

What is iMols?

iMols is a cloud WebApp to manage your chemical libraries including and integrating different tools and source database. Tools includes, searches, virtual profiling, compound selection and more.

Who is it for?

iMols is designed for all those chemists and life sciences researchers, from wet laboratory to computational, that want to manage all computational tools and databases in a single framework.

Why you have to use it?

To skip browsing on different databases, installing software, paying licenses and to forget your backups. iMols do all of it for you.

CLOUD TECHNOLOGY FOR YOUR RESEARCH

iMols applies the philosophy of cloud technology to your computational research, which means you do not need to be worried about licenses, backups and hardware maintenance. iMols do all of it for you. Based on the trusted and robust infrastructure of the best worldwide cloud provider, Amazon Web Services, iMols provides you the licenses, hardware and secure backups you need for your research, and you only pay for the real use.

ALL MEMBERS OF YOUR TEAM IN THE SAME PLACE

iMols can be used by a single researcher but is also a collaborative tool. You can sign up as a administrator of your team and invite all your collaborators. All of you will be able to communicate, share computational experiments, results, projects, molecules, projects and databases. Forgot to send molecule files, protein pdbs and results by mail, iMols is for your team allowing you to share information and save time.

ALL IN ONE

Manage all your computational research in one environment. Stop browsing different databases, copying files to an other webservice, learn how to manage different software and serches tools,... iMols integrates different databases and tools allowing you to have all your computational research in a single place.

KEY FEATURES

Manage your libraries

iMols allow you to store all your chemical compounds, add comments and synonyms and group them in your team private libraries. All libraries can be also grouped in projects allowing you to centralize all your computational drug discovery process in a single place

Explore public libraries

Explore all public libraries including more than 1,3 million of chemical structures and more than 9000 protein targets. Explore all their properties and biological activities. Search them by descriptors, similarity, 3D, bioactivity,...

Discover and compute

iMols allow you to discover new targets for your chemical compounds, these virtual screening techniques predict the biological activity of a given molecule resulting in a list of probable targets. With iMols will be also able to search for similar compounds for a given molecules (with different technologies you can choice when you start the experiment) and screen databases looking for active compounds for an starting protein.

Teams

iMols can be used by a single user but it has been designed to work in teams. With iMols you will be able to share all your information, compounds, proteins, experiments and libraries and you can also share comments in proteins and molecules