LURA 2021 Submission Response 2

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1 - Name

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2 - Email address

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3 - Academic Major

Biochemistry and Molecular Biology

4 - Level

Senior

5 - How did you hear about the Libraries Undergraduate Research Award? - Selected Choice

From an instructor or faculty member

Other - Text

N/A

See next page for Project Abstract, Files Names, and Reflection Prompt Responses.

6 - Project Abstract or Description (100 words or less)

In silico methods is a cost- and time-effective way to synthesize materials. Refractive index (n) is an important characteristic of an optical material. This work contains a quantitative structure–property relationship (QSPR) model that was developed to predict the (n) of 262 polymers collected from various sources. Several models were created, where a four-variable model showed the best predictive performance. The best model's predictability was validated using the leave-one-out technique, external set, and y-scrambling methods. For (n), ionization potential, polarizability, 2D and 3D geometrical descriptors were the most influential. The model can be used to predict (n) for untested polymers.

7_Name - Please upload your project file here - Name

molecules-25-03772 (2).pdf F_abh2WoN4ee2206J

8_Name - Please upload your bibliography file here. If you have any trouble loading your file, contact nicole.km.juve@ndsu.edu - Name

Bibliography_list.docx F_2BtSFv7uv7JrI1z

9 - Reflection Prompt 1 How did you select your research topic or question? Did your topic or question change in any way during the research process? (100 words minimum)

The topic was suggested by my supervisor, Prof. Rasulev. Prof. Rasulev and his graduate student, Meade Erickson, were working on development of the machine learning model to predict a refractivity index of polymers. They asked me to help them to collect additional data for this project and then check chemical structures on correctness in the collected computational dataset. Since I was already experienced in chemical structures drawing and collecting chemical data by working on another project in Prof. Rasulev group, the new task was the one I could do the best. The data on refractivity index were extracted from several papers I collected using the online access provided by NDSU Library service. No, the selected topic didn't change during the research process. Moreover, the research was successfully completed, and a scientific manuscript was written based on it and published in one of the top chemical journals- Molecules

10 - Reflection Prompt 2 Did interactions with librarians, your professor(s), peers, and/or others influence the direction of your research?(100 words minimum)

The overall direction of my research never changed. In overall, I was working with chemical data collection and chemical structures analysis and characterization by computational methods. However, depending on particular project the sub-topics were changing. For example, I was working with refractivity data of polymers, then with biodegradation data of organic compounds and polymers, as well as computational investigating the interactions of cyclodextrins with food flavor compounds. During this time, the projects discussed with my professor and graduate students and necessary changes and improvements in the direction are made. I was always interacting with graduate students in the lab, asking them project related questions and at the same time discussing with them my findings and collected data from bibliographical sources.

11 - Reflection Prompt 3How did you find the sources you used in your research? Which specific search tools or databases - library or otherwise - did you use? If you encountered any challenges while searching for sources, how did you overcome them? (100 words minimum)

Since the performed research is happened during the pandemic time, I had only a possibility to use NDSU's library service remotely, from the lab. Mainly I was searching for the scientific papers through the Google Scholar and Scopus. Then, if I found a relevant paper, I was downloading the full text (in many cases the access to these papers was provided for free by NDSU Library). For example, Google Scholar or Scopus were forwarding me through the link to Sciencedirect.com database where specific paper was located, and I downloaded it from the database. It was very important to have access to a full text of many papers, since only in this case I was able to collect necessary information on chemical structures and their refractivity values. Thus, the research that was published with my co-authorship in journal Molecules (MDPI) is based on data collected for 262 polymers. These data were collected from many previously published papers by other researchers, and some of these data were collected by me, in addition to data that were collected by the graduate student. The only challenges during this research that I experienced were when some of the resources had no free access through the NDSU Library service and I had to ask my supervisor to use his professional contacts at other universities to download these papers of interest.

12 - Reflection Prompt 4Reflecting back on your research experience, is there anything you would do differently? Are there any resources or services the library could offer to better support student research? (100 words minimum)

Of course, I would work on this research more efficiently, if I could get proper training on how to work with bibliographic information, how to do a search on particular data efficiently, what databases to use and etc. In my case I had to learn everything on the way, by getting advise from the supervisor, through emails and conversations in person, with students and the professor. I think the NDSU Library is doing a good job by providing a free access to many resources at main publishers. In 90% of the cases during my data collection work, I was able to find and download necessary papers without any problems. It would be good if NDSU library will organize more training for undergraduate students on effective work with library resources to do a better research. I know that NDSU library every year organizes various trainings, but probably not all of them are getting advertised efficiently and therefore not many undergraduate students know about it.