Software and Code, and Data Availability

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## Software, Code and Data Availability

All calculations were performed using R version 4.3.0 (2023-04-21), with the following packages and versions:

* creation of raincloud plots: ggrain v0.0.3
* general plotting: ggplot2 v3.4.2
* calculation of principal component variances and associates: visualizationQualityControl v0.4.10 (Github moseleybioinformaticslab/visualizationqualitycontrol@7590a72)
* receiver operating curves and plots: pROC v1.18.5
* UpSet plots and heatmaps: ComplexHeatmap v2.16.0
* ICI-Kendall-tau calculations: ICIKendallTau v1.0.5 (Github moseleybioinformaticslab/icikendalltau@a9ca36b)
* Hierarchical clustering reordering: dendsort v0.3.4
* Workflow control: targets v1.0.0

A full list of all installed R packages can be found in the renv.lock file in the Zenodo repository at https://dx.doi.org/10.5281/zenodo.12190086.

All code used for the analysis is available on GitHub at https://github.com/MoseleyBioinformaticsLab/conwell-manuscript.ChronicPancreatitisUrineMetabolomics/, and on Zenodo at https://dx.doi.org/10.5281/zenodo.12190086.