

## Foreword

One of the real perks of this job is being able to put together a Special Issue honoring the career of a central figure in Mass Spectrometry for the past three decades. That certainly is the case here, where the honoree is Alan Marshall whose career is synonymous with the emergence and development of FT-ICR as a powerful new technique in Mass Spectrometry. The objective nuts and bolts of Alan's career are summarized in his CV and publication list which follow. Alan is perhaps exhibit A in making the case Mass Spectrometry is a scientific discipline not just an analytical technique. From my perspective of 36 years in the field, my colleagues have always accorded scientific status to those doing NMR, but have not been as generous to Mass Spectroscopists, even though Mass Spectrometry has more Nobel Laureates. Hence Alan's move from near 100% NMR starting his career at UBC (1969), to a mix between NMR and FT-ICR on moving to Ohio State (1980) to essentially pure FT-ICR on moving to FSU (1993) runs counter to this perception, and in no small measure helped our discipline achieve the respect accorded to it today. Alan is a great spokesman for our field. Anyone who has heard one of his "global" talks comes away with the impression that unique, important and often seminal results pour forth from his mystical laboratory at FSU. He is the master of collaboration, while at the same time moving the core of FT-ICR forward with new methods development and deeper analysis. Most of us don't give "gee whiz" lectures (but wish we did), yet Alan routinely does so. And he understands what he's talking about, whether its crude oil collected from the Gulf Coast or complex biological systems.

Of course, there is a personal side to Alan. I remember the International Mass Spectrometry meeting at Tampere, Finland in 1997. On one afternoon, there were a number of "outings" the delegates could select. There was a traditional Finnish sauna held on the shores of the local (very large) lake or there was a tour of the lake on several lovely ships. Being sophisticated, I chose the tour and was rewarded not only with lovely vistas but was served delicious, near frozen vodka along with appropriate hors d'oeuvres. Genteel conversation with my wife and fellow travelers was a further reward. Alan, on the other hand, chose the sauna. On quizzing him later I found out that the participants who deposited their clothes in a basket before entering, were given tree branches with leaves still attached, and got to sit in a hot sweaty room beating themselves with the branches. I

think an overseer was present and just as they were about to pass out this overseer screamed at them to leave the sauna enclosure and race at full speed into the lake. Now this is Finland and even though it was August the lake temperature was no higher than the low 50 °F. I think the survivors were eventually given a towel and led back to their rumpled clothes stored in the basket. Lest you think a redeeming feature might have been coed participation, forget it. Women could participate, but they had their own sauna some 100 yards down the beach.

Those of you who have socialized with Alan realize he is a connoisseur of red wine. Some might contend consumer is the correct word but what do they know. Several years ago Alan was asked to give the coveted Saturday evening lecture at the Lake Arrowhead Ion Chemistry Conference (I'll save that story for another day) and he spent several days at my house following his lecture. Of course I had stocked up on good red wine knowing his predilection, and the first night we opened a bottle or two. Now, one of my predilections is a nice single malt scotch, so when we retreated to the living room after dinner I brought out a selection. It turns out this was a new experience for Alan but if he could do the sauna he could do the Scotch. I explained about "more peaty" and "less peaty" and he eventually settled in on a Macallan 12 years old. [For you non-single malt drinkers that's a very full flavored, non-peaty, very smooth drink with maybe a hint of honey in the finish.] In spite of being treated like a king, Alan eventually left Santa Barbara. I got an e-mail on his first day home asking about that Scotch he'd been sampling and I gave him the details. I wasn't sure if it had become one of his "predilections", however, until I ran into Alan on the Royal Mile in Edinburgh during last years IMSC meeting. Our meeting took place inside the best Scotch shop in Edinburgh!! And Alan had a horrendous cold at the time. He was literally shopping 'til he dropped. He had a predilection!

There are other things I could add in this vein, but Elsevier keeps close track of my word count in order to keep them solvent! However, Naresh Dalal has added a personal foreword that gives another and more reliable view of Alan Marshall and I encourage you to read it.

Before finishing, I want to add a little science. Those of you that have heard Alan give a talk may well have heard him quip that he can spell his name in one letter amino acid code. From the dawn of history, it has been axiomatic that

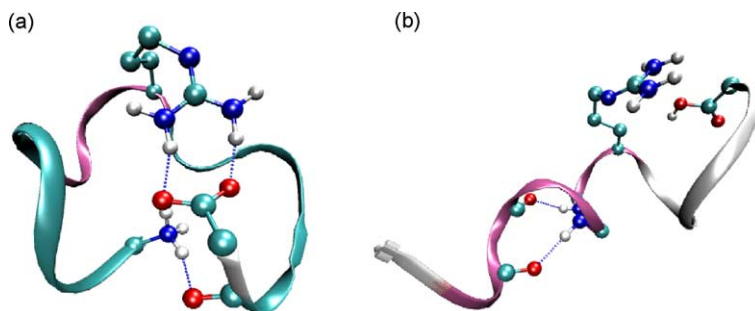


Fig. 1. Low energy configurations of ALANMARSHALL. (a) Salt bridge form; (b) charge solvation form.

to really know a person you must know their name. This need has always puzzled me a bit so I decided to do something about it. I had Summer Bernstein and Nick Dupuis, two of my graduate students, do high level MM/MD modeling of ALANMARSHALL with our AMBER suite of programs. Being a creative sort, we felt our name sake peptide might have multiple configurations so we modeled both the “charge solvation” form with only the arginine protonated (R to you non-peptide types) and also the salt bridge form with both the arginine and N-terminus protonated and the C-terminus deprotonated. This made especially good sense as I remembered how Alan became enamored of salt bridges during some H/D exchange work with Mike Freitas on various forms of Bradykinin several years ago. Well we took our ALANMARSHALL and ran it through a rather torturous annealing process and generated a very large number of structures of both forms. A distinct low energy family of structures emerged for each form. Representative structures are given in Fig. 1.

Just as I expected, ALANMARSHALL is not as simple as it appears. Depending on the energetics of charge solvation/salt bridge, ALANMARSHALL is either a quasi closed loop with the N-terminus and C-terminus essentially holding hands (salt bridge form) or it is a beautiful  $\alpha$ -helix pep-

tide with the N-terminus and C-terminus at opposing ends (charge solvation form). At this stage, further calculations will not solve the puzzle as ALANMARSHALL is too big for accurate DFT calculations, at least on my computers.

Of course the answer, as almost always occurs, will be found only by experiment. The cross-sections projected for the two low energy families are sufficiently different that they can be distinguished by ion mobility experiments ( $\sim 283 \text{ \AA}^2$  for the salt bridge and  $\sim 300 \text{ \AA}^2$  for the helix). Do we have any volunteers with a peptide synthesizer who will make us some ALANMARSHALL? What ALANMARSHALL actually looks like will have to wait until we do the experiments so just keep scanning the internet for ALANMARSHALL and eventually you will learn who he actually is!

I hope you enjoy this issue. There are 22 outstanding research articles from Alan’s students, postdocs, and colleagues. He was clearly a dominant force in Mass Spectrometry the last quarter of the 20th century and I fully expect he will exceed this record in the first quarter of the 21st century. Best wishes and may the wind continue to be at your back.

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