**Pathway Tools Navigator Tutorial Script**

**Desktop Mode**

**To the Instructor:**

 The Navigator tutorial is done via live demonstration on the desktop software.

 Rather than strictly script your exact words, each section lists information you need to convey and actions to demonstrate.

 One way to slow down a bit and enhance clarity is to clearly announce what you are clicking on, and whether you are right or left clicking.

 It’s also helpful to the tutorial participants if you mouse over any item you’re discussing, and perhaps change your mouse cursor to make it easier to see.

**-- Pathway Tools Navigator tutorial script starts here --**

Start on the Pathway Tools all-organisms (Home) page:

***All organisms page***

Select *E. coli* as current organism.

Select MetaCyc and back again

***Organism summary page***

Click on EcoCyc.

 Organism summary page lists info like authors, taxonomy, summary of stats

 Remember that each line is clickable

 Click on the Pathways link

*Current organism.*

 “Current organism” selector chooses where your searches look

 The “current organism” can be different from the one in the frame you’re currently on

 Easy way to search into another organism without backing up to list of organisms

***Protein page***

Go to page for enzyme adenosine phosphorylase/DeoD

* + Get sequence
	+ Show TU for deoCp2
	+ Show DeoR protein page (from Reg Summary diagram of DeoD)

 Buttons for nucleotide sequence, protein sequence, and “advanced nucleotide sequence” that lets you get nearby sequence – good for PCR primers

 Unification and other links – ways to crosslink to relevant resources, such as PDB if the protein has a crystal structure

 Summary

*Gene-regulation schematic*

*Gene-reaction schematic*

 This shows the relationship between genes, proteins, and reactions

 Purple boxes are genes, circles are proteins, blue boxes are reactions

 Get a second set of boxes, with a number, for a multimer

 A fast way of seeing how genes, proteins, and reactions relate

 Below the gene-reaction schematic, we have GO terms and essentiality data

*Enzymatic reactions*

 Enzymatic reactions capture how *this* specific enzyme carries out a *general* reaction

 It’s where we have Kms, cofactors, and regulators that are specific to this enzyme

 This is how we can capture different regulatory or other data for isozymes, for example

 Also where we have the evidence code

*Protein search*

Protein Curation Search

 Protein Search by Modulation

Protein Advanced Search

* + Search for proteins with 100<MW<200 and 10<pI
	+ Search for proteins in the periplasm
	+ Search for proteins with lipid binding sites
		- Adv Search > Features > Amino-Acid-Sites-That-Bind > Lipid-Binding-Sites
	+ Search for proteins with metal binding sites
	+ Search for proteins with L-arginine as a ligand
		- Adv Search > Ligand > L-arginine

*Evidence codes*

 You’ll see these icons across the database

 Indicate how we know what we know

 A flask means experimental evidence, a computer means it was predicted, a book means “We think this is true, but can’t link it to other evidence”

 There are lots of types of evidence – for example, from a purified protein *in vitro* versus inferred from a mutant phenotype

***Gene searches, RNA searches***

 Can search for genes and RNAs by the usual methods

 Remember that gene searches will take you to combined gene/protein pages

*Genetic information*

 Search genes for argC

 Click on argCBG TU

 This is a transcription unit – most of the time, that’s the same as an operon

 Shows the genes in their local context, with transcription factors

 Promoters, transcription factor bindings sites, evidence for regulatory interactions

 Search genes by GO term; expand Biological Process, select Locomotion

 Gene Advanced Search: search for RNA genes less than 200 nucleotides in length

***Compound search***

 Two universal searches – by name or object ID, and by substring

 Search by exact name for “adenine”

*Compound page*

 Show the compound names, structure, molecular formula

 Collects links to literally everywhere the compound appears in the database, whether that’s in reactions or as regulators or cofactors

 InChI and SMILES are text codings for organic molecules – can be handy for searching for “features” like an aromatic ring

***Pathway search***

 Search pathway “adenine and adenosine salvage V” via substring “adenine”

*What’s in a pathway page*

 We show pathway with major intermediates and all the reaction steps

 Can zoom in and out

 Zoom in – see side compounds, names of enzymes and associated genes

 Zoom in again – see structure for those side compounds

 Can also zoom all the way out to see the “conceptual” pathway

 Useful if you mainly care about the pathway as a whole, like for regulation

 Feedback regulation shown via lines

 The +/- shows what the regulating factor does

*Genetic regulation schematic*

 At the bottom of the page, genetic regulation schematic

 Shows all the genetic regulation that controls the genes for this pathway

 Genes grouped by operon

 This is a one-stop, at-a-glance view of regulation

 For complex features like this, note the question mark icon

 Click on the question mark to get a full explanation of that feature

***Reaction page***

 Click on first rxn (2.4.2.1) in previous pathway “pathway adenine and adenosine salvage V”

 Lists pathways the reaction is involved in, and enzymes carrying out the reaction

 Note that reactions *just* show the molecular transformation

 Details about how specific enzymes do the reaction live with those enzymes

 In other words, reaction frame shows the molecular change, but the enzyme will talk about things like Kms, Kcats, and so forth

*Reaction search*

 Can search by name or substring, as before

 Search by E.C. number

 Search by pathway (Biosyn > … L-tryptophan biosynthesis)

 Search by substrates (left: L-methionine ; right: S-adenosyl-methionine)

 Show use of Answer List

 Then use history list to go back to 2.4.2.1

***Multi-Organism Search***

 Select organisms in Altered Schaedler Flora

 Protein search: biotin synthase

 Compound: spermidine

 Pathway: tryptophan