Supplementary information

Seasonal plasticity of the polar lipidome of *Ulva rigida* cultivated in a sustainable integrated multi-trophic aquaculture

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Table S1. Glycolipids identified by LC–MS and MS/MS on *Ulva rigida* samples collected during winter, spring, summer and autumn (mass error < 5 ppm). Observed *m/z* and respective error were checked for all samples, but those presented were obtained from one summer sample. Numbers in parenthesis (C:N) indicate the number of carbon atoms (C) and double bonds (N) in the fatty acyl chains. *, Molecular species identified only by retention time and mass accuracy.

Lipid species (C:N)	Theoretical *m/z*	Observed *m/z*	Error (ppm)	Fatty acyl chain(s)	Formula
MGMG identified as $[M + NH_4]^+$					
MGMG (16:4)	502.3016	502.3015	-0.2170	(16:4)	C25H44NO9
MGMG (16:3)	504.3173	504.3168	-0.9101	(16:3)	C25H46NO9
MGMG (16:2)	506.3329	506.3332	0.5747	(16:2)	C25H48NO9
MGMG (16:1)	508.3486	508.3488	0.4741	(16:1)	C25H50NO9
MGMG (16:0)	510.3642	510.3642	0.0000	(16:0)	C25H52NO9
MGMG (18:4)	530.3329	530.3330	0.1716	(18:4)	C27H48NO9
DGMG identified as $[M + NH_4]^+$					
DGMG (14:0)	644.3857	644.3877	3.0510	(14:0)	C29H58NO14
DGMG (16:4)	664.3544	664.3549	0.7014	(16:4)	C31H54NO14
DGMG (16:3)	666.3701	666.3683	-2.6772	(16:3)	C31H56NO14
DGMG (16:2)	668.3857	668.3860	0.3980	(16:2)	C31H58NO14
DGMG (16:1)	670.4014	670.4021	1.0680	(16:1)	C31H60NO14
DGMG (16:0)	672.4170	672.4178	1.1897	(16:0)	C31H62NO14
MGDG identified as $[M + NH_4]^+$					
MGDG (32:8)	732.4687	732.4682	-0.6826	(16:4/16:4)	C41H66NO10
MGDG (32:7)	734.4843	734.4838	-0.6807	(16:4/16:3)	C41H68NO10
MGDG (32:5)	738.5156	738.5146	-1.3866	(16:4/16:1)	C41H72NO10
MGDG (32:4)	740.5307	740.5316	1.2153	(16:4/16:0) and (16:3/16:1)	C41H74NO10
MGDG (34:8)	760.5000	760.5005	0.6917	(18:4/16:4)	C43H70NO10
MGDG (34:3)	770.5782	770.5779	-0.4205	(18:3/16:0) and (18:2/16:1)	C43H80NO10
MGDG (36:9)	786.5156	786.5153	-0.3814	(20:5/16:4)	C45H72NO10
MGDG (36:8)	788.5313	788.5297	-1.9910	(18:4/18:4)	C45H74NO10
MGDG (36:7)	790.5469	790.5465	-0.5060	(18:4/18:3)	C45H76NO10
DGDG identified as $[M + NH_4]^+$					
DGDG (32:1)	908.6310	908.6290	-2.2011	(16:1/16:0) and (18:1/14:0)	C47H90O15N
DGDG (32:0)	910.6467	910.6496	3.1846	(16:0/16:0)	C47H92O15N
DGDG (34:8)	922.5528	922.5533	0.5420	(18:4/16:4)	C49H80O15N
DGDG (34:6)	926.5841	926.5826	-1.6188	*	C49H84O15N
DGDG (34:5)	928.5997	928.5979	-1.9384	*	C49H86O15N
DGDG (34:4)	930.6154	930.6140	-1.5044	*	C49H88O15N
DGDG (34:3)	932.6310	932.6307	-0.3217	(18:3/16:0)	C49H90O15N
DGDG (34:2)	934.6467	934.6439	-2.9958	(18:2/16:0)	C49H92O15N
DGDG (34:1)	936.6623	936.6611	-1.2811	(18:1/16:0)	C49H94O15N
DGDG (36:7)	952.5997	952.5999	0.2100	(18:3/18:4) and (20:5/16:2)	C51H86O15N
DGDG (36:6)	954.6154	954.6134	-2.0951	(18:3/18:3) and (18:2/18:4)	C51H88O15N
DGDG (36:5)	956.6310	956.6286	-2.5088	(18:2/18:3) and (18:1/18:4)	C51H90O15N
DGDG (36:4)	958.6467	958.6446	-2.1906	(18:1/18:3)	C51H92O15N

Table S1. [Continued]

SQMG identified as $[M - H]^-$					
SQMG (14:0)	527.2526	527.2538	2.2532	(14:0)	C23H43O11S
SQMG (16:1)	553.2683	553.2697	2.5991	(16:1)	C25H45O11S
SQMG (16:0)	555.2839	555.2851	2.1394	(16:0)	C25H47O11S
SQMG (18:3)	577.2683	577.2692	1.6249	(18:3)	C27H45O11S
SQMG (18:1)	581.2996	581.3013	2.9916	(18:1)	C27H49O11S
SQDG identified as $[M - H]^-$					
SQDG (28:0)	737.4510	737.4522	1.6584	(14:0/14:0) and (12:0/16:0)	C37H69O12S
SQDG (30:1)	763.4666	763.4668	0.2266	(14:0/16:1)	C39H71O12S
SQDG (30:0)	765.4823	765.4830	0.9445	(14:0/16:0)	C39H73O12S
SQDG (32:4)	785.4510	785.4520	1.3024	(18:4/14:0) and (16:4/16:0)	C41H69O12S
SQDG (32:3)	787.4666	787.4696	3.7754	(18:3/14:0) and (16:3/16:0)	C41H71O12S
SQDG (32:2)	789.4823	789.4844	2.6891	(18:2/14:0) and (16:2/16:0)	C41H73O12S
SQDG (32:1)	791.4979	791.4993	1.7347	(16:1/16:0) and (18:1/14:0)	C41H75O12S
SQDG (32:0)	793.5136	793.5149	1.6685	(16:0/16:0)	C41H77O12S
SQDG (34:7)	807.4353	807.4357	0.4620	(18:3/16:4)	C43H67O12S
SQDG (34:5)	811.4666	811.4693	3.2940	(20:5/14:0)	C43H71O12S
SQDG (34:4)	813.4823	813.4835	1.5034	(18:4/16:0)	C43H73O12S
SQDG (34:3)	815.4979	815.4993	1.6836	(18:3/16:0)	C43H75O12S
SQDG (34:1)	819.5292	819.5303	1.3093	(18:1/16:0)	C43H79O12S
SQDG (36:5)	839.4979	839.4989	1.1590	(20:5/16:0)	C45H75O12S
SQDG (36:4)	841.5136	841.5146	1.2169	(20:4/16:0) and (18:1/18:3)	C45H77O12S
SQDG (36:3)	843.5292	843.5256	-4.2998	(20:3/16:0)	C45H79O12S
SQDG (36:2)	845.5449	845.5463	1.6829	(20:2/16:0)	C45H81O12S
SQDG (36:1)	847.5605	847.5597	-0.9757	(18:0/18:1) and (20:1/16:0)	C45H83O12S
SQDG (38:5)	867.5292	867.5314	2.5048	(22:5/16:0)	C47H79O12S
SQDG (38:0)	877.6075	877.6083	0.9378	(22:0/16:0)	C47H89O12S

Table S2. Phospholipids identified by LC–MS and MS/MS of *Ulva rigida* samples collected during winter, spring, summer and autumn (mass error < 5 ppm). Observed *m/z* and respective error were checked for all samples, but those presented were obtained from one summer sample. Numbers in parenthesis (C:N) indicate the number of carbon atoms (C) and double bonds (N) in the fatty acyl chains. *, Molecular species identified only by retention time and mass accuracy. **, Molecular species identified by retention time, mass accuracy and MS/MS of $[M + H]^+$ ions.

Lipid species (C:N)	Theoretical *m/z*	Observed *m/z*	Error (ppm)	Fatty acyl chain(s)	Formula
PC identified as $[M + H]^+$ (determination of fatty acyl chains by MS/MS of $[M + CH_3COO]^-$)					
PC (30:0)	706.5387	706.5384	-0.3991	**	C38H77NO8P
PC (32:2)	730.5387	730.5381	-0.7967	(16:1/16:1)	C40H77NO8P
PC (34:3)	756.5543	756.5535	-1.0984	**	C42H79NO8P
PC (34:2)	758.5700	758.5690	-1.2945	**	C42H81NO8P
PC (34:1)	760.5856	760.5851	-0.6995	**	C42H83NO8P
PC (36:3)	784.5856	784.5861	0.5965	(18:1/18:2)	C44H83NO8P
PC (36:2)	786.6013	786.6006	-0.8670	(18:1/18:1)	C44H85NO8P
PC (38:6)	806.5700	806.5685	-1.8374	**	C46H81NO8P
PC (38:5)	808.5856	808.5853	-0.4106	**	C46H83NO8P
LPC identified as $[M + H]^+$ (determination of fatty acyl chains by MS/MS of $[M + CH_3COO]^-$)					
LPC (16:0)	496.3403	496.3397	-1.2411	(16:0)	C24H51NO7P
LPC (16:1)	494.3247	494.3248	0.2691	(16:1)	C24H49NO7P
LPC (18:1)	522.3560	522.3569	1.7861	(18:1)	C26H53NO7P
LPC (18:2)	520.3403	520.3386	-3.2978	(18:2)	C26H51NO7P
LPC (18:3)	518.3247	518.3241	-1.0939	**	C26H49NO7P
LPC (18:4)	516.3090	516.3080	-1.9698	**	C26H47NO7P
LPC (20:4)	544.3403	544.3405	0.3380	**	C28H51NO7P
LPC (20:5)	542.3247	542.3244	-0.4923	(20:5)	C28H49NO7P
LPC (22:6)	568.3403	568.3401	-0.3801	(22:6)	C30H51NO7P
PE identified as $[M - H]^-$					
PE (32:2)	686.4761	686.4755	-0.8740	**	C37H69O8NP
PE (32:1)	688.4917	688.4928	1.5977	**	C37H71NO8P
PE (34:2)	714.5074	714.5093	2.6592	**	C39H73NO8P
LPE identified as $[M - H]^-$					
LPE (16:0)	452.2777	452.2784	1.5101	*	C21H43NO7P
LPE (18:1)	478.2934	478.2943	1.9507	(18:1)	C23H45NO7P
LPE (20:4)	500.2777	500.2789	2.3647	(20:4)	C25H43NO7P
LPE (22:5)	526.2934	526.2947	2.5328	(22:5)	C27H45NO7P
PI identified as $[M - H]^-$					
PI (34:1)	835.5337	835.5330	-0.8378	(16:0/18:1)	C43H80O13P
PI (34:2)	833.5180	833.5171	-1.0798	(16:0/18:2)	C43H78O13P
PI (34:3)	831.5024	831.5024	0.0000	(16:0/18:3)	C43H76O13P
LPI identified as $[M - H]^-$					
LPI (16:0)	571.2883	571.2894	1.8520	(16:0)	C25H48O12P

Table S2. [Continued]

PG identified as [M - H]$^-$					
PG (30:1)	691.4550	691.4562	1.7355	(14:0/16:1)	C36H68O10P
PG (32:1)	719.4863	719.4872	1.2509	(16:0/16:1) and (14:0/18:1)	C38H72O10P
PG (32:2)	717.4707	717.4723	2.2301	(16:1/16:1)	C38H70O10P
PG (34:2)	745.5020	745.5035	2.0121	(16:1/18:1) and (16:0/18:2)	C40H74O10P
PG (34:3)	743.4863	743.4844	-2.5555	(16:1/18:2) and (16:0/18:3)	C40H72O10P
PG (34:4)	741.4707	741.4720	1.7533	(16:1/18:3)	C40H70O10P
PG (34:5)	739.4550	739.4569	2.5695	(16:1/18:4) and (16:2/18:3)	C40H68O10P
PG (36:2)	773.5333	773.5347	1.8099	(18:1/18:1)	C42H78O10P
PG (36:3)	771.5176	771.5200	3.1108	(18:1/18:2)	C42H76O10P
PG (36:5)	767.4863	767.4876	1.6938	(16:0/20:5), (16:1/20:4) and (18:2/18:3)	C42H72O10P
LPG identified as [M - H]$^-$					
LPG (16:0)	483.2723	483.2740	3.5218	(16:0)	C22H44O9P
LPG (16:1)	481.2566	481.2576	1.9782	(16:1)	C22H42O9P
LPG (18:1)	509.2879	509.2894	2.8510	(18:1)	C24H46O9P
LPG (18:3)	505.2566	505.2579	2.4779	(18:3)	C24H42O9P

Table S3. Betaine lipids identified by LC–MS and MS/MS of *Ulva rigida* samples collected during winter, spring, summer and autumn. Observed *m/z* and respective error were checked for all samples, but those presented were obtained from one summer sample. Numbers in parenthesis (C:N) indicate the number of carbon atoms (C) and double bonds (N) in the fatty acyl chains. [§], with contribution of sodium adducts.

Lipid species (C:N)	**Theoretical *m/z***	**Observed *m/z***	**Error (ppm)**	**Fatty acyl chain(s)**	**Formula**
DGTS identified as [M + H]$^+$					
DGTS (30:4)	676.5152	676.5149	-0.4434	(12:0/18:4) and (14:0/16:4)	C40H70O7N
DGTS (30:1)	682.5622	682.5621	-0.1465	(14:0/16:1)	C40H76O7N
DGTS (30:0)	684.5778	684.5784	0.8765	(14:0/16:0)	C40H78O7N
DGTS (32:4)	704.5465	704.5466	0.1419	(14:0/18:4) and (16:0/16:4)	C42H74O7N
DGTS (32:3)	706.5622	706.5605	-2.4060	(14:0/18:3), (16:0/16:3) and (16:1/16:2)	C42H76O7N
DGTS (32:2)	708.5778	708.5779	0.1411	(14:0/18:2), (16:1/16:1) and (16:0/16:2)	C42H78O7N
DGTS (32:1)	710.5935	710.5935	0.0000	(16:0/16:1) and (14:0/18:1)	C42H80O7N
DGTS (32:0)	712.6091	712.6092	0.1403	(16:0/16:0)	C42H82O7N
DGTS (34:7)	726.5309	726.5303	-0.7969	(16:4/18:3)[§]	C44H72O7N
DGTS (34:6)	728.5465	728.5467	0.2745	(16:2/18:4)	C44H74O7N
DGTS (34:5)	730.5622	730.5624	0.2738	(16:4/18:1), (16:2/18:3) and (16:1/18:4)	C44H76O7N
DGTS (34:4)	732.5778	732.5779	0.1365	(16:0/18:4)	C44H78O7N
DGTS (34:3)	734.5935	734.5920	-2.0419	(16:0/18:3)	C44H80O7N
DGTS (34:2)	736.6091	736.6079	-1.6291	(16:0/18:2) and (16:1/18:1)	C44H82O7N
DGTS (34:1)	738.6248	738.6244	-0.5415	(16:0/18:1)	C44H84O7N
DGTS (36:8)	752.5465	752.5465	-0.0266	(18:4/18:4)	C46H74O7N
DGTS (36:7)	754.5622	754.5609	-1.7229	(18:3/18:4)[§]	C46H76O7N
DGTS (36:6)	756.5778	756.5759	-2.5113	(18:3/18:3) and (18:2/18:4)	C46H78O7N

Table S3. [Continued]

DGTS (36:5)	758.5935	758.5934	-0.1318	(18:1/18:4)	C46H80O7N
DGTS (36:4)	760.6091	760.6076	-1.9721	(18:0/18:4), (18:1/18:3) and (16:0/20:4)	C46H82O7N
DGTS (36:2)	764.6404	764.6410	0.7847	(18:1/18:1)	C46H86O7N
DGTS (38:9)	778.5622	778.5619	-0.3853	(20:5/18:4) and (16:4/22:5)	C48H76O7N
DGTS (38:8)	780.5778	780.5763	-1.9217	(20:4/18:4) and (20:5/18:3)	C48H78O7N
DGTS (38:7)	782.5935	782.5917	-2.3000	(20:4/18:3) and (20:3/18:4)	C48H80O7N
DGTS (38:6)	784.6091	784.6099	1.0196	(16:1/22:5) and (20:5/18:1)	C48H82O7N
DGTS (38:5)	786.6248	786.6249	0.1271	(16:0/22:5) and (20:4/18:1)	C48H84O7N
DGTS (40:9)	806.5935	806.5939	0.4959	(22:5/18:4) and (20:5/20:4)	C50H80O7N
DGTS (40:8)	808.6091	808.6087	-0.4947	(22:5/18:3)	C50H82O7N
DGTS (40:7)	810.6248	810.6235	-1.6037	(22:5/18:2)	C50H84O7N
DGTS (40:6)	812.6404	812.6413	1.1075	(22:5/18:1)	C50H86O7N
DGTS (40:4)	816.6717	816.6729	1.4694	(22:0/18:4)	C50H90O7N
DGTS (42:10)	832.6091	832.6089	-0.2738	(22:5/20:5)	C52H82O7N
DGTS (44:10)	860.6404	860.6397	-0.8470	(22:5/22:5)	C54H86O7N
MGTS identified as $[M + H]^+$					
MGTS (14:0)	446.3482	446.3481	-0.1434	(14:0)	C24H48O6N
MGTS (16:4)	466.3169	466.3170	0.2916	(16:4)	C26H44O6N
MGTS (16:2)	470.3482	470.3486	0.9270	(16:2)	C26H48O6N
MGTS (16:1)	472.3638	472.3640	0.3938	(16:1)	C26H50O6N
MGTS (16:0)	474.3795	474.3794	-0.2108	(16:0)	C26H52O6N
MGTS (18:5)	492.3325	492.3307	-3.6845	(18:5)[§]	C28H46O6N
MGTS (18:4)	494.3482	494.3482	0.0728	(18:4)	C28H48O6N
MGTS (18:3)	496.3638	496.3626	-2.4458	(18:3)[§]	C28H50O6N
MGTS (18:1)	500.3951	500.3950	-0.2278	(18:1)	C28H54O6N
MGTS (20:5)	520.3638	520.3638	-0.0269	(20:5)	C30H50O6N
MGTS (20:4)	522.3795	522.3780	-2.8026	(20:4)[§]	C30H52O6N
MGTS (20:1)	528.4264	528.4261	-0.5942	(20:1)	C30H58O6N
MGTS (20:0)	530.4421	530.4423	0.4449	(20:0)	C30H60O6N
MGTS (22:5)	548.3951	548.3952	0.1568	(22:5)	C32H54O6N
MGTS (22:0)	558.4734	558.4735	0.2435	(22:0)	C32H64O6N

Table S4. Contribution (%) of each variable to principal components (PC) 1 and 2 of the PCA of fatty acids dataset, and respective change in PC1 and PC2 positive.

Fatty acids	PC1 contrib.	PC2 contrib.	PC1 change	PC2 change
14:0	0.7	16.3	none	DOWN
16:0	14.9	0.0	DOWN	none
16:1*n*-7	0.6	22.4	none	DOWN
16:1*n*-9	1.6	3.6	DOWN	UP
16:4*n*-3	14.3	0.5	UP	none
18:0	5.8	0.1	DOWN	none
18:1	1.1	5.2	DOWN	DOWN
18:2*n*-6	0.2	17.2	none	DOWN
18:3*n*-6	0.5	20.0	none	DOWN
18:3*n*-3	7.3	2.4	UP	UP
18:4*n*-3	14.7	0.7	UP	none
20:4*n*-3	14.1	0.0	UP	none
20:5*n*-3	8.2	10.0	UP	DOWN
22:0	2.0	1.0	UP	DOWN
22:5*n*-3	14.2	0.6	UP	none

Table S5. Variables ordered by contribution (%) to principal component (PC) 1 of the PCA of lipid classes dataset, and respective change in PC1 positive.

Lipid class	PC1 contrib.	Change	Lipid class	PC1 contrib.	Change
DGTS	12.61	DOWN	LPG	4.84	UP
LPE	12.32	DOWN	DGMG	4.81	UP
PG	12.21	DOWN	PC	3.89	DOWN
PE	11.14	DOWN	PI	3.62	DOWN
DGDG	8.82	DOWN	SQMG	3.17	UP
MGTS	6.35	DOWN	LPI	1.74	DOWN
MGDG	6.26	DOWN	MGMG	1.74	UP
SQDG	6.00	DOWN	LPC	0.50	none

Table S6. Top 25 variables contributing to principal component (PC) 1 of the PCA of lipid species dataset, and respective change in PC1 positive. Numbers in parenthesis (C:N) indicate the number of carbon atoms (C) and double bonds (N) in the fatty acyl chains.

Lipid species	PC1 contrib.	Change	Lipid species	PC1 contrib.	Change
MGDG (36:8)	1.63	DOWN	DGTS (30:4)	1.43	DOWN
LPC (20:5)	1.57	DOWN	DGTS (40:8)	1.41	DOWN
LPC (18:4)	1.55	DOWN	SQDG (36:4)	1.40	DOWN
DGDG (36:7)	1.53	DOWN	MGDG (32:7)	1.39	DOWN
LPC (20:4)	1.50	DOWN	DGTS (40:9)	1.38	DOWN
PG (36:3)	1.49	DOWN	MGDG (34:8)	1.38	DOWN
DGDG (36:6)	1.47	DOWN	LPG (16:0)	1.38	DOWN
DGTS (40:6)	1.46	DOWN	DGTS (40:7)	1.38	DOWN
DGTS (32:4)	1.46	DOWN	DGTS (36:8)	1.37	DOWN
MGDG (36:9)	1.45	DOWN	DGTS (42:10)	1.37	DOWN
DGTS (38:5)	1.45	DOWN	MGDG (36:7)	1.36	DOWN
SQDG (34:5)	1.44	DOWN	SQDG (34:7)	1.36	DOWN
MGDG (32:8)	1.43	DOWN			

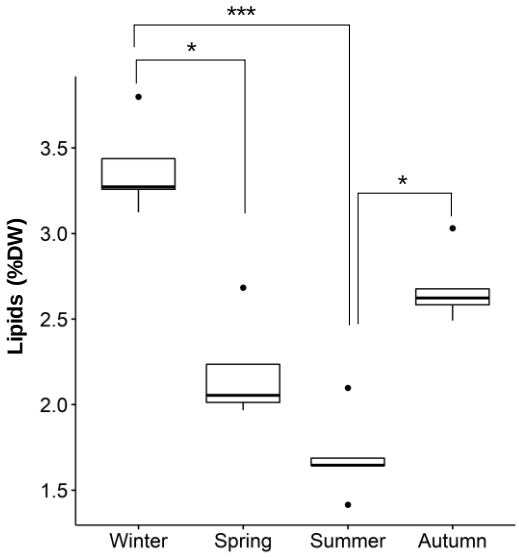

Figure S1. Lipid contents, expressed as percentage of biomass dry weight (%DW), of *Ulva rigida* samples cultivated in different seasons: winter, spring, summer and autumn. Kruskal-Wallis test followed by Dunn's multicomparison test was used to determine significant variations, marked with * if $q < 0.05$ and *** if $q < 0.001$.

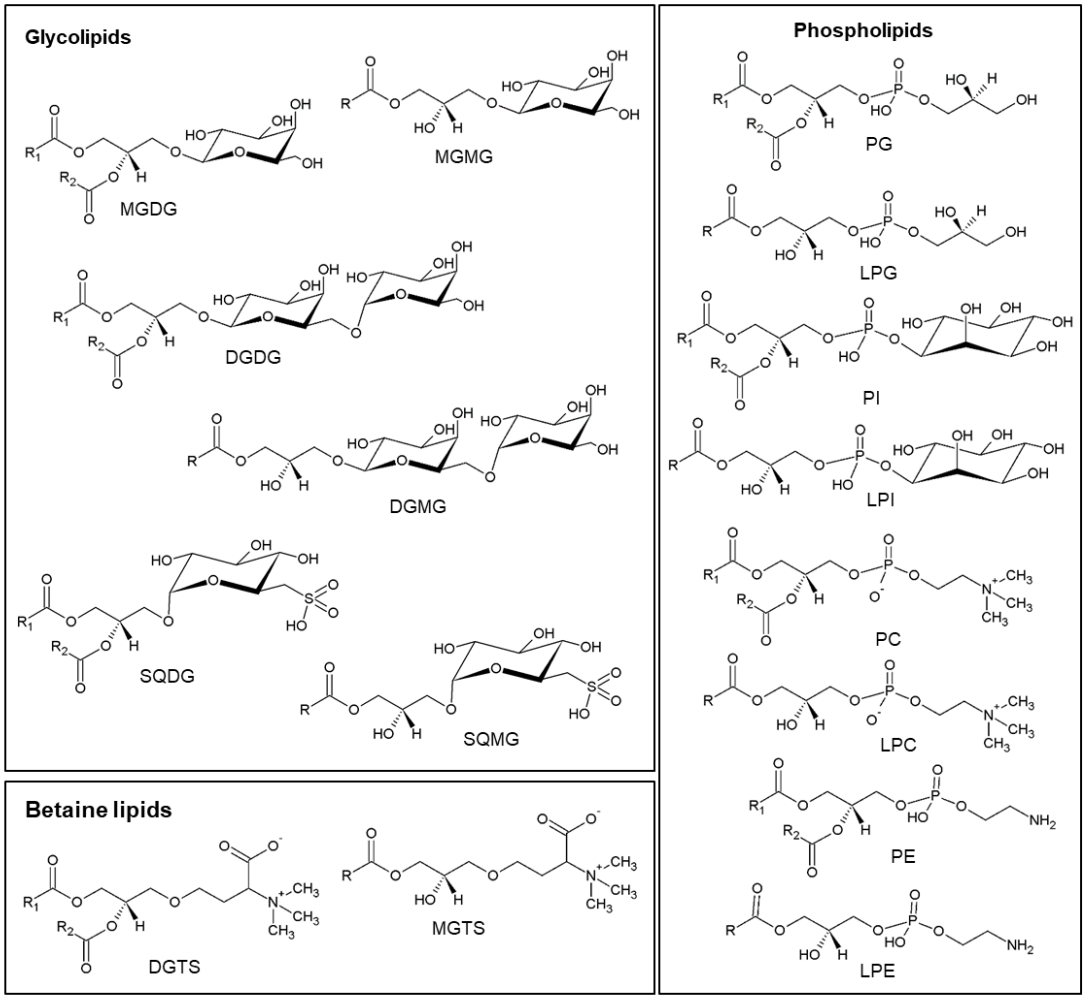

Figure S2. Structures of the glycolipid, phospholipid, and betaine lipid classes identified from samples of *Ulva rigida* cultivated in winter, spring, summer and autumn. Different species within the same class have distinct fatty acyl chains, represented by R1 and R2 for the diacyl-forms, or R for lyso forms carrying a single fatty acyl chain. All structures are represented as in LIPID MAPS® structure database [1].

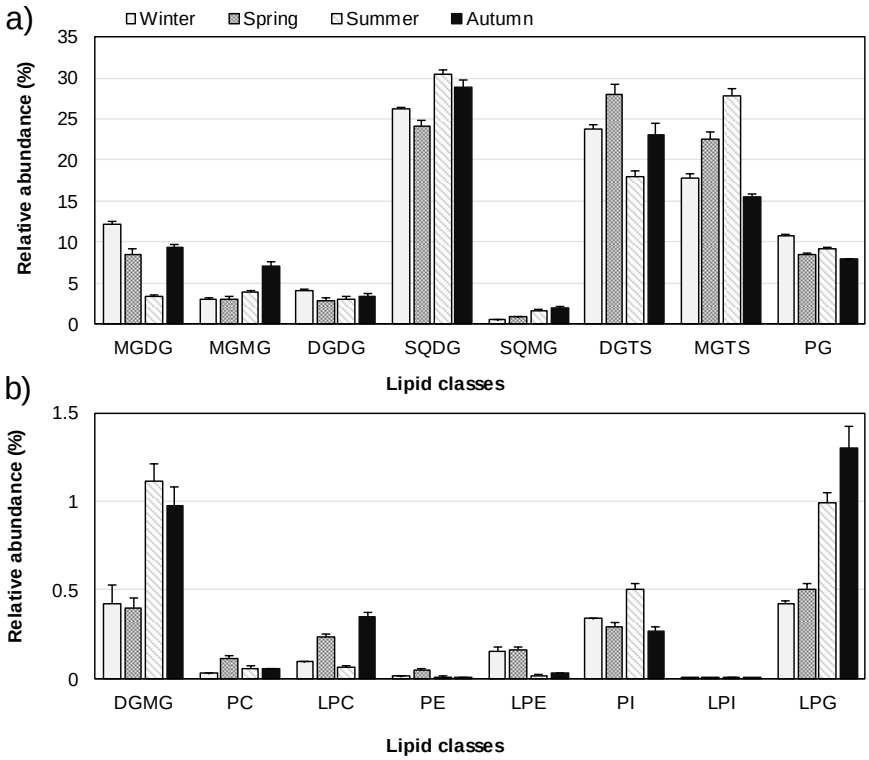

Figure S3. Relative abundance (RA, %) of the lipid classes identified by LC–MS and MS/MS of *Ulva rigida* samples collected during winter, spring, summer and autumn: (a) classes with RA higher than 2% in at least one of the four seasons, and (b)) classes with RA lower than 2% in the four seasons.

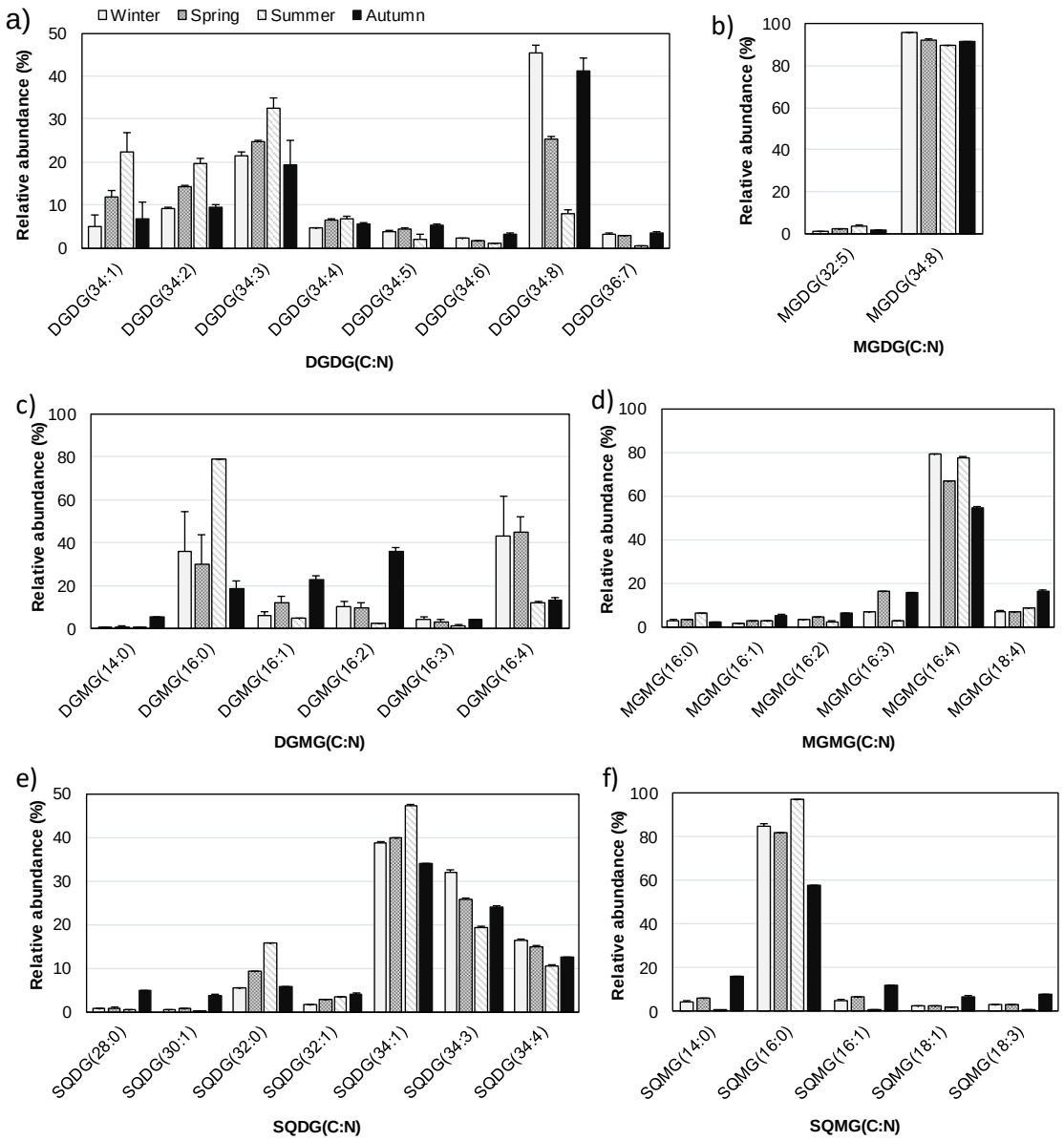

Figure S4. Relative abundance (%) of glycolipids identified by LC–MS and MS/MS of *Ulva rigida* samples collected during winter, spring, summer and autumn: (a) DGDG, (b) MGDG, (c) DGMG, (d) MGMG, (e) SQDG, and (f) SQMG. For simplicity and considering that the most abundant species (not the vestigial ones) are the most important from a perspective of valorisation for potential applications, only species with relative abundance higher than 3% in at least one of the four seasons are shown. Numbers in parenthesis (C:N) indicates the number of carbon atoms (C) and double bonds (N) in the fatty acyl chains.

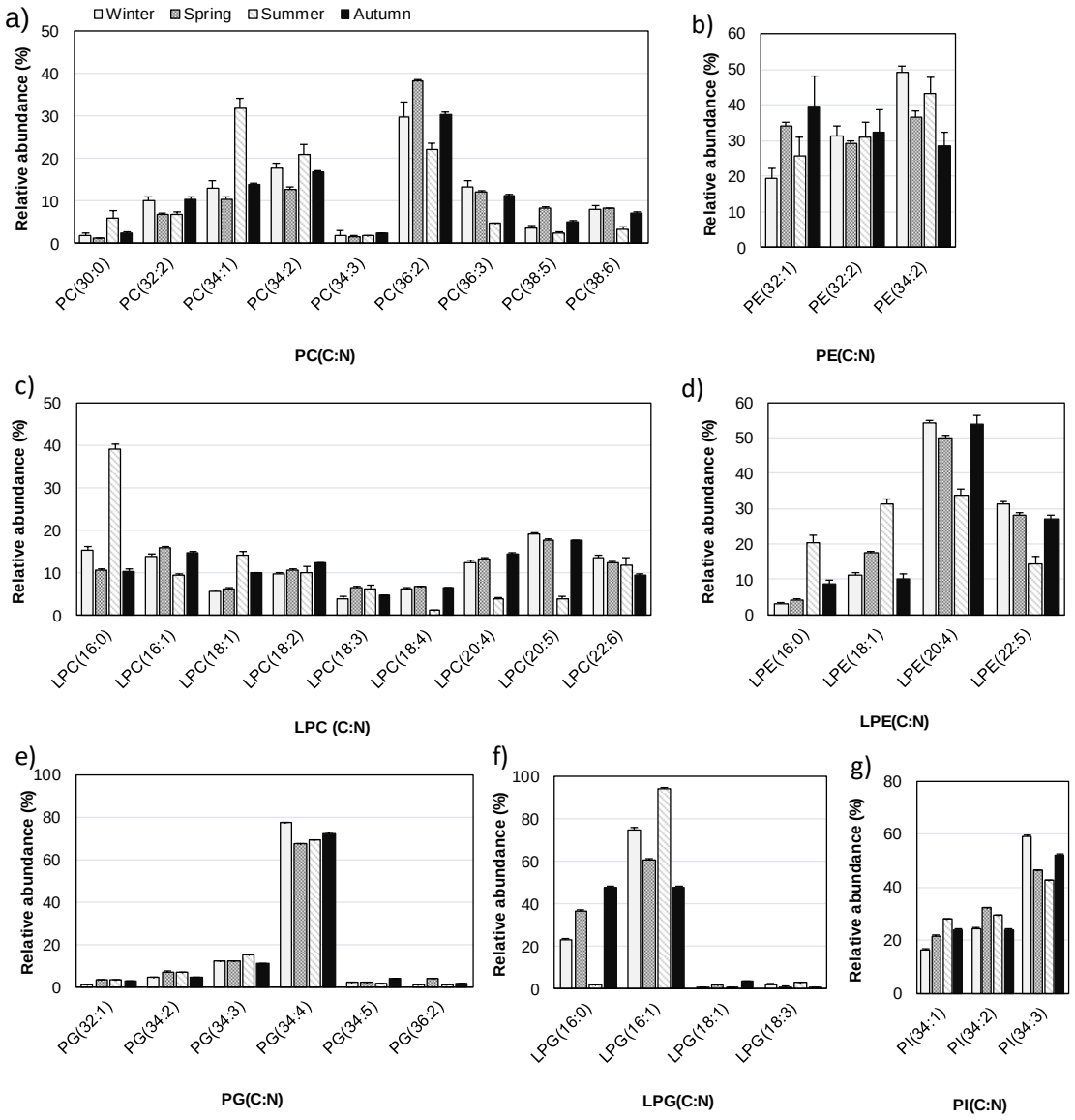

Figure S5. Relative abundance (%) of phospholipids identified by LC–MS and MS/MS of *Ulva rigida* samples collected during winter, spring, summer and autumn: (a) PC, (b) PE, (c) LPC, (d) LPE, (e) PG, (f) LPG, and (g) PI species. For simplicity and considering that the most abundant species (not the vestigial ones) are the most important from a perspective of valorisation for potential applications, only species with relative abundance higher than 3% in at least one of the four seasons are shown. Numbers in parenthesis (C:N) indicates the number of carbon atoms (C) and double bonds (N) in the fatty acyl chains.

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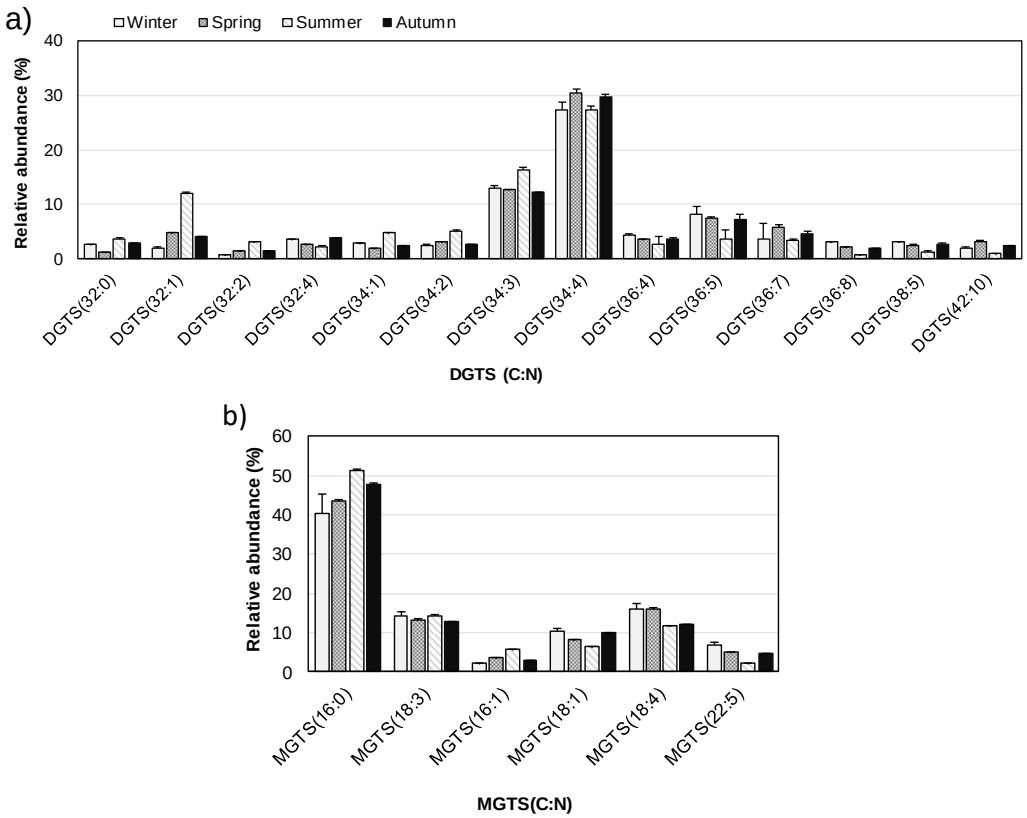

Figure S6. Relative abundance (%) of betaine lipids identified by LC–MS and MS/MS of *Ulva rigida* samples collected during winter, spring, summer and autumn: (a) DGTS and (b) MGTS species. For simplicity and considering that the most abundant species (not the vestigial ones) are the most important from a perspective of valorisation for potential applications, only species with relative abundance higher than 3% in at least one of the four seasons are shown. Numbers in parenthesis (C:N) indicates the number of carbon atoms (C) and double bonds (N) in the fatty acyl chains.

Reference

[1] Sud, M.; Fahy, E.; Cotter, D.; Brown, A.; Dennis, E. A.; Glass, C. K.; Merrill, A. H., Jr.; Murphy, R. C.; Raetz, C. R. H.; Russell, D. W.; Subramaniam, S. LMSD: LIPID MAPS structure database. *Nucleic Acids Res.* **2007**, *35*, D527-D532.