ChemMaps.com V2 – Exploring the Environmental Chemical Universe

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Easily navigating chemical space has become more important due to the increasing size and diversity of publicly accessible databases such as DrugBank, ChEMBL, and DSSTox, and associated compendiums of high-throughput screening (HTS) and other data. Construction of computationally based visualization tools to accomplish this relies on complex projection techniques using molecular descriptors. However, the multiple cheminformatics steps required to prepare, characterize, compute, and explore these molecules typically require 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 U.S. Food and Drug Administration-approved drugs and over 6,000 drug candidates from the DrugBank database (https://www.drugbank.ca/). ChemMaps.com was later extended to include a second map of about 47,000 environmental chemicals. The chemical space of ChemMaps.com V2, released 2022, now includes approximately one million environmental chemicals from the Distributed Structure-Searchable Toxicity (DSSTox) inventory, updated in 2021. ChemMaps.com V2 incorporates mapping to 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 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. Each chemical is linked to the U.S. Environmental Protection Agency CompTox Chemicals Dashboard (https://comptox.epa.gov/dashboard/), which allows users to quickly retrieve additional chemical and assay information. 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 a customizable color mapping based on chemical properties. The user can now upload their own set of chemicals and visualize them on the available maps. Finally, we updated and improved the 3D navigation to be more responsive and faster for a better user experience.

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