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1 **Improving plant bioaccumulation science through consistent reporting of**
2 **experimental data**

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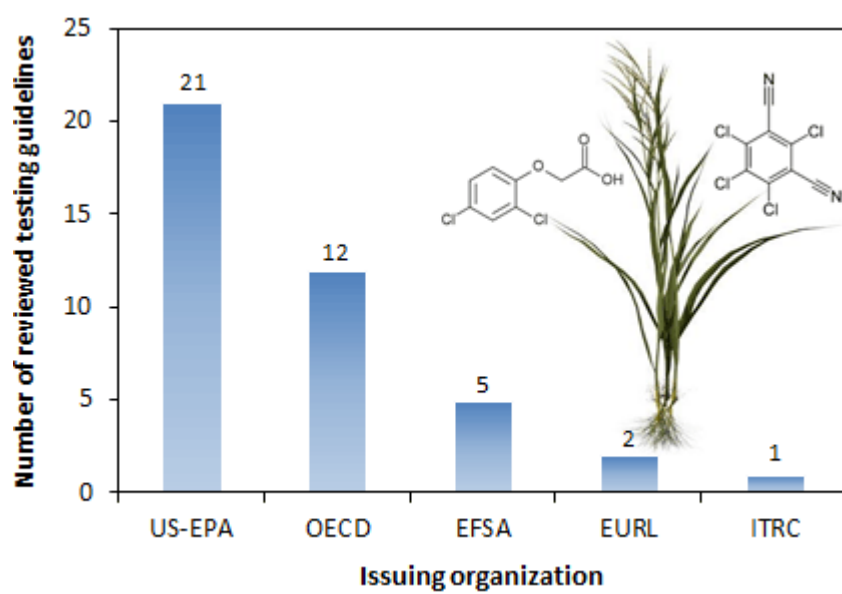
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14 **TOCart**



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17 **Abstract**

18 Experimental data and models for plant bioaccumulation of organic contaminants play
19 a crucial role for assessing the potential human and ecological risks associated with chemical
20 use. Plants are receptor organisms and direct or indirect vectors for chemical exposures to all
21 other organisms. As new experimental data are generated they are used to improve our
22 understanding of plant-chemical interactions that in turn allows for the development of better
23 scientific knowledge and conceptual and predictive models. The interrelationship between
24 experimental data and model development is an ongoing, never-ending process needed to
25 advance our ability to provide reliable quality information that can be used in various contexts
26 including regulatory risk assessment. However, relatively few standard experimental
27 protocols for generating plant bioaccumulation data are currently available and because of
28 inconsistent data collection and reporting requirements, the information generated is often less
29 useful than it could be for direct applications in chemical assessments and for model
30 development and refinement. We review existing testing guidelines, common data reporting
31 practices, and provide recommendations for revising testing guidelines and reporting
32 requirements to improve bioaccumulation knowledge and models. This analysis provides a
33 list of experimental parameters that will help to develop high quality datasets and support
34 modeling tools for assessing bioaccumulation of organic chemicals in plants and ultimately
35 addressing uncertainty in ecological and human health risk assessments.

36

37 **Keywords:** bioaccumulation modeling; biotransformation; plant uptake; organic
38 contaminants; reporting requirements; testing guidelines

39

40 1. Introduction

41 Terrestrial plants constitute the largest global mass fraction of living organisms and
42 are the primary food source for humans and most terrestrial animals (Houghton et al., 2009).
43 Plants take up, translocate, transform, and accumulate organic chemicals that are not essential
44 for plant growth and development (ITRC, 2011; U.S. EPA, 2012f), thereby contributing to the
45 cycling of organic contaminants from local to global scales (Collins et al., 2011). Plants are
46 subject to toxic effects from exposure to chemical stressors. Plants are also direct and indirect
47 vectors for chemical exposures to higher trophic level organisms. Environmental
48 concentrations and plant bioaccumulation (toxicokinetics) determine the likelihood for
49 adverse effects to plants directly and to subsequent exposures and potential adverse effects to
50 higher trophic level organisms. The extent of bioaccumulation is a function of substance-
51 specific physicochemical properties, plant species-specific characteristics, and environmental
52 conditions (Collins et al., 2011; Fantke et al., 2014; Trapp, 2015). Understanding plant uptake
53 and bioaccumulation is crucial for a variety of regulatory applications including the
54 authorization of formulations containing pesticides (EC, 2009) or biocides (EC, 1998), and
55 for commercial chemicals falling under the REACH regulation (EC, 2006). Plant uptake has
56 also been exploited to phytoremediate chemically contaminated sites and to delineate the
57 extent of groundwater plumes using plants as biomonitors. The potential influence of plants in
58 the overall fate and persistence of chemicals in the environment has been modelled at various
59 scales but is largely unknown, particularly for chemicals that may be subject to degradation
60 on or in plants (Cousins and Mackay, 2001; Undeman and McLachlan, 2011).

61 Experimentally, plant bioaccumulation data are collected from *in vivo* and *in vitro*
62 studies. *In vivo* studies (field and greenhouse grown plants) usually focus on accumulation
63 and dissipation from harvested plant components or whole plants and attempt to simulate
64 realistic environmental conditions (Burrows et al., 2002). In contrast, *in vitro* studies (cell
65 cultures) provide information on transport and degradation processes in plant cells under

66 controlled laboratory conditions (Schwitzguébel et al., 2011). Data from *in vivo* and *in vitro*
67 studies demonstrate the capacity of plants to biotransform and bioaccumulate a wide range of
68 organic contaminants (Bacci et al., 1990; Eggen et al., 2011; Fantke and Juraske, 2013; Jones
69 and Duarte-Davidson, 1997; Liu et al., 2009; Macherius et al., 2012; Mikes et al., 2009;
70 Samsøe-Petersen et al., 2002; Scheunert et al., 1994; Sharma et al., 2007; St-Amand et al.,
71 2007; Stahl et al., 2009; Willis and McDowell, 1987). For most chemical-plant species
72 combinations no experimental bioaccumulation and biotransformation data exist (Arnot et al.,
73 2013; Fantke et al., 2014) and in the few cases where data are available, the critical
74 information necessary to assess data reproducibility and interpretability are often lacking
75 (Fantke and Juraske, 2013).

76 Mathematical models are used to complement expensive and time-consuming
77 experimental studies for generalizing and extrapolating findings from specific experimental
78 scenarios and as input for decisions in exposure- and risk-related science-policy fields.
79 Models thereby show considerable potential for improving the basic understanding of
80 contaminant transport processes in plants (Gobas et al., 2016). In this study, we seek to help
81 identifying key test parameters that are required to improve the interpretation and evaluation
82 of plant bioaccumulation data, and to support the development, parameterization, application
83 and evaluation of plant bioaccumulation models.

84 We first review existing plant bioaccumulation testing guidelines and their reporting
85 requirements to identify whether information crucial for interpreting experimental data and
86 for supporting modeling is reported. Next, we give a brief overview of data that are essential
87 for developing and testing plant bioaccumulation models. Finally, we evaluate how data
88 reporting requirements in current test protocols can be improved to better support the
89 interpretation of experimental data and their use in plant bioaccumulation modeling. We will
90 thereby emphasize that reporting the most relevant additional data is usually feasible and does
91 not provide additional financial challenges. Overall, our study aims to improve the

92 understanding of plant bioaccumulation in support of various regulatory and non-regulatory
93 applications.

94

95 **2. Available bioaccumulation testing and data reporting guidelines**

96 2.1. Existing guidelines and their scope

97 Current plant bioaccumulation testing guidelines were reviewed ($n = 41$) with focus
98 on the following key question: Do the reporting recommendations in current testing
99 guidelines include the key parameters needed to adequately interpret and quantify the
100 experimental results and facilitate the use of measured data in models for risk and impact
101 assessment? Guidelines were categorized according to their relevance for quantifying
102 bioaccumulation and/or biotransformation in terrestrial plants via modeling approaches. High
103 relevance is given when either plant uptake, accumulation or transformation/other removal
104 was addressed in a quantitative way. Medium relevance is given when uptake, accumulation
105 or transformation was addressed, but could not be quantitatively associated with chemical
106 application (e.g. pesticides) or emission or when specifically residue sampling and analysis
107 procedures were addressed. Low relevance is given when neither plant uptake, accumulation
108 or transformation was the focus, but when other metrics associated with plant
109 bioaccumulation were addressed, such as crop damage, human contact levels (as input for
110 occupational exposure), or transformation products in soil that could enter the plant.

111 Few guidelines from national and international organizations address one or more
112 aspects involved in the testing of uptake, translocation and bioaccumulation of chemicals in
113 plants as listed in **Table 1**. The U.S. Environmental Protection Agency (US-EPA) established
114 a series of ecological effect, residue chemistry, fate, transport and transformation, as well as
115 occupational and residential exposure test guidelines developed by the Office of Chemical
116 Safety and Pollution Prevention and the Office of Prevention, Pesticides and Toxic
117 Substances for use in the experimental testing of chemicals (U.S. EPA, 1996a, b, c, d, e, f, g,

118 h, i, j, k, l, m, 2008a, b, 2012a, b, c, d, e, f). The EU Reference Laboratories for Residues of
 119 Pesticides (EURL) and the European Food Safety Authority (EFSA) developed guidelines
 120 focusing on the sampling of plants in the frame of pesticide residue testing (EFSA, 2010,
 121 2012, 2013, 2014a, b; EU RLRP, 2011, 2013). The Interstate Technology and Regulatory
 122 Council (ITRC) provides guidelines for the evaluation of contaminated sediment sites,
 123 thereby also addressing plant uptake (ITRC, 2011). Finally the Organisation for Economic
 124 Co-operation and Development (OECD) established several guidelines for the testing of
 125 chemicals for use in studies measuring the distribution of chemicals in the plant environment
 126 (OECD, 1992, 1997, 2002, 2006a, b, 2007a, b, c, d, e, 2008, 2009).

127
 128 **Table 1** Existing guidelines and standards for different contexts of testing bioaccumulation of
 129 chemicals in plants, plant environments and plant-based commodities, and their relevance for
 130 quantification of bioaccumulation and/or biotransformation in terrestrial plants.

Issuing organization	Guideline	Purpose	Relevance
U.S. Environmental Protection Agency	Fate, Transport and Transformation Test Guidelines: Terrestrial Field Dissipation, OPPTS 835.6100 (U.S. EPA, 2008a)	Plant uptake is assessed as one of several field dissipation pathways; restricted to pesticides; bioaccumulation or biotransformation in plants not considered	Medium
	Fate, Transport and Transformation Test Guidelines: Forestry Dissipation, OPPTS 835.6300 (U.S. EPA, 2008b)	Uptake into tree litter assessed as one of several field dissipation pathways; restricted to bioaccumulation in tree litter, soil and water	High
	Ecological Effects Test Guidelines: Background and Special Considerations - Tests with Terrestrial and Aquatic Plants, Cyanobacteria, and Terrestrial Soil-Core Microcosms, OCSP 850.4000 (U.S. EPA, 2012a)	Exposure damage to plants and other organisms including non-target plants is assessed; quantitative bioaccumulation or biotransformation not considered	Low
	Ecological Effects Test Guidelines: Seedling	Effects of substances on plants during early critical development	Low

Issuing organization	Guideline	Purpose	Relevance
	Emergence and Seedling Growth, OCSPP 850.4100 (U.S. EPA, 2012b)	stages are measured; quantitative bioaccumulation or biotransformation not considered	
	Ecological Effects Test Guidelines: Vegetative Vigor, OCSPP 850.4150 (U.S. EPA, 2012c)	Effects of foliar applied substances on plants during vegetative growth are measured; restricted to spray application (i.e. not applicable for root uptake); quantitative bioaccumulation or biotransformation not considered	Low
	Ecological Effects Test Guidelines: Early Seedling Growth Toxicity Test, OCSPP 850.4230 (U.S. EPA, 2012d)	Data on the phytotoxicity of substances are provided; quantitative bioaccumulation or biotransformation not considered	Low
	Ecological Effects Test Guidelines: Terrestrial Plants Field Study, OCSPP 850.4300 (U.S. EPA, 2012e)	Field experiments with focus on plant damage are conducted; bioaccumulation or biotransformation not considered	Low
	Ecological Effects Test Guidelines: Plant Uptake and Translocation Test, OCSPP 850.4800 (U.S. EPA, 2012f)	Data on the quantity of substances incorporated in plant tissues and the potential for entry into food chains are provided; consideration of quantitative plant uptake and bioaccumulation	High
	Residue Chemistry Test Guidelines: Nature of the Residue – Plants, Livestock, OPPTS 860.1300 (U.S. EPA, 1996d)	Qualitative metabolic fate of an active ingredient applied to a plant is assessed; quantitative bioaccumulation or biotransformation not considered; restricted to pesticides	High
	Residue Chemistry Test Guidelines: Residue Analytical Method, OPPTS 860.1340 (U.S. EPA, 1996e)	Analytical methods are tested to determine all components of the total toxic residue; quantitative bioaccumulation or biotransformation not considered	Medium
	Residue Chemistry Test Guidelines: Multiresidue Method, OPPTS 860.1360 (U.S. EPA, 1996f)	Analytical methods are applied to confirm the presence or absence of many pesticides and their metabolites in commodities; quantitative bioaccumulation or biotransformation not considered	Low
	Residue Chemistry Test Guidelines: Storage Stability Data, OPPTS 860.1380 (U.S. EPA, 1996g)	Stability or decomposition rate of total toxic residue in or on raw/processed agricultural commodity between harvest or	Medium

Issuing organization	Guideline	Purpose	Relevance
		sample collection and analysis are validated; quantitative bioaccumulation or biotransformation not considered	
	Residue Chemistry Test Guidelines: Water, Fish, and Irrigated Crops, OPPTS 860.1400 (U.S. EPA, 1996h)	Levels of pesticide residues are assessed in water, fish, and irrigated crops; restricted to application to water to control aquatic pests; restricted to pesticides	High
	Residue Chemistry Test Guidelines: Crop Field Trials, OPPTS 860.1500 (U.S. EPA, 1996i)	Magnitude of pesticide residues are assessed in or on raw agricultural commodities; designed for field experiments, but restricted to pesticides	High
	Residue Chemistry Test Guidelines: Processed Food/Feed, OPPTS 860.1520 (U.S. EPA, 1996j)	It is assessed whether residues in raw commodities may be expected to degrade or concentrate during food processing (i.e. not applicable for plant uptake); restricted to time after harvest, restricted to pesticides	High
	Residue Chemistry Test Guidelines: Proposed Tolerances, OPPTS 860.1550 (U.S. EPA, 1996k)	Tolerance levels are obtained based on maximum residues during field trials; quantitative bioaccumulation or biotransformation not considered	Low
	Residue Chemistry Test Guidelines: Confined Accumulation in Rotational Crops, OPPTS 860.1850 (U.S. EPA, 1996l)	Nature and amount of pesticide residue uptake in rotational crops are assessed; restricted to pesticides	High
	Residue Chemistry Test Guidelines: Field Accumulation in Rotational Crops, OPPTS 860.1900 (U.S. EPA, 1996m)	Amount of pesticide residue uptake in rotational crops is assessed under actual field-use conditions; restricted to pesticides	High
	Occupational and Residential Exposure Test Guidelines: Background for Post-application Exposure Monitoring Test Guidelines, OPPTS 875.2000 (U.S. EPA, 1996a)	Time necessary is assessed for pesticide residues at the treated site to decline to allowable human reentry levels (i.e. not applicable for plant uptake); restricted to pesticides	Low

Issuing organization	Guideline	Purpose	Relevance
	Occupational and Residential Exposure Test Guidelines: Foliar Dislodgeable Residue Dissipation, OPPTS 875.2100 (U.S. EPA, 1996b)	Pesticide residues are assessed which are deposited on and remain on surfaces after pesticide application (i.e. not applicable for plant uptake); restricted to pesticides	Medium
	Occupational and Residential Exposure Test Guidelines: Data Reporting and Calculations, OPPTS 875.2900 (U.S. EPA, 1996c)	Detectable dislodgeable residues are assessed of the pesticide on surfaces to which the pesticide was applied (i.e. not applicable for plant uptake); restricted to pesticides	Low
EU Reference Laboratories for Residues of Pesticides	Method Validation & Quality Control Procedures for Pesticide Residues Analysis in Food & Feed, SANCO/12495/2011 (EU RLRP, 2011)	Sampling procedure is evaluated as part of laboratory tests (i.e. not applicable for plant uptake or transformation tests); restricted to pesticides	Medium
	Guidance Document on Analytical Quality Control and Validation Procedures for Pesticide Residues Analysis in Food and Feed, SANCO/12571/2013 (EU RLRP, 2013)	Sampling procedure and sampling quality control are evaluated as part of laboratory tests (i.e. not applicable for plant uptake or transformation tests); restricted to pesticides	Medium
European Food Safety Authority	Standard Sample Description for Food and Feed (EFSA, 2010)	Sampling procedure is evaluated as part of laboratory tests (i.e. not applicable for plant uptake or transformation tests); restricted to pesticides	Medium
	Use of the EFSA Standard Sample Description for the Reporting of Data on the Control of Pesticide Residues in Food and Feed According to Regulation (EC) No 396/2005; including revision 1 and version 2013 data collection (EFSA, 2012, 2013, 2014b)	Sampling procedure is evaluated part of laboratory tests for the reporting of the national results of the pesticide monitoring (i.e. not applicable for plant uptake or transformation tests); restricted to pesticides	Medium
	EFSA Guidance Document for Evaluating Laboratory and Field Dissipation Studies to Obtain DegT50 Values of Active Substances of Plant Protection Products and Transformation Products of	Degradation rates of active substances and transformation products in soil are assessed and crop interception values are selected (i.e. not applicable for plant uptake or transformation tests); restricted to pesticides	Low

Issuing organization	Guideline	Purpose	Relevance
	these Active Substances in Soil (EFSA, 2014a)		
Interstate Technology and Regulatory Council	Incorporating Bioavailability Considerations into the Evaluation of Contaminated Sediment Sites (ITRC, 2011)	Plant uptake is assessed as one out of several considered pathways of sediment dissipation; bioaccumulation or biotransformation in plants not considered	Medium
Organisation for Economic Co-operation and Development	OECD Guidelines for the Testing of Chemicals, Terrestrial Plant Test: Seedling Emergence and Seedling Growth Test, Test no. 208 (OECD, 2006a)	Negative effects on seedling emergence and growth are assessed; restricted to soil application (i.e. not applicable for foliar uptake); bioaccumulation or biotransformation not considered	Low
	OECD Guidelines for the Testing of Chemicals, Terrestrial Plant Test: Vegetative Vigour Test, Test no. 227 (OECD, 2006b)	Negative effects on vegetative vigor of plants are assessed; restricted to spray application (i.e. not applicable for root uptake); bioaccumulation or biotransformation not considered	Low
	OECD Guidelines for the Testing of Chemicals: Ready Biodegradability, Test no. 301 (OECD, 1992)	Chemicals are screened for ready biodegradability in an aerobic aqueous medium; not applicable for plant uptake or plant tissue sample testing	Medium
	OECD Guidelines for the Testing of Chemicals: Aerobic and Anaerobic Transformation in Soil, Test no. 307 (OECD, 2002)	Aerobic and anaerobic transformation in soil is evaluated; includes formation and decline of transformation products (i.e. not applicable for plant uptake or transformation tests)	Low
	OECD Guidelines for the Testing of Chemicals: Metabolism in Crops, Test no. 501 (OECD, 2007a)	Total radioactive residues, transformation products and pathways are estimated in crops after treatment; rates of uptake and degradation not considered; intended for pesticides	High
	OECD Guidelines for the Testing of Chemicals: Metabolism in Rotational Crops, Test no. 502 (OECD, 2007b)	Potential of chemicals and their soil transformation products to accumulate in rotational crops is assessed; restricted to pesticides	High
	OECD Guidelines for the Testing of Chemicals:	Residues from accumulation in rotational crops via soil uptake	High

Issuing organization	Guideline	Purpose	Relevance
	Residues in Rotational Crops, Limited Field Studies, Test no. 504 (OECD, 2007c)	under field conditions are assessed; restricted to pesticides	
	OECD Guidelines for the Testing of Chemicals: Stability of Pesticide Residues in Stored Commodities, Test no. 506 (OECD, 2007d)	Stability time period in crop commodities is analyzed between sampling and analysis (i.e. not applicable for plant uptake or transformation tests)	Low
	OECD Guidelines for the Testing of Chemicals: Nature of the Pesticide Residues in Processed Commodities - High Temperature Hydrolysis, Test no. 507 (OECD, 2007e)	Magnitude of residues in processed food commodities is assessed (compared to raw agricultural commodities); restricted to post-harvest processes	Medium
	OECD Guidelines for the Testing of Chemicals: Magnitude of the Pesticide Residues in Processed Commodities, Test no. 508 (OECD, 2008)	Distribution of residues of active ingredients and degradation products is quantified in processed commodities resulting from processing; not applicable for plant uptake; restricted to post-harvest processes	High
	OECD Guidelines for the Testing of Chemicals: Crop Field Trial, Test no. 509 (OECD, 2009)	Magnitude of residues is assessed in or on raw agricultural commodities and dissipation rate after field application; restricted to pesticides	High
	OECD Series on Testing and Assessment, Guidance Document for the Conduct of Studies of Occupational Exposure to Pesticides During Agricultural Application, OCDE/GD(97)148 (OECD, 1997)	Worker exposure during and after field application of pesticides is assessed (i.e. not applicable for plant uptake or transformation tests); restricted to pesticides	Low

131

132 2.2. The role of data reporting requirements

133 Most test guidelines provide general reporting recommendations for test species,

134 pathway analysis and sample extraction. Of these, some US-EPA and OECD guidelines

135 provide a good starting point to improve the quantitative understanding of bioaccumulation

136 and biotransformation in plants. These guidelines focus on general bioaccumulation in plant

137 tissue (U.S. EPA, 2012f), biotransformation in crops (OECD, 2007a) and rotational crops
138 (OECD, 2007b), accumulation of pesticides in rotational crops under confined (U.S. EPA,
139 1996l) and actual field conditions (OECD, 2007c; U.S. EPA, 1996m), and residual pesticide
140 concentrations and biotransformation after harvest in raw (OECD, 2009; U.S. EPA, 1996i)
141 and processed agricultural crop-based commodities (OECD, 2008; U.S. EPA, 1996j). EURL
142 provides extensive reporting guidelines for sampling of pesticide residues in plants (EU
143 RLRP, 2011, 2013). A key limitation is that none of the existing guidelines discusses or
144 provides guidance on how to further use the experimental data (study conditions,
145 measurement results, etc.) to support plant bioaccumulation modeling that is used to
146 complement experimental data in several science-policy fields. Further, except EURL (EU
147 RLRP, 2011, 2013), existing guidelines do not provide information on how to determine
148 uncertainty associated with measurement, sampling and analytical tools with respect to a
149 standardized interpretability of different testing designs and with respect to reporting
150 measurement uncertainty.

151 All in all, there is no existing testing guideline that provides sufficient information of
152 how to consistently report and interpret testing data or how to use experimental results as such
153 and as input in plant bioaccumulation models applied in regulation and decision support. Most
154 importantly, guidelines do not include requirements for relevant plant and exposure medium
155 characteristics, relevant environmental condition parameters, and applied formulation and
156 substance properties, although most of these aspects can be readily obtained and do not
157 require additional experimental equipment. As a consequence, current data reporting gaps in
158 experimental testing studies and underlying guidelines are recognized important limitations in
159 plant bioaccumulation models (Arnot et al., 2013; Environment Agency, 2006; Fantke and
160 Juraske, 2013; Fryer and Collins, 2003; Gobas et al., 2016; McKone and Maddalena, 2007).
161 However, several existing guidelines already provide a good starting point in terms of data
162 reporting requirements and these guidelines could be slightly modified to provide critical

163 information that could be used to improve plant bioaccumulation modeling. For that, it is
164 important to understand the data that are required in bioaccumulation modeling, which is
165 outlined in the following.

166

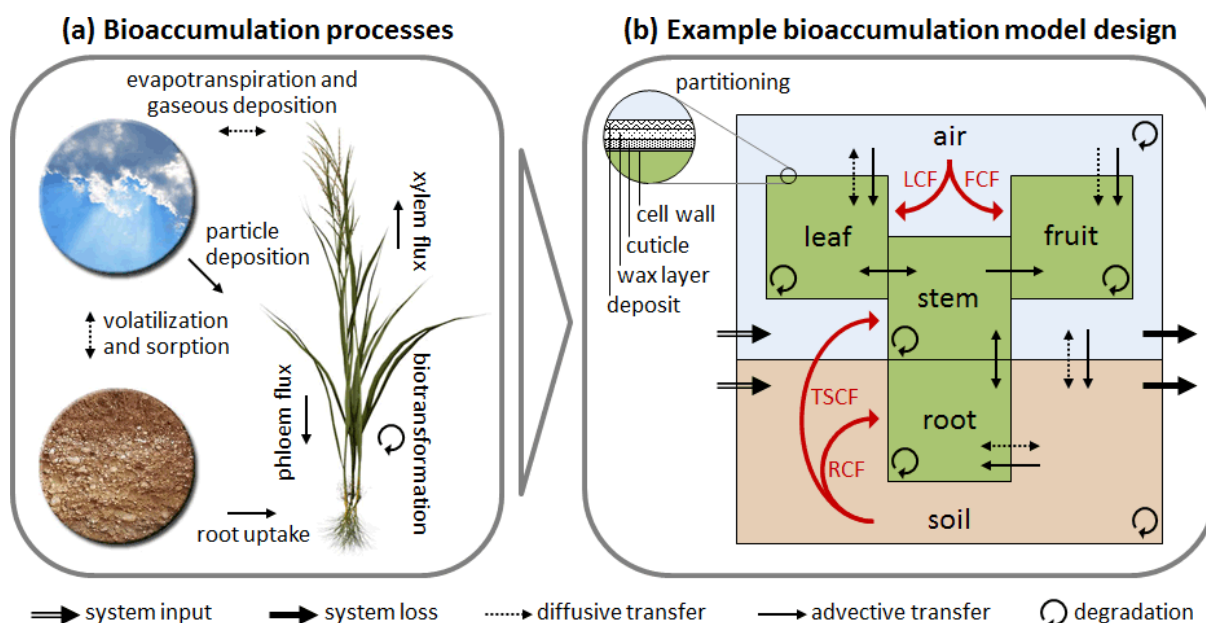
167 **3. Plant bioaccumulation models and their application**

168 3.1. Framework for plant bioaccumulation modeling

169 Mathematical models are often used to better understand experimental data obtained
170 under defined test conditions. Models also help the extrapolation of experimental data from
171 defined test conditions to specific environmental scenarios in an attempt to address various
172 regulatory questions. Key processes described in plant bioaccumulation models are direct
173 application onto the plant (e.g. agricultural pesticide applications), gaseous and dry/wet
174 particle deposition from air onto cuticles, evaporation from cuticles and transpiration through
175 leaf stomata, root uptake with soil pore water, diffusion between soil gas and root phases,
176 chemical and microbial transformation in plant tissue, chemical partitioning between tissues
177 and phases, as well as translocation with xylem transpiration and phloem assimilation
178 streams. Furthermore, re-volatilization from soil, leaching toward groundwater, soil surface
179 run-off, wash-off from plants, wind-drift in air and plant growth are often modeled processes
180 influencing the distribution and accumulation of chemicals in plants. Detailed process
181 descriptions are found elsewhere (Collins et al., 2006; Collins et al., 2011; Fantke et al., 2011;
182 Riederer, 1990; Trapp and Legind, 2011; Trapp and Mc Farlane, 1995). Different types of
183 plant bioaccumulation models are described elsewhere (e.g. Gobas et al., 2016).

184 Models are generally not accepted until they can be evaluated using results from tests
185 collected under a variety of conditions. Most models rely on measured data from field and
186 laboratory tests with respect to various input variables (e.g. air temperature, plant water
187 content) and process-related parameters (e.g. degradation rates in plant components),
188 depending on each model's scope and level of detail. Fig. 1 shows conceptually how key

189 uptake, partitioning, translocation and degradation processes measured in experimental plant
 190 bioaccumulation tests (Fig. 1a) can be translated into modeled systems based on
 191 interconnected environmental and plant compartments (Fig. 1b).
 192



194 **Fig. 1** – Schematic representation of main processes relevant in plant bioaccumulation studies
 195 (a) and their representation in a mechanistic plant bioaccumulation models (b): Red arrows
 196 indicate steady-state concentration ratios between leaf (LCF), fruit (FCF), stem (TSCF), root
 197 (RCF) and external solution, respectively; black arrows indicate process rates.

199 3.2. Input data requirements

200 Typically, when doing experiments more data are collected than reported in
 201 experimental plant bioaccumulation studies, often because it is not clear which of the
 202 measured data are in fact useful as relevant aspects for decisions and/or as input for models.
 203 To address the latter, the present section provides insight into typical input data requirements
 204 for plant bioaccumulation models.

205 In a typical mass balance model (Fig. 1b), bioaccumulation of a chemical is the net
 206 result of competing uptake and elimination processes. Plants take up chemicals from air (via

207 aerial surfaces, predominantly leaves) and soil (via roots). Elimination of chemicals from
208 plants includes losses to the environment (e.g. volatilization), losses due to plant growth
209 (biodilution), and degradation within plants. To quantify these processes, input data are
210 required for each level of model detail and scope. For example, to estimate chemical uptake
211 through the air-leaf interface, a simple model might require the leaf concentration factor
212 (LCF, Fig. 1b) defined as the concentration ratio in leaf and in air at equilibrium (Calamari,
213 1993). In contrast, a more complex model might quantify each competitive process
214 contributing to leaf uptake, such as dry and wet deposition, as a function of particle
215 concentration, aerosol washout and rain occurrence in air (Fantke et al., 2011), diffusion
216 through the leaf-air boundary layer derived from stomatal and cuticular resistances (Schreiber
217 and Schönherr, 2009), and concentration dilution as function of plant growth rates. In any
218 case, specific input variables must be given to model plant uptake. If these input variables
219 cannot be estimated based on e.g. available regressions, models rely on experimental studies
220 to obtain required input data. Input variables that are reported in 25 plant uptake modeling
221 studies to strongly affect bioaccumulation processes and that typically have to be obtained
222 from experimental testing studies are listed in Table 2.

223 Partition coefficients K_{OW} and K_{AW} along with half-lives in plants are by far the
224 substance properties most frequently reported to be relevant for plant bioaccumulation
225 modeling followed by molecular mass and pKa. Most frequently reported plant characteristics
226 are plant lipid and water contents, growth rates, and xylem flow (transpiration stream). Air
227 temperature and soil organic carbon (OC) content are the most frequently reported
228 environmental conditions relevant for plant bioaccumulation modeling along with scenario-
229 specific time between substance application (e.g. in case of intentionally applied pesticides)
230 and plant harvest. Many additional parameters are less frequently reported to be relevant (see
231 Table 2). This demonstrates that generally multiple parameters are required as input for
232 bioaccumulation models including substance properties, plant characteristics, and

233 environmental and scenario conditions – most of these parameters need to be provided by
 234 experimental testing studies.

235

236 **Table 2** Relevant input parameters identified in 25 plant bioaccumulation models.

Key parameters		Plant bioaccumulation modeling studies																										
		a	b	c	d	e	f	g	h ⁽¹⁾	i	j	k	l	m ⁽¹⁾	n ⁽¹⁾	o	p ⁽¹⁾	q	r	s	t	u	v	w	y	z		
substance properties	Molecular mass		x		x		x	x																		x		
	Vapor pressure	x							x																			
	pKa	x	x																x							x		
	K _{OW}		x	x		x	x	x	x		x	x	x	x	x		x	x	x	x	x	x	x	x	x	x	x	x
	K _{AW}		x	x								x				x		x			x	x		x		x		x
	K _{OC}							x															x					
	Half-life in plant					x	x	x		x	x	x	x				x									x		
	Half-life in soil							x																				
plant characteristics	Plant mass																x											
	Plant temperature																											x
	Leaf area index											x													x	x		
	Leaf thickness	x																										
	Plant conductance																									x	x	
	Plant growth rate		x									x							x	x					x	x	x	
	Plant lipid content		x		x						x	x	x	x						x				x	x			
	Plant pH	x																		x					x			
	Plant water content					x							x	x	x										x	x	x	
	Plant xylem flow																											x
environmental conditions	Soil mass																											x
	Air temperature								x			x	x	x	x	x										x		x
	Air humidity												x															
	Soil OC content		x					x																	x	x		x
	Soil pH												x													x		
	Soil water content																									x		x
	Sunlight																											
	Wind speed																											
	Time to harvest ⁽²⁾																											

237 ^aBuchholz and Trapp (2015); ^bCollins et al. (2011); ^cCzub and McLachlan (2004); ^dDoucette
 238 et al. (2005); ^eFantke et al. (2011); ^fFantke et al. (2012); ^gFantke et al. (2013); ^hFantke et al.
 239 (2014); ⁱFantke and Jolliet (2016); ^jFryer and Collins (2003); ^kJacobsen et al. (2015); ^lJuraske
 240 et al. (2008); ^mKömp and McLachlan (1997b); ⁿKömp and McLachlan (1997a); ^oLegind et al.
 241 (2011); ^pMcLachlan (1995); ^qRein et al. (2011); ^rRendal et al. (2011); ^sTakaki et al. (2014);
 242 ^tTrapp et al. (1990); ^uTrapp et al. (2007); ^vTrapp and Legind (2011); ^wTrapp (2015);
 243 ^yUndeman et al. (2009); ^zUndeman and McLachlan (2011).

244 ¹Studies refer to “plant characteristics” in general as key aspect influencing bioaccumulation.

245 ²Specific for chemicals applied in pulses to plants, such as pesticides.

246

247 Not all data that are summarized in [Table 2](#) as being relevant for bioaccumulation
248 models are commonly reported in experimental studies. We seek to identify and close gaps
249 between data provided by studies following current testing guidelines and data required for
250 improving plant bioaccumulation science by adapting current experimental methods (and
251 reporting requirements). In most cases these gaps can be addressed with minimal additional
252 resources.

253

254 **4. Current practice in plant bioaccumulation testing**

255 4.1. Reviews of experimental plant bioaccumulation studies

256 Experimental plant bioaccumulation tests are usually conducted under well-defined
257 environmental conditions (field and greenhouse studies) or under controlled conditions
258 (laboratory studies). Laboratory studies are usually carried out at 25°C and 14 hours light
259 cycle. Plants are exposed to known substance concentrations applied as a pulse or
260 continuously over a certain time period; one example of significant differences in exposure
261 design. Plants and the exposure media (soils or hydroponic solutions) are sampled at different
262 times during and after exposure, but at least once at the end of the experimental period.
263 Concentrations of contaminants are normally reported for plants and soil/hydroponic solution.

264 To highlight the state of science in experimental plant bioaccumulation testing, we
265 summarize key findings from two recent compilations of experimental data. The first
266 compilation focuses on plant bioaccumulation studies published in the peer-reviewed
267 literature for a broad range of chemical classes including PAHs, legacy pesticides, current use
268 pesticides (CUPs), PCBs, polybrominated diphenyl ethers (PBDEs), perfluorinated
269 compounds (PFCs), pharmaceutical and veterinary chemicals and others ([Arnot et al., 2013](#)).
270 This review focused on key words pertaining to quantitative metrics of plant bioaccumulation,
271 such as “bioconcentration factor” (BCF), “root concentration factor” (RCF), “transpiration
272 stream concentration factor” (TSCF), and other plant/exposure medium-based metrics as well

273 as plant uptake and biotransformation rate constants. The resulting dataset includes 3,644
274 unique entries for 358 chemicals from 166 scientific references. Only 11 of the 166 studies
275 included any mention of plant biotransformation and only 3 of the 11 included
276 biotransformation rate information (for lindane and a series of phenols). Proximate composite
277 analysis of the plants (i.e., lipid contents, water contents) was reported in only about 10% of
278 all studies.

279 The second compilation focuses on experimentally derived pesticide dissipation half-
280 lives in plants obtained from key word searches with regard to “dissipation”, “persistence”
281 and “degradation” of pesticides in plants or certain plant components. This compilation
282 identified 4,513 unique data points for 346 substances applied to almost 200 different plant
283 species collected from 811 scientific references (Fantke and Juraske, 2013). Key points are to
284 analyze the variability across substances, plant species and harvested plant components as
285 well as to discuss different substance, vegetation and environmental aspects influencing
286 pesticide dissipation kinetics. Only 18% of all reviewed references assessed one or more of
287 these aspects, such as the influence of temperature on pesticide dissipation from plants.
288 Furthermore, most reported data regarding substance (e.g. purity), plant characteristics (e.g.
289 growth stage), application and sampling settings (e.g. treated plant components), and
290 environmental conditions (e.g. air humidity) were incomplete (see Table 3 for an example).

291

292 4.2. Limitations of reported data for use in bioaccumulation modeling

293 Screening various experimental studies reveals there are few parameters that are
294 consistently reported, such as the sampled plant component and the substance application rate
295 (typically for pesticide treatment) or assumed exposure concentrations (typically for non-
296 pesticide contaminants). In contrast, many parameters considered essential for interpreting
297 experimental data and serving as important input for plant bioaccumulation models are
298 infrequently reported, such as mean air temperature, substance fraction that is intercepted by

299 plants or water content of the sampled plant components or soil characteristics. To
 300 demonstrate differences in reporting data, we compared six studies that assessed the same
 301 substance-plant species combination, namely cypermethrin applied to eggplant, and analyzed
 302 residues in the same sampled plant components, i.e. eggplant fruits (Arora, 2009; Kaur et al.,
 303 2011; Lu, 2011; Mukherjee et al., 2012; Sinha and Gopal, 2002; Walia et al., 2010). Data
 304 reported in each of the compared studies are summarized in Table 3.
 305
 306 Table 3 Comparison of data reported in experimental plant bioaccumulation test studies
 307 analyzing the same combination of chemical, plant species, and plant component, i.e.
 308 cypermethrin residues measured in sampled eggplant fruits. For full parameter descriptions
 309 see Table 4.

Parameter	Reported in experimental testing study					
	a	b	c	d	e	f
Study location(s)	✓ ¹	✓ ¹	✓ ¹	✓ ¹	✓ ¹	✓ ¹
Study year(s)		✓		✓		
Study characteristics	✓		✓	✓		
Application rate	✓	✓	✓	✓	✓	✓
Application date (or days after planting)		✓				
Application duration					✓	
Application type	✓ ²	✓ ²	✓ ²	✓ ²		✓ ²
Treated component			✓			
Formulation	✓	✓	✓	✓		✓
Substance purity	✓		✓			✓
Relative air humidity	✓	✓				
Rain rate	✓ ³	✓				
Wind speed		✓				
Air temperature	✓	✓				
Binomial plant name (including variety)	✓	✓	✓	✓	✓ ⁴	✓
Plant growth period		✓		✓		
Plant stage	✓			✓		✓
Planting density	✓	✓				
Sampled component	✓	✓	✓	✓	✓	✓
Sampled mass	✓	✓	✓	✓	✓	✓
Sampling date(s)/time(s)	✓	✓	✓	✓		✓
Sampling specifics	✓		✓	✓	✓	✓
Residue analysis setup	✓ ⁵	✓	✓	✓ ⁵	✓	✓ ⁵
Analysis temperature(s)	✓	✓	✓	✓		✓

Parameter	Reported in experimental testing study					
	a	b	c	d	e	f
Solvents used	✓	✓	✓	✓	✓	✓
Fate processes studied			✓	✓	✓	
Kinetic models used	✓					✓

310 ^aSinha and Gopal (2002); ^bArora (2009); ^cWalia et al. (2010); ^dKaur et al. (2011); ^eLu (2011);
311 ^fMukherjee et al. (2012).

312 ¹Reported in a way that does not allow deriving exact geographical coordinates; ²Application
313 height not given; ³Total rainfall (mm) during experiment given, but explicit duration of
314 experiment not stated; ⁴Variety not given; ⁵Analytical limits of detection not given.

315
316 Many aspects of the sampling and analysis methods are reported by all studies
317 compared in [Table 3](#). In contrast, several key parameters considered as important input to
318 plant bioaccumulation models and required by existing testing guidelines, are not consistently
319 reported (e.g. pesticide application dates, treated plant components, air temperature and
320 relative humidity, plant growth stage during treatment and at sampling times), or not reported
321 by any study (e.g. substance CAS number, pH of soil or hydroponic solution, plant root to
322 shoot ratio, plant leaf area index). Inconsistent collection or presentation of data makes it
323 difficult to use or compare results from different studies. For non-pesticide chemicals, there
324 are generally even less data reported, because testing requirements are less stringent ([Arnot et
325 al., 2013](#)). The inconsistency of key bioaccumulation information reported in the literature is
326 primarily because studies either do not follow any official guideline or they do not comply
327 with reporting recommendations when following existing guideline.

328 329 **5. Toward consistent bioaccumulation testing data sets**

330 5.1. Sampled plant components

331 With respect to harvested plant samples, most modeling approaches either require
332 information on individual plant components, such as leaves, fruits, roots, etc. ([Fantke et al.,
333 2011; Trapp and Legind, 2011](#)), or specific component parts or tissues like fruit peel, fruit
334 pulp, epicuticular wax, nectar, etc. ([Satchivi et al., 2006](#)). In contrast, composite plant parts

335 (straw, shoot, etc.) are often mixed and homogenized before analysis, thus assigning chemical
336 quantities in individual interconnected components is usually impossible. The best case
337 scenario is when sampled plant components are well distinguished and terms like “rind” or
338 “fruit-surface” are avoided as these are difficult to allocate to specific plant components. As
339 an example of good practice, using “bark” or “peel” are unambiguous terms referring to
340 specific plant components.

341 To get the maximum benefit from an experimental study, we recommend to separately
342 sample and report plant components and to provide a description of each sampled component.
343 However, when facing sample mass limitations, i.e. not enough mass of specific components
344 or tissue is sampled to allow a proper analysis, the reporting focus should be on the tissue or
345 component that is most relevant for subsequent exposure studies, such as fruits harvested for
346 human or animal consumption. This would require consistently describing each sampled
347 component in terms of sampled mass and composition (e.g. water content). Moreover, we
348 recommend reporting not only the day of sampling, but also the day of planting or at least the
349 different plant component growth stages at sampling time, such as flowering. This does not
350 require additional equipment, but provides important information about for example growth
351 dilution.

353 5.2. Considered (fate) processes

354 Most experimental studies measure overall dissipation from plant samples (Braun et
355 al., 1980; Galiotta et al., 2011; Lee and Cheng, 1983; Willis and McDowell, 1987) or focus on
356 particular dissipation processes, such as volatilization (Bedos et al., 2010; Guth et al., 2004;
357 Kubiak et al., 1995; Stork et al., 1998), photodecomposition (Burrows et al., 2002; Katagi,
358 2004; McCrady and Maggard, 1993) or microbial degradation (Azaizeh et al., 2011; Quistad
359 et al., 1974; Roy et al., 2001). However, whereas this might be sufficient to ensure
360 compliance with regulatory thresholds for plant uptake and bioaccumulation, it does not help

361 to understand bioaccumulation mechanisms as relevant in other science-policy fields.
362 Moreover, mechanistic models typically rely on information of all contributing dissipation
363 processes to arrive at a complete set of rate coefficients as input (Fantke et al., 2014). Such
364 processes include dry and wet deposition, advective root and foliar uptake, volatilization (gas-
365 exchange), wash-off from plant surfaces, chemical concentration dilution due to plant growth,
366 direct and indirect photolysis, microbiological, chemical and photodecomposition,
367 metabolism due to hydroxylation and oxidation, and plant-internal translocation in xylem and
368 phloem (Collins et al., 2011; Fantke and Juraske, 2013). It is often impractical to
369 simultaneously report rate constants for various individual dissipation processes. However, if
370 this information is reported, it allows for a much more detailed analysis and understanding of
371 the dynamics of chemicals in the plant-environment systems relevant for different science-
372 policy fields.

373 We recommend reporting rate constants for specific processes whenever possible, e.g.
374 for biodegradation when metabolites are known based on metabolite concentrations or for
375 volatilization based on measuring air concentrations. When only overall dissipation can be
376 reported, we recommend testing different kinetic models instead of simply assuming first-
377 order kinetics for best interpretability of actual dissipation. While reporting data for specific
378 processes may require additional equipment (e.g. when sampling air), testing different kinetic
379 models can easily be implemented without additional costs, and an overview of different
380 kinetic models is for example given in Fantke and Juraske (2013). Further, we recommend
381 reporting environmental conditions to the extent feasible. This includes most importantly air
382 temperature, air humidity, and soil properties like pH and organic carbon content. If air
383 temperature cannot be measured directly, average temperature over the study duration at the
384 study site can serve as proxy, and if air humidity is not available, recording the number of rain
385 events can serve as alternative.

386 Partitioning of neutral organic chemicals is predominantly controlled by the quantity
387 and quality of organic carbon; hence, organic carbon content of the soil can contribute to
388 variance in the plant bioaccumulation of neutral organics exposed from soils (Seth et al.,
389 1999). While analyzing soil samples for carbon content might come at the expense of
390 additional resources, classifying the soil (e.g. as podzol) and providing a basic description of
391 the soil horizons will already give some information about potential soil characteristics.
392 Quantifying the environmental fate and sorption of ionizable organic chemicals is generally
393 more uncertain. Evidence suggests that the cation exchange capacity (CEC) of the soil is a
394 key determinant for the sorption of cations (Droge and Goss, 2013). For anionic chemicals,
395 the sorption to soils may be adequately characterized by soil organic carbon and soil pH (Kah
396 and Brown, 2007). At present, we recommend reporting CEC for soil exposures to cations.
397 Revisions to guidelines and reporting requirements for plant bioaccumulation for ionizable
398 organic chemicals should consider the emerging science on chemical distribution of these
399 chemicals in multimedia environments.

400 Finally, bioaccumulation processes are usually chemical-specific and, hence,
401 physicochemical properties need to be considered in modeling approaches. However, most if
402 not all relevant chemical data are already reported elsewhere, e.g. in the database on
403 registered substances of the European Chemicals Agency ([http://echa.europa.eu/information-](http://echa.europa.eu/information-on-chemicals)
404 [on-chemicals](http://echa.europa.eu/information-on-chemicals)), except the CAS registry number that is essential to identify a chemical
405 unambiguously. We hence recommend to at least reporting CAS registry numbers.

406

407 5.3. Recommendations for reported bioaccumulation testing data

408 Based on the findings of our review of experimental plant bioaccumulation testing
409 studies and our knowledge regarding bioaccumulation models, we present a set of
410 recommended parameters to be included in future testing studies (Table 4). Parameters that
411 have been identified being of high relevance for interpreting test results and for developing

412 plant bioaccumulation models are specified in the “priority data list” of **Table 4**. Parameters
 413 providing additional information for interpreting experimental results and for use in
 414 bioaccumulation modeling are given in the “complementary data list” of **Table 4**.

415
 416 **Table 4** Priority and complementary data recommended to be reported in testing studies
 417 referring to parameters relevant to improve the interpretation of measured data and to support
 418 quantification of bioaccumulation in plants with modeling approaches.

Parameter (unit)	Description
PRIORITY DATA LIST (recommended to be reported by all testing studies)	
CAS-RN	Chemical Abstracts Service Registry Number; unique identifier of a tested chemical
Study location(s)	Location (geographic coordinates) or city/specific area within country) of experimental study site(s)
Study characteristics	Specific conditions, such as field or greenhouse study
Application or release rate (kg day ⁻¹ or L ha ⁻¹ day ⁻¹)	Application or release rate of chemical; number of applications during study
Application or release date(s)	For purposely applied chemicals (e.g. pesticides), application or release date(s) of chemical (exposure time of the plant) or application or release in days after planting; for single exposure events (e.g. spill), exposure concentration and duration
Treated plant component(s) or exposure medium	Treated (exposed) plant component (leaf, pulp, etc.) or environmental compartment/matrix (soil, hydroponic solution, etc.)
Formulation (%)	Fraction of applied or released substance/active ingredient, if applied or released as formulation (e.g. refers to active ingredient of interest plant protection product formulation)
Air temperature (°C)	Mean daily temperature in air (at soil surface level) and min/max range
Soil pH	pH of treated/exposed/sampled soil
Soil OC content (kg kg ⁻¹)	Organic carbon content in treated/exposed/sampled soil for neutral organic chemicals; alternatively, the soil type and horizons can be described
Soil CEC (meq g ⁻¹)	Cation exchange capacity of treated/exposed/sampled soil for ionizable organic chemicals
Binomial plant name	Unambiguous identification of plant species and, if required, variety or cultivar

Parameter (unit)	Description
Plant stage	Growth stage of the treated/exposed/sampled plant (mature, seedling, etc.)
Capture coefficient (–)	Substance capture coefficient as average substance fraction that is intercepted by plant during sampling period and min/max range
Plant transpiration (L kg ⁻¹ or L day ⁻¹)	Plant transpiration as inverse of weight unit of plant dry mass produced per weight unit of consumed water or as volumetric transpiration stream per time unit
Sampled component(s)	Sampled plant component(s) (leaf, pulp, etc.) or tissue(s) (wax layer, etc.) and proximate composition (lipids, organic carbon, carbohydrates, water)
Sampled mass (kg)	Dry and/or wet mass of plant sample(s)
Sampling date(s)/time(s)	Sampling date(s) or sampling days or times after application or release or exposure (day)
Sampling specifics	Specific sampling conditions, such as cold storage, washing or food processing after harvest/sampling
Fate processes studied	Considered fate processes (including post-harvest) either contributing to bioaccumulation (penetration, deposition, etc.) or biodilution (volatilization, metabolism, etc.)
Kinetic models used	Applied assessment models in case of calculating rate coefficients (pseudo-first order, second order, biexponential, etc.); this is only required if the underlying raw data (e.g. concentration at any sampled time) is not provided

COMPLEMENTARY DATA LIST (recommended to be reported when feasible)

Study year(s)	Year(s) of experimental study
M (g mol ⁻¹)	Molecular mass
log K _{AW} (–)	Air/water partition coefficient; alternatively, the Henry's law constant (Pa m ³ mol ⁻¹), or the combination of saturation vapor pressure (Pa) and water solubility (g m ⁻³)
log K _{OW} (–)	<i>N</i> -octanol/water partition coefficient
log K _{OA} (–)	<i>N</i> -octanol/air partition coefficient; alternatively, K _{oa} can be calculated from K _{aw} and K _{ow} as log K _{oa} = log K _{ow} – log K _{aw}
K _{OC} (L kg ⁻¹)	Organic carbon normalized soil sorption coefficient
pK _a (–)	Acid dissociation constant
Chiral configuration	Specification of (<i>S</i>)-(+)-enantiomer and (<i>R</i>)-(–)-enantiomer status
Application or release duration (day)	Application or release duration of chemical (exposure duration of the plant)
Application or release type	Application or release type or method (for pesticides aerial spray, drip irrigation, soil injection, etc.) including release or application height (m)

Parameter (unit)	Description
Substance purity (%)	Purity of chemical analytical standard or substance/active ingredient as part of mixture; radio purity, if applicable
Rain rate (mm day ⁻¹)	Daily average precipitation rate (1 mm = 1 L m ⁻²) and min/max range; alternatively, average relative air humidity or number of rain events over the study duration can be reported
Wind speed (m day ⁻¹)	Mean wind speed at 2 m above soil surface level and min/max range
Soil temperature (°C)	Mean temperature of treated/exposed/sampled soil
Soil water content (L L ⁻¹)	Fraction of volumetric water in bulk soil
Soil porosity (L L ⁻¹)	Volumetric porosity in soil or fraction of volumetric pores in bulk soil
Plant growth rates (day ⁻¹)	Plant growth rates for different plant components the differences in plant component masses (kg) per time period(s) during the study (day)
Planting density ($n_{\text{plants}} \text{ ha}^{-1}$)	Number of plants grown per defined area (only in field and greenhouse studies)
Root to shoot ratio (-)	Average ratio between below-ground and aerial plant components
Leaf fraction (-)	Average fraction of aerial plant components that is leaf
Fruit fraction (-)	Average fraction of aerial plant components that is fruit
Stem fraction (-)	Average fraction of aerial plant components that is stem/trunk
LAI (-)	Leaf area index at different times between substance application or release and plant harvest/sampling; for plants with only 1 leaf layer the leaf cover (m ⁻²) can be reported instead
Leaf/fruit/stem/root water (L kg ⁻¹)	Average water content of plant leaf/fruit/stem/root
Leaf/fruit/stem/root lipid (L kg ⁻¹)	Average lipid content of plant leaf/fruit/stem/root
Stem height (m)	Average height of plant stem/trunk during study period
Residue analysis setup	Description of all post-sampling procedures and analysis steps including durations of individual processing and analysis steps and analytical detection limits
Analysis temperature(s) (°C)	Temperatures at all post-sampling processing and analysis stages
Solvents used	Solvents and solvent concentrations/purity used at all post-sampling processing and analysis stages

420 **6. Conclusions and implications for future research and policy making**

421 We have highlighted current data gaps that need to be addressed to improve the
422 quantitative understanding of organic chemical bioaccumulation and biotransformation in
423 plants. For non-organic contaminants, the reader is referred to the respective literature
424 ([Pulford and Watson, 2003](#); [Raskin and Ensley, 2000](#); [Salt et al., 1995](#); [Weis and Weis, 2004](#)).

425 We emphasize the key experimental parameters that would need to be measured and reported
426 in priority and without much additional effort or equipment in order to improve models for
427 use in various regulatory and decision support contexts. The focus is on terrestrial plants, but
428 similar concepts should also be considered for aquatic plants.

429 Our reporting recommendations ([Table 4](#)) are intended to optimize existing testing
430 guidelines for improved mechanistic bioaccumulation knowledge in a cost-effective manner.
431 This includes reducing unnecessary or redundant testing of the same chemical-plant
432 combinations and to keep study areas and sampling mass reasonably small. Ultimately, the
433 focus of future experimental testing should be to improve data quality and to better facilitate
434 the interpretation and use of testing study results in decision support models.

435

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440

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