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November 6, no comments Why smart posting is incredibly important for biologists? Simply writing is fundamental to any scientific discipline as it is an easy method scientist and university students talk about their clinical collected information and ideas. Great penning competencies basically topic in biology and that is a organic discipline about whole life at the majority stages as well as all existing microorganisms. Coming up with is a vital an element of the technological task. It is vital for almost any scientist to focus but not only on scientific research content and articles along with on posting. Quite a lot of professionals can deal with some problems and complications concerning this matter. Specialists and trainees through the biological faculty may get good at all exact aspects and key features of the scientific coming up with in biology. An experienced biologist will probably acquire many of these important talents in composing as awareness of characteristics, business, serious research and information based mostly decision making. Forms of composing in biology There are many different brands of penning in biology such as abstracts, article papers, laboratory research, researching manuscripts, major literature critiques, research proposals or grants or loans, laboratory notebooks, cards and talking about scientific disciplines. Abstract is really small breakdown of an investigation pieces of paper. Reviewed newspaper serves as a breakdown of the revealed findings in a few region of biology. This can be a coherent, designed and precisely referenced sms. Research laboratory review explains concerning the findings of this experiments. Investigation manuscript is truly a number one literature in respect to the rewards research experiments. Leading literature critique examines and evaluates the quality of a publication, its content material, with its crafting form, portrays the weak points and muscle of an tests. Studies offer or offer features a justification of your medical run, hypotheses, suggested plans and required resulted. Poster serves as a graphic aid which is made by the scientist for his mouth presentation. Covering art boasts enticing essays, revealing items within scientific well written articles, articles or content and discourse forums. But, you will find conferences all biologists will need to conform with inside of their writing. You should use only precise Language and write within your viewers in third guy. You must stay clear of rates. Usually, use past tense and active tone of voice. Salary amazing focus on Latin leaders and chemical formulae. To the brief description with your solutions you should use desks and numbers. Use scientific citation style. Be highly accurate and brief inside the formulating. About some peculiarities and complications of article writing in biology we should confess which not all biologists can cope with them. In some cases, it is best to uncover the aid of knowledgeable generating company to discuss your scientific preliminary research, ideas and information within optimal way. Firm article writing is extremely important for establishments, businesses, manufacturers and nations since it is how they talk about facts and techniques. Modernized persons seriously should interpret the need for sector making skill sets. It is vital to convey basics and ideas in the right way in the industry scene. Home business generating skill sets are important for advertising and firm correspondence. The skilled firm authoring is indeed so necessary that a multitude of business companies and businesses hire commercial specialists or freelance writers to compose endeavor words. In certain not easy examples it is far better to acquire the help from knowledgeable made to order help as online business simply writing is pretty specific. Varieties business enterprise authoring Opportunity penning works as a general part when it includes lots of different models of operation documents. Regardless of sorts of company records and documents you could be article writing it should be well-defined and concise. Organization letter regarded as a traditional kind of company correspondence around reputable companies, valued clients, buyers, builders and leaders. Message of difficulty is penned whenever you are disappointed with a product or service and is particularly designated to handle a disorder instance. Sales page is the lead snail mail which is certainly authored to encourage the reader to purchase distinct solution or simply a supplement. The Memorandum is really fairly short subject matter delivered from a single man or woman to an alternative and to several

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Chapter 2 : Cheminfostream: Structural Biology and Structure-based Drug Design

Focuses on DNA as a starting point for the consideration of the evolution of information and complexity in the natural world. This volume is the second of two providing introduction to the "Design.

Designed objects, like Mount Rushmore, exhibit characteristic features that point to an intelligence. Such features or patterns constitute signs of intelligence. Proponents of intelligent design, known as design theorists, purport to study such signs formally, rigorously, and scientifically. Intelligent design may therefore be defined as the science that studies signs of intelligence. Intelligent design is controversial because it purports to find signs of intelligence in nature and specifically in biological systems. Intelligent design therefore directly challenges Darwinism and other naturalistic approaches to the origin and evolution of life. Although intelligent design is incompatible with a naturalized, nonteleological understanding of evolution, it has no complaint against evolution per se. Intelligent design is compatible with common descent, the claim that all organisms trace their lineage to some last universal common ancestor. At the same time intelligent design is also compatible with special creation, the claim that organisms, except for small-scale evolutionary changes, were all separately created. Given this flexibility, intelligent design is not readily shoehorned into the usual spectrum of explanations for evolutionary change, which places naturalistic evolution at one end, scientific creationism at the other, and theistic evolution somewhere in the middle. Intelligent design argues that intelligence played a discernible role in the history of life. Whether that intelligence acted through an evolutionary process or by special creations is a separate question, and proponents of intelligent design come down on both sides of this question. Behe, for instance, accepts common descent. Defining Signs of Intelligence The idea that an intrinsic intelligence or teleology inheres in and is expressed through nature has a long history and is embraced by many religious traditions. What has kept design outside the scientific mainstream since the rise of Darwinism has been the lack of precise methods for distinguishing intelligently caused objects from unintelligently caused ones. For design to be a fruitful scientific concept, scientists have to be sure they can reliably determine whether something is designed. Johannes Kepler, for instance, thought the craters on the moon were intelligently designed by moon dwellers. It is now known that the craters were formed by purely material factors like meteor impacts. This fear of falsely attributing something to design only to have it overturned later has hindered design from entering the scientific mainstream. But design theorists argue that they now have formulated precise methods for discriminating designed from undesigned objects. To say intelligent causes are empirically detectable is to say there exist well-defined methods that, based on observable features of the world, can reliably distinguish intelligent causes from undirected natural causes. Many special sciences have already developed such methods for drawing this distinction— notably forensic science, cryptography, archaeology, and the search for extraterrestrial intelligence SETI. Essential to all these methods is the ability to eliminate chance and necessity. Why do the radio astronomers in Contact draw such a design inference from the signals they monitored from distant space? SETI researchers run signals collected from space through computers programmed to recognize preset patterns. These patterns serve as a sieve. Signals that do not match any of the patterns pass through the sieve and are classified as random. After years of receiving apparently meaningless, random signals, the Contact researchers discover a pattern of beats and pauses that corresponds to the sequence of all the prime numbers between 2 and Prime numbers are divisible only by themselves and by one. That startles the astronomers, and they immediately infer an intelligent cause. When a sequence begins with 2 beats and then a pause, 3 beats and then a pause, and continues through each prime number all the way to beats, researchers must infer the presence of an extraterrestrial intelligence. The rationale for this inference is that nothing in the laws of physics requires radio signals to take one form or another. The prime sequence is therefore contingent rather than necessary. Also the prime sequence is long and hence complex. Note that if the sequence were extremely short and therefore lacked complexity, it could easily have happened by chance. Finally, the sequence is not merely complex but also exhibits an independently given pattern or specification it is not just any sequence of numbers but a mathematically significant one—the prime numbers. Intelligence leaves behind a characteristic trademark or

signature—what within the intelligent design community is now called specified complexity. An event exhibits specified complexity if it is contingent and therefore not necessary, if it is complex and therefore not readily reproducible by chance, and if it is specified in the sense of exhibiting an independently given pattern. Note that a merely improbable event is not sufficient to eliminate chance—by flipping a coin long enough, one will witness a highly complex or improbable event. Even so, one will have no reason to attribute it to anything other than chance. The important thing about specifications is that they be objectively given and not arbitrarily imposed on events after the fact. On the other hand, if the targets are set up in advance specified and then the archer hits them accurately, one legitimately concludes that it was by design. The combination of complexity and specification convincingly points the radio astronomers in the movie *Contact* to an extraterrestrial intelligence. Note that the evidence is purely circumstantial—the radio astronomers know nothing about the aliens responsible for the signal or how they transmit it. Design theorists contend that specified complexity provides compelling circumstantial evidence for intelligence. Moreover design theorists argue that purely material factors cannot adequately account for specified complexity. Biological Design In determining whether biological organisms exhibit specified complexity, design theorists focus on identifiable systems e. These systems are not only specified by their independent functional requirements but also exhibit a high degree of complexity. For Behe, irreducible complexity is a sure indicator of design. One irreducibly complex biochemical system that Behe considers is the bacterial flagellum. The flagellum is an acid-powered rotary motor with a whiplike tail that spins at twenty thousand revolutions per minute and whose rotating motion enables a bacterium to navigate through its watery environment. Behe shows that the intricate machinery in this molecular motor—including a rotor, a stator, O-rings, bushings, and a drive shaft—requires the coordinated interaction of approximately forty complex proteins and that the absence of any one of these proteins would result in the complete loss of motor function. Behe argues that the Darwinian mechanism faces grave obstacles in trying to account for such irreducibly complex systems. Once an essential constituent of an organism exhibits specified complexity, any design attributable to that constituent carries over to the organism as a whole. To attribute design to an organism one need not demonstrate that every aspect of the organism was designed. Organisms, like all material objects, are products of history and thus subject to the buffeting of purely material factors. Automobiles, for instance, get old and exhibit the effects of corrosion, hail, and frictional forces. But that does not make them any less designed. Likewise design theorists argue that organisms, though exhibiting the effects of history and that includes Darwinian factors such as genetic mutations and natural selection, also include an ineliminable core that is designed. Paley published his argument in a book titled *Natural Theology*. The subtitle of that book is revealing: *So too, according to Paley, the marvelous adaptations of means to ends in organisms like the intricacy of the human eye with its capacity for vision ensure that organisms are the product of an intelligence.* In arguing for the design of natural systems, intelligent design is more modest than the design arguments of natural theology. For natural theologians like Paley, the validity of the design argument did not depend on the fruitfulness of design-theoretic ideas for science but on the metaphysical and theological mileage one could get out of design. A natural theologian might point to nature and say, "Clearly the designer of this ecosystem prized variety over neatness. Far from rejecting the design argument, Kant objected to overextending it. For Kant, the design argument legitimately establishes an architect that is, an intelligent cause whose contrivances are constrained by the materials that make up the world, but it can never establish a creator who originates the very materials that the architect then fashions. Intelligent design is entirely consonant with this observation by Kant. Creation is always about the source of being of the world. Intelligent design, as the science that studies signs of intelligence, is about arrangements of preexisting materials that point to a designing intelligence. Creation and intelligent design are therefore quite different. One can have creation without intelligent design and intelligent design without creation. For instance, one can have a doctrine of creation in which God creates the world in such a way that nothing about the world points to design. Even if Dawkins is right about the universe revealing no evidence of design, it would not logically follow that it was not created. It is logically possible that God created a world that provides no evidence of design. On the other hand, it is logically possible that the world is full of signs of intelligence but was not created. This was the ancient Stoic view, in which the

world was eternal and uncreated and yet a rational principle pervaded the world and produced marks of intelligence in it. The implications of intelligent design for religious belief are profound. The rise of modern science led to a vigorous attack on all religions that treat purpose, intelligence, and wisdom as fundamental and irreducible features of reality. In other words, Darwin appeared to show that the design in biology and by implication in nature generally was dispensable. By showing that design is indispensable to the scientific understanding of the natural world, intelligent design is reinvigorating the design argument and at the same time overturning the widespread misconception that the only tenable form of religious belief is one that treats purpose, intelligence, and wisdom as by-products of unintelligent material processes. Dembski and Michael Ruse, pp. Law, Darwinism, and Public Education: Examines whether intelligent design is inherently religious and thus, on account of church-state separation, must be barred from public school science curricula. The Biochemical Challenge to Evolution. New York , An impassioned defense of Darwinism against any form of teleology or design. Answering the Toughest Questions about Intelligent Design. From Darwin to DNA. This anthology places intelligent design in conversation with Darwinian, self-organizational, theistic approaches to evolution. A history of the intelligent design movement by a critic of that movement. A Theology of Evolution. A theological critique of intelligent design. Evolution and the Problem of Evil. Grand Rapids , Mich. Provides an interesting analysis of how intelligent design and Darwinism play off the problem of evil. Critique of Pure Reason. The Teleological Argument and Modern Science. This anthology situates intelligent design within broader discussions about teleology.

Chapter 3 : Design and Information in Biology

Following an introductory chapter on design as understood in biology, the various aspects of the biological information revolution are addressed. Areas discussed include molecular structure, the genome, development, and neural networks.

Advanced Search Understanding complex systemsâ€™ their origin, maintenance, and designâ€™ is perhaps the major integrating theme across all of modern science. We live in the so-called Information Age, propelled by an increasingly rich and detailed understanding of the genomic architecture of life, as well as ever-improving computational power. A major emerging theme of our age is that man can continue to learn from, and put to use, the impressive design of natural systems. This book ambitiously champions the growing connection between engineering and biology. This is the second volume in a series, Design and Nature, a project whose goal is to bring together perspectives from biology, engineering, mathematics, physics, and computer science to explore the origin, evolution, and maintenance of complexity in both natural and man-made systems. Complexity is thus both a theme of the book and an appropriate metaphor for its ambitious scope. All of the chapters are information-rich, and many review the historical development of the questions they address, providing a detailed context for the subject. Unfortunately, it is impossible to cover these topics simply, and this fact makes it extremely difficult to find a level at which most readers could connect major themes across the chapters. Nonetheless, chapters on genetics and genomics will reinforce these topics for bioengineers while, for biologists, chapters on thermodynamics bring physical laws into the explanation of biological systems at the most fundamental level. Engineers will benefit from chapters that draw examples and lessons from natural systems. The breadth of this book is challenging, but I find it difficult to imagine how integration of design technologies and biological systems could occur without such a wide purview. A major contribution is the detailed chapter on the origin of life, self-assembly, and evolution contributed by M. Reflections on Life, Self-replication, and Evolution. This piece demonstrates how far we have come in understanding and studying life, but also reveals that we have a long way to go before our own self-replicating machines can match the organization and complexity of even the simplest living organism. Many would consider the design of insect locomotory appendages and sensory apparatuses, or the morphology and physiology of a palm, to be among the best simple systems to mimic in engineering. Excellent review chapters on the mechanisms of insect flight R. Wootton , walking and behavior M. Randall , as well as a review of the general properties of sensory perception as information optimization M. Abdallah reveal that mimicking these systems is far from simple, and their complexity and success reflect millions of years of natural selection shaping well-integrated and efficient strategies for survival. Robotics engineers are actively incorporating elements from these organisms into their latest designs and the chapters in this volume lay out the general principles that make these among the best systems in the natural world from which to copy. This book of contributed reviews concludes with several highly readable and interesting chapters that describe, from an engineering perspective, nature-based strategies for optimization and sustainability with increasing complexity in societies and human organizations, engineered products, and intelligent systems. A final chapter covers the factors that promote the emergence of behavior in robotic systems and draws parallels to selection for group behavior in natural populations. It could be argued that all scientific inquiry is based on the assertion that gathering information increases our understanding of the natural world, and that we should use this information to further improve countless diverse, human agendas. A great amount of information is gathered and disseminated in this second volume of the Design and Nature seriesâ€™ and it amounts to a sometimes overwhelming and always stimulating array of biological and engineering questions. The high cost of the book will limit its audience to academic and corporate buyers, but it is this same group who has the most to gain from integrating scientific disciplines to a level beyond simple metaphor. That complexity is an inherent and unavoidable outcome of natural systems is a major theme of this book and I have little doubt that such complexity will be replicated in subsequent editions in the series.

Chapter 4 : design and information in biology | Download eBook PDF/EPUB

20 Design and Information in Biology Figure 3: The induction by lactose of gene expression in the lac operon of the bacterium E. coli. The three genes of the operon, Z, Y and A, are under the control of a single promoter.

History[edit] Figure 1: Simple schematic for a data warehouse. The Extract, transform, load ETL process extracts information from the source databases, transforms it and then loads it into the data warehouse. Simple schematic for a data-integration solution. A system designer constructs a mediated schema against which users can run queries. The virtual database interfaces with the source databases via wrapper code if required. Issues with combining heterogeneous data sources, often referred to as information silos , under a single query interface have existed for some time. In the early s, computer scientists began designing systems for interoperability of heterogeneous databases. IPUMS used a data warehousing approach, which extracts, transforms, and loads data from heterogeneous sources into a single view schema so data from different sources become compatible. The data warehouse approach offers a tightly coupled architecture because the data are already physically reconciled in a single queryable repository, so it usually takes little time to resolve queries. Difficulties also arise in constructing data warehouses when one has only a query interface to summary data sources and no access to the full data. This problem frequently emerges when integrating several commercial query services like travel or classified advertisement web applications. As of [update] the trend in data integration favored loosening the coupling between data[citation needed] and providing a unified query-interface to access real time data over a mediated schema see figure 2 , which allows information to be retrieved directly from original databases. This is consistent with the SOA approach popular in that era. This approach relies on mappings between the mediated schema and the schema of original sources, and transform a query into specialized queries to match the schema of the original databases. Such mappings can be specified in 2 ways: The latter approach requires more sophisticated inferences to resolve a query on the mediated schema, but makes it easier to add new data sources to a stable mediated schema. As of [update] some of the work in data integration research concerns the semantic integration problem. This problem addresses not the structuring of the architecture of the integration, but how to resolve semantic conflicts between heterogeneous data sources. For example, if two companies merge their databases, certain concepts and definitions in their respective schemas like "earnings" inevitably have different meanings. In one database it may mean profits in dollars a floating-point number , while in the other it might represent the number of sales an integer. A common strategy for the resolution of such problems involves the use of ontologies which explicitly define schema terms and thus help to resolve semantic conflicts. This approach represents ontology-based data integration. On the other hand, the problem of combining research results from different bioinformatics repositories requires bench-marking of the similarities, computed from different data sources, on a single criterion such as positive predictive value. This enables the data sources to be directly comparable and can be integrated even when the natures of experiments are distinct. This data isolation is an unintended artifact of the data modeling methodology that results in the development of disparate data models. Disparate data models, when instantiated as databases, form disparate databases. Enhanced data model methodologies have been developed to eliminate the data isolation artifact and to promote the development of integrated data models. As a result of recasting multiple data models, the set of recast data models will now share one or more commonality relationships that relate the structural metadata now common to these data models. Commonality relationships are a peer-to-peer type of entity relationships that relate the standardized data entities of multiple data models. Multiple data models that contain the same standard data entity may participate in the same commonality relationship. When integrated data models are instantiated as databases and are properly populated from a common set of master data, then these databases are integrated. Since , data hub approaches have been of greater interest than fully structured typically relational Enterprise Data Warehouses. Since , data lake approaches have risen to the level of Data Hubs. See all three search terms popularity on Google Trends. Example[edit] Consider a web application where a user can query a variety of information about cities such as crime statistics, weather, hotels, demographics, etc. Traditionally, the

information must be stored in a single database with a single schema. But any single enterprise would find information of this breadth somewhat difficult and expensive to collect. Even if the resources exist to gather the data, it would likely duplicate data in existing crime databases, weather websites, and census data. A data-integration solution may address this problem by considering these external resources as materialized views over a virtual mediated schema, resulting in "virtual data integration". This means application-developers construct a virtual schema—the mediated schema—to best model the kinds of answers their users want. Next, they design "wrappers" or adapters for each data source, such as the crime database and weather website. These adapters simply transform the local query results those returned by the respective websites or databases into an easily processed form for the data integration solution see figure 2. When an application-user queries the mediated schema, the data-integration solution transforms this query into appropriate queries over the respective data sources. This solution offers the convenience of adding new sources by simply constructing an adapter or an application software blade for them. It contrasts with ETL systems or with a single database solution, which require manual integration of entire new dataset into the system. The virtual ETL solutions leverage virtual mediated schema to implement data harmonization; whereby the data are copied from the designated "master" source to the defined targets, field by field. Advanced data virtualization is also built on the concept of object-oriented modeling in order to construct virtual mediated schema or virtual metadata repository, using hub and spoke architecture. Each data source is disparate and as such is not designed to support reliable joins between data sources. Therefore, data virtualization as well as data federation depends upon accidental data commonality to support combining data and information from disparate data sets. Because of this lack of data value commonality across data sources, the return set may be inaccurate, incomplete, and impossible to validate. One solution is to recast disparate databases to integrate these databases without the need for ETL. The recast databases support commonality constraints where referential integrity may be enforced between databases. The recast databases provide designed data access paths with data value commonality across databases. Theory[edit] The theory of data integration [1] forms a subset of database theory and formalizes the underlying concepts of the problem in first-order logic. Applying the theories gives indications as to the feasibility and difficulty of data integration.

Chapter 5 : Design and information in biology : from molecules to systems (eBook,) [calendrierdelascience

Download Citation on ResearchGate | On Jan 1, , Kenn Kaufman and others published Design and Information in Biology: From Molecules to Systems }.

October 02, Structural Biology and Structure-based Drug Design On 16 October we will hold an eCheminfo Community of Practice conference session at Bryn Mawr College, Philadelphia to discuss latest advances in structural biology related to drug discovery. The session will be chaired by Max Cummings Tibotec Pharmaceuticals and includes a knowledgeable panel of speakers and discussion leaders: A description of the session with presentation abstracts follows: In the affinity optimization phase of a medicinal chemistry effort the timely determination of the 3D structure of a relevant protein-ligand complex can have a huge positive impact. At the same time it is important to note that a wide range of structural information can be useful in guiding drug design efforts - from a single lowly 2D ligand structure to a set of high resolution 3D structures of protein-ligand complexes. Ligand structures and their known activities can help to predict side effects, as well as possible new uses for known drugs. How reliable is a given 3D protein structure, and how can users evaluate this for themselves? Positioning of hydrogen atoms for biomolecular calculations is a longstanding issue, and a new approach to solving this problem is presented. Aspects of the recently popular concept of druggability are explored by two of the speakers. Protein flexibility is discussed in the context of protein-ligand structures related to the regulation of drug metabolism. Attendees will be exposed to various ways in which structural information is used in drug design, and should gain an appreciation for a few currently emerging challenges in the fields of structural biology and structure-based drug design. Please follow continuation to read abstracts of sessions talks. This induction of metabolism negatively impacts drug exposure and forms the basis for detrimental drug-drug interactions. We have engineered a constitutively-active PXR ligand binding domain and demonstrated that it is capable of binding known PXR ligands. Moreover, we used this construct in an inverse structure-assisted drug design effort to understand the structural basis of ligand binding to PXR. During this analysis, we were presented with unexpected binding modes which underscore the plasticity of the PXR ligand binding pocket. Fundamental differences between high- and low-affinity complexes of enzymes and non-enzymes Heather A. Ligand efficiencies were found to be much higher in non-enzymes. This implies they may be more "druggable" targets than enzymes because drug-like affinities can be obtained with smaller molecules which are more easily absorbed and have less functional groups for potential toxicity concerns. Additional data also suggest that divergent approaches may be needed to improve the affinity of ligands for the two classes of proteins. High-affinity ligands are much larger than low-affinity ligands for enzyme complexes. The addition of complementary functional groups is likely to improve the affinity of an enzyme inhibitor through more contact with the pocket, but this process may not be as fruitful for ligands of non-enzymes. High- and low-affinity inhibitors are the same size in non-enzymes. The inherent differences between enzymes and non-enzymes have significant ramifications for scoring functions and structure-based drug design. Gerard J Kleywegt, Uppsala University, Uppsala, Sweden The recent debacle with the ABC transporter structures has shown not for the first time, unfortunately - and probably not for the last time either that the mere fact that a pretty crystal structure is reported in the pages of a glossy journal does not guarantee that the structure is even close to being correct. Some of the causes of serious errors in biomacromolecular crystal structures will be discussed. In addition, a few examples of such errors will be given, and simple ways in which non-experts can assess the overall reliability of a protein crystal structure will be discussed. However, even when the overall structure is reliable, this is not necessarily true for each and every detail. Particularly relevant in this respect are the protein residues that interact with substrates or inhibitors and the interacting molecules themselves. A few examples will be used to demonstrate that the structures of ligands etc. Obviously, for users of protein structures these observations have important implications. First and foremost, crystal structures should be treated with healthy scepticism rather than reverence. The best way to assess the reliability of critical aspects of a structure ligands, active-site residues, metal-binding sites, interface residues, etc. Our efforts to provide such maps, and information derived from

them, for all crystal structures for which structure factors have been deposited with the wwPDB will be discussed. Assignment of Protonation States and Geometries to Macromolecular Structures using Unary Quadratic Optimization Paul Labute, CCG Many computational methodologies relating to macromolecular structures depend significantly on the assignment of protonation states and proton coordinates. The complexity of hydrogen bond networks, tautomers, ionization states and metal ligands often make automated protonation assignment quite difficult. A method based upon Unary Quadratic Optimization is presented to address this problem. The algorithm and thermodynamic theory is described along with some validation results on high resolution crystal structures. Structure-based prediction of small-molecule druggability Alan C. Cheng, Amgen Over half of drug discovery efforts fail in lead identification or in optimization of leads for drug-like properties. We set out to reduce the failure rate by identifying the more druggable targets early on, and discovered that a model based on basic biophysical principles does this very well. These estimates turn out to correlate reasonably well with drug discovery outcomes and are useful in the prioritization of small-molecule drug targets. Computer-aided approaches that have potential in tackling difficult druggability targets will also be presented. Systematic annotation of their primary targets reveals that over of these modulate approximately 85 biological targets. The results of multiple analyses, based exclusively on ligand-focused modeling, will be discussed. Drug pairs sharing a target had significantly higher similarity than drug pairs sharing no target. Also, target pairs with no overlap in annotated drug specificity shared lower similarity than target pairs with increasing overlap. Clustering analysis suggested that side effects and drug-drug interactions might be revealed by modeling many targets. Ligand-based models of diverse targets were constructed and tested in virtual screening protocols. Excellent enrichment was possible against backgrounds of screening molecules. More interesting, however, was that by crossing all drugs against all targets, it becomes possible to identify a number of known side effects, drug specificities, and drug-drug interactions that have a rational basis in molecular structure.

Chapter 6 : Scientific Method Worksheets

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In brief, living organisms are distinguished by their specified complexity. Crystals are usually taken as the prototypes of simple well-specified structures, because they consist of a very large number of identical molecules packed together in a uniform way. Lumps of granite or random mixtures of polymers are examples of structures that are complex but not specified. The crystals fail to qualify as living because they lack complexity; the mixtures of polymers fail to qualify because they lack specificity. Another contribution to the book was written by William A. Dembski, who took this up as the basis of his subsequent work. Specified complexity is fundamental to his approach to intelligent design, and each of his subsequent books has also dealt significantly with the concept. He has stated that, in his opinion, "if there is a way to detect design, specified complexity is it". He provides the following examples to demonstrate the concept: A long sentence of random letters is complex without being specified. A Shakespearean sonnet is both complex and specified. In that context, "specified" meant what in later work he called "pre-specified", that is specified by the unnamed designer before any information about the outcome is known. The value of the universal probability bound corresponds to the inverse of the upper limit of "the total number of [possible] specified events throughout cosmic history", as calculated by Dembski. The terms "specified complexity" and "complex specified information" are used interchangeably. In more recent papers Dembski has redefined the universal probability bound, with reference to another number, corresponding to the total number of bit operations that could possibly have been performed in the entire history of the universe. Dembski asserts that CSI exists in numerous features of living things, such as in DNA and in other functional biological molecules, and argues that it cannot be generated by the only known natural mechanisms of physical law and chance, or by their combination. He argues that this is so because laws can only shift around or lose information, but do not produce it, and because chance can produce complex unspecified information, or simple specified information, but not CSI; he provides a mathematical analysis that he claims demonstrates that law and chance working together cannot generate CSI, either. Moreover, he claims that CSI is holistic, with the whole being greater than the sum of the parts, and that this decisively eliminates Darwinian evolution as a possible means of its "creation". Dembski maintains that by process of elimination, CSI is best explained as being due to intelligence, and is therefore a reliable indicator of design. Law of conservation of information[edit] Dembski formulates and proposes a law of conservation of information as follows: This strong proscriptive claim, that natural causes can only transmit CSI but never originate it, I call the Law of Conservation of Information. Immediate corollaries of the proposed law are the following: The specified complexity in a closed system of natural causes remains constant or decreases. The specified complexity cannot be generated spontaneously, originate endogenously or organize itself as these terms are used in origins-of-life research. The specified complexity in a closed system of natural causes either has been in the system eternally or was at some point added exogenously implying that the system, though now closed, was not always closed. In particular any closed system of natural causes that is also of finite duration received whatever specified complexity it contains before it became a closed system. Quoting Dembski [18] Thus, the event E might be a die toss that lands six and T might be the composite event consisting of all die tosses that land on an even face. Kolmogorov complexity provides a measure of the computational resources needed to specify a pattern such as a DNA sequence or a sequence of alphabetic characters.

Chapter 7 : Controlled experiments (article) | Khan Academy

This is the second volume in a series, Design and Nature, a project whose goal is to bring together perspectives from biology, engineering, mathematics, physics, and computer science to explore the origin, evolution, and maintenance of complexity in both natural and man-made systems. Integration of information and insights from multiple.

A new model of laboratory design is emerging, one that creates lab environments that are responsive to present needs and capable of accommodating future demands. Several key needs are driving the development of this model: The need to create "social buildings" that foster interaction and team-based research; The need to achieve an appropriate balance between "open" and "closed" labs ; The need for flexibility to accommodate change; The need to design for technology to provide access to electronic communications systems throughout the building, which has immense implications on lab design; The need for environmental sustainability ; and The need, in some cases, to develop science parks to facilitate partnerships between government, private-sector industry, and academia. They display an astonishing capacity to adopt new research approaches and tools as quickly as they become available. Thus, science functions best when it is supported by architecture that facilitates both structured and informal interaction, flexible use of space, and sharing of resources.

Meeting Places A critical consideration in designing such an environment is to establish places—break rooms, meeting rooms, atrium spaces—where people can congregate outside their labs to talk with one another. Even stairways, fire stairs, or stairs off an atrium with built-in window seats can provide opportunities for people to meet and exchange ideas. Designers must look for opportunities for such uses in public spaces, making optimal use of every square foot of the building. Atrium spaces are usually very active, popular spaces that support better communication.

Team-Based Labs Laboratories should have casework and engineering services that can easily be changed to support each research team. The CDC building project, see photograph below, right, was designed with generic architectural and engineering services. At move in, the research teams were able to create over 60 different custom laboratory configurations. Collaborative research requires teams of scientists with varying expertise to form interdisciplinary research units. As networks connect people and organizations, sharing data within a team and with other research teams becomes less complicated. So, designers are organizing space in new ways. Laboratory designers can support collaborative research by:

- Creating flexible engineering systems and casework that encourage research teams to alter their spaces to meet their needs
- Designing offices and write-up areas as places where people can work in teams
- Creating "research centers" that are team-based
- Creating all the space necessary for research team members to operate properly near each other
- Minimizing or eliminating spaces that are identified with a particular department
- Establishing clearly defined circulation patterns
- Provide interior glazing to allow people to see one another.

The open lab concept is significantly different from that of the "closed" lab of the past, which was based on accommodating the individual principle investigator. In open labs, researchers share not only the space itself but also equipment, bench space, and support staff. The open lab format facilitates communication between scientists and makes the lab more easily adaptable for future needs. A wide variety of labs—from wet biology and chemistry labs, to engineering labs, to dry computer science facilities—are now being designed as open labs. Most laboratory facilities built or designed since the mid-1990s in the U.S. For the Phase 2 Neuroscience facility at NIH above, right the open labs are designed with the offices to the right and direct access to the labs and the lab support to the left. The open labs are the focal point. There can be two or more open labs on a floor, encouraging multiple teams to focus on separate research projects. Closed labs are still needed for specific kinds of research or for certain equipment. Nuclear magnetic resonance NMR equipment, electron microscopes, tissue culture labs, darkrooms, and glass washing are examples of equipment and activities that must be housed in separate, dedicated spaces. Moreover, some researchers find it difficult or unacceptable to work in a lab that is open to everyone. They may need some dedicated space for specific research in an individual closed lab. In some cases, individual closed labs can directly access a larger, shared open lab. When a researcher requires a separate space, an individual closed lab can meet his or her needs; when it is necessary and beneficial to work as a team, the main open lab is used. Equipment and bench space

can be shared in the large open lab, thereby helping to reduce the cost of research. This concept can be taken further to create a lab module that allows glass walls to be located almost anywhere. The glass walls allow people to see each other, while also having their individual spaces. Flexibility Maximizing flexibility has always been a key concern in designing or renovating a laboratory building. Flexibility can mean several things, including the ability to expand easily, to readily accommodate reconfigurations and other changes, and to permit a variety of uses. The engineering systems may need to be designed to enable fume hoods to be removed or added, to allow the space to be changed from a lab environment to an office and then back again, or to allow maintenance of the controls outside the lab. At NC State, these engineering laboratories are supported by highly flexible mechanical systems that allow for equipment setups to be completed in almost endless number of scenarios. Change is encouraged and seen as beneficial in most cases. From the start, mechanical systems need to be designed for a maximum number of fume hoods in the building. Ductwork can be sized to allow for change and growth and vertical exhaust risers provided for future fume hoods in the initial construction. When a hood is required, the duct can simply be run from the hood to the installed vertical riser. The mechanical systems will need to be re-balanced when a fume hood is added or deleted to efficiently accommodate the numbers of hoods in use and the air changes necessary through each room. Vertical risers are primarily used for the hoods that exhaust special chemicals such as radioactive and perchloric fumes that cannot be mixed into the main laboratory exhaust system. Installing vertical risers during initial construction takes little time and costs approximately one-third of what it costs for retrofitting to add vertical risers later on. Space should be allowed in utility corridors, ceilings, and vertical chases for future heating, ventilation, and air conditioning HVAC , plumbing, and electrical needs. Service shutoff valves should be easily accessible, located in a box in the wall at the entry to the lab or in the ceiling at the entry. All pipes, valves, and clean-outs should be clearly labeled to identify the contents, pressure, and temperature. Equipment Zones It typically takes about three years for a 10, square meter lab building to be designed and built. In either case, there is a good chance that the purpose of the lab will change. If the entire lab is fitted with new casework, the casework may have to be changed before anyone occupies the new laboratory. The equipment zone shown in the dark rectangular color in the photo to the right becomes a type of swing space. Equipment zones are usually fitted out when the research team moves into the lab—that is, when the team knows exactly what will be needed to do the work. The creation of equipment zones that accommodate change easily is a cost-effective design opportunity. The casework is usually located on the outside wall, with islands defined as equipment zones. It may also be helpful to locate 3 ft. Generic Labs When a laboratory facility is designed generically, all the labs are the same size and are outfitted with the same basic engineering services and casework. Generic labs are a sensible option when it is not known who will occupy the space or what specific type of research will be conducted there. Generic lab design may also make sense from an administrative standpoint, since each team or researcher is given the same basic amenities. The best generic labs have some flexibility built in and can be readily modified for the installation of equipment or for changes to the engineering services or casework. Many new labs are designed with mobile casework everywhere except for the fixed fume hoods and sinks. Mobile Casework Technological advances allow for more research procedures to be automated. There are several types of movable casework to consider. Storage cabinets that are 7 ft. Mobile write-up stations can be moved into the lab whenever sit-down space is required for data collection. Casework truly works like a kit of parts with the ability to add or subtract casework easily by the research team. Notice that none of the casework is on wheels to reduce cost and vibration concerns. Only carts are typically built with wheels. Mobile carts make excellent equipment storage units. Often used in research labs as computer workstations, mobile carts allow computer hardware to be stacked and then moved to equipment stations as needed. Data ports are also located adjacent to electrical outlets along the casework. Instrument cart assemblies are designed to allow for the sharing of instruments between labs. Carts are typically designed to fit through a 3 ft. Many mobile carts are load tested to support 2, lbs. The depth of the shelving can vary to allow efficient stacking of equipment and supplies. Mobile base cabinets are constructed with a number of drawer and door configurations and are equipped with an anti-tipping counterweight. The drawer units can be equipped with locks. The typical height of mobile cabinets is 29 in. Also, mobile tables are now available for robotic analyzers and designed to

support lbs. A mobile cabinet can also be designed to incorporate a computer cabinet, which can be hooked up to the robotic analyzers. Carts incorporate a pullout shelf for the server and a pullout tray for the keyboard in front of the monitor. Wire management is designed as a part of the cart. Using the Full Volume of the Lab Space Many labs today are equipment intensive and require as much bench space as possible. Using the full volume of the lab space to stack equipment and supplies can be very helpful and cost-effective. Mobile carts, as mentioned earlier, can be used to stack computer hardware as well as other lab equipment. Overhead cabinets allow for storage above the bench, making good use of the volume of a space. Flexibility can also be addressed with adjustable shelving instead of cabinets. Adjustable shelving allows the researcher to use the number of shelves required, at the height and spacing necessary. If tall equipment is set on the bench, the shelving can be taken down to allow space for the equipment. The bottom shelf should be 19"20 in. These laboratories have high, sloped ceilings which allow natural indirect light in, provide engineering services above the laboratory equipment, and provide enough space to stack the equipment easily and safely. Overhead Service Carriers An overhead service carrier is hung from the underside of the structural floor system. The utility services are run above the ceiling, where they are connected to the overhead service carrier. The utility services that are run above the ceiling should have quick connect and disconnect features for easy hookups to the overhead service carriers. Overhead service carriers come in standard widths and accommodate electrical and communication outlets, light fixtures, service fixtures for process piping, and exhaust snorkels. Wet and Dry Labs Research facilities typically include both wet labs and dry labs. Wet labs have sinks, piped gases, and usually, fume hoods. Dry labs are usually computer intensive, with significant requirements for electrical and data wiring. Their casework is mobile; they have adjustable shelving and plastic laminate counters.

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