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A structure-activity relationship study on the mechanisms of methacrylate-induced toxicity using NMR chemical shift of β-carbon, RP-HPLC log P and semiempirical molecular descriptor

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Abstract:
To clarify the mechanism of methacrylate-induced toxicity, a total of 24 acrylates, methacrylates, and dimethacrylates were chosen for a structure-activity relationship (SAR) study in terms of NMR chemical shifts, semiempirical molecular descriptors, and reverse phase (RP)-HPLC log P. Molecular descriptors as well as bulk, electronic, and energy descriptors were calculated using the PM3/CONFLEX method. A significant multiple linear regression equation for methacrylates in mice was denoted as log $1/LD_{50}$ (which was function [$-(E_{HOMO}+E_{LUMO})/2$, log P]). Besides, significant linear regression equations for methacrylates were denoted as log $1/ED_{50}$ in HeLa S3 and in HGF cells as function [E_{HOMO} and/or log P]. Results showed that the ^{13}C NMR chemical shift of β-carbon for methacrylates was correlated with their E_{HOMO}. Findings of this study thus suggested that it might be possible to predict methacrylate-induced toxicity using physicochemical properties.

Key words:
Methacrylates, Structure-activity relationships (SAR), Physicochemical properties

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