Genetics Algorithm Approaches of Cheminformatics Reengineering Process

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ABSTRACT

The important features of Information system and Technology, as it explores the many different technologies inherent in the field of information technology and impact on information systems design, function, operations, and management to its people, organisation as well as science today. Sciences tend to make full usage of information system and technology to seek a description and understanding of the natural world and its physical properties. Hence this study examines the concept of information system, technology and how it affected science namely Cheminformatics. The utilization of Cheminformatics instruments is picking up significance in the field of translational exploration from Medicinal Chemistry to Neuropharmacology. Specifically, require for it the investigation of substance data on huge datasets of bioactive mixes. These mixes frame vast multi-target complex systems it is a drug-target interactome system, that bringing about an extremely difficult information examination issue. Counterfeit Neural Network in short for CNN, algorithms may offer some support with anticipating the collaboration of medications and focuses on CNS interactome. Here, this study to find out the effective and efficient solution through Cheminformatics approach.

KEYWORDS: Cheminformatic; Dataset; Medical chemistry; Counterfeit neural network; Structure activity Relationship; Genetic algorithms

INTRODUCTION

Information system is similar to Information and Communication Technology. It consists of raw data collection (Input); that can be processed into an additional value for an organization (output). After being analysed and processed, it would turn into information data or facts that could be used to answer questions, solve problems or to conduct a project. Moreover, information system also known as a software which is being used in an organization to help organize and analyse databases into a useful information that can be used in the decision making. In other hand, Information technology has been around for quite a long time. Essentially the length of individuals have been around, information technology has been around on the grounds that there were always ways of communicating through innovation accessible at that point in time. There are 4 main ages that divide up the historical background information of information technology. Just the latest age (electronic) and a percentage of the electromechanical age absolutely influence us today. Information technology can be referred to as comprising of three fundamental parts: computational information processing, decision support, and business programming. Information Technology or IT are broadly utilized as a part of business and the field of computing. Individuals use the terms generically when alluding to different sorts of PC related work [1-10].

LITERATURE REVIEW

The usage of technology is very crucial in this modern world. The newly improved advanced technology has changed our life dramatically and make it much easier to anticipate the demand of...
our needs and wants. Information system (IS) is practically being used everywhere and it has been evolving over since the form of device such as smartphone. Now it has been moving to home appliances such as television, which is currently called as a “smart television”. Information system or IS is integrated components that collect, manipulate, store and disseminate data, information and provide a feedback mechanism to meet objectives for individual, group and organization. It is a vital processor that every computer needs because without it, information technology in short IT and information communication technology or ICT will not be able to function properly or follow the instruction given by us. This is because information system is built with software that comes from manufacturer itself where it has its own function and follows the task given by us.

In today’s world, technology has taken a huge part in improving our life. Now, Information system in short IS could take part in helping science to improvised their medical methods into a new whole dimension of science in order to improve the development and assimilation of human life and capabilities of technology. Not only those, but it could also help scientists to conduct practical research to find a new discovery in science to find solutions to the problems of what human has been facing as such, new remedies are yet to be created to fight diseases. Every day, scientists all around the world are working hard to uncover mysterious solutions to what we, the human, are actually facing not only in the term of medicine but also, new methods in the field of surgeon and technology. How information system could help science would depend on the characteristic and how it is being used. Development in advanced technology and human capabilities; by using information system software it could help to gather all the raw data and molecule from the past research by synthesis with the new finding. Hence, it would uncover the mysterious of what it might be a new discovery in medicine or drugs to cure unsolved diseases. Especially by emerging technology combine with high instrumentation will help in advance the process without any complication. For instance, how research being conducted for the past couple of decades was immensely complicated because they have to go through every practical research and books unlikely how it is now because we have advance machinery, technology, information and internet to help us [11-25].

**DISCUSSION**

Range of definition given for this concept; however, information does not have a specific and uniform definition. The definition stated by N. Winer, who determines the content of the information gleaned from the outside world in the process of our adjustment to it and adapt it to our senses (McGarry M., 2008). Information system is the combination of people’s innovation and computer that processes or unravels information. Information and communication technology in short ICT; that organization uses, as well as a way of communication people use to interact which leads in support for business processes. There are no specific and clear distinction between information systems, computer system, and business processes. Nowadays information systems mainly use to gain maximum benefits by processing data from inputs to generate information system, a combination of hardware, coordination, and decision-making in an organization. It is also known as decision-making support system. It is a collective combination of collection of people, procedure, software, database, and device that support problem specific decision making. The main usage of information system in an organisation is communication. Which it allows people to communicate easily, for instance the method of communication, which is electronic mail or E-mail, which are delivered extremely fast, it can be sent and received from any devices all around the world, that has an internet connection. In addition, the availability of cloud function which allows people to make changes, add information and share with one another in a community cloud. Thus, it makes communication better and faster, as most information are now accessible, which people could gain the right information at the right time. In order to meet one’s need and want as it is important to obtain accurate and complete information [26-30].

Business process may be difficult, as entrepreneurial culture and the degree to which the existing information systems tend to represent compatibility and application functionality significantly affect a firm’s propensity to adopt cloud computing technologies. The discovery supports our abstract development and suggest complementarities between innovation diffusion theory and the information processing view. Industry professionals to aid in making more informed adoption decisions in regard to cloud computing technologies in order to support of the supply chain. Due to the fact that Information System play a major role mainly in Business by creating new products and services, make it possible for managers to use real time data when making a decision, therefore information must be relevant and reliable in order to help people in their organization to achieve their goals and perform tasks more effectively that then lead to competitive advantage and these systems make their jobs easier as possible. Z. Messner stated that information as data on monetary phenomena and processes used in decision-making processes (Messner Z., 1991). Namely for human resource management, marketing and administration.

Moreover, Information system could stores documents, histories, communication records as well as operational data, that could be use in the future for better references, as it act as a useful historical information. It improves efficiency of certain organisation’s operation in order to achieve aims, objectives and goals, namely to achieve higher profitability. Information system needs to be flexible, which able to accommodate certain amount of variation, regarding the requirement in terms of supporting business process. The impact of information system being flexible, enable cost efficiency for the business. Information technology tend be to be applied within business operations that can save a great deal of time during the fulfilment of daily tasks. Business tends to include knowledge management, artificial intelligence, expert system, multimedia, and virtual reality system. Papwork is processed immediately, and financial transactions are automatically calculated by information system. Although businesses may view this expediency as a boon, there are untoward effects to such levels of automation. As technology amend, tasks that were formerly performed by human employees are now carried out by computer and information systems. This leads to the elimination of jobs and, in some cases, alienation of clients, thus lack of face-to-face interaction. Unemployed specialists and once-loyal employees may have difficulty securing future employment [26-30].

Therefore, as much as information system could help make tasks easier for an organisation, it has certain issues and obstacles, which for an organisation to have to face. Firstly, is culture challenges, to state the fact that each countries and regional areas have their own intellectual awareness or culture as well as their own customs that could significantly affect individuals and organization involved in global trade, by means that it is a contagious issues with an influence affecting our culture. An organisation should also be aware of the
best way to approach global demographics, which had profound on the global landscape as well as on profession of globalization.

Secondly, limitation of language usage, by means that language differences create an issue that can make it difficult to translate the actual meaning of a conversation for instance. Due to the fact that meanings from another language may be different which leads to misunderstandings, irritations, feelings of exclusion and a sense of inferiority, are daily challenges for not having spoken the language of English speakers trying to communicate in the language of global business. As English mainly use all across the world for conversation. Moreover, on the internet there are no facial expressions, body language, or other non-verbal cues, which makes communication even more complex [31-35].

Thirdly, time and distance challenges whereby these issues can be difficult to overcome for an individual and organisations involved with global trade in remote locations. Moreover, large time differences make it difficult to communicate directly to people on the other side of the world. With long distance, it can take days to get the products or part from one location to another. Although Information System as well and technology may be able to make communication faster and easier to use for individuals and organisation, it may lead to difficulty in terms of different time zone, and the distance, where schedule for instance a meeting will be hardly organized to get group of individuals from all over the country to have a meeting through video conversation.

Fourthly, technology transfer issues, where most government does not allow certain military-related equipment and systems to be sold in some countries. As access to capital is limited, the capital costs of ESTs are generally higher than those of standard technologies. Also, the fact that risks of identifying existence for new technologies, financing costs will tend to be higher. Moreover, the availability of FDI is restricted and unevenly distributed around the world. Although many countries are review their trade policies in order to loosen restrictions in terms of the markets, substantial tariff barriers as an obstacle remain in many cases for imports of external technologies including energy supply equipment. This limits exposure to energy in terms of productivity, resulting improvement pressures from foreign competition on national suppliers and avert early introduction of sustainable energy that are able to maintain on certain level by alternation from abroad. Where foreign exchange of restrictions and public revenue deliberation make across-the-board tariff removal difficult.

Lastly, regarding trade agreement. An international agreement on condition of trade in goods and services. Countries often enter into trade agreements with each other. Although it creates a dynamic business climate where business are protected by the agreement, lower government spending where numbers of government may put the fund for better use, increase in number of expertise that leads to misunderstandings, irritations, feelings of exclusion and a sense of inferiority, are daily challenges for not having spoken the language of English speakers trying to communicate in the language of global business. As English mainly use all across the world for conversation. Moreover, on the internet there are no facial expressions, body language, or other non-verbal cues, which makes communication even more complex [31-35].

In terms of education, Information Technology makes it conceivable to have online education. Unlike in the past when education was tied to particular limits, now the education sector has changed. With the establishment of online education services, students can learn from anywhere utilizing internet. This has helped in spreading of vital education materials to all individual mainly students across the globe. Online education is also being improved by the making of portable application which empowers
students’ access to educational material via their mobile phones. In terms of agriculture, information technology plays a major part in advancing the agricultural sector. These days farmers can sell their products right from the homestead utilizing the internet. All they need to do is create a site to advertise their products, orders will be placed directly by means of the site and the farmers will deliver fresh goods to the consumers once orders have been made. This gets rid of the middlemen who tend to increase cost of farming products with the aim of making profits. In this case, Information Technology benefits both the farmer and the consumer. The consumer gets the product at a low price when it is still fresh, and the farmer gains additional income [36,37].

Somehow, most likely the best point of interest of data innovation is the making of new and intriguing occupations. PC software engineers, Systems analysts, Hardware and Software designers and Web fashioners are only a portion of the numerous new business opportunities made with the assistance of Information Technology. In addition to that, job posting sites usually use Information Technology as a classification in their databases. The class incorporates an extensive variety of employment across architecture, engineering, and management functions. Individuals with occupations in these areas commonly have a progress on education mainly in software engineering and or information systems which they may also possess related industry certifications. Short courses in Information Technology fundamentals can also be discovered online and are particularly helpful for the individuals who want to get some introduction to the field before focusing on it as a career. A career in Information Technology can include working in or leading Information Technology departments, product advancement teams, or research groups.

Headways in data innovation have had numerous huge points of interest on society and might be the crown gem of our time and indicate the progression of humankind, be that as it may, this has not come without its disadvantages to Information Technology or Information Systems that leave individuals thinking about whether the great exceeds the terrible. A few weaknesses of data innovation incorporate while data innovation might have streamlined the business process it has additionally made occupation redundancies, cutting back and outsourcing. This implies a ton of lower and center level occupations have been done away with bringing on more individuals to end up unemployed. Despite the fact that unemployment made, and occupation made due to Information Technology is no place close in examination as Information Technology has unquestionably delivered inconceivable number of employment. Change tragically is constant and in business terms you need to move with movement or be abandoned.

Despite the fact that data innovation might have made correspondence speedier, less demanding and more advantageous, it has additionally purchased along security issues. From wireless sign block attempts to email hacking, individuals are currently agonized over their once private at get ting to be open information. Significant measure of individuals is uninformed of the endeavours substantial organizations go to gather information on individuals and the utilization and offering of this information. By and large thoughts, for example, online treats which promote the web client’s hobbies can be seen as something to be thankful for yet one could think about whether faculty data processing is something worth being thankful for in the hands of extensive organizations whose essential premium is to inspire you to spend your well-deserved cash.

On the other hand, industry specialists trust that the web has made professional stability a major issue as since alternation continues changing with every day. This suggest one must be in a steady learning mode, on the off chance that he or she wishes for their business to be secured. This of the disservices of Information technology or Information System has been around since the presentation of all innovation and one must not overlook that life is a ceaseless learning cycle and that you should stick to it or be abandoned. Moreover, as computing systems and capabilities keep growing worldwide, information overload has turned into an undeniably critical issue for many Information Technology experts.

Efficiently processing immense measures of information to produce beneficial business intelligence necessitates a lot of processing power, sophisticated software, and human analytic expertise. As data innovation might have made the world a worldwide town, it has likewise added to one society overwhelming another weaker one. For instance, it is currently contended that US impacts how most youthful young people everywhere throughout the world now act, dress and carry on. Dialects too have gotten to be dominated, with English turning into the essential method of correspondence for business and everything else. Loss of dialect and society is never something worth being thankful for, yet Information Technology or Information System additionally impressive at holding learning of society, dialect and one-of-a-kind practices, so it is hence down to individuals to hold their character or social personality.

Over dependence on innovation where Computers and the Internet has turned into a fundamental part of this current life, a few individuals, particularly youths who grow up with it, would not have the capacity to work without it. The Internet is conceivably making individuals sluggish, especially with regards to task or venture research as opposed to perusing books in a library, individuals can simply do a Google search. Also, the usage of technology in an organization, company or business decreases the number of hours that a human works at that company. This may even result in some people losing their work because technology is doing it for them. However, this is advantageous for the organization as their profit will increase because they do not need to pay their workers as much because they are not needed as much. With the ever-growing variety of social networking sites such as Facebook and Twitter, it is not impossible that the traditional communication skills will be lost. Especially children who always engrossed in these websites because exchange of information and responsive skills are not important with computers. Emails and instant messaging have replaced the old tradition of handwritten letters. Although this is advantageous considering time constraints, but a personal touch and sense of feeling are lost in comparison to consuming the time to sit down and handwrite a letter.

In terms of health, studies have proved that technology can create a number of problems with a person’s health. Many scientists, doctors and researchers are worried about potential links between technology and heart problems, eye strain, obesity, muscle problems and deafness. Waste released from technology can contaminate the environment which not only makes people ill, but it also harms the environment.

CHEMINFORMATICS

The availability of open access and online chemical databases has made it easier for the people to know more about what is going on in the chemistry world and to keep updated with the recent findings. Integrating databases with other resources, including
journal writing, it was important for advance scientific progress. Enhancement of data and information integration specifically in scientific software system has become an issue of awareness among the chemists and the cheminformatics community for the past few years, but the issue has been solved by the development of the Semantic Web techniques. In the field of sciences, in order to develop new research, it is always based on the previous findings. Therefore, it is crucial to keep record of the previous concepts of sciences, so that it can be used in the future whether for improvements on the finding or for the benefit of references. The Semantic Web technique itself is the inclusion of machine-processable data in web documents and it is aimed to transform information which has not been structured or only semi-structured into a fully organized web document which will be made accessible both to humans and machines. There are actually three major sections in the Semantic Web technique, they are the Dublin Core, Open Archives Initiative Object Reuse and Exchange in short OAI-ORE and finally Simple Knowledge Organization in short SKOS. In this modern world, information system plays a very important role especially in collecting, organizing and storing data or information. It is almost impossible for an organization to not have information system department. Information system also consists of a series of advanced technology such as the latest software and hardware. In order to achieve information faster and in an organized manner, software such as Microsoft Excel might be of help in such situation. These sophisticated technologies can only be functioned to its full potential by people who have the accomplishment in handling those technologies. Basically, information system is initially created for supporting operations, management and decision making in an organization. It also helps an organization in terms of communication networking, processing, and interpreting data.

Science is the body of knowledge of the physical and natural world which often requires the support of technology. The advancement of science is largely maintained by the frequently updated technology. Especially in the field of research, technology is probably the most significant necessity in ensuring the success of that certain research. Even tools and equipment used in science cannot be developed without the help of technology. The results of a science research which is made possible by the existence of technology are usually used for the benefits of the society such as drug discovery in the medical world. For instance, drug discovery nowadays requires proper management system and the enhancement of the accessibility of potentially useful data. This can only be achieved by the existence of an information system and technology. If information system and technology were to be combined in the advancement of science, surely, they will produce an efficient and a more effective finding in any research. This is due to the requirements needed for research to be conducted, such as the complicated comprehensions of words in chemistry which can only be interpreted using a certain program such as the Semantic Web techniques, Borkum 2014.

Semantic as we know it is the study of meanings of words, phrases, signs, and symbols. In chemistry alone there are plenty of words, phrases, signs, and symbols which are not familiar to the people who are not in the field of chemistry. Fortunately, with this newly founded technology, it is easier for the consumers to search for the meaning of a certain word, phrases, signs, or symbols. A Semantic Web technique is especially created for the purpose of smoothing of any chemistry research. The Dublin Core specifically focuses on definitions of specifications, vocabularies, and best practice for the assertion of metadata on the web. Dublin core is an initiative to create a digital “library card catalogue” for the Web the elements that offer extended categorize information and improved document indexing.

Similarly, OAI-ORE Open Archives Initiative Object Reuse and Exchange in short OAI-ORE, is when some resources have meaningful relationship with other resources or becoming a part of other resources, such as a figure or a table which belongs to another resource of a scientific publication. Another example is when a resource is being associated with another resource such as when a review is made; it is related back to its original text of the scientific publication. The automated software system will then manipulate these sources instead of separating them. This technique can make a certain research or reference a lot more efficient, effective and less time consuming. Then finally, the Simple Knowledge Organization System in short SKOS, is a project that encouraged publication of controlled vocabularies on the Semantic Web, it is also highly dependent upon informal methods, including natural language. Another few important aspects of information system and technology in terms of supporting science are validity, accountability, and value proposition. Validity is deeply important, for instance in a laboratory environment an invalid risk assessment could have negative consequences, endangerment of human life inclusive. In the case of accountability, an organization or an individual is accountable or responsible for the validity of the information that they provided, while value proposition depends on individual perspective and organizational perspective. From an individual perspective, it is less time consuming in doing work and the data or information provided have been standardized so that it is easier to carry out research. From an organizational perspective, it is risky to provide a source of information as an unauthorized access can easily condemn or leak out valuable information on the website if the website has a weak safety system.

Science, innovation and advancement each speaks to a progressively bigger classification of exercises which are profoundly associated however particular. Science adds to innovation in no less than six ways. Firstly, new learning which serves as an immediate wellspring of thoughts for new mechanical potential outcomes. Secondly, wellspring of devices and methods for more proficient building outline and an information base for assessment of attainability of plans. Thirdly, research instrumentation, lab strategies and expository techniques utilized as a part of examination that in the end discover their way into configuration or mechanical practices, frequently through middle of the road disciplines.

Next, routine of exploration as a hotspot for improvement and absorption of new human aptitudes and abilities in the end helpful for innovation. Moreover, formation of an information base that turns out to be progressively critical in the appraisal of innovation as far as its more extensive social and natural effects. Lastly, information base that empowers more productive methodologies of connected examination, advancement, and refinement of new innovations. The opposite effect of innovation on science is of in any event measure up to significance that through giving a ripe wellsprings of novel exploratory inquiries and in this manner additionally defending the assignment of assets expected to address these inquiries in an effective and auspicious way, amplifying the motivation of science and as a wellsprings of generally inaccessible instrumentation and methods expected to address novel and more troublesome investigative inquiries all the more effectively. Illustrations of each of these two-way connections are stated. Due
to numerous backhanded and coordinate associations in the middle of science and innovation, the exploration arrangement of potential social advantage is much more extensive and more looking so as to differ than would be recommended just at the immediate associations in the middle of science and innovation.

The Institute has previously distributed contextual investigations one of advancements that have been come regarding the interest driven material science research. The studies show the long-time scales over which the procedure between the first disclosures and the advancement of items that use the examination can happen. Four key advances highlighted in these distributions that empowered a number of the innovation-based developments found in the administration areas are portrayed beneath. First example is Fibre Optics where the advancement of fiber optic advances has taken into consideration broadband web associations and quick overall correspondence of data, empowering online developments in the administration areas, for example, virtual interfaces, online medicinal services checking and remote systems administration. The innovation has its roots in material science research by John Tyndall in the 1800s and in later research into photonics. Secondly, the utilization of lasers has took into consideration both quick correspondence through broadband systems, furthermore for quick information stockpiling and recovery through Compact Disc in short CD and Digital versatile Disc or Digital Video Disc, DVD advances. The guideline behind the laser was produced by Albert Einstein and it took over 40 years before the principal obvious wavelength laser was built. Analysts at the University of Surrey are as of now attempting to control quantum course lasers which could be utilized for restorative analysis, for instance, glucose observing for diabetics. Thirdly, Liquid Crystal Display in short as LCD innovation empowers cell phones through lightweight, low-control utilization and ease screens. The first exploratory examination that supports LCD innovation was led over 100 years prior, with further advancement in the second 50% of the most recent century. Basic LCD showcases are found in watches and number crunchers with more intricate shows now in cell telephones, personal computer or PC screens and televisions. Lastly is GPS where the capacity to precisely decide the position of an article or individual has empowered advancements, for example, web-based robbery following of autos and satellite route. GPS is supported by an extensive variety of material science research, from nuclear timekeepers to the hypothesis of General Relativity, consolidated with space science and innovation.

CHEMINFORMATICS: GENETIC ALGORITHM

Genetic Algorithm, also called by partial-least-square methods with functions to find out and predicting comprehensive bioactive parts, most likely to be beneficial for science field today equally to the world globally. The integration of chemistry and information system has proven to be advantages as it assist chemist to comprehended and gather all the feature of molecules with certain pharmacological has improved. This innovation and accessible of database have help to measure and analyze in the discovery of potential new drug. Moreover, because of the unlimited accessible in the field of cheminformatics, chemists have the ultimate pleasure in the use enormous tools and methods that are advanced, safe, and bioavailable. Cheminformatics, and compound informatics, is the utilization of personal computer and instructive procedures connected to a scope of issues in the field of science. These in silico strategies are utilized as a part of, for instance, pharmaceutical organizations during the time spent medication disclosure. The utilization of Cheminformatics instruments is picking up significance in the field of translational exploration from Medicinal Chemistry to Neuropharmacology. Specifically, require for it the investigation of substance data on huge datasets of bioactive mixes. These mixes frame vast multi-target complex systems it is a drug-target interactome system, that bringing about an extremely difficult information examination issue. Counterfeit Neural Network in short for CNN, calculations may offer some support with anticipating the collaboration of medications and focuses on CNS interactome. However, Cheminformatics can be simple with the right devices, as it begins with database. It keeps all your basic data and delegate information readily available. In any case, all the more imperatively, a cheminformatics framework like CDD Vault. CDD is a hosted database solution for secure analysis, management and sharing chemical biological data, where it let intuitively organise chemical structure and biological structure data and allows collaboration within the organization internal or external partners through web interface and it incorporates every one of the instruments important for a simple to utilize, end-to-end arrangement. That registration, synthetic drawing, looking, and representation, and additionally SAR and different examinations. CDD Vault even serves as the storehouse for more than two million open mixes and examine results. CDD Vault gives a complete medication revelation informatics framework, effortlessly information for action, compound similitude, and selectivity.

CDD Vault makes the testing objectives of cheminformatics less troublesome where commonplace web interface makes cheminformatics more available to learners. In addition, incorporated diagrams offer some assistance with visualizing the relationship in the middle of action and properties. Information base instructional exercises also offer some assistance with navigating the cheminformatics scene such as submerge seek on exercises, structure, or naturally figured physical properties. What is more, as a protected, facilitated cloud application, CDD Vault is a practical arrangement that is ideal for scholastic gatherings, charities, and little organizations. Current facilitated cloud design gives cost investment funds, additionally makes it conceivable to fabricate more natural interfaces, better than legacy frameworks. At the point when cheminformatics work includes others, CDD Vault makes coordinated effort simple with implicit correspondence and sharing capacities. The precise cut of the information with just the accomplices determined. For instance Cheminformatics Analysis of Organic Substituents which identify most of common substituents, it calculation of substituent properties, and as well as mechanical recognition of drug-like bio isosteric groups.

Namely, Enterprise Capability as an industrial strength database with all the benefits of the cloud which is easy to use. State the fact that there are zero footprint web interference run on all major browser, served from the certified cloud for immediate turnkey deployment. As for the cloud technology provide private, multi-tenant architecture that are able to provide affordable security and has demonstrate 99.999% history availability. Moreover, it provides management tool that are easy to track in real time changes, showing full details for new compounds and data. The fact that it is customizable, where it could define protocols, data fields, preferred graphs, and even chemical registration business rules, however customization services are available for more complex requests. The entire combinatorial science is likewise considering the idea of substituents, acting for this situation under the name building squares. The present study concentrates on natural substituents from the perspective of cheminformatics and tries to
reply to questions about the aggregate number of substituents in known natural science space and the ramifications of this number for the span of virtual natural space science. The portrayal of substituents by ascertainment properties is too examined, including a technique for computing substituent drug-resemblance in view of an examination of the dissemination of substituents in a vast database of medications versus an extensive database of non-drugs. At long last an illustration of the application of a vast database of medication such as substituents with computed properties is presented a Web-based instrument for programmed distinguishing proof of bio isosteric gatherings.

CONCLUSION

The advancement of information technology achieved a turning point with the improvement of the Internet. Through the course of its improvement, specialists started finding different utilizations for the network, and utilization of the technology spread around the world. Access to the Internet today by people, organizations, and institutions alike has created a worldwide business sector for Internet service and has spurred an increase in productivity in the technological communication field. Information technology continuously developed in order to enhance today's organization system to be more manageable, productive and systematic. Constant improvements can possibly create new applications of information technology that can affect all the areas of the society which includes the economy, households, government, and private sectors. Therefore, it is important to always be aware of the latest update of the technology in order to use the information system and technology to their maximum potential; it will definitely result in improvement, not just in an organization but also among individuals of the society.

RECOMMENDATION

Although information system has already beneficial to almost all organizations, it is still open to embrace improvements. One of them is to create a Technology Usage Agreement for the staffs of that certain organization. For instance, an organization has the right to control its staffs from browsing or visiting inappropriate web sites that are known to house viruses such as torrent and file sharing sites. In addition, the organization could also develop limitation for data or music downloading policy and include terms and conditions for data confidentiality. This is to assure that the organization confidentiality is safely guarded by its staffs.

The second improvement that can be made is having a back-up plan. It is impossible to know what will happen to an organization in the future, to be safe; hence a backup plan is essential. One solution for this issue is to hire or consult one of the many firms that provide an off-site storage where an organization can keep record of the key documents and important databases. So that when an unexpected disaster happens, the organization can still recover by referring to the back-up plan. The third betterment that can also be made is by setting up a schedule periodic maintenance downtime. Where the employees of the information system and technology department can manage update, scan for viruses, backup all the data, fixing errors. This is due to the prevention of data loss and system malfunction. Then the fourth method that can be considered is to contact the Internet Service Provider of an organization. An organization can request to increase its bandwidth. Increasing bandwidth has a lot of advantages for the organization such as making multitasking much easier, and it could also reduce application hang-ups caused by slow updating of the software of that certain application. After that, the organization may also create a comprehensive technology plan. Comprehensive technology plan is where an organization can monitor the updates of technologies nowadays and hence use it for the benefit of the organization. The results of the monitoring on the latest technologies can be evaluated closely and then it can be adopted into the organization to replace aging workstations that are no longer efficient and effective in today's modern world.

Finally, an organization must at least make the effort to create a web site which is user-friendly. This can be done by considering software as a service. The organization then can provide many options for functions such as word processing, search engine, contact person or email and most importantly customer relationship management function.

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