国立医薬品食品衛生研究所・特別講演会

日時

2024年12月3日（火）14:00 – 15:00

場所

国立医薬品食品衛生研究所2階【共用会議室】
神奈川県川崎市川崎区殿町3-25-26

講師

Naomi Kruhlak, PhD (US Food and Drug Administration/Center for Drug Evaluation and Research, USA)

タイトル

Application of (Q)SAR Modeling to the Safety Assessment of Pharmaceuticals

要旨

(Quantitative) structure-activity relationship ((Q)SAR) computational models can make a prediction of toxicity based solely on a chemical's structure and are used by the US Food and Drug Administration's (FDA) Center for Drug Evaluation and Research (CDER) to provide predictions for chemical substances under review when robust experimental data are unavailable. Examples include: 1) the mutagenicity assessment of drug impurities under the ICH M7(R2) guideline using complementary (Q)SAR models in combination with expert knowledge; 2) the general toxicity assessment of extractable and leachable compounds using read-across from a structurally-related surrogate compound; and 3) the prediction of carcinogenic potency of nitrosamine impurities using the Carcinogenic Potency Categorization Approach (CPCA).

This presentation will provide an introduction to the (Q)SAR modeling methodology, followed by examples of the practical use of (Q)SAR analysis for regulatory decision-making in drug safety. Additionally, FDA/CDER's Computational Toxicology Consultation Service review workflow will be presented, including the role of chemical structure-based databasing of (Q)SAR assessments to promote consistency and efficiency across new and generic drug evaluations.

お問い合わせ

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