Supplementary Materials for

In silico identification and biological evaluation of antioxidant food components endowed with IX and XII *h*CA inhibition

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Figure S1. 2D chemical structures of the already approved inhibitors of both *h*CA isoforms.

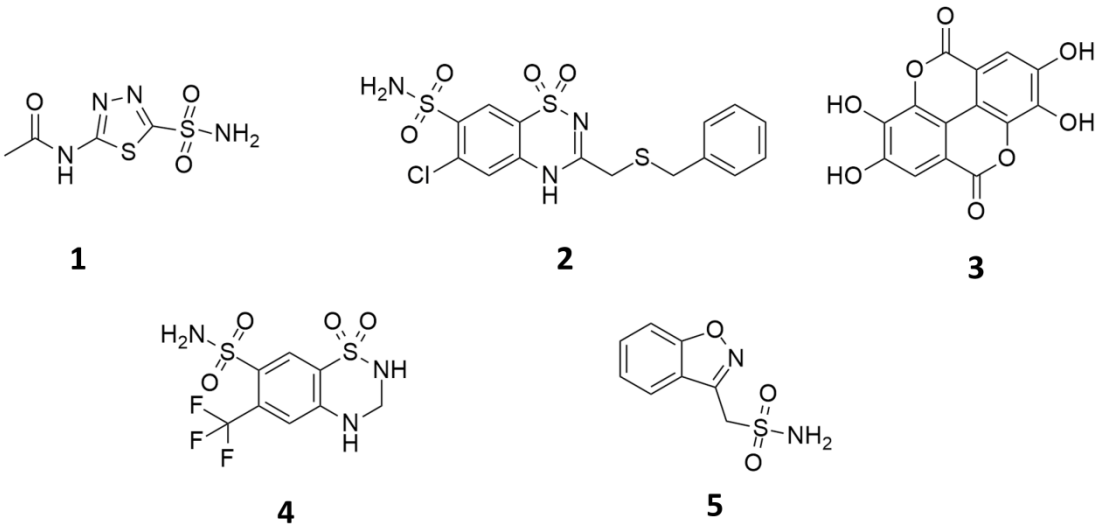

Table S1. 2D chemical structures, G-score and ΔE values for each already approved inhibitor of the *h*CA XII isoform.

Compound	Name	G-Score *(kcal/mol)*	ΔE *(kcal/mol)*
1	Acetazolamide	-4.56	-28.56
2	Benzthiazide	-5.62	-34,12
3	Ellagic acid	-5.51	-30.10
4	Hydroflumethiazide	-5.86	-28.30
5	Zonisamide	-5.34	-19.86

Table S2. 2D chemical structures, G-score and ΔE values for each already approved inhibitor of the *h*CA IX isoform.

Compound	Name	G-Score *(kcal/mol)*	ΔE *(kcal/mol)*
2	Benzthiazide	-4.96	-23.30
3	Ellagic acid	-5.18	-26.60
4	Hydroflumethiazide	-5.10	-12.57
5	Zonisamide	-5.22	-25.21

Table S3. Name, FooDB ID, G-score and ΔE values of the 9 best dual *hits* related to both *h*CA isoforms.

			***h*AC IX**		***h*AC XII**	
Number	**Name**	**FooDB ID**	**G-Score** *(kcal/mol)*	**ΔE** *(kcal/mol)*	**G-Score** *(kcal/mol)*	**ΔE** *(kcal/mol)*
6	(-)-Dehydrodiconiferyl Alcohol	FDB021188	-5.76	-37.89	-6.15	-43.75
7	13'-carboxy-α-tocopherol	FDB029121	-5.88	-35.86	-7.23	-58.88
8	8-Hydroxy-3-methoxy-1-methylanthraquinone-2-carboxylic acid	FDB016091	-7.10	-32.99	-8.42	-35.20
9	Albafuran A	FDB001381	-5.59	-35.25	-6.49	-33.59
10	Cartormin	FDB013856	-6.02	-45.64	-6.45	-62.46
11	Licoagroaurone	FDB014047	-5.50	-41.16	-6.18	-42.89
12	Lithospermic acid	FDB006174	-5.14	-23.42	-7.32	-31.82
13	Piperoic acid	FDB020410	-6.99	-40.69	-7.50	-51.16
14	Syringin	FDB011657	-5.12	-31.22	-6.12	-43.81

Figure S2. 2D chemical structures of the best 9 selected *hits*.