

Nanosafety Assessment of ENMs under Dermal Exposure Scenario: From Key Molecular Events to *In Silico* Modeling Tools

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Table of Abbreviations

Acronym	Term
AAS	atomic absorption spectroscopy
AD	applicability domain
AFM	atomic force microscope
AI	artificial intelligence
ANN	artificial neural network
AOPs	adverse outcome pathways
BSA	bovine serum albumin
CER	long-chain ceramide
CG-MD	coarse-grained molecular dynamics
CHOL	cholesterol
CLSM	confocal laser scanning microscope
DFT	density functional theory
DLS	dynamic light scattering
DOPC	1,2-dioleoyl-sn-glycero-3-phosphocholine
DPPC	1,2-dipalmitoyl-sn-glycero-3-phosphocholine
ECHA	European Chemicals Agency
ENMs	engineered nanomaterials
ETC	electron transport chain
FFA	free fatty acid
FRET	fluorescence resonance energy transfer

GSH	glutathione
HAADF	high-angle annular dark field
HCA	high content analysis
HI	human insulin
HRTEM	high resolution transmission electron microscope
HTS	high throughput screening
IATA	integrated approaches to testing and assessment
ICCR	International Cooperation on Cosmetics Regulation
ICP-MS	inductively coupled plasma-mass spectrometry
LC-MS	liquid chromatography-mass spectrometry
LDH	lactate dehydrogenase
LMO	leave-more-out
LOO	leave-one-out
MD	molecular dynamics
MeOx NPs	metal oxide nanoparticles
ML	machine learning
MLR	multiple linear regression
MTT	3- (4,5)-dimethylthiahiazio (-z-y1)-3,5-di- phenytetrazoliumromide
NGO	graphene oxide
NPs	nanoparticles
NPT	isothermal-isobaric
NTA	nanoparticle tracking analysis
NVT	isothermal-isochoric
OECD	Organization for Economic Cooperation and Development
PBPK	physiologically-based pharmacokinetic
PCA	principal component analysis
PLS	partial least-squares
POPC	1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine
q-RASAR	quantitative read-across structure-activity relationship
QSAR	quantitative structure activity relationship
RA	read-across
REO	rare earth oxide
RF	random forest
ROS	reactive oxygen species
SAED	selected area electron diffraction
SAR	structure-activity relationship
SCCS	Scientific Committee on Consumer safety
SEM	scanning electron microscope
SMILE	simplified molecular input-line entry
SOD	superoxide dismutase
SPRM	surface plasmon resonance microscope
SVM	support vector machine
TEM	transmission electron microscope

UV-Vis	ultraviolet–visible spectroscopy
XRD	X-ray Diffraction
XTT	2,3- bis (2-methoxy-4-nitro-5-sulfophenyl)-5- [(phenylamino)carbonyl] -2H-tetrazolium hydroxide
