Quantitative analysis of chemiluminescence intensity and toxicity \textit{in silico}

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The chemiluminescence detection technique is highly sensitive. Chemiluminescence is produced by a chemical reaction, the sensitivity and intensity of which depends on the reactivity of super oxide. The intensity of chemiluminescence was quantitatively analyzed using computational chemical calculations based on a radical reaction mechanism where a keto-enol rearrangement produces super oxide, and the super oxide reacts with luminol or lusigenin to produce the chemiluminescence. The partial charge of the carbon atoms of a carbonyl group, calculated using the MOPAC function of the CAChe™ program, changed significantly and strongly correlated with the relative intensity of the chemiluminescence. This computational chemical analytical method can be used to determine the relative sensitivity of the chemiluminescence reaction using luminol and lusigenin.

Super oxide is toxic in vivo. The chemiluminescence was therefore related to the toxicity. The toxicity was calculated using the TOPKAT™ program from Fujitsu. The correlation coefficient between the intensity of the chemiluminescence of phenacylalcohol derivatives and rat oral LD50 was 0.949 ($n = 5$) and that between the partial charge change and the rat oral LD50 was 0.912 ($n = 5$). These results indicate that measurement of the intensity can provide a quantitative measurement of the toxicity of an analyte. Furthermore, the calculation of the partial charge change by the computational chemical method can be used to estimate the rat oral LD50. These experimental and computational chemical methods will help to speed-up screening of certain drug candidates by chemiluminescence assays.

Many steroid-drugs are used for the treatment of skin diseases. Super oxide produced from steroids should also produce chemiluminescence by the same mechanism. Therefore, the above approaches were applied to study the efficacy, i.e., toxicity, of steroid drugs. The intensity of the chemiluminescence strongly correlated with the partial charge change of targeted atoms as well as with the rat oral LD50.