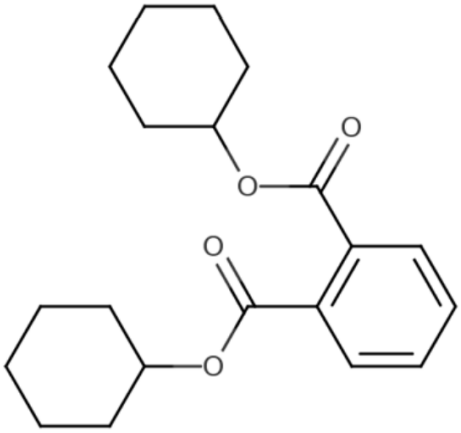
United States
Environmental Protection Agency

December 2024
Office of Chemical Safety and
Pollution Prevention

Draft Data Quality Evaluation and Data Extraction Information for Environmental Fate and Transport for Dicyclohexyl Phthalate (DCHP) (1,2- Benzenedicarboxylic acid, 1,2-dicyclohexyl ester)

Systematic Review Support Document for the Draft Risk Evaluation

CASRN: 84-61-7



December 2024

This supplemental file contains information regarding the data extraction and evaluation results for data sources that were considered for the *Draft Risk Evaluation for Dicyclohexyl Phthalate (DCHP)* and that underwent systematic review. EPA used the TSCA systematic review process described in the *Draft Systematic Review Protocol Supporting TSCA Risk Evaluations for Chemical Substances* (also referred to as the '2021 Draft Systematic Review Protocol'). The systematic review steps are further described in the *Draft Risk Evaluation for Dicyclohexyl Phthalate (DCHP) – Systematic Review Protocol*. EPA conducted data extractions and data quality evaluations based on author-reported descriptions and results; additional analyses (*e.g.*, statistical analyses) potentially conducted by EPA are not contained in this supplemental file. Additionally, the overall quality determination (OQD) for each reference represents the data as a whole for each study and not for individual metric domains within a study.

Table of Contents

Study Citation:	EC/HC, (2015). State of the science report: Phthalate substance grouping: Medium-chain phthalate esters: Chemical Abstracts Service Registry Numbers: 84-61-7; 84-64-0; 84-69-5; 523-31-9; 5334-09-8;16883-83-3; 27215-22-1; 27987-25-3; 68515-40-2; 71888-89-6.
OECD Harmonized Template:	Biodegradation in Water
HERO ID:	3688160

EXTRACTION

Parameter	**Data**
CASRN and Test Material	84-61-7; DCHP
Confidentiality, EndPoint, Type, Guideline	none; Aerobic biodegradability; experimental; other: not specified
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR; NR Notes: NR
Blank and Control	not reported; not reported
Oxygen and Inoculum	not reported; not specified: not reported
Duration, Parameter, System, and Sampling Frequency	28 days; %BOD; %biodegradation: not reported; not reported
pH Adjusted and pH	not reported; not reported
Concentration	not reported not reported - not reported not reported
Composition and Test Temperature	not reported; not reported
CEC, Water Aeration Dilution, Continuous Darkness, and Other Design	not reported; not reported; not reported; not reported
Results Details Method, Results per Degradation Parameter, and Direct Quantum Yield Results	not reported; %BOD; %biodegradation; not reported
Results Value, Results Standard Deviation, Results Sample Time, and Results Reference Substance Compartments	68.5; 91; not reported; 28 days; not reported
Results Remarks and Results Details	not reported; not reported
Results Mean Total Recovery and Results per Recovery	not reported; not reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified.
	Metric 2:	Test Substance Purity	Medium	The test substance purity was not reported; however, the omission was not likely to have a substantial impact on the study results.
Domain 2: Test Design				
	Metric 3:	Study Controls	Medium	Details were not reported in this gray literature source; however, further details may be provided in source cited.
	Metric 4:	Test Substance Stability	Medium	Details were not reported in this gray literature source; however, further details may be provided in source cited.

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Study Citation:	EC/HC, (2015). State of the science report: Phthalate substance grouping: Medium-chain phthalate esters: Chemical Abstracts Service Registry Numbers: 84-61-7; 84-64-0; 84-69-5; 523-31-9; 5334-09-8;16883-83-3; 27215-22-1; 27987-25-3; 68515-40-2; 71888-89-6.
OECD Harmonized Template:	Biodegradation in Water
HERO ID:	3688160

			EVALUATION	
Domain		Metric	Rating	Comments
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	High	The test method is suitable.
	Metric 6:	Testing Conditions	Medium	Details were not reported in this gray literature source; however, further details may be provided in source cited.
	Metric 7:	Testing Consistency	Medium	Details were not reported in this gray literature source; however, further details may be provided in source cited.
	Metric 8:	System Type and Design	Medium	Details were not reported in this gray literature source; however, further details may be provided in source cited.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	Medium	The inoculum was reported with limited details; however, further details may be provided in source cited.
	Metric 10:	Sampling Methods	N/A	The metric is not applicable to this study.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Medium	Details were not reported in this gray literature source; however, further details may be provided in source cited.
	Metric 12:	Test Substance Purity	Medium	Details were not reported in this gray literature source; however, further details may be provided in source cited.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	Medium	Details were not reported in this gray literature source; however, further details may be provided in source cited.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	The metric is not applicable to this source.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Medium	Details were not reported in this gray literature source; however, further details may be provided in source cited.
	Metric 16:	Statistical Methods and Kinetic Calculations	Medium	Details were not reported in this gray literature source; however, further details may be provided in source cited.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Medium	Gray literature source citing ECHA profile.
	Metric 18:	QSAR Models	N/A	The metric is not applicable to this study.

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Study Citation:	EC/HC, (2015). State of the science report: Phthalate substance grouping: Medium-chain phthalate esters: Chemical Abstracts Service Registry Numbers: 84-61-7; 84-64-0; 84-69-5; 523-31-9; 5334-09-8;16883-83-3; 27215-22-1; 27987-25-3; 68515-40-2; 71888-89-6.
OECD Harmonized Template:	Biodegradation in Water
HERO ID:	3688160

EVALUATION

Domain	Metric	Rating	Comments
Overall Quality Determination		**Medium**	

* Related References: [ECHA] European Chemicals Agency. c2007–2014c. Registered substances database. Search for CAS RN 84-61-7 [DCHP]. Helsinki (FI): ECHA. [cited 2014 Sept]. Available from: http://echa.europa.eu/information-on-chemicals/registered-substances?p_auth=UvS8Lp1d&p_p_id=registeredsubstances_WAR_regsubsportlet&p_p_lifecycle=1&p_p_state=normal&p_p_mode=view&p_p_col_id=column-1&p_p_col_pos=1&p_p_col_count=6&_registeredsubstances_WAR_regsubsportlet_javax.portlet.action=registeredSubstancesAction

Study Citation:	NCBI, (2020). PubChem database: compound summary: dicyclohexyl phthalate.
OECD Harmonized Template:	Biodegradation in Water
HERO ID:	6629414

EXTRACTION

Parameter	**Data**
CASRN and Test Material	84-61-7; Dicyclohexyl phthalate
Confidentiality, EndPoint, Type, Guideline	None; ready biodegradability; Experimental; OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I)): Japanese MITI Test
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR; NR
Blank and Control	Not reported; Not reported
Oxygen and Inoculum	aerobic; activated sludge (adaptation not specified): activated sludge 30 mg/L
Duration, Parameter, System, and Sampling Frequency	4 weeks; ThOD: Not reported; Not reported
pH Adjusted and pH	Not Reported; Not reported
Concentration	100 mg/L
Composition and Test Temperature	Not reported; Not reported
CEC, Water Aeration Dilution, Continuous Darkness, and Other Design	Not reported; Not reported; Not Reported; Not reported
Results Details Method, Results per Degradation Parameter, and Direct Quantum Yield Results	Not reported; BOD; Not Reported
Results Value, Results Standard Deviation, Results Sample Time, and Results Reference Substance Compartments	68.5%; Not reported; 4 weeks; Not reported
Results Remarks and Results Details	Not reported; Not reported
Results Mean Total Recovery and Results per Recovery	Not reported; Not reported

EVALUATION

Domain	Metric	Rating	Comments
Domain 1: Test Substance			
Metric 1:	Test Substance Identity	High	The test substance was identified clearly.
Metric 2:	Test Substance Purity	Medium	The test substance purity was not reported.
Domain 2: Test Design			
Metric 3:	Study Controls	Medium	Limited data is presented in this secondary source.
Metric 4:	Test Substance Stability	Medium	Limited data is presented in this secondary source.
Domain 3: Test Conditions			
Metric 5:	Test Method Suitability	Medium	Limited data is presented in this secondary source.

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Study Citation:	NCBI, (2020). PubChem database: compound summary: dicyclohexyl phthalate.
OECD Harmonized Template:	Biodegradation in Water
HERO ID:	6629414

Domain		Metric	EVALUATION Rating	Comments
	Metric 6:	Testing Conditions	Medium	Limited data is presented in this secondary source.
	Metric 7:	Testing Consistency	Medium	Limited data is presented in this secondary source.
	Metric 8:	System Type and Design	Medium	Limited data is presented in this secondary source.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	Medium	Limited data is presented in this secondary source.
	Metric 10:	Sampling Methods	N/A	The metric is not applicable to the study type.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	N/A	The intended outcome is reported for the target substance.
	Metric 12:	Test Substance Purity	Medium	Limited data is presented in this secondary source.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	Medium	Limited data is presented in this secondary source.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	This metric is not applicable to this type of study.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Medium	Limited data is presented in this secondary source.
	Metric 16:	Statistical Methods and Kinetic Calculations	Medium	Limited data is presented in this secondary source.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Medium	Due to limited information, evaluation of the reasonableness of the study results was not possible.
	Metric 18:	QSAR Models	N/A	This metric is not applicable to this type of study.

Overall Quality Determination — Medium

* Related References: NITE; Chemical Risk Information Platform (CHRIP). Biodegradation and Bioconcentration. Tokyo, Japan: Natl Inst Tech Eval. Available from, as of Mar 2, 2016: http://www.safe.nite.go.jp/english/db.html

Study Citation:	NCBI, (2020). PubChem database: compound summary: dicyclohexyl phthalate.
OECD Harmonized Template:	Biodegradation in Sediment
HERO ID:	6629414

EXTRACTION

Parameter	**Data**
CASRN and Test Material	84-61-7; Dicyclohexyl phthalate
Confidentiality, EndPoint, Type, Guideline	None; Not Reported; Experimental; other: Biodegradation in sediment
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	Not Reported; NR; NR; NR
Oxygen and Inoculum	aerobic/anaerobic; natural sediment: Six river sediment samples from Taiwan rivers
Duration, Parameter, System, and Sampling Frequency	Not reported; not specified; Not reported; Not reported
Results Sample Time, Compartment, Sludge Compartment, Water Compartment, CEC, and pH	Not reported; Not reported; Not reported; Not reported; Not reported; Not reported
Control Dark, Control, and Blank	Not Reported; Not reported; Not reported
Concentration	Not reported
Analytical Method, Analytical Details, and Results Per Degredation Parameter	Not reported; Not reported; Not Reported
Results Remarks	Not reported
Halflife, Standard Deviation Results, Reference Substance Results, and Reference Substance Compartment Results	average aerobic half-life=11.1 days; average anaerobic half-life=26.4 days; Not reported; Not reported; Not reported
Results Details	Not reported
Mean Total Recovery Results and Results Per Recovery	Not reported; Not reported
Results Value, Direct Quantum Yield Results, and Transformation Products	Not reported; Not Reported; Not reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified clearly.
	Metric 2:	Test Substance Purity	Medium	Details regarding this metric were not reported; however, additional information may be included in the primary source.
Domain 2: Test Design				
	Metric 3:	Study Controls	Medium	Detail regarding this metric were not reported; however, additional information may be included in the primary source.
	Metric 4:	Test Substance Stability	Medium	Detail regarding this metric were not reported; however, additional information may be included in the primary source.

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Study Citation:	NCBI, (2020). PubChem database: compound summary: dicyclohexyl phthalate.
OECD Harmonized Template:	Biodegradation in Sediment
HERO ID:	6629414

			EVALUATION	
Domain		Metric	Rating	Comments
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	Medium	Detail regarding this metric were not reported; however, additional information may be included in the primary source.
	Metric 6:	Testing Conditions	Medium	Detail regarding this metric were not reported; however, additional information may be included in the primary source.
	Metric 7:	Testing Consistency	Medium	Detail regarding this metric were not reported; however, additional information may be included in the primary source.
	Metric 8:	System Type and Design	Medium	Detail regarding this metric were not reported; however, additional information may be included in the primary source.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	Medium	Detail regarding this metric were limited; however, additional information may be included in the primary source.
	Metric 10:	Sampling Methods	N/A	The metric is not applicable to this study type.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Medium	Detail regarding this metric were not reported; however, additional information may be included in the primary source.
	Metric 12:	Test Substance Purity	Medium	Detail regarding this metric were not reported; however, additional information may be included in the primary source.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	Medium	Detail regarding this metric were not reported; however, additional information may be included in the primary source.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	This metric is not applicable to this type of study.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Medium	Detail regarding this metric were limited; however, additional information may be included in the primary source.
	Metric 16:	Statistical Methods and Kinetic Calculations	Medium	Detail regarding this metric were not reported; however, additional information may be included in the primary source.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Medium	Due to limited information, evaluation of the reasonableness of the study results was not possible; however, additional information may be included in the primary source.
	Metric 18:	QSAR Models	N/A	The metric is not applicable to this study type.

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Study Citation:	NCBI, (2020). PubChem database: compound summary: dicyclohexyl phthalate.
OECD Harmonized Template:	Biodegradation in Sediment
HERO ID:	6629414

EVALUATION

Domain	Metric	Rating	Comments
Overall Quality Determination		**Medium**	

* Related References: Yuan SY et al; Chemosphere 49: 1295-9 (2002)

Study Citation:	Yuan, S. Y., Liu, C., Liao, C. S., Chang, B. V. (2002). Occurrence and microbial degradation of phthalate esters in Taiwan river sediments. Chemosphere 49(10):1295-1299.
OECD Harmonized Template:	Biodegradation in Sediment
HERO ID:	5541359

EXTRACTION

Parameter	Data
CASRN and Test Material	84-61-7; DCHP
Confidentiality, EndPoint, Type, Guideline	None; other; Experimental; other: Not reported; biodegradation kinetics in Taiwanese river sediment
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; Chem Service (West Chester, PA); NR; 99.0%
Oxygen and Inoculum	anaerobic; natural sediment: freshwater: Top 10 cm layer sediment samples collected from the Zhonggang, Keya, Erren, Gaoping, Donggang, and Danshui Rivers, Taiwan, from January - August 2000
Duration, Parameter, System, and Sampling Frequency	Not reported; formulation; 125 mL serum bottles with 45 mL medium, 5 g river sediment, and 5 ug/g mixture of phthalic acid esters; Not reported
Results Sample Time, Compartment, Sludge Compartment, Water Compartment, CEC, and pH	Not reported; Sediment; Natural river sediment; Not reported; Not reported; Not reported
Control Dark, Control, and Blank	Not Reported; Not reported; Not reported
Concentration	5 ug/g
Analytical Method, Analytical Details, and Results Per Degredation Parameter	GC/MS, analytes separated on DB-5 capillary column, 0.25 um film thickness, 0.25 m i.d., 30 m length; detection limit 100 ug/L; Sediment extracted 3x by rotating shaker with hexane; Not Reported
Results Remarks	Range half-life: 24.9 - 28.8 daysAverage background test substance sediment concentration (range): 0.2 ug/g (N.D. - 1.9 ug/g)Danshui River sed. half-life: 14.8 dDanshui River sed. background conc.: NDZhonggang River sed. half-life: 27.2 dZhonggang River sed. background conc.: NDIndustrial discharge into the Danshui River has occurred for longer than the Zhonggang River, faster degradation may be due to microbial adaptation.
Halflife, Standard Deviation Results, Reference Substance Results, and Reference Substance Compartment Results	26.4 d; Not Reported; Not reported; Not reported
Results Details	First order kinetics: S=S_0*exp(-k*t), t0.5=0.693/k
Mean Total Recovery Results and Results Per Recovery	98.1%; Not reported
Results Value, Direct Quantum Yield Results, and Transformation Products	Not Reported; Not Reported; Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified by name and CASRN.
	Metric 2:	Test Substance Purity	High	The test substance source and purity were reported.
Domain 2: Test Design				
	Metric 3:	Study Controls	Medium	Controls were not explicitly included.

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Study Citation:	Yuan, S. Y., Liu, C., Liao, C. S., Chang, B. V. (2002). Occurrence and microbial degradation of phthalate esters in Taiwan river sediments. Chemosphere 49(10):1295-1299.
OECD Harmonized Template:	Biodegradation in Sediment
HERO ID:	5541359

		EVALUATION		
Domain		Metric	Rating	Comments
	Metric 4:	Test Substance Stability	Medium	Test substance preparation and storage conditions were not reported.
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	High	The test method is suitable for the test substance.
	Metric 6:	Testing Conditions	Low	Minimal test conditions were reported, omissions include sediment characteristics, pH, temperature, incubation time, and sample frequency.
	Metric 7:	Testing Consistency	High	Test set up was consistent across study groups.
	Metric 8:	System Type and Design	N/A	Not applicable.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	High	The inoculum sources were reported and are commonly used for similar studies.
	Metric 10:	Sampling Methods	N/A	Not applicable.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	High	The outcome assessment methodology was appropriate for determining degradation kinetics.
	Metric 12:	Test Substance Purity	Medium	Sample preparation was described and appropriate, frequency was not reported.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	Medium	Many study details were omitted.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	Not applicable.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	High	The analytical method was reported; limits of detection and extraction efficiency were reported. Raw data was not reported.
	Metric 16:	Statistical Methods and Kinetic Calculations	High	Kinetic calculations were described and applied appropriately.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Medium	The results were reasonable based on the method however many key study details were not reported, which reduces the reliability of this study.
	Metric 18:	QSAR Models	N/A	Not applicable.

Overall Quality Determination — High

Study Citation:	Yuan, S. Y., Liu, C., Liao, C. S., Chang, B. V. (2002). Occurrence and microbial degradation of phthalate esters in Taiwan river sediments. Chemosphere 49(10):1295-1299.
OECD Harmonized Template:	Biodegradation in Sediment
HERO ID:	5541359

EXTRACTION

Parameter	Data
CASRN and Test Material	84-61-7; DCHP
Confidentiality, EndPoint, Type, Guideline	None; other; Experimental; other: Not reported; biodegradation kinetics in Taiwanese river sediment
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; Chem Service (West Chester, PA); NR; 99.0%
Oxygen and Inoculum	aerobic; natural sediment: freshwater: Top 10 cm layer sediment samples collected from the Zhonggang, Keya, Erren, Gaoping, Donggang, and Danshui Rivers, Taiwan, from January - August 2000
Duration, Parameter, System, and Sampling Frequency	Not reported; formulation; 125 mL serum bottles with 45 mL medium, 5 g river sediment, and 5 ug/g mixture of phthalic acid esters; Not reported
Results Sample Time, Compartment, Sludge Compartment, Water Compartment, CEC, and pH	Not reported; Sediment; Natural river sediment; Not reported; Not reported; Not reported
Control Dark, Control, and Blank	Not Reported; Not reported; Not reported
Concentration	5 ug/g
Analytical Method, Analytical Details, and Results Per Degredation Parameter	GC/MS, analytes separated on DB-5 capillary column, 0.25 um film thickness, 0.25 m i.d., 30 m length; detection limit 100 ug/L; Sediment extracted 3x by rotating shaker with hexane; Not Reported
Results Remarks	Range half-life: 2.3 - 37.5 daysAverage background test substance sediment concentration (range): 0.2 ug/g (N.D. - 1.9 ug/g)Danshui River sed. half-life: 5.0 dDanshui River sed. background conc.: NDZhonggang River sed. half-life: 9.2 dZhonggang River sed. background conc.: NDIndustrial discharge into the Danshui River has occurred for longer than the Zhonggang River, faster degradation may be due to microbial adaptation.
Halflife, Standard Deviation Results, Reference Substance Results, and Reference Substance Compartment Results	11.1 d; Not Reported; Not reported; Not reported
Results Details	First order kinetics: S=S_0*exp(-k*t), t0.5=0.693/k
Mean Total Recovery Results and Results Per Recovery	98.1%; Not reported
Results Value, Direct Quantum Yield Results, and Transformation Products	Not Reported; Not Reported; Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified by name and CASRN.
	Metric 2:	Test Substance Purity	High	The test substance source and purity were reported.
Domain 2: Test Design				
	Metric 3:	Study Controls	Medium	Controls were not explicitly included.
	Metric 4:	Test Substance Stability	Medium	Test substance preparation and storage conditions were not reported.

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Study Citation:	Yuan, S. Y., Liu, C., Liao, C. S., Chang, B. V. (2002). Occurrence and microbial degradation of phthalate esters in Taiwan river sediments. Chemosphere 49(10):1295-1299.
OECD Harmonized Template:	Biodegradation in Sediment
HERO ID:	5541359

		EVALUATION	
Domain	Metric	Rating	Comments
Domain 3: Test Conditions			
Metric 5:	Test Method Suitability	High	The test method is suitable for the test substance.
Metric 6:	Testing Conditions	Low	Minimal test conditions were reported, omissions include sediment characteristics, pH, temperature, incubation time, and sample frequency.
Metric 7:	Testing Consistency	High	Test set up was consistent across study groups.
Metric 8:	System Type and Design	N/A	Not applicable.
Domain 4: Test Organisms			
Metric 9:	Outcome Assessment Methodology	High	The inoculum sources were reported and are commonly used for similar studies.
Metric 10:	Sampling Methods	N/A	Not applicable.
Domain 5: Outcome Assessment			
Metric 11:	Test Substance Identity	High	The outcome assessment methodology was appropriate for determining degradation kinetics.
Metric 12:	Test Substance Purity	Medium	Sample preparation was described and appropriate, frequency was not reported.
Domain 6: Confounding/Variable Control			
Metric 13:	Confounding Variables	Medium	Many study details were omitted.
Metric 14:	Health Outcomes Unrelated to Exposure	N/A	Not applicable.
Domain 7: Data Presentation and Analysis			
Metric 15:	Data Reporting	High	The analytical method was reported; limits of detection and extraction efficiency were reported. Raw data was not reported.
Metric 16:	Statistical Methods and Kinetic Calculations	High	Kinetic calculations were described and applied appropriately.
Domain 8: Other			
Metric 17:	Verification or Plausibility of Results	Medium	The results were reasonable based on the method however many key study details were not reported, which reduces the reliability of this study.
Metric 18:	QSAR Models	N/A	Not applicable.

Overall Quality Determination — High

* Related References: Cited in HSDB

Study Citation:	EC/HC, (2017). Draft screening assessment: Phthalate substance grouping.
OECD Harmonized Template:	Aquatic Bioconcentration
HERO ID:	5353181

EXTRACTION

Parameter	Data
CASRN and Test Material	84-61-7; Not Reported
Confidentiality, Type, and Guideline	None; Not specified; other: Not reported
Solvent, Reactivity, Storage, Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, Purity	Not Reported; Not Reported; Not Reported; Not Reported
Test Organism and Test Organism Details	Not Reported; Not Reported
Lipid Content, Test Temperature, pH, and Depuration Time	Not Reported; Not Reported; Not Reported; Not Reported
Media Type, TOC, and Salinity	Not Reported; Not Reported; Not Reported
Dissolved Oxygen, Conductivity, and Hardness	Not Reported; Not Reported; Not Reported
Exposure Route, Elimination, and Nominal Measurements	Not Reported; Not Reported; Not Reported
Test Type, Test Temperature, and Test Condition Comments	Not Reported; Not Reported; Not Reported
Duration, Parameter, and Sampling Frequency	Not Reported; Not Reported; Not Reported
Concentration	Not Reported
Analytical Method and Analytical Details	Not Reported; Not Reported;
Rate Constant and Results per Recovery	Not Reported; Not Reported
Statistics, Basis, and Calculation Basis	Not Reported; Not Reported; Not Reported
Results Value and Results Details	Not Reported; BAF: 92
Metabolites, Reference, and Results Reference Substance	Not Reported; Not Reported; Not Reported

EVALUATION

Domain	Metric	Rating	Comments
Domain 1: Test Substance			
Metric 1:	Test Substance Identity	High	The test substance was identified by common nomenclature.
Metric 2:	Test Substance Purity	Low	Details regarding the test substance purity were not reported in the secondary source.
Domain 2: Test Design			
Metric 3:	Study Controls	Low	Details regarding the use of control groups were not reported in the secondary source.
Metric 4:	Test Substance Stability	Low	The test substance stability, homogeneity, preparation, and storage conditions were not reported in the secondary source.
Domain 3: Test Conditions			
Metric 5:	Test Method Suitability	Uninformative	The test method was not reported in the secondary source.
Metric 6:	Testing Conditions	Uninformative	Testing conditions were not reported in the secondary source.

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Study Citation:	EC/HC, (2017). Draft screening assessment: Phthalate substance grouping.
OECD Harmonized Template:	Aquatic Bioconcentration
HERO ID:	5353181

			EVALUATION	
Domain		Metric	Rating	Comments
	Metric 7:	Testing Consistency	Low	The testing consistency could not be evaluated due to limited information reported by the secondary source.
	Metric 8:	System Type and Design	Uninformative	The system type was not reported in the secondary source.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	The metric is not applicable to the study type.
	Metric 10:	Sampling Methods	Uninformative	No details were provided in the secondary source regarding the test organism.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Uninformative	The outcome assessment methodology was not reported in the secondary source.
	Metric 12:	Test Substance Purity	Low	Details regarding the sampling methods were not reported in the secondary source.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	Low	Sources of variability and uncertainty were not reported.
	Metric 14:	Health Outcomes Unrelated to Exposure	Low	Health outcomes were not described in the secondary source.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Low	The analytical method and chemical concentrations were not reported in the secondary source.
	Metric 16:	Statistical Methods and Kinetic Calculations	Low	Statistical analysis and kinetic calculations were not reported in the secondary source.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Low	Due to limited information, evaluation of the reasonableness of the study results was not possible.
	Metric 18:	QSAR Models	N/A	The metric is not applicable to the study type.

Overall Quality Determination — Uninformative

* Related References: Environmental Canada, Health Canada 2015a, 2015b, 2015c, 2015d. (HERO IDs: 7264200, 3688160, 3688004, 7264199)

Study Citation:	Lee, Y. M., Lee, J. E., Choe, W., Kim, T., Lee, J. Y., Kho, Y., Choi, K., Zoh, K. D. (2019). Distribution of phthalate esters in air, water, sediments, and fish in the Asan Lake of Korea. Environment International 126:635-643.
OECD Harmonized Template:	Aquatic Bioconcentration
HERO ID:	5043593

EXTRACTION

Parameter	Data
CASRN and Test Material	84-61-7; Dicyclohexyl phthalate
Confidentiality, Type, and Guideline	None; Experimental; other: Not reported; Bioaccumulation field study
Solvent, Reactivity, Storage, Stability	NA; NR; Water samples stored in amber glass bottles with formaldehyde; sediment samples stored in amber straight sided glass jars; organisms wrapped in aluminum foil; all samples except water stored at -20°C; NR
Radiolabel, Source, State, Purity	NA; Asan Lake, Korea; NA; NA
Test Organism and Test Organism Details	four fish species including crucian carp, skygager, bluegill, and bass; n=30
Lipid Content, Test Temperature, pH, and Depuration Time	Not reported; Not reported; Not reported; Not reported
Media Type, TOC, and Salinity	natural water / sediment; Not reported; Not reported
Dissolved Oxygen, Conductivity, and Hardness	Not reported; Not reported; Not reported
Exposure Route, Elimination, and Nominal Measurements	Water (BAF), sediment (BSAF); Not applicable; Measured (mean): 0.001 ug/L (water), 0.7 ug/kg dw (sediment) detection frequency = 2.1% (water) and 6.4% (sediment)
Test Type, Test Temperature, and Test Condition Comments	field study; Not reported; Water, sediment, and fish samples collected from Asan Lake, a large artificial lake in Korea surrounded by industrial complex and farmlands
Duration, Parameter, and Sampling Frequency	Not applicable; Not Reported; October 2016. January 2017 (water and sediment only), May and July 2017
Concentration	not detected - 21.9 ug/kg dw
Analytical Method and Analytical Details	GC-MS in selected ion monitoring mode with an electron impact ionization, analytes separated on DB-5 MS UI capillary column; LOD 0.001 - 0.021 ug/L (water), 0.104 - 1.32 ug/kg dw (sediment), 0.17 - 0.53 ug/kg dw (fish); Water extracted by C18-E cartridge, eluted with methanol and hexane, evaporated to dryness, resuspended in acetone; Sediment and fish extracted by sonication with DCM, concentrated by roto-evap, cleaned up on Florisil-silica cartridge;
Rate Constant and Results per Recovery	Not applicable; 77 - 112% (water), 88-108% (sediment), 89-118% (fish) from matrix spiked samples
Statistics, Basis, and Calculation Basis	Spearman correlation and Kruskal-Wallis tests conducted with SPSS significance $p < 0.05$; principal component analysis with R v. 3.5.1;log BAF positive correlation with log Kow ($r=0.606$, $p < 0.01$), high bioavailability in water; Tissue, dry wt.; steady state
Results Value and Results Details	Not Reported; BAF = 23.9 ug/kg (mean fish conc.)/0.001 ug/L (mean water conc.) = 23,900 L/kg (SRC calculated); BSAF = 23.9 ug/kg (mean fish conc.)/0.7 ug/L (mean water conc.) = 34.1 L/kg (SRC calculated). Detection frequency in fish = 13.3%
Metabolites, Reference, and Results Reference Substance	Not reported; Not reported; Not reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified by name.
	Metric 2:	Test Substance Purity	High	The sample source was reported.
Domain 2: Test Design				
	Metric 3:	Study Controls	Medium	Analytical blanks or reference organisms were not explicitly included.

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Study Citation:	Lee, Y. M., Lee, J. E., Choe, W., Kim, T., Lee, J. Y., Kho, Y., Choi, K., Zoh, K. D. (2019). Distribution of phthalate esters in air, water, sediments, and fish in the Asan Lake of Korea. Environment International 126:635-643.
OECD Harmonized Template:	Aquatic Bioconcentration
HERO ID:	5043593

			EVALUATION	
Domain		Metric	Rating	Comments
	Metric 4:	Test Substance Stability	High	Sample storage and preparation was reported.
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	High	The field study was appropriate for the test substance.
	Metric 6:	Testing Conditions	Medium	No environmental conditions were provided; these omitted details are not expected to impact study results.
	Metric 7:	Testing Consistency	High	Samples were collected, analyzed, and processed consistently.
	Metric 8:	System Type and Design	High	Field sites are assumed to be in dynamic equilibrium.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	The metric is not applicable to this study type.
	Metric 10:	Sampling Methods	Medium	Organism species was reported, other details may be included in supplemental information.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	High	The outcome assessment methodology allowed for BAF and BSAF determination.
	Metric 12:	Test Substance Purity	High	Sampling methods were appropriate and were able to account for seasonal variance.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	Medium	Standard deviation was not reported, seasonal variation in fish samples was not addressed.
	Metric 14:	Health Outcomes Unrelated to Exposure	High	No differences in organism health were reported.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Medium	Analytical method was appropriate and limits of detection and percent recovery of spiked samples was reported. Lipid content was not reported and BAF was not lipid normalized.
	Metric 16:	Statistical Methods and Kinetic Calculations	High	Statistical methods were described and applied appropriately.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	High	The results were reasonable based on the method and were comparable to previous studies.
	Metric 18:	QSAR Models	N/A	The metric is not applicable to this study type.

Overall Quality Determination — High

Study Citation:	Lu, C. (2009). Prediction of environmental properties in water-soil-air systems for phthalates. Bulletin of Environmental Contamination and Toxicology 83(2):168-173.
OECD Harmonized Template:	Adsorption and Desorption
HERO ID:	807140

EXTRACTION

Parameter	**Data**
CASRN and Test Material	84-61-7; 0
Confidentiality, Type, Guideline	None; QSAR; other: Quantitative Structure-Property relationship model for estimation of Koc
Solvent, Reactivity, Storage, Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, Purity	Not Reported; Not Reported; Not Reported; Not Reported
Sampling Frequency, Sampling Details, and Number of Replicates	Not reported; Not reported; Not reported
pH, Test Temperature, Buffer, and Test Details	Not reported; Not reported; Not reported; QSPR model using the Lu index, which is based on the shortest distance matrix.
Matrix, Clay Silts and Organic Carbon, and CEC	Not Reported; Not reported; Not reported
Bulk Density and Matrix Details	Not reported; Not reported
Media, Recovery, and Statistics	Not reported; Not reported; Not reported
Transformation Products, Equilibrium Adsorption Details, and Equilibrium Desorption Details	Not reported; Not reported; Not reported
Reference Substance, Reference Substance Results, and Percent Adsorption	Not reported; Not reported; Not reported
Adsorption Coefficient Type, Adsorption Coefficient Results, Adsorption Coefficient Results Comments, and Adsorption Desorption Type	Not reported; Not reported; Not reported; Not reported
Partition Coefficient Type and Partition Coefficient Results	Log Koc; 4.47
Partition Coefficient Phase and Partition Coefficient Results	Not Reported; Not reported
Mass Balance	Not reported

EVALUATION

Domain	Metric	Rating	Comments
Domain 1: Test Substance			
Metric 1:	Test Substance Identity	High	The test substance was identified by common name and CASRN.
Metric 2:	Test Substance Purity	N/A	The metric is not applicable to the study type.
Domain 2: Test Design			
Metric 3:	Study Controls	N/A	The metric is not applicable to the study type.
Metric 4:	Test Substance Stability	N/A	The metric is not applicable to the study type.
Domain 3: Test Conditions			

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Study Citation:	Lu, C. (2009). Prediction of environmental properties in water-soil-air systems for phthalates. Bulletin of Environmental Contamination and Toxicology 83(2):168-173.
OECD Harmonized Template:	Adsorption and Desorption
HERO ID:	807140

			EVALUATION	
Domain		Metric	Rating	Comments
	Metric 5:	Test Method Suitability	N/A	The metric is not applicable to the study type.
	Metric 6:	Testing Conditions	N/A	The metric is not applicable to the study type.
	Metric 7:	Testing Consistency	N/A	The metric is not applicable to the study type.
	Metric 8:	System Type and Design	N/A	The metric is not applicable to the study type.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	The metric is not applicable to the study type.
	Metric 10:	Sampling Methods	N/A	The metric is not applicable to the study type.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	N/A	The metric is not applicable to the study type.
	Metric 12:	Test Substance Purity	N/A	The metric is not applicable to the study type.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	N/A	The metric is not applicable to the study type.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	The metric is not applicable to the study type.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	N/A	The metric is not applicable to the study type.
	Metric 16:	Statistical Methods and Kinetic Calculations	N/A	The metric is not applicable to the study type.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	N/A	The metric is not applicable to the study type.
	Metric 18:	QSAR Models	Uninformative	The QSPR model failed the standard error threshold of <0.3 and is therefore rated unacceptable.

Overall Quality Determination — Uninformative

Study Citation:	Cheng, X., Ma, L., Xu, D., Cheng, H., Yang, G., Luo, M.,in (2015). Mapping of phthalate esters in suburban surface and deep soils around a metropolis-Beijing, China. Journal of Geochemical Exploration 155:56-61.
OECD Harmonized Template:	Miscellaneous
HERO ID:	3022721

EXTRACTION

Parameter	**Data**
CASRN and Test Material	NR; dicyclohexyl phthalate
Confidentiality, Type, Guideline	None; Experimental - monitoring; Calculation - volatilization (not reported); Experimental - monitoring; Calculation - volatilization (not reported)
Solvent, Reactivity, Storage, Stability	NA; NR; NR; NR
Radiolabel, Source, State, Purity	NR; Soil from Beijing, China; NR; NA
Test Method Details, Test Condition Details, and Test Consistency Details	Data collected in monitoring study; 47 surface soil samples and core samples and 16 vicinal sub-samples weremixed fully to obtain one composite surface sample; NA
System Type Design	NA
Sampling Frequency and Sampling Details	1 sample time; Not Reported
Test Temperature	NA
Results Details	0.06 ±0.11 mg/kg in surface soil (mean) and 0.03 ±0.09 mg/kg in deep soil; volatility calculated but not reported
Analytical Method and Analytical Details	GC-FID; confirmation of the compounds by GC-MSD-EI-SIM
Transformation Products, Statistics, and Kinetics	NR; range, median and mean concentrations reported; NA
Reference Substance and Reference Substance Results	Analytical blank, spiked blank, spiked matrix; Average recoveries of PAEs were 75–130% with the relative standard deviations of 3–13% (n = 5)

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified definitively.
	Metric 2:	Test Substance Purity	N/A	Test purity is not applicable to this study type (monitoring).
Domain 2: Test Design				
	Metric 3:	Study Controls	N/A	The study did not require concurrent control groups.
	Metric 4:	Test Substance Stability	N/A	This metric is not applicable to monitoring studies.
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	High	The test method was suitable for the test substance.
	Metric 6:	Testing Conditions	Medium	There were reported deviations or omissions in testing conditions; however, sufficient data were reported to determine that the deviations and omissions were not likely to have a substantial impact on study results.
	Metric 7:	Testing Consistency	N/A	This metric is not applicable to monitoring studies.
	Metric 8:	System Type and Design	N/A	This metric is not applicable to monitoring studies.

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Study Citation:	Cheng, X., Ma, L., Xu, D., Cheng, H., Yang, G., Luo, M.,in (2015). Mapping of phthalate esters in suburban surface and deep soils around a metropolis-Beijing, China. Journal of Geochemical Exploration 155:56-61.
OECD Harmonized Template:	Miscellaneous
HERO ID:	3022721

			EVALUATION	
Domain		Metric	Rating	Comments
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	The metric is not applicable to this study type.
	Metric 10:	Sampling Methods	N/A	The metric is not applicable to this study type.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Low	Deficiencies in the outcome assessment methodology of the assessment or reporting were likely to have a substantial impact on results. Soil transport and volatility can be inferred from these monitoring results.
	Metric 12:	Test Substance Purity	High	The study reported the use of sampling methods that address the outcome(s) of interest, and used widely accepted methods/approaches for the chemical and media being analyzed.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	Low	Sources of variability and uncertainty in the measurements were reported in the study and there is concern that variability or uncertainty was likely to have a substantial impact on the results.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	The metric is not applicable to this study type.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Low	There was insufficient evidence presented to confirm that parent compound disappearance was not likely due to some other process.
	Metric 16:	Statistical Methods and Kinetic Calculations	High	Statistical methods or kinetic calculations were clearly described and address the dataset(s).
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Low	Due to limited information, evaluation of the reasonableness of the study results was not possible.
	Metric 18:	QSAR Models	N/A	A QSAR model was not reported.

Overall Quality Determination **Low**

Study Citation:	Cheng, Z., Li, H. H., Yu, L., Yang, Z. B., Xu, X. X., Wang, H. S., Wong, M. H. (2018). Phthalate esters distribution in coastal mariculture of Hong Kong, China. Environmental Science and Pollution Research 25(18):17321-17329.
OECD Harmonized Template:	Miscellaneous
HERO ID:	4728634

EXTRACTION

Parameter	**Data**
CASRN and Test Material	Not reported; DCHP
Confidentiality, Type, Guideline	None; Experimental; Experimental
Solvent, Reactivity, Storage, Stability	NA; NA; NA; NA
Radiolabel, Source, State, Purity	NA; NA; NA; NA Notes: DCHP
Test Method Details, Test Condition Details, and Test Consistency Details	Fish and sediment samples collected from 6 mariculture sites in Hong Kong and China; Surface sediment (0-5 cm; mariculture and non-mariculture) and farmed fish species collected: Red snapper (Lutjanus campechanus) (n = 26), orange spotted grouper (Epinephelus coioides) (n = 26), and snubnose pompano (Trachinotus blochii) (n = 17); Not applicable
System Type Design	Field study
Sampling Frequency and Sampling Details	Not applicable; sampling dates not provided; Sediment samples were collected via a stainless steel grab sampler; fish samples were collected, wrapped in foil, delivered and stored at -20C prior to analysis
Test Temperature	Site specific temperatures not reported
Results Details	Approximate concentrations in mariculture (MS) and nonmariculture (NS) sediment (mg/kg dw) and corresponding concentrations fish samples (mg/kg ww): Site M1: 1 (MS), 1 (NS), 0.04 (snubnose pompano), 0.02 (orange-spotted grouper), 0.10 (red snapper); Site M2: 2 (MS), 3 (NS), 0.08 (snubnose pompano), 0.04 (orange-spotted grouper), 0.03 (red snapper); Site H1: 5 (MS), 6 (NS), 0.08 (orange-spotted grouper), 0.15 (red snapper); Site H2: 1 (MS), 7 (NS), 0.02 (orange-spotted grouper); Site H3: 1 (MS), 1 (NS), 0.06 orange-spotted grouper), 0.10 (red snapper); Site H4: 8 (MS), 5 (NS), 0.11 (snubnose pompano), 0.02 (orange-spotted grouper), 0.02 (red snapper)
Analytical Method and Analytical Details	Preparation and measurements in sediment and fish samples were conducted following a method in a cited reference.; Analytical details described in Supplementary Materials, only available to authorized users.
Transformation Products, Statistics, and Kinetics	Not applicable; Analysis of the data was performed by two independent t tests, Wilcoxon rank sum test, one-way ANOVA, and Duncan's multiple range test ($p < 0.05$); Not applicable
Reference Substance and Reference Substance Results	Not applicable; Not applicable

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	Medium	The chemical of interest was identified by common acronym used for this phthalate ester; however the acronym was not defined in the paper.
	Metric 2:	Test Substance Purity	Low	Field sample sources reported; analytical standard source and purity not reported.
Domain 2: Test Design				
	Metric 3:	Study Controls	Medium	Procedural blanks were not included.
	Metric 4:	Test Substance Stability	Medium	Sample storage and limited preparation details were reported.
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	High	The monitoring study method was appropriate for the chemical of interest.

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Study Citation:	Cheng, Z., Li, H. H., Yu, L., Yang, Z. B., Xu, X. X., Wang, H. S., Wong, M. H. (2018). Phthalate esters distribution in coastal mariculture of Hong Kong, China. Environmental Science and Pollution Research 25(18):17321-17329.
OECD Harmonized Template:	Miscellaneous
HERO ID:	4728634

			EVALUATION	
Domain		Metric	Rating	Comments
	Metric 6:	Testing Conditions	Medium	No environmental conditions were reported.
	Metric 7:	Testing Consistency	N/A	This metric is not applicable to this type of study.
	Metric 8:	System Type and Design	High	Field samples are assumed to be in dynamic equilibrium.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	This metric is not applicable to this type of study.
	Metric 10:	Sampling Methods	Low	Organism species were reported; specific details were not reported for individual species.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Low	The outcome assessment did not quantify accumulation or report numerical concentrations in sediment.
	Metric 12:	Test Substance Purity	High	Sampling focused on appropriate species with acceptable sample sizes, and processing was appropriate. The same tissues for fish were analyzed across species.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	N/A	This metric is not applicable to this type of study.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	The metric is not applicable to this study type.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Low	The analytical method was not reported, detail in SI which was not available.
	Metric 16:	Statistical Methods and Kinetic Calculations	High	Statistical methods were described.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Low	The results were reasonable however BCF values were not reported.
	Metric 18:	QSAR Models	N/A	The metric is not applicable to this study type.

Overall Quality Determination — Medium

Study Citation:	Wu, J., Ma, T., Zhou, Z., Yu, N.,a, He, Z., Li, B., Shi, Y., Ma, D. (2019). Occurrence and fate of phthalate esters in wastewater treatment plants in Qingdao, China. Human and Ecological Risk Assessment 25(6):1547-1563.
OECD Harmonized Template:	Miscellaneous
HERO ID:	5442818

EXTRACTION

Parameter	**Data**
CASRN and Test Material	Not reported; Dicyclohexyl phthalate
Confidentiality, Type, Guideline	None; Experimental; Experimental
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; Standard solution of 16 PAEs purchased from O2SI, Inc (USA); Standard solution; NR Notes: DCHP
Test Method Details, Test Condition Details, and Test Consistency Details	WWTP Removal efficiency; Qingdao, China Rivers: Chengyang, Licun, and Haibo, which employ different treatment processes; A procedural blank, solvent blank, spiked blank, and sample duplicate were tested for every10 samples for quality control and quality assurance (QC/QA).
System Type Design	6890 gas chromatograph connected to a 5973 mass spectrometer(GC-MS) (Agilent Technologies, Avondale, PA, USA) equipped with electron impact and selective ion monitoring modes.
Sampling Frequency and Sampling Details	57 sewage and 9 sludge samples; PAEs were extracted from 100 mL liquid samples thrice using 50 mL n-hexane, evaporated extracts were reduced to 1 mL and measured using gas chromatography-mass spectrometry (GC-MS).
Test Temperature	column initial temperature of 80°C maintained for 1.0 min, increased to 180C at a rate of 20C/min with 10 min holding time, and increased to 300°C at 2°C/min and maintained for 10 min
Results Details	Removal % Chengyang: 69.38, Licun: 68.60, Haibo: 97.97
Analytical Method and Analytical Details	GC-MS equipped with electron impact and selective ion monitoring modes; instrument detection limits ranged from 1-9 pg
Transformation Products, Statistics, and Kinetics	Not reported; Not reported; Not reported
Reference Substance and Reference Substance Results	Not reported; Not reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified clearly.
	Metric 2:	Test Substance Purity	Medium	Purity of standard solution was not provided but not likely to influence the study results.
Domain 2: Test Design				
	Metric 3:	Study Controls	N/A	This metric is not applicable to this type of study.
	Metric 4:	Test Substance Stability	Medium	Details regarding the test substance homogeneity, preparation, and storage conditions were not reported but their omission is not likely to influence the study results.
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	High	This metric met the criteria for high confidence as expected for this type of study.
	Metric 6:	Testing Conditions	High	This metric met the criteria for high confidence as expected for this type of study.
	Metric 7:	Testing Consistency	High	This metric met the criteria for high confidence as expected for this type of study.
	Metric 8:	System Type and Design	High	This metric met the criteria for high confidence as expected for this type of study.

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Study Citation:	Wu, J., Ma, T., Zhou, Z., Yu, N.,a, He, Z., Li, B., Shi, Y., Ma, D. (2019). Occurrence and fate of phthalate esters in wastewater treatment plants in Qingdao, China. Human and Ecological Risk Assessment 25(6):1547-1563.
OECD Harmonized Template:	Miscellaneous
HERO ID:	5442818

		EVALUATION		
Domain		Metric	Rating	Comments
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	High	This metric met the criteria for high confidence as expected for this type of study.
	Metric 10:	Sampling Methods	N/A	The metric is not applicable to this study type.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	High	The outcome assessment methodology addressed the intended outcome of interest.
	Metric 12:	Test Substance Purity	High	This metric met the criteria for high confidence as expected for this type of study.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	High	No confounding variables were noted or identified.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	The metric is not applicable to this study type.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	High	This metric met the criteria for high confidence as expected for this type of study.
	Metric 16:	Statistical Methods and Kinetic Calculations	N/A	This metric is not applicable to this type of study.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Medium	The study results were reasonable.
	Metric 18:	QSAR Models	N/A	The metric is not applicable to this study type.

Overall Quality Determination — High

Study Citation:	Zeng, F., Cui, K., Xie, Z., Liu, M., Li, Y., Lin, Y., Zeng, Z., Li, F. (2008). Occurrence of phthalate esters in water and sediment of urban lakes in a subtropical city, Guangzhou, South China. Environment International 34(3):372-380.
OECD Harmonized Template:	Miscellaneous
HERO ID:	698257

EXTRACTION

Parameter	**Data**
CASRN and Test Material	Not Reported; Dicyclohexyl phthalate
Confidentiality, Type, Guideline	None; Environmental monitoring of both sediment and water; Environmental monitoring of both sediment and water
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; monitoring study of 15 urban lakes in Guangzhou city; NR; NR Notes: Analytical standards from Dr. Ehrenstorfer (Augsburg, Germany)
Test Method Details, Test Condition Details, and Test Consistency Details	NA; 15 urban lakes in Guangzhou city. Water DOC and sediment TOC in the urban lake of this area were investigated and ranged from 1.13 to 6.87%, 0.281 to 3.76 mg L−1, with the average value of 3.34%, 1.97 mg L−1, respectively.; To eliminate randomicity, each sample consisted of 5 subsamples collected within a surface area of 100×100 m, about 20 m far from the shore, and were well mixed.
System Type Design	NR
Sampling Frequency and Sampling Details	Not Reported; 30 samples, 15 water and sediment samples each, collected from May 10–15, 2005. Water samples were collected in 10 L pre-cleaned glass bottles using a frame that allows the bottle to be opened underwater to avoid the collection of the surface microlayer. The samples were stored at 4±2 °C in a cooler. Sediments were collected using a stainless steel grab sampler. The top 10-cm layer of sediments was scooped, using a pre-cleaned stainless steel scoop, into solvent rinsed glass jars. The samples were cooled in a refrigerator (0 °C) during transport to the laboratory where they were stored at −20 °C.
Test Temperature	mean air temperature of 21.8 °C for Guangzhou area of about 7500 sq. km
Results Details	Dissolved phase: ND-0.076 ug/L (0.076 Mean), Detectable frequency 7%. Sediment phase: ND-0.22 ug/g dw (0.074 Mean), Detectable frequency 53%
Analytical Method and Analytical Details	GC-MS; For each batch of 10 field samples, a procedural blank, a spiked blank, a spiked matrix sample, a spiked matrix duplicate, and a sample duplicate were processed.
Transformation Products, Statistics, and Kinetics	NR; Not Reported; NR
Reference Substance and Reference Substance Results	NR; NR

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified definitively.
	Metric 2:	Test Substance Purity	N/A	Not applicable: Monitoring study
Domain 2: Test Design				
	Metric 3:	Study Controls	N/A	The study did not require concurrent control groups.
	Metric 4:	Test Substance Stability	High	The test substance stability, homogeneity, preparation, and storage conditions were reported (e.g., mixing temperature, stock concentration, stirring methods, centrifugation or filtration), and were appropriate for the study
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	High	The test method was suitable for the test substance.

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Study Citation:	Zeng, F., Cui, K., Xie, Z., Liu, M., Li, Y., Lin, Y., Zeng, Z., Li, F. (2008). Occurrence of phthalate esters in water and sediment of urban lakes in a subtropical city, Guangzhou, South China. Environment International 34(3):372-380.
OECD Harmonized Template:	Miscellaneous
HERO ID:	698257

			EVALUATION	
Domain		Metric	Rating	Comments
	Metric 6:	Testing Conditions	N/A	The metric is not applicable to this study type.
	Metric 7:	Testing Consistency	N/A	The metric is not applicable to this study type.
	Metric 8:	System Type and Design	N/A	The metric is not applicable to this study type.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	The metric is not applicable to this study type.
	Metric 10:	Sampling Methods	N/A	The metric is not applicable to this study type.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Medium	There were minor differences between the assessment methodology and the intended outcome assessment; concentrations in soil and water measured, but partition coefficients were not calculated.
	Metric 12:	Test Substance Purity	High	The study reported the use of sampling methods that address the outcome of interest, and used widely accepted methods/approaches for the chemical and media being analyzed and no notable uncertainties or limitations were expected to influence results.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	Low	Sources of variability and uncertainty in the measurements and statistical techniques and between study groups (if applicable) were reported in the study.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	The metric is not applicable to this study type.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Medium	The target chemical concentration, extraction efficiency, percent recovery, or mass balance were not reported; however, these omissions were not likely to have a substantial impact on study results.
	Metric 16:	Statistical Methods and Kinetic Calculations	High	Statistical methods or kinetic calculations were clearly described and address the dataset(s).
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Medium	The study results were reasonable
	Metric 18:	QSAR Models	N/A	The metric is not applicable to this study type.

Overall Quality Determination — Medium

List of Abbreviations and Acronyms for Data Quality Evaluation and Extraction Tables

Term	Definition
BAF	Biaccumulation Factor
BCF	Bioconcentration Factor
BMF	Biomagnification Factor
BSAF	Biota-sediment Accumulation Factor
C	Concentration
CASRN	Chemical Abstract Service registry number
DOC	Dissolved Organic Carbon
dw	Dry weight
DW	Drinking Water
DWTP	Drinking Water Treatment Plant
EPA	Environmental Protection Agency
ESI	Electrospray Ionisation
FID	Flame Ionisation Detector
FPD	Flame Photometric Detector
GC	Gas Chromatography
g/L	Grams per Liter
HLC	Henry's Law Constant
HPLC	High-performance liquid chromatography
ISO	International Organization for Standardization
K_{oa}	Octanol-Air partition coefficient
K_{oc}	Organic carbon-water partition coefficient
K_{ow}	Octanol-Water partition coefficient
L/d	Liters per day
LOD	Limit of Detection
LOQ	Limit of Quantification
lw	Lipid weight
M	Molarity (mol/L = moles per Liter)
mL/min	Milliliters per minute
mM	Millimolar
MDL	Method Detection Limit
mg/kg	Milligrams per Kilogram
mg/L	Milligrams per Liter
mg/m^3	Milligrams per cubic meter
MRL	Method Reporting Limit
MS	Mass Spectrometry
n	Sample Size
N/A	Not applicable
ND	Non-Detection
ng/L	Nanograms per Liter

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Term	Definition
nm	Nanometers
NR	Not Reported
OECD	Organisation for Economic Co-operation and Development
· OH	Hydroxyl radical
OPE	Organophosphate Ester
pg/L	Picograms per Liter
ppm	parts per million
QSAR	Quantatative Structure Activity Relationship
RSD	Relative Standard Deviation
SI	Supplemental Information
SIM	Selected Ion Monitoring
SPE	Solid Phase Extraction
STP	Sewage Treatment Plant
TMF	Trophic Magnification Factor
TOC	Total Organic Carbon
TOF	Time of Flight
μg/L or μg/mL	micrograms per liter or per milliliter
UPLC	Ultra-performance liquid chromatography
US or USA	United States of America
UV (UV-Vis)	Ultra Violet (Visible)
ww	Wet Weight
WWTP	Wastewater Treatment Plant