Systematization of computational toxicology for decision making in drug discovery and development

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Furthermore, in the “Go”, “No-Go” decision of drug development, supportive utilization of a scientifically interpretable computational toxicology system is required for human safety evaluation. Pharmaceutical safety evaluator as a related toxicologist who is facing to practical decision does not need a data-driven AI (Artificial Intelligence) system that calls for the final consequence, rather requires an explainable AI that can provide comprehensive information necessary for evaluation and can help decision making. Through the explication and suggestion of information on the mechanism of toxic effects to safety assessment scientists, ultimately a subsidiary partnership system for risk assessment is to be a powerful tool that can indicate project-vector with data weight for the corresponding counterparts.

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