Recrutement M2 - Edition 2021

Recensement des Projets des Equipes et Plateformes

EQUIPE/PLATEFORME

Intitulé : Machine-learning scoring functions for structure-based virtual screening

Chef(s) d'équipe ou responsable(s) scientifique(s) de plateforme
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SUJET DE MASTER PROPOSE et PI DU SUJET

Titre : Machine-learning scoring functions for structure-based virtual screening

PI du sujet (Nom, Prénom) : BALLESTER, Pedro
HDR X Oui ☐ Non
Etudiants en thèse X Oui ☐ Non
(si oui, préciser le nb):

RESUME DU PROJET

Molecular docking is a family of computational tools frequently used in drug design. Docking aims at predicting whether and how a small molecule binds to a macromolecular target. Classical scoring functions (SFs), based on linear regression, have reached a plateau in their performance to carry out such prediction. By contrast, machine-learning SFs have been widely praised by the degree with which they have outperformed classical SFs at binding affinity prediction. Research on the optimal application of Machine Learning (ML) to the related problem of Structure-Based Virtual Screening (SBVS) is highly promising, but it is still in its infancy.

References

1.Fresnais, L., Ballester, P.J. (2020) "Briefings in Bioinformatics, bbaa095 (jointly with a 2019 M2 student). https://doi.org/10.1093/bib/bbaa095
2. Li, H., Sze, K-H., Lu, G., Ballester, P.J. (2020) WIREs Computational Molecular Science, e1478. https://onlinelibrary.wiley.com/doi/abs/10.1002/wcms.1478
3. Li, H., Sze, K-H., Lu, G., Ballester, P.J. (2020) WIREs Computational Molecular Science, e1467. https://onlinelibrary.wiley.com/doi/10.1002/wcms.1465
4. Hongjian Li, Jiangjun Peng, Yee Leung, Kwong-Sak Leung, Man-Hon Wong, Gang Lu, Ballester, P.J. (2019) Bioinformatics 35, 3989-95. http://dx.doi.org/10.1093/bioinformatics/btz183

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