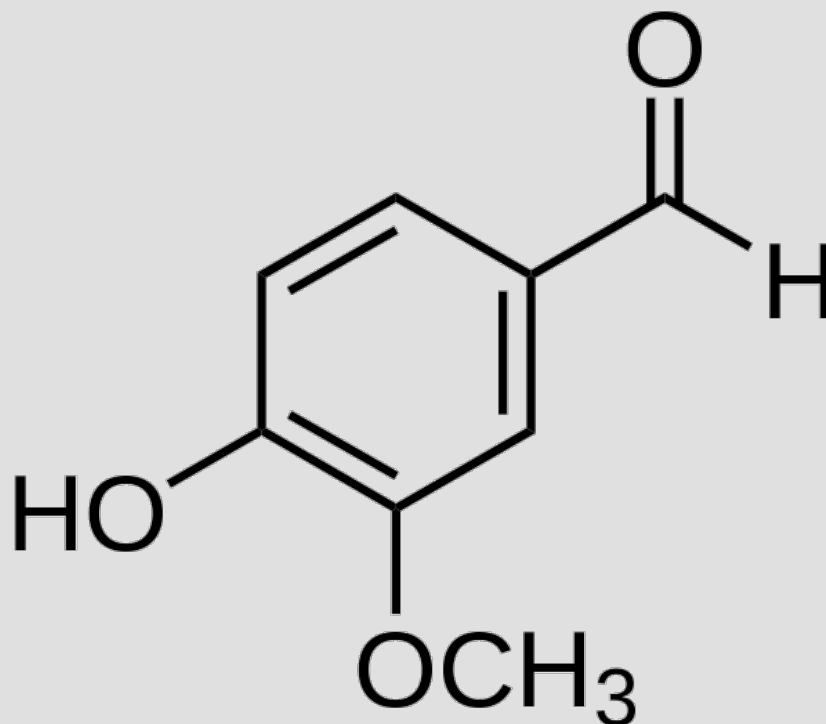


Drug discovery

string representation of a molecule

SMILES: COC1=C(C=CC(=C1)C=O)O



SMILES = Simplified Molecular Input Line Entry Specification

