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Conception of trapping cidal spray constituents using blend masks in agricultural practices within western region of India

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Abstract
For farmers, pesticides and insecticides are both allies and enemies. The long-term risks they generate can have significant adverse effects on farmers. In order to avoid pests and insects, the application of these chemicals in the field is also important. In the recent years, serious attention has been paid to the harmful effects of pesticides on the environment and human health by the public authorities. It is necessary for farmers to wear protective equipment in this condition to avoid the inhalation as well as absorption of these chemicals (by skin). These chemicals cause have side effects ranging from nausea, headache, temporary blindness to adverse health conditions like permanent blindness, respiratory disorder, nervous system problem, and cancer. A survey was conducted in the western region of India where 30 chemicals were auditioned among which malathione, pyrethroids and cyhalothrin got selected for further progress. Upon docking these chemicals with neutrophil elastase, cholestrerly ester transfer, G alpha, β-arrestin proteins. We found that these chemicals showed affinity with a high binding interaction towards the aromatic amino acids residues that can form H- bonds with a higher binding interaction. Therefore, from our in-silico findings we hypothesize that peptide matrix will be a good candidate for preparing blended masks to entrap the hazardous chemicals from the sprays.

Keywords: Toxic cidal spray, molecular docking, blended masks

Introduction
The foundation of Indian economy is agriculture. 70% of individuals are directly or indirectly active in agriculture sector. With the increase in production of crops, attack of pests and an increase in plant disease is eminent. Regular use of pesticides to control plant diseases and pest attacks impose health hazards. The use of toxic pesticides to manage pest problems has become a common practice around the world. Pesticides are designed to kill and because their mode of action is not specific to one species, they often kill or harm organisms other than pests, including humans (Mori *et al*., 2010) [5]. Use of large amounts of pesticides has raised human health and ecological concerns (Deshpande *et al*., 2011) [3]. Over the past three decades, the indiscriminate use and improper handling of pesticides in agriculture have caused serious human health problems in many developing countries. Unfortunately, due to lack of adequate facility to equip them with a protective gear such as mask, eye covers, body covers and head gears the farmers had symptoms showing up due to toxicity induced by the chemicals. In this research we focus on designing a mask containing binding agent for the specified chemicals (Ajayabhai C *et al*., 2018) [1].

Study site and questionnaire
The study was conducted in the western region of India like Maharashtra, Goa, Gujrat, Rajasthan (Fig 1). In Maharashtra, the baseline survey was conducted in 45 districts all around the region.

The survey questionnaire was prepared to target the awareness status of the farmer on pesticide, to find the culprit spray that causes the hazardous effect on people health and the environment. The questionnaire was divided into three parts (Table 1). The first part contains the basic information of the respondent (Name, Age, Address, Nature of respondent, crop under cultivation). The second part deals with the farmer's knowledge and awareness (knowledge on pesticide specificity, safety measures. In routine practice, awareness status, information from cide-seller) and the third part is about the effect of pesticide observed by farmers such as toxicity symptoms, pre-incidence health issue, causalities, number of deaths, permanent disable, general sufferers and the possible reason of mishaps.

Fig 1: The study site of the survey: Maharashtra, Goa, Gujrat, Rajasthan

Table 1: Survey questionnaire

Name	Basic information about the respondent
Age	
Nature of the respondent	
Address	
Nature of the respondent	
Crop under cultivation	
Type of chemical spray used	Farmer's knowledge and awareness
Pesticide specificity	
Safety measures in routine practice	
Awareness status	

Sampling procedure

The survey was conducted through telephone communication by translating the questionnaire into the local language for better results. The translated questionnaire was also sent through WhatsApp. The filled form was sent by farmers in the same mode. About 116 questionnaires were surveyed.

Data analysis

The data from the questionnaire have been entered into Microsoft Excel

The plots were performed using Excel to depict the number of the respondent in each selected category (Fig 1) (Farmers, Press Reporter, Agriculture Businessman, B.Sc., Agriculture students, Agriculture Officer) and the frequency of crop cultivated in the study area (Fig 2).

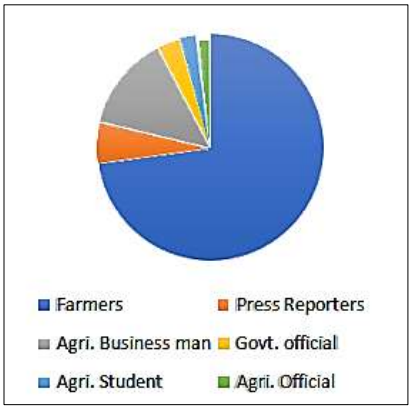


Fig 2: Respondents of survey

Materials and Methods

Among the chemicals (cides) from baseline survey four culprit (harmful) chemicals that are causing adverse effects on farmers were selected for molecular docking studies with specific target proteins.

Selection of specific target proteins

The canonical smiles of chemicals were obtained from PubChem database (Kim *et al*., 2019) [3], canonical smiles of chemicals were submitted in Swiss target prediction web server and the list of target proteins were retrieved. The proteins having low resolution value were selected for each chemical from RCSB PDB (Chen *et al*., 2007) [2].

Docking studies

Molecular docking studies were done using Autodock 4.2 (Morris *et al*., 2009) [6]. The chemicals were docked against target proteins to find the appropriate orientation and conformations in the binding pockets. The Autodock software predicts the binding free energies of chemicals to target proteins. The autodock results were evaluated based on two parameters i.e., binding energy and dissociation constant. The conformation having high binding energy (more negative charge) is chosen as final model and interactions between protein and chemical were observed.

Results

- The various crops cultivated are Rice, Jowar, Bajra, Wheat, Mango, Cashew, Coconut, Banana, Pineapple, Jackfruit, Maize and Pulses. Amongst these, 65% contributes to *Rabi* crops, 30% to pulses, 5% to the rest of the crops cultivated.
- About 50% of farmers used safety measures like wearing a mask, gloves, goggles, helmet, and full sleeve clothes. But no farmers have used specific PPE suitable for specific crops. It is being analysed that 28 out of 50 farmers who were aware of pesticide, 6 out of 25 farmers who are unaware, 20 out of 50 farmers who have incomplete knowledge undertaken the safety measures.
- The primary source of toxicity information was provided by cide-sellers to 60% of farmers.
- 90% of the farmer had 'No' pre-incidence health issue, 5% are 'Not Sure' and 3% of the farmer has 'Preincidence health issue'.
- The various causalities observed after the exposure of pesticides are health disorder (50%), Temporary disability (12%), Permanent disability (2%), death (3%), and no disability was observed in 27% of farmers.
- The toxicity symptoms observed after the exposure to pesticides are headache, dizziness, confusion, nausea, vomiting, convulsion, irritation in eyes and skin, diarrhoea, and difficulty in breathing.

Table 2: The culprit spray used for various crops like rice, jowar, bajra, wheat

Commercial name	Technical name	Crop to which the cides are used
Delegate Bioclaim	Delegate -Spinetoram Bioclaim -Emamectin Benzoate	Jowar
Monocrown Prahar Malathion, Tafgor	Monocrown-Monocrotophos, Prahar- Profenofos, Malathion- Acephate Tafgor- Dimethoate 30 EC	Wheat
Tafgor	Tafgor-Dimethoate 30% EC	Pulses
Colt Hi-Yield	Pyrethroids Benzoepin Thiodan	Black Gram
Chess Applaud Nagata Targa super Rifit plus Monocrown Brodan Ferio herbicide Furadan, Blastin Bayer Mancozeb Taspa Indofil avtar Indofil M-45 Chempa Roundup 32 EC Fipscort Malathion Tata Panida Token Eradex Cartap Coragen Lamda	Chess- Pymetrozine Applaud-Buprofezin Nagata-Flubendiamide Targa super-Quizalofop ethyl 5% Monocrown Monocrotophos Brodan - Brodan chlorpyrifos Ferio herbicide - Glufosinate ammonium. Furadan- Carbofuran Blastin -Tricyclazole Bayer-Carbendazim Mancozeb- Indofil M-45 Chempa- pyrazosulfuron 32 EC-Glyphosate Acephate Tata Panida-Pendimethalin Token- Dinotefuran Cartap- Cartap hydrochloride Coragen- Chlorantraniliprole Lamda-Cyhalothrin	Rice
Paraxzone Gramo Sumax Kataar	Paraquat methosulfate Paraquat I Paraquat dimetilsulfate Paraquat-dimethylsulfate	Bajra

- It was reported that 102 people have died, 1200 were disabled permanently. And, about 2500 are general sufferers.
- The possible reason for the mishaps listed by the farmer was: using the pesticide above the normal dosage, lack of proper knowledge, long-term exposure to pesticides by sprayers to increase their earnings, absence of concrete preventive measures, and negligence.
- Among the chemicals from baseline survey, three chemicals which are culprit were chosen based on their effect on the farmers. Namely malathione, pyrethroids and cyhalothrin. These chemicals were used for molecular docking studies through which they were docked with specific proteins.
- The molecular docking studies were performed using AtoDock 4.2.
- Results obtained provided information on the binding orientation of ligand-receptor interaction. Autodock results were assessed based on binding energy and dissociation constant. The results were shown below.

Table 3: Protein: crystal structure of malathione docking with human neutrophile elastase protein

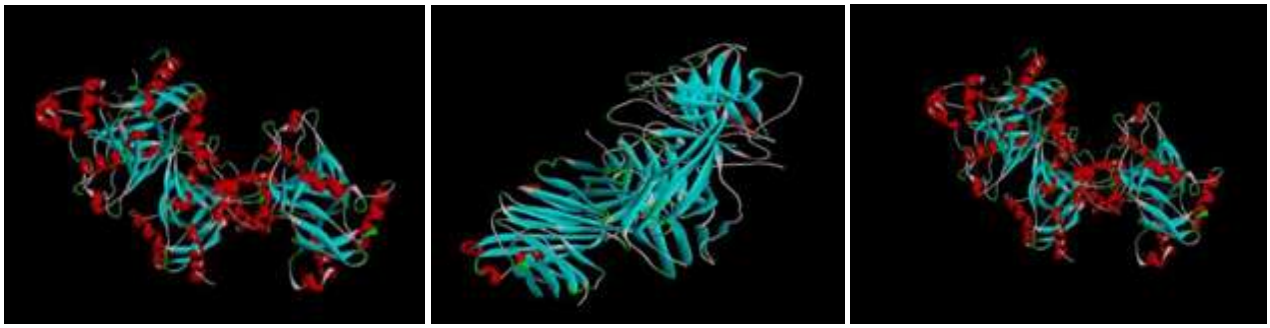
S. No.	Compound name	Interacting amino acids	Binding energy ΔG (Kcal/Mol)	Dissociation constant (kI) (μM)
1	Malathione	SER195	-33.8	7.74

Table 4: Protein: crystal structure of pyrethroids with beta-arrestin 1 protein

S. No.	Compound name	Interacting amino acids	Binding energy ΔG (Kcal/Mol)	Dissociation constant (kI) (μM)
2	Pyrethroids	ARG67, SER31, GLN39	-9.1	3.91

Table 5: Protein: crystal structure of cyhalothrin with cholesteryl ester transfer protein

S. No.	Compound name	Interacting amino acids	Binding energy ΔG (Kcal/Mol)	Dissociation constant (kI) (μM)
3	Cyhalothrin	SER342, ILE367	0	0



1 **2** **3**

Fig 3: Molecular docking chemicals-target proteins

Conclusion

- The toxicity information provided by the cide- seller is negatively correlated with farmers undertaking safety measures.
- There is no association was found between pre- incidence health issues and causalities.
- In the present study, the selected chemicals were docked with specific target proteins. The molecular docking studies shown interactions between the chemicals and proteins. So, the chemicals were having affinity towards the proteins.

- From the above docking studies, it is observed that the chemicals are having affinity towards the specific target proteins, so the hypothesis is that these proteins when used in preparing masks as a matrix can trap the cidal spray constituents (chemicals) i.e., the chemicals bind to the target proteins therefore inhalation of harmful chemicals by farmers can be controlled.

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