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Theoretical I.R Spectroscopy Confirmation of 2, 4- Dibromo Aniline and its Possible Toxicity Effects in Dye Shampoos

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Abstract

The aim of this pilot study is to retrieve structural information through theoretical methods and highlight infrared (I.R) spectrophotometric confirmation of 2,4dibromoaniline/benzene, which used in hair dye manufacture sector. Density function theory approach with the assistance of computational simulating is used. In the next step its possible toxicity effects on human skin calculated through QSAR (Quantitative structure–activity relationship modelling) method. Four different types of cell lines applied to calculate three different oral toxicity predictions. The aforementioned aniline is belong to class 4 according to Globally Harmonised System. After obtaining theoretical results, we will able to suggest that the mentioned molecule is not suitable for cosmetic and food items manufacturing. The I.R spectrogram of 1, 2, 4 tri substrate results are compiled in a comprehensive way to conform structure. Toxicity results of mentioned organic precursor molecule is not acceptable for humans use.

Keywords: Virtual calculation, 2, 4di bromo benzene amine, dermal toxicity aniline.

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1. Introduction

The use of aniline in dye manufacturing is an open secret that makes aniline the best choice for dyes. Is this safe? A fundamental question arises [1] before development and regulation of any pharmaceutical chemical and their toxicity effect on humans. This type of study provided vital information to dermatologists and others. Hair is the showcase of beauty for any human [2]. In USA 75%, Europe nearly 70% women use some form of hair dyes. This growing trend of coloring hair has increased the sales of hair dye production and every day new technology being introduce in cosmetic industry [3]. Most of the world's population has dark black colored hair [4], every individual select their hair care products based on their specific hair needs [5] .Which mean there is a great demand of dark-colored hair dyes. Higher concentrations of chemicals, which produce dark colour, could pose greater potential risks for health. There are two major types of adverse effects, external, which damage skin and other internal, which puts an effect on vital organs [6].

Chemically induced skin sensitization is a complex immunological disease with a high impact on the quality of life. Humans can exposed to chemical by the usage of a variety of synthetic products made with chemicals, which meet food and plastic [7]. There are many mechanisms and pathways by which toxicity can spread [8]. With the advancement in science, the practice of chemicals on animals and harming the animal is no more required [9] and the sale of product tested on animals is also banned in developing countries. There many alternatives to animal testing methods for the evaluation of chemical potency among which QSAR model is one [10]. Molecular visualization provides the edge to examine the 3D virtual confirmation of any molecule. I.R spectrogram is able to confirm the structure easily and note the vibration modes. Structure plays a role in drug toxicity [11]. The study of Hao jin is limited to chlorinated aniline [12]. Study of Bushra T. Al Quadeib *et al* is limited to ordinary shampoos and highlight there ingredients [13] know a day's dyes shampoo also capture the portion of cosmetic market. Until a date according to authorize knowledge no study found which explain the toxicity effect and structural determination of 2, 4 di bromo aniline.

1.1. Stereochemistry

Aniline molecule contains an amino group with one simple aromatic ring with the attachment of two Bromine atoms. There six carbons atoms present in the aromatic ring. There are five hydrogen atoms. Three double bonds, no triple bond is present, as shown in (Figure 1).smile notation NC1=CC=C(Br)C=C1Br

2. Methodology

Avogadro 1.2 Molecular Editor is used for molecular structure [14], ProTox-III is used for prediction of GHS nature of chemical [15] KnowIt All Informatics Systems is used for the comparison of theoretical results. Virtual calculation of I.R Spectra obtained through GAMESS

[16]. Assessing skin sensitization is through [17]. Calculation in basic set B3LYP and to utilize People basis 6-31G*.

3. Results and discussion

3.1. Results

3.1.1. I.R spectrometer

2, 4-dibromo aniline I.R spectrograms is mention in figure 2. (i)Amine: 3556cm/1 medium anti symmetric stretch of NH while the symmetric stretch of NH is 3443cm/1.C-H medium stretch 1320.NH2 1670 medium peak. (ii) Halogen: C-Br strong peak 687-630cm/1. Structure contains two bromine atoms. (iii)Ring confirmation: 1, 2, 4 tri substrate are attached with ring. 1680 stretching, 1444 medium, CH bending 1000-1200cm/1 as shown in spectrogram.

3.1.2. Dermatological evaluation

Is the mentioned organic precursor molecule safe for humans? A fundamental question arises before development and regulation of any cosmetic chemicals and their toxicity impact on human skin. With the advancement in science, cosmetic products tested in advance through QSAR model [18]. Murine local lymph node assay is a popular nonclinical test for assessing the potential of chemicals sensitization by xenobiotic. Skin responses identified by their ability to provoke proliferative responses in mouse local lymph node. The human Cell Line Activation test is a cell-based assay that identifies skin sensitizers by examining changes in the expression of cell surface markers. The Keratino Sens assay is useful in vitro system for evaluating the skin responses towards oxidative stress or electrophilic compounds. Table 1 shows that above aniline molecule is a skin sensitizer, this theoretical evidence proves that when human skin comes into contact with it, it can lead to sensitization this causes problems like damaging the immune system, interferes with hormones and finally leads to cancer. Patho-mechanisms of the allergic response is complex mechanism although all the findings needs confirmation in humans [19]. Contact hypersensitivity is due to activation of both innate and adaptive immunity in response to haptens. Cosmetic products directly used by human may release into the environment as an indirect consequence of their use like atopic dermatitis (Rastogi *et al.*, 2018).

3.1.3. Oral toxicity

According to LD_{50}: 1120mg/kg assessment, concern molecule belong to toxicity class 4 as define by "The Globally Harmonized System of Classification and Labelling of Chemicals" (GHS) which mean harmful if deglutition. The GUSAR software and DL-AOT prediction acute oral toxicity [20] show same results. Which mean 2, 4 di Bromo aniline is also not suitable for artificial food coloring agent.

3.1.4. Carcinogenic potential

Carcinogenicity is active as per evaluation. Certain kinds of aromatic amines ascertained to be carcinogens, more particularly if exposed to for lengthy periods or high concentration. As for the primary substance, Bromo-aniline, the compound is not investigated in regards to its carcinoma properties in detail, however, precaution should be used because of its chemical relation to other carcinogen [21] the aromatic amines.

3.2. Discussion

The field now days as "computational prediction" is a product of the digital age. Through digital molecular editing, it is possible to see actually issue in comprehensible way [22] but it does not aim to replace experiment. I.R spectrophotometry used to elaborate the structural information, as already mention structure role in any scientific query is the initial key to understand. The dye tolerance and their possible adverse effects maximize the chance of autoimmune disease and cancer. QSAR model only computes that chemical is sensitive or not. However, information about the relative sensitization potency of any chemical is still underway. Similarly, the International office for Research on Cancer disclose that some of the synthetic chemicals in hair dye are presumable cancer causing to those who exposed to them occupationally (e.g., hairdressers and barbers). Media effect on individuals have started to mould their mind to color their hair from prior ages, presenting them to firmly sharpening substances that can possibly expand the danger of hypersensitive responses. Now a day's hair dye shampoos is easily available in market normally during bathing contact of shampoo with body parts become easy and increase the contact of hazed chemical, which cause skin allergy. As such, it becomes paramount when dealing with dye shampoos to look at the concentration of the specific product, in this case bromo-aniline and the rate at which one responds to the shampoo. It is therefore common to find that regulatory agencies put specific restrictions concerning the levels of aromatic amines present in consumer products.

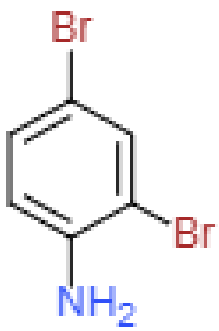

Figure 1. Arrangement of atoms

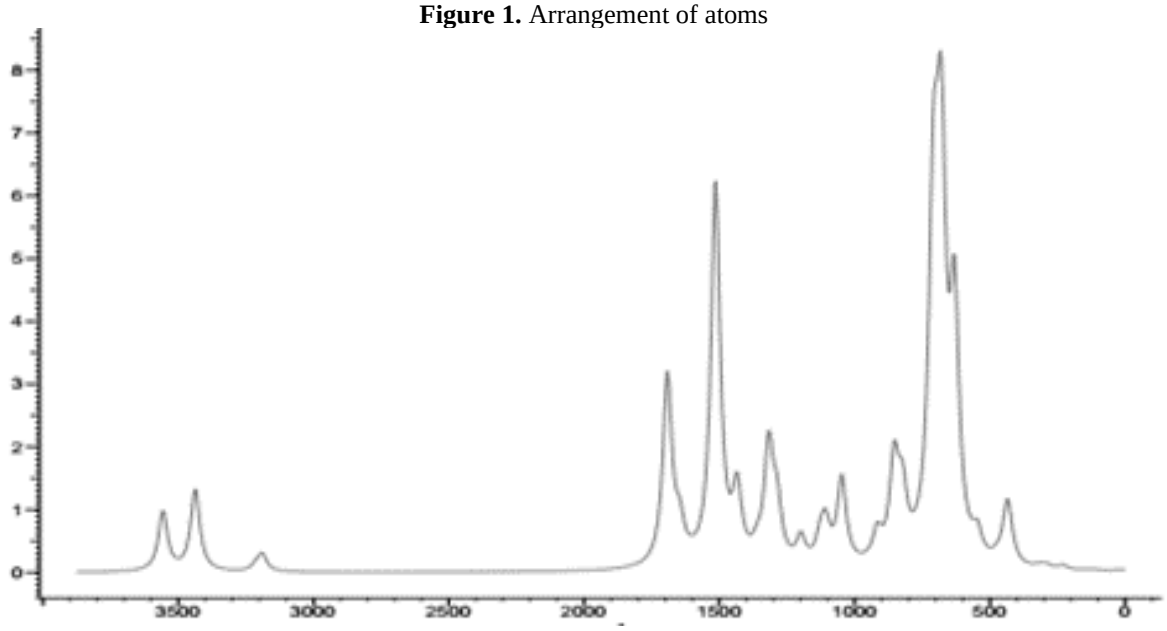

Figure 2. Show a spectrogram of 2, 4-di bromo aniline

Table 1. QSAR models based skin response results

Test name	2,4 di,Br aniline Probability	Remark
1.Human skin	80%	sensitization
2. Murine local lymph node assay	60%	sensitization
3.Human cell line activation test	90%	sensitization
4.Keratino Sens	90%	sensitization

Each perdition is perform in triplet

4. Conclusion

Current glimpse study is limited to 2,4diBromo aniline, but the syngeneic effect of hair dyes, dye shampoos with other chemicals like Hydrogen per oxide put effects that are more lethal. Due to a lack interest show by concern authorities, different hazardous chemicals used in hair dyes products that cause health complication. Approved chemical for hair dyes development and provided guideline of cosmeceutical compounds minimize the risk of dermal and oral toxicity. To prevent any unwanted risks of bromoaniline in the shampoos containing dyes, many factors come into consideration, which are as follows: Manufacturers have to follow the legal requirements of the governments, perform various safety analyses, and give a label about how the product should use and the dangers associated with it. Consumers should also ensure that these instructions followed to the latter to avoid coming into contact with the virus and seek medical attention if any unpleasant symptoms are experienced.

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