BioCyc: Metabolic Pathway Databases and Informatics Tools
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LanzaTech, the carbon recycling company, began trading on the Nasdaq Stock Exchange on Friday, February 10th, following the successful completion of the business combination with AMCI Acquisition Corp. II. LanzaTech is both the first carbon capture and transformation ("CCT") company and the first gas fermentation company to go public in the US. The proceeds from this transaction provide a significant runway for the company to continue scaling its technology to convert waste carbon into the everyday items of our material economy—from sustainable fuels and running shorts to packaging and perfume. Read more about the announcement here:

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**Style**

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**Symbols, acronyms and measurement**

Define all symbols and spell out all acronyms the first time they are used. All weights and measures must be in the metric system (SI units). Abbreviations may be used for units of weight or measurement that describe data without definition.

**Figures and photos**

Acceptable formats: EPS, TIFF, JPG, and PDF are the acceptable file formats for figures and photos. Original native documents may be requested if any issues with the figure quality arise.

**File submission**

All figures must be submitted as separate files either electronically or on a CD/DVD. Figures embedded in Word files will not be accepted.

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All figures and photos should be high quality. Raster line art and grayscale or color work should be a minimum of 300 ppi (pixels per inch) resolution at the desired print dimensions. Enlarging the dimensions of an image will also reduce its resolution inversely. For example, if the dimensions are increased by 25% then the resolution will be reduced by 25%.

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Reminder:  
2023 SIMB Election for Board of Directors

The SIMB Election for positions on the Board of Directors will commence March 1 and end March 31 at noon EST.

Current members have received login instructions for accessing the voting module.

After voting ends, the SIMB Election Committee, currently chaired by Kristien Mortelmans, SRI International and consisting of a minimum of two SIMB members, receives access to the voting module. The committee certifies counts from online voting, as well as any paper ballots previously requested and postmarked no later than the deadline date for electronic voting, and delivers the results to the SIMB President and SIMB Secretary for announcement.
NSF Releases Diversity in STEM Report

The National Science Foundation’s (NSF) National Center for Science and Engineering Statistics (NCSES) recently released their Diversity and STEM: Women, Minorities, and Persons with Disabilities 2023 report, which presents the federal government’s most comprehensive analysis of diversity trends in STEM employment and education.

The report, published every 2 years, provides statistical information about three groups—women, minorities, and persons with disabilities—who have been historically underrepresented in STEM.

The latest iteration shows more women, as well as Black, Hispanic, American Indian, and Alaska Native people collectively, worked in STEM jobs over the past decade and are earning more degrees in science and engineering fields at all levels compared to previous years. However, those groups, as well as people with disabilities, largely still remain underrepresented in STEM compared to their overall distribution in the U.S. population.

According to the report, nearly a quarter (24 percent) of the U.S. workforce—34.9 million people ages 18 to 74—was employed in STEM occupations in 2021, up 20 percent from 2011. It found that the STEM workforce has been gradually diversifying. Underrepresented minorities made up nearly a quarter (24 percent) of the STEM workforce in 2021, up from 18 percent in 2011. Representation of women increased from 32 percent in 2011 to 35 percent in 2021.

STEM workers have higher median earnings and lower unemployment rates than non-STEM workers, the report found. However, Hispanic, Black, American Indian, and Alaska Native STEM workers have lower median earnings than white or Asian STEM workers. While women earned half of science and engineering bachelor’s degrees and associate’s degrees, they represented a third of the STEM workforce, and their wages were consistently lower than men’s.
Newsworthy

Survey Shows Bipartisan Support for Federal Investment in Science

According to a recent survey commissioned by Research! America, Americans across the political spectrum agree that federal investments in research and development (R&D) drive job creation, innovation, and global leadership.

A large majority of Americans, about 91 percent, think it is important for the U.S. to be a global leader in science and technology (S&T). About 77 percent of Americans are concerned that China will surpass the U.S. as the global S&T leader, with 6 in 10 Americans agreeing that Congress should invest more taxpayer dollars to advance S&T.

Notably, more than 8 in 10 Americans, including 92 percent of Democrats, 78 percent of Republicans, and 76 percent of independents, think that the federal government should support basic research.

The survey also found that 63 percent of Americans are willing to pay $1 dollar more per week in taxes in support of medical and health research. More than 3 in 4 Americans agree that R&D investments are creating job opportunities for people across the country.

Another interesting finding was that public confidence in scientists and healthcare providers is very high overall, with nurses (89 percent), doctors (87 percent), and scientists (78 percent) ranked as the three most trusted professions—each up 8 to 10 points over 2022. On the other hand, confidence in research institutions has dropped 9 points from 76 to 67 percent.
Abstract

This article describes a coordinated set of bioinformatics databases and software tools designed to solve multiple problems faced by metabolic engineers and microbiologists related to metabolic pathways. Those problems include the following: (1) Answering basic questions about the metabolism of a given organism; that is, what pathways does a given bacterium possess and what enzymes and metabolites participate in a given pathway? (2) Predicting the metabolism of an organism from its genome sequence. (3) Engineering new pathways into an organism. (4) Predicting pathway activation levels from omics datasets. (5) Comparative analyses of metabolism. BioCyc.org provides 20,000 Pathway/Genome databases for sequenced microbes that describe their reconstructed metabolic networks. The MetaCyc DB provides a universal encyclopedia of metabolism across all domains of life. BioCyc computational tools provide search, comparison, and multiple analysis operations, including omics data analysis.
Introduction

The immense diversity of microbial metabolism presents microbiologists with great challenges: How do we capture and interrogate the huge mass of information about microbial metabolism? For any given microbe, how do we navigate and analyze its metabolic network to gain an in-depth understanding of its capabilities? And how do we compare the metabolism of multiple microbes to understand the differences in their networks? BioCyc, a resource that has benefited from more than 20 years of research and development, is designed to address these challenges (Karp et al., 2019).

BioCyc.org provides a collection of 20,000 microbial Pathway/Genome Databases (PGDBs), each of which describing the genome and metabolic network of a single sequenced organism. Each PGDB is based on a computational reconstruction of the organism’s metabolism computed from its sequenced genome (Karp et al., 2011). For some organisms, that reconstruction is supplemented with manually curated information. The metabolic information present in each database includes the reactions, metabolites, enzymes, and pathways that make up each metabolic network.

BioCyc.org also provides dozens of computational tools for searching and analyzing genome and metabolic information. Search tools enable users to find a given metabolite, reaction, enzyme, or pathway. Visualization tools enable users to inspect search results, including information pages for metabolites, reactions, and pathways. Visualization tools also enable navigation through full metabolic networks. Analysis tools include RouteSearch, which searches for novel metabolic routes from a feedstock to a target compound, and tools for visualizing and analyzing transcriptomics and metabolomics data on individual pathway diagrams and on full metabolic map diagrams. A suite of comparison tools is available to differentiate the metabolic networks of two or more organisms.

The computational tools present in the BioCyc.org website are provided by the Pathway Tools software. A local Pathway Tools installation can serve as a full data management environment for genome and metabolism information for thousands of organisms. For example, Pathway Tools includes a genome browser, BLAST searches, sequence pattern searches, and a multiple sequence alignment tool. It also includes interactive editing tools for modifying a PGDB, such as adding a new metabolite, changing the function of a gene, adding a transcriptional regulatory interaction, and modifying a metabolic pathway.

A local Pathway Tools installation supports the analysis of genomes not present in the BioCyc website by enabling the generation of new PGDBs for any annotated genomes, including proprietary genomes or a multi-organism metagenome. In addition, a local Pathway Tools
installation enables the RouteSearch tool to add new reactions from MetaCyc when generating routes.

BioCyc Databases
The MetaCyc Database

The MetaCyc DB (MetaCyc.org) is a key reference database for metabolism that contains experimentally studied metabolic pathways, reactions, enzymes, and metabolites from all domains of life. It has received extensive curation from 74,000 publications to ensure the accuracy and completeness of its information (Caspi et al., 2020).

In addition to serving scientists as an online encyclopedic reference on metabolism, MetaCyc plays a central role in several BioCyc computational tools. MetaCyc provides the reference metabolic information for BioCyc tools for computing metabolic reconstructions; those tools copy relevant metabolites, reactions, and pathways from MetaCyc into a new database containing the reconstruction. MetaCyc is also the source of exogenous reactions for the RouteSearch tool that designs novel pathways from a specified start-to-end metabolite. In addition, our gap-filling tool draws from MetaCyc reactions to fill gaps in metabolic models.

MetaCyc metabolite pages, such as that for L-tryptophan, include a list of chemical names and synonyms, molecular weight and monoisotopic mass, chemical formula and structure, unique identifiers (e.g., InChI and SMILES), Gibbs free energy of formation, and links to many other chemical databases.

The Regulation tab lists the regulatory influences of the compound on enzymes within MetaCyc.

The Reactions tab lists the reactions known to produce, consume, and transport the compound across all domains of life, with associated pathway(s) indicated when relevant. Clicking on a reaction opens a MetaCyc reaction page, such as that for the L-tryptophan aminotransferase reaction. The reaction page shows the reaction equation with the chemical structures automatically colored to show substructures that are conserved between the reactants and the products and the bonds that are made and broken by this reaction, based on the atom-mapping information that we compute for most MetaCyc reactions (Figure 1). For most reactions, the reaction page lists one or more enzymes that catalyze them, the organisms from which those enzymes were isolated, and the metabolic pathways in which the reaction participates.
Clicking on a pathway name opens a MetaCyc pathway page (Figure 2). Different organisms have evolved alternative mechanisms for accomplishing a given biochemical transformation (e.g., degradation of L-tryptophan). We call these alternative mechanisms pathway variants, and append roman numerals to the pathway name to designate variants, such as L-tryptophan degradation VIII (to tryptophol). Pathway drawings are generated automatically by the BioCyc software, and the user can control which aspects of a pathway are included in the diagrams, such as metabolite chemical structures or allosteric regulation of pathway’s enzymes. Pathway pages also list some specific organisms that are known to possess the pathway and list the taxonomic groups in which the pathway is expected to be found. Pathway pages contain a mini-review of the literature describing that pathway. Mini-reviews are found in other pages as well; those for pathway and enzyme pages tend to be the most extensive (Caspi et al., 2013).

Clicking on an enzyme name opens a MetaCyc gene/protein page, such as that for the TrpE subunit of anthranilate synthase of E. coli. Enzyme pages collect information regarding the reaction(s) catalyzed by the enzyme and the pathways in which they participate. Enzyme pages also list the cellular location(s), the activators, inhibitors, and cofactors affecting the enzyme, and, when relevant, the multimeric complex in which the protein is a subunit of. When available, the page lists kinetic parameters for the enzyme as well as its temperature and pH optima. Some proteins are annotated by GO terms and protein features (known regions and residues of interest within the protein, such as metal ion binding sites, active sites, and phosphorylation sites), which can be accessed via the Go Terms and Protein Features tabs, respectively.

The overall data content of MetaCyc is summarized and compared with the content of the KEGG pathway database in Table 1. MetaCyc contains more data (7.3 times as many pathways and 1.6 times as many reactions) and more in-depth summaries of the literature in its mini-reviews.

To clarify the relationship between MetaCyc and BioCyc, one major aim of MetaCyc is to integrate experimentally derived information on metabolism from all domains of life to provide a solid reference source for performing metabolic reconstructions and developing metabolic models. Thus, the collection of information for any one organism in MetaCyc will necessarily be limited to information from experimental studies. For example, MetaCyc contains 22 pathways recorded as being

<table>
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<tr>
<td>Mini-Reviews [textbook pages]</td>
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</table>

A comparison of MetaCyc version 26.5 (December 2022) with KEGG version 104.0+/0415 (December 2022). The first line compares the number of genomes in BioCyc versus those in the KEGG Genome database (not including viral genomes). Subsequent lines compare the number of pathways and reactions in MetaCyc with the number in KEGG (obtained from the KEGG PATHWAY and KEGG REACTION databases, respectively). To calculate the number of textbook pages in commentary, we collected the total lines of commentary in MetaCyc and in KEGG reference databases and converted them to the number of textbook pages by using the formula 3050 words = 1 page.
Figure 2

MetaCyc Pathway: L-tryptophan degradation VIII (to tryptophol)

L-tryptophan:2-oxoglutarate aminotransferase (Sc): Sc-ARO8
2.6.1.27

L-tryptophan:phenylpyruvate aminotransferase (Sc): Sc-ARO9
2.6.1.28

2-oxoglutarate → L-glutamate

3-phenyl-2-oxopropanoate → L-phenylalanine

(indol-3-yl)pyruvate decarboxylase (Sc): Sc-PDC1
indole-3-pyruvate carboxy-lyase (Sc): Sc-PDC5
indole-3-pyruvate carboxy-lyase (Sc): Sc-PDC6
3-(indol-3-yl)pyruvate carboxy-lyase (Sc): Sc-ARO10
4.1.1.74

H⁺ → CO₂

(indol-3-yl)ethanol dehydrogenase (Sc): Sc-ADH5
indole-3-ethanol dehydrogenase (Sc): Sc-ADH3
indole-3-ethanol dehydrogenase (Sc): Sc-ADH2
indole-3-ethanol dehydrogenase (Sc): Sc-ADH1
indole-3-ethanol:NAD+ oxidoreductase (Sc): Sc-SFA1
1.1.1.190

NAD⁺ → NADH

(indol-3-yl)acetaldehyde
experimentally studied in *Pseudomonas putida* KT2440. In contrast, the BioCyc DB for *Pseudomonas putida* KT2440 contains 334 metabolic pathways (including those present in MetaCyc), most of which were predicted during the computational metabolic reconstruction for this strain.

**BioCyc Organism-Specific Databases**

BioCyc organism-specific databases contain the full genome of the organism; database objects describing every gene and protein in the organism; and a mixture of computationally predicted information about the metabolic reactions, pathways, and metabolites of this organism. These databases are created through a series of operations that include computational inferences, import of data from other bioinformatics databases, and, for selected organisms, manual curation.

**Computational inferences**

» Metabolic reconstruction (computational prediction of metabolic pathways and reactions)

» Prediction of pathway holes (genes likely to code for enzymes catalyzing pathway reactions with no assigned enzyme)

» Prediction of transport reactions

» Prediction of operons

» Prediction of protein complexes

» Determination of orthologs to other BioCyc genomes

» Data import

» Creation of database links to UniProt

» Import of Gene Ontology terms and protein features from UniProt

» Import of protein localization data from PSORTdb

» Import of gene essentiality data from OGEE

**Manual curation**

» Curation of gene functions from the literature, including enzymatic activities and regulatory functions

» Curation of protein complexes

» Deletion of incorrectly-predicted enzymatic activities and pathways

» Curation of missing pathways

Some of the BioCyc databases describe organisms that are used extensively in the fields of synthetic biology and metabolic engineering and may be of particular interest to researchers in these fields. The following databases received manual curation.

*Escherichia coli* K-12 MG 1655 (EcoCyc). K-12 strains of *E. coli* serve as the most common hosts for recombinant DNA technology. The EcoCyc DB is arguably the most comprehensive organism knowledgebase available. It has been manually curated by teams from multiple institutions for over 25 years from 42,000 publications. Its contents span protein function, metabolic pathways, transport, and regulation (Keseler et al., 2021).

*Bacillus subtilis* 168. Following *E. coli*, *B. subtilis* is the second most commonly used bacterium in synthetic biology. In addition to being the best-characterized Gram-positive bacterium, the organism can secrete proteins in the gram per liter range and does not produce any toxic by-products (van Dijl & Hecker, 2013).

*Pseudomonas putida* KT2440. *P. putida* is a well-established host for cloning and gene expression, displays solvent tolerance, has a remarkable capability to degrade aromatic compounds, and has a high tolerance to oxidative stress. It is considered a model organism for biodegradation studies and as production platform and is currently used for bioremediation, small molecule production, and bioplastics production (Nikel et al., 2016).

*Saccharomyces cerevisiae* S288c (YeastCyc). *S. cerevisiae* is used in brewing, baking, and as the main source of nutritional yeast. The yeast genome, which was the first eukaryotic genome to be completely sequenced, is highly accessible to manipulation, making it an excellent model for genome engineering and a preferred host for expression of eukaryotic proteins. The *S. cerevisiae* database was generated in 2002 by the *Saccharomyces* Genome Database (SGD) team and benefited from
significant curation by SGD curators. In 2012, the database was transferred to SRI International, where it is curated by members of the SRI Bioinformatics Research Group (Caspi et al., 2014).

*Corynebacterium glutamicum* ATCC 13032. *C. glutamicum* has been traditionally used industrially for large-scale production of amino acids. This “work horse” of the amino acid fermentation industry is nonpathogenic, does not produce any toxins, and has been used for over 70 years for multi-million-ton scale production of glutamate and lysine. It is now commonly engineered to allow the production of a wide range of industrially relevant compounds using a variety of carbon sources (Becker et al., 2018).

*Lactobacillus plantarum* WCSF1. *L. plantarum* is one of the most studied species that are extensively used in the food industry. The bacterium is widely used in the manufacture of dairy products, fermented foods, and bacteriocins (Behera et al., 2018). It is also considered a probiotic and serves as a source of commercially important enzymes such as esterases and lipases (Andersen et al., 1995; Kim et al., 2017; Uppada et al., 2017).

*Lactobacillus rhamnosus* GG. *L. rhamnosus* has been used for various health effects including the prevention and treatment of gastro-intestinal infections and diarrhea and stimulation of immune responses and is currently one of the most widely studied probiotic strains. It has antibacterial activity and anti-inflammatory effects on its host. It also produces and secretes proteins that reduce the inflammatory state and apoptosis of intestinal epithelial cells (Claes et al., 2012; Yan et al., 2007).

The following databases received no manual curation:

*Clostridium acetobutylicum* ATCC 824. Solventogenic clostridia are attractive hosts for anaerobic biosyntheses because they produce a broad spectrum of chemicals that can be used as precursors to or directly as biofuels and industrial chemicals (Tracy et al., 2012). *C. acetobutylicum* natively produces acetone, butanol, and ethanol and has been used for production of chemicals for the biofuels, flavoring, cosmetics, and plasticizers fields. However, clostridia-based bioproduction remains economically unfavorable on an industrial-scale because of the inefficient fermentation process, leading to intensive efforts to modify their metabolic network to remove bottlenecks (Cheng et al., 2019; Liao et al., 2018; Yang et al., 2016).

*Shewanella oneidensis* MR-1: Microbial fuel cells convert organic compounds to electricity (Logan & Rabaey, 2012). The process requires that the microorganisms transfer electrons to electrodes. This is enabled by microbial nanowires, electrically conductive filaments that facilitate long-range extracellular electron transfer. Bacterial nanowires are involved in several additional processes such as electromethanogenesis (Kato et al., 2012) and microbial electrosynthesis (Rabaey & Rozendal, 2010). *S. oneidensis* produces nanowires that conduct current by electron hopping between cytochromes surrounding a filament of an unspecified composition (El-Naggar et al., 2010; Pirbadian & El-Naggar, 2012).

*Geobacter sulfurreducens* PCA: Like *S. oneidensis*, *G. sulfurreducens* produces nanowires, but these nanowires are completely different, comprising pili that have metal-like conductivity attributed to overlapping pi–pi orbitals of aromatic amino acids (Malvankar & Lovley, 2014; Reguera et al., 2005).

*Bacteroides thetaiotaomicron*: This organism is a prevalent and stable resident of the human gut. It possesses an extensive collection of saccharolytic enzymes and serves as a primary fermenter of host-, diet-, or microbially derived polysaccharides. Genetic modification of this bacterium to sense and respond to stimuli in the gut has been suggested as providing a foundation for microbiome engineering (Mimee et al., 2015).

*Deinococcus radiodurans* R1: *Deinococcus* spp. are among the most radiation-resistant microorganisms, showing a remarkable resistance towards ionizing radiation, desiccation, UV radiation, and oxidizing agents. Several studies have used *D. radiodurans* for small molecule production or bioremediation of toxic compounds under stress conditions, such as radioactive environments (Brim et al., 2000; Gerber et al., 2015; Lange et al., 1998).

*Synechocystis* sp. PCC 6803: Photosynthetic cyanobacteria attract significant attention as a promising alternative to traditional hosts due to their ability to use solar irradiation...
and CO2 as their sole energy and carbon sources, respectively. Cyanobacteria have been successfully engineered to produce more than 20 fuels and small molecules directly from CO2. Synechocystis sp. PCC 6803 is one of the cyanobacterial species with the most developed genetic tools and is a favorite cyanobacterium for genetic engineering (Wang et al., 2013; Wang et al., 2016; Yu et al., 2013).

*Klebsiella pneumoniae*: This organism natively produces large amounts of 2,3-butanediol (2,3-BD), a compound that has many industrial applications. The organism is easy to cultivate, grows rapidly in a simple medium, and can metabolize all the major sugars in hemicellulose and cellulose hydrolysates into 2,3-BD (Ji et al., 2011). Despite a certain risk of opportunistic infection by the organism, it has been used extensively for the production of 2,3-BD from many substrates, including wood hemicellulose (Yu & Saddler, 1982; Yu et al., 1985); sugar cane juice (Berbert-Molina et al., 2001); starch (Zheng et al., 2008); Jerusalem artichoke tubers (Sun et al., 2009); and corn cob molasses (Wang et al., 2010).

**BioCyc Software Tools**

**Search Tools and Information Seeking**

One major task for industrial users of BioCyc is finding information about the genome or metabolism of their organism of interest or related organisms. Multiple search tools are available for finding information in BioCyc databases. The quick search box near the top of most BioCyc pages enables name-based searches across the
currently selected database, whether MetaCyc or a BioCyc organism-specific database. Searching for a term such as “pyruvate” or “utilization” produces a list of entities within that database whose name contains the search term, sorted by the type of entity. For example, results from the pyruvate search would include pathways such as pyruvate fermentation to acetate, enzymes such as pyruvate carboxylase, metabolites such as 3-hydroxypyruvate, and reactions involving a metabolite with pyruvate in its name.

Additional search tools are available under the Tools > Search menu. For example, the command Tools > Search > Search Genes, Proteins, or RNAs would enable searching a BioCyc database for enzymes with any combination of the following specified properties: molecular weight range, pI range, number of subunits, protein features, small molecule regulator, cofactor, substrate, or ligand.

The full metabolic network browser generates an organism-specific metabolic chart from an organism PGDB. This diagram can be interactively zoomed in real time in a web browser. As the diagram enlarges, it progressively depicts metabolites, enzyme names, and gene names. The user can search the diagram for the names of metabolites, enzymes, genes, and pathways. The diagram can also be overlayed with omics data and with predicted reaction fluxes, and it can be used for comparing two or more metabolic networks.

Metabolic Engineering Tools

Metabolic Network Explorer provides interactive exploration of the metabolic network of an organism starting with a compound of interest (see Figure 3). Once the user selects the initial compound, the tool shows all the reactions in the organism’s metabolic network that either produce or consume that compound. Selecting one of those reactions generates a short pathway consisting of that reaction. The user can add reactions either leading to the first compound of the pathway or continuing from the pathway’s last compound. Adding more reactions in this fashion builds a novel pathway based on enzymes available in the organism.

When executing this tool in the MetaCyc DB, the user can design pathways that consist of enzymes from multiple organisms. In that scenario, the tool may alert the designer to the presence of metabolic transformations that they are not familiar with and are otherwise difficult to find (Paley & Karp, 2021).

Metabolic Route Search (MRS, see Figure 4) aims to find possible metabolic routes connecting a specified starting molecule to a specified product metabolite. The version of the tool that is available at BioCyc.org can search a single organism-specific database or a user-defined combination of organism-specific databases. The version of the tool available by installing a local copy of the Pathway Tools software also enables reactions to be drawn from the broad collection of metabolic reactions present in
MetaCyc, which covers enzymes that are characterized from thousands of organisms (Krummenacker et al., 2019; Latendresse et al., 2014).

In addition to specifying the feedstock and goal compounds, the user can specify the number of routes to compute and the maximum route length (number of reactions). The software searches for minimal cost routes where the cost of a route depends on the included number of reactions (reactions imported from MetaCyc can be assigned a higher cost), and the number of feedstock atoms lost along the route (which are computed from MetaCyc atom mappings). The user can also specify compounds or reactions to avoid.

The RouteSearch tool can search only fully balanced reactions in which all the components have complete chemical structures. As a result, polymeric reactions are currently not included in the tool’s results.

Metabolic Modeling: When installed locally, the Pathway Tools software enables the user to generate quantitative metabolic flux models. The modeling toolkit includes functions such as flux balance analysis, flux variability analysis, and reaction gap filling.

Omics Data Analysis

In many industrial applications, scientists generate transcriptomics and metabolomics data to better understand the response of their organisms to conditions of interest. BioCyc contains multiple tools that facilitate analysis of these data.

» Transcriptomics data analysis tools include the following capabilities:

» Visually overlay transcriptomics data onto individual pathway diagrams

» Visually overlay transcriptomics data onto multi-pathway diagrams

» Visually overlay transcriptomics data onto full metabolic network diagrams (Figure 5)

» Sort pathways according to a pathway activation score computed from the transcriptomics data

Figure 5

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Pathway Tools Omics Dashboard for *Escherichia coli* K-12 substr. MG1655
GSE71562 Anaerobic–Aerobic transition, significant genes only.

**Figure 6**
» Analyze data using the interactive Omics Dashboard tool (Figure 6)

» Perform gene-set enrichment analysis

» Metabolomics data analysis tools include the following capabilities:
   » Search BioCyc for metabolites based on monoisotopic mass and/or chemical formula
   » Visually overlay metabolomics data onto individual pathway diagrams
   » Visually overlay metabolomics data onto multi-pathway diagrams
   » Visually overlay metabolomics data onto full metabolic network diagrams
   » Sort pathways according to a pathway activation score computed from the metabolomics data
   » Analyze data using the interactive Omics Dashboard tool
   » Calculate metabolomics-based pathway-covering sets
   » Perform metabolite-set enrichment analysis

Comparative Pathway Analysis tools include:

» A comparative analysis tool that visually highlights shared reactions on a full metabolic network diagram.

» A tool that generates tables of the pathways that are shared by a set of organisms. In this tool, the user selects a pathway category of interest, such as amino acid biosynthesis or carbohydrate catabolism pathways; the comparison table is based all pathways within that category.

Availability

BioCyc.org is available by subscription to all users. The E. coli database at EcoCyc.org is freely available.

The Pathway Tools software is freely available to academics and is available for a fee to commercial institutions.

Funding

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Yang, Y., Lang, N., Yang, G., Yang, S., Jiang, W., & Gu, Y. 2016. Improving the performance of solventogenic clostridia by reinforcing the biotin synthetic pathway. *Metab Eng* 35:121-128.


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**Figure Legends**

- **Figure 1.** BioCyc shows full structures for compounds in compound, reaction, and pathway pages; users can specify the level of details in pathway diagrams. Compound structures are uniformly protonated to the typical cellular pH of 7.3. All balanceable reactions are balanced, and an optional atom-mapping coloring helps users follow the chemical transformations. The control panel on the left allows zooming in/out and printing the diagram to a PDF file.

- **Figure 2.** Pathway diagrams show compounds, reactions, EC numbers, enzymes catalyzing the reactions, genes encoding the enzymes, and links to upstream and/or downstream pathways. The flask icon in the upper right corner indicates experimental evidence for the pathway. Every object can be clicked to navigate to its own page, providing additional details. A Detail Level button allows the user to select which features are displayed.

- **Figure 3.** The Metabolic Network Explorer provides interactive exploration of the metabolic network of an organism. This figure shows a user constructed route consisting of two reactions. The route can be expanded or modified by clicking on the circled plus symbols flanking the reactions.

- **Figure 4.** The Metabolic Route Search tool aims to find possible metabolic routes connecting a specified starting molecule to a specified product metabolite. Reactions imported from MetaCyc (indicating the enzymes catalyzing them are not present in the explored organism) are shown in red.

- **Figure 5.** The Cellular Overview Omics Viewer allows painting omics data on a diagram that shows all pathways and enzymatic reactions of an organism. The diagram can accept many types of omics data, such as transcriptomics, proteomics, and metabolomics. A control panel allows the user to control many aspects of the diagram. When multiple time points are recorded, the tool supports animation, moving automatically from one time point to another. Sophisticated zooming controls display more information as the zooming level increases. Popups can show information for individual enzymes in multiple plot types.

- **Figure 6.** The Omics Dashboard consists of a series of panels that summarize omics data for different cellular systems. Each panel contains a set of plots representing one subsystem, with large dots showing the average of multiple values. Clicking on a panel opens a new panel with more data (insert at bottom right corner) enabling to user to move from a high-level view representing the whole organism into individual enzymes with only a few clicks.
45th Symposium on Biomaterials, Fuels and Chemicals (SBFC)

Hilton Portland
Portland, Oregon

April 30–May 3, 2023
www.simbhq.org/sbfc

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Housing deadline: April 3, 2023. SIMB has secured a discounted room rate of $195 (plus taxes and fees) at the Hilton Portland.

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Be sure to check simbhq.org/sbfc for the most up-to-date program details!

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**BIOFUELS, BIOPRODUCTS, AND SYNTHETIC BIOLOGY**

Sessions:
- The Agile BioFoundry and Advanced Bioproducts and Biofuels Process Demonstration Unit: Engines to Drive Biomanufacturing
  - Systems Biology, Artificial Intelligence and Machine Learning within the DBTL cycle
  - Metabolic engineering to improve bioproduction titers, rates and yields
  - Hybrid biological and chemical approaches for production of sustainable aviation fuel and other “hard to electrify” fuels

**TOPIC AREA 2**

**ALTERNATIVE FEEDSTOCKS AND NOVEL BIOBASED MATERIALS**

Sessions:
- Organic Waste Valorization
- Plastic Upcycling
- C1 Metabolism
- New Bio-Based Materials

**TOPIC AREA 3**

**ENGINEERING AND DECONSTRUCTION OF BIOMASS AND RECALCITRANT POLYMERS**

Sessions:
- Engineering bioenergy crops
- Biomass/lignin deconstruction
- Biomass active enzyme discovery, mechanisms, & engineering
- Integration and scale up for lignocellulosic biomass bioconversion

**SPECIAL SESSIONS**

- Biofuels and negative emissions
- Poster Sessions
- Student Oral Presentations with Poster Rapid Fire
2023 SIMB Annual Meeting and Exposition

Hyatt Regency Minneapolis
Minneapolis, Minnesota

July 30–August 2, 2023
www.simbhq.org/annual

Registration, Housing and Abstract Information

» Registration Open: Early Deadline April 21
» Housing Open: Rate $169 +taxes/fees
» Abstract Submission Closes: May 15

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Biocatalysis Sessions:
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» Advanced process and engineering for biomanufacturing of pharmaceuticals
» Fermentation 4.0 - from Data to Value
» Tech Transfer - Increasing the likelihood of success (Panel Discussion)

Environmental Sessions:
» Biodegradation and Bioremediation: groundwater contaminants, plastic waste, plant biomass waste
» Energy and nutrient recovery from municipal and industrial wastewater
» Bio-enabled metal recovery and processing: Discovery and application in biomining
» Microbes and built environment
» Microbiomes of the natural and contaminated environment: genome to function

Metabolic Engineering Sessions:
» Domesticating and Engineering Non-model Organisms
» Metabolic Engineering for Alternative Feedstocks
» Automated and Computational Approaches to Metabolic Engineering
» Metabolic Engineering for Fuels and Chemicals I (commodity chemicals)
» Metabolic Engineering for Fuels and Chemicals II (specialty chemicals)

Natural Products Sessions:
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» Enzymology in Natural Product Biosynthesis
» Synthetic and Systems Biology of Natural Products
» New Modes of Natural Product Bioactivity
» Informatics and Data Science for Natural Products Research

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» Poster Sessions & Science Slam
» Student Oral Talks

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» Early Career Award: Distinguish and encourage young investigators
» SIMB Fellowship Status: Special grade of SIMB membership
» Waksman Outstanding Teaching Award: Recognize the important role of educators and allow SIMB to help support their endeavors

Sponsorship and Exhibit Prospectus
Look for this to be available and sent out in mid-to-late March.
Additional SIMB Conferences

Looking for the recap of the 2022 Recent Advances of Fermentation Technology (RAFT® 14)?

This was published in the previous issue, Oct/Nov/Dec 2022, or available online at simbhq.org/2022/12/13/recap-raft14/

Reminder that RAFT® 15 will be held October 29–November 1, 2023, in Naples, Florida.

Looking for the recap of the 4th International Conference on Natural Product Discovery and Development in the Genomic Era?

Stay tuned for this in the next issue, and save the date for the conference to come back in January 2025!

Newly Announced!

SIMB is holding a new specialized conference, Connecting Microbiome Communities (CMiC). This will be held November 3–6, 2024, in San Diego, California. Learn more at simbhq.org/cmic or stay tuned for the next issue of SIMB News.
A string of events over many years brought me to read *For Blood and Money* by Nathan Vardi. In searching the Norton website for books to review, I noticed a listing on Vardi’s book. Vardi’s career includes having written for Forbes and serving as a managing editor for MarketWatch. His writing shows his understanding of people, their complicated interactions, and their competitiveness. He also understands the nuances of the finances of startups, conglomerates, and hedge funds. In addition, he shows the potential impacts of L. Ron Hubbard and the Church of Scientology on how corporations may be run. Vardi expanded his knowledge of biotechnology and biopharmaceuticals through interviews and conversations with the scientists within the pharmaceutical companies plus the physicians and patients involved in the clinical trials. This is a sweeping review of the development of treatments/vaccines for cancers – potential problems for people as well as domesticated animals. The book is dedicated to people who volunteer to participate in clinical trials and acknowledges to impacts these trials have on themselves and their families.

Several students I met in graduate school opted for careers in pharmaceutical companies. Maintaining contacts with these friends has led to my continued interest in these companies including their products, their interactions, and the personnel involved. The publicity on the companies involved in the development of the COVID vaccines/boosters continued my interest in pharmaceutical companies. These interests led to my recent review of *The Great Secret* by Jennet Conant which covered the launch of the war on cancer and now to the review of Vardi’s book.

The prologue drops the reader into a scenario of Ahmed Hamby’s reaction to unexpectedly being fired from Pharmaclytics, a biotech company in California. Among the stockpile of compounds this biotech company owned was a BTK inhibitor which Pharmaclytics had picked up mainly by chance but was pursuing as a treatment for blood cancer. Although the drug showed promise and was close to finalizing clinical trials, Pharmaclytics decided to drop the drug and to cut the personnel involved which is a not uncommon event in pharmaceuticals. The book included
an unusual turn of events when these same personnel rallied and developed another effective anti-cancer drug. A dual success story woven among the intriguing interactions of the companies and participants.

The remainder of the book covers many topics including

» how much biopharma wants to develop one-in-a million cancer drugs,

» how hard it is for the companies to develop successful drugs,

» how expensive drug development is,

» how important the profits are to the companies as well as to the individuals involved in drug development,

» how dependent the companies are on investors,

» how profit-driven investors are impacting medicine,

» how dependent cancer patients are on the drugs being developed, and

» how participation in clinical trials impacts the patients involved.

The book included an unusual turn of events when the same personnel fired during the development of the BTK product rallied and developed another effective anti-cancer drug. Having a dual success story woven among the intriguing interactions of the companies and participants made Nathan Vardi’s book a fascinating read.
## Upcoming SIMB Meetings

**APR. 30–MAY 3, 2023**
45th Symposium on Biomaterials, Fuels and Chemicals (SBFC)
Hilton Portland • Portland, OR
www.simbhq.org/sbfc

**JUL. 30–AUG. 2, 2023**
SIMB Annual Meeting and Exhibition
Hyatt Regency Minneapolis • Minneapolis, MN
www.simbhq.org/annual

**OCT. 29–NOV. 1, 2023**
RAFT®15 – Recent Advances in Fermentation Technology
Naples Grande Hotel • Naples, FL
www.simbhq.org/raft

## Upcoming Industry Meetings

**MAR. 20–21, 2023**
ICMA 2023: 17. International Conference on Microbiome Analysis
Tokyo, Japan
waset.org/microbiome-analysis-conference-in-march-2023-in-tokyo

**APR. 25–27, 2023**
INTERPHEX 2023
Javits Center • New York City, NY
www.interphex.com/en-us.html

**JUNE 14–15, 2023**
3rd Edition of Chemistry World Conference
Rome, Italy
chemistryworldconference.com/program/scientific-sessions/natural-products-chemistry

**JAN. 21–22, 2024**
ICBFT 2024: 18. International Conference on Bioprocess and Fermentation Technology
Amsterdam, Netherlands

**JUL. 15–16, 2024**
ICABBB 2024: 18. International Conference on Applications of Biotechnology, Bioinformatics and Bioengineering
Stockholm, Sweden

**JUL. 28–AUG. 2, 2024**
Natural Products and Bioactive Compounds Gordon Research Conference
Proctor Academy
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www.grc.org/natural-products-and-bioactive-compounds-conference/2024
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<td>2023</td>
<td>Tae Seok Moon, Thomas Alexander, Charles Isaac</td>
<td>Haley Cox</td>
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