

Colorants: Dyes, Pigments and Databases

Nelson R. Vinueza

Associate Professor

Department of Textile Engineering, Chemistry and Science

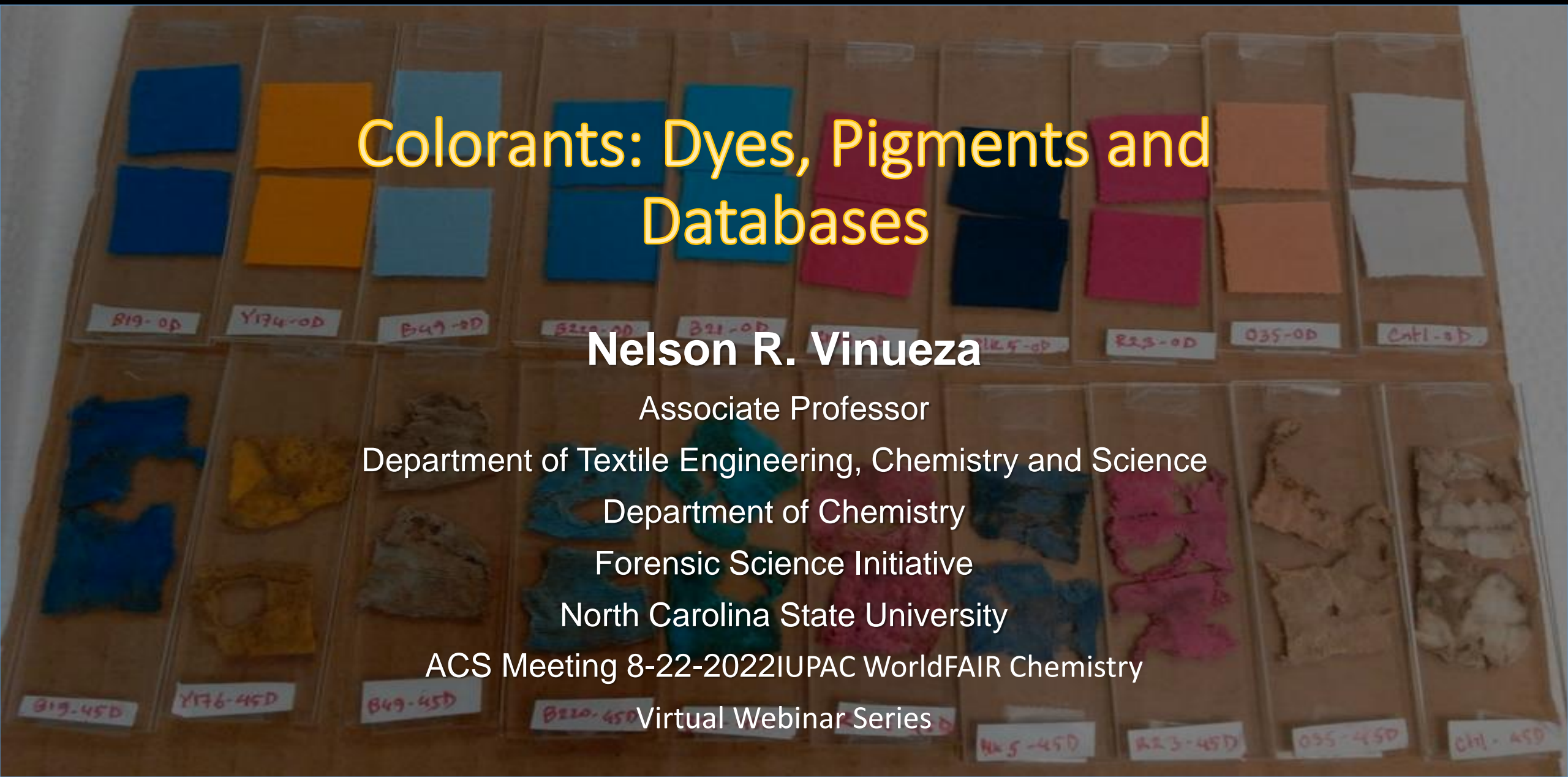
Department of Chemistry

Forensic Science Initiative

North Carolina State University

ACS Meeting 8-22-2022 IUPAC WorldFAIR Chemistry

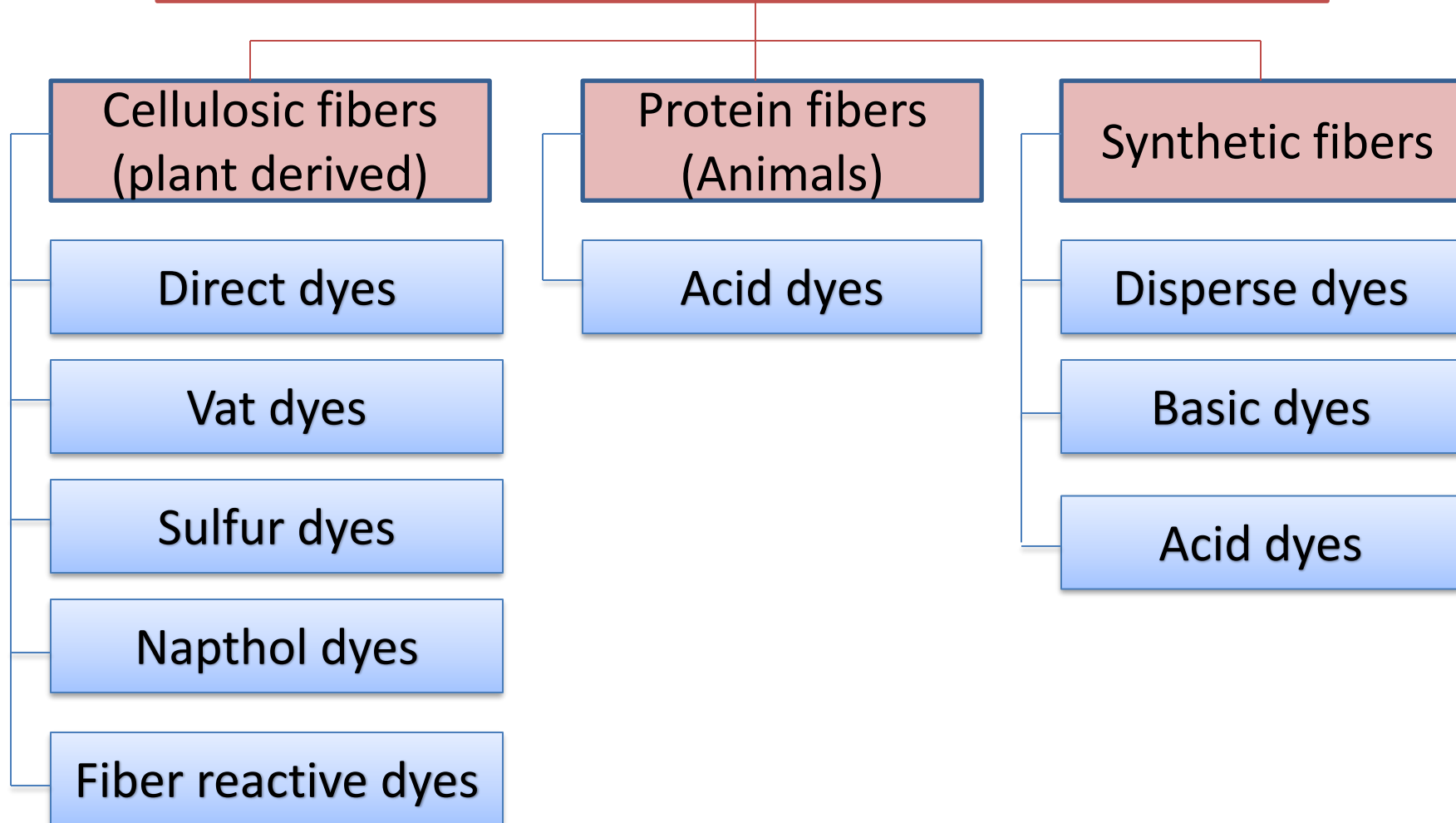
Virtual Webinar Series



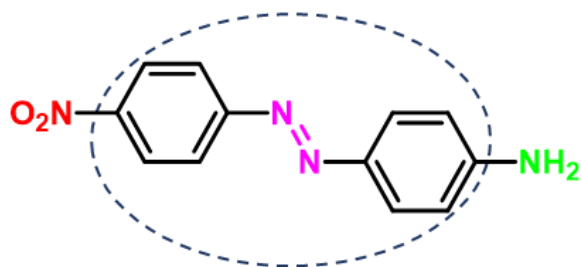
Colorants

- Colorants are characterized by their ability to absorb or emit light in the visible range (400-700 nm)
- In terms of chemical structure, colorants may either be inorganic or organic compounds
- Colorants are either **dyes** or **pigments**. These two terms are used indiscriminately.
 - **Pigments** consist of small particles that are practically insoluble in those media in which they are applied.
 - **Dyes** are applied to various substrates from liquid in which they are completely, or at least partly, soluble.

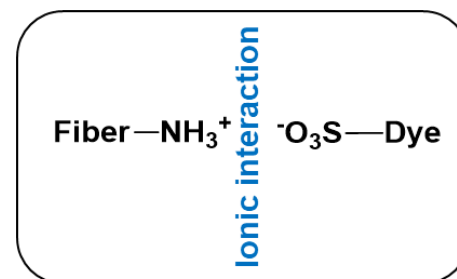
Dye classification based on fiber type



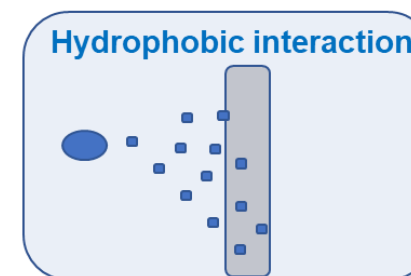
Organic dyes and their interaction to textile substrates



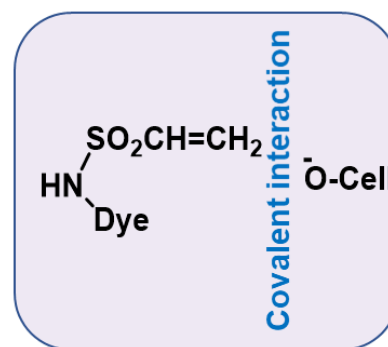
Chromophore
Auxochrome
Antiauxochrome
Extended Conjugation



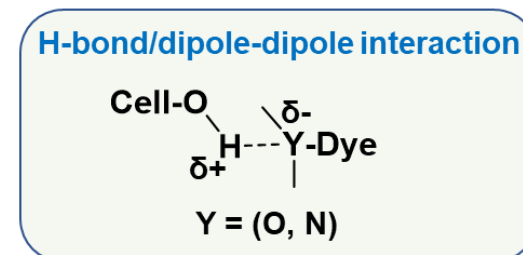
Acid dye - polyamide fiber



Disperse dye - acetate/PET fiber



Reactive dye - cellulosic fiber



Direct dye - cellulosic fiber

Colour Index™ Classification Overview

- **Colour Index™ Generic Name:** The prime descriptor, in that it is the one most commonly used in discussions by colorant users and is the one easier to remember, is the Colour Index™ Generic Name (often abbreviated to CIGN). This is related to the **application process**.
- **Colour Index™ Constitution Number:** **Chemical-structure related** (often abbreviated to CIGN). For example, monoazo 11000-19999, acridine 46000-46999 and inorganic pigments 77000-77999.

Example of a Colour Index™ Table

| C.I. Generic Name | C.I. Constitution Number | Shade | Commercial Products |
|--------------------------|---------------------------------|--------------|----------------------------|
| Acid Red 1 | 18050 | Red | 60 |
| Acid Red 2 | 13020 | Red | 1 |
| Acid Red 3 | 14910 | Bluish Red | 1 |
| Acid Red 4 | 14710 | Red | 15 |

Challenges

- Colorant structures can be limited due to patents
- Dyes structures sometimes do not correlate with structures available to the public
- Faster quality control tests
- Toxicological data of dyes and their effects on the environment (e.g., Sudan dyes)

Enhancing dye databases

Max Weaver Dye Library

NC STATE'S DYE LIBRARY BY THE NUMBERS

Estimated samples of dyed textiles and light stability data:

250,000

Decade oldest dyes in the library were synthesized:

1940s

Approximate years of research represented:

50

Estimated replacement value:

\$112 million

Approximate number of dye compounds:

98,000



Max Weaver Dye Library

- Large collection of organic dyes offers a powerful database for
 - Solar energy research
 - Forensic science
 - Chemical education
 - Electronic structure methodology benchmarking
 - Fundamental studies on spectroscopic substituent-dependent spectroscopic properties relevant to dye-design strategies
 - Color-structure relationships
 - Molecular modeling structure-activity relationships

How Novel the Max Weaver Dyes Are?

- An examination of the novelty of the dyes was performed by searching the first part of the **InChI keys** for **150 newly registered structures** of dyes across the ChemSpider database, which contains over **58 million** unique chemicals as of March 2017.

What We Found?

- 143 structures were newly registered chemicals to the database while, **7** already had existing forms based on the InChI key skeleton

How to share this Treasure Trove?

- Not everybody can come to NC State and visit the library
 - Digitalize the library
- How we can reach scientists from different fields to get interested in these rich aromatic compounds?
 - Cheminformatics
- How we can enhance STEM education using this library?
 - Combining analytical chemistry, modeling and technology

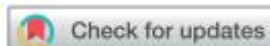
How to share this Treasure Trove?

Chemical
Science



EDGE ARTICLE

View Article Online
View Journal | View Issue



Cite this: *Chem. Sci.*, 2017, 8, 4334

Weaver's historic accessible collection of synthetic dyes: a cheminformatics analysis^{†‡}

Melaine A. Kuenemann, ^{id}^b Malgorzata Szymczyk, ^{id}^a Yufei Chen, ^{id}^a
Nadia Sultana, ^{id}^a David Hinks, ^{id}^a Harold S. Freeman, ^{id}^a Antony J. Williams, ^{id}^c
Denis Fourches ^{id}^{*b} and Nelson R. Vinueza ^{id}^{*a}

We present the Max Weaver Dye Library, a collection of ~98 000 vials of custom-made and largely sparingly water-soluble dyes. Two years ago, the Eastman Chemical Company donated the library to North Carolina State University. This unique collection of chemicals, housed in the College of Textiles, also includes tens of thousands of fabric samples dyed using some of the library's compounds. Although the collection lies at the core of hundreds of patented inventions, the overwhelming majority of this chemical treasure trove has never been published or shared outside of a small group of scientists. Thus, the goal of this donation was to make this chemical collection, and associated data, available to interested parties in the research community. To date, we have digitized a subset of 2700 dyes which allowed us to start the constitutional and structural analysis of the collection using cheminformatics approaches. Herein, we open the discussion regarding the research opportunities offered by this unique library.

Received 7th February 2017
Accepted 5th April 2017

DOI: 10.1039/c7sc00567a

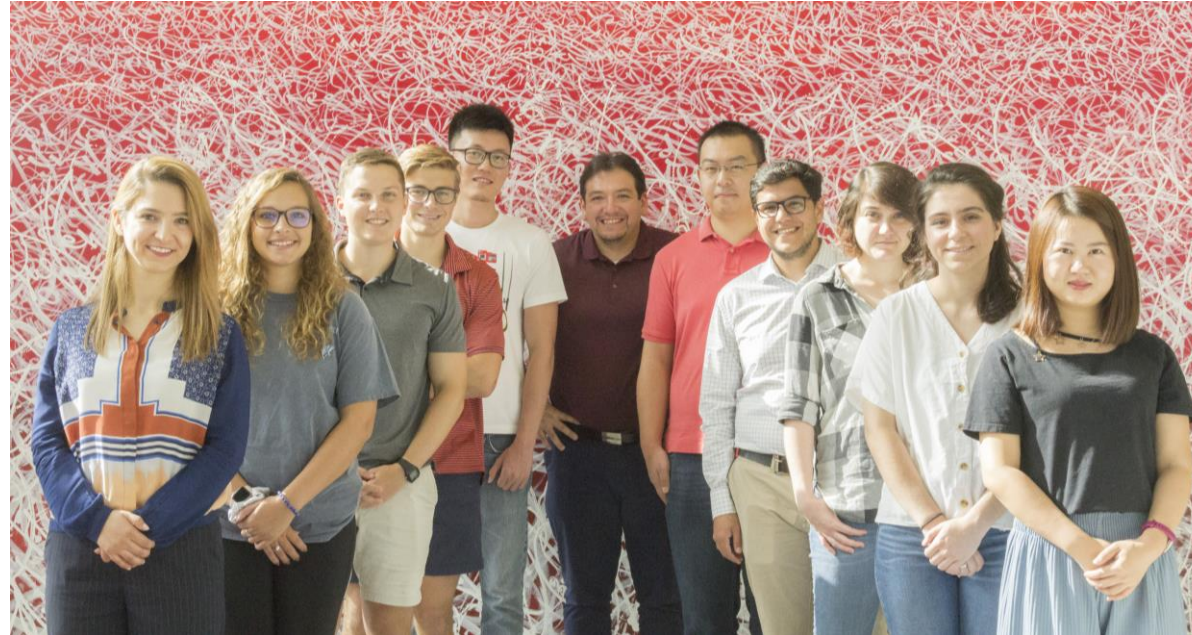
rsc.li/chemical-science

sed under a Creative Commons Attribution 3.0 Unported Licence.

Melaine A. Kuenemann, Malgorzata Szymczyk, Yufei Chen, Nadia Sultana, David Hinks, Harold S. Freeman, Antony J. Williams, Denis Fourches and Nelson R. Vinueza. *Chem. Sci.* **2017**, 8, 4334-4339

Acknowledgements

- **Vinueza Labs**
 - Dr. Xinyi Sui
 - Dr. Chengcheng Feng
 - Zoe Millbern
 - Morgan Demmler
 - Alison Trettin
 - Rachel Wu
 - Michelle Sipple
 - Jacob Best

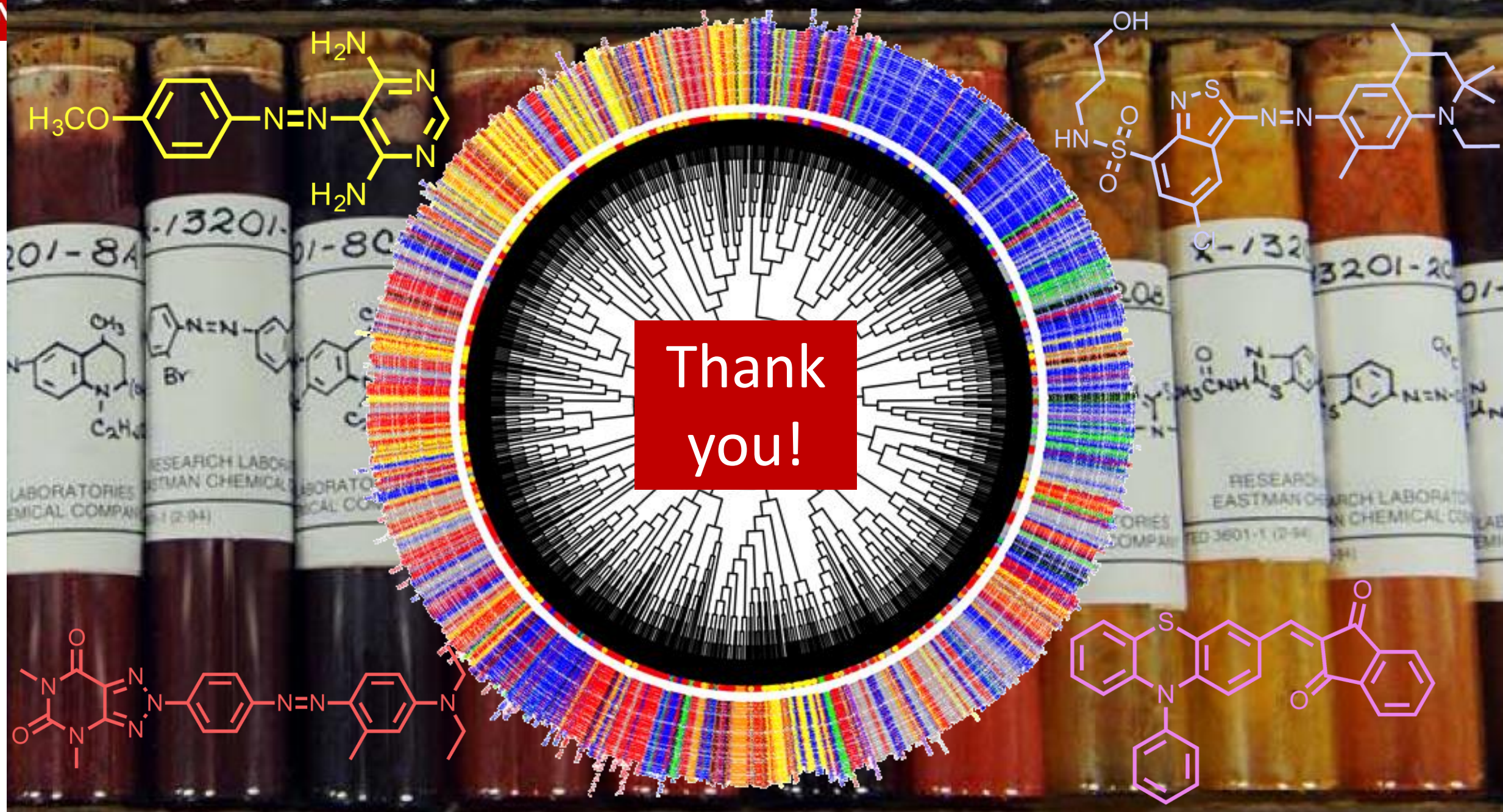


NIST National Institute of
Standards and Technology
U.S. Department of Commerce

Grant No. 60NANB19D115

ThermoFisher
S C I E N T I F I C

 Follow us!
[@nrvinueza](https://twitter.com/nrvinueza)
[@VinuezaLabs](https://twitter.com/VinuezaLabs)



Thank
you!



Follow us: @nrvinueza; @VinuezaLabs