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Welcome to Volume 12 of *Future Medicinal Chemistry*

Harriet Wall*,¹

¹Future Science Group, Unitec House, London, N3 1QB, UK

*Author for correspondence: h.wall@future-science.com

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We would like to welcome our readers to Volume 12 of *Future Medicinal Chemistry*! In this foreword, we will discuss some of the highlights that the journal has seen over the last 12 months – as well as what there is to expect in 2020. Thanks must be given to our editorial board members, authors, peer reviewers and readers – we look forward to continuing to work with all of our contributors again in 2020.

Content Highlights of 2019

One of our most read articles this year, ‘*Peeking at G-protein-coupled receptors through the molecular dynamics keyhole*’ [1], reviewed the main contributions of molecular dynamics (MD) to the study of GPCRs. Where most systems can be partially explained using static parameters, MD allows for the time-dependent description of biological processes – giving rise to a more accurate description of GPCR–ligand recognition, activation mechanisms and biased agonism. Understanding the dynamics of a target is integral to the development of related drugs – making MD a key asset to this field.

In addition to this, a wide range of review style articles were published in 2019, which aimed to highlight recent significant advances in research, ongoing challenges and unmet needs. Of note, ‘*Recent progress on inhibitors of the type II transmembrane serine proteases, hepsin, matriptase and matriptase-2*’ [2] was particularly popular among our readers. This review focused on the structure–activity relationships (SARs) of type II transmembrane serine protease inhibitors, as well as the design strategy for these small molecules.

Primary research plays an integral role in the development of medicinal chemistry. Many research articles were published in *Future Medicinal Chemistry* last year – popular titles among these included ‘*Discovery of arginine-containing tripeptides as a new class of pancreatic lipase inhibitors*’ [3], ‘*Synthesis and evaluation of novel 7H-pyrrolo-[2,3-d]pyrimidine derivatives as potential anticancer agents*’ [4] and ‘*A structure-guided molecular chaperone approach for restoring the transcriptional activity of the p53 cancer mutant Y220C*’ [5].

In addition to our core content of Reviews, Perspectives and Original Research, the journal also featured content on topical areas of debate relevant to academia and industry; including Editorials, Commentaries, and more. Of interest is ‘*Multitarget-directed ligands for neurodegenerative diseases: real opportunity or blurry mirage?*’ [6]. In this Editorial, Mohamed Benchekroun, Université Paris-Saclay (Paris, France) and Samuele Maramai, University of Sussex (Brighton, UK) discussed alternatives to the mono-target approach for the treatment of neurodegenerative diseases. Multitarget-directed ligands have the potential to modulate multiple biological processes – once an effective combination of targets has been selected, drug candidates can be developed which provide synergistic therapy for disease.

Further, Elisabetta Chiarparin, AstraZeneca (Cambridge, UK), discussed the analysis of free ligand conformations and trends in their SARs in the popular commentary piece entitled ‘*Experimental free ligand conformations: a missing link in structure-based drug discovery*’ [7].

As with last year, we have seen a huge engagement in the topic of computational chemistry in drug discovery. Popular articles concerning this include ‘*Deep learning for molecular generation*’ [8], ‘*Second-generation activity cliffs identified on the basis of target set-dependent potency difference criteria*’ [9], and ‘*Computational chemical biology on the rise*’ [10]. From QSAR modeling to big data, computational chemistry has become an essential tool for modern

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Figure 1. Percentage readership by geographic location.

Figure 2. Percentage authorship by geographic location.

day drug discovery – and the interest we have seen in this field proves its importance for the future of medicinal chemistry.

Demographics

Future Medicinal Chemistry has seen a continued increase in readership over the past year, with the majority of readers based in Asia, followed by Europe and North America (Figure 1).

Future Medicinal Chemistry continues to receive submissions from all around the globe. The authorship demographics largely reflect that of our readership – with the majority of authors submitting from institutions in Europe, Asia and North America (Figure 2).

Article outreach & online presence

Future Medicinal Chemistry continues to be active across social media, and we are keen for you to engage. Follow us on Twitter at @fsgfmc [11] and on LinkedIn [12] to stay updated with our latest content – including our journal highlights and the latest medicinal chemistry news.

We also recommend you to get involved through our partnered digital site, RxNet [13], which provides a free interactive resource for you to engage with. RxNet covers up-to-date news, views and research on the entire drug discovery pipeline. The site posts regular updates on developments in medicinal chemistry, including exclusive interviews from the authors of *Future Medicinal Chemistry*.

Conclusion

We appreciate the support and engagement that has been provided over the past year, and look forward to what is to come in 2020. As always, we are happy for you to submit any unsolicited articles to the journal – whether they are original research, reviews or opinion pieces. If you have a submission that you would like us to consider, you can find details on article preparation or submission online [14] or get in touch.

Finally, we would like to thank everyone for their continued feedback and support – we look forward to working with all of you over the coming year.

Financial & competing interests disclosure

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References

1. Deganutti G, Moro S, Reynolds CA. Peeking at G-protein-coupled receptors through the molecular dynamics keyhole. *Future. Med. Chem.* 11(6), 599–615 (2019).
2. Damalanka VC, Janetka JW. Recent progress on inhibitors of the type II transmembrane serine proteases, hepsin, matriptase and matriptase-2. *Future. Med. Chem.* 11(7), 743–769 (2019).
3. Stefanucci A, Luisi G, Zengin G. Discovery of arginine-containing tripeptides as a new class of pancreatic lipase inhibitors. *Future. Med. Chem.* 11(1), 5–19 (2019).
4. Liu YM, Chen CH, Yeh TK, Liou JP. Synthesis and evaluation of novel 7H-pyrrolo-[2,3-d]pyrimidine derivatives as potential anticancer agents. *Future. Med. Chem.* 11(9), 959–974 (2019).
5. Bauer MR, Jones RN, Tareque RK. A structure-guided molecular chaperone approach for restoring the transcriptional activity of the p53 cancer mutant Y220C. *Future. Med. Chem.* 11(19), 2491–2504 (2019).
6. Benchekroun M, Maramai S. Multitarget-directed ligands for neurodegenerative diseases: real opportunity or blurry mirage? *Future. Med. Chem.* 11(4), 261–263 (2019).
7. Chiarparin E, Packer MJ, Wilson DM. Experimental free ligand conformations: a missing link in structure-based drug discovery. *Future. Med. Chem.* 11(2), 79–82 (2019).
8. Xu Y, Lin K, Wang S. Deep learning for molecular generation. *Future. Med. Chem.* 11(6), 567–597 (2019).
9. Hu H, Stumpfe D, Bajorath J. Second-generation activity cliffs identified on the basis of target set-dependent potency difference criteria. *Future. Med. Chem.* 11(5), 379–394 (2019).
10. Brown JB, Bajorath J. Computational chemical biology on the rise. *Future. Med. Chem.* 11(1), 1–3 (2019).
11. Future Medicinal Chemistry, Twitter page (2020). twitter.com/fsgfmc
12. Future Medicinal Chemistry, LinkedIn group (2020). www.linkedin.com/groups/2822505
13. Rx Net (2020). www.rx-network.com/
14. Future Medicinal Chemistry (2020). www.future-science.com/loi/fmc