

Meenu Ravi
R Skills: PNNL Write Up
November 25 2020

Part 1: Question 1 and 2

Part 2-9: Question 3 (run consecutively)

Part 10-11: Question 4 (run consecutively)

Part 1

This file contains:

- my installation and formatting initial files given
 - Unzipped both given files
 - Read phosphopeptides into a table
- Map RefSeq IDs to gene IDs
 - Use biomaRt to get gene ids
 - Added that to phosphopeptides table
 - Wrote result into a text file called phosphogene.txt

Part 2

This file contains:

- Convert sapiens fasta file to a table by reading it in as a csv first
- Then remove '>'
- Save result as formattedProteins.txt

Part 3

This file contains:

- Merged dataset containing the refseq, peptide, gene id and associated protein sequence
- The substring for all peptides from right before the first *

- Saved resulting table in proteinp1.txt

RStudio

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Go to file/function Addins

ex.R × part2 × ex2.R × ex3.R × combined × phosphogene × ex4.R × ex5.R × ex6.R × ex7.R × ex8.R × ex9.R ×

Filter

refSeq	Peptide	external_gene_name	X	sequence	part1
1 NP_000007	R.S*DPDPKAPANKA	ACADM	19163	MAAGGRCRCVLRISRFHWRSQHTKANRQREPLGFSFEFEQ...	S*DPDPKAPANKA
2 NP_000009	K.SDSHP5*DALTRK	ACADVL	10123	MQAARMAASLGRQLRLGGSSRLTALGGPRGPARRPVAGG...	S*DALTRK
3 NP_000012	R.S*LGHPEPLSNRPGQNSR.Q	PSEN1	16939	MTLPAPLSYFQNAQMSDNHLSNTVRSQNDNRERQEHNDRL...	S*LGHPEPLSNRPGQNSR.Q
4 NP_000012	R.AAVQELSS*S*ILAGEDPEER.G	PSEN1	16939	MTLPAPLSYFQNAQMSDNHLSNTVRSQNDNRERQEHNDRL...	S*ILAGEDPEER.G
5 NP_000012	R.S*LGHPEPLSNR.P	PSEN1	16939	MTLPAPLSYFQNAQMSDNHLSNTVRSQNDNRERQEHNDRL...	S*LGHPEPLSNR.P
6 NP_000012	K.Y*NAESTERESQDTVAENDDGGFSEWEAQR.D	PSEN1	16939	MTLPAPLSYFQNAQMSDNHLSNTVRSQNDNRERQEHNDRL...	Y*NAESTERESQDTVAENDDGGFSEWEAQR.D
7 NP_000012	R.AAVQELSS*S*ILAGEDPEER.G	PSEN1	16939	MTLPAPLSYFQNAQMSDNHLSNTVRSQNDNRERQEHNDRL...	S*S*ILAGEDPEER.G
8 NP_000015	R.FHVQNLS*QVEQDGR.T	ADRB2	19579	MGQGGNGSAFLAPNRSHAPDHDTQQRDEVWVVMGIVM...	S*QVEQDGR.T
9 NP_000022	K.SS*PAFGDR.R	ALAD	24018	MQPQSVLHSGYFHLRLAWQTATTILNASNLVPIFVTDVDDIQ...	S*PAFGDR.R
10 NP_000022	K.SS*PAFGDR.R	ALAD	24018	MQPQSVLHSGYFHLRLAWQTATTILNASNLVPIFVTDVDDIQ...	S*PAFGDR.R
11 NP_000028	R.ITHSP1*VS*QVTER.S	ANK1	936	MPYVSGFREDAATSFLRAARSGNLDKALDHRLNGVDINTCNQ...	T*VS*QVTER.S
12 NP_000028	R.LGVIS*VTDVLK.V	ANK1	936	MPYVSGFREDAATSFLRAARSGNLDKALDHRLNGVDINTCNQ...	S*VTDVLK.V
13 NP_000028	R.RDS*RDVDEEKE	ANK1	936	MPYVSGFREDAATSFLRAARSGNLDKALDHRLNGVDINTCNQ...	S*RDVDEEKE
14 NP_000028	K.NGAS*PNEVSSDGTTLPLAIK.R	ANK1	936	MPYVSGFREDAATSFLRAARSGNLDKALDHRLNGVDINTCNQ...	S*PNEVSSDGTTLPLAIK.R
15 NP_000028	K.LST*PPPLAEFGLASR.J	ANK1	936	MPYVSGFREDAATSFLRAARSGNLDKALDHRLNGVDINTCNQ...	T*PPPLAEFGLASR.J
16 NP_000028	K.LDQVVS*PAIRL.J	ANK1	936	MPYVSGFREDAATSFLRAARSGNLDKALDHRLNGVDINTCNQ...	S*PAIRL.J
17 NP_000028	R.TP1*PLAURL.Y	ANK1	936	MPYVSGFREDAATSFLRAARSGNLDKALDHRLNGVDINTCNQ...	T*PLAURL.Y
18 NP_000028	R.ITHS*PTVS*QVTER.S	ANK1	936	MPYVSGFREDAATSFLRAARSGNLDKALDHRLNGVDINTCNQ...	S*PTVS*QVTER.S
19 NP_000028	M.PYS*VGFRE	ANK1	936	MPYVSGFREDAATSFLRAARSGNLDKALDHRLNGVDINTCNQ...	S*VGFRE
20 NP_000028	R.ITHS*PTVS*QVTER.S	ANK1	936	MPYVSGFREDAATSFLRAARSGNLDKALDHRLNGVDINTCNQ...	S*PTVS*QVTER.S

Showing 1 to 21 of 72,504 entries. 6 total columns

Part 4

This file contains:

- The substring for all peptides with 2 *
- Saved this table as proteinsp2.txt

RStudio

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Go to file/function Addins

ex.R × part2 × ex2.R × ex3.R × combined × phosphogene × ex4.R × proteins × ex5.R × ex6.R × ex7.R × ex8.R × ex9.R ×

Filter

refSeq	Peptide	external_gene_name	X	sequence	part1	part2
1 NP_000007	R.S*DPDPKAPANKA	ACADM	19163	MAAGGRCRCVLRISRFHWRSQHTKANRQREPLGFSFEFEQ...	S*DPDPKAPANKA	NA
2 NP_000009	K.SDSHP5*DALTRK	ACADVL	10123	MQAARMAASLGRQLRLGGSSRLTALGGPRGPARRPVAGG...	S*DALTRK	NA
3 NP_000012	R.S*LGHPEPLSNRPGQNSR.Q	PSEN1	16939	MTLPAPLSYFQNAQMSDNHLSNTVRSQNDNRERQEHNDRL...	S*LGHPEPLSNRPGQNSR.Q	NA
4 NP_000012	R.AAVQELSS*S*ILAGEDPEER.G	PSEN1	16939	MTLPAPLSYFQNAQMSDNHLSNTVRSQNDNRERQEHNDRL...	S*ILAGEDPEER.G	NA
5 NP_000012	R.S*LGHPEPLSNR.P	PSEN1	16939	MTLPAPLSYFQNAQMSDNHLSNTVRSQNDNRERQEHNDRL...	S*LGHPEPLSNR.P	NA
6 NP_000012	K.Y*NAESTERESQDTVAENDDGGFSEWEAQR.D	PSEN1	16939	MTLPAPLSYFQNAQMSDNHLSNTVRSQNDNRERQEHNDRL...	Y*NAESTERESQDTVAENDDGGFSEWEAQR.D	NA
7 NP_000012	R.AAVQELSS*S*ILAGEDPEER.G	PSEN1	16939	MTLPAPLSYFQNAQMSDNHLSNTVRSQNDNRERQEHNDRL...	S*S*ILAGEDPEER.G	NA
8 NP_000015	R.FHVQNLS*QVEQDGR.T	ADRB2	19579	MGQGGNGSAFLAPNRSHAPDHDTQQRDEVWVVMGIVM...	S*QVEQDGR.T	NA
9 NP_000022	K.SS*PAFGDR.R	ALAD	24018	MQPQSVLHSGYFHLRLAWQTATTILNASNLVPIFVTDVDDIQ...	S*PAFGDR.R	NA
10 NP_000022	K.SS*PAFGDR.R	ALAD	24018	MQPQSVLHSGYFHLRLAWQTATTILNASNLVPIFVTDVDDIQ...	S*PAFGDR.R	NA
11 NP_000028	R.ITHSP1*VS*QVTER.S	ANK1	936	MPYVSGFREDAATSFLRAARSGNLDKALDHRLNGVDINTCNQ...	T*VS*QVTER.S	S*QVTER.S
12 NP_000028	R.LGVIS*VTDVLK.V	ANK1	936	MPYVSGFREDAATSFLRAARSGNLDKALDHRLNGVDINTCNQ...	S*VTDVLK.V	NA
13 NP_000028	R.RDS*RDVDEEKE	ANK1	936	MPYVSGFREDAATSFLRAARSGNLDKALDHRLNGVDINTCNQ...	S*RDVDEEKE	NA
14 NP_000028	K.NGAS*PNEVSSDGTTLPLAIK.R	ANK1	936	MPYVSGFREDAATSFLRAARSGNLDKALDHRLNGVDINTCNQ...	S*PNEVSSDGTTLPLAIK.R	NA
15 NP_000028	K.LST*PPPLAEFGLASR.J	ANK1	936	MPYVSGFREDAATSFLRAARSGNLDKALDHRLNGVDINTCNQ...	T*PPPLAEFGLASR.J	NA
16 NP_000028	K.LDQVVS*PAIRL.J	ANK1	936	MPYVSGFREDAATSFLRAARSGNLDKALDHRLNGVDINTCNQ...	S*PAIRL.J	NA
17 NP_000028	R.TP1*PLAURL.Y	ANK1	936	MPYVSGFREDAATSFLRAARSGNLDKALDHRLNGVDINTCNQ...	T*PLAURL.Y	NA
18 NP_000028	R.ITHS*PTVS*QVTER.S	ANK1	936	MPYVSGFREDAATSFLRAARSGNLDKALDHRLNGVDINTCNQ...	S*PTVS*QVTER.S	S*QVTER.S
19 NP_000028	M.PYS*VGFRE	ANK1	936	MPYVSGFREDAATSFLRAARSGNLDKALDHRLNGVDINTCNQ...	S*VGFRE	NA

Part 5

This file contains:

- From the part 1 and part 2 that we got, I remove the non alphanumeric characters: * and . and any -
- This will be saved as proteinsStripped.txt

rsite	external_gene_name	X	sequence	part1	part2	part1Stripped	part2Stripped
'D'PDKAPANKA	ACADM	19163	MAAGGRCRCVLSISRFHWSQHTKANRQREPGLGSEFTEQ...	S'DPDKAPANKA	NA	SDPDKAPANKA	NA
'S'HP'S'DALTRK	ACADVL	10123	MQAARMAASLGRQLRLGGSSRLTALLGQPRGPARRPVAGG...	S'DALTRK	NA	SDALTRK	NA
'L'GHPEPLSNGRPGQNSRQ	PSEN1	16939	MTLPAPLSYFQNAQMSDNHLSNTVRSQNDNRERQEHNDRR...	S'LGHPEPLSNGRPGQNSRQ	NA	SLGHPEPLSNGRPGQNSRQ	NA
'AVQELSS'S'ILAGEDPEER.G	PSEN1	16939	MTLPAPLSYFQNAQMSDNHLSNTVRSQNDNRERQEHNDRR...	S'ILAGEDPEER.G	NA	SILAGEDPEER.G	NA
'L'GHPEPLSNGR.P	PSEN1	16939	MTLPAPLSYFQNAQMSDNHLSNTVRSQNDNRERQEHNDRR...	S'LGHPEPLSNGR.P	NA	SLGHPEPLSNGR.P	NA
'YNAESTERESQDTVAENDGGFSEWEAQR.D	PSEN1	16939	MTLPAPLSYFQNAQMSDNHLSNTVRSQNDNRERQEHNDRR...	YNAESTERESQDTVAENDGGFSEWEAQR.D	NA	YNAESTERESQDTVAENDGGFSEWEAQR.D	NA
'AVQELSS'S'ILAGEDPEER.G	PSEN1	16939	MTLPAPLSYFQNAQMSDNHLSNTVRSQNDNRERQEHNDRR...	S'ILAGEDPEER.G	S'ILAGEDPEER.G	SSILAGEDPEER.G	SILAGEDPEER.G
'VQNL'S'QVEQDGR.T	ADRB2	19579	MGQPGNSGAFLLAPNRSHAPDHDTQGRDEVWVWGMGIVM...	S'QVEQDGR.T	NA	SQVEQDGR.T	NA
'S'PAFGDR.R	ALAD	24018	MQPQSVLHSGYFHPILRAWQTATTTLNASNLVPIFVTDVDDIQ...	S'PAFGDR.R	NA	SPAFGDRR	NA
'S'PAFGDR.R.C	ALAD	24018	MQPQSVLHSGYFHPILRAWQTATTTLNASNLVPIFVTDVDDIQ...	S'PAFGDR.R.C	NA	SPAFGDRRC	NA
'HSPT'S'QVTER.S	ANK1	936	MPYSVGFREADAATSFUAAARSGNLDKALDHLRNGVDINTCNQ...	T'S'QVTER.S	S'QVTER.S	TVSQVTER.S	SQVTER.S
'S'YIS'VTDVLK.V	ANK1	936	MPYSVGFREADAATSFUAAARSGNLDKALDHLRNGVDINTCNQ...	S'YIS'VTDVLK.V	NA	SVTDVLKV	NA
'DS'RDVDEEKE	ANK1	936	MPYSVGFREADAATSFUAAARSGNLDKALDHLRNGVDINTCNQ...	S'RDVDEEKE	NA	SRDVDEEKE	NA
'GAS'PNEVSSDGTTPLAIAKR	ANK1	936	MPYSVGFREADAATSFUAAARSGNLDKALDHLRNGVDINTCNQ...	S'PNEVSSDGTTPLAIAKR	NA	SPNEVSSDGTTPLAIAKR	NA
'T'PPPLAEEEGLASRJ	ANK1	936	MPYSVGFREADAATSFUAAARSGNLDKALDHLRNGVDINTCNQ...	S'PPPLAEEEGLASRJ	NA	TPPPLAEEEGLASRJ	NA
'DQVVS'PAIPRI	ANK1	936	MPYSVGFREADAATSFUAAARSGNLDKALDHLRNGVDINTCNQ...	S'PAIPRI	NA	SPAIPRI	NA
'T'PLALRY	ANK1	936	MPYSVGFREADAATSFUAAARSGNLDKALDHLRNGVDINTCNQ...	S'PLALRY	NA	TPLALRY	NA
'HS'PTVS'QVTER.S	ANK1	936	MPYSVGFREADAATSFUAAARSGNLDKALDHLRNGVDINTCNQ...	S'PTVS'QVTER.S	S'QVTER.S	SPTVSQVTER.S	SQVTER.S

Part 6

This file contains:

- Using the part1Stripped and part2Stripped columns that we just got, I get the amino acid position within the protein sequence
- This is saved as proteinsPositions.txt

part1	part2	part1Stripped	part2Stripped	part1Loc	part2Loc
S'DPDKAPANKA	NA	SDPDKAPANKA	NA	207	NULL
S'DALTRK	NA	SDALTRK	NA	57	NULL
S'LGHPEPLSNGRPGQNSRQ	NA	SLGHPEPLSNGRPGQNSRQ	NA	43	NULL
S'ILAGEDPEER.G	NA	SILAGEDPEER.G	NA	367	NULL
S'LGHPEPLSNGR.P	NA	SLGHPEPLSNGR.P	NA	43	NULL
YNAESTERESQDTVAENDGGFSEWEAQR.D	NA	YNAESTERESQDTVAENDGGFSEWEAQR.D	NA	315	NULL
S'ILAGEDPEER.G	S'ILAGEDPEER.G	SSILAGEDPEER.G	SILAGEDPEER.G	366	367
S'QVEQDGR.T	NA	SQVEQDGR.T	NA	246	NULL
S'PAFGDR.R	NA	SPAFGDRR	NA	215	NULL
S'PAFGDR.R.C	NA	SPAFGDRRC	NA	215	NULL
T'S'QVTER.S	S'QVTER.S	TVSQVTER.S	SQVTER.S	1688	1690
S'YIS'VTDVLK.V	NA	SVTDVLKV	NA	781	NULL
S'RDVDEEKE	NA	SRDVDEEKE	NA	834	NULL
S'PNEVSSDGTTPLAIAKR	NA	SPNEVSSDGTTPLAIAKR	NA	759	NULL
T'PPPLAEEEGLASRJ	NA	TPPPLAEEEGLASRJ	NA	961	NULL
S'PAIPRI	NA	SPAIPRI	NA	856	NULL
T'PLALRY	NA	TPLALRY	NA	1380	NULL
S'PTVS'QVTER.S	S'QVTER.S	SPTVSQVTER.S	SQVTER.S	1686	1690

Part 7

This file contains:

- I get the amino acid S, T, or Y and save it in amino 1 for the first one and amino2 for the second position
- This table is saved in proteinsAminos.txt

RStudio

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ex.R x part2 x ex2.R x ex3.R x combined x phosphogene x ex4.R x proteins x ex5.R x ex6.R x ex7.R x proteins x proteins x ex8.R x ex9.R x

Filter

part1	part2	part1Stripped	part2Stripped	part1Loc	part2Loc	amino1	amino2	pos1	pos2	dash	site
ANRQREPLGLGSFFETEQ...	S*DPPDKAPANKA	SODPKAPANKA	NA	207	NULL	S	NULL	S207	NA	-	ACADM-S207
LLGQPRPGPARPRVAGG...	S*DALTRK	SDALTRK	NA	57	NULL	S	NULL	S57	NA	-	ACADVL-S57
RSQNDNRRQEHNDRR...	S*LGHPEPLSNGRPQNSRQ	SLGHPEPLSNGRPQNSRQ	NA	43	NULL	S	NULL	S43	NA	-	PSEN1-S43
RSQNDNRRQEHNDRR...	S*ILAGEDPEER.G	SILAGEDPEER.G	NA	367	NULL	S	NULL	S367	NA	-	PSEN1-S367
RSQNDNRRQEHNDRR...	S*LGHPEPLSNGRP	SLGHPEPLSNGRP	NA	43	NULL	S	NULL	S43	NA	-	PSEN1-S43
RSQNDNRRQEHNDRR...	Y*NAESTERESQDTVAENDDGGFSEWEAQRD	YNAESTERESQDTVAENDDGGFSEWEAQRD	NA	315	NULL	Y	NULL	Y315	NA	-	PSEN1-Y315
RSQNDNRRQEHNDRR...	S*SIILAGEDPEER.G	SSIILAGEDPEER.G	SILAGEDPEER.G	366	367	S	S	S366	S367	-	PSEN1-S366S367
QQRDEVVWVGMGIVM...	S*QVEQDGR.T	SQVEQDGR.T	NA	246	NULL	S	NULL	S246	NA	-	ADRB2-S246
VASNLVPIFVTDVPDDIQ...	S*PAFGDR.R	SPAFGDRR	NA	215	NULL	S	NULL	S215	NA	-	ALAD-S215
VASNLVPIFVTDVPDDIQ...	S*PAFGDRR.C	SPAFGDRRC	NA	215	NULL	S	NULL	S215	NA	-	ALAD-S215
ALDHLRNGVDINTCNQ...	T*VS*QVTERS	TVSQVTERS	SQVTERS	1688	1690	T	S	T1688	S1690	-	ANK1-T1688S1690
ALDHLRNGVDINTCNQ...	S*VTDVLK.V	SVTDVLKV	NA	781	NULL	S	NULL	S781	NA	-	ANK1-S781
ALDHLRNGVDINTCNQ...	S*RDVDEEKE	SRDVDEEKE	NA	834	NULL	S	NULL	S834	NA	-	ANK1-S834
ALDHLRNGVDINTCNQ...	S*PNEVSSDGTPLAIK.R	SPNEVSSDGTPLAIK.R	NA	759	NULL	S	NULL	S759	NA	-	ANK1-S759
ALDHLRNGVDINTCNQ...	T*PPPLAEEGLASRI	TPPPLAEEGLASRI	NA	961	NULL	T	NULL	T961	NA	-	ANK1-T961
ALDHLRNGVDINTCNQ...	S*PAIPRI	SPAIPRI	NA	856	NULL	S	NULL	S856	NA	-	ANK1-S856
ALDHLRNGVDINTCNQ...	T*PLALR.Y	TPLALRY	NA	1380	NULL	T	NULL	T1380	NA	-	ANK1-T1380
ALDHLRNGVDINTCNQ...	S*PTVS*QVTERS	SPTVSQVTERS	SQVTERS	1686	1690	S	S	S1686	S1690	-	ANK1-S1686S1690
ALDHLRNGVDINTCNQ...	S*QVTERS	SQVTERS	NA	1	NA	S	NA	S1	NA	-	ANK1-S1

Showing 1 to 19 of 72,504 entries. 17 total columns

Part 10

This file contains:

- Asks user for input: The geneld
- Saves the input in a txt file called input.txt

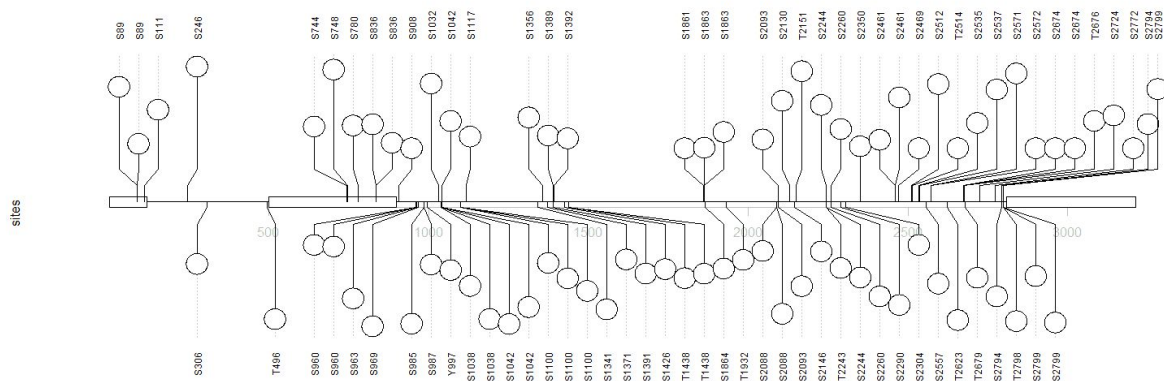
Part 11

This file contains:

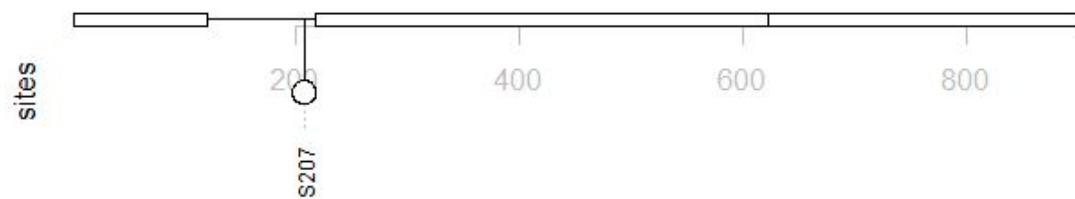
- The visualization

Below is an example for APC and ACADM (Also attached as png for clarity)

APC:



ACADM



What I learned:

- Bioconductor library for R and its various libraries and how they can be used for bioinformatics and gene mapping
- How to find position of substring in string
- How to create gene map visualizations using lollipop plots
- How to handle large datasets
- I got more experience with R