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Integrating Inference, Simulation and Deduction in Molecular Domain Analysis and Synthesis with Peculiar Attention to Drug Discovery

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Abstract : Standard molecular modeling is traditionally done through Schroedinger equations via the help of powerful tools helping to manage them atom by atom, often needing High Performance Computing. Here, a full portfolio of new tools, conjugating statistical inference in the so called eXplainable Artificial Intelligence framework (in the form of Machine Learning of understandable rules) to the more traditional modeling and simulation control theory of mixed dynamic logic hybrid processes, is offered as quite a general purpose even if making an example to a popular chemical physics set of problems.

Keywords : understandable rules ML, k-means, PCA, PieceWise Affine Auto Regression with eXogenous input
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