

Supplementary material

Bioprospecting of targeted phenolic compounds of *Dictyota dichotoma*, *Cystoseira barbata*, *Ericaria amentacea*, *Sargassum hornschurchii* and *Ellisolandia elongata* from the Adriatic Sea extracted by two green methods

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Table S1. Target polyphenols. CAS number, molecular mass, retention time and MS/MS transitions.

Polyphenols	CAS	Molecular mass (g mol ⁻¹)	Retention time (min)	MS/MS transitions*		
				Precursor ion	Product ions	Collision energy, eV
Gallic acid	149-91-7	170.1	2.35	<u>169.0</u>	<u>125.0</u> , 153.1	<u>17</u> , 15
2,4,6-trihydroxybenzoic acid	71989-93-0	188.1	3.37	<u>168.9</u>	<u>150.9</u> , 107.0	<u>17</u> , 22
Galocatechin	970-73-0	306.3	3.80	<u>305.0</u>	<u>175.1</u> , 158.4	<u>19</u> , 12
3,4-dihydroxybenzoic acid	99-50-3	154.1	3.88	<u>152.9</u>	<u>109.0</u> , 91.0, 108.0	<u>17</u> , 19, 23
2,4-dihydroxybenzoic acid	89-86-1	154.1	4.41	<u>153.0</u>	<u>109.0</u> , 65.0, 67.0	<u>16</u> , 19, 23
2,5-dihydroxybenzoic acid	490-79-9		4.44	<u>153.0</u>	<u>109.0</u> , 65.0, 67.0	<u>16</u> , 19, 23
Caftaric acid	67879-58-7	312.2	4.48	<u>310.9</u>	<u>178.9</u> , 310.9, 148.9	<u>17</u> , 14, 14
2,5-dihydroxybenzaldehyde	1194-98-5	138.1	4.63	<u>136.9</u>	<u>81.0</u> , 109.0	<u>21</u> , 18, 14
3,4-dihydroxybenzaldehyde	139-85-5	138.1	4.64	<u>136.9</u>	<u>81.0</u> , 109.04	<u>21</u> , 24, 25
3-hydroxybenzoic acid	99-06-9	138.1	5.15	<u>137.0</u>	<u>93.0</u> , 65.0	<u>17</u> , 27
4-hydroxybenzoic acid	99-96-7	138.1	5.18	<u>137.0</u>	<u>93.0</u> , 65.0	<u>17</u> , 27
Procyanidin B1	20315-25-7	578.5	5.30	<u>577.0</u>	<u>407.0</u> , 288.9, 424.9	<u>26</u> , 25, 26
Catechin	18829-70-4	290.3	5.34	<u>289.0</u>	<u>245.0</u> , 203.1	<u>17</u> , 22
2,6-dihydroxybenzoic acid	303-07-1	154.1	5.54	<u>153.0</u>	<u>109.0</u> , 135.0	<u>17</u> , 16
3,5-dihydroxybenzoic acid	99-10-5	154.1	5.54	<u>153.0</u>	<u>109.0</u> , 135.0	<u>17</u> , 16
3-hydroxybenzaldehyde	100-83-4	122.1	5.67	<u>121.0</u>	<u>93.0</u> , 92.0, 120.0	<u>20</u> , 23, 19
4-hydroxybenzaldehyde	123-08-0	122.1	5.67	<u>121.0</u>	<u>93.0</u> , 92.0, 120.0	<u>20</u> , 23, 19

3,4-dimethoxybenzoic acid	93-07-2	182.0	6.03	<u>182.9</u>	<u>137.0</u> , 106.9	<u>6</u> , 22
Procyanidin B2	29106-49-8	578.5	6.10	<u>577.0</u>	<u>407.0</u> , 288.9, 424.9	<u>26</u> , 25, 26
Chlorogenic acid	327-97-9	354.3	6.12	<u>353.0</u>	<u>191.0</u> , 85.0, 93.0	<u>22</u> , 43, 45
Ampelopsin	27200-12-0	320.25	6.20	<u>319.0</u>	<u>193.1</u> , 301.1, 125.1	<u>15</u> , 13, 27
Caffeic acid	331-39-5	180.2	6.50	<u>178.8</u>	<u>135.0</u> , 134.0	<u>19</u> , 28
Procyanidin C1	37064-30-5	866.8	6.52	<u>577.0</u>	<u>288.3</u> , 407.0, 424.9	<u>26</u> , 25, 26
Epicatechin	35323-91-2	290.3	6.56	<u>289.0</u>	<u>245.0</u> , 203.1	<u>17</u> , 22
Epigallocatechingallate	989-51-5	458.4	6.79	<u>457.1</u>	<u>169.0</u> , 125.0, 305.0	<u>21</u> , 42, 21
Procyanidin A1	12798-56-0	576.5	6.80	<u>577.0</u>	<u>407.0</u> , 288.9, 424.9	<u>26</u> , 25, 26
Gallocatechingallate	84650-60-2	458.4	7.29	<u>457.1</u>	<u>169.0</u> , 125.0, 305.0	<u>21</u> , 42, 21
Procyanidin A2	41743-41-3	576.5	7.32	<u>577.0</u>	<u>287.0</u> , 136.9, 425.0	<u>32</u> , 62, 13
Orientine	28608-75-5	448.4	7.38	<u>477.1</u>	<u>327.1</u> , 357.1	<u>23</u> , 22
7-hydroxycoumarin	93-35-6	162.1	7.80	<u>162.9</u>	<u>107.0</u> , 77.0, 91.0	<u>22</u> , 34, 20
4-hydroxycinnamic acid	501-98-4	164.2	7.89	<u>163.0</u>	<u>119.0</u> , 93.0, 117.0	<u>17</u> , 37, 38
Epicatechingallate	1257-08-5	442.4	7.92	<u>441.1</u>	<u>289.1</u> , 125.0, 169.0	<u>20</u> , 42, 24
Polidatin	27208-80-6	390.4	7.98	<u>389.1</u>	<u>227.1</u> , 185.1, 143.1	<u>22</u> , 38, 48
Taxifolin	480-18-2	304.25	8.06	<u>303.0</u>	<u>285.1</u> , 125.1, 175.1	<u>14</u> , 23, 22
Catechingallate	130405-40-2	442.3	8.12	<u>441.1</u>	<u>289.1</u> , 125.0, 169.0	<u>20</u> , 42, 24
3,4-dimethoxybenzaldehyde	120-14-9	166.2	8.33	<u>167.0</u>	<u>139.0</u> , 108.0, 124.0	<u>13</u> , 21, 18
Trans-ferulic acid	537-98-4	194.2	8.92	<u>192.8</u>	<u>177.9</u> , 133.9	<u>12</u> , 16
4-methoxybenzaldehyde	123-11-5	136.1	9.11	<u>136.9</u>	<u>109.0</u> , 77.0, 94.0	<u>12</u> , 23, 18
Resveratrol	501-36-0	228.07	9.31	<u>227.1</u>	<u>185.1</u> , 115.1, 117.1	<u>21</u> , 47, 20
Robinetin	490-31-3	302.23	9.50	<u>301.2</u>	<u>162.6</u> , 273.0	<u>20</u> , 20
Quercetin-3-glucuronide	22688-79-5	478.4	9.54	<u>479.0</u>	<u>461.5</u> , 302.9	<u>14</u> , 18
Quercetin-3-rutinoside	153-18-4	610.5	9.72	<u>609.1</u>	<u>270.9</u> , 178.8, 300.0	<u>96</u> , 44, 37
Quercetin-3-glucoside	482-35-9	463.4	9.75	<u>465.0</u>	<u>256.9</u> , 302.9	<u>41</u> , 14
Myricetin	529-44-2	318.2	10.09	<u>319.0</u>	<u>153.0</u> , 217.0, 245.0	<u>31</u> , 31, 27
Ellagic acid	476-66-4	302.19	10.21	<u>301.0</u>	<u>145.1</u> , 185.1, 173.1	<u>39</u> , 29, 36
Rosmarinic acid	20283-92-5	360.3	10.37	<u>359.0</u>	<u>161.1</u> , 133.1, 135.1	<u>23</u> , 42, 38
3,4,5-trimethoxycinnamic acid	90-50-6	238.2	11.13	<u>239.0</u>	<u>221.0</u> , 162.9, 190.0	<u>11</u> , 27, 19
Astragalin	480-10-4	448.4	11.16	<u>447.0</u>	<u>255.1</u> , 284.1, 227.1	<u>40</u> , 28, 49
3,5-dimethoxybenzaldehyde	7311-34-4	166.2	11.26	<u>167.1</u>	<u>124.0</u> , 77.0	<u>17</u> , 26
Fisetin	528-48-3	286.2	11.50	<u>285.0</u>	<u>135.0</u> , 163.0	<u>15</u> , 15
Daidzein	486-66-8	254.2	11.53	<u>253.0</u>	<u>133.1</u> , 91.1, 135.1	<u>34</u> , 40, 30
Epsilon-viniferin	62218-08-0	454.5	11.82	<u>455.1</u>	<u>361.1</u> , 349.1, 350.1	<u>20</u> , 20, 20
Quercetine	117-39-5	302.2	11.83	<u>303.0</u>	<u>229.1</u> , 153.0	<u>28</u> , 33
Naringenin	67604-48-2	272.2	11.89	<u>272.0</u>	<u>119.0</u> , 147.0	<u>20</u> , 22
Luteolin	491-70-3	286.2	12.17	<u>285.0</u>	<u>199.0</u> , 175.0, 241.0	<u>20</u> , 22, 20
Kaempferol	520-18-3	286.2	12.35	<u>285.0</u>	<u>184.9</u> , 239.1	<u>30</u> , 35
Isorhamnetin	480-19-3	316.3	12.52	<u>317.0</u>	<u>302.0</u> , 165.0, 257.0	<u>20</u> , 24, 35
Diosmetin	520-34-3	300.26	12.64	<u>299.0</u>	<u>133.1</u> , 63.1, 65.1	<u>46</u> , 48, 54
Apigenin	520-36-5	270.2	12.63	<u>269.0</u>	<u>117.1</u> , 149.1, 151.0	<u>37</u> , 26, 26
Chrysin	480-40-0	254.2	13.24	<u>253.1</u>	<u>143.1</u> , 63.2, 145.1	<u>30</u> , 34, 31

* Underlined MS transition is used for quantification purpose