SUPPORTING INFORMATION

Meniran (*Phyllanthus niruri* L) Embedded Zeolitic Imidazolate Framework (ZIF-8) Nanoparticle for Cancer Chemotherapy: Supported Molecular Docking Analysis

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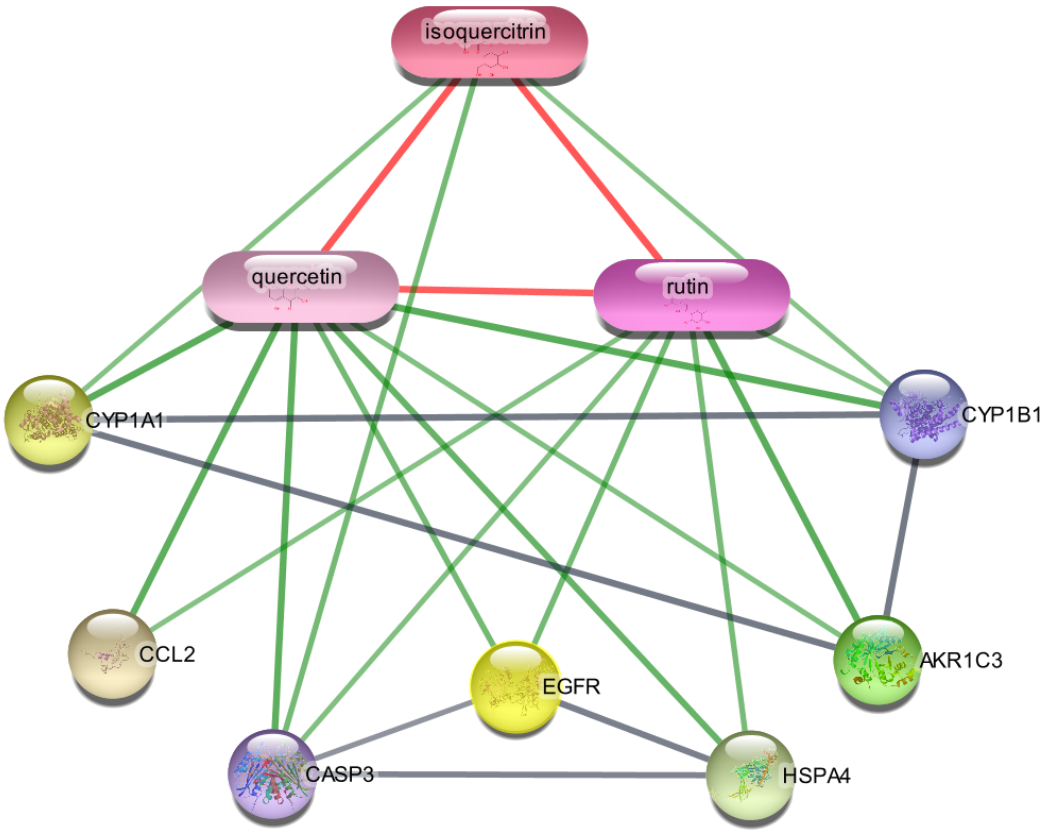


Figure S1. Interaction prediction of between Meniran compounds and proteins.

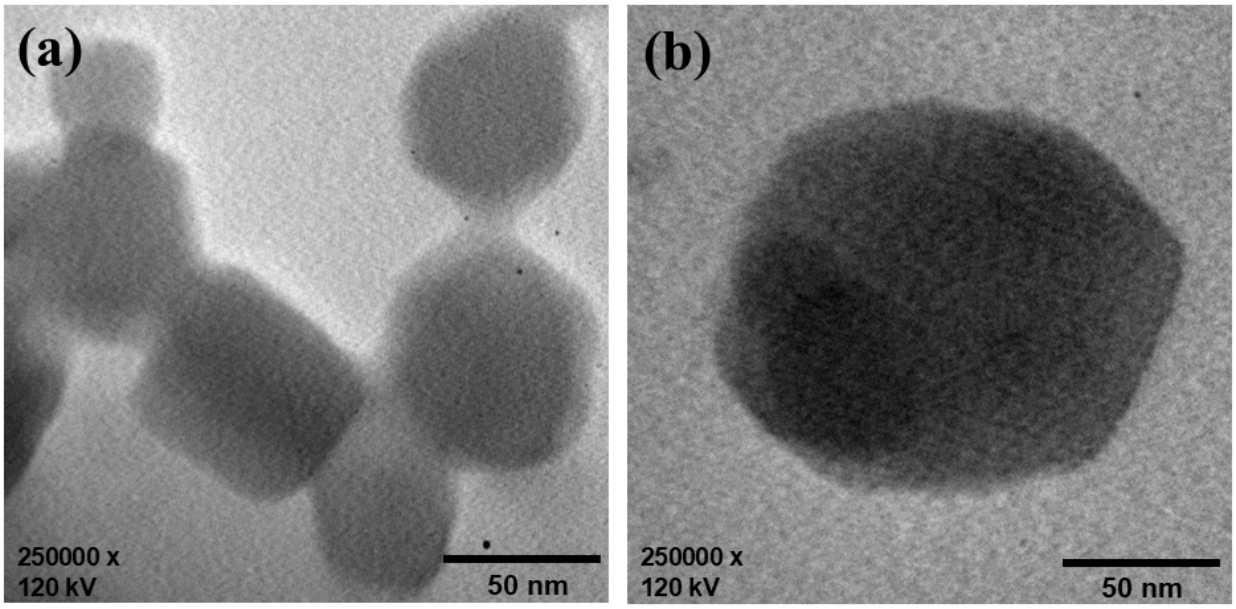


Figure S2. TEM bright field of **(a)** ZIF-8 nanoparticles, and **(b)** Meniran-incorporated ZIF-8 nanoparticles.

Table S1. Characteristics of active compound from Meniran.

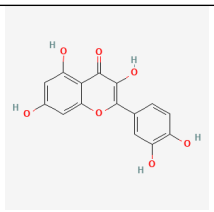
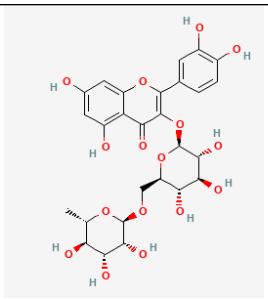
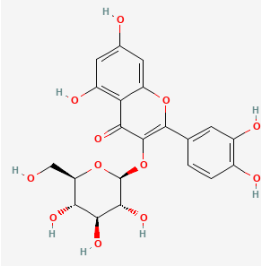
Name	Structure	Formula	Calc. MW	RT [min]	Area (Max.)	mzCloud Best Match
Quercetin		C15 H10 O7	302.04061	23.525	10,266,492.12	92.7
Rutin		C27 H30 O16	610.15007	23.523	57,315,267.66	92.6
Quercetin-3β-D-glucoside		C21 H20 O12	464.09319	23.803	8,823,643.46	91.1

Table S2. Drug-loading content (DLC) and drug-loading efficiency (DLE) of Meniran-incorporated ZIF-8 nanoparticles

Meniran/ZIF-8	Meniran/ZIF-8 (weight ratio)	DLC ± SD (%)	DLE ± SD (%)
Meniran/ZIF-8	1 : 1	2.45 ± 0.71	17.11 ± 1.09
	1.5 : 1	4.39 ± 0.53	15.64 ± 1.98
	2 : 1	5.01 ± 0.85	11.05 ± 1.28

Table S3. Binding affinity between compounds and AKT-1 or MDM2.

Ligand	**Binding Affinity (kcal/mol)**		
	AKT-1	**MDM2**	**EGFR**
ZIF-8	-10.8	-9.4	-8.5
Imidazole		-9.6	
AZD5363	-9.1		
MTX-531			-8.2