Supplementary Materials: Identification and Characterization of Two New Degradation Products of Saikosaponin A under Acid Hydrolytic Conditions

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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
☑	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 hydroxy-saikosaponin A.

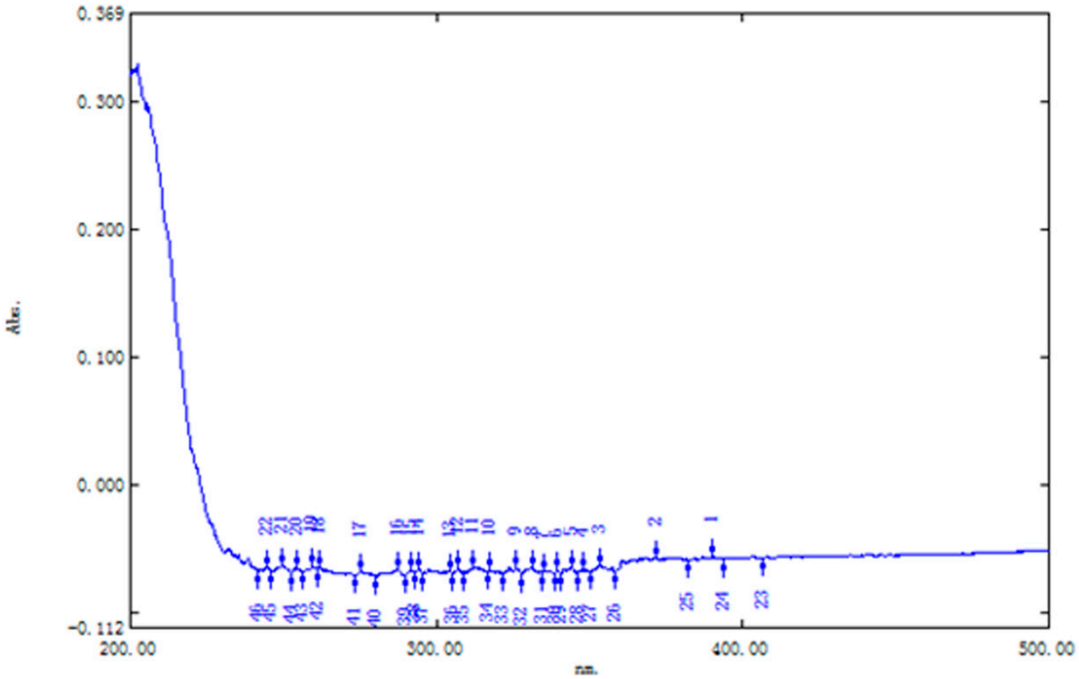

Figure S2. UV spectrum of hydroxy-saikosaponin A.

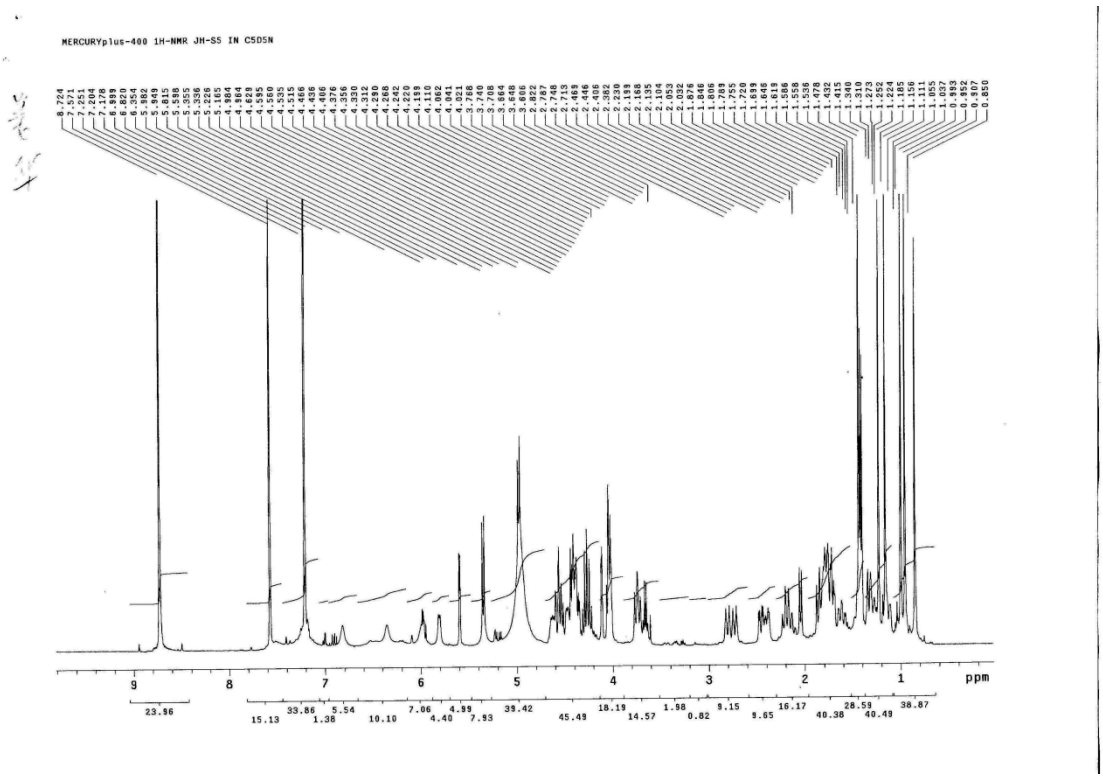

Figure S3. [1]H-NMR spectrum of hydroxy-saikosaponin A.

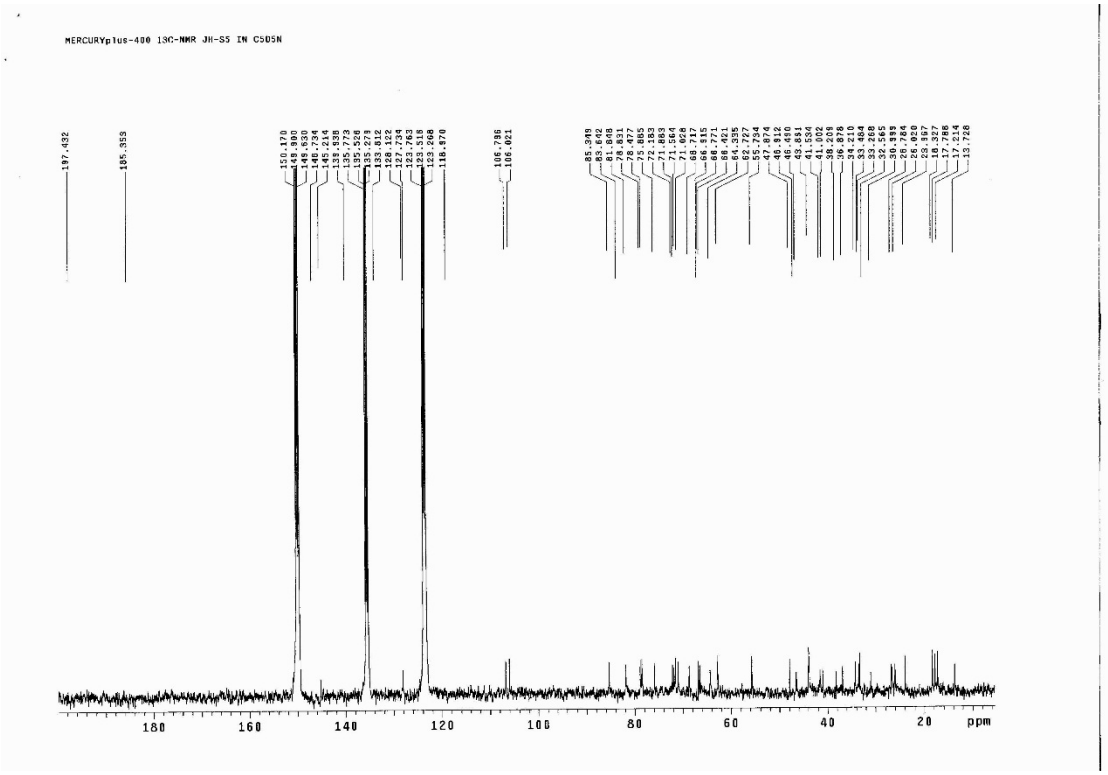

Figure S4. [13]C-NMR spectrum of hydroxy-saikosaponin A.

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	Spaci
☑	C42 H68 O13	C42 H68 Na O13	99.91		780.4667	780.466	803.4552	-0.97	0.97	99.97	99.76	

Figure S5. HRESI-MS data of saikosaponin B2.

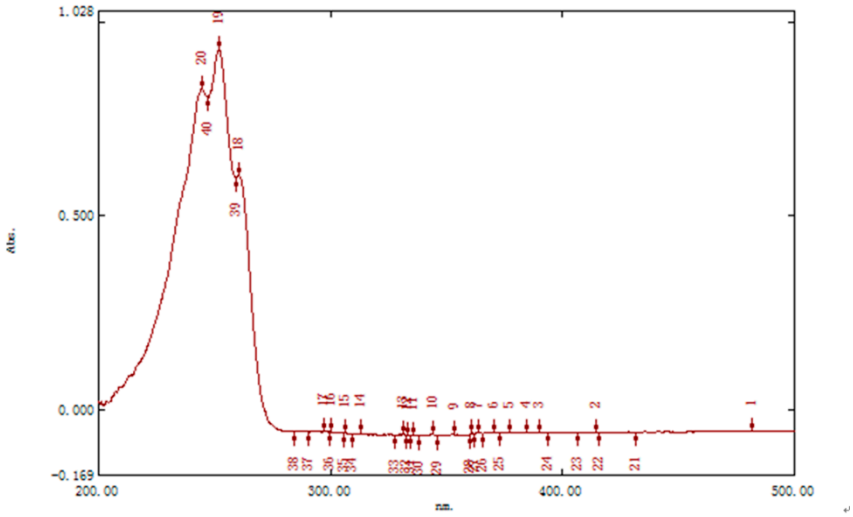

Figure S6. UV spectrum of saikosaponin B2.

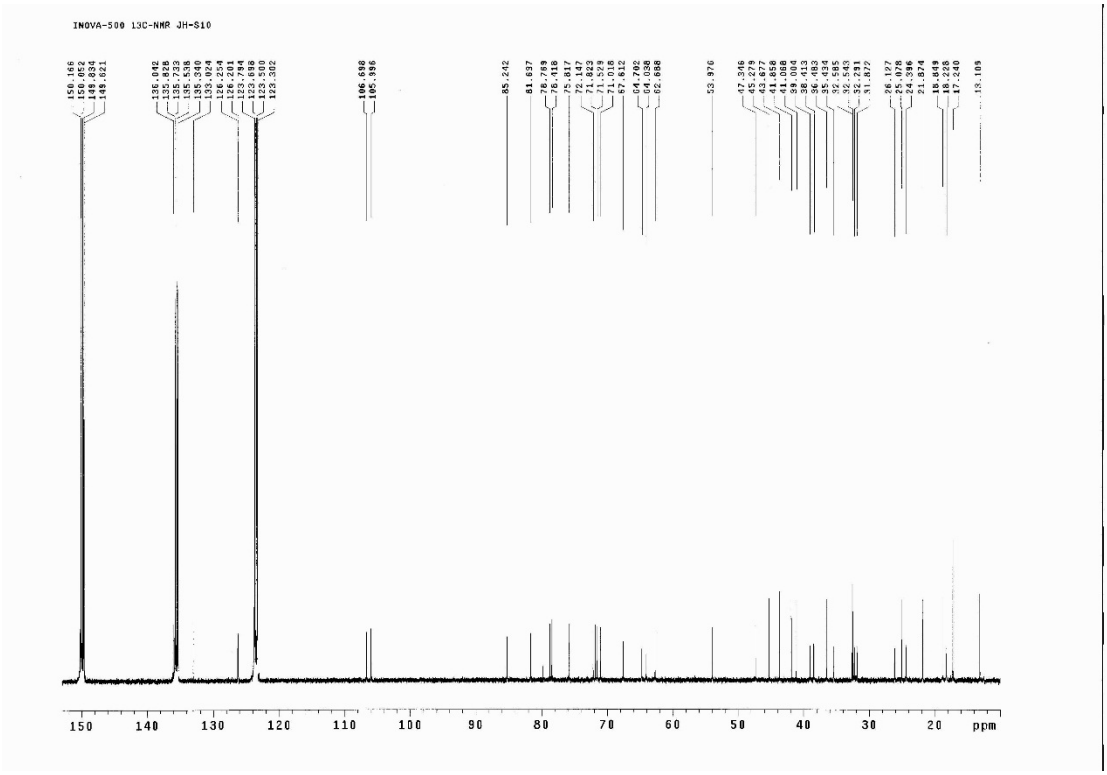

Figure S7. ^{13}C-NMR spectrum of saikosaponin B2.

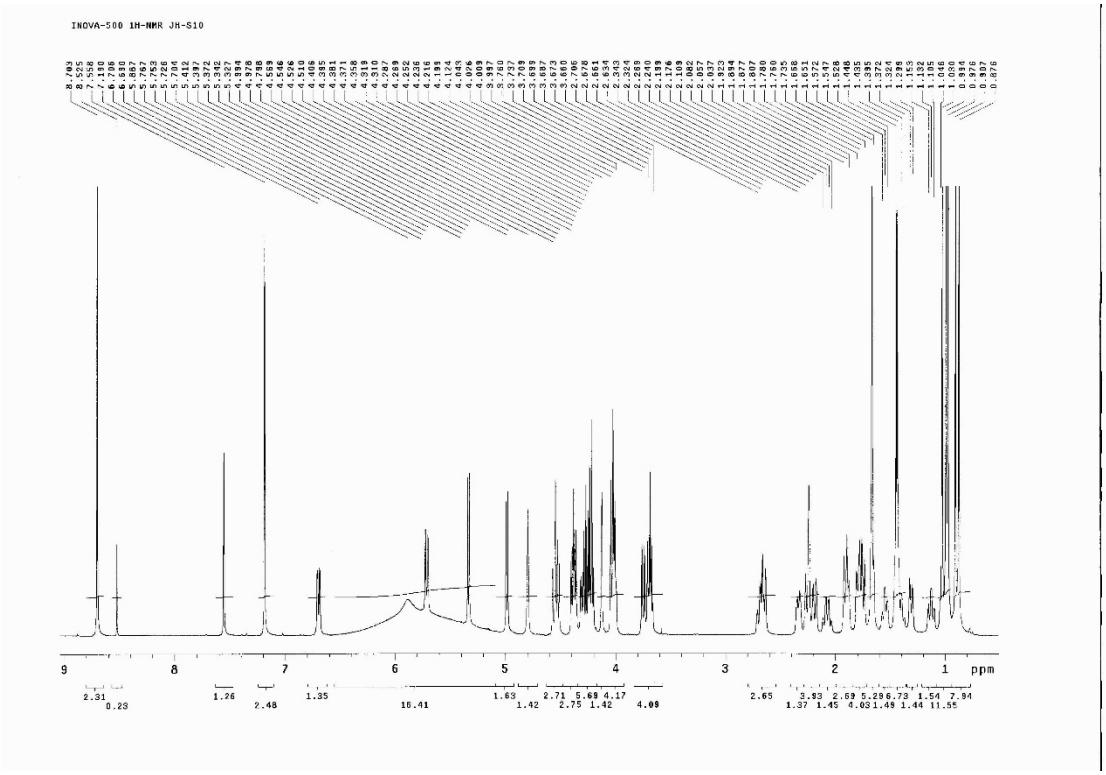

Figure S8. [1]H-NMR spectrum of saikosaponin B2.