KEMIJSKI INŠTITUT

Vabilo na inštitutsko predavanje / Invitation to the institute lecture

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Velika predavalnica Kemijskega inštituta / Great Lecture Hall, National Institute of Chemistry; Hajdrihova 19, Ljubljana

Chemical and Biological Data

From Compound Selection to Mode of Action Analysis (and Back Again)

More and more chemical and biological information is becoming available, both in public databases as well as in company repositories. However, how to make use of this information in chemical biology and drug discovery settings is much less clear.

In this work, we will discuss how chemical and biological information from different domains – such as compound bioactivity data, pathway annotations from the bioinformatics domain, and gene expression data – can be used for a variety of purposes, such as the mode-of-action analysis from phenotypic readouts, anticipating compound toxicities in early discovery and during lead optimization based on gene expression data, and for designing and selecting compounds with the desired bioactivities against a range of protein targets as well as cell lines. Another application of much relevance to screening is the design of screening libraries, where we have explored the impact of cytotoxicity in such libraries, iterative screening and the utilization of 'informer sets'. Finally, the modelling of compound mixtures will be discussed in this overview presentation of the work taking place in our research group, where we will present prospective research projects covering diverse biological systems, such as *Plasmodium falciparum* screens and others.

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2. Drakakis G, *et al. MedChemComm* **2014**, 5, 386 – 396.
3. Verbist B, *et al. Drug Discov. Today* **2015**, 20, 505 – 513.
4. Van Westen GJP, *et al. PLoS Comp. Biol.* **2013**, 9, e1002899.
5. Cortes-Ciriano I, *et al. Bioinformatics* **2016**, 32, 85 – 95.
6. Mervin, LH, *et al. ACS Chem. Biol.* **2016** *(ASAP Article, DOI: 10.1021/acschembio.6b00538)*
7. Paricharak S, *et al. ACS Chem. Biol.* **2016,** 1255 – 1264.
8. Paricharak S, *et al. J. Chem. Inf. Model.* **2016**, 56, 1622 – 1630.
9. Bulusu KC*, et al. Drug Discov. Today* **2016**, 21, 225 – 238**.**

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Vljudno vabljeni / Kindly invited