Virtual screening and collaborative computing: a new frontier in drug discovery

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The term *collaborative computing* includes technologies and informatics resources based on a network communication system that allows to share documents between the people that are working on the same projects. All activities are managed by a variety of devices such as desktops, laptops, tablets and smartphones. This is the most common definition of this term, in which the shared resources are mainly information and more generally data flows, but in a computational chemistry laboratory, it may be interesting to share also hardware resources in order to increase the global computational power. In the last years, the computational power demand is increased not only to perform more complex calculations or longer simulations, but also to carry out a large amount of relatively simple calculations as those for the virtual screening, one of the most powerful computational approaches to identify hit compounds in the drug discovery process. The typical scenario of a computational chemistry lab consists in a local network in which several PCs are connected each other to share the local resources and to access to Internet. In this situation, the global computational power is very high, but almost unusable because fragmented over the net. The classical grid computing paradigm can be applied successfully to take advantage of this computational power but it requires dedicated hardware, specific software and skilled people to implement it. Starting from this ground and with the aim to collect the unused computational power without interfering with the normal user activity, WarpEngine was developed. It’s a client-server system included in VEGA ZZ package that allows to perform several types of calculations thanks to its flexible script-based programmability.
The communication will describe the WarpEngine features, how to use it efficiently in the structure-based virtual screening and how to choose the best molecular docking software on the basis of its performances in terms of speed and quality of the results.