

ToxAlerts: Database of structural alerts

ToxAlerts is a OCHEM-based platform for collecting and storing toxicological structural alerts from literature and for virtual screening of chemical libraries to flag potentially toxic chemicals and compounds that can cause adverse side effects. An alert is uniquely identified by a SMARTS template, a toxicological endpoint, and a publication where the alert was described. Additionally, the system allows storing complementary information such as name, comments, and mechanism of action, as well as other data. Most importantly, the platform can be easily used for fast virtual screening of large chemical datasets, focused libraries, or newly designed compounds against the toxicological alerts, providing a detailed profile of the chemicals grouped by structural alerts and endpoints.