

## ASSOCIATED CONTENT

### **Molecular Approach of the Synergistic Effect on Astringency Elicited by Mixtures of Flavanols**

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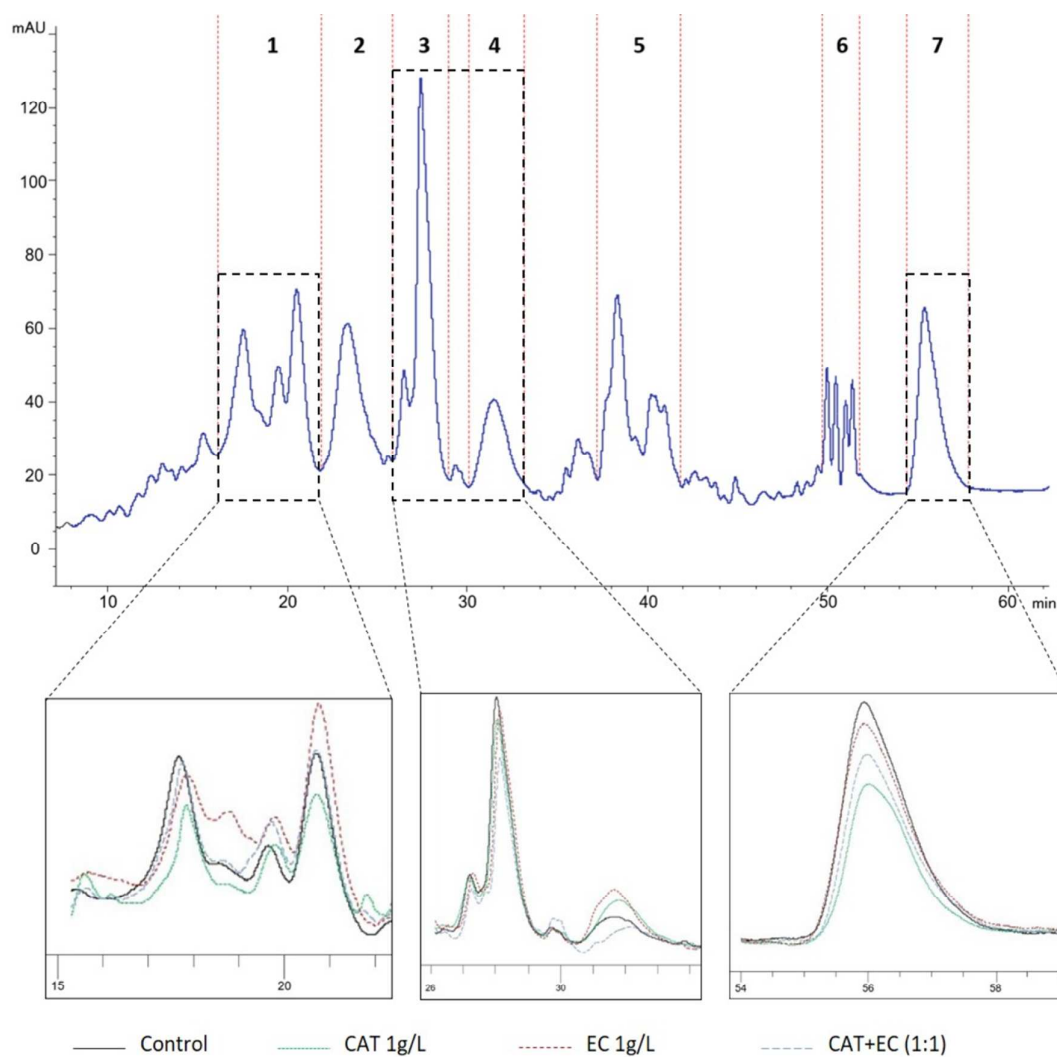
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**Table S1**

The binding of eight molecules (CAT and/or EC) to four IB7<sub>14</sub> PRP fragments was analysed by number of flavanols bound in simultaneous to each peptide throughout the first 25 ns of simulations.

System		1 flavanol	2 flavanols	3 flavanols
CAT	IB714_1	0.1	-	-
	IB714_2	3.7	-	-
	IB714_3	7.9	-	-
	IB714_4	3.9	-	-
	<i>average</i>	3.9	-	-
	<i>sum</i>	15.6	-	-
EC	IB714_1	3.3	0.0	-
	IB714_2	1.2	0.0	-
	IB714_3	6.1	0.1	-
	IB714_4	1.5	0.1	-
	<i>average</i>	3.0	0.1	-
	<i>sum</i>	12.0	0.2	-
CAT+EC	IB714_1	13.3	0.5	0.0
	IB714_2	5.0	2.8	0.7
	IB714_3	7.1	0.0	0.0
	IB714_4	5.0	0.0	0.0
	<i>average</i>	7.6	0.8	0.2
	<i>sum</i>	30.4	3.3	0.7

**Figure S1.** Total chromatographic salivary profile (upper) and chromatographic profiles of the fractions 1, 3, 4 and 7 that underwent significant changes after addition of CAT + EPI (---) and CAT (—) or EPI (---). See table 1 for the identification of the fractions.



**Figure S2.** Enlarged illustration of representative geometries of the binding of different flavanols to one IB714 peptide extracted from MD simulations of the (IB714)<sub>4</sub>:(CAT)<sub>8</sub>, (IB714)<sub>4</sub>:(EC)<sub>8</sub> and (IB714)<sub>4</sub>:(CAT)<sub>4</sub>:(EC)<sub>4</sub> systems. The peptides are depicted with sticks, and are colored by element type. The CAT and EC molecules are depicted with balls and sticks representation and are colored by element type (except the CAT compounds in the third system that are colored in orange).

