

Supplementary Materials

Identification and characterization of two new forced degradation products of saikosaponin a under the stress of acid hydrolytic condition

Jun Li, Qiang Xu, Jiang Hua *

Supplementary Figure

MS Formula Results: + Scan (8.264 min) Sub (2014102903.d)

m/z	Ion	Formula	Abundance
821.4546	(M+Na) ⁺	C42 H70 Na O14	130068

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
17	C42 H70 O14	C42 H70 Na O14	99.86		798.4698	798.4711	821.4603	1.65	1.65	99.91	99.75	99.89	9

Figure S1 HRESI-MS data for hydroxyl-saikosaponin a

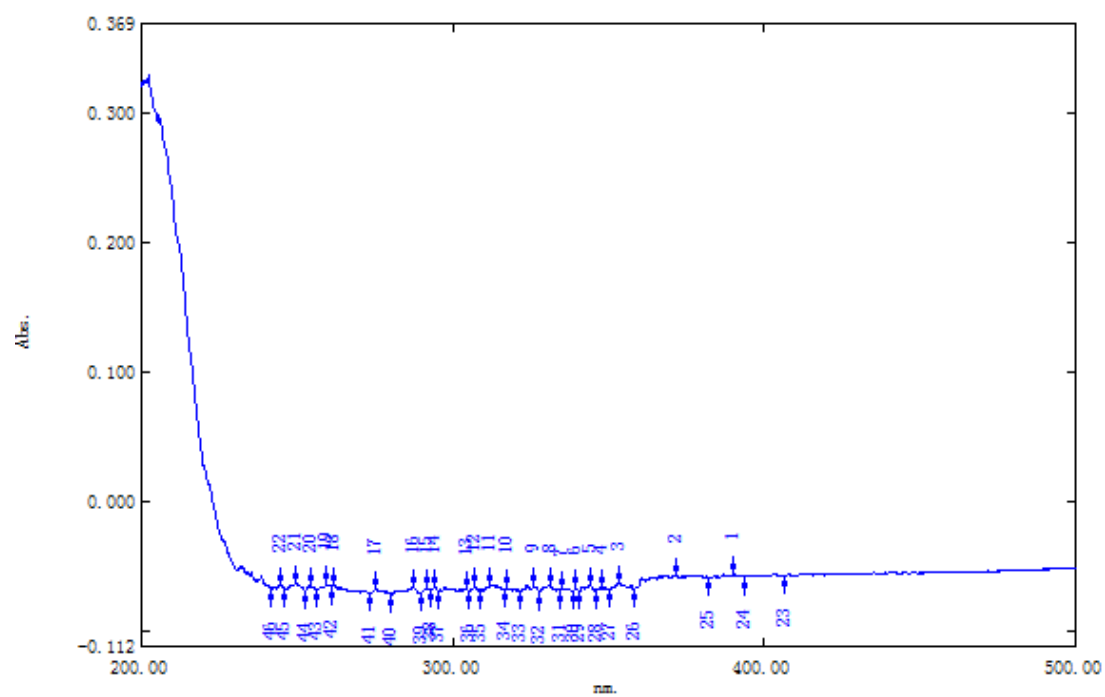


Figure S2 UV spectrum of hydroxyl-saikosaponin a

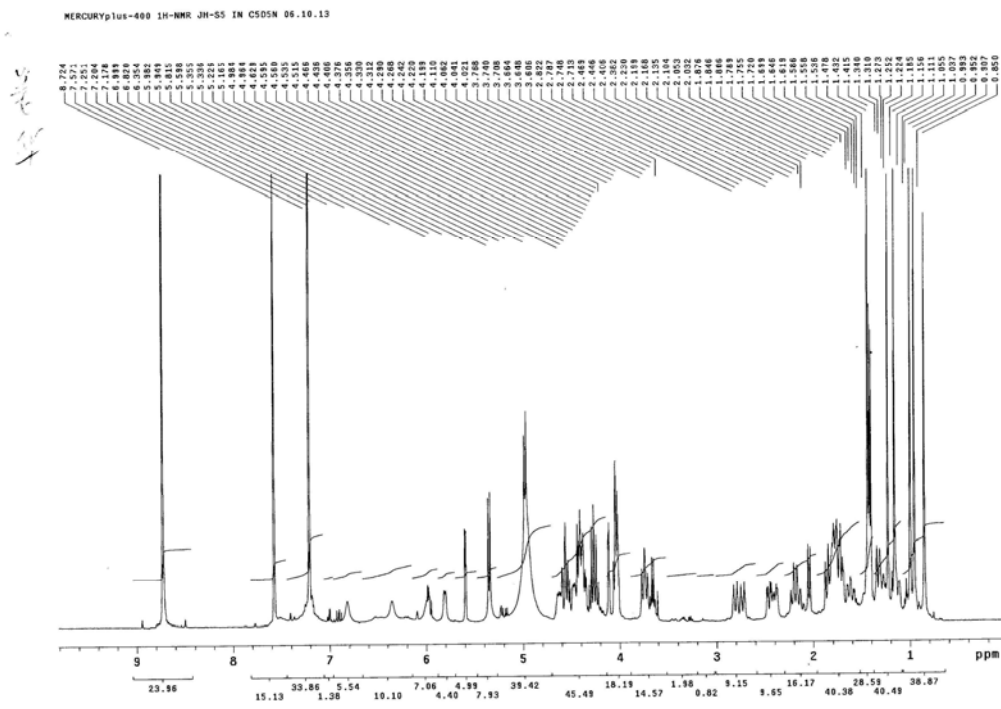


Figure S3 ¹H-NMR spectrum of hydroxyl-saikosaponin a

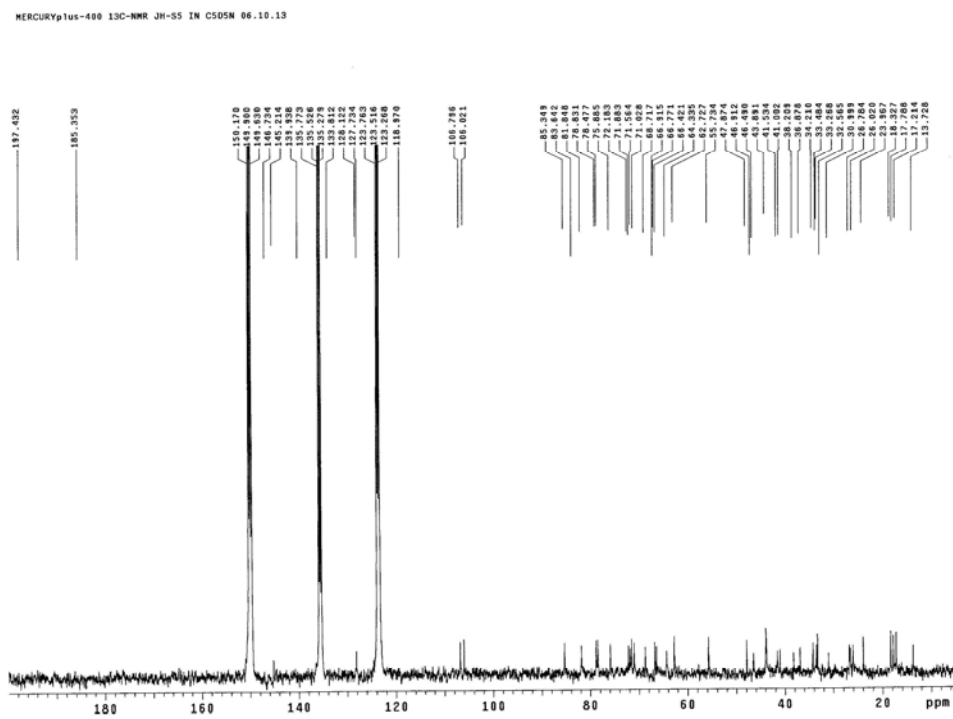


Figure S4 ¹³C-NMR spectrum of hydroxyl-saikosaponin a

MS Formula Results: + Scan (8.231 min) Sub (2014102901.d)

m/z	Ion	Formula	Abundance
803.4559	(M+Na) ⁺	C42 H68 Na O13	1085403.5

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
1	C42 H68 O13	C42 H68 Na O13	99.91		780.4667	780.466	803.4552	-0.97	0.97	99.97	99.76	99.98	9

Figure S5 HRESI-MS data of saikosaponin b²

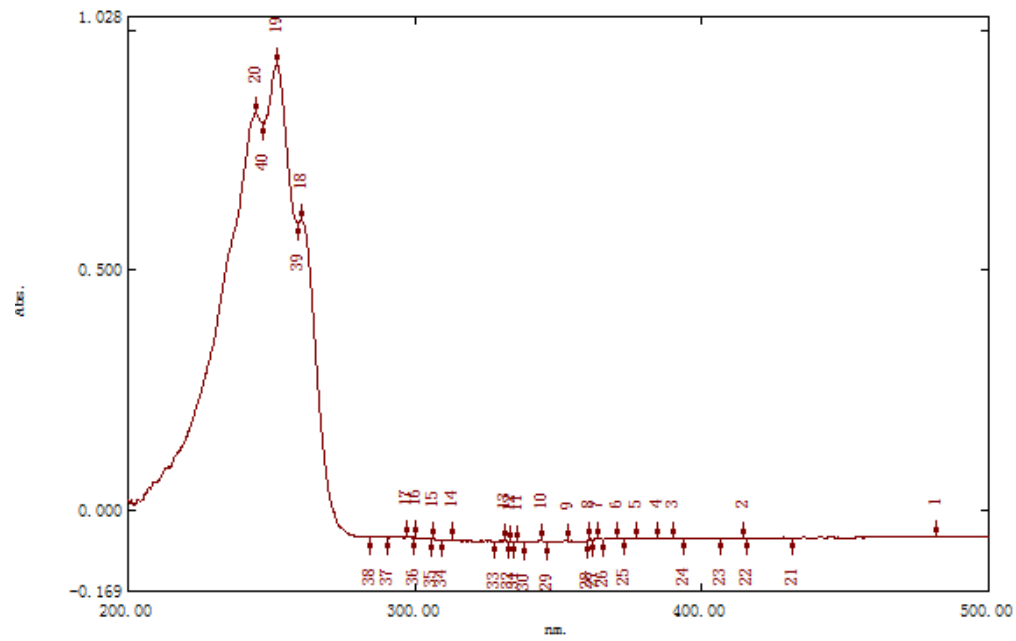


Figure S6 UV spectrum of saikosaponin b₂

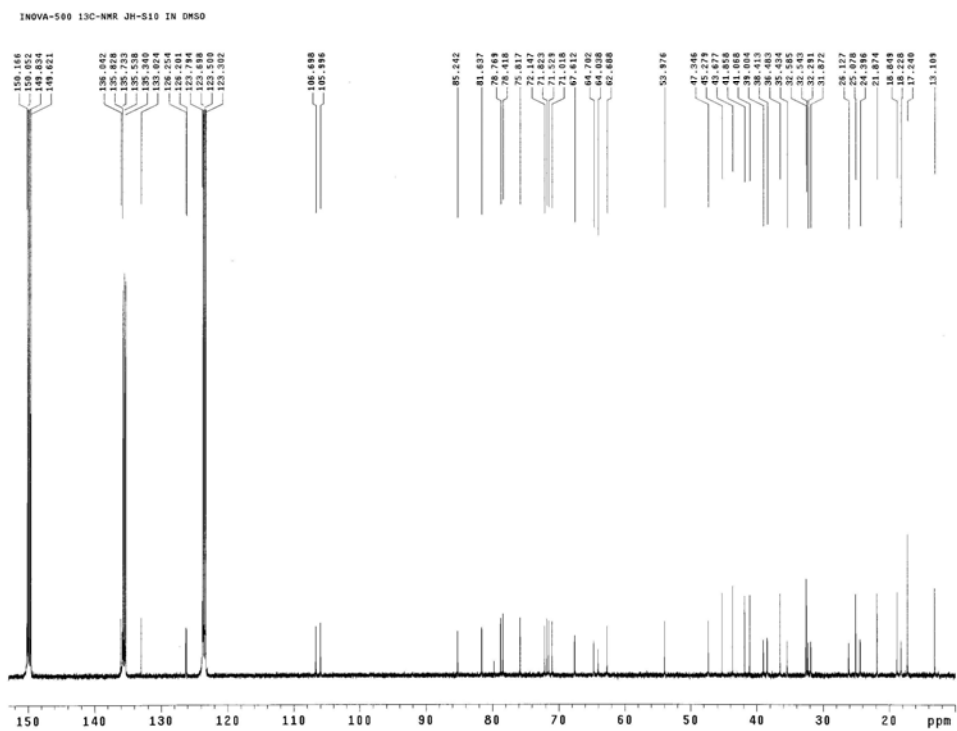


Figure S7 ^{13}C -NMR spectrum of saikosaponin b_2

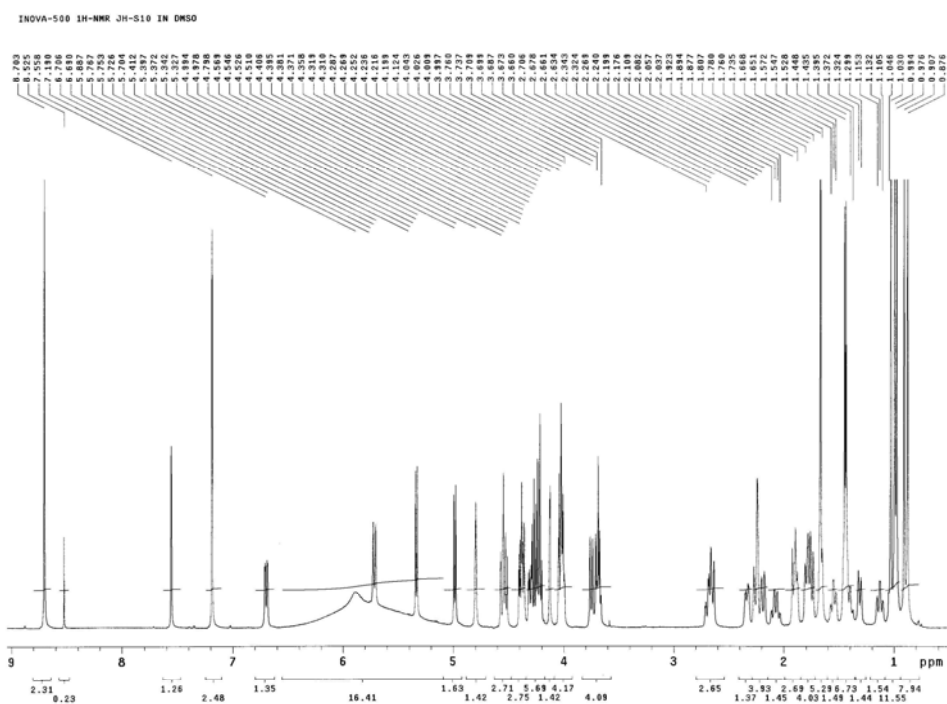


Figure S8 ^1H -NMR spectrum of saikosaponin b_2