Kaempferol as selective human MAO-A inhibitor: analytical detection in Calabrian red wines, biological and molecular modelling studies

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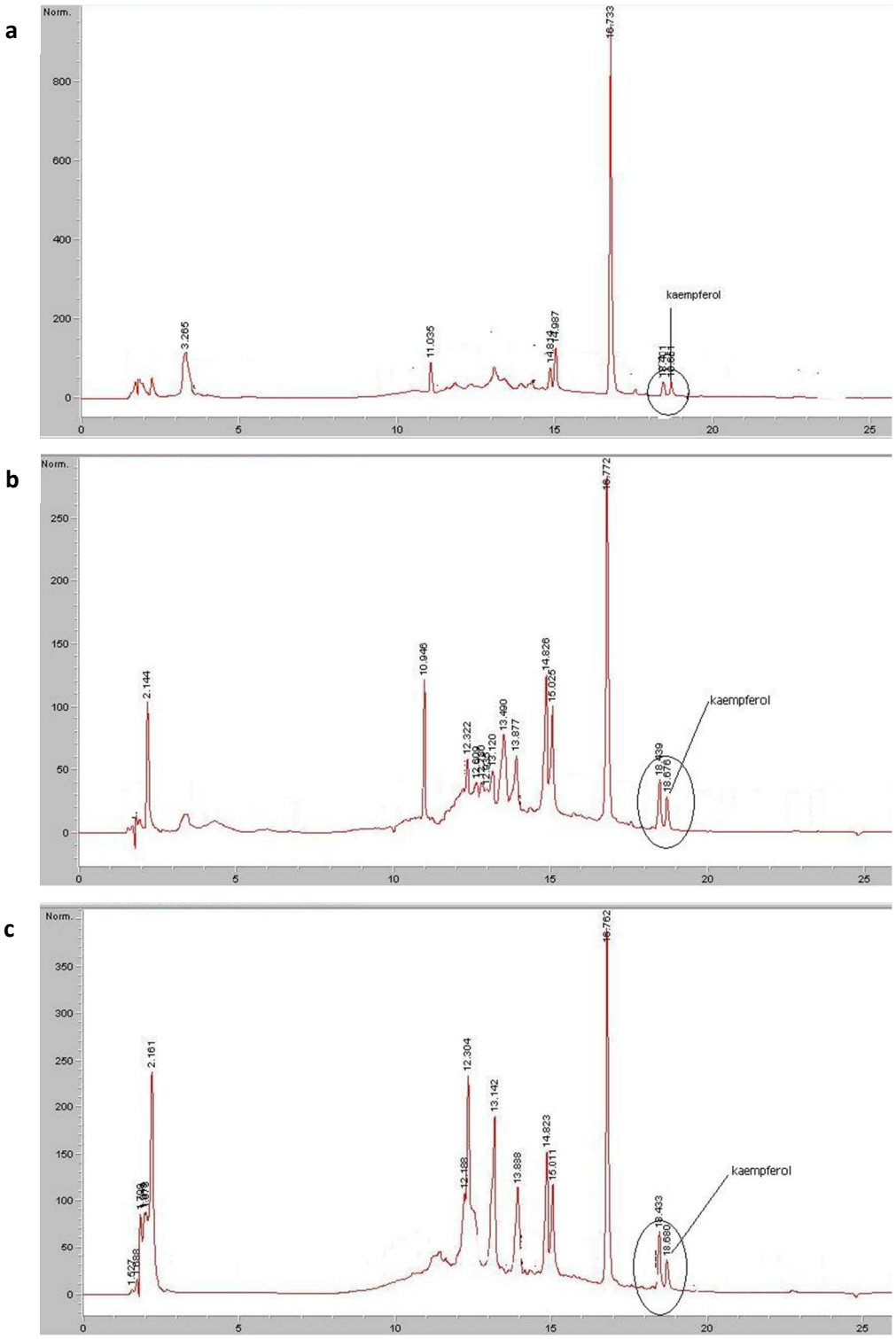

Figure 1S. HPLC chromatograms of the three Calabrian red wine samples from the 2013 vintage: Magliocco (**a**), Gaglioppo (**b**) and Nerello (**c**) containing the kaempferol peak in evidence.

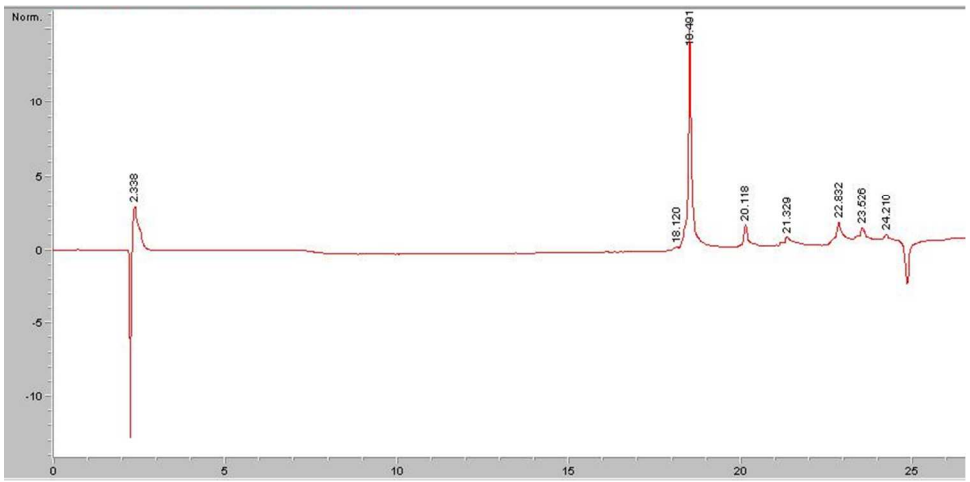

Figure 2S: The retention time of Kaempferol in the standard solution equal to 18.5 min.

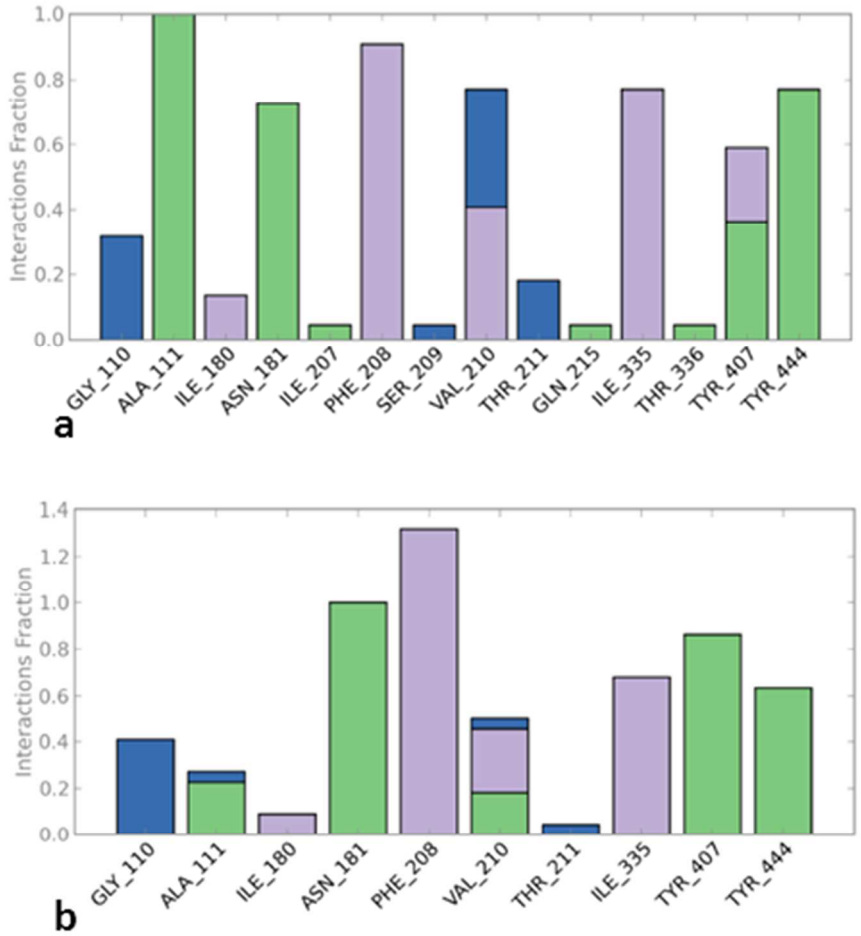

Figure 3S: SID plots showing the protein-ligand interactions, established during the MD simulation, between the amino acid residues of hMAO-A binding site and the flavonoids kaempferol (**a**) and quercetin (**b**). The stacked bar charts are categorized as follow: hydrogen bond (green), hydrophobic (violet) and water bridge (blue).

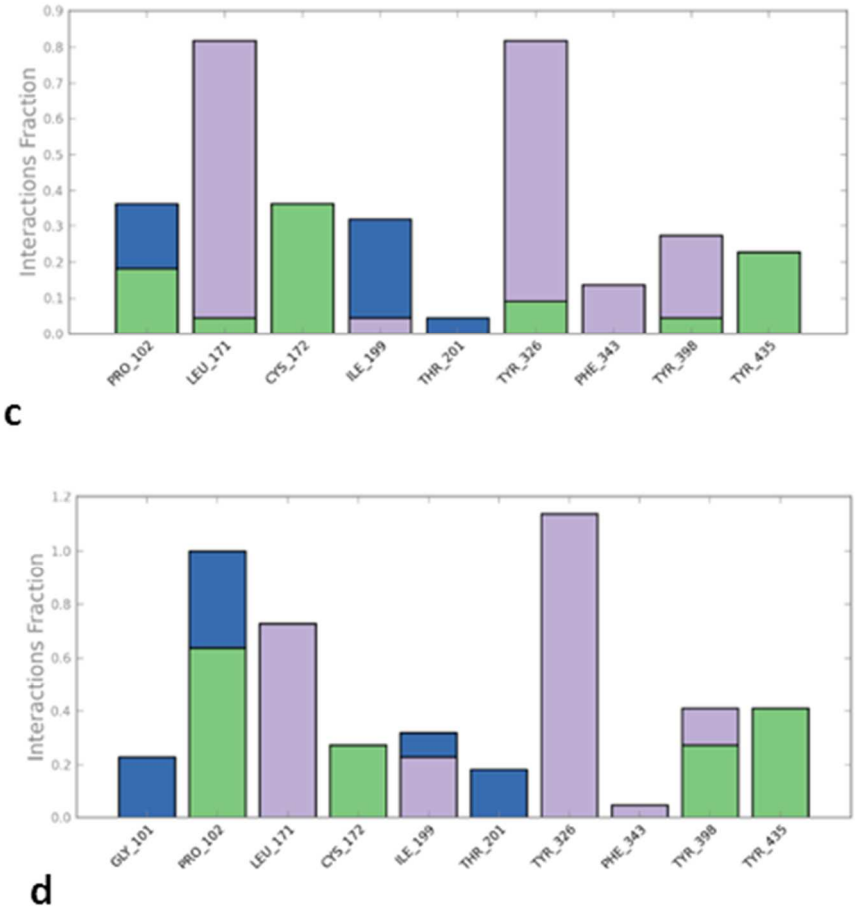

Figure 4S: SID plots showing the protein-ligand interactions, established during the MD simulation, between the amino acid residues of hMAO-B binding site and the flavonoids kaempferol (**c**) and quercetin (**d**). The stacked bar charts are categorized as follow: hydrogen bond (green), hydrophobic (violet) and water bridge (blue).