



AOARD-114035

Nanobioinformatics: emerging computational tools to understand nano-bio interact

Upadhyayula Murty
INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
UPPAL ROAD, TARNAKA
HYDERABAD, 500007
IN

09/06/2019
Final Report

DISTRIBUTION A: Distribution approved for public release.

Air Force Research Laboratory
Air Force Office of Scientific Research
Asian Office of Aerospace Research and Development
Unit 45002, APO AP 96338-5002

REPORT DOCUMENTATION PAGE					<i>Form Approved</i> OMB No. 0704-0188	
<p>The public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing the burden, to Department of Defense, Executive Services, Directorate (0704-0188). Respondents should be aware that notwithstanding any other provision of law, no person shall be subject to any penalty for failing to comply with a collection of information if it does not display a currently valid OMB control number.</p> <p>PLEASE DO NOT RETURN YOUR FORM TO THE ABOVE ORGANIZATION.</p>						
1. REPORT DATE (DD-MM-YYYY) 06-09-2019		2. REPORT TYPE Final		3. DATES COVERED (From - To) 14 Sep 2011 to 13 Sep 2014		
4. TITLE AND SUBTITLE Nanobioinformatics: emerging computational tools to understand nano-bio interaction				5a. CONTRACT NUMBER		
				5b. GRANT NUMBER FA2386-11-1-4035		
				5c. PROGRAM ELEMENT NUMBER 61102F		
6. AUTHOR(S) Upadhyayula Murty				5d. PROJECT NUMBER		
				5e. TASK NUMBER		
				5f. WORK UNIT NUMBER		
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY UPPAL ROAD, TARNAKA HYDERABAD, 500007 IN				8. PERFORMING ORGANIZATION REPORT NUMBER		
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) AOARD UNIT 45002 APO AP 96338-5002				10. SPONSOR/MONITOR'S ACRONYM(S) AFRL/AFOSR IOA		
				11. SPONSOR/MONITOR'S REPORT NUMBER(S) AOARD-114035		
12. DISTRIBUTION/AVAILABILITY STATEMENT A DISTRIBUTION UNLIMITED: PB Public Release						
13. SUPPLEMENTARY NOTES						
14. ABSTRACT Final originally sent to DTIC by some manner on 11/16/2012. However, deliverables were not in PK Award File. Initiated this WF to re-submit & complete deliverables in PK Award File.						
15. SUBJECT TERMS Nanobio devices						
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT SAR	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON CHEN, JERMONT	
a. REPORT Unclassified	b. ABSTRACT Unclassified	c. THIS PAGE Unclassified			19b. TELEPHONE NUMBER (Include area code) 315-227-7007	

Project Final Report

Title of the project:

"Nanobioinformatics:

Emerging Computational
Tools to understand nano-bio
interaction".

Submitted To

ASIAN OFFICE OF AEROSPACE
R&D
7-23-17, ROPPONGI,
MINATO-KU TOKYO
160-0032 JAPAN

Submitted by

Principal Investigator:

Dr USN Murty

Chief Scientist
Head, Biology Division
CSIR-Indian Institute of
Chemical Technology
Tarnaka,
Hyderabad - 500 007

Email: murty_usn@yahoo.com

Tel: 040-7193134

Mobile: 0944082794

Index

	Page No.
General Information about project	03
Abstract	03
Introduction	04
Phase wise project details	05
Phase-I: Data collection	05
Phase-II: Self Organising Maps	06
Steps involved in SOM algorithm	07
SOM Results	09
Phase-III-Nano-database	10
Data flow	11
Web interface & application	14
Description of database	15
Database screen shots	17
Results	27
Conclusions	27
Outcome of the project	27
Future programs	28

General information about Project (AOARD- Grant 114035):

PROJECT TITLE: "Nanobioinformatics: Emerging Computational Tools to understand nano-bio interaction".

Name of the Principal Investigators: **Dr U.S.N.Murty**
Head, Biology Division
CSIR-Indian Institute of Chemical Technology
Tarnaka, Hyderabad-607, INDIA
Email address: usnmurty@iict.res.in
Tel: +91-40-27160123-40

ABSTRACT:

Nanoparticles have become a part of our daily life due to the advancement in various product developments ranging from cosmetics to medicine to other primary and secondary utility products. There is a requirement of much more regulation for quality check of the products developed from nano particles. Therefore, various toxicity assessment of these tiny particle derived products are the need of the time and development of organized and regulated protocol is essential for the upcoming future and booming market of products made of nanoparticles. Especially, products nanoparticles based products applied in the area of medicine including imaging, drug delivery agents, cosmetics are to be strictly assessed for toxicity before reaching the market.

Observing the future need, it is easily understandable that the cost, time, labour of the experimental assessment will also rise exponentially as on a range of products will keep on occupying the market. The need of a well established computational system which can efficiently share the cost, time and labour of the experimental requirement with certain amount of accuracy is going to expedite the overall process of toxicity assessment professionally.

Development of prediction tool for nanotoxicity studies is a novel approach using computational techniques by which we can predict the nature of particular nanoparticle easily when compared to the traditional *in-vivo* methods where animals are used as test organisms and experiments are conducted for days, weeks even months depending on the need and nature of the experiment.

This computational system will aid in easy categorization of the particles depending on several parameters utilized. The application of the artificial intelligence system for classifying the data depending on the parameters considered will easily identify the compounds within the certain toxicity ranges.

The developed database in this regard will grow further depending on the upcoming raw data deposition in the public domain databases and in the literatures which will in turn raise the strength of the prediction further due to availability of more data points.

INTRODUCTION:

Development of prediction tool for toxicity of nanoparticles requires huge amount of data, data based on which the tool is developed it can be generated by conducting the studies on the Wister male/female mice, these mice are very good test subject for carrying out the studies because these have similar genome as of the humans almost of 90%, these are easy to handle, morphological changes occurring in them can be easily noticed through naked eye.

PHASE WISE PROJECT DETAILS:

Phase I: Data collection

Collected data on nanoparticles from the different manuscripts published in different journals, these articles are downloaded and data is collected from it. There are many online journals which report studies of NANOPARTICLES toxicity these are: Nature Nanotechnology, SCIENCE DIRECT, ACS NANO, BMC, Small, Nano Today, Current Nano science, Nano Letters, Nanotechnology. The key words which were used for searching in the site are Nanotoxicity, Nano-particles, Nanoparticles AND toxicity. These were among the few words used for searching the articles. Huge number of articles have been found, all the relevant articles were downloaded and studied for the data. These articles were sorted based on the source and the particles upon which it is studied and sorted according to element and its source from where it is found like science direct, acs nano, wiley publications, etc.

Elements like Gold, silver, titanium are few among upon which most of the studies are concentrated, other elements are also reported but few numbers of articles had been found

comparing to these elements in conjugated form had also been studied such as silver nitrate, titanium dioxide, and many more. Many studies had been reported until now as these NP individually are not potent but in conjugated form proved to be very dangerous to use. These data reported in the journals are collected in an excel sheet, each article deals with different nanoparticles and as each investigator will one conducts different experiments for his own purpose, this make challenging for the data collection and as every journal has different type of data represented in different fashion like tables, graphs, percentages, ratios and etc.

Phase –II: Application of SOM algorithm

Self Organizing Maps (SOM)

Briefly, SOM is a data clustering technique invented by Professor Teuvo Kohonen of Helsinki University of Technology, Finland, in 1960's which reduce the dimensions of data through the use of self-organizing neural networks. In SOM the neurons are organized in a lattice, usually a one or two-dimensional array, which is placed in the input space and is spanned over the inputs distribution. The processing units in the SOM lattice are associated with weights of the same dimension of the input data. Using the weights of each processing unit as a set of coordinates the lattice can be positioned in the input space. During the learning stage the weights of the units change their position and "move" towards the input points. This "movement" becomes slower and at the end of the learning stage the network is "frozen" in the input space. After the learning stage the inputs can be associated to the nearest network unit. When the map is visualized the inputs can be associated to each cell on the map. One or more cell that clearly contains similar objects can be considered as a cluster on the map. These clusters are generated during the learning phase without any other information. Hence, the main applications of the SOM is to visualize high-dimensional data in a two dimensional manner, and the creation of abstractions like in many clustering techniques.

The characteristic that distinguishes the SOM net from the other cluster algorithms is that not only similar inputs are associated to the same cell but also neighborhood cells contain similar types of documents. This property together with the easy visualization makes the SOM map a useful tool for visualization and clustering of large amount of data.

Steps involved in the algorithm

1. **Initialization:** Randomly initialize a weight vector (W_i) for each neuron i

$$W_i = [w_{i1}, w_{i2}, \dots, w_{in}], n \text{ denotes dimension of input data}$$

2. **Sampling:** Select an input vector $X = [x_1, x_2, \dots, x_n]$

3.

4. **Similarity matching:** Find the winning neuron whose weight vector best matches with the input vector

$$j(t) = \arg \min \{ \|X - W_i\| \}$$

5. **Updating:** Update weight vector of winning neuron, such that it becomes still closer to the input vector. Also update weight vectors of neighbouring neurons – farther the neighbour, lesser the change.

$$W_i(t+1) = W_i(t) + \alpha(t) * h_{ij}(t) * [X(t) - W_i(t)]$$

$\alpha(t)$: Learning rate that decreases with time t , $0 < \alpha(t) \leq 1$

$$h_{ij}(t) = \exp(-\|r_j - r_i\|^2 / 2 * \sigma(t)^2)$$

$\|r_j - r_i\|^2$ = Distance between winning neuron and other neurons

$\sigma(t)$ = Neighbourhood radius that decreases with time t

6. **Continuation:** Repeat steps 2 to 4 until there is no change in weight vectors or up to certain number of iterations For each input vector, find the best matching weight vector and allot the input vector to the corresponding neuron/cluster

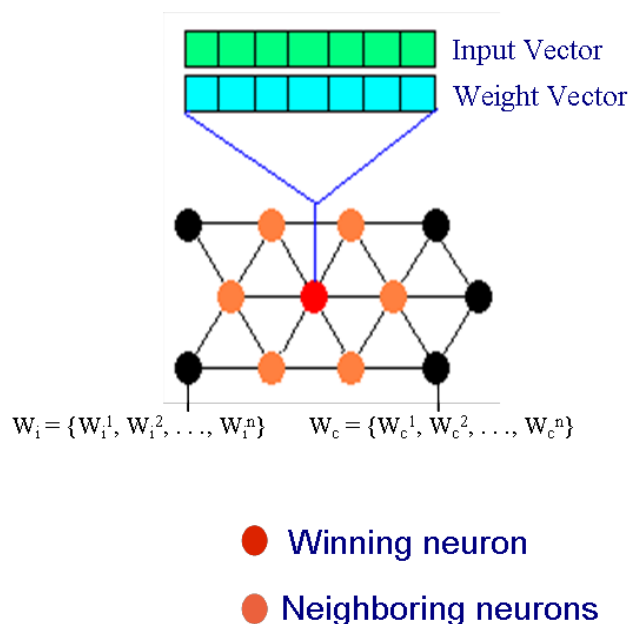


Figure1. Illustration of an SOM neural network

Data Normalization:

Summarized data is normalized linearly in such a way that minimum value in each category is 0 and the maximum is 1. This is done to ensure that all the parameters are given to equal importance when clustering is done. The neuron weightage was adjusted by the learning rate. The learning rates and distance threshold values for the SOM are generally default values. Unsupervised learning was done using the data learning constant of 0.01 with 5000 iterations that yielded clusters based on the neighborhood distance.

Parameters identified for application of SOM:

Parameters are Size, Shape, Concentration, Exposure time, Mode of exposure, Surface group, present on it Stress response, Cell viability, Up regulation and down regulation of enzymes (GSH, SOD, GSSH, MDA, ALK, ALT, LDH), Cell lines.

Preprocessing: After collection of data from the published articles preprocessing of the data is done the process of pre processing include

- Decide which fields to include in that data collected (document the rational for inclusion/exclusion)

- Collect additional data if needed
- Select data subsets to use
- Consider use of sampling techniques to reduce size of data set decide if data balancing is required

SOM result:

The obtained results of the SOM analysis helps us to integrate the parameters depending on their proximity to each other applying artificial intelligent based analysis of each data points and their respective statistical importance. The output of the analysis clustered the data points with a human understandable color gradation ranging from red to dark black. The objective of this color gradation is to represent the appropriate visual representation of each considered datapoints under the analysis along with their exact position in the dataset under consideration. An example of such representation is provided below in figure 2. The result was generated with 10,000,00 iteration during the analysis.

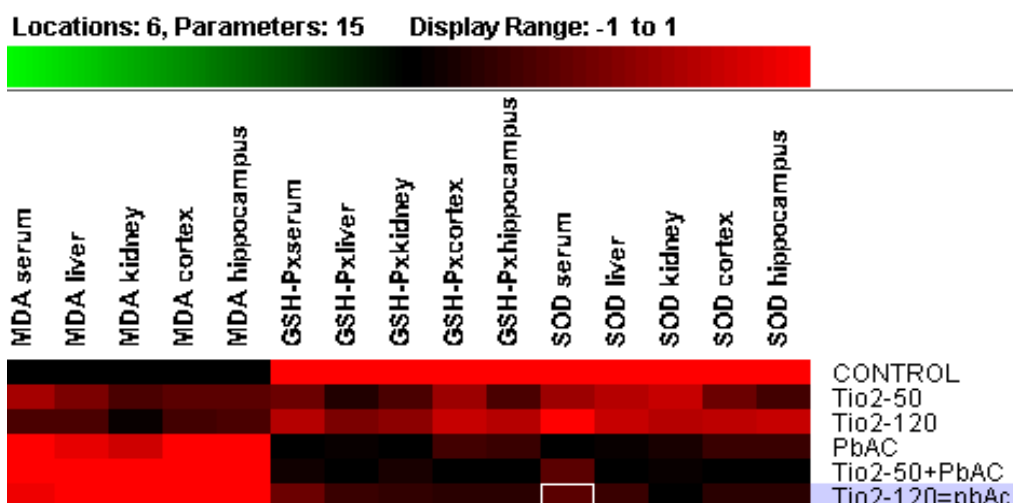


Figure2. Result from SOM, shows that the stress response of Titanium Dioxide when injected orally single dose with and without lead acetate, titanium dioxide when injected alone not much change in enzymes (Malondialdehyde, Glutathione reductase, superoxide Dismutase) concentration is seen (light region), but with conjugation of lead acetate on surface of TiO₂ an elevated concentration of these enzymes found (dark regions).

In this clustering system any amount of data related to the nanoparticle toxicity properly preprocessed according to the need of the analysis could be used for clustering and the position of the new data points could be easily determined to understand their relative position with relation to the training data set applied for the model development.

Phase-III: Development of database:

Back end database support is an integral part of any tool development project which not only yields in the organized categorizing and querying of the available data points also leaves the scope of future large scale development and commercial product development.

The database development details are provided in the later section in details:

Database design and architecture:

The database was constructed as a relational database management system (RDBMS) for data storage in Microsoft SQL Server in the back-end on a web server, as it is the leading open source industrial strength database, and is competitive in quality and performance with the major proprietary databases. The relational architecture of nanoinformatics ensures data integrity and future expandability. In addition, nanoinformatics makes use of custom-designed lookup tables that ensures rapid responses to search queries. The database structure was designed to be modular, to avoid unnecessary redundancy and to allow fast queries. The database schema conforms to a set of functional dependencies designed to avoid unnecessary data duplication. Functional dependencies are considered standard practice in establishing good database designs. The data inserted into this SQL Server database can have its origin in different kinds of sources. Once the data are available in the SQL Server database, uniform access via a standardized query language is provided. The contents of the database are then made available for interactive querying using a standard three tier approaches consisting of the SQL Server database as the back-end, a web server capable to dynamically create hyper text markup language (HTML) pages as the middle tier, and web browsers as light-weight clients. In addition to data access via web browsers, the query language of the underlying RDBMS can be used directly to access data at different integration levels by the database administrator. Since the data in nanotox database is

purely based on experimental results, it is reasonable to assume that additional entries in future would continue to improve the scope of the database.

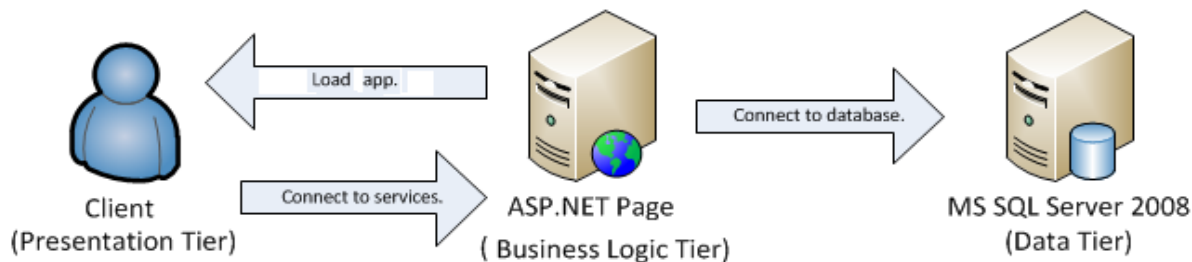
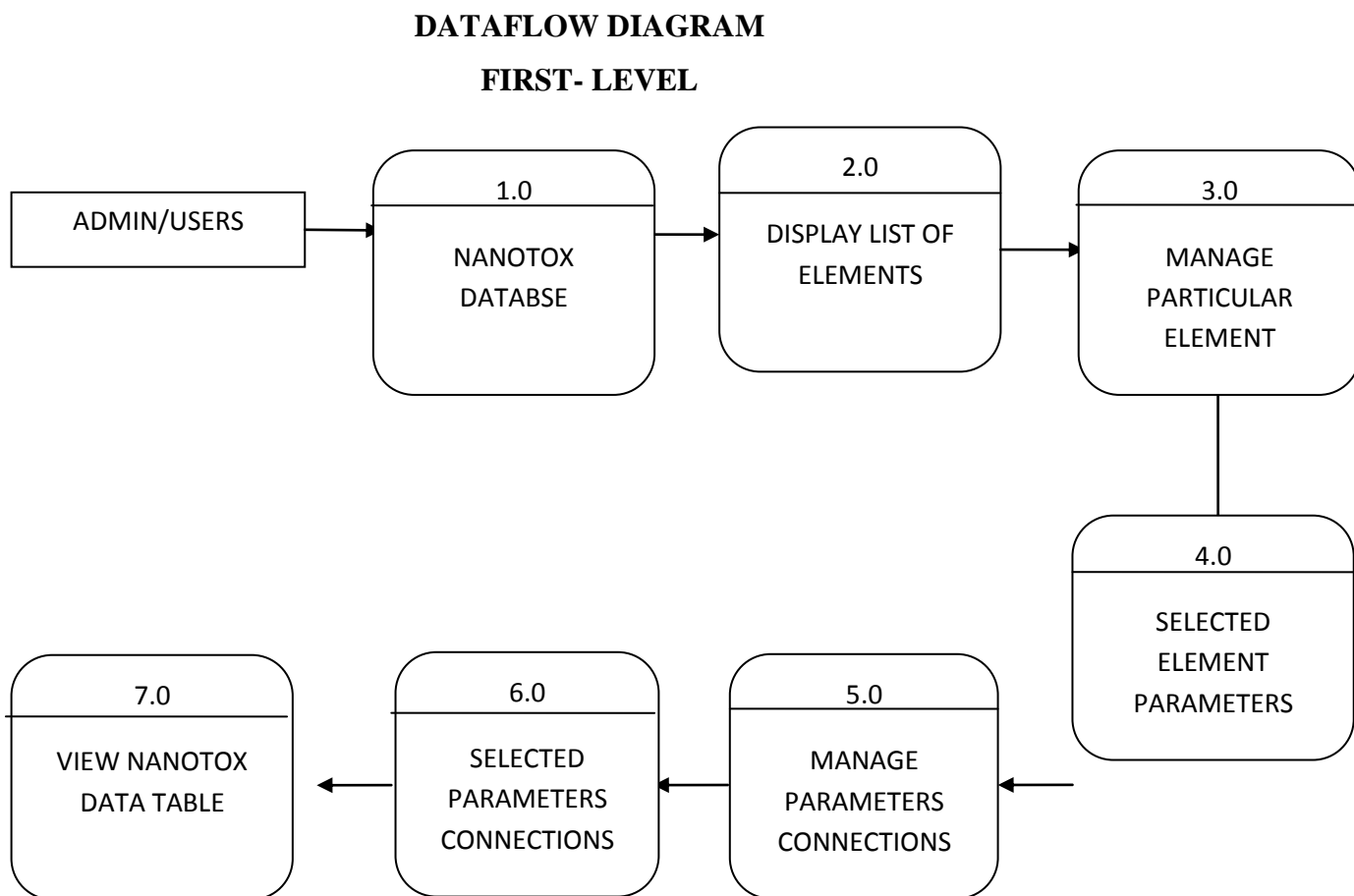
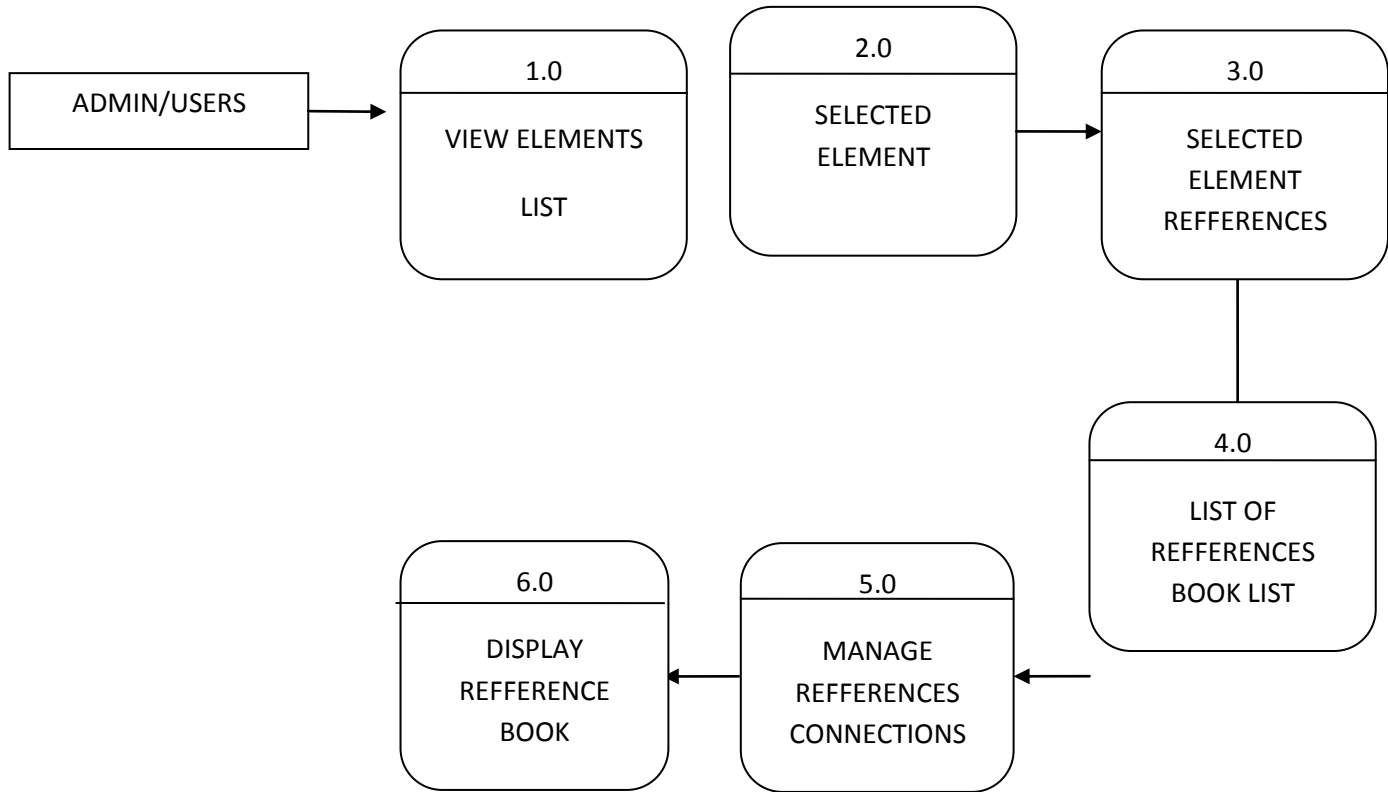


Figure3.Client server relation representation.

The level wise data flow diagram is provided in the following section:



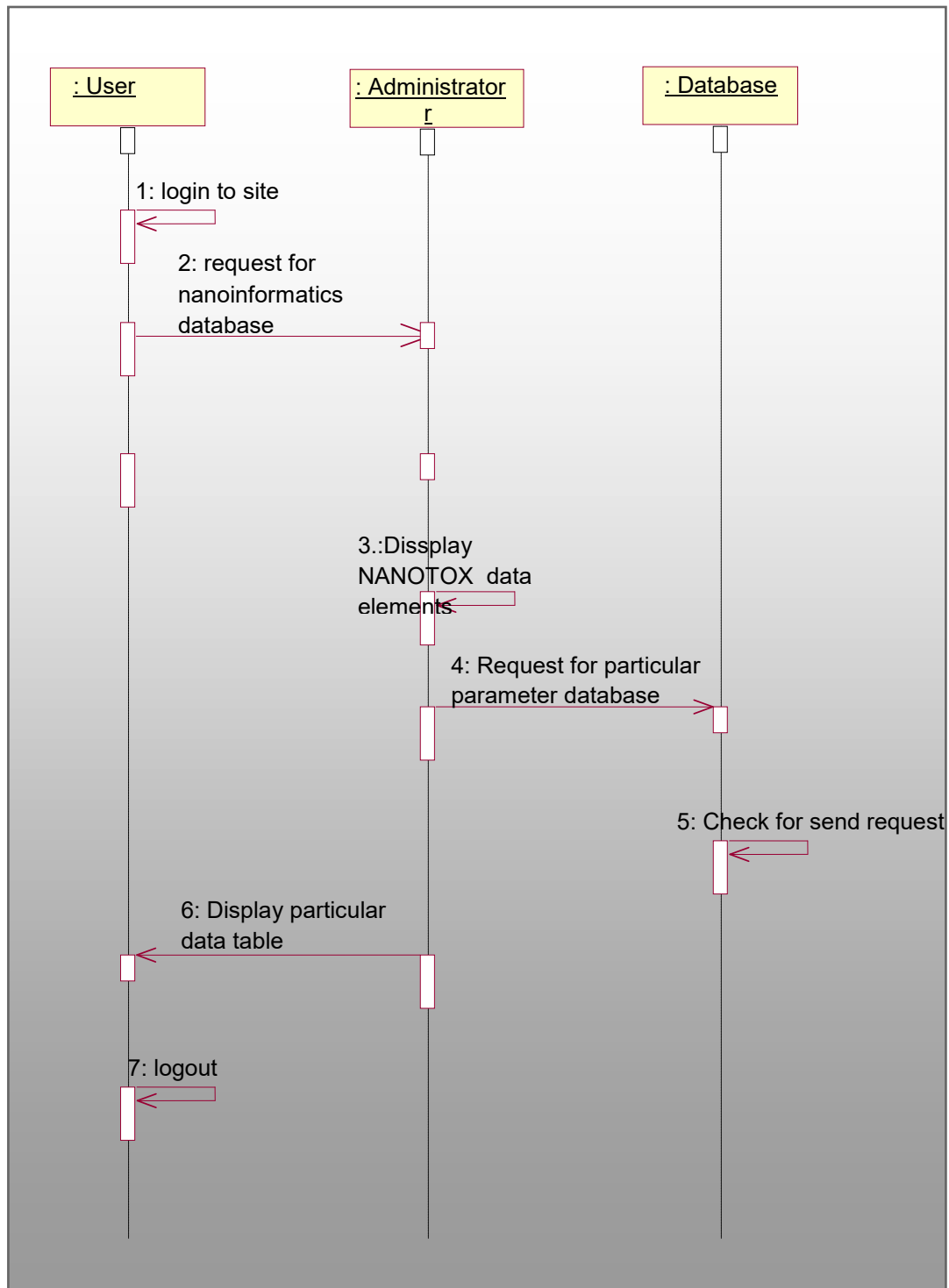
DATAFLOW DIAGRAM
SECOND- LEVEL



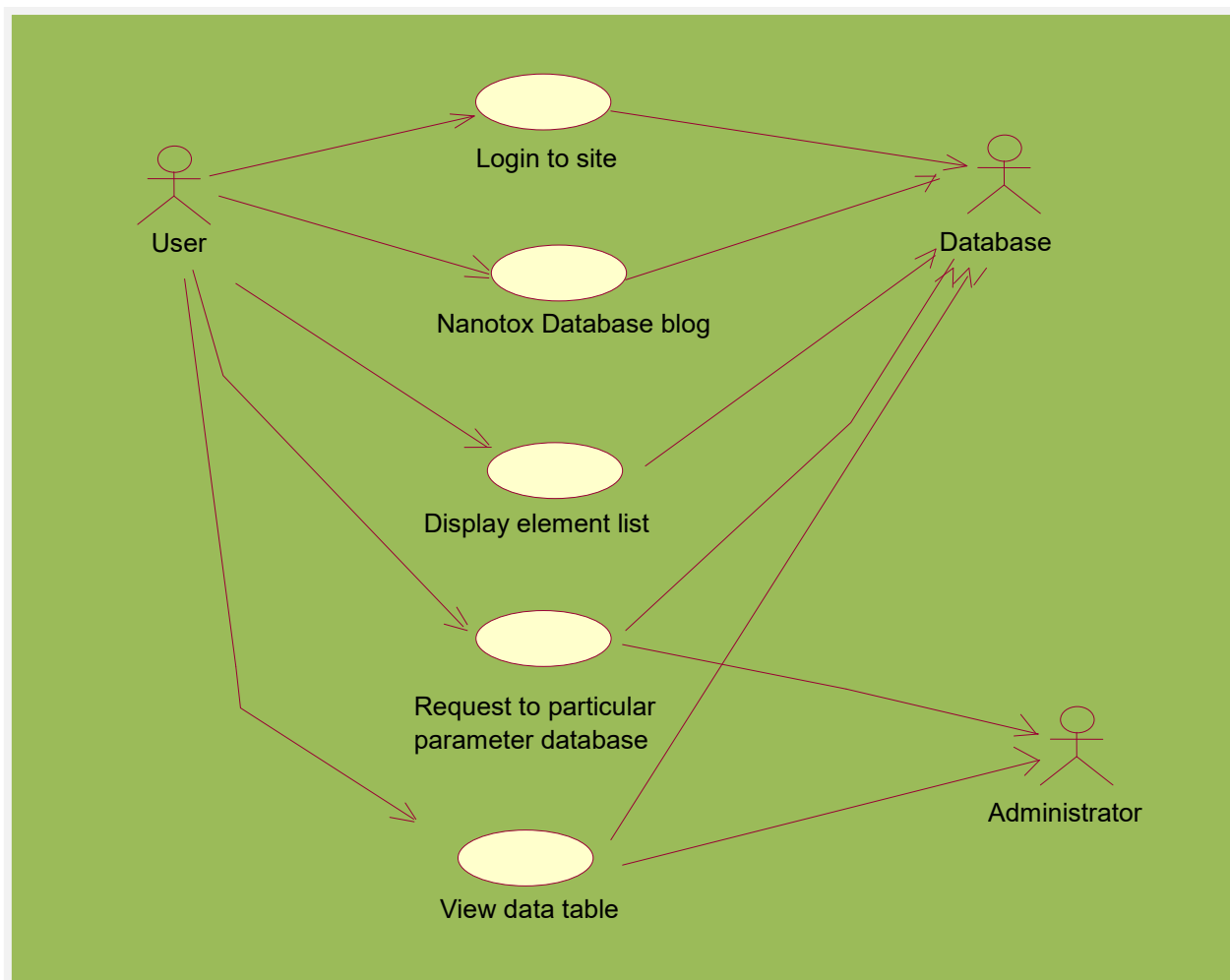
The detail of the entity relationship diagram is area as follows:

ENTITY-RELATIONSHIP DIAGRAMS

Sequence diagram for Nanoinformatics:



Use case diagram for Nanoinformatics:



Web Interface and Application:

The whole database is running under Microsoft SQL Server, MicroSoft.NET technology, integration of open source softwares. HTML and ASP.NET technologies have been used to build the dynamic web interface. SQL Server, a relational database management system (RDBMS), works at the backend and provide commands to retrieve stored NANOTOX data. C#, a server side scripting language, provides interface and functions to fetch data from database. MicroSoft.NET and SQL Server combination is quite efficient and powerful for database management.

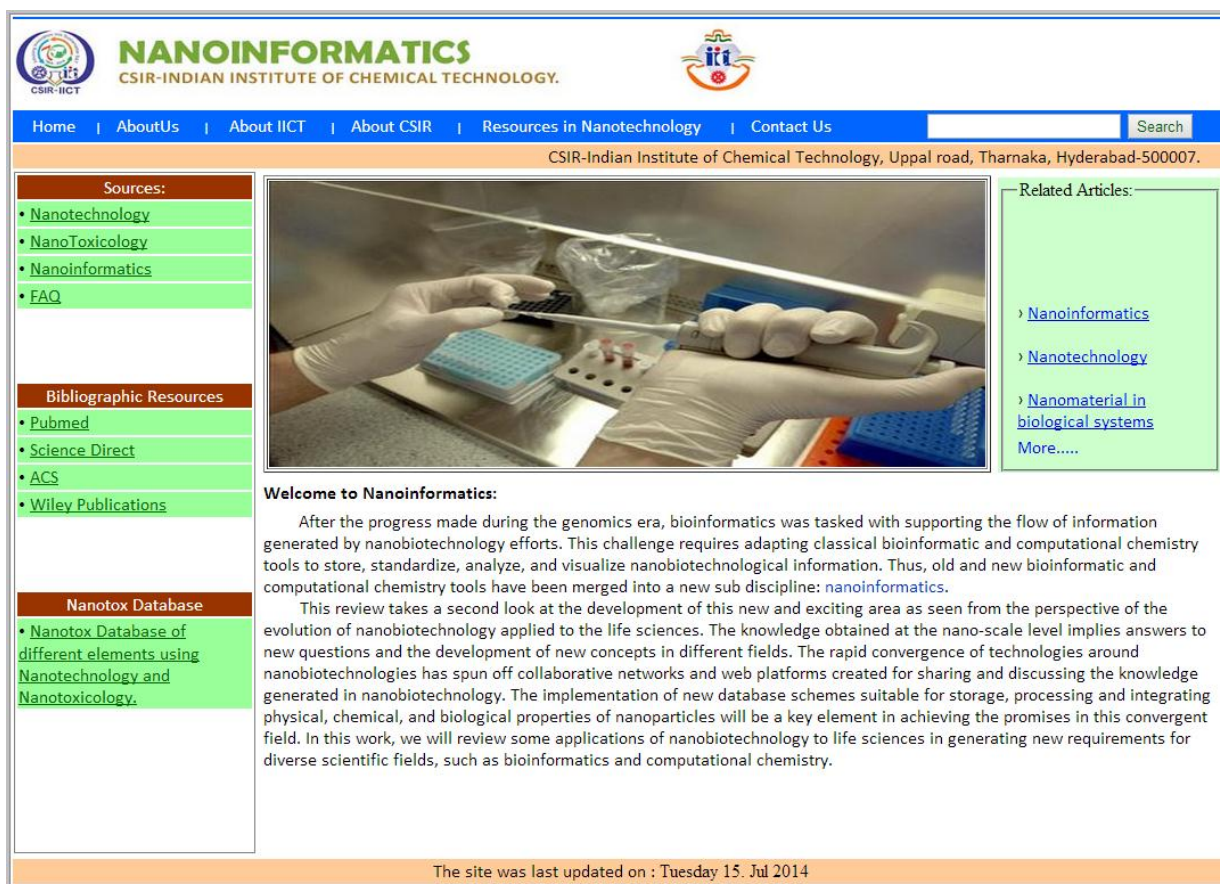


Figure4. Home page of the Nanoinformatics web application.

Description of the Database:

The database contains a home page consisting of the initial information related to the database and introduction and link of the Institute involved and contact details. In the same page there is the links to the relevant pages.

PROJECT MODULES:

The application is accessed by two types of users: Administrator and Customer. The following are the modules in Nanoinformatics:

Modules:

1. Nanotox Database module &
2. Database connection module

1. Nanotox Database module:

This is First module of our Nanoinformatics where the customers can view the different types of elements list for the nanotox database. This module is managed by the administrator who manages different types of element's nanotox database. Our Project having the option to select from various elements for nanotox database like Gold, Silver, Titanium etc... These elements provide all the parameters are listed to our users. It is very much useful for the user to select the particular parameter.

2. Database connection module:

Administrator will be managing this module where each Customer who had logged in the Application can view the different elements with their parameters listed by the administrator.

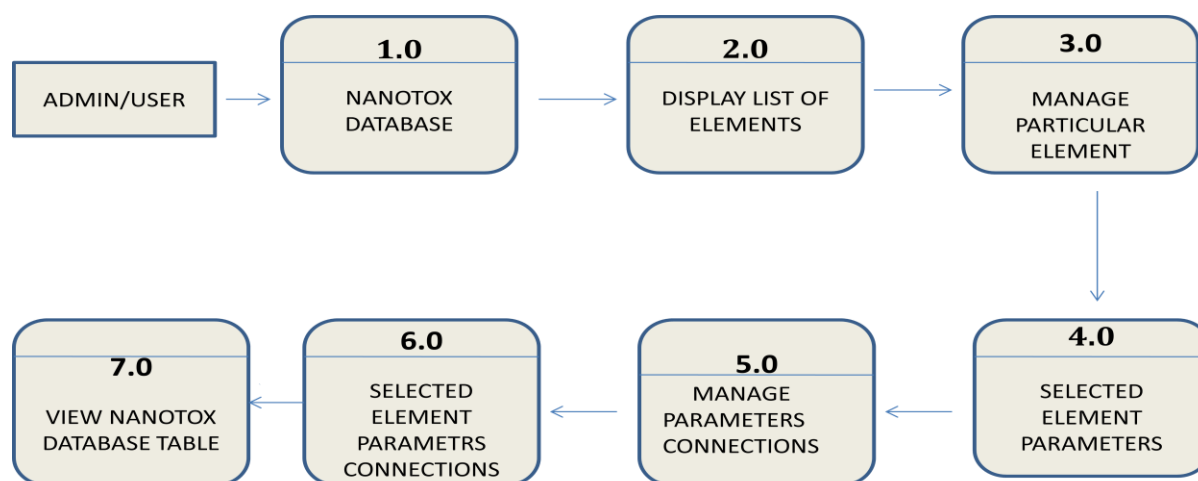


Figure5. Data flow information of the Nanotox Database of different Nanoparticles.

Screen shots of Nano database:

NANOINFORMATICS
CSIR-INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY.

Home | About Us | About IICT | About CSIR | Resources in Nanotechnology | Contact Us

CSIR-Indian Institute of Chemical Technology, Uppal road, Tharnaka, Hyderabad-500007.

Sources:

- Nanotechnology
- NanoToxicology
- Nanoinformatics
- FAQ

Bibliographic Resources

- Pubmed
- Science Direct
- ACS
- Wiley Publications

Nanotox Database

- Nanotox Database of different elements using Nanotechnology and Nanotoxicology.

Gold nano Related Database

The optoelectronic and physicochemical properties of nanoscale matter are a strong function of particle size. Nanoparticle shape also contributes significantly to modulating their electronic properties. Several shapes ranging from rods to wires to plates to teardrop structures may be obtained by chemical methods; triangular nanoparticles have been synthesized by using a seeded growth process. Here, we report the discovery that the extract from the lemongrass plant, when reacted with aqueous chloraurate ions, yields a high percentage of thin, flat, single-crystalline gold nanotriangles. The nanotriangles seem to grow by a process involving rapid reduction, assembly and room-temperature sintering of 'liquid-like' spherical gold nanoparticles. The anisotropy in nanoparticle shape results in large near-infrared absorption by the particles, and highly anisotropic electron transport in films of the nanotriangles.

Gold-DNA Nanoparticle Drug Delivery Vehicle

Diagram illustrating the Gold-DNA Nanoparticle Drug Delivery Vehicle. The vehicle is shown interacting with a Cancer Cell and a DNA molecule. The vehicle is labeled "Au" and "Doxorubicin Anticancer Drug on DNA".

Database Category

Choose on which type of Database you want: Surface coating on the Biodistribution

References

The site was last updated on : Monday 14. Jul 2014

Figure shows Gold Nanoparticle data page.

NANOINFORMATICS
CSIR-INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY.

Home | About Us | About IICT | About CSIR | Resources in Nanotechnology | Contact Us

CSIR-Indian Institute of Chemical Technology, Uppal road, Tharnaka, Hyderabad-500007.

Acute toxicity and biodistribution of different sized titanium dioxide particles in mice after oral administration:

MALE Database:

Groups	body weight Before	Body weight after	Liver(mg/g)	spleen(mg/g)	kidneys(mg/g)
control	20.2	26.4	45.5	2.21	19.6
25nm	20.2	26.5	44.6	2.29	18.4
80 nm	21	26.3	44.3	2.54	18.9
fine	19.6	27.6	44.2	2.3	18.5

FEMALE Database:

Groups	body weight Before	Body weight after	Liver(mg/g)	spleen(mg/g)	kidneys(mg/g)
control	20.1	27.4	48.1	3.54	13.5
25nm	20.6	26.7	52.4	3.1	14
80 nm	20.1	26.8	54.5	3.95	14.5
fine	19.1	25.9	49.1	3.59	13.6

The site was last updated on : Monday 14. Jul 2014

Figure shows acute toxicity and distribution of different sized TiO₂ particles.





[Home](#) | [AboutUs](#) | [About IICT](#) | [About CSIR](#) | [Resources in Nanotechnology](#) | [Contact Us](#)

CSIR-Indian Institute of Chemical Technology, Uppal road, Tharnaka, Hyderabad-500007.

Sources:

- [Nanotechnology](#)
- [NanoToxicology](#)
- [Nanoinformatics](#)
- [FAQ](#)

Bibliographic Resources

- [Pubmed](#)
- [Science Direct](#)
- [ACS](#)
- [Wiley Publications](#)

Nanotox Database

- [Nanotox Database of different elements using Nanotechnology and Nanotoxicology.](#)



Related Articles:

- [Nanoinformatics](#)
- [Nanotechnology](#)
- [More.....](#)




Welcome to Nanoinformatics:

After the progress made during the genomics era, bioinformatics was tasked with supporting the flow of information generated by nanobiotechnology efforts. This challenge requires adapting classical bioinformatic and computational chemistry tools to store, standardize, analyze, and visualize nanobiotechnological information. Thus, old and new bioinformatic and computational chemistry tools have been merged into a new sub discipline: *nanoinformatics*.

This review takes a second look at the development of this new and exciting area as seen from the perspective of the evolution of nanobiotechnology applied to the life sciences. The knowledge obtained at the nano-scale level implies answers to new questions and the development of new concepts in different fields. The rapid convergence of technologies around nanobiotechnologies has spun off collaborative networks and web platforms created for sharing and discussing the knowledge generated in nanobiotechnology. The implementation of new database schemes suitable for storage, processing and integrating physical, chemical, and biological properties of nanoparticles will be a key element in achieving the promises in this convergent field. In this work, we will review some applications of nanobiotechnology to life sciences in generating new requirements for diverse scientific fields, such as bioinformatics and computational chemistry.

The site was last updated on : Tuesday 14. Oct 2014

Home Page of the Nanoinformatics.

[Home](#) | [AboutUs](#) | [About IICT](#) | [About CSIR](#) | [Resources in Nanotechnology](#) | [Contact Us](#)

CSIR-Indian Institute of Chemical Technology, Uppal road, Tharnaka, Hyderabad-500007.

Sources:

- [Nanotechnology](#)
- [NanoToxicology](#)
- [Nanoinformatics](#)
- [FAQ](#)

Bibliographic Resources

- [Pubmed](#)
- [Science Direct](#)
- [ACS](#)
- [Wiley Publications](#)

Nanotox Database

- [Nanotox Database of different elements using Nanotechnology and Nanotoxicology.](#)

Nano-technology and Nanotoxicology:

Nanotechnology (sometimes shortened to "nanotech") is the manipulation of matter on an atomic and molecular scale. The earliest, widespread description of nanotechnology referred to the particular technological goal of precisely manipulating atoms and molecules for fabrication of macroscale products, also now referred to as molecular nanotechnology. A more generalized description of nanotechnology was subsequently established by the National Nanotechnology Initiative, which defines nanotechnology as the manipulation of matter with at least one dimension sized from 1 to 100 nanometers. This definition reflects the fact that quantum mechanical effects are important at this quantum-realm scale.

Nanotoxicology is a branch of bionanoscience which deals with the study and application of toxicity of nanomaterials. Nanomaterials, even when made of inert elements like gold, become highly active at nanometer dimensions.



Keywords: nano-technology, nano-toxicology, nano-particle(s).

Nanotox Database based on Nanoparticles:

- [Titanium](#)
- [Gold](#)
- [Carbon](#)
- [Silica](#)
- [Silver](#)
- [Iron](#)
- [Au](#)
- [Aluminium Oxide](#)

The site was last updated on : Tuesday 14. Oct 2014

Database home page of different nanoparticles.


NANOINFORMATICS
 CSIR-INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY.
 

[Home](#) | [AboutUs](#) | [About IICT](#) | [About CSIR](#) | [Resources in Nanotechnology](#) | [Contact Us](#)

CSIR-Indian Institute of Chemical Technology, Uppal road, Tharnaka, Hyderabad-500007.

Sources:

- [Nanotechnology](#)
- [NanoToxicology](#)
- [Nanoinformatics](#)
- [FAQ](#)

Bibliographic Resources

- [Pubmed](#)
- [Science Direct](#)
- [ACS](#)
- [Wiley Publications](#)

Nanotox Database


- [Nanotox Database of different elements using Nanotechnology and Nanotoxicology.](#)

Titanium nano Related Database

The element titanium is finding more and more applications in today's society. The use of titanium metal in aerospace, sports and medicine is well known; in fact, over 96% of the worldwide use of titanium is in the oxide form, TiO₂ (titanium dioxide), thus creating a high demand.

The disinfectant and self-cleaning qualities of TiO₂ (titanium dioxide) are being widely employed in Japan and many European countries today for such products as coated ceramic tile for use in homes. This coating is reported to last the life of the tile and is activated by a UV light source and water. Other applications are TiO₂ (titanium dioxide) coated self-cleaning roof tiles for homes and buildings, which are also activated by the UV light of the sun.



In addition, TiO₂ (titanium dioxide) is currently being used to treat the air in fruit, vegetable and cut flower storage areas to prevent spoilage and increase the products shelf life. The photocatalytic properties of TiO₂ (titanium dioxide) remove ethylene gas from the air. Ethylene is a naturally occurring gaseous hormone produced by plant tissue that in low concentrations triggers the ripening of fruits and vegetables. Ethylene is also produced from other sources including internal combustion engines, certain fungi, and cigarette smoke.



Database Category
 Choose on which type of Database you want

The site was last updated on : Tuesday 14. Oct 2014

Titanium Database Page.


NANOINFORMATICS
 CSIR-INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY.
 

[Home](#) | [AboutUs](#) | [About IICT](#) | [About CSIR](#) | [Resources in Nanotechnology](#) | [Contact Us](#)

CSIR-Indian Institute of Chemical Technology, Uppal road, Tharnaka, Hyderabad-500007.

Sources:

- [Nanotechnology](#)
- [NanoToxicology](#)
- [Nanoinformatics](#)
- [FAQ](#)

Bibliographic Resources

- [Pubmed](#)
- [Science Direct](#)
- [ACS](#)
- [Wiley Publications](#)

Nanotox Database



- [Nanotox Database of different elements using Nanotechnology and Nanotoxicology.](#)

Titanium Publications:

- In vitro evidence of dysregulation of blood-brain barrier function after acute and repeated/long-term exposure to TiO₂ nanoparticles. [Download](#)
- Titanium Dioxide (P25) Produces Reactive Oxygen Species in Immortalized Brain Microglia (BV2): Implications for Nanoparticle Neurotoxicity. [Download](#)
- The effect of titanium dioxide nanoparticles on pulmonary surfactant function and ultrastructure. [Download](#)
- Pulmonary Instillation Studies with Nanoscale TiO₂ Rods and Dots in Rats: Toxicity Is not Dependent upon Particle Size and Surface Area. [Download](#)
- Correlating Nanoscale Titania Structure with Toxicity: A Cytotoxicity and Inflammatory Response Study with Human Dermal Fibroblasts and Human Lung Epithelial Cells. [Download](#)
- Crystal structure mediates mode of cell death in TiO₂ nanotoxicity. [Download](#)
- Acute toxicity study of the interaction between titanium dioxide nanoparticles and lead acetate in mice. [Download](#)
- Acute toxicity and biodistribution of different sized titanium dioxide particles in mice after oral administration. [Download](#)
- Exposure to Titanium Dioxide Nanomaterials Provokes Inflammation of an in Vitro Human Immune Construct. [Download](#)
- Internalisation of hybrid titanium dioxide/para-amino benzoic acid nanoparticles in human dendritic cells did not induce toxicity and changes in their functions. [Download](#)
- Modest effect on plaque progression and vasodilatory function in atherosclerosis-prone mice exposed to nanosized TiO₂. [Download](#)
- TiO₂ Nanoparticles in the Marine Environment: Impact on the Toxicity of Tributyltin to Abalone (Haliotis diversicolor supertexta) Embryos. [Download](#)

The site was last updated on : Tuesday 14. Oct 2014

Titanium Publications Page.


NANOINFORMATICS
 CSIR-INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY.
 

[Home](#) | [About Us](#) | [About IICT](#) | [About CSIR](#) | [Resources in Nanotechnology](#) | [Contact Us](#)

CSIR-Indian Institute of Chemical Technology, Uppal road, Tharnaka, Hyderabad-500007.

Acute toxicity and biodistribution of different sized titanium dioxide particles in mice after oral administration:

MALE Database:



Groups	body weight Before	Body weight after	Liver(mg/g)	spleen(mg/g)	kidneys(mg/g)
control	20.2	26.4	45.5	2.21	19.6
25nm	20.2	26.5	44.6	2.29	18.4
80 nm	21	26.3	44.3	2.54	18.9
fine	19.6	27.6	44.2	2.3	18.5

FEMALE Database:

Groups	body weight Before	Body weight after	Liver(mg/g)	spleen(mg/g)	kidneys(mg/g)
control	20.1	27.4	48.1	3.54	13.5
25nm	20.6	26.7	52.4	3.1	14
80 nm	20.1	26.8	54.5	3.95	14.5
fine	19.1	25.9	49.1	3.59	13.6

The site was last updated on : Tuesday 14. Oct 2014

Toxicity and biodistribution of different sized titanium


NANOINFORMATICS
 CSIR-INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY.
 

[Home](#) | [AboutUs](#) | [About IICT](#) | [About CSIR](#) | [Resources in Nanotechnology](#) | [Contact Us](#)

CSIR-Indian Institute of Chemical Technology, Uppal road, Tharnaka, Hyderabad-500007.

Sources:

- [Nanotechnology](#)
- [NanoToxicology](#)
- [Nanoinformatics](#)
- [FAQ](#)

Bibliographic Resources

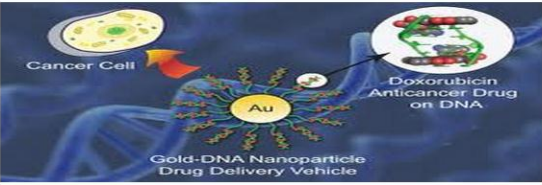
- [Pubmed](#)
- [Science Direct](#)
- [ACS](#)
- [Wiley Publications](#)

Nanotox Database

- [Nanotox Database of different elements using Nanotechnology and Nanotoxicology.](#)

Gold nano Related Database

The optoelectronic and physicochemical properties of nanoscale matter are a strong function of particle size. Nanoparticle shape also contributes significantly to modulating their electronic properties. Several shapes ranging from rods to wires to plates to teardrop structures may be obtained by chemical methods; triangular nanoparticles have been synthesized by using a seeded growth process. Here, we report the discovery that the extract from the lemongrass plant, when reacted with aqueous chloroaurate ions, yields a high percentage of thin, flat, single-crystalline gold nanotriangles. The nanotriangles seem to grow by a process involving rapid reduction, assembly and room-temperature sintering of 'liquid-like' spherical gold nanoparticles. The anisotropy in nanoparticle shape results in large near-infrared absorption by the particles, and highly anisotropic electron transport in films of the nanotriangles.





The diagram illustrates a Gold-DNA Nanoparticle Drug Delivery Vehicle. It shows a central gold nanoparticle (Au) with a DNA strand wrapped around it. The DNA strand is labeled 'Doxorubicin Anticancer Drug on DNA'. The nanoparticle is shown interacting with a 'Cancer Cell'.

Database Category
 Choose on which type of Database you want

The site was last updated on : Tuesday 14. Oct 2014

Gold Database Page


NANOINFORMATICS
 CSIR-INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY.
 

[Home](#) | [About Us](#) | [About IICT](#) | [About CSIR](#) | [Resources in Nanotechnology](#) | [Contact Us](#)

CSIR-Indian Institute of Chemical Technology, Uppal road, Tharnaka, Hyderabad-500007.

Sources:

- Nanotechnology
- NanoToxicology
- Nanoinformatics
- FAQ

Bibliographic Resources

- Pubmed
- Science Direct
- ACS
- Wiley Publications

Nanotox Database



- Nanotox Database of different elements using Nanotechnology and Nanotoxicology.

Gold Publications:

- Bioaccumulation and toxicity of gold nanoparticles after repeated administration in mice. [Download](#)
- Effect of surface coating on the biodistribution profile of gold nanoparticles in the rat. [Download](#)
- Biocompatible gellan gum-reduced gold nanoparticles:cellular uptake and subacute oral toxicity studies. [Download](#)
- Effects and uptake of gold nanoparticles deposited at the air-liquid interface of a human epithelial airway model. [Download](#)
- Particle size-dependent organ distribution of gold nanoparticles after intravenous administration. [Download](#)
- Particle size-dependent and surface charge-dependent biodistribution of gold nanoparticles after intravenous administration. [Download](#)
- Subchronic inhalation toxicity of gold nanoparticles. [Download](#)
- Cisplatin-loaded Au-Au2S nanoparticles for potential cancer therapy: Cytotoxicity, in vitro carcinogenicity, and cellular uptake. [Download](#)
- Targeting Gold Nanoshells on Silica Nanorattles: a Drug Cocktail to Fight Breast Tumors via a Single Irradiation with Near-Infrared Laser Light. [Download](#)
- Cellular uptake and toxicity of gold nanoparticles in prostate cancer cells: a comparative study of rods and spheres. [Download](#)

The site was last updated on : Tuesday 14. Oct 2014

Gold Publications.


NANOINFORMATICS
 CSIR-INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY.
 

[Home](#) | [About Us](#) | [About IICT](#) | [About CSIR](#) | [Resources in Nanotechnology](#) | [Contact Us](#)

CSIR-Indian Institute of Chemical Technology, Uppal road, Tharnaka, Hyderabad-500007.

Biocompatible gellan gum-reduced gold nanoparticles cellular uptake and subacute oral toxicity studies.

Male Database


Parameters	Control	300 ppm
hematocrit(%)	38.9	36.15
hemoglobin (g dl)	15.62	14.42
RBC (milli cmm)	7.28	6.97
WBC (milli cmm)	13275	12350
erythrocyte sedimentation Rate (mm after 1h)	2	1.5
Neutrophils (%)	21	15.25
Lymphocytes	73.5	79
Eosinophils (%)	1.5	1.25
Monocytes (%)	4	4.5
Basophils (%)	0	0
aspartate aminotransferase (u/l)	227.75	234
alkaline phosphatase(u/l)	412	287.75
alanine aminotransferase(u/l)	65.25	67.75
blood sugar level(mg/dl)	133.75	133.75
Bilirubin (mg/dl)	44.75	47.25
cholesterol(mg/dl)	52	64
Total protein (mg dl)	7.47	7.2
Albumin (mg/dl)	3.55	3.32
Urea (mg/dl)	78.5	75.75
creatinine (mg/dl)	0.61	0.51
sodium (mEQ/l)	143	146
potassium(mEQ/l)	3.82	3.85


Female Database

Parameters	Control	300 ppm
hematocrit(%)	32.35	34.92
hemoglobin (g dl)	13.55	14.87
RBC (milli cmm)	5.87	6.58
WBC (milli cmm)	9575	8675
erythrocyte sedimentation Rate (mm after 1h)	1.5	1.75
Neutrophils (%)	20.25	15.5
Lymphocytes	74.25	78.25
Eosinophils (%)	2.25	2
Monocytes (%)	3.25	4.25
Basophils (%)	0	0
aspartate aminotransferase (u/l)	285.5	232.75
alkaline phosphatase(u/l)	414.25	224.5
alanine aminotransferase(u/l)	62	56.75
blood sugar level(mg/dl)	131.75	124.75
Bilirubin (mg/dl)	60	62.5
cholesterol(mg/dl)	60.75	57
Total protein (mg dl)	8.15	8.27
Albumin (mg/dl)	4.1	4.12
Urea (mg/dl)	60.6	58
creatinine (mg/dl)	0.61	0.61
sodium (mEQ/l)	141	142.2
potassium(mEQ/l)	4.6	4.62

The site was last updated on : Tuesday 14. Oct 2014

Bio compatible gellan of gold nanoparticle.


NANOINFORMATICS
 CSIR-INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY.



[Home](#) | [About Us](#) | [About IICT](#) | [About CSIR](#) | [Resources in Nanotechnology](#) | [Contact Us](#)

CSIR-Indian Institute of Chemical Technology, Uppal road, Tharnaka, Hyderabad-500007.

Sources:

- [Nanotechnology](#)
- [NanoToxicology](#)
- [Nanoinformatics](#)
- [FAQ](#)

Bibliographic Resources

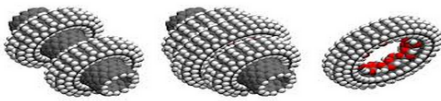
- [Pubmed](#)
- [Science Direct](#)
- [ACS](#)
- [Wiley Publications](#)

Nanotox Database

- [Nanotox Database of different elements using Nanotechnology and Nanotoxicology.](#)

Carbon nano Related Database


NANOSHEL produces more than 350 types of nanotechnology products, among which the main products are Carbon Nanotubes, Metal and Alloy Nanoparticles, and Oxides and Allied nanoparticles and nanoparticles of high quality and purity. All the products are manufactured using Arc Discharge, CVD and various other techniques. The range of purity percentage of our carbon nanotubes (CNTs), metal nanoparticles, Oxide nanoparticles, Compound nanoparticles is from 90% to 99.99%. We supply nanomaterials for commercial purposes as well as scientific research projects, from small quantities (grams) to larger quantities (kilograms).




Database Category
 Choose on which type of Database you want

The site was last updated on : Tuesday 14. Oct 2014

Carbon Database Page.


NANOINFORMATICS
 CSIR-INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY.



[Home](#) | [About Us](#) | [About IICT](#) | [About CSIR](#) | [Resources in Nanotechnology](#) | [Contact Us](#)

CSIR-Indian Institute of Chemical Technology, Uppal road, Tharnaka, Hyderabad-500007.

Challenges for assessing Carbon nanomaterial toxicity to the skin:

Fisher CARBON BLACK

Time	Control	0.1 mg/ml	0.2 mg/ml	0.4 mg/ml
1 Hrs	20	25	15	10
2 Hrs	30	35	25	25
4 Hrs	40	50	55	45
8 Hrs	65	120	130	125
12 Hrs	70	140	170	150
24 Hrs	100	290	340	390

Cabot CARBON BLACK

Time	Control	0.1 mg/ml	0.2 mg/ml	0.4 mg/ml
1 Hrs	15	10	10	5
2 Hrs	20	20	15	10
4 Hrs	30	28	30	10
8 Hrs	45	50	45	25
12 Hrs	50	80	75	50
24 Hrs	75	160	150	130

Printex 90(A)


Time	Control	0.1 mg/ml	0.2 mg/ml	0.4 mg/ml
1 Hrs	15	2	2	1
2 Hrs	25	5	3	2
4 Hrs	50	5	2	2
8 Hrs	60	10	2	2
12 Hrs	60	20	2	5
24 Hrs	90	40	3	2

Printex 90(B) 14-16 nm


Time	Control	0.1 mg/ml	0.2 mg/ml	0.4 mg/ml
1 Hrs	15	2	2	1
2 Hrs	25	5	3	2
4 Hrs	50	5	2	2
8 Hrs	60	10	2	2
12 Hrs	60	20	2	5
24 Hrs	90	40	3	2

The site was last updated on : Tuesday 14. Oct 2014

Carbon nanomaterial toxicity to the skin



NANOINFORMATICS
 CSIR-INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY.



[Home](#) | [About Us](#) | [About IICT](#) | [About CSIR](#) | [Resources in Nanotechnology](#) | [Contact Us](#)

CSIR-Indian Institute of Chemical Technology, Uppal road, Tharnaka, Hyderabad-500007.

Sources:

- Nanotechnology
- NanoToxicology
- NanoInformatics
- FAQ

Bibliographic Resources

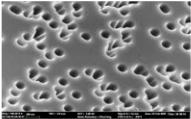
- Pubmed
- Science Direct
- ACS
- Wiley Publications

Nanotox Database

- Nanotox Database of different elements using Nanotechnology and Nanotoxicology.

Silica nano Related Database


We have developed uniform core/shell nanoparticles, consisting of a silica layer coating and pigments or magnetite core, using a water-in-oil microemulsion method. The nanoparticles are highly luminescent and photostable with the size ranging from 5 nm to 400 nm. Bioconjugation of these silica nanoparticles adds unique biofunctions with various molecules such as enzymes, antibodies, and DNA molecules. Significant advantages have been shown in using bioconjugated nanoparticles for biosensing and bioimaging, such as cell staining, DNA detection and separation, rapid single bacterium detection, and biotechnological application in DNA protection.




Database Category
 Choose on which type of Database you want

The site was last updated on : Tuesday 14. Oct 2014

Silica Database Page.



NANOINFORMATICS
 CSIR-INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY.



[Home](#) | [About Us](#) | [About IICT](#) | [About CSIR](#) | [Resources in Nanotechnology](#) | [Contact Us](#)

CSIR-Indian Institute of Chemical Technology, Uppal road, Tharnaka, Hyderabad-500007.

In vitro developmental toxicity test detects inhibition of stem cell differentiation by Silica nanoparticles:

Effects of silica NP on the metabolic activity of D3 cells after 24 hr and 10 days of incubation:

	Duration 24 Hours					Duration 10 Days				
Size	10 nm	30 nm	80 nm	400 nm	10 nm	30 nm	80 nm	400 nm		
Control	100	100	100	100	100	100	100	100		
0.3 µg/ml	100	105	90	110	100	100	108	105		
1 µg/ml	108	120	98	112	90	100	100	100		
3 µg/ml	122	130	110	120	95	98	105	100		
10 µg/ml	125	140	115	125	95	108	105	96		
30 µg/ml	120	135	110	122	95	90	100	88		
100 µg/ml	110	120	105	115	60	58	96	96		

	In deionized water				ID50			
Nominal size [nm]	TEM size [nm]	zeta potential ζ [mV]	pH	DLSb size [nm]	PDI	Mass [µg/ml]	Number [particles/ml]	Surface area nm ² /ml
10	10.96	-43.3	7.2	103.1	0.792	59	3.9	1.46
30	33.73	-33.7	6.5	77.9	0.259	29	6.4	2.33
80	33.71	-10.6	6.3	65.9	0.374	100	2.2	8
400	247.91	-49.1	8.7	269	0.049	100	5.7	1.1

The site was last updated on : Tuesday 14. Oct 2014

Silica invitro development toxicity.

[Home](#) | [About Us](#) | [About IICT](#) | [About CSIR](#) | [Resources in Nanotechnology](#) | [Contact Us](#)

CSIR-Indian Institute of Chemical Technology, Uppal road, Tharakur, Hyderabad-500007.

Sources:

- Nanotechnology
- NanoToxicology
- Nanoinformatics
- FAQ

Bibliographic Resources

- Pubmed
- Science Direct
- ACS
- Wiley Publications

Nanotox Database

- Nanotox Database of different elements using Nanotechnology and Nanotoxicology.

Silver nano Related Database

Nanosilver technologies appear in a variety of manufacturing processes and end products. It can appear imbedded in a coating which is applied to the product by the manufacturer (coating). Some products come in a liquid form and are meant to be applied to form a coating (coating & spray). Nanosilver can be presented in a liquid form such as a homeopathy colloid or contained within a shampoo (liquid). It can also be embedded in a solid such as a polymer master batch or be suspended in a bar of soap (solid). Nanosilver can also be utilized in the textile industry by incorporating it into the fiber (spun) or produced as a powder (powder).

Database Category

Choose on which type of Database you want

References

The site was last updated on : Tuesday 14. Oct 2014

Silver nano Related Database

[Home](#) | [About Us](#) | [About IICT](#) | [About CSIR](#) | [Resources in Nanotechnology](#) | [Contact Us](#)

CSIR-Indian Institute of Chemical Technology, Uppal road, Tharakur, Hyderabad-500007.


The following table links nanoparticle size with mass, atomic molarity, mass percent, particle concentration, and peak optical density for BioPure solutions.

BioPure Silver Nanoparticles:


Size (nm)	Mass Concentration (mg/mL)	Atomic (Ag) Molarity (mmol/L)	Particle Concentration (particles/mL)	Ag Mass Percent (%)	Max Optical Density (cm-1)	Peak Wave-length (nm)
10	1.0	9.27	1.8 x 10	0.1	125	395
20	1.0	9.27	2.3 x 10	0.1	125	400
30	1.0	9.27	6.7 x 10	0.1	110	400
40	1.0	9.27	2.8 x 10	0.1	135	410
50	1.0	9.27	1.5 x 10	0.1	120	420
60	1.0	9.27	8.4 x 10	0.1	95	435
70	1.0	9.27	5.3 x 10	0.1	85	440
80	1.0	9.27	3.6 x 10	0.1	70	460
90	1.0	9.27	2.5 x 10	0.1	65	480
100	1.0	9.27	1.8 x 10	0.1	45	500
110	1.0	9.27	1.4 x 10	0.1	40	515

The site was last updated on : Tuesday 14. Oct 2014

BioPure Silver Nanoparticles:



NANOINFORMATICS
 CSIR-INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY.



[Home](#) | [About Us](#) | [About IICT](#) | [About CSIR](#) | [Resources in Nanotechnology](#) | [Contact Us](#)

CSIR-Indian Institute of Chemical Technology, Uppal road, Tharnaka, Hyderabad-500007.

Sources:

- Nanotechnology
- NanoToxicology
- Nanoinformatics
- FAQ

Bibliographic Resources

- Pubmed
- Science Direct
- ACS
- Wiley Publications


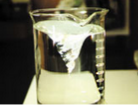
Nanotox Database

- Nanotox Database of different elements using Nanotechnology and Nanotoxicology.

Au nano related Database:

Properties of materials change at the nanoscale. In bulk at the macroscale, the element of gold is gold colored, but at the in particles nanoscale, the element of gold is red to purple in color. The formation of gold nanoparticles can be therefore observed by a change in color since small nanoparticles of gold are red. The layer of absorbed citrate anions on the surface of the nanoparticles keep the nanoparticles separated, and the presence of this colloidal suspension can be detected by the reflection of a laser beam from the particles. Switching to a smaller anion allows the particles to approach more closely and another color change is observed.


Before the addition of the reducing agent, the gold is in solution in the Au+3 form. When the reducing agent is added, gold atoms are formed in the solution, and their concentration rises rapidly until the solution exceeds saturation. Particles then form in a process called nucleation. The remaining dissolved gold atoms bind to the nucleation sites and growth occurs.


Database Category
 Choose on which type of database you want:

The site was last updated on : Tuesday 14. Oct 2014

Au nano related Database



NANOINFORMATICS
 CSIR-INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY.



[Home](#) | [About Us](#) | [About IICT](#) | [About CSIR](#) | [Resources in Nanotechnology](#) | [Contact Us](#)


CSIR-Indian Institute of Chemical Technology, Uppal road, Tharnaka, Hyderabad-500007.

Interference in EGF signal transduction by 10 nm Ag,Au abd Spion:


Group	Ag NP- 5nm	Au Np - 5 nm	SPION - 5nm	Au NP- 25 nm	SPION - 25 nm
Akt phosphorylation (% control)	75	80	96	85	80
Erk phosphorylation (% control)	80	66	86	74	84
Akt Activity (% control)	100	85	95	80	100
ATF 1	1.53	2.02	1.83	0	0
BRAF	3.3	0	0	2.58	3.63
DUSP1	0	0	0	3.97	4.98
DUSP6	0	0	0	3.29	0
EGFR	0	2.43	0	4.3	5.32
EP88	0	0	0	-2.03	0
FN1	0	0	0	3.24	3.11
MAPK9	-1.16	0	0	-1.33	-2.03
NFATC3	0	0	-1.45	-1.74	2.72
PDGFB	-1.26	0	0	2.49	4.37
PLAT	0	0	0	-1.96	-3.2
TP53	-1.45	0	0	-1.91	-2.5

The site was last updated on : Tuesday 14. Oct 2014

EGF signal transduction of Au.



NANOINFORMATICS
 CSIR-INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY.



[Home](#) | [About Us](#) | [About IICT](#) | [About CSIR](#) | [Resources in Nanotechnology](#) | [Contact Us](#)

CSIR-Indian Institute of Chemical Technology, Uppal road, Tharnaka, Hyderabad-500007.

Sources:

- Nanotechnology
- NanoToxicology
- Nanoinformatics
- FAQ

Bibliographic Resources

- Pubmed
- Science Direct
- ACS
- Wiley Publications


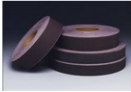

Nanotox Database

- Nanotox Database of different elements using Nanotechnology and Nanotoxicology.

Aluminium Oxide nano related Database:

Corundum is a crystalline form of aluminium oxide (Al₂O₃) with traces of iron, titanium and chromium. It is a rock-forming mineral. It is one of the naturally clear transparent materials, but can have different colors when impurities are present. Transparent specimens are used as gems, called ruby if red and padparadscha if pink-orange. All other colors are called sapphire, e.g., "green sapphire" for a green specimen. The name "corundum" is derived from the Sanskrit word kuruvinda meaning "ruby". Because of corundum's hardness (pure corundum is defined to have 9.0 Mohs), it can scratch almost every other mineral. It is commonly used as an abrasive on everything from sandpaper to large machines used in machining metals, plastics, and wood. Some emery is a mix of corundum and other substances, and the mix is less abrasive, with an average Mohs hardness of 8.0. In addition to its hardness, corundum is unusual for its density of 4.02 g/cm³, which is very high for a transparent mineral composed of the low atomic mass elements aluminium and oxygen.


Corundum occurs as a mineral in mica schist, gneiss, and some marbles in metamorphic terranes. It also occurs in low silica igneous syenite and nepheline syenite intrusives. Other occurrences are as masses adjacent to ultramafic intrusives, associated with lamprophyre dikes and as large crystals in pegmatites. It commonly occurs as a detrital mineral in stream and beach sands because of its hardness and resistance to weathering. The largest documented single crystal of corundum measured about 65×40×40 cm (26×16×16 in), and weighed 152 kg (335 lb). The record has since been surpassed by certain synthetic boules. Corundum for abrasives is mined in Zimbabwe, Russia, Sri Lanka and India. Historically it was mined from deposits associated with dunites in North Carolina, USA and from a nepheline syenite in Craigmont, Ontario. Emery grade corundum is found on the Greek island of Naxos and near Peekskill, New York, USA. Abrasive corundum is synthetically manufactured from bauxite. Four corundum axes dating back to 2500 BCE from the Liangzhou culture have been discovered in China. The surfaces of the axes are remarkably smoothly polished


Database
 Choose on which type of Database you want :

The site was last updated on : Tuesday 14. Oct 2014

Aluminium Oxide nano related Database



NANOINFORMATICS
 CSIR-INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY.



[Home](#) | [About Us](#) | [About IICT](#) | [About CSIR](#) | [Resources in Nanotechnology](#) | [Contact Us](#)

CSIR-Indian Institute of Chemical Technology, Uppal road, Tharnaka, Hyderabad-500007.

Acute effect of alluminum oxide NP and bulk on reduced GSH content in various tissues of rats on day 3 and 14:

Tissue	Dose(mg/kg)	Control	Day 3-30nm	Day 3-40nm	Day 3-bulk	Day 14-30nm	Day 14-40nm	Day 14-bulk	
Liver	2000	592.5	427.1	42.6	494.1	519.6	524.3	520.3	
	-	1000	592.5	439.6	478.4	501.7	565.6	564.1	575.8
	-	500	592.5	506	507.2	520.2	591.9	593.4	586.9
Kidney	2000	409.5	310.9	306.4	307.1	381.2	388.9	382.2	
	-	1000	409.5	318	324	327.4	395.2	383.4	379.9
	-	500	409.5	352.4	355	346.9	409	406.3	404
Brain	2000	248.5	138.2	145.9	154.4	241	225.9	232.8	
	-	1000	248.5	169.3	168.7	169.9	233.2	249.9	249.6
	-	500	248.5	187.6	182.6	186.4	265.4	248.7	236
Heart	2000	85.2	84.1	84.5	84.5	89.6	85.7	82.8	
	-	1000	85.2	82.3	88.2	84.9	88.9	74.9	82.6
	-	500	85.2	83.5	85.6	83.6	83.6	81	73.6

The site was last updated on : Tuesday 14. Oct 2014

Acute effect of alluminum oxide NP in various tissues of rats on day 3 and 14

RESULTS:

This database was constructed mainly to create a resource that would facilitate easy retrieval of nanotox data of nanoparticle information. It is an attempt has been made to create a comprehensive database on different elements of nanoparticles. This database tries to bring the experimental data out into the open in a succinct and consolidated form.

By using prediction tools the problems raised above will be minimized to greater extent and we will obtain results in no time. By providing the parameters required to the tool, it will be efficiently predicting the nature of the particle and detect with certain amount of accuracy whether the particles are toxic to humans or not. Through this prediction tool we can infer maximum permissible limit of NP for humans as well as animals.

CONCLUSION:

Nanoinformatics is the Web database providing comprehensive information on Nanotox database of nanoparticles. It is a schema-free database that can be accessed as a Web service from modern C# programming language using a simple HTTP call. Nanoinformatics provides interfaces to freely retrieve visualize and analyze the nanoparticle database. The Nanoinformatics Web site can also be used to access the integrative information about the Nanotoxicology.

OUTCOME OF THE PROJECT:

1. In this project data integration is performed from various literature sources and initially they were categorized for individual inspection.
2. Integration of the data is performed under MYSQL and the whole dataset was made search able through different types of query framing.
3. The front-end of the database is developed using ASP.NET and it has been connected with the back-end MYSQL server where user friendly query can generate different types of report depending on the need of the user.
4. SOM based clustering is performed to understand and compare each data points with relation to their various properties along with toxicity.

FUTURE PROGRAM:

As the availability of the data will increase in future the following addition in the present database and classification system could be incorporated:

1. More data will be incorporated in the present database
2. The number of parameters for classification and clustering can be increased
3. More types of query framing could be incorporated in the present database.