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Data Article

Data on the inner filter effect, suspended solids and nitrate interferences in fluorescence measurements of wastewater organic matter

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ABSTRACT

Data presented in this article show the extent of the inner filter effect (IFE) in fluorescence measurements of wastewater and wastewater-impacted surface water samples. Particularly, data show the effectiveness of a commonly used method for IFE correction based on UV absorbance measurement to reinstate the linearity of the relationship between fluorescence intensities and absorbance values. Data report also the effect of nitrates in fluorescence measurements of wastewater samples. Finally, data presented in this work show the effect of total suspended solids (TSS) in the UV absorbance and fluorescence measurements of different waters. Particularly, data describe the TSS effect in fluorescence intensities acquired at different pairs of excitation-emission wavelengths, and in waters with different TSS concentration. Data of this article are related to the publication "*M. Sgroi, E. Gagliano, F.G.A. Vagliasindi, P. Roccaro, Inner filter effect, suspended solids and nitrite/nitrate interferences in fluorescence measurements of wastewater organic matter, Sci. Total Environ., In press*" [1]. Raw data are available in a public repository (https://doi.org/10.17632/4zss49jycj.1).

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Specifications Table

Subject area	*Environmental Science*
More specific subject area	*Spectroscopic measurements of wastewater and surface water samples*
Type of data	*Table, figure*
How data was acquired	*Shimadzu UV-1800 spectrophotometer; Shimadzu RF-5301PC fluorescence spectrophotometer.*
Data format	*Raw, processed*
Experimental factors	*Spectroscopic analyses were performed in dilution series produced using filtered (0.7 μm) and unfiltered samples.*
Experimental features	*Deviation from linearity of the relationship between fluorescence and absorbance to assess the effectiveness of inner filter effect (IFE) correction. Comparison between spectroscopic measurements of filtered and unfiltered samples. Nitrate interference in the inner filter correction*
Data source location	*Sicily (Italy)*
Data accessibility	*Processed data are provided in this article. Raw data are deposited in a public repository (https://doi.org/10.17632/4zss49jycj.1*
Related research article	*M. Sgroi, E. Gagliano, F.G.A. Vagliasindi, P. Roccaro, Inner filter effect, suspended solids and nitrite/nitrate interferences in fluorescence measurements of wastewater organic matter, Sci. Total Environ., In press* [1]

Value of the Data

- Data in this article are useful to assess possible interferences that can occur during fluorescence measurements of wastewater organic matter.
- These data can help researchers to address future research on the on-line monitoring of water quality by the use of portable fluorescence sensors, which need to be installed in-situ.
- Data can be used by researchers as a benchmark for future investigations on inner filter effect and dissolved organic matter characterization of wastewater and surface water.

1. Data

The datasets in this article describe typical interferences, such as the inner filter effect and the presence of suspended solids and quenchers (i.e., nitrite/nitrate) in water, which can affect the fluorescence measurements of wastewater organic matter.

Fig. 1, Fig. 2 and Fig. 3 show the relationship between different fluorescence intensities (denoted as I_1, I_2, I_3, I_4, I_5) and total absorbance values measured in dilution series of different wastewater and wastewater-impacted surface water samples. Data shown are both corrected and uncorrected for inner filter effect (IFE).

Fig. 4 shows the UV absorbance spectra of nitrates and nitrites dissolved in Milli-Q water. In Fig. 5 are reported the excitation-emission matrix (EEM) fluorescence spectra of wastewater samples, where

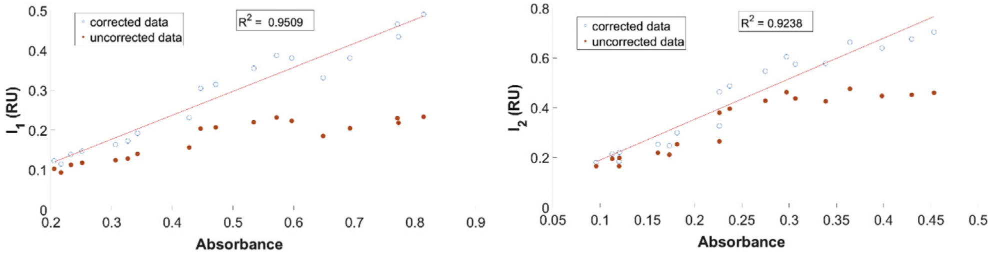

Fig. 1. Relationship between fluorescence intensities of peaks I_1, I_2 and total absorbance values for filtered samples corrected and uncorrected for inner filter effect of Paternò1 wastewater.

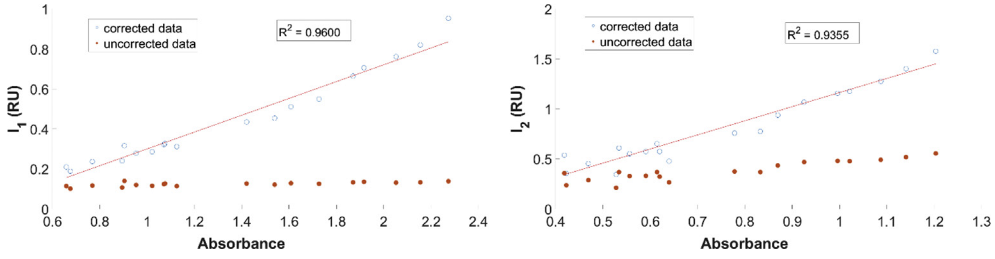

Fig. 2. Relationship between fluorescence intensities of peaks I_1, I_2 and total absorbance values for filtered samples corrected and uncorrected for inner filter effect of Bronte wastewater.

spikes of different amounts of nitrate were performed. EEMs shown in Fig. 5 are corrected and uncorrected for IFE.

Fig. 6 shows the absorbance spectra of filtered and unfiltered samples for different wastewaters and a surface water. In filtered samples, total suspended solids (TSS) were removed by 0.7 μm filtration. Fig. 7 reports the fluorescence spectra of filtered and unfiltered samples for Pozzillo surface water (TSS = 21 mg/L), and Bronte wastewater (TSS = 2 mg/L). In Fig. 8, Fig. 9 and Fig. 10 are reported scatter plots that compare selected fluorescence intensities (denoted as I_1, I_2, I_3, I_4, I_5) and total absorbance values (denoted as Abs_1, Abs_2, Abs_3, Abs_4, Abs_5) measured in dilution series of filtered and unfiltered samples produced using different wastewaters and a wastewater-impacted surface water. Fig. 11 shows the location of the fluorescence intensities I_1, I_2, I_3, I_4, I_5 in a typical EEM of wastewater sample.

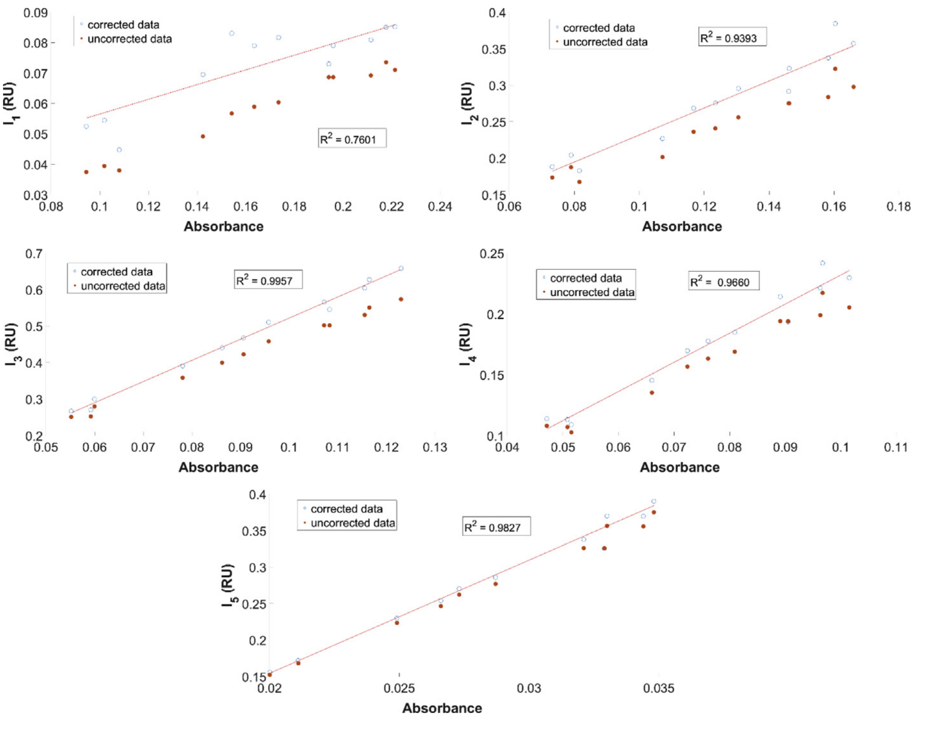

Fig. 3. Relationship between fluorescence intensities of peaks I_1, I_2, I_3, I_4, I_5 and total absorbance values for filtered samples corrected and uncorrected for inner filter effect of Pozzillo water.

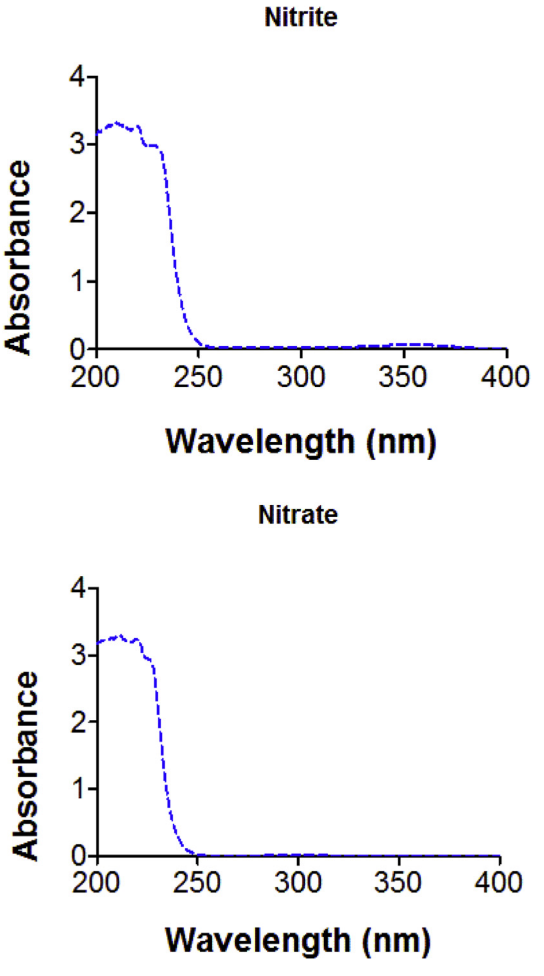

Fig. 4. UV absorbance spectra of spiked nitrate and nitrite concentration (40 mg/L) in Milli-Q water.

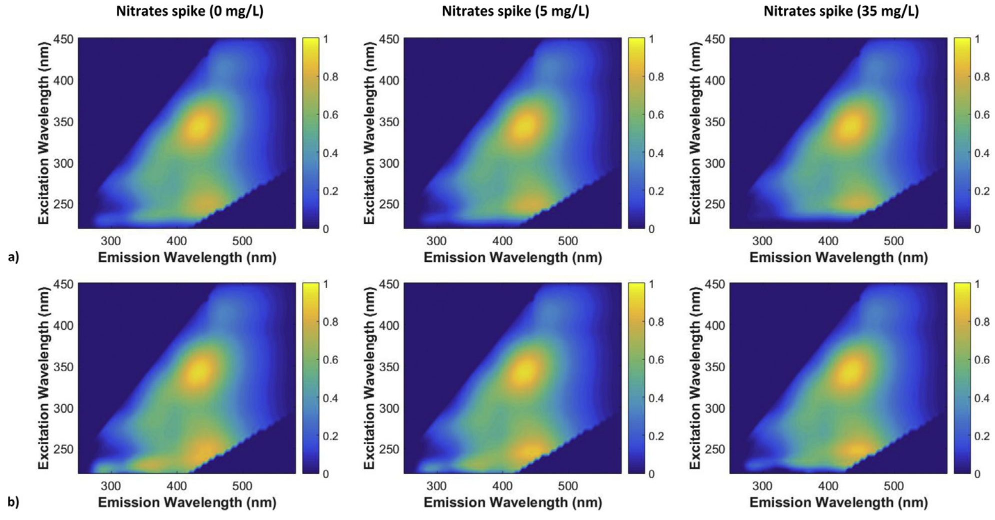

Fig. 5. Fluorescence EEMs of a wastewater secondary effluent with different nitrate concentration spikes. EEMs are shown for samples a) uncorrected for inner filter effect and b) corrected for inner filter effect.

Finally, Table 1 gives a description of the aquatic systems investigated in Sgroi et al. [1] and located in Sicily (Italy), where samples were collected to perform fluorescence and UV absorbance measurements reported in this Data Article.

2. Experimental design, materials, and methods

Data shown in this Data Article are related to samples collected from the primary wastewater effluent at Lentini wastewater treatment plant (WWTP), from the unchlorinated final effluents of Paternò WWTP and Bronte WWTP, and from Pozzillo Lake, which is a wastewater-impacted surface water (Table 1). Different samplings performed in same aquatic systems were denoted by different numbers.

Fig. 11 shows the location of pairs of excitation/emission wavelengths in a typical EEM of wastewater sample related to five fluorescence peaks, which were selected by pick-peaking method, and that can be considered representative of different dissolved organic matter (DOM) components [2–4]. In Fig. 11, the selected fluorescence peaks are denoted as I_1, I_2, I_3, I_4, I_5 and their coordinates selected by peak-picking method are described in Sgroi et al. [1]. Total absorbance values denoted as Abs_1, Abs_2, Abs_3, Abs_4, Abs_5 were calculated as the sum of the absorbance of excitation and emission wavelengths of fluorescence peaks I_1, I_2, I_3, I_4, I_5, respectively [5].

Deviation from the linearity of the relationship between fluorescence and total absorbance of the peaks I_1, I_2, I_3, I_4, I_5 was used to assess the effectiveness of IFE correction method proposed by Lakowicz [6] for different DOM components. For this purpose, dilution series were prepared by diluting the original sample with Milli-Q water.

Effect of TSS in fluorescence measurements was also evaluated for these abovementioned five fluorescence intensities. Particularly, the effect of TSS in fluorescence measurements was accomplished

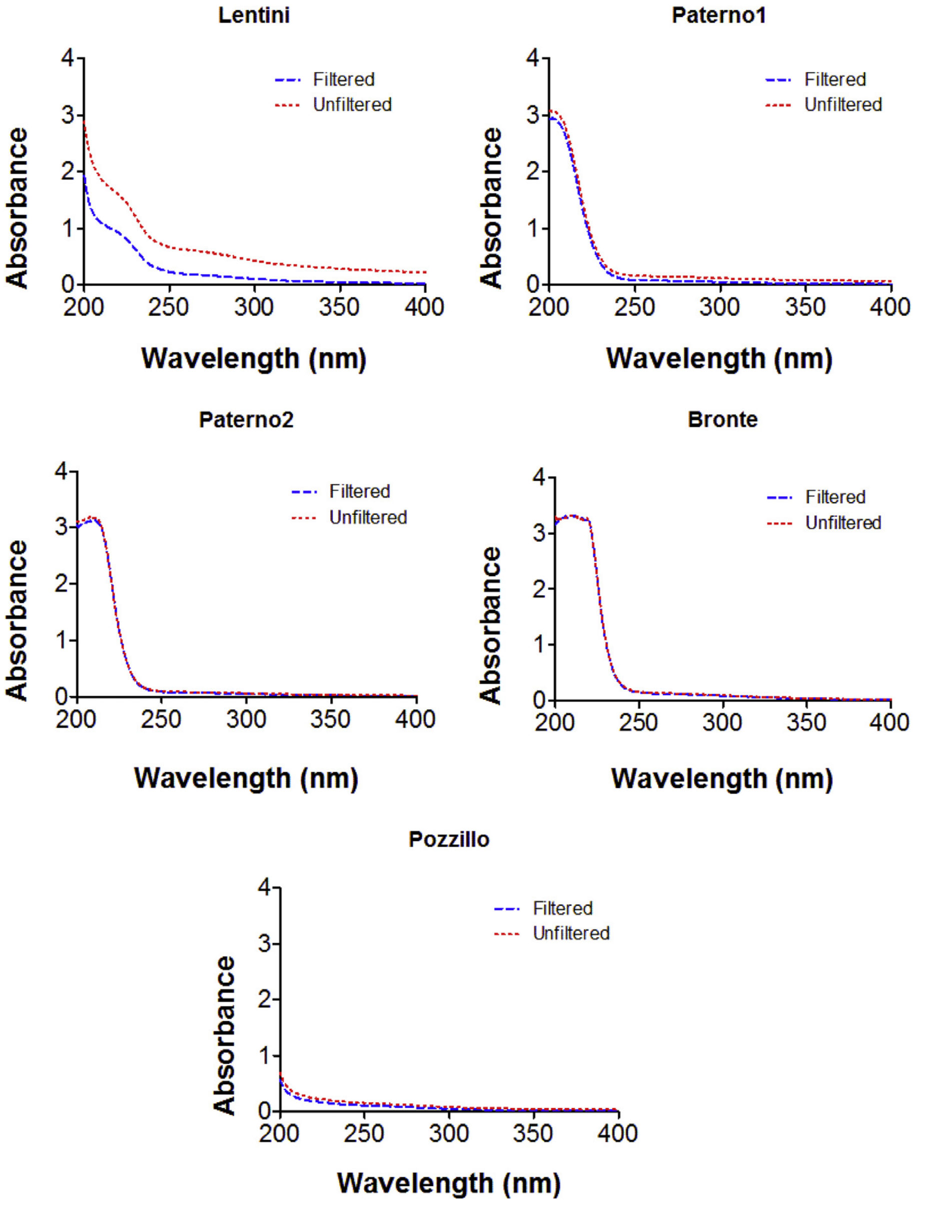

Fig. 6. UV absorbance spectra for filtered and unfiltered samples of tested waters.

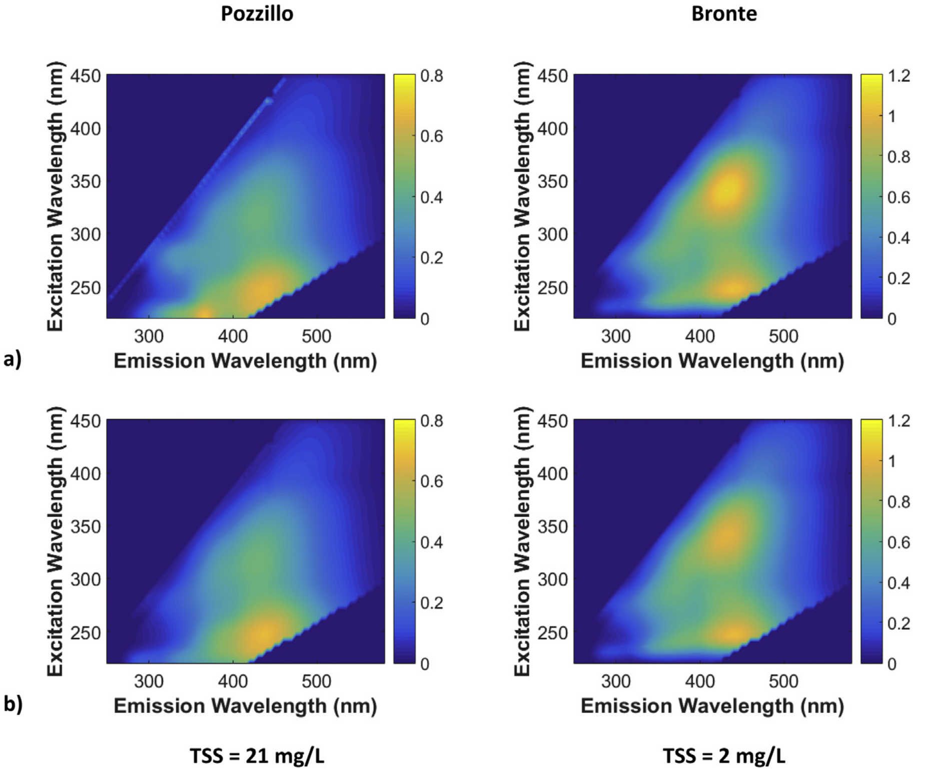

Fig. 7. EEMs non corrected for inner filter effect of a) unfiltered and b) filtered (0.7 μm) samples of Pozzillo and Bronte waters with indication of TSS concentration.

comparing the fluorescence measurements of unfiltered and 0.7 μm filtered samples. For this comparison, fluorescence spectra were not corrected for IFE [1].

Ultraviolet light absorbance was analyzed using a Shimadzu UV-1800 spectrophotometer (Kyoto, Japan). Absorbance spectra were measured from 200 to 800 nm at 1 nm intervals in a 1 cm quartz cuvette with Milli-Q water used as a blank.

Fluorescence data were collected using a Shimadzu RF-5301PC fluorescence spectrophotometer (Kyoto, Japan) with the scanning range from excitation wavelength 220 nm–450 nm at an interval of 5 nm and emission wavelength from 250 nm to 580 nm at the interval of 1 nm. Excitation and emission slit widths were both set at 5 nm. The Raman scatter effect was minimized by subtracting EEMs of pure Milli-Q water from the sample EEMs; any negative intensity values produced by this subtraction were converted to zero values. Then, the emission intensity data were normalized to the Raman peak area of an emission wavelengths scan of Milli-Q water samples collected at the interval of 1 nm and related to an excitation wavelength of 350 nm to produce fluorescence intensities in Raman unit (RU). All the EEMs were subjected to inner filter effect correction according to the methodology proposed by Lakowicz [6]. Non-trilinear data related to the Rayleigh scattering were eliminated [7].

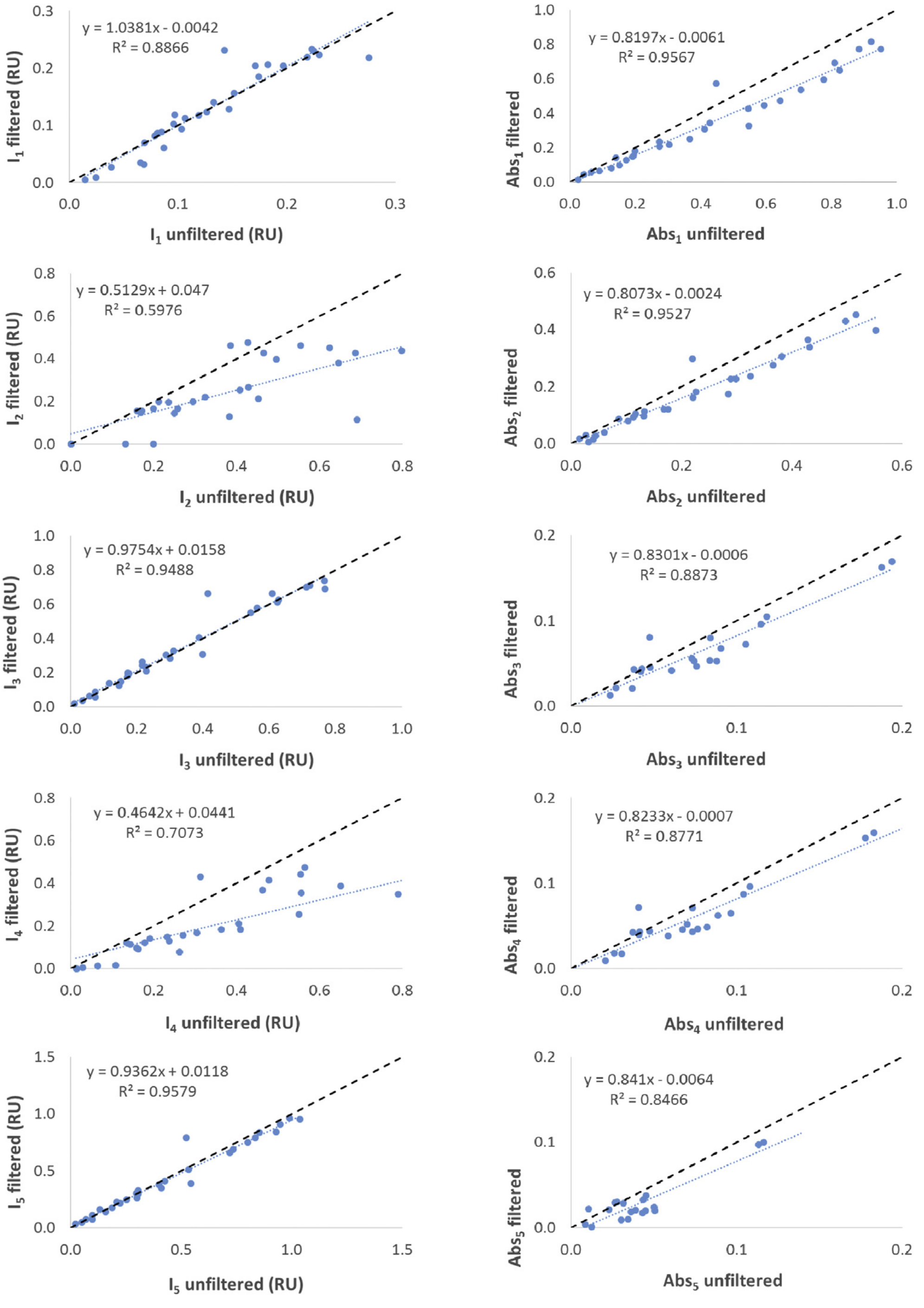

Fig. 8. Comparison between fluorescence intensities (uncorrected for inner filter) and total absorbance values in filtered and unfiltered diluted samples of Paternò1 wastewater (TSS = 94 mg/L). Dashed line indicates the first bisector.

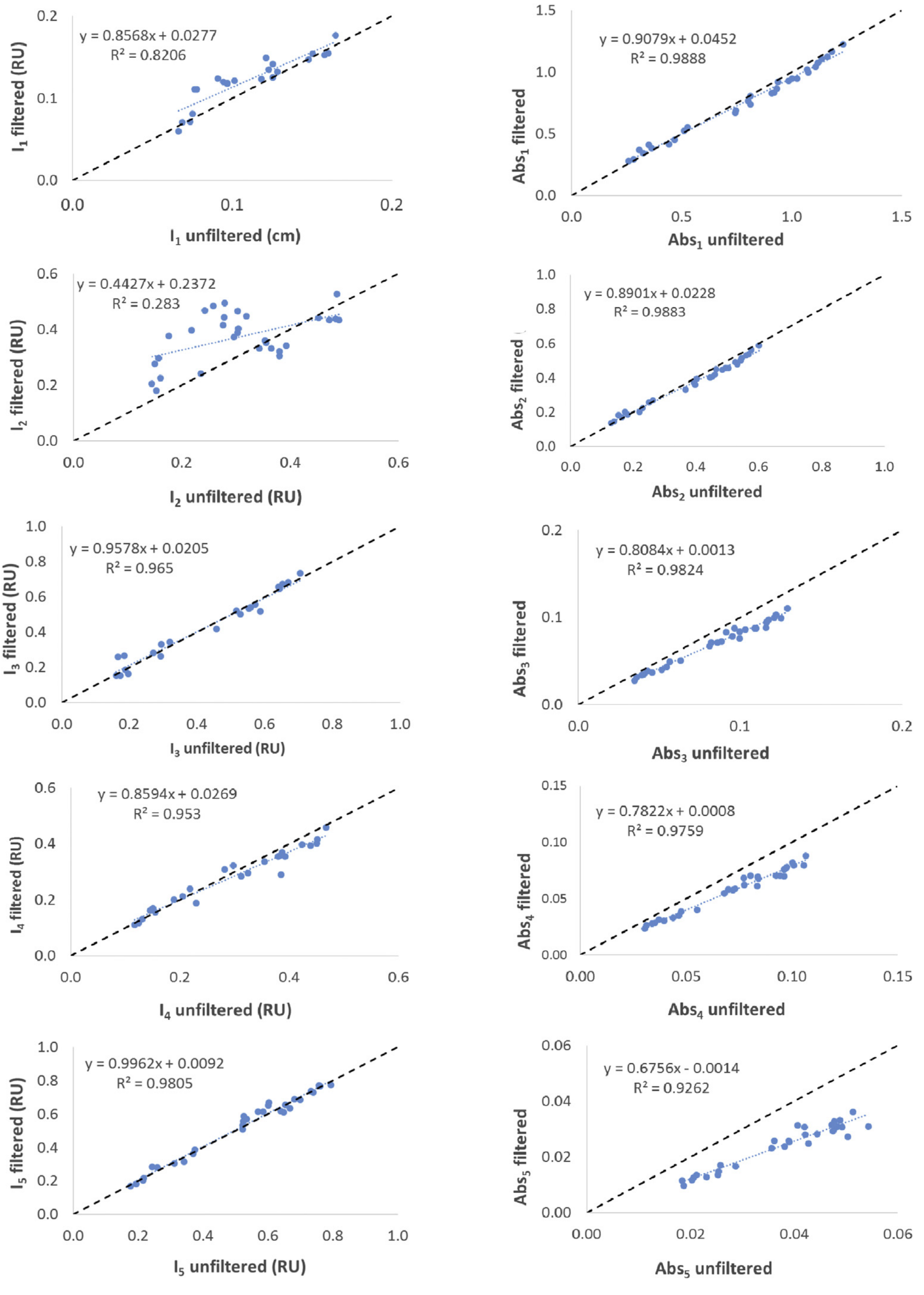

Fig. 9. Comparison between fluorescence intensities (uncorrected for inner filter) and total absorbance values in filtered and unfiltered diluted samples of Paternò2 wastewater (TSS = 4 mg/L). Dashed line indicates the first bisector.

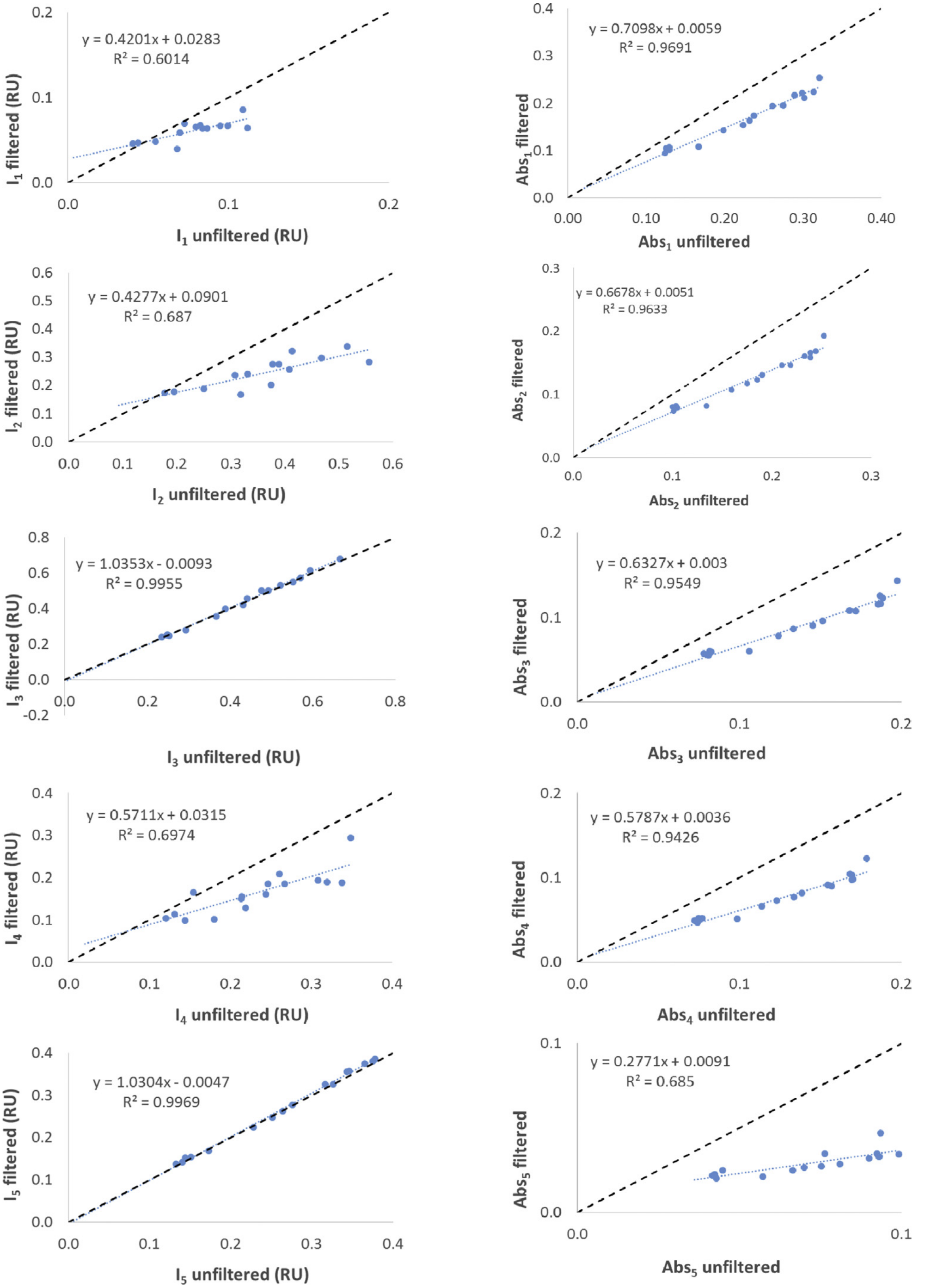

Fig. 10. Comparison between fluorescence intensities (uncorrected for inner filter) and total absorbance values in filtered and unfiltered diluted samples of Pozzillo wastewater impacted surface water (TSS = 21 mg/L). Dashed line indicates the first bisector.

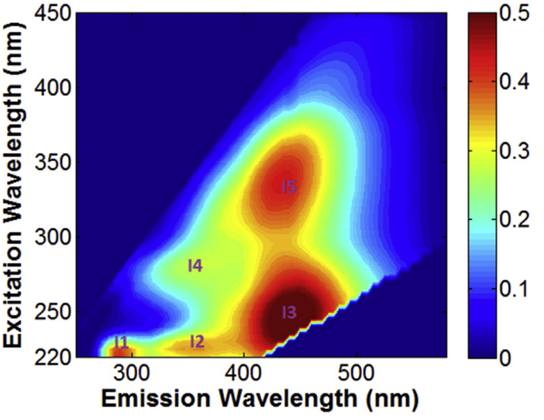

Fig. 11. Locations of excitation/emission pairs in a typical EEM of wastewater sample related to peaks I_1, I_2, I_3, I_4, and I_5.

Table 1
Description of the investigated aquatic systems.

Water system	Description	Geographic coordinates	
		Latitude	Longitude
Lentini	Municipal wastewater treatment plant – Treatment train: Preliminary treatments, primary sedimentation, biological treatment (activated sludge), secondary sedimentation, chlorination	37.304803°	14.987647°
Paternò	Municipal wastewater treatment plant – Treatment train: Preliminary treatments, primary sedimentation, biological treatment (activated sludge), secondary sedimentation, chlorination	37.555581°	14.875595°
Bronte	Municipal wastewater treatment plant – Treatment train: Preliminary treatments, biological treatment (activated sludge – extended aeration), secondary sedimentation, sand filtration, UV disinfection	37.784821°	14.811374°
Adrano	Municipal wastewater treatment plant – Treatment train: preliminary, primary, secondary (activated sludge, nitrifying), chlorination	37.651933°	14.837083°
Taormina	Municipal wastewater treatment plant – Treatment train: preliminary, primary, secondary (activated sludge, nitrification, denitrification), chlorination	37.808720°	15.256122°
Letojanni	Municipal wastewater treatment plant – Treatment train: preliminary, primary, secondary (activated sludge, nitrification, denitrification), chlorination	37.808720°	15.256122°
Pozzillo	Artificial lake - Surface water impacted by wastewater discharge	37.659966°	14.595029°
Contrasto	Artificial lake - Surface water impacted by wastewater discharge	37.662783°	14.791933°
Ponte Barca	Artificial lake - Surface water impacted by wastewater discharge	37.547133°	14.863233°

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Architecture, Project “Advanced treatment processes for the removal of emerging contaminants from water (PACEm)”. Authors are thankful to Davide Gionfriddo, master student at the University of Catania, for his support during sampling, analysis of water quality parameters and spectroscopic measurements.

Conflict of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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