smiles validity ecfp4 range qed range physchem range ecfp6 range physchem range ecfp4 counts range physchem range ecfp4 range physchem range ap range physchem maxsim ecfp6 range physchem maxsim ecfp4 range physchem maxsim ap range physchem range ecfp4 counts range ecfp4 maxsim ecfp6 maxsim ecfp4 maxsim ap filters validity ecfp4 Synthetic Accessibility Score Distribution