

Artificial Neural Networks: a tool for science

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Ph. D. Seminars - XD 107

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“*Artificial Neural Networks*” (ANNs) can be applied in different scientific fields (and in particular to chemistry).

The seminar comprises a brief introduction to artificial neural networks, their structure, the working principle and learning capabilities. Also, the advantages the use of Experimental Design in conjunction with ANNs will be discussed. The capabilities of ANNs will be shown through several examples (i) the use of ANNs as tools for “soft” modelling of the Nernst equation, complex cases like (ii) multicomponent kinetic determination (iii) optimization of chemical synthesis, (iv) synthesis of nano-materials (v) estimation of kinetic rate constants and (vi) analysis of cytotoxic activity of mixtures of compounds, etc. More emphasis will be given to their practical use rather than to theoretical aspects. General applicability of ANNs in science will be stressed.

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