

Supporting information

Bioactive Compounds from the stems of *Clausena lansium*

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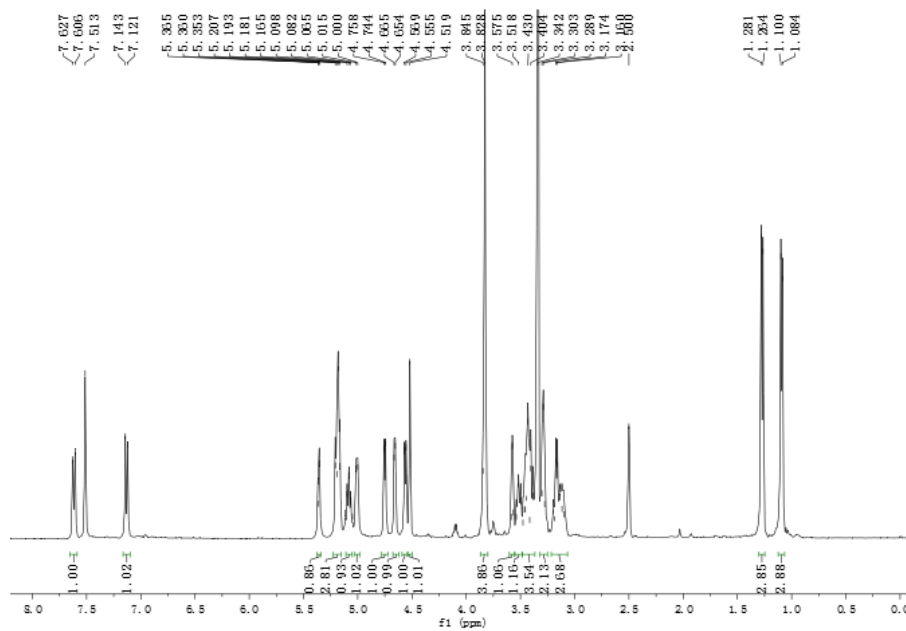


Figure S1. The ^1H NMR Spectrum of compound 1 (400 MHz, $\text{DMSO}-d_6$)

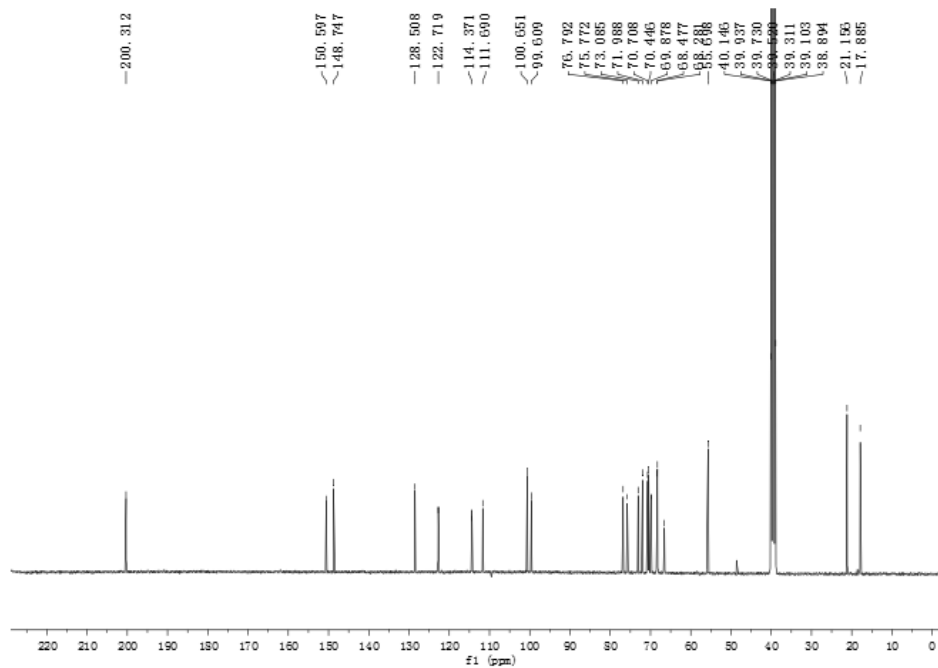


Figure S2. The ^{13}C NMR Spectrum of compound 1 (100 MHz, $\text{DMSO-}d_6$)

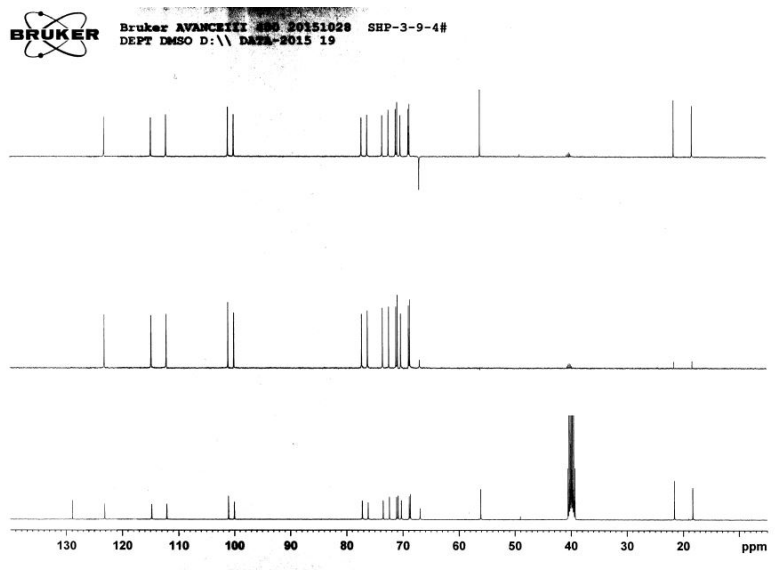


Figure S3. The DEPT Spectrum of compound 1

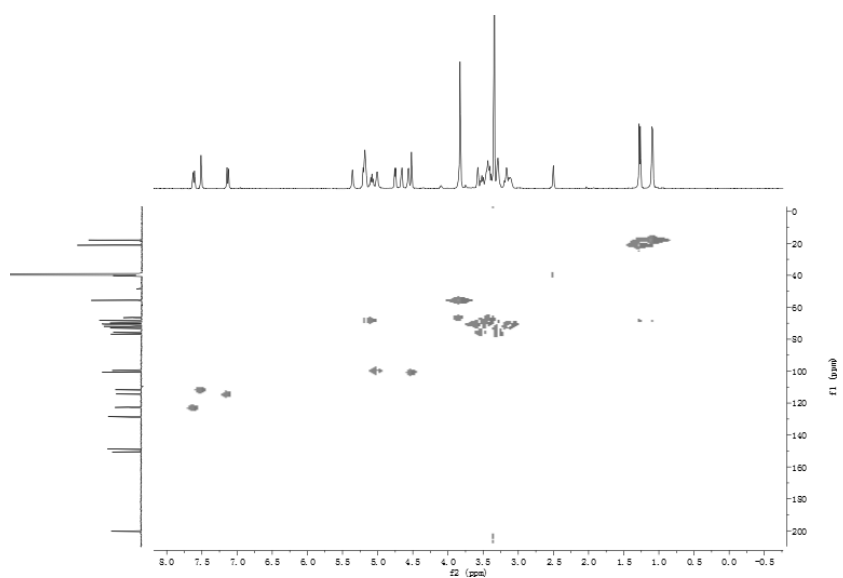


Figure S4. The HSQC Spectrum of compound 1

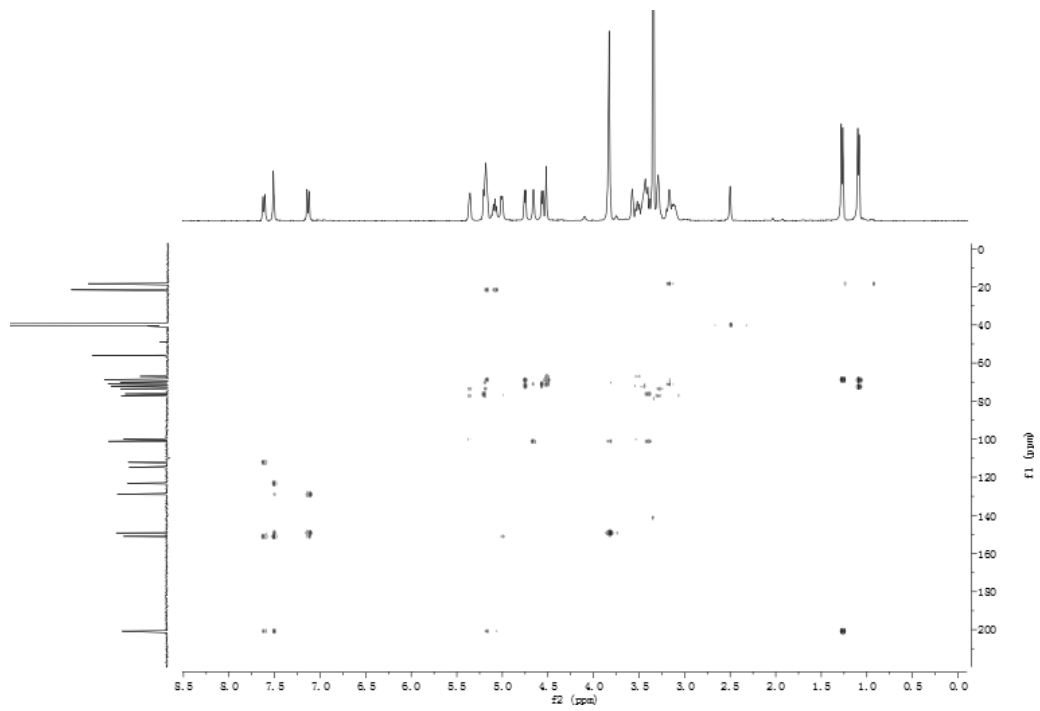


Figure S5. The HMBC Spectrum of compound 1

MS Formula Results: + Scan (3.658 min) Sub (2016031801.d)

m/z	Ion	Formula	Abundance
527.1731	(M+Na) ⁺	C22 H32 Na O13	55974.3

Best	Formula (M)	Ion Formula	Score	Cross Sco	Mass	Calc Mass	Calc m/z	Diff (ppm)	Abs Diff (ppm)	Mass Match	Abund Match
✓	C22 H32 O13	C22 H32 Na O13	99.93		504.1839	504.1843	527.1735	0.82	0.82	99.98	99.93
	C35 H24 N2 O2	C35 H24 N2 Na O2	96.5		504.1839	504.1838	527.173	-0.2	0.2	100	87.95

Figure S6. The HRESIMS Spectrum of compound 1

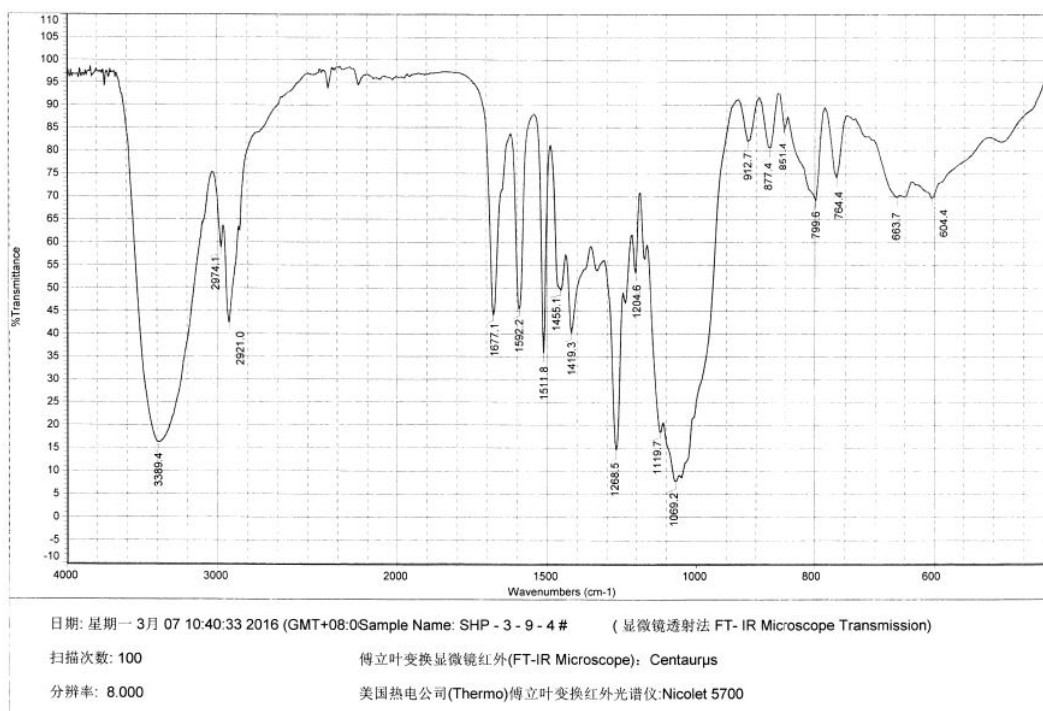


Figure S7. The IR Spectrum of compound 1

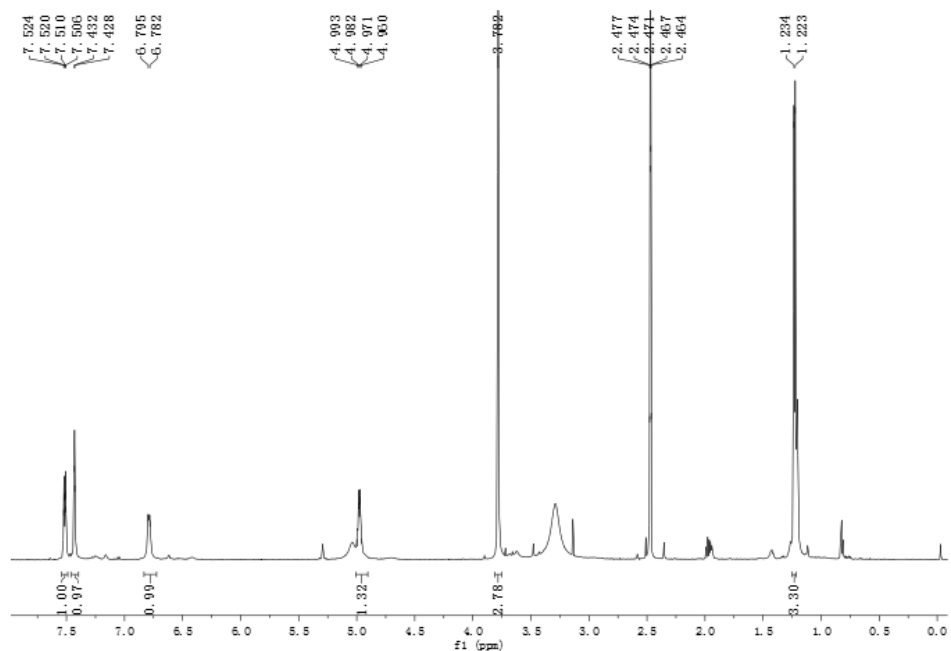


Figure S8. The ^1H NMR Spectrum of compound 1a (600 MHz, $\text{DMSO-}d_6$)

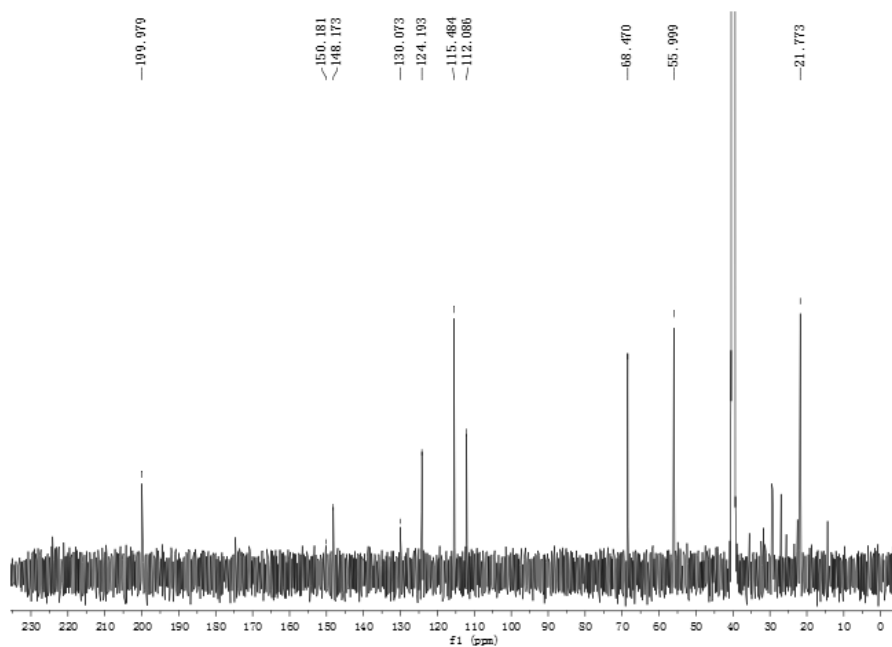


Figure S9. The ^{13}C NMR Spectrum of compound 1a (150 MHz, DMSO- d_6)

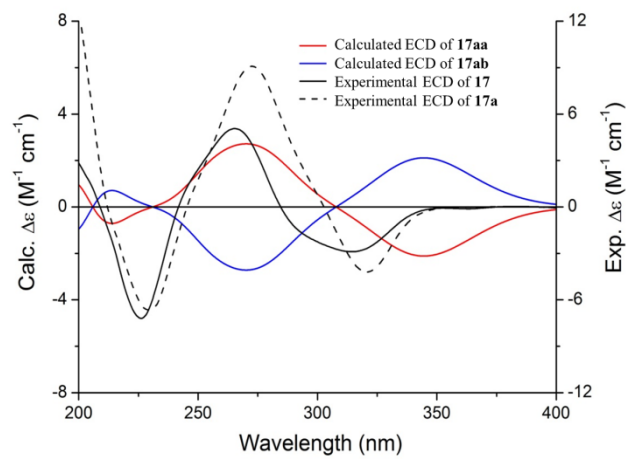


Figure S10. Calculated ECD spectra of (8S)1a and (8R)1a and the experimental ECD of 1a and 1

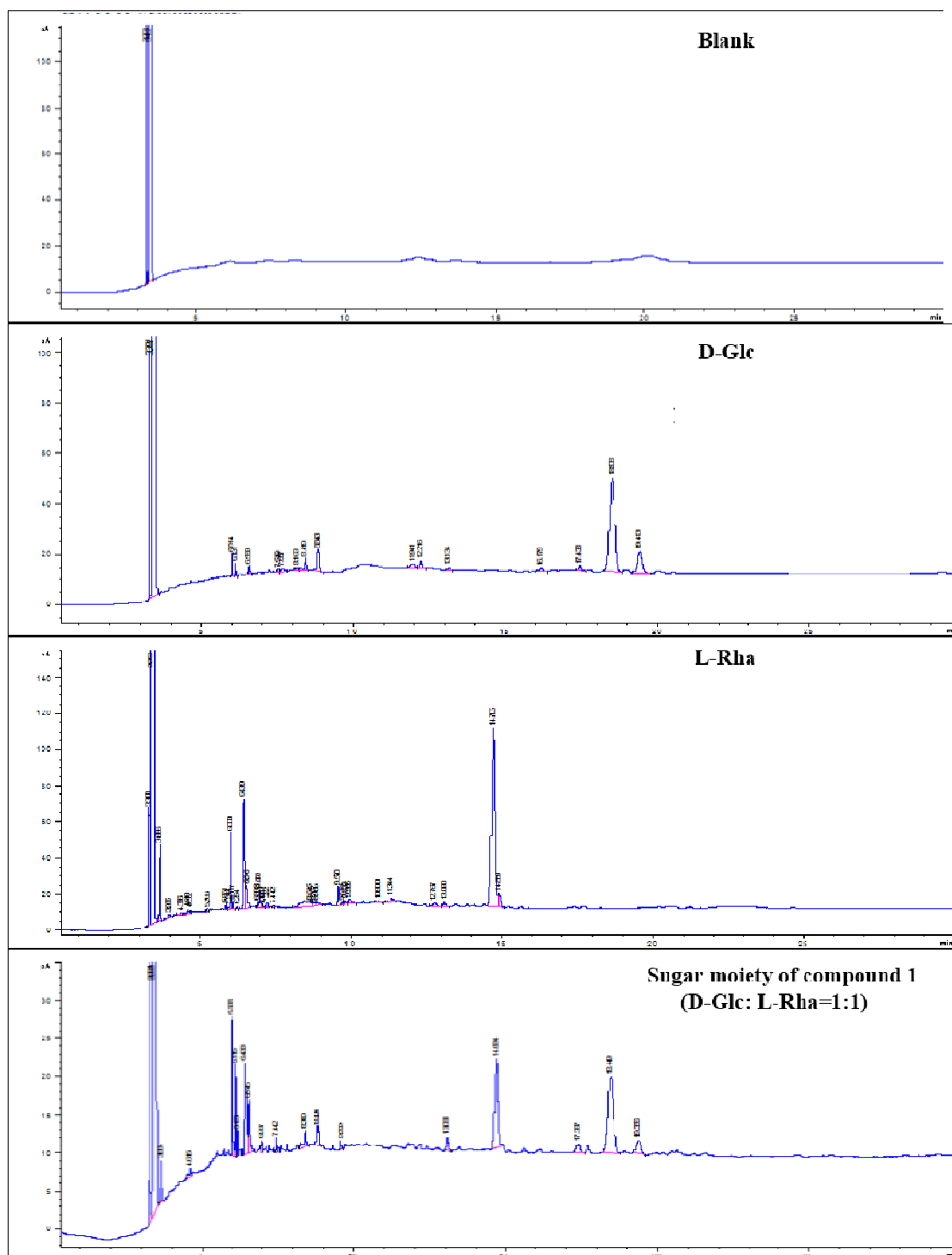


Figure S11. GC chromatogram of sugar moieties silylated after acid hydrolysis of 1

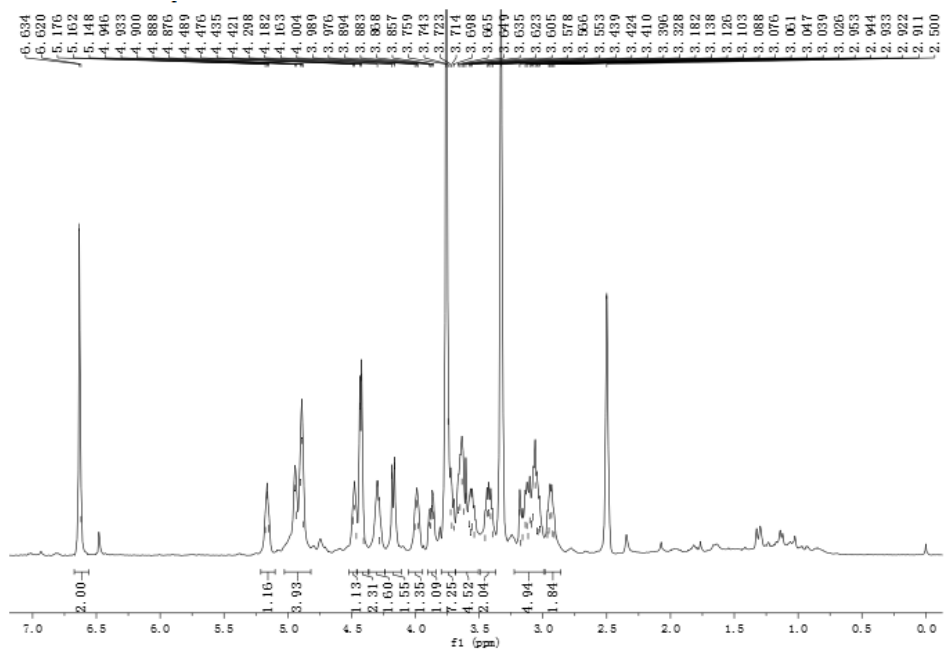


Figure S12. The ^1H NMR Spectrum of compound 2 (400 MHz, $\text{DMSO-}d_6$)

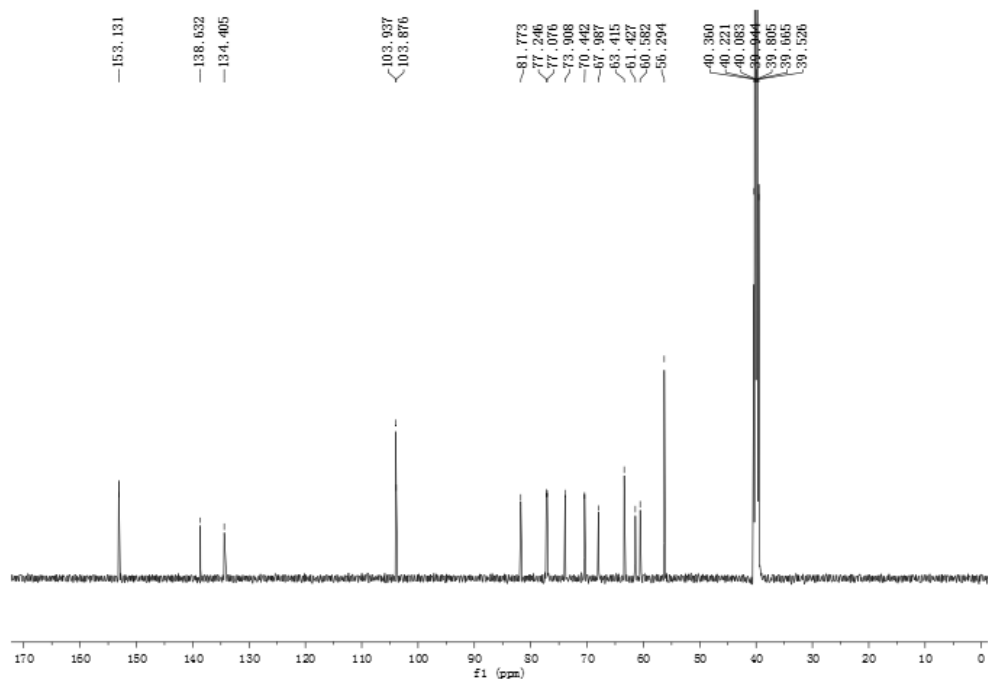


Figure S13. The ^{13}C NMR Spectrum of compound 2 (100 MHz, $\text{DMSO-}d_6$)



Bruker AVANCEIII 400 20151023 SHP-3-5-2#
DEPT DMF D:\\ DATA-2015 38

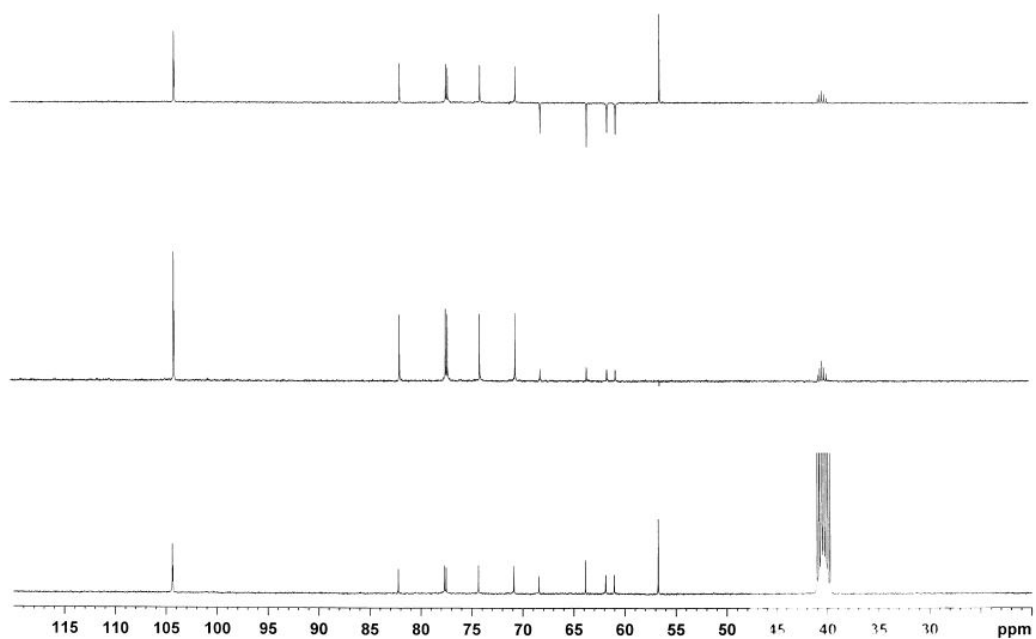


Figure S14. The DEPT Spectrum of compound 2

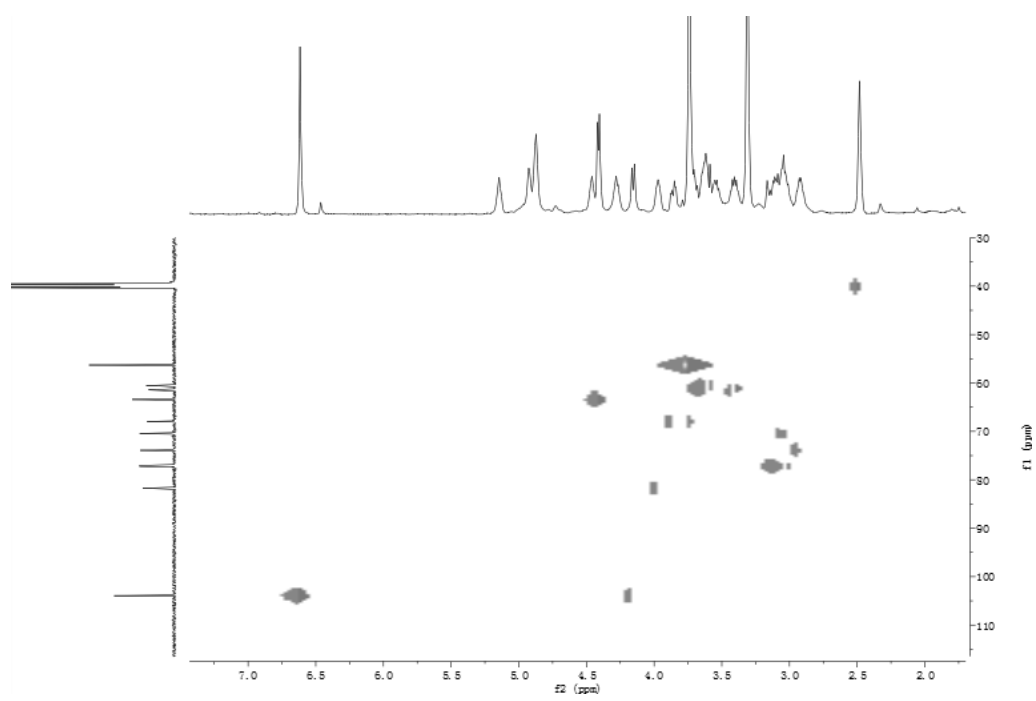


Figure S15. The HSQC Spectrum of compound 2

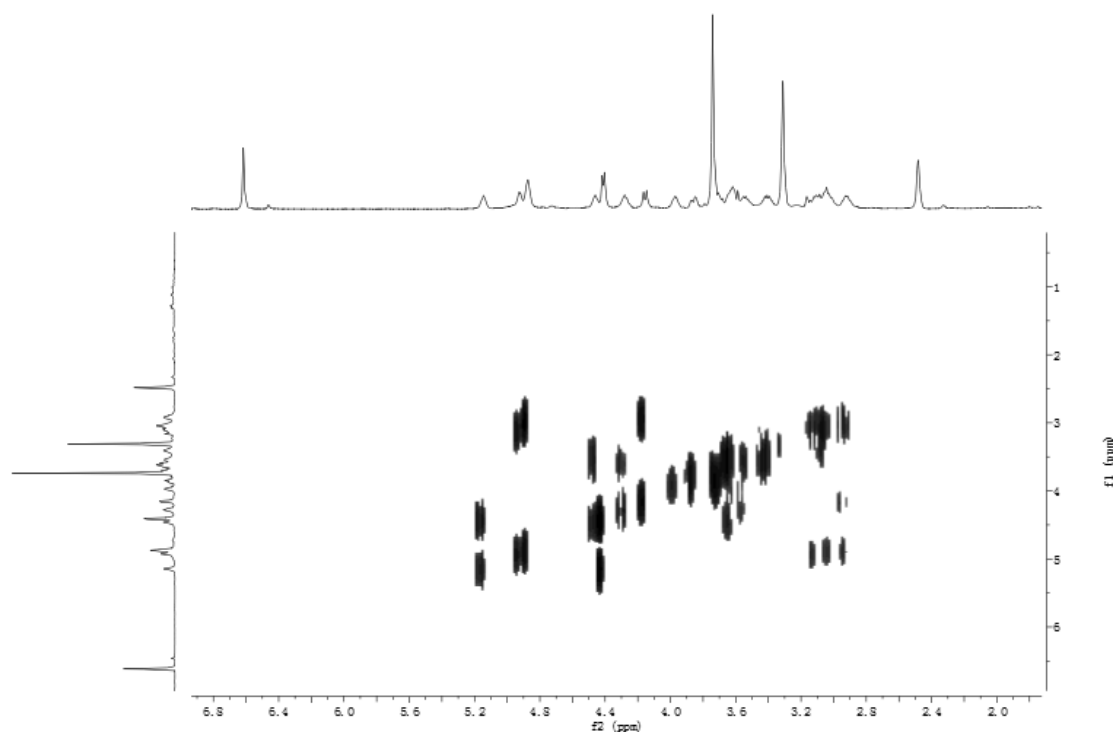


Figure S16. The ^1H , ^1H -COSY Spectrum of compound 2

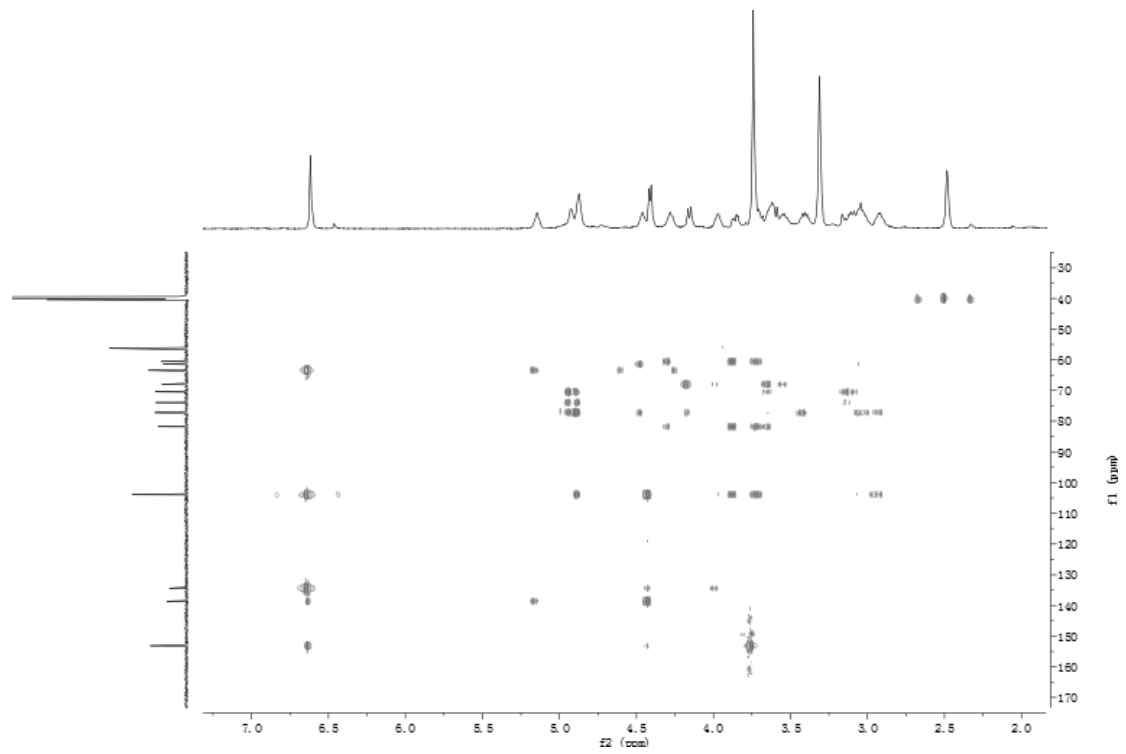


Figure S17. The HMBC Spectrum of compound 2

MS Formula Results: + Scan (3.831 min) Sub (2016031802.d)

m/z	Ion	Formula	Abundance
443.1532	(M+Na) ⁺	C18 H28 Na O11	355264.8

Best	Formula (M)	Ion Formula	Score	Cross Sco	Mass	Calc Mass	Calc m/z	Diff (ppm)	Abs Diff (ppm)	Mass Match	Abund Match	Spacing Match	DBE
✓	C18 H28 O11	C18 H28 Na O11	99.89		420.164	420.1632	443.1524	-1.95	1.95	99.89	99.89	99.9	5
	C31 H20 N2	C31 H20 N2 Na	94.87		420.164	420.1626	443.1519	-3.17	3.17	99.7	82.71	99.81	23

Figure S18. The HRESIMS Spectrum of compound 2

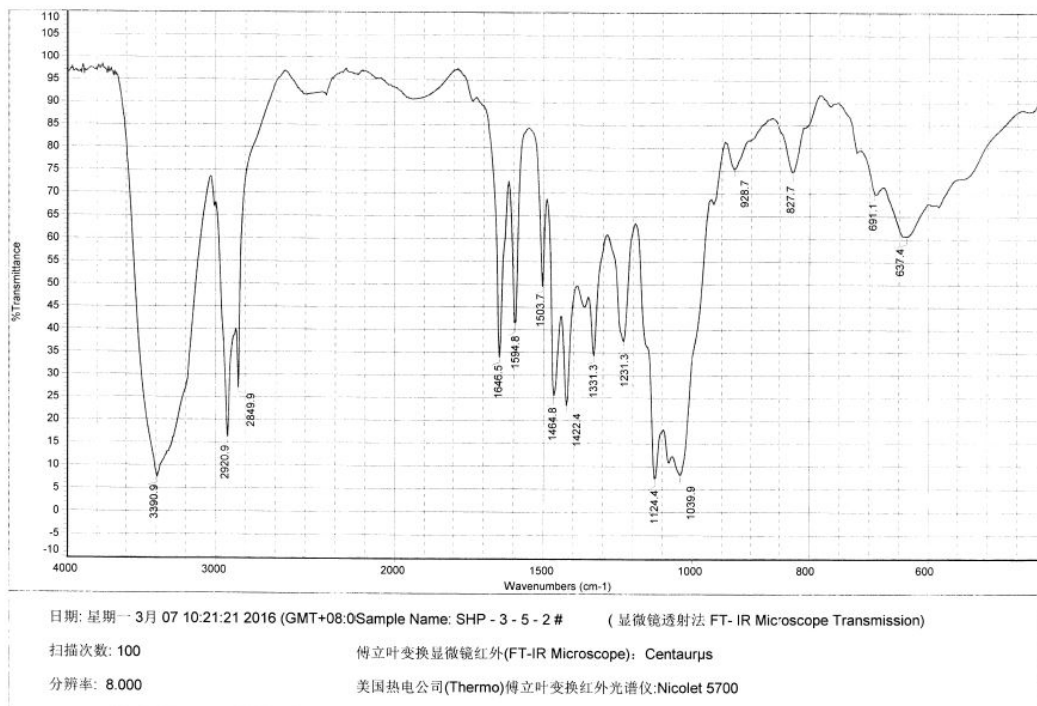


Figure S19. The IR Spectrum of compound 2

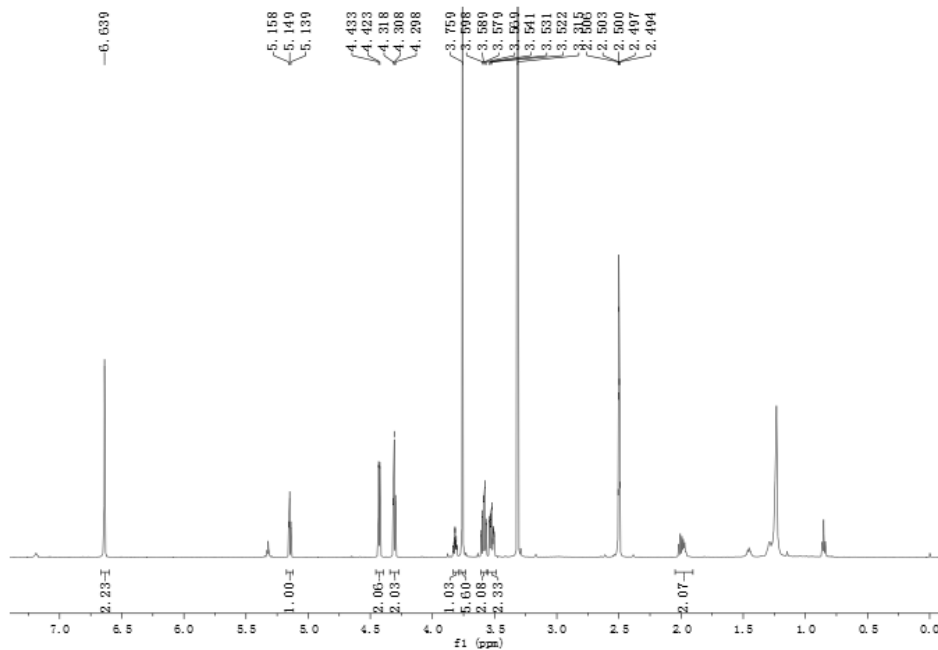


Figure S20. The ^1H NMR Spectrum of compound 2a (600 MHz, $\text{DMSO-}d_6$)

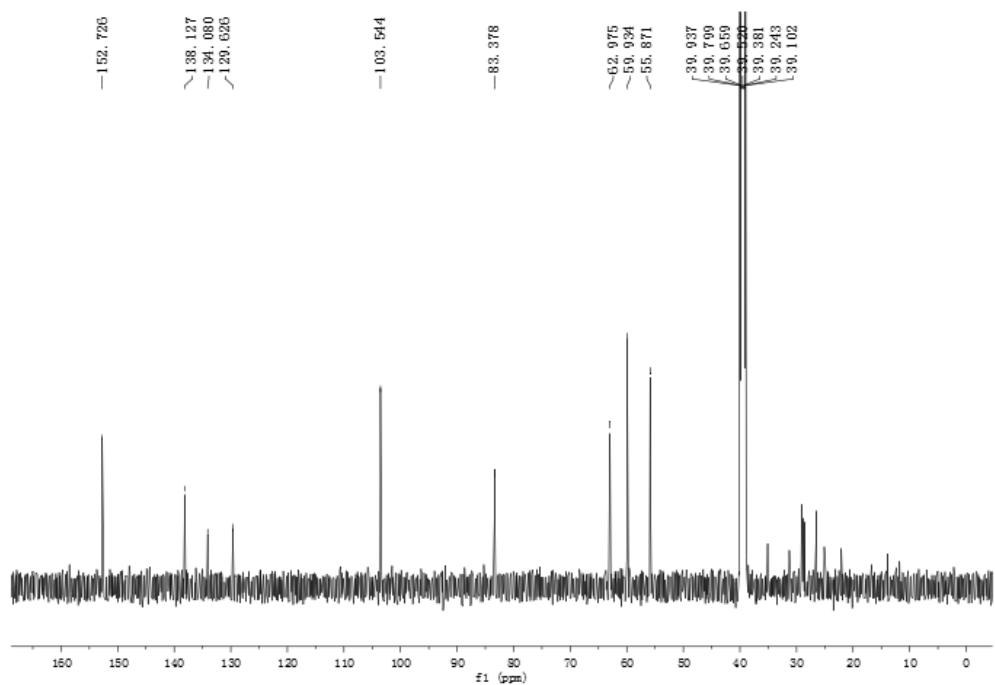


Figure S21. The ^{13}C NMR Spectrum of compound 2a (150 MHz, $\text{DMSO-}d_6$)

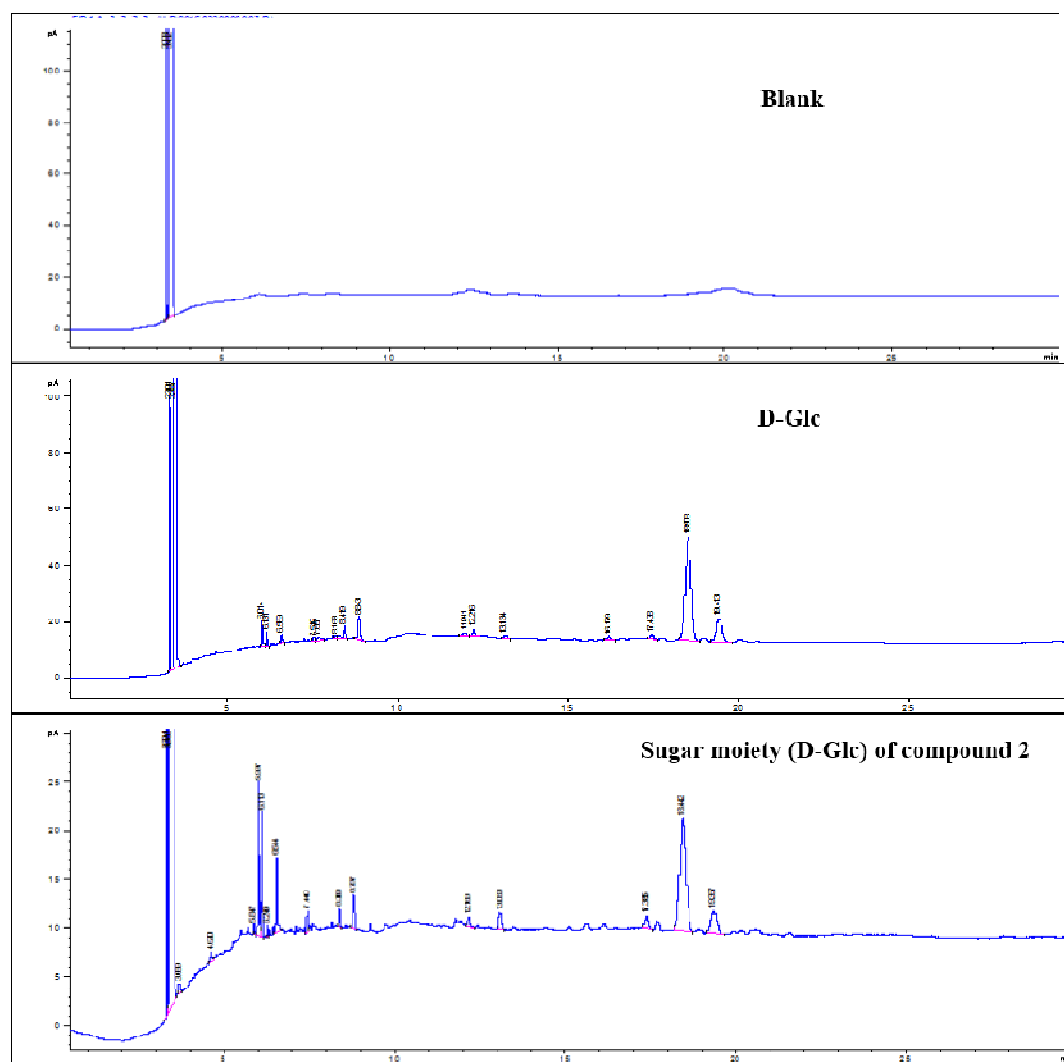


Figure S22. GC chromatogram of sugar moiety silylated after acid hydrolysis of 2

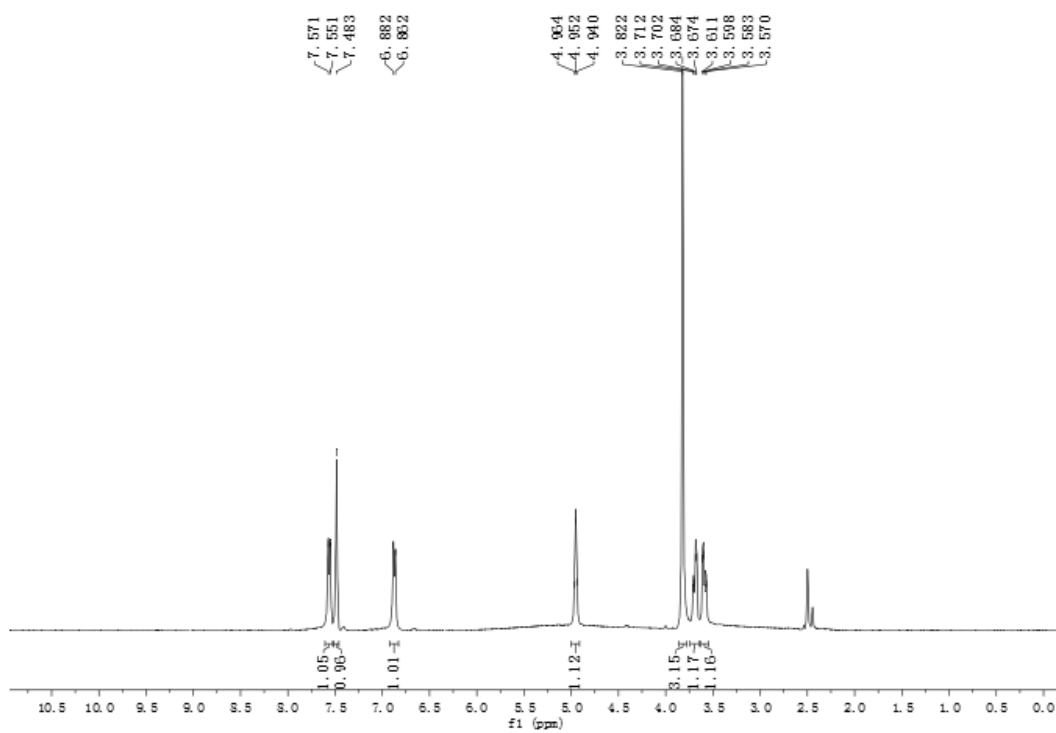


Figure S23. The ^1H NMR Spectrum of compound 3 (400 MHz, $\text{DMSO-}d_6$)

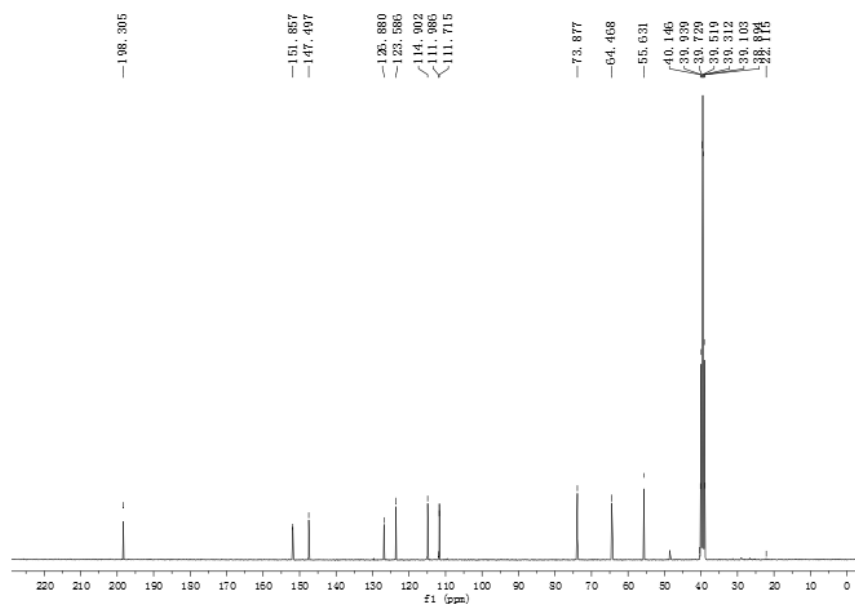


Figure S24. The ^{13}C NMR Spectrum of compound 3 (100 MHz, $\text{DMSO-}d_6$)

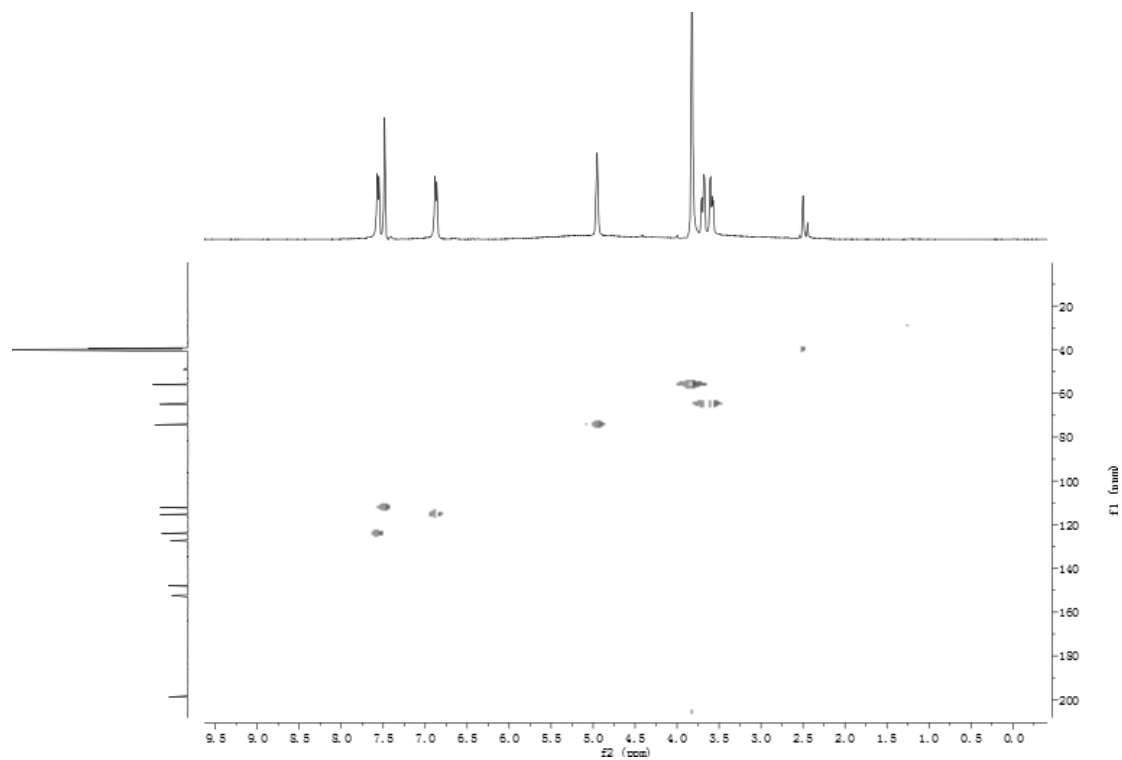


Figure S25. The HSQC Spectrum of compound 3

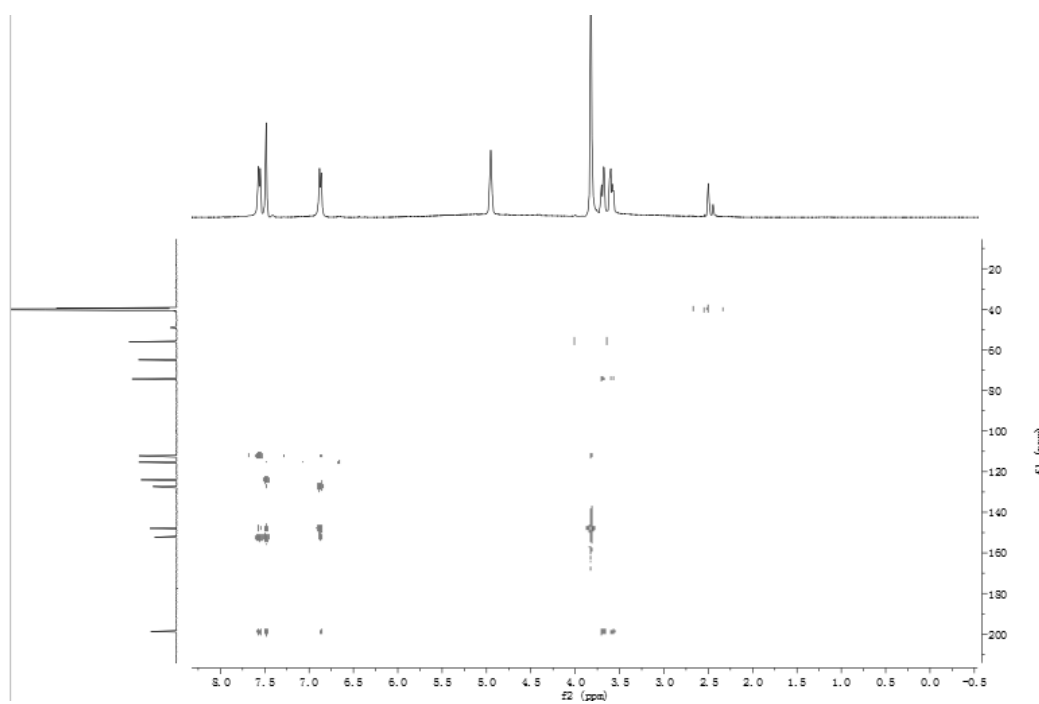


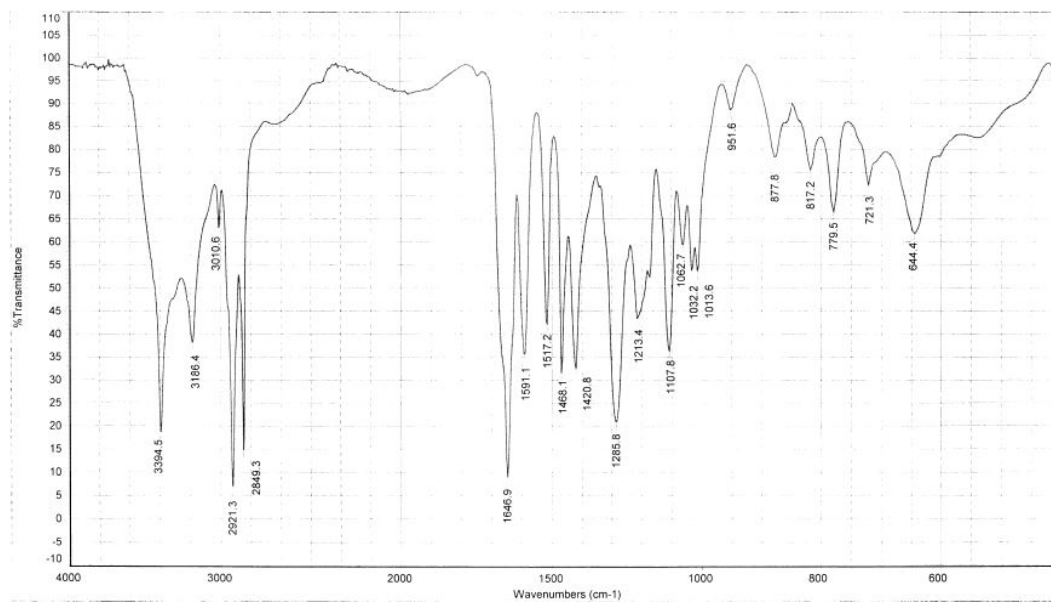
Figure S26. The HMBC Spectrum of compound 3

MS Formula Results: + Scan (1.789 min) Sub (2016031803.d)

m/z	Ion	Formula	Abundance
235.0573	(M+Na) ⁺	C ₁₀ H ₁₂ NaO ₅	76301.2

Best	Formula (M)	Ion Formula	Score	Cross Sco	Mass	Calc Mass	Calc m/z	Diff (ppm)	Abs Diff (ppm)	Mass Match	Abund Match	Spacing Match	DBE
✓	C ₁₀ H ₁₂ O ₅	C ₁₀ H ₁₂ NaO ₅	99.92		212.0681	212.0685	235.0577	1.83	1.83	99.92	99.88	99.95	5

Figure S27. The HRESIMS Spectrum of compound 3



日期: 星期一 3月 07 10:54:50 2016 (GMT+08:0) Sample Name: SHP - 11 - 1# - 1# (显微镜透射法 FT-IR Microscope Transmission)

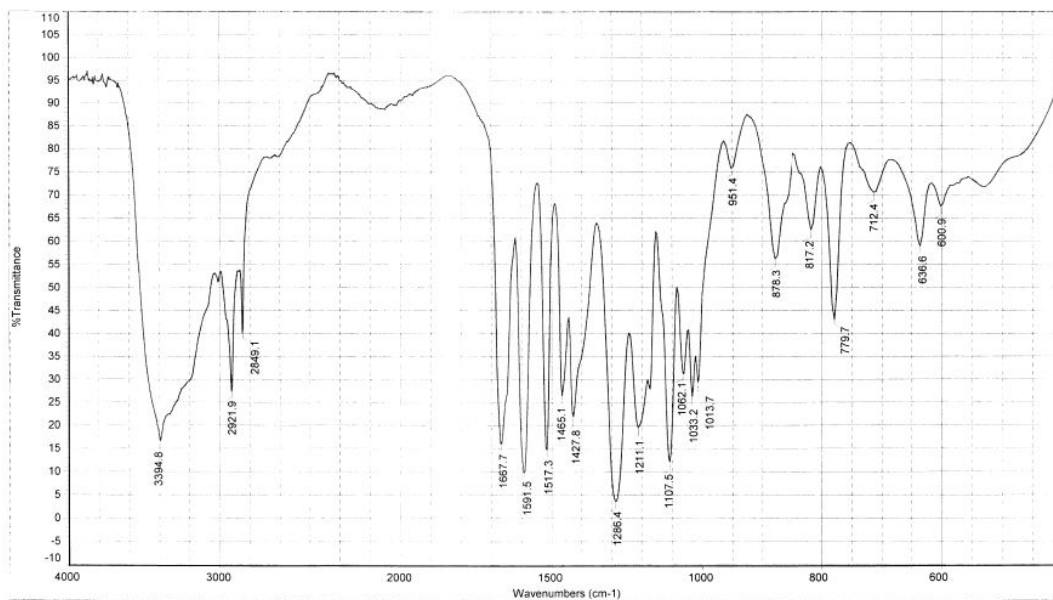
扫描次数: 100

傅立叶变换显微镜红外 (FT-IR Microscope): Centaurus

分辨率: 8.000

美国热电公司 (Thermo) 傅立叶变换红外光谱仪: Nicolet 5700

Figure S28. The IR Spectrum of compound 3a



日期: 星期一 3月 07 10:47:33 2016 (GMT+08:00) Sample Name: SHP - 11 - 1# - 2# (显微镜透射法 FT- IR Microscope Transmission)

扫描次数: 100

傅立叶变换显微镜红外(FT-IR Microscope): Centaurus

分辨率: 8.000

美国热电公司(Thermo)傅立叶变换红外光谱仪:Nicolet 5700

Figure S29. The IR Spectrum of compound 3b

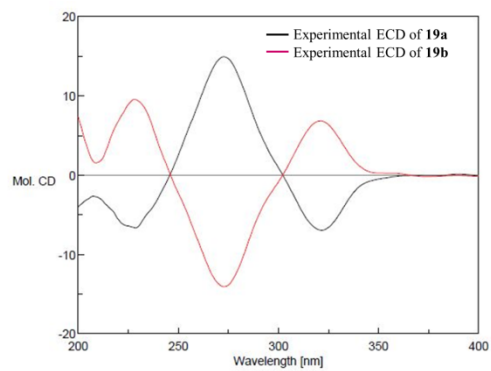


Figure S30. The experimental CD Spectrum of compound 3a and 3b in

MeOH

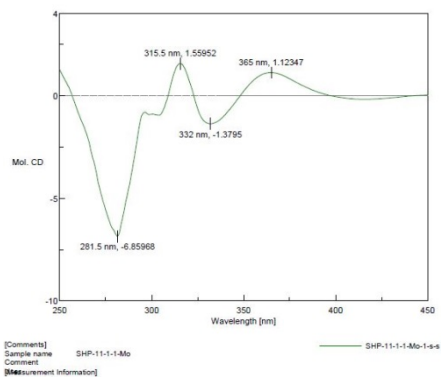


Figure S31. The $\text{Mo}_2(\text{OAc})_4$ Induced CD Spectrum of compound 3a

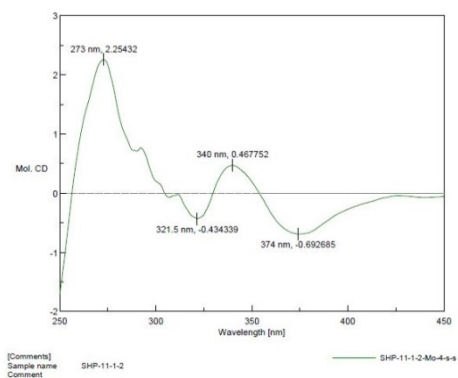


Figure S32. The $\text{Mo}_2(\text{OAc})_4$ Induced CD Spectrum of compound 3b

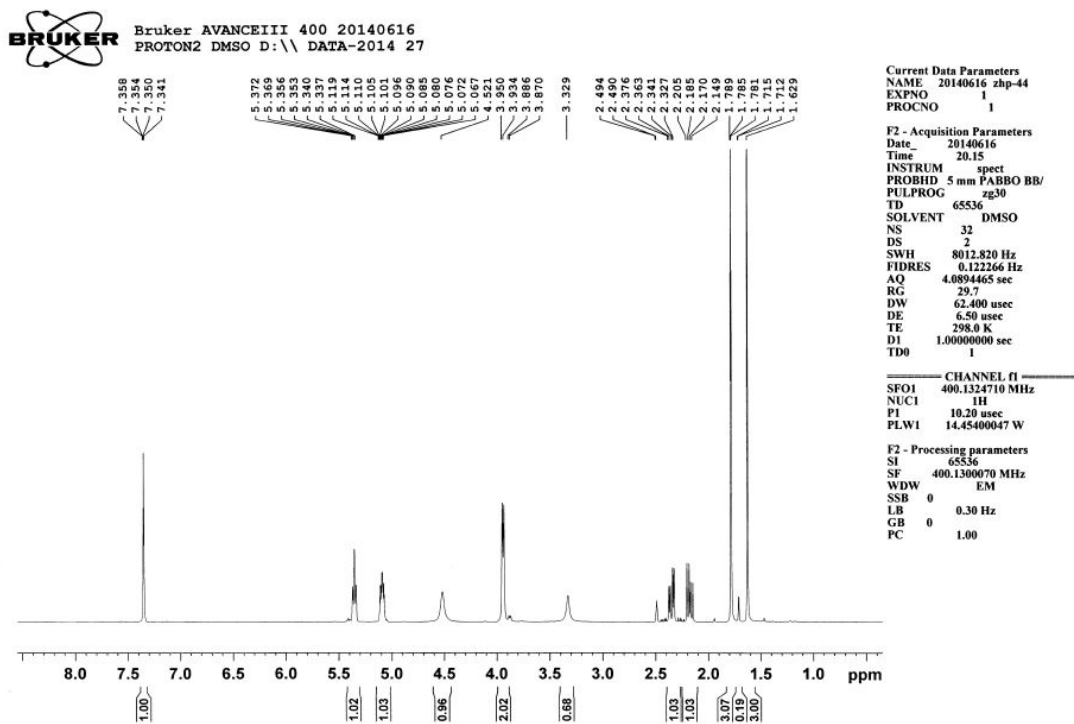
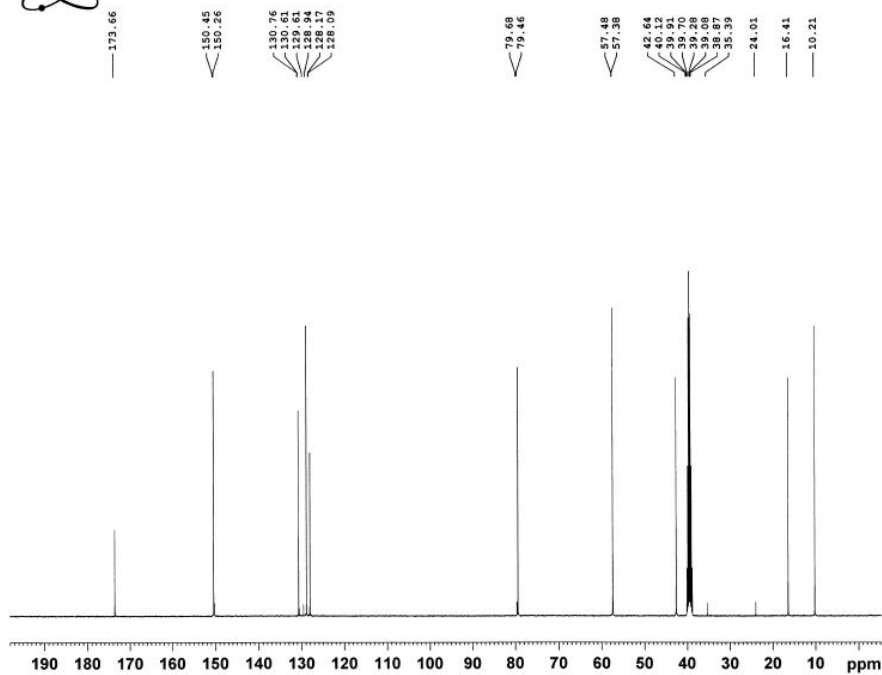


Figure S33. The ^1H NMR Spectrum of compound 4 (600 MHz, $\text{DMSO-}d_6$)



Bruker AVANCEIII 400 20140604
C13 DMSO D:\ DATA-2014 13



Current Data Parameters
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EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
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FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 194.76
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 400

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NUC1 13C
P1 10.00 usec
PLW1 70.00000000 W

==== CHANNEL f2 =====
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NUC2 1H
CPDPRG2 waltz16
PCPD2 80.00 usec
PLW2 14.45400047 W
PLW12 0.23497000 W
PLW13 0.15038000 W

F2 - Processing parameters
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SF 100.6128163 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S34. The ^{13}C NMR Spectrum of compound 4 (150 MHz, $\text{DMSO-}d_6$)



Bruker AVANCEIII 400 20140604 ZHP-44
DEPT DMSO D:\ DATA-2014 13

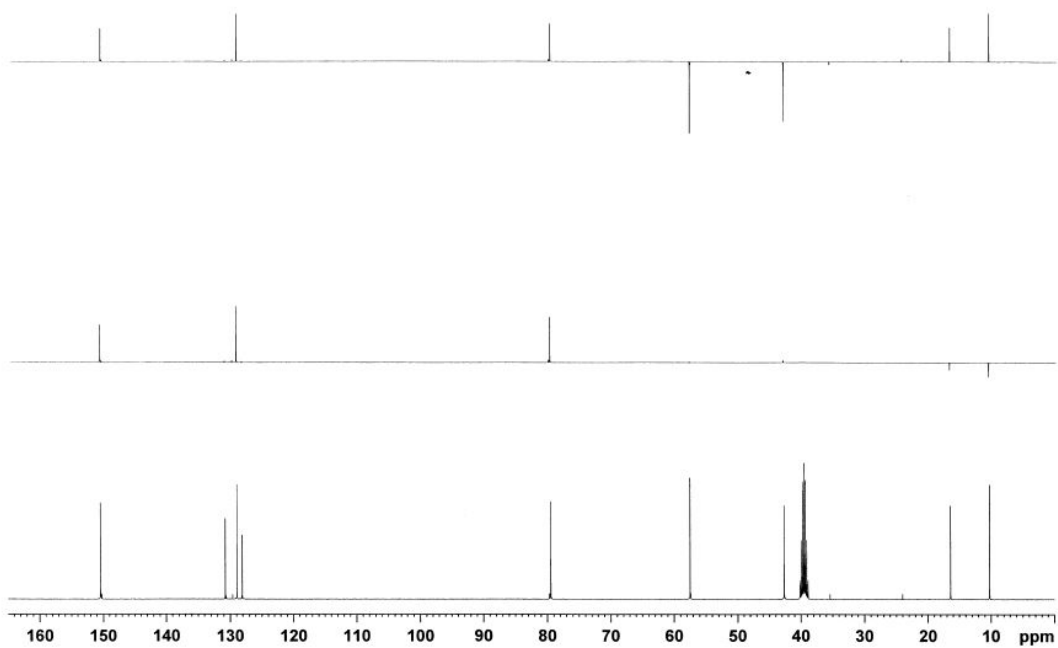
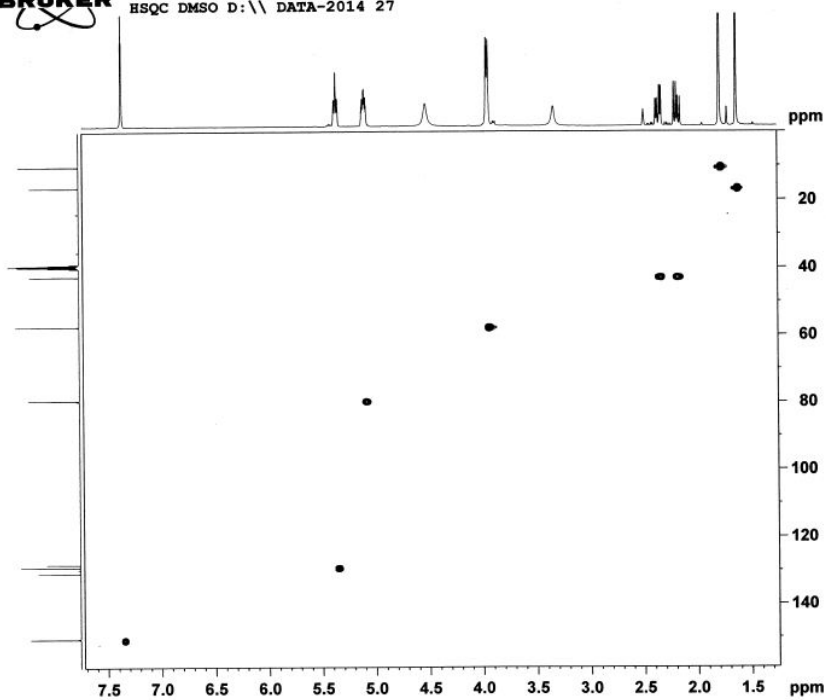


Figure S35. The DEPT Spectrum of compound 4



Bruker AVANCEIII 400 20140616
HSQC DMSO D:\ DATA-2014 27



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EXPNO 4
PROCNO 1

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TD 1024
SOLVENT DMSO
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DS 16
SWH 5597.015 Hz
FIDRES 5.465835 Hz
AQ 0.0914773 sec
RG 194.76
DW 89.333 usec
DE 6.50 usec
TE 298.1 K
CNS12 145.0000000
CNS17 1.0000000
D0 0.00000300 sec
D1 1.00000000 sec
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D24 0.00110000 sec
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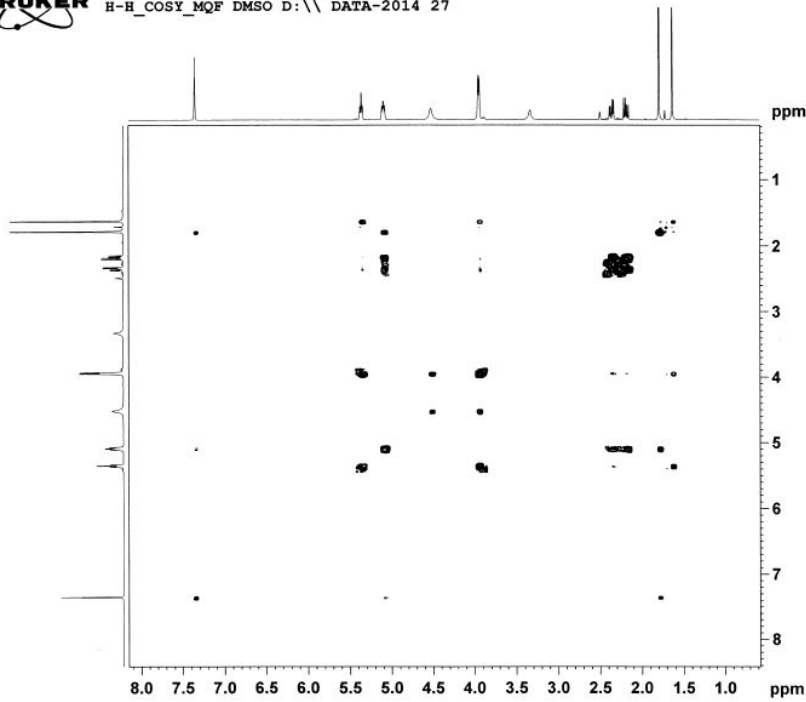
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P2 20.40 usec
P28 1000.00 usec
PLW1 14.45400047 W

CHANNEL f2
SFO2 100.6228284 MHz
NUC2 13C
CPDPRG2 garp
P3 10.05 usec
P14 500.00 usec
P24 2000.00 usec
PCPD2 70.00 usec
PLW0 0 W
PLW2 69.38400116 W
PLW12 1.50660002 W
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SFOAL3 0.500
SFOFS3 0 Hz
SPW3 10.80000019 W
SPNAM[7] Crp60comp.4
SFOAL7 0.500
SFOFS7 0 Hz
SPW7 10.80000019 W

Figure S36. The HSQC Spectrum of compound 4



Bruker AVANCEIII 400 20140616
H-H_COSY_MQF DMSO D:\\ DATA-2014 27



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Current Data Parameters
NAME 20140616 zhp-44
EXPNO 6
PROCNO 1

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TD 2048
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DS 16
SWH 5341.830 Hz
FIDRES 2.608340 Hz
AQ 0.1916928 sec
RG 194.76
DW 93.600 usec
DE 6.50 usec
TE 298.0 K
D0 0.00000300 sec
D1 2.00000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00018720 sec

----- CHANNEL f1 -----
SFO1 400.1324857 MHz
NUC1 1H
PI 10.20 usec
PLW1 14.45400047 W

----- GRADIENT CHANNEL -----
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GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 16.00 %
GPZ2 12.00 %
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
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FIDRES 41.733440 Hz
SW 13.350 ppm
FqMODE QF

F2 - Processing parameters
SI 1024
SF 400.1300088 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 400.1300000 MHz
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Figure S37. The ^1H , ^1H -COSY Spectrum of compound 4



Bruker AVANCEIII 400 20140604 ZHP-44
DEPT DMSO D:\ \ DATA-2014 13

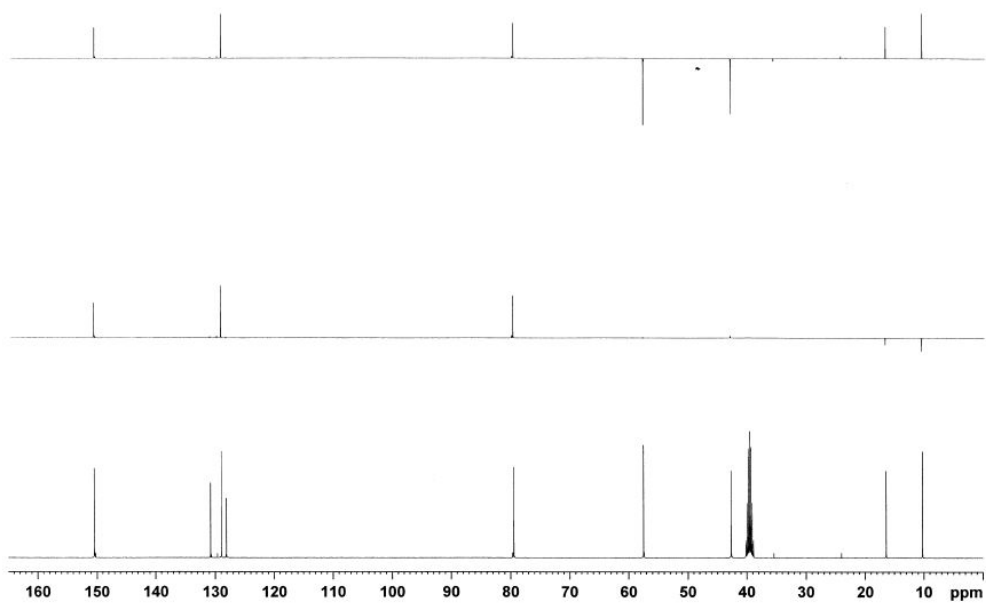


Figure S38. The HMBC Spectrum of compound 4

MS Formula Results: + Scan (4.334 min) Sub (2014061603.d)

m/z	Ion	Formula	Abundance
205.0835	(M+Na) ⁺	C ₁₀ H ₁₄ NaO ₃	1367869.5

Best	Formula (M)	Ion Formula	Score	Cross Sco	Mass	Calc Mass	Calc m/z	Diff (ppm)	Abs Diff (ppm)	Mass Match	Abund Match	Spacing Match	DBE
☑	C ₁₀ H ₁₄ O ₃	C ₁₀ H ₁₄ NaO ₃	99.99		182.0942	182.0943	205.0835	0.33	0.33	100	99.99	99.98	4

Figure S39. The HRESIMS Spectrum of compound 4

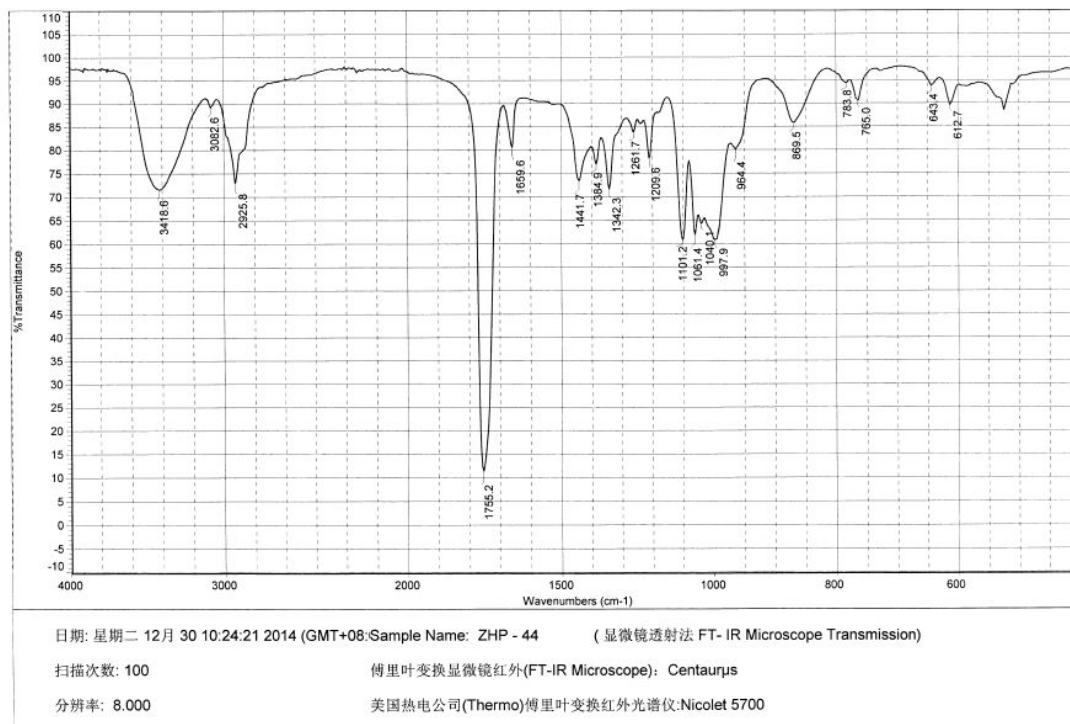


Figure S40. The IR Spectrum of compound 4

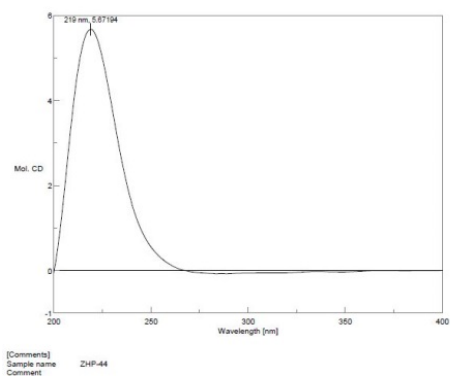


Figure S41. The CD Spectrum of compound 4

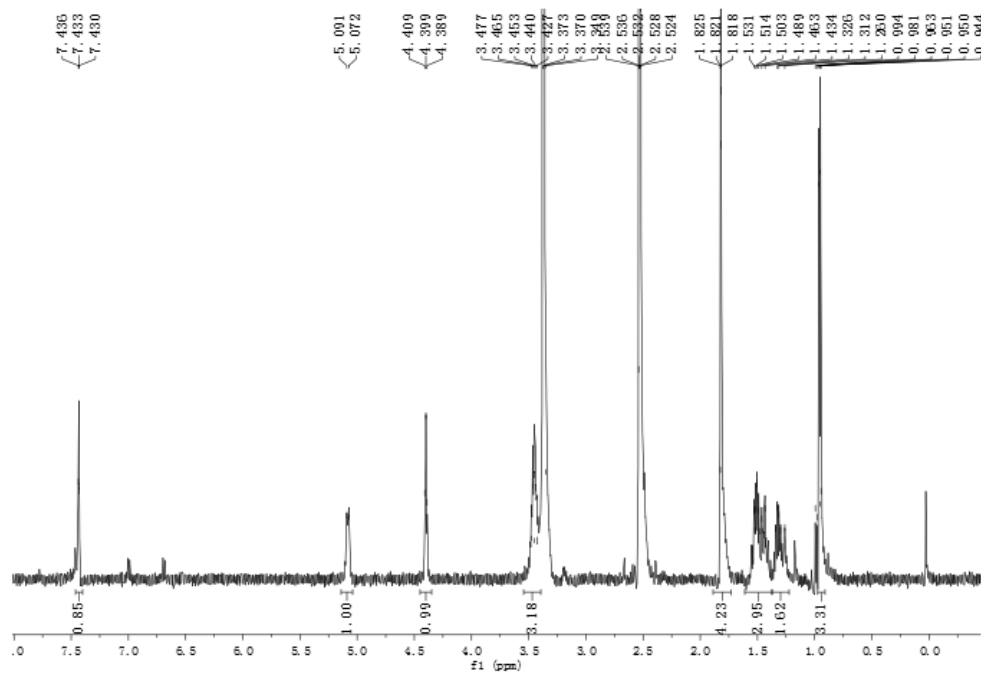


Figure S42. The ^1H NMR Spectrum of compound 5 (600 MHz, $\text{DMSO-}d_6$)

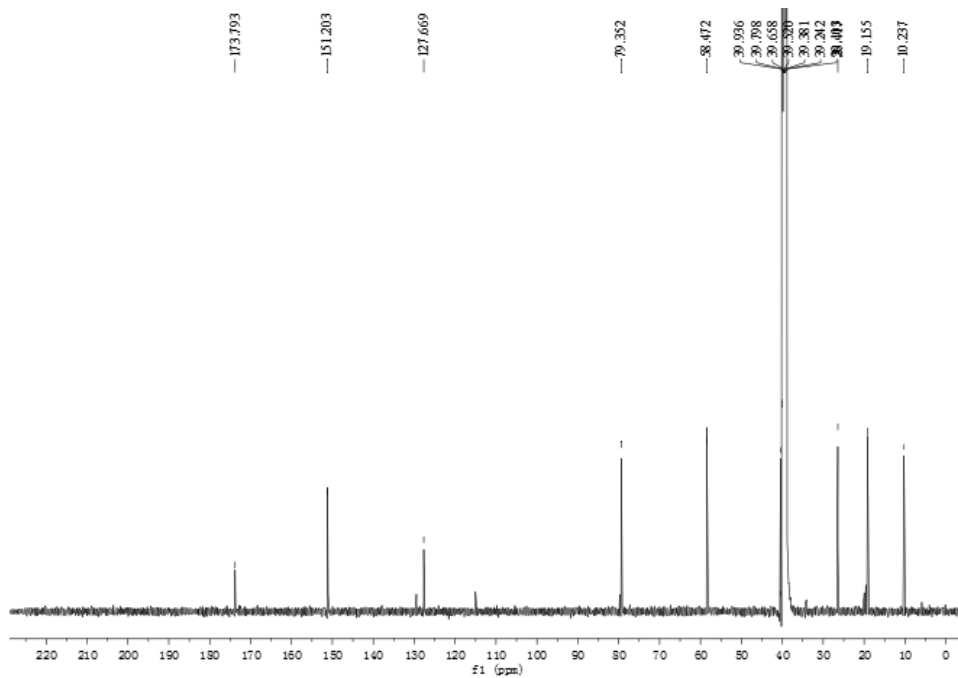


Figure S43. The ^{13}C NMR Spectrum of compound 5 (150 MHz, $\text{DMSO-}d_6$)



Bruker AVIIIHD 600 20150529
DEPT DMSO D:\\ DATA2015 27

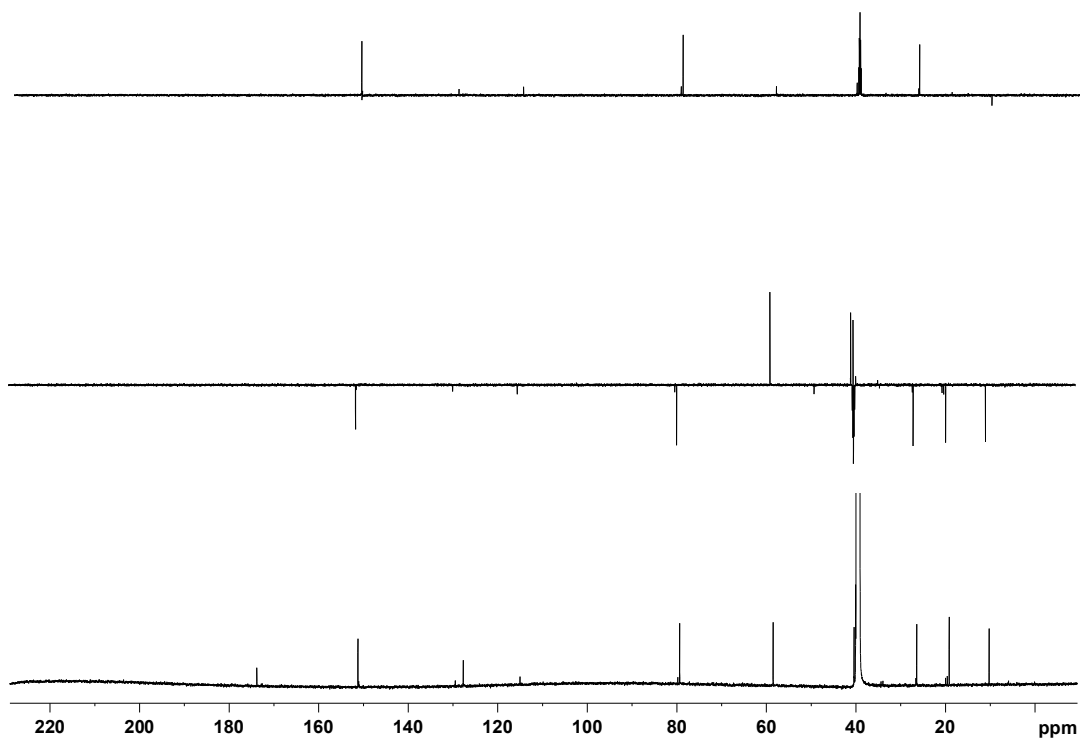


Figure S44. The DEPT Spectrum of compound 5

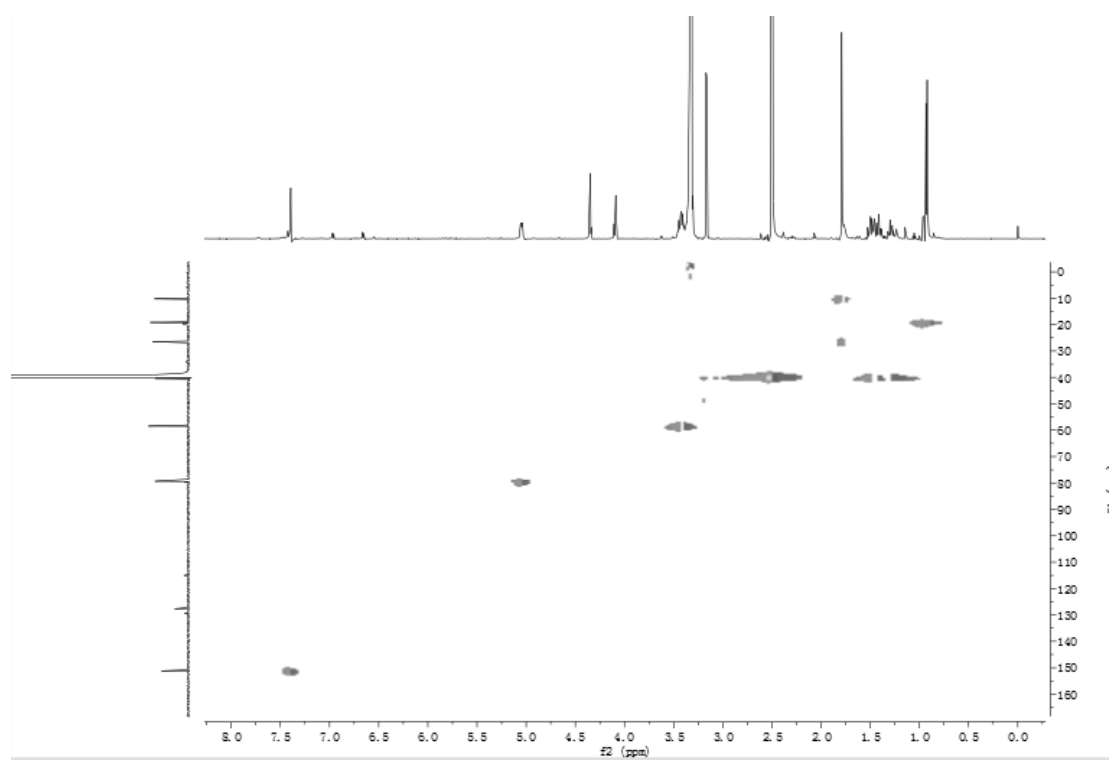


Figure S45. The HSQC Spectrum of compound 5

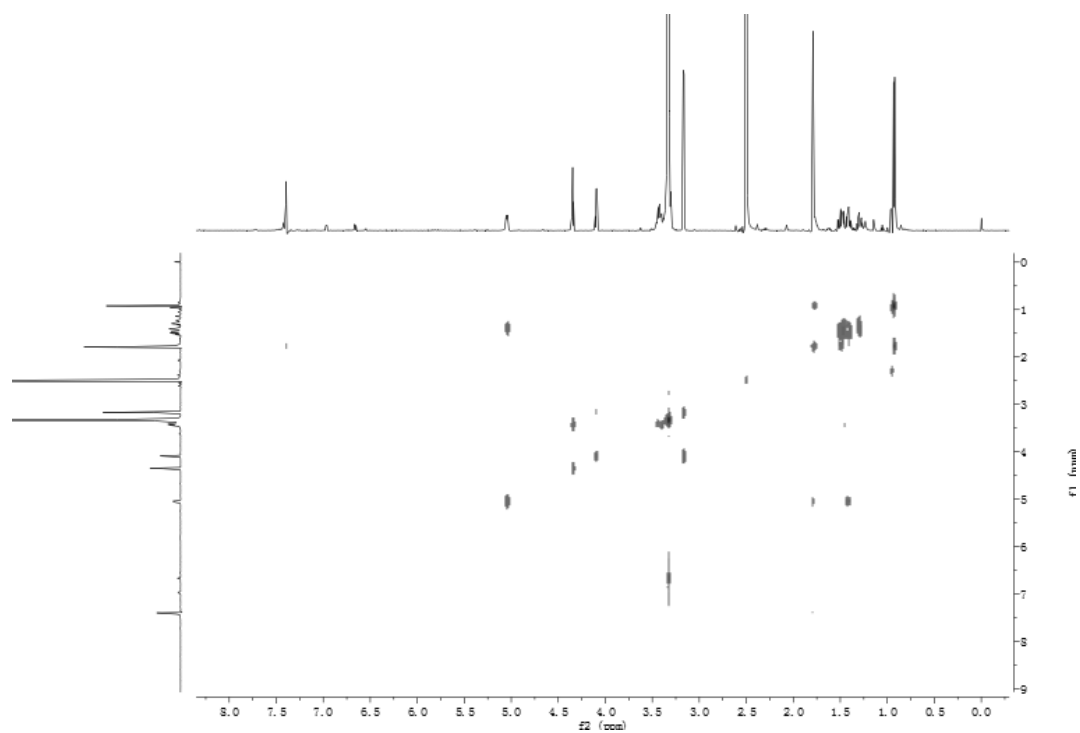


Figure S46. The ^1H , ^1H -COSY Spectrum of compound 5

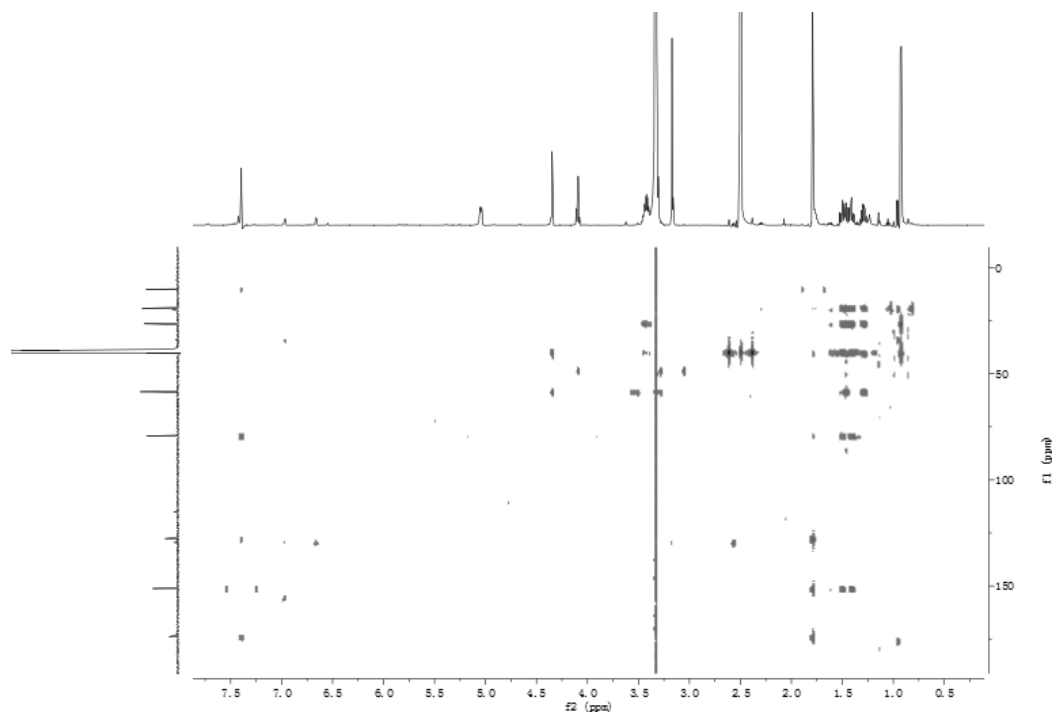


Figure S47. The HMBC Spectrum of compound 5

MS Formula Results: + Scan (4.882 min) Sub (2016031804.d)

m/z	Ion	Formula	Abundance
207.0993	(M+Na) ⁺	C ₁₀ H ₁₆ NaO ₃	89198.8

Best	Formula (M)	Ion Formula	Score	Cross Sco	Mass	Calc. Mass	Calc. m/z	Diff (ppm)	Abn Diff (ppm)	Mass Match	Abund Match	Spacing Match	DBE
✓	C ₁₀ H ₁₆ O ₃	C ₁₀ H ₁₆ NaO ₃	97.42		184.1101	184.1099	207.0992	-0.64	0.64	99.99	99.65	89.59	3

Figure S48. The HRESIMS Spectrum of compound 5

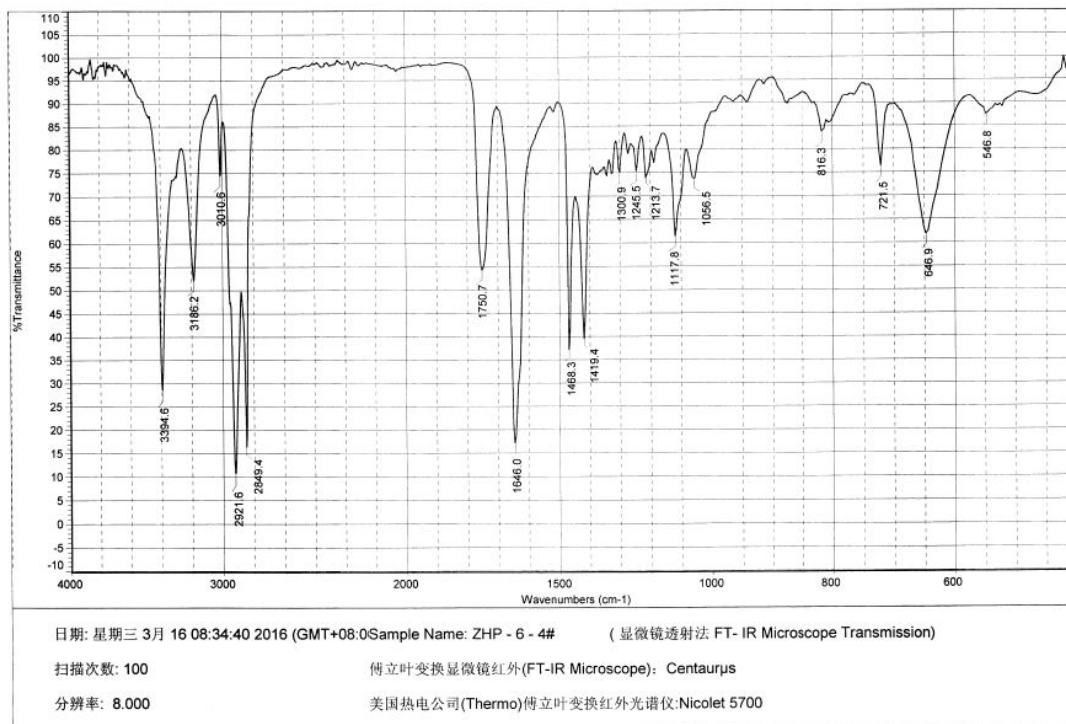


Figure S49. IR Spectrum of compound 5

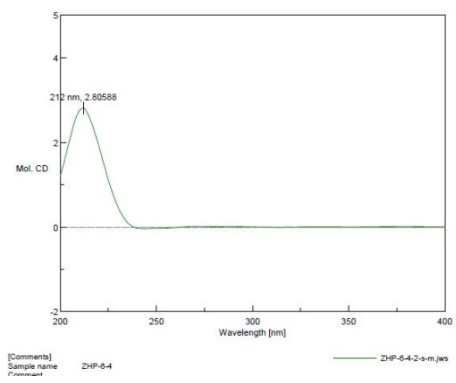


Figure S50. CD Spectrum of compound 5