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Applications of proteochemometrics: From species extrapolation to cell line sensitivity modelling

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Proteochemometrics (PCM) is a computational method to simultaneously model the bioactivity of multiple ligandsagainst multiple protein targets, and therefore permits to explore the selectivity and promiscuity of ligands on different protein classes. Indeed, the simultaneous inclusion of both chemical and target information enables the extra- andinterpolation to predict the bioactivity of compounds on targets, which can be not present in the training set. In thiscontribution, we will firstly show a methodological advance in the field, namely how Bayesian inference (GaussianProcesses) can be successfully applied in the context of PCM for (i) the prediction of compounds bioactivity along withthe error estimation of the prediction; (ii) the determination of the applicability domain of a PCM model; and (iii) theinclusion of experimental uncertainty of bioactivity measurements. Additionally, we will describe how the applicationof PCM can be useful in medicinal chemistry to concomitantly optimize compounds selectivity and potency, in thecontext of two application scenarios, which are: (a) Modellingisoform-selective cyclooxygenase inhibition; and (b)large-scale cancer cell line drug sensitivity prediction.

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