Development of Nanostructure-Activity Relationships Assisting the Nanomaterial Hazard Categorization for Risk Assessment and Regulatory Decision-Making

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Content:

Influence of Discretization Thresholds on Model Performances

Before building models, the influences of discretization thresholds on model performances were taken into consideration. For global models, a series of thresholds were chosen to examine the tendency of model predictability with the shift of thresholds. Values of the thresholds were set to be 0.1, 0.3, 0.5, 0.7, 1.0, 2.0, 4.0, 6.0, 8.0, 10.0, 30, 50, 70, and 100.0 mg/L for the case studies of LC50 and EC50, and 1.0, 2.0, 4.0, 6.0, 8.0, 10.0, 50.0 and 100.0 mg/L for MIC due to a narrower variation of toxicity values. Within each dataset the records were ranked based on the values of toxicity endpoints. ENMs with toxicity values less than the threshold values were assigned to the 'active' class, and the rest of ENMs were labeled as 'inactive'. On the basis of different classification performances, the thresholds that lead to the most balanced predictive performances for both active and inactive groups were considered for the three case studies. Referring to the regulations and directives nowadays in force, choice of the thresholds for global models was restricted to the values of 0.1, 1.0, 10.0 and 100.0 mg/L, which are, for instance, used by the CLP-Regulation (EC) No 1272/2008 and the EU Directive 93/67/EEC to rank the hazard effects of chemicals. As results, selected cut-off values for case studies I, II and III are respective 1, 10 and 10 mg/L, as described in Figure S1.

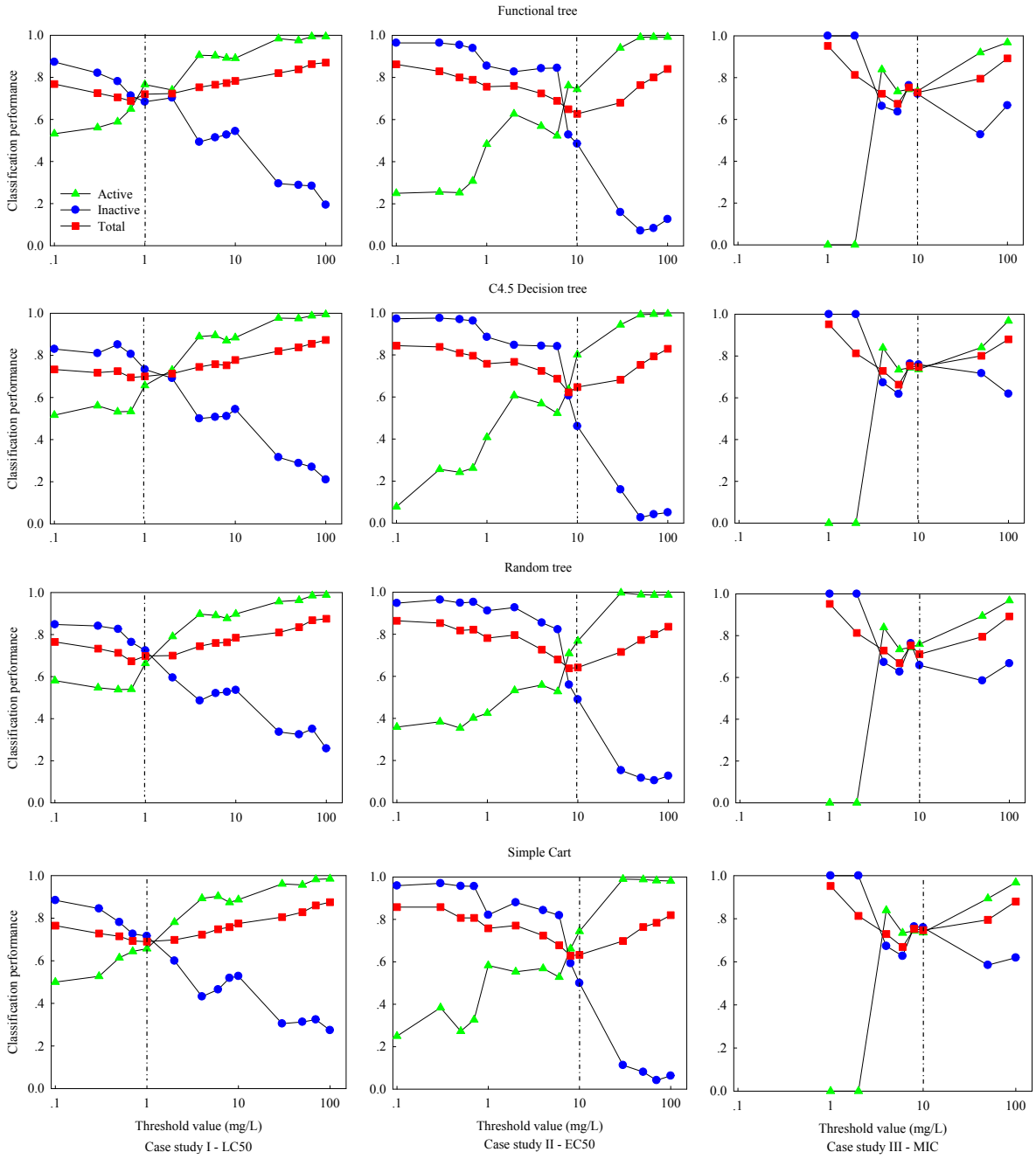
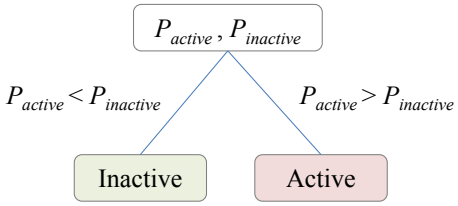


Figure S1. Effect of classification threshold values on model performances. Case study I: LC50 values of 400 ENMs, the optimal threshold value is 1 mg/L for discretizing the numerical values; Case study II: EC50 values of 450 ENMs, the optimal threshold value is 10 mg/L; Case study III: MIC values of 166 ENMs, the optimal threshold value is 10 mg/L.

Developed Global Classification Models

Case study I LC50:

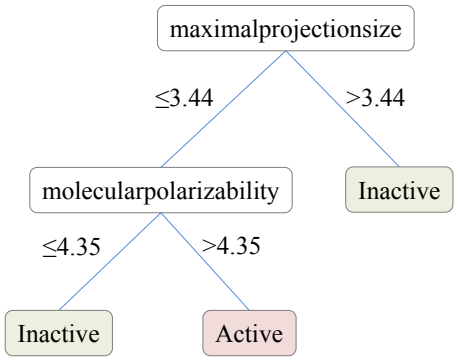
Functional tree



$$P_{active}=\frac{\exp(f_{active})}{\exp(f_{active})+\exp(f_{inactive})}, P_{inactive}=\frac{\exp(f_{inactive})}{\exp(f_{active})+\exp(f_{inactive})}$$

f_{active} = 2.28 - 0.07×[tholepolarizability_a_zz] - 0.01×[volume] - 0.03×[polarsurfacearea] - 0.1×[SddTi] + 0.14×[SsAg] - 15.18×[SdAg] - 0.63×[Se1Al1Al1] - 0.34×[SsCo] - 5.56×[SdCa] - 0.26×[SsSn] + 0.37×[SsNi] - 0.21×[SsSe] + 1.48×[ALogPS_logP] = $-f_{inactive}$

C4.5 decision tree

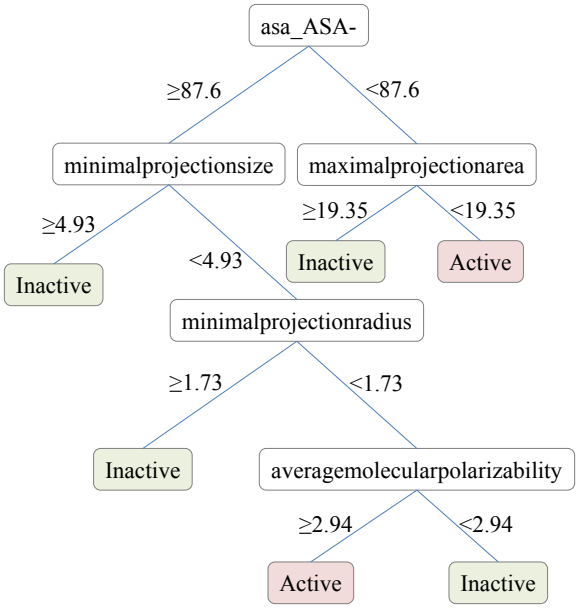


Random tree

```
asa_ASA_P< 78
|  minimalprojectionarea < 10.3
|  |  exactmass < 82.45
|  |  |  ALogPS_logS < 0.45
|  |  |  |  ALogPS_logS < 0.1 : Inactive (3/1)
|  |  |  |  ALogPS_logS >= 0.1 : Active (2/0)
|  |  |  ALogPS_logS >= 0.45 : Inactive (4/0)
|  |  exactmass >= 82.45
|  |  |  maximalprojectionradius < 3.01
|  |  |  |  wienerindex < 0.5
|  |  |  |  |  ALogPS_logP < -1.31
|  |  |  |  |  |  ALogPS_logS < 0.1
|  |  |  |  |  |  |  ALogPS_logS < 0.02 : Active (4/1)
|  |  |  |  |  |  |  ALogPS_logS >= 0.02 : Active (7/0)
|  |  |  |  |  |  ALogPS_logS >= 0.1
|  |  |  |  |  |  |  ALogPS_logS < 0.13 : Inactive (1/0)
|  |  |  |  |  |  |  ALogPS_logS >= 0.13
|  |  |  |  |  |  |  |  ALogPS_logS < 0.31 : Active (1/0)
```

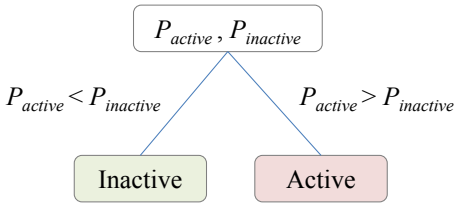
```
|  |  |  |  |  |  |  |  ALogPS_logS >= 0.31
|  |  |  |  |  |  |  |  |  ALogPS_logS < 0.86
|  |  |  |  |  |  |  |  |  |  ALogPS_logS < 0.64 : Inactive (17/8)
|  |  |  |  |  |  |  |  |  |  ALogPS_logS >= 0.64 : Active (31/15)
|  |  |  |  |  |  |  |  |  ALogPS_logS >= 0.86 : Inactive (1/0)
|  |  |  |  |  ALogPS_logP >= -1.31 : Active (15/0)
|  |  |  |  wienerindex >= 0.5 : Active (18/8)
|  |  |  maximalprojectionradius >= 3.01
|  |  |  |  logd < -0.87 : Active (1/0)
|  |  |  |  logd>= -0.87 : Active (57/16)
|  minimalprojectionarea >= 10.3 : Inactive (8/0)
asa_ASA_P >= 78
|  asa_ASA- < 89.7
|  |  tholepolarizability_a_xx < 5.05
|  |  |  tholepolarizability_a_xx < 3.26 : Inactive (2/0)
|  |  |  tholepolarizability_a_xx >= 3.26
|  |  |  |  exactmass < 101.45
|  |  |  |  |  maximalprojectionradius < 2.45
|  |  |  |  |  |  minimalprojectionradius < 1.68 : Active (4/2)
|  |  |  |  |  |  minimalprojectionradius >= 1.68 : Inactive (40/12)
|  |  |  |  |  maximalprojectionradius >= 2.45
|  |  |  |  |  |  minimalprojectionradius < 1.67 : Inactive (4/0)
|  |  |  |  |  |  minimalprojectionradius >= 1.67 : Inactive (22/9)
|  |  |  |  exactmass >= 101.45 : Active (2/0)
|  |  tholepolarizability_a_xx >= 5.05 : Active (1/0)
|  asa_ASA- >= 89.7
|  |  molecularpolarizability < 6.67
|  |  |  chainbondcount < 1.5 : Inactive (3/0)
|  |  |  chainbondcount >= 1.5
|  |  |  |  minimalprojectionradius < 2.49
|  |  |  |  |  dreidingenergy < 61.85 : Inactive (2/0)
|  |  |  |  |  dreidingenergy >= 61.85
|  |  |  |  |  |  chainatomcount < 4 : Inactive (43/6)
|  |  |  |  |  |  chainatomcount >= 4 : Inactive (8/1)
|  |  |  |  minimalprojectionradius >= 2.49 : Inactive (8/2)
|  |  molecularpolarizability >= 6.67 : Inactive (11/0)
```

Simple CART



Case study II EC50:

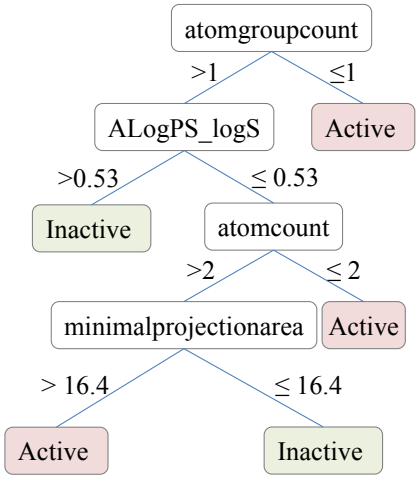
Functional tree



$$P_{active}=\frac{\exp(f_{active})}{\exp(f_{active})+\exp(f_{inactive})}, P_{inactive}=\frac{\exp(f_{inactive})}{\exp(f_{active})+\exp(f_{inactive})}$$

f_{active} = 0.46 - 0.22×[rotatablebondcount] - 0.11×[SsAg] - 0.35×[Se2Ni1O1] + 0.49×[Se1Au1Au1] - 0.44×[SdsDy] + 0.61×[Se1Er2O2ds] - 0.6×[SsFe] + 0.23×[SsAl] + 0.18×[SdsSb] = - $f_{inactive}$

C4.5 decision tree



Random tree

```
balabanindex < 1.32
|  molecularpolarizability < 4.33
|  |  maximalprojectionarea < 13.35
|  |  |  logp < -0.65
|  |  |  |  minimalprojectionarea < 7.07 : Inactive (1/0)
|  |  |  |  minimalprojectionarea >= 7.07 : Active (66/31)
|  |  |  logp >= -0.65
|  |  |  |  minimalprojectionsize < 4.73 : Active (59/29)
|  |  |  |  minimalprojectionsize >= 4.73 : Active (2/0)
|  |  maximalprojectionarea >= 13.35 : Inactive (5/0)
|  molecularpolarizability >= 4.33
|  |  minimalprojectionsize < 6.45
|  |  |  maximalprojectionsize < 0.9
|  |  |  |  ALogPS_logS < -0.03 : Active (16/6)
|  |  |  |  ALogPS_logS >= -0.03
|  |  |  |  |  ALogPS_logS < 0.7
|  |  |  |  |  |  ALogPS_logP < -1.11
|  |  |  |  |  |  |  ALogPS_logS < 0.31 : Active (3/0)
```

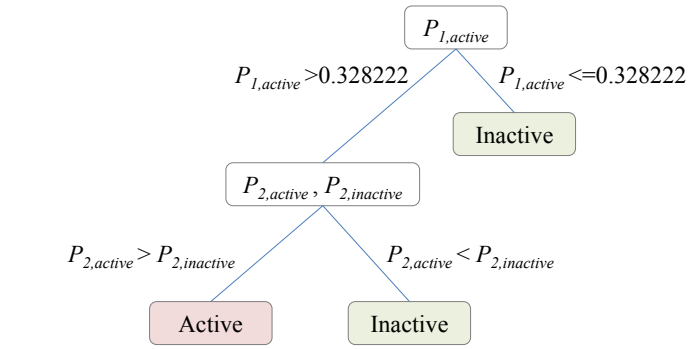
```
|  |  |  |  |  |  |  ALogPS_logS >= 0.31
|  |  |  |  |  |  |  |  ALogPS_logS < 0.54 : Active (34/4)
|  |  |  |  |  |  |  |  ALogPS_logS >= 0.54 : Active (1/0)
|  |  |  |  |  |  ALogPS_logP >= -1.11 : Active (8/2)
|  |  |  |  |  ALogPS_logS >= 0.7
|  |  |  |  |  |  ALogPS_logS < 0.95 : Active (24/8)
|  |  |  |  |  |  ALogPS_logS >= 0.95 : Active (3/0)
|  |  |  maximalprojectionsize >= 0.9
|  |  |  |  maximalprojectionradius < 3.19 : Active (12/0)
|  |  |  |  maximalprojectionradius >= 3.19 : Active (18/4)
|  |  minimalprojectionsize >= 6.45 : Inactive (1/0)
balabanindex >= 1.32
|  logd < -0.43
|  |  atomcount < 4
|  |  |  molecularsurfacearea < 88.1
|  |  |  |  minimalprojectionradius < 2.25 : Inactive (68/22)
|  |  |  |  minimalprojectionradius >= 2.25 : Inactive (3/0)
|  |  |  molecularsurfacearea >= 88.1 : Inactive (26/11)
|  |  atomcount >= 4 : Active (2/0)
|  logd >= -0.43 : Inactive (8/0)
```

Simple CART

```
asa_ASA_H < 61.0
| minimalprojectionsize < 4.93
| | minimalprojectionarea < 7.029999999999999: Active(2.0/0.0)
| | minimalprojectionarea >= 7.029999999999999
| | | averagemolecularpolarizability < 2.94: Active(35.0/31.0)
| | | averagemolecularpolarizability >= 2.94: Active(30.0/29.0)
| minimalprojectionsize >= 4.93
| | averagemolecularpolarizability < 7.52
| | | tholepolarizability_a_xx < 3.4349999999999996
| | | | minimalprojectionarea < 12.55
| | | | | tholepolarizability_a_yy < 4.4: Inactive(15.0/11.0)
| | | | | tholepolarizability_a_yy >= 4.4: Inactive(46.0/22.0)
| | | | minimalprojectionarea >= 12.55: Inactive(3.0/0.0)
| | | tholepolarizability_a_xx >= 3.4349999999999996: Inactive(14.0/0.0)
| | averagemolecularpolarizability >= 7.52: Active(2.0/0.0)
asa_ASA_H >= 61.0: Active(95.0/25.0)
```

Case study III MIC:

Functional tree



$$P_{1,active}=\frac{\exp(f_{1,active})}{\exp(f_{1,active})+\exp(f_{1,inactive})}$$

$$P_{2,active}=\frac{\exp(f_{2,active})}{\exp(f_{2,active})+\exp(f_{2,inactive})},\ P_{2,inactive}=\frac{\exp(f_{2,inactive})}{\exp(f_{2,active})+\exp(f_{2,inactive})}$$

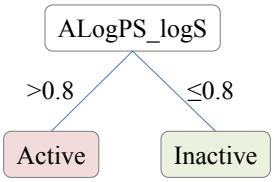
192

193 $f_{1,active}$ = 5.1 + 0.14×[minimalprojectionarea] + 0.01×[asa_ASA_H] - 1.07×[balabanindex] -
194 0.14×[hararyindex] - 0.01×[asa_ASA+] - 0.61×[SsCu] + 5.91×[ALogPS_logP] + 0.91×[ALogPS_logS]
195 = -$f_{1,inactive}$

196 $f_{2,active}$ = 59.21 - 0.29×[averagemolecularpolarizability] + 0.14×[minimalprojectionarea] +
197 0.01×[asa_ASA_H] -1.07×[balabanindex] -0.14×[hararyindex] - 0.01×[asa_ASA+] - 0.61×[SsCu] +
198 46.68×[ALogPS_logP] + 0.39×[ALogPS_logS] = -$f_{2,active}$

199

200 *C4.5 decision tree*

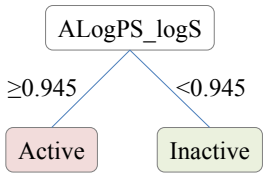


201

202 *Random tree*

```
203 tholepolarizability_a_yy < 2.05
204 |   ALogPS_logP < -1.31
205 |   |   ALogPS_logS < 0.11 : Inactive (5/0)
206 |   |   ALogPS_logS >= 0.11
207 |   |   |   ALogPS_logS < 0.31 : Inactive (27/13)
208 |   |   |   ALogPS_logS >= 0.31 : Inactive (13/4)
209 |   ALogPS_logP >= -1.31 : Active (66/14)
210 tholepolarizability_a_yy >= 2.05
211 |   maximalprojectionarea < 21 : Inactive (18/0)
212 |   maximalprojectionarea >= 21
213 |   |   chainatomcount < 3.5 : Inactive (3/1)
214 |   |   chainatomcount >= 3.5 : Inactive (1/0)
215
216
```

217 *Simple CART*



218

219

Table S1. Performances of the LC50 related nano-SARs for *Danio rerio* and *Daphnia magna*. The best performance of the models were bolded in the table

	Threshold (mg/L)	Data set	Sensitivity	Specificity	Accuracy	CCR
Danio rerio, $n_{training}$ = 76, n_{test} = 18						
Functional tree	1	Training set	0.389	0.828	0.724	0.609
		Test set	0.750	0.714	0.722	0.732
	10	Training set	0.868	0.632	0.750	0.750
		Test set	0.667	0.556	0.611	0.612
	100	Training set	**0.943**	**0.913**	**0.934**	0.928
		Test set	**1**	**1**	**1**	1
C4.5 decision tree	1	Training set	0.056	0.948	0.737	0.502
		Test set	0	1	0.778	0.500
	10	Training set	0.947	0.632	0.789	0.790
		Test set	1	0.556	0.778	0.778
	100	Training set	**0.906**	**0.913**	**0.908**	0.910
		Test set	**1**	**1**	**1**	1
Daphnia magna, $n_{training}$ = 82, n_{test} = 20						
Functional tree	1	Training set	**0.843**	**0.968**	**0.890**	0.906
		Test set	**0.750**	**1**	**0.850**	0.875
	10	Training set	0.971	0.250	0.866	0.611
		Test set	0.941	0.333	0.850	0.637
	100	Training set	1	0	0.927	0.500
		Test set	0.947	0	0.900	0.474
C4.5 decision tree	1	Training set	**0.843**	**0.968**	**0.890**	0.906
		Test set	**0.750**	**1**	**0.850**	0.875
	10	Training set	0.957	0.250	0.854	0.604
		Test set	0.941	0.333	0.850	0.637
	100	Training set	1	0	0.927	0.500
		Test set	1	0	0.950	0.500

Table S2. Performances of the EC50 related nano-SARs for *Daphnia magna* and *Pseudokirchneriella subcapitata*. The best performance of the models were bolded in the table

	Threshold (mg/L)	Data set	Sensitivity	Specificity	Accuracy	CCR
Daphnia magna, $n_{training}$ = 84, n_{test} = 21						
Functional tree	1	Training set	0.552	0.909	0.738	0.731
		Test set	0.500	1	0.762	0.750
	10	Training set	0.926	0.313	0.810	0.620

	100	Test set	1	0.500	0.905	0.750
		Training set	1	0	0.929	0.500
		Test set	1	0	0.905	0.500
C4.5 decision tree	1	Training set	0.550	0.909	0.738	0.730
		Test set	0.500	1	0.762	0.750
	10	Training set	0.912	0.375	0.810	0.644
		Test set	0.824	0.750	0.810	0.787
	100	Training set	1	0	0.929	0.500
		Test set	1	0	0.905	0.500
Pseudokirchneriella subcapitata, $n_{training}$ = 53, n_{test} = 13						
Functional tree	1	Training set	**0.944**	**0.914**	**0.925**	0.929
		Test set	**0.750**	**1**	**0.923**	0.875
	10	Training set	0.813	0.667	0.755	0.740
		Test set	0.750	0.800	0.769	0.775
	100	Training set	1	0	0.906	0.500
		Test set	1	0	0.846	0.500
C4.5 decision tree	1	Training set	**0.944**	**0.914**	**0.925**	0.929
		Test set	**0.750**	**1**	**0.923**	0.875
	10	Training set	0.781	0.667	0.736	0.724
		Test set	0.750	0.800	0.769	0.775
	100	Training set	1	0	0.906	0.500
		Test set	1	0	0.846	0.500

Table S3. Performances of the MIC related nano-SARs for *Escherichia coli* and *Staphylococcus aureus*. The best performance of the models were bolded in the table

	Threshold (mg/L)	Data set	Sensitivity	Specificity	Accuracy	CCR
Escherichia coli, $n_{training}$ = 33, n_{test} = 8						
Functional tree	10	Training set	0	1	0.636	0.500
		Test set	0	1	0.625	0.500
	100	Training set	1	0	0.515	0.500
		Test set	0.882	0.563	0.727	0.723
C4.5 decision tree	10	Training set	0.250	0.905	0.667	0.578
		Test set	0	1	0.625	0.500
	100	Training set	0	1	0.5	0.500
		Test set	0.750	1	0.875	0.875
Staphylococcus aureus, $n_{training}$ = 32, n_{test} = 7						
Functional tree	10	Training set	1	0	0.563	0.500
		Test set	0.750	0.667	0.714	0.709

C4.5 decision tree	100	Training set	1	0	0.750	0.500
		Test set	0.800	1	0.857	0.900
	10	Training set	0.667	0.357	0.531	0.512
		Test set	0.750	0.667	0.714	0.709
	100	Training set	**0.833**	**0.875**	**0.844**	0.854
		Test set	**0.800**	**1**	**0.857**	0.900

232 Table S4. Data resources of LC50 data

Data resources of LC50 toxicity endpoint	Number of toxicity endpoint
Silver nanoparticles: behaviour and effects in the aquatic environment.	20
Acute toxicities of six manufactured nanomaterial suspensions to Daphnia magna	4
Fractionating nanosilver: importance for determining toxicity to aquatic test organisms.	16
Toxicity and bioaccumulation of TiO2 nanoparticle aggregates in Daphnia magna.	3
Acute and chronic effects of nano- and non-nano-scale TiO(2) and ZnO particles on mobility and reproduction of the freshwater invertebrate Daphnia magna.	1
Toxicity Assessment of Titanium (IV) Oxide Nanoparticles Using Daphnia magna (Water Flea).	3
Daphnia magna mortality when exposed to titanium dioxide and fullerene (C60) nanoparticles.	2
Biological surface coating and molting inhibition as mechanisms of TiO2 nanoparticle toxicity in Daphnia magna.	2
Effects of particle composition and species on toxicity of metallic nanomaterials in aquatic organisms.	23
In Vivo Toxicity of Silver Nanoparticles and Silver Ions in Zebrafish (Danio rerio)	1
In vitro evaluation of cytotoxicity of engineered metal oxide nanoparticles.	7
Acute toxicity of cerium oxide, titanium oxide and iron oxide nanoparticles using standardized tests	3
Effects of nano-scale TiO2, ZnO and their bulk counterparts on zebrafish: acute toxicity, oxidative stress and oxidative damage.	5
Toxicity of nanosized and bulk ZnO, CuO and TiO2 to bacteria Vibrio fischeri and crustaceans Daphnia magna and Thamnocephalus platyurus.	9
Exposure to copper nanoparticles causes gill injury and acute lethality in zebrafish (Danio rerio).	1
Comparative toxicity of several metal oxide nanoparticle aqueous suspensions to Zebrafish (Danio rerio) early developmental stage.	1
Scientific Report No. 12	1
Fate and effects of CeO2 nanoparticles in aquatic ecotoxicity tests.	3
Toxicity of two types of silver nanoparticles to aquatic crustaceans Daphnia magna and Thamnocephalus platyurus.	4
Toxicity Test of Ag+, Nano-Ag0 and Nano-Ag2O using Green Algae (Chlorella sp.) and Water Flea (Moina Macrocopa)	1
Toxicity of Nanoscale CuO and ZnO to Daphnia magna	2
Ecotoxicology of nanomaterials: the role of invertebrate testing	15
Zebrafish as a correlative and predictive model for assessing biomaterial nanotoxicity.	1
Dispersion and toxicity of selected manufactured nanomaterials in natural river water samples: effects of water chemical composition.	12
Acute and chronic toxicity of nano-scale TiO 2 particles to freshwater fish, cladocerans, and green algae, and effects of organic and inorganic substrate on TiO 2 toxicity	3
Effects from filtration, capping agents, and presence/absence of food on the toxicity of silver nanoparticles to Daphnia magna.	9
Differentiation of the toxicities of silver nanoparticles and silver ions to the Japanese medaka (Oryzias latipes) and the cladoceran Daphnia magna.	2
The effects of silver nanoparticles on fathead minnow (Pimephales promelas) embryos.	6
Ecotoxicity of nanoparticles of CuO and ZnO in natural water.	8

Toxicity of manufactured zinc oxide nanoparticles in the nematode Caenorhabditis elegans.	3
Toxicogenomic responses of nanotoxicity in Daphnia magna exposed to silver nitrate and coated silver nanoparticles.	11
Toxicity of nanoparticulate and bulk ZnO, Al2O3 and TiO2 to the nematode Caenorhabditis elegans.	6
Importance of surface coatings and soluble silver in silver nanoparticles toxicity to Daphnia magna.	5
Toxicity of silver nanoparticles in zebrafish models	1
Silver nanoparticle toxicity in the embryonic zebrafish is governed by particle dispersion and ionic environment.	4
Effect of nanoparticle stabilization and physicochemical properties on exposure outcome: acute toxicity of silver nanoparticle preparations in zebrafish (Danio rerio).	14
Toxicity of Silver Nanoparticles in Aquatic Ecosystems: Salinity as the Main Cause in Reducing Toxicity	1
Toxicity assessments of multisized gold and silver nanoparticles in zebrafish embryos.	4
Toxicity of Silver and Titanium Dioxide Nanoparticle Suspensions to the Aquatic Invertebrate, Daphnia magna	2
Toxicity comparison of colloidal silver nanoparticles in various life stages of rainbow trout (Oncorhynchus mykiss)	3
Effects of Nanotoxicity on Female Reproductivity and Fetal Development in Animal Models	2
Nanomaterials and the environment: a review for the biennium 2008-2010.	1
Effects of silver nanoparticles on the development and histopathology biomarkers of Japanese medaka (Oryzias latipes) using the partial-life test.	2
The primacy of physicochemical characterization of nanomaterials for reliable toxicity assessment: a review of the zebrafish nanotoxicology model.	6
Engineered Nanoparticles: Review of Health and Environmental Safety	10
The toxicity of silver nanoparticles to zebrafish embryos increases through sewage treatment processes.	4
Acute effects of Fe_2O_3, TiO_2, ZnO and CuO nanomaterials on Xenopus laevis.	6
Silver nanoparticles and silver nitrate induce high toxicity to Pseudokirchneriella subcapitata, Daphnia magna and Danio rerio.	3
Comparison of nanosilver and ionic silver toxicity in Daphnia magna and Pimephales promelas.	6
Effects of Cu2O nanoparticle and CuCl2 on zebrafish larvae and a liver cell-line.	1
Acute toxicity of 31 different nanoparticles to zebrafish (Danio rerio) tested in adulthood and in early life stages - comparative study.	18
Determination of the mechanism of photoinduced toxicity.xls	4
Determination of the mechanism of photoinduced toxicity of selected metal oxide nanoparticles (ZnO, CuO, Co3O4 and TiO2) to E. coli bacteria	4
Ecotoxicity of manufactured ZnO nanoparticles--a review.	8
Toxicity of TiO(2) nanoparticles to cladocerans, algae, rotifers and plants - effects of size and crystalline structure.	4
Accumulation and toxicity of metal oxide nanoparticles in a soft-sediment estuarine amphipod.	4
Metal-based nanoparticles in soil: fate, behavior, and effects on soil invertebrates.	6
Developmental toxicity of Japanese medaka embryos by silver nanoparticles and released ions in the presence of humic acid.	2
The impact of size on the fate and toxicity of nanoparticulate silver in aquatic systems.	2
Toxicity of copper oxide nanoparticle suspensions to aquatic biota.	3

Phototoxicity of TiO2 nanoparticles under solar radiation to two aquatic species: Daphnia magna and Japanese medaka.	3
Acute and chronic toxicity of nano-scale TiO2 particles to freshwater fish, cladocerans, and green algae, and effects of organic and inorganic substrate on TiO2 toxicity	8
Effects of Silica Dioxide Nanoparticles on the Embryonic Development of Zebrafish	1
Freshwater snail vital rates affected by non-lethal concentrations of silver nanoparticles	1
Initial Study on the Toxicity of Silver Nanoparticles (NPs) against Paramecium caudatum	4
Investigating potential toxicity of phenanthrene adsorbed to nano-ZnO using Daphnia magna	4
Toxicity of silver, titanium and silicon nanoparticles on the root-knot nematode, Meloidogyne incognita, and growth parameters of tomato	1
Determination of the mechanism of photoinduced toxicity of selected metal oxide nanoparticles (ZnO, CuO, Co3O4 and TiO2) to E. coli bacteria.	8
Assessment of nanosilver toxicity during zebrafish (Danio rerio) development.	1
Ceriodaphnia dubia as a potential bio-indicator for assessing acute aluminum oxide nanoparticle toxicity in fresh water environment.	3
Comparative toxicity of nano-ZnO and bulk ZnO suspensions to zebrafish and the effects of sedimentation, ˙OH production and particle dissolution in distilled water.	1
Differential gene expression in Daphnia magna suggests distinct modes of action and bioavailability for ZnO nanoparticles and Zn ions.	1
Effect of subacute exposure to silver nanoparticle on some hematological and plasma biochemical indices in silver carp (Hypophthalmichthys molitrix).	4
Effects of nano-sized zero-valent iron (nZVI) on DDT degradation in soil and its toxicity to collembola and ostracods.	1
Elemental selenium particles at nano-size (Nano-Se) are more toxic to Medaka (Oryzias latipes) as a consequence of hyper-accumulation of selenium: a comparison with sodium selenite.	1
Evaluation of the toxic impact of silver nanoparticles on Japanese medaka (Oryzias latipes).	1
Histopathological studies and oxidative stress of synthesized silver nanoparticles in Mozambique tilapia (Oreochromis mossambicus).	1
Interaction of silver nanoparticles with biological surfaces of Caenorhabditis elegans.	1
Photoinactivation of Escherichia coli by sulfur-doped and nitrogen-fluorine-codoped TiO2 nanoparticles under solar simulated light and visible light irradiation.	10
Phototoxicity of TiO2 nanoparticles to zebrafish (Danio rerio) is dependent on life stage.	3
Silver nanocolloids disrupt medaka embryogenesis through vital gene expressions.	1
Silver nanoparticle toxicity to Daphnia magna is a function of dissolved silver concentration.	9
Silver nanoparticles cause oxidative damage and histological changes in medaka (Oryzias latipes) after 14 days of exposure.	3
Silver nanoparticle-specific mitotoxicity in Daphnia magna.	1
Surface interactions affect the toxicity of engineered metal oxide nanoparticles toward Paramecium.	4
The zerovalent iron nanoparticle causes higher developmental toxicity than its oxidation products in early life stages of medaka fish.	1
Titanium dioxide nanoparticles produce phototoxicity in the developing zebrafish.	1
Toxicity assessment of iron oxide nanoparticles in zebrafish (Danio rerio) early life stages.	1
Toxicity of silver and titanium dioxide nanoparticle suspensions to the aquatic invertebrate, Daphnia magna.	2
Zinc oxide nanoparticles toxicity to Daphnia magna: size-dependent effects and dissolution.	1

233

234

235 Table S5. Data resources of EC50 data

Data resources of EC50 toxicity endpoint	Number of toxicity endpoint
Acute toxicities of six manufactured nanomaterial suspensions to Daphnia magna	5
Toxicity of silver nanoparticles to Chlamydomonas reinhardtii.	10
Toxicity and bioaccumulation of TiO2 nanoparticle aggregates in Daphnia magna.	1
Acute and chronic effects of nano- and non-nano-scale TiO(2) and ZnO particles on mobility and reproduction of the freshwater invertebrate Daphnia magna.	5
Biological surface coating and molting inhibition as mechanisms of TiO2 nanoparticle toxicity in Daphnia magna.	2
Effects of particle composition and species on toxicity of metallic nanomaterials in aquatic organisms.	4
Acute toxicity of cerium oxide, titanium oxide and iron oxide nanoparticles using standardized tests	2
Aggregation and toxicity of titanium dioxide nanoparticles in aquatic environment--a review.	2
Toxicity of nanosized and bulk ZnO, CuO and TiO2 to bacteria Vibrio fischeri and crustaceans Daphnia magna and Thamnocephalus platyurus.	8
Comparative toxicity of several metal oxide nanoparticle aqueous suspensions to Zebrafish (Danio rerio) early developmental stage.	1
Toxicity of nanoparticles of CuO, ZnO and TiO2 to microalgae Pseudokirchneriella subcapitata.	9
Toxicity of various silver nanoparticles compared to silver ions in Daphnia magna.	3
Algal testing of titanium dioxide nanoparticles--testing considerations, inhibitory effects and modification of cadmium bioavailability.	4
Fate and effects of CeO2 nanoparticles in aquatic ecotoxicity tests.	9
Ecotoxic effect of photocatalytic active nanoparticles (TiO2) on algae and daphnids.	2
Toxicity of two types of silver nanoparticles to aquatic crustaceans Daphnia magna and Thamnocephalus platyurus.	6
Ecotoxicity of TiO2 to Daphnia similis under irradiation.	6
Acute toxicity of TiO2 nanoparticles to Ceriodaphnia dubia under visible light and dark conditions in a freshwater system.	2
Acute toxicity of nanosized TiO(2) to Daphnia magna under UVA irradiation.	4
Changes in the Daphnia magna midgut upon ingestion of copper oxide nanoparticles: a transmission electron microscopy study.	2
Toxicity Test of Ag+, Nano-Ag0 and Nano-Ag2O using Green Algae (Chlorella sp.) and Water Flea (Moina Macrocopa)	1
Toxicity of Nanoscale CuO and ZnO to Daphnia magna	3
Microbial toxicity of metal oxide nanoparticles (CuO, NiO, ZnO, and Sb2O3) to Escherichia coli, Bacillus subtilis, and Streptococcus aureus.	17
Differentiation of the toxicities of silver nanoparticles and silver ions to the Japanese medaka (Oryzias latipes) and the cladoceran Daphnia magna.	2
Ecotoxicity of nanoparticles of CuO and ZnO in natural water.	12
Ecotoxicity of nanosized TiO2. Review of in vivo data.	3
Toxicity of manufactured zinc oxide nanoparticles in the nematode Caenorhabditis elegans.	3
Development of a base set of toxicity tests using ultrafine TiO2 particles as a component of	7

nanoparticle risk management.	
Silver nanoparticle toxicity in the embryonic zebrafish is governed by particle dispersion and ionic environment.	4
The toxicity of silver nanoparticles to zebrafish embryos increases through sewage treatment processes.	6
Acute effects of Fe_2O_3, TiO_2, ZnO and CuO nanomaterials on Xenopus laevis.	13
Silver nanoparticles and silver nitrate induce high toxicity to Pseudokirchneriella subcapitata, Daphnia magna and Danio rerio.	3
Toxicity of nanoparticles of ZnO, CuO and TiO2 to yeast Saccharomyces cerevisiae.	13
Toxicity of ZnO and CuO nanoparticles to ciliated protozoa Tetrahymena thermophila.	12
Nano-silver induces dose-response effects on the nematode Caenorhabditis elegans.	2
Ecotoxicity of manufactured ZnO nanoparticles--a review.	2
Toxicity of TiO(2) nanoparticles to cladocerans, algae, rotifers and plants - effects of size and crystalline structure.	12
Chronic toxicity of ZnO nanoparticles, non-nano ZnO and ZnCl2 to Folsomia candida (Collembola) in relation to bioavailability in soil.	1
Evaluation of toxicity and oxidative stress induced by copper oxide nanoparticles in the green alga Chlamydomonas reinhardtii.	1
Ecotoxicity of non-aged and aged CeO2 nanomaterials towards freshwater microalgae.	3
The impact of size on the fate and toxicity of nanoparticulate silver in aquatic systems.	8
Toxicity of copper oxide nanoparticle suspensions to aquatic biota.	1
Acute toxicity of Ag and CuO nanoparticle suspensions against Daphnia magna: the importance of their dissolved fraction varying with preparation methods.	32
Nanomaterial-Biological Interactions Knowledgebase	14
ER_li_data.xlsx	1
Responses of Ceriodaphnia dubia to TiO2 and Al2O3 nanoparticles: a dynamic nano-toxicity assessment of energy budget distribution.	2
Acute and chronic toxicity of nano-scale TiO2 particles to freshwater fish, cladocerans, and green algae, and effects of organic and inorganic substrate on TiO2 toxicity	7
A comparative cytotoxicity study of TiO2 nanoparticles under light and dark conditions at low exposure concentrations	4
Cytotoxicity of TiO2 nanoparticles and their detoxification in a freshwater system	2
Responses of algae to photocatalytic nano-TiO2 particles with an emphasis on the effect of particle size	5
Studies on toxicity of aluminum oxide (Al2O3) nanoparticles to microalgae species: Scenedesmus sp and Chlorella sp	2
Toxicity of oxide nanoparticles to the green algae Chlorella sp	1
A new medium for Caenorhabditis elegans toxicology and nanotoxicology studies designed to better reflect natural soil solution conditions.	1
Ag nanoparticles: size- and surface-dependent effects on model aquatic organisms and uptake evaluation with NanoSIMS.	12
Aquatic toxicity of nanosilver colloids to different trophic organisms: contributions of particles and free silver ion.	6
Assay-dependent effect of silver nanoparticles to Escherichia coli and Bacillus subtilis.	1
Biotoxicity of nickel oxide nanoparticles and bio-remediation by microalgae Chlorella vulgaris.	2
Comparative toxicity assessment of nanosilver on three Daphnia species in acute, chronic and multi-	3

generation experiments.	
Comparative toxicity of nanoparticulate ZnO, bulk ZnO, and ZnCl2 to a freshwater microalga (Pseudokirchneriella subcapitata): the importance of particle solubility.	2
Differential effect of common ligands and molecular oxygen on antimicrobial activity of silver nanoparticles versus silver ions.	1
Dissolution of silver nanowires and nanospheres dictates their toxicity to Escherichia coli.	2
Effect of light on toxicity of nanosilver to Tetrahymena pyriformis.	1
Effect of ZnO and TiO_2 nanoparticles preilluminated with UVA and UVB light on Escherichia coli and Bacillus subtilis.	8
Effects of nano-sized zero-valent iron (nZVI) on DDT degradation in soil and its toxicity to collembola and ostracods.	1
Effects of natural water chemistry on nanosilver behavior and toxicity to Ceriodaphnia dubia and Pseudokirchneriella subcapitata.	4
Effects of zinc oxide and titanium dioxide nanoparticles on green algae under visible, UVA, and UVB irradiations: no evidence of enhanced algal toxicity under UV pre-irradiation.	3
High throughput kinetic Vibrio fischeri bioluminescence inhibition assay for study of toxic effects of nanoparticles.	4
Ion-release kinetics and ecotoxicity effects of silver nanoparticles.	2
Mechanism of silver nanoparticle toxicity is dependent on dissolved silver and surface coating in Caenorhabditis elegans.	14
Physicochemical characterization and ecotoxicological assessment of CeO2 nanoparticles using two aquatic microorganisms.	24
Phytotoxicity of silver nanoparticles to Lemna minor L.	8
Profiling of the reactive oxygen species-related ecotoxicity of CuO, ZnO, TiO2, silver and fullerene nanoparticles using a set of recombinant luminescent Escherichia coli strains: differentiating the impact of particles and solubilised metals.	35
Silver nanotoxicity using a light-emitting biosensor Pseudomonas putida isolated from a wastewater treatment plant.	12
The chronic toxicity of ZnO nanoparticles and ZnCl2 to Daphnia magna and the use of different methods to assess nanoparticle aggregation and dissolution.	1
The critical importance of defined media conditions in Daphnia magna nanotoxicity studies.	1
Toxic effects of ZnO nanoparticles towards marine algae Dunaliella tertiolecta.	1
Toxicity assessment of iron oxide nanoparticles in zebrafish (Danio rerio) early life stages.	1
Toxicity of CuO nanoparticles to yeast Saccharomyces cerevisiae BY4741 wild-type and its nine isogenic single-gene deletion mutants.	10
Zinc oxide nanoparticles toxicity to Daphnia magna: size-dependent effects and dissolution.	4

236

237

238 Table S6. Data resources of MIC data

Data resources of MIC toxicity endpoint	**Number of toxicity endpoint**
Effect of Surfactants and Polymers on Stability and Antibacterial Activity of Silver Nanoparticles (NPs)	50

Silver colloid nanoparticles: synthesis, characterization, and their antibacterial activity.	44
Toxicity of nanosized and bulk ZnO, CuO and TiO2 to bacteria Vibrio fischeri and crustaceans Daphnia magna and Thamnocephalus platyurus.	8
Antimicrobial efficacy of nanosilver, sodium hypochlorite and chlorhexidine gluconate against Enterococcus faecalis	2
Synthesis and antibacterial activity of a Fe3O4-AgCl nanocomposite against Escherichia coli	1
Adsorbed polymer and NOM limits adhesion and toxicity of nano scale zerovalent iron to E. coli.	4
Antibacterial efficacy of silver nanoparticles of different sizes, surface conditions and synthesis methods.	32
Comparative toxicity assessment of CeO2 and ZnO nanoparticles towards Sinorhizobium meliloti, a symbiotic alfalfa associated bacterium: use of advanced microscopic and spectroscopic techniques.	1
Impacts of silver nanoparticles on cellular and transcriptional activity of nitrogen-cycling bacteria.	3
Non-cytotoxic nanomaterials enhance antimicrobial activities of cefmetazole against multidrug-resistant Neisseria gonorrhoeae.	2
Poly-L-lysine-modified reduced graphene oxide stabilizes the copper nanoparticles with higher water-solubility and long-term additively antibacterial activity.	4
Selective toxicity of ZnO nanoparticles toward Gram-positive bacteria and cancer cells by apoptosis through lipid peroxidation.	3
Strain specificity in antimicrobial activity of silver and copper nanoparticles.	12

239

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241 Table S7. Detailed information of the LC50 data used for building nano-SARs

Information of nanoparticles in the Online Chemical Modeling Environment (OCHEM) platform					Sub-dataset	Classification (threshold value 1.0 mg/L)	Species tested
Material Nanoparticles of Elements	**SMILES**	**RECORDID in OCHEM**	**MOLECULEID in OCHEM**	**Identifier in article**			
Silver	[Ag].[Ag]	R2691529	M2645220	AUTO_7	training set	Active	*Zebrafish embryo*
Silver, colloid	[Ag].[Ag]	R9889878	M2645220	AUTO_8	training set	Active	*Danio rerio*
Silver	[Ag].[Ag]	R21028214	M2645220	AUTO_190	training set	Active	*Ceriodaphnia dubia*
Copper(II) oxide	O=[Cu].O=[Cu]	R9870385	M2652894	AUTO_11	training set	Active	*Daphnia pulex*
Copper(II) oxide	O=[Cu].O=[Cu]	R21028034	M2652894	AUTO_9	training set	Active	*Leptocheirus plumulosus*
Silver, colloid	[Ag].[Ag]	R9889873	M2645220	AUTO_3	training set	Active	*Danio rerio*
Silver, colloid	[Ag].[Ag]	R9889877	M2645220	AUTO_7	training set	Active	*Danio rerio*
Silver	[Ag].[Ag]	R9870394	M2645220	AUTO_1	training set	Active	*Ceriodaphnia dubia*
Zinc oxide	O=[Zn].O=[Zn]	R9870389	M2652893	AUTO_15	training set	Active	*Thamnocephalus platyurus*
Zinc oxide	O=[Zn].O=[Zn]	R21028035	M2652893	AUTO_10	training set	Active	*Leptocheirus plumulosus*
Silver	[Ag].[Ag]	R21028074	M2645220	AUTO_49	training set	Active	*Ceriodaphnia dubia*
Silver	[Ag].[Ag]	R9870396	M2645220	AUTO_3	training set	Active	*Ceriodaphnia dubia*
Silver, rod	[Ag].[Ag]	R9889882	M2645220	AUTO_12	training set	Active	*Danio rerio*
Silver, colloid	[Ag].[Ag]	R9889874	M2645220	AUTO_4	training set	Active	*Danio rerio*
Silver oxide	O=[Ag].O=[Ag]	R9876467	M3728112	AUTO_2	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R9879040	M2645220	AUTO_4	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21028094	M2645220	AUTO_70	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21028145	M2645220	AUTO_121	training set	Active	*Daphnia magna*
Silver oxide	O=[Ag].O=[Ag]	R9876466	M3728112	AUTO_1	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R9889043	M2645220	AUTO_3	training set	Active	*Daphnia magna*
Copper(II) oxide	O=[Cu].O=[Cu]	R9870386	M2652894	AUTO_12	training set	Active	*Ceriodaphnia dubia*
Copper(I) oxide	[Cu]O[Cu].[Cu]O[Cu]	R21028100	M84341516	AUTO_76	training set	Active	*Danio rerio*
Silver, colloid	[Ag].[Ag]	R9889881	M2645220	AUTO_11	training set	Active	*Danio rerio*
Silver	[Ag].[Ag]	R9879043	M2645220	AUTO_7	training set	Active	*Daphnia*

							magna
Silver, colloid	[Ag].[Ag]	R9889879	M2645220	AUTO_9	training set	Active	*Danio rerio*
Silver	[Ag].[Ag]	R9879046	M2645220	AUTO_10	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R2642961	M2645220	AUTO_2	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R9879037	M2645220	AUTO_1	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R9889042	M2645220	AUTO_2	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21028146	M2645220	AUTO_122	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21028215	M2645220	AUTO_191	training set	Active	*Ceriodaphnia dubia*
Silver	[Ag].[Ag]	R21028279	M2645220	AUTO_256	training set	Active	*Daphnia magna*
Copper	[Cu].[Cu]	R21028077	M2655006	AUTO_52	training set	Active	*Ceriodaphnia dubia*
Silver	[Ag].[Ag]	R21028198	M2645220	AUTO_174	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21028143	M2645220	AUTO_119	training set	Active	*Physa acuta*
Silver	[Ag].[Ag]	R21028192	M2645220	AUTO_168	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R9890206	M2645220	AUTO_1	training set	Active	*Daphnia magna neonates*
Silver	[Ag].[Ag]	R21028265	M2645220	AUTO_242	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21028199	M2645220	AUTO_175	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21028193	M2645220	AUTO_169	training set	Active	*Daphnia magna*
Zinc oxide	O=[Zn].O=[Zn]	R9870387	M2652893	AUTO_13	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21028097	M2645220	AUTO_73	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R2642963	M2645220	AUTO_4	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R2642962	M2645220	AUTO_3	training set	Active	*Daphnia magna*
Copper(II) oxide	O=[Cu].O=[Cu]	R9870384	M2652894	AUTO_10	training set	Active	*Thamnocephalus platyurus*
Silver	[Ag].[Ag]	R9879039	M2645220	AUTO_3	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R9870395	M2645220	AUTO_2	training set	Active	*Ceriodaphnia dubia*
Silver	[Ag].[Ag]	R21028076	M2645220	AUTO_51	training set	Active	*Ceriodaphnia dubia*
Silver	[Ag].[Ag]	R9997786	M2645220	AUTO_1	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R2642969	M2645220	AUTO_11	training set	Active	*Pimephales promelas*
Copper(II) oxide	O=[Cu].O=[Cu]	R9870383	M2652894	AUTO_9	training set	Active	*Daphnia magna*
Zinc oxide	O=[Zn].O=[Zn]	R9870388	M2652893	AUTO_14	training set	Active	*Daphnia magna*

Silver	[Ag].[Ag]	R21028204	M2645220	AUTO_180	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R9879038	M2645220	AUTO_2	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R9979589	M2645220	AUTO_1	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21028055	M2645220	AUTO_30	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R2642965	M2645220	AUTO_6	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R9979590	M2645220	AUTO_2	training set	Active	*Daphnia magna*
Silver, colloid	[Ag].[Ag]	R9889876	M2645220	AUTO_6	training set	Active	*Danio rerio*
Silver, colloid	[Ag].[Ag]	R9889884	M2645220	AUTO_14	training set	Active	*Danio rerio*
Silver, colloid	[Ag].[Ag]	R9889883	M2645220	AUTO_13	training set	Active	*Danio rerio*
Silver	[Ag].[Ag]	R21028195	M2645220	AUTO_171	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21028196	M2645220	AUTO_172	training set	Active	*Daphnia magna*
Aluminium oxide	O=[Al]O[Al]=O.O=[Al]O[Al]=O	R9870382	M2652898	AUTO_8	training set	Active	*Ceriodaphnia dubia*
Silver	[Ag].[Ag]	R2642966	M2645220	AUTO_7	training set	Active	*Daphnia magna*
Titanium	O=[Ti]=O.O=[Ti]=O	R2646241	M2645228	AUTO_9	training set	Active	*Daphnia magna*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R9870376	M2645228	AUTO_2	training set	Active	*Daphnia magna*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21028060	M2645228	AUTO_35	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R9879041	M2645220	AUTO_5	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21028098	M2645220	AUTO_74	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R2642967	M2645220	AUTO_8	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R2642970	M2645220	AUTO_12	training set	Active	*Pimephales promelas*
Silver	[Ag].[Ag]	R21028056	M2645220	AUTO_31	training set	Active	*Daphnia magna*
Silver, colloid	[Ag].[Ag]	R9889871	M2645220	AUTO_1	training set	Active	*Danio rerio*
Silver	[Ag].[Ag]	R9997787	M2645220	AUTO_2	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R9877327	M2645220	AUTO_1	training set	Active	*Oryzias latipes*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21028186	M2645228	AUTO_162	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21028123	M2645220	AUTO_99	training set	Active	*Oryzias latipes*
Silver	[Ag].[Ag]	R21028099	M2645220	AUTO_75	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R2691536	M2645220	AUTO_14	training set	Active	*Daphnia pulex*
Silver	[Ag].[Ag]	R9895726	M2645220	AUTO_7	training set	Active	*Daphnia pulex*

Silver	[Ag].[Ag]	R2642971	M2645220	AUTO_13	training set	Active	*Pimephales promelas*
Copper	[Cu].[Cu]	R9870398	M2655006	AUTO_5	training set	Active	*Ceriodaphnia dubia*
Copper	[Cu].[Cu]	R21028078	M2655006	AUTO_53	training set	Active	*Ceriodaphnia dubia*
Zinc oxide	O=[Zn].O=[Zn]	R12182880	M2652893	AUTO_1	training set	Active	*Escherichia coli*
Zinc oxide	O=[Zn].O=[Zn]	R21028068	M2652893	AUTO_43	training set	Active	*Escherichia coli*
Copper	[Cu].[Cu]	R21028079	M2655006	AUTO_54	training set	Active	*Ceriodaphnia dubia*
Silver	[Ag].[Ag]	R2642972	M2645220	AUTO_14	training set	Active	*Pimephales promelas*
Copper	[Cu].[Cu]	R9926573	M2655006	AUTO_3	training set	Active	*Daphnia pulex*
Silver	[Ag].[Ag]	R2642973	M2645220	AUTO_15	training set	Active	*Pimephales promelas*
Silver	[Ag].[Ag]	R2642974	M2645220	AUTO_16	training set	Active	*Pimephales promelas*
Silver	[Ag].[Ag]	R2691537	M2645220	AUTO_15	training set	Active	*Ceriodaphnia*
Silver	[Ag].[Ag]	R9895729	M2645220	AUTO_10	training set	Active	*Ceriodaphnia dubia neonates*
Silver	[Ag].[Ag]	R21028104	M2645220	AUTO_80	training set	Active	*Ceriodaphnia dubia*
Silver	[Ag].[Ag]	R9727605	M2645220	AUTO_3	training set	Active	*Thamnocephalus platyurus, freshwater*
Silver	[Ag].[Ag]	R2642976	M2645220	AUTO_18	training set	Active	*Pimephales promelas*
Silver	[Ag].[Ag]	R9997788	M2645220	AUTO_3	training set	Active	*Fathead Minnow*
Silver, colloid	[Ag].[Ag]	R9890169	M2645220	AUTO_1	training set	Active	*Rainbow trout*
Silver	[Ag].[Ag]	R21028059	M2645220	AUTO_34	training set	Active	*Pimephales promelas*
Silver	[Ag].[Ag]	R2642968	M2645220	AUTO_9	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R9979591	M2645220	AUTO_3	training set	Active	*Daphnia magna*
Zinc oxide	O=[Zn].O=[Zn]	R21028069	M2652893	AUTO_44	training set	Active	*Escherichia coli*
Zinc oxide	O=[Zn].O=[Zn]	R9890186	M2652893	AUTO_5	training set	Active	*Thamnoplatyurus platyurus*
Zinc oxide	O=[Zn].O=[Zn]	R12601997	M2652893	AUTO_5	training set	Active	*Thamnocephalus platyurus*
Copper(II) oxide	O=[Cu].O=[Cu]	R12182881	M2652894	AUTO_2	training set	Active	*Escherichia coli*
Copper(II) oxide	O=[Cu].O=[Cu]	R21028064	M2652894	AUTO_39	training set	Active	*Escherichia coli*
Silver	[Ag].[Ag]	R2691542	M2645220	AUTO_20	training set	Active	*Chlamydomonas reinhardtii*
Zinc oxide	O=[Zn].O=[	R2707692	M2652893	AUTO_33	training set	Active	*Thamnocep*

	Zn]						*halus platyurus*
Zinc oxide	O=[Zn].O=[Zn]	R12601994	M2652893	AUTO_2	training set	Active	*Thamnocephalus platyurus*
Zinc oxide	O=[Zn].O=[Zn]	R12714707	M2652893	AUTO_2	training set	Active	*Thamnocephalus platyurusb*
Zinc oxide	O=[Zn].O=[Zn]	R21028259	M2652893	AUTO_236	training set	Active	*Thamnocephalus platyurus*
Silver	[Ag].[Ag]	R2691540	M2645220	AUTO_18	training set	Active	*Pseudokirchneriella subcapitata*
Silver	[Ag].[Ag]	R9895734	M2645220	AUTO_15	training set	Active	*Pseudokirchneriella subcapitata*
Silver	[Ag].[Ag]	R9727604	M2645220	AUTO_2	training set	Active	*Thamnocephalus platyurus, river water*
Silver	[Ag].[Ag]	R21028089	M2645220	AUTO_64	training set	Active	*Hypophthalmichthys molitrix*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R9870378	M2645228	AUTO_4	training set	Active	*Caenorhabditis elegans*
Zinc oxide	O=[Zn].O=[Zn]	R2707691	M2652893	AUTO_32	training set	Active	*Thamnocephalus platyurus*
Silver	[Ag].[Ag]	R9890208	M2645220	AUTO_1	training set	Active	*Rainbow trout, eleutheroembryos*
Silver	[Ag].[Ag]	R9727603	M2645220	AUTO_1	training set	Active	*Thamnocephalus platyurus, freshwater*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R9890211	M2645228	AUTO_1	training set	Active	*Danio rerio*
Silver	[Ag].[Ag]	R9727606	M2645220	AUTO_4	training set	Active	*Thamnocephalus platyurus, river water*
Nickel	[Ni].[Ni]	R9895737	M2655007	AUTO_18	training set	Active	*Pseudokirchneriella subcapitata*
Silver	[Ag].[Ag]	R21028090	M2645220	AUTO_65	training set	Active	*Hypophthalmichthys molitrix*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R9870375	M2645228	AUTO_1	training set	Active	*Daphnia magna*
Copper	[Cu].[Cu]	R21028107	M2655006	AUTO_83	training set	Active	*Ceriodaphnia dubia*
Silver	[Ag].[Ag]	R2691538	M2645220	AUTO_16	training set	Active	*Ceriodaphnia dubia*
Copper(II) oxide	O=[Cu].O=[Cu]	R21028233	M2652894	AUTO_210	training set	Active	*Brachionus calyciflorus*
Copper	[Cu].[Cu]	R9895735	M2655006	AUTO_16	training set	Active	*Pseudokirchneriella*

							subcapitata
Nickel	[Ni].[Ni]	R9895733	M2655007	AUTO_14	training set	Active	*Ceriodaphnia dubia neonates*
Nickel	[Ni].[Ni]	R9926576	M2655007	AUTO_6	training set	Active	*Ceriodaphnia dubia*
Nickel	[Ni].[Ni]	R21028108	M2655007	AUTO_84	training set	Active	*Ceriodaphnia dubia*
Silver	[Ag].[Ag]	R9890209	M2645220	AUTO_2	training set	Active	*Rainbow trout, larvae*
Silver	[Ag].[Ag]	R2691541	M2645220	AUTO_19	training set	Active	*Chlamydomonas reinhardtii*
Titanium	O=[Ti]=O.O=[Ti]=O	R2646991	M2645228	AUTO_7	training set	Active	*Daphnia magna*
Copper	[Cu].[Cu]	R9895721	M2655006	AUTO_2	training set	Active	*Danio rerio*
Silver	[Ag].[Ag]	R21028092	M2645220	AUTO_67	training set	Active	*Hypophthalmichthys molitrix*
Silver	[Ag].[Ag]	R21028201	M2645220	AUTO_177	training set	Active	*Oryzias latipes*
Copper	[Cu].[Cu]	R9926572	M2655006	AUTO_2	training set	Active	*Danio rerio*
Copper	[Cu].[Cu]	R21028115	M2655006	AUTO_91	training set	Active	*Danio rerio*
Copper(II) oxide	O=[Cu].O=[Cu]	R21028207	M2652894	AUTO_183	training set	Active	*Paramecium multimicronucleatum*
Silver	[Ag].[Ag]	R2691558	M2645220	AUTO_36	training set	Inactive	*Autotrophic nitrifying bacteria*
Silver	[Ag].[Ag]	R2691559	M2645220	AUTO_37	training set	Inactive	*Nitrifying bacteria*
Selenium	[Se].[Se]	R21028121	M17788121	AUTO_97	training set	Inactive	*Oryzias latipes*
Zinc oxide	O=[Zn].O=[Zn]	R21028159	M2652893	AUTO_135	training set	Inactive	*Daphnia magna*
Silver	[Ag].[Ag]	R9926262	M2645220	AUTO_1	training set	Inactive	*Oryzias latipes*
Silver	[Ag].[Ag]	R21028120	M2645220	AUTO_96	training set	Inactive	*Oryzias latipes*
Silver	[Ag].[Ag]	R21028202	M2645220	AUTO_178	training set	Inactive	*Oryzias latipes*
Silver	[Ag].[Ag]	R21028049	M2645220	AUTO_24	training set	Inactive	*Danio rerio*
Zinc oxide	O=[Zn].O=[Zn]	R9889292	M2652893	AUTO_6	training set	Inactive	*Daphnia magna*
Silver	[Ag].[Ag]	R21028212	M2645220	AUTO_188	training set	Inactive	*Pimephales promelas*
Silver	[Ag].[Ag]	R9963620	M2645220	AUTO_2	training set	Inactive	*Danio rerio embryos*
Silver	[Ag].[Ag]	R21028216	M2645220	AUTO_192	training set	Inactive	*Danio rerio*
Silver, sonicated	[Ag].[Ag]	R9877332	M2645220	AUTO_4	training set	Inactive	*Pimephales promelas embryos*
Silver	[Ag].[Ag]	R21028203	M2645220	AUTO_179	training set	Inactive	*Oryzias latipes*
Silver	[Ag].[Ag]	R21028191	M2645220	AUTO_167	training set	Inactive	*Oryzias latipes*
Silver	[Ag].[Ag]	R21028070	M2645220	AUTO_45	training set	Inactive	*Oryzias*

							latipes
Copper	[Cu].[Cu]	R9870393	M2655006	AUTO_1	training set	Inactive	*Danio rerio*
Copper	[Cu].[Cu]	R9926550	M2655006	AUTO_4	training set	Inactive	*Danio rerio*
Zinc oxide	O=[Zn].O=[Zn]	R21028160	M2652893	AUTO_136	training set	Inactive	*Daphnia magna*
Zinc oxide	O=[Zn].O=[Zn]	R12601996	M2652893	AUTO_4	training set	Inactive	*Daphnia magna*
Copper	[Cu].[Cu]	R9926574	M2655006	AUTO_4	training set	Inactive	*Danio rerio*
Copper	[Cu].[Cu]	R21028124	M2655006	AUTO_100	training set	Inactive	*Danio rerio*
Titanium	O=[Ti]=O.O=[Ti]=O	R2647004	M2645228	AUTO_21	training set	Inactive	*Daphnia magna*
Cobalt	[Co].[Co]	R9895732	M3728136	AUTO_13	training set	Inactive	*Ceriodaphnia dubia neonates*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R12174312	M2645228	AUTO_3	training set	Inactive	*Escherichia coli*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R12182882	M2645228	AUTO_3	training set	Inactive	*Escherichia coli*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21028066	M2645228	AUTO_41	training set	Inactive	*Escherichia coli*
Copper(II) oxide	O=[Cu].O=[Cu]	R9890182	M2652894	AUTO_1	training set	Inactive	*Thamnoplatyurus platyurus*
Silver	[Ag].[Ag]	R9963619	M2645220	AUTO_1	training set	Inactive	*Danio rerio embryos*
Zinc oxide	O=[Zn].O=[Zn]	R12601999	M2652893	AUTO_7	training set	Inactive	*Danio rerio*
Silver	[Ag].[Ag]	R21028217	M2645220	AUTO_193	training set	Inactive	*Danio rerio*
Zinc oxide	O=[Zn].O=[Zn]	R12714708	M2652893	AUTO_3	training set	Inactive	*Danio rerio*
Titanium	O=[Ti]=O.O=[Ti]=O	R2647003	M2645228	AUTO_20	training set	Inactive	*Daphnia magna*
Zinc oxide	O=[Zn].O=[Zn]	R12602000	M2652893	AUTO_8	training set	Inactive	*Danio rerio*
Copper(II) oxide	O=[Cu].O=[Cu]	R2707722	M2652894	AUTO_63	training set	Inactive	*Thamnocephalus platyurus*
Copper(II) oxide	O=[Cu].O=[Cu]	R9926580	M2652894	AUTO_10	training set	Inactive	*Thamnocephalus platyurus*
Zinc oxide	O=[Zn].O=[Zn]	R21028161	M2652893	AUTO_137	training set	Inactive	*Daphnia magna*
Zinc oxide	O=[Zn].O=[Zn]	R9890189	M2652893	AUTO_8	training set	Inactive	*Thamnoplatyurus platyurus*
Silver	[Ag].[Ag]	R9890210	M2645220	AUTO_3	training set	Inactive	*Rainbow trout*
Zinc oxide	O=[Zn].O=[Zn]	R12643422	M2652893	AUTO_5	training set	Inactive	*Caenorhabditis elegans*
Zinc oxide	O=[Zn].O=[Zn]	R21028244	M2652893	AUTO_221	training set	Inactive	*Caenorhabditis elegans*
Zinc oxide	O=[Zn].O=[Zn]	R9887903	M2652893	AUTO_1	training set	Inactive	*Caenorhabditis elegans*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21028187	M2645228	AUTO_163	training set	Inactive	*Oryzias latipes*
Zinc oxide	O=[Zn].O=[Zn]	R21028162	M2652893	AUTO_138	training set	Inactive	*Daphnia magna*

Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21028223	M2645228	AUTO_199	training set	Inactive	*Daphnia magna*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21028026	M2645228	AUTO_1	training set	Inactive	*Ceriodaphnia dubia*
Zinc oxide	O=[Zn].O=[Zn]	R12643420	M2652893	AUTO_3	training set	Inactive	*Folsomia candida*
Zinc oxide	O=[Zn].O=[Zn]	R9890187	M2652893	AUTO_6	training set	Inactive	*Thamnoplatyurus platyurus*
Copper(II) oxide	O=[Cu].O=[Cu]	R2707713	M2652894	AUTO_54	training set	Inactive	*Daphnia magna*
Zinc oxide	O=[Zn].O=[Zn]	R9926577	M2652893	AUTO_7	training set	Inactive	*Daphnia magna*
Copper(II) oxide	O=[Cu].O=[Cu]	R9926578	M2652894	AUTO_8	training set	Inactive	*Daphnia magna*
Zinc oxide	O=[Zn].O=[Zn]	R12601993	M2652893	AUTO_1	training set	Inactive	*Daphnia magna*
Copper(II) oxide	O=[Cu].O=[Cu]	R12714709	M2652894	AUTO_4	training set	Inactive	*Daphnia magna*
Copper(II) oxide	O=[Cu].O=[Cu]	R21028231	M2652894	AUTO_208	training set	Inactive	*Nitellopsis obtusa*
Silver	[Ag].[Ag]	R21028071	M2645220	AUTO_46	training set	Inactive	*Oryzias latipes*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21028027	M2645228	AUTO_2	training set	Inactive	*Ceriodaphnia dubia*
Copper	[Cu].[Cu]	R11895743	M2655006	AUTO_46	training set	Inactive	*Danio rerio*
Nickel	[Ni].[Ni]	R9895728	M2655007	AUTO_9	training set	Inactive	*Daphnia pulex*
Nickel	[Ni].[Ni]	R9926575	M2655007	AUTO_5	training set	Inactive	*Daphnia pulex*
Zinc oxide	O=[Zn].O=[Zn]	R21028053	M2652893	AUTO_28	training set	Inactive	*Danio rerio*
Aluminium	[Al].[Al]	R9895731	M3728130	AUTO_12	training set	Inactive	*Ceriodaphnia dubia neonates*
Aluminium	[Al].[Al]	R21028105	M3728130	AUTO_81	training set	Inactive	*Ceriodaphnia dubia*
Copper	[Cu].[Cu]	R11895742	M2655006	AUTO_45	training set	Inactive	*Danio rerio*
Copper(II) oxide	O=[Cu].O=[Cu]	R21028065	M2652894	AUTO_40	training set	Inactive	*Escherichia coli*
Zinc oxide	O=[Zn].O=[Zn]	R21028102	M2652893	AUTO_78	training set	Inactive	*Danio rerio*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21028270	M2645228	AUTO_247	training set	Inactive	*Brachionus plicatilis*
Silver	[Ag].[Ag]	R9848059	M2645220	AUTO_1	training set	Inactive	*Moina macrocopa*
Silver	[Ag].[Ag]	R2691539	M2645220	AUTO_17	training set	Inactive	*Ceriodaphnia dubia*
Silver	[Ag].[Ag]	R2691527	M2645220	AUTO_5	training set	Inactive	*Zebrafish*
Silver	[Ag].[Ag]	R9926571	M2645220	AUTO_1	training set	Inactive	*Danio rerio*
Silver	[Ag].[Ag]	R21028112	M2645220	AUTO_88	training set	Inactive	*Danio rerio*
Silver	[Ag].[Ag]	R9895720	M2645220	AUTO_1	training set	Inactive	*Danio rerio*
Zinc oxide	O=[Zn].O=[Zn]	R12601995	M2652893	AUTO_3	training set	Inactive	*Daphnia magna*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R9876464	M2645228	AUTO_2	training set	Inactive	*Ceriodaphnia dubia*
Titanium	O=[Ti]=O.O	R9890207	M2645228	AUTO_2	training set	Inactive	*Daphnia*

dioxide	=[Ti]=O						*magna neonates*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21028266	M2645228	AUTO_243	training set	Inactive	*Daphnia magna*
Aluminium	[Al].[Al]	R9895736	M3728130	AUTO_17	training set	Inactive	*Pseudokirchneriella subcapitata*
Zinc oxide	O=[Zn].O=[Zn]	R2707682	M2652893	AUTO_23	training set	Inactive	*Daphnia magna*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R9876465	M2645228	AUTO_3	training set	Inactive	*Daphnia pulex*
Silver, stirred	[Ag].[Ag]	R9877329	M2645220	AUTO_1	training set	Inactive	*Pimephales promelas embryos*
Silver	[Ag].[Ag]	R9889345	M2645220	AUTO_2	training set	Inactive	*Danio rerio embryos*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21028272	M2645228	AUTO_249	training set	Inactive	*Brachionus plicatilis*
Silver, stirred	[Ag].[Ag]	R9877330	M2645220	AUTO_2	training set	Inactive	*Pimephales promelas embryos*
Copper(II) oxide	O=[Cu].O=[Cu]	R21028232	M2652894	AUTO_209	training set	Inactive	*Thamnocephalus platyurus*
cerium oxide	O=[Ce]=O.O=[Ce]=O	R21028042	M2659378	AUTO_17	training set	Inactive	*Daphnia magna*
Silver	[Ag].[Ag]	R21028144	M2645220	AUTO_120	training set	Inactive	*Oreochromis mossambicus*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21028032	M2645228	AUTO_7	training set	Inactive	*Daphnia pulex*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21028271	M2645228	AUTO_248	training set	Inactive	*Brachionus plicatilis*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21028174	M2645228	AUTO_150	training set	Inactive	*Escherichia coli*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21028030	M2645228	AUTO_5	training set	Inactive	*Ceriodaphnia dubia*
Silver	[Ag].[Ag]	R2691545	M2645220	AUTO_23	training set	Inactive	*Paramecium caudatum*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21028044	M2645228	AUTO_19	training set	Inactive	*Daphnia magna*
Silver	[Ag].[Ag]	R2691530	M2645220	AUTO_8	training set	Inactive	*Zebrafish*
Silver	[Ag].[Ag]	R9890190	M2645220	AUTO_1	training set	Inactive	*Danio rerio*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21028183	M2645228	AUTO_159	training set	Inactive	*Danio rerio*
Zinc oxide	O=[Zn].O=[Zn]	R21028153	M2652893	AUTO_129	training set	Inactive	*Escherichia coli*
Silver	[Ag].[Ag]	R9889347	M2645220	AUTO_4	training set	Inactive	*Danio rerio embryos*
Zinc oxide	O=[Zn].O=[Zn]	R9926551	M2652893	AUTO_5	training set	Inactive	*Danio rerio embryos*
Copper	[Cu].[Cu]	R11895744	M2655006	AUTO_47	training set	Inactive	*Danio rerio eggs*
Copper	[Cu].[Cu]	R11895745	M2655006	AUTO_48	training set	Inactive	*Danio rerio eggs*
Silver	[Ag].[Ag]	R2691531	M2645220	AUTO_9	training set	Inactive	*Zebrafish*
Silver	[Ag].[Ag]	R2691532	M2645220	AUTO_10	training set	Inactive	*Zebrafish*

Silver	[Ag].[Ag]	R9890192	M2645220	AUTO_3	training set	Inactive	*Danio rerio*
Silver	[Ag].[Ag]	R2691533	M2645220	AUTO_11	training set	Inactive	*Zebrafish*
Zinc oxide	O=[Zn].O=[Zn]	R2707287	M2652893	AUTO_2	training set	Inactive	*Zebrafish*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21028184	M2645228	AUTO_160	training set	Inactive	*Danio rerio*
Cobalt(II) oxide	O=[Co].O=[Co].O=[Co]O[Co]=O.O=[Co]O[Co]=O	R12174313	M4394264	AUTO_4	training set	Inactive	*Escherichia coli*
Cobalt(II) oxide	O=[Co].O=[Co].O=[Co]O[Co]=O.O=[Co]O[Co]=O	R12182883	M4394264	AUTO_4	training set	Inactive	*Escherichia coli*
Silver	[Ag].[Ag]	R21028155	M2645220	AUTO_131	training set	Inactive	*Paramecium caudatum*
cerium oxide	O=[Ce]=O.O=[Ce]=O	R21028132	M2659378	AUTO_108	training set	Inactive	*Daphnia magna*
Silver	[Ag].[Ag]	R9889339	M2645220	AUTO_1	training set	Inactive	*Danio rerio embryos*
Silver	[Ag].[Ag]	R21028156	M2645220	AUTO_132	training set	Inactive	*Paramecium caudatum*
Silver	[Ag].[Ag]	R21028157	M2645220	AUTO_133	training set	Inactive	*Paramecium caudatum*
Silver	[Ag].[Ag]	R9889344	M2645220	AUTO_1	training set	Inactive	*Danio rerio embryos*
cerium oxide	O=[Ce]=O.O=[Ce]=O	R21028131	M2659378	AUTO_107	training set	Inactive	*Daphnia magna*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21028179	M2645228	AUTO_155	training set	Inactive	*Escherichia coli*
Iron(III) oxide	O=[Fe]O[Fe]=O.O=[Fe]O[Fe]=O	R21028230	M2652899	AUTO_207	training set	Inactive	*Danio rerio*
Silver	[Ag].[Ag]	R21028158	M2645220	AUTO_134	training set	Inactive	*Caenorhabditis elegans*
Cobalt(II) oxide	O=[Co].O=[Co].O=[Co]O[Co]=O.O=[Co]O[Co]=O	R21028063	M4394264	AUTO_38	training set	Inactive	*Escherichia coli*
Copper(II) oxide	O=[Cu].O=[Cu]	R21028148	M2652894	AUTO_124	training set	Inactive	*Escherichia coli*
Titanium	O=[Ti]=O.O=[Ti]=O	R2645347	M2645228	AUTO_6	training set	Inactive	*Daphnia magna*
cerium oxide	O=[Ce]=O.O=[Ce]=O	R21028133	M2659378	AUTO_109	training set	Inactive	*Daphnia magna*
Aluminium oxide	O=[Al]O[Al]=O.O=[Al]O[Al]=O	R21028050	M2652898	AUTO_25	training set	Inactive	*Ceriodaphnia dubia*
Copper(II) oxide	O=[Cu].O=[Cu]	R9890184	M2652894	AUTO_3	training set	Inactive	*Thamnoplatyurus platyurus*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21028243	M2645228	AUTO_220	training set	Inactive	*Caenorhabditis elegans*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R9887905	M2645228	AUTO_3	training set	Inactive	*Caenorhabditis elegans*

Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R12643418	M2645228	AUTO_1	training set	Inactive	*Caenorhabditis elegans*
Aluminium oxide	O=[Al]O[Al]=O.O=[Al]O[Al]=O	R21028242	M2652898	AUTO_219	training set	Inactive	*Caenorhabditis elegans*
Aluminium oxide	O=[Al]O[Al]=O.O=[Al]O[Al]=O	R12643419	M2652898	AUTO_2	training set	Inactive	*Caenorhabditis elegans*
Aluminium oxide	O=[Al]O[Al]=O.O=[Al]O[Al]=O	R21028051	M2652898	AUTO_26	training set	Inactive	*Ceriodaphnia dubia*
Copper(II) oxide	O=[Cu].O=[Cu]	R2707721	M2652894	AUTO_62	training set	Inactive	*Thamnocephalus platyurus*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21028180	M2645228	AUTO_156	training set	Inactive	*Danio rerio*
Nickel	[Ni].[Ni]	R9926558	M2655007	AUTO_12	training set	Inactive	*Danio rerio embryos*
Aluminium oxide	O=[Al]O[Al]=O.O=[Al]O[Al]=O	R21028052	M2652898	AUTO_27	training set	Inactive	*Ceriodaphnia dubia*
Titanium	O=[Ti]=O.O=[Ti]=O	R2692112	M2645228	AUTO_16	training set	Inactive	*Zebrafish*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21028101	M2645228	AUTO_77	training set	Inactive	*Danio rerio*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21028185	M2645228	AUTO_161	training set	Inactive	*Danio rerio*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21028173	M2645228	AUTO_149	training set	Inactive	*Escherichia coli*
Magnesium(II) oxide	O=[Mg].O=[Mg]	R11895725	M4394239	AUTO_21	training set	Inactive	*Danio rerio*
Magnesium(II) oxide	O=[Mg].O=[Mg]	R11895726	M4394239	AUTO_22	training set	Inactive	*Danio rerio*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R9889289	M2645228	AUTO_3	training set	Inactive	*Daphnia magna*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21028188	M2645228	AUTO_164	training set	Inactive	*Oryzias latipes*
Aluminium oxide	O=[Al]O[Al]=O.O=[Al]O[Al]=O	R9889287	M2652898	AUTO_1	training set	Inactive	*Daphnia magna*
Copper(II) oxide	O=[Cu].O=[Cu]	R2707712	M2652894	AUTO_53	training set	Inactive	*Daphnia magna*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21028175	M2645228	AUTO_151	training set	Inactive	*Escherichia coli*
Nickel	[Ni].[Ni]	R9926557	M2655007	AUTO_11	training set	Inactive	*Danio rerio embryos*
Silicon dioxide	O=[Si]=O.O=[Si]=O	R21028116	M2652900	AUTO_92	training set	Inactive	*Danio rerio*
Calcium(II) oxide	O=[Ca].O=[Ca]	R11895737	M4394240	AUTO_37	training set	Inactive	*Danio rerio*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21028273	M2645228	AUTO_250	training set	Inactive	*Brachionus plicatilis*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21028181	M2645228	AUTO_157	training set	Inactive	*Danio rerio*
Calcium(II) oxide	O=[Ca].O=[Ca]	R11895739	M4394240	AUTO_39	training set	Inactive	*Danio rerio eggs*
Calcium(II) oxide	O=[Ca].O=[Ca]	R11895740	M4394240	AUTO_40	training set	Inactive	*Danio rerio eggs*
Titanium	O=[Ti]=O.O	R21028182	M2645228	AUTO_158	training set	Inactive	*Danio rerio*

dioxide	=[Ti]=O						
Aluminium oxide	O=[Al]O[Al]=O.O=[Al]O[Al]=O	R21028147	M2652898	AUTO_123	training set	Inactive	*Escherichia coli*
Nickel	[Ni].[Ni]	R9926555	M2655007	AUTO_9	training set	Inactive	*Danio rerio embryos*
Nickel	[Ni].[Ni]	R9926556	M2655007	AUTO_10	training set	Inactive	*Danio rerio embryos*
Copper(II) oxide	O=[Cu].O=[Cu]	R11895718	M2652894	AUTO_14	training set	Inactive	*Danio rerio*
Silicon dioxide	O=[Si]=O.O=[Si]=O	R21028209	M2652900	AUTO_185	training set	Inactive	*Paramecium multimicron ucleatum*
Lanthanum oxide	O=[La]O[La]=O.O=[La]O[La]=O	R21028150	M2652906	AUTO_126	training set	Inactive	*Escherichia coli*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R9876463	M2645228	AUTO_1	training set	Inactive	*fathead minnow*
Titanium	O=[Ti]=O.O=[Ti]=O	R2645343	M2645228	AUTO_2	training set	Inactive	*Daphnia magna*
Zinc oxide	O=[Zn].O=[Zn]	R21028210	M2652893	AUTO_186	training set	Inactive	*Paramecium multimicron ucleatum*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21028067	M2645228	AUTO_42	training set	Inactive	*Escherichia coli*
Iron(III) oxide	O=[Fe]O[Fe]=O.O=[Fe]O[Fe]=O	R21028149	M2652899	AUTO_125	training set	Inactive	*Escherichia coli*
Zinc oxide	O=[Zn].O=[Zn]	R9879033	M2652893	AUTO_1	training set	Inactive	*Caenorhabditis elegans*
Tin	[Sn].[Sn]	R11895762	M4394242	AUTO_65	training set	Inactive	*Danio rerio*
Tin	[Sn].[Sn]	R11895763	M4394242	AUTO_66	training set	Inactive	*Danio rerio*
Tin	[Sn].[Sn]	R11895764	M4394242	AUTO_67	training set	Inactive	*Danio rerio eggs*
Zinc oxide	O=[Zn].O=[Zn]	R12643423	M2652893	AUTO_6	training set	Inactive	*Caenorhabditis elegans*
Copper(II) oxide	O=[Cu].O=[Cu]	R11895720	M2652894	AUTO_16	training set	Inactive	*Danio rerio eggs*
Copper(II) oxide	O=[Cu].O=[Cu]	R12584191	M2652894	AUTO_2	training set	Inactive	*Leptocheirus plumulosus*
Titanium	O=[Ti]=O.O=[Ti]=O	R2645345	M2645228	AUTO_4	training set	Inactive	*Daphnia magna*
Zinc oxide	O=[Zn].O=[Zn]	R21028235	M2652893	AUTO_212	training set	Inactive	*Caenorhabditis elegans*
Silver	[Ag].[Ag]	R2691526	M2645220	AUTO_4	training set	Inactive	*Zebrafish*
Copper(II) oxide	O=[Cu].O=[Cu]	R9890185	M2652894	AUTO_4	training set	Inactive	*Thamnoplatyurus platyurus*
Tin dioxide	O=[Sn]=O.O=[Sn]=O	R21028151	M2652902	AUTO_127	training set	Inactive	*Escherichia coli*
Zinc oxide	O=[Zn].O=[Zn]	R9890213	M2652893	AUTO_3	training set	Inactive	*Danio rerio*
Zinc oxide	O=[Zn].O=[Zn]	R21028234	M2652893	AUTO_211	training set	Inactive	*Caenorhabditis elegans*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R12714711	M2645228	AUTO_6	training set	Inactive	*Daphnia magna*
Silver	[Ag].[Ag]	R21028269	M2645220	AUTO_246	training set	Inactive	*Meloidogyn*

							e incognita
Silver, colloid	[Ag].[Ag]	R9889880	M2645220	AUTO_10	test set	Active	*Danio rerio*
Silver	[Ag].[Ag]	R21028073	M2645220	AUTO_48	test set	Active	*Ceriodaphnia dubia*
Silver	[Ag].[Ag]	R21028075	M2645220	AUTO_50	test set	Active	*Ceriodaphnia dubia*
Silver	[Ag].[Ag]	R9879042	M2645220	AUTO_6	test set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21028095	M2645220	AUTO_71	test set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21028096	M2645220	AUTO_72	test set	Active	*Daphnia magna*
Nickel(II) oxide	O=[Ni].O=[Ni]	R9870392	M2652904	AUTO_18	test set	Active	*Ceriodaphnia dubia*
Copper	[Cu].[Cu]	R9870397	M2655006	AUTO_4	test set	Active	*Ceriodaphnia dubia*
Nickel(II) oxide	O=[Ni].O=[Ni]	R9870391	M2652904	AUTO_17	test set	Active	*Daphnia pulex*
Silver	[Ag].[Ag]	R21028200	M2645220	AUTO_176	test set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R2642964	M2645220	AUTO_5	test set	Active	*Daphnia magna*
Zinc oxide	O=[Zn].O=[Zn]	R9870390	M2652893	AUTO_16	test set	Active	*Caenorhabditis elegans*
Silver, colloid	[Ag].[Ag]	R9889872	M2645220	AUTO_2	test set	Active	*Danio rerio*
Silver	[Ag].[Ag]	R21028280	M2645220	AUTO_257	test set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21028194	M2645220	AUTO_170	test set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21028197	M2645220	AUTO_173	test set	Active	*Daphnia magna*
Silver oxide	O=[Ag].O=[Ag]	R9876468	M3728112	AUTO_3	test set	Active	*Daphnia magna*
Silver, colloid	[Ag].[Ag]	R9889875	M2645220	AUTO_5	test set	Active	*Danio rerio*
Silver	[Ag].[Ag]	R9889041	M2645220	AUTO_1	test set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R9879047	M2645220	AUTO_11	test set	Active	*Daphnia magna*
Zinc oxide	O=[Zn].O=[Zn]	R12174310	M2652893	AUTO_1	test set	Active	*Escherichia coli*
Copper	[Cu].[Cu]	R9895727	M2655006	AUTO_8	test set	Active	*Daphnia pulex*
Silver	[Ag].[Ag]	R9877328	M2645220	AUTO_2	test set	Active	*Oryzias latipes*
Silver	[Ag].[Ag]	R2650124	M2645220	AUTO_2	test set	Active	*Zebra danio*
Silver	[Ag].[Ag]	R2642975	M2645220	AUTO_17	test set	Active	*Pimephales promelas*
Copper(II) oxide	O=[Cu].O=[Cu]	R12174311	M2652894	AUTO_2	test set	Active	*Escherichia coli*
Zinc oxide	O=[Zn].O=[Zn]	R9926579	M2652893	AUTO_9	test set	Active	*Thamnocephalus platyurus*
Zinc oxide	O=[Zn].O=[Zn]	R9890188	M2652893	AUTO_7	test set	Active	*Thamnoplatyurus platyurus*

Iron(II,III)oxide	O=[Fe].O=[Fe].O=[Fe]O[Fe]=O.O=[Fe]O[Fe]=O	R21028043	M2659379	AUTO_18	test set	Active	*Daphnia magna*
Aluminium oxide	O=[Al]O[Al]=O.O=[Al]O[Al]=O	R9870379	M2652898	AUTO_5	test set	Active	*Caenorhabditis elegans*
Copper	[Cu].[Cu]	R9895730	M2655006	AUTO_11	test set	Active	*Ceriodaphnia dubia neonates*
Silver	[Ag].[Ag]	R21028091	M2645220	AUTO_66	test set	Active	*Hypophthalmichthys molitrix*
Copper	[Cu].[Cu]	R21028114	M2655006	AUTO_90	test set	Active	*Danio rerio*
Iron(III) oxide	O=[Fe]O[Fe]=O.O=[Fe]O[Fe]=O	R21028208	M2652899	AUTO_184	test set	Active	*Paramecium multimicronucleatum*
Copper(II) oxide	O=[Cu].O=[Cu]	R9866147	M2652894	AUTO_1	test set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R9890798	M2645220	AUTO_1	test set	Inactive	*Oryzias latipes*
Silver, sonicated	[Ag].[Ag]	R9877331	M2645220	AUTO_3	test set	Inactive	*Pimephales promelas embryos*
Zinc oxide	O=[Zn].O=[Zn]	R21028281	M2652893	AUTO_258	test set	Inactive	*Daphnia magna*
Zinc oxide	O=[Zn].O=[Zn]	R9866148	M2652893	AUTO_2	test set	Inactive	*Daphnia magna*
Zinc oxide	O=[Zn].O=[Zn]	R9889291	M2652893	AUTO_5	test set	Inactive	*Daphnia magna*
Cobalt	[Co].[Co]	R21028106	M3728136	AUTO_82	test set	Inactive	*Ceriodaphnia dubia*
Zinc oxide	O=[Zn].O=[Zn]	R12643421	M2652893	AUTO_4	test set	Inactive	*Eisenia veneta*
Zinc oxide	O=[Zn].O=[Zn]	R21028054	M2652893	AUTO_29	test set	Inactive	*Danio rerio*
Copper(II) oxide	O=[Cu].O=[Cu]	R12714710	M2652894	AUTO_5	test set	Inactive	*Thamnocephalus platyurusb*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21028177	M2645228	AUTO_153	test set	Inactive	*Escherichia coli*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21028178	M2645228	AUTO_154	test set	Inactive	*Escherichia coli*
Zinc oxide	O=[Zn].O=[Zn]	R2707683	M2652893	AUTO_24	test set	Inactive	*Daphnia magna*
Zinc oxide	O=[Zn].O=[Zn]	R12714706	M2652893	AUTO_1	test set	Inactive	*Daphnia magna*
Titanium	O=[Ti]=O.O=[Ti]=O	R2646990	M2645228	AUTO_6	test set	Inactive	*Daphnia magna*
Zinc oxide	O=[Zn].O=[Zn]	R12601998	M2652893	AUTO_6	test set	Inactive	*Danio rerio*
Zinc oxide	O=[Zn].O=[Zn]	R2707288	M2652893	AUTO_3	test set	Inactive	*Zebrafish*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21028031	M2645228	AUTO_6	test set	Inactive	*Daphnia pulex*
Silver	[Ag].[Ag]	R21028113	M2645220	AUTO_89	test set	Inactive	*Danio rerio*
Silver	[Ag].[Ag]	R9889346	M2645220	AUTO_3	test set	Inactive	*Danio rerio embryos*

Silver	[Ag].[Ag]	R21028213	M2645220	AUTO_189	test set	Inactive	*Pimephales promelas*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21028028	M2645228	AUTO_3	test set	Inactive	*Ceriodaphnia dubia*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21028029	M2645228	AUTO_4	test set	Inactive	*Ceriodaphnia dubia*
Silver	[Ag].[Ag]	R21028154	M2645220	AUTO_130	test set	Inactive	*Paramecium caudatum*
Zinc oxide	O=[Zn].O=[Zn]	R21028072	M2652893	AUTO_47	test set	Inactive	*Daphnia magna*
Silver	[Ag].[Ag]	R9890191	M2645220	AUTO_2	test set	Inactive	*Danio rerio*
Silver	[Ag].[Ag]	R9890193	M2645220	AUTO_4	test set	Inactive	*Danio rerio*
Cobalt(II) oxide	O=[Co].O=[Co].O=[Co]O[Co]=O.O=[Co]O[Co]=O	R21028062	M4394264	AUTO_37	test set	Inactive	*Escherichia coli*
Silver	[Ag].[Ag]	R2691544	M2645220	AUTO_22	test set	Inactive	*Paramecium caudatum*
Silver	[Ag].[Ag]	R2691547	M2645220	AUTO_25	test set	Inactive	*MetPlate-Bacterial bioassay*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21028036	M2645228	AUTO_11	test set	Inactive	*Daphnia magna*
Iron	[Fe].[Fe]	R21028103	M84326991	AUTO_79	test set	Inactive	*Heterocypris incongruens*
Aluminium oxide	O=[Al]O[Al]=O.O=[Al]O[Al]=O	R9887904	M2652898	AUTO_2	test set	Inactive	*Caenorhabditis elegans*
Silver	[Ag].[Ag]	R2691548	M2645220	AUTO_26	test set	Inactive	*MetPlate-Bacterial bioassay*
Copper(II) oxide	O=[Cu].O=[Cu]	R9890183	M2652894	AUTO_2	test set	Inactive	*Thamnoplatyurus platyurus*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21028176	M2645228	AUTO_152	test set	Inactive	*Escherichia coli*
Iron	[Fe].[Fe]	R21028218	M84326991	AUTO_194	test set	Inactive	*Oryzias latipes*
Calcium(II) oxide	O=[Ca].O=[Ca]	R11895738	M4394240	AUTO_38	test set	Inactive	*Danio rerio*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21028219	M2645228	AUTO_195	test set	Inactive	*Danio rerio*
Copper(II) oxide	O=[Cu].O=[Cu]	R11895717	M2652894	AUTO_13	test set	Inactive	*Danio rerio*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21028033	M2645228	AUTO_8	test set	Inactive	*Pimephales promelas*
Zinc oxide	O=[Zn].O=[Zn]	R12584190	M2652893	AUTO_1	test set	Inactive	*Leptocheirus plumulosus*
Tin	[Sn].[Sn]	R11895765	M4394242	AUTO_68	test set	Inactive	*Danio rerio eggs*
Copper(II) oxide	O=[Cu].O=[Cu]	R11895719	M2652894	AUTO_15	test set	Inactive	*Danio rerio eggs*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21028152	M2645228	AUTO_128	test set	Inactive	*Escherichia coli*
Silver	[Ag].[Ag]	R5065867	M2645220	AUTO_47	test set	Inactive	*Daphnia Magna*

							Stratus

242

243

244 Table S8. Detailed information of the EC50 data used for building nano-SARs

Information of nanoparticles in the Online Chemical Modeling Environment (OCHEM) platform					Sub-dataset	Classification (threshold value 10.0 mg/L)	Species tested
Material Nanoparticles of Elements	**SMILES**	**RECORDID in OCHEM**	**MOLECULEID in OCHEM**	**Identifier in article**			
Silver	[Ag].[Ag]	R21027757	M2645220	AUTO_124	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R9877325	M2645220	AUTO_1	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R9979588	M2645220	AUTO_3	training set	Active	*Daphnia magna*
Gold	[Au].[Au]	R18891663	M2660068	AUTO_7	training set	Active	*Zebrafish embryo*
Silver	[Ag].[Ag]	R9877326	M2645220	AUTO_2	training set	Active	*Daphnia magna*
Silver, colloid	[Ag].[Ag]	R9728762	M2645220	AUTO_2	training set	Active	*Daphnia magna neonates*
Silver	[Ag].[Ag]	R21027880	M2645220	AUTO_253	training set	Active	*Pseudokirchneriella subcapitata*
Gold	[Au].[Au]	R18891691	M2660068	AUTO_64	training set	Active	*Zebrafish embryo*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027666	M2652894	AUTO_28	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21027737	M2645220	AUTO_101	training set	Active	*Pseudokirchneriella subcapitata*
Silver	[Ag].[Ag]	R21027881	M2645220	AUTO_254	training set	Active	*Pseudokirchneriella subcapitata*
Silver	[Ag].[Ag]	R21027884	M2645220	AUTO_257	training set	Active	*Pseudokirchneriella subcapitata*
Silver	[Ag].[Ag]	R21027756	M2645220	AUTO_123	training set	Active	*Daphnia magna*
Gold	[Au].[Au]	R18891659	M2660068	AUTO_2	training set	Active	*Zebrafish embryo*
Silver	[Ag].[Ag]	R21027705	M2645220	AUTO_69	training set	Active	*Daphnia pulex*
Silver	[Ag].[Ag]	R21027656	M2645220	AUTO_18	training set	Active	*Daphnia magna*
Gold	[Au].[Au]	R18891690	M2660068	AUTO_63	training set	Active	*Zebrafish embryo*
Silver	[Ag].[Ag]	R21027658	M2645220	AUTO_20	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21027659	M2645220	AUTO_21	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R9979587	M2645220	AUTO_2	training set	Active	*Daphnia magna*
Gold	[Au].[Au]	R18891662	M2660068	AUTO_6	training set	Active	*Zebrafish embryo*
Silver	[Ag].[Ag]	R21027660	M2645220	AUTO_22	training set	Active	*Daphnia magna*
Gold	[Au].[Au]	R18891689	M2660068	AUTO_62	training set	Active	*Zebrafish*

							embryo
Silver	[Ag].[Ag]	R21027806	M2645220	AUTO_173	training set	Active	*Lemna minor*
Silver	[Ag].[Ag]	R21027883	M2645220	AUTO_256	training set	Active	*Pseudokirchneriella subcapitata*
Silver	[Ag].[Ag]	R21027689	M2645220	AUTO_51	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21027740	M2645220	AUTO_104	training set	Active	*Pseudokirchneriella subcapitata*
Silver	[Ag].[Ag]	R21027940	M2645220	AUTO_314	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R18891681	M2645220	AUTO_42	training set	Active	*Zebrafish embryo*
Silver	[Ag].[Ag]	R9979586	M2645220	AUTO_1	training set	Active	*Pseudokirchneriella subcapitata*
Silver	[Ag].[Ag]	R21027680	M2645220	AUTO_42	training set	Active	*Desmodesmus subspicatus*
Silver	[Ag].[Ag]	R21027882	M2645220	AUTO_255	training set	Active	*Pseudokirchneriella subcapitata*
Silver	[Ag].[Ag]	R21027807	M2645220	AUTO_174	training set	Active	*Lemna minor*
Zinc oxide	O=[Zn].O=[Zn]	R9727613	M2652893	AUTO_1	training set	Active	*Pseudokirchneriella subcapitata*
Silver	[Ag].[Ag]	R21027939	M2645220	AUTO_313	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21027811	M2645220	AUTO_178	training set	Active	*Lemna minor*
Zinc oxide	O=[Zn].O=[Zn]	R21027914	M2652893	AUTO_288	training set	Active	*Pseudokirchneriella subcapitata*
Silver	[Ag].[Ag]	R9727601	M2645220	AUTO_3	training set	Active	*Daphnia magna, freshwater*
Copper(II) oxide	O=[Cu].O=[Cu]	R12714722	M2652894	AUTO_10	training set	Active	*Daphnia magna*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027675	M2652894	AUTO_37	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R9727600	M2645220	AUTO_2	training set	Active	*Daphnia magna, river water*
Zinc oxide	O=[Zn].O=[Zn]	R21027706	M2652893	AUTO_70	training set	Active	*Pseudokirchneriella subcapitata*
Silver	[Ag].[Ag]	R21027812	M2645220	AUTO_179	training set	Active	*Lemna minor*
Silver	[Ag].[Ag]	R21027808	M2645220	AUTO_175	training set	Active	*Lemna minor*
Silver	[Ag].[Ag]	R21027925	M2645220	AUTO_299	training set	Active	*Chlamydomonas reinhardtii*
Silver	[Ag].[Ag]	R21027926	M2645220	AUTO_300	training set	Active	*Chlamydomonas reinhardtii*

Gold	[Au].[Au]	R18891677	M2660068	AUTO_28	training set	Active	*Zebrafish embryo*
Copper(II) oxide	O=[Cu].O=[Cu]	R12714718	M2652894	AUTO_6	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21027927	M2645220	AUTO_301	training set	Active	*Chlamydomonas reinhardtii*
Silver	[Ag].[Ag]	R21027758	M2645220	AUTO_125	training set	Active	*Caenorhabditis elegans*
Copper(II) oxide	O=[Cu].O=[Cu]	R12714716	M2652894	AUTO_4	training set	Active	*Daphnia magna*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027677	M2652894	AUTO_39	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21027928	M2645220	AUTO_302	training set	Active	*Chlamydomonas reinhardtii*
Copper(II) oxide	O=[Cu].O=[Cu]	R12714717	M2652894	AUTO_5	training set	Active	*Daphnia magna*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027668	M2652894	AUTO_30	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21027687	M2645220	AUTO_49	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21027813	M2645220	AUTO_180	training set	Active	*Lemna minor*
Silver	[Ag].[Ag]	R21027809	M2645220	AUTO_176	training set	Active	*Lemna minor*
Zinc oxide	O=[Zn].O=[Zn]	R21027876	M2652893	AUTO_249	training set	Active	*Daphnia magna*
Zinc oxide	O=[Zn].O=[Zn]	R21027947	M2652893	AUTO_321	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R9727602	M2645220	AUTO_4	training set	Active	*Daphnia magna, river water*
Silver	[Ag].[Ag]	R2659286	M2645220	AUTO_6	training set	Active	*Chlamydomonas reinhardtii*
Silver, suspension	[Ag].[Ag]	R9728763	M2645220	AUTO_3	training set	Active	*Daphnia magna neonates*
Silver	[Ag].[Ag]	R2659284	M2645220	AUTO_4	training set	Active	*Chlamydomonas reinhardtii*
Silver	[Ag].[Ag]	R2659283	M2645220	AUTO_3	training set	Active	*Chlamydomonas reinhardtii*
Mixture: Copper(II) oxide/Zinc oxide	O=[Cu].O=[Cu].O=[Zn].O=[Zn]	R9866146	M3728107	AUTO_3	training set	Active	*Daphnia magna*
cerium oxide	O=[Ce]=O.O=[Ce]=O	R21027800	M2659378	AUTO_167	training set	Active	*Anabaena sp.*
Erbium oxide	O=[Er]O[Er]=O.O=[Er]O[Er]=O	R18891676	M84250880	AUTO_27	training set	Active	*Zebrafish embryo*
Silver	[Ag].[Ag]	R21027766	M2645220	AUTO_133	training set	Active	*Caenorhabditis elegans*
Copper(II)	O=[Cu].O=	R12714720	M2652894	AUTO_8	training set	Active	*Daphnia*

oxide	[Cu]						*magna*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027673	M2652894	AUTO_35	training set	Active	*Daphnia magna*
Zinc oxide	O=[Zn].O=[Zn]	R21027948	M2652893	AUTO_322	training set	Active	*Daphnia magna*
Nickel	[Ni].[Ni]	R21027744	M2655007	AUTO_108	training set	Active	*Pseudokirchneriella subcapitata*
Gold	[Au].[Au]	R18891666	M2660068	AUTO_12	training set	Active	*Zebrafish embryo*
Silver	[Ag].[Ag]	R21027929	M2645220	AUTO_303	training set	Active	*Chlamydomonas reinhardtii*
Silver	[Ag].[Ag]	R21027768	M2645220	AUTO_135	training set	Active	*Caenorhabditis elegans*
Silver	[Ag].[Ag]	R21027718	M2645220	AUTO_82	training set	Active	*Escherichia coli*
Copper(II) oxide	O=[Cu].O=[Cu]	R9866144	M2652894	AUTO_1	training set	Active	*Daphnia magna*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21027892	M2645228	AUTO_265	training set	Active	*Daphnia magna*
Zinc oxide	O=[Zn].O=[Zn]	R9889048	M2652893	AUTO_5	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21027661	M2645220	AUTO_23	training set	Active	*Daphnia magna*
Copper	[Cu].[Cu]	R21027743	M2655006	AUTO_107	training set	Active	*Pseudokirchneriella subcapitata*
cerium oxide	O=[Ce]=O.O=[Ce]=O	R21027797	M2659378	AUTO_164	training set	Active	*Anabaena sp.*
Zinc oxide	O=[Zn].O=[Zn]	R12602002	M2652893	mg/l	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21027690	M2645220	AUTO_52	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21027719	M2645220	AUTO_83	training set	Active	*Escherichia coli*
Gold	[Au].[Au]	R18891664	M2660068	AUTO_8	training set	Active	*Zebrafish embryo*
Copper(II) oxide	O=[Cu].O=[Cu]	R9727617	M2652894	AUTO_5	training set	Active	*Pseudokirchneriella subcapitata*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21027699	M2645228	AUTO_63	training set	Active	*Daphnia magna*
Zinc oxide	O=[Zn].O=[Zn]	R9866145	M2652893	AUTO_2	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21027695	M2645220	AUTO_59	training set	Active	*Danio rerio*
Titanium dioxide ((Degussa P25)	O=[Ti]=O.O=[Ti]=O	R9729291	M2645228	AUTO_2	training set	Active	*Daphnia magna, UVA photoperiod*
Silver	[Ag].[Ag]	R21027759	M2645220	AUTO_126	training set	Active	*Caenorhabditis elegans*
cerium oxide	O=[Ce]=O.O=[Ce]=O	R21027788	M2659378	AUTO_155	training set	Active	*Pseudokirchneriella subcapitata*

Copper(II) oxide	O=[Cu].O=[Cu]	R21027912	M2652894	AUTO_286	training set	Active	*Pseudokirchneriella subcapitata*
Silver	[Ag].[Ag]	R21027692	M2645220	AUTO_56	training set	Active	*Raphidocelis subcapitata*
Zinc oxide	O=[Zn].O=[Zn]	R9728758	M2652893	AUTO_2	training set	Active	*Daphnia magna*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21027640	M2645228	AUTO_1	training set	Active	*Pseudokirchneriella subcapitata*
Silver	[Ag].[Ag]	R9963618	M2645220	AUTO_2	training set	Active	*Danio rerio embryos*
Silver	[Ag].[Ag]	R21027886	M2645220	AUTO_259	training set	Active	*Danio rerio*
Silver	[Ag].[Ag]	R9963617	M2645220	AUTO_1	training set	Active	*Danio rerio embryos*
Silver	[Ag].[Ag]	R21027887	M2645220	AUTO_260	training set	Active	*Danio rerio*
Silver	[Ag].[Ag]	R21027662	M2645220	AUTO_24	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21027889	M2645220	AUTO_262	training set	Active	*Danio rerio*
Silver	[Ag].[Ag]	R21027697	M2645220	AUTO_61	training set	Active	*Danio rerio*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027667	M2652894	AUTO_29	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21027763	M2645220	AUTO_130	training set	Active	*Caenorhabditis elegans*
Silver	[Ag].[Ag]	R21027663	M2645220	AUTO_25	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21027767	M2645220	AUTO_134	training set	Active	*Caenorhabditis elegans*
Zinc oxide	O=[Zn].O=[Zn]	R21027945	M2652893	AUTO_319	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21027739	M2645220	AUTO_103	training set	Active	*Pseudokirchneriella subcapitata*
Silver	[Ag].[Ag]	R21027696	M2645220	AUTO_60	training set	Active	*Danio rerio*
Zinc oxide	O=[Zn].O=[Zn]	R21027946	M2652893	AUTO_320	training set	Active	*Daphnia magna*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21027709	M2645228	AUTO_73	training set	Active	*Scenedesmus obliquus*
Zinc oxide	O=[Zn].O=[Zn]	R2707670	M2652893	AUTO_11	training set	Active	*Vibrio fischeri*
Silver	[Ag].[Ag]	R21027769	M2645220	AUTO_136	training set	Active	*Caenorhabditis elegans*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027669	M2652894	AUTO_31	training set	Active	*Daphnia magna*
Zinc oxide	O=[Zn].O=[Zn]	R2707671	M2652893	AUTO_12	training set	Active	*Vibrio fischeri*
Zinc oxide	O=[Zn].O=[Zn]	R9968654	M2652893	AUTO_3	training set	Active	*Vibrio fischeri*
Zinc oxide	O=[Zn].O=[Zn]	R21027921	M2652893	AUTO_295	training set	Active	*Vibrio fischeri*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21027641	M2645228	AUTO_2	training set	Active	*Pseudokirchneriella subcapitata*

Silver	[Ag].[Ag]	R21027715	M2645220	AUTO_79	training set	Active	*Escherichia coli*
Zinc oxide	O=[Zn].O=[Zn]	R9968655	M2652893	AUTO_4	training set	Active	*Danio rerio*
Zinc oxide	O=[Zn].O=[Zn]	R21027708	M2652893	AUTO_72	training set	Active	*Danio rerio*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027670	M2652894	AUTO_32	training set	Active	*Daphnia magna*
dysprosium oxide	O=[Dy]O[Dy]=O.O=[Dy]O[Dy]=O	R18891672	M3728214	AUTO_22	training set	Active	*Zebrafish embryo*
Silver	[Ag].[Ag]	R21027679	M2645220	AUTO_41	training set	Active	*Desmodesmus subspicatus*
Silver	[Ag].[Ag]	R21027878	M2645220	AUTO_251	training set	Active	*Phaeodactylum tricornutum*
Zinc oxide	O=[Zn].O=[Zn]	R21027890	M2652893	AUTO_263	training set	Active	*Dunaliella tertiolecta*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21027642	M2645228	AUTO_3	training set	Active	*Ceriodaphnia dubia*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21027745	M2645228	AUTO_109	training set	Active	*Pseudokirchneriella subcapitata*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027830	M2652894	AUTO_198	training set	Active	*Escherichia coli*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027671	M2652894	AUTO_33	training set	Active	*Daphnia magna*
Copper(II) oxide	O=[Cu].O=[Cu]	R9890170	M2652894	AUTO_1	training set	Active	*Daphnia magna*
Zinc oxide	O=[Zn].O=[Zn]	R9890174	M2652893	AUTO_5	training set	Active	*Daphnia magna*
Zinc oxide	O=[Zn].O=[Zn]	R12602003	M2652893	mg/l	training set	Active	*Daphnia magna*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027672	M2652894	AUTO_34	training set	Active	*Daphnia magna*
Titanium dioxide ((Degussa P25)	O=[Ti]=O.O=[Ti]=O	R9729293	M2645228	AUTO_4	training set	Active	*Daphnia magna, UVA photoperiod*
Silver	[Ag].[Ag]	R21027781	M2645220	AUTO_148	training set	Active	*Caenorhabditis elegans*
Silver	[Ag].[Ag]	R21027651	M2645220	AUTO_12	training set	Active	*Caenorhabditis elegans*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21027746	M2645228	AUTO_110	training set	Active	*Pseudokirchneriella subcapitata*
Silver	[Ag].[Ag]	R21027819	M2645220	AUTO_186	training set	Active	*Escherichia coli*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R12572776	M2645228	AUTO_2	training set	Active	*Daphnia magna*
Copper(II) oxide	O=[Cu].O=[Cu]	R12714719	M2652894	AUTO_7	training set	Active	*Daphnia magna*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027831	M2652894	AUTO_199	training set	Active	*Escherichia coli*

Copper(II) oxide	O=[Cu].O=[Cu]	R21027901	M2652894	AUTO_275	training set	Active	*Saccharomyces cerevisiae*
Silver	[Ag].[Ag]	R21027760	M2645220	AUTO_127	training set	Active	*Caenorhabditis elegans*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R12572777	M2645228	AUTO_311	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21027879	M2645220	AUTO_252	training set	Active	*Phaeodactylum tricornutum*
Silver	[Ag].[Ag]	R21027682	M2645220	AUTO_44	training set	Active	*Desmodesmus subspicatus*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21027934	M2645228	AUTO_308	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21027820	M2645220	AUTO_187	training set	Active	*Escherichia coli*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21027700	M2645228	AUTO_64	training set	Active	*Daphnia magna*
Zinc oxide	O=[Zn].O=[Zn]	R21027754	M2652893	AUTO_121	training set	Active	*Vibrio fischeri*
Silver	[Ag].[Ag]	R21027665	M2645220	AUTO_27	training set	Active	*Daphnia magna*
Zinc oxide	O=[Zn].O=[Zn]	R10003996	M2652893	AUTO_2	training set	Active	*Tetrahymena thermophila*
Copper(II) oxide	O=[Cu].O=[Cu]	R9848050	M2652894	AUTO_1	training set	Active	*Daphnia magna*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027922	M2652894	AUTO_296	training set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21027694	M2645220	AUTO_58	training set	Active	*Raphidocelis subcapitata*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027902	M2652894	AUTO_276	training set	Active	*Saccharomyces cerevisiae*
Zinc oxide	O=[Zn].O=[Zn]	R10003995	M2652893	AUTO_1	training set	Active	*Tetrahymena thermophila*
Silver	[Ag].[Ag]	R21027764	M2645220	AUTO_131	training set	Active	*Caenorhabditis elegans*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027903	M2652894	AUTO_277	training set	Active	*Saccharomyces cerevisiae*
cerium oxide	O=[Ce]=O.O=[Ce]=O	R21027790	M2659378	AUTO_157	training set	Active	*Pseudokirchneriella subcapitata*
Zinc oxide	O=[Zn].O=[Zn]	R21027755	M2652893	AUTO_122	training set	Active	*Vibrio fischeri*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027904	M2652894	AUTO_278	training set	Active	*Saccharomyces cerevisiae*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21027647	M2645228	AUTO_8	training set	Active	*Bacillus licheniformis*

cerium oxide	O=[Ce]=O.O=[Ce]=O	R21027786	M2659378	AUTO_153	training set	Active	*Pseudokirchneriella subcapitata*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027905	M2652894	AUTO_279	training set	Active	*Saccharomyces cerevisiae*
Zinc oxide	O=[Zn].O=[Zn]	R21027944	M2652893	AUTO_318	training set	Active	*Tetrahymena thermophila*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R12572781	M2645228	AUTO_8	training set	Active	*Brachionus plicatilis*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027906	M2652894	AUTO_280	training set	Active	*Saccharomyces cerevisiae*
cerium oxide	O=[Ce]=O.O=[Ce]=O	R21027725	M2659378	AUTO_89	training set	Active	*Pseudokirchneriella subcapitata*
Silver	[Ag].[Ag]	R21027825	M2645220	AUTO_193	training set	Active	*Escherichia coli*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R9727615	M2645228	AUTO_3	training set	Active	*Pseudokirchneriella subcapitata*
Silver	[Ag].[Ag]	R9889342	M2645220	AUTO_3	training set	Active	*Danio rerio embryos*
Zinc oxide	O=[Zn].O=[Zn]	R21027942	M2652893	AUTO_316	training set	Active	*Tetrahymena thermophila*
cerium oxide	O=[Ce]=O.O=[Ce]=O	R21027794	M2659378	AUTO_161	training set	Active	*Anabaena sp.*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21027710	M2645228	AUTO_74	training set	Active	*Scenedesmus obliquus*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027836	M2652894	AUTO_204	training set	Active	*Escherichia coli*
Zinc oxide	O=[Zn].O=[Zn]	R21027846	M2652893	AUTO_214	training set	Active	*Escherichia coli*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027907	M2652894	AUTO_281	training set	Active	*Saccharomyces cerevisiae*
Zinc oxide	O=[Zn].O=[Zn]	R9890176	M2652893	AUTO_7	training set	Active	*Daphnia magna*
Zinc oxide	O=[Zn].O=[Zn]	R10004000	M2652893	AUTO_6	training set	Active	*Tetrahymena thermophila*
Zinc oxide	O=[Zn].O=[Zn]	R9728759	M2652893	AUTO_3	training set	Active	*Daphnia magna*
cerium oxide	O=[Ce]=O.O=[Ce]=O	R21027803	M2659378	AUTO_170	training set	Active	*Anabaena sp.*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R9727607	M2645228	AUTO_1	training set	Active	*Daphnia similis*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027908	M2652894	AUTO_282	training set	Active	*Saccharomyces cerevisiae*
Aluminium	[Al].[Al]	R21027742	M3728130	AUTO_106	training set	Active	*Pseudokirchneriella subcapitata*
cerium	O=[Ce]=O.	R21027791	M2659378	AUTO_158	training set	Active	*Pseudokirc*

oxide	O=[Ce]=O						*hneriella subcapitata*
cerium oxide	O=[Ce]=O.O=[Ce]=O	R21027792	M2659378	AUTO_159	training set	Active	*Pseudokirchneriella subcapitata*
Zinc oxide	O=[Zn].O=[Zn]	R9890178	M2652893	AUTO_9	training set	Active	*Tetrahymena thermophila*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21027936	M2645228	AUTO_310	training set	Active	*Daphnia magna*
cerium oxide	O=[Ce]=O.O=[Ce]=O	R21027787	M2659378	AUTO_154	training set	Active	*Pseudokirchneriella subcapitata*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21027913	M2645228	AUTO_287	training set	Active	*Pseudokirchneriella subcapitata*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027909	M2652894	AUTO_283	training set	Active	*Saccharomyces cerevisiae*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21027938	M2645228	AUTO_312	training set	Active	*Daphnia magna*
Zinc oxide	O=[Zn].O=[Zn]	R9890177	M2652893	AUTO_8	training set	Inactive	*Daphnia magna*
Zinc oxide	O=[Zn].O=[Zn]	R12584192	M2652893	AUTO_1	training set	Inactive	*Folsomia candida*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027827	M2652894	AUTO_195	training set	Inactive	*Escherichia coli*
Zinc oxide	O=[Zn].O=[Zn]	R9968656	M2652893	AUTO_5	training set	Inactive	*Xenopus laevis*
Zinc oxide	O=[Zn].O=[Zn]	R21027653	M2652893	AUTO_14	training set	Inactive	*Xenopus laevis*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R12572782	M2645228	AUTO_9	training set	Inactive	*Brachionus plicatilis*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R12572778	M2645228	AUTO_5	training set	Inactive	*Phaeodactylum tricornutum*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027828	M2652894	AUTO_196	training set	Inactive	*Escherichia coli*
Copper(II) oxide	O=[Cu].O=[Cu]	R9727618	M2652894	AUTO_6	training set	Inactive	*Pseudokirchneriella subcapitata*
Silver	[Ag].[Ag]	R21027770	M2645220	AUTO_137	training set	Inactive	*Caenorhabditis elegans*
cerium oxide	O=[Ce]=O.O=[Ce]=O	R9727307	M2659378	AUTO_114	training set	Inactive	*Pseudokirchneriella subcapitata*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R9727608	M2645228	AUTO_2	training set	Inactive	*Daphnia similis*
cerium oxide	O=[Ce]=O.O=[Ce]=O	R21027783	M2659378	AUTO_150	training set	Inactive	*Pseudokirchneriella subcapitata*
Copper(II) oxide	O=[Cu].O=[Cu]	R9997798	M2652894	AUTO_7	training set	Inactive	*Saccharomyces cerevisiae*
Silver	[Ag].[Ag]	R21027780	M2645220	AUTO_147	training set	Inactive	*Caenorhabditis elegans*

Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R12572780	M2645228	AUTO_7	training set	Inactive	*Phaeodactylum tricornutum*
Zinc oxide	O=[Zn].O=[Zn]	R9890181	M2652893	AUTO_12	training set	Inactive	*Tetrahymena thermophila*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027829	M2652894	AUTO_197	training set	Inactive	*Escherichia coli*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R9887907	M2645228	AUTO_2	training set	Inactive	*Pseudokirchneriella subcapitata*
cerium oxide	O=[Ce]=O.O=[Ce]=O	R21027793	M2659378	AUTO_160	training set	Inactive	*Pseudokirchneriella subcapitata*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21027649	M2645228	AUTO_10	training set	Inactive	*Bacillus licheniformis*
Silver	[Ag].[Ag]	R21027816	M2645220	AUTO_183	training set	Inactive	*Escherichia coli*
Zinc oxide	O=[Zn].O=[Zn]	R9890179	M2652893	AUTO_10	training set	Inactive	*Tetrahymena thermophila*
cerium oxide	O=[Ce]=O.O=[Ce]=O	R9727308	M2659378	AUTO_115	training set	Inactive	*Pseudokirchneriella subcapitata*
Silver	[Ag].[Ag]	R9889341	M2645220	AUTO_2	training set	Inactive	*Danio rerio embryos*
Titanium dioxide ((Degussa P25)	O=[Ti]=O.O=[Ti]=O	R9729290	M2645228	AUTO_1	training set	Inactive	*Daphnia magna, dark*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21027650	M2645228	AUTO_11	training set	Inactive	*Bacillus licheniformis*
cerium oxide	O=[Ce]=O.O=[Ce]=O	R21027749	M2659378	AUTO_116	training set	Inactive	*Daphnia magna*
Copper(II) oxide	O=[Cu].O=[Cu]	R9997794	M2652894	AUTO_3	training set	Inactive	*Saccharomyces cerevisiae*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R9887908	M2645228	AUTO_3	training set	Inactive	*Pseudokirchneriella subcapitata*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21027711	M2645228	AUTO_75	training set	Inactive	*Pseudokirchneriella subcapitata*
Silver	[Ag].[Ag]	R21027693	M2645220	AUTO_57	training set	Inactive	*Raphidocelis subcapitata*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027917	M2652894	AUTO_291	training set	Inactive	*Saccharomyces cerevisiae*
Zinc oxide	O=[Zn].O=[Zn]	R21027843	M2652893	AUTO_211	training set	Inactive	*Escherichia coli*
cerium oxide	O=[Ce]=O.O=[Ce]=O	R21027750	M2659378	AUTO_117	training set	Inactive	*Daphnia magna*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21027644	M2645228	AUTO_5	training set	Inactive	*Ceriodaphnia dubia*

Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21027652	M2645228	AUTO_13	training set	Inactive	*Daphnia magna*
Zinc oxide	O=[Zn].O=[Zn]	R9890180	M2652893	AUTO_11	training set	Inactive	*Tetrahymena thermophila*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R9728765	M2645228	AUTO_2	training set	Inactive	*Ceriodaphnia dubia, dark*
Titanium dioxide ((Degussa P25)	O=[Ti]=O.O=[Ti]=O	R9729292	M2645228	AUTO_3	training set	Inactive	*Daphnia magna, dark*
Copper(II) oxide	O=[Cu].O=[Cu]	R9866153	M2652894	AUTO_1	training set	Inactive	*Escherichia coli*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027776	M2652894	AUTO_143	training set	Inactive	*Escherichia coli*
Silver	[Ag].[Ag]	R9889340	M2645220	AUTO_1	training set	Inactive	*Danio rerio embryos*
Silver	[Ag].[Ag]	R9848057	M2645220	AUTO_1	training set	Inactive	*Chlorella sp.*
Silver	[Ag].[Ag]	R21027821	M2645220	AUTO_188	training set	Inactive	*Escherichia coli*
Zinc oxide	O=[Zn].O=[Zn]	R21027730	M2652893	AUTO_94	training set	Inactive	*Bacillus subtilis*
Zinc oxide	O=[Zn].O=[Zn]	R21027734	M2652893	AUTO_98	training set	Inactive	*Escherichia coli*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21027720	M2645228	AUTO_84	training set	Inactive	*Desmodesmus subspicatus*
Nickel(II) oxide	O=[Ni].O=[Ni]	R21027701	M2652904	AUTO_65	training set	Inactive	*Chlorella vulgaris*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027832	M2652894	AUTO_200	training set	Inactive	*Escherichia coli*
cerium oxide	O=[Ce]=O.O=[Ce]=O	R21027795	M2659378	AUTO_162	training set	Inactive	*Anabaena sp.*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R9879036	M2645228	AUTO_3	training set	Inactive	*Daphnia magna*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R9889045	M2645228	AUTO_2	training set	Inactive	*Daphnia magna*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R9727616	M2645228	AUTO_4	training set	Inactive	*Pseudokirchneriella subcapitata*
Iron	[Fe].[Fe]	R21027736	M84326991	AUTO_100	training set	Inactive	*Heterocypris incongruens*
cerium oxide	O=[Ce]=O.O=[Ce]=O	R9727310	M2659378	AUTO_5	training set	Inactive	*Daphnia magna*
cerium oxide	O=[Ce]=O.O=[Ce]=O	R21027799	M2659378	AUTO_166	training set	Inactive	*Anabaena sp.*
Aluminium oxide	O=[Al]O[Al]=O.O=[Al]O[Al]=O	R21027872	M2652898	AUTO_245	training set	Inactive	*Scenedesmus sp.*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027833	M2652894	AUTO_201	training set	Inactive	*Escherichia coli*
cerium oxide	O=[Ce]=O.O=[Ce]=O	R9727309	M2659378	AUTO_4	training set	Inactive	*Daphnia magna*
Titanium	O=[Ti]=O.	R21027857	M2645228	AUTO_226	training set	Inactive	*Ceriodaphn*

dioxide	O=[Ti]=O						*ia dubia*
cerium oxide	O=[Ce]=O.O=[Ce]=O	R21027804	M2659378	AUTO_171	training set	Inactive	*Anabaena sp.*
cerium oxide	O=[Ce]=O.O=[Ce]=O	R21027751	M2659378	AUTO_118	training set	Inactive	*Daphnia magna*
Titanium	O=[Ti]=O.O=[Ti]=O	R2692103	M2645228	AUTO_7	training set	Inactive	*Desmodesmus subspicatus*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R9727312	M2645228	AUTO_1	training set	Inactive	*Desmodesmus subspicatus*
Nickel(II) oxide	O=[Ni].O=[Ni]	R21027702	M2652904	AUTO_66	training set	Inactive	*Chlorella vulgaris*
Silver	[Ag].[Ag]	R9889343	M2645220	AUTO_4	training set	Inactive	*Danio rerio embryos*
Silver	[Ag].[Ag]	R21027771	M2645220	AUTO_138	training set	Inactive	*Caenorhabditis elegans*
Zinc oxide	O=[Zn].O=[Zn]	R21027731	M2652893	AUTO_95	training set	Inactive	*Bacillus subtilis*
Aluminium oxide	O=[Al]O[Al]=O.O=[Al]O[Al]=O	R21027856	M2652898	AUTO_225	training set	Inactive	*Ceriodaphnia dubia*
Aluminium oxide	O=[Al]O[Al]=O.O=[Al]O[Al]=O	R21027871	M2652898	AUTO_244	training set	Inactive	*Chlorella sp.*
Silver	[Ag].[Ag]	R21027685	M2645220	AUTO_47	training set	Inactive	*Vibrio fischeri*
cerium oxide	O=[Ce]=O.O=[Ce]=O	R21027802	M2659378	AUTO_169	training set	Inactive	*Anabaena sp.*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027834	M2652894	AUTO_202	training set	Inactive	*Escherichia coli*
Silver	[Ag].[Ag]	R21027765	M2645220	AUTO_132	training set	Inactive	*Caenorhabditis elegans*
Silver	[Ag].[Ag]	R21027861	M2645220	AUTO_234	training set	Inactive	*Pseudomonas putida*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21027852	M2645228	AUTO_221	training set	Inactive	*Pseudokirchneriella subcapitata*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027835	M2652894	AUTO_203	training set	Inactive	*Escherichia coli*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R9727609	M2645228	AUTO_3	training set	Inactive	*Daphnia similis*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027899	M2652894	AUTO_273	training set	Inactive	*Chlorella sp.*
cerium oxide	O=[Ce]=O.O=[Ce]=O	R21027805	M2659378	AUTO_172	training set	Inactive	*Anabaena sp.*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21027714	M2645228	AUTO_78	training set	Inactive	*Pseudokirchneriella subcapitata*
Copper(II) oxide	O=[Cu].O=[Cu]	R9866157	M2652894	AUTO_5	training set	Inactive	*Bacillus subtilis*
Copper(II) oxide	O=[Cu].O=[Cu]	R9866161	M2652894	AUTO_9	training set	Inactive	*Streptococcus aureus*
Zinc oxide	O=[Zn].O=[Zn]	R21027847	M2652893	AUTO_215	training set	Inactive	*Escherichia coli*
Copper(II) oxide	O=[Cu].O=[Cu]	R9968657	M2652894	AUTO_6	training set	Inactive	*Vibrio fischeri*

Copper(II) oxide	O=[Cu].O=[Cu]	R21027753	M2652894	AUTO_120	training set	Inactive	*Vibrio fischeri*
cerium oxide	O=[Ce]=O.O=[Ce]=O	R9727311	M2659378	AUTO_6	training set	Inactive	*Daphnia magna*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R9846671	M2645228	AUTO_53	training set	Inactive	*Pseudokirchneriella subcapitata*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R9879035	M2645228	AUTO_2	training set	Inactive	*Pseudokirchneriella subcapitata*
Copper(II) oxide	O=[Cu].O=[Cu]	R2707701	M2652894	AUTO_42	training set	Inactive	*Vibrio fischeri*
Zinc oxide	O=[Zn].O=[Zn]	R21027735	M2652893	AUTO_99	training set	Inactive	*Escherichia coli*
Silver	[Ag].[Ag]	R21027862	M2645220	AUTO_235	training set	Inactive	*Pseudomonas putida*
Zinc oxide	O=[Zn].O=[Zn]	R21027848	M2652893	AUTO_216	training set	Inactive	*Escherichia coli*
Zinc oxide	O=[Zn].O=[Zn]	R9866159	M2652893	AUTO_7	training set	Inactive	*Bacillus subtilis*
Zinc oxide	O=[Zn].O=[Zn]	R21027849	M2652893	AUTO_217	training set	Inactive	*Escherichia coli*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21027712	M2645228	AUTO_76	training set	Inactive	*Pseudokirchneriella subcapitata*
Silver	[Ag].[Ag]	R21027863	M2645220	AUTO_236	training set	Inactive	*Pseudomonas putida*
Zinc oxide	O=[Zn].O=[Zn]	R21027850	M2652893	AUTO_218	training set	Inactive	*Escherichia coli*
Copper(II) oxide	O=[Cu].O=[Cu]	R10004001	M2652894	AUTO_7	training set	Inactive	*Tetrahymena thermophila*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R9727610	M2645228	AUTO_4	training set	Inactive	*Daphnia similis*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R9727611	M2645228	AUTO_5	training set	Inactive	*Daphnia similis*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R9727612	M2645228	AUTO_6	training set	Inactive	*Daphnia similis*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R9887906	M2645228	AUTO_1	training set	Inactive	*Daphnia magna*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21027853	M2645228	AUTO_222	training set	Inactive	*Pseudokirchneriella subcapitata*
Silver	[Ag].[Ag]	R21027865	M2645220	AUTO_238	training set	Inactive	*Pseudomonas putida*
Aluminium oxide	O=[Al]O[Al]=O.O=[Al]O[Al]=O	R9889044	M2652898	AUTO_1	training set	Inactive	*Daphnia magna*
Zinc oxide	O=[Zn].O=[Zn]	R21027779	M2652893	AUTO_146	training set	Inactive	*Escherichia coli*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21027924	M2645228	AUTO_298	training set	Inactive	*Chlorella sp.*
Zinc oxide	O=[Zn].O=[Zn]	R9997792	M2652893	AUTO_1	training set	Inactive	*Saccharomyces cerevisiae*
Zinc oxide	O=[Zn].O=[Zn]	R21027918	M2652893	AUTO_292	training set	Inactive	*Saccharomyces cerevisiae*

Nickel(II) oxide	O=[Ni].O=[Ni]	R9866158	M2652904	AUTO_6	training set	Inactive	*Bacillus subtilis*
Nickel(II) oxide	O=[Ni].O=[Ni]	R21027773	M2652904	AUTO_140	training set	Inactive	*Bacillus subtilis*
Zinc oxide	O=[Zn].O=[Zn]	R9866163	M2652893	AUTO_11	training set	Inactive	*Streptococcus aureus*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21027854	M2645228	AUTO_223	training set	Inactive	*Pseudokirchneriella subcapitata*
Copper(II) oxide	O=[Cu].O=[Cu]	R10003997	M2652894	AUTO_3	training set	Inactive	*Tetrahymena thermophila*
Zinc oxide	O=[Zn].O=[Zn]	R9997796	M2652893	AUTO_5	training set	Inactive	*Saccharomyces cerevisiae*
Zinc oxide	O=[Zn].O=[Zn]	R21027919	M2652893	AUTO_293	training set	Inactive	*Saccharomyces cerevisiae*
Copper(II) oxide	O=[Cu].O=[Cu]	R9890172	M2652894	AUTO_3	training set	Inactive	*Daphnia magna*
Silver	[Ag].[Ag]	R21027867	M2645220	AUTO_240	training set	Inactive	*Pseudomonas putida*
Antimony(III) oxide	O=[Sb]O[Sb]=O.O=[Sb]O[Sb]=O	R21027774	M69142	AUTO_141	training set	Inactive	*Bacillus subtilis*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R9846672	M2645228	AUTO_54	training set	Inactive	*Pseudokirchneriella subcapitata*
Silver	[Ag].[Ag]	R21027868	M2645220	AUTO_241	training set	Inactive	*Pseudomonas putida*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027748	M2652894	AUTO_112	training set	Inactive	*Chlamydomonas reinhardtii*
Zinc oxide	O=[Zn].O=[Zn]	R9997797	M2652893	AUTO_6	training set	Inactive	*Saccharomyces cerevisiae*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027943	M2652894	AUTO_317	training set	Inactive	*Tetrahymena thermophila*
Copper(II) oxide	O=[Cu].O=[Cu]	R9890171	M2652894	AUTO_2	training set	Inactive	*Daphnia magna*
Nickel(II) oxide	O=[Ni].O=[Ni]	R21027777	M2652904	AUTO_144	training set	Inactive	*Escherichia coli*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027941	M2652894	AUTO_315	training set	Inactive	*Tetrahymena thermophila*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21027732	M2645228	AUTO_96	training set	Inactive	*Escherichia coli*
Zinc oxide	O=[Zn].O=[Zn]	R21027840	M2652893	AUTO_208	training set	Inactive	*Escherichia coli*
Silver	[Ag].[Ag]	R21027683	M2645220	AUTO_45	training set	Inactive	*Vibrio fischeri*
Zinc oxide	O=[Zn].O=[Zn]	R21027841	M2652893	AUTO_209	training set	Inactive	*Escherichia coli*
Silver	[Ag].[Ag]	R21027870	M2645220	AUTO_243	training set	Inactive	*Pseudomonas putida*

Zinc oxide	O=[Zn].O=[Zn]	R21027842	M2652893	AUTO_210	training set	Inactive	*Escherichia coli*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027752	M2652894	AUTO_119	training set	Inactive	*Vibrio fischeri*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21027728	M2645228	AUTO_92	training set	Inactive	*Bacillus subtilis*
Zinc oxide	O=[Zn].O=[Zn]	R21027844	M2652893	AUTO_212	training set	Inactive	*Escherichia coli*
Magnetite	O=[Fe].O=[Fe].O=[Fe]O[Fe]=O.O=[Fe]O[Fe]=O	R2678284	M2659379	AUTO_5	training set	Inactive	*Vibrio fischeri*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R9846670	M2645228	AUTO_4	training set	Inactive	*Pseudokirchneriella subcapitata*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R9879034	M2645228	AUTO_1	training set	Inactive	*Pseudokirchneriella subcapitata*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21027691	M2645228	AUTO_55	training set	Inactive	*Pseudokirchneriella subcapitata*
Antimony(III) oxide	O=[Sb]O[Sb]=O.O=[Sb]O[Sb]=O	R21027778	M69142	AUTO_145	training set	Inactive	*Escherichia coli*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R9889046	M2645228	AUTO_3	training set	Inactive	*Daphnia magna*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21027855	M2645228	AUTO_224	training set	Inactive	*Pseudokirchneriella subcapitata*
Silver	[Ag].[Ag]	R21027822	M2645220	AUTO_189	training set	Inactive	*Escherichia coli*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21027645	M2645228	AUTO_6	training set	Inactive	*Pimephales promelas*
Silver	[Ag].[Ag]	R21027824	M2645220	AUTO_192	training set	Inactive	*Escherichia coli*
Silver	[Ag].[Ag]	R21027826	M2645220	AUTO_194	training set	Inactive	*Escherichia coli*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21027646	M2645228	AUTO_7	training set	Inactive	*Pimephales promelas*
Zinc oxide	O=[Zn].O=[Zn]	R9879032	M2652893	AUTO_1	training set	Inactive	*Caenorhabditis elegans*
Copper(II) oxide	O=[Cu].O=[Cu]	R9997799	M2652894	AUTO_8	training set	Inactive	*Saccharomyces cerevisiae*
Copper(II) oxide	O=[Cu].O=[Cu]	R9968660	M2652894	AUTO_9	training set	Inactive	*Xenopus laevis*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R9968662	M2645228	AUTO_11	training set	Inactive	*Xenopus laevis*
Iron(III) oxide	O=[Fe].O=[Fe].O=[Fe]O[Fe]=O.O=[Fe]O[Fe]=O	R9968663	M2659379	AUTO_12	training set	Inactive	*Xenopus laevis*
Copper(II) oxide	O=[Cu].O=[Cu]	R9890173	M2652894	AUTO_4	training set	Inactive	*Daphnia magna*
Silver	[Ag].[Ag]	R21027727	M2645220	AUTO_91	training set	Inactive	*Tetrahymena*

							pyriformis
Copper(II) oxide	O=[Cu].O=[Cu]	R10003998	M2652894	AUTO_4	training set	Inactive	*Tetrahymena thermophila*
Copper(II) oxide	O=[Cu].O=[Cu]	R10004002	M2652894	AUTO_8	training set	Inactive	*Tetrahymena thermophila*
Titanium	O=[Ti]=O.O=[Ti]=O	R2707661	M2645228	AUTO_2	training set	Inactive	*Vibrio fischeri*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R2707662	M2645228	AUTO_3	training set	Inactive	*Vibrio fischeri*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R9968661	M2645228	AUTO_10	training set	Inactive	*Vibrio fischeri*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R9997800	M2645228	AUTO_9	training set	Inactive	*Saccharomyces cerevisiae*
Silver	[Ag].[Ag]	R21027688	M2645220	AUTO_50	test set	Active	*Daphnia magna*
Silver, colloid	[Ag].[Ag]	R9728761	M2645220	AUTO_1	test set	Active	*Daphnia magna neonates*
Silver	[Ag].[Ag]	R21027877	M2645220	AUTO_250	test set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21027657	M2645220	AUTO_19	test set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21027703	M2645220	AUTO_67	test set	Active	*Daphnia galeata*
Silver	[Ag].[Ag]	R21027810	M2645220	AUTO_177	test set	Active	*Lemna minor*
Silver	[Ag].[Ag]	R21027738	M2645220	AUTO_102	test set	Active	*Pseudokirchneriella subcapitata*
Zinc oxide	O=[Zn].O=[Zn]	R9727614	M2652893	AUTO_2	test set	Active	*Pseudokirchneriella subcapitata*
Silver	[Ag].[Ag]	R21027885	M2645220	AUTO_258	test set	Active	*Pseudokirchneriella subcapitata*
Silver	[Ag].[Ag]	R9727599	M2645220	AUTO_1	test set	Active	*Daphnia magna, freshwater*
Zinc oxide	O=[Zn].O=[Zn]	R21027707	M2652893	AUTO_71	test set	Active	*Pseudokirchneriella subcapitata*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027676	M2652894	AUTO_38	test set	Active	*Daphnia magna*
Gold	[Au].[Au]	R18891661	M2660068	AUTO_5	test set	Active	*Zebrafish embryo*
Silver	[Ag].[Ag]	R21027704	M2645220	AUTO_68	test set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R2659285	M2645220	AUTO_5	test set	Active	*Chlamydomonas reinhardtii*
Silver	[Ag].[Ag]	R21027741	M2645220	AUTO_105	test set	Active	*Pseudokirchneriella subcapitata*
Gold	[Au].[Au]	R19004350	M2660068	AUTO_32	test set	Active	*Zebrafish*

							embryo
Silver	[Ag].[Ag]	R21027681	M2645220	AUTO_43	test set	Active	*Desmodesmus subspicatus*
Silver	[Ag].[Ag]	R21027684	M2645220	AUTO_46	test set	Active	*Vibrio fischeri*
Samarium oxide	O=[Sm]O[Sm]=O.O=[Sm]O[Sm]=O	R18891675	M3728215	AUTO_25	test set	Active	*Zebrafish embryo*
Zinc oxide	O=[Zn].O=[Zn]	R9889047	M2652893	AUTO_17	test set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R2659282	M2645220	AUTO_2	test set	Active	*Chlamydomonas reinhardtii*
Silver	[Ag].[Ag]	R21027762	M2645220	AUTO_129	test set	Active	*Caenorhabditis elegans*
cerium oxide	O=[Ce]=O.O=[Ce]=O	R21027785	M2659378	AUTO_152	test set	Active	*Pseudokirchneriella subcapitata*
Zinc oxide	O=[Zn].O=[Zn]	R9728760	M2652893	AUTO_4	test set	Active	*Daphnia magna*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R12572775	M2645228	AUTO_1	test set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21027888	M2645220	AUTO_261	test set	Active	*Danio rerio*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027900	M2652894	AUTO_274	test set	Active	*Saccharomyces cerevisiae*
Copper(II) oxide	O=[Cu].O=[Cu]	R12714721	M2652894	AUTO_9	test set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21027664	M2645220	AUTO_26	test set	Active	*Daphnia magna*
Copper(II) oxide	O=[Cu].O=[Cu]	R12714715	M2652894	AUTO_3	test set	Active	*Daphnia magna*
cerium oxide	O=[Ce]=O.O=[Ce]=O	R21027789	M2659378	AUTO_156	test set	Active	*Pseudokirchneriella subcapitata*
Copper(II) oxide	O=[Cu].O=[Cu]	R12714713	M2652894	AUTO_1	test set	Active	*Daphnia magna*
Copper(II) oxide	O=[Cu].O=[Cu]	R12714714	M2652894	AUTO_2	test set	Active	*Daphnia magna*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21027747	M2645228	AUTO_111	test set	Active	*Pseudokirchneriella subcapitata*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027674	M2652894	AUTO_36	test set	Active	*Daphnia magna*
Silver	[Ag].[Ag]	R21027698	M2645220	AUTO_62	test set	Active	*Escherichia coli*
Zinc oxide	O=[Zn].O=[Zn]	R9968653	M2652893	AUTO_2	test set	Active	*Vibrio fischeri*
Zinc oxide	O=[Zn].O=[Zn]	R9890175	M2652893	AUTO_6	test set	Active	*Daphnia magna*
cerium oxide	O=[Ce]=O.O=[Ce]=O	R21027724	M2659378	AUTO_88	test set	Active	*Pseudokirchneriella subcapitata*
Zinc oxide	O=[Zn].O=[Zn]	R9968652	M2652893	AUTO_1	test set	Active	*Vibrio fischeri*

Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21027648	M2645228	AUTO_9	test set	Active	*Bacillus licheniformis*
Zinc oxide	O=[Zn].O=[Zn]	R21027845	M2652893	AUTO_213	test set	Active	*Escherichia coli*
cerium oxide	O=[Ce]=O.O=[Ce]=O	R21027726	M2659378	AUTO_90	test set	Active	*Pseudokirchneriella subcapitata*
Zinc oxide	O=[Zn].O=[Zn]	R10003999	M2652893	AUTO_5	test set	Active	*Tetrahymena thermophila*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027837	M2652894	AUTO_205	test set	Active	*Escherichia coli*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R9728764	M2645228	AUTO_1	test set	Active	*Ceriodaphnia dubia, photoperiod*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21027643	M2645228	AUTO_4	test set	Active	*Ceriodaphnia dubia*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027838	M2652894	AUTO_206	test set	Active	*Escherichia coli*
cerium oxide	O=[Ce]=O.O=[Ce]=O	R9727306	M2659378	AUTO_113	test set	Inactive	*Pseudokirchneriella subcapitata*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R12572779	M2645228	AUTO_6	test set	Inactive	*Phaeodactylum tricornutum*
cerium oxide	O=[Ce]=O.O=[Ce]=O	R21027782	M2659378	AUTO_149	test set	Inactive	*Pseudokirchneriella subcapitata*
Zinc oxide	O=[Zn].O=[Zn]	R21027839	M2652893	AUTO_207	test set	Inactive	*Escherichia coli*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21027713	M2645228	AUTO_77	test set	Inactive	*Pseudokirchneriella subcapitata*
Silver	[Ag].[Ag]	R21027817	M2645220	AUTO_184	test set	Inactive	*Escherichia coli*
Silver	[Ag].[Ag]	R21027818	M2645220	AUTO_185	test set	Inactive	*Escherichia coli*
Zinc oxide	O=[Zn].O=[Zn]	R21027729	M2652893	AUTO_93	test set	Inactive	*Bacillus subtilis*
Zinc oxide	O=[Zn].O=[Zn]	R21027733	M2652893	AUTO_97	test set	Inactive	*Escherichia coli*
cerium oxide	O=[Ce]=O.O=[Ce]=O	R21027798	M2659378	AUTO_165	test set	Inactive	*Anabaena sp.*
cerium oxide	O=[Ce]=O.O=[Ce]=O	R21027784	M2659378	AUTO_151	test set	Inactive	*Pseudokirchneriella subcapitata*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R21027851	M2645228	AUTO_219	test set	Inactive	*Pseudokirchneriella subcapitata*
Silver	[Ag].[Ag]	R21027859	M2645220	AUTO_232	test set	Inactive	*Pseudomonas putida*
Iron(III) oxide	O=[Fe]O[Fe]=O.O=[Fe]O[Fe]=O	R21027898	M2652899	AUTO_272	test set	Inactive	*Danio rerio*
Silver	[Ag].[Ag]	R21027761	M2645220	AUTO_128	test set	Inactive	*Caenorhabditis*

							elegans
Silver	[Ag].[Ag]	R21027860	M2645220	AUTO_233	test set	Inactive	*Pseudomonas putida*
cerium oxide	O=[Ce]=O.O=[Ce]=O	R21027801	M2659378	AUTO_168	test set	Inactive	*Anabaena sp.*
Silver	[Ag].[Ag]	R21027823	M2645220	AUTO_191	test set	Inactive	*Escherichia coli*
Titanium	O=[Ti]=O.O=[Ti]=O	R2692104	M2645228	AUTO_8	test set	Inactive	*Desmodesmus subspicatus*
Zinc oxide	O=[Zn].O=[Zn]	R21027911	M2652893	AUTO_285	test set	Inactive	*Caenorhabditis elegans*
Copper(II) oxide	O=[Cu].O=[Cu]	R21027772	M2652894	AUTO_139	test set	Inactive	*Bacillus subtilis*
cerium oxide	O=[Ce]=O.O=[Ce]=O	R21027796	M2659378	AUTO_163	test set	Inactive	*Anabaena sp.*
Copper(II) oxide	O=[Cu].O=[Cu]	R9968659	M2652894	AUTO_8	test set	Inactive	*Vibrio fischeri*
Zinc oxide	O=[Zn].O=[Zn]	R21027775	M2652893	AUTO_142	test set	Inactive	*Bacillus subtilis*
Silver	[Ag].[Ag]	R21027864	M2645220	AUTO_237	test set	Inactive	*Pseudomonas putida*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R9728757	M2645228	AUTO_1	test set	Inactive	*Daphnia magna*
Zinc oxide	O=[Zn].O=[Zn]	R9866155	M2652893	AUTO_3	test set	Inactive	*Escherichia coli*
Nickel(II) oxide	O=[Ni].O=[Ni]	R9866162	M2652904	AUTO_10	test set	Inactive	*Streptococcus aureus*
Silver	[Ag].[Ag]	R21027866	M2645220	AUTO_239	test set	Inactive	*Pseudomonas putida*
Zinc oxide	O=[Zn].O=[Zn]	R9997793	M2652893	AUTO_2	test set	Inactive	*Saccharomyces cerevisiae*
Silver	[Ag].[Ag]	R21027869	M2645220	AUTO_242	test set	Inactive	*Pseudomonas putida*
Nickel(II) oxide	O=[Ni].O=[Ni]	R9866154	M2652904	AUTO_2	test set	Inactive	*Escherichia coli*
Copper(II) oxide	O=[Cu].O=[Cu]	R9848051	M2652894	AUTO_2	test set	Inactive	*Daphnia magna*
Copper(II) oxide	O=[Cu].O=[Cu]	R9968658	M2652894	AUTO_7	test set	Inactive	*Vibrio fischeri*
Iron(II,III)oxide	O=[Fe].O=[Fe].O=[Fe]O[Fe]=O.O=[Fe]O[Fe]=O	R21027678	M2659379	AUTO_40	test set	Inactive	*Vibrio fischeri*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R12572783	M2645228	AUTO_10	test set	Inactive	*Brachionus plicatilis*
Silver	[Ag].[Ag]	R21027686	M2645220	AUTO_48	test set	Inactive	*Vibrio fischeri*
Zinc oxide	O=[Zn].O=[Zn]	R21027910	M2652893	AUTO_284	test set	Inactive	*Caenorhabditis elegans*
Copper(II) oxide	O=[Cu].O=[Cu]	R9997795	M2652894	AUTO_4	test set	Inactive	*Saccharomyces cerevisiae*
Copper(II) oxide	O=[Cu].O=[Cu]	R2707700	M2652894	AUTO_41	test set	Inactive	*Vibrio fischeri*

	Titanium dioxide	O=[Ti]=O. O=[Ti]=O	R9997801	M2645228	AUTO_10	test set	Inactive	*Saccharomyces cerevisiae*

245

246

247 Table S9. Detailed information of the MIC data used for building nano-SARs

Information of nanoparticles in the Online Chemical Modeling Environment (OCHEM) platform					Sub-dataset	Classification (threshold value 10.0 mg/L)	Species tested
Material Nanoparticles of Elements	**SMILES**	**RECORDID in OCHEM**	**MOLECULEID in OCHEM**	**Identifier in article**			
Silver	[Ag].[Ag]	R21027989	M2645220	AUTO_49	training set	Active	*Nitrosomonas europaea*
Silver	[Ag].[Ag]	R2644427	M2645220	AUTO_4	training set	Active	*Escherichia coli CCM 3954*
Silver	[Ag].[Ag]	R2644428	M2645220	AUTO_5	training set	Active	*Pseudomonas aeruginosa CCM 3955*
Silver	[Ag].[Ag]	R2644429	M2645220	AUTO_6	training set	Active	*Pseudomonas aeruginosa*
Silver	[Ag].[Ag]	R2644431	M2645220	AUTO_8	training set	Active	*Staphylococcus epidermidis methicillin-resistant*
Silver	[Ag].[Ag]	R2644432	M2645220	AUTO_9	training set	Active	*Staphylococcus aureus MRSA*
Silver	[Ag].[Ag]	R2644450	M2645220	AUTO_27	training set	Active	*Staphylococcus epidermidis methicillin-susceptible*
Silver	[Ag].[Ag]	R2644425	M2645220	AUTO_2	training set	Active	*Enterococcus faecalis CCM 4224*
Silver	[Ag].[Ag]	R2644433	M2645220	AUTO_10	training set	Active	*Enterococcus faecium vancomycin-resistant*
Silver	[Ag].[Ag]	R2644434	M2645220	AUTO_11	training set	Active	*Klebsiella pneumoniae ESBL*
Silver	[Ag].[Ag]	R2644437	M2645220	AUTO_14	training set	Active	*Escherichia coli CCM 3954*
Silver	[Ag].[Ag]	R2644440	M2645220	AUTO_17	training set	Active	*Staphylococcus epidermidis methicillin-susceptible*
Silver	[Ag].[Ag]	R2644446	M2645220	AUTO_23	training set	Active	*Staphylococcus aureus CCM 3953*
Silver	[Ag].[Ag]	R2644447	M2645220	AUTO_24	training set	Active	*Escherichia*

							coli CCM 3954
Silver	[Ag].[Ag]	R2644448	M2645220	AUTO_25	training set	Active	*Pseudomonas aeruginosa CCM 3955*
Silver	[Ag].[Ag]	R2644451	M2645220	AUTO_28	training set	Active	*Staphylococcus epidermidis methicillin-resistant*
Silver	[Ag].[Ag]	R2644457	M2645220	AUTO_34	training set	Active	*Escherichia coli CCM 3954*
Silver	[Ag].[Ag]	R2644459	M2645220	AUTO_36	training set	Active	*Pseudomonas aeruginosa*
Silver	[Ag].[Ag]	R2644460	M2645220	AUTO_37	training set	Active	*Staphylococcus epidermidis methicillin-susceptible*
Silver	[Ag].[Ag]	R2644461	M2645220	AUTO_38	training set	Active	*Staphylococcus epidermidis methicillin-resistant*
Silver	[Ag].[Ag]	R2644469	M2645220	AUTO_46	training set	Active	*Pseudomonas aeruginosa*
Silver	[Ag].[Ag]	R2644470	M2645220	AUTO_47	training set	Active	*Staphylococcus epidermidis methicillin-susceptible*
Silver	[Ag].[Ag]	R2644471	M2645220	AUTO_48	training set	Active	*Staphylococcus epidermidis methicillin-resistant*
Silver	[Ag].[Ag]	R2644472	M2645220	AUTO_49	training set	Active	*Staphylococcus aureus MRSA*
Silver	[Ag].[Ag]	R2650100	M2645220	AUTO_21	training set	Active	*Staphylococcus epidermidis methicillin-resistant*
Silver	[Ag].[Ag]	R21027983	M2645220	AUTO_41	training set	Active	*Staphylococcus aureus*
Silver	[Ag].[Ag]	R21027972	M2645220	AUTO_26	training set	Active	*Salmonella sp.*
Silver	[Ag].[Ag]	R21027963	M2645220	AUTO_17	training set	Active	*Escherichia coli*
Silver	[Ag].[Ag]	R21027971	M2645220	AUTO_25	training set	Active	*Salmonella sp.*
Silver	[Ag].[Ag]	R21027984	M2645220	AUTO_42	training set	Active	*Staphylococcus aureus*
Silver	[Ag].[Ag]	R2644436	M2645220	AUTO_13	training set	Active	*Staphylococcus aureus*

							CCM 3953
Silver	[Ag].[Ag]	R2644438	M2645220	AUTO_15	training set	Active	*Pseudomonas aeruginosa CCM 3955*
Silver	[Ag].[Ag]	R2644442	M2645220	AUTO_19	training set	Active	*Staphylococcus aureus MRSA*
Silver	[Ag].[Ag]	R2644445	M2645220	AUTO_22	training set	Active	*Enterococcus faecalis CCM 4224*
Silver	[Ag].[Ag]	R2644449	M2645220	AUTO_26	training set	Active	*Pseudomonas aeruginosa*
Silver	[Ag].[Ag]	R2644453	M2645220	AUTO_30	training set	Active	*Enterococcus faecium vancomycin-resistant*
Silver	[Ag].[Ag]	R2644458	M2645220	AUTO_35	training set	Active	*Pseudomonas aeruginosa CCM 3955*
Silver	[Ag].[Ag]	R2644462	M2645220	AUTO_39	training set	Active	*Staphylococcus aureus MRSA*
Silver	[Ag].[Ag]	R2644463	M2645220	AUTO_40	training set	Active	*Enterococcus faecium vancomycin-resistant*
Silver	[Ag].[Ag]	R2644464	M2645220	AUTO_41	training set	Active	*Klebsiella pneumoniae ESBL*
Silver	[Ag].[Ag]	R2644467	M2645220	AUTO_44	training set	Active	*Escherichia coli CCM 3954*
Silver	[Ag].[Ag]	R2644473	M2645220	AUTO_50	training set	Active	*Enterococcus faecium vancomycin-resistant*
Silver	[Ag].[Ag]	R2650096	M2645220	AUTO_17	training set	Active	*Escherichia coli CCM 3954*
Silver	[Ag].[Ag]	R2650098	M2645220	AUTO_19	training set	Active	*Pseudomonas aeruginosa*
Silver	[Ag].[Ag]	R21027953	M2645220	AUTO_6	training set	Active	*Escherichia coli*
Silver	[Ag].[Ag]	R21027954	M2645220	AUTO_7	training set	Active	*Escherichia coli*
Silver	[Ag].[Ag]	R21027962	M2645220	AUTO_15	training set	Active	*Escherichia coli*
Silver	[Ag].[Ag]	R21027964	M2645220	AUTO_18	training set	Active	*Escherichia coli*
Silver	[Ag].[Ag]	R21027975	M2645220	AUTO_29	training set	Active	*Staphylococcus aureus*
Silver	[Ag].[Ag]	R21027982	M2645220	AUTO_39	training set	Active	*Staphylococcus aureus*
Silver	[Ag].[Ag]	R21027990	M2645220	AUTO_50	training set	Active	*Pseudomonas stutzeri*

Iron	[Fe].[Fe]	R21027949	M84326991	AUTO_1	training set	Active	*Escherichia coli*
Silver	[Ag].[Ag]	R21027981	M2645220	AUTO_37	training set	Active	*Staphylococcus aureus*
Silver	[Ag].[Ag]	R2644435	M2645220	AUTO_12	training set	Active	*Enterococcus faecalis CCM 4224*
Silver	[Ag].[Ag]	R2644443	M2645220	AUTO_20	training set	Active	*Enterococcus faecium vancomycin-resistant*
Silver	[Ag].[Ag]	R2644444	M2645220	AUTO_21	training set	Active	*Klebsiella pneumoniae ESBL*
Silver	[Ag].[Ag]	R2644455	M2645220	AUTO_32	training set	Active	*Enterococcus faecalis CCM 4224*
Silver	[Ag].[Ag]	R2644465	M2645220	AUTO_42	training set	Active	*Enterococcus faecalis CCM 4224*
Silver	[Ag].[Ag]	R2644474	M2645220	AUTO_51	training set	Active	*Klebsiella pneumoniae ESBL*
Silver	[Ag].[Ag]	R2650081	M2645220	AUTO_2	training set	Active	*Staphylococcus aureus CCM 3953*
Silver	[Ag].[Ag]	R2650091	M2645220	AUTO_12	training set	Active	*Staphylococcus epidermidis methicillin-susceptible*
Silver	[Ag].[Ag]	R2650095	M2645220	AUTO_16	training set	Active	*Staphylococcus aureus CCM 3953*
Silver	[Ag].[Ag]	R2650097	M2645220	AUTO_18	training set	Active	*Pseudomonas aeruginosa CCM 3955*
Silver	[Ag].[Ag]	R2650101	M2645220	AUTO_22	training set	Active	*Staphylococcus aureus MRSA*
Silver	[Ag].[Ag]	R2650105	M2645220	AUTO_26	training set	Active	*Staphylococcus aureus CCM 3953*
Silver	[Ag].[Ag]	R2650109	M2645220	AUTO_30	training set	Active	*Staphylococcus epidermidis methicillin-susceptible*
Silver	[Ag].[Ag]	R2650110	M2645220	AUTO_31	training set	Active	*Staphylococcus epidermidis methicillin-resistant*
Silver	[Ag].[Ag]	R21028005	M2645220	AUTO_65	training set	Active	*Staphylococcus aureus*
Silver	[Ag].[Ag]	R21028008	M2645220	AUTO_69	training set	Active	*Staphylococcus aureus*
Silver	[Ag].[Ag]	R21027960	M2645220	AUTO_13	training set	Active	*Escherichia coli*

Silver	[Ag].[Ag]	R21027988	M2645220	AUTO_48	training set	Inactive	*Azotobacter vinelandii*
Silver	[Ag].[Ag]	R21027985	M2645220	AUTO_43	training set	Inactive	*Enterococcus faecalis*
Silver	[Ag].[Ag]	R21027992	M2645220	AUTO_52	training set	Inactive	*Neisseria gonorrhoeae*
Silver	[Ag].[Ag]	R2650084	M2645220	AUTO_5	training set	Inactive	*Pseudomonas aeruginosa*
Silver	[Ag].[Ag]	R2650085	M2645220	AUTO_6	training set	Inactive	*Staphylococcus epidermidis methicillin-susceptible*
Silver	[Ag].[Ag]	R2650094	M2645220	AUTO_15	training set	Inactive	*Enterococcus faecalis CCM 4224*
Silver	[Ag].[Ag]	R2650107	M2645220	AUTO_28	training set	Inactive	*Pseudomonas aeruginosa CCM 3955*
Silver	[Ag].[Ag]	R2650108	M2645220	AUTO_29	training set	Inactive	*Pseudomonas aeruginosa*
Silver	[Ag].[Ag]	R21028000	M2645220	AUTO_60	training set	Inactive	*Enterococcus faecalis*
Copper	[Cu].[Cu]	R21028012	M2655006	AUTO_74	training set	Inactive	*Bacillus subtilis*
Silver	[Ag].[Ag]	R2650083	M2645220	AUTO_4	training set	Inactive	*Pseudomonas aeruginosa CCM 3955*
Silver	[Ag].[Ag]	R2650087	M2645220	AUTO_8	training set	Inactive	*Staphylococcus aureus MRSA*
Silver	[Ag].[Ag]	R2650088	M2645220	AUTO_9	training set	Inactive	*Klebsiella pneumoniae (ESBL-positive)*
Silver	[Ag].[Ag]	R2650090	M2645220	AUTO_11	training set	Inactive	*Pseudomonas aeruginosa*
Silver	[Ag].[Ag]	R2650111	M2645220	AUTO_32	training set	Inactive	*Staphylococcus aureus MRSA*
Silver	[Ag].[Ag]	R21028003	M2645220	AUTO_63	training set	Inactive	*Escherichia coli*
Silver	[Ag].[Ag]	R21028004	M2645220	AUTO_64	training set	Inactive	*Escherichia coli*
Silver	[Ag].[Ag]	R21028007	M2645220	AUTO_68	training set	Inactive	*Staphylococcus aureus*
Zinc oxide	O=[Zn].O=[Zn]	R21027987	M2652893	AUTO_47	training set	Inactive	*Sinorhizobium meliloti*
Silver	[Ag].[Ag]	R21028011	M2645220	AUTO_73	training set	Inactive	*Bacillus subtilis*
Silver	[Ag].[Ag]	R21028013	M2645220	AUTO_75	training set	Inactive	*Escherichia coli*
Silver	[Ag].[Ag]	R21027986	M2645220	AUTO_44	training set	Inactive	*Enterococc*

							us faecalis
Silver	[Ag].[Ag]	R2650092	M2645220	AUTO_13	training set	Inactive	*Staphylococcus epidermidis methicillin-resistant*
Silver	[Ag].[Ag]	R2650093	M2645220	AUTO_14	training set	Inactive	*Staphylococcus aureus MRSA*
Silver	[Ag].[Ag]	R2650104	M2645220	AUTO_25	training set	Inactive	*Enterococcus faecalis CCM 4224*
Silver	[Ag].[Ag]	R2650112	M2645220	AUTO_33	training set	Inactive	*Enterococcus faecium (VRE)*
Silver	[Ag].[Ag]	R21028001	M2645220	AUTO_61	training set	Inactive	*Enterococcus faecalis*
Silver	[Ag].[Ag]	R21028010	M2645220	AUTO_71	training set	Inactive	*Staphylococcus aureus*
Silver	[Ag].[Ag]	R21027955	M2645220	AUTO_8	training set	Inactive	*Escherichia coli*
Silver	[Ag].[Ag]	R21027966	M2645220	AUTO_20	training set	Inactive	*Salmonella sp.*
Iron	[Fe].[Fe]	R21027950	M84326991	AUTO_3	training set	Inactive	*Escherichia coli*
Silver	[Ag].[Ag]	R21028014	M2645220	AUTO_76	training set	Inactive	*Escherichia coli*
Silver	[Ag].[Ag]	R21028021	M2645220	AUTO_83	training set	Inactive	*Staphylococcus aureus*
Zinc oxide	O=[Zn].O=[Zn]	R21027999	M2652893	AUTO_59	training set	Inactive	*Staphylococcus aureus*
Silver	[Ag].[Ag]	R21028015	M2645220	AUTO_77	training set	Inactive	*Escherichia coli*
Copper	[Cu].[Cu]	R21028017	M2655006	AUTO_79	training set	Inactive	*Escherichia coli*
Copper	[Cu].[Cu]	R21028022	M2655006	AUTO_86	training set	Inactive	*Staphylococcus aureus*
Silver	[Ag].[Ag]	R21028016	M2645220	AUTO_78	training set	Inactive	*Escherichia coli*
Silver	[Ag].[Ag]	R21027969	M2645220	AUTO_23	training set	Inactive	*Salmonella sp.*
Silver	[Ag].[Ag]	R21027973	M2645220	AUTO_27	training set	Inactive	*Staphylococcus aureus*
Zinc oxide	O=[Zn].O=[Zn]	R2707679	M2652893	AUTO_20	training set	Inactive	*Vibrio fischeri*
Copper(II) oxide	O=[Cu].O=[Cu]	R2707710	M2652894	AUTO_51	training set	Inactive	*Vibrio fischeri*
Copper	[Cu].[Cu]	R21028018	M2655006	AUTO_80	training set	Inactive	*Escherichia coli*
Zinc oxide	O=[Zn].O=[Zn]	R21028025	M2652893	AUTO_91	training set	Inactive	*Vibrio fischeri*
Copper	[Cu].[Cu]	R21028019	M2655006	AUTO_81	training set	Inactive	*Escherichia coli*
Copper	[Cu].[Cu]	R21027994	M2655006	AUTO_54	training set	Inactive	*Escherichia coli*
Silver	[Ag].[Ag]	R21027976	M2645220	AUTO_31	training set	Inactive	*Staphylococcus aureus*
Silver	[Ag].[Ag]	R21027979	M2645220	AUTO_35	training set	Inactive	*Staphylococcus aureus*

Copper	[Cu].[Cu]	R21028020	M2655006	AUTO_82	training set	Inactive	*Escherichia coli*
Silver	[Ag].[Ag]	R21027956	M2645220	AUTO_9	training set	Inactive	*Escherichia coli*
Copper	[Cu].[Cu]	R21027995	M2655006	AUTO_55	training set	Inactive	*Escherichia coli*
Copper	[Cu].[Cu]	R21027996	M2655006	AUTO_56	training set	Inactive	*Escherichia coli*
Silver	[Ag].[Ag]	R21027957	M2645220	AUTO_10	training set	Inactive	*Escherichia coli*
Silver	[Ag].[Ag]	R21027961	M2645220	AUTO_14	training set	Inactive	*Escherichia coli*
Silver	[Ag].[Ag]	R21027977	M2645220	AUTO_32	training set	Inactive	*Staphylococcus aureus*
Silver	[Ag].[Ag]	R21027978	M2645220	AUTO_33	training set	Inactive	*Staphylococcus aureus*
Silver	[Ag].[Ag]	R21027980	M2645220	AUTO_36	training set	Inactive	*Staphylococcus aureus*
Zinc oxide	O=[Zn].O=[Zn]	R21027997	M2652893	AUTO_57	training set	Inactive	*Escherichia coli*
Iron	[Fe].[Fe]	R21027952	M84326991	AUTO_5	training set	Inactive	*Escherichia coli*
Iron(II,III)oxide	O=[Fe].O=[Fe].O=[Fe]O[Fe]=O.O=[Fe]O[Fe]=O	R21028023	M2659379	AUTO_89	training set	Inactive	*Escherichia coli*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R2707665	M2645228	AUTO_6	training set	Inactive	*Vibrio fischeri*
Titanium dioxide	O=[Ti]=O.O=[Ti]=O	R2707666	M2645228	AUTO_7	training set	Inactive	*Vibrio fischeri*
Copper(II) oxide	O=[Cu].O=[Cu]	R21028024	M2652894	AUTO_90	training set	Inactive	*Vibrio fischeri*
Silver	[Ag].[Ag]	R2644430	M2645220	AUTO_7	test set	Active	*Staphylococcus epidermidis methicillin-susceptible*
Silver	[Ag].[Ag]	R2644426	M2645220	AUTO_3	test set	Active	*Staphylococcus aureus CCM 3953*
Silver	[Ag].[Ag]	R2644441	M2645220	AUTO_18	test set	Active	*Staphylococcus epidermidis methicillin-resistant*
Silver	[Ag].[Ag]	R2644452	M2645220	AUTO_29	test set	Active	*Staphylococcus aureus MRSA*
Silver	[Ag].[Ag]	R2644468	M2645220	AUTO_45	test set	Active	*Pseudomonas aeruginosa CCM 3955*
Silver	[Ag].[Ag]	R2650099	M2645220	AUTO_20	test set	Active	*Staphylococcus epidermidis methicillin-susceptible*
Silver	[Ag].[Ag]	R21027965	M2645220	AUTO_19	test set	Active	*Salmonella*

							sp.
Silver	[Ag].[Ag]	R2644439	M2645220	AUTO_16	test set	Active	*Pseudomonas aeruginosa*
Silver	[Ag].[Ag]	R2644456	M2645220	AUTO_33	test set	Active	*Staphylococcus aureus CCM 3953*
Silver	[Ag].[Ag]	R2644466	M2645220	AUTO_43	test set	Active	*Staphylococcus aureus CCM 3953*
Silver	[Ag].[Ag]	R21028002	M2645220	AUTO_62	test set	Active	*Escherichia coli*
Silver	[Ag].[Ag]	R21027970	M2645220	AUTO_24	test set	Active	*Salmonella sp.*
Silver	[Ag].[Ag]	R21027959	M2645220	AUTO_12	test set	Active	*Escherichia coli*
Silver	[Ag].[Ag]	R2644454	M2645220	AUTO_31	test set	Active	*Klebsiella pneumoniae ESBL*
Silver	[Ag].[Ag]	R2650086	M2645220	AUTO_7	test set	Active	*Staphylococcus epidermidis methicillin-resistant*
Silver	[Ag].[Ag]	R2650103	M2645220	AUTO_24	test set	Active	*Klebsiella pneumoniae (ESBL-positive)*
Silver	[Ag].[Ag]	R21028006	M2645220	AUTO_67	test set	Active	*Staphylococcus aureus*
Silver	[Ag].[Ag]	R21027991	M2645220	AUTO_51	test set	Inactive	*Neisseria gonorrhoeae*
Silver	[Ag].[Ag]	R2650102	M2645220	AUTO_23	test set	Inactive	*Enterococcus faecium (VRE)*
Silver	[Ag].[Ag]	R2650082	M2645220	AUTO_3	test set	Inactive	*Escherichia coli CCM 3954*
Silver	[Ag].[Ag]	R2650106	M2645220	AUTO_27	test set	Inactive	*Escherichia coli CCM 3954*
Silver	[Ag].[Ag]	R21028009	M2645220	AUTO_70	test set	Inactive	*Staphylococcus aureus*
Silver	[Ag].[Ag]	R2650089	M2645220	AUTO_10	test set	Inactive	*Staphylococcus aureus CCM 3953*
Silver	[Ag].[Ag]	R2650113	M2645220	AUTO_34	test set	Inactive	*Klebsiella pneumoniae (ESBL-positive)*
Zinc oxide	O=[Zn].O=[Zn]	R2707680	M2652893	AUTO_21	test set	Inactive	*Vibrio fischeri*
Iron	[Fe].[Fe]	R21027951	M84326991	AUTO_4	test set	Inactive	*Escherichia coli*
Silver	[Ag].[Ag]	R21027958	M2645220	AUTO_11	test set	Inactive	*Escherichia coli*
Copper	[Cu].[Cu]	R21027993	M2655006	AUTO_53	test set	Inactive	*Escherichia coli*

Silver	[Ag].[Ag]	R21027974	M2645220	AUTO_28	test set	Inactive	*Staphylococcus aureus*
Silver	[Ag].[Ag]	R21027967	M2645220	AUTO_21	test set	Inactive	*Salmonella sp.*
Silver	[Ag].[Ag]	R21027968	M2645220	AUTO_22	test set	Inactive	*Salmonella sp.*
Zinc oxide	O=[Zn].O=[Zn]	R21027998	M2652893	AUTO_58	test set	Inactive	*Pseudomonas aeruginosa*
Copper(II) oxide	O=[Cu].O=[Cu]	R2707709	M2652894	AUTO_50	test set	Inactive	*Vibrio fischeri*

248