Open for Innovation
KNIME

KNIME Pros Learnathon

Building Reliable and Reusable Components

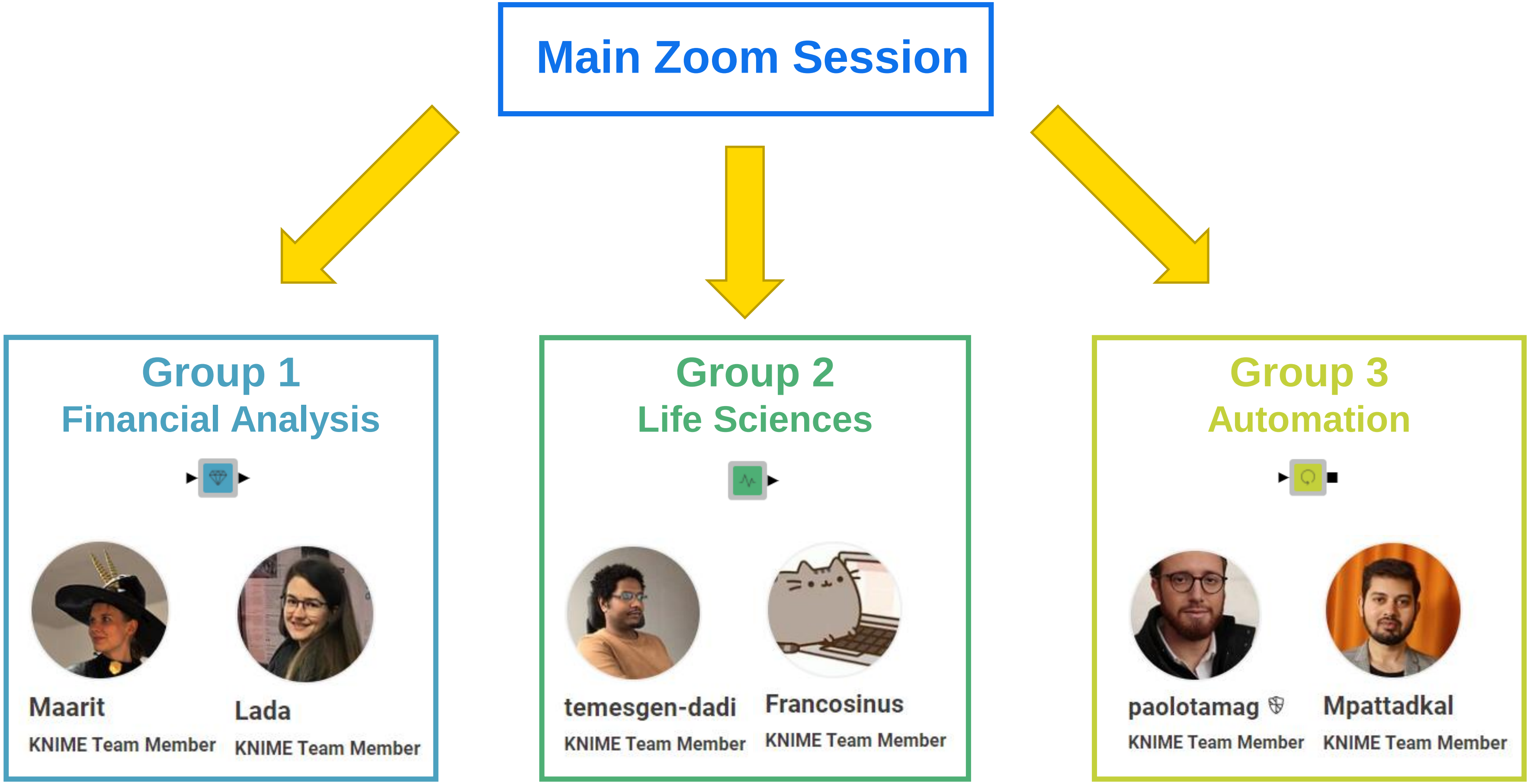
Group 2: Life Sciences

KNIME Team

@KNIME
#Learnathon

tinyurl.com/KNIME-Pros-Stuff

See you soon in a Breakout Room!



Main Zoom Session

Group 1
Financial Analysis

Maarit
KNIME Team Member

Lada
KNIME Team Member

Group 2
Life Sciences

temesgen-dadi
KNIME Team Member

Francosinus
KNIME Team Member

Group 3
Automation

paolotamag
KNIME Team Member

Mpattadkal
KNIME Team Member

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Three Parallel Tracks via Zoom Breakout Rooms!

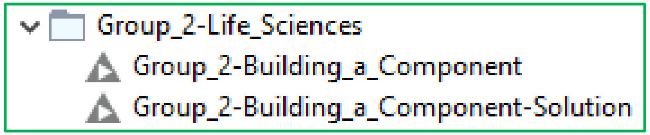
Main Zoom Session

Welcome to:
Group 2.
Life Sciences

Group 2
Life Sciences

temesgen-dadi
KNIME Team Member

Francosinus
KNIME Team Member



Group_2-Life_Sciences
- Group_2-Building_a_Component
- Group_2-Building_a_Component-Solution

- Download exercises from:
  tinyurl.com/KNIME-Pros-Stuff

OR

- Search **hub.knime.com** :
  “KNIME Pros Learnathon Group 2”

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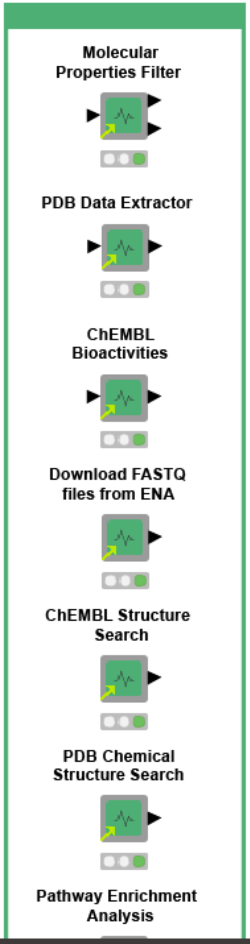
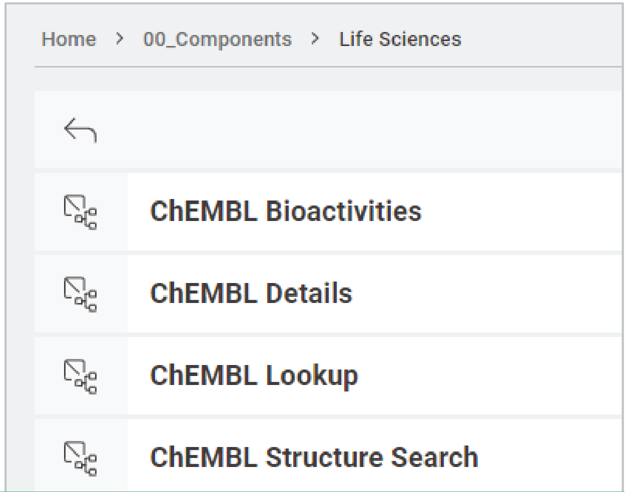
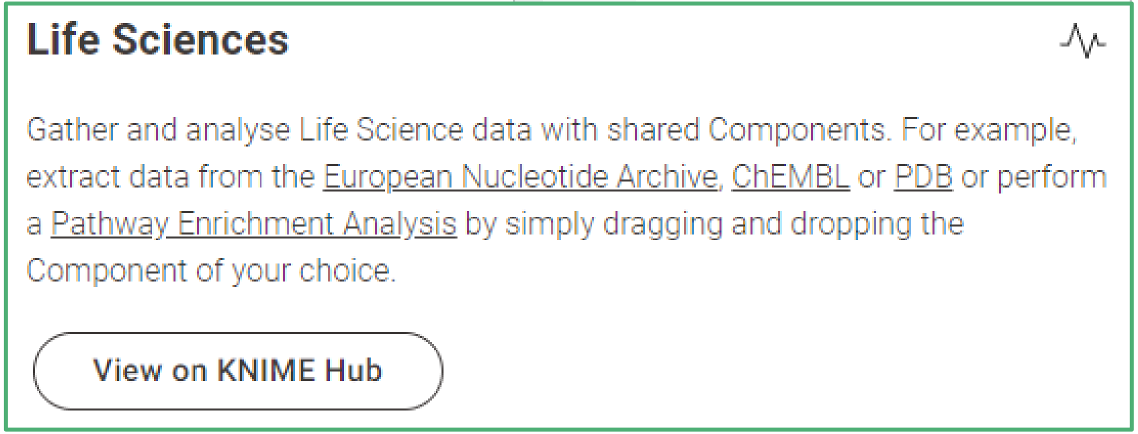
Life Sciences Verified Components


Molecular Properties Filter
PDB Data Extractor
ChEMBL Bioactivities
Download FASTQ files from ENA
ChEMBL Structure Search
PDB Chemical Structure Search
Pathway Enrichment Analysis

Available on hub.knime.com



- ChEMBL Bioactivities
- ChEMBL Details
- ChEMBL Lookup
- ChEMBL Structure Search

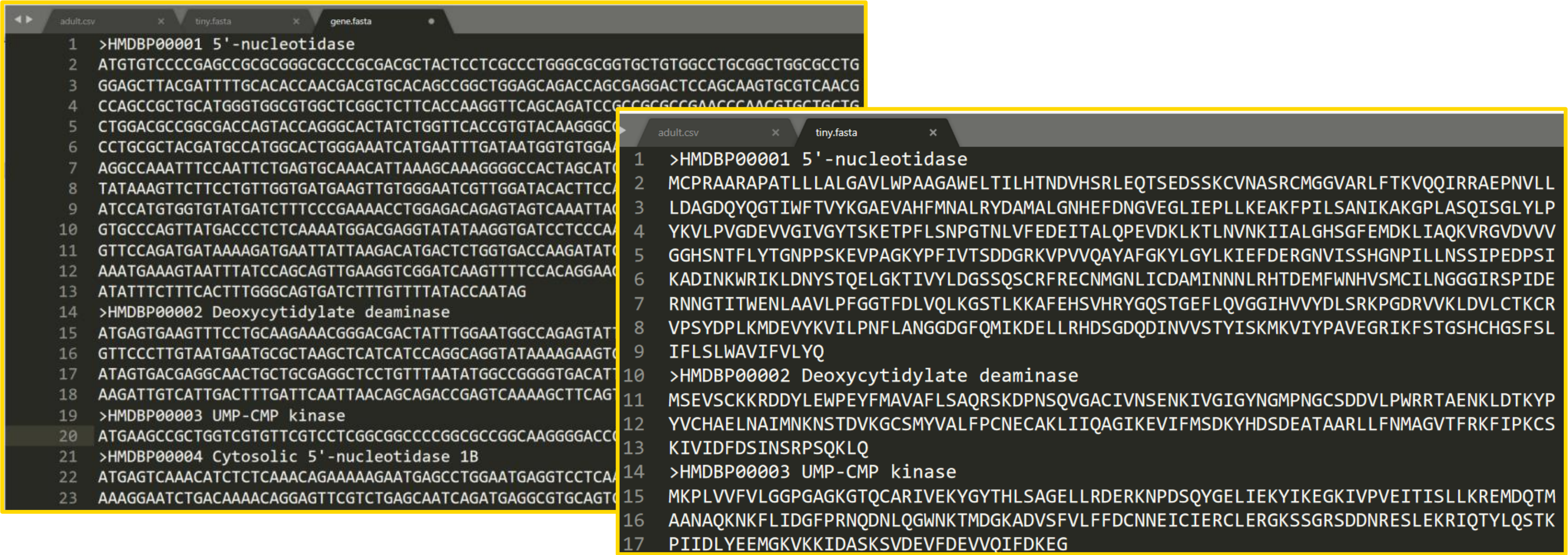


Life Sciences

Gather and analyse Life Science data with shared Components. For example, extract data from the European Nucleotide Archive, ChEMBL or PDB or perform a Pathway Enrichment Analysis by simply dragging and dropping the Component of your choice.

FASTA File Format

- common file format in bioinformatics and biochemistry
- text-based format for representing either nucleotide sequences or amino acid (protein) sequences
- allows for sequence names and comments to precede the sequences



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CTGGACGCCGGCGACCAGTACCAGGGCACTATCTGGTTCACCGTGTACAAGGGCC
CCTGCGCTACGATGCCATGGCACTGGGAAATCATGAATTTGATAATGGTGTGGAA
AGGCCAAATTTCCAATTCTGAGTGCAAACATTAAAGCAAAGGGGCCACTAGCATC
TATAAAGTTCTTCCTGTTGGTGATGAAGTTGTGGGAATCGTTGGATACACTTCCA
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AAATGAAAGTAATTTATCCAGCAGTTGAAGGTCGGATCAAGTTTTCCACAGGAAC
ATATTTCTTTCACTTTGGGCAGTGATCTTTGTTTTATACCAATAG
>HMDBP00002 Deoxycytidylate deaminase
ATGAGTGAAGTTTCCTGCAAGAAACGGGACGACTATTTGGAATGGCCAGAGTATT
GTTCCCTTGTAATGAATGCGCTAAGCTCATCATCCAGGCAGGTATAAAAGAAGTC
ATAGTGACGAGGCAACTGCTGCGAGGCTCCTGTTTAATATGGCCGGGGTGACATT
AAGATTGTCATTGACTTTGATTCAATTAACAGCAGACCGAGTCAAAAGCTTCAGT
>HMDBP00003 UMP-CMP kinase
ATGAAGCCGCTGGTCGTGTTCGTCCTCGGCGGCCCCGGCGCCGGCAAGGGGACCC
>HMDBP00004 Cytosolic 5'-nucleotidase 1B
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```

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YKVLPVGDEVVGIVGYTSKETPFLSNPGTNLVFEDEITALQPEVDKLKTLNVNKIIALGHSGFEMDKLIAQKVRGVDVVV
GGHSNTFLYTGNPPSKEVPAGKYPFIVTSDDGRKVPVVQAYAFGKYLGYLKIEFDERGNVISSHGNPILLNSSIPEDPSI
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RNNGTITWENLAAVLPFGGTFDLVQLKGSTLKKAFEHSVHRYGQSTGEFLQVGGIHVVYDLSRKPGDRVVKLDVLCTKCR
VPSYDPLKMDEVYKVILPNFLANGGDGFQMIKDELLRHDSGDQDINVVSTYISKMKVIYPAVEGRIKFSTGSHCHGSFSL
IFLSLWAVIFVLYQ
>HMDBP00002 Deoxycytidylate deaminase
MSEVSCKKRDDYLEWPEYFMAVAFLSAQRSKDPNSQVGACIVNSENKIVGIGYNGMPNGCSDDVLPWRRTAENKLDTKYP
YVCHAELNAIMNKNSTDVKGCSMYVALFPCNECAKLIIQAGIKEVIFMSDKYHDSDEATAARLLFNMAGVTFRKFIPKCS
KIVIDFDSINSRPSQKLQ
>HMDBP00003 UMP-CMP kinase
MKPLVVFVLGGPGAGKGTQCARIVEKYGYTHLSAGELLRDERKNPDSQYGELIEKYIKEGKIVPVEITISLLKREMDQTM
AANAQKNKFLIDGFPRNQDNLQGWNKTMDGKADVSFVLFFDCNNEICIERCLERGKSSGRSDDNRESLEKRIQTYLQSTK
PIIDLYEEMGKVKKIDASKSVDEVFDEVVQIFDKEG
```

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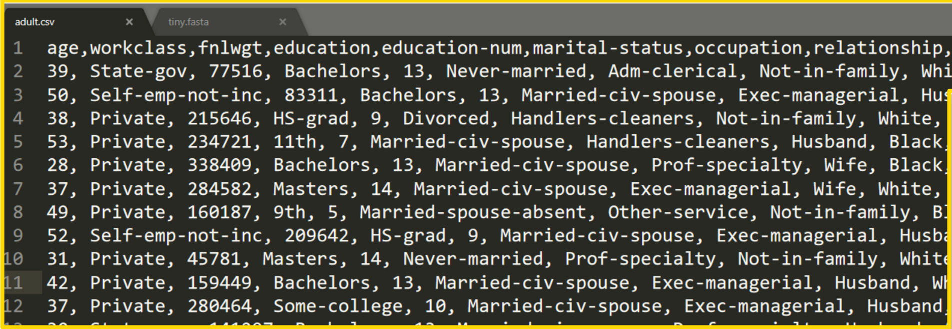
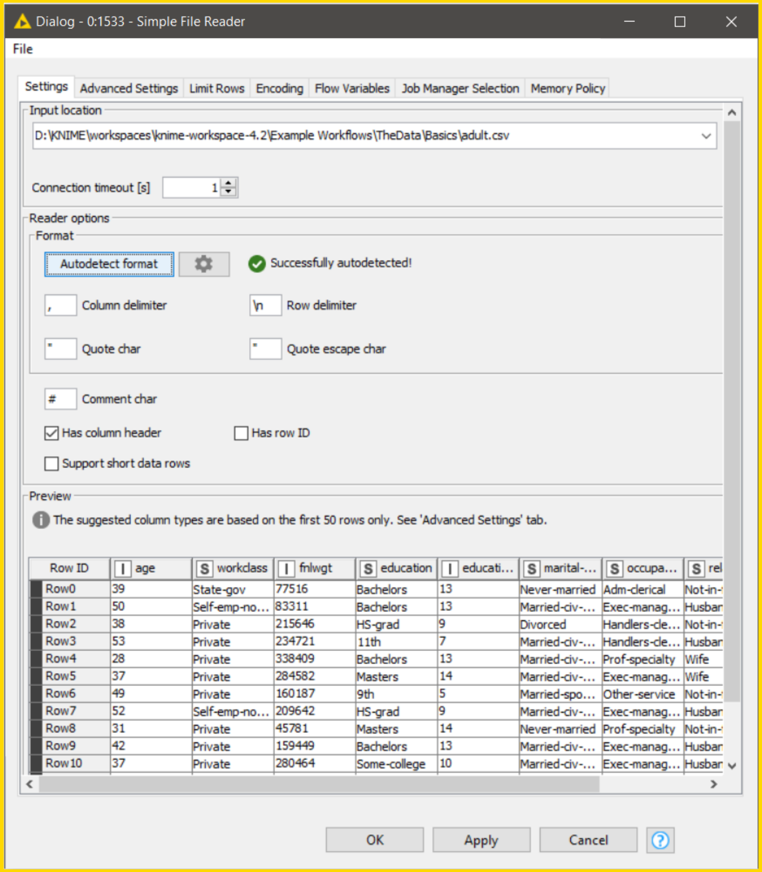
KNIME Nodes (File Readers)



adult.csv tiny.fasta

```
age,workclass,fnlwgt,education,education-num,marital-status,occupation,relationship,race,sex,capital-gain,capital-loss,hours-per-week,native-country,income
39, State-gov, 77516, Bachelors, 13, Never-married, Adm-clerical, Not-in-family, White, Male, 2174, 0, 40, United-States, <=50K
50, Self-emp-not-inc, 83311, Bachelors, 13, Married-civ-spouse, Exec-managerial, Hus
38, Private, 215646, HS-grad, 9, Divorced, Handlers-cleaners, Not-in-family, White,
53, Private, 234721, 11th, 7, Married-civ-spouse, Handlers-cleaners, Husband, Black
28, Private, 338409, Bachelors, 13, Married-civ-spouse, Prof-specialty, Wife, Black
37, Private, 284582, Masters, 14, Married-civ-spouse, Exec-managerial, Wife, White,
49, Private, 160187, 9th, 5, Married-spouse-absent, Other-service, Not-in-family, Bl
52, Self-emp-not-inc, 209642, HS-grad, 9, Married-civ-spouse, Exec-managerial, Husba
31, Private, 45781, Masters, 14, Never-married, Prof-specialty, Not-in-family, White
42, Private, 159449, Bachelors, 13, Married-civ-spouse, Exec-managerial, Husband, Wh
37, Private, 280464, Some-college, 10, Married-civ-spouse, Exec-managerial, Husband
```



Dialog - 0:1533 - Simple File Reader

File

Settings | Advanced Settings | Limit Rows | Encoding | Flow Variables | Job Manager Selection | Memory Policy

Input location

D:\KNIME\workspaces\knime-workspace-4.2\Example Workflows\TheData\Basics\adult.csv

Connection timeout [s] 1

Reader options

Format

Autodetect format ✓ Successfully autodetected!

Column delimiter: ,

Row delimiter: \n

Quote char: "

Quote escape char: "

Comment char: #

☑ Has column header ☐ Has row ID

☐ Support short data rows

Preview

The suggested column types are based on the first 50 rows only. See 'Advanced Settings' tab.

Row ID	I age	S workclass	I fnlwgt	S education	I educati...	S marital-...	S occupa...	S rel
Row0	39	State-gov	77516	Bachelors	13	Never-married	Adm-clerical	Not-in-
Row1	50	Self-emp-no...	83311	Bachelors	13	Married-civ-...	Exec-manag...	Husbar
Row2	38	Private	215646	HS-grad	9	Divorced	Handlers-cle...	Not-in-
Row3	53	Private	234721	11th	7	Married-civ-...	Handlers-cle...	Husbar
Row4	28	Private	338409	Bachelors	13	Married-civ-...	Prof-specialty	Wife
Row5	37	Private	284582	Masters	14	Married-civ-...	Exec-manag...	Wife
Row6	49	Private	160187	9th	5	Married-spo...	Other-service	Not-in-
Row7	52	Self-emp-no...	209642	HS-grad	9	Married-civ-...	Exec-manag...	Husbar
Row8	31	Private	45781	Masters	14	Never-married	Prof-specialty	Not-in-
Row9	42	Private	159449	Bachelors	13	Married-civ-...	Exec-manag...	Husbar
Row10	37	Private	280464	Some-college	10	Married-civ-...	Exec-manag...	Husbar

OK
Apply
Cancel

File Reader **CSV Reader** **CSV Reader (Labs)** **Simple File Reader**

- Well suited to read tabular data

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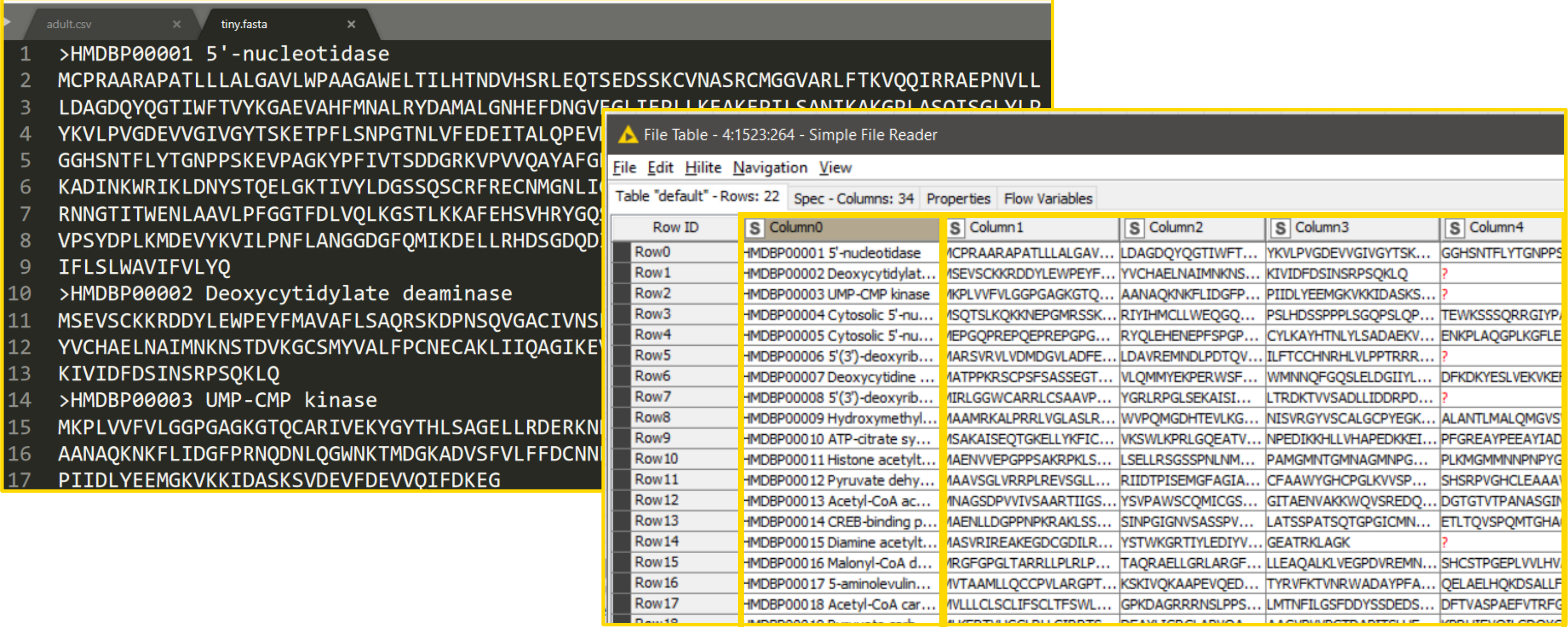
FASTA File as Tabular Data


adult.csv
tiny.fasta
File Table - 4:1523:264 - Simple File Reader
File Edit Hilite Navigation View
Table "default" - Rows: 22
Spec - Columns: 34
Properties
Flow Variables

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>HMDBP00001 5'-nucleotidase
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YKVLPVGDEVVGIVGYTSKETPFLSNPGTNLVFEDEITALQPEV
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RNNGTITWENLAAVLPFGGTFDLVQLKGSTLKKAFEHSVHRYGQ
VPSYDPLKMDEVYKVILPNFLANGGDGFQMIKDELLRHDSGDQD
IFLSLWAVIFVLYQ
>HMDBP00002 Deoxycytidylate deaminase
MSEVSCKKRDDYLEWPEYFMAVAFLSAQRSKDPNSQVGACIVNS
YVCHAELNAIMNKNSTDVKGCSMYVALFPCNECAKLIIQAGIKE
KIVIDFDSINSRPSQKLQ
>HMDBP00003 UMP-CMP kinase
MKPLVVFVLGGPGAGKGTQCARIVEKYGYTHLSAGELLRDERKN
AANAQKNKFLIDGFPRNQDNLQGWNKTMDGKADVSFVLFFDCNN
PIIDLYEEMGKVKKIDASKSVDEVFDEVVQIFDKEG
```

Row ID	S Column0	S Column1	S Column2	S Column3	S Column4
Row0	HMDBP00001 5'-nucleotidase	MCPRAARAPATLLLALGAV...	LDAGDQYQGTIWFT...	YKVLPVGDEVVGIVGYTSK...	GGHSNTFLYTGNPPS
Row1	HMDBP00002 Deoxycytidylat...	MSEVSCKKRDDYLEWPEYF...	YVCHAELNAIMNKNS...	KIVIDFDSINSRPSQKLQ	?
Row2	HMDBP00003 UMP-CMP kinase	MKPLVVFVLGGPGAGKGTQ...	AANAQKNKFLIDGFP...	PIIDLYEEMGKVKKIDASKS...	?
Row3	HMDBP00004 Cytosolic 5'-nu...	MSQTSLKQKKNEPGMRSSK...	RIYIHMCLLWEQGQ...	PSLHDSSPPPLSGQPSLQP...	TEWKSSSQRRGIYPA
Row4	HMDBP00005 Cytosolic 5'-nu...	MEPGQPREPQEPREPGPG...	RYQLEHENEPFSPGP...	CYLKAYHTNLYLSADAEKV...	ENKPLAQGPLKGFLE
Row5	HMDBP00006 5'(3')-deoxyrib...	MARSVRVLVDMDGVLADFE...	LDAVREMNDLPDTQV...	ILFTCCHNRHLVLPPTRRR...	?
Row6	HMDBP00007 Deoxycytidine ...	MATPPKRSCPSFSASSEGT...	VLQMMYEKPERWSF...	WMNNQFGQSLELDGIIYL...	DFKDKYESLVEKVKEI
Row7	HMDBP00008 5'(3')-deoxyrib...	MIRLGGWCARRLCSAAVP...	YGRLRPGLSEKAISI...	LTRDKTVVSADLLIDDRPD...	?
Row8	HMDBP00009 Hydroxymethyl...	MAAMRKALPRRLVGLASLR...	WVPQMGDHTEVLKG...	NISVRGYVSCALGCPYEGK...	ALANTLMALQMGVSV
Row9	HMDBP00010 ATP-citrate sy...	MSAKAISEQTGKELLYKFIC...	VKSWLKPRLGQEATV...	NPEDIKKHLLVHAPEDKKEI...	PFGREAYPEEAYIAD
Row10	HMDBP00011 Histone acetylt...	MAENVVEPGPPSAKRPKLS...	LSELLRSGSSPNLNM...	PAMGMNTGMNAGMNPG...	PLKMGMMNNPNPYG
Row11	HMDBP00012 Pyruvate dehy...	MAAVSGLVRRPLREVSGLL...	RIIDTPISEMGFAGIA...	CFAAWYGHCPGLKVVSP...	SHSRPVGHCLEAAAV
Row12	HMDBP00013 Acetyl-CoA ac...	MNAGSDPVVIVSAARTIIGS...	YSVPAWSCQMICGS...	GITAENVAKKWQVSREDQ...	DGTGTVTPANASGIN
Row13	HMDBP00014 CREB-binding p...	MAENLLDGPPNPKRAKLSS...	SINPGIGNVSASSPV...	LATSSPATSQTGPGICMN...	ETLTQVSPQMTGHAG
Row14	HMDBP00015 Diamine acetylt...	MASVRIREAKEGDCGDILR...	YSTWKGRTIYLEDIYV...	GEATRKLAGK	?
Row15	HMDBP00016 Malonyl-CoA d...	MRGFGPGLTARRLLPLRLP...	TAQRAELLGRLARGF...	LLEAQALKLVEGPDVREMN...	SHCSTPGEPLVVLHVA
Row16	HMDBP00017 5-aminolevulin...	MVTAAMLLQCCPVLARGPT...	KSKIVQKAAPEVQED...	TYRVFKTVNRWADAYPFA...	QELAELHQKDSALLF
Row17	HMDBP00018 Acetyl-CoA car...	MVLLLCLSCLIFSCLTFSWL...	GPKDAGRRRNSLPPS...	LMTNFILGSFDDYSSDEDS...	DFTVASPAEFVTRFG

SequenceID

← Sequence →

- Re-think Row/Column delimiters
  - “>” Row delimitr
  - “\n” Column delimeter

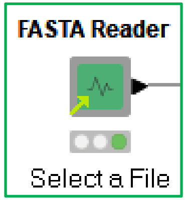
Today’s Challenge: FASTA Reader Component

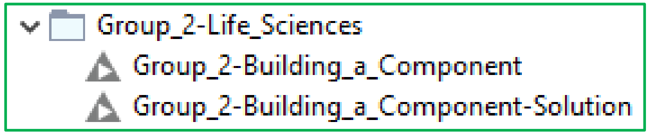
- Download Exercises from **link** and import .knar file to your KNIME Analytics Platform LOCAL Workspace!

OR

- Download from KNIME Hub!

hub.knime.com/knime/spaces/Education/latest/Learnathons
or Search for “**KNIME Pros Learnathon - Group 2**”

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