Electronic Supplementary Material (ESI) for RSC Advances.

Anti-inflammatory alkaloid Glycoside and Quinoline alkaloid derivates from the stems of *Clausena lansium*

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Supporting Information

List of Supporting Information

Figure S1. The ^{1}H NMR (400 MHz) spectrum of Clausenaside A (1) in DMSO-d_6

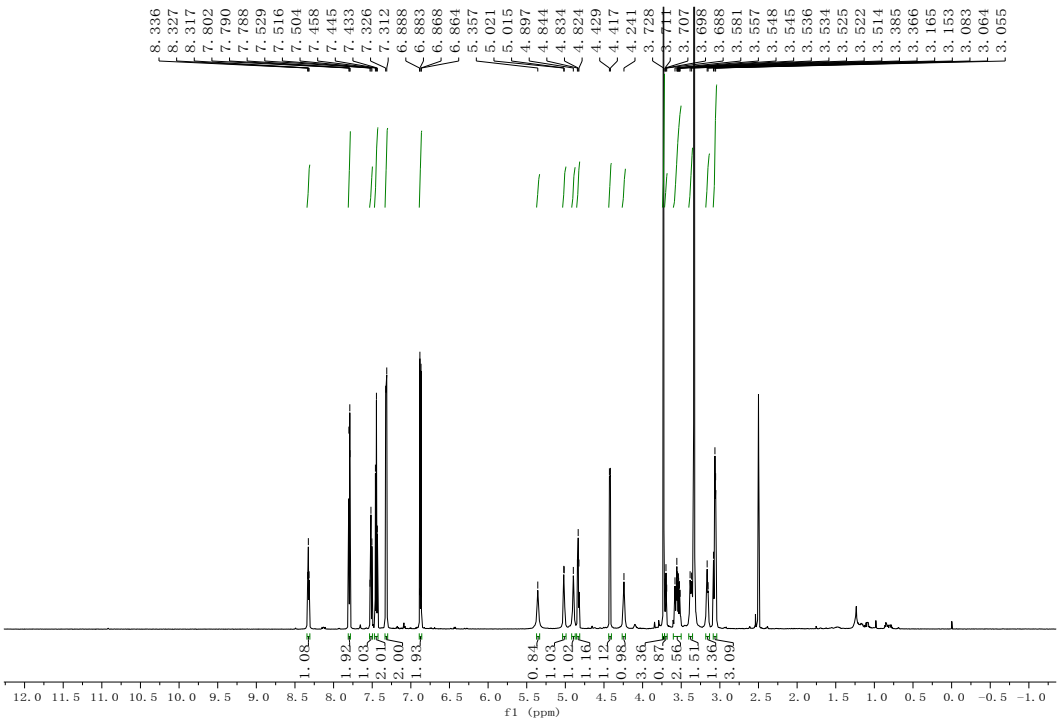


Figure S2. The ^{13}C NMR (100 MHz) spectrum of Clausenaside A (1) in DMSO-d_6

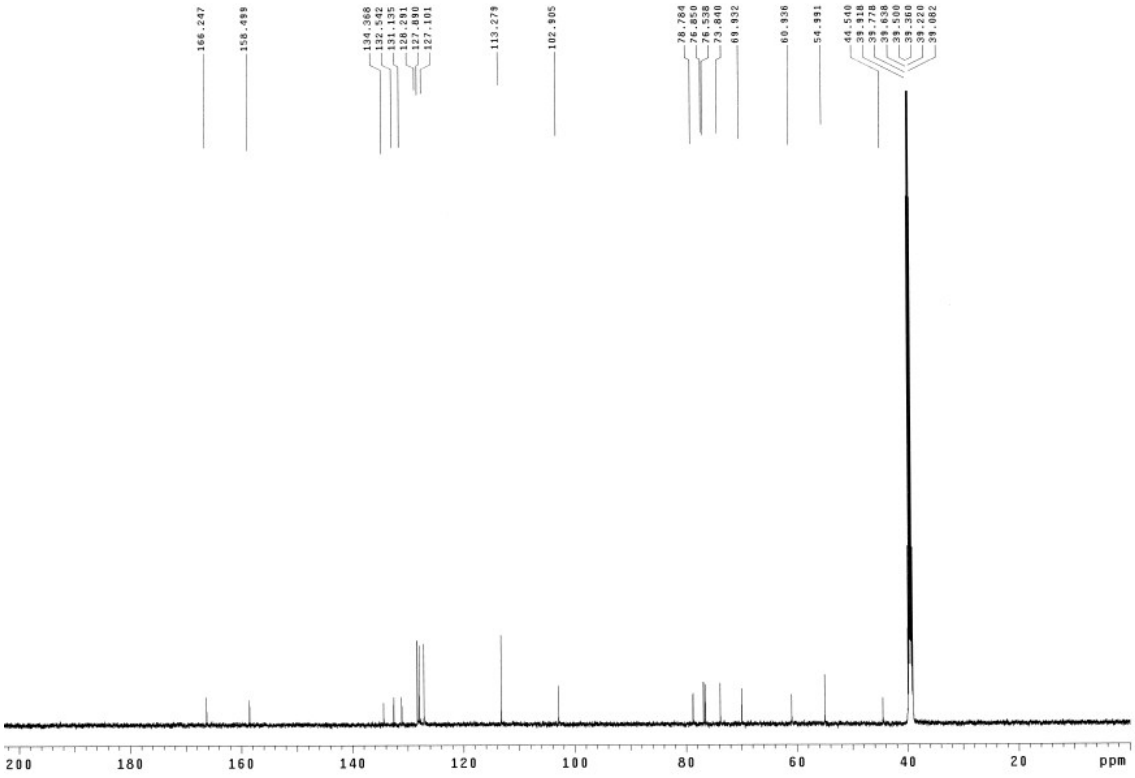


Figure S3. The DEPT spectrum of Clausenaside A (1) in DMSO-d_6

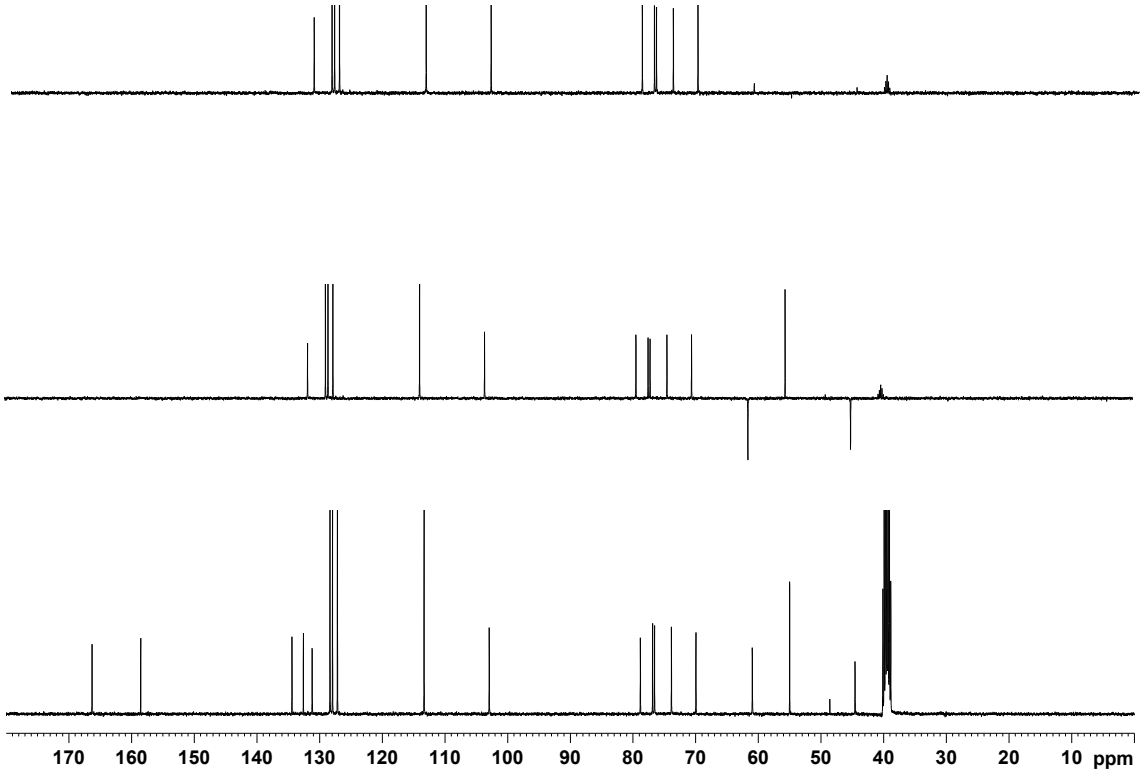


Figure S4. The HSQC spectrum of Clausenaside A (1) in DMSO-d_6

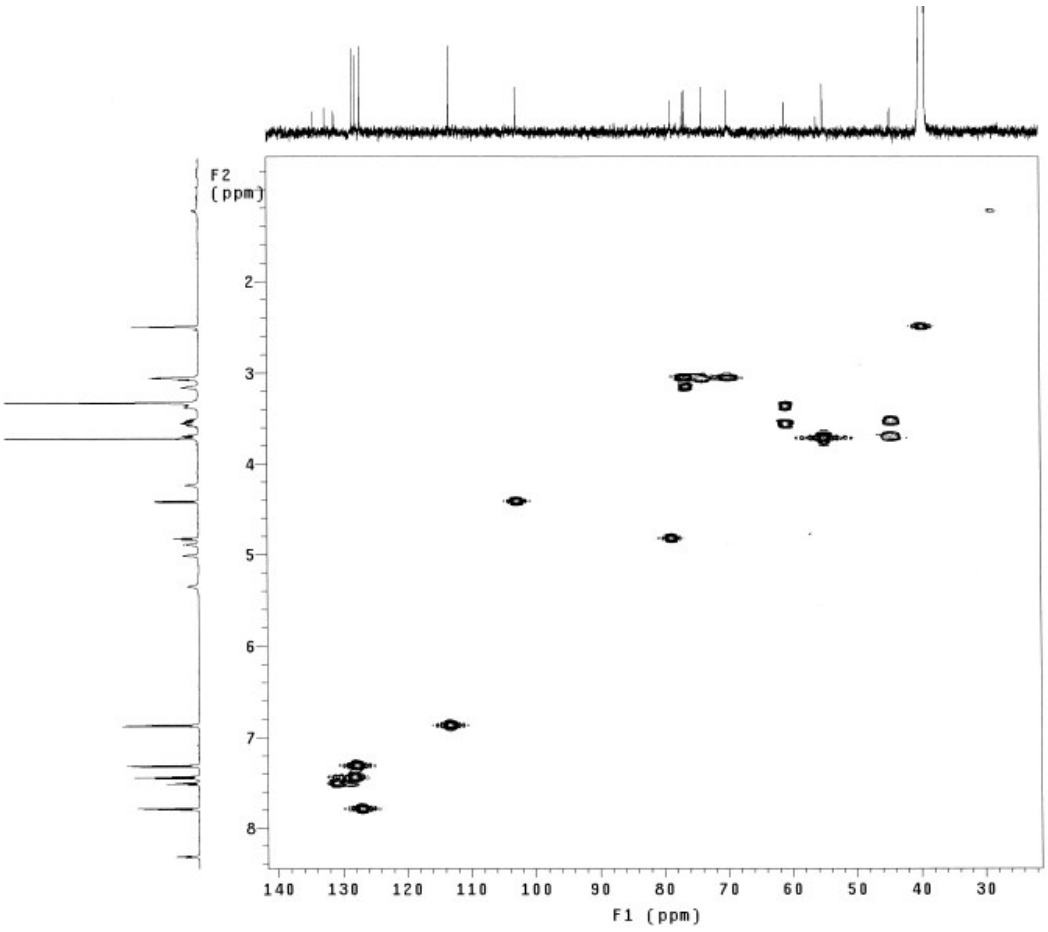


Figure S5. The HMBC spectrum of Clausenaside A (1) in DMSO-d_6

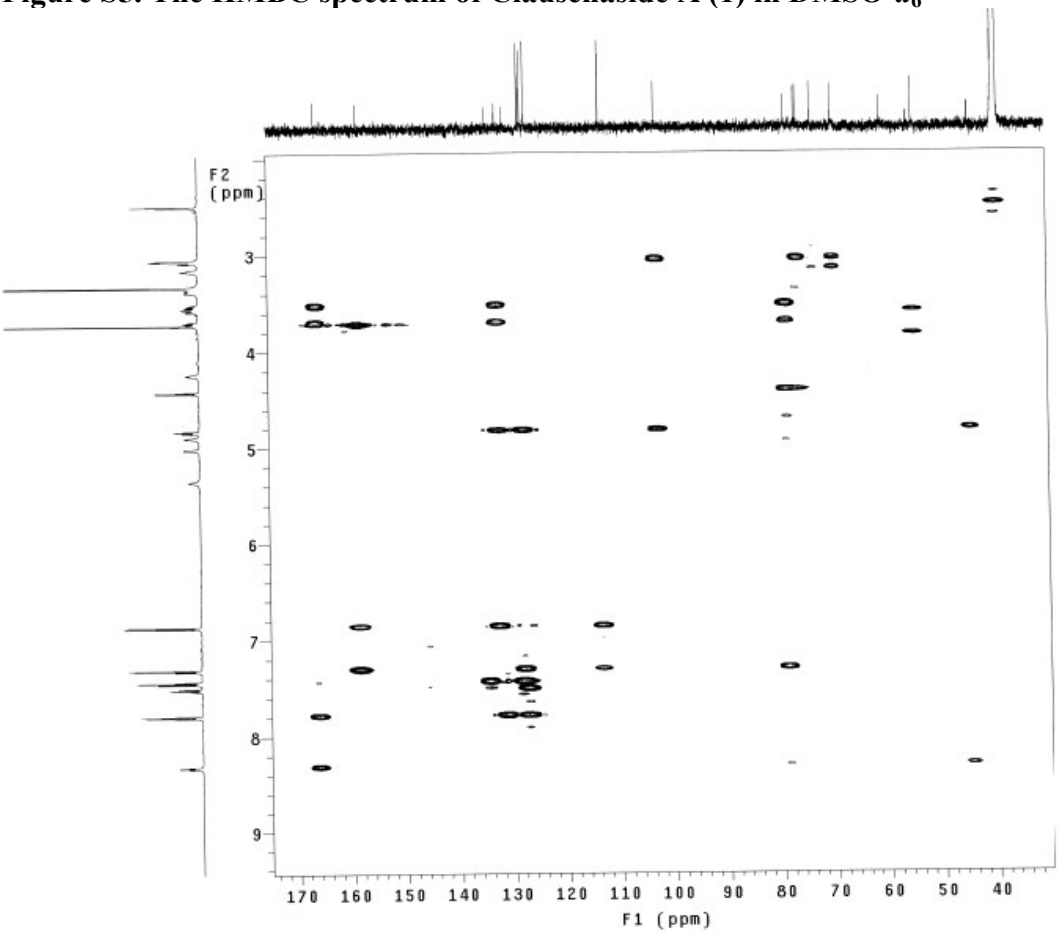


Figure S6. The ^{1}H-^{1}H COSY spectrum of Clausenaside A (1) in DMSO-d_6

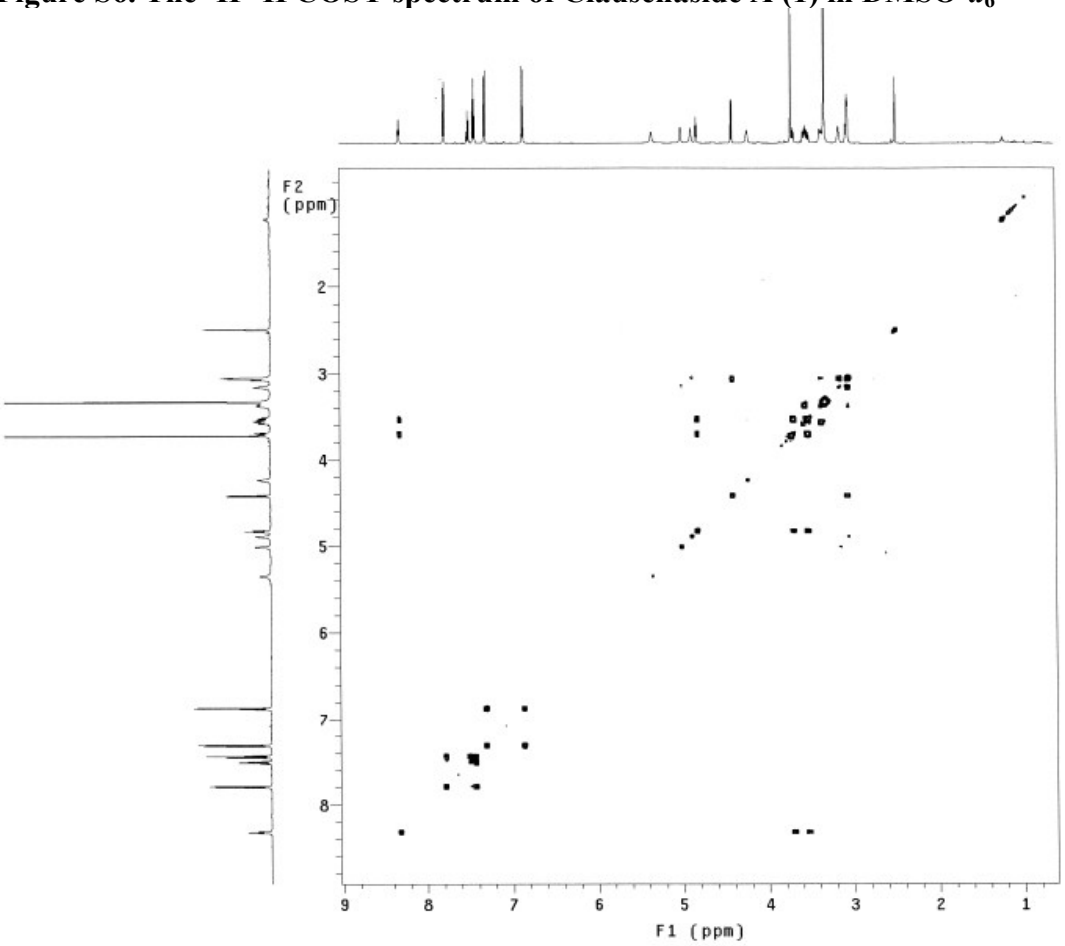


Figure S7. The experimental CD spectrum of Clausenaside A (1)

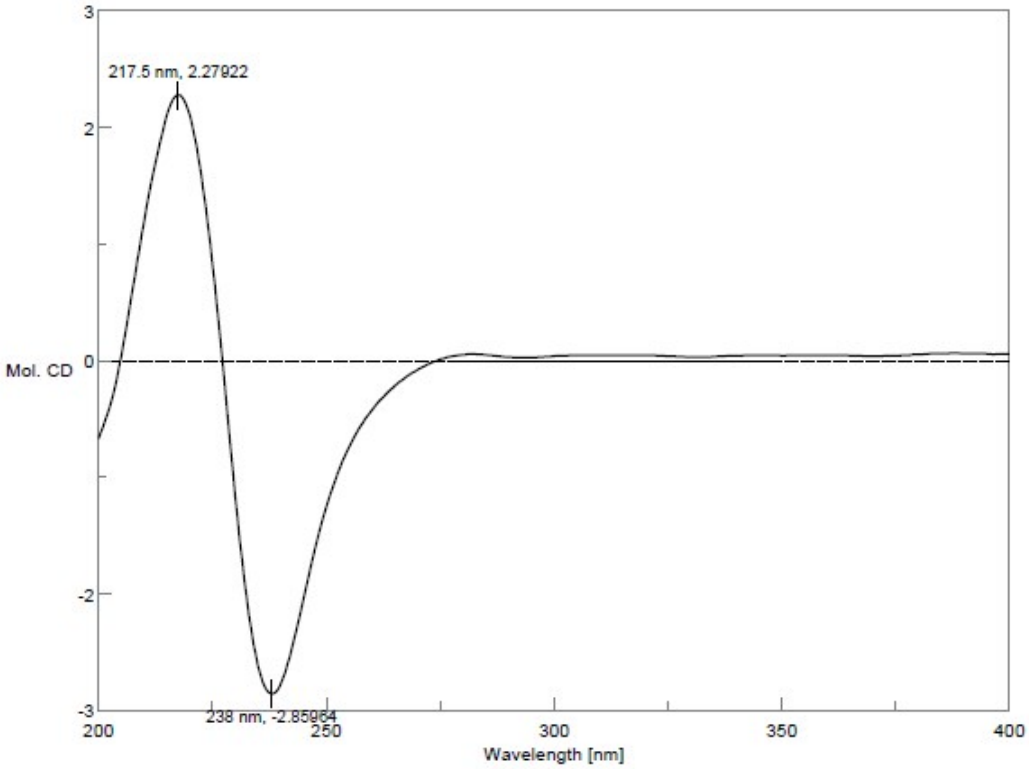


Figure S8. The IR spectrum of Clausenaside A (1)

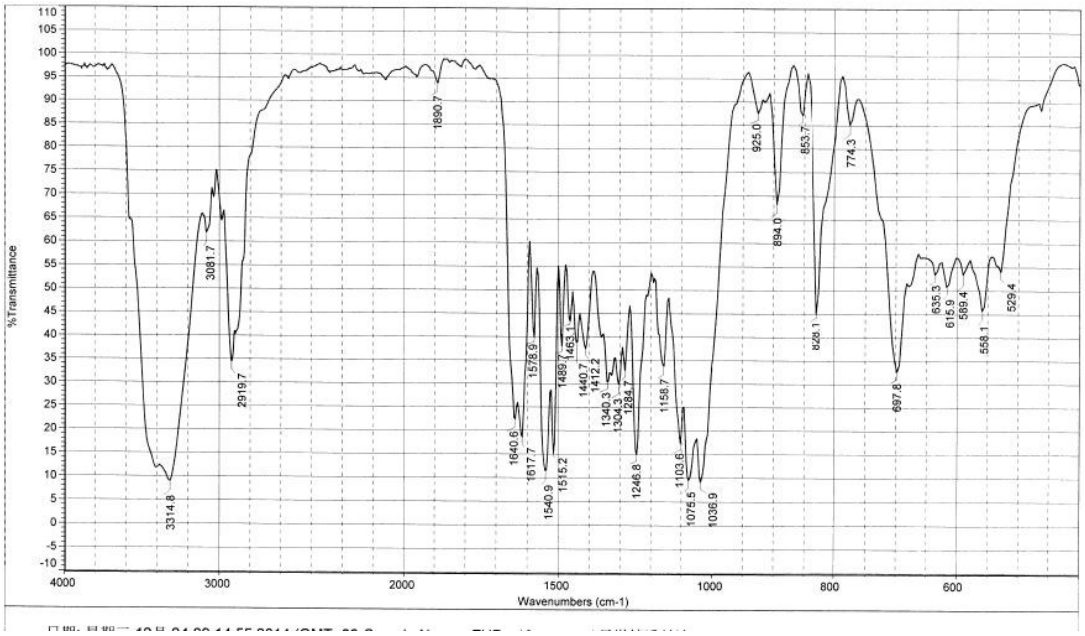


Figure S9. The HRESIMS of Clausenaside A (1)

MS Formula Results: + Scan (5.735 min) Sub (2014011001.d)

	m/z	Ion	Formula	Abundance
-	456.1634	(M+Na)+	C22 H27 N Na O8	499566.3

	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
+	☑	C22 H27 N O8	C22 H27 N Na O8	456.1629	99.97		433.1741	433.1737	-1.09	1.09	99.99	99.94	99.96	456.1634	10
+	☐	C23 H23 N5 O4	C23 H23 N5 Na O4	456.1642	99.79		433.1741	433.175	1.98	1.98	99.48	99.99	99.88	456.1634	15
+	☐	C23 H31 N O3 S2	C23 H31 N Na O3 S2	456.1638	97.45		433.1741	433.1745	0.9	0.9	91.52	99.52	99.98	456.1634	9
+	☐	C14 H31 N3 O10 S	C14 H31 N3 Na O10 S	456.1622	97.41		433.1741	433.173	-2.61	2.61	91.57	99.65	99.79	456.1634	1

Figure S10. The ^{1}H NMR (400 MHz) spectrum of (*S*)-(+)-tembamide (1a) in DMSO-d_6

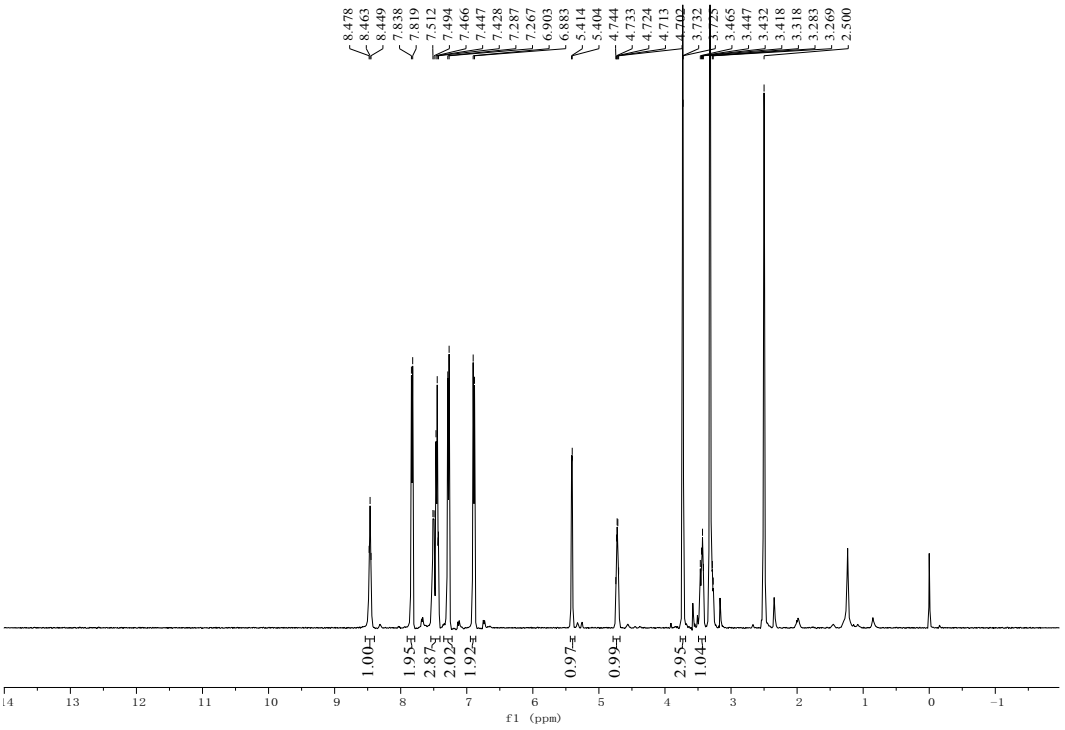


Figure S11. The ^{13}C NMR (150 MHz) spectrum of (*S*)-(+)-tembamide (1a) in DMSO-d_6

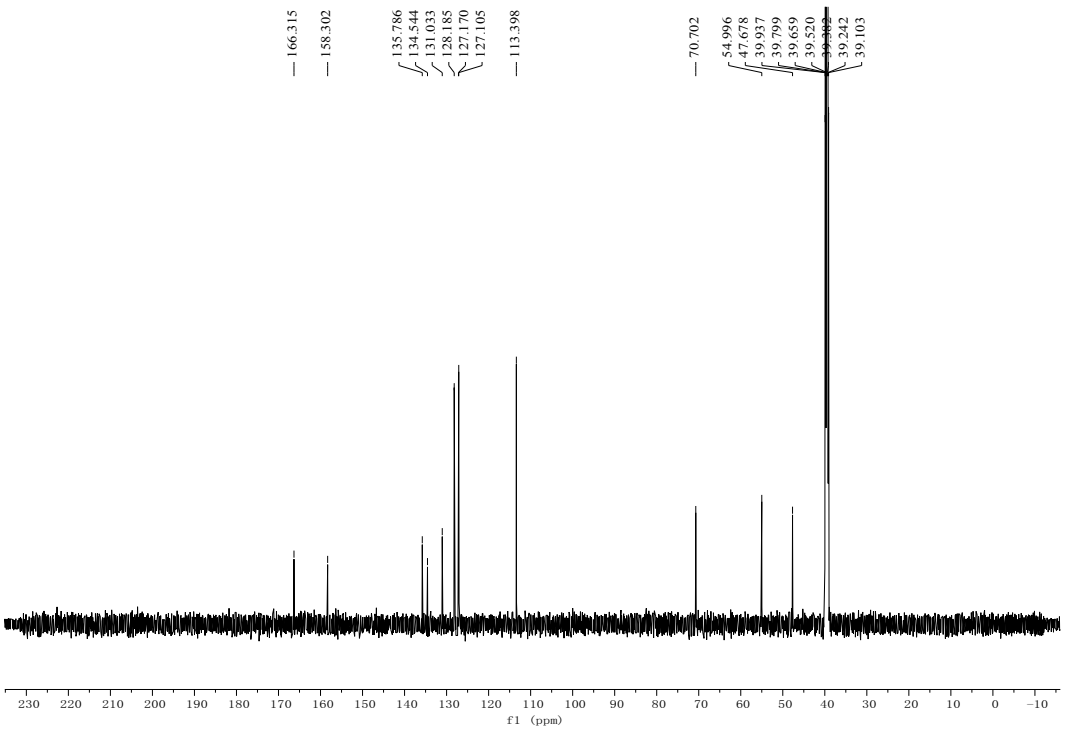


Figure S12. The experimental CD spectrum of (*S*)-(+)-tembamide (1a)

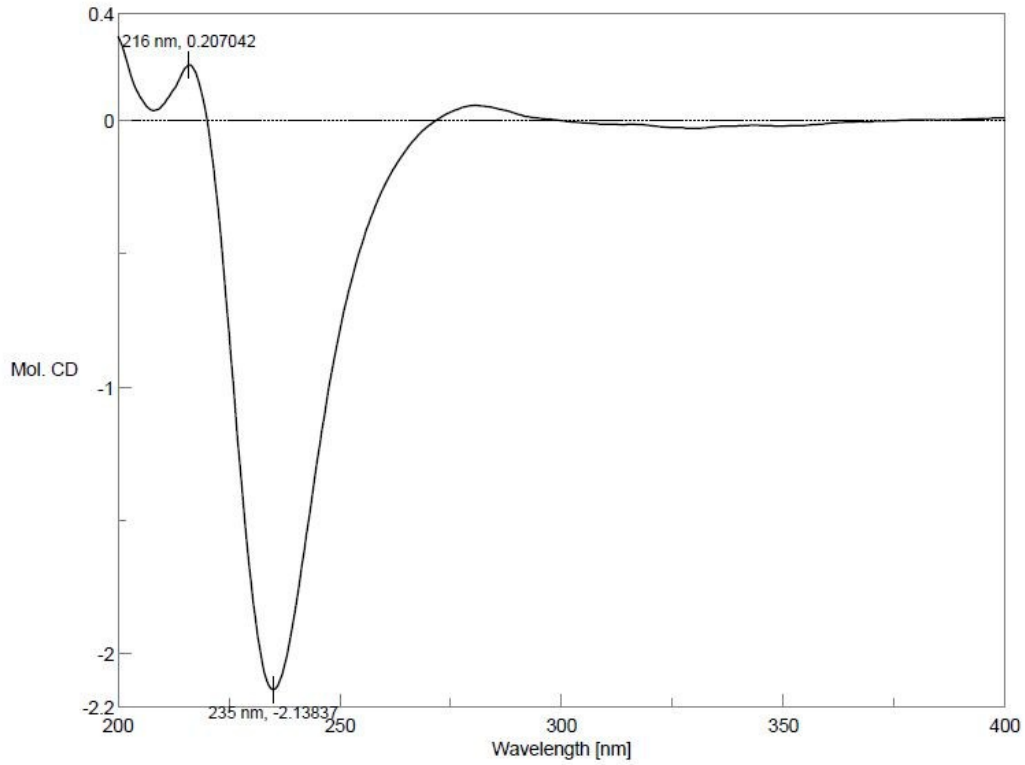


Figure S13. The HRESIMS of (*S*)-(+)-tembamide (1a)

MS Formula Results: + Scan (5.910 min) Sub (2015010601.d)

	m/z	Ion	Formula	Abundance
-	294.1109	(M+Na)+	C16 H17 N Na O3	792599.5

	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
•	✓	C16 H17 N O3	C16 H17 N Na O3	99.85		271.1217	271.1208	294.1101	-3.05	3.05	99.76	99.94	99.94	9
•		C13 H18 F N O4	C13 H18 F N Na O4	99.43		271.1217	271.122	294.1112	1.17	1.17	99.96	98.11	99.94	5
•		C13 H22 F N S Si	C13 H22 F N Na S Si	97.39		271.1217	271.1226	294.1118	3.5	3.5	99.68	91.75	99.59	4

Figure S14. The ^{1}H NMR (600 MHz) spectrum of (*S*)-MTPA-ester (1aa) in DMSO-d_6

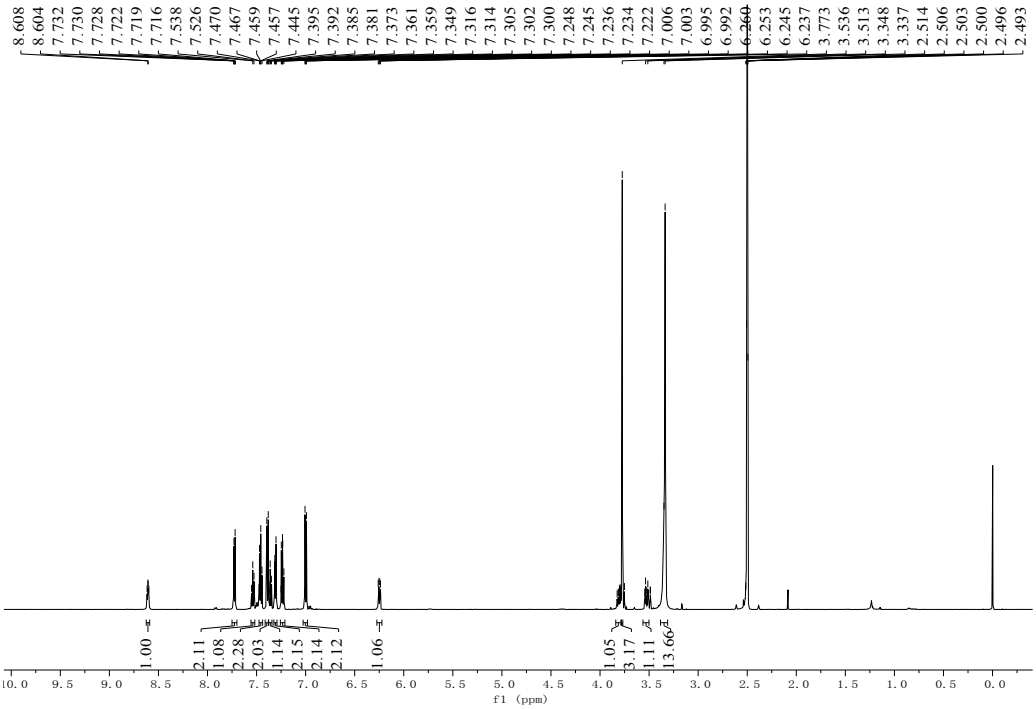


Figure S15. The ^{13}C NMR (150 MHz) spectrum of (*S*)-MTPA-ester (1aa) in DMSO-d_6

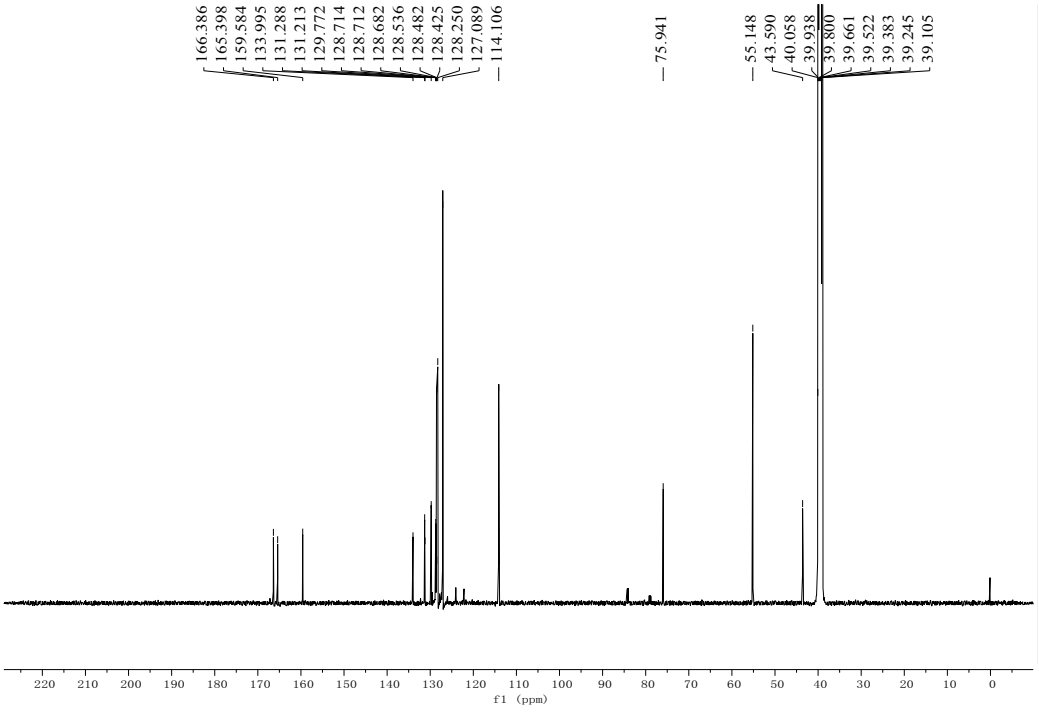


Figure S16. The HSQC spectrum of (*S*)-MTPA-ester (1aa) in DMSO-d_6

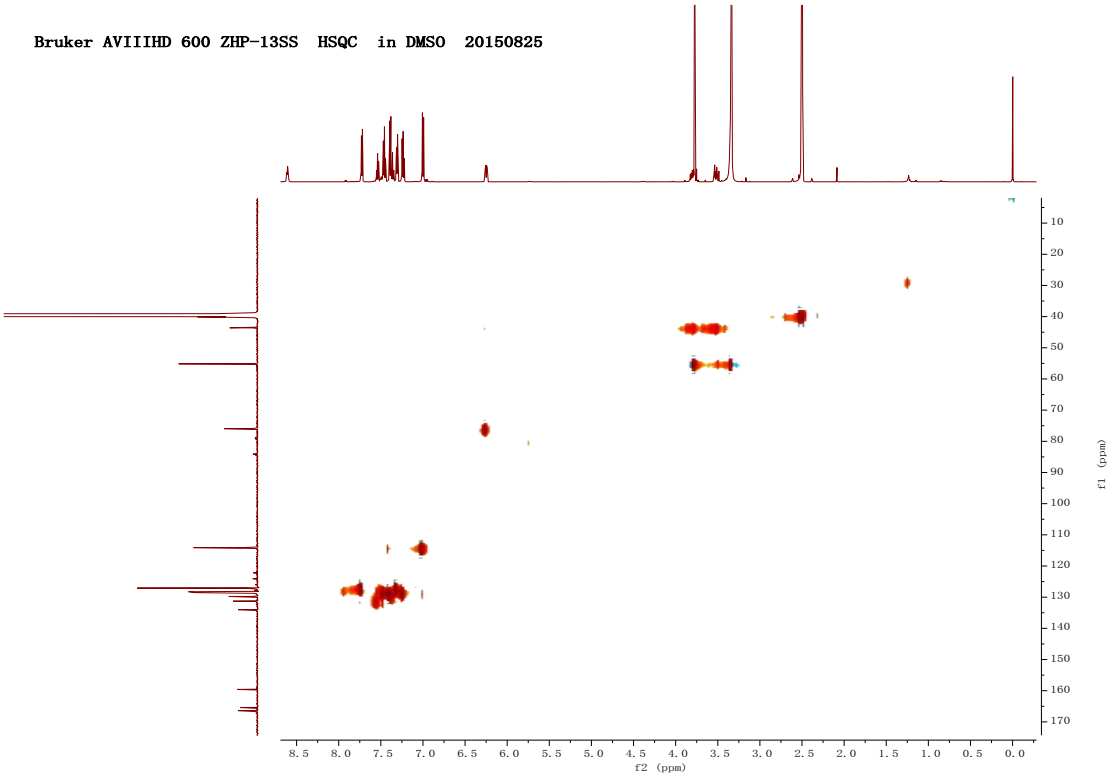


Figure S17. The HMBC spectrum of (*S*)-MTPA-ester (1aa) in DMSO-d_6

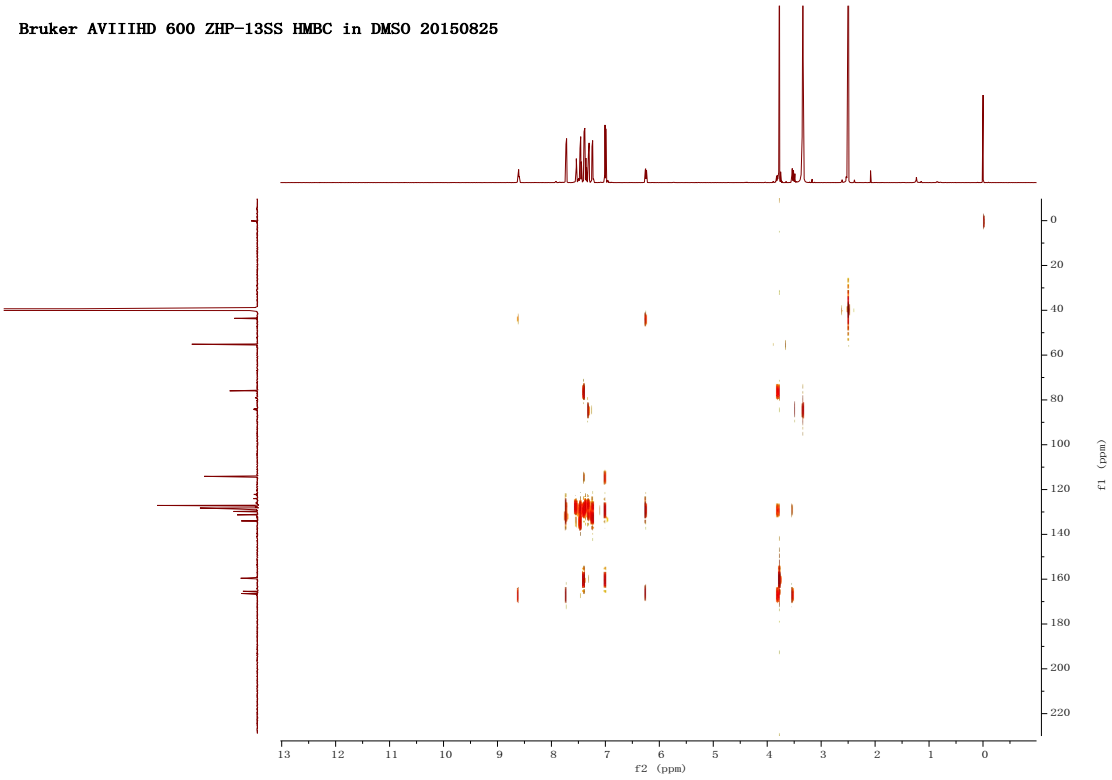


Figure S18. The ^{1}H NMR (600 MHz) spectrum of (*R*)-MTPA-ester (1ab) in DMSO-d_6

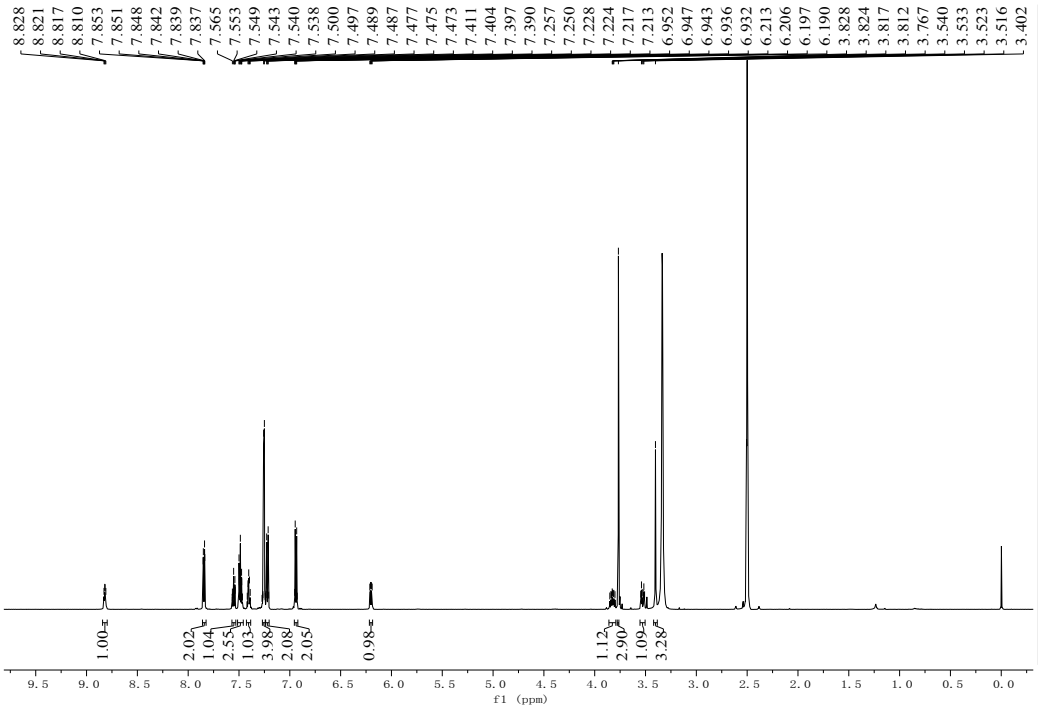


Figure S19. The ^{13}C NMR (150 MHz) spectrum of (*R*)-MTPA-ester (1ab) in DMSO-d_6

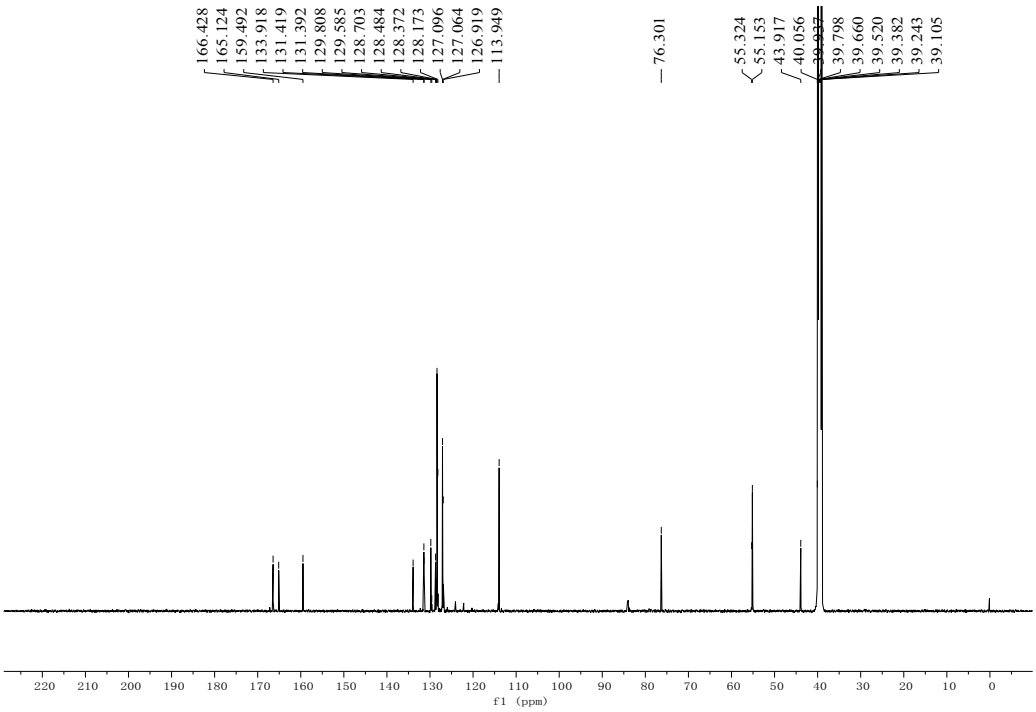


Figure S20. The HSQC spectrum of (*R*)-MTPA-ester (1ab) in DMSO-d_6

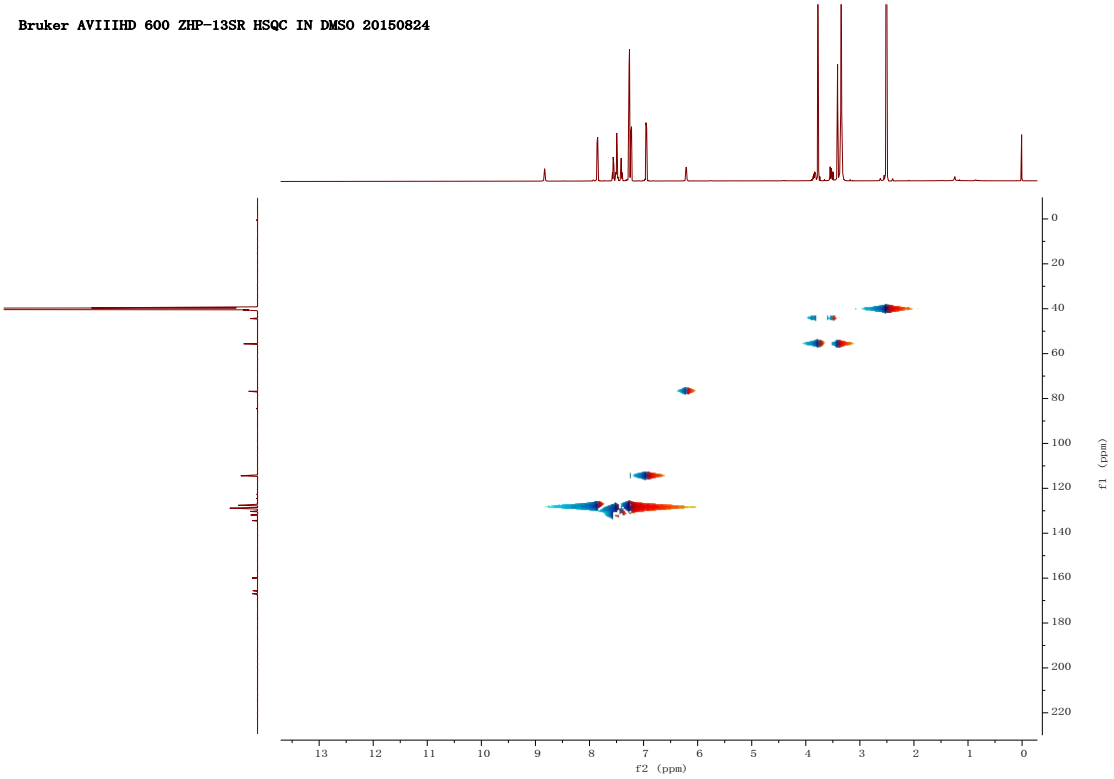


Figure S21. The HMBC spectrum of (*R*)-MTPA-ester (1ab) in DMSO-d_6

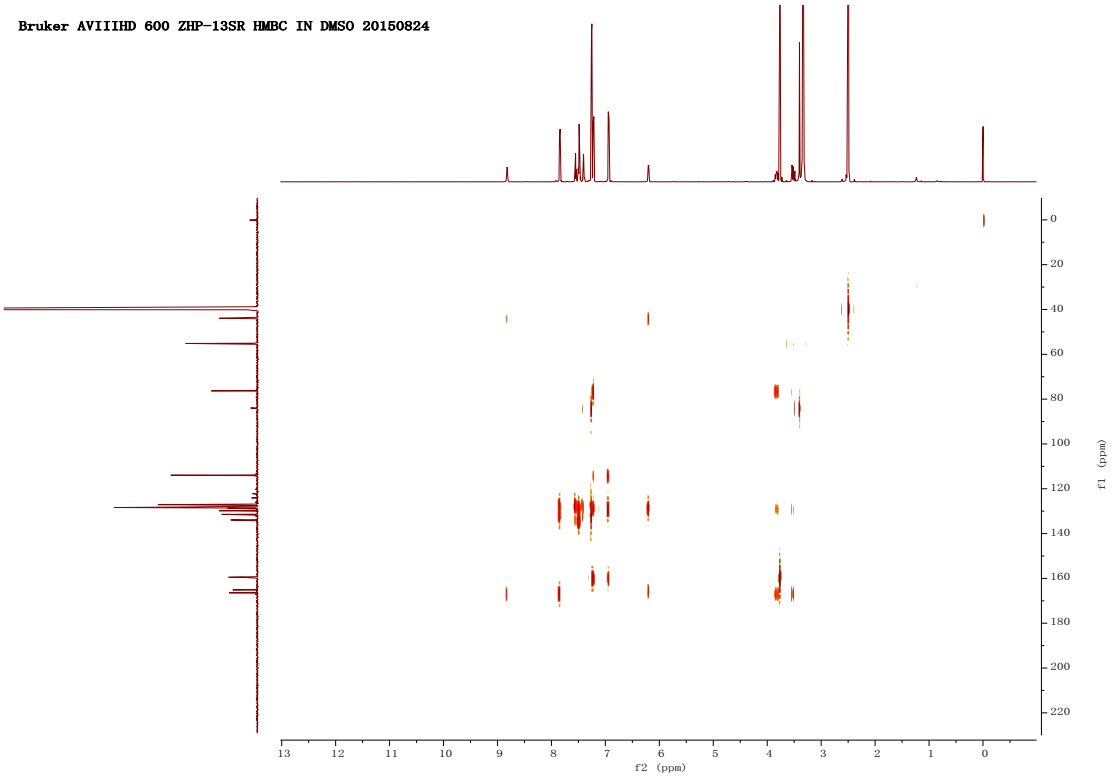


Figure S22. The ^{1}H NMR (400 MHz) spectrum of Clausenaside B (2) in DMSO-d_6

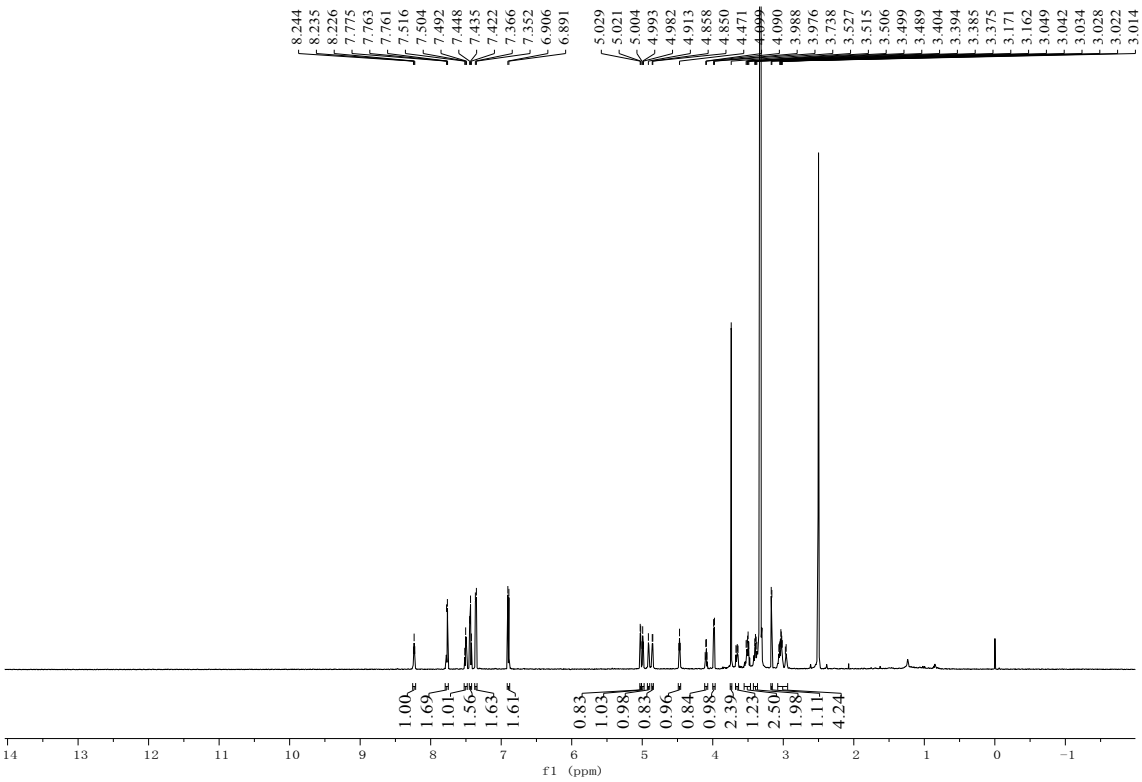


Figure S23. The ^{13}C NMR (100 MHz) spectrum of Clausenaside B (2) in DMSO-d_6

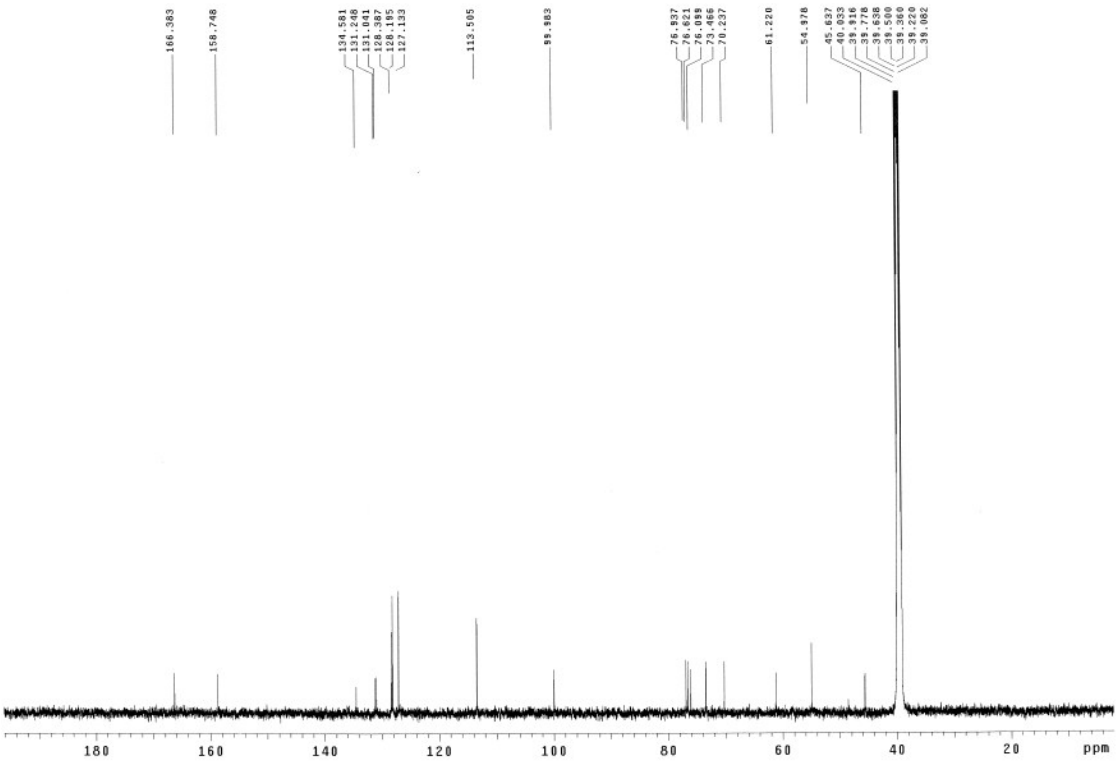


Figure S24. The DEPT spectrum of Clausenaside B (2) in DMSO-d_6

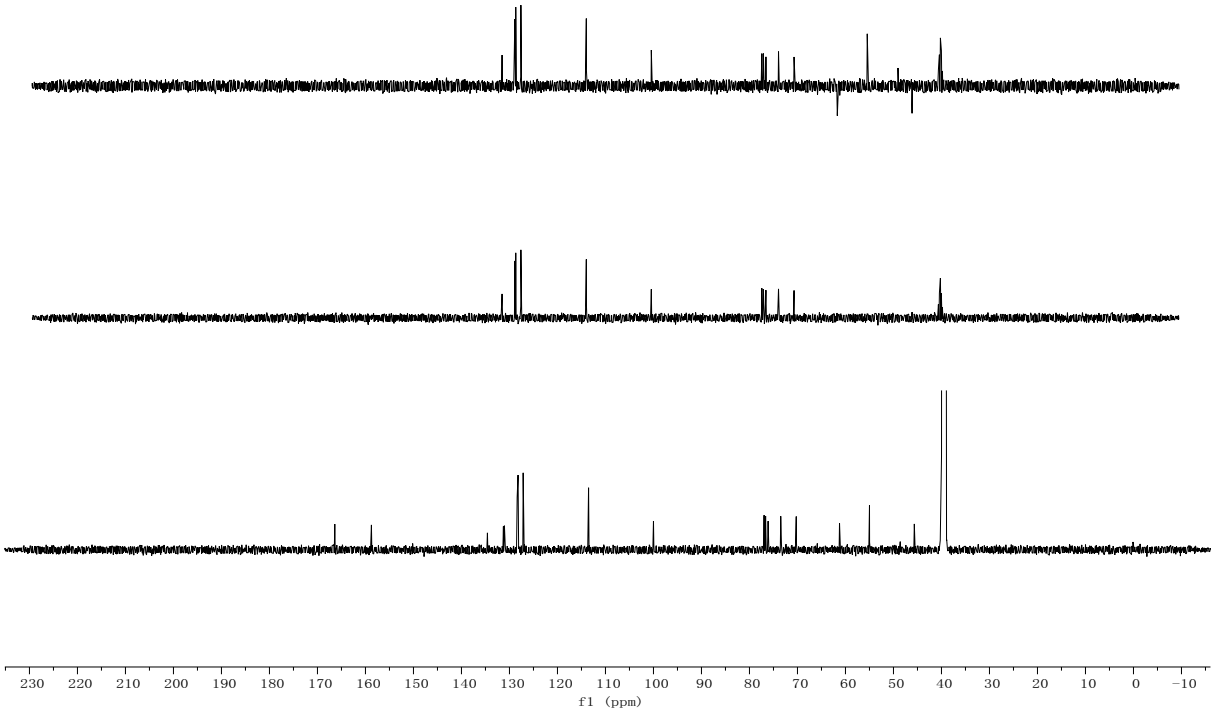


Figure S25. The HSQC spectrum of Clausenaside B (2) in DMSO-d_6

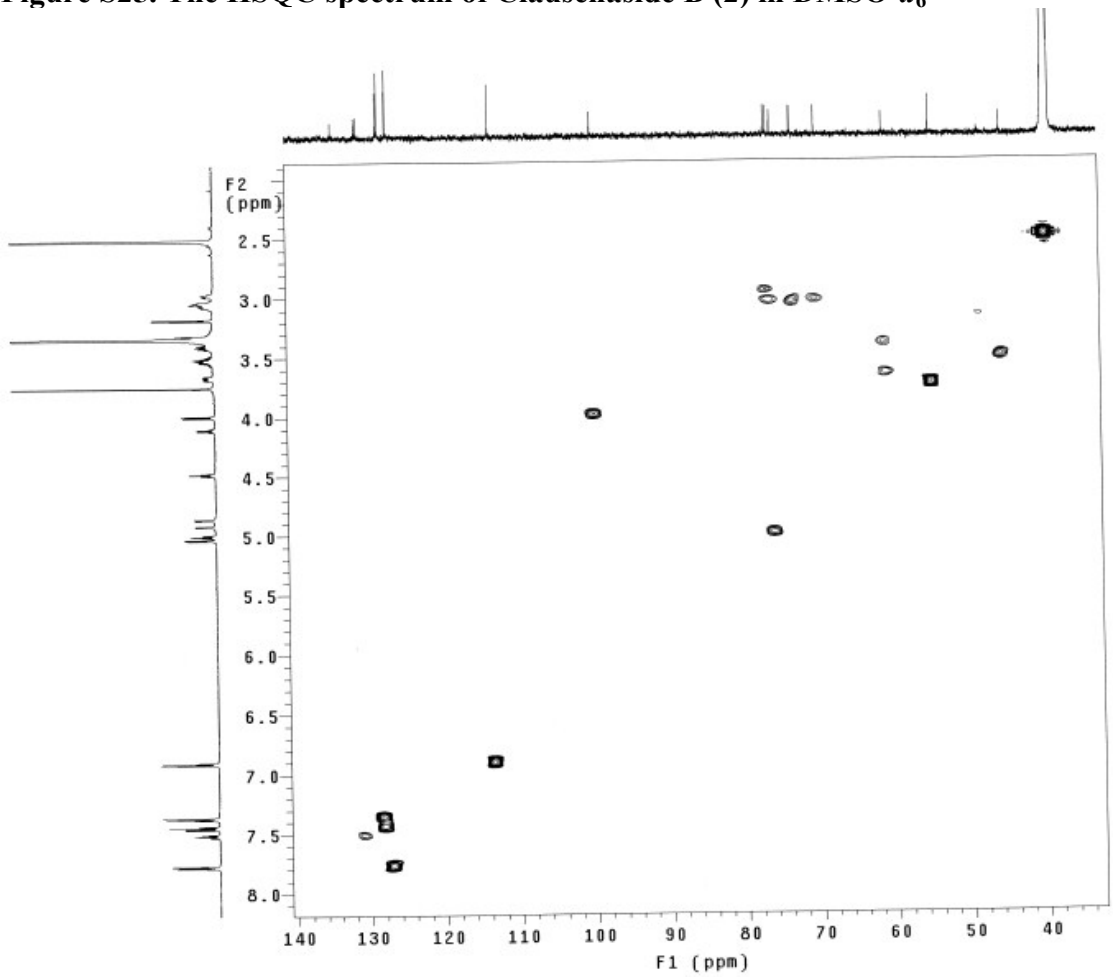


Figure S26. The HMBC spectrum of Clausenaside B (2) in DMSO-d_6

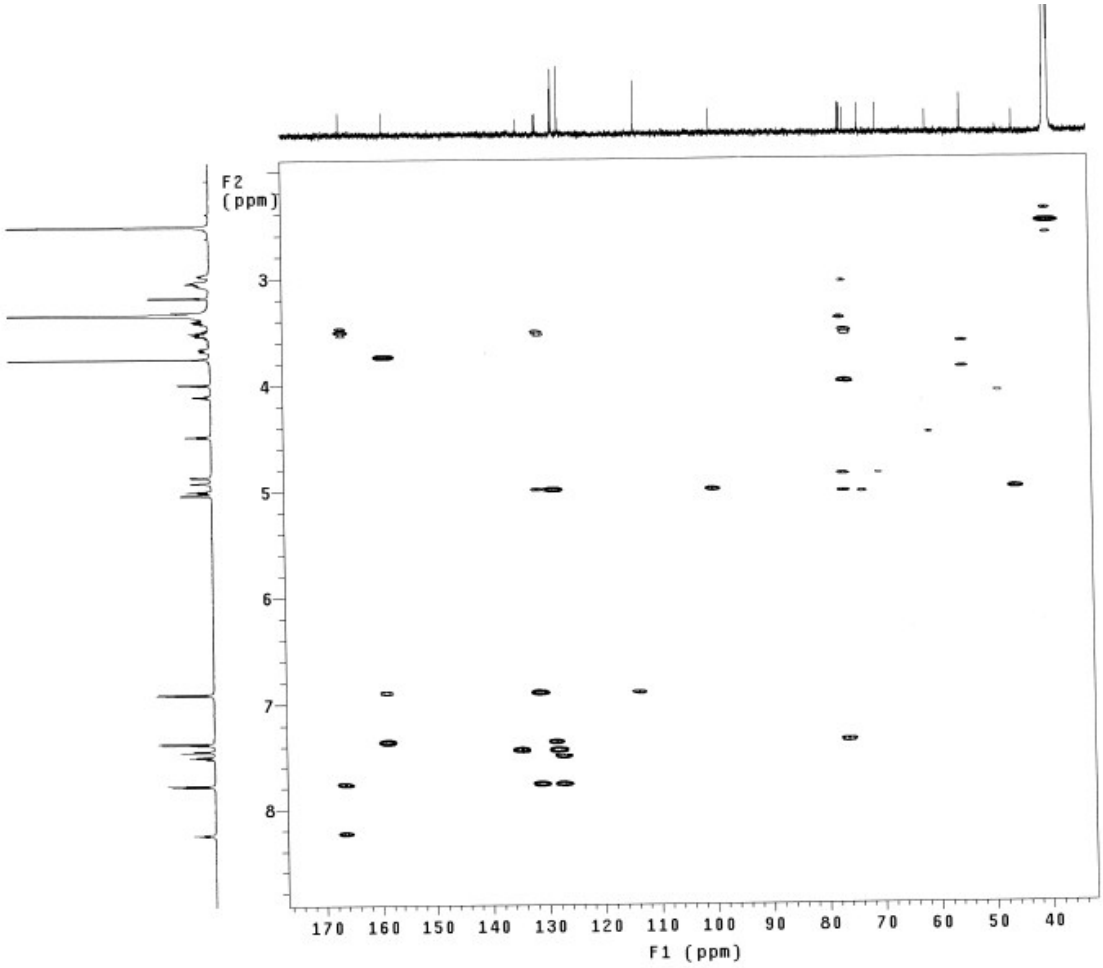


Figure S27. The ^{1}H-^{1}H COSY spectrum of Clausenaside B (2) in DMSO-d_6

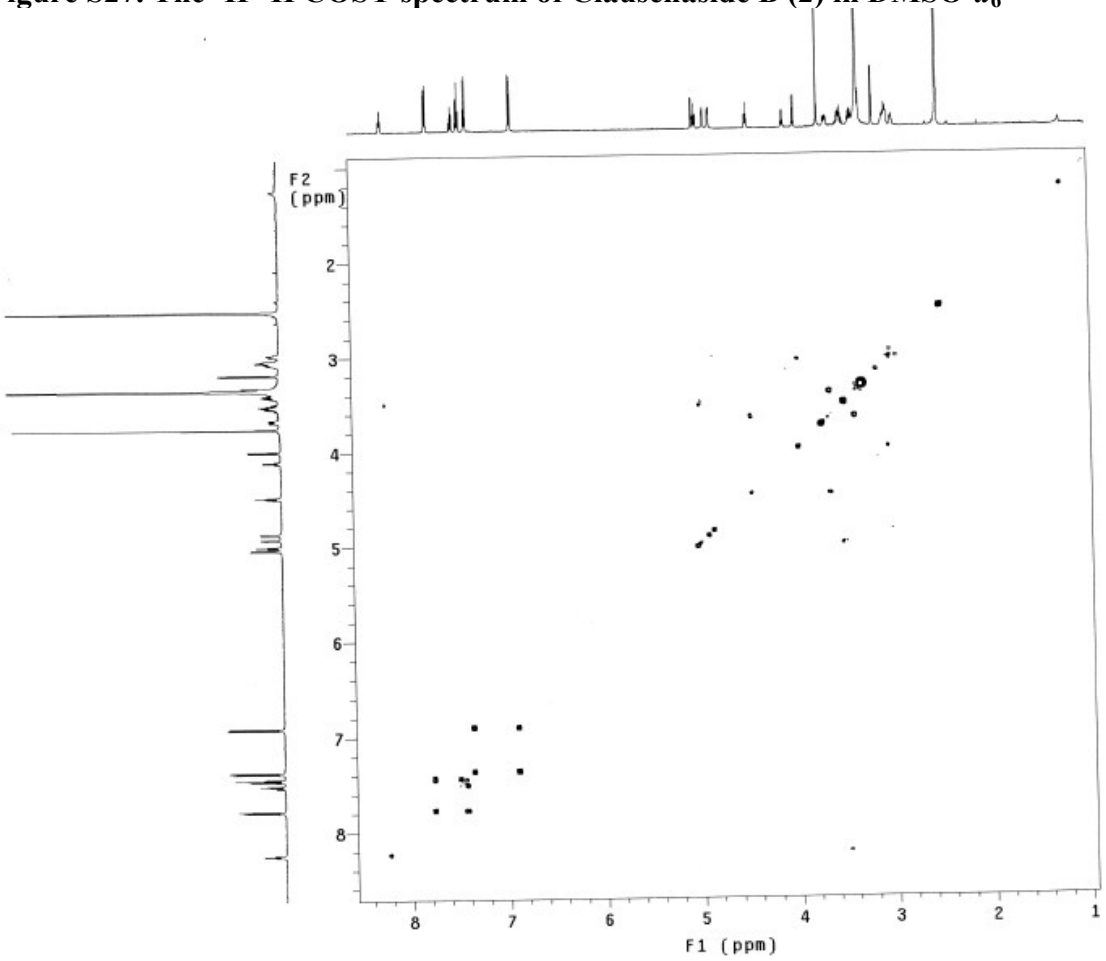


Figure S28. The experimental CD spectrum of Clausenaside B (2)

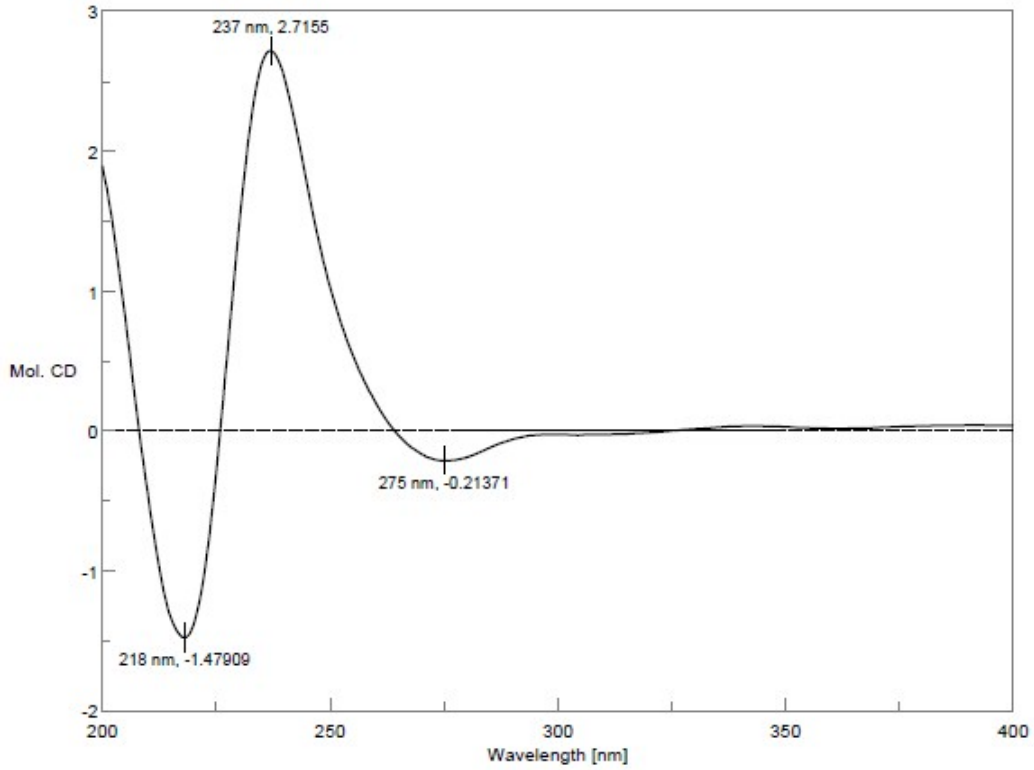


Figure S29. The IR spectrum of Clausenaside B (2)

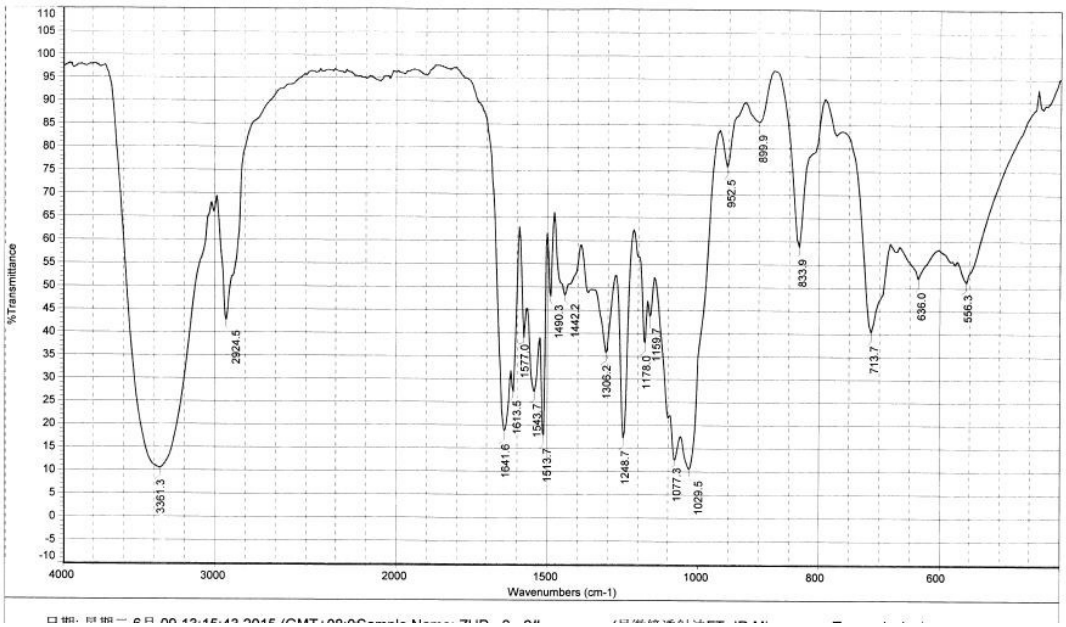


Figure S30. The HRESIMS of Clausenaside B (2)

MS Formula Results: + Scan (5.615 min) Sub (2014121501.d)

m/z	Ion	Formula	Abundance
456.1635	(M+Na)+	C22 H27 N Na O8	1592229.4

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
☑	C22 H27 N O8	C22 H27 N Na O8	99.93		433.1743	433.1737	456.1629	-1.5	1.5	99.93	99.9	99.97	10
☐	C19 H28 F N O9	C19 H28 F N Na O9	99.49		433.1743	433.1748	456.164	1.14	1.14	99.96	98.31	99.97	6
☐	C21 H28 N3 O5 P	C21 H28 N3 Na O5 P	99.49		433.1743	433.1767	456.1659	5.4	5.4	99.11	99.74	99.93	10
☐	C22 H29 F N3 O P S	C22 H29 F N3 Na O P S	99.43		433.1743	433.1753	456.1645	2.26	2.26	99.84	98.66	99.54	10
☐	C21 H29 F N3 O2 P Si	C21 H29 F N3 Na O2 P Si	99.4		433.1743	433.1751	456.1643	1.71	1.71	99.91	98.43	99.56	10
☐	C25 H28 N3 P S	C25 H28 N3 Na P S	99.32		433.1743	433.1742	456.1634	-0.38	0.38	100	97.93	99.61	14
☐	C25 H25 F N3 O P	C25 H25 F N3 Na O P	99.3		433.1743	433.1719	456.1611	-5.52	5.52	99.08	99.16	99.93	15
☐	C23 H28 F N O4 S	C23 H28 F N Na O4 S	99.05		433.1743	433.1723	456.1615	-4.64	4.64	99.35	98.08	99.64	10
☐	C18 H31 N O9 Si	C18 H31 N Na O9 Si	98.95		433.1743	433.1768	456.166	5.72	5.72	99.01	98.31	99.59	5
☐	C22 H28 F N O5 Si	C22 H28 F N Na O5 Si	98.9		433.1743	433.1721	456.1613	-5.19	5.19	99.18	97.81	99.65	10
☐	C24 H28 N3 O P Si	C24 H28 N3 Na O P Si	98.82		433.1743	433.1739	456.1631	-0.93	0.93	99.97	96.21	99.63	14
☐	C13 H31 N3 O11 Si	C13 H31 N3 Na O11 Si	98.46		433.1743	433.1728	456.162	-3.58	3.58	99.61	95.78	99.38	1
☐	C19 H32 F N O5 S Si	C19 H32 F N Na O5 S Si	97.87		433.1743	433.1754	456.1647	2.58	2.58	99.8	93.48	99.28	5
☐	C22 H31 N O4 S Si	C22 H31 N Na O4 S Si	97.74		433.1743	433.1743	456.1635	-0.05	0.05	100	92.61	99.36	9
☐	C23 H31 N O3 S2	C23 H31 N Na O3 S2	97.59		433.1743	433.1745	456.1638	0.5	0.5	99.99	92.1	99.36	9
☐	C20 H32 F N O4 S2	C20 H32 F N Na O4 S2	97.22		433.1743	433.1757	456.1649	3.13	3.13	99.7	91.38	99.29	5
☐	C15 H36 N O7 P S Si	C15 H36 N Na O7 P S Si	97.1		433.1743	433.1719	456.1612	-5.53	5.53	99.07	92.09	99.16	0
☐	C14 H31 N3 O10 S	C14 H31 N3 Na O10 S	97.03		433.1743	433.173	456.1622	-3.02	3.02	99.72	90.53	99.44	1

Figure S31. The ^{1}H NMR (400 MHz) spectrum of Clausenaside C (3) in DMSO-d_6

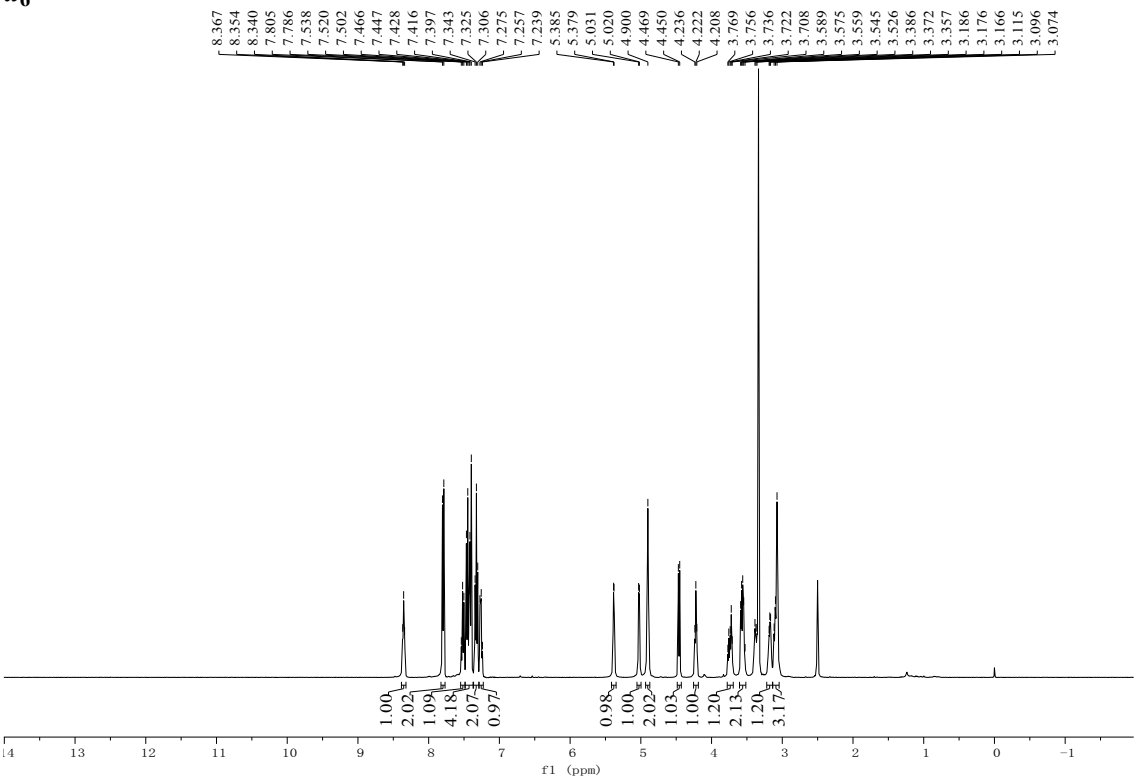


Figure S32. The ^{13}C NMR (100 MHz) spectrum of Clausenaside C (3) in DMSO-d_6

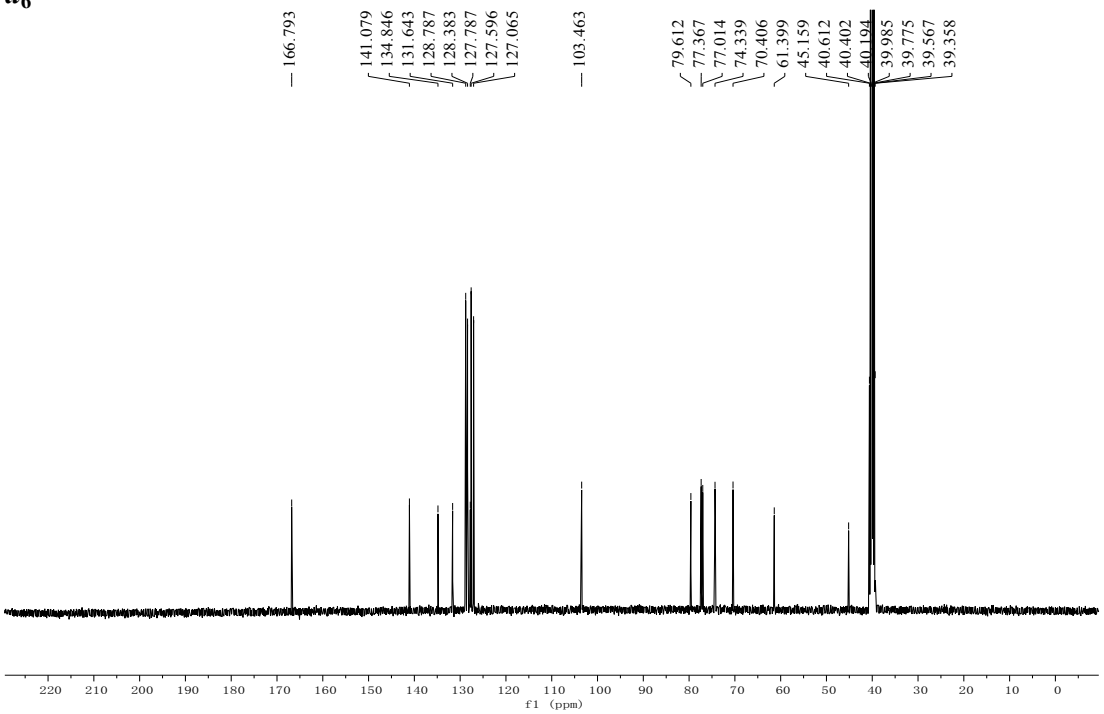


Figure S33. The DEPT spectrum of Clausenaside C (3) in DMSO-d_6

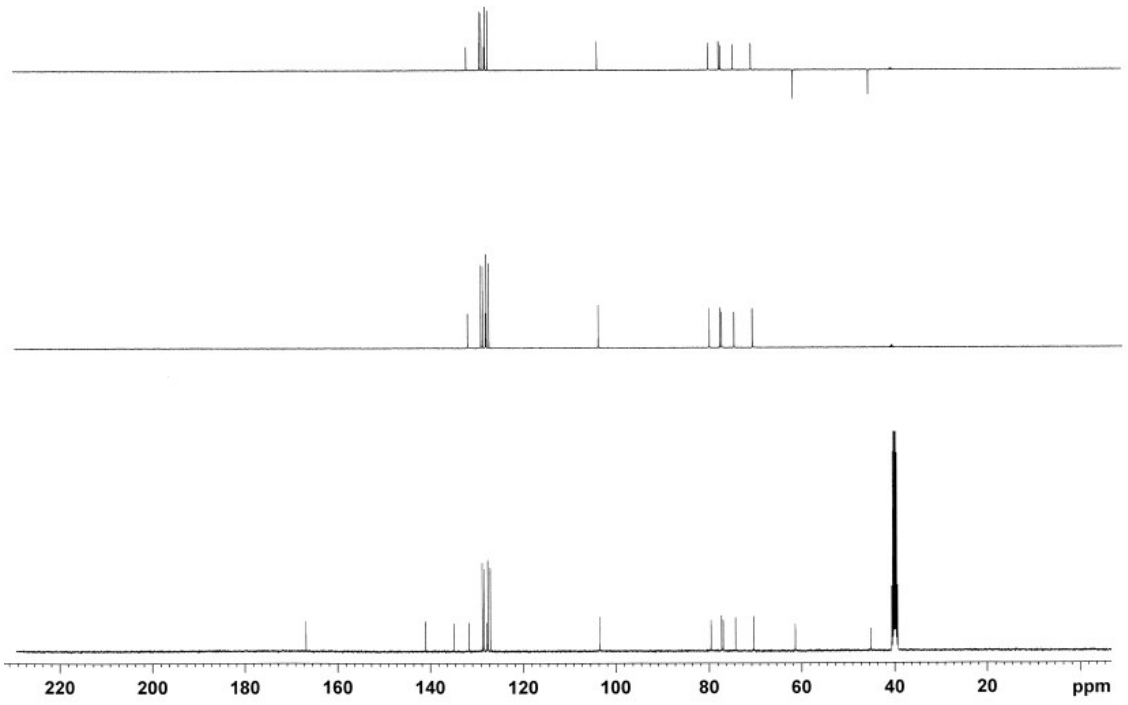


Figure S34. The HSQC spectrum of Clausenaside C (3) in DMSO-d_6

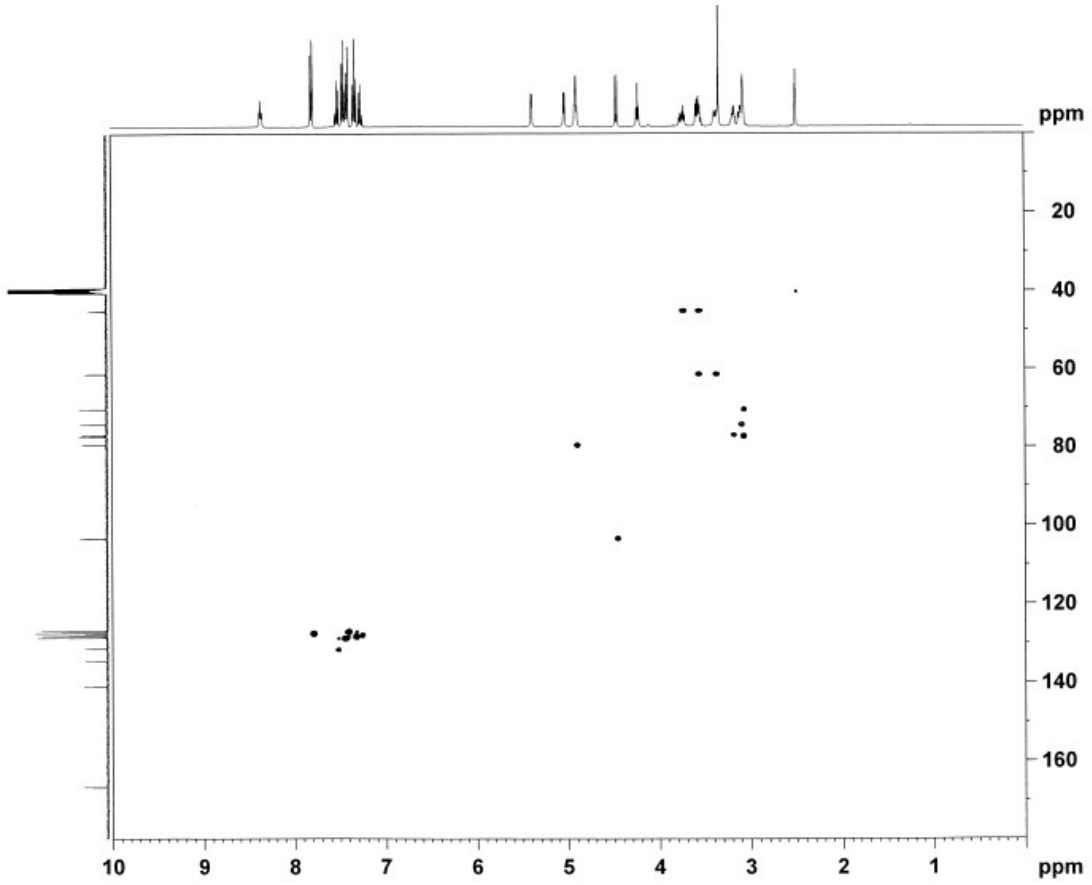


Figure S35. The HMBC spectrum of Clausenaside C (3) in DMSO-d_6

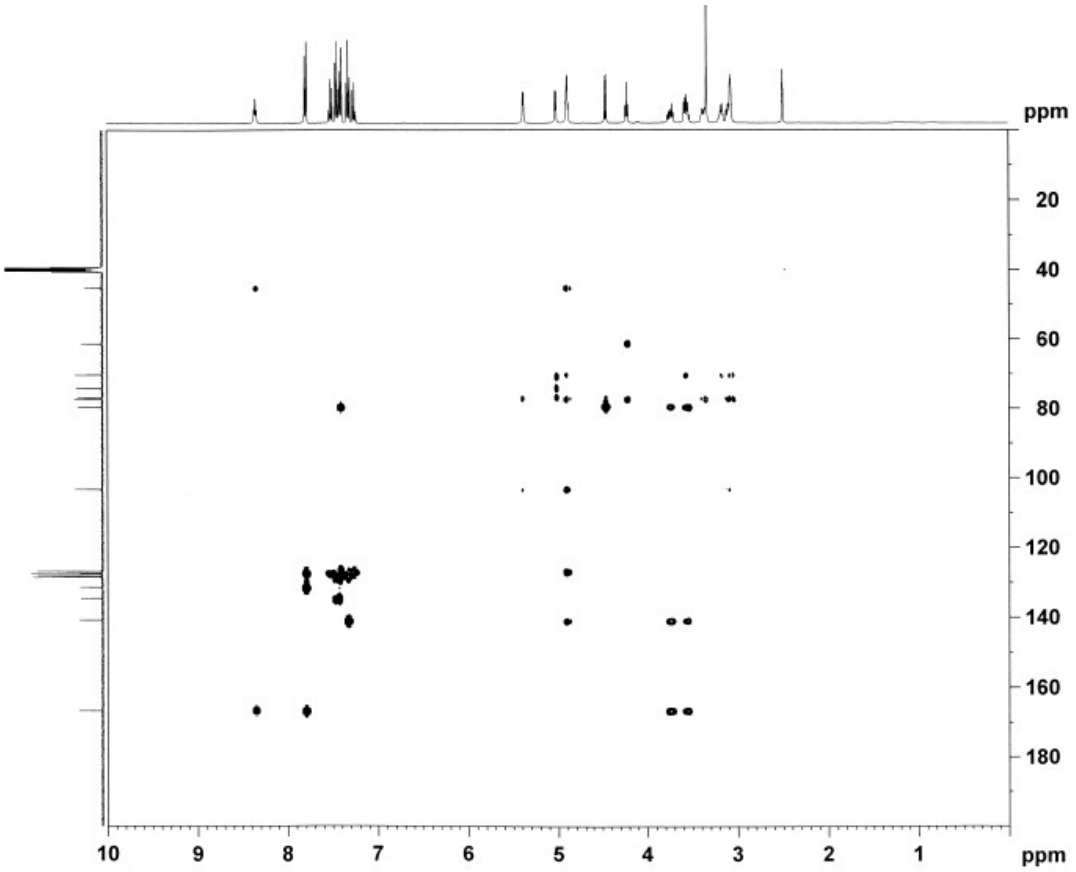


Figure S36. The ^{1}H-^{1}H COSY spectrum of Clausenaside C (3) in DMSO-d_6

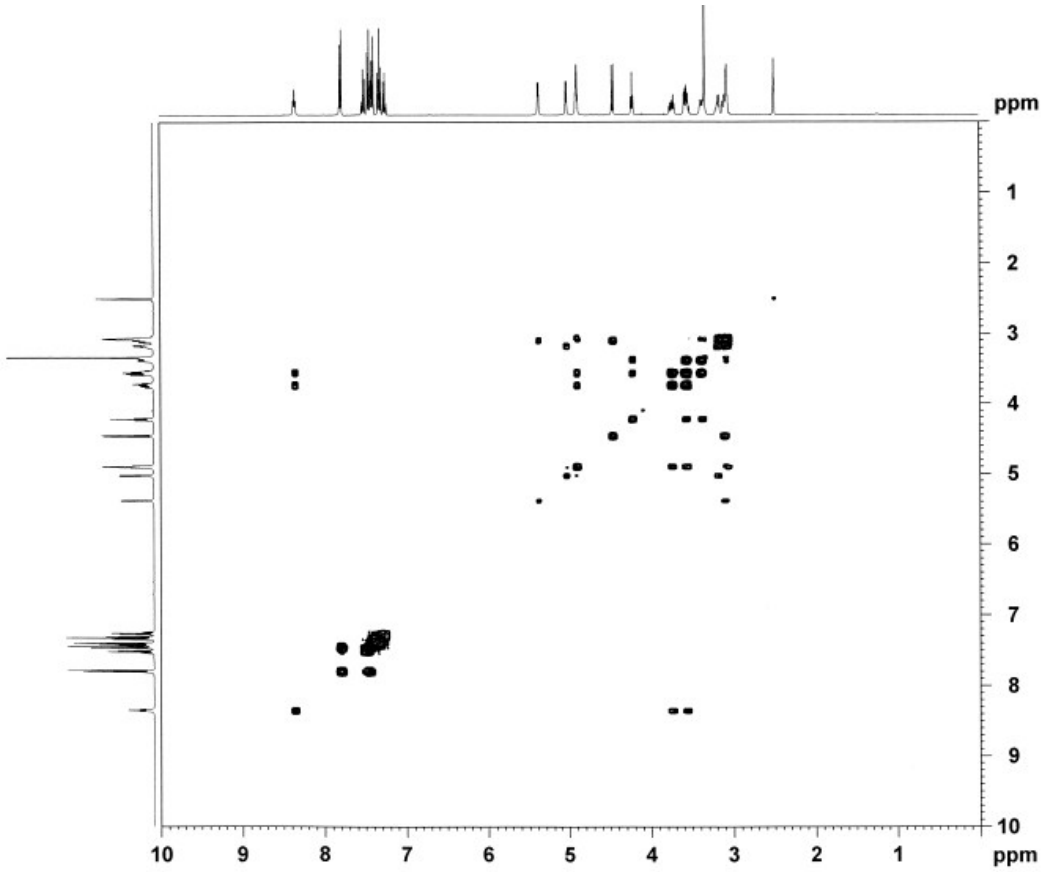


Figure S37. The experimental CD spectrum of Clausenaside C (3)

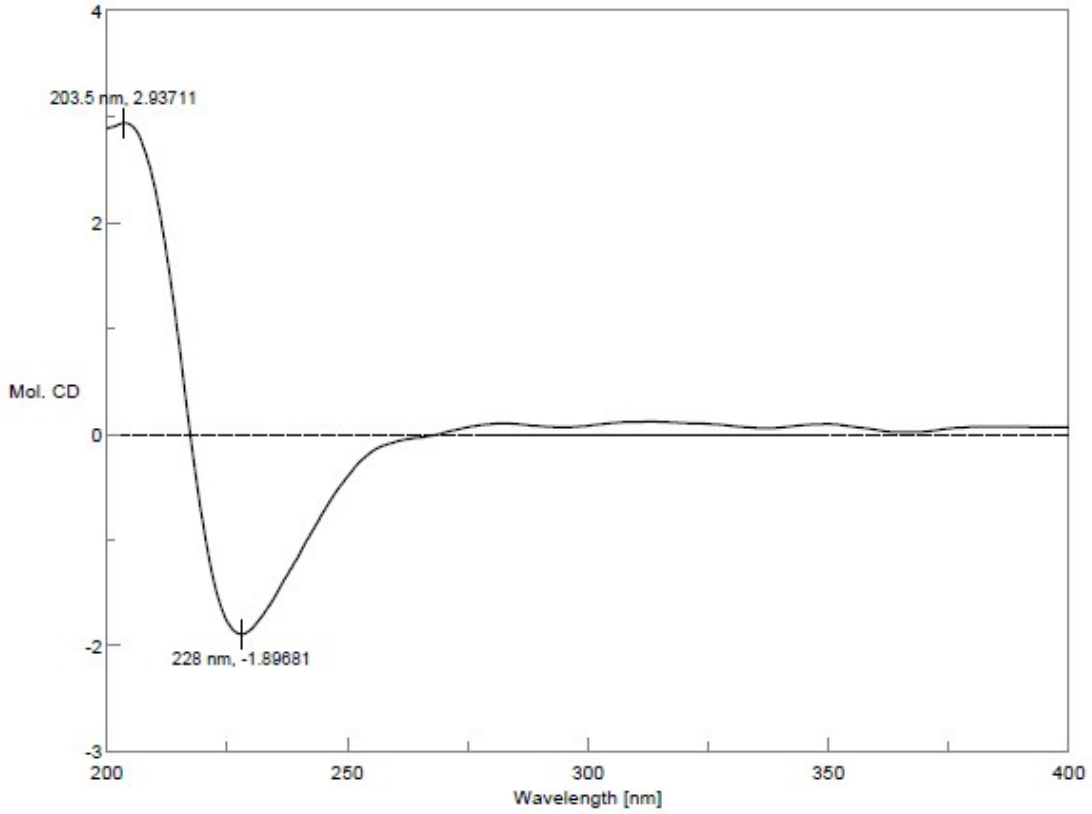


Figure S38. The IR spectrum of Clausenaside C (3)

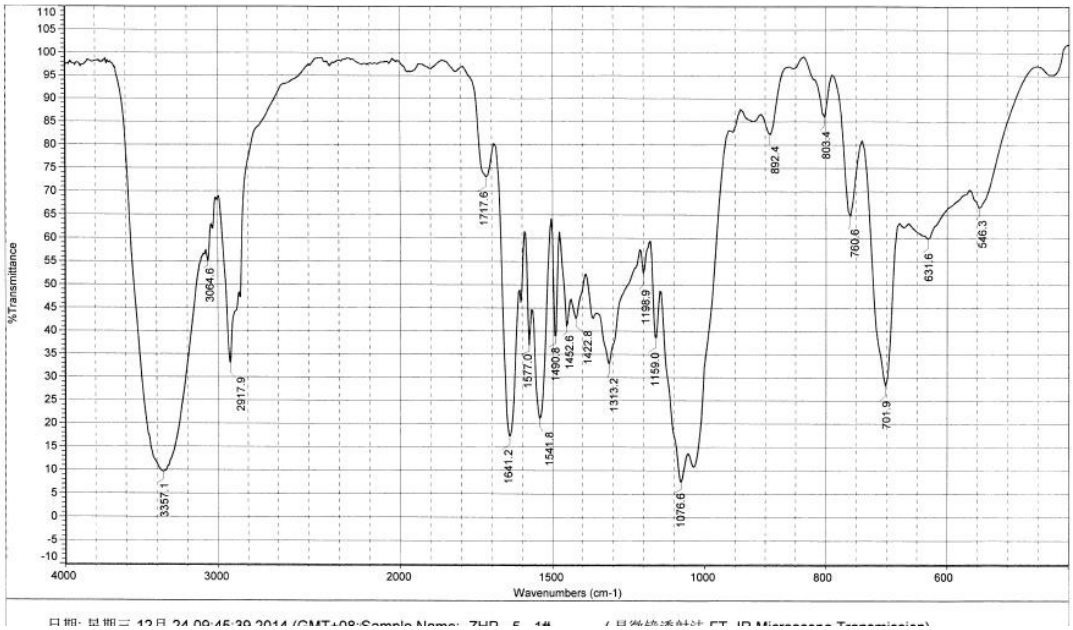


Figure S39. The HRESIMS of Clausenaside C (3)

MS Formula Results: + Scan (5.566 min) Sub (2014031201.d)

m/z	Ion	Formula	Abundance
404.171	(M+H)+	C21 H26 N O7	771528.8

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
☑	C21 H25 N O7	C21 H26 N O7	404.1704	99.91		403.1637	403.1631	-1.46	1.46	99.96	99.81	99.93	404.171	10
☐	C22 H21 N5 O3	C22 H22 N5 O3	404.1717	99.67		403.1637	403.1644	1.84	1.84	99.1	99.92	99.89	404.171	15
☐	C19 H23 N4 O6	C19 H24 N4 O6	404.169	99.59		403.1637	403.1618	-4.8	4.8	99.91	99.91	99.24	404.171	10.5
☐	C24 H23 N2 O4	C24 H24 N2 O4	404.1731	99.12		403.1637	403.1658	5.18	5.18	98.51	99.83	99.12	404.171	14.5
☐	C16 H27 N4 O6 S	C16 H28 N4 O6 S	404.1724	98.79		403.1637	403.1651	3.55	3.55	96.75	99.62	99.59	404.171	5.5
☐	C15 H31 O10 S	C15 H32 O10 S	404.1711	98.09		403.1637	403.1638	0.25	0.25	93.69	99.55	100	404.171	0.5
☐	C20 H27 N4 O S2	C20 H28 N4 O S2	404.1699	97.68		403.1637	403.1626	-2.66	2.66	92.73	99.43	99.77	404.171	9.5
☐	C13 H29 N3 O9 S	C13 H30 N3 O9 S	404.1697	97.62		403.1637	403.1625	-3.1	3.1	92.52	99.6	99.68	404.171	1
☐	C22 H29 N O2 S2	C22 H30 N O2 S2	404.1712	97.59		403.1637	403.164	0.68	0.68	92.07	99.44	99.98	404.171	9

m/z	Ion	Formula	Abundance
426.1524	(M+Na)+	C21 H25 N Na O7	1251080.3

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
☑	C21 H25 N O7	C21 H25 N Na O7	426.1523	99.94		403.1632	403.1631	-0.18	0.18	99.83	99.97	100	426.1524	10
☐	C22 H21 N5 O3	C22 H21 N5 Na O3	426.1537	99.8		403.1632	403.1644	3.12	3.12	99.85	99.93	99.71	426.1524	15
☐	C19 H23 N4 O6	C19 H23 N4 Na O6	426.151	99.64		403.1632	403.1618	-3.52	3.52	99.41	99.95	99.63	426.1524	10.5
☐	C16 H27 N4 O6 S	C16 H27 N4 Na O6 S	426.1544	98.15		403.1632	403.1651	4.83	4.83	94.97	99.67	99.3	426.1524	5.5
☐	C20 H27 N4 O S2	C20 H27 N4 Na O S2	426.1518	97.61		403.1632	403.1626	-1.38	1.38	92.15	99.5	99.94	426.1524	9.5
☐	C22 H29 N O2 S2	C22 H29 N Na O2 S2	426.1532	97.5		403.1632	403.164	1.96	1.96	91.79	99.61	99.88	426.1524	9
☐	C15 H31 O10 S	C15 H31 Na O10 S	426.153	97.37		403.1632	403.1638	1.53	1.53	91.11	99.77	99.93	426.1524	0.5

Figure S40. The ^{1}H NMR (600 MHz) spectrum of Clausenaside D (4) in DMSO-d_6

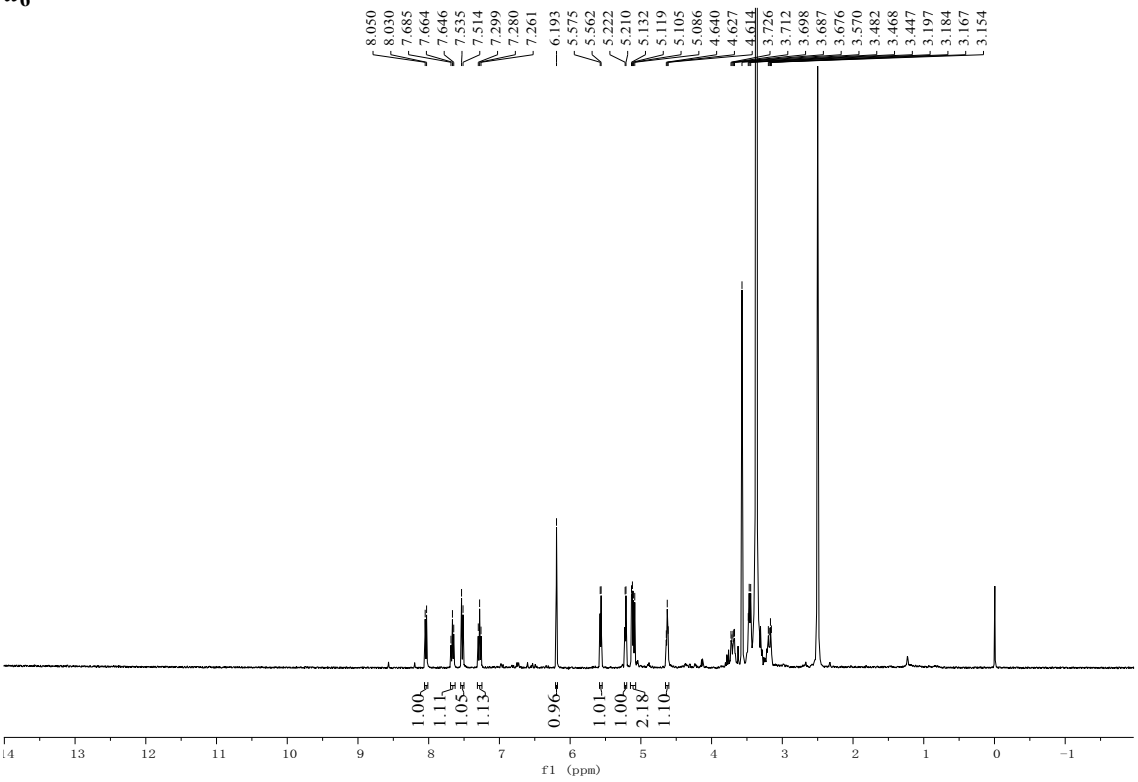


Figure S41. The ^{13}C NMR (150 MHz) spectrum of Clausenaside D (4) in DMSO-d_6

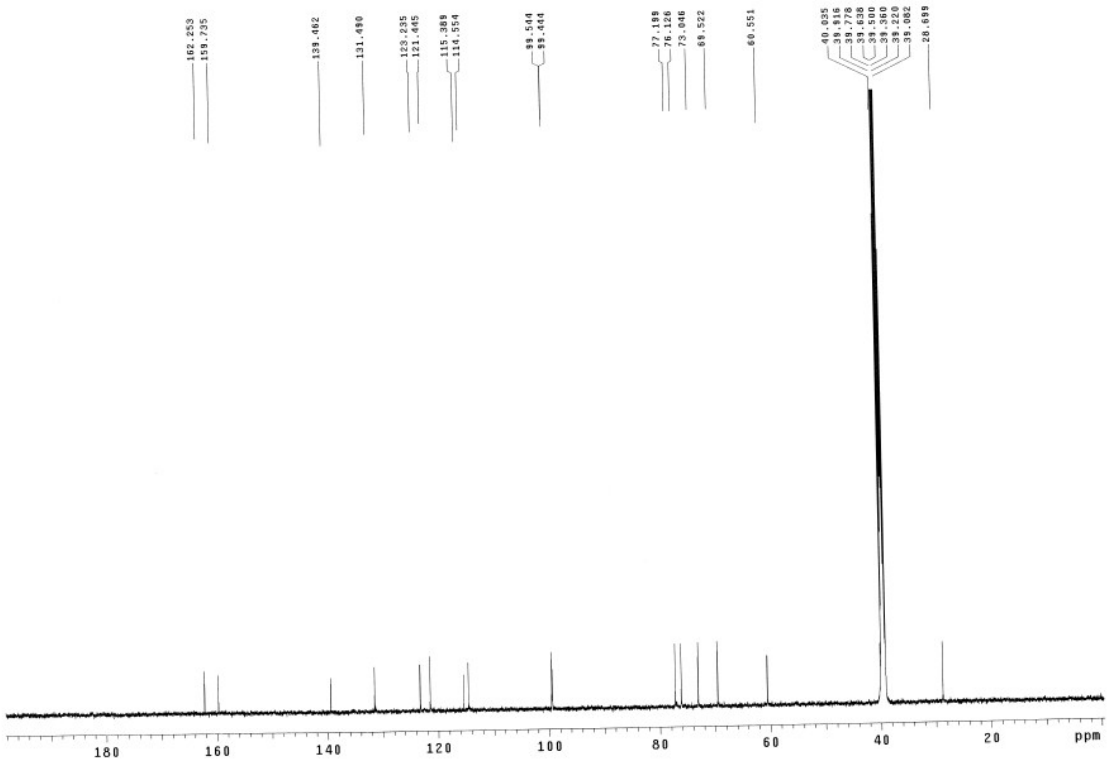


Figure S42. The DEPT spectrum of Clausenaside D (4) in DMSO-d_6

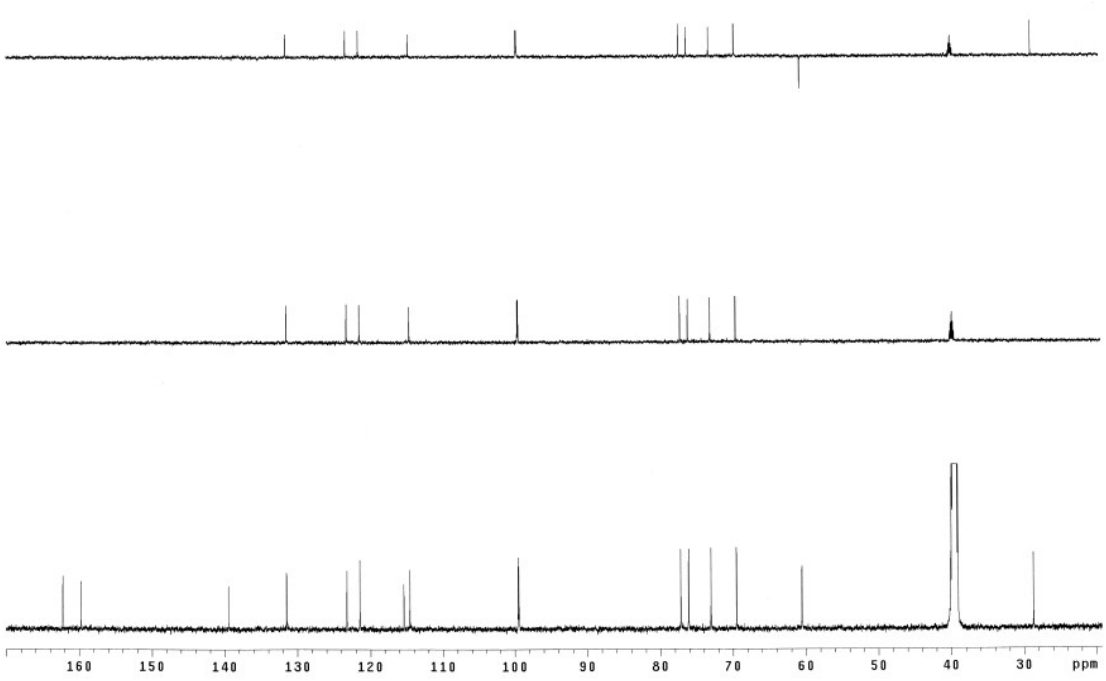


Figure S43. The HSQC spectrum of Clausenaside D (4) in DMSO-d_6

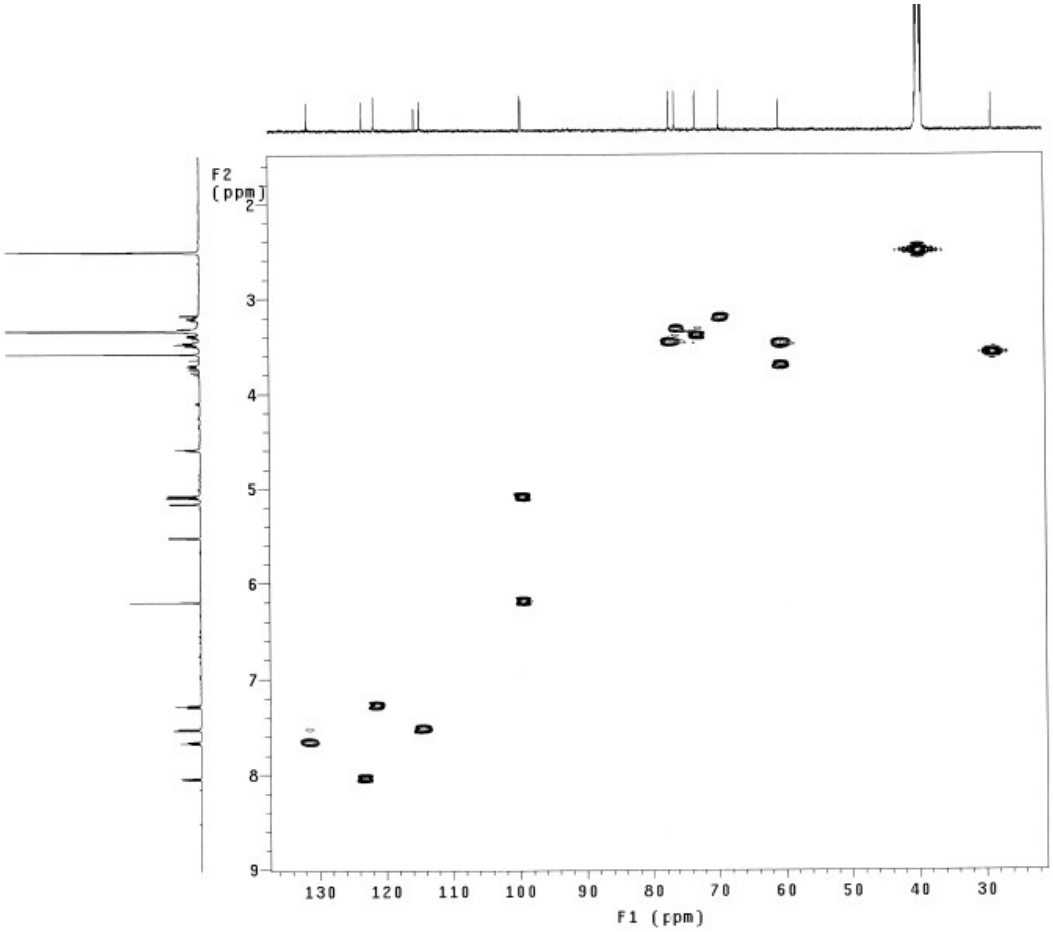


Figure S44. The HMBC spectrum of Clausenaside D (4) in DMSO-d_6

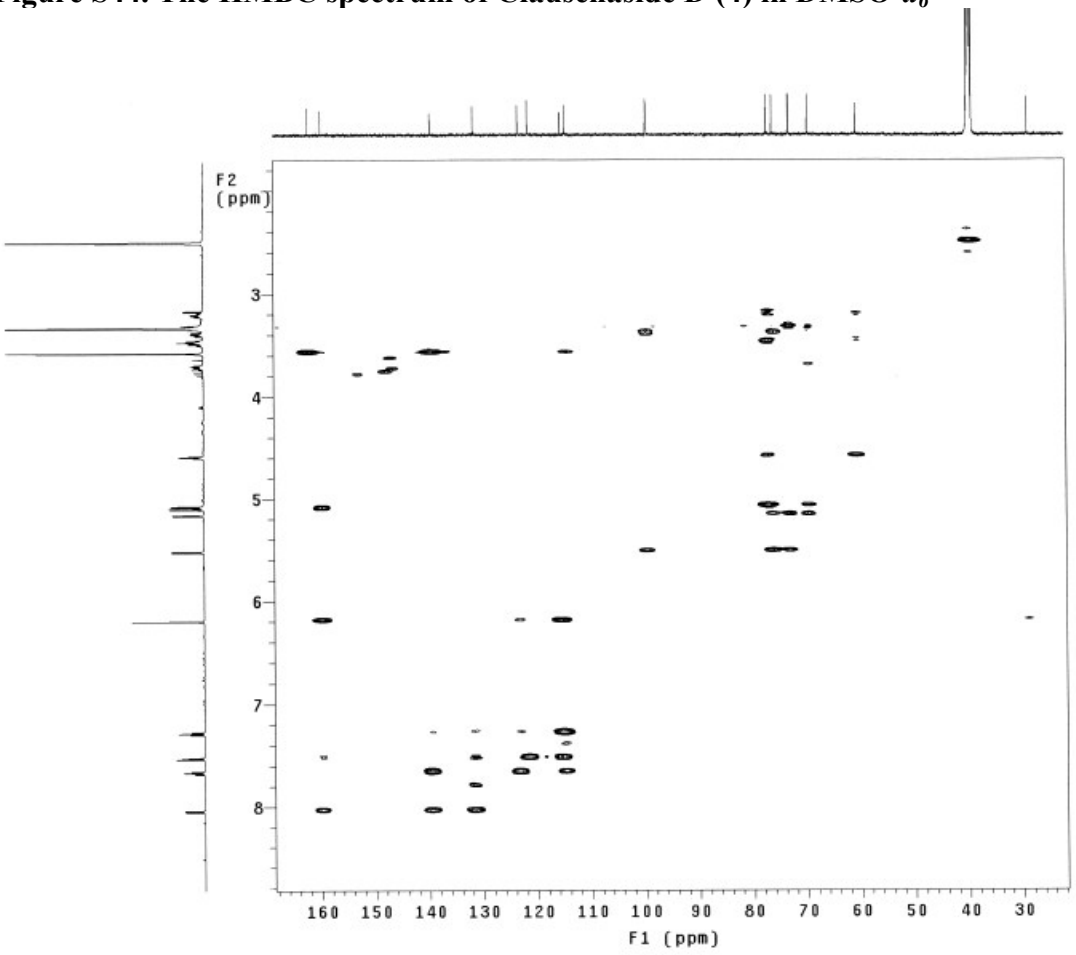


Figure S45. The ^{1}H-^{1}H COSY spectrum of Clausenaside D (4) in DMSO-d_6

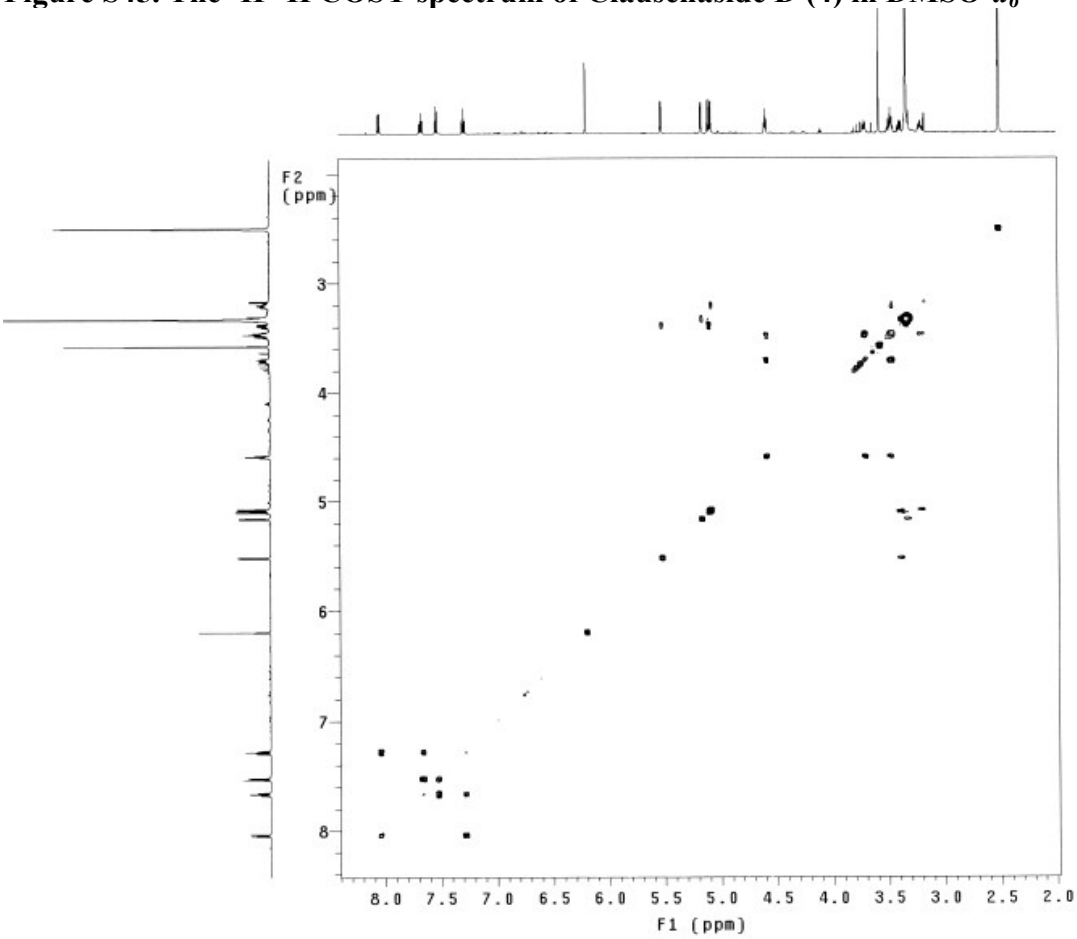


Figure S46. The IR spectrum of Clausenaside D (4)

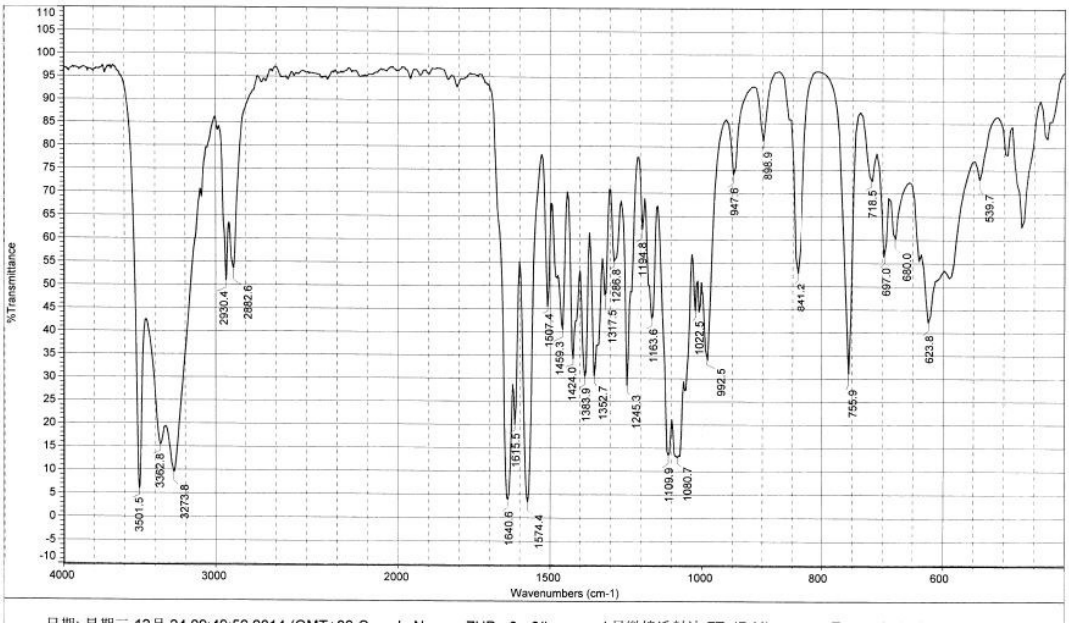


Figure S47. The HRESIMS of Clausenaside D (4)

MS Formula Results: + Scan (4.227 min) Sub (2014051402.d)

m/z	Ion	Formula	Abundance
338.1232	(M+H)+	C16 H20 N O7	118451.9

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
☑	C16 H19 N O7	C16 H20 N O7	338.1234	99.96		337.116	337.1162	0.54	0.54	99.9	99.97	99.99	338.1232	8
☐	C17 H15 N5 O3	C17 H16 N5 O3	338.1248	99.57		337.116	337.1175	4.5	4.5	99.67	99.86	99.36	338.1232	13

Figure S48. The ^{1}H NMR (600 MHz) spectrum of Clausenaside E (5) in DMSO-d_6

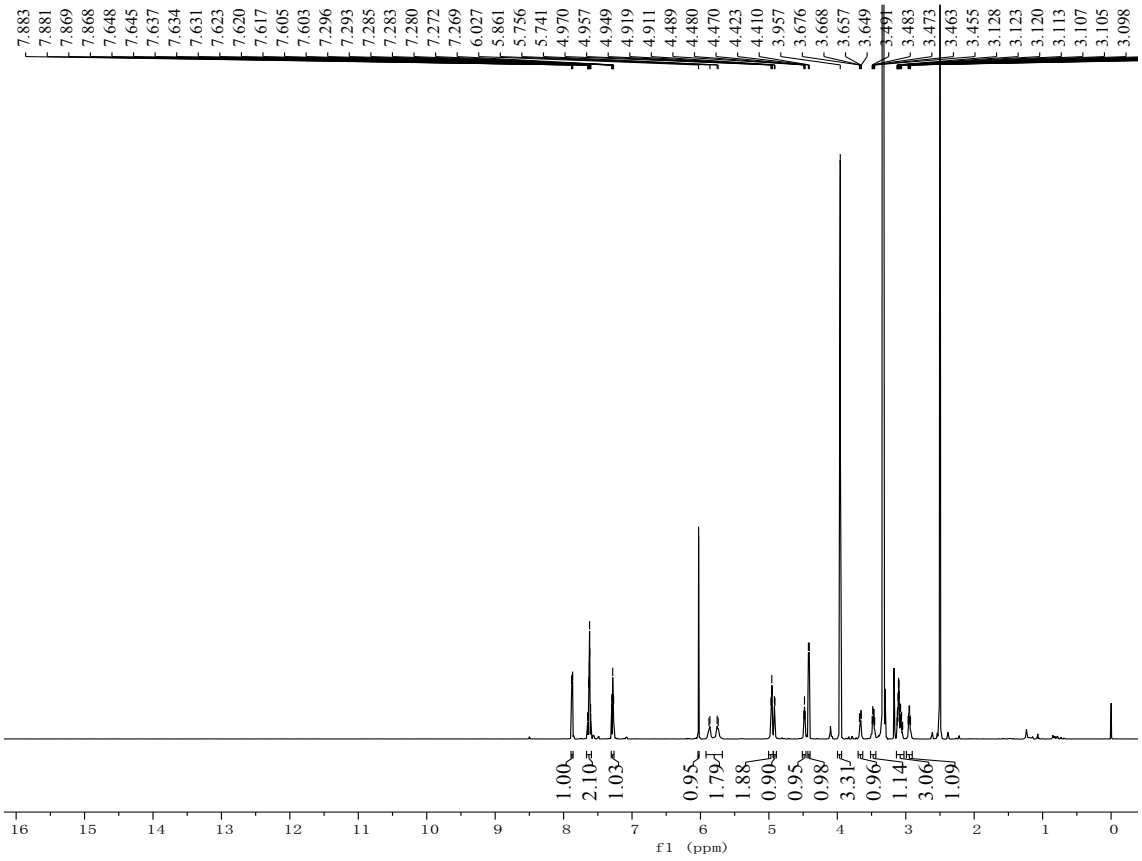


Figure S49. The ^{13}C NMR (150 MHz) spectrum of Clausenaside E (5) in DMSO-d_6

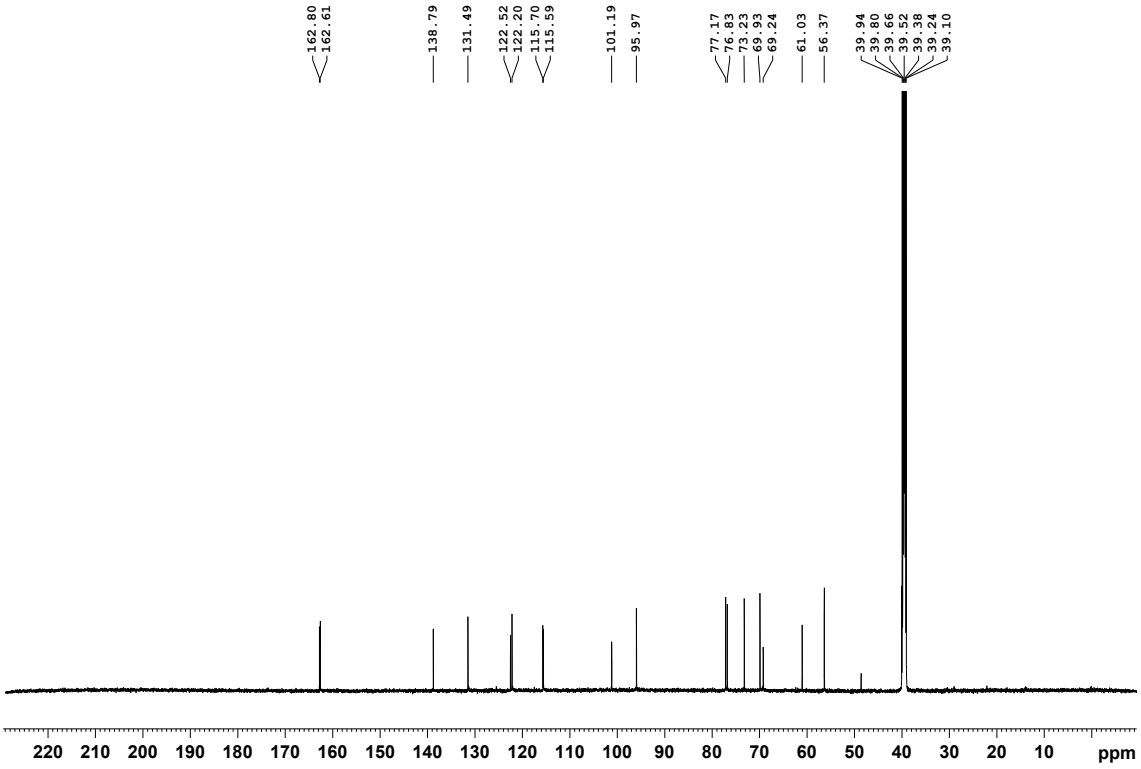


Figure S50. The DEPT spectrum of Clausenaside E (5) in DMSO-d_6

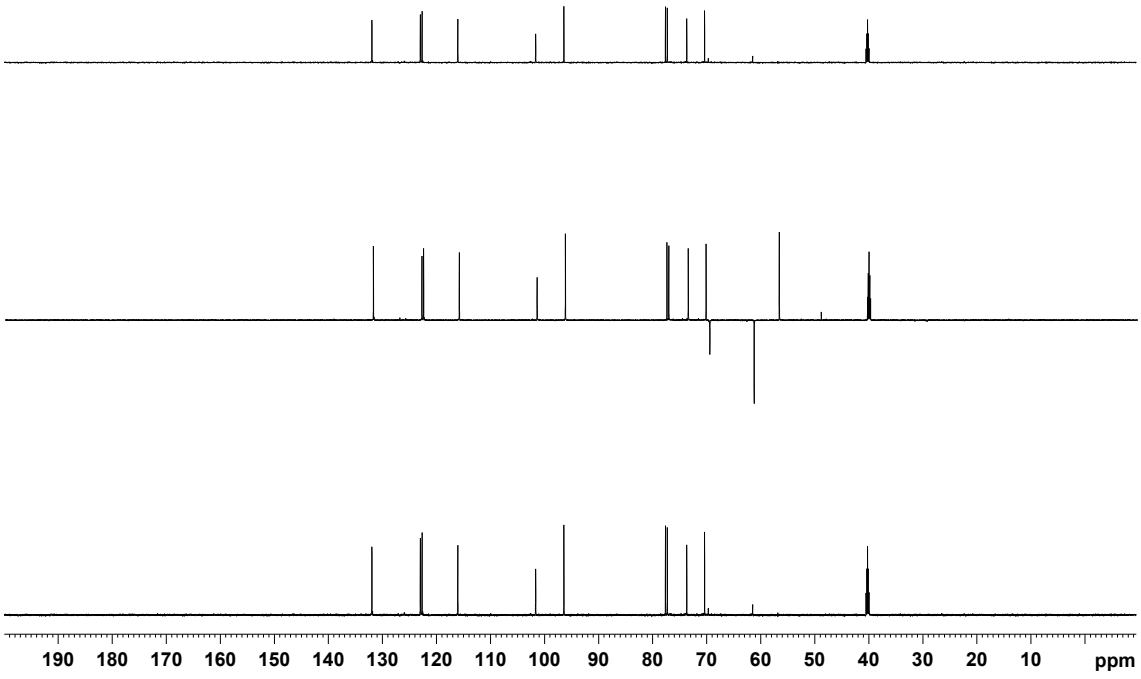


Figure S51. The HSQC spectrum of Clausenaside E (5) in DMSO-d_6

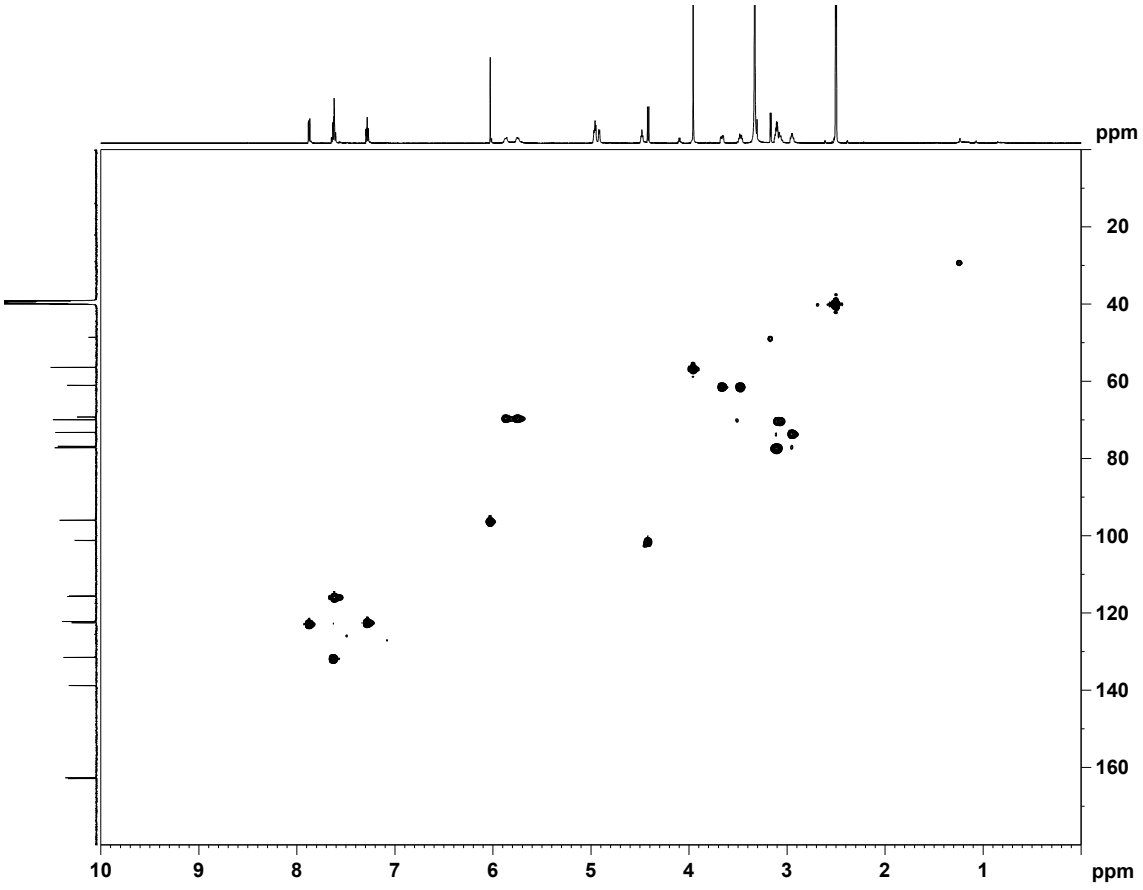


Figure S52. The HMBC spectrum of Clausenaside E (5) in DMSO-d_6

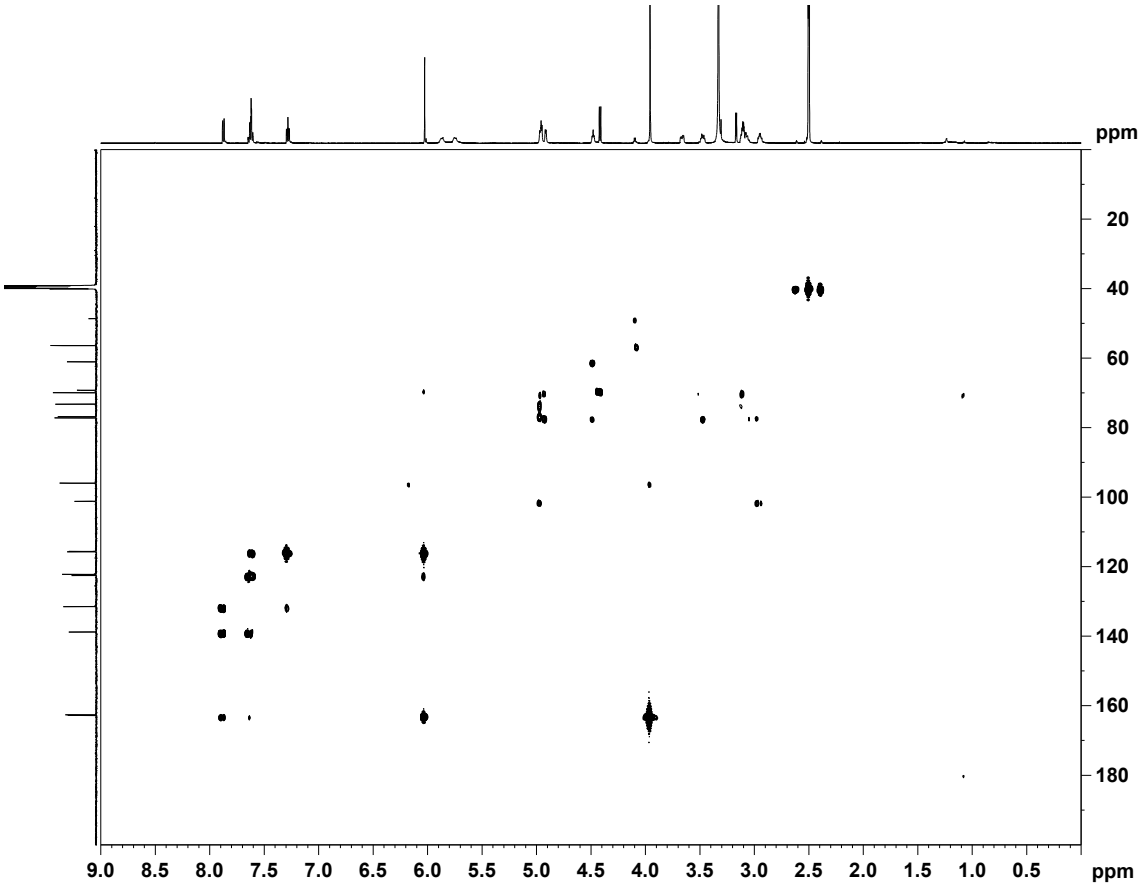


Figure S53. The ^{1}H-^{1}H COSY spectrum of Clausenaside E (5) in DMSO-d_6

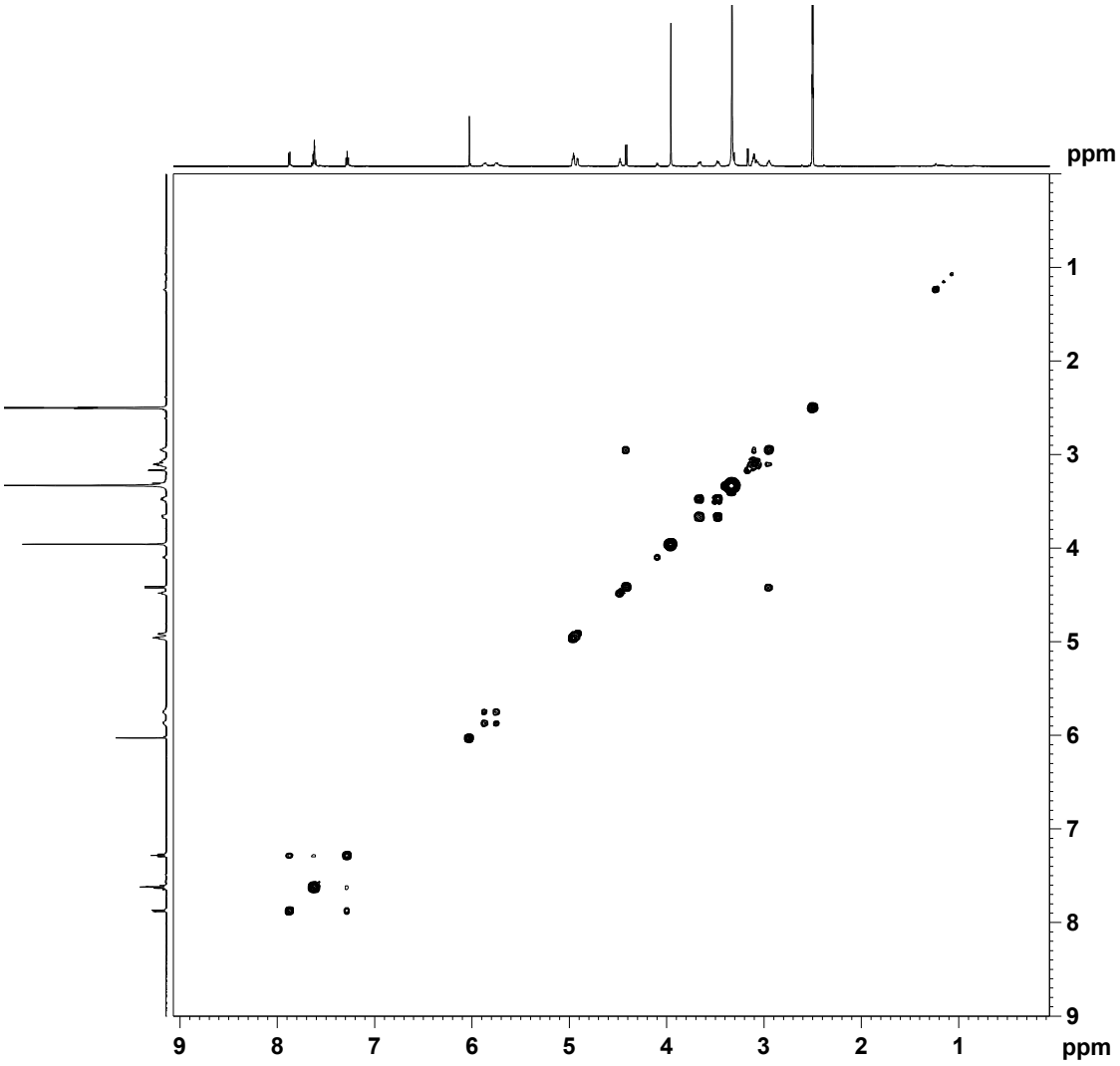


Figure S54. The IR spectrum of Clausenaside E (5)

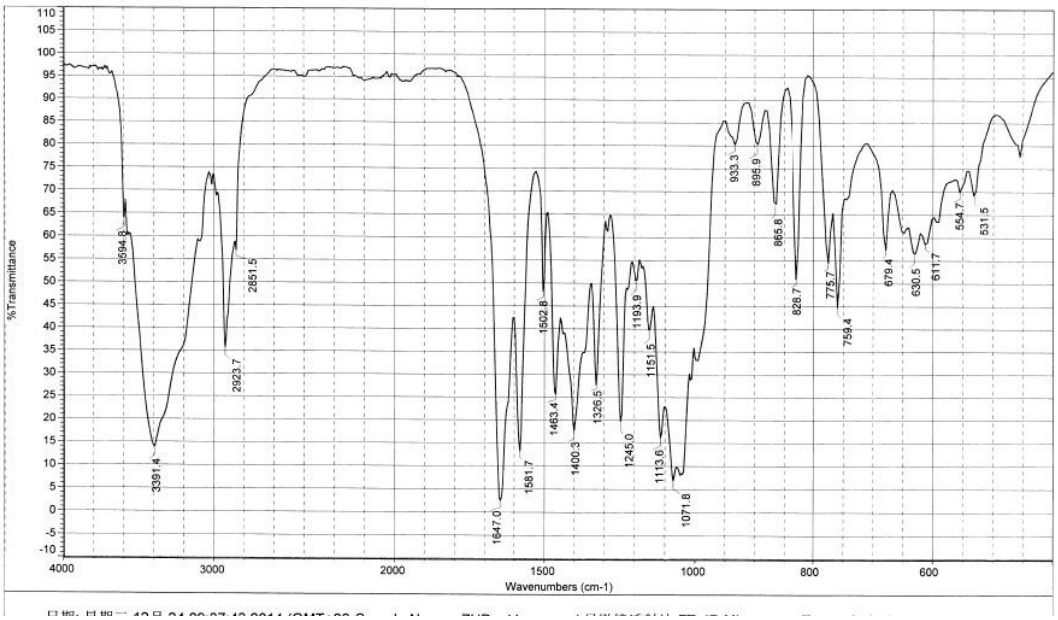


Figure S55. The HRESIMS of Clausenaside E (5)

MS Formula Results: + Scan (5.158 min) Sub (2014090101.d)

	m/z	Ion	Formula	Abundance
-	368.1346	(M+H)+	C17 H22 N O8	889722.2

	Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match	DBE
+	✔	C17 H21 N O8	C17 H22 N O8	99.9		368.134	-1.68	99.91	99.84	99.95	8
+		C14 H22 F N O9	C14 H23 F N O9	99.34		368.1351	1.43	99.93	97.86	99.95	4
+		C16 H23 F N3 O2 P Si	C16 H24 F N3 O2 P Si	99.31		368.1354	2.11	99.86	98.08	99.7	8
+		C19 H22 N3 O P Si	C19 H23 N3 O P Si	98.6		368.1343	-1	99.97	95.34	99.77	12

	m/z	Ion	Formula	Abundance
-	390.1161	(M+Na)+	C17 H21 N Na O8	471258.3

	Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match	DBE
+	✔	C17 H21 N O8	C17 H21 N Na O8	99.96		390.1159	-0.36	100	99.87	99.99	8
+		C14 H22 F N O9	C14 H22 F N Na O9	99.69		390.1171	2.75	99.78	99.28	100	4
+		C20 H19 F N3 O P	C20 H19 F N3 Na O P	98.88		390.1142	-5.1	99.24	97.35	99.99	13
+		C16 H23 F N3 O2 P Si	C16 H23 F N3 Na O2 P Si	98.81		390.1173	3.44	99.66	96.69	99.68	8
+		C17 H22 F N O5 Si	C17 H22 F N Na O5 Si	98.47		390.1143	-4.7	99.36	95.9	99.78	8
+		C19 H22 N3 O P Si	C19 H22 N3 Na O P Si	97.91		390.1162	0.33	100	92.89	99.75	12

Figure S56. The ^{1}H NMR (600 MHz) spectrum of Clausenaside F (6) in MeOH-d_4

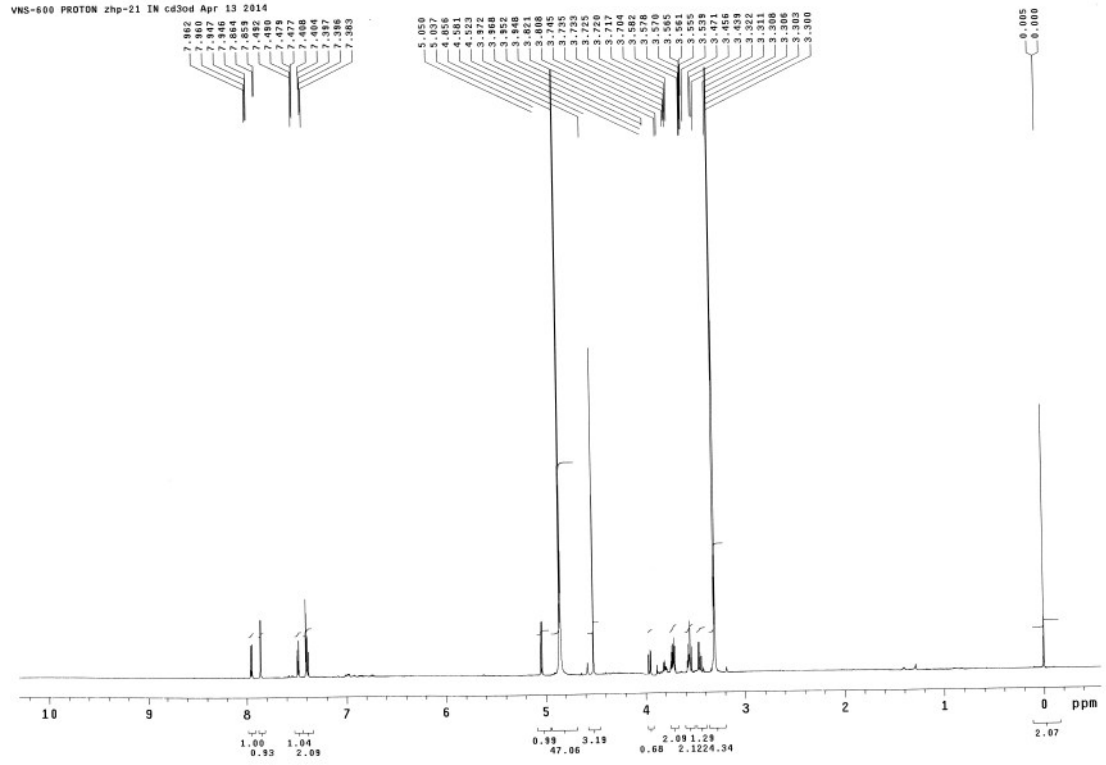


Figure S57. The ^{13}C NMR (150 MHz) spectrum of Clausenaside F (6) in MeOH-d_4

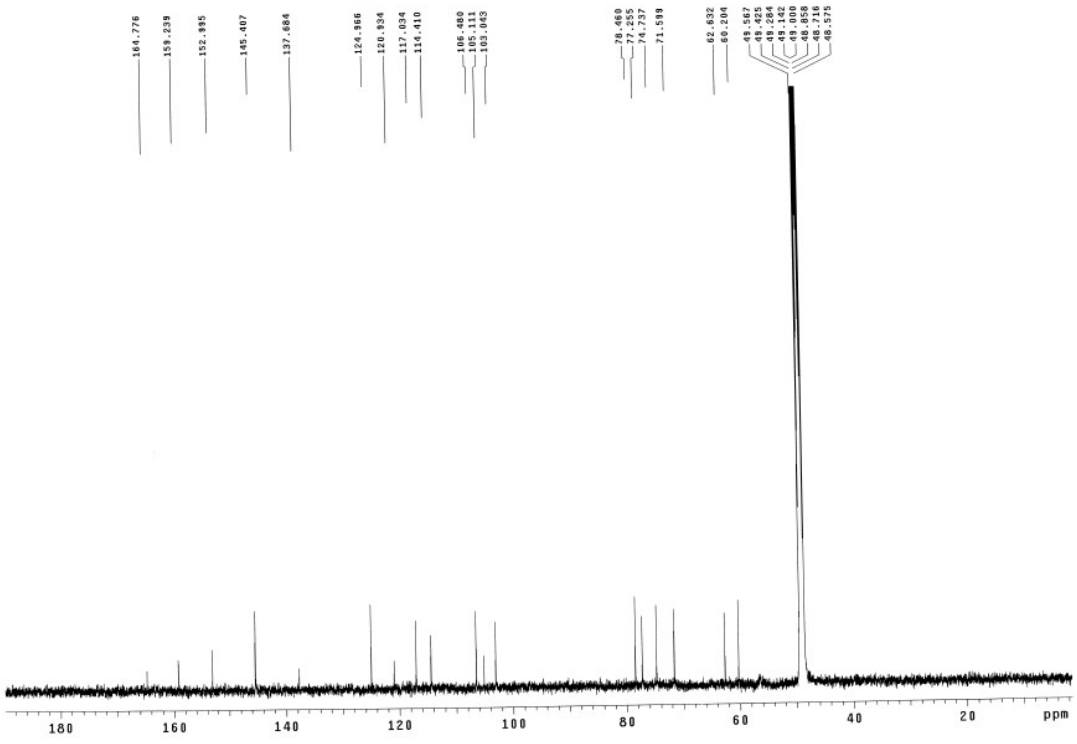


Figure S58. The HSQC spectrum of Clausenaside F (6) in MeOH-d_4

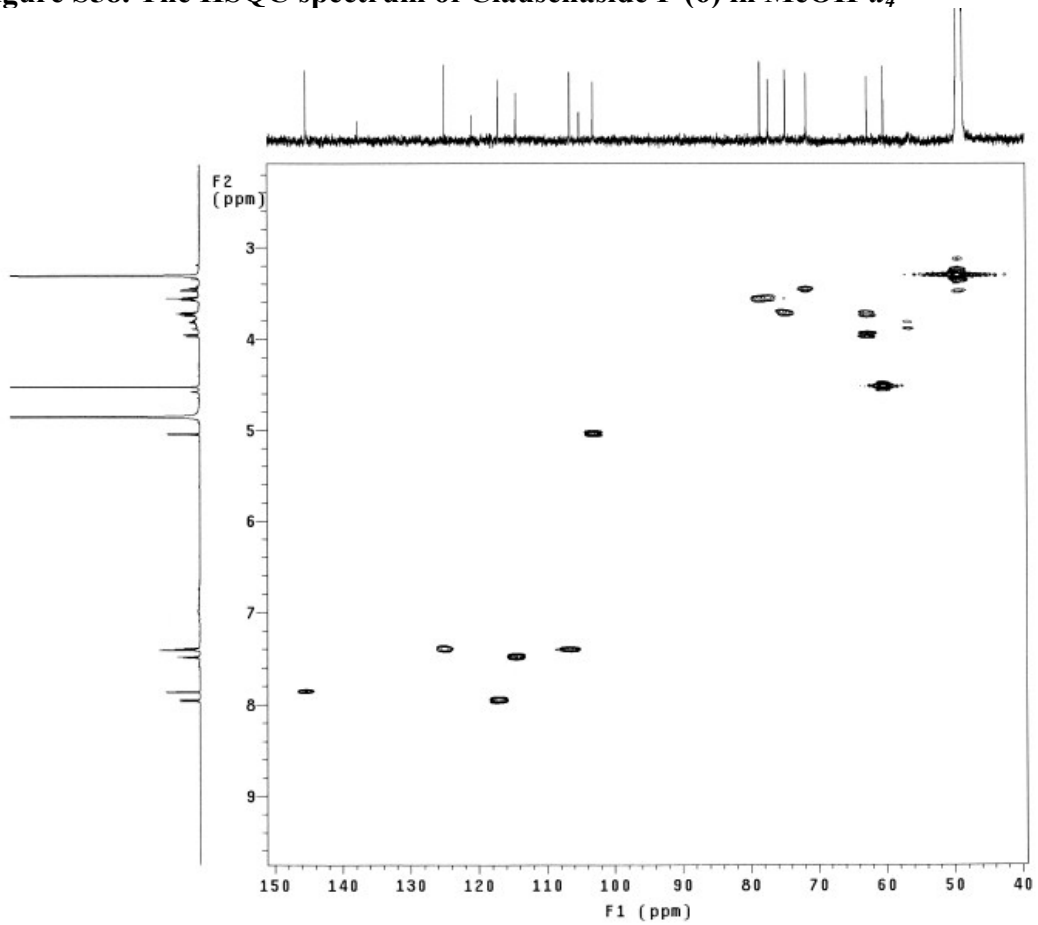


Figure S59. The HMBC spectrum of Clausenaside F (6) in MeOH-d_4

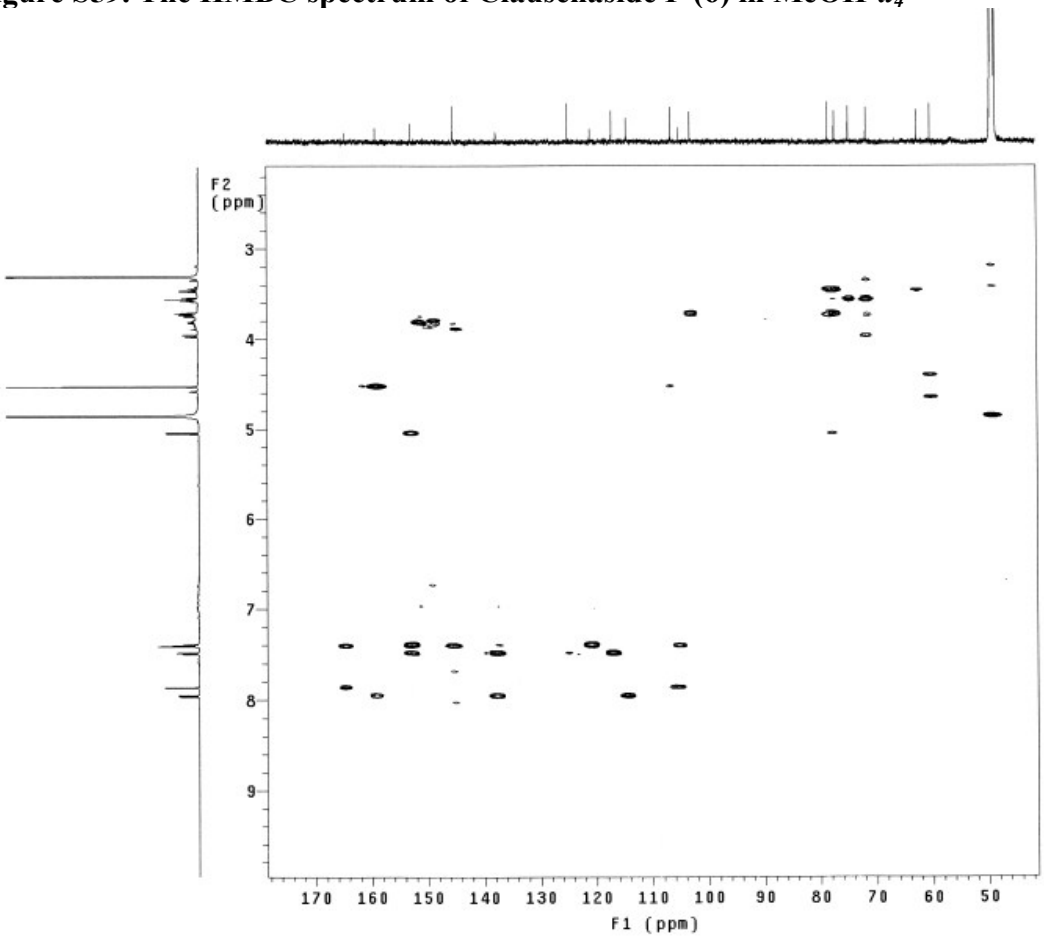


Figure S60. The ^{1}H-^{1}H COSY spectrum of Clausenaside F (6) in MeOH-d_4

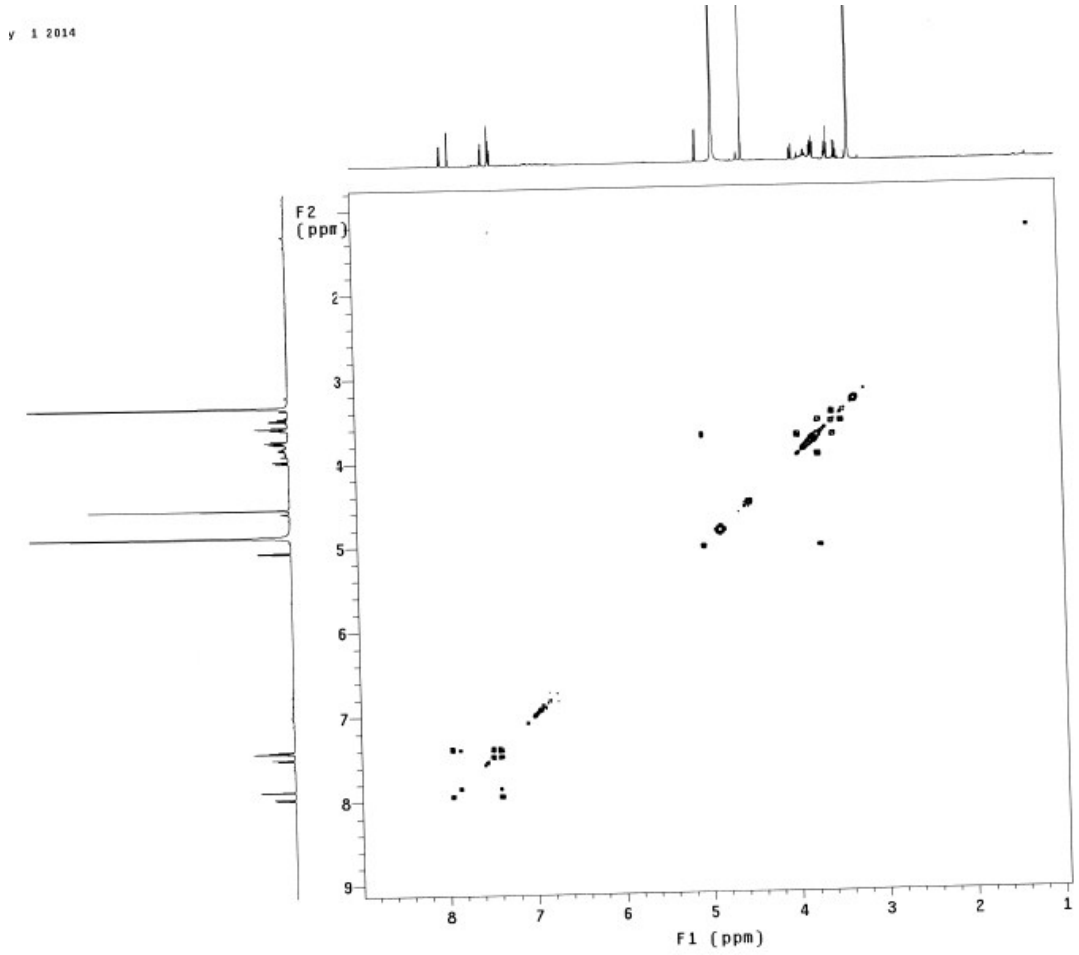


Figure S61. The IR spectrum of Clausenaside F (6)

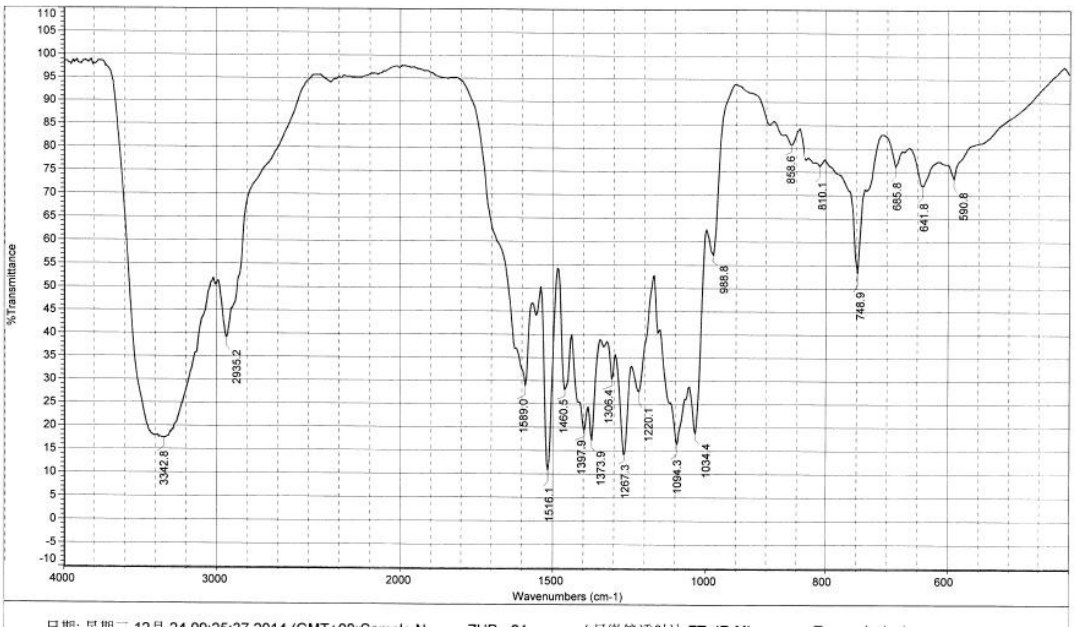


Figure S62. The HRESIMS of Clausenaside F (6)

MS Formula Results: + Scan (5.404 min) Sub (2014031202.d)

m/z	Ion	Formula	Abundance
378.118	(M+H)+	C18 H20 N O8	398447.1

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
☑	C18 H19 N O8	C18 H20 N O8	378.1183	99.97		377.1107	377.1111	0.85	0.85	99.93	100	99.98	378.118	10
☐	C16 H17 N4 O7	C16 H18 N4 O7	378.117	99.77		377.1107	377.1097	-2.72	2.72	99.62	99.98	99.76	378.118	10.5
☐	C19 H15 N5 O4	C19 H16 N5 O4	378.1197	99.61		377.1107	377.1124	4.39	4.39	99.68	99.98	99.38	378.118	15
☐	C22 H19 N O3 S	C22 H20 N O3 S	378.1158	98.42		377.1107	377.1086	-5.79	5.79	96.51	99.73	98.92	378.118	14
☐	C25 H17 N2 S	C25 H18 N2 S	378.1185	98.13		377.1107	377.1112	1.32	1.32	93.76	99.76	99.94	378.118	18.5
☐	C17 H21 N4 O2 S2	C17 H22 N4 O2 S2	378.1179	97.46		377.1108	377.1106	-0.42	0.42	91.66	99.36	99.99	378.118	9.5
☐	C12 H25 O11 S	C12 H26 O11 S	378.119	97.21		377.1107	377.1118	2.68	2.68	90.91	99.64	99.77	378.118	0.5
☐	C19 H23 N O3 S2	C19 H24 N O3 S2	378.1192	97.2		377.1107	377.1119	3.15	3.15	91.19	99.46	99.68	378.118	9

m/z	Ion	Formula	Abundance
400.0999	(M+Na)+	C18 H19 N Na O8	244098.8

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
☑	C18 H19 N O8	C18 H19 N Na O8	400.1003	99.95		377.1107	377.1111	0.96	0.96	99.92	99.95	99.97	400.0999	10
☐	C16 H17 N4 O7	C16 H17 N4 Na O7	400.0989	99.8		377.1107	377.1097	-2.61	2.61	99.62	100	99.8	400.0999	10.5
☐	C19 H15 N5 O4	C19 H15 N5 Na O4	400.1016	99.52		377.1107	377.1124	4.5	4.5	99.32	100	99.41	400.0999	15
☐	C22 H19 N O3 S	C22 H19 N Na O3 S	400.0978	98.63		377.1107	377.1086	-5.68	5.68	97.07	99.66	99.06	400.0999	14
☐	C25 H17 N2 S	C25 H17 N2 Na S	400.1005	98.2		377.1107	377.1112	1.43	1.43	94.03	99.71	99.94	400.0999	18.5
☐	C17 H21 N4 O2 S2	C17 H21 N4 Na O2 S2	400.0998	97.91		377.1107	377.1106	-0.31	0.31	93.27	99.29	100	400.0999	9.5
☐	C19 H23 N O3 S2	C19 H23 N Na O3 S2	400.1012	97.63		377.1107	377.1119	3.26	3.26	92.77	99.36	99.69	400.0999	9
☐	C12 H25 O11 S	C12 H25 Na O11 S	400.101	97.62		377.1107	377.1118	2.79	2.79	92.44	99.55	99.77	400.0999	0.5
☐	C10 H23 N3 O10 S	C10 H23 N3 Na O10 S	400.0996	97.27		377.1107	377.1104	-0.78	0.78	90.87	99.52	99.96	400.0999	1
☐	C16 H25 O6 S2	C16 H25 Na O6 S2	400.0985	97.18		377.1107	377.1093	-3.85	3.85	91.41	99.33	99.57	400.0999	4.5

Figure S63. The ^{1}H NMR (600 MHz) spectrum of Clausenaside G (7) in DMSO-d_6

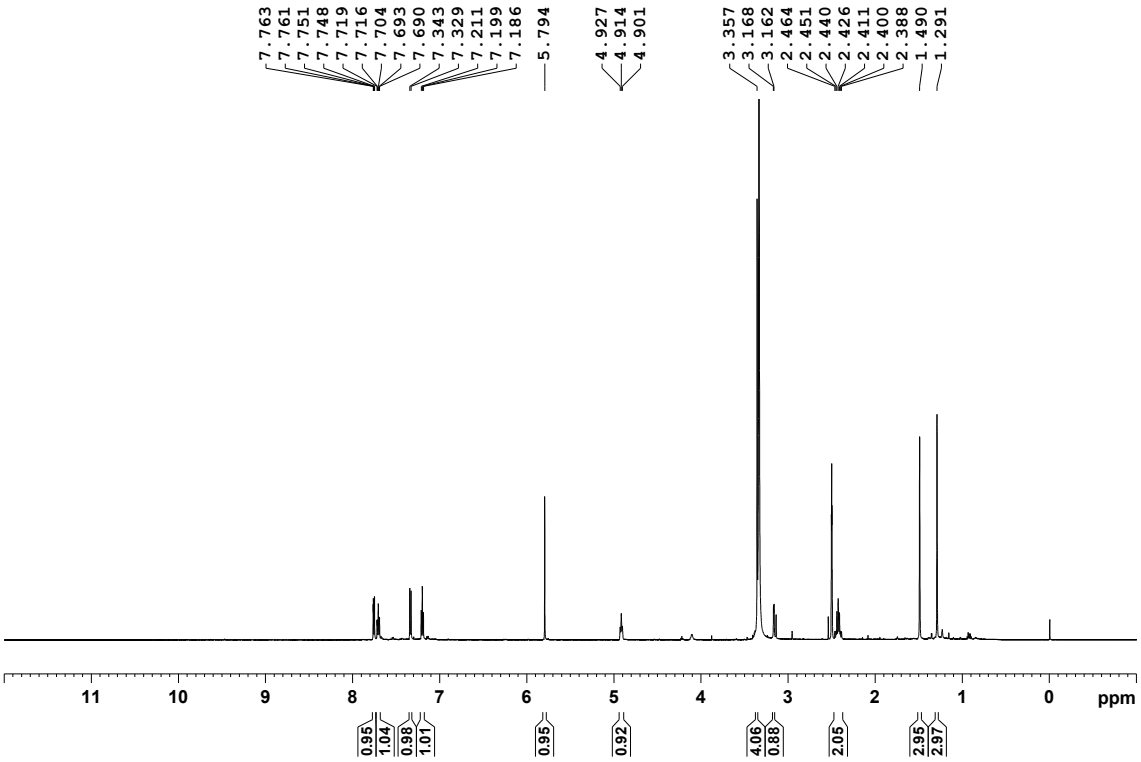


Figure S64. The ^{13}C NMR (150 MHz) spectrum of Clausenaside G (7) in DMSO-d_6

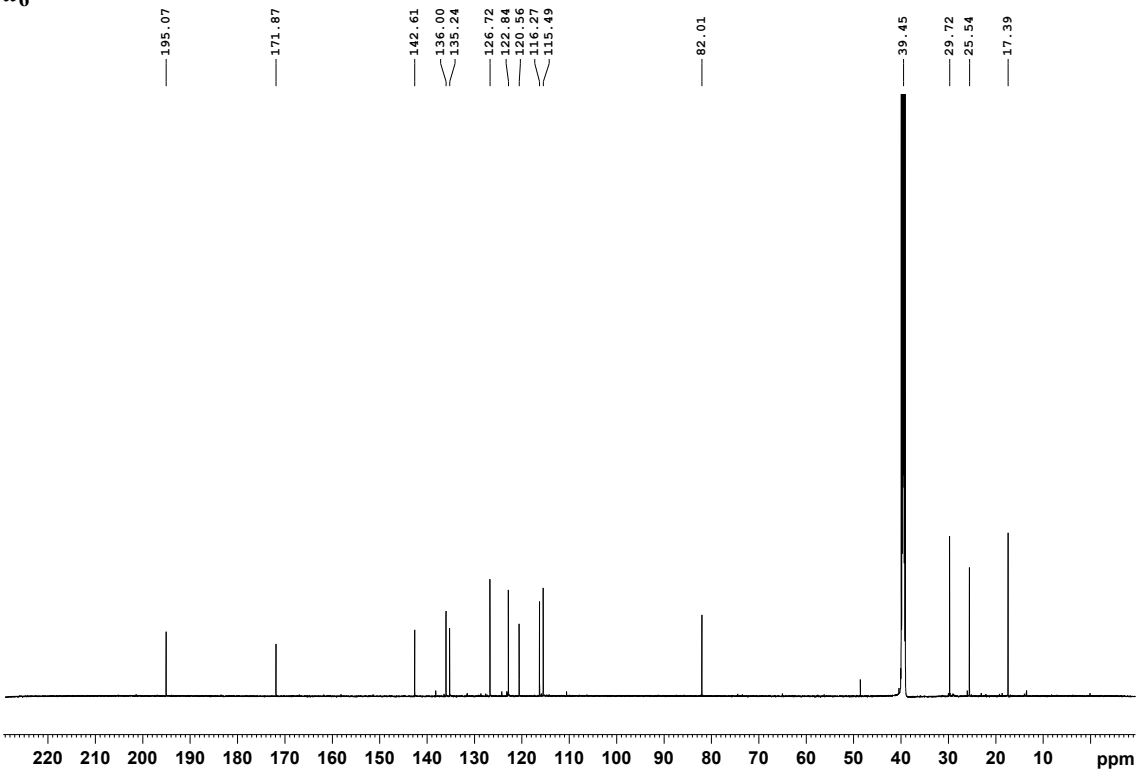


Figure S65. The HSQC spectrum of Clausenaside G (7) in DMSO-d_6

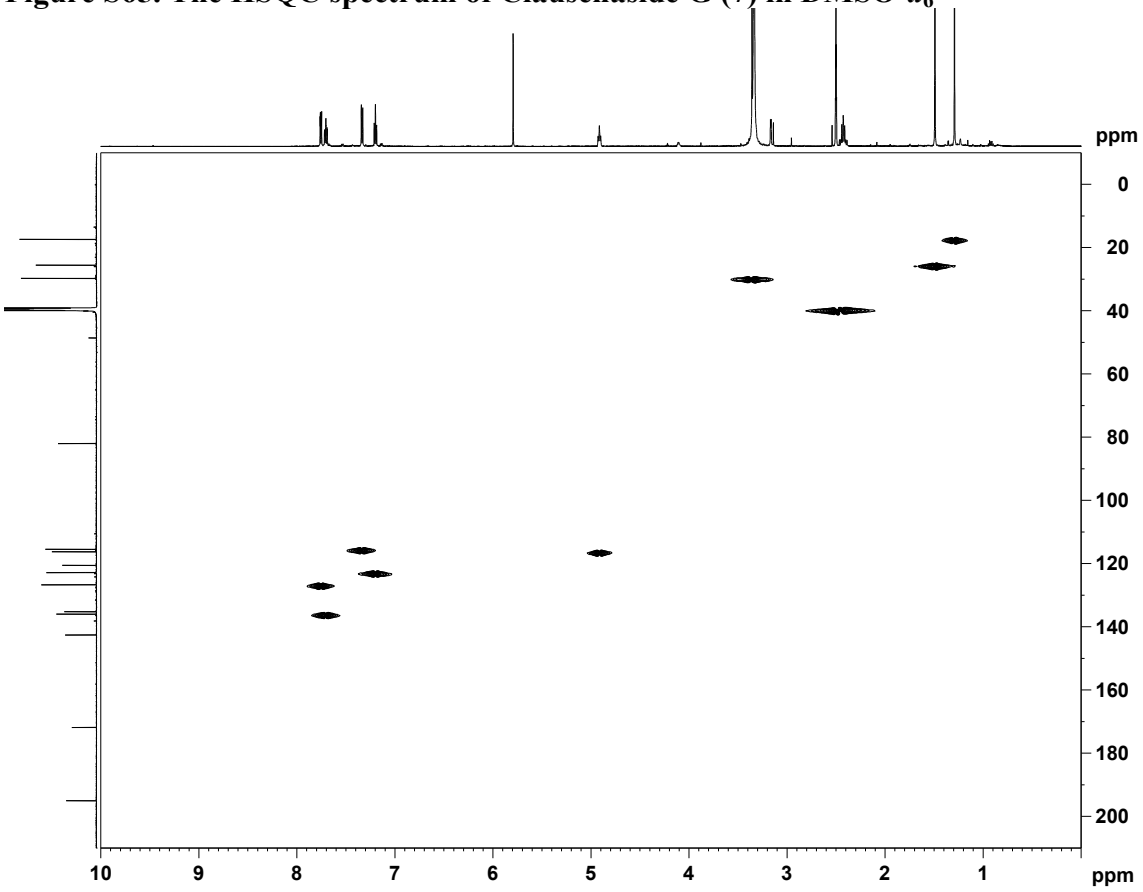


Figure S66. The HMBC spectrum of Clausenaside G (7) in DMSO-d_6

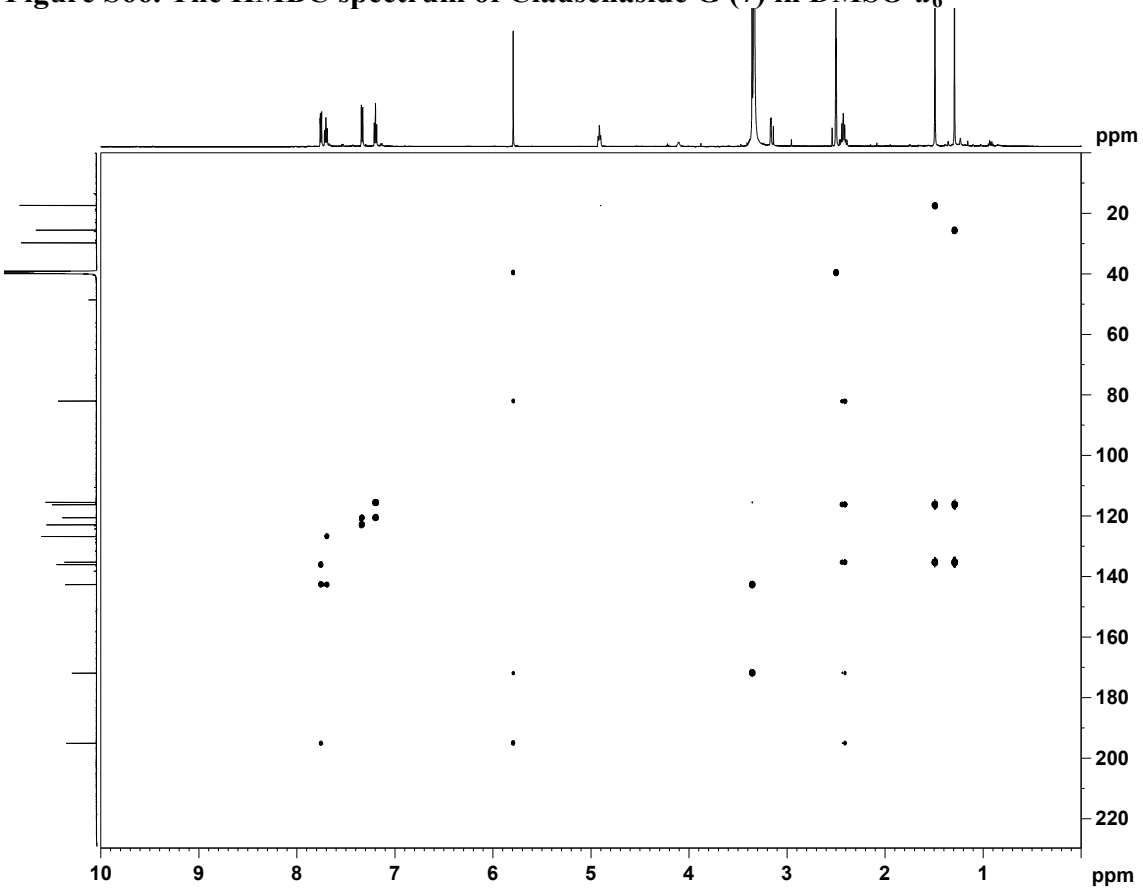


Figure S67. The ^{1}H-^{1}H COSY spectrum of Clausenaside G (7) in DMSO-d_6

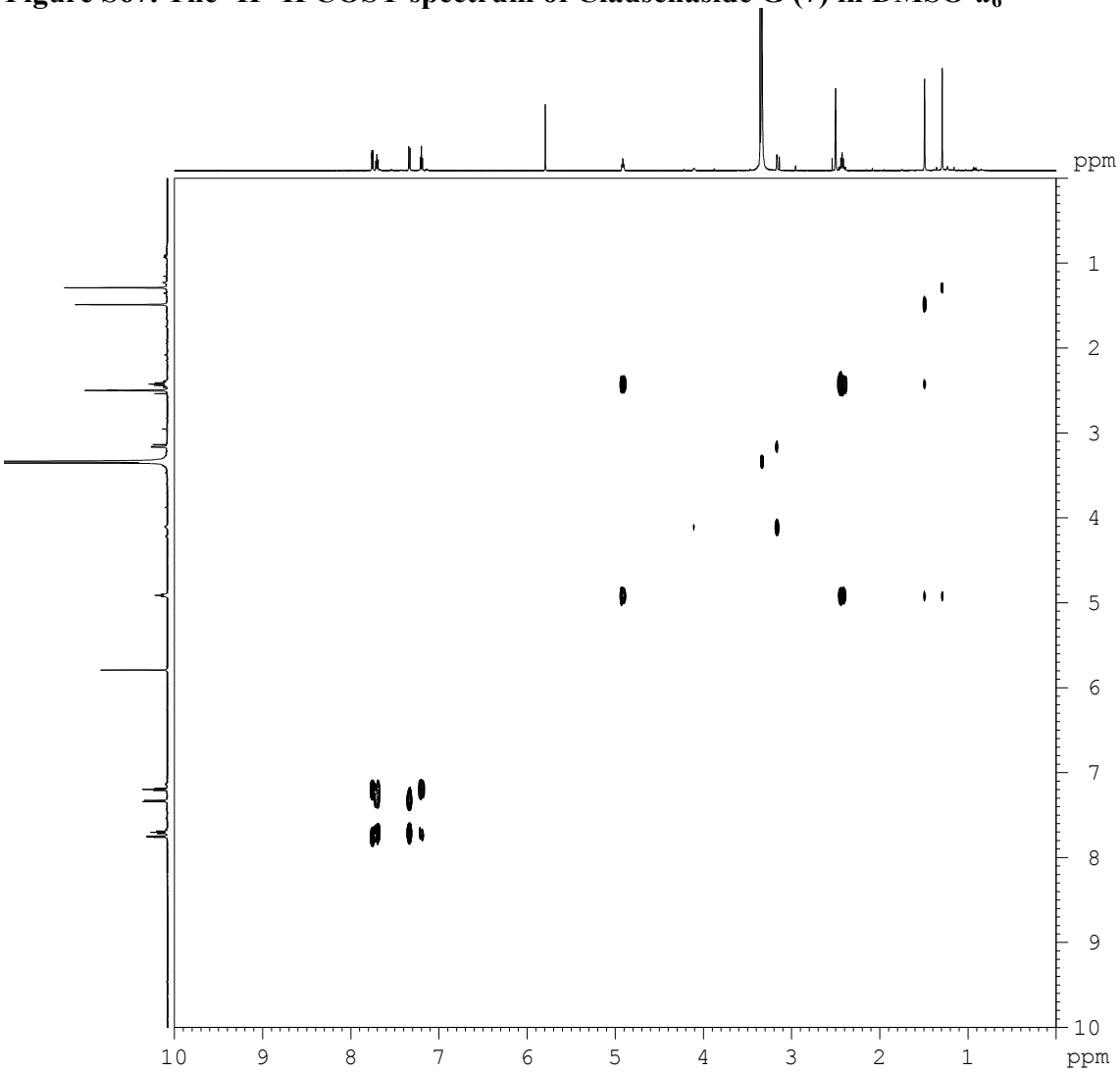


Figure S68. The IR spectrum of Clausenaside G (7)

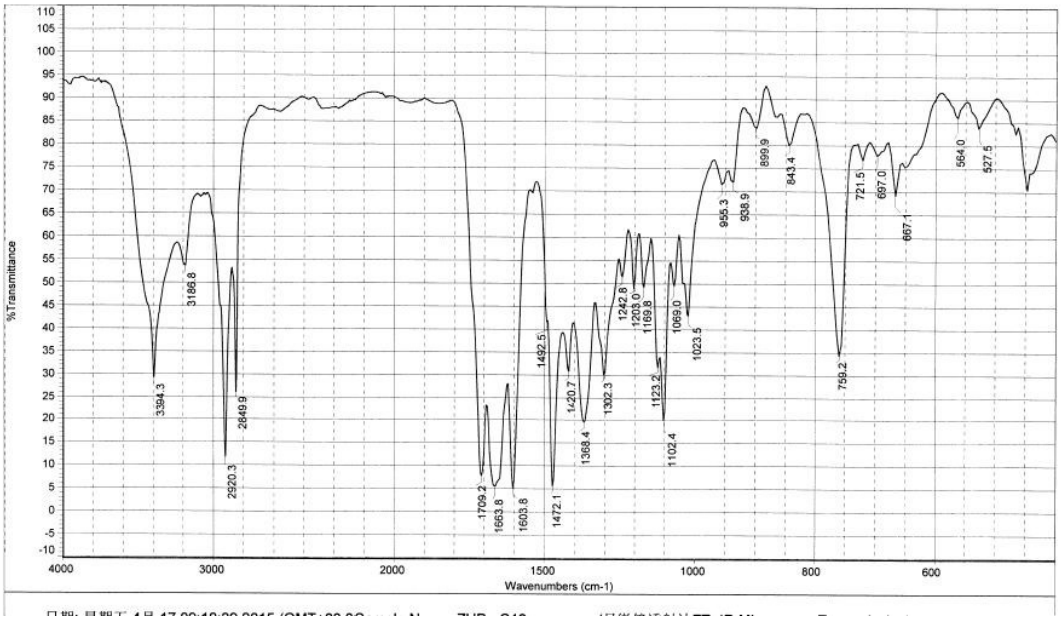


Figure S69. The HRESIMS of Clausenaside G (7)

MS Formula Results: + Scan (6.414 min) Sub (2014110201.d)

	m/z	Ion	Formula	Abundance
-	282.1107	(M+Na)+	C15 H17 N Na O3	361227.5

	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
+	☑	C15 H17 N O3	C15 H17 N Na O3	98.24		259.1215	259.1208	282.1101	-2.49	2.49	99.84	97.03	96.49	8

Figure S70. Two conformations of Clausenaside G (7)

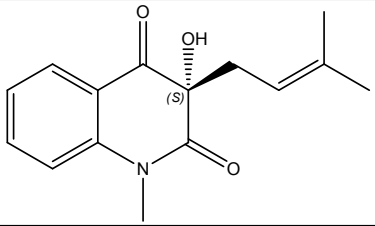
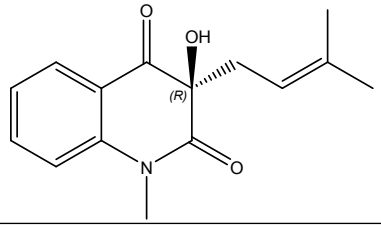
7a	
7b	

Figure S71. Calculated ECD spectra of 3*S* (7a), Calculated ECD spectra of 3*R* (7b) and experimental ECD spetrum of Clausenaside G (7)

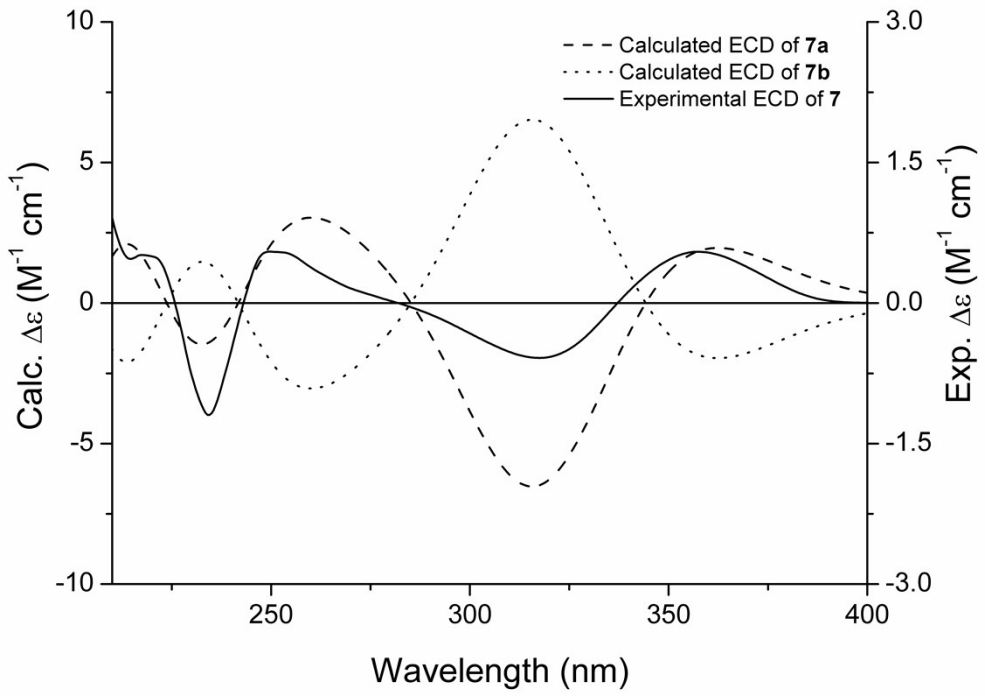


Figure S72. The ^{1}H NMR (400 MHz) spectrum of Clausenaside H (8) in DMSO-*d*$_6$

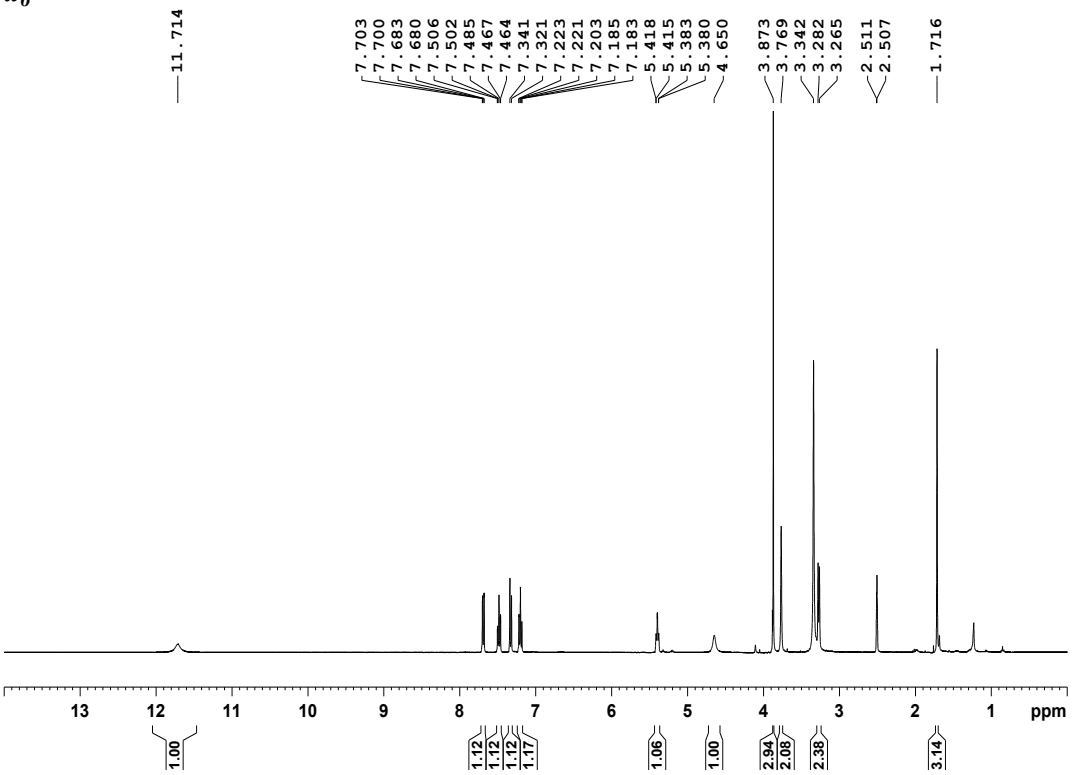


Figure S73. The ^{13}C NMR (100 MHz) spectrum of Clausenaside H (8) in DMSO-d_6

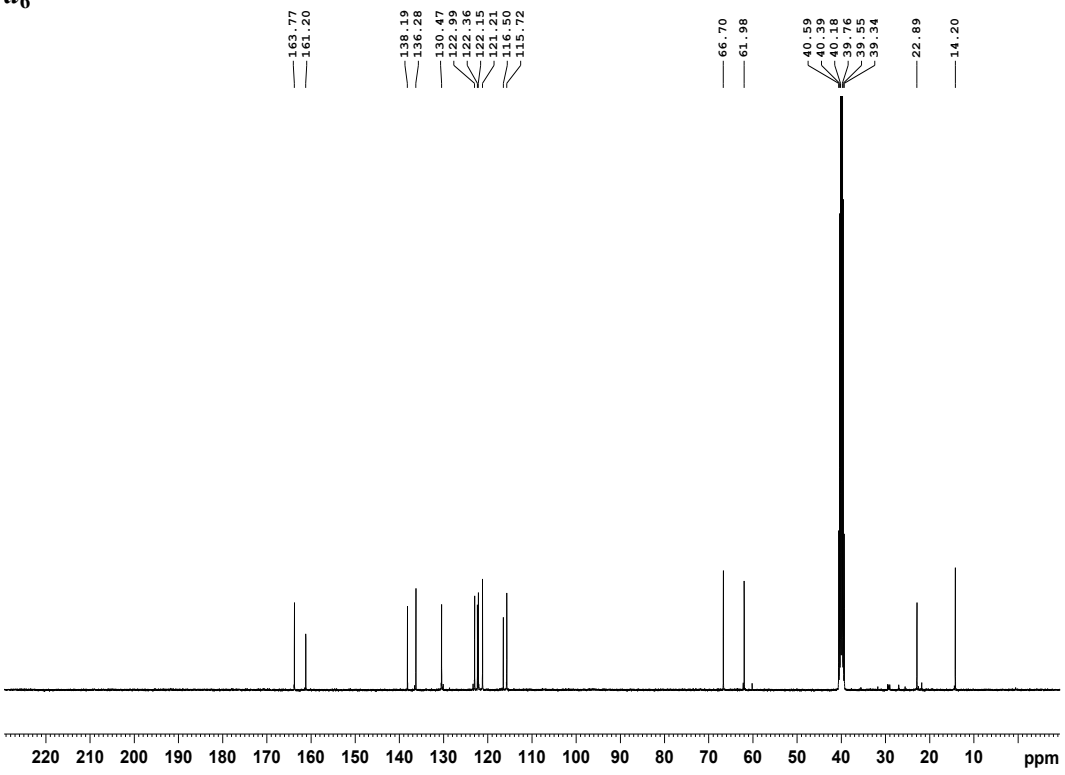


Figure S74. The DEPT spectrum of Clausenaside H (8) in DMSO-d_6

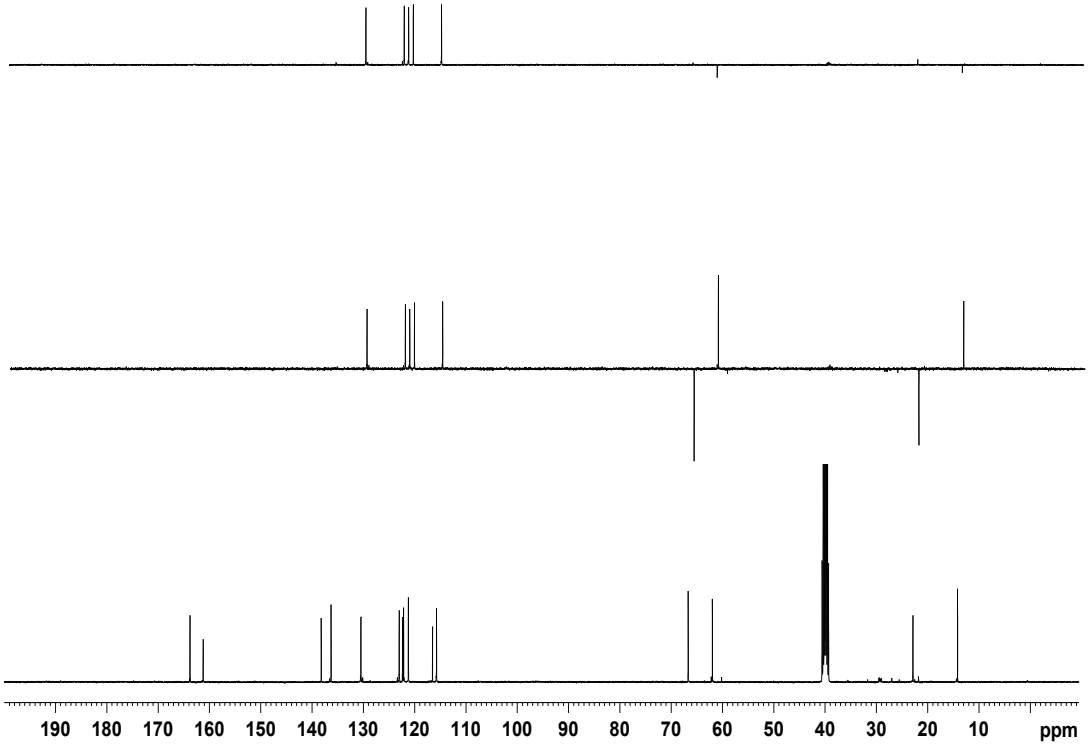


Figure S75. The HSQC spectrum of Clausenaside H (8) in DMSO-d_6

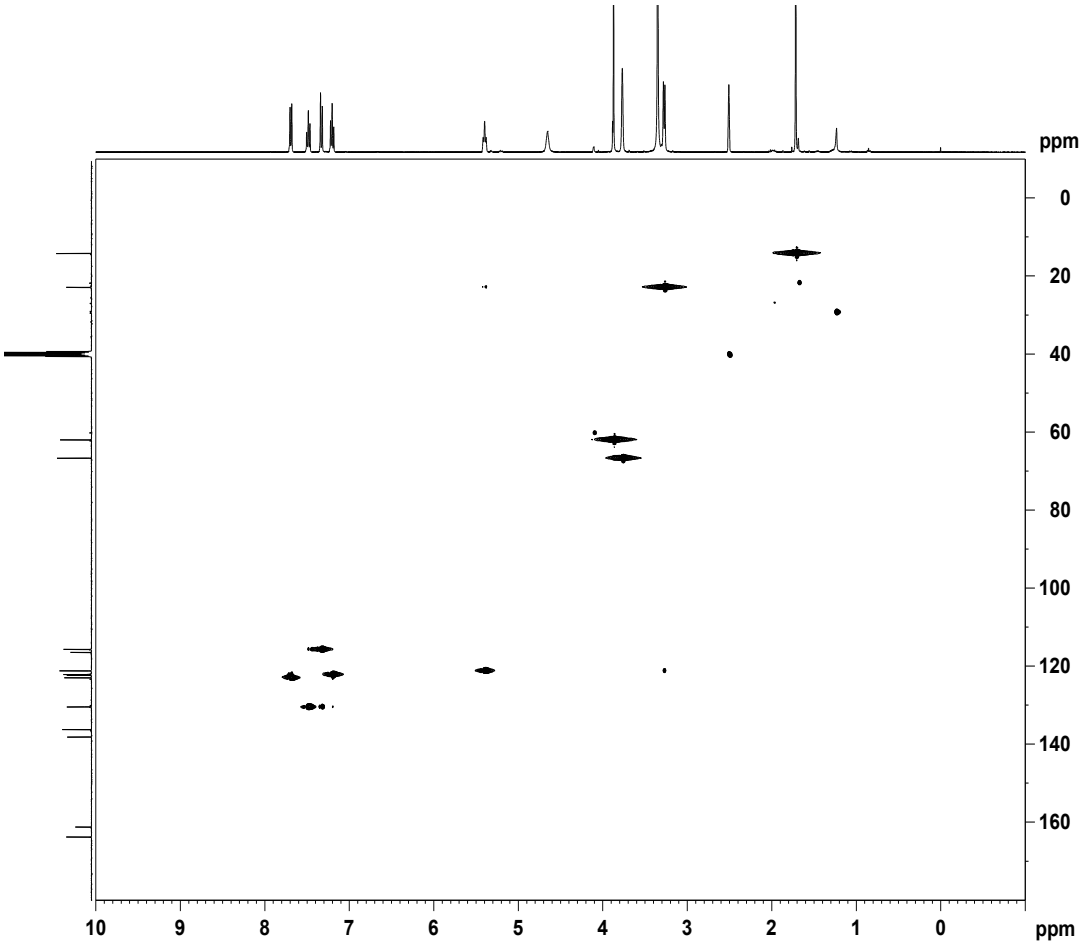


Figure S76. The HMBC spectrum of Clausenaside H (8) in DMSO-d_6

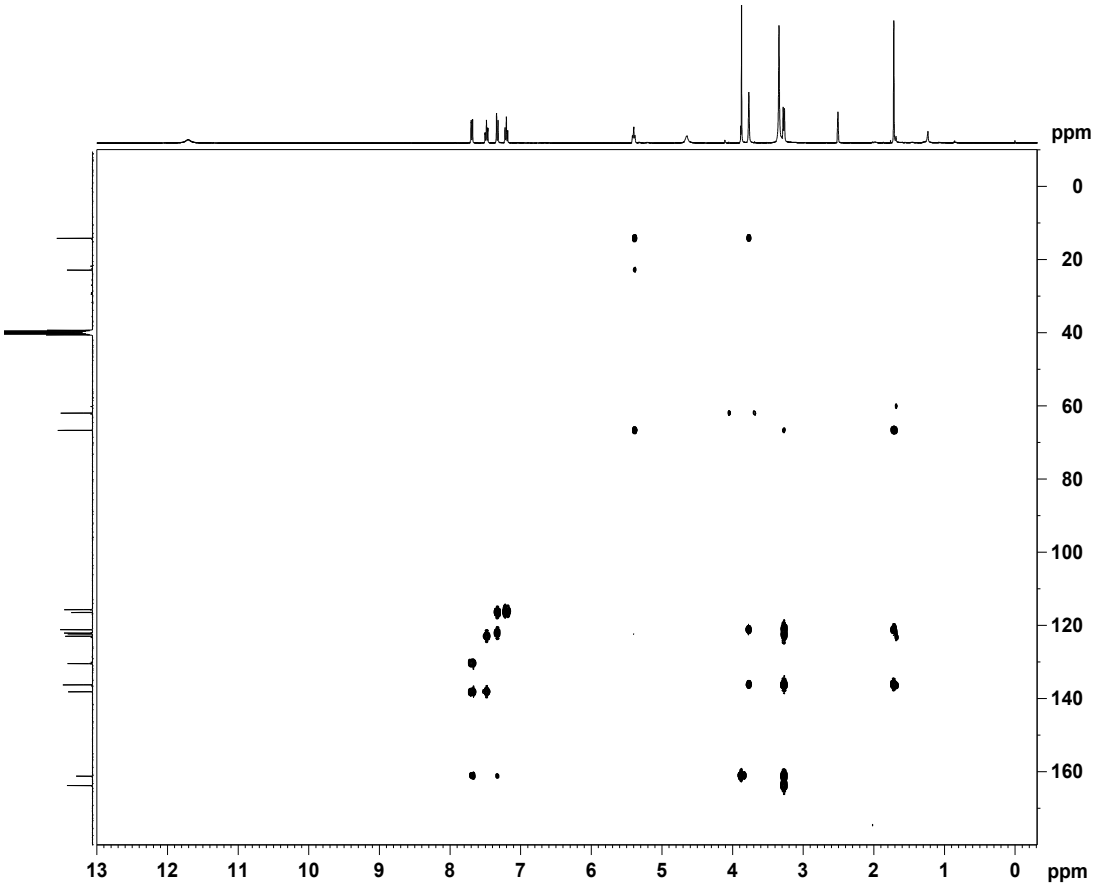


Figure S77. The ^{1}H-^{1}H COSY spectrum of Clausenaside H (8) in DMSO-d_6

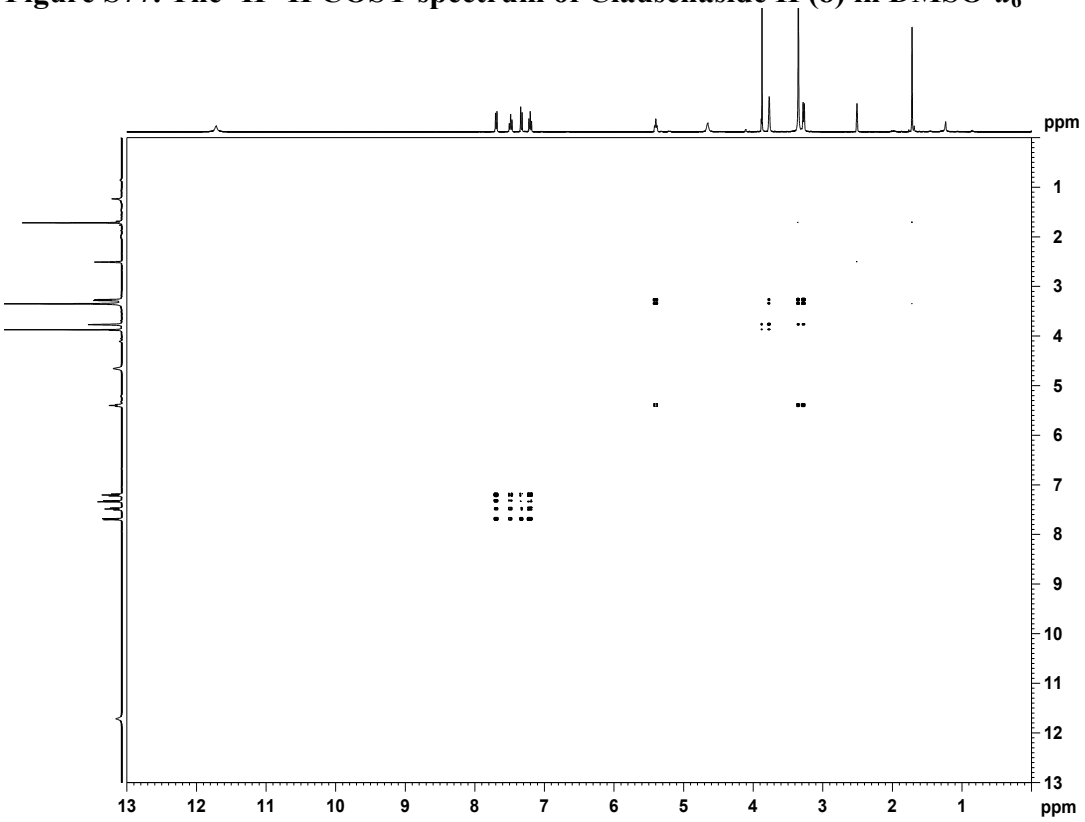


Figure S78. The NOE difference spectrum of Clausenaside H (8) in DMSO-d_6

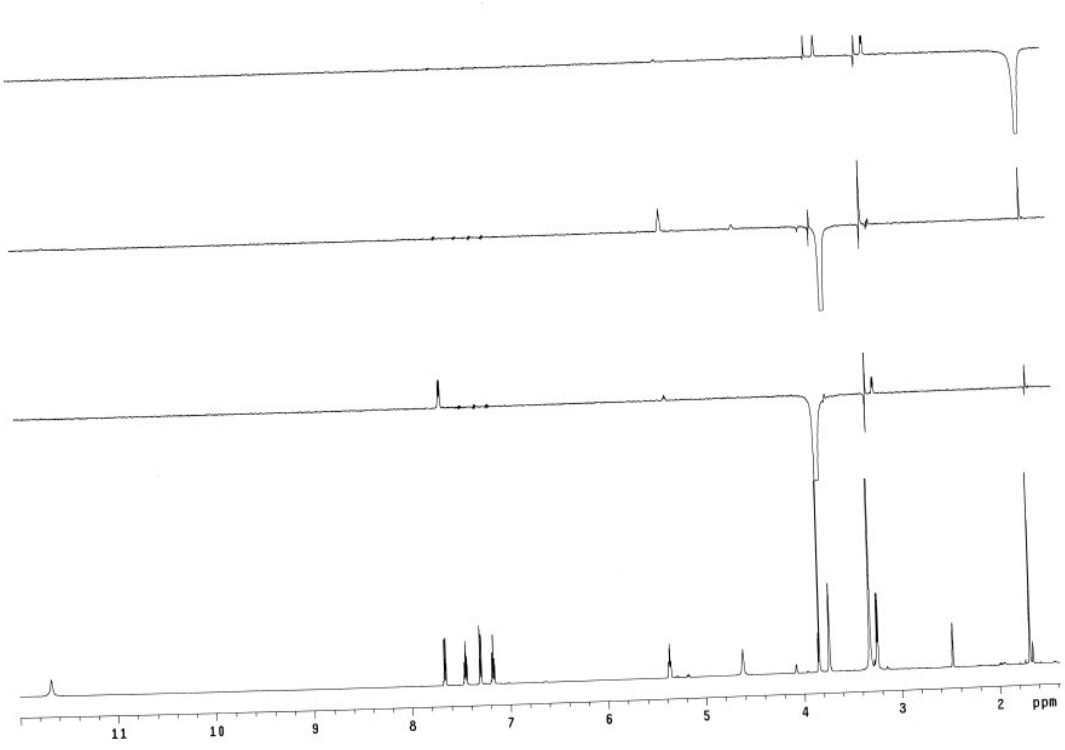


Figure S73. The IR spectrum of Clausenaside H (8)

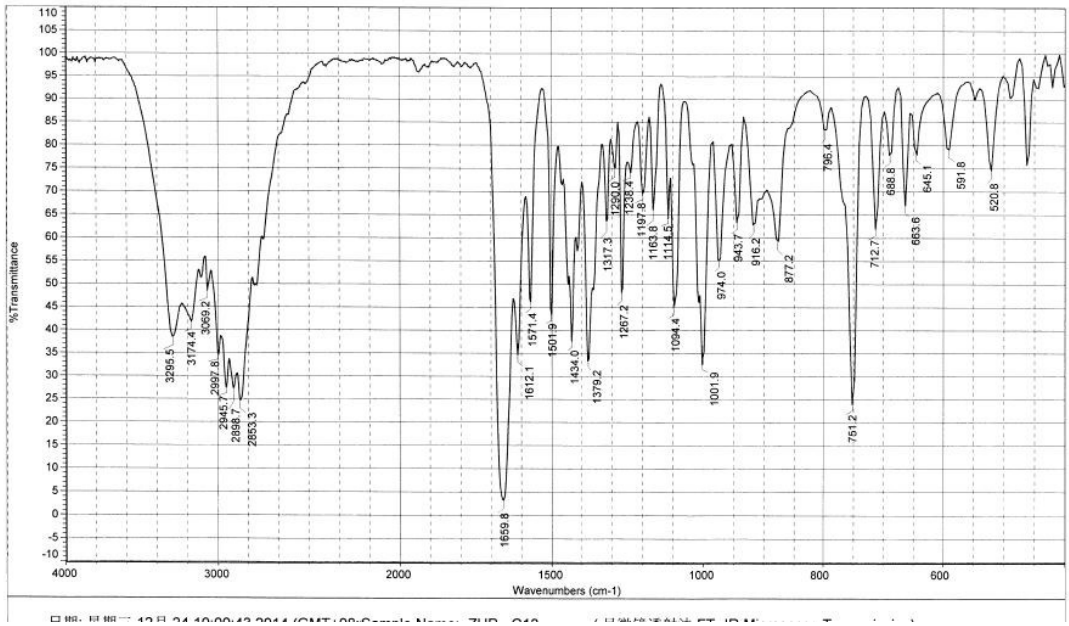
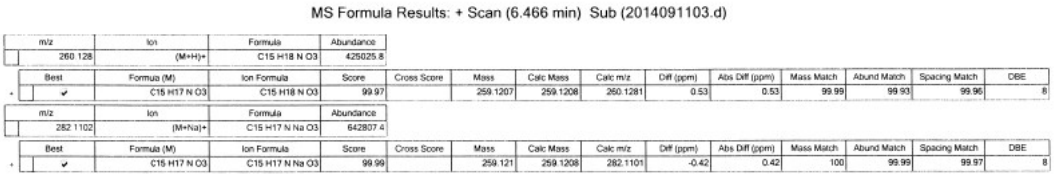


Figure S74. The HRESIMS of Clausenaside H (8)



MS Formula Results: + Scan (6.466 min) Sub (2014091103.d)

	m/z	Ion	Formula	Abundance
-	260.128	(M+H)+	C15 H18 N O3	425025.8

	Best	Formula (M)	Ion Formula	Score	Cross Score	Mass	Calc Mass	Calc m/z	Diff (ppm)	Abs Diff (ppm)	Mass Match	Abund Match	Spacing Match	DBE
+	✔	C15 H17 N O3	C15 H18 N O3	99.97		259.1207	259.1208	260.1281	0.53	0.53	99.99	99.93	99.96	8

	m/z	Ion	Formula	Abundance
-	282.1102	(M+Na)+	C15 H17 N Na O3	642807.4

	Best	Formula (M)	Ion Formula	Score	Cross Score	Mass	Calc Mass	Calc m/z	Diff (ppm)	Abs Diff (ppm)	Mass Match	Abund Match	Spacing Match	DBE
+	✔	C15 H17 N O3	C15 H17 N Na O3	99.99		259.121	259.1208	282.1101	-0.42	0.42	100	99.99	99.97	8