Critical review of plant-derived compounds as possible inhibitors of SARS-Cov2 proteases: a comparison with experimentally validated molecules

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Common fragments in the 648 predicted molecules.

The fragment analysis of all the unique molecules using Recap generates a total of 1042 different fragments (the full list can be seen in Supplementary Material 1B). Because of the large number of fragments (and the wide chemical diversity) we included the top frequent fragments (with more than 4 non-hydrogen atoms and from 0.25 to 24% of abundance) in Figure S1. The fragments were arranged in groups and we can easily identify the fragments related to: gallic and caffeic acids (Group I, Group II, Group V), fragments or even portions of the double ring fragments which are associated with the molecules with higher evidence (quercetin, luteolin, kaempferol, etc) (Group I and Group IX). We also found several monosaccharides, disaccharides and glucuronic fragments which are consistent with glycosylated flavonoids (Group III). On the other hand, we found fragments present in molecules like piperine, coumaperine, piperundecalidi and quinic acids and different aliphatic substituents commonly found in the dataset.

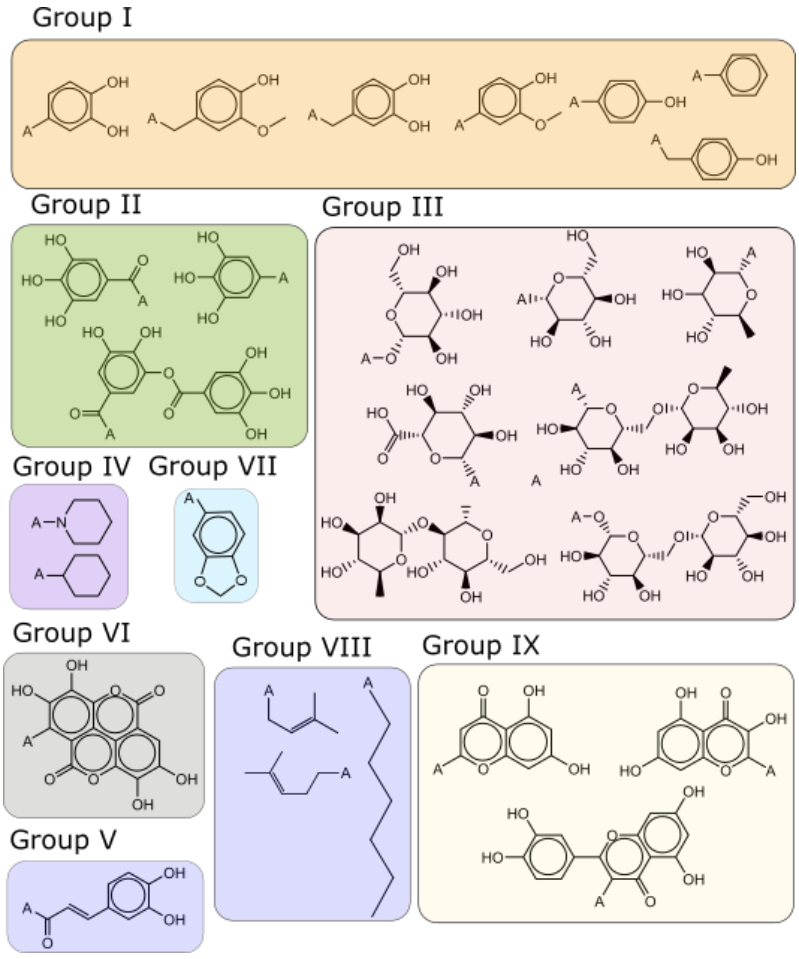

Figure S1. Top frequent fragments identified in all unique molecules.