Richard L. Apodaca

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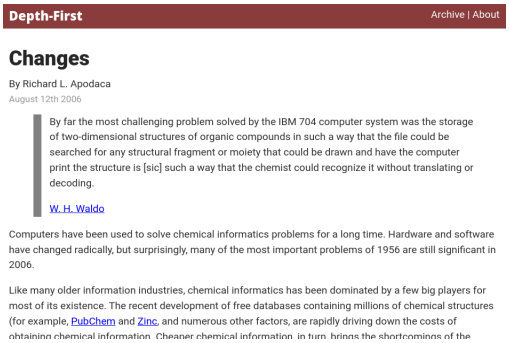
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Changes

By Richard L. Apodaca

August 12th 2006

> By far the most challenging problem solved by the IBM 704 computer system was the storage of two-dimensional structures of organic compounds in such a way that the file could be searched for any structural fragment or moiety that could be drawn and have the computer print the structure is [sic] such a way that the chemist could recognize it without translating or decoding.
>
> W. H. Waldo

Computers have been used to solve chemical informatics problems for a long time. Hardware and software have changed radically, but surprisingly, many of the most important problems of 1956 are still significant in 2006.

Like many older information industries, chemical informatics has been dominated by a few big players for most of its existence. The recent development of free databases containing millions of chemical structures (for example, PubChem and Zinc, and numerous other factors, are rapidly driving down the costs of obtaining chemical information. Cheaper chemical information, in turn, brings the shortcomings of the

If you are into openscience chemistry or chemistry blogging, then you probably heard of Rich Apodaca's Depth-First blog. Rich started blogging in 2006 but this is not how I discovered his work originally. I know that we at least already had contact in 2005, because that is when he wrote about an integration between his Octet library and the Chemistry Development Kit in the CDK News (volume 2, issue 2), *CDKTools: The CDK-Octet Bridge*. In 2006 he reviewed our use of the Open Journal System for CDK News .

But I did find we have been blogging about our work a lot. Searching for Rich gives false positives, but plenty of discussions of his work. At the same time, my name shows up multiple times in Depth-First too. Looking back at our shared history, we find, for example, Rich has blogged a lot about using the Chemistry Development Kit in Ruby .

Rich blogged about a lot of cheminformatics innovation. For example, in 2006 he was working on multi-atom bonding , such as in ferrocene, something that is even today not routinely used in cheminformatics. I replied to that in this post. Another thing he explored was embedding chemical graph notations in PNG images. In 2007 he wrote how to Never Draw the Same Molecule Twice: Image Metadata for Cheminformatics . This was picked up by several others, including me with an implementation in JChemPaint.

Another tool that I really liked was his Chempedia which collected "[f]ree chemical information resources created and reviewed by chemists". One of the things it did was link chemical names to chemical structures, e.g. for this compound . And because of the open license I was able to generate an RDF representation of Chempedia. This resulted perhaps in one of my first online SPARQL endpoints.

One and a half year ago he was confronted with health issues . Rich blogged openly about the months after that. Rereading this post is still hard, having seen cancer in action on my mother. It turned out to be cancer, a brain tumor . Just this Thursday I attended a fascinating ^{2}H NMR presentation, showing how much better we got at recognizing tumors, but Rich' MRI was obvious. He blogged for months on his plan. Until the end of May this year.

Some weeks ago I received confirmation our fear; he passed away. Richard L. Apodaca was born in 1968, completed his PhD at the University of Texas at Austin in 1996 on *Studies in enantioselective catalysis: (1) a new class of chiral C_2-symmetric bisphenols; (2) Diorganotin dihalides* (wikidata:Q131405461). Rich published multiple papers in the field of medicinal chemistry (see his Scholia profile), was very active in open science and held many patents. His latest work was about *Balsa: A Compact Line Notation Based on SMILES* (see doi:10.26434/chemrxiv-2022-01ltp).

The Depth-First blog has a CC-BY 2.0 license and perhaps Rogue Scholar can archive it? It helps us remember Rich and his contributions to open science cheminformatics.