Prediction of Environmental Toxicity of Active Chemical Constituents of *Ipomoea Carnea* through GUSAR Software

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Abstract

Stability of environment is based upon the proper ecological balance and better environmental conditions, but the stability of earth is affected by the pollution and it also endangers the life and survival of all living beings on this planet. According to a report published by Lancet Commission on Pollution and Health in October month of 2017, total number of deaths caused by all type of Pollution were found to be 9 million throughout the year which was around 15times more than total deaths occur due to War, and even sometimes brutality caused byhumans. Factors that are calculated for the measurement of Eco-toxicity includes Fathead Minnow LC50 Log10 (mmol/L), Daphnia magna LC50 -Log10 (mol/L), Tetrahymena pyriformis IGC50 -Log10 (mol/L), Bioaccumulation factor Log10 (BCF) etc. As the environmental toxicity increases day by day and affects human life, so there is a need for measuring the environmental toxicity and need to take crucial steps to control it. *Ipomoea carnea* a plant of natural origin and it falls under the family of Convolvulaceae. This

plant can also be named as Bush Morning Glory is used for measurement of environmental toxicity.In this research study it was aimed to predict environmental toxicity caused by active chemical constituents of *I. carnea*..This research study was conducted through GUSAR online software. The environmental toxicity caused by active chemical constituents of *I.carnea* was predicted. As per the study results, the active chemical constituents of *I. carnea*were predicted to cause environmental toxicity.

Keywords: Bioaccumulation factor Log10 (BCF), Convolvulaceae, Daphnia magna LC50 -Log10(mol/L), Ecological Balance, Environment, Environmental toxicity, Fathead Minnow LC50Log10 (mmol/L), GUSAR online software, Human beings, Ipomoea carnea, Lancet Commission on Pollution and Health, Panic, Pollution, Prediction, Tetrahymena pyriformisIGC50 -Log10 (mol/L).

Introduction

Pollution has become the most threatening theme for human beings and the environment. Pollution can be described as process of addition of harmful contaminants in the environment that may lead to harmful changes in the natural environment (Pollution – Definition from the Merriam-Webster Online Dictionary, 2010). There are lot of ways in which environment may get polluted which includes air, noise, chemicals, heat, or light and even plants also. Number of deaths occurs due to pollution have been found to be around 9 million throughout the globe in the year 2015 (Beil, 2017; Carrington, 2017). According to WHO report (2007), it was reported that in India, air pollution becomes the cause of death for about 5 lakhs persons (Chinese Air Pollution Deadliest in World, 2007). Environmental pollution shows harmful effects over human health as well as natural flora and fauna. Ozone depletion is one of the most common factors responsible for causing diseases like throat inflammation, congestion, cardio-vascular disease, respiratory disease and even skin cancer. According to a report published by Lancet Commission on Pollution and Health in October month of 2017, total number of deaths caused by all type of pollution have been reported to be approximately 9 million throughout the year which was around 15 times more than total deaths occurred due to War in past, and even sometimes brutality caused by humans (Stanglin, 2017). Stability of environment is based upon the proper ecological balance and better environmental conditions; however, the stability of earth is affected by the pollution and also endangers the life and survival of all living beings on this planet (Carrington, 2017). Some harmful effects of pollution over environment include global warming, ocean acidification, allelopathy and debries caused by invasive plants, ozone depletion, organic pollution etc.

BAF or Bioaccumulation Factor is a ratio which is defined as the concentration of contaminant in an organism to the amount in the favorable environment at a steady state and organism can either ingest the contaminant with food or may ingest directly (bioaccumulation factor. (n.d.) Segen's Medical Dictionary, 2011).

BCF or Bio-Concentration Factor can be described as the occurrence of bio-concentration up to a certain degree and the only way to measure it includes the controlled laboratory conditions in which there is no any intentional consumption of those chemicals that have nutritional value and these should not be included (Arnot & Gobas, 2006) . Some other factors that are calculated for the measurement of eco-toxicity includes Fathead Minnow LC50 Log10 (mmol/L), Daphnia magna LC50 -Log10 (mol/L), Tetrahymena pyriformis IGC50 -Log10 (mol/L) etc.

All these values are useful for determination of environmental toxicity caused by the herbal plants. *Ipomoea carnea,* a medicinal plant of natural origin belongs to the family: Convolvulaceae. This plant is commonly known as "Bush Morning Glory" (Frey, 1995) .This plant is generally known for its wide range of pharmacological activities. Some of the pharmacological activities of Bush Morning Glory include antioxidant, (Arshad, *et al,* 2010; Gaur *et al,* 2014; Adsul *et al*, 2012) immuno-stimulatory, (Cook, 1987; Sahayaranj & Ravi, 2008) anti-diabetic, (Khalid *et al,* 2011; Latif *et al,* 2012) anti-cancer, (Kumar *et al,*2014; Sharma & Bachheti, 2013) sedative, (Bhattacharya *et al*, 1975; Rout & Kar, 2013) etc.

A tool known for the measurement of eco-toxicity called Way 2 drug have been used for the purpose of determining the Eco-toxicity of active chemical constituents of Bush Morning Glory (Poroikov *et al,* 2003). In this tool GUSAR software provide a source for measurement of Eco-toxicity.

Material and methods

Prediction of environmental toxicity by GUSAR online tool

The use of https://www.way2drug.com/, a bioinformatic tool was utilized for the purpose of prediction of Environmental Toxicity. The GUSAR online server of this Bioinformatic tool is capable of prediction of Environmental Toxicity on the basis of chemical structures of the active organic chemical constituents of *Ipomoea carnea.*

Screening of environmental toxicity by GUSAR online tool

Smile structures of active chemical constituents of *Ipomoea carnea* was sync in the search bar column of this tool to obtain the data of Environmental Toxicity and after obtaining the data we digitized it in our computer in xls. format.

Data analysis

Prediction value is the basic consideration moiety for analyzing the data obtained from above prediction of active chemical constituents of *Ipomoea carnea*. All chemical moieties which exhibit higher prediction value show Environmental Toxicity. The results are given in Table 1.

Results

In the present research study, we predicted the environmental toxicity of active chemical constituents of *Ipomoea carnea*on the basis of Bioaccumulation factor Log10 (BCF), Fathead Minnow LC50 Log10 (mmol/L), Daphnia magna LC50 -Log10 (mol/L), Tetrahymena pyriformis IGC50 -Log10 (mol/L). The interpretation of results suggested that the active chemical constituents of *Ipomoea carnea* shows environmental toxicity as predicted using the GUSAR software analysis.

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Table 1. Prediction of environmental toxicity of active chemical constituents of *Ipomoea carnea*(as listed from S. No. 1 to S. No. 17)

S. No.	Active Chemical Constituents	Bioaccumulation factor Log10(BCF)	Daphnia magna LC50 - Log10(mol/L)	Fathead Minnow LC50 Log10(mmol/L)	Tetrahymena pyriformis IGC50 - Log10(mol/L)
		Prediction Values	Prediction Values	Prediction Values	Prediction Values
1	Swainsonine (Balogh *et al*, 1999)	0,313	2,871	0,951	-1,307
2	Squalene (Sahayaraj *et al*, 2015)	1,360	5,723	-7,640	3,994
3	2-Ethyl-1,3-dimethylbenzene (Sahayaraj *et al*, 2015)	0,000	0,000	0,000	0,000
4	2-(12-Pentadecynyloxy)-tetrahydro2H-pyran (Sahayaraj *et al*, 2015)	1,321	5,232	-3,229	2,281
5	Hexadecanoic Acid (Sahayaraj *et al*, 2015)	2,285	4,446	-3,326	2,692
6	Linoleic Acid (Sahayaraj *et al*, 2015)	1,902	5,146	-4,203	2,951

7	Epiglobulol (Sahayaraj *et al*, 2015)	1,731	4,398	-1,234	0,632
8	1-Octadecanol (Sahayaraj *et al*, 2015; Tirkey *et al*, 1998)	2,208	4,227	-4,243	3,233
9	Stearic Acid Tirkey *et al*, 1998)	2,084	4,671	-4,061	3,150
10	1, 2-diethyl phthalate (Tirkey *et al*, 1998)	0,000	0,000	0,000	0,000
11	Octacosane (Tirkey *et al*, 1998)	1,053	5,774	-8,582	5,158
12	Hexatriacontane (Tirkey *et al*, 1998)	0,345	6,203	-11,150	5,481
13	Tetracontane (Tirkey *et al*, 1998)	0,172	6,380	-12,200	5,187
14	3-diethylamino-1-propanol (Tirkey *et al*, 1998)	0,296	3,133	0,738	-0,873
15	Calystegine B1 (Balogh *et al*, 1999)	0,247	2,958	0,510	-1,441
16	Calystegine B2 (Balogh *et al*, 1999)	0,221	2,713	0,589	-1397
17	Calystegine C1 (Balogh *et al*, 1999)	0,232	2,579	0,595	-1,457