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Integration of Bioinformatics in Bioremediation

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Abstract

Currently bioinformatics assists in the expansion and implementation of bioremediation in a more efficient way by utilizing computational tools to catalogue numerous microbes with biodegrading capabilities. Besides recognition of microbial enzymes involved in biodegradation cycle, knowledge of structural biochemistry of different pollutants and their toxicity helps in *in silico* study of bioremediation pathways.

Keywords: Biocyc; BRENDA; EcoCycsystem; KEGG; Database of biodegradative oxygenases

Introduction

Bioremediation is a useful waste managing technique used at contaminated areas and sites to remove waste [1]. It particularly involves the use of organisms to eat up or neutralize the pollutants [2]. Bioremediation exploits data from different biological databases such as databases of chemical structure, organic compounds, RNA/protein expression, catalytic enzymes, comparative genomics, microbial degradation pathways etc. [3,4] to interpret the underlying degradation mechanism carried out by a specific organism for a specific pollutant [5]. All these sources are interpreted by various bioinformatics tools to study bioremediation for the development of better environmental cleaning technology [6]. Bioremediation implementation has been limited because of scarcity of data on factors controlling the growth and metabolism of microorganisms with bioremediation potential [7]. With the help of bioinformatics, microorganisms with bioremediation capabilities are profiled along with detailed information about their mineralization pathways mechanisms [8]. Using proteomic approaches such as two-dimensional polyacrylamide gel electrophoresis, mass spectrometry and microarrays also plays a crucial role in exploring bioremediation [9]. It significantly enhances the structural characterization of microbial proteins with contaminant degradable capabilities [10].

How Bioinformatics Assists in Bioremediation?

Bioinformatics helps in understanding bioremediation by covering the following aspects of this biological degradation process which is enlisted below:

- Physical/chemical characteristics of degradation pathway: An important aspect of microbial degradation is its kinetics, specificity and reaction physicochemical parameters [11]. Chemical characterization includes the data on physical/chemical properties, fate and transport, properties related to potential for exposure, bioaccumulation and toxicity [12]. A number of databases provide information like name, synonyms, SMILES code, molecular weight, chemical formula, chemical structure image, canonical three-dimensional structure in PDB format, density, evaporation rate, melting point, d-point boiling, solubility in etc.
- Toxicity: Determination of toxicity level which is lethal for the survival of the degrading microbe is very important [13]. Therefore *in silico* approaches are employed for the prediction of toxicity of chemicals [14].
- Microbes: Detailed catalogue of biodegradative microbial strains is available in numerous bioinformatic databases [15].
- Microbial Enzymes: Detailed catalogue of microbial enzymes from different organism involved in bioremediation is available in databases [16].
- Proteomics: Bioinformatics covers the identification and characterization of protein related properties, and the reconstruction of biodegradation metabolic and regulatory pathways.
- Phylogenetic studies: Using phylogenetic analysis, new microbes have been identified from known microbes related to the degradation process [17].
- Molecular interaction: Bioinformatics tools can be used to screen for pollutants for their already characterized degradation sensitivity by specific enzyme [18].

Given below is a list of different bioinformatics tools/databases that assists in the implementation of bioremediation (Table 1).

S.no	Purpose	Bioinformatics Database/Tools
1	Protein-ligand docking tool	AutoDock/AutodockVina [19] DOCK [20] DockoMatic [21] FINDSITE LHM [22] GalaxyDock [23] GlamDock [24] Glide [25] GOLD [26] GriDock [27] Haddock [28] HomDock Rosetta Ligand [29]

		LeadFinder [30] Molegro Virtual Docker [31] PAR-3D [32] ParaDockS [33] PROCAT [34] Pocket-finder [35] rDock [36] VinaMPI [37] YASARA Structure [38]
2	Metabolic pathways databases	BioCarta and WIT [39] Biocyc BRENDA [40] EcoCycsystem [41] ExPASy [42] KEGG [43] MetaCyc [44] MetaRouter [45] PANTHER [46] Roche Biochemical Pathways UM-BBD [47]
3	Physical chemical properties related databases	ChemDplus [48] Chemogenesis [49] PubChem [50]
4	Toxicity prediction	ACD / TOx suite [51] CAESAR [52] Comparative Toxicogenomics Database ECOSAR [53] ECOTOX [54] GENE-TOX [55] Hazard Expert [56] PBT profiler [57] Toxicity Estimation Tool (TEST) [58]
5	Catalog of microbes degrading pathways	Database of Biodegradative Oxygenases [59] KEGG [60]
6	Phylogenetic study of the microbes involved in bioremediation	Phylemon2 [61] Phylip [62] Phylodendron [63] PHYML [64] T-Rex [65]

Table 1: Bioinformatics tools/databases utilized in studying bioremediation.

Conclusion

This review inspects possible bioinformatic approaches in numerous biodegradation pathways, physiochemical analysis of toxins, toxicity level prediction, genomic and proteomic approaches to microbial enzymes, path prediction, and reaction kinetics. Thus for the development of cheaper microbial environmental cleaning technology, Bioinformatics hold potential applications.

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