

In-silico SMILES-Based Toxicity Prediction of Fluorescent Dye (Rh-B)

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Abstract

The aim of this study was to investigate the toxicity of Rhodamine B (Rh-B) via computational tools. Rh-B is a fluorescent organic dye and it has much importance because of its photo-physical properties. The 'International Agency for Research on Cancer' classified Rh-B in the risk category for human cancer (CAS No. 81-88-9) This illegally used food colorant was here assessed for its toxicity via computational tools. For this assessment we used LAZAR Toxicity Predictions, PROTOX and pkCSM to explore about the pharmacokinetic and toxicological properties of Rh-B. We simulated Rh-B structure based on SMILES build by ACD/ChemSketch. This assessment shows that Rh-B provides carcinogenic, hepatotoxic risk for humans with a maximum recommended tolerated dose of 0.423 log(mg/kg/day).

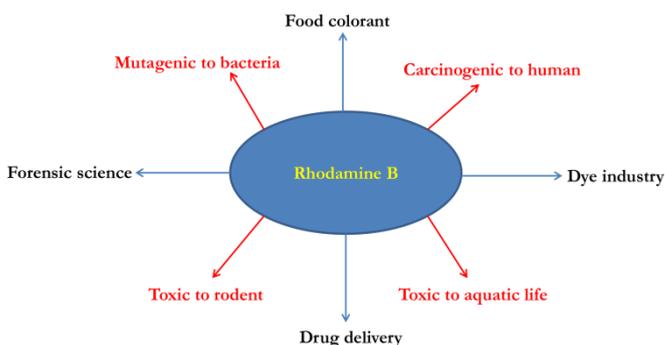


Figure1. Rh-B is economically important but toxic

Recent Publications

1. Cheng, Y.Y. and Tsai, T.H., 2017. Pharmacokinetics and Biodistribution of the Illegal Food Colorant Rhodamine B in Rats. *Journal of Agricultural and Food Chemistry*, 65(5), pp.1078-1085.
2. Elumalai, S. and Muthuraman, G., 2015. Studies on rhodamine B dye transport through a supported liquid membrane from basic aqueous solutions using phenol as a membrane phase. *RSC Advances*, 5(96), pp. 78799-78806.
3. International Agency for Research on Cancer classified Rh-B as a carcinogenic agent. http://monographs.iarc.fr/ENG/Classification/latest_classif.php web site accessed on 2017-05-10.
4. Mottram, L.F., Forbes, S., Ackley, B.D. and Peterson, B.R., 2012. Hydrophobic analogues of rhodamine B and rhodamine 101: potent fluorescent probes of mitochondria in living *C. elegans*. *Beilstein Journal of Organic Chemistry*, 8(1), pp. 2156-2165.
5. Padhi, B.S., 2012. Pollution due to synthetic dyes toxicity & carcinogenicity studies and remediation. *International Journal of Environmental Sciences*, 3(3), p.940.
6. Tatebe, C., Zhong, X., Ohtsuki, T., Kubota, H., Sato, K. and Akiyama, H., 2014. A simple and rapid chromatographic method to determine unauthorized basic colorants (rhodamine B, auramine O, and pararosaniline) in processed foods. *Food Science & Nutrition*, 2(5), pp. 547-556.
7. Theaker, B.J., Hudson, K.E. and Rowell, F.J., 2008. Doped hydrophobic silica nano- and micro-particles as novel agents for developing latent fingerprints. *Forensic Science International*, 174(1), pp.26-34.
8. Zheng, L., Wang, C., Shu, Y., Yan, X. and Li, L., 2015. Utilization of diatomite/ chitosan-Fe (III) composite for the removal of anionic azo dyes from wastewater: equilibrium, kinetics and thermodynamics. *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, 468, pp. 129-139.



Biography

Dahms Hans-Uwe received his PhD and DSc degree in Biology from the University of Oldenburg, Germany. He is currently a Professor of the Department of Biomedical Science and Environmental Biology at Kaohsiung Medical University (KMU). His current research is about antibiotics and public health.

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Biography

Charli Deepak Arulanandam was born in 1990. He is a PhD student in Kaohsiung Medical University (KMU), Taiwan. His current research interests are the screening of multi drug resistant bacteria from the marine environment and the impact of emerging antibiotic resistant genes on public health. In his currently assigned work, he assessed Rhodamine-B (fluorescent dye) toxicological properties using *in silico* tools.

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Notes/Comments: