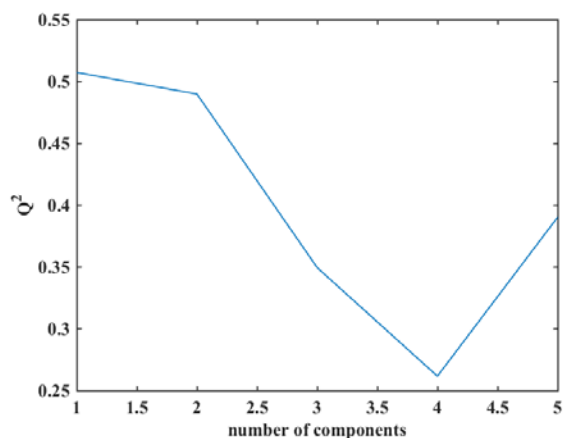
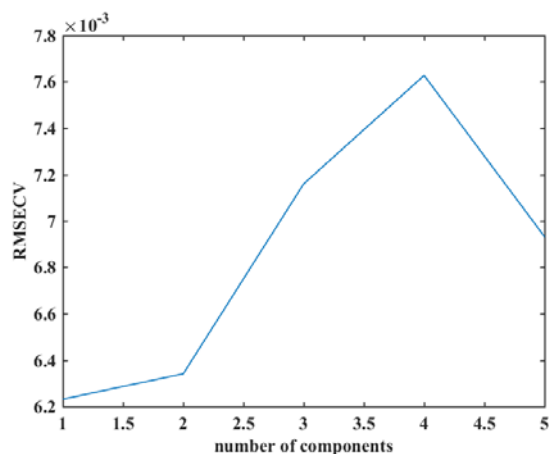


Supplementary materials:

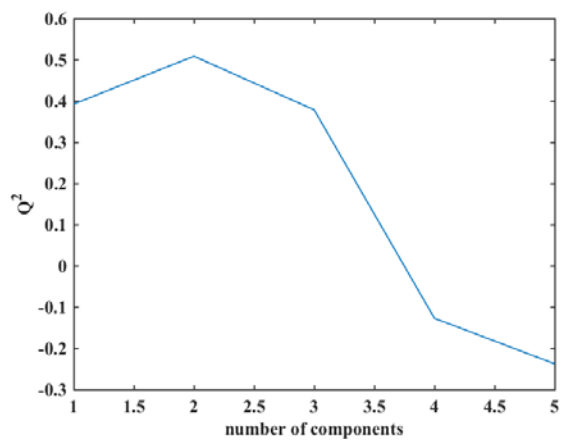
(a)



(b)



(c)



(d)

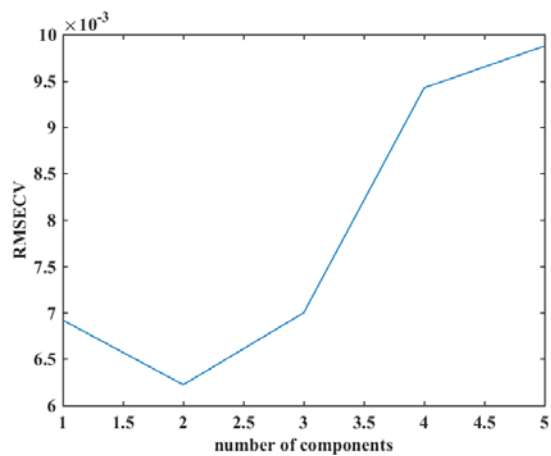


Figure S1. Leave-one-out cross validation for PLS model (a) and (b) plasma NMR data, (c) and (d) urine NMR data. (a) Q^2 value for PLS on plasma data, and (b) RMSECV for PLS model on plasma data. (c) Q^2 value for PLS on urine data, and (d) RMSECV for PLS model on urine data.