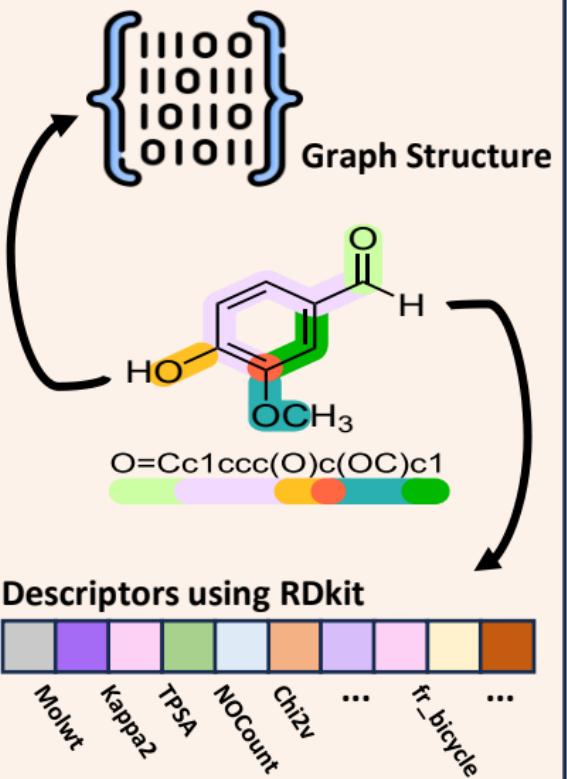
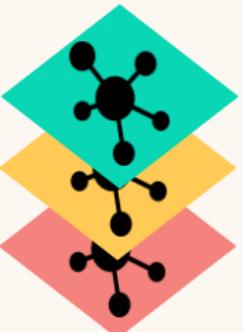


Stage #1. Structural & Descriptor extraction



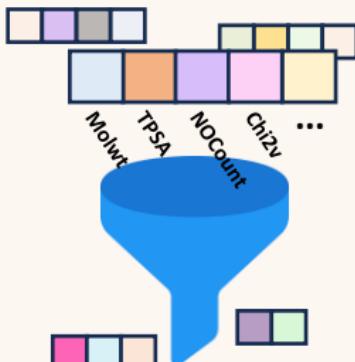
Stage #2. Multimodal Fusion

Graph modality



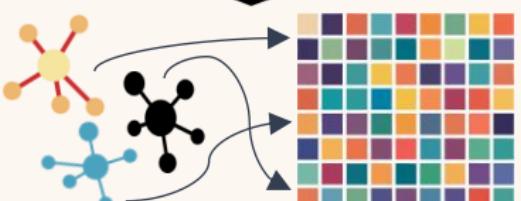
Capturing Atomic–bond
relational patterns

Descriptor modality



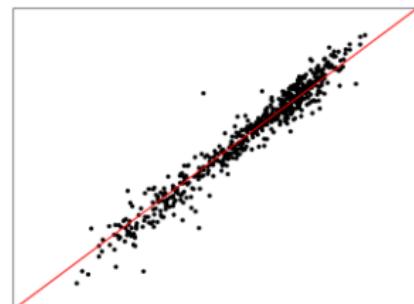
Enforcing parsimonious
variable selection

Kronecker-product

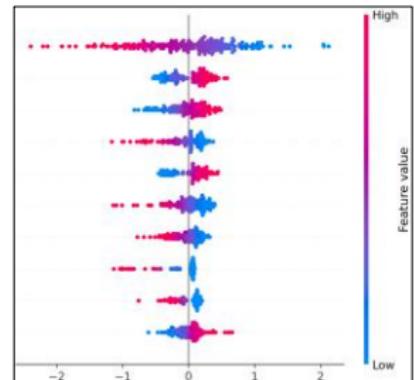


Modeling sparse cross-modal interactions

Stage #3. Predictive & Explanatory outputs



Prediction



Interpretation