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Trapping cidal spray constituents using blend masks in agricultural practices

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Abstract
India ranks twelfth in the world for the use of pesticides. Exposure to pesticides causes tremendous health effects in people as well as in the environment. But the effect can be controlled when it is handled properly. The baseline survey was conducted to know the awareness status of the farmer, the hazardous effect faced, and the culprit spray responsible for mishaps. The various districts of Tamil Nadu, Telangana, Andhra Pradesh, Karnataka and the Union territory, Puducherry were under the survey area.
The chi-square value (32.9938) suggests that there is a strong bearing between the awareness status of the farmer and the farmers undertaking safety measures. The toxicity information provided by the cide-seller is negatively correlated with farmers undertaking safety measures (r= -0.0382). There is no association was found between pre-incidence health issues and causalities (chi-square value= 151.9).
The five culprit sprays such as Methoxychlor, Profenofos, Glyphosate, Diafenthiuron and Imidacloprid were selected for further study. These chemicals were docked against the target proteins. The target protein can be blended on the mask to trap the culprit spray. This would prevent the entry of pesticides into the respiratory tract of farmers and thereby prevent the mishaps.

Keywords: cidal spray constituents, blend masks, agricultural practices

Introduction
India is a country with a population of 139 crores in 2020. As the population grows linearly, the production and use of pesticides also increase to meet the demand for food. The synthetic pesticide was first introduced during World War 2 to destruct food resources. But, later it was used in agriculture for the process of cultivation. (Abubakar *et al*., 2019) [1]. Exposure to pesticides causes tremendous health effects in people as well as in the environment. India ranks twelfth in the world for the use of pesticides. The toxic effect of pesticides can be controlled by various factors such as handling of pesticides with proper application strategy (Glunt *et al*., 2018) [2] and awareness status of the farmer. (Maitah *et al*., 2015) [4]. Therefore, the survey conducted was focused on finding the awareness status of the farmer, the hazardous effect faced by farmers, the culprit spray responsible for mishaps find the protein that could be coated on the mask so that the culprit spray could be trapped and prevent entry into the respiratory tract of the farmer who is spraying the pesticide.

Study site
The survey was conducted in the southern region of India like Telangana, Andhra Pradesh, Karnataka, Tamil Nadu, and Union territories like Pondicherry (Fig 1). In Karnataka, the baseline survey was conducted in various districts like Ballari, Dharwad, Shivamogga, Mandya, Bidar, Bijapur, Banglore, and Gulbarga. 21 districts of Telangana were under the survey. Districts like Chittor, Kurnool, East Godavari, West Godavari, Vijayawada were under the survey in Andhra Pradesh. Districts of Tamil Nadu under survey are Erode, Tiruppur, Salem, Thoothukudi, Thanjavur, Madurai, Sivagangi, and Dindugal.

Survey questionnaire
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 death, permanent disable, general sufferers and the possible reason of mishaps.

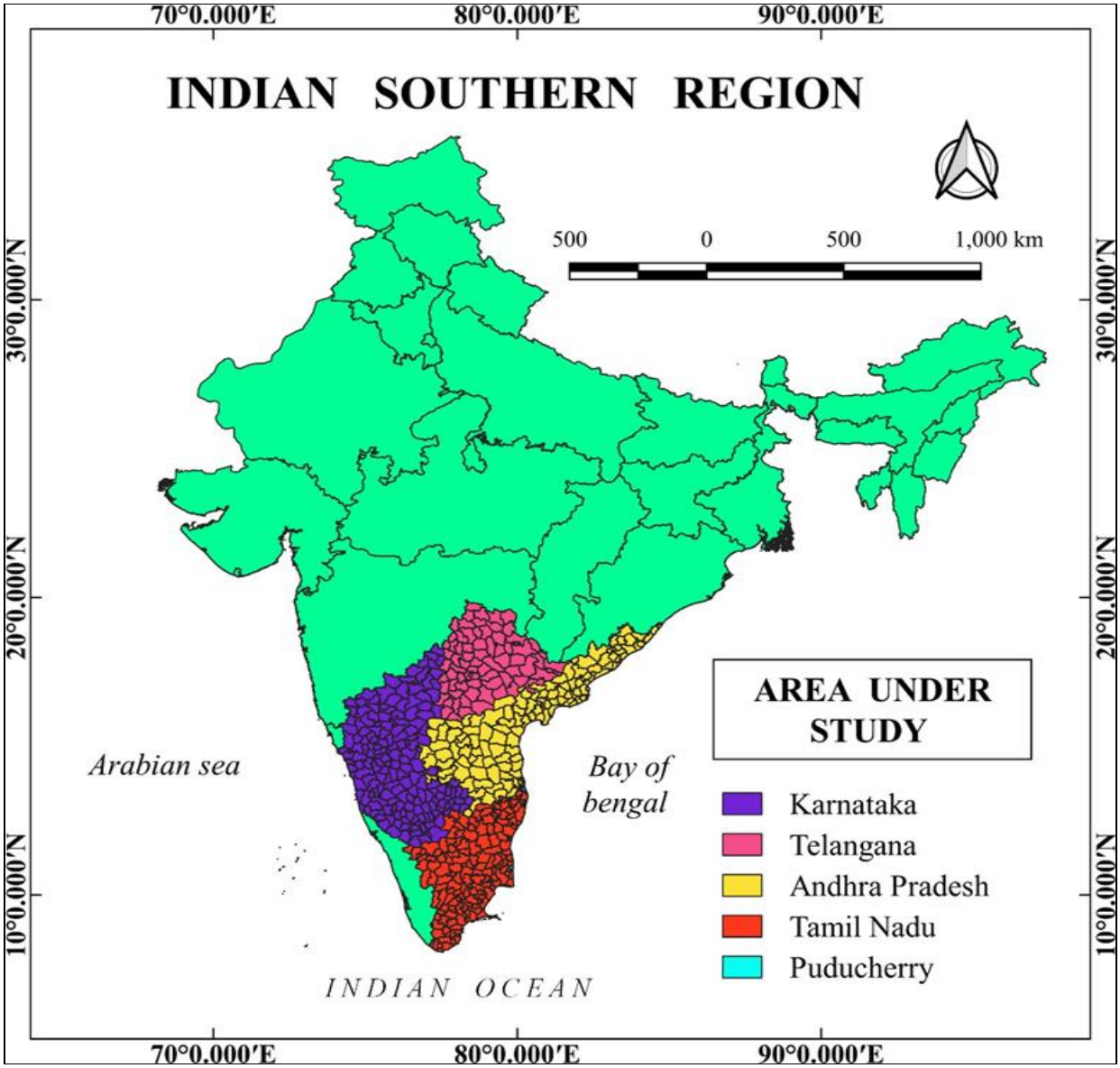


Fig 1: The study site of the survey: Karnataka, Andhra Pradesh, Telangana, Tamil Nadu, and Puducherry

Table 1: Survey questionnaire

Name	
Age	Basic information about 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	
Information from cide-seller	
Toxicity symptoms	Effect of pesticide observed by farmers
Pre-incidence health issue	
Causalities	
Number of deaths	
Permanent disable	
General sufferers	
The possible reason for mishaps.	

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 chi-square test was performed to conclude whether there is an association between the awareness status of the farmer and usage of Personal Protective Equipment (PPE) at (P<0.05). The chi-square was

also performed to check the independence of the variables such as pre-incidence health issues and causalities observed at $P<0.05$.

The correlation test was performed to check the correlation between safety measures undertaken by farmers and the information provided by the cide-seller.

The plots were performed using Excel to depict the number of the respondent in each selected category (Fig1) (Farmers, Press Reporter, Agriculture Businessman, B.Sc., Agriculture students, Agriculture Officer) and the frequency of crop cultivated in the study area (Fig 2)

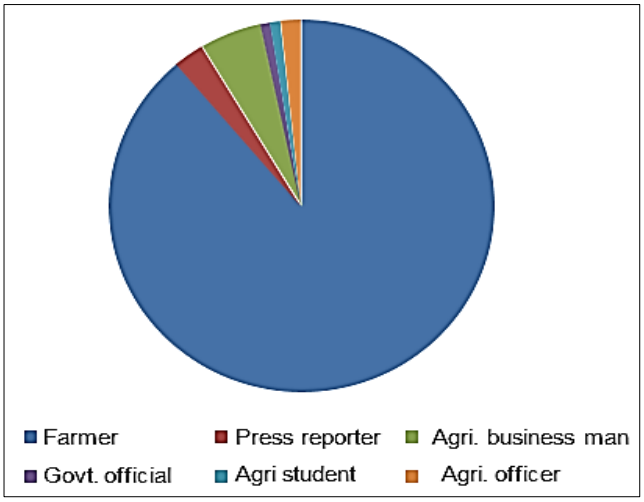


Fig 2: Respondents of the survey

Materials and Methods

Among the chemicals (cides) from baseline survey five 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.

Docking studies

Molecular docking studies were done using Autodock 4.2 (Morris *et al*., 2009) [5]. 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 paddy, maize, cotton, vegetables, sugarcane, chili, turmeric, jowar, groundnuts, sesame, black gram, potato, and mustard. Among these, 45% contributes to paddy, 34% to cotton, 14% to maize, and 7% to the rest of the crops cultivated.
- About 68% 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 analyzed that 50 out of 55 farmers who were aware of pesticide, 6 out of 25 farmers who are unaware, 24 out of 36 farmers who have incomplete knowledge undertaken the safety measures.
- The chi-square value on the awareness status of the farmer and the farmers undertaking safety measures is 32.9938.
- The primary source of toxicity information was provided by cide-sellers to 78% of farmers.
- The correlation value was found between the toxicity information provided by the cide- seller and the farmers undertaking safety measures is -0.0382.
- 94% of the farmer had ‘No’ pre-incidence health issue, 3% are ‘Not Sure’ and 1.7% of the farmer has ‘Pre-incidence health issue’.
- The various causalities observed after the exposure of pesticides are health disorder (54%), Temporary disability (12.9%), Permanent disability (1.7%), death (3.4%), and no disability was observed in 27% of farmers.
- The chi-square value of independence between pre-incidence health issues and causalities is 151.9.
- The toxicity symptoms observed after the exposure to pesticides are headache, dizziness, confusion, nausea, vomiting, convulsion, irritation in eyes and skin, diarrhea, and difficulty in breathing.

The culprit spray used for various crops is listed in Table 2 and 3.

Table 2: The culprit spray used for various crops like paddy, cotton, Maize

Commercial name	Technical name	Crop to which the cides are used
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% Rifit plus-Pretilachlor 37 Monocrown-Monocrotophos Brodan - Brodan chlorpyrifos Ferio herbicide - Glufosinate ammonium. Furadan- Carbofuran Blastin –Tricyclazole Bayer-Carbendazim Mancozeb-Dithiocarbamate Taspa- Propicanozole+Difenaconazole Indofil avtar- zineb+hexaconazol Indofil M-45 Chempa- pyrazosulfuron Roundup 32 EC-Glyphosate Fipscort- Fipronil Malathion-Acephate Tata Panida-Pendimethalin Token- Dinotefuran Cartap- Cartap hydrochloride Coragen-Chlorantraniliprole Lamda-Cyhalothrin Eradex- Chloropyrifos	Paddy
Confidor Malathion Cyperfil Polo Parachute Glyphosate Indofil Wapkil 20 SP Endosul Monocrown	Confidor -Imidacloprid, Malathion -Acephate Cybergirl-Cypermethrin Polo-Diaenthifuron Parachute-Paraquat dichloride Indofil -Novaluron Wapkil 20 SP- Acetamiprid Endosul-Endoslfan 35 EC Monocrown-Monocrotophos	cotton

Table 3: The culprit spray used for various crops like vegetables maize jowar chilli

Commercial name	Technical name	Crop to which the cides are used
Monocrown Tata Panida Vapona Dermin lotion	Monocrown- Monocrotophos, Tata Panida-Pendimethalin Vapona- Dichlorvos Dermin lotion- Benzoate	Vegetables
Delegate Laudis Sevin	Delegate –Spinetoram Laudis – Tembotrione Sevin-Carbaryl	Maize
Delegate Bioclaim	Delegate –Spinetoram Bioclaim -Emamectin Benzoate	Jowar
Monocrown Prahar Malathion, Tafgor	Monocrown-Monocrotophos, Prahar -Profenofos, Malathion- Acephate Tafgor-Dimethoate 30 EC	Groundnuts
Atratop 50% WP Furadan	Atratop 50% WP- Atrazine Furadan- Carbofuran	Sorghum
Krush KC	Krush KC -Quinalphos 25 EC	Sesame
Tafgor	Tafgor -Dimethoate 30% EC	Black gram
Evident	Evident -Thiamethoxam 25%	potato
Tremor 75 SP Benevia Delegate.	Tremor 75 SP- Acephate Benevia- Cyantraniliprole Delegate- Spinetoram	Chilli
Metrigold	Metrigold -Metribuzin	Sugarcane
Basudin	Basudin -Diazinon	Turmeric

- It was reported that 62 people have died, 989 were disabled permanently. And, about 1783 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, five chemicals which are culprit were chosen based on their effect on the farmers. The five chemicals are Methoxychlor, Diafenthiuron, profenofos, glyphosate, acephate. These chemicals were used for molecular docking studies through which they were docked with specific proteins. The molecular docking studies were performed using AtoDock4.2.
- 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 4: Protein: Crystal structure of rap. GMPPNP in complex with the RAS-binding-domain of C-RAF1 KINASE (RAFRBD)

S. No.	Compound name	Interacting amino acids	Binding energy ΔG (Kcal/Mol)	Dissociation constant (kI) (µM)
1	Methoxychlor	ASN64, ARG67, ARG67	-6.42	19.58

Table 5: Protein: Progesterone receptor with bound asoprisnil and a peptide from the co-repressor NCoR

S. No.	Compound name	Interacting amino acids	Binding energy ΔG (Kcal/Mol)	Dissociation constant (kI) (µM)
2	Profenofos	ARG766	-6.67	12.94

Table 6: Protein: Crystal structure of the GluA2o LBD in complex with glutamate and compound-2

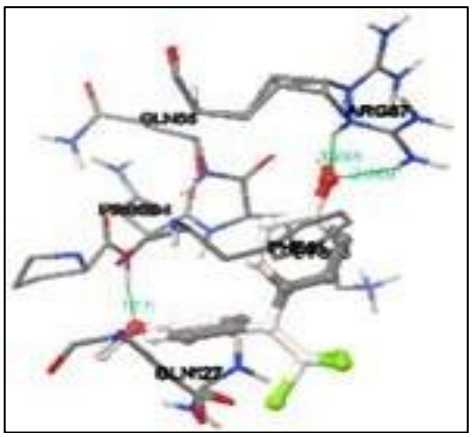
S. No.	Compound name	Interacting amino acids	Binding energy ΔG (Kcal/Mol)	Dissociation constant (kI) (µM)
3	Glyphosate	THR501,ARG506, SER675	-5.58	48.92

Table 7: Protein: Crystal structure of PYK2 complexed with BIRB796

S. No.	Compound name	Interacting amino acids	Binding energy ΔG (Kcal/Mol)	Dissociation constant (kI) (µM)
4	Diafenthiuron	ASP567	-7.54	2.99

Table 8: Protein: Crystal structure of human D-amino acid oxidase

S. No.	Compound name	Interacting amino acids	Binding energy ΔG (Kcal/Mol)	Dissociation constant (kI) (µM)
5	Imidacloprid	GLY50, LEU51	-5.29	132.1



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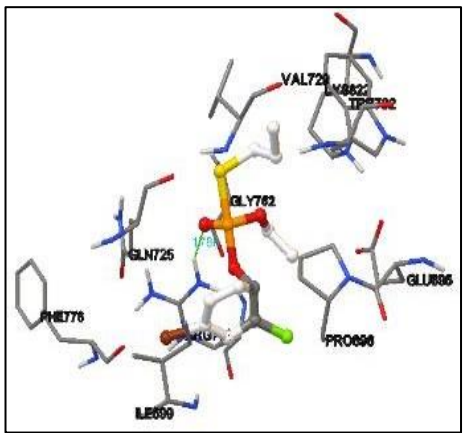

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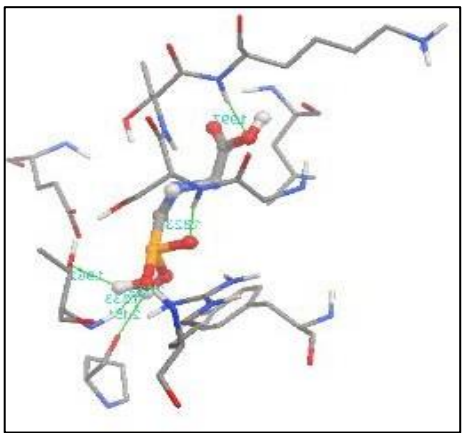

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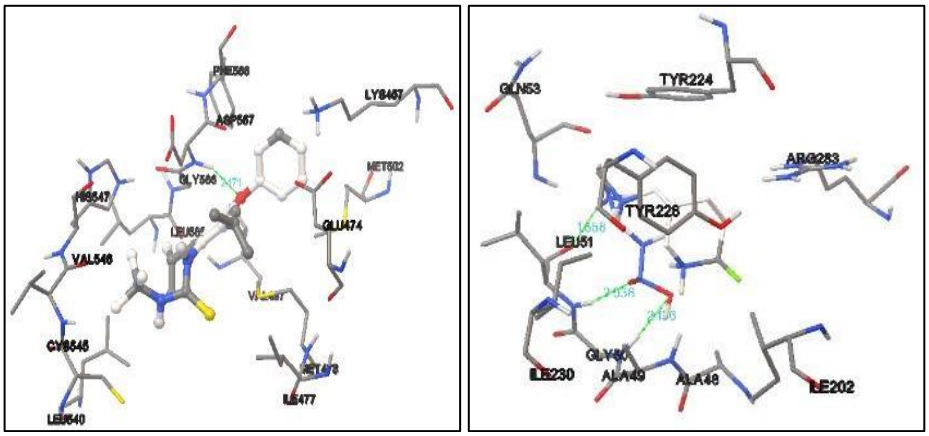

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Fig 3: Molecular docking chemicals-target proteins

Conclusion

- The chi-square test suggested that there is a strong bearing between the awareness status of the farmer and the farmers undertaking safety measures. (Chi-square value= 32.9938)
- The toxicity information provided by the cide-seller is negatively correlated with farmers undertaking safety measures. (r=-0.0382)
- There is no association was found between pre-incidence health issues and causalities (chi- square value= 151.9).
- 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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