

1125-33-3002

Atila Sit* (atilla.sit@eku.edu) and **Daisuke Kihara**. *Three dimensional Krawtchouk descriptors for local comparison of protein surfaces.*

Direct comparison of images or 3D structures is computationally expensive and inefficient due to problems such as scaling and rotation. Also, in many applications, information about specific local structures rather than the entire image is of more interest. Thus, finding invariant descriptors that can retrieve local image patches or subimages becomes necessary. We have recently developed a set of 2D moment invariants based on discrete orthogonal Krawtchouk polynomials for comparison of local image patches. In this work, we extend them to 3D and construct three dimensional Krawtchouk descriptors (3DKD) that are invariant under translation, rotation, and scaling. We present the new formulation of 3DKDs and apply them to local comparison of protein surface patches for detecting ligand binding sites. (Received September 20, 2016)