DALHOUSIE UNIVERSITY
FACULTY OF ENGINEERING

Department of Electrical and Computer Engineering

Design of an Online User Interface for Informatics – Guided Classification of Miscible and Immiscible Aqueous Solutions

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BACKGROUND

Aqueous two-phase systems (ATPSs) form when two immiscible solutions are mixed at specific temperatures and concentrations. ATPSs are used for biomedical purposes, such as separating and extracting viruses, enzymes and other biomolecules. [1]

Testing various solutions for the formation of an ATPS is a tedious process. Dr. Frampton's team have developed and trained four different machine learning algorithms to predict the formation of ATPSs. [2]
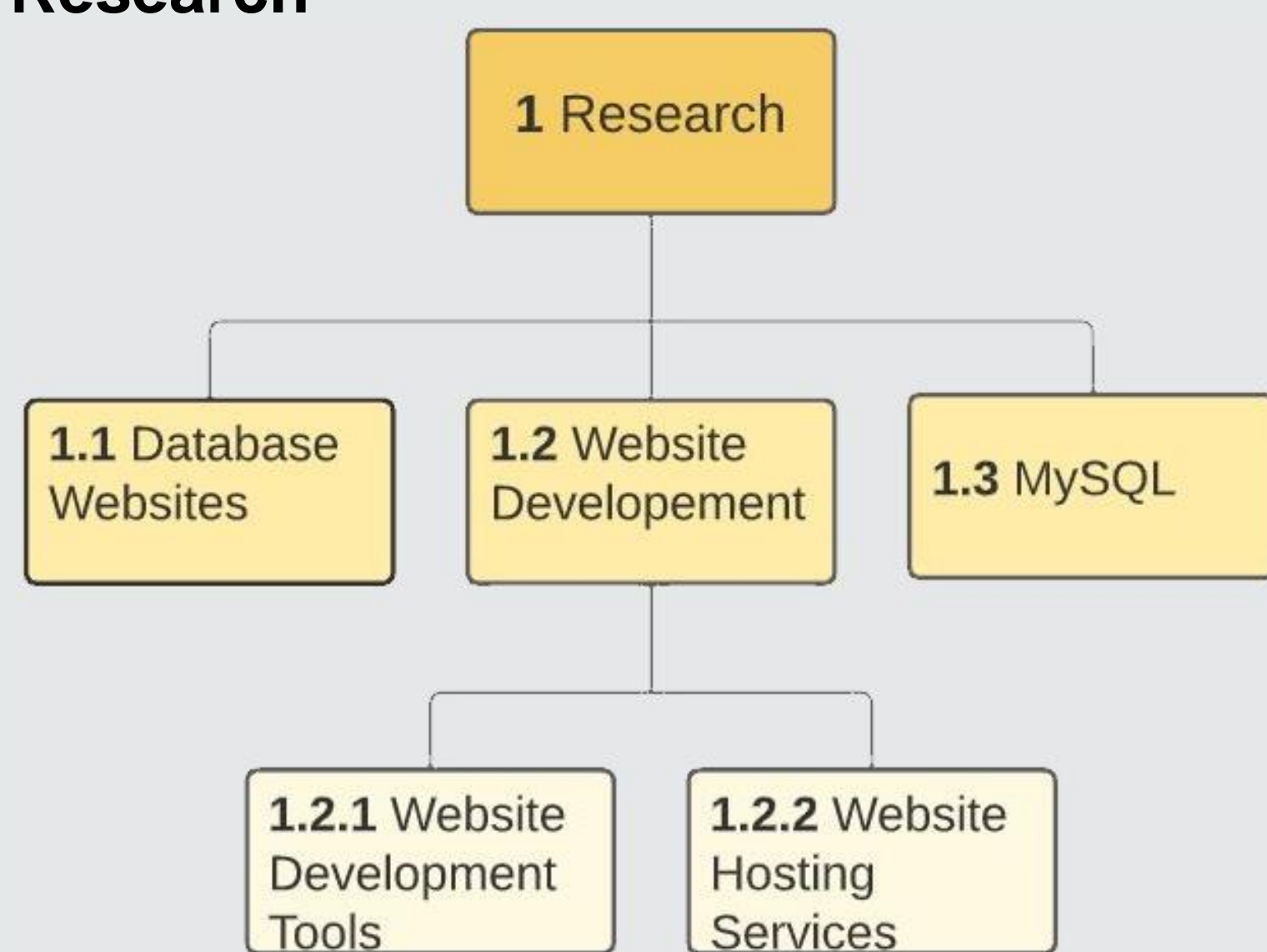
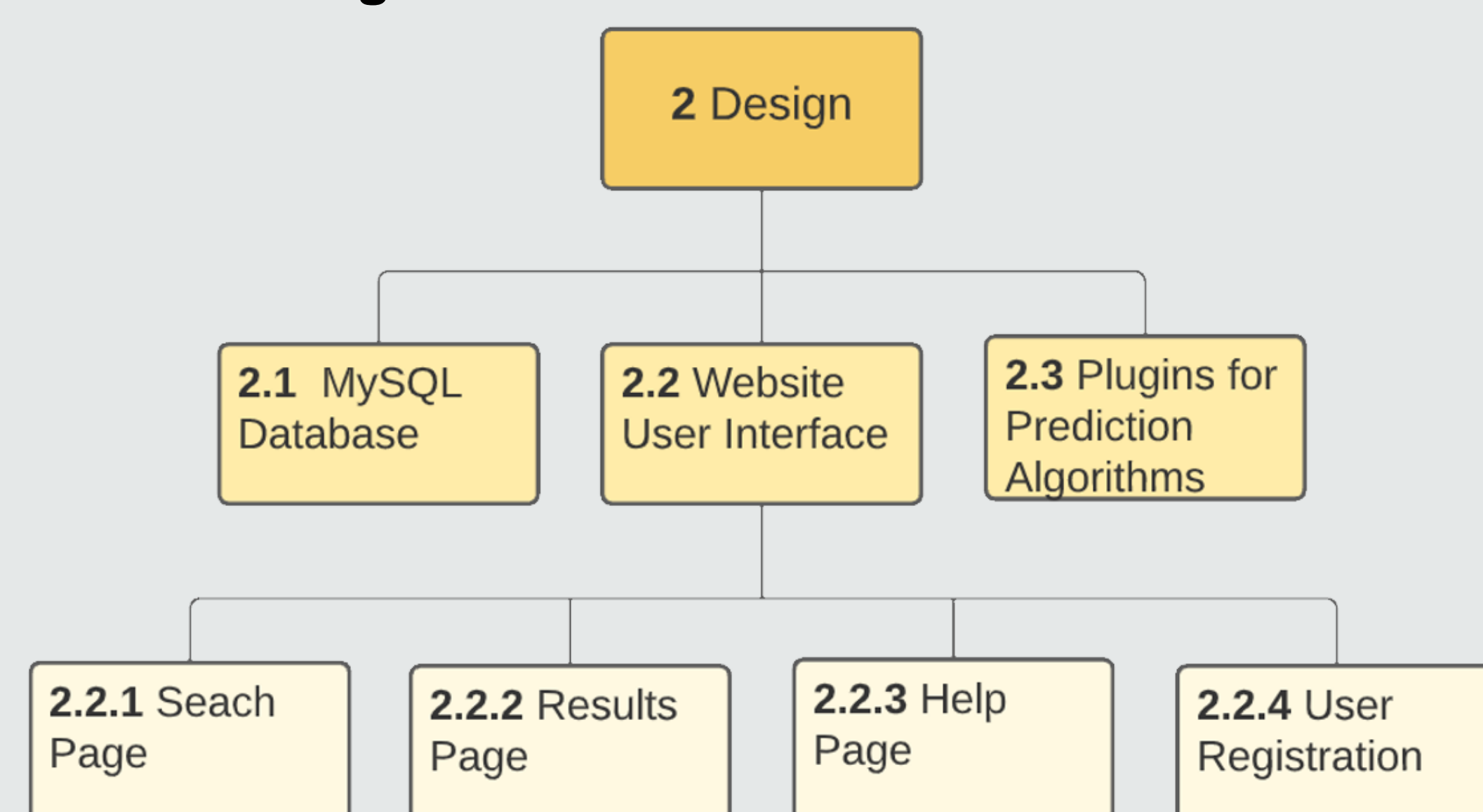## OBJECTIVE

Develop a website which:

- Houses Frampton Lab's solution database.
- Makes the four machine learning algorithms available for ATPS predictions.
- Provides users with a confidence metric for their prediction.
- Allows user contribution to the database.
- Has a user registration and login system.
- Includes a troubleshooting system.

DESIGN PROCESS

Phase 1: Research

Phase 2: Design

WORK COMPLETED

The work completed to date includes a comparison of various website hosting services. Table 1 presents a compact version of the evaluated shared hosting providers

The hosts were compared based upon their offered content management systems (CMS), cost per month, storage space, support for MySQL databases, and support for python plugins.

From the hosts assed, Dreamhost was selected because of its low cost and support for python plugins.

Table 1: Comparison of Website Hosting Services

	Plan	Cost/per month	CMS	Storage Space	Number of MySQL Databases
Bluehost	Basic	$19.42	WordPress	50 GB	Unmetered
	Plus	$23.31	WordPress	Unmetered	Unmetered
Dreamhost	Starter	$8.99	WordPress	50 GB	6
	Unlimited	$13.99	WordPress	Unlimited	Unlimited
GoDaddy	Economy	$36.39	WordPress Joomla	100 GB	10
	Deluxe	$39.39	WordPress Joomla	Unlimited	25
HostGator	Hatchling	$10.94	WordPress Joomla Drupal	Unlimited	Unlimited
	Baby	$13.94	WordPress Joomla Drupal	Unlimited	Unlimited

Table 2 displays an analysis of websites housing chemical and metal alloy databases.

The sites were evaluated based upon their searching system, troubleshooting mechanisms, formats for exportable data, login/ user registration system, and publication system.

This table identifies the key attributes of a database website.

**Table 2: Website Architecture Evaluation**

	Database Searching	Trouble Shooting	Exporting Data
NIST Alloy Data	• Search bar • Graphical input	• Error pop-ups • Feedback email • "Report data issue" button	• Figure windows • PNG for plots • CSV for data
CINDAS LLC HPAD	• Search bar • Drop-down menus	• Instructional document • Video tutorials • FAQ	• Print plots directly from site • PNG, JPG, PDF or SVG for plots
PhaSepDB	• Search bar • Drop-down filters	• Instructional page • Contact emails • Example inputs	• Excel for database(s)
AFLOW	• Search bar • Filter buttons • Graphical input	• External forum • Contact emails	• CIF, STATE, JPG, PNG for images • PNG for plots • TXT for data
NOMAD Laboratory	• Graphical input • Filter buttons	• Pop-up instructions • External forum • Virtual tutorials	• TXT for data • JSON for structures

Webpage layouts were created to organize the contents of each potential webpage. The figure to the left shows the layout for the search page which will be used to navigate through the database.

Layouts were created for the home, sign-in, account creation, FAQ, data entry, search, and results pages.

The layouts will be used as a reference for the design of the website.
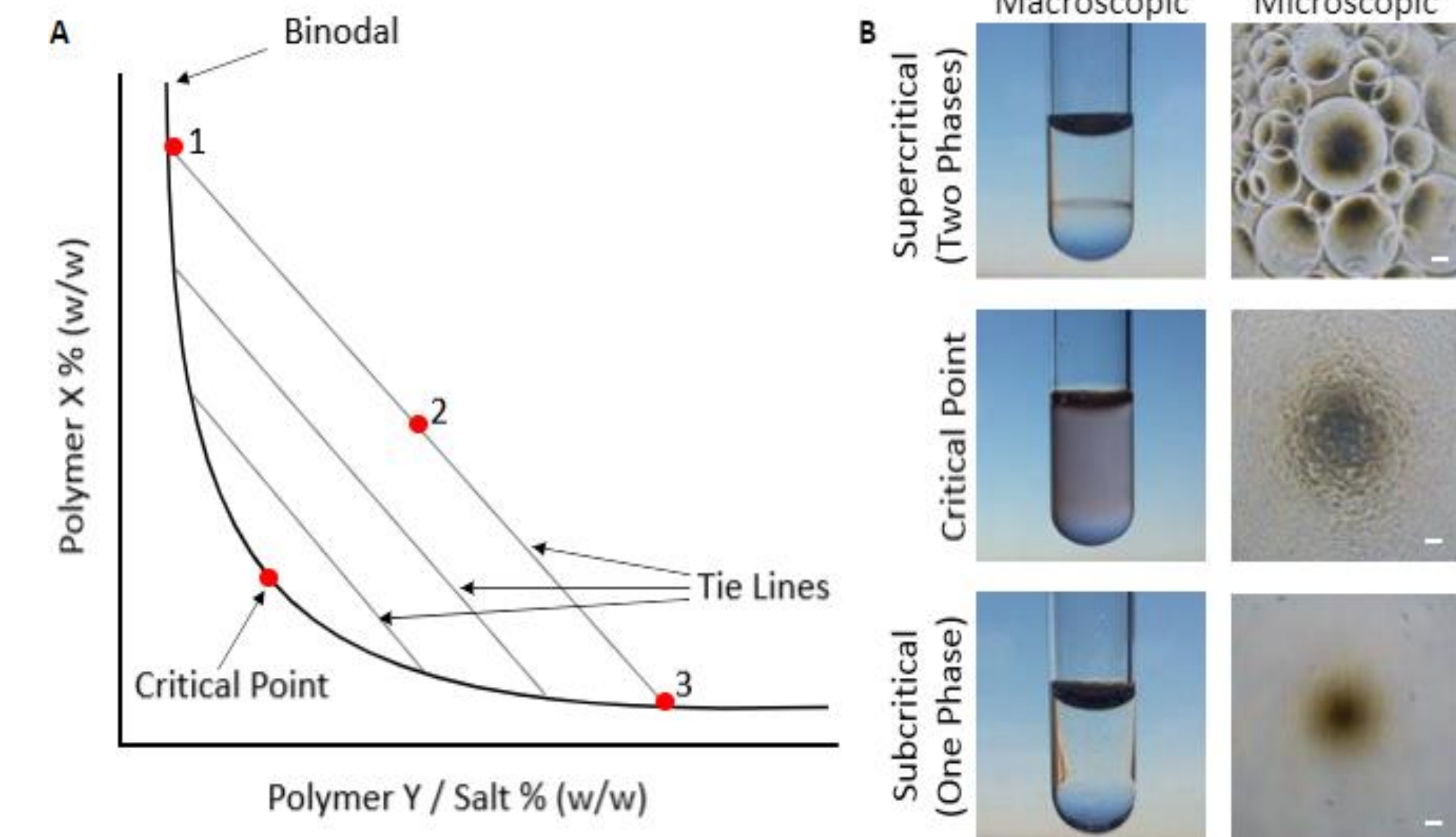
Depiction of an ATPS [3]

FUTURE WORK

- Displaying the database on the website
- Publication System
- Searching System
- Data export system
- WordPress plugins for the machine learning algorithms.
- User registration and login system
- Troubleshooting system
- Testing and debugging the site

CONCLUSION

This project is on schedule to be completed in December 2021.

To date, the team has evaluated and selected tools for building the website, chosen a web hosting service to fit the clients needs, and created a preliminary website layout.

The next steps are to upload the ATPS database to the website, create and format each webpage, and implement the required systems starting with the search page.

REFERENCES

1. Iqbal, M., Tao, Y., Xie, S. *et al.* Aqueous two-phase system (ATPS): an overview and advances in its applications. *Biol Proced Online* **18,** 18 (2016). https://doi.org/10.1186/s12575-016-0048-8
2. Peacock, C. J., Lamont, C., Sheen, D. A., Shen, V. K., Kreplak, L., & Frampton, J. P. (2021). Predicting the Mixing Behavior of Aqueous Solutions Using a Machine Learning Framework. *ACS Applied Materials & Interfaces, 13*(9), 11449-11460. doi:10.1021/acsami.0c21036
3. Teixeira, A. G., Agarwal, R., Ko, K. R., Grant-Burt, J., Leung, B. M., Frampton, J. P., *Adv. Healthcare Mater.* 2018, 7, 1701036. https://doi.org/10.1002/adhm.201701036