

Supporting Information for:

A Sequential Algorithm for Multiblock Orthogonal Projections to Latent Structures

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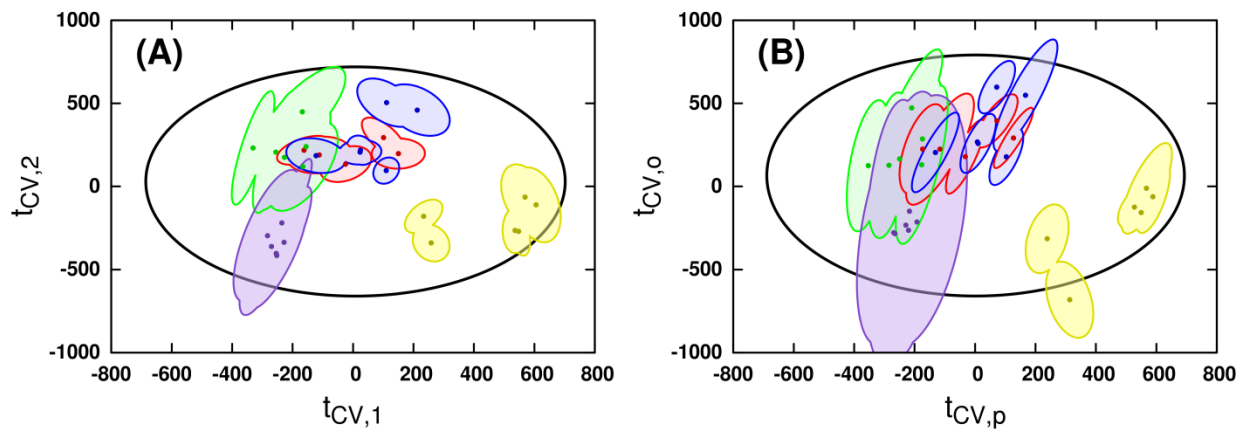


Figure S-1. Cross-validated super scores from (A) MB-PLS and (B) MB-OPLS models of the joint ^1H NMR and DI-ESI-MS data matrices. Points indicate mean values for each observation, and filled regions represent the union of all observations' confidence intervals from Monte Carlo iterations. Class colors are identical to those in Figure 2.

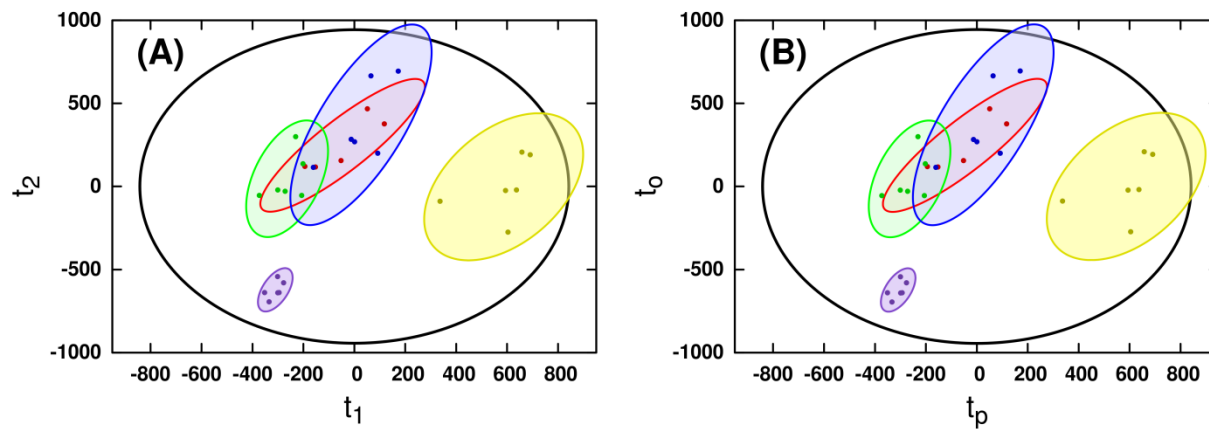


Figure S-2. Block scores from (A) MB-PLS and (B) MB-OPLS models of the ¹H NMR data matrix. Ellipses represent the 95% confidence intervals for each class. Class colors are identical to those in Figure 2.

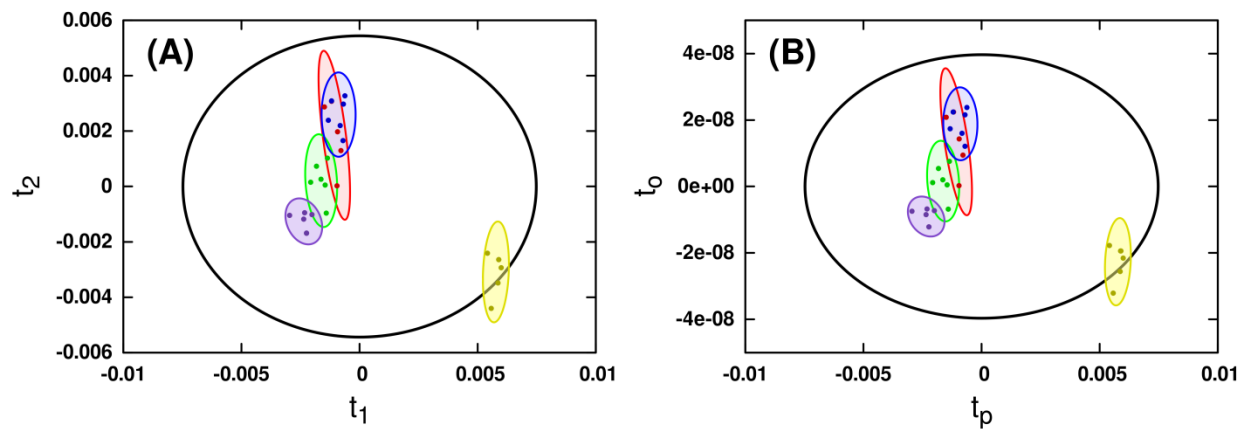


Figure S-3. Block scores from (A) MB-PLS and (B) MB-OPLS models of the DI-ESI-MS data matrix. Ellipses represent the 95% confidence intervals for each class. Class colors are identical to those in Figure 2.

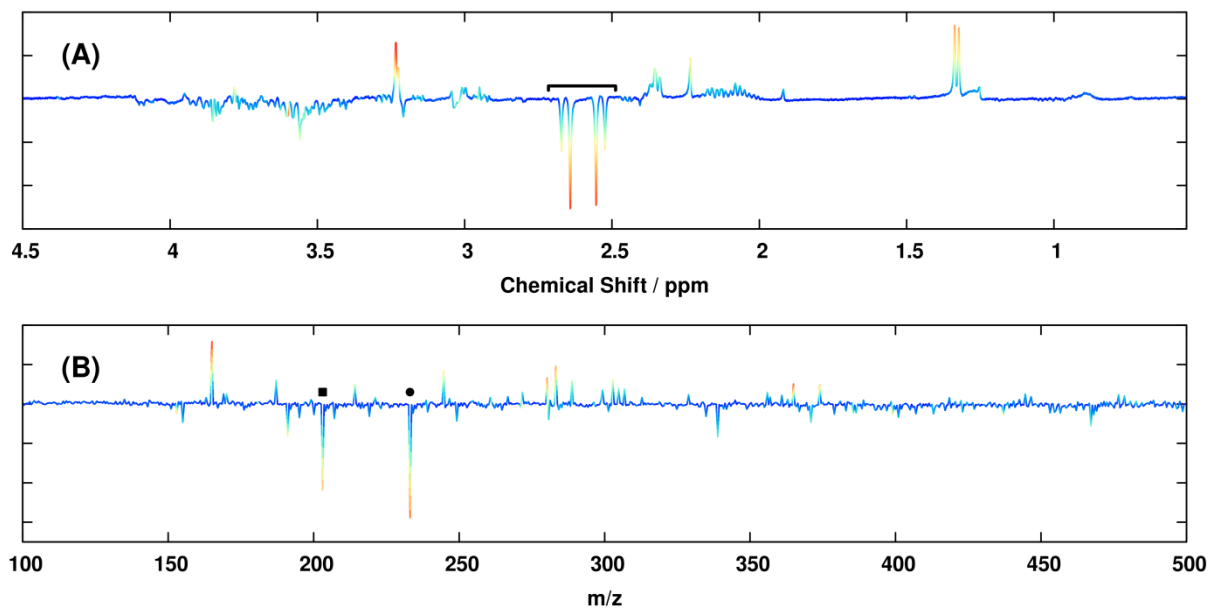


Figure S-4. Backscaled orthogonal block loadings from the MB-OPLS model of the (A) ^1H NMR and (B) DI-ESI-MS data matrices. Coloring of each loading vector is identical to that of Figure 3.

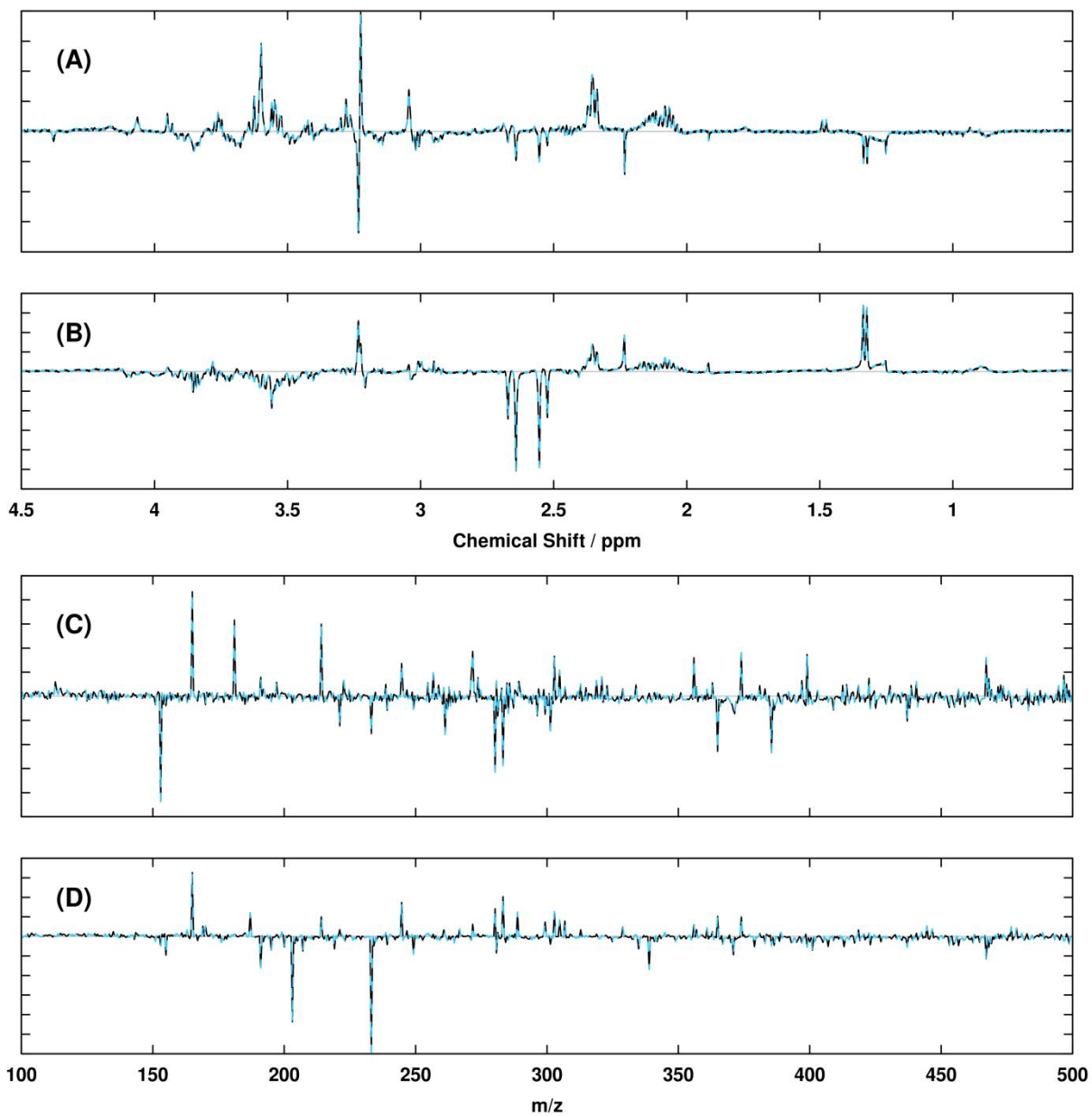


Figure S-5. Backscaled predictive (**A**, **C**) and orthogonal (**B**, **D**) block loadings from the MB-OPLS model of the (**A**, **B**) ^1H NMR and (**C**, **D**) DI-ESI-MS data matrices. Black lines indicate loadings from the algorithm in section 2.3.2 of the main text, dashed blue lines indicate loadings from the algorithm in section 2.3.4, and grey lines indicate their differences.