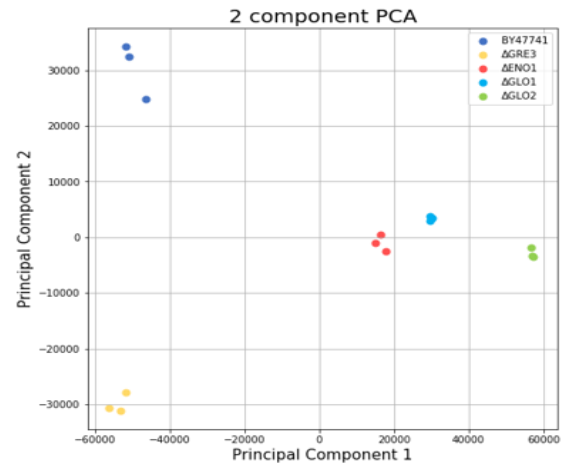
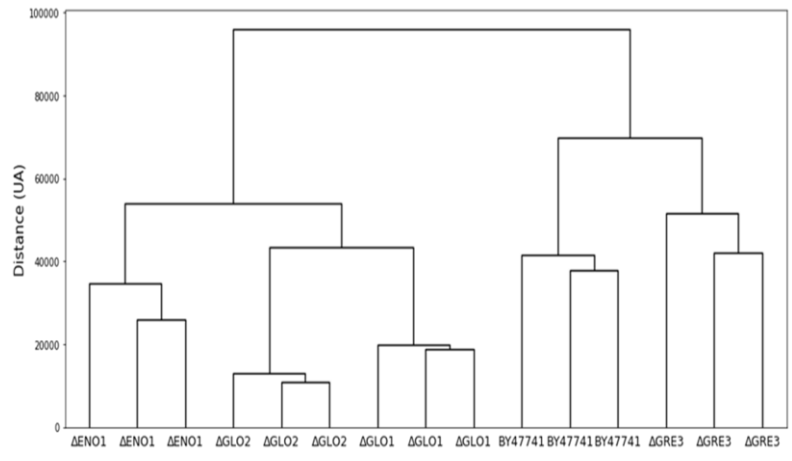
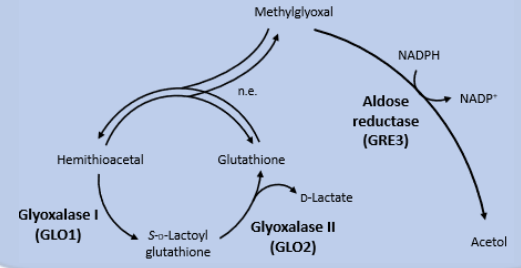


Introduction and methods

S. cerevisiae has only 6000 genes, most of which can be deleted without noticeable consequences. We searched for “hidden effects” of single-gene deletions through an untargeted FT-ICR-MS metabolomic analysis of 5 isogenic strains, mainly related to methylglyoxal, a toxic by-product of glycolysis.



Hierarchical Clustering dendrogram (left) and Principal Component Analysis score plot (right) of the FT-ICR-MS data

Hierarchical Clustering and Principal Component Analysis plots reveal greater similarity between samples of the same strain, which always cluster together

Results

We were able to discriminate between all strains using multivariate statistical analysis of extreme resolution FT-ICR-MS data.

Furthermore, inter-strain comparisons revealed the existence of two groups:

- One formed by the reference strain (BY4741) and aldose reductase mutant (ΔGRE3)
- The other formed by the two glyoxalase mutant strains (ΔGLO1/2) and the enolase mutant strain (ΔENO1)

Mass (Da)	Metabolite Name	Molecular Formula	VIP Score	Relative concentration
307.0838	Glutathione	C ₁₀ H ₁₇ N ₃ O ₆ S	8.418	BY4741 ΔGLO1 ΔGLO2 ΔGRE3 ΔENO1
493.3168	PC(16:1(9Z)/0:0)	C ₂₄ H ₄₈ NO ₇ P	5.993	
624.0873	N/A	C ₁₄ H ₂₈ N ₁₀ O ₁₀ S ₄	5.588	
257.1029	Glycerophosphocholine	C ₈ H ₂₀ NO ₆ P	4.837	

Glutathione is the most relevant metabolite for strain differentiation in agreement with its role as catalytic cofactor of the glyoxalase pathway