HUBUNGAN KUANTITATIF ANTARA STRUKTUR DAN TOKSISITAS SENYAWA KLOROFENOL

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ABSTRACT

Quantitative Structure-Activity Relationship (QSAR) for the toxicity of chlorophenols (CPs) from mono to pentachlorine substituted compounds has been done. The structural parameters are obtained from geometry structure optimization by computational chemistry using *ab initio* methods and the experimental data of acute toxicity (-log EC_{50}) of chlorophenols to *Daphnia magna* were taken from the literature. The best QSAR model obtained by multilinier regression analysis, using the systematic approach for variable selection and the result showed that QSAR equations i.e:

$$-\log EC_{50\ pre} = -99.545 - 83.402\ r_{OH} + 145.879\ r_{CO} - 0.053\ q_O + 26.198\ q_H + 0.568\ E_H - 2.599\ E_L - 0.067\ HE - 0.134\ Rm + 0.133\ \mu$$

(n = 18, R = 0.971, R^2 = 0.943, SD = 0.447794, F_{cal}/F_{tab} = 3.956)

Keywords: *Chlorophenol, QSAR, toxicity*

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