

Endpoint	Mutagenicity in vitro micronucleus test		
Endpoint description	Mutagenicity - mutagenic effect in mammalian cell lines treated in vitro with TiO ₂ nanoforms, using micronucleus test performed according to scientifically valid, recognized protocols, including OECD TG 487.		
Nanoform	TiO ₂		
Data quality control	The QSAR model utilizes extracted literature data subjected to a quality control including the evaluation of: i) relevance of the test material, ii) reliability of genotoxicity studies, and iii) relevance of genotoxicity studies.		
Type of model	L-PCA + kNN		
Descriptors	The model includes descriptors of nanoform physicochemical characteristics and cell line characteristics.		
Dataset		training set	validation set
	positive	19	5
	negative	26	7
			total
			57
Statistics		training set	validation set
	accuracy	0.822	0.750
	precision	0.867	0.750
	recall	0.684	0.600
	F1 score	0.765	0.667
	MCC	0.636	0.478
Inclusion criteria to applicability domain	Chemical composition of nanoform: 'TiO ₂ ' Shape of nanoform: 'spherical' Crystal structure: 'anatase' OR 'rutile' OR 'anatase+rutile' Surface area, value up to: 220.0 Minimum particle size, range: 5.0 - 90.0 Mean particle size, range: 6.2 - 110.0 Maximum particle size, range: 6.2- 262.0		

Endpoint	Mutagenicity in vitro micronucleus test		
Endpoint description	Mutagenicity – mutagenic effect in mammalian cell lines treated in vitro with SiO ₂ nanoforms, using micronucleus test performed according to scientifically valid, recognized protocols, including OECD TG 487.		
Nanoform	SiO ₂		
Data quality control	The QSAR model utilizes extracted literature data subjected to a quality control including the evaluation of: i) relevance of the test material, ii) reliability of genotoxicity studies, and iii) relevance of genotoxicity studies.		
Type of model	L-PCA + SVM		
Descriptors	The model includes descriptors of nanoform physicochemical characteristics and cell line characteristics.		
Dataset		training set	validation set
	positive	7	3
	negative	12	6
			total
			28
Statistics		training set	validation set
	accuracy	0.895	0.778
	precision	0.857	0.667
	recall	0.857	0.667
	F1 score	0.857	0.677
	MCC	0.774	0.5
Inclusion criteria to applicability domain	Chemical composition of nanoform: 'SiO ₂ ' Shape of nanoform: 'spherical' Surface area, value up to: 183.0 Minimum particle size, range: 5.0 – 224.8 Mean particle size, range: 6.0 – 200.0 Maximum particle size, range: 6.0 – 200.0		