EDITORIAL

Editorial

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All your results are good results!

THE ALL RESULTS JOURNALS

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Editorial

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Dear readers of the *All Results Journals:Chem*,

We are pleased to introduce you to *The All Results Journals: Chem* (All Res. J. Chem.). A very particular journal, as it publishes fully indexed chemical articles and reviews that challenge current models, tenets and dogmas. This journal represents the first open access source for chemical research concerning negative results and will be a valuable resource for researchers all over the world, including those who are already experts and those entering the field.

The All Results Journals: Chem immediate goal is to provide scientists with responsible and balanced information in order to avoid unproductive synthetic routes, improve experimental designs and economical decisions. Many journals skew towards only publishing "positive" data; that is, data that successfully proves a hypothesis. *The All Results Journals: Chem* is the home for negative or "secondary" data: experimental documentation of hypotheses that turn out not to be true, or other experiments that do not lead to an advance of a specific hypothesis but are nevertheless a true rendering of that experiment. For example, if a researcher sets up an organic reaction and a variety of molecules do not react in exactly those conditions, it would be very useful for other researchers to know this (to avoid time and wasting money).

There is a huge mass of experimental data locked up in lab notebooks that could be of great service to the scientific community at large. Many experiments fail to produce results or expected discoveries. Some have even pointed out the different types of negative data we can obtain.[1] This high percentage of "failed" research can still generate high quality knowledge. The main objective of *The All Results Journals: Chem* is to recover and publish these valuable pieces of scientific information.

As we publish negative results, the newer generation of researchers will not waste their time and money repeating the same studies and finding the same results (negative in this case). We believe that negative results are high-level pieces of knowledge that deserves to be published.

The All Results Journals: Chem is a peer reviewed journal developed to publish original, innovative and novel research articles resulting in negative results. This peer-reviewed scientific journal publishes theoretical and empirical papers that report negative findings and research failures in Chemistry and all related sub-fields. Submissions should have a negative focus, which means the output of research yielded in negative results is being given more preference. All theoretical and methodological perspectives are welcomed. We also encourage the submission of short papers/communications presenting counter-examples to usually accepted conjectures or to published papers.

The tip of the iceberg problem and The All Results Journals: Chem

Normally when presenting a paper/study only a small part of what the researcher have done is shown; the negative results are not reported (biased). This is not favorable to advancing Science. Some authors have pointed out elsewhere the problem of publication bias, a well known phenomenon in clinical literature, in which positive results have a better chance of being published, are published earlier, and are published in journals with higher impact factors.[2] We truly believe that today a bigger problem is the submission bias, that is, the authors' resistance to

publish negative results. Science is a deeply frustrating pursuit. One reason we're so resistant to publish negative results might be that researchers want their competitors to think they succeed at every project designed. Other times we get negative results and both, don't find a place where all these results can fit properly and/or there is no specific journal to publish only negative findings. Another reason is rooted in the way the human brain works. We carefully edit our reality, searching for evidence that confirms what we already believe. The problem with science, then, isn't that some experiments have negative results — it's that most negative results are ignored and never published. There is another important reason: what happens with the results that are not 100% reproducible? We all have performed experiments that only work 6 times of 10. Where do these experiments fit? Are these experiments less worthy to communicate?
Last but not least, authors might not consider the undertaking to be worth the effort. For *The All Results Journals: Chem* these experiments have high value because they will avoid wastes of time and could help prevent repetitions worldwide.

Publication of the negative results in *The All Results Journals: Chem* will have two main positive aspects for a scientist:
1. *The All Results Journals: Chem* paper can be presented as a proof of ALL the work that has been done before reaching an original result, and this can be helpful, v.gr., when referees in others journals asked for more data.
2. Others' negative results could also be helpful for an author, if this prevents him from duplicating useless methodologies. This feedback will be essential for boosting authors research.

The question of why we are named The All Results Journals

Many people have asked us why we are named *The All Results Journals*. The name is related to the so-called "file drawer" problem.[3] Of all experiments conducted (in all fields, not only Chemistry), just the tip of the iceberg are being published; only positive results. *The All Results Journals: Chem* target to publish rigorously performed chemical studies producing negative results. *The All Results Journals* are trying to get out the water the complete iceberg (the whole study, showing "All Results" of the author, the complete picture of his research topic, the real job done, not only the positive outcomes). Scientists have the responsibility to study Nature and report everything, and this includes reporting the negative findings. Even more: the research projects might have been funded by public agencies, and that means public money... In part, funding agencies have some responsibility, they should also incentivize the publishing of all results (specially negative results) not only positive. Naturally someone can think it would also bring more bureaucracy to the system, but this might be another topic for a next editorial.

This problematic is the starting point of *The All Results Journals: Chem*. Considering that all results are good results, our target is to bring out all the results that have already been obtained but not published (the negative ones). Exposing the whole iceberg, the only way to improve Science and one of our biggest commitments.

In this issue

In this first issue of the journal, we published two articles related to the experimental determination of values of CMC (critical micelle concentration) on bile salt solutions and to stereoselective organocatalyst, respectively.
Bile salts, natural amphiphilic compounds synthesized in the liver and stored in the gallbladder, are the most important natural surfactants. Unlike ordinary surfactants bile salts do not possess the polar head groups and the non-polar aliphatic tail. They exhibit planar polarity with hydroxyl groups generally located on one face and methyl groups on the opposite. For this reason the shape of the bile salt aggregates is different from classical surfactant micelles. In this sense, the aggregation feature and the shape of the micelles of the bile anions are different from those of common alkyl surfactants. In their article, Professor P. Perez-Tejeda and her colleagues have studied the aggregation behaviour of cholate and deoxycholate anions (as sodium salts) in aqueous solutions. They used TMA-DPH (NNN-Trimethyl-4-(6-phenyl-1, 3,5-hexatriene-1-yl) phenylammonium-p-toluenesulfonate) as a probe molecule in order to obtain information about the CMC considering the shifts of TMA-DPH absorption spectrum as a function of bile salt concentration.
Recently there have been studies of electron transfer reactions between two metal complexes in the presence of different types of receptors (DNA, micelles cyclodextrins, bile salt aggregates, etc.). From the analysis of these charge transfer processes, usually from the rate constant variation when the concentration of a receptor changes, it is possible to determine the free energy of binding between the receptor and one or both reactants (ligands). For this purpose, the two states model (free ligand and associated ligand to the receptor) can be used as a starting point. The advantage of using an electron-transfer process as a probe resides in its apparent simplicity: in this reaction an electron is transferred from a donor to an acceptor, without breaking or forming new bonds, a pure electron-transfer reaction and one of the simplest chemical processes. Unlike other receptors, for the cases of alkyl surfactant micelles and bile salt aggregates, it is necessary to know CMC values and if these concentrations change in the presence of the reactants (ligands). The authors have been confronted with the need to determine CMC values of bile salts in the presence of a cationic metal complex such as [Ru(NH3)5pz]2+ (pz=pyrazine) to explain previous results concerning to the electron transfer reaction between [Ru(NH3)5pz]2+ (pz=pyrazine) and [Co(C2O4)3]3- in the presence of these amphiphilic compounds. The studies using the probe molecule (TMA-DPH) show the existence of two CMCs for two types of

bile salts, NaC and NaDC. However the author states that results can also be explained taking into account a single CMC due to the sigmoid curve observed for the shifts of TMA-DPH absorption spectrum as a function of bile salt concentration. That is, the two concentrations of NaC and NaDC that cause abrupt changes in the positions (wavelengths) of the TMA-DPH spectrum can also be taken as the beginning and the end of the aggregation process rather than as two CMCs. In fact, a sigmoidal dependence is also characteristic of common alkyl surfactant micelles in which only a single CMC instead of two is considered. In this sense the authors explain how the probe molecule (TMA-DPH) does not provide sufficient information on the existence of the secondary aggregates of bile salts. Although the method proposed by the authors is suitable for the determination of CMC in the presence of other ligands different from surfactants theirself, the authors reflect the negative results obtained in distinguishing between different types of CMC or different structural aggregates. These results state that the probe molecule (TMA-DPH) does not provide sufficient information on the existence of the secondary aggregates of bile salts.

The second paper of this first issue of *All. Res. J. Chem*. focus on the development of stereoselective organocatalysts. Organocatalysis have reached the standards of modern well-established asymmetric reactions in terms of chemical efficiency and selectivity. In the first part, the mini-review of Dr. Bernal and Monge, describes the development of the Jørgensen catalyst highlighting the importance of analyzing negative results for the development of new improved catalysts To do this, they use the example of O-TMS protected diarylprolinols. In asymmetric catalysis, as in others branches of Chemistry, many experiments are necessary in order to design and optimize a process. In this regard, the analysis of the results concerning reactivity and enantioselectivity is highly time demanding and here lies the importance of careful examination of all the negative results.
Asymmetric catalysis corresponds to a subject that has been extensively studied for several decades. It is a topic that exercises the interest of teh many sub-sections of chemistry from synthetic chemist to catalytic chemists. The main drive has been to find new, exciting routes to chiral molecules. In the first introductory part the authors reflect how among the different ways to synthesize chiral molecules, asymmetric catalysis represents the most efficient strategy. As examples of asymmetric aminocatalysis, connection between enamine and iminium catalysis is described and also the general mechanisms for both. It is showed the enormous possibilities of aminocatalysis and how the field reached its maturity over 2005, when Jørgensen and co-workers reported on the synthesis of a new class of general organocatalysts: trimethylsilyl (TMS) O-protected diarylprolinols. The authors accurately reflect how their success came up step by step from careful observation and analysis of negative results. The family of O-TMS protected diarylprolinols has found wide applicability in organocatalysis and nowadays, commercially available, contribute to the fast-growing research field with a scope that know goes beyond aminocatalyzed reactions. In the last part of the minireview the authors highlight the importance of analyzing negative results for some important α-functionalization of aldehydes: α-fluorination, α-arylation of aldehydes, 1,4-conjugated additions and the direct Mannich reaction using acetaldehyde. Using the example of O-TMS protected diarylprolinols they show the development of new improved catalysts, starting from erroneous synthetic routes.
These two articles open the venue for new submissions to the journal; comments on the articles are also welcomed and our registered readers are invited to send them to foster debate.

Conclusion

Scientists spend much of their time doing work that doesn't get published. The time and money spent to produce such data (that we like to call them "secondary data") are essentially wasted. Should we not make an effort to increase our society's return on its investment? *The All Results Journals: Chem* is taking it. Our goal is to establish an online medium for the publication of the negative results that otherwise may be lost. Now, we request the collaboration of researchers to succeed.

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