

XIAO HU

PHD

15 Trinity Court

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SOFTWARE SKILLS

Programming language:

C++, Python, R, Bash shell scripting

Software experiences:

MD simulations, 3D-RISM, MM-PB/GBSA calculations (AMBER package), docking and virtual screening (PLANTS, MOE, Autodock4.0, and Autodock Vina), QM calculations (Gaussian09), SAR and molecular modelling (MOE, VMD, Chimera, and PyMOL), and other software (TAC4.0, Cytoscape, Spartan, and MATLAB), WordPress

LANGUAGES

English (mastery), Chinese (native speaker)

REFERENCES

Prof. Alessandro Contini

Principle Investigator for PhD

Email: alessandro.contini@unimi.it

Dr. Olga Tura Ceide

Supervisor of a PhD project

Email: tura@clinic.ca

Prof. Ian Gould

Supervisor for master's thesis

Email: i.gould@imperial.ac.uk

Prof. Robert. J. Woods

Supervisor for undergraduate thesis

Email: rwoods@ccrc.uga.edu

RESEARCH EXPERIENCES

PhD research projects:

- **Computational analysis of a specific glycolytic enzyme relevant for atherosclerosis therapy, design of allosteric modulators and in vitro testing**
- **Standardisation and assessment of virtual screening protocol with MM-PB/GBSA re-evaluation**
- **Incorporating explicit hydration into virtual screening: Protocol development and protocol optimisation**
- **Industry Intern in Bioinformatics, Biomax Informatics**

AG, Germany

Feb 2016 – May 2019

University of Milan, Italy

University of Barcelona, Spain

Master's research project:

- **Investigation of protein tyrosine phosphatase 1B (PTP1B) allosteric inhibition mechanism using MD simulations**

Oct 2014 – Oct 2015

Institute of Chemical Biology, Imperial College London, UK

WORKING EXPERIENCE

Oct 2020 – present

Computational Chemist

University of Dundee

Dundee, United Kingdom

August 2019 – June 2020

Engineer of Research and Development

Fundacio Clinic Per la Recerca Biomedica

Barcelona, Spain

May 2019 – July 2019

Laboratory Technician in Bioinformatics

Institut d'investigacions Biomèdiques August Pi i Sunyer (IDBAPS)

Barcelona, Spain

EDUCATION

Feb 2016 – May 2019

ITN-European Joint Doctorate in Pharmaceutical Science

University of Milan (Italy)

Hospital Clínic, University of Barcelona (Spain)

Oct 2014 – Oct 2015

Master by research (MRes.) in Chemical Biology

Imperial College London (United Kingdom)

Final result: Distinction (>70%)

Sept 2010 – June 2014

B.Sc. (honours) Biopharmaceutical Chemistry

National University of Ireland, Galway (Ireland)

Final results: 73.16% (First class honours)

POSTER PRESENTATIONS

"Beware of Solute Dielectric Constants in MM-PBSA Calculations", 14th German Conference on Chemoinformatics, Mainz, Germany, 2018

"Docking and Virtual Screening with Flexible Hydration and Potentials in MM-PBSA rescoring", 13th German Conference on Chemoinformatics, Mainz, Germany, 2017

"Flexible Water Docking and Virtual Screening Using PLANTS Combined with Tuned Water Selection", WATOC 2017: 11th Triennial Congress of the World Association of Theoretical and Computational Chemists, Munich, Germany, 2017

"Docking with Flexible Explicit Water Molecules: The Application of WSELECT, A Water Selection Program", 12th German Conference on Chemoinformatics, Fulda, Germany, 2016

"Combining 3D-RISM with hydrophobic characteristic water evaluation: first step preparation for further PLANTS virtual screening with flexible explicit water molecules", eCheminfo 2016 workshop, Milan, Italy, 2016

"Mechanism of Enzymatic Activity Interference from Glycans: MD Simulations of Ligand-bound Complexes of Ribonuclease A/B", Warren Workshop, Galway, Ireland, 2014