
Supporting Information to Analysing cytotoxic effects of selected isothiazol-3-one biocides using the "Toxic Ratio" concept and the "T-SAR" approach

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Concentration response curves for all isothiazol-3-ones tested in this study are shown in Figure S 1. EC_{50} values and $\log EC_{50}$ values with 95 % confidence intervals for the three test systems are listed in Tables S 1, 2, and 3. The statistical parameters listed in the tables are as provided by the R package drfit [1], which is an extension of the R software for statistical computing [2].

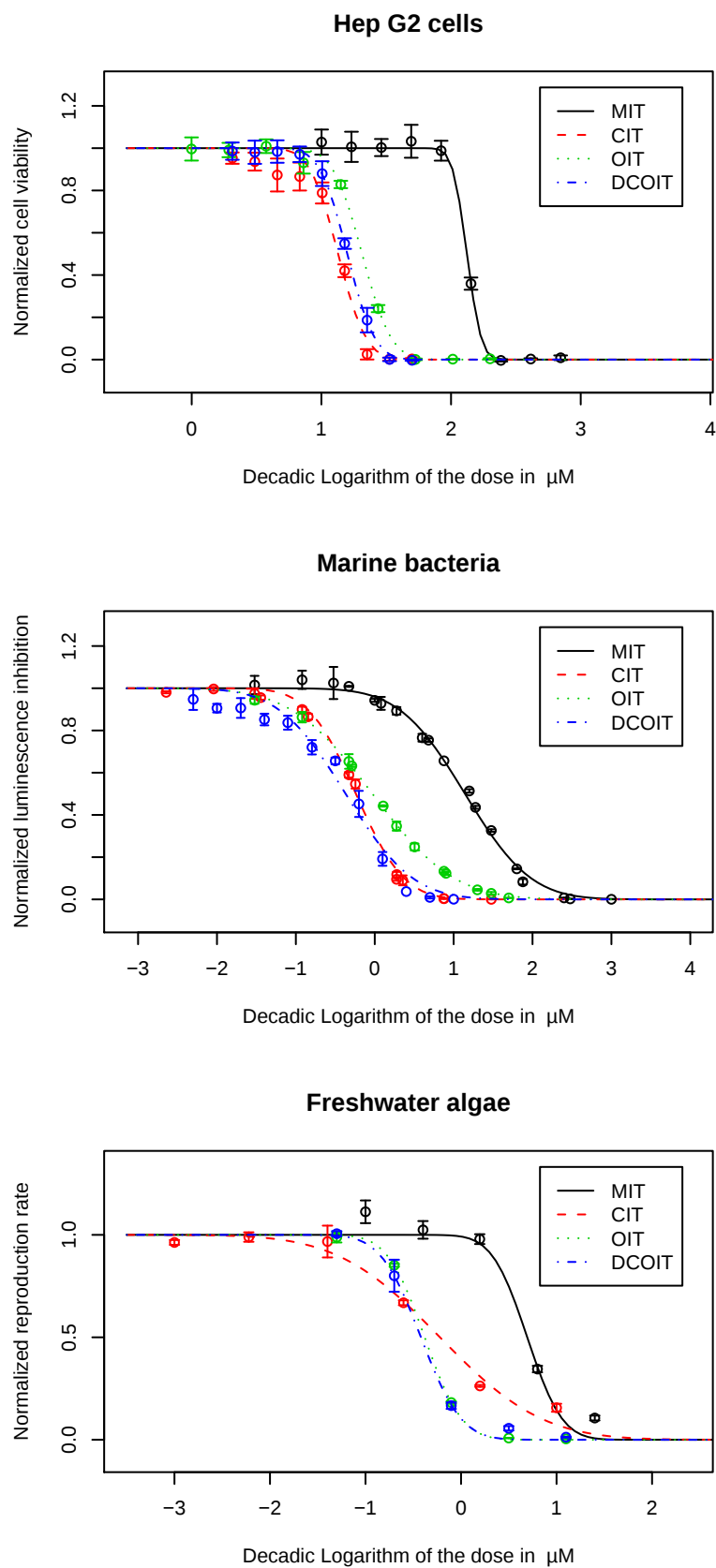


Figure S 1: Concentration response curves for Hep G2 cell viability after 48 h, luminescence inhibition in *Vibrio fischeri* after 30 min, and cell growth in freshwater green algae *Scenedesmus vacuolatus* after 24 h

Table S 1: Cytotoxicity in the WST-1 assay with Hep G2 cells

	mtype	EC ₅₀	unit	log EC ₅₀	sigma	a	b
MIT	probit	130	μ M	2.12	0.0425	2.12	0.0867
CIT	probit	13	μ M	1.13 (1.11-1.15)	0.0752	1.13	0.17
OIT	probit	21	μ M	1.31 (1.3-1.33)	0.034	1.31	0.177
DCOIT	probit	16	μ M	1.2 (1.19-1.21)	0.0408	1.2	0.166

Table S 2: Acute toxicity towards *Vibrio fischeri*

	mtype	EC ₅₀	unit	log EC ₅₀	sigma	a	b
MIT	probit	14	μ M	1.14 (1.11-1.18)	0.0339	1.14	0.654
CIT	probit	0.58	μ M	-0.239 (-0.26-0.217)	0.0281	-0.239	0.478
OIT	probit	0.94	μ M	-0.029 (-0.0475-0.0105)	0.02	-0.029	0.811
DCOIT	probit	0.43	μ M	-0.369 (-0.434-0.305)	0.0677	-0.369	0.665

Table S 3: Acute toxicity towards *Scenedesmus vacuolatus*

	mtype	EC ₅₀	unit	log EC ₅₀	sigma	a	b
MIT	probit	4.9	μ M	0.693	0.0816	0.693	0.288
CIT	probit	0.6	μ M	-0.221 (-0.36-0.0767)	0.0572	-0.221	0.84
OIT	probit	0.42	μ M	-0.38 (-0.397-0.364)	0.0116	-0.38	0.306
DCOIT	probit	0.38	μ M	-0.42 (-0.477-0.362)	0.04	-0.42	0.332

Table S 4: HPLC reference substances for the determination of the $\log K_{ow}$ values of the isothiazol-3-ones.

Substance	$\log K_{ow}$	
Adenosine	-1.05	[3]
Propan-2-one	-0.24	[4]
Butan-2-one	0.29	[5]
Pyridine	0.65	[6]
Aniline	0.90	[3]
Pentan-2-one	0.91	[3]
Hexan-2-one	1.38	[6]
Heptan-2-one	1.98	[7]
Toluene	2.73	[3]
Benzophenone	3.18	[3]
1,2-Dichlorobenzene	3.43	[8]
n-Butylbenzene	4.38	[8]
Triphenylamine	5.74	[3]

References

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