<p style="text-align:center">WORKSHOP #14</p>

<p style="text-align:center">New Science Enabled by Ultra-high Throughput Crystallography</p>

<p style="text-align:center">Organizer: Alexei Soares</p>

Proponents of high data rate crystallography will be invited to discuss their science and their experimental needs, particularly the synchrotron capabilities that will enable transformative research. We will invite participants with expertise in areas such as high throughput screening of chemical libraries, protein engineering, protein dynamics, mechanistic studies, and perturbation studies. However, any scientist who could benefit from ultra-high throughput protein crystallography with a high level of automation and streamlined access is invited to participate. The goal of the workshop is to benchmark the experimental priorities of the ultra-high throughput crystallography community, and to investigate the potential new science that these instrumental investments could be expected to support.

Start Time (ET)	Title	Speaker (Affiliation)
9:45 a.m.	Introduction/Welcome Remarks	Sean McSweeney
10:00 a.m.	Discovering New Ligands for the SARS CoV 2 Macrodomain enabled by High Throughput X-ray Crystallography	C.J. San Felipe (University of California, San Francisco)
10:45 a.m.	Protein dynamics and fragment screening using high throughput MX including advanced structural analysis	Rebecca Page (University of Connecticut School of Health)
11:30 a.m.	High-throughput structural analyses of metabolite and effector binding for biofuel and environmental research	Joseph Jez (Washington University in Saint Louis)
12:15 p.m.	Break	
1:30 p.m.	Towards an integrated and highly automated facility for fragment screening: sample preparation, data collection, structure analysis, and post-processing	Dale Kreitler (BNL)
2:15 p.m.	Ultra-high throughput autonomous data collection: current state of the art, outlook, and scientific opportunities	Jean Jakoncic (BNL)
3:00 p.m.	Discussion	Alexei Soares (moderator)