

Supplementary Materials

Pleiotropic Potential of *Evernia prunastri* Extracts and Their Main Compounds Evernic Acid and Atranorin: In Vitro and In Silico Studies

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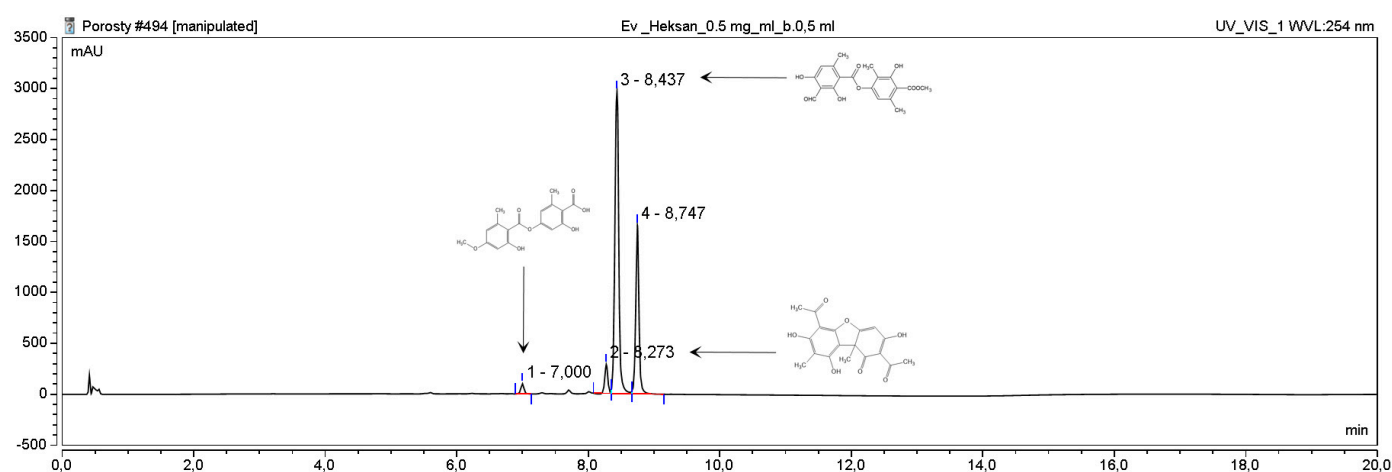


Figure S1. The chromatogram of hexane extract from *E. prunastri*, showing the identified compounds, i.e., evernic acid, atranorin and (+)-usnic acid, respectively.

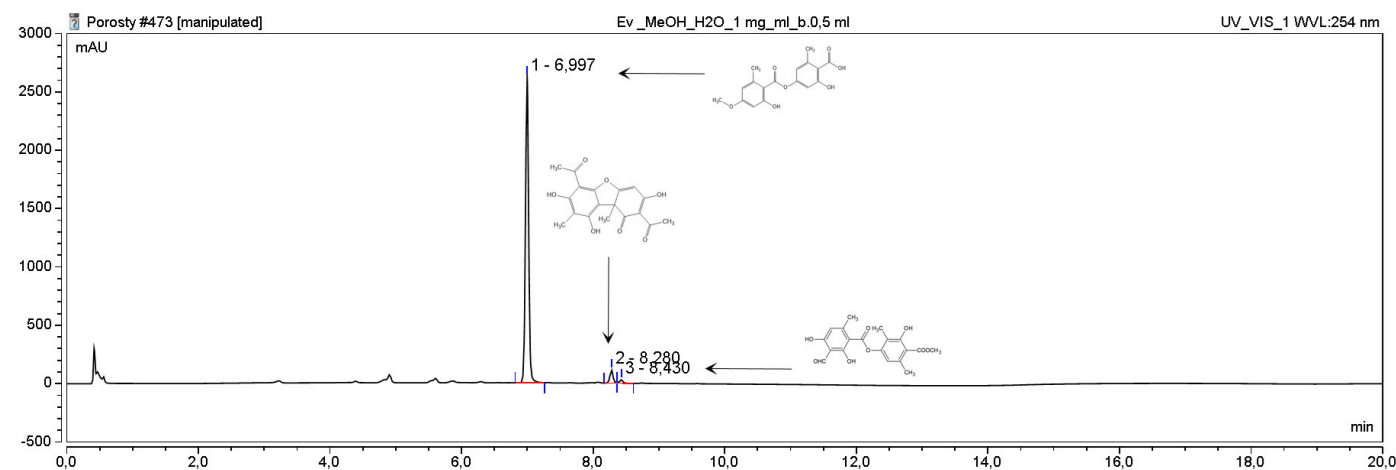
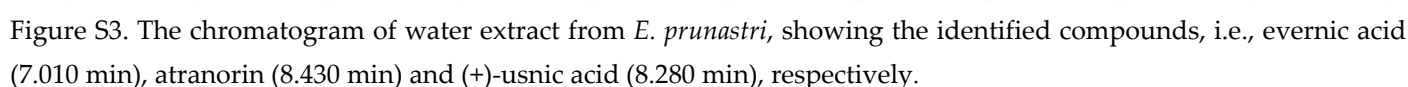


Figure S2. The chromatogram of methanol-water extract from *E. prunastri*, showing the identified compounds, i.e., evernic acid (6.997 min), atranorin (8.430 min) and (+)-usnic acid (8.280), respectively.



Target molecule	PDB code	Binding Energy [kcal/mol]		K_i [nM]		Receptor contact	
		evernic acid	atranorin	evernic acid	atranorin		
						evernic acid	atranorin
COX-2*	5F1A	-11.85	- 12.47	2.08	0.72	ALA168	ALA168
						GLN172	HIS176
						PHE179	PHE179
						THR181	THR181
						ASN351	ASN351
						HIS355	TYR354
						TRP356	HIS355
						HIS357	TRP356
						LEU360	HIS357
AChE*	4BDT	−11.97	−13.22	1.69	0.21		ASP70
						THR79	THR79
						TRP82	TRP82
						GLY116	GLY116
						TYR129	TYR120
						TYR333	TYR129
						HIS443	TYR333
							TRP435
							TYR445
BChE	4BDS	−10.67	−11.47	15.07	3.92	TRP79	
						GLY113	GLY113
						TYR125	SER195
						SER195	LEU283
						ALA325	PHE326
						TYR329	HIS433
						TRP425	
HIS433							
Tyrosinase	2Y9X	−9.49	−10.42	110.47	23.01	HIS60	HIS60
						HIS84	HIS84
						HIS243	HIS243

						ASN259	ASN259
						HIS262	PHE263
						PHE263	ALA285
						MET279	HIS295
						VAL282	
						ASP197	
α -glucosidase*	2QMJ	−8.66	+51.81	448.87	na	TRP400	na
						PHE444	
						ARG520	

K_i – estimated inhibition constant, “na” – not active *– indicates statistically significant differences ($p \leq 0.05$) in enzyme activity (the significance determined based on the comparison of binding energies).