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BIMM143 Project

Questions:

[Q1] Tell me the name of a protein you are interested in. Include the species and the accession number. This can be a human protein or a protein from any other species as long as it's function is known.

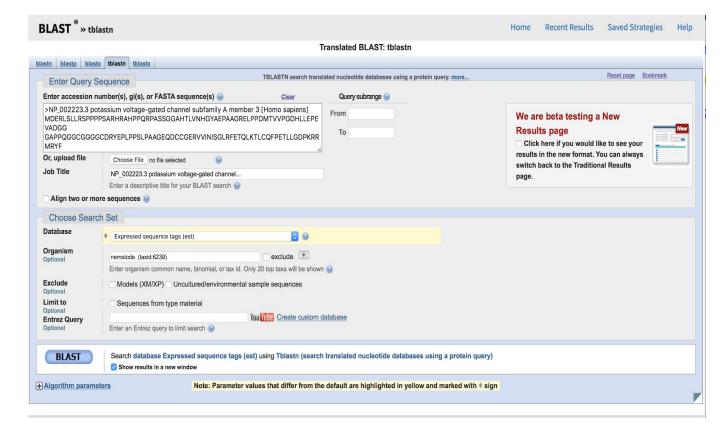
Name: Potassium voltage-gated channel subfamily A member 3

Accession: NP_002223.3 Species: Homo sapiens

[Q2] Perform a BLAST search against a DNA database, such as a database consisting of genomic DNA or ESTs. The BLAST server can be at NCBI or elsewhere. Include details of the BLAST method used, database searched and any limits applied (e.g. Organism).

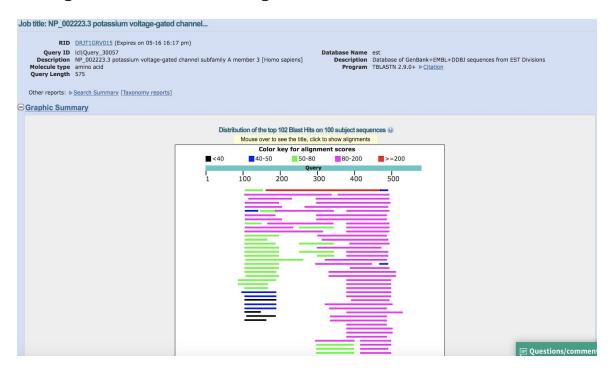
Method: TBLASTN (2.9.0) Database: Expressed Sequence Tags (est)

Organism: Nematodes(Taxid: 6239)

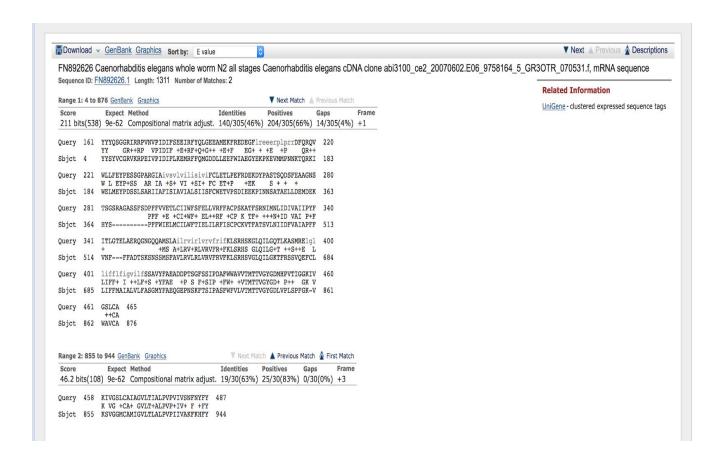


On the BLAST results, clearly indicate a match that represents a protein sequence, encoded from some DNA sequence, that is homologous to your query protein. I need to be able to inspect the pairwise alignment you have selected, including the E value and score. It should be labeled a "genomic clone" or "mRNA sequence", etc. - but include no functional annotation.

Chosen match: Accession FN892626.1, a 1311 base pair clone from *C.Elegans* See below for alignment details.



	Description	Max Score	Total Score	Query Cover	E	Per. Ident	Accession
FN	892626 Caenorhabditis elegans whole worm N2 all stages Caenorhabditis elegans cDNA clone abi3100_ce2_20070602.E06_9758164_5_GR3OTR_070531.f, mRNA ser	211	258	56%	9e-62	37.38%	FN892626.1
FN	892628 Caenorhabditis elegans whole worm N2 all stages Caenorhabditis elegans cDNA clone abi3100_ce2_20030813.E06_9758164_SL1_3_030813.r, mRNA sequence	191	191	40%	2e-56	40.34%	FN892628.1
OS	tTR30005E07 pDONR201 Entry vector Caenorhabditis elegans cDNA, mRNA sequence	174	174	34%	2e-49	44.16%	CV123089.1
OS	tTR30005F06 pDONR201 Entry vector Caenorhabditis elegans cDNA, mRNA sequence	163	163	34%	4e-45	41.21%	CV123100.1
FN	881339 Caenorhabditis elegans whole worm N2 all stages Caenorhabditis elegans cDNA clone abi3100_ce2_20060527.B12_8305806_5_GR3OTR_060526.f, mRNA ser	145	145	38%	1e-37	39.66%	FN881339.1
BJ	793488 unpublished oligo-capped cDNA library Caenorhabditis elegans cDNA clone yk1676g02 3', mRNA sequence	134	134	24%	5e-35	46.38%	BJ793488.1
BJ.	141226 unpublished oligo-capped cDNA library, C. elegans L1 stage Caenorhabditis elegans cDNA clone yk1168a01 3', mRNA sequence	133	133	20%	6e-35	53.04%	BJ141226.1
BJ	781564 unpublished oligo-capped cDNA library Caenorhabditis elegans cDNA clone yk1500f10 3', mRNA sequence	134	134	32%	6e-35	37.17%	BJ781564.1
BJ	781447 unpublished oligo-capped cDNA library Caenorhabditis elegans cDNA clone yk1499c12 3', mRNA sequence	134	134	32%	6e-35	37.17%	BJ781447.1
BJ	784946 unpublished oligo-capped cDNA library Caenorhabditis elegans cDNA clone yk1540h10 3', mRNA sequence	134	134	20%	7e-35	53.04%	BJ784946.1
BJ.	140991 unpublished oligo-capped cDNA library, C. elegans L1 stage Caenorhabditis elegans cDNA clone yk1164g03 3', mRNA sequence	134	134	20%	9e-35	53.04%	BJ140991.1
BJ	133820 unpublished oligo-capped cDNA library. C. elegans L1 stage Caenorhabditis elegans cDNA clone yk1081d09 3', mRNA sequence	134	134	20%	9e-35	53.04%	BJ133820.1
BJ	783576 unpublished oligo-capped cDNA library Caenorhabditis elegans cDNA clone yk1524c12 3', mRNA sequence	132	132	32%	3e-34	37.43%	BJ783576.1
FN	892625 Caenorhabditis elegans whole worm N2 all stages Caenorhabditis elegans cDNA clone abi3100_ce2_20021105.E06_9758164_021105.r, mRNA sequence	102	159	34%	3e-32	33.33%	FN892625.1
FN	881340 Caenorhabditis elegans whole worm N2 all stages Caenorhabditis elegans cDNA clone abi3100_ce2_20051114.B12_8305806f_5_dT35V_051114.ft mRNA seque	128	128	30%	2e-31	40.66%	FN881340.1
FN	892624 Caenorhabditis elegans whole worm N2 all stages Caenorhabditis elegans cDNA clone abi3100_ce2_20021105.E06_9758164_021105.f, mRNA sequence	123	123	30%	6e-31	36.93%	FN892624.1
BJ	793280 unpublished oligo-capped cDNA library Caenorhabditis elegans cDNA clone yk1674c01 3', mRNA sequence	119	119	18%	4e-30	50.47%	BJ793280.1
BJ	147254 unpublished oligo-capped cDNA library, C. elegans L1 stage Caenorhabditis elegans cDNA clone yk1244g01 3', mRNA sequence	119	119	29%	7e-30	37.93%	BJ147254.1
os	STR185D3_2 AD-wrmcDNA Caenorhabditis elegans cDNA, mRNA sequence	118	118	19%	8e-30	50.88%	CB397258.1
os	STR185D3_1 AD-wrmcDNA Caenorhabditis elegans cDNA, mRNA sequence	118	118	19%	8e-30	50.88%	CB397221.1
OS	STR143H5_1 AD-wrmcDNA Caenorhabditis elegans cDNA, mRNA sequence	117	117	28%	8e-30	35.71%	CB394726.1
BJ	106154 unpublished oligo-capped cDNA library, C. elegans L1 stage Caenorhabditis elegans cDNA clone yk1081d09 5', mRNA sequence	115	115	26%	3e-29	37.75%	BJ106154.2
AU	214472 unpublished oligo-capped cDNA library, stage L2 Caenorhabditis elegans cDNA clone yk813e07 3', mRNA sequence	116	116	18%	4e-29	50.00%	AU214472.1
C7	1245 Yuji Kohara unpublished cDNA Caenorhabditis elegans cDNA clone yk442g4 5', mRNA sequence	112	112	20%	2e-28	45.69%	C71245.1
OS	sTR182G8_2 AD-wrmcDNA Caenorhabditis elegans cDNA, mRNA sequence	112	112	31%	1e-:	Oues	tions/com



Alignment Details:

FN892626 Caenorhabditis elegans whole worm N2 all stages Caenorhabditis elegans cDNA clone abi3100_ce2_20070602.E06_9758164_5_GR3OTR_070531.f, mRNA sequence

Length = 1311,

Score = 211 bits (538) for Range 1 and 46.2 bits (108) for Range 2

Expect = 9e-62

Method = Compositional matrix adjust.

Identities = 140/305(46%) for Range 1 and 19/30(62%) for Range 2

Positives = 204/305(66%) for Range 1 and 25/30(83%) for Range 2

Gaps = 14/3055(3%) for Range 1 and 0/30(0%) for Range 2

Frame = +1 for Range 1 and +3 for Range 2

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Range 1:
Query 161 YYYQSGGRIRRPVNVPIDIFSEEIRFYQLGEEAMEKFREDEGFIreeerplprrDFQRQV 220
               GR++RP VPIDIF +E+RF+Q+G++ +E+F EG+ + +E +P QR++
Sbjct 4
         YYSYVCGRVKRPEIVPIDIFLKEMRFFQMGDDLLEEFWIAEGYEKPKEVMMPNNKTQRKI 183
Query 221 WLLFEYPESSGPARGIAivsvlvilisiviFCLETLPEFRDEKDYPASTSQDSFEAAGNS 280
         W L EYP+SS AR IA +S+VI+SI+ FC ET+P +EK
                                                     S+++
Sbjct 184 WELMEYPDSSLSARIIAFISIAVIALSIISFCWETVPSDIEEKPINNSATAELLDEMDEK 363
Query 281 TSGSRAGASSFSDPFFVVETLCIIWFSFELLVRFFACPSKATFSRNIMNLIDIVAIIPYF 340
           PFF +E +CI+WF+ EL++RF +CP K TF+ +++N+ID VAI P+F
Sbjct 364 HYS------PFFWIELMCILWFTIELILRFISCPCKVTFATSVLNIIDFVAIAPFF 513
Query 341 ITLGTELAERQGNGQQAMSLAilrvirlvrvfrifKLSRHSKGLQILGQTLKASMREIgI 400
             +MS A+LRV+RLVRVFR+FKLSRHS GLQILG+T ++S++E L
Sbjct 514 VNF---FFADTSKSNSSMSFAVLRVLRLVRVFRVFKLSRHSVGLQILGKTFRSSVQEFCL 684
Query 401 lifflfigvilfSSAVYFAEADDPTSGFSSIPDAFWWAVVTMTTVGYGDMHPVTIGGKIV 460
         LIFF+ I ++LF+S +YFAE +P S F+SIP +FW+ +VTMTTVGYGD+ P++ GK V
Sbjct 685 LIFFMAIALVLFASGMYFAEQGEPNSKFTSIPASFWFVLVTMTTVGYGDLVPLSPFGK-V 861
Query 461 GSLCA 465
          ++CA
Sbjct 862 WAVCA 876
Range 2:
Query 458 KIVGSLCAIAGVLTIALPVPVIVSNFNYFY 487
         K VG +CA+ GVLT+ALPVP+IV+ F +FY
Sbjct 855 KSVGGMCAMIGVLTLALPVPIIVAKFKHFY 944
```

[Q3] Gather information about this "novel" **protein**. At a minimum, show me the protein sequence of the "novel" protein as displayed in your BLAST results from [Q2] as FASTA format (you can copy and paste the aligned sequence subject lines from your BLAST result page if necessary) or translate your novel DNA sequence using a tool called EMBOSS Transeq at the EBI. Don't forget to translate all six reading frames; the ORF (open reading frame) is likely to be the longest sequence without a stop codon. It may not start with a methionine if you don't have the complete coding region. Make sure the sequence you provide includes a header/subject line and is in traditional FASTA format.

Chosen Sequence (From Emboss TransSeqResult):

>FN892626.1_1 Caenorhabditis elegans whole worm N2 all stages Caenorhabditis elegans cDNA clone abi3100_ce2_20070602.E06_9758164_5_GR3OTR_070531.f, mRNA sequence HYYSYVCGRVKRPEIVPIDIFLKEMRFFQMGDDLLEEFWIAEGYEKPKEVMMPNNKTQRK IWELMEYPDSSLSARIIAFISIAVIALSIISFCWETVPSDIEEKPINNSATAELLDEMDE KHYSPFFWIELMCILWFTIELILRFISCPCKVTFATSVLNIIDFVAIAPFFVNFFFADTS

KSNSSMSFAVLRVLRLVRVFRVFKLSRHSVGLQILGKTFRSSVQEFCLLIFFMAIALVLF ASGMYFAEQGEPNSKFTSIPASFWFVLVTMTTVGYGDLVPLSPFGKVWAVCAQ*LVS*HW HFQFLLLLPNSNTSTDQKNGLASMKSKGDDANNDFS*RGEGL*NKCETERTPFAPKARHP LGGTFGLLSSIKPFQPLTISRALQLCFPILKVFYFPTPFSPNFFFLKKRGGKTPCGPPGN SPPPPPKKILFSPSPP

>FN892626.1_2 Caenorhabditis elegans whole worm N2 all stages Caenorhabditis elegans cDNA clone abi3100_ce2_20070602.E06_9758164_5_GR3OTR_070531.f, mRNA sequence IIIHMCAEE*NDLKLCRLTYF*KKCDFSKWVMIFWKNSG*LRVMKNQKK**CQIIKPKEK YGN*WNIRIVHFPRELLHSFQLLLLHYPSSHSAGKQYHLTSKKNQSIIQQLRNYWMKWTK NIIPHFSGLSSCVFCGLLLN*FFGLFHVLVK*HLPRLC*ILLTLWQLLRFLLTFSSRTQA NPIHRCRLQCSVCSDWFEYSEFSNLVDIPLVFKFLEKLSDPLSKSFVFSFSSWQLLWFSL HQECILRSKGSQTQSSLQFQQASGLYWSQ*QQSDMEIWFR*VHLEKCGRYVRNDWCLDIG TSSSYYCCQIQTLLPTKKTVLLQ*NQRVTMQTTTSHDGVKAFETSVKPKEPHLPRKLAIP WGEPSDC*APSSPFSPSPSPSPSPSPSPFSPSPFPFFFKKFIFQPLFPPIFFFLKKGGGKPLVAPPEI PPPPPLQKKFFSLPLPP

>FN892626.1_3 Caenorhabditis elegans whole worm N2 all stages Caenorhabditis elegans cDNA clone abi3100_ce2_20070602.E06_9758164_5_GR3OTR_070531.f, mRNA sequence LLFICVRKSETT*NCAD*HIFERNAIFPNG**SSGRILDS*GL*KTKRSDDAK**NPKKN MGTNGISG*FTFRENYCIHFNCCYCIIHHLILLGNSTI*HRRKTNQ*FSNCGTIG*NGRK TLFPIFLD*AHVYFVVYY*INSSVYFMSL*SDICHVCVEYY*LCGNCSVFC*LFLRGHKQ IQFIDVVCSAPCAPIGSSIQSFQT*STFRWSSNSWKNFPILCPRVLSSHFLHGNCSGSLC IRNVFCGARGAKLKVHFNSSKLLVCTGHNDNSRIWRFGSAESIWKSVGGMCAMIGVLTLA LPVPIIVAKFKHFYRPKKRSCFNEIKG*RCKQRLLMTG*RPLKQV*NRKNPICPESSPSP GGNLRIVKLHQALSAPHHLQGPPTLFSNFKSFLFSNPFFPQFFFS*KKGGENPLWPPRKF PPPPPSKKNSFLSLSPX

>FN892626.1_4 Caenorhabditis elegans whole worm N2 all stages Caenorhabditis elegans cDNA clone abi3100_ce2_20070602.E06_9758164_5_GR3OTR_070531.f, mRNA sequence GGRGREKNFFWRGGGGGISGGATRGFPPPFFKKKKIGGKRGWKIKNF*NWKTKLEGPGDG EGLKGLDGA*QSEGSPQGMASFRGKWGSFGFTLVSKAFTPS*EVVVCIVTL*FH*SKTVF LVGRSV*IWQQ**ELEVPMSRHQSLRTYRPHFSKWTQRNQISISDCCHCDQYKPEACWN* SEL*VWLPLLRKIHS*CKENQSNCHEENEKTKLLDRGSESFSKNLKTNGMSTKFENSEYS NQSEHTEHCKRHR*IGFACVREEKVNKKRSNCHKVNNIQHRRGKCHFTRT*NKPKN*FNS KPQNTHELNPEKWGIMFFVHFIQ*FRSC*IIDWFFFDVRWYCFPAE*DDG*CNNSN*NEC NNSRGK*TIRIFH*FPYFSLGFIIWHHHFFWFFITLSYPEFFQKIITHLEKSHFFQKYVN RHNFRSFHSSAHI*IIM

>FN892626.1_5 Caenorhabditis elegans whole worm N2 all stages Caenorhabditis elegans cDNA clone abi3100_ce2_20070602.E06_9758164_5_GR3OTR_070531.f, mRNA sequence GERERKEFFLEGGGGGNFRGGHKGFSPPFF*EKKNWGKKGLENKKLLKLENKVGGPWRW* GAERA*WSLTIRRFPPGDGELSGQMGFFRFHTCFKGLHPVMRSRCLHRHPLISLKQDRFF GR*KCLNLATIIGTGSANVKTPIIAHIPPTLFQMDSAEPNLHIRLLSL*PVQTRSLLELK *TLSLAPLAPQNTFLMQREPEQLP*RK*EDKTLGQRIGKFFQEFEDQRNVD*V*KL*ILE PIGAHGALQTTSMNWICLCPRRKS*QKTEQLPQSQ*YSTQTWQMSLYKDMK*TEELIQ**

TTKYT*AQSRKMGNNVFRPFHPIVPQLLNY*LVFLRCQMVLFPSRMR*WIMQ*QQLK*MQ
*FSRKVNYPDIPLVPIFFFGFYYLASSLLLVFHNPQLSRILPEDHHPFGKIAFLSKICQS
AQFQVVSLFRTHMNNNX

>FN892626.1_6 Caenorhabditis elegans whole worm N2 all stages Caenorhabditis elegans cDNA clone abi3100_ce2_20070602.E06_9758164_5_GR3OTR_070531.f, mRNA sequence GGEGEKRIFFGGGGGGEFPGGPQGVFPPLFLRKKKLGEKGVGK*KTFKIGKQSWRALEMV RG*KGLMELNNPKVPPRGWRAFGANGVLSVSHLFQRPSPRHEKSLFASSPFDFIEARPFF WSVEVFEFGNNNRNWKCQCQDTNHCAHTAHTFPNGLSGTKSPYPTVVIVTSTNQKLAGIE VNFEFGSPCSAKYIPDAKRTRAIAMKKMRRQNSWTEDRKVFPRI*RPTECRLSLKTLNTR TNRSTRSTANDIDELDLLVSAKKKLTKNGAIATKSIIFNTDVANVTLQGHEINRRINSIV NHKIHMSSIQKNGE*CFSSISSNSSAVAELLIGFSSMSDGTVSQQNEMMDNAITAIEMNA IILAESELSGYSISSHIFLWVLLFGIITSFGFS*PSAIQNSSRRSSPIWKNRISFKNMSI GTISGRFTLPHTYE**X

Here, tell me the name of the novel protein, and the species from which it derives. It is very unlikely (but still definitely possible) that you will find a novel gene from an organism such as S. cerevisiae, human or mouse, because those genomes have already been thoroughly annotated. It is more likely that you will discover a new gene in a genome that is currently being sequenced, such as bacteria or plants or protozoa.

Name of Protein: Not found Species Caenorhabditis elegans

Eukaryota; Metazoa; Ecdysozoa; Nematoda; Chromadorea;

Rhabditida; Rhabditina; Rhabditomorpha;

Rhabditoidea; Rhabditidae; Peloderinae; Caenorhabditis.

[Q4] Prove that this gene, and its corresponding protein, are novel. For the purposes of this project, "novel" is defined as follows. Take the protein sequence (your answer to [Q3]), and use it as a query in a blastp search of the nr database at NCBI.

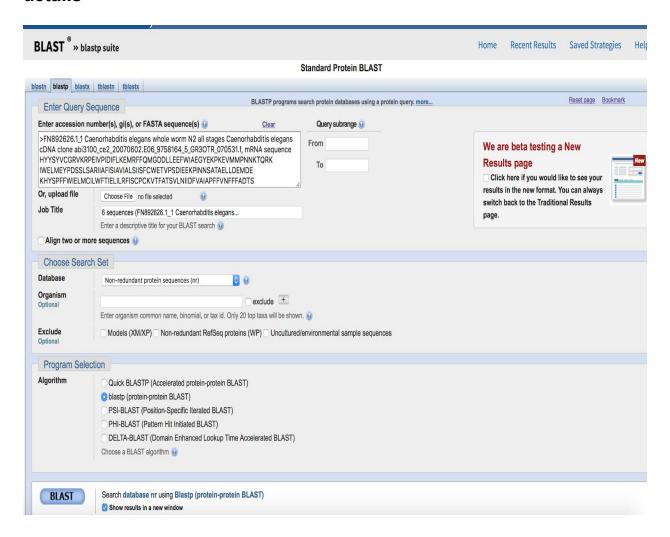
- If there is a match with 100% amino acid identity to a protein in the database, from the same species, then your protein is NOT novel (even if the match is to a protein with a name such as "unknown"). Someone has already found and annotated this sequence, and assigned it an accession number.
- If the top match reported has less than 100% identity, then it is likely that your protein is novel, and you have succeeded.

- If there is a match with 100% identity, but to a different species than the one you started with, then you have likely succeeded in finding a novel gene.
- If there are no database matches to the original query from [Q1], this indicates that you have partially succeeded: yes, you may have found a new gene, but no, it is not actually homologous to the original query. You should probably start over.

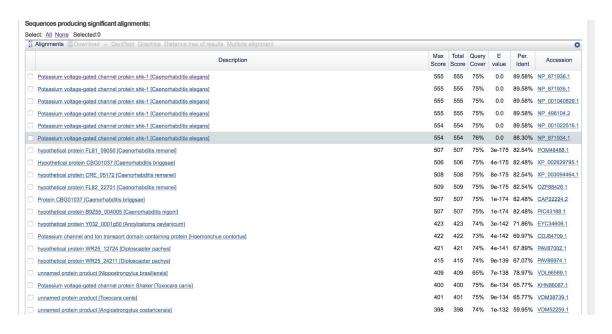
Details:

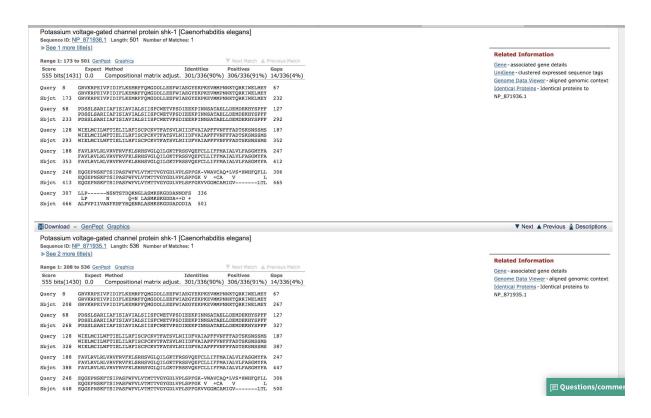
A BLASTP search against NR database (see setup in the first screen-shot below) yielded a top hit result is to a protein from C.Elegans.

See additional screenshots below for top hits and selected alignment details



The top result is to a protein from Caenorhabditis elegans with identity lower than 100%, see second screenshot below for alignment details:





[Q5] Generate a multiple sequence alignment with your novel protein, your original query protein, and a group of other members of this family from different species. A typical number of proteins to use in a multiple sequence alignment for this assignment purpose is a minimum of 5 and a maximum of 20 - although the exact number is up to you. Include the multiple sequence alignment in your report. Use Courier font with a size appropriate to fit page width.

Side-note: Indicate your sequence in the alignment by choosing an appropriate name for each sequence in the input unaligned sequence file (i.e. edit the sequence file so that the species, or short common, names (rather than accession numbers) display in the output alignment and in the subsequent answers below). The goal in this step is to create an interesting an alignment for building a phylogenetic tree that illustrates species divergence.

Potassium channel and Ion transport domain containing protein [Haemonchus contortus]	422	422	73%	4e-142 69.97%	CDJ84709.1
hypothetical protein WR25_24211 [Diploscapter pachys]	415	415	74%	9e-139 67.07%	PAV86974.1
unnamed protein product [Nippostrongylus brasiliensis]	409	409	65%	7e-138 78.97%	VDL66569.1
Potassium voltage-gated channel protein Shaker [Toxocara canis]	400	400	75%	6e-134 65.77%	KHN86087.1
unnamed protein product [Toxocara canis]	401	401	75%	9e-134 65.77%	VDM38739.1
unnamed protein product [Angiostrongylus costaricensis]	398	398	74%	1e-132 59.95%	VDM52259.1
transporter, cation channel family protein [Ancylostoma caninum]	388	388	70%	3e-130 70.35%	RCN37415.1
unnamed protein product [Anisakis simplex]	395	395	65%	1e-129 73.43%	VDK46358.1
unnamed protein product [Enterobius vermicularis]	380	380	64%	7e-127 70.71%	VDD95068.1
unnamed protein product [Thelazia callipaeda]	379	379	65%	2e-124 71.43%	VDN08188.1
K+ channel tetramerization domain protein [Onchocerca flexuosa]	368	368	66%	2e-120 67.58%	OZC11969.1
unnamed protein product [Onchocerca flexuosa]	368	368	66%	3e-120 67.92%	VDP12905.1
unnamed protein product [Haemonchus placei]	355	355	73%	1e-116 63.66%	VDO32825.1
unnamed protein product [Onchocerca ochengi]	353	353	66%	2e-115 68.94%	VDK62583.1
unnamed protein product [Brugia timori]	346	346	66%	2e-112 69.62%	VDO32192.1
BMA-SHK-1, isoform e [Brugia malayi]	346	346	66%	3e-112 69.62%	CDP90796.1
unnamed protein product [Wuchereria bancrofti]	342	342	62%	7e-112 70.80%	VDM12676.1
BMA-SHK-1, isoform g [Brugia malayi]	347	347	66%	9e-112 69.62%	CDP90793.1
Potassium voltage-gated channel protein Shaker [Strongyloides ratti]	346	346	65%	7e-111 62.50%	XP_024509009.1
hypothetical protein LOAG_01893 [Loa loa]	342	342	66%	7e-111 68.94%	XP_020303708.1
unnamed protein product [Dracunculus medinensis]	337	337	62%	9e-110 68.50%	VDN55395.1
BMA-SHK-1, isoform c [Brugia malayi]	340	340	66%	1e-109 68.00%	CDP90795.1

(Figure shows the clicked links corresponding to the different species selected)

>Human_K+_Channel_Protein | NP_002223.3 | potassium voltage-gated channel subfamily A member 3 | [Homo sapiens]

MDERLSLLRSPPPPSARHRAHPPQRPASSGGAHTLVNHGYAEPAAGRELPPDMTVVPGDHLLEPEVADGG
GAPPQGGCGGGGCDRYEPLPPSLPAAGEQDCCGERVVINISGLRFETQLKTLCQFPETLLGDPKRRMRYF
DPLRNEYFFDRNRPSFDAILYYYQSGGRIRRPVNVPIDIFSEEIRFYQLGEEAMEKFREDEGFLREEERP
LPRRDFQRQVWLLFEYPESSGPARGIAIVSVLVILISIVIFCLETLPEFRDEKDYPASTSQDSFEAAGNS
TSGSRAGASSFSDPFFVVETLCIIWFSFELLVRFFACPSKATFSRNIMNLIDIVAIIPYFITLGTELAER
QGNGQQAMSLAILRVIRLVRVFRIFKLSRHSKGLQILGQTLKASMRELGLLIFFLFIGVILFSSAVYFAE
ADDPTSGFSSIPDAFWWAVVTMTTVGYGDMHPVTIGGKIVGSLCAIAGVLTIALPVPVIVSNFNYFYHRE
TEGEEQSQYMHVGSCQHLSSSAEELRKARSNSTLSKSEYMVIEEGGMNHSAFPQTPFKTGNSTATCTTNN
NPNSCVNIKKIFTDV

>C.Elegans K+_Protein(Shaker-1) | NP_871936.1 | Potassium voltage-gated channel protein shk-1 | [Caenorhabditis elegans]
MIDSLIRRLEQVLNVHPEKYQNGCSSQRPSRQPSPVEQLAPIRSHSADFGRAAEMASGNSEEGKGMLLRN
GDDRIRLPSPQRGTPDTSSTQGHPYTDQIVTINVSGMRFQTFESTLSRYPNSLLGDRNKRQHFFVSDTNE
FFFDRHRTTSSSFTFEIRNYLFESILYIYQSGGRVKRPEIVPIDIFLKEMRFFQMGDDLLEEFWIAEGYE
KPKEVMMPNNKTORKIWELMEYPDSSLSARIJAFISTAVJALSIJSFCWETVPSDIFEKPINNSATAFIJ

KPKEVMMPNNKTQRKIWELMEYPDSSLSARIIAFISIAVIALSIISFCWETVPSDIEEKPINNSATAELL DEMDEKHYSPFFWIELMCILWFTIELILRFISCPCKVTFATSVLNIIDFVAIAPFFVNFFFADTSKSNSS MSFAVLRVLRLVRVFRVFKLSRHSVGLQILGKTFRSSVQEFCLLIFFMAIALVLFASGMYFAEQGEPNSK FTSIPASFWFVLVTMTTVGYGDLVPLSPFGKVVGGMCAMIGVLTLALPVPIIVANFKHFYRQENRLASMK SKGDDADDDIA

>Barber's_pole_worm K+_Channel_Protein | CDJ84709.1 | Potassium channel and Ion transport domain containing protein | [Haemonchus contortus]

MWRLRRYRGPPILDLDEANGNLLVDDSTRNASPQRGTPQGDERLRSSDLVTINVSGLRFQTFERTLARFP

NTLLGCKSKRERYYMQDTNEYFFDRHRSTFESILYIYQSGGRVKRPESVPIDIFLREMRFFQMGEQLIEE

FWIAEGYEKPEEAILPKNLSQRRLWELMEYPDSSLAARIIAFISVFVIVISIVSFCWETVPSGDVRDTNG

TTGVTSPDKDEGRLVWNPFFWLELVCIVWFTIELTLRFISCPSKVTFMMSFLNIIDFVAIAPFFVNLIWA

DANKSSGSMSFAVLRVLRLVRVFRIFKLSRHSAGLQILGKTFRASVQEFCLLIFFMAIALVLFSSGMYFA

EQGEANSKFTSIPASFWFVLVTMTTVGYGDLVPLSTQGKIVGSMCALIGVLTLALPVPIIVANFKHFYRQ

ENRLATMRSAGKDLETAESIDDS

>Dog_roundworm K+_Channel_Protein | KHN86087.1 | Potassium voltage-gated channel protein Shaker [Toxocara canis]

MIPEEEAVNVIPPTDGISSNMSENNSIVTINVSGLKFQTFNSTLSRYPETLLGDPVKRARFWNGHDGEYF FDRHRGSFESILYIYQSHGIVKRPEAVPIDIFLKEMKFFEMTDDILEAFWISEGYEKPKEAKMPQNIHQR RIWELMEYPDSSLSARILAFVSIIVITVSIVSFCLETLPSLKPADIEGVRDWSNPFLWVEFVCIIWFTIE LLLRFASCPCKLTFMRSIPNIIDFIAIAPFFVNLVWSDVSKSNSSMSFAVLRVLRLVRVFRIFKLSRHSV GLQILGKTFRASIQEFCLLIFFMAIALVLFASGMYFAEQGEPDTKFTSIPASFWFVLVTMTTVGYGDLTP TGVYGKLVGSVCALIGVLTLALPVPIIVANFKHFYRQETRLATMRANADEEDEECSQDSSRT

>Deer_roundworm K+_Channel_Protein | OZC11969.1 | K+ channel tetramerization domain protein, partial [Onchocerca flexuosa]

RQIEHLLNVHPEKYRSRSGQSIETSTSVHLNQMGCHHRSRSVDYLSPMMDASNKEINEEKSNNGSIFPMI

TEEESSNIMYNDTSLTKRRERVTINVSGLRFQTYESTLRRYPLTLLGNSFKRNRFWDPKNKEYFFDRHRT

SFESILYTYQSGGVVKRPESVPIDMFIKELKFFEMGEELLEKFWISEGYEKPKEIQMPKNVLLRKLWELV

EYPDSSLFARIFALLSIFVISISIISFCLETLPSMKVNPGDVRDWSNPFFHIELFCIIWFTTELLLRFIS

CPNKLSFLRSALNIIDFIAIAPFFGNLLWMDSAKSSMSFAILRVLRLVRVFRIFKLSRHSVGLQILGKTF

RASIQEFCLLIFFMIIALVLFSSGIYFAEQNEPNTKFTSIPASFWFVLVTMTTVGYGDLTPTGVYGKLVG

GLCALIGVLTLALPVPIIVANFKHFYRQETRLAQMRASVEDDETASEKSSKSP

>Rat_roundworm K+Channel Protein | XP_024509009.1 | Potassium voltage-gated channel protein Shaker [Strongyloides ratti]
MNKKTFSCEGNDDISFSFRQKIEQILHVHPEKYRARGGVGSRRSTPGKRGSYDDRLHVRSASEELRQRSL QSSSSDSPSINDSNNSKQLEELSIPIPVECINSGVNKSNDSEYRNPLTSHHNHIPDNGDIKWKNEEVITI NVSGLRFQTYESTLARFPNSLLGHPAKRAKYWNNKTKEYFLDHSRYCFESILNIYQTNGDVRRPELVPLE IYLKELKFYEMNEEVMENFWLSEGYEKPIEHIMPNNFIQKYIWELMEYPDSSVPARVLAFISISVIVTSI VSFCLETLPDFREASETLTEIGYSKWNNPFLILESLCIVWFSIELFLRFISCPSKSLFMKSFLNIVDFIA IAPFFINLILSEGNKNNSSTTSFAVLRVLRLVRVFRIFKLSRHSVGLQILGKTFRASIQEFCLLVFFMVI ALVLFSSAIFYVEQGEADTRFTSIPASFWFVVATMTTVGYGDLVPTGTYGKLVGSLCALLGVLTLALPVP IIVANFKHFYRQECRLAAMRVSREIDDASRYNESDEEYTT

>Human_Lymphatic_Roundworm Shaker 1 Protein | CDP90795.1 | BMA-SHK-1, isoform c [Brugia malayi]

MDTPSNREVSDEKPNNGSIFPMITEEEPNNIMFNDTSSAKQLERNLITINVSGLRFQTYESTLERYPLTL LGNSFKRNRFWDPKNEEYFFDRHRTSFESILYAYQSGGIMKRPESVPIDMFVKELKFFEVNPKLQKMGEE LLEKFWISEGYEKPKEIQMPQNVLQRQLWELVEYPDSSLFARIFALLSIFVISISIISFCLETLPSMKEN PGDVRDWSNPFFYIELFCIIWFTIELLLRFISCPNKFSFLRSVLNIIDFVAIAPFFGNLMWMDSTKSSSS MSFAVLRVLRLVRVFRIFKLSRHSVGLQILGKTFRASIQEFCLLIFFMVIALVLFSSGVYFAEQNEPNTK FTSIPASFWFVLVTMTTVGYGDLTPTGVYGKLVGGLCALIGVLTLALPVPIIVANFKHFYRQETRLAQMR ASAEEDETNSEHSSKSP

Alignment: (Obtained using MUSCLE (version 3.8) at EBI:

Human_K+_Channel_Protein -----MDERLSLLRSPPPPSARHRAHPPORPASSGGAHTLVNHGYAEP Rat roundworm MNKKTFSCEGNDDISFSFRQKIEQILHVHPEKYRARGGVGSRRSTPGKRGSYDDRLHVRS Dog roundworm _____ Deer_roundworm -----RQIEHLLNVHPEKYRSRSGQSIETSTSVHLNQMGCHHRSRS -----RQ1EHLLNVHPEKYRSRSGQSIETSTSVHLNQMGCHHRSRS
Human_Lymphatic_Roundworm

C.Elegans
------MIDSLIRRLEQVLNVHPEKYQNGCSSQRPSRQPSPVEQLAPIRSHS-Barber's pole worm Human_K+_Channel_Protein AAGRELPPDMTVVPGDHLLEPEVADGG----GAPPQGGCGGGGCDR-----YEPL Rat roundworm ASEELRQRSLQSSSSDSPSINDSNNSKQLEELSIPIPVECINSGVNKSNDSEYRNPLTSH Deer_roundworm DTSLTKRRE-----RVTINVSGLRFQTYESTLRRYPLTLLGNSFKRNRFWDPKNKE
Human_Lymphatic_Roundworm DTSSAKQLE-----RNLITINVSGLRFQTYESTLERYPLTLLGNSFKRNRFWDPKNEE
C.Elegans QRGTPDTSSTQGHPYTDQIVTINVSGMRFQTFESTLSRYPNSLLGDRNKRQHFFVSDTNE
Barber's_pole_worm QRGTPQGDE---RLRSSDLVTINVSGLRFQTFERTLARFPNTLLGCKSKRERYYMQDTNE Deer_roundworm :.**:**: ** ** .:* :*** Human_K+_Channel_Protein YFFDRNRPS------FDAILYYYQSGGRIRRPVNVPIDIFSEEIRFYQ----Rat roundworm YFLDHSRYC------FESILNIYOTNGDVRRPELVPLEIYLKELKFYE-----Rat roundworm YFLDHSRYC----FESILNIYQTNGDVRRPELVPLEIYLKELKFYE----YFFDRHRGS-----FESILYIYQSHGIVKRPEAVPIDIFLKEMKFFE-----Dog roundworm Dog_roundworm
Deer_roundworm Deer_roundworm YFFDRHRTS------FESILYTYQSGGVVKRPESVPIDMFIKELKFFE----Human_Lymphatic_Roundworm YFFDRHRTS------FESILYAYQSGGIMKRPESVPIDMFVKELKFFEVNPKLQ
C.Elegans FFFDRHRTTSSSFTFEIRNYLFESILYIYQSGGRVKRPEIVPIDIFLKEMRFFQ----Barber's_pole_worm YFFDRHRST------FESILYIYQSGGRVKRPESVPIDIFLREMRFFQ-----*::** **: * :.** **:::: *:.*:: Human_K+_Channel_Protein -LGEEAMEKFREDEGFLREEERPLPRRDFQRQVWLLFEYPESSGPARGIAIVSVLVILIS
Rat roundworm -MNEEVMENFWLSEGYEKPIEHIMPNNFIQKYIWELMEYPDSSVPARVLAFISISVIVTS Dog_roundworm -MTDDILEAFWISEGYEKPKEAKMPQNIHQRRIWELMEYPDSSLSARILAFVSIIVITVS
Deer_roundworm -MGEELLEKFWISEGYEKPKEIQMPKNVLLRKLWELVEYPDSSLFARIFALLSIFVISIS
Human_Lymphatic_Roundworm KMGEELLEKFWISEGYEKPKEIQMPQNVLQRQLWELVEYPDSSLFARIFALLSIFVISIS
C.Elegans -MGDDLLEEFWIAEGYEKPKEVMMPNNKTQRKIWELMEYPDSSLSARIIAFISIAVIALS
Barber's_pole_worm -MGEQLIEEFWIAEGYEKPEEAILPKNLSQRRLWELMEYPDSSLAARIIAFISVFVIVIS : :: :* *. **: . * :*.. . :* *.*** ** :*::*: ** * Human K+ Channel Protein IVIFCLETLPEFRDEKDYPASTSQDSFEAAGNSTSGSRAGASSFSDPFFVVETLCIIWFS

Rat roundworm Dog roundworm Deer roundworm C.Elegans Barber's_pole_worm Human K+ Channel Protein

Rat_roundworm Dog roundworm Deer roundworm Human Lymphatic Roundworm C.Elegans Barber's pole worm

Human K+ Channel Protein Rat roundworm Dog roundworm Deer roundworm C.Elegans Barber's pole worm

Human_K+_Channel_Protein Rat roundworm Dog roundworm Deer roundworm Barber's_pole_worm

Human_K+_Channel_Protein Rat roundworm Dog roundworm Deer roundworm Human Lymphatic_Roundworm C.Elegans Barber's pole worm

Human_K+_Channel_Protein Rat roundworm Dog roundworm Deer roundworm Human_Lymphatic_Roundworm C.Elegans Barber's pole worm

IVSFCLETLPDFRE------ASETLTEIGYSKWNNPFLILESLCIVWFS IVSFCLETLPSLK--------PADIEGVRDWSNPFLWVEFVCIIWFT IISFCLETLPSMKV------NPGD---VRDWSNPFFHIELFCIIWFT IISFCWETVPSDIE-----EKPINNSATAELLDEMDEKHYS-PFFWIELMCILWFT IVSFCWETVPSGDV------RDTNGTTGVTSPDKDEGRLVWN-PFFWLELVCIVWFT *: ** **:*. :. **: :* .**:**:

> FELLVRFFACPSKATFSRNIMNLIDIVAIIPYFITLGTELAERQGNGQQAMSLAILRVIR IELFLRFISCPSKSLFMKSFLNIVDFIAIAPFFINL--ILSEGNKNNSSTTSFAVLRVLR IELLLRFASCPCKLTFMRSIPNIIDFIAIAPFFVNL--VWSDVSKSNSS-MSFAVLRVLR TELLLRFISCPNKLSFLRSALNIIDFIAIAPFFGNL--LWMDSAKSS---MSFAILRVLR IELLLRFISCPNKFSFLRSVLNIIDFVAIAPFFGNL--MWMDSTKSSSS-MSFAVLRVLR IELILRFISCPCKVTFATSVLNIIDFVAIAPFFVNF--FFADTSKSNSS-MSFAVLRVLR IELTLRFISCPSKVTFMMSFLNIIDFVAIAPFFVNL--IWADANKSSGS-MSFAVLRVLR

LVRVFRIFKLSRHSKGLQILGQTLKASMRELGLLIFFLFIGVILFSSAVYFAEADDPTSG LVRVFRIFKLSRHSVGLQILGKTFRASIQEFCLLVFFMVIALVLFSSAIFYVEQGEADTR LVRVFRIFKLSRHSVGLQILGKTFRASIQEFCLLIFFMAIALVLFASGMYFAEQGEPDTK LVRVFRIFKLSRHSVGLQILGKTFRASIQEFCLLIFFMIIALVLFSSGIYFAEQNEPNTK Human_Lymphatic_Roundworm LVRVFRIFKLSRHSVGLQILGKTFRASIQEFCLLIFFMVIALVLFSSGVYFAEQNEPNTK LVRVFRVFKLSRHSVGLQILGKTFRSSVQEFCLLIFFMAIALVLFASGMYFAEQGEPNSK LVRVFRIFKLSRHSAGLQILGKTFRASVQEFCLLIFFMAIALVLFSSGMYFAEQGEANSK

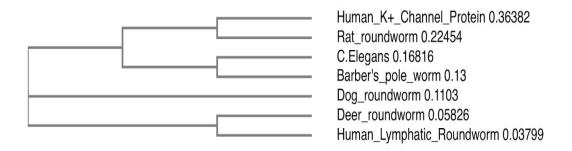
FSSIPDAFWWAVVTMTTVGYGDMHPVTIGGKIVGSLCAIAGVLTIALPVPVIVSNFNYFY FTSIPASFWFVVATMTTVGYGDLVPTGTYGKLVGSLCALLGVLTLALPVPIIVANFKHFY FTSIPASFWFVLVTMTTVGYGDLTPTGVYGKLVGSVCALIGVLTLALPVPIIVANFKHFY FTSIPASFWFVLVTMTTVGYGDLTPTGVYGKLVGGLCALIGVLTLALPVPIIVANFKHFY Human_Lymphatic_Roundworm FTSIPASFWFVLVTMTTVGYGDLTPTGVYGKLVGGLCALIGVHILLDLTLTLT....
FTSIPASFWFVLVTMTTVGYGDLVPLSPFGKVVGGMCAMIGVLTLALPVPIIVANFKHFY FTSIPASFWFVLVTMTTVGYGDLVPLSTQGKIVGSMCALIGVLTLALPVPIIVANFKHFY *:*** :**:.:.******* **:**::**: ****:**:**:**

> HRETEGEEQSQYMHVGSCQHLSSSAEELRKARSNSTLSKSEYMVIEEGGMNHSAFPQTPF RQEC-----RLAAMRVSREIDDASRYNESDEEYTT------RQET-----RLATMRANADEEDEECSQDSSRT-----RQET-----RLAQMRASVEDDETASEKSSKSP-----RQET-----RLAQMRASAEEDETNSEHSSKSP------RQEN-----RLASMKSKGDDADDDIA-----RQEN-----RLATMRSAGKDLETAESIDDS-----..* :

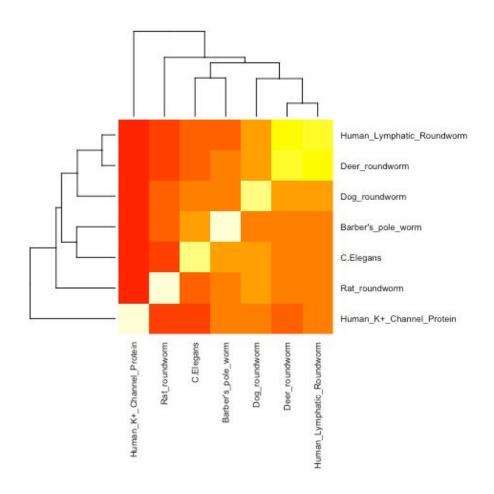
KTGNSTATCTTNNNPNSCVNIKKIFTDV _____ _____ _____ _____

[Q6] Create a phylogenetic tree, using either a parsimony or distance-based approach. Bootstrapping and tree rooting are optional. Use "simple phylogeny" online from the EBI or any respected phylogeny program (such as MEGA, PAUP, or Phylip). Paste an image of your Cladogram or tree output in your report.

Using "simple phylogeny" online from the EBI, we got this tree:



[Q7] Generate a sequence identity based **heatmap** of your aligned sequences using R.

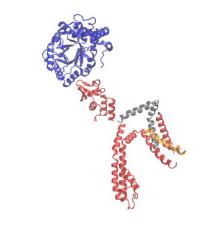


[Q8] Using R/Bio3D (or an online blast server if you prefer), search the main protein structure database for the most similar atomic resolution structures to your aligned sequences.

List the top 3 unique hits (i.e. not hits representing different chains from the same structure) along with their Evalue and sequence identity to your query. Please also add annotation details of these structures. For example include the annotation terms PDB identifier (structureld), Method used to solve the structure (experimentalTechnique), resolution (resolution), and source organism (source).

ID	Technique	Resolution	Source	Evalue	Identity
2A79_B	X-RAY DIFFRACTION	2.9	Rattus norvegicus	6.64e-140	51.523
3LUT_B	X-RAY DIFFRACTION	2.9	Rattus norvegicus	7.08e-140	51.523
2R9R_B	X-RAY DIFFRACTION	2.4	Rattus norvegicus	3.98e-134	49.744

[Q9] Generate a molecular figure of one of your identified PDB structures using VMD. You can optionally highlight conserved residues that are likely to be functional. Please use a white or transparent background for your figure (i.e. not the default black). Based on sequence similarity. How likely is this structure to be similar to your "novel" protein?



2A79 is chosen to generate the VMD PDB structures (Rendered in internal Tachyon, saved as tga file and then converted to JPG in order to be put in the google doc). Based on sequence similarity (~50%) and the rule of thumb mentioned in the lecture, since they have more than 45% identity, they should have similar structures.

[Q10] Perform a "Target" search of ChEMBEL (https://www.ebi.ac.uk/chembl/) with your novel sequence. Are there any **Target Associated Assays** and **ligand efficiency data** reported that may be useful starting points for exploring potential inhibition of your novel protein?

https://www.ebi.ac.uk/chembl/target_report_card/CHEMBL4106173/

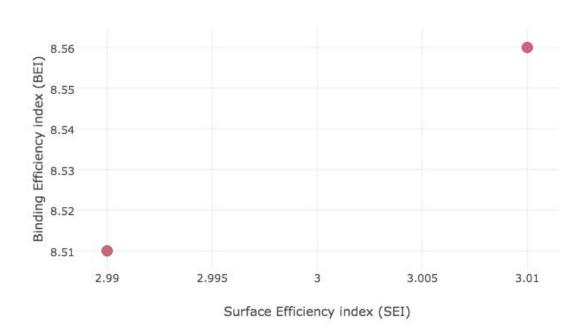
CHEMBL Details 8 Binding Assays

ChEMBL ID	\$	Description	\$	Organism 🕏	Compounds	\$	Document 🕏	BAO Format	Source \$
CHEMBL4009	564	Inhibition of recombinant rat Kv1.1/1.1/1. expressed in HEK293 cells at 10 uM at -90 holding potential by whole cell patch clam method relative to control) mV	Rattus norvegicus	By Mol. Wt.:	_	CHEMBL4007435	cell-based format	Scientific Literature
CHEMBL4009	568	Inhibition of recombinant rat Kv(1.1)3/Kv: expressed in HEK293 cells assessed as tin for activation of Kv1.1 channel current at -90 mV holding potential by whole cell pat Qpatch method (Rvb = 3.1 +/- 0.2 ms)	ne constant 10 uM at	Rattus norvegicus	By Mol. Wt.:	_	CHEMBL4007435	cell-based format	Scientific Literature
CHEMBL4009	563	Inhibition of recombinant rat Kv1.2/1.1/1. expressed in HEK293 cells at 10 uM at -90 holding potential by whole cell patch clam method relative to control) mV	Rattus norvegicus	By Mol. Wt.:	_	CHEMBL4007435	cell-based format	Scientific Literature
CHEMBL4009	567	Inhibition of recombinant rat $Kv(1.1)2/Kv$ expressed in HEK293 cells assessed as tin for activation of $Kv1.1$ channel current at -90 mV holding potential by whole cell pat Qpatch method ($Rvb = 2.8 + /-0.4 \text{ ms}$)	ne constant 10 uM at	Rattus norvegicus	By Mol. Wt.:	_	CHEMBL4007435	cell-based format	Scientific Literature
CHEMBL4009	561	Inhibition of recombinant rat Kv1.1/Kv(1.3 expressed in HEK293 cells at -90 mV hold potential by whole cell patch clamp Qpatcl	ing	Rattus norvegicus	By Mol. Wt.:		CHEMBL4007435	cell-based format	Scientific Literature
CHEMBL40095	60	Inhibition of recombinant rat $Kv(1.1)2/Kv($ expressed in HEK293 cells at -90 mV holdi potential by whole cell patch clamp Q patch	ng	Rattus norvegicus	By Mol. Wt.:	_	CHEMBL4007435	cell-based format	Scientific Literature
CHEMBL40095	65	Inhibition of recombinant rat Kv1.2/1.2/1. expressed in HEK293 cells at 10 uM at -90 holding potential by whole cell patch clam method relative to control	mV	Rattus norvegicus	By Mol. Wt.:		CHEMBL4007435	cell-based format	Scientific Literature
CHEMBL40095	59	Inhibition of recombinant rat Kv(1.1)3/Kv1 expressed in HEK293 cells at -90 mV holdi potential by whole cell patch clamp Qpatch	ng	Rattus norvegicus	By Mol. Wt.:	_	CHEMBL4007435	cell-based format	Scientific Literature

Link to one of the binding assay linked articles:

https://pubs.acs.org/doi/10.1021/acs.jmedchem.6b01262

ChEMBL Ligand Efficiency Plot for Target CHEMBL4106173



Ligand Efficiency session has the following plots. Both points are associated with molecule CHEMBL4079366 (Different standard values) that is possible to inhibit the novel protein.

Information about this molecule:

Name And Classification

