

Supplementary Materials: **The distribution of asterosaponins, polyhydroxysteroids and related glycosides in different body components of the Far Eastern starfish *Lethasterias fusca***

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Figure S4. Calibration curve for 5α -cholestan- $3\beta,4\beta,6\alpha,7\alpha,8,15\beta,16\beta,26$ -octaol (for the sum of ion intensities $[M-H]^-$ at m/z 499.33 and $[M+FA]^-$ at m/z 545.3).

Table S4. Content of detected compounds in different organs and coelomic fluid of the starfish *L. fusca* (ng/g wet weight of the organs for BW, G, PC, and S and ng/ml for CF) and result of statistical analysis (ANOVA followed by Tukey HSD test of multiple comparisons was performed for BW, G, PC, and S groups; q -value < 0.05 was considered statistically significant).

Table S1. Description of studied individuals of *L. fusca*.

Individual	Animal size, mm	Animal weight, g	Wet weight of the organs, g				Volume of coelomic fluid, ml
			BW	G	PC	S	
1	178	286.2	163.76	3.04	67.80	3.69	15.0
2	153	220.3	85.39	0.70	32.37	3.26	24.0
3	128	103.6	53.63	-*	19.33	1.21	7.5
4	101	57.3	27.51	0.25	6.11	0.50	3.0
5	109	87.8	45.66	0.19	10.51	0.80	7.0

* Starfish #3 has undeveloped gonads. BW: body wall, G: gonads, PC: pyloric caeca, S: stomach

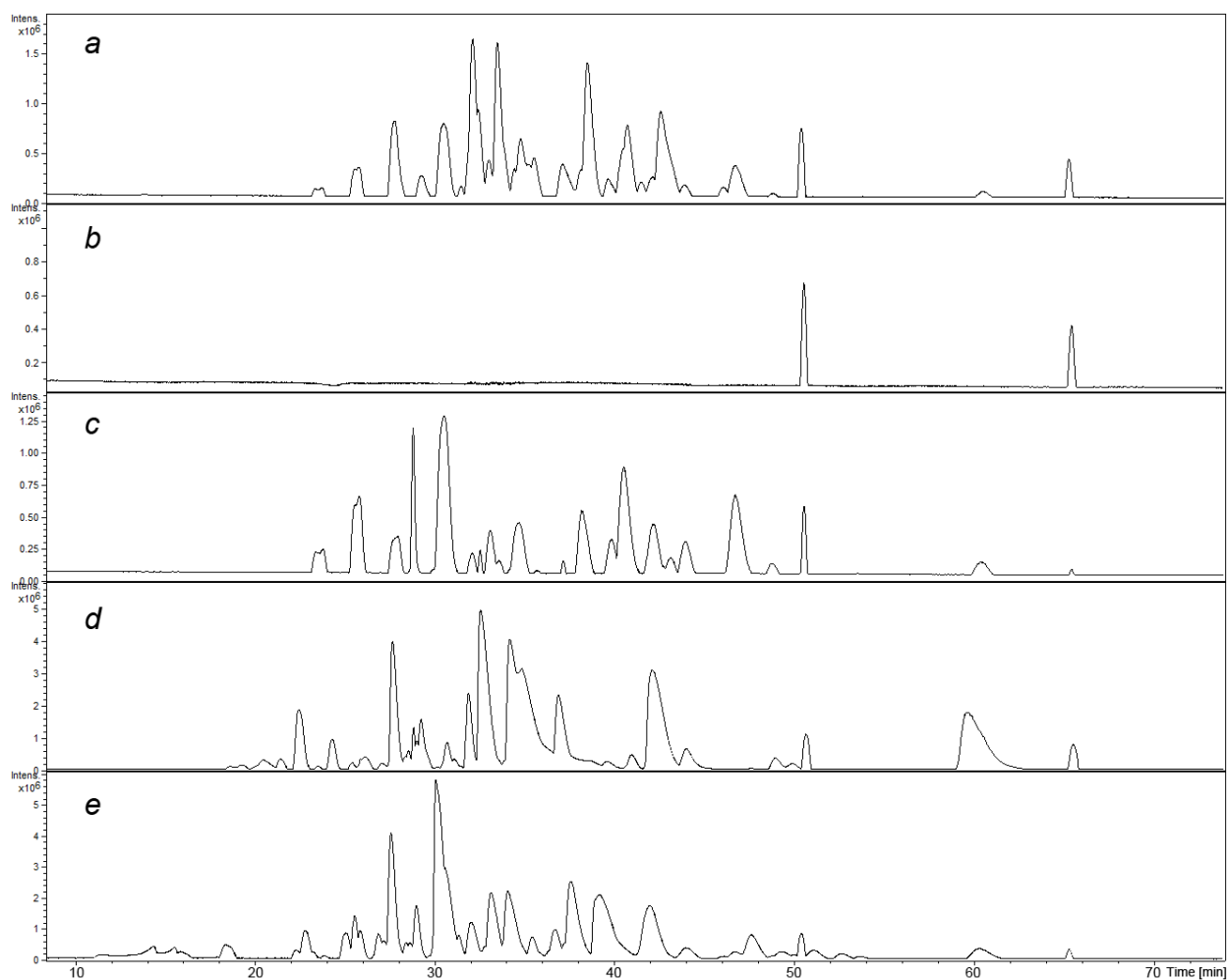


Figure S1. Typical nLC/ESI-QTOF-MS base-peak chromatograms of purified fractions of polar steroid compounds of different body components of the starfish *L. fusca* in negative ion mode: (a) body walls, sample BW#5; (b) coelomic fluid, sample CF#5; (c) gonads, sample G#5; (d) stomach, sample S#1; (e) pyloric caeca, sample PC#1.

Table S2 Batch steps and parameters used for data preprocessing in MZmine

Batch step	Module	Parameters	
Raw data import	-		
Raw data filtering	Crop filter	Retention time:	5 – 80 min
Chromatogram detection	Targeted peak detection	Noise level:	300
		<i>m/z</i> tolerance:	5 ppm
		Retention time tolerance:	3 %
Chromatogram deconvolution	Local minimum search	Chromatographic threshold:	85 %
		Search minimum in Rt range:	0.15
		Minimum absolute height:	1000
		Minimum ratio of peak top/edge:	2
		Peak duration range:	0.1 – 2.0 min
Normalization of retention time	Retention time normalizer	<i>m/z</i> tolerance:	3 ppm
		Retention time tolerance:	0.5 min
		Minimum standard intensity:	50000
Alignment	Join aligner	<i>m/z</i> tolerance:	5 ppm
		Retention time tolerance:	0.5 min
Gap filling	Same RT and <i>m/z</i> range gap filler	<i>m/z</i> tolerance:	5 ppm
Export to CSV			

Table S3. Polar steroids of the starfish *L. fusca* detected by nLC/CSI-QTOF-MS

No ^a	Rt (min)	Elemental composition	Calculated <i>m/z</i>	Measured <i>m/z</i>	Δ (ppm)	Ion type	Proposed structures
1	8.96	C ₃₂ H ₅₆ O ₁₀	599.3801	599.3805	-0.7	[M-H] ⁻	24-O-pentosyl-5 α -cholestane-3 β ,6,8,15 α ,16 β ,24-hexaol
			645.3856	645.3862	-0.9	[M+FA] ⁻	
2	9.15	C ₃₃ H ₅₈ O ₁₂	645.3856	645.3857	-0.2	[M-H] ⁻	24-O-hexosyl-5 α -cholestane-3 β ,6,7,8,15 α ,16 β ,24-heptaol
			691.391	691.3913	-0.4	[M+FA] ⁻	
3	12.69	C ₅₆ H ₉₁ O ₃₂ SNa	1307.522	1307.5223	-0.2	[M-Na] ⁻	Hex-dHex-Hex-Xyl(-Qui)-Qui-AG I
4	13.3	C ₂₇ H ₄₆ O ₈	499.3276	499.3279	-0.6	[M-H] ⁻	5 α -cholestane-3 β ,4 β ,6 α ,7 α ,8,15 α ,16 β ,26-octaol
			545.3331	545.3330	0.2	[M+FA] ⁻	
5	13.77	C ₃₇ H ₆₄ O ₁₃	715.4274	715.4280	-0.8	[M-H] ⁻	fuscaside B
			761.4329	761.4333	-0.5	[M+FA] ⁻	
6	14.06	C ₂₇ H ₄₆ O ₁₁ SNa	575.2532	575.2535	-0.5	[M-Na] ⁻	Hex-AG I
7	14.2	C ₃₃ H ₅₈ O ₁₀	613.3957	613.3962	-0.8	[M-H] ⁻	28-O-pentosyl-5 α -ergostane-3 β ,6,8,15,16 β ,28-hexaol
			659.4012	659.4015	-0.5	[M+FA] ⁻	
8	14.39	C ₅₇ H ₉₄ NO ₂₇ SNa	1256.5739	1256.5743	-0.3	[M-Na] ⁻	dHex-dHex-Qui(-Qui)-(C ₆ H ₉ NO ₃)-AG III
9	14.67	C ₂₇ H ₄₆ O ₁₁ SNa	575.2532	575.2534	-0.3	[M-Na] ⁻	Hex-AG I
10	14.7	C ₃₇ H ₆₄ O ₁₃	715.4274	715.4271	0.4	[M-H] ⁻	distolasteroside D ₁
			761.4329	761.4331	-0.3	[M+FA] ⁻	
11	14.8	C ₂₇ H ₄₆ O ₇	483.3327	483.3337	-2.1	[M-H] ⁻	5 α -cholestane-3 β ,6 α ,7 α ,8,15 α ,16 β ,26-heptaol
			529.3382	529.3387	-0.9	[M+FA] ⁻	
12	14.93	C ₃₃ H ₅₈ O ₁₀	613.3957	613.3963	-1.0	[M-H] ⁻	24-O-hexosyl-5 α -cholestane-3 β ,6,8,15 β ,24-pentaol
			659.4012	659.4019	-1.1	[M+FA] ⁻	
13	15.66	C ₄₉ H ₇₉ O ₂₆ SNa	1115.4586	1115.4599	-1.2	[M-Na] ⁻	dHex-Pent-Xyl(-Qui)-Qui-AG I
14	15.85	C ₃₇ H ₆₂ O ₁₃	713.4118	713.4124	-0.8	[M-H] ⁻	distolasteroside D ₂
			759.2172	759.2172	0.0	[M+FA] ⁻	
15	16.02	C ₂₇ H ₄₆ O ₈	499.3276	499.3284	-1.6	[M-H] ⁻	5 α -cholestane-3 β ,4 β ,6 α ,7 α ,8,15 β ,16 β ,26-octaol
			545.3331	545.3337	-1.1	[M+FA] ⁻	
16	16.14	C ₅₃ H ₈₅ O ₂₈ SNa	1201.4964	1201.4966	-0.2	[M-Na] ⁻	dHex-dHex-Qui(-Qui)-Hex-AG IV
17	16.58	C ₅₆ H ₈₉ O ₃₂ SNa	1305.5063	1305.5068	-0.4	[M-Na] ⁻	Hex-dHex-Hex-Xyl(-Qui)-Qui-AG II
18	17.15	C ₃₂ H ₅₆ O ₉	583.3852	583.3856	-0.7	[M-H] ⁻	pyncnopodioside A
			629.3906	629.3918	-1.9	[M+FA] ⁻	
19	17.7	C ₂₇ H ₄₆ O ₇	483.3327	483.3332	-1.0	[M-H] ⁻	5 α -cholestane-3 β ,6 α ,7 α ,8,15 β ,16 β ,26-heptaol
			529.3382	529.3383	-0.2	[M+FA] ⁻	
20	17.72	C ₅₀ H ₈₁ O ₂₆ SNa	1129.4742	1129.4741	0.1	[M-Na] ⁻	dHex-Pent-Qui(-Qui)-Qui-AG I
21	18.17	C ₃₂ H ₅₄ O ₉	581.3695	581.3704	-1.5	[M-H] ⁻	desulfated minutoside A
			627.375	627.3757	-1.1	[M+FA] ⁻	
22	18.85	C ₅₀ H ₇₉ O ₂₇ SNa	1143.4535	1143.4539	-0.3	[M-Na] ⁻	dHex-Hex-Xyl(-Qui)-Qui-AG II
23	18.86	C ₃₂ H ₅₆ O ₁₁ SNa	695.3318	695.3315	0.4	[M-Na] ⁻	3-O-pentosyl-5 α -cholestane-3 β ,6,7,8,15,16 β ,26-heptaol 26-O-sulfate
24	19.04	C ₂₇ H ₄₆ O ₆	467.3378	467.3375	0.6	[M-H] ⁻	5 α -cholestane-3 β ,6 α ,8,15 β ,16 β ,26-hexaol
			513.3433	513.3428	1.0	[M+FA] ⁻	
25	19.07	C ₅₇ H ₉₃ O ₃₁ SNa	1289.5478	1289.5483	-0.4	[M-Na] ⁻	dHex-dHex-Glc(-Qui)-Qui-AG VI
26	19.16	C ₂₇ H ₄₆ O ₁₁ SNa	559.2582	559.2582	0.0	[M-Na] ⁻	dHex-AG I
27	19.35	C ₅₁ H ₈₁ O ₂₇ SNa	1157.4691	1157.4692	-0.1	[M-Na] ⁻	dHex-dHex-Glc(-Qui)-Qui-AG II
28	19.47	C ₃₈ H ₆₁ O ₁₈ SNa	837.3584	837.3582	0.2	[M-Na] ⁻	Qui-Xyl-Qui-AG I
29	20.01	C ₄₉ H ₇₇ O ₂₆ SNa	1113.4429	1113.4422	0.6	[M-Na] ⁻	dHex-Pent-Xyl(-Qui)-Qui-AG II
30	20.08	C ₂₇ H ₄₆ O ₈ SNa	529.2841	529.2832	1.7	[M-Na] ⁻	-
31	20.11	C ₃₉ H ₆₃ O ₁₉ SNa	867.369	867.3688	0.2	[M-Na] ⁻	Qui-Glc-Qui-AG I
32	20.2	C ₅₇ H ₉₃ O ₃₁ SNa	1289.5478	1289.5472	0.5	[M-Na] ⁻	dHex-dHex-Qui(-Qui)-DXU-AG VI
33	20.25	C ₅₁ H ₈₁ O ₂₇ SNa	1157.4691	1157.4690	0.1	[M-Na] ⁻	dHex-dHex-Qui(-Qui)-DXU-AG II
34	20.3	C ₂₁ H ₃₃ O ₆ SNa	413.2003	413.2003	0.0	[M-Na] ⁻	AG I
35	20.68	C ₅₁ H ₈₁ O ₂₇ SNa	1157.4691	1157.4694	-0.3	[M-Na] ⁻	dHex-dHex-Qui(-Qui)-DXU-AG II
36	21.17	C ₅₁ H ₈₁ O ₂₇ SNa	1157.4691	1157.4681	0.9	[M-Na] ⁻	dHex-Hex-Qui(-Qui)-Qui-AG II
37	21.55	C ₅₀ H ₈₁ O ₂₆ SNa	1129.4742	1129.4743	-0.1	[M-Na] ⁻	dHex-Pent-Qui(-Qui)-Qui-AG I
38	21.72	C ₃₉ H ₆₁ O ₁₉ SNa	865.3533	865.3536	-0.3	[M-Na] ⁻	Qui-Glc-Qui-AG II
39	22.12	C ₃₉ H ₆₃ O ₁₈ SNa	851.3741	851.3747	-0.7	[M-Na] ⁻	Qui-Qui-Qui-AG I
40	22.33	C ₆₂ H ₁₀₁ O ₃₄ SNa	1421.59	1421.5907	-0.5	[M-Na] ⁻	Hex-dHex-Hex-Xyl(-Qui)-Qui-AG VII
41	22.55	C ₆₂ H ₉₉ O ₃₄ SNa	1419.5744	1419.5748	-0.3	[M-Na] ⁻	Hex-dHex-Hex-Xyl(-Qui)-Qui-AG VIII
42	22.57	C ₂₇ H ₄₆ O ₁₁ SNa	559.2582	559.2581	0.2	[M-Na] ⁻	dHex-AG I
43	22.59	C ₅₀ H ₇₉ O ₂₆ SNa	1127.4586	1127.4595	-0.8	[M-Na] ⁻	dHex-Pent-Qui(-Qui)-Qui-AG II

No ^a	Rt (min)	Elemental composition	Calculated <i>m/z</i>	Measured <i>m/z</i>	Δ (ppm)	Ion type	Proposed structures
44	22.94	C ₆₂ H ₁₀₁ O ₃₄ SNa	1421.59	1421.5902	-0.1	[M-Na] ⁻	Hex-dHex-Hex-Xyl(-Qui)-Hex-AG V
45	23.13	C ₃₃ H ₅₇ O ₁₄ SNa	709.3475	709.3480	-0.7	[M-Na] ⁻	24-O-hexosyl-5 α -cholestane-3 β ,6,8,15,16 β ,24-hexaol 3-O-sulfate
46	23.51	C ₃₈ H ₆₅ O ₁₇ SNa	825.3948	825.3951	-0.4	[M-Na] ⁻	3-O-pentosyl-24-O-sulfohexosyl-5 α -cholestane-3 β ,6,8,15,24-pentaol
47	23.56	C ₅₁ H ₈₅ O ₂₆ SNa	1143.4899	1143.4906	-0.6	[M-Na] ⁻	dHex-dHex-Que(-Qui)-Qui-AG I
48	23.8	C ₃₃ H ₅₇ O ₁₄ SNa	693.3525	693.3532	-1.0	[M-Na] ⁻	24-O-hexosyl-5 α -cholestane-3 β ,6,8,15,24-pentaol 3-O-sulfate
49	23.92	C ₆₁ H ₉₉ O ₃₂ SNa	1391.5795	1391.5805	-0.7	[M-Na] ⁻	Hex-dHex-Hex-Xyl(-Qui)-Qui-AG X
50	24.01	C ₅₁ H ₈₅ O ₂₆ SNa	1141.4742	1141.4742	0.0	[M-Na] ⁻	dHex-dHex-Que(-Qui)-Qui-AG II
51	24.36	C ₃₈ H ₆₁ O ₁₈ SNa	837.3584	837.3588	-0.5	[M-Na] ⁻	Qui-Xyl-Que-AG I
52	24.38	C ₅₁ H ₈₁ O ₂₆ SNa	1141.4742	1141.4745	-0.3	[M-Na] ⁻	dHex-dHex-Que(-Qui)-Qui-AG II
53	24.5	C ₃₃ H ₅₇ O ₁₄ SNa	709.3475	709.3487	-1.7	[M-Na] ⁻	24-O-sulfohexosyl-5 α -cholestane-3 β ,6,8,15,16 β ,24-hexaol
54	24.64	C ₂₇ H ₄₁ O ₁₀ SNa	557.2426	557.2422	0.7	[M-Na] ⁻	dHex-AG II
55	24.65	C ₃₂ H ₅₅ O ₁₂ SNa	663.342	663.3420	0.0	[M-Na] ⁻	3-O-pentosyl-5 α -cholestane-3 β ,6,8,15,26-pentaol 26-O-sulfate
56	25	C ₃₃ H ₅₅ O ₁₄ SNa	707.3318	707.3313	0.7	[M-Na] ⁻	26-O-sulfohexosyl-5 α -cholest-22-ene-3 β ,6,8,15,16 β ,26-hexaol
57	25.2	C ₃₉ H ₆₇ O ₁₇ SNa	839.4104	839.4101	0.4	[M-Na] ⁻	3-O-pentosyl-28-O-sulfohexosyl-5 α -ergostane-3 β ,6,8,15,28-pentaol
58	25.29	C ₃₂ H ₅₅ O ₁₃ SNa	677.3212	677.3209	0.4	[M-Na] ⁻	-
59	25.35	C ₃₂ H ₅₅ O ₁₂ SNa	663.342	663.3415	0.8	[M-Na] ⁻	3-O-pentosyl-5 α -cholestane-3 β ,6,8,15,26-pentaol 26-O-sulfate
60	25.43	C ₅₆ H ₉₁ O ₂₈ SNa	1259.5372	1259.5361	0.9	[M-Na] ⁻	dHex-Hex-Xyl(-Qui)-Hex-AG V
61	25.5	C ₅₂ H ₈₀ NO ₂₆ SNa	1166.4695	1166.4698	-0.3	[M-Na] ⁻	dHex-dHex-Que(-Qui)-(C ₇ H ₉ NO ₄)-AG II
62	25.52	C ₅₅ H ₉₁ O ₂₇ SNa	1215.5474	1215.5478	-0.3	[M-Na] ⁻	dHex-Pent-Xyl(-Qui)-Qui-AG XI
63	25.68	C ₂₇ H ₄₇ O ₁₁ SNa	579.2845	579.2857	-2.1	[M-Na] ⁻	5 α -cholestane-3 β ,4,6,7,8,15 α ,16 β ,26-octaol 6-O-sulfate
64	25.74	C ₃₇ H ₆₃ O ₁₆ SNa	795.3842	795.3841	0.1	[M-Na] ⁻	3-O-sulfo-pentosyl-24-O-pentosyl-5 α -cholestane-3 β ,6,8,15,24-pentaol
65	25.97	C ₅₇ H ₉₉ O ₂₈ SNa	1253.5267	1253.5273	-0.5	[M-Na] ⁻	dHex-dHex-Que(-Qui)-Hex-AG XII
66	25.99	C ₅₇ H ₉₉ O ₂₉ SNa	1273.5529	1273.5537	-0.6	[M-Na] ⁻	dHex-dHex-Glc(-Qui)-Qui-AG VII
67	26.11	C ₆₃ H ₁₀₃ O ₃₄ SNa	1435.6057	1435.6061	-0.3	[M-Na] ⁻	Hex-dHex-Hex-Xyl(-Qui)-Hex-AG XIII
68	26.11	C ₃₂ H ₅₅ O ₁₂ SNa	679.3369	679.3379	-1.5	[M-Na] ⁻	24-O-pentosyl-5 α -cholestane-3 β ,6,8,15,16 β ,24-hexaol 3-O-sulfate
69	26.18	C ₃₈ H ₆₅ O ₁₇ SNa	823.3791	823.3797	-0.7	[M-Na] ⁻	3-O-pentosyl-26-O-sulfohexosyl-27-nor-5 α -ergost-22-ene-3 β ,6,8,15,26-pentaol
70	26.27	C ₅₇ H ₉₉ O ₂₉ SNa	1273.5529	1273.5532	-0.2	[M-Na] ⁻	dHex-dHex-Glc(-Qui)-Hex-AG V
71	27.1	C ₃₃ H ₅₅ O ₁₄ SNa	707.3318	707.3323	-0.7	[M-Na] ⁻	26-O-sulfohexosyl-27-nor-5 α -ergost-22-ene-3 β ,6,8,15,16 β ,26-hexaol
72	27.13	C ₃₄ H ₅₇ O ₁₄ SNa	721.3475	721.3464	1.5	[M-Na] ⁻	28-O-sulfohexosyl-5 α -ergost-20(22)-ene-3 β ,6,8,15,16 β ,28-hexaol
73	27.17	C ₂₁ H ₃₁ O ₆ SNa	411.1847	411.1857	-2.4	[M-Na] ⁻	3-O-sulfoasterone (AG II)
74	27.18	C ₅₇ H ₉₉ O ₂₉ SNa	1271.5372	1271.5380	-0.6	[M-Na] ⁻	dHex-dHex-Que(-Qui)-DXU-AG VIII
75	27.3	C ₃₃ H ₅₇ O ₁₂ SNa	677.3576	677.3588	-1.8	[M-Na] ⁻	3-O-pentosyl-5 α -ergostane-3 β ,6,8,15,26-pentaol 26-O-sulfate
76	27.4	C ₃₉ H ₆₅ O ₁₇ SNa	837.3948	837.3953	-0.6	[M-Na] ⁻	3-O-pentosyl-28-O-sulfohexosyl-5 α -ergost-22-ene-3 β ,6,8,15,28-pentaol
77	27.55	C ₅₇ H ₉₉ O ₂₉ SNa	1273.5529	1273.5533	-0.3	[M-Na] ⁻	dHex-dHex-Que(-Qui)-DXU-AG VII
78	27.67	C ₆₂ H ₁₀₁ O ₃₂ SNa	1405.5951	1405.5958	-0.5	[M-Na] ⁻	Hex-dHex-Hex-Xyl(-Qui)-Qui-AG V
79	27.81	C ₅₆ H ₉₉ O ₂₇ SNa	1229.563	1229.5639	-0.7	[M-Na] ⁻	dHex-Pent-Que(-Qui)-Qui-AG XI
80	27.81	C ₅₆ H ₉₁ O ₂₈ SNa	1243.5423	1243.5426	-0.2	[M-Na] ⁻	dHex-dHex-Glc(-Qui)-Qui-AG X
81	27.89	C ₃₂ H ₅₅ O ₁₂ SNa	663.342	663.3426	-0.9	[M-Na] ⁻	24-O-pentosyl-5 α -cholestane-3 β ,6,8,15,24-pentaol 3-O-sulfate
82	27.98	C ₃₃ H ₅₅ O ₁₂ SNa	675.342	675.3424	-0.6	[M-Na] ⁻	3-O-pentosyl-5 α -ergost-20(22)-ene-3 β ,6,8,15,28-pentaol 28-O-sulfate
83	28.1	C ₃₄ H ₅₉ O ₁₄ SNa	723.3631	723.3638	-1.0	[M-Na] ⁻	28-O-sulfohexosyl-5 α -ergostane-3 β ,6,8,15,16 β ,28-hexaol
84	28.15	C ₃₃ H ₅₅ O ₁₂ SNa	691.3369	691.3378	-1.3	[M-Na] ⁻	28-O-pentosyl-5 α -ergost-22-ene-3 β ,6,8,15,16 β ,28-hexaol 3-O-sulfate
85	28.17	C ₃₉ H ₆₅ O ₁₇ SNa	837.3948	837.3958	-1.2	[M-Na] ⁻	3-O-pentosyl-28-O-sulfohexosyl-5 α -ergost-22-ene-3 β ,6,8,15,28-pentaol
86	28.38	C ₃₉ H ₆₅ O ₁₈ SNa	851.3741	851.3750	-1.1	[M-Na] ⁻	Qui-Que-Que-AG I
87	28.5	C ₅₄ H ₈₇ O ₂₇ SNa	1199.5161	1199.5167	-0.5	[M-Na] ⁻	dHex-Pent-Xyl(-Qui)-Qui-AG X
88	28.5	C ₆₃ H ₁₀₃ O ₃₂ SNa	1419.6108	1419.6115	-0.5	[M-Na] ⁻	Hex-dHex-dHex-Glc(-Qui)-Qui-AG V
89	28.59	C ₅₂ H ₈₀ NO ₂₆ SNa	1166.4695	1166.4709	-1.2	[M-Na] ⁻	dHex-dHex-Que(-Qui)-(C ₇ H ₉ NO ₄)-AG II
90	28.6	C ₅₈ H ₉₅ O ₃₁ SNa	1303.5634	1303.5638	-0.3	[M-Na] ⁻	dHex-dHex-Glc(-Qui)-Qui-AG XIV
91	28.69	C ₃₃ H ₅₅ O ₁₄ SNa	707.3318	707.3324	-0.8	[M-Na] ⁻	26-O-sulfohexosyl-27-nor-5 α -ergost-22-ene-3 β ,6,8,15,16 β ,26-hexaol
92	28.93	C ₃₇ H ₆₃ O ₁₆ SNa	795.3842	795.3849	-0.9	[M-Na] ⁻	3-O-pentosyl-24-O-sulfo-pentosyl-5 α -cholestane-3 β ,6,8,15,24-pentaol
93	29	C ₅₇ H ₉₉ O ₂₈ SNa	1257.558	1257.5590	-0.8	[M-Na] ⁻	dHex-dHex-Que(-Qui)-Hex-AG V
94	29.21	C ₃₉ H ₆₅ O ₁₇ SNa	837.3948	837.3953	-0.6	[M-Na] ⁻	3-O-pentosyl-26-O-sulfohexosyl-5 α -ergost-22-ene-3 β ,6,8,15,26-pentaol
95	29.23	C ₆₁ H ₉₉ O ₃₂ SNa	1375.5846	1375.5842	0.3	[M-Na] ⁻	Hex-dHex-Pent-Xyl(-Qui)-Qui-AG IX
96	29.23	C ₃₂ H ₅₅ O ₁₃ SNa	677.3212	677.3203	1.3	[M-Na] ⁻	24-O-pentosyl-5 α -cholest-22-ene-3 β ,6,8,15,16 β ,24-hexaol 3-O-sulfate
97	29.25	C ₅₆ H ₉₅ O ₂₇ SNa	1229.563	1229.5624	0.5	[M-Na] ⁻	dHex-Pent-Xyl(-Qui)-Qui-AG XV
98	29.44	C ₆₂ H ₁₀₃ O ₃₂ SNa	1391.6159	1391.6155	0.3	[M-Na] ⁻	Hex-dHex-Pent-Xyl(-Qui)-Qui-AG XV
99	29.53	C ₃₄ H ₅₇ O ₁₄ SNa	721.3475	721.3471	0.6	[M-Na] ⁻	28-O-sulfohexosyl-5 α -ergost-20(22)-ene-3 β ,6,8,15,16 β ,28-hexaol
100	29.64	C ₃₇ H ₆₃ O ₁₆ SNa	795.3842	795.3835	0.9	[M-Na] ⁻	3-O-pentosyl-24-O-sulfo-pentosyl-5 α -cholestane-3 β ,6,8,15,24-pentaol
101	29.7	C ₂₇ H ₄₇ O ₁₀ SNa	563.2895	563.2901	-1.1	[M-Na] ⁻	5 α -cholestane-3 β ,6,7,8,15 α ,16 β ,26-heptaol 6-O-sulfate
102	29.87	C ₃₅ H ₅₉ O ₁₄ SNa	735.3631	735.3628	0.4	[M-Na] ⁻	29-O-sulfohexosyl-5 α -stigmast-20(22)-ene-3 β ,6,8,15,16 β ,29-hexaol

No ^a	Rt (min)	Elemental composition	Calculated m/z	Measured m/z	Δ (ppm)	Ion type	Proposed structures
103	29.92	C ₃₄ H ₅₇ O ₁₄ SNa	705.3525	705.3527	-0.3	[M-Na] ⁻	28-O-sulfohexosyl-5 α -ergost-20(22)-ene-3 β ,6,8,15,28-pentaol
104	30.11	C ₅₆ H ₉₅ O ₂₈ SNa	1245.558	1245.5576	0.3	[M-Na] ⁻	dHex-Hex-Xyl(-Qui)-Hex-AG XX
105	30.3	C ₅₈ H ₉₅ O ₂₈ SNa	1287.5685	1287.5681	0.3	[M-Na] ⁻	dHex-dHex-Glc(-Qui)-Hex-AG XIII
106	30.3	C ₆₂ H ₁₀₁ O ₃₂ SNa	1389.6002	1389.6003	-0.1	[M-Na] ⁻	dHex-dHex-Hex-Xyl(-Qui)-Qui-AG V
107	30.39	C ₃₃ H ₅₇ O ₁₃ SNa	693.3525	693.3533	-1.2	[M-Na] ⁻	pyncopodioside C
108	30.41	C ₃₈ H ₆₅ O ₁₆ SNa	809.3999	809.4004	-0.6	[M-Na] ⁻	3-O-pentosyl-24-O-methylsulfohexosyl-5 α -cholestane-3 β ,6,8,15,24-pentaol
109	30.63	C ₃₂ H ₅₅ O ₁₂ SNa	661.3263	661.3266	-0.5	[M-Na] ⁻	24-O-pentosyl-5 α -cholest-22-ene-3 β ,6,8,15,24-pentaol 3-O-sulfate
110	30.67	C ₆₂ H ₁₀₁ O ₃₂ SNa	1389.6002	1389.6007	-0.4	[M-Na] ⁻	Hex-dHex-dHex-Xyl(-Qui)-Qui-AG V
111	30.86	C ₅₇ H ₉₅ O ₂₈ SNa	1273.5529	1273.5538	-0.7	[M-Na] ⁻	dHex-Hex-Glc(-Qui)-Qui-AG V
112	30.99	C ₆₂ H ₁₀₁ O ₃₂ SNa	1405.5951	1405.5959	-0.6	[M-Na] ⁻	Hex-dHex-Hex-Xyl(-Qui)-Hex-AG XVII
113	31.05	C ₃₄ H ₅₇ O ₁₃ SNa	721.3475	721.3486	-1.5	[M-Na] ⁻	26-O-sulfohexosyl-5 α -ergost-22-ene-3 β ,6,8,15,16 β ,26-hexaol
114	31.39	C ₃₈ H ₆₅ O ₁₆ SNa	807.3842	807.3844	-0.2	[M-Na] ⁻	3-O-pentosyl-28-O-sulfohexosyl-5 α -ergost-20(22)-ene-3 β ,6,8,15,28-pentaol
115	31.46	C ₃₅ H ₅₅ O ₁₃ SNa	691.3369	691.3380	-1.6	[M-Na] ⁻	24-O-sulfohexosyl-5 α -cholest-20(22)-ene-3 β ,6,8,15,24-pentaol
116	31.71	C ₆₃ H ₁₀₅ O ₃₃ SNa	1419.6108	1419.6112	-0.3	[M-Na] ⁻	Hex-dHex-Hex-Xyl(-Qui)-Qui-AG XIII
117	31.72	C ₂₇ H ₄₇ O ₉ SNa	547.2946	547.2953	-1.3	[M-Na] ⁻	5 α -cholestane-3 β ,6,8,15 α ,16 β ,26-hexaol 6-O-sulfate
118	31.77	C ₅₆ H ₉₁ O ₂₈ SNa	1243.5423	1243.5423	0.0	[M-Na] ⁻	Fuc-Gal-Xyl(-Qui)-Qui-AG V (thornasteroside A)
119	32.14	C ₄₀ H ₆₇ O ₁₈ SNa	867.4054	867.4058	-0.5	[M-Na] ⁻	28-O-[sulfohexosyl-hexosyl]-5 α -ergost-22-ene-3 β ,6,8,15,28-pentaol
120	32.22	C ₃₄ H ₅₉ O ₁₄ SNa	723.3631	723.3636	-0.7	[M-Na] ⁻	28-O-sulfohexosyl-5 α -ergostane-3 β ,6,8,15,16 β ,28-hexaol
121	32.27	C ₅₇ H ₉₅ O ₂₈ SNa	1259.5736	1259.5748	-1.0	[M-Na] ⁻	dHex-Hex-Qui(-Qui)-Hex-AG XX
122	32.31	C ₅₇ H ₉₅ O ₂₈ SNa	1257.558	1257.5581	-0.1	[M-Na] ⁻	Fuc-Qui-Glc(-Qui)-Qui-AG V (luidiaquinoside)
123	32.36	C ₆₂ H ₁₀₅ O ₃₂ SNa	1391.6159	1391.6166	-0.5	[M-Na] ⁻	Hex-dHex-Hex-Xyl(-Qui)-Qui-AG XX
124	32.71	C ₃₂ H ₅₅ O ₁₂ SNa	679.3369	679.3380	-1.6	[M-Na] ⁻	24-O-sulfohexosyl-5 α -cholestane-3 β ,6,8,15,16 β ,24-hexaol
125	32.88	C ₃₃ H ₅₅ O ₁₃ SNa	691.3369	691.3377	-1.2	[M-Na] ⁻	-
126	33.07	C ₃₄ H ₅₉ O ₁₃ SNa	707.3682	707.3686	-0.6	[M-Na] ⁻	28-O-sulfohexosyl-5 α -ergostane-3 β ,6,8,15,28-pentaol
127	33.37	C ₃₄ H ₅₇ O ₁₄ SNa	721.3475	721.3487	-1.7	[M-Na] ⁻	26-O-sulfohexosyl-5 α -ergost-22-ene-3 β ,6,8,15,16 β ,26-hexaol
128	33.47	C ₅₆ H ₉₅ O ₂₇ SNa	1229.563	1229.5636	-0.5	[M-Na] ⁻	dHex-Pent-Qui(-Qui)-Hex-AG XX
129	33.56	C ₆₃ H ₁₀₅ O ₃₂ SNa	1403.6159	1403.6164	-0.4	[M-Na] ⁻	Hex-dHex-dHex-Qui(-Qui)-Qui-AG V
130	33.78	C ₆₂ H ₁₀₁ O ₃₂ SNa	1389.6002	1389.6006	-0.3	[M-Na] ⁻	Hex-dHex-Pent-Xyl(-Qui)-Qui-AG XIII
131	33.84	C ₃₃ H ₅₅ O ₁₃ SNa	691.3369	691.3371	-0.3	[M-Na] ⁻	26-O-sulfohexosyl-27-nor-5 α -ergost-20(22)-ene-3 β ,6,8,15,26-pentaol
132	33.85	C ₅₅ H ₈₉ O ₂₇ SNa	1213.5317	1213.5320	-0.2	[M-Na] ⁻	dHex-Pent-Xyl(-Qui)-Qui-AG IX
133	34.08	C ₂₇ H ₄₇ O ₉ SNa	547.2946	547.2960	-2.6	[M-Na] ⁻	5 α -cholestane-3 β ,6,8,15 β ,16 β ,26-hexaol 6-O-sulfate
134	34.13	C ₃₃ H ₅₅ O ₁₂ SNa	675.342	675.3421	-0.1	[M-Na] ⁻	3-O-pentosyl-5 α -ergost-22-ene-3 β ,6,8,15,26-pentaol 26-O-sulfate
135	34.34	C ₅₇ H ₉₅ O ₂₈ SNa	1257.558	1257.5589	-0.7	[M-Na] ⁻	dHex-dHex-Qui(-Qui)-DXU-AG V
136	34.36	C ₂₇ H ₄₇ O ₉ SNa	531.2997	531.3002	-0.9	[M-Na] ⁻	5 α -cholestane-3 β ,6,8,15,24-pentaol 24-O-sulfate
137	34.41	C ₆₁ H ₁₀₁ O ₃₁ SNa	1361.6053	1361.6050	0.2	[M-Na] ⁻	Hex-dHex-Pent-Xyl(-Qui)-Qui-AG XX
138	34.51	C ₃₃ H ₅₅ O ₁₃ SNa	691.3369	691.3367	0.3	[M-Na] ⁻	26-O-sulfohexosyl-27-nor-5 α -ergost-20(22)-ene-3 β ,6,8,15,26-pentaol
139	34.6	C ₃₂ H ₅₅ O ₁₂ SNa	663.342	663.3413	1.1	[M-Na] ⁻	coscinasteroside B
140	34.72	C ₅₇ H ₉₅ O ₂₇ SNa	1243.5787	1243.5788	-0.1	[M-Na] ⁻	dHex-dHex-Qui(-Qui)-Hex-AG XX
141	34.8	C ₂₇ H ₄₇ O ₉ SNa	547.2946	547.2960	-2.6	[M-Na] ⁻	5 α -cholestane-3 β ,6,8,15,16 β ,24-hexaol 3-O-sulfate
142	35.03	C ₃₂ H ₅₅ O ₁₂ SNa	663.342	663.3426	-0.9	[M-Na] ⁻	-
143	35.52	C ₅₆ H ₈₉ O ₂₇ SNa	1225.5317	1225.5310	0.6	[M-Na] ⁻	dHex-Pent-Qui(-Qui)-Hex-AG XXI
144	35.66	C ₆₂ H ₁₀₁ O ₃₁ SNa	1373.6053	1373.6041	0.9	[M-Na] ⁻	Hex-dHex-dHex-Xyl(-Qui)-Qui-AG XXII
145	35.7	C ₃₈ H ₆₅ O ₁₆ SNa	809.3999	809.4002	-0.4	[M-Na] ⁻	3-O-pentosyl-24-O-methylsulfohexosyl-5 α -cholestane-3 β ,6,8,15,24-pentaol
146	35.74	C ₂₈ H ₄₇ O ₁₀ SNa	575.2895	575.2903	-1.4	[M-Na] ⁻	5 α -ergost-22-ene-3 β ,6,7,8,15 α ,16 β ,26-heptaol 6-O-sulfate
147	36.02	C ₃₅ H ₅₉ O ₁₄ SNa	735.3631	735.3623	1.1	[M-Na] ⁻	29-O-sulfohexosyl-5 α -stigmast-20(22)-ene-3 β ,6,8,15,16 β ,29-hexaol
148	36.2	C ₃₄ H ₅₇ O ₁₄ SNa	721.3475	721.3478	-0.4	[M-Na] ⁻	28-O-sulfohexosyl-5 α -ergost-22-ene-3 β ,6,8,15,16 β ,28-hexaol
149	36.33	C ₆₂ H ₁₀₅ O ₃₁ SNa	1375.621	1375.6209	0.1	[M-Na] ⁻	Hex-dHex-dHex-Xyl(-Qui)-Qui-AG XX
150	36.87	C ₅₇ H ₉₁ O ₂₇ SNa	1239.5474	1239.5470	0.3	[M-Na] ⁻	dHex-dHex-Qui(-Qui)-Hex-AG XXI
151	37.13	C ₃₃ H ₅₅ O ₁₃ SNa	691.3369	691.3371	-0.3	[M-Na] ⁻	28-O-sulfohexosyl-5 α -ergost-20(22)-ene-3 β ,6,8,15,16 β ,28-hexaol
152	37.34	C ₅₇ H ₉₅ O ₂₈ SNa	1257.558	1257.5578	0.2	[M-Na] ⁻	dHex-dHex-Glc(-Qui)-Hex-AG XXII
153	37.56	C ₂₈ H ₄₇ O ₉ SNa	559.2946	559.2942	0.7	[M-Na] ⁻	5 α -ergost-22-ene-3 β ,6,8,15,16 β ,26-hexaol 6-O-sulfate
154	37.92	C ₃₄ H ₅₇ O ₁₃ SNa	705.3525	705.3525	0.0	[M-Na] ⁻	28-O-sulfohexosyl-5 α -ergost-22-ene-3 β ,6,8,15,28-pentaol
155	37.99	C ₃₂ H ₅₅ O ₁₂ SNa	663.342	663.3417	0.5	[M-Na] ⁻	24-O-sulfohexosyl-5 α -cholestane-3 β ,6,8,15,24-pentaol
156	38.49	C ₃₈ H ₉₂ NO ₂₈ SNa	1282.5532	1282.5519	1.0	[M-Na] ⁻	dHex-dHex-Glc(-Qui)-(C ₇ H ₉ NO ₄)-AG V
157	38.53	C ₅₇ H ₉₅ O ₂₈ SNa	1257.558	1257.5571	0.7	[M-Na] ⁻	dHex-Hex-Qui(-Qui)-Hex-AG XXII
158	38.58	C ₆₄ H ₁₀₅ O ₃₃ SNa	1433.6264	1433.6251	0.9	[M-Na] ⁻	Hex-dHex-Hex-Xyl(-Qui)-Qui-AG XVI
159	38.62	C ₅₆ H ₉₅ O ₂₇ SNa	1229.563	1229.5628	0.2	[M-Na] ⁻	Fuc-Gal-Xyl(-Qui)-Qui-AG XVIII (lethasteroside B)

No ^a	Rt (min)	Elemental composition	Calculated m/z	Measured m/z	Δ (ppm)	Ion type	Proposed structures
160	38.88	C ₅₈ H ₉₅ O ₂₈ SNa	1271.5736	1271.5733	0.2	[M-Na] ⁻	dHex-dHex-Glc(-Qui)-Qui-AG XIII
161	39.07	C ₄₅ H ₇₅ O ₂₃ SNa	965.4421	965.4422	-0.1	[M-Na] ⁻	Qui-Glc-Qui-AG V
162	39.19	C ₃₅ H ₆₁ O ₁₅ SNa	753.3737	753.3748	-1.5	[M-Na] ⁻	29-O-sulfohexosyl-5 α -stigmastane-3 β ,6,7,8,15,16 β ,29-heptaol
163	39.36	C ₃₅ H ₆₁ O ₁₅ SNa	737.3788	737.3794	-0.8	[M-Na] ⁻	29-O-sulfohexosyl-5 α -stigmastane-3 β ,6,8,15,16 β ,29-hexaol
164	39.45	C ₃₄ H ₅₇ O ₁₄ SNa	705.3525	705.3533	-1.1	[M-Na] ⁻	26-O-sulfohexosyl-5 α -ergost-22-ene-3 β ,6,8,15,26-pentaol
165	39.47	C ₃₄ H ₅₇ O ₁₄ SNa	721.3475	721.3481	-0.8	[M-Na] ⁻	28-O-sulfohexosyl-5 α -ergost-22-ene-3 β ,6,8,15,16 β ,28-hexaol
166	39.55	C ₆₂ H ₁₀₁ O ₃₂ SNa	1389.6002	1389.6001	0.1	[M-Na] ⁻	Gal-Fuc-Gal-Xyl(-Qui)-Qui-AG XVII (anasteroside A)
167	39.55	C ₃₅ H ₅₉ O ₁₄ SNa	735.3631	735.3635	-0.5	[M-Na] ⁻	29-O-sulfohexosyl-5 α -stigmast-20(22)-ene-3 β ,6,8,15,16 β ,29-hexaol
168	39.92	C ₅₇ H ₉₅ O ₂₇ SNa	1243.5787	1243.5785	0.2	[M-Na] ⁻	dHex-dHex-Glc(-Qui)-Qui-AG XX
169	40.11	C ₃₂ H ₅₅ O ₁₂ SNa	663.342	663.3421	-0.2	[M-Na] ⁻	24-O-sulfopentosyl-5 α -cholestane-3 β ,6,8,15,24-pentaol
170	40.12	C ₅₈ H ₉₅ O ₂₈ SNa	1271.5736	1271.5730	0.5	[M-Na] ⁻	dHex-dHex-Glc(-Qui)-Qui-AG XIII
171	40.47	C ₃₄ H ₅₇ O ₁₄ SNa	705.3525	705.3534	-1.3	[M-Na] ⁻	28-O-sulfohexosyl-5 α -ergost-22-ene-3 β ,6,8,15,28-pentaol
172	40.47	C ₃₃ H ₅₇ O ₁₂ SNa	677.3576	677.3584	-1.2	[M-Na] ⁻	24-O-methylsulfopentosyl-5 α -cholestane-3 β ,6,8,15,24-pentaol
173	40.68	C ₅₆ H ₉₁ O ₂₇ SNa	1227.5474	1227.5465	0.7	[M-Na] ⁻	dHex-Pent-Qui(-Qui)-Hex-AG XXII
174	40.8	C ₂₇ H ₄₁ O ₈ SNa	525.2528	525.2523	1.0	[M-Na] ⁻	AG VIII
175	40.87	C ₅₇ H ₉₅ O ₂₇ SNa	1241.563	1241.5623	0.6	[M-Na] ⁻	dHex-dHex-Qui(-Qui)-Qui-AG V
176	40.87	C ₆₃ H ₁₀₃ O ₃₂ SNa	1403.6159	1403.6157	0.1	[M-Na] ⁻	Hex-dHex-dHex-Glc(-Qui)-Qui-AG XXII
177	41.41	C ₅₅ H ₉₁ O ₂₆ SNa	1199.5525	1199.5522	0.3	[M-Na] ⁻	dHex-Pent-Xyl(-Qui)-Qui-AG XVIII
178	41.8	C ₂₇ H ₄₃ O ₈ SNa	527.2684	527.2682	0.4	[M-Na] ⁻	AG VII
179	41.98	C ₃₄ H ₅₇ O ₁₄ SNa	705.3525	705.3539	-2.0	[M-Na] ⁻	26-O-sulfohexosyl-5 α -ergost-22-ene-3 β ,6,8,15,26-pentaol
180	42.17	C ₅₇ H ₉₅ O ₂₆ SNa	1221.5368	1221.5369	-0.1	[M-Na] ⁻	dHex-dHex-Qui(-Qui)-(C ₆ H ₅ O ₂)-AG V
181	42.2	C ₃₅ H ₆₁ O ₁₄ SNa	737.3788	737.3792	-0.5	[M-Na] ⁻	29-O-sulfohexosyl-5 α -stigmastane-3 β ,6,8,15,16 β ,29-hexaol
182	42.31	C ₅₇ H ₉₅ O ₂₇ SNa	1241.563	1241.5628	0.2	[M-Na] ⁻	dHex-dHex-Qui(-Qui)-Hex-AG XXII
183	42.4	C ₃₅ H ₅₉ O ₁₄ SNa	735.3631	735.3632	-0.1	[M-Na] ⁻	29-O-sulfohexosyl-5 α -stigmast-22-ene-3 β ,6,8,15,16 β ,29-hexaol
184	42.55	C ₃₃ H ₅₅ O ₁₂ SNa	675.342	675.3424	-0.6	[M-Na] ⁻	28-O-sulfopentosyl-5 α -ergost-20(22)-ene-3 β ,6,8,15,28-pentaol
185	42.96	C ₃₅ H ₆₁ O ₁₄ SNa	721.3838	721.3845	-1.0	[M-Na] ⁻	29-O-sulfohexosyl-5 α -stigmastane-3 β ,6,8,15,29-pentaol
186	43.07	C ₅₈ H ₉₂ NO ₂₇ SNa	1266.5583	1266.5584	-0.1	[M-Na] ⁻	dHex-dHex-Qui(-Qui)-(C ₆ H ₅ NO ₂)-AG V
187	43.19	C ₅₇ H ₈₉ O ₂₆ SNa	1221.5368	1221.5374	-0.5	[M-Na] ⁻	dHex-dHex-Qui(-Qui)-(C ₆ H ₅ O ₂)-AG V
188	43.69	C ₃₃ H ₅₅ O ₁₂ SNa	675.342	675.3427	-1.0	[M-Na] ⁻	28-O-sulfopentosyl-5 α -ergost-20(22)-ene-3 β ,6,8,15,28-pentaol
189	43.86	C ₃₅ H ₅₉ O ₁₄ SNa	735.3631	735.3640	-1.2	[M-Na] ⁻	29-O-sulfohexosyl-5 α -stigmast-22-ene-3 β ,6,8,15,16 β ,29-hexaol
190	43.97	C ₅₇ H ₉₅ O ₂₇ SNa	1243.5787	1243.5799	-1.0	[M-Na] ⁻	dHex-dHex-Qui(-Qui)-DXU-AG XVIII
191	44.75	C ₅₈ H ₉₅ O ₂₈ SNa	1271.5436	1271.5448	-0.9	[M-Na] ⁻	dHex-dHex-Qui(-Qui)-DXU-AG XIII
192	44.81	C ₆₂ H ₁₀₁ O ₃₁ SNa	1373.6053	1373.6056	-0.2	[M-Na] ⁻	dHex-dHex-Hex-Xyl(-Qui)-Qui-AG XXII
193	45.81	C ₆₂ H ₁₀₁ O ₃₁ SNa	1373.6053	1373.6053	0.0	[M-Na] ⁻	Hex-dHex-dHex-Xyl(-Qui)-Qui-AG XVII
194	45.82	C ₆₃ H ₁₀₃ O ₃₂ SNa	1403.6159	1403.6164	-0.4	[M-Na] ⁻	Hex-dHex-Hex-Xyl(-Qui)-Qui-AG XXIII
195	45.99	C ₅₇ H ₉₁ O ₂₇ SNa	1239.5474	1239.5473	0.1	[M-Na] ⁻	dHex-dHex-Qui(-Qui)-DXU-AG XIX
196	46.45	C ₃₂ H ₅₅ O ₁₂ SNa	661.3263	661.3261	0.3	[M-Na] ⁻	24-O-sulfopentosyl-5 α -cholest-22-ene-3 β ,6,8,15,24-pentaol
197	47.6	C ₃₅ H ₆₁ O ₁₄ SNa	737.3788	737.3793	-0.7	[M-Na] ⁻	29-O-sulfohexosyl-5 α -stigmastane-3 β ,6,8,15,16 β ,29-hexaol
198	48.4	C ₅₆ H ₉₁ O ₂₇ SNa	1227.5474	1227.5470	0.3	[M-Na] ⁻	Fuc-Gal-Xyl(-Qui)-Qui-AG XVII (lethasteroside A)
199	48.83	C ₅₈ H ₉₂ NO ₂₇ SNa	1266.5583	1266.5580	0.2	[M-Na] ⁻	dHex-dHex-Qui(-Qui)-(C ₆ H ₅ NO ₂)-AG V
200	50.2	C ₅₇ H ₉₅ O ₂₇ SNa	1241.563	1241.5635	-0.4	[M-Na] ⁻	dHex-dHex-Glc(-Qui)-Qui-AG XVII
201	50.98	C ₆₃ H ₁₀₃ O ₃₁ SNa	1387.621	1387.6211	-0.1	[M-Na] ⁻	Hex-dHex-dHex-Qui(-Qui)-Qui-AG XVII
202	52.5	C ₃₃ H ₅₇ O ₁₂ SNa	677.3576	677.3588	-1.8	[M-Na] ⁻	24-O-methylsulfopentosyl-5 α -cholestane-3 β ,6,8,15,24-pentaol
203	53.28	C ₅₇ H ₉₅ O ₂₇ SNa	1241.563	1241.5636	-0.5	[M-Na] ⁻	dHex-dHex-Qui(-Qui)-DXU-AG XVII
204	55.29	C ₃₄ H ₅₉ O ₁₃ SNa	707.3682	707.3689	-1.0	[M-Na] ⁻	29-O-sulfopentosyl-5 α -stigmastane-3 β ,6,8,15,16 β ,29-hexaol
205	59.82	C ₂₇ H ₄₅ O ₇ SNa	511.2735	511.2749	-2.7	[M-Na] ⁻	3-O-sulfothornasterol A (AG V)
206	66.76	C ₅₇ H ₉₅ O ₂₆ SNa	1225.5681	1225.5685	-0.3	[M-Na] ⁻	dHex-dHex-Qui(-Qui)-Qui-AG XVII
207	72.27	C ₂₇ H ₄₅ O ₈ SNa	495.2786	495.2795	-1.8	[M-Na] ⁻	3-O-sulfo-24,25-dihydromarthasterone (AG XVII)

^a The number of the peaks on (-)LC/MS chromatogram

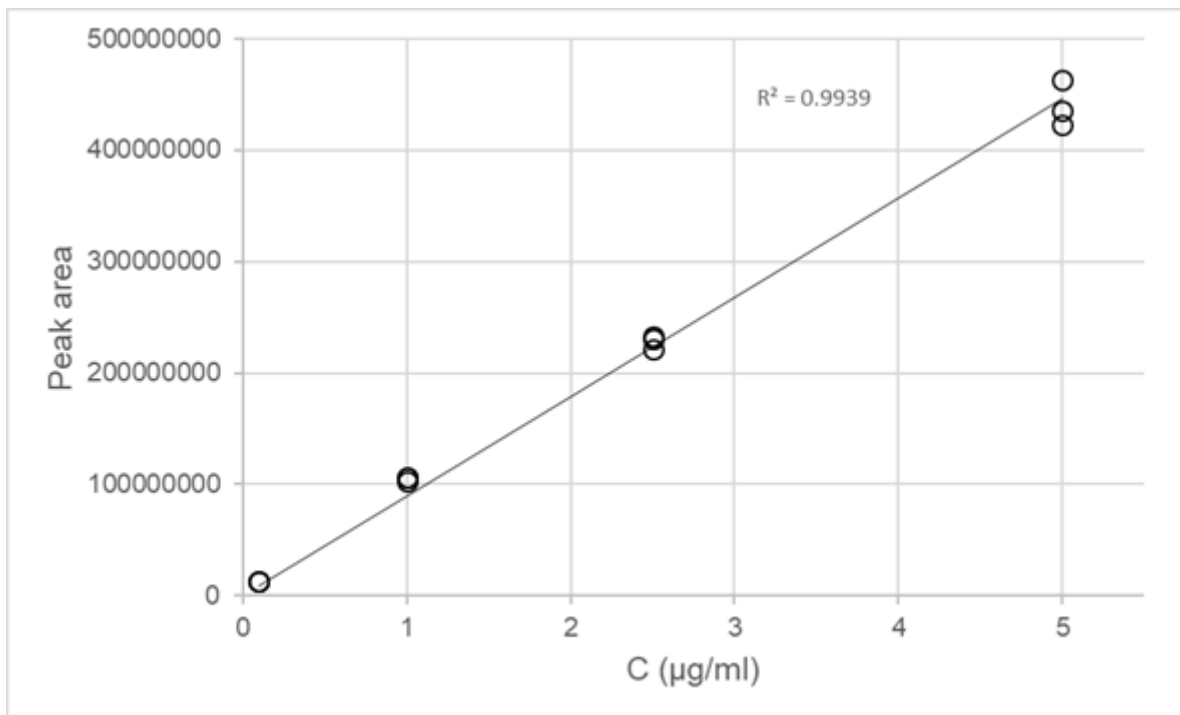


Figure 2S. Calibration curve for fuscaside A (ion $[M - \text{Na}]^-$ at m/z 795.38)

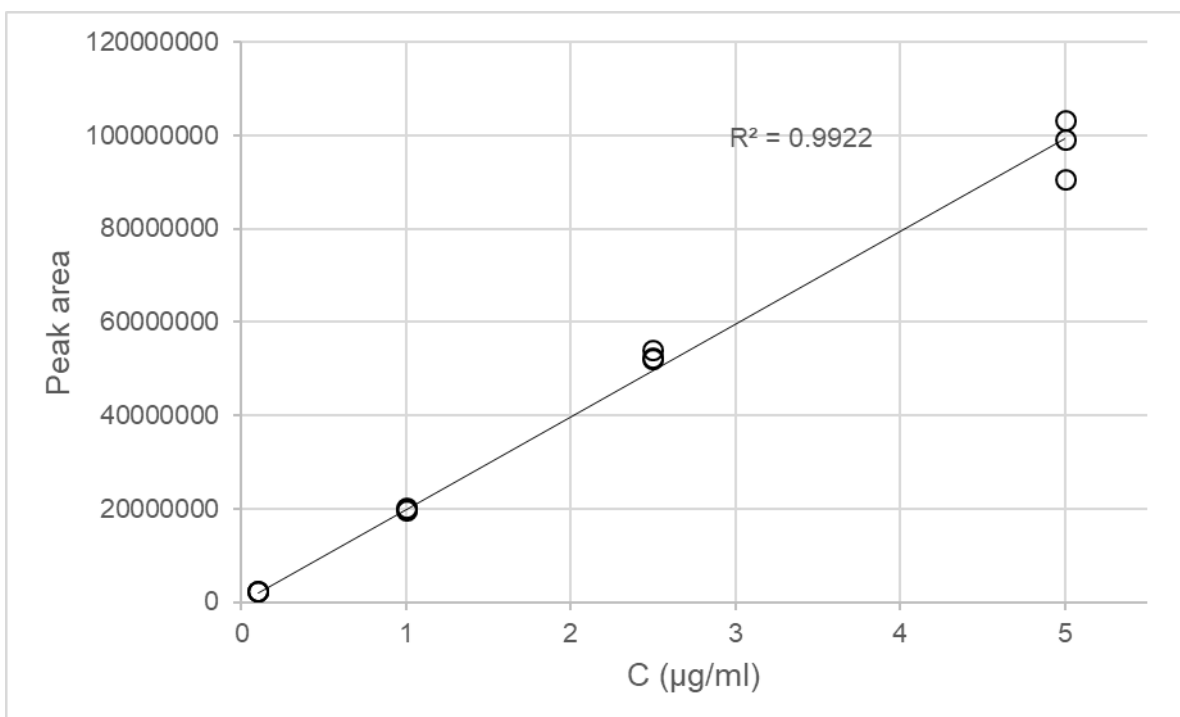


Figure 3S. Calibration curve for lethasterioside A (ion $[M - \text{Na}]^-$ at m/z 1227.54)

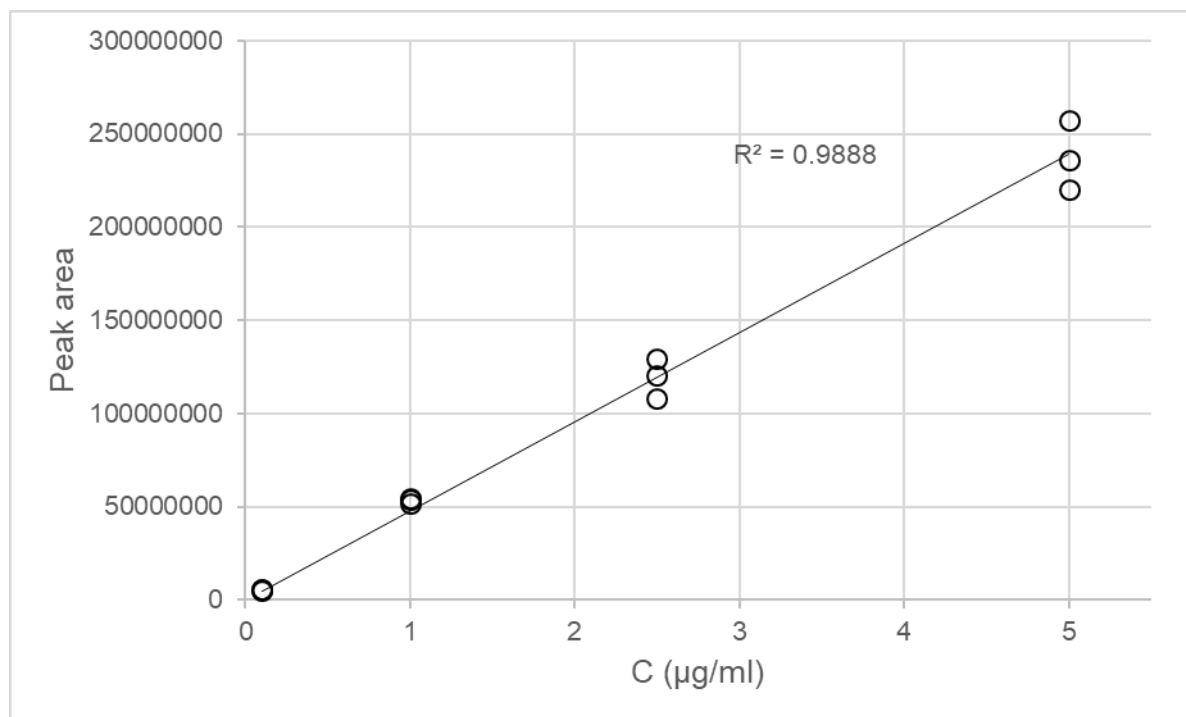


Figure 4S. Calibration curve for 5 α -cholestan-3 β ,4 β ,6 α ,7 α ,8,15 β ,16 β ,26-octal (for the sum of ion intensities [M - H]⁻ at m/z 499.33 and [M + FA]⁻ at m/z 545.3)

Table S4 Content of detected compounds in different organs and coelomic fluid of the starfish *L. fusca* (ng/g wet weight of the organs for BW, G, PC, and S and ng/ml for CF) and result of statistical analysis (ANOVA followed by Tukey HSD test of multiple comparisons was performed for BW, G, PC, and S groups; q-value < 0.05 was considered statistically significant).

N	Body Walls					Coelomic fluid					Gonads					Pyloric caeca					Stomach					p-value	q-value	Tukey's HSD
	BW#1	BW#2	BW#3	BW#4	BW#5	CF1	CF2	CF3	CF4	CF5	G#1	G#2	G#4	G#5	PC#1	PC#2	PC#3	PC#4	PC#5	S#1	S#2	S#3	S#4	S#5				
1	0.1	1.0	1.3	2.1	0.9	nd	nd	nd	nd	nd	0.5	<0.1	1.6	15.2	152.9	175.5	334.7	757.5	428.4	3.8	2.1	20.2	14.0	6.9	0.001	0.003	PC-BW; PC-G; S-PC	
2	0.4	0.2	0.9	3.9	2.2	nd	nd	nd	nd	nd	0.2	nd	2.7	11.1	167.7	171.0	375.4	952.5	441.0	8.4	3.3	12.5	22.7	9.3	0.002	0.009	PC-BW; PC-G; S-PC	
3	1.1	55.1	40.1	36.2	4.8	0.1	0.1	nd	nd	nd	nd	0.8	1.9	0.3	0.1	0.2	0.2	2.3	1.4	5.3	6.6	7.0	7.9	4.1	0.011	0.034	G-BW; PC-BW; S-BW	
4	0.2	0.1	0.1	0.3	0.1	nd	nd	nd	nd	nd	nd	nd	nd	1.0	122.8	52.8	132.6	202.4	108.4	1.3	0.6	1.2	1.5	0.8	<0.001	<0.001	PC-BW; PC-G; S-PC	
5	28.4	11.6	4.3	23.4	4.5	nd	0.1	nd	nd	nd	54.0	38.7	26.1	33.1	3304.0	12328.5	681.4	3065.1	262.5	56.7	101.7	19.2	64.2	7.5	0.068	0.105	-	
6	242.4	1244.9	2.4	17.9	1059.9	0.6	2.5	nd	nd	1.8	26.0	37.8	4.3	57.8	32.2	31.0	33.9	86.5	70.2	15.8	24.2	39.0	46.2	33.8	0.068	0.133	-	
7	0.3	0.7	2.9	21.6	168.2	nd	nd	nd	nd	nd	3.7	1.3	9.8	307.3	372.0	239.2	1207.3	3870.7	13159.6	6.4	4.7	28.4	69.0	84.0	0.137	0.161	-	
8	0.1	nd	0.2	0.3	nd	nd	nd	nd	nd	nd	61.5	3.3	2.0	1.7	2.2	1.5	1.6	6.3	2.6	32.6	26.4	45.7	172.0	32.3	0.046	0.099	-	
9	85.1	441.5	3.3	6.7	305.6	0.3	1.3	0.1	<0.1	0.7	23.4	23.2	2.8	23.7	13.6	11.4	20.5	49.8	32.7	28.4	36.1	43.0	97.7	47.6	0.126	0.198	-	
10	29.8	449.3	0.4	3.1	4.2	<0.1	0.3	<0.1	<0.1	nd	34.7	21.4	3.7	14.9	5697.7	21395.2	687.9	3043.8	441.0	84.2	149.3	8.2	39.0	9.0	0.117	0.145	-	
11	0.6	0.2	0.1	0.5	0.6	nd	nd	nd	nd	nd	0.1	<0.1	0.4	3.6	340.6	89.4	171.3	752.5	275.9	5.6	2.2	7.2	19.0	7.2	0.003	0.01	PC-BW; PC-G; S-PC	
12	0.4	0.4	3.1	9.5	78.3	nd	nd	nd	nd	nd	3.0	0.8	7.3	323.1	391.1	238.7	428.9	4106.0	13195.0	1.2	2.1	18.3	38.2	124.9	0.164	0.186	-	
13	2.2	335.1	0.8	0.6	78.4	nd	1.0	nd	nd	nd	15.3	17.4	nd	5.0	9.0	17.0	10.8	28.7	19.8	11.6	11.5	10.4	6.0	5.2	0.369	0.426	-	
14	2.2	12.0	<0.1	<0.1	nd	nd	nd	nd	nd	nd	1.9	1.2	nd	0.1	502.1	1299.9	17.0	38.9	20.0	6.2	9.0	nd	2.6	0.7	0.147	0.171	-	
15	2.4	0.9	1.3	4.4	2.1	nd	nd	nd	nd	nd	1.4	0.7	4.4	24.6	855.5	734.2	1036.8	1989.9	467.7	14.6	5.3	20.7	28.8	7.0	<0.001	0.001	PC-BW; PC-G; S-PC	
16	nd	0.1	nd	nd	0.4	nd	nd	nd	nd	nd	nd	nd	nd	nd	0.6	1.0	3.0	9.2	5.2	85.5	156.7	nd	29.2	167.1	0.006	0.024	S-BW; S-G; S-PC	
17	22.2	84.9	14.0	3.0	126.4	nd	nd	nd	nd	nd	70.2	34.7	12.0	42.0	95.3	143.2	7.8	21.7	128.4	442.5	670.4	425.3	777.0	975.2	<0.001	<0.001	S-BW; S-G; S-PC	
18	3.4	13.4	13.8	39.8	44.2	nd	nd	nd	nd	nd	9.0	4.4	36.7	232.3	752.0	1594.4	2317.6	7797.0	3920.7	11.5	78.7	185.8	387.0	174.8	0.007	0.018	PC-BW; PC-G; S-PC	
19	0.1	nd	0.3	0.2	<0.1	nd	nd	nd	nd	nd	nd	nd	nd	0.2	32.0	3.9	294.4	95.7	12.6	2.4	1.4	35.0	5.8	1.3	0.127	0.15	-	
20	25.8	159.8	0.8	0.2	26.9	nd	0.7	nd	nd	nd	93.3	12.5	nd	2.8	27.4	10.7	5.0	12.6	7.1	202.2	25.9	8.1	12.7	10.2	0.738	0.738	-	
21	3.2	21.2	19.0	25.3	20.1	nd	nd	nd	nd	nd	11.3	7.1	28.1	117.8	1226.7	1934.7	2332.9	4028.9	1244.5	16.0	78.9	109.9	152.2	44.4	<0.001	0.001	PC-BW; PC-G; S-PC	
22	55.2	79.0	45.4	2.9	104.6	nd	nd	nd	nd	nd	2283.3	295.6	56.8	132.5	401.7	294.5	33.7	64.5	574.2	1810.9	302.4	346.7	554.8	724.3	0.243	0.316	-	
23	24.4	46.0	0.3	0.3	60.3	<0.1	nd	nd	nd	nd	16.6	5.4	3.3	304.2	2056.6	1794.4	63.9	247.1	3736.0	79.4	46.6	9.9	20.5	145.8	0.016	0.036	PC-BW; PC-G; S-PC	
24	0.1	nd	0.3	8.7	0.1	nd	nd	nd	nd	nd	1.6	nd	9.6	8.1	23.7	4.5	161.9	1924.3	1.4	3.0	1.5	52.2	277.4	0.8	0.408	0.413	-	
25	0.5	0.8	0.5	1.5	0.4	nd	nd	nd	nd	nd	24.9	6.4	8.5	19.5	5.1	8.3	6.1	21.0	7.8	609.4	801.7	229.4	3538.2	460.4	0.058	0.119	-	
26	60.9	2463.1	535.4	5561.0	98.7	4.5	15.2	0.9	7.1	1.0	342.8	157.4	1453.2	140.3	75.4	62.7	41.6	207.8	52.6	134.0	76.9	821.2	279.2	67.3	0.199	0.269	-	
27	96.0	15.1	351.7	69.9	204.4	0.1	nd	nd	1.0	nd	962.8	208.3	574.3	179.6	117.7	185.8	120.0	196.1	228.5	1569.7	2859.7	18224.1	27866.8	4666.2	0.028	0.07	-	
28	28.0	1787.1	3301.8	4144.6	120.0	3.2	11.4	2.4	3.7	0.1	25.4	131.3	985.5	92.8	19.7	46.2	42.4	125.4	39.7	322.5	323.2	1743.4	372.7	142.1	0.063	0.126	-	
29	24.0	30.6	0.9	0.1	12.4	nd	nd	nd	nd	nd	1555.7	40.7	13.2	16.7	91.5	5.2	7.7	15.5	11.7	634.5	38.2	98.8	47.4	33.7	0.394	0.442	-	
30	0.2	164.2	50.0	53.6	2.3	0.2	0.9	0.3	0.1	<0.1	9.6	7.4	12.9	6.1	14.4	21.2	52.6	122.9	74.6	15.6	405.3	683.9	1215.8	24.4	0.051	0.085	-	
31	1.0	50.4	9.5	18.2	9.1	nd	nd	nd	nd	nd	104.4	10.2	30.5	33.9	21.2	18.0	17.5	53.0	60.5	818.5	685.0	2984.7	8560.5	1376.3	0.044	0.099	-	
32	0.2	1.1	2.0	0.7	0.1	nd	nd	nd	nd	nd	4.4	2.2	0.7	6.6	5.2	7.0	3.7	12.6	8.4	1247.7	931.4	44.4	1379.4	487.3	0.001	0.004	S-BW; S-G; S-PC	

N	Body Walls					Coelomic fluid					Gonads					Pyloric caeca					Stomach					p-value	q-value	Tukey's HSD
	BW#1	BW#2	BW#3	BW#4	BW#5	CF1	CF2	CF3	CF4	CF5	G#1	G#2	G#4	G#5	PC#1	PC#2	PC#3	PC#4	PC#5	S#1	S#2	S#3	S#4	S#5				
33	161.7	22.0	13.2	1.3	29.0	nd	nd	nd	0.4	nd	1085.2	41.3	40.1	16.0	50.8	17.2	5.8	14.3	13.5	2298.9	1451.8	1744.3	5812.5	2437.7	0.001	0.005	S-BW; S-G; S-PC	
34	25.8	83.3	144.2	161.8	51.0	0.1	0.3	0.1	<0.1	0.2	18.7	3.0	11.0	9.0	20.1	6.2	9.8	21.5	11.6	96.2	23.2	68.3	31.0	23.7	0.008	0.026	G-BW; PC-BW	
35	39.0	10.0	8.5	1.9	11.8	nd	nd	nd	nd	nd	1838.9	21.3	20.7	6.6	62.2	7.7	4.2	9.1	8.2	3387.0	235.0	341.7	793.1	338.6	0.199	0.269	-	
36	28.3	10.5	9.6	2.3	12.0	nd	nd	nd	nd	nd	1083.7	18.1	12.9	5.9	31.5	6.3	4.7	11.9	8.7	951.2	165.3	249.4	571.6	244.7	0.098	0.171	-	
37	53.5	2.1	1.0	0.2	1.8	nd	nd	nd	nd	nd	363.1	23.2	2.6	0.7	279.0	7.8	4.9	12.1	6.4	2880.2	105.3	3.1	28.0	31.9	0.477	0.509	-	
38	0.2	32.5	389.3	143.4	1.9	<0.1	nd	nd	<0.1	nd	356.8	6.2	202.1	27.7	28.7	13.8	305.2	681.5	82.2	179.5	68.7	21617.9	18196.8	110.2	0.109	0.177	-	
39	2.0	362.1	727.6	1029.4	3.3	0.3	1.7	0.1	0.7	nd	36.3	28.0	129.9	15.9	41.3	29.4	38.0	84.0	24.1	457.5	96.3	415.0	107.1	72.2	0.109	0.177	-	
40	15.8	26.6	7.6	3.2	66.1	nd	nd	nd	nd	nd	5.8	4.5	0.4	40.7	17.4	22.8	1.1	7.5	42.8	766.2	920.0	34.8	393.6	962.7	0.001	0.004	S-BW; S-G; S-PC	
41	0.4	1.3	0.4	0.6	1.7	nd	nd	nd	nd	nd	1.3	1.5	nd	20.1	4.1	6.9	0.3	1.8	15.9	299.0	513.3	16.6	286.2	511.3	<0.001	0.003	S-BW; S-G; S-PC	
42	9.5	1334.4	29.4	88.8	13.1	2.5	5.1	2.2	1.6	2.3	126.9	58.4	24.8	23.7	76.3	42.1	45.6	156.6	47.6	352.1	442.9	6963.1	6687.8	162.4	0.081	0.151	-	
43	409.1	8.7	0.2	0.4	4.0	<0.1	nd	nd	0.6	1.0	18306.4	92.9	110.7	13.0	1073.3	17.0	6.3	17.1	11.6	13986.7	265.0	71.2	85.0	137.2	0.509	0.53	-	
44	42.9	69.0	24.8	2.1	183.4	nd	0.1	nd	nd	0.1	18.3	3.2	0.5	13.8	6.7	5.9	0.5	3.5	11.2	730.2	310.0	161.4	136.4	412.9	0.002	0.01	S-BW; S-G; S-PC	
45	48.5	14.8	0.1	1.8	0.9	nd	nd	nd	nd	nd	12.4	1.3	1.6	9.4	2787.4	477.6	34.8	94.5	92.2	137.4	8.5	2.1	8.4	7.7	0.25	0.277	-	
46	13.5	80.0	0.2	4.3	19.9	nd	<0.1	nd	nd	nd	12.7	5.3	3.0	40.2	743.7	2117.0	60.9	243.7	344.9	57.7	51.3	6.3	20.6	17.1	0.06	0.094	-	
47	16.0	1.3	0.8	1.1	1.8	nd	nd	nd	nd	nd	91.6	5.0	2.3	2.4	98.8	4.5	3.7	10.8	7.8	952.6	17.4	28.1	41.5	30.3	0.407	0.451	-	
48	3.7	2.0	2.8	2.4	199.6	0.3	0.1	<0.1	<0.1	0.1	9.2	1.8	5.9	718.4	295.4	75.4	107.8	207.4	7882.2	30.4	7.6	26.0	17.1	473.0	0.423	0.423	-	
49	29.9	156.4	88.4	2.0	153.8	nd	0.2	nd	nd	nd	36.9	8.4	1.6	8.6	8.0	8.8	4.5	4.2	4.7	203.2	199.9	805.2	126.7	78.7	0.052	0.108	-	
50	100.1	6.3	3.5	0.9	3.8	nd	nd	nd	<0.1	nd	139.5	29.0	72.2	12.4	452.3	30.5	9.8	32.8	36.7	140.6	145.5	367.3	660.0	381.7	0.023	0.06	-	
51	5.8	385.9	1.0	31.9	5.7	nd	0.1	nd	nd	nd	55.2	32.1	4.9	13.3	51.4	66.9	25.3	38.6	45.0	843.1	2228.3	291.3	1226.2	709.9	0.002	0.009	S-BW; S-G; S-PC	
52	82.0	14.7	8.3	1.1	23.7	nd	nd	nd	0.1	nd	7071.3	26.7	44.3	5.1	42.1	4.1	4.3	14.2	8.1	6736.8	57.9	87.0	102.4	107.8	0.505	0.53	-	
53	1.9	3.4	2.4	45.1	0.3	nd	nd	nd	nd	nd	2.1	0.6	17.4	13.3	139.2	92.1	253.5	299.3	39.7	11.7	4.6	13.4	103.7	3.5	0.003	0.01	PC-BW; PC-G; S-PC	
54	21.7	114.3	34.3	140.5	10.1	0.3	0.7	0.1	0.1	nd	7473.3	80.6	268.9	45.8	507.0	30.2	133.8	396.3	54.9	835.4	72.8	3892.5	1345.9	260.7	0.383	0.434	-	
55	13.7	35.5	24.9	146.9	20.5	0.3	0.2	0.2	0.1	0.1	5.3	7.4	64.6	80.0	829.8	110.1	3241.0	8552.8	196.7	13.6	13.2	141.4	418.6	14.8	0.121	0.147	-	
56	2.8	3.0	8.7	39.6	0.1	nd	nd	nd	nd	nd	2.5	1.1	16.4	10.9	227.0	219.1	502.4	2626.5	22.2	13.1	10.5	20.1	95.6	2.8	0.165	0.186	-	
57	1.4	30.2	0.6	0.2	4.8	nd	nd	nd	nd	nd	3.4	2.2	0.6	10.2	158.9	767.9	49.7	63.8	123.3	6.1	13.9	2.9	5.3	4.1	0.092	0.124	-	
58	43.1	39.9	105.7	103.8	31.6	<0.1	nd	<0.1	<0.1	nd	15.1	8.3	47.8	144.2	2348.6	1420.6	4231.9	5110.9	1115.1	89.0	64.4	160.4	251.9	61.4	<0.001	0.002	PC-BW; PC-G; S-PC	
59	34.1	142.0	9.6	33.2	30.0	0.5	0.7	0.3	0.2	0.3	28.7	9.2	19.6	97.6	2323.1	5039.5	414.5	1843.3	1027.4	122.8	175.6	27.2	136.1	47.2	0.006	0.018	PC-BW; PC-G; S-PC	
60	44.0	70.7	28.5	2.0	258.2	<0.1	0.1	nd	nd	nd	93.2	28.9	9.1	76.8	74.3	49.1	18.0	29.0	166.1	1841.5	1075.2	620.6	657.9	1964.5	<0.001	0.001	S-BW; S-G; S-PC	
61	0.7	0.1	0.6	nd	0.5	nd	nd	nd	nd	nd	215.6	3.0	2.8	0.7	14.9	1.0	2.4	9.0	3.1	142.7	37.4	58.6	401.9	142.9	0.049	0.104	-	
62	32.0	1.2	0.3	0.1	1.8	nd	nd	nd	nd	nd	1483.7	5.9	11.3	3.4	117.8	1.6	7.5	57.9	7.0	943.7	5.0	8.8	4.1	10.1	0.511	0.53	-	
63	9.4	23.6	0.5	0.6	26.9	<0.1	nd	0.1	nd	<0.1	5.2	1.5	0.9	60.0	530.5	829.1	60.6	41.4	815.8	19.6	43.1	8.3	12.9	30.1	0.008	0.019	PC-BW; PC-G; S-PC	
64	62.7	116.2	472.1	2212.9	610.7	1.0	1.1	1.1	0.7	1.2	74.6	28.6	988.5	2157.7	2987.5	2438.9	17721.8	64535.2	15898.9	261.3	152.3	1204.6	3448.2	612.0	0.078	0.115	-	
65	0.6	0.9	<0.1	0.4	0.3	nd	nd	nd	nd	nd	0.2	0.4	nd	4.3	1.6	2.3	2.0	7.7	6.1	260.8	859.3	1.7	94.0	660.6	0.017	0.046	S-BW; S-G; S-PC	
66	22.4	51.4	37.3	8.2	65.4	0.1	<0.1	nd	0.6	nd	16.8	37.4	22.9	72.2	36.0	69.6	50.5	132.7	124.7	2048.8	1763.3	465.0	15822.2	1742.5	0.147	0.22	-	
67	47.4	443.0	61.9	10.0	449.9	0.5	1.5	nd	nd	nd	4.6	10.5	0.1	15.4	3.1	7.8	0.3	2.1	7.6	82.7	355.3	40.5	71.3	73.6	0.1	0.172	-	
68	41.4	113.9	7.8	16.0	1.2	<0.1	0.1	nd	<0.1	nd	20.8	7.4	4.0	8.2	2263.3	3657.0	238.2	384.4	69.6	155.8	58.1	10.3	24.7	6.8	0.06	0.094	-	

N	Body Walls					Coelomic fluid					Gonads					Pyloric caeca					Stomach					p-value	q-value	Tukey's HSD
	BW#1	BW#2	BW#3	BW#4	BW#5	CF1	CF2	CF3	CF4	CF5	G#1	G#2	G#4	G#5	PC#1	PC#2	PC#3	PC#4	PC#5	S#1	S#2	S#3	S#4	S#5				
69	12.3	78.1	1.5	9.0	11.4	nd	0.1	nd	nd	nd	12.0	6.0	4.8	32.4	684.6	2114.1	132.2	459.5	353.5	42.7	38.9	7.6	22.1	10.3	0.03	0.058	-	
70	38.7	43.1	35.8	8.5	48.0	0.4	0.2	nd	0.2	1.0	55.3	35.7	14.8	51.8	14.5	23.9	13.4	26.6	41.4	1897.0	2821.0	1854.2	3607.9	3845.4	<0.001	<0.001	S-BW; S-G; S-PC	
71	17.3	16.5	9.1	10.3	0.1	<0.1	nd	nd	nd	nd	5.7	2.0	5.0	5.2	1055.4	482.8	387.7	596.2	24.4	44.1	13.9	13.7	24.2	2.9	0.002	0.007	PC-BW; PC-G; S-PC	
72	33.1	15.3	5.9	69.8	2.5	<0.1	0.1	<0.1	nd	nd	11.4	4.0	35.4	25.5	2031.1	599.4	360.6	4368.5	92.6	98.3	22.3	19.2	180.9	8.2	0.06	0.094	-	
73	167.6	100.7	78.6	30.3	172.6	0.8	0.8	0.3	0.6	0.9	2986.5	147.1	135.1	154.8	1276.5	430.1	194.4	673.2	382.3	2266.6	614.8	1669.2	2807.9	1149.3	0.045	0.099	-	
74	1.6	8.5	1.2	5.7	7.2	0.4	0.4	nd	<0.1	1.4	18.4	6.5	6.5	16.7	8.1	7.8	7.7	18.4	16.2	1490.5	1492.8	215.2	2879.9	1265.2	<0.001	0.004	S-BW; S-G; S-PC	
75	0.5	5.3	37.0	39.3	0.4	nd	nd	nd	nd	nd	2.0	2.6	21.4	14.3	51.0	184.4	1946.5	2297.2	27.3	4.2	13.7	107.0	116.0	2.2	0.076	0.115	-	
76	0.8	1.8	16.9	10.0	1.5	nd	nd	nd	nd	nd	0.4	1.1	5.1	6.4	37.1	11.4	963.1	595.9	44.8	2.2	4.1	32.0	19.9	2.2	0.091	0.124	-	
77	11.2	17.2	8.4	9.1	19.2	0.1	0.1	nd	nd	0.1	66.2	12.2	11.8	32.2	23.6	21.0	11.0	32.8	28.1	4120.9	3021.4	302.2	4763.9	2234.7	<0.001	0.002	S-BW; S-G; S-PC	
78	1247.1	4523.6	960.5	226.2	5384.2	5.6	9.3	1.2	5.9	7.7	2984.7	1785.1	372.0	2382.7	1179.5	1300.9	71.3	121.9	2092.6	25461.0	22508.6	17412.0	16285.3	35490.6	<0.001	<0.001	S-BW; S-G; S-PC	
79	28.3	7.3	5.8	1.1	9.0	nd	nd	nd	nd	nd	682.6	4.2	6.7	0.2	68.5	1.5	3.8	9.4	4.7	863.5	5.2	13.2	7.8	11.0	0.579	0.584	-	
80	32.3	21.9	114.0	0.9	37.4	nd	nd	nd	nd	0.1	198.1	25.2	11.4	19.2	28.1	15.7	34.4	16.8	19.3	401.3	407.8	4922.6	829.8	231.1	0.159	0.231	-	
81	192.7	222.8	33.2	83.3	356.9	0.8	1.0	0.6	0.5	0.6	76.0	21.0	49.7	1205.1	10565.5	7590.5	1793.2	5272.2	10762.4	597.2	137.5	77.5	190.2	547.2	<0.001	0.001	PC-BW; PC-G; S-PC	
82	0.5	4.1	163.8	147.5	0.7	1.3	1.2	1.5	1.1	1.5	9.9	10.7	83.4	50.7	100.1	165.6	7589.5	7869.6	104.2	13.5	36.2	476.4	456.4	9.7	0.101	0.132	-	
83	19.6	46.4	1.7	21.2	1.8	nd	<0.1	nd	nd	nd	9.9	4.6	11.2	9.8	1093.5	1578.9	123.0	1371.5	20.0	57.5	48.6	6.8	61.0	3.7	0.007	0.019	PC-BW; PC-G; S-PC	
84	24.3	24.9	152.2	96.1	9.8	0.1	<0.1	0.2	<0.1	nd	4.2	5.9	45.4	30.5	113.1	116.3	6812.0	5248.2	82.8	12.3	27.3	201.5	182.6	6.7	0.101	0.132	-	
85	14.9	88.6	1.0	7.3	11.7	nd	0.1	nd	nd	nd	13.7	9.5	3.5	36.3	661.1	2014.7	144.3	242.3	381.7	39.8	49.9	7.4	19.1	14.0	0.043	0.076	-	
86	13.2	50.0	1.6	0.6	1.6	nd	nd	nd	nd	nd	201.5	13.6	5.7	9.0	120.9	162.0	34.6	30.9	55.2	2873.5	562.2	124.8	445.3	233.3	0.127	0.198	-	
87	16.1	20.8	14.3	2.6	37.2	nd	nd	nd	nd	nd	1447.0	20.1	12.7	5.4	44.6	4.0	2.5	5.1	4.6	109.0	14.5	19.0	5.1	6.6	0.325	0.387	-	
88	28.3	137.9	49.4	12.3	159.7	0.3	0.2	nd	0.1	nd	127.7	125.6	34.6	154.0	29.7	47.5	6.1	14.9	68.9	3448.1	4412.0	2704.2	5002.3	7808.1	<0.001	<0.001	S-BW; S-G; S-PC	
89	0.1	<0.1	0.1	nd	<0.1	nd	nd	nd	nd	nd	10.0	0.8	0.1	0.4	56.9	2.7	0.5	5.5	4.3	139.0	45.8	66.0	857.7	430.9	0.041	0.095	-	
90	nd	0.4	0.4	nd	0.3	nd	nd	nd	nd	nd	nd	0.1	nd	0.1	0.3	1.7	1.1	6.7	3.4	45.8	149.4	29.6	165.0	29.2	0.004	0.017	S-BW; S-G; S-PC	
91	21.5	22.1	5.5	5.9	0.4	nd	nd	nd	nd	nd	8.1	2.4	3.7	7.4	1529.7	936.9	334.6	397.2	74.7	31.4	31.5	13.0	21.7	4.4	0.009	0.021	PC-BW; PC-G; S-PC	
92	12.8	70.9	17.5	45.5	29.2	0.2	0.3	0.2	0.2	0.3	10.2	7.0	8.6	72.7	699.1	2149.6	294.6	619.2	858.0	26.5	31.4	13.3	37.2	22.9	0.003	0.01	PC-BW; PC-G; S-PC	
93	56.2	119.4	20.7	8.1	315.5	0.7	0.7	nd	0.6	0.1	189.6	101.7	12.0	184.3	93.5	77.1	9.8	17.7	159.0	5113.8	4837.0	530.3	1557.1	12851.9	0.017	0.046	S-BW; S-G; S-PC	
94	13.0	38.9	1.9	8.9	18.7	nd	nd	nd	nd	nd	12.0	6.5	4.8	53.2	679.0	961.2	67.6	412.2	639.2	41.8	25.5	6.2	23.0	22.6	<0.001	0.002	PC-BW; PC-G; S-PC	
95	864.7	1253.2	96.3	7.6	1935.5	2.2	4.5	nd	1.1	3.6	5766.1	200.9	52.4	209.9	535.4	37.3	11.1	8.9	62.6	10790.0	975.5	2583.0	287.6	472.0	0.384	0.434	-	
96	76.6	41.4	3.4	8.5	1.0	nd	<0.1	nd	nd	nd	19.6	3.8	4.3	7.8	4116.9	1373.3	173.7	438.3	57.8	209.0	24.9	7.8	20.6	7.0	0.118	0.145	-	
97	121.4	2.2	0.3	0.9	4.0	nd	nd	nd	nd	0.5	1569.6	10.4	14.4	2.1	169.8	1.5	1.9	8.2	7.4	1147.9	10.4	11.4	15.0	21.9	0.546	0.555	-	
98	156.9	35.0	19.6	0.6	50.3	0.2	0.2	nd	nd	0.4	462.3	6.1	4.0	3.3	70.2	3.8	0.4	11.0	9.4	1881.6	14.2	42.9	29.1	17.9	0.536	0.551	-	
99	5.5	7.6	3.6	16.4	19.0	<0.1	nd	<0.1	nd	nd	4.4	3.9	9.2	49.3	663.2	318.0	261.8	1088.7	582.6	24.5	16.8	15.0	51.3	26.5	<0.001	0.001	PC-BW; PC-G; S-PC	
100	6.1	32.2	82.8	134.9	10.0	0.3	0.4	0.4	0.2	0.3	6.8	7.2	73.0	55.4	174.5	349.8	5086.2	7383.7	147.6	13.4	26.6	140.2	229.6	8.1	0.087	0.122	-	
101	1.7	7.1	28.8	0.1	4.1	nd	nd	nd	nd	nd	2.3	2.1	0.4	15.7	297.2	281.6	1491.4	21.3	187.1	8.5	22.8	96.1	7.8	8.2	0.093	0.124	-	
102	2.2	46.0	0.3	26.3	0.4	<0.1	<0.1	nd	nd	nd	7.8	5.3	14.1	9.6	188.5	1149.1	62.5	1016.1	41.7	11.2	33.8	6.2	65.4	3.5	0.042	0.076	-	
103	3.7	11.7	10.6	24.0	105.0	0.4	0.3	0.2	0.1	0.1	6.1	6.5	14.1	314.9	320.7	408.7	509.3	1407.5	3597.6	17.6	23.7	40.2	76.7	185.2	0.047	0.08	-	
104	106.5	815.9	19.1	14.5	1201.8	0.3	1.7	nd	nd	nd	178.9	215.9	11.3	118.2	51.8	82.1	3.6	12.4	90.6	379.8	1241.2	94.4	358.6	642.5	0.149	0.22	-	

N	Body Walls					Coelomic fluid					Gonads					Pyloric caeca					Stomach					p-value	q-value	Tukey's HSD
	BW#1	BW#2	BW#3	BW#4	BW#5	CF1	CF2	CF3	CF4	CF5	G#1	G#2	G#4	G#5	PC#1	PC#2	PC#3	PC#4	PC#5	S#1	S#2	S#3	S#4	S#5				
177	130.1	968.7	278.5	19.4	1419.9	0.3	1.9	nd	nd	nd	1522.4	112.7	24.8	91.2	64.2	23.3	4.1	3.2	54.0	470.9	147.0	176.7	29.5	45.3	0.29	0.361	-	
178	1.8	0.7	0.5	10.5	10.2	1.1	0.2	0.1	0.4	0.1	28.6	8.4	9.5	54.8	197.5	106.8	94.9	505.1	193.7	1474.2	900.9	162.4	1728.2	852.3	0.001	0.004	S-BW; S-G; S-PC	
179	176.4	517.7	39.1	116.6	532.1	1.6	2.1	1.0	0.7	0.9	129.8	70.0	99.4	1845.8	10130.1	14976.0	2479.3	7496.3	19375.3	639.9	806.0	219.7	619.2	1123.6	<0.001	0.002	PC-BW; PC-G; S-PC	
180	24.5	18.6	66.0	29.8	116.3	nd	nd	nd	0.1	nd	2316.3	209.7	140.8	235.4	169.5	94.4	22.6	94.1	94.6	2643.2	2111.4	4624.6	11194.8	3774.3	0.004	0.017	S-BW; S-G; S-PC	
181	11.4	99.4	108.1	40.8	7.8	0.2	0.3	0.2	<0.1	<0.1	17.8	17.5	25.2	27.0	761.0	3737.7	5788.2	2598.7	133.8	37.6	179.3	280.1	148.0	9.2	0.009	0.021	PC-BW; PC-G; S-PC	
182	2497.1	4167.9	983.3	627.0	8925.0	10.2	12.7	2.1	7.5	14.0	4003.8	1902.6	165.7	1779.7	714.0	826.4	43.4	83.4	1405.5	48534.8	47305.1	1990.1	9162.0	75914.8	0.008	0.026	S-BW; S-G; S-PC	
183	47.6	60.5	4.2	12.5	0.1	<0.1	0.1	nd	<0.1	nd	16.9	10.0	7.6	7.1	2334.3	1980.8	231.1	834.3	27.1	146.8	106.2	17.8	61.7	5.0	0.017	0.036	PC-BW; PC-G; S-PC	
184	3.1	22.7	115.5	56.2	35.5	0.4	0.5	0.4	0.2	0.2	6.1	8.1	35.8	107.8	96.5	349.9	5133.3	3205.6	1340.6	10.4	50.5	526.7	205.6	86.4	0.033	0.063	-	
185	4.9	3.6	37.5	20.2	204.6	0.1	<0.1	<0.1	nd	<0.1	10.3	5.6	15.2	692.9	404.8	300.9	2095.2	1379.7	8216.7	49.2	36.8	161.3	94.9	368.0	0.114	0.145	-	
186	4.4	7.2	14.1	0.8	12.3	7.1	8.5	7.6	6.0	7.7	2342.1	80.1	60.7	50.4	110.1	25.1	22.8	47.1	44.7	2829.6	974.5	1702.8	9603.1	3777.1	0.016	0.046	S-BW; S-G; S-PC	
187	46.9	9.9	22.2	16.6	29.2	0.1	<0.1	nd	<0.1	nd	7138.4	62.3	69.5	43.2	360.9	27.9	6.8	17.4	18.1	1998.2	120.8	798.9	1544.7	185.8	0.353	0.412	-	
188	2.8	46.6	24.6	17.9	369.6	1.1	1.1	0.8	0.4	0.7	20.3	18.2	24.3	1212.6	146.5	1811.8	823.7	845.5	13910.6	11.2	166.5	141.0	121.4	811.8	0.268	0.289	-	
189	31.4	57.0	11.9	12.2	9.3	0.1	0.2	nd	nd	nd	19.3	9.7	9.0	32.8	2229.9	2326.5	659.8	834.3	385.9	100.4	106.9	37.8	64.7	19.3	0.002	0.006	PC-BW; PC-G; S-PC	
190	819.0	1272.3	694.4	231.8	763.6	2.5	3.4	nd	0.9	2.0	16433.3	253.1	226.9	96.1	166.1	25.1	4.8	6.6	30.2	8230.7	921.5	428.3	222.5	922.7	0.454	0.489	-	
191	0.5	83.0	3.3	0.4	62.1	<0.1	0.5	nd	nd	nd	46.5	16.5	<0.1	7.1	0.1	2.5	nd	0.1	4.8	33.7	57.6	92.9	32.8	17.0	0.101	0.172	-	
192	26.1	18.1	620.7	198.9	44.7	0.3	0.1	nd	nd	nd	8.2	0.3	18.2	3.5	0.1	nd	5.2	6.6	0.9	9.7	6.0	118.8	7.6	6.1	0.166	0.235	-	
193	89.8	48.0	477.0	183.9	89.2	0.7	0.1	nd	nd	0.1	31.6	1.0	18.4	5.9	2.8	nd	1.6	1.9	0.8	35.3	15.3	321.8	10.5	5.6	0.11	0.177	-	
194	65.1	558.5	473.1	26.5	351.7	0.9	1.7	nd	nd	nd	8.3	10.0	2.5	16.6	0.1	3.0	2.7	6.6	10.9	15.1	21.2	98.4	4.9	12.0	0.006	0.024	G-BW; PC-BW; S-BW	
195	653.1	1543.8	4173.5	1751.9	1557.2	2.6	2.7	0.5	1.5	2.1	458.7	110.4	230.8	112.4	22.2	9.8	8.8	17.0	14.9	421.6	407.3	2181.8	368.9	352.3	0.009	0.029	G-BW; PC-BW	
196	19.8	32.8	230.7	530.9	863.3	1.6	1.0	0.9	0.5	0.7	45.3	23.3	298.1	2944.5	1540.8	1460.9	11699.2	33181.6	25318.7	119.1	135.0	1016.8	1905.3	2044.4	0.022	0.045	PC-BW; PC-G; S-PC	
197	59.1	15.2	2.3	1.6	4.8	0.1	<0.1	nd	<0.1	nd	15.7	3.1	0.5	13.0	3978.5	620.8	52.6	35.1	113.8	228.2	23.6	4.3	7.9	18.2	0.289	0.308	-	
198	157.3	122.3	5574.0	3952.7	551.7	0.2	nd	nd	nd	nd	255.1	56.0	443.0	91.1	43.3	9.7	173.6	268.5	58.9	190.5	59.0	744.3	100.0	69.6	0.097	0.171	-	
199	16.1	3.5	2.2	1.1	1.1	4.4	4.2	4.1	3.1	4.1	175.3	22.3	18.9	30.0	226.6	25.1	14.4	38.7	38.1	4126.3	1289.7	1714.1	17776.5	11203.0	0.017	0.046	S-BW; S-G; S-PC	
200	93.8	249.6	2325.5	2064.5	430.0	0.9	nd	<0.1	1.2	nd	483.4	70.5	614.2	116.5	54.2	19.1	164.5	319.7	51.5	409.4	722.2	8208.9	1435.2	613.8	0.281	0.354	-	
201	7.2	6.5	1075.1	527.6	26.7	0.1	nd	0.1	0.1	<0.1	5.0	0.9	56.7	10.2	0.3	0.1	3.2	7.5	2.0	55.7	19.7	351.9	30.3	46.5	0.212	0.283	-	
202	14.5	12.8	1.2	0.1	47.5	<0.1	nd	nd	nd	nd	7.3	2.7	2.5	175.2	1195.2	633.9	48.2	211.7	2531.8	66.8	40.5	9.2	22.4	97.6	0.039	0.072	-	
203	368.5	263.8	5114.3	1743.7	277.9	1.6	0.1	1.3	1.9	1.5	403.2	86.5	621.5	78.3	22.6	5.1	24.3	34.3	10.7	1068.4	783.4	11283.8	958.3	550.5	0.335	0.395	-	
204	0.6	1.8	9.4	78.1	5.6	<0.1	<0.1	nd	nd	nd	3.6	1.1	44.6	45.1	32.9	56.6	448.3	5233.9	222.9	3.7	5.5	44.9	324.4	13.1	0.342	0.35	-	
205	1597.0	1008.3	795.8	359.8	1721.4	22.3	20.4	17.4	24.6	19.7	30876.2	3304.3	2029.5	4245.0	13186.6	4638.6	2979.9	9927.2	7953.1	42662.0	23410.4	52198.3	77821.2	30560.5	<0.001	0.002	S-BW; S-G; S-PC	
206	16.4	75.5	547.4	799.2	73.4	nd	nd	nd	<0.1	nd	42.3	17.7	189.5	37.8	10.4	3.7	32.4	63.2	11.2	77.2	75.7	544.1	94.7	94.3	0.223	0.294	-	
207	675.3	471.0	774.9	149.1	319.1	12.3	14.0	13.3	6.8	8.2	385.9	62.9	61.6	107.3	196.6	300.5	457.0	274.4	372.8	446.3	322.6	775.6	1042.3	735.4	0.017	0.046	S-G; S-PC	

BW: body wall, G: gonads, PC: pyloric caeca, S: stomach; nd: not detected