KP10

Calculation of quantitative structure activity relationship(QSAR) of sensitizing disperse dye and an application to an allergic contact dermatitis.

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The 26 kinds of sensitization reported disperse dyes calculated Quantitative Structure-Activity Relationship (QSAR, Skin sensitization). As a result, some azo type disperse dyes cannot detect sensitizing potential. Azo type disperse dyes receives reduction reaction by an enzyme in skin. And an Azo bond is reduced, as a result, formation an amine compound. Input a chemical structure of the formation amine compound into QSAR system, and it calculated sensitizing potential. A result, detect ability of sensitizing potential betterment. We improved QSAR calculation method can use for cause investigation of the allergic contact dermatitis that azo type disperse dyes. However, some sensitization azo type disperse dyes cannot detected sensitizing potential. In addition, about C.I.Disperse Blue 124 cannot detect sensitization in QSAR, executed base data and Guinea Pig Maximization Test (GPMT) of QSAR, and confirmed strong sensitizing potential. These data will be useful for improvement of QSAR.