Class: AIzymes_MAIN

Main class for managing AIzymes workflow, including setup, initialization, control, and plotting functions.

Function: init

Initializes an instance of the AIzymes_MAIN class.

Function: setup

Sets up the AIzymes project environment with specified parameters.

Parameters:

FOLDER_HOME (str): Path to the main folder.

FOLDER_PARENT (str): Path to the parent folder.

CST_NAME (str): Constraint name.

WT (str): Wild type information.

LIGAND (str): Ligand data.

DESIGN (str): Design specifications.

MAX_JOBS (int): Maximum number of jobs to run concurrently.

N_PARENT_JOBS (int): Number of parent jobs.

MAX_DESIGNS (int): Maximum number of designs.

KBT_BOLTZMANN (list): Boltzmann constant values.

CST_WEIGHT (float): Constraint weight.

ProteinMPNN_PROB (float): Probability parameter for ProteinMPNN.

ProteinMPNN_BIAS (float): Bias parameter for ProteinMPNN.

LMPNN_PROB (float): Probability parameter for LMPNN.

FOLDER_MATCH (str): Path to match folder.

ProteinMPNN_T (str): Temperature for ProteinMPNN.

LMPNN_T (str): Temperature for LMPNN.

LMPNN_BIAS (float): Bias parameter for LMPNN.

SUBMIT_PREFIX (str): Submission prefix.

SYSTEM (str): System information.

MATCH (str): Match specifications.

ROSETTA_PATH (str): Path to Rosetta source.

EXPLORE (bool): Whether to explore parameter space.

FIELD_TOOLS (str): Path to FieldTools script.

LOG (str): Logging level.

PARENT_DES_MED (str): Parent design method.

Function: initialize

Initializes Alzymes with given parameters.

Parameters:

FOLDER_HOME (str): Path to the main folder.

UNBLOCK_ALL (bool): Flag to unblock all processes.

PRINT_VAR (bool): Flag to print variables.

PLOT_DATA (bool): Flag to plot data.

LOG (str): Logging level.

Function: controller

Controls the Alzymes project based on scoring and normalization parameters.

Parameters:

HIGHSCORE (float): High score threshold for evaluation.

NORM (dict): Normalization values for different scores.

Function: plot

Generates plots based on Alzymes data, including main, tree, and landscape plots.

Parameters:

main_plots (bool): Flag to generate main plots.

tree_plot (bool): Flag to generate tree plot.

landscape_plot (bool): Flag to generate landscape plot.

print_vals (bool): Flag to print values on plots.

NORM (dict): Normalization values for different scores.

HIGHSCORE_NEGBEST (dict): High score and negative best score for different metrics.