ChemMaps.com V2 - Exploring the Environmental Chemical Universe

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Access to computationally based visualization tools to navigate chemical space has become more important due to the increasing size and diversity of publicly accessible databases and associated compendiums of high-throughput screening (HTS) and other descriptor and effects data. Construction of visualization tools relies on complex projection techniques using molecular descriptors. However, application of these techniques requires advanced programming skills that are beyond the capabilities of many stakeholders. Inspired by the popular Google Maps application, we developed the ChemMaps.com webserver (https://sandbox.ntp.niehs.nih.gov/chemmaps/) to easily navigate chemical space. The first version of ChemMaps.com enabled users to browse and visualize a space of 2,000 FDA-approved drugs and over 6,000 drug candidates from the DrugBank database (https://www.drugbank.ca/). The chemical space of ChemMaps.com V2, released in 2022, includes approximately one million environmental chemicals from the EPA Distributed Structure-Searchable Toxicity (DSSTox) inventory. ChemMaps.com V2 incorporates mapping to HTS assay data from the U.S. federal Tox21 research collaboration program, which includes results from around 2,000 assays tested on up to 10,000 chemicals. ChemMaps.com V2 users can now visualize chemical activity both by assay and target directly on the map and compare chemical spaces occupied by active and inactive chemicals. ChemMaps.com V2 also has new navigation options, including an on-the-fly distance measurement between two chemicals selected on the 3D map, a map screenshot button, and customizable color mapping based on chemical properties. Project was funded by NIEHS under Contract No. HHSN273201500010C.