

Description of Additional Supplementary Files

File name: Supplementary Data 1

Description: Classification metrics for all odor labels across feature types and classifiers. Supports main Figure 1.

File name: Supplementary Data 2

Description: Average feature importance scores for FG and MD models. Supports main Figure 2.

File name: Supplementary Data 3

Description: Raw distributions and model-optimal values for three MD descriptors (MolLogP, MolWt, TPSA). Supports main Figure 3.

File name: Supplementary Data 4

Description: Contains the 1024-dimensional fingerprint importance vectors (one per odor label), UMAP-embedded coordinates, and the corresponding 2D MDS projection values. Supports main Figure 4.