

# A validation study of the COMPACT and HazardExpert techniques with 40 chemicals

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...Such features direct the course of **metabolism** by the P450s, and also determine the rates and positions of **metabolism**. In particular, COMPACT can provide...toxic consequences of P450-mediated **metabolism**, especially when used in conjunction...

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**Abbreviations:** COMPACT, computer-optimized molecular parametric analysis of chemical toxicity; QSARs, quantitative structure-activity relationships; HOMO, highest occupied molecular orbital; LUMO, lowest unoccupied molecular orbital; EIP, electrostatic isopotential;  $E(\text{HOMO})$ , energy of the HOMO;  $E(\text{LUMO})$ , energy of the LUMO; AAF, 2-acetylaminofluorene;  $\Delta E$ ,  $E(\text{LUMO})-E(\text{HOMO})$ ;  $k_e$ , electron uptake rate constant; Ah, aryl hydrocarbon; log P, logarithm of the octanol-water partition coefficient; ROS, reactive oxygen species; CYP, cytochrome P450

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