

iCEED: Integrated customized extraction of enzyme data

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Abstract

Enzymes catalyze diverse biochemical reactions and are building blocks of cellular and metabolic pathways. Data and metadata of enzymes are distributed across databases and are archived in various formats. The enzyme databases provide utilities for efficient searches and downloading enzyme records in batch mode but do not support organism-specific extraction of subsets of data. Users are required to write scripts for parsing entries for customized data extraction prior to downstream analysis. Integrated Customized Extraction of Enzyme Data (iCEED) has been developed to provide organism-specific customized data extraction utilities for seven commonly used enzyme databases and brings these resources under an integrated portal. iCEED provides dropdown menus and search boxes using typehead utility for submission of queries as well as enzyme class-based browsing utility. A utility to facilitate mapping and visualization of functionally important features on the three-dimensional (3D) structures of enzymes is integrated. The customized data extraction utilities provided in iCEED are expected to be useful for biochemists, biotechnologists, computational biologists, and life science researchers to build curated datasets of their choice through an easy to navigate web-based interface. The integrated feature visualization system is useful for a fine-grained understanding of the enzyme structure-function relationship. Desired subsets of data, extracted and curated using iCEED can be subsequently used for downstream processing, analyses, and knowledge discovery. iCEED can also be used for training and teaching purposes.

Keywords: Enzyme; biodata curation; bioinformatics; data curation; data extraction; data visualization; databases; pathway.

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