Supplement of Biogeosciences, 22, 2461–2484, 2025
https://doi.org/10.5194/bg-22-2461-2025-supplement

Biogeosciences
Open Access

Supplement of

Relationships between the concentration of particulate organic nitrogen and the inherent optical properties of seawater in oceanic surface waters

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The supporting information provides the best-fit coefficients and their standard deviation of the relationships between PON and IOPs for the open-ocean dataset (Table S1) and the whole dataset (Table S2 and S3). In addition, the supporting information includes the slope (*S*), intercept (*I*), and statistical metrics of the relationships between PON derived from IOP-based algorithms and measured PON for the open-ocean dataset (Table S4) and the whole dataset (Table S5).

Table S1. Best-fit coefficients of the relationships between PON (mg m^{-3}) and IOPs(λ) (m^{-1}) for the open-ocean dataset (OOD). *R^2* is the coefficient of determination and *N* the number of samples.

PON = A IOP(λ)^B	A	B	R^2	N
PON = $A\ b_{bp}(442)^B$	245739.14 ± 260832.07	1.51 ± 0.10	0.75	70
PON = $A\ b_{bp}(510)^B$	206544.76 ± 196112.79	1.44 ± 0.09	0.80	63
PON = $A\ b_{bp}(555)^B$	105514.11 ± 72139.11	1.31 ± 0.07	0.84	74
PON = $A\ a_{p}(412)^B$	246.10 ± 54.57	0.73 ± 0.03	0.87	71
PON = $A\ a_{p}(442)^B$	229.69 ± 50.62	0.74 ± 0.03	0.86	71
PON = $A\ a_{p}(490)^B$	284.23 ± 61.70	0.71 ± 0.03	0.88	71
PON = $A\ a_{p}(510)^B$	356.71 ± 79.86	0.69 ± 0.03	0.89	71
PON = $A\ a_{p}(555)^B$	468.23 ± 127.04	0.62 ± 0.03	0.86	69
PON = $A\ a_{p}(670)^B$	265.76 ± 66.94	0.56 ± 0.03	0.84	71
PON = $A\ a_{ph}(412)^B$	223.93 ± 57.02	0.65 ± 0.04	0.82	71
PON = $A\ a_{ph}(442)^B$	215.76 ± 54.12	0.68 ± 0.04	0.82	71
PON = $A\ a_{ph}(490)^B$	259.53 ± 65.26	0.66 ± 0.03	0.84	71
PON = $A\ a_{ph}(510)^B$	310.04 ± 81.39	0.62 ± 0.03	0.84	71
PON = $A\ a_{ph}(555)^B$	309.01 ± 92.82	0.49 ± 0.03	0.80	69
PON = $A\ a_{ph}(670)^B$	249.45 ± 66.11	0.53 ± 0.03	0.82	71
PON = $A\ a_{d}(412)^B$	1195.9 ± 601.35	0.85 ± 0.06	0.74	71
PON = $A\ a_{d}(442)^B$	1264.5 ± 693.80	0.82 ± 0.06	0.71	71
PON = $A\ a_{d}(490)^B$	1212.0 ± 756.50	0.75 ± 0.07	0.65	71
PON = $A\ a_{d}(510)^B$	1109.51 ± 711.43	0.72 ± 0.07	0.63	71
PON = $A\ a_{d}(555)^B$	878.97 ± 617.02	0.64 ± 0.07	0.56	71
PON = $A\ a_{d}(670)^B$	251.02 ± 185.26	0.41 ± 0.06	0.38	71

Table S2. Best-fit coefficients of the relationships between PON (mg m^{-3}) and $b_{bp}(\lambda)$ (m^{-1}) for the whole dataset (WD). R^2 is the coefficient of determination and N the number of samples.

	a_0	a_1	a_2	a_3	R^2	N
$\log_{10}(PON) = a_0 + a_1(\log_{10}(b_{bp}(442))) + a_2(\log_{10}(b_{bp}(442)))^2 + a_3(\log_{10}(b_{bp}(442)))^3$	2.21	0.57	0.34	0.10	0.60	289
$\log_{10}(PON) = a_0 + a_1(\log_{10}(b_{bp}(510))) + a_2(\log_{10}(b_{bp}(510)))^2 + a_3(\log_{10}(b_{bp}(510)))^3$	2.63	1.40	0.74	0.15	0.62	279
$\log_{10}(PON) = a_0 + a_1(\log_{10}(b_{bp}(555))) + a_2(\log_{10}(b_{bp}(555)))^2 + a_3(\log_{10}(b_{bp}(555)))^3$	2.62	1.32	0.68	0.14	0.63	284

Table S3. Best-fit coefficients of the relationships between PON (mg m^{-3}) and the spectral absorption coefficients (m^{-1}) of different seawater particulate constituents for the whole dataset (WD). R^2 is the coefficient of determination and N the number of samples.

PON = A IOP$a(\lambda)^B$	A	B	R^2	N
PON = $A\,a_p(412)^B$	134.53 ± 8.32	0.62 ± 0.02	0.80	392
PON = $A\,a_p(442)^B$	152.42 ± 9.50	0.65 ± 0.02	0.82	392
PON = $A\,a_p(490)^B$	221.56 ± 16.02	0.67 ± 0.02	0.82	392
PON = $A\,a_p(510)^B$	254.27 ± 19.62	0.64 ± 0.02	0.82	392
PON = $A\,a_p(555)^B$	326.86 ± 30.76	0.59 ± 0.02	0.79	389
PON = $A\,a_p(670)^B$	278.87 ± 21.81	0.59 ± 0.01	0.83	392
PON = $A\,a_{ph}(412)^B$	209.99 ± 16.29	0.63 ± 0.02	0.79	392
PON = $A\,a_{ph}(442)^B$	220.73 ± 16.96	0.67 ± 0.02	0.80	392
PON = $A\,a_{ph}(490)^B$	323.53 ± 27.80	0.69 ± 0.02	0.82	392
PON = $A\,a_{ph}(510)^B$	359.60 ± 31.47	0.64 ± 0.02	0.82	392
PON = $A\,a_{ph}(555)^B$	363.03 ± 35.65	0.52 ± 0.01	0.79	389
PON = $A\,a_{ph}(670)^B$	273.66 ± 21.93	0.55 ± 0.01	0.82	392
PON = $A\,a_d(412)^B$	184.38 ± 16.10	0.55 ± 0.02	0.73	392
PON = $A\,a_d(442)^B$	223.29 ± 21.18	0.55 ± 0.02	0.73	392
PON = $A\,a_d(490)^B$	303.97 ± 34.60	0.56 ± 0.02	0.70	392
PON = $A\,a_d(510)^B$	351.94 ± 42.41	0.57 ± 0.02	0.70	392
PON = $A\,a_d(555)^B$	504.51 ± 72.94	0.58 ± 0.02	0.68	392
PON = $A\,a_d(670)^B$	787.80 ± 160.15	0.56 ± 0.02	0.58	392

Table S4. Slope (*S*), intercept (*I*), and statistical metrics of the relationships between PON derived from IOP-based algorithms and measured PON for the open-ocean dataset (OOD). *RMSD* is the Root Mean Square Deviation (mg m^{-3}), *MdB* the Median Bias (mg m^{-3}), *MdR* the Median Ratio, *MdAPD* the Median Absolute Percentage Difference (%), *MdSA* the Median Symmetric Accuracy (%), and *N* the number of samples.

	S	*I*	*R*	*RMSD*	*MdB*	*MdR*	*MdAPD*	*MdSA*	*N*
$b_{bp}(442)$	1.06	-0.07	0.87	6.35	0.34	1.01	28.56	35.41	70
$b_{bp}(510)$	1.04	-0.04	0.90	4.30	0.56	1.07	20.11	22.02	63
$b_{bp}(555)$	1.02	-0.03	0.92	6.17	0.28	1.05	23.68	28.30	74
$a_{p}(412)$	0.98	0.02	0.93	4.57	0.06	1.01	18.08	19.84	71
$a_{p}(442)$	0.98	0.02	0.93	4.81	0.31	1.04	18.29	21.50	71
$a_{p}(490)$	0.98	0.04	0.94	4.46	0.31	1.03	17.99	19.88	71
$a_{p}(510)$	0.98	0.02	0.94	4.39	0.10	1.03	18.91	19.56	71
$a_{p}(555)$	0.97	0.03	0.93	4.79	-0.09	0.98	20.21	24.51	69
$a_{p}(665)$	0.95	0.05	0.92	5.35	-0.10	0.98	18.76	21.18	71
$a_{ph}(412)$	0.96	0.05	0.91	4.63	0.22	1.04	17.64	18.69	71
$a_{ph}(442)$	0.96	0.04	0.91	4.85	0.28	1.04	18.81	18.88	71
$a_{ph}(490)$	0.96	0.03	0.92	4.48	0.22	1.01	18.81	19.56	71
$a_{ph}(510)$	0.96	0.04	0.92	4.32	0.25	1.03	17.42	18.65	71
$a_{ph}(555)$	0.93	0.07	0.90	4.55	0.42	1.04	17.66	17.66	69
$a_{ph}(665)$	0.94	0.06	0.91	5.19	0.20	1.04	19.45	19.80	71
$a_{d}(412)$	0.97	0.03	0.86	7.14	-0.04	0.99	30.44	34.20	71
$a_{d}(442)$	0.96	0.04	0.84	7.60	0.22	1.03	31.98	36.90	71
$a_{d}(490)$	0.94	0.06	0.81	8.35	0.30	1.07	35.83	42.91	71
$a_{d}(510)$	0.92	0.08	0.79	8.58	0.46	1.07	37.21	40.62	71
$a_{d}(555)$	0.87	0.13	0.75	9.20	0.63	1.10	38.90	54.67	69
$a_{d}(665)$	0.63	0.36	0.62	10.83	0.72	1.12	47.09	58.05	71

Table S5. Slope (*S*), intercept (*I*), and statistical metrics of the relationships between PON derived from IOP-based algorithms and measured PON for the whole dataset (WD). *RMSD* is the Root Mean Square Deviation (mg m^{-3}), *MdB* the Median Bias (mg m^{-3}), *MdR* the Median Ratio, *MdAPD* the Median Absolute Percentage Difference (%), *MdSA* the Median Symmetric Accuracy (%), and *N* the number of samples.

	S	*I*	*R*	*RMSD*	*MdB*	*MdR*	*MdAPD*	*MdSA*	*N*
$b_{bp}(442)$	0.80	0.28	0.83	29.85	0.23	1.02	36.99	47.87	289
$b_{bp}(510)$	0.80	0.27	0.83	28.91	0.65	1.04	34.50	38.79	279
$b_{bp}(555)$	0.82	0.24	0.85	28.18	0.41	1.03	35.88	43.75	284
$a_p(412)$	0.95	0.08	0.89	27.52	-0.48	0.98	30.93	38.94	392
$a_p(442)$	0.96	0.06	0.90	25.36	0.31	1.02	30.47	36.88	392
$a_p(490)$	0.96	0.06	0.91	25.72	0.25	1.02	29.17	34.87	392
$a_p(510)$	0.96	0.06	0.91	26.09	-0.11	0.99	28.49	33.47	392
$a_p(555)$	0.94	0.09	0.89	27.72	0.24	1.02	30.14	37.01	389
$a_p(665)$	0.95	0.07	0.91	23.27	0.08	1.01	25.28	31.62	392
$a_{ph}(412)$	0.95	0.08	0.89	24.77	0.05	1.00	30.30	37.58	392
$a_{ph}(442)$	0.96	0.07	0.90	23.35	0.37	1.03	29.37	35.70	392
$a_{ph}(490)$	0.96	0.06	0.90	23.77	0.33	1.03	29.29	33.57	392
$a_{ph}(510)$	0.96	0.06	0.91	23.80	0.42	1.03	27.33	33.77	392
$a_{ph}(555)$	0.93	0.11	0.89	26.82	0.61	1.03	28.28	33.94	389
$a_{ph}(665)$	0.94	0.08	0.90	23.76	-0.10	0.99	24.91	30.20	392
$a_d(412)$	0.91	0.13	0.85	32.77	0.41	1.02	33.53	43.15	392
$a_d(442)$	0.91	0.13	0.85	32.56	0.62	1.03	34.10	41.24	392
$a_d(490)$	0.90	0.15	0.84	33.19	0.22	1.01	34.32	41.30	392
$a_d(510)$	0.90	0.14	0.84	33.21	0.23	1.01	34.05	42.22	392
$a_d(555)$	0.90	0.15	0.82	33.88	-0.08	0.99	37.67	44.05	389
$a_d(665)$	0.85	0.23	0.76	35.41	0.46	1.03	39.90	48.77	392