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## Shape retrieval methods for the classification of protein surfaces

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Macromolecular complexes play a crucial role in almost all biological functions in living cells. Elucidating structural features in proteins is essential to understanding their underlying functions and binding activity. With the rapid accumulation of protein-structure data through AI methods and experimental techniques, such as cryo-electron microscopy, there is a growing demand for efficient approaches to detect protein-structure similarity in real-time database searches. Recently, high-speed computer vision methods have been adapted to perform efficient protein surface comparisons by computing geometric invariant descriptors of 3D features. Here, we present a pipeline that maps 3D surface shape descriptors of proteins using matching and clustering algorithms to identify structure similarity across the Protein Data Bank. We represent the surface shapes of proteins with moment-based 3D Zernike descriptors and spectral signatures. Using matching algorithms based on functional maps and distances can retrieve local similarities between protein surfaces. This pipeline will be integrated into the PDBe and PDBe Knowledge Base infrastructure. Its primary goal is to improve the classification of macromolecular structures and interfaces, which can significantly aid in identifying similarities in protein conformations and facilitate the use of AI methods for predicting macromolecular complexes.

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**Primary author:** DIAZ LEINES, Grisell (EMBL-EBI)

**Co-authors:** Prof. KIHARA, Daisuke (Purdue University); Dr UHLMANN, Virginie (EMBL-EBI); VELANKAR, Sameer (EMBL-EBI)

**Presenter:** DIAZ LEINES, Grisell (EMBL-EBI)

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