Tap water fingerprinting using convolutional neural network built from coffee-ring effect images

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Research goal

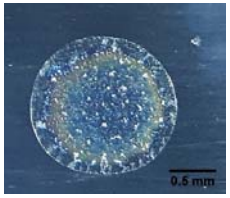
1. Develop a new low-cost water fingerprinting method

- Water analysis usually requires different methods/instruments for each analyte class
- Few of the multiplex, fast, low-cost methods are sensitive, accurate, and precise enough for reliable tap water monitoring
- We are working to harness water fingerprints created using the coffee-ring effect for low-cost, multiplex water chemistry monitoring

2. Develop an algorithm (CNN model) to harness water fingerprints

- Water fingerprints are images
- Water fingerprints sensitive to water chemistry
- Current models are not strong enough to extract chemistry information from water fingerprints

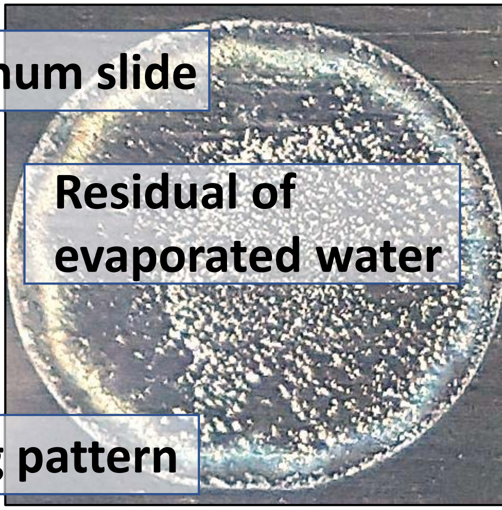
MSU academic hall

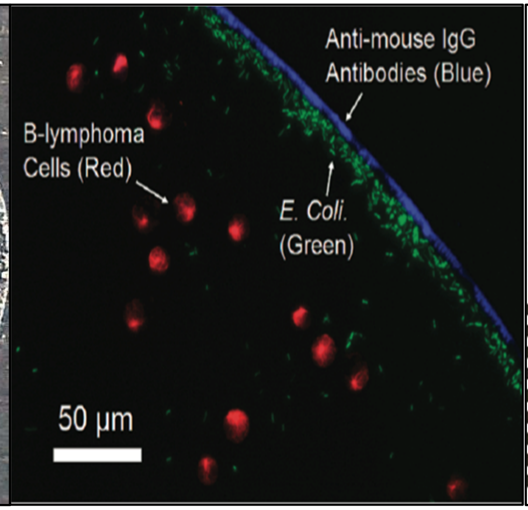


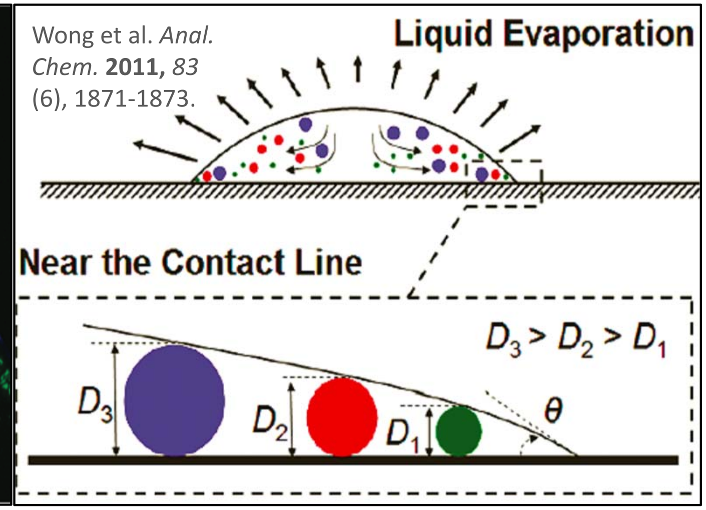
To harness the Coffee Ring Effect

Dried Detroit water

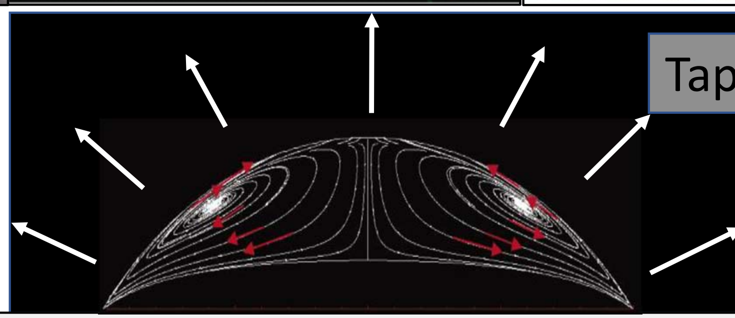
Solid Separated by size (Wong 2011)







Evaporation

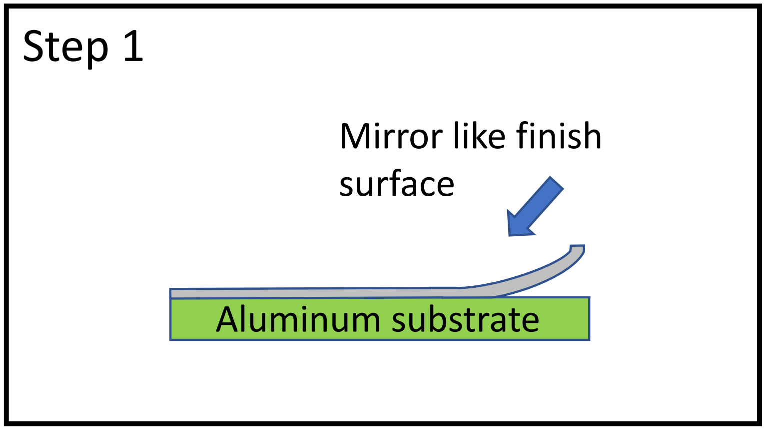


Aluminum Substrate

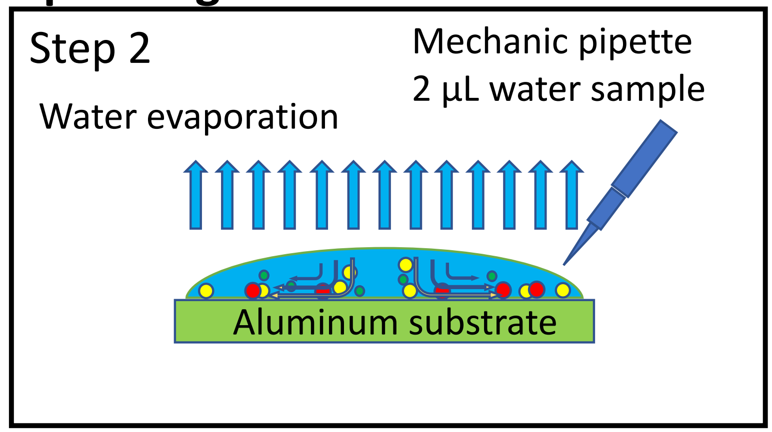
Hu & Larson. *J. Phys. Chem. B* **2006,** *110* (14), 7090-7094.

Simple setup to harness coffee ring effect

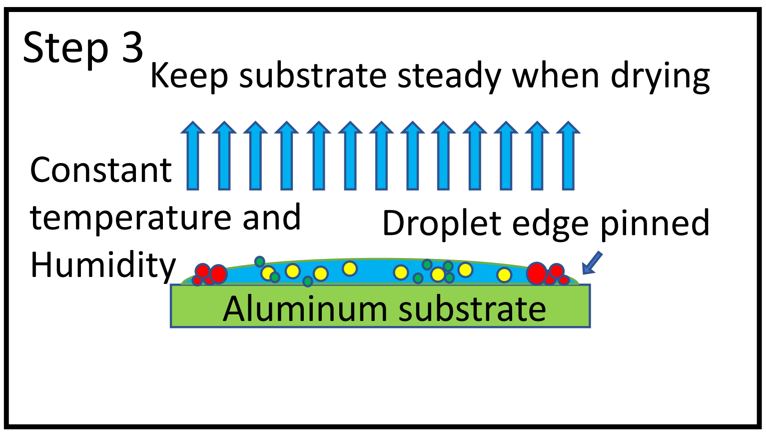
Step 1: Peel off plastic film and clean the slide surface



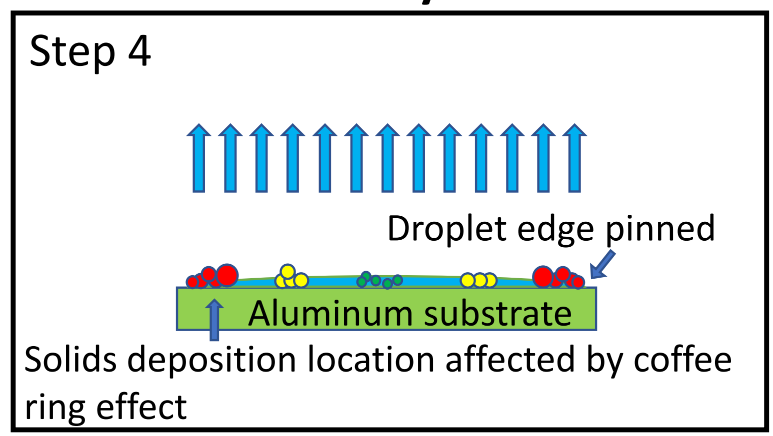
Step 2: Coffee ring effect brings particles to droplet edge



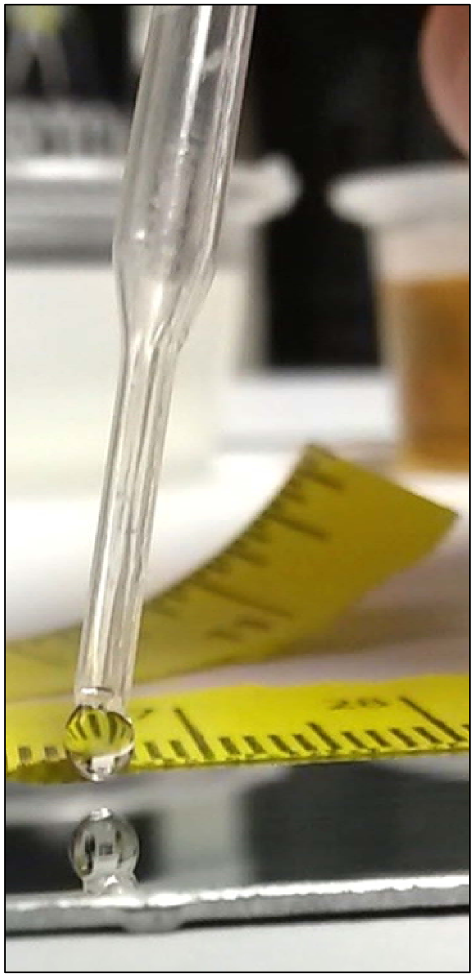
Step 3: Less soluble crystals formed first



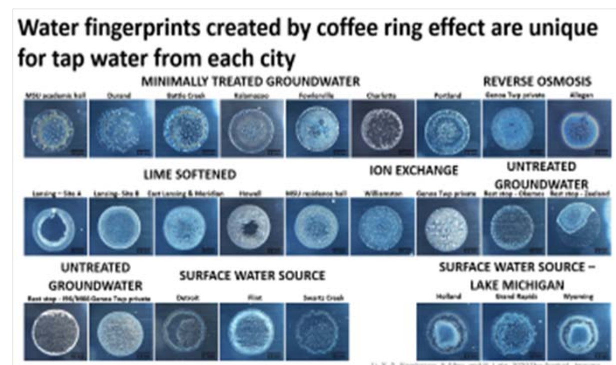
Step 4: More soluble crystals formed later



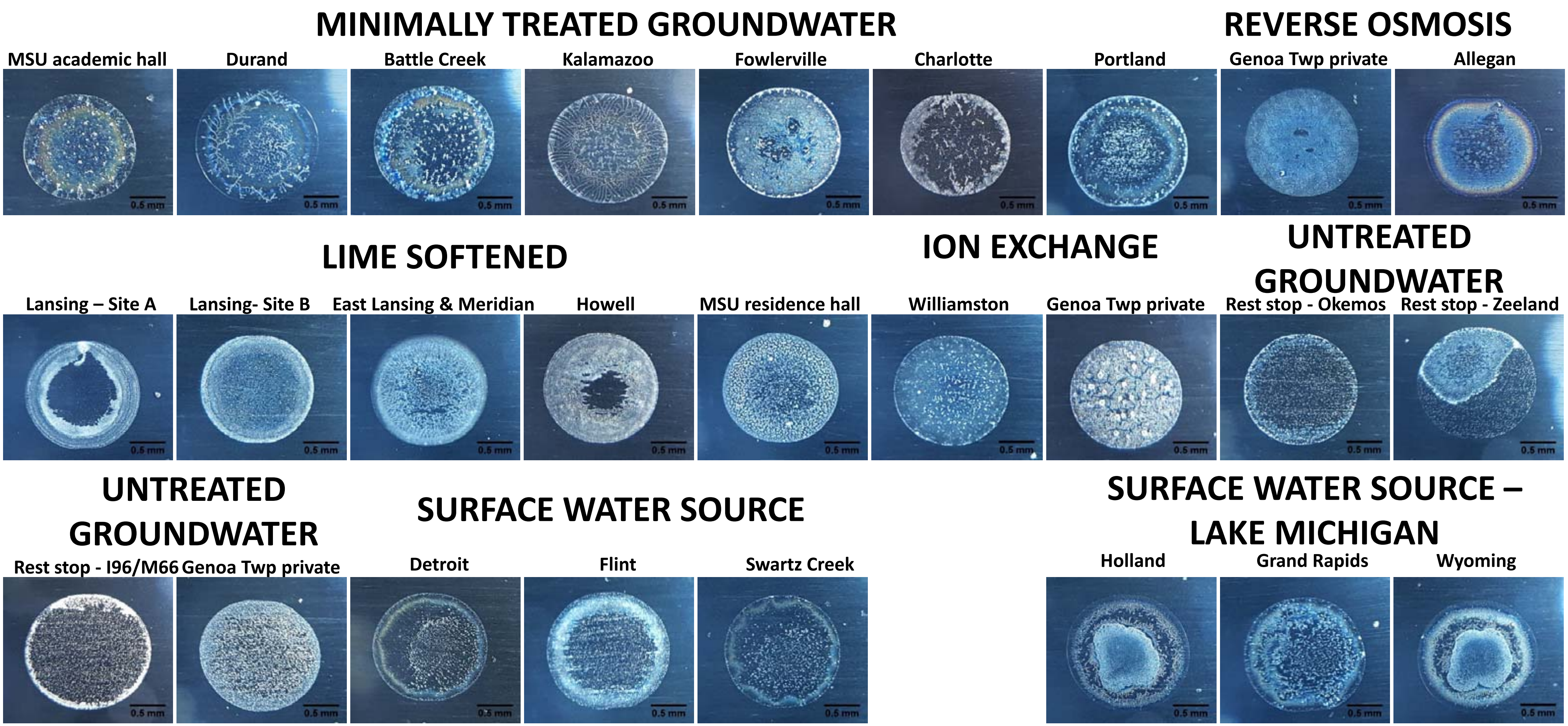
Li, X, A. Sanderson, S Allen, and R. Lahr. 2020*The Analyst*, January.



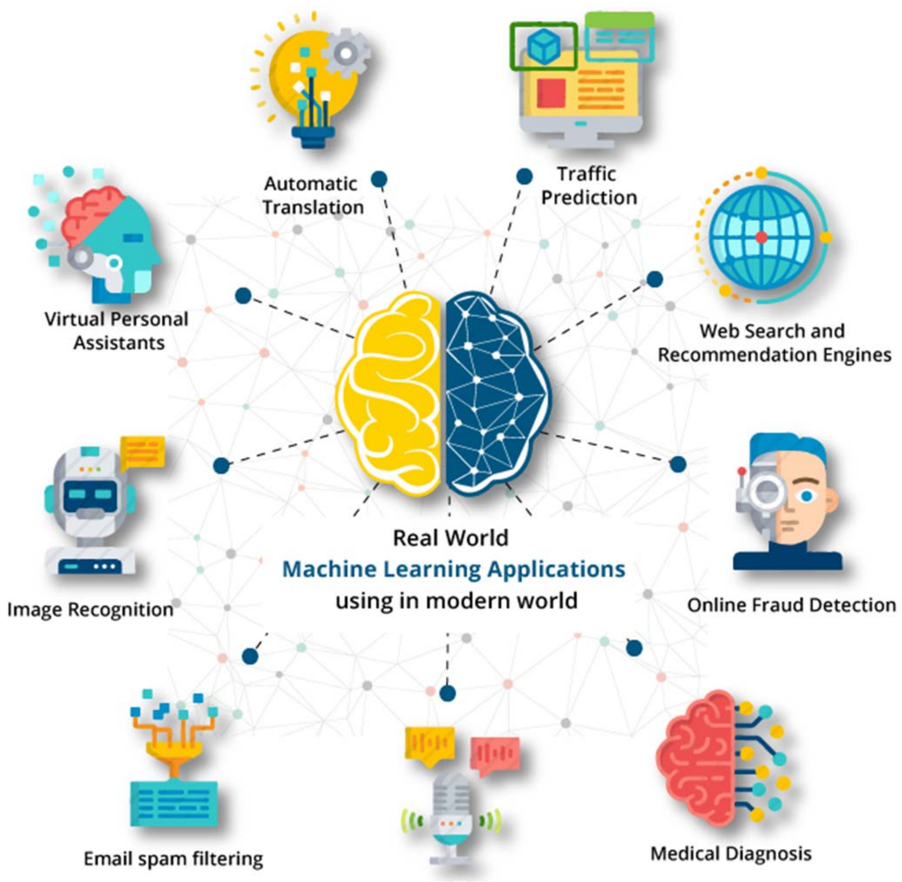
Dropping sample droplet and take the picture



Water fingerprints created by coffee ring effect are unique for tap water from each city



Li, X, A. Sanderson, S Allen, and R. Lahr. 2020 *The Analyst*, January.



Machine Learning techniques have been used to solve many complex problems

https://www.quora.com/What-are-some-real-world-examples-of-applications-of-machine-learning-in-the-field

Different deep learning networks are used to analyze each different data type

Convolutional neural network

For image data, for example, medical image data, face recognition and object detection

Long short-term memory network

For series data, for example time series data, speech data, robot control, grammar learning

Recurrent neural networks

For series data, for example text data, speech data, machine translation

Generative adversarial network

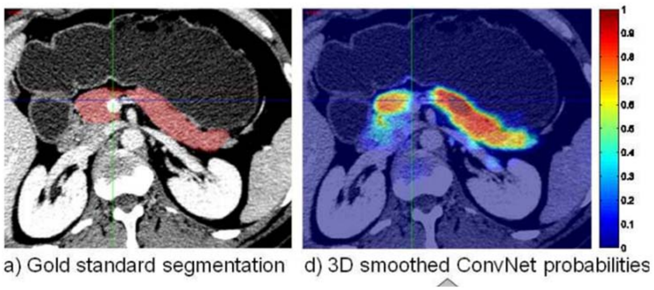
For two networks contest with each other, for example, fashion, science, video games, Miscellaneous applications

Reinforcement learning

Along side of supervised learning and unsupervised learning, for example, AlphaGo

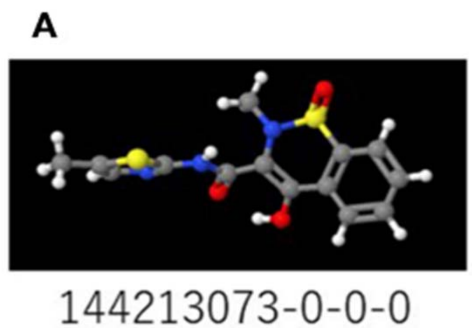
Convolutional neural network (CNN) have been used for image analysis in many different fields

Magnetic resonance images and Computerized tomography images



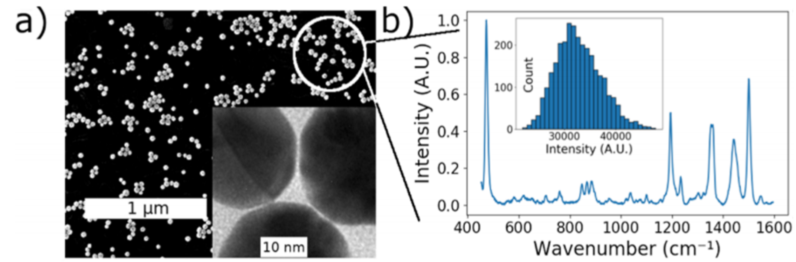
H. R. Roth, A. Farag, L. Lu, E. B. Turkbey and R. M. Summers, in Medical Imaging 2015: Image Processing, International Society for Optics and Photonics, 2015, vol. 9413, p. 94131G.

Molecular structure for toxicity prediction



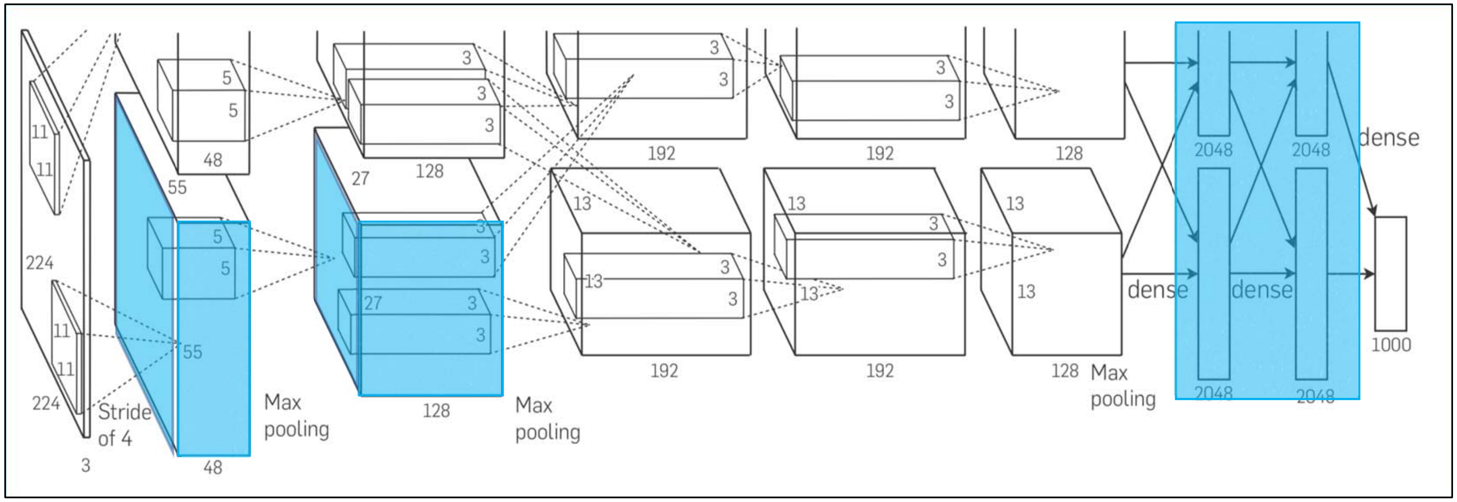
Y. Matsuzaka and Y. Uesawa, Optimization of a Deep-Learning Method Based on the Classification of Images Generated by Parameterized Deep Snap a Novel Molecular-Image-Input Technique for Quantitative Structure–Activity Relationship (QSAR) Analysis, Front. Bioeng. Biotechnol., 2019, 7, 65.

Quantification of Analyte Concentration in the Single Molecule Regime



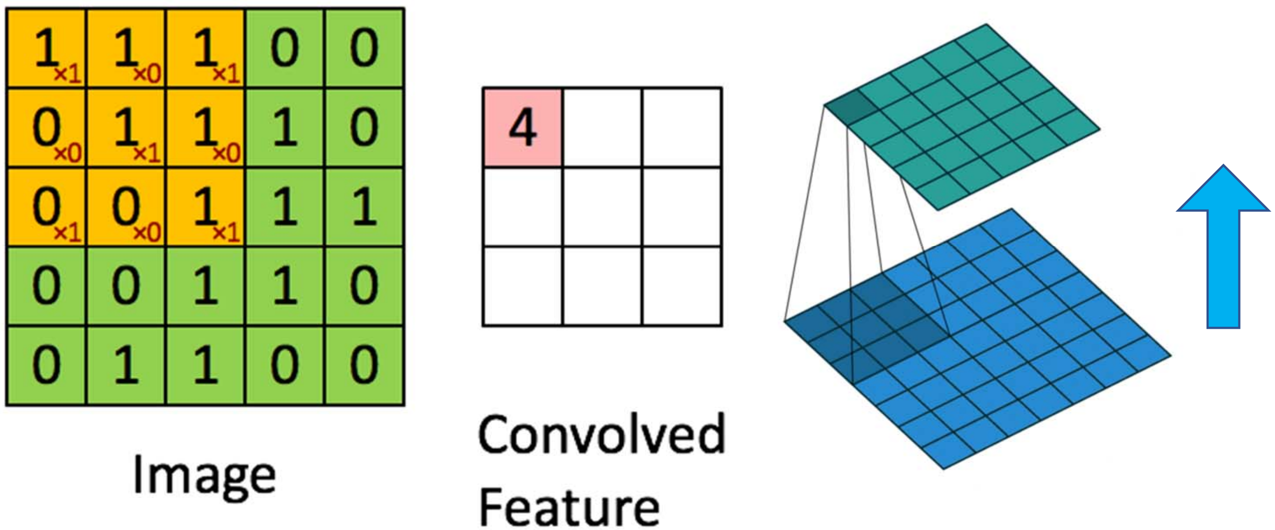
W. J. Thrift and R. Ragan, Quantification of Analyte Concentration in the Single Molecule Regime Using Convolutional Neural Networks, Anal. Chem., 2019, 91, 13337–13342.

Convolutional Neural Networks structure includes convolutional layers, max pooling layers and fully connected layers to take input images and extract features of interest



A. Krizhevsky, I. Sutskever and G. E. Hinton, in Proceedings of the 25th International Conference on Neural Information Processing Systems, vol. 1, pp. 1097–1105.

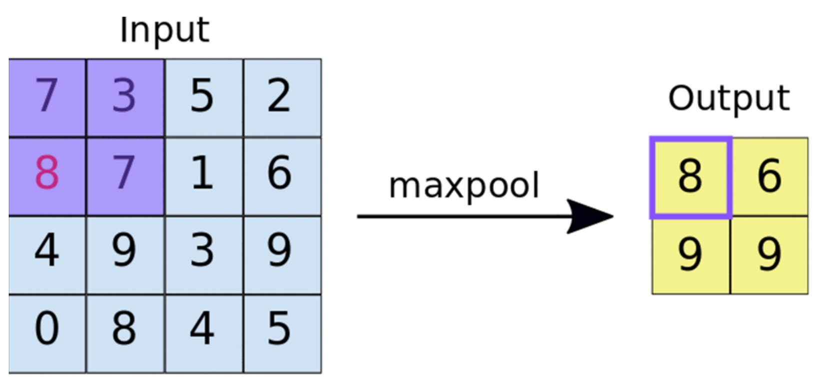
Convolutional layers work to extract nonlinear features by multiplying by the feature parameter matrix with image matrix



Convolutional layer illustration

https://towardsdatascience.com/a-comprehensive-guide-to-convolutional-neural-networks-the-eli5-way-3bd2b1164a53

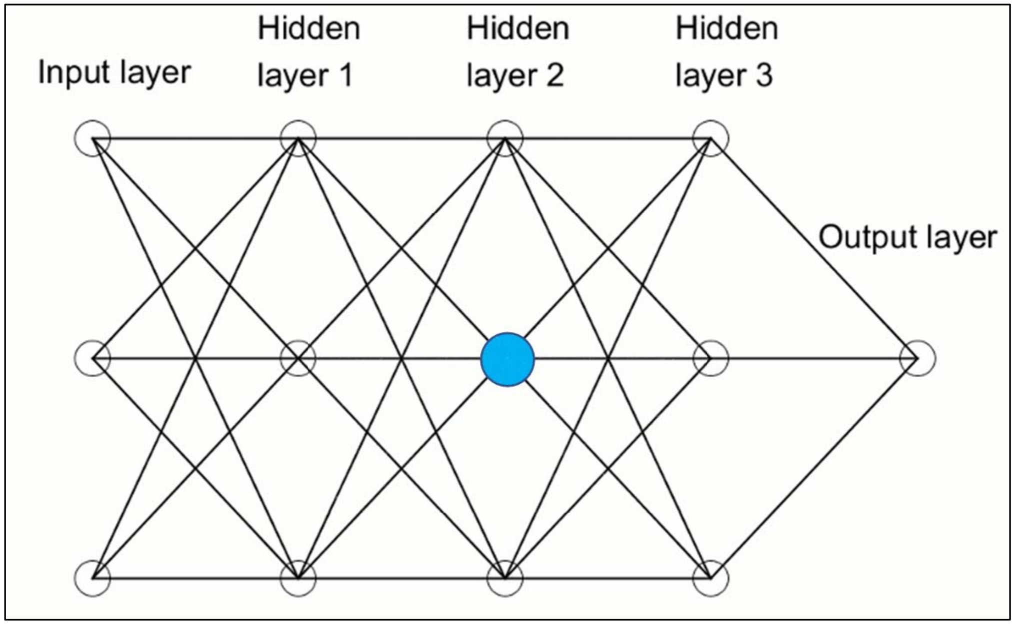
Max pooling layers work to extract the most important information (features) from convolutional layers processed layers.



Max pooling illustration

https://developers.google.com/machine-learning/practica/image-classification/convolutional-neural-networks

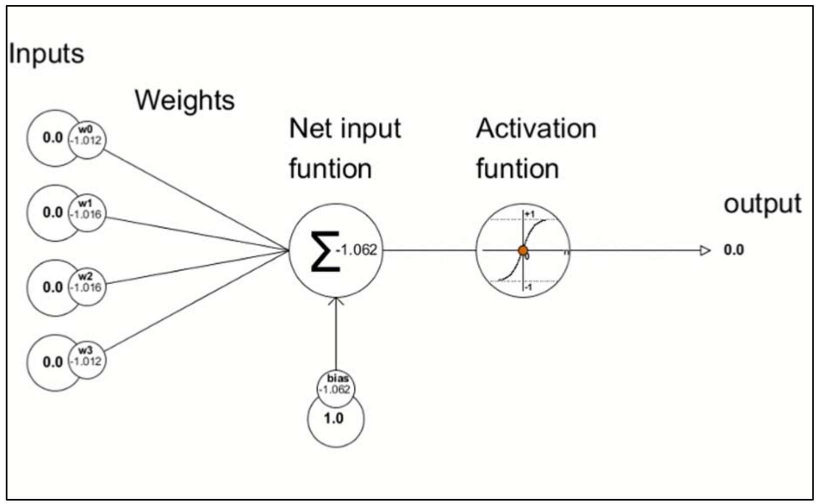
Fully connected layers work to correlate image features with nonlinear activation function to reduce 2-D image to 1-D data



Fully connected layer

https://www.mql5.com/en/blogs/post/724245

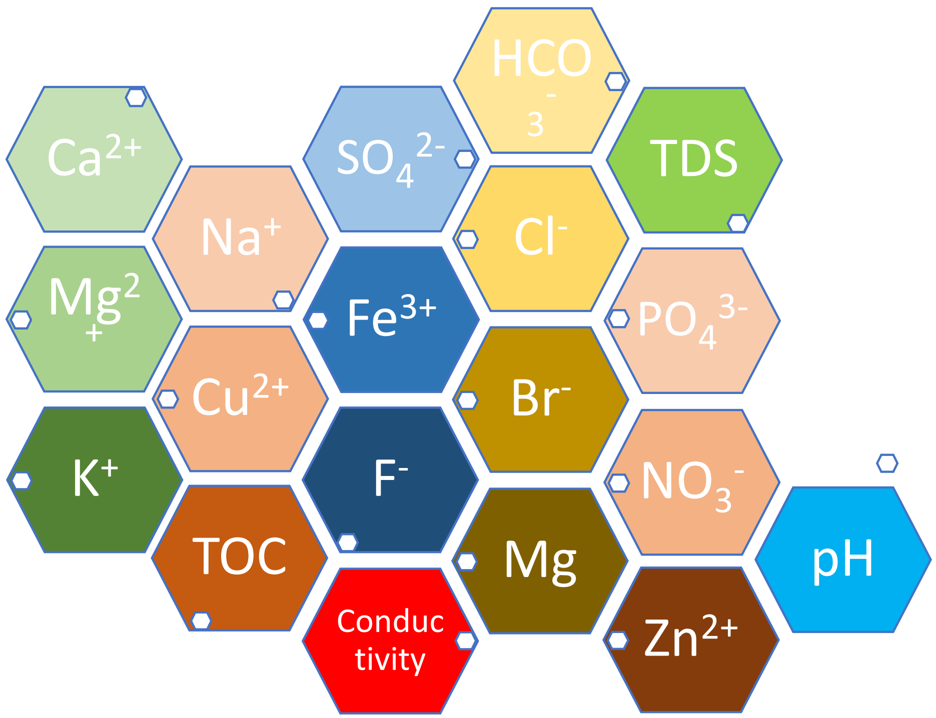
Parameters in the fully connected layers will be updated by backpropagation based on the target output



Activation Node

https://www.mql5.com/en/blogs/post/724245

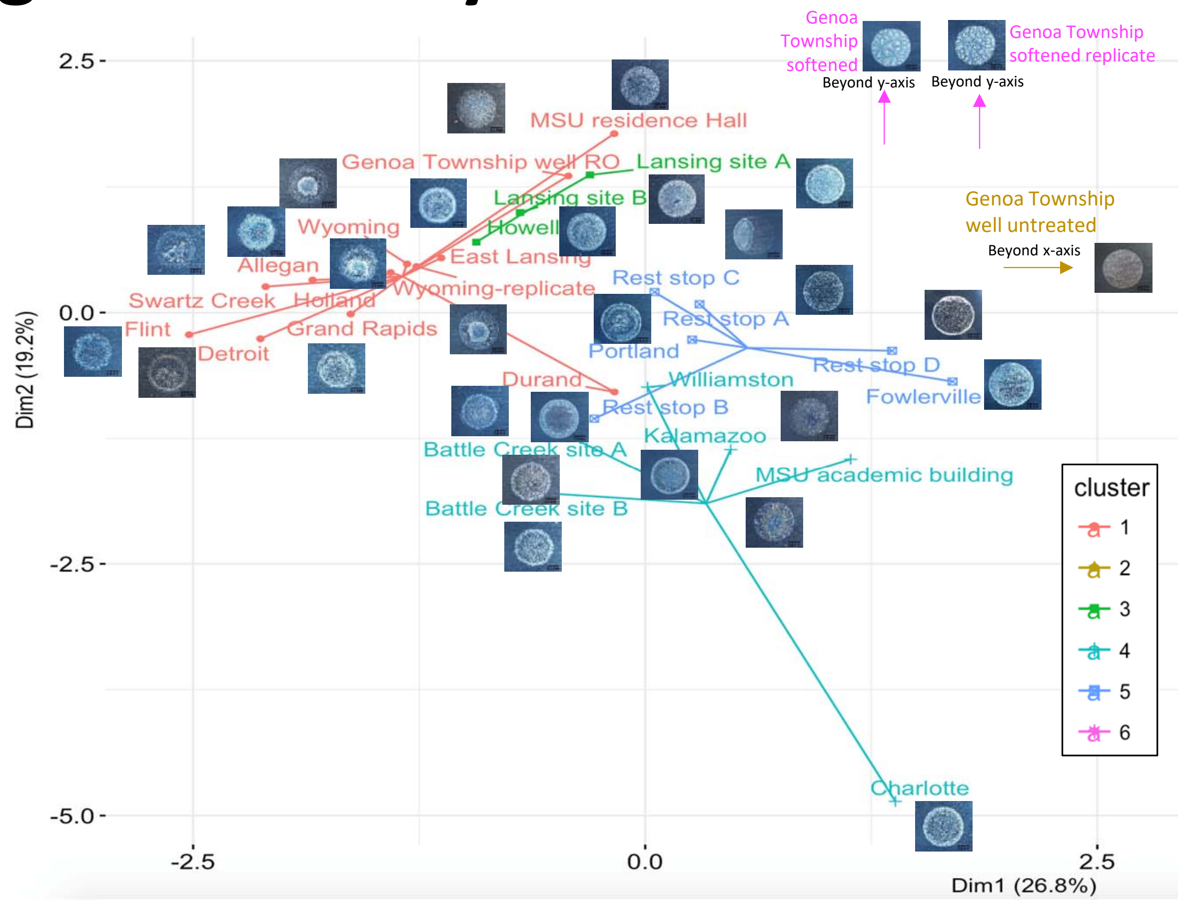
Used standard methods for analysis of water to measure chemistry and used for residue analysis



30 water collected across Michigan State
Instruments: ICP-OES, IC, pH meter, oven, AA, conductivity meter
Time consumed: **around 3 month**

Li, X, A. Sanderson, S Allen, and R. Lahr. 2020*The Analyst*, January.

Samples were grouped based on their water chemistry using cluster analysis



Clustering method groups water samples based on their chemistry data

Is that possible to correlate water samples coffee ring effect pattern with chemistry data?

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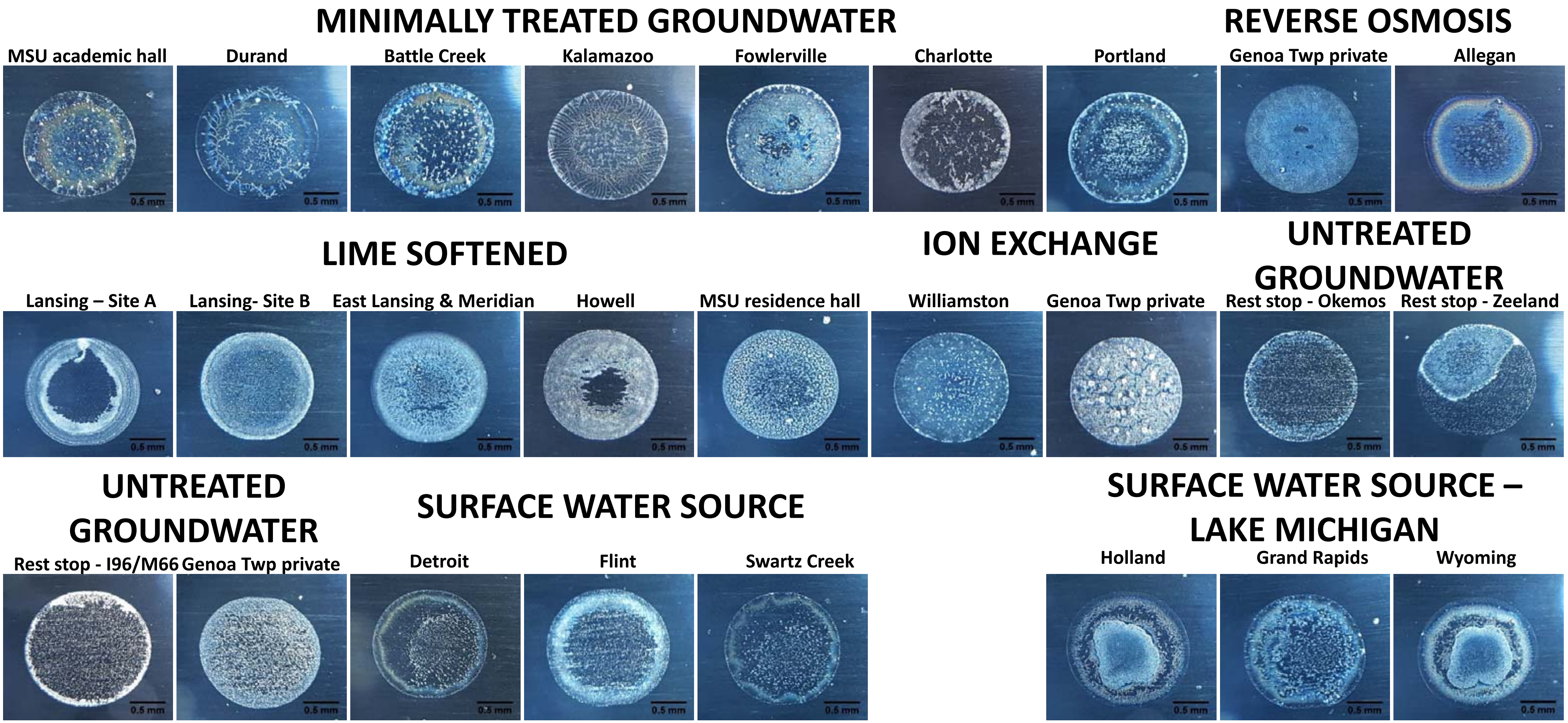
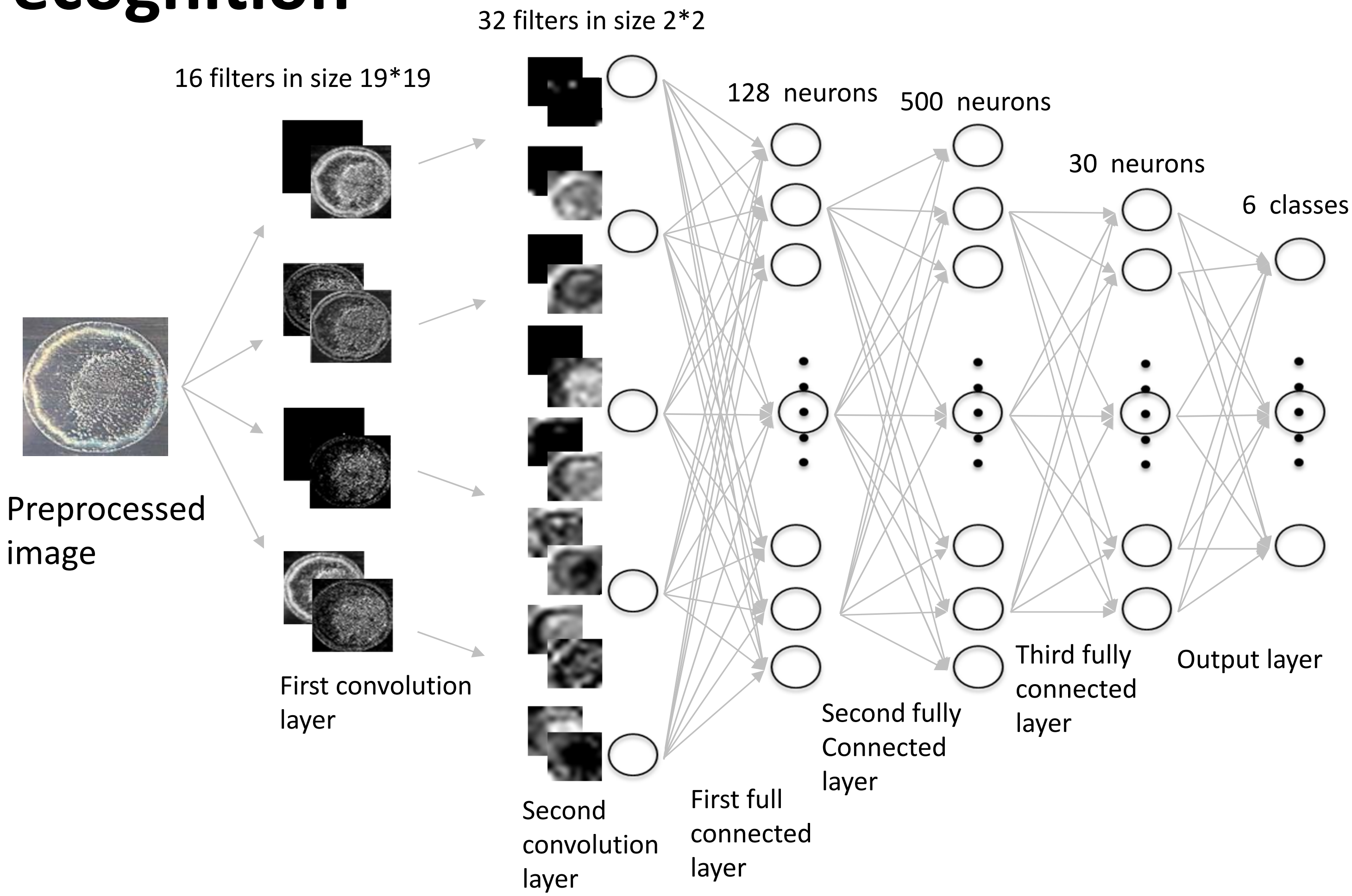
Water fingerprints created by coffee ring effect are unique for tap water from each city



Li, X, A. Sanderson, S Allen, and R. Lahr. 2020 *The Analyst*, January.

Convolutional Neural Network model for water residue pattern recognition



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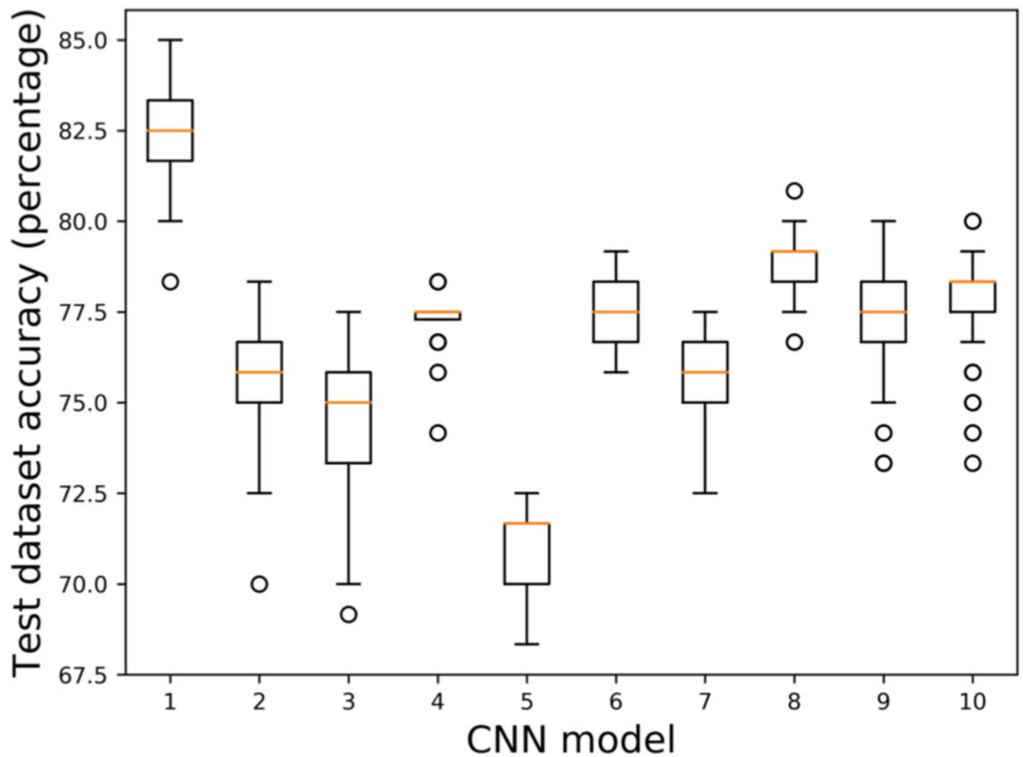
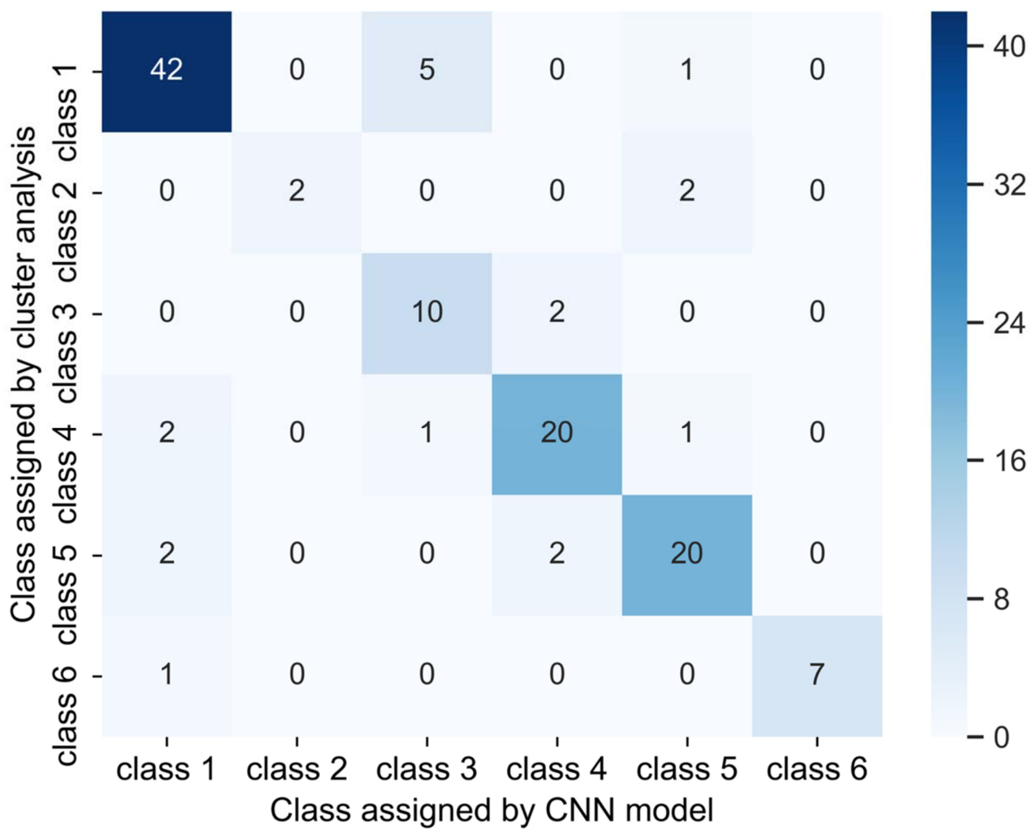
Ten CNN models were created, and assigned the image to a group with similar water chemistry (cluster analysis) with an accuracy of 77 ± 3 %



Classes with more images were more accurate.



Class	Waters included
1	Surface waters, RO, others (MSU residence hall, East Lansing
2	Untreated well water with high TDS
3	Lime softened
4	Minimally treated groundwater, other (Williamston)
5	Untreated groundwater, some minimally treated
6	Well water with high TDS after ion exchange

Larger dataset needed to achieve higher accuracy

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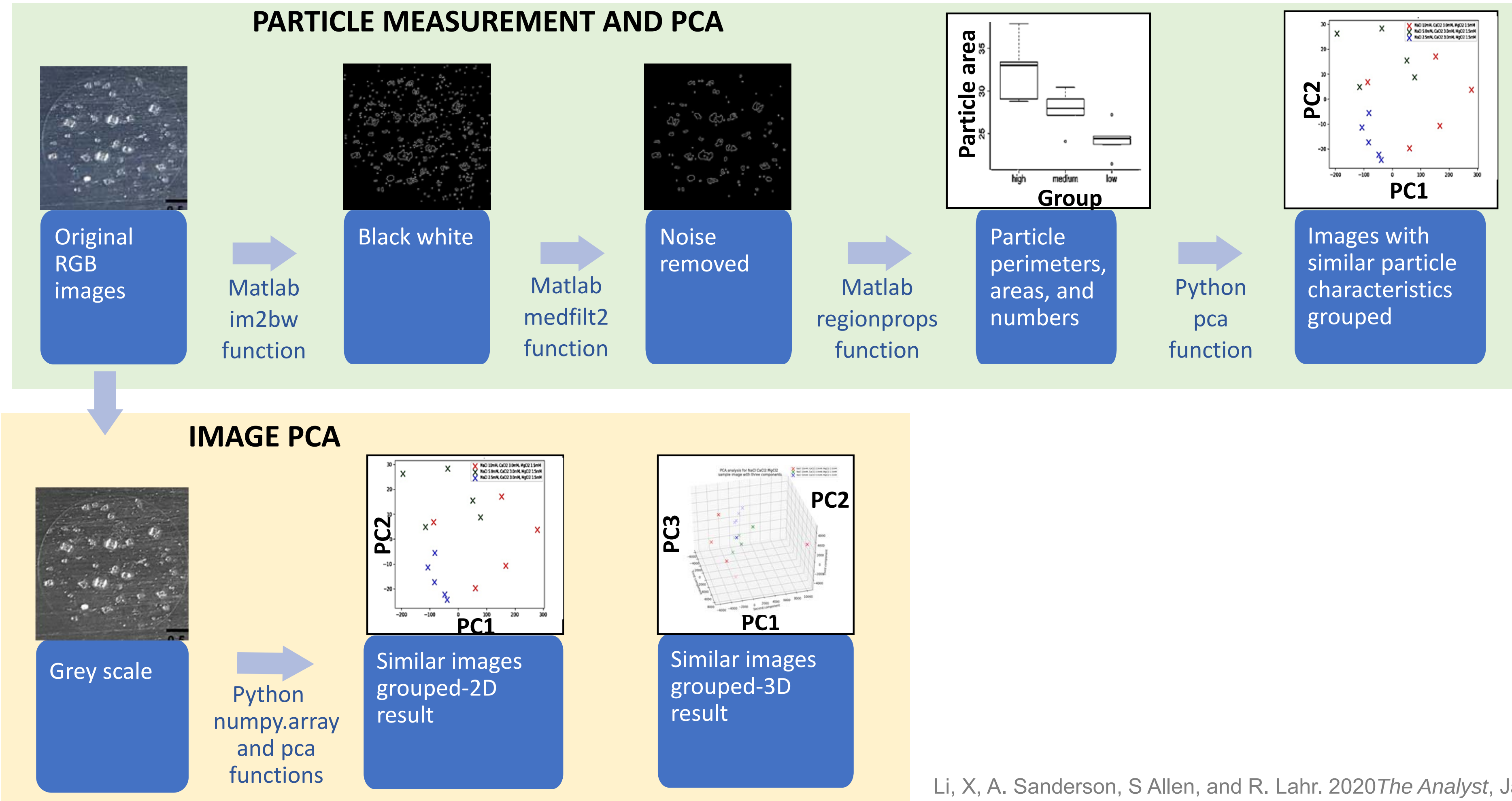
Images were analyzed using Matlab particle analysis and python image analysis



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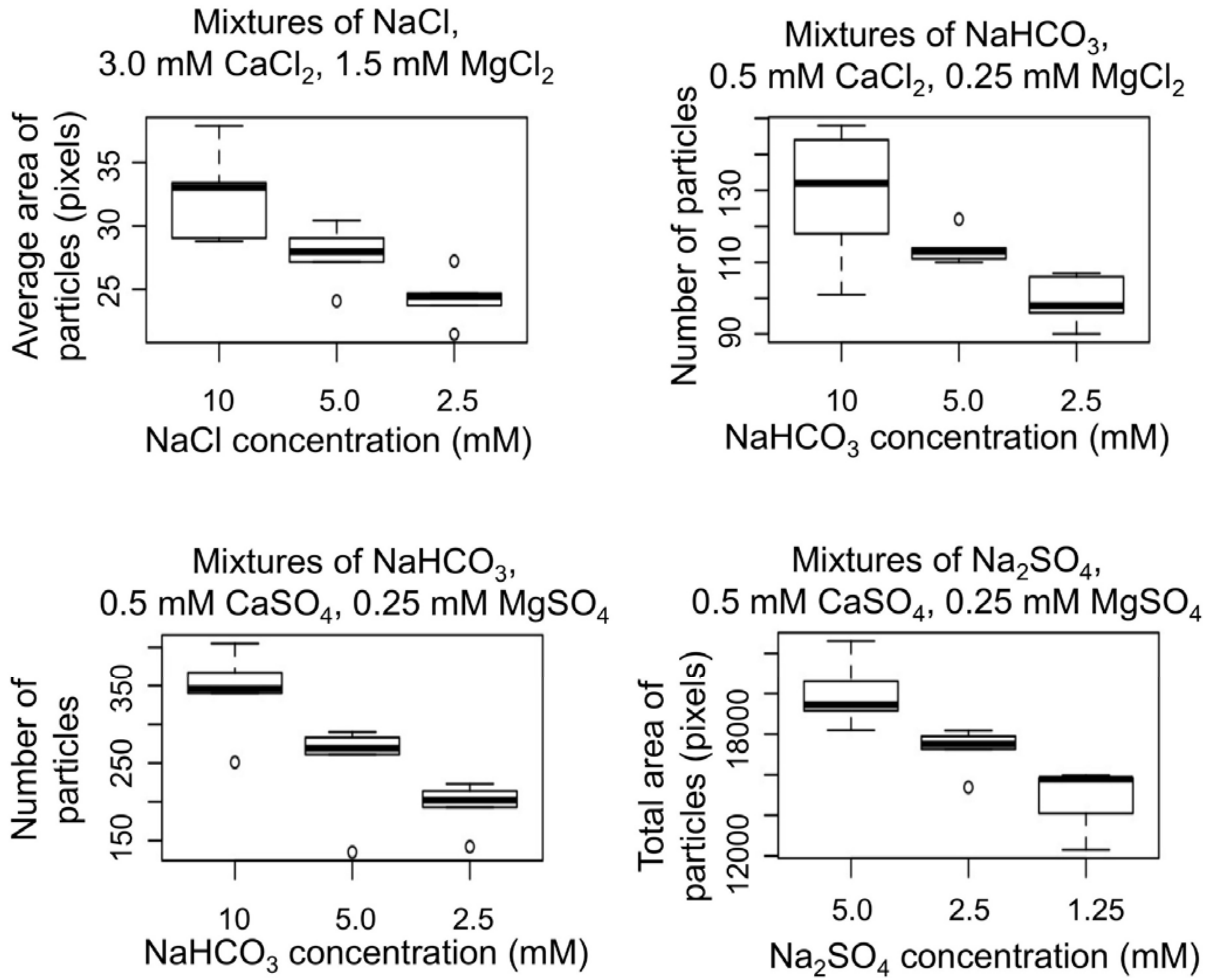

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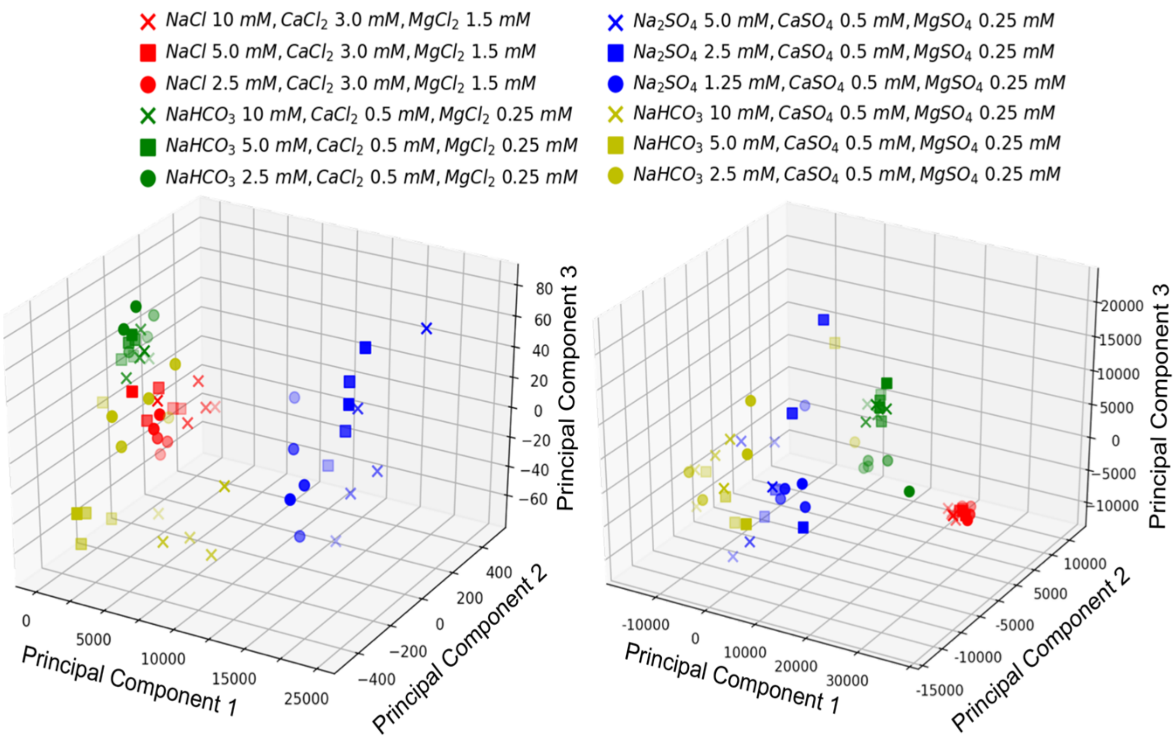
Principal component analysis (PCA) aids in classification of samples into groups with similar ions



PCA on particle measurement data

PCA on image files

PCA method couldn't recognize nonlinear features so the classification result is not good enough

Oliveira et al., 2017. *International Conference on Digital Image Computing: Techniques and Applications,* 1–8.

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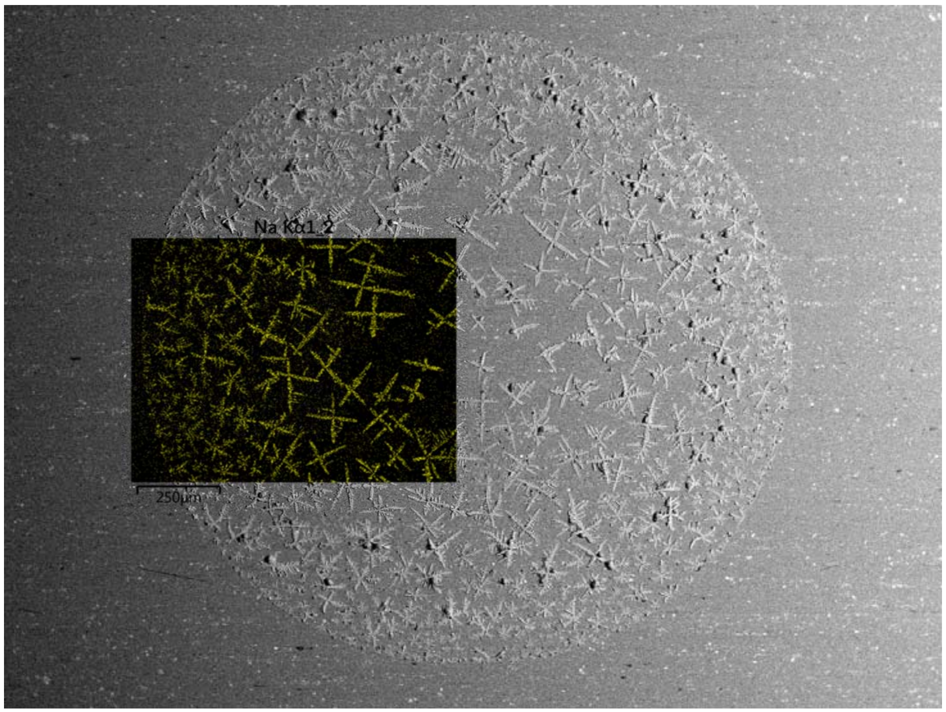
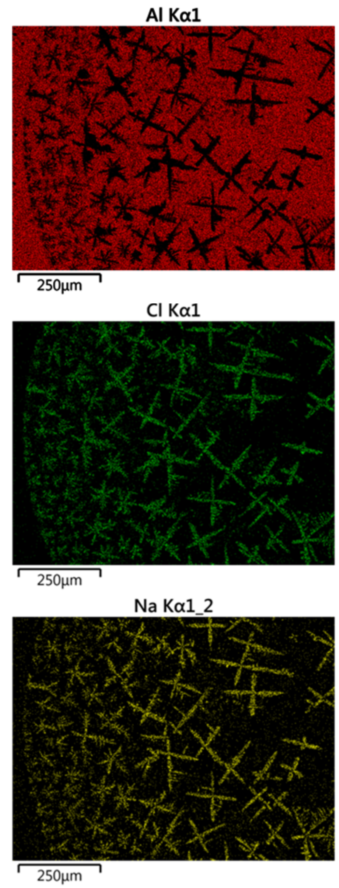
Future Work: To build a CNN model to predict where elements deposit and use it to quantify the element

$CaCl_2$, $MgCl_2$, NaCl mixture

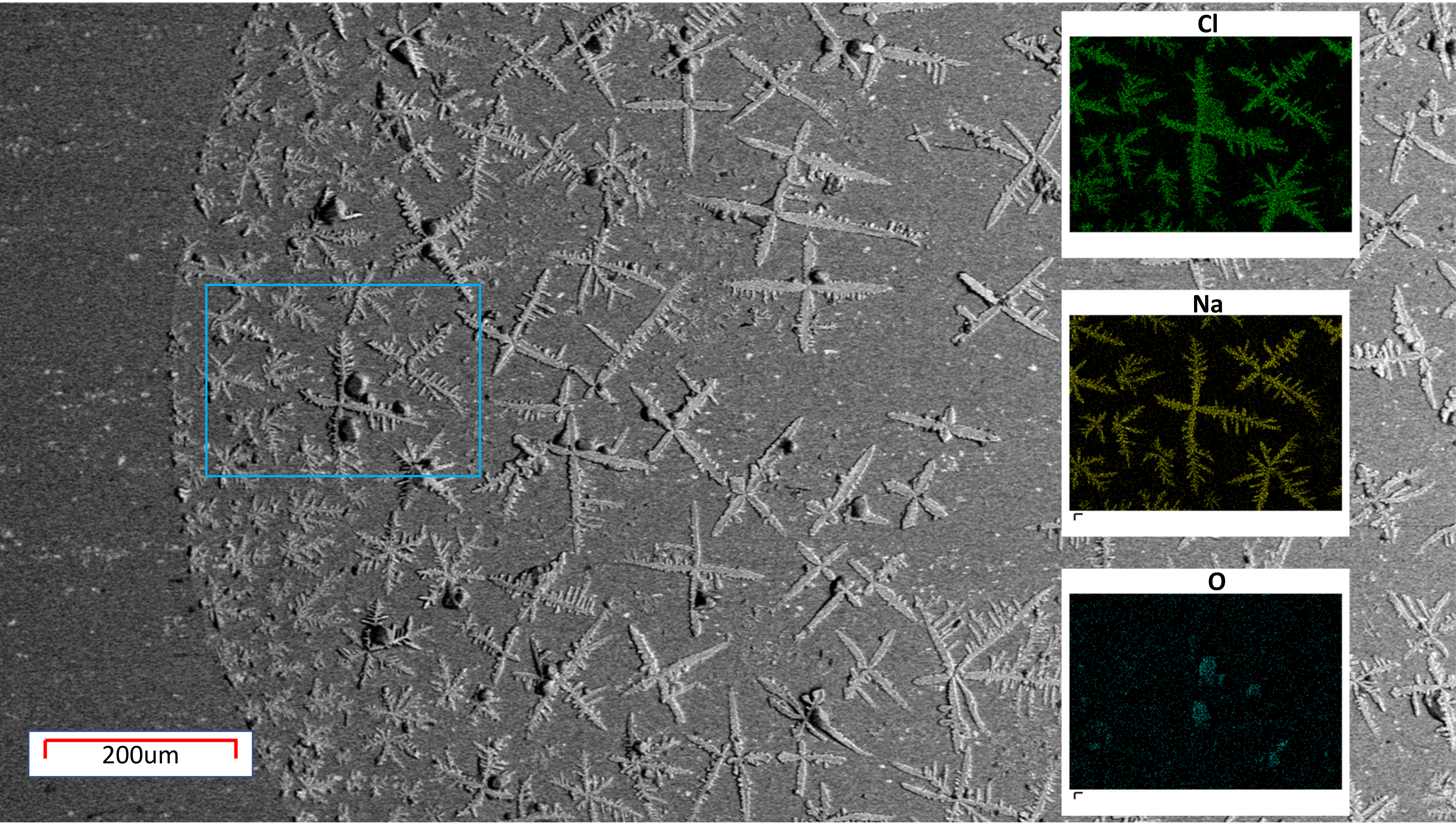


scanning electron microscope (SEM) image



SEM-EDS, elemental analysis map

Li, X, R. Lahr. Paper unpublished


Cl
Na
O
200um

Conclusion-Coffee ring effect with CNN model could monitor water components

- There is correlation between water samples coffee ring effect pattern and water chemistry

- Cluster analysis could classify water samples based on their chemistry data

- Principal component analysis on water sample residue patterns couldn't classify water samples well because data is non-linear

- CNN model could effectively recognize tap water residue patterns and classify water samples based on the patterns

Thank you!

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Zoe Wilton
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EPA United States Environmental Protection Agency