

Bioactive 18(4→3)-*abeo*-abietanoids Derivatives from the Leaves of *Tripterygium Wilfordii*

Chao Wang,^{ab} Chuang-Jun Li,^a Jie Ma,^a Jing-Zhi Yang,^a Xiao-Guang Chen,^a Li Li,^a and Dong-Ming Zhang^{*a}

^a State Key Laboratory of Bioactive Substance and Function of Natural Medicines, Institute of Materia Medica, Chinese Academy of Medical Sciences and Peking Union Medical College, Beijing 100050, People's Republic of China

^b College of Pharmacy, Dalian Medical University, Dalian 116044, China

Supporting Information

List of Supporting Information

Figure S1. The ^1H NMR (600 MHz) spectrum of tripterlide A (1) in actone- d_6	4
Figure S2. The ^{13}C NMR (150 MHz) spectrum of tripterlide A (1) in actone- d_6	5
Figure S3. The DEPT spectrum of tripterlide A (1) in actone- d_6	6
Figure S4. The HSQC spectrum of tripterlide A (1) in actone- d_6	7
Figure S5. The HMBC spectrum of tripterlide A (1) in actone- d_6	8
Figure S6. The ^1H - ^1H COSY spectrum of tripterlide A (1) in actone- d_6	9
Figure S7. The NOESY spectrum of tripterlide A (1) in actone- d_6	10
Figure S8. The IR spectrum of tripterlide A (1).....	11
Figure S9. The HRESIMS of tripterlide A (1).....	12
Figure S10. The ^1H NMR (400 MHz) spectrum of tripterlide B (2) in actone- d_6	13
Figure S11. The ^{13}C NMR (150 MHz) spectrum of tripterlide B (2) in actone- d_6	14
Figure S12. The DEPT spectrum of tripterlide B (2) in actone- d_6	15
Figure S13. The HSQC spectrum of tripterlide B (2) in actone- d_6	16
Figure S14. The HMBC spectrum of tripterlide B (2) in actone- d_6	17
Figure S15. The ^1H - ^1H COSY spectrum of tripterlide B (2) in actone- d_6	18
Figure S16. The NOESY spectrum of tripterlide B (2) in actone- d_6	19
Figure S17. The IR spectrum of tripterlide B (2).....	20
Figure S18. The HRESIMS of tripterlide B (2).....	21
Figure S19. The ^1H NMR (500 MHz) spectrum of tripterlide C (3) in CDCl_3	22
Figure S20. The ^{13}C NMR (125 MHz) spectrum of tripterlide C (3) in CDCl_3	23
Figure S21. The HSQC spectrum of tripterlide C (3) in CDCl_3	24
Figure S22. The HMBC spectrum of tripterlide C (3) in CDCl_3	25
Figure S23. The ^1H - ^1H COSY spectrum of tripterlide C (3) in CDCl_3	26
Figure S24. The NOESY spectrum of tripterlide C (3) in CDCl_3	27
.....	27
Figure S25. The IR spectrum of tripterlide C (3).....	28
Figure S26. The HRESIMS of tripterlide C (3).....	29
Figure 27. Optimized conformations of 1	30
Figure S28. Calculated ECD spectra of 5 <i>R</i> , 20 <i>S</i> , 12 <i>S</i> (1a , 1aC2) and experimental ECD spectrum of 1	30
Figure 29. Optimized conformations of 2	31
Figure S30. Calculated ECD spectra of 5 <i>R</i> , 20 <i>S</i> , 12 <i>R</i> (2a , 2aC2) and experimental ECD spectrum of 2 , and 3	31
Figure S31. The ^1H NMR (600 MHz)spectrum of tripterlide D (4) in CDCl_3	32
Figure S32. The ^{13}C NMR (150 MHz) spectrum of tripterlide D (4) in CDCl_3	33
Figure S33. The HSQC spectrum of tripterlide D (4) in CDCl_3	34
Figure S34. The HMBC spectrum of tripterlide D (4) in CDCl_3	35
Figure S35. The ^1H - ^1H COSY spectrum of tripterlide D (4) in CDCl_3	36
Figure S36. The NOESY spectrum of tripterldie D (4) in CDCl_3	37
Figure S37. The HRESIMS spectrum of tripterlide D (4).....	38
Figure S38. The ^1H NMR (600 MHz) spectrum of tripterlide E (5) in CDCl_3	39

Figure S39. The ^{13}C NMR (150 MHz) spectrum of tripterlide E (5) in CDCl_3	40
Figure S40. The HSQC spectrum of tripterlide E (5) in CDCl_3	41
Figure S41. The HMBC spectrum of tripterlide E (5) in CDCl_3	42
Figure S42. The ^1H - ^1H COSY spectrum of tripterlide E (5) in CDCl_3	43
Figure S43. The NOESY spectrum of tripterlide E (5) in CDCl_3	44
Figure S44. The IR spectrum of tripterlide E (5) in CDCl_3	45
Figure S45. The HRESIMS spectrum of tripterlide E (5) in CDCl_3	46
Figure S46. The ^1H NMR (400 MHz) spectrum of tripterlide F (6) in CDCl_3	47
Figure S47. The ^{13}C NMR (100 MHz) spectrum of tripterlide F (6) in CDCl_3	48
Figure S48. The HSQC spectrum of tripterlide F (6) in CDCl_3	49
Figure S49. The HMBC spectrum of tripterlide F (6) in CDCl_3	50
Figure S50. The ^1H - ^1H COSY spectrum of tripterlide F (6) in CDCl_3	51
Figure S51. The 1D NOE spectrum of tripterlide F (6) in CDCl_3	52
Figure S52. The IR spectrum of tripterlide F (6)	53
Figure S53. The HRESIMS spectrum of tripterlide F (6).....	54

Figure S1. The ^1H NMR (600 MHz) spectrum of tripterlide A (1) in actone- d_6

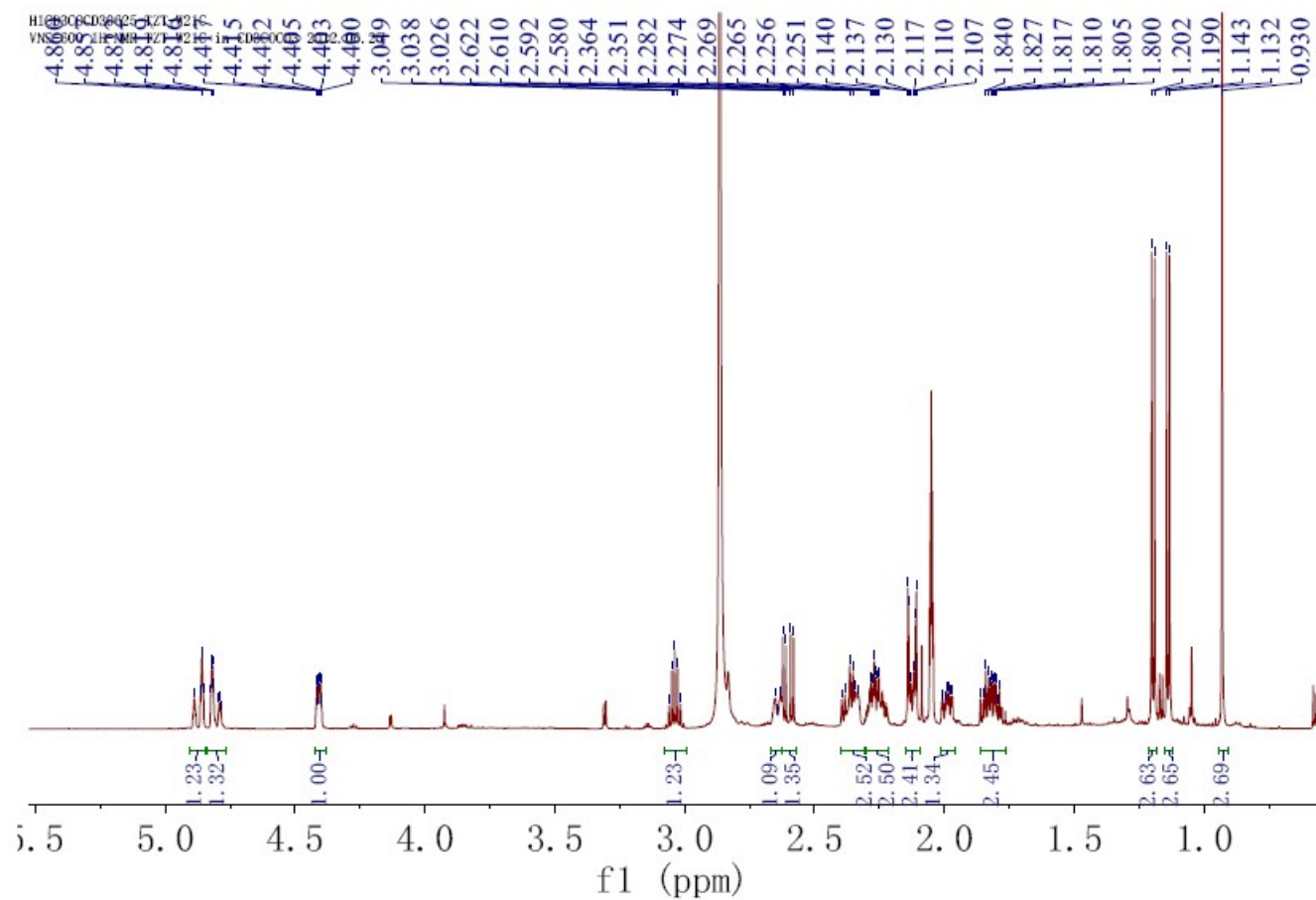


Figure S2. The ^{13}C NMR (150 MHz) spectrum of tripterlide A (1) in acetone- d_6

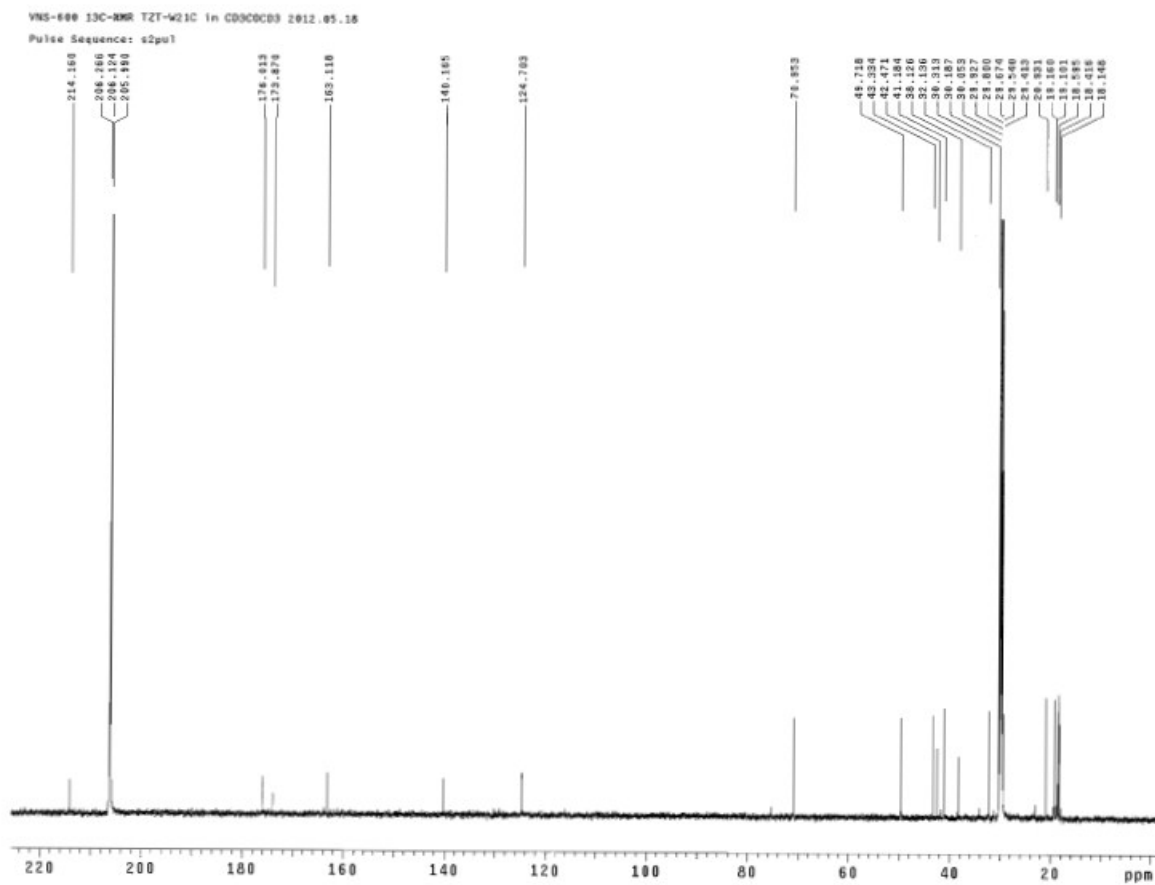


Figure S3. The DEPT spectrum of tripterlide A (1) in actone- d_6

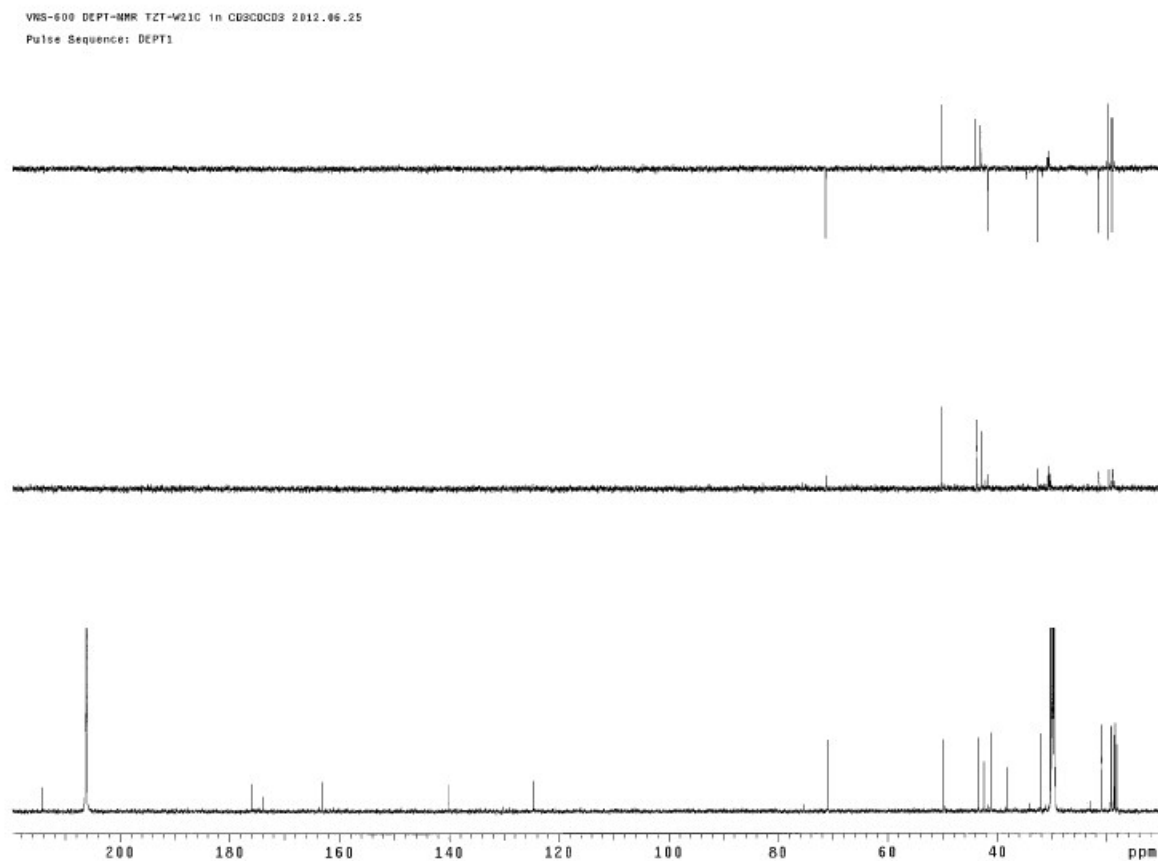


Figure S4. The HSQC spectrum of tripterlide A (1) in actone- d_6

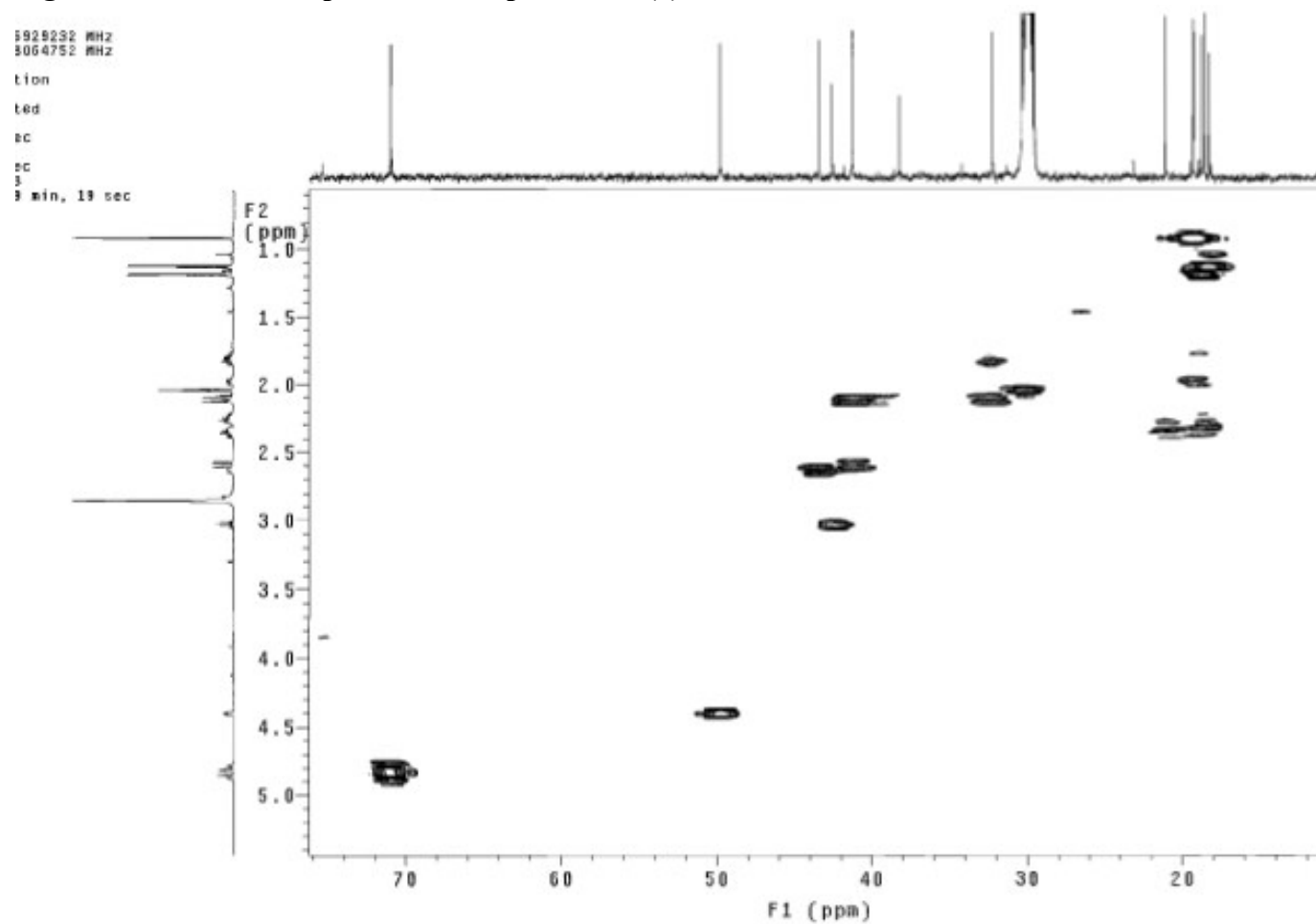


Figure S5. The HMBC spectrum of tripterlide A (1) in actone- d_6

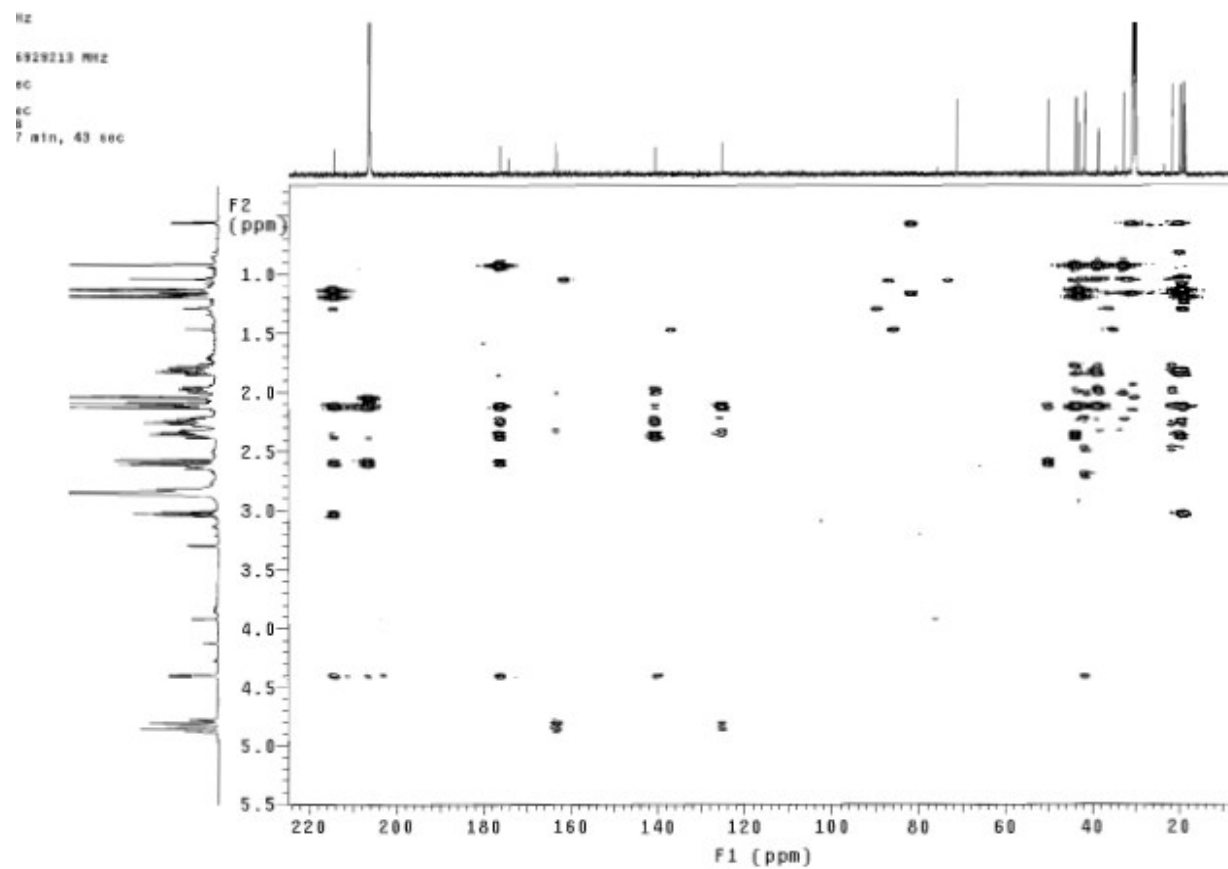


Figure S6. The ^1H - ^1H COSY spectrum of tripterlide A (1) in actone- d_6

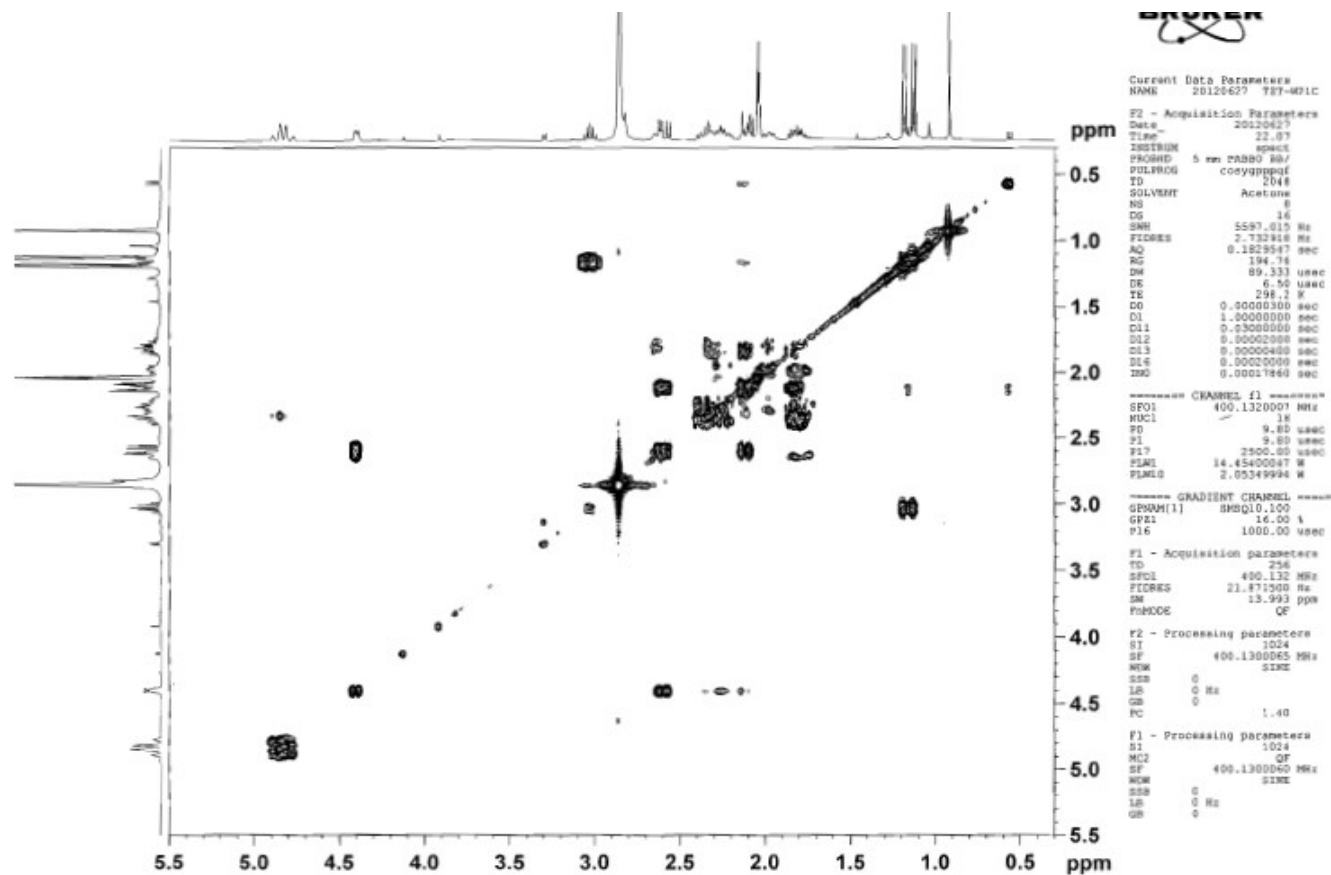


Figure S7. The NOESY spectrum of tripterlide A (1) in actone- d_6

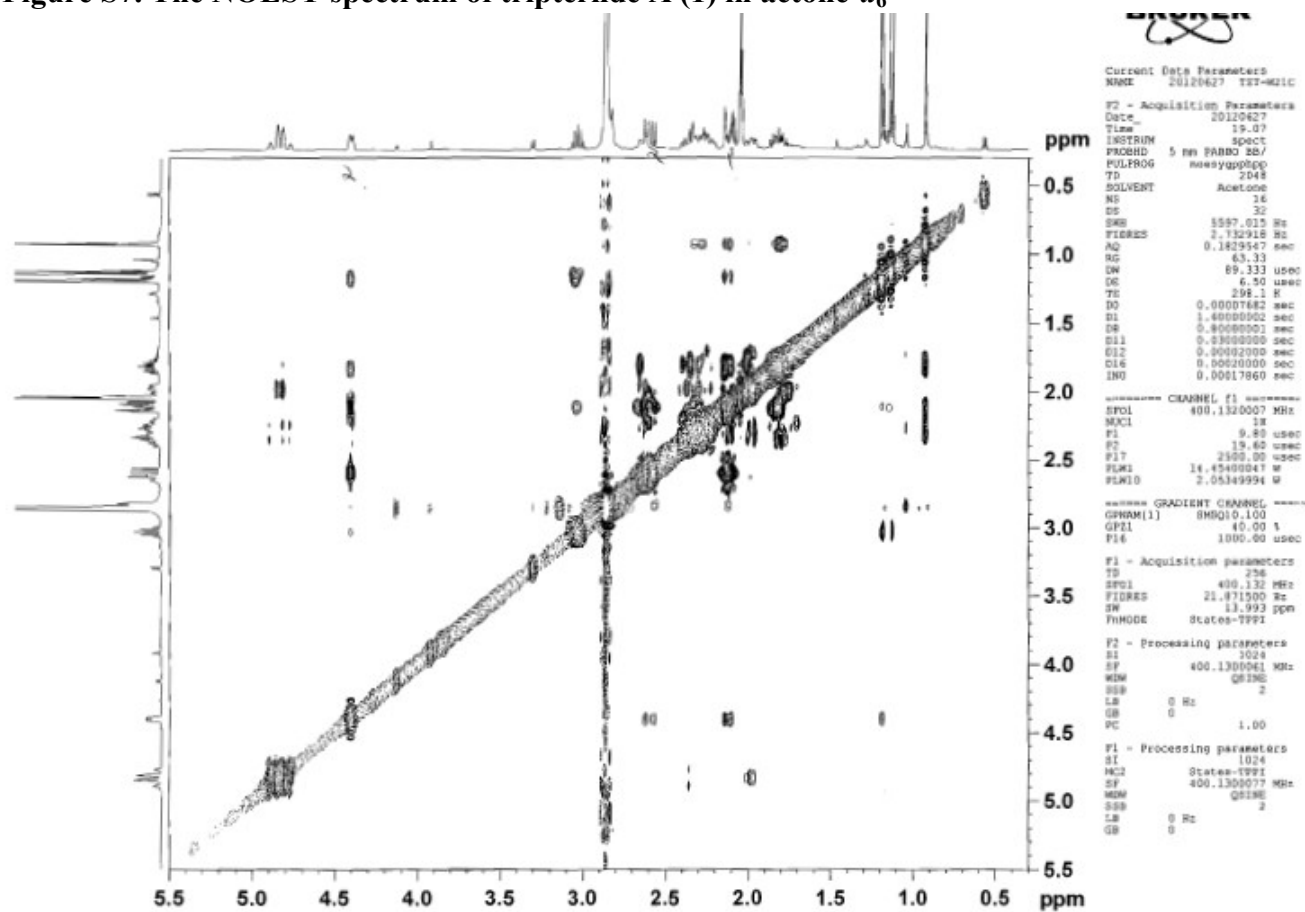


Figure S8. The IR spectrum of tripterlide A (1)

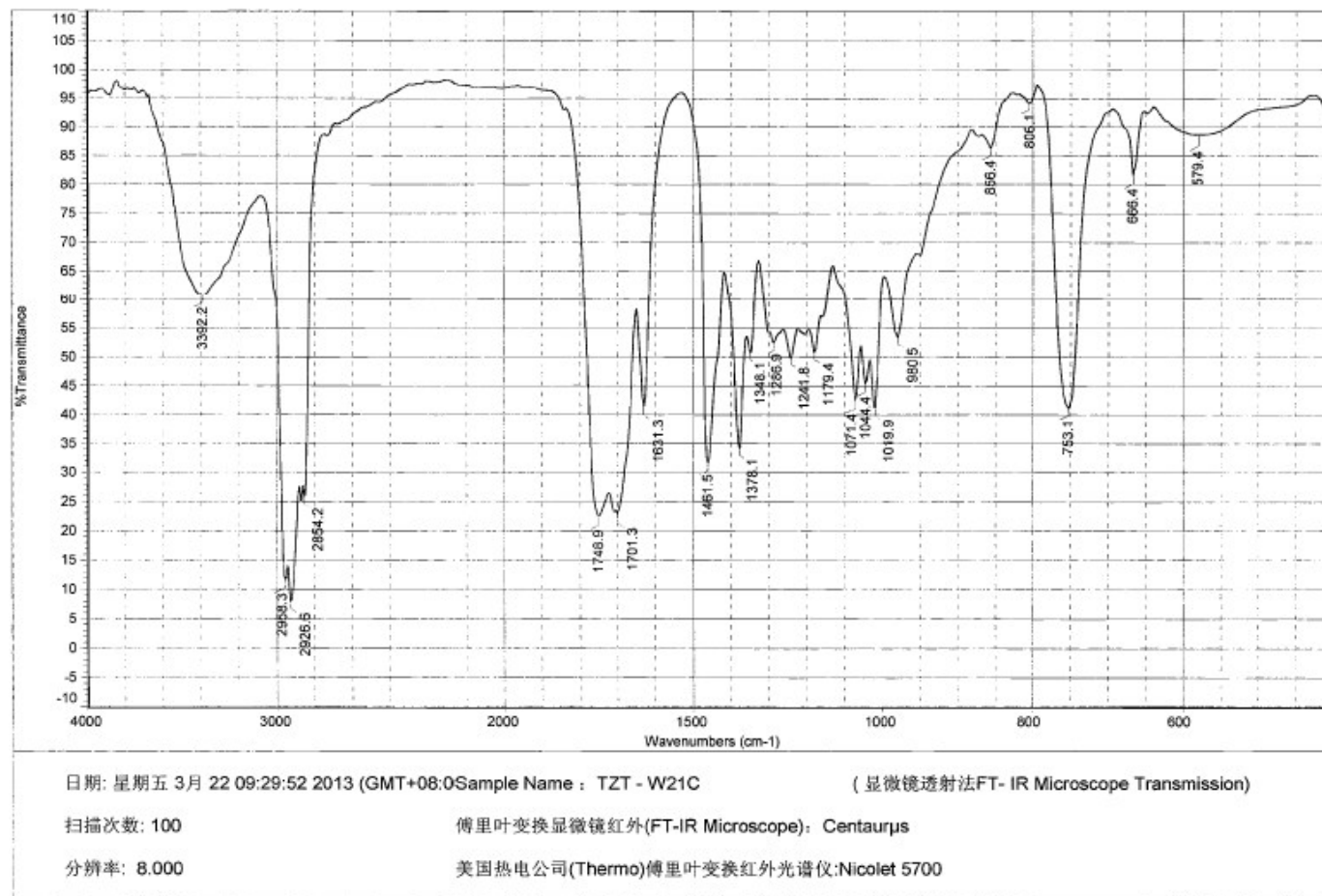


Figure S9. The HRESIMS of tripterlide A (1)

MS Formula Results: + Scan (5.977 min) Sub (2012060501.d)

m/z	Ion	Formula	Abundance
329.1759	[M+H] ⁺	C29 H25 O4	775358.9

Base	Formula (M)	Ion Formula	Calc m/z	Score	Cross S	Mass	Calc Mass	Diff (ppm)	Alt Diff (ppm)	Abund Match	Spacing Mat	Mass Match	m/z	DBE
[2]	C20 H24 O4	C29 H25 O4	329.1747	99.76		329.1686	329.1675	-3.58	3.58	99.88	99.94	99.6	329.1759	9
[14]	C21 H20 N4	C21 H21 N4	329.1791	99.76		329.1686	329.1689	0.49	0.49	99.15	100	99.99	329.1759	14
[8]	C17 H28 O4 S	C17 H29 O4 S	329.1791	99.39		329.1686	329.1708	6.69	6.69	97.3	99.29	98.6	329.1759	4

m/z	Ion	Formula	Abundance
351.1573	[M+Na] ⁺	C20 H24 Na O4	1674053.6

Base	Formula (M)	Ion Formula	Calc m/z	Score	Cross S	Mass	Calc Mass	Diff (ppm)	Alt Diff (ppm)	Abund Match	Spacing Mat	Mass Match	m/z	DBE
[2]	C20 H24 O4	C20 H24 Na O4	351.1567	99.87		329.1681	329.1675	-1.88	1.88	99.88	99.79	99.9	351.1573	9
[14]	C21 H20 N4	C21 H20 N4 Na	351.158	99.78		329.1681	329.1689	2.19	2.19	99.74	99.64	99.87	351.1573	14

Figure S10. The ^1H NMR (400 MHz) spectrum of tripterlide B (2) in acetone- d_6

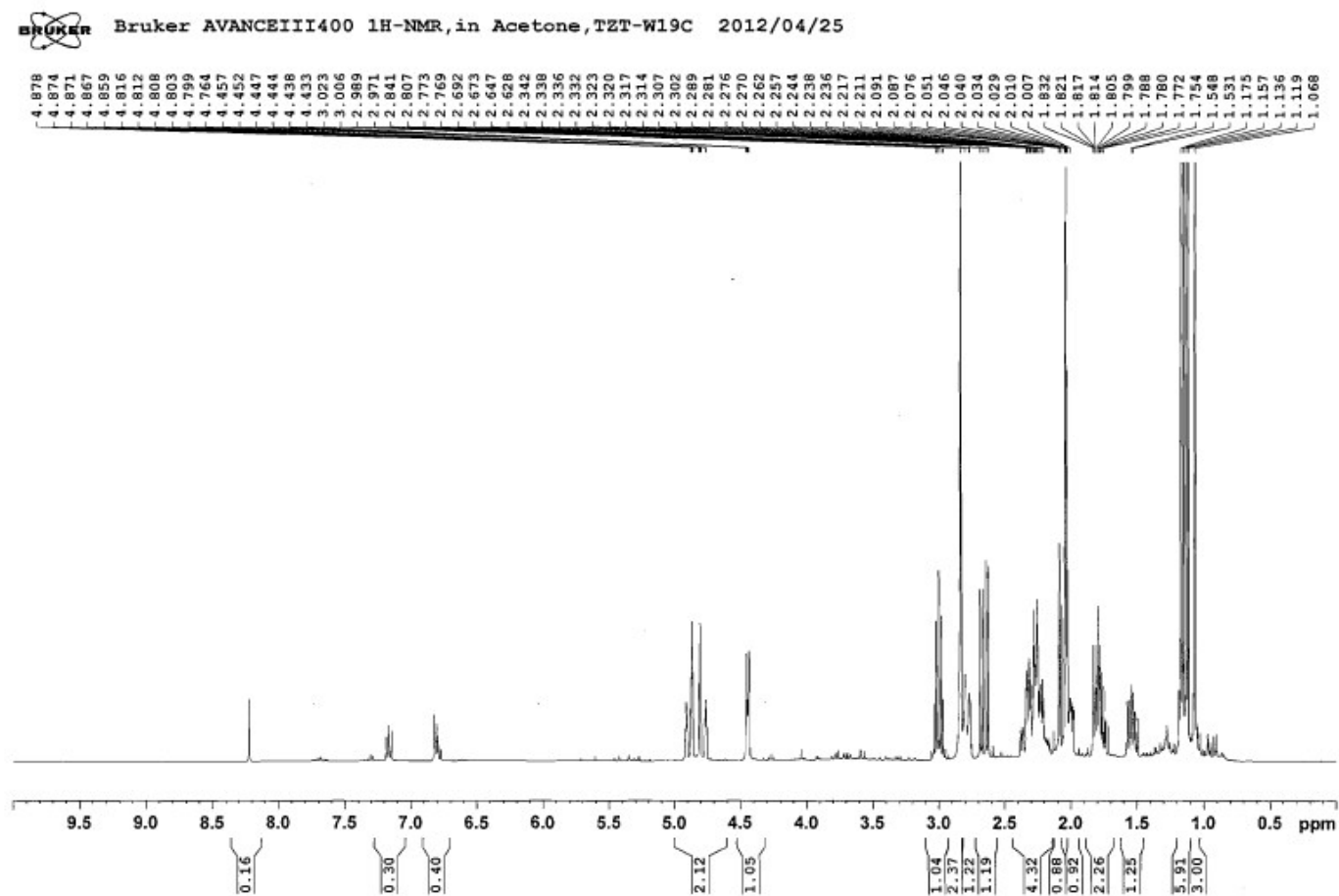


Figure S11. The ^{13}C NMR (150 MHz) spectrum of tripterlide B (2) in actone- d_6

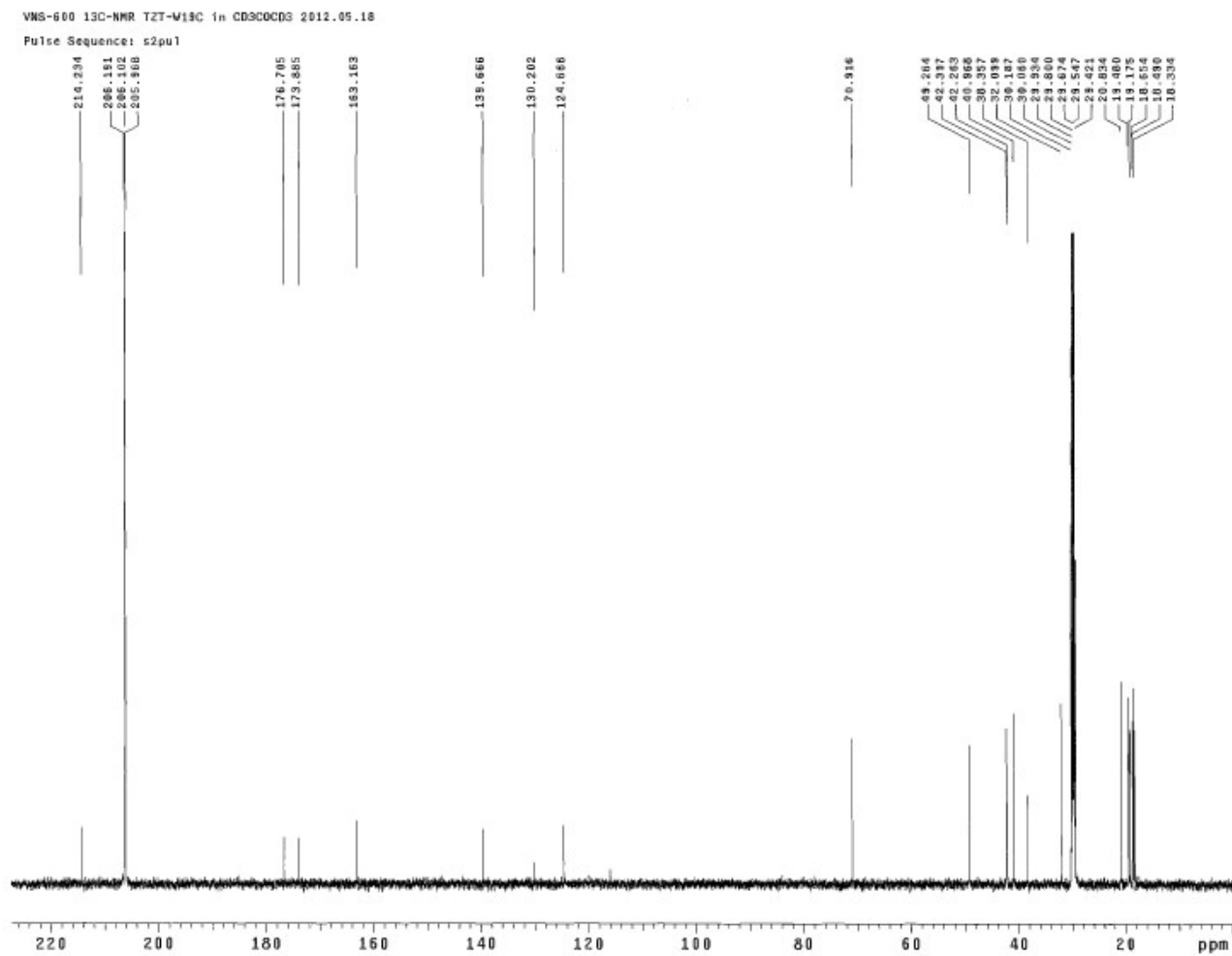


Figure S12. The DEPT spectrum of tripterlide B (2) in acetone- d_6

VNS-600 DEPT 121-V19C IN acetone Jul 19 2012

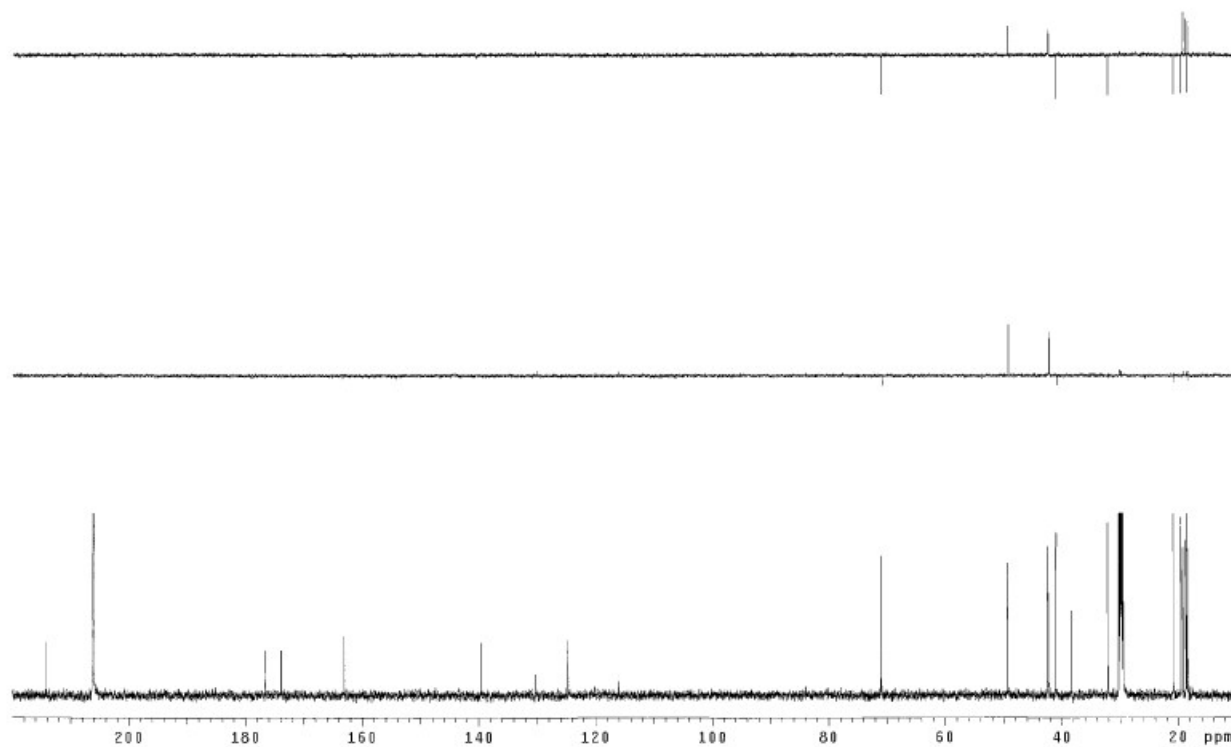


Figure S13. The HSQC spectrum of tripterlide B (2) in actone- d_6

tone Jul 19 2012

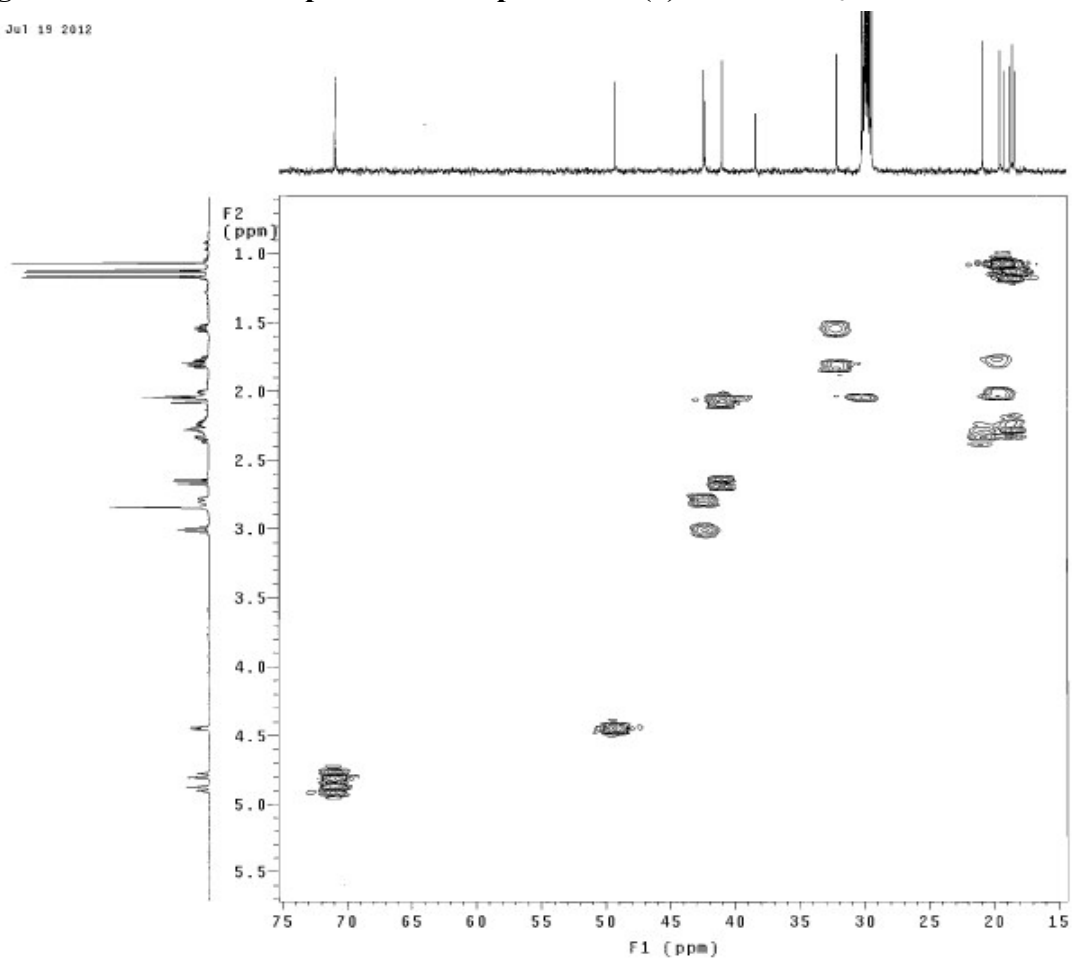


Figure S14. The HMBC spectrum of tripterlide B (2) in actone- d_6

itone Jul 19 2012

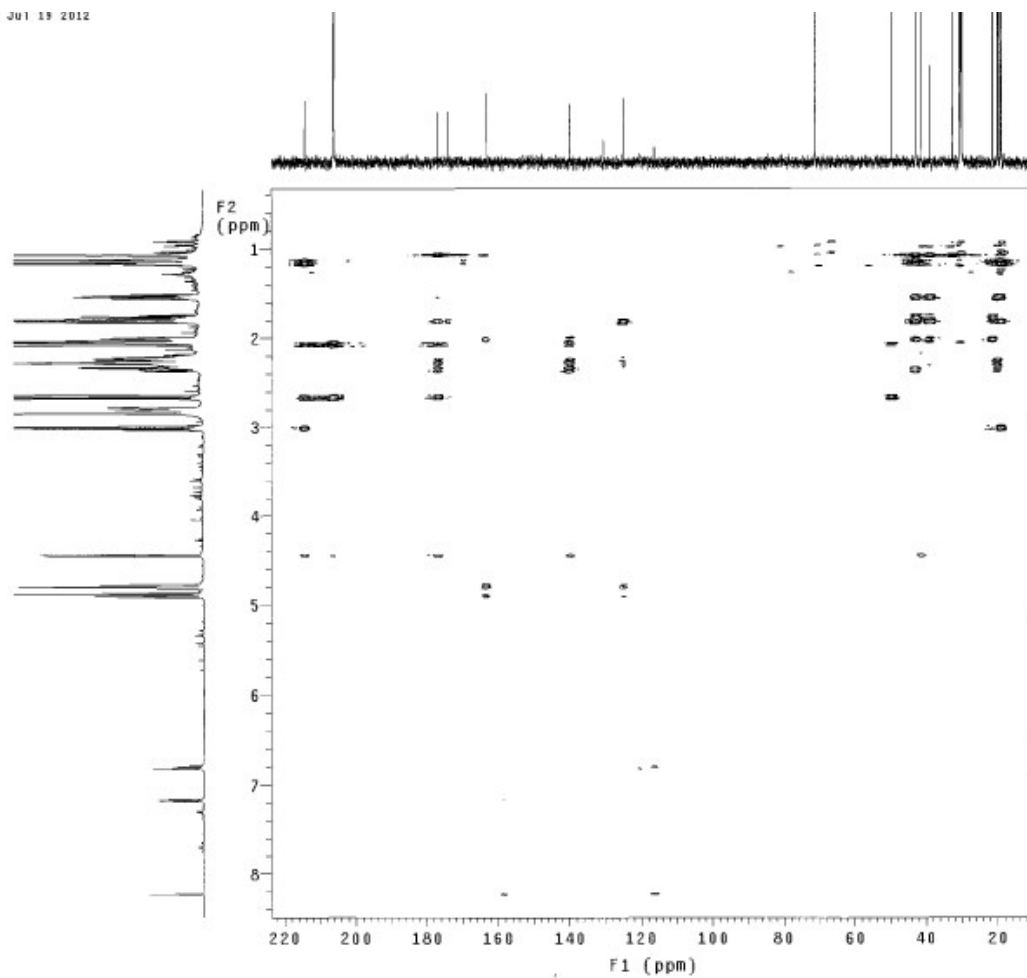


Figure S15. The ^1H - ^1H COSY spectrum of tripterlide B (2) in acetone- d_6

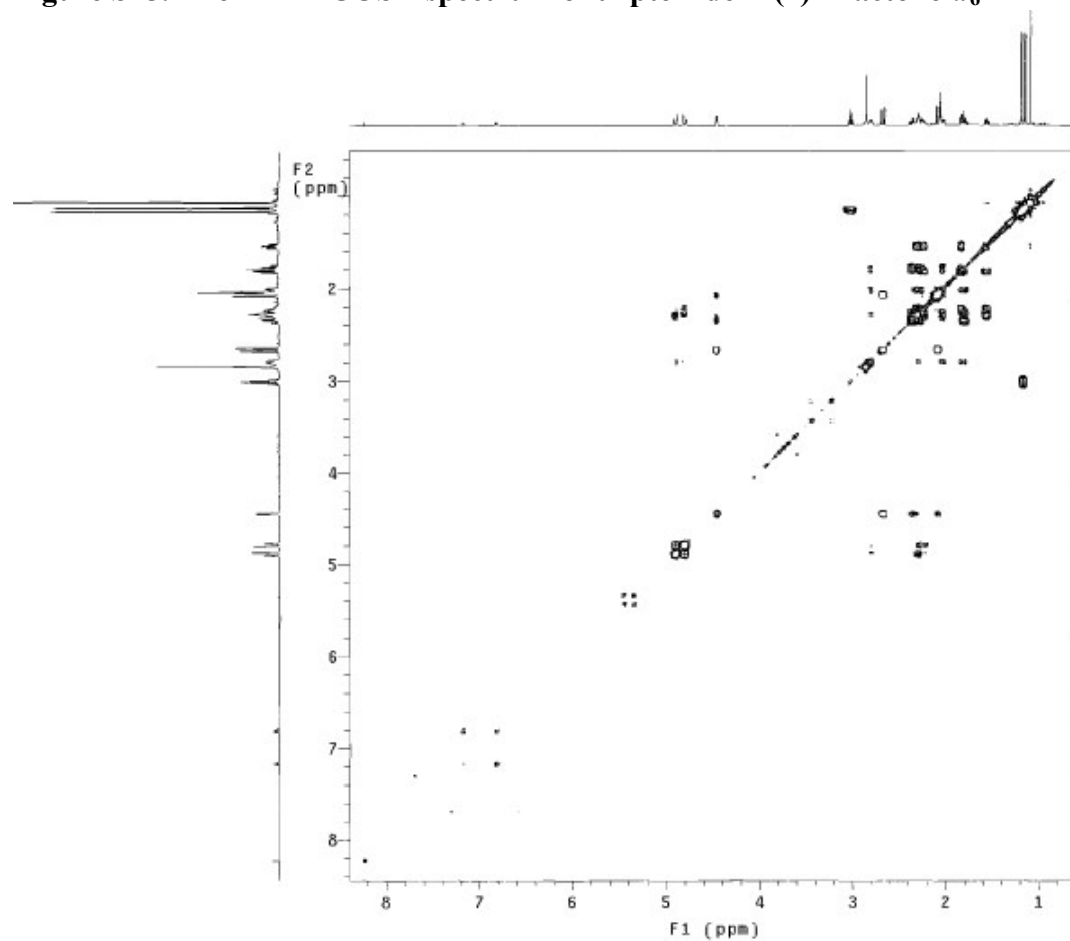


Figure S16. The NOESY spectrum of tripterlide B (2) in actone- d_6

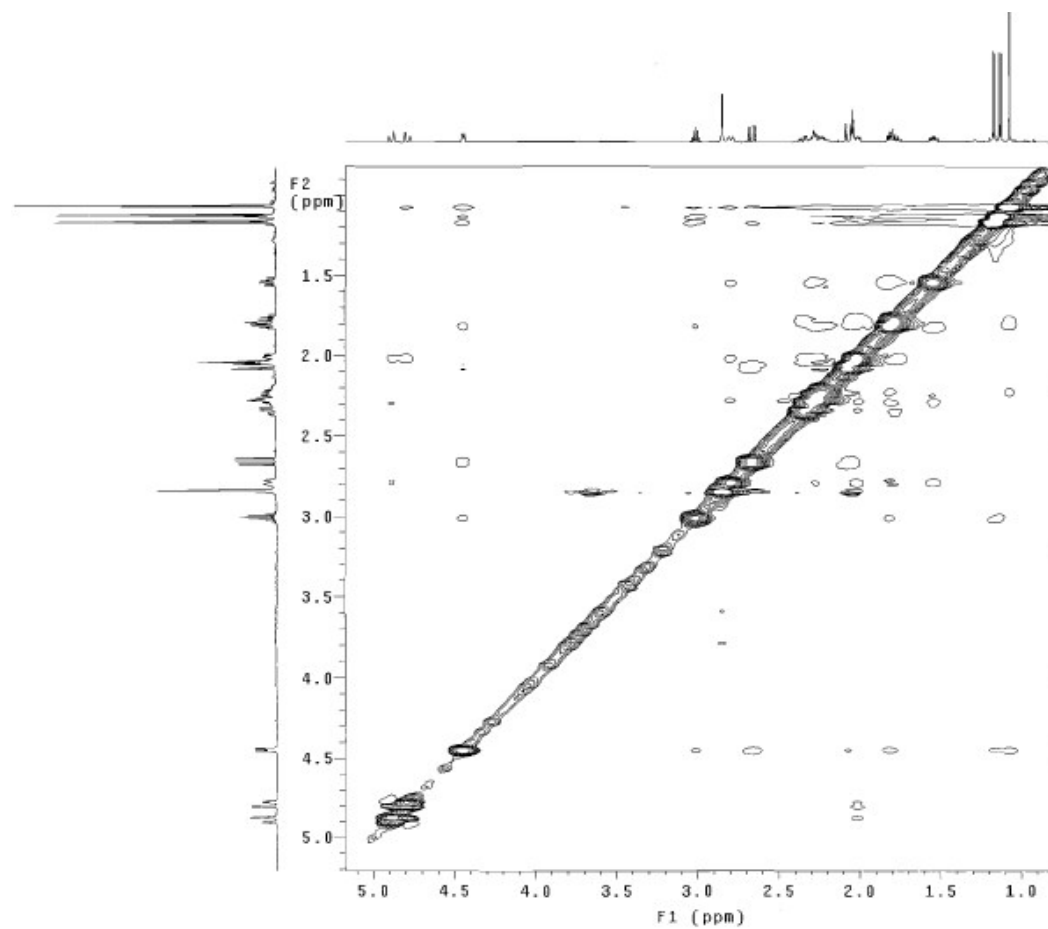


Figure S17. The IR spectrum of tripterlide B (2)

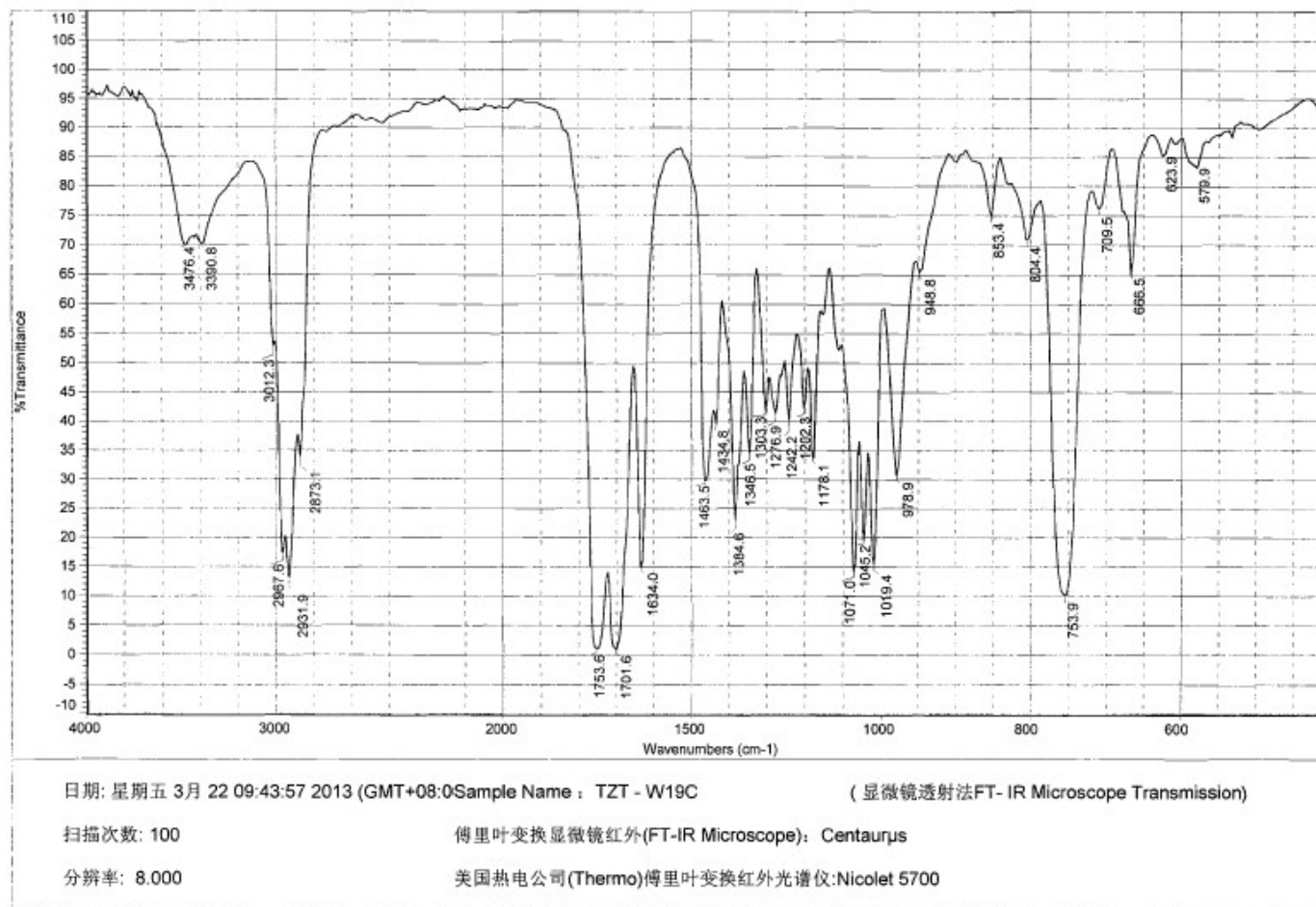


Figure S18. The HRESIMS of tripterlide B (2)

MS Formula Results: + Scan (5.850 min) Sub (2012071601.d)

m/z	Ion	Formula	Abundance											
329.1753	(M+H) ⁺	C29 H25 O4	5217935											
Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross S	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Mat	Mass Match	m/z	DBE
329.1747	C29 H24 O4	C29 H25 O4	329.1747	99.48		329.168	329.1675	-1.34	1.34	98.35	99.87	99.9	329.1753	9
m/z	Ion	Formula	Abundance											
346.2021	(M+NH4) ⁺	C30 H28 N O4	860529.1											
Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross S	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Mat	Mass Match	m/z	DBE
346.2013	C30 H28 N O4	C30 H28 N O4	346.2013	98.31		329.1682	329.1675	-2.11	2.11	97.06	98.7	99.67	346.2021	9
m/z	Ion	Formula	Abundance											
351.1571	(M+Na) ⁺	C30 H24 Na O4	1729496.9											
Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross S	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Mat	Mass Match	m/z	DBE
351.1567	C30 H24 Na O4	C30 H24 Na O4	351.1567	99		329.1670	329.1675	+1.25	1.25	99.6	99.38	99.99	351.1571	9

Figure S19. The ^1H NMR (500 MHz) spectrum of tripterlide C (3) in CDCl_3

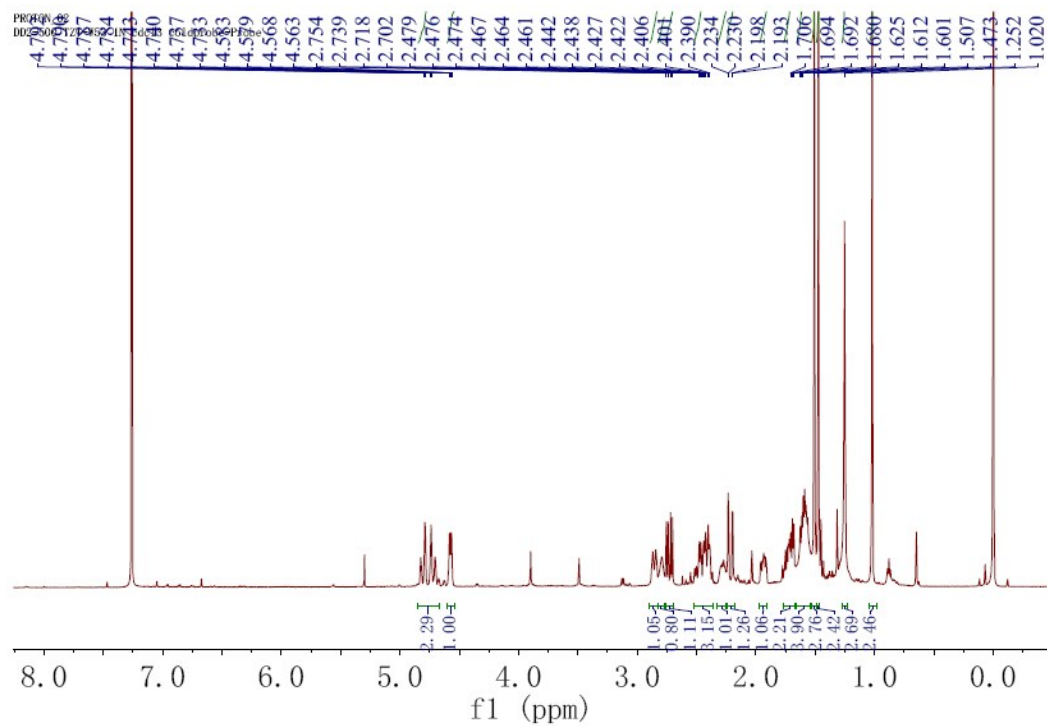


Figure S20. The ^{13}C NMR (125 MHz) spectrum of tripterlide C (**3**) in CDCl_3

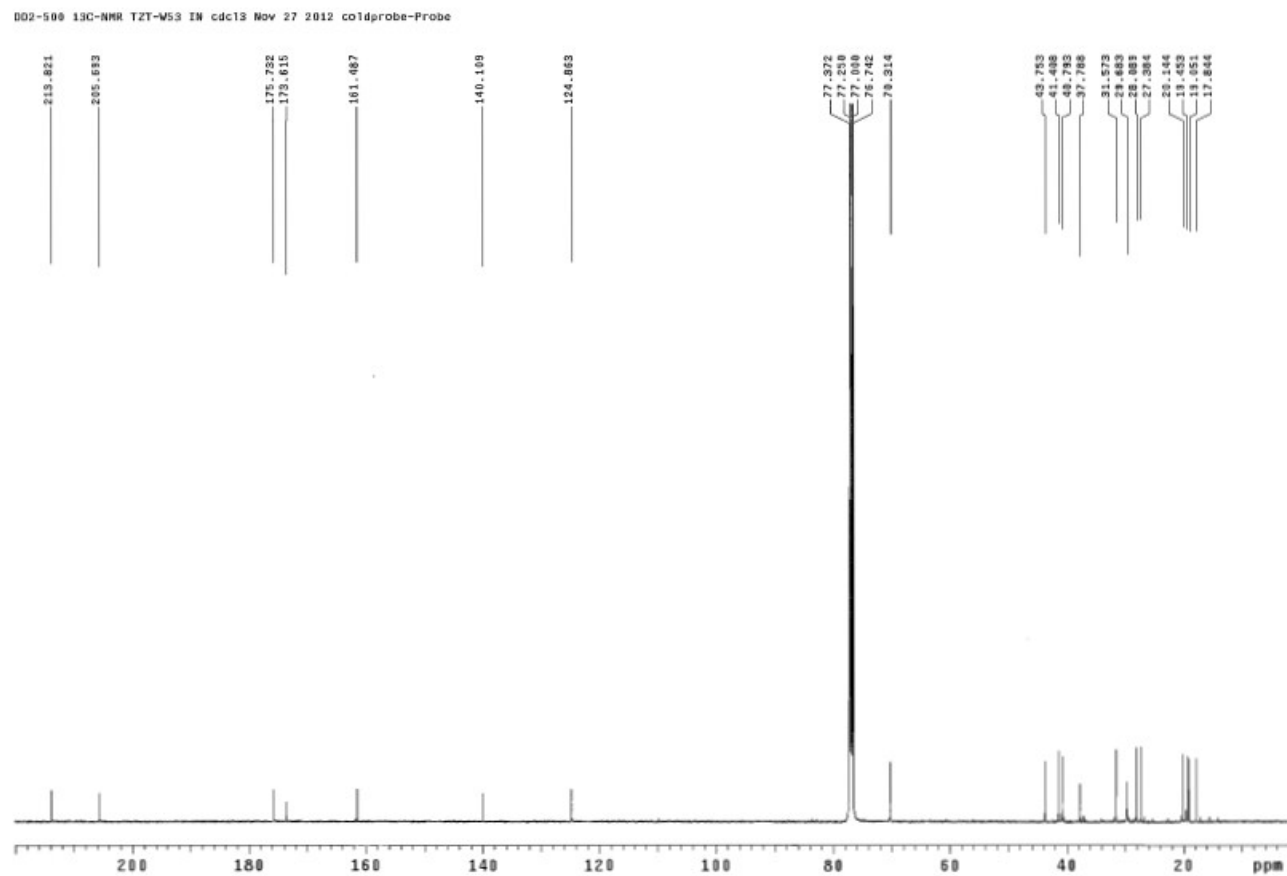


Figure S21. The HSQC spectrum of tripterlide C (3) in CDCl₃

dc13 Nov 27 2012 coldprobe

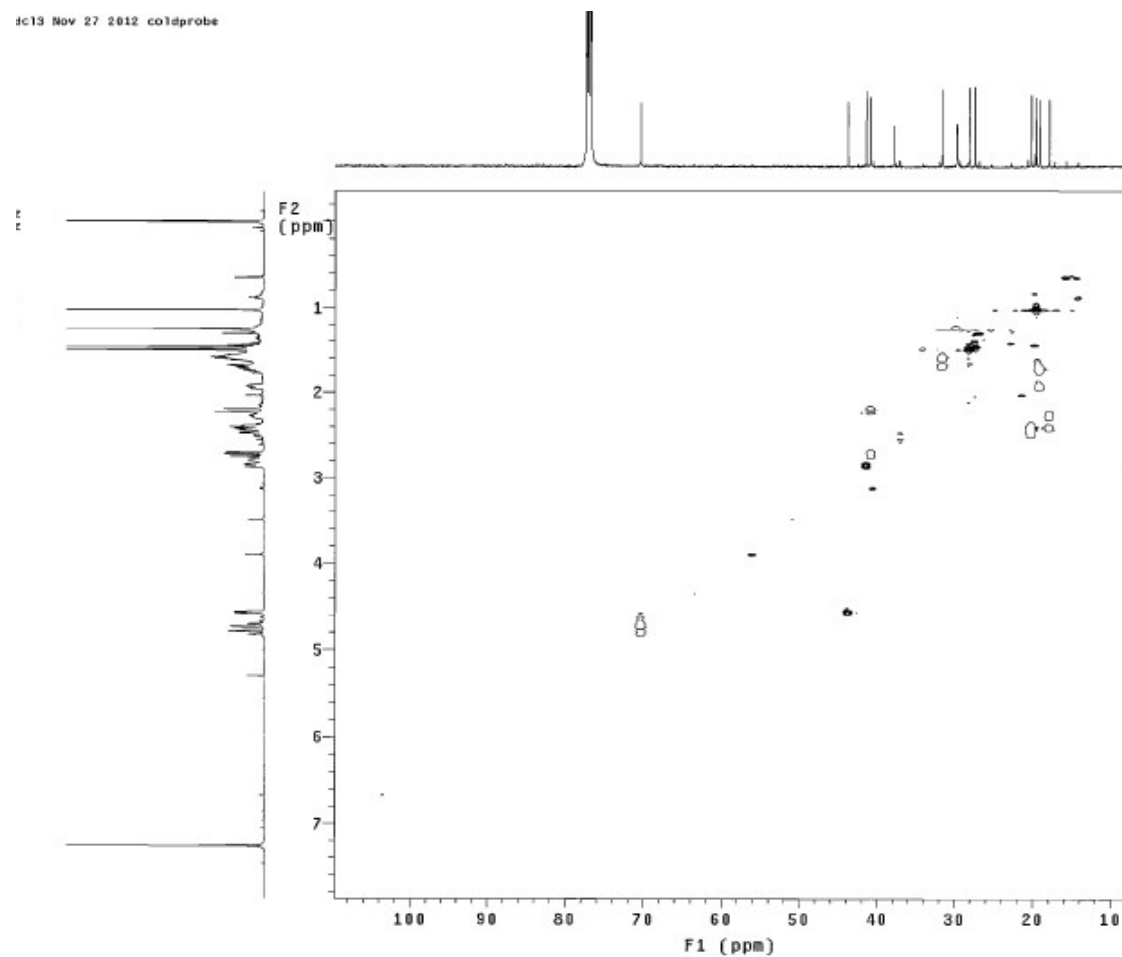


Figure S22. The HMBC spectrum of tripterlide C (3) in CDCl₃

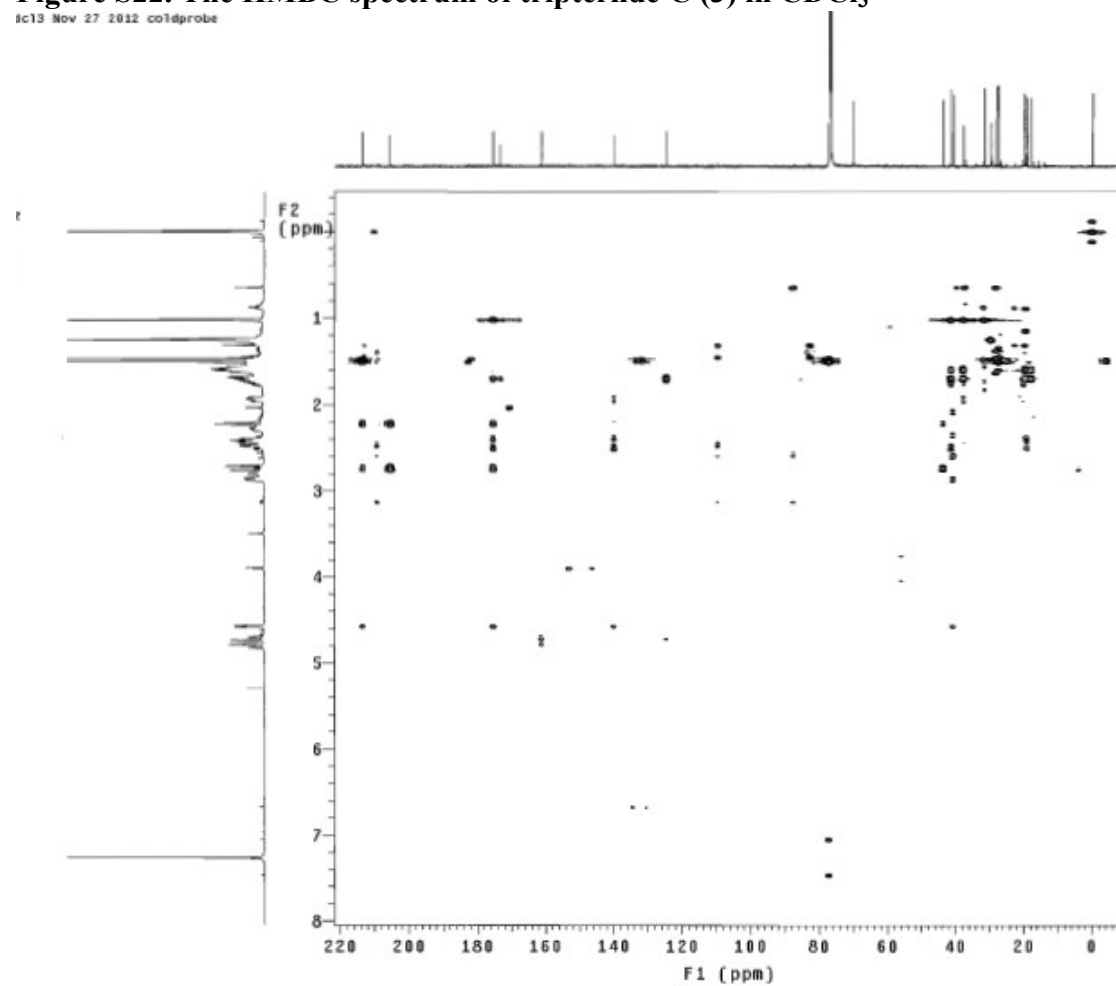


Figure S23. The ^1H - ^1H COSY spectrum of tripterlide C (**3**) in CDCl_3

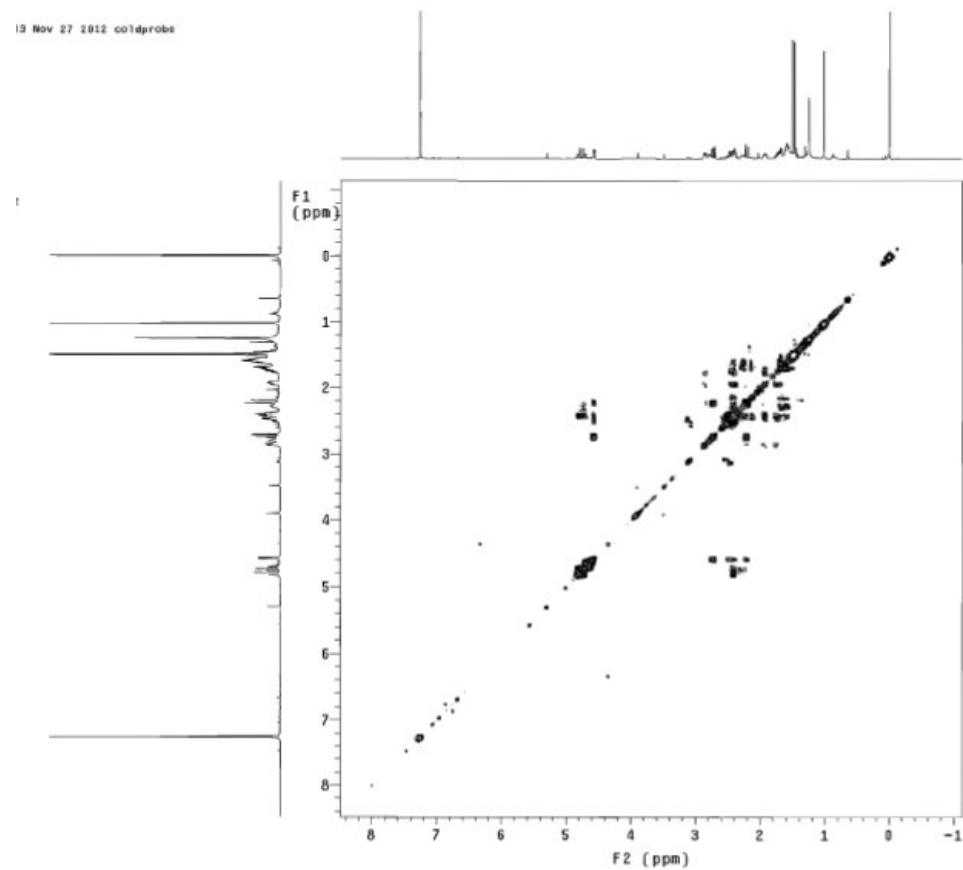


Figure S24. The NOESY spectrum of tripterlide C (3) in CDCl₃

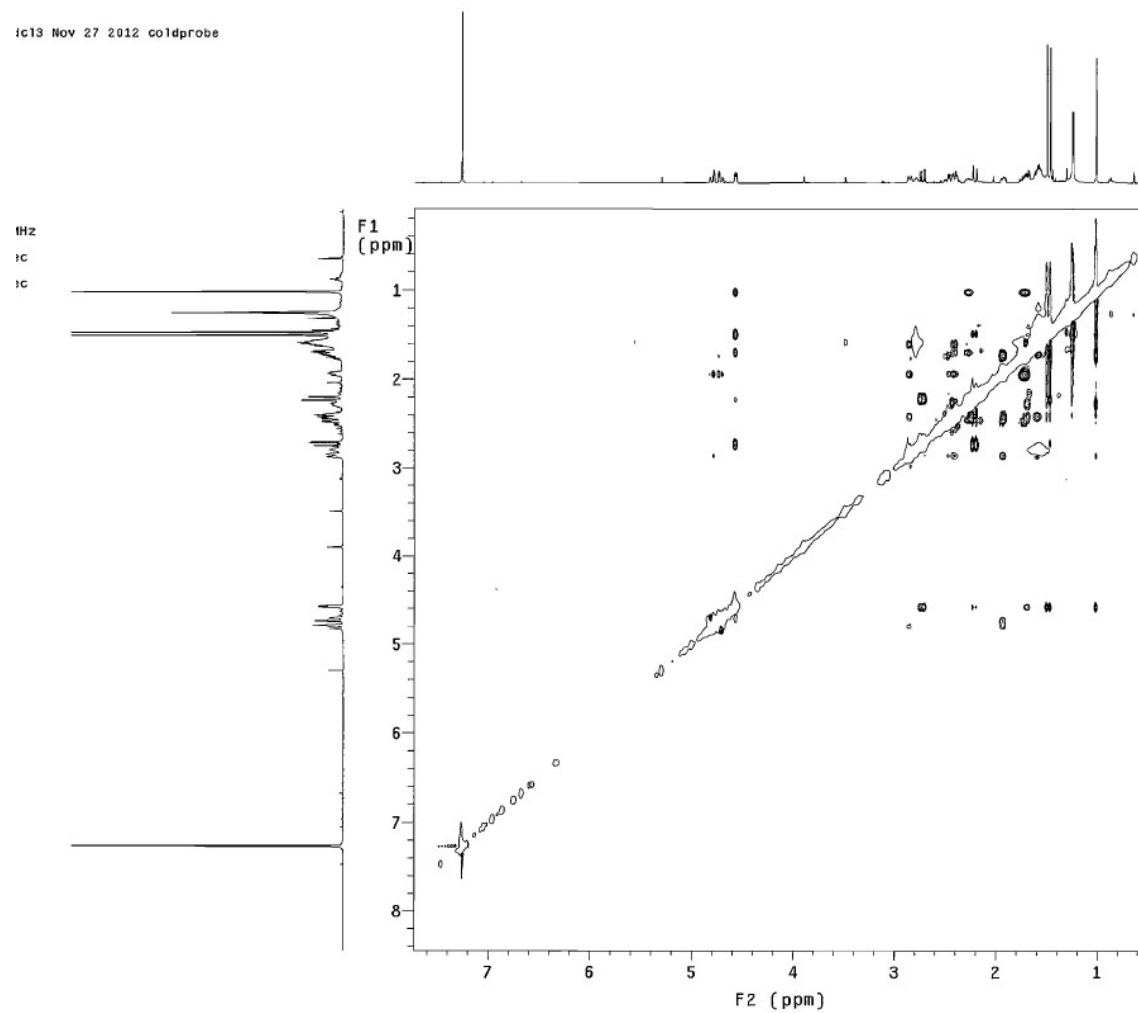


Figure S25. The IR spectrum of tripterlide C (3)

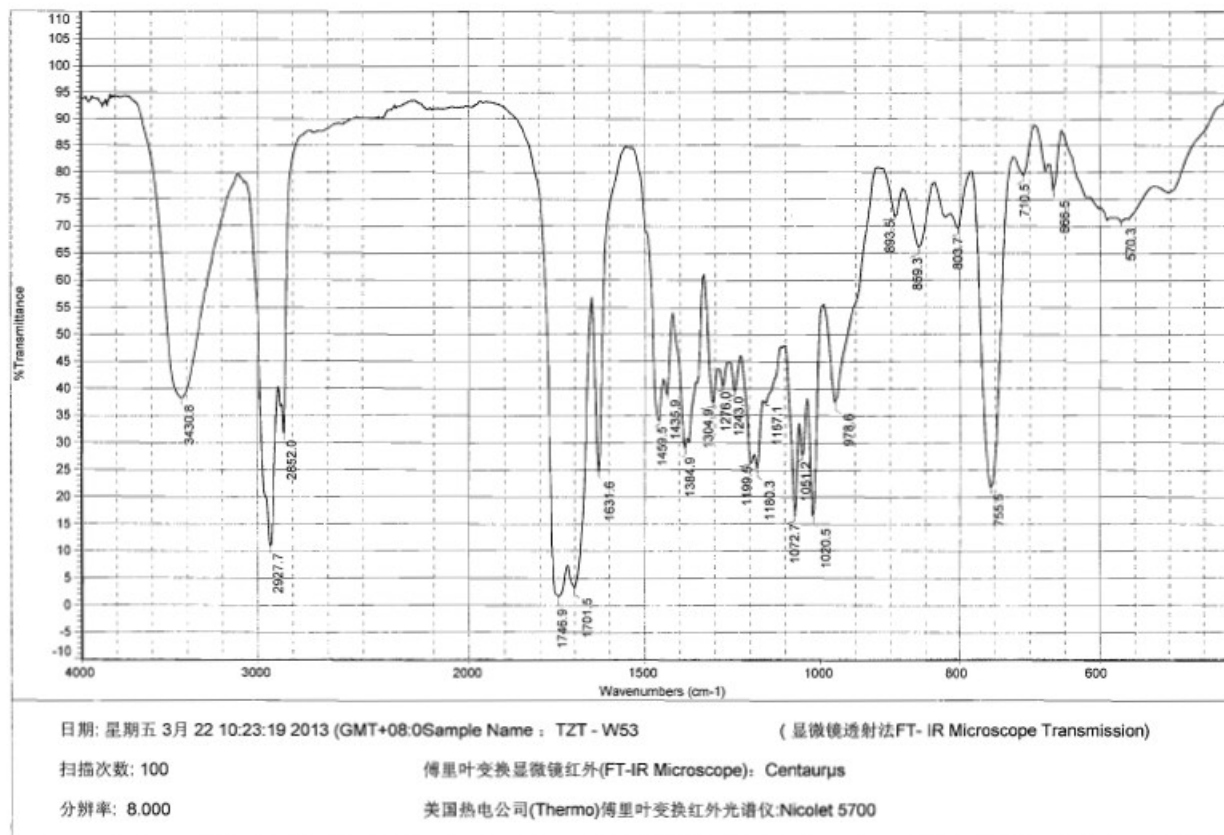


Figure S26. The HRESIMS of tripterlide C (3)

MS Formula Results: + Scan (5.421 min) Sub (2012091301.d)

m/z	Ion	Formula	Abundance													
345.1701	(M+H) ⁺	C20 H25 O5	4884524.5													
3	Best	Formula (M)	Ion Formula	Calc. m/z	Score	1	Cross S	Mass	Calc. Mass	Diff (ppm)	Abs. Diff (ppm)	Abund. Match	Spacing Max	Mass Match	m/z	DBE
3	[P]	C20 H24 O5	C20 H25 O5	345.1697	99.41			344.1628	344.1624	-1.22	1.22	98.25	99.75	99.95	345.1701	9
4	[F]	C24 H24 S	C24 H25 S	345.1671	98.85			344.1628	344.1590	-8.5	8.5	99.23	99.62	97.72	345.1701	13
5	[F]	C21 H28 S2	C21 H29 S2	345.1730	98.12			344.1628	344.1632	1.28	1.28	94.04	99.36	99.95	345.1701	8
6	[F]	C17 H28 O5 S	C17 H29 O5 S	345.173	97.29			344.1628	344.1667	8.56	8.56	94.04	99.67	97.69	345.1701	4
7	[F]	C12 H28 N2 O7 S	C12 H29 N2 O7 S	345.159	95.84			344.1628	344.1617	-3.14	3.14	98.39	99.51	99.88	345.1701	0
m/z	Ion	Formula	Abundance													
367.1519	(M+Na) ⁺	C20 H24 Na O5	1790355.6													
3	Best	Formula (M)	Ion Formula	Calc. m/z	Score	1	Cross S	Mass	Calc. Mass	Diff (ppm)	Abs. Diff (ppm)	Abund. Match	Spacing Max	Mass Match	m/z	DBE
3	[P]	C20 H24 O5	C20 H24 Na O5	367.1516	99.41			344.1627	344.1624	-1.06	1.06	97.73	45.72	99.97	367.1519	9
4	[F]	C24 H24 S	C24 H24 Na S	367.1491	93.83			344.1627	344.1596	-8.34	8.34	91.42	45.5	98.03	367.1519	13
5	[F]	C17 H28 O5 S	C17 H28 Na O5 S	367.155	92.86			344.1627	344.1667	8.73	8.73	89.75	45.47	97.85	367.1519	4
6	[F]	C21 H28 S2	C21 H28 Na S2	367.1525	91.97			344.1627	344.1632	1.45	1.45	82.61	45.27	99.94	367.1519	8
7	[F]	C12 H28 N2 O7 S	C12 H28 N2 Na O7 S	367.1539	81.73			344.1627	344.1617	-2.97	2.97	82.41	44.88	99.75	367.1519	0

Figure 27. Optimized conformations of 1

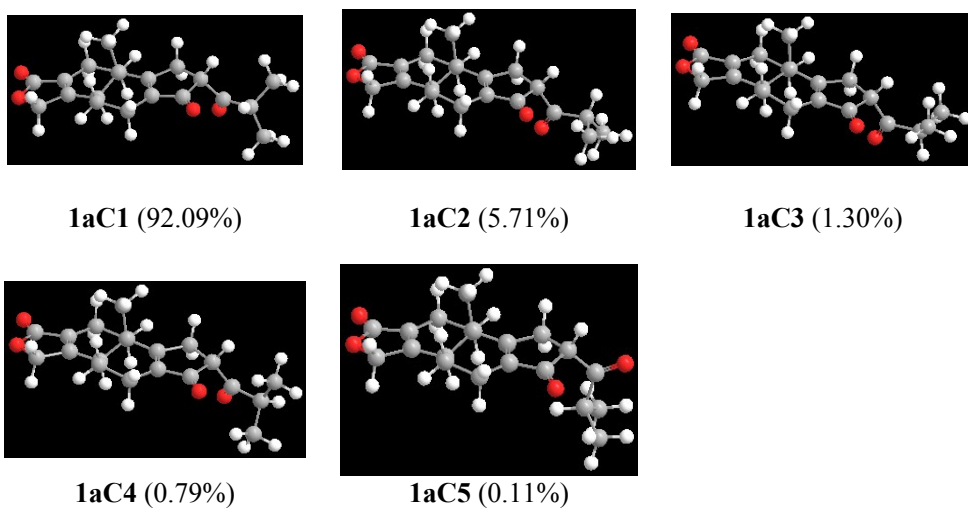


Figure S28. Calculated ECD spectra of 5*R*, 20*S*, 12*S* (1a, 1aC2) and experimental ECD spectrum of 1

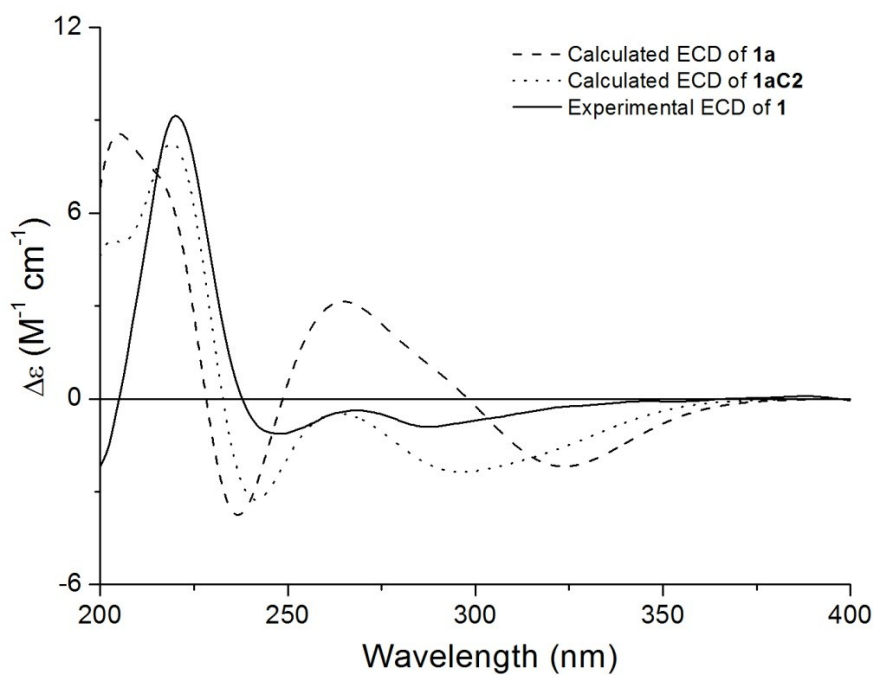


Figure 29. Optimized conformations of 2

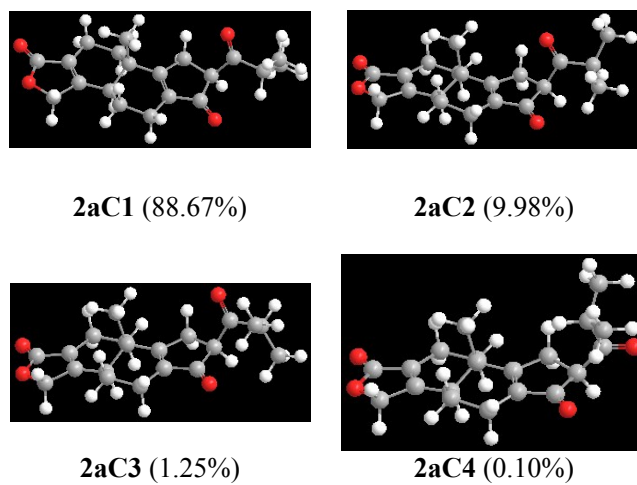


Figure S30. Calculated ECD spectra of 5*R*, 20*S*, 12*R* (2a, 2aC2) and experimental ECD spectrum of 2, and 3

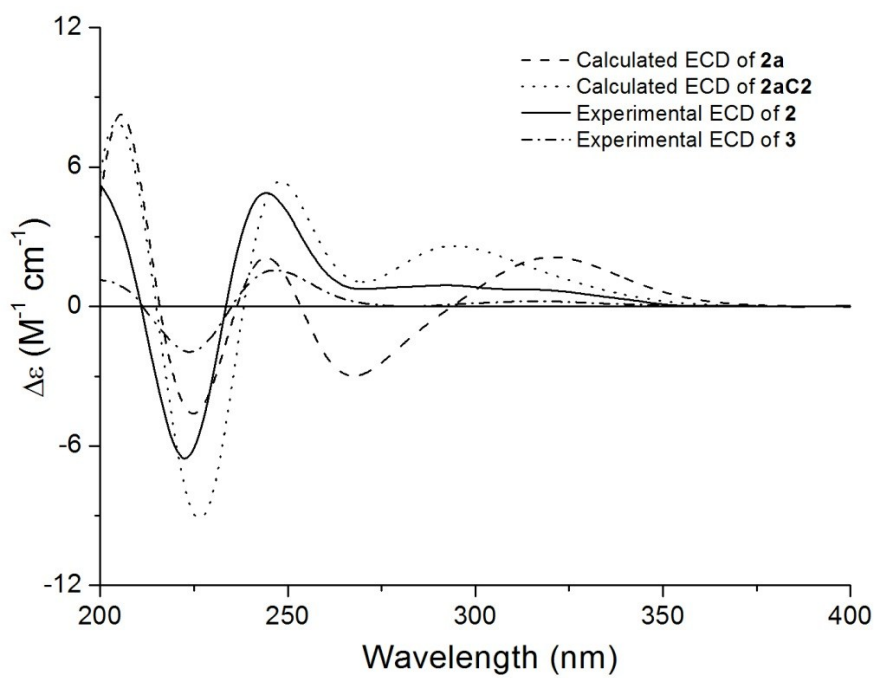


Figure S31. The ^1H NMR (600 MHz) spectrum of tripterlide D (4) in CDCl_3

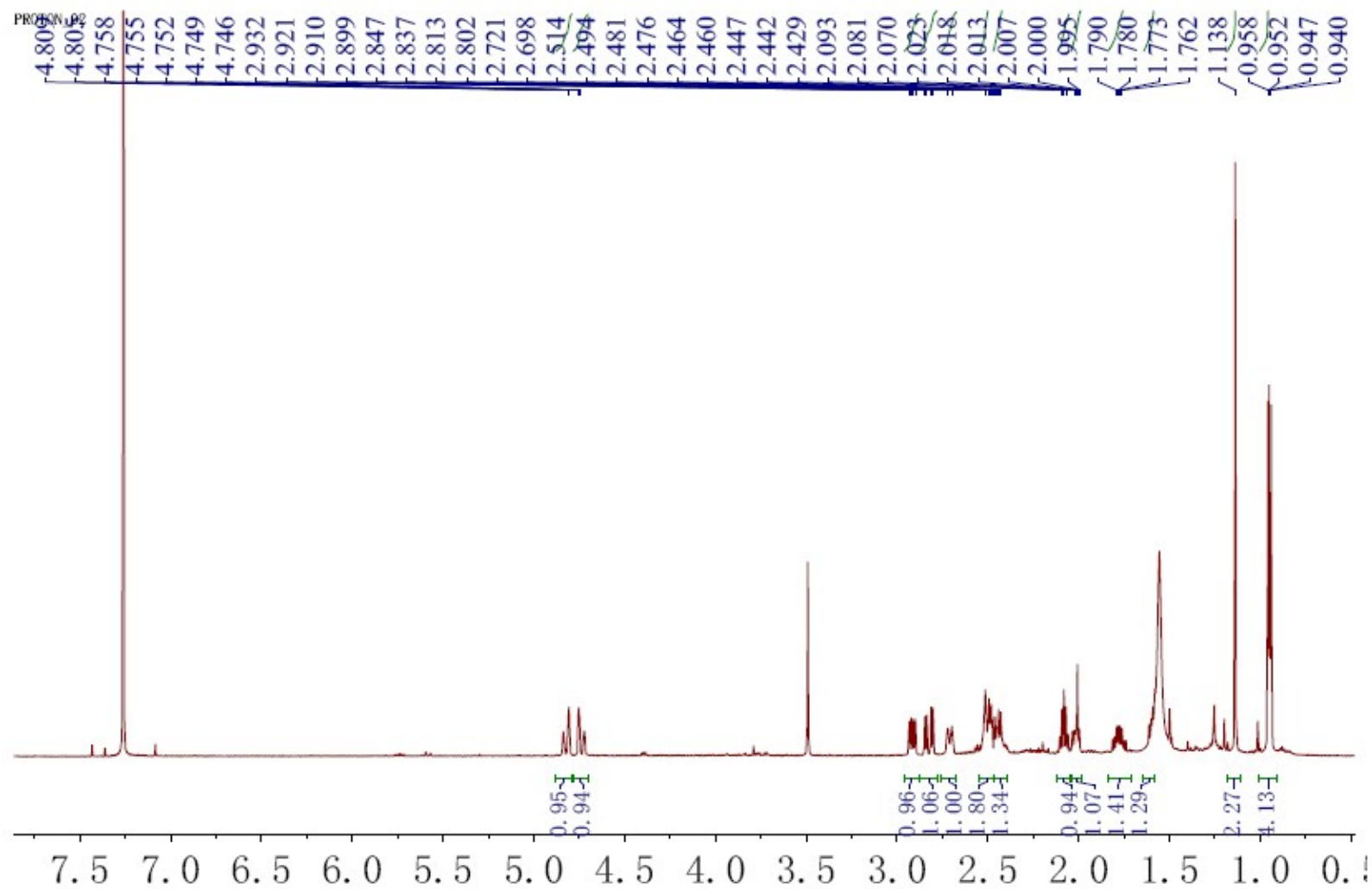


Figure S32. The ^{13}C NMR (150 MHz) spectrum of tripterlide D (4) in CDCl_3

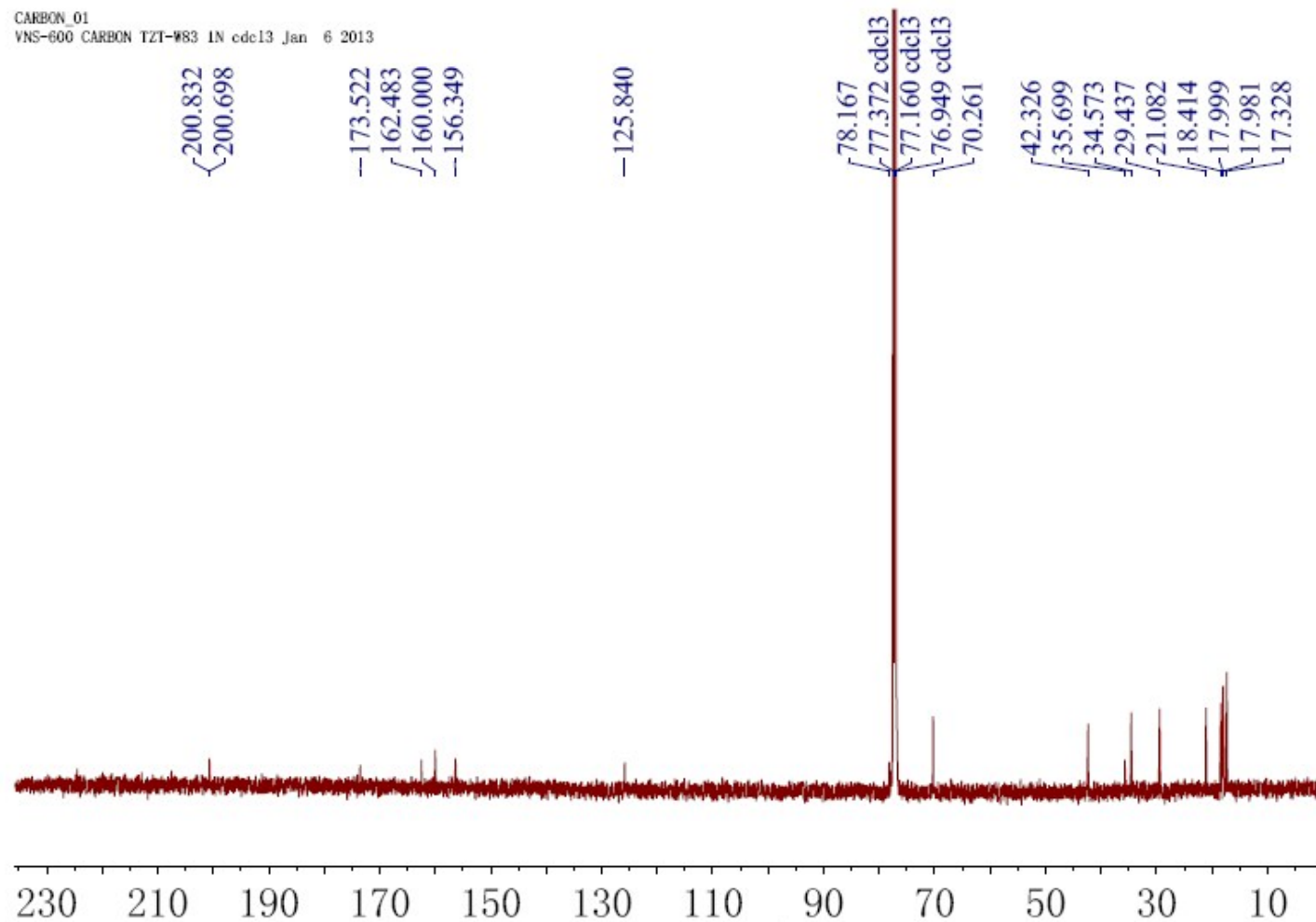


Figure S33. The HSQC spectrum of tripterlide D (4) in CDCl₃

VNS-600 gHSQCAD T2T-WB3 IN cdc13 Jan 11 2013

Temp. 25.0 C / 298.1 K
Sample #5, Operator: vjwalk

Relax. delay 1.000 sec
Acq. time 0.256 sec
Width 5630.6 Hz
2D Width 30154.5 Hz
64 repetitions
140 increments
OBSERVE H1, 599.6898042 MHz
DECOUPLE C13, 150.8056925 MHz
Power 35 dB
on during acquisition
off during delay
W40_NEW-SW modulated
DATA PROCESSING
Sine bell 0.033 sec
F1 DATA PROCESSING
Sine bell 0.005 sec
FT size 4096 x 2048
Total time 2 hr, 59 min

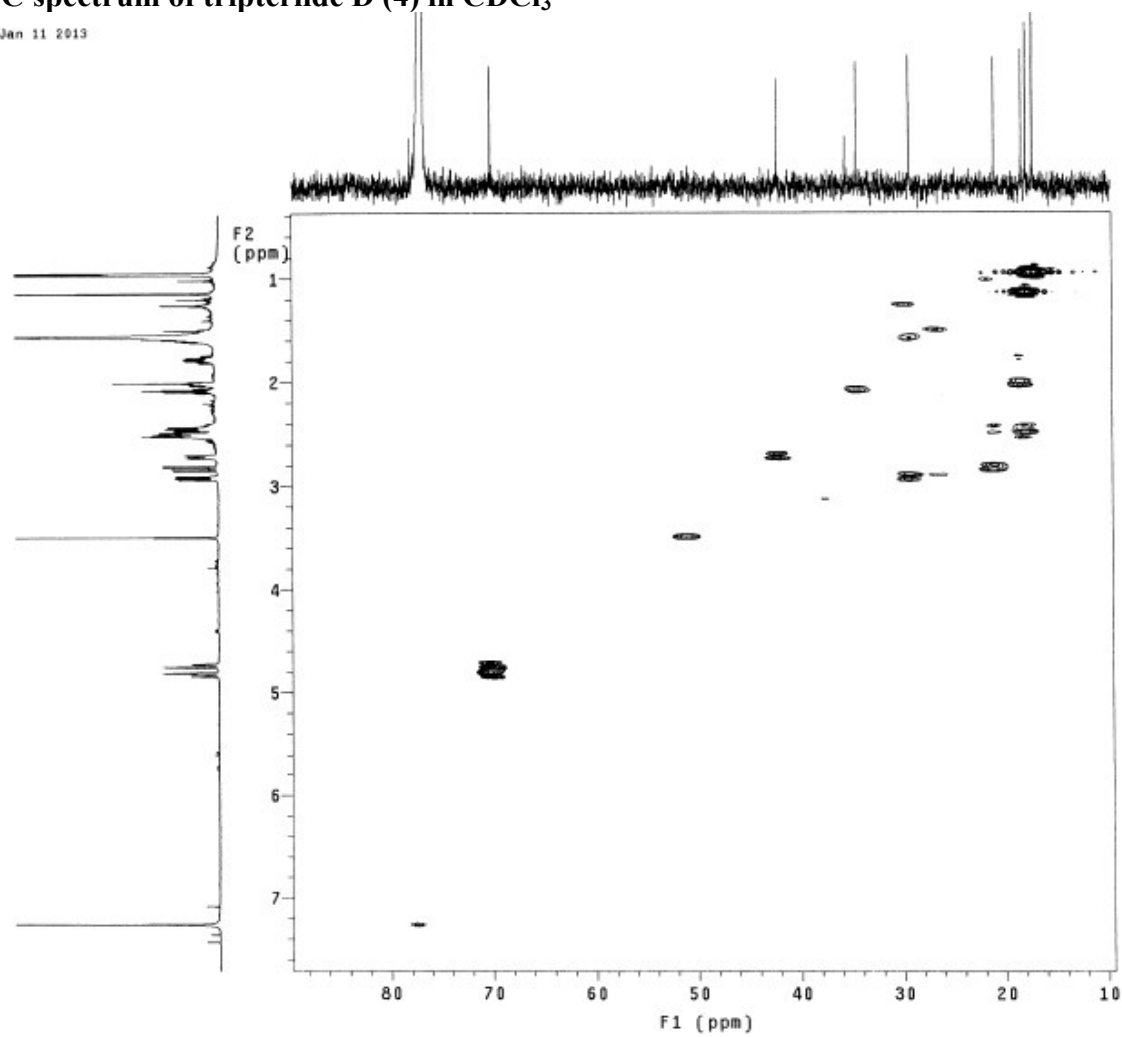


Figure S34. The HMBC spectrum of tripterlide D (4) in CDCl₃

VNS-600 gHMBCAD T2T-W83 IN cdc13 Jan 11 2013

Temp. 25.0 C / 298.1 K
Sample #5, Operator: vjwalk

Relax. delay 1.000 sec
Acq. time 0.258 sec
Width 5630.6 Hz
2D width 36182.7 Hz
128 repetitions
160 increments
OBSERVE H1, 500.136042 MHz
DATA PROCESSING
Sine bell 0.057 sec
F1 DATA PROCESSING
Sine bell 0.004 sec
FT size 4096 x 2048
Total time 7 hr, 1 min

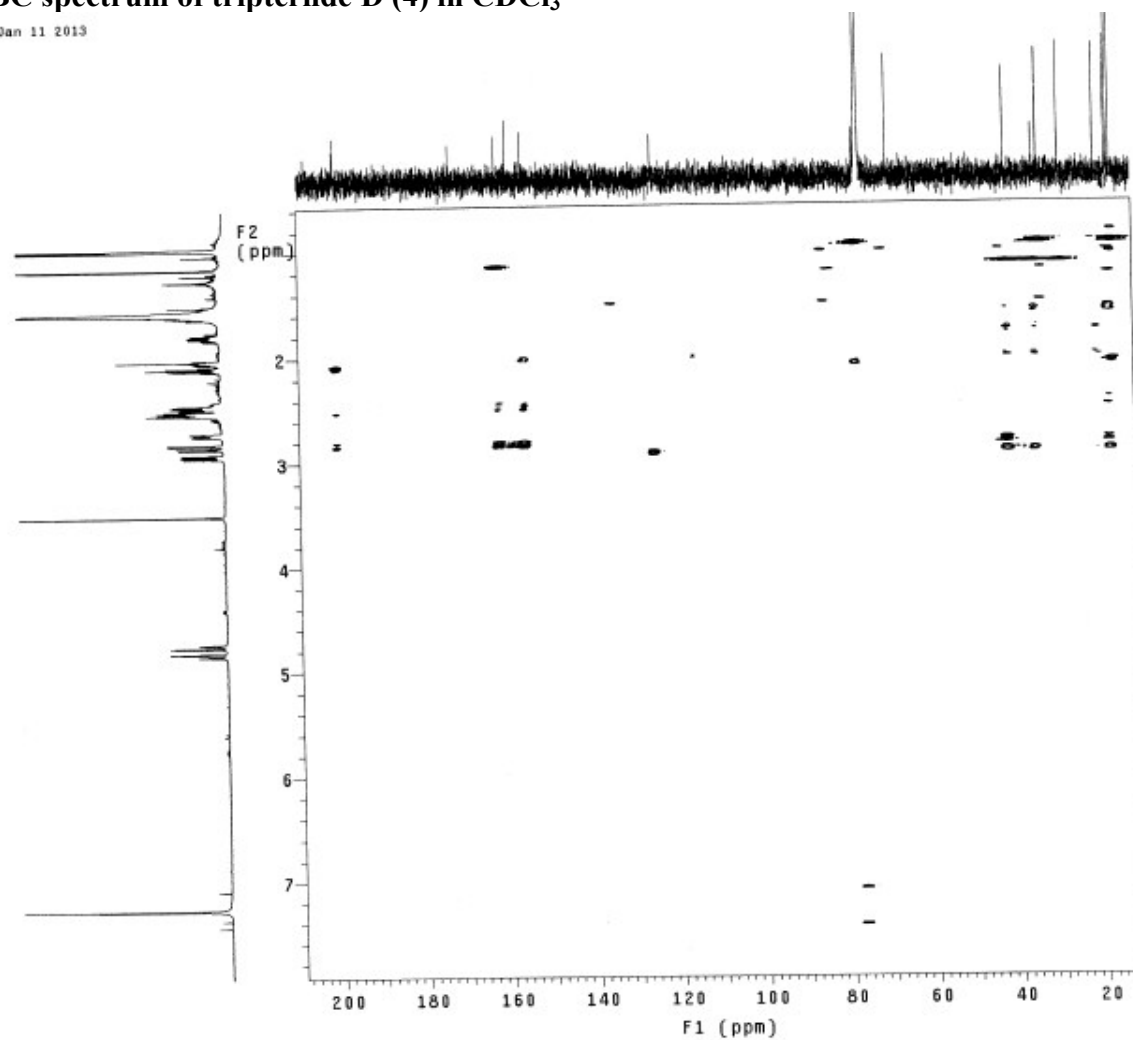


Figure S35. The ^1H - ^1H COSY spectrum of tripterlide D (4) in CDCl_3

VNS-600 gCOSY T2T-W83 IN cdc13 Jan 11 2013

Temp. 25.0 C / 298.1 K
Sample #5, Operator: vjwaik
Relax. delay 1.000 sec
Acq. time 0.150 sec
Width 5630.6 Hz
ZD Width 5630.6 Hz
4 repetitions
128 increments
OBSERVE H1, 599.6898042 MHz
DATA PROCESSING
Sg. sine bell 0.075 sec
F1 DATA PROCESSING
Sg. sine bell 0.023 sec
FT size 2048 x 2048
Total time 10 min

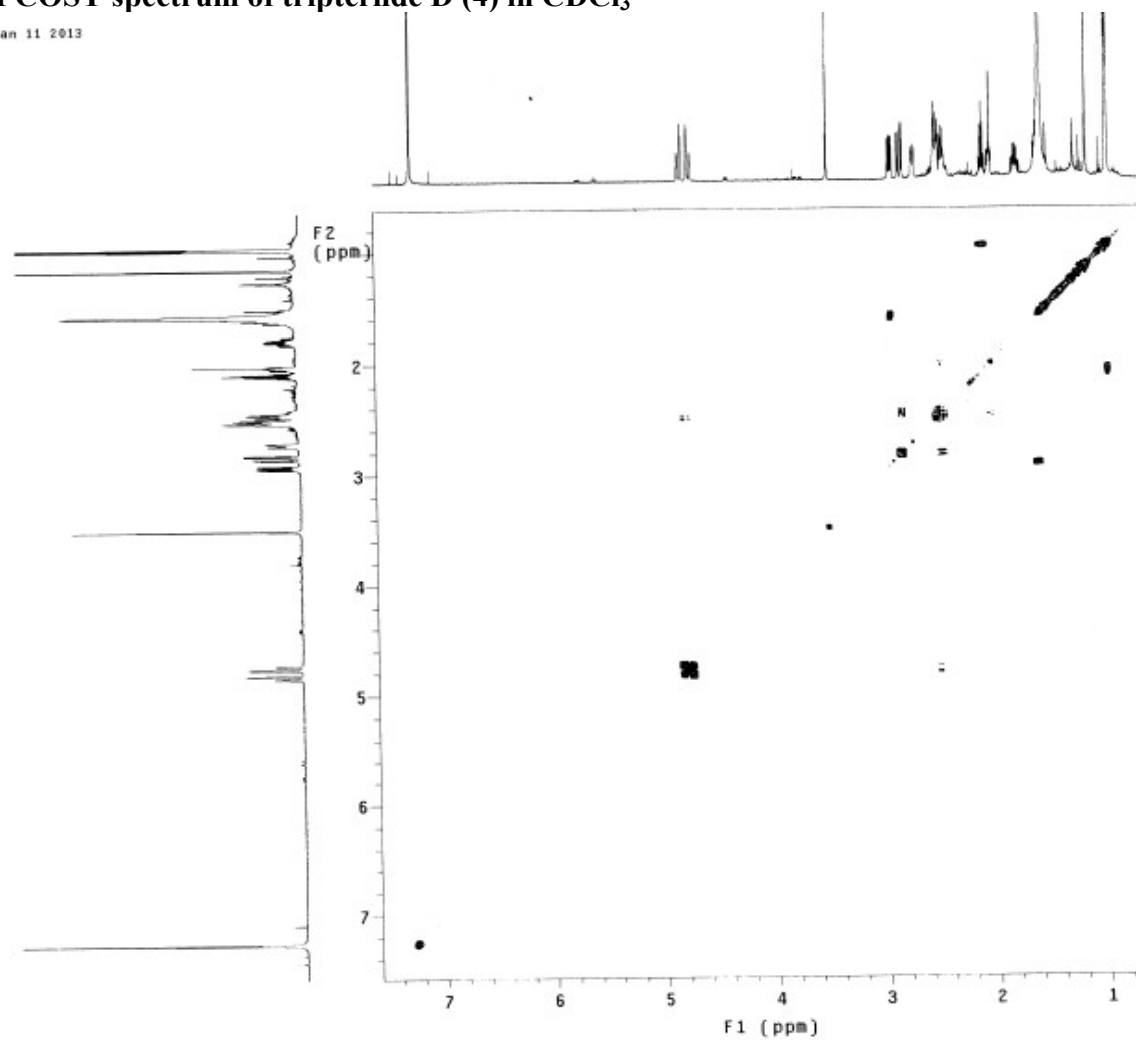


Figure S36. The NOESY spectrum of tripterldie D (4) in CDCl₃

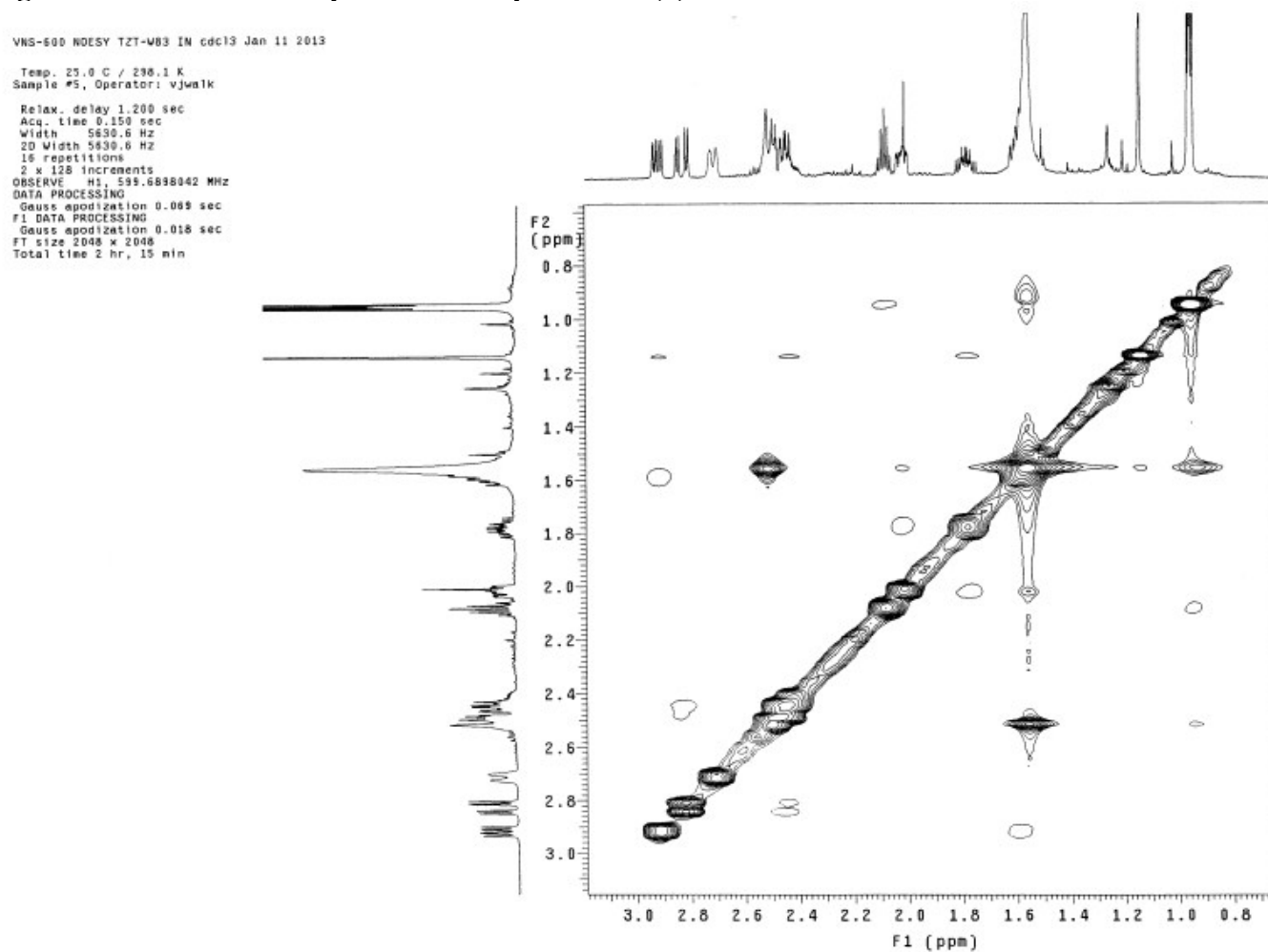


Figure S37. The HRESIMS spectrum of tripterlide D (4)

MS Formula Results: + Scan (5.731 min) Sub (2013011701.d)

m/z	Ion	Formula	Abundance
331.1543	(M+H) ⁺	C ₁₉ H ₂₃ O ₅	135966

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross S	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Mat	Mass Match	m/z	DBE
1	C ₁₉ H ₂₂ O ₅	C ₁₉ H ₂₃ O ₅	331.154	99.73		330.147	330.1467	-0.84	0.84	99.15	99.93	99.98	331.1543	9

m/z	Ion	Formula	Abundance
353.137	(M+Na) ⁺	C ₁₉ H ₂₂ NaO ₅	285638.9

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross S	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Mat	Mass Match	m/z	DBE
1	C ₁₉ H ₂₂ O ₅	C ₁₉ H ₂₂ NaO ₅	353.1359	87.46		330.1478	330.1467	-3.22	3.22	98.4	49.84	99.71	353.137	9
2	C ₁₆ H ₂₆ O ₅ S	C ₁₆ H ₂₆ NaO ₅ S	353.1363	84.66		330.1478	330.1501	6.98	6.98	91.57	49.78	98.63	353.137	4
3	C ₁₁ H ₂₆ N ₂ O ₇ S	C ₁₁ H ₂₆ N ₂ NaO ₇ S	353.1353	83.68		330.1478	330.1461	-5.21	5.21	86.65	49.6	99.24	353.137	0
4	C ₂₀ H ₂₆ S ₂	C ₂₀ H ₂₆ NaS ₂	353.1368	83.18		330.1478	330.1476	-0.6	0.6	83.04	49.73	99.99	353.137	8

Figure S38. The ^1H NMR (600 MHz) spectrum of tripterlide E (5) in CDCl_3

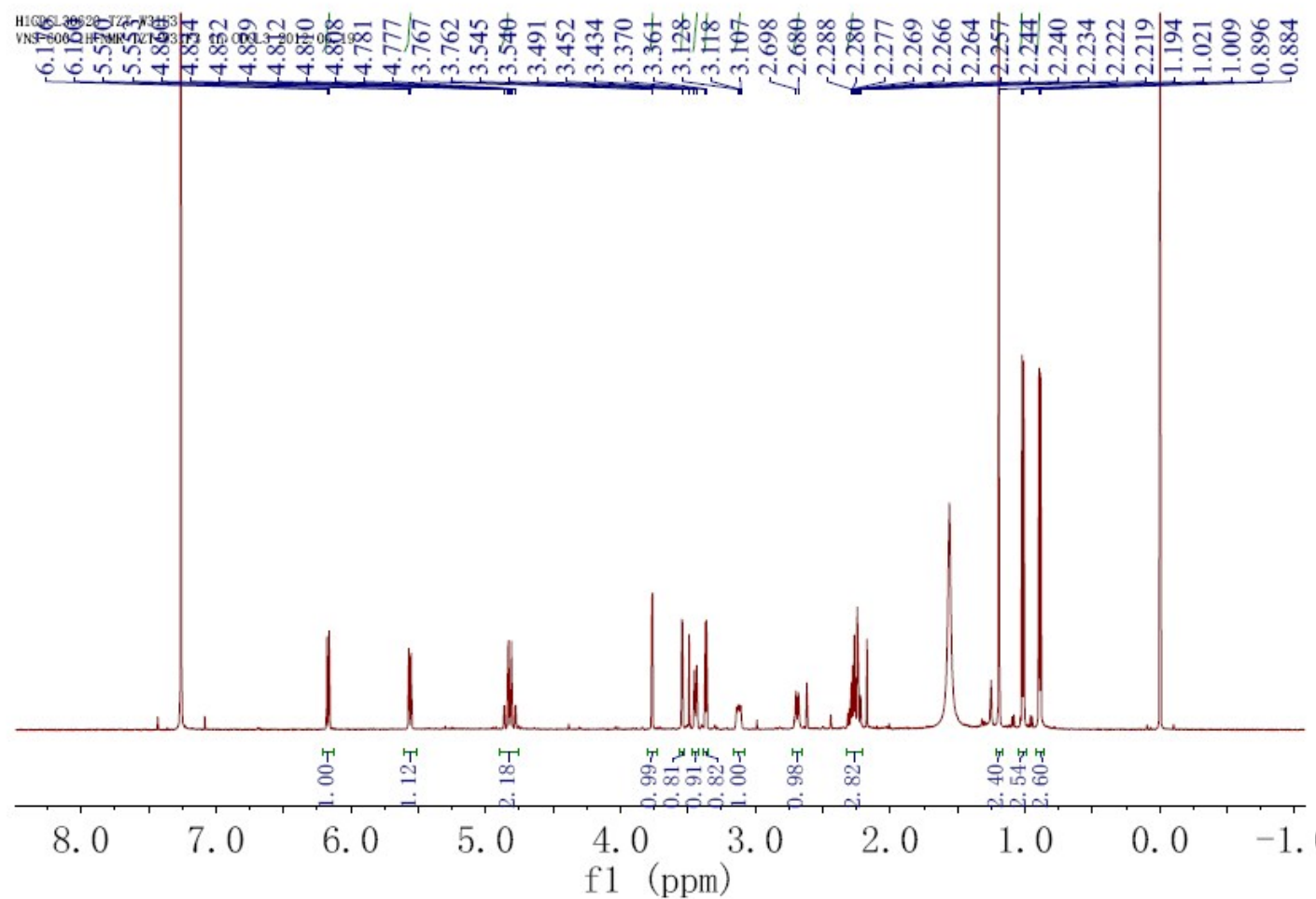


Figure S39. The ^{13}C NMR (150 MHz) spectrum of tripterlide E (5) in CDCl_3

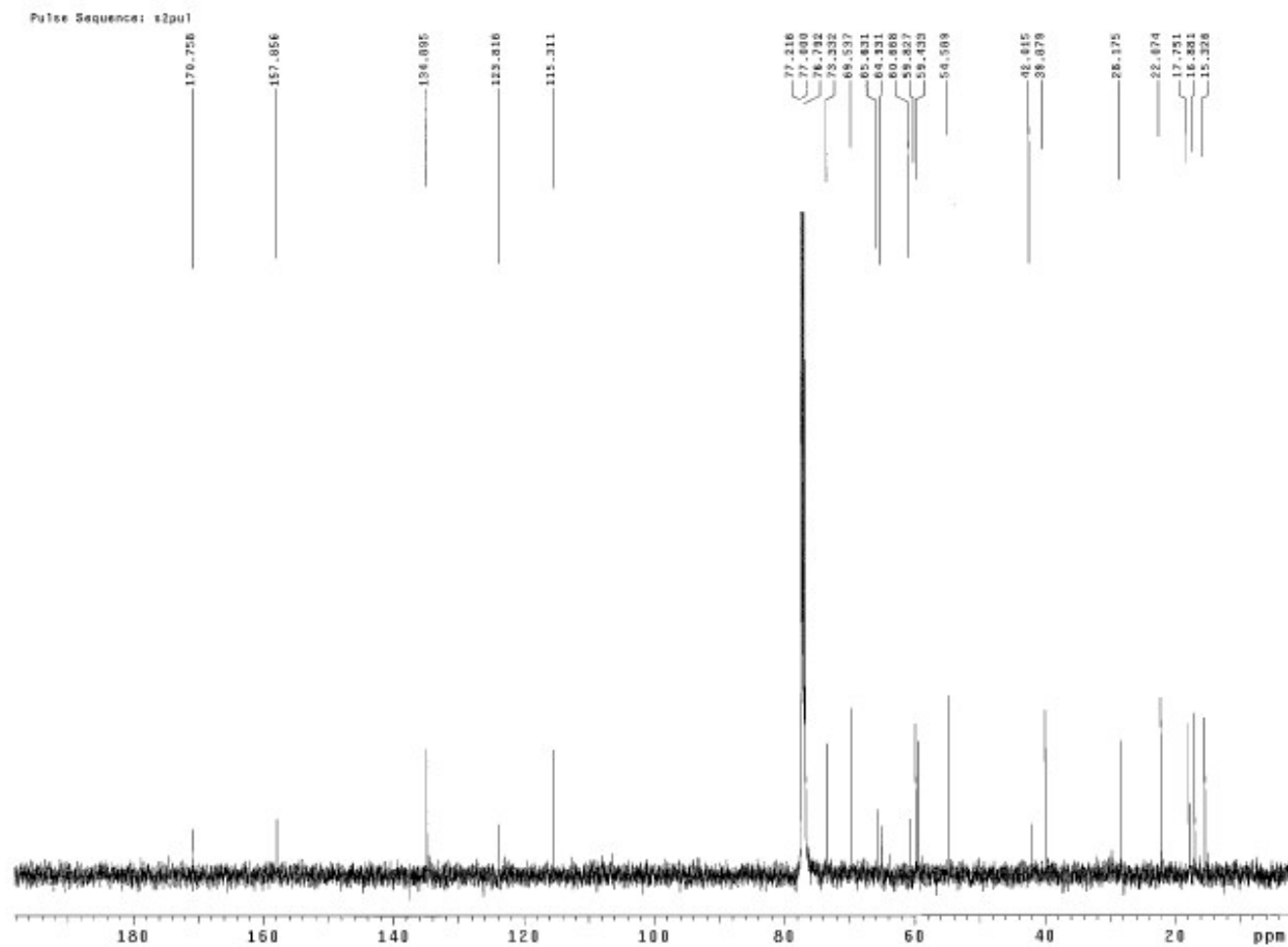


Figure S40. The HSQC spectrum of tripterlide E (5) in CDCl₃

VNS-600 gHSQC T2T-W31F3 in CDCl₃ 2012.06.19

Pulse Sequence: gHSQC

Solvent: cdc13

Temp: 25.0 C / 288.1 K

Sample #7, Operator: walkup

File: ghsqc

VNMR-600 "wormhole"

Relax. delay 1.000 sec

Acq. time 0.199 sec

Width 5733.3 Hz

2D Width 28653.3 Hz

48 repetitions

140 increments

OBSERVE H1, 599.6698039 MHz

DECOUPLE C13, 150.8049385 MHz

Power 35 dB

on during acquisition

off during delay

WDS_NEW-SU modulated

DATA PROCESSING

Sine bell 0.025 sec

F1 DATA PROCESSING

Sine bell 0.004 sec

FT size 4096 x 2048

Total time 2 hr, 19 min, 19 sec

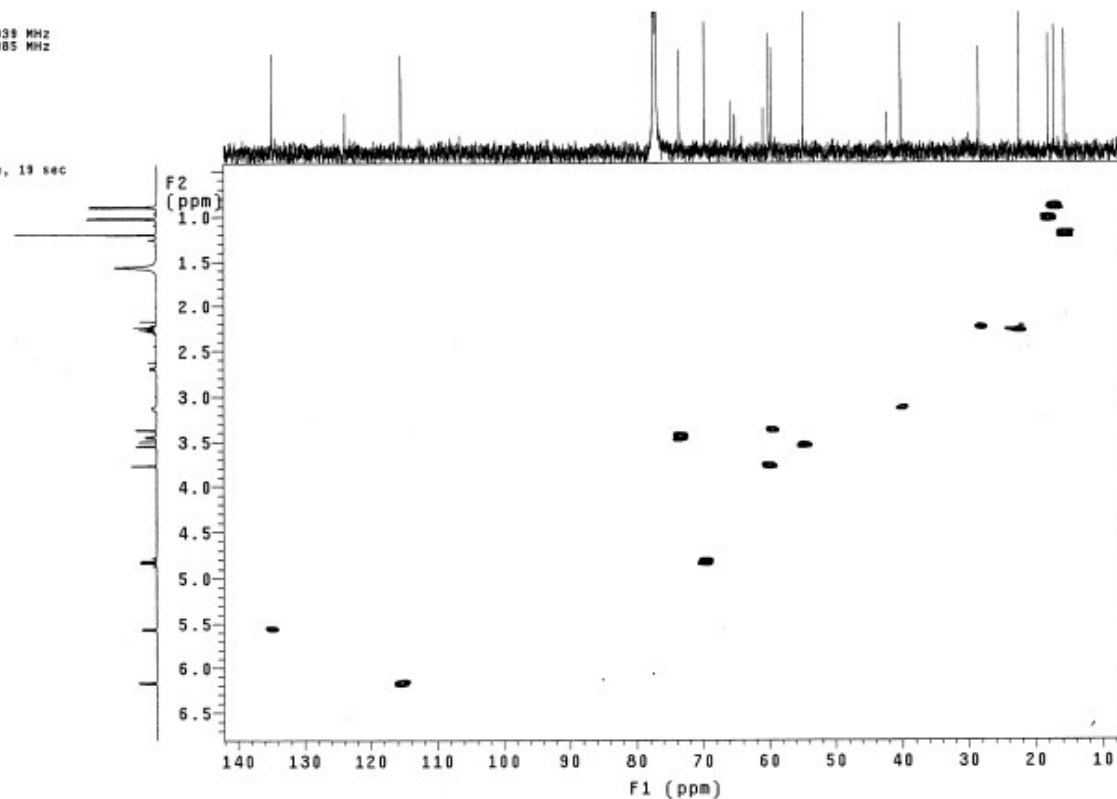


Figure S41. The HMBC spectrum of tripterlide E (5) in CDCl₃

VNS-600 gHMBC T2T-W31F3 in CDCl3 2012.06.19

Pulse Sequence: gHMBC

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Sample #7, Operator: Walkup

File: gHMBC

VNS-600 "wormhole"

Relax. delay 1.000 sec

Mixing 0.080 sec

Acq. time 0.128 sec

Width 5733.9 Hz

SD Width 36182.7 Hz

60 repetitions

150 increments

OBSERVE H1: 599.686842 MHz

DATA PROCESSING

Sine bell 0.084 sec

F1 DATA PROCESSING

Sine bell 0.084 sec

FT size 4096 x 2048

Total time 4 hr, 17 min, 42 sec

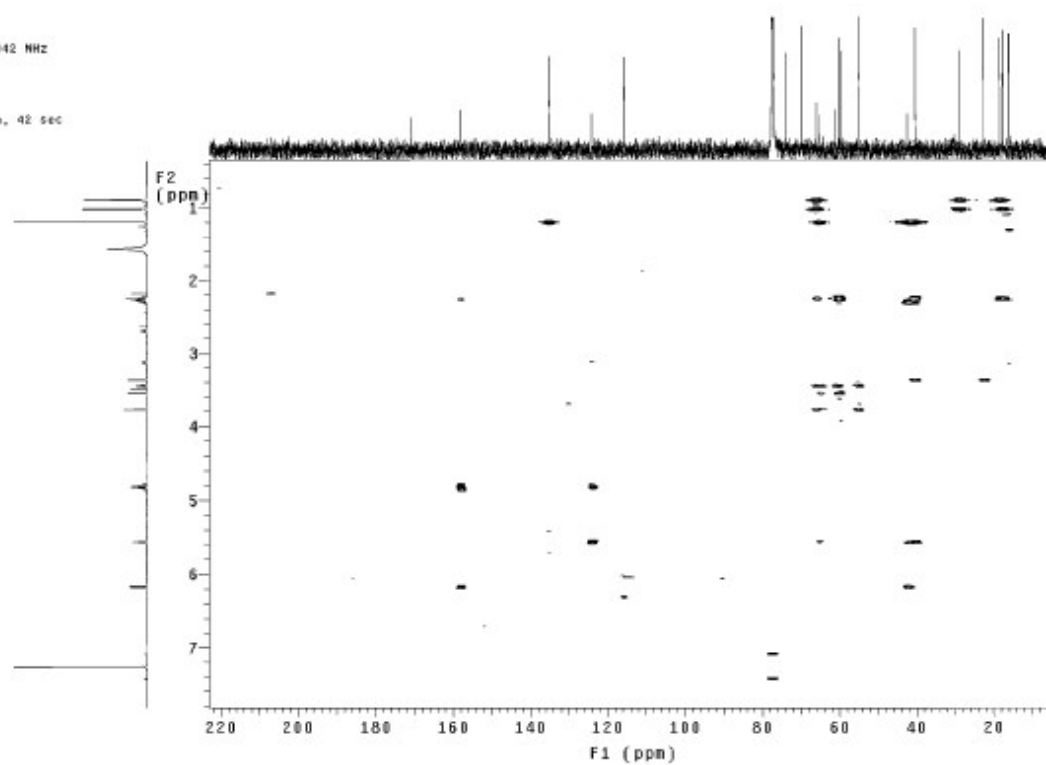


Figure S42. The ^1H - ^1H COSY spectrum of tripterlide E (5) in CDCl_3

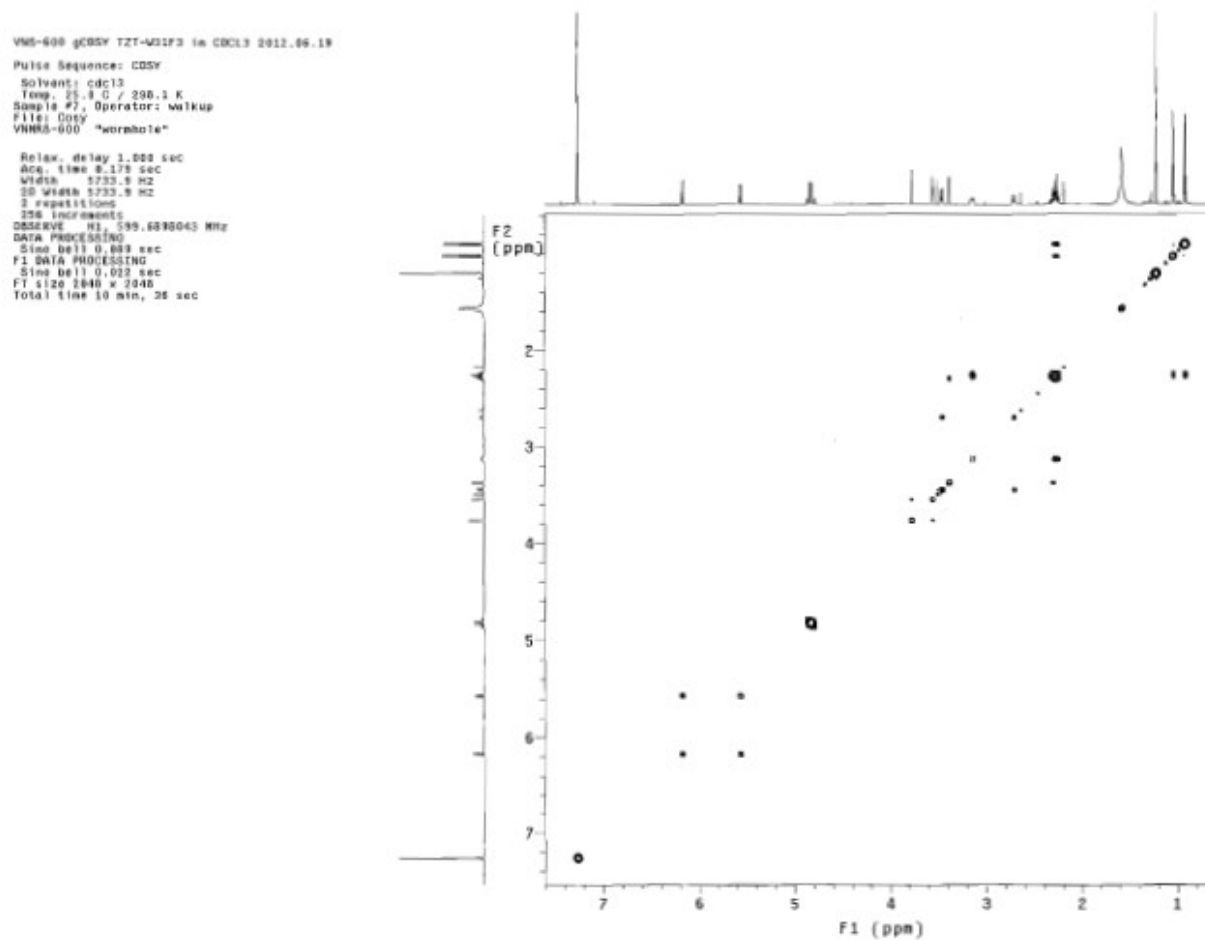


Figure S43. The NOESY spectrum of tripterlide E (5) in CDCl₃

Bruker AVANCEIII400 NOESY-NMR, in CDCl₃, T2T-W31F3 2012/06/26

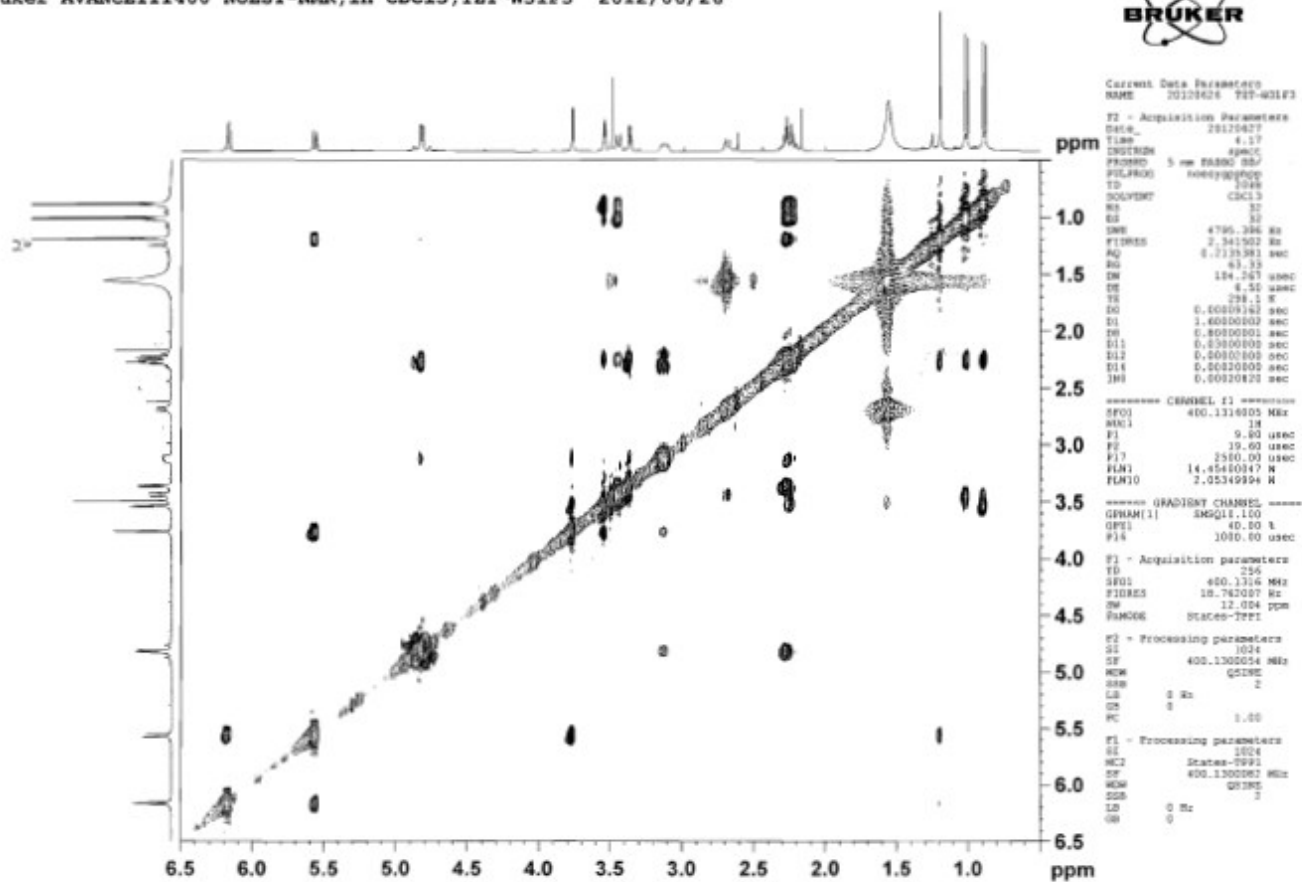


Figure S44. The IR spectrum of tripterlide E (5) in CDCl_3

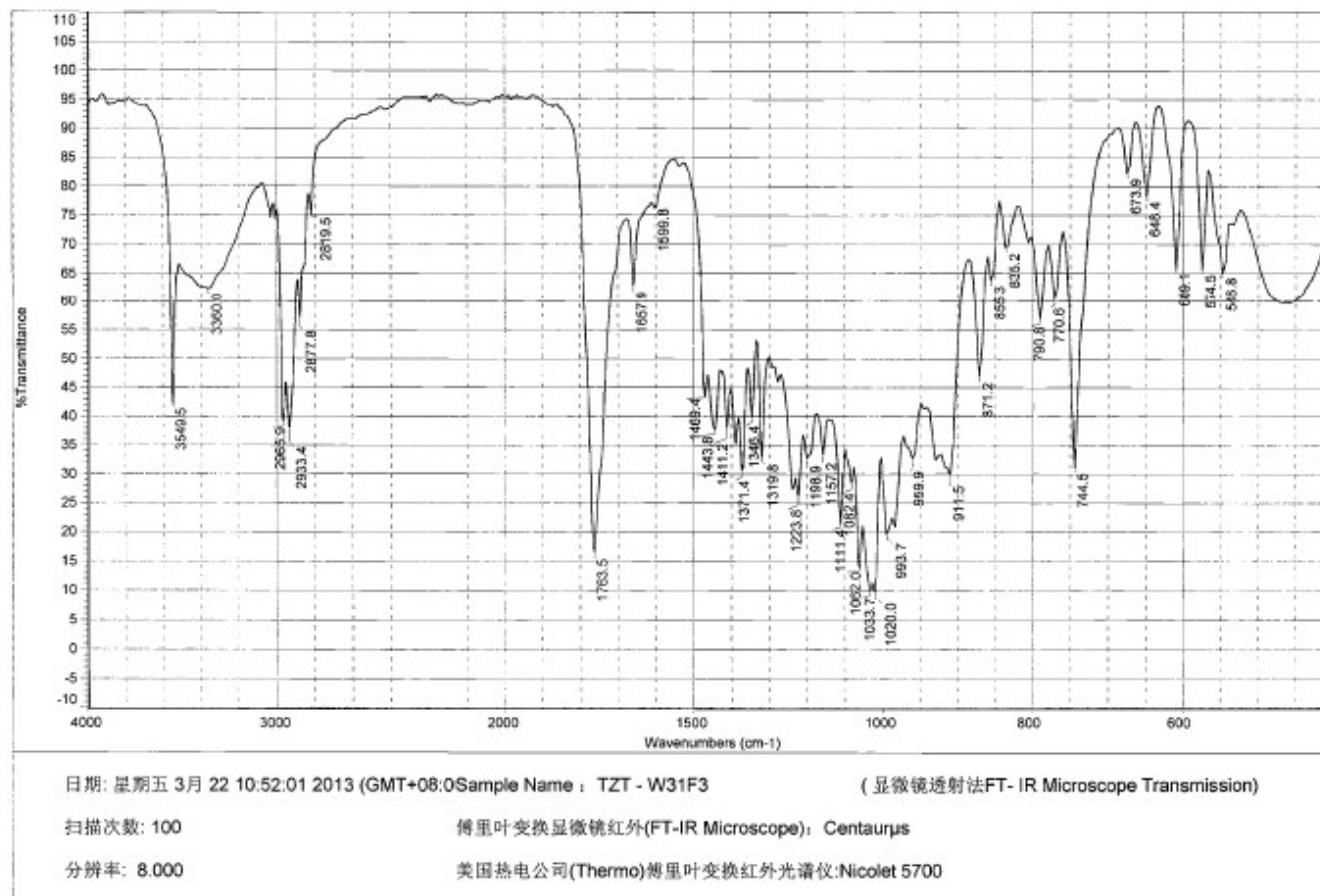


Figure S45. The HRESIMS spectrum of tripterlide E (5) in CDCl₃

MS Formula Results: + Scan (5.909 min) Sub (2012071302.d)

m/z	Ion	Formula	Abundance											
355.1495	[M+H] ⁺	C20H23O6	518525.7											
Base	Formula (M)	Ion Formula	Calc m/z	Score	Cross S	Mass	Calc Mass	Diff (ppm)	Alt Diff (ppm)	Abund Match	Spacing Met	Mass Match	m/z	DBE
3	[M]	C20H22O6	C20H22O6	355.1489	95.31	355.1424	355.1419	-3.03	2.53	98.91	99.17	99.01	355.1496	10
4	[M-1]	C17H20O6S	C17H20O6S	355.1523	97.65	355.1434	355.145	7.37	7.37	99.24	99.8	99.26	355.1466	5
5	[M-2]	C21H23O5S2	C21H23O5S2	355.1498	97.19	355.1434	355.1425	0.38	0.38	99.43	99.78	99.5	355.1496	8
6	[M-3]	C24H25O5S	C24H25O5S	355.1484	97.38	355.1434	354.1391	-9.02	9.02	97.87	98.4	97.47	355.1496	14
7	[M-4]	C12H25N2O6S	C12H25N2O6S	355.1483	97.14	355.1424	355.141	-3.87	3.87	98.0	98.47	98.52	355.1496	7
375.1762	[M+H] ⁺	C20H26N2O6	528751.8											
Base	Formula (M)	Ion Formula	Calc m/z	Score	Cross S	Mass	Calc Mass	Diff (ppm)	Alt Diff (ppm)	Abund Match	Spacing Met	Mass Match	m/z	DBE
3	[M]	C20H26N2O6	C20H26N2O6	375.1755	95.51	358.1425	358.1418	-1.21	1.21	98.42	99.71	99.68	375.1762	10
4	[M-1]	C17H24N2O6S	C17H24N2O6S	375.1789	96.13	358.1425	358.145	7.49	7.49	99.35	99.78	99.35	375.1762	5
5	[M-2]	C21H28N2O5S2	C21H28N2O5S2	375.1764	97.89	358.1425	358.1425	0.5	0.5	99.62	99.91	99.66	375.1762	8
6	[M-3]	C24H30N2O5S	C24H30N2O5S	375.1773	97.42	358.1425	358.1391	-8.9	8.9	97.97	98.7	97.88	375.1762	14
7	[M-4]	C12H28N2O6S	C12H28N2O6S	375.1749	97.4	358.1425	358.141	-3.79	3.79	99.02	99.52	99.58	375.1762	7
385.1270	[M+H] ⁺	C20H22N2O6	434172.8											
Base	Formula (M)	Ion Formula	Calc m/z	Score	Cross S	Mass	Calc Mass	Diff (ppm)	Alt Diff (ppm)	Abund Match	Spacing Met	Mass Match	m/z	DBE
3	[M]	C20H22N2O6	C20H22N2O6	385.1269	98.49	358.1425	358.1419	-1.86	1.86	98.97	97.69	98.8	385.1275	10
4	[M-1]	C17H20N2O6S	C17H20N2O6S	385.1342	97.14	358.1425	358.145	7.64	7.64	99.25	99.75	99.37	385.1315	5
5	[M-2]	C21H26N2O5S2	C21H26N2O5S2	385.1317	97.13	358.1425	358.1425	0.54	0.54	97.78	99.01	98.98	385.1315	8
6	[M-3]	C24H28N2O5S	C24H28N2O5S	385.1294	98.51	358.1425	358.1391	-8.85	8.85	97.3	98.07	97.75	385.1315	14
7	[M-4]	C12H26N2O6S	C12H26N2O6S	385.1332	98.38	358.1425	358.141	-3.71	3.71	94.99	97.5	98.8	385.1315	7
397.1092	[M+H] ⁺	C20H22K2O6	57780.9											
Base	Formula (M)	Ion Formula	Calc m/z	Score	Cross S	Mass	Calc Mass	Diff (ppm)	Alt Diff (ppm)	Abund Match	Spacing Met	Mass Match	m/z	DBE
3	[M]	C21H25O5S2	C21H25O5S2	397.1097	96.87	358.1421	358.1425	1.22	1.22	97.89	99.46	99.66	397.1092	8
4	[M-1]	C20H22K2O6	C20H22K2O6	397.1045	95.7	358.1421	358.1419	-1.19	1.19	94.98	97.71	95.98	397.1092	10
5	[M-2]	C17H26O6S	C17H26O6S	397.1087	96.18	358.1421	358.145	8.22	8.22	97.63	99.38	99.2	397.1092	5
6	[M-3]	C24H28O5S	C24H28O5S	397.1023	95.96	358.1421	358.1391	-8.17	8.17	96.11	97.03	96.22	397.1092	14
7	[M-4]	C12H28K2O6S	C12H28K2O6S	397.1041	96.84	358.1421	358.141	-3.03	3.03	93.65	99.88	99.75	397.1092	7

Figure S46. The ^1H NMR (400 MHz) spectrum of tripterlide F (6) in CDCl_3

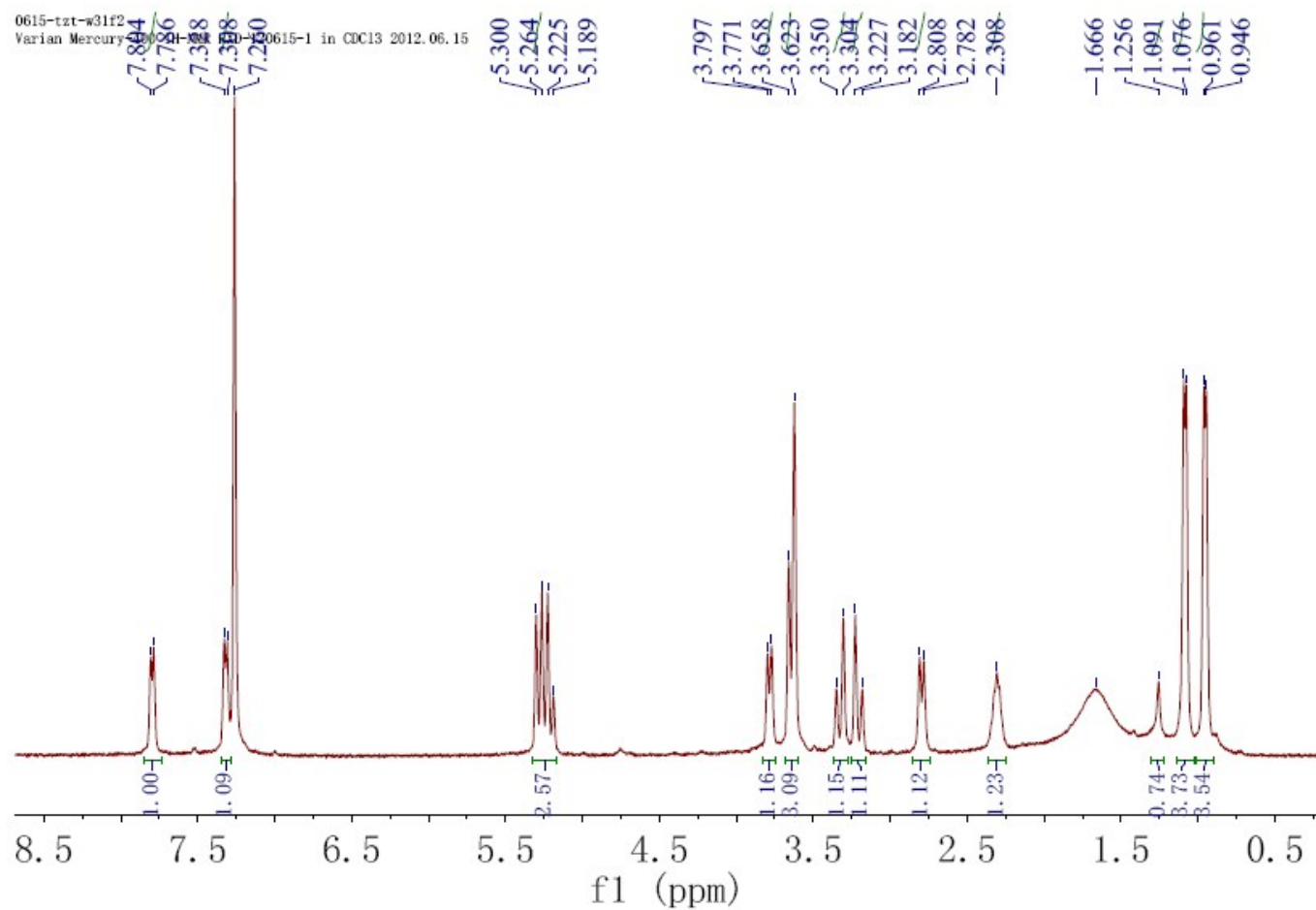


Figure S47. The ^{13}C NMR (100 MHz) spectrum of tripterlide F (6) in CDCl_3

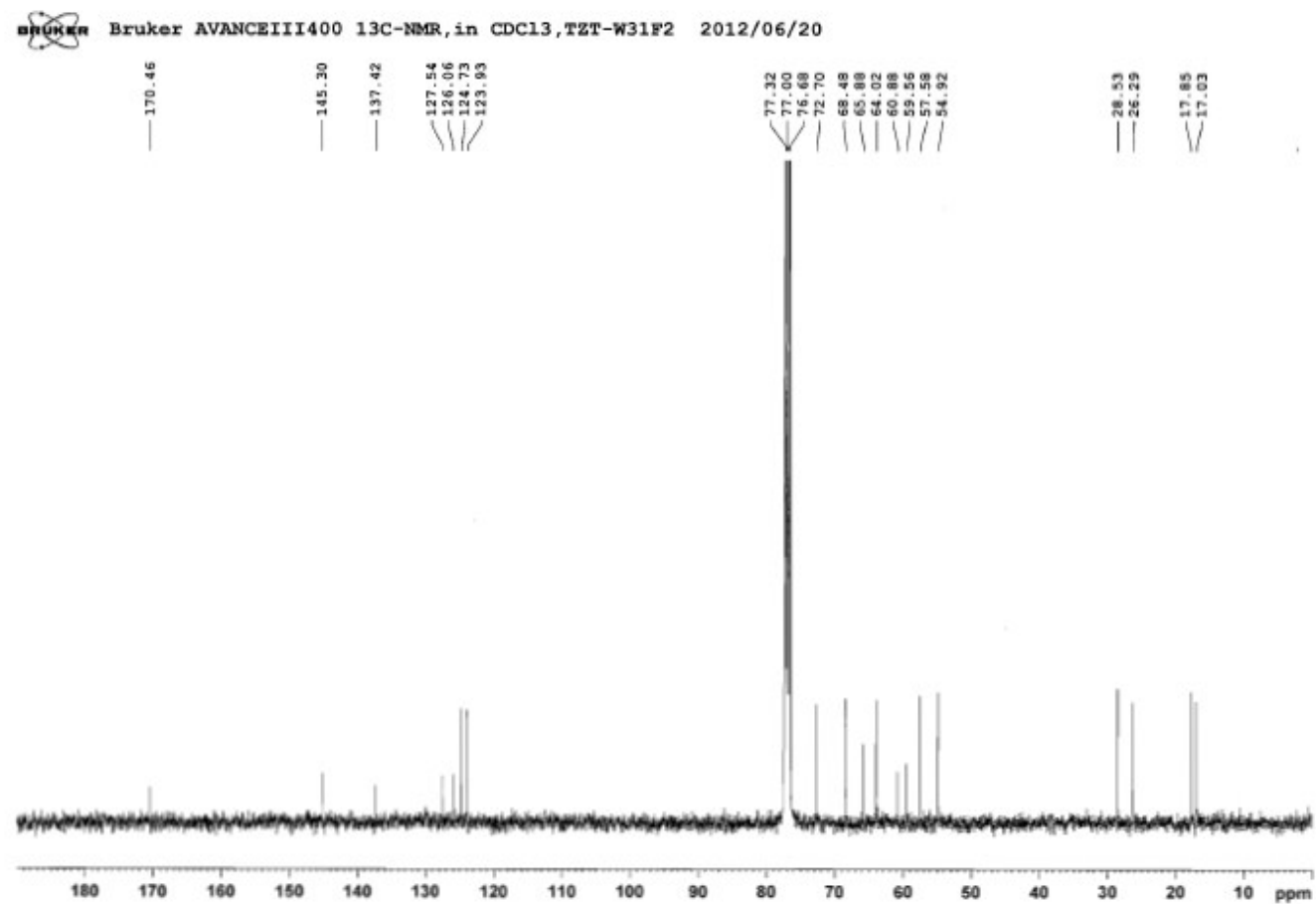


Figure S48. The HSQC spectrum of tripterlide F (6) in CDCl₃

Bruker AVANCEIII400 HSQC-NMR, in CDCl₃, T2T-W31F2 2012/07/06

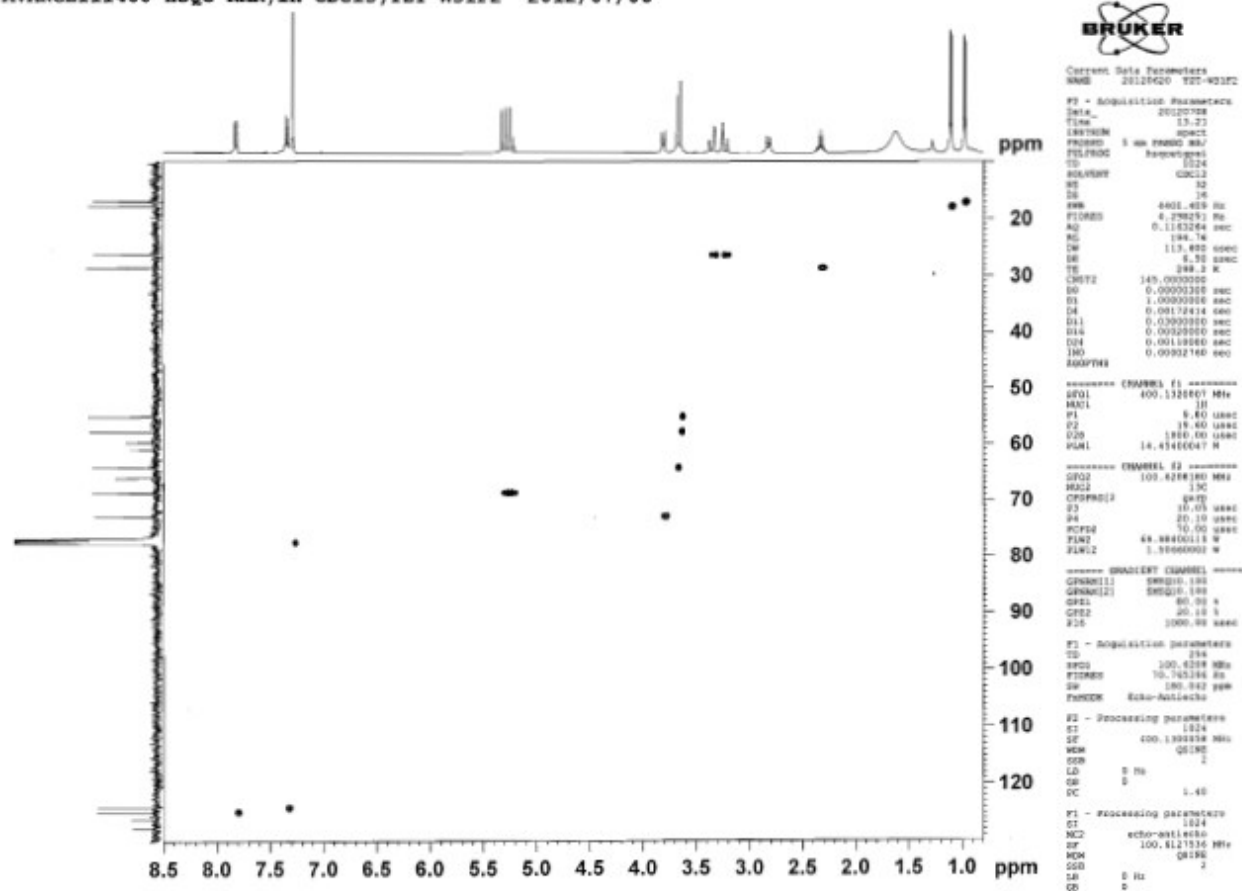


Figure S49. The HMBC spectrum of tripterlide F (6) in CDCl_3

Bruker AVANCEIII400 HMBC-NMR, in CDCl_3 , TET-W31F2 2012/07/06

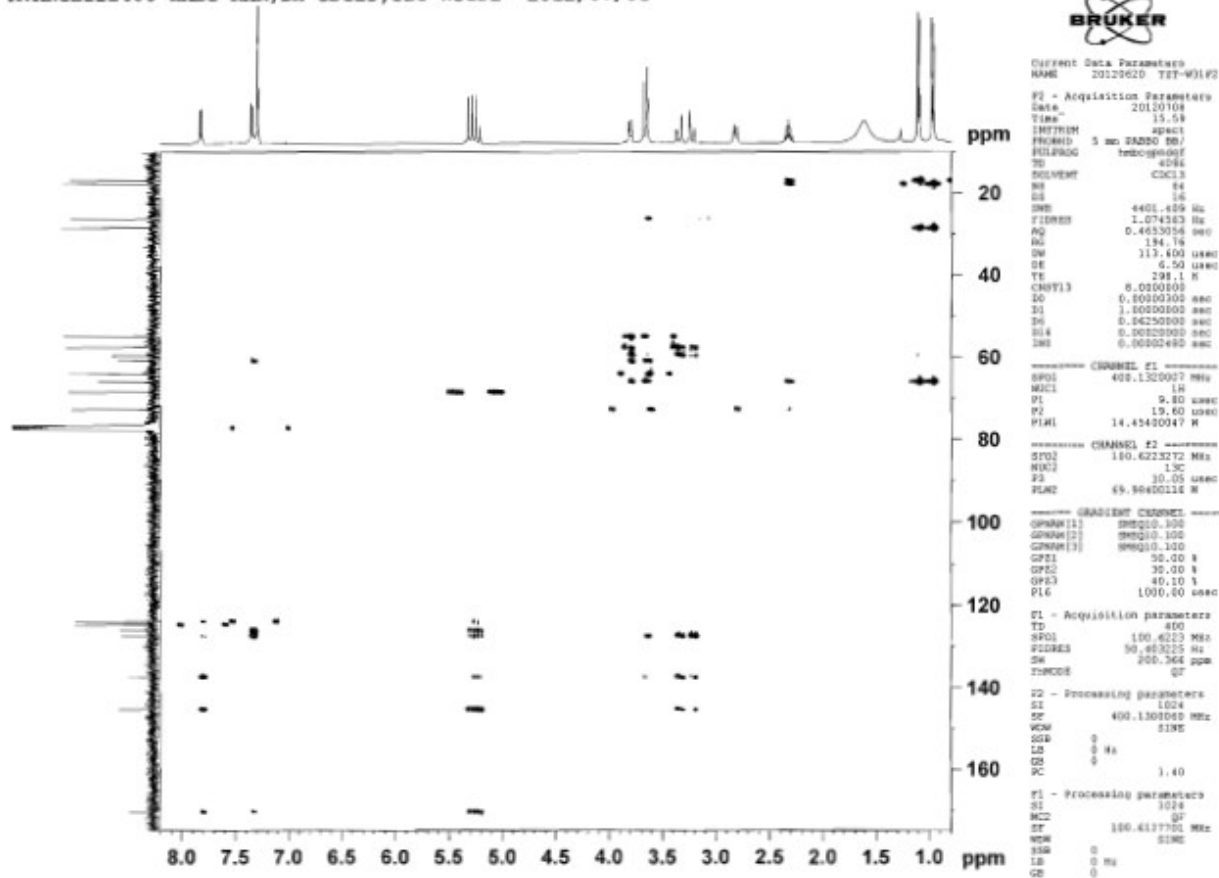


Figure S50. The ^1H - ^1H COSY spectrum of tripterlide F (6) in CDCl_3

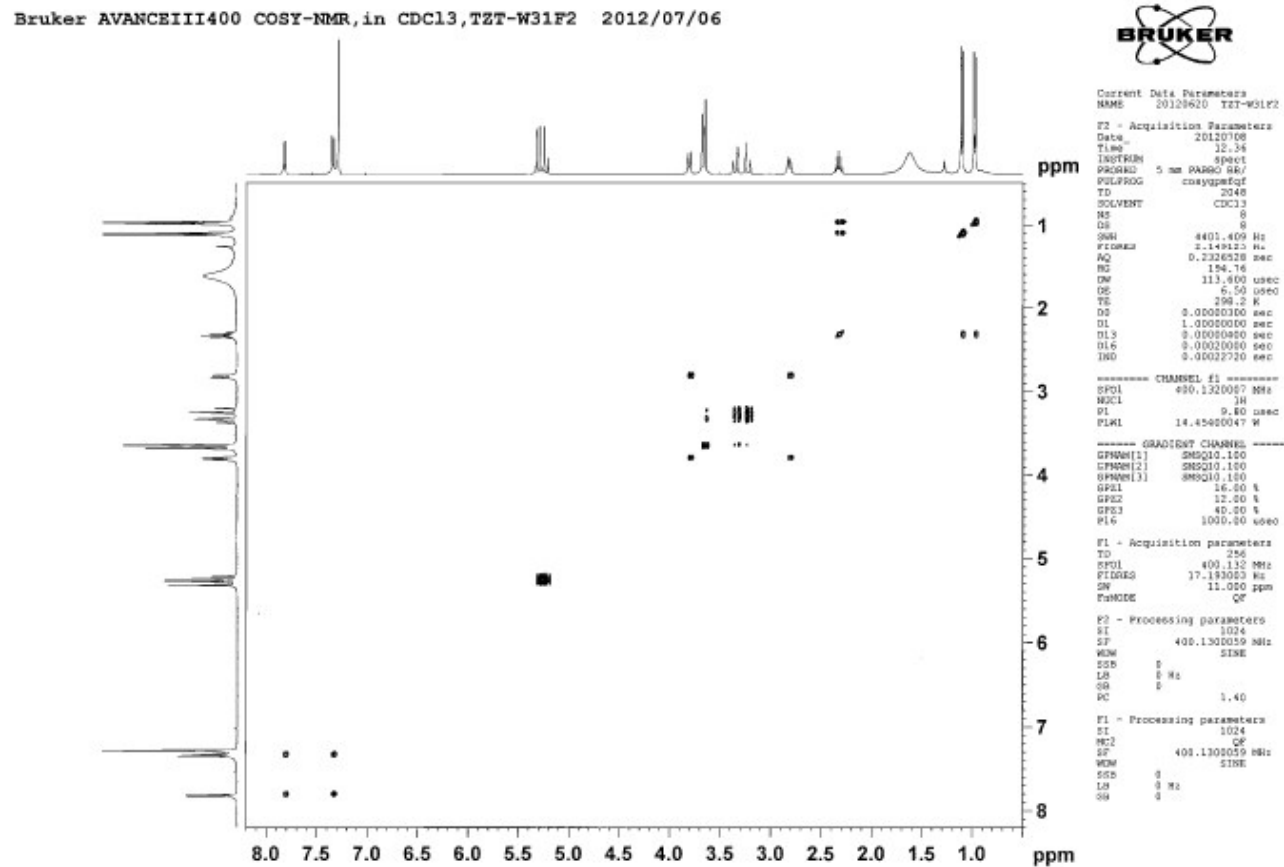


Figure S51. The 1D NOE spectrum of tripterlide F (6) in CDCl₃

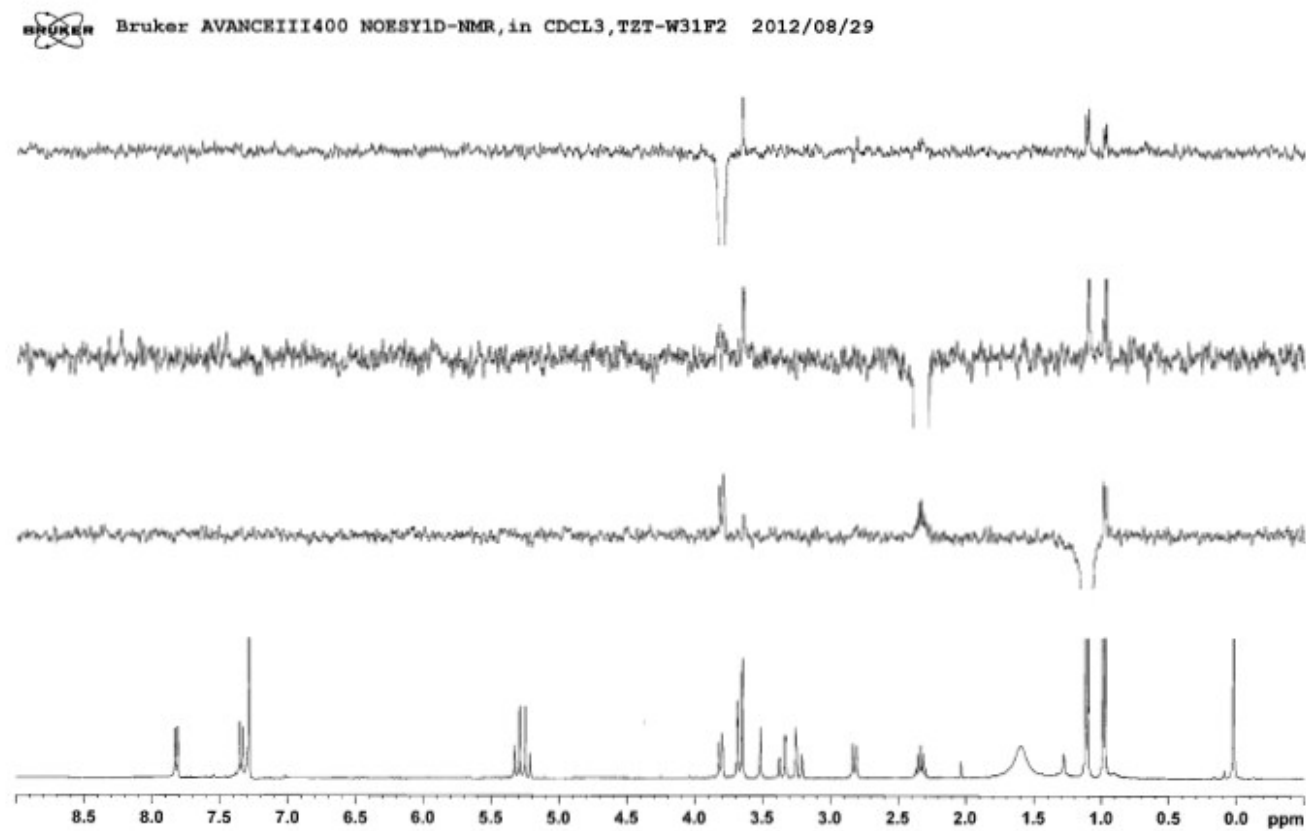


Figure S52. The IR spectrum of tripterlide F (6)

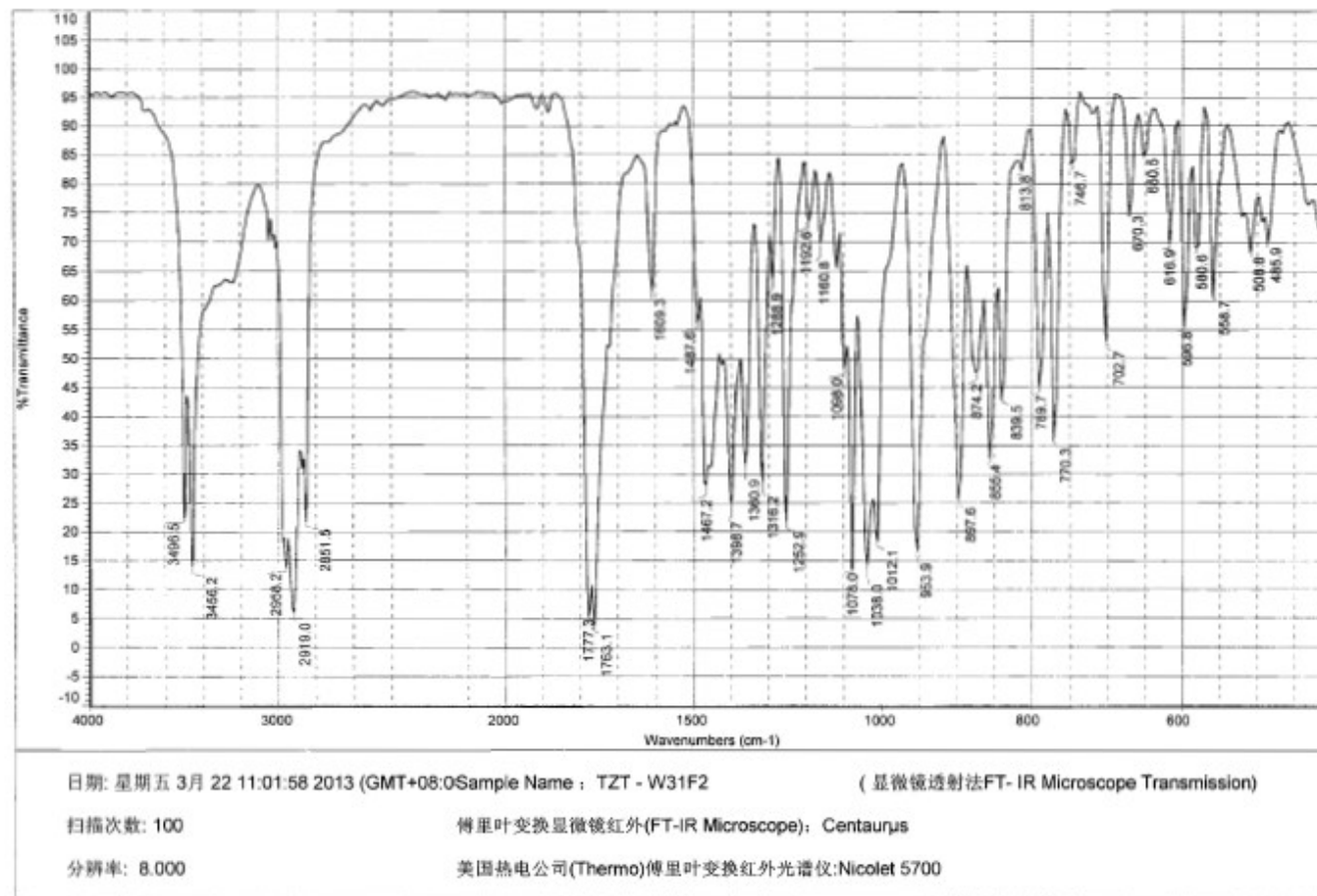


Figure S53. The HRESIMS spectrum of tripterlide F (6)

MS Formula Results: + Scan (5.766 min) Sub (2012071303.d)

m/z	Ion	Formula	Abundance
343.1170	(M+H) ⁺	C ₁₉ H ₁₈ O ₈	184044

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross S	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Mat	Mass Match	m/z	DBE	
1	[M]	C ₁₉ H ₁₈ O ₈	C ₁₉ H ₁₈ O ₈	343.1178	99.05		342.1107	342.1103	-4.30	6.98	98.65	98.97	98.97	343.1179	11
2	[M-1]	C ₁₉ H ₁₇ O ₈	C ₁₉ H ₁₇ O ₈	343.1151	98		342.1107	342.1106	-0.27	6.27	98.64	98.98	97.84	343.1179	15
3	[M-2]	C ₁₉ H ₁₆ O ₈	C ₁₉ H ₁₆ O ₈	343.1121	97.4		342.1107	342.1107	0.00	6.89	98.49	98.47	97.51	343.1179	8
4	[M-3]	C ₁₉ H ₁₅ O ₈	C ₁₉ H ₁₅ O ₈	343.1188	97.35		342.1107	342.1112	1.37	1.57	91.44	98.22	99.82	343.1179	10
5	[M-4]	C ₁₉ H ₁₄ O ₈	C ₁₉ H ₁₄ O ₈	343.117	96.55		342.1107	342.1207	-2.80	2.88	98.51	98.27	98.74	343.1179	2

m/z	Ion	Formula	Abundance
345.1448	(M+H) ⁺	C ₁₉ H ₂₂ N ₂ O ₈	1248324.8

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross S	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Mat	Mass Match	m/z	DBE	
1	[M]	C ₁₉ H ₂₂ N ₂ O ₈	C ₁₉ H ₂₂ N ₂ O ₈	345.1442	98.85		342.1111	342.1103	-2.32	2.32	99.61	98.23	99.89	345.1448	11
2	[M-1]	C ₁₉ H ₂₁ N ₂ O ₈	C ₁₉ H ₂₁ N ₂ O ₈	345.1417	97.91		342.1111	342.1206	-9.34	9.34	97.94	98.3	97.48	345.1448	15
3	[M-2]	C ₁₉ H ₂₀ N ₂ O ₈	C ₁₉ H ₂₀ N ₂ O ₈	345.140	97.67		342.1111	342.1112	0.91	0.91	97.87	98.95	98.99	345.1448	10
4	[M-3]	C ₁₉ H ₁₉ N ₂ O ₈	C ₁₉ H ₁₉ N ₂ O ₈	345.1379	97.6		342.1111	342.1131	2.82	2.82	95.8	98.53	98.29	345.1448	8
5	[M-4]	C ₁₉ H ₁₈ N ₂ O ₈	C ₁₉ H ₁₈ N ₂ O ₈	345.1358	96.25		342.1111	342.1247	-3.95	3.95	98.69	98.54	98.55	345.1448	2

m/z	Ion	Formula	Abundance
385.1088	(M+H) ⁺	C ₁₉ H ₁₈ Na ₂ O ₈	166862.8

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross S	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Mat	Mass Match	m/z	DBE	
1	[M]	C ₁₉ H ₁₈ Na ₂ O ₈	C ₁₉ H ₁₈ Na ₂ O ₈	385.1098	99.85		342.1114	342.1103	-3.32	3.32	98.69	98.95	98.74	385.1088	11
2	[M-1]	C ₁₉ H ₁₇ Na ₂ O ₈	C ₁₉ H ₁₇ Na ₂ O ₈	385.1078	98.38		342.1114	342.1107	0.85	0.85	98.69	98.75	98.69	385.1088	8
3	[M-2]	C ₁₉ H ₁₆ Na ₂ O ₈	C ₁₉ H ₁₆ Na ₂ O ₈	385.1059	97.32		342.1114	342.1207	-4.32	4.32	92.01	98.73	98.31	385.1088	2
4	[M-3]	C ₁₉ H ₁₅ Na ₂ O ₈	C ₁₉ H ₁₅ Na ₂ O ₈	385.1034	97.24		342.1114	342.1112	-0.20	0.48	90.84	98.95	98.99	385.1088	10