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

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Supporting Information

List of Supporting Information

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

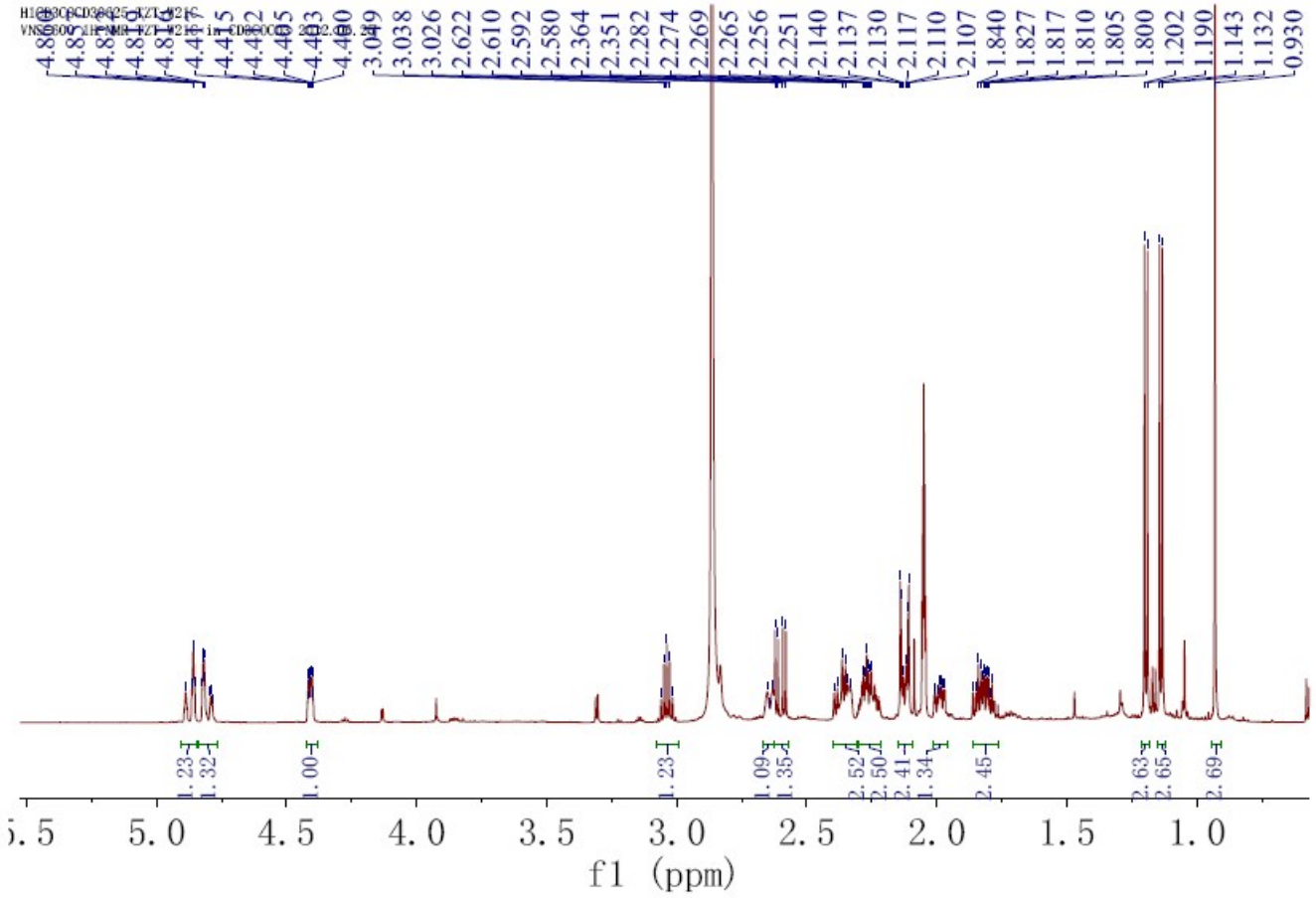


Figure S2. The ^{13}C NMR (150 MHz) spectrum of tripterlide A (1) in actone-d_6

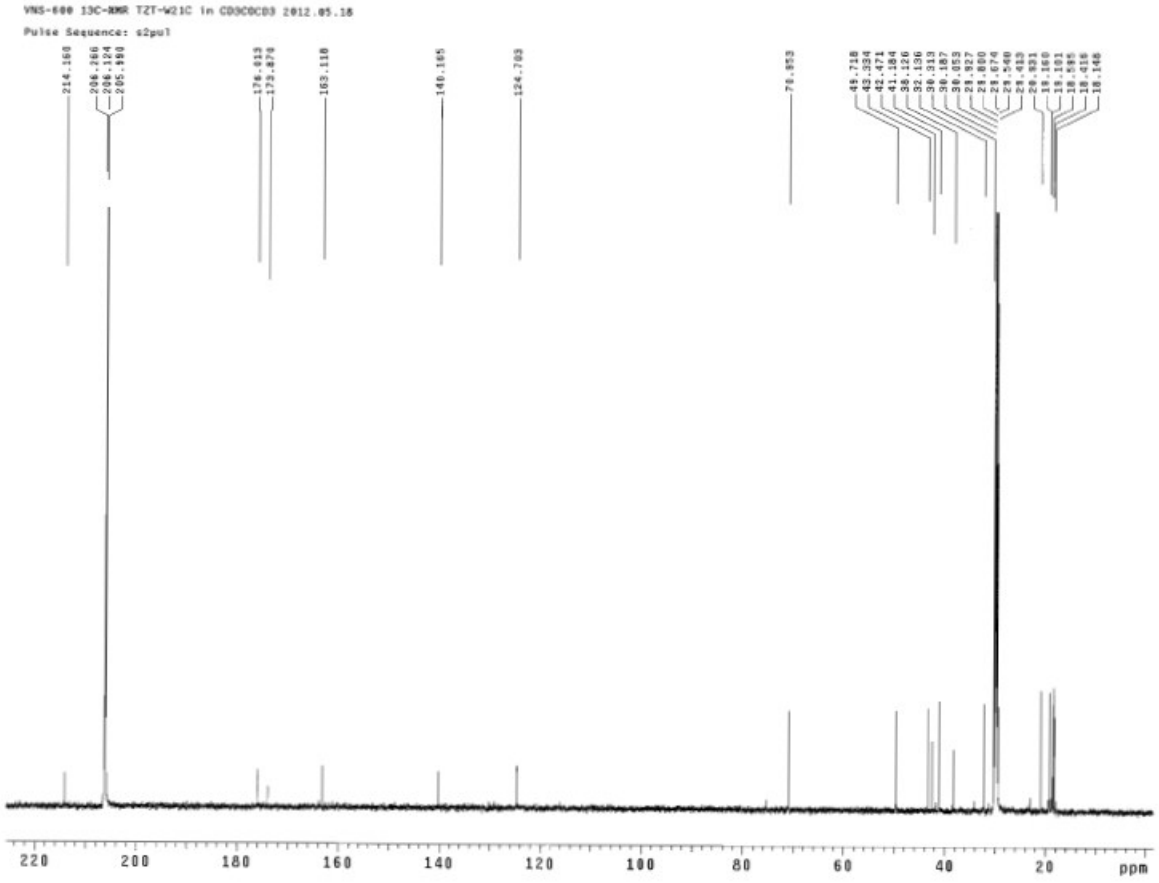


Figure S3. The DEPT spectrum of tripterlide A (1) in actone-d_6

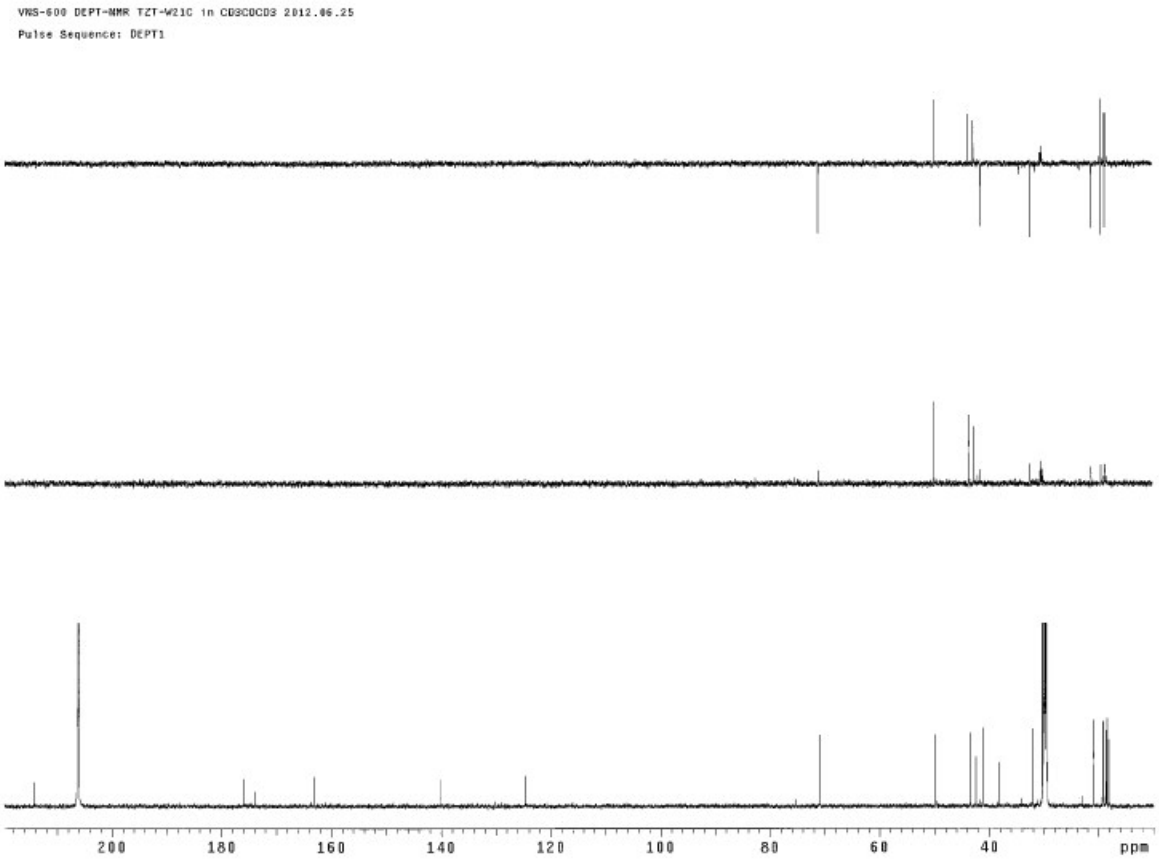


Figure S4. The HSQC spectrum of tripterlide A (1) in actone-d_6

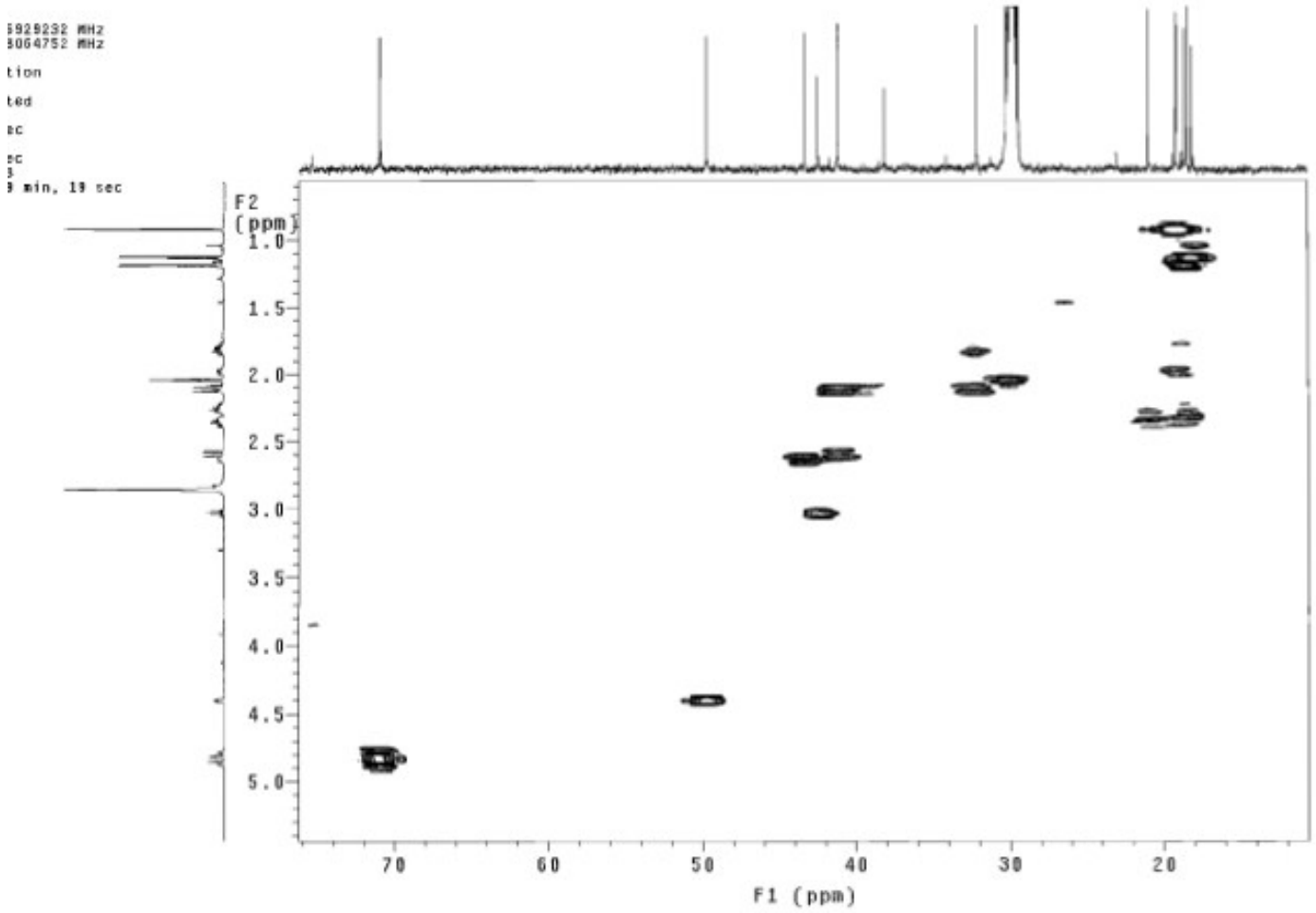


Figure S5. The HMBC spectrum of tripterlide A (1) in actone-d_6

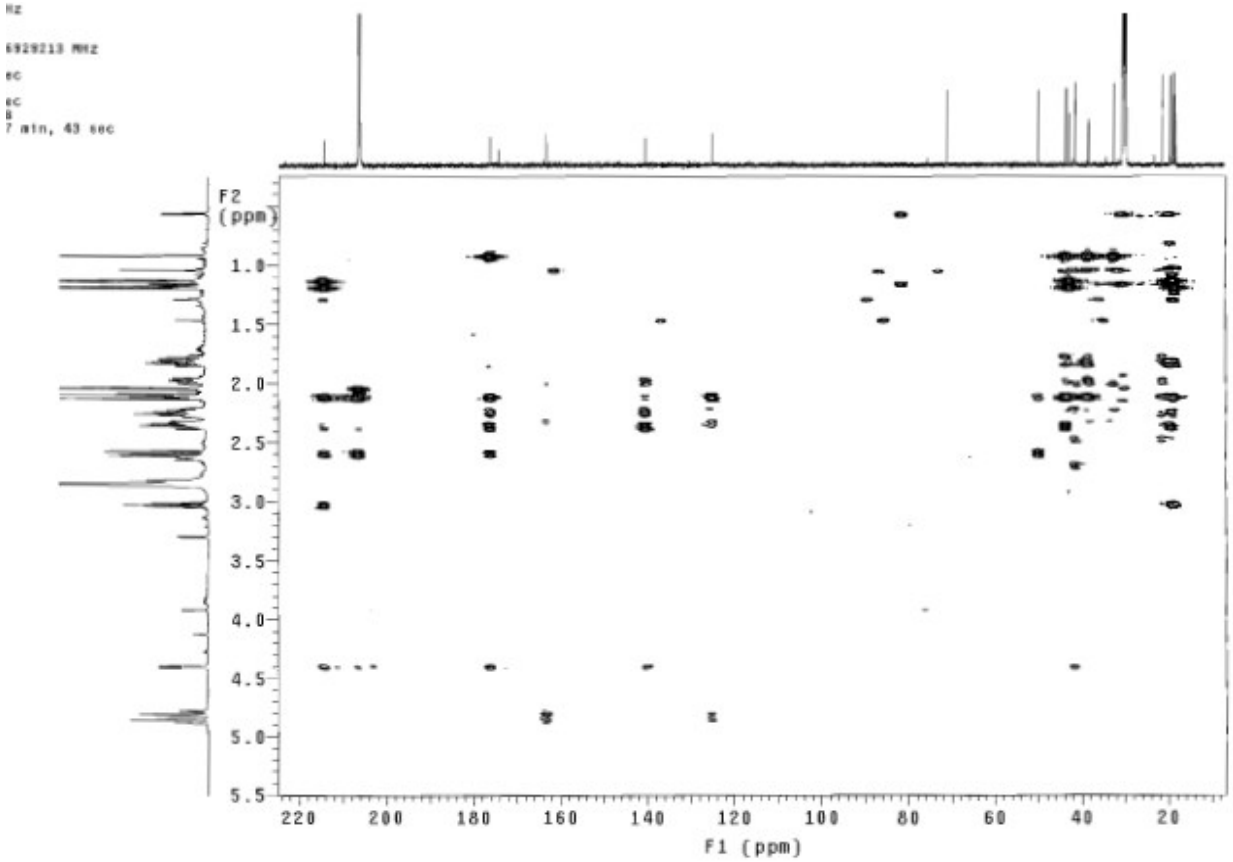
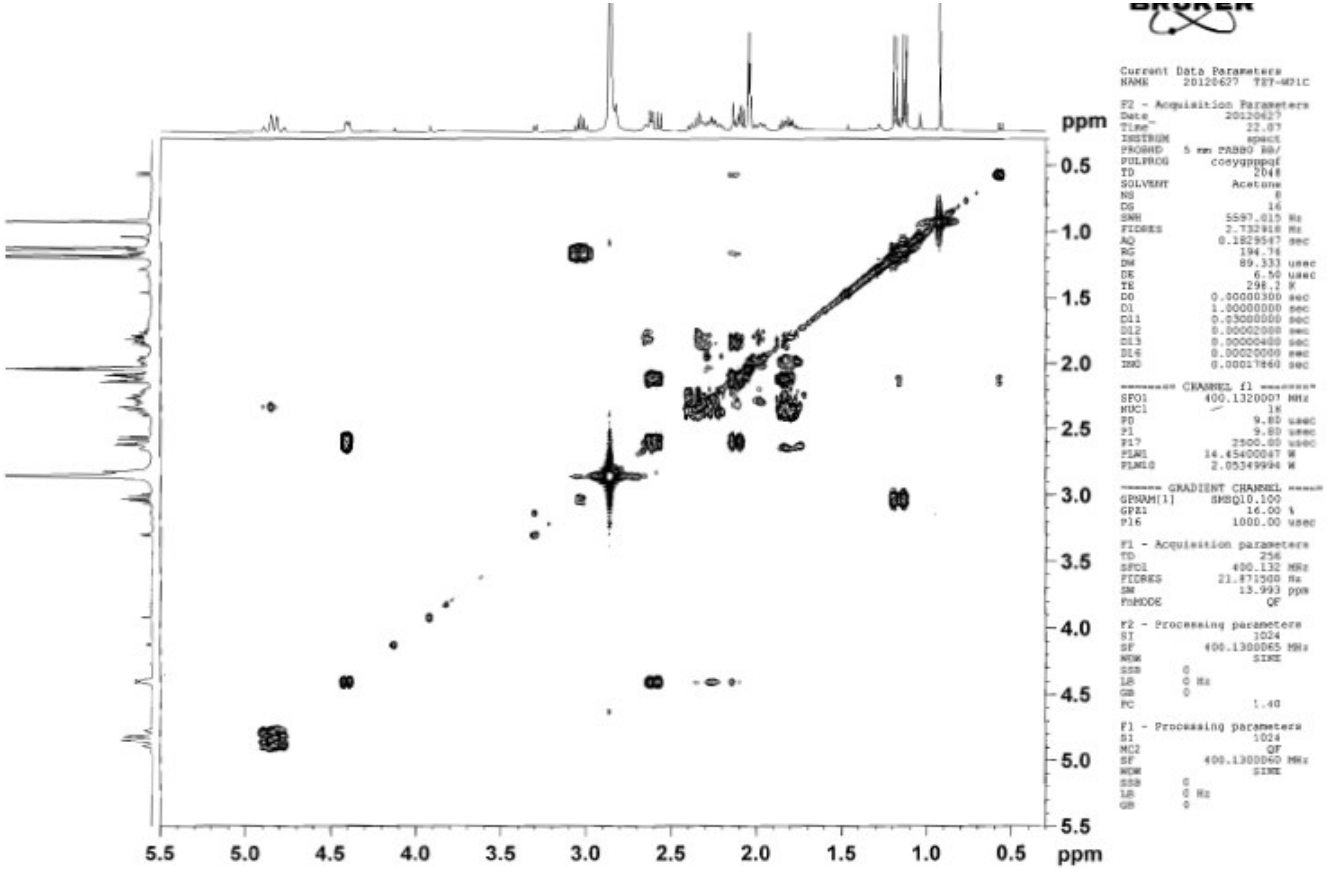


Figure S6. The ^{1}H-^{1}H COSY spectrum of tripterlide A (1) in actone-d_6



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TD 2048
SOLVENT Acetone
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FIDRES 2.732918 Hz
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RG 194.76
DW 89.333 usec
DE 6.50 usec
TE 298.2 K
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D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00017860 sec

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LB 0 Hz
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PC 1.40

F1 - Processing parameters
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WDW SINE
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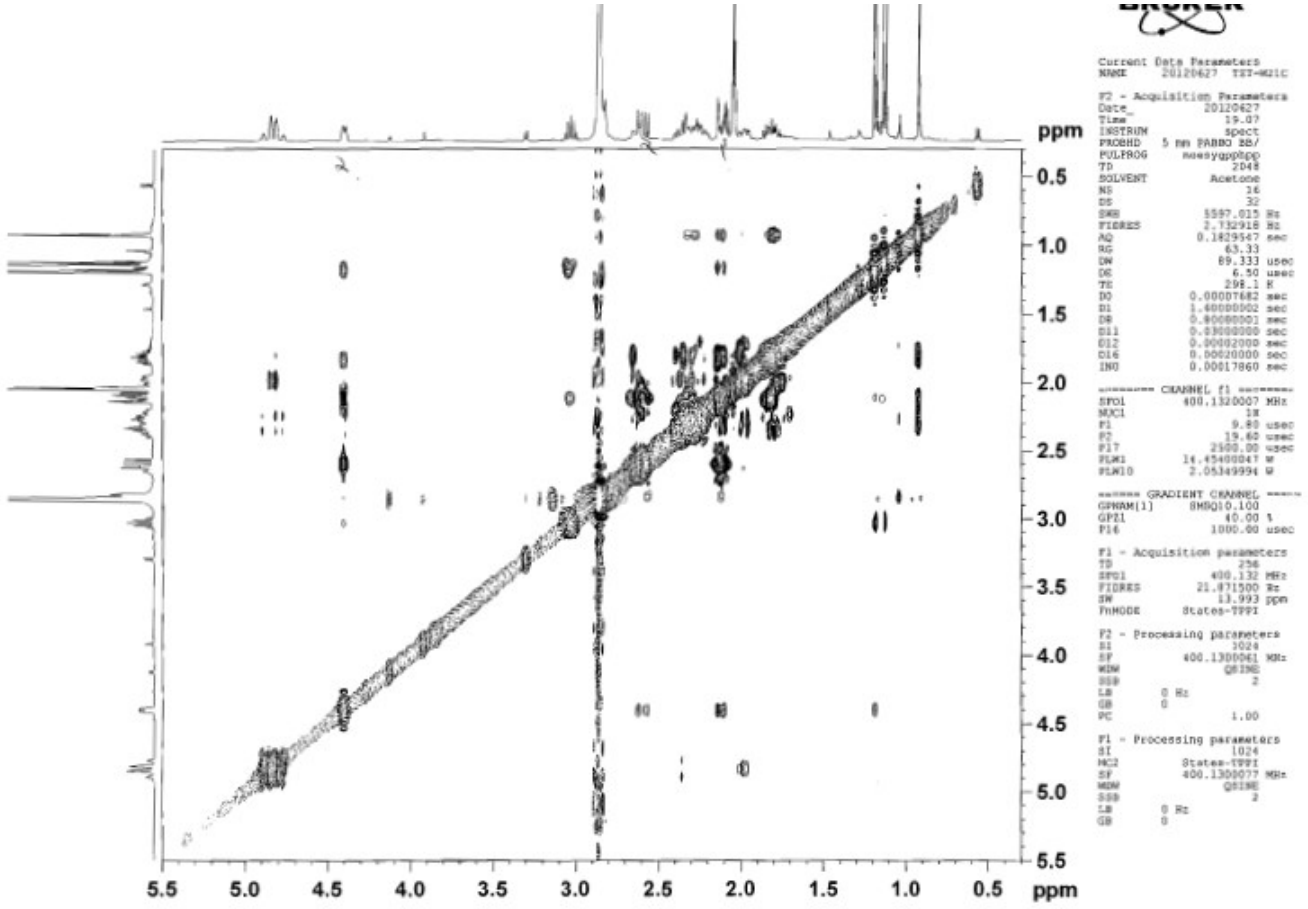
GB 0

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



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SOLVENT Acetone
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RG 63.33
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DE 6.50 usec
TE 298.1 K
D0 0.00007682 sec
D1 1.40000002 sec
D8 0.80000001 sec
D11 0.03000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
IN0 0.00017860 sec

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NUC1 1H
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P2 19.60 usec
P17 2500.00 usec
PLW1 14.45400047 W
PLW10 2.05349994 W

====== GRADIENT CHANNEL =====
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FIDRES 21.471500 Hz
SW 13.993 ppm
FnMODE States-TPPI

F2 - Processing parameters
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SF 400.1300041 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
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MC2 States-TPPI
SF 400.1300077 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0

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

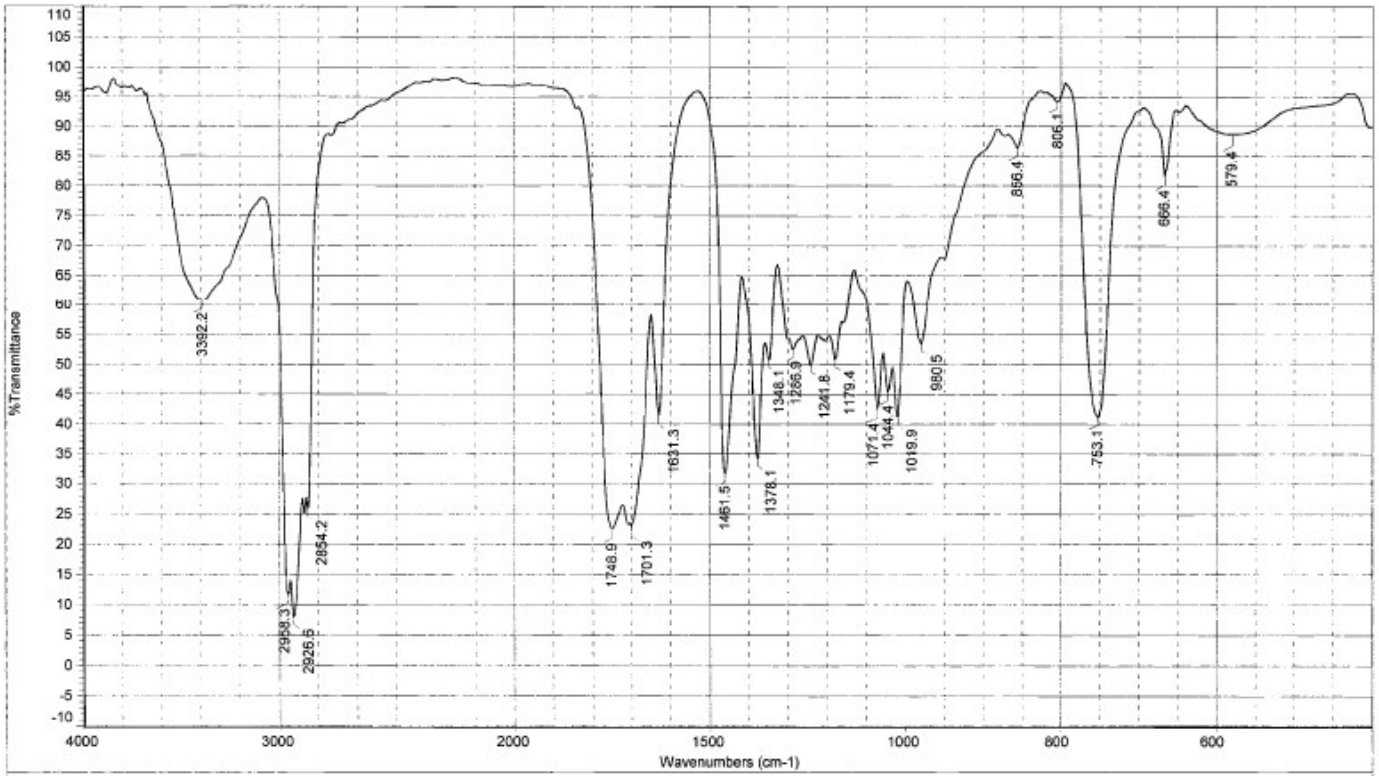
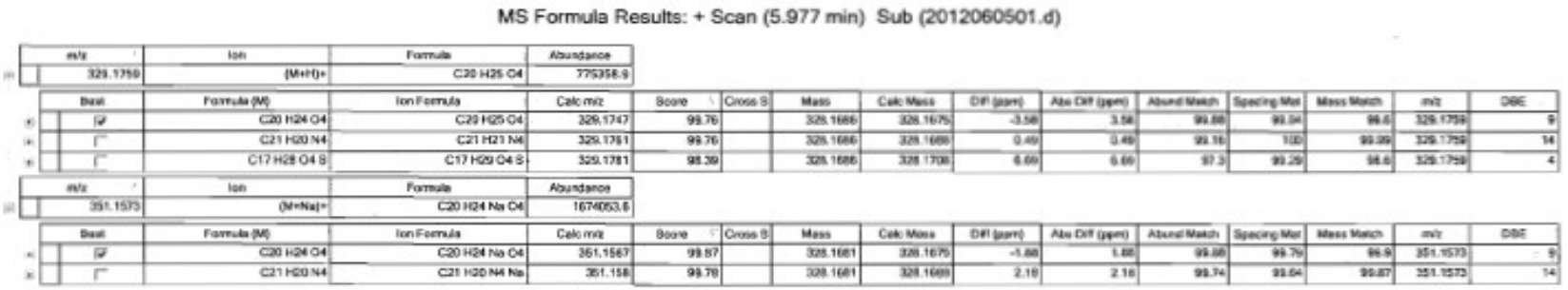


Figure S9. The HRESIMS of tripterlide A (1)



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

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1	329.1759	(M+H)+	C20 H25 O4	775358.9

	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	☑	C20 H24 O4	C20 H25 O4	329.1747	99.76		328.1680	328.1675	-3.58	3.58	99.68	99.94	98.6	329.1759	9
2	☐	C21 H20 N4	C21 H21 N4	329.1761	99.76		328.1680	328.1689	0.49	0.49	99.16	100	99.09	329.1759	14
3	☐	C17 H28 O4 S	C17 H29 O4 S+	329.1781	98.39		328.1686	328.1708	6.69	6.69	97.3	99.29	98.6	329.1759	4

	m/z	Ion	Formula	Abundance
2	351.1573	(M+Na)+	C20 H24 Na O4	1674063.6

	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	☑	C20 H24 O4	C20 H24 Na O4	351.1567	99.87		328.1681	328.1675	-1.68	1.68	99.68	99.79	99.9	351.1573	9
2	☐	C21 H20 N4	C21 H20 N4 Na	351.158	99.78		328.1681	328.1689	2.18	2.18	99.74	99.64	99.87	351.1573	14

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

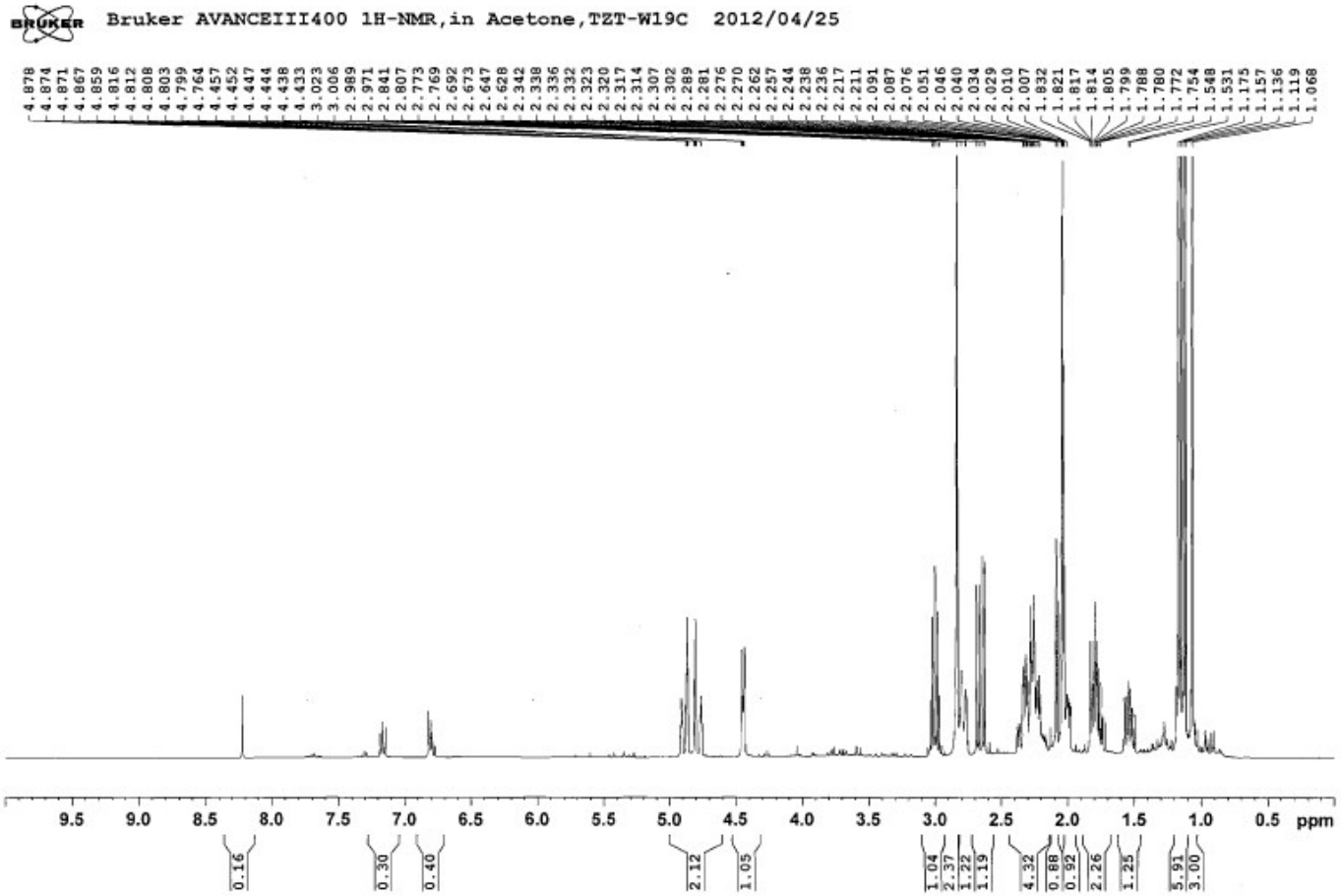


Figure S11. The ^{13}C NMR (150 MHz) spectrum of tripterlide B (2) in actone-d_6

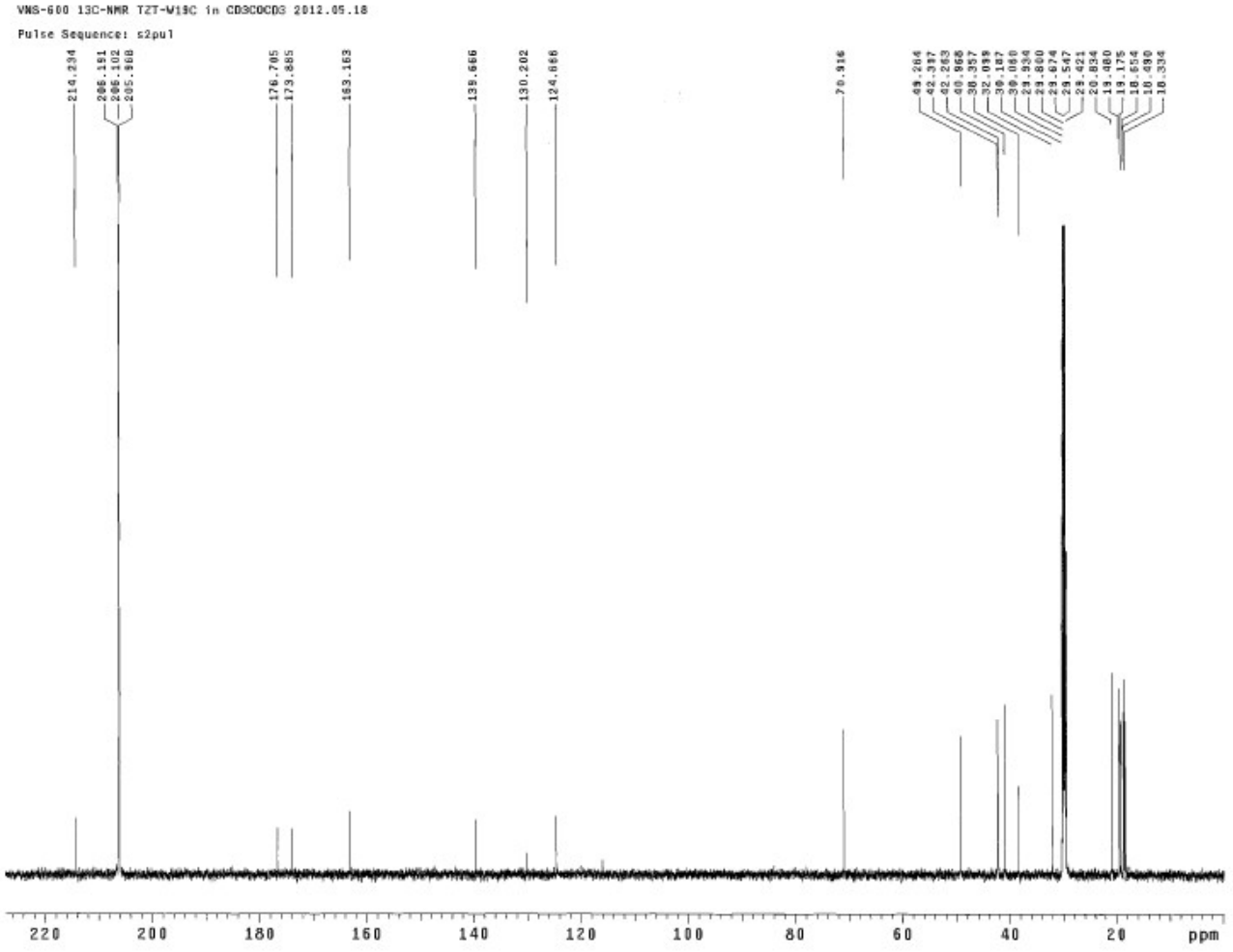


Figure S12. The DEPT spectrum of tripterlide B (2) in actone-d_6

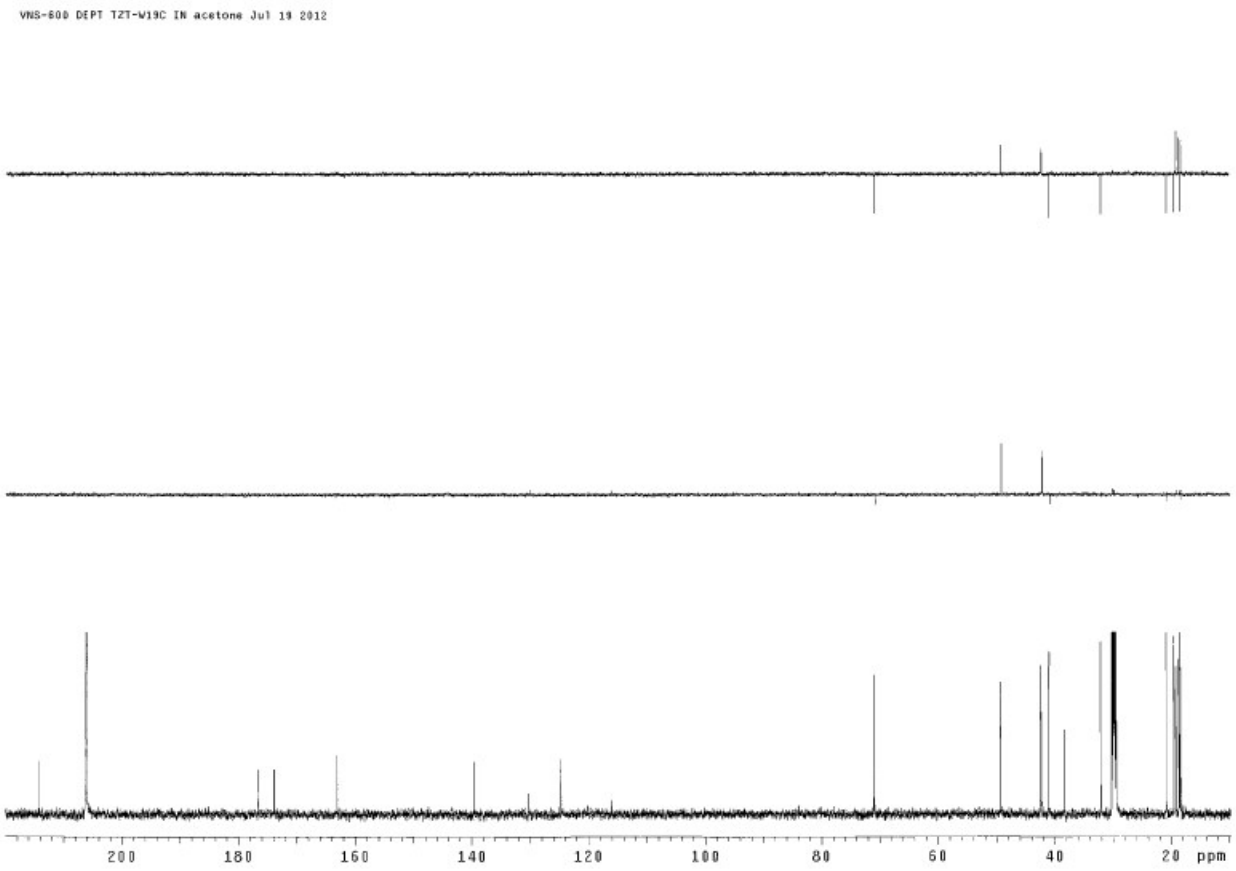


Figure S13. The HSQC spectrum of tripterlide B (2) in actone-d_6

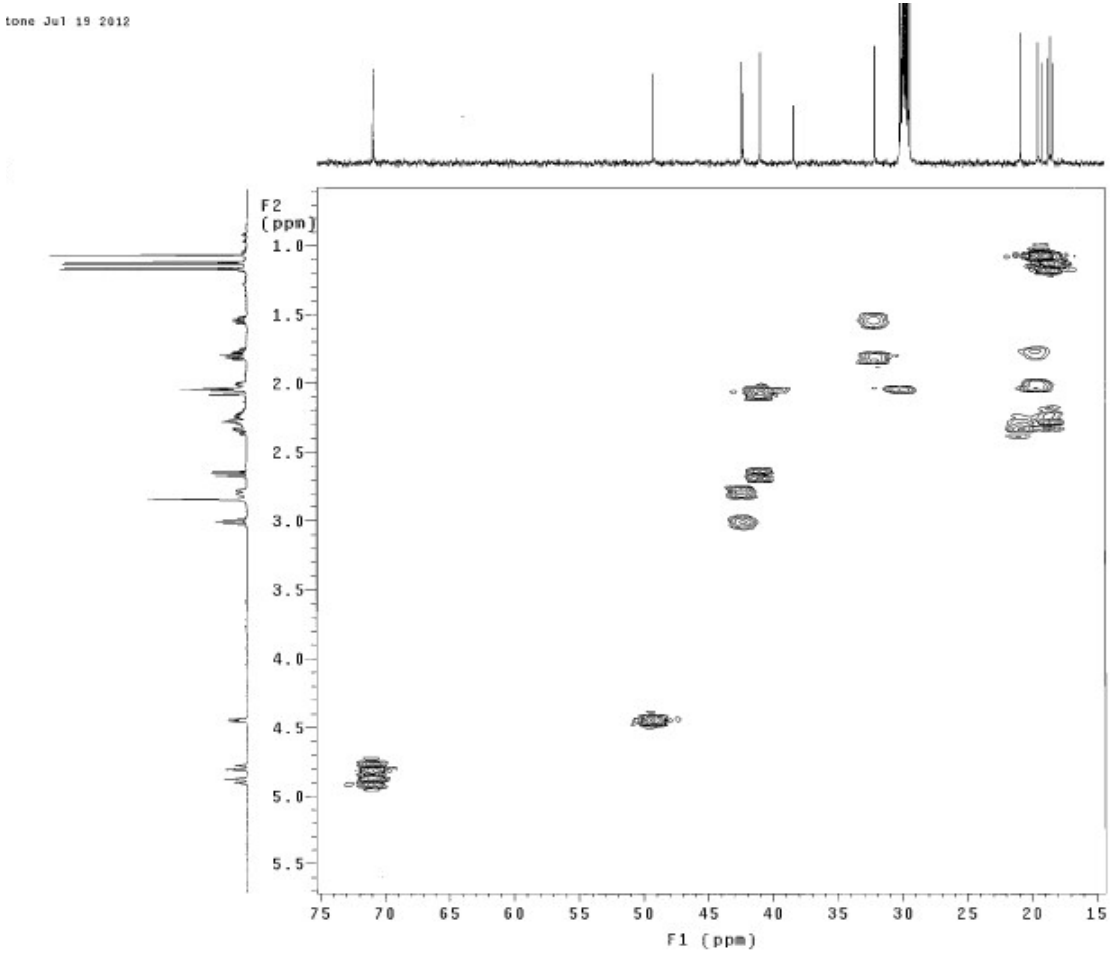


Figure S14. The HMBC spectrum of tripterlide B (2) in actone-d_6

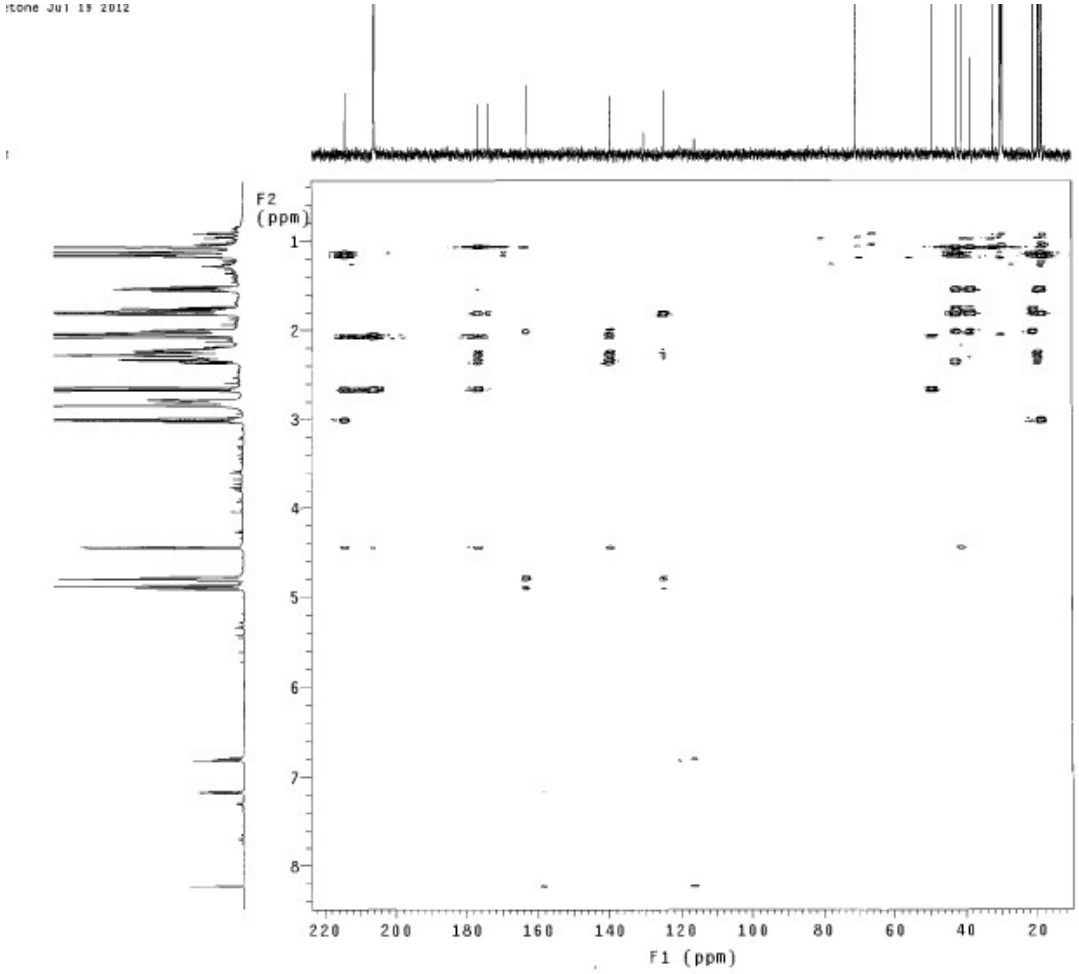


Figure S15. The ^{1}H-^{1}H COSY spectrum of tripterlide B (2) in actone-d_6

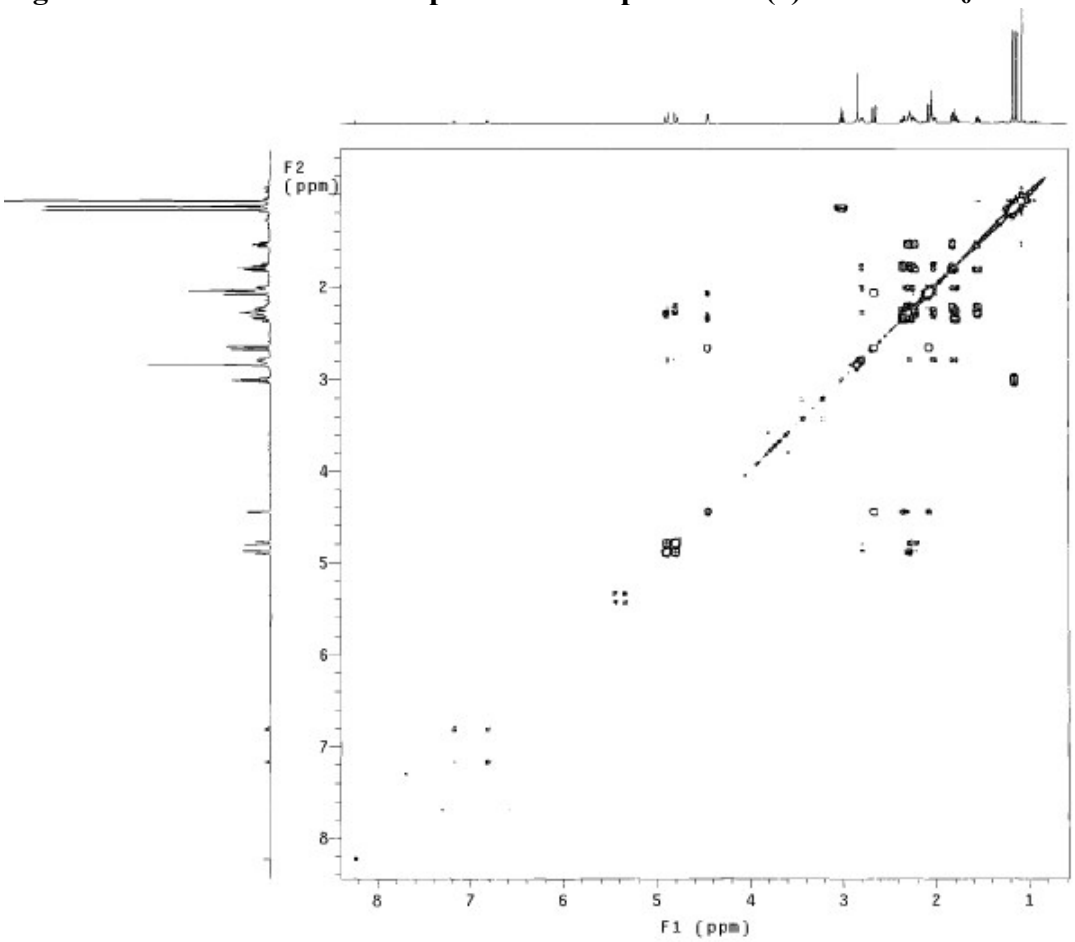


Figure S16. The NOESY spectrum of tripterlide B (2) in actone-d_6

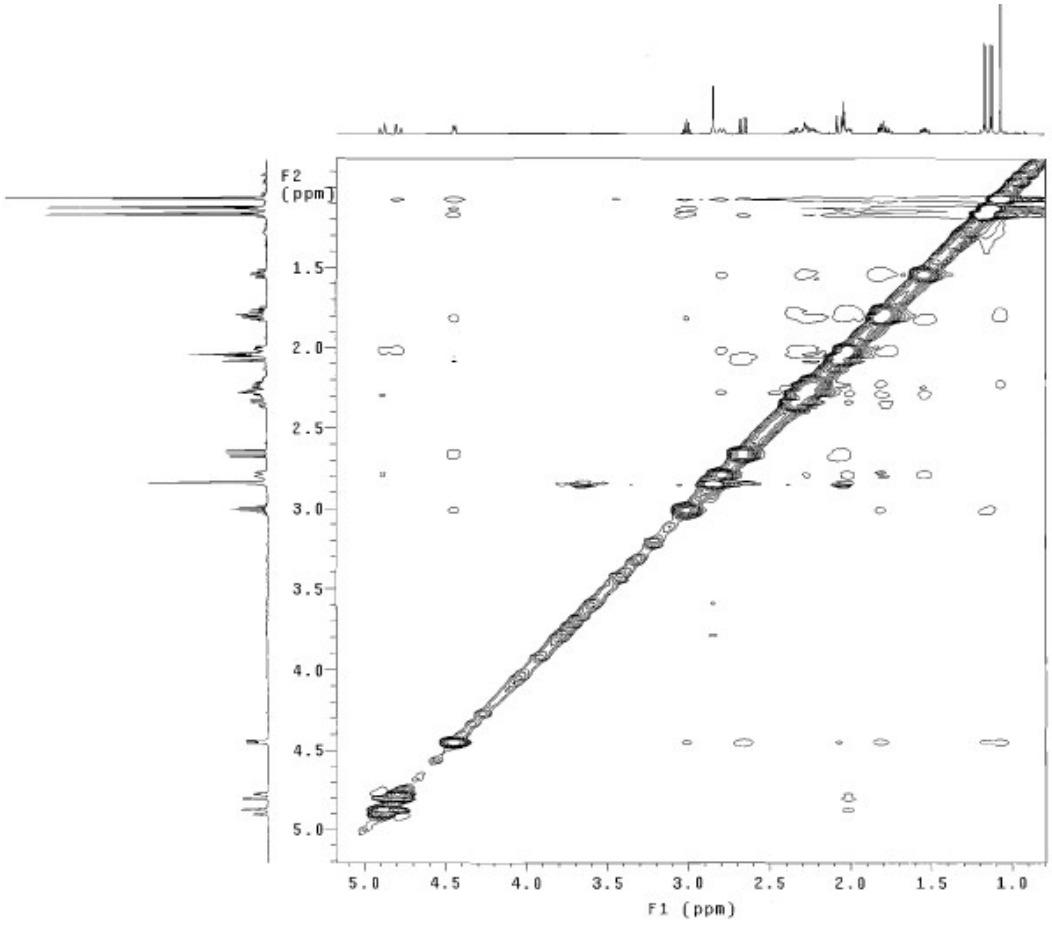


Figure S17. The IR spectrum of tripterlide B (2)

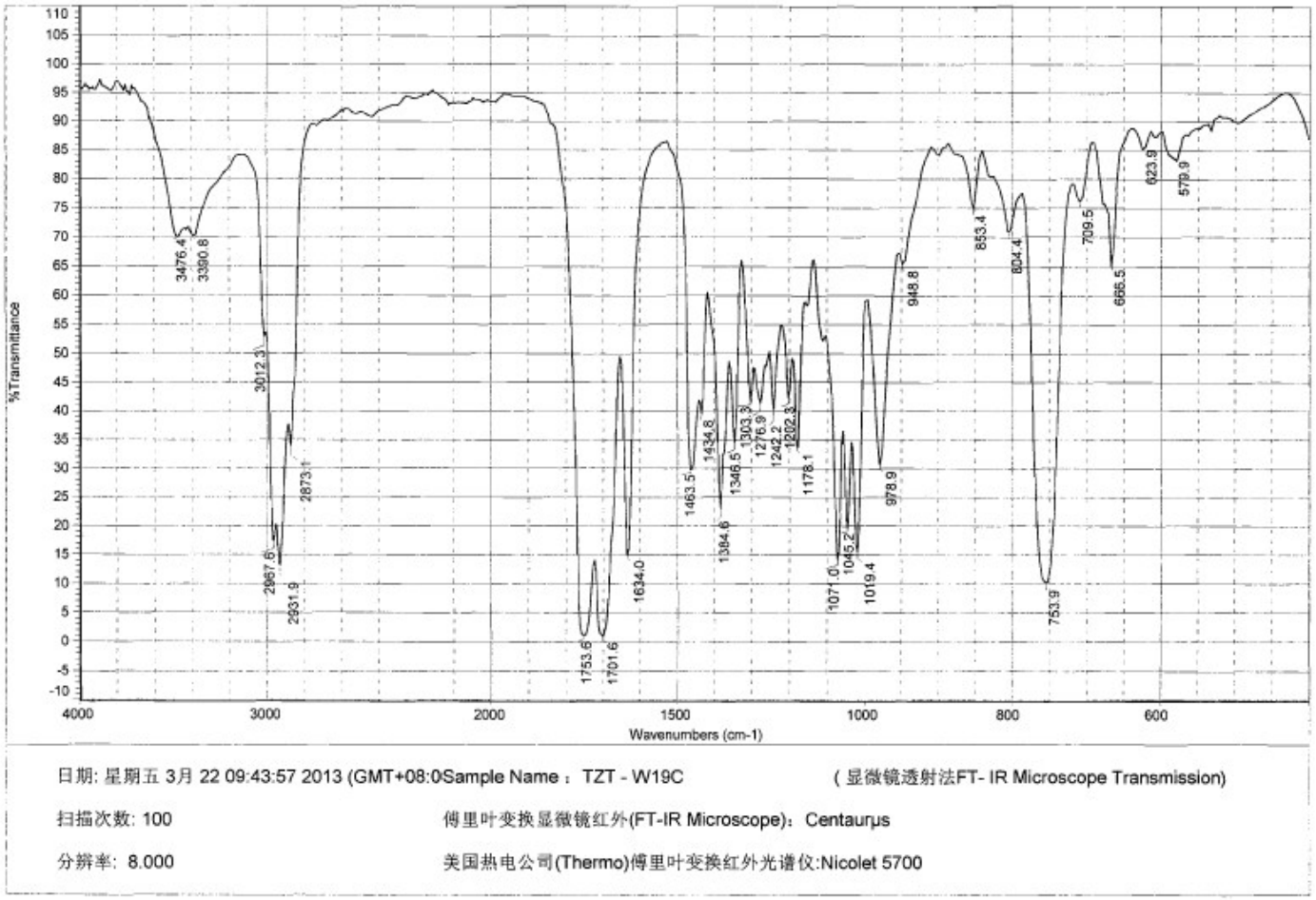


Figure S18. The HRESIMS of tripterlide B (2)

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

m/z	Ion	Formula	Abundance
329.1753	(M+H)+	C20 H25 O4	521788

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
☑	C20 H24 O4	C20 H25 O4	329.1747	99.48		328.168	328.1675	-1.74	1.74	98.35	99.97	99.9	329.1753	9

m/z	Ion	Formula	Abundance
346.2021	(M+NH4)+	C20 H28 N O4	860629.1

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
☑	C20 H24 O4	C20 H28 N O4	346.2013	98.31		328.1682	328.1675	-2.11	2.11	97.06	90.7	99.67	346.2021	9

m/z	Ion	Formula	Abundance
351.1571	(M+Na)+	C20 H24 Na O4	1729499.9

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
☑	C20 H24 O4	C20 H24 Na O4	351.1567	99		328.1679	328.1675	-1.25	1.25	99.6	96.36	99.96	351.1571	9

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

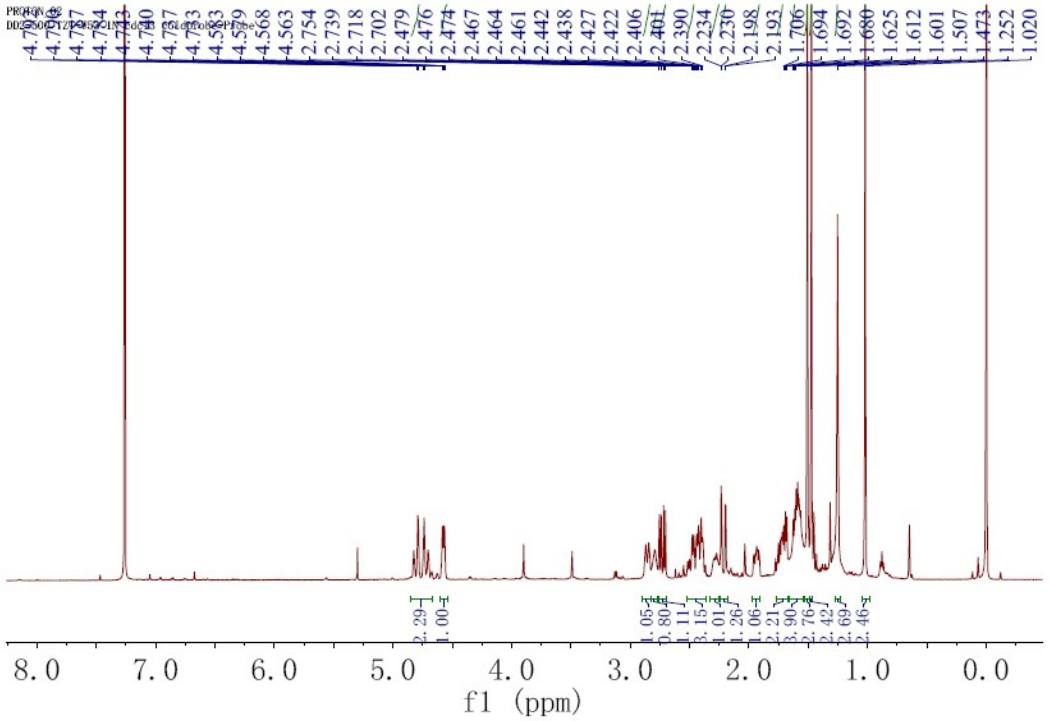


Figure S20. The ^{13}C NMR (125 MHz) spectrum of tripterlide C (3) in $CDCl_3$

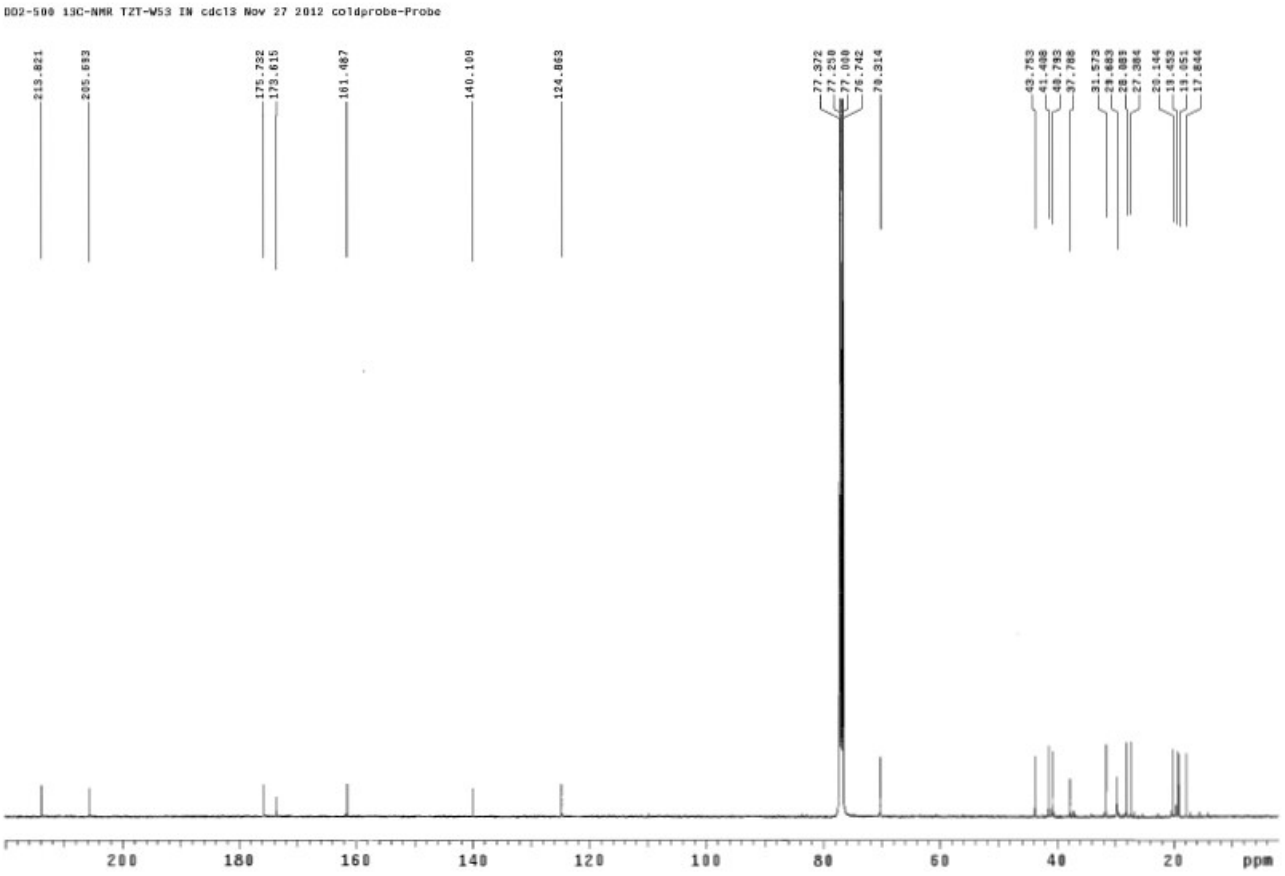


Figure S21. The HSQC spectrum of tripterlide C (3) in $CDCl_3$

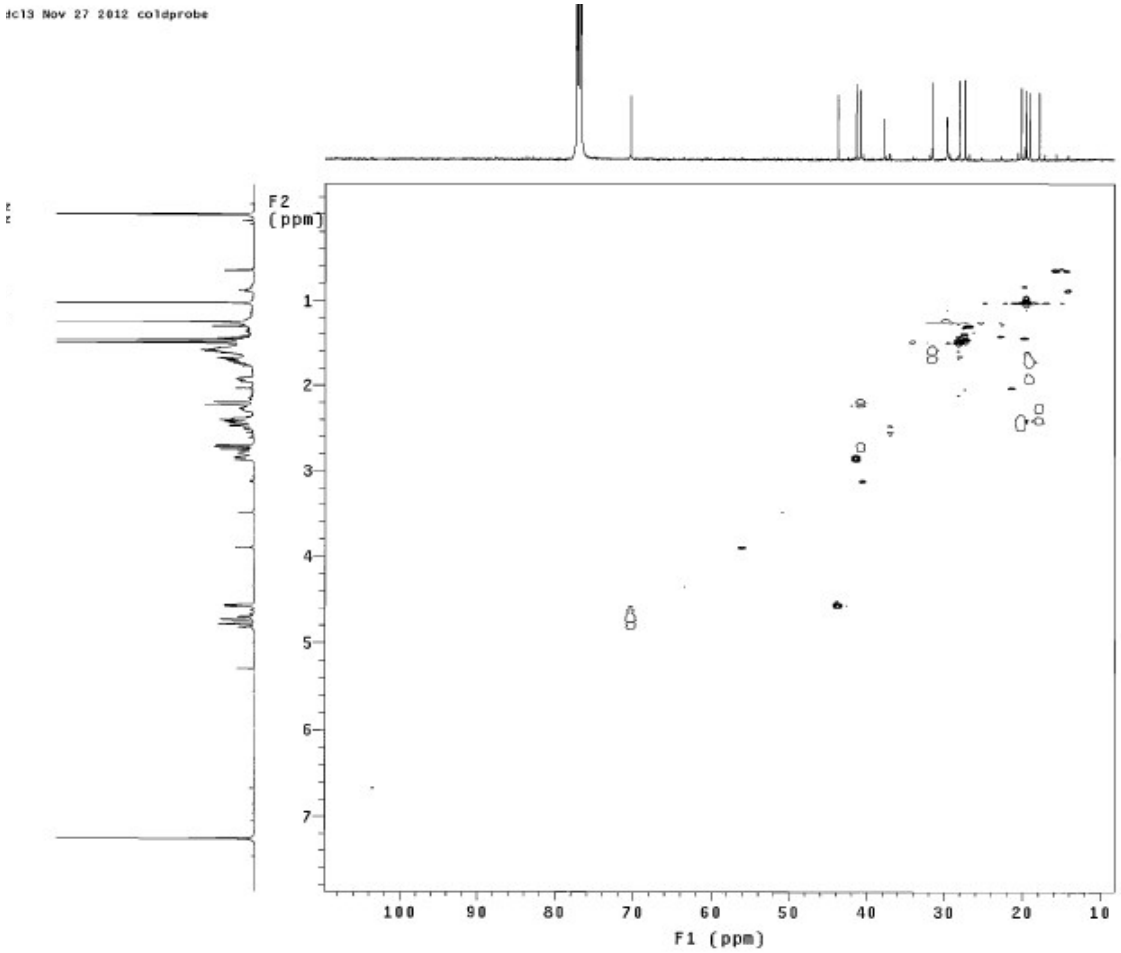


Figure S22. The HMBC spectrum of tripterlide C (3) in $CDCl_3$

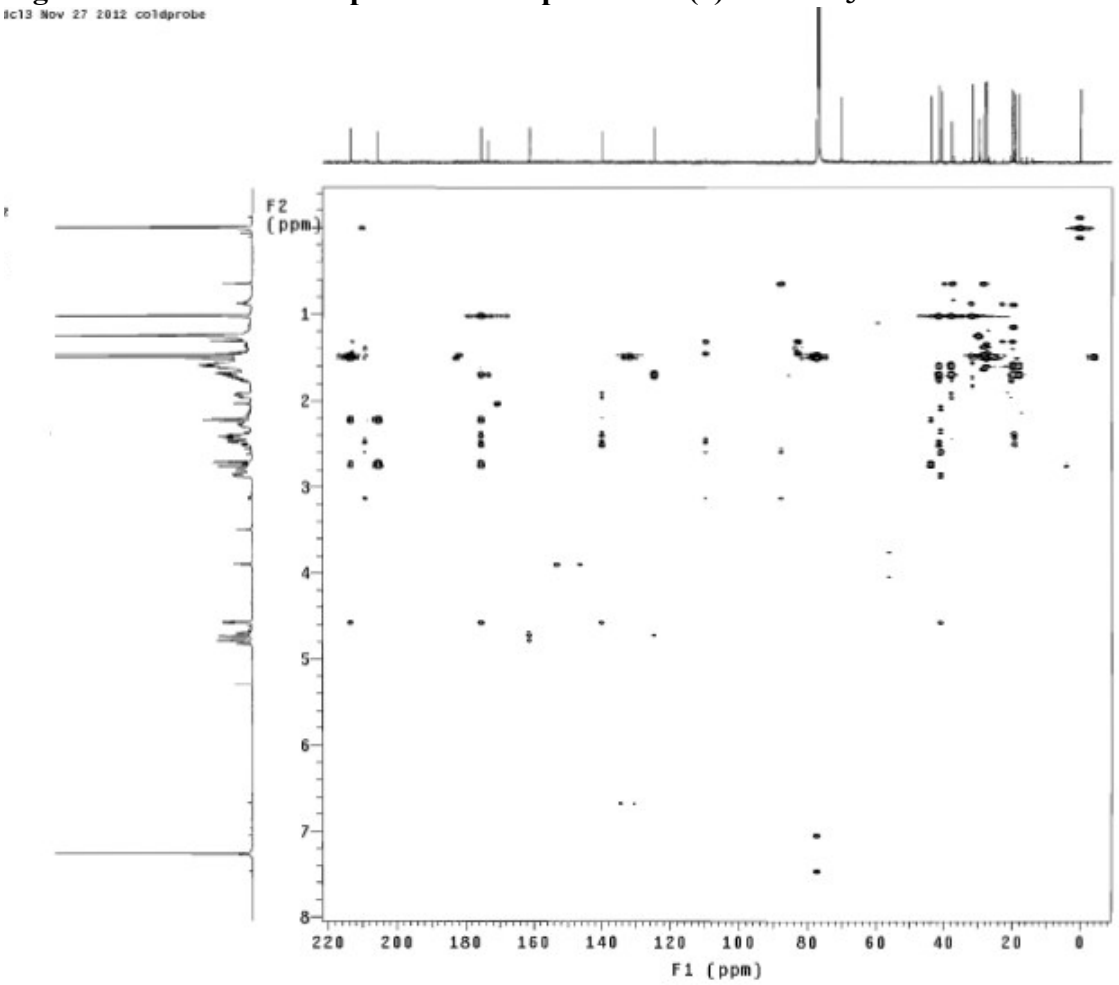


Figure S23. The ^{1}H-^{1}H COSY spectrum of tripterlide C (3) in $CDCl_3$

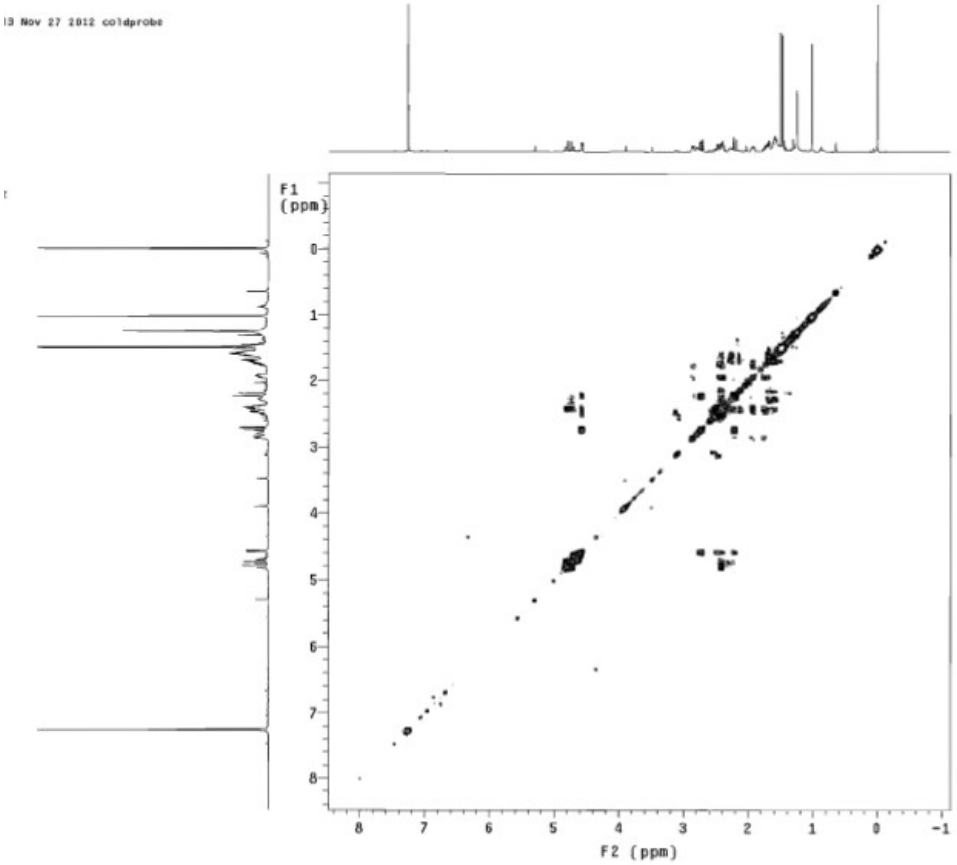


Figure S24. The NOESY spectrum of tripterlide C (3) in $CDCl_3$

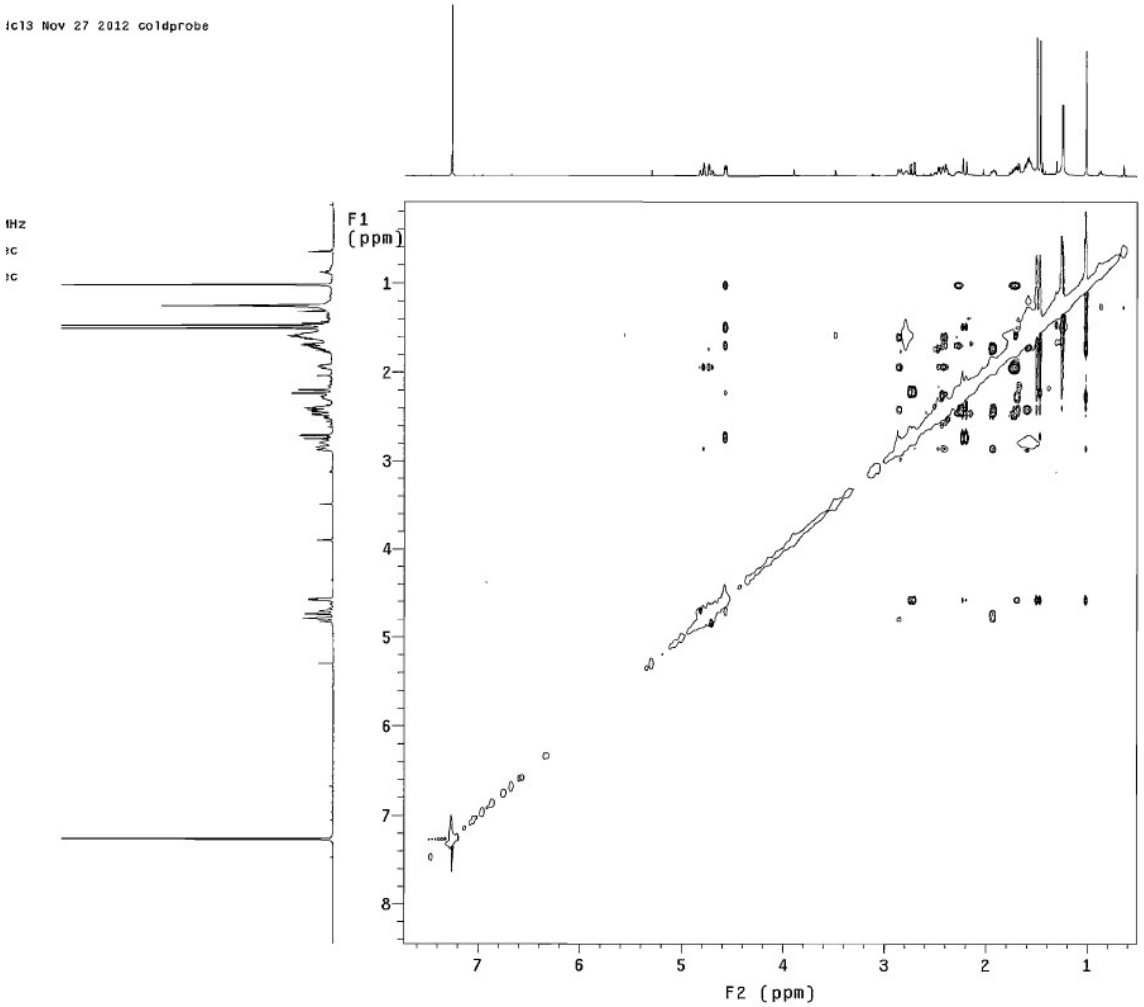


Figure S25. The IR spectrum of tripterlide C (3)

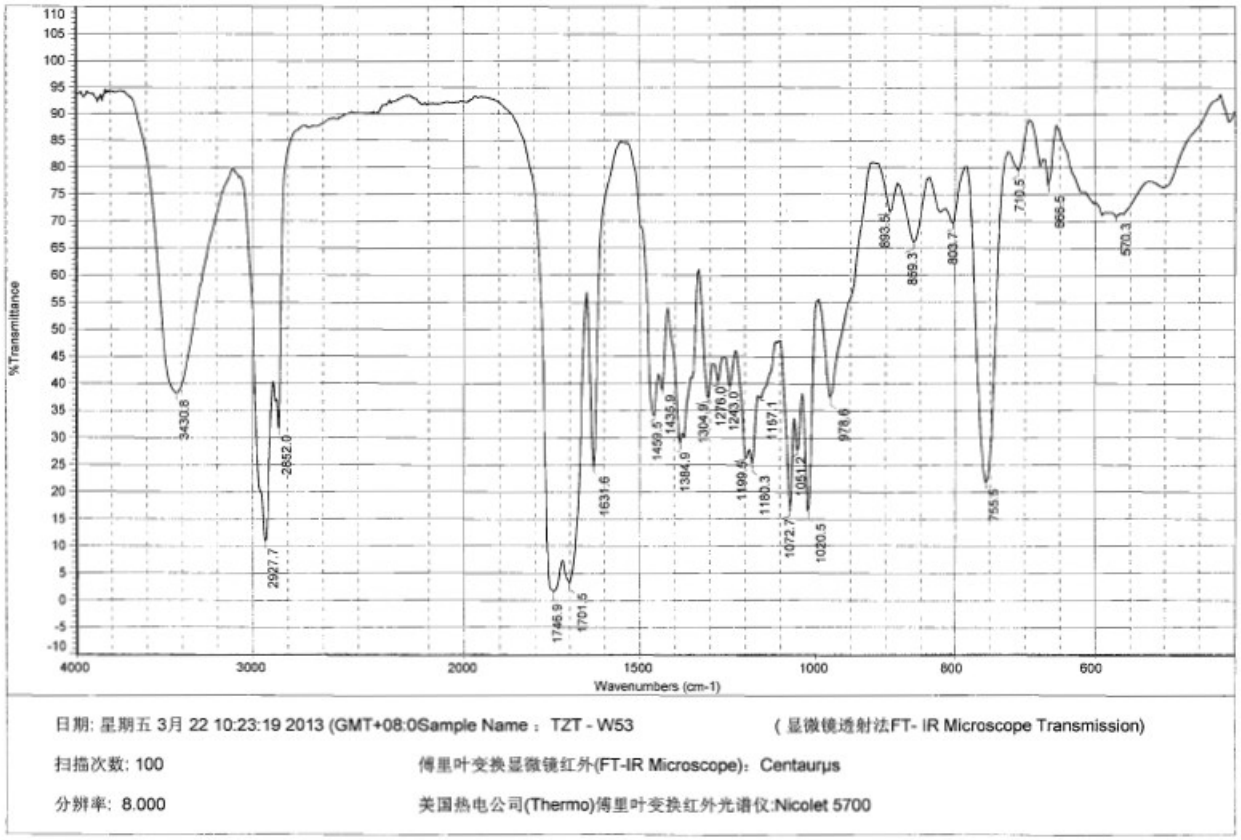
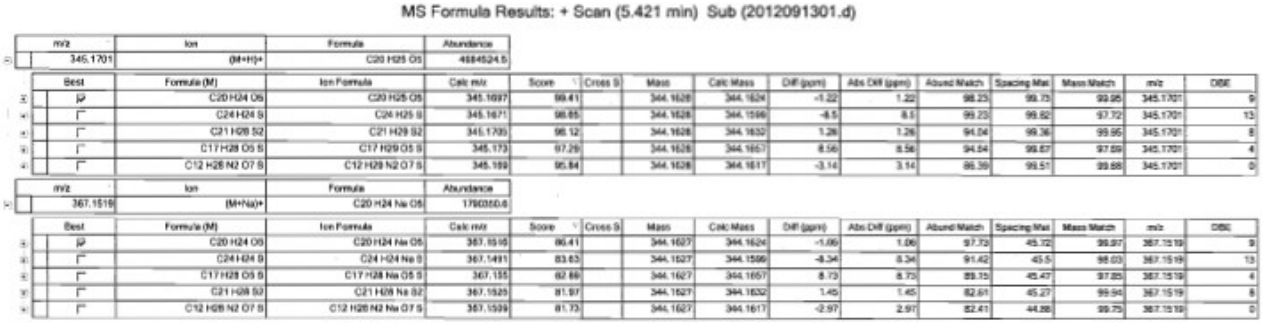


Figure S26. The HRESIMS of tripterlide C (3)



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

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1	345.1701	(M+H)+	C20 H25 O5	4884524.5

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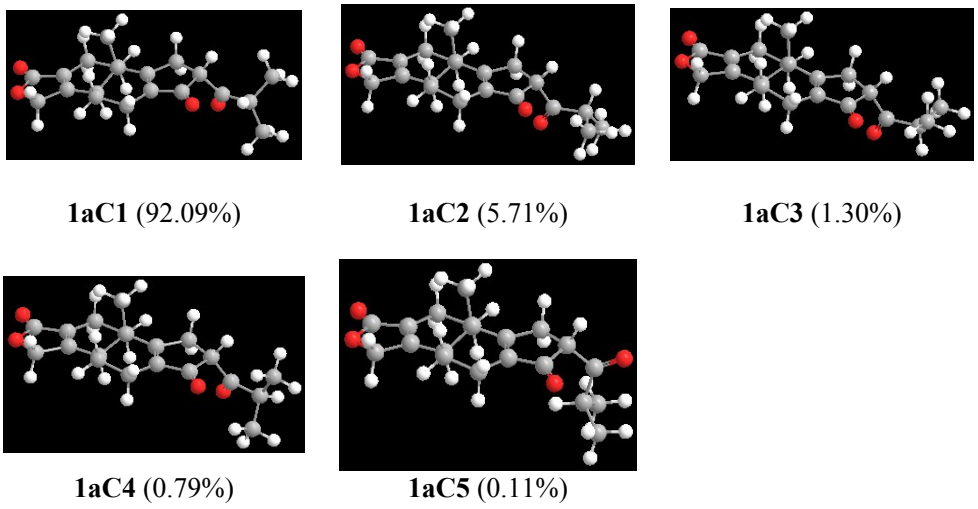
2	✓	C20 H24 O5	C20 H25 O5	345.1697	99.41		344.1628	344.1624	-1.22	1.22	98.23	99.73	99.95	345.1701	9
3		C24 H24 S	C24 H25 S	345.1671	98.65		344.1628	344.1599	-8.5	8.5	99.23	99.82	97.72	345.1701	13
4		C21 H28 S2	C21 H29 S2	345.1709	98.12		344.1628	344.1632	1.26	1.26	94.04	99.36	99.95	345.1701	8
5		C17 H28 O5 S	C17 H29 O5 S	345.173	97.29		344.1628	344.1657	8.56	8.56	94.64	99.67	97.59	345.1701	4
6		C12 H26 N2 O7 S	C12 H29 N2 O7 S	345.169	95.84		344.1628	344.1617	-3.14	3.14	86.39	99.51	99.66	345.1701	0

	m/z	Ion	Formula	Abundance
1	367.1519	(M+Na)+	C20 H24 Na O5	1790350.6

	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
2	✓	C20 H24 O5	C20 H24 Na O5	367.1516	99.41		344.1627	344.1624	-1.09	1.09	97.73	45.72	99.97	367.1519	9
3		C24 H24 S	C24 H24 Na S	367.1491	83.63		344.1627	344.1599	-8.34	8.34	91.42	45.5	98.03	367.1519	13
4		C17 H28 O5 S	C17 H28 Na O5 S	367.155	92.88		344.1627	344.1657	8.73	8.73	89.15	45.47	97.85	367.1519	4
5		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
6		C12 H26 N2 O7 S	C12 H26 N2 Na O7 S	367.1539	91.73		344.1627	344.1617	-2.97	2.97	82.41	44.88	99.75	367.1519	0

Figure 27. Optimized conformations of 1



1aC1 (92.09%) **1aC2** (5.71%) **1aC3** (1.30%)

1aC4 (0.79%) **1aC5** (0.11%)

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

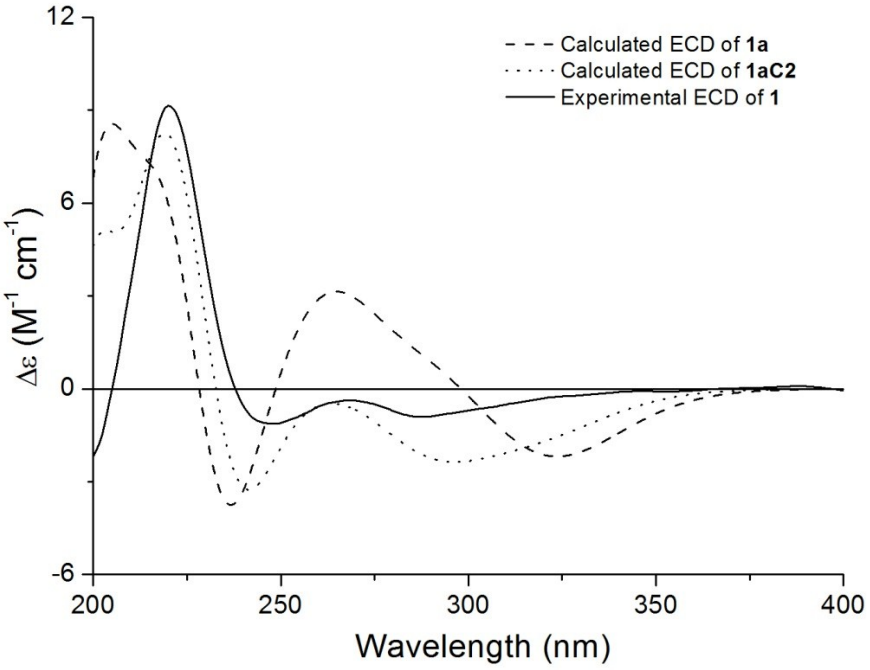


Figure 29. Optimized conformations of 2

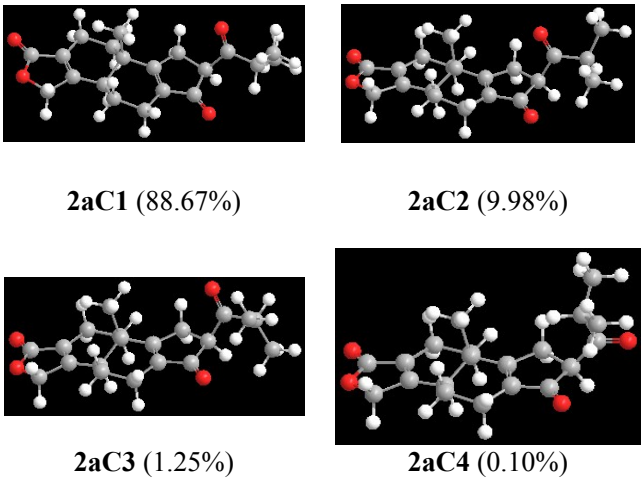


Figure S30. Calculated ECD spectra of 5*R*, 20*S*, 12*R* (2a, 2aC2) and experimental ECD spetrum of 2, and 3

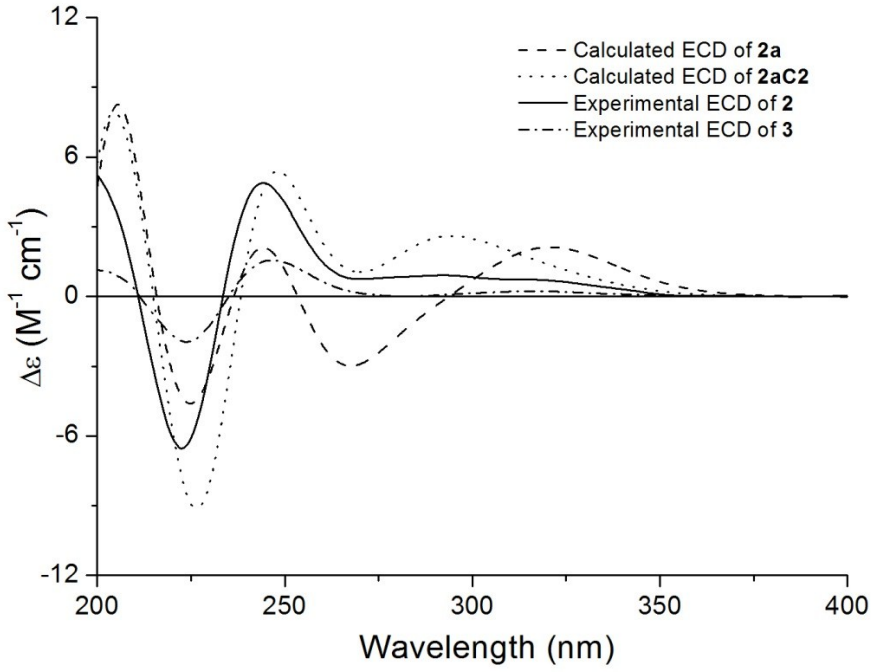


Figure S31. The ^{1}H NMR (600 MHz)spectrum of tripterlide D (4) in $CDCl_3$

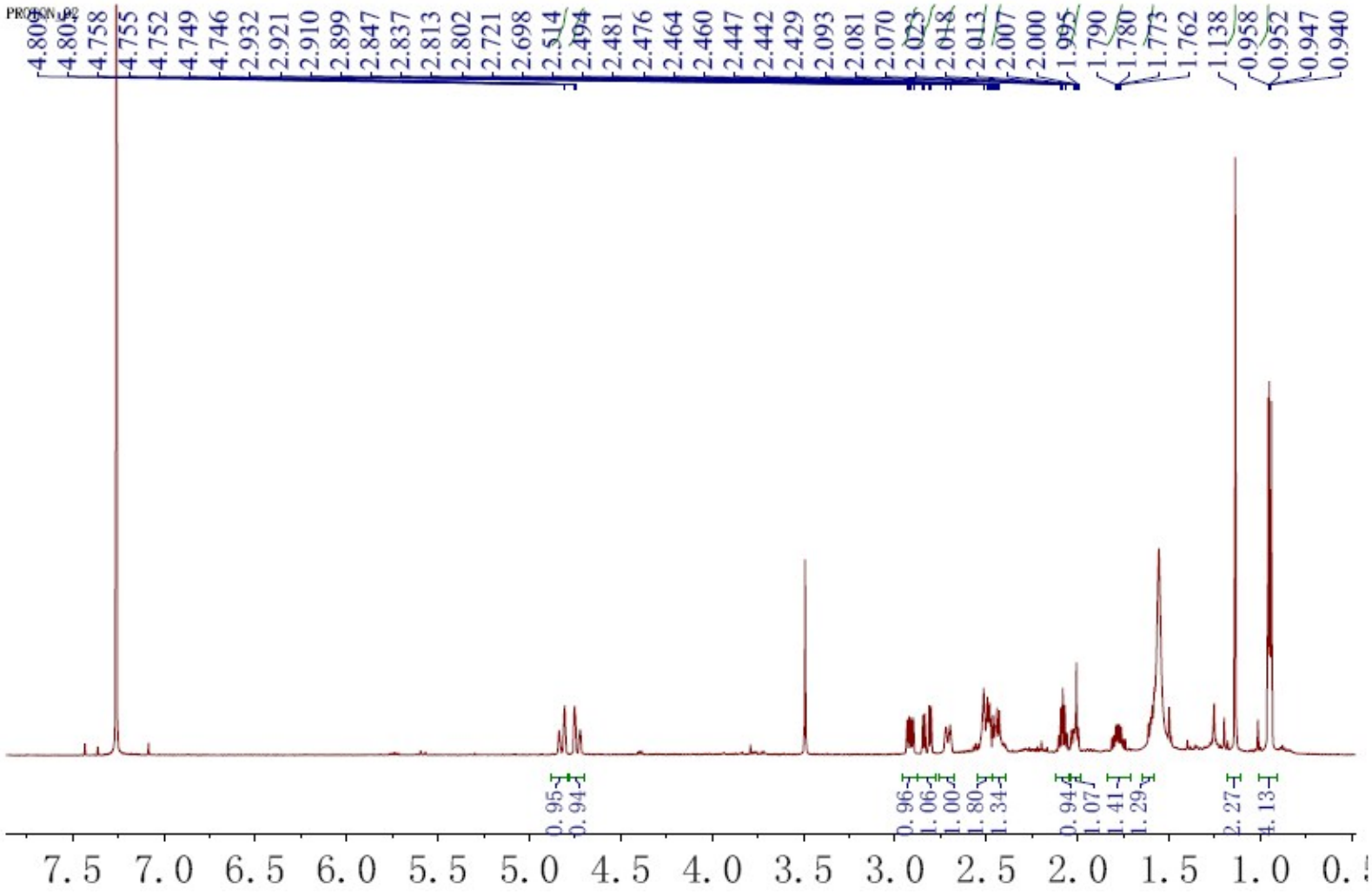


Figure S32. The ^{13}C NMR (150 MHz) spectrum of tripterlide D (4) in $CDCl_3$

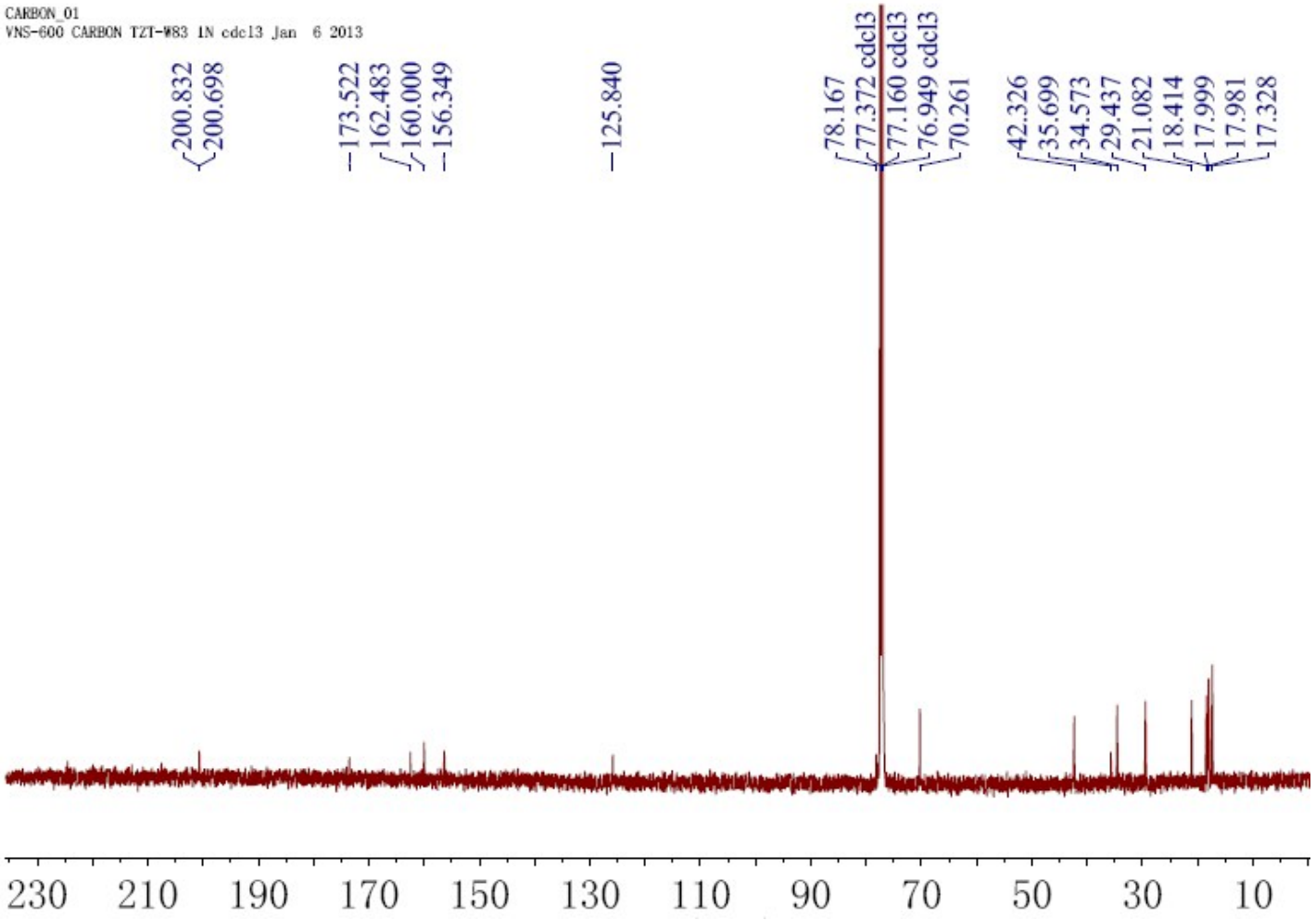


Figure S33. The HSQC spectrum of tripterlide D (4) in $CDCl_3$

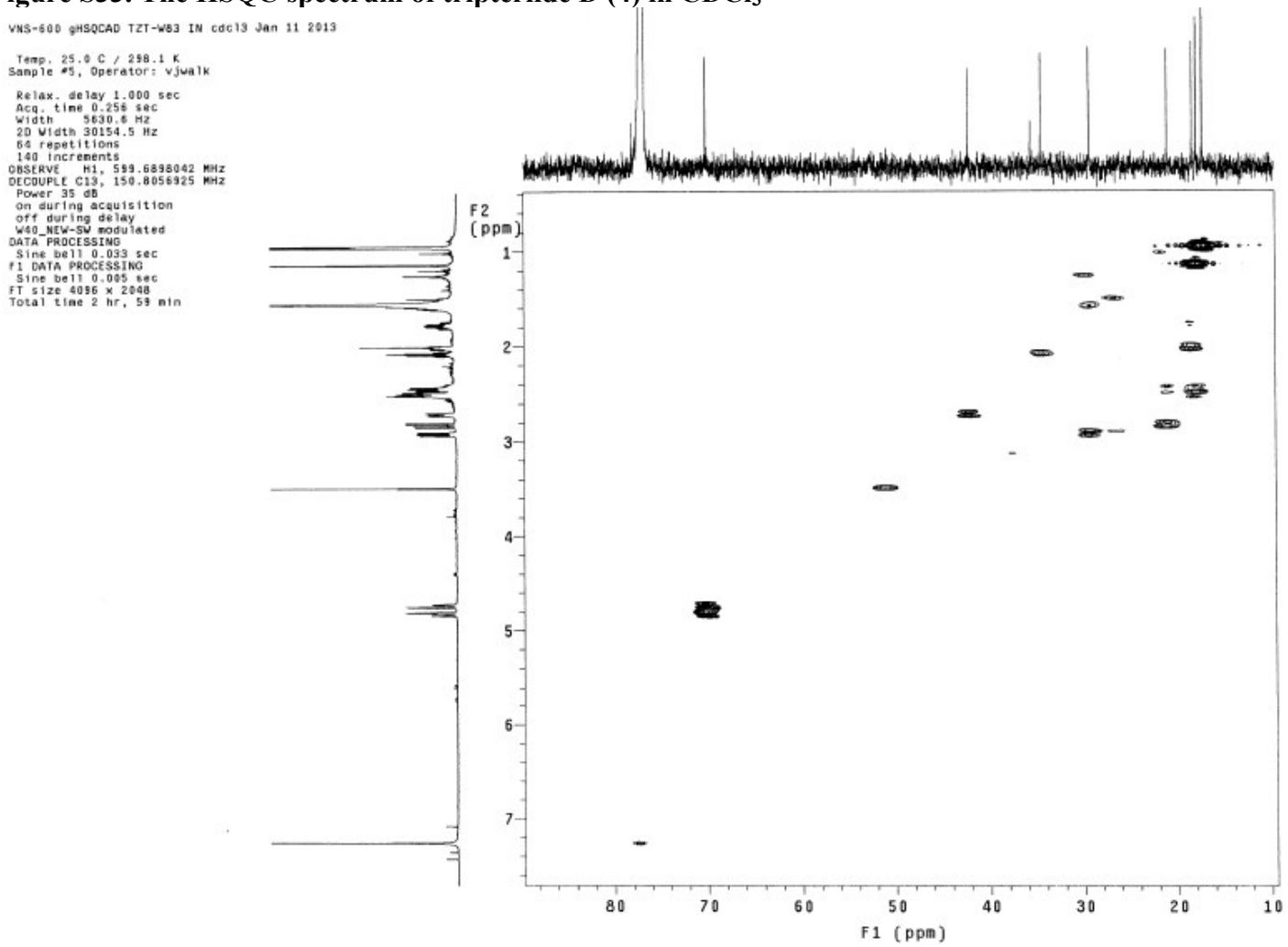


Figure S34. The HMBC spectrum of tripterlide D (4) in $CDCl_3$

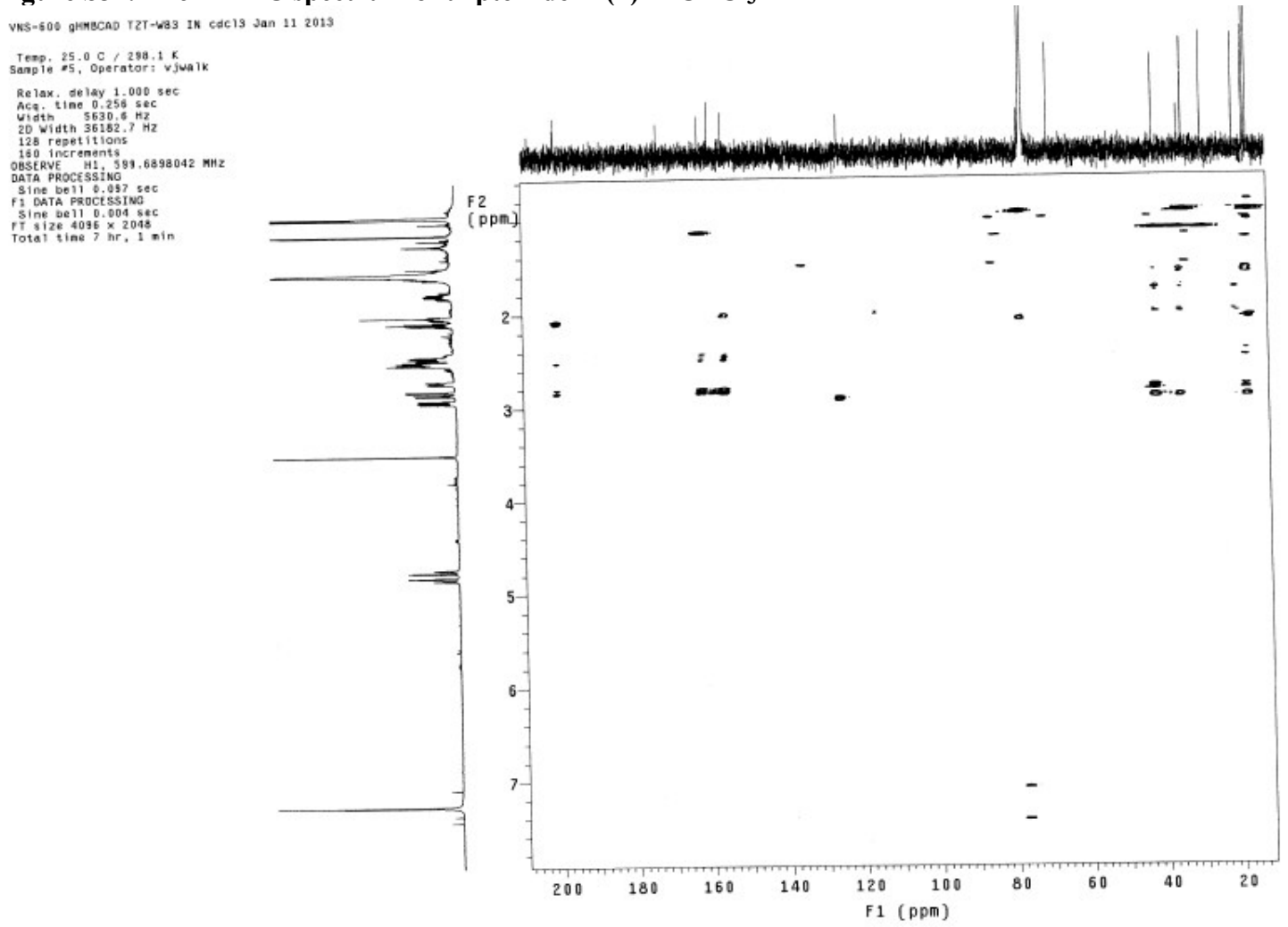


Figure S35. The ^{1}H-^{1}H COSY spectrum of tripterlide D (4) in $CDCl_3$

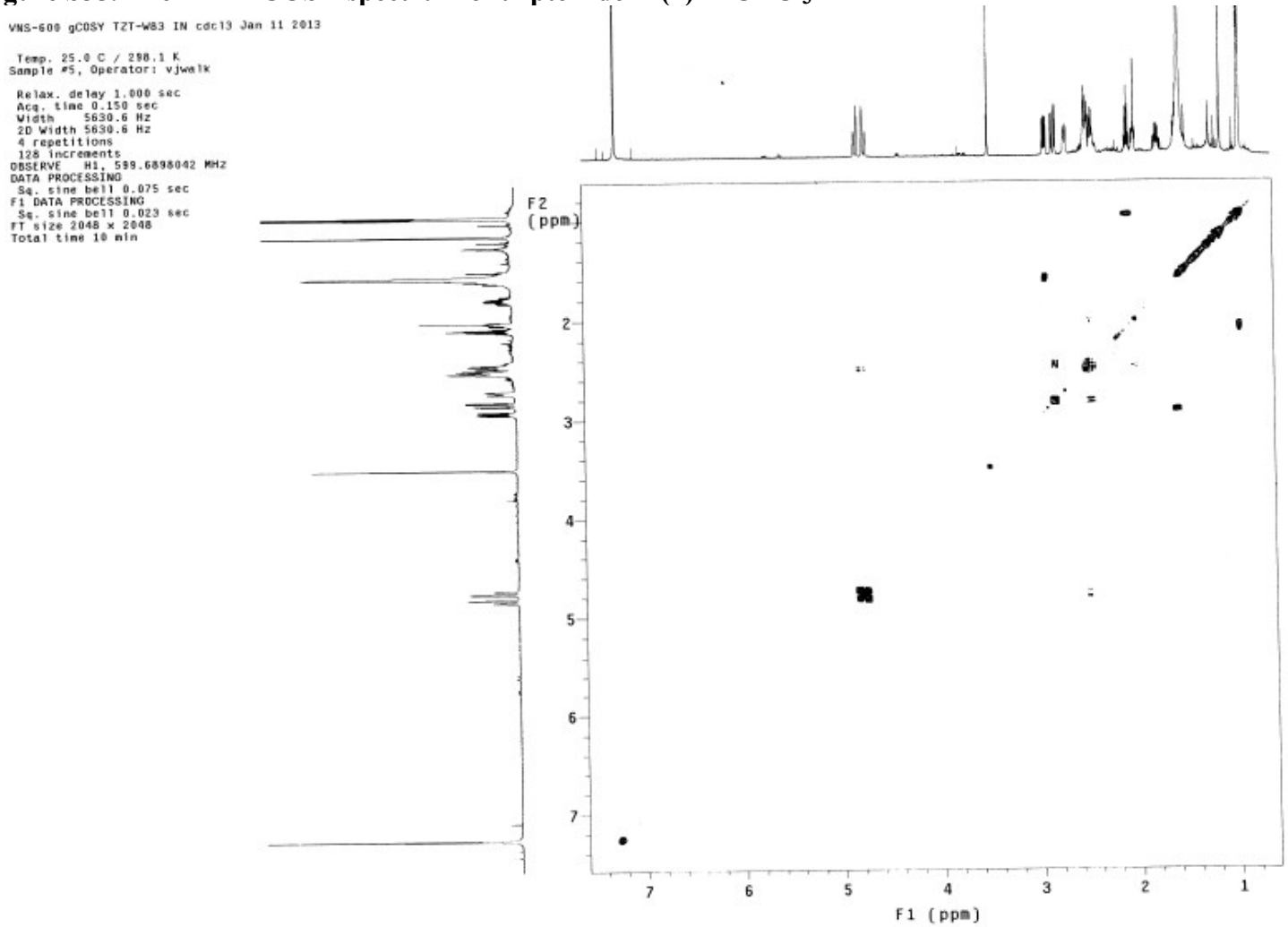


Figure S36. The NOESY spectrum of tripterldie D (4) in $CDCl_3$

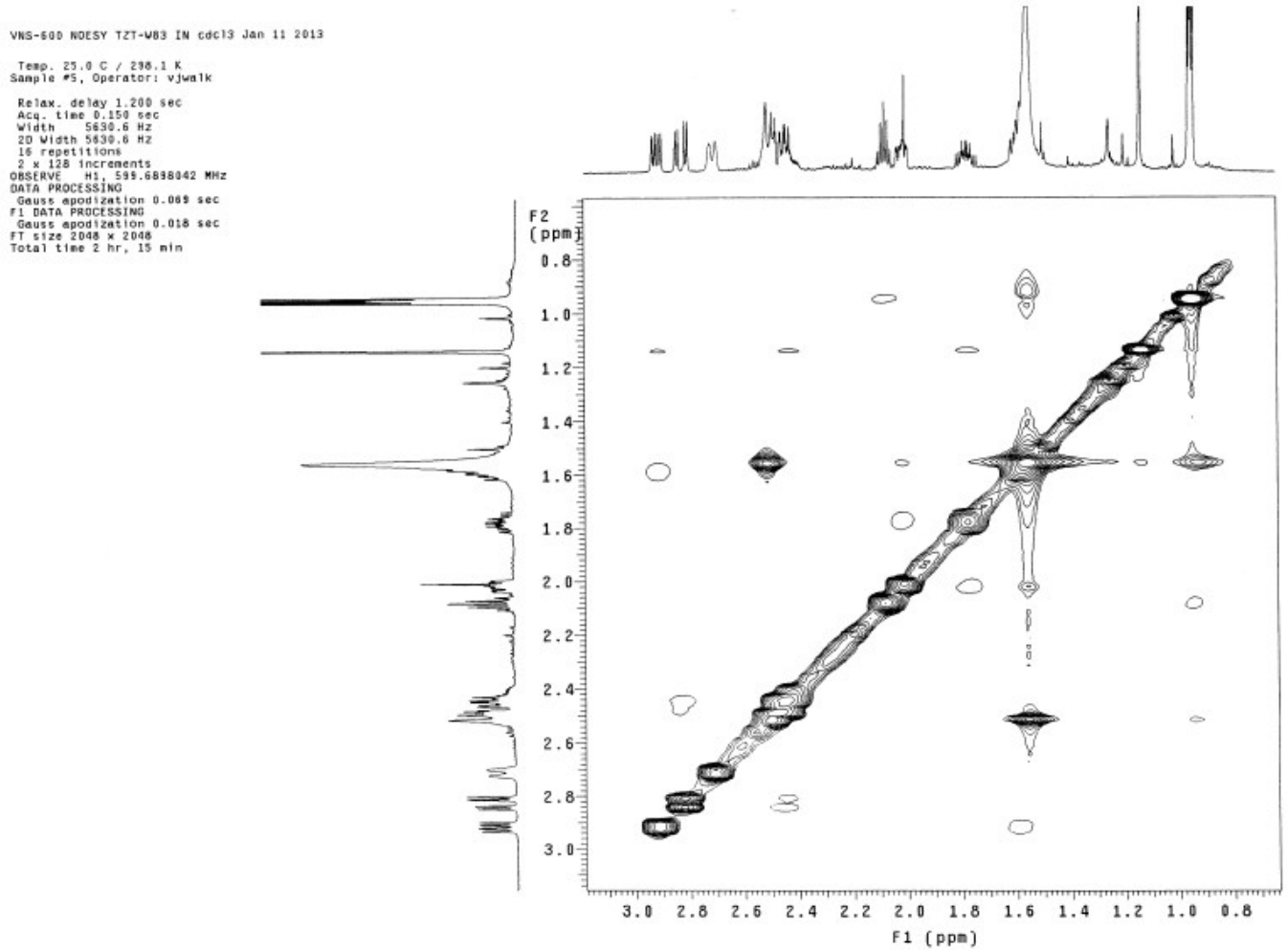


Figure S37. The HRESIMS spectrum of tripterlide D (4)

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

	m/z	Ion	Formula	Abundance
-	331.1543	(M+H)+	C19 H23 O5	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
+	☑	C19 H22 O5	C19 H23 O5	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)+	C19 H22 Na O5	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
+	☑	C19 H22 O5	C19 H22 Na O5	353.1359	87.46		330.1478	330.1467	-3.22	3.22	98.4	49.84	99.71	353.137	9
+	☐	C16 H26 O5 S	C16 H26 Na O5 S	353.1393	84.98		330.1478	330.1501	6.98	6.98	91.57	49.78	98.63	353.137	4
+	☐	C11 H26 N2 O7 S	C11 H26 N2 Na O7 S	353.1353	83.88		330.1478	330.1461	-5.21	5.21	86.85	49.6	99.24	353.137	0
+	☐	C20 H26 S2	C20 H26 Na S2	353.1368	83.18		330.1478	330.1476	-0.6	0.6	83.04	49.73	99.99	353.137	8

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

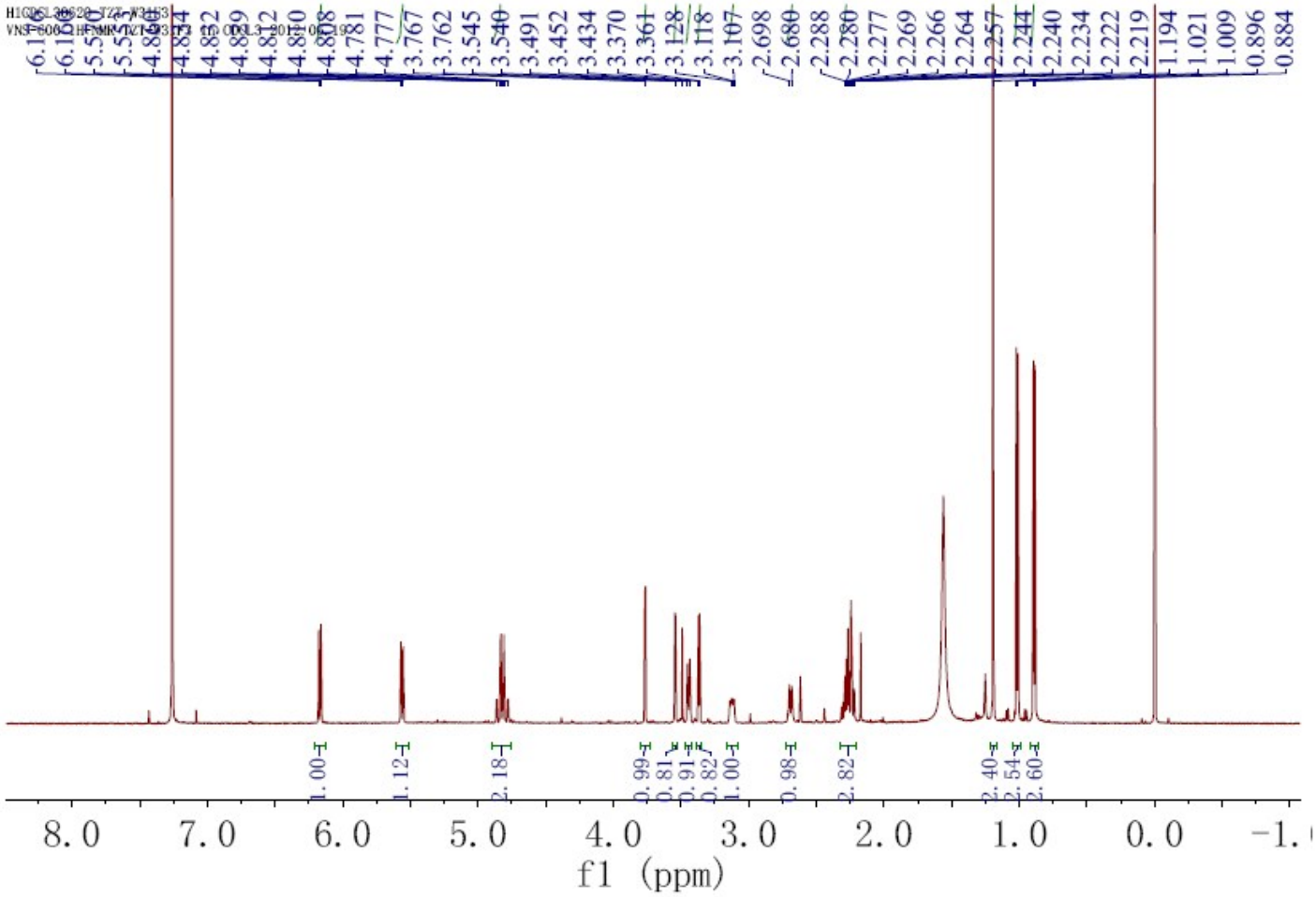


Figure S39. The ^{13}C NMR (150 MHz) spectrum of tripterlide E (5) in $CDCl_3$

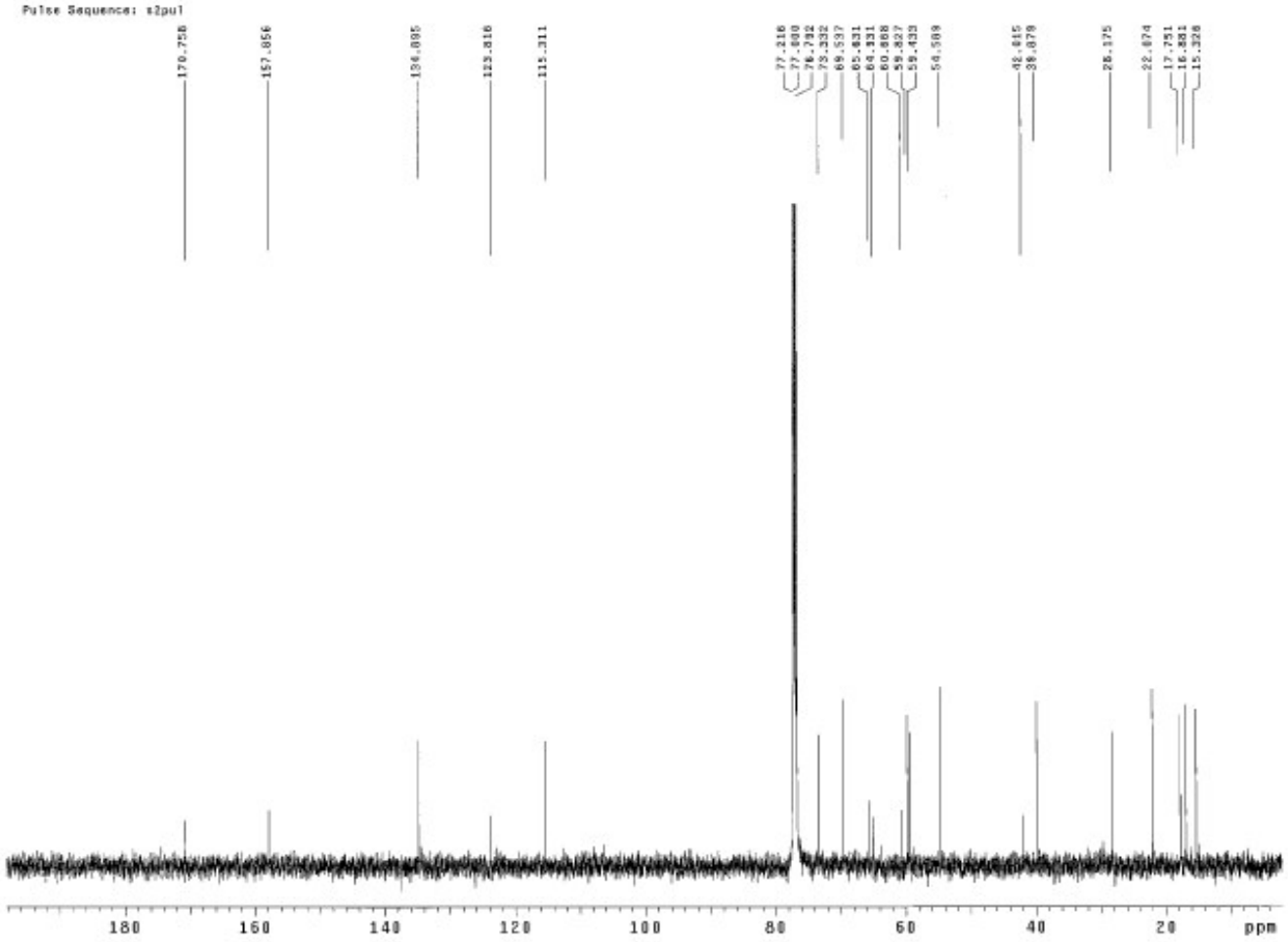


Figure S40. The HSQC spectrum of tripterlide E (5) in $CDCl_3$

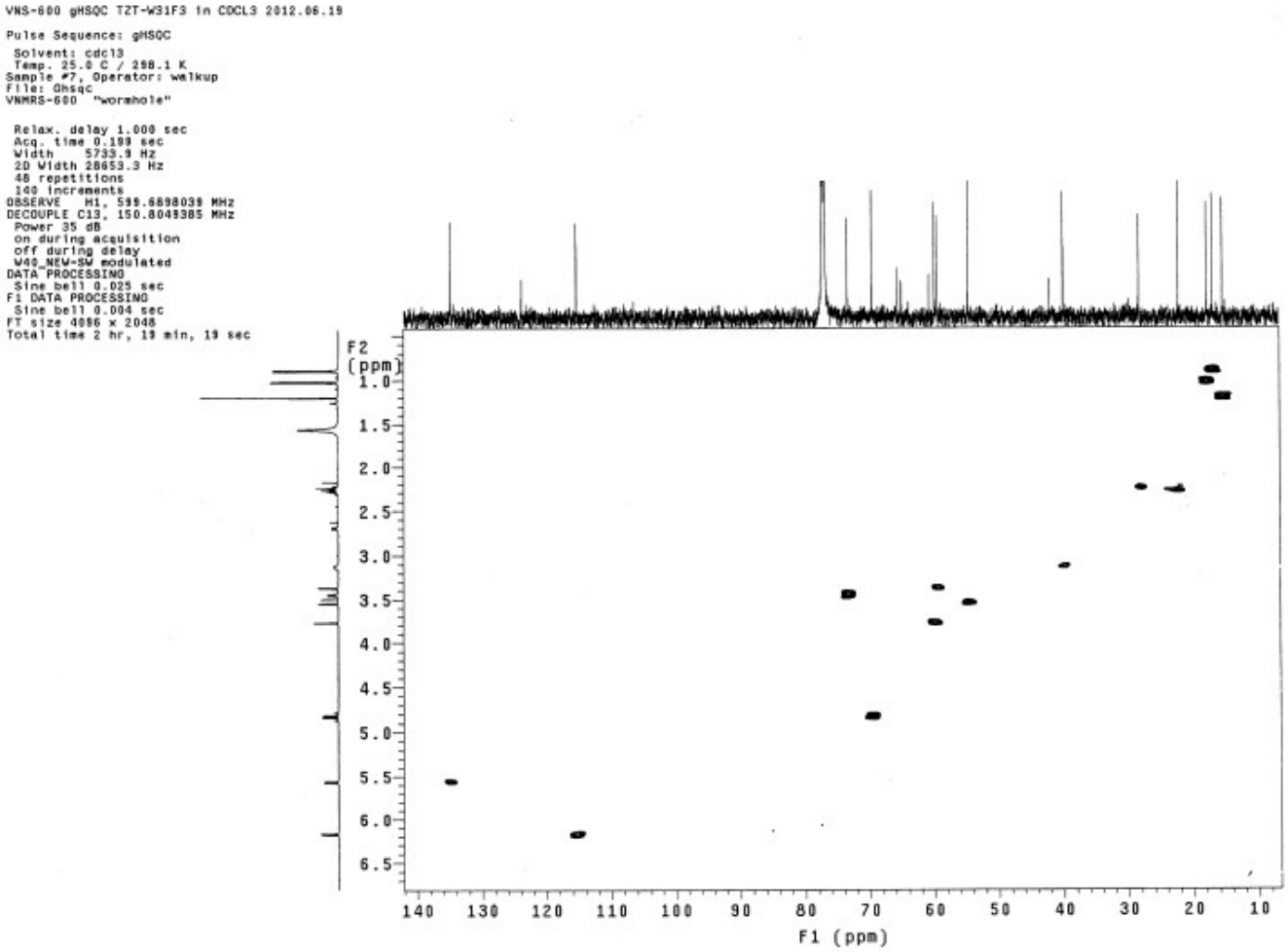


Figure S41. The HMBC spectrum of tripterlide E (5) in $CDCl_3$

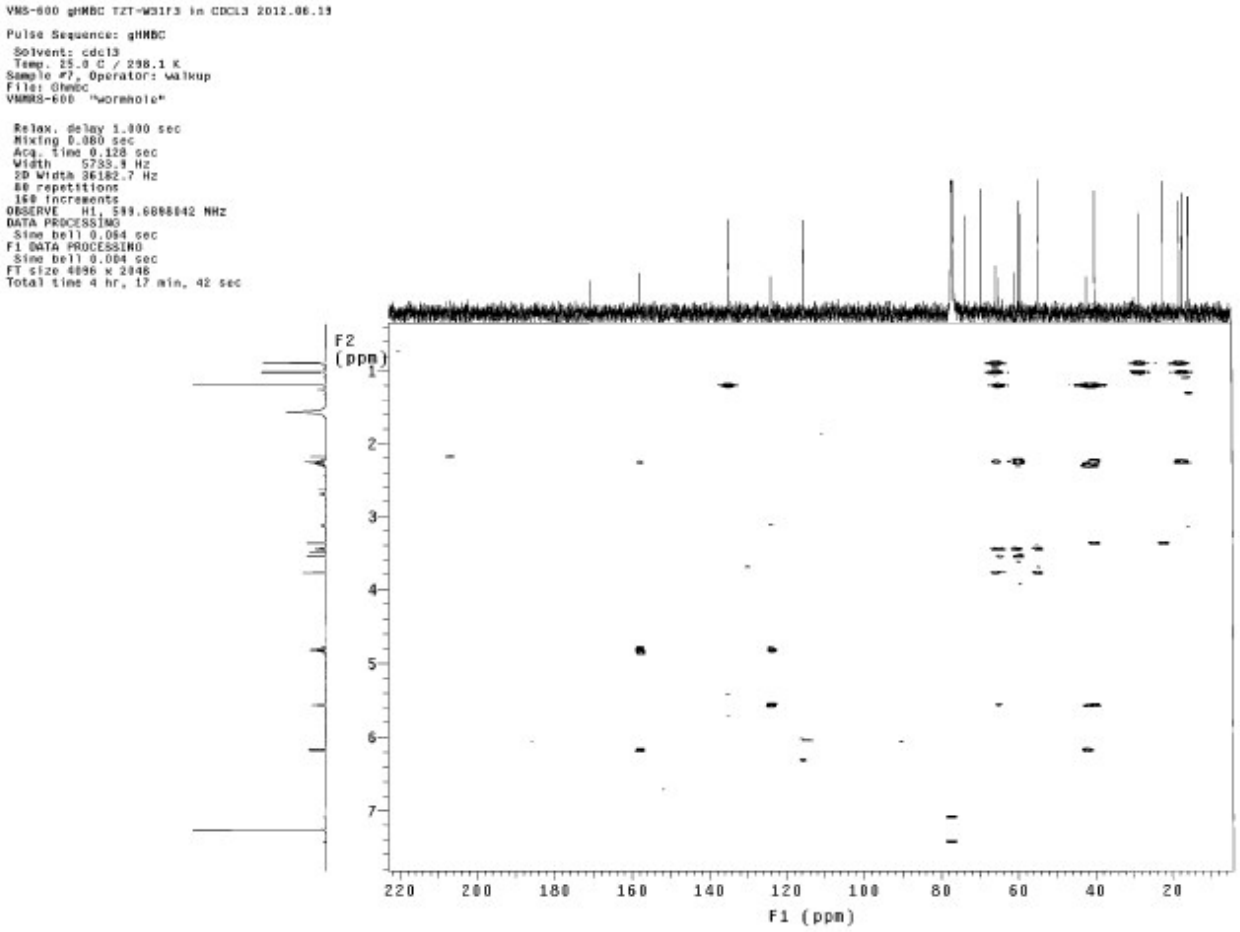


Figure S42. The ^{1}H-^{1}H COSY spectrum of tripterlide E (5) in $CDCl_3$

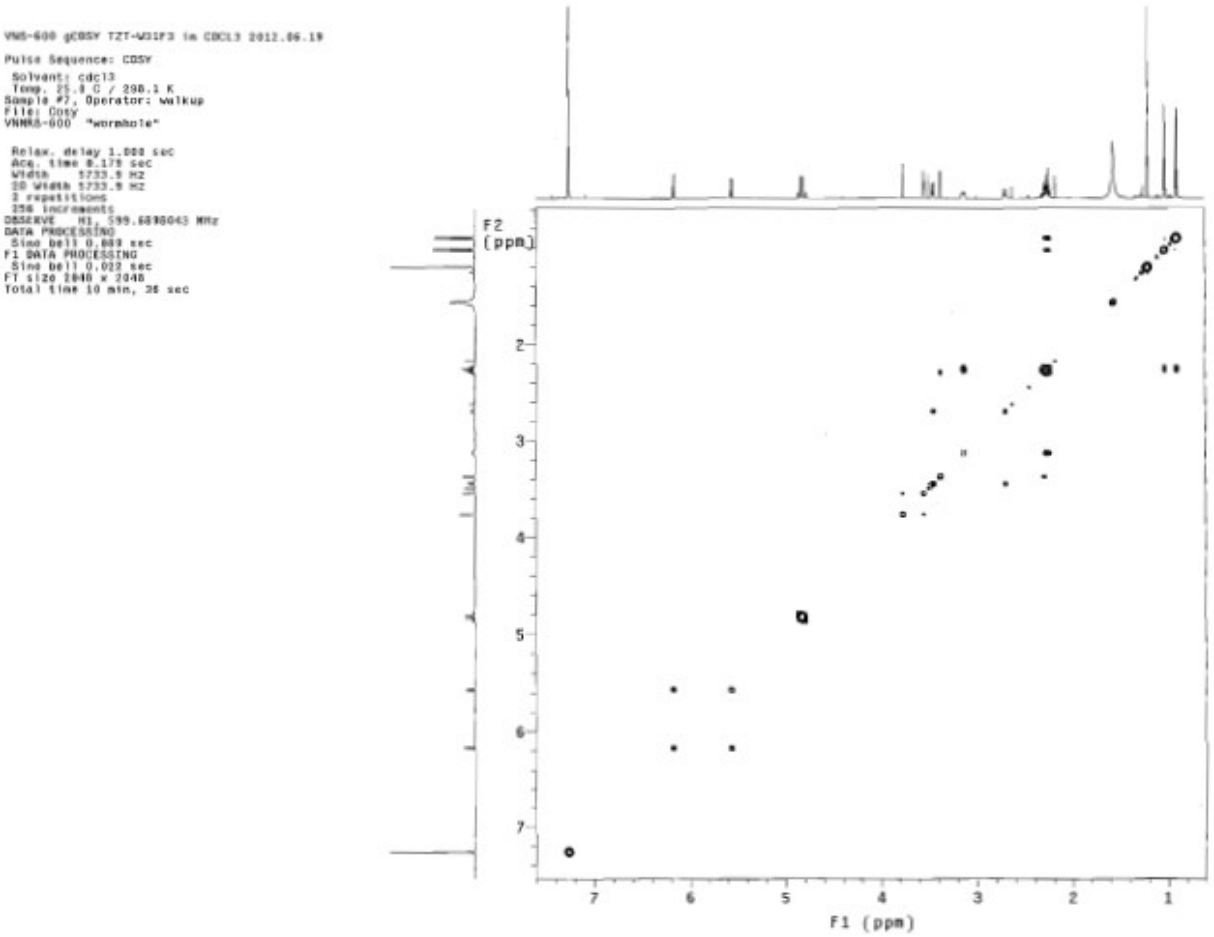


Figure S43. The NOESY spectrum of tripterlide E (5) in $CDCl_3$

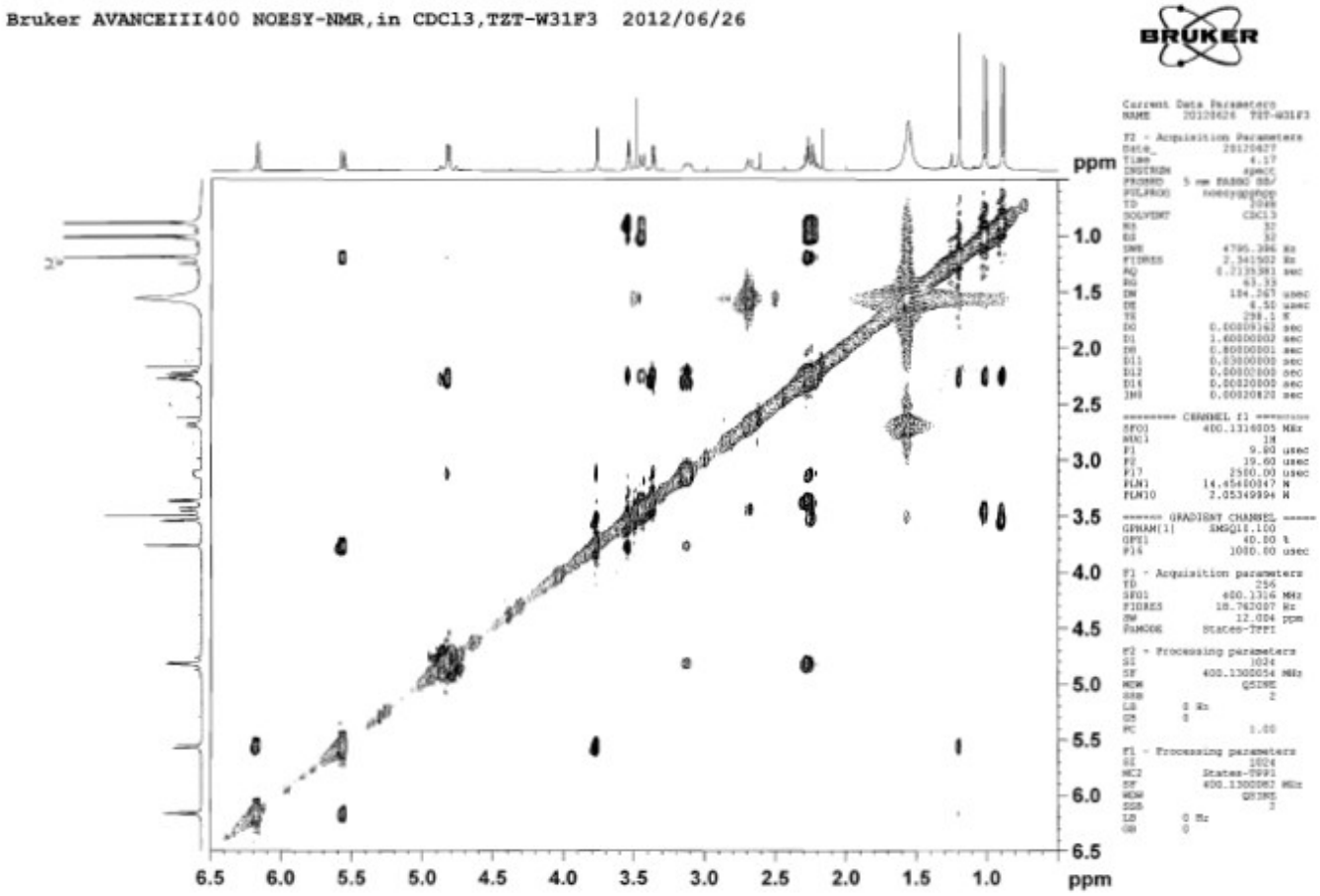


Figure S44. The IR spectrum of tripterlide E (5) in $CDCl_3$

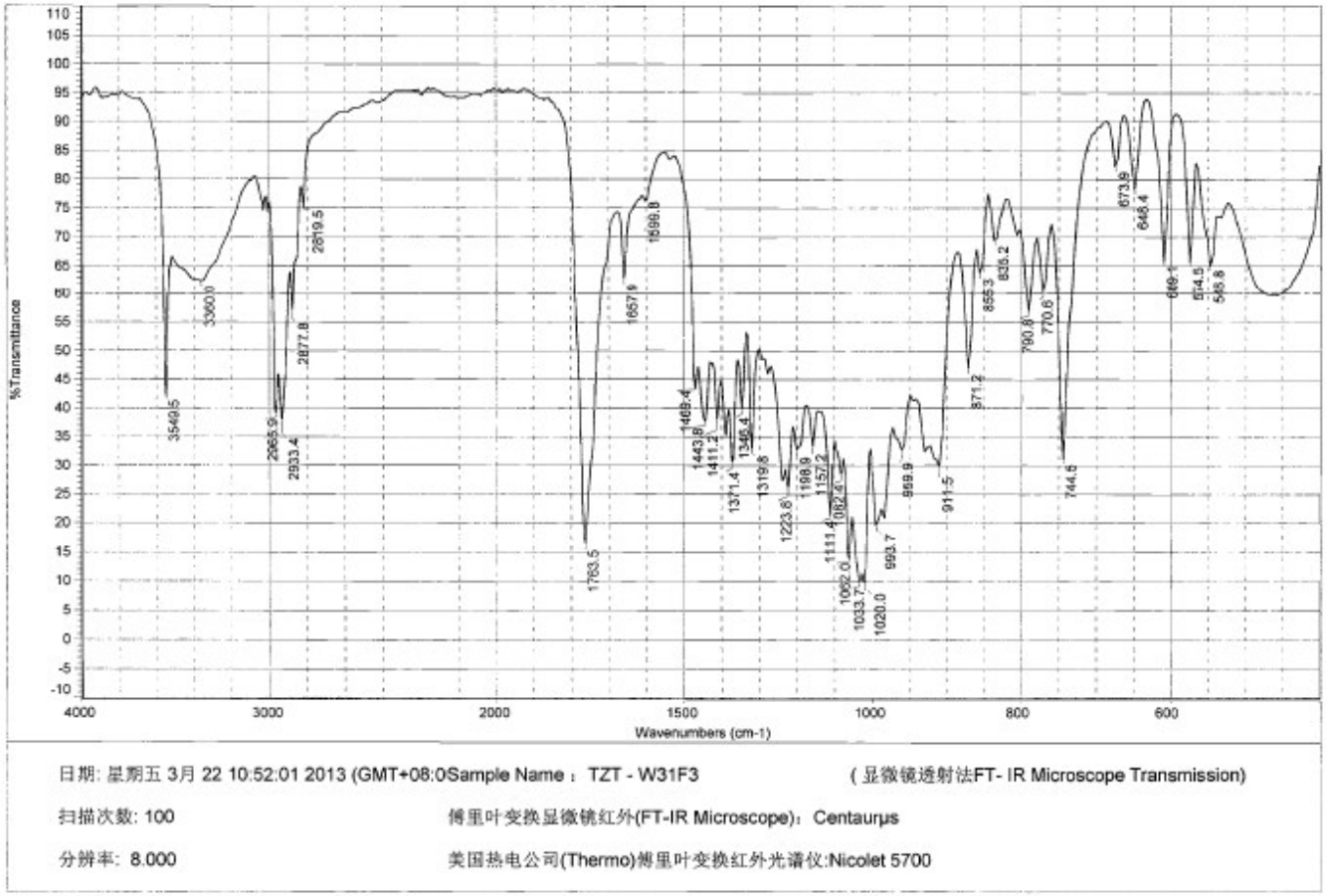
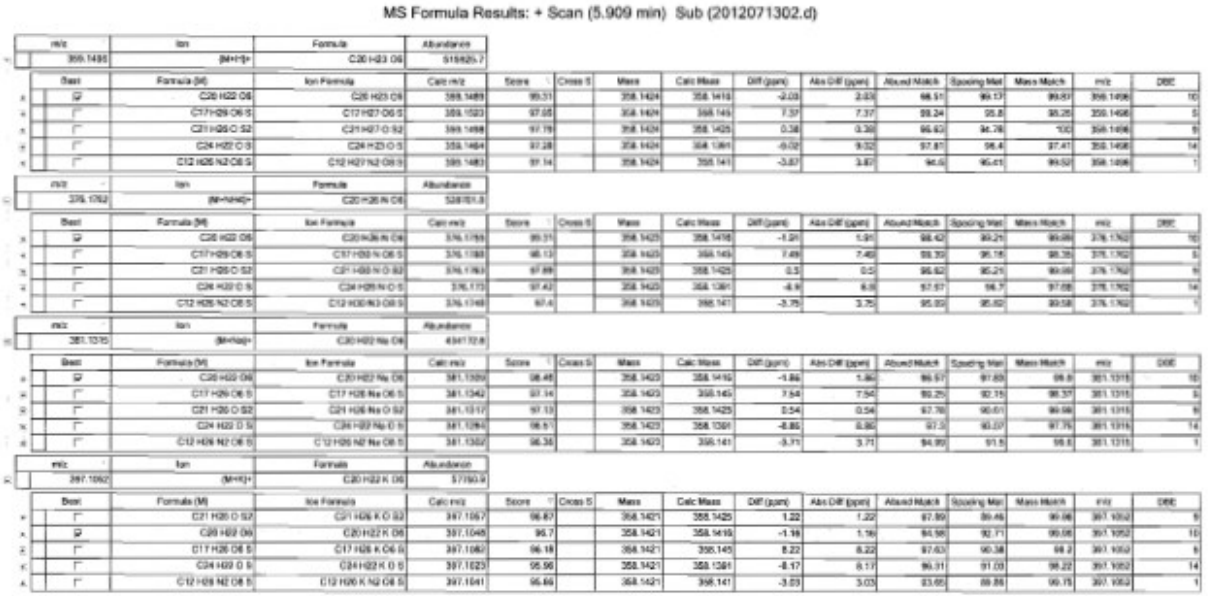


Figure S45. The HRESIMS spectrum of tripterlide E (5) in $CDCl_3$



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

	m/z	Ion	Formula	Abundance
1	359.1496	[M+H]+	C20 H23 O6	515926.7

	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	☑	C20 H22 O6	C20 H23 O6	359.1489	99.31		358.1424	358.1416	-2.03	2.03	98.51	99.17	99.83	359.1496	10
2	☐	C17 H26 O6 S	C17 H27 O6 S	359.1523	97.05		358.1424	358.145	7.37	7.37	93.24	95.8	96.25	359.1496	5
3	☐	C21 H26 O S2	C21 H27 O S2	359.1498	97.79		358.1424	358.1425	0.38	0.38	96.62	94.28	100	359.1496	9
4	☐	C24 H22 O 5	C24 H23 O 5	359.1464	97.28		358.1424	358.1361	-9.02	9.02	97.87	98.4	97.47	359.1496	14
5	☐	C12 H26 N2 O6 S	C12 H27 N2 O6 S	359.1483	97.14		358.1424	358.141	-3.87	3.87	94.6	95.41	99.52	359.1496	1

	m/z	Ion	Formula	Abundance
2	376.1762	[M+NH4]+	C20 H26 N O6	528781.8

	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	☑	C20 H22 O6	C20 H26 N O6	376.1759	99.31		358.1424	358.1416	-1.91	1.91	98.42	99.21	99.68	376.1762	10
2	☐	C17 H29 O6 S	C17 H30 N O6 S	376.1788	98.13		358.1424	358.145	7.49	7.49	93.39	96.18	98.39	376.1762	5
3	☐	C21 H26 O S2	C21 H30 N O S2	376.1763	97.89		358.1424	358.1425	0.3	0.3	96.62	95.24	99.68	376.1762	9
4	☐	C24 H22 O 5	C24 H26 N O 5	376.1713	97.42		358.1424	358.1361	-8.9	8.9	97.87	98.7	97.68	376.1762	14
5	☐	C12 H26 N2 O6 S	C12 H30 N3 O6 S	376.1748	97.4		358.1424	358.141	-3.75	3.75	95.92	95.92	99.58	376.1762	1

	m/z	Ion	Formula	Abundance
3	381.1315	[M+Na]+	C20 H22 Na O6	4341728

	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	☑	C20 H22 O6	C20 H22 Na O6	381.1309	98.48		358.1423	358.1416	-1.84	1.84	96.97	97.69	98.8	381.1315	10
2	☐	C17 H26 O6 S	C17 H26 Na O6 S	381.1342	97.14		358.1423	358.145	7.54	7.54	93.25	92.15	96.37	381.1315	5
3	☐	C21 H26 O S2	C21 H26 Na O S2	381.1317	97.13		358.1423	358.1425	0.54	0.54	97.76	90.61	99.68	381.1315	9
4	☐	C24 H22 O 5	C24 H22 Na O 5	381.1264	96.5		358.1423	358.1361	-6.86	6.86	97.3	93.07	97.75	381.1315	14
5	☐	C12 H26 N2 O6 S	C12 H26 N2 Na O6 S	381.1302	96.36		358.1423	358.141	-3.71	3.71	94.99	91.5	98.8	381.1315	1

	m/z	Ion	Formula	Abundance
4	397.1052	(M+K)+	C20 H22 K O6	57193.9

	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	☐	C21 H26 O S2	C21 H26 K O S2	397.1057	96.87		358.1421	358.1425	1.22	1.22	97.89	89.46	99.06	397.1052	9
2	☑	C20 H22 O6	C20 H22 K O6	397.1046	96.7		358.1421	358.1416	-1.18	1.18	94.58	92.71	99.06	397.1052	10
3	☐	C17 H26 O6 S	C17 H26 K O6 S	397.1082	96.18		358.1421	358.145	8.22	8.22	97.63	90.38	98.2	397.1052	5
4	☐	C24 H22 O 5	C24 H22 K O 5	397.1023	95.96		358.1421	358.1361	-8.17	8.17	96.31	91.09	98.22	397.1052	14
5	☐	C12 H26 N2 O6 S	C12 H26 K N2 O6 S	397.1041	95.86		358.1421	358.141	-3.03	3.03	83.65	89.86	99.15	397.1052	1

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

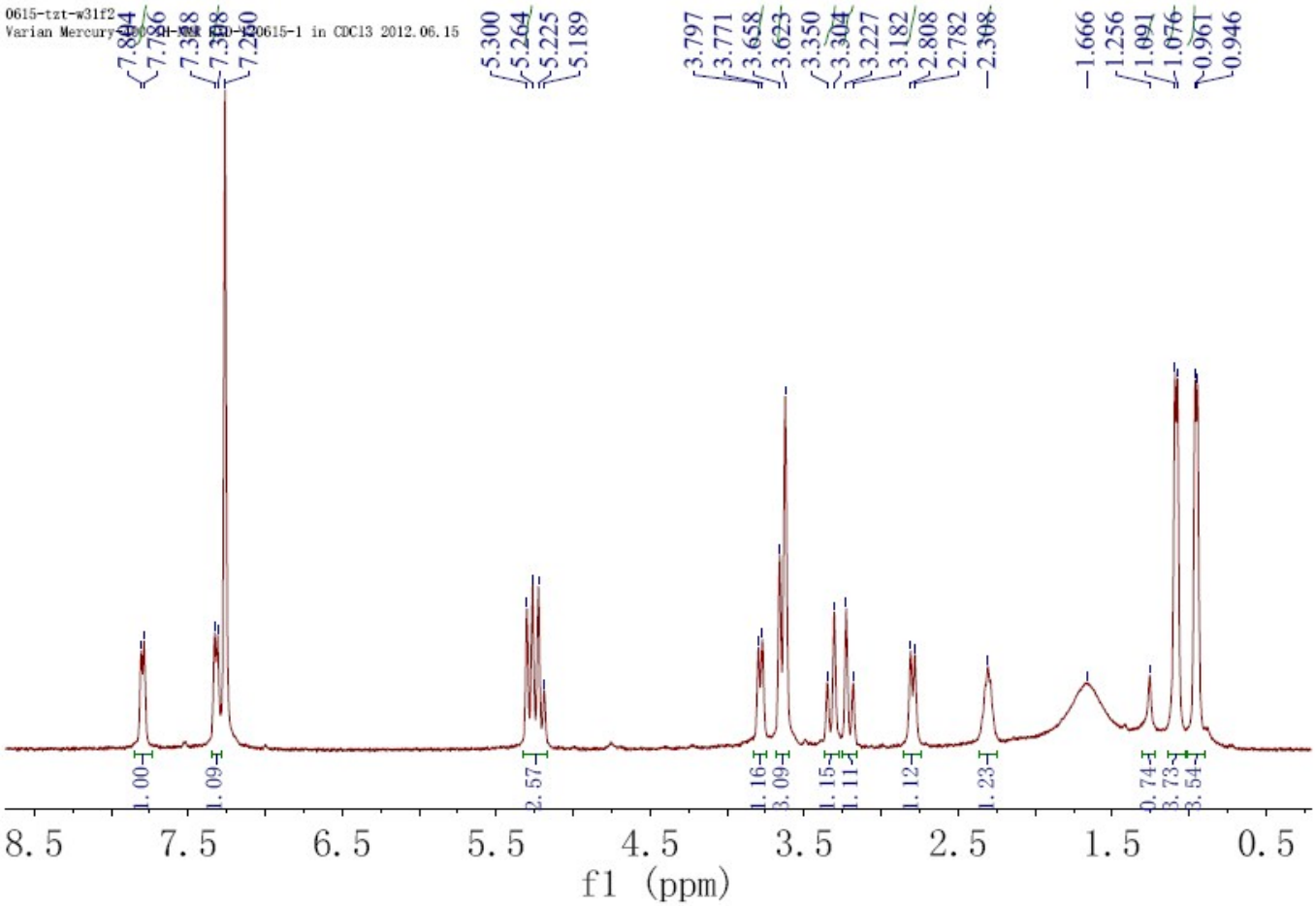

Figure S47. The ^{13}C NMR (100 MHz) spectrum of tripterlide F (6) in $CDCl_3$

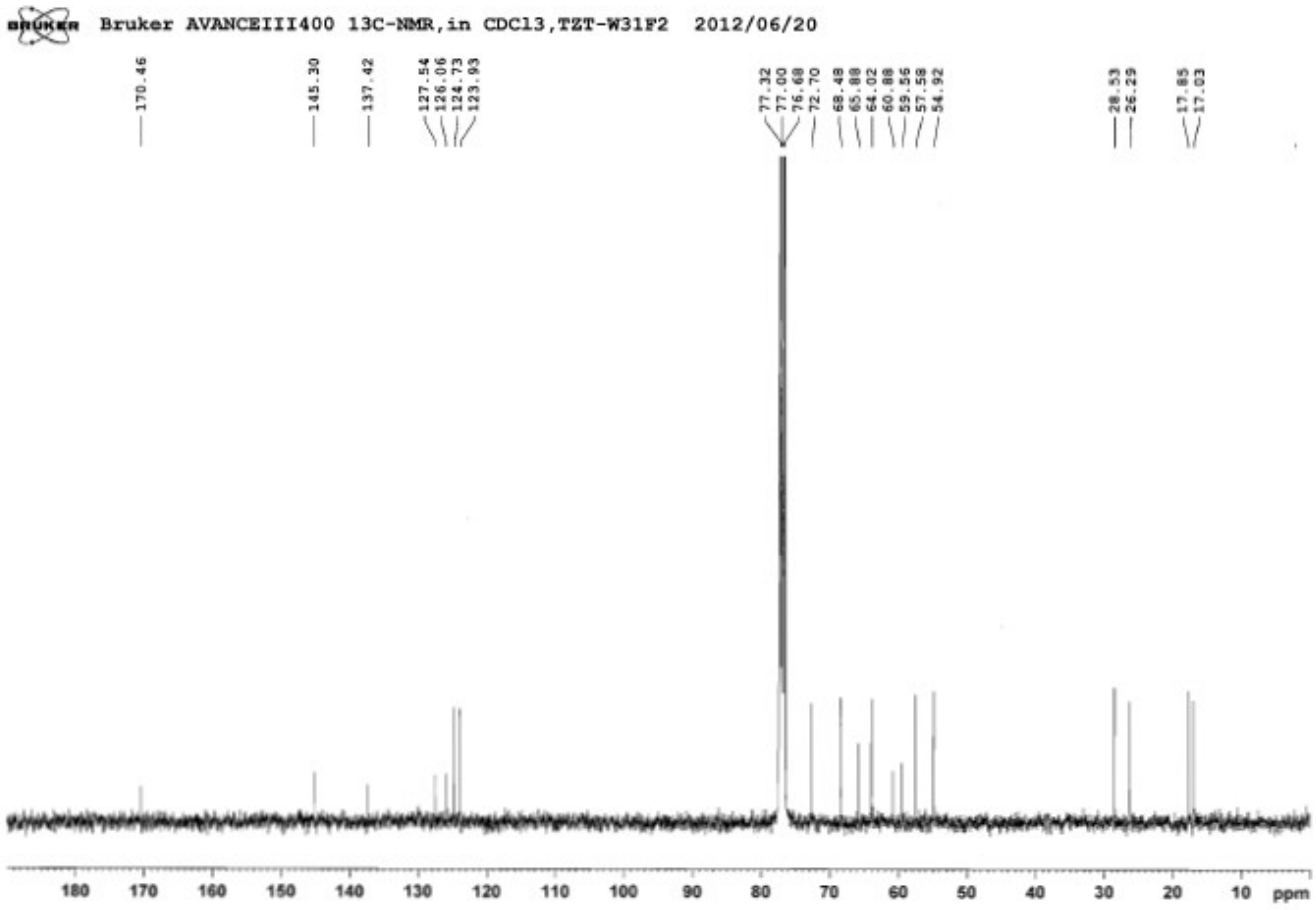

Figure S48. The HSQC spectrum of tripterlide F (6) in $CDCl_3$

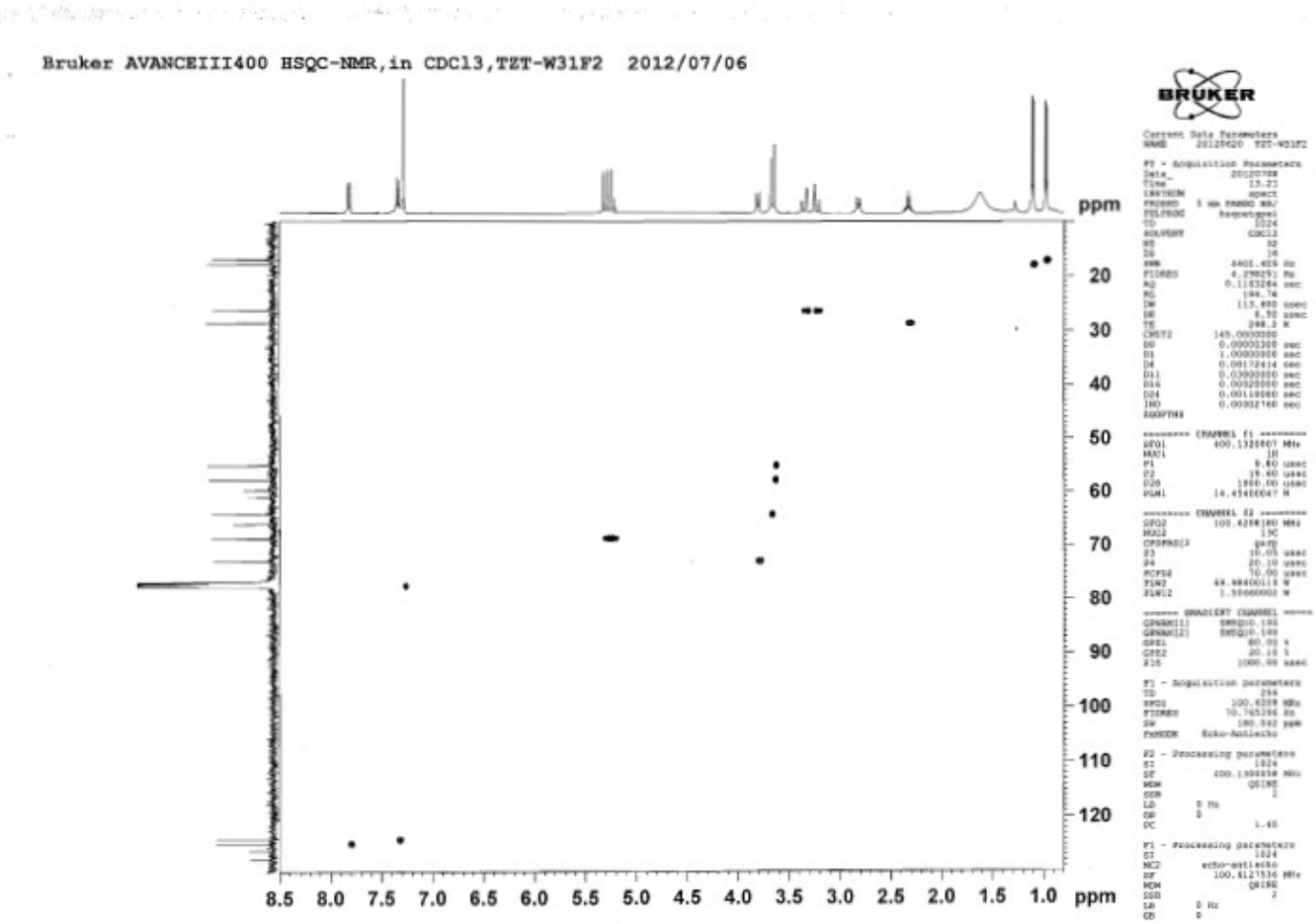

Figure S49. The HMBC spectrum of tripterlide F (6) in $CDCl_3$

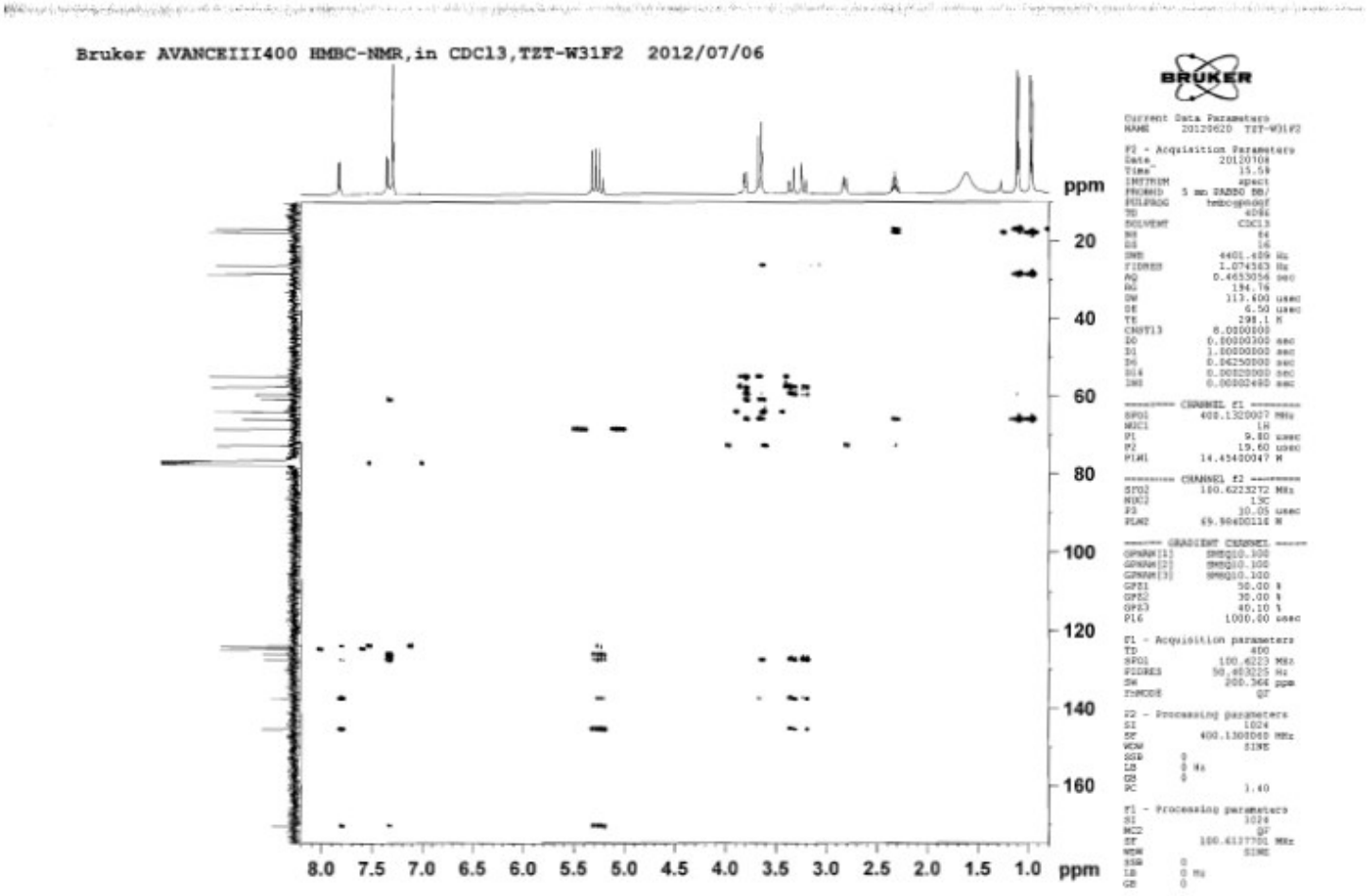

Figure S50. The ^{1}H-^{1}H COSY spectrum of tripterlide F (6) in $CDCl_3$

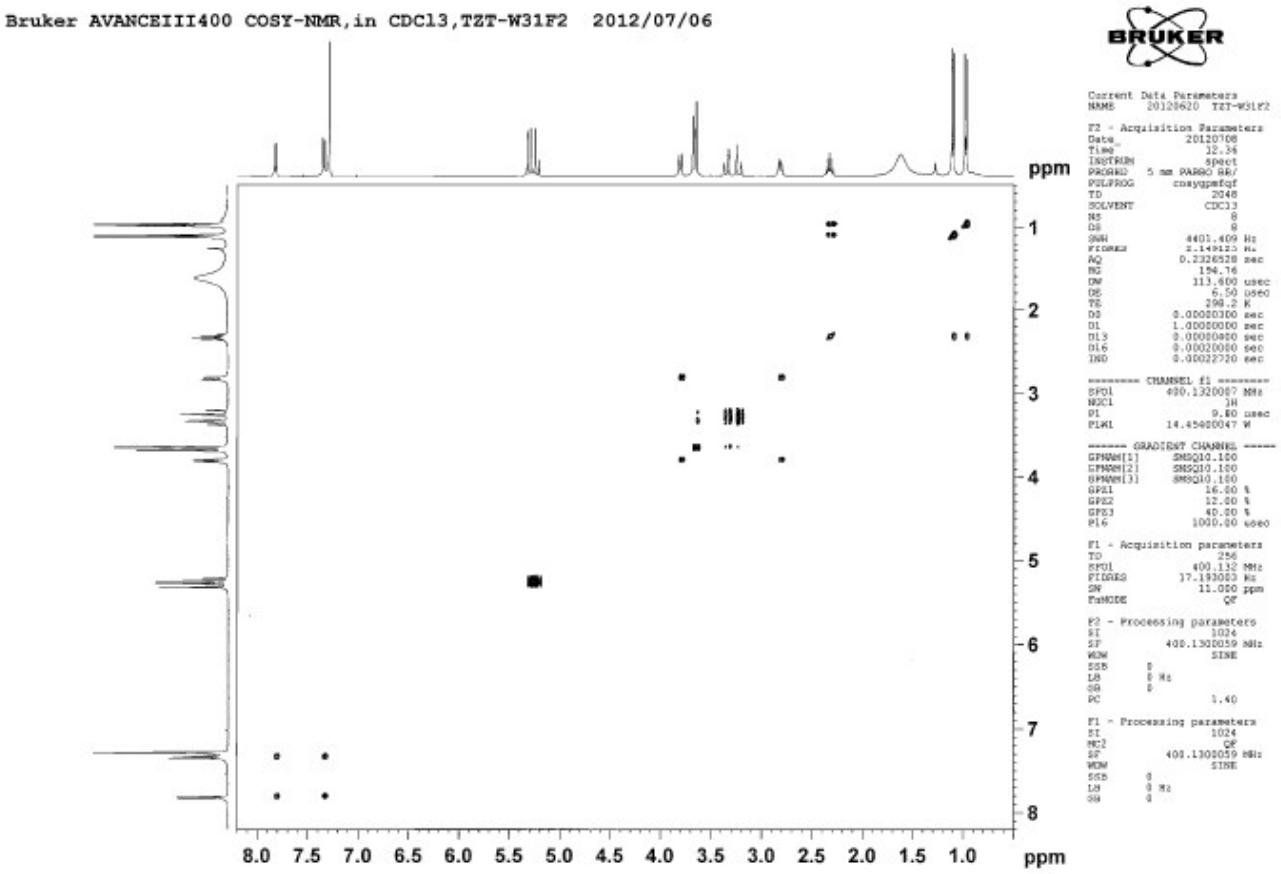

Figure S51. The 1D NOE spectrum of tripterlide F (6) in $CDCl_3$

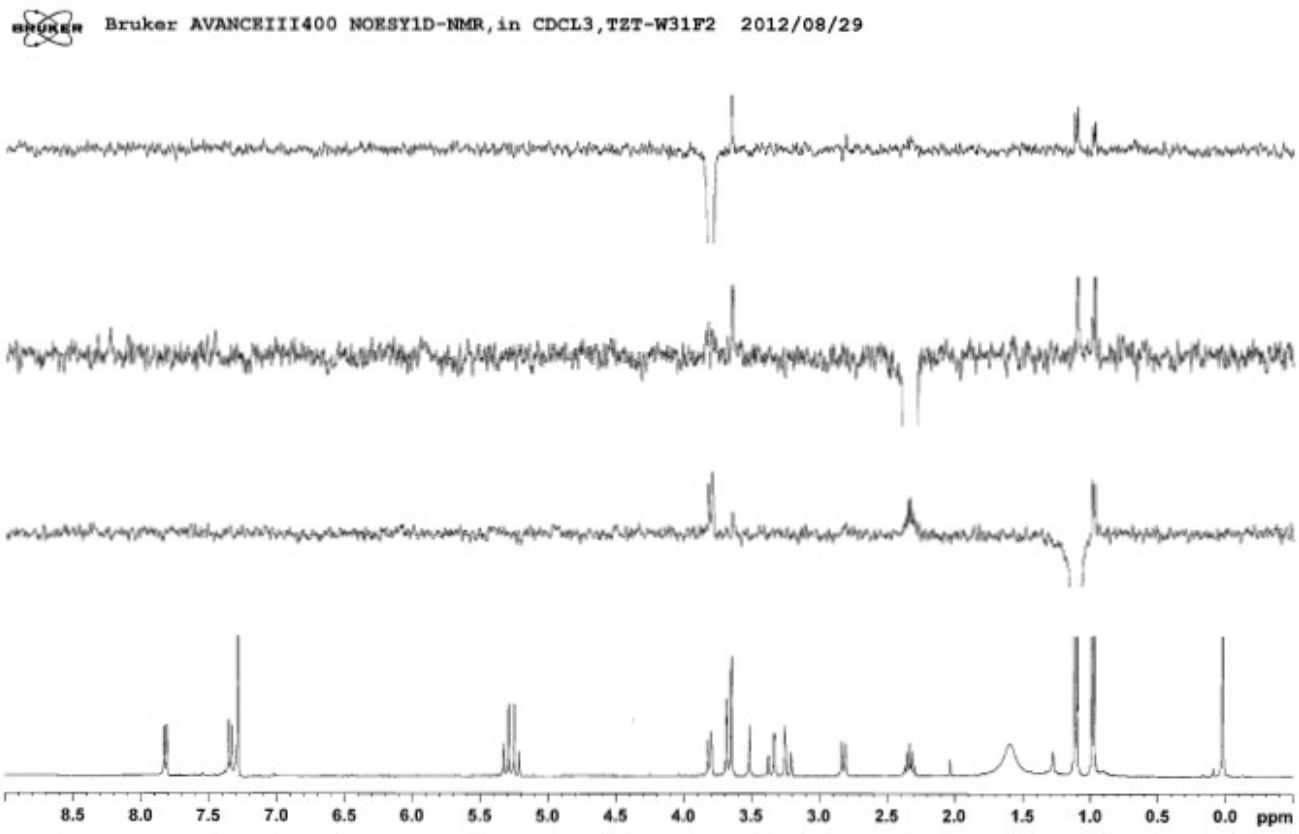

Figure S52. The IR spectrum of tripterlide F (6)

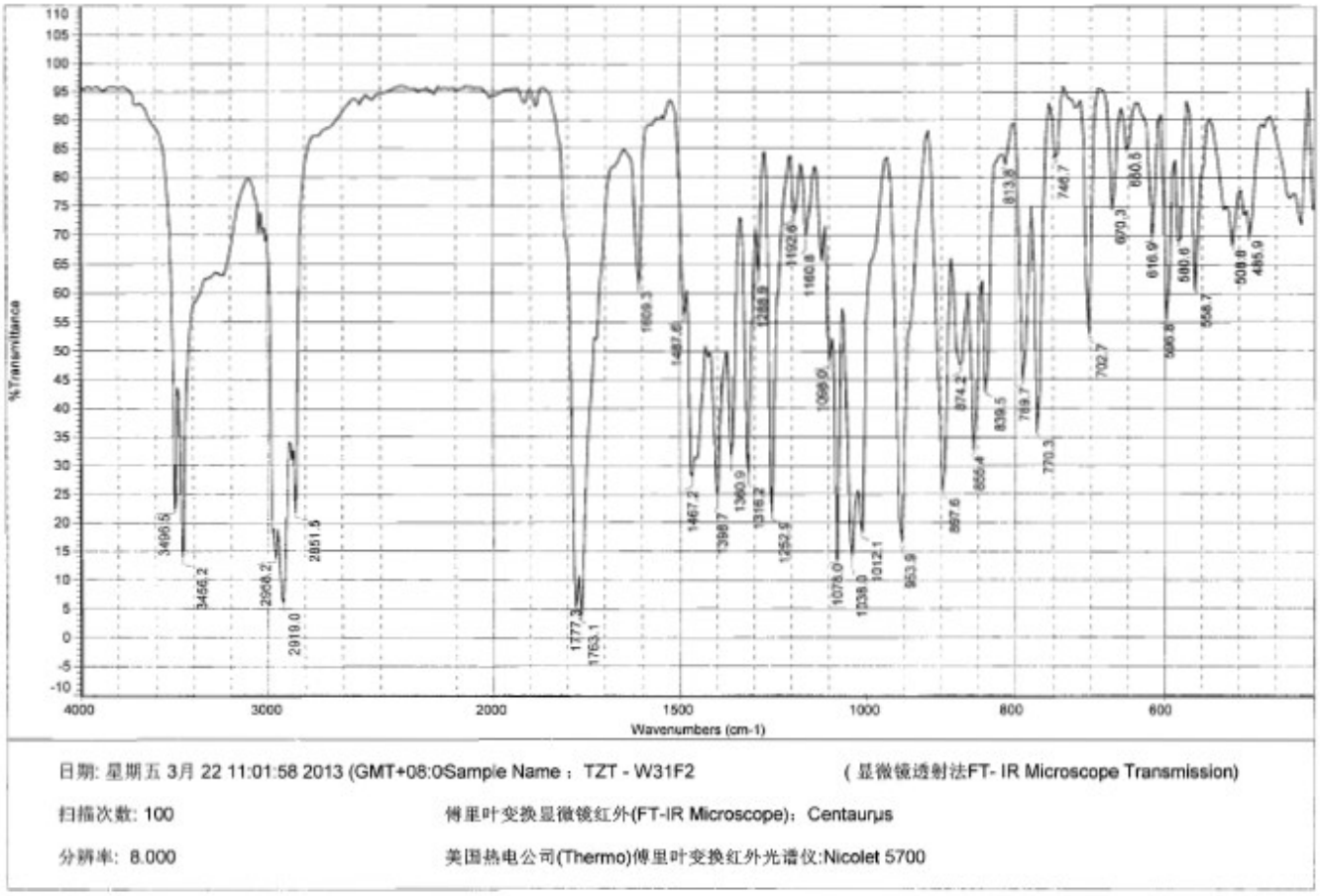

Figure S53. The HRESIMS spectrum of tripterlide F (6)