

Supplement Tables

Tab.S1 Core targets prediction of peptides intervention in acute colitis

Tab.S2 KEGG (Kyoto Encyclopedia of Genes and Genomes) signaling pathways of the predicted core targets (organism: *Mus musculus*) ($p < 0.05$)

Tab.S3 Results of molecular docking between core targets and peptides

Tab.S1

Rank	Gene symbol	Protein name	UniProt ID
1	Acat	Acetyl-CoA acetyltransferase, mitochondrial	Q8QZT1
2	Akr1b1	Aldose reductase	P45376
3	Akt1	RAC-alpha serine/threonine-protein kinase	P31750
4	Akt2	RAC-beta serine/threonine-protein kinase	Q60823
5	Alb	Serum albumin	Q546G4
6	Ang	Angiogenin	P21570
7	Arf1	ADP-ribosylation factor 1	P84078
8	Btk	Tyrosine-protein kinase BTK	P35991
9	Casp1	Caspase-1	P29452
10	Casp3	Caspase-3	P70677
11	Cat	Catalase	Q91XI2
12	Clic1	Chloride intracellular channel protein 1	Q9Z1Q5
13	Cma1	Chymase	A4QPC5
14	Dhfr	Dihydrofolate reductase	P00375
15	Dpp4	Dipeptidyl peptidase 4	P28843
16	Eea1	Early endosome antigen 1	Q8BL66
17	Egfr	Epidermal growth factor receptor	Q01279
18	Eif4e	Eukaryotic translation initiation factor 4E	P63073
19	F2	Prothrombin	Q3TJ94
20	Fabp5	Fatty acid-binding protein, epidermal	Q05816
21	G6pd	Glucose-6-phosphate 1-dehydrogenase	Q43727
22	Gsk3b	Glycogen synthase kinase-3 beta	Q5KU03
23	Gss	Glutathione synthetase	P51855
24	Gsta1	Glutathione S-transferase A1	P13745
25	Gstm1	Glutathione S-transferase Mu 1	P10649
26	Hadh	Hydroxyacyl-coenzyme A dehydrogenase, mitochondrial	Q61425
27	Hsp90aa1	Heat shock protein HSP 90-alpha	P07901
28	Insr	Insulin receptor	P15208
29	Lck	Proto-oncogene tyrosine-protein kinase LCK	P06240
30	Lcn2	Neutrophil gelatinase-associated lipocalin	P11672
31	Mapk10	Mitogen-activated protein kinase 10	Q61831
32	Mif	Macrophage migration inhibitory factor	P34884
33	Mme	Neprilysin	Q61391
34	Mmp12	Macrophage metalloelastase	Q61391
35	Mmp2	72 kDa type IV collagenase	P33434
36	Mmp3	Stromelysin-1	P28862
37	Nos3	Nitric oxide synthase, endothelial	P70313
38	Nr1h2	Oxysterols receptor LXR-beta	Q60644
39	Nr1i2	Nuclear receptor subfamily 1 group I member 2	O54915
40	Plau	Urokinase-type plasminogen activator	P06869
41	Plg	Plasminogen	P20918
42	Pnpo	Pyridoxine-5-phosphate oxidase	Q91XF0
43	Ptk2	Focal adhesion kinase 1	P34152
44	Ptpn1	Tyrosine-protein phosphatase non-receptor type 1	P35821
45	Rab11a	Ras-related protein Rab-11A	E9PZB2
46	Rab5a	Ras-related protein Rab-5A	Q9CQD1
47	Rac1	Ras-related C3 botulinum toxin substrate 1	Q3TLP8
48	Raf1	RAF proto-oncogene serine/threonine-protein kinase	F6TUC4
49	Sele	E-selectin	Q00690
50	Sult1a1	Sulfotransferase 1A1	P52840
51	Sult2a1	Sulfotransferase 2A1	P52843
52	Tgfb2	Transforming growth factor beta-2	P27090

Tab.S2

Rank	Term ID	Term description	Gene count	FDR	Matching proteins
1	mmu05210	Colorectal cancer	8	5.08E-06	Mapk10, Gsk3b, Tgfb2, Akt2, Casp3, Akt1, Rac1, Raf1
2	mmu05205	Proteoglycans in cancer	10	4.63E-05	Tgfb2, Plau, Akt2, Mmp2, Casp3, Akt1, Rac1, Raf1, Egfr, Ptk2
3	mmu05212	Pancreatic cancer	7	4.63E-05	Mapk10, Tgfb2, Akt2, Akt1, Rac1, Raf1, Egfr
4	mmu04931	Insulin resistance	8	5.38E-05	Mapk10, Gsk3b, Ptpn1, Nos3, Insr, Akt2, Nr1h2, Akt1
5	mmu05200	Pathways in cancer	12	1.15E-04	Mapk10, Gsk3b, Tgfb2, Hsp90aa1, Akt2, Mmp2, Casp3, Akt1, Rac1, Raf1, Egfr, Ptk2
6	mmu04012	ErbB signaling pathway	7	1.15E-04	Mapk10, Gsk3b, Akt2, Akt1, Raf1, Egfr, Ptk2
7	mmu04068	FoxO signaling pathway	8	1.15E-04	Mapk10, Tgfb2, Insr, Akt2, Cat, Akt1, Raf1, Egfr
8	mmu04910	Insulin signaling pathway	8	1.34E-04	Mapk10, Gsk3b, Ptpn1, Insr, Akt2, Akt1, Raf1, Eif4e
9	mmu04915	Estrogen signaling pathway	7	1.72E-04	Hsp90aa1, Nos3, Akt2, Mmp2, Akt1, Raf1, Egfr
10	mmu04151	PI3K-Akt signaling pathway	11	1.72E-04	Gsk3b, Hsp90aa1, Nos3, Insr, Akt2, Akt1, Rac1, Raf1, Eif4e, Egfr, Ptk2
11	mmu04370	VEGF signaling pathway	6	1.72E-04	Nos3, Akt2, Akt1, Rac1, Raf1, Ptk2
12	mmu04664	Fc epsilon RI signaling pathway	6	2.91E-04	Mapk10, Akt2, Btk, Akt1, Rac1, Raf1
13	mmu04662	B cell receptor signaling pathway	6	3.09E-04	Gsk3b, Akt2, Btk, Akt1, Rac1, Raf1
14	mmu05152	Tuberculosis	8	3.38E-04	Eea1, Mapk10, Tgfb2, Akt2, Casp3, Akt1, Raf1, Rab5a
15	mmu04380	Osteoclast differentiation	7	4.29E-04	Mapk10, Tgfb2, Lck, Akt2, Btk, Akt1, Rac1
16	mmu05215	Prostate cancer	6	7.55E-04	Gsk3b, Hsp90aa1, Akt2, Akt1, Raf1, Egfr
17	mmu04510	Focal adhesion	8	7.77E-04	Mapk10, Gsk3b, Akt2, Akt1, Rac1, Raf1, Egfr, Ptk2
18	mmu05014	Amyotrophic lateral sclerosis (ALS)	5	9.82E-04	Casp3, Cat, Casp1, Rac1, Rab5a
19	mmu05213	Endometrial cancer	5	0.001003258	Gsk3b, Akt2, Akt1, Raf1, Egfr
20	mmu04932	Non-alcoholic fatty liver disease (NAFLD)	7	0.001073187	Mapk10, Gsk3b, Insr, Akt2, Casp3, Akt1, Rac1
21	mmu05231	Choline metabolism in cancer	6	0.001073187	Mapk10, Akt2, Akt1, Rac1, Raf1, Egfr
22	mmu04066	HIF-1 signaling pathway	6	0.001073187	Nos3, Insr, Akt2, Akt1, Eif4e, Egfr
23	mmu04014	Ras signaling pathway	8	0.001073187	Mapk10, Insr, Akt2, Akt1, Rac1, Raf1, Rab5a, Egfr
24	mmu04668	TNF signaling pathway	6	0.001375863	Mapk10, Akt2, Casp3, Mmp3, Akt1, Sele
25	mmu05164	Influenza A	7	0.001377226	Mapk10, Gsk3b, Akt2, Casp1, Akt1, Plg, Raf1
26	mmu04010	MAPK signaling pathway	8	0.001660417	Mapk10, Tgfb2, Akt2, Casp3, Akt1, Rac1, Raf1, Egfr

Rank	Term ID	Term description	Gene count	FDR	Matching proteins
27	mmu05211	Renal cell carcinoma	5	0.001983279	Tgfb2, Akt2, Akt1, Rac1, Raf1
28	mmu04722	Neurotrophin signaling pathway	6	0.001983279	Mapk10, Gsk3b, Akt2, Akt1, Rac1, Raf1
29	mmu04071	Sphingolipid signaling pathway	6	0.002062824	Mapk10, Nos3, Akt2, Akt1, Rac1, Raf1
30	mmu04917	Prolactin signaling pathway	5	0.002346233	Mapk10, Gsk3b, Akt2, Akt1, Raf1
31	mmu05160	Hepatitis C	6	0.002936129	Mapk10, Gsk3b, Akt2, Akt1, Raf1, Egfr
32	mmu05161	Hepatitis B	6	0.003912034	Mapk10, Tgfb2, Akt2, Casp3, Akt1, Raf1
33	mmu04914	Progesterone-mediated oocyte maturation	5	0.004121783	Mapk10, Hsp90aa1, Akt2, Akt1, Raf1
34	mmu04660	T cell receptor signaling pathway	5	0.006934534	Gsk3b, Lck, Akt2, Akt1, Raf1
35	mmu05145	Toxoplasmosis	5	0.007760522	Mapk10, Tgfb2, Akt2, Casp3, Akt1
36	mmu05223	Non-small cell lung cancer	4	0.010302019	Akt2, Akt1, Raf1, Egfr
37	mmu04062	Chemokine signaling pathway	6	0.012224552	Gsk3b, Akt2, Akt1, Rac1, Raf1, Ptk2
38	mmu05230	Central carbon metabolism in cancer	4	0.014221754	Akt2, Akt1, Raf1, Egfr
39	mmu05214	Glioma	4	0.014471488	Akt2, Akt1, Raf1, Egfr
40	mmu04015	Rap1 signaling pathway	6	0.016365292	Insr, Akt2, Akt1, Rac1, Raf1, Egfr
41	mmu05218	Melanoma	4	0.017442493	Akt2, Akt1, Raf1, Egfr
42	mmu05220	Chronic myeloid leukemia	4	0.017442493	Tgfb2, Akt2, Akt1, Raf1
43	mmu04520	Adherens junction	4	0.017442493	Ptpn1, Insr, Rac1, Egfr
44	mmu04666	Fc gamma R-mediated phagocytosis	4	0.026000943	Akt2, Akt1, Rac1, Raf1
45	mmu04022	cGMP-PKG signaling pathway	5	0.028204425	Nos3, Insr, Akt2, Akt1, Raf1
46	mmu04912	GnRH signaling pathway	4	0.028204425	Mapk10, Mmp2, Raf1, Egfr
47	mmu05204	Chemical carcinogenesis	4	0.031106979	Sult1a1, Gstm1, Gsta1, Sult2a1
48	mmu04620	Toll-like receptor signaling pathway	4	0.039044863	Mapk10, Akt2, Akt1, Rac1
49	mmu05142	Chagas disease (American trypanosomiasis)	4	0.040278532	Mapk10, Tgfb2, Akt2, Akt1
50	mmu04650	Natural killer cell mediated cytotoxicity	4	0.041520682	Lck, Casp3, Rac1, Raf1
51	mmu05219	Bladder cancer	3	0.043197962	Mmp2, Raf1, Egfr
52	mmu04024	cAMP signaling pathway	5	0.045944969	Mapk10, Akt2, Akt1, Rac1, Raf1
53	mmu04919	Thyroid hormone signaling pathway	4	0.048540352	Gsk3b, Akt2, Akt1, Raf1

Tab.S3

Peptides-target	Hydrogen Bonds	Electrostatic	Hydrophobic
AFKDEDQTQ-Gstm1	GLU5:HN - LEU59:O GLN8:HT - TYR115:OH ARG42:HH21 - GLU5:OE1 TRP45:HE1 - GLU5:OE2 TRP7:HD1 - GLU5:O ILE3:HN2 - ILE4:O GLU1:HN1 - ASN58:OD1 TYR6:HH - GLU1:O	LYS49:HZ3 - GLU5:OE2 ARG42:NE - GLU5:OE2 ARG42:NE - ASP6:OD2	-
ESIINF-Gstm1	ARG42:HH21 - GLU1:OE1 TYR115:HH - SER2:O GLU1:HA - LEU59:O TRP7:HD1 - GLU1:O PHE1:HN1 - ASN58:OD1 ALA7:HN - PRO57:O ARG42:HE - ILE4:O ARG42:HH21 - ILE4:O	GLU1:HN2 - GLU1:OE2 ILE3:N - GLU1:OE2 ARG42:NE - GLU1:OE2	ILE3 - LEU12 PHE6 - MET108 TYR115 - ILE3 TYR115 - ILE4 PHE208 - ILE3
FDSITGA-Gstm1	LYS49:HZ1 - ALA7:O1 LEU59:HN - THR5:O THR5:HB - LEU59:O GLY6:HA2 - ASN58:OD1 ALA7:HA - PRO57:O	-	ILE4 - MET211
LHPIQDL-Gstm1	GLN5:HE21 - ASN58:OD1 GLN5:HE21 - LEU59:O TRP7:HE1 - GLN5:O TYR115:HH - ASP6:OD1	ASP6:OD2 - TYR115	ILE4 - LEU12 LEU7 - LEU59 HIS2 - LEU12 TRP45 - LEU7 HIS107 - ILE4 TYR115 - PRO3 PHE208 - ILE4
AFKDEDQTQ-Rac1	LYS3:HZ2 - GLY30:O LYS3:HZ3 - ALA1:O LYS3:HZ3 - GLY30:O LYS116:HE1 - GLU5:OE2	LYS3:NZ - GLU31:OE2 LYS116:NZ - GLU5:OE2	ALA1 - LEU160 PHE2 - ALA13 PHE28 - ALA1
ESIINF-Rac1	ILE4:HN - GLU1:O GLU1:HN3 - ALA13:O TYR32:HN - ASN5:OD1 SER83:HG - GLU1:OE1 LYS116:HZ2 - PHE6:OCT LYS116:HZ2 - GLU1:OE1 LYS116:HZ2 - GLU1:O ILE4:HA - GLU1:O ALA13:HA - ILE4:O VAL14:HA - GLU1:OE2 SER83:HB1 - GLU1:OE2 ILE4:HN - PHE1:O PHE1:HN1 - GLY30:O PHE1:HN2 - GLY30:O THR5:HG1 - ILE4:O ALA7:HN - GLY30:O GLY15:HA1 - ASP2:OD1 LYS116:HE1 - ASP2:OD1	LYS116:HZ3 - GLU1:OE2	PHE6 - PHE28 ALA13 - ILE4 PHE6 - LEU160 TYR32 - ILE4
FDSITGA-Rac1		LYS116:HZ1 - ASP2:OD2,	PHE1 - PHE28 PHE1 - YS116 PHE1 - LEU160

Peptides-target	Hydrogen Bonds	Electrostatic	Hydrophobic
LHPIQDL - Rac1	TYR32:HN - HIS2:NE2		LEU1 - LEU7
	LYS116:HZ2 - ASP6:O		ALA13 - ILE4
	HIS2:HE1 - GLY30:O		ALA13 - PRO3
	LEU7:HC - ASP6:O	-	CYS18 - ILE4
	GLU31:HA - HIS2:NE2		VAL85 - LEU7
	LYS116:HE1 - ASP6:O		TYR32 - ILE4
	LYS3:HZ1 - CYS481:SG		
	LYS3:HZ2 - THR410:O		
	LYS3:HN - LEU408:O		
	GLN8:OCT - GLN412:OE1		
AFKDEDQ - Btk	THR410:HN - LYS3:O		LYS3 - VAL416
	GLN412:HN - ASP6:O		CYS481 - LYS3
	CYS481:HN - PHE2:O	ARG525:NE -GLU5:OE1	PHE2 - LEU408
	LYS558:HZ1 - GLN8:OCT		
	LYS558:HZ1 - GLN8:OE1		
	GLY411:HA1 - ASP6:O		
	GLY480:HA2 -:PHE2:O		
	LYS558:HE1 - GLN8:OCT		
	LYS558:HE2 - GLN8:OE1		
	ASN5:HN - LEU408:O		
ESIINF - Btk	ASN5:HD22 - THR410:O		GLY409:N - PHE6
	PHE6:HN - LEU408:O		ILE3 - LEU528
	PHE6:OCT - LEU408:O		ILE4 - LEU408
	GLU1:HN1 - ASN526:OD1	GLU1:N - GLU1:OE2	ILE4 - LEU528
	THR410:HN - ASN5:OD1	GLU1:N - ASP539:OD2	VAL416 - ILE3
	GLN412:HN - SER2:O	LYS558:NZ - GLU1:OE2	VAL416 - ILE4
	SER2:CA - ARG525:O		
	GLY409:HA2 - ASN5:OD1		
	GLY411:HA1 - GLU1:OE2		
	PHE1:HN2 - LEU408:O		
FDSITG - Btk	THR5:HN - ARG525:O		ILE4 - LEU528
	GLY6:HN - CYS481:SG		CYS481 - ILE4
	ALA7:HN - THR410:O		PHE1 - LEU408
	GLN412:HN - ILE4:O		
	MET477:HN - ASP2:OD1	-	
	CYS481:HN - PHE1:O		
	SER3:HB2 - LEU408:O		
	THR5:HA - ARG525:O		
	GLY6:HA2 - THR410:O		
	GLY411:HA2 - ILE4:O		
LHPIQDL - Btk	LEU1:HN1 - ASN526:OD1		ILE4 - LEU408
	LEU7:HT - GLU407:O		ILE4 - LEU528
	GLN412:HN - LEU1:O		PRO3 - LEU528
	ASN484:HD22 - GLN5:OE1		LEU7 - LEU408
	ASN484:HD22 - ASP6:OD1	LEU1:HN1 - ASP539:OD2	VAL416 - ILE4
	PRO3:HD1 - ARG525:O	LEU1:N - ASP521:OD2	CYS481 - PRO3
	HIS2:HA - ARG525:O		HIS2 - ARG525
	LEU1:HA - ASN526:OD1		
	GLY409:HA2 - GLN5:O		
	GLY409:HA2 - ASP6:O		
GLY411:HA1 - HIS2:O			
GLY411:HA2 - HIS2:O			