The Pathway Tools Software in 2009: Supplementary Figures

Some of the figures herein are difficult to read at low magnification settings. We recommend that the reader increase the magnification of their PDF viewer to approximatly 300% to read figures such as Supplementary Figure 3.

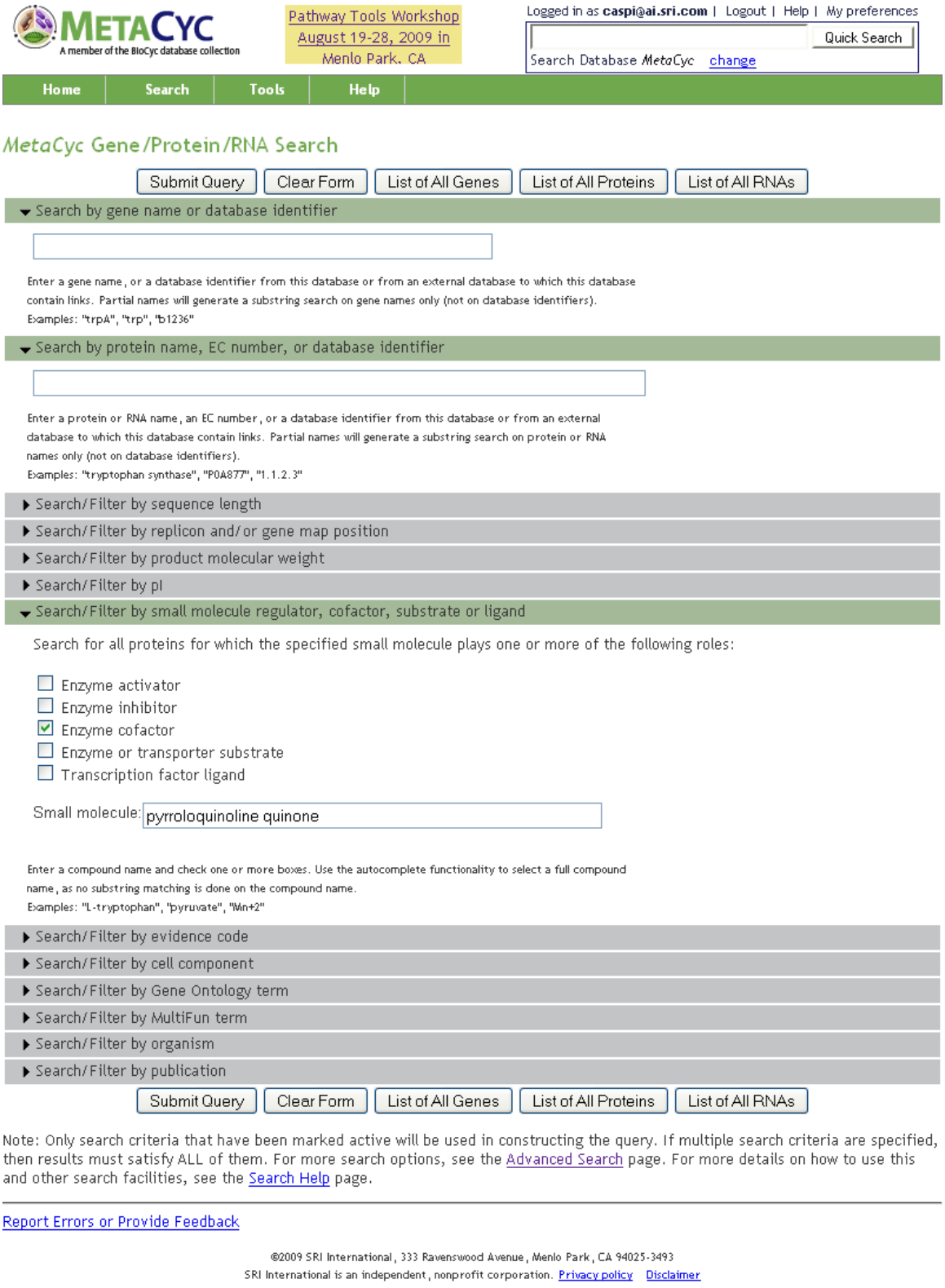


Figure 1: Object-specific query tool for genes, proteins, and RNAs. The user selects which query fields are active by clicking on the triangles to the left. In this example the user is searching for proteins that contain a PQQ (pyrroloquinoline quinone) cofactor.

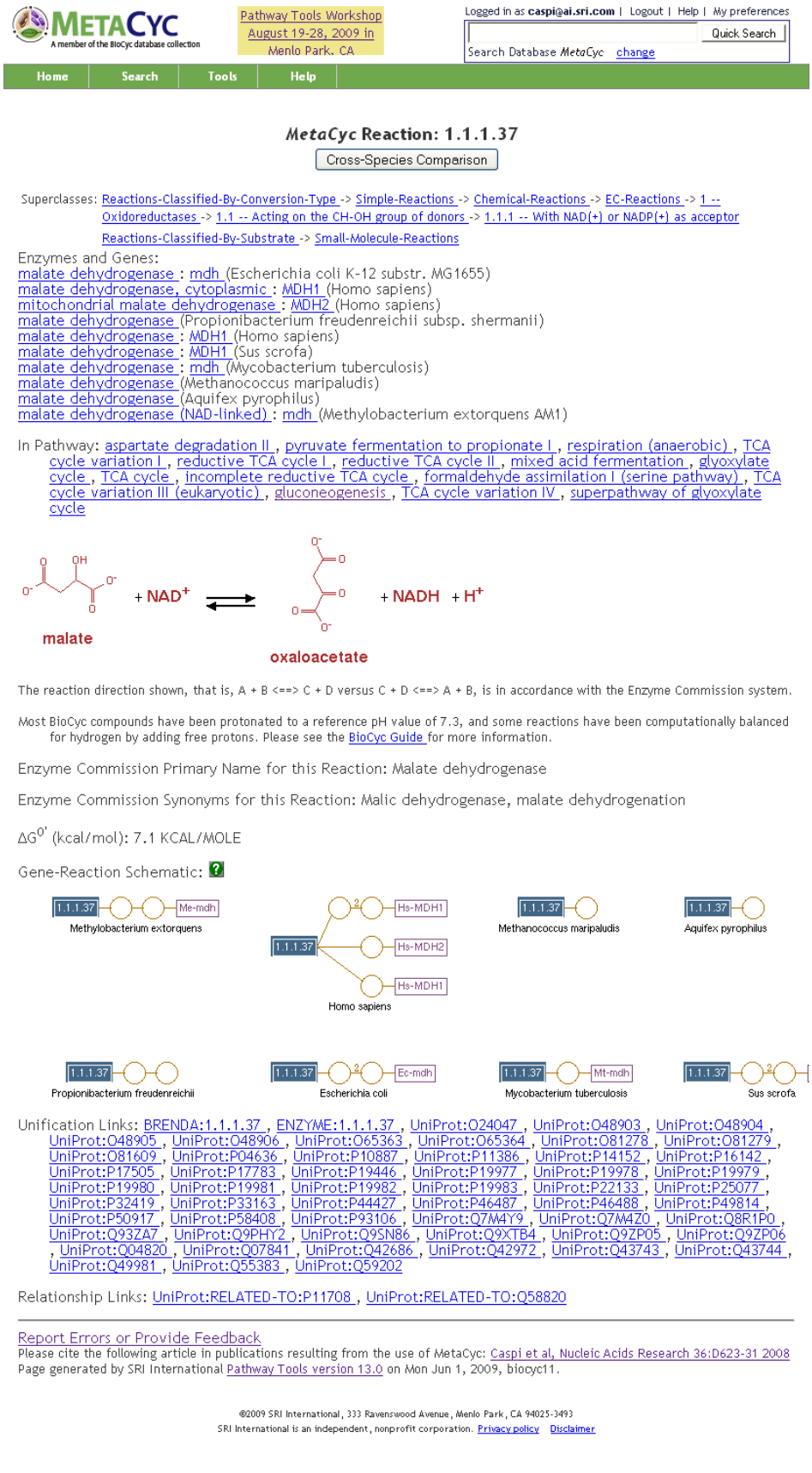


Figure 2: In addition to the reaction equation, the reaction display page contains many additional information fields, including a list of enzymes in the database that catalyze the reaction, a list of pathways in which the reaction participates, computationally calculated standard free energy, gene-reaction schematics that display relationships between genes, enzymes and reactions, unification links and more.

Figure 3: The protein display page is divided into several sections. The top section provides general information about the protein and includes an optional summary, synonyms, subunit composition (in the case of protein complexes), molecular weight, links to external databases, a gene-reaction schematic that links genes, proteins, and the reactions they catalyze, and optional GO terms. If the protein is an enzyme and catalyzes one or more reactions, the next section(s) provide information about the enzymatic reaction(s). There is a different section for each enzymatic activity, and each section includes the reaction equation, a list of pathways in which the reaction participates, information about the reaction directionality (if known), a list of known inhibitors, cofactors, and activators. Additional sections provide sequence features and references.

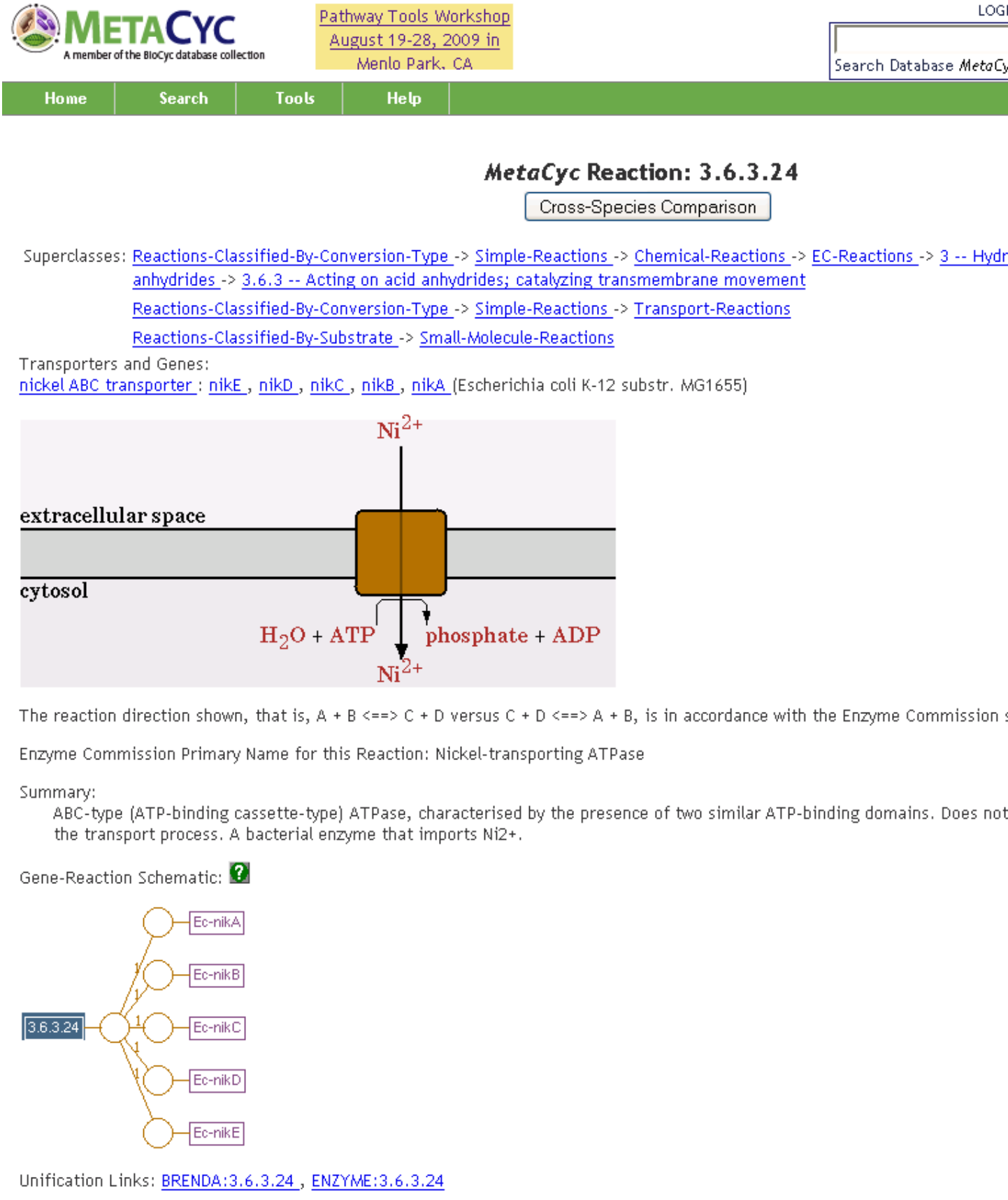
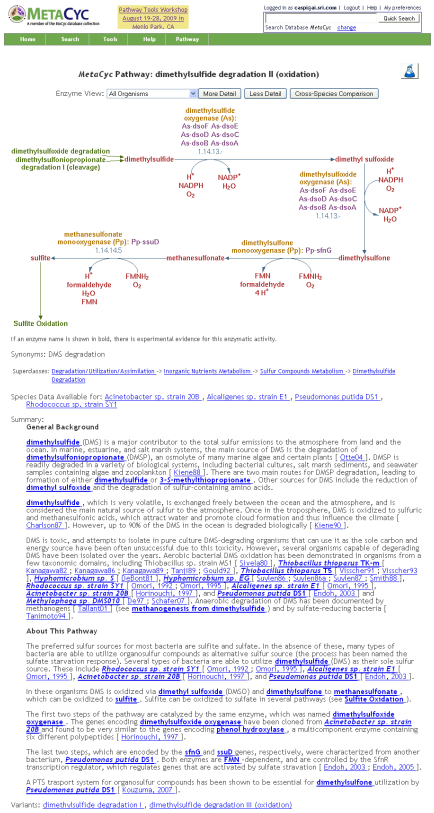


Figure 4: Transport reaction pages include a diagram that depicts the compartments across the membrane and the direction of transport. Like regular reactions, the page includes a list of the genes and proteins associated with the transport reaction, and a gene-reaction schematic.

Figure 5: Unlike other proteins, the display page for transcription factors (TFs) includes a graphical display of all of the transcription units that are controlled by the TF. The functionality of the TF is indicated by color, and additional information, such as distance from the transcription start site and evidence code is displayed when available by hovering the mouse in top of the TF.



If an enzyme name is shown in bold, there is experimental evidence for this enzymatic activity.

Synonyms: DMS degradation

Superclasses: Degradation/Utilization/Assimilation -> Inorganic Nutrients Metabolism -> Sulfur Compounds Metabolism -> Dimethylsulfide Degradation

Species Data Available for: Acinetobacter sp. strain 20B , Alcaligenes sp. strain E1 , Pseudomonas putida DS1 , Rhodococcus sp. strain ST1

Summary:

General Background

dimethylsulfide (DMS) is a major contributor to the total sulfur emissions to the atmosphere from land and the ocean. In marine, estuarine, and salt marsh systems, the main source of DMS is the degradation of **dimethylsulfoniopropionate** (DMSP), an osmolyte of many marine algae and certain plants [Otte04]. DMSP is readily degraded in a variety of biological systems, including bacterial cultures, salt marsh sediments, and seawater samples containing algae and zooplankton [Kiene88]. There are two main routes for DMSP degradation, leading to formation of either **dimethylsulfide** or **3-S-methylthiopropionate** . Other sources for DMS include the reduction of **dimethyl sulfoxide** and the degradation of sulfur-containing amino acids.

dimethylsulfide , which is very volatile, is exchanged freely between the ocean and the atmosphere, and is considered the main natural source of sulfur to the atmosphere. Once in the troposphere, DMS is oxidized to sulfuric and methanesulfonic acids, which attract water and promote cloud formation and thus influence the climate [Charlson87]. However, up to 90% of the DMS in the ocean is degraded biologically [Kiene90].

DMS is toxic, and attempts to isolate in pure culture DMS-degrading organisms that can use it as the sole carbon and energy source have been often unsuccessful due to this toxicity. However, several organisms capable of degrading DMS have been isolated over the years. Aerobic bacterial DMS oxidation has been demonstrated in organisms from a few taxonomic domains, including Thiobacillus sp. strain M5 [Sivola80], ***Thiobacillus thioparus* TK-m** [Kanagawa82 ; Kanagawa84 ; Tani89 ; Gould92], ***Thiobacillus thioparus* T5** [Visscher91 ; Visscher93], ***Hyphomicrobium sp. S*** [DeBont81], ***Hyphomicrobium sp. EG*** [Suylen86 ; Suylen86b ; Suylen87 ; Smith88], ***Rhodococcus sp. strain ST1*** [Omori, 1992 ; Omori, 1995], ***Alcaligenes sp. strain E1*** [Omori, 1995], ***Acinetobacter sp. strain 20B*** [Horinouchi, 1997], and ***Pseudomonas putida* DS1** [Endoh, 2003] and ***Methylophaga sp. DMS010*** [Boe97 ; Schafer07]. Anaerobic degradation of DMS has been documented by methanogens [Tallan01] (see **methanogenesis from dimethylsulfide**) and by sulfate-reducing bacteria [Tanimoto94].

About This Pathway

The preferred sulfur sources for most bacteria are sulfite and sulfate. In the absence of these, many types of bacteria are able to utilize organosulfur compounds as alternative sulfur source (the process has been named the sulfate starvation response). Several types of bacteria are able to utilize **dimethylsulfide** (DMS) as their sole sulfur source. These include ***Rhodococcus sp. strain ST1*** [Omori, 1992 ; Omori, 1995], ***Alcaligenes sp. strain E1*** [Omori, 1995], ***Acinetobacter sp. strain 20B*** [Horinouchi, 1997], and ***Pseudomonas putida* DS1** [Endoh, 2003].

In these organisms DMS is oxidized via **dimethyl sulfoxide** (DMSO) and **dimethylsulfone** to **methanesulfonate** , which can be oxidized to **sulfite** . Sulfite can be oxidized to sulfate in several pathways (see **Sulfite Oxidation**).

The first two steps of the pathway are catalyzed by the same enzyme, which was named **dimethylsulfide oxygenase** . The genes encoding **dimethylsulfide oxygenase** have been cloned from ***Acinetobacter sp. strain 20B*** and found to be very similar to the genes encoding **phenol hydroxylase** , a multicomponent enzyme containing six different polypeptides [Horinouchi, 1997].

The last two steps, which are encoded by the **sfnG** and **ssuD** genes, respectively, were characterized from another bacterium, ***Pseudomonas putida* DS1** . Both enzymes are **FMN**-dependent, and are controlled by the SfnR transcription regulator, which regulates genes that are activated by sulfate starvation [Endoh, 2003 ; Endoh, 2005].

A PTS trasport system for organosulfur compounds has been shown to be essential for **dimethylsulfone** utilization by ***Pseudomonas putida* DS1** [Kouzuma, 2007].

Variants: dimethylsulfide degradation I , dimethylsulfide degradation III (oxidation)

Credits:
Created 29-Sep-2008 by Caspi R , SRI International

References

Charlson, R.J., Lovelock, J.E., Andreae, M.O., Warren, S.G. (1987). "Oceanic phytoplankton, atmospheric sulphur, cloud albedo and climate." Nature 326:655-661.

De Zwart J., Sluis J., Kuenen J.G. (1997). "Competition for Dimethyl Sulfide and Hydrogen Sulfide by Methylophaga sulfidovorans and Thiobacillus thioparus T5 in Continuous Cultures." Appl Environ Microbiol 63(8):3318-3322. PMID: 10535680

DeBont J. A. M., Dijken J. P. van, Harder W. (1981). "Dimethyl sulphoxide and dimethyl sulphide as a carbon, sulphur and energy source for growth of Hyphomicrobium S." J. Gen. Microbiol. 127: 315-323.

Endoh T., Kasuga K., Horinouchi M., Yoshida T., Habe H., Nojiri H., Omori T. (2003). "Characterization and identification of genes essential for dimethyl sulfide utilization in Pseudomonas putida strain DS1." Appl Microbiol Biotechnol 62(1):85-91. PMID: 12835962

Endoh T., Habe H., Nojiri H., Yamane H., Omori T. (2005). "The sigma54-dependent transcriptional activator SfnR regulates the expression of the Pseudomonas putida sfnFG operon responsible for dimethyl sulphone utilization." Mol Microbiol 55(3):897-911. PMID: 15661012

Gould, WD., Kanagawa, T. (1992). "Purification and properties of methyl-lmercaptan oxidase from Thiobacillus thioparu TK-m." J. Gen. Microbiol. 138: 217 - 221.

Horinouchi M., Kasuga K., Nojiri H., Yamane H., Omori T. (1997). "Cloning and characterization of genes encoding an enzyme which oxidizes dimethyl sulfide in Acinetobacter sp. strain 20B." FEMS Microbiol Lett 155(1):29-105. PMID: 9345770

Kanagawa, T., Dazai, M., Kukuoka, S. (1982). "Degradation of D, D-dimethyl phosphodithioate by Thiobacillus thioparus TK-1 and Pseudomonas AK-2." Agric. Biol. Chem. 46: 2671-2678.

Kanagawa, T., Kelly, D.P. (1986). "Breakdown of dimethylsulphide by mixed cultures and by Thiobacillus thioparus." FEMS Microbiol. Lett. 34: 13 - 19.

Kanagawa T, Mikami E (1989). "Removal of methanethiol, dimethyl sulfide, dimethyl disulfide, and hydrogen sulfide from contaminated air by Thiobacillus thioparus TK-m." Appl Environ Microbiol 55(3):555-8. PMID: 2930168

Kiene RP, Taylor BF (1988). "Demethylation of Dimethylsulfoniopropionate and Production of Thiols in Anoxic Marine Sediments." Appl Environ Microbiol 54(9):2208-2212. PMID: 16347732

Kiene, R. P., Bates, T. S. (1990). "Biological removal of dimethyl sulfide from sea-water." Nature 345:702-705.

Kouzuma A, Endoh T, Omori T, Nojiri H, Yamane H, Habe H (2007). "The ptsP gene encoding the PTS family protein EI(Ntr) is essential for dimethyl sulfone utilization by Pseudomonas putida." FEMS Microbiol Lett 275(1):175-81. PMID: 17711492

Omori T., Monna L., Saiki Y., Kodama T. (1992). "Desulfurization of dibenzothiophene by Corynebacterium sp. strain ST1." Appl Environ Microbiol 58(3):911-5. PMID: 1575493

Omori, T., Saiki, Y., Kasuga, K., Kodama, T. (1995). "Desulfurization of Alkyl and Aromatic Sulfides and Sulfonates by Dibenzothiophene-desulfurizing Rhodococcus sp. Strain ST1." Bioscience, biotechnology, and biochemistry 59(7):1195-1198.

Otte ML., Wilson G., Morris JT., Moran BM. (2004). "Dimethylsulphoniopropionate (DMSP) and related compounds in higher plants." J Exp Bot 55(404):1919-25. PMID: 15181109

Schafer H (2007). "Isolation of Methylophaga spp. from marine dimethylsulfide-degrading enrichment cultures and identification of polypeptides induced during growth on dimethylsulfide." Appl Environ Microbiol 73(8):2580-91. PMID: 17322322

Sivela S (1980). "Dimethylsulphide as a growth substrate of an obligate-tely chemolithotrophic Thiobacillus." Commentationi Physico-Mathe-matical Dissertations 1: 1-93.

Smith NA, Kelly DP (1988). "Isolation and physiological characteris-tization of authotrophic sulphur bacteria oxidizing dimethyldisulphide as sole source of energy." J. General Microbiol., 134: 1407 - 1417.

Suylen GM, Kuenen JG (1986). "Chemostat enrichment and isolation of Hyphomicrobium EG. A dimethyl-sulphide oxidizing methylotroph and reevaluation of Thiobacillus M5." Antonie Van Leeuwenhoek 52(4):281-93. PMID: 3767349

Suylen, G. M. H., Stefess, G. C., Kuenen, J. G. (1986). "Chemolithotrophic potential of a Hyphomicrobium species, capable of growth on methylated sulphur compounds." Arch Microbiol 146:192 - 198.

Suylen GMH, Large P.J, van Dijken JP, Kuenen JG (1987). "Methyl-mercaptan oxidase, a key enzyme in the metabolism of methylated sulphur compounds by Hyphomicrobium EG." J. Gen. Microbiol., 133: 2989 - 2997.

Tallant TC, Paul L, Krzycki JA (2001). "The MtaA subunit of the methylthiolcoenzyme M methyltransferase of Methanosarcina barkeri catalyses both half-reactions of corrinoid-dependent dimethylsulfide: coenzyme M methyl transfer." J Biol Chem 276(6):4485-93. PMID: 11073950

Tanimoto Y, Bak F (1994). "Anaerobic degradation of methylmercaptan and dimethyl sulfide by newly isolated thermophilic sulfate-reducing bacteria." Appl Environ Microbiol 60(7):2480-5. PMID: 8074526

Tanii, Y., Kanagawa, T., Mikami, E. (1989). "Removal of dimethyl sulphide, methyl mercaptan, and hydrogen sulphide by immobilized Thioba-cillus thioparus TK-m." J. Ferment. Bioeng. 67(4): 280 - 285.

Visscher PT, Quist P, van Gemerden H (1991). "Methylated sulfur compounds in microbial mats: in situ concentrations and metabolism by a colorless sulfur bacterium." Appl Environ Microbiol 57(6):1758-63. PMID: 1872604

Visscher PT, Taylor BF (1993). "A new mechanism for the aerobic catabolism of dimethyl sulfide." Appl Environ Microbiol 59(11):3784-9. PMID: 8285684

Other References Related to Enzymes, Genes, Subpathways, and Substrates of this Pathway

Andreae M. O. (1980). "Dimethylsulfoxide in marine and freshwaters." Limnol. Oceanogr. 25: 1054-1063.

Borodina E, Kelly DP, Rainey FA, Ward-Rainey NL, Wood AP (2000). "Dimethylsulfone as a growth substrate for novel methylotrophic species of Hyphomicrobium and Arthrobacter." Arch Microbiol 173(5-6):425-37. PMID: 10896224

Howard EC, Henriksen JR, Buchan A, Reisch CR, Burgmann H, Welsh R, Ye W, Gonzalez JM, Mace K, Joye SB, Kiene RP, Whitman WB, Moran MA (2006). "Bacterial taxa that limit sulfur flux from the ocean." Science 314(5799):649-52. PMID: 17068264

Kelly DP, Murrell JC (1999). "Microbial metabolism of methanesulfonic acid." Arch Microbiol 172(6):341-8. PMID: 10591843

Murakami-Nitta T, Kurimura H, Kirimura K, Kino K, Usami S (2002). "Continuous degradation of dimethyl sulfoxide to sulfate ion by Hyphomicrobium denitrificans WUK-217." J Biosci Bioeng 94(1):52-6. PMID: 16233269

Report Errors or Provide Feedback
Please cite the following article in publications resulting from the use of MetaCyc: Caspi et al, Nucleic Acids Research 36:D623-31 2008
Page generated by SRI International Pathway Tools version 13.0 on Mon Jun 1, 2009, biocyc6.

Figure 6: Pathway display pages include a pathway diagram, classification of the pathway based on an internal pathway ontology, a summary, and a list of references. The pathway diagram includes enzymes and genes, and the level of details shown can be controlled through buttons at a top. In addition, the pathway diagram can be modified extensively through the "Pathway" menu.

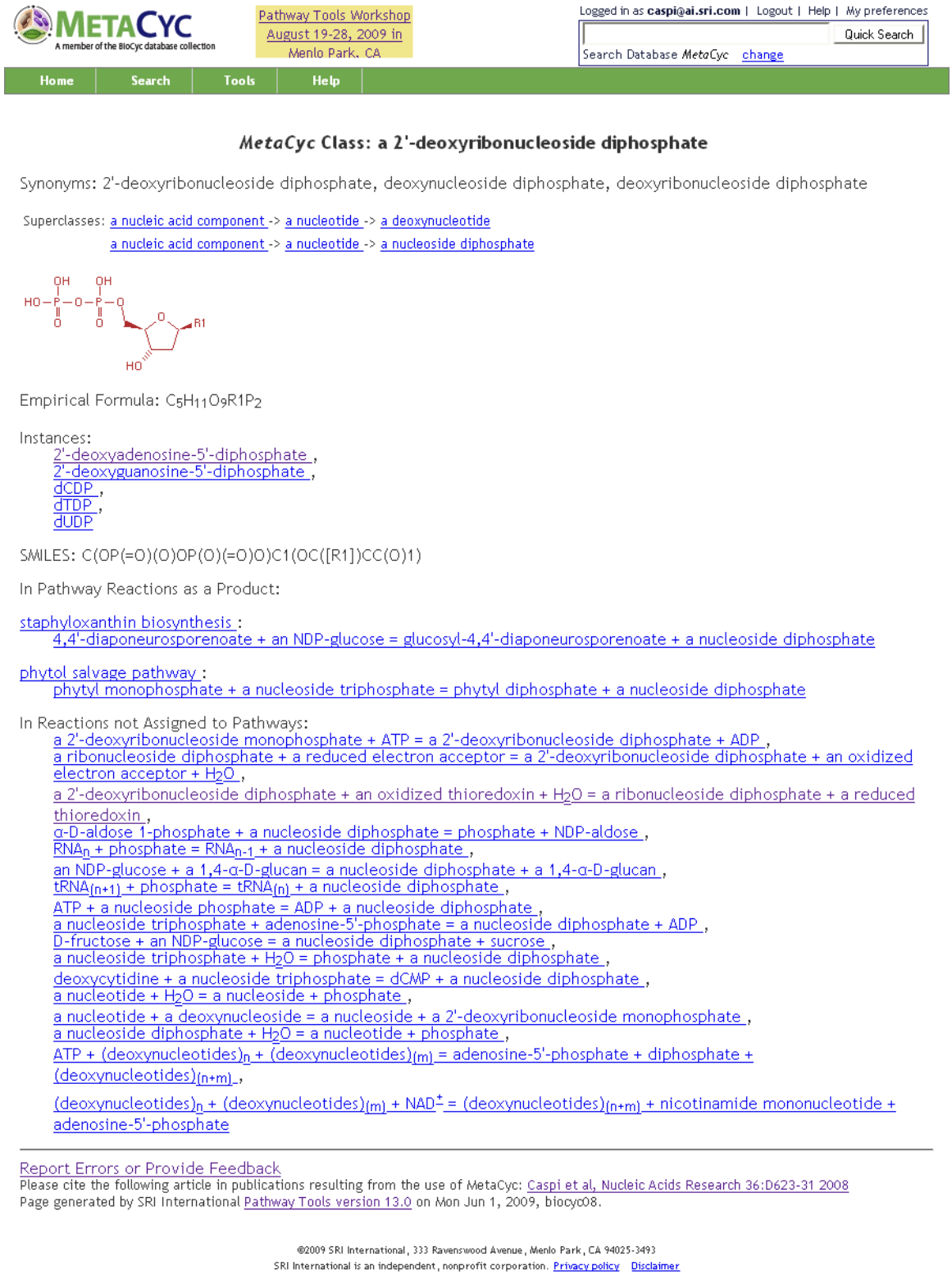


Figure 7: Compound display pages include synonyms, classification, structure, empirical formula, smiles and InChI strings, and lists of all the reactions and pathways present in the database in which the compound participates. Class compounds can include an R residue in their structures, as shown in this figure, and specify the children compound classes and instances that reside within the class. Class compounds do not have an InChI string.

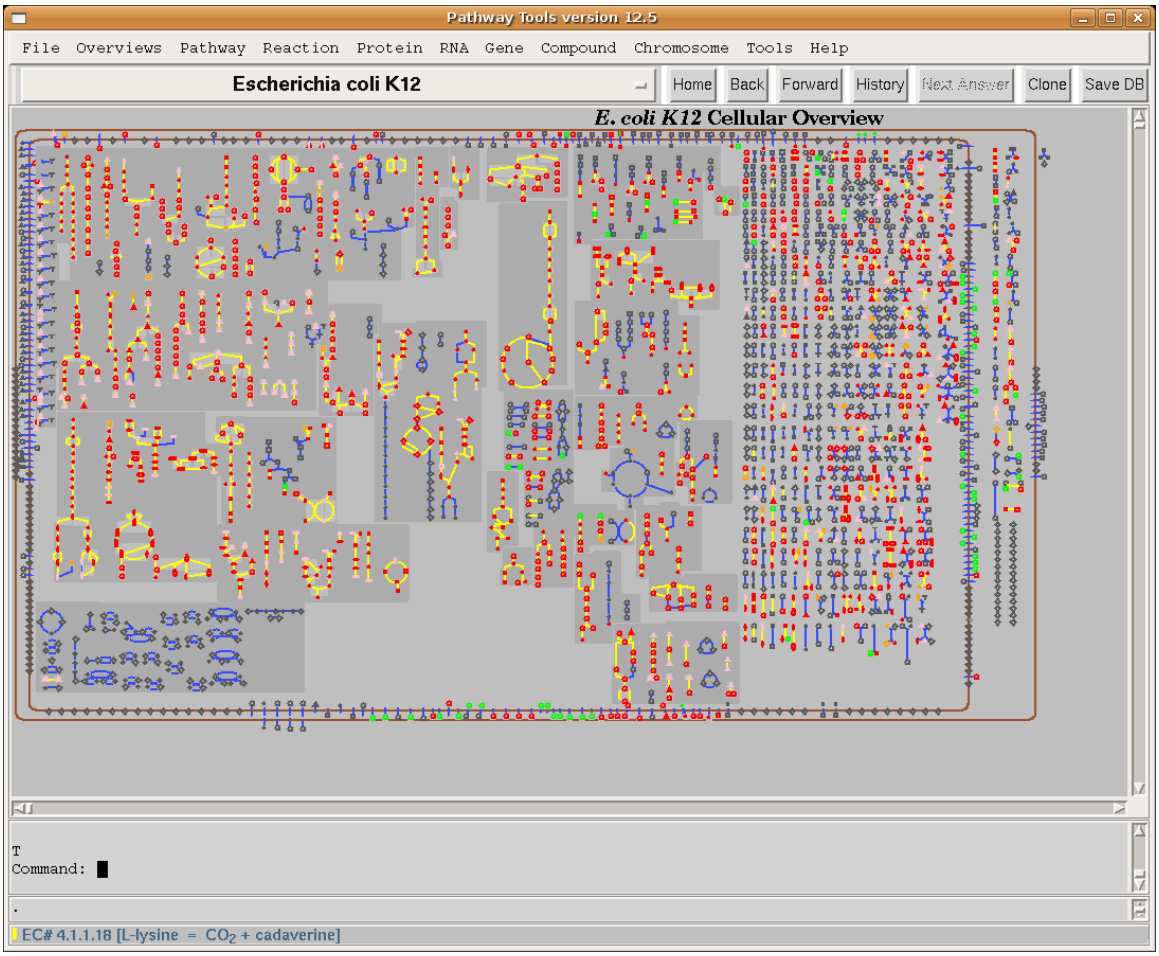


Figure 8: Reachability analysis for EcoCyc. The results are visualized by highlighting reactions and compounds on the cellular overview in different colors. Fired reactions are yellow lines, produced biomass metabolites are pink, other produced metabolites are red. Green metabolites are supplied by the growth medium, and orange indicates auxiliary metabolites.

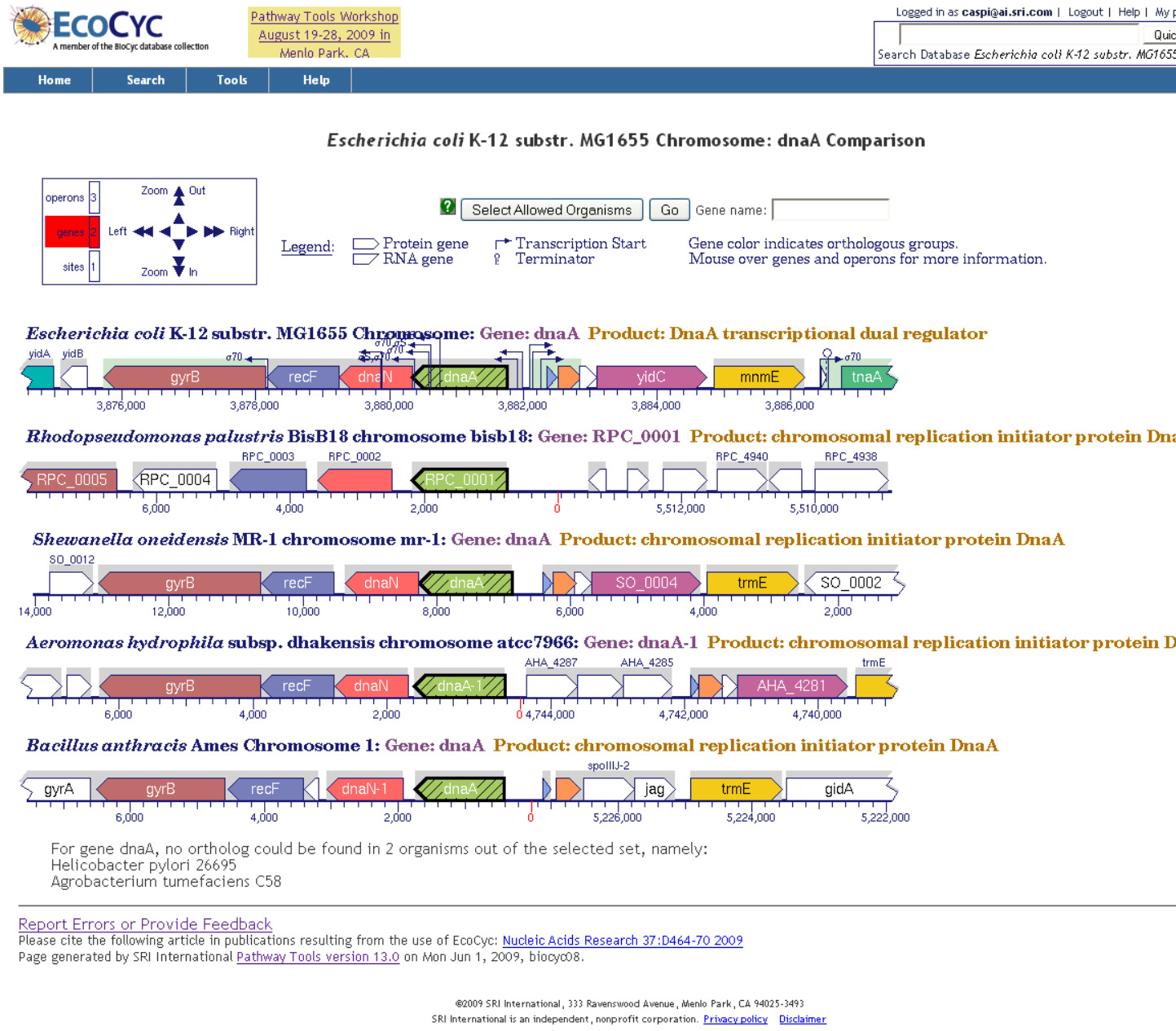


Figure 9: Comparative genome browser displaying chromosomal regions around the *dnaA* genes in several organisms.

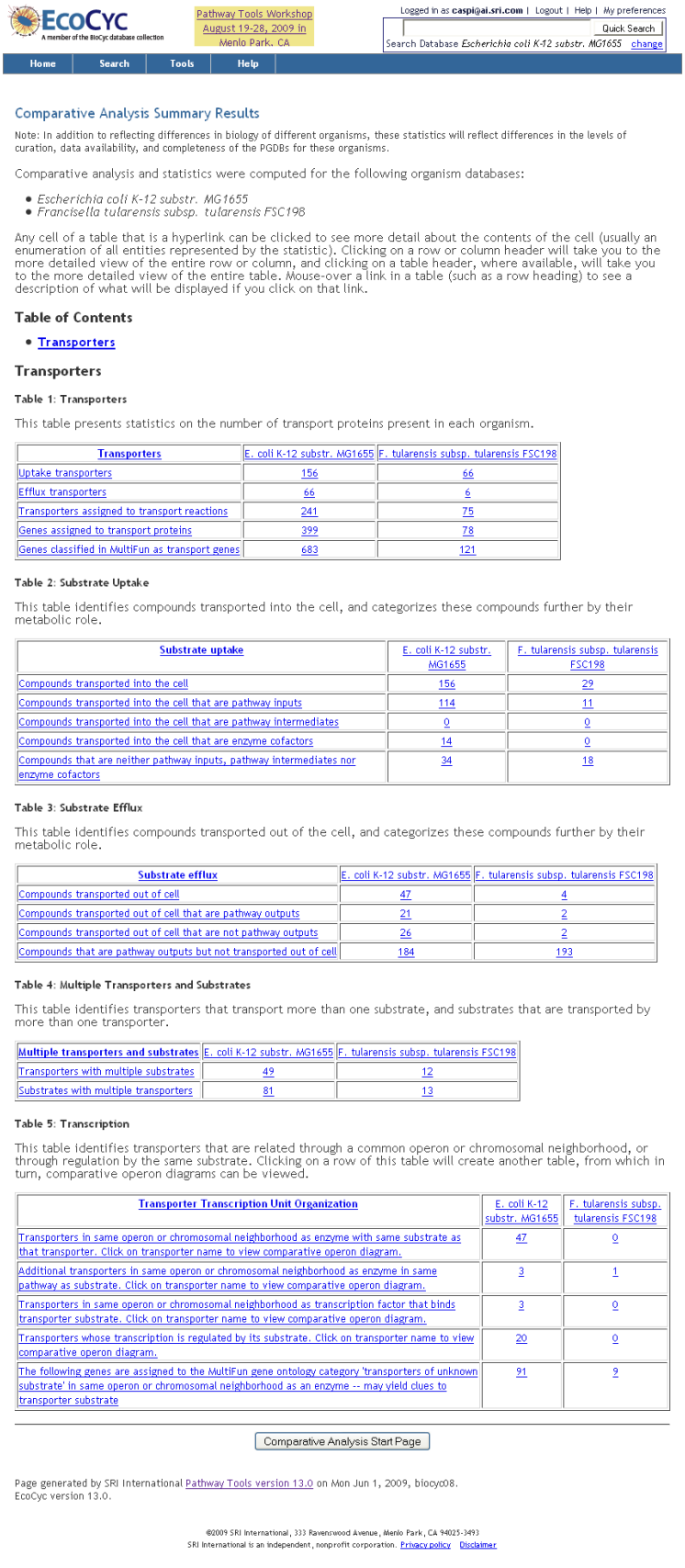


Figure 10: Comparative transporter report for *E. coli* K-12 MG1655 and *Francisella tularensis* FSC198.

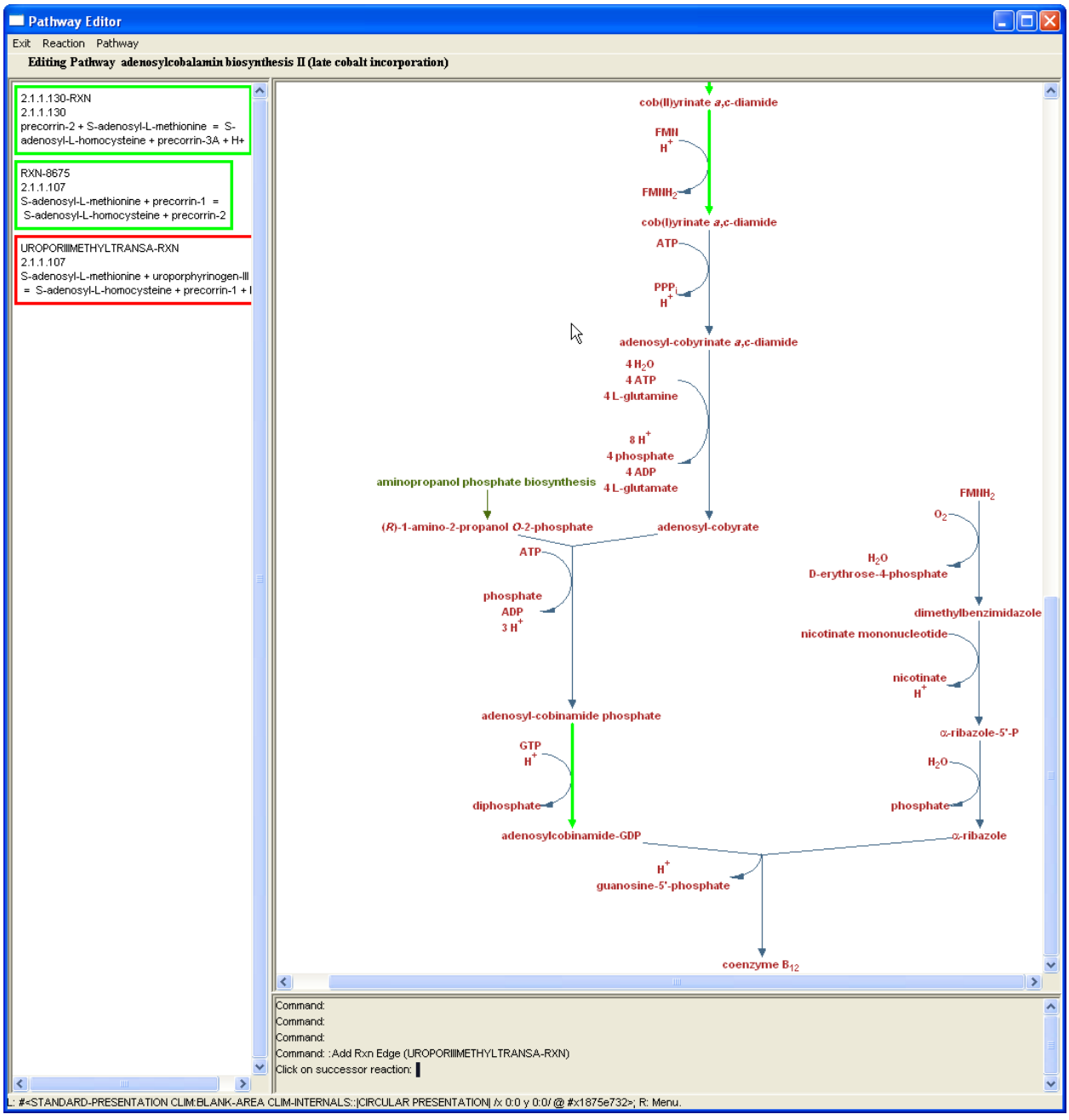


Figure 11: Pathway Tools Pathway Editor.

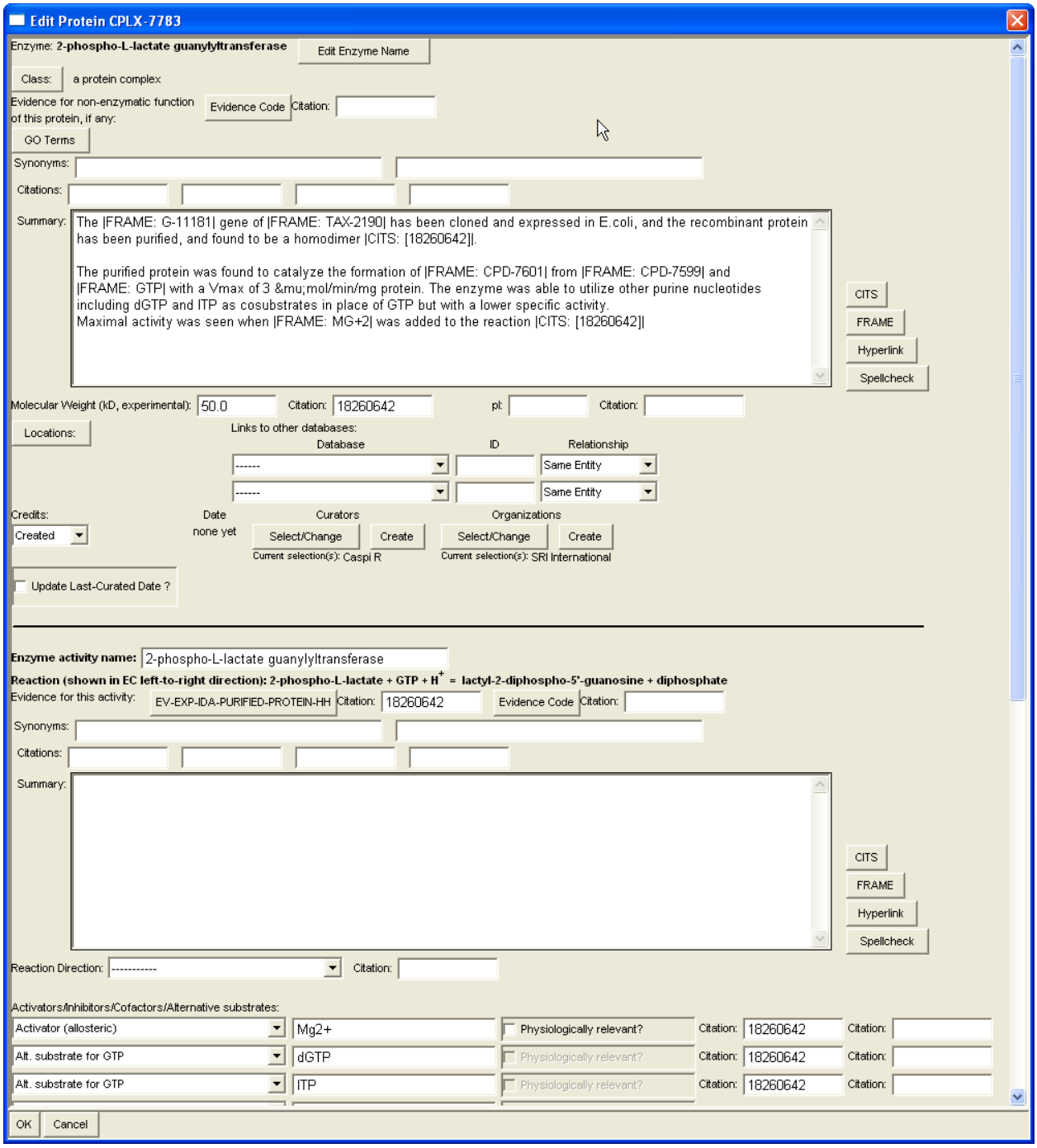


Figure 12: Pathway Tools Protein Editor.

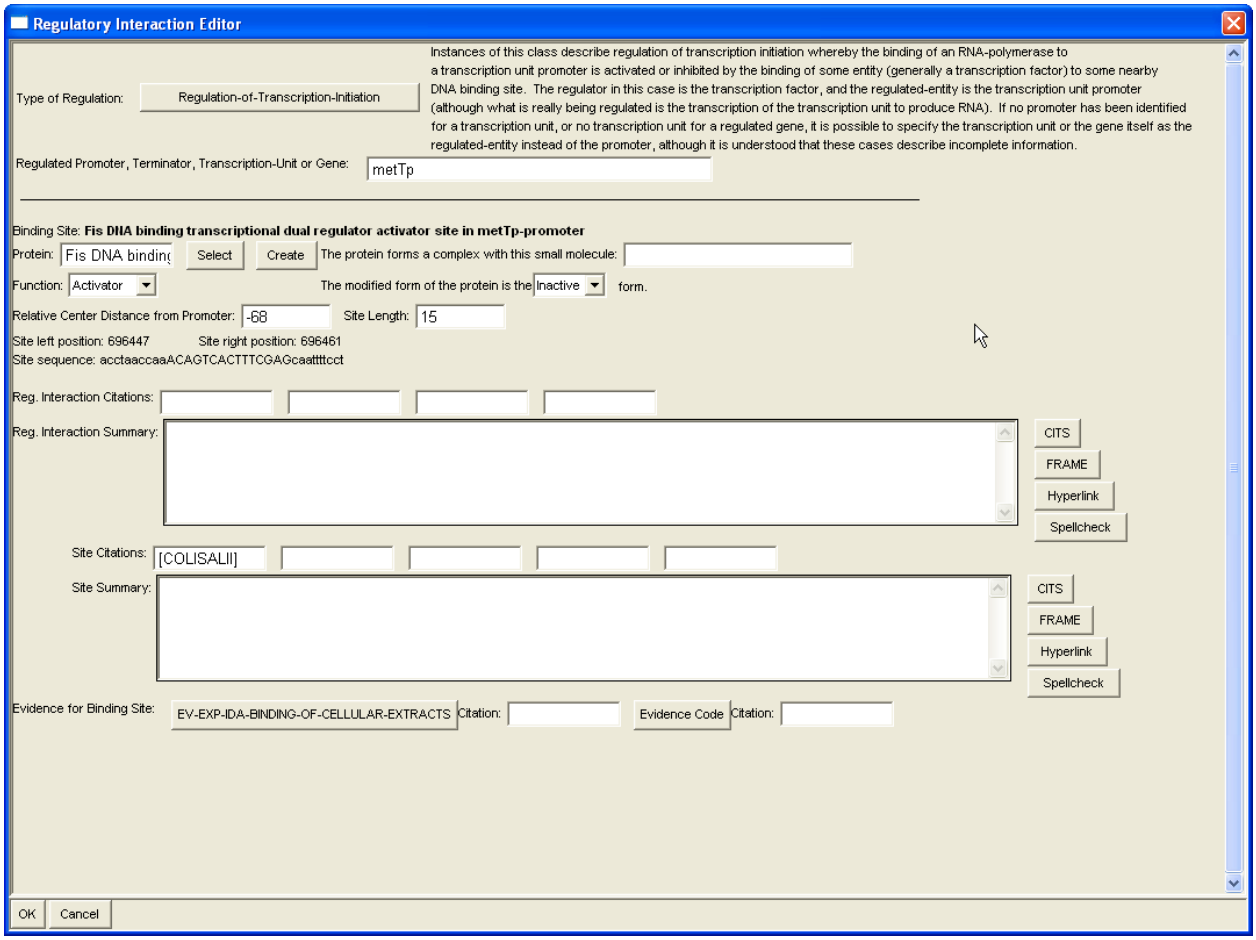


Figure 13: Pathway Tools Regulation Editor.