

Comparative biochemical composition and exploratory UPLC–ESI– QTOF– MS^E metabolite profiling of marine macrophytes from the Mekong Delta Coast, Vietnam

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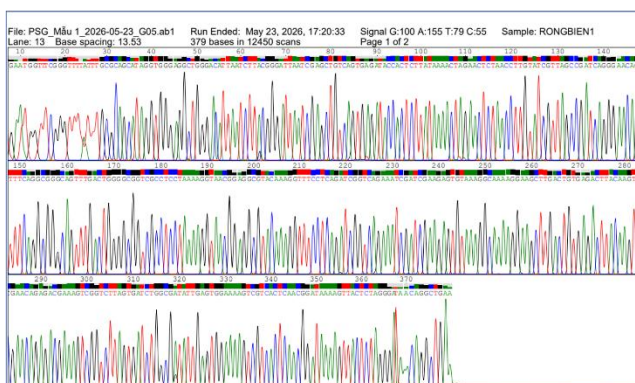
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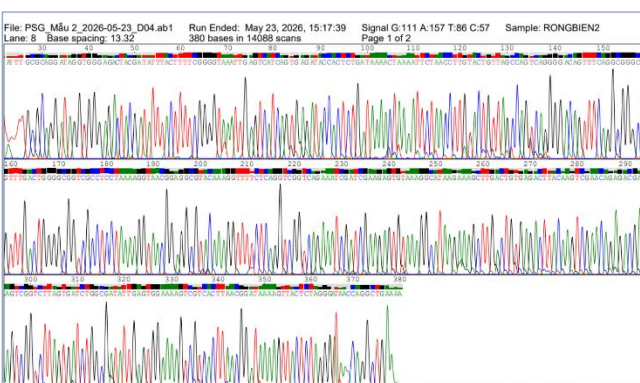
Supplementary Materials

Comparative Biochemical Composition and Putative Metabolite Profiling of Selected Marine Macrophytes from the Mekong Delta Coast of Vietnam

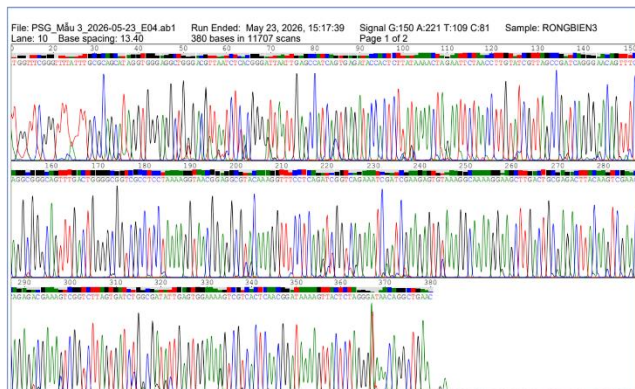
(A) MM1-*Sargassum* sp.



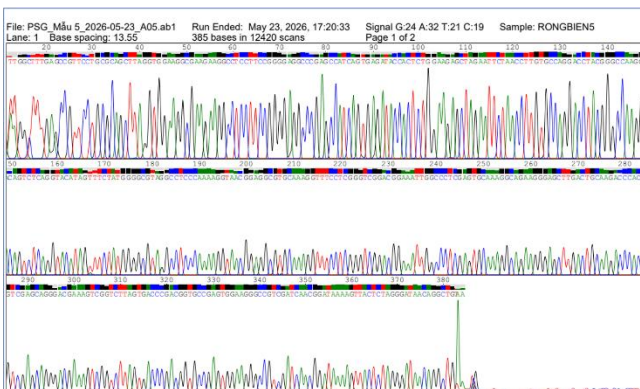
(B) MM2-*Padina* sp.



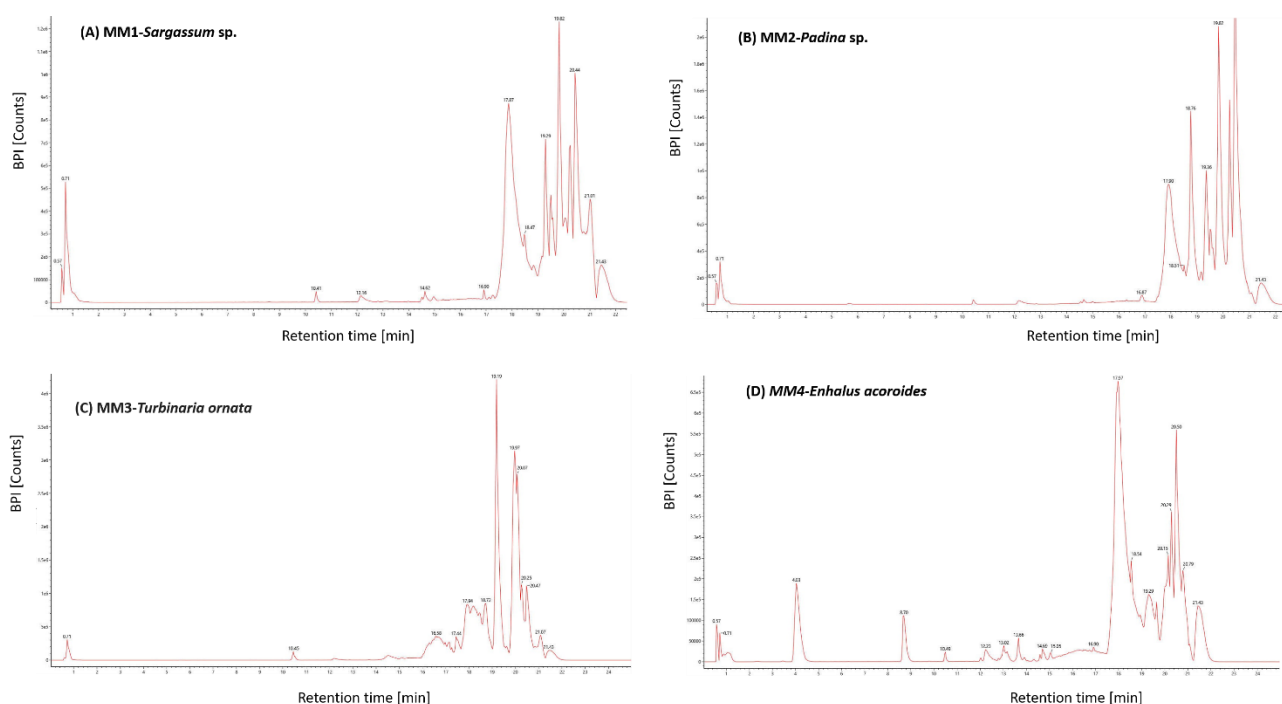
(C) MM3-*Turbinaria ornata*



(D) MM4-*Enhalus acoroides*



Supplementary Figure S1. Representative Sanger sequencing chromatograms of partial chloroplast 23S rRNA amplicons from MM1–MM4.



Supplementary Figure S2. Base peak chromatograms (BPCs) of pooled extracts from MM1–MM4, generated from the low-energy TOF-MS acquisition function of the UPLC–ESI–QTOF–MS^E analysis in negative-ion mode. The y-axis represents base peak intensity (BPI, counts).

Supplementary Text S1: The sequences are presented in the 5′–3′ direction. Each sequence was generated from one representative specimen and trimmed after chromatogram quality assessment.

MM1 | *Sargassum* sp. | partial chloroplast 23S rRNA | 369 bp

TGGTTTCGGGTTTTATTTGCGCAGCATAGGTGGGAGGCTGGGACATTAATCTTACGGGAT
TAATCGAGCTGTCAGTGAGATACCACTCTTATAAACTAGAACTCTAACCTTGTATCGTTA
GCCGATCAGGGAACAGTTTCAGGCGGGCAGTTTGACTGGGGCGGTCGCCTCCTAAAAG
GTAACGGAGGCGTACAAAGGTTTCCTCAGATCGGTCAGAAATCGATCGAAGAGTGTA
GGCAAAGGAAGCTTGACTGTGAGACTTACAAGTCGAACAGAGACGAAAGTCGGTCTT
AGTGATCTGGCGATATTGAGTGGAAAAGTCGTCCTCAACGGATAAAAGTTACTCTAGG
GATAACAGGCTGAA

MM2 | *Padina* sp. | partial chloroplast 23S rRNA | 351 bp

TGCGCAGGATAGGTGGGAGACTACGATATTTACTTTTCGGGGTAAATTGAGTCATCAGTG
AGATAACCACTCTGATAAACTAAAATTCTAACCTTGTACTGTTAGCCAGTCAGGGGACAG
TTTCAGGCGGGCAGTTTGACTGGGGCGGTTCGCCTCCTAAAAGGTAACGGAGGCGTACA
AAGGTTTTCTCAGGTCGGTCAGAAATCGATCGAAGAGTGTAAGGCATAAGAAAGCTTG
ACTGTGAGACTTACAAGTCGAACAGAGACGAAAGTCGGTCTTAGTGATCTGGCGATATT
GAGTGGAAGAGTCGTCACTTAACGGATAAAAGTTACTCTAGGGATAACCAGGCTG

MM3 | *Turbinaria ornata* | partial chloroplast 23S rRNA | 368 bp

TGGTTTCGGGTTTTATTTGCGCAGCATAGGTGGGAGGCTGGGACGTTAATCTCACGGGAT
TAATTGAGCCATCAGTGAGATAACCACTCTTATAAACTAGAATTCTAACCTTGTATCGTTA
GCCGATCAGGGAACAGTTTCAGGCGGGCAGTTTGACTGGGGCGGTTCGCCTCCTAAAAG
GTAACGGAGGCGTACAAAGGTTTCCTCAGATCGGTCAGAAATCGATCGAAGAGTGTAAG
GGCAAAGGAAGCTTGACTGCGAGACTTACAAGTCGAACAGAGACGAAAGTCGGTCTT
AGTGATCTGGCGATATTGAGTGGAAGAGTCGTCACTCAACGGATAAAAGTTACTCTAGG
GATAACAGGCTGA

MM4 | *Enhalus acoroides* | partial chloroplast 23S rRNA | 371 bp

TTGGCTTTGAGCCGTTCTGCGCAGCTTAGGTGGAAGGCGAAGAAGGCCTCCTTCCGGG
GAGGCCCCGAGCCATCAGTGAGATAACCACTCTGGAAGAGCTAGAATTCTAACCTTGTGCC
AGGACCTACGGGCCAAGGGACAGTCTCAGGTACATAGTTTCTATGGGGCGTAGGCCTCC
CAAAAGGTAACGGAGGCGTGCAAAGGTTTCCTCGGGTCGGACGGAAATTGGCCCTCGA
GTGCAAAGGCAGAAGGGAGCTTGACTGCAAGACCCACCCGTCGAGCAGGGACGAAAG
TCGGTCTTAGTGACCCGACGGTGCCGAGTGGAAGGGCCGTCGATCAACGGATAAAAGTT
ACTCTAGGGATAACAGGCTG

Supplementary Table S1. Tentatively assigned molecular features detected by UPLC–ESI–QTOF–MS^E in pooled extracts from four marine macrophytes.

Sample code	Taxonomic name used in manuscript	No.	Software-generated annotation	Conservative reported assignment	Retention time (min)	Observed m/z	Adduct(s)	Molecular formula	Mass error (mDa)	Mass error (ppm)	Peak response
MM1	<i>Sargassum</i> sp.	1	(E)-Labda-8(17),12-diene-15,16-dial	C20H30O2 labdane-related feature	19.31	301.2179	-H	C20H30O2	0.6	2.1	192,484
MM1	<i>Sargassum</i> sp.	2	6-Octadecenoic acid	C18:1 fatty-acid-related feature	20.49	281.2493	-H, +HCOO	C18H34O2	0.7	2.5	346,885
MM1	<i>Sargassum</i> sp.	3	Arachidonic acid	C20:4 fatty-acid-related feature	19.84	303.2337	-H	C20H32O2	0.8	2.5	337,127
MM1	<i>Sargassum</i> sp.	4	ent-16 α ,17-Hydroxy-19-kauranoic acid	C20H32O3 oxygenated diterpenoid-related feature	17.12	365.2338	+HCOO, -H	C20H32O3	0.5	1.3	6,238
MM1	<i>Sargassum</i> sp.	5	Mannitol	C6H14O6 sugar-alcohol-related feature	1.16	181.0723	-H, +HCOO	C6H14O6	0.6	3.2	5,095
MM1	<i>Sargassum</i> sp.	6	Periplogenin	C23H34O5 steroid-related feature	17.27	435.2390	+HCOO	C23H34O5	0.1	0.3	13,591
MM1	<i>Sargassum</i> sp.	7	Spathulenol	C15H24O sesquiterpenoid-related feature	15.36	265.1806	+HCOO	C15H24O	-0.4	-1.4	3,790
MM2	<i>Padina</i> sp.	1	(E)-Labda-8(17),12-diene-15,16-dial	C20H30O2 labdane-related feature	19.65	301.2180	-H	C20H30O2	0.7	2.2	104,415

MM2	<i>Padina</i> sp.	2	2,3-Dihydrofarnesol	C15H28O terpenoid-related feature	18.45	269.2129	+HCOO	C15H28O	0.7	2.6	66,758
MM2	<i>Padina</i> sp.	3	3,5,7-Trihydroxychromone	C9H6O5 polyhydroxylated chromone-related feature	5.69	193.0146	-H	C9H6O5	0.4	1.9	1,854
MM2	<i>Padina</i> sp.	4	3-Acetylaleuritic acid	C32H50O4 triterpenoid-related feature	20.80	497.3635	-H	C32H50O4	-0.2	-0.3	10,708
MM2	<i>Padina</i> sp.	5	6-Octadecenoic acid	C18:1 fatty-acid-related feature	20.49	281.2492	-H, +HCOO	C18H34O2	0.6	2.1	636,792
MM2	<i>Padina</i> sp.	6	Arachidonic acid	C20:4 fatty-acid-related feature	19.85	303.2339	-H	C20H32O2	0.9	3.1	542,125
MM2	<i>Padina</i> sp.	7	Cryptomeridiol	C15H28O2 oxygenated sesquiterpenoid-related feature	16.91	285.2074	+HCOO	C15H28O2	0.3	0.9	19,978
MM2	<i>Padina</i> sp.	8	ent-16 α ,17-Hydroxy-19-kauranoic acid	C20H32O3 oxygenated diterpenoid-related feature	17.75	319.2281	-H	C20H32O3	0.2	0.6	3,301
MM2	<i>Padina</i> sp.	9	Inosine [*]	C10H12N4O5 nucleoside-related feature	1.50	267.0736	-H	C10H12N4O5	0.1	0.4	859
MM2	<i>Padina</i> sp.	10	Mannitol	C6H14O6 sugar-alcohol-related feature	1.07	181.0722	-H	C6H14O6	0.4	2.4	1,209
MM2	<i>Padina</i> sp.	11	Methyl 7,10-	C17H30O2 fatty-acid	18.15	311.2218	+HCOO	C17H30O2	-1.0	-3.2	5,346

			hexadecadienoate	ester-related feature							
MM2	<i>Padina</i> sp.	12	Palmitoleic acid	C16:1 fatty-acid-related feature	19.56	253.2179	-H	C16H30O2	0.6	2.5	164,568
MM2	<i>Padina</i> sp.	13	Ricinoleic acid [†]	C18H34O3 hydroxy-fatty-acid-related feature	19.59	297.2438	-H	C18H34O3	0.3	0.9	53,195
MM2	<i>Padina</i> sp.	14	Stearidonic acid	C18:4 fatty-acid-related feature	18.79	275.2024	-H, +HCOO	C18H28O2	0.8	2.8	354,298
MM2	<i>Padina</i> sp.	15	γ -Linolenic acid	C18:3 fatty-acid-related feature	19.38	277.2180	-H	C18H30O2	0.7	2.4	236,677
MM3	<i>Turbinaria ornata</i>	1	(E)-Labda-8(17),12-diene-15,16-dial	C20H30O2 labdane-related feature	19.36	301.2178	-H	C20H30O2	0.5	1.6	64,955
MM3	<i>Turbinaria ornata</i>	2	6-Methyl-5-hepten-2-one [†]	C8H14O unsaturated aliphatic ketone-related feature	8.87	171.1033	+HCOO	C8H14O	0.6	3.6	491
MM3	<i>Turbinaria ornata</i>	3	6-Octadecenoic acid	C18:1 fatty-acid-related feature	20.53	281.2490	-H, +HCOO	C18H34O2	0.4	1.3	342,604
MM3	<i>Turbinaria ornata</i>	4	Arachidonic acid	C20:4 fatty-acid-related feature	19.86	303.2334	-H	C20H32O2	0.4	1.4	128,970
MM3	<i>Turbinaria ornata</i>	5	Citric acid	C6H8O7 organic-acid-related feature	0.98	191.0200	-H	C6H8O7	0.3	1.5	1,225
MM3	<i>Turbinaria ornata</i>	6	γ -Linolenic acid	C18:3 fatty-acid-related feature	19.39	277.2179	-H	C18H30O2	0.6	2.0	149,007
MM3	<i>Turbinaria ornata</i>	7	γ -Octalactone [†]	C8H14O2 lactone-	8.67	187.0983	+HCOO	C8H14O2	0.7	3.9	494

				related feature							
MM4	<i>Enhalus acoroides</i>	1	6-Octadecenoic acid	C18:1 fatty-acid-related feature	20.53	281.2489	-H	C18H34O2	0.3	1.1	194,448
MM4	<i>Enhalus acoroides</i>	2	Arachidonic acid	C20:4 fatty-acid-related feature	19.89	303.2331	-H	C20H32O2	0.1	0.4	15,985
MM4	<i>Enhalus acoroides</i>	3	p-Hydroxybenzoic acid [†]	C7H6O3 hydroxybenzoic-acid-related feature	3.46	137.0250	-H	C7H6O3	0.6	4.2	438
MM4	<i>Enhalus acoroides</i>	4	Ricinoleic acid [†]	C18H34O3 hydroxy-fatty-acid-related feature	18.11	297.2433	-H	C18H34O3	-0.2	-0.8	846
MM4	<i>Enhalus acoroides</i>	5	γ-Octalactone [†]	C8H14O2 lactone-related feature	8.71	187.0981	+HCOO	C8H14O2	0.5	2.7	1,159

Peak response represents relative instrument signal intensity and should not be interpreted as absolute concentration. Software-generated annotations are retained for traceability, whereas selected features were conservatively reported at the molecular-formula or chemical-class level because specific isomeric or stereochemical identities could not be confirmed. All annotations are reported at MSI Level 3; the UNIFI terms “Identified” and “Confirmed” are software workflow labels rather than standard-confirmed identifications. † Low-response molecular feature; tentative assignment requiring confirmation by replicated targeted analysis.

Supplementary Table S2. Species-level mean values used as the input matrix for principal component analysis (PCA).

Sample	Moisture (%FW)	Crude protein (%DW)	n-Hexane- extractable lipid (% DW)	Total ash (% DW)	Total polyphenol (mg GAE/g DW)	Total flavonoid (mg CE/g DW)	Total chlorophyll (mg/g DW)	Total carotenoid (mg/g DW)
<i>Sargassum</i> sp.	92.12	23.22	1.2	20.77	14.55	6.52	1.07	0.65
<i>Padina</i> sp.	90.29	22.19	0.69	22.84	18.48	11.21	3.31	0.31
<i>Turbinaria ornata</i>	88.77	18.94	1.64	20.67	13.04	5.94	2.38	0.74
<i>Enhalus acoroides</i>	86.22	14.45	1.31	20.57	2.56	1.05	0.9	0.21