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Applications of QSAR Method in Painting and Coating Industry

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Outline

- Introduction to QSAR: Basics and Principles
- Applications of QSAR and Strategic Drivers to use
- The Study Profile
- QSAR Results and Comparison with Test/Calculation Data for Selected Substances
- Discussion and Conclusions

Introduction: QSAR Basics

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(Q)SAR = (Quantitative) Structure-Activity Relationship

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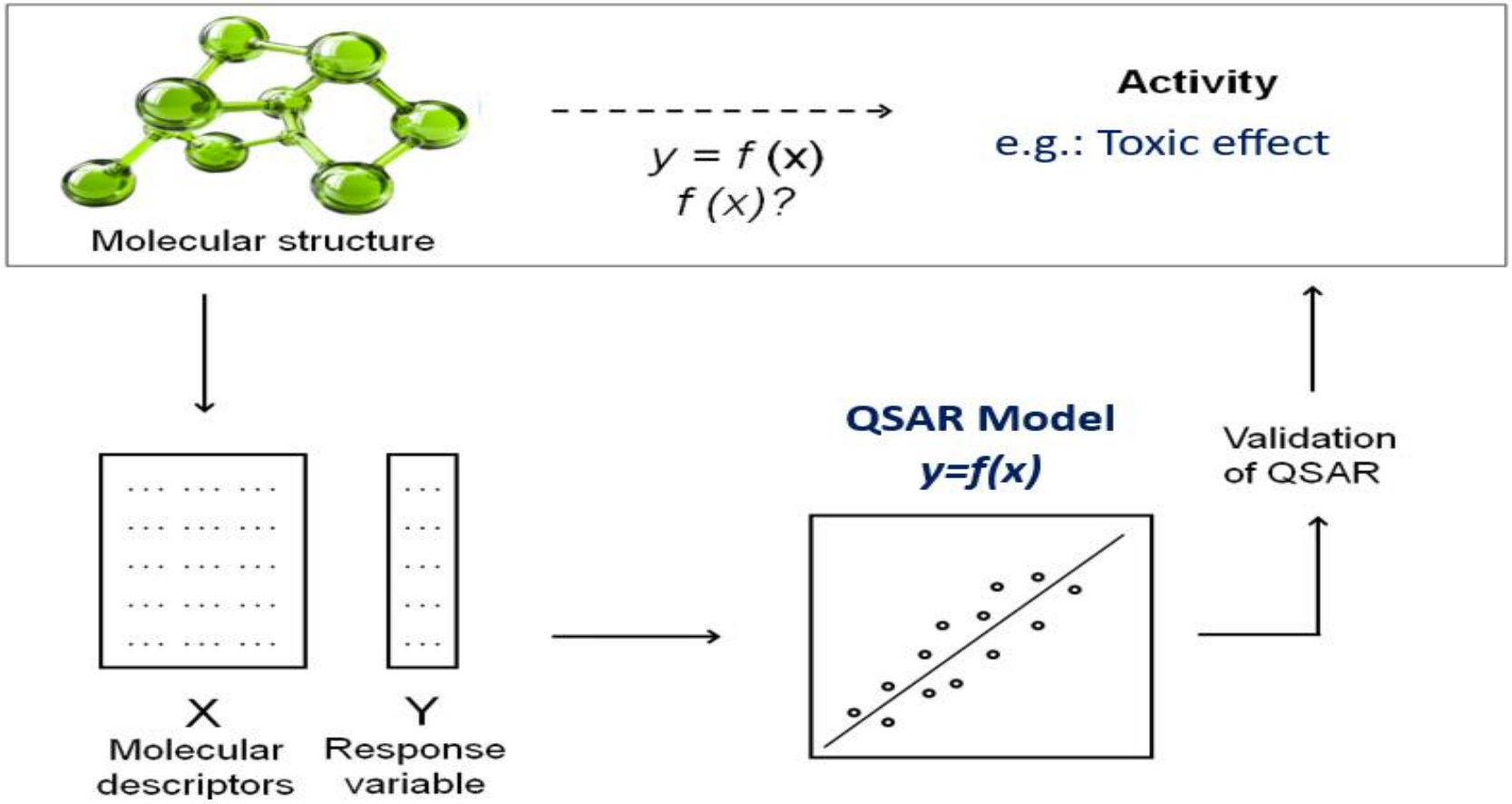
Introduction: QSAR Principle



QSAR Applications

Data production of

- Physical Chemical Properties
- Environmental Fate and Transport
- Ecotoxicological Information
- Human Health Hazard (Toxicological Information)

For

- Chemical Safety Assessment
  - Safety Data Sheet (SDS) Preparation/Compliance
  - Certification
- New Molecule and Formulation Development (R&D)
- Regulatory Compliance (REACH like regulations)
  - Chemical Safety Assessment
  - Notification
  - Registration & Authorizations

Reasons to use QSAR

- Regulatory Encouragements/Obligations
- Animal welfare
- Innovation
- Time for experiments
- Occurrence of enough laboratories/resources
- Costs
- Prioritization needs
- Pro-active approach for safer chemicals

The Study Profile

- Aim: Investigation of applicability/reliability of QSAR Method for common chemicals used in paint industry for Regulatory Compliance, R&D and Quality certification by comparing the test results with QSAR results
- Method: QSAR Toolbox 4.7.1 Software (OECD)
- Selected Chemicals
  1. Pigment Red 170
  2. Bisphenol A
  3. Toluene
- Investigated endpoints (if applicable)
  - Physical Chemical Properties
  - Environmental Fate and Transport
  - Ecotoxicological Information
  - Human Health Hazard (Toxicological Information)

Results: 1. Pigment Red 170
Physical Chemical Properties and Environmental Fate

Endpoint	Measured Value	QSAR Calculation
Melting/Freezing Point (°C)	M: Decomposition takes place at ca. 313 °C.	Q: 321 -350 °C (hypothetical)
N-Octanol/Water	Not available	Q: 6.04
Vapour Pressure (mmHg)	Not available	Q: 1.35E-29 - 3.77E-16 mm Hg
Water Solubility (mg/L)	M: 0.0119 mg/L	Q: 0.0135 mg/L
Biodegradation	M: Not inherently biodegradable (0 %, 29d)	Q: Not Readily Biodegradable
Bioaccumulation (BCF-Animals)	M:10-169.6 L/kg	Q:10 -194 L/kg

Results: 1. Pigment Red 170
Toxicological and Ecotoxicological Information

Endpoint	Measured Value	QSAR Calculation/Prediction
Acute Aquatic Toxicity (Algea and Cynobacteria, EC50, mg/L, 72h)	M: > 1.00 mg/L (alg, 72h)	Q: 0.238-1.83 mg/L (alg, 72h)
NOEC (Chronic)	M: 1.0 mg/L (NOEC, 21 d)	Q: 1.17 (calculated NOEC from 1.66 mg/L ChV)
Acute Toxicity (Oral, LD50, mg/kg)	M: >2E+03 mg/kg M: >1.5E+04 mg/kg	Q: 2.72E+03 mg/kg (LD50, oral rat)
Repeated dose toxicity, NOAEL	M: ≥1E+03 mg/kg bdwt/d (NOAEL	Predicted: 1E+3 mg/kg bdwt/d (NOAEL)
Genetic Toxicity (Mutagenicity)	M: Negative (19 in vitro test data)	Q: Negative
Eye irritation/Corrosion	M: Not irritating	Q: Not Corrosive to eye
Skin irritation	M: Not irritating	Q: Not irritating
Skin Sensitisation	M: Not sensitising (LLNA)	Q: Not sensitising (+ 1 positive), There are CLP notifications ➔ sensitizing!

Results: 2. Bisphenol A
Physical Chemical Properties and Environmental Fate

Endpoint	Measured Value	QSAR Calculation
Boiling Point (°C)	M: 360 °C with decomposition M: 250 - 252°C with potential decomposition.	Q: 364 °C
Melting/Freezing Point (°C)	M: 153 °C	Q: 181 °C
Flash Point (°C)	M: 227 °C	Q: 158 °C
N-Octanol/Water	M: 3.32	Q: 3.64
Vapour Pressure (mmHg)	M: 2.97E-07 hPa	M: 2.76E-07 hPa
Water Solubility (mg/L)	M: 120 mg/L	M: 161mg/L
Biodegradation	M: Readily biodegradable	Q: Not ready (?)
Bioaccumulation (BCF-Animals)	M: 38 and 73 L/kg	Q: 72.44 L/kg

Results: 2. Bisphenol A
Toxicological and Ecotoxicological Information

Endpoint	Measured Value	QSAR Calculation/Prediction
Acute Aquatic Toxicity (Algea and Cynobacteria, EC50, mg/L, 96h)	M: 2.5 mg/L, 96h, algea	Q: 1.33 mg/L, 96h, algea
Acute Aquatic Toxicity (Daphnia) (EC50-mg/L)-48 saat	M: EC50 values were in the range of 0.885 to 34.7 mg/L.	Q: 1.35 mg/L Daphnia Magna, 48h, EC50,
Acute Aquatic Toxicity (Fish, EC50, mg/L, 96hh)	M: 4.7 mg/L, 96h, fish	Q: 4.76 mg/L, 96h, fish
NOEC (Chronic)	M: 0,25-3.5 mg/L	Predicted: 1.21 mg/L
Acute Toxicity (Oral, LD50, mg/kg)	M: 3E+03 - 5.2 E+03 mg/kg	T: 1.77E+03 mg/kg
Acute Toxicity (Dermal, LD50, mg/kg)	M: ca.3E+03 mg/kg	T: 3.26E+03 mg/kg
Repeated dose toxicity, NOAEL	Not a selective reproductive toxicant	Q: Development toxicity→Negative
Genetic Toxicity (Mutagenicity)	M: Negative	Q: Negative
Eye irritation/Corrosion	M: Eye irritiant	Q: Unknown
Skin irritation	M: Not Irritating or Corrosive to skin	Q: Not Irritating or Corrosive to skin
Skin Sensitisation	M: Not sensitising in REACH registration	Q: Sensitizing

Results: 3. Toluene
Physical Chemical Properties and Environmental Fate

Endpoint	Measured Value	QSAR Calculation
Auto flammability/ self ignition temperature (°C)	M: 480 °C	Q: 426 C
Boiling Point (°C)	M: 111 °C	Q: 126 °C
Melting/Freezing Point (°C)	M: -95 °C	Q: -78.1 °C
N-Octanol/Water	M: 2.73	Q: 2.54
Vapour Pressure (mmHg)	M: 23,16 mmHg	Q: 22.3 mm Hg
Biodegradation	M: 53 %-86%==> Readily biodegradable	Q: Readily biodegradable
Bioaccumulation (BCF-Animals)	M: 90 (test, 3d) Estimated: 42	Q: 27.54

Results: 3. Toluene
Toxicological and Ecotoxicological Information

Endpoint	Measured Value	QSAR Calculation/Prediction
Acute Aquatic Toxicity (Algea and Cynobacteria, EC50, mg/L, 96h)	M: 134 mg/L	Q: 17.5 -29.1 mg/LL
Acute Aquatic Toxicity (Daphnia) (EC50-mg/L)-48 saat	M: 3.78 mg/L	Q: 4.27-6.6 mg/L
Acute Aquatic Toxicity (Fish, EC50, mg/L, 96hh)	M: 5.5 mg/L.	Q: 24.8 mg/L
NOEC (Chronic)	M: 0.74 mg/L	Q: 1.173 (NOEC calculated from CrV)
Acute Toxicity (Oral, LD50, mg/kg)	M: 5.58E+03 mg/kg	Q: 3.3E+03 mg/kg
Acute Toxicity (Dermal, LD50, mg/kg)	M: >5E+03 mg/kg	Q: NA
Repeated dose toxicity, NOAEL	M: 625 mg/kg (oral, rat)	Q: 56.6 mg/kg
Genetic Toxicity (Mutagenicity)	M: Negative	Q: Negative
Eye irritation/Corrosion	M: Irritating	Q: Not estimated
Skin irritation	M: Irritating	Q: Irritating /Not irritating
Skin Sensitisation	M: Not sensitising	M: Not sensitising

Conclusions and Recommendations

- High Correlation Observed:

The comparison between experimentally measured and QSAR-predicted values across selected endpoints demonstrates high consistency.

- Interpretation of Findings:

QSAR predictions for Pigment Red 170, Bisphenol A, and Toluene align closely with existing experimental datasets. Minor deviations observed were within acceptable regulatory thresholds and can be attributed to data availability and model domain applicability.

- Implications for the Paint Industry:

The study confirms the reliability of QSAR models as a screening tool for regulatory submissions.

Reinforces the potential of QSAR in reducing the need for in vivo/in vitro testing, contributing to cost efficiency and animal welfare.

Supports broader application in SDS preparation, substance notification, and certification processes

- Recommendations

Further studies on specific chemicals might be projected for further confirmation of the applicability of the method

New QSAR models should be developed to enrich availability of models in domain by collaboration with Universities

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