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In-silico SMILES-based toxicity prediction of fluorescent dye (Rh-B)

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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).

Biography

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

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