

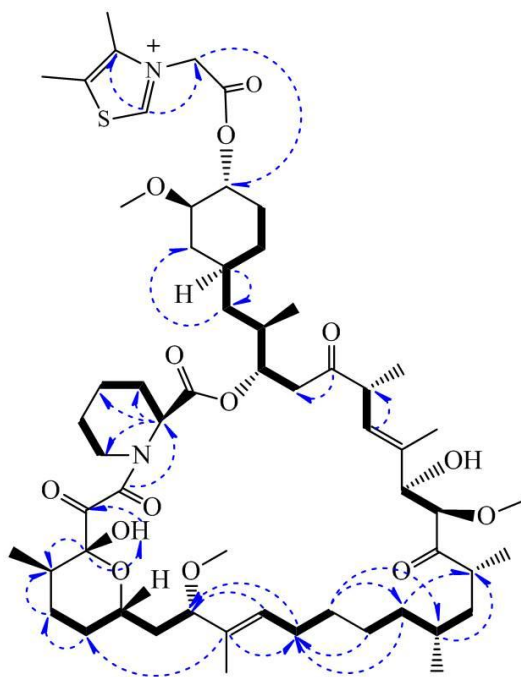
Supplementary File

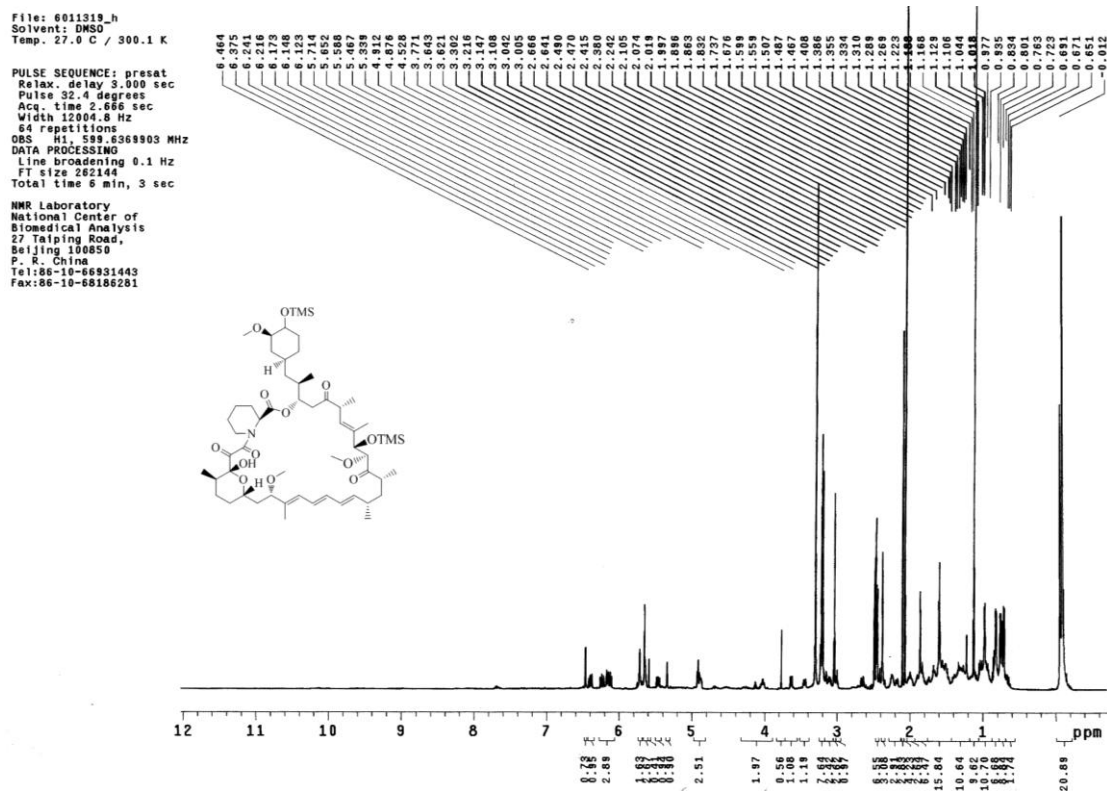
Content

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1. The Complete Simulate 3D Structure and Selected COSY and HMBC Correlations Exhibited by Compound **1**

Figure S1. Selected COSY and HMBC correlations exhibited by compound **1**.





3. 1D, 2D NMR, LCMS and IR Spectra of Compound 1–11

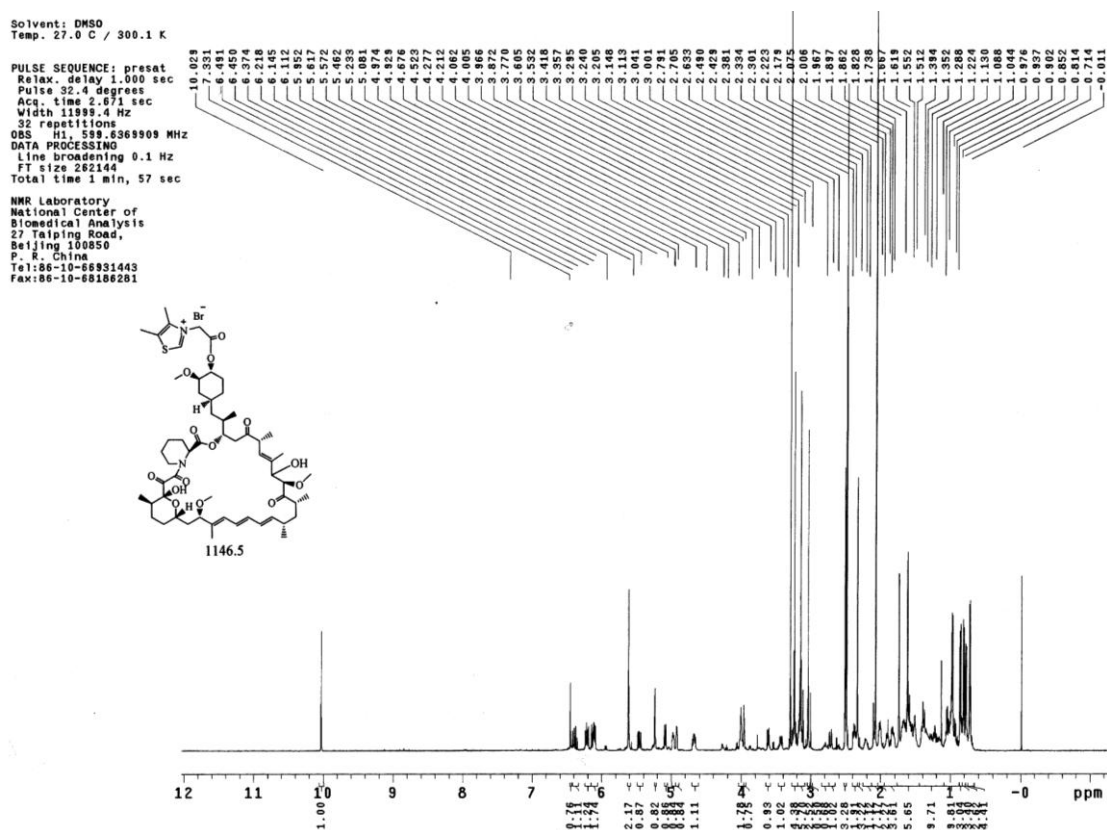
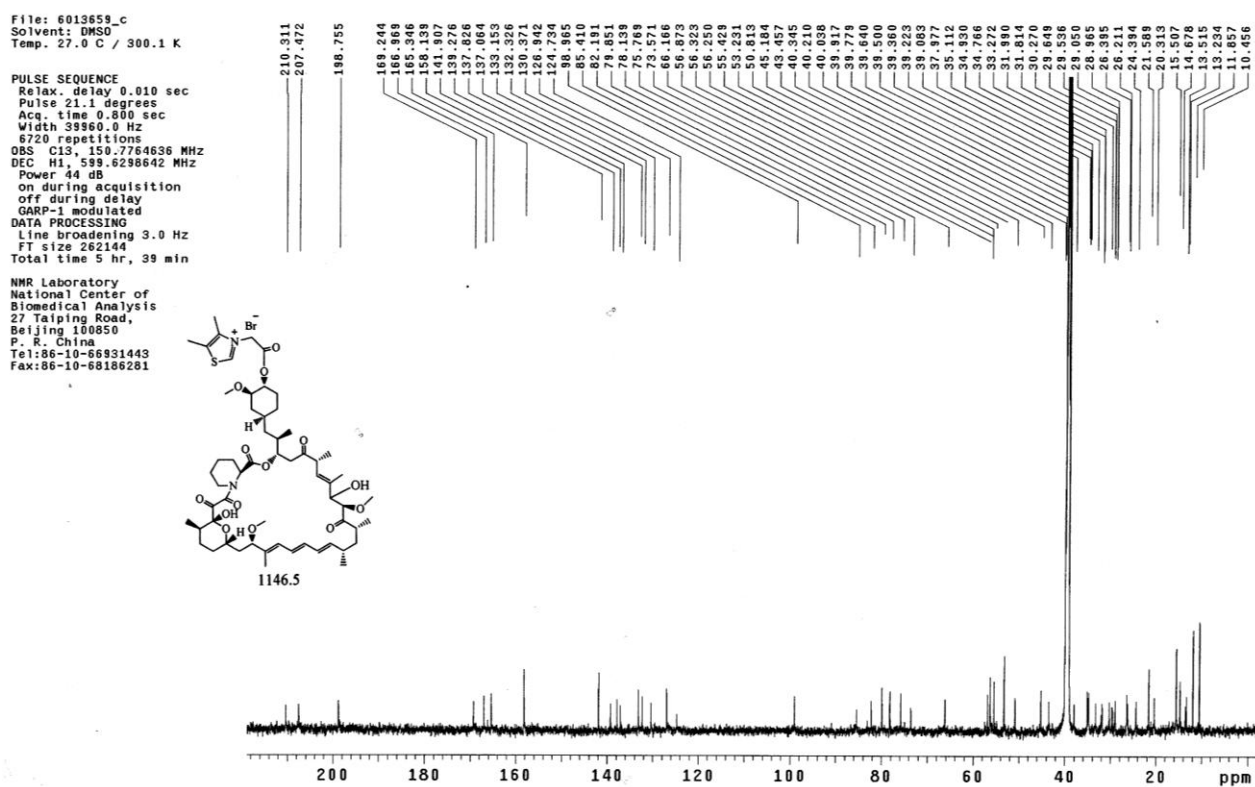
Figure S4. ^1H -NMR of compound 1.Figure S5. ^{13}C -NMR of compound 1.

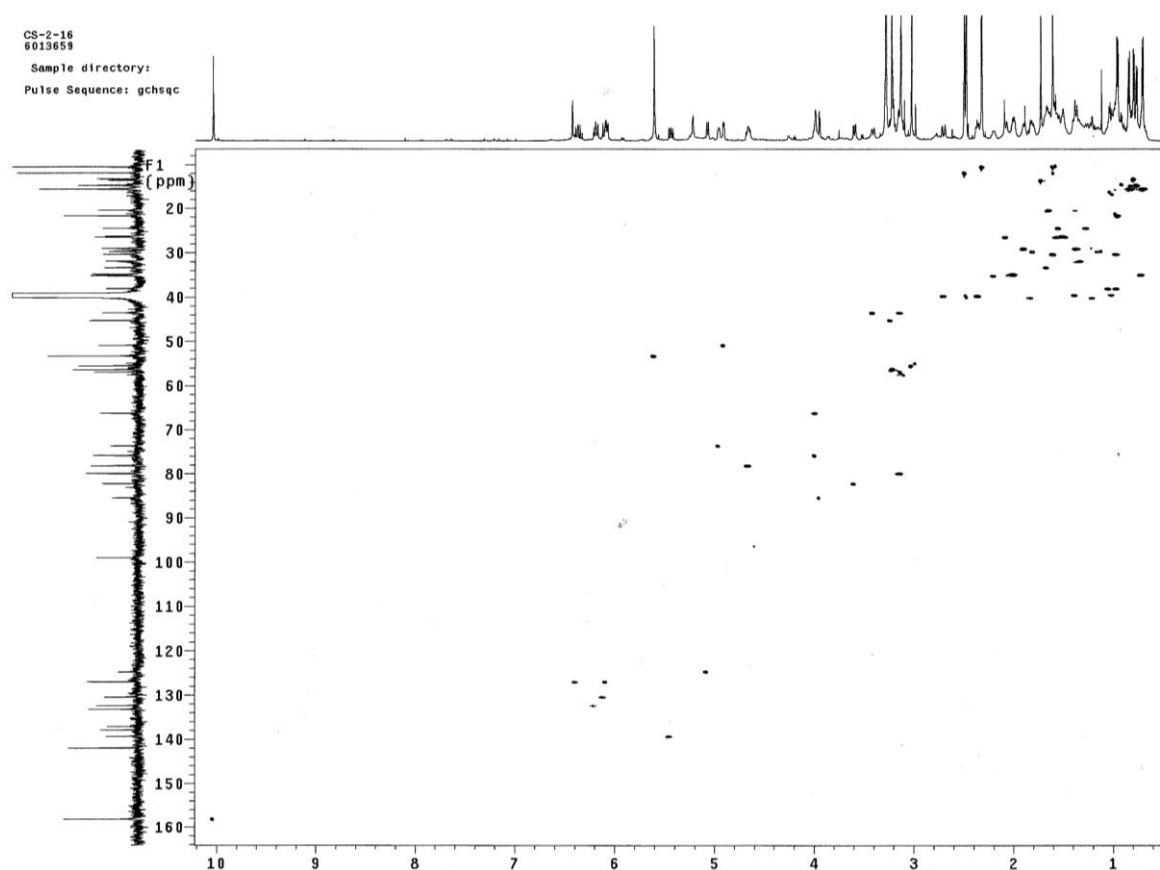
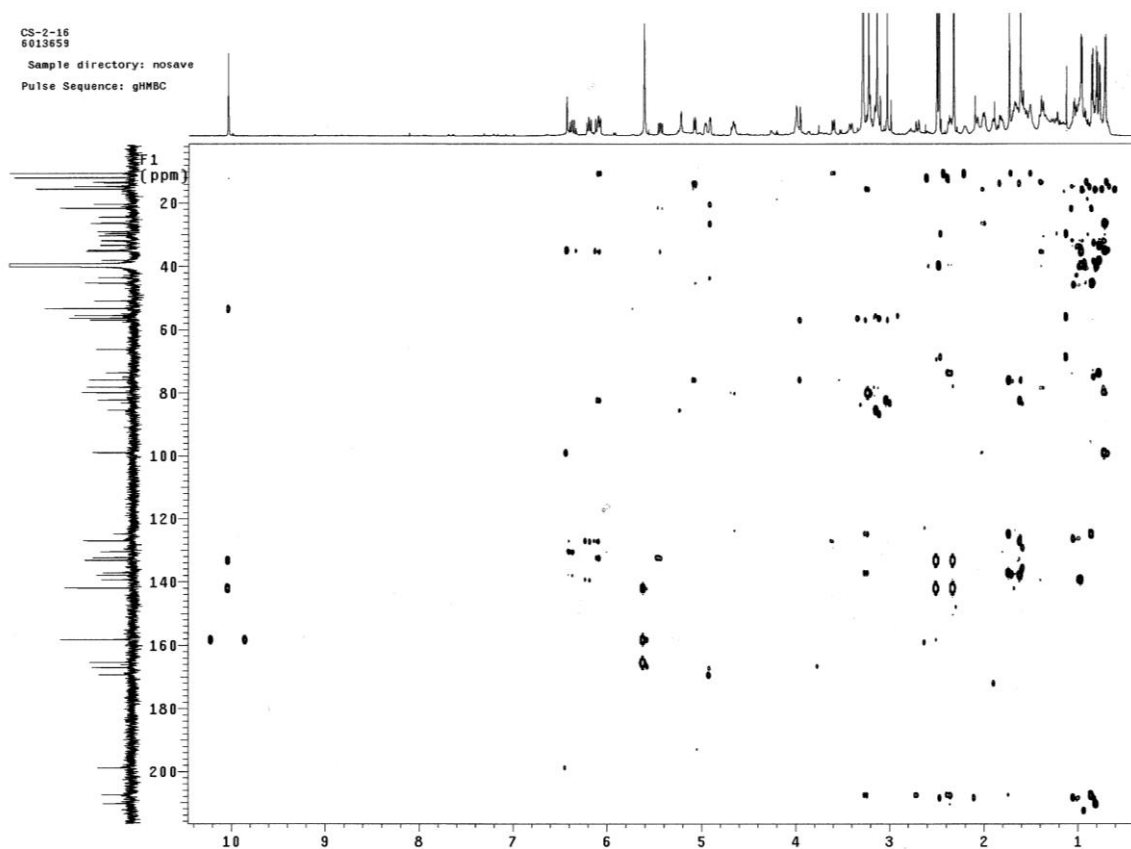
Figure S6. HSQC of compound 1.**Figure S7. HMBC of compound 1.**

Figure S8. COSY of compound 1.

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6013659
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Pulse Sequence: gCOSYpr
Spectrometer: "ncba600"
VARIAN INOVA 600
File: 6013659_cosy_2
Solvent: DMSO
Temp. 27.0 C / 300.1 K

PULSE SEQUENCE: gCOSYpr
Relax. delay 1.000 sec
Acq. time 0.293 sec
Width 6982.6 Hz
2D Width 6982.6 Hz
8 repetitions
512 increments
OBS H1, 599.6272226 MHz
DATA PROCESSING
Sq. sine bell 0.147 sec
F1 DATA PROCESSING
Sq. sine bell 0.037 sec
FT size 4096 x 4096
Total time 1 hr, 32 min

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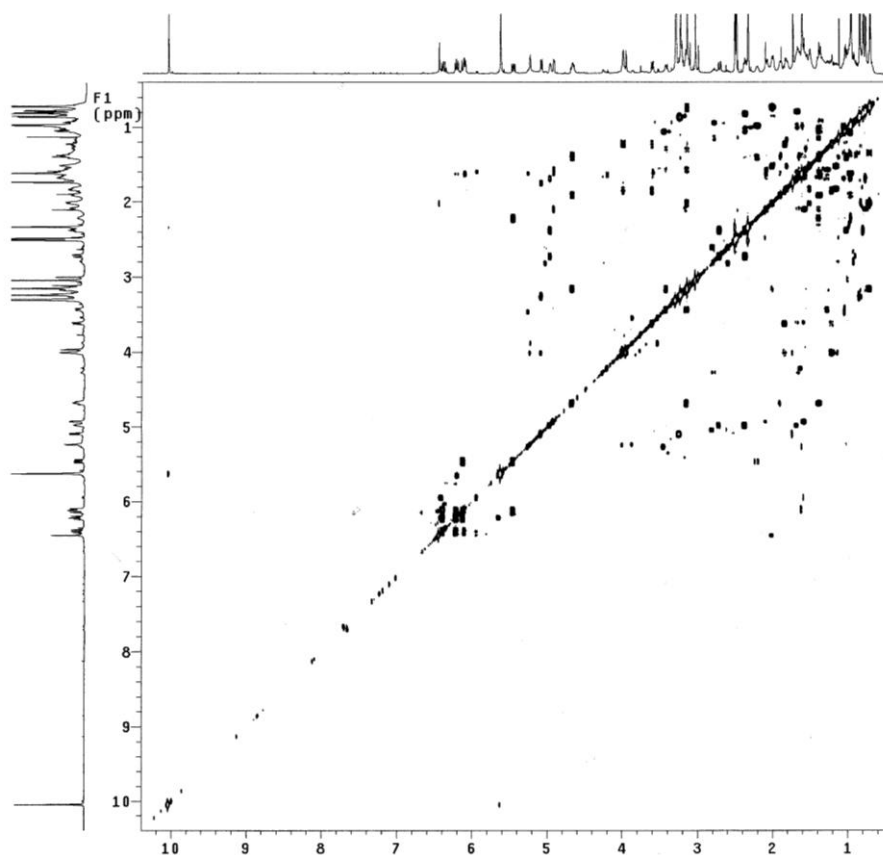


Figure S9. ROESY of compound 1.

CS-2-16
6013659
Sample directory: nosave
Pulse Sequence: ROESY
Spectrometer: "ncba600"
VARIAN INOVA 600
File: 6013659_roesy
Solvent: DMSO
Temp. 27.0 C / 300.1 K

PULSE SEQUENCE: ROESY
Relax. delay 1.000 sec
Mixing 0.250 sec
Acq. time 0.293 sec
Width 6982.6 Hz
2D Width 6982.6 Hz
32 repetitions
2 x 256 increments
OBS H1, 599.6272226 MHz
DATA PROCESSING
Sq. sine bell 0.293 sec
Shifted by -0.233 sec
F1 DATA PROCESSING
Sq. sine bell 0.073 sec
Shifted by -0.073 sec
FT size 4096 x 4096
Total time 7 hr, 11 min

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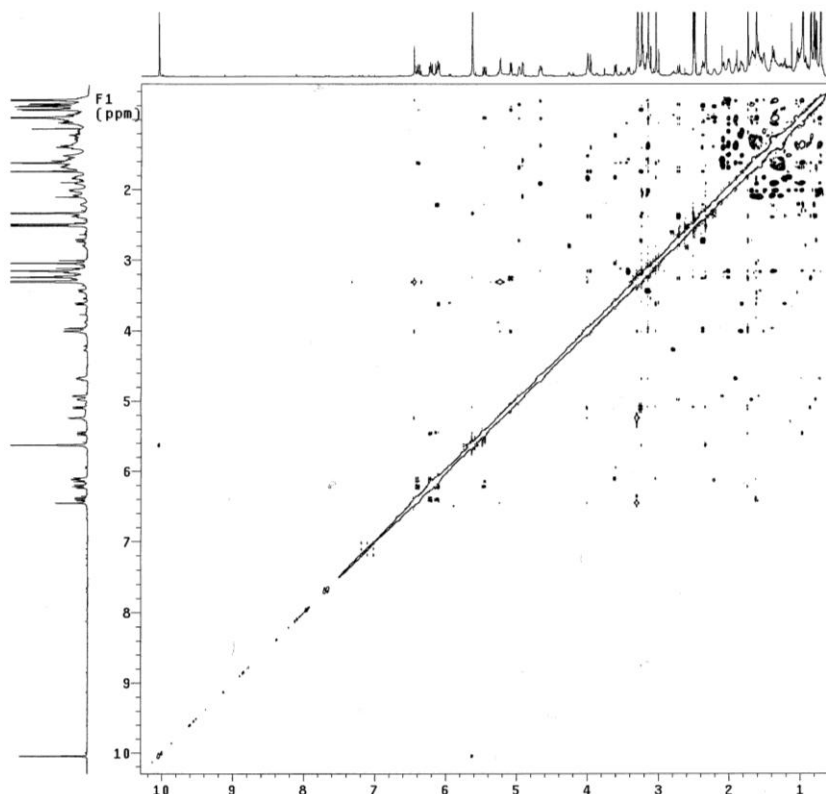


Figure S10. TOCSY of compound 1.

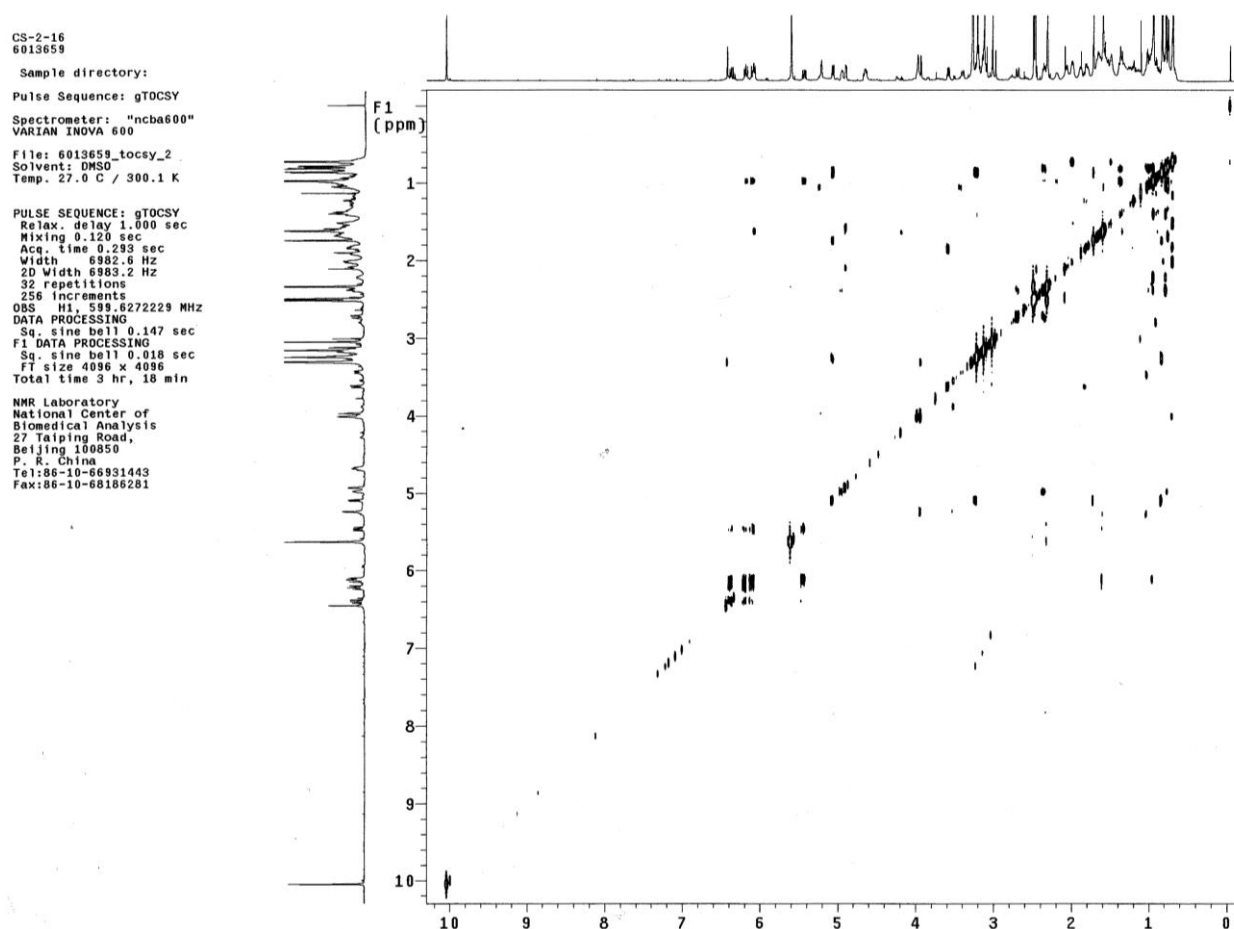


Figure S11. MS of compound 1.

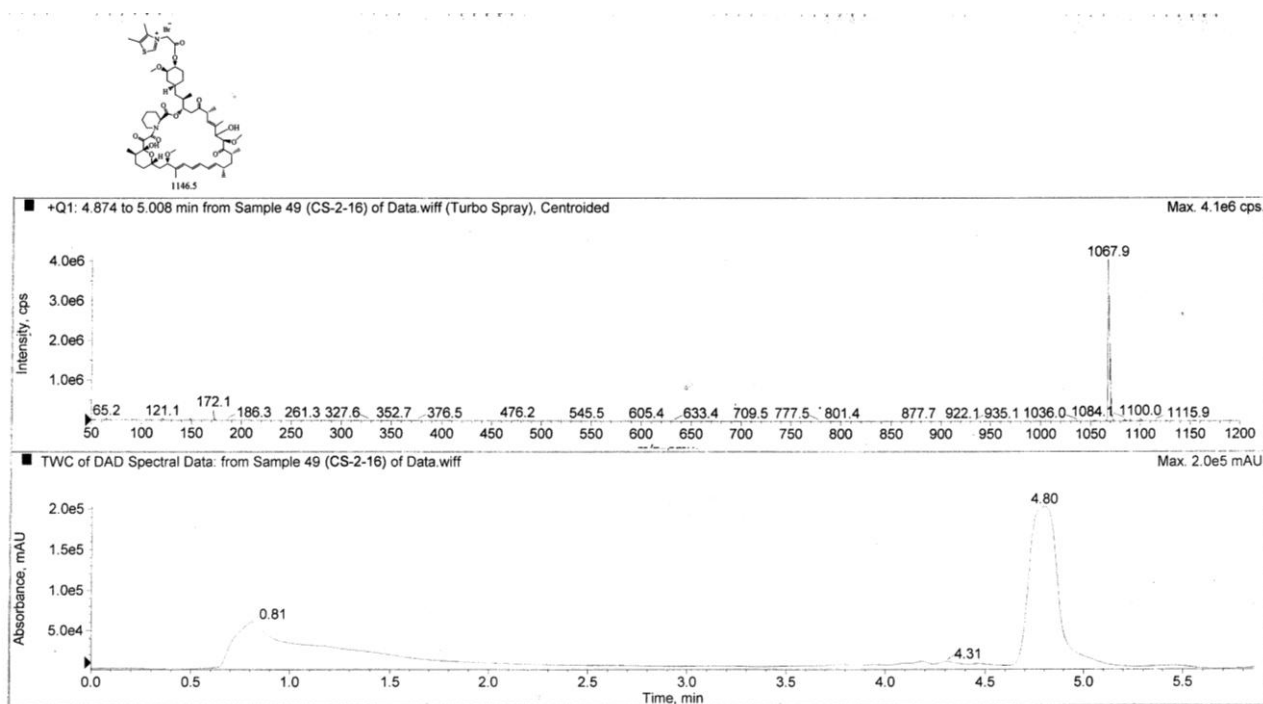


Figure S12. IR of compound **1**.

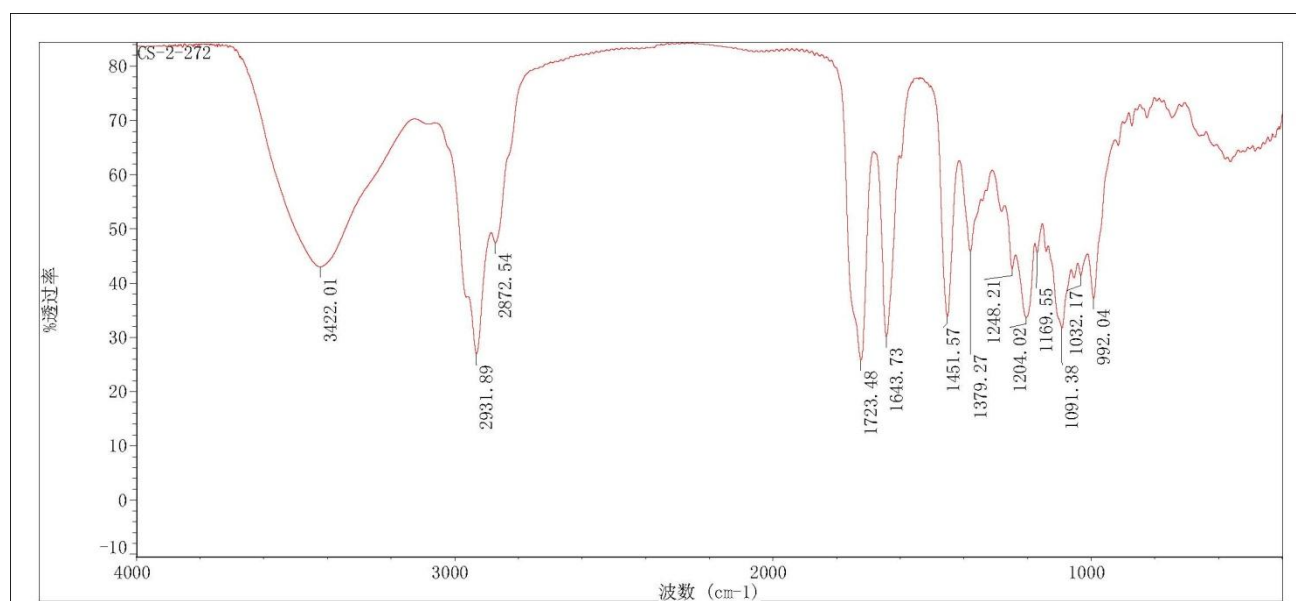


Figure S13. ^1H -NMR of compound 2.

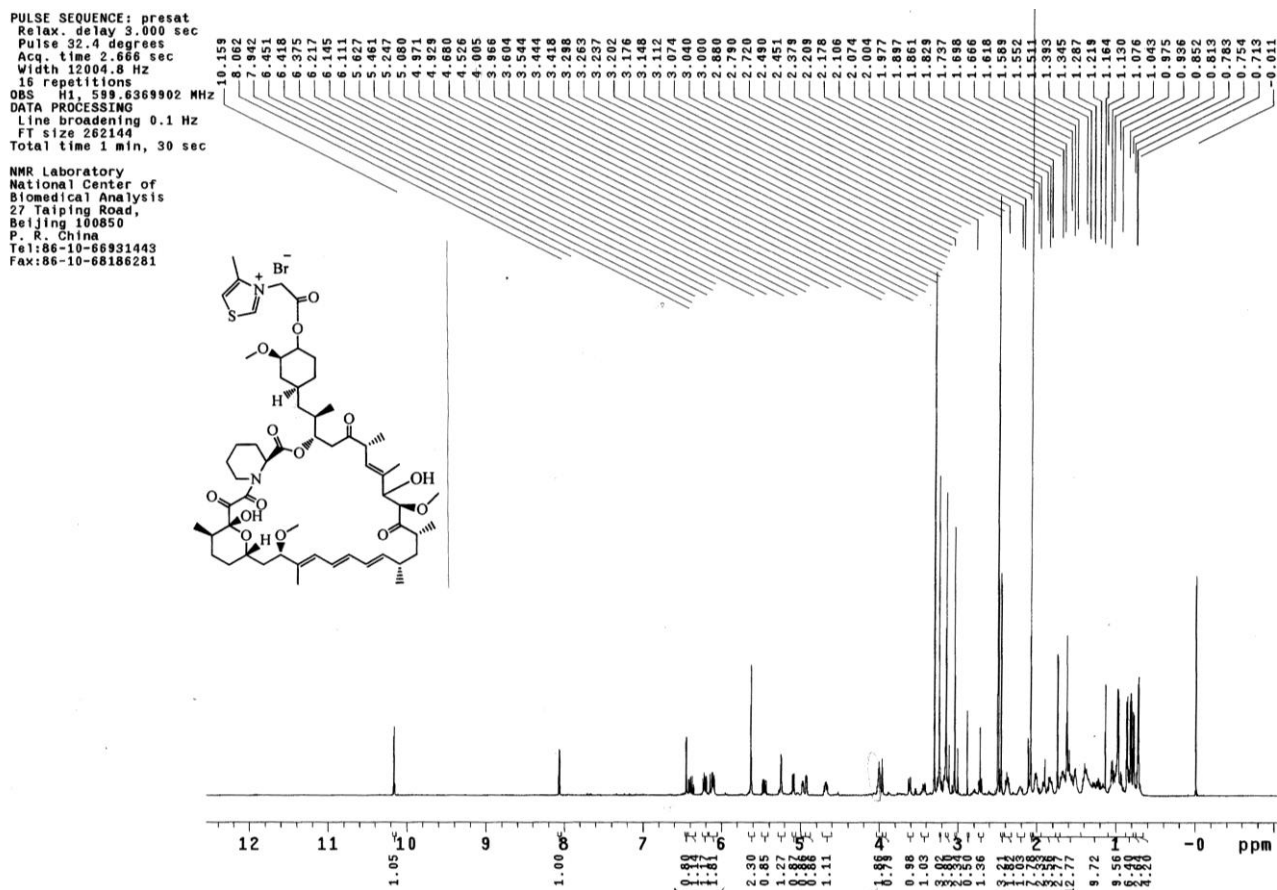


Figure S14. ^{13}C -NMR of compound 2.

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 Scans = 950
 Temp_get = 18.5[dC]
 Solvent = CHLOROFORM-D

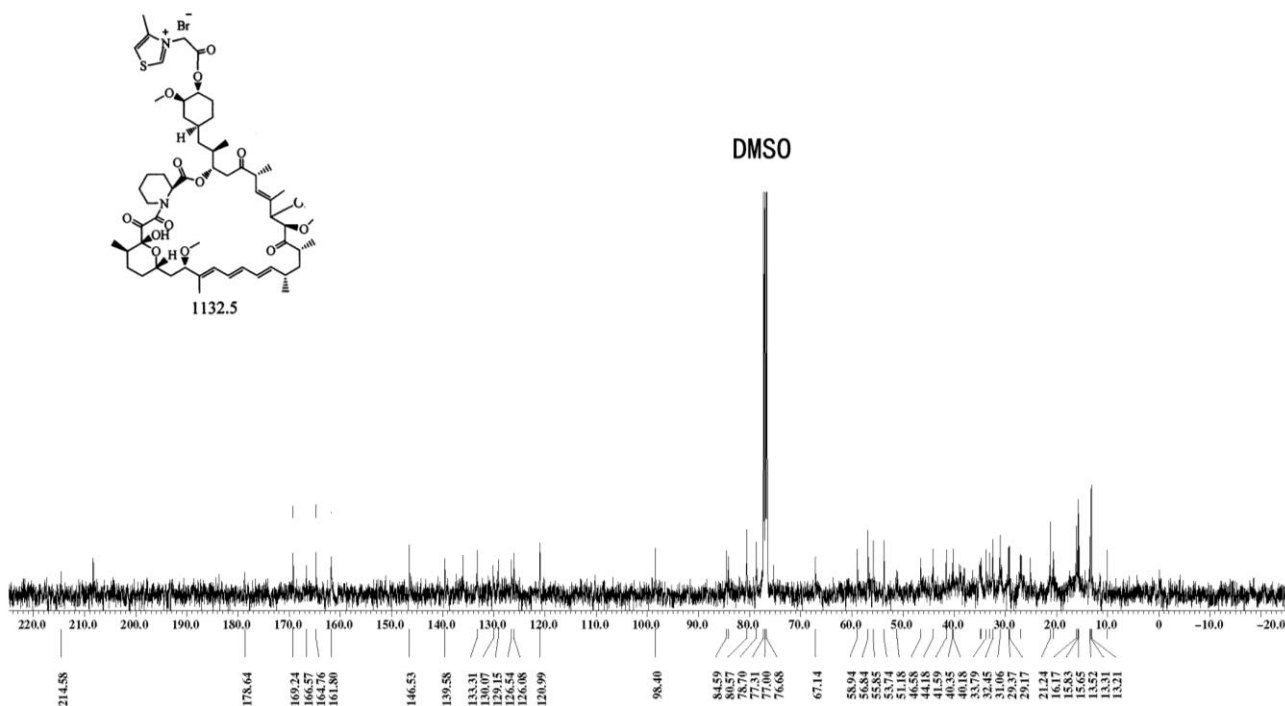


Figure S15. MS of compound 2.

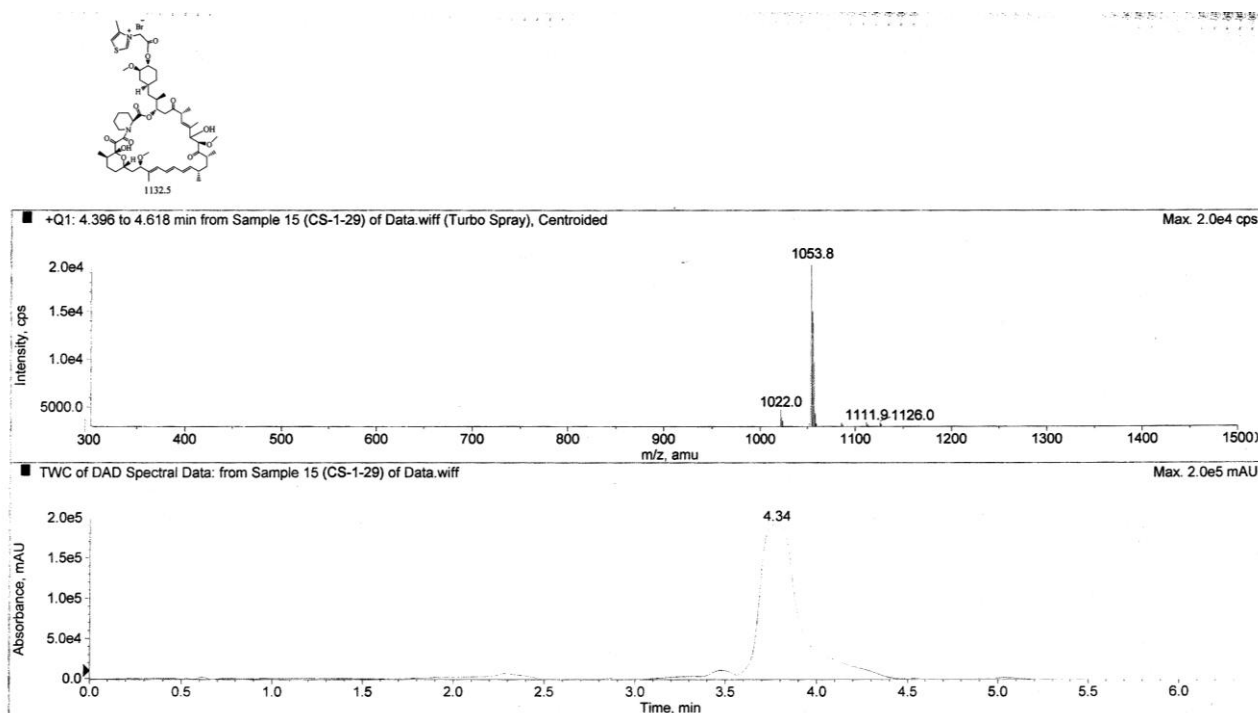


Figure S16. IR of compound 2.

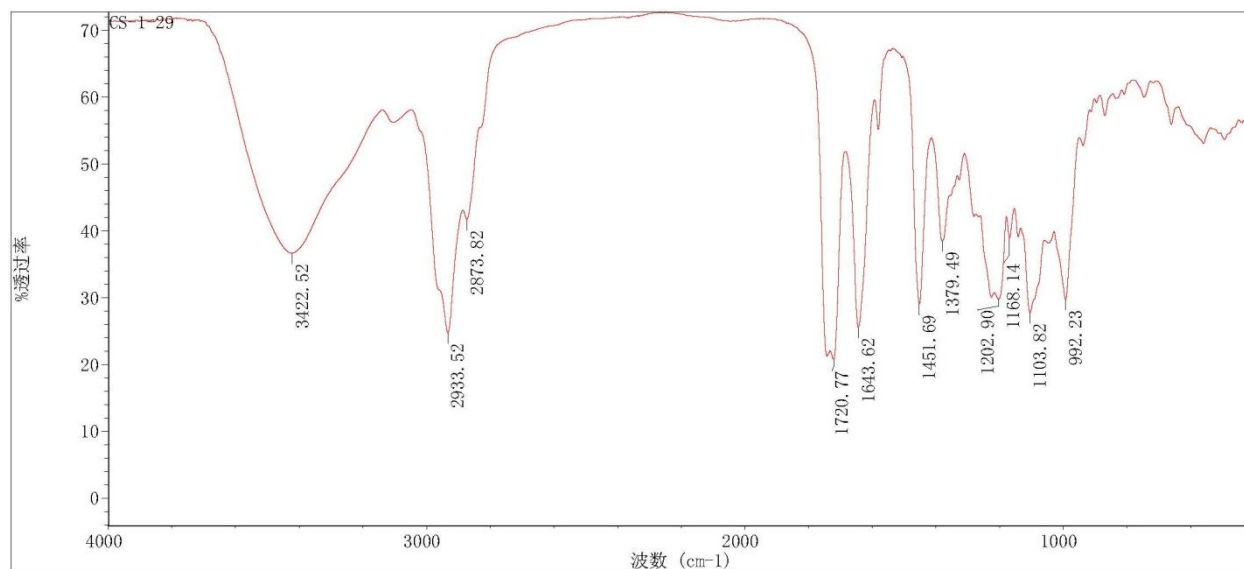
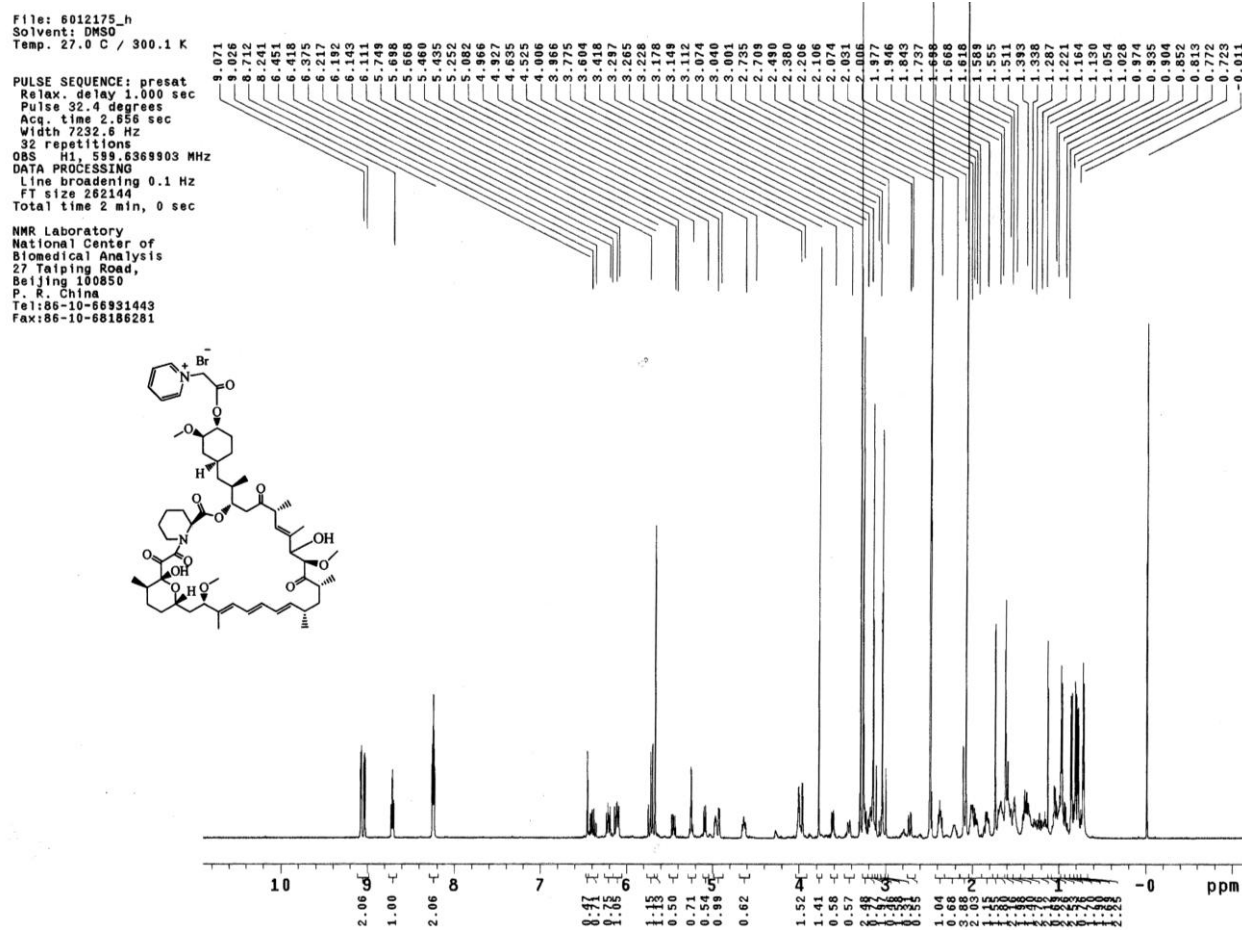
Figure S17. ¹H-NMR of compound 3.

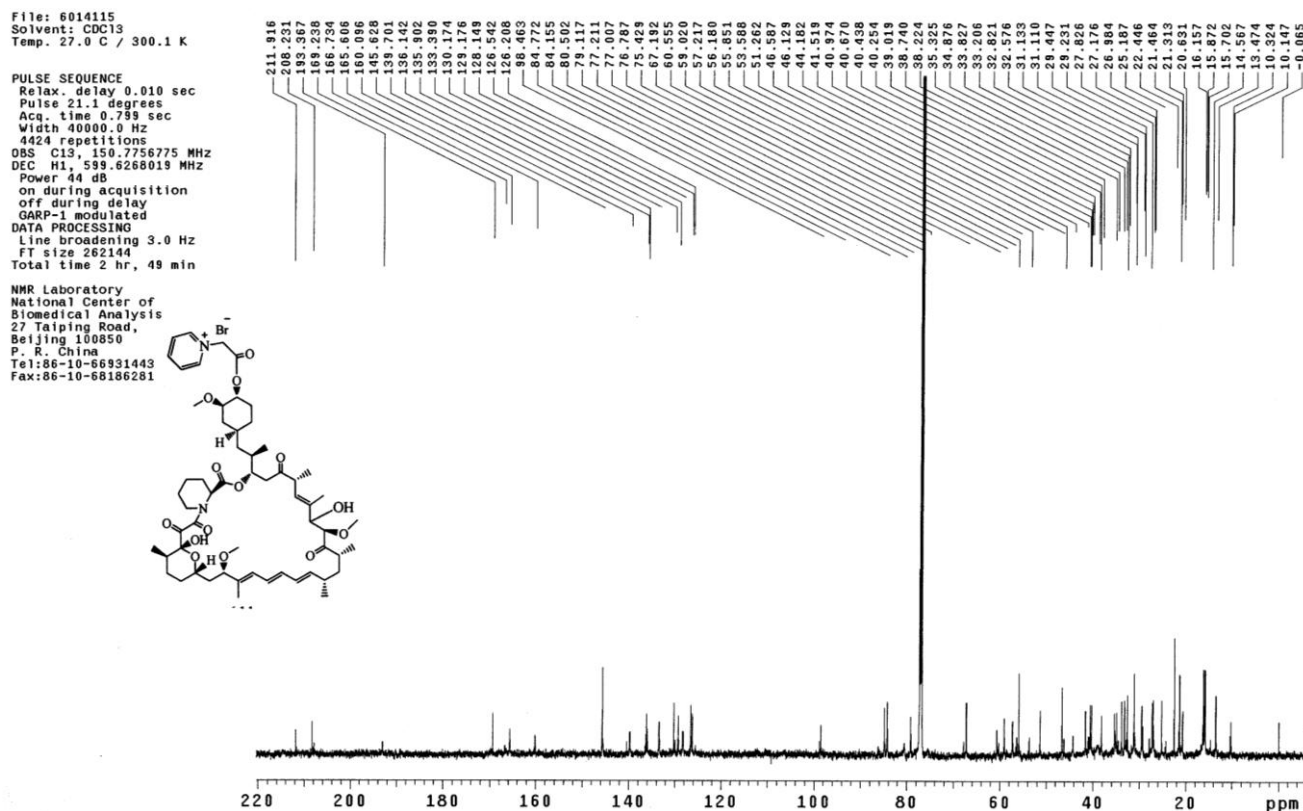
Figure S18. ^{13}C -NMR of compound 3.

Figure S19. MS of compound 3.

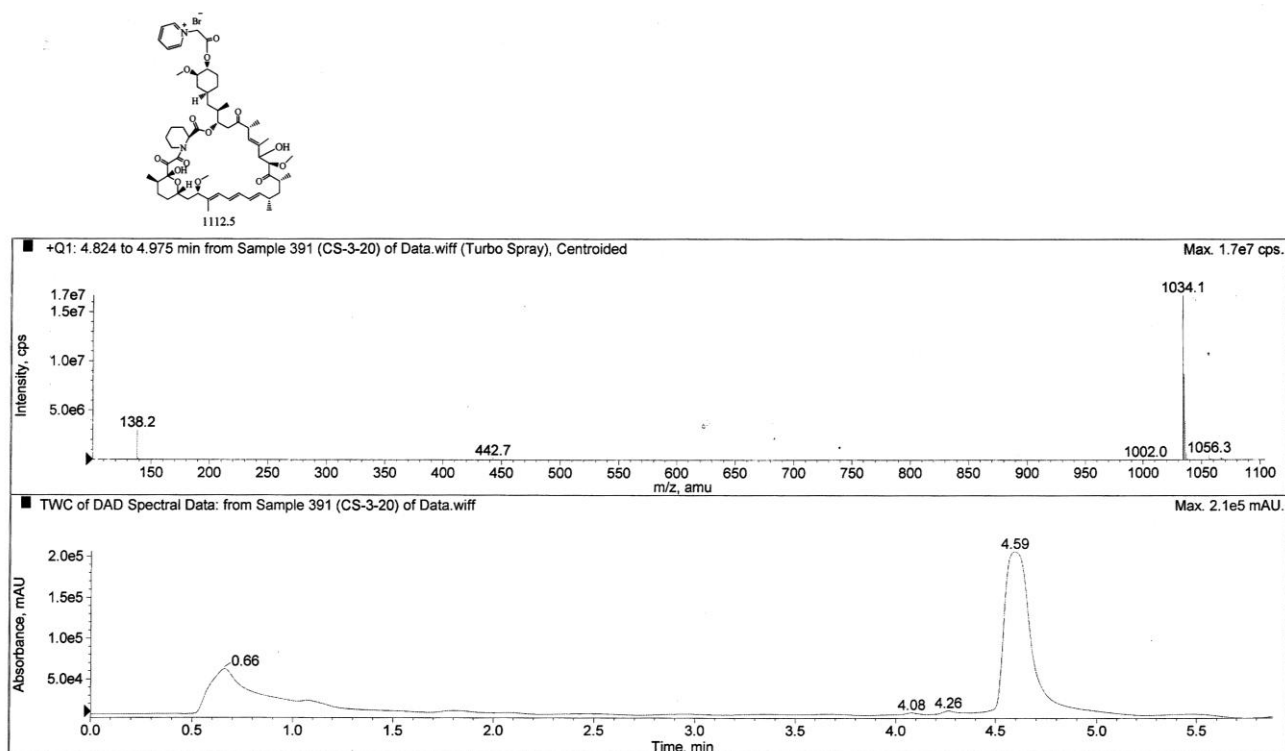


Figure S20. IR of compound 3.

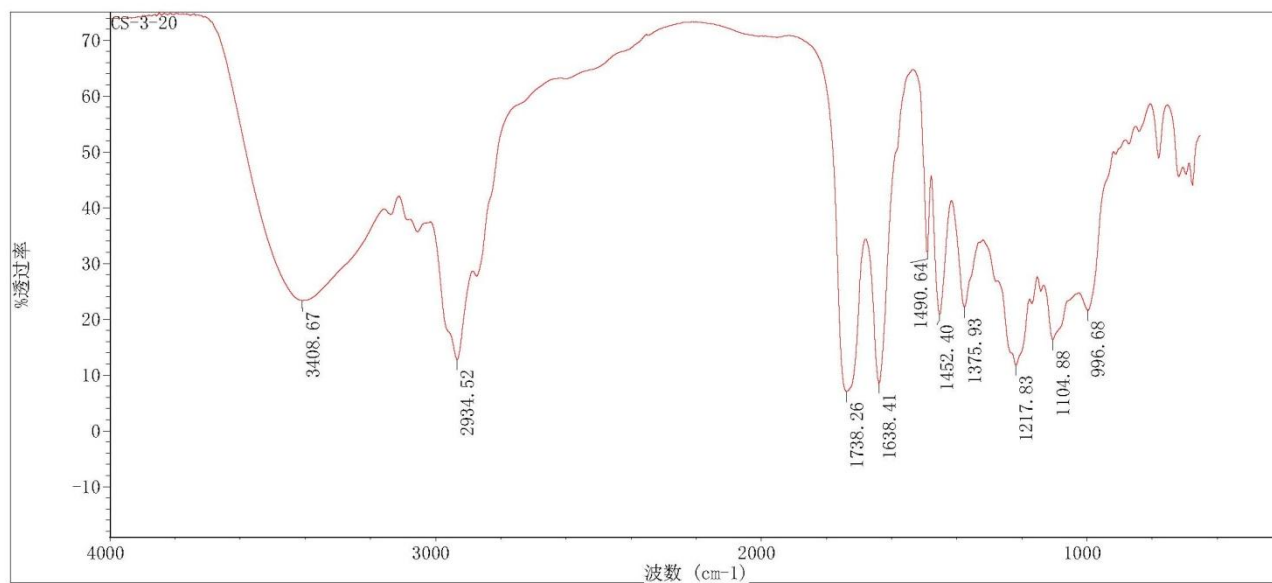
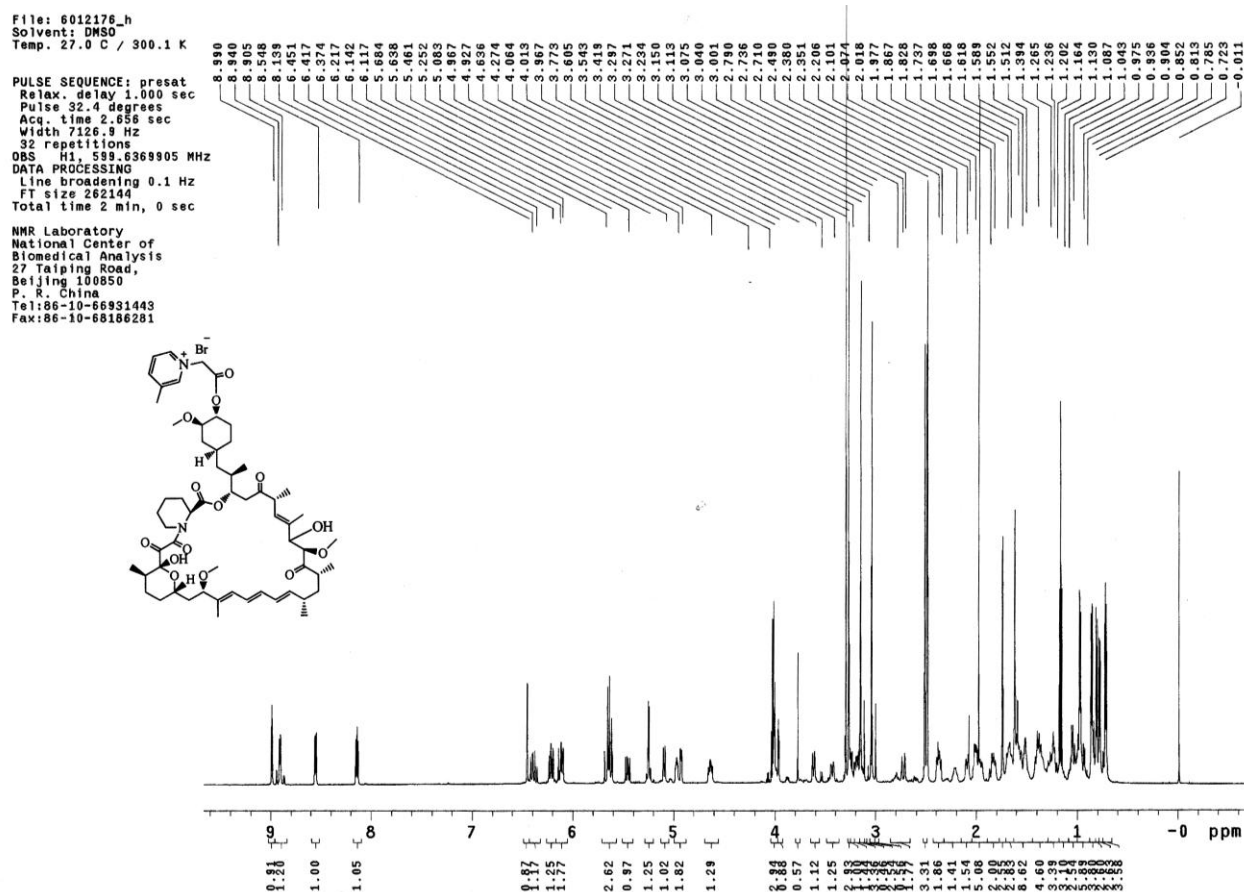
Figure S21. ¹H-NMR of compound 4.

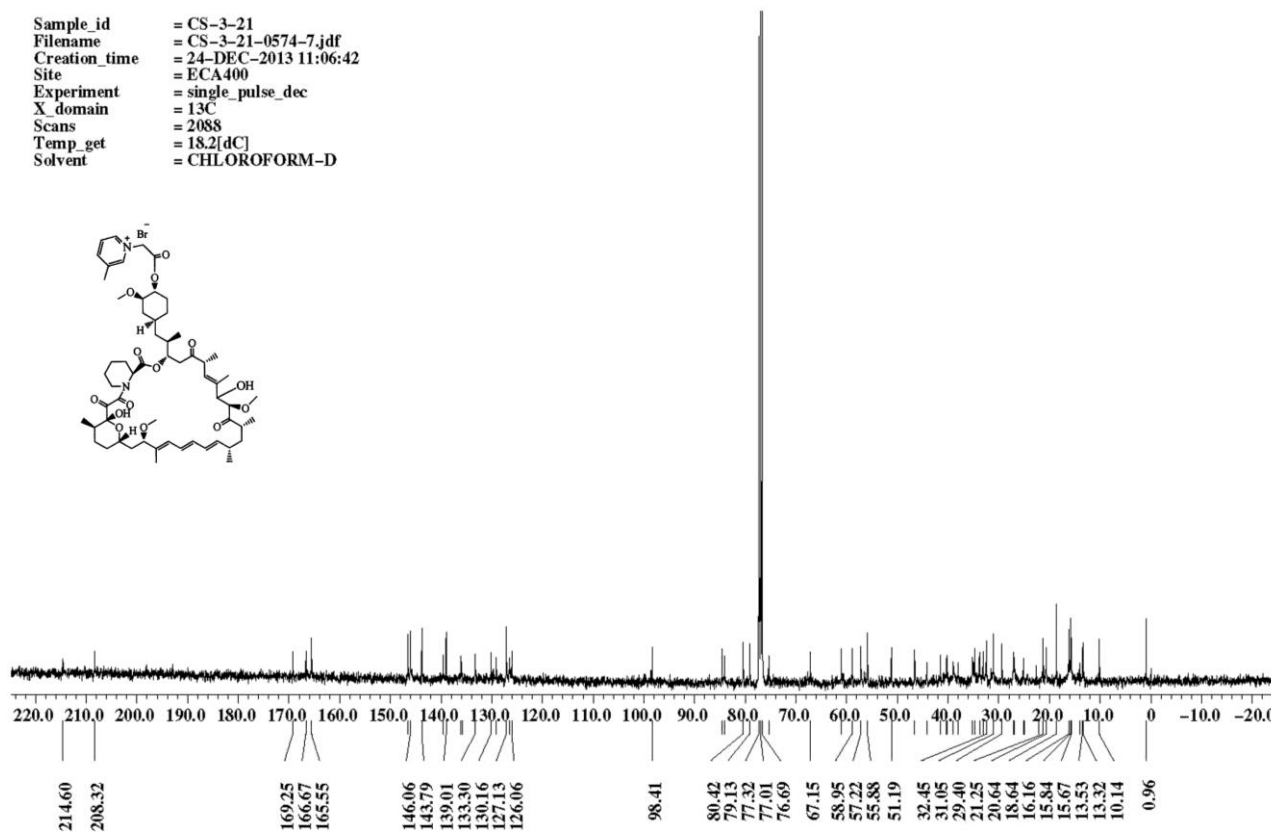
Figure S22. ^{13}C -NMR of compound 4.

Figure S23. MS of compound 4.

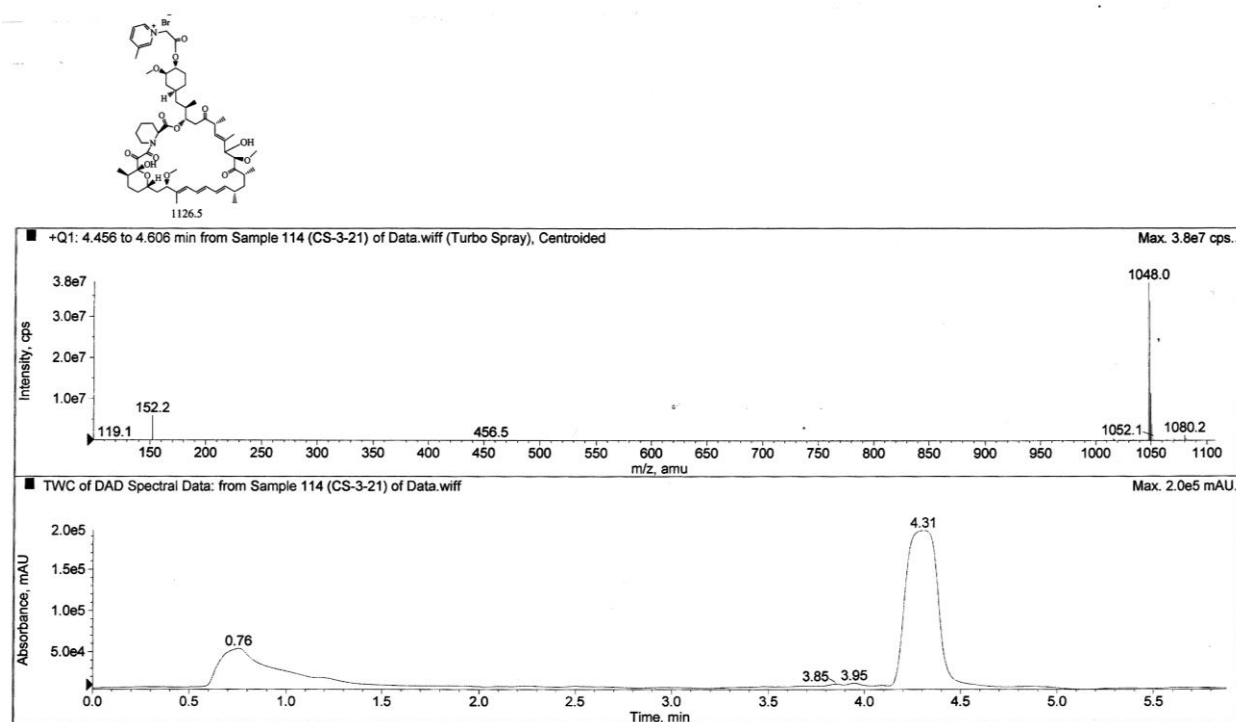


Figure S24. IR of compound 4.

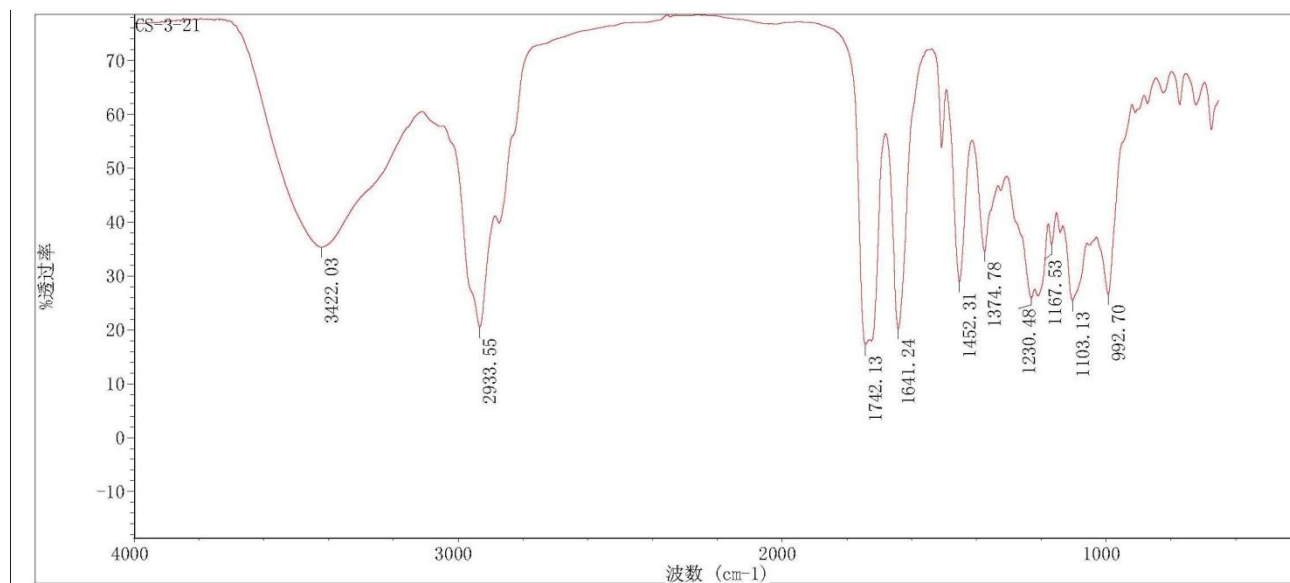
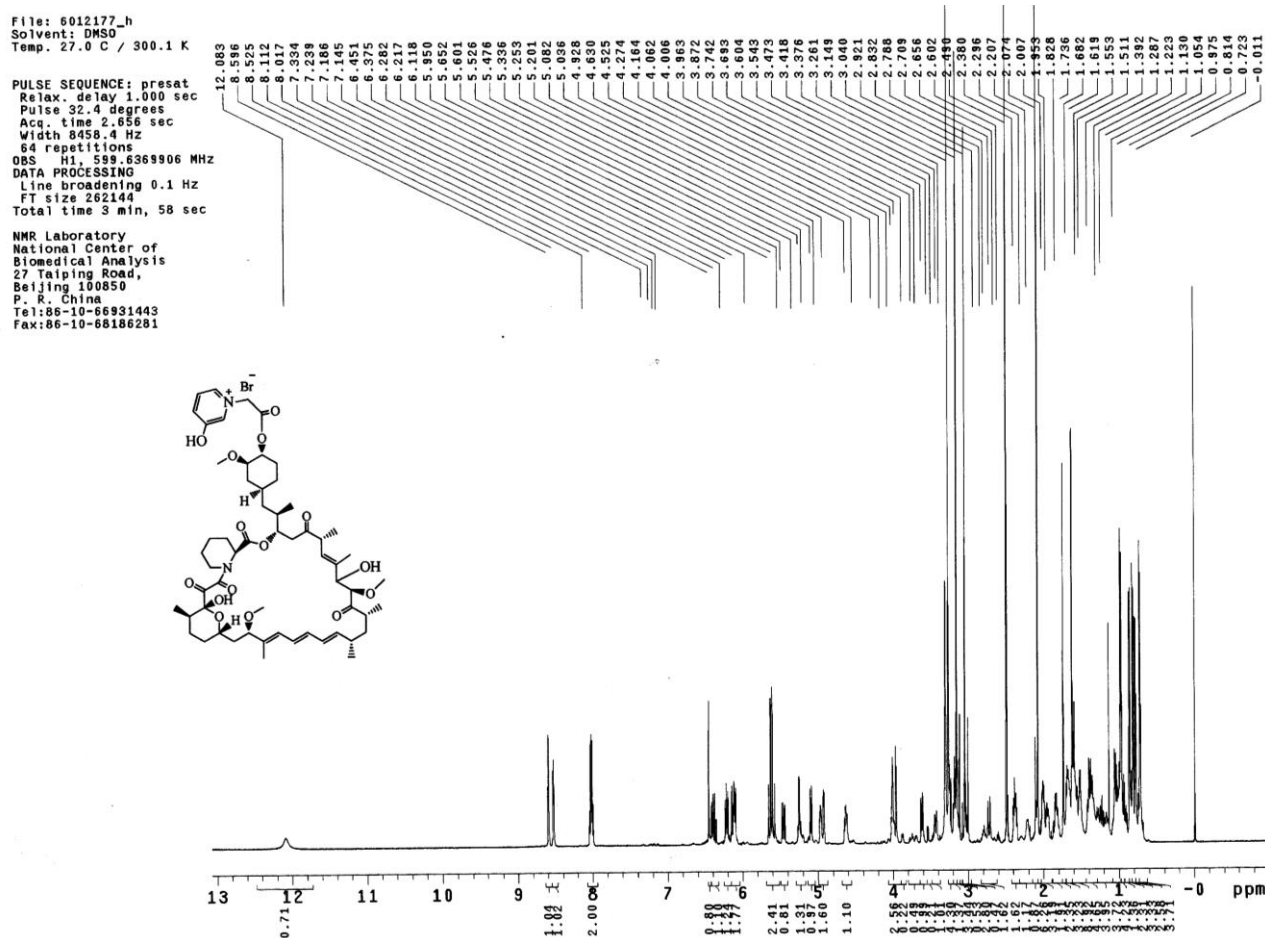
Figure S25. ¹H-NMR of compound 5.

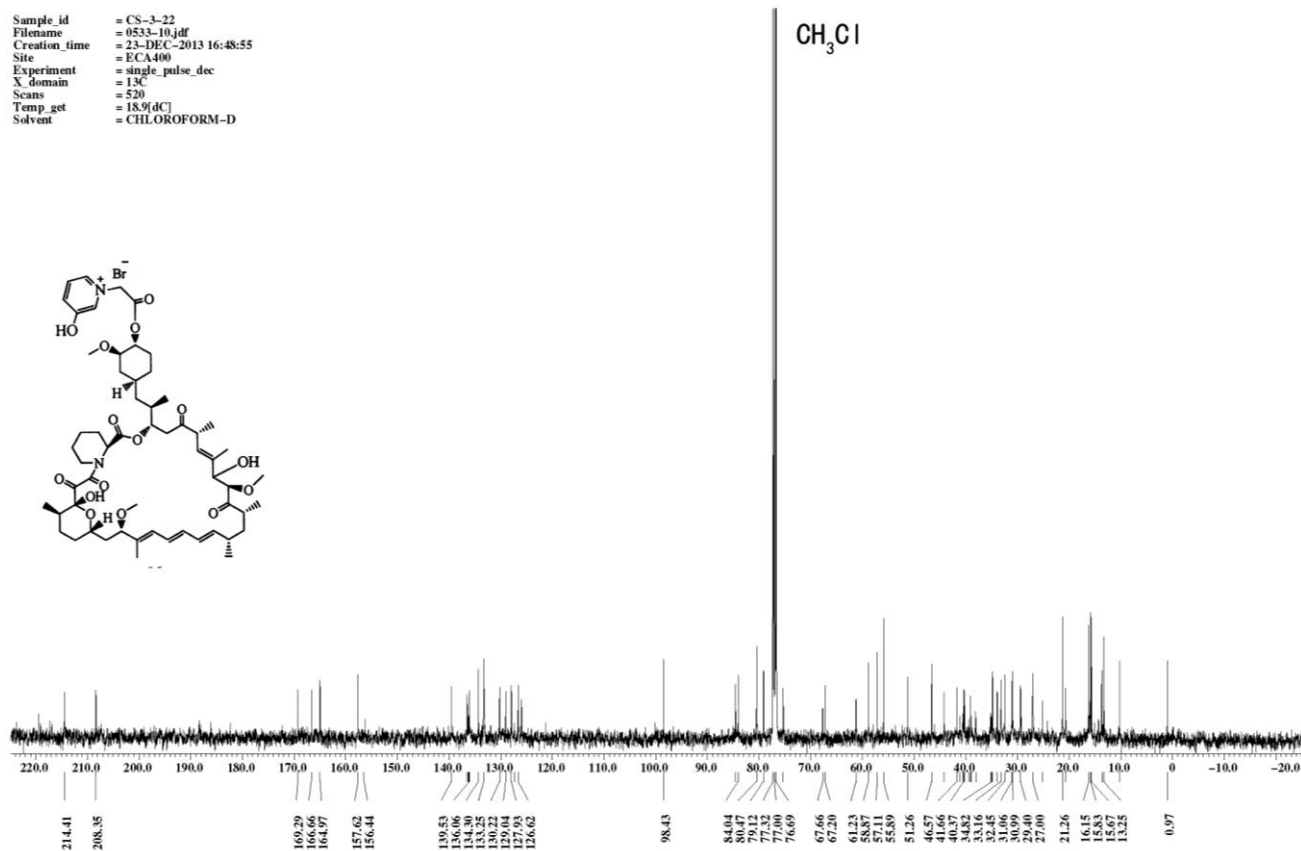
Figure S26. ^{13}C -NMR of compound 5.

Figure S27. MS of compound 5.

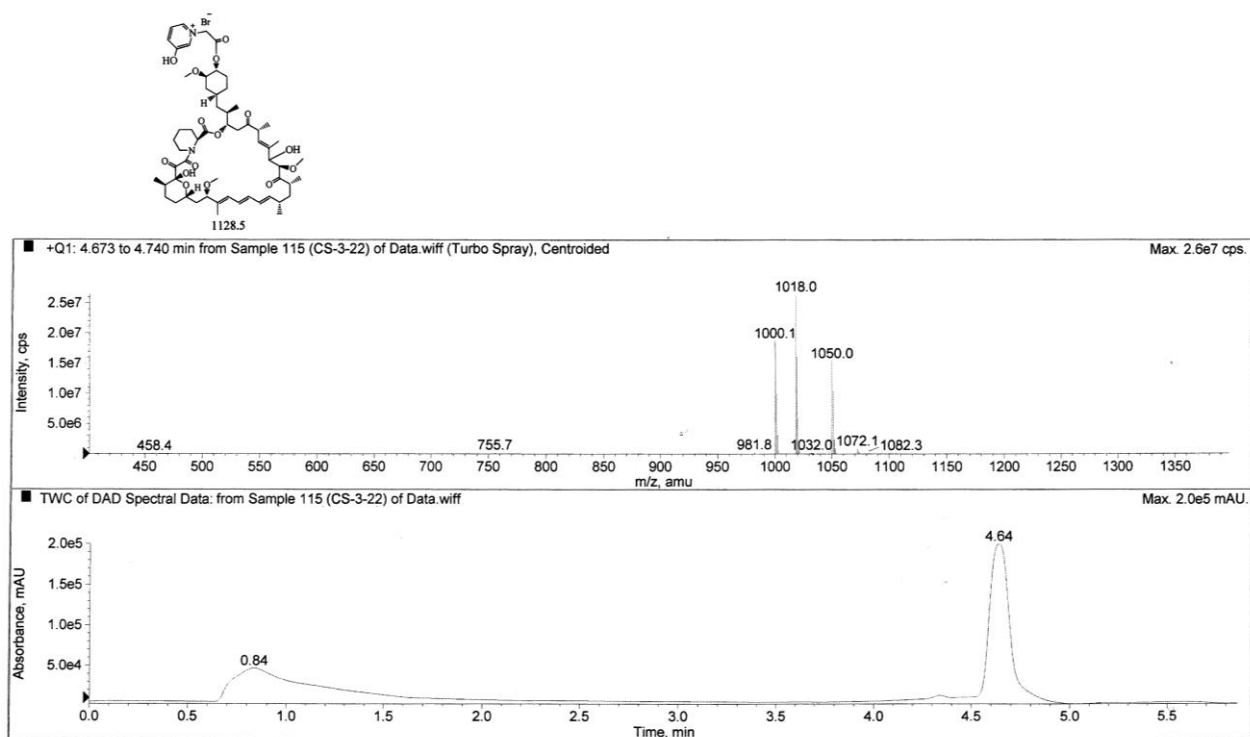


Figure S28. IR of compound 5.

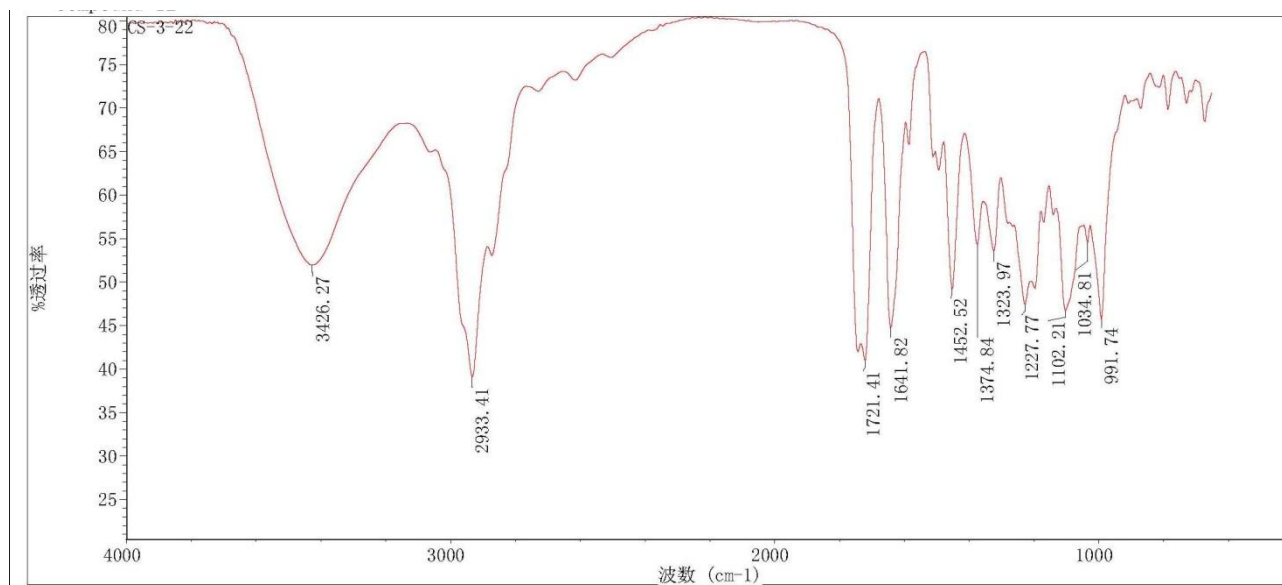
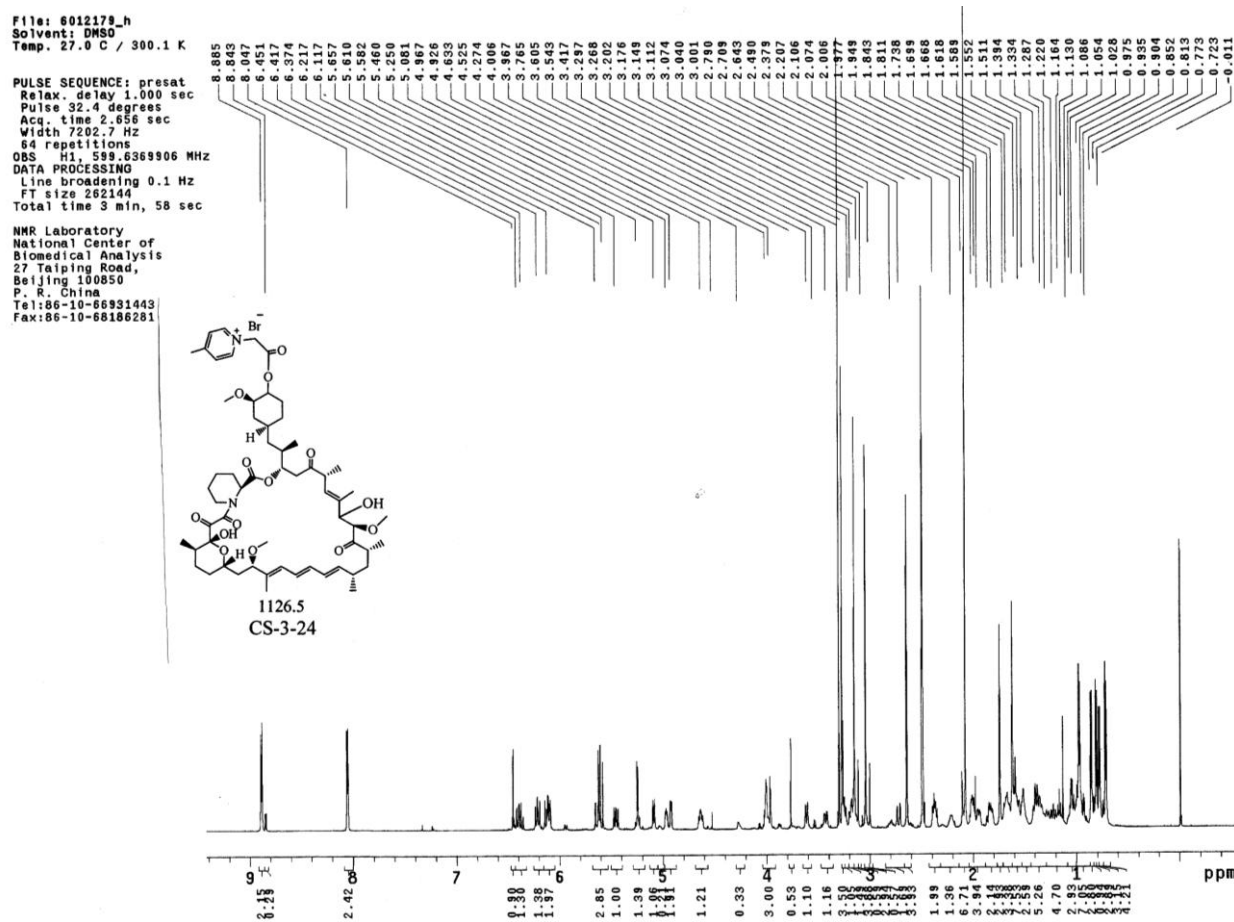


Figure S29. ^1H -NMR of compound **6**.

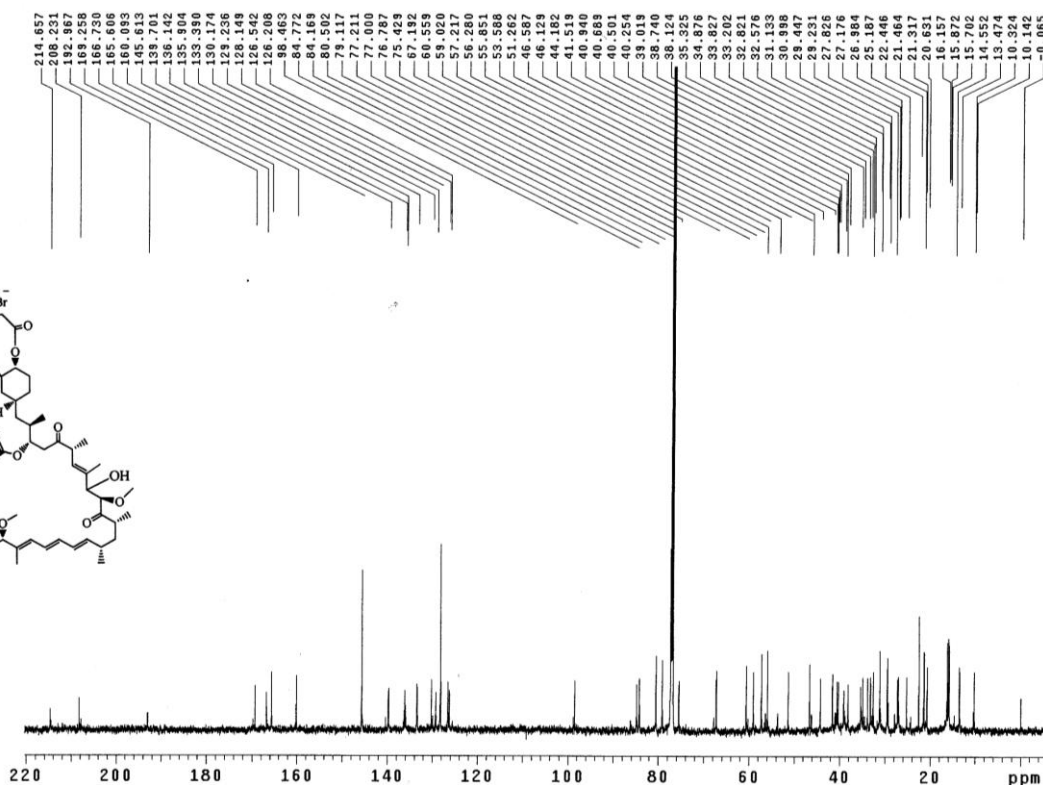
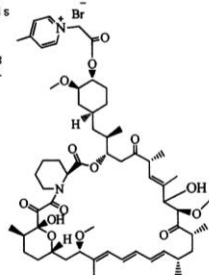


Spectrometer: "ncba600"
VARIAN INOVA 600

File: 6014023_c
Solvent: CDCl₃
Temp. 27.0 C / 300.1 K

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PULSE SEQUENCE
Pulse. delay 0.010 sec
Pulse 21.1 degrees
Acq time 0.75 sec
Width 40000.0 Hz
4424 repetitions
OBS C13 150.7756729 MH
DEC H1, 599.6268019 MHZ
Power 44 dB
on during acquisition
off during delay
GARP-1 modulated
DATA PROCESSING
Line broadening 3.0 Hz
FT size 262144
Total time 2 hr, 49 min
```

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1126.5

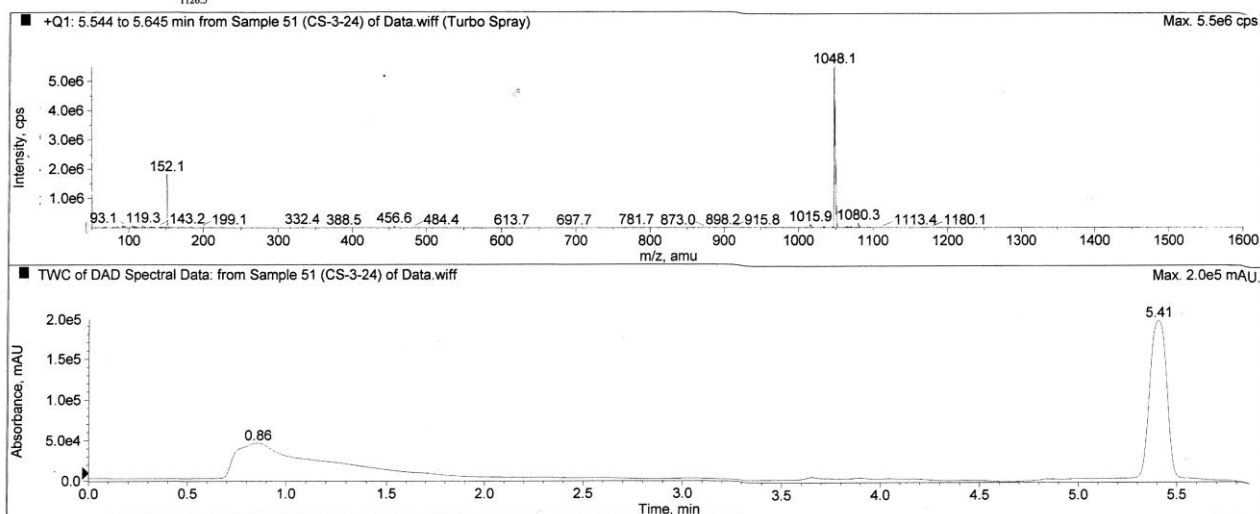


Figure S32. IR of compound 6.

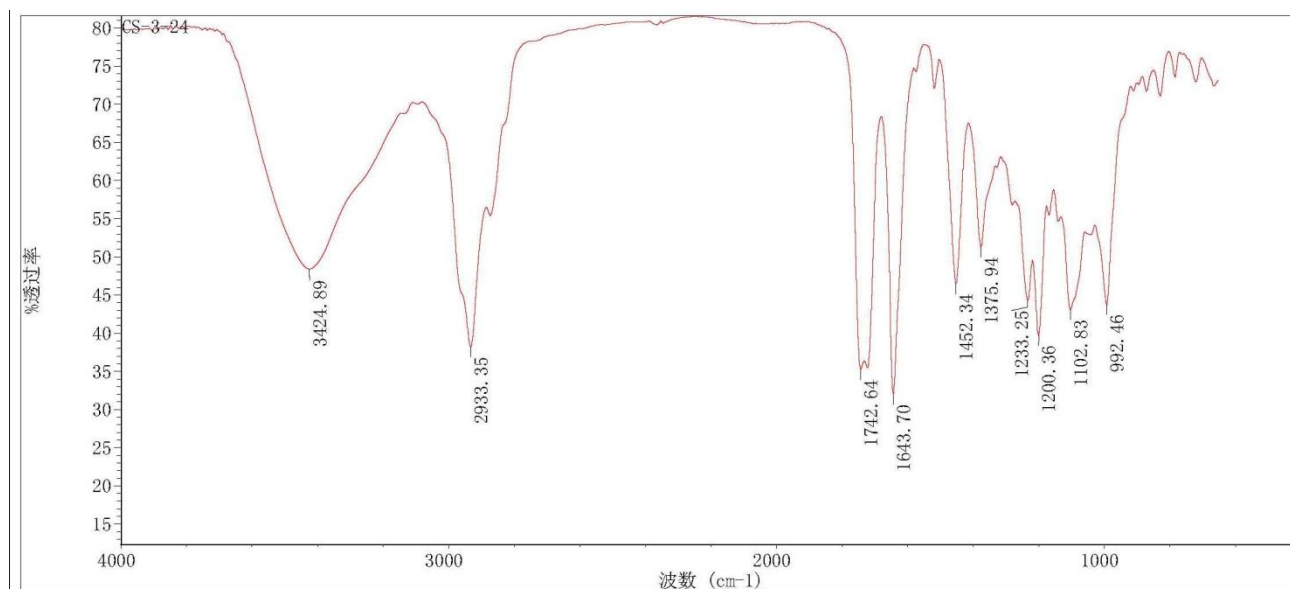
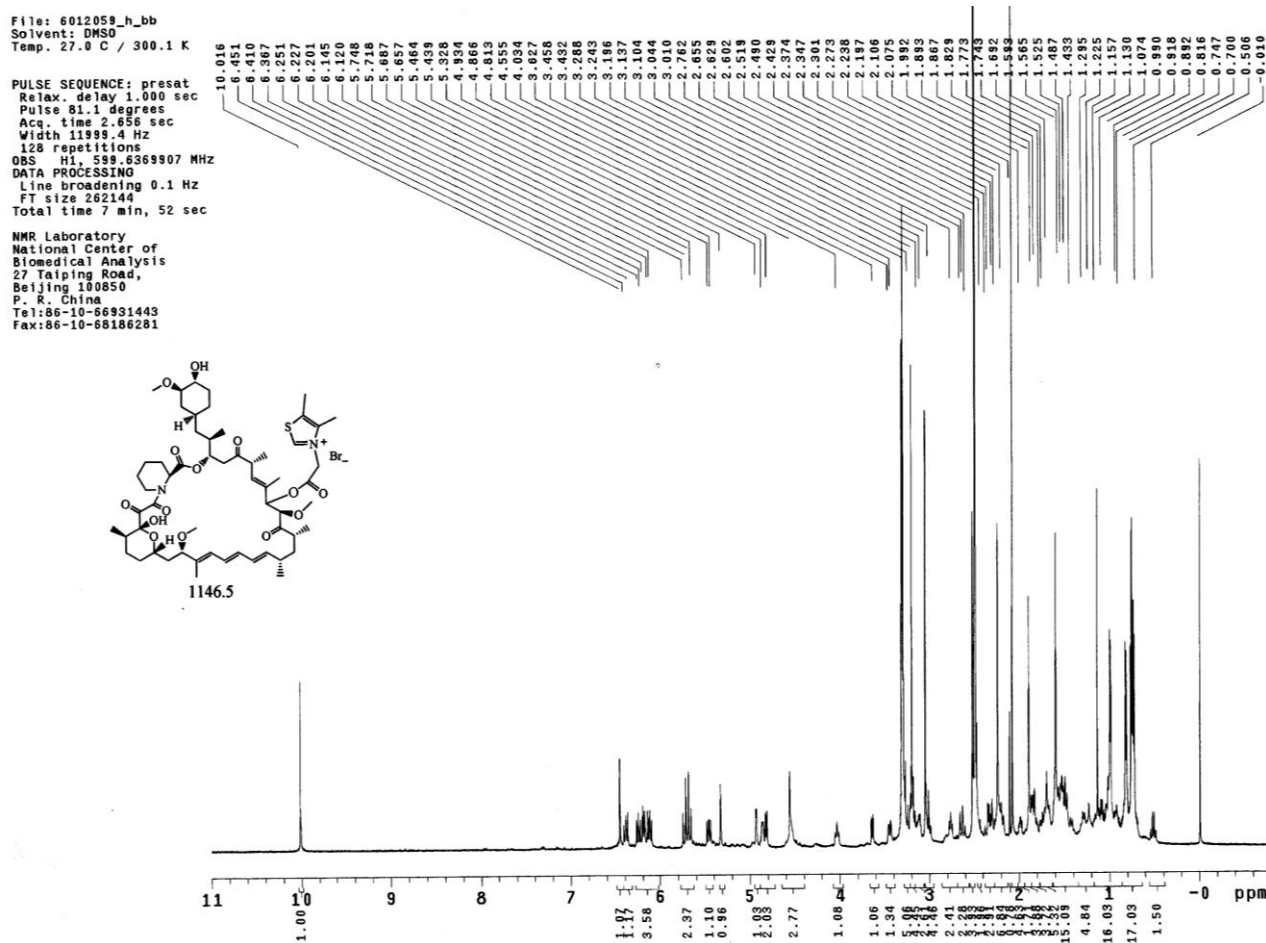
Figure S33. ¹H-NMR of compound 7.

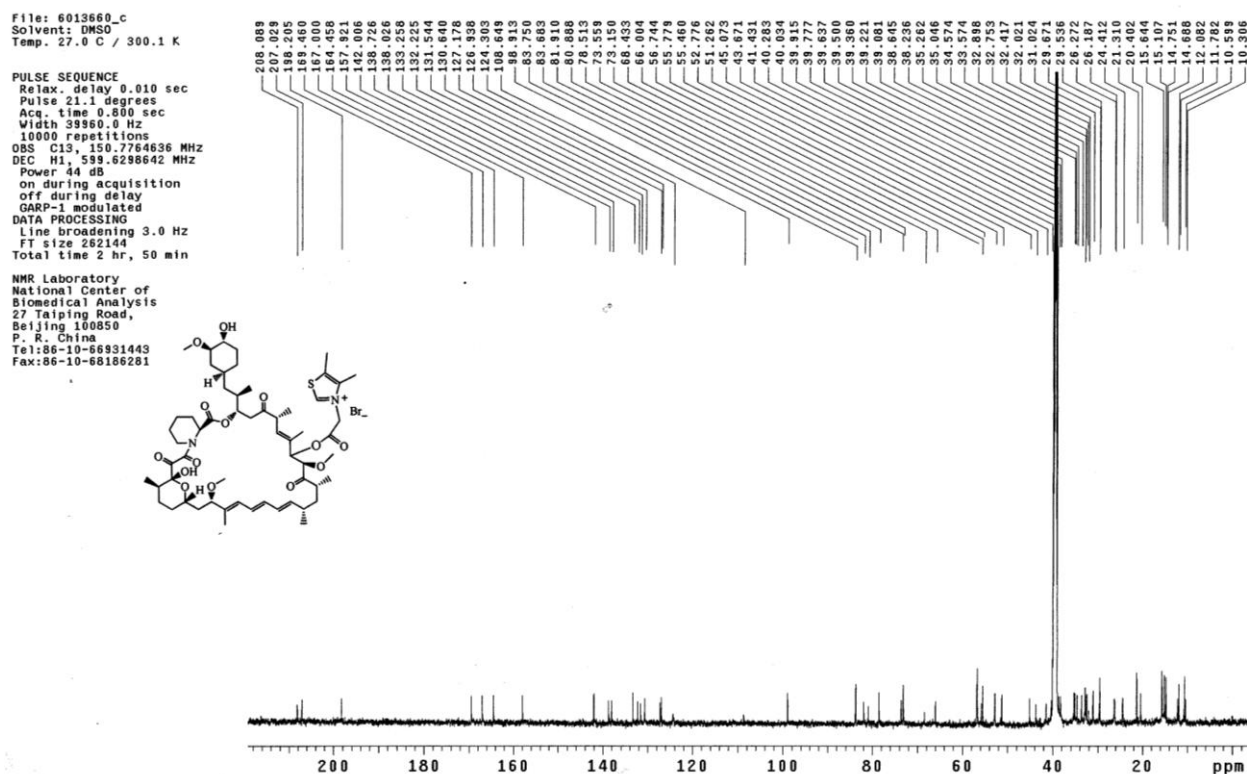
Figure S34. ^{13}C -NMR of compound 7.

Figure S35. HSQC of compound 7.

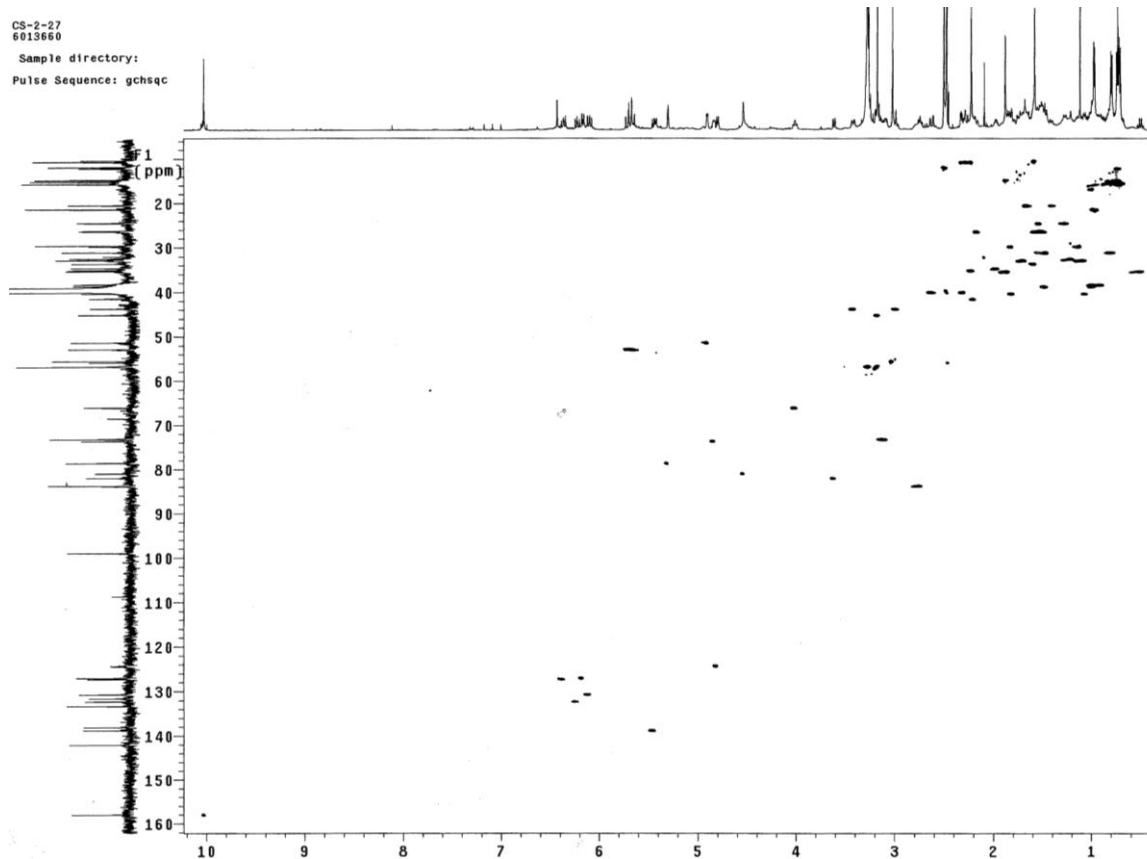


Figure S36. HMBC of compound 7.

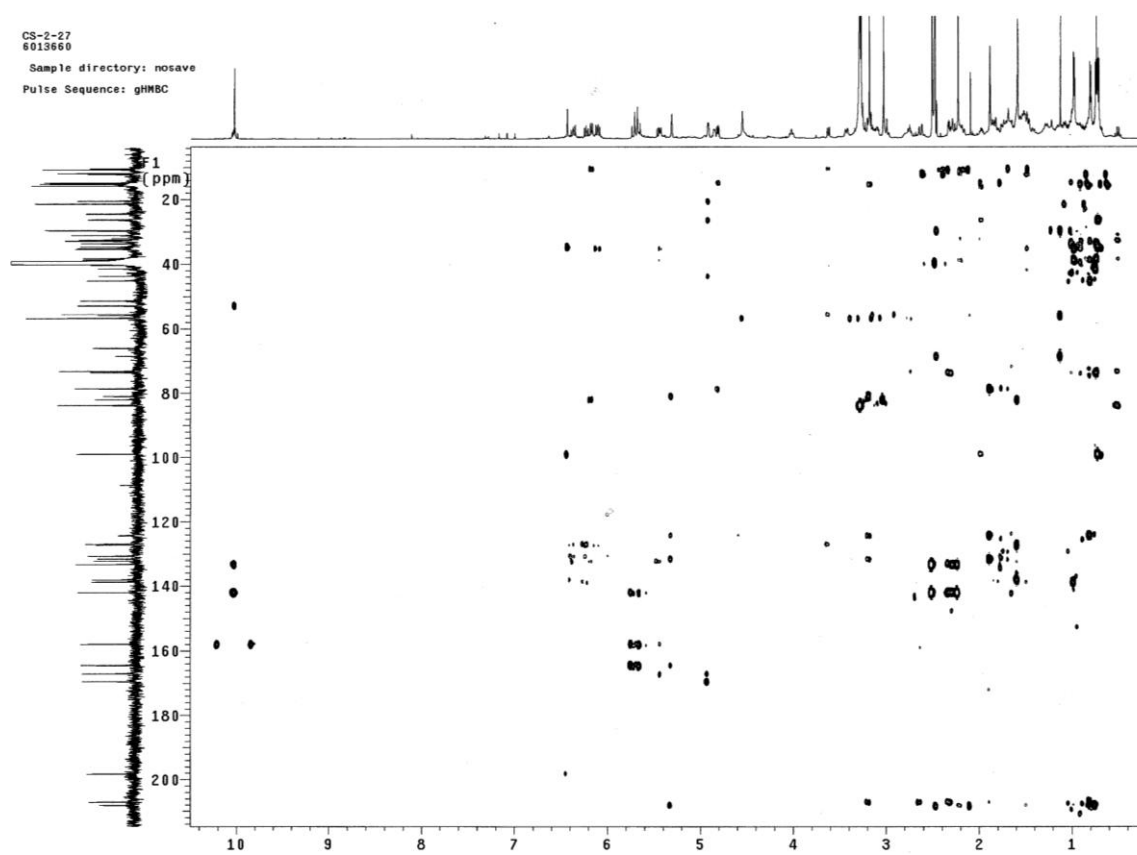


Figure S37. COSY of compound 7.

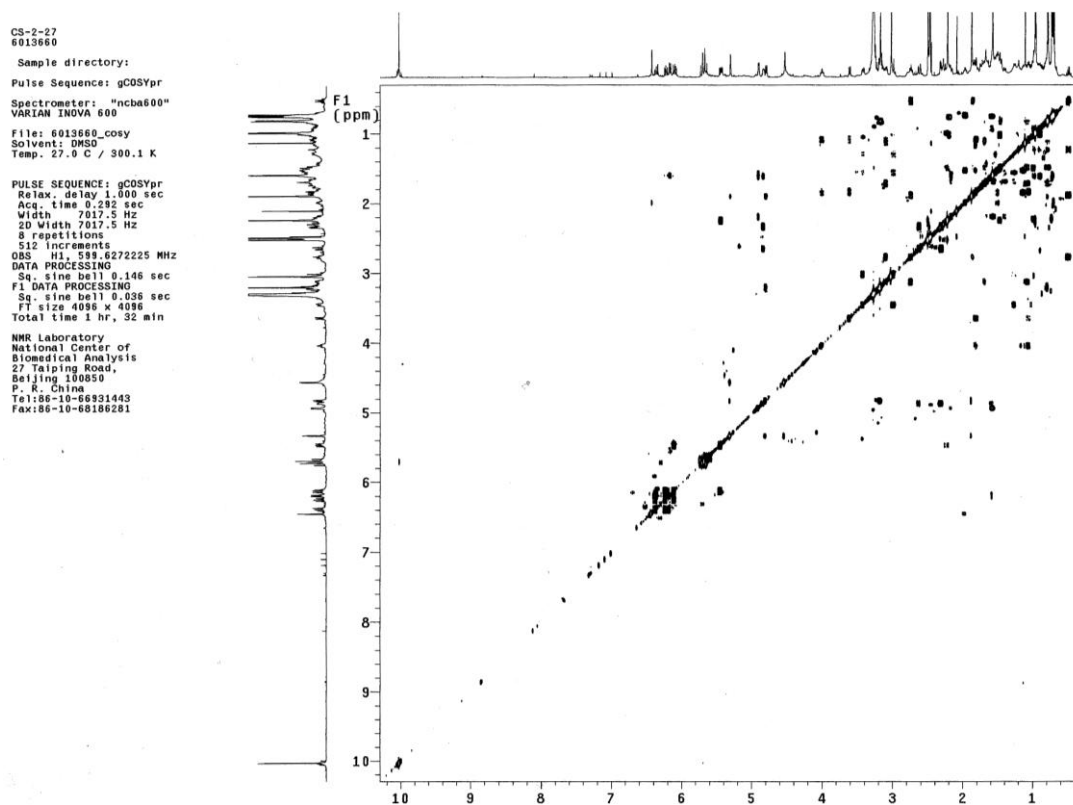


Figure S38. ROESY of compound 7.

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Pulse Sequence: ROESY
Spectrometer: "ncba600"
VARIAN INOVA 600
File: 6013660_roesy
Solvent: DMSO
Temp: 27.0 C / 300.1 K

PULSE SEQUENCE: ROESY
Relax. delay 1.000 sec
Mixing 0.250 sec
Acq. time 0.292 sec
Width 7017.5 Hz
2D Width 7017.5 Hz
32 repetitions
2 x 256 increments
DSS H1, 599.6272230 MHz
DATA PROCESSING
Sg. sine bell 0.292 sec
Shifted by -0.292 sec
F1 DATA PROCESSING
Sg. sine bell 0.073 sec
Shifted by -0.073 sec
FT size 4096 x 4096
Total time 7 hr, 10 min

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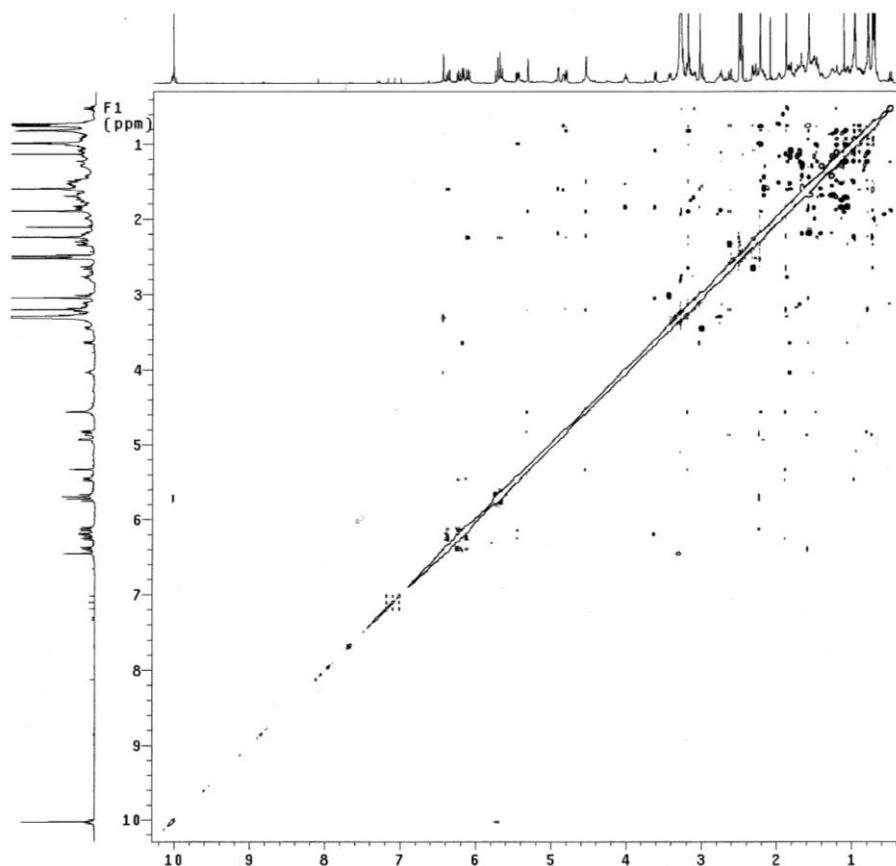


Figure S39. TOCSY of compound 7.

CS-2-27
6013660
Sample directory:
Pulse Sequence: gTOCSY
Spectrometer: "ncba600"
VARIAN INOVA 600
File: 6013660_tocsy
Solvent: DMSO
Temp: 27.0 C / 300.1 K

PULSE SEQUENCE: gTOCSY
Relax. delay 1.000 sec
Mixing 0.120 sec
Acq. time 0.293 sec
Width 7017.5 Hz
2D Width 6985.2 Hz
32 repetitions
256 increments
DSS H1, 599.6272230 MHz
DATA PROCESSING
Sg. sine bell 0.147 sec
F1 DATA PROCESSING
Sg. sine bell 0.018 sec
FT size 4096 x 4096
Total time 3 hr, 18 min

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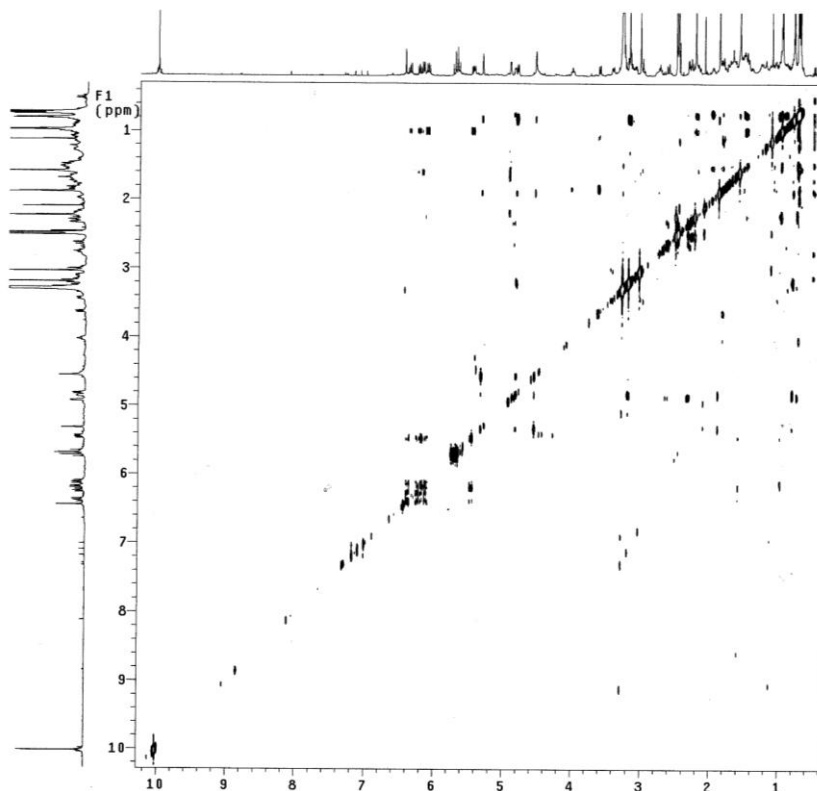


Figure S40. MS of compound 7.

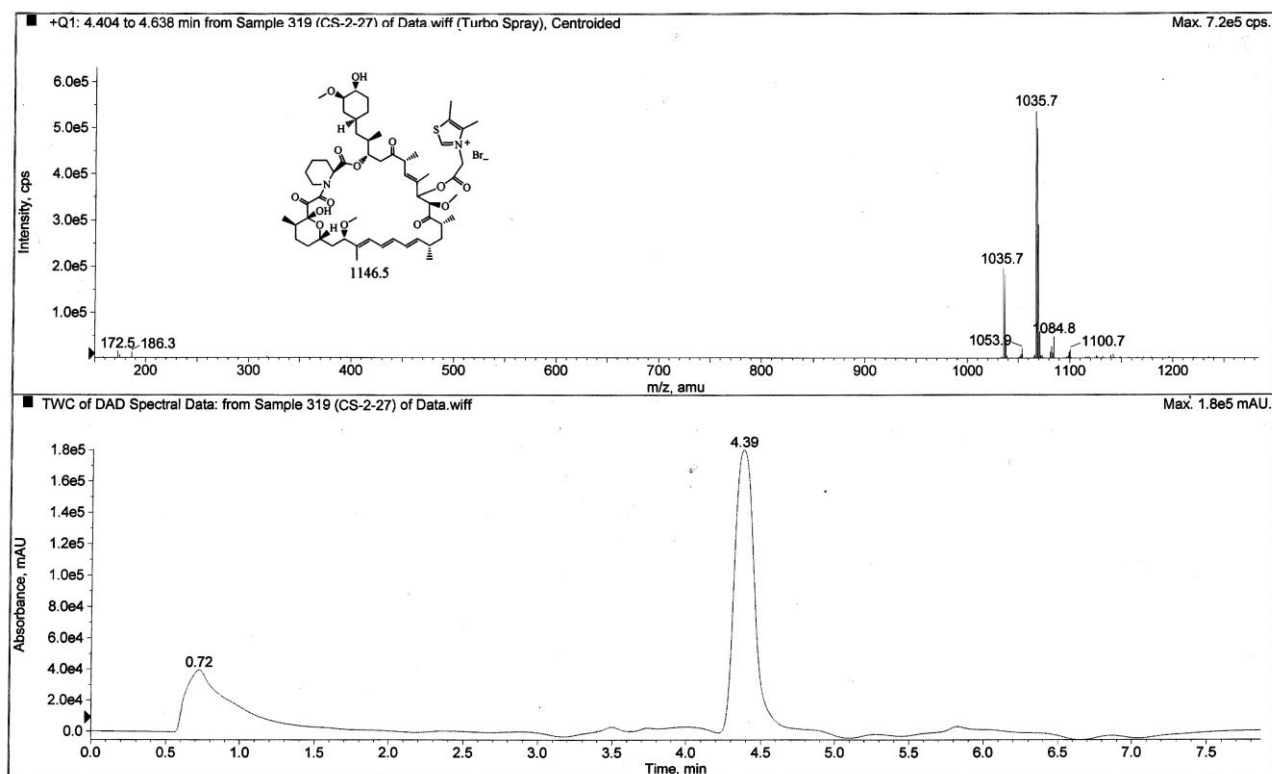
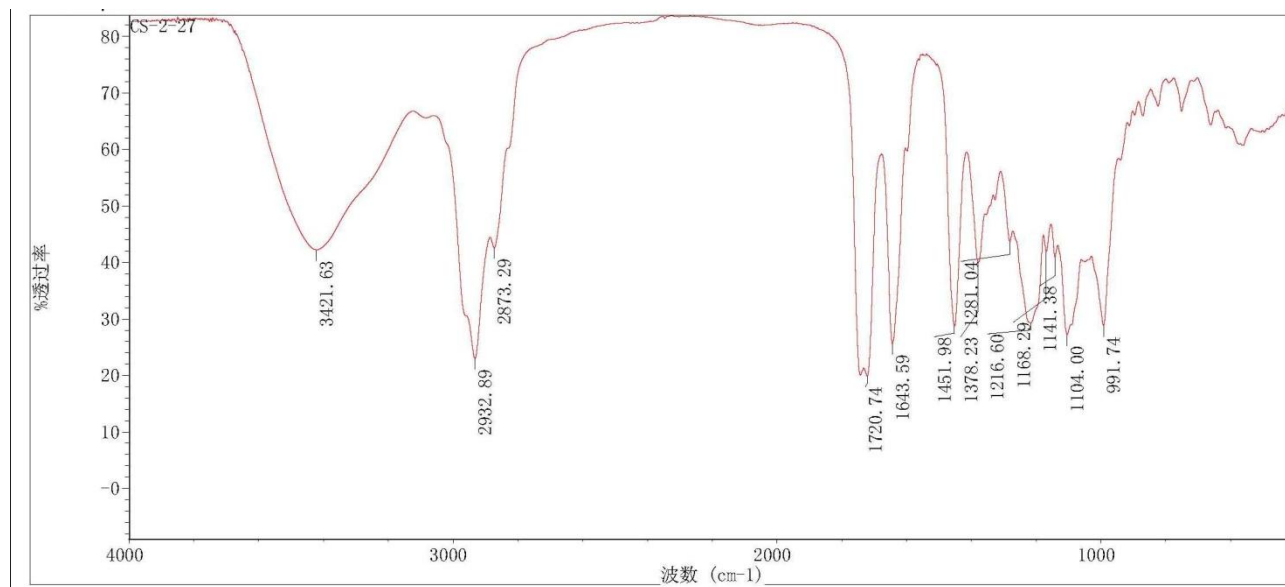


Figure S41. IR of compound 7.



[illegible]

File: 6013628_C
Solvent: DMSO
Temp. 27.0 C / 300.1 K

PULSE SEQUENCE
Relax. delay 0.010 sec
Pulse 21.1 degrees
Acq. time 0.800 sec
Width 39960.0 Hz
10000 repetitions
OBS C13, 150.7764663 MHz
DEC H1, 599.6308648 MHz
Power 44 dB
on during acquisition
off during delay
GARP-1 modulated

DATA PROCESSING
Line broadening 3.0 Hz
FT size 262144
Total time 2 hr, 50 min

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212.110
207.021
186.205
186.205
189.487
187.008
187.008
187.952
187.952
182.016
182.016
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186.056
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182.255
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181.544
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184.389
180.648
180.648
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86.913
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83.663
83.663
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81.810
80.668
80.668
78.513
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10.306

1134.3

Figure S44. MS of compound 8.

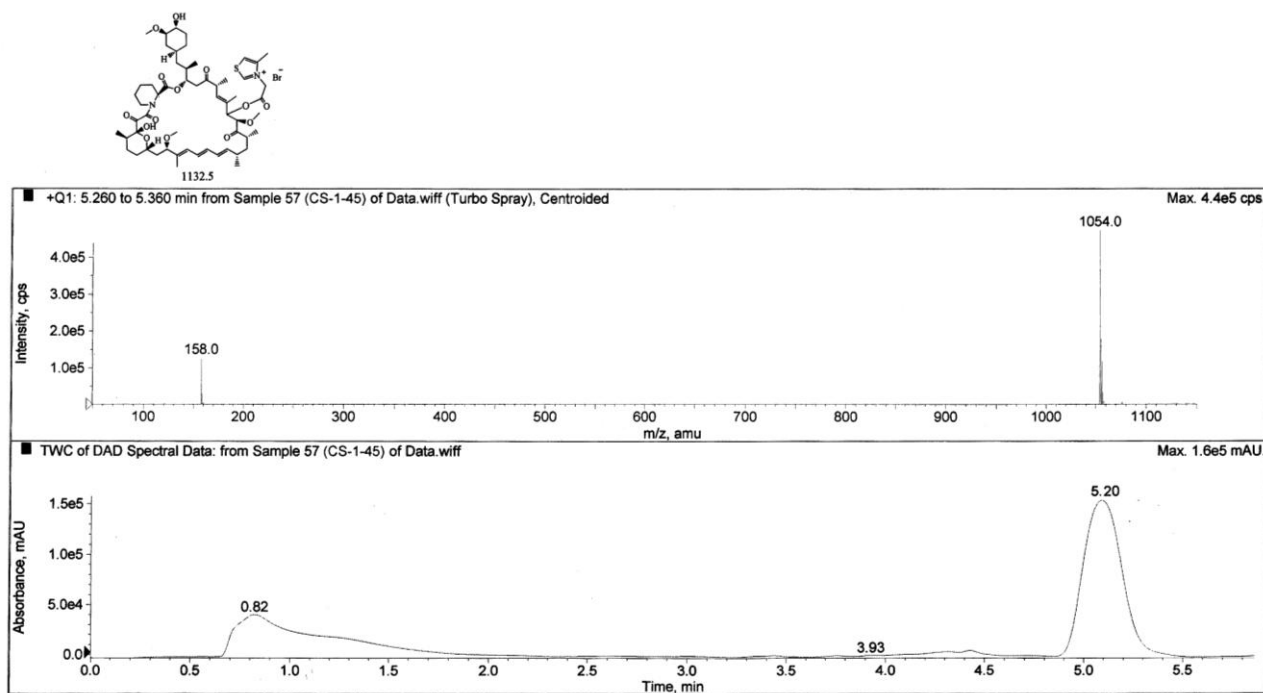


Figure S45. IR of compound 8.

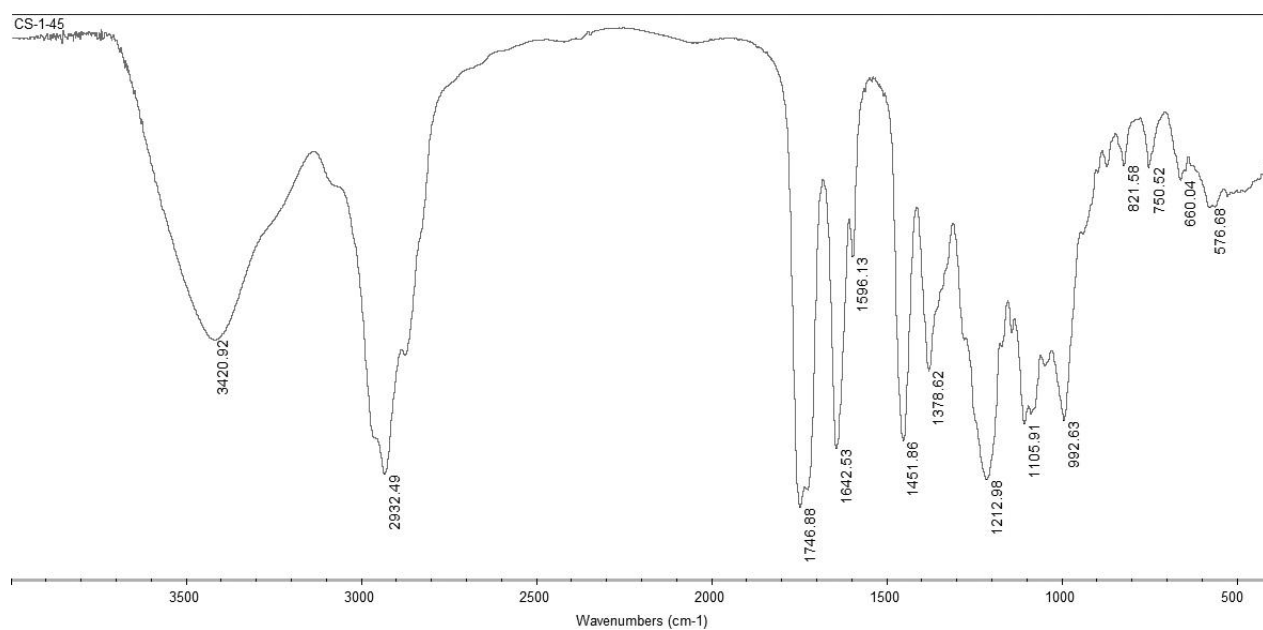


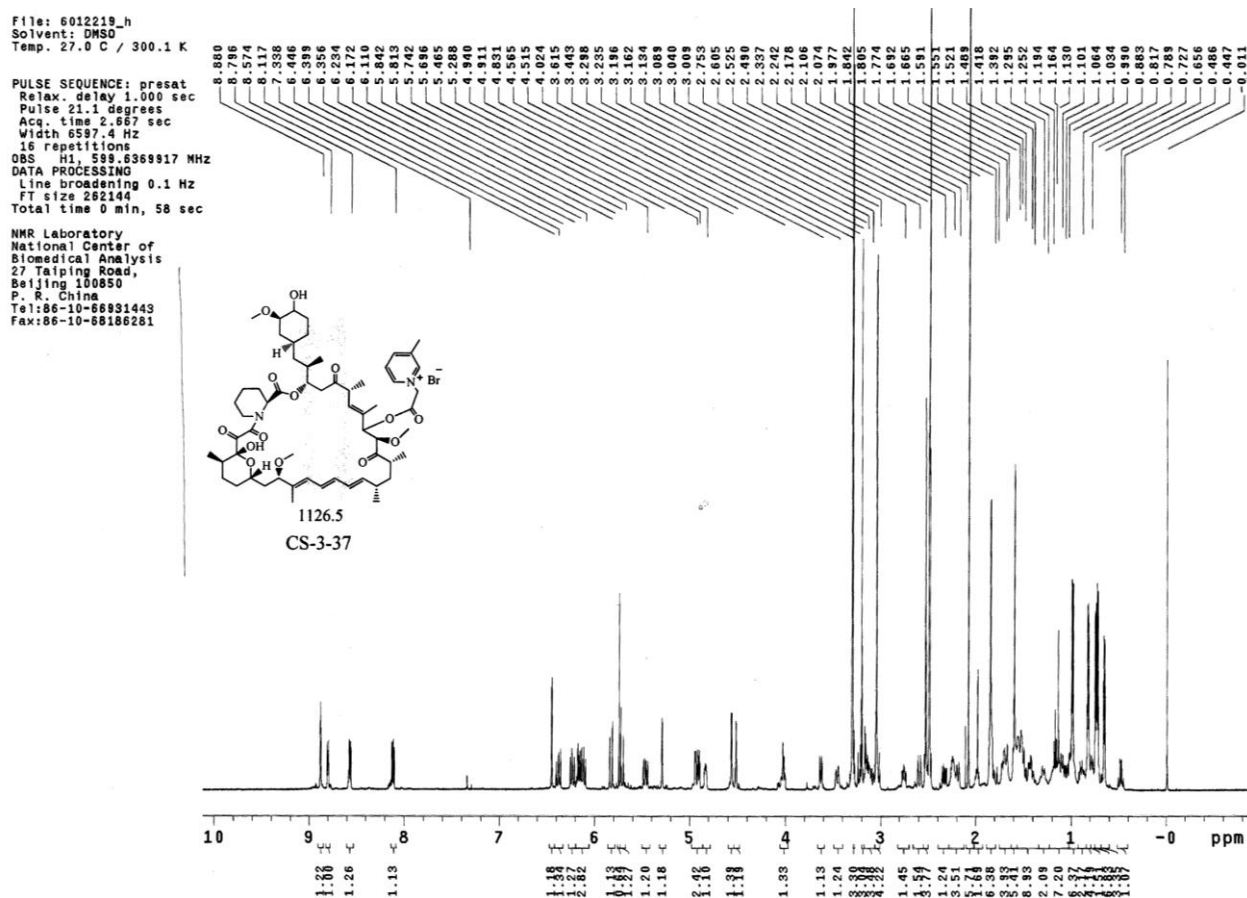
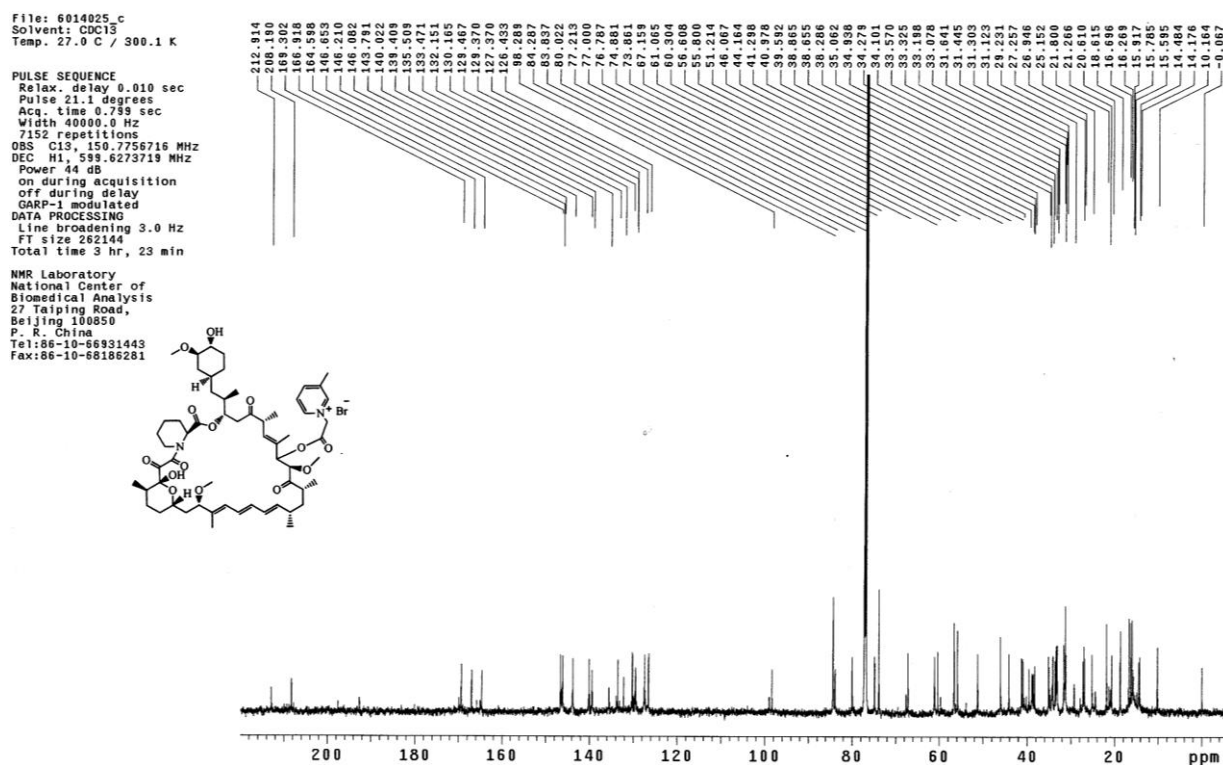
Figure S46. ^1H -NMR of compound 9.Figure S47. ^{13}C -NMR of compound 9.

Figure S48. MS of compound 9.

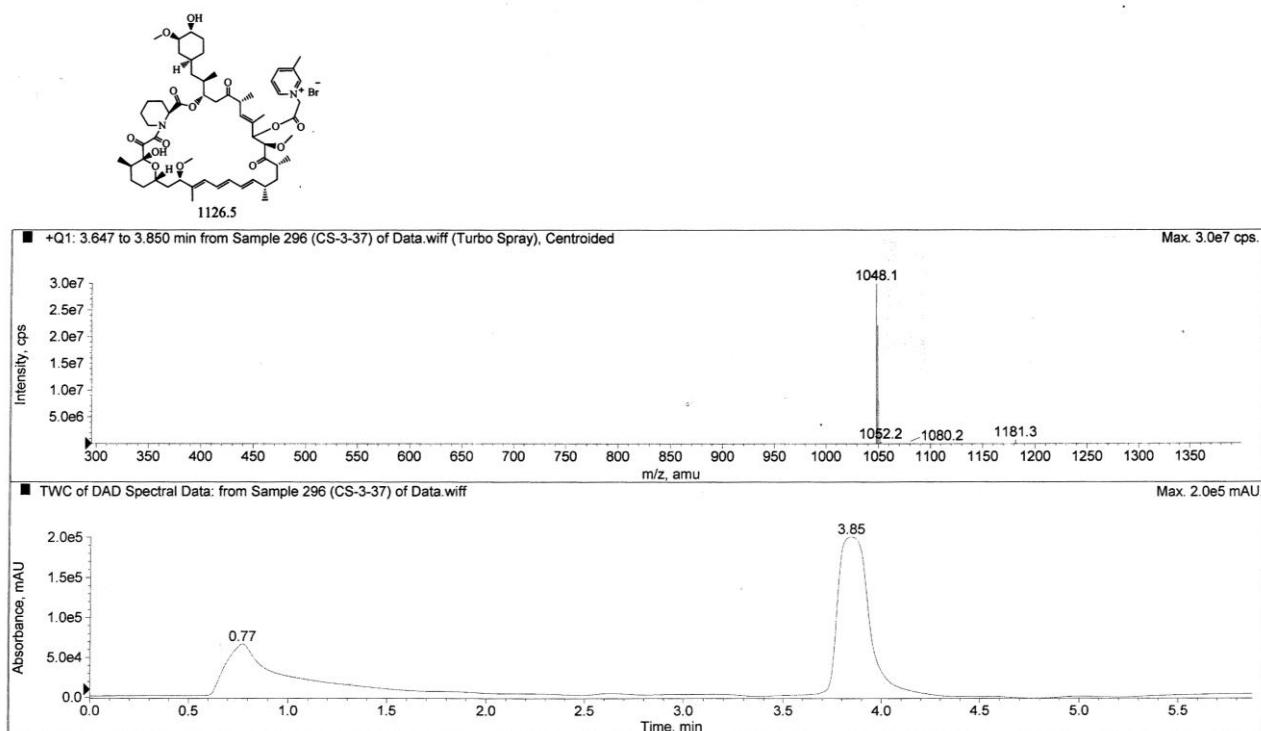


Figure S49. IR of compound 9.

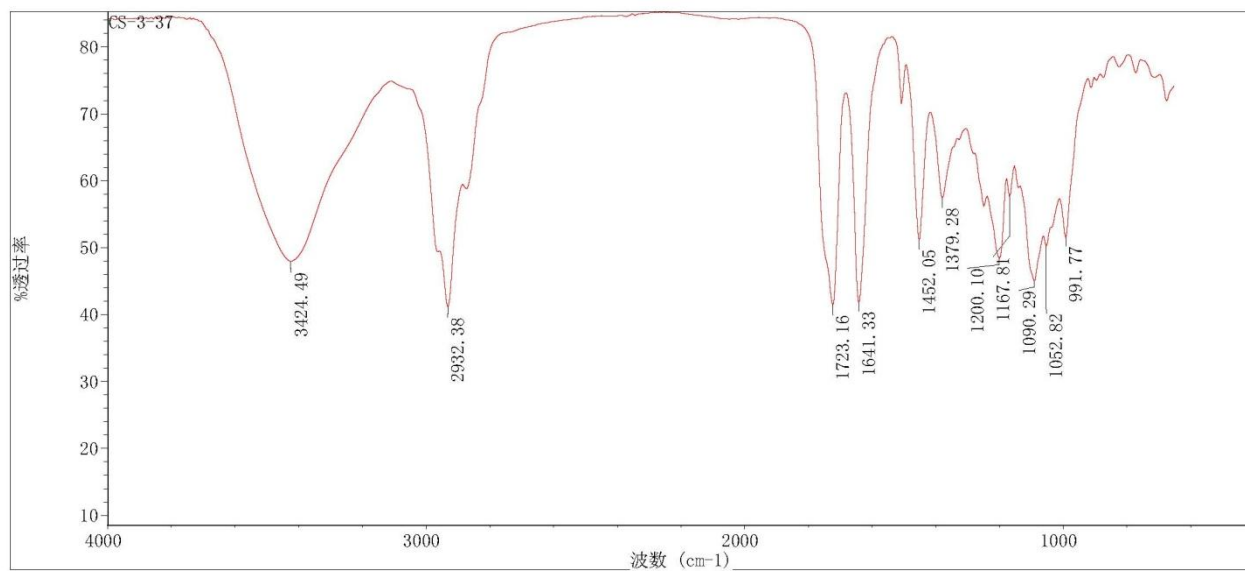


Figure S52. MS of compound 10.

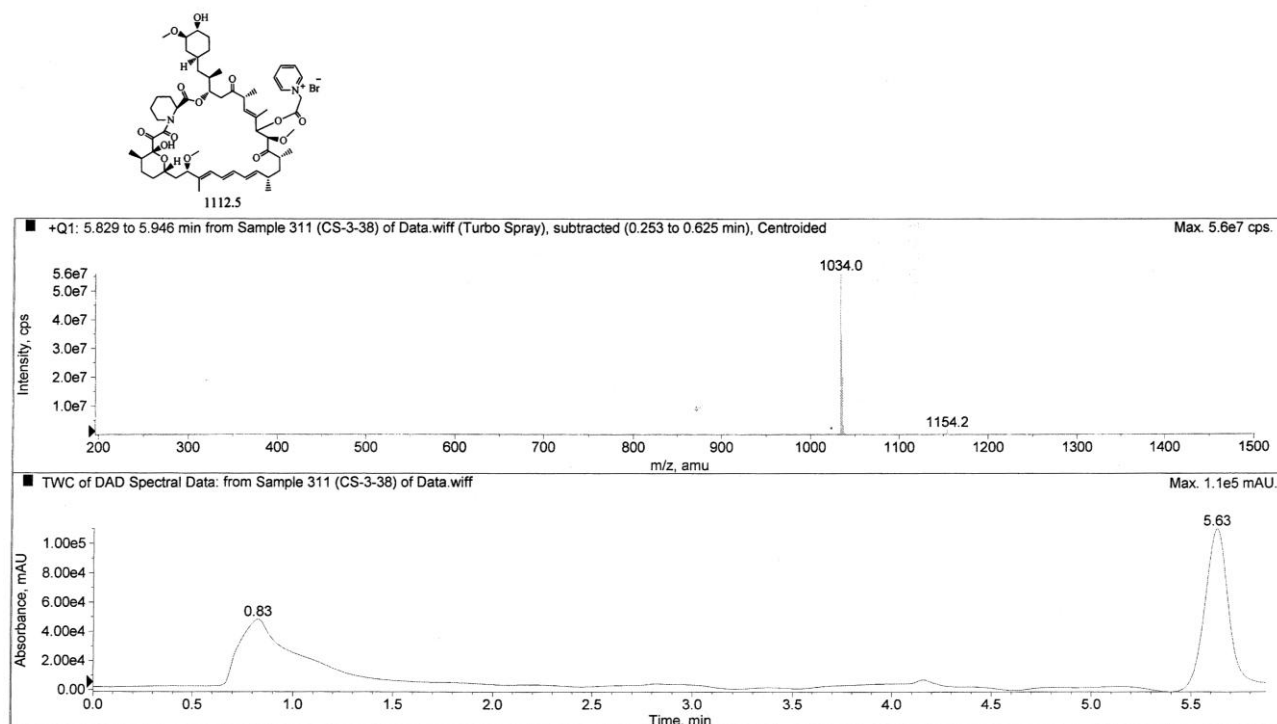
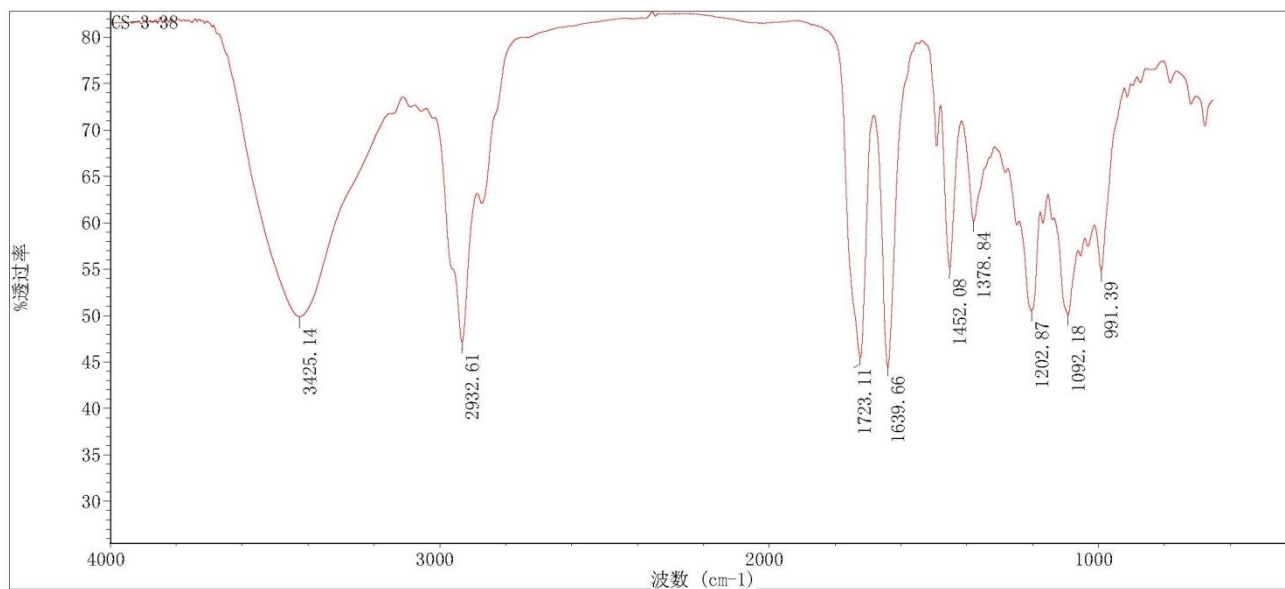


Figure S53. IR of compound 10.



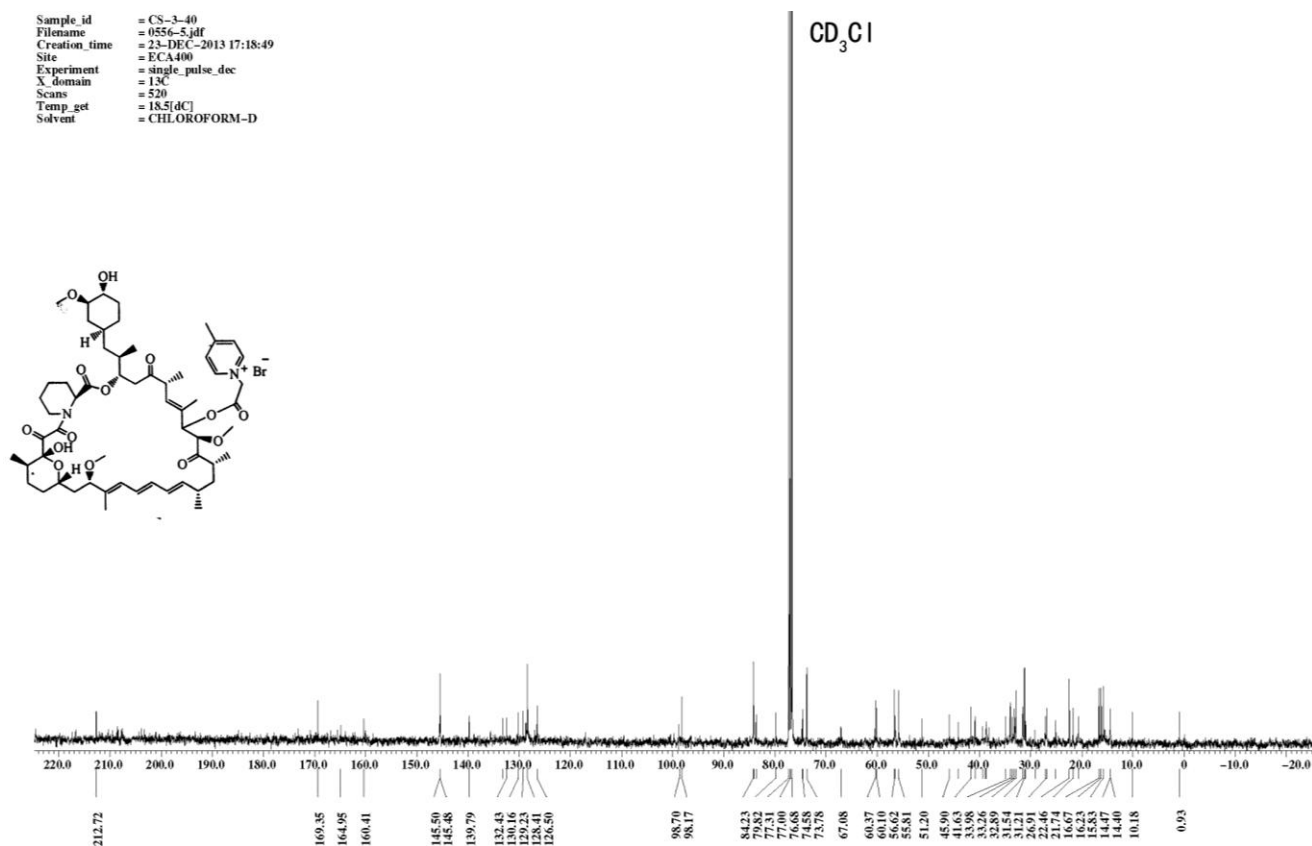
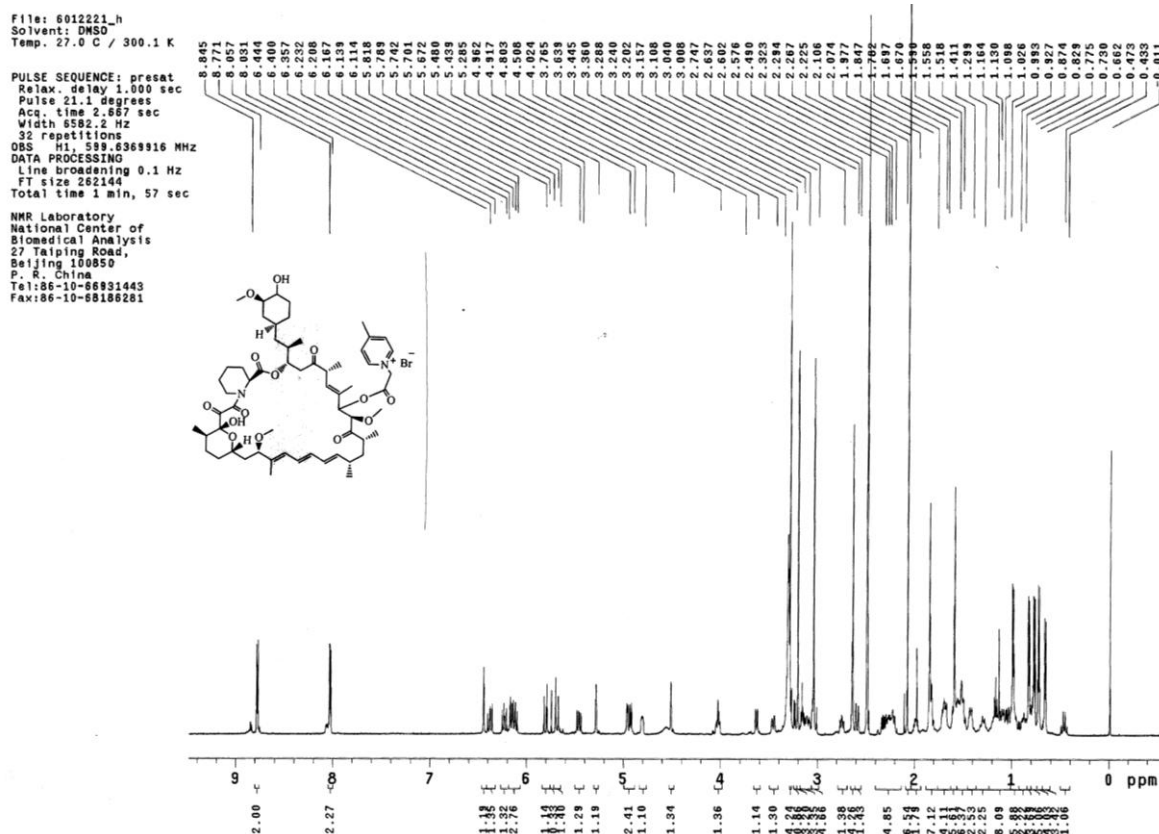


Figure S56. MS of compound 11.

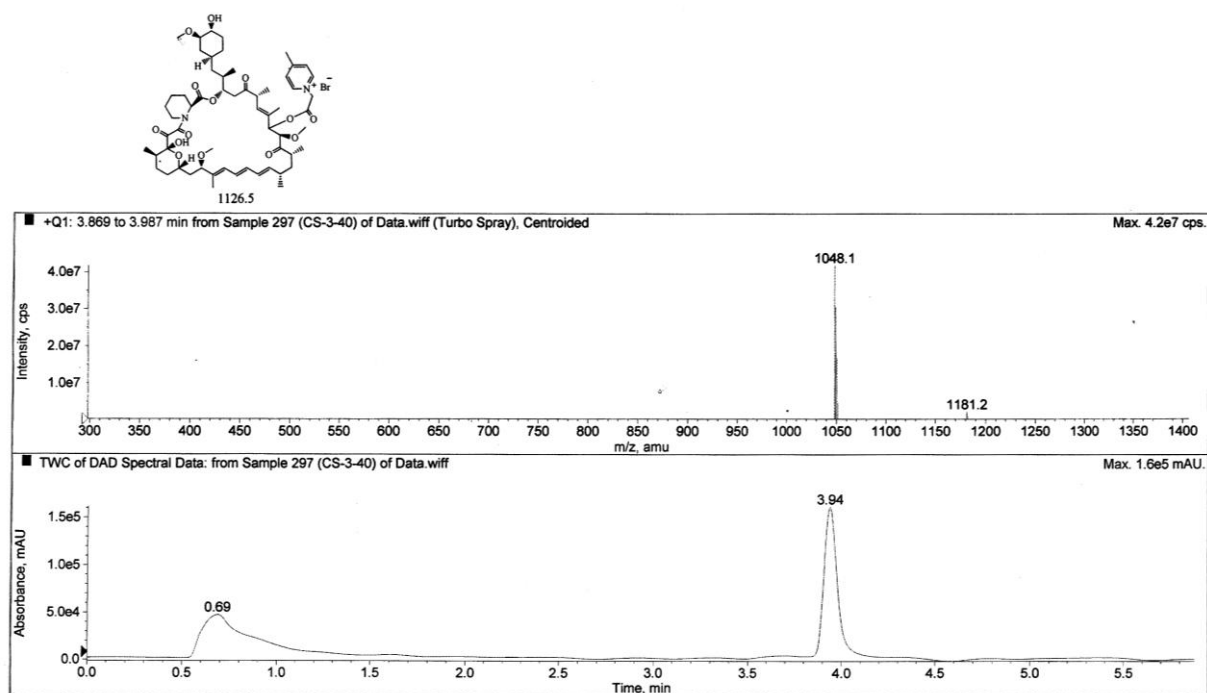


Figure S57. IR of compound 11.

