SAB 2020

Biofísica en tiempos de COVID-19

Libro de Resúmenes

3 y 4 de diciembre de 2020
Argentina

Sociedad Argentina de Biofísica
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Ernesto Ambroggio, Soledad Celej, Axel Hollmann, Juan Pablo Acierno

Diseño de Tapa y Logo

Comité Organizador

Asistencia Técnica Web

Juan Pablo Acierno

Sociedad Argentina de Biofísica

Member of the International Union for Pure and Applied Biophysics

Primeras jornadas virtuales de la Sociedad Argentina de Biofísica

3 y 4 de diciembre 2020

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Welcoming words

Dear members, participants and friends,

This is a very special year in our lives. The Covid-19 pandemic has changed the way in how societies communicate, imposing modern modes of virtual interaction. Naturally, SAB was not unsympathetic to this turn of events and, therefore, in the spirit of maintaining our yearly gathering, we faced the challenge of organizing these first virtual sessions of the Argentinean Society of Biophysics.

We sincerely hope that during this two-day meeting, we enjoy this new proposal, where keynote lectures, lightning talks and round tables will be shared as open access events contributing to scientific outreach activities to the community. Not only these open sessions will be held, but also all registered participants (SAB members and invited colleagues) will be able to participate online in two workshops, presenting their scientific research as mini-videos and being able to discuss with pairs and mentors through separate virtual channels.

Lastly, we all know that this pandemic situation has already had a terrible impact on the economic situation of our country. Therefore, we thank in advance to all participants for their personal contributions along these days and to everybody for sharing their research and joining the scientific discussions.

The SAB Executive Council

Scientific programme

Thursday, December 3

9:45 – 10:00 h *Entry to virtual platform*

10:00 – 10:10 h ***Opening Ceremony***

José María Delfino, IQUIFIB-CONICET, FFyB-UBA, Buenos Aires, Argentina

10:15 – 12:15 h ***Poster session I***

Only for registered participants

12:15 – 12:30 h ***Lightning talks***

Chair: José María Delfino

Horizontal and Collaborative against the clock work in pandemic: Production, characterization and distribution of a low-cost SARS-CoV-2 antigen by the Argentinian AntiCovid Consortium

María Florencia Pignataro, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, Buenos Aires, Argentina

12:30 – 13:45 h *Lunch*

13:45 – 14:00 h *Entry to virtual platform*

14:00 – 16:00 h Round Table 1 – Enseñanza virtual y presencial en biociencias

Chairs: Irene Mangialavori, Lía Pietrasanta and José María Delfino

Intervenciones educativas en línea: Desafíos y potencialidades

Karina Alleva. Facultad de Farmacia y Bioquímica, UBA, Buenos Aires, Argentina

Educomunicación ubicua para el nuevo escenario de convivencia

Fernando Irigaray. Director de la Maestría Digital Interactiva, Facultad de Ciencia Política, UNR, Rosario, Argentina

Los desafíos de evaluar con mediación tecnológica. Escenarios y propuestas

Carina Lion. Facultad de Filosofía y Letras, UBA. Instituto de Investigaciones en Ciencias de la Comunicación, Buenos Aires, Argentina

La enseñanza de ciencias experimentales en tiempos de pandemia: ¿es posible evaluar aprendizajes desde la virtualidad?

Marcelo Mariscal. Vicedecano, Facultad de Ciencias Químicas, UNC, Córdoba, Argentina

16:00 – 17:00 h Keynote Lecture

Chair: José María Delfino

ECA2: ¿ángel o demonio? Mariela Gironacci. IQUIFIB, UBA, Buenos Aires, Argentina

Friday, December 4

8:45 – 9:00 h *Entry to virtual platform*

9:00 – 12:00 h ***Interactive workshops***

Only for registered participants

Workshop 1: Uniprot: explorando secuencias y función de proteínas

Cecilia Arighi. Department of Computer & Information Sciences, University of Delaware and Department of Biochemistry and Molecular & Cell Biology, Georgetown University Medical Center

Workshop 2: Biofísica de Biomembranas

Ernesto Ambroggio (CIQUIBIC-UNC, Córdoba), Luis Bagatolli (INIMEC-UNC, Córdoba), Laura Fanani (CIQUIBIC-UNC, Córdoba), Axel Hollmann (CIBAAL-UNSE, Santiago del Estero) and Natalia Wilke (CIQUIBIC-UNC, Córdoba).

12:00 – 13:00 h *Lunch*

13:00 – 14:50 h ***Poster session II***

Only for registered participants

14:50 – 15:00 h *Entry to virtual platform*

15:00 – 17:00 h ***Round Table 2 – Políticas integrales para la equidad de géneros en ciencia y técnica***

Chairs: M. Natalia Lisa, Noelia Burgardt and M. Soledad Celej

***Paula Lenguita*.** Responsable del Programa de Género Agencia I+D+i, Argentina

***Victoria Prieto*.** Comisión de Género y Comité de Calidad con Equidad Institut Pasteur de Montevideo, Comisión de Género Pedeciba (Programa de Desarrollo de Ciencias Básicas), Uruguay

***Erica Hynes*.** Diputada provincial de Santa Fe por el Frente Progresista Cívico y Social. Especialista en tecnología de alimentos y política argentina, Argentina

***Victoria Tignino*.** Secretaria ejecutiva del Programa Nacional para la Igualdad de Géneros en Ciencia y Tecnología del MinCyT, Argentina

***Azul Hermida*.** Integrante del Observatorio de violencia laboral y de género (OVLG) y Comisión de Igualdad de Oportunidades y Trato (CIOT) de CONICET, Argentina

17:00 – 18:00 h Keynote Lecture

Chair: Lía Pietrasanta

Desarrollo de un suero equino hiperinmune para el tratamiento de COVID-19 en Argentina. Fernando Goldbaum. CRIP, Inmunova, UNSAM, Buenos Aires, Argentina

18:00 – 18:30 h Poster Awards and Closing Ceremony

M. Soledad Celej and José María Delfino

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Inhibition of lanosterol 14 alpha-demethylase: Molecular modeling study of triazole derivatives acting against the phytopathogen *Botrytis cinerea*

Sirur Flores J[a], Parravicini O[a], Rojas S[a], Gutiérrez LJ[a], Herrera Cano N[b], Feresin G[b], **Andújar S**[a]

a - Facultad de Química, Bioquímica y Farmacia, Universidad Nacional de San Luis, Instituto Multidisciplinario de Investigaciones Biológicas (IMIBIO-SL)

b - Instituto de Biotecnología, Facultad de Ingeniería, Universidad Nacional de San Juan, CONICET–CCT

Botrytis cinerea is a phytopathogenic fungus that causes the gray mold disease. It is considered a main factor in post-harvest losses in fresh fruit crops, causing serious economic losses in the agricultural industry. In addition, it has become an important model for the molecular study of necrotrophic fungi. Although there are fungicides for its control, many of them have failed since *B. cinerea* has evolved a variety of infection mechanisms due to its genetic variability. In this regard, triazoles have been used for the control of several pathogenic fungi. These compounds act as inhibitor of the lanosterol 14 alpha-demethylase, a cytochrome p450 (CYP54B)-dependent enzyme system involved in the synthesis of ergosterol.

In order to explain the biological behavior of different CYP54B-triazole complexes we performed a combined molecular modeling study. In this way, we determined the conformational aspects of the currently available triazole antifungal agents when complexed with CYP54B. Furthermore, a new series of novel triazole derivatives was synthesized and their inhibitory activity was assessed. Some of them showed strong inhibitory effects comparable to that observed for commercial antifungal drugs. The molecular modeling study was carried out in three stages. First, we conducted molecular docking calculations. Next, we performed molecular dynamics (MD) simulations and free energy of the different complexes was calculated. Finally, we performed a per-residue analysis in order to identify the amino acids involved in the intermolecular interactions of the complexes.

Our molecular modeling study indicated that all active compounds are bounded in a similar spatial arrangement. Thus, it is reasonable to assume that the compounds studied here interact with the same region of the enzyme. MD simulations enable us to explain the different activities displayed by these compounds. The main stabilizing interactions are Tyr101, Thr105, Tyr115, Phe208, Ala287, His290 and Ile353.