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Multiblock omics data fusion using the Consensus OPLS R package



Céline Bougel^{1,2}, Van Du Tran³, Julien Bocard⁴, Marie Tremblay-Franco^{1,2}, Florence Mehl³

¹ Toxalim (Research Center in Food Toxicology), Toulouse University, INRAE, ENVT, INP-Purpan, UPS, Toulouse, France

² MetaboHUB-Metatoul, National Infrastructure of Metabolomics and Fluxomics, Toulouse, France

³ Vital-IT Group, SIB Swiss Institute for Bioinformatics, 1015 Lausanne, Switzerland

⁴ School of Pharmaceutical Sciences, University of Geneva, 1211, Geneva 4, Switzerland



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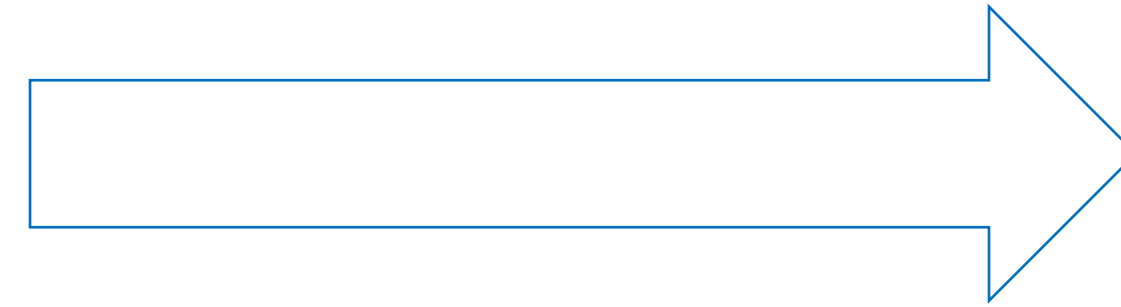
Introduction

Omics approaches have proven their value in providing a broad monitoring of biological systems. However, despite the wealth of data generated by modern analytical platforms, the analysis of a single dataset is still limited and insufficient to reveal the full biochemical complexity of biological samples. The fusion of information from several data sources constitutes therefore a relevant approach to assessing biochemical events more comprehensively. However, inherent problems encountered when analyzing

single tables are amplified with the generation of multi-block datasets. Finding the relationships between data layers of increasing complexity constitutes a challenging task. Here we propose an extension to the versatile methodology combining the strength of established data analysis strategies, multi-block approaches with Orthogonal Partial Least Squares Discriminant analysis (OPLS-DA) framework [1], to offer an efficient tool as an R package for the fusion of Omics data obtained from multiple sources.



MATLAB in-house scripts available at [GitHub Unige](#) with demo_data [2]



R package available in [CRAN](#)
New features



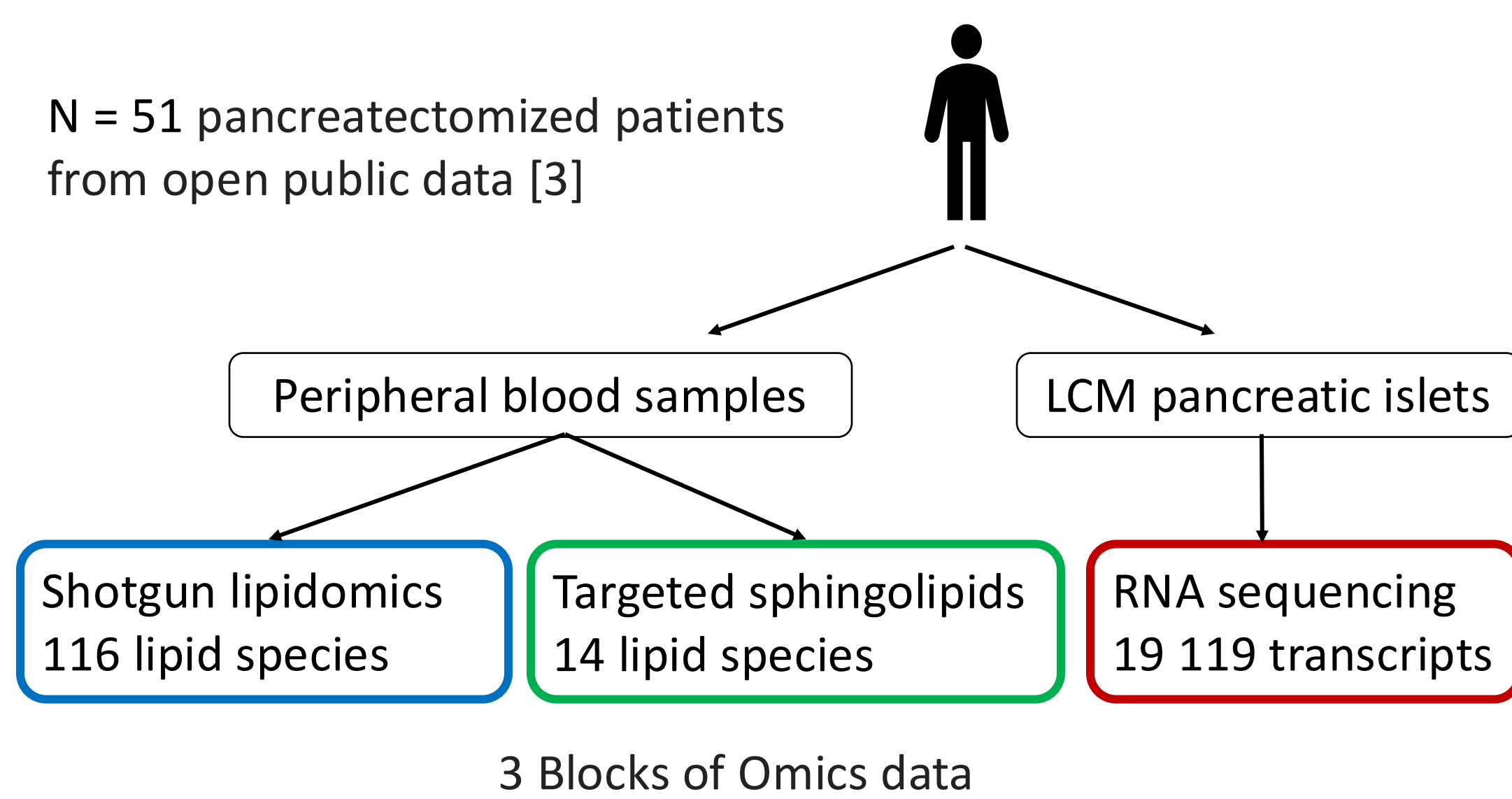
Upgrades

Kernels non-linear
Multiple predictive components

Variable Importance in Projection (VIP)
Prediction of new samples

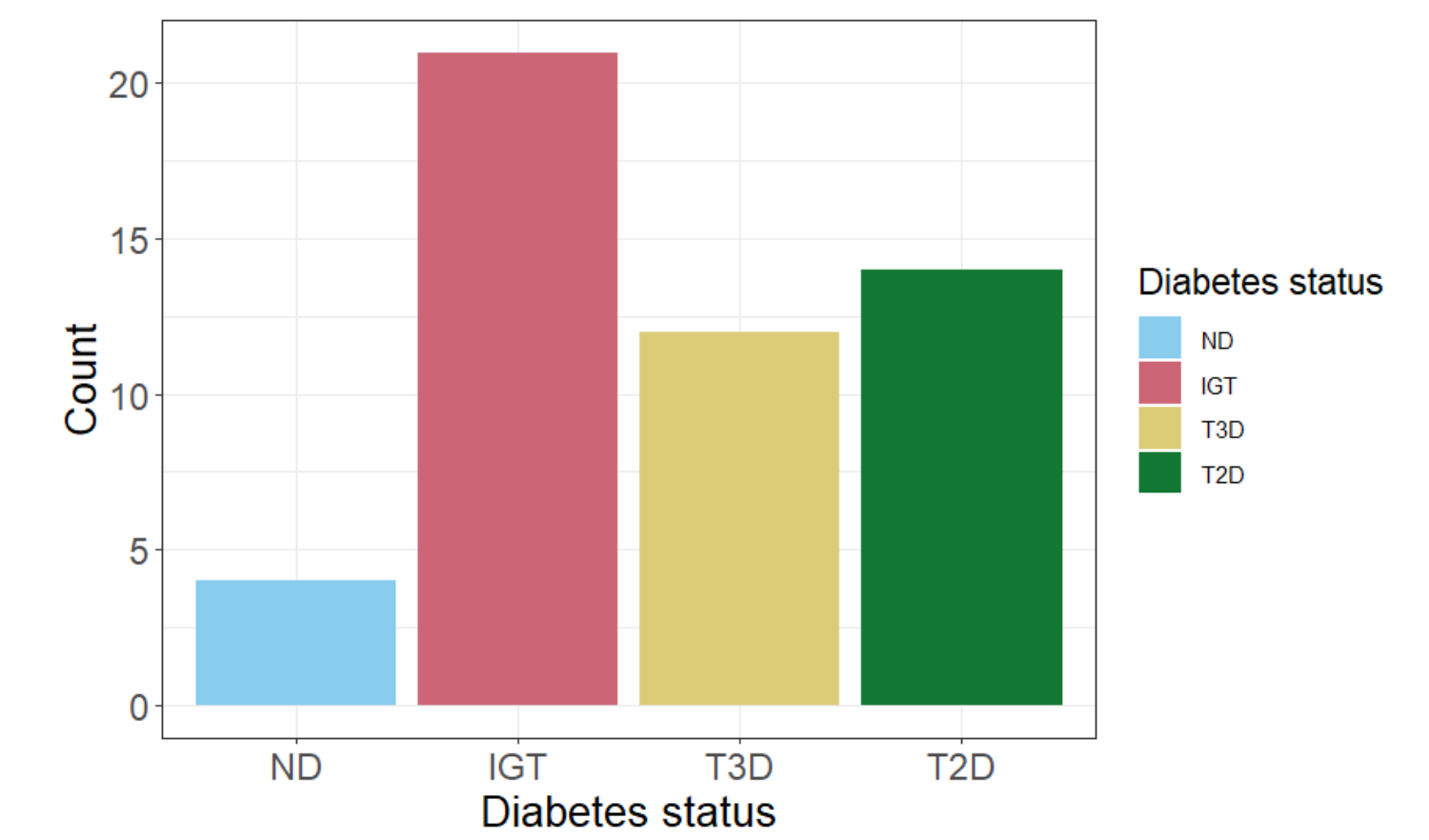
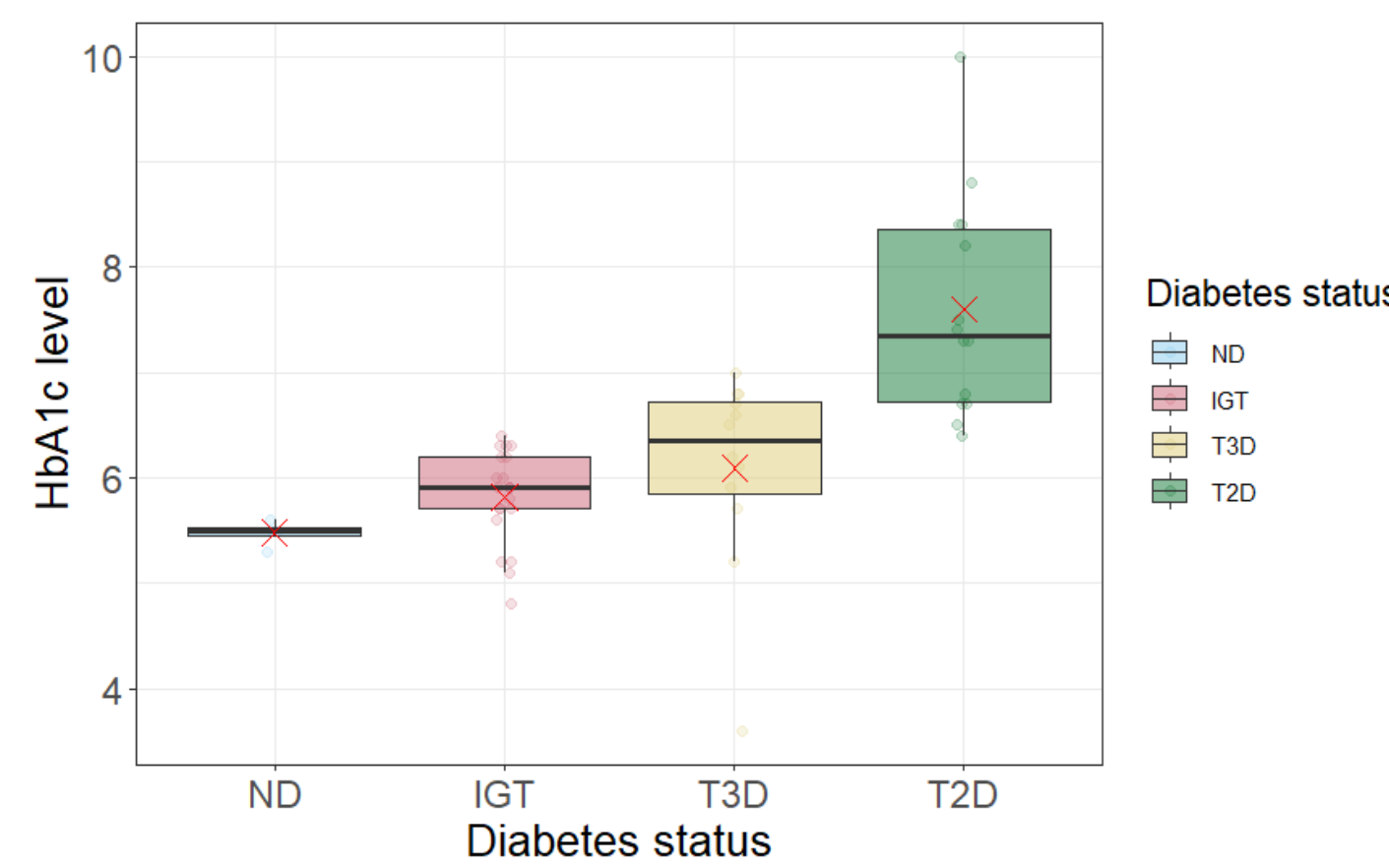
Parallel computing

N = 51 pancreatized patients from open public data [3]



Use case

4 groups of patients based on glycemic values at fasting and at the 2-hour timepoint of an oral glucose tolerance test, using the thresholds defined in the guidelines of the American Diabetes Association : Non-diabetic (ND); impaired glucose tolerance (IGT); type 2 diabetes (T2D); type 3c diabetes (T3D).



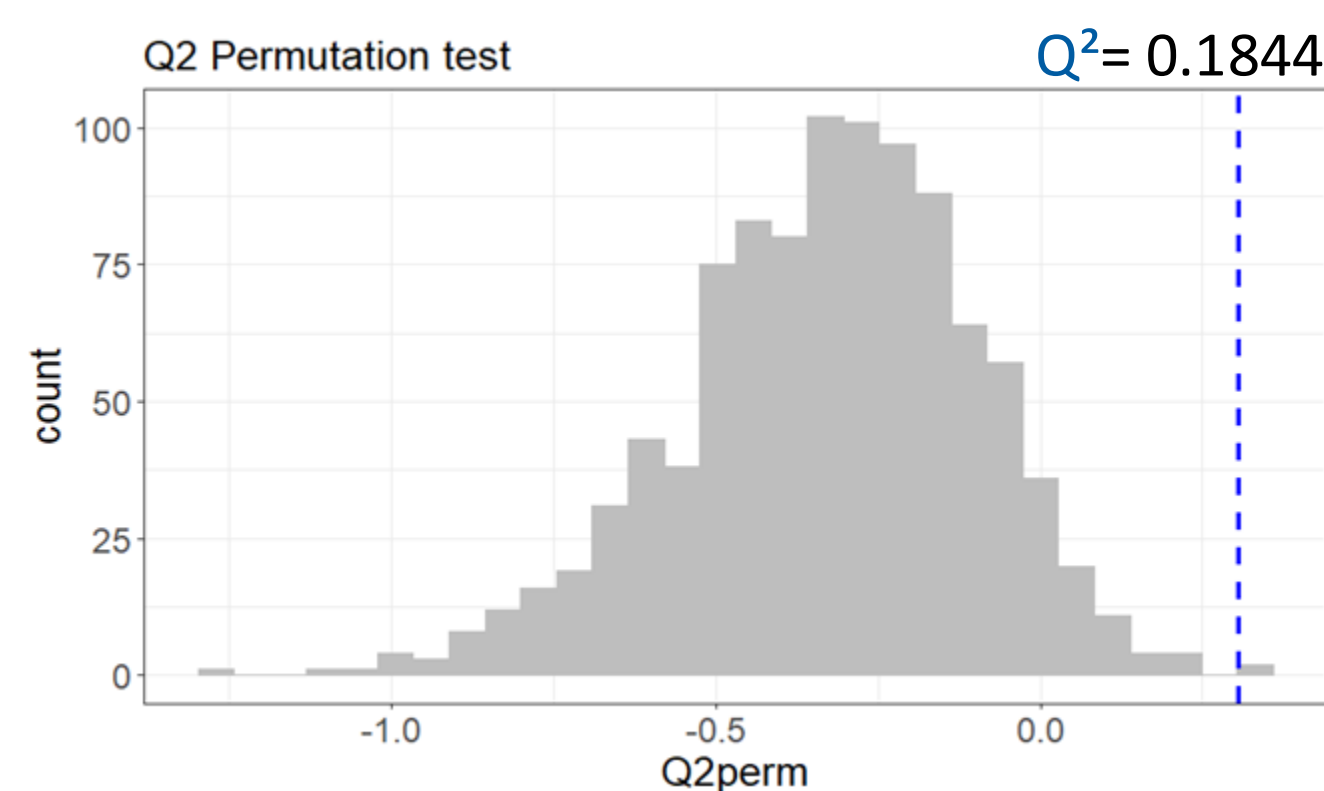
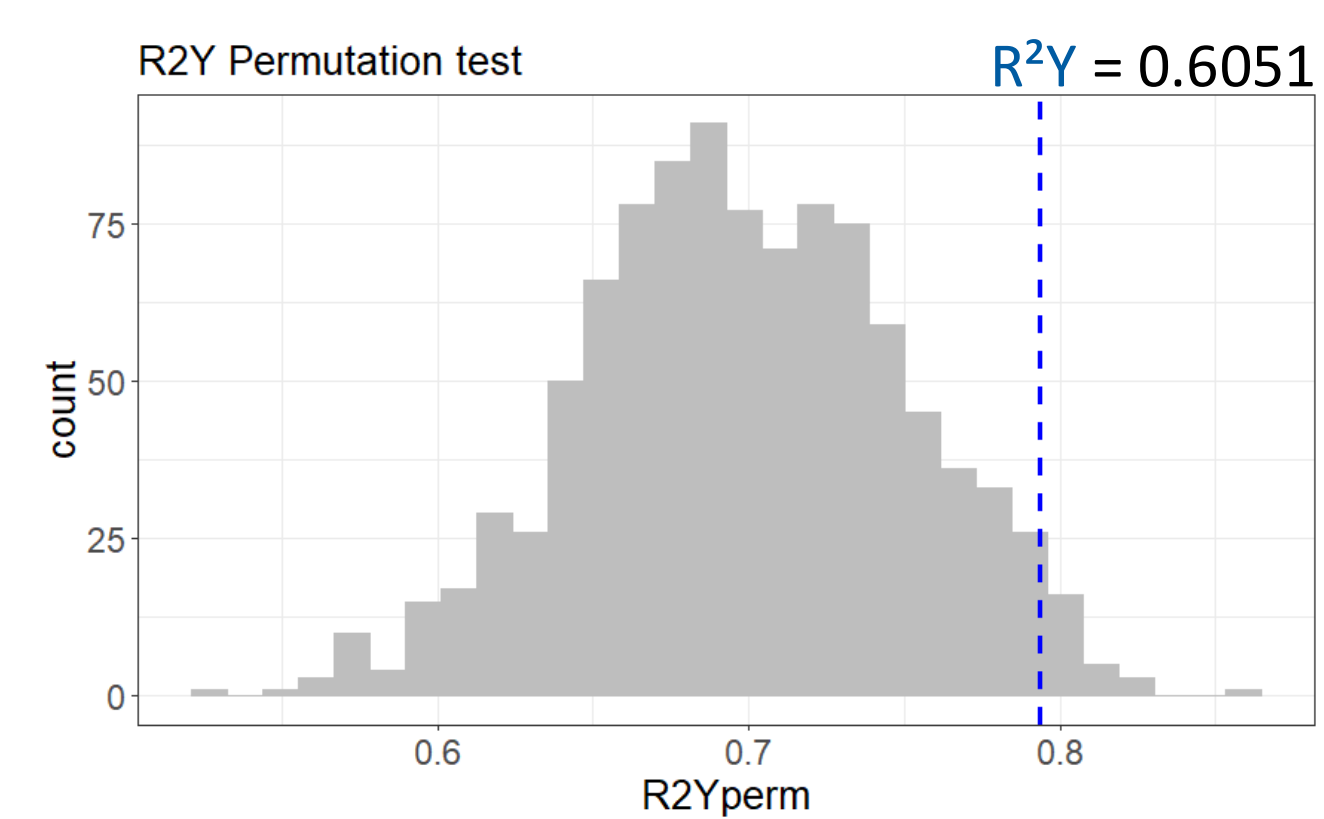
Results and discussion

Model computation

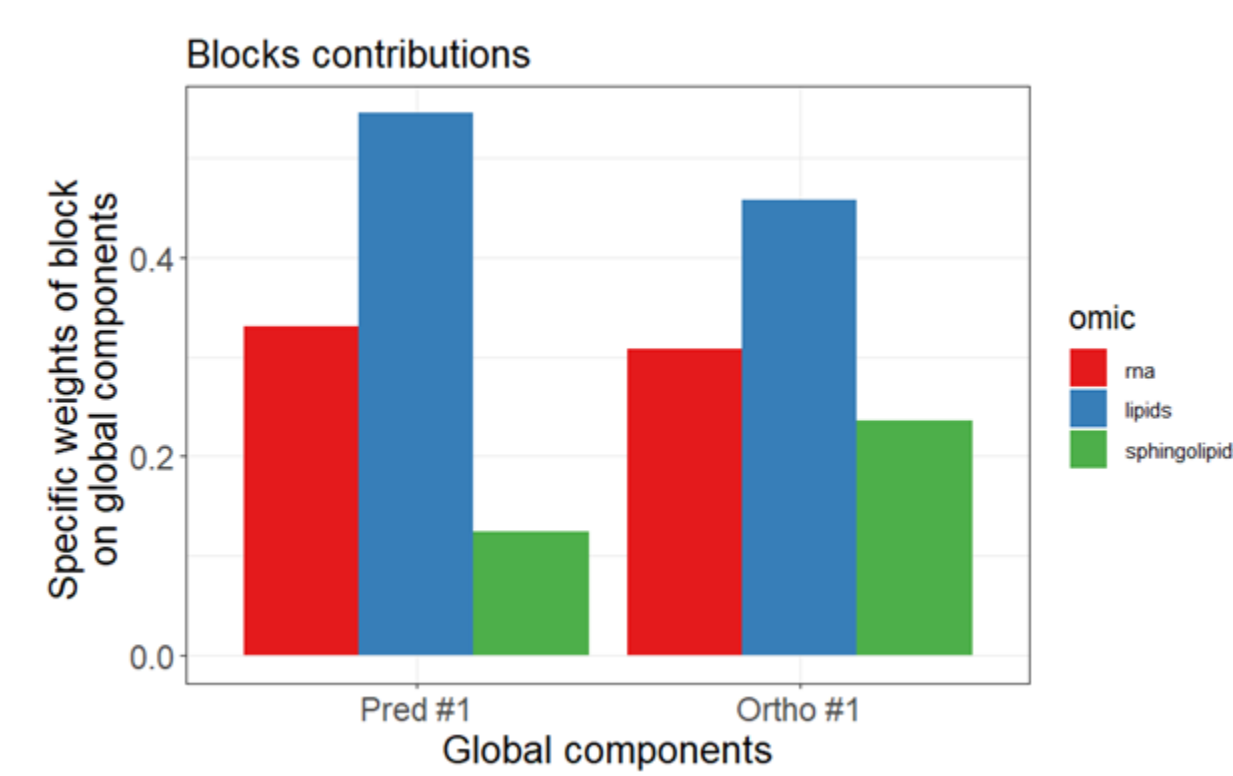
```
COPLS_results <- ConsensusOPLS(
  data = my_data_with_3_blocks_of_omics_data,
  Y = response_HbA1c_variables,
  maxComp = 1, #one predictive component
  maxOrtho = 1, #one orthogonal component
  modelType = "reg", #regression model
  nperm = 1000, #number of permutations
  cvType = "nfold", #type of cross-validation
  nfold = 51, #number of subjects = leave-one-out
  kernelParams = list(type = "p",
    params = c(order = 1)), #linear polynomial kernel
  mc.cores = 1, #how many cores for parallelization
)
```

Quality assessment

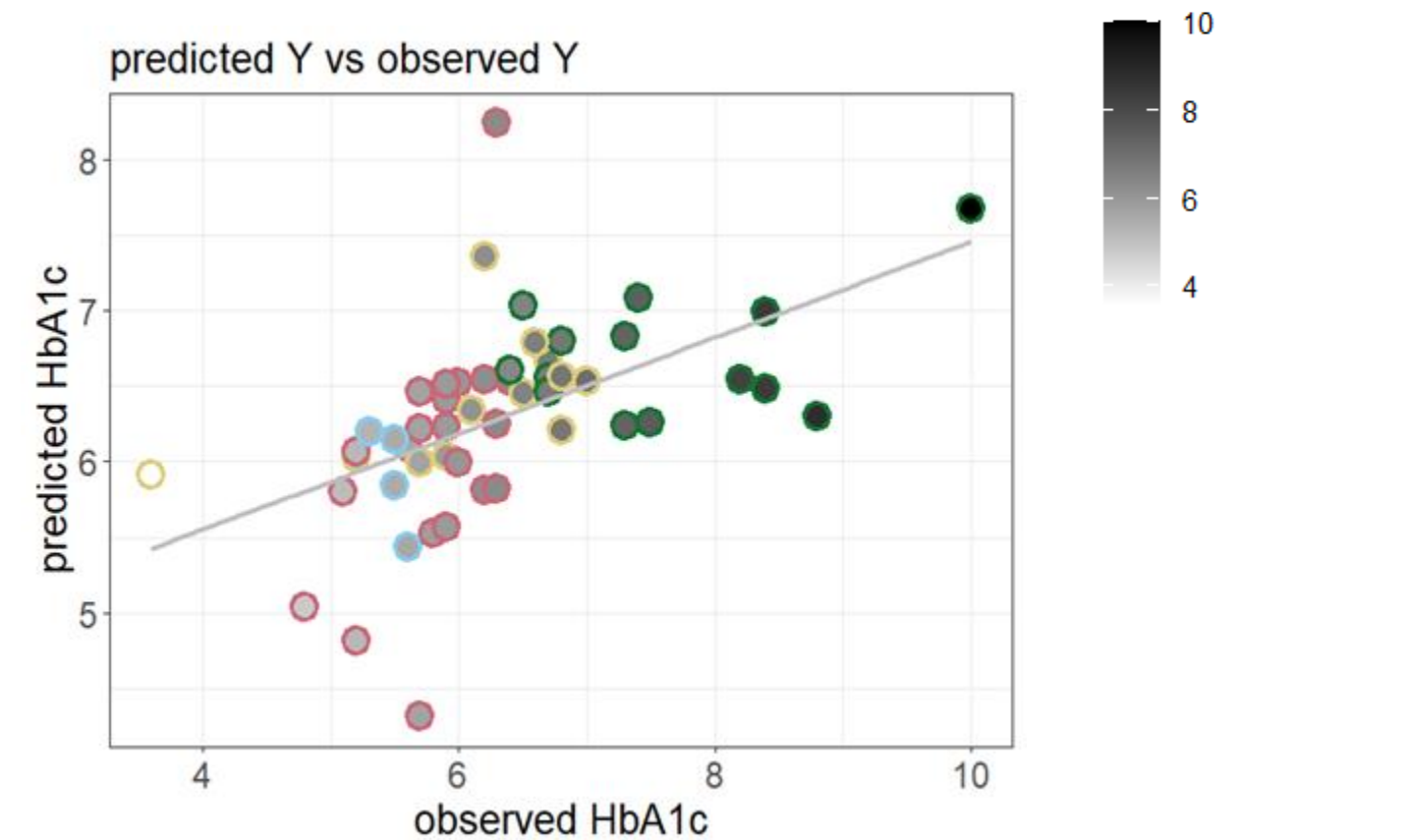
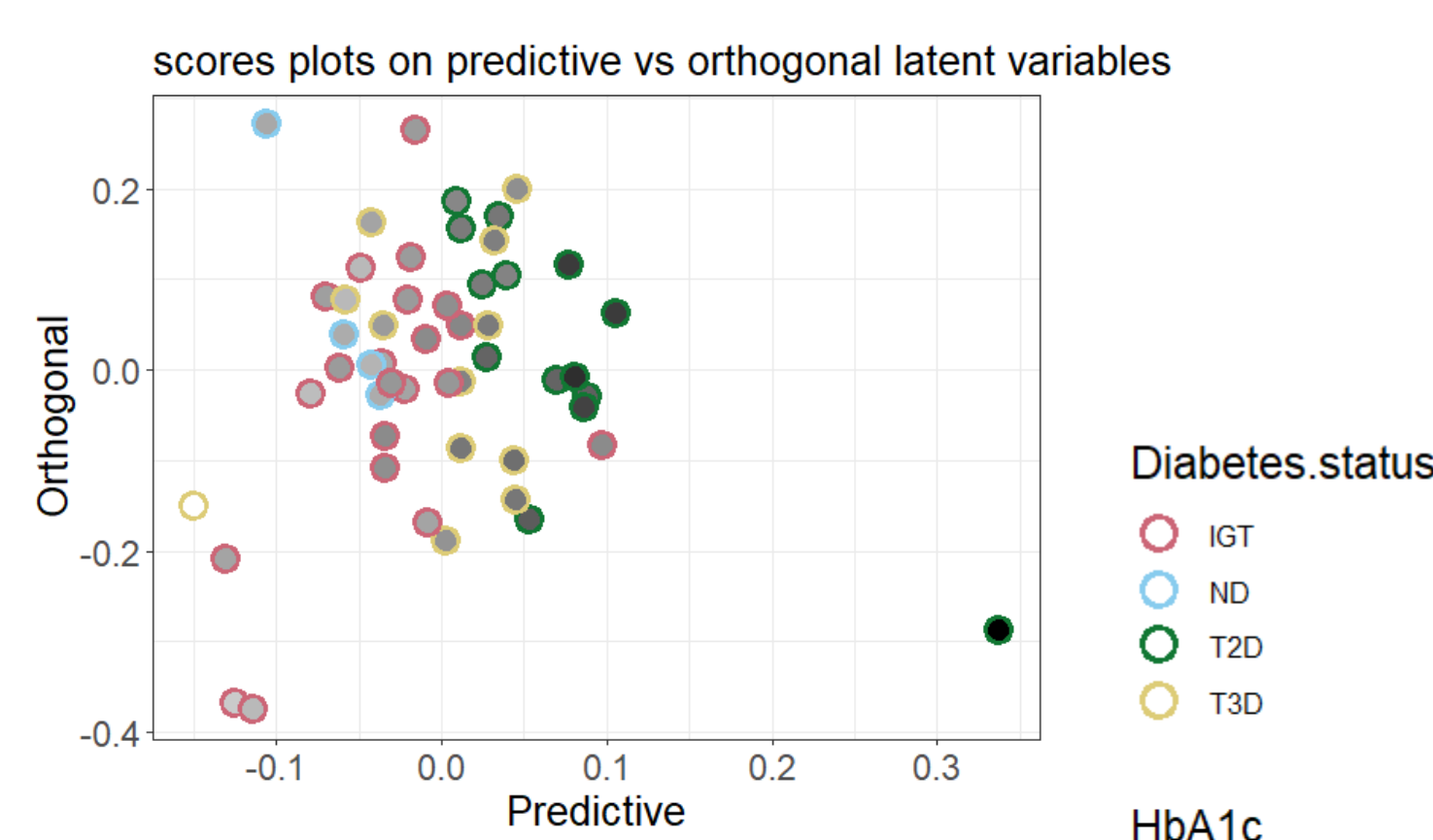
1000 models are computed with permuted Y values. The results of the optimal model are significantly different from the results of the permuted models.



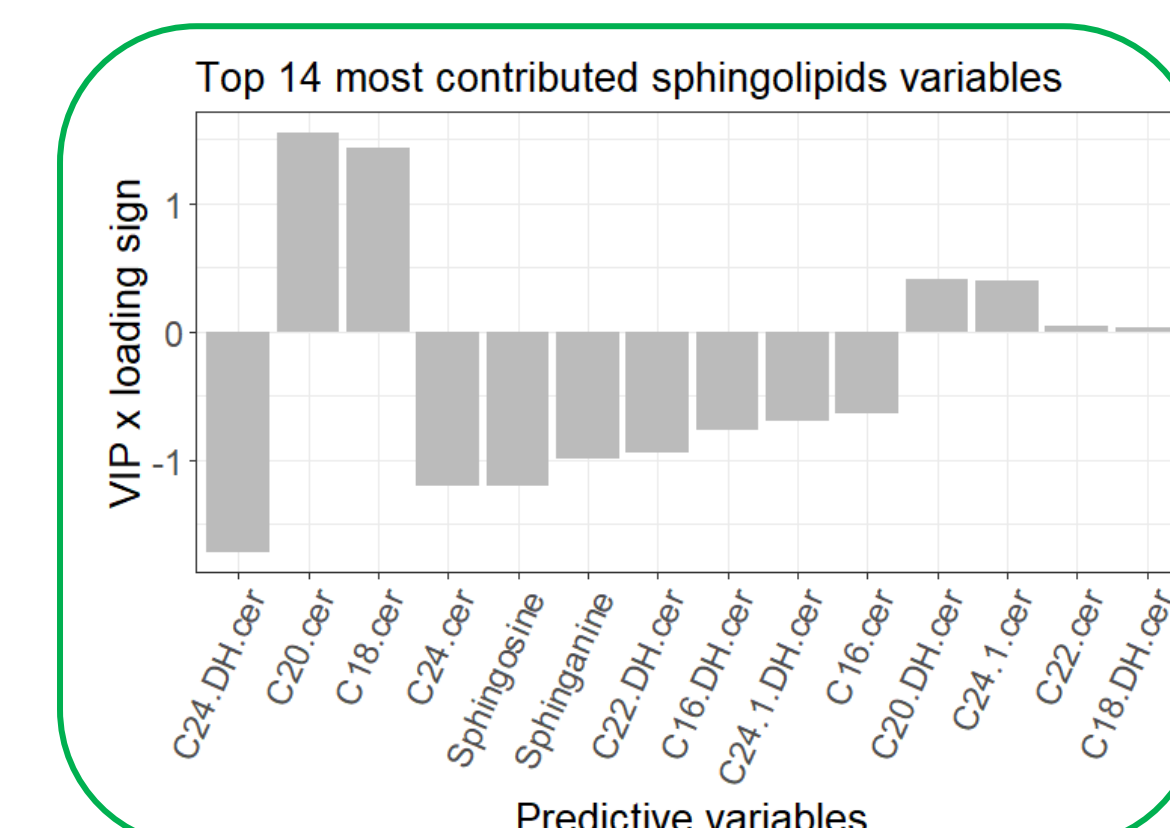
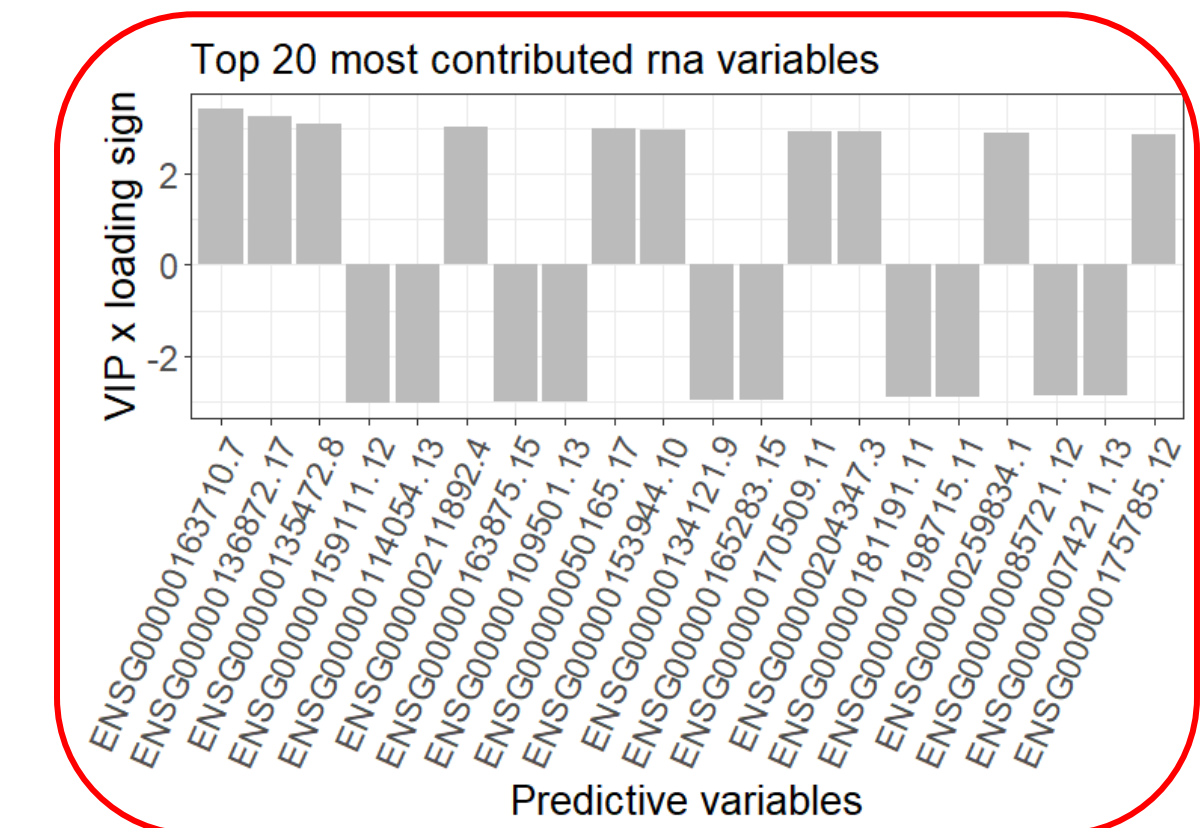
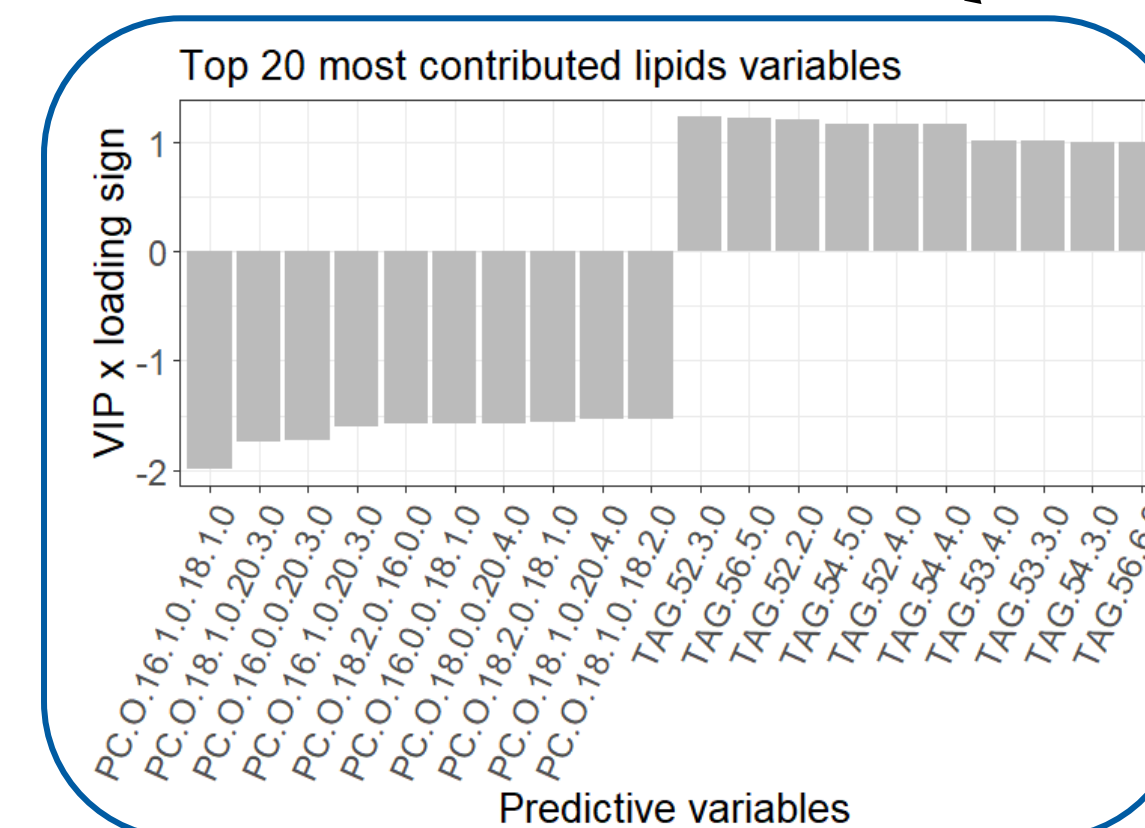
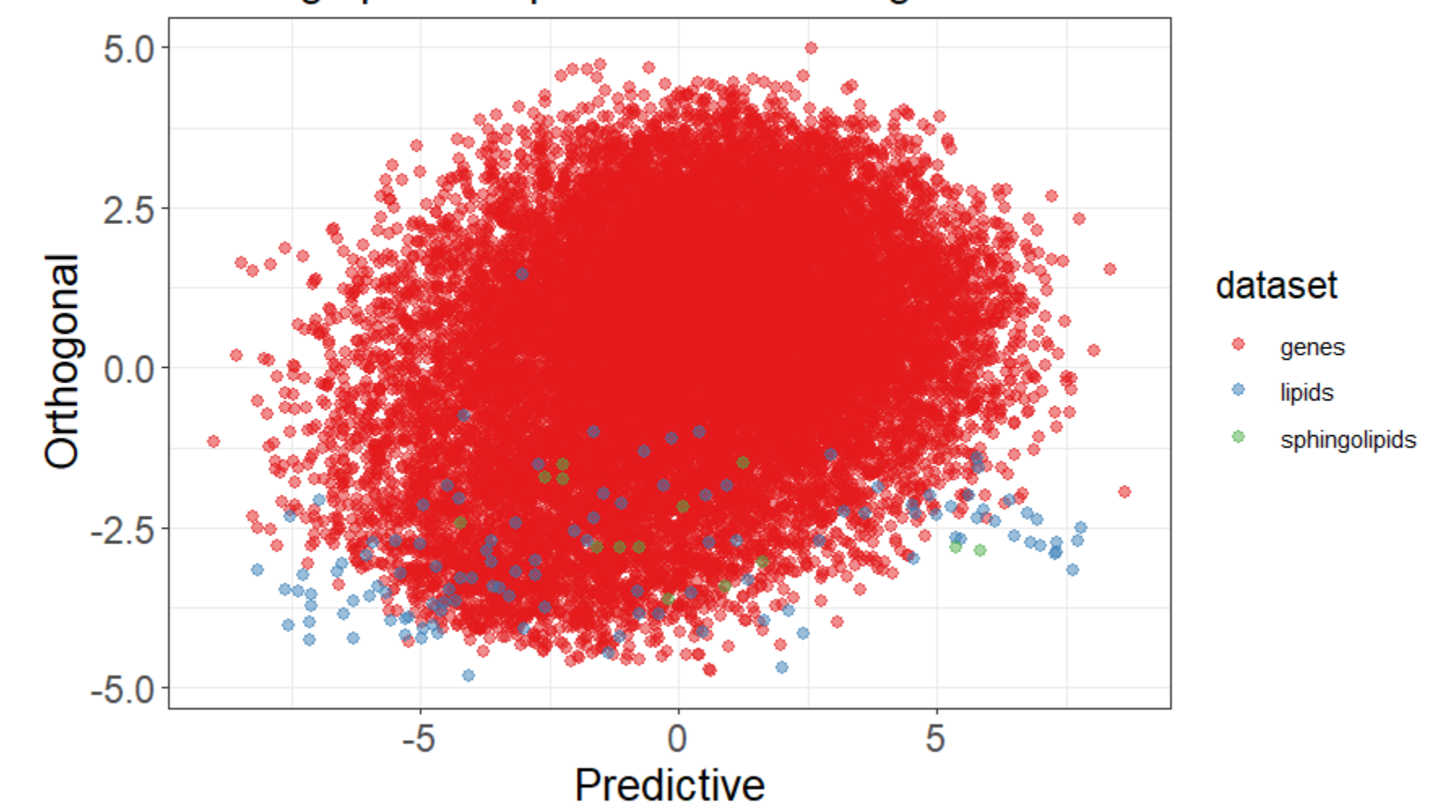
Regression Analysis (ConsensusOPLS-reg) of HbA1c levels



The 3 omics contribute to the modelization of HbA1c levels. The untargeted lipidomics dataset brings the largest part of the information.



Loadings plots on predictive vs orthogonal latent variables



Conclusions

The **ConsensusOPLS R package** proposes a **free, open-source, and easy-to-use software** for the Consensus OPLS method, which was demonstrated as a **relevant and widely applicable** method for the **horizontal integration of omics data**, with multiple functionality upgrades.

References

The **ConsensusOPLS R package** is available at <https://CRAN.R-project.org/package=ConsensusOPLS>.

[1] J. Bocard, D.N. Rutledge. 2013. "A Consensus Orthogonal Partial Least Squares Discriminant Analysis (OPLS-DA) Strategy for Multiblock Omics Data Fusion." Analytica Chimica Acta 769 (March): 30–39. <https://doi.org/10.1016/j.aca.2013.01.022>.

[2] R.H. Shoemaker. 2006. "The NCI60 Human Tumour Cell Line Anticancer Drug Screen." Nature Reviews. Cancer 6 (10): 813–823. <https://doi.org/10.1038/nrc1951>.

[3] Wigger L, Barovic M, Brunner AD, et al. 2021. "Multi-omics profiling of living human pancreatic islet donors reveals heterogeneous beta cell trajectories towards type 2 diabetes." Nat Metab. 2021 Jul;3(7):1017-1031. PMID: 34183850. <https://doi.org/10.1038/s42255-021-00420-9>.

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- Vital-IT Group, SIB Swiss Institute for Bioinformatics.
- School of Pharmaceutical Sciences, University of Geneva.

Contacts

- marie.tremblay-franco@inrae.fr
- florence.mehl@sib.swiss