Q&A
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A vision of Medicinal Chemistry for the future
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Q1: What would you tell your younger self to go off learn and train themselves up with if you could do it again?

My background is an interesting one and an unusual one and taking that risk, I don't think necessarily what I would tell myself, but in some ways, I'm proud of some of those decisions and proud of taking a risk to go and do something else. Rather than going down a very specialised, narrow focus on the thing you're currently doing, go and do something completely different. Go and build a mixed skill set that then enables you to operate at the interface between those two disciplines taking the positives of each one and combining it. Then see the things that those who only have one of those skill sets might not necessarily see. It's kind of by chance I've ended up with this kind of mixed computational medicinal chemistry skill set and by slight design. I've certainly seen that the way I operate on projects is different to some of my more computational colleagues or medicinal colleagues and I would like to think that there's some aspects of what the future could look like.

Q2: So, I recall when you launched your assistant to Eli Lilly and I remember when we had chatted about this before and you were saying some people are actually replying to the chat box going "thank you very much" which was great. I was just wondering in the complete cycle of doing all the tasks (and I will come on to talk about this). Is there a point where chemists went "no stop now, that's too much, that's too much automation". So, you really encountered resistance?

I don't think so. We never ran a huge number of those cycles because often the complexity of molecules being made on a project means that the intersection between computational design ideas and those that could be easily executed on the robot, often they didn't intersect. So often the mode was, the assistant creates those ideas, ranks them, scores them, and then they would be sent to the team and the team would then act upon them if they wanted to. So, they went into the funnel of designs being considered and there are examples of where team members will go "oh yeah, we thought about doing that, but we'd parked it" for whatever reason, but seeing the predictions stacked up alongside it, that's enough to then tip them over the edge to try. I think whenever you try and change things and do something new, you'll always come up with some resistance, and that's why I put 'support from management' on this slide, because you need that vision to say we are going to do things differently. We're going to see how they were going to see if they're better, but also being dissatisfied with the status quo which I think most drug discovery organisations are, in many ways, anything you do should always be unsatisfied with how you're doing today and think about how you could be better in the future. But to try something you always carry some risk, and so you'll always come up against some resistance to change people who'll say, "what we do is fine". So, if you want to drive improvement, which often management, say that's what they would like to do. And so organisationally you think about how that all plays together nicely and to move in that direction.