

Supplementary materials

Seasonal Variations in the Metabolome and Bioactivity Profile of *Fucus vesiculosus* Extracted by an Optimised, Pressurised Liquid Extraction Protocol

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Table S1. Dereplication of compounds identified in monthly *F. vesiculosus* organic extracts from Jan. 2017 – Dec. 2017, based on UPLC-PDA-(ESI+)MS² data.

Comp. ID	t _R (min)	Chemical class	Putative identification	Mol. Formula (M)	MS ¹ (m/z)	Error (Δppm)	Confidence level ^a	MS ² (m/z)	UV λ _{max} (nm) ^b
1	0.98	Phlorotannin	Fucodiphlorethol A, B, C, D, E, G or Difucophlorethol A or Tetrafulcol A, B or Tetraphlorethol A, C, E	C ₂₄ H ₁₈ O ₁₂	499.084 [M+H] ⁺	7.3	2	481.09, 463.08, 411.08, 395.09, 393.07, 355.06, 337.05, 327.06, 287.07, 285.05, 271.04, 269.05, 139.04	
2	6.12	Phosphatidylcholine	LysoPC ^c 20:5	C ₂₈ H ₄₈ NO ₇ P	542.321 [M+H] ⁺	6.8	2	524.33, 184.08, 104.11	
3	6.27	Betaine lipid	LysoDGTSA ^d 14:0	C ₂₄ H ₄₇ NO ₆	446.339 [M+H] ⁺	20.5 ^f	2	428.35, 285.25, 236.16, 144.11	
4	6.29	Betaine lipid	LysoDGTSA 18:3	C ₂₈ H ₄₉ NO ₆	496.350 [M+H] ⁺	27.8 ^f	2	478.37, 236.15, 144.11	
5	6.31	Betaine lipid	LysoDGTSA 20:5	C ₃₀ H ₄₉ NO ₆	520.354 [M+H] ⁺	18.9 ^f	2	502.37, 236.15	
6	6.68	Phosphatidylethanolamine	LysoPE ^e 20:4	C ₂₅ H ₄₃ NO ₇ P	502.283 [M+H] ⁺	20.6 ^f	2	422.16, 379.17, 361.28	
7	6.81	Betaine lipid	LysoDGTSA 18:2	C ₂₈ H ₅₁ NO ₆	498.376 [M+H] ⁺	6.9	2	480.37, 361.29, 236.16, 144.11	
8	6.88	Betaine lipid	LysoDGTSA 20:4	C ₃₀ H ₅₁ NO ₆	522.377 [M+H] ⁺	4.7	2	504.38, 236.16, 173.03	
9	7.27	Betaine lipid	LysoDGTSA 20:3	C ₃₀ H ₅₃ NO ₆	546.369 [M+Na] ⁺	14.7 ^f	2	528.39, 236.16	
10	7.45	Betaine lipid	LysoDGTSA 16:0	C ₂₆ H ₅₁ NO ₆	474.373 [M+H] ⁺	13.6 ^f	2	456.40, 351.14, 313.29, 236.16, 144.11	
11	7.52	Betaine lipid	LysoDGTSA 18:1	C ₂₈ H ₅₃ NO ₆	500.392 [M+H] ⁺	6.2	2	482.39, 422.15, 236.16	
12	7.76	Carotenoid	Fucoxanthin dehydrated	C ₄₂ H ₅₈ O ₆	641.427 [M+H- H ₂ O] ⁺	10.0 ^f	2	549.37, 221.16, 203.15	
13	8.40	Carotenoid	Violaxanthin or Neoxanthin	C ₄₀ H ₅₆ O ₄	583.420 [M+H- H ₂ O] ⁺	8.4	2	491.37, 283.22, 221.16, 165.10	
14	9.30	Chlorophyll	Chlorophyll <i>c</i> 2	C ₃₅ H ₂₈ MgN ₄ O ₅	609.204 [M+H] ⁺	8.5	2	591.23, 549.21, 534.23, 532.19	
15	9.61	Chlorophyll			623.413 [M+H] ⁺		3	605.42, 587.42, 549.34, 531.34, 295.17, 259.13	224, 450
16	10.71	Phosphatidylcholine			782.590 [M+H] ⁺		3	750.57, 572.39, 554.39, 446.37, 428.35, 184.08	
17	10.71	Chlorophyll	Pheophytin <i>b</i>	C ₅₅ H ₇₂ N ₄ O ₆	885.602 [M+H] ⁺	55.3 ^f	2	607.30, 547.28	
18	10.93	Carotenoid	Fucoxanthinol	C ₄₀ H ₅₆ O ₅	599.408 [M+H- H ₂ O] ⁺	3.4	2	581.42, 411.28, 355.25, 277.21, 263.19, 213.13, 199.15, 185.14, 173.14, 127.11, 109.10	224, 265, 330, 447, 470
19	10.94	Carotenoid	Fucoxanthin	C ₄₂ H ₅₈ O ₆	681.421 [M+Na] ⁺	11.6 ^f	1 ^g	663.42, 621.41, 603.40, 527.33	224, 265, 330, 447, 470
					659.435 [M+H] ⁺	6.4	1	641.46, 581.43, 109.11	
20	11.20	Chlorophyll	Pheophorbide <i>a</i>	C ₃₅ H ₃₆ N ₄ O ₅	593.279 [M+H] ⁺	4.4	2	533.27	224, 265, 330, 409, 505, 535
21	11.35	Phosphatidylcholine			810.625 [M+H] ⁺		3	778.60, 313.28, 184.08	
22	11.40	Betaine lipid	DGTSA 32:4	C ₄₂ H ₇₃ NO ₇	704.553 [M+H] ⁺	9.2	2	494.37, 476.35, 446.38, 428.35,	

			(18:4/14:0 or 14:0/18:4)						144.11	
23	11.47	Chlorophyll	Pheophytin c2	C ₃₅ H ₃₀ N ₄ O ₅	587.231 [M+H] ⁺	2.6	2	543.25, 527.22, 511.23		224, 450
24	11.47	Phosphatidylcholine		C ₄₅ H ₈₂ NO ₇ P	780.594 [M+H] ⁺	4.2	3	520.38, 502.37, 496.38, 478.36, 184.08		
25	11.55	Betaine lipid	DGTSA 30:2 (16:2/14:0 or 14:0/16:2)	C ₄₀ H ₇₃ NO ₇	680.551 [M+H] ⁺	6.6	2	470.35, 452.35, 446.36, 428.36, 144.10		
26	11.60	Betaine lipid	DGTSA 34:5 (20:5/14:0 or 14:0/20:5)	C ₄₄ H ₇₅ NO ₇	730.575 [M+H] ⁺	17.6 ^f	2	520.38, 502.36, 446.36, 428.35, 144.10		
27	11.68	Phosphatidylcholine			806.611 [M+H] ⁺		3	702.53, 522.39, 520.39, 504.38, 502.37, 184.08		
28	11.72	Betaine lipid	DGTSA 32:3 (18:3/14:0 or 14:0/18:3)	C ₄₂ H ₇₅ NO ₇	706.569 [M+H] ⁺	9.7	2	496.37, 478.36, 446.36, 428.35, 144.10		
29	11.80	Phosphatidylcholine		C ₄₅ H ₈₄ NO ₇ P	782.607 [M+H] ⁺	0.8	3	678.53, 184.08		
30	11.84	Carotenoid		C ₄₀ H ₅₂ O ₃	581.401 [M+H] ⁺	2.6	3	563.42, 411.29, 355.26, 277.21, 251.20, 185.14, 127.12, 109.11		225, 265, 330, 442, 470
31	11.86	Betaine lipid	DGTSA 28:0 (14:0/14:0)	C ₃₈ H ₇₃ NO ₇	656.550 [M+H] ⁺	5.3	2	446.38, 428.37, 109.11		
32	11.91	Betaine lipid	DGTSA 34:4 (20:4/14:0 or 14:0/20:4)	C ₄₄ H ₇₇ NO ₇	732.589 [M+H] ⁺	15.2 ^f	2	522.41, 504.40, 446.37, 428.37, 144.11		
33	12.08	Betaine lipid	DGTSA 32:2 (18:2/14:0 or 14:0/18:2)	C ₄₂ H ₇₇ NO ₇	708.593 [M+H] ⁺	21.4 ^f	2	498.41, 480.40, 446.38, 428.37, 144.11		
34	12.09	Phospholipid		C ₄₃ H ₈₄ NO ₇ P	758.605 [M+H] ⁺	1.8	3	654.53, 520.37, 502.36, 474.40, 456.39, 184.08		
35	12.13	Phospholipid		C ₄₅ H ₈₆ NO ₇ P	784.623 [M+H] ⁺	1.3	3	647.54, 522.41, 504.39, 498.42, 480.40, 184.09, 144.11		
36	12.26	Betaine lipid		C ₄₄ H ₇₉ NO ₇	734.605 [M+H] ⁺	15.7	3	524.43, 506.42, 496.40, 474.41, 456.40, 446.38, 428.36, 144.11		
37	12.30	Phosphatidylethanolamine		C ₄₇ H ₈₈ NO ₇ P	810.637 [M+H] ⁺	0.8	3	669.51, 522.41, 504.39, 164.02		
38	12.50	Betaine lipid	DGTSA 30:0 (16:0/14:0 or 14:0/16:0)	C ₄₀ H ₇₇ NO ₇	684.585 [M+H] ⁺	10.5 ^f	2	474.40, 456.39, 446.37, 428.35		
39	12.56	Betaine lipid	DGTSA 32:1 (18:1/14:0 or 14:0/18:1)	C ₄₂ H ₇₉ NO ₇	710.599 [M+H] ⁺	7.8	2	500.42, 482.40, 446.36, 428.36, 144.11		
40	12.59	Chlorophyll	Methylpheophorbide	C ₃₆ H ₃₈ N ₄ O ₅	607.292 [M+H] ⁺	0.1	2	547.29		

<i>a</i>								
41	12.73	Betaine lipid		C ₄₄ H ₈₁ NO ₇	736.619 [M+H] ⁺	13.4 ^f	3	498.40, 480.38, 474.39, 456.38
42	13.26	Tocopherol	α -Tocopherol	C ₂₉ H ₅₀ O ₂	429.364 [M+H-H ₂] ⁺	21.6 ^f	2	311.30, 205.12, 191.11, 165.09, 163.11
43	13.37	Chlorophyll	Pheophytin <i>a</i>	C ₅₅ H ₇₄ N ₄ O ₅	871.582 [M+H] ⁺	9.5	2	593.32, 533.29
44	13.59	Carotenoid	Zeaxanthin	C ₄₀ H ₅₆ O ₂	569.433 [M+H] ⁺	5.0	2	477.42

^a Confidence level of the metabolite identification based on Sumner *et al.* 2007 and Blaženovic *et al.* 2018.

^b When no λ_{\max} indicated, either no absorbance, or compound in too low amount to be detected

^c LysoPC: lysophosphatidylcholine

^d DGTSA: either DGTS [1,2-diacylglycerol-*O*-2'-(hydroxymethyl)-(N,N,N-trimethyl)homoserine] or DGTA [1,2-diacylglycerol-*O*-2'-(hydroxymethyl)-(N,N,N-trimethyl)- β -alanine]

^e LysoPE: lysophosphatidylethanolamine

^f High Δ ppm (≥ 10 ppm) due to a detection saturation or to a very low intensity of the ion in the UPLC-MS chromatogram

^g Identification confirmed by comparison with a purchased commercial standard

Table S2. Dereplication table of the 54 compounds significantly varying with collection month.

Box plot ID	Compound ID	RT (min)	Chemical class	Tentative identification	Formula (M)	MS ¹ (<i>m/z</i>)	Error (Δ ppm)	Confidence level ^a	MS ² (<i>m/z</i>)	UV λ_{\max} (nm) ^b
I	1	0.98	Phlorotannins	Fucodiphlorethol A, B, C, D, E, G or Difucophlorethol A or Tetrafulcol A, B or Tetraphlorethol A, C, E	C ₂₄ H ₁₈ O ₁₂	499.084 [M+H] ⁺	7.3	2	481.09, 463.08, 411.08, 395.09, 393.07, 355.06, 337.05, 327.06, 287.07, 285.05, 271.04, 269.05 139.04	
II		5.23				507.251				
III		6.19				535.285				
IV	3	6.27	Betaine lipids	LysoDGTSA ^c 14:0	C ₂₄ H ₄₇ NO ₆	446.339 [M+H] ⁺	20.5 ^d	2	428.35, 285.25, 236.16, 144.11	
V	7	6.81	Betaine lipids	LysoDGTSA 18:2	C ₂₈ H ₅₁ NO ₆	498.376 [M+H] ⁺	6.9	2	480.37, 361.29, 236.16, 144.11	
VI	10	7.45	Betaine lipids	LysoDGTSA 16:0	C ₂₆ H ₅₁ NO ₆	474.373 [M+H] ⁺	13.6 ^d	2	456.40, 351.14, 313.29, 236.16, 144.11	
VII	12	7.76	Carotenoids	Fucoxanthin (dehydrated)	C ₄₂ H ₅₈ O ₆	641.427 [M+H- H ₂ O] ⁺	10.0 ^d	2	549.37, 221.16, 203.15	
VIII	14	9.30	Chlorophylls	Chlorophyll <i>c</i> 2	C ₃₅ H ₂₈ MgN ₄ O ₅	609.204 [M+H] ⁺	8.5	2	591.23, 549.21, 534.23, 532.19	

IX		9.37				658.532			448.34, 446.36, 430.34, 428.35	224, 450
X		9.61				600.420			291.19, 263.20, 145.11, 121.11	224, 450
XI	15	9.61	Chlorophylls			623.413 [M+H] ⁺	3		605.42, 587.42, 549.34, 531.34, 295.17, 259.13 750.57	224, 450
XII		9.87				768.576				
XIII		10.25				686.562				
XIV	16	10.71	Phosphatidylcholines			782.590 [M+H] ⁺	3		750.57, 572.39, 554.39, 446.37, 428.35, 184.08	
XV	18	10.93	Carotenoids	Fucoxanthinol	C ₄₀ H ₅₆ O ₅	599.408 [M+H- H ₂ O] ⁺	3.4	2	581.42, 411.28, 355.25, 277.21, 263.19, 213.13, 199.15, 185.14, 173.14, 127.11, 109.10	224, 265, 330, 447, 470

XVI	19	10.94	Carotenoids	Fucoxanthin	C ₄₂ H ₅₈ O ₆	681.421 [M+Na] ⁺	11.6 ^d	1 ^g	663.42, 621.41, 603.40, 527.33, 641.46, 581.43, 109.11	224, 265, 330, 447, 470
XVII	20	11.20	Chlorophylls	Pheophorbide <i>a</i>	C ₃₅ H ₃₆ N ₄ O ₅	593.279 [M+H] ⁺	4.4	2	533.27	224, 265, 330, 409, 505, 535
XVIII	21	11.35	Phosphatidylcholines			810.625 [M+H] ⁺		3	778.60, 313.28, 184.08	
XIX	22	11.40	Betaine lipids	DG TSA 32:4 (18:4/14:0 or 14:0/18:4)	C ₄₂ H ₇₃ NO ₇	704.553 [M+H] ⁺	9.2	2	494.37, 476.35, 446.38, 428.35, 144.11	
XX	23	11.47	Chlorophylls	Pheophytin <i>c</i> 2	C ₃₅ H ₃₀ N ₄ O ₅	587.231 [M+H] ⁺	2.6	2	543.25, 527.22, 511.23	224, 450
XXI	24	11.47	Phosphatidylcholines			780.594 [M+H] ⁺	4.2	3	520.38, 502.37, 496.38, 478.36, 184.08	
XXII	25	11.55	Betaine lipids	DG TSA 30:2 (16:2/14:0 or 14:0/16:2)	C ₄₀ H ₇₃ NO ₇	680.551 [M+H] ⁺	6.6	2	470.35, 452.35, 446.36, 428.36, 144.10	
XXIII	26	11.60	Betaine lipids	DG TSA 34:5 (20:5/14:0 or 14:0/20:5)	C ₄₄ H ₇₅ NO ₇	730.575 [M+H] ⁺	17.6 ^d	2	520.38, 502.36, 446.36, 428.35, 144.10	
XXIV	27	11.68	Phosphatidylcholines			806.611		3	702.53,	

										[M+H] ⁺	522.39, 520.39, 504.38, 502.37, 184.08	
XXV	28	11.72	Betaine lipids	DGTSA 32:3 (18:3/14:0 or 14:0/18:3)	C ₄₂ H ₇₅ NO ₇	706.569 [M+H] ⁺	9.7	2			496.37, 478.36, 446.36, 428.35, 144.10	
XXVI	29	11.80	Phosphatidylcholines		C ₄₅ H ₈₄ NO ₇ P	782.607 [M+H] ⁺	0.8	3			678.53, 184.08	
XXVII	30	11.84	Carotenoids		C ₄₀ H ₅₂ O ₃	581.401 [M+H] ⁺	2.6	3			563.42, 411.29, 355.26, 277.21, 251.20, 185.14, 127.12, 109.11	225, 265, 330, 442, 470
XXVIII		11.86				641.427					581.42, 411.29, 251.20, 109.10	225, 330, 442
XXIX		11.86				681.415					663.42, 603.39, 527.33	225, 330, 442
XXX	31	11.86	Betaine lipids	DGTSA 28:0 (14:0/14:0)	C ₃₈ H ₇₃ NO ₇	656.550 [M+H] ⁺	5.3	2			446.38, 428.37, 109.11	
XXXI	32	11.91	Betaine lipids	DGTSA 34:4 (20:4/14:0 or 14:0/20:4)	C ₄₄ H ₇₇ NO ₇	732.589 [M+H] ⁺	15.2 ^d	2			522.41, 504.40, 446.37, 428.37, 144.11	
XXXII		11.93				682.569					603.41, 527.34	225, 265, 330, 442, 470

XXXIII		11.95				808.623			704.58, 522.40, 504.38, 377.33
XXXIV		12.01				710.593			498.40, 480.39, 446.37, 428.35, 144.11
XXXV		12.05				708.793			
XXXVI	33	12.08	Betaine lipids	DG TSA 32:2 (18:2/14:0 or 14:0/18:2)	$C_{42}H_{77}NO_7$	708.593 [M+H] ⁺	21.4 ^d	2	498.41, 480.40, 446.38, 428.37, 144.11
XXXVII	35	12.13	Phospholipids		$C_{45}H_{86}NO_7P$	784.623 [M+H] ⁺	1.3	3	647.54, 522.41, 504.39, 498.42, 480.40, 184.09, 144.11
XXXVIII		12.15				333.223			241.21, 161.14, 145.11, 133.11, 121.11, 119.09, 107.09, 105.07, 95.09, 93.07, 91.06, 81.07
XXXIX		12.16				635.473			617.48, 543.44, 359.27, 285.23, 267.22, 241.20, 201.17, 161.14,

XL		12.17				976.626			147.12, 133.16	
XLI	36	12.26	Betaine lipids		C ₄₄ H ₇₉ NO ₇	734.605 [M+H] ⁺	15.7	3	524.43, 506.42, 496.40, 474.41, 456.40, 446.38, 428.36, 144.11	225
XLII	37	12.30	Phosphatidylethanolamines		C ₄₇ H ₈₈ NO ₇ P	810.637 [M+H] ⁺	0.8	3	669.51, 522.41, 504.39, 164.02	
XLIII		12.31				957.580			795.53, 679.36	
XLIV		12.48				760.623			697.31, 656.55, 522.4, 504.39, 474.40, 456.38, 236.57, 144.11	
XLV	38	12.50	Betaine lipids	DG TSA 30:0 (16:0/14:0 or 14:0/16:0)	C ₄₀ H ₇₇ NO ₇	684.585 [M+H] ⁺	10.5 ^d	2	474.40, 456.39, 446.37, 428.35	
XLVI	39	12.56	Betaine lipids	DG TSA 32:1 (18:1/14:0 or 14:0/18:1)	C ₄₂ H ₇₉ NO ₇	710.599 [M+H] ⁺	7.8	2	500.42, 482.40, 446.36, 428.36, 144.11	
XLVII	40	12.59	Chlorophylls	Methylpheophorbide <i>a</i>	C ₃₆ H ₃₈ N ₄ O ₅	607.292 [M+H] ⁺	0.1	2	547.29	
XLVIII		12.66				983.600			705.37, 681.37	225
XLIX		12.69				767.482			519.32, 489.27	
L	41	12.73	Betaine lipids		C ₄₄ H ₈₁ NO ₇	736.619	13.4 ^d	3	498.40,	

			[M+H] ⁺	480.38, 474.39, 456.38	
LI	12.84		793.501	517.30	
LII	12.94		762.639	658.56, 520.48, 506.40, 474.41, 456.38, 144.09	
LIII	13.13		635.473		200, 225, 450, 475
LIV	13.29		795.519	517.30	

^a Confidence level of the metabolite identification based on Sumner *et al.* 2007 and Blaženovic *et al.* 2018.

^b When no λ_{\max} indicated, either no absorbance, or compound in too low amount to be detected

^c DGTSA: either DGTS [1,2-diacylglyceryl-*O*-2'-(hydroxymethyl)-(N,N,N-trimethyl)homoserine] or DGTA [1,2-diacylglyceryl-*O*-2'-(hydroxymethyl)-(N,N,N-trimethyl)- β -alanine]

^d High Δ ppm (≥ 10 ppm) due to a detection saturation or to a very low intensity of the ion in the UPLC-MS chromatogram

Table S3. Pathogen strains and their strain-specific culture conditions.

Pathogen	Strain	Medium	Positive control	Pre-culture incubation temperature (°C)	Start optical density	Incubation temperature (°C)	Incubation time (h)
<i>Enterococcus faecium</i>	DSM 20478)	M92 ^a	Ampicillin	37	0.01	37	4
Methicillin-resistant <i>Staphylococcus aureus</i> (MRSA)	DSM 18827	TSB12 ^b	Chloramphenicol	28	0.01	37	5
<i>Klebsiella pneumoniae</i>	DSM 30104	TSB12 ^b	Chloramphenicol	28	0.01	37	5
<i>Acinetobacter baumannii</i>	DSM 30007	TSB12 ^b	Ampicillin	28	0.01	37	5
<i>Pseudomonas aeruginosa</i>	DSM 1128	TSB12 ^b	Chloramphenicol	37	0.01	37	5
<i>Escherichia coli</i>	DSM 1576	TSB12 ^b	Chloramphenicol	28	0.01	37	5
<i>Candida albicans</i>	DSM 1386	M186 ^c	Nystatin	28	0.03	37	5
<i>Cryptococcus neoformans</i>	DSM 6973	M186 ^c	Amphotericin B	28	0.03	28	6-7
<i>Vibrio anguillarum</i>	DSM 21597	TM ^d	Chloramphenicol	28	0.01	28	5
<i>Pseudoalteromonas bacteriolytica</i>	CIP 105725	TM ^d	Chloramphenicol	28	0.03	28	6-7
<i>Pseudoalteromonas elyakovii</i>	CIP 105338	TM ^d	Chloramphenicol	28	0.03	28	6-7

^a 30 g tryptic soy broth, 3 g yeast extract, 1000 mL H₂O, pH 7.0-7.2

^b 12 g tryptic soy broth, 5 g NaCl, 1000 mL H₂O

^c 10 g glucose, 5 g peptone from soybeans, 3 g yeast extract, 3 g malt extract, 1000 mL H₂O

^d 5 g peptone from soybeans, 1 g yeast extract, 30 g Tropic Marin artificial sea salt, 1000 mL H₂O

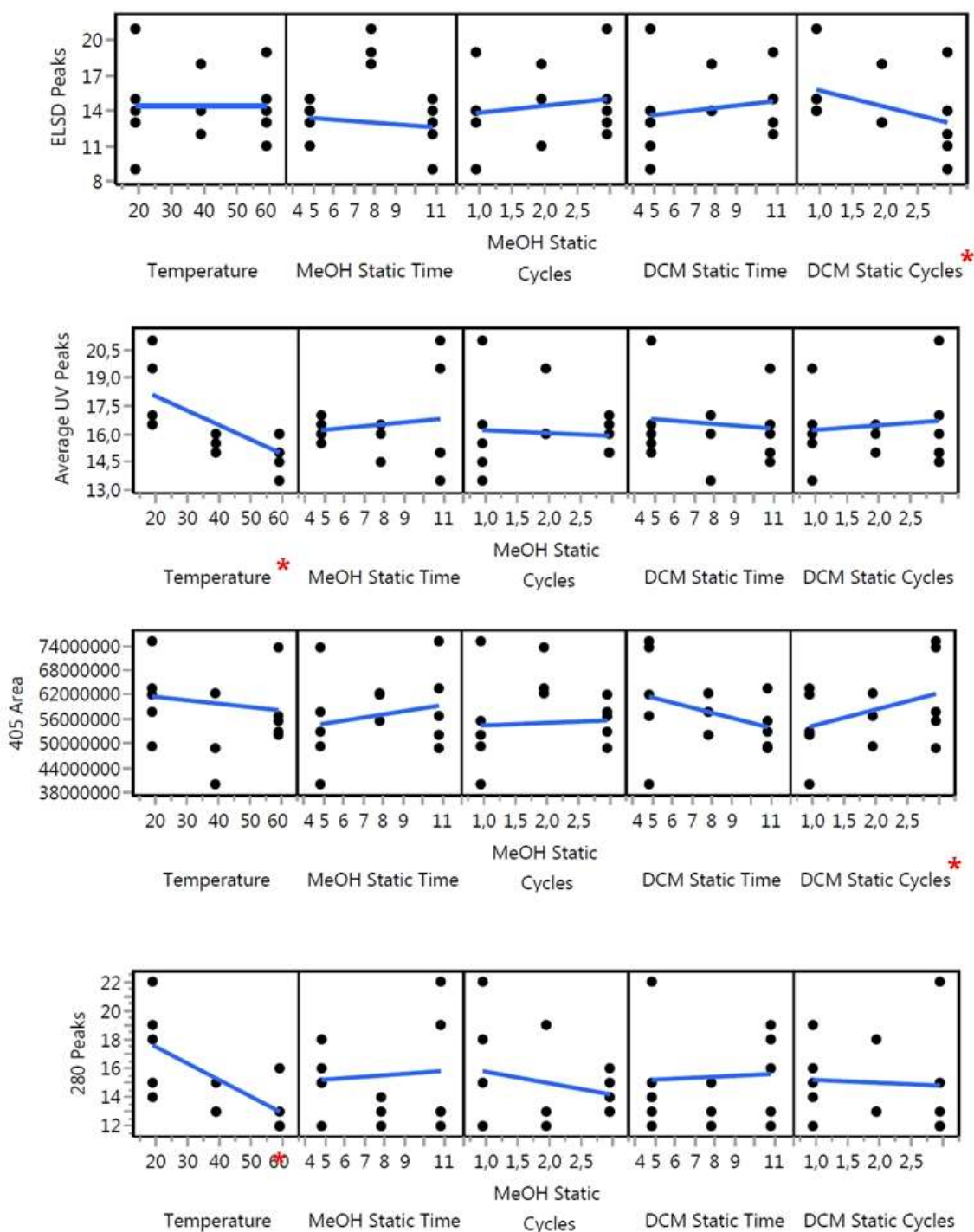


Figure S1. Statistical linear regression analyses of the relationships between the five extraction variables and: (A) number of ELSD signal peaks (1st repeat); (B) average number of UV peaks (2nd repeat); (C) 405 nm UV peak area (2nd repeat); (D) number of 280 nm UV peaks (2nd repeat).

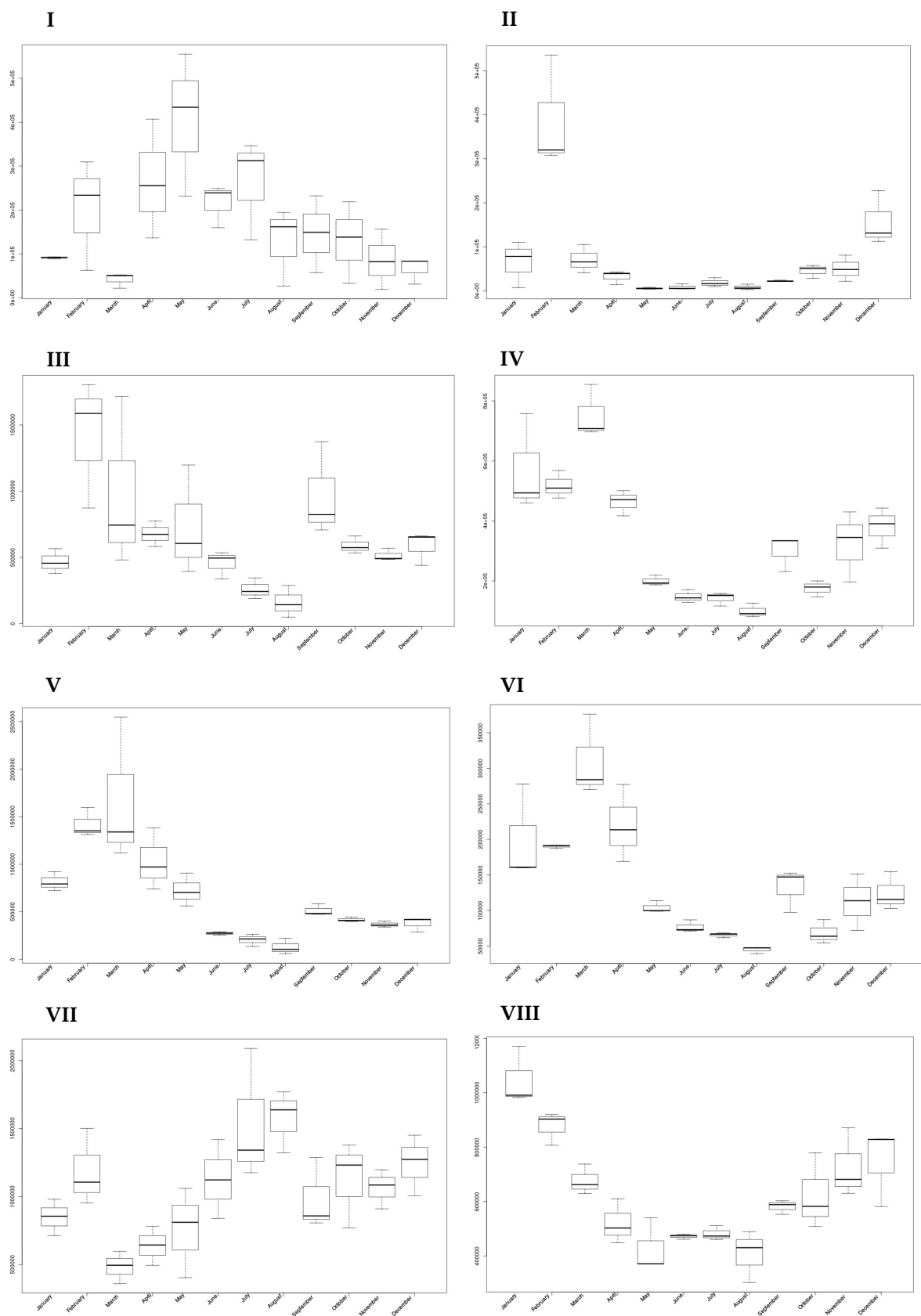


Figure S2. Seasonality box plots depicting monthly median (bold), 1st-3rd quartiles (lower-upper box limits), and minimum and maximum (lower and upper bars) total ion count for compounds I-VIII.

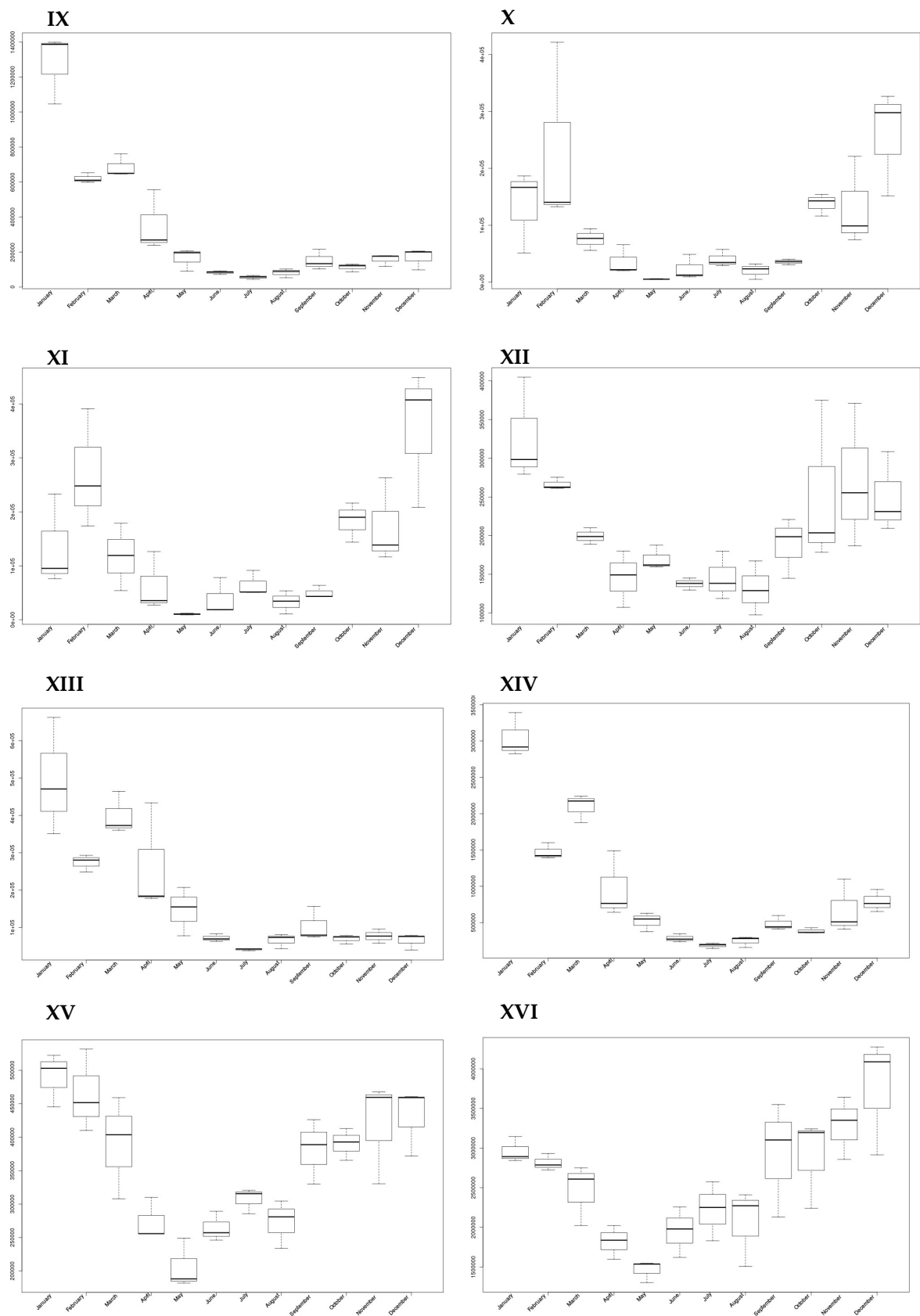


Figure S3. Seasonality box plots depicting monthly median (bold), 1st-3rd quartiles (lower-upper box limits), and minimum and maximum (lower and upper bars) total ion count for compounds IX-XVI.

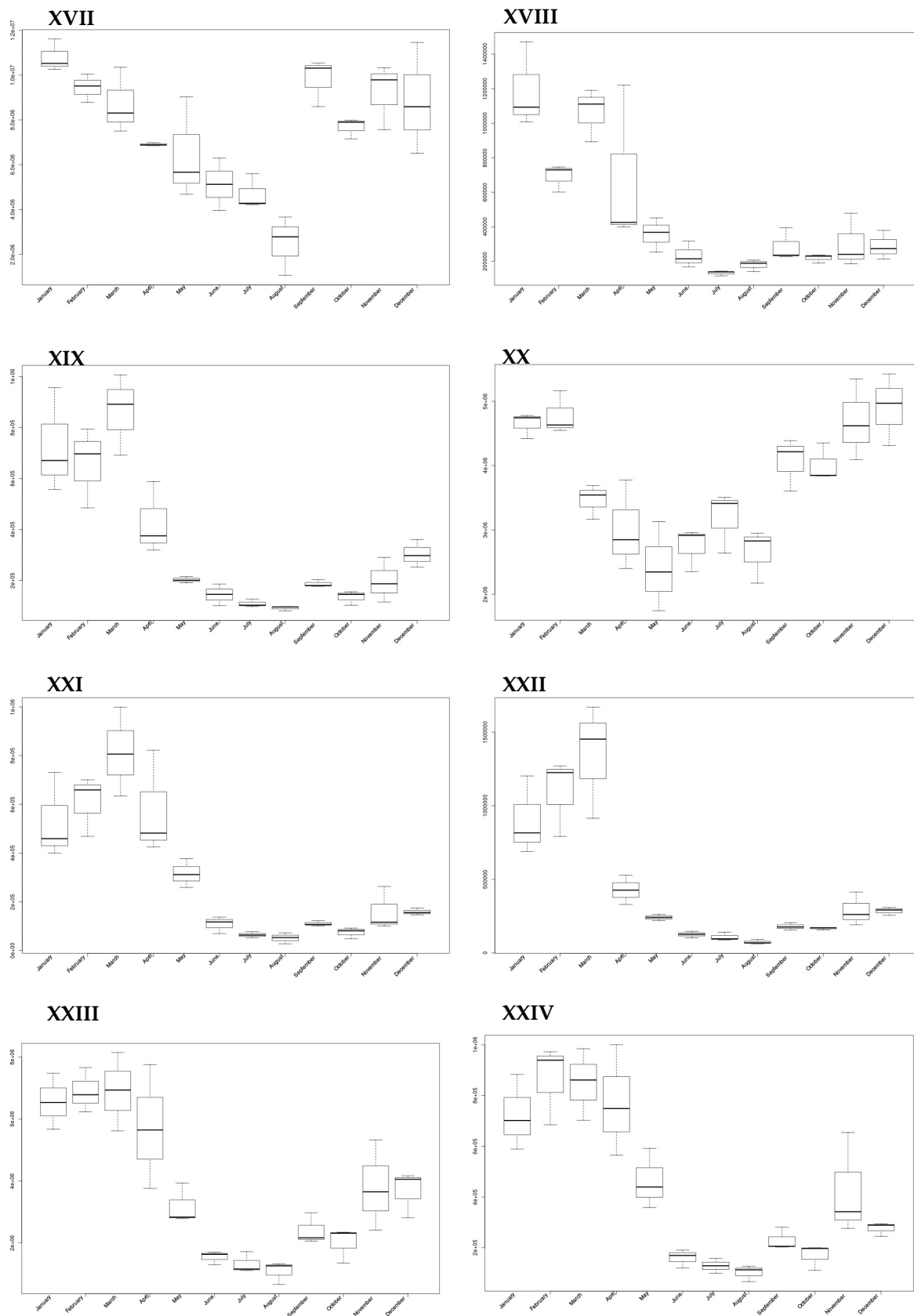


Figure S4. Seasonality box plots depicting monthly median (bold), 1st-3rd quartiles (lower-upper box limits), and minimum and maximum (lower and upper bars) total ion count for compounds XVII-XXIV.

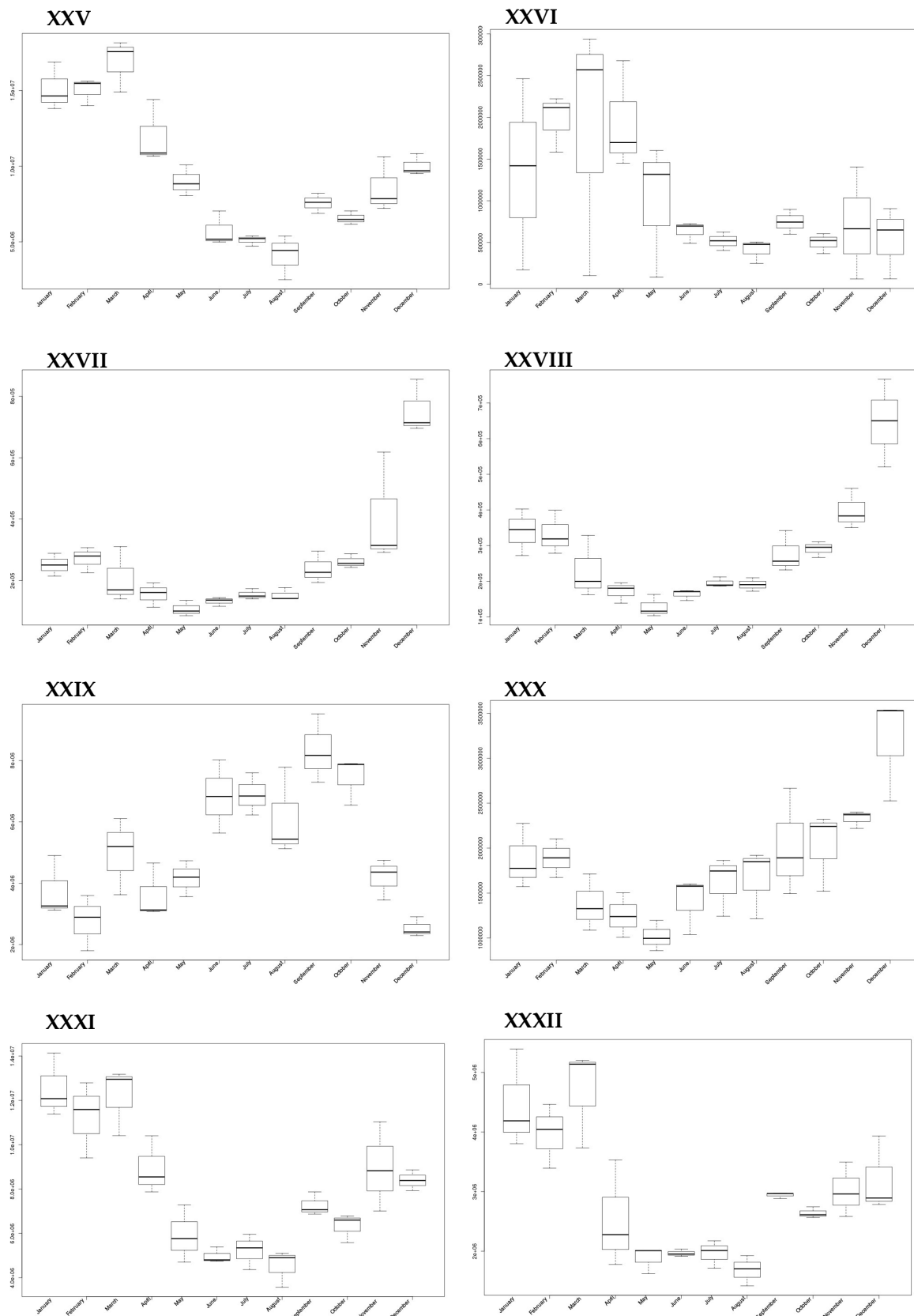


Figure S5. Seasonality box plots depicting monthly median (bold), 1st-3rd quartiles (lower-upper box limits), and minimum and maximum (lower and upper bars) total ion count for compounds XXV-XXXII.

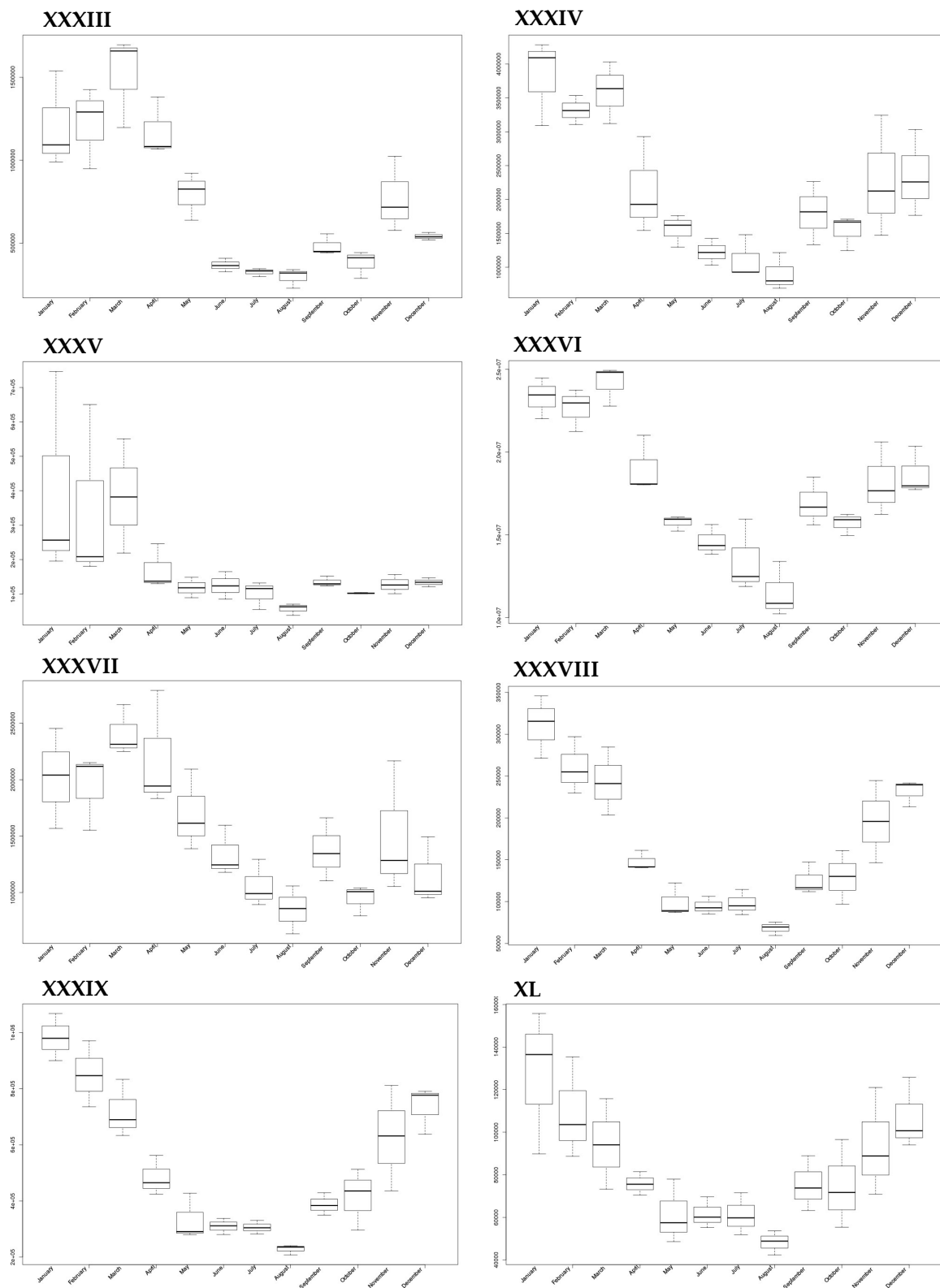


Figure S6. Seasonality box plots depicting monthly median (bold), 1st-3rd quartiles (lower-upper box limits), and minimum and maximum (lower and upper bars) total ion count for compounds XXXIII-XL.

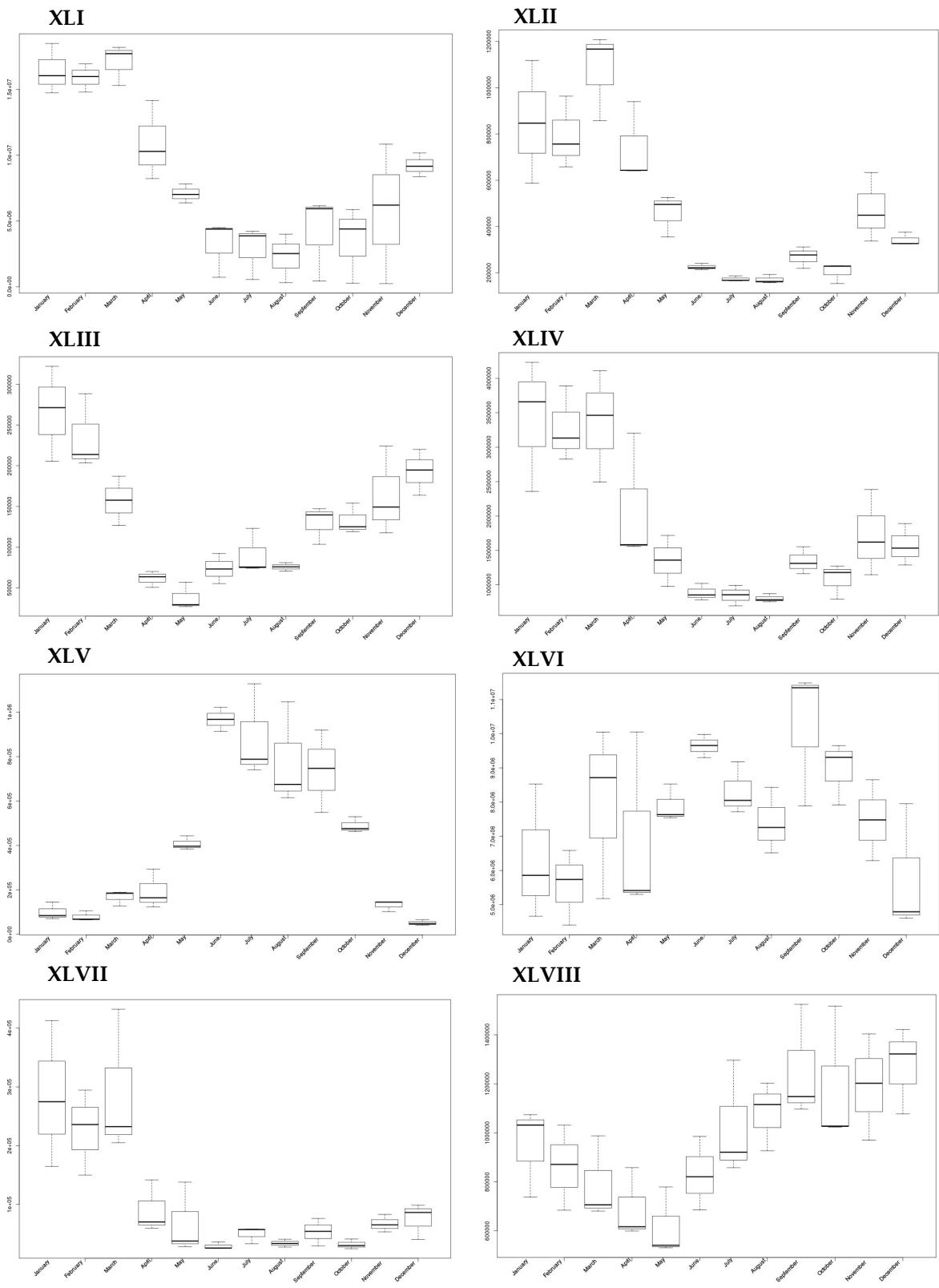


Figure S7. Seasonality box plots depicting monthly median (bold), 1st-3rd quartiles (lower-upper box limits), and minimum and maximum (lower and upper bars) total ion count for compounds XLI-XLVIII.

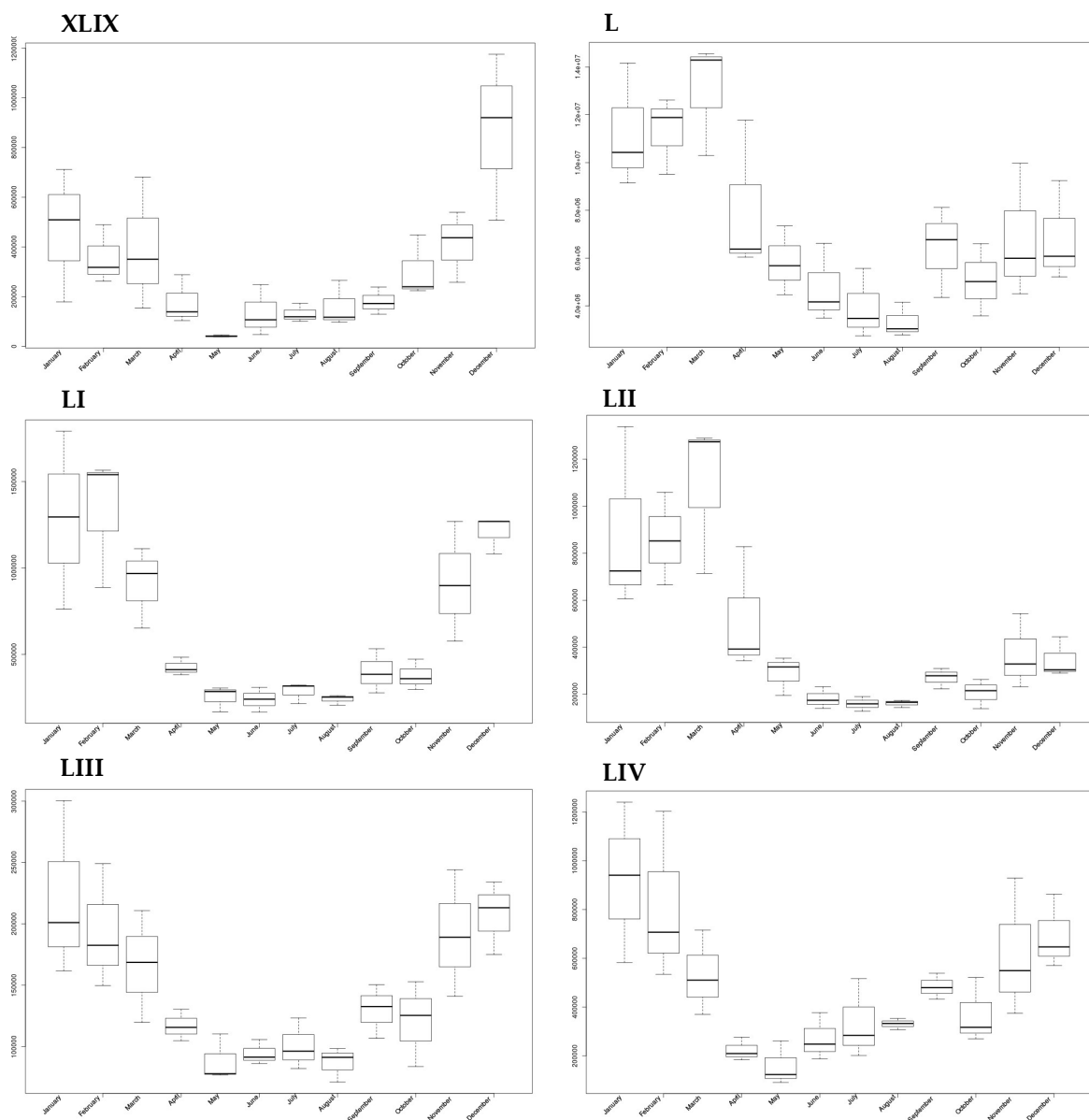


Figure S8. Seasonality box plots depicting monthly median (bold), 1st-3rd quartiles (lower-upper box limits), and minimum and maximum (lower and upper bars) total ion count for compounds XLIX-LIV.