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Research Article

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In silico investigation of polycyclic aromatic hydrocarbons against bacterial 1-2 dioxygenase

Tripti Sharma

Altius Institute of Universal Studies, Indore (MP), India

ABSTRACT

Polycyclic aromatic hydrocarbons (PAHs) are the major soil contaminants formed as a result of combustion of organic materials, road traffic and industrial activities. PAHs are constituted by fused benzene rings thus contain only carbon and hydrogen atoms which are sometimes substituted by atoms of nitrogen, sulfur, oxygen or alkyl groups to form heterocyclic aromatic compounds. Present study is a step towards bioremediation of two major PAHs, Benzo[a]pyrene and Chrysene whose aim is to find out possible interactions of these pollutants with bacterial 1-2 dioxygenase from Rhodococcus opacus and Acinetobacter radioresistens respectively. Crystal structures of bacterial enzymes (PDB ID-3HGI, 2XSR) are retrieved from RCSB Protein Data Bank and in silico docking studies were performed against Benzo[a]pyrene (CID 2336) and Chrysene (CID 9171) respectively as ligands by using autodock 4.2. Binding score in terms of binding energies is calculated and binding stability in terms of interactions between macromolecule and ligand is determined. Findings of present work suggest that both the Dioxygenases from Rhodococcus opacus and Acinetobacter radioresistens show stable binding with the ligands. Binding efficiency of Rhodococcus opacus dioxygenase with Benzo[a]pyrene is slightly better with lesser binding energy than Chrysene while in case of Acinetobacter radioresistens Chrysene binds with lesser binding energy as compared to Benzo[a]pyrene, suggesting that Rhodococcus opacus can be the better choice for Benzo[a]pyrene and Acinetobacter radioresistens for Chrysene biodegradation. Both of these organisms can be used for field trials for bioremediation of Benzo[a]pyrene and Chrysene.

Key words: Polycyclic aromatic hydrocarbon (PAH), Dioxygenase, Docking

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INTRODUCTION

Polycyclic aromatic hydrocarbons (PAHs) are hydrophobic organic compounds consist of two or more than two fused benzene rings [1]. Many Polycyclic aromatic hydrocarbons have deleterious effects on respiratory, immunological, neurological and reproductive organs of mammals including humans [2, 3, 4]. PAHs also cause inhibited reproduction and increased mortality of aquatic invertebrates and fin erosion, liver abnormalities, cataracts, and immune system impairments in fish [5.6], therefore presence of PAHs in the environment is the major environmental concern .Presence of PAHs in urban and agricultural soil is directly impacted by human activity. Soil can also be contaminated with PAHs when bio wastes are used as fertilizers. Another source of PAH is the coal tar refinery. Microorganisms can be used for bioremediation of wide range of environmentally toxic substances including PAHs. [7]. Polycyclic aromatic hydrocarbon (PAH) degradation by soil mycobacterium isolates has been well demonstrated. PAH-degrading isolates *Mycobacterium vanbaalenii* PYR-1 and *Mycobacterium gilvum* PYR-GCK have been isolated and identified as PAH degraders.[8,9], these isolates degraded pyrene and phenanthrene,

but only few have been reported to degrade benzo[a]pyrene [10]. Dioxygenases are oxidoreductase enzymes produced by many bacteria and eukaryotic organisms, these enzymes utilize dioxygen as a biological oxidant for Xenobiotic degradation. The catechol dioxygenases, some of the most well-studied dioxygenase enzymes, use dioxygen to cleave a carbon-carbon bond of an aromatic catechol ring system.[11]. In the present study interactions between bacterial dioxygenases and PAHs (Benzo[a]pyrene and Chrysene) are seen by performing molecular docking.

EXPERIMENTAL SECTION

The NCBI Entrez protein database (protein data bank) was accessed at internet. Crystal structure of 1,2-Dioxygenase from Rhodococcus opacus and Acinetobacter radioresistens (PDB IDs-3HGI and 2XSR) are retrieved from RCSB Protein Data Bank, which is a repository for the 3-D protein structural data. These structures are obtained by X-ray crystallography or NMR spectroscopy, submitted by scientists around the world. In the present study 1,2-Dioxygenases from Rhodococcus opacus and Acinetobacter radioresistens are docked with Benzo[a]pyrene and Chrysene (CID 2336 and 9171) which are two major polycyclic aromatic hydrocarbon (PAHs) soil contaminants. Structures of these ligands are retrieved from pubchem which is a database for chemical molecules. Openbabel which allows us to search, convert, analyze data from molecular modeling is used to prepare ligands for docking. For preparation of macromolecules, Discovery studio 3.5 from Accelrys which is a well-known suite of softwares for macromolecule simulation systems is used. Docking is performed by using Autodock 4.2, which is simulation software for molecular modeling and Protein-ligand docking, available under General Public License. Autodock is frequently used for calculating and displaying feasible docking modes of pairs of protein and corresponding ligands (protein-ligand docking) and for calculating binding energies of their interactions .It has two main programs:- AutoDock for docking of the ligand to a set of grids describing the target protein and AutoGrid for pre-calculating these grids, maintained by The Scripps Research Institute and Olson Laboratory [12]. In the present study entire surface of the macromolecule is searched for docking and very large grid maps are created. Docked structures are analyzed by using Discovery studio 3.5 and Pymol 1-1 [13,14]

RESULTS

Fig 1 and 2 (a) show interacting residues of 1,2-Dioxygenase from Rhodococcus opacus with Benzo[a]pyrene. Fig 1 and 2 (b) show interacting residues of 1,2-Dioxygenase from Rhodococcus opacus with Chrysene. Fig 3 and 4 (a) show interacting residues of 1,2-Dioxygenase from Acinetobacter radioresistens with Benzo[a]pyrene Fig 3 and 4 (b) show interacting residues of 1,2-Dioxygenase from Acinetobacter radioresitens with Chrysene.

Table 1 shows binding energies of macromolecules with Benzo[a]pyrene for which the values are -7.36 kcal and -6.1 kcal for Rhodococcus opacus and Acinetobacter radioresistens respectively. Table 2 shows binding energies of Macromolecules with Chrysene. Binding energies of 1-2 Dioxygenase from Rhodococcus opacus, with Chrysene is -6.8 Kcal and binding energies of 1-2 dioxygenase from Acinetobacter radioresistens with Chrysene is -7.09 Kcal/ respectively. Results suggest that dioxygenase from Rhodococcus opacus binds more efficiently to Benzo[a]pyrene than Chrysene while reverse is the case with dioxygenase from Acinetobacter radioresistens which binds more efficiently with Chrysene than Benzo[a]pyrene.

Table-1 shows Binding Energies of 1,2-Dioxygenase with Benzo[a]pyrene

Macromolecule	PDB-ID	Binding Energy with Benzo [a] pyrene	Intermolecular Energy with Benzo [a] pyrene
Dioxygenase (Rhodococcus opacus)	3HGI	-7.36kcal/	-7.36kcal
Dioxygenase (Acinetobacter adioresistens)	2XSR	-6.1 Kcal/	-6.1 Kcal

Table-2 shows Binding Energies of 1,2-Dioxygenase with Chrysene

Macromolecule	PDB-ID	Binding Energy with Chrysene	Intermolecular Energy with Chrysene
Dioxygenase (Rhodococcus opacus)	3HGI	-6.8kcal/	-6.8kcal
Dioxygenase (Acinetobacter radioresistens)	2XSR	-7.09 Kcal/	-7.09 Kcal

Fig 1 and 2 (a) - Interacting residues of 1,2-Dioxygenase from Rhodococcus opacus with Benzo[a]pyrene.

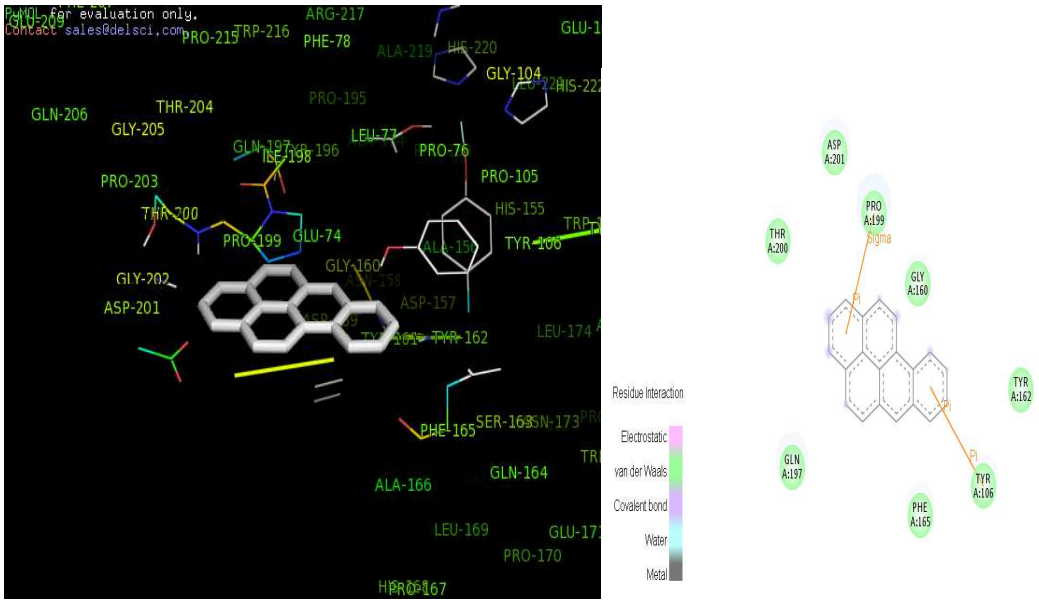


Fig 1 and 2 (b) - Interacting residues of 1,2-Dioxygenase from Rhodococcus opacus with Chrysene

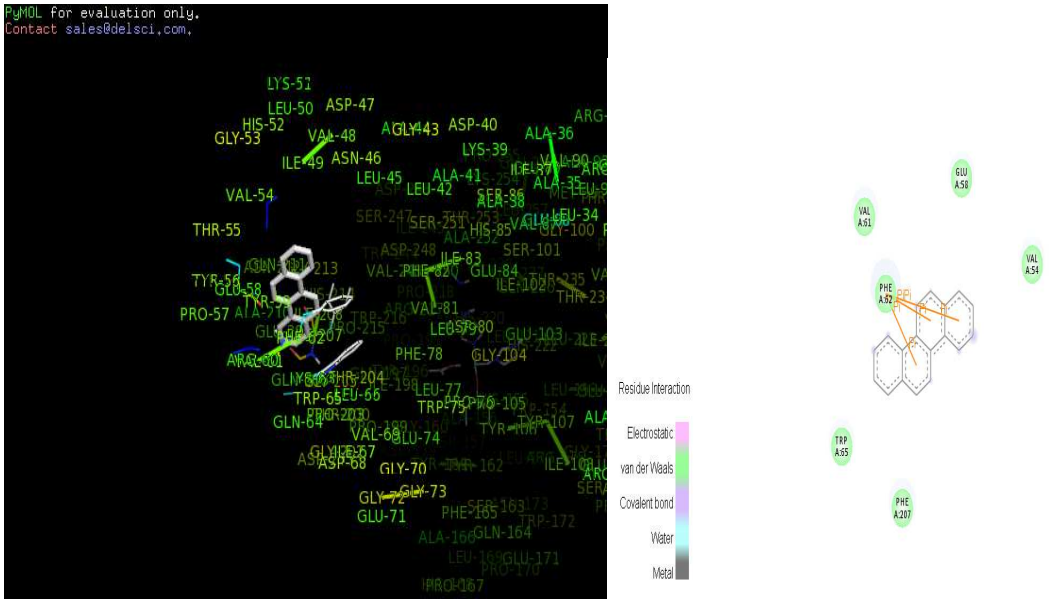


Fig 3 and 4 (a) - Interacting residues of 1,2-Dioxygenase from Acinetobacter radioresistens with Benzo[a]pyrene

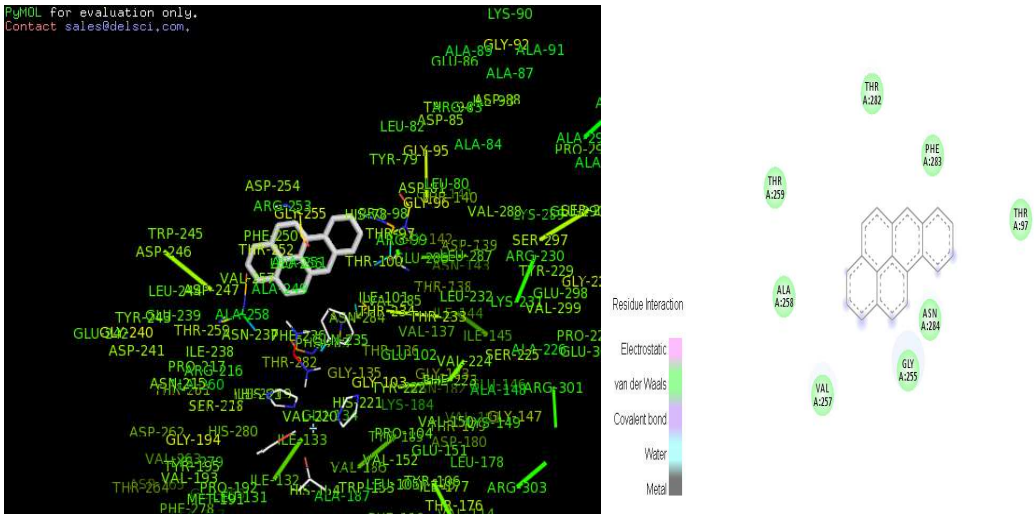
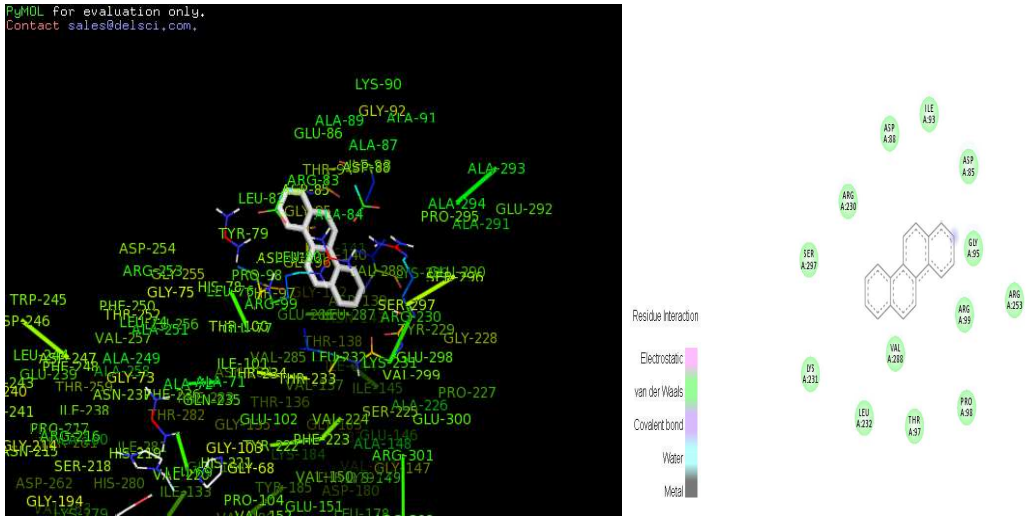


Fig 3 and 4 (b) - Interacting residues of 1,2-Dioxygenase from Acinetobacter radioresitens with Chrysene



DISCUSSION AND CONCLUSION

PAH contamination of soil is a major environmental concern that needs to be resolved. Incineration used to destroy organic contaminants makes soil sterile and depletes its organic matter. Hence, other methods including bioremediation have been developed. Microorganisms have the potential to degrade a wide variety of soil contaminants. Mycobacterium gilvum is well known for its ability to degrade four-benzene-ring aromatic hydrocarbon pyrene, 16 PAHs (Naphthalene, Acenaphthene, Acenaphthylene, Fluorene Phenanthrene, 1-Methylanthracene, Pyrene, Fluoranthene, Benzo[a]anthracene, Chrysene, Benzo[k]fluoranthene, Benzo[b]fluoranthene, Benzo[a]pyrene, Dibenz[a,h]anthracene, Indeno[1,2,3-cd]pyren,e Benzo[ghi]perylene, Benzo[a]pyrene) are designated as primary pollutants by United States Environmental Protection Agency (US-EPA). Present study is designed to investigate possible methods for biological remediation to accomplish PAHs degradation and to observe possible interactions of two major poly aromatic hydrocarbons Benzo[a]pyrene and Chrysene with Fe (lll) containing dioxygenase enzymes specialized in aerobic degradation of catechols from Rhodococcus opacus and Acinetobacter radioresistens. These dioxygenases show effective binding with Benzo[a]pyrene and Chrysene suggesting that these two microorganisms can be used for experimental trials with Benzo[a]pyrene and Chrysene as sole source of carbon or along with other naturally occurring carbon sources.

Microorganisms may cause transformations rather than degradation of polycyclic aromatic hydrocarbons (PAHs) so careful optimization and observation is must before field trials.

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