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## Publications clés

### Année de publication : 2021

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Thomas Barbot, Veronica Beswick, Cédric Montigny, Éric Quiniou, Nadège Jamin and Liliane Mouawad (2021 Feb 4)

**Deciphering the mechanism of inhibition of SERCA1a by sarcolipin using molecular simulations**

*Frontiers in Molecular Biosciences* : 7 : 606254 : [DOI : 10.3389/fmolb.2020.606254](https://doi.org/10.3389/fmolb.2020.606254)

### Année de publication : 2019

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El Hassen Mokrani, Abderrahmane Bensegueni, Ludovic Chaput, Claire Beauvineau, Hanane Djeghim, Liliane Mouawad (2019 May 1)

**Identification of New Potent Acetylcholinesterase Inhibitors Using Virtual Screening and *In Vitro* Approaches.**

*Molecular informatics* : 38 : 1800118 : [DOI : 10.1002/minf.201800118](https://doi.org/10.1002/minf.201800118)

M Schmidt-Cernohorska, I Zhernov, E Steib, M Le Guennec, R Achek, S Borgers, D Demurtas, L Mouawad, Z Lansky, V Hamel, P Guichard (2019 Jan 19)

**Flagellar microtubule doublet assembly *in vitro* reveals a regulatory role of tubulin C-terminal tails.**

*Science (New York, N.Y.)* : 363 : 285-288 : [DOI : 10.1126/science.aav2567](https://doi.org/10.1126/science.aav2567)

### Année de publication : 2017

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Chaput Ludovic, Mouawad Liliane (2017 Jun 12)

**Efficient conformational sampling and weak scoring in docking programs?**

**Strategy of the wisdom of crowds**

*Journal of Cheminformatics* : 9 : 37 : [DOI : 10.1186/s13321-017-0227-x](https://doi.org/10.1186/s13321-017-0227-x)

Mélanie J Domingues, Juan Martinez-Sanz, Laura Papon, Lionel Larue, Liliane Mouawad, Jacky Bonaventure (2017 Mar 9)

**Structure-based mutational analysis of ICAT residues mediating negative regulation of  $\beta$ -catenin co-transcriptional activity.**

*PloS ONE* : 12(3) : e0172603 : [DOI : 10.1371/journal.pone.0172603](https://doi.org/10.1371/journal.pone.0172603)

Année de publication : 2016

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Chaput L., Martinez-Sanz J., Saettel N., Mouawad L. (2016 Oct 17)

**Benchmark of four popular virtual screening programs: construction of the active/decoy dataset remains a major determinant of measured performance**

*Journal of Cheminformatics* : 8:56 : [DOI : 10.1186/s13321-016-0167-x](https://doi.org/10.1186/s13321-016-0167-x)

Chaput L., Martinez-Sanz J., Quiniou E., Rigolet P., Saettel N., Mouawad L. (2016 Jan 18)

**vSDC: a method to improve early recognition in virtual screening when limited experimental resources are available**

*Journal of Cheminformatics* : 8:1 : [DOI : 10.1186/s13321-016-0112-z](https://doi.org/10.1186/s13321-016-0112-z)

Année de publication : 2013

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Eric Quiniou, Paul Guichard, David Perahia, Sergio Marco, Liliane Mouawad (2013 May 7)

**An atomistic view of microtubule stabilization by GTP.**

*Structure (London, England : 1993)* : 21 : 833-843 : [DOI : 10.1016/j.str.2013.03.009](https://doi.org/10.1016/j.str.2013.03.009)

Année de publication : 2009

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Liliane Mouawad, Adriana Isvoran, Eric Quiniou, Constantin T Craescu (2009 Jan 22)

**What determines the degree of compactness of a calcium-binding protein?**

*The FEBS journal* : 276 : 1082-1093 : [DOI : 10.1111/j.1742-4658.2008.06851.x](https://doi.org/10.1111/j.1742-4658.2008.06851.x)