AYUsearch: a repository to facilitate the biochemical understanding of natural products-derived chemical substances

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Ayurveda – a traditional Indian medicinal (TIM) practice advocates a lifestyle regimen utilizing natural products to cure complex ailments. The famous Ayurveda classics, viz. *Charak Samhita*, *Ashtanga Hridayam* and *Sushruta Samhita*, elaborate on various plant and animal products, in which the descriptions are narrated in Sanskrit and often signified through a metaphor. The particulars are empirical and usually lack experimental evidence. Its efficacy needs to be ensured towards the gold standard of biomedical sciences. Indeed, an ordered catalogue on a natural product is quintessential to designing the validation strategies for TIM. We obtained evidence on 60 natural products with a mentioned history in Ayurveda. For this, we manually curated a list of natural products-derived molecules (NDMs). Next, they were sorted into universally accepted chemical identifiers and processed into SDF formats. The 1004 gene targets were identified for 636 NDMs through molecular and reverse docking studies. Subsequently, the functional annotation of differentially expressed genes using KEGG pathways and Gene Ontology analysis unravelled the role of the scrutinized ligands on cell functions. AYUsearch (database) is an attempt to redefine the information embedded in Ayurveda, where the biological role of natural chemical products is decoded through network pharmacology.

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(TMs) alone[2]. Mainly, TMs contain a cocktail of bioactive chemical substances, unlike active lead in allopathic drugs. However, over the last two decades, drug designing and development has gradually shifted to a multidrug–multitarget strategy instead of a single drug–single target approach, formally known as poly-drug or network pharmacology (NP)[3]. NP integrates interactions of bioactive molecules with a large set of cellular targets and predicts a relatable association[4,5]. Using NP, bioactive molecules are continuously examined for their efficacy in treating complex disorders often derived from natural origin and known to exert a synergistic impact on the host target/s[6].

Countless computational tools have been developed to predict such interactions and are now considered essential to initiate drug screening. Such tools are classified into three broad categories: (i) catalogues or databases that collect and sort information on the ligands, (ii) suits that analyse and visualize the affinities of ligands and biological targets and (iii) functional annotation tools that predict the biological role of such ligands. Eventually, these tools have enhanced the speed of the drug screening process, which was earlier considered relatively slow-paced. Here, the only rate-limiting step is the availability of information on bioactive molecules scattered in numerous records and not readily available to drug practitioners. Towards this, various datasets have been developed and are openly accessible at the web interface. HIT[7], TCMID[8], TCMSP[9], TCM-Mesh[10], NutriChem[11], TCMChemDB[12] and plant metabolite data-