



Corrigendum: Fluorescence Quantum Yields of Natural Organic Matter and Organic Compounds: Implications for the Fluorescence-based Interpretation of Organic Matter Composition

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A Corrigendum on

Fluorescence Quantum Yields of Natural Organic Matter and Organic Compounds: Implications for the Fluorescence-based Interpretation of Organic Matter Composition.

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The authors wish to include the following corrections to the original article. Some data presented in the published article were inaccurate due to improper instrumental correction factors resulting in incorrect fluorescence intensities. Moreover, we have corrected an error in the aquaDOM toolbox that affected the molar fluorescence and absorbance of organic compounds reported in the original article. Since these issues influenced data reported in **Tables 1, 2** and figures (**Figures 1–9**), there is a need for this corrigendum. The findings of the original manuscript were unaffected by these issues and remain the same.

Corrections are listed below in bold and underlined font. For page numbers, section heading, and paragraph numbers please refer to <http://dx.doi.org/10.3389/fmars.2015.00098>.

PAGE 1. ABSTRACT

- Range of Φ of organic compounds changed from 0.00079–0.35 to **0.001–0.37**
- Range of DOM AQY changed from 0.011 ± 0.003 to **0.012 \pm 0.004**
- Number of studies that contained matches with this study changed from 16 to **21**

PAGE 4. MATERIALS AND METHODS. (APPARENT) QUANTUM YIELD CALCULATION.

- Paragraph 1: The MATLAB toolbox is now available at <https://github.com/urbanwuensch/aquaDOM/releases>. The toolbox published with the original article is available as v1.0.0. For the corrigendum, v1.0.1 was used. Further updates will be published on this website if necessary.
- Paragraph 3: The molar fluorescence of the cross-reference salicylic acid was previously underestimated and led to the conclusion that 0.54 is the true reference quantum yield for

TABLE 1 | Optical properties of organic compounds dissolved in 1 mmol L⁻¹ phosphate buffer (pH 7.5).

Name	Molecular formula	Molecular weight (g mol ⁻¹)	λ_{\max} (nm)	λ_{em} (nm)	Molar fluorescence (R.U. μmol^{-1} L)	Molar absorbance (L mol ⁻¹ cm ⁻¹)	Stokes shift (eV)	Φ ($\pm\%$)
Caffeine	C ₈ H ₁₀ N ₄ O ₂	194.19	258	–	–	15,791	–	–
Coniferyl alcohol	C ₁₀ H ₁₂ O ₃	180.2	262	337	5.2	11,860	–	–
			292		1.8	4887	0.49	0.1 (9)
Coumarin	C ₉ H ₆ O ₂	146.14	276	376	0.019	11,100	–	–
			306		0.018	6356	1.26	0.001 (5)
Cresol	C ₇ H ₈ O	108.14	279	304	1.4	1928	0.41	0.155 (28)
Ferulic acid	C ₁₀ H ₁₀ O ₄	194.18	286	414	0.062	14,425	1.33	0.002 (13)
Gallic acid	C ₇ H ₆ O ₅	170.12	252	340	0.133	8280	1.38	0.006 (4)
Indole	C ₈ H ₇ N	117.15	269	340	4.6	5240	1.01	0.335 (9)
Benzoic acid	C ₇ H ₆ O ₂	122.12	223	314	–	7772	–	–
			266		0.002	550	0.31	0.001 (17)
Phenylalanine	C ₉ H ₁₁ NO ₂	165.19	256	281	0.036	153	0.43	0.039 (7)
L-dihydroxyphenylalanine	C ₉ H ₁₁ NO ₄	197.19	279	312	1.0	2723	0.48	0.085 (25)
Salicylic acid	C ₇ H ₆ O ₃	138.12	295	407	3.8	3469	1.16	0.365 (4)
Syringic acid	C ₉ H ₁₀ O ₅	198.17	260	332	0.538	14,604	1.03	0.012 (30)
DL-Tryptophane	C ₁₁ H ₁₂ N ₂ O ₂	204.23	277	350	2.3	5368	0.96	0.162 (8)
L-Tyrosine	C ₉ H ₁₁ NO ₃	181.19	274	301	1.3	1206	0.42	0.193 (32)
Vanillic acid	C ₈ H ₈ O ₄	168.14	250	324	1.1	8832	–	–
			284		0.590	4051	0.53	0.039 (13)

Molar fluorescence and absorbance are reported for the absorbance maximum and the secondary absorbance peak in if present. The quantum yield precision was estimated using the 95% confidence interval (see section 2.3) and is stated as the percentage of the estimated quantum yield.

quinine sulfate. As both 0.51 and 0.54 appear in the literature and 0.51 results in smaller errors during the cross calibration, the reference quantum yield of quinine sulfate was changed from 0.54 to **0.51**.

PAGE 5. RESULTS. OPTICAL PROPERTIES OF SAMPLES AND ORGANIC COMPOUNDS. PARAGRAPH 2.

- Molar fluorescence range changed from 0.003–38.50 (indole) to **0.002–5.2 Raman units L μmol^{-1} (coniferyl alcohol)**
- Stokes shift range changed from 0.32–1.38 eV (ferulic acid) to **0.31–1.38 eV (gallic acid)**
- Stokes shift range “group 1” changed from 0.32–0.57 eV with emission maxima of 281–339 nm to **0.32–0.49 eV and emission maxima of 281–337 nm**
- Stokes shift range group 2 changed from 0.97–1.38 eV with emission maxima of 333–413 nm to **1.01–1.38 eV and emission maxima of 340–414 nm**
- Φ of p-cresol and tyrosine changed from 0.11 and 0.13 to **0.16, and 0.19**; Stokes shift changed from 0.45 and 0.49 eV to **0.41 and 0.42 eV**
- Φ of tryptophan and indole changed from 0.15 and 0.28 to **0.16 and 0.34**

PAGE 7. RESULTS. METHOD COMPARISON: APPARENT QUANTUM YIELD CALCULATIONS.

- AQY accuracy for both approaches changed from 0.1–6% to **0.1–2.5%**
- Zero-intercept approach wavelength extent changed from 565 nm to **570 nm**
- Precision estimates of variable- and zero-intercept approach changed from $\pm 2.4\%$ and $\pm 1.3\%$ to **2.3% and 1.02%**, respectively.

PAGE 7. RESULTS. APPARENT QUANTUM YIELDS OF CDOM AND Φ OF ORGANIC COMPOUNDS. PARAGRAPH 1.

- Range of AQY₃₅₀ changed from 0.006–0.021 to **0.007–0.022**

PAGE 7. RESULTS. APPARENT QUANTUM YIELDS OF CDOM AND Φ OF ORGANIC COMPOUNDS. PARAGRAPH 2.

- Average surface water AQY changed from 0.009 to **0.010**
- Average deep-sea water AQY changed from 0.014 ± 0.003 to **0.016 ± 0.003**

TABLE 2 | Similarities between fluorescence spectra of PARAFAC components in the OpenFluor database and the spectra of organic compounds.

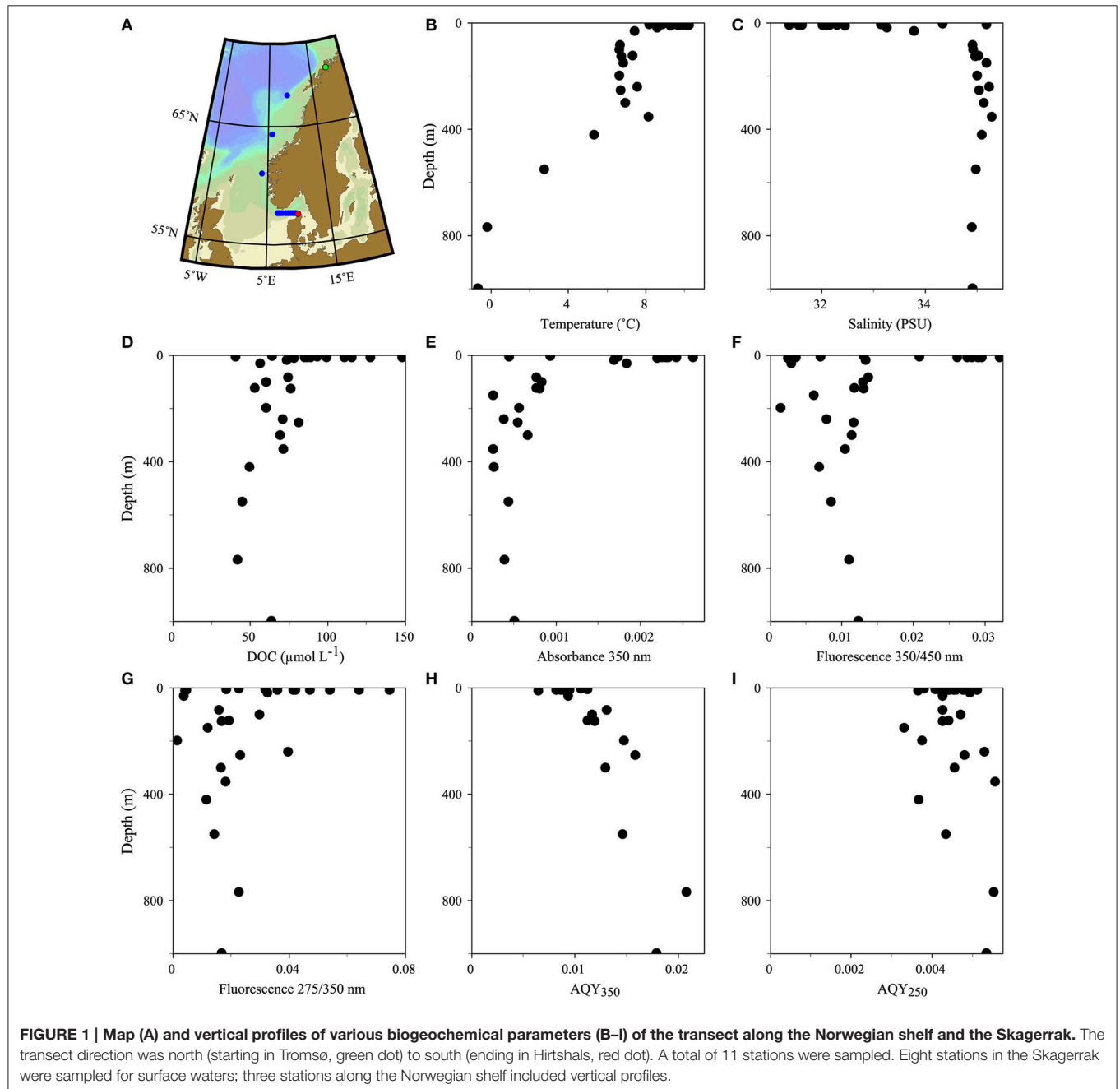
Organic compound	Study	Component	TCC Excitation	TCC Emission	TCC Excitation × Emission
Benzoic acid	Kauai ^a	2	0.99	0.96	0.95
	CS-Galathea ^b	3	0.95	0.90	0.86
	Recycle_StMary ^c	4	0.97	0.93	0.90
Coumarine	Swimpool ^d	1	0.95	0.95	0.90
	CS-Flocc ^e	2	1.00	0.95	0.95
p-Cresol	BWE7 ^f	1	0.98	0.98	0.96
	Recycle_WRAMS ^g	3	0.97	0.93	0.90
	FloridaKeys ^g	3	0.98	0.96	0.94
	Atlantic6AMT20 ^h	4	0.98	1.00	0.97
	CWT ⁱ	4	0.97	0.95	0.93
	Kauai	5	0.91	0.96	0.87
	LiverpoolBay ^j	6	0.95	0.97	0.92
	HF2005 ^k	8	0.97	0.97	0.94
L-DOPA	Recycle_WRAMS	3	0.95	0.99	0.94
	FloridaKeys	3	0.96	0.98	0.94
	Atlantic6AMT20	4	0.93	0.93	0.87
	CWT	4	0.96	0.98	0.94
	Beringia2005 ^l	5	0.92	0.97	0.89
	ONR ^m	6	0.96	0.97	0.93
	Kauai	6	0.95	0.94	0.90
	HF2005	8	0.96	0.92	0.89
Indole	Antarctic ⁿ	3	0.93	0.99	0.92
	Atlantic6AMT20	3	0.98	0.94	0.92
	CS-Bergen ⁿ	4	0.97	0.92	0.90
	TropicalRivers ^b	5	0.94	0.90	0.85
	LiverpoolBay	5	0.91	0.98	0.89
	CS-Bergen	6	0.92	0.94	0.87
	BWE7 ^o	6	0.96	0.95	0.91
	FCEP	7	0.98	0.91	0.89
Salicylic acid	Atlantic6AMT20	5	0.99	0.98	0.97
	Beringia2005	6	0.99	0.99	0.98
Syringic acid	TropicalRivers	5	0.93	0.93	0.86
	FCE	7	0.95	0.95	0.90
Tryptophan	Antarctic	3	0.98	0.94	0.92
	Atlantic6AMT20	3	0.98	0.92	0.91
	Recycle_StMary	5	0.92	0.92	0.84
	Horsens5 ^q	5	0.94	0.93	0.87
	HF2005	7	0.94	0.99	0.93
	Kauai	7	0.90	0.98	0.89
	Tyrosine	BWE7	1	1.00	1.00
FloridaKeys		3	0.97	0.93	0.90
Atlantic6AMT20		4	1.00	1.00	0.99
CWT		4	0.96	0.91	0.87
Kauai		5	0.95	0.94	0.89
Recycle_StMary		6	0.96	0.92	0.88
LiverpoolBay		6	0.96	0.98	0.94
HF2005		8	0.95	0.96	0.91

(Continued)

TABLE 2 | Continued

Organic compound	Study	Component	TCC Excitation	TCC Emission	TCC Excitation × Emission
Vanillic acid	Recycle_StMary	4	0.92	0.92	0.85
	DONKEY ^f	5	0.93	0.96	0.89
	FCE	7	0.97	0.95	0.92

Matches were restricted to Tucker congruence coefficients (TCC) of >0.9 and peak deviations <15 nm. ^a(Murphy et al., 2008); ^b(Jørgensen et al., 2011); ^c(Murphy et al., 2011); ^d(Seredyńska-Sobecka et al., 2011); ^e(Søndergaard et al., 2003); ^f(Murphy et al., 2006); ^g(Yamashita et al., 2013); ^h(Kowalczyk et al., 2013); ⁱ(Yamashita et al., 2011a); ^j(Yamashita et al., 2011b); ^k(Stedmon and Markager, 2005a); ^l(Walker et al., 2009); ^m(Osburn and Stedmon, 2011); ⁿ(Stedmon et al., 2011); ^o(Stedmon and Markager, 2005b); ^p(Yamashita et al., 2010); ^q(Murphy et al., 2014); ^r(Stedmon et al., 2007).



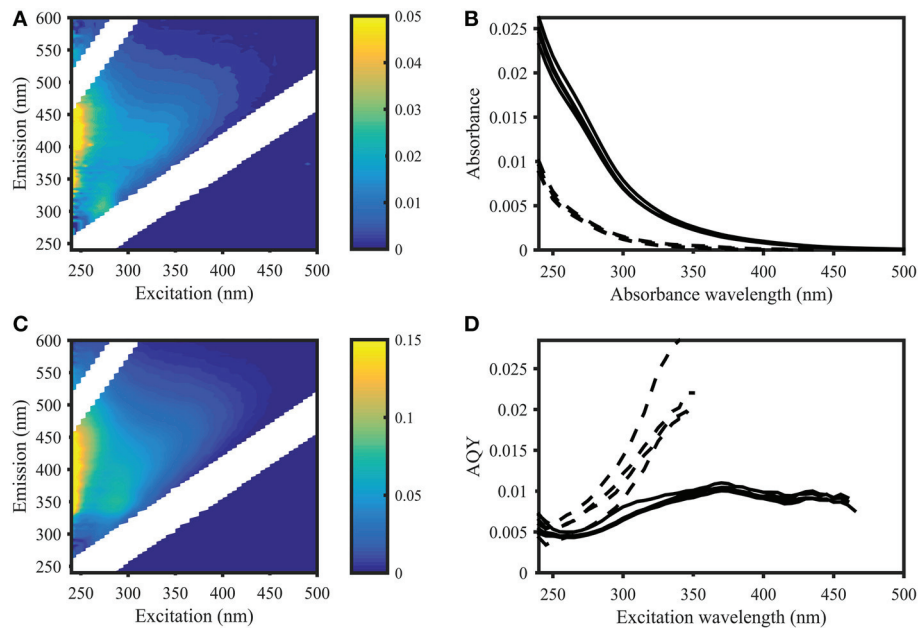


FIGURE 2 | Apparent quantum yield and fluorescence in samples from the Norwegian Sea (Station 2, deep sea) and Skagerrak (Station 14, surface water). Left panel: EEMs of deep (A) and surface (C) samples in Raman units (different scales as indicated by colorbar). Right panel: CDOM absorbance (B) and CDOM apparent fluorescence quantum yields (D) of four deep sea samples (dashed lines) and four surface water samples (solid lines), showing deep sea AQYs consistently higher than in surface waters. AQYs at wavelengths where signal to noise ratios were below 25 are missing values.

- Average AQY_{250} changed from 0.004 ± 0.0006 to 0.005 ± 0.0007
- **Figure 4:** water depth changed from 30, 10, and 200 m (A–C, respectively) to **6 m, 30 m and 200 m (A–C, respectively).**

PAGE 7. RESULTS. APPARENT QUANTUM YIELDS OF CDOM AND Φ OF ORGANIC COMPOUNDS. PARAGRAPH 3.

- Recalculation of AQYs eliminated the outlier at 197 m
- **Table 1:** Molar absorbance and fluorescence is reported for all mentioned peaks in the corrected version of the paper. Most values reported in the original version of the document have changed slightly. The correct values are reported in **Table 1**.

PAGE 7–8. RESULTS. APPARENT QUANTUM YIELDS OF CDOM AND Φ OF ORGANIC COMPOUNDS. PARAGRAPH 4.

- Range of Φ for organic compounds changed from 0.00079–0.35 to **0.001–0.37**
- Wavelength dependence of Φ for salicylic acid changed from 0.35 at 295 nm and 0.15 at 250 nm to **0.37 at 295 nm and 0.18 at 250 nm.**
- Distinct minima of coniferyl alcohol changed from 300 nm: 0.06, 250 nm: 0.11, 315 nm: 0.16 to **280 nm: 0.07, 250 nm: 0.14, 312 nm: 0.17**

PAGE 8. RESULTS. SPECTRAL MATCHING OF ORGANIC COMPOUNDS WITH PARAFAC SPECTRA

- List of potential matches for organic compounds changed from p-cresol, tryptophan, indole, L-dihydroxyphenylalanine, tyrosine, coumarin, salicylic acid, ferulic acid, and benzoic acid to **indole, p-cresol, L-diphenylalanine, tyrosine, tryptophan, vanillic acid, benzoic acid, syringic acid, and salicylic acid**
- Similarity of spectra changed from p-cresol and tryptophan, as well as indole and tyrosine to **p-cresol and tyrosine, as well as indole and tryptophan**

PAGE 8–9. DISCUSSION. DOM APPARENT FLUORESCENCE QUANTUM YIELDS. PARAGRAPH 1.

- Maximum Φ of organic compounds changed from 0.35 to **0.37**
- AQY of equimolar mixture of caffeine and salicylic acid changed from 0.0046 to **0.0054**
- Range of AQY of 1 mol L^{-1} salicylic acid and 0.01 to 1 mol L^{-1} caffeine changed from 0.15–0.0046 to **0.19–0.0054**
- AQY of mixture for mixture of caffeine and salicylic acid above 310 nm changed from 0.35 to **0.37**

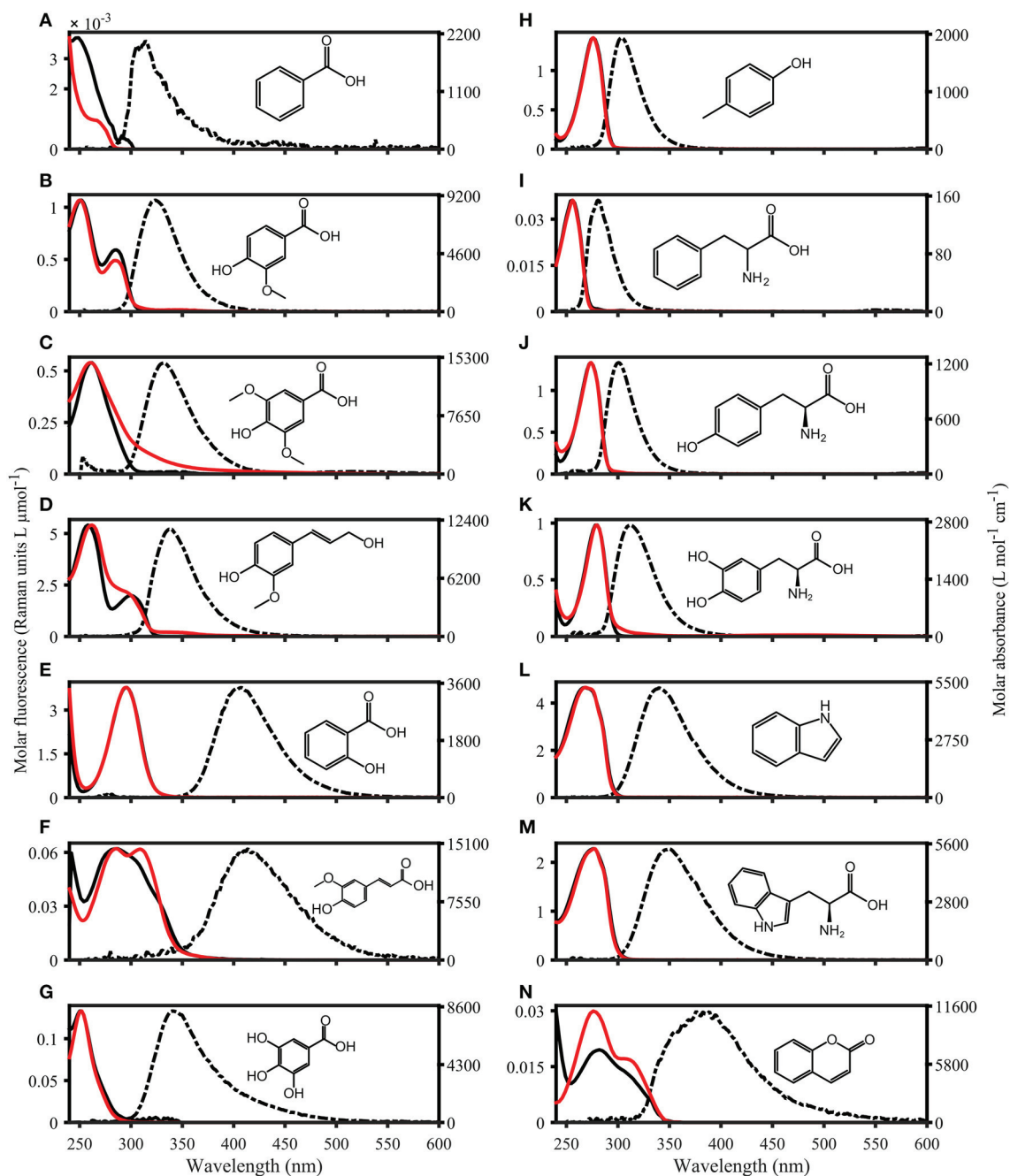


FIGURE 3 | Absorbance and Fluorescence spectra of organic compounds dissolved in water with 1 mmol L⁻¹ PO₄ buffer (pH 7.5). The molar absorptivity is shown as a solid red line, excitation loadings are solid black lines, and emission loadings are dashed black lines. **(A–G)** Benzoic acid, vanillic acid, syringic acid, coniferyl alcohol, salicylic acid, ferulic acid, gallic acid. **(H–N)** p-Cresol, phenylalanine, tyrosine, dihydroxyphenylalanine, indole, tryptophan, coumarin.

PAGE 9. DISCUSSION. DOM APPARENT FLUORESCENCE QUANTUM YIELDS. PARAGRAPH 2.

- Average AQY at 350 nm changed from 0.011 ± 0.003 to 0.012 ± 0.004
- **Figure 5A** legend: Recalculation eliminated outlier at 197 m

PAGE 10–11. DISCUSSION. METHOD COMPARISON: QUANTUM YIELD CALCULATIONS. PARAGRAPH 4.

- %-difference between reference study and this study for optical properties of salicylic acid changed from 1.3, 2.9, and 0.4 (molar absorbance, Φ , and Stokes shift, respectively) to

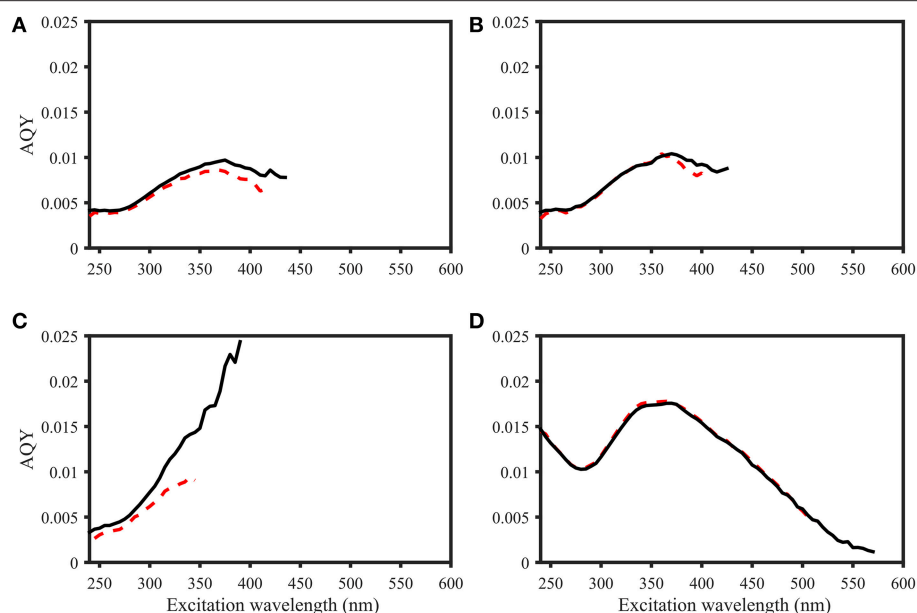


FIGURE 4 | Comparison of AQY calculations for four samples. Black line: Zero-intercept approach. Red dashed line: Variable-intercept approach. **(A–C)** Norwegian shelf DOM, water depth: 6, 30, and 200 m **(A–C, respectively).** **(D)** 2.5 mg L^{-1} Suwannee River XAD-8 fulvic acid extract. Figures do not include error bars for ease of viewing, but in all cases, AQY values of the two calculation approaches were within the precision estimates.

1.3, 2.7, and 0.3 (molar absorbance, Φ , and Stokes shift, respectively).

- Φ of phenylalanine changed from 0.018 to 0.039. This matches previously published values (Feitelson, 1964). Therefore, the last three sentences of paragraph 4 are redundant.
- **Table 2:** The erroneous spectral correction factors resulted in slightly inaccurate peak shapes for many organic compounds. This affected similarity scores between organic compounds such that some previously-matched PARAFAC components were excluded, while new hits were added to the table.

PAGE 13. DISCUSSION. LINKING OPTICAL AND CHEMICAL PROPERTIES. PARAGRAPH 1.

- Range of molar fluorescence and absorbance of a 1 nmol L^{-1} equivalent changed from 35×10^{-5} – 0.0036 m^{-1} , and 25×10^{-5} – 0.038 Raman units to **3.5×10^{-5} to 0.0036 m^{-1} for absorbance, and 2.1×10^{-6} to 0.0052 Raman units**

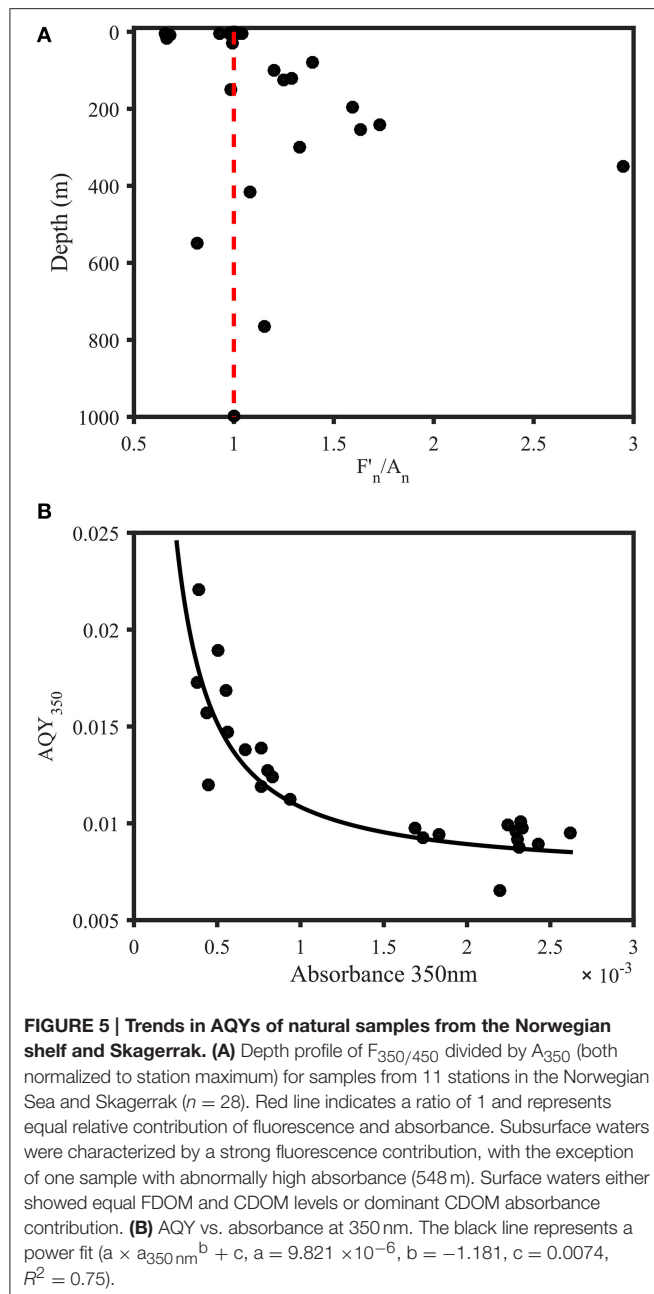
- **Figure 9** legend: AQY decrease changed from 0.15–0.0046 changed to **0.19–0.0054**

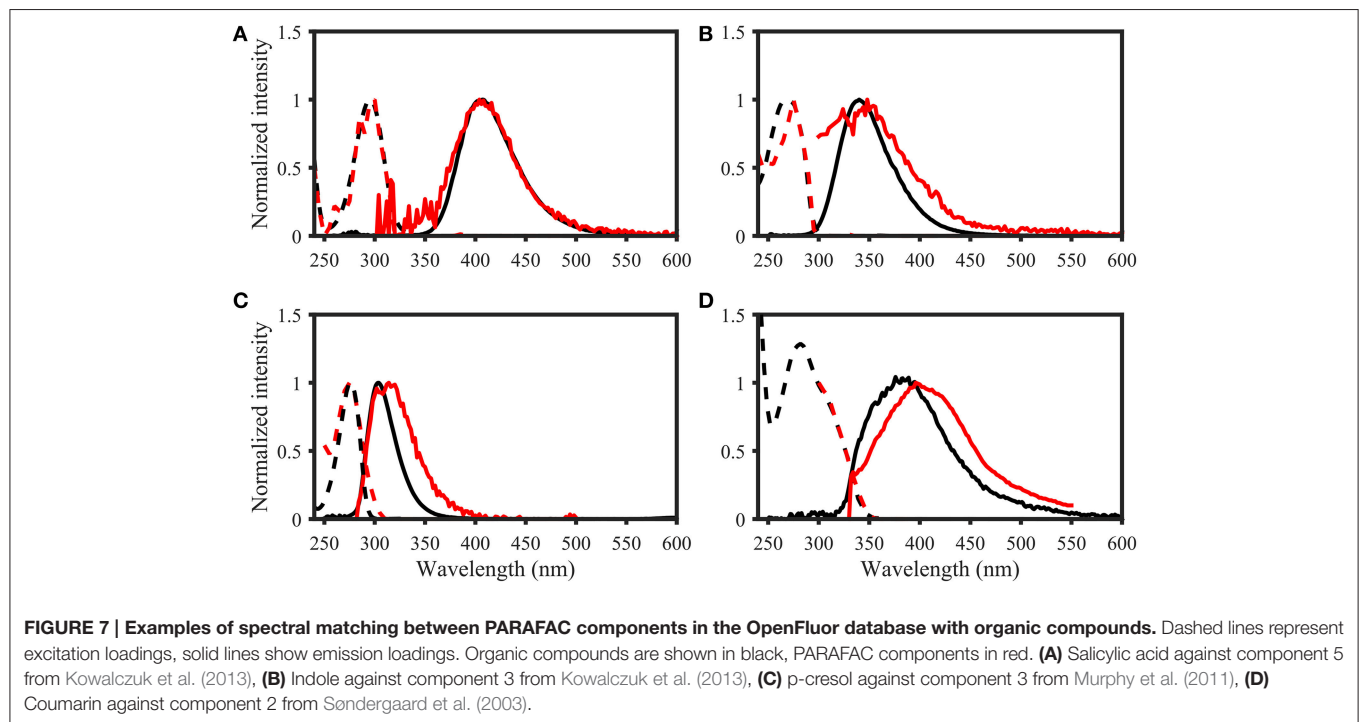
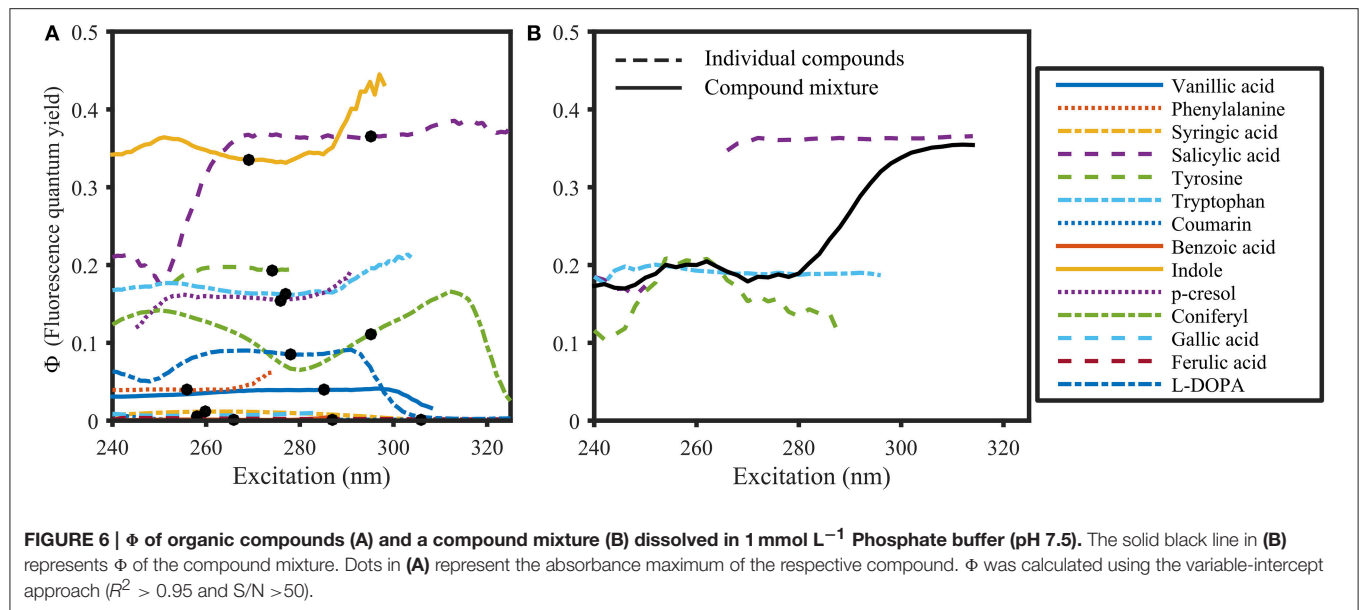
AUTHOR CONTRIBUTIONS

All authors (UW, KM, and CS) contributed substantially to the text of the submitted corrigendum. UW performed the data analysis and correction, CS and KM assisted during the correction process.

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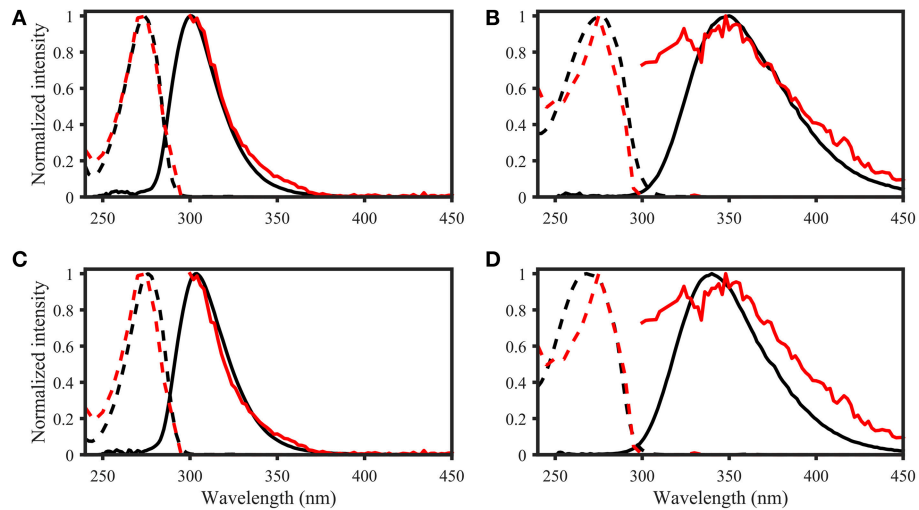


FIGURE 8 | OpenFluor matches of (A) tyrosine, (B) tryptophan, (C) p-cresol, and (D) indole (all in black) with PARAFAC components (all in red) from Kowalczyk et al. (2013). Dashed lines represent excitation loadings, solid lines show emission loadings. Tryptophan and indole, as well as tyrosine and p-cresol yield matches with the same PARAFAC component.

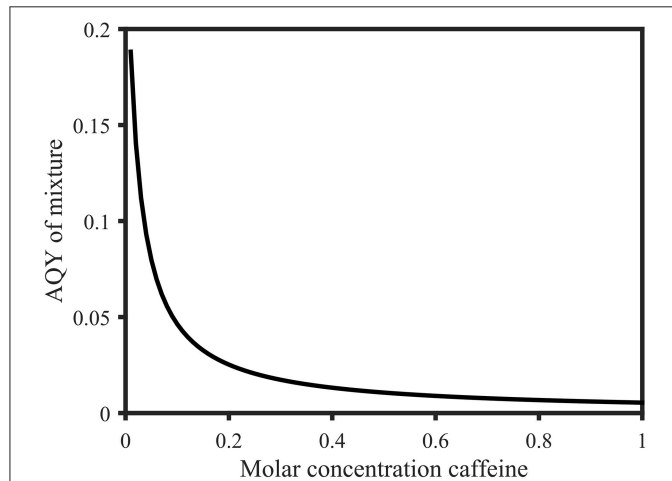


FIGURE 9 | Calculated apparent quantum yields of a mixture of 1 mol L⁻¹ salicylic acid solution with variable molar parts of caffeine (0.01 to 1 mol L⁻¹) at 258 nm. The apparent quantum yield decreases from 0.19 (0.01 mol L⁻¹ caffeine) to 0.0054 (1 mol L⁻¹ caffeine). Calculations were based on Eq. 5 and are explained in the Supplementary Material.

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The Guest Associate Editor CO declares that, despite co-authoring a paper with author CAS, the review process was handled objectively and no conflict of interest exists.

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