MMsINC®: a new public large-scale chemoinformatics database system

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MMSinc is a database of commercially available compounds. It currently contains over 4 million */non-redundant/* chemical compounds in 3D format. The whole database was studied in term of uniqueness, diversity, frameworks, chemical reactivity, drug-like and lead-like properties. There are more than 175.000 frameworks in our database. There are 3.89 millions (98%) of drug-like molecules among which more than 3.61 millions (91%) are lead-like. Moreover, 3.45 million (87%) are considered chemically stable compounds. The druglikeness and leadlikeness are estimated using Lipinski and Oprea cut-off values. The compounds are stored in a PostgreSQL database and the code to manage this database is in Java. Moreover, MMsINC is nicely integrated with PubChem and PDB databases facilitating the cross exchange of ligand information. We are developing tools for efficient database access and analysis, for virtual screening and chemoinformatic applications. MMsINC is accessible at the following web address: http://mms.dsfarm.unipd.it/MMsINC/.