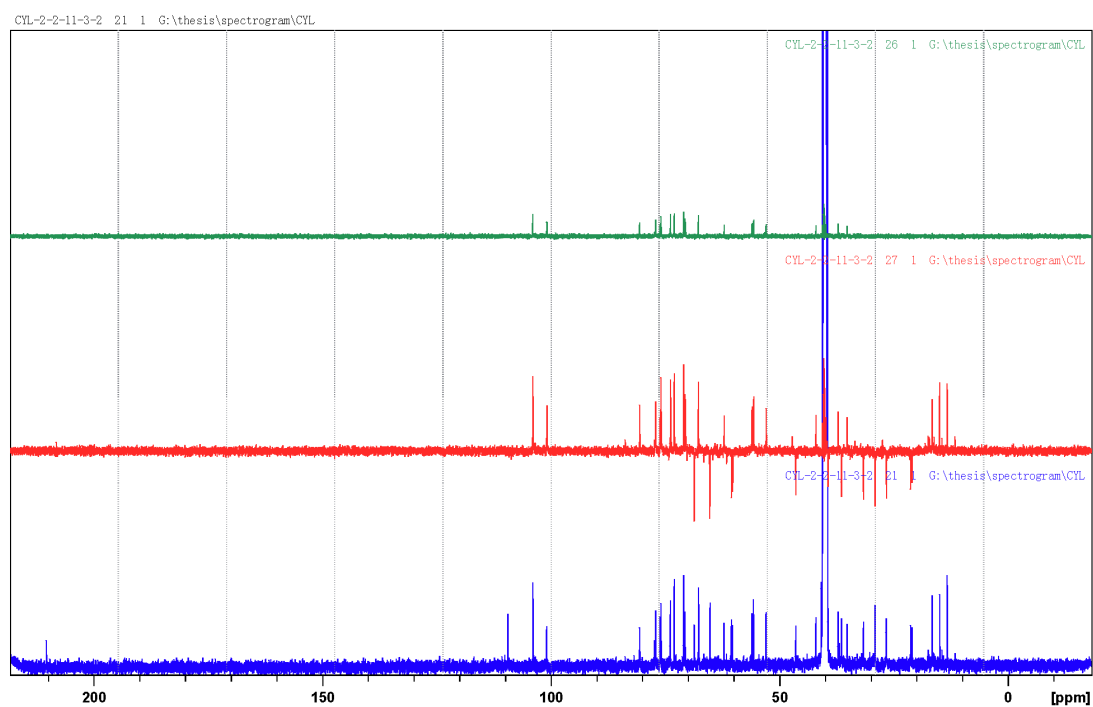


Figure S56. HSQC spectrum of compound 7.

