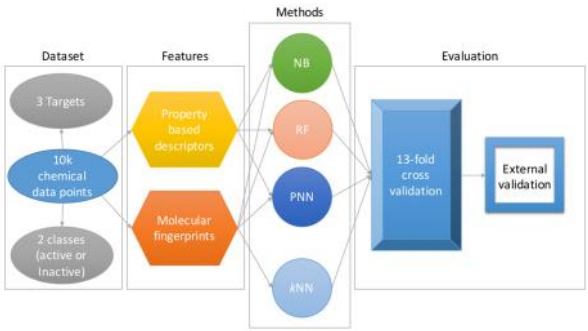
Newsletter

Berlin-Brandenburg research platform BB3R – Issue 1 April 2017

BB3R introduces: Structural Bioinformatics Group (AG Preissner, Charité)

Our interdisciplinary research spans a broad range of topics in Bio/Cheminformatics and Personalized Medicine with a special emphasis on understanding of the evolution, structure, function and interaction of chemicals, proteins and disease relationships. We create freely accessible databases and web applications that are useful to the community as one stop sources for integrated data and computational predictions. We developed fast and reliable computational models [1, 2] for predicting the interference of chemical structures in nuclear receptor and stress response pathways. The models were recognized as relevant and useful by the US National Institute of Health's screening initiative "Toxicology in 21st century" and are likely to be used in screening large libraries of chemical structures whose activity in these two pathways is unknown. We felt the need to create a one-stop resource that serves as a hub of drugs or drug products that were recalled from global markets due to safety concerns. Therefore, we developed "WITHDRAWN - a database of withdrawn and discontinued drugs" [3]. The resource is not only useful in exploring the toxicities associated with the withdrawals but also in elucidating mechanisms of toxicity. We developed a web-based application, ProTox [4], for prediction of oral toxicity in rodents. Overall, we accept the challenge to predict the results of *in vitro* experiments *via* computational modeling, simulation and screening to complement the principles of the 3Rs (Replacement, Reduction and Refinement). We believe our models could significantly reduce the number of experiments needed to estimate chemical toxicity and assessment of toxic doses of chemicals in rodents.



Schematic representation of methodology involved in construction and validation of *in silico* prediction models [1]

References: **[1]** J Cheminform. (2016) 8:51 **[2]** Front Environ Sci. 3(July):1–9 **[3]** Nucleic Acids Res. 2016 Jan 4;44(D1):D1080-6 **[4]** Nucleic Acids Res. 2014 Jul;42(Web Server issue):W53-8

Upcoming Events

- April 24th 2017: public discussion at the **Urania** Berlin: "A future without animal tests – will Berlin be the capital of alternative methods? "
  BB3R Prof. Dr. Sarah Hedtrich will present her research about in vitro skin disease models [more information]
- summer semester 2017: the second lecture and webinar about "Alternative methods in research and education" takes place at the Freie Universität Berlin [more information]
- June 27th 2017: BB3R will present the latest 3R related research at the „Lange Nacht der Wissenschaften" in Berlin and Potsdam [more information]

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