

**EXECUTIVE SUMMARY [NON-CONFIDENTIAL, NON-TECHNICAL ABSTRACT FOR PUBLIC INFORMATION OR PROGRAM PROMOTION]:** The explosive increase in the size of structural (both protein and small molecule) databases and their importance in contemporary biology and drug discovery, underlines the necessity for fast and accurate techniques for determining molecular similarity. Such techniques form the basis for querying information from structural databases. Current approaches to structure-based querying typically use simplistic molecular representation, primarily based on 2D graph-based description of molecules. Such representations fail to adequately capture the biochemical characteristics of molecules that depend on interactions across the molecular surface. These interactions have been known to play a significant role in mediating molecule-molecule as well as molecule-membrane interactions which are often the focus of study in structural biology and drug discovery.

This research seeks to address this issue by developing techniques for supporting surface-based query-retrieval from molecular databases that are both accurate and rapid enough to be used in a wide variety of real-world applications including the aforementioned areas of structural biology and drug discovery. It will help researchers retrieve structural data in manners that have greater bio-chemical relevance than what is possible today. This will lead to a reduction in time and cost of conducting research and development in many critical areas of biological and pharmaceutical sciences.