

Table SI. Molecular docking between PF and indicated molecules.

No.	Target Protein	PDB ID	Associated disease	Predicted binding energy (ΔG , kcal/mol) ¹	Key interacting residues
1	MAPK1	4QTB	AS; UC; RA; OA; GBM; AKI; cholestasis; muscle atrophy; ALI; IRI; cholestatic liver injury; pancreatic cancer	-8.7	GLU-343, TYR-156, ARG-370
2	MAPK3	7NRB	AS; UC; RA; OA; GBM; AKI; cholestasis; muscle atrophy; ALI; IRI; cholestatic liver injury; pancreatic cancer	-7.3	VAL-344, TYR-219, THR-287, ASP-347, ASP-345
3	TP53	8svi	AS; UC; RA; OA; GBM; AKI; cholestasis; muscle atrophy; ALI; IRI; cholestatic liver injury; pancreatic cancer	-8.4	GLLU-16, HIS-68, LYS-66
4	HSP90A A1	5j2x	AS; UC; RA; OA; GBM; AKI; cholestasis; muscle atrophy; ALI; IRI; pancreatic cancer	-7.4	ALA-137, GLY-135, THR-126
5	ESR1	1A52	AS; UC; RA; OA; GBM; AKI; cholestasis; muscle atrophy; ALI; IRI; pancreatic cancer	-7.6	ARG-477
6	BCL2	8hts	AS; UC; RA; OA; GBM; AKI; cholestasis; muscle atrophy; ALI; IRI; pancreatic cancer	-7.4	GLN-118
7	HIF1A	6gmr	AS; UC; RA; OA; GBM; AKI; cholestasis; muscle atrophy; ALI; IRI; pancreatic cancer	-8.1	LYS-72, SER-94
8	IL6	4cni	AS; UC; RA; OA; GBM; AKI; cholestasis; muscle atrophy; ALI; chronic colitis; IRI; cholestatic liver injury; pancreatic cancer	-6.5	LYS-120, GLU-99, PRO-139
9	IL10	8sve	AS; UC; RA; OA; GBM; AKI; Cholestasis; ALI; IRI; pancreatic cancer	-6.7	GLY-58, CYS-62, ARG-110
10	FGF2	5x1o	AS; UC; RA; OA; GBM; AKI; cholestasis; ALI; chronic colitis; IRI; Pancreatic cancer	-6.9	LYS-135, LYS-125, ARG-120
11	IL1B	5r8n	Chronic colitis; Cholestatic liver injury	-7.7	GLN-39
12	ALB	6yg9	Chronic colitis; Cholestatic liver injury	-8.1	GLU-244
13	PTGS2	5F19	Chronic colitis	-8.9	ASP-515, PRO-191, HIS-351, SER-581, GLY-193, VAL-582
14	CASP3	4ps0	Chronic colitis	-7.7	GLY-45, MET-44, LYS-82

15	IFNG	5D48	Chronic colitis	-9.6	ASP-2, VAL-44, ARG--4, GLY-46
16	TLR4	3FXI	Chronic colitis	-8.5	LYS-39, MET-145
17	TGFB1	1KLA	Chronic colitis	-7.6	ALA-72, PRO-76
18	NFKB1	8tqd	Chronic colitis	-9.9	ALA-137, GLY-135, THR-126
19	TNF	6OP0	Cholestatic liver injury	-8.4	LEU-142, PHE-144
20	IL18	4G74	Muscle atrophy; Cholestatic liver injury	-7.3	ARG-492

¹Binding energy was calculated using AutoDock Vina. The binding affinity was classified as follows: Binding Energy $\leq$ -5.0 kcal/mol was considered as candidate binding; $\leq$ -7.0 kcal/mol as strong binding; and $\leq$ -9.0 kcal/mol as very strong binding. These thresholds are empirical and used for comparative ranking of docking poses; experimental validation is required to confirm actual binding. RA, rheumatoid arthritis; UC, ulcerative colitis; OA, osteoarthritis; GBM, glioblastoma multiforme; AKI, acute kidney injury; ALI, acute lung injury; IRI, ischemia-reperfusion injury; AS, atherosclerosis.

Table SII. Sensitivity analysis of hub gene selection across 10 diseases.

Disease	MCC vs. Degree Overlap	MCC vs. betweenness Overlap	Overlapping Genes (MCC $\cap$ Degree / MCC $\cap$ Betweenness)
Atherosclerosis	7/10	6/10	MAPK1, MAPK3, HSP90AA1, TP53, ESR1, IL6, IL10 / MAPK1, MAPK3, HSP90AA1, TP53, IL6, IL10
Acute lung injury	7/10	6/10	MAPK1, MAPK3, TP53, HSP90AA1, ESR1, IL6, IL10 / MAPK1, MAPK3, TP53, HSP90AA1, IL6, IL10
Hepatic ischemia-reperfusion injury	8/10	7/10	MAPK1, MAPK3, HSP90AA1, TP53, ESR1, BCL2, IL6, IL10 / MAPK1, MAPK3, HSP90AA1, TP53, ESR1, IL6, IL10
ANIT-induced cholestatic liver injury	6/10	4/10	MAPK1, MAPK3, TP53, ESR1, BCL2, IL6 / MAPK1, TP53, IL6, ESR1
Chronic colitis	7/10	5/10	IL6, IL1B, ALB, PTGS2, CASP3, TLR4, NFKB1 / IL6, IL1B, ALB, PTGS2, NFKB1
Ulcerative colitis	7/10	6/10	MAPK1, MAPK3, HSP90AA1, TP53, ESR1, IL6, IL10 / MAPK1, MAPK3, HSP90AA1, TP53, IL6, IL10
Ischemia/reperfusion-induced acute kidney injury	7/10	6/10	MAPK1, MAPK3, TP53, HSP90AA1, ESR1, IL6, IL10 / MAPK1, MAPK3, TP53, HSP90AA1, IL6, IL10
Rheumatoid arthritis	8/10	7/10	MAPK1, MAPK3, HSP90AA1, TP53, ESR1, BCL2, IL6, IL10 / MAPK1, MAPK3, HSP90AA1, TP53, ESR1, IL6, IL10
Osteoarthritis	7/10	5/10	MAPK1, HSP90AA1, MAPK3, TP53, IL6, IL10, BCL2 / MAPK1, HSP90AA1, TP53, IL6, ESR1
Cisplatin-induced muscle wasting	6/10	5/10	MAPK1, MAPK3, TP53, HSP90AA1, ESR1, IL6 / MAPK1, MAPK3, TP53, HSP90AA1, ESR1
Overlap Genes: Shared genes between MCC-identified top 10 hub genes and those ranked by Degree or Betweenness centrality (top 10).			