

Fluorescence spectroscopic characterisation of algal organic matter: towards improved in-situ fluorometer development

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Table S1: Characteristics of bloom forming species

Characteristics	<i>Dolichospermum circinalis</i>	<i>Cylindrospermopsis raciborskii</i>	<i>Microcystis aeruginosa</i>				<i>Chlorella vulgaris</i>
Strain	CS-533/02	CS-508	CS-555	CS-554	CS-564	CS-566	CS-42/7
Type	Cyanobacteria	Cyanobacteria	Cyanobacteria	Cyanobacteria	Cyanobacteria	Cyanobacteria	Algae
Geometric shape	Filamentous	Chained filaments (Trichomes)	Sphere	Sphere	Sphere	Sphere	Sphere
Dimensions	L = 2-3 μm ; W = 2-3 μm	L = 50-300 μm , W = 1.7–4.2 μm	D = 4-6 μm	D = 4-6 μm	D = 4-6 μm	D = 4-6 μm	D = 2-10 μm
Fluorescent pigment	Phycocyanin Chlorophyll-a	Phycocyanin Chlorophyll-a	Phycocyanin Chlorophyll-a	Phycocyanin Chlorophyll-a	Phycocyanin Chlorophyll-a	Phycocyanin Chlorophyll-a	Chlorophyll-a
Strain origin	Canning river, Perth	Townsville, North Queensland	Lake burley, Griffin	Irrigation canal, Griffith	St Marys STP, TAS	Werribee, STP, Victoria	Unknown
Toxicity	Below detection	Non-toxic	Toxic	below detection	below detection	Toxic	Non-toxic

Table S2: Comparisons between individual models versus the unified model

Component	C 1	C 2	C 3	C 4	C 5	C 6
MA555	0.99/0.99*	0.97/0.98	0.97/0.99		0.97/0.95	0.99/0.97
MA564	0.96/0.98	1.00/0.93	1.00/0.86	0.95/0.94	1.00/0.97	
MA554	1.00/0.99		0.95/0.94	0.91/0.72	1.00/0.52	0.90/0.70
MA566	1.00/0.81	1.00/0.85	0.95/0.94	0.91/0.71	0.99/0.90	
DC	0.99/0.89	0.96/0.93	0.96/0.94	0.92/0.91	0.98/0.87	0.97/0.86
CV	0.82/0.67	0.95/0.92	0.94/0.92	0.91/0.87	0.97/0.85	
CR		0.96/0.94	0.97/0.94	0.98/0.96	0.95/0.94	0.95/0.96

* Correspondence is indicated by Tucker correlation coefficients for excitation/emission spectra

Table S3A: Statistical analysis for the AOM properties of algae and cyanobacterial species two-way ANOVA (*p* value analysis) with $\alpha=0.01$

	DOC	DC	CR	CV	MA555	MA554	MA564	MA566
C1	0.156	0.42	0.14	0.39	0.23	0.002	0.007	0.004
C2	0.0002	0.02	0.004	0.01	0.001	0.35	0.21	0.74
C3	0.0008	0.01	0.006	0.003	0.004	0.69	0.35	0.65
C4	0.001	0.31	0.61	0.2	0.53	0.013	0.001	0.001
C5	0.120	0.26	0.26	0.19	0.31	0.45	0.34	0.48
C6	0.004	0.73	0.74	0.23	0.47	0.37	0.26	0.56
Normalised C1	0.120	0.21	0.11	0.16	0.19	0.006	0.003	0.002
Normalised C2	0.004	0.001	0.003	0.003	0.0006	0.54	0.19	0.39
Normalised C3	0.006	0.004	0.002	0.002	0.002	0.32	0.28	0.47
Normalised C4	0.005	0.13	0.24	0.14	0.46	0.001	0.0007	0.003
Normalised C5	0.07	0.17	0.16	0.16	0.62	0.16	0.46	0.29
Normalised C6	0.002	0.32	0.35	0.52	0.37	0.18	0.71	0.34
C1: (C2+C4)	0.11	-	-	-	-	-	-	-
C2:C4	0.02	-	-	-	-	-	-	-
C2:C1	0.004	-	-	-	-	-	-	-
C3:C2	0.004	-	-	-	-	-	-	-

Table S3B: Statistical analysis between PARAFAC component and LC-OCD fractions two-way ANOVA (*p* value analysis) with $\alpha=0.01$

	C1	C2	C3	C4	C5	C6
Biopolymers	0.78	0.85	0.002	0.47	0.43	0.0006
Proteins	0.63	0.36	0.003	0.24	0.51	0.003
Polysaccharides	0.58	0.24	0.41	0.36	0.85	0.14
BBlocks	0.64	0.16	0.94	0.79	0.76	0.16
LMW acids	0.23	0.54	0.14	0.26	0.18	0.001

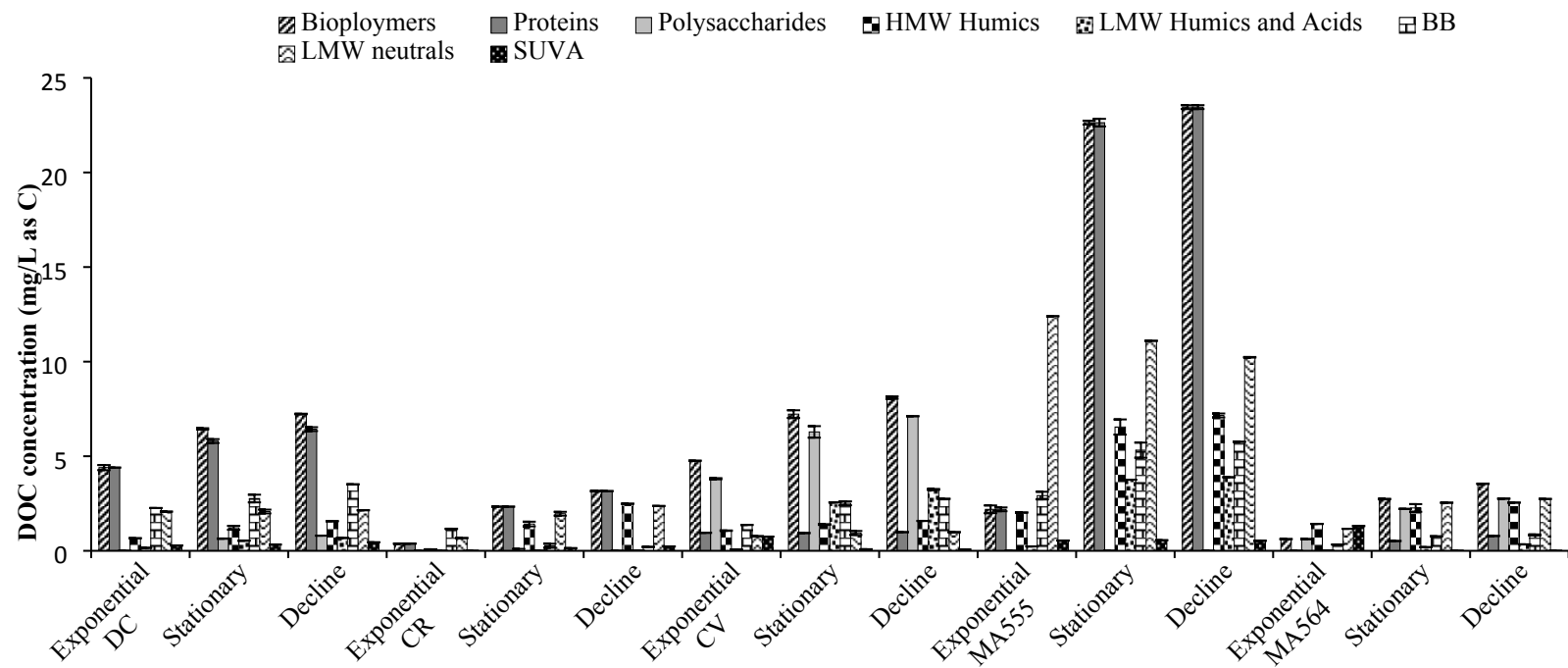


Figure S1: AOM composition of (i) DC (ii) CR (iii) CV (iv) MA555) and (v) MA564 at different growth phases

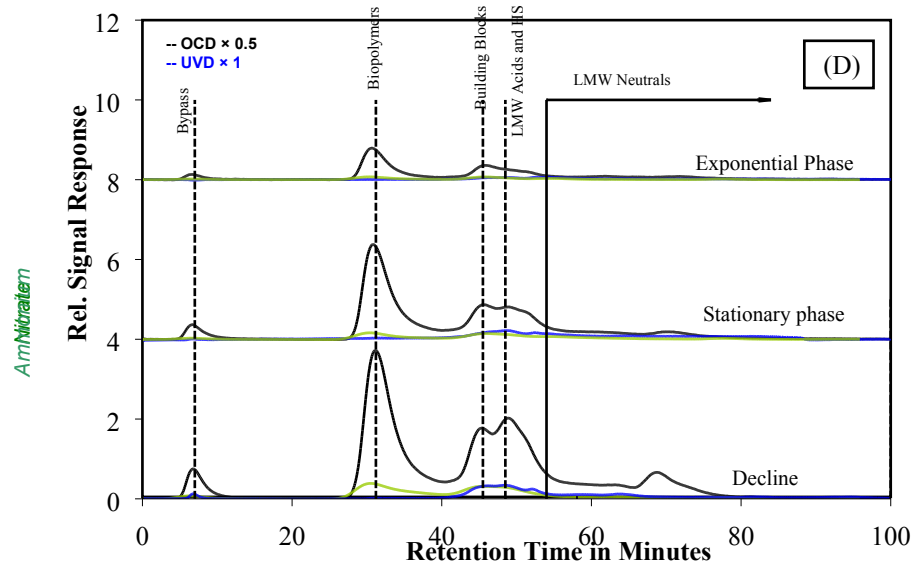
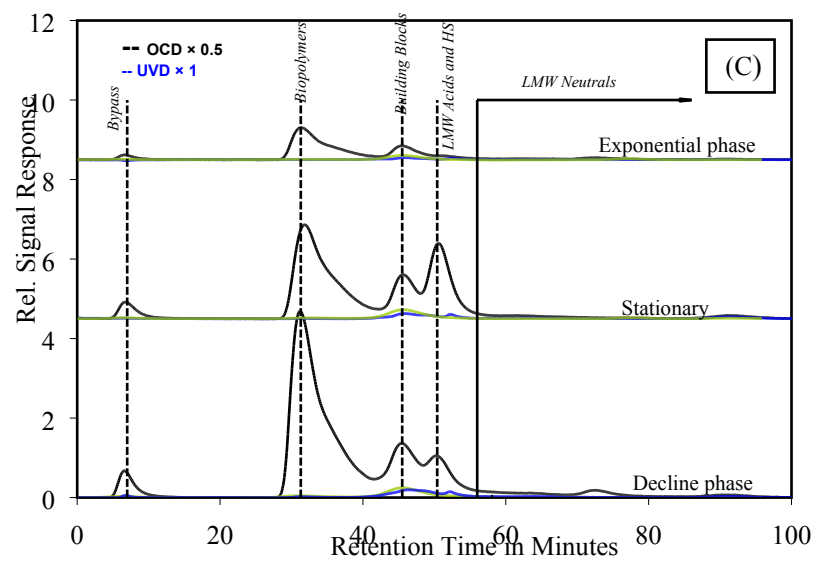
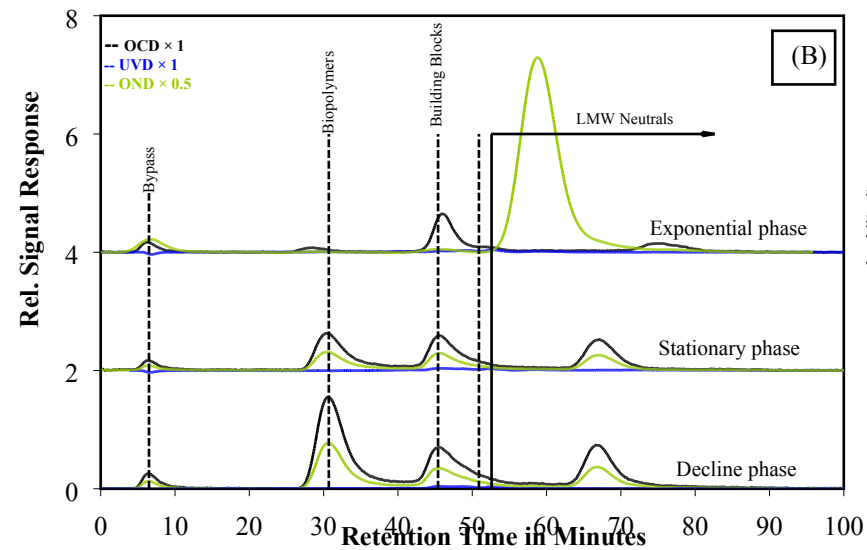
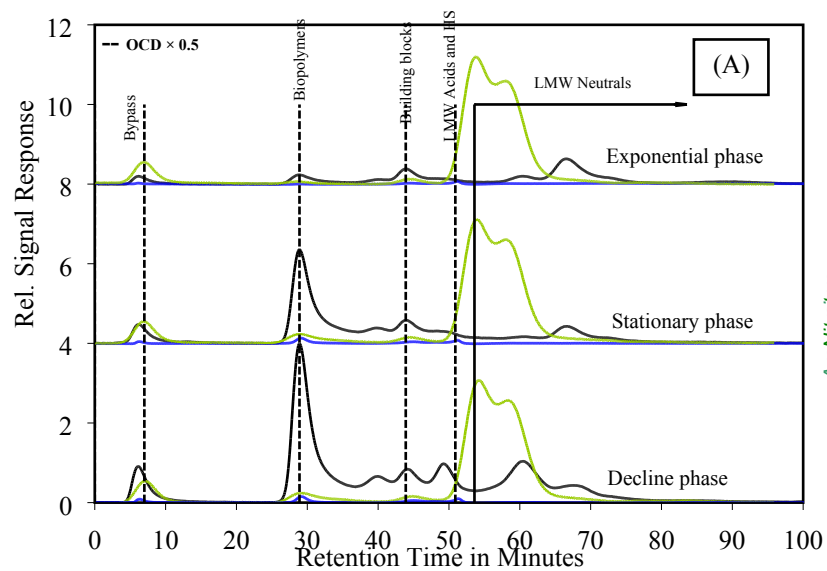


Figure S2: LC-OCD chromatograms of AOM from (A) MA555 (B) CR (C) CV and (D) DC at different growth phase

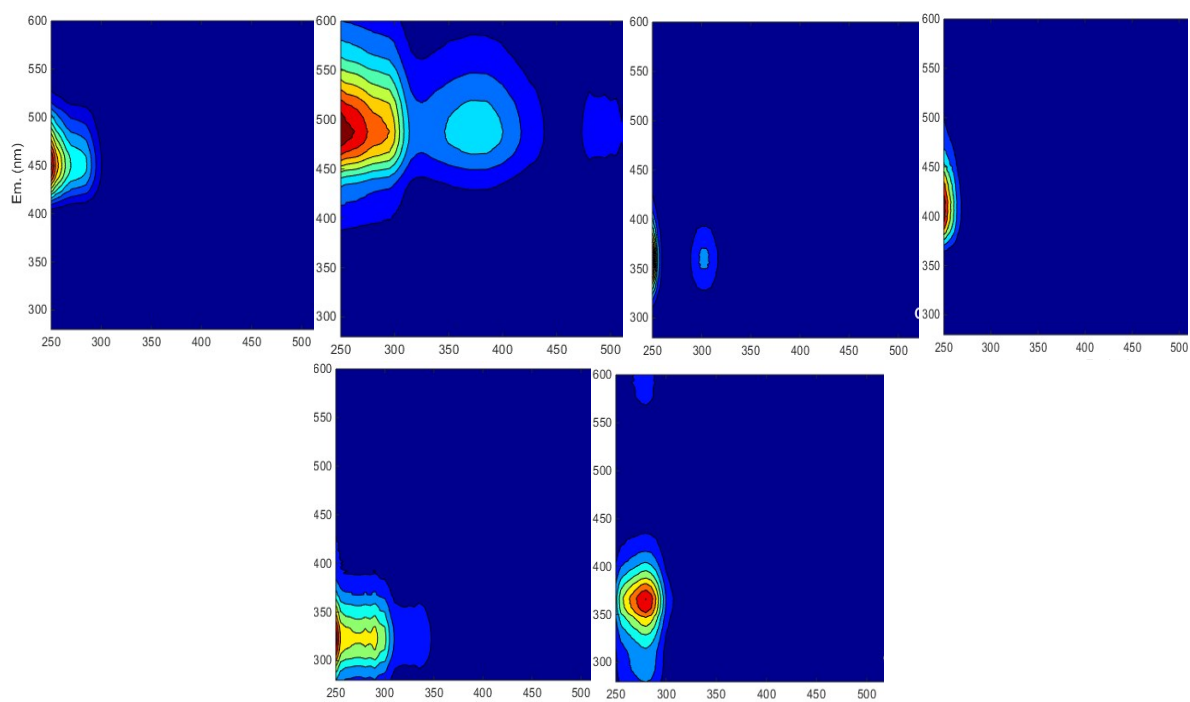


Figure S3: Contour plots of the six AOM components identified from the complete F-EEMs dataset

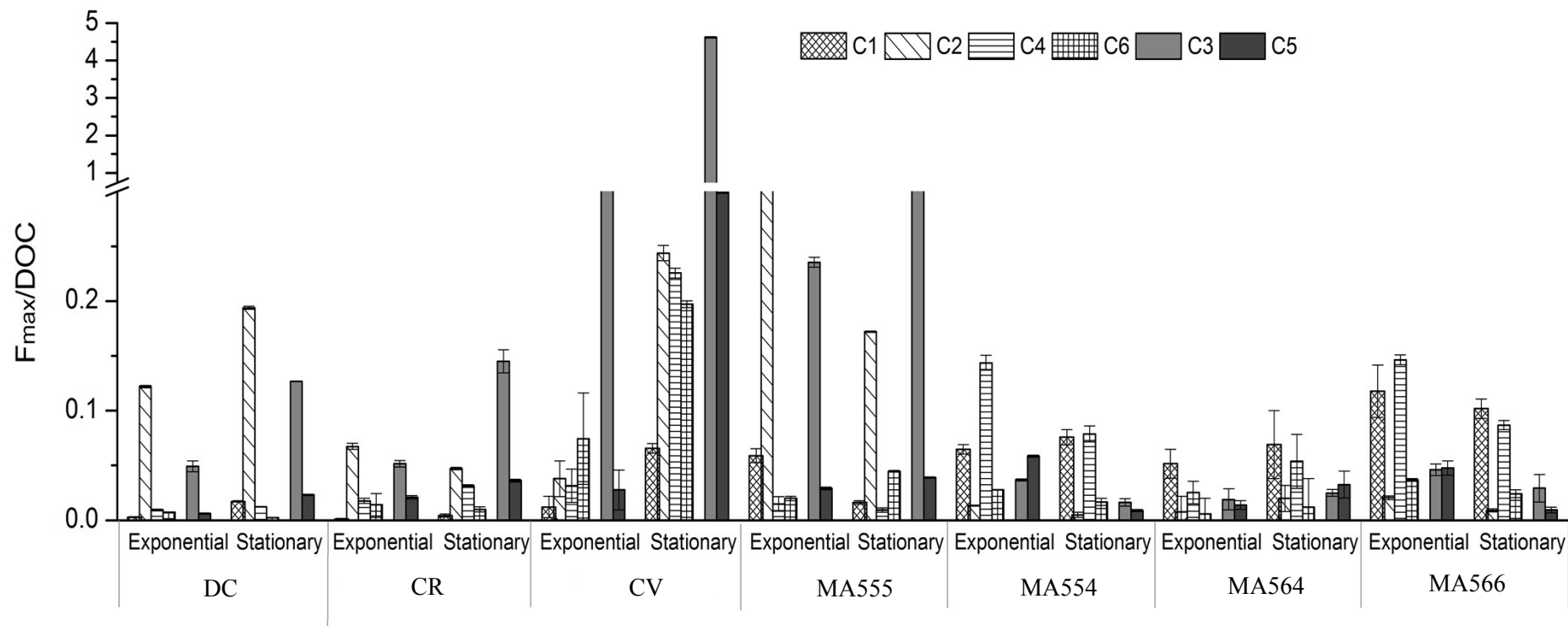


Figure S4: Normalized fluorescence intensity of observed AOM components along the growth phase of species

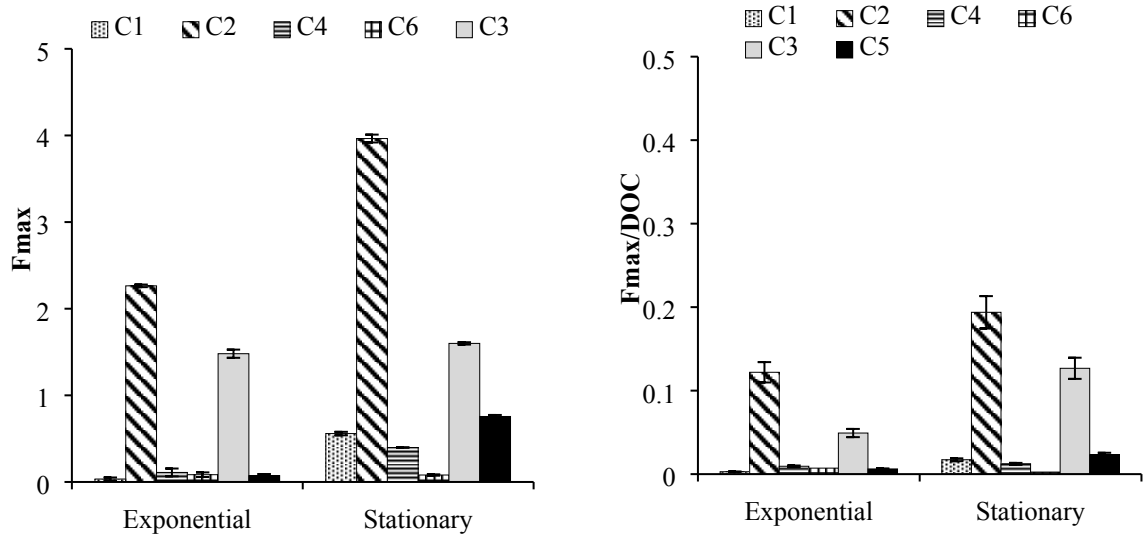


Figure S5: F_{max} and F_{max}/DOC for DC for observed AOM components

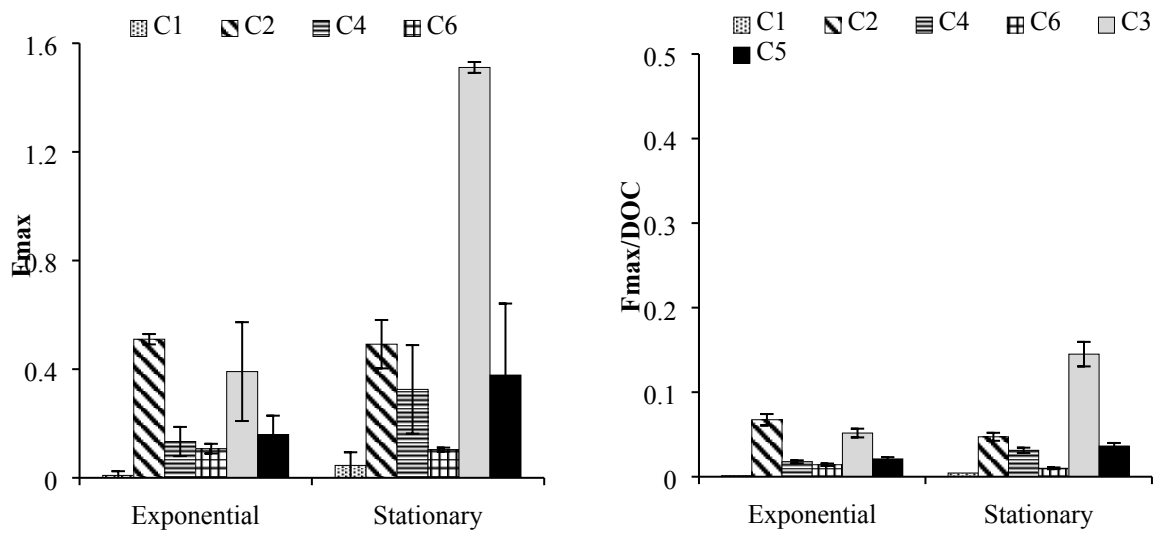


Figure S6: F_{max} and F_{max}/DOC for CR for observed AOM components

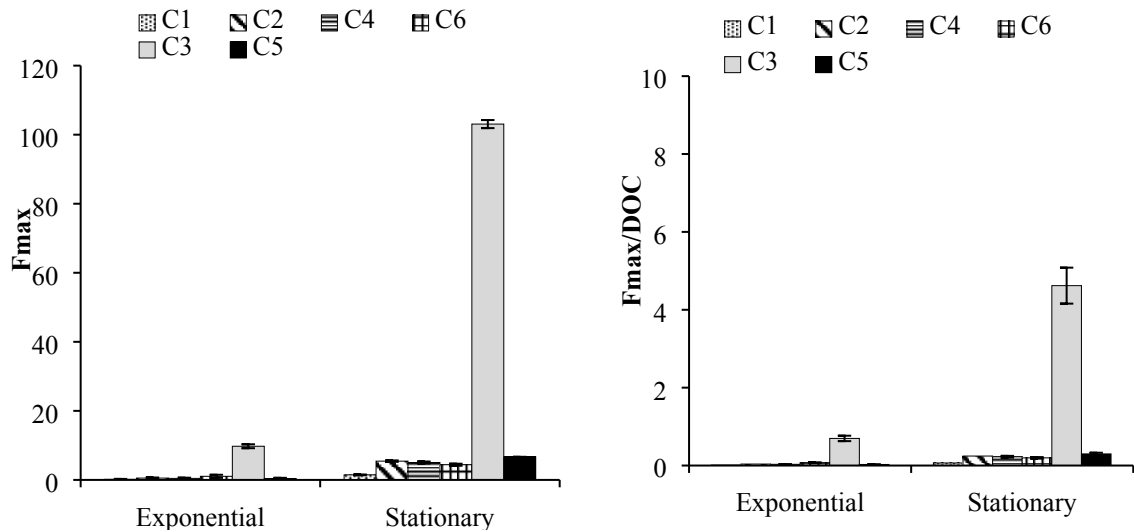


Figure S7: F_{max} and F_{max}/DOC for CV for observed AOM components

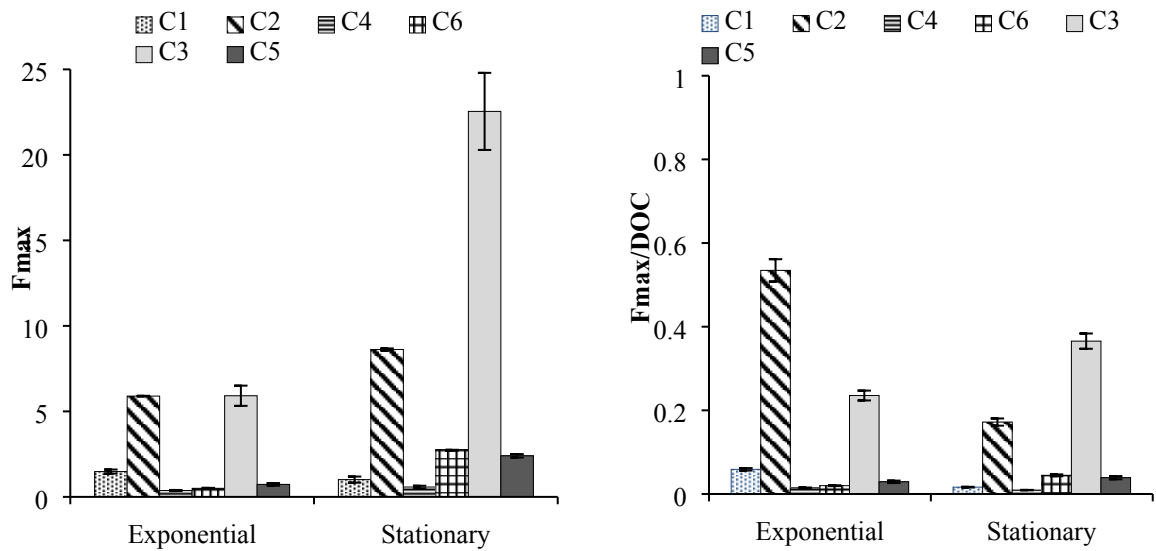


Figure S8: F_{max} and F_{max}/DOC for MA555 for observed AOM components

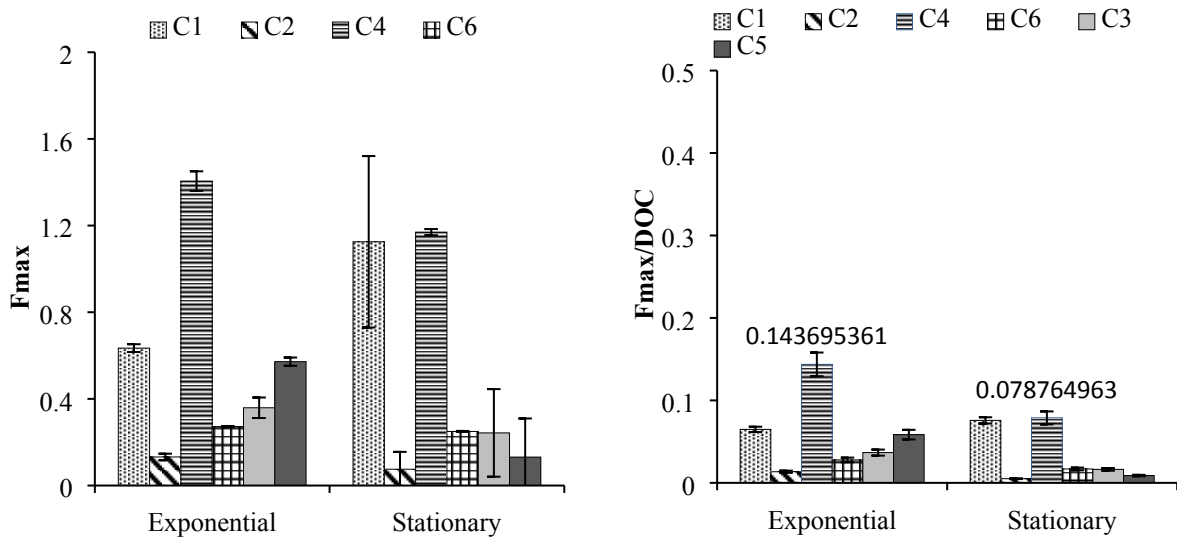


Figure S9: F_{max} and F_{max}/DOC for MA554 for observed AOM components

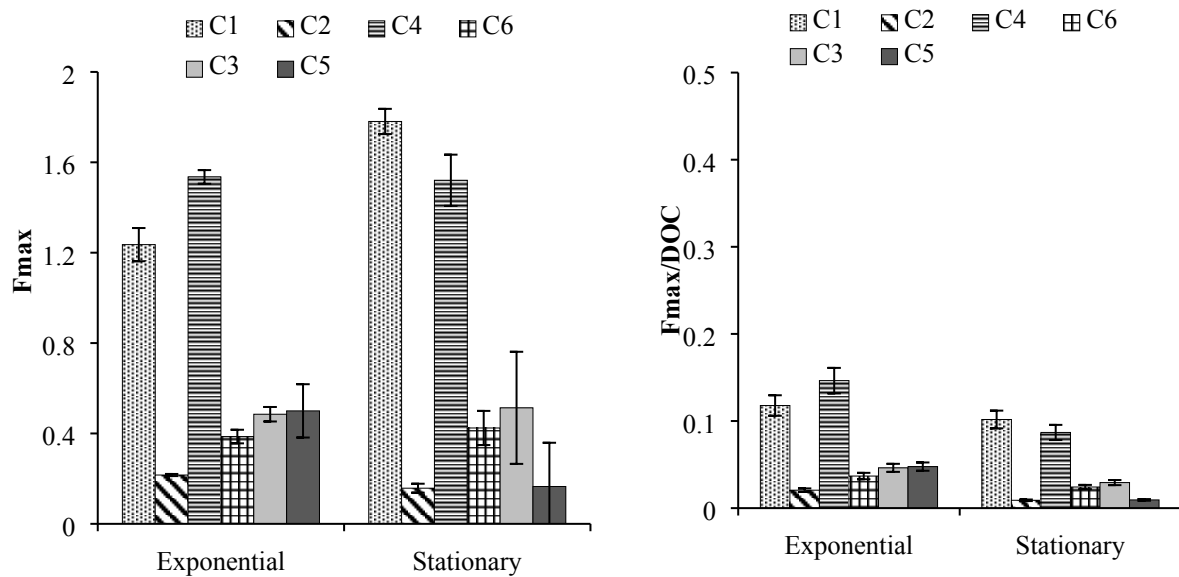


Figure S10: F_{max} and F_{max}/DOC for MA566 for observed AOM components

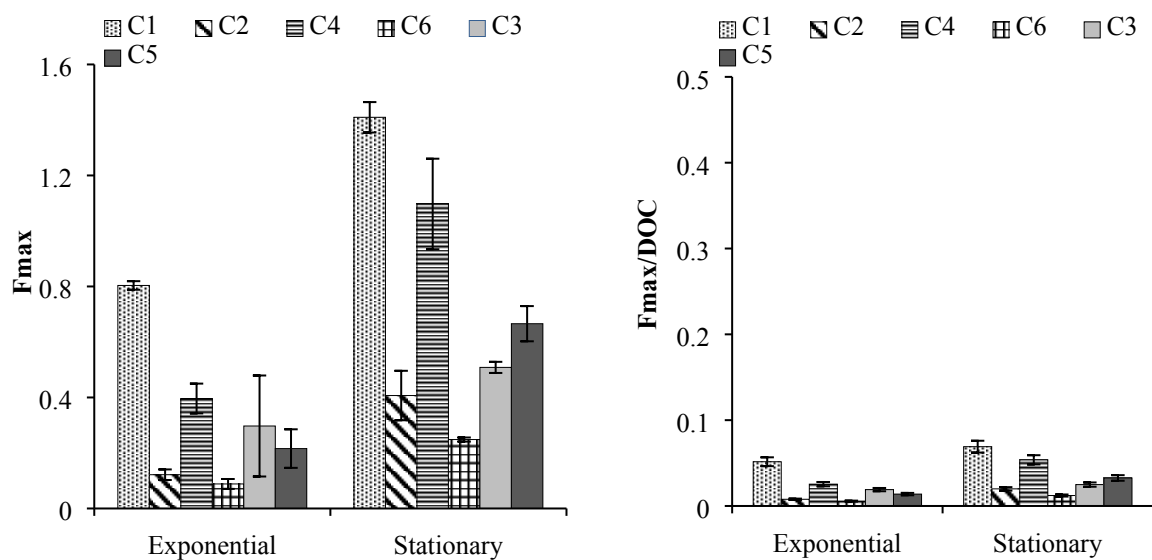


Figure S11: F_{max} and F_{max}/DOC for MA564 for observed AOM components

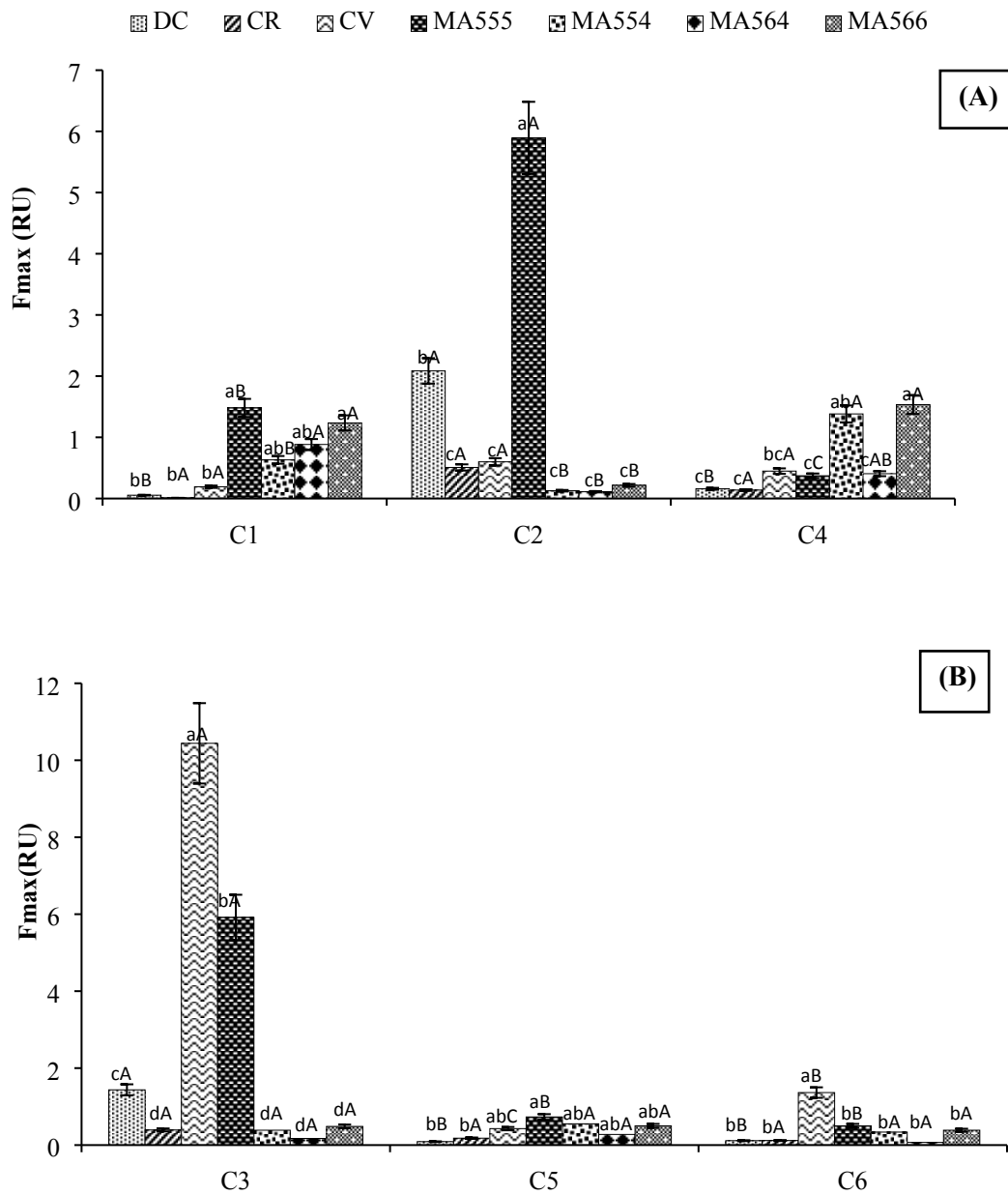


Figure S12 (A & B): Interaction averages of observed fluorophores during exponential phase

For statistical comparison of means, same upper-case letters indicate no significant effect of changes in AOM fluorophores for a same species, and same lower-case letters indicate no significant difference among species for a particular AOM component

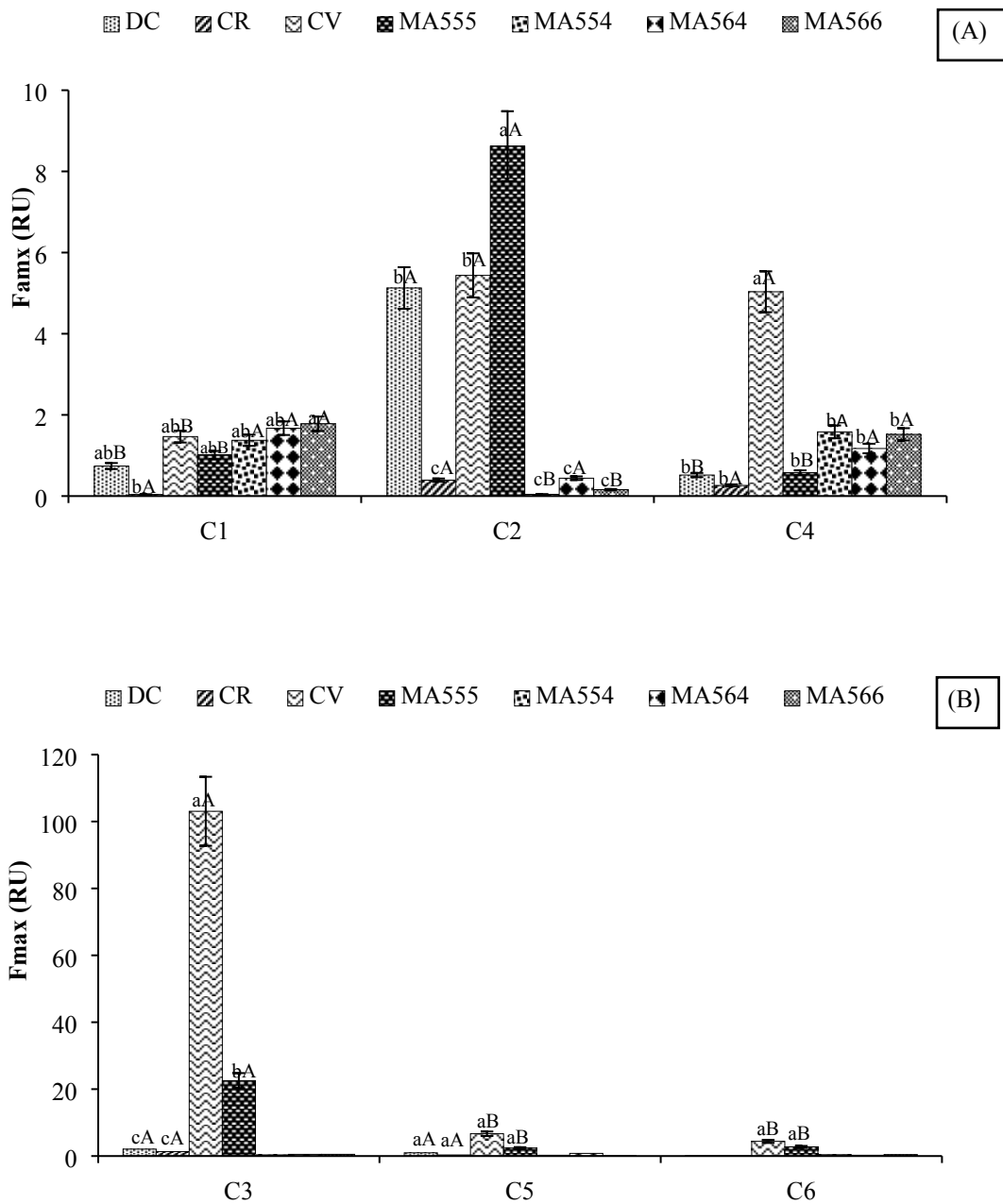


Figure S13 (A & B): Interaction averages of observed AOM components during stationary phase

For statistical comparison of means, same upper-case letters indicate no significant effect of changes in AOM fluorophores for a same species, and same lower-case letters indicate no significant difference among species for a particular AOM component

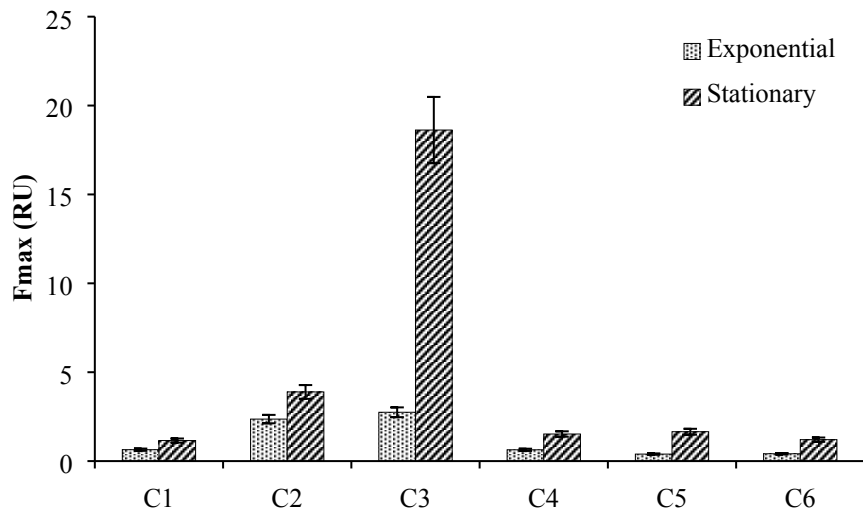


Figure S14: Single factor averages of observed AOM components (C1-C6) across exponential and stationary phase