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Article

Application of Network Pharmacology, Molecular Docking and in vitro Experimental Evaluation to Decipher the Anti-inflammatory Mechanisms of *Cirsium japonicum*

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Supplementary Materials

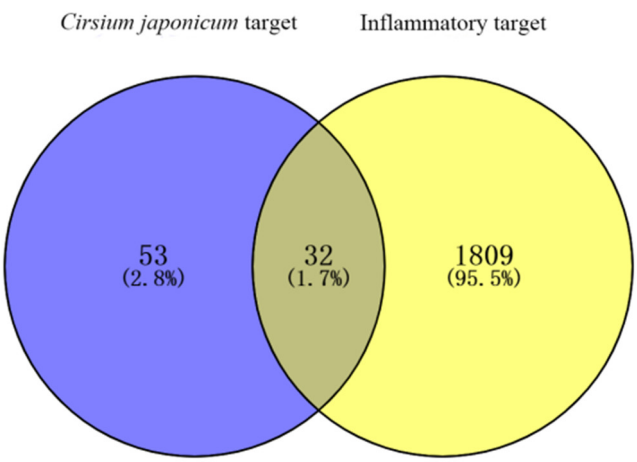


Figure S1. Venn diagram of intersecting targets between anti-inflammatory genes and active compounds of *C. japonicum*.

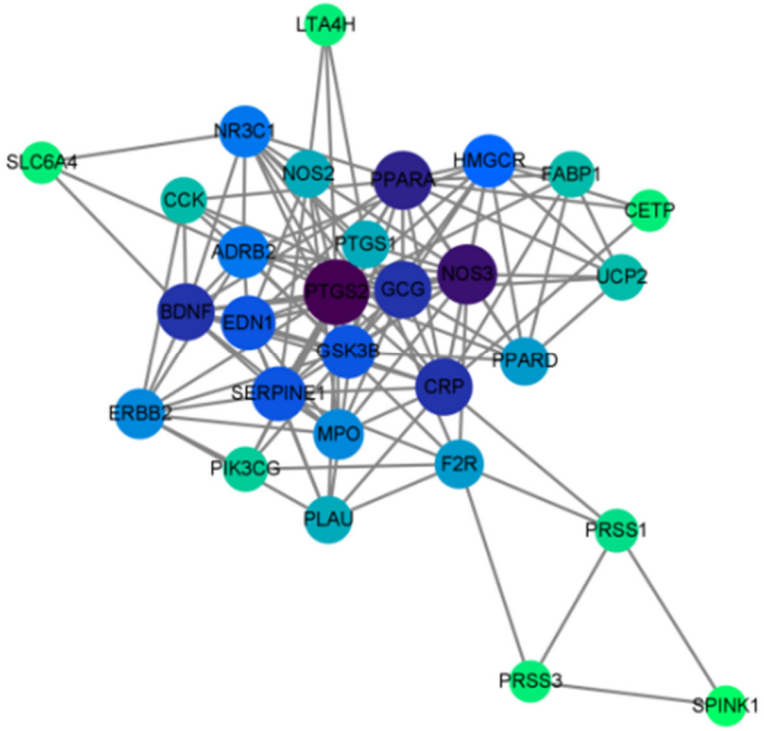


Figure S2. Protein-protein interaction (PPI) network analysis.

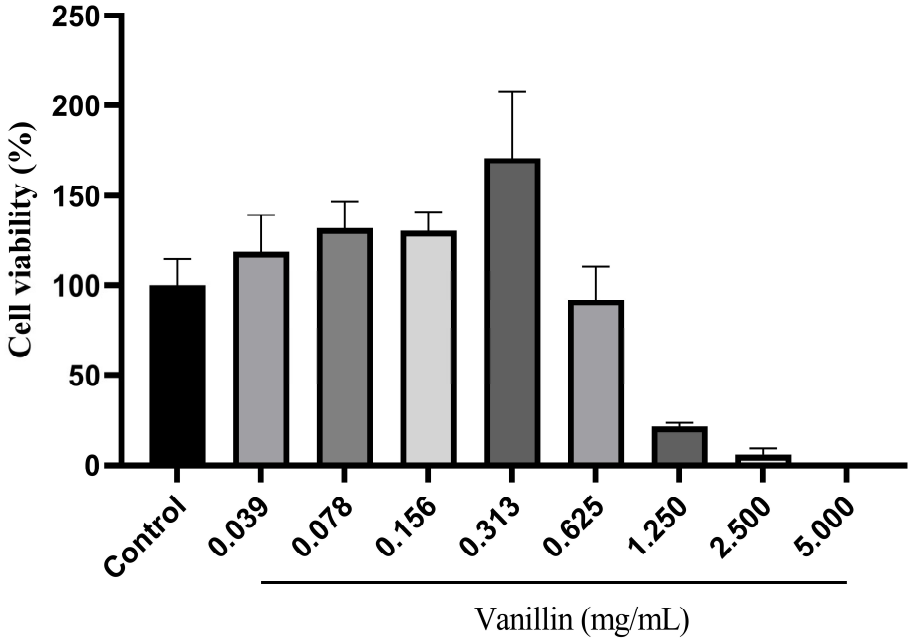


Figure S3. Cytotoxicity of vanillin against RAW 264.7 cells.

Table S1. Binding energies of key anti-inflammatory protein targets docked to active compounds of *C. japonicum.*

Molecular ID	Molecular name	Key target	PDB ID	AutoDock Docking score
MOL000675	Oleic acid	PPARG	1ZGY	-5.78
MOL000675	Oleic acid	PTGS2	5F19	-1.56
MOL000675	Oleic acid	BDNF	1BND11	-2.43
MOL000675	Oleic acid	GCG	6PHI	-2.58
MOL000675	Oleic acid	PPARA	6KAX	-3.86
MOL000675	Oleic acid	EDN1	1EDN	-2.74
MOL001641	Methyl linoleate	PPARG	1ZGY	-4.4
MOL001641	Methyl linoleate	PTGS2	5F19	-2.82
MOL001641	Methyl linoleate	BDNF	1BND11	-1.95
MOL001641	Methyl linoleate	GCG	6PHI	-3.04
MOL001641	Methyl linoleate	PPARA	6KAX	-4.71
MOL001641	Methyl linoleate	EDN1	1EDN	-2.69
MOL000359	Sitosterol	PPARG	1ZGY	-7.37
MOL000359	Sitosterol	PTGS2	5F19	-6.09
MOL000359	Sitosterol	BDNF	1BND11	-5.39
MOL000359	Sitosterol	GCG	6PHI	-6.38
MOL000359	Sitosterol	PPARA	6KAX	-8.67
MOL000359	Sitosterol	EDN1	1EDN	-6.66
MOL000449	Stigmasterol	PPARG	1ZGY	-8.61
MOL000449	Stigmasterol	PTGS2	5F19	-5.18
MOL000449	Stigmasterol	BDNF	1BND11	-6.83
MOL000449	Stigmasterol	PPARA	6KAX	-8.2
MOL000449	Stigmasterol	EDN1	1EDN	-6.46
MOL000635	Vanillin	PPARG	1ZGY	-4.47
MOL000635	Vanillin	PTGS2	5F19	-4.04
MOL000635	Vanillin	BDNF	1BND11	-5.54
MOL000635	Vanillin	GCG	6PHI	-3.35
MOL000635	Vanillin	PPARA	6KAX	-4.82
MOL000635	Vanillin	EDN1	1EDN	-3.92