Supplement of Biogeosciences, 23, 5377–5397, 2026
https://doi.org/10.5194/bg-23-5377-2026-supplement

Biogeosciences Open Access EGU

Supplement of

Selective accumulation of dissolved organic matter in the sea surface microlayer: integrated multi-spectral CDOM and FDOM characterization and a novel FDOM/CDOM index at a Mediterranean coastal site

Elli Pitta et al.

Correspondence to: Elli Pitta (ellip@hcmr.gr)

Table S1. Measured environmental and physicochemical variables during samplings.

Sampling date	**SML thickness d_{SML}**	**Wind speed**	**Solar irradiance E**	**Seawater Temperature T**	**Seawater Salinity**	**DOC**	
	µm	m s^{-1}	W m^{-2}	°C	psu	mg L^{-1}	
				At 1m depth		*SML*	*ULW*
2/06/2016	45.99	0-0.8	600-750	17.2	38.5	3.039	0.964
16/06/2016	50.79	0.9-1.8	600-850	23.0	38.5	3.584	1.019
1/07/2016	52.60*	0.8-2.0	650-800	22.1	38.9	6.561	0.917
2/08/2016	41.05	0-0.8	650-900	25.8	38.9	3.208	0.916
18/08/2016	50.42	0-1.8	650-900	26.3	38.9	2.865	0.977
6/09/2016	45.22	0-0.9	500-650	26.0	38.9	-	0.996
21/09/2016	42.85*	0-1.4	500-650	26.5	38.9	3.876	0.924
7/10/2016	48.62*	0	300-450	25.7	38.8	1.585	1.263
21/10/2016	49.07*	0-1.9	250-350	24.4	38.8	3.008	0.871
3/11/2016	51.81*	0-1.5	200-320	23.0	38.6	1.462	0.913
18/11/2016	58.71*	0-1.5	200-320	21.8	38.7	3.714	0.864
2/12/2016	54.99*	0- 2.0	200-300	20.7	38.9	3.228	0.887
20/12/2016	51.59*	0.4-1.7	200-250	19.0	38.7	2.498	0.860
4/01/2016	57.02	0-1.5	200-350	17.2	38.6	1.830	0.815
28/01/2017	60.05*	0-2.2	130-200	15.6	38.6	2.321	0.777
9/02/2017	56.37	3.5	150-280	14.1	38.5	1.090	0.787
22/02/2017	48.83	0-0.7	400-500	14.2	39.0	1.215	0.832
7/03/2017	51.22*	0.5-2.1	200-450	14.3	39.0	1.990	0.891
3/04/2017	49.47	0-0.1	520-690	15.5	38.2	1.116	0.832
25/04/2017	44.29*	0-1.3	550-690	15.5	38.9	1.909	0.879
4/05/2017	47.09*	0-1.7	580-750	17.0	39.0	6.85	0.850
10/06/2017	56.79	0-0.7	600-820	19.1	38.3	3.575	0.938
Average				20.2	38.8	2.480	0.908
Standard Deviation				4.5	0.5	0.942	0.102
CV (%)				22.0	1.1	38.0	11.2

*Visible slicks

Table S2. Spectral position of the PARAFAC components deconvoluted by the 2 different models using the seawater (SML and UWL) EEMs and for the rainwater EEMs.

Seawater	Rainwater
C1 Ex/Em= 240,370/ 485 Peak A, C	R1 Ex/Em= 240,290/ 394 Peak A, M
C2 Ex/Em= 240,280/ 325 Peak T	R2 Ex/Em= 245,335/ 456 Peak A, C
C3 Ex/Em= 240,295/ 415 Peak A, M	R3 Ex/Em= 240,270/ 299 Peak B
C4 Ex/Em= 265/296 Peak B	

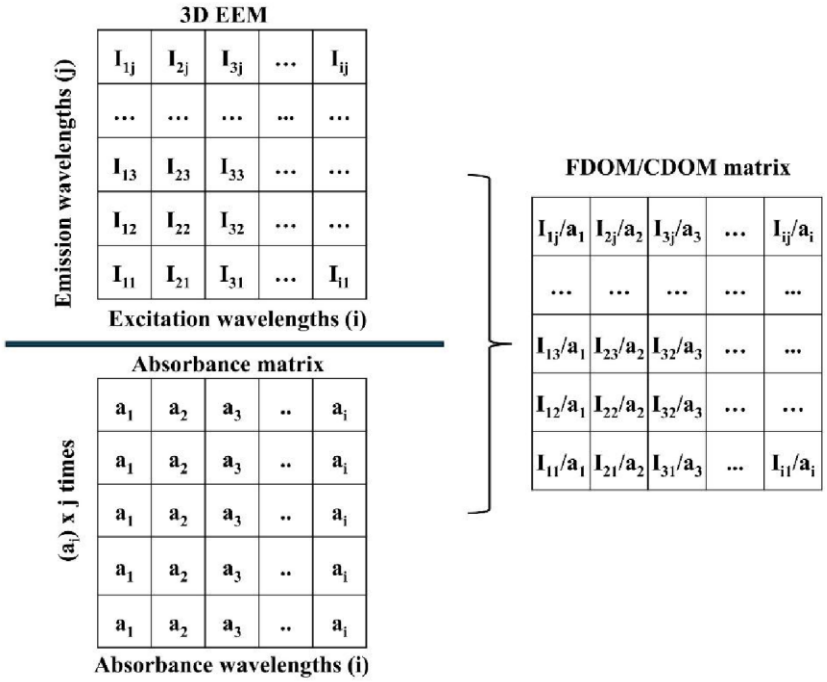

Fig. S1 The FDOM/CDOM index is calculated as follows: The fluorescence intensity (I_{ij}) at each excitation wavelength (Ex_i) of the EEM matrix is divided by the corresponding absorption coefficient (a_i) obtained from the absorption measurements. This is repeated for all emission wavelengths (Emj) (a_i x j times), thus yielding the ratio I_{ij}/a_i i.e. the FDOM/CDOM (R.U.m) index, in the form of a 3-dimensional matrix where Ex=250-450nm and Em=260-550nm

Table S3 Absorption coefficients $a_{(\lambda)}$ (m^{-1}) and spectral slope $S_{275-295}$ (nm^{-1}) for the SML and ULW samples

Sampling date	**a_{265} (m^{-1})**		**a_{280} (m^{-1})**		**a_{300} (m^{-1})**		**a_{370} (m^{-1})**		**$S_{275-295}$ (nm^{-1})**	
	SML	*ULW*	*SML*	*ULW*	*SML*	*ULW*	*SML*	*ULW*	*SML*	*ULW*
2/06/2016	-	2.546	-	1.810	-	0.979	-	0.198	-	0.031
16/06/2016	5.002	1.102	3.719	0.748	2.403	0.367	0.892	0.083	0.023	0.035
1/07/2016	12.29	1.372	9.429	0.921	6.362	0.483	2.896	0.122	0.020	0.033
2/08/2016	4.992	1.219	3.635	0.810	2.133	0.421	0.695	0.121	0.026	0.034
18/08/2016	4.073	0.910	3.282	0.599	1.991	0.282	0.686	0.090	0.023	0.037
6/09/2016	5.852	1.424	4.293	0.964	2.666	0.451	0.777	0.084	0.023	0.036

21/09/2016	5.761	0.953	4.180	0.635	2.452	0.306	0.766	0.062	0.027	0.037
7/10/2016	2.552	1.890	1.845	1.474	1.017	0.740	0.291	0.140	0.029	0.030
21/10/2016	4.898	1.406	3.633	0.927	2.216	0.434	0.693	0.092	0.024	0.037
3/11/2016	2.564	1.313	1.815	0.853	1.021	0.391	0.329	0.070	0.029	0.038
18/11/2016	7.402	1.109	5.757	0.724	3.741	0.327	1.466	0.073	0.021	0.039
2/12/2016	6.339	1.248	4.794	0.843	3.031	0.418	1.208	0.096	0.023	0.035
20/12/2016	5.923	1.506	4.419	1.035	2.538	0.560	0.829	0.157	0.028	0.031
4/01/2016	3.006	0.956	2.211	0.653	1.223	0.302	0.404	0.060	0.030	0.036
28/01/2017	4.948	1.161	3.925	0.803	2.286	0.404	0.740	0.099	0.025	0.034
9/02/2017	1.772	1.790	1.304	1.418	0.758	0.685	0.251	0.119	0.027	0.031
22/02/2017	2.119	1.254	1.531	0.897	0.852	0.528	0.270	0.184	0.030	0.027
7/03/2017	4.651	1.147	3.536	0.780	2.335	0.425	0.894	0.090	0.021	0.030
3/04/2017	1.591	0.905	1.119	0.621	0.569	0.338	0.138	0.103	0.034	0.031
25/04/2017	3.443	1.403	2.610	0.963	1.592	0.530	0.635	0.140	0.026	0.030
4/05/2017	12.91	1.116	12.73	1.084	9.347	0.638	5.877	0.202	0.015	0.027
10/06/2017	6.264	1.682	4.965	1.197	3.332	0.700	1.453	0.174	0.021	0.026
Average	4.376	1.337	3.293	0.944	2.565	0.487	0.706	0.116	0.025	0.033
Standard Deviation	1.725	0.381	1.349	0.303	0.908	0.173	0.381	0.044	0.004	0.004
CV (%)	39.4	28.5	41.0	32.1	45.2	35.5	54.0	37.5	16.7	11.6

Table S4. Enrichment Factors (EFs) of DOC, absorption coefficients (a_i) and fluorescence intensities (I_{1-4}) of the identified PARAFAC components (all EFs are significantly greater than unity, $p<0.05$). Average values and ranges in parentheses.

	All (July 2016 and May 2017 excluded)	**July 2016**	**May 2017**
DOC	2.7 (1.3 - 4.3)	7.2	8.1
a_{265}	3.6 (1.5 - 4.8)	8.2	13.3
a_{280}	3.8 (1.6 - 5.4)	10.2	13.5

a_{300}	4.8 (1.8 - 7.0)	12.7	17.8
a_{370}	7.4 (2.3 - 13.0)	22.4	37.1
I1	4.2 (2.8 - 5.7)	10.9	24.3
I2	4.5 (2.1 - 6.7)	25.0	18.5
I3	3.4 (2.2 - 4.8)	110.9	33.7
I4	2.8 (1.1 - 5.9)	9.7	16.6

Table S5. Parameter estimates for the selected generalized linear models (GLMs). Intercept terms and parameter estimates (B) are presented together with their standard errors (SE), Wald χ^2 statistics, and associated p values for all predictors retained in the selected models.

Response	**Predictor**	**B**	**SE**	**Wald χ^2**	**p**
a300	Intercept	-1.252	0.0892	197.087	<0.001
	DOC	0.507	0.0706	51.443	<0.001
	Layer	0.595	0.1399	18.083	<0.001
$S_{275-295}$	Intercept	-3.129	0.0608	2645.923	<0.001
	a300	-0.618	0.1283	23.200	<0.001
	Layer	-0.285	0.0745	14.595	<0.001
	a300 x Layer	0.493	0.1298	14.399	<0.001
I1	Intercept	-4.007	0.0618	4208.789	<0.001
	a300	0.348	0.0633	30.203	<0.001
	Layer	0.727	0.1217	35.609	<0.001
I2	Intercept	-4.063	0.0737	3042.595	<0.001
	a300	0.231	0.0741	9.673	0.002
	Layer	1.085	0.1447	56.274	<0.001
I3	Intercept	-4.242	0.0820	2677.384	<0.001
	a300	0.328	0.0853	14.741	<0.001
	Layer	0.582	0.1622	12.885	<0.001
I4	Intercept	-4.547	0.2127	456.964	<0.001
	a300	0.587	0.1407	17.374	<0.001

Table S6. Diagnostic summary for the selected generalized linear models (GLMs). Maximum absolute standardized deviance residuals and Cook's distance values are shown for each selected model. Standardized deviance residuals were examined to identify potential departures from model assumptions, with values exceeding |2| considered noteworthy and values exceeding |3| considered indicative of possible outliers. Cook's distance was used to assess observation influence, with values greater than 4/n (0.111; n = 36) considered potentially influential and values approaching or exceeding 0.5 considered indicative of substantial influence. Several models contained observations with standardized deviance residuals slightly greater than |2| and Cook's distance values exceeding the 4/n threshold; however, no standardized deviance residual exceeded |2.5| and no Cook's distance value exceeded 0.25. These results indicate adequate model fit and the absence of highly influential observations.

Model	Max std. deviance residual	Max Cook's distance
a300 ~ DOC + layer	2.127	0.164
$S_{275\text{-}295}$ ~ a300 + layer + a300 x layer	2.052	0.163
I1 ~ a300 + layer	2.113	0.172
I2 ~ a300 + layer	2.271	0.212
I3 ~ a300 + layer	2.435	0.233
I4 ~ a300	2.230	0.190

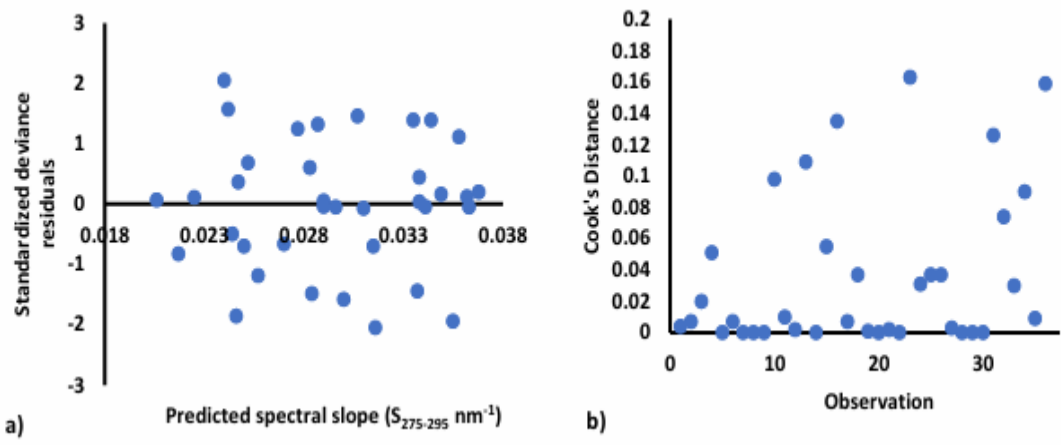

Fig. S2. Diagnostic evaluation of the selected generalized linear model describing the relationship between spectral slope ($S_{275–295}$), CDOM absorption coefficient at 300 nm (a300), water layer (SML, ULW), and their interaction. (a) Standardized deviance residuals plotted against predicted values. (b) Cook's distance values for individual observations.

Table S7. Maximum fluorescence intensities (I_{1-4}) (R.U.) of the 4 components resolved by the PARAFAC seawater model.

Sampling date	**I_1 (R.U.)**		**I_2 (R.U.)**		**I_3 (R.U.)**		**I_4 (R.U.)**	
	SML	*ULW*	*SML*	*ULW*	*SML*	*ULW*	*SML*	*ULW*
2/06/2016	0.140	0.019	0.099	0.017	0.083	0.013	0.126	0.011
16/06/2016	0.056	0.022	0.051	0.019	0.050	0.016	0.024	0.037
1/07/2016	0.241	0.027	0.429	0.023	1.249	0.016	0.141	0.016
2/08/2016	0.083	0.018	0.073	0.017	0.064	0.009	0.051	0.009
18/08/2016	0.068	0.014	0.065	0.014	0.053	0.008	0.106	0.011
6/09/2016	0.080	0.017	0.060	0.015	0.056	0.007	0.058	0.017
21/09/2016	0.087	0.022	0.075	0.021	0.052	0.017	0.048	0.017
7/10/2016	0.051	0.036	0.046	0.035	0.039	0.036	0.022	0.046
21/10/2016	0.098	0.016	0.092	0.017	0.072	0.015	0.057	0.012

3/11/2016	0.045	0.026	0.047	0.024	0.030	0.021	0.032	0.013
18/11/2016	0.106	0.017	0.093	0.016	0.058	0.011	0.035	0.003
2/12/2016	0.112	0.027	0.106	0.022	0.075	0.022	0.041	0.009
20/12/2016	0.100	0.031	0.136	0.021	0.064	0.025	0.036	0.009
4/01/2016	0.086	0.016	0.110	0.021	0.048	0.018	0.027	0.022
28/01/2017	0.112	0.017	0.116	0.019	0.078	0.018	0.080	0.014
9/02/2017	0.038	0.023	0.038	0.020	0.039	0.021	0.020	0.009
22/02/2017	0.061	0.025	0.093	0.019	0.032	0.011	0.001	0.011
7/03/2017	0.095	0.015	0.077	0.010	0.044	0.013	0.012	0.007
3/04/2017	0.033	0.020	0.051	0.019	0.016	0.016	0.002	0.004
25/04/2017	0.067	0.021	0.085	0.015	0.040	0.015	0.021	0.004
4/05/2017	0.398	0.020	0.315	0.017	0.394	0.013	0.196	0.013
10/06/2017	0.101	0.017	0.117	0.014	0.057	0.010	0.048	0.004
Average	0.081	0.081	0.053	0.045	0.122	0.019	0.016	0.014
Standard Deviation	0.028	0.028	0.017	0.031	0.006	0.005	0.006	0.010
CV (%)	34.8	34.0	32.8	70.4	27.0	26.6	40.4	76.5

Table S8. Rainwater data of DOC (mg L^{-1}), absorbance coefficients a_i (m^{-1}) and maximum fluorescence intensities (I_{1-3}) (R.U.) of the 3 components resolved by the PARAFAC rainwater model.

Sampling date	**DOC (mg L^{-1})**	**a_{265} (m^{-1})**	**a_{280} (m^{-1})**	**a_{300} (m^{-1})**	**a_{370} (m^{-1})**	***$S_{275-295}$*** (nm^{-1})	**I_1 (R.U.)**	**I_2 (R.U.)**	**I_3 (R.U.)**
15/12/2016	5.745	16.26	12.81	8.001	2.361	0.025	0.786	0.389	0.203
28-29/12/2016	2.494	5.128	4.123	2.424	0.734	0.026	0.374	0.126	0.223
09-10/01/2017	3.471	11.99	9.381	6.049	1.659	0.022	1.091	0.302	0.336
15/01/2017	1.238	4.645	3.580	2.396	0.683	0.021	0.375	0.134	0.101
24/01/2017	2.798	4.689	3.826	2.287	0.567	0.023	0.315	0.138	0.197
07/02/2017	1.257	7.115	6.258	3.567	0.741	0.023	0.453	0.295	0.381
08/02/2017	0.681	2.219	1.733	1.124	0.393	0.023	0.162	0.065	0.071
07/03/2017	6.266	16.50	12.82	8.070	2.331	0.023	0.741	0.376	0.457
08-09/03/2017	0.596	2.895	2.432	1.465	0.452	0.023	0.120	0.057	0.145
09/03/2017	1.186	3.381	2.869	1.707	0.537	0.023	0.192	0.072	0.186
11/03/2017	-	2.186	2.081	0.931	0.161	0.030	0.108	0.025	0.123
18/05/2017	3.463	10.09	7.871	4.658	1.368	0.025	0.297	0.187	0.223
21/05/2017	0.886	2.611	2.063	1.361	0.367	0.021	0.114	0.074	0.056
22/05/2017	2.281	7.947	5.965	3.486	0.871	0.026	0.156	0.090	0.082
Average	2.489	6.976	5.558	3.395	0.945	0.024	0.377	0.166	0.199
Standard Deviation	1.851	4.969	3.831	2.431	0.711	0.002	0.299	0.123	0.120
CV (%)	74.4	71.2	68.9	71.6	75.3	10.0	79.2	74.2	60.5