ENM DICTIONARY

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Term or abbreviation	Explanation
AMBIT.Js	*A Java Script Library for interaction with AMBIT instances;*
AMBIT	*AMBIT (http://ambit.sf.net) is an open source web application for cheminformatics data management, modelling and read across. It offers graphical user interface and REST web services, including implementation of OpenTox API and eNanoMapper API extensions. The eNanoMapper database http://data.enanomapper.net runs a customized version of AMBIT.*
API	**A**pplication **P**rogramming **I**nterface *A way computer programs talk to one another. Can be understood in terms of how a programmer sends instructions between programs. The API specifies how software components should interact. A good API makes it easier to develop a program by providing all the building blocks. A programmer then puts the blocks together.*
ArrayAnalysis.org	*Offers user-friendly solutions for gene expression data analysis, from raw data to biological pathways. It contains modules of three types that can be launched individually or successively as an integrated workflow; QC and pre-processing, statistical analysis and pathway analysis.*
ArrayExpress	*A database with data from high-throughput functional genomics experiments stored in a standardized format, providing these data for reuse to the research community. It also includes data on nanomaterials.* *https://www.ebi.ac.uk/arrayexpress/*
Bioclipse	*A Java-based, open source advanced workbench for chem- and bioinformatics. It provides 2D-editing and 3D-visualization of molecules, proteins and sequences, calculation of chemical properties, QSAR and much more; all fully integrated into a user-friendly desktop application. http://www.bioclipse.net/*
caNanoLab	**ca**ncer **Nano**technology **Lab**oratory *is a data sharing portal providing support for the annotation of nanomaterials with characterizations resulting from physico-chemical,* in vitro *and* in vivo *assays and the sharing of these characterizations and associated nanotechnology protocols in a secure fashion.* *https://cananolab.nci.nih.gov/caNanoLab/*
ChEMBL	*A manually curated chemical database of bioactive molecules with drug-like properties developed at the European Molecular Biology Laboratory. It also contains data on nanomaterials. https://www.ebi.ac.uk/chembl/*
Chipster	*An open source user-friendly analysis software for omics and high-throughput data. It contains over 350 analysis tools for next generation sequencing (NGS), microarray, proteomics and sequence data. Users can save and share automatic analysis workflows, and visualize data interactively.*
CTD	**C**omparative **T**oxicogenomics **D**atabase *is a manually curated robust, publicly available database providing information about chemical–gene/protein interactions, chemical–disease and gene–disease relationships, integrated with functional and pathway data to aid in development of hypotheses about the mechanisms underlying environmentally influenced diseases. It also contains data on nanomaterials. http://ctdbase.org/*
eNM	*eNanoMapper – A Database and Ontology Framework for Nanomaterials Design and Safety Assessment (EU Project)*
GEO	*A database with data from high-throughput functional genomics experiments*

	stored in a standardized format, providing these data for reuse to the research community. It also includes data on nanomaterials. http://www.ncbi.nlm.nih.gov/geo/
ISA-TAB	The **I**nvestigation / **S**tudy / **A**ssay **tab** - delimited *format is a general purpose framework with which to collect and communicate complex metadata (i.e. sample characteristics, technologies used, type of measurements made) from experiments employing a combination of technologies. In particular, ISA - TAB has been developed for —but not limited to — experiments using genomics, transcriptomics, proteomics or metabol/nomics techniques. For example, consider an investigation into the effect of a compound that induces liver damage, which looks at changes in (i) the metabolite profile of urine and (ii) gene expression in the liver (by mass spectrometry and microarray technologies, respectively). The general motivation for this work is the fulfillment of the needs of two group. http://www.isa-tools.org/*
ISO 13528:2015	*Statistical methods for use in proficiency testing by interlaboratory comparison; from International Standard Organization (ISO)*
IUCLID5	**I**nternational **U**niform **C**hemica**l** **I**nformation **D**atabase version **5** *plays a central role in the IT environments of all organisations that have to cope with data submission requirements of REACH and other programs (OECD HPV, EU Biocides and others). Industry stakeholders, EU Member States, the European CHemicals Agency (ECHA) , and any other interested party obtain the IUCLID installation kit from the web site; once installed, the local IUCLIDs are the essential tool to capture & store, submit, and exchange data on chemical substances stored according the format of the OECD Harmonised Templates http://iuclid.eu/*
Jaqpot Quattro	*An eNanoMapper developed web application that currently supports data preprocessing, as well as statistical, data mining and machine learning algorithms and methods for defining the Domain of Applicability of a predictive nQSAR model. It is an extension of the Jaqpot web application, which was originally developed during the OpenTox project.*
JSON	**J**ava**S**cript **O**bject **N**otation *is a lightweight data-interchange format. It is easy for humans to read and write. It is easy for machines to parse and generate. JSON is a text format that is completely language independent but uses conventions that are familiar to programmers of the C-family of languages, including C, C++, C#, Java, JavaScript, Perl, Python, and many others. It is based on a subset of the JavaScript Programming Language, Standard ECMA-262 3rd Edition - December 1999. http://json.org/*
MOPAC	**M**olecular **O**rbital **PAC**kage *is a semiempirical quantum chemistry program for generating QSAR descriptors.*
MySQL	**My**-**S**tructural **Q**uery **L**anguage *is an open-source relational database management system, enabling delivery of reliable, high-performance and scalable Web-based and embedded database applications. "My" is the name of daughter to one of the founders. https://www.mysql.com/*
Nano-lazar	**Nano**-**Laz**y structure-**a**ctivity **r**elationships *is an eNanoMapper developed tool for read across toxicity prediction (https://nano-lazar.in-silico.ch/predict).*
NanoWiki	*Originally developed as an internal knowledgebase of the toxicity of, primarily, metal oxides at the Karolinska Institutet and Maastricht University. Uses https://semantic-mediawiki.org/ for data input. The data is exported as RDF*

	dump , available at http://dx.doi.org/10.6084/m9.figshare.1330208. *The NanoWiki RDF dump is converted with a custom parser and imported into the eNanoMapper database at http://data.enanomapper.net*
OECD HT	The **OECD H**armonized **T**emplates (OHTs) *are structured (XML) data formats for reporting safety-related studies on chemical substances. The OHTs http://www.oecd.org/ehs/templates/) and the supporting IT tool (IUCLID5, http://iuclid.eu) are used in a regulatory context, for preparation of substance dossiers for REACH and for other regulatory frameworks operating in Europe; as well as by the JRC NanoHub database*
Ontology	*A relational controlled vocabulary; deals with questions concerning what entities exist or may be said to exist, and how such entities may be grouped, related within a hierarchy, and subdivided according to similarities and differences.*
OpenTox	*A predictive toxicology framework with a unified access to toxicological data, (Q)SAR models and supporting information developed under the grant agreement FP7-HEALTH-2007-A- 200787*
Open Source	**Open-source** software (OSS) *is computer software with its source code made available with a license in which the copyright holder provides the rights to study, change, and distribute the software to anyone and for any purpose. Open-source software may be developed in a collaborative public manner.*
PathVisio	*An open-source and free pathway analysis and pathway drawing software. Allows drawing, editing and analysis of biological pathways. http://www.pathvisio.org/*
PROAST	*An R-based software package that has been developed by RIVM for the statistical analysis of dose-response data. It can be used for 1) dose-response modelling, 2) deriving a Bench Mark Dose in human risk assessment, and 3) deriving an effect concentration in ecotoxicological risk assessment.*
PubChem	The **PubChem** Compound Database *contains validated chemical depiction information provided to describe substances in PubChem Substance. Structures stored within PubChem Compounds are pre-clustered and cross-referenced by identity and similarity groups. It also contains data on nanomaterials. https://pubchem.ncbi.nlm.nih.gov/*
RDF	The **R**esource **D**escription **F**ramework *is one of the core common standards and data exchange formats of the Semantic Web. RDF it is based upon the idea of making statements about resources (in particular web resources) in the form of subject–predicate–object expressions. These expressions are known as triples in RDF terminology. https://www.w3.org/RDF/* *Example: "The sky has the color blue" in RDF is as the triple: a subject denoting "the sky", a predicate denoting "has", and an object denoting "the color blue".*
REST	**Re**presentational **s**tate **t**ransfer *is an abstraction of the architecture of the World Wide Web; more precisely, REST is an architectural style consisting of a coordinated set of architectural constraints applied to components, connectors, and data elements, within a distributed hypermedia system. REST ignores the details of component implementation and protocol syntax in order to focus on the roles of components, the constraints upon their interaction with other components, and their interpretation of significant data elements. OpenTox web services are based on the REST architecture.*
RO	**R**esearch **O**bject *are semantically rich aggregations of resources that bring together data, methods and people in scientific investigations.*

RRegrs	*An eNanoMapper developed tool. It is an R package based on a collection of regression tools from R that can be used to search the best regression models for any dataset. The initial use of the script is aimed at finding QSAR models for chemoinformatics / nanotoxicology.*
SPARQL	**S**imple **P**rotocol **A**nd **R**DF **Q**uery **L**anguage *is a semantic query language for databases, able to retrieve and manipulate data stored in RDF format.*
ToxBank	*A dedicated web-based warehouse for toxicity data management and modelling, a 'gold standards' compound database and repository of selected test compounds, and a reference resource for cells, cell lines and tissues of relevance for in vitro systemic toxicity research carried out across the FP7 HEALTH.2010.4.2.9 Alternative Testing Strategies SEURAT program.*

Abbreviation	Explanation
1D	*1-Dimensional*
3D	*3-Dimensional*
A&A	*Authentication and Authorisation*
AAI	*Authentication and Authorisation Interface*
ANOVA	*Analysis of Variance*
ARFF	*Attribute-Relation File Format*
BAO	*BioAssay Ontology*
bao (namespace)	http://www.bioassayontology.org/bao#
BFO	*Basic Formal Ontology*
BMD	*Benchmark Dose*
BP	*Biological Processes*
CC	*Cellular Components*
CC	*Creative Commons*
CCZero	*Creative Commons Zero waiver*
CDK	*Chemistry Development Kit*
ChEBI	*Chemical Entities of Biological Interest*
CHEMINF	*Chemical Information Ontology*
CL	*Cell Ontology*
clo (namespace)	http://purl.obolibrary.org/obo/
CML	*Chemical Markup Language*
CMS	*Content Management System*
CSV	*Comma-separated values*
CV	*Cross-Validation*
DB	*Database*
DC	*Dublin Core Metadata Ontology*
DFT	*Density Functional Theory*
DoA	*Domain of Applicability*
DoW	*Description of Work*
EC	*European Commission*
EHS	*Environment and Health Safety*
EJB	*Enterprise JavaBeans*
EN	*Elastic Net*
ENET	*Elastic Net regression*

ENM	*Engineered Nano Materials*
ENPRA	*Risk Assessment Of Engineered Nanoparticles (EU Project)*
ENVO	*Environment Ontology*
EU	*European Union*
FFNN	*Feed Forward Neural Network*
GLM	*Generalized Linear Model with Stepwise Feature Selection*
GNU GPL	*GNU General Public License*
GO	*Gene Ontology*
GPW	*Gaussian and plane waves*
GSEA	*Gene Set Enrichment Analysis*
GUI	*Graphical User Interface*
HC	*Hierarchical Clustering*
HF	*Hartree-Fock*
HOMO	*Highest Occupied Molecular Orbital*
HTTP	*Hypertext Transfer Protocol*
IAO	*Information Artifact Ontology*
ID3	*Iterative Dichotomiser 3*
IRI	*International Resource Identifier*
JPDI	*Jaqpot Protocol of Data Interchange JQ Jaqpot Quattro*
JRC	*Joint Research Centre https://ec.europa.eu/jrc/*
JSF	*JavaServer Faces*
KEGG	*Kyoto Encyclopedia of Genes and Genomes*
kNN	*K Nearest Neighbour*
KS-DFT	*Kohn-Sham density functional theory*
LASSO	*Least Absolute Shrinkage and Selection Operator*
LC-MS/MS	*Liquid chromatography–Mass Spectrometry/ Mass Spectrometry*
LDAP	*Lightweight Directory Access Protocol*
LM	*Linear Model*
LOO	*Leave-One-Out*
LOOCV	*Leave one out cross validation*
LUMO	*Lowest Unoccupied Molecular Orbital*
MARINA	*Managing Risks of Nanomaterials (EU Project)*
MeOx	*Metal oxides*
MF	*Molecular Functions*
MIREOT	*Minimum Information to Reference an External Ontology Term*
MLR	*Multiple Linear Regression*
MODENA	*Modelling Nanomaterial Toxicity (EU COST Action)*
ModNanoTox	*Modelling nanoparticle toxicity: principles, methods, novel approaches (EU Project)*
MOPAC	*Molecular Orbital PACkage*
MS	*Mass Spectrometry*
MSigDB	*Molecular Signature Databases*
NANOSOLUTIONS	*Biological Foundation for the Safety Classification of Engineered Nanomaterials (ENM): Systems Biology Approaches to Understand Interactions of ENM with Living Organisms and the Environment (EU Project)*
NANoPUZZLES	*Nanoparticles safety collaboration platform*
nanoQSAR	*Nano- Quantitative Structure-Activity Relationship*
NANoREG	*A common European approach to the regulatory testing of Manufactured*

	Nanomaterials (EU Project)
NCBI	*National Center for Biotechnology Information*
NM	*Nanomaterial*
NN	*Neural Networks*
NPO	*NanoParticle Ontology*
NPs	*Nanoparticles*
nQSAR	*Nano- Quantitative Structure-Activity Relationship*
NSC	*NanoSafety Cluster*
OBI	*Ontology for Biomedical Investigations*
OECD	*Organisation for Economic Co-operation and Development*
OLS	*Ordinary Least Squares*
OpenAM	*OpenAM is an open source access management, entitlements and federation server platform http://en.wikipedia.org/wiki/OpenAM. OpenAM is the software that allows OpenTox services running at each partner facility to use one and the same user credentials (user name and password) this is known as Single Sign On capability.*
OWL	*Web Ontology Language, a family of knowledge representation languages for authoring ontologies*
PATO	*Phenotype and Trait Ontology*
PLS	*Partial Least Squares*
PMML	*Predictive Model Markup Language*
PR	*Protein Ontology (alternative abbreviation)*
PRO	*Protein Ontology*
PubMed	*US National Library of Medicine National Institutes of Health*
QC	*Quality Control*
QM	*Quantum Mechanics*
QSAR	*Quantitative Structure-Activity Relationship*
RA	*Risk Assessment*
RBF	*Radial Basis Function*
RBF-DDA	*Radial Basis Dynamic Decay Adjustment*
RF	*Random Forest*
RFE	*Recursive Feature Elemination*
RMSE	*Root Mean Square Error*
RO	*Relations Ontology*
RO	*Research Object*
RSS	*Rich Site Summary*
SAB	*Scientific Advisory Board*
SDF	*Structure Data File*
SME	*Small and Medium Enterprise*
SEO	*Search Engine Optimization*
SMILES	*Simplified molecular-input line-entry system*
SMW	*Semantic MediaWiki*
SOP	*Standard Operating Procedure*
SPARQL	*SPARQL Protocol and RDF Query Language (recursive acronym)*
SSL	*Secure Sockets Layer*
SSO	*Single Sign-On*
SUN	*Sustainable Nanotechnologies (EU Project)*
SUNDS	*Sustainable Nanotechnologies Decision Support System*

SVM	*Support Vector Machines*
SVN	*SubVersioN*
SVR	*Support Vector Regression*
TEM	*Transmission Electron Microscopy*
TLS	*Transport Layer Security*
UI	*User Interface*
UniProt	*Universal Protein Database*
UO	*Unit Ontology*
URI	*Uniform Resource Identifier*
URL	*Uniform Resource Locator*
UX Design	*User eXperience Design*
VIP	*Very Important Person*
VIP	*Variable Importance to Projection*
WP	*Work Package*
WS	*Web Services*
XLS	*eXceL Spreadsheet*
XML	*eXtensible Markup Language*
Xvfb	*X virtual framebuffer*