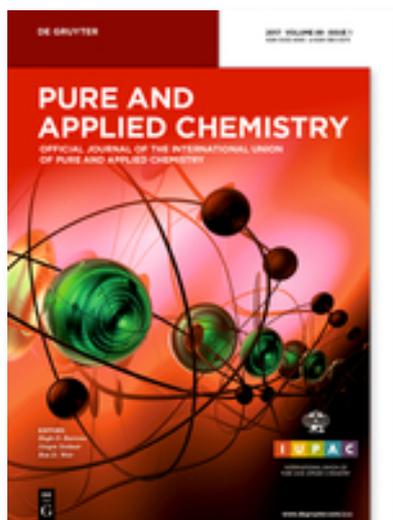


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# Medicinal chemistry in the new millennium. A glance into the future

**Paul W. Erhardt**

**Published Online:** 2009-01-01 | **DOI:** <https://doi.org/10.1351/pac200274050703>

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The future of medicinal chemistry as both a pure and an applied science has been

considered relative to trends that are already having a significant impact upon drug discovery and development. After quickly reviewing how medicinal chemistry has been practiced to date, topics considered into the future include: pursuing therapeutic efficacy, addressing 3D structure within database settings, assuring absorption, directing distribution, controlling metabolism, optimizing elimination, and avoiding toxicity. It is suggested that as the exploration of these topics proceeds into the new millennium by deploying combinatorial chemistry coupled to high-throughput screening, medicinal chemistry will play a key role as a central interpreter of the underlying structure–activity relationships such that the overall process of drug discovery and development will be knowledge-generating. As fundamental knowledge accumulates across all of these areas, virtual approaches will eventually become firmly anchored to experimental and theoretical databases having validated clinical predictability. The potential impact of some of the recent trends in process chemistry, and in analytical chemistry using X-ray diffraction as an exemplary method, are additionally highlighted before reiterating the article's major points in a summary section. From this purview, the summary also considers the education of future medicinal chemists, notes potential issues related to the future of pharmaceutical-related intellectual property, and concludes by alluding to a brewing paradox between enhanced knowledge and enhanced molecular diversity relative to the future discovery of new drugs.

## About the article

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