

W0192

A Prediction System for Protein Crystallization Conditions. Koji Inaka¹, Shigeru Sugiyama¹, Fujiko Shibata¹, Yoshiko Kobayashi¹, Kaoru Sugimori², Michiyo Takeuchi², Jose Martin Ciloy², Masato Kitajima² ¹MARUWA Food Industries, Inc. Yamatokoriyama, Japan, ²Fujitsu Kyushu System Engineering Ltd. Fukuoka, Japan.

A prediction system for crystallization conditions has been developed. This system will help guide the user to a rational and highly confident crystallization method. This system consists of a database that contains not only detailed information on crystallization conditions extracted from published crystallization and structural analysis reports, but also biological information for each macromolecule that is essential for protein crystallization experiments. Each crystallization condition related to a specific target protein can be easily searched and extracted by providing only the amino acid sequence information and a few keywords. Moreover, crystallization data stored by each user can be linked conveniently to the system. Since comparison and data mining of the search results readily reveal trends in the crystallization parameters, each crystallization parameter can be narrowed down and estimated before any screening experiment is started. This prediction system is an efficient approach to crystallization since it helps reduce unnecessary screenings in the process.