Optical tastebuds for water analysis

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Abstract: We demonstrate a preliminary nano-tastebud sensor comprised of tailored plasmonic metasurfaces that, once fully developed, could be integrated into water treatment facilities as an early warning system to warn of imminent system failures.

The gold-standard method for monitoring the health of centralized drinking water treatment works (DWTW) involves regular and routine sampling and laboratory analysis to monitor the complex mixture of molecules and ions in the effluent water [1]. While this method yields an accurate picture of all the components in the water, it is crucial that we find alternative methods to ensure new technological advances in the water sector are sustainable and scalable.

Here, we demonstrate a preliminary water quality sensor comprised of an array of tailored plasmonic metasurfaces. Instead of developing multiple sensors for each component of interest, our label-free, array-based design mimics the biological system of taste [2-5], where each sensor in the array acts as a tastebud that responds uniquely to different components within the mixture. In this label-free, cross-reactive system, each nano-tastebud selectively permits certain components within the mixture to enter it's plasmonic sensing region, shifting it's resonance condition. Monitoring the shift across multiple, differently-responsive tastebuds [6] generates a unique fingerprint for that sample liquid, which can be used to build an identification model [2,7,8] through statistical analysis techniques like principal component analysis [9] and linear discriminant analysis [10].

To train and test our sensor, Scottish Water provided us with samples of influent (x2), effluent (x2), and tap (x3) water from various DWTW facilities and randomly selected consumer taps across Scotland, and we calculated the average resonance shift from DI Water, for each nano-tastebud for each sample measured on that nano-tastebud. Figure 1a shows the 3D scatterplot of the three canonicals of an LDA [10] classifying by 'DI Water' (black), 'effluent water' (blue), 'tap water' (green), and 'influent water' (red), and Table 1a shows the resulting classification matrix for this LDA, using leave-one-out cross validation. In all instances, the sensor was successfully able to classify DI Water; for effluent water, the accuracy rate was 93%; for tap water, it was 90.5%; and for influent water, it was 93%, resulting in an overall accuracy of 93%.

As both effluent and tap water are considered 'treated' water, the few misclassifications between these two is not too surprising. In any DWTW effluent water sensor, the crucial outcome is the sensor's ability to differentiate between water that passes quality control ('treated': effluent or tap) and water that does not ('untreated': influent water). The violin plot and classification matrix of a second LDA classifying between 'treated' and 'untreated' water are shown in Figure 1b and Table 1b, respectively. For this analysis, the sensor performed with an overall accuracy of 98% (0 misclassifications for treated water [100% accurate] and 1 misclassification for untreated water [93% accurate]).

In conclusion, we have successfully demonstrated a preliminary nano-tastebud sensor that has the potential to be developed into a fully usable optical nano-tastebud for DWTW quality control measurements. Once fully developed, this technology could be fully integrated into water treatment facilities and provide non-expert end-users with a warning for imminent system failures.

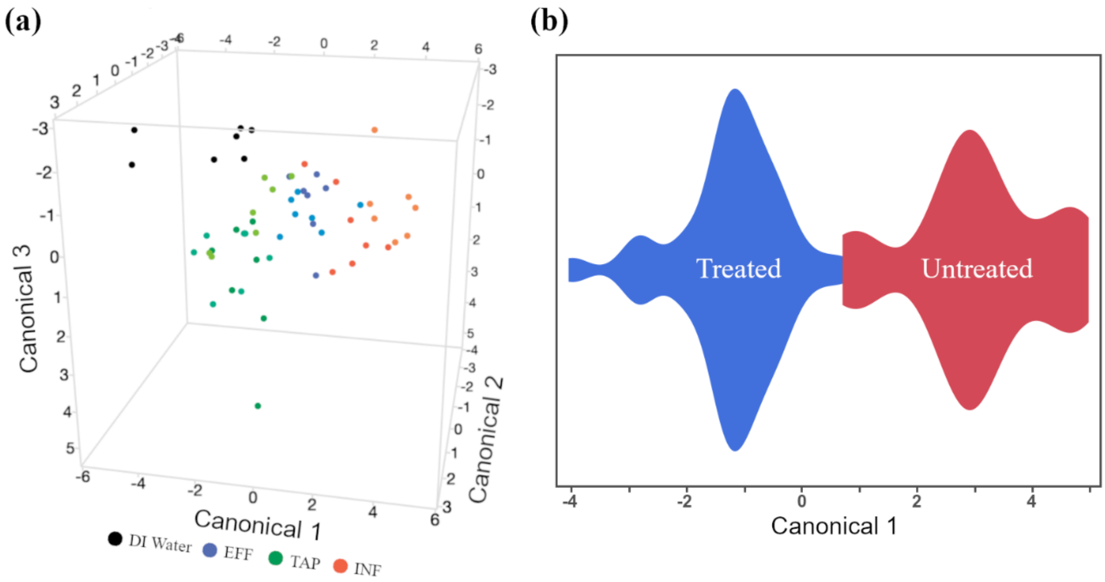

Figure 1. Linear discriminant analysis of transmission peaks (average shift from DI Water) of water samples from various sites across Scotland. (a) LDA of the first three canonicals using groups: DI Water (black), tap (TAP, green), influent (INF, red), and effluent (EFF, blue). (b) LDA combining tap and effluent samples as ‘treated’ (blue) and influent as ‘untreated’ (red).

Table 1. Classification matrices for LDA shown in (a) Figure 1a and (b) Figure 1b.

(a)

		Predicted			
	Label	DI	EFF	INF	TAP
Actual	DI	100%	0%	0%	0%
	EFF	0%	93%	0%	7%
	INF	0%	7%	93%	0%
	TAP	0%	9.5%	0%	90.5%

(b)

		Predicted	
	Label	Treated	Untreated
Actual	Treated	100%	0%
	Untreated	7%	93%

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