

SUPPLEMENTARY DATA

ROCK2-specific inhibitor KD025 suppresses adipocyte differentiation by inhibiting casein kinase 2

Nhu Nguyen Quynh Tran, Kwang-Hoon Chun*

*Gachon Institute of Pharmaceutical Sciences, College of Pharmacy, Gachon University,
Incheon 21936, Republic of Korea*

Correspondence to:

Kwang-Hoon Chun, Ph.D.

Gachon Institute of Pharmaceutical Sciences, College of Pharmacy, Gachon University, Incheon 21936, Republic of Korea

Tel.: 82-32-820-4951

E-mail address: khchun@gachon.ac.kr

Supplemental Figures

(A)

NW Score		Identities	Positives	Gaps
1306		242/263 (92%)	255/263 (96%)	0/263 (0%)
ROCK1	76	YEVVKVIGRGAFGEVQLVRHKSTRKVYAMKLLSKFEMIKRSDSAFFWEERDIMAFANSPW Y+VVKVIGRGAFGEVQLVRHK+++KVYAMKLLSKFEMIKRSDSAFFWEERDIMAFANSPW		135
ROCK2	92	YDVVKVIGRGAFGEVQLVRHKASQKVYAMKLLSKFEMIKRSDSAFFWEERDIMAFANSPW		151
ROCK1	136	VVQLFYAFQDDRYLYMVMEYMPGGDLVNLMSNYDVPEKWARFYTAEVVLALDAIHSMGFI VVQLFYAFQDDRYLYMVMEYMPGGDLVNLMSNYDVPEKWA+FYTAEVVLALDAIHSMG I		195
ROCK2	152	VVQLFYAFQDDRYLYMVMEYMPGGDLVNLMSNYDVPEKAWKFYTAEVVLALDAIHSMGLI		211
ROCK1	196	HRDVKPDNMLLDKSGHLKLADFGTCMKMKEGMVRCDTAVGTPDYISPEVLKSQGGDGY HRDVKPDNMLLDK GHLKLADFGTCMKM++ GMV CDTAVGTPDYISPEVLKSQGGD+Y		255
ROCK2	212	HRDVKPDNMLLDKHGHLKLADFGTCMKMDETGMVHCDTAVGTPDYISPEVLKSQGGDGFY		271
ROCK1	256	GRECDWWSVGVFLYEMLVGDTPFYADSLVGTYSKIMNHKNSLTFPDDNDISKEAKNLICA GRECDWWSVGVFLYEMLVGDTPFYADSLVGTYSKIM+HKNSL FP+D +ISK AKNLICA		315
ROCK2	272	GRECDWWSVGVFLYEMLVGDTPFYADSLVGTYSKIMDHKNSLCPEDAIEISKHAKNLICA		331
ROCK1	316	FLTDREVRLGRNGVEEIKRHLFF FLTDREVRLGRNGVEEI++H FF	338	
ROCK2	332	FLTDREVRLGRNGVEEIRQHPPF	354	

(B)

NW Score		Identities	Positives	Gaps
1381		253/286 (88%)	271/286 (94%)	0/286 (0%)
CK2α	39	YQLVRKLRGKGYSEVFEAINITNNEKVVVKILKPVKKKIKREIKILENLRGGPNIITLA YQLVRKLRGKGYSEVFEAINITNNE+VVVKILKPVKKKIKRE+KILENLRG NII L		98
CK2α'	40	YQLVRKLRGKGYSEVFEAINITNNERVVVKILKPVKKKIKREVKILENLRGGTNIKLI		99
CK2α	99	DIVKDPVSRTPALVFEHVNNTDFKQLYQLTDYDIRFYMYEILKALDYCHSMGIMHRDVK D VKDPVS+TPALVFE++NNTDFKQLYQ LTD+DIRFYMYE+LKALDYCHS GIMHRDVK		158
CK2α'	100	DTVKDPVSKTPALVFEYINNNTDFKQLYQLTDFDIRFYMYELKALDYCHSKGIMHRDVK		159
CK2α	159	PHNVMIDHEHRKRLRIDWGLAEFYHPQEYNVRVASRYFKGPELLVDYQMYDYSLDMWSL PHNVMIDH+ +KRLRIDWGLAEFYHP QEYNVRVASRYFKGPELLVDYQMYDYSLDMWSL		218
CK2α'	160	PHNVMIDHQKRLRIDWGLAEFYHPAQEYNVRVASRYFKGPELLVDYQMYDYSLDMWSL		219
CK2α	219	GCMLASMIFRKEPFFHGHNDYDQLVRIAKVLGTELDYDYIDKYNIELDPRFNDILGRHSR GCMLASMIFR+EPFFHG DNYDQLVRIAKVLGTE+LY Y+ KY+I+LDP FNDILG+HSR		278
CK2α'	220	GCMLASMIFRREPFFHGHNDYDQLVRIAKVLGTEELYGYLKKYHIDLDPHFNDILGQHSR		279
CK2α	279	KRWERFVHSENQHLVSPEALDFLDKLLRYDHSRLTAREAMEHPYF KRWE F+HSEN+HLVSPEALD LDKLLRYDHS RLTA+EAMEHPYF	324	
CK2α'	280	KRWENFIHSENRLVSPEALDLDKLLRYDHSRLTAKEAMEHPYF	325	

Figure S1. Pairwise alignment of kinase domains between ROCK1 and ROCK2 (A) and between CK2 α and CK2 α ' (B). Protein sequences were aligned using NCBI BLAST global alignment tool (<https://blast.ncbi.nlm.nih.gov/>). NCBI protein ID: NP_005397.1 (ROCK1), NP_004841.2 (ROCK2), NP_001886.1 (CK2 α), NP_001887.1 (CK2 α ').

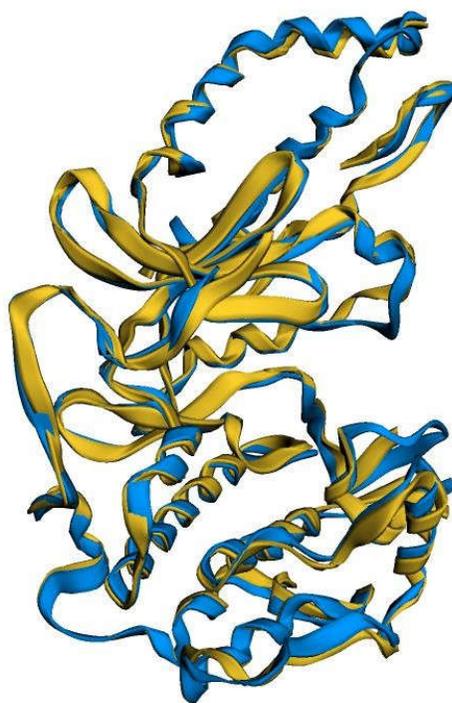


Figure S2. The structural alignment of ROCK1 and ROCK2. The structures were aligned using FATCAT program (<https://fatcat.godziklab.org/>). PDB IDs: 6E9W (ROCK1), 7JOV (ROCK2).