Table S1. Phenolic compounds contained to the examined herbs, derived from extensive literature review.

Family	***Lamiaceae***					***Asteraceae***		***Verbenaceae***	***Elaeagnaceae***	***Hypericaceae***	
											Ref.
	O. majorana [1]	*O. vulgare*	*T. capitatus*	*M. pulegium*	*M. spicata*	*E. purpurea*	*M. chamomilla*	*L. citriodora*	*H. rhamnoides*	*H. perforatum*	
Compounds											
3,4-Dihydroxyphenyllactic acid (Danshensu)	- [2]	√ [3]	-	-	-	-	-	-	-	-	[1]
3,1-Caffeoylquinic (Neochlorogenic acid)	-	-	-	-	√	-	-	-	-	-	[2]
3-Feruloylquinic acid	-	-	-	-	-	-	-	-	-	√	[3]
3-O-methyl-catechin (Meciadanol)	√	-	-	-	-	-	-	-	-	-	[4]
3-p-Coumaroylquinic acid	-	-	-	-	-	-	-	-	-	√	[3]

4-Hydroxybenzoic acid	√	√	-	-	-	-	√	-	-	-	[4–6]
5-O-Caffeoylquinic acid	-	-	-	-	-	-	-	-	-	√	[1]
6-Methylscutellarein	-	-	-	-	-	-	-	√	-	-	https://foodb.ca/
Acacetin rutinoside	-	-	-	√	-	-	-	-	-	-	[4]
Acacetin-7-diglucuronide	-	-	-	√	-	-	-	-	-	-	[7]
Apigenin	√	√	√	-	√	-	-	-	-	-	[1,2,6,8]
Apigenin-7-o-glucoside	-	-	-	-	-	-	√	-	-	-	[6]
Caffeic acid	√	√	√	√	√	√	√	-	√	-	[1,2,4–9]
Caffeoyl-arbutin	√	-	-	-	-	-	-	-	-	-	[4]
Caftaric acid	-	-	-	-	√	√	-	-	-	-	[2,10]
Carnosic acid	-	√	-	-	-	-	-	-	-	-	[1]
Carnosol	-	√	-	-	-	-	-	-	-	-	[1]
Catechin	-	-	-	√	-	-	-	-	√	√	(https://foodb.ca/) [4]
Chlorogenic acid	√	√	√	√	√	-	√	-	-	-	[1,3–6,8]
Chrysoeriol	-	√	-	-	-	-	-	-	-	-	[1]
Chrysoeriol-7-diglucuron	-	-	-	-	-	-	-	√	-	-	[7]
Cichoric acid	-	-	-	-	-	√	-	-	-	-	[10]
Cinapic acid	-	√	-	-	-	-	-	-	-	-	[5]
Cinnamic acid	-	√	-	-	-	-	-	-	-	-	[5]

Cirsilineol	-	-	-	-	-	-	-	√	-	-	[7]
Cirsimaritin	-	-	-	-	-	-	-	√	-	-	[7]
Diosmetin	-	√	-	-	-	-	-	-	-	-	[1]
Diosmin	√	-	-	√	-	-	-	-	-	-	[4]
Ellagic acid	-	-	-	-	-	-	-	-	√	-	(https://foodb.ca/)
Ellagic acid pentoside	√	-	-	-	-	-	-	-	√	-	(https://foodb.ca/)
Epicatechin	-	-	-	-	-	-	-	-	-	√	[1]
Eriodictyol	√	√	-	-	-	-	-	-	-	-	[1,4]
Eriodictyol-7-o-glucuronide	-	-	√	-	-	-	-	-	-	-	[8]
Eukovoside	-	-	-	√	-	-	-	-	-	-	[4]
Eupafolin	-	-	-	-	-	-	-	√	-	-	(https://foodb.ca/)
Eupatorin	-	-	-	-	-	-	-	√	-	-	(https://foodb.ca/)
Ferullic acid	-	-	-	√	-	-	-	-	-	-	[1]
Feruloylquinic acid	-	-	-	-	√	-	-	-	-	√	[2,3][2-3]
Gallic acid	√	√	√	-	√	-	-	-	√	-	[1,5,9]
Gallocatechin	√	-	√	√	-	-	-	-	-	-	[4]
Gentisic acid	√	-	-	-	-	-	-	-	-	-	[4]
Guaijaverin (quercetin 3-O-arabinoside)	-	-	-	-	-	-	-	-	-	√	[3]
Hesperidin	√	-	-	√	-	-	-	-	-	-	[4]
Hydroxyphenyllactic acid	-	√	-	-	√	-	-	-	-	-	[1,2]
Hyperoside (quercetin 3-O-galactoside)	-	-	-	-	-	-	-	-	-	√	[3]
Isoorientin	√	-	-	-	-	-	-	-	-	-	[4]
Isoquercitirn	-	-	-	-	-	-	-	-	-	√	[1]
Isoquerutrin	-	-	-	-	-	-	-	-	-	√	[1]

Isorhamnetin	-	-	-	-	-	-	√	-	√	-	(https://foodb.ca/) [6]
Isosalvianolic acid B	-	-	-	√	-	-	-	-	-	-	[4]
Jaceosidin	-	-	-	-	-	-	-	√	-	-	(https://foodb.ca/)
Kaempferol	-	-	-	-	-	-	√	-	-	-	[6]
Kaempferol 3-O-rutinoside	-	-	-	-	-	-	-	-	-	√	[3]
Laricitrin-3-o-glucoside	-	-	-	-	-	-	√	-	-	-	[6]
Lithospermic acid	-	-	-	√	√	-	-	-	-	-	[2,4]
Luteolin	√	√	√	-	-	-	√	√	-	-	[1,4,6,8]
Luteolin 7-O-glucoside	-	√	√	√	√	-	√	√	-	-	[1,2,4,7]
Medioresinol	-	√	-	-	-	-	-	-	-	-	(https://foodb.ca/)
Myricetin 3-O-glucoside	-	√	-	-	-	-	-	-	-	-	[1]
Naringenin	-	√	√	-	-	-	-	-	-	-	[1,5]
Narirutin	-	-	-	√	√	-	-	-	-	-	[2,4]
Orientin	√	-	-	-	√	-	-	-	-	-	[4]
p-Coumaric acid	√	-	√	-	√	-	√	-	√	-	[4,6,8,9]
Protocatechuic acid	-	√	-	-	-	-	-	-	√	√	[1,5]
Quercetin	√	√	√	-	-	-	√	√	√	-	[1,4,6,8,11]
Quercetin rutinoside / Rutin	√	-	-	-	-	√	-	-	-	√	[2,3,6]
Quercetin-3-O-glucoside	-	-	√	-	-	-	-	-	-	√	(https://foodb.ca/)
Quercitrin	-	-	-	-	-	-	-	-	-	√	[1,3]

Quinic acid	-	√	-	-	-	-	-	-	-	√	[1,3]
Resveratrol	-	-	-	-	-	-	-	-	-	√	(https://foodb.ca/)
Rosmarinic acid	√	√	√	√	√	-	-	-	-	-	[1,2,4,8]
Sagerinic acid	-	-	-	-	√	-	-	-	-	-	[2]
Sakuranetin	√	-	-	-	-	-	-	-	-	-	[4]
Salicylic acid	-	-	-	-	-	-	√	-	√	-	[6,9]
Salvianolic acid A	-	-	-	-	√	-	-	-	-	-	[2]
Salvianolic acid B	-	-	-	√	√	-	-	-	-	-	[2,4]
Salvianolic acid F	-	-	-	-	√	-	-	-	-	-	[2]
Salvianolic acid I	√	-	-	-	-	-	-	-	-	-	[4]
Salvianolic acid J	-	-	-	-	√	-	-	-	-	-	[2]
Syringetin	-	-	-	√	-	-	-	-	-	-	[4]
Syringic acid	√	√	√	√	-	-	-	-	-	-	(https://foodb.ca/) [4,8]
Taxifolin	√	√	-	-	-	-	-	-	-	-	[1,4]
Thymol	-	-	√	-	-	-	-	-	-	-	[8]
Vanillic acid	√	√	√	√	√	-	-	-	-	√	(https://foodb.ca/) [4,5,8,9]
Vanillyl alcohol	-	-	-	√	-	-	-	-	-	-	[4]
Vitexin	√	-	-	-	-	-	-	-	-	-	[4]

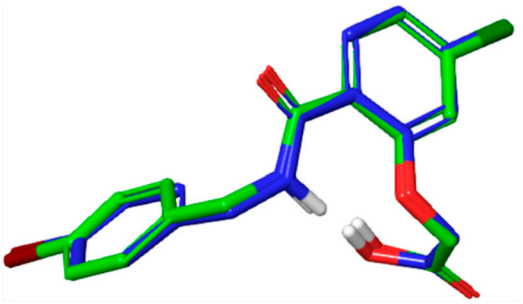
[1] *O. majorana: Origanum majorana, O. vulgare: Origanum vulgare, T. capitatus: Thymus capitatus, M. pulegium: Mentha pulegium, M. spicata: Mentha spicata, E. purpurea: Echinacea purpurea, M. chamomilla: Matricaria chamomilla, L. citriodora: Lippia citriodora, H. rhamnoides: Hippophae rhamnoides, H. perforatum: Hypericum perforatum,*
[2] The symbol declares the absence of the phenolic compound from the herbal infusion, [3] The symbol declares the presence of phenolic compound in the herbal infusion

Table S2. Molecular target prediction results derived from all collected phenolic compounds, by applying Ensemble TargetNet (http://targetnet.scbdd.com/calcnet/index_ensemble/) calculations [12].

Fingerprint Types (Daylight fingerprint and ECFP4)	
Compounds	**AUC value - aldose reductase**
3,4-Dihydroxyphenyllactic acid (Danshensu)	1.0
31-Caffeoylquinic (Neochlorogenic acid)	1.0
3-Feruloylquinic acid	0.667
3-O-methyl-catechin (Meciadanol)	1.0
3-p-Coumaroylquinic acid	0.67
4-Hydroxybenzoic acid	1.0
5-O-Caffeoylquinic acid	0.667
6-Methylscutellarein	1.0
Acacetin rutinoside	0.665
Acacetin-7-diglucuronide	1.0
Apigenin	0.667
Apigenin-7-o-glucoside	1.0
Caffeic acid	1.0
Caffeoyl-arbutin	1.0
Caftaric acid	1.0
Carnosic acid	1.0
Carnosol	0.316
Catechin	1.0
Chlorogenic acid	0.667
Chrysoeriol	1.0
Chrysoeriol-7-diglucuronide	1.0
Cichoric acid	1.0
Cinapic acid	0.667
Cinnamic acid	1.0
Cirsilineol	1.0
Cirsimaritin	1.0
Diosmetin	0.667
Diosmin	1.0
Ellagic acid	1.0
Ellagic acid pentoside	1.0
Epicatechin	1.0
Eriodictyol	1.0
Eriodictyol-7-o-glucuronide	1.0
Eukovoside	0.563
Eupafolin	1.0
Eupatorin	1.0
Ferullic acid	1.0
Feruloylquinic acid	0.667

Gallic acid	1.0
Gallocatechin	0.667
Gentisic acid	1.0
Guaijaverin (quercetin 3-O-arabinoside)	1.0
Hesperidin	0.628
Hydroxyphenyllactic acid	0.695
Hyperoside (quercetin 3-O-galactoside)	1.0
Isoorientin	1.0
Isoquercitirn	1.0
Isoquerutrin	1.0
Isorhamnetin	1.0
Isosalvianolic acid B	0.667
Jaceosidin	1.0
Kaempferol	1.0
Kaempferol 3-O-rutinoside	1.0
Laricitrin-3-o-glucoside	1.0
Lithospermic acid	0.605
Luteolin	1.0
Luteolin 7-O-glucoside	1.0
Medioresinol	1.0
Myricetin 3-O-glucoside	1.0
Naringenin	0.329
Narirutin	1.0
Orientin	1.0
p-Coumaric acid	1.0
Protocatechuic acid	1.0
Quercetin	1.0
Quercetin rutinoside / Rutin	1.0
Quercetin-3-O-glucoside	0.996
Quercitrin	1.0
Quinic acid	1.0
Resveratrol	0.695
Rosmarinic acid	0.662
Sagerinic acid	1.0
Sakuranetin	0.667
Salicylic acid	1.0
Salvianolic acid A	0.605
Salvianolic acid B	0.667
Salvianolic acid F	0.670
Salvianolic acid I	0.667
Salvianolic acid J	0.667
Syringetin	1.0
Syringic acid	1.0
Taxifolin	0.481
Thymol	1.0
Vanillic acid	0.695
Vanillyl alcohol	0.659

Vitexin	1.0



Aldose Reductase (Chain A)
PDB ID: 4LAU, Resolution: 0.84 Å
({2-[(4-bromobenzyl)carbamoyl]-5-chlorophenoxy}acetic acid - W8X)
Docking score = -11.61 kcal·mol^{-1}
RMSD = 0.1894 Å

Figure S1. The similarity in the overlapping between crystallographic (blue) and docked (green) poses, derived from aldose reductase (AR) enzyme.

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