Supplementary Information

Label-free cell phenotypic profiling identifies pharmacologically active compounds in two Traditional Chinese Medicinal plants

Xiuli Zhang[a,‡], Huayun Deng[b,‡], Yuansheng Xiao[a], Xingya Xue[a], Ann M. Ferrie[b], Elizabeth Tran[b], Xinmiao Liang[a,*], and Ye Fang[b,*]

[a] Key Laboratory of Separation Science for Analytical Chemistry, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, Liaoning 116023, China

[b] Biochemical Technologies, Science and Technology Division, Corning Incorporated, Corning, New York 14831, United States of America.

‡ These authors contributed equally to this work.

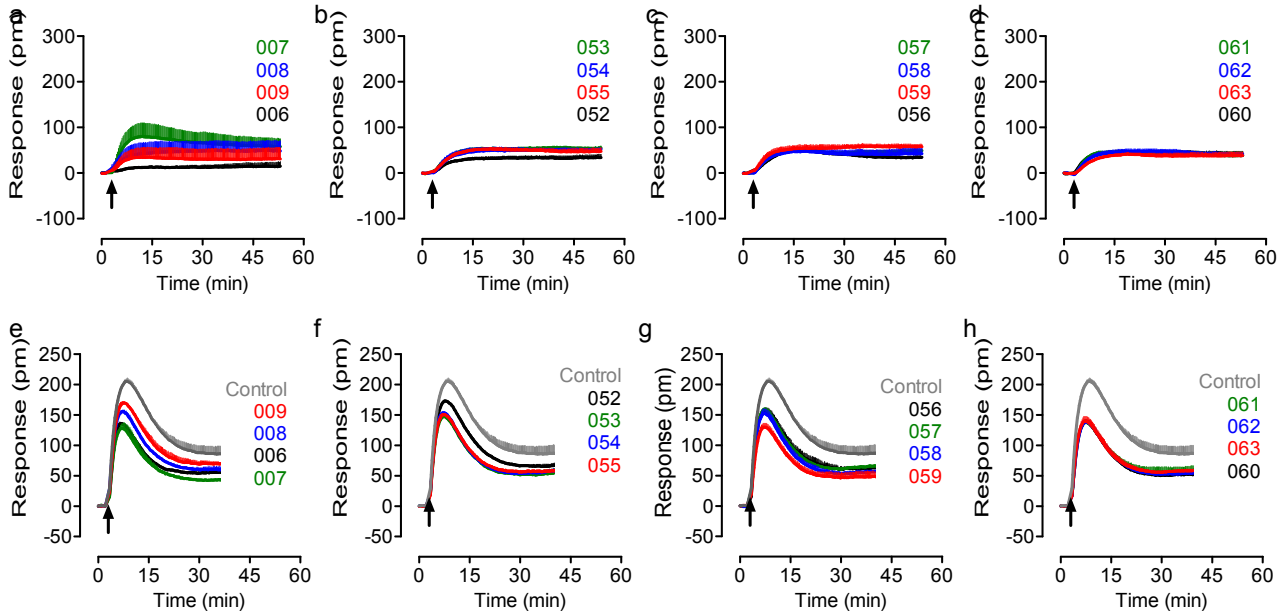
* E-mail: liangxm@dicp.ac.cn (X.L.); fangy2@corning.com (Y.F.).

Supplementary Figure S1-S5: The DMR signals of fractions versus the DMR of YE210 after pretreatment with the active fractions in HT-29.

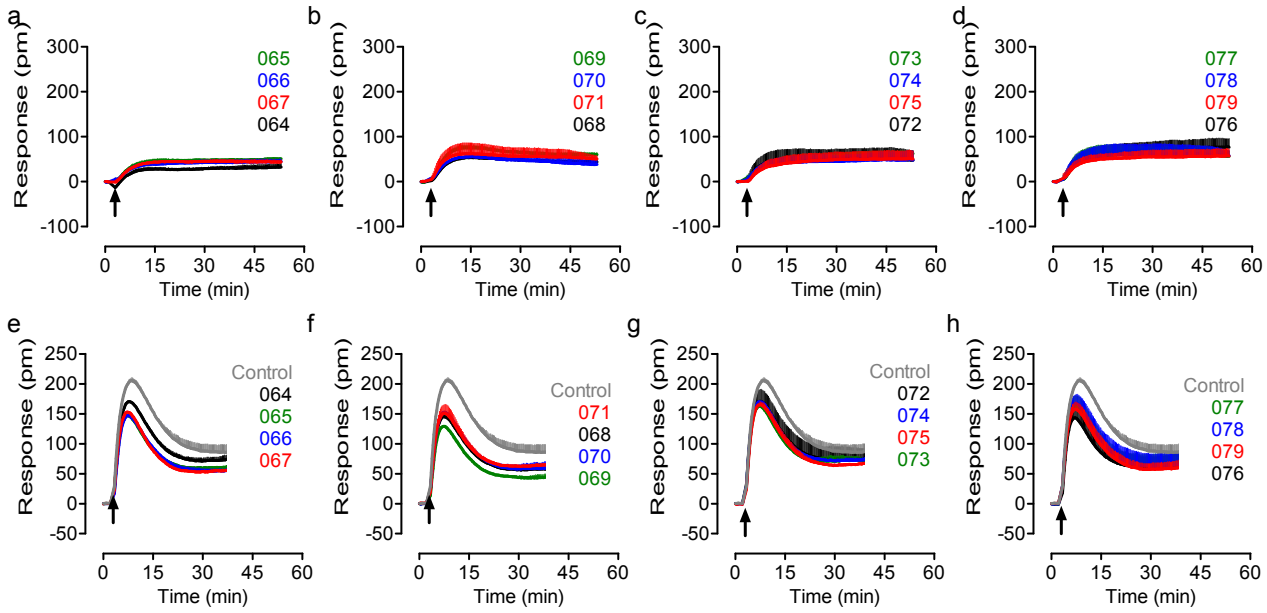
Supplementary Figure S6: Mass spectra of purified compound C2.

Supplementary Figure S7: 1H-NMR and 13C-NMR spectra of purified compound C2.

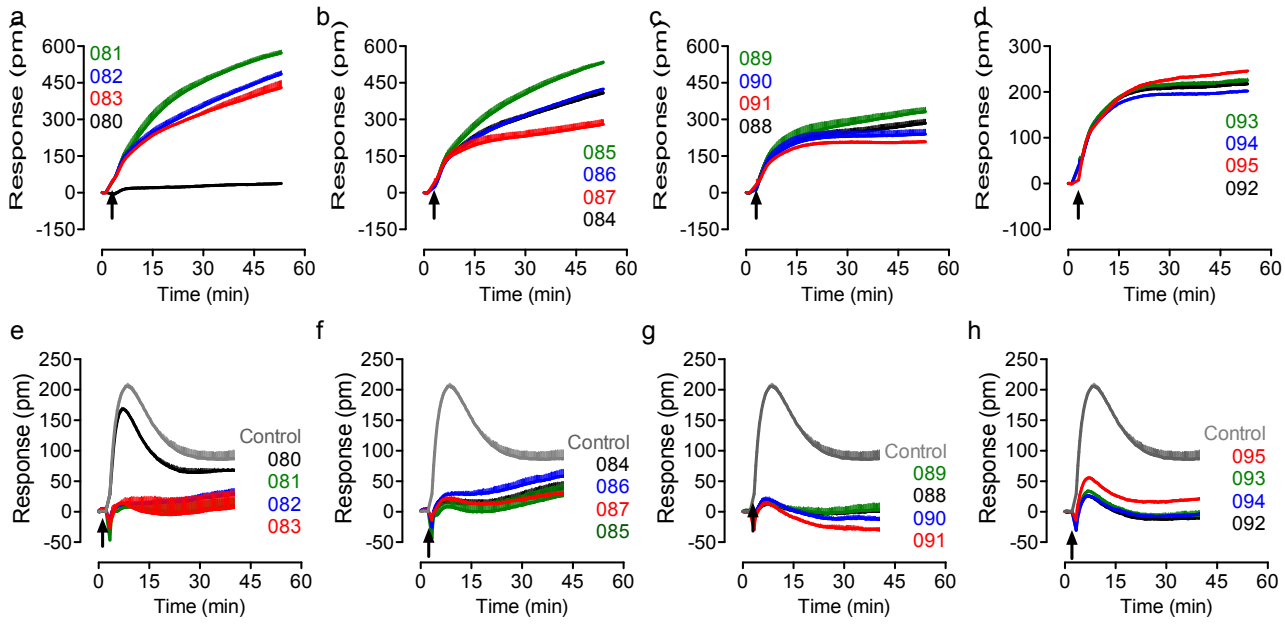
Supplementary Figure S8: LC-MS spectra with a targeted m/z of 124 of the fraction group of DYT-001 to 005.



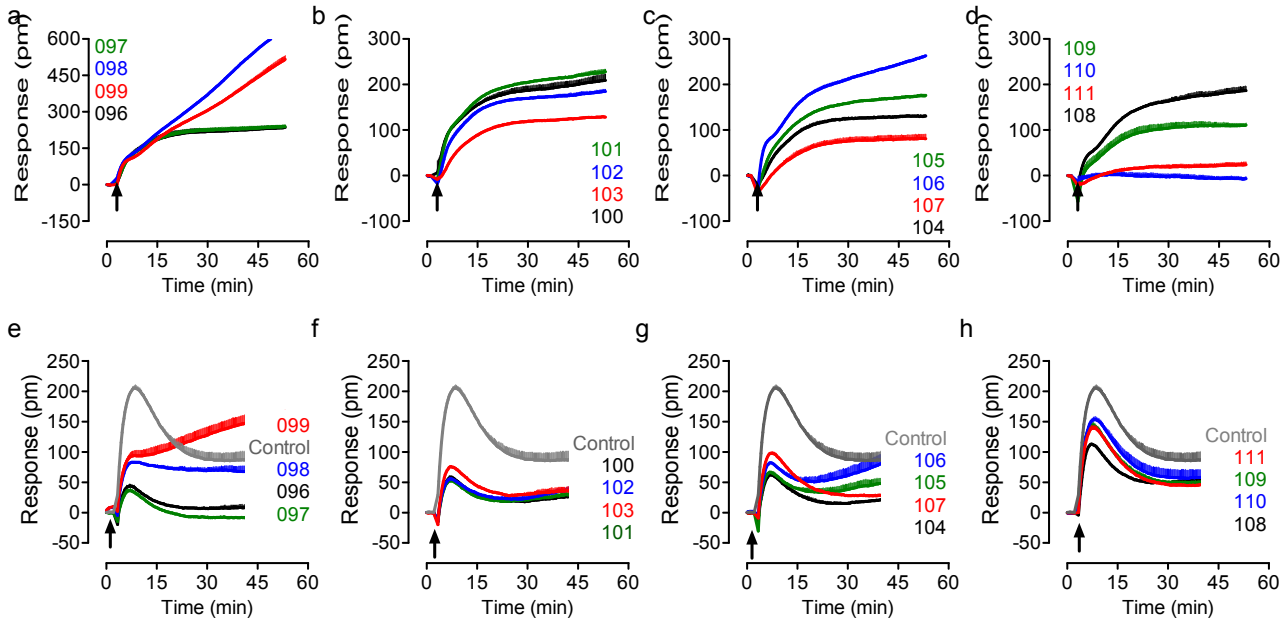
Supplementary Figure S1. The real-time DMR signals of fractions of Millettia pachyloba extracts in HT29 (a-d) versus the DMR of 1μM YE210 after one-hour pretreatment with the corresponding fractions (e-h). (a,e) fractions DYT-006, 007, 008 and 009. (b,f) fractions DYT-052, 053, 054, and 055. (c,g) fractions DYT-056, 057, 058 and 059. (d,h) fractions DYT-060, 061, 062 and 063. In (e-h) the control represents the DMR of YE210 after pretreatment with DMSO at a concentration equal to those of all fractions. Data represents mean±s.d. (n=4).



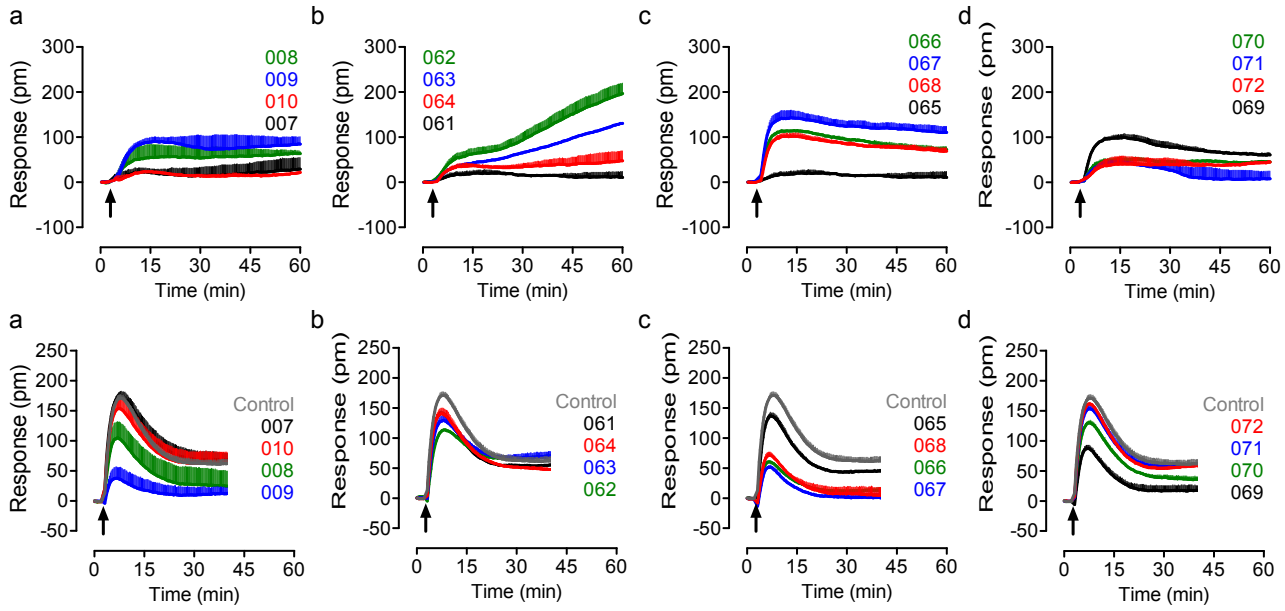
Supplementary Figure S2. The real-time DMR signals of fractions of Millettia pachyloba extracts in HT29 (a-d) versus the DMR of 1μM YE210 after one-hour pretreatment with the corresponding fractions (e-h). (a,e) fractions DYT-064, 065, 066 and 067. (b,f) fractions DYT-068, 069, 070, and 071. (c,g) fractions DYT-072, 073, 074 and 075. (d,h) fractions DYT-076, 077, 078, and 079. In (e-h) the control represents the DMR of YE210 after pretreatment with DMSO at a concentration equal to those of all fractions. Data represents mean±s.d. (n=4).



Supplementary Figure S3. The real-time DMR signals of fractions of Millettia pachyloba extracts in HT29 (a-d) versus the DMR of 1μM YE210 after one-hour pretreatment with the corresponding fractions (e-h). (a,e) fractions DYT-080, 081, 082 and 083. (b,f) fractions DYT-084, 085, 086, and 087. (c,g) fractions DYT-088, 089, 090 and 091. (d,h) fractions DYT-092, 093, 094, and 095. In (e-h) the control represents the DMR of YE210 after pretreatment with DMSO at a concentration equal to those of all fractions. Data represents mean±s.d. (n=4).



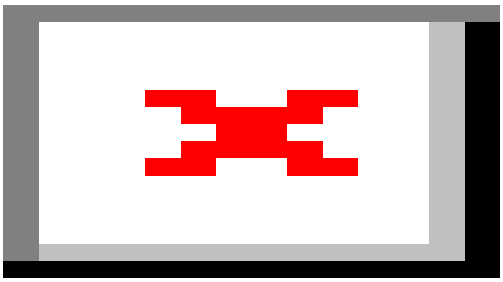
Supplementary Figure S4. The real-time DMR signals of fractions of Millettia pachyloba extracts in HT29 (a-d) versus the DMR of 1μM YE210 after one-hour pretreatment with the corresponding fractions (e-h). (a,e) fractions DYT-096, 097, 098 and 099. (b,f) fractions DYT-100, 101, 102, and 103. (c,g) fractions DYT-104, 105, 106 and 107. (d,h) fractions DYT-108, 109, 110, and 111. In (e-h) the control represents the DMR of YE210 after pretreatment with DMSO at a concentration equal to those of all fractions. Data represents mean±s.d. (n=4).



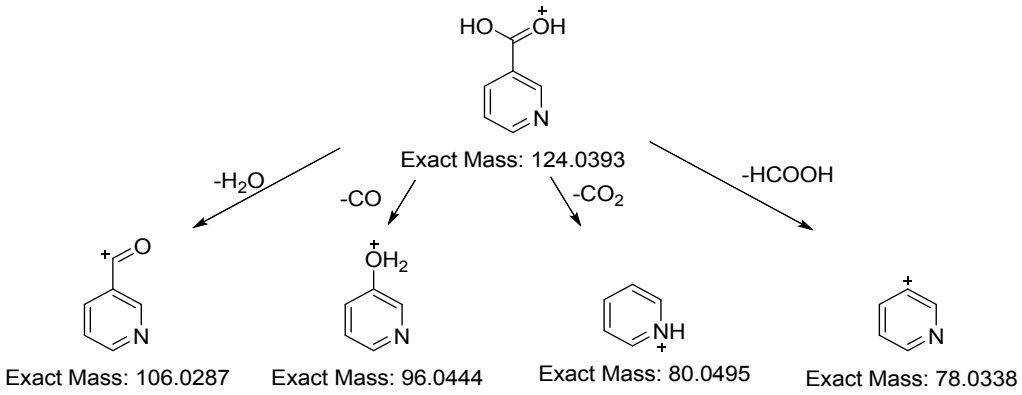
Supplementary Figure S5. The real-time DMR signals of fractions of Paederia scandens extracts in HT29 (a-d) versus the DMR of 1μM YE210 after one-hour pretreatment with the corresponding fractions (e-h). (a,e) fractions JST-007, 008, 009 and 010. (b,f) fractions JST-061, 062, 063, and 064. (c,g) fractions JST-065, 066, 067 and 068. (d,h) fractions JST-069, 070, 071, and 072. In (e-h) the control represents the DMR of YE210 after pretreatment with DMSO at a concentration equal to those of all fractions. Data represents mean±s.d. (n=4).

a

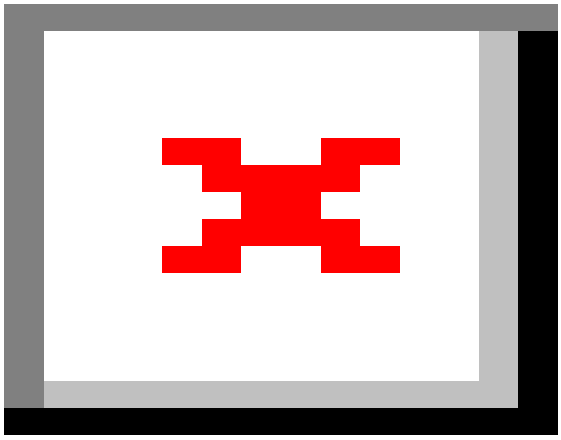
b



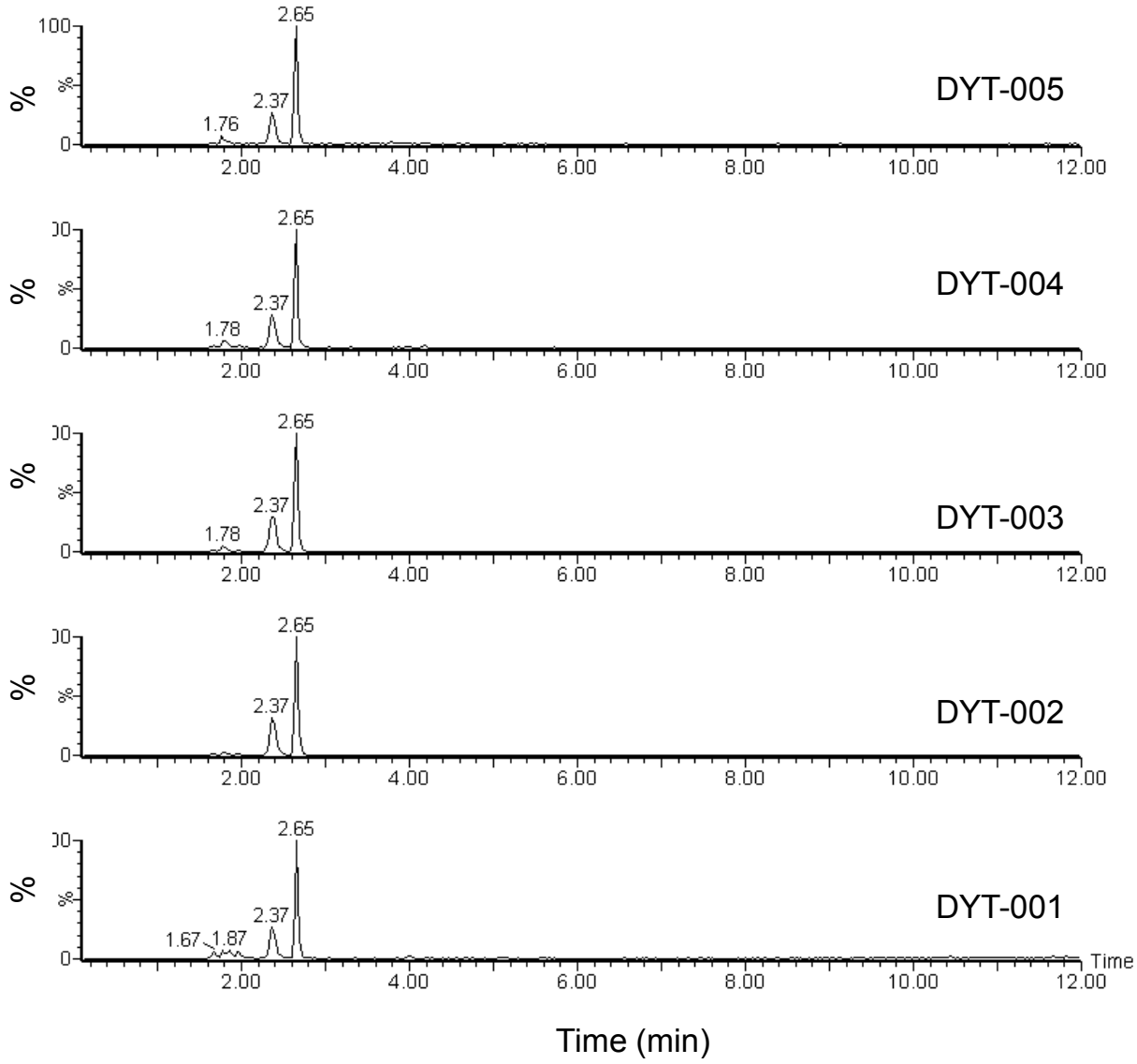
c



Supplementary Figure S6. Mass spectroscopic characterization of **C2**. (a) MS spectrum of **C2**. (b) MS spectrum of niacin. Both were obtained using positive ESI mode with a cone voltage of 35 V. (c) The deconvolution of fragmentation path of niacin. Noticed is that m/z is slightly different from the exact mass of ionized niacin and its fragments calculated.



Supplementary Figure S7. 1H and 13C-NMR of **C2** in D_2O.



Supplementary Figure S8. LC-MS analysis of the fraction group of DYT-001 to 005 using selected ion chromatography with a targeted m/z of 124 at positive ESI mode. Mobile phase A is 0.1% (v) formic acid in water and B is 0.1% (v) formic acid in acetonitrile. The gradient of separations was 0 min (5%, phase B)-15 min (95%, phase B). The flow rate was 1 ml/min.