



Front page for deliverables

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1. Glossary

CASRN	Chemical Abstract Service Registry Number.
CO ₂	Max. amount of CO ₂ production (and time-point) in soil.
DT ₅₀	Time in which 50% of the parent compound has disappeared from soil by transformation.
RIVM	National Institute of Public Health and Environmental Protection.
SMILES	Simplified Molecular Input Line Entry System. This is a chemical notation system that is used to represent the 2D molecular structure by a linear string of symbols.

2. Introduction

This report provides an overview of the collected data for biodegradability in soil. All data could be grouped in three types. First type of data includes a set of 219 pesticides with information about the most important properties which describe biodegradability and mobility, such as DT₅₀ and CO₂ production. The second set of data includes 183 chemicals with documented maps for biodegradation in soil. The third set of chemicals includes 20 pesticides having information about the maximum amount of their major metabolites, biodegradability DT₅₀ and observed metabolic maps in soil.

3. Collected data for biodegradability in soil

3.1. Rate of biodegradation in soil

A set of 219 pesticides with biodegradability data were collected from the report provided by the National Institute of Public Health and Environmental Protection (RIVM) [1]. The data mentioned are based on confidential information supplied by the manufactures of the pesticides. Most of the data are derived from laboratory experiments under aerobic conditions with the active ingredient of a pesticide. For some pesticides only data from field studies are available. The collected information for the chemicals includes common name, arithmetic mean or median of DT₅₀ (days), range of variation of DT₅₀, maximum amount of CO₂ calculated as a percentage of the total CO₂ that the chemicals could theoretically produce (ThCO₂ %) and the duration of the test period.

The available information for the pesticides is summarized in Table 1. It should be noted that in the table a dash means that data are not available; data derived from less reliable studies due to inadequate experimental design are marked with an asterisk. 218 out of 219 pesticides have data for DT₅₀, 156 have data for CO₂, and 155 compounds have information for both the DT₅₀ and CO₂.

Table 1. List of pesticides with their rate of biodegradation in soil.

CASRN	Chemical name	DT ₅₀ (days) mean/median	Range of variation of DT ₅₀ (days)	ThCO ₂ (%)	Test period (days)
542-75-6	1,3-dichloropropene	13	2-24	-	-
94-75-7	2,4-D pH < 5	8	2-14	49-83	51-150
74070-46-5	acetonifene	71	43-99	3	90-104
101007-06-1	acrinathrin	23	9-37	32-55	120
15972-60-8	alachlor	22	14-29	5.5-30	62-175
116-06-3	aldicarb	2.4	1.3-3.5	65	90
55635-13-7	Alloxydim sodium	20	2-38	17-23	28
101-05-3	anilazine	1	-	0.3-1.3	28-112
3337-71-1	asulam	24	9-39	<1-3.2	56-77
1912-24-9	atrazine	50	38-62	4-14	90-375
86-50-0	azinphos-methyl	52*	-	5-19	222-365
68038-71-1	Bacillus thuringiensis	2.7	-	13	23
22781-23-3	bendiocarb	28*	5-63*	10-42	60-62
17606-31-4	bensultap	7	-	62-79	365
25057-89-0	bentazone	48	19-77	2	60
8001-54-5	benzalkonium chloride	-	-	33	64
82657-04-3	bifenthrin	219*	169-292*	13-37	120-180
13181-17-4	bromofenoxim	73	0.7-145	29-51	210-214
4824-78-6	bromophos-ethyl	8*	6-10*	-	-
18181-80-1	bromopropylate	59*	47-70*	44-69	180-365
51249-05-9	buminafos	9*	6-13*		-
41483-43-6	bupirimate	79	67-91	1-53	329-365
63-25-2	carbaryl	<14*	-	3-64	28-60
16118-49-3	carbetamide	10	5-15	47-72	82-182
5234-68-4	carboxin	7*	-	-	-

13360-45-7	chlorbromuron	39*	18-60*	5-15	60
470-90-6	chlorfenvinphos	36	-	16	100
1698-60-8	chloridazon	31	15-46	-	-
7003-89-6	chlormequat	1.3*	-	-	-
1897-45-6	chlorothalonil	10	-	-	-
15545-48-9	chlorotoluron	63	42-83	0.7	120
1982-47-4	chloroxuron	36	-	5-29	30-168
101-21-3	chlorpropham	40	36-44	16-28	200
2921-88-2	chlorpyrifos	94*	16-172*	27-89	360
105512-06-9	clodinafop-propargyl	0.6	-	49-61	336
74115-24-5	clofentezine	39	19-59	46	180
420-04-2	cyanamide	3.5*	0.4-6.6*	-	-
21725-46-2	cyanazine	16*	13-19*	-	-
1134-23-2	cycloate	61*	9.4-133*	-	-
101205-02-1	cycloxydim	1	-	2.5-32	90
68359-37-5	cyfluthrin	116*	74-172*	32-36	190
57966-95-7	cymoxanil	0.7	0.01-1.3	64-75	40
52315-07-8	cypermethrin (cis)	90*	61-119*	6-69*	112-175
52315-07-8	cypermethrin (trans)	32*	22-42*	6-69*	112-175
94361-06-5	cyproconazole	110	-	40	140
66215-27-8	cyromazine	93	75-110	1-8	28-367
75-99-0	dalapon	3.6	1-7	-	-
1596-84-5	daminozide	4.5*	3-4.5*	75-84*	14
533-74-4	dazomet	<1	-	-	-
52918-63-5	deltamethrin	25	18-30	26-73	64-128
17040-19-6	demeton-S-methylsulphon	2.7*	0.5-5.1*	10-31	73
13684-56-5	desmedipham	49	8-101	27-50	100-448
1014-69-3	desmetryn	9	8-10	1.2-20	30-168
333-41-5	diazinon	21	10-31	35-56	140-166
1918-00-9	dicamba	48	5-91	2-45	70-189
1194-65-6	dichlobenil	70*	24-116*	6.1	110
97-17-6	dichlofenthion	6*	4-9*	-	-
1085-98-9	dichlofluanid	2.9*	2.3-3.5*	78-99	63
120-36-5	dichlorprop	15	10-20	-	-
15165-67-0	dichlorprop-P	15	10-20	-	-
62-73-7	dichlorvos	2	1-2	60-80	1-60
99-30-9	dicloran	282	-	8	360
115-32-2	dicofol op	15*	-	-	-
7173-51-5	dodecyldimethylammoniumchloride	23	14-31	-	-
38727-55-8	diethyl-ethyl	114*	98-131*	4	56
87130-20-9	diethofencarb	5.4	1.5-9.2	31-57	270
119446-68-3	difenoconazole	140	-	4	107
14214-32-5	difenoxuron	18	-	17-29	30-168
35367-38-5	diflubenzuron	3	2-4	26	28

83164-33-4	diflufenican	192	116-277	46	365
52508-35-7	dikegulac-sodium	>195	-	-	-
34205-21-5	dimefuron	170*	-	-	-
60-51-5	dimethoate	16	10-21	20-30	7-30
110488-70-5	dimethomorph (E-isomer)	41	-	17-28	362-365
1420-07-1	dinoterb	9.8	9.2-10.4	23-24	50-63
3347-22-6	dithianon	5*	5-9*	14-16	98
330-54-1	diuron	94*	79-108*	3-18	40-105
534-52-1	DNOC	8.5	4-13	11-65	59-80
1593-77-7	dodemorph	190*	152-228*	-	-
759-94-4	EPTC	47*	42-52*	-	-
16672-87-0	ethephon	1*	-	0.06	98
29973-13-5	ethiofencarb	37*	34-131*	43	82
26225-79-6	ethofumesate	37	-	38	316
13194-48-4	ethoprophos	32	8-56	56-60	90
80844-07-1	etofenprox	11*	10-11*	38	56
2593-15-9	etridiazole	23*	12-33*	6-29	10-42
38260-54-7	etrimfos	12.5	8-17	25-60	70
140-56-7	fenaminosulf	17*	-	-	-
22224-92-6	fenamiphos	21	14-28	0.4-39	35-180
103112-35-2	fenchlorazole-ethyl	2.4	1.6-3.1	0.4-0.9	97
122-14-5	fenitrothion	28	14-42	12-70	60-365
66441-23-4	fenoxaprop-ethyl	<1	-	1.4-55	10-64
71283-80-2	fenoxaprop-P-ethyl	0.65	0.6-0.7	10-33	100
74738-17-3	fenpiclonil	308*	210-458*	27-45	270-365
39515-41-8	fenpropathrin	34	13-54	38-55	60-168
67306-00-7	fenpropidin	111	73-149	50-67	180
67564-91-4	fenpropimorph	67*	16-145*	9-18	45
900-95-8	fentin acetate	46*	29-62*	27-75	63-280
76-87-9	fentin hydroxide	26*	5-53*	-	-
51630-58-1	fenvalerate	83	30-135	4-48	30-90
79622-59-6	fluazinam	107	48-165	6	361
113036-88-7	flucycloxuron	208	146-269	21-39	175-364
69377-81-7	fluroxypyr	2.4	-	-	-
81406-37-3	fluroxypyr 1-methylheptyl ester	27	-	47-76	365
85509-19-9	flusilazole	600*	-	0.2-1.1	365
66332-96-5	flutolanil	601*	445-712*	0.4-6	180
69409-94-5	fluvalinate	7*	4-10*	3-9	56
944-22-9	fonofos	99*	48-150*	-	-
2540-82-1	formothion	<1	-	55-75	60
39148-24-8	fosetyl-aluminium	0.07	0.03-0.11	70-75	4
65907-30-4	furathiocarb	1*	-	52	365
81591-81-3	glyphosate-trimesium (glyph.part)	8*	-	83	376
81591-81-3	glyphosate-trimesium (trim.part)	4*	-	75	211

108173-90-6	guazatine	20*	-	28-45	190-454
87237-48-7	haloxyfop ethoxyethyl	1.5	-	33-36	180
23560-59-0	heptenophos	0.7	0.07-1.8	27-48	7
79983-71-4	hexaconazole	122	49-200	13-39	280
51235-04-2	hexazinone	62	59-64	35	175
81405-85-8	imazamethabenz-methyl (m-isomer)	51	45-57	11-58	240-360
81334-34-1	imazapyr	510*	-	14	360
138261-41-3	imidacloprid	180	159-200	6-10	100
36734-19-7	iprodisone	41	-	9-14	385
25311-71-1	isofenphos	64*	40-88*	10	92
82558-50-7	isoxaben	262*	165-389*	12-15	252
91465-08-6	lambda-cyhalothrin	41	13-69	36-70	92-181
2164-081	lenacil	179	-	47	365
58-89-9	lindane	1406	-	5	336
330-55-2	linuron	131	47-236	2.6-3	180
8018-017	mancozeb	5	3-7	-	-
12427-38-2	maneb	f 56	-	-	-
94-74-6	MCPA	15	6-24	-	-
7085-19-0	mecoprop	11	6-14	-	-
16484-77-8	mecoprop-P	11	6-14	-	-
57837-19-1	metalaxyl	42	29-54	14-25	180-360
108-62-3	metaldehyde	10*	9-12*	13	91
41394-05-2	metamitron	30	20-40	28-33	84-470
137-42-8	metam-sodium	0.009	0.003-0.018	-	-
67129-08-2	metazachlor	18	10-27	-	-
18691-97-9	methabenzthiazuron	135	117-153	0.2-6.6	77-126
10265-92-6	methamidophos	2.6	1.2-4	-	-
950-37-8	methidathion	4.5	-	14-61	28-365
2032-65-7	methiocarb	61*	42-80*	-	-
16752-77-5	methomyl	8	2-14	30-45	40
74-83-9	methyl bromide	15*	1-29*	-	-
556-61-6	methyl isothiocyanate	6	4-8	-	-
9006-42-2	metiram	6*	0.05-12*	-	-
51218-45-2	metolachlor	101	59-144	5-7	84-112
19937-59-8	metoxuron	f 18.5*	f 16-21*	-	-
74223-64-6	metsulfuron-methyl	31	27-34	36	168
26718-65-0	mevinphos	1.2*	0.4-2*	-	-
1746-81-2	monolinuron	50	33-66	9-54	112
88671-89-0	myclobutanil	282*	200-393"	3-28	240
10552-74-6	nitrothal-isopropyl	4*	1.2-9*	15-53	44-45
63284-71-9	nuarimol	306	213-399	-	-
1113-02-6	omethoate	1	0.9-1.2	19-49	49-112
23135-22-0	oxamyl	18*	10-26*	51-59	28-42
301-12-2	oxydemeton-methyl	0.5	-	59-79	57-60
56-38-2	parathion	49	18-92	40	135

298-00-0	parathion-methyl	19	14-23	60	135
66246-88-6	penconazole	197	194-200	1.4-65	364-546
66063-05-6	pencycuron	64*	42-86*	12-26	60
40487-42-1	pendimethalin	171	129-207	-	-
52645-53-1	permethrin	13	-	2-83	28-84
13684-63-4	phenmedipham	45*	16-74*	8-35	224-365
2310-17-0	phosalone	7	4.6-9.4	7-10	29-85
732-11-6	phosmet	5.6*	3.4-7*	53-80	308
13171-21-6	phosphamidon	4.5*	0.8-5.3*	80	66
51-03-6	piperonyl butoxide	13*	12-14*	-	-
23103-98-2	pirimicarb	108	8-222	0.5-97	84-490
29232-93-7	pirimiphos-methyl	12.5	12-13	1-17	210
7287-19-6	prometryn	41	37-45	0-6	180-360
1918-16-7	propachlor	5.2	3.4-7.0	0.5-13	98-126
24579-73-5	propamocarb	25	16-38	49-95	31-360
111479-05-1	propaquizafop	10	-	33-40	360
139-40-2	propazine	132	92-157	1-9	225-364
122-42-9	propham	11	6-15	25-40	200
60207-90-1	propiconazole	96*	67-125*	3	364
114-26-1	propoxur	79	26-131	20-35	330
23950-58-5	propyzamide	25	12-37	-	-
52888-80-9	prosulfocarb	24	9-39	52	370
13457-18-6	pyrazophos	39*	23-53*	14	77
8003-34-7	pyrethrins	8*	6-10*	-	-
96489-71-3	pyridaben	55	26-84	21 -50	360
55512-33-9	pyridate	5*	3.5-6*	13-25	70
88283-41-4	pyrifenoxy	66	60-72	5-16	365
90717-03-6	quinmerac	68	35-101	0.8-30	31-365
76578-14-8	quizalofop-ethyl	0.3	0.26-0.35	2-10	60
100646-51-3	quizalofop-P-ethyl	2*	-	-	-
122931-48-0	rimsulfuron	31	-	1-6	365
74051-80-2	sethoxydim	1.2	0.9-1.5	1-15	30-60
122-34-9	simazine	58	31-85	8	365
3689-24-5	sulfotep	28*	14-42*	-	-
107534-96-3	tebuconazole	652*	355-841*	0.7-32	433
79538-32-2	tefluthrin	13	-	11-65	60-180
3383-96-8	temephos	<2*	-	-	-
13071-79-9	terbufos	8*	6-11*	46	365
886-50-0	terbutryn	74	22-125	0.1-18.5	28-181
79277-27-3	thifensulfuron-methyl	6	3-9	31-44	140
31895-22-4	thiocyclam hydrogen oxalate	2.2*	0.5-3.8*	38-59	32
59669-26-0	thiodicarb	2	1.5-3	64-90	35-57
39196-18-4	thiofanox	4	2-6	75	153

640-15-3	thiometon	2*	1.9-7*	-	-
137-26-8	thiram	18*	7-35*	-	-
57018-04-9	tolclofos-methyl	66	45-95	19-38	90-240
731-27-1	tolylfluanid	1	1-1	25-40	99
55219-65-3	triadimenol	114*	-	-	-
2303-17-5	tri-allate	103	101-104	5-28	28-119
76608-88-3	triapenthenol	81*	65-95*	31-48	196
24017-47-8	triazophos	65*	27-102*	6-22	21-88
52-68-6	trichlorfon	18*	7-30*	-	-
55335-06-3	triclopyr	20	12-27	19-20	101-300
24602-86-6	tridemorph	34*	11-56*	12-23	49
99387-89-0	triflumizole	13	7-19	3-6	70-98
1582-09-8	trifluralin	221*	186-255*	-	-
26644-46-2	triforine	19	11-27	38	90
2275-23-2	vamidotion	1.8	1.5-2.1	9-10	14
50471-44-8	vinclozolin	23*	4-43*	0.5	45
81-81-2	warfarin	5	-	-	-
137-30-4	ziram	40*	-	-	-

3.2. Database with observed biodegradation pathways

An electronic database with documented biodegradation pathways in soil were collected and entered into the MetaPath database at different levels of completeness. Using MetaPath software (developed under the grant CR-83199501-0 with US EPA, Athens USA) the experimental information on observed metabolites, biotransformations and relative biotransformation rates can be systematically compiled into a searchable database. The created database includes observed biodegradation pathways for 183 chemicals, mainly pesticides which are presented in Table 2. Amongst them there are herbicides, insecticides, fungicides, acaricides, etc. The later includes substances with a variety of chemical functionality, such as acid amides, anilines and nitrobenzenes, dithio and thiolcarbamates, five- and six- membered heterocyclic compounds, phenyl (aryl) carbamates, phosphoro(di)thiolates, sulfonyleureas, etc. All chemicals are tested in soil but for most of them the microbial species are unknown and in these cases in

the database is entered the general name microorganism. For 44 chemicals from the database the microbial species is bacteria and for 25 of them there is an additional information about bacteria species and/or bacteria strain. 46 chemicals from the database have additional information about the conditions of biodegradation (aerobic or anaerobic metabolism).

Table 2. List of chemicals with observed biodegradation pathways.

Map No.	Study No.	Chemical name	CASRN	References	Study name	Species	Strain	Biotism
1	1	Urea	000057-13-6	2	Soil, Microorganisms	Microorganisms		
2	1	Isopropylbenzene	000098-82-8	3	Soil, Microorganisms	Microorganisms		
3	1	N-Butylbenzene	000104-51-8	3	Soil, Microorganisms	Microorganisms		
4	1	Isobutylbenzene	000538-93-2	3	Soil, Fungi	Fungi		
5	1	2-Phenylpentane	002719-52-0	3	Soil, Fungi	Fungi		
6	1	3-Phenylpentane	001196-58-3	3	Soil, Microorganisms	Microorganisms		
7	1	Anthracene	000120-12-7	4	Soil, Microorganisms	Microorganisms		
8	1	2,4-Dichlorophenoxyacetic acid	000094-75-7	5	Soil, Microorganisms	Microorganisms		
9	1	Permethrin	052645-53-1	6	Soil, Microorganisms	Microorganisms		
10	1	Chlorothalonil	001897-45-6	7	Soil, Microorganisms	Microorganisms		
11	1	Chlorotoluron	015545-48-9	8	Soil, Microorganisms	Microorganisms		
12	1	Chloroacetamide	000079-07-2	9	Soil, Microorganisms	Microorganisms		
13	1	Chloroacetonitrile	000107-14-2	9	Soil, Microorganisms	Microorganisms		
14	1	Chloroacetic_acid	000079-11-8	9	Soil, Microorganisms	Microorganisms		
15	1	Fenamiphos	022224-92-6	10	Soil, Microorganisms	Microorganisms		
15	2	Fenamiphos	022224-92-6	10	Soil, Microorganisms	Microorganisms		
15	3	Fenamiphos	022224-92-6	10	Soil, Microorganisms	Microorganisms		
16	1	Pentachloronitrobenzene	000082-68-8	11	Soil, Microorganisms	Microorganisms		
17	1	Carbaryl	000063-25-2	12	Soil, Microorganisms	Microorganisms		
18	1	Pendimethalin	040487-42-1	13	Soil, Microorganisms	Microorganisms		
18	2	Pendimethalin	040487-42-1	13	Soil, Microorganisms	Microorganisms		
18	3	Pendimethalin	040487-42-1	13	Soil, Microorganisms	Microorganisms		
19	1	Bromuconazole	116255-48-2	14	Soil, Microorganisms	Microorganisms		
20	1	Fenbuconazole	114369-43-6	14	Soil, Microorganisms	Microorganisms		
21	1	Flusilazole	085509-19-9	14	Soil, Fungi	Fungi		
22	1	Imazalil	035554-44-0	14	Soil, Microorganisms	Microorganisms		
23	1	Acetonitrile	000075-05-8	9	Soil, Microorganisms	Microorganisms		
24	1	Diphenylamine	000122-39-4	15	Soil, Microorganisms	Microorganisms		

25	1	Kerb	023950-58-5	16	Soil, Microorganisms	Microorganisms		
26	1	MT-101	052570-16-8	16	Soil, Microorganisms	Microorganisms		
27	1	Chloroanisidine	005345-54-0	16	Soil, Microorganisms	Microorganisms		
28	1	Alachlor	015972-60-8	16	Soil, Microorganisms	Microorganisms		
29	1	N-sec-Butyl-4-tert-butyl-2,6-dinitroaniline	033629-47-9	16	Soil, Microorganisms	Microorganisms		
30	1	Chloronitrofen	001836-77-7	16	Soil, Microorganisms	Microorganisms		
31	1	Ethylene_bis-dithiocarbamic_acid	000111-54-6	16	Soil, Microorganisms	Microorganisms		
32	1	Benthiocarb	028249-77-6	16	Soil, Microorganisms	Microorganisms		
33	1	Molinate	002212-67-1	16	Soil, Microorganisms	Microorganisms		
34	1	3-(3,5-Dichlorophenyl)-5,5-dimethyl-2,4-oxazolidinedione	024201-58-9	16	Soil, Microorganisms	Microorganisms		
35	1	Oxadiazone	019666-30-9	16	Soil, Microorganisms	Microorganisms		
36	1	Procymidone	032809-16-8	16	Soil, Microorganisms	Microorganisms		
37	1	BPMC	003766-81-2	16	Soil, Microorganisms	Microorganisms		
38	1	Fluoroimide	041205-21-4	16	Soil, Microorganisms	Microorganisms		
39	1	Thiofanox	039196-18-4	16	Soil, Microorganisms	Microorganisms		
40	1	Dichlorfop-methyl	051338-27-3	16	Soil, Microorganisms	Microorganisms		
41	1	Isothiazolinone	002682-20-4	16	Soil, Microorganisms	Microorganisms		
42	1	Thiophanate_methyl	023564-05-8	16	Soil, Microorganisms	Microorganisms		
43	1	Methabenzthiazuron	018691-97-9	16	Soil, Microorganisms	Microorganisms		
44	1	MIPC	002631-40-5	16	Soil, Microorganisms	Microorganisms		
45	1	M-(1-methylbutyl)phenyl_methyl_carbamate	002282-34-0	16	Soil, Microorganisms	Microorganisms		
46	1	M-(1-ethylpropyl)phenyl_methyl_carbamate	000672-04-8	16	Soil, Microorganisms	Microorganisms		
47	1	Clearcide	033439-45-1	16	Soil, Microorganisms	Microorganisms		
48	1	Carpropamid	104030-54-8	17	Soil, Microorganisms	Microorganisms		
49	1	Buturon	003766-60-7	16	Soil, Fungi	Rhizoctonia solani		
50	1	Dyfonate	000944-22-9	16	Soil, Microorganisms	Microorganisms		
51	1	Surecide	013067-93-1	16	Soil, Microorganisms	Microorganisms		
52	1	Cyanox	002636-26-2	16	Soil, Microorganisms	Microorganisms		
53	1	BAY-NTN-9306	035400-43-2	16	Soil, Microorganisms	Microorganisms		

54	1	Supracide	000950-37-8	16	Soil, Microorganisms	Microorganisms		
55	1	Phosalone	002310-17-0	16	Soil, Microorganisms	Microorganisms		
56	1	Cypermethrins_(cis, trans)	052315-07-8	16	Soil, Microorganisms	Microorganisms		
57	1	Sencor	021087-64-9	16	Soil, Microorganisms	Microorganisms		
58	1	3,6-Dichloro-alfa-picolic_acid	001702-17-6	16	Soil, Microorganisms	Microorganisms		Aerobic
59	1	Chloroneb	002675-77-6	16	Soil, Microorganisms	Microorganisms		
60	1	Metazachlor	067129-08-2	17	Soil, Bacteria	Bacillus		
61	1	Thenylchlor	096491-05-3	17	Soil, Fungi	Fungi		Aerobic
62	1	Haloxypop-methyl	069806-40-2	17	Soil, Fungi	Fungi		Anaerobic
63	1	1,3-Dichloropropene	000542-75-6	17	Soil, Bacteria	Bacteria		
64	1	Carbetamide	016118-49-3	17	Soil, Microorganisms	Microorganisms		Aerobic
65	1	Diethofencarb	087130-20-9	17	Soil, Bacteria	Nocardiosis sp.		
66	1	Fenothiocarb	062850-32-2	17	Soil, Microorganisms	Microorganisms		Aerobic
67	1	Fenothiocarb_sulfoxide	103614-75-1	17	Soil, Bacteria	Arthrobacter atrocyaneus	MCM B- 425	
68	1	Orbencarb	034622-58-7	17	Soil, Bacteria	Bacillus megaterium	MCM B- 423	
69	1	Fenpyroximate	134098-61-6	17	Soil, Bacteria	Bacillus sp.		Aerobic
70	1	Imidacloprid	105827-78-9	17	Soil, Bacteria	Methylosinus trichosporium	OB-3B	
71	1	Pyrazolate	058011-68-0	17	Soil, Bacteria	Methylosinus trichosporium	OB-3B	
72	1	Spiroxamine	118134-30-8	17	Soil, Bacteria	Methylosinus trichosporium	OB-3B	
73	1	Cloransulam-methyl	147150-35-4	17	Soil, Microorganisms	Methylosinus trichosporium	OB-3B	
74	1	Buprofezin	069327-76-0	17	Soil, Microorganisms	Microorganisms		
75	1	Mepanipyrim	110235-47-7	17	Soil, Bacteria	Streptomyces sp.	D7	
76	1	Chlorbromuron	013360-45-7	17	Soil, Microorganisms	Microorganisms		
77	1	Pencycuron	066063-05-6	17	Soil, Microorganisms	Microorganisms		
78	1	Amido-sulfuron	120923-37-7	17	Soil, Bacteria	Delftia acidovorans	WDL34	

79	1	Bensulfuron_methyl	083055-99-6	17	Soil, Microorganisms	Microorganisms		
80	1	Chlorimuron_ethyl	090982-32-4	17	Soil, Microorganisms	Microorganisms		
81	1	Metsulfuron_methyl	074223-64-6	17	Soil, Microorganisms	Microorganisms		Aerobic & anaerobic
82	1	Prosulfuron	094125-34-5	18	Soil, Microorganisms	Microorganisms		
83	1	Rimsulfuron	122931-48-0	19	Soil, Bacteria	Bacteria		
84	1	Thifensulfuron_methyl	079277-27-3	17	Soil, Microorganisms	Microorganisms		Aerobic
85	1	Sulfometuron_methyl	074222-97-2	17	Soil, Microorganisms	Microorganisms		
86	1	Hexazinone	051235-04-2	20	Soil, Microorganisms	Microorganisms		
87	1	Tribenuron_methyl	101200-48-0	17	Soil, Microorganisms	Microorganisms		
88	1	Vanilic acid	000121-34-6	21	Soil, Microorganisms	Microorganisms		
89	1	Chlorsulfuron	064902-72-3	22	Soil, Microorganisms	Microorganisms		
90	1	Trans - Anethole	004180-23-8	23	Soil, Microorganisms	Microorganisms		Aerobic & anaerobic
91	1	Clethodim	099129-21-2	24	Soil, Bacteria	Bacillus brevis	625	Aerobic & anaerobic
92	1	Tetradifon	000116-29-0	25	Soil, Microorganisms	Microorganisms		
93	1	Chlordimeform	006164-98-3	26	Soil, Microorganisms	Microorganisms		Aerobic & anaerobic
94	1	1,2,3,4-Tetrachlorobenzene	000634-66-2	27	Soil, Microorganisms	Microorganisms		Aerobic
95	1	Thiometon	000640-15-3	28	Soil, Microorganisms	Microorganisms		Anaerobic
96	1	Bentazone	025057-89-0	29	Soil, Bacteria	Pseudomonas acidovorans	M3GY	
97	1	2-Chloroethylphosphonic_acid	016672-87-0	30	Soil, Fungi	Fungi		Aerobic & anaerobic
98	1	Ioxynil	001689-83-4	31	Soil, Bacteria	Bacteria		
99	1	Ioxynil octanoate	003861-47-0	32	Soil, Microorganisms	Microorganisms		Aerobic
100	1	Trifluralin	001582-09-8	33	Soil, Microorganisms	Microorganisms		Aerobic &

								anaerobic
100	2	Trifluralin	001582-09-8	33	Soil, Bacteria	Flavobacterium sp.		
101	1	Diclosulam	145701-21-9	34	Soil, Microorganisms	Microorganisms		Aerobic
102	1	Teflubenzuron	083121-18-0	35	Soil, Microorganisms	Microorganisms		Aerobic
103	1	Tebuconazole	107534-96-3	36	Soil, Bacteria	Acinetobacter sp.	BEM2	Aerobic
104	1	Dicyclopentadiene	000077-73-6	37	Soil, Bacteria	Pseudomonas sp.	PEM1	Aerobic
105	1	Myclobutanil	088671-89-0	38	Soil, Bacteria	Bacteria		Aerobic
106	1	Sodium acifluorofen	062476-59-9	39	Soil, Bacteria	Bacteria		
107	1	Monocrotophos	006923-22-4	40	Soil, Bacteria	Bacteria		
107	2	Monocrotophos	006923-22-4	40	Soil, Bacteria	Bacteria		
108	1	Fenpropimorph	067306-03-0	41	Soil, Microorganisms	Microorganisms		Aerobic & anaerobic
109	1	Methomyl	016752-77-5	42	Soil, Bacteria	Bacteria		
110	1	Benomyl	017804-35-2	43	Soil, Bacteria	Pseudomonas desmolytica		
111	1	Spinosyn_A	131929-60-7	44	Soil, Bacteria	Pseudomonas desmolytica		
112	1	Aldicarb	000116-06-3	45	Soil, Bacteria	Pseudomonas desmolytica		
113	1	Spinosyn_D	131929-63-0	44	Soil, Bacteria	Pseudomonas desmolytica		
114	1	Carfentrazone - ethyl	128639-02-1	46	Soil, Bacteria	Pseudomonas desmolytica		
115	1	Dimethylammonium_[(4-chloro-o-tolyl)oxy]acetate	002039-46-5	47	Soil, Bacteria	Pseudomonas sp.		
116	1	Dimethylammonium_(+)-2-[(4-chloro-o-tolyl)oxy]propionate	053404-32-3	47	Soil, Microorganisms	Microorganisms		Aerobic
117	1	Dimethylammonium_3,6-dichloro-2-methoxybenzoate	002300-66-5	47	Soil, Microorganisms	Microorganisms		
118	1	Fipronil	120068-37-3	48	Soil, Bacteria	Bacteria		Aerobic

								& anaerobic
119	1	Linuron	000330-55-2	49	Soil, Microorganisms	Microorganisms		Aerobic & anaerobic
120	1	Acetochlor	034256-82-1	50	Soil, Bacteria	Bacteria		
121	1	Fluometuron	002164-17-2	50	Soil, Bacteria	Bacteria		
122	1	Eptam	000759-94-4	51	Soil, Microorganisms	Microorganisms		
123	1	Pebulate	001114-71-2	51	Soil, Microorganisms	Microorganisms		
124	1	Diallate	002303-16-4	51	Soil, Microorganisms	Microorganisms		
125	1	Triallate	002303-17-5	51	Soil, Microorganisms	Microorganisms		
126	1	Bitertanol	055179-31-2	52	Soil, Microorganisms	Microorganisms		
127	1	Perchloroethylene	000127-18-4	53	Soil, Microorganisms	Microorganisms		
128	1	Hexachlorobenzene	000118-74-1	53	Soil, Microorganisms	Microorganisms		
129	1	1,1-Dichloro-2,2-bis(4-chlorophenyl)ethylene	000072-55-9	54	Soil, Microorganisms	Microorganisms		
130	1	Fenitrothion	000122-14-5	55	Soil, Microorganisms	Microorganisms		
131	1	N-Dodecyl_benzenesulphonate	N/A	56	Soil, Bacteria	Bacteria		
132	1	Methyl_bromide	000074-83-9	57	Soil, Bacteria	Arthrobacter oxydans	P52	
133	1	Methyl_tert-butyl_ether	001634-04-4	58	Soil, Bacteria	Bacteria		
134	1	Chlorpyrifos	002921-88-2	45	Soil, Bacteria	Pseudomonas chlororaphis	RW71	Aerobic
135	1	Alloxydim sodium	055635-13-7	45	Soil, Microorganisms	Microorganisms		Aerobic & anaerobic
136	1	Clodinafop-propargyl	105512-06-9	45	Soil, Microorganisms	Microorganisms		Aerobic
137	1	Atrazine	001912-24-9	59	Soil, Microorganisms	Microorganisms		Aerobic
138	1	Cycloxydim	101205-02-1	45	Soil, Microorganisms	Microorganisms		Aerobic
139	1	Dazomet	000533-74-4	60	Soil, Microorganisms	Microorganisms		Anaerobic
140	1	Desmedipham	013684-56-5	61	Soil, Microorganisms	Microorganisms		
141	1	Metam-Sodium	000137-42-8	62	Soil, Bacteria	Bacteria		
142	1	Phenmedipham	013684-63-4	61	Soil, Bacteria	Bacteria	M91-3	Aerobic &

								anaerobic
143	1	Metalaxyl	057837-19-1	63	Soil, Bacteria	Arthrobacter sp.		Aerobic
144	1	Lufenuron	103055-07-8	64	Soil, Microorganisms	Microorganisms		
145	1	2,6-Dichlorobenzonitrile	001194-65-6	65	Soil, Microorganisms	Microorganisms		Aerobic & anaerobic
146	1	Diflubenzuron	035367-38-5	66	Soil, Microorganisms	Microorganisms		Aerobic & anaerobic
147	1	Etrinfos	038260-54-7	45	Soil, Microorganisms	Microorganisms		Aerobic
148	1	Fenoxaprop-ethyl	066441-23-4	67	Soil, Microorganisms	Microorganisms		Anaerobic
149	1	Fenoxaprop-P-ethyl	071283-80-2	45	Soil, Bacteria	Bacteria		
150	1	Isoxaben	082558-50-7	68	Soil, Bacteria	Bacteria		Aerobic & anaerobic
151	1	Phosmet	000732-11-6	69	Soil, Microorganisms	Microorganisms		
152	1	Formothion	002540-82-1	70	Soil, Microorganisms	Microorganisms		
153	1	LGC-42153	412928-75-7	71	Soil, Microorganisms	Microorganisms		
154	1	4-Chloroaniline	000106-47-8	72	Soil, Bacteria	Pseudomonas sp.		
154	2	4-Chloroaniline	000106-47-8	72	Soil, Bacteria	Arthrobacter aurescens	TA13	
155	1	Furathiocarb	065907-30-4	73	Soil, Microorganisms	Microorganisms		
156	1	Glyphosate-trimesium	081591-81-3	45	Soil, Microorganisms	Microorganisms		
157	1	Glyphosate	001071-83-6	74	Soil, Microorganisms	Microorganisms		
158	1	Glufosinate-ammonium	077182-82-2	75	Soil, Microorganisms	Microorganisms		
159	1	Haloxypop-etotyl	087237-48-7	76	Soil, Microorganisms	Microorganisms		
159	2	Haloxypop-etotyl	087237-48-7	76	Soil, Microorganisms	Microorganisms		Aerobic & anaerobic
160	1	Imazamethabenz-methyl (p-isomer)	081405-85-8	77	Soil, Bacteria	Bacteria		
161	1	Imazamethabenz-methyl (m-isomer)	N/A	77	Soil, Bacteria	Bacteria		
162	1	Propaquizafop	111479-05-1	78	Soil, Microorganisms	Microorganisms		Aerobic
163	1	Pyridate	055512-33-9	79	Soil, Microorganisms	Microorganisms		

163	2	Pyridate	055512-33-9	79	Soil, Microorganisms	Microorganisms	
164	1	Quizalofop-P-ethyl	100646-51-3	80	Soil, Microorganisms	Microorganisms	
165	1	Sethoxydim	074051-80-2	81	Soil, Microorganisms	Microorganisms	
166	1	Fluazifop-P-butyl	079241-46-6	82	Soil, Microorganisms	Microorganisms	Aerobic & anaerobic
167	1	Acephate	030560-19-1	83	Soil, Microorganisms	Microorganisms	Aerobic
168	1	Thiodicarb	059669-26-0	84	Soil, Bacteria	Arthrobacter sp.	Aerobic
168	2	Thiodicarb	059669-26-0	84	Soil, Microorganisms	Microorganisms	
169	1	Tolylfluanid	000731-27-1	85	Soil, Microorganisms	Microorganisms	
170	1	Triclopyr	055335-06-3	86	Soil, Microorganisms	Microorganisms	
171	1	Chlordane	000057-74-9	87	Soil, Microorganisms	Microorganisms	
172	1	Nitrofen	001836-75-5	88	Soil, Microorganisms	Microorganisms	Anaerobic
173	1	Diazinon	000333-41-5	89	Soil, Microorganisms	Microorganisms	Aerobic
174	1	Picolinafen	137641-05-5	90	Soil, Microorganisms	Microorganisms	Aerobic
175	1	Zoxamide	156052-68-5	91	Soil, Microorganisms	Microorganisms	Aerobic
175	2	Zoxamide	156052-68-5	91	Soil, Microorganisms	Microorganisms	
176	1	Flumioxazin	103361-09-7	92	Soil, Microorganisms	Microorganisms	Anaerobic
177	1	Tebufenozide	112410-23-8	93	Soil, Microorganisms	Microorganisms	Aerobic
178	1	Tebuthiuron	034014-18-1	94	Soil, Microorganisms	Microorganisms	Aerobic
178	2	Tebuthiuron	034014-18-1	94	Soil, Microorganisms	Microorganisms	Aerobic & anaerobic
179	1	Fenvalerate	051630-58-1	95	Soil, Microorganisms	Microorganisms	Aerobic & anaerobic
180	1	Lactofen	077501-63-4	96	Soil, Microorganisms	Microorganisms	Aerobic
181	1	Malathion	000121-75-5	97	Soil, Microorganisms	Microorganisms	
182	1	Propachlor	001918-16-7	98	Soil, Microorganisms	Microorganisms	
182	2	Propachlor	001918-16-7	98	Soil, Microorganisms	Microorganisms	Anaerobic
183	1	Norflurazon	027314-13-2	99	Soil, Microorganisms	Microorganisms	Aerobic

Information about the chemicals is organized in the following fields:

1. Data fields.

Map information:

- *Map info*
 - Map title
 - References
- *Parent info*
 - Structure, CAS, name, chemical use
 - Test compound
 - IUPAC name
- *Studies*
 - Test subjects (species) – strain
 - Additional information

Chemical information:

- SMILES
- Chemical name + Synonyms
- Chemical use class

Figure 1 represents an example for the documented biodegradation pathway for acetonitrile. On the left the observed metabolic pathway is presented, and on the right part of the window additional information for the chemical is given:

- **reference** – “Castro, Ch. E., S. K. O’Shea, W. Wang, E. W. Bartnicki, Environ. Sci. and Technol., vol. 30, N 4, 1996, pp. 1180-1184”;
- name of the **study** – “Soil, Microorganism”;
- **species** name – “Methylosinus trichosporium”
- **strain** – “OB-3B”.

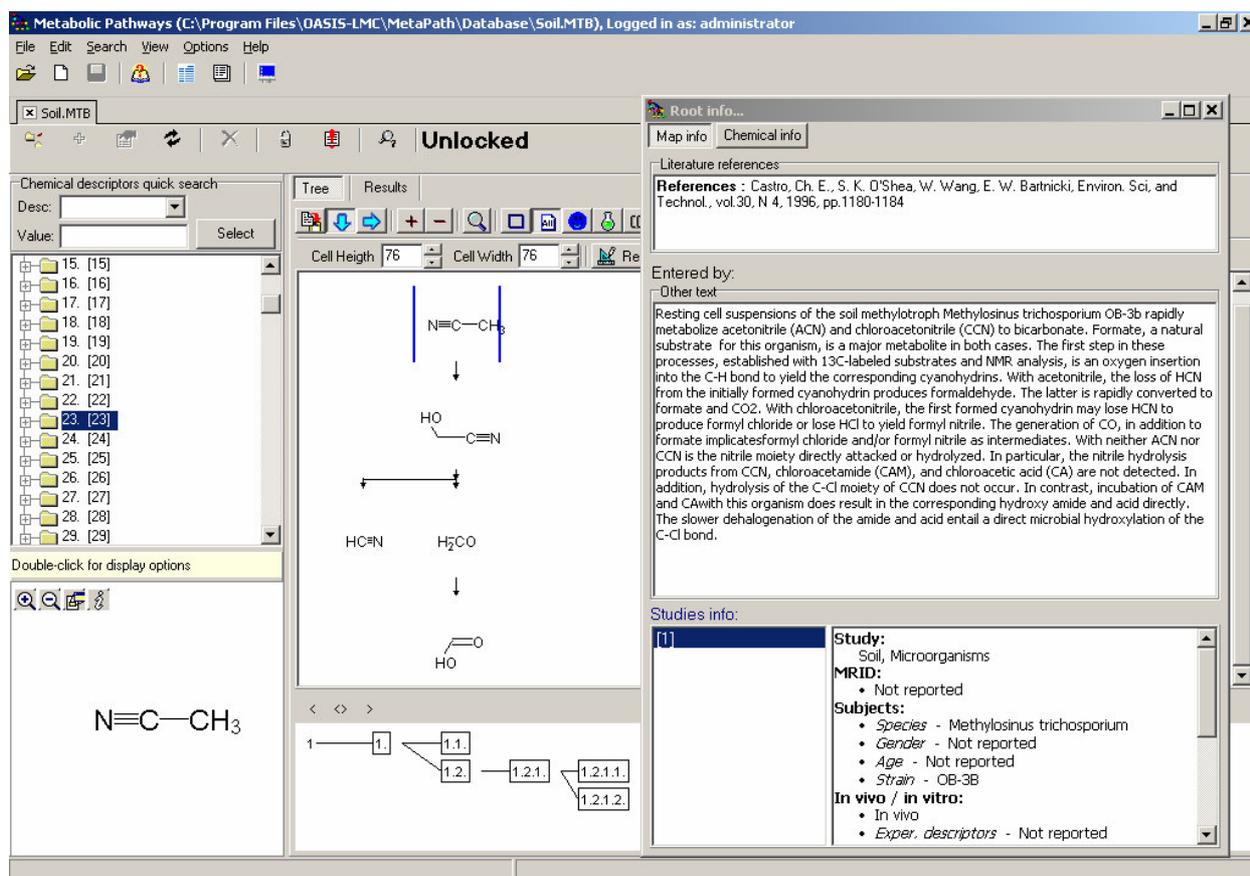


Figure 1. Illustration of the MetaPath file format for documented biodegradation pathway of acetonitrile.

In some cases there are documented metabolic maps including more than one study. This means that for one parent chemical there are metabolites generated by different soil microorganisms and/or at different conditions. In such cases there is a possibility the metabolites from different studies are indicated with different colors as presented on Figure 2. As can be seen from Figure 2, the illustrated metabolic pathway for pendimethalin combines metabolites generated in three studies. The red arrows indicate metabolites generated in the presence of soil

bacteria, while the blue and green arrows indicate metabolites generated in the presence of soil fungi in aerobic and anaerobic conditions, respectively.

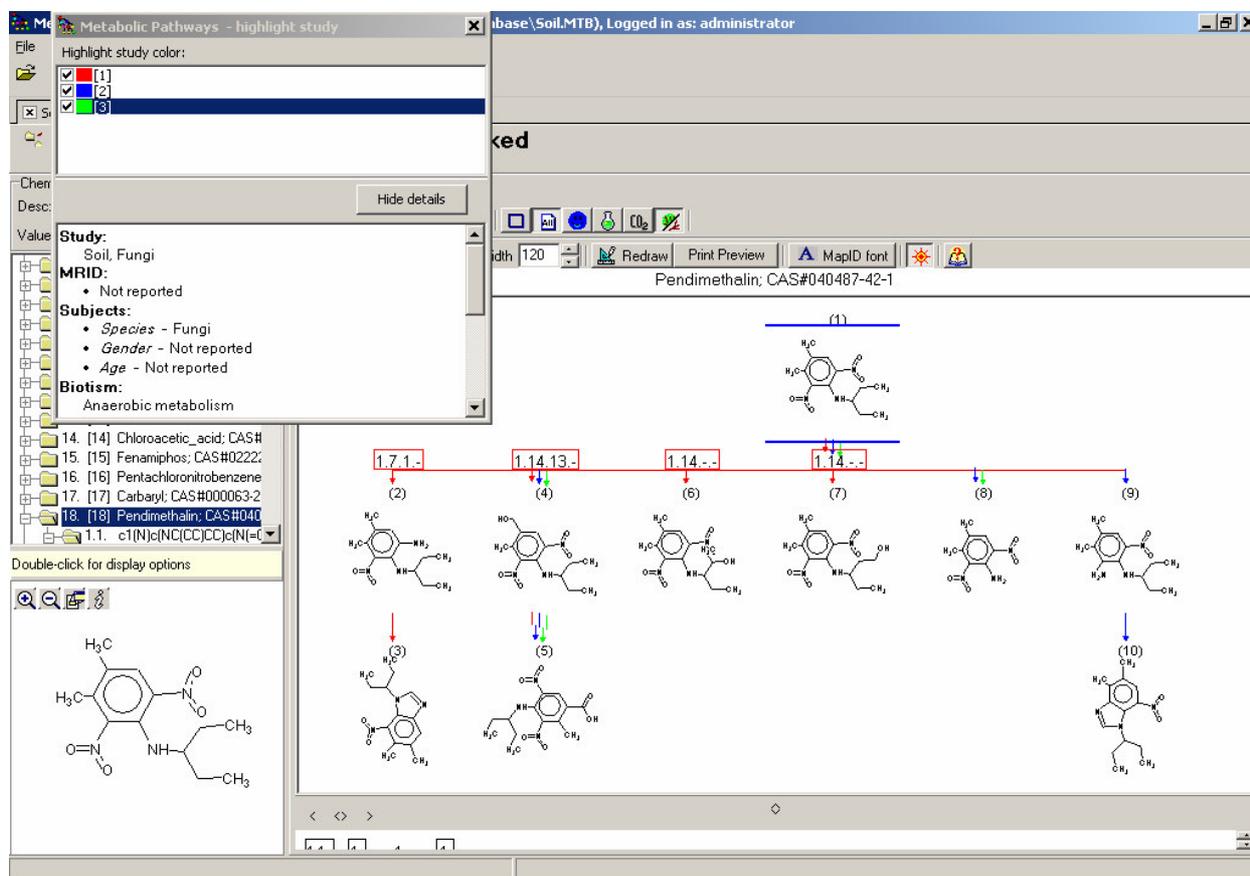


Figure 2. Example of a metabolic pathway including metabolites generated in different study conditions.

3.3. Behavior in soil and major metabolites

For 20 pesticides with documented biodegradation pathways additional data for the amount of their major metabolites and DT_{50} values have been collected. These chemicals are part of the electronic database with observed biodegradation pathways in soil created in MetaPath file format. Information about the time in which 50% of the parent compound has disappeared from

soil was taken from the report provided by the National Institute of Public Health and Environmental Protection (RIVM) [1]. In Table 3 the available data for the 20 pesticides are presented.

Table 3. Major metabolites – behavior in soil.

Parent chemical	Parent CASRN	Metabolite name	Reference	Study name	Species	Strain	Biotism	Maximum amount, %	DT50 (days)	Test Period (days)?
Aldicarb	116-06-3	Aldicarb sulfoxide	45	Soil, Microorganisms	Microorganisms			90	22	16-28
		Aldicarb sulfone	45	Soil, Microorganisms	Microorganisms			20	48	9-87
Chlorpyrifos	2921-88-2	3,5,6-trichloro-2-pyridinol	45	Soil, Microorganisms	Microorganisms			38	91	12-217
Alloxydim sodium	55635-13-7	methyl 6,6-dimethyl-2-propyl-4-oxo-4,5,6,7-tetrahydrobenzoxazol-5-carboxylate	45	Soil, Microorganisms	Microorganisms			10	19*	15-22*
Clodinafop-propargyl	105512-06-9	clodinafop	45	Soil, Microorganisms	Microorganisms			95	8*	-
Atrazine	1912-24-9	desethyl-atrazine	59	Soil, Bacteria	Bacteria	M91-3	Aerobic & anaerobic	21	45*	-
		2-hydroxy atrazine	59	Soil, Bacteria	Bacteria	M91-3	Aerobic & anaerobic	33	164*	-
Cycloxydim	101205-02-1	TSO (2-(1-(ethoxyimino)butyl)-3-hydroxy-5-(tetrahydro-2H-thiopyransulfoxide-3-yl)-2-cyclohexen-1-one)	45	Soil, Microorganisms	Microorganisms			25*	45*	-
		T2SO (2-(2*-propyl)oxazolyl-5-(tetrahydro-2-H-thiopyran-3-yl)-2-cyclohexen-1-one)	45	Soil, Microorganisms	Microorganisms			25*	45*	-
Dazomet	533-74-4	methylisothiocyanate	60	Soil, Microorganisms	Microorganisms			-	6	4-8
Desmedipham	13684-56-5	ethyl-N-(3-hydroxyphenyl)-carbamate	61	Soil, Bacteria	Arthrobacter oxydans	P52		49	101	14-221
Metam-Sodium	137-42-8	Methyl isothiocyanate	62	Soil, Microorganisms	Microorganisms			48	6	4-8
Phenmedipham	13684-63-4	methyl(3-hydroxyphenyl)-carbamate	61	Soil, Bacteria	Bacteria			31	56*	-
Metalaxyl	57837-19-1	N-(2,6-DIMETHYLPHENYL)-N-(2*-RNETHOXYACETYL)ALANINE	63	Soil, Bacteria	Bacteria			54	58	-
2,6-Dichlorobenzonitrile	1194-65-6	2.6-Dichlorobenzamide	65	Soil, Bacteria	Bacteria			66	660*	-

Diflubenzuron	35367-38-5	4-chlorophenyl-urea	66	Soil, Fungi	Fungi		Aerobic & anaerobic	68	51*	37-65*
Etrimfos	38260-54-7	6-ethoxy-2-ethyl-4-hydroxypyrimidine	45	Soil, Microorganisms	Microorganisms			85	98*	13-186*
Fenoxaprop-ethyl	66441-23-4	2-(4-(6-chloro-benzoxazol-2-ylloxy)-phenoxy)propanoic acid	67	Soil, Microorganisms	Microorganisms			>10	12	12-13
Fenoxaprop-P-ethyl	71283-80-2	Propanoic acid, 2-(4-((6-chloro-2-benzoxazolyl)oxy)phenoxy)-, (R)-	45	Soil, Microorganisms	Microorganisms			81	16	14-18
Isoxaben	82558-50-7	N-[3-(1-hydroxy-1-methylpropyl)-5-isoxazolyl]-2,6-dimethoxybenzamide	68	Soil, Bacteria	Bacteria			20	51*	-
Formothion	2540-82-1	dimethoate	70	Soil, Microorganisms	Microorganisms		Aerobic & anaerobic	70	16	10-21
Furathiocarb	65907-30-4	carbofuran	73	Soil, Bacteria	Arthrobacter sp.		Aerobic	80	36	16-56
Glyphosate-trimesium	81591-81-3	1-Aminomethylphosphonic acid	45	Soil, Microorganisms	Microorganisms			15	37	26-44
		Aldicarb sulfone						20	48	9-87
		2-hydroxy-atrazine						33	164*	-
		T2SO (2-(2*-propyl)oxazolyl-5-(tetrahydro-2-H-thiopyran-3-yl-2-cyclohexen-1-one)						25*	45*	-

4. Summary

Information for biodegradation rate of 219 chemicals, and metabolic fate in soil for 183 chemicals was collected from literature. In progress is the development of an electronic website database that will provide remote access by means of browsing the records as well as creating and executing search queries. The collected biodegradation data will be used for the development of a metabolic simulator for biodegradation in soil.

5. References

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http://umbbd.ahc.umn.edu/2,4-d/2,4-d_map.html; Supplemental Environmental Impact Statement Assessments of Aquatic Herbicides: Volume 3 - 2,4-D, Section 3 - Environmental Fate, pp. 41-48, February 2001; <http://www.24d.org/govtrev/Washington-State-Review.pdf>
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