Name	Last name	Affiliation	Poster Title	Poster ID	Category
Shubham	Chatterjee	The University of Texas at Dallas	Impact of an Ionic Liquid Solution on Horseradish Peroxidase Activity	Comp001	#LatinXChemComp
Nicolas Ignacio	Neuman	CONICET	Computational studies on Corroles and Metallocorroles	Comp002	#LatinXChemComp
Luis Daniel	Goyzueta Mamani	Universidad Católica de Santa María	Targeting Leishmania infantum Mannosyl-oligosaccharide glucosidase with natural products: potential pH-dependent inhibition explored through CADD	Comp003	#LatinXChemComp
Rafael	Souza Mattos	Aix-Marseille Université	Quantum dynamics from Classical Trajectories	Comp004	#LatinXChemComp
Jose Pablo	Rodríguez-Zúñiga	Universidad de Costa Rica	UnravelingThe Encrypted Lipophilicity Of Disulfide Bridges In The Molecular Architecture Of Peptides: Bioactivity Of Antimicrobial Peptides	Comp005	#LatinXChemComp
José A.	Alcalá González	Universidad de Carabobo	Aggregation of fatty acids in the aqueous phase and its application in the solubilization of biomolecules through molecular simulations	Comp006	#LatinXChemComp
Diana Marlen	Castañeda Bagatella	New Jersey Institute of Technology	DFT investigations of the enantioselective phase-transfer-catalyzed aza-Michael cyclization of ureas	Comp007	#LatinXChemComp
Valentina	Sierra Jimenez	Washington State University	Biochar Data into Structure: A Methodology for Generating Large-Scale Atomistic Representations	Comp008	#LatinXChemComp
Shanti Kinari	Castillo Avila	UNAM	CADMA-CHEM: Un protocolo computacional para el estudio de fármacos neuroprotectores.	Comp009	#LatinXChemComp
Sakshi	Nain	Institute of Nano Science and Technology	Spin-Phonon Coupling and Magnetic Anisotropy in Sandwiched Single Molecule Magnets	Comp010	#LatinXChemComp
Fernando Ivàn	Molina Herrera	Universidad de guanajuato	Aplicación de la Mecánica Computacional de Fluidos en la Optimización de Sistemas de Aireación de Granos	Comp011	#LatinXChemComp
Antonio Miguel	Bosch Fernandez	Universidad Autonoma de Madrid	Adsorption-Driven Deformation and Footprints of the RBD Proteins in SARS-CoV-2 Variants on Biological and Inanimate Surfaces	Comp012	#LatinXChemComp
Carlos Andrés	Castillo-Orellana	Universidad de Concepción	Non-bonded force field parameters derived from Atom-In-Molecules approaches reproduce interactions in proteins from first principles calculations	Comp013	#LatinXChemComp
Francisco	Villanueva-Mejía	TecNM/ITPA	ANTIFUNGAL ALLIODORIN COMPOUND STUDY VIA MOLECULAR DOCKING	Comp014	#LatinXChemComp
Gabriel	da Hora	University of Utah	Deciphering Lasso Peptide Folding: Merging Chemical Intuition and Machine Learning	Comp015	#LatinXChemComp
Marcia	Castillo	Universidad de los Andes	Machine Learning Applied to Drug Discovery for the Treatment of Colorectal Cancer	Comp016	#LatinXChemComp
Miguel	Gallegos	University of Oviedo	Decoding Molecular Energies: Integrating IQA and Machine Learning	Comp017	#LatinXChemComp
Nelson	Barrios	North Carolina State University	Decarbonizing the Energy-Intensive Drying of Cellulosics: Exploring Bound-Water Removal through Computer Simulations	Comp018	#LatinXChemComp
Jose Antonio	Sandoval Mendoza	Universidad de Guanajuato	Lawesson and Woollins reagents: Elimination instead of substitution.	Comp019	#LatinXChemComp
Manuel Alejandro	Treto Suárez	Universidad Autónoma de Chile	Quantum-mechanical study of a MO2 (cyclam)+ complexes series with M= Mn, Tc, Re	Comp020	#LatinXChemComp
Emilio	Piña Betancourt	CINVESTAV Unidad Mérida	Could oxalic acid be present in interstellar space? and would we be able to detect it? An exploration of the chemical space of the isomers of C2H2O4	Comp021	#LatinXChemComp
Hassan	Khartabil	University of Reims Champagne-Ardenne - Reims Institute of Molecular Chemistry (UMR CNRS 7312)	IGMPlot: A More Comprehensive Toolkit for Better Understanding the Structure and Reactivity of Complex Chemical Systems	Comp022	#LatinXChemComp
Alma	Barragán Labastida	Universidad Autónoma del Estado de Morelos	Optimizing baclofen: a Computer Aided Drug Design of novel GABAB receptor agonists.	Comp023	#LatinXChemComp
Estefany	Bello Vargas	Universidad Autónoma del Estado de Morelos	A Computational Method for the Binding Mode Prediction of COX1 and COX2 Inhibitors: Analyzing the Union of Coxibs, Oxicams, Propionic and Acetic Acids	Comp024	#LatinXChemComp
Farzin	Sohraby	TU Berlin	Characterization of the bottlenecks and pathways for inhibitor dissociation from [NiFe] hydrogenase	Comp025	#LatinXChemComp
Peter Ludwig	Rodríguez-Kessler	Centro de Investigaciones en Optica A. C.	Structures of Ni-doped Bn (n= 1-13) clusters: A computational study	Comp026	#LatinXChemComp
Itzel Montserrat	Mercado Sánchez	Universidad de Guanajuato	Evaluación de doxorrubicina, β-lapachona y sus análogos como agentes anticancerígenos, un estudio biológico y computacional	Comp027	#LatinXChemComp
Soumya Ranjan	Dash	CSIR- National Chemical Laboratory, Pune, India	Going where Experimentalists Fear to Tread: Computational Chemistry to the Rescue in Understanding XeO3 Chemistry	Comp028	#LatinXChemComp
Ajeet Kumar	Singh	Institute of Chemical Technology Mumbai-IOC Odisha Campus Bhubaneswar India	A DFT Study on Nickel-Based Water Oxidation Catalysis and Identification of Reactivity Descriptor to Design Novel Catalysts	Comp029	#LatinXChemComp
Williams Mesías	García Argote	Andres Bello University	Aromatic Germanium Clusters: Assembly and Persistence of M6Ge5 and M12Ge10 (M = Li-Rb) Units.	Comp030	#LatinXChemComp
Cristian Abraham	Medina Jiménez	Universidad de Guanajuato - División de Ingeniería Campus Irapuato Salamanca	Predicción de propiedades ópticas NO-lineales a partir de la DTF y el Machine Learning	Comp031	#LatinXChemComp
Sasha José Agustín	Gazzari Jara	Pontificia Universidad Católica de Chile	ESTUDIO TEÓRICO DE CARBENOIDES METÁLICOS DE Cu(I), Y SU ROL EN REACCIONES DE INSERCIÓN C−H	Comp032	#LatinXChemComp
Javier Emilio	Alfonso Ramos	Chimie ParisTech - PSL	Repurposing quantum chemical descriptor datasets for on-the-fly generation of informative reaction representations.	Comp033	#LatinXChemComp
Santiago Jr	Bolivar Avila	Universidad Nacional de Rosario	Identification of a new natural Argentine inhibitor for KRAS G12C through molecular modeling and DFT calculations.	Comp034	#LatinXChemComp
Damián Alberto	Delgado Montiel	Centro de Investigación de Materiales Avanzados S.C.	ESTUDIO TEÓRICO SOBRE LAS PROPIEDADES ÓPTICAS Y ELECTRÓNICAS DE COLORANTES DERIVADOS DE TRIFENILAMINA Y FENIL PARA SU USO EN DSSC.	Comp035	#LatinXChemComp
Sindy Julieth	Rodríguez Sotelo	Ben-Gurion University of the Negev	Can Heavy-Atom Tunneling Determine the Stability of Tricyclic Benzene Isomers?	Comp036	#LatinXChemComp
Kenneth	Lopez Perez	University of Florida	BitBIRCH: Efficient molecular clustering algorithm	Comp037	#LatinXChemComp
Milton Nahúm	Márquez Zárate	Benemérita Universidad Autónoma de Puebla	Implementación de herramientas bioinformáticas para el estudio de 2,4-dinitrofenilhidrazonas frente a biomoléculas con actividad terapéutica	Comp038	#LatinXChemComp

Juan Julián	Santoyo Flores	Ben Gurion University of the Negev	Heavy Atom Quantum Tunnelling in N-Heterocyclic Pentalenes	Comp039	#LatinXChemComp
Pamella Cristiny	Carneiro da Silva	Universidade Estadual de Campinas (UNICAMP)	Solvation effects of choline-derived Ionic Liquids on Plasmodium falciparum AMA1 protein	Comp040	#LatinXChemComp
Eduardo	Mayo Yanes	Technion - Israel Institute of Technology	Hetero-Polycyclic Aromatic Systems: a data-driven analysis	Comp041	#LatinXChemComp
Lisset	Noriega de los Santos	CINVESTAV-Mérida	Reveling the unlikely: an exploration of Ethane-1,1,1-triol and its structural isomers	Comp042	#LatinXChemComp
Maria Elane	Soares da Cunha	Universidade Estadual do Piauí	ESTUDO DE DOCKING MOLECULAR E DFT DE CONSTITUINTES DA CROTON HELIOTROPIIFOLIUS KUNTH COM POTENCIAL AÇÃO ANTICONVULSIVANTE	Comp043	#LatinXChemComp
Aura Ximena	Gómez Heredia	Cinvestav	Implementación de la teoría RRKM en Eyringpy para el cálculo de la constante de velocidad de reacciones unimoleculares	Comp044	#LatinXChemComp
Raúl Rodolfo	Flores Mena	UNIVERSIDAD AUTÓNOMA DE CHIHUAHUA	Electronic properties of hole-transporting materials based on heterocyclic derivatives	Comp045	#LatinXChemComp
José G.	Parra	Universidad de Carabobo	Exploring the influence of charge distribution of hydrophilic headgroup on interfacial properties of the vacuum/SDS/water system	Comp046	#LatinXChemComp
Adalid	Armenta	CIMAV	Theoretical Evaluation of Beryllium-Coordinated Graphitic Carbon Nitride for Effective Metformin Capture	Comp047	#LatinXChemComp
Félix	Reboiro Sáez	Universidad de La Rioja	A computational and topological study of Au(I)···Ir(I) interactions in cationic models	Comp048	#LatinXChemComp
Carlos Iván	Oliva López	Universidad Veracruzana	Theoretical study of interactions between polycyclic aromatic compounds and deep eutectic solvents	Comp049	#LatinXChemComp
Diego	Román	Universidad Veracruzana	Computational study of solvents on the extraction of biofuel compounds found in biomass	Comp050	#LatinXChemComp
Luis Ignacio	Perea-Ramírez	Instituto de Química Aplicada	Chemical reactivity of sulfur compounds present in crude oil: A CDFT and ML approach	Comp051	#LatinXChemComp
Dumer Stiven	Sacanambo y Papamija	Universidad Andrés Bello	Searching Planar Tetracoordinate Atoms in Aromatic Rings with Group 13-15 Atoms	Comp052	#LatinXChemComp
Bruno	Bercini de Araújo	UFRGS	Photo-deactivation process of low-lying excited states of Isothiazolinones, a non-adiabatic dynamics investigation	Comp053	#LatinXChemComp
José G.	Parra	Universidad de Carabobo, Facultad Experimental de Ciencias y Tecnología, Dpto. de Química, Lab. SiMolQuimEx	Exploring the adsorption of a model humic acid on cristobalite with different surface charge densities	Comp054	#LatinXChemComp
Alejandro	Castro Méndez	Benemérita Universidad Autónoma de Puebla	Analisis estadístico bioinformático de Di-metilhidrazonas frente a biomoléculas	Comp055	#LatinXChemComp
Laura Milena	Pedraza González	University of Pisa	How the pH Controls Photoprotection in the Light-Harvesting Complex of Mosses	Comp056	#LatinXChemComp
Jeremy M	Carr	Central Alabama Community College	Evidence of H-Bonding in the CF3•••H-N(sp2) Motif Using Stewart's PM6-ORG Hamiltonian	Comp057	#LatinXChemComp
Stephany	Ortega Alarcon	Universidad Tecnológica de Pereira	Obtaining coprinol scaffolds by virtual screening for activity against tyrosinase enzyme	Comp058	#LatinXChemComp
Maurizio Alejandro	Pantoja Hernández	Universidad Veracruzana	Theoretical study of the oxidative desulfurization with new perturbed chemical reactivity descriptors	Comp059	#LatinXChemComp
Brenda	Manzanilla Viveros	Universidad de Zaragoza	AQME: Automating Computational Chemistry Protocols and Descriptor Generation for Machine Learning Models	Comp060	#LatinXChemComp
Surajit	Das	Research Scholar	Machine Learning Prediction of NMR Chemical Shifts Using Discrete Representation	Comp061	#LatinXChemComp
Atreyee	Majumdar	Tata Institute of Fundamental Research Hyderabad, India	Resilience of Hund's rule in the chemical space of small organic molecules	Comp062	#LatinXChemComp
yeison felipe	rodriguez lopez	Universidad de pamplona	In-Silico Evaluation of Gas-Phase Bimolecular Reactions in the Interstellar Medium: A DFT and Kinetic Study	Comp063	#LatinXChemComp
Darien Isaac	Martínez-Valencia	Universidad de Guanajuato	Interacción entre iluros útiles en la reacción de polihomologación	Comp064	#LatinXChemComp
Julián	Hernández Herrera	Universidad Santiago de Cali	In silico study of potential inhibitors of Pseudomonas aeruginosa aminoaldehyde dehydrogenase enzyme PauC	Comp065	#LatinXChemComp
Xhuu Naxhi Huini	Medina Toledo	Universidad Veracruzana	THEORETICAL STUDY OF INTERACTIONS BETWEEN QUERCETIN AND A NATURAL DEEP EUTECTIC SOLVENT	Comp066	#LatinXChemComp
Mariano	Rodriguez	Conjunto Centro de Investigación de Química Sustentable	Formación del sigma hole en compuestos di-halógenos y aromáticos halogenados.	Comp067	#LatinXChemComp
Tomás	Rojas Solórzano	Universidad de Costa Rica	Computational Study of Carbon Nano Scrolls as Cathodes in Aluminum-Based Batteries	Comp068	#LatinXChemComp
Elier Enrique	Abreu Martínez	Cinvestav	Towards a KNIME workflow for SAR and QSAR	Comp069	#LatinXChemComp
Eliana Rocio	Herrera Giraldo	Universidad Pedagógica y Tecnológica de Colombia- UPTC	Estudio mecanístico de la sililación de grupos O-H en benzodiazepinas con BSTFA	Comp070	#LatinXChemComp
Daniel	Aragon	Universidad del Quindio	Optimización de Síntesis Orgánica mediante Química Computacional	Comp071	#LatinXChemComp
Cristian J.	Guerra Madera	Universidad Andrés Bello	On the electron density redistribution in electronically excited states	Comp072	#LatinXChemComp
Jesús Alfredo	Lara Cerón	Universidad de Guadalajara	Analytical and traditional reactivity descriptors of carbon dots (CDs) using deMon2k software	Comp073	#LatinXChemComp
Claudia Ximena	Torres Benítez	Universidad Autónoma del Estado de México	Polaron formation in PDTODT oligomers studied via Advanced DFT analysis	Comp074	#LatinXChemComp
Carlos Alberto	Lobato Tapia	Universidad Politécnica Metropolitana de Puebla	Molecular docking de compuestos presentes en plantas medicinales como posibles inhibidores de la enzima macrólido 2-fosfotransferasa	Comp075	#LatinXChemComp
Jeremy M	Carr	Central Alabama Community College	Getting Smart with SARMs: Can PM7/COSMO Thermochem Provide Reasonable log P Values?	Comp076	#LatinXChemComp
Alexis	Rodriguez-Resendiz	UAEH	Estudio de las propiedades ópticas de absorción y emisión de 5-(ariletinil)fenil)benzoxazoles mediante estudios DFT	Comp077	#LatinXChemComp
Manuel Alonso	Luque Román	Universidad Autónoma de Sinaloa	Estudio teórico y experimental de un ion líquido y su evaluación teórica de la interacción con la superficie de Fe como potencial inhibidor	Comp078	#LatinXChemComp
Cinthia	Ramírez Martínez	Universidad Autónoma del Estado de Hidalgo	MODELO QSTR EN DERIVADOS DEL ÁCIDO BENZOICO UTILIZANDO DESCRIPTORES LOCALES DE C-DFT Y QTAIM	Comp079	#LatinXChemComp

Rodrigo	Moreira	Facultad de Química, Universidad de la República	Interaction of metalates in the active site of Trypanosoma cruzi protein tyrosine phosphatase	Comp080	#LatinXChemComp
Hazel Uriel	Vázquez Hernández	Universidad Autónoma Metropolitana Unidad Iztapalapa	Molecular packing similarity index based on dual quaternions	Comp081	#LatinXChemComp
Fernando Jose	Martinez-Villarino	Cinvestav - Merida	Calculation of ring-current strengths in Aromagnetic programa by using Ampere-Maxwell integration	Comp082	#LatinXChemComp
Jhoan	Londoño Restrepo	Universidad de Antioquia	More please: what drives the formation of unsaturated molecules in Interstellar medium?	Comp083	#LatinXChemComp
Guadalupe	Castro González	Univeridad Autónoma Metropolitana	Extracting knowledge of 2D-Hybrid Halide Perovskite materials, a data mining approach.	Comp084	#LatinXChemComp
Ana María	Vanegas Castro	Universidad de Antioquia	Estudio Teórico de la Reactividad de Intermediarios Cocristalinos en Reacciones de activación Mediadas por Complejos de Rodio e Iridio	Comp085	#LatinXChemComp
Salomón de Jesús	Alas Guardado	Universidad Autónoma Metropolitana Cuajimalpa	Effect of the Lys62Ala Mutation on the Thermal Stability of BstHPr Protein by Molecular Dynamics	Comp086	#LatinXChemComp
Daniela	Quadros de Azevedo	Universidade Federal de Minas Gerais	Antiviral Medicinal Plants and Natural Products Database (avMpNp DB): a reference platform for medicinal plants and natural antiviral products.	Comp087	#LatinXChemComp
Sebastian David	Vargas Vergara	Universidad de Sucre	Structural and functional performance evaluation of graphene-grafted polymer nanocomposites using molecular dynamics	Comp088	#LatinXChemComp
Royle	Pérez Castillo	National University of Quilmes	Transient-absorption spectroscopy of dendrimers via nonadiabatic excited-state dynamics simulations	Comp089	#LatinXChemComp
Manuela	Jaramillo Vanegas	Universidad de los Andes	Computational Insights into the Interactions Between Membrane Cholesterol and the CB1 Receptor	Comp090	#LatinXChemComp
Joanatan Michael	Bautista Renedo	Universidad Autónoma Metropolitana - Iztapalapa	Machine Learning Force Fields for the efficient exploration of oxalic acid polymorphs	Comp091	#LatinXChemComp
Noé	Brigido Salvador	Benemérita Universidad Autónoma de Puebla	Estudio computacional de la adsorción de compuestos organoboranos de tipo RB-NR sobre nanoestructuras fullerénicas de nitruro de boro	Comp092	#LatinXChemComp
Marilina	Cathcarth	Instituto de Investigaciones Fisicoquímicas Teóricas y Aplicadas (INIFTA)	Negatively charged protein adsorption on silica surface by Molecular Theory simulations	Comp093	#LatinXChemComp
Wilson Alberto	Tárraga	INIFTA, Instituto de Investigaciones Fisicoquímicas Teóricas y Aplicadas	Protein adsorption mediated by silica binding peptide on silica-like surface model via thermodynamic simulations	Comp094	#LatinXChemComp
Paulina	Escobar Martinez	Universidad Tecnologica de Pereira	Computational Analysis of N-Phenylmaleimide HIT Compounds: Influence of Deactivating groups on Biological Activity	Comp095	#LatinXChemComp
Lexin	Chen	University of Florida	Molecular pathways through Sampling Hierarchical Intrinsic N-ary Ensembles (SHINE)	Comp096	#LatinXChemComp
Lexin	Chen	University of Florida	MDANCE: flexible and versatile n-ary clustering package	Comp097	#LatinXChemComp
Juan Esteban	Pulgarin Restrepo	Universidad tecnológica de Pereira	Computational Analysis of N-Phenylmaleimide HIT Compounds: Influence of activating groups on Biological Activity.	Comp098	#LatinXChemComp
Nicandro Noel	Uribe Lopez	Centro Conjunto de Investigación de Química Sustentable UAEM-UNAM, Instituto de química UNAM	Estabilización de aniones en complejos de inclusión a través de agujero sigma.	Comp099	#LatinXChemComp
Enoch	Robles-Diaz	Universidad Autónoma de Sinaloa	Estudio del uso de azometina para modificar un colorante basado en carbazol mejorando la eficiencia de la DSSC.	Comp100	#LatinXChemComp
Maria Jose	Lara Genne	Universidad de Sucre	Construction of an atomistic model of starch to investigate its physicochemical behavior through molecular dynamics	Comp101	#LatinXChemComp
Angie Paola	Mogollón Rivero	Universidad de Pamplona	In silico evaluation of the gas trapping of HFCs R23, R-236fa, and R143a in deep eutectic solvents (DES).	Comp102	#LatinXChemComp
Lady Johanna	Rosero Carvajal	Universidad Tecnología de pereira	Estudio foodinformatics del fruto del aguacate Hass (Persea americana) para aplicaciones en la industria alimentaria	Comp103	#LatinXChemComp
Rugwed Anil	Lokhande	University of Florida	FANPT: Flexible Ansatz for N-body Perturbation Theory	Comp104	#LatinXChemComp
Rugwed Anil	Lokhande	University of Florida	2nd order FANPT	Comp105	#LatinXChemComp
Merlys	Borges	Comisión Chilena de Energía Nuclear	A theoretical study of simultaneous extraction of magnesium and boron using ionic liquids	Comp106	#LatinXChemComp
Viviana	Roman Ventura	Universidad Andres Bello	η5-C5H5Fe(η5-Li5B5H5): A Novel Sandwich Complex with an Aromatic Boron Ring	Comp107	#LatinXChemComp
Etzael Alexis	Mendoza García	Benémerita Universidad Autónoma de Puebla	Computational analysis of phytochemicals with anticancer activity	Comp108	#LatinXChemComp
Joan	Cardona Olives	Universitat de Barcelona	Computational Insight of Hyperfine Coupling in Molecular Qubits	Comp109	#LatinXChemComp
Arnau	Garcia Duran	Universitat de Barcelona	Computational Study Of Spin-Crossover Systems Embedded In Carbon Nanohoops	Comp110	#LatinXChemComp
Valeria	Bedoya Jiménez	Universidad San Francisco de Quito	KLD: a program to elucidate the localization of the Fermi and Coulomb holes in molecular systems	Comp111	#LatinXChemComp
Alvaro	Muñoz-Castro	Universidad San Sebastian	Modern Aspects of Chemical Bonding in Cluster Chemistry From Computational Chemistry	Comp112	#LatinXChemComp
Luis Roy	Quispe Corimayhua	Universidad Andrés Bello	Exploration of local and global magnetic properties in U(III) inverted-sandwich structure: A theoretical study.	Comp113	#LatinXChemComp
Liana Margarita	Diaz Ortiz	Universidad de Medellín	Adsorption of drugs on Calcium Oxides: A computational study	Comp114	#LatinXChemComp
Arley Santiago	Lesmes Gacha	Universidad Pedagógica y Tecnológica de Colombia	DFT study on the reaction mechanism for the synthesis of imino ligands from aniline derivatives and 2-formylpyridine.	Comp115	#LatinXChemComp
Wendy Michelle	Rodríguez	Universidad San Francisco de Quito	A Redefinition of CDFT Reactivity Indexes by means of the Cubic Expansions of the Energy	Comp116	#LatinXChemComp
Isaac Rafael	Gutiérrez Campos	Cinvestav	Molecular structure clustering based on morphological patterns using machine learning tools	Comp117	#LatinXChemComp
Jesús Israel	Espinoza Castañeda	Universidad Nacional Autónoma de México	Automated analysis of structure-multiple property relationships: Impacts on SMARTs	Comp118	#LatinXChemComp
Rafael	Flores Larrañaga	Benemérita Universidad Autónoma de Puebla	DFT study of the reaction between formaldehyde and relevant astronomical radicals and cations	Comp119	#LatinXChemComp

Andrea	Moreno-Ceballos	Benemérita Universidad Autónoma de Puebla	Evaluación teórica de los efectos mutagénicos de caespitato.	Comp120	#LatinXChemComp
Mari Toña	Juárez Méndez	Benemérita Universidad Autónoma de Puebla	Efecto del disolvente en los parámetros de reactividad global de triterpenos de origen natural con posible actividad antiviral	Comp121	#LatinXChemComp
Miguel Osvaldo	Juárez Tecua	Benemérita Universidad Autónoma de Puebla	Computational analysis of the adsorption energies between glyphosate derivatives and calix[4]arene.	Comp122	#LatinXChemComp
María Paula	Gamarra Madera	Universidad de Sucre	Computational Exploration of Complex Phospholipid Membranes via MD: Modeling, Simulation, and Analysis of Bioactive Compound Interactions	Comp123	#LatinXChemComp
Ana María	Arango Ortiz	Universidad de Antioquia	El octámero de agua	Comp124	#LatinXChemComp
Xquenda Guadalupe	Rios Aguilar	Benemérita Universidad Autónoma de Puebla	Análisis computacional de isoflavonas de soya en la activación de receptores de estrógeno	Comp125	#LatinXChemComp
Ernesto Alejandro	Fajardo Díaz	Universidad de la Habana	STDock: Automating the “STD-NMR Informed” Docking Pipelines in Drug Discovery	Comp126	#LatinXChemComp
Leonardo Israel	Lugo Fuentes	Universidad de Guanajuato	Water Reduction by bisborylphosphine (BPB) and borylphosphine (BP) FLPs: Reaction Mechanism and Energy Barrier Differences	Comp127	#LatinXChemComp
Ximena	Fernández Sánchez	Facultad de Medicina, Universidad Nacional Autónoma de México	Antidepressant drugs, gene perturbation profiles and adverse effects: a network pharmacology approach	Comp128	#LatinXChemComp
Erick Henrique de Souza	Alves	Universidade de São Paulo	Investigation of Visible Light-induced Enantioselective 6pi-Photoelectrocyclizations	Comp129	#LatinXChemComp
José Ángel	Hernández Martínez	Universidad de Sucre	Fungal Pigments for industrial applications: a Computational Approach to Properties Evaluation	Comp130	#LatinXChemComp
José Ángel	Espinoza Basopoli	Universidad Autonoma de Sinaloa	Estructura molecular y espectro de absorción de colorante orgánico con estructura D-π-A mediante cálculos computacionales	Comp131	#LatinXChemComp
Javier Yahir	Izaguirre Navarro	Universidad Autónoma de Sinaloa	Análisis de las propiedades electrónicas de un compuesto de Zinc con M06	Comp132	#LatinXChemComp
Edgar	Higuera Ruiz	Universidad Autónoma de Sinaloa	Análisis de la estructura electrónica de un compuesto de Zinc empleando M06	Comp133	#LatinXChemComp
Jordan Edilberto	Ruiz Castelán	Benemérita Universidad Autónoma de Puebla	Efectos estructurales de la subunidad β3 sobre el canal de sodio hNav1.7	Comp134	#LatinXChemComp
Vanessa	Gallego Montoya	Universidad de Antioquia	Stabilization of the Chikungunya virus - cellular receptor complex by molecular dynamics simulations.	Comp135	#LatinXChemComp
Vicente	Martí-Centelles	Universitat Politècnica de València	CageCavityCalc (C3) software to calculate and visualize cavities in Molecular Cages	Comp136	#LatinXChemComp
Edwin Reji	Chacko	McMaster University	Spectro: A multi-modal machine learning approach for molecule elucidation using IR and NMR data	Comp137	#LatinXChemComp
Jhon Erick	Aceros Ramirez	Universidad del Atlántico	Estudio In silico sobre la acción hepatoprotectora de PGA1 y PGA3 mediante inhibición de GSK3α	Comp138	#LatinXChemComp
Ana María	Rodelo Cabarcas	Universidad del Atlántico	Evaluación in silico de la propiedad coagulante de eicosanoides tromboxánicos sobre trombina	Comp139	#LatinXChemComp
Rubén	Marrero Carballo	Universidad Autónoma de Yucatán	Estudio del acoplamiento molecular de nitrobencenesulfonamidas derivadas de tiazol y la ferredoxina de Trichomonas vaginalis	Comp140	#LatinXChemComp
Alexandre	de Camargo	McMaster	Leveraging Normalizing Flows for Orbital-Free Density Functional Theory	Comp141	#LatinXChemComp
Flor María Montserrat	Briceño Vargas	Universidad Autónoma de Yucatán	Topological electron density study of n→p* interactions in amides and thioamides.	Comp142	#LatinXChemComp
Anaid	Flores	Universidad Autónoma Metropolitana Unidad Iztapalapa	Dipole Moment and Charge Transfer in Hydrogen Bonds	Comp143	#LatinXChemComp
Estefanía del Alba	Lizama García	Benemérita Universidad Autónoma de Puebla	Estudio de la reactividad química de la Casiarina A y sus derivados para el tratamiento de la malaria	Comp144	#LatinXChemComp
Erick Daniel	Salazar Calzada	Benemérita Universidad Autónoma de Puebla	POTENCIAL ACTIVIDAD BIOLÓGICA DE DERIVADOS DEL TROZAMICOL: UN ENFOQUE IN SILICO	Comp145	#LatinXChemComp
María Elena	Astorga Huerta	Benemérita Universidad Autónoma de Puebla	Estudio computacional de la interacción del segmento 1-42 del péptido beta-amiloide con carnosol	Comp146	#LatinXChemComp
María Fernanda	Muñoz Pastori	Universidad Central de Venezuela	Estudio computacional de benzotiazoles como posibles antivirales para COVID-19	Comp147	#LatinXChemComp
Camila Alexandra	Rosas Roldán	Benemérita Universidad Autónoma de Puebla	Diseño in silico de metioninas protegidas y su potencial uso farmacológico.	Comp148	#LatinXChemComp
Boris Daniel	Gutiérrez Cortés	Universidad Autónoma Mexicana	Free energy energy determination of molecular crystals using ab inito methods	Comp149	#LatinXChemComp
Monica Lucia	Suarez Gutierrez	Universidad del Atlántico	Potencial efecto anticancerígeno de la AACOCF3 por inhibición de la lipasa monoglicérido mediante método in silico	Comp150	#LatinXChemComp
Nicolas	Molina Trujillo	Universidad Nacional de Colombia	Assessing water force fields by predicting vibrational observables using the MD-IFM method	Comp151	#LatinXChemComp
Gabriela	Valle Núñez	UNAM - Facultad de Química	Desarrollo de modelos de predicción para la identificación de compuestos con actividad antiviral	Comp152	#LatinXChemComp
Nicolás Damián	Gómez	Instituto de Investigaciones Fisicoquímicas Teóricas y Aplicadas	Cálculo de las constantes de velocidad de las reacciones de CCl2FCH2CF3 (HCFC-234fb) con los radicales OH y Cl	Comp153	#LatinXChemComp
Yoslainy	Echevarria Valdés	Universidad Andrés Bello	Computational study of the Luminescence Activation/Deactivation Mechanism in the UiO-66-(COOH)2 type MOF by including Eu(III) as a dopant specie	Comp154	#LatinXChemComp
Yoslainy	Echevarria Valdés	Universidad Andrés Bello	Quantum Chemistry Insights into the Electronic Properties of UiO-66 type MOF doped with Eu(III) ions: Selective Sensing of Hg(II) ions	Comp155	#LatinXChemComp
Mario	Saavedra	Millenium Nuclei on Catalytic Process towards Sustainable Chemistry (CSC)	Computational study of the Crotonaldehyde adsorption over PtSn(110), Pt3Sn(111)/Pt(111), Pt3Sn(111) and PtSn4(010): A periodic DFT study	Comp156	#LatinXChemComp
Viviana	Acevedo López	Universidad Tecnológica de Pereira	In silico evaluation of the antibacterial bioactivity of nitrophenylmaleimide isomers (NPMI)	Comp157	#LatinXChemComp
Luis Antonio	Cobos Ontiveros	Benemérita Universidad Autónoma de Puebla	Estudio conformacional y de reactividad química del 5-ALA en diferentes disolventes	Comp158	#LatinXChemComp
Asma	Jamali Rafsanjani	School of Computational and Science Engineering at McMaster University	MOLPIPx, a fully differentiable library for Permutationally Invariant Polynomials in Python and Rust	Comp159	#LatinXChemComp
Araceli	Cahuantzi Cuamatzi	Benemérita Universidad Autónoma de Puebla	Estudio computacional de la actividad farmacológica de compuestos antimaláricos.	Comp160	#LatinXChemComp

Angel Jesus	Suarez Bustos	Instituto Tecnologico de Mexico en Celaya	Study of cellulose degradation with an aqueous solution of sodium hydroxide using molecular dynamics	Comp161	#LatinXChemComp
Leandro	Martinez Heredia	Universidad Nacional de La Plata	NaturAr: A database of natural products from Argentina	Comp162	#LatinXChemComp
Mesías	Orozco-Ic	Donostia International Physics Center (DIPC), 20018 Donostia, Euskadi, Spain. / Instituto de Ciencias Físicas, Universidad Nacional Autónoma de México, 62210 Cuernavaca, México	Core-electron contributions to the magnetic response of molecules with heavy elements	Comp163	#LatinXChemComp
Luis Armando	Gonzalez Ortiz	CINVESTAV-IPN Mérida	Búsqueda metaheurística de isómeros para sistemas orgánicos usando SMILES	Comp164	#LatinXChemComp
Yoan	Hidalgo-Rosa	Centro de Nanotecnología Aplicada, Facultad de Ciencias, Ingeniería y Tecnología, Universidad Mayor, Camino La Pirámide 5750, Huechuraba, Santiago, Chile	Investigating the Electronic and Photophysical Properties of Metalloporphyrin-Based Ti-MOFs for Photocatalysis Applications via Quantum Chemistry	Comp165	#LatinXChemComp
Andrés Felipe	Flor López	Universidad de Chile	Identificando el origen de estados de transición ambimodales producto de modos normales específicos en Cicloaromatizaciones altamente competitivas.	Comp166	#LatinXChemComp
Heriberto	Miranda Nieto	Tecnológico Nacional de México en Celaya	METODOLOGÍA PARA SELECCIÓN DE SOLVENTES PARA DESTILACIÓN EXTRACTIVA	Comp167	#LatinXChemComp
Carlos Andrés	Padilla Jaramillo	Universidad Industrial de Santander	AI-guided design of Electron Transfer MALDI matrices for analyzing small labile and unstable compounds	Comp168	#LatinXChemComp
Paolo G.	Zucchini	INIFTA, Instituto de Investigaciones Fisicoquímicas, Teóricas y Aplicadas	Comparison of the thermal decomposition reactions for different isomers of dichloropropene	Comp169	#LatinXChemComp
Yamil	Hernandez Urquieta	BUAP	Caracterización de las interacciones intramoleculares Mg-N en la clorofila-a con la cadena de fitol completa	Comp170	#LatinXChemComp
Ana María	Cruz González	INIFTA	Polymer Nanogels Responsive to Solvent Quality Changes as Biomaterial Carriers: Studies through Computer Simulations	Comp171	#LatinXChemComp
Joshua	Mercado	University of Pittsburgh	Evaluating Binding Stability of Molecular Fragments in LARP1 via Molecular Dynamics	Comp172	#LatinXChemComp
Leticia	Adao Gomes	Northeastern University	Benchmarking Density Functional Methods for Accurate Prediction of Ground and Excited State Redox Potentials of Organic Photoredox Catalysts	Comp173	#LatinXChemComp
Montserrat	Ávila Cuautle	Benemérita Universidad Autónoma de Puebla	Análisis bioinformático de compuestos derivados de Fenilhidrazona para la identificación de dianas terapéuticas	Comp174	#LatinXChemComp
Thiago Mineo	Mizumoto	Instituto de Química da Universidade de São Paulo (IQUSP)	Creating a cluster: size and structural distortion	Comp175	#LatinXChemComp
Carlos Osmar	Farfan Vazquez	Benemérita Universidad Autónoma de Puebla	Estudio In Silico de la interacción de una sapogenina sintética sobre la pared celular de Staphylococcus aureus.	Comp176	#LatinXChemComp
Alisson Dayana	Cabrera Felicita	Universidad San Francisco de Quito	NeuralRho: A Neural-Networks Model for the Electron Density	Comp177	#LatinXChemComp
Juan Emanuel	López Cervantes	Universidad Autónoma del Estado de Hidalgo	DFT-ChemDescriptors: Una herramienta para el cálculo de descriptores cuánticos y su aplicación en QSAR	Comp178	#LatinXChemComp
Luis Antonio	Castillo Felix	Tecnológico Nacional de México en Celaya	Estudio teórico-experimental del comportamiento reológico del líquido iónico 1-butil-2,3-dimetilimidazolio tetrafluoroborato	Comp179	#LatinXChemComp
Luis Moises	Leyva Parra	Universidad Central de Chile	New Perspectives on Delocalization Pathways in Aromatic Molecular Chameleons	Comp180	#LatinXChemComp
Luz Maria	Diego Ramon	Universidad Andres Bello	Electronic stability in planar pentacoordinate atoms of group 13 (B, Al and Ga)	Comp181	#LatinXChemComp
Lucas Welington	de Lima	Universidade de São Paulo	Temperature Dependence of the CO2 and Cyclohexene Oxide Polymerization and Cyclic Carbonate Formation Reactions	Comp182	#LatinXChemComp
Sebastian	Richter	Universidad de Chile	Reaction Force Constant As a Descriptor of the Principle of Non-Perfect Synchronization	Comp183	#LatinXChemComp
Eduardo	Naranjo Adorno	Tecnológico Nacional de Mexico en Celaya	Estudio comparativo de la dureza de PLA y PE mediante nanoindentación usando Dinámica Molecular	Comp184	#LatinXChemComp
Omar	Méndez-Fernández	Benemérita Universidad Autónoma de Puebla	Computational investigation of agents able to modulate the Cyclic Nucleotide Binding Domain (CNBD) of the HCN channels	Comp185	#LatinXChemComp
Enzo	Sampronha	Polytechnic School, Universidade de São Paulo	Study of CO2 adsorption on 13X zeolite using GCMC and KS-DFT methods	Comp186	#LatinXChemComp
Fernando	Murillo	Centro de Investigación y de Estudios Avanzados	The mechanism of transformation between B10H14 and B10H14(2–): Solving a conundrum	Comp187	#LatinXChemComp
Yurimar	Ruiz Rocha	Universidad de Sucre	Full Atom Amylose and Amylopectin in Water Solubility Analysis via Molecular Dynamics	Comp188	#LatinXChemComp
Arturo	Sauza	Universidad de Chicago	Comprehensive chemical bonding study of lanthanide/actinide complexes with anionic/radical ligands.	Comp189	#LatinXChemComp
Leandro Ramos	Marques	University of São Paulo	Investigating the charge transfer of a Frustrated Lewis Pairs in the resonance Raman spectrum	Comp190	#LatinXChemComp
Jessica Olinda	Valero Rojas	Universidad de Concepción	AlzyFinder: An ML-driven platform for ligand-based virtual screening and network pharmacology	Comp191	#LatinXChemComp
Diana	López López	Universidad Autónoma del Estado de Morelos	Diseño de iridoides con base en la estructura de genipina mediante estudios in vitro e in silico contra cáncer cervicouterino	Comp192	#LatinXChemComp
Bryan Ashley	Acosta García	Cinvestav	Towards a theoretical justification of Mayr scales using Chemical Reactivity	Comp193	#LatinXChemComp
Yeljair Enrique	Monascal Rodríguez	Instituto de Investigaciones Fisicoquímicas Teóricas y Aplicadas (INIFTA), UNLP, CONICET.	A computational analysis of the gas-phase thermal decomposition of cyclopropanesulfonyl fluoride	Comp194	#LatinXChemComp
Krisztina Anna	Zsigmond	University of Florida	Breaking particle-number symmetry in Coupled-Cluster wavefunctions	Comp195	#LatinXChemComp