SCIENCES DU VIVANT
Sciences
Université de Paris

MASTER «*In Silico* Drug Design»

Second Year

OFFER AN INTERNSHIP
year 2021 / 20212

send to Pr Camproux
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Name of the head of laboratory or company:

Evotec AG

Computational Chemistry department

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Name of training supervisors:

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Specialty training : Research X Professional X

a few key words to describe the subject of training :

QSAR, PCA, chemical space, RNA binders

Title of internship:

Study of the chemical space of RNA binders and development of QSAR models to distinguish RNA selective binders from other families of compounds

this subject is a first step towards a thesis: No

Short text describing your project

This work will involve the following tasks:

1. Keep up-to-date with relevant literature on this topic.
2. Compilation of a dataset of RNA selective binders and decoys.

3. Visualization and study of the RNA binders chemical subspace (PCA, tSNE …).
4. Building of high-quality QSAR models to distinguish RNA selective binders.
5. Application of the QSAR models to automatically filter internal/commercial databases of compounds.
6. Present work results at group and department meetings.

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