In Memory of Richard Lerner

Venue Information

Broad Institute
415 Main St.
Cambridge, MA

Organizers

Yun Ding (*GSK*)
Lisa Marcaurelle (*GSK*)
Ying Zhang (*X-Chem*)

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Thursday - November 3, 2022 - Day 1

8:30 - 8:55	Registration
8:55 - 9:00	Information & Opening Yun Ding *(GSK)*
9:00 - 9:20	In Memorium - Richard Lerner

Session 1: Advances in Selection
Chair: Chris Dimitri (*GSK*)

9:20 - 9:45	Quantification of DEL selections and implications for good selection protocols Dario Neri *(ETH Zurich)*
9:50 - 10:15	Development of selective PDE3B inhibitors from an ELT screen Westley Tear *(GSK)*
10:15 - 10:45	Coffee break & Poster session (Day 1)

Session 2: Advances in Chemistry
Chair: Yun Ding (*GSK*)

10:45 -11:10	Photoredox chemistry in the service of building DELs Gary Molander *(University of Pennsylvania)*
11:15-11:40	DNA-encoded chemistry development for heterocycles based library synthesis Xiaojie Lu *(Shanghai Institute of Materia Medica, CAS)*
11:45 - 12:10	Cyclopropanation on DNA: Towards uncharted chemical space of DELs Matthieu Richter *(Broad Institute/Novartis)*
12:10 - 13:30	Lunch Break

Session 3: Case Studies
Chair: Jack Scott (*Merck*)

13:30 - 13:55	When to use DEL? Tim Foley *(Pfizer)*
14:00 - 14:25	DNA-encoded libraries in drug discovery: Identification of a novel NKG2d inhibitor class with a unique mechanism of action Pei-Pei Kung *(Janssen)*
14:30 - 14:55	Expanding the target landscape for DNA-encoded library (DEL) screening Adrian Saldanha *(Merck)*
15:00 - 15:30	Coffee break & Poster session (Day 1)

Session 4: Technology Development
Chair: John Guilinger (*X-Chem*)

15:30 - 15:55	DELs in cells Nils Hansen *(Vipergen)*
16:00 - 16:25	DEL selections via enzymatic proximity labeling for selective enrichment of GPCR biased agonists Casey Krusemark (*Purdue University)*
16:30 - 16:55	Fragment DEL Guansai Liu (*HitGen*)
17:00-18:00	Poster session (Day 1)
17:00- 20:00	Reception

Friday - November 4, 2022 - Day 2

8:30 - 8:55 Registration

8:55 - 9:00 Information & Opening

Session 5: Advances in Chemistry

Chair: Frederic Berst (*Novartis*)

9:00 - 9:25 Micellar mediated approaches to the synthesis of DNA-encoded libraries
Mike Waring (*Newcastle University)*

9:30 - 9:55 Confirming DEL hits by protein NMR analysis of on-DNA compounds
Matthew Katcher *(AbbVie)*

10:00 - 10:30 Coffee break & Poster session (Day 2)

Session 6: Case Studies

Chair: Dario Neri (*ETH & Philogen*)

10:30 - 10:55 DNA-encoded libraries for novel SARS-CoV-2 Mpro inhibitors
Damian Young *(Baylor College of Medicine)*

11:00 - 11:25 Leveraging DELs for efficient discovery of novel crop protection chemistries
Tim Panosian *(Enko Chem)*

11:30 - 11:55 Discovery of novel Mer kinase inhibitors for immuno-oncology through DEL screening
Emma Rivers *(AstraZeneca)*

11:55- 13:30 Lunch Break

Session 7: Data Analysis/Machine Learning

Chair: Ying Zhang (*X-Chem*)

13:30 - 13:55 DEL/ML: Teaching an old dog new tricks
Jeff Messer *(GSK)*

14:00 - 14:25 X-Chem's ArtemisAI platform: A flexible approach to AI for drug discovery
Noor Shaker *(X-Chem)*

14:30 - 14:55 Apples to oranges, A tale of DEL data similarity
Letian Kuai *(Wuxi AppTec)*

15:00 - 16:00 Coffee break & Poster session (Day 2)

Session 8: Keynote Presentation

Chair: Lisa Marcaurelle (*GSK*)

16:00 - 17:00 The rise of molecular glues and bifunctional compounds
Stuart Schreiber *(Broad Institute)*

17:00 - 17:05 Closing remarks
Lisa Marcaurelle *(GSK)*

17:05 - 19:00 Happy hour/poster session (Day 2)

Posters
Nov. 3rd, 2022 (Day 1)

1	Andrew MacConnell	Ultra-High-throughput SAR profiling and hypothesis-driven screening by the rapid cycling through chemical space with >70K-member molecular libraries on a microfluidic discovery platform
2	Priyanka Patel	Impact of Post-Selection Processes' Optimization on Quality of Sequencing Data
3	Martin Fillmore	Using DEL screening to identify a selective c-MET inhibitor with a novel binding mode
4	Ramkumar Modukuri	Discovery of highly potent and BMPR2-selective kinase inhibitors using DNA-encoded chemical library screening
5	Murugesan Palaniappan	Discovery and Characterization of Estrogen Receptor Mutant Inhibitors Using DNA-Encoded Chemical Libraries
6	Qi Ouyang	switchSENSE for DEL hit validation
7	Jing Chai	On-DNA Macrocyclization via Intramolecular Benzimidazole Formation
8	Anton Kozhushnyan	Discovery of Novel Efflux Pump Inhibitors Using DEL Technology
9	Daniel Riley	Counter Screening Strategy Rapidly Identifies Selective Kinase Inhibitors from a DNA Encoded Library
10	Lijun Fan	Novel Methods for On-DNA Macrocyclic Peptide Cyclization
11	Hongyao Zhu	Estimate Data Noise Level in DNA-Encoded Library Selection
12	Paige Dickson	DEL-Enabled Identification of Novel Irreversible Covalent BTK inhibitors
13	Patrick Fitzgerald	Integrating photochemical compound dosing with activity-based DNA-encoded library screening
14	Vijay Siripuram	DNA-Compatible Suzuki-Miyaura Cross-Coupling Reaction of Aryl Iodides with (Hetero)Aryl Boronic Acids for DNA-Encoded Libraries
15	Fong Sang Lam	DNA-encoded chemical libraries for macrocycle ligand discovery
16	Ying Zhang	DNA-Encoded Macrocyclic Compound Libraries for Hit Identification for Challenging Targets
17	Jack Pruneau	Automated Discovery: Streamlining processes to enable rapid discovery of lead molecules via DEL and IVP
18	Will Evenson	Comparing DEL and HTS: Case studies with two unique success stories
19	Pratik Rajesh Chheda	Enabling on-DNA palladium mediated cross coupling reactions: on-DNA Carbonylative Suzuki and C-N cross couplings

20	Ryan Walsh	ML-powered Prediction of the Suitability of Building Blocks for Incorporation in DELs
21	Yiran Huang	Target-Specific Labeling of Membrane Proteins for Ligand Discovery and Other Applications
22	Takashi Nakai	Highly Selective Novel Heme Oxygenase-1 Inhibitor Discovery by DNA Encoded Library (DEL) Based Deep Learning Model beyond the DEL Chemical Space
23	Jason Deng	DELvision: a protein-DEL experimental database connecting the proteome with small molecule chemical space
24	Sebastian Oehler	A compact and stereo-defined DNA-Encoded Chemical Library enables the discovery of stereo-selective isozyme-specific tumor targeting agents
25	Adam Skiredj	On-DNA Kinugasa Reaction for β-Lactam DEL Synthesis
26	Yuntian Bai	Random Dimerization of Headpiece DNA Encoded Chemical Libraries for Increasing Library Diversity
27	Brian M. Paegel	Liposomal Permeation Assay for Droplet-Scale Pharmacokinetic DEL Screening

Posters
Nov. 4th, 2022 (Day 2)

1	Jian-yuan Li	Summary of DNA Compatible Reactions Developed in the Center for Drug Discovery
2	Srinivas Chamakuri	DNA-Encoded Chemistry Technology Yields Expedient Access to SARS-CoV-2 Mpro Inhibitors
3	Emily Ziperman	Directed Evolution of Sugar Clusters on 2’-F RNA Backbones to Bind Protein Targets
4	Satoru Horiya	DNA ligated to the 3'-ends of mRNA mediates aberrant translations in mRNA display
5	Mark Mantell	One Reaction Served Three Ways: The on-DNA Ugi 4C-3R reaction for the formation of lactams
6	Rodrigo Ortiz-Meoz	The Impact of Blocking DNA on DEL Selection Outcomes
7	Anthony Harris	Driving Efficiency for DNA-Encoded Library Selection Campaigns and Hit Confirmation
8	Noor Shaker	TBD
9	Philipp Sander	PhenoDEL: Towards Phenotypic DNA-encoded chemical library selections in mammalian cells
10	Fei Ma	Metal-Catalyzed One-Pot On-DNA Syntheses of Diarylmethane and Thioether Derivatives

11	Yashoda Krishna Sunkari	Large-scale multi-parameters screening to quantify the impact of organic chemistry conditions on DNA durability in the context of DNA-encoded library technology
12	Wenyin Shen	Development of the next generation of DNA-encoded dynamic libraries
13	Yuhan Gui	Converting double-stranded DNA-encoded libraries (DELs) to single-stranded libraries for more versatile selections
14	Alba L. Montoya	Development of TNKS1 Inhibitors as a Model for Using DNA Encoded Libraries as a Platform for Structure-Based Exploration and Pharmacophore Design
15	Kyle Denton	Selectivity Assessment through Parallel Selections: A Case Study with Phosphodiesterases
16	Kelly McCarthy	Helical domain deletion enables discovery of potent PARP1 inhibitors from a DEL selection
17	Ali Chou	Applying Machine Learning (ML) to DNA-Encoded Library (DEL) Screening Output Data for Small Molecule Drug Discovery
18	Amol Mhetre	DNA-encoded chemistry under Schotten-Baumann conditions
19	Alex Satz	Covalent DEL: a new way of drug discovery
20	Wenji Su	DEL Enables a Record-breaking Target-to-IND in 2.5 Years: Discovery of Potent SARS-CoV-2 3CLpro inhibitors
21	Letian Kuai	Apples and Oranges, a Tale of DEL Data Similarity
22	Bing Xia	From DEL to X-DEL, XtalPi's Holistic Approach
23	Adam Skiredj	Novel DEL design tactics evolved by a new linker
24	Adam Skiredj	Copper-Catalyzed Oxidization and Amindation of Terminal Alkynes on DNA oligo
25	Ilaria Proietti Silvestri	Synthetically Validated, 3d-Rich, Multifunctional, Novel Synthons for High Quality DELs
26	Jason Deng	DEL+ML: New Coming Wave for Hit Discovery
27	Wenji Su	Discovery and Structural Characterization of Small Molecule Binder of the Human CTLH E3 Ligase Subunit GID4

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