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Nanobioinformatics: emerging computational tools to understand nano-bio interact

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IN

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Final Report

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Project Final Report

Title of the project:

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

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<u>General information about Project</u> *(AOARD- Grant 114035)*:

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

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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 i*n-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.

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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 NANOPATICLES 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 where among the few words used for searching the articles. Huge number of articles have been found, all the relevant articles was downloaded and studied for the data. These articles where 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

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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.

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Steps involved in the algorithm

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

   Wi = [wi1, wi2, ..., win], n denotes dimension of input data

2. **Sampling:** Select an input vector X = [x1, x2, ..., xn]
3.
4. **Similarity matching:** Find the winning neuron whose weight vector best matches with the input vector

   j(t) = arg min { || X – Wi|| }

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.

   Wi(t+1) = Wi(t) + α(t) * hij(t) * [X(t) – Wi(t)]

   α(t): Learning rate that decreases with time t, 0 < α(t) <= 1

   hij(t) = exp(-||rj – ri||2 / 2 * σ(t)2)

   ||rj – ri||2 = Distance between winning neuron and other neurons

   σ(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

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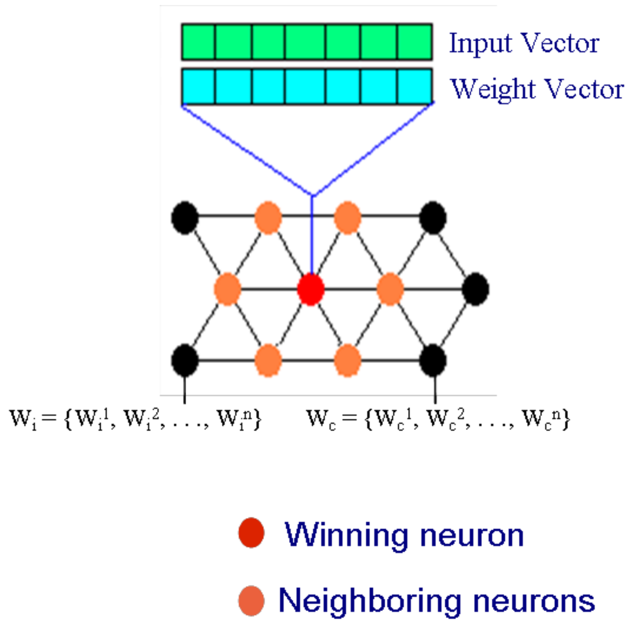

Figure1. Illustration of an SOM neural network

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)

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- 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 datap points under the analysis along with their exact position in the dataset under consderation.An example of such representation is provided below in figure 2.The result was geerated with 10,000,00 iteration during the analysis.

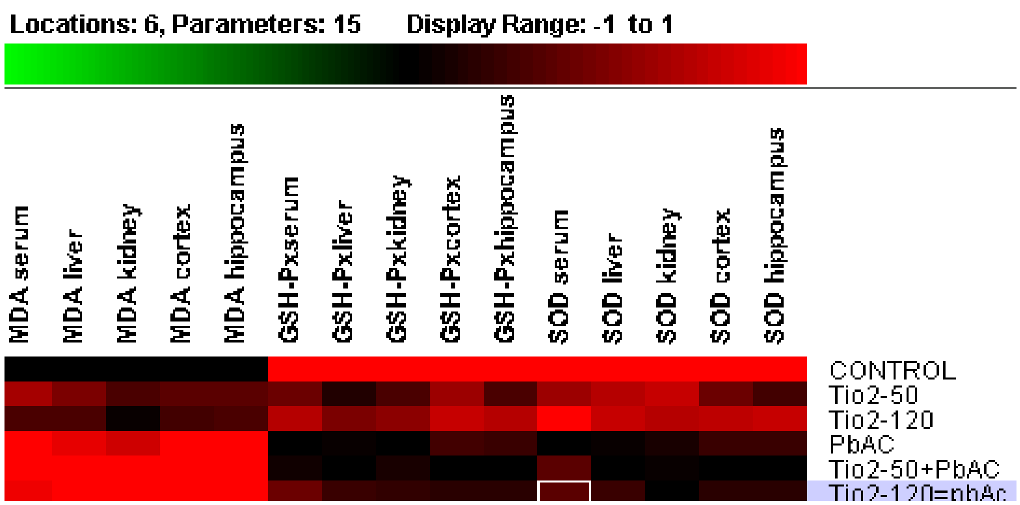

Figure2. Result from SOM, shows that the stress response of Titaninum Dioxide when injected orally single dose with and without lead acetate, titanium dioxide when injected alone not much change in enzymes (Malondialdehyde, Glutathione reductase, superoxide Dismutase) concentration is seen (light region),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

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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

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

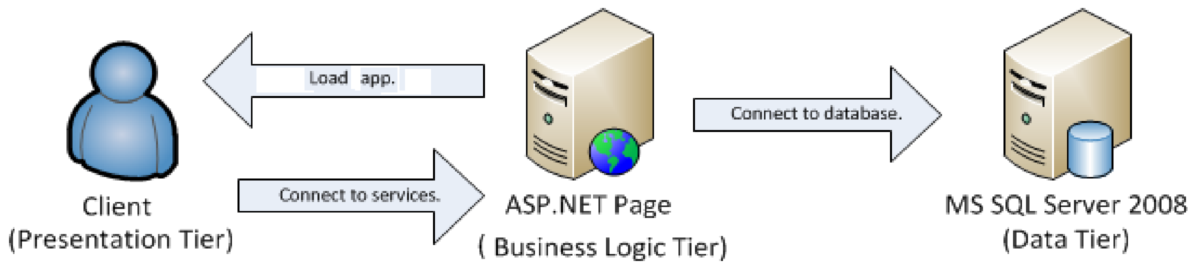
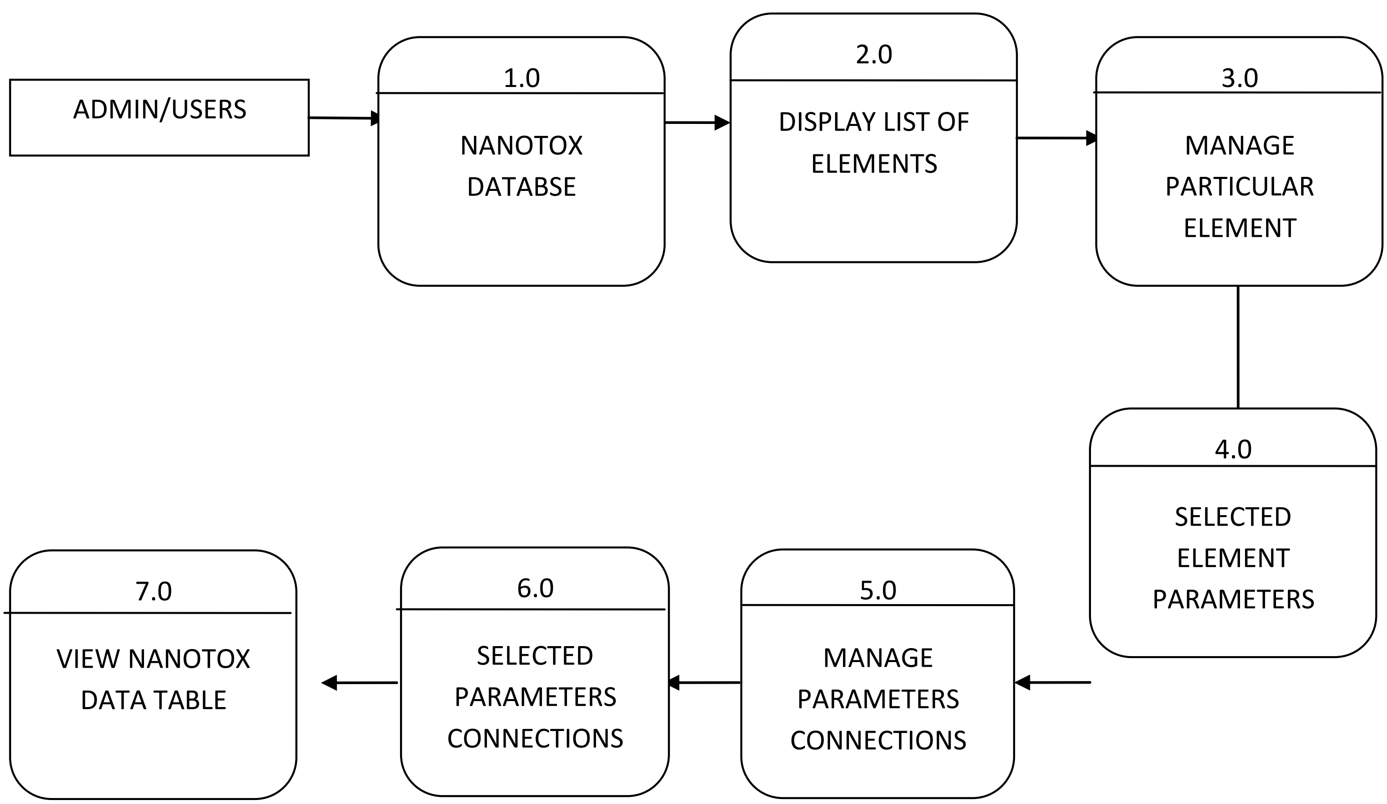


Figure3.Client server relation representation.

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

DATAFLOW DIAGRAM

FIRST- LEVEL



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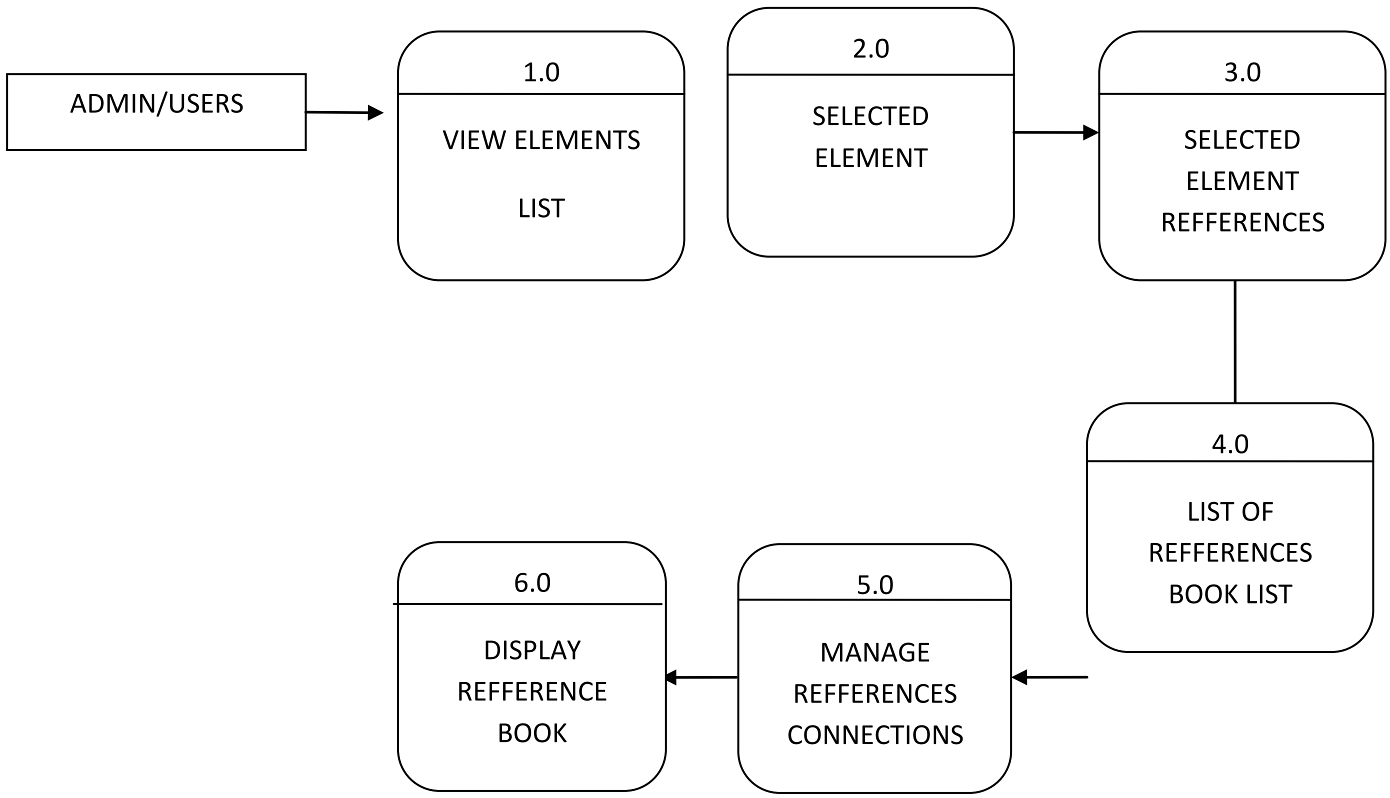
DATAFLOW DIAGRAM
SECOND- LEVEL



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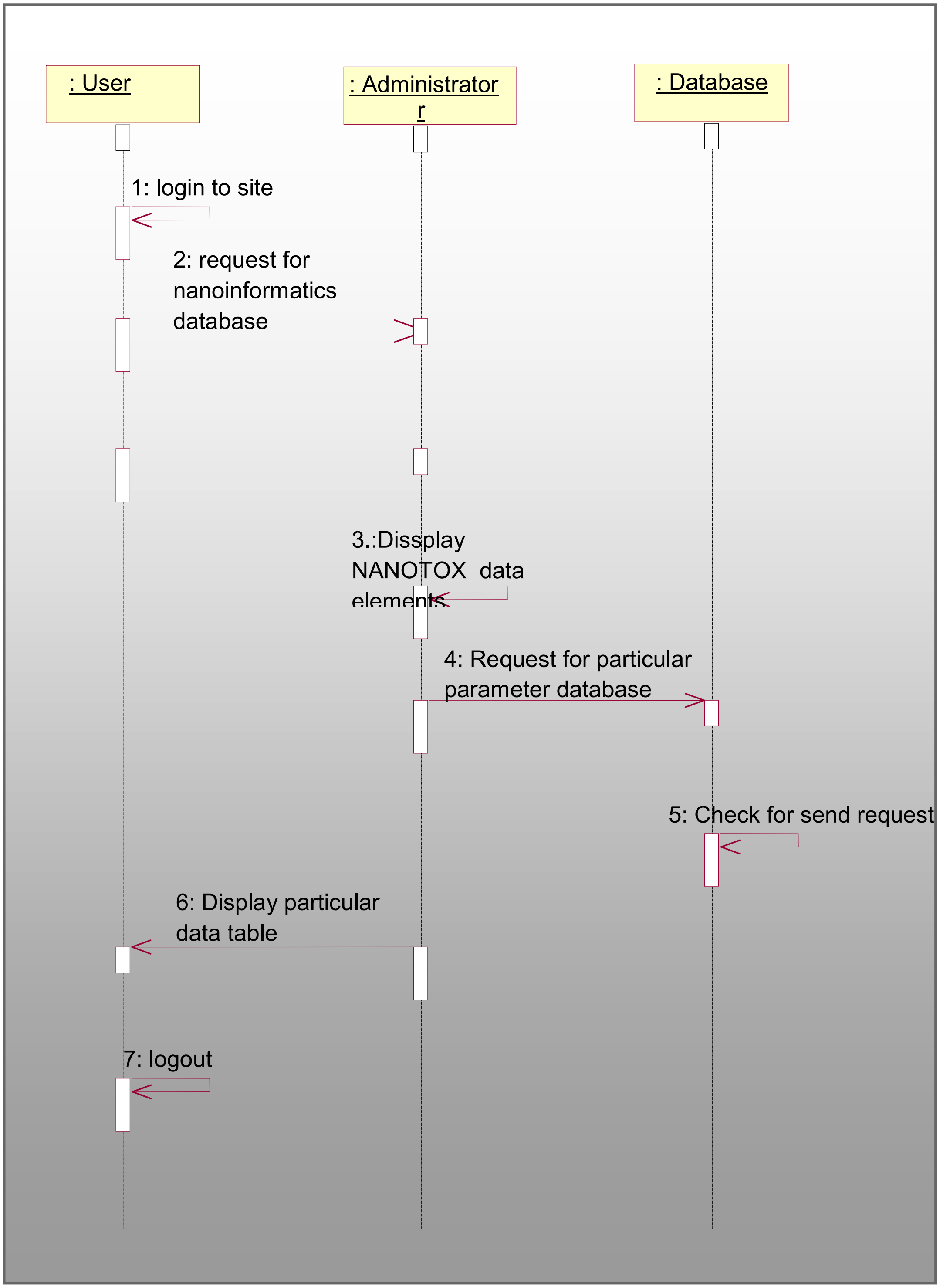
The detail of the entity relationship diagram is area as follows:

ENTITY-RELATIONSHIP DIAGRAMS

Sequence diagram for Nanoinformatics:



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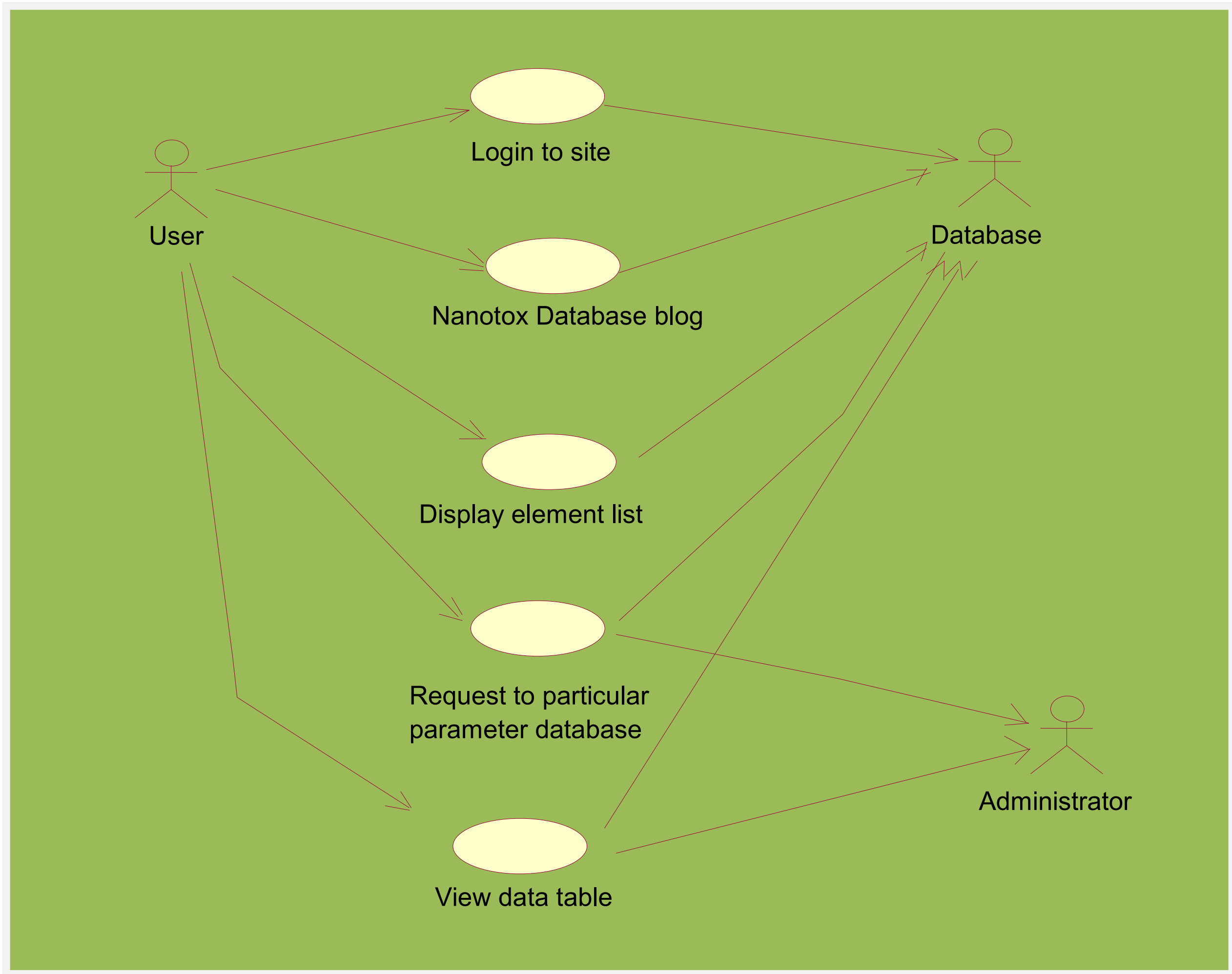
Use case diagram for Nanoinformatics:



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.

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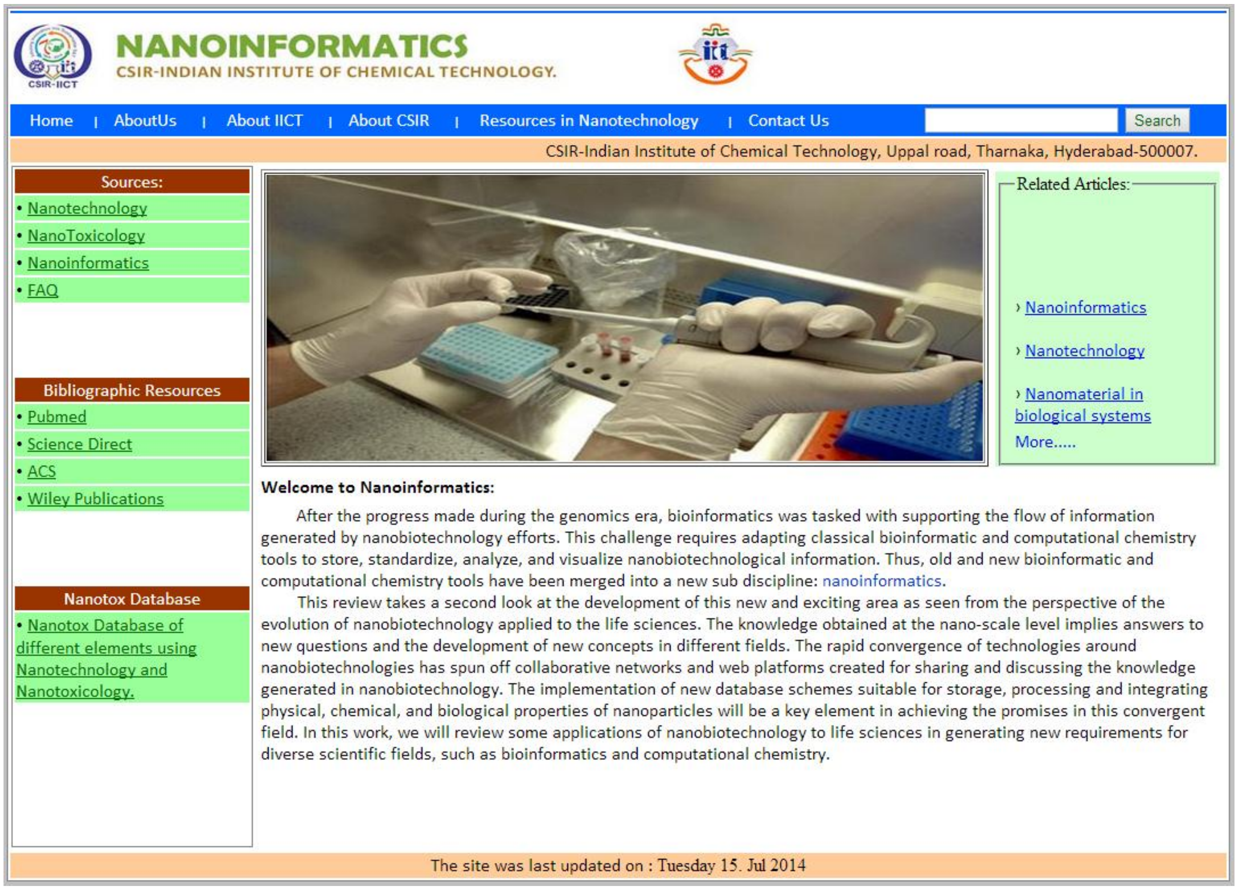

Figure4. Home page of the Nanoinformatics web application.

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

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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.

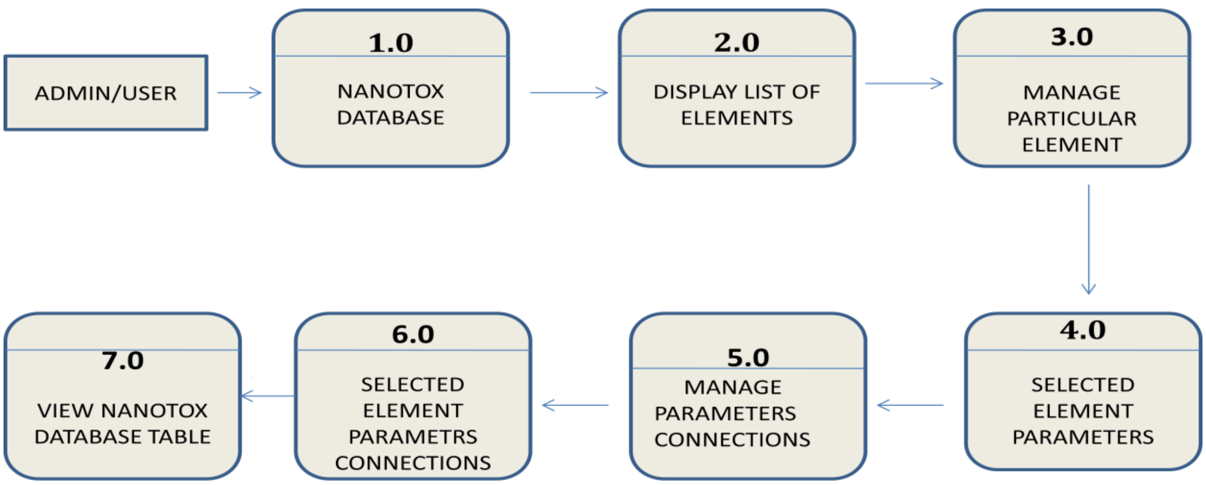

Figure5. Data flow information of the Nanotox Database of different Nanoparticles.

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Screen shots of Nano database:

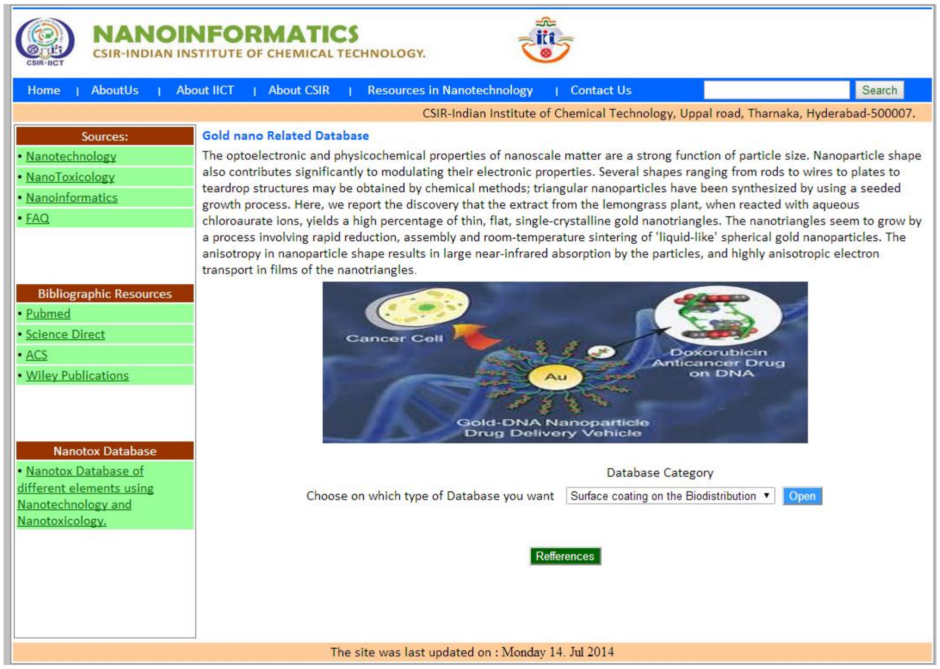
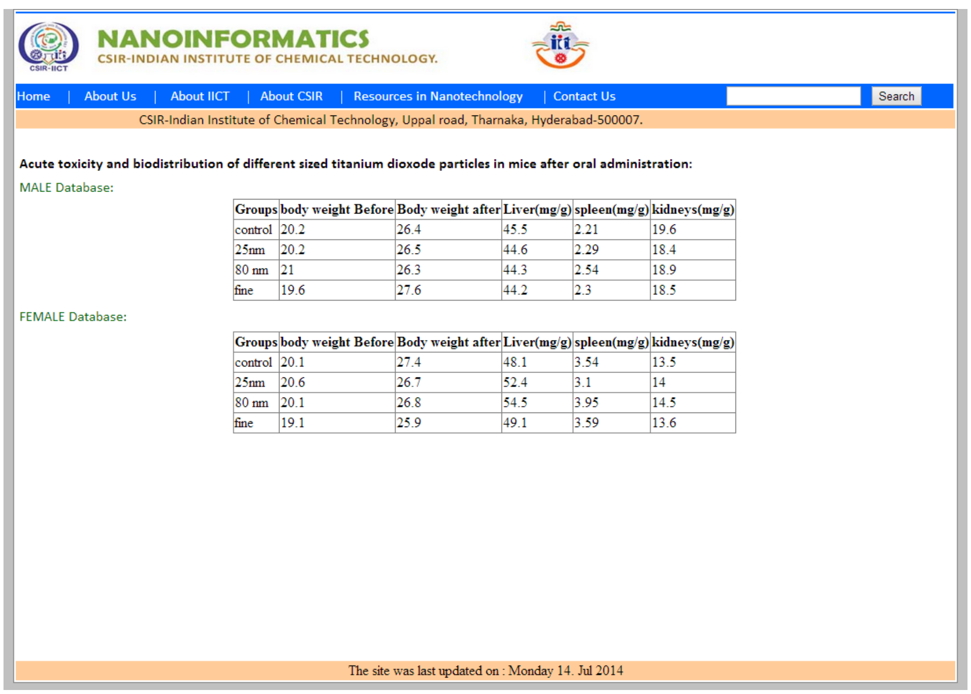


Figure shows Gold Nanoparticle data page.



Acute toxicity and biodistribution of different sized titanium dioxode 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

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

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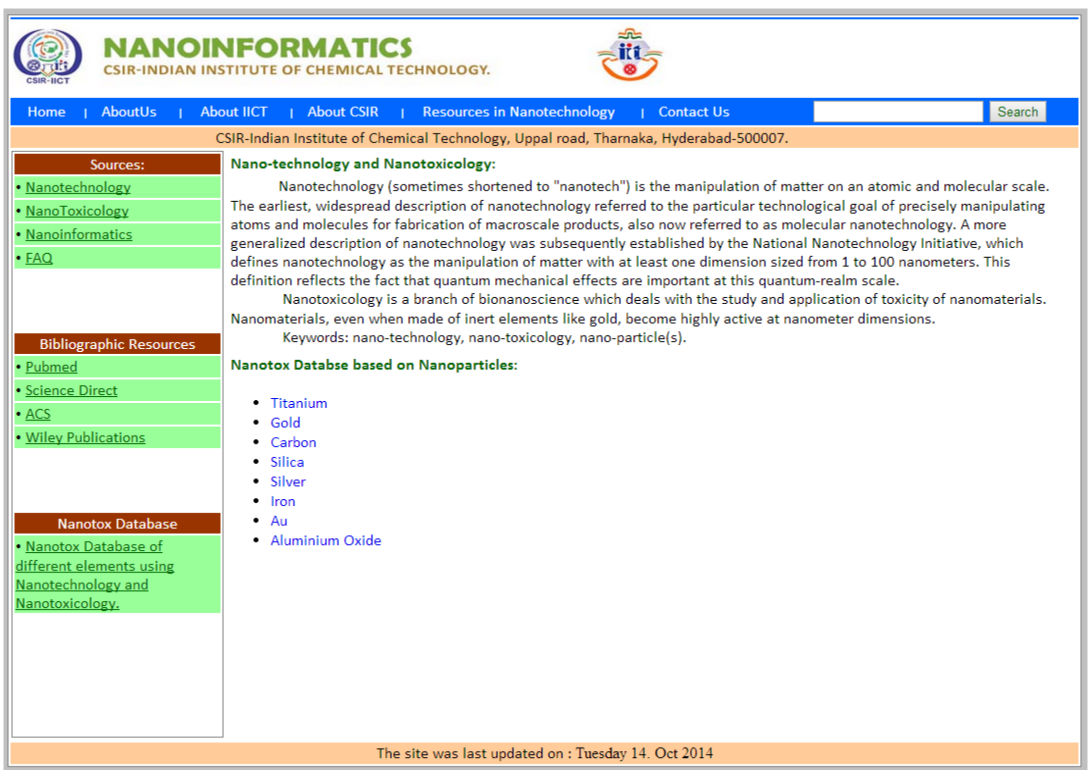
Home Page of the Nanoinformatics.



Database home page of different nanoparticles.

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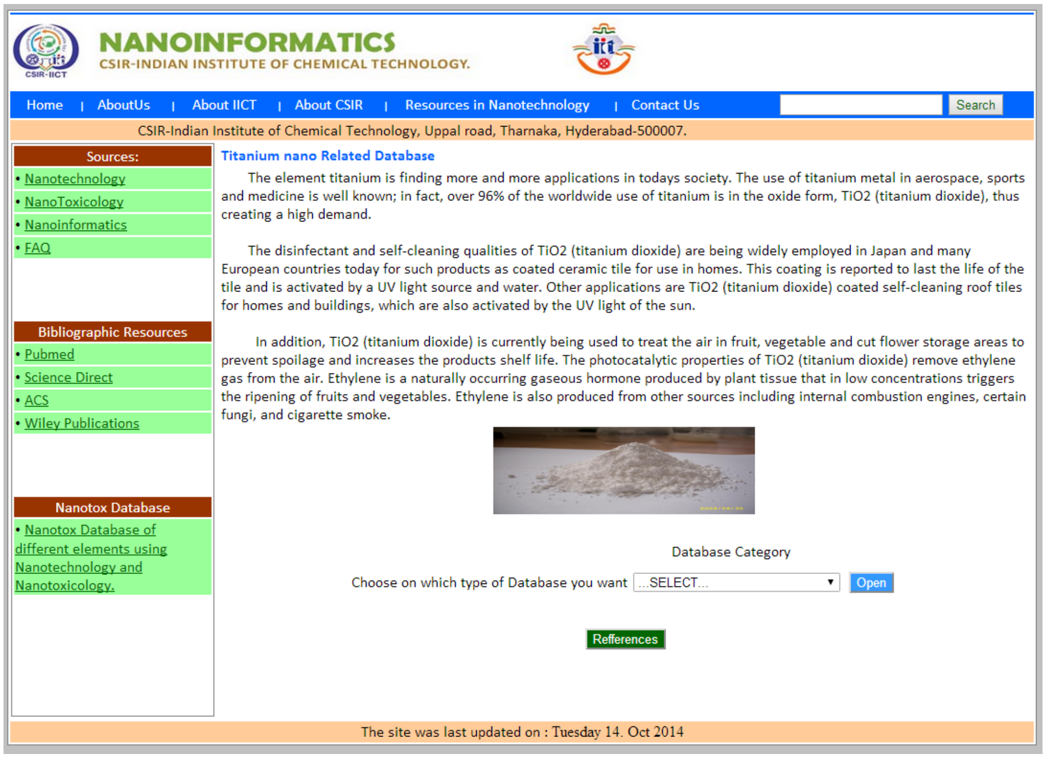
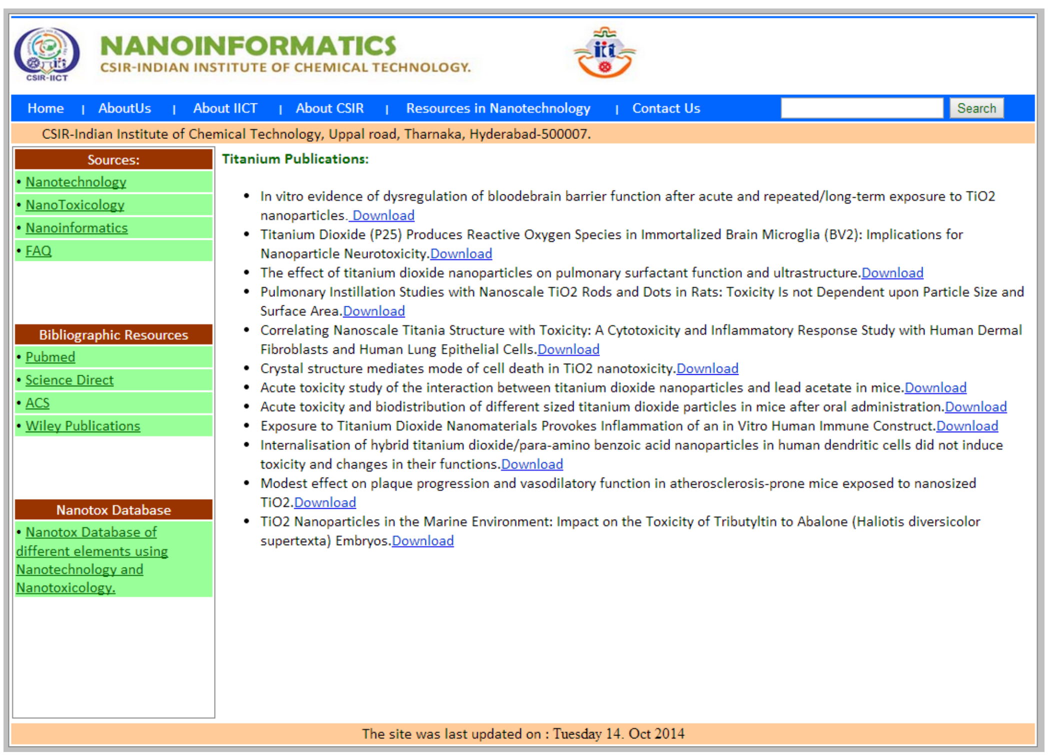


Titanium Database Page.



Titanium Publucations Page.

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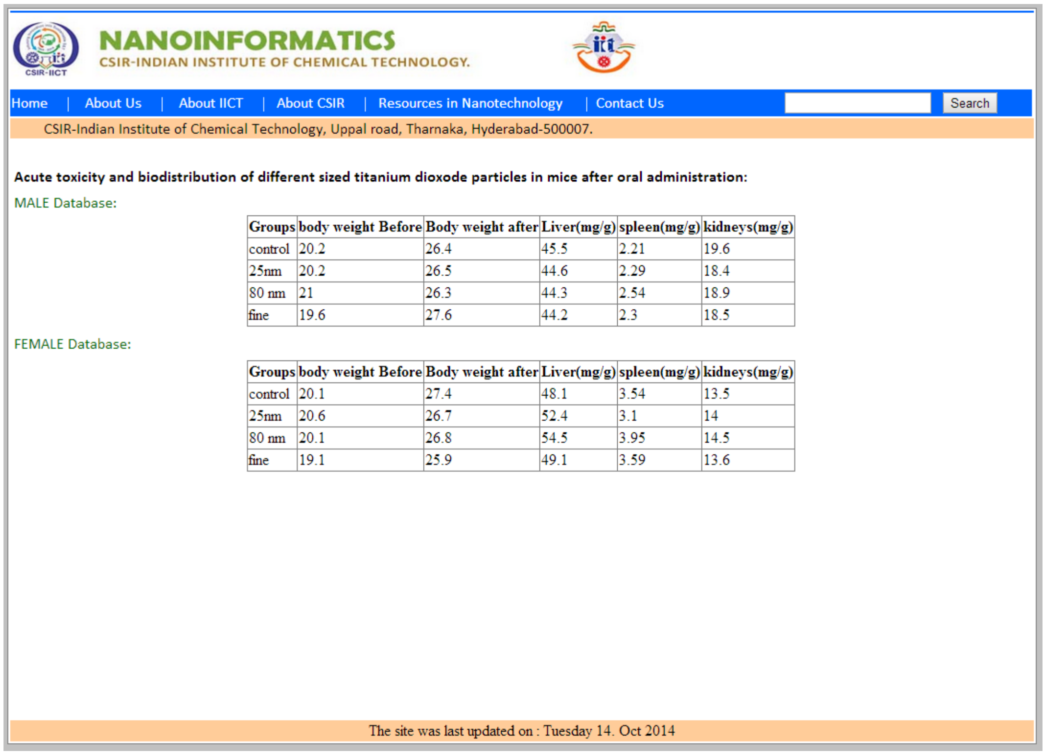

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Acute toxicity and biodistribution of different sized titanium dioxode particles in mice after oral administration:

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

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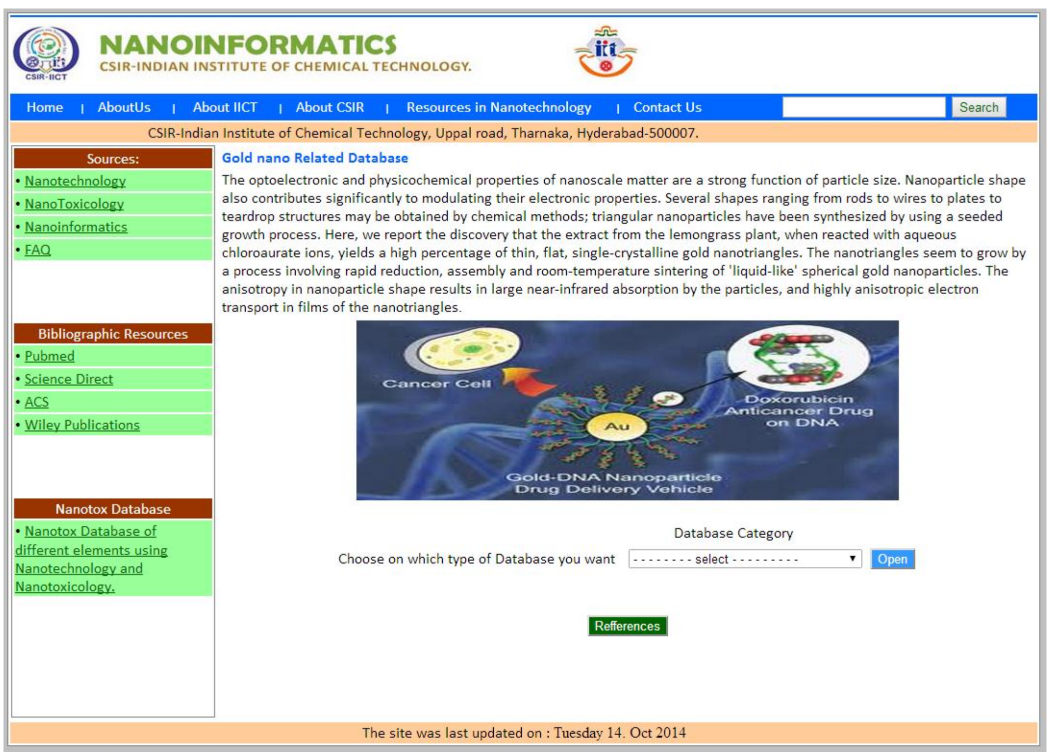
Toxicity and biodistribution of different sized titanium



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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.

Database Category

Choose on which type of Database you want -------- select --------- Open

Refferences

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Gold Database Page

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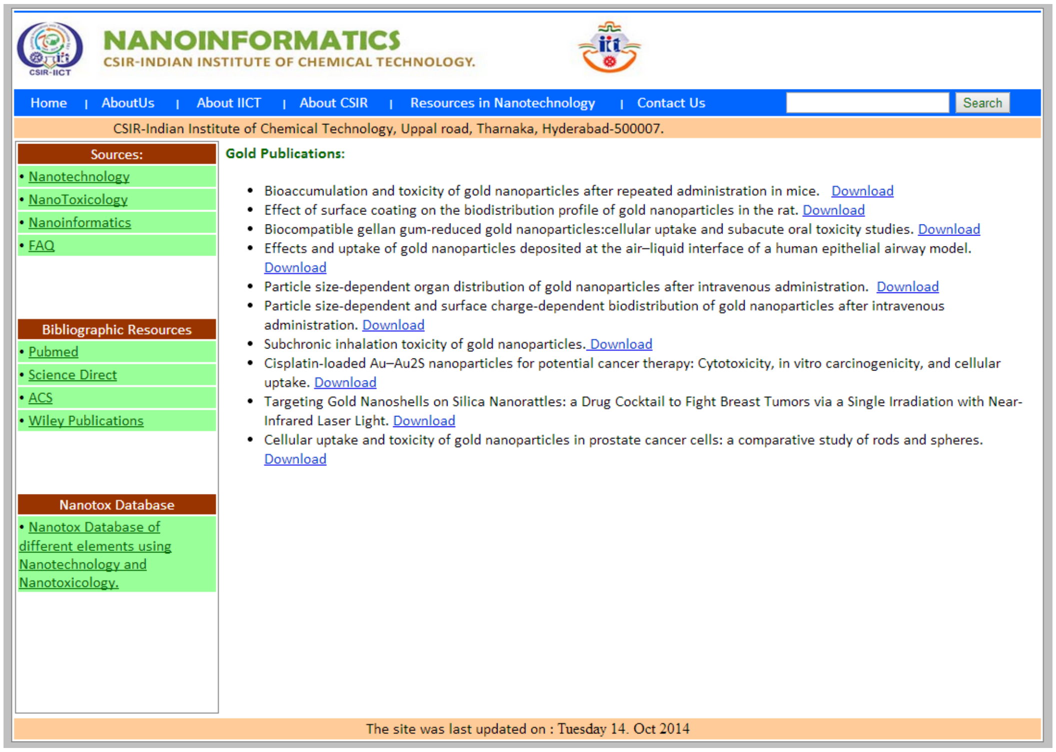
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- NanoToxicology
- Nanoinformatics
- FAQ

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

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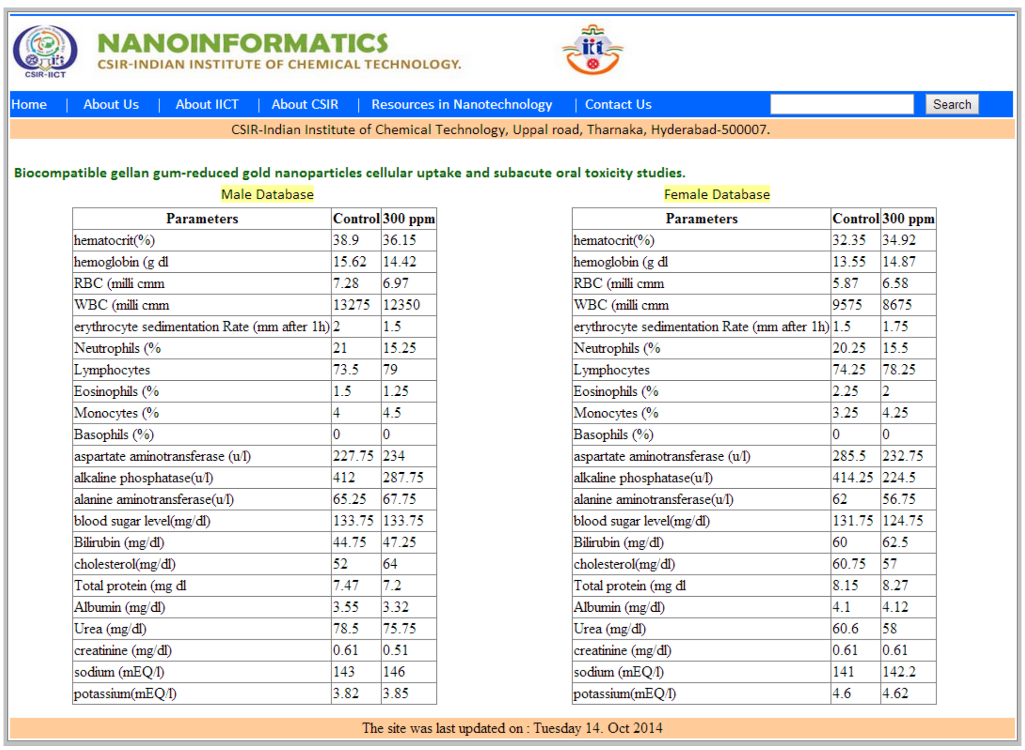
Gold Publications.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Biocompatible gellan gum-reduced gold nanoparticles cellular uptake and subacute oral toxicity studies.

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

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Bio compatible gellan of gold nanoparticle.

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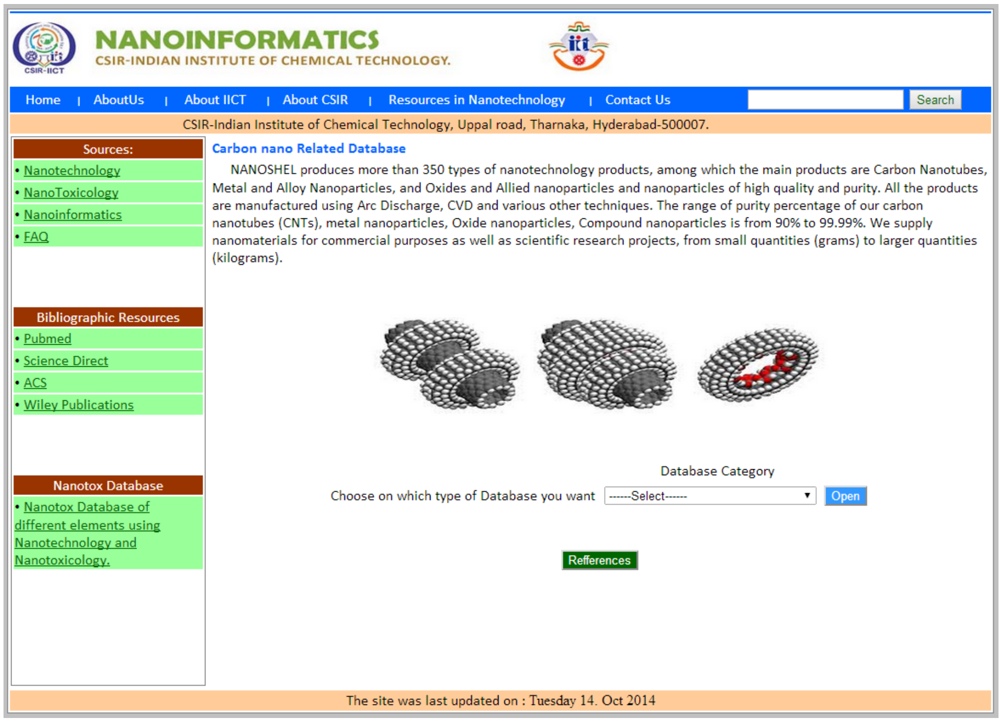

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Sources:
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- NanoToxicology
- Nanoinformatics
- FAQ

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
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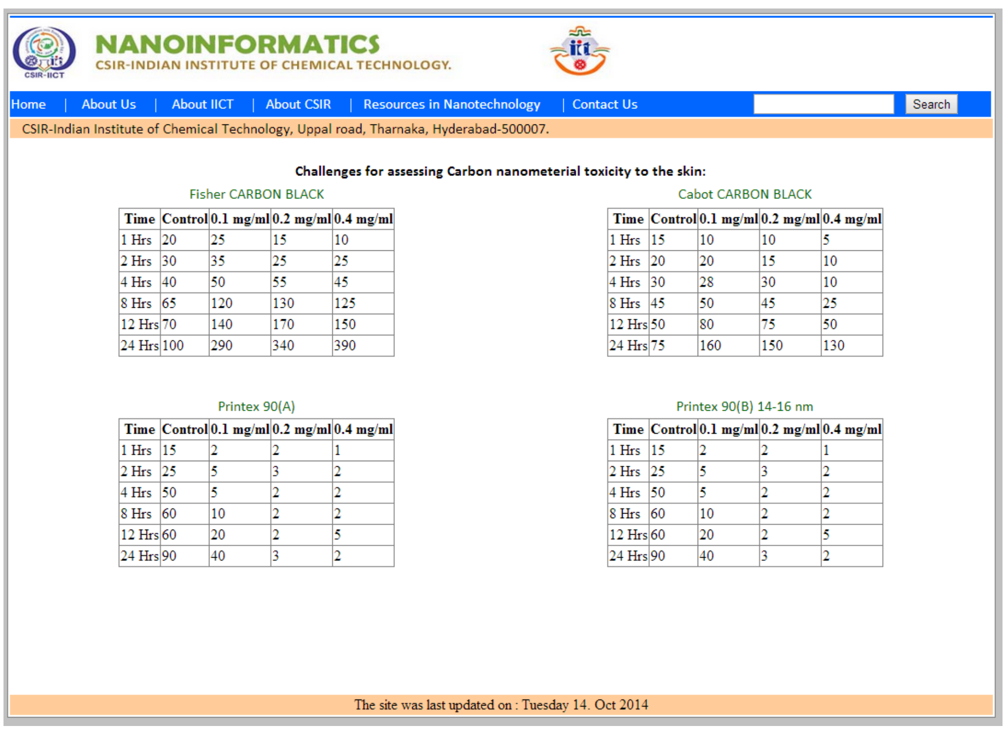
Carbon Database Page.



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Challenges for assessing Carbon nanometerial 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

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Carbon nanometerial toxicity to the skin

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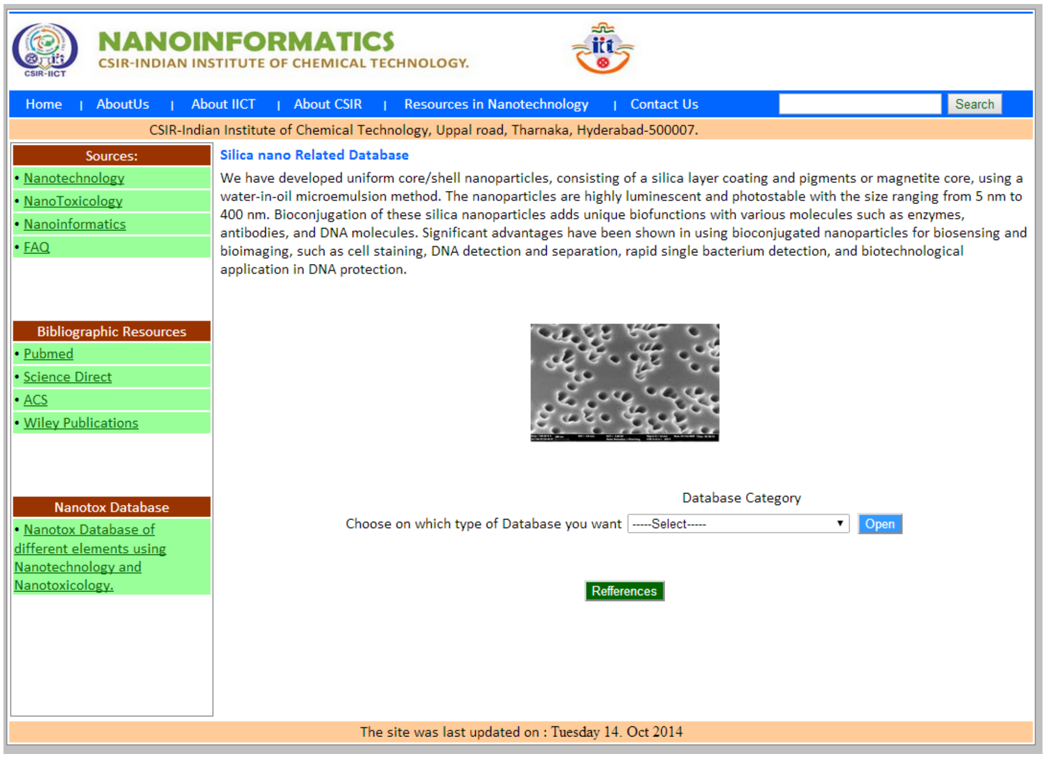
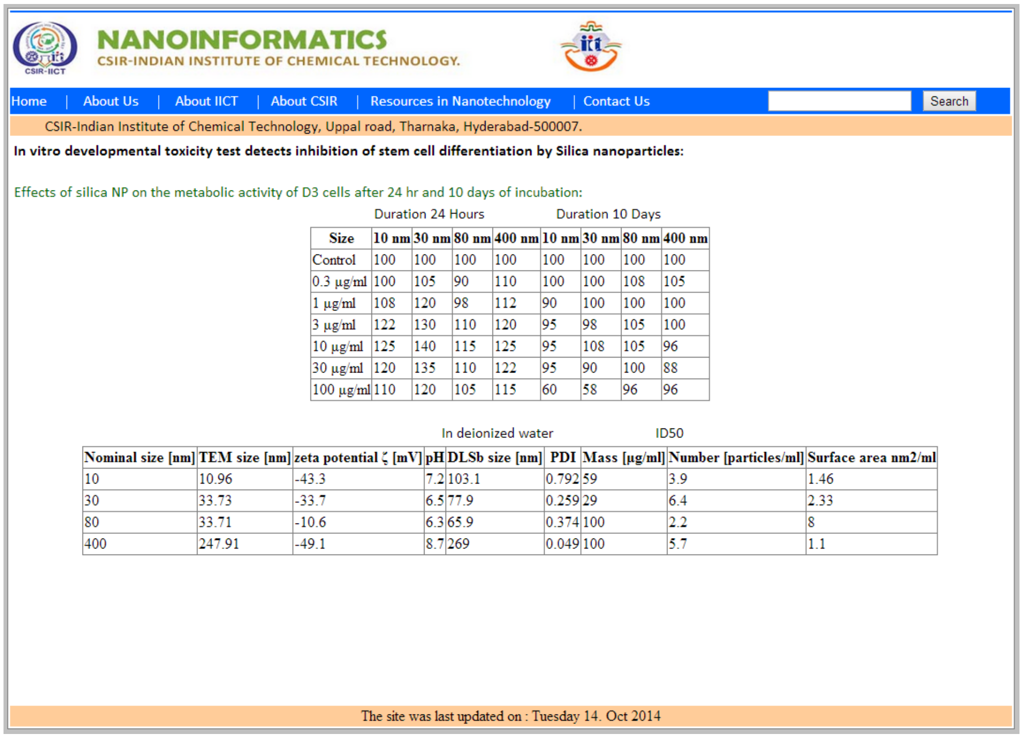


Silica Database Page.



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

Nominal size [nm]	TEM size [nm]	zeta potential ζ [mV]	pH	DLSb size [nm]	PDI	Mass [μg/ml]	Number [particles/ml]	Surface area nm2/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

Silica invitro development toxicity.

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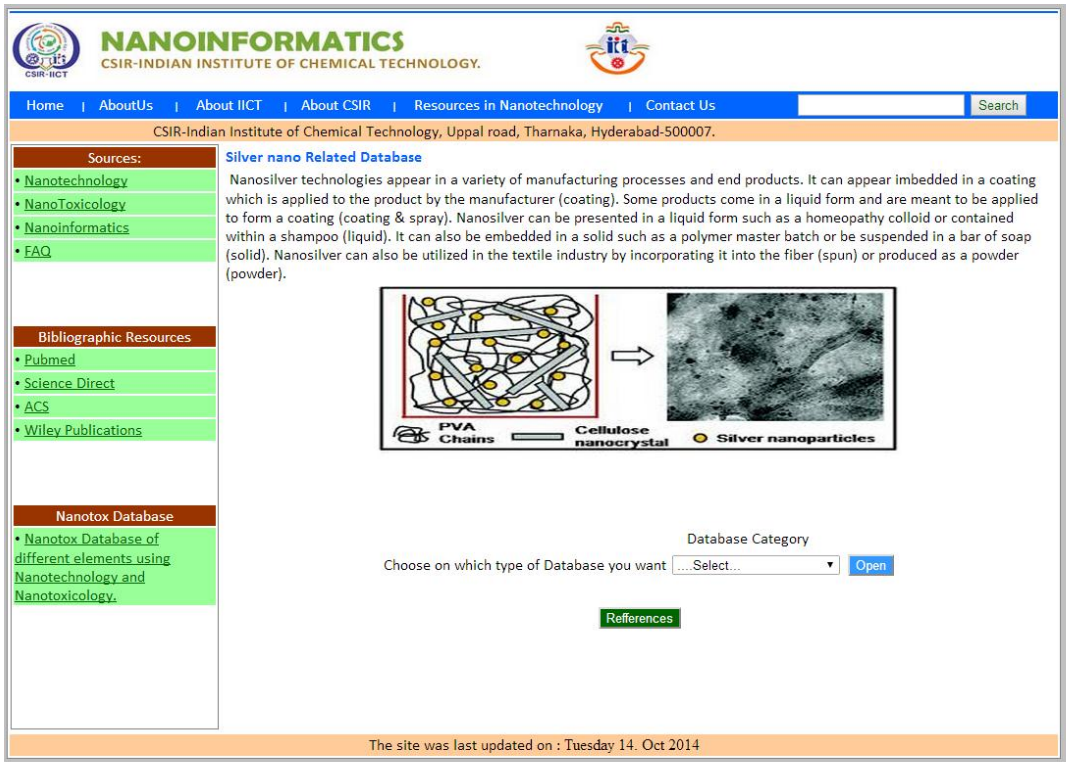
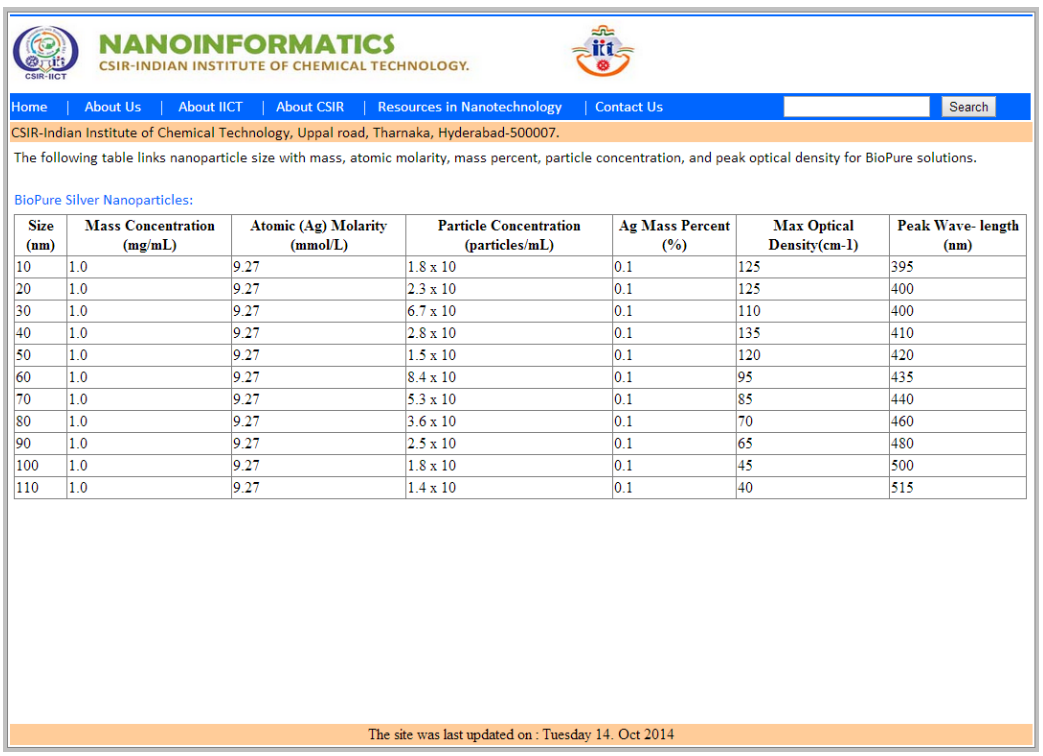


Silver nano Related Database



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

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BioPure Silver Nanoparticles:

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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.

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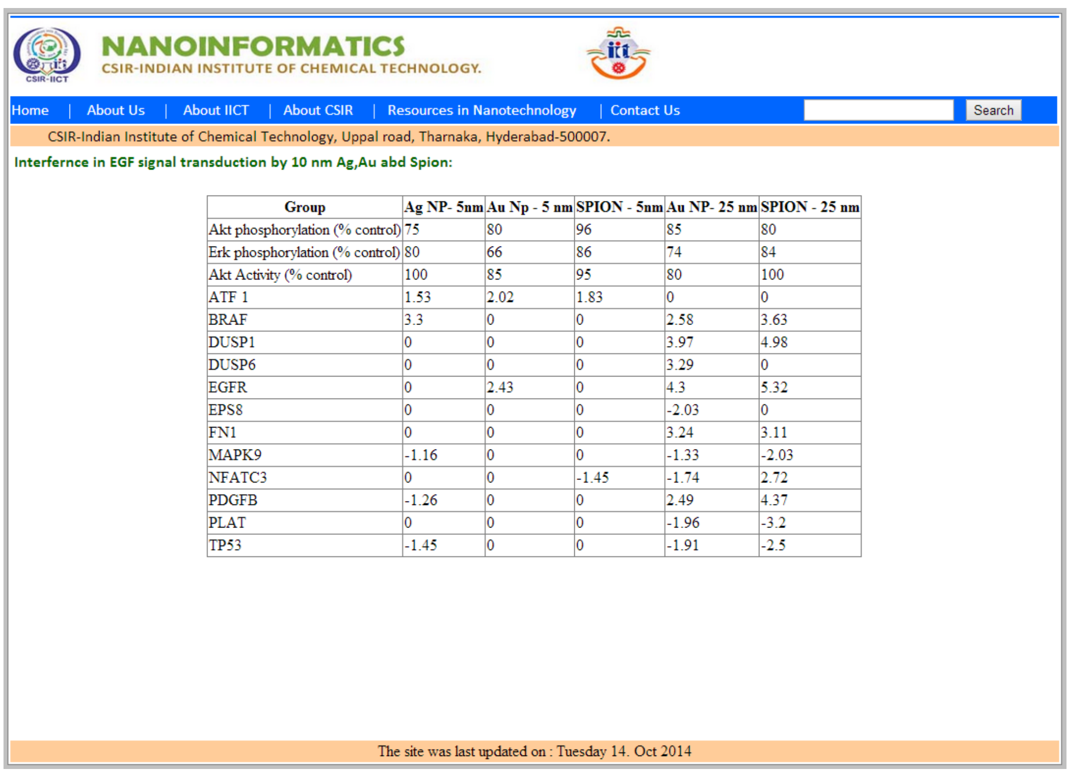
Au nano related Database



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Interfernce 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
EPS8	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

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EGF signal transduction of Au.

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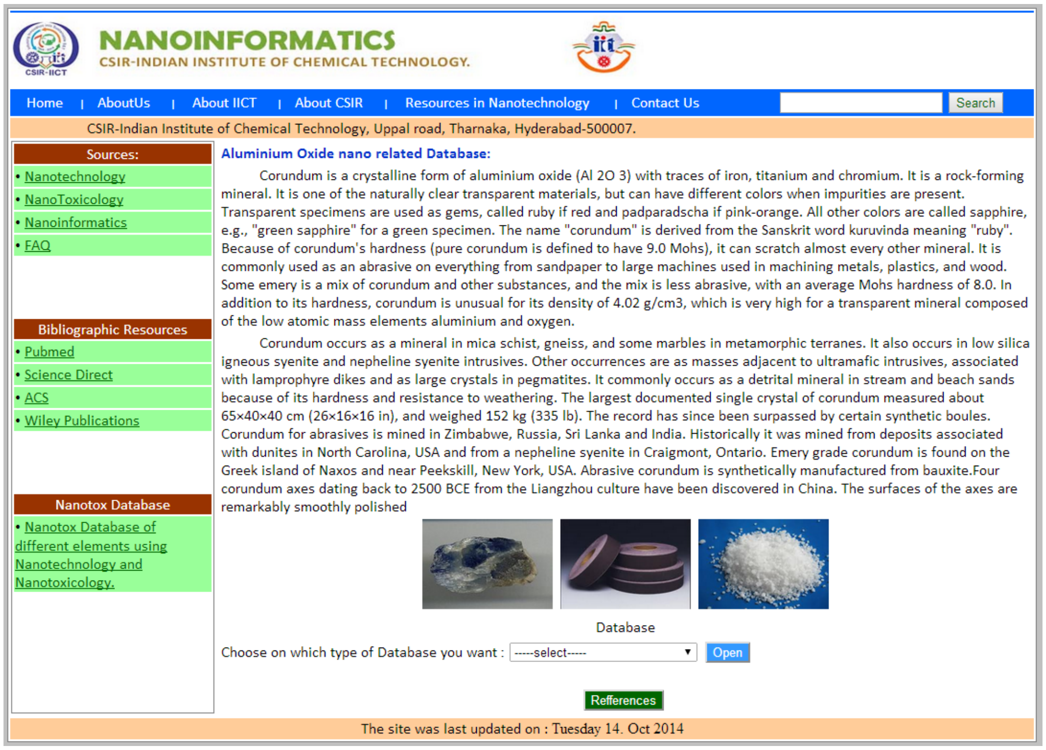

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Nanotox Database
- Nanotox Database of different elements using Nanotechnology and Nanotoxicology.

Aluminium Oxide nano related Database:

Corundum is a crystalline form of aluminium oxide (Al 2O 3) 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

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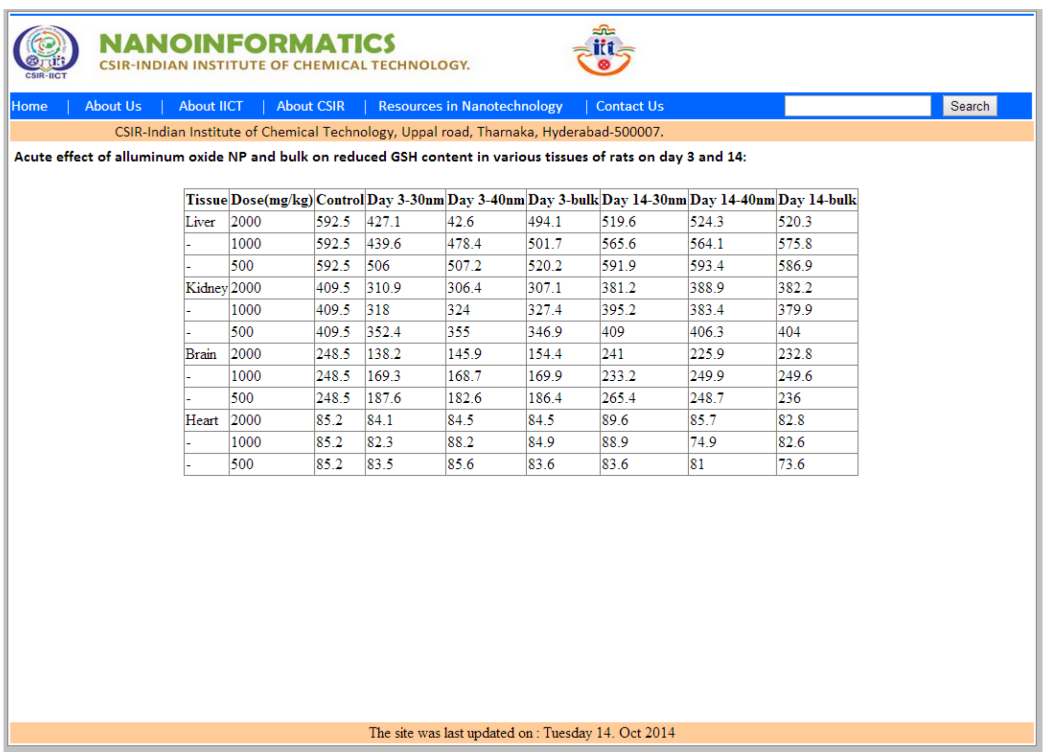
Aluminium Oxide nano related Database



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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

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

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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.

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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.

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