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PELE Studio: The next generation drug design software

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We are clearly assisting a rise of computational predictions in drug design; top pharmaceutical companies are signing large contracts with modeling software companies. This, has been made possible by the improvement in the techniques (algorithms) but also by the rise in computational power, such as the use of graphic processing units in molecular dynamics of docking program. Next generation drug design software, however, will embrace additional (current) technological developments. In this line we are combining PELE, our Monte Carlo sampling technique highlighted as an outstanding achievement in the latest CSAR blind test, with machine learning algorithms, high performance computing and improved 2D/3D visualization techniques. Our aim is to provide a drug design software capable of: i) interactive: Instantaneous answers; ii) accurate: Quantitative answers; iii) smart: Self-learning capabilities; iv) connecting: Providing a virtual working space. Our efforts and initial results in this line will be provided in this talk.

Biography

Victor Guallar completed his PhD in collaboration between UAB (Spain) and UC Berkeley (USA) and Postdoctoral studies from Columbia University. He worked as an Assistant Professor at Washington University School of Medicine (USA), he was awarded an ICREA Professor position at the Barcelona Supercomputing Center. He is also the Founder of Nostrum Biodiscovery. He has published more than 100 papers in reputed journals and has been the recipient of prestigious grants like Advanced ERC from the European Union.

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