Digitalization and the Medicinal Chemistry – Chemical Biology Continuum

Medicinal chemistry is a constantly developing science and rapidly expands towards biology, providing pharmacological and imaging tools to set up assays, interrogate cellular pathways and explore various pathologies. It also develops quickly to take advantage of the new technologies enabled by digitalization. These forces will shape the evolution of medicinal chemistry over the next few years, and represent a fantastic opportunity to take advantage of synergies with other disciplines and increase scientific creativity.

In this sense, the 55th edition of the International Conference on Medicinal Chemistry, RICT 2019, is a perfect occasion to keep abreast of the newest developments: Focusing on the interface between Chemical Biology and Drug Discovery, it also includes a session on artificial intelligence.

A successful scientific career in drug discovery increasingly requires awareness of the full scientific continuum across medicinal chemistry and chemical biology. Research projects can be looked at as intellectual adventures starting with the most basic biological questions related to target selection, for which medicinal chemists can provide the necessary pharmacological tools. Subsequently, medicinal chemists play a critical role in identifying and optimising drug candidates, as well as in providing imaging tools for characterisation of drug candidates in the clinic. The extended role of medicinal chemists over the life of a project creates opportunities for multiple impactful contributions. It also requires an understanding of the needs of all their scientific partners, from in vitro biologists to pharmacologists and clinicians. It is a tall order, and what makes medicinal chemistry scientifically so fascinating.

The second trend, digitalization, is beginning to enable a different approach to medicinal chemistry. While some applications are still in their infancy, many begin to show their potential to free chemists' minds from repetitive and low-value activities. This will give us more time to address the right problems and take full advantage of our creativity. There are two main applications of digitalization: The first is purely related to data acquisition, data management and interpretation, as illustrated by automatised synthesis systems, electronic notebooks, database exploration tools, and recommender programs. The reliability and efficiency of these tools is improving quickly, and many are already implemented. In contrast, applications related to true artificial intelligence still need to demonstrate their usefulness in chemical biology and medicinal chemistry, and the session on this topic will be a good starting point to discuss the potential of future applications. The convergence of life sciences and digital technologies is clearly happening: wearable diagnostics, robotics, big data mining from clinical trials and many other examples are becoming reality. At some point, AI will also influence medicinal chemistry.

Another area, unrelated to chemical science, impacts the practice of medicinal chemistry: outsourcing, which has expanded from providing starting materials, to subcontracting multi-step organic synthesis and established biological assays. The cost of research, particularly in Europe and in the USA, pushes both academia and industry to find alternatives for segments of organic chemistry that have low added value, and for standard profiling activities. The time of researchers is precious; it is important that they do not have to spend hours on activities that can be done faster and cheaper by a machine or a service lab, sparing their time for creative work – a skill that won't be replaced by artificial intelligence and robotic systems anytime soon. It is worth talking to exhibitors to keep abreast of new offers, and to let them know which services are expected from them.

This conference is attracting a number of highly influential researchers, including Herbert Waldmann, who will deliver the Paul Ehrlich Award Lecture. There will be sessions on cancer and therapeutic breakthroughs, as well as on complex carbohydrates, antibodies and protein engineering. While low-molecular weight compounds will remain the mainstay of medicinal chemistry, these new areas provide added opportunities to demonstrate its impact. The combination of biologics and skillful chemical optimisation provides access to novel classes of drug candidates, with the potential to address diseases that were so far difficult to treat. This is scientifically very promising.

Such an environment provides key opportunities for networking, a must in a community where collaboration is a requirement for successful funding and scientific impact. By organising RICT on an annual basis, the Société de Chimie Thérapeutique contributes to a lively medicinal chemistry community. They deserve our continuous support and appreciation for bringing together such an attractive program.

I wish you a very successful participation in RICT 2019, enjoying new scientific insights among a growing network of medicinal chemistry and chemical biology enthusiasts.

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