

2nd Women in Bioinformatics & Data Science LA Conference

Fostering collaboration among women

**VIRTUAL MEETING
FROM 22ND TO 24TH
SEPTEMBER 2021**



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Latin American Congress of Women in Bioinformatics and Data Science
2nd Latin American Congress of Women in Bioinformatics and Data Science: Abstract
Book / compilado por Women in Bioinformatics and Data Science. - 1a ed . - Ciudad
Autónoma de Buenos Aires.

Libro digital, PDF
Archivo Digital: descarga y online

1. Bioingeniería. 2. Biología. 3. Aplicaciones Informáticas.

Este libro es una obra colectiva basada en los resúmenes enviados por los autores y presentados en el Segundo Congreso Latinoamericano de Mujeres en Bioinformática y Ciencia de Datos, realizado los días 22 al 24 de septiembre de 2021.

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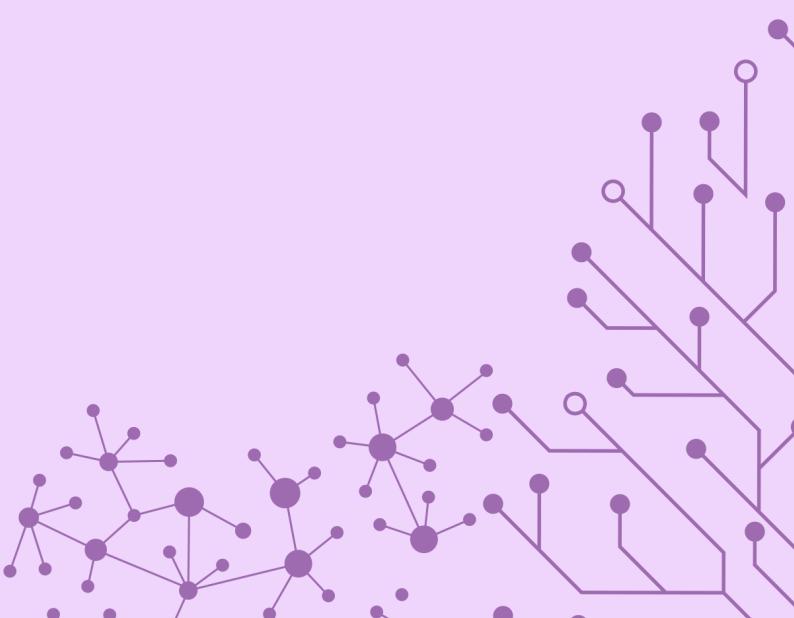
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GENERAL INFORMATION



2nd Women in Bioinformatics & Data Science LA Conference

The 2nd Women in Bioinformatics & Data Science LA Conference is a free event open to the entire community, which brings together professionals, students, academics, businesswomen, public officials, and hobbyists.

The main purpose of the meeting is to promote and make visible the research carried out by women and dissidents in the field of Bioinformatics and Data Science. This congress focuses on the areas of systems biology, omics technologies, artificial intelligence, machine learning, data science, data mining, and high-performance computing with biological applications in public and private sectors.



Targeting Protein Pockets with Halogen Bonds

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Halogen bonds (X-bonds) are directional interactions involving an attractive force between an electrophilic region on the halogen and interaction partners with nucleophilic properties, X-bond has gained recognition as an atypical molecular interaction useful in modeling halogens computationally to develop new pharmaceutical drugs. X-bonds in protein-ligand complexes are surrounded by residues that conform the "X-bond environment". Since sigma-hole formation in X-bonds is a consequence of the anisotropy of the charge density distribution around the halogen, protein residues that surround the halogen atom might perturb its charge distribution and X-bond strength. In this work we proposed a protocol to study the feasibility of protein pockets to form X-bond with halogenated ligands, based on the environment. First, a structural survey of X-bonded protein-ligand complexes in public databases was performed to get a description of the "X-bond environment" based on the charge density, with help of the Quantum Theory of Atoms in Molecules (QTAIM). In the second step, the "X-bond environment" is used as a reference system to judge the propensity of protein pockets to host an X-bond. To test the protocol, we generated poses in which chlorobenzene is forming: (a) the known X-bond and (b) a different X-bond in a nearby protein sub-pocket with no structural evidence about its existence. We termed this last as "decoy X-bond". Fifty poses were generated with the docking algorithm for both known and decoys X-bonds. Charge density-based X-bond environments for the docking poses were estimated by mapping the chloro protein neighborhood, into the X-bond environment pre-computed on the reference system. The protocol was able to prioritize docking poses that reproduce the actual X-bond in crystal structures based on their X-bond environments, since "real X-bonds" have stronger X-bond environments than decoy X-bonds, as expected. The results suggest that X-bond formation might require a proper protein environment to be established.

Keywords: halogen bond, drug design, X-bond environment, QTAIM.