

## DIGITAL SEED GRANT WINNERS AND FINAL PROJECTS 2019-2020

### ABOUT

Walker Library *Digital Scholarship Initiatives* supports individual and collaborative digital projects in research, teaching, and public outreach from any discipline on campus. The Digital Seed Grant is an annual award for start-up funds, developed to encourage and create opportunities for faculty, staff, and graduate students to use digital technologies in their research, service or teaching.

The Digital Seed Grant ([dsi.mtsu.edu/dsgrant](https://dsi.mtsu.edu/dsgrant)) had an impressive applications for its third year (award period 2019-2020), which initially launched in 2016 for the award period of 2017-2018. The Digital Seed Grant Review Committee and Dean of Libraries decided to award two grants for the 2019-2020 academic year. One recipient later declined due to scheduling conflicts.

The AY 19-20 awardee was announced on the website at <https://dsi.mtsu.edu/dsgrant19-20>. Below is the brief summary of the winning project and resulting outcomes.

### Use of Spectral Interpretation and Database Resources

**Primary Investigator (PI):** Dr. Ngee-Sing Chong, Chemistry Department

**PI's Project Description:** Through research projects undertaken at MTSU, the identification of chemical compounds via the acquisition of NMR, Raman, IR, and mass spectra have played a central role in advancing research in the interdisciplinary areas of forensic, materials, and environmental analyses. The use of Walker Library's Digital Seed Grant was used for the purchase of ACD Labs and Mestrenova software programs that have enabled the editing and conversion of the spectral data into formats that can be shared online. Spectral data of color dyes, environmental toxicants, and polymers are now available for supporting analytical courses and research in relevant fields.

**Purpose and Audience:** The outcome of this project includes the creation of spectral data that can be shared among different student and faculty researchers at MTSU and other institutions. This will improve the productivity of research in forensic, materials, and environmental fields by allowing researchers to calculate the spectral match index through database searching. It will also support the instructional activities related to CHEM 6230 Intermediate Analytical Chemistry as well as CHEM 4230 and FSCH 4230 Instrumental Analysis courses by Forensic Science and Chemistry majors to download the spectral data remotely, which is helpful for remote instruction under the current pandemic restrictions. Students will learn spectral interpretation skills and procedures for searching a spectral database using the sample spectra acquired for this project.

#### Project News:

The creation of dynamic spectra database is complete, upload to searchable online database is pending (expected upload by June 2021).

Examples of Spectral Match of Dyes in "CC Red" Color Run Powders to Allura Red AC are shown in the following images:

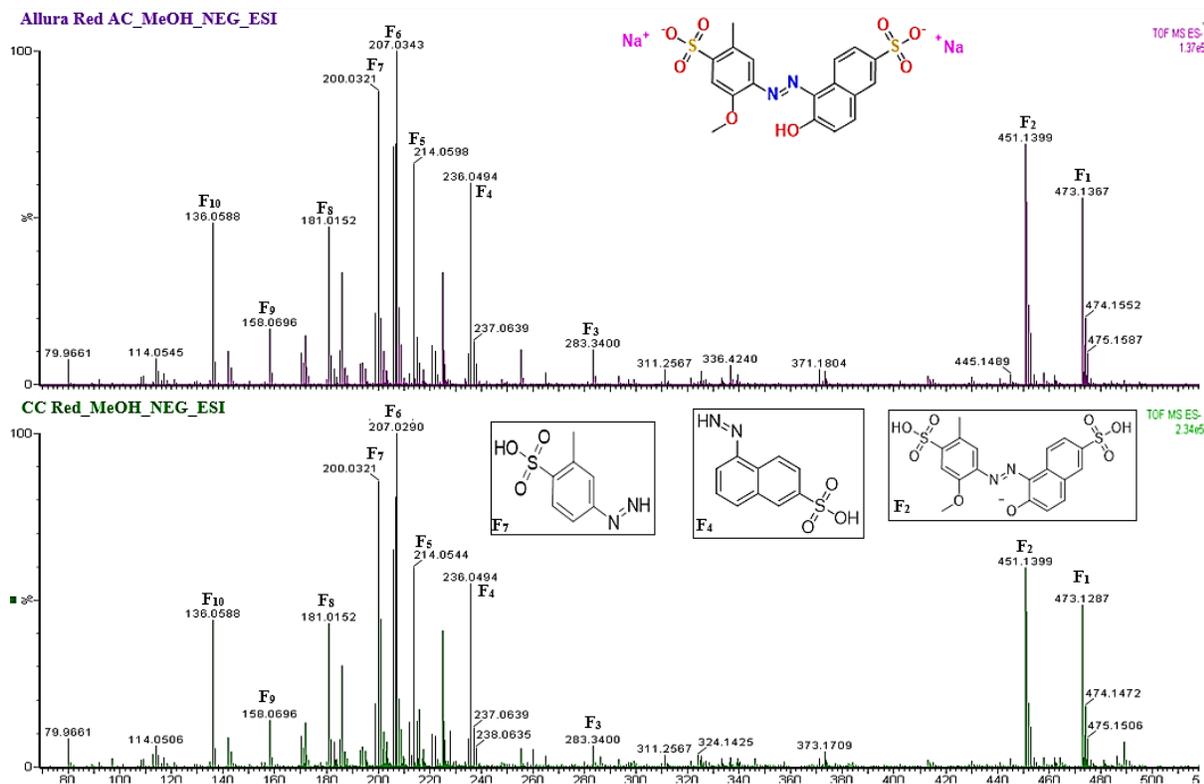


Figure 1. Mass Spectra of Allura Red AC and CC Red dye in methanol acquired in negative mode of ESI-MS.

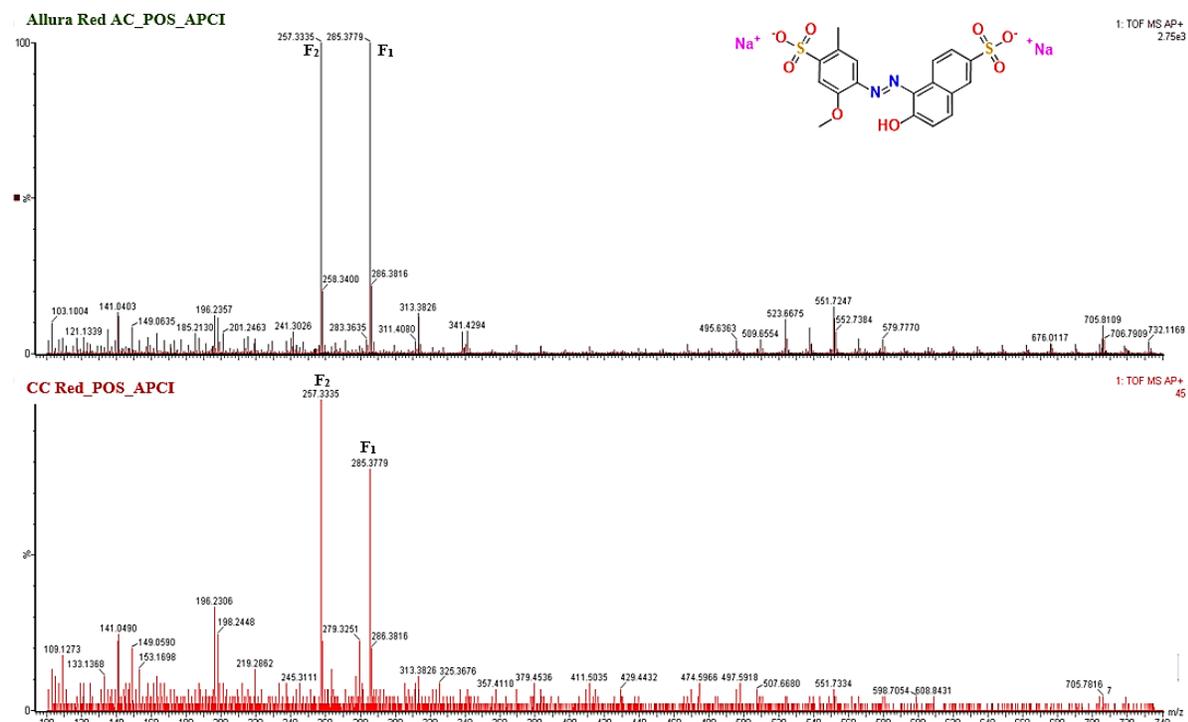


Figure 2. Mass Spectra of Allura Red AC and CC Red acquired in positive mode of APCI-MS using the ASAP probe analysis.

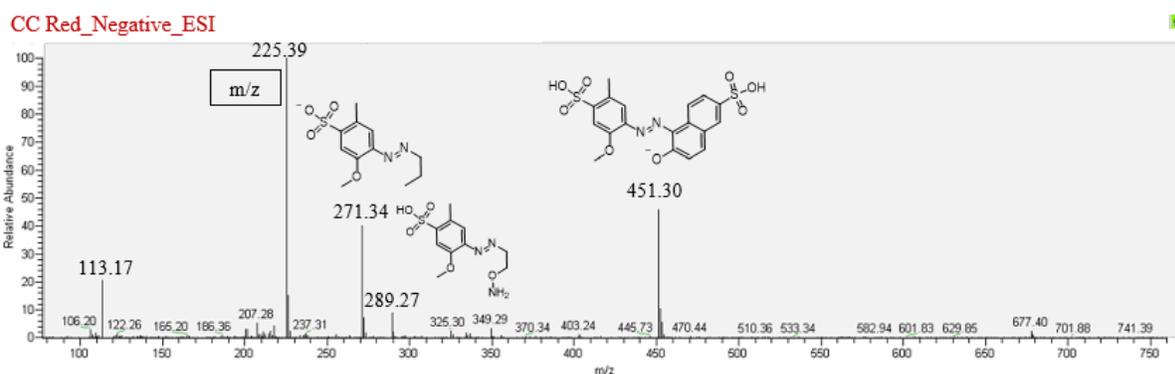
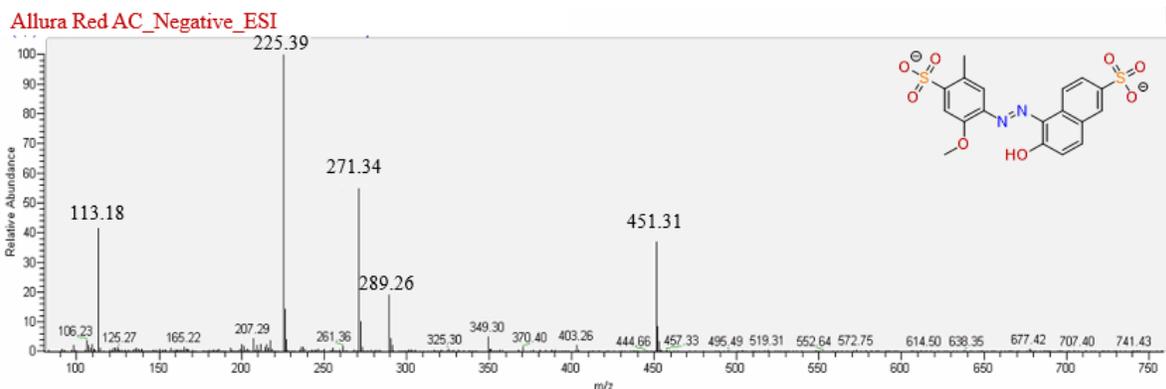


Figure 3. HPLC's Mass Spectrum of Allura Red AC (RT: 14.20) and CC Red (14.20) under ESI negative mode.

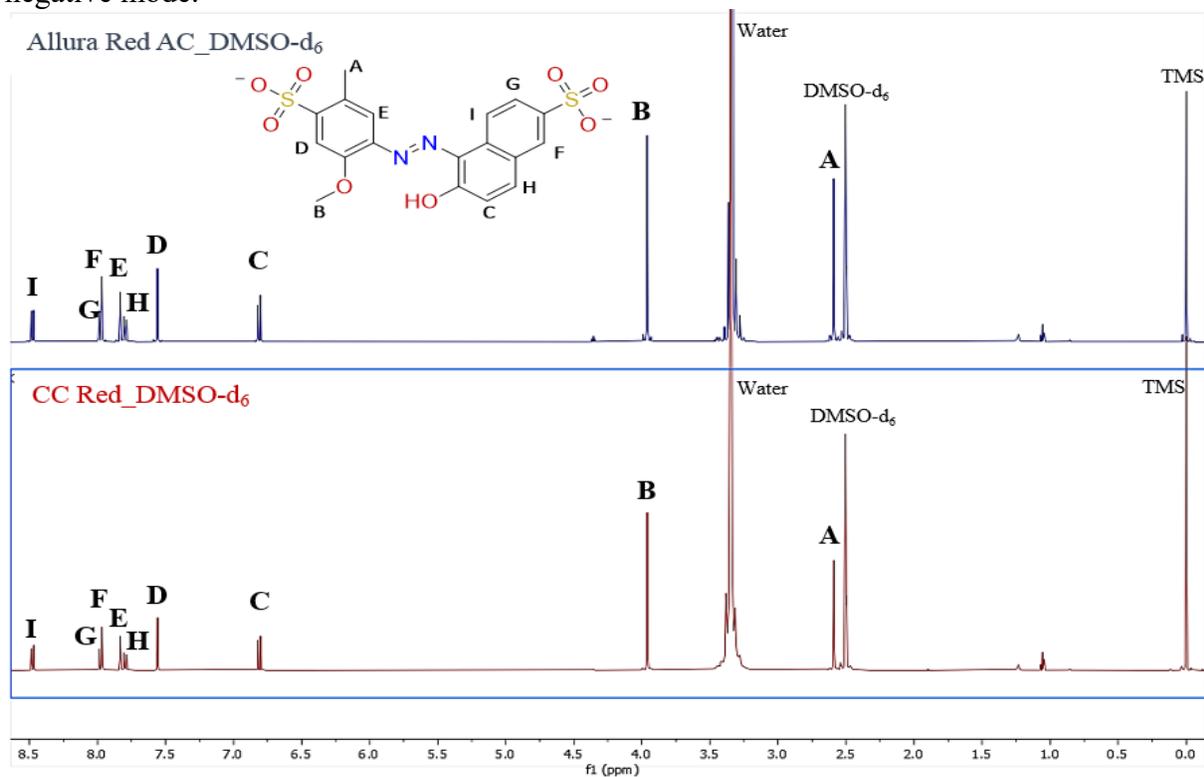


Figure 4. Comparison of H-NMR spectra of Allura Red AC and CC Red dye in DMSO-d<sub>6</sub> at 256 and 1024 scans, respectively.

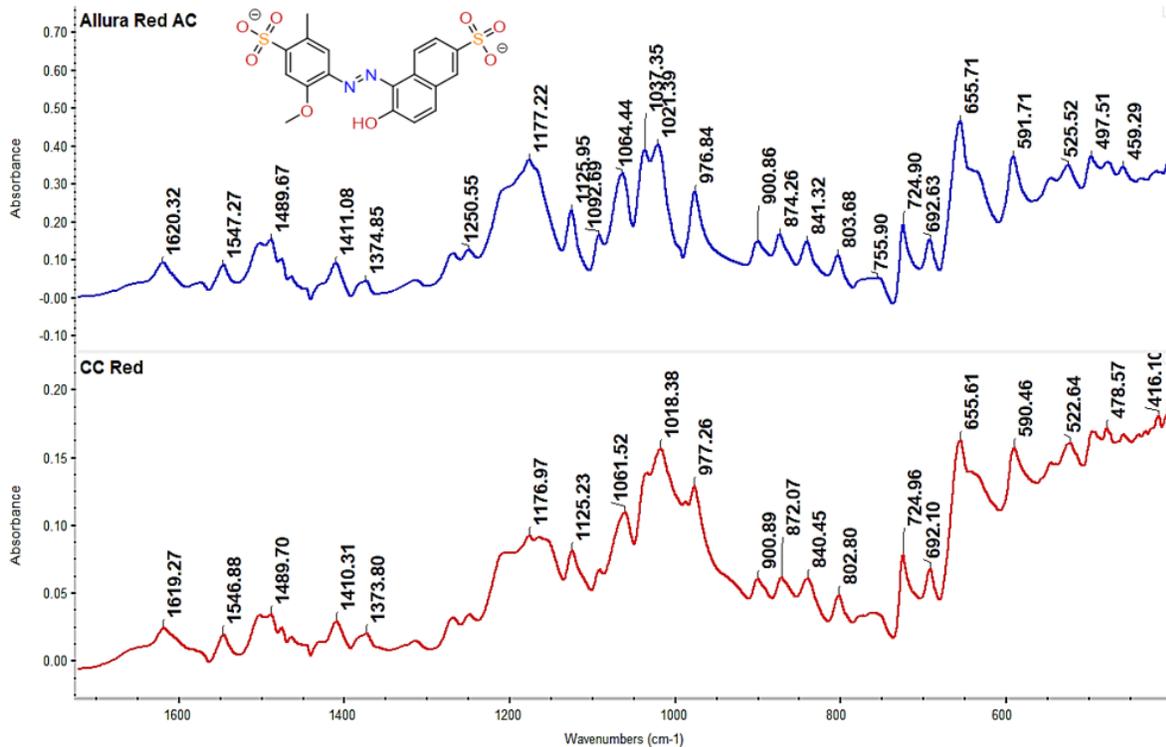


Figure 19. Stacked FTIR of Allura Red AC and CC Red dyes with a HQI of 92.02% for CC Red.

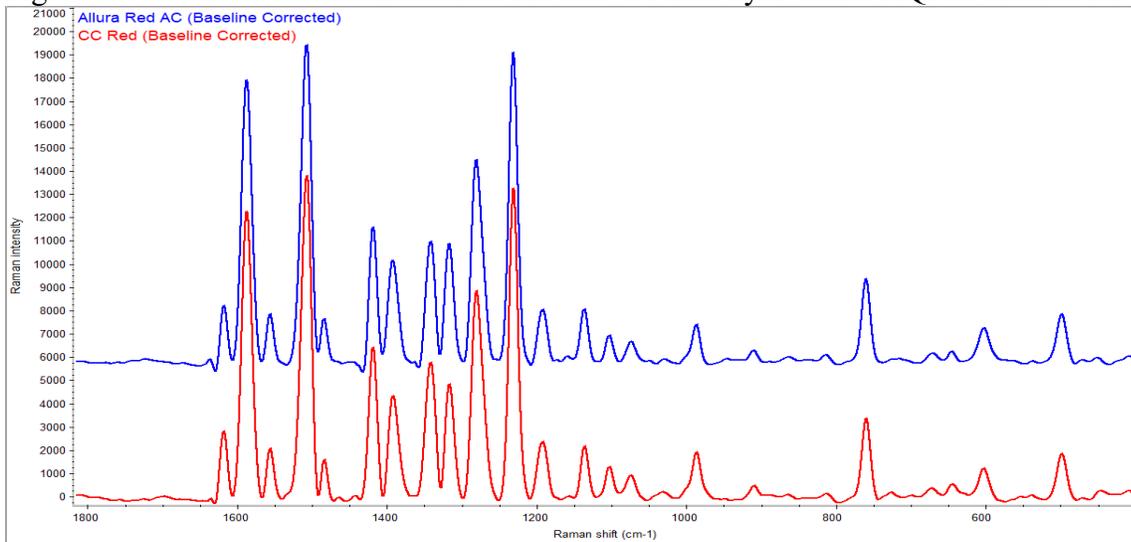


Figure 20. Baseline Corrected Raman Spectral Match of Allura Red AC and CC Red with a HQI match of 99.49%.

## FUNDING AND SUPPORT

The Digital Seed Grant is made possible by generous funding and support from the Dean of Libraries and the Digital Scholarship Initiatives project team. For many, this is a starter grant, which can lead to national grant opportunities in the future and Walker Library wants to encourage and support such creativity activity.

As a competitive grant, evaluation of applications and assessment of digital lifecycles of selected projects takes time. The Digital Seed Grant is indebted to the time of the Review Committee, comprised of digital project experts from Walker Library and the Digital Partners (a rotating member from the Department of History, Center for Historic Preservation, Center for Popular Music, Albert Gore Research Center and the University Archives). The Walker Library also thanks those that help promote the grant and encourage participation.

The 2020-2021 call for proposals closed; and those projects will continue until August 2021 and January 2022. As those projects are completed, the following website will be updated: <https://dsi.mtsu.edu/dsgrant20-21>.

The 2021-2022 call for proposals will open March 1, 2021 and the application deadline is April 16, 2021. For more information on the Digital Seed Grant and access the application, visit <https://dsi.mtsu.edu/dsgrant>.