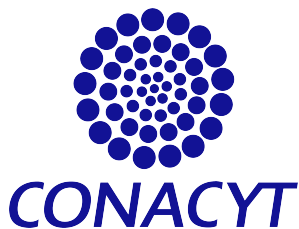




6^o CONGRESO DE LA RAMA DE FISICOQUÍMICA, ESTRUCTURA Y DISEÑO DE PROTEÍNAS



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 virus 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 allostereism 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

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 Juárez 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 H₂S and Akt on the mechanism of action of vasodilators isoxsuprine 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, Maria 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-Martinez, 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; Rodríguez 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-Jimenez, 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-Sanchez, Jose Luis; Caro-Gomez, Luis; Briebe-de Castro, Luis G; Arroyo-Verastegui, Rossana; Ortega-Lopez, Jaime; Rojo-Dominguez, Arturo; Benítez-Cardoza, 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-Espinosa, 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

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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.

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.; Ezquerro-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; Cossio-Ayala, Mayte; García-Hernández, Enrique

39

Thermosonication 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

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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.; Martiñón, Susana; Medina-Mora, María Elena; Mixcoha, Edgar

44

Application of the nonbonded dummy model of Cu(ii) in metallopeptides: plastocyanin and 1-16 amyloid β -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-Bolóm, 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 GlcN6P 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^{2+} + 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 phosphomimic modification on the structure and dynamics of an intrinsically disordered protein

Ramírez-Martínez, Marco; Pastor-Colón, Nina

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

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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

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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

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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

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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

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

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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.

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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

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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