

Table S5. Result for feature selection by 200 LASSO runs using the untargeted metabolomics data in the discovery cohort

Var1	Freq
X10.3_193.09mz_neg	200
X10.3_380.033mz_neg	200
X13.6_289.164mz_pos	200
X13_329.233mz_neg	200
X13_750.519mz_pos	200
X14.3_329.233mz_neg	200
X14.7_357.228mz_neg	200
X16.8_420.807mz_pos	200
X16.9_637.157mz_neg	200
X17_448.315mz_pos	200
X19.9_637.105mz_pos	200
X21.3_612.425mz_pos	200
X21.4_512.336mz_neg	200
X22.7_543.376mz_pos	200
X23.4_490.686mz_pos	200
X26.2_398.18mz_neg	200
X26.6_483.297mz_neg	200
X27.8_353.212mz_neg	200
X28.5_368.169mz_neg	200
X29.3_319.264mz_neg	200
X29.9_447.312mz_neg	200
X33.6_279.233mz_neg	200
X34.6_578.25mz_pos	200
X42.1_572.415mz_pos	200
X7.4_461.196mz_pos	200
X28.9_475.116mz_neg	180
X14.2_513.363mz_pos	177
X26.7_502.015mz_pos	177
X7.8_384.259mz_pos	177
X24_355.228mz_neg	152
X1_197.068mz_neg	150
X15.9_584.729mz_pos	150