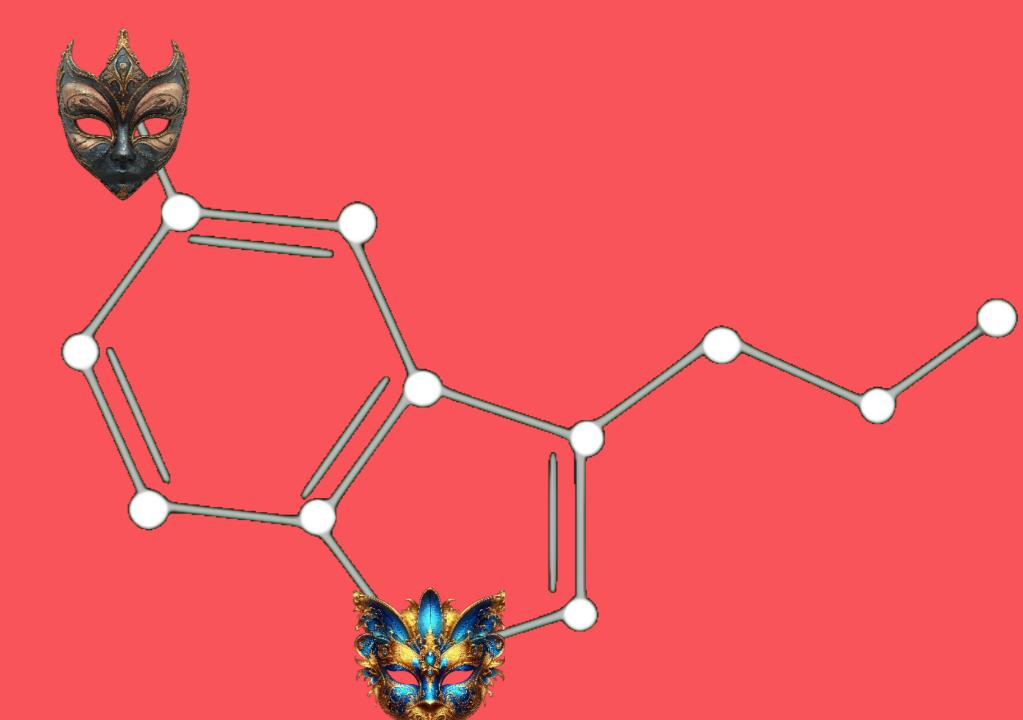


ENHANCING CHEMICAL EXPLAINABILITY THROUGH COUNTERFACTUAL MASKING



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MOTIVATION: Molecular Masking Is Broken

When atoms or bonds are naively masked (by zeroing features or deleting parts of molecule), the resulting molecules often become **chemically implausible or physically impossible**, producing examples that fall outside the training distribution. This **out-of-distribution problem** undermines the reliability of both the explanations and their evaluation metrics.

