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EDITORIAL NOTES

Editorial

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Introduction

This is a rare special issue of JCAMD, dedicated to Yvonne Martin. We are using her recent retirement from Abbott as an excuse to recognize and honor her founding role in computer-aided molecular design, her leadership, her example, and her accomplishments.

Yvonne is one of founders of the field of computer-assisted drug design. There have been other highly accomplished contributors from academia, pharmaceutical companies, and the software industry. However, Yvonne is unique among them not only in her early involvement but also because she has in essence spanned all three areas. It is clear from her work that her goals have been first and foremost to solve problems. She has attacked real world problems faced by her company and the industry as a whole without regard of whether it could be addressed by her prior expertise or a particular approach. When faced with a problem, she found the best way of approaching it, whether that was by using available tools, developing her own, collaborating with others, or learning a new field, often combining all of these.

So many are now applying computational methods and there are so many programs and publications that it could almost be possible to forget that Yvonne set the path for us all, if in fact her contributions had not been so many, so steady, and so significant. Of course, we can not separate QSAR from Yvonne. However, she also pioneered the use of molecular graphics, structure-based drug design, molecular property analysis, combinatorial chemistry, pharmacophore analysis, and similarity analysis, among others. It is fair to say that if Yvonne has not developed an expertise in a method, it probably has not been of direct application to drug discovery.

Many of the results of Yvonne's scientific career are recorded in her 135 publications, in addition to her innumerable conference presentations around the world. Thus far (as of 25th October 2006), her seven books, 60 research articles, 61 book chapters and seven patents have attracted 2798 citations in the Thomson ISI Science Citation Index. These citations have appeared across the medicinal chemistry and chemoinformatics literatures, with the top-five journals for citations to her work being *Journal of Medicinal Chemistry*, followed by *Journal of Chemical Information and Computer Sciences*, *Journal of Computer-Aided Molecular Design*, *Quantitative Structure-Activity Relationships* and then *European Journal of Medicinal Chemistry*.

Yvonne played a key role in the early days of QSAR in publicising the strengths of the new techniques that were then becoming available to the practicing medicinal chemist. It is thus hardly surprising that her most cited publication is her 1978 book on *Quantitative Drug Design* [1]; this has received 497 citations, with its continuing importance being reflected by the five citations it has attracted even in 2006. There are a further 18 publications that have attracted more than 50 citations, these covering not just specific aspects of chemoinformatics in which she has made significant contributions such as molecular similarity, pharmacophore mapping molecular

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diversity analysis and 3D substructure searching, but also molecular modeling and medicinal chemistry more generally (see, e.g., [2–10]).

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It goes without saying for anyone even on the periphery of our field that Yvonne is highly respected and even loved by the community. It is not a coincidence or contrivance that most of the pictures on this cover show her with the other leaders in her field. In fact, it seems that it is hard to find pictures of Yvonne by herself! She is constantly surrounded by friends and respectful colleagues. She often went to other leaders in the field for advice and collaboration and likely more often the roles were reversed.

This issue is a testimony to that respect and devotion. It started with a short list of invitees who were asked to adhere to short time limits and strict deadlines. Editors are used to waiting days and weeks for responses to requests, which normally ask the recipient for time and effort. Yet, for this issue responses arrived within the hour of the initial email, 6–7 within a few hours, and all invitees shortly thereafter. There were only a few sad, deep regrets caused by busy schedules, which conflicted with this issue's editorial deadlines.

For a computational chemist in Pharma, there is no greater testimony to one's accomplishments than the praise of fellow employees. Good theory can be done without solving applied problems. Elegant science can be done without collaboration. However neither is true in her industry. That several of the papers in this issue were enthusiastically contributed by her Abbott colleagues (and unfortunately, one that could not make the deadline), shows her contributions were not only to the field and literature, but to her workplace as well.

Yvonne's career has also been defined by her considerate, courteous, thoughtful nature; qualities that elevate a great scientist to the status of statesperson. Not only has she done outstanding science, but she also delights in sharing it with whoever has the interest to ask a question, regardless of credentials.

A personal story by one of us (TRS) illustrates this. Early in the 1980s I attended my first scientific meeting as the only graduate student at a Drug Information Agency meeting on QSAR in Philadelphia. I was excited to hear the giants of the field for the first time, having known them only by their publications. At the time, Yvonne was concerned about the treatment of molecular electrostatics, an immediate point of concern for me as well. After her talk, as the large crowd of attendees swarmed from the conference room to a reception, I mustered the courage to approach her, introduce myself, and ask for additional information. She listened intently, but before she could answer an entourage of notables whisked her off. To my surprise, later in the day Yvonne, dodging several nascent conversations, made her way to the back of the room to slip me a thoughtful, detailed note answering my question and providing several solutions and references. She took time and effort to see through her answer to the question of a young student and ensure that it was delivered.

Despite her knowledge, Yvonne sits quietly through the talks of others, often preferring to ask questions in private. The center picture on the cover is indicative of the deep thought and consideration so many of us are used to seeing in her. Although she maintains a low profile during the talks of others, she is no shrinking violet. Cutting questions or implications addressed to her are met with composure, civility, and a considered scientific response

Retirement is a milestone in a career. We were all a little saddened and startled to hear that she was to retire from Abbott. Truly, few in our field have known a time without Yvonne behind her computer at Abbott Park. However, it is a relief to know that although her status at Abbott is changing, she is just doing as she has done many times before, simply shifting focus. Her active mind will not let the problems of the field rest and she has already formulated new research projects and started another book.

Let's all join the prominent contributors of this issue in thanking Yvonne for over 40 years of accomplishments, for helping to found our field, for continually showing us how to do our jobs right, for setting an example, and for promising to continue for many more years to come.