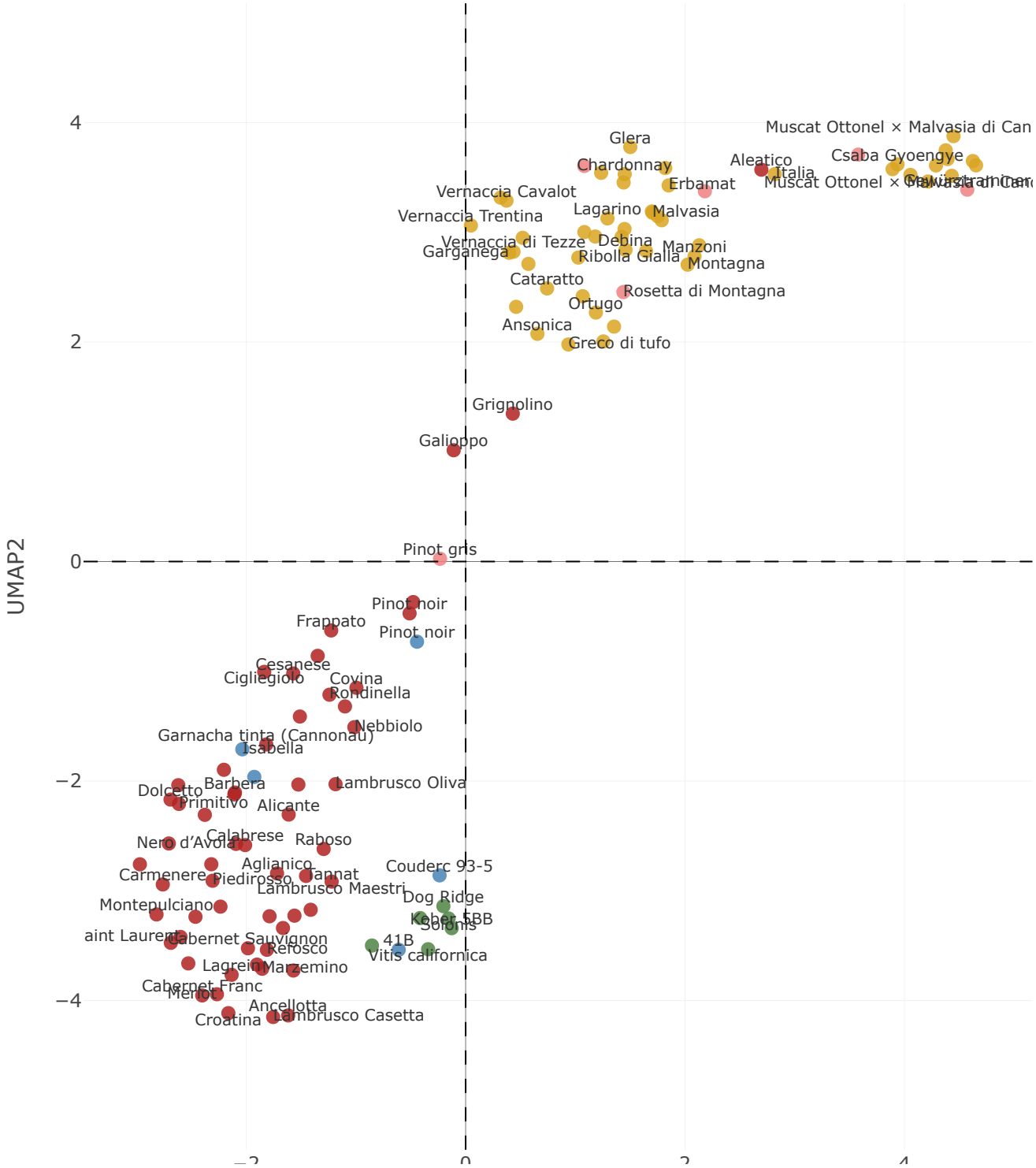
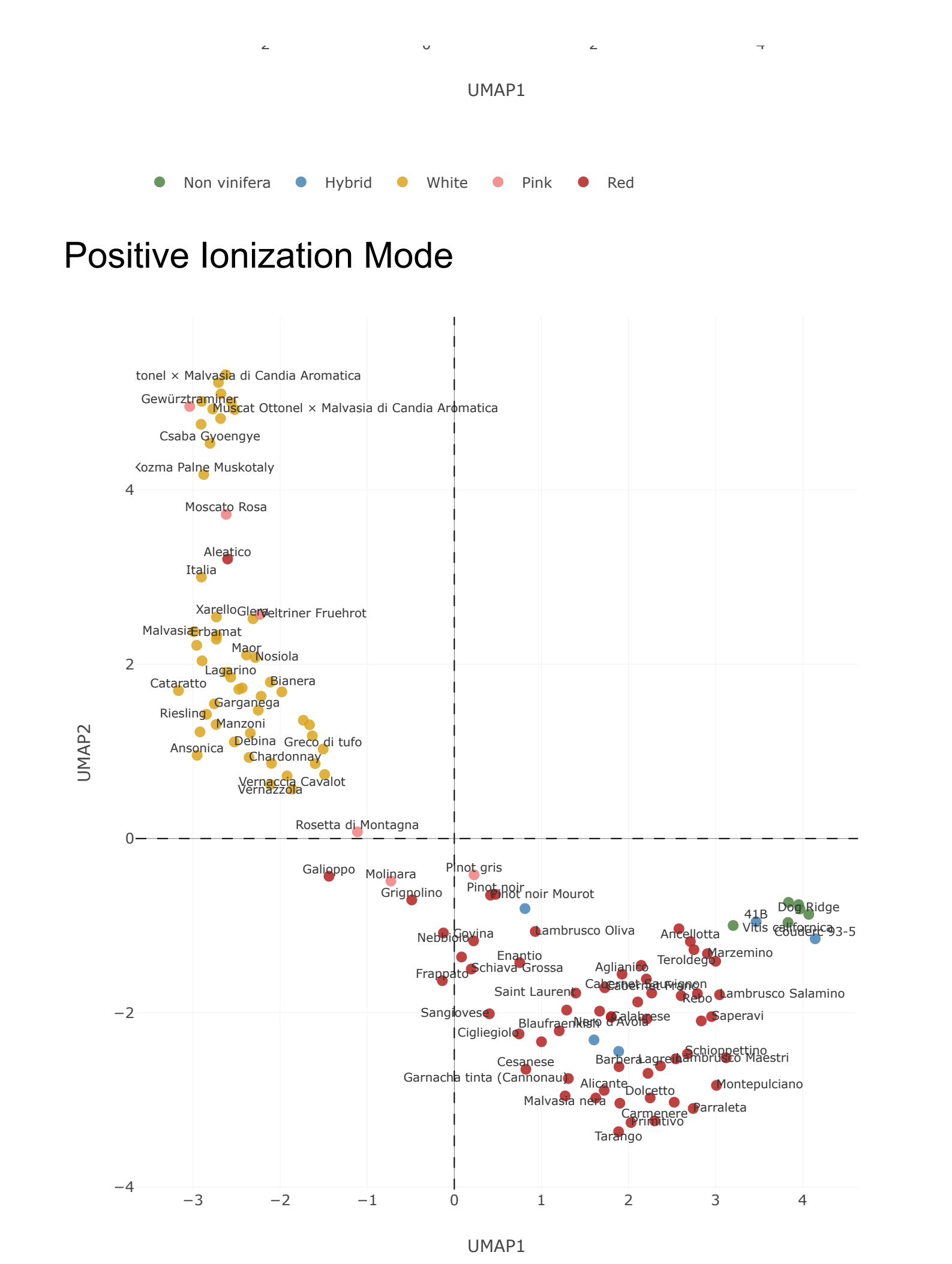
Grape Metabolome — Per-Variety UMAP Explorer

2026-09-04

This page shows one interactive UMAP per ionization mode (NEG, POS), with one point per grape variety. Hover over a point to see its name and group. Zoom in to reveal more variety names as they spread apart; zoom back out to see the overall structure. See the methods page (methods.html) for how these maps were built and the UMAP parameters used.

Negative Ionization Mode




UMAP1
Non vinifera
Hybrid
White
Pink
Red
tonel × Malvasia di Candia Aromatica
Gewürztraminer
Muscat Ottonel × Malvasia di Candia Aromatica
Csaba Gyoengye
Kozma Palne Muskotaly
Moscato Rosa
Aleatico
Italia
Xarello
Glera
Veltriner Fruehrot
Malvasia Erbamat
Maor
Nosiola
Lagarino
Cataratto
Bianera
Garganega
Riesling
Manzoni
Ansonica
Debina
Greco di tufo
Chardonnay
Vernaccia
Cavalot
Vernazzola
Rosetta di Montagna
Galioppo
Molinara
Grignolino
Pinot gris
Pinot noir
Pinot noir Mourot
Dog Ridge
41B
Vitis californica
Couderc 93-5
Nebbiolo
Covina
Lambrusco Oliva
Ancellotta
Marzemino
Enantio
Schiava Grossa
Teroldego
Aglianico
Frappato
Cabernet Sauvignon
Cabernet Franc
Rebo
Saint Laurent
Lambrusco Salamino
Sangiovese
Calabrese
Saperavi
Blaufraenkisch
Nero d'Avola
Ciligiegiolo
Schiopettino
Barbera
Lagrein
Lambrusco Maestri
Cesanese
Garnacha tinta (Cannonau)
Alicante
Montepulciano
Dolcetto
Malvasia nera
Parraleta
Carmenere
Primitivo
Tarango
UMAP2
Positive Ionization Mode

A note on reading these maps. UMAP preserves *local neighbourhood structure*, not a global distance metric: two points sitting close together are more similar than two points far apart, but the exact distance between them — or between two clusters — carries no quantitative meaning. Distances should not be compared across regions of the plot, and the size of the gap between two clusters should never be read as “how different” those clusters are. Only relative closeness is informative.

Citation. This dataset and its variety groupings come from:

Arapitsas, P.; Franceschi, P.; Garcia-Aloy, M.; Vrhovsek, U.; Narduzzi, L.; Masuero, D.; Stefanini, M.; Bettinelli, P.; Grando, M. S.; Emanuelli, F.; Wehrens, R.; Theodoridis, G.; Mattivi, F. A Metabolome Atlas of Grape Biodiversity. *J. Agric. Food Chem.* **2026**. DOI: 10.1021/acs.jafc.6c04648 (https://pubs.acs.org/jafcau/article/doi/10.1021/acs.jafc.6c04648/5328347/A-Metabolome-Atlas-of-Grape-Biodiversity).

Download the full maps. Static, print-quality PDF versions of both maps, with every variety labelled: Negative Ionization Mode (PDF) (gm_umap_explorer_NEG.pdf) · Positive Ionization Mode (PDF) (gm_umap_explorer_POS.pdf)

Methods. For details on how these maps were built — per-variety averaging, outlier handling, batch correction, and the UMAP parameters used — see the methods page (methods.html).