**MicroCycle: a Machine Learning Driven, Automated and Integrated Platform for Drug Discovery**

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Abstract:

What if we could develop an integrated drug discovery platform to accelerate drug discovery, which utilises micro-scale chemistry, real-time biological and physicochemical characterisation and machine learning driven compound design? At NIBR this is a reality! Our automated medicinal chemistry 'design-make-test-analyse' cycle is powered by machine learning, enables sequential multi-parameter optimisation and generates knowledge in a timeframe never before possible. We have built MicroCycle; a modular technology platform which benefits from recent advances in plate based micro-scale chemistry, micropurification,[1] *in-situ* quantification and machine learning thus ensuring rapid access to high quality chemical matter already formatted for assay. Furthermore, by reorienting existing high throughput assay technology we can generate a full package of relevant data on each set of compounds in every learning cycle.

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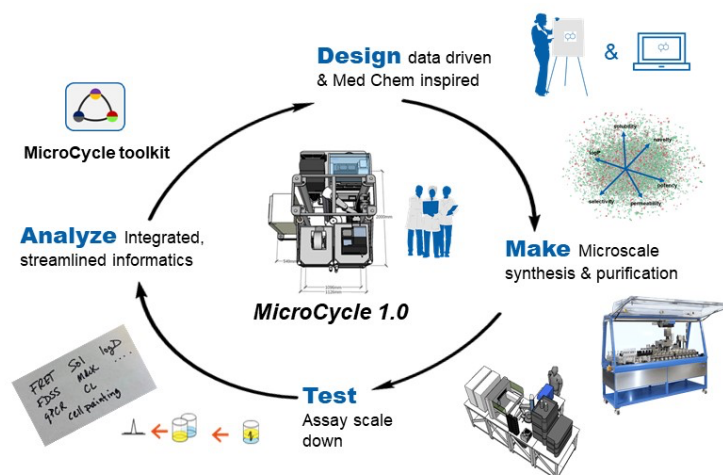
[1] 'Integrated and Automated High-Throughput Purification of Libraries on Microscale' C. Ginsburg-Moraff, J. Grob, K. Chin, G. Eastman, S. Wildhaber, M. Bayliss, H. M. Mues, M. Palmieri, J. Poirier, M. Reck, A. Luneau, S. Rodde, J. Reilly, T. Wagner, C. E. Brocklehurst, R. Wyler, D. Dunstan, A. N. Marziale, *SLAS Technology*, **2022**, manuscript available online

Dr. Cara Brocklehurst is currently Director and Head SynTech Basel within Global Discovery Chemistry at Novartis Institutes for Biomedical Research. After a PhD with Prof. Nick Turner in Edinburgh and a postdoc with Prof. Andreas Pfaltz in Basel, Cara joined Novartis Basel in 2005 in the Global Discovery Chemistry, Prep Labs. A group based in the Novartis research arm, Novartis Institutes for Biomedical Research (NIBR), primarily concerned with the optimisation of synthetic routes and scale up of intermediates and drug candidates. The group has evolved over time and become SynTech, and Cara now leads the group. The global SynTech team works across the portfolio, optimising synthetic routes for scale up, testing novel chemical transformations to open up chemical space for project teams, applying chemical technologies such as flow chemistry, photochemistry and building automated workflows to catalyse drug discovery.