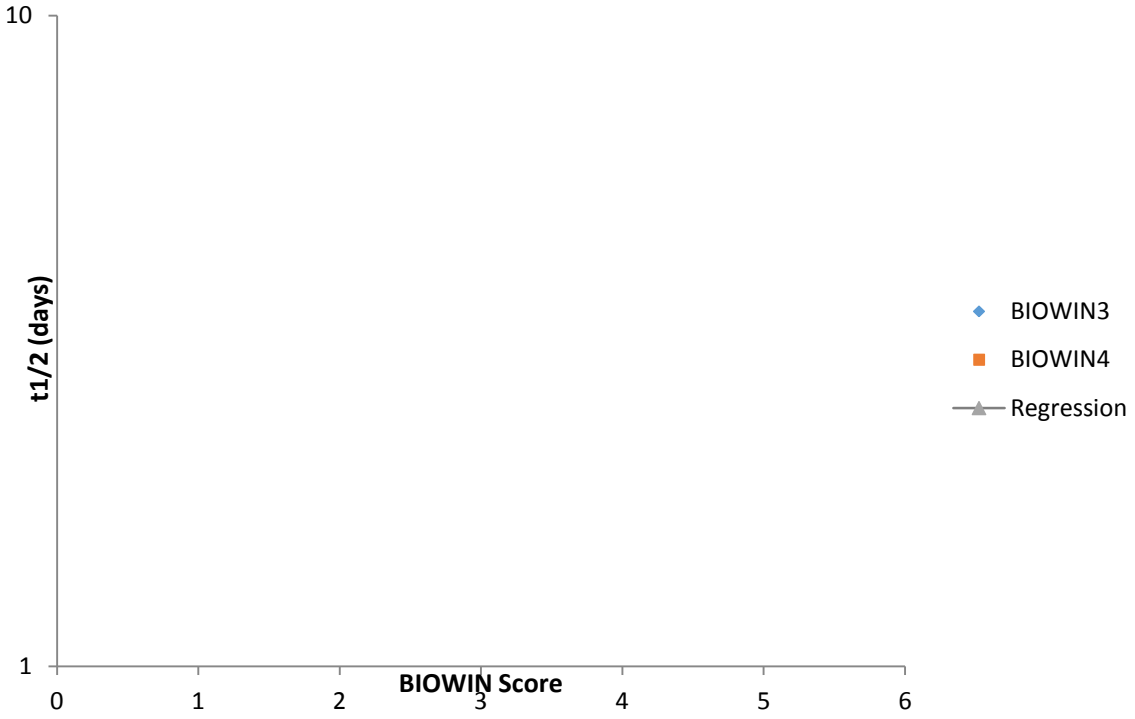
Doplňte vybarvená pole

Chemical	Smiles	Cas No	Log Kaw	Log Kow	BIOWIN3	$t_{½}$ (Days)	BIOWIN4
n hexane	C(CCCC)C	110-54-3	1.87	3.9			
cyclohexane	C(CCCC1)C1	110-82-7	0.79	3.44			
p-xylene	c(ccc(c1)C)(c1)C	106-42-3	-0.55	3.15			
1,4-dichloroben	c(ccc(c1)Cl)(c1)(	106-46-7	-1.01	3.44			
octachlorodiben	Clc3c(Cl)c(Cl)c2(	3268-87-9	-3.06	7.57			
2,2',3,4,5,5',6'-o	c1(Cl)c(Cl)cc(Cl)(	52663-75-9	-3.39	8.91			
octabromodiphe	Brc1c(c(c(c(c1Br	32536-52-0	-4.6	10.17			



$t_{½}$ (Days)

Aronson et al 2(Table 4

Descriptor	*model output*	*half-life (days)*
Hours	*>4.75*	*0.17*
Hours-days	*4.25-4.75*	*1.25*
Days	*3.75-4.25*	*2.33*
Days–weeks	*3.25–3.75*	*8.67*
Weeks	*2.75–3.25*	*15*
Weeks–months	*2.25–2.75*	*37.5*
Months	*1.75–2.25*	*120*
Recalcitrant	*<1.75*	*180*
–	*1.25–1.75*	*240*
–	*<1.25*	*720*

Regression line

Score	t 1/2
0	
1	
2	
3	
4	
5	

	BIOWIN 3		Ultimate biodeg
	Structural fragments	Coeff	Value
OCDD	8 * Aromatic Chloride	-0.2066	-1.6528
	2 * Aromatic Ether	-0.0581	-0.1162
octa-BDE	8 * Aromatic Bromide	-0.1360	-1.0880
	1 * Aromatic Ether	-0.0581	-0.0581

BIOWIN 4		**Primary biodeg**
Structural fragments	Coeff	Value
8 * Aromatic Chloride	-0.1653	-1.3224
2 * Aromatic Ether	0.0771	0.1542
8 * Aromatic Bromide	-0.1535	-1.228
1 * Aromatic Ether	0.0771	0.0771

Coefficients from Table 1 in Boethling et al (1994)

	primary coeff	ultimate coeff
yclic aromatic hydrocarbon (≥4	-0.702	-0.799
nsubstituted aromatic (≤3 rings	-0.343	-0.586
tertiary amine	-0.288	-0.255
trifluoromethyl (CF3)	-0.274	-0.513
aromatic Cl	-0.165	-0.207
aromatic Br	-0.154	-0.136
rbon with 4 single bonds and nc	-0.153	-0.212
aromatic I	-0.127	-0.045
aromatic NO2	-0.108	-0.17
aromatic NH2 or NH	-0.108	-0.135
aliphatic Cl	-0.101	-0.173
lkyl substituent on aromatic rin	-0.069	-0.075
cyanideinitrile (C≡N)	-0.065	-0.082
triazine ring	-0.058	-0.246
azo group (N=N)	-0.053	-0.3
ketone (CC(=O)C)	-0.022	-0.023
pyridine ring	-0.019	-0.214
aliphatic ether	-0.0097	-0.0087
molecular weight	-0.00144	-0.00221
nsubstituted phenyl group (C6H	0.0049	0.022
aromatic (C(=O)OH)	0.0078	0.088
N-nitroso (NN=O)	0.019	-0.385
aromatic sulfonic acid or salt	0.022	0.142
aliphatic Br	0.035	0.029
aromatic OH	0.04	0.056
aliphatic NH2 or NH	0.043	0.024
aromatic ether	0.077	-0.058
aliphatic OH	0.129	0.16
aromatic F	0.135	-0.407
aliphatic sulfonic acid or salt	0.177	0.193
caibamate	0.194	-0.047
aldehyde (CHO)	0.197	0.022
amide (C(=O)N or C(=S)N)	0.205	-0.054
ester (C(=O)OC)	0.229	0.14
r C4 terminal alkyl (CH2CH2CH2	0.269	0.298
aliphatic (C(=O)OH)	0.386	0.365
phosphate ester	0.465	0.154
equation constant	3.848	3.199