Proceedings of the
Merck Young Chemists' Symposium
XXIII edition

Edited by: I. Arduino, C. Bonfio, M. Bonomo, M. Da Pian, A. Dall'Anese, I. Fierri, A. M. Fiore, A. Marotta, M. Mendolicchio, C. M. Montone, E. Paone, F. Pizzetti, A. Polo, L. Rivoira, A. Rossetti, I. Romeo, M. Sambucci, C. Sergi, S. Tortorella, F. Vincenti.

ISBN: 978-88-94952-50-6

Welcome to the 23nd edition of the Merck Young Chemists' Symposium (MYCS), formerly also known as SAYCS and MEYCS. This international conference is organized by the Young Group of Società Chimica Italiana (SCI Giovani) and the National Interuniversity Consortium of Materials Science and Technology (INSTM) with the financial support from Merck and several other sponsors, that you will meet during the conference.

The symposium covers all the disciplines of Chemistry, aiming to connect young researchers, inspire new ideas, and potentially trigger new collaborations. With the contributions of our five invited plenary speakers, and the international environment guaranteed by the presence of people coming from different countries, we truly hope that you will all enjoy this great event with us. We have worked hard to organize this meeting with 230 participants, prioritizing high-level scientific topics and other themes of crucial importance in our modern society. Thank you for the great trust shown towards SCI Giovani, Merck and all our supporters. Enjoy the conference and have a nice stay with us!

Marta Da Pian

SCI Giovani Coordinator

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FL048

Novel 6,7-dimethoxy-4-piperazinylquinoline derivatives as promising antibacterial agents against Staphylococcus aureus

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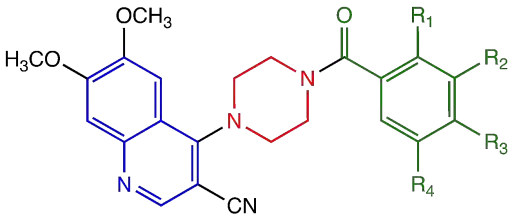
In the field of medicinal chemistry, significant research efforts are dedicated to developing new antibiotics targeting clinically validated enzymes such as DNA gyrase and topoisomerase IV, which are crucial for bacterial DNA replication. Among the frontline classes of agents against broad-spectrum bacterial infections, quinolines and their analogues are particularly effective in inhibiting both targets [1]. However, the recent emergence of resistance, due to mutations that impair drug accumulation in bacterial cells and target recognition, has driven the development of new approaches for discovering innovative inhibitors. Drawing on our experience in the synthesis of quinoline-based compounds, we have focused on the study of piperazinylquinoline derivatives with potential antibiotic activity [2].



1a-k

Figure 1. General structure of 6,7-dimethoxy-4-piperazinylquinoline compounds **1a-k**.

Induced Fit Docking (IFD) studies were performed on the DNA gyrase of *S. aureus* (PDB code 6FM4), to assess protein-ligand interactions between our molecular dataset and the target binding sites. The 6,7-dimethoxy-4-piperazinylquinoline compounds **1a-k** (Figure 1) showed remarkable binding affinity to the DNA gyrase comparable to that of the reference ligand. The selected molecules were synthesized using appropriate synthetic strategies and characterized spectroscopically. Preliminary antibacterial tests showed promising activity of piperazinyl quinolines against *S. aureus*, known for its resistance to many conventional antibiotic therapies. Further *in vitro* studies are currently underway to elucidate the mechanism of action and validate the efficacy and therapeutic potential of these compounds.

[1] K. B. Patel, P Kumari, *Journal of Molecular Structure* (2022) 133634

[2] G. La Monica, G. Pizzolanti, C. Baiamonte, A. Bono, F. Alamia, F. Mingoia, A. Lauria, A. Martorana, *ACS Omega* (2023) 6;8(50):48582.

Società Chimica Italiana

Società Chimica Italiana (SCI) is a scientific association that includes more than 5000 members. It was founded in 1909 and erected as a Legal Institution with R.D. n. 480/1926. SCI members carry out their activities in universities, public and private research institutes, schools, industries, or as freelancers. They are joined not only by the interest in chemical sciences, but also by the desire to contribute to the cultural and economic growth of the national community, within a global framework, improving the quality of human life and the protection of the environment. SCI is organized in Divisions and Sections: Divisions are thematic branches, gathering members working in the same field or sharing the same scientific interests; Sections are local branches, gathering people working or living in the same territory.

For new members

All the participants to the *Merck Young Chemists' SymposiumXXII edition* are (or are going to be) SCI members. Those who were not yet SCI members before the conference, must fill the request form included in the Conference bag in order to complete the membership procedure. Those who chose the 1-year subscription will be enrolled until 31/12/2024; those who chose the 2-year subscription will be SCI members up to the end of 2025.

SCI Giovani / SCI Young

All SCI members younger than 35 years old belong to SCI Giovani, an interdisciplinary group organizing multiple initiatives precisely devoted to youngers, such as prizes, workshops, and the very congress you are attending.

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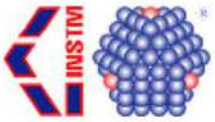

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