| Endpoint                                      | <b>Genotoxicity</b><br>in vitro comet assay   |  |  |       |
|---|---|--|--|-------|
| <b>Endpoint description</b>                   | Genotoxicity – genotoxic effect in mammalian cell lines<br>using comet assay performed according to scientifical<br>including those described in Collins, A., Møller, P., Gajski,<br>with the comet assay: a compendium of protocols. Nat   |  |  |       |
| Nanoform                                      | TiO <sub>2</sub>  |  |  |       |
| Data quality control                          | The QSAR model utilizes extracted literature data subje<br>the evaluation of: i) relevance of the test material, ii) re<br>and iii) relevance of genotoxicity studies.  |  |  |       |
| Type of model                                 | L-PCA + KNN   |  |  |       |
| Descriptors                                   | The model includes descriptors of nanoform physicoch<br>line characteristics.   |  |  |       |
| Dataset                                       | positive<br>negative  | <b>training set</b><br>69<br>19                                  | <b>validation set</b><br>18<br>5                                   | total |
| Statistics                                    | accuracy<br>precision<br>recall<br>F1 score<br>MCC  | <b>training set</b><br>0.977<br>1.000<br>0.971<br>0.985<br>0.937 | <b>validation set</b><br>0.870<br>0.895<br>0.944<br>0.919<br>0.592 |       |
| Inclusion criteria to<br>applicability domain | Chemical composition of nanoform: ' $TiO_2$ '<br>Shape of nanoform: 'spherical'<br>Crystal structure: 'anatase' OR 'rutile' OR 'anatase+rutile'<br>Surface area, value up to: 343.7<br>Minimum particle size, range: $3.9 - 142.0$<br>Mean particle size, range: $3.9 - 280.0$<br>Maximum particle size, range: $4.0 - 400.0$ |  |  |       |
|   |   |  |  |       |

nes treated in vitro with TiO<sub>2</sub> nanoforms, cally valid, recognized protocols, ski, G. et al. Measuring DNA modifications at Protoc 18, 929–989 (2023).

jected to a quality control including reliability of genotoxicity studies,

chemical characteristics and cell

| <b>Genotoxicity</b><br>in vitro comet assay   |  |   |  |
|---|--|---|--|
| Genotoxicity – genotoxic effect in mammalian cell line<br>using comet assay performed according to scientifica<br>including those described in Collins, A., Møller, P., Gajski<br>with the comet assay: a compendium of protocols. Nat                          |  |   |  |
| SiO <sub>2</sub>  |  |   |  |
| The QSAR model utilizes extracted literature data subject<br>the evaluation of: i) relevance of the test material, ii) re<br>and iii) relevance of genotoxicity studies.  |  |   |  |
| L-PCA + Decision tree   |  |   |  |
| The model includes descriptors of nanoform physicoch<br>line characteristics.   |  |   |  |
| positive<br>negative  | <b>training set</b><br>34<br>18  | <b>validation set</b><br>9<br>4   | <b>tota</b><br>65  |
| accuracy<br>precision<br>recall<br>F1 score<br>MCC  | <b>training set</b><br>0.865<br>0.966<br>0.824<br>0.889<br>0.736   | <b>validation set</b><br>0.769<br>0.800<br>0.889<br>0.842<br>0.426  |  |
| Chemical composition of nanoform: 'SiO <sub>2</sub> '<br>Shape of nanoform: 'spherical'<br>Surface area, value up to: 450.0<br>Minimum particle size, range: 5.0 - 166.1<br>Mean particle size, range: 6.0 - 169.2<br>Maximum particle size, range: 6.0 - 172.3 |  |   |  |
|   | in vitro com<br>Genotoxicity<br>using come<br>including th<br>with the cor<br>SiO <sub>2</sub><br>The QSAR m<br>the evaluati<br>and iii) relevant<br>L-PCA + Dea<br>The model i<br>line charact<br><b>positive</b><br><b>negative</b><br><b>accuracy</b><br><b>precision</b><br><b>recall</b><br><b>F1 score</b><br><b>MCC</b> | in vitro comet assay<br>Genotoxicity – genotoxic eff<br>using comet assay perform<br>including those described ir<br>with the comet assay: a cor<br>SiO <sub>2</sub><br>The QSAR model utilizes extra<br>the evaluation of: i) relevand<br>and iii) relevance of genoto<br>L-PCA + Decision tree<br>The model includes description<br>line characteristics.<br><b>training set</b><br><b>positive</b> 34<br><b>negative</b> 18<br><b>training set</b><br><b>accuracy</b> 0.865<br><b>precision</b> 0.966<br><b>recall</b> 0.824<br><b>FI score</b> 0.889<br><b>MCC</b> 0.736<br>Chemical composition of name<br>Shape of nanoform: 'spherical<br>Surface area, value up to: 450 | in vitro comet assay<br>Genotoxicity – genotoxic effect in mammalian<br>using comet assay performed according to so<br>including those described in Collins, A., Møller, I<br>with the comet assay: a compendium of proto<br>SiO <sub>2</sub><br>The QSAR model utilizes extracted literature do<br>the evaluation of: i) relevance of the test mate<br>and iii) relevance of genotoxicity studies.<br>L-PCA + Decision tree<br>The model includes descriptors of nanoform p<br>line characteristics.<br><b>training set</b> validation set<br><b>positive</b> 34 9<br><b>negative</b> 18 4<br><b>training set</b> validation set<br>accuracy 0.865 0.769<br><b>precision</b> 0.966 0.800<br><b>recall</b> 0.824 0.889<br>Fl score 0.889 0.842<br>MCC 0.736 0.426<br>Chemical composition of nanoform: 'SiO <sub>2</sub> '<br>Shape of nanoform: 'spherical'<br>Surface area, value up to: 450.0 |

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