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**InModelia : Design of experiments, Molecule properties.**

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InModelia is a software reseller and a consulting services company involved in:

- Neural networks for nonlinear regression.
- Design of experiments for explicit nonlinear algebraic functions and nonlinear ordinary differential equations. Knowing/computing the optimal points help reduce the number of experiments and return more accurate models, even in a nonlinear environment like thermodynamic models.  
Software Neuro Pex
- Graph machines, a special construction that uses neural networks, to compute in silico molecule properties, QSAR and QSPR. We get outstanding results, even with small datasets. This work is conducted with ESPCI-ParisTech.  
A. Goulon, T. Picot, A. Duprat, and G. Dreyfus  
Predicting activities without computing descriptors: graph machines for QSAR  
SAR and QSAR in Environmental Resesarch, vol. 18, pp. 141 - 153 (2007)

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**Keywords:** neural networks, design of experiments, graph machines, QSAR, QSPR.