

# ***In silico* exploration of the chemical space of natural compounds from Ayurveda traditional medicine**

***Honey Polur***

DTU Systems Biology, Technical University of Denmark  
s081185@student.dtu.dk

Natural products and their derivatives have historically been invaluable as a source of therapeutic agents and our natural environment remains a non-exhausted creative pool for the discovery and synthesis of new drug compounds. It has long been recognized that natural-product structures have the characteristics of high-chemical diversity, biochemical specificity and other molecular properties that make them favorable as lead structures for drug discovery, which serve to differentiate them from libraries of synthetic and combinatorial compounds. Natural products can be viewed as a population of privileged structures selected by evolutionary pressures to interact with a wide variety of proteins and other biological targets for specific purposes. On the basis of this concept, a guiding principle has emerged that natural products, by virtue of their molecular evolution to preferentially bind to the protein folds, are validated starting points for drug-development.

In the proposed project advanced chemoinformatics tools will be used for the mapping of the chemicals space of natural compounds from plants used in Ayurveda, the traditional Indian medicine. Our approach will consist of the following consecutive steps:

1. Curation of the Ayurveda database: Each natural compound will be eventually described with its 2D chemical structure in SMILES and sdf format. A database will then be constructed that will include: a) chemical name, b) structural information, c) plant source and d) medicinal use according to Ayurveda.
2. As most part of the chemical space of Ayurveda medicine is virtual 'terra incognita', a detailed structural analysis of the natural compounds from the database will be performed including the distribution of properties related to drug-likeness, such as molecular weight and hydrogen bond donors and acceptors .
3. The structural similarity of the natural compounds with compounds from the databases included in ChemProt server: (<http://www.cbs.dtu.dk/services/ChemProt-1.0/>) will be evaluated to propose potential new ligands of natural origin. The part of the database that consists of natural compounds with known and documented biological activities (if any) will be analyzed and these will be compared to the traditional medicinal use. Two types of descriptors, MACCS fingerprints and pharmacophore-based descriptors will be evaluated.
4. Finally, the natural compounds from the Ayurvedic plants will be compared with the human metabolites from the Human Metabolome Database (<http://www.hmdb.ca/>) to investigate whether they potentially interfere with human metabolic pathways.