

Table S1. Molecular composition and presence of molecular groups (percentage with respect to the total of formulas) for the different extractions in different solvents: water (dH_2O), dH_2O :Ethanol (EtOH) (1:1), dH_2O :EtOH (1:4), dH_2O :Methanol (MeOH) (1:1), dH_2O :MeOH (1:4), from the biomass of *Asparagopsis armata* and *Rugulopteryx okamurae*. Values are expressed as average \pm standard deviation (SD) (n=3).

	Sample Name	Total Number of formulae	% of exclusive formulae	Aromatic		Highly unsaturated		Polyphenols		Unsaturated		Saturated	
				O rich	O poor	O rich	O poor	O rich	O poor	O rich	O poor	O rich	O poor
<i>A. Armata</i>	dH_2O	320 \pm 44	15	11 \pm 3	26 \pm 4	16 \pm 2	12 \pm 2	8 \pm 1	0 \pm 0	17 \pm 2	17 \pm 6	11 \pm 2	0 \pm 0
	dH_2O :EtOH (1:1)	315 \pm 57	4	4 \pm 1	11 \pm 0	6 \pm 1	22 \pm 1	11 \pm 2	1 \pm 0	11 \pm 1	40 \pm 2	25 \pm 3	2 \pm 0
	dH_2O :EtOH (1:4)	286 \pm 56	2	4 \pm 0	14 \pm 2	9 \pm 1	21 \pm 1	9 \pm 1	1 \pm 0	12 \pm 1	35 \pm 4	29 \pm 2	2 \pm 0
	dH_2O :MeOH (1:1)	279 \pm 48	2	5 \pm 0	13 \pm 1	7 \pm 0	20 \pm 2	11 \pm 2	0 \pm 0	13 \pm 0	37 \pm 2	29 \pm 1	2 \pm 1
	dH_2O :MeOH (1:4)	447 \pm 75	4	4 \pm 1	12 \pm 2	12 \pm 4	35 \pm 8	10 \pm 1	0 \pm 0	9 \pm 1	25 \pm 7	20 \pm 7	1 \pm 0
<i>R. Okamurae</i>	dH_2O	233 \pm 12	6	5 \pm 2	20 \pm 5	8 \pm 3	18 \pm 2	10 \pm 1	1 \pm 0	10 \pm 3	35 \pm 14	5 \pm 0	2 \pm 1
	dH_2O :EtOH (1:1)	372 \pm 20	5	2 \pm 0	12 \pm 1	5 \pm 1	42 \pm 1	9 \pm 1	1 \pm 0	7 \pm 0	30 \pm 2	6 \pm 2	1 \pm 0
	dH_2O :EtOH (1:4)	357 \pm 87	4	1 \pm 0	10 \pm 2	3 \pm 1	51 \pm 4	10 \pm 1	2 \pm 0	8 \pm 0	24 \pm 4	9 \pm 6	2 \pm 0
	dH_2O :MeOH (1:1)	210 \pm 48	1	2 \pm 0	13 \pm 3	6 \pm 1	51 \pm 3	8 \pm 1	1 \pm 0	6 \pm 1	19 \pm 5	3 \pm 1	2 \pm 0
	dH_2O :MeOH (1:4)	525 \pm 108	3	1 \pm 0	10 \pm 1	3 \pm 0	52 \pm 0	8 \pm 1	1 \pm 0	8 \pm 1	24 \pm 1	5 \pm 1	1 \pm 0

* Unsaturated with N are part already of the Unsaturated O rich and O poor groups, therefore, do not quantify as an independent group.

Table S2. Pearson coefficient (r) between the different variables analyzed in this work for the different extractions in different solvents: water (dH_2O), $\text{dH}_2\text{O}:\text{Ethanol}$ (EtOH) (1:1), $\text{dH}_2\text{O}:\text{EtOH}$ (1:4), $\text{dH}_2\text{O}:\text{Methanol}$ (MeOH) (1:1), $\text{dH}_2\text{O}:\text{MeOH}$ (1:4), from the biomass of *Asparagopsis armata* and *Rugulopteryx okamurae*. Green: Positive correlation, Red: Negative correlations. **: p<0.01, *p<0.05.

	TPC	TPC (PVPP)	ABTS	DPPH	CHO	CHON	CHOS	CHOP	Arom. Or	Arom. Op	H satur. Or	H satur. Op	Unsatur. Or	Unsatur. Op	Unsatur. N	Satur. Or	Satur. Op
TPC	1,0000	,8785**	,7994**	,7717**	,9056**	-,8589**	-,6846**	,6083**	-,6584**	-,3526	-,6449**	,7277**	-,7148**	-,1164	-,6856**	-,0592	-,4858**
TPC-PVPP		1,0000	,5738**	,5782**	,8334**	-,8257**	-,5656**	,5909**	-,5615**	-,2981	-,5824**	,7023**	-,6195**	-,1940	-,6796**	-,0523	-,4978**
ABTS			1,0000	,9744**	,7805**	-,7114**	-,3926*	,2139	-,3711**	-,0455	-,3378	,3718*	-,5331**	-,0447	-,6353**	,0239	-,4522*
DPPH				1,0000	,7867**	-,7370**	-,3430	,2173	-,3156	,0271	-,3104	,3201	-,4993**	-,0477	-,6758**	,0226	-,4536*
CHO					1,0000	-,9012**	-,6435**	,5234**	-,6520**	-,3281	-,5244**	,7228**	-,7458**	-,1477	-,8036**	-,1188	-,5864**
CHON						1,0000	,3836*	-,6780**	,4071*	,1294	,3984*	-,6538**	,5573**	,3163	,9267**	,3162	,7011**
CHOS							1,0000	-,4949**	,8961**	,7176**	,6992**	-,7614**	,7245**	-,0894	,1918	-,0675	,2060
CHOP								1,0000	-,4741**	-,4132*	-,4325*	,7372**	-,3130	-,3449	-,5735**	-,4047*	-,5414**
Arom. Or									1,0000	,7987**	,7477**	-,7387**	,6449**	-,1810	,1991	-,0794	,1510
Arom. Op										1,0000	,6080**	-,5692**	,5148**	-,3648*	-,0638	,0721	-,0764
H satur. Or											1,0000	-,4623**	,5516**	-,4470*	,0702	-,1226	-,0824
H satur. Op												1,0000	-,6926**	-,4332*	-,5712**	-,1862	-,5631**
Unsatur. Or													1,0000	-0,0605	,4486*	,1298	,2317
Unsatur. Op														1,0000	,5142**	,1517	,6412**
Unsatur. N															1,0000	,4064*	,7911**
Satur. Or																1,0000	,3727*
Satur. Op																	1,0000

TPC: Total phenolic compounds; Arom. Or: Aromatic oxygen rich; Arom. Op: Aromatic oxygen poor; H. satur. Or: Highly saturated oxygen rich; H. satur. Op: Highly saturated oxygen poor; Unsatur. Or: Unsaturated oxygen rich, Unsatur. Op: Unsaturated oxygen poor; Unsatur. N: Unsaturated Nitrogen; Satur. Or: Saturated oxygen rich; Satur. Op: Saturated oxygen poor.

Figure S1. ChemCrawler Interface (a) and an example of molecular search (b)

ChemCrawler

Welcome, Teresa S. Catalá!

formula

3 3 isomers

3 3 references per source

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C9H11NO6S

Top 3 isomers

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2,3-Dimethoxy-5-sulfamoylbenzoic Acid

A target-agnostic screen identifies approved drugs to stabilize the endoplasmic reticulum-resident proteome

pubmed 2021 Cell reports

"Endoplasmic reticulum (ER) dysregulation is associated with pathologies including neurodegenerative, muscular, and diabetic conditions. Depletion of ER calcium can lead to the loss of resident proteins in a process termed exodosis. To identify compounds that attenuate the redistribution of ER proteins under pathological conditions, we performed a quantitative high-throughput screen using the Gaussia luciferase (GLuc)-secreted ER calcium modulated protein (GERCAmP) assay, which monitors secretion of ER-resid..."

Therapeutic candidates for the Zika virus identified by a high-throughput screen for Zika protease inhibitors

pubmed 2020 Proceedings of the National Academy of Sciences of the United States of America

"When Zika virus emerged as a public health emergency there were no drugs or vaccines approved for its prevention or treatment. We used a high-throughput screen for Zika virus protease inhibitors to identify several inhibitors of Zika virus infection. We expressed the NS2B-NS3 Zika virus protease and conducted a biochemical screen for small-molecule inhibitors. A quantitative structure-activity relationship model was employed to virtually screen ~138,000 compounds, which increased the identification of activ..."