



SIMPOSIO NACIONAL DE QUÍMICA ORGÁNICA
CÓRDOBA - ARGENTINA 2021



Estimados colegas,

Tal como comunicamos anteriormente, en esta edición del SINAQO hemos decidido incluir en el marco de las actividades virtuales, tres Ciclos de Conferencias denominados XXIII SINAQO - Virtual Opening Meetings (VOMs). A continuación, les hacemos llegar el programa del **XXIII SINAQO - 2nd Virtual Opening Meeting: From the Benchtop to Technological Innovation - 2^{da} VOM Desde la Mesada a la Innovación Tecnológica**, a realizarse el día 26 de agosto del corriente:

8:30 -9:00 am (ARG): Apertura. Dra. Miriam Strumia y Ministro Pablo De Chiara (MinCyT-Cba)

9:00 - 9:40 am (ARG): Conferencia: "HTE in Medicinal Chemistry". Dr. Spencer Dreher (Merck & Co., Inc., USA). Modera: Dra. Natalia Pacioni

9:40 - 11:00 am (ARG): Mesa redonda: Dra. Isabel N. Vega (Y-TEC); Sr. Leonardo Castagna (Jose Guma S.A.); Dra. Silvia Goyanes (UBA); Dr. Alejandro Rago (INTA) y Mg. Bqa. Marisa Cordi (ARCOR SAIC). Moderan: Dr. Gabriel Raya (MinCyT-Cba) y Dr. Fabricio Bisogno

11:00 - 11:50 am (ARG): Mesa redonda, sección de P&R. Moderan: Dr. Gabriel Raya (MinCyT-Cba) y Dr. Fabricio Bisogno

11:50 am (ARG): Cierre y presentación del 3^{er} VOM.

¡Esperamos contar con su participación!!!

Cordialmente,

**Comisión Organizadora
XXIII SINAQO**



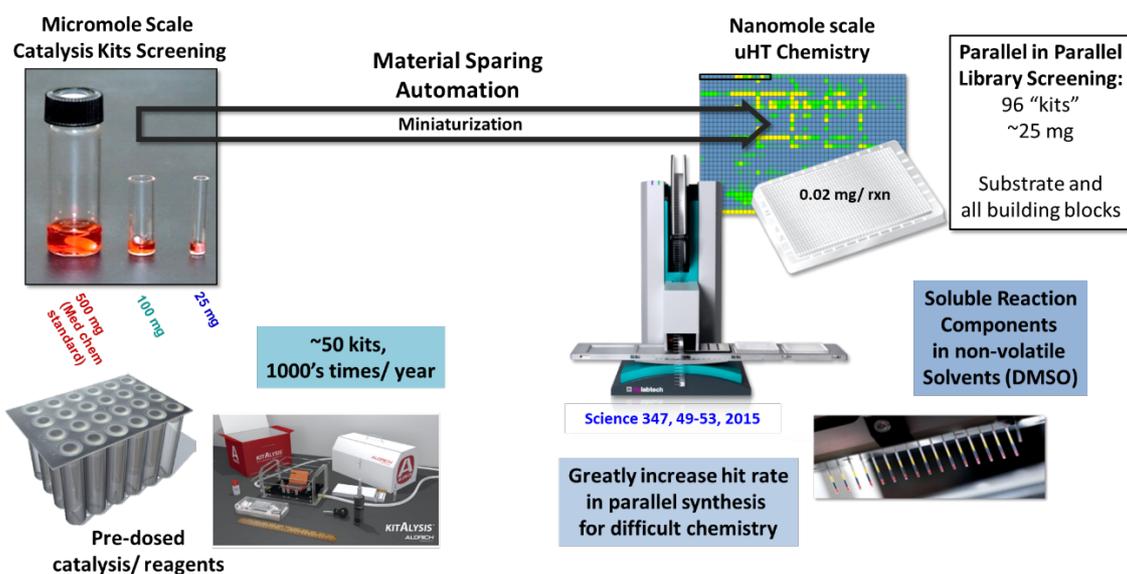
HTE IN MEDICINAL CHEMISTRY

Dreher, Spencer

HTE and Lead Discovery Capabilities. 2000 Galloping Hill Rd, Merck & Co., Inc., Kenilworth, NJ 07033, USA

Keywords: HTE, Medicinal Chemistry

High throughput experimentation (HTE) chemistry has been evolving in leaps and bounds. In industry and academic labs, reactions are run in increasingly miniaturized and parallelized format changing the very nature of what we can make and the overall cost-structure of synthesis. At Merck, HTE was initiated in Process Chemistry to rapidly solve difficult problems and has more recently become pervasive in Medicinal Chemistry labs for problem-solving and library synthesis. In Med-chem, nanomole-scale screening can uncover unique conditions for micromole scale parallel synthesis libraries to greatly increase hit rates. In addition, increasingly, direct-to-biology approaches allow for nanomole-scale reaction arrays wherein parallel conditions are applied to parallel reactions and successful reactions are tested directly in biology, without chromatographic purification. In the very near future, the data that is generated in these experiments will be used to create models to help predict successful conditions to minimize the need for screening. Massively parallel, integrated chemistry/ biology with data-driven conditions prediction is on the horizon for discovering new drugs rapidly, and cheaply.



References:

^a Krska, S.W., DiRocco, D.A., Dreher, S.D., Shevlin, M. *Acc. Chem. Res.* **2017**, 2976-2985.