

12:08:59 From Dan Iverson : The link to join IVAN Spinsights is https://join.slack.com/t/ivan-spinsights/shared_invite/zt-fbfzblja-vET5Gp5VsQdoCFbeBrNAfg

12:16:14 From Claudia Nascimento to MR Resources Inc(Privately) : please, could you give access to one of my students? his name is Joaquim Knox

12:18:25 From MR Resources Inc to Claudia Nascimento(Privately) : They needed to sign up previously to the meeting. if you forward the email to that person they can sign up and then when they get the return email they can ask to be admitted.

12:19:00 From MR Resources Inc to Claudia Nascimento(Privately) : The email you need to send them is the original invite email not the one you received back with the join link

12:19:05 From Claudia Nascimento to MR Resources Inc(Privately) : ok; thanks

12:22:08 From Wei Wang : will the slides be made available after this meeting?

12:23:25 From Jeffrey Walton : Or the recording?

12:23:46 From MR Resources Inc to Wei Wang(Privately) : This entire video meeting will be available in 2 3 days via our youtube channel.

12:24:00 From Bob Berno : The recording will be available soon.

12:24:27 From Bob Berno : There will be a link on the IVAN YouTube page.

12:24:29 From MR Resources Inc : YEs the entire video meeting will be available on our youtube channel in about 2-3 days

12:26:52 From Roberto Gil : Feel free to email me if you need more information or further material in addition to the material that will be available as a video.

12:27:47 From Roberto Gil : My email is rgil@andrew.cmu.edu or roberto.r.gil@gmail.com

12:28:21 From Bob Berno : How do you know if your calculated tensors are good without the solid state powder pattern data?

12:32:10 From Roberto Gil : You don't know the tensor a-priori. You perform SVD fitting to all the possible structure in your ensemble (your solution structure must be part of the pool). For each compound the SVD will create a tensor and back calculate the RDC, RCSA or RQC value. The calculated values are compared with the experimental ones for each structure and the best fit is your solution.

12:34:13 From Roberto Gil : The most popular score of the fitting is the Cornilescu Q factor. A que Q factor less that 0.1 is good, less that 0.050 excellent.

12:53:00 From David Rice : The content is great! Everyone is here - we should not worry about time!

12:55:52 From Ping YU : It'll be great if the slides are posted online after the meeting

12:59:57 From Hugh Dannatt : Sadly I have to leave early. Thanks to all, very interesting talks

13:11:25 From Gary Martin : David will you post PDFs of the slides for everyone?

13:14:41 From David Rice : Yes - Eric will post the slides on the IVAN web site. We need to arrange to get them all to him. Also Eric will post the link to the recording.

13:15:58 From yizhou liu : To answer Bob Berno's question about how we know the tensors from DFT are accurate, the proof is in the pudding. When we fit exp RCSA to DFT-calculated shielding tensors, we always get good results, and with higher quality exp data, we get better results, which means the bottle neck is actually not in the DFT, but in the experiments.

13:33:34 From Bob Berno : Thanks Roberto for organizing this. Thanks also to the presenters.. I have to run.

13:34:59 From Prashansa Agrawal : It was great presentation. Looking forward to the next one.

13:35:28 From Katja Pedersen : For RDCs it was mentioned that F1 coupled CLIP-HSQC spectra was preferred. What is the advantage compared to F2 coupled?

13:37:08 From Pablo Trigo Mouriño : The extraction of RDCs is simpler and there is less influence of H-H couplings. On top, F1 experiments allow for scaling of the couplings.

13:40:36 From Chunqing Zhao : thank you very much for everyone. it was a good one.

13:42:24 From Darcy Burns : Thanks all . . . super informative; we've managed to on-board a couple of students with this technique here at the UofToronto. Its been a great complementary tool so far . . the challenge is getting more students interested / over the learning curve ;) Gotta run, but thanks again for a great set of talks (and NMR tools!).

13:43:42 From Padmanava Pradhan : Thanks for the nice talks. Is PBLG recyclable.

13:43:55 From Jonathan FARJON : We are all specialists explaining why questions are rare ;)

13:45:00 From philippe Lesot : Yes the PBLG can be recycled.

13:45:10 From Gary Martin : You can crash your compound out of PBLG with EtOAc to recover the analyte, but we've never bothered to try to recover the PBLG, although there is no reason why you couldn't. You would have to wash it thoroughly though.

13:45:46 From Padmanava Pradhan : Thanks Gary and Phillippe

13:46:46 From Clemens Anklin : Thanks Roberto for moderating this and thanks for the great presentations

13:49:01 From Jonathan FARJON : NMR people like poisons ;)

13:49:53 From Gary Martin : In a previous life, I was a pharmacist... back in the dark ages of pharmacy, there was an Iron, Quinine and Strychnine that was used as a "tonic" to promote muscle tone...

13:51:29 From Jonathan FARJON : everything can be a poison it depends on the quantity even water on spectra also ;)

13:51:47 From Gary Martin : Absolutely correct, Jonathan

13:52:16 From Gabriel Cornilescu : Gorgeous meeting, thanks much Roberto for your continuous enthusiasm and generosity over the years! Thanks to all the speakers for the interesting methods and applications shared.

13:52:51 From Jonathan FARJON : curing poisoning two faces of the same coin ;)