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Physicochemical study of opium industry effluent and toxicity prediction using *in silico* method

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Industrial effluent discharge is a major concern in developing countries like India. Opioids and alkaloids serve as raw materials for production of important pharmaceutical drugs like codeine, morphine, papaverine, thebaine, etc. Proper effluent discharge and waste management from opioids processing and similar industries is still a challenge. The present study focuses on collection, characterization and toxicity prediction of pollutants found in opioids processing industries in India. The wastewater was collected from Government Opium Alkaloid Works, Ghazipur, Uttar Pradesh, India. The collected effluent was subjected to physicochemical characterization, identification and quantification of different pollutants. Physicochemical tests revealed Chemical oxygen demand of 10015 mg/L, Biological oxygen demand 3870 mg/L, and Total dissolved solid (TDS) 1275 mg/L, with an pH of 9.47 having dark brown appearance accompanied by a pungent odour. Gas chromatography mass spectrometry followed by Fourier transform infrared spectroscopy was performed to identify the chemical composition of the effluent which revealed the presence of butanol, toluene, methyl isocyanide, 2-methylpentane, and benzeamine, N, N-dimethyl in major concentrations. Toluene is one of the hazardous pollutants found in up to 5.17% in the effluent. Prolonged exposure to toluene leads to disorders of muscles, cardiovascular effects, permanent neuropsychiatric effects, renal tubular damage, and sudden death. The toxicity of toluene was predicted by Toxicity estimation software tool. The software provided the LD₅₀ value for oral rat as 1.77 -log₁₀ mol/kg and for human 0.28 -log₁₀ mol/kg. The authors propose to develop a methodology to bioremediate toluene from wastewater to prevent harmful effects on aquatic and higher living organisms.

Keywords: Alkaloids, Opium effluent, Pollutants, Toluene, Waste management