

First QSTR Report on *Allium Cepa* Phytotoxicity of Pesticides

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ABSTRACT

With the aim of identification of the toxic nature of the diverse pesticides on *Allium cepa*, experimental data (EC₂₅ and NOEL) were collected from the OPP database and was subjected to QSTR analysis. All the developed MLR models were found to be robust ($Q^2_{LOO} = 0.619 - 0.748$) and predictive enough ($Q^2_{Fn} = 0.662 - 0.845$, $CCC = 0.844 - 0.867$). The prediction reliability was assured by the application of the leverage approach of applicability domain (AD). Finally, prediction and prioritization of the pesticides with no experimental data for two endpoints (EC₂₅ and NOEL) were done by the first theoretical phytotoxicity model of onion. The occurrence of similar prioritized pesticides for both endpoints indicated that either of the endpoints can be used for the ecotoxicological study of the pesticides.

KEYWORDS

AD, GA, MLRNOEL, Pesticides, Phytotoxicity

1. INTRODUCTION

For a very long time, plants have been blessing us with their usefulness. But our altering lifestyle has turned to be a curse in disguise. With the rise in global population that crossed 7.83 billion (World Population Clock 2021), agriculture faces tremendous pressure to supply food, fibres, and fuel ([https://www.worldometers.info/worldpopulation/#:~:text=7.9%20Billion%20\(2021\), Nations%20estimates%20elaborated%20by%20Worldometer](https://www.worldometers.info/worldpopulation/#:~:text=7.9%20Billion%20(2021),Nations%20estimates%20elaborated%20by%20Worldometer)). To overcome these situations, the consumption of fertilizers and pesticides has increased drastically. Our modern agriculture is incomplete without pesticides and fertilizers to kill or inhibit pests, control diverse diseases, suppress the growth of undesirable plants that compete with crops, prevent and reduce the damage due to various fungal species, thereby improving the crop quality and minimizing crop loss. Generally, the pesticides are used intentionally to protect crops, but they or their degradation may affect their non-treated neighbouring crops, which may result in the alteration of the equilibrium of the ecosystem as every organism in the ecosystem depends on each other for their necessities (Chhipa, 2017).

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Allium Cepa (Onion) that originated in Central Asia is the second most and oldest cultivated plant (<https://www.medicalnewstoday.com/articles/276714>). With three varieties of onion (red/white or yellow/brown) and specific flavour ranging from mildly sweet to strong, it is a regularly used vegetable in daily life around the globe. Onions are very rich source of various phytonutrients and are used as both food and therapeutic application in the treatment of cardiovascular and neurological disease, cancers, diabetes, and other dysfunctions related to oxidative stress (Ferioli & D'Antuono 2016).

Food stuff contamination by pesticides and other pollutants is a major concern in recent days. This results in accumulation of persistent nature of pesticides which finally in turn appear in food travelling various compartments of the environment.

The interaction of the plants with all the compartments of environments is the advantageous nature of plants through the bio-indications (Silveira et al. 2017; Vishvkarma et al. 2021). Evaluation of ecotoxicological effects of environmental pollutants is gaining much more attention in recent years. Search/development of the simple and cost effective toxicity screening assays/ tests is always advantageous. Phytotoxicity is one of the important simple, cost-effective bio indicator assays able to identify the presence or absence of pollutant and their subsequent environmental impact either positive or negative. Among the various plants, *Allium Cepa* is one of the plant species recommended by regulatory bodies such as OECD (OECD Guideline no 208) for the phytotoxicity study. The early germination and seedling development can be microscopically observed after exposure of pollutant or mixtures of pollutant in this type of assay. A lot of experimental phytotoxicity determination assays were carried out for onion by various research groups (Ogeleka et al. 2016; Kim et al. 2004; Téllez Vargas et al. 2017) which clearly demonstrated the environmental impacts of agrochemicals and pollutants. Besides this, onion is also being used for cytogenotoxic study (Grant 1999). The number of recently existing environmental pollutants including pesticides in the environment are very large as highlighted by different chemical databases and the experimental toxicity values are very few (5%). Besides these, continuous newer ones are also being added to the existing ones. In order to assess the environmental impacts in a rapid way, computational studies like QSAR with reliable estimates are regularly applied with confidence. For a very long time, QSAR models are being applied in the field of pre-synthesis and even for the regulatory assessments of pharmaceuticals, pesticides, and other chemicals. QSAR aims to discover possible relationships between molecular properties and biological activity patterns of drug applicants. These relationships are developed by using a mathematical approach to predict the activities and properties of untested chemical compounds. QSAR can be seen to have continued to play an important role in toxicity estimation in a cost-effective way in terms of time, money, and manpower as well as minimizing ethical issues arising in experimental toxicity study (Tandon et al. 2019; Tandon et al. 2020; Toropova et al. 2019; Toropov et al. 2020; Tandon et al. 2019; Toropov et al. 2020). To date, many *in silico* phytotoxicity studies are available in the literature but none of them are based on onion as per our knowledge (Bettiol et al. 2016; Freitas et al. 2013; Hulzebos et al. 1991, 1993; Wang et al. 2001, 2002).

In order to get a well-validated QSAR models, the OECD has established five principles of QSAR model validation. They are 1) a defined endpoint; 2) an unambiguous algorithm; 3) a defined domain of applicability; 4) appropriate measures of goodness-of-fit, robustness, and predictive power; 5) a mechanistic interpretation, *if possible*. The details of these 5 principles were given elsewhere in the literature (Banjare et al. 2021; Dearden 2016; Gramatica 2020, <https://www.oecd.org/env/ehs/riskassessment/guidancedocumentsandreportsrelatedtoqsars.htm>). Nowadays, the QSAR studies have become one of the necessary tools for ecotoxicological risk assessments for the environmental fate of chemicals.

In view of these contexts, this research work is aimed at establishing the local predictive QSTR models for the phytotoxicity estimation of pesticides on onion and the application of developed models to pesticides having no experimental phytotoxicity value. The identification of possible structural feature responsible for the toxicity of pesticides on onion was another objective of this research work. In this regard, in the present research work, the authors have gathered 57 pesticides with 21 days

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