Contamination Detection of Water with Varying Routine Backgrounds by UV-Spectrophotometry

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Abstract: Water is a resource that affects every aspect of life. Intentional or accidental contamination events in the water supply system could have a tremendous impact on public health. Quick detection of such events can reduce the expected damage. Continuous online monitoring is the first line of defense for reducing contamination-associated damage. One of the available tools for such detection is ultraviolet (UV)-absorbance spectrophotometry, where the absorbance spectra are compared against a set of normal and contaminated water fingerprints. However, because there are many factors at play that affect this comparison, it is an elusive and tedious task. This study presents a new scheme for early detection of drinking water contamination events through UV absorbance. The detection mechanism is based on a new affinity measure, Fitness, which is flexible enough to identify the source of the drinking water being monitored and alert if contaminants are present. The potential of the method is presented in a set of comprehensive experiments with various contaminants in drinking water extracted directly from a real supply system with mixed sources. **DOI: 10.1061/(ASCE)WR.1943-5452.0000965.** *© 2018 American Society of Civil Engineers.*

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Introduction

Ensuring the safety of drinking water is a primary objective of drinking water suppliers and other stakeholders. Intentional contaminations of drinking water by toxic substances as an act of war and terrorism, as well as unintentional or accidental contaminations, were recorded historically (Green et al. 2003; Winston et al. 2003; Gleick 2006). Rapid detection of such events close to their occurrence is a key factor in reducing response times and applying effective responses that could prevent the contaminated water from reaching the consumers or, in a less optimistic scenario, minimize the potential risk and thus maintain public confidence in the water supply system.

Typically, ensuring the quality of drinking water in a water supply system is done by sampling and analyzing water samples in a laboratory (Storey et al. 2011; Glassmeyer et al. 2017). Though laboratory methods are accurate and precise, they are labor intensive and costly. Furthermore, because laboratory analyses of samples are conducted offline, results usually reflect only a very small portion of the water supplied, and might arrive only after the water has been consumed.

Advances in sensor and communication technologies have facilitated the development of water quality sensors that provide a denser grid both temporally (sampling frequency) and spatially (locations over the water network). These sensors allow continuous real-time in-situ monitoring of water properties, such as oxidation-reduction potential, electrical conductivity, residual chlorine concentration, pH, and ultraviolet-visible (UV-Vis) absorbance (Ikonen et al. 2017; Wang et al. 2017). These new data not only improve water security and public health, they provide new means of water resource management and planning by allowing the network operator to plan for and react in case of contamination in its very early stages.

Among the various pollutants, organic contaminants such as pesticides, fuel residues, and organic solvents can cause acute poisoning at relatively low concentrations within a relatively short exposure time. Therefore, they are among the most important groups of contaminants requiring detection, for which instruments that can react in real time to the presence of organic materials in water provide important advantages.

A feasible means of monitoring organic and some inorganic compounds (both natural and anthropogenic contaminants) is by measuring indicators for such substances with online water quality sensors and to use these measurements for quantification of these compounds. This can be achieved by using a Ultra-Violet to VISual light (UV-Vis) spectrophotometer (SP). The SP offers a fast and simple method for this task and does not require advanced equipment or chemical reagents (Albrektienė et al. 2012). Spectrophotometry is based on the Beer–Lambert law (Harris 2003), which states that when light hits a sample, the irradiance decreases because some of the light is absorbed by the sample. To this end, Albrektienė et al. (2012) found good correlations between total organic carbon (TOC) and UV_{254} ($R^2 = 0.94$), and between chemical oxygen demand by potassium permanganate (COD_{Mn}) and UV_{254} ($R^2 = 0.88$) in groundwater. Etheridge et al. (2014) tested the use of UV-Vis SP for estimating the concentrations of nitrate, total nitrogen, dissolved organic carbon (DOC), phosphate, total phosphorus, total suspended solids, and salinity in brackish water. Their method applied regression models to examine the relationships between the concentrations measured in the laboratory and the UV-Vis absorbance. The regression models for all substances except phosphate and total phosphorus showed R^2 values higher than 0.86. Zitko (2001) qualitatively evaluated the chlorination dose at the treatment stage of surface water by examining drinking water in a supply system with residual chlorine below the detection threshold by measuring changes in UV spectra of natural organic

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matter. Hou et al. (2014) applied probabilistic principal component analysis together with a multivariate monitoring chart to UV-Vis absorption spectroscopy data in order to modulate contaminant events in water supply systems. The USEPA (2012) tested two fluorescent sensors as a contaminant detection tool in water with a stable baseline. One sensor had a single excitation and emission wavelength, whereas the other had multiple wavelengths and also the capability to measure absorbance. The research found that the tested fluorimeters alone were not as effective in detecting contaminants as standard water quality sensors. Still, both sensors detected most contaminants. That study suggested that further research, with more wavelengths, may expand the range of contaminants detected. Recent studies (Hu and Wang 2017; Carré et al. 2017) associated absorption patterns with the chemical characteristics of the substance by using a dynamic partitioning algorithm and partial least-squares linear regression, respectively. However, in both cases, in order to assess changes in absorption patterns, one must acquire the routine background.

A practical example for UV-Vis SP is a commercial instrument (Messtechnik, Vienna, Austria), that works online to measure the absorption spectrum between 190 and 720 nm (UV-Vis); it detects changes in water quality by monitoring the shape of the spectrum and responding to abnormal changes (spectral alarms). The spectrum is also used to derive more specific parameters, such as turbidity, nitrate concentration, spectral absorbance coefficient at 254 nm (SAC254), TOC, and DOC. To operate the device, a training round is required, in which a baseline of normal patterns is established for all parameters relative to each other and alarm levels are set. Additional software modules integrate all results into one “anomaly detection module.” Alarms can be generated by using four different approaches: static alarm thresholds, dynamic alarm thresholds (time gradients), a pattern-recognition–based alarm parameter, and composite alarms (Langergraber et al. 2004).

The above review strongly suggests that research on water contamination detection through SP has proliferated in recent years. However, though SP devices have shown a great potential, they are still not mature enough to be deployed on a large scale (Storey et al. 2011). A careful analysis of the methods that have been suggested for analyzing UV-SP data reveals that many of them still have major shortcomings. All the aforementioned methods essentially assume that a routine, stable background does exist. However, because the number of substances and factors that affect water quality is so large, creating this routine pattern is challenging. The difficulty of finding such a pattern may be amplified by the complexity of the water supply system and the simultaneous use of several drinking water sources (or drinking water types, depending on the context). In Israel, for example, the drinking water supply system uses water from several sources whose chemical composition varies: groundwater from several aquifers with different water compositions, desalinated brackish water and seawater, and surface water.

In this study, the UV-SP absorbances of drinking water that originated from various sources at three configurations are characterized. (1) each water type tested alone; (2) several pesticide contaminants added to drinking water from each of the sources, which served as background water; and (3) mixtures of drinking water from the various sources, in varied proportions, which simulated stochastic background. All were applied to drinking water extracted from real water supply systems and subjected to comprehensive laboratory tests. The results of water spectral absorbance measurements served as an index of changes in organic and inorganic contents in the drinking water—both pollutants and natural. Thus, the contribution of this paper to the current knowledge base is twofold. First, it presents a new contamination detection scheme, which is evaluated over a significantly large set of real samples. Second, the large data set allows not only for the evaluation of the proposed detection scheme, but for assessment of how the different contaminants in different quantities affect the absorption spectra of various drinking water types. Previous studies that suggested early detection schemes either used synthetic [e.g., Pickard et al. (2011); Oliker and Ostfeld (2014)] or limited experimental data (Hall et al. 2007; Kroll and King 2007), limiting their findings.

Materials and Methods

Experimental Setup

Instrumentation

The Israeli water supply system uses water from several sources that differ significantly in their chemical composition: desalinated seawater, treated surface water, and treated groundwater from several aquifers. The various drinking water types contain organic and inorganic compounds, according to their sources and treatment processes, and each water source has its typical characteristics. In this study, we analyzed drinking water, extracted from the national system itself and derived from surface water, groundwater, and desalinated seawater. In addition, we also tested distilled water with an electrical conductivity of 0.15–0.57 $\mu\mathrm{S/cm}$, serving as a reference, that is, water with no substances. The surface water, which originated from the Sea of Galilee (Lake Kinneret), was characterized by relatively high DOC levels, and its treatment was mostly physiochemical, consisting of sedimentation and filtration. The groundwater originated from two wells on the Mountain Aquifer, and was characterized by relatively high concentrations of nitrates and carbonates and low levels of TOC and DOC. Desalinated water originated from the Mediterranean Sea, and was characterized by low concentrations of organic and inorganic compounds. Water of all types was chlorinated. Table 1 specifies the typical concentrations of the main compounds in the three water types.

All experiments were performed in a 50-L mixing tank connected to the UV-SP and equipped with a recirculating pump and 1.27 cm (0.5 in.) input and output lines. Water was continuously circulated between the tank and UV-SP during the experiments. Data were acquired by an online continuous spectroscopy analyzer (Real-Spectrum Analyzer, model PL3000-TOC-UVA-PC; Real-Tech, Canada) with a deuterium lamp and a path-length (cell) of 1 cm, absorption range of 0.0–1.5 cm^{-1}, and flow rate of 300–800 $\mathrm{mL/min}$. Each measurement determined the absorbance of UV light by the water at 117 different wavelengths within the range of 197.8–370.8 nm at intervals of 1.4–1.6 nm.

Experimental Configurations

Three experiments were conducted with drinking water, extracted from a real-life system and originating from the three different sources, measuring the absorbance of (1) nitrate and bicarbonate that are naturally present in the water, (2) the contaminants to be tested, and (3) the three different water types on their own and in various mixed ratios.

The aim for the experiments with nitrate and bicarbonate was to understand the natural background absorbance of the several types of drinking water tested. Knowing the contents of the various water types, we added the most prominent ones to distilled water simulating their absorbance patterns. The tested components were nitrate at 1, 3, 10, and 30 $\mathrm{mg/L}$ and bicarbonate at 150, 300, 450, and 600 $\mathrm{mg/L}$. The absorbance results of these experiments were compared with those obtained with drinking water from the tested sources. This set of experiments identified the main natural components that affected absorbance the most.

Table 1. Concentration ranges and averages of the main compounds in the examined waters, as measured since 2010; average values are computed over *n* samples and presented against the normal ranges for each water source

Drinking water source	NO_3 (mg/L)	DOC (mg/L)	TOC (mg/L)	EC (μS/cm)	HCO_3^- (mg/L)	Turbidity (NTU)
Surface water						
Sample size	505	481	NM	22	41	479
Average value	0.006	2.49		1,164	139	0.13
Normal range	0–3	1.9–3.1		1,024–1,273	126.82–174.3	0.07–0.5
Groundwater Well Number 1						
Sample size	10	NM	2	3	1	25
Average value	23		0.2	1,019	382.8	0.21
Normal range	21–24		—	1,014–1,026	—	0.1–0.5
Groundwater Well Number 2						
Sample size	10	NM	1	2	1	19
Average value	27.2		<0.2	997	349.9	0.42
Normal range	23–29		—	975–979	—	0.27–0.69
Desalinated water						
Sample size	NM	NM	NM	3	453	981
Average value				238	110.4	0.19
Normal range	LDT		LDT	220–255	63.4–165.8	0.05–0.82

Note: NM = not measured; and LDT = less than detection threshold.

Table 2. NOAEL or NOEL dosage, the oral LD50 values, and the pesticide group of the contaminants used at the spiking experiments

Pesticide group	Acute exposure—oral LD50 values (mg/kg of body weight)	Criterion	NOAEL or NOEL dosage (mg/kg of body weight per day)	Contaminant
Chlorophenol	27–177	NOAEL of short-term exposure	3	A
Carbamate	0.487–1.3	NOAEL of short-term exposure	0.05–0.06	B
Organophosphates	2.2–18	NOEL of chronic exposure	0.025	C
Carbamate	3–19	NOAEL of short-term exposure	0.22–0.3	D
Organophosphates	2	NOAEL of short-term exposure	<1.5	E

Spiking experiments were performed with five different organic pesticides, designated as A, B, C, D, and E. Table 2 specifies, according to World Health Organization (WHO), the no-observed-adverse-effect-level (NOAEL or NOEL) dosages, the oral lethal dose that is expected to kill 50% of the exposed population (LD50) values, and the pesticide groups of these contaminants (U.S. Environmental Protection Agency 1998). Each of the experiments comprised two or three stages, each taking 2 h. In the first stage, uncontaminated drinking water—groundwater, surface water, desalinated seawater, or distilled water—was continuously monitored. Then, an organic contaminant was added to the water at 1 mg/L, while monitoring continued. In the third stage, the same water sample was monitored with a higher contaminant concentration that gave a total dosage of 2, 3, or 5 mg/L. This procedure was repeated for each water type with each of the five contaminants. Each such experiment yielded several tens of absorbance spectra for each of the stages. This set of tests characterized the absorbance of each of the contaminants with respect to each water type and thereby facilitated evaluation of the effects on absorbance of interactions between each water type and the various contaminants and, within the examined range, with additional contaminants. The characteristic absorbance spectrum of each of the contaminants with respect to each water type was generated by computing the elementwise median of the obtained spectra for each combination of water type and contaminant. The marginal contribution of each of the contaminants was then computed by subtracting the characteristic medians obtained in the first stage (background water only) from those obtained in the second and third stages to obtain the net medians of the contamination effect. These net medians were normalized by dividing each spectrum by the contaminant concentration. The resulting net-normalized medians were then compared to evaluate the differences between them.

Mixed drinking water experiments were conducted to simulate water mixtures that might flow in the supply system. The experiments were conducted in several stages, with a different baseline water type for each experiment. At successive stages, measured

Table 3. Mixed water experiments: volumes and proportions of water mixtures used

Surface water (L)	Desalinated water (L)	Groundwater (L)	Surface water (%)	Desalinated water (%)	Groundwater (%)
Experiment Number 1					
10	0	0	100.0	0.0	0.0
10	2.5	0	80.0	20.0	0.0
10	5	0	66.7	33.3	0.0
10	5	0.5	64.5	32.3	3.2
10	7	0.5	57.1	40.0	2.9
10	7	1	55.6	38.9	5.6
10	10	1	47.6	47.6	4.8
Experiment Number 2					
0	10	0	0.0	100.0	0.0
2.5	10	0	20.0	80.0	0.0
5	10	0	33.3	66.7	0.0
5	10	0.5	32.3	64.5	3.2
7	10	0.5	40.0	57.1	2.9
7	10	1	38.9	55.6	5.6
10	10	1	47.6	47.6	4.8
Experiment Number 3					
25	0	2.5	90.9	0	9.1
25	0	5	83.3	0	16.7
25	0	10	71.4	0	28.6
25	0	20	55.6	0	44.4
25	0	25	50.0	0	50.0

amounts of water of a certain type were added to the sample in proportions that might normally occur in the water supply system. Each step ran for at least 20 min, that is, 10 readings. These experiments are described in more detail in Table 3. These tests were intended to determine whether the natural compounds reacted additively or otherwise when waters of differing types were blended.

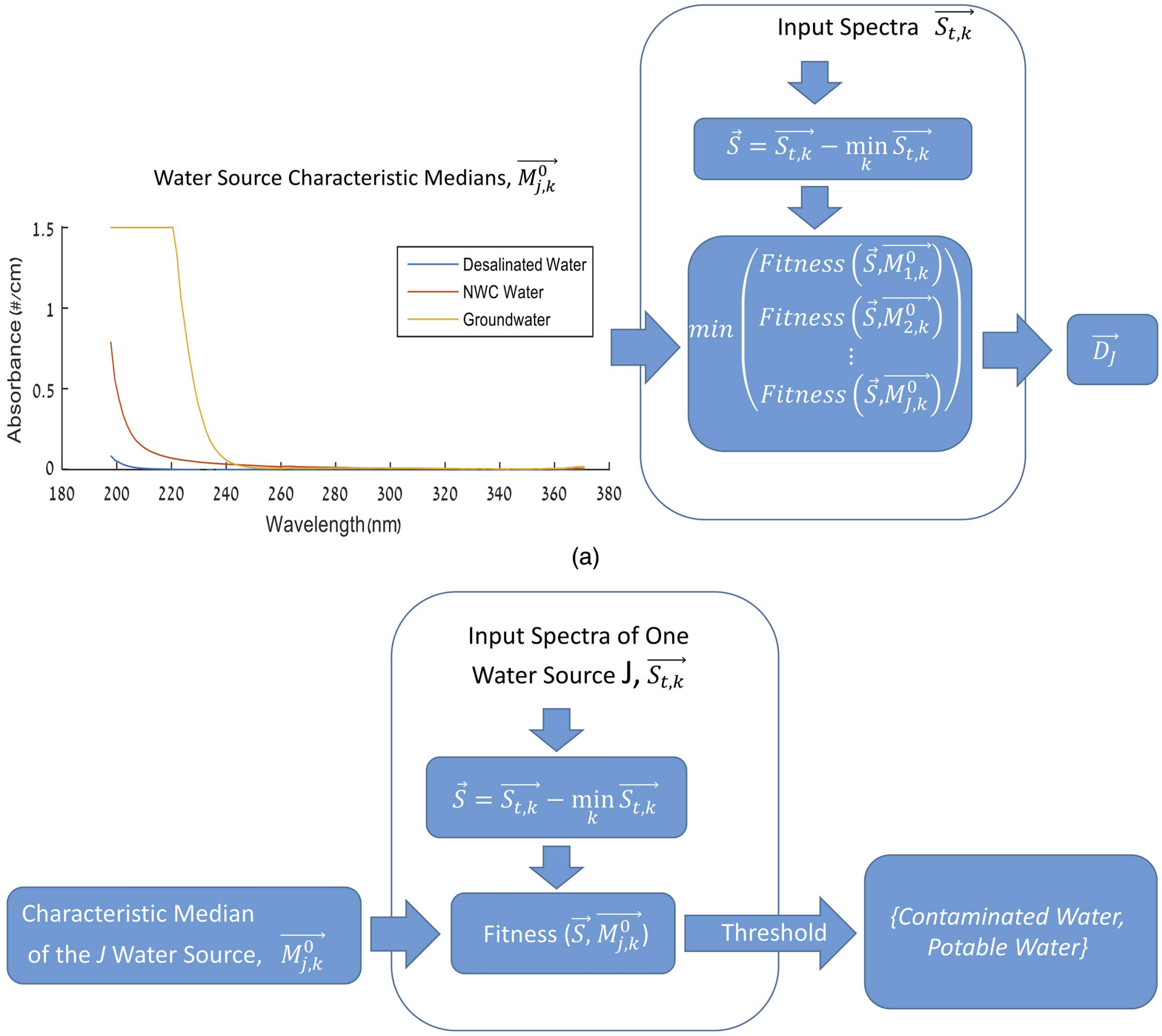
Methodology

Fitness Measure

A new measure of affinity between records—the Fitness Measure—was developed. It was tested as a means to distinguish between drinking water sources and between contaminated and potable water. The following notations are used to formulate the Fitness Measure. Let $\overrightarrow{S_{t,k}}$ be the input absorbance spectrum acquired at time $t \in T$. Each vector element of the spectra is the absorbance at the $k \in K$ wavelength, where, in the present study, $|K| = 117$. Let $\overrightarrow{M^0_{j,k}}$ be the median absorbance computed over all spectrum measurements acquired for a specific drinking water type $j \in J$, where $|J| = 3$ in the present case, when no contamination was present. The obtained $\overrightarrow{M^0_{j,k}}$ is used to characterize drinking water type j. The median is preferred over the mean because it is less sensitive to extreme values that might bias the results. It is noteworthy that samples of contaminated water may be used to generate $\overrightarrow{M^0_{j,k}}$, as long as the lion's share of the measurements are of potable water.

The Fitness Measure is a product of two components: the Pearson correlation and the Euclidian distance, between a template vector and a given measurement. Specifically, when there is a set of $|T|$ spectra acquired from a specific water sample, the Pearson correlation between each of the spectra and the median vectors, $\overrightarrow{M^0_{j\in J,k\in K}}$ of the drinking water types is computed, resulting in a correlation matrix, **CCMat**, of the size $[T \times J]$, with $\mathbf{CCMat}(t,j) = \mathrm{corr}(\overrightarrow{S_{t\in T,k\in K}}, \overrightarrow{M^0_{j\in J,k\in K}})$. Similarly, a distance matrix, **DistMat**, of the size $[T \times J]$, is computed; it represents at location (t,j), that is, $\mathbf{DistMat}_{(t,j)}$, the Euclidian distance between $\overrightarrow{S_{t\in T,k\in K}}$ and $\overrightarrow{M^0_{j\in J,k\in K}}$. The Fitness Matrix, which expresses the overall compatibility between a measurement $\overrightarrow{S_{t,k}}$ and a median $\overrightarrow{M^0_{j,k}}$, is than calculated as follows:

$$\mathbf{Fitness}_{(t,j)} = (1 - \mathbf{CCMat}_{(t,j)}) \cdot\times (\mathbf{DistMat}_{(t,j)}) \qquad (1)$$



(a)

(b)

Fig. 1. Fitness measure usage to distinguish between (a) water sources; and (b) potable and contaminated water.

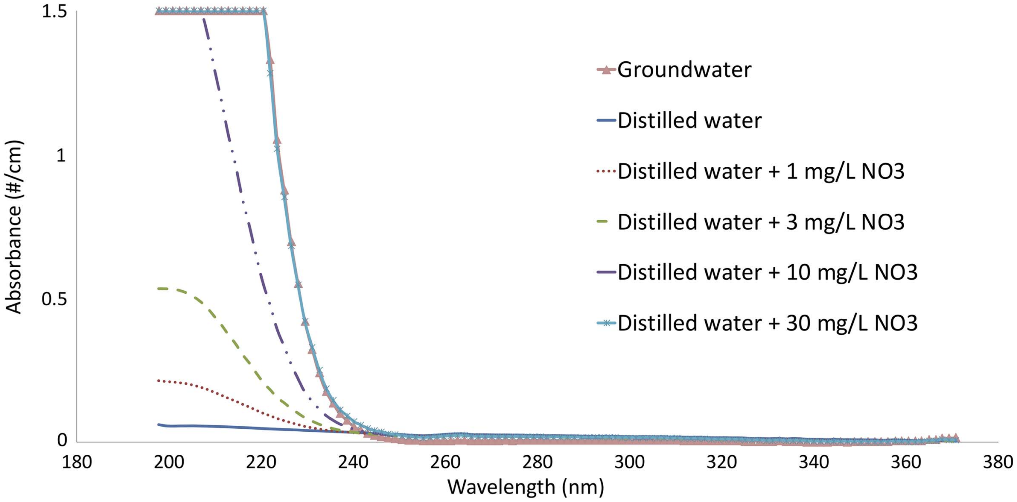


Fig. 2. Adding nitrate to distilled water at increasing concentrations of 1, 3, 10, and 30 mg/L. Results are averages of at least 10 readings per concentration.

where $(\cdot\times)$ = elementwise multiplication operator. In this formulation, the closer the results are to zero, the better the fitness.

Fitness Application

The baseline of the water measurements may drift after a long operating time because of fouling, which would lead to increased absorbance values. Hence, each spectrophotometric application of the Fitness Measure began with preprocessing: in light of the knowledge that spectra of all drinking water types include some wavelengths at which there is no absorption; for each measurement $\overrightarrow{S_{t,k}}$, the lowest absorbance value among those found for all wavelengths covered by the same measurement was subtracted, which eliminated most of the drift effect.

In order to test the performance of the Fitness Measure in associating readings with drinking water types, a randomly chosen 25% of the data ($293 \leq n \leq 631$), where n is the number of readings per water type, were used to calculate the medians, and the remaining 75% to perform classification.

The inference of whether a sample is of contaminated water was carried out in two phases. At the first stage, the Fitness of the sample was computed against all medians of the drinking water types with no contaminants, that is, $\overrightarrow{M^0_{j\in J,k\in K}}$. Then, once the water type j is determined, the decision about whether the water is contaminated or potable is done by computing the sample's Fitness against the results obtained from the spiking experiments. A Fitness threshold value was recommended based on the Fitness values obtained for the potable and contaminated water. The building blocks of the Fitness applications are described in Fig. 1.

Results and Discussion

Experiments with Natural Components

The aim of these experiments was to characterize the natural absorbance of the tested drinking water when its contents, such as nitrate and bicarbonate, were known. The addition of nitrate to distilled water at 30 mg/L resulted in absorbance values very similar to those of the tested groundwater from the two wells, which contained 23 and 27 mg/L of nitrate on average (Fig. 2). Adding bicarbonate to distilled water at 150 mg/L resulted in increased absorbance values that were slightly higher than those of the tested desalinated water, which contained 110 mg/L of bicarbonate on average and showed an absorption curve of similar shape (Fig. 3).

Differentiating between Drinking Water Types

The differences in the UV absorbance spectra between water types are well observed (Fig. 4). The water types were classified using the

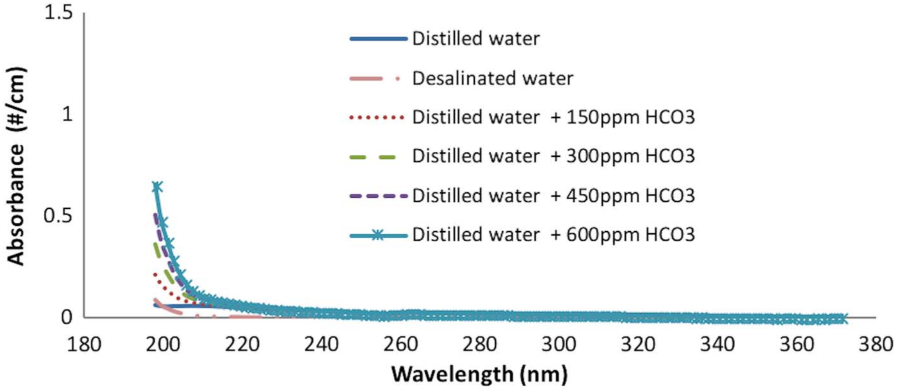


Fig. 3. Adding bicarbonate to distilled water at increasing concentrations of 150, 300, 450, and 600 mg/L. Results are averages of at least 10 readings per concentration.

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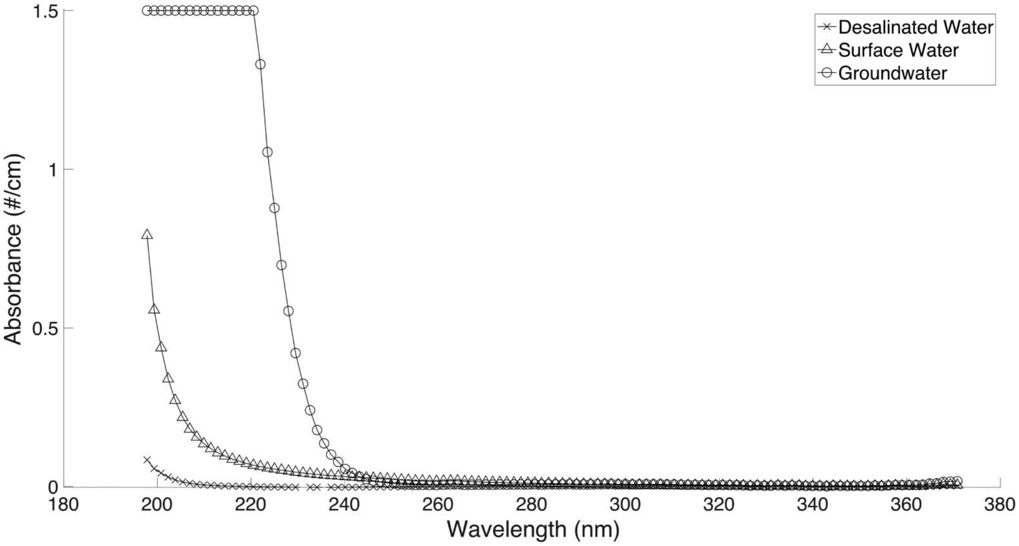

Fig. 4. Medians of the examined drinking water types ($293 < n < 631$).

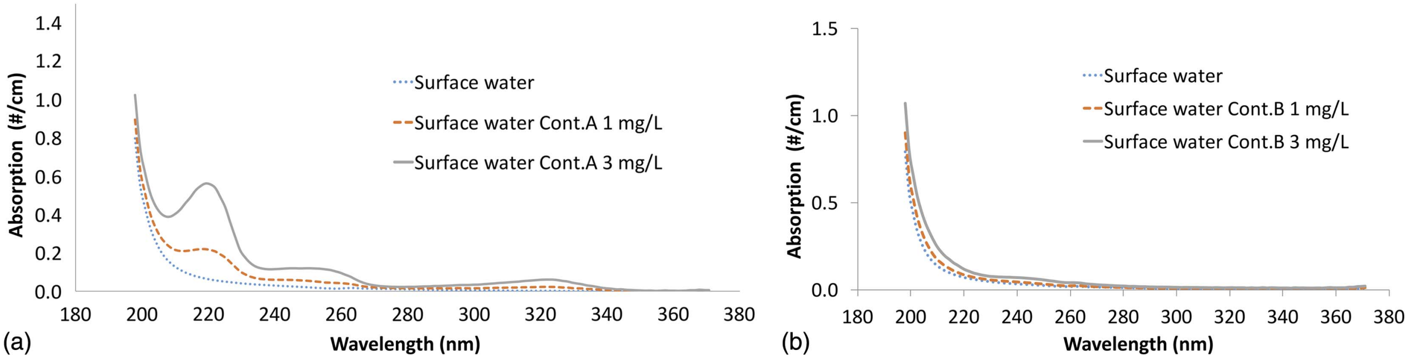

Fig. 5. Surface water average absorption without any contaminants, and with contaminant: (a) A; and (b) B at 1 or 3 mg/L (for each series $43 \leq n \leq 78$, $\sigma < 0.05$).

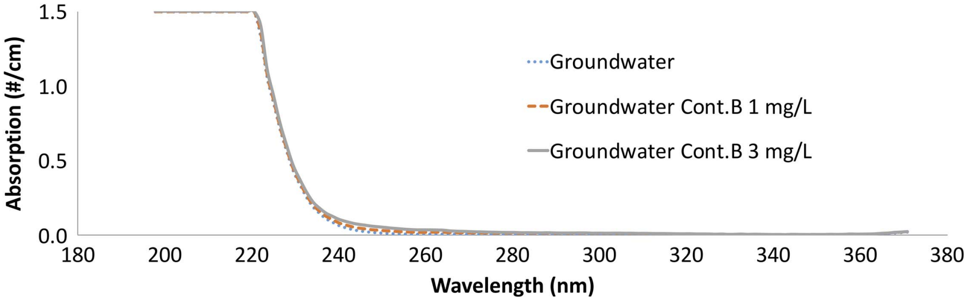

Fig. 6. Groundwater average absorption without any contaminants and with contaminant B at 1 and 3 mg/L, (for each series $58 \leq n \leq 87$, $\sigma < 0.009$).

Fitness Measure, and classification was performed without any mistakes.

Differentiating between Potable and Contaminated Water

Contaminant-Spiking Experiments

The data yielded by 19 different contaminated-water experiments included 1,705 and 1,968 readings from uncontaminated and contaminated water, respectively. Fig. 5 shows that some contaminant absorbance, for example, contaminant A, had noticeable impacts on the absorbance spectra, whereas others, e.g., contaminant B, elicited less pronounced effects and were hard to detect. For all tested contaminants, the highest absorbance values occurred at the shorter wavelengths, between 197.8 and 208.4–228.0 nm. Groundwater from the tested wells absorbed UV light at wavelengths between 197.8 and 220.5 nm above the measurement threshold. Therefore, contaminants, which absorb mainly in this range, would be very hard to detect in water from these wells (Fig. 6).

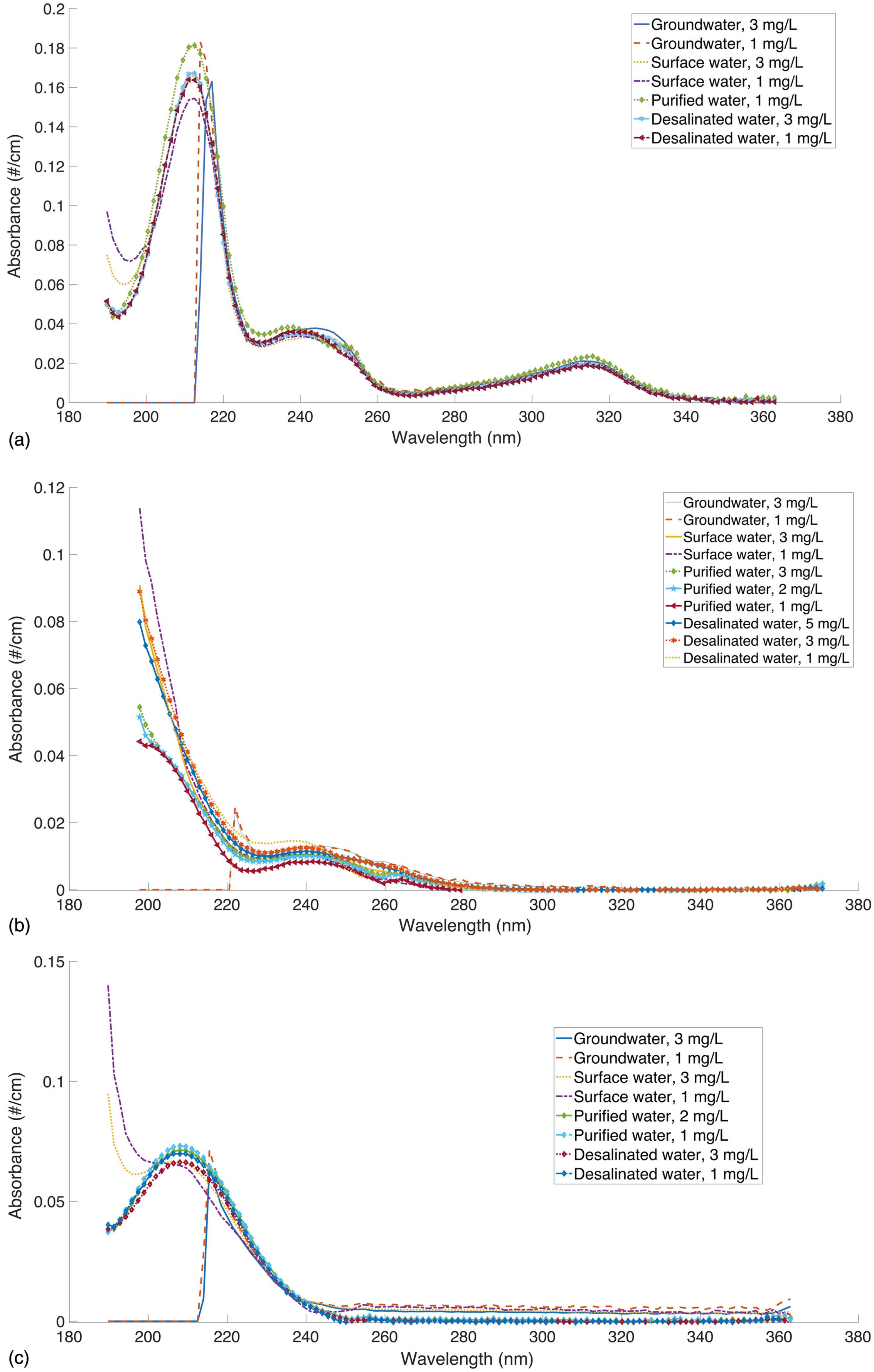

Fig. 7. Median absorbance of net-normalized contaminant concentrations of 1, 2, or 3 mg/L with different background waters: (a) contaminant A; (b) contaminant B; (c) contaminant C; (d) contaminant D; and (e) Contaminant E. Graphs use different Y scales.

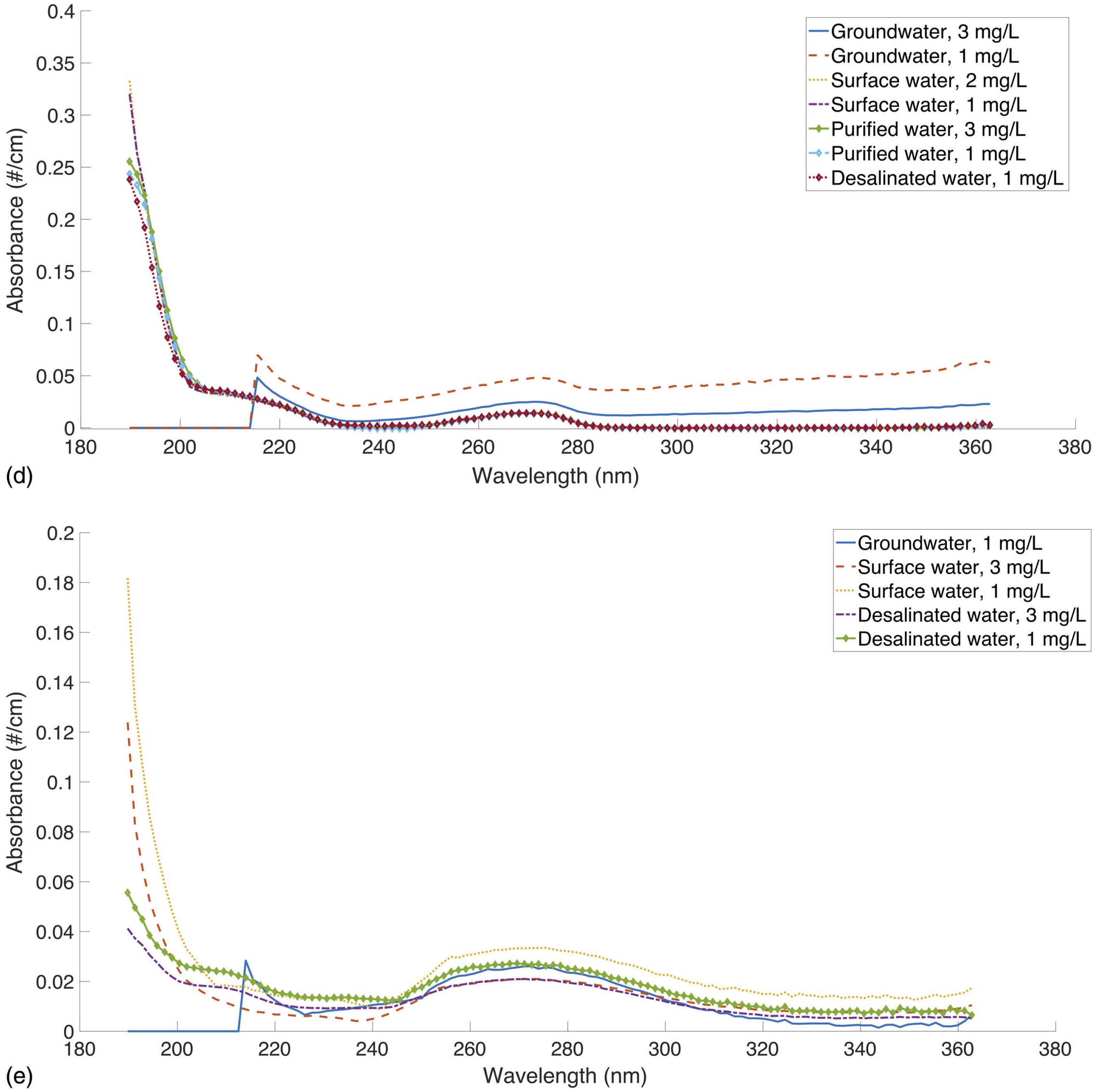

Fig. 7. (*Continued.*)

Absorbance Patterns of Contaminants at Varied Concentrations and from Different Drinking Water Sources

Different contaminants absorb light differently, according to their chemical structure and the character of the chemical bonds within and between the components of their molecular groups. We examined whether the absorbances of samples containing the tested contaminants differed when background drinking water from different sources was used. Also, we examined whether the absorbance caused by contaminants increased linearly with increases in contaminant concentrations within the examined range. Fig. 7 illustrates the results for the various tested contaminants. The results show that, at short wavelengths (~197.8–208.4 nm), there were only minor differences between the absorbance of contaminants in surface water and those in desalinated and purified water.

Differentiating between Contaminated and Potable Water: Fitness Measurement Results

Contaminated and potable water were distinguished by using the Fitness method; Fitness values for drinking water with and without contaminants were calculated for water from each source. The median Fitness values of potable water derived from surface water, desalinated seawater, and groundwater were 5.087×10^{-6}, 8.89×10^{-5}, and 3.31×10^{-7}, respectively. These Fitness values of potable water are between 1 and 4 orders of magnitude lower than those of contaminated water, depending on the background drinking water source and the contaminant and its concentration.

Table 4 illustrates the intuitive notion that contaminants with high absorbance, such as contaminant A, had relatively high Fitness values, whereas those with low absorbance, such as contaminant D, had relatively low Fitness values, especially at low contaminant concentrations.

Mixed Drinking Water Experiments

The data yielded by these experiments include 412 measurements of drinking water from various sources, mixed in known proportions; Fig. 8 presents an example of an experiment result. When the total absorbance of a water mixture was calculated as the sum of the partial absorbance of drinking water from each source, the results were very similar to those measured for actual water mixtures. Over the whole spectrum of 117 wavelengths, the range, median, and mean of the absolute differences between the calculated and measured absorbance were 0.00–0.3312, 0.0028, and 0.0141, respectively. The Fitness value between each pair of the calculated and measured absorbances was evaluated. The range, median, and mean of the

Table 4. Fitness median values of potable and contaminated water for each tested water source

Water source	Potable	Contaminant A 1 mg/L	Contaminant A 3 mg/L	Contaminant B 1 mg/L	Contaminant B 3 or 2[a] mg/L	Contaminant C 1 mg/L	Contaminant C 3 or 2[a] mg/L	Contaminant D 1 mg/L	Contaminant D 3 or 2[a] mg/L	Contaminant E 1 mg/L	Contaminant E 3 mg/L
Surface water	5.087×10^{-6}	0.016	0.30	2.81×10^{-4}	3.4×10^{-3}	2.4×10^{-3}	0.044	8.42×10^{-4}	2.91×10^{-3}[a]	9.36×10^{-4}	5.5×10^{-3}
Desalinated water	8.89×10^{-5}	0.38	1.34	0.0176	0.090.16[a]	0.013	0.50[a]	0.019	—	0.016	
Groundwater	3.31×10^{-7}	4.54×10^{-4}	0.01	1.53×10^{-5}	1.44×10^{-4}	4.15×10^{-5}	8.13×10^{-4}	8.24×10^{-5}	4.58×10^{-4}	8.83×10^{-6}	—

[a] 2 mg/L contaminant concentrations.

Fitness values between them were $3.397 \times 10^{-6} - 0.0028$, 3.972×10^{-4}, and 5.957×10^{-4}, respectively. It can therefore be concluded that there was no interaction between water types; that is, their effects were additive.

Conclusions

This paper presents a comprehensive characterization of drinking water, encompassing the presence of natural and contaminant substances, the source of the water, and changes in the mixing ratios of the different types due to operational practices at the water supply system. This was obtained using three different arrays of experiments that used spectrophotometry to measure UV absorbance, from 197.8 to 370.8 nm, of drinking water from three different sources: surface water, desalinated seawater, and groundwater. Specifically, these sets of experiments enabled the evaluation of UV absorbance patterns of water from the drinking water supply system that are affected by: (1) natural substances that may be found in drinking water, i.e., bicarbonate and nitrate; (2) various contaminants introduced into the drinking water from several different sources; and (3) mixtures of drinking water from different sources that differed in their dissolved contents.

A measure of affinity between records, dubbed Fitness, was also developed. This suggested measure was shown to allow for a distinction to be made between drinking water from different sources and between contaminated and potable water. Additionally, by evaluating the Fitness between the calculated and measured absorbances, it can be concluded that there is no interaction between the different water types.

The findings of the experiments with nitrate and bicarbonate indicate that the UV absorbance at wavelengths ranging from 197.8 to 240 nm in the groundwater from the Mountain Aquifer that was used in the present study could be attributed to the presence of nitrate and bicarbonate, which absorb mainly at these UV wavelengths. The absorbance at wavelengths from 197.8 to 215 nm in desalinated Mediterranean seawater could be attributed to the presence of bicarbonate.

Tests with five different organic pesticides, representative of contaminants that might reach drinking water, revealed that these contaminants significantly absorb in a UV wavelength range of up to 228 nm. We therefore recommend that for testing water containing nitrate or other components that significantly absorb UV light at short wavelengths, a spectrophotometer with a path-length cell narrow enough to account for the natural background and the contaminant absorbance should be used. However, it also should be considered that the narrower the cell, the lower the measurement sensitivity and consequently the lower the ability to detect contamination.

A comparison between the increases in UV absorbance caused by addition of the various contaminants to drinking water from the various sources revealed only minor absorbance differences at short wavelengths, about 197.8–208.4 nm when tested with the water originating from surface water only. Thus, it can be concluded that absorbance of water from all sources—but perhaps from the tested surface water and only at the short wavelengths—and for all tested contaminants was proportionally affected by increasing contaminant concentrations within the tested range.

With regard to mixtures of drinking water derived from several different sources, no interaction was found among the tested water types. This means that when drinking water from several different sources was mixed in order to simulate the mixing in a drinking water supply system, the absorbance increments were additive.

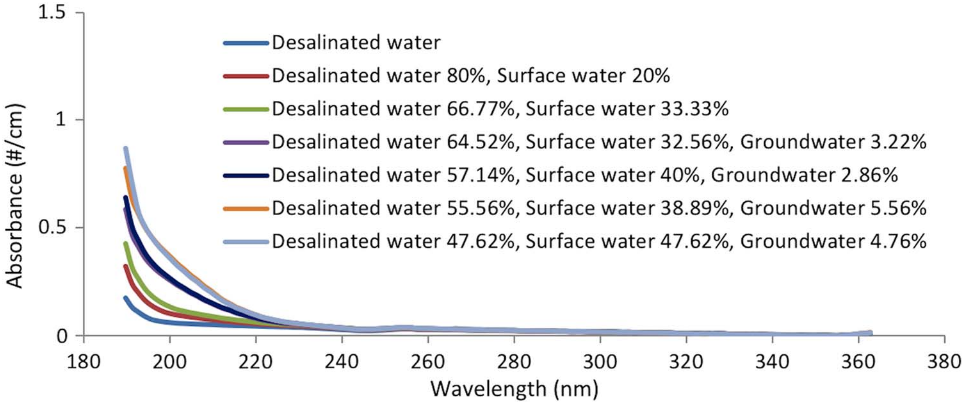

Fig. 8. Mean absorbance by mixtures of water sources in various proportions—groundwater, desalinated seawater and surface water—measured during a mixed water experiment (for each series, $11 \leq n \leq 13$, $\sigma < 0.031$).

Use of the Fitness Measure to identify the source of the drinking water was 100% successful. Also, the Fitness Measure enabled us to distinguish between contaminated and potable water; because all the tested contaminated drinking water exhibited Fitness values higher by at least 1 or 2 orders of magnitude than those of potable water from the same source, even contaminants with a low spectral absorbance could be detected at concentrations as low as 1 mg/L.

In light of our findings with the drinking water tested in the present study, we recommend that in cases where absorbance of potable water is below the measurement threshold for all UV wavelengths, a threshold Fitness value more than 2 orders of magnitude greater than that of the potable background water be used to distinguish between potable and contaminated water. Thus, it is concluded that using the Fitness Measure for UV-spectrophotometry readings is a highly effective means for identifying water sources and classifying water as potable or contaminated. Further research is needed to enable expansion of the use of the Fitness Measure as presented here to drinking water from supply systems that use mixtures of water from several sources in unknown, varying proportions.

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