

Supplementary Materials

Aqueous extracts of fish roe as a source of several bioactive compounds

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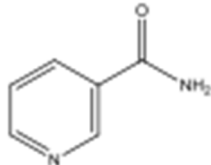
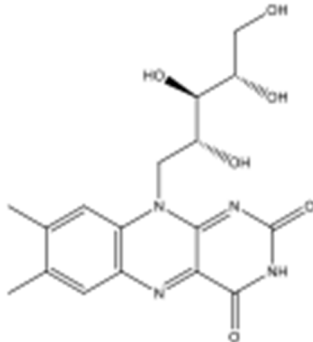
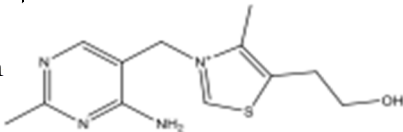
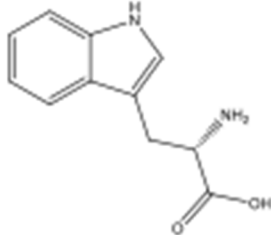
3 TOXRUN – Toxicology Research Unit, University Institute of Health Sciences, CESPU, CRL Rua Central de Gandra, 1317, 4585-116 Gandra PRD, Portugal

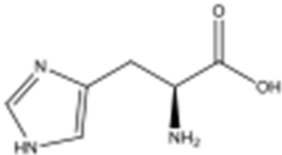
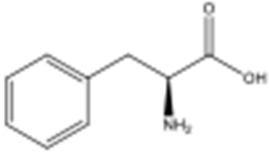
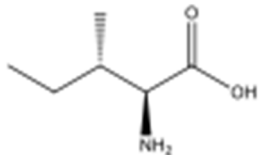
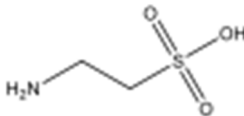
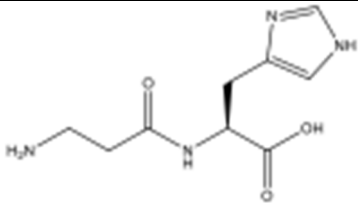
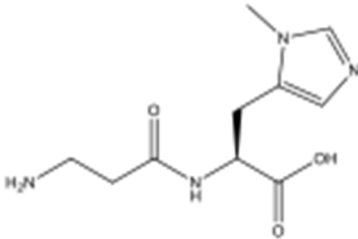
4 Interdisciplinary Centre of Marine and Environmental Research (CIIMAR), University of Porto, Terminal de Cruzeiros do Porto de Leixões, Avenida General Norton de Matos, S/N, 4450-208 Matosinhos, Portugal

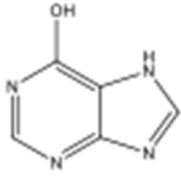
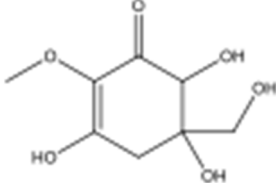
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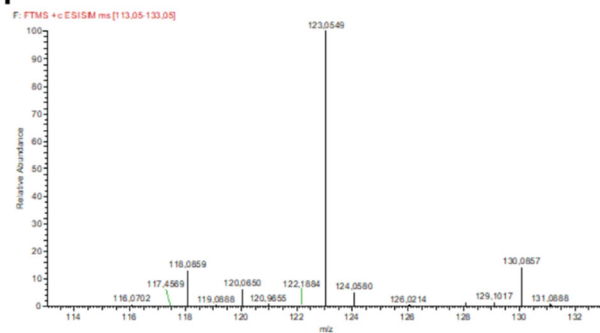
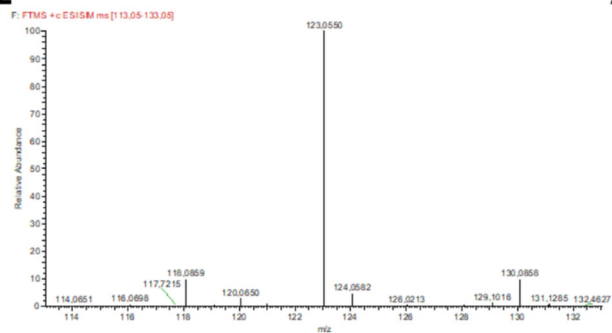
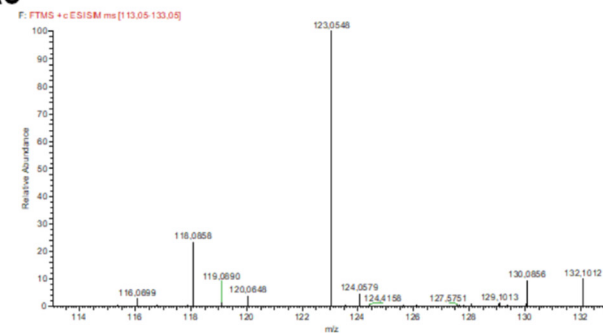
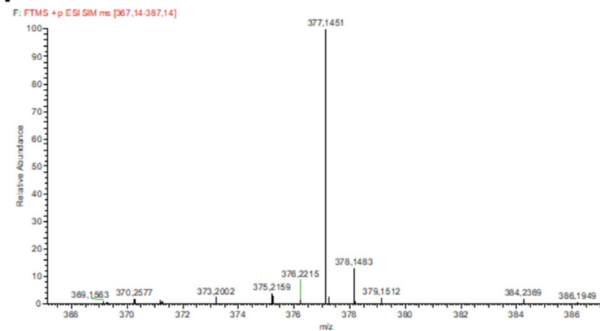
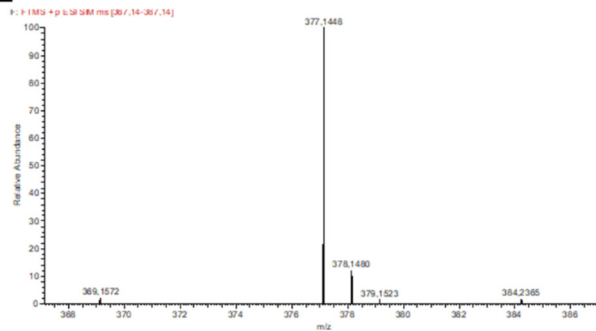
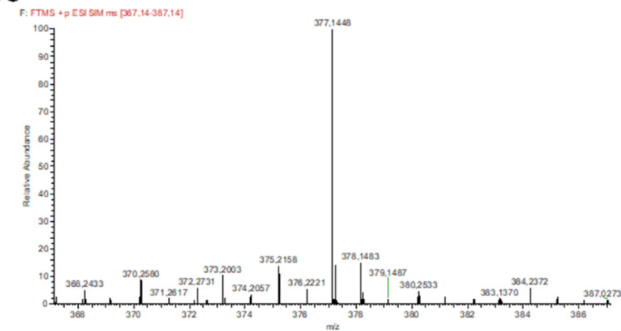
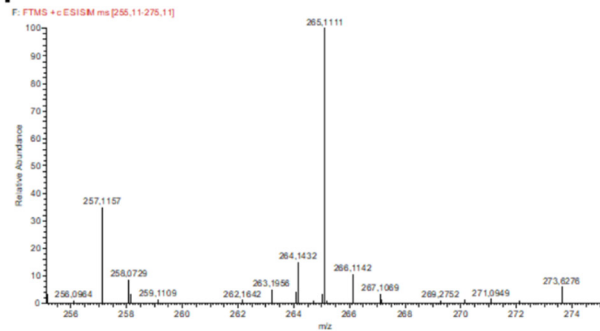
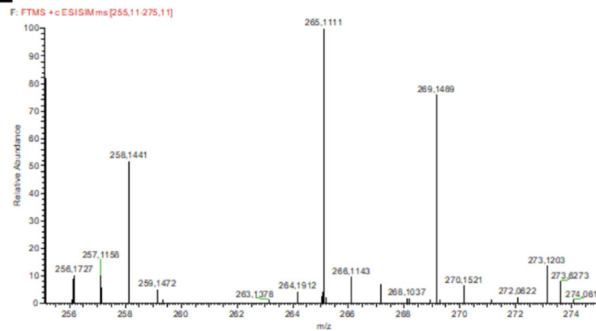
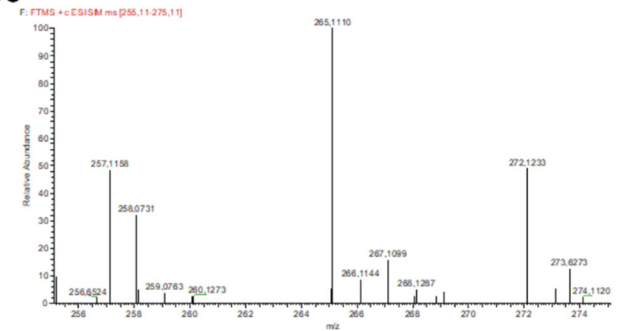
Table S1. IUPAC name, chemical structure, CAS number, molecular formula, mass exact and pKa values of the water-soluble compounds identified in sardine, horse mackerel and sea bass roe-derived aqueous extracts.*

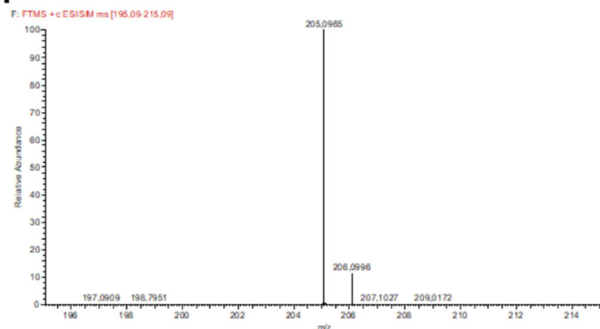
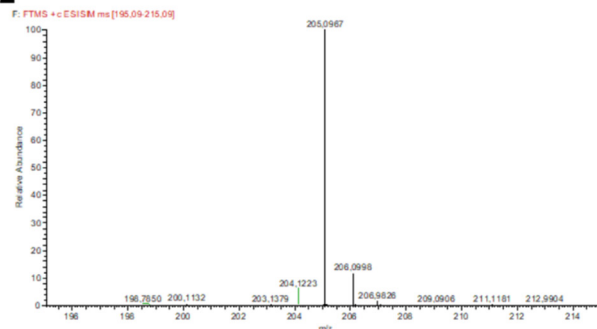
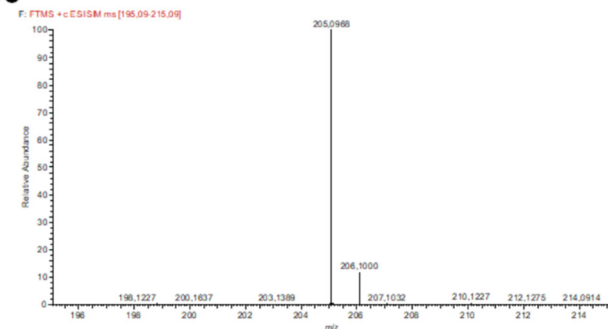
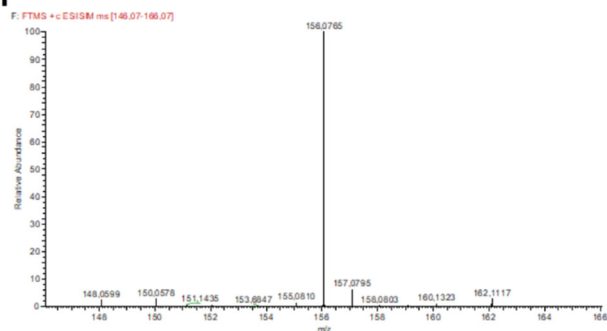
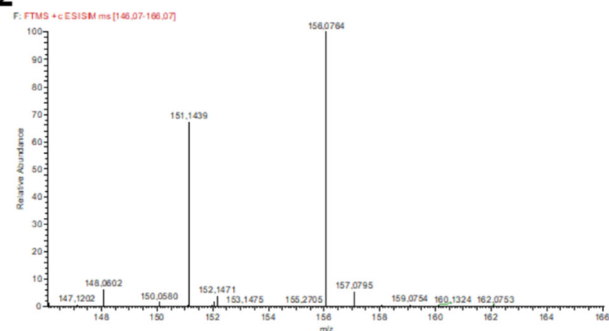
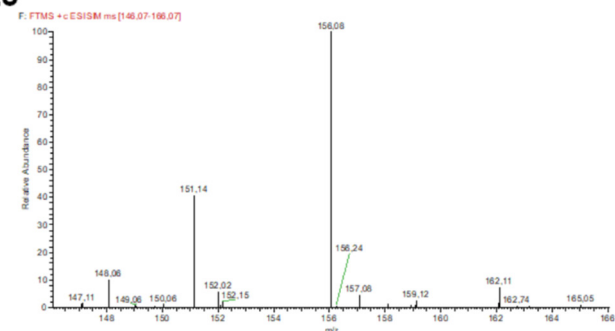
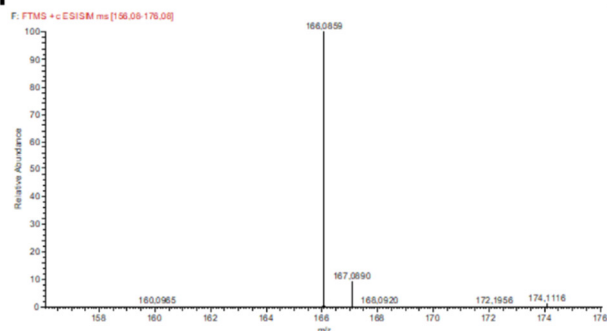
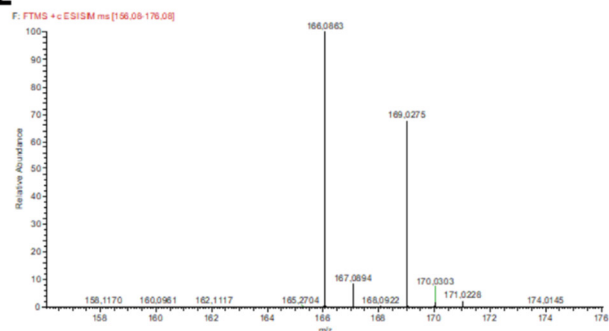
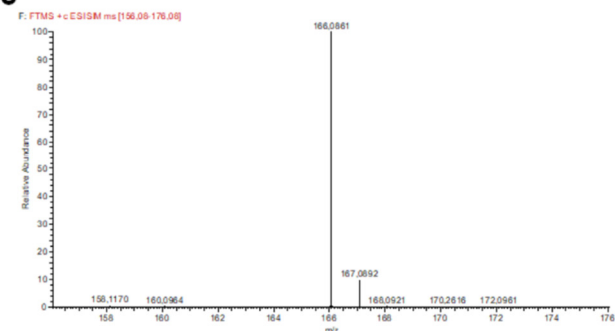
Compound		IUPAC Name	Chemical structure	CAS Number	Molecular formula	Mass exact (g/mol)	pKa	
Vitamins	Nicotinamide	pyridine-3-carboxamide		98-92-0	C ₆ H ₆ N ₂ O	122.048013	13.39	3.63
	Riboflavin	7,8-dimethyl-10-[(2S,3S,4R)-2,3,4,5-tetrahydroxypentyl]benzo[g]pteridine-2,4-dione		83-88-5	C ₁₇ H ₂₀ N ₄ O ₆	376.138284	5.97	- 2.60
	Thiamine	2-[3-[(4-amino-2-methylpyrimidin-5-yl)methyl]-4-methyl-1,3-thiazol-3-ium 5-yl]ethanol		70-16-6	C ₁₂ H ₁₇ N ₄ OS ⁺	265.112307	15.50	5.54
Amino acids	L-Tryptophan	(2S)-2-amino-3-(1H-indol-3-yl)propanoic acid		73-22-3	C ₁₁ H ₁₂ N ₂ O ₂	204.089878	2.54	9.40

	L-Histidine	(2S)-2-amino-3-(1H-imidazol-5-yl)propanoic acid		71-00-1	C6H9N3O2	155.069477	1.85	9.44
	L- Phenylalanine	(2S)-2-amino-3-phenylpropanoic acid		63-91-2	C9H11NO2	165.078979	2.47	9.45
	L-Isoleucine	(2S,3S)-2-amino-3-methylpentanoic acid		73-32-5	C6H13NO2	131.094629	2.79	9.59
	Taurine	2-aminoethanesulfonic acid		107-35-7	C2H7NO3S	125.014664	- 1.5	9.34
Peptides	Anserine	(2S)-2-(3-aminopropanoylamino)-3-(3-methylimidazol-4-yl)propanoic acid		584-85-0	C10H16N4O3	240.12224	7.15	
	Carnosine	(2S)-2-(3-aminopropanoylamino)-3-(1H-imidazol-5-yl)propanoic acid		305-84-0	C9H14N4O3	226.10659	7.01	

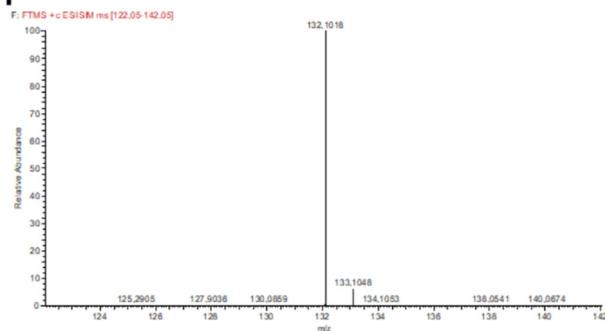
Purine derivative	Hypoxanthine	1,7-dihydropurin-6-one		68-94-0	C ₅ H ₄ N ₄ O	136.038511	8.72	1.73
	Gadusol	3,4,5-trihydroxy-5-(hydroxymethyl)-2-methoxycyclohex-2-en-1-one		76663-30-4	C ₈ H ₁₂ O ₆	204.063388	7.07	- 3.10

*Data obtained from PubChem (IUPAC name, chemical structure, CAS number, molecular formula, mass exact) and Food DB (pKa values) databases, and from the manuscript of Perrone et al. (pKa values of anserine and carnosine) [1].

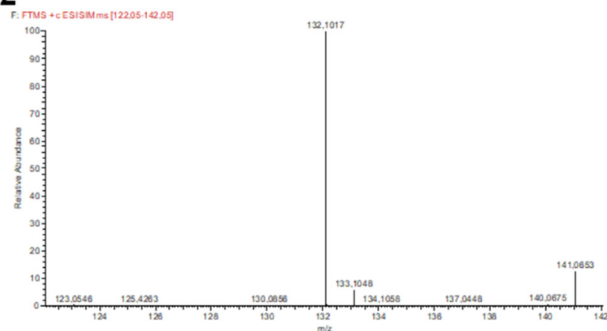
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D1**D2****D3****E1****E2****E3****F1****F2****F3**

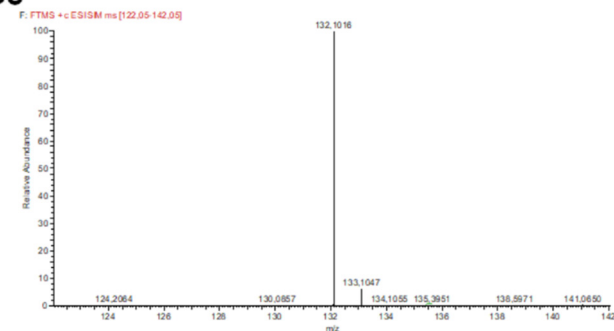
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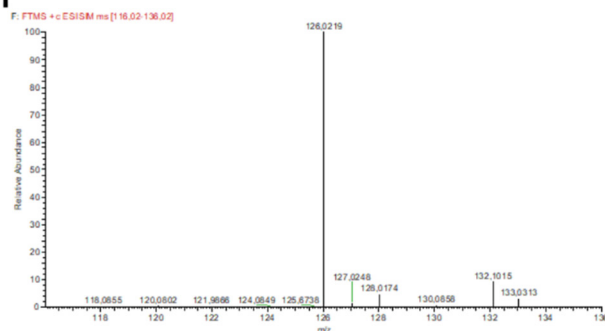
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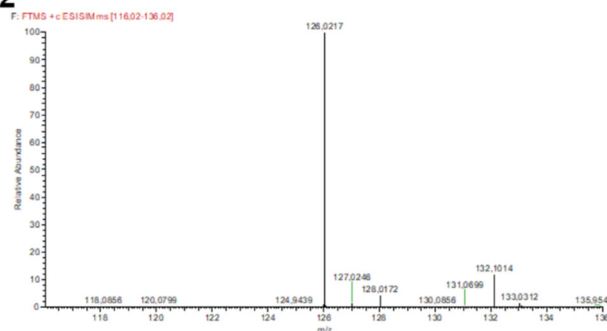
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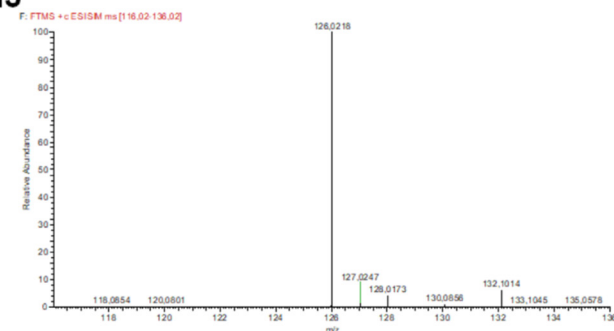
H1



H2



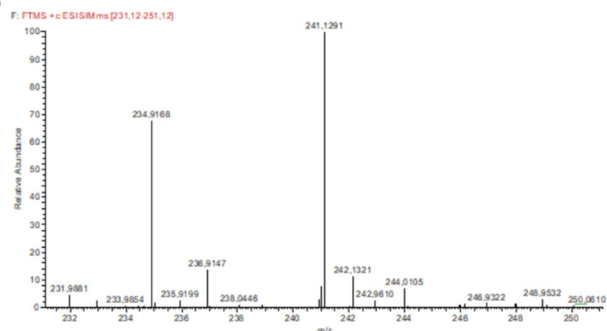
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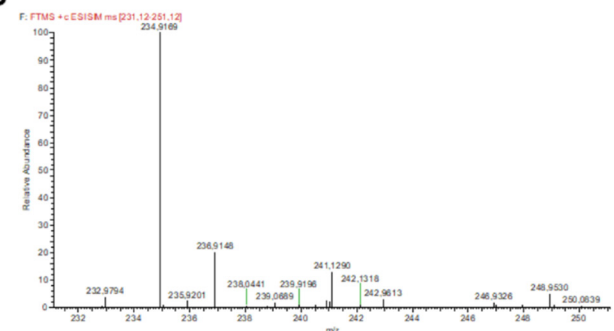
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I2



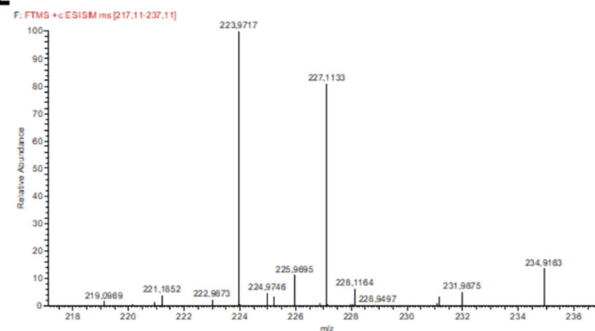
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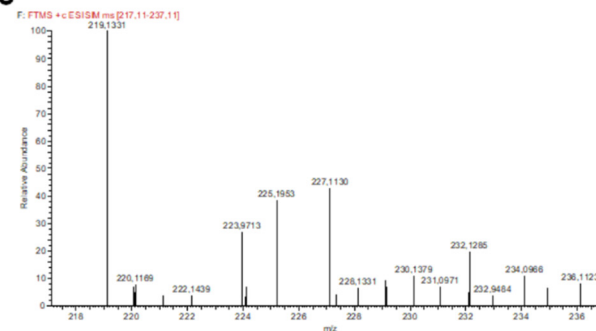
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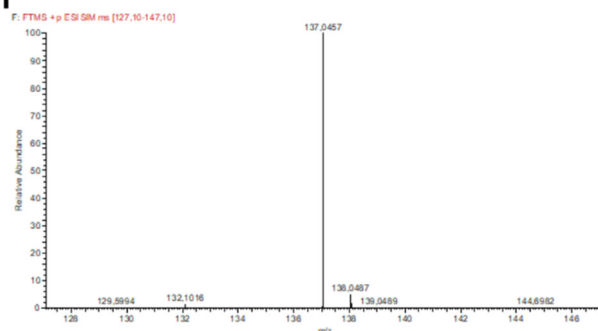
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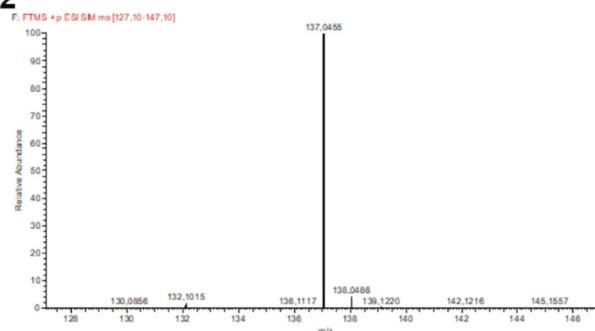
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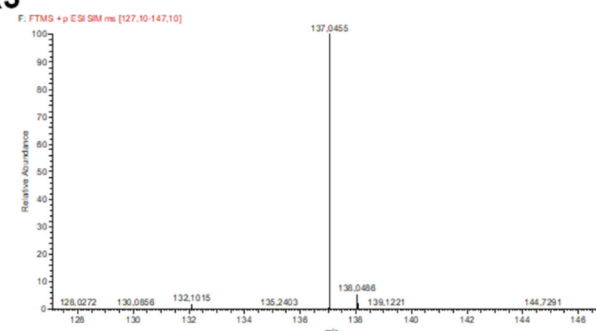
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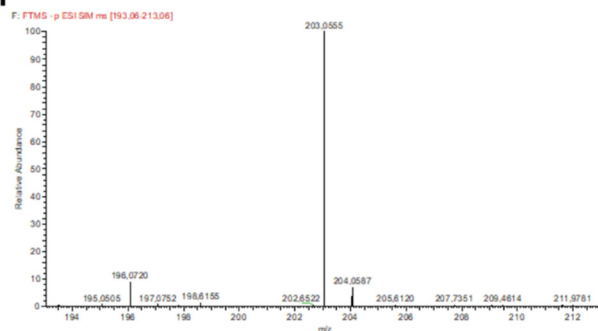
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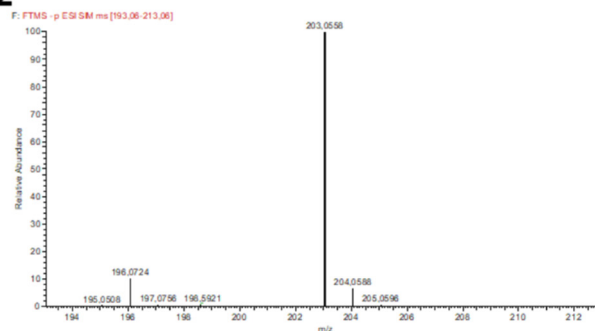
K3



L1



L2



L3

Not detected

Figure S1. MS spectra of nicotinamide (A), riboflavin (B), thiamine (C), tryptophan (D), histidine (E), phenylalanine (F), isoleucine (G), taurine (H), anserine (I), carnosine (J), hypoxanthine (K) and gadusol (L) in the sardine (1), horse mackerel (2) and sea bass (3) roe-derived aqueous extracts.

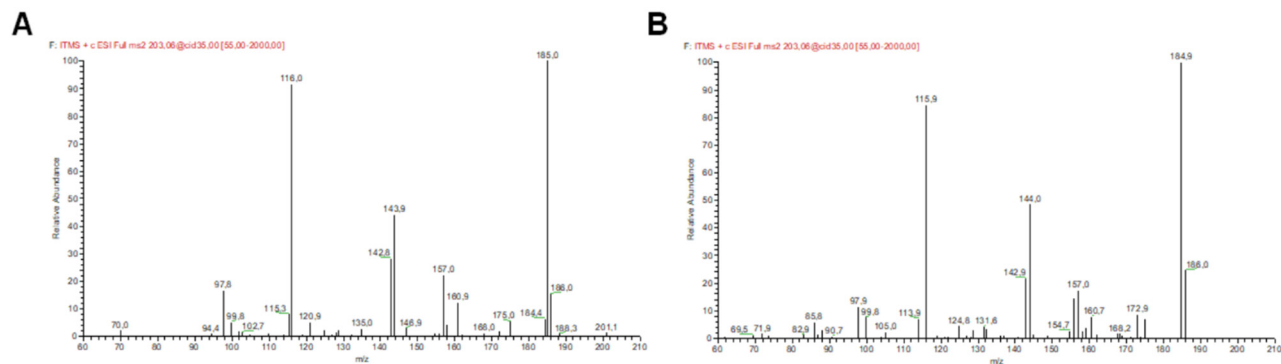


Figure S2. MS² spectra of gadusol in the sardine (A) and horse mackerel (B) roe-derived aqueous extracts.

References

1. Perrone, D.; Monteiro, M.; Castelo-Branco, V.N. The Chemistry of Imidazole Dipeptides. In *Imidazole Dipeptides: Chemistry, Analysis, Function and Effects*, Preedy, V.R., Ed.; Food and Nutritional Components in Focus; 2015; Volume 8, pp. 43-60.