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Volatile compounds of some popular Mediterranean seafood species

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Supplementary Data
["Volatile compounds of some popular Mediterranean seafood species"
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PCA component matrix (Because of the large number of volatile compounds, only those present in at least half of the studied species are shown)

	Component								
	1	2	3	4	5	6	7	8	9
Heptanal	0.985	-0.024	0.045	-0.043	-0.086	-0.067	-0.026	0.108	0.014
2-Nonanone	0.972	-0.082	-0.053	0.068	-0.005	-0.115	0.120	-0.112	-0.017
2,4-dimethyl-heptane,	0.952	-0.118	-0.184	0.056	-0.044	-0.095	0.171	-0.041	0.013
Octanal	0.950	-0.291	0.022	-0.029	-0.066	-0.066	0.005	0.052	0.020
Unknown (3-Nonen-2-one)	0.930	0.076	-0.038	-0.282	0.157	0.018	0.039	-0.150	0.015
4-Heptanone	0.905	-0.360	0.062	-0.142	-0.103	-0.088	-0.032	-0.088	-0.014
Unknown (4,7-dimethyl-undecane	0.901	0.242	-0.275	0.095	0.067	-0.165	0.113	0.026	-0.031
Toluene	0.885	-0.247	0.179	-0.250	0.205	-0.087	-0.053	-0.083	0.036
Pentanal	0.874	-0.481	-0.001	-0.051	-0.006	-0.027	-0.003	-0.030	-0.015
Decanal	0.861	-0.321	0.014	-0.121	-0.225	-0.011	-0.047	0.297	0.007
2,3-Dimethyl hexane	0.854	-0.221	-0.152	0.173	0.079	-0.310	0.077	-0.246	0.003
Benzaldehyde	0.842	-0.527	-0.003	-0.020	0.030	-0.039	-0.059	-0.074	-0.049
2,4-Dimethyl-1-heptene	0.834	-0.459	-0.128	0.081	0.074	-0.111	0.212	-0.079	0.042
Nonanal	0.824	-0.512	-0.015	-0.064	-0.057	-0.161	0.061	0.130	-0.068
2-Methyl butanal	0.821	-0.371	0.250	0.181	-0.048	0.264	-0.060	-0.128	-0.038
Unknown	0.810	0.512	0.090	-0.026	-0.027	-0.243	0.038	0.008	-0.112
3-Methylthio-propanal	0.805	-0.076	0.265	0.469	0.031	0.134	-0.192	-0.019	0.011
3-Pentanol	0.797	0.340	0.151	-0.331	0.175	-0.147	0.224	0.025	0.116
1-Methylthiopropene,	0.793	-0.066	0.000	0.499	-0.218	0.174	0.187	0.075	0.000
Octane	0.791	-0.601	-0.013	-0.084	-0.023	-0.066	-0.002	0.018	-0.016
Tetrahydrofuran	0.790	0.468	0.121	-0.145	0.125	-0.272	-0.127	-0.109	-0.062
4-Methyloctane	0.785	-0.609	-0.041	-0.069	0.018	-0.057	-0.008	-0.057	-0.007
Ethylbenzene	0.777	-0.501	0.230	-0.025	0.078	-0.081	0.045	0.195	-0.197
p-Xylene	0.769	-0.605	-0.048	0.061	0.107	0.060	0.045	-0.142	-0.009
1-Pentanol	0.760	-0.640	-0.012	-0.023	-0.044	0.035	-0.077	-0.021	0.047
Furfural	0.759	-0.632	-0.040	-0.017	0.121	0.000	0.009	-0.085	0.004
Hexanal	0.758	0.598	-0.050	-0.124	-0.088	-0.069	-0.039	0.155	0.112
1-(2-Furanyl)-ethanone	0.758	-0.645	-0.024	-0.066	0.010	-0.037	0.008	-0.058	-0.020
Pyridine	0.745	-0.649	-0.037	-0.106	0.008	-0.072	-0.045	-0.067	0.000
5-methyl-2-furancarboxaldehyde	0.732	-0.533	0.007	0.265	-0.128	0.201	-0.228	-0.040	0.019
D-Limonene	0.719	-0.650	-0.034	-0.112	-0.125	0.053	-0.038	0.135	0.097
Nonadecane	0.717	-0.163	-0.390	0.228	-0.064	-0.210	0.405	-0.208	0.020
3-Methyl butanal,	0.715	-0.362	0.279	0.391	0.075	0.237	-0.164	-0.192	0.044
1-Octadecene	0.679	0.097	0.241	-0.381	0.222	0.338	0.074	0.103	-0.384
Benzeneacetaldehyde	0.662	-0.475	0.212	0.354	-0.164	0.275	-0.245	-0.009	0.065
o-Xylene	0.656	-0.647	0.153	0.193	0.020	-0.132	-0.169	0.072	0.195
2-Pentenal	0.364	0.915	0.107	0.011	-0.073	0.014	0.083	0.078	0.004
4-Ethyl-benzaldehyde	0.376	0.913	0.077	0.022	-0.041	0.025	0.096	0.008	0.084
trans-2-(2-pentenyl)-furan	0.330	0.902	-0.097	0.158	-0.103	0.158	0.022	0.083	-0.023
2-Methoxy-2-methyl-butane	0.240	-0.897	0.090	0.257	-0.214	0.096	0.078	-0.029	0.033
1-Penten-3-ol	0.359	0.885	0.203	0.130	-0.133	0.086	0.045	0.040	0.039
2,3-pentanedione	0.366	0.883	0.029	0.018	0.043	-0.011	0.270	-0.094	0.034

(continued)

(continued)

	Component								
	1	2	3	4	5	6	7	8	9
Heptanal	0.985	-0.024	0.045	-0.043	-0.086	-0.067	-0.026	0.108	0.014
3,5-Octadiene	0.395	0.860	0.244	-0.166	0.054	-0.088	-0.066	-0.056	0.001
<i>trans,trans</i> -2,4-Heptadienal	0.449	0.854	0.114	-0.172	-0.017	0.044	0.064	0.090	0.110
<i>trans</i> -2-Penten-1-ol-(Z)-	0.442	0.849	0.056	0.110	-0.092	-0.184	-0.103	0.014	0.122
3,5-Octadien-2-one	0.458	0.848	0.080	-0.111	0.025	-0.203	-0.087	-0.018	0.055
4-Ethyl phenol	0.353	0.828	0.345	0.046	-0.156	0.050	-0.140	0.131	0.072
1,4-Cyclohexadiene	0.114	0.824	0.049	-0.432	-0.030	-0.223	0.082	-0.249	-0.017
<i>cis,trans</i> -2,6-Nonadienal	0.544	0.817	0.115	-0.043	-0.036	-0.100	0.086	0.038	-0.019
Unknown	0.133	-0.810	-0.282	-0.402	0.226	-0.132	0.039	0.123	0.010
2-Hexenal	0.503	0.802	0.064	-0.046	0.087	-0.260	-0.062	-0.108	-0.089
All <i>cis</i> -1,3,5-Octatriene	0.248	0.749	0.451	-0.010	0.024	0.318	0.212	-0.112	0.116
2-Pentyl furan	0.602	0.749	-0.018	-0.137	-0.057	0.167	-0.057	0.144	-0.034
Dimethyl trisulfide	0.285	0.712	0.118	0.482	0.011	0.015	-0.338	-0.222	-0.043
<i>trans</i> -4-Heptenal	0.655	0.703	0.127	0.181	-0.062	-0.147	0.001	0.012	-0.050
Hexadecanoic acid ethylester	0.253	0.702	-0.621	-0.015	-0.017	0.134	-0.173	-0.006	0.098
2,4-Heptadienal	0.616	0.667	0.084	-0.361	0.161	0.017	-0.043	-0.088	0.045
2,3-Octanedione	0.528	0.650	0.136	-0.496	0.120	0.095	-0.077	0.067	-0.025
1-Nonadecene	0.370	-0.646	0.293	-0.296	0.414	0.088	0.190	0.157	-0.182
2-Acetyl-5-methyl-furan	0.322	0.602	0.233	0.397	-0.377	-0.212	0.003	-0.012	-0.367
1,3,5-Trimethyl benzene	0.440	-0.592	0.168	0.241	0.379	-0.270	-0.321	0.121	0.189
Unknown ester	0.138	0.368	-0.756	0.404	0.257	0.166	0.084	-0.060	-0.081
Unknown ester	-0.166	-0.158	-0.755	0.298	0.013	0.450	0.289	0.038	-0.018
1-Octadecanol	0.129	0.528	-0.753	-0.081	-0.045	0.216	-0.173	0.227	-0.021
2,6,11-trimethyl-dodecane	0.527	0.294	-0.736	0.116	0.123	0.152	-0.099	0.179	0.018
Tetradecane	0.303	0.003	-0.733	-0.264	0.254	0.443	-0.199	0.013	-0.016
2-methyl-undecane	0.659	0.210	-0.695	0.162	-0.009	0.062	-0.010	0.083	-0.030
Octadecane	0.114	0.620	-0.691	0.049	-0.144	0.003	-0.027	0.056	0.314
Tridecane	0.285	-0.321	-0.656	-0.266	0.279	0.456	-0.00	0.020	0.171
Octadecanoic acid ethylester	0.347	0.639	-0.642	-0.019	0.060	0.081	-0.213	0.060	0.015
Acetophenone	-0.123	0.310	0.633	-0.221	0.579	0.200	-0.148	0.111	0.171
Styrene	-0.069	0.027	0.601	-0.534	0.499	0.109	-0.098	0.232	0.153
2-Thiophene carboxaldehyde	0.432	0.046	0.593	0.350	-0.087	0.476	-0.225	0.132	0.187
Unknown	0.557	0.258	-0.559	-0.272	0.388	0.089	-0.062	-0.269	0.041
1-Hexadecene	0.405	0.118	0.559	-0.457	-0.106	0.168	0.173	0.379	-0.296
Phlorobutyrophenone 2-butyl-5(2-methyl-propyl) thiophene	0.113	0.137	0.345	0.773	0.354	-0.217	0.191	0.177	0.107
Unknown	-0.069	0.021	0.289	0.749	-0.404	0.326	-0.221	0.166	-0.062
2-Acetylthiazole	0.148	-0.060	0.327	0.704	0.296	0.467	0.072	-0.170	0.177
2,4-Decadienal	0.449	0.218	0.207	-0.692	0.086	0.352	0.042	0.125	0.284
Hexadecanoic acid methylester	-0.185	-0.282	0.354	-0.669	-0.286	0.050	-0.183	-0.399	0.189
Octadecanoic acid methylester	-0.293	-0.186	0.323	-0.647	-0.301	0.137	-0.251	-0.409	0.133
2-Hydroxy-3-pentanone	0.367	0.238	0.395	0.571	-0.191	0.523	0.041	-0.077	-0.089
2-Phenylpropenal	0.025	0.437	0.236	0.489	0.400	0.304	0.377	-0.344	0.027
2,5-Cyclohexadiene-1,4-dione 2,6-bis(1,1-dimethylethyl)-	-0.144	0.093	-0.013	0.384	0.845	-0.109	-0.256	0.086	-0.156
Dimethyl disulfide	-0.115	0.269	0.075	0.357	0.793	-0.248	-0.302	-0.001	-0.006
Dimehtyl carbamic chloride	-0.476	-0.180	0.074	0.361	0.706	-0.286	-0.034	0.148	0.041
Pyrazine	0.100	-0.252	0.068	-0.561	0.146	0.622	0.425	0.106	-0.084
3-Hydroxy-2-butanone	-0.273	0.031	0.266	0.215	0.326	-0.003	0.814	-0.060	0.187
3-Penten-2-ol	0.132	-0.270	0.011	0.264	-0.421	-0.435	0.288	0.397	0.483