

Chemical profiling and quantification of potential bio-active components in Gandouling Pills by ultra-high performance liquid chromatography coupled with high quadrupole-Qorbitrap mass spectrometry

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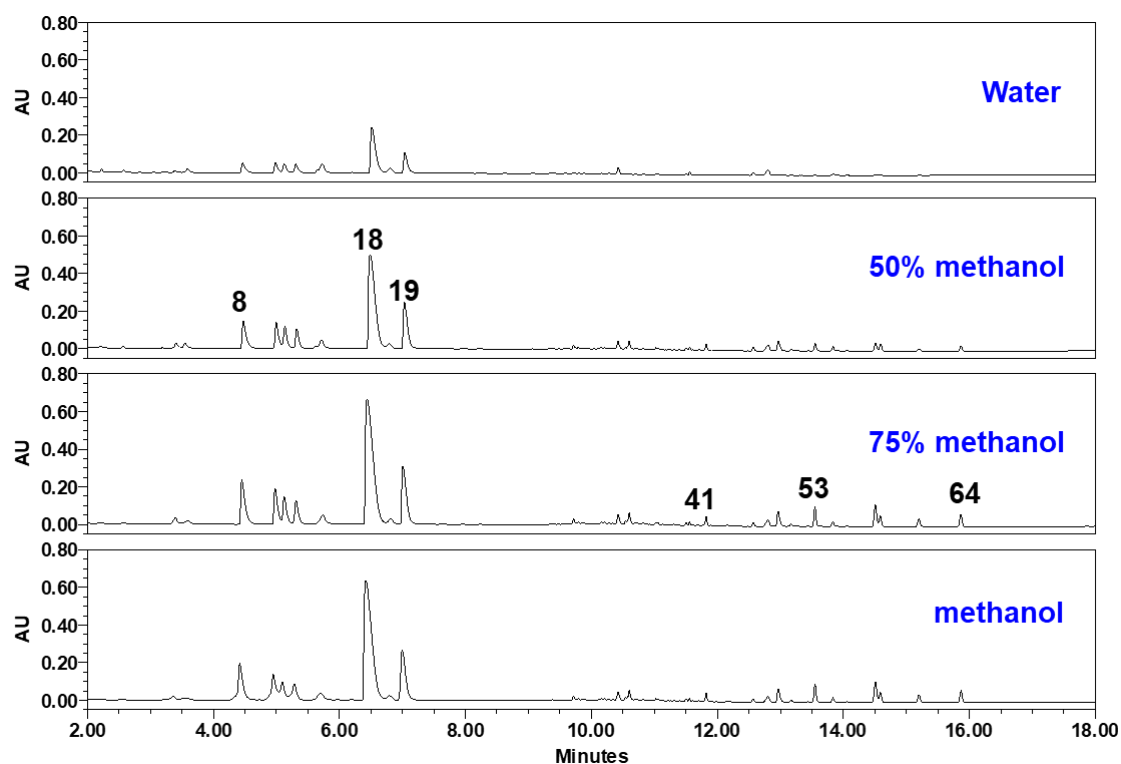


Figure S1 Extraction efficiency of compounds in GDL Pills using different solvents (270 nm).

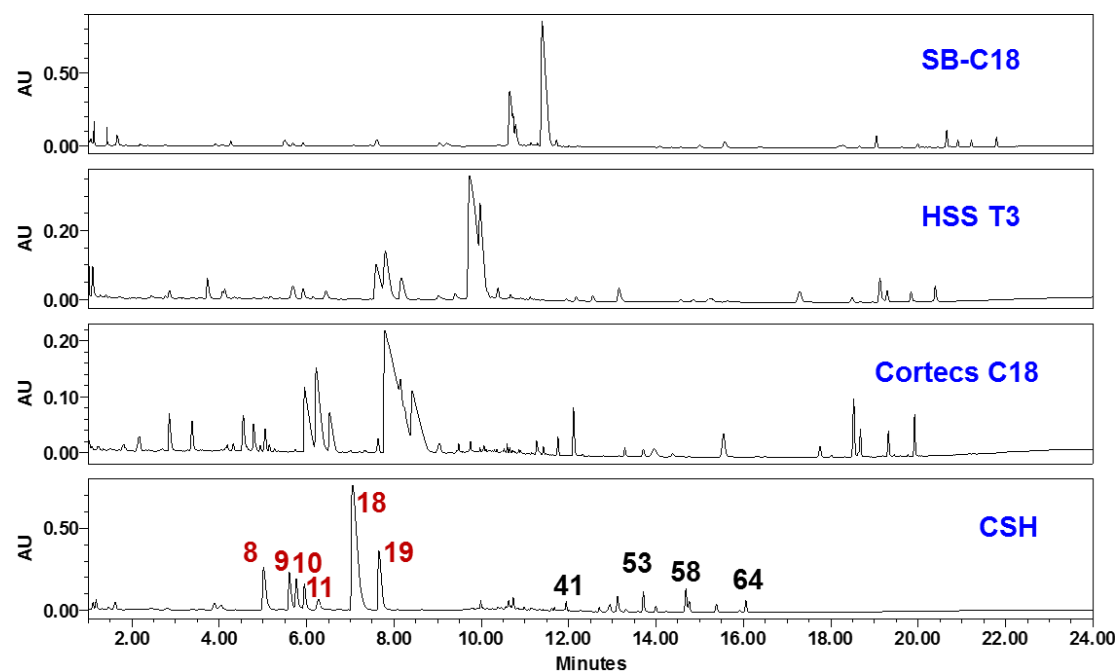


Figure S2 Separation efficiency of compounds in GDL Pills using different stationary phases. The alkaloids were marked in red and other compounds marked in black (270 nm).

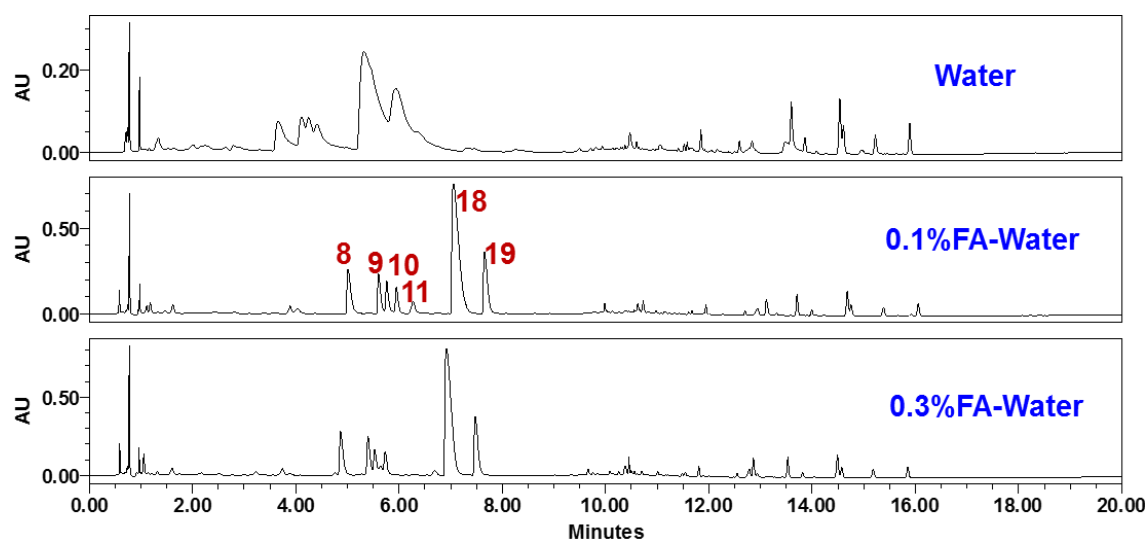


Figure S3 Separation efficiency of compounds in GDL Pills using different mobile phases (270 nm).

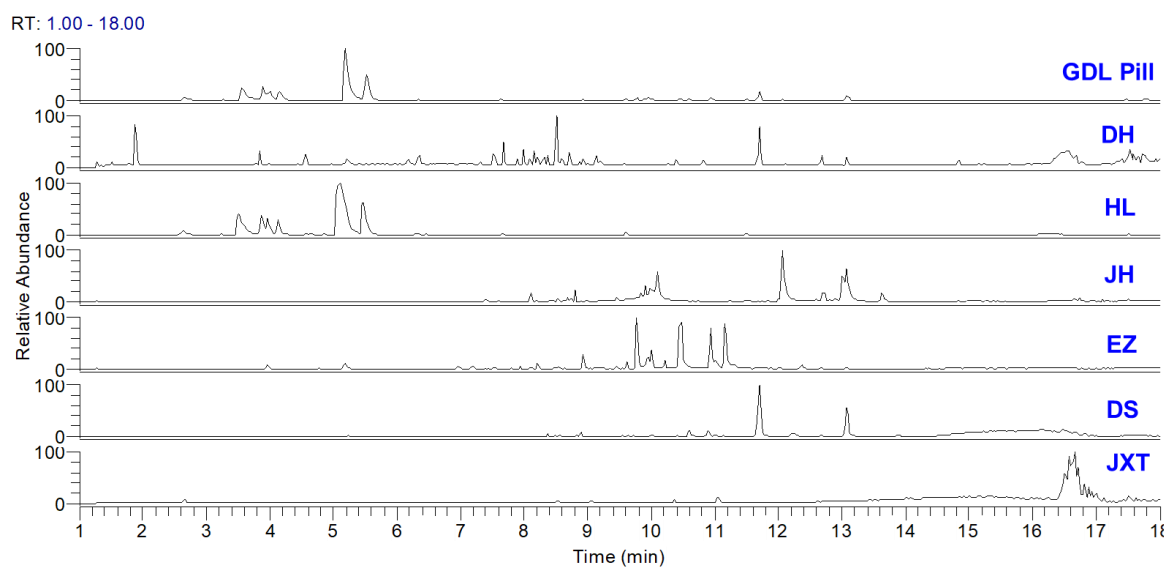


Figure S4 The LC/MS chromatograms of GDL Pill and separate herbs in the positive ion mode.

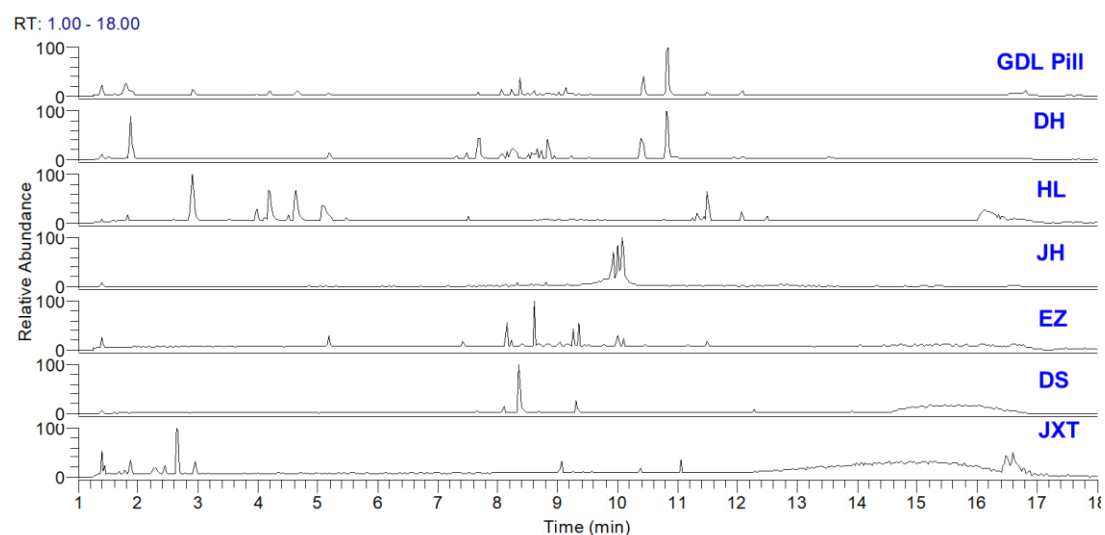


Figure S5 The LC/MS chromatograms of GDL Pill and separate herbs in the negative ion mode.

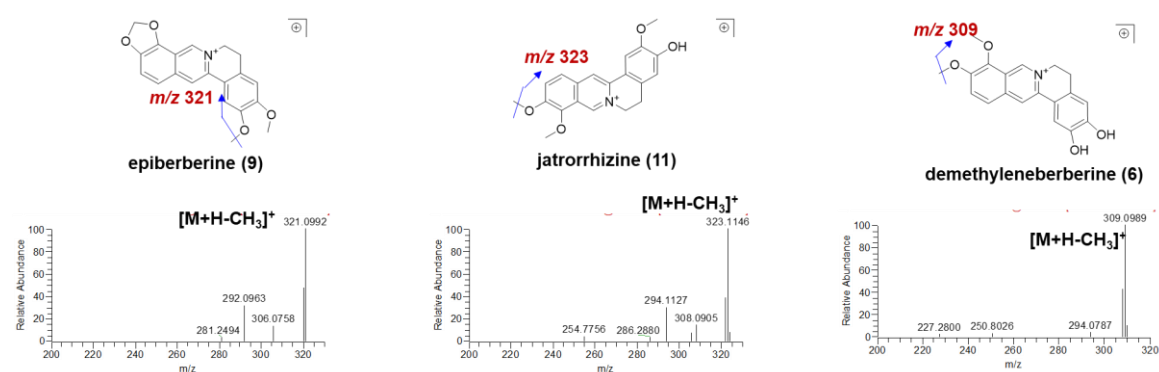


Figure S6 The MS/MS spectra of representative alkaloids identified in GDL Pill.

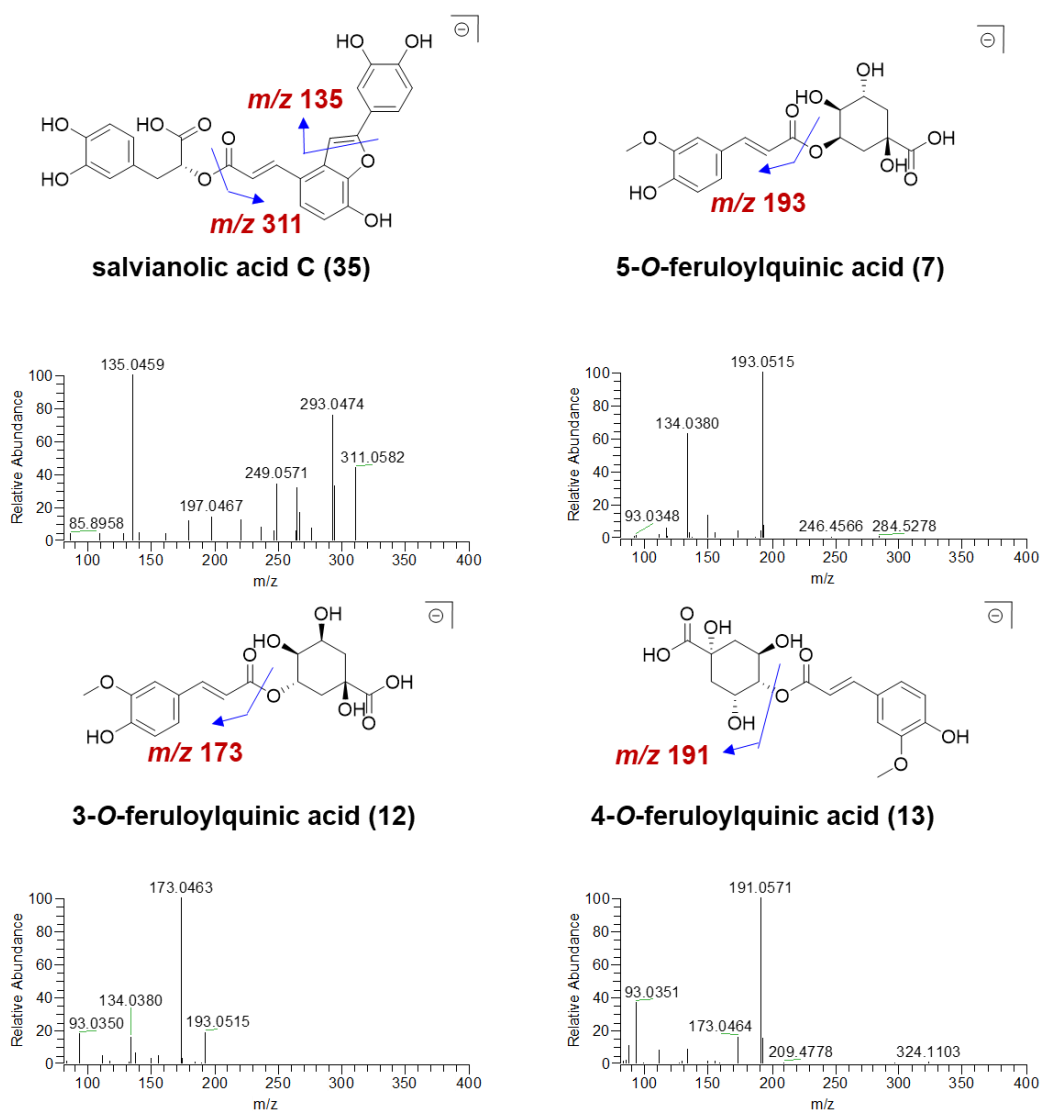


Figure S7 The MS/MS spectra of representative organic acids identified in GDL Pill.

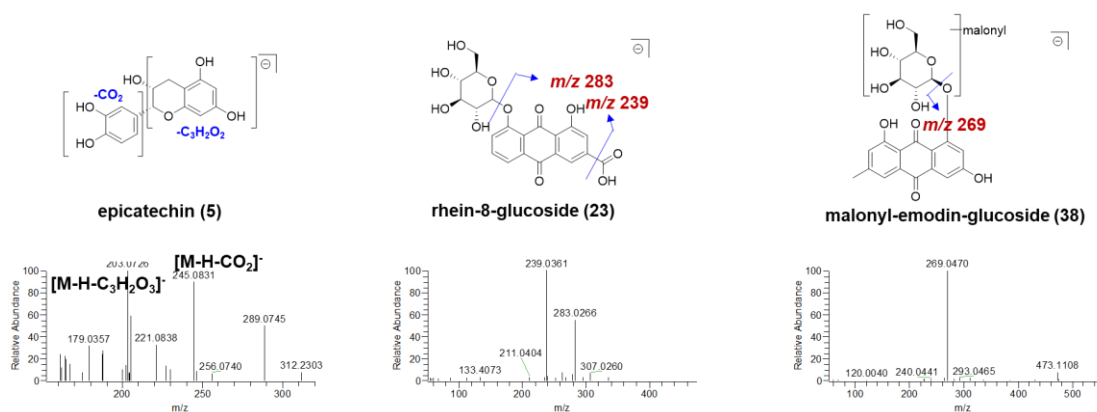


Figure S8 The MS/MS spectra of representative phenolics identified in GDL Pill.

Table S1 Comparison of extraction recovery (%) of 6 major compounds in GDL Pill
by using different kinds of extraction solvent.

Peaks	water	50% methanol	75% methanol	methanol
8	75.06	92.31	100.00	99.00
18	72.95	89.42	100.00	98.22
19	68.42	84.37	99.87	100.00
41	55.61	83.31	100.00	96.55
53	57.48	86.74	100.00	97.77
64	57.69	81.23	99.45	100.00