Protein features as determinants of wild-type glycoside hydrolase thermostability - DTU Orbit (30/08/2017)

Protein features as determinants of wild-type glycoside hydrolase thermostability

Thermostable enzymes for conversion of lignocellulosic biomass into biofuels have significant advantages over enzymes with more moderate thermostability due to the challenging application conditions. Experimental discovery of thermostable enzymes is highly cost intensive, and the development of in-silico methods guiding the discovery process would be of high value. To develop such an in-silico method and provide the data foundation of it, we determined the melting temperatures of 602 fungal glycoside hydrolases from the families GH5, 6, 7, 10, 11, 43 and AA9 (formerly GH61). We, then used sequence and homology modeled structure information of these enzymes to develop the ThermoP melting temperature prediction method. Furthermore, in the context of thermostability, we determined the relative importance of 160 molecular features, such as amino acid frequencies and spatial interactions, and exemplified their biological significance. The presented prediction method is made publicly available at http://www.cbs.dtu.dk/services/ThermoP. This article is protected by copyright. All rights reserved.

General information
State: Accepted/In press
Organisations: Novo Nordisk Foundation Center for Biosustainability, Department of Bio and Health Informatics, Immunoinformatics and Machine Learning, Integrative Systems Biology, Metagenomics, Novozymes A/S, Technical University of Denmark
Authors: Geertz-Hansen, H. M. (Intern), Kiemer, L. (Ekstern), Nielsen, M. (Intern), Stanchev, K. (Ekstern), Blom, N. (Ekstern), Brunak, S. (Intern), Petersen, T. N. (Intern)
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Proteins
ISSN (Print): 0887-3585
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.25 SJR 1.293 SNIP 0.747
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.417 SNIP 0.813 CiteScore 2.4
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.487 SNIP 0.893 CiteScore 2.55
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.997 SNIP 0.986 CiteScore 3.21
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.137 SNIP 1.037 CiteScore 3.28
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.945 SNIP 0.983 CiteScore 3.08
ISI indexed (2011): ISI indexed no
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.87 SNIP 0.908
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.959 SNIP 0.985
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 2.225 SNIP 1.017
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.13 SNIP 1.02
Scopus rating (2006): SJR 2.388 SNIP 1.096