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Development of a 3D protein motif dictionary management system

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For knowledge discovery based on 3D structural feature analysis of proteins, we have investigated to construct a dictionary of 3D partial structures that are conformed to the motifs in PROSITE, and systematic extensive analysis of 3D protein structures based on the 3D motif dictionary established. For every PROSITE motif, 3D structure files for the corresponding motif segments, a list of enumerated cluster pattern, a representative 3D pattern, and other related information are registered in the dictionary. In the present work, the WWW-based user interface programs are developed for managing and using this motif dictionary. First, the user can input some keywords or ID numbers for not only the PROSITE motifs but also proteins to retrieve the dictionary. Then, a list of corresponding motif information with the representative 3D pattern is displayed, and the user can easily browse a table of other corresponding segments for each motif, and alternative cluster patterns. For displaying 3D structural information of proteins, MDL's Chime plug-in is required, and RasMol scripts are used for instruction of the view models. For each 3D segment stored in this dictionary, a whole protein structure and the corresponding motif sites are also interactively displayed.