

## ALLERGIC REACTION OF P-PHENYLENEDIAMINE ON SKIN

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## ABSTRACT

This paper describes in detail the interaction between para phenylenediamine and keratin protein. This interaction triggers inflammatory response for those people who are allergic to para phenylenediamine diamine. The autodock analysis of the interaction shows that the energy involved for the process is  $-2.55$  kcal/mol.

**Keywords:** Para phenylene diamine, allergic, autodock

## INTRODUCTION

Para phenylenediamine diamine (PPD) is a compound which is commonly found in dye. Keratin is a protein which is present in the epidermis along with other skin proteins. P-Phenylenediamine is an organic compound with the formula  $C_6H_4(NH_2)_2$ . PPD is a derivative of aniline. It is a white solid which darkens due to air oxidation. It is mainly used as a component of engineering polymers and composites. Also it is an ingredient used in hair dyes.

PPD is used in several industries for dyeing furs, photochemical processes, tyre vulcanisation industries, oxidisable hair dye, etc. Allergic effect is well established and many studies are devoted to the subject, but PPD systemic poisoning is well not understood [1]. Several PPD poisoning cases had been reported where it is traditionally used mixed with Henna to color palms of hands and soles of feet and to dye hair. Despite the wide spread use of natural henna, specially, in countries where henna art is traditionally practiced, reports of allergic contact dermatitis to natural henna are very rare in the literature. It can therefore be assumed that natural henna is a very weak skin allergen [2]. Severe cases of immediate type hypersensitivity to PPD described in which the patients developed severe edema, irritation of the eyes and face and also difficulty in breathing [6]. Short-term exposure to high levels of PPD (acute effects) may cause severe dermatitis, eye irritation and tearing, asthma, gastritis, renal failure, vertigo, tremors, convulsions, and coma in humans. Eczematous contact dermatitis may result from long-term exposure (chronic effect) in humans. *para*-Phenylenediamine (PPD) is an allergen; even if someone does not have a reaction the first time they are exposed to it, they can become

“sensitized” to PPD over time and can have adverse reaction upon re-exposure.

In addition, PPD provokes cross-allergy, making people allergic to other substances which contain *para*-substituted amino compounds. PPD is demonstrated to be mutagenic [5]. PPD together with hydrogen peroxide may be carcinogenic. *para*-phenylenediamine has been mixed with natural henna to give an ebony color (black henna) instead of the orange/reddish color given by natural henna. The adverse health effects associated with the use of henna containing PPD (black henna) include acute allergic contact dermatitis, eczema, chemical burn, acute renal failure, acute and severe angioneurotic edema, abdominal pain and vomiting

## MATERIALS AND METHODS

## Chemsketch

It is a molecular modeling freeware software used to design molecules for docking [4]. Apart from designing the molecule various chemical as well as physical properties of the molecule can be calculated from chemsketch. PPD structure consists of a benzene ring and two amino groups (Fig.1).

## Protein data bank

The structure of various proteins can be obtained from protein data bank (PDB). It describes in details the method by which structure of the protein was derived as well as other structural details of the protein molecule. The structure of keratin protein was obtained from PDB (Fig.2).

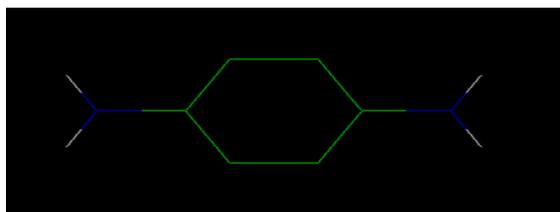


Fig. 1: Structure of P-phenylenediamine in Chemsketch

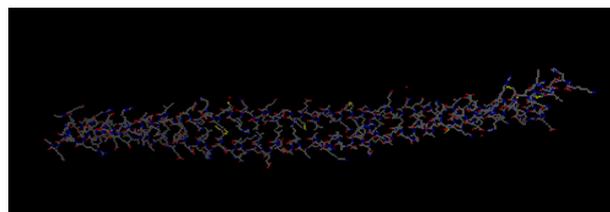


Fig. 2: Structure of Keratin protein from pdb

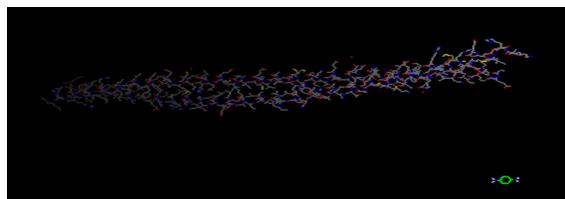


Fig. 3: PDB structure of PPD and keratin in Autodock before docking

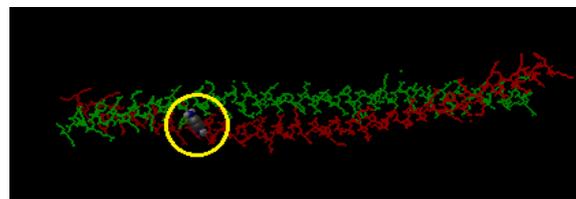


Fig. 4: Docked Structure of Keratin and Parabenzene diamine

**Autodock**

It is software used for docking and simulation of ligand and protein [3].

The compounds can be viewed in different format. A grid box can be specified to faster docking.

Various energies can be calculated from autodock. These energies show whether there is interaction between the protein and ligand and the extent of the interaction.

**RESULT AND DISCUSSIONS****Autodock Results**

The pdb formats of the ppd and keratin protein were loaded in autodock (Fig.3). Molecular Modeling and simulation analysis was carried out to understand the extent of interaction between the protein and the ligand. The position at which ppd was interacting with keratin was seen after the generation of the dlq file from Autodock (Fig.4). The results obtained after docking are shown in Table I.

**Table I: Energy obtained from Autodock**

S. No.	Type	Energy
1	Estimated Free Energy of Binding	-2.55 kcal/mol
2	Estimated Inhibition Constant, Ki	13.54 mM
3	Final Intermolecular Energy	-3.15 kcal/mol
	Vdw + Hbond + desolv Energy	-3.03 kcal/mol
	Electrostatic Energy	-0.11 kcal/mol
4	Final Total Internal Energy	+0.02 kcal/mol
5	Torsional free energy	+0.60 kcal/mol
6	Unbound System's Energy	+ 0.02 kcal/mol

The Table I show the energy obtained from Autodock. Estimated energy of free binding was observed to be -2.55 kcal/mol.

**CONCLUSION**

The free energy of binding was found to be -2.55 kcal/mol. This indicated that there is a stable interaction between ppd and keratin protein. Hence it causes contact dermatitis in patients who are sensitive to the compound ppd which is present in hair dye. Hence people allergic to ppd has to go for other alternatives as using dyes having ppd can be fatal and result in various health hazards.

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