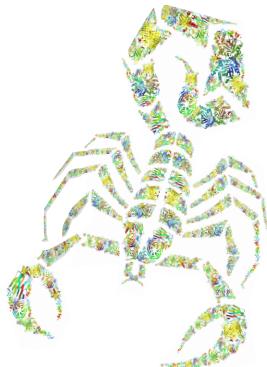




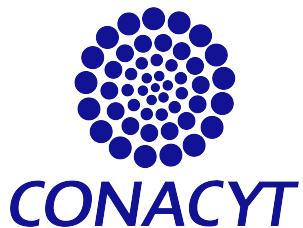
# 6º CONGRESO DE LA RAMA DE FISICOQUÍMICA, ESTRUCTURA Y DISEÑO DE PROTEÍNAS



UNIVERSIDAD JUÁREZ DEL ESTADO DE DURANGO  
6 AL 10 DE NOVIEMBRE 2017  
DURANGO, MÉXICO



Red  
Estructura  
Función y  
Evolución de  
Proteínas





# Lunes 6 de noviembre

17:30 Inauguración

18:00

Joseph W. Thornton (*University of Chicago, EUA*)

**Ancient mechanisms for the evolution of protein specificity: insights from ancestral protein reconstruction**

19:00 Brindis

# Martes 7 de noviembre

9:00

Rosario A. Muñoz-Clares (*Fac. Química, Universidad Nacional Autónoma de México*)

**Biochemical and structural studies on the complex allosteric regulation of the photosynthetic phosphoenolpyruvate carboxylases from C4 plants**

9:50 Presentaciones orales M1 (Trabajos del 1 al 11)

10:40 Café

11:00 Presentaciones orales M2 (Trabajos del 22 al 32)

11:50

R. Brian Dyer (*Emory University, EUA*)

**Membrane Protein Folding and Functional Dynamics**

12:40 Presentaciones orales M3 (Trabajos del 43 al 53)

13:30 Comida

15:30 Presentaciones orales M4 (Trabajos del 63 al 73)

16:20

Alejandro J. Vila (*Universidad Nacional del Rosario, Argentina*)

**Molecular traits improving fitness in zinc-dependent carbapenemases: Mind the gap!**

17:10

Daniel Maturana Nanotemper Technologies  
**Biophysics at the Cutting Edge: MicroScale Thermophoresis and nanoDSF**

17:25 Presentación de Carteles (Trabajos del 1 al 73)

# Miércoles 8 de noviembre

9:00

Georgina Garza (*Fac. Medicina, Universidad Nacional Autónoma de México*)

**Structural and functional studies of bacterial nitrilases and the challenges for their biotechnological application**

9:50

Chris D. Bahl (*Institute for Protein Innovation, EUA*)

**De novo design of antivirulence therapeutics based on genetically encodable, hyperstable constrained peptides**

10:40 Café

11:00

Wilhelm Hansberg (*I. Fisiología Celular, Universidad Nacional Autónoma de México*)

**Catalase and catalase-peroxidase: complex enzymes for a simple reaction**

11:50

Birte Hocker (*Universitat Bayreuth, Alemania*)

**Evolution and design of proteins**

12:40

Braulio Gutiérrez (*Instituto Potosino de Investigación Científica y Tecnológica*)

**Protein dynamics and kinetics under the light**

13:30 Comida

Tarde libre

20:00 Evento cultural

# Jueves 9 de noviembre

9:00

Gloria Saab (*I. Biotecnología, Universidad Nacional Autónoma de México*)

**Exploring Sequence-Space in TIM Barrel Proteins**

9:50 Presentaciones orales J1. Trabajos del 74 al 84

10:40 Café

11:00 Presentaciones orales J2. Trabajos del 94 al 104

11:50

Marcelo A. Comini (*Institut Pasteur de Montevideo, Uruguay*)

**Glucose- 6-phosphate dehydrogenase from the human pathogen Trypanosoma cruzi: unique structural features and steroid-binding mode**

12:40 Presentaciones orales J3. Trabajos del 115 al 125

13:30 Comida

15:30 Presentaciones orales J4. Trabajos del 135 al 149

16:20

Glacius Oliva (*Universidad de São Paulo, Brasil*)

**Structural biology and drug discovery of Zika vírus proteins**

17:10 Presentación de Carteles. Trabajos del 74 al 150

# Viernes 10 de noviembre

9:50

Doug Barrick (*Johns Hopkins University, EUA*)

**Using consensus sequences to learn about folding cooperativity, stability, and function**

10:40 Café

11:00

Edgar Morales (*Centro de Investigación y de Estudios Avanzados*)

**One step closer to the atomic structure of the ATP synthase**

11:50

Susan Marqusee (*University of California, Berkeley, EUA*)

**Touring the Landscape: the view depends on how and when you look**

12:50 Clausura

# Martes 7 de noviembre

**1**

## **Structural and phylogenetic studies of choline monooxygenase**

Carrillo Campos, Javier; Riveros Rosas, Héctor; Rodríguez Sotres, Rogelio; Muñoz Clares, Rosario A.

**2**

## **Exploration of the structural ensemble of an intrinsically disordered protein using MD simulations.**

Hernandez-Segura, Teresa; Pastor-Colón, Carmen Nina

**3**

## **Expression of *Taenia solium* cysticercus antigenic proteins for cysticercosis immunodiagnosis**

Gomez-Fuentes, S; Sánchez, F; Ochoa-Leyva, A; Parada-Colin, MC; Espitia Clara; Adalid-Peralta, L

**4**

## **Heterologous expression of Exl1 expansin from *Pectobacterium carotovorum* in cells of the Rhizobiaceae family and analysis of the modification of biofilm production by these bacteria.**

Acosta-Hernandez, Luis Armando; Martínez-Anaya, Claudia

**5**

## **New paradigms in the study of allosterism of membrane proteins**

Guevara-Hernández, Eduardo; Contreras-Cervera, Ricardo; Rangel-Yezcas, Gisela; Rosenbaum-Emir, Tamara; Islas-Suárez, León

**6**

## **Interplay between Protein Thermal Flexibility and Kinetic Stability**

Quezada, Andrea G.; Díaz-Salazar, Jessica A; Cabrera, Nallely; Pérez-Montfort, Ruy; Piñeiro, Ángel; Costas, Miguel

*Martes*

**7**

**Regulatory Tcell induction by excretion-secretion products from *Taenia crassiceps* cysticerci for possible antiinflammatory use**

Morales-Ruiz, Valeria; López-Recinos, Dina; Guevara-Salinas, Adrián; Gómez-Fuentes, Sandra; Parada-Colín, Cristina; Espitia-Pinzón, Clara; Hernández-González, Marisela; Mora-Herrera, Ivonne; Adalid-Peralta, Laura.

**8**

**Structural and functional relation of a group of plant proteins with a protective action during water deficit**

Rendón-Luna, David Felipe; De Luna-Valenciano, Haydée; Covarrubias-Robles, Alejandra

**9**

**Interaction between *Aedes aegypti* CPB1 and viral proteins.**

López-López, Edgar; Barrientos-Salcedo, Carlina

**10**

**Characterization of the coupling mechanism of peptide variants of Discrepin on Kv4.3 potassium channel.**

**Molecular Dynamics Simulations**

Montero Dominguez Andrei; Garduño Juarez Ramon

**11**

**The importance of the imidazole group in the evolution of biological catalysis**

Vázquez-Salazar, Alberto; Becerra, Arturo; Lazcano, Antonio

**12**

**Quantum-mechanics consistent prediction of the substrate-activator-enzyme ternary complex of a mitosomal inorganic soluble pyrophosphatase from *Entamoeba histolytica***

Rodríguez-Sotres, Rogelio; Ramos-Ibarra, Marco Antonio; Melendez-López, Samuel G

**13**

**Copper-induced aggregation of the human gamma C- and S-crystallin proteins: Relevance to cataracts disease**

Martínez-Jurado, Eduardo; Domínguez-Calva, José; Serebryany, Eugene; Haasse-Pettingell, Cammie; King, Jonathan; Quintanar-Vera, Liliana

**14**

**Dynamic in two families of glycoside hydrolases (GH11, GH12)**

Homobono-Fuentes, Luis; Maldonado-Puga, Saira; Sosa-Peinado, Alejandro.

**15**

**Participation of H<sub>2</sub>S and Akt on the mechanism of action of vasodilators isoxsuprime and carvedilol: in silico and in vitro studies.**

Medina-Ruiz, Daniella; Mendoza-Ángeles, Diego; Romo-Mancillas, Antonio; Ibarra-Alvarado, César

**16**

**Amyloid fibers inhibition by aminoacids**

Cerón, Ricardo; Peimbert, Mariana; Rojo, Arturo; Nájera, Hugo

**17**

**Studying Cu(II) interactions with ABeta and Prion Protein: Insights into the molecular features of the fight for Cu(II) in Alzheimer Disease**

Posadas, Yanahi; Parra-Ojeda, Lili; Pérez-Cruz, Claudia; Quintanar, Liliana

**18**

**Structural analysis of the conformational changes generated by damage in laccase crystals exposed to different doses of deposited radiation**

Miranda-Blancas, Ricardo; Rudiño-Piñera, Enrique

**19**

**Proteomic analysis of cell wall of *Candida glabrata* and *Candida parapsilosis* resistant to fluconazol**

Corral-Pérez, Karina; Saucedo-Mendiola, María Leticia; López-Rodríguez, Angélica; Tinoco-Favila, Juan Carlos; Martínez-Aguilar, Gerardo; Salcido-Gutiérrez, Lorena; Ruiz-Baca, Estela

**20**

**Structural and kinetic characterization of a bi-functional Kunitz-STI protease inhibitor of aspartate and serine proteases: insights into its binding modes.**

Guerra, Yasel; Valiente Flores, Pedro A; Pons, Tirso; Berry, Colin; Rudiño-Piñera, Enrique

**21**

**Analysis of pyruvate kinases production using *E. coli* as a host**

Hernández-Alcántara, Gloria; Alba-Martínez, Zoe; Ramírez-Silva, Leticia

**22**

**Enzymatic assisted refolding**

Hernández-Tapia, Jacob Alejandro; Cano-Sánchez, Patricia; Del Rio-Portilla, José Federico

**23**

**Structural and thermodynamic determinants of ligand binding in a periplasmic binding protein**

Vergara-Gutiérrez, Jesús Renan; Romero-Romero, Sergio; Velázquez-López, Isabel; Sosa-Peinado, Alejandro; Fernández-Velasco, Daniel Alejandro

**24**

**Functional prediction on hypothetical transcription factors of *Escherichia coli* K-12**

Flores-Bautista, Emanuel; Ludeña Cronick, Carenne Cumanda; Rodriguez Fersaca, Anny; Perez-Rueda, Ernesto

**25**

**Porcine kidney betaine aldehyde dehydrogenase: Overexpression, purification and structural characteristics**

Muñoz-Bacasehua, César; Rosas-Rodríguez, Jesús A; Soñanez-Organis, José G; Arvizu-Flores, Aldo A; Yepiz-Plascencia, Gloria; Figueroa-Soto, Ciria G; Valenzuela-Soto, Elisa M

**26**

**Change in protein-ligand specificity inspired by Statistical Coupling Analysis**

Banda-Vázquez, Jesús; Shanmugaratnam, Sooruban; Rodríguez-Sotres, Rogelio; Torres-Larios, Alfredo; Höcker, Birte; Sosa-Peinado, Alejandro

**27**

**The interaction of the transcription factor NagC from *Escherichia coli* with its ligands: a physicochemical approach**

Díaz-Jiménez, Dana M; Zonszein-Strauss, Sergio; Alvarez-Añorve, Laura I; Plumbridge, Jacqueline; Calcagno, Mario

**28**

**Role of the expansin Exl1 from *Pectobacterium carotovorum* and *P. atrosepticum* during plant infection**  
Narváez-Barragán, Delia A.; Humphris, Sonia; Toth, Ian K.; Martínez-Anaya, Claudia

**29**

**Probable interaction of new drugs against *T. vaginalis***  
Vique-Sánchez, Jose Luis; Caro-Gómez, Luis; Brieba-de Castro, Luis G; Arroyo-Verastegui, Rossana; Ortega-López, Jaime; Rojo-Dominguez, Arturo; Benítez-Carriba, Claudia

**30**

**Biochemical and functional characterization of a lysozyme of *Solanum elaeagnifolium***  
Gutiérrez-Esparza, Brenda; Pelayo-Benavides, Helvia; Díaz-Sánchez, Ángel; Jiménez-Vega, Florinda; Hernández-Santoyo, Alejandra; Vargas-Requena, Claudia

**31**

**The TATA binding proteins of eukaryotic parasites reveal specific surface structural features and potential druggable sites**

Santiago, Angel; Pastor, Nina

**32**

**Analyzing the influence of effective electrostatic potentials of increasing size on the active sites of metalloenzymes using reactivity parameters**

Lozano-Espinoza, Mayra; Guevara-García, Alfredo; Galván, Marcelo

**33**

***In silico* identification of potentially functional motifs in components of the 5' to 3' mRNA decay pathway of plants**  
Maldonado-Bonilla, Luis

**34**

**Disulfiram inhibition of NADH Oxidase from the human parasite *Giardia lamblia***

Castillo-Villanueva, Adriana; Ramírez-Fonseca, Paola R; Méndez-Cruz, Sara Teresa; Oria-Hernández, Jesús

**35**

**Synthesis and application of metal-organic framework using trimesic acid and terephthalic acid to inhibit the aggregation of an amiloidogenic protein model**

Martínez Fuentes, Rubén; Nájera, Hugo; Beltrán, Hiram I.

*Martes*

**36**

**Bacterial expression, purification and biophysical characterization of wheat germ agglutinin and its four hevein-like domains**

Leyva, Eduardo; Medrano-Cerano, Jorge L.; Cano-Sánchez, Patricia; López-González, Itzel; Gómez-Velasco, Homero; García-Hernández, Enrique

**37**

**Activation energies and thermodynamic parameters of trypsins III mutants of sardine (*Sardinops sagax caerulea*)**

Carretas-Valdez, Manuel I.; Costas-Basín, Miguel A.; Cinco-Moroyoqui; Francisco J.; Ezquerra-Brauer, Marina J.; Márquez-Ríos, Enrique; Sotelo-Mundo, Rogerio R.; Arvizu-Flores, Aldo A.

**38**

**Biophysical characterization of the antimicrobial activity of a synthetic peptide derived from the C-terminal region of human chemokine CCL13.**

Portillo-Téllez, María del Carmen; Cossío-Ayala, Mayte; García-Hernández, Enrique

**39**

**Thermosonation effect on whey proteins isolate by infrared spectroscopy**

Barajas-Flores, Juanita; Delgado-Macuil, Raúl; Amador-Espejo, Genaro; Contreras-Rozo, José Antonio.

**40**

**Study of the function of the L9 loop in the regulation of the activity of a bi-functional protease inhibitor of the Kunitz-STI family**

Campuzano-González, Alexis; Guerra, Yasel; Rudiño-Piñera, Enrique

**41**

**Expression of the E1 gene of human papillomavirus type**

**16**

Campos-Parga, Bianca Nayeli; Gándara-Mireles, Alonso; Anguiano-Vega, Gerardo; Urtiz-Estrada, Norma; Saucedo-Mendiola, María Leticia

**42**

**A comparative evaluation of *de novo* assembly parameters for *Centruroides suffusus* transcriptome**

Carreño-Díaz, Ismael; Dozal-Rodríguez, Ricardo; López-Rodríguez, Angélica

**43**

**Two different peptide ligands of Human mu opioid receptor drive different atomic displacements in Molecular Dynamics simulations**

Cisneros-Caballero, Ángel Fernando; Matus-Ortega, Maura E.; Martíñon, Susana; Medina-Mora, María Elena; Mixcoha, Edgar

**44**

**Application of the nonbonded dummy model of Cu(II) in metallopeptides: plastocyanin and 1-16 amyloid  $\beta$ -peptide.**

Monjaraz-Rodríguez, Alejandra; Zubillaga, Rafael A.; Moreno-Razo, José Antonio; Vargas, Rubicelia

**45**

**Structural analysis of vasoinhibins: A Molecular Dynamics simulation approach**

Robles, Juan Pablo; Velasco-Bolom, José Luis; Garduño-Juarez, Ramón; Triebel, Jakob; Martínez de la Escalera, Gonzalo; Clapp, Carmen

**46**

**Optimization of the culture media for the production of laccases and zymography of *Pycnoporus cinnabarinus***

Cuevas-Reyes, Elizabeth; Diaz-Godinez, Gerardo; Villegas-Villarreal, Elba

**47**

**A New Mechanism of Cooperativity and Allostery in the SIS Fold GlcNAc Deaminase**

Marcos-Viquez, Jorge; Medina-García ,Andrea; Rodríguez-Hernández, Annia; Rodríguez-Romero, Adela; Calcagno-Montans, Mario; Bustos-Jaimes, Ismael

**48**

**Digestion and inhibition of Ca<sup>2+</sup> + ATPase of sarcoplasmic reticulum of rabbit muscle by the venom of the snake *Crotalus molossus*.**

Rivas-Valles, Cesar; Plenge-Tellechea, Luis

**49**

**The effects of phosphorylation versus phosphomimetic modification on the structure and dynamics of an intrinsically disordered protein**

Ramírez-Martínez, Marco; Pastor-Colón, Nina

*Martes*

**50**

**Disaggregation of HPV-16 virus like particles complex by non-functionalized gold nanoparticles**

Palomino-Vizcaino, Giovanni; Valencia-Reséndiz, Diana Gabriela; Benítez-Hess, María Luisa; Martínez-Acuña, Natalia; Tapia-Vieyra, Juana Virginia; Bahena, Daniel; Díaz-Sánchez, Mauricio; García-González, Octavio Patricio; Alvarez-Sandoval, Brenda Arizaí; Alvarez-Salas, Luis Marat.

**51**

**Insights into the chaperone-like protection mechanism of AtLEA4, an intrinsically disordered protein**

Romero-Pérez, Paulette S.; Cuevas-Velazquez, Cesar L.; Covarrubias, Alejandra A.

**52**

**Energetic effects of allosteric communication within the catalytic domain of oncogenic Bcr-Abl tyrosine kinase.**

López-González, Itzel; Cruz-Castañeda, Roberto; García-Curiel, Manuel Bernardo; Luviano-Jardón, Christian Axel; Badillo-Angeles, Eliud Horacio; García-Hernández, Enrique

**53**

**Reconstruction of ancestral eukaryotic triosephosphate isomerases**

Pérez-Niño, Jorge Alejandro; Fernández-Velasco, Daniel Alejandro

**54**

**Energetic and structural determinants of the effect of allosteric inhibition on the interaction between inhibitory molecules and the kinase Bcr-Abl.**

Cruz- Castañeda, Roberto; López-González, Itzel; García-Curiel, Manuel Bernardo; García-Hernández Enrique; Luviano-Jardón, Christian Axel

**55**

**Biochemical characterization of the trypsin III A233N mutant of sardine (*Sardinops sagax caerulea*)**

Cota-Núñez, Iris D.; Ramos-Osorio, Yamel D.; Carretas-Valdez, Manuel I.; Arvizu-Flores, Aldo A

**56**

**Protein profiles of germinated and non-germinated alfalfa (*Medicago sativa*) and antioxidant capacity of protein hydrolysates by reducing power**

Sauce-Guevara, Mildred; Diaz-Avendaño, Yael; González-Montoya, Marcela

**57**

**Design of fluorescent biosensors based on protein ligand interactions.**

Cabrera-Calderón, Leticia; Sosa-Peinado Alejandro

**58**

**Evaluating the effect of Cu(II) ions and a non-natural bifunctional tetrapeptide in the aggregation of an amyloidogenic prion protein fragment**

Villegas, Atenea; Vallejo, Luis Alberto; Quintanar, Liliana

**59**

**Computational study of omentin protein stability**

Nava-Andrade, Israel; Robles-Martínez, José L.; Rosas-Trigueros, Jorge L.; Palma-Orozco, Rosaura

**60**

**Detection of RB tumor suppressor in blood samples**

Salazar-Campos, Karla Lorena; Olivares-Illana, Vanesa.

**61**

**Histone deacetylase class 1 as a potential target against *trichinella spiralis*: An in silico approach.**

Montaño, Sarita; Correa, José; Pineda, Yolanda; Martínez, Marlet

**62**

**Construction of EF-hand sensor protein from a modulator protein**

Arévalo-Salina, Emma Liliana; Osuna-Quintero, Joel; Flores-Soto, Humberto; Saab-Rincón, Gloria

**63**

**Compositional and structural characterization of inclusion bodies of *Escherichia coli* during recombinant protein production with a thermo-inducible system**

Restrepo-Pineda, Sara; Bando-Campos, Carlos G.; Valdez-Cruz, Norma A.; Trujillo-Roldán, Mauricio A.

**64**

**Insights in protein radiation damage resistance.**

Venancio-Landeros, Alberto-Antony; Rudiño-Piñera, Enrique; Cardona-Félix, César-Salvador

**65**

**Deciphering the structural analysis of the heterodimeric complex of Alix-syntenin-1 on human papilloma Virus**

Pineda, Yolanda; Correa, José; Martínez, Marlet; Montaño, Sarita

*Martes*

**66**

**Analysis of contacts between protein residues as a tool to identify structural determinants of the transglycosylation function of the alpha-amylase family**

Arreola-Barroso, Rodrigo A.; Miranda-Molina, Alfonso; Xolalpa-Villanueva, Wendy; Olvera-Rodríguez, Leticia; Saab-Rincón, Gloria

**67**

**A computational approach to the study of the interactions of P-glycoprotein with ligands**

Mares-Sámano, Sergio; Garduño-Juárez, Ramón

**68**

**The first crystal structure of a three-domain cyclodextrin glucanotransferase**

Posso-Dradá, Jackeline; Virgen-Ortíz, Raúl; Guerra, Yasel; López-Munguía, Agustín; Rudiño-Piñera, Enrique; Centeno-Leija, Sara; Serrano-Posada, Hugo

**69**

**Design of peptide antimicrobials and their activity against pathogenic strains of clinical interest**

Hermenegildo-Rosas, Héctor Daniel; Corzo Burguete, Gerardo A.; Rodríguez Solís, Alexis J; Villegas Villarreal, Elba C.

**70**

**Revealing structural insights of HDAC1 by Molecular Dynamic simulations**

Sixto-López, Yudibeth; Bello, Martiniano; Correa-Basurto, José

**71**

**Modifications at the dimerization surface shift the mode of oligomeric assembly and determine catalytic activity of nitrilase from *Rhodococcus* sp. V51B.**

Aguirre Sampieri, Sergio; Gómez-Aguilar, Agustin; Garza-Ramos Martínez, Georgina

**72**

**Evolution of the Hemerythrin-Like Domain Superfamily**

Alvarez-Carreño, Claudia; Becerra, Arturo; Lazcano, Antonio

**73**

**Obtaining and characterization of enzymatic hydrolysates  
with biological activity from primary and secondary whey  
of dairy products**

Mares-Mares, Everardo; Herrera-Castillo, Fátima Luz  
Maria; León-Galván, Ma. Fabiola

*Martes*

# Jueves 9 de noviembre

**74**

**TvTIM as a biomolecular tool: Crystallization scaffold.**

Alamán-Zárate, Marcel; Diaz-Quezada, Corina; Brieba de Castro, Luis

**75**

**The conformational landscape of *de novo* designed TIM barrels**

Romero-Romero, Sergio; Silva-Manzano, Daniel-Adriano; Costas, Miguel; Shanmugaratnam, Sooruban; Höcker, Birte; Baker, David; Fernández-Velasco, Daniel Alejandro.

**76**

**Study about the disaggregation of amyloids fibers in human lysozyme**

López-Guzmán, Santos Arturo ; Nájera-Peña, Hugo

**77**

**Expression of recombinant glycoproteins of *M. tuberculosis* in yeast**

Bando-Campos, Giroshi; Juárez-López, Daniel; Olvera, Clarita; Trujillo-Roldán, Mauricio A.; Valdez-Cruz, Norma A.

**78**

**Modification of aggregation properties, cytotoxicity and ROS production of Amyloid  $\beta$  peptide through insertion of key amino acid point mutations.**

Estrada-Rodríguez, Ana; Treviño-Garza, Alejandro; Martínez-Rodríguez, Herminia Guadalupe; Rivas-Estilla, Ana María; Vidaltamayo-Ramírez, Román; Zomosa-Signoret, Viviana

*Jueves*

**79**

**The contribution of two isozymes to the pyruvate kinase activity of *Vibrio cholera*: one K+-dependent constitutively active and another K+-independent with essential allosteric activation**

Ramírez-Silva, Leticia; Guerrero-Mendiola, Carlos; García-Trejo, José; Saavedra, E; Encalda, R; Hernández-Alcántara, Gloria

**80**

**Role of DNA glycosylase MutY in transcription associated mutagenesis**

Leyva-Sánchez, Hilda Cecilia; Débora-Nayar, Bernardo; Gómez-Marroquín, Martha; Pedraza-Reyes, Mario

**81**

**Characterization of *Taenia crassiceps* secretion-excretion proteins with immunomodulator activity to control inflammatory processes**

López-Recinos, Dina; Morales-Ruiz, Valeria; Guevara-Salinas, Adrián; Gómez-Fuentes, Sandra; Parada-Colín, Cristina; Espitia-Pinzón, Clara; Hernández-González, Marisela; Mora-Herrera, Ivonne; Adalid-Peralta, Laura

**82**

**Effects on activity and stability of site-specific mutations along C-terminal end of nitrilase from *Rhodococcus sp. V51B*.**

Larrañaga-Ramírez, Hugo; Garza-Ramos, Georgina

**83**

**Interactions between Flavonoids and  $\alpha$ -Amylase.**

Martinez-Gonzalez, Alejandra I; Díaz-Sánchez, Ángel G; de la Rosa, Laura A; Vargas-Requena, Claudia L; Bustos-Jaimes, Ismael; and Alvarez-Parrilla, Emilio

**84**

***Moringa oleifera* leaf extract effect on mitochondrial function of diabetic rats hearts.**

Sánchez-Muñoz, María Alejandra; Flores-Molina, Loammi; Valdez-Solana, Mónica Andrea; García-Arenas, Guadalupe; Avitia-Domínguez, Claudia; Tellez-Valencia Alfredo; Sierra-Campos, Erick

**85**

**Homo and heterodimerization of cannabinoids receptors CB1, CB2, GPR55 and GPR18 as binding targets of cannabinoids**

Hurtado-S., Edna; Romo-Mancillas, Antonio

**86**

**Four CNG channel subunits evidenced from the scorpion *Centruroides suffusus***

Dozal-Rodríguez, Ricardo; Carreño-Díaz, Ismael; Saucedo-Mendiola, Leticia; Ruiz-Baca Estela; López-Rodríguez Angélica.

**87**

**Overcoming drug-resistance: specific inhibition of ATP synthase from pathogenic organisms**

Cofas-Vargas, Luis Fernando; Mendoza-Espinosa, Paola; Avila-Barrientos, Luis Pablo, Salcedo-Barrientos, Guillermo; Hernández-García, Enrique; Ruiz-Blanco, Yasser B.; García-Hernández, Enrique

**88**

**Native 3d information of isolated and highly conserved in silico-built loops belonging to proteins that refold *in vitro***

Rodríguez-Flores, Brenda Nataly; Padilla-Zuñiga, Jaqueline

**89**

**Improving the stability of a *de novo* TIM barrel.**

Avilés-Sánchez, Octavio; Fernández-Velasco, Daniel Alejandro

**90**

**Cloning, purification, and characterization of shikimate kinase from methicillin resistant *Staphylococcus aureus*. Kinetic and Molecular Dynamics studies**

Favela-Candia, Alejandro; Téllez-Valencia, Alfredo; Cisneros-Martínez, Jorge; Gómez Palacio- Gastellum, Marcelo; Avitia- Domínguez, Claudia

**91**

**Docking and molecular dynamics simulations of protein-ligand complexes on TRPA1 receptor: insights of binding site specificity**

Uribe-Piña, Ignacio; Romo-Mancillas, Antonio

**92**

**Using magnetic particles to analyze biomolecular interaction**

Orozco-Macías, Mariana; Moctezuma-Martíñon, Rosario;  
Olivares-Illana, Vanesa.

**93**

**Towards a multi-player activation model of Bax: effect of NaCl concentration**

Rosas-Trigueros, Jorge L.; García-Pérez, Francisco J.;  
Palma-Orozco, Rosaura

**94**

**Identification and characterization of two novel class-I chitinase isoforms from *Agave tequilana* with antifungal activity.**

Sierra-Gómez, Yusvel; Rodríguez-Hernández, Annia;  
Rodríguez-Romero, Adela

**95**

**Inactivation of Polyphenol oxidase from Hass avocado (*Persea americana*).**

Tobías-Juárez, Ileana; Nájera-Peña, Hugo.

**96**

**Repair of ultraviolet photodimers with *Bacillus subtilis* UV-endonuclease YwjD and low-fidelity DNA polymerases YqjH and YqjW**

Patlán Vázquez, Adriana G.; Corona-Bautistaand, Saúl U.;  
Pedraza Reyes, Mario

**97**

**Ancestral reconstruction of ligand binding proteins: Clues to understand protein specificity evolution**

Maldonado-Puga, Saira; Banda-Vazquez, Jesus; Sosa-  
Peinado, Alejandro

**98**

**Virtual screening studies to identify potential inhibitors of protein tyrosine phosphatase 1B**

Chaidez-Avila, Alondra; Avitia-Domínguez, Claudia; Sierra-  
Campos Erick; Valdez-Solana Monica, Téllez-Valencia,  
Alfredo

**99**

**Simple sequences in early evolution of life**

Sánchez-Rocha, Alma Carolina; Becerra-Bracho, Arturo  
Carlos II

**100**

**Modeling of protein structure using machine learning**

Del Río Guerra, Gabriel; Fontove Herrera, Fernando

**101**

**Dynamics of the interaction between the essential GTPases Gpn1 and Gpn3**

Cristóbal-Mondragón, Gema; Santiago, Ángel; De la Rosa-Jiménez, Victor; Ladrón de Guevara, Ernesto; Rangel-Yescas, Gisela E; Pastor, Nina; Islas-Suárez, León; Sánchez-Olea, Roberto and Calera-Medina, Monica

**102**

**Expression of the different fragments of the gene of soybean 2S albumin (gm2S-1) in *Escherichia coli***

Jara-Romero, Guadalupe Janet; Luna-Suárez Silvia

**103**

**Discovery inhibitors of arginase from *Leishmania mexicana* by virtual screening.**

Betancourt-Conde, Irene; Vázquez-Raygoza, Alejandra; Avitia-Domínguez, Claudia; Romo-Mancillas, Antonio; Hernández-Campos, Alicia; Tellez-Valencia, Alfredo

**104**

**Theoretical study of  $\alpha$ -synuclein by a biological complexity approach**

García-Romero, Ezra Michelet; Barrientos-Salcedo, Carolina

**105**

**Structural and energetic characterization of molecular recognition of the human Abl tyrosine kinase domain**

Garcia-Curiel, Manuel Bernardo; Cruz-Castañeda, Roberto; Luviano-Jardon, Christian Axel; Garcia-Hernandez, Enrique.

**106**

**Theoretical study of anti viral agents in HAART therapy**

Márquez-Hernández, Carmen Guadalupe; Aguirre-Cabrera, Carla; Cabrera-Vivas, Blanca Martha; Ramirez-García, Juan Carlos

**107**

**Cloning and expression of the hexokinase 2 of *Entamoeba histolytica***

Alcazar-Medina, Tania Libertad; Sandoval-Carrillo, Ada; Ruiz-Baca, Estela; López-Rodríguez, Angélica María; Saucedo-Mendiola, María Leticia

**108**

**Expression of the e2 gene of human papillomavirus type 16**

Gándara-Mireles Jesús Alonso, Campos- Parga Bianca Nayeli , López-Rodríguez Angélica María, Ruíz-Baca Estela, Saucedo-Mendiola Leticia

**109**

**Thermal stability and lytic properties of Lecithin-dependent Hemolysin from *Vibrio parahaemolyticus* pathogenic for shrimp**

López-Zavala, Alonso A.; Morado-Vazquez, Luis E.; Robles-Ruíz Ana G.; Sotelo-Mundo, Rogerio R.; Arvizu-Flores Aldo A.

**110**

**Purification, characterization and inactivation of polyphenol oxidase from Mexican Golden Delicious apple (*Malus domestica*)**

Marrufo-Hernández, Norma A.; Palma-Orozco, Gisela; Beltrán-Conde, Hiram I.; Nájera, Hugo

**111**

**Spectroscopic and redox studies of Cu(II) complexes at the N-terminal of alpha and beta synuclein proteins**

Rodríguez, Esaú E.; Arcos-López, Trinidad; Trujano-Ortiz, Lidia G.; Fernández, Claudio O.; J. González, Felipe; Vela, Alberto; Quintanar, Liliana.

**112**

**Different salts effect and *Moringa oleifera* leaf extract activation on human and murine paraoxonase-1 activity**

Pedroza-Dávila, Ulrik; Pérez-Velázquez Jesús; Campos-Almazán Mara; Téllez-Valencia, Alfredo; Avitia-Domínguez, Claudia, Valdez-Solana Mónica, García-Arenas, Guadalupe; Sierra-Campos, Erick.

**113**

**Identification of redox regulation targets in triose-phosphate isomerase from *Synechocystis* sp PCC 6803**

Castro-Torres, Eduardo; Díaz-Quesada, Corina; Luis G. Brieba

**114**

**Determination of the optimal extraction process for storage proteins in seeds of chicayota (*Cucurbita argyrosperma* subsp. *sororia*)**

Herrera-Castillo, Fátima Luz María; Mares-Mares, Everardo; León Galván Ma. Fabiola

**115**

**Intraspecific venom variation of the Mojave rattlesnake (*C. scutulatus scutulatus*) from the Mexican Chihuahuan Desert**

Borja, Miguel; Castañeda-Gaytán, Gamaliel; Neri-Castro, Edgar; Strickland, Jason; Espinoza-Femmat, Jorge; Alagón-Cano, Alejandro; Pérez-Morales, Rebeca

**116**

**Proteínas reguladoras de hierro en *E. histolytica*.**

Gastelum-Martínez, Aurora Alicia; Plata-Guzmán, Laura Yuliana; Soto-Castro, Liliana; Figueroa-Angulo, Elisa Elvira; Arroyo Rossana; Garzón-Tiznado, José Antonio; Puga-Barraza, Francisco; Hernández-Valenzuela, Marco Antonio; López-Moreno, Héctor Samuel; De la Garza, Mireya; Reyes-López, Magda; León-Sicairos, Claudia

**117**

**Characterizing the structural ensemble of gamma-secretase using a multiscale molecular dynamics approach**

Aguayo-Ortiz, Rodrigo; Chávez-García, Cecilia; Straub, John E.; Domínguez, Laura

**118**

**Polymorphism pro12ala in the ppar $\gamma$ 2 gen associated with biochemical indicators and metabolic therapeutical analysis *in silico***

Motta-Pardo, Angelo; Acosta-Conchucos, Oscar

**119**

**Horizontal Gene Transfer of a triose-phosphate isomerase (TIM21) between Pacific whiteleg shrimp and their microbiome**

Martínez-Hernández, Omar; Sanchez-López, Filiberto; Brieba-Castro, Luis G.; Saab-Rincón, Gloria; López-Zavala, Alonso; Cornejo-Granados, Fernanda; López-Leal, Gamaliel; Sotelo-Mundo, Rogerio; Ochoa-Leyva, Adrián

**120**

**Finding inhibitors of shikimate dehydrogenase from methicillin resistant *Staphylococcus aureus*. Kinetic and biological activity studies.**

Enríquez-Mendiola, Daniel; Sierra-Campos, Erick; Valdez-Solana, Monica; Téllez-Valencia, Alfredo; Avitia-Domínguez, Claudia

**121**

**The Organellar DNA primase helicase from *Arabidopsis thaliana* recognizes a unique trinucleotide sequence on ssDNA and synthesizes primers for the DNA polymerase**  
Peralta-Castro, Antolín; Baruch-Torres, Noe; Diaz-Quezada, Corina; Brieba de Castro, Luis

**122**

**Role of cis-trans Proline isomerization in the function of pathogenic enterobacterial Periplasmic Binding Proteins.**  
Cortes-Hernandez, Paulina; Dominguez-Ramirez, Lenin

**123**

**Thermodynamic and kinetic characterization of the inhibition of *Escherichia coli* ATP synthase by polyphenols**

Avila-Barrientos, Luis Pablo; Mendoza-Espinosa, Paola; Cofas-Vargas, Luis Fernando; Salcedo-Barrientos, Guillermo; García-Hernández, Enrique

**124**

**Correlation between calculated and experimental thermal fluctuations of TRPV1 ion channel**

Ladrón-de-Guevara, Ernesto; Islas, León D.

**125**

**Heterologous expression of VS\_VI, a therapeutic fusion protein consisting of vasostatin 30 and vasoinhibin ii-14.1, secreted from a multicopy strain of *Pichia pastoris*.**

Calderón-Salais, Sergio; Balderas-Hernández, Victor E.; Barba-de la Rosa, Ana P.; De León-Rodríguez, Antonio

**126**

**Kinetic and structural studies on the role of metals over the activity of a Mu- Class Glutathione S-transferase from *Litopenaeus vannamei***

Escudero-García, Angela; Juárez-Martínez, Ariadna B; Rudiño-Piñera, Enrique.

**127**

**Repair of deaminated bases and AP sites initiated by Endonuclease V proceeds in a pathway that involve DNA-polymerase I in *Bacillus subtilis***

Ayala-García, Víctor M; Valenzuela-García, Luz I; Vargas-Arias, Pedro L; Brieba, Luis G; Pedraza-Reyes, M.

**128**

**Crystal structure of the endochitinase ChiA74 of *Bacillus thuringiensis* reveals a unique domain assembly**

Jimenez-Sandoval, Pedro; Juárez-Hernández, Estefania O; Barboza-Corona, José E.; Brieba, Luis G.

**129**

**Characterization of the coupling mechanism of peptide variants of Discrepin on Kv4.3 potassium channel.**

**Molecular Dynamics Simulations**

Montero-Dominguez, Andrei; Mares-Sámano, Sergio; Pérez-Mejía, Ana E.; Garduño-Juárez Ramón

**130**

**The transcriptome of *Palaemonetes argentinus* as a tool for protein structure and evolution studies**

Sotelo-Mundo, Rogerio; Garcia, C. Fernando; Pedrini, Nicolas; Lavarias, Sabrina; Fernandez-Gimenez, Analia; Lukaszewicz, German; Lopez-Zavala, Alonso; Ochoa-Leyva, Adrian; Criscitiello, Michael F.

**131**

**Performance assessment of several enhanced sampling methodologies used in molecular dynamics simulations.**

Amador Herrera, Jorge Alejandro; Arciniega Castro, Marcelino

**132**

**Virtual screening in the domain n of protein E1 of HPV16**

Corral-Pérez, Karina; Ruiz-Baca, Estela; López-Rodríguez, Angélica; Saucedo-Mendiola, María Leticia

**133**

**Peptidomic analysis of chicayota seed globulins obtained by ultrasonic hydrolysis**

Rocha-Mendoza, María Azucena; León Galván, Ma. Fabiola

**134**

**Recombinant expression and purification of wild-type and mutants of trypsin III from sardine (*Sardinops sagax caerulea*)**

Ramos-Osorio, Yamel; Cota-Nuñez, Iris; Hoyos-González, Nallely; Casas-Flores, Sergio; Osuna-Amarillas, Pablo; Carretas-Valdez, Manuel; Arvizu-Flores, Aldo.

**135**

**Specie-specific inactivators of triosephosphate isomerase from *Trypanosoma brucei***

Vazquez-Raygoza, Alejandra Guadalupe; Avitia-Domínguez, Claudia Isela; Betancourt-Conde, María Irene; Hernández-Campos, María Alicia; Téllez-Valencia Alfredo

**136**

**Biosynthesis of scorpion toxin (tamapin) mutants against metastatic cancer cells**

Mayorga-Flores, M; Melchor-Meneses, CM; Toledano-Magaña, Y; Galindo-Murillo, R; Del Río Portilla, JF.

**137**

**Quantitative measurement of expansin activity: biochemical characterization of the fungal protein ExlX1 from *Schizophyllum commune***

Tovar-Herrera, Omar Eduardo; Martínez-Anaya, Claudia

**138**

**Insomnia drug design. Searching potential Orexine antagonist through virtual screening.**

Rosales-Ronquillo, Humberto Israel; Avitia-Domínguez, Claudia Isela; Cisneros-Martínez, Jorge Arturo; Gómez Palacio-Gastelum, Marcelo; Téllez-Valencia, Alfredo.

**139**

**A single mutation enables LAO Binding Protein to visit a closed state without ligands**

Granados, Diego S.; Banda-Vazquez Jesús; Sosa-Peinado Alejandro

**140**

**rGM-CSF bacterial expression under oscillating conditions of glucose, dissolved oxygen and pH**

Reynoso-Cereceda, Greta I.; Valdez-Cruz, Norma A.; Trujillo-Roldán, Mauricio A.

**141**

**Finding potential PTP1B inhibitors through pharmacophore modeling**

Campos Almazán, Mara Ibeth; Téllez Valencia, Alfredo; Sierra Campos, Erick; Valdez Solana, Mónica Andrea; Cisneros Martínez, Jorge Arturo; Gómez Palacio Gastelum, Marcelo; Avitia Domínguez, Claudia Isela.

**142**

**Cloning, expression, and characterization of the binding to cellulose, of the modular expansin ScExl1-CBM from *Sorangium cellulosum*, and four truncated mutants.**

Salazar-Cortés, Juan; Martínez-Anaya, Claudia

**143**

**Deltalactoferrin a transcription factor controled by a crosstalk between several post-translational modifications**

Escobar-Ramirez, Adelma; Vercoutter-Edouart, Anne-Sophie; Huvent, Isabelle; Mortuaire, Marlène; Tony, Lefebvre; Pierce, Annick

**144**

**The zwitterionic state drives the dipeptide self-assembly**

González-Díaz, Norma E.; López-Rendón, Roberto; Ireta-Moreno, Joel

**145**

**Design of antibiofilms peptides from samples of patients with diabetic foot**

Salazar-Aguilar, Airam Soledad; Barrientos Salcedo, Carolina

**146**

**The production and O-mannosylation of a recombinant glycolantigen in *Streptomyces lividans* is affected by the oxygen transfer rate in submerged culture.**

Gamboa-Suasnávar, Ramsés A.; Valdez-Cruz, Norma A., Marín-Palacio, Luz D., Klöckner, Wolf; Büchs, Jochen; Trujillo-Roldán, Mauricio A.

**147**

**Inhibition of shikimate dehydrogenase from methicillin resistant *Staphylococcus aureus*.**

Urban-Martínez, José Luis; Valdez-Solana, M; Sierra Campos, Erik; Téllez-Valencia Alfredo; Avitia-Domínguez, Claudia Isela.

**148**

**AKT3 homology model: structural approach towards the search for inhibitors**

Sanabria-Chanaga, Elkin; Hernandez-Campos, Alicia; Castillo, Rafael

**149**

**Molecular recognition between the flavivirus protein NS3 and Alix a host protein**

Gabriel-León, José-Correa; Martínez, Marlet; Montaño, Sarita

**150**

**Análisis in silico de proteínas de superficie de *Trypanosoma cruzi***

Robles Ramirez, Oscar; Barrientos Salcedo, Carolina

*Jueves*

# Comité organizador

**Claudia Avitia Dominguez**

Facultad de Medicina y Nutrición UJED

**Luis Brieba de Castro**

CINVESTAV

**D. Alejandro Fernández Velasco**

Universidad Nacional Autónoma de México

**Mariana Peimbert Torres**

Universidad Autónoma Metropolitana

**Erik Sierra Campos**

Facultad de Ciencias Químicas G.P. UJED

**Alfredo Tellez Valencia**

Facultad de Medicina y Nutrición UJED

# Comité local

**Mayra Cisneros Quintero**

Facultad de Medicina y Nutrición UJED

**Susuky Mar Aldana**

Facultad de Medicina y Nutrición UJED

**Martha Quintanar Escorza**

Facultad de Medicina y Nutrición UJED

**Estela Ruiz Baca**

Facultad de Ciencias Químicas UJED

**Iván Salazar**

Facultad de Medicina y Nutrición UJED

**Mónica Valdez Solana**

Facultad de Ciencias Químicas G.P. UJED

*Jueves*



**Presidente**

**Irene Beatriz Castaño Navarro**

*División de Biología Molecular, IPICYT*



Red  
Estructura  
Función y  
Evolución de  
Proteínas

**Responsable Técnico**

**Liliana Quintanar Vera**

*Departamento de Química, CINVESTAV*



**Rector**

**Oscar Erasmo Návar García**

*Jueves*