

Supplementary Information for:

Generalized Adaptive Intelligent Binning of Multiway Data

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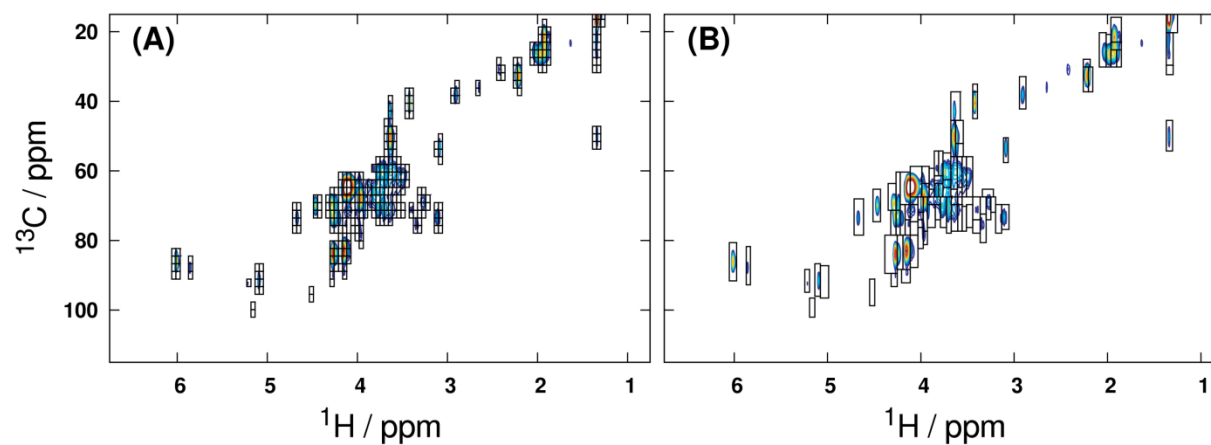


Figure S-1. Processed ^1H - ^{13}C HSQC mean spectrum of the fibroblast data tensor, with overlaid uniform (A) and GAI (B) bin boundaries. The dataset was binned with minimum bin widths along ^1H and ^{13}C of 0.025 ppm and 2.5 ppm, respectively. Retained bins all have maximum intensities no less than three times the standard deviation of the noise floor.

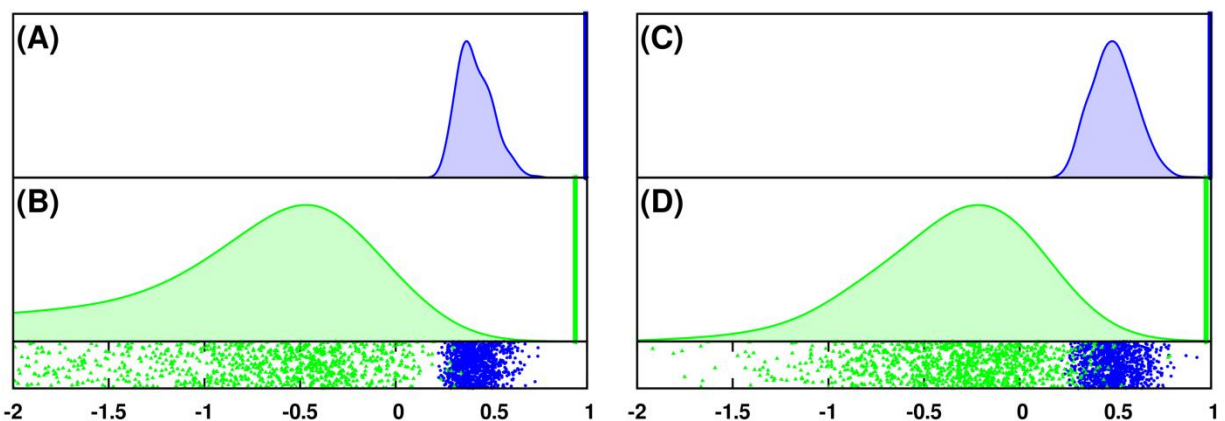


Figure S-2. Response permutation test results for OPLS-DA models of the uniformly binned (integrated) liver (**A, B**) and the fibroblast (**C, D**) data tensors. Model fit (R^2_Y) statistics (**A, C**) are shown in blue, and model predictive ability (Q^2) statistics (**B, D**) are shown in green. True values of R^2_Y and Q^2 are represented by vertical bars, and null distributions are computed through kernel density estimation of the values from permutation. Scatter plots of the permutation R^2_Y and Q^2 statistics are shown in the lower panes.

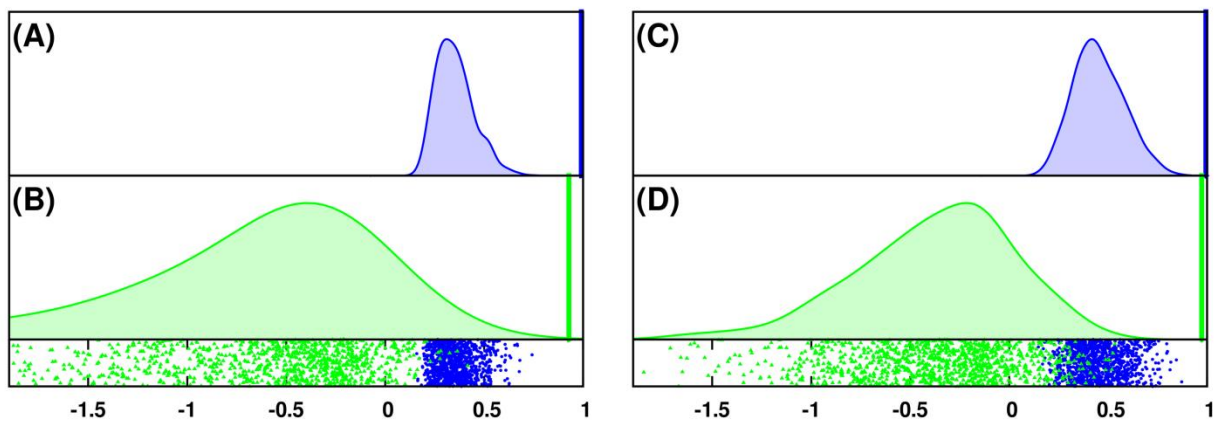


Figure S-3. Response permutation test results for OPLS-DA models of the GAI-binned (integrated) liver (**A, B**) and the fibroblast (**C, D**) data tensors. See the caption of Figure S-2 for a complete description of the figure contents.

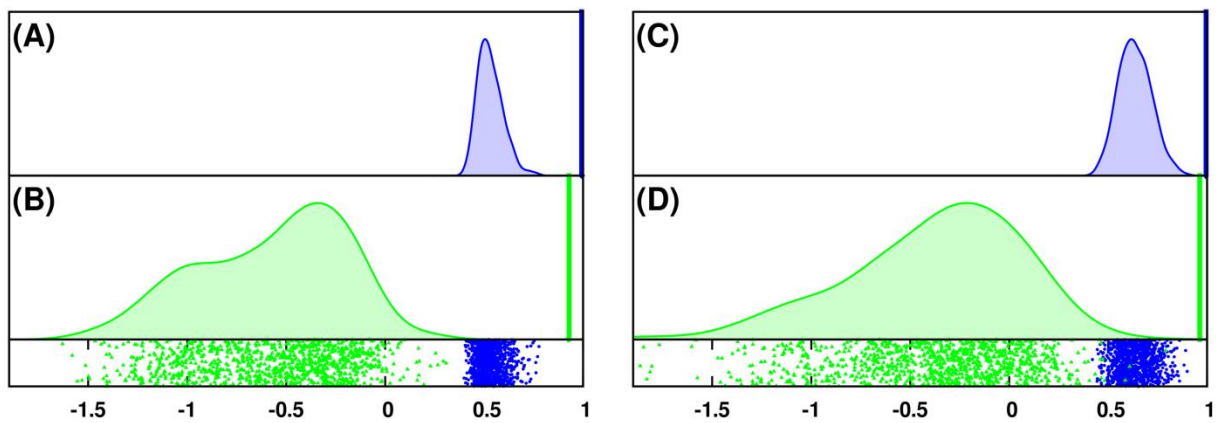


Figure S-4. Response permutation test results for OPLS-DA models of the uniformly binned (vectorized) liver (**A, B**) and the fibroblast (**C, D**) data tensors. See the caption of Figure S-2 for a complete description of the figure contents.

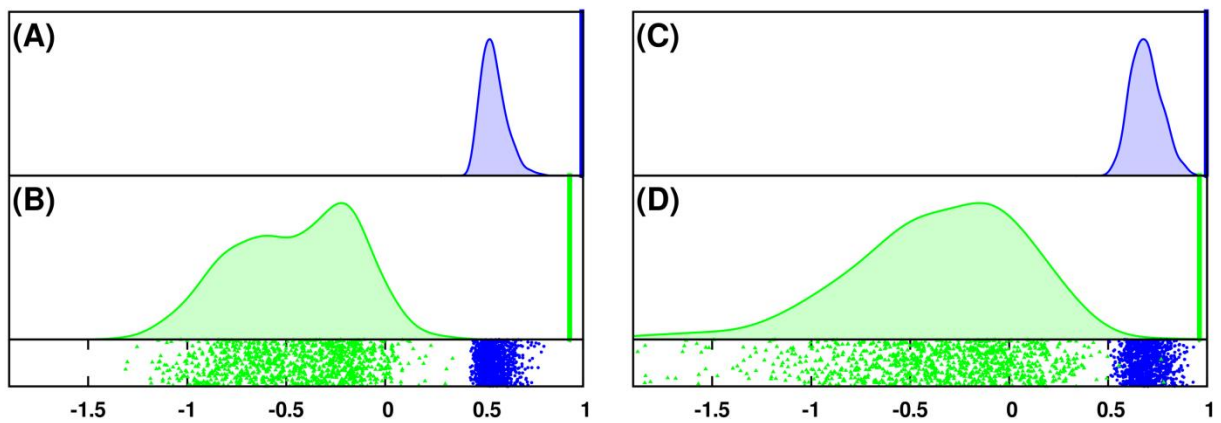


Figure S-5. Response permutation test results for OPLS-DA models of the GAI-binned (vectorized) liver (**A, B**) and the fibroblast (**C, D**) data tensors. See the caption of Figure S-2 for a complete description of the figure contents.