Cup of Carbon: Smartphone-based analysis of dissolved organic carbon in water for use in citizen science

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Supplementary Information

SI. 1 Verification of water DOC concentration by TOC analysis

The DOC concentration of samples was determined directly from UV/Vis spectra using the dual wavelength model of Carter et al., (2012), which estimates the DOC concentration of samples based on the absorbance at 270 and 350 nm using a model parametrised with DOC and absorbance data from ~1700 surface water samples from Europe and North America. Eleven samples collected in August were also analysed using a total organic carbon (TOC) analyser (Thermolox, Sercon) to ensure the accuracy of the UV/Vis modelled DOC concentrations. The results of the UV/Vis method showed excellent agreement with the TOC analyser, with a regression coefficient of $R^2 = 0.9987$ (figure S1) and Lin's Concordance Correlation Coefficient (CCC) of $r_c=0.997$ (Lin, 1989; Muir & Innes, 2024). The UV/vis method gave results which were slightly higher than those measured by TOC, with an average recovery of 104.30 %, however all the DOC concentrations measured by the UV/vis method were within the 95 % confidence intervals (CI) reported by Carter et al., (2012), of 2 mg L^{-1} for concentrations from 5 – 20 mg L^{-1}, and 4 mg L^{-1} for concentrations from 20 – 80 mg L^{-1} (table S1).

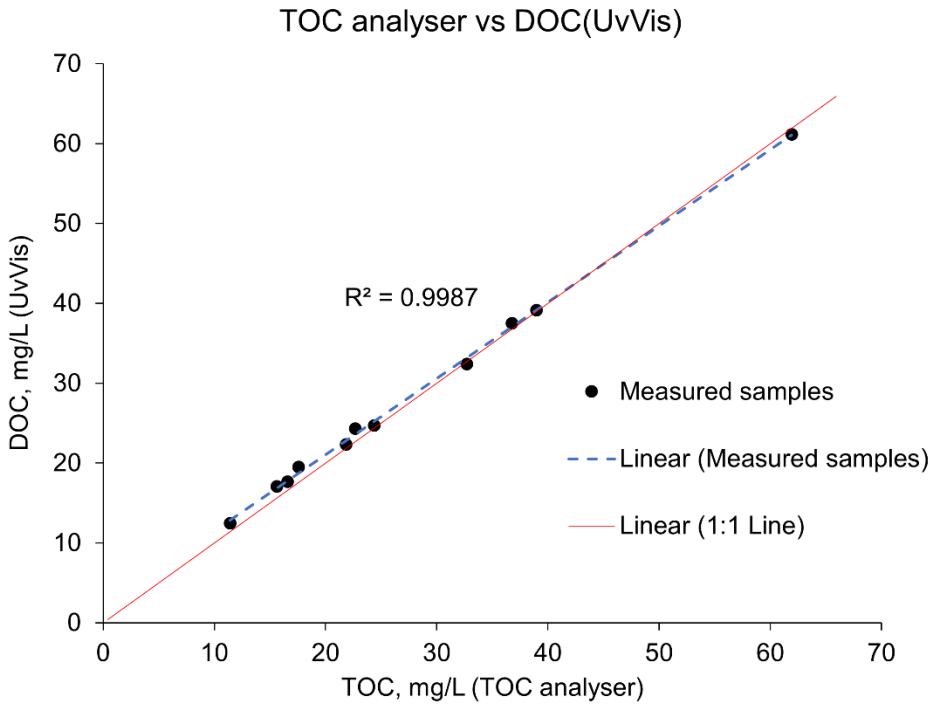

Figure S1. Scatter plot showing the comparison of the DOC concentration measured by the direct UV/Vis spectrophotometer method compared to the reference TOC analyser method. The 1:1 line is shown in red, and the blue dashed line shows the linear regression between the two methods.

Table S1. Results of the analysis of DOC by the UV/Vis and TOC analyser methods

TOC analyser (mg L^{-1})	DOC, UV/vis (mg L^{-1})	Difference (mg L^{-1})	95 % CI from Carter et al., (2012)	Recovery (%)
16.57	17.67	1.10	± 2 mg L^{-1}	106.61
11.41	12.48	1.07	± 2 mg L^{-1}	109.40
17.59	19.50	1.91	± 2 mg L^{-1}	110.88
21.84	22.35	0.52	± 4 mg L^{-1}	102.38
32.70	32.42	-0.28	± 4 mg L^{-1}	99.13
22.68	24.33	1.65	± 4 mg L^{-1}	107.26
15.64	17.05	1.42	± 2 mg L^{-1}	109.06
36.78	37.50	0.71	± 4 mg L^{-1}	101.94
38.99	39.16	0.17	± 4 mg L^{-1}	100.44
61.92	61.15	-0.77	± 4 mg L^{-1}	98.76
24.38	24.73	0.35	± 4 mg L^{-1}	101.44
			Average	**104.30 %**
			Standard deviation	**4.43 %**

Carter, H. T., Tipping, E., Koprivnjak, J. F., Miller, M. P., Cookson, B., & Hamilton-Taylor, J. (2012). Freshwater DOM quantity and quality from a two-component model of UV absorbance. *Water Research*, *46*(14), 4532–4542. https://doi.org/10.1016/j.watres.2012.05.02

Lin, L. I.-K. (1989). A Concordance Correlation Coefficient to Evaluate Reproducibility. *Biometrics*, *45*(1), 255–268. https://www.jstor.org/stable/2532051

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