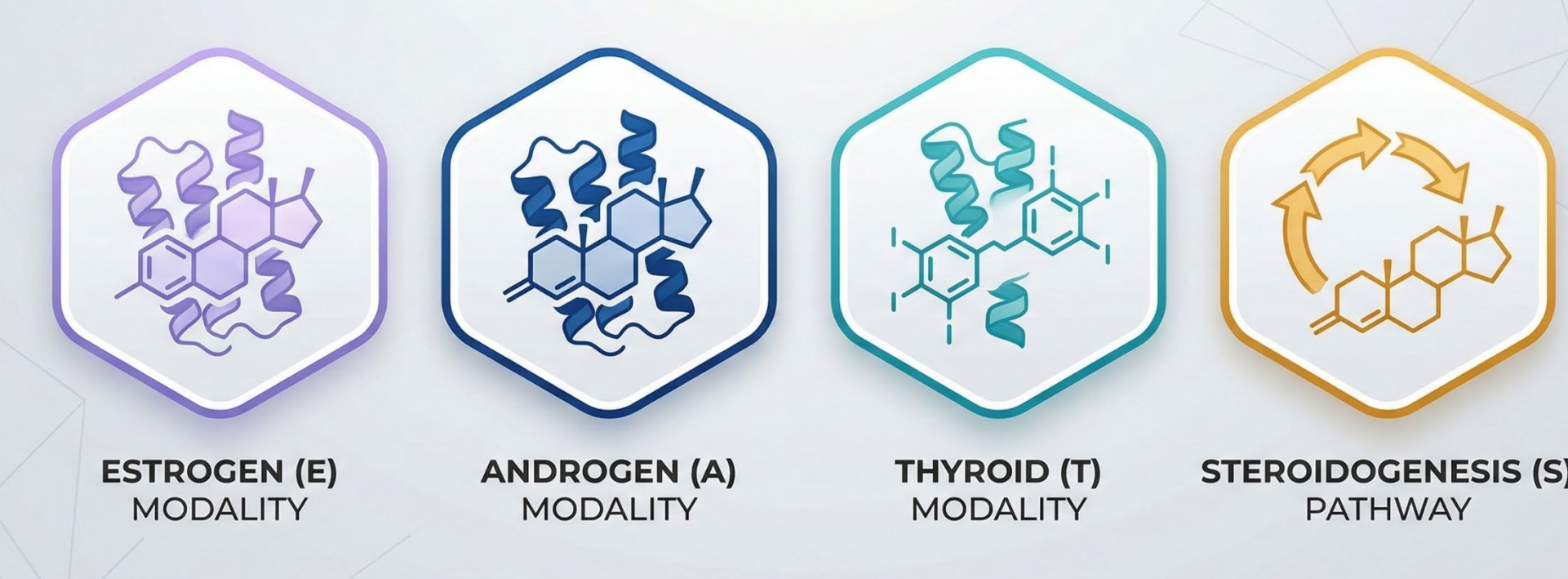




High-throughput in silico screening for endocrine-related activity using a KNIME-based decision tree framework

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Multi-Tool VEGA, OPERA, Percepta and OECD QSAR Toolbox • High-Sensitivity OR-Gate Logic • Automated KNIME Workflow • R & C Scoring System

INTRODUCTION

In 2023, new hazard class for endocrine disruptors (ED) was introduced under ECHA's CLP Regulation. A reliable, efficient and reproducible solution for early-stage identification of this hazard is required to enable rapid screening of a large industrial dataset for potential endocrine-related activity.

METHODOLOGY

