Syntax for search in Scopus

((TITLE-ABS-KEY (carrier) OR TITLE-ABS-KEY (support) OR TITLE-ABS-KEY (matrix) OR TITLE-ABS-KEY (matrices) OR TITLE-ABS-KEY (framework))) AND (TITLE-ABS-KEY (enzyme)) AND ((TITLE-ABS-KEY (immobiliz*) OR TITLE-ABS-KEY (immobilis*) OR TITLE-ABS-KEY (stabiliz*) OR TITLE-ABS-KEY (stabilis*) OR TITLE-ABS-KEY (adsorption) OR TITLE-ABS-KEY (adsorb*) OR TITLE-ABS-KEY (encapsulat*) OR TITLE-ABS-KEY (entrap*) OR TITLE-ABS-KEY (cross-link*) OR TITLE-ABS-KEY (covalent* bound*) OR TITLE-ABS-KEY (covalent* bind*) OR TITLE-ABS-KEY (covalent* bond*))) AND ((TITLE-ABS-KEY ("in silico") OR TITLE-ABS-KEY (bioinformatic*) OR TITLE-ABS-KEY (comput*) OR TITLE-ABS-KEY (dock*) OR TITLE-ABS-KEY (simulat*) OR TITLE-ABS-KEY (comput* model*)))

Syntax for search in Web of Science

(TS=(carrier) OR TS=(support) OR TS=(matrix) OR TS=(matrices) OR TS=(framework)) AND (TS=(enzyme)) AND (TS=(immobiliz*) OR TS=(immobilis*) OR TS=(stabiliz*) OR TS=(stabilis*) OR TS=(adsorption) OR TS=(adsorb*) OR TS=(encapsulat*) OR TS=(entrap*) OR TS=(cross-link*) OR TS=(covalent* bound*) OR TS=(covalent* bind*) OR TS=(covalent* bond*)) AND (TS=("in silico") OR TS=(bioinformatic*) OR TS=(comput*) OR TS=(dock*) OR TS=(simulat*) OR TS=(comput* model*))

Supplementary Tables

Table S1. Docking method and its detail in the included studies.

Software	Type of docking	Reference
Autodock 4.2	-	[1]
Autodock vina	Flexible ligand docking	[2, 3]
Dock v.6.522	Rigid body docking	[4]
Autodock 4.2	-	[5]
Hex 8.0	Flexible-ligand docking	[6]
AutoDock 3.05	-	[7]
AutoDock 4.2	Flexible-Ligand docking	[8]
-	-	[9]
AutodockVina	-	[10]
PatchDock server & FireDock server	Rigid body docking	[11, 12]
AutoDock Vina	Enzyme: flexible and rigid Surface modifier: flexible and rigid	[13]
HaddDock online tool & Firedock (for refinement of the results)	-	[14]
Autodock vina	Flexible docking	[15, 16]

Table S2. The employed tools for the analysis of enzyme structure and surface.

Software/Tool and its function	Reference
PyMol: Visualization software	17
PyMol: Visualization software	18
- GetArea tool: Calculation the solvent accessible surface - APBS plugin of visual molecular dynamics (VMD): Visualization of surface charges	19
- PDB2PQR server: Determination of enzyme protonation sate - APBS software: To solve the PBE - PyMol sotware: Visualization of surface charges	20
- FUZZPRO available at EBI SRS server: Searching protein motifs to recognize N-glycosylation sites - GRID program version 22: Calculation of the molecular fields which are produced through interaction between the enzyme and hydrophilic/hydrophobic probes	21
- DSSP program: Computation of solvent accessibility - RASMOL: Visualization - A neural network-based program: Prediction the cysteine tendency for disulfide bond formation	22
- MarvinSketch V6.2.0: Prediction of physicochemical properties - MSMS package: Displaying hydrophilic surface - PropKa and PDB2PQR in UCSF Chimera: Determination of enzyme protonation state - APBS: Computation of surface electrostatic potential of enzyme	11
- SwissPdb Viewer 4.1.0 software: Identification of exposed residues on the enzyme surface - Maestro 10.3 software: Visualization of the hydrophobic and charged residues	23
- PropKa program: Determination of enzyme protonation state - APBS plugin in PyMol: Visualization of surface charges	24
APBS function of PyMol: Visualization of surface charges	25
- GRASP program: Computation of surface electrostatic potential of the enzymes	26
- Maestro: Visualization of the hydrophobic and charged surface	27
- PyMol: Visualization software - Calculation the solvent accessible surface via a web server (available at: http://cib.cf.ocha.ac.jp/bitool/ASA/	28

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