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Intereses de la investigación

Los receptores a coplados a proteína G (GPCRs) representan una de las mas grandes familias del genoma humano y blancos de interés farmacológico. Mi investigación está enfocada en el estudio de la estructura y funcionamiento de estas proteínas de membrana por medio de métodos *in Silico* tales como simulaciones de dinámica molecular, estudios de acoplamiento molecular, además del uso de técnicas experimentales, tales como bioquímicas y farmacológicas para su caracterización.

Resultado de la investigación

In Silico Screening of Drugs That Target Different Forms of E Protein for Potential Treatment of COVID-19

Ramírez Salinas, G. L., López Rincón, A., García Machorro, J., Correa Basurto, J. & Martínez Archundia, M., feb. 2023, En: *Pharmaceuticals*. 16, 2, 296.

The Advantage of Using Immunoinformatic Tools on Vaccine Design and Development for Coronavirus

García-Machorro, J., Ramírez-Salinas, G. L., Martínez-Archundia, M. & Correa-Basurto, J., nov. 2022, En: *Vaccines*. 10, 11, 1844.

The Advantage of Using Immunoinformatic Tools on Vaccine Design and Development for Coronavirus

Martínez Archundia, M. T., García Machorro, J., Gema, L. R. S. & Correa Basurto, J., 28 oct. 2022, En: *Vaccines*. 10, 11, p. 1844 1890 p., 11.

Unveiling the G4-PAMAM capacity to bind and protect Ang-(1-7) bioactive peptide by molecular dynamics simulations

Chi, L. A., Asgharpour, S., Correa-Basurto, J., Bandala, C. R. & Martínez-Archundia, M., sep. 2022, En: *Journal of Computer-Aided Molecular Design*. 36, 9, p. 653-675 23 p.

The β_2 -Subunit (AMOG) of Human Na^+ , K^+ -ATPase Is a Homophilic Adhesion Molecule

Roldán, M. L., Ramírez-Salinas, G. L., Martínez-Archundia, M., Cuellar-Perez, F., Vilchis-Nestor, C. A., Cancino-Díaz, J. C. & Shoshani, L., jul. 2022, En: *International Journal of Molecular Sciences*. 23, 14, 7753.

Searching Epitope-Based Vaccines Using Bioinformatics Studies

Martínez-Archundia, M., Ramírez-Salinas, G. L., García-Machorro, J. & Correa-Basurto, J., 2022, *Methods in Molecular Biology*. Humana Press Inc., p. 471-479 9 p. (Methods in Molecular Biology; vol. 2412).

Design, Docking Simulations, Synthesis, and *in vitro* and *in vivo* Behavioral Assessment of m-Aminobenzoic Acid Analogues as GABA-AT Inhibitors

Altamirano-Espino, J. A., Córdova-Moreno, R., Andrade-Jorge, E., Martínez-Archundia, M., García-Machorro, J. & Trujillo-Ferrara, J. G., 14 sep. 2021, En: *ChemistrySelect*. 6, 34, p. 8959-8970 12 p.

Liver disorders in COVID-19, nutritional approaches and the use of phytochemicals

Vargas-Mendoza, N., García-Machorro, J., Angeles-Valencia, M., Martínez-Archundia, M., Madrigal-Santillán, E. O., Morales-González, Á., Anguiano-Robledo, L. & Morales-González, J. A., 14 sep. 2021, En: *World Journal of Gastroenterology*. 27, 34, p. 5630-5665 36 p.

Drug repositioning to target NSP15 protein on SARS-CoV-2 as possible COVID-19 treatment

Sixto-López, Y. & Martínez-Archundia, M., 15 may. 2021, En: *Journal of Computational Chemistry*. 42, 13, p. 897-907 11 p.

Current advances in mass spectrometry-based proteomic studies on childhood acute lymphoblastic leukemia
Bermudez-Lugo, J. A., Martínez-Archundia, M., Correa-Basurto, J. & Zapata-Tarres, M. M., 2021, En: Current Topics in Peptide and Protein Research. 22, p. 1-15 15 p.

Repositioning of ligands that target the spike glycoprotein as potential drugs for sars-cov-2 in an in silico study
Ramírez-Salinas, G. L., Martínez-Archundia, M., Correa-Basurto, J. & García-Machorro, J., 1 dic. 2020, En: Molecules. 25, 23, 5615.

Acetylcholinesterase Inhibition (Potential Anti-Alzheimer Effects) by Aminobenzoic Acid Derivatives: Synthesis, in Vitro and in Silico Evaluation
Altamirano-Espino, J. A., Sánchez-Labastida, L. A., Martínez-Archundia, M., Andrade-Jorge, E. & Trujillo-Ferrara, J. G., 30 nov. 2020, En: ChemistrySelect. 5, 44, p. 14177-14182 6 p.

Molecular dynamics simulations reveal structural differences among wild-type NPC1 protein and its mutant forms
Martínez-Archundia, M., Hernández Mojica, T. G., Correa-Basurto, J., Montaño, S. & Camacho-Molina, A., 12 ago. 2020, En: Journal of Biomolecular Structure and Dynamics. 38, 12, p. 3527-3532 6 p.

Machine learning-based ensemble recursive feature selection of circulating miRNAs for cancer tumor classification
López-Rincon, A., Mendoza-Maldonado, L., Martínez-Archundia, M., Schönthuth, A., Kraneveld, A. D., Garssen, J. & Tonda, A., jul. 2020, En: Cancers. 12, 7, p. 1-27 27 p., 1785.

Immunoinformatics study to search epitopes of spike glycoprotein from SARS-CoV-2 as potential vaccine
Martínez-Archundia, M., Correa Basurto, J., García Machorro, J. & Gema, L. R. S., 25 jun. 2020, En: Journal of Biomolecular Structure and Dynamics. p. 1-14 p.

Identification of two arylimides as cholinesterase inhibitors and testing of propranolol addition on impaired rat memory
Ciprés-Flores, F. J., Farfán-García, E. D., Andrade-Jorge, E., Cuevas-Hernández, R. I., Tamay-Cach, F., Martínez-Archundia, M., Trujillo-Ferrara, J. G. & Soriano-Ursúa, M. A., 1 abr. 2020, En: Drug Development Research. 81, 2, p. 256-266 11 p.

Studying the collective motions of the adenosine A2A receptor as a result of ligand binding using principal component analysis
Martínez-Archundia, M., Correa-Basurto, J., Montaño, S. & Rosas-Trigueros, J. L., 12 dic. 2019, En: Journal of Biomolecular Structure and Dynamics. 37, 18, p. 4685-4700 16 p.

Automatic discovery of 100-miRNA signature for cancer classification using ensemble feature selection
López-Rincon, A., Martínez-Archundia, M., Martínez-Ruiz, G. U., Schoenhuth, A. & Tonda, A., 18 sep. 2019, En: BMC Bioinformatics. 20, 1, 480.

A model for the homotypic interaction between Na^+, K^+ -ATPase $\beta 1$ subunits reveals the role of extracellular residues 221-229 in its Ig-like domain
Páez, O., Martínez-Archundia, M., Villegas-Sepúlveda, N., Roldan, M. L., Correa-Basurto, J. & Shoshani, L., 2 sep. 2019, En: International Journal of Molecular Sciences. 20, 18, 4538.

Docking analysis provide structural insights to design novel ligands that target PKM2 and HDC8 with potential use for cancer therapy
Martínez-Archundia, M., Colin-Astudillo, B., Gómez-Hernández, L., Abarca-Rojano, E. & Correa-Basurto, J., 13 jun. 2019, En: Molecular Simulation. 45, 9, p. 685-693 9 p.

Oenothera rosea L'Hér. ex Ait attenuates acute colonic inflammation in TNBS-induced colitis model in rats: in vivo and in silico myeloperoxidase role
Calva-Candelaria, N., Meléndez-Camargo, M. E., Montellano-Rosales, H., Estrada-Pérez, A. R., Rosales-Hernández, M. C., Fragoso-Vázquez, M. J., Martínez-Archundia, M., Correa-Basurto, J. & Márquez-Flores, Y. K., dic. 2018, En: Biomedicine and Pharmacotherapy. 108, p. 852-864 13 p.

Computational study of the binding modes of diverse DPN analogues on estrogen receptors (ER) and the biological evaluation of a new potential antiestrogenic ligand

Martínez-Archundia, M., García-Vázquez, J. B., Colín-Astudillo, B., Bello, M., Prestegui-Martel, B., Chavez-Blanco, A., Dueñas-González, A., Fragoso-Vázquez, M. J., Mendieta-Wejebe, J., Abarca-Rojano, E., Ordaz-Rosado, D., García-Becerra, R., Castillo-Bautista, D. & Correa Basurto, J., 2018, En: Anti-Cancer Agents in Medicinal Chemistry. 18, 11, p. 1508-1520 13 p.

Design of drugs by filtering through ADMET, physicochemical and ligand-target flexibility properties

Martínez-Archundia, M., Bello, M. & Correa-Basurto, J., 2018, *Methods in Molecular Biology*. Humana Press Inc., p. 403-416 14 p. (Methods in Molecular Biology; vol. 1824).

Selection of a GPER1 ligand via ligand-based virtual screening coupled to molecular dynamics simulations and its anti-proliferative effects on breast cancer cells

Martínez-Muñoz, A., Prestegui-Martel, B., Méndez-Luna, D., Fragoso-Vázquez, M. J., García-Sánchez, J. R., Bello, M., Martínez-Archundia, M., Chávez-Blanco, A., Dueñas-González, A., Mendoza-Lujambio, I., Trujillo-Ferrara, J. & Correa-Basurto, J., 2018, En: Anti-Cancer Agents in Medicinal Chemistry. 18, 11, p. 1629-1638 10 p.

Ligand recognition properties of the vasopressin V2 receptor studied under QSAR and molecular modeling strategies

Martínez-Archundia, M., Colín-Astudillo, B., Moreno-Vargas, L. M., Ramírez-Galicia, G., Garduño-Juárez, R., Deeb, O., Contreras-Romo, M. C., Quintanar-Stephano, A., Abarca-Rojano, E. & Correa-Basurto, J., nov. 2017, En: Chemical Biology and Drug Design. 90, 5, p. 840-853 14 p.

Study of new interactions of glitazone's stereoisomers and the endogenous ligand 15d-PGJ2 on six different PPAR gamma proteins

Álvarez-Almazán, S., Bello, M., Tamay-Cach, F., Martínez-Archundia, M., Alemán-González-Duhart, D., Correa-Basurto, J. & Mendieta-Wejebe, J. E., 15 oct. 2017, En: Biochemical Pharmacology. 142, p. 168-193 26 p.

Searching the conformational complexity and binding properties of HDAC6 through docking and molecular dynamic simulations

Sixto-López, Y., Bello, M., Rodríguez-Fonseca, R. A., Rosales-Hernández, M. C., Martínez-Archundia, M., Gómez-Vidal, J. A. & Correa-Basurto, J., 3 oct. 2017, En: Journal of Biomolecular Structure and Dynamics. 35, 13, p. 2794-2814 21 p.

Design, synthesis and biological evaluation of a phenyl butyric acid derivative, N-(4-chlorophenyl)-4-phenylbutanamide: A HDAC6 inhibitor with anti-proliferative activity on cervix cancer and leukemia cells

Alberto, R. F. R., Yudibeth, S. L., Jonathan, F. V. M., Raúl, F. M., Cristina, C. P. L., Ismael, V. M., Cecilia, R. H. M., Bello, M., Martínez-Archundia, M., Guadalupe, T. F. J., Elvia, B. M. & José, C. B., 2017, En: Anti-Cancer Agents in Medicinal Chemistry. 17, 10, p. 1441-1454 14 p.

Is there something else besides the proapoptotic AVPI-segment in the Smac/DIABLO protein?

Victoria-Acosta, G., Martínez-Archundia, M., Moreno-Vargas, L., Meléndez-Zajgla, J. & Martínez-Ruiz, G. U., 1 nov. 2016, En: Boletín Medico del Hospital Infantil de Mexico. 73, 6, p. 365-371 7 p.

Current tools and methods in Molecular Dynamics (MD) simulations for drug design

Hernández-Rodríguez, M., Rosales-Hernández, M. C., Mendieta-Wejebe, J. E., Martínez-Archundia, M. & Basurto, J. C., 1 oct. 2016, En: Current Medicinal Chemistry. 23, 34, p. 3909-3924 16 p.

Deciphering the GPER/GPR30-agonist and antagonists interactions using molecular modeling studies, molecular dynamics, and docking simulations

Méndez-Luna, D., Martínez-Archundia, M., Maroun, R. C., Ceballos-Reyes, G., Fragoso-Vázquez, M. J., González-Juárez, D. E. & Correa-Basurto, J., 3 oct. 2015, En: Journal of Biomolecular Structure and Dynamics. 33, 10, p. 2161-2172 12 p.

Identification of the antiepileptic racetam binding site in the synaptic vesicle protein 2A by molecular dynamics and docking simulations

Correa-Basurto, J., Cuevas-Hernández, R. I., Phillips-Farfán, B. V., Martínez-Archundia, M., Romo-Mancillas, A., Ramírez-Salinas, G. L., Pérez-González, Ó. A., Trujillo-Ferrara, J. & Mendoza-Torreblanca, J. G., 10 abr. 2015, En:

Theoretical studies, synthesis, and biological activity of 1-[(4-methylphenyl)sulfonyl]-5-oxo-2,3,4,5-tetrahydro-1H-1-benzazepine-4- carbonitrile (C9) as a non-peptide antagonist of the arginine vasopressin V1a and V2 receptors

Contreras-Romo, M. C., Correa-Basurto, J., Padilla-Martínez, I., Martínez-Archundia, M., Martínez-Ramos, F., Ślusarz, M. J., López-Pérez, G. & Quintanar-Stephano, A., mar. 2014, En: Medicinal Chemistry Research. 23, 3, p. 1581-1590 10 p.

Exploring the ligand recognition properties of the human vasopressin V1a receptor using QSAR and molecular modeling studies

Contreras-Romo, M. C., Martínez-Archundia, M., Deeb, O., Ślusarz, M. J., Ramírez-Salinas, G., Garduño-Juárez, R., Quintanar-Stephano, A., Ramírez-Galicia, G. & Correa-Basurto, J., feb. 2014, En: Chemical Biology and Drug Design. 83, 2, p. 207-223 17 p.

Molecular dynamics simulations reveal initial structural and dynamic features for the A₂AR as a result of ligand binding

Martínez-Archundia, M. & Correa-Basurto, J., 2014, En: Molecular Simulation. 40, 13, p. 996-1014 19 p.

Automated docking for novel drug discovery

Bello, M., Martínez-Archundia, M. & Correa-Basurto, J., jul. 2013, En: Expert Opinion on Drug Discovery. 8, 7, p. 821-834 14 p.

Morphological changes, chitinolytic enzymes and hydrophobin-like proteins as responses of Lecanicillium lecanii during growth with hydrocarbon

Rocha-Pino, Z., Del Carmen Marín-Cervantes, M., Martínez-Archundia, M., Soriano-Blancas, E., Revah, S. & Shirai, K., may. 2013, En: Bioprocess and Biosystems Engineering. 36, 5, p. 531-539 9 p.

Molecular modeling of the M3 acetylcholine muscarinic receptor and its binding site

Martinez-Archundia, M., Cordomi, A., Garriga, P. & Perez, J. J., 2012, En: Journal of Biomedicine and Biotechnology. 2012, 789741.

Salt effects on the conformational stability of the visual G-protein-coupled receptor rhodopsin

Reyes-Alcaraz, A., Martínez-Archundia, M., Ramon, E. & Garriga, P., 7 dic. 2011, En: Biophysical Journal. 101, 11, p. 2798-2806 9 p.