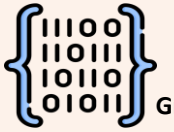
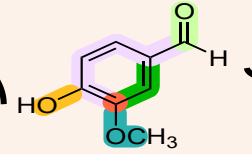
Stage #1. Structural & Descriptor extraction

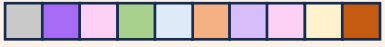


Graph Structure



O=Cc1ccc(O)c(OC)c1

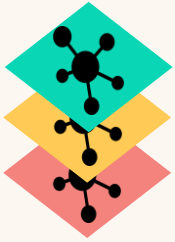
Descriptors using RDkit



Molwt | Kappa2 | TPSA | NOCount | Chi2v | ... | fr_bicycle | ...

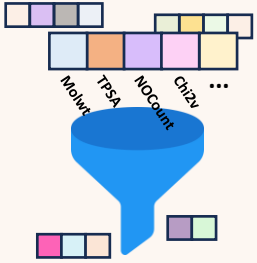
Stage #2. Multimodal Fusion

Graph modality



Capturing Atomic–bond relational patterns

Descriptor modality

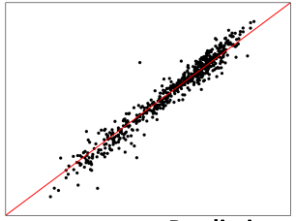


Enforcing parsimonious variable selection

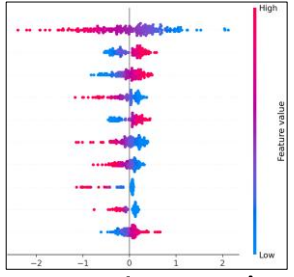
Kronecker-product

Modeling sparse cross-modal interactions

Stage #3. Predictive & Explanatory outputs



Prediction



Interpretation