

QMR Number	Title	Keywords	Endpoint 1	Endpoint 2
Q2-10-1-136	QSAR for acute toxicity to fish (Danio rerio)	acute toxicity, fish, Danio rerio, QSARModel 3.3.8, LC50, Molcode	3. Ecotoxic effects	3. 3. Acute toxicity to fish (lethality)
Q2-10-6-83	QSAR for mutagenicity (Salmonella typhimurium TA98 strain)	mutagenicity, Salmonella typhimurium, TA98, Molcode	4. Human Health Effects	4.10. Mutagenicity
Q2-10-14-119	QSAR for honey bee acute contact toxicity (ester derivatives)	honey bee acute contact toxicity, ester derivatives, QSARModel 3.5.0	3.Ecotoxic effects	3.13.b.Toxicity to honeybees. Acute contact toxicity
Q2-10-14-174	QSAR for acute toxicity to fathead minnow	acute toxicity, fathead minnow, Molcode	3.Ecotoxic effects	3.3.Acute toxicity to fish (lethality)
Q2-10-25-177	QSAR for human serum albumin binding	Molcode, immobilized albumin, Toxicokinetics	5.Toxicokinetics	5.9.Toxicokinetics.Protein-binding
Q2-10-25-184	QSAR for blood-brain barrier (BBB) partitioning	Molcode, blood-brain barrier partitioning, rat, Toxicokinetics	5.Toxicokinetics	5.4.Toxicokinetics.Blood-brain barrier penetration
Q2-10-26-179	QSAR for soil adsorption coefficient Koc	Molcode, ecotoxic effects, adsorption, desorption, multilinear regression QSAR	2.Environmental fate parameters	2.6.Partition coefficient. Organic carbon-adsorption partition coefficient (organic carbon: Koc)
Q2-15-8-108	QSAR for skin sensitisation via Schiff base formation	skin sensitisation, LLNA, EC3, Schiff base	4.Human Health Effects	4.6.Skin sensitisation
Q2-17-11-126	QSAR for acute toxicity to Pimephales promelas (Fathead Minnow)	QSAR, fathead minnow, Pimephales promelas, acute toxicity	3.3.Acute toxicity to fish (lethality)	203Fish, Acute Toxicity Test
Q2-17-16-140	QSAR for bioconcentration factor in fish	BCF, bioconcentration factor, fish	2.Environmental fate parameters	2.4.a.Bioconcentration . BCF fish
Q2-18-14-144	QSAR for honey bee acute contact toxicity (amide derivatives)	honey bee, acute contact toxicity, Molcode	3.Ecotoxic effects	3.13.b.Toxicity to honeybees. Acute contact toxicity
Q2-22-1-135	QSAR for eye irritation (Draize test)	eye irritation, Draize eye test, MMAS, Molcode	4.Human Health Effects	4.9.Eye irritation/corrosion
Q7-17-11-112	QSAR for the Global Half-Life Index (GHLI) of Persistent Organic Pollutants (POPs)	GHLI, MOBYDIGS, Persistence Global Half-Life Index, DRAGON	2.Environmental fate parameters	2.2.b.Persistence: Abiotic degradation in air (Phototransformation). Indirect photolysis (OH-radical reaction, ozone-radical reaction, other)

Q8-10-1-309	QSAR for toxicity to activated sludge	Molcode, activated sludge, bacterial respiration inhibition, biodegradation, Shk1, wastewater	3.Ecotoxic effects	3.6.Microbial inhibition (activated sludge respiration inhibition, inhibition of nitrification. other)
Q8-10-13-121	QSAR for honey bee acute contact toxicity (amine derivatives)	Honeybees acute contact toxicity, QSARModel 3.5.0, amine derivatives	3.Ecotoxic effects	3.13.b.Toxicity to honeybees. Acute contact toxicity
Q8-10-14-150	QSAR for acute toxicity to rainbow trout	Molcode, acute fish toxicity, rainbow trout	3.Ecotoxic effects	3.3.Acute toxicity to fish (lethality)
Q8-10-14-153	QSAR for female rat carcinogenicity (TD50) of nitro compounds	Molcode, female rat carcinogenicity, TD50	4.Human Health Effects	4.12. Carcinogenicity
Q8-10-14-169	QSAR for honey bee acute contact toxicity (ether derivatives not containing amide groups)	Molcode, honey bee, acute contact toxicity	3.Ecotoxic effects	3.13.b.Toxicity to honeybees. Acute contact toxicity
Q8-10-14-171	QSAR for Relative Binding Affinity to Estrogen Receptor	Molcode, rat uterine cytosol, estrogen receptor binding	4.Human Health Effects	4.18.a.Endocrine Activity. Receptor-binding (specify receptor)
Q8-10-14-175	QSAR for bioconcentration (flow through fish test) of pesticides	BCF, bioconcentration, flow through test, bluegill, Molcode	2.Environmental fate parameters	2.4.a.Bioconcentration . BCF fish
Q8-10-14-176	QSAR for acute oral toxicity (in vitro)	Molcode, acute oral toxicity, cytotoxicity	4. 2. Acute Oral toxicity	OECD 420 Acute Oral Toxicity-Fixed Dose Method, OECD 423 Acute Oral Toxicity - Acute Toxic Class Method
Q8-10-14-207	QSAR for the bioconcentration factor of non-ionic organic compounds	Molcode, bioconcentration factors, nonionic organic compounds, rainbow trout, guppies, fathead minnow, bluegill	2.Environmental fate parameters	2.4.a.Bioconcentration . BCF fish
Q8-10-24-173	QSAR for bioconcentration (flow-through fish test) of polychlorinated biphenyls	BCF, bioconcentration, flow through test, fish, Molcode	2.Environmental fate parameters	2.4.a.Bioconcentration . BCF fish
Q8-10-27-209	QSAR for acute toxicity to algae	Molcode, Toxicity to algae, Benzene derivatives, Chlorella vulgaris	3.Ecotoxic effects	3.2.Short-term toxicity to algae (inhibition of the exponential growth rate)
Q8-10-28-208	QSAR for algae toxicity of benzene derivatives	Molcode, algae toxicity of benzene derivatives, Chlorella vulgaris	3.Ecotoxic effects	3.2.Short-term toxicity to algae (inhibition of the exponential growth rate)

Q8-10-29-220	QSAR for acute oral toxicity of benzene derivatives - Acute Toxic Class Method	acute oral toxicity, benzene derivatives, Molcode, Acute Toxic Class Method, Rat	4.Human Health Effects	4.2.Acute Oral toxicity
Q8-10-30-221	QSAR for abiotic degradation in air (OH tropospheric degradation of volatile organic compounds)	Molcode, abiotic degradation in air, OH tropospheric degradation, volatile organic compounds	2.Environmental fate parameters	2.2.b.Persistence: Abiotic degradation in air (Phototransformation). Indirect photolysis (OH-radical reaction, ozone-radical reaction, other)
Q8-10-30-222	QSAR for abiotic degradation in air (NO ₃ radical reaction of volatile organic compounds)	Molcode, abiotic degradation in air, NO ₃ radical reaction, volatile organic compounds	2.Environmental fate parameters	2.2.b.Persistence: Abiotic degradation in air (Phototransformation). Indirect photolysis (OH-radical reaction, ozone-radical reaction, other)
Q8-10-30-224	QSAR for abiotic degradation in air (O ₃ radical reaction of volatile organic compounds)	Molcode, abiotic degradation in air, O ₃ radical reaction, volatile organic compounds	2.Environmental fate parameters	2.2.b.Persistence: Abiotic degradation in air (Phototransformation). Indirect photolysis (O ₃ -radical reaction)
Q8-10-30-265	QSAR for persistence: abiotic degradation in water	Molcode, Persistence, Abiotic degradation, water	2.Environmental fate parameters	2.1.c.Persistence: Abiotic degradation in water. Other
Q8-10-30-266	QSAR for persistence: abiotic degradation in air	Molcode, Persistence, Abiotic degradation, air, Biodegradation	2.Environmental fate parameters	2.2.a.Persistence: Abiotic degradation in air
Q8-10-30-288	QSAR for rat chronic LOAEL	Molcode, Rat, chronic LOAEL, Multilinear regression	4.Human Health Effects	4.14.Repeated dose toxicity
Q8-26-8-155	QSAR for haloacetic acid mutagenicity	Ames mutagenicity, TOPS-MODE, haloacetic acid	4.Human Health Effects	4.10.Mutagenicity
Q8-29-23-53	Catalogic QSAR for aquatic toxicity	Catalogic, basesurface narcosis, aquatic toxicity, Daphnia Magna	3.Ecotoxic effects	3.1.Short-term toxicity to Daphnia (immobilisation)
Q9-21-18-132	Catalogic Hybrid Expert System for biodegradation	Catalogic, expert system, biodegradation, BOD, MITI database, University of Minnesota Biocatalysis/Biodegradation database	2.3.a.Persistence: Biodegradation. Ready/not ready biodegradability	301Ready Biodegradability
Q10-23-19-143	Nonlinear QSAR: artificial neural network for acute aquatic toxicity	ANNE, neural network, acute fish toxicity, Pimephales Promelas, fathead minnow	3.Ecotoxic effects	3.3.Acute toxicity to fish (lethality)

Q11-25-20-154	TOPKAT NTP Rodent Carcinogenicity Model (Female Mouse)	Accelrys, TOPKAT, OPS, female mouse carcinogenicity	4.Human Health Effects	4.12.Carcinogenicity
Q13-33-36-312	Derek for Windows - Mutagenicity	Lhasa, Derek for Windows, Ames, mutagenicity	4.Human Health Effects	4.10.Mutagenicity
Q13-33-36-314	Derek for Windows - Carcinogenicity	Lhasa Limited, Carcinogenicity, Derek for Windows, mammal, rat and mouse	4.Human Health Effects	4.12.Carcinogenicity
Q13-34-36-313	Derek for Windows - Chromosome damage	Lhasa Limited, Chromosome damage, Derek for Windows, Mammal (primarily hamster, mouse and human)	6.Other	6.6.Other Chromosome damage
Q13-34-36-315	Derek for Windows - Skin sensitisation	Lhasa Limited, Derek for Windows - Skin sensitisation, Mammal (mainly Guinea Pig, Mouse and Human)	4. Human Health Effects	4. 6. Skin sensitisation
Q14-26-8-158	QSAR for Ames test of alpha, beta-unsaturated carbonyl compounds	Ames mutagenicity, alpha, beta-unsaturated carbonyl compound	4.Human Health Effects	4.10.Mutagenicity
Q14-26-8-160	QSAR for mammalian cell mutagenicity of alpha, beta-unsaturated carbonyl compounds	mammalian cell mutagenicity, alpha, beta-unsaturated carbonyl compound	4.Human Health Effects	4.10.Mutagenicity
Q14-37-8-303	TOPS-MODE QSAR for Ames test of alpha, beta-unsaturated carbonyl compounds	Ames mutagenicity, TOPS-MODE, alpha beta-unsaturated carbonyl compounds	4.Human Health Effects	4.10.Mutagenicity
Q15-28-8-162	QSAR for narcosis to fathead minnow, including non-polar and polar narcosis.	acute fish toxicity, narcosis, fathead minnow	3.Ecotoxic effects	3. 3. Acute toxicity to fish (lethality)
Q17-10-1-225	Nonlinear QSAR: artificial neural network for mouse carcinogenicity	Molcode, Nonlinear QSAR, artificial neural network, mouse carcinogenicity, Mouse	4.Human Health Effects	4.12.Carcinogenicity
Q17-10-1-226	Nonlinear QSAR: artificial neural network for biodegradation: activated sludge respiration inhibition test	Molcode, nonlinear QSAR, artificial neural network, biodegradation, activated sludge, respiration inhibition test	3.Ecotoxic effects	3.6.Microbial inhibition (activated sludge respiration inhibition, inhibition of nitrification, other)

Q17-10-1-241	Nonlinear QSAR: artificial neural network for classification of skin sensitisation potential	skin sensitisation, local lymph node assay, neural network, Molcode, QSARModel	4.Human Health Effects	4.6.Skin sensitisation
Q17-10-1-267	Nonlinear QSAR: artificial neural network for acute toxicity to Daphnia magna	Molcode, nonlinear QSAR, artificial neural network, acute toxicity, Daphnia magna	3.Ecotoxic effects	3.4.Long-term toxicity to Daphnia (lethality, inhibition of reproduction)
Q17-10-1-289	Nonlinear QSAR: artificial neural network for in vitro chromosome aberrations in mammalian cells	Molcode, ANN QSAR, in vitro chromosome aberrations, mammalian cells, Chinese Hamster Lung Cells	4.Human Health Effects	4.10.Mutagenicity
Q17-10-1-297	Nonlinear QSAR: artificial neural network for acute oral toxicity (rat cell line)	Molcode, artificial neural network, acute oral toxicity, rat, cell line	4.Human Health Effects	4.2.Acute Oral toxicity
Q17-10-1-311	Nonlinear QSAR: artificial neural network for in vitro chromosomal aberration	Molcode, artificial neural network, in vitro chromosome aberration, Chinese Hamster Lung cell	4.Human Health Effects	4.10.Mutagenicity
Q17-10-31-264	Nonlinear QSAR: artificial neural network for classification of repeated dose toxicity	Molcode, ANN QSAR, Repeated Dose, Reproduction/Developmental Toxicity, Rat (male; female)	4.Human Health Effects	4.14.Repeated dose toxicity
Q17-22-1-332	Nonlinear QSAR: artificial neural network for dermal irritation	skin irritation, PII, Draize, Molcode	4.Human Health Effects	4.4.Skin irritation /corrosion
Q18-32-33-245	TerraQSAR - LOGP	TerraQSAR, logP, neural network	1.Physical Chemical Properties	1.6.Octanol-water partition coefficient (Kow)
Q19-10-30-299	QSAR for acute toxicity to Daphnia magna (LC50)	Molcode, acute toxicity, Daphnia, immobilisation	3.Ecotoxic effects	3.1.Short-term toxicity to Daphnia (immobilisation)
Q19-10-30-300	QSAR for octanol-water partition coefficient (logP) for pesticides	Molcode, logP, octanol-water partition coefficient, pesticide	1.Physical Chemical Properties	1.6.Octanol-water partition coefficient (Kow)
Q19-22-1-333	Nonlinear QSAR: artificial neural network for acute toxicity of birds	acute toxicity, birds, LD50, Molcode, artificial neural network	3.Ecotoxic effects	3.12.aToxicity to birds. Short term toxicity (feeding, gavage, other)
Q19-22-1-336	Nonlinear QSAR: artificial neural network for the Daphnia magna reproduction test	Daphnia magna, reproduction, Molcode, artificial neural network	3.Ecotoxic effects	3.4.Long-term toxicity to Daphnia (lethality, inhibition of reproduction)

Q19-30-8-242	TOPS-MODE QSAR for mammalian cell mutagenicity of alpha,beta-unsaturated carbonyl compounds	TOPS MODE, mutagenicity, alpha,beta-unsaturated carbonyl compound	4.Human Health Effects	4.10.Mutagenicity
Q19-35-35-290	Toxtree QSAR 6: mutagenicity aromatic amines in Salmonella typhimurium TA100, with S9 metabolic activation	Toxtree, mutagenicity, Salmonella typhimurium TA100, S9 metabolic activation, aromatic amines.	4.Human Health Effects	4.10.Mutagenicity
Q19-35-35-291	Toxtree QSAR 8: carcinogenicity of aromatic amines	Toxtree, rulebase, carcinogenicity, aromatic amines, Rodents (rats and mice)	4.Human Health Effects	4.12.Carcinogenicity
Q19-35-35-292	Toxtree QSAR 13: mutagenicity of alpha,beta unsaturated aliphatic aldehydes in Salmonella typhimurium TA100	Toxtree, Mutagenicity, Salmonella typhimurium TA100, α β -unsaturated aliphatic aldehydes	4.Human Health Effects	4.10.Mutagenicity
Q19-39-8-317	Non polar narcosis QSAR for fathead minnow acute toxicity	fathead minnow, Pimephales promelas, acute fish toxicity, non-polar narcosis	3.3.Acute toxicity to fish (lethality)	C.1.Acute Toxicity for Fish
Q19-39-8-318	Polar narcosis QSAR for fathead minnow acute toxicity	fathead minnow, Pimephales promelas, acute fish toxicity, polar narcosis	3.3.Acute toxicity to fish (lethality)	C.1.Acute Toxicity for Fish
Q19-41-37-331	MultiCASE model for in vitro chromosome aberration in mammalian (CHL) cells	MultiCASE, Danish National Food Institute, in vitro chromosome aberration, Chinese Hamster Lung Cell	4.Human Health Effects	4.10.Mutagenicity
Q26-35-35-295	Toxtree: Benigni-Bossa rulebase for genotoxic and non-genotoxic carcinogenicity	Toxtree, Benigni-Bossa rulebase, genotoxic and nongenotoxic carcinogenicity, Rodents (rats and mice)	4. Human Health Effects	4.12. Carcinogenicity
Q26-35-35-296	Toxtree: rulebase for mutagenicity (in vivo micronucleus assay)	Toxtree, ToxMic rulebase, in vivo, mutagenicity, Rodents (rats and mice)	4. Human Health Effects	4.10.Mutagenicity
Q27-39-8-319	Polar narcosis QSAR for tetrahymena pyriformis acute toxicity	tetrahymena pyriformis, acute fish toxicity, polar narcosis	3.Ecotoxic effects	3. 3. Acute toxicity to fish (lethality)

Q27-40-8-320	Non polar narcosis QSAR for tetrahymena pyriformis acute toxicity	tetrahymena pyriformis, acute fish toxicity, non-polar narcosis	3.Ecotoxic effects	3. 3. Acute toxicity to fish (lethality)
Q31-47-42-424	ACD/Percepta model for genotoxicity (Ames test)	ACD/Percepta;genotoxicity; mutagenicity; Ames ; S. Typhimurium; E. Coli	QMRF 4. Human Health Effects	QMRF 4.10. Mutagenicity
Q32-48-43-425	ACD/Percepta model for rat acute oral toxicity	ACD/Percepta;acute oral toxicity; LD50; rat	QMRF 4. Human Health Effects	QMRF 4. 2. Acute Oral toxicity
Q32-48-43-426	ACD/Percepta model for mouse acute oral toxicity	ACD/Percepta;acute oral toxicity; LD50; mouse;	QMRF 4. Human Health Effects	QMRF 4. 2. Acute Oral toxicity
Q34-49-44-428	QSAR for non-polar narcosis to fish	Chronic fish toxicity, non-polar narcosis, QSARCHE	QMRF 3. Ecotoxic effects	QMRF 3. 5. Long-term toxicity to fish (egg/sac fry, growth inhibition of juvenile fish, early life stage, full life cycle)
Q33-49-44-427	QSAR for polar narcosis to fish	Chronic fish toxicity, polar narcosis, QSARCHE	QMRF 3. Ecotoxic effects	QMRF 3. 5. Long-term toxicity to fish (egg/sac fry, growth inhibition of juvenile fish, early life stage, full life cycle)
Q28-43-38-420	Lazar model for rodent carcinogenicity	Lazar;rat;mouse;carcinogenicity	QMRF 4. Human Health Effects QMRF	4.12. Carcinogenicity
Q30-45-40-421	Chronic fish toxicity model for predicting sub-lethal NOEC values for non-polar narcotics.	Chronic fish toxicity, NOEC, non-polar narcotic	QMRF 3. Ecotoxic effects	QMRF 3. 5. Long-term toxicity to fish (egg/sac fry, growth inhibition of juvenile fish, early life stage, full life cycle)
Q19-46-41-422	iSafeRat@HA-QSAR based on a holistic approach for predicting physicochemical and ecotoxicological endpoints	iSafeRat; HA-QSAR; holistic; physicochemical; Log Kow; Solubility; Ecotoxicity	[1]QMRF 1. Physical Chemical Properties [2]QMRF 1. Physical Chemical Properties (Kow) [3]QMRF 3. Ecotoxic effects [4]QMRF 3. Ecotoxic effects [5]QMRF 3. Ecotoxic effects	[1]QMRF 1. 3. Water solubility [2]QMRF 1. 6. Octanol-water partition coefficient (Kow) [3]QMRF 3. 1. Short-term toxicity to Daphnia (immobilisation) [4]QMRF 3. 2. Short-term toxicity to algae (inhibition of the exponential growth rate) [5]QMRF 3. 3. Acute toxicity to fish (lethality)
Q29-44-39-423	Lazar models for carcinogenic potency (TD50) in the rat and mouse	Lazar, TD50, automated read/across, rat, mouse	QMRF 4.12. Carcinogenicity	OECD 451 Carcinogenicity Studies