

**Table S5** UHPLC-HR-ESI-MS/MS data of compounds **a-f** detected in the *Citrus aurantium* albedo (A), but not found in bread samples enriched with A.

Peak*	Compound	<i>t<sub>R</sub></i> (min)	HR-[M-H] <sup>-</sup> ( <i>m/z</i> )	Negative Product Ions ( <i>m/z</i> )**	Error (ppm)
<b>a</b>	Caffeic acid glucoside	4.9	341.1239	<b>179.03</b> , 135.0	-0.29
<b>b</b>	Feruloyl acid glucoside	6.1	355.1035	193.05, <b>175.04</b> , 149.06	0.00
<b>c</b>	Lucenin-2 4'-methyl ether (diosmetin 6,8-di-C- glucoside)	8.9	623.1619	503.12, 413.09, 383.08, <b>312.06</b>	+0.16
<b>d</b>	Naringin glucoside	9.2	741.2254	579.17, <b>271.06</b> , 151.00	+0.94
<b>e</b>	Diosmetin 8-C- glucoside/6-C-glucoside	10.8	461.1091	361.08, 341.07, <b>298.05</b>	+0.43
<b>f</b>	3-Hydroxy-3-methyl- glutaryl- neoericitrin/eriocitrin	11.9	739.2099	595.17, 287.06, <b>151.00</b>	+1.08

\*Peak numbers correspond with those in Figure 1S. \*\*The base ion peaks generated in the ESI-MS/MS experiments are shown in bold.