

## Activity Characterization of Triazines Analogues: Statistical Parameters for Models Assessment

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### Abstract

Correlation coefficients and associated squared values are used as parameters in validation of structure-activity relationship models. By using of the molecular descriptors family on structure-activity relationship method [1] the herbicidal activity of a sample of triazines analogues was modelled [2]. A number of three multivariate models proved to have estimation and prediction abilities [2].

Starting from the hypothesis that the measured activity of triazines analogue is a semi-quantitative variable, the aim of the research was to analyzed the three previously reported models by using the Pearson, Spearman, Kendall's and Gamma correlation coefficients.

The structure-activity relationship models were previously reported [2]. The measured herbicidal activity of triazines analogues and the value estimated by the previously reported models were investigated by using the Pearson, Spearman, Kendall's  $\tau_a$ ,  $\tau_b$ ,  $\tau_c$  and Gamma correlation coefficients ( $r_{Prs}$ ,  $\rho_{Spm}$ ,  $\tau_{Ken,a}$ ,  $\tau_{Ken,b}$ ,  $\tau_{Ken,c}$ ,  $\Gamma$ ) and associated squared correlation coefficient ( $r_{Prs}^2$ ,  $\rho_{Spm}^2$ ,  $\tau_{Ken,a}^2$ ,  $\tau_{Ken,b}^2$ ,  $\tau_{Ken,c}^2$ ,  $\Gamma^2$ ).

The results of investigation, express as correlation coefficients and associated 95% confidence intervals, squared correlation coefficient and Student's t, respectively the parameter of the Z test were calculated and analyzed.

The correlation coefficients obtained with all methods were statistical significant ( $p < 0.0001$ ). The correlation coefficients vary according with the model as follow:

- Model with two descriptors: from  $r = 0.6889$  ( $\tau_{Ken,c}$ ) - 95%CI [0.4370-0.8405] to  $r = 0.9855$  ( $r_{Prs}$ ) - 95% CI [0.9694-0.9931];
- Model with three descriptors: from 0.7489 ( $\tau_{Ken,c}$ ) - 95%CI [0.5321-0.8734] to the value equal with 0.9883 ( $r_{Prs}$ ) - 95% CI [0.9752-0.9944];

- Model with four descriptors: from 0.7444 ( $\tau_{\text{Ken,c}}$ ) - 95%CI [0.5248-0.8710] to the value equal with 0.9925 ( $r_{\text{Prs}}$ ) - 95% CI [0.9841-0.9964].

If there is considered that the herbicidal activity of triazines analogues is a quantitative variable, the Pearson correlation coefficients is the statistical parameter that must be used in evaluation of relationship between the measured and estimated activity.

Considering the measured activity of triazines analogues as a semi-quantitative variable, a rank correlation coefficient is the statistical parameter able to provide more reliable estimation rather than Pearson correlation coefficient. However, which is the proper rank correlation coefficients that can be use in this circumstance? The comparisons between the rank correlation coefficients are discussed and the further plan of research is highlighted.

**Keywords:** Triazines Analogues, Statistical Models, Correlation Coefficients

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### **References**

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