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Preface to the special issue in memory of Phil Magee

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Shortly after Phil Magee died of cancer in June 2005, Marvin Charton approached me at the end of an AGRO Division QSAR Symposium and asked me if I would be willing to help him organize a memorial Symposium in Phil's honor. I was happy to do so, and was pleased to be joined in the effort by John Block the next June. Lowell Hall and Lemont Kier offered to pitch in later that year. Sponsoring organizations eventually included the AGRO, COMP and CINF Divisions of the American Chemical Society and the Cheminformatics and QSAR Society.

Corporate sponsorship was provided by this Journal, Tripos International, Chemical Computing Group, eduSoft, ChemSilico, BioSAR Research, Hall Associates Consulting and Magee Real Estate. Their generous contributions were used to offset the travel expenses of several Symposium speakers who would not have been able participate otherwise.

The response to our calls for Symposium papers was nearly overwhelming. Over 40 abstracts for oral presentations were submitted, with several of Phil's friends and colleagues writing to express their regret at not being able to attend the meeting. The memorial symposium, formally titled "QSAR Reborn: A Symposium in Memory of Dr. Phillip Magee", consisted of six well-attended sessions spread across all five days (19–23 August 2007) of the 234th National ACS Meeting in Boston MA.

The idea of putting together the Memorial issue of the Journal of Computer-Aided Molecular Design that you now hold in your hands—physically or virtually—grew in parallel to the organization of the Symposium. Symposium participants were invited to contribute, of course, but the topics were not restricted to what had been presented at the meeting. The call for papers solicited manuscripts for the Journal from the entire community, including those who were unable to attend or to speak at the Boston meeting.

Just as for the Symposium, the response for Journal contributions was more than could reasonably have been hoped for. I trust that you will find the 15 papers collected here a fitting tribute to Phil's memory. The authors hail from across the continent and around the world, representing ten states and provinces and nine different countries. They are drawn from industrial as well as academic research organizations.

The collection begins with Marvin Charton's brief biography of the man and his place in QSAR and its history. About half of the technical papers deal with 2D descriptors and about half involve 3D (or higher) levels of description, with some comparing—or even integrating—the two levels. Topics range from the practical (e.g., predicting solubility or developing a better insecticide) to the esoteric (e.g., scaling descriptors by molecular size to decorrelate them or choosing between ligand- and receptor-based alignment methods). Most deal with QSAR at the level of the intact organism, just as Phil himself often did. The organisms considered range in size from viruses to guppies to humans. Although in vitro assays of one kind or another underlie some of the analyses, most concern physical, metabolic or toxicological properties. They include two studies on dermal sensitivity, one of which makes use of a data set compiled by Phil himself.

In summary: the papers collected here embrace nearly as broad a chunk of the QSAR world as Phil Magee did himself. I think he would approve, and hope that you will as well.

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