**Pathway Tools Navigator Tutorial Script**

**Web Mode**

**To the Instructor:**

 The Navigator tutorial is done via live demonstration on the BioCyc.org site.

 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 --**

***Database selection***

Ways to select an organism:

* Start on BsubCyc.org
* “Sites” menu at top of page
* [Change Current Database] button
	+ Review the basic selection mechanisms
	+ Select *E. coli* as current organism for rest of demo

***Organism summary page***

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

***Gene/Protein page***

Quicksearch for adenosine phosphorylase or deoD

* + Review tabs with different information types
		- Operon tab – click on deoCp2
	+ Evidence codes
	+ Gene-regulation schematic -- click on DeoR
	+ Gene-reaction schematic
	+ Get sequence
		- Show both protein and nucleotide
		- Explain right-sidebar menu

*Enzymatic reactions*

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

 Kms, cofactors, and regulators that are specific to this enzyme

*Protein advanced search*

* + Search for proteins with 100<MW<200 and 10<pI
	+ Search for proteins with Lipid binding sites
		- [search/filter by protein features -> Lipid-Binding-Sites]
	+ Search for proteins by GO term: biological process -> biological adhesion
	+ Search for proteins with L-arginine as a ligand

***Compound search and compound page***

 Quicksearch area

 Search by exact name for “adenine”

*Compound page*

 Show the compound names, structure, molecular formula

 Shows links to 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

**Layout of BioCyc Pages**

 Point out top menu bar

Point out tabs on compound page or gene page

***Pathway search and pathway page***

 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

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

 Zoom in again – see structure for those side compounds

 Turn on display of regulatory information

**Quick Search – more detail**

 Items that can be entered to Quick Search:

* Name or substring for a
	+ Compound
	+ Gene
	+ Protein
	+ Pathway
* Identifier from BioCyc, UniProt, KEGG, ChEBI
* GenBank locus-id

 Quick search results grouped by object type

***Multi-Organism Search***

 Go into Search > Genes/Proteins/RNAs, click box next to “Search across multiple organisms/genomes”

 Select organisms in Altered Schaedler Flora

 Protein search: biotin synthase

 Compound: spermidine

 Pathway: tryptophan

***BLAST Search***

Search against *E. coli*:

MVKERKTELV EGFRHSVPYI NTHRGKTFVI MLGGEAIEHE NFSSIVNDIG LLHSLGIRLV

VVYGARPQID ANLAAHHHEP LYHKNIRVTD AKTLELVKQA AGTLQLDITA RLSMSLNNTP

LQGAHINVVS GNFIIAQPLG VDDGVDYCHS GRIRRIDEDA IHRQLDSGAI VLMGPVAVSV

TGESFNLTSE EIATQLAIKL KAEKMIGFCS SQGVTNDDGD IVSELFPNEA QARVEAQEEK

GDYNSGTVRF LRGAVKACRS GVRRCHLISY QEDGALLQEL FSRDGIGTQI VMESAEQIRR

ATINDIGGIL ELIRPLEQQG ILVRRSREQL EMEIDKFTII QRDNTTIACA ALYPFPEEKI

GEMACVAVHP DYRSSSRGEV LLERIAAQAK QSGLSKLFVL TTRSIHWFQE RGFTPVDIDL

LPESKKQLYN YQRKSKVLMA DLG

***Sequence Pattern Search***