

Session Program

1-3 Dec 2026



International Meeting on

Theoretical and Experimental Chemistry:

How to Design and Study
New Compounds with
Potential Application

International Meeting on Theoretical and Experimental Chemistry: How to Design and Study New Compounds with Potential Application

Session 2. Chair: Monika Kijewska

Wrocław, Poland, WEBINAR (ONLINE CONFERENCE, FREE OF CHARGE, time zone: CET, UTC+1)
ul. F. Joliot-Curie 14 50-383 Wrocław, Poland

Tuesday 1 December

14:00

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Session |**Location:** Wrocław, Poland, WEBINAR (ONLINE CONFERENCE, FREE OF CHARGE, time zone: CET, UTC+1), ul. F. Joliot-Curie 14 50-383 Wrocław, Poland

14:00–14:30

From Molecular Dynamics to Machine Learning: A Local-to-Global Strategy for Predicting Protein-RNA Binding Affinity

Speaker

Dr Parisa Aletayeb

14:30–15:00

Design and synthesis of (2-)piperidinyl methanol-derived quinolines and their structural determinants for antiparasitic activity

Speaker

Dr Diogo Rodrigo Moreira

15:00–15:30

Charting Natural Product Chemical Space: Cheminformatics and Artificial Intelligence for Drug Discovery

Speaker

Prof. José L. Medina-Franco

15:30