

Supplementary material:

Table 1: The primary targets of thymoquinone identified from reverse screening approaches

PDB ID	Protein Target	Procedure of reverse screening	Experimental Evidence	Binding energy (kcal/mol)
2FGI	Basic fibroblast growth factor receptor 1	PharmMapper/ ReverseScreen3D	CancerResource	-4.65
1P62	Deoxycytidine kinase	PharmMapper	CancerResource	-4.75
2X0V	Cellular tumor antigen p53	ReverseScreen3D	NPACT	-4.6
1DB1	Vitamin D3 receptor	PharmMapper/ ReverseScreen3D	CancerResource	-5.17
1R9O	Cytochrome P450 2CP	PharmMapper/ ReverseScreen3D	CancerResource	-4.63
1E3G	Androgen receptor	PharmMapper/ ReverseScreen3D	CancerResource	-5.28
2C6T	Cyclin A2	PharmMapper	CancerResource	-4.77
3BL1	Carbonic Anhydrase II	PharmMapper/ ReverseScreen3D	CancerResource	-4.33
1HFQ	Dihydrofolate reductase	PharmMapper/ ReverseScreen3D	CancerResource	Error
3CP9	Vascular endothelial growth factor 2	PharmMapper/ ReverseScreen3D	CancerResource	-7.57
1B41	Acetylcholine esterase	Target Hunter	NCBI PubChem	-4.09
2QG0	Heat shock protein HSP-90 alpha	PharmMapper	CancerResource	-4.14
3F7H	Baculoviral IAP repeat-containing protein 7	PharmMapper/ ReverseScreen3D	CancerResource	-3.73
2FZ8	Aldose reductase	PharmMapper/ ReverseScreen3D	CancerResource	-5.99
1RW8	TGF-beta receptor type-1	PharmMapper/ ReverseScreen3D	CancerResource	-5.21
1GRE	Glutathione reductase, mitochondrial	PharmMapper	CancerResource	-4.65
2R7B	3-phosphoinositide-dependent protein kinase 1	PharmMapper/ ReverseScreen3D	CancerResource	-4.59
1NME	Caspase 3	ReverseScreen3D	CancerResource	-3.99
1YSG	Apoptosis regulator Bcl-X	ReverseScreen3D	NPACT	-3.89
3PXZ	Cell division protein kinase 2	PharmMapper, ReverseScreen3D	CancerResource	-5.21
1GKC	Matrix metalloprotease 9	PharmMapper, ReverseScreen3D	CancerResource	-5.64
2RG6	MAP kinase 14	PharmMapper, ReverseScreen3D	CancerResource	-4.81