NC STATE UNIVERSITY

Comparative Medicine Institute

Denis Fourches

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Computer-aided Molecular Design

Research emphasis:

Our research goal is to analyze, model, and forecast complex interactions between chemical structures and various types of biological targets (e.g., kinases, GPCRs, HLAs, HDACs) to design novel compounds with the desired activity and safety profiles. We develop cheminformatics approaches to establish ligand-based and structure-based quantitative structure-activity relationships, and screen large libraries of virtual compounds for prioritizing hits to be tested and confirmed experimentally.

Application:

- Drug Discovery
- Chemical Risk Assessment
- Agrochemicals
- Nanomaterials

Collaboration potential:

- Virtual screening
- *In Silico* lead optimization
- Molecular dynamics

Selected publications:

Fourches D, Sassano MF, Roth BL, Tropsha A. HTS navigator: freely accessible cheminformatics software for analyzing high-throughput screening data. Bioinformatics. 2014 Feb 15;30(4):588-9.

Fourches D, Politi R, Tropsha A. Target-specific native/decoy pose classifier improves the accuracy of ligand ranking in the CSAR 2013 benchmark. J Chem Inf Model. 2015 Jan 26;55(1):63-71.

Fourches D, Muratov E, Tropsha A. Curation of chemogenomics data. Nature Chem Biol. 2015 Aug;11(8):535.

Fourches D, Pu D, Li L, Zhou H, Mu Q, Su G, Yan B, Tropsha A. Computer-aided design of carbon nanotubes with the desired bioactivity and safety profiles. Nanotoxicology. 2015 Nov 2:1-10.