

Supplementary Materials: Statistical Correlations between HPLC Activity-Based Profiling Results and NMR/MS Microfractions Data to Deconvolute Bioactive Compounds in Mixture

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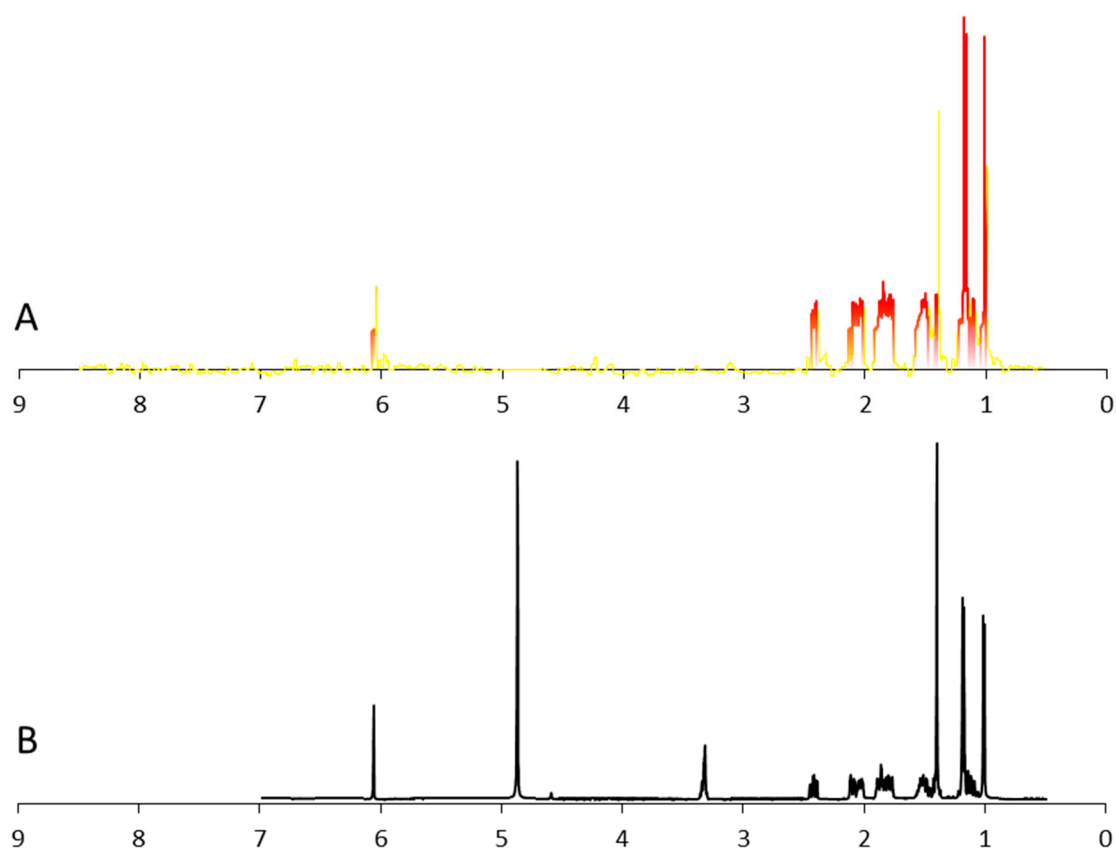


Figure S1. Example of statistical deconvolution on the coelution of artemisinin and 4'-bromoflavone. (A) filtered ¹H-NMR pseudospectrum corresponding to feature RT = 2.18 min and $m/z = 283.1566$ (PI) – artemisinin as $[M + H]^+$ adduct; (B) real spectrum of artemisinin in deuterated methanol.

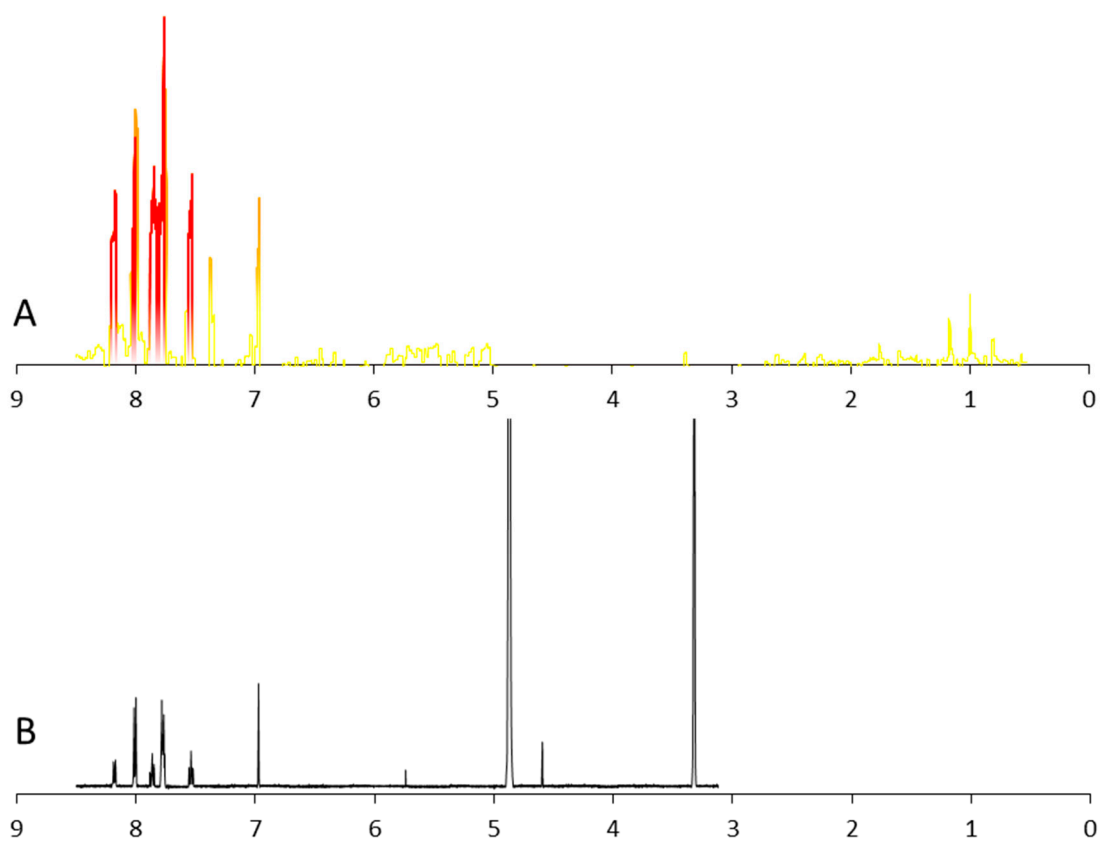


Figure S2. Example of statistical deconvolution on the coelution of artemisinin and 4'-bromoflavone. (A) filtered ¹H-NMR pseudospectrum corresponding to feature RT = 2.37 min and $m/z = 300.9882$ (PI)–4'-bromoflavone as $[M + H]^+$ adduct; (B) real spectrum of 4'-bromoflavone in deuterated methanol.