



6 months internship Chemoinformatics

Title : 3D implementation and validation of Discngine Pharmacophore Graph

Description :

Discngine Pharmacophore Graph is a molecular reduction scheme to simplify complex molecular data to a graph. This reduced graph representation of small molecules allows powerful molecular comparison and scaffold hopping applications of interest during drug optimization processes. Discngine developed the first set of methods for applications on 2D representations of small molecules. We now seek a highly motivated trainee to advance all developed technology to the third dimension.

The candidate will be in charge of

- (i) adapting the existing pharmacophore reduction scheme to 3D molecules,
- (ii) adapting the existing pharmacophore graph matching procedures,
- (iii) developing a novel 3D pharmacophore graph comparison algorithm,
- (iv) validating the previously developed functionalities on publicly available data.

About the company :

Discngine is a Paris based start-up. Ideally situated at Paris Bastille, Discngine provides since 2004 informatics services in knowledge and sample management to pharmaceutical & cosmetics industry customers. We strongly encourage research & development of novel methodologies in the areas of chemoinformatics & bioinformatics for direct industrial application.

Required skills :

The candidate should be self-motivated, highly skilled or proficient in Java programming. He should be familiar with small molecules, chemoinformatics & common molecular interactions. Previous experience in using Pipeline Pilot is a plus.

Salary :

Wages are fixed according to French law for internships + advantages. Discngine is constantly seeking talented people. Outstanding candidates for this position could definitely be considered for a later permanent position.

Duration :

6 months

Contact :

Please send your curriculum & letter of intent to :

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For more information on pharmacophore graph :

<ftp://ftp.discngine.com/collections/docs/Discngine%20Pharmacophore%20Graph.pdf>

About the company :

<http://www.discngine.com>