Structure-guided phylogenetic reconstruction of the superfamily of proteins sharing the metallo-β-lactamase fold

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April 28, 2020

Abstract

The superfamily of metallo-β-lactamases (MBL) comprises an ancient group of proteins found in all domains of life, sharing a characteristic αββα fold and a histidine-rich motif for binding of transition metal ions, with the ability to catalyze a variety of hydrolysis and redox reactions. Herein, structural homology and sequence similarity network (SSN) analysis are used to assist the phylogenetic reconstruction of the MBL superfamily, introducing tanglegrams to evaluate structure-function relationships. SSN neighborhood connectivity is applied for spotting protein families within SSN clusters, showing that 98 % of the superfamily remains to be explored experimentally. Further SSN research is suggested in order to determine their topological properties, which will be instrumental for the improvement of automated sequence annotation methods.

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