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Supplementary information

The NCATS Assay Guidance Manual programme: advancing the practice and rigour of preclinical translation

In the format provided by the authors

Supplementary Table 1 | Table of contents of the Assay Guidance Manual electronic book, including specific sections and distribution of chapters within each section

Table of Contents	Number of Chapters
Preface	N/A
Considerations for Early Phase Drug Discovery	1
In Vitro Biochemical Assays	11
In Vitro Cell Based Assays	24
In Vivo Assay Guidelines	2
Assay Artifacts and Interferences	5
Assay Validation, Operations and Quality Control	6
Assay Technologies	2
Instrumentation	3
Pharmacokinetics and Drug Metabolism	1
Glossary	1
Total Number of Chapters	**56**

*Note: The AGM is a dynamic ebook which is updated regularly. This data is as of September 2022.

Supplementary Table 2 | Dates, locations, number of sessions/lectures, and organizing institutions of the multiple assay guidance workshops for high-throughput screening and lead discovery that were held since 2015

Date(s)	Location	Sessions	Organizer(s)
October 18-19, 2022	Bethesda, MD	16	NCATS
Feb 5, 2022	Boston, MA	9	SLAS, NCATS
Nov 18-19, 2020	Virtual*	24	NCATS
Jan 25, 2020	San Diego, CA	10	SLAS, NCATS
Sep 11-12, 2019	Cambridge, MA	19	NCATS, Pfizer
Feb 2, 2019	Washington, DC	9	SLAS, NCATS
Sep 10-11, 2018	Potomac, MD	17	NCATS
Mar 26-27, 2018	Potomac, MD	17	NCATS
Feb 3, 2018	San Diego, CA	9	SLAS, NCATS
Oct 23, 2017	Chapel Hill, NC	12	UNC Catalyst for Rare Diseases, Promega, NCATS
Aug 7, 2017	Potomac, MD	10	NCATS
Feb 4, 2017	Washington, DC	9	SLAS, NCATS
Oct 27, 2016	Madison, WI	9	Promega, ICBS, NCATS
Apr 5-6, 2016	College Park, MD	10	US FDA, NCATS
Jan 23, 2016	San Diego, CA	9	SLAS, NCATS
Jul 17, 2015	College Park, MD	7	US FDA, NCATS
Feb 6, 2015	Rockville, MD	5	NCATS

Abbreviations:
National Center for Advancing Translational Sciences (NCATS)
Society for Laboratory Automation and Screening (SLAS)
University of North Carolina (UNC)
International Chemical Biology Society (ICBS)
US Food and Drug Administration (US FDA)

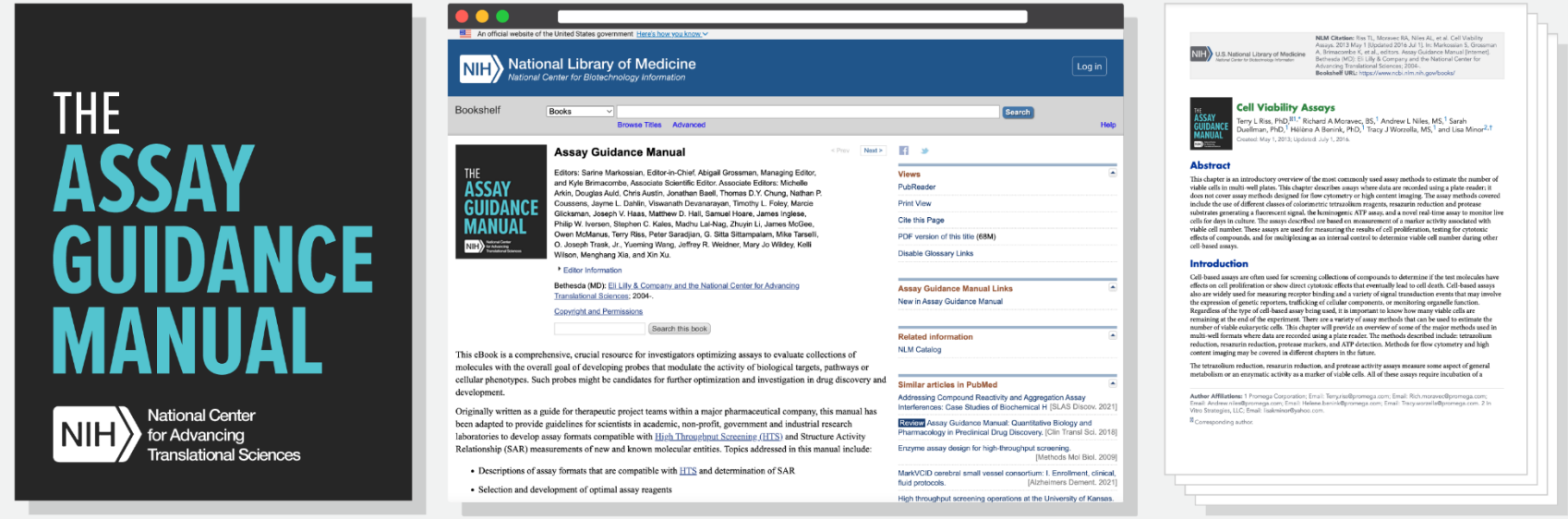
*Event information and video recordings from November 18-19, 2020: https://ncats.nih.gov/events/Assay-Guidance-Workshop-for-High-Throughput-Screening-and-Lead-Discovery

Supplementary Table 3 | Information on various topic-focused workshops conducted by the AGM programme

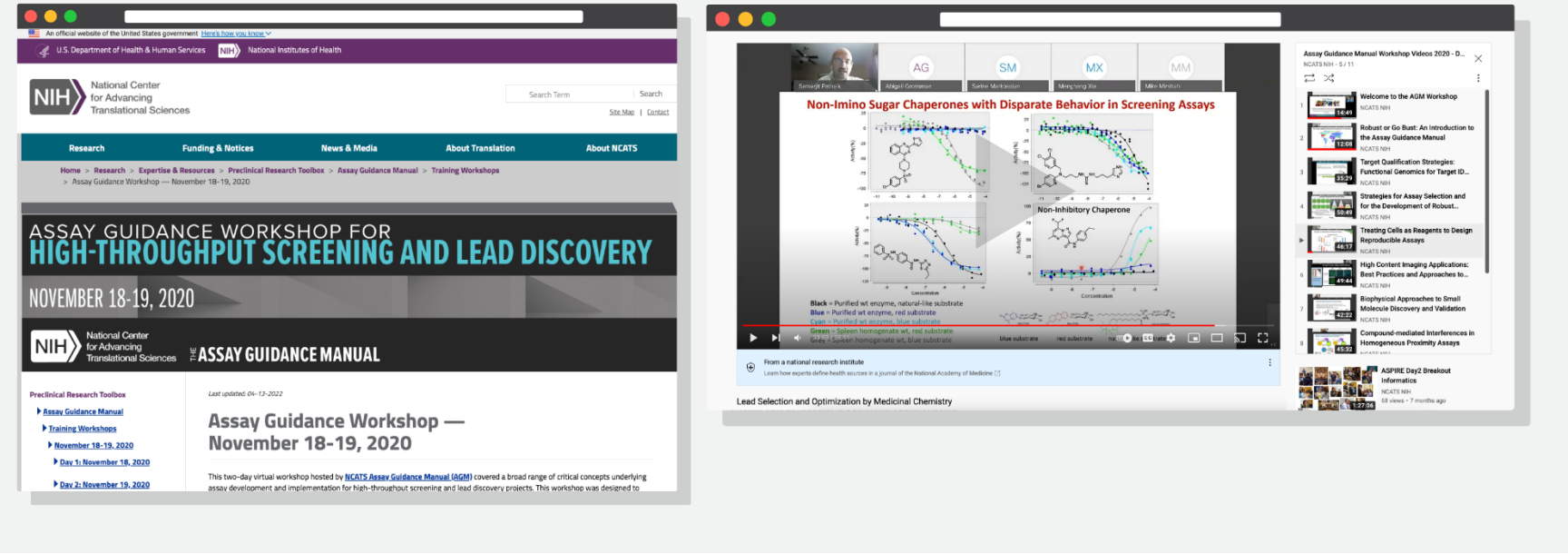
Event name	Summary/goal	Dates	Location	Organizers	Related links
Assay Guidance Workshop on 3D Tissue Models for Antiviral Drug Development	This workshop aimed to provide participants with a roadmap for developing robust and reproducible tissue models to study pandemic threat viruses	June 7-8, 2022	Virtual	NCATS, NIAID, Bill & Melinda Gates Foundation	Event information: https://ncats.corsizio.com/c/62153215b176e58b1884dfc5 Day 1 on June 7, 2022: https://videocast.nih.gov/watch=45399 Day 2 on June 8, 2022: https://videocast.nih.gov/watch=45401
Assay Guidance Workshop for Cell-Based Assays and Lead Discovery	This workshop aimed to inform the translational science community on the fundamentals and applications of image-based and 3D cellular assay technologies and to provide a future perspective on the utility of complex cellular models in drug discovery	November 16-17, 2021	Virtual	NCATS, Promega, PerkinElmer	Event information: https://ncats.corsizio.com/c/610be47733a68a57165e9db7 Day 1 on November 16, 2021: https://videocast.nih.gov/watch=44132 Day 2 on November 17, 2021: https://videocast.nih.gov/watch=44130
Assay Guidance Workshop on DNA-Encoded Libraries (DEL) for Lead Discovery	This workshop aimed to inform the translational science community on the fundamentals and applications of DEL technology and to bring together those practicing the art to share insights and perspectives in an open forum	September 1-2, 2021	Virtual	NCATS, Pfizer, Nurix Therapeutics, HitGen Inc., GlaxoSmithKline	Event information: https://ncats.corsizio.com/c/608b1547ba86ce418b3c2b5b Day 1 on September 1, 2021: https://videocast.nih.gov/watch=42626 Day 2 on September 2, 2021: https://videocast.nih.gov/watch=42628

Assay Development Principles and Good Research Practices for Rigor and Reproducibility in *In Vitro* Toxicology	This course aimed to provide participants with guidelines and principles for rigor and reproducibility in high throughput *in vitro* toxicological assays	March 10, 2019	Baltimore, MD	Society of Toxicology, NCATS	Event Information and booklet: https://www.toxicology.org/education/ce/docs/SOT-AM19_CE_AM03_v7.pdf
The Opioid Crisis and the Future of Addiction and Pain Therapeutics: Opportunities, Tools, and Technologies Symposium	This symposium highlighted challenges and opportunities in the pre-competitive, preclinical stage of development for addiction- and pain-related medications and provided a framework for more focused efforts within the research community	February 7-8, 2019	NIH Campus, Bethesda, MD	NCATS, NIDA, NINDS	Event information and related publications: https://ncats.nih.gov/pubs/features/heal-symposium https://events-support.com/events/NCATS-Pain-Addiction-Symposium https://pubmed.ncbi.nlm.nih.gov/31481516/ Day 1 on February 7, 2019: https://videocast.nih.gov/watch=31404 Day 2 on February 8, 2019: https://videocast.nih.gov/watch=31408

Abbreviations:
National Center for Advancing Translational Sciences (NCATS)
National Institute of Allergy and Infectious Diseases (NIAID)
National Institute on Drug Abuse (NIDA)
National Institute of Neurological Disorders and Stroke (NINDS)



Supplementary Figure 1 | A screenshot of the cover and landing page of the *Assay Guidance Manual* electronic book on the National Library of Medicine (NLM), National Center for Biotechnology Information (NCBI) Bookshelf. Also shown is an example of a highly cited and accessed chapter on cell viability assays that can be downloaded in a PDF format.



Supplementary Figure 2 | A screenshot of the landing page of the virtual *Assay Guidance Workshop for High-throughput Screening and Lead Discovery* that was conducted in 2020. Also highlighted is an example of a highly viewed video recording from the workshop on lead selection and optimization by medicinal chemistry.