Angel J. Ruiz-Moreno

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AngelRuizMoreno

LENGUAJES

Spanish (Native) English (C1)

SOFTWARE

- **Operative Systems** (Advanced): MacOs, Linux, and Windows.
- **Programing**: Python (Proficient), R (intermediate).
- **Data Sciences, Biostatistics,** and **Machine Learning**: Pandas, NumPy, SciPy, SciKit-Learn, Matplotlib, Jupyter, GraphPad Prism.
- **Drug Design, Chem/Bioinformatics**: RDKit, OpenBabel, PyMol, BioPython, MDAnalysis, Modeller, ChemAxon, Schrodinger Suite, CSD Suite, ChemDraw, Reaxis.

EDUCATION

Ph.D. in Drug Design
09/2017- 12/2021
University of Groningen (UG). The Netherlands.

Ph.D. in Biomedical Sciences
09/2017- 01/2022
Universidad Nacional Autónoma de México (UNAM). Mexico.

M.Sc. Biochemical Sciences
09/2015 – 05/2017
Instituto Politécnico Nacional (IPN). Mexico. 100/100

B.Sc.Pharmaceutical chemistry
08/2009 – 03/2015
Universidad Nacional Autónoma de México (UNAM). Mexico. 80/100

HOBBIES

Reading, writing, photography, music lover.

EXPERIENCE

Postdoctoral Fellowship 01/2022 – PRESENT

Place: Genetics Department, UMCG.
Role: Cheminformatics and metabolomics in gut microbiome metabolism
Supervisor: Prof. dr. Jingyuan Fu.

Ph.D. in Drug Design 09/2017- 12/2021

Place: Dömling's lab, Drug Design Department, UG.
Role: Ligand/Structure-based Drug Design using computational methodologies and Multicomponent Reaction (MCR) synthesis.

- Development and implementation of computational methodologies for combinatorial computational chemistry, cheminformatics, and drug design such as molecular docking, small molecule design, pharmacophore modeling, and molecular dynamics simulations.
- Structure-based search and analysis of interesting targets using crystallographic data and protein modeling. Development of bioinformatic workflows for protein structures and annotations. Usage of unsupervised machine learning algorithms for the classification of small molecules.
- Implementation of explicit solvent molecular dynamics for the analysis of ligand-protein interactions, free energy calculations and protein conformational changes determination.
- Organic synthesis of small molecules using MCR routes. Structure determination using NMR and purification by chromatography.

Results: Several publications reporting the design or repurposing of novel compounds as therapeutics using computational methodologies. Design and cheminformatic analysis of novel MCR-based compound libraries.
Supervisor: Prof. dr. Alexander Dömling.

Ph.D. in Biomedical Sciences 09/2017- 01/2021

Place: Molecular Pharmacology Lab, UNAM.
Role: Computer-aided design and Pre-clinical evaluation of compounds as potential treatments for cancer.

- Virtual screening and cheminformatic analysis of massive compound libraries for identification and repurposing of novel compound as treatments for breast cancer.
- Bioinformatics workflows for public servers containing genomic and phenotypic annotations as tools for the establishment of interesting targets and cell line selection as models for cancer research.

Results: Publications and patents for new the therapeutic usage of known drugs as cancer treatments. Development of computational/bioinformatic workflows currently implemented in the group for drug repurposing and cell line selection for compound testing.
Supervisor: Prof. dr. Marco A. Velasco-Velázquez.

M.Sc. Biochemical Sciences 09/2015 – 05/2017

Place: Development and Bioprocesses Research Unit (UDIBI) and Molecular Pharmacology Lab, IPN/UNAM.

- Ligand-binding analysis using experimental methodologies as ELISA, flow cytometry and ITC.
- Pre-clinical evaluation of small molecules in eukaryotic cells, analyzing *in vitro* cytotoxicity, mamosphere formation and cell adhesion assays, PCR and qRT-PCR, western blotting, and animal models.

Results: Training in experimental immunopharmacology and molecular biology techniques for the evaluation of small molecules as potential inhibitors of novel targets.
Supervisor: Prof. dr. Marco A. Velasco-Velázquez.