

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: Chemistry, Physical Chemistry and Chemical Engineering

Subfield: Chemistry

Title: In silico design of unescapable influenza therapies

ParisTech School: Chimie ParisTech | PSL

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Research group/Lab: CTM / i-CLeHS

Lab location: Chimie Paris Tech, 11 rue Pierre et Marie Curie, F-75005 Paris

Lab/Advisor website: <https://www.quanthic.fr/>

Short description of possible research topics for a PhD:

Influenza is a major Public Health threat. A single anti-influenza drug, oseltamivir, is available in Europe but resistance mutations against this drug can occur. Our goal is to develop anti-influenza drugs with little or no possibility of viral escape. For this purpose, *in silico* work allows us to describe new therapeutic targets that should reduce viral escape and to propose inhibitors potentially clinging to these targets. We have already defined a reusable data processing (DP) pipeline shown opposite.

During this project, the PhD student will participate to the (1) *in silico* design of antiviral targets and (2) drug design of potential inhibitors. Iterative cycles involving bioinformatics and chemoinformatics will allow us to refine both the targets (to consider the maximum of sub-types of influenza viruses) and the chemical structure of the inhibitors.

Required background of the student:

Molecular modeling, computational chemistry or bioinformatics

Representative publications of the group:

1. Perrier, A. *et al.* J. Phys. Chem. B 2019,123, 582-592. DOI: [10.1021/acs.jpcc.8b10767](https://doi.org/10.1021/acs.jpcc.8b10767).
2. Ozeel, V. *et al.* Symmetry 2019, 11(5), 662; DOI:[10.3390/sym11050662](https://doi.org/10.3390/sym11050662).
3. Sharma, A. *et al.* Phys. Chem. Chem. Phys. 2016, 18, 30029-30039. DOI: [10.1039/C6CP05105G](https://doi.org/10.1039/C6CP05105G)

