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BIOCIDE RUNOFF FROM BUILDING FACADES: DEGRADATION KINETICS IN SOIL

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Table S1 Extraction recoveries [%] for biocides in soil (n=20, concentration range: 0.03-300 µg g^{-1}) as well as limits of detection (LOD) [10^{-3} µg g^{-1}].

	MI	BIT	IP	IPBC	DR	TB	IRG	OIT	TBU	DCOIT	PPZ	CD	MCPP
Recovery	88	70	104	103	101	108	109	91	98	84	112	104	67
StDev	14	20	6	16	7	9	8	21	22	45	13	14	32
LOD	3.6	4.9	1.8	0.9	0.6	0.2	0.1	0.1	0.4	0.2	0.4	0.2	0.6

MI: Methylisothiazolinone, BIT: Benzisothiazolinone, IP: Isoproturon, IPBC: Iodocarb, DR: Diuron, TB: Terbutryn, IRG: Cybutryn, OIT: Octyl- isothiazolinone, TBU: Tebuconazole, DCOIT: Dichloroctylisothiazolinone, PPZ: Propiconazole, CD: Carbendazim: MCPP: Mecoprop

Table S2 Extraction recoveries [%] for terbutryn degradation products in soil (n=4, concentration: 300 ng g^{-1}) as well as limits of detection (LOD) [ng g^{-1}].

	TBM	TB-SO	M1	TB-DesS	TB-DesS-DesE	TB-DesS-DesB	TB-OH-DesB	TB-OH-DesE	TB-OH
Recovery	141	79	145	95	108	91	53	92	106
StDev	7	4	6	4	6	7	8	2	3
LOD	0.16	0.59	0.46	0.19	0.39	0.32	0.07	0.34	0.06

TBM: Terbumeton, TB-SO: Terbutryn-sulfoxide, M1: Desethyl-terbutryn, TB-DesS: Desthiomethyl-terbutryn, TB-DesS-DesE: Desethyl-desthiomethyl-terbutryn, TB-DesS-DesB: Desbutyl-desthiomethyl-terbutryn, TB-OH-DesB: Desbutyl-2-hydroxy-terbutryn, TB-OH-DesE: Desethyl-2-hydroxy-terbutryn, TB-OH: 2-hydroxy-terbutryn

Table S3 Extraction recoveries [%] for octylisothiazolinone degradation products in soil (n=4, concentration: 0300 ng g^{-1}) as well as limits of detection (LOD) [ng g^{-1}].

	OAM	OFA	OAA	OPA	OT	OMA	OOA
Recovery	65	94	101	104	100	245	85
StDev	0.5	1	1	1	1	14	12
LOD	6.5	3.5	0.7	0.9	6.8	1.9	4.0

OAM: Octylamine, OFA: *N*-Octylformamide, OAA: *N*-Octylacetamide, OPA: *N*-Octylprop-2-enaminde, OT: 3-Octylthiazol-2(3*H*)-one, OMA: *N*-Octyl malonamic acid, OOA: *N*-Octyl oxamic acid

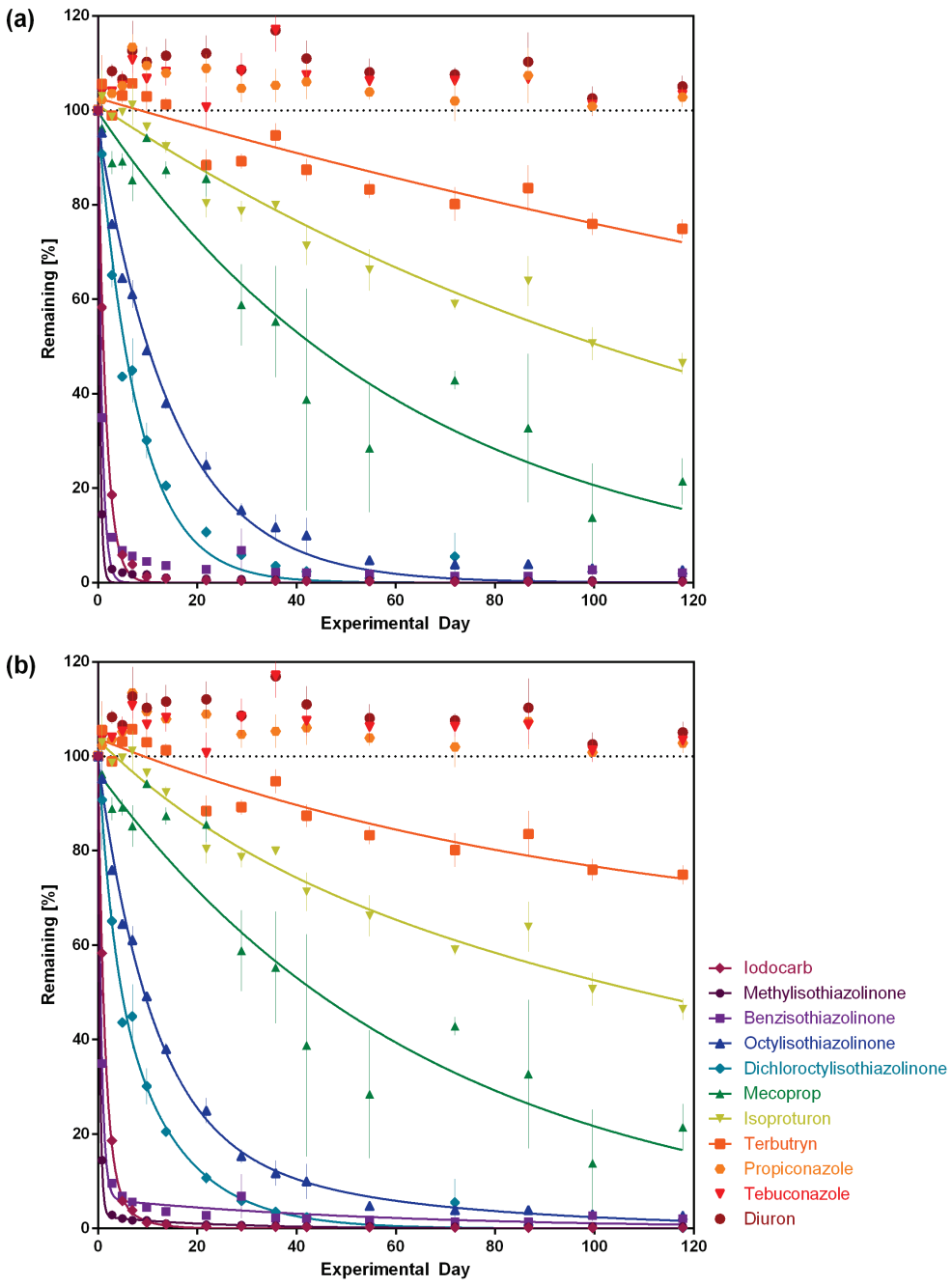

Figure S1 Comparison of (a) single first order kinetic and (b) two-phase first order kinetic fits.

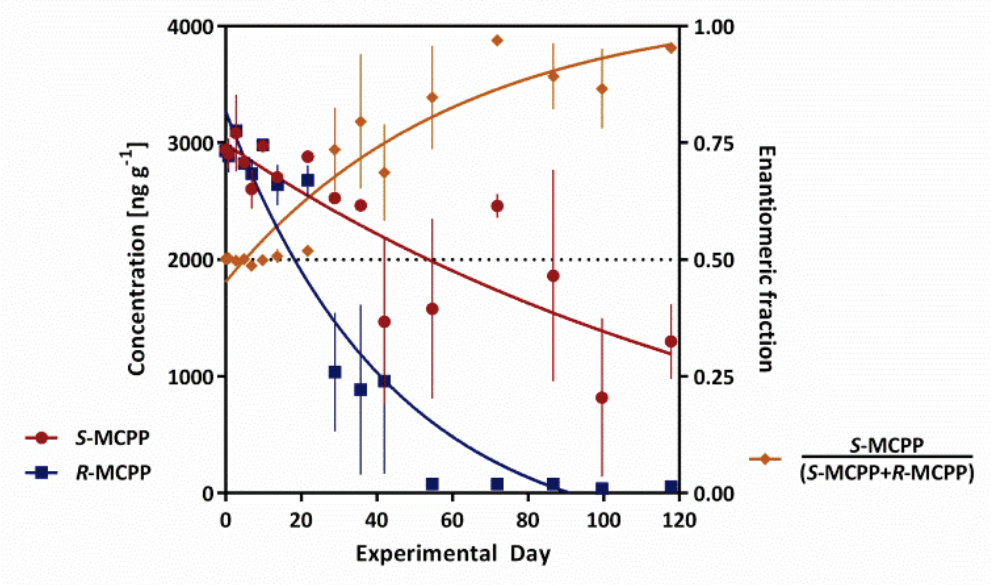

Figure S2 Enantioselective degradation of mecoprop; error bars: standard error of mean (n=3).

Note S1 Estimation of half-lives for PPZ, TBU, and DR.

With an experimental standard deviation of 6% the maximum removal after 120 d would be 6% (Remaining fraction after 120 d: $RF_{120} > 94\%$). Using the following formula for the first-order degradation kinetic (Eq. 1) the degradation rate constant was estimated to be $k < 0.0005\ d^{-1}$.

$$RF=RF_0*\exp(-k*t) \quad \text{(Eq. 1)}$$

Hence, degradation half-lives of $T_{1/2} > 2500$ d are expected.

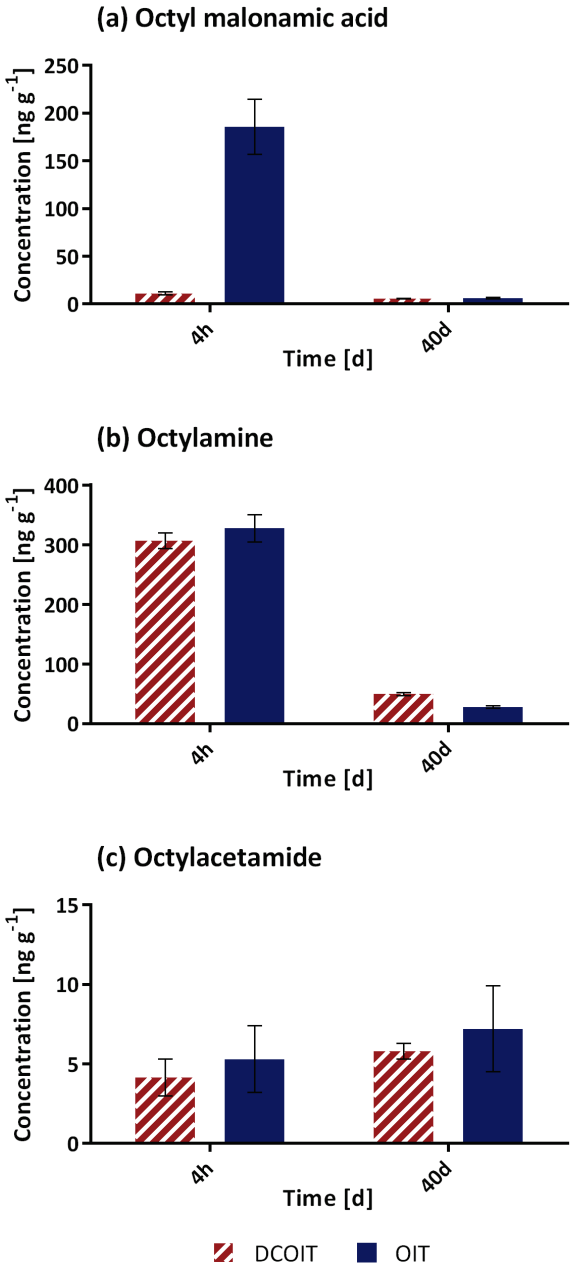

Figure S3 Concentrations of (a) octyl malonamic acid, (b) octylamine, and (c) octylacetamide in incubations of DCOIT & OIT alone (soil concentration 50 µg g^{-1}; incubation for 4 h and 40 d; error bars: range, n=2).

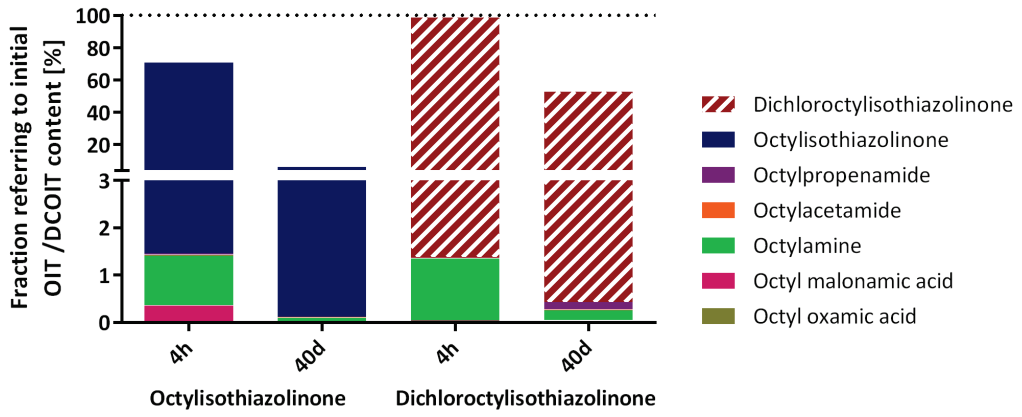

Figure S4 Mass balances for DCOIT and OIT and their studied transformation products in incubations of DCOIT & OIT alone (soil concentration 50 µg g^{-1}; incubation for 4 h and 40 d).

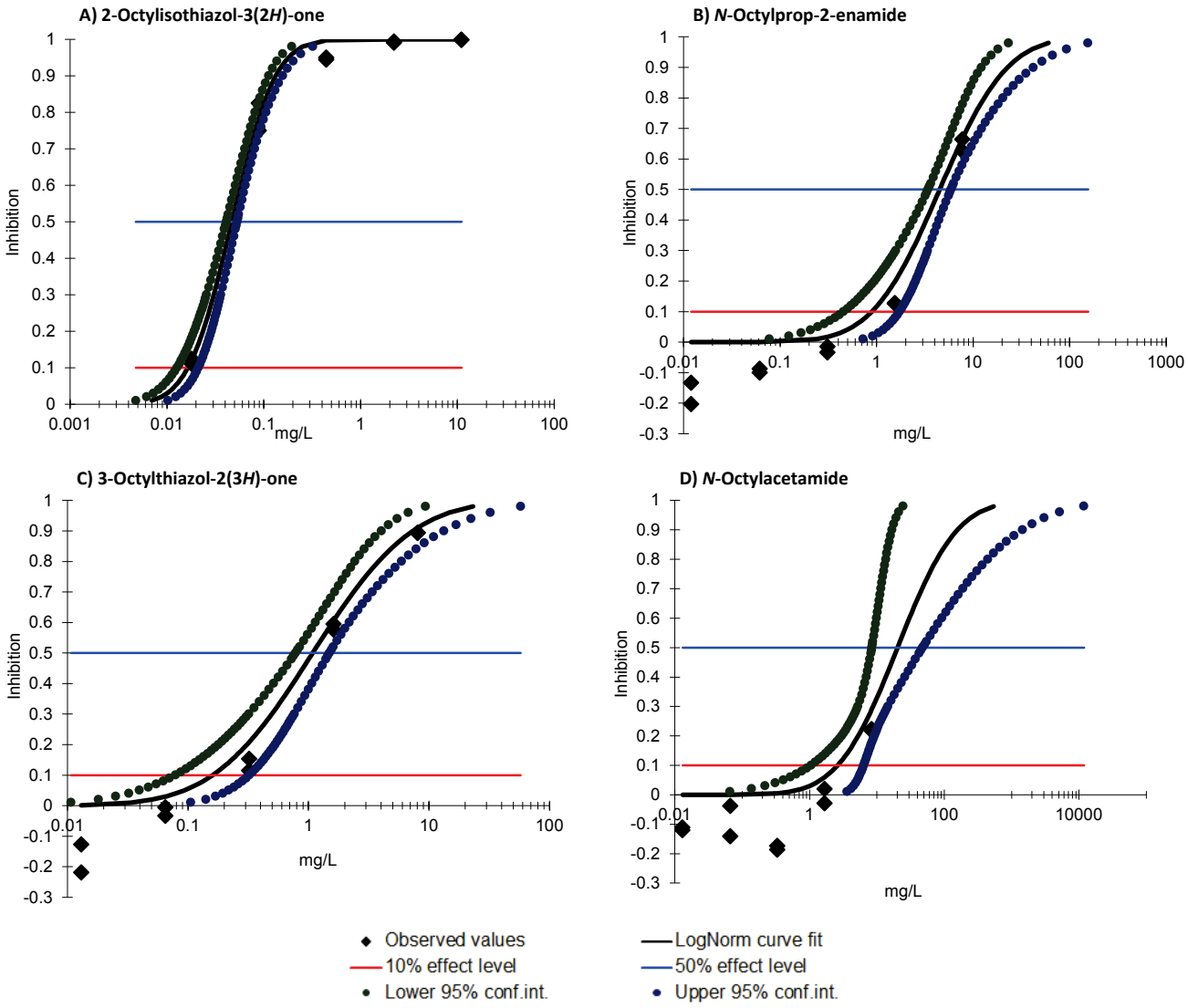

Figure S5 Treatment-effect curves from Microtox-tests for the bactericide 2-Octylisothiazol-3(2*H*)-one (A) and three of its degradation products [*N*-octylprop-2-enamide (B), 3-octylthiazol-2(3*H*)-one (C), and *N*-octylacetamide (D)] showing fitted logarithmic curves, confidence intervals (95%), and inhibition at 10% and 50% (horizontal lines).

Table S4 Ecotoxicological data for terbutryn and octylisothiazolinone degradation products found in the literature.

Compound	CAS-No	Test species	Endpoint	Ref.
Octylisothiazolinone (OIT)	26530-20-1	Fathead minnow	LC_{50} (96 h) = 0.14 mg L^{-1}	[1]
		Daphnia magna	EC_{50} (48 h) = 0.11-0.32 mg L^{-1}	[1]
Octylamine	111-86-4	Fathead minnow	LC_{50} (96 h) = 5.19 mg L^{-1}	[1]
		Daphnia magna	EC_{50} (48 h) = 1.9 mg L^{-1}	[1]
		Green algae	EC_{50} (72 h) = 0.23 mg L^{-1}	[1]
Terbutryn (TB)	886-50-0	Rainbow trout	LC_{50} (96 h) = 1.1 mg L^{-1}	[2]
		Daphnia magna	EC_{50} (48 h) = 2.66 mg L^{-1}	[2]
		Green algae	EC_{50} (72 h) = 0.0036 mg L^{-1}	[2]
2-Hydroxy-terbutryn	66753-07-9	Rainbow trout	LC_{50} (96 h) > 100 mg L^{-1}	[2]
		Daphnia magna	EC_{50} (48 h) > 2.5 mg L^{-1}	[2]
		Green algae	EC_{50} (72 h) > 3.96 mg L^{-1}	[2]
Terbumeton	33693-04-8	Fathead minnow	LC_{50} (96 h) = 38 mg L^{-1}	[1]
		Daphnia magna	EC_{50} (48 h) = 44 mg L^{-1}	[1]
		Green algae	EC_{50} (72 h) = 0.059 mg L^{-1}	[1]
Terbutryn sulfoxide	82985-33-9	Aliivibrio fischeri	similar toxicity as terbutryn	[3]
Desethyl-terbutryn	30125-65-6	Daphnia magna	EC_{50} (48 h) = 11 mg L^{-1}	[1]
		Green algae	EC_{50} (72 h) = 0.019 mg L^{-1}	[1]
Desethyl-2-hydroxy-terbutryn	66753-06-8	Rainbow trout	LC_{50} (96 h) > 100 mg L^{-1}	[2]
		Daphnia magna	EC_{50} (48 h) > 100 mg L^{-1}	[2]
		Green algae	EC_{50} (72 h) = 35.4 mg L^{-1}	[2]

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2. ECHA *CLH Report: Terbuthylazine*; 2014
3. Luft, A.; Wagner, M.; Ternes, T. A., Transformation of Biocides Irgarol and Terbutryn in the Biological Wastewater Treatment. *Environ. Sci. Technol.* **2013,** *48*, (1), 244-254.