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National Food Institute
Technical University of Denmark

Exact Mass Pesticide Database for use by GC-HRMS

Report 1

(08042015)

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CONTENT:

1. Introduction

This report describes an exact database of 53 pesticides for use with gas chromatography high resolution mass spectrometry (GC-HRMS). For each pesticide the chemical formula and molecular weight is listed as well as the formula and exact mass of a number of characteristic fragment ions.

The intention is to use the database in conjunction with Agilent MassHunter software. A preliminary test have been conducted with the build of a custom Agilent library (PCDL) and analysis of a pesticide standard mixture.

2. Analytical conditions for the GC-HRMS

Gas chromatograph:

Inlet: PTV

Inlet temperature: 60 °C

Injection volume: 5 µl

Carrier gas: Helium

Carrier flow: 1.2 ml/min (column 1) and 1.4 ml/min /column 2)

Columns: 2 identical columns. HP-5MS UI, 15m x 250 µm x 0.25 µm

Oven temperature program: 60 °C in 3 min., 30 °C/min. to 180 °C, hold in 0.8 min, 5 °C/min. to 300 °C. Total run time 31.8 min.

Mass Spectrometer

Ion source temperature: 230 °C

Transfer line temperature: 300 °C

Ionization: electron impact

Electron energy: 70 eV

Sampling rate: 4 GHz

Mass range: 50 - 500 AMU

3. Exact mass database of 53 pesticides for use by GC-HRMS

Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
2,4-D Butyl ester	94-80-4	12.607	276.032000	C12H14O3Cl2		
2,4-D Butyl ester	94-80-4	12.607		C8H6O3Cl2	219.968851	219.969399
2,4-D Butyl ester	94-80-4	12.607		C8H6O3Cl	184.999998	185.000547
2,4-D Butyl ester	94-80-4	12.607		C7H5OCl2	174.971197	174.971745
2,4-D Butyl ester	94-80-4	12.607		C6H4OCl2	161.963372	161.963920
2,4-D Butyl ester	94-80-4	12.607		C6H3Cl2	144.960632	144.961181
2.4.5-T-methylester	1928-37-6	11.387	267.946077	C9H7O3Cl3		
2.4.5-T-methylester	1928-37-6	11.387		C9H7O3Cl2	232.976676	232.977225
2.4.5-T-methylester	1928-37-6	11.387		C7H4OCl3	208.932224	208.932773
2.4-DB-methylester	18625-12-2	12.196	262.016350	C11H12O3Cl2		
2.4-DB-methylester	18625-12-2	12.196		C10H9O2Cl2	230.997411	230.997960
2.4-DB-methylester	18625-12-2	12.196		C6H4OCl2	161.963372	161.963920
2.4-DB-methylester	18625-12-2	12.196		C5H9O2	101.059706	101.060255
4,4'-Dichlorobenzophenone	90-98-2	14.183	249.995220	C13H8OCl2		
4,4'-Dichlorobenzophenone	90-98-2	14.183		C13H8OCl	215.025819	215.026368
4,4'-Dichlorobenzophenone	90-98-2	14.183		C7H4OCl	138.994519	138.995067
4,4'-Dichlorobenzophenone	90-98-2	14.183		C6H4Cl	110.999604	111.000153
Acetochlor	34256-82-1	12.709	269.118257	C14H20NO2Cl		
Acetochlor	34256-82-1	12.709		C14H20NO2	234.148855	234.149404
Acetochlor	34256-82-1	12.709		C12H14NOCl	223.075843	223.076392
Acetochlor	34256-82-1	12.709		C11H12NO	174.091340	174.091889
Acetochlor	34256-82-1	12.709		C10H12NO	162.091340	162.091889
Acetochlor	34256-82-1	12.709		C10H12N	146.096426	146.096974
Acetochlor	34256-82-1	12.709		C9H10N	132.080776	132.081324
Allethrin	584-79-2	15.357	302.188195	C19H26O3		
Allethrin	584-79-2	15.357		C9H15	123.116827	123.117375
Allethrin	584-79-2	15.357		C9H12O	136.088266	136.088815
Allethrin	584-79-2	15.357		C8H11	107.085527	107.086075
Aspon	3244-90-4	13.969	378.085338	C12H28O5P2S2		
Aspon	3244-90-4	13.969		C9H22O5P2S2	336.037840	336.038388
Aspon	3244-90-4	13.969		C6H17O5P2S2	294.998714	294.999263
Aspon	3244-90-4	13.969		C3H11O5P2S2	252.951764	252.952313
Aspon	3244-90-4	13.969		H5O5P2S2	210.904814	210.905363
Aspon	3244-90-4	13.969		H4O5P2S2	209.896989	209.897538
Aspon	3244-90-4	13.969		H3O4P2S2	192.894249	192.894798

Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
Aziprotryne	4658-28-0		225.079664	C7H11N7S		
Aziprotryne	4658-28-0			C6H8N7S	210.055640	210.056189
Aziprotryne	4658-28-0			C7H11N5S	197.072967	197.073516
Aziprotryne	4658-28-0			C7H10N5S	196.065142	196.065691
Aziprotryne	4658-28-0			C6H8N5S	182.049492	182.050041
Aziprotryne	4658-28-0			C5H5N5S	167.026017	167.026566
Aziprotryne	4658-28-0			C6H8N5	150.077422	150.077970
Barban (endo) (isomerA)	101-27-9	16.832	257.001034	C11H9NO2Cl2		
Barban (endo) (isomerA)	101-27-9	16.832		C11H9NO2Cl	222.031633	222.032181
Barban (endo) (isomerA)	101-27-9	16.832		C7H4NOCl	152.997593	152.998141
Barban (endo) (isomerA)	101-27-9	16.832		C10H9N	143.072951	143.073499
Barban (endo) (isomerA)	101-27-9	16.832		C6H6NCl	127.018328	127.018877
Barban (endo) (isomerA)	101-27-9	16.832		C6H4NCl	125.002678	125.003227
Benfluralin	1861-40-1	10.153	335.109291	C13H16N3O4F3		
Benfluralin	1861-40-1	10.153		C10H9N3O4F3	292.053967	292.054515
Benfluralin	1861-40-1	10.153		C10H9N3O3F3	276.059052	276.059601
Benfluralin	1861-40-1	10.153		C8H5N3O4F3	264.022667	264.023215
Bensulide	741-58-2		397.060507	C14H24NO4PS3		
Bensulide	741-58-2			C7H8NO2S	170.027026	170.027574
Bensulide	741-58-2			C6H5O2S	141.000476	141.001025
Bensulide	741-58-2			C6H5	77.038577	77.039125
Benzoylprop-ethyl	22212-55-1	20.827	365.058549	C18H17NO3Cl2		
Benzoylprop-ethyl	22212-55-1	20.827		C15H12NOCl2	292.029046	292.029594
Benzoylprop-ethyl	22212-55-1	20.827		C7H5O	105.033491	105.034040
Benzoylprop-ethyl	22212-55-1	20.827		C6C(13)H5O	106.036846	106.037395
Benzoylprop-ethyl	22212-55-1	20.827		C6H5	77.038577	77.039125
Butachlor	23184-66-9	16.283	311.165207	C17H26NO2Cl		
Butachlor	23184-66-9	16.283		C17H26NO2	276.195805	276.196354
Butachlor	23184-66-9	16.283		C13H16NOCl	237.091493	237.092042
Butachlor	23184-66-9	16.283		C13H16NO	202.122641	202.123189
Butachlor	23184-66-9	16.283		C11H14NO	176.106990	176.107539
Butachlor	23184-66-9	16.283		C11H14N	160.112076	160.112624
Butachlor	23184-66-9	16.283		C12H14NO	188.106990	188.107539
Butamifos	36335-67-8	16.552	332.095964	C13H21N2O4PS		
Butamifos	36335-67-8	16.552		C13H21NO2PS	286.102513	286.103061
Butamifos	36335-67-8	16.552		C11H17NO2PS	258.071212	258.071761
Butamifos	36335-67-8	16.552		C7H7NO4PS	231.982791	231.983340
Butamifos	36335-67-8	16.552		C7H7NO4P	200.010721	200.011269
Butylate (Sutan)	2008-41-5	8.137	217.150035	C11H23NOS		

Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
Butylate (Sutan)	2008-41-5	8.137		C8H16NOS	174.094711	174.095260
Butylate (Sutan)	2008-41-5	8.137		C9H18NO	156.138291	156.138839
Butylate (Sutan)	2008-41-5	8.137		C7H16NS	146.099797	146.100345
Carbetamide	16118-49-3	14.158	236.116092	C12H16N2O3		
Carbetamide	16118-49-3	14.158		C6C(13)H5NO	120.039920	120.040469
Carbetamide	16118-49-3	14.158		C7H5NO	119.036565	119.037114
Carbetamide	16118-49-3	14.158		C6H5N	91.041651	91.042199
Carbetamide	16118-49-3	14.158		C3H6NO	72.044390	72.044939
Chinomethionate	2439-01-2	15.760	233.992154	C10H6N2OS2		
Chinomethionate	2439-01-2	15.760		C9H6N2S2	205.996691	205.997240
Chinomethionate	2439-01-2	15.760		C9H6N2S	174.024620	174.025169
Chinomethionate	2439-01-2	15.760		C9H5N2S	173.016795	173.017344
Chinomethionate	2439-01-2	15.760		C8H6NS	148.021546	148.022095
Chinomethionate	2439-01-2	15.760		C8H6N	116.049476	116.050024
Chlorthiamid	1918-13-4	12.521	204.951975	C7H5NSCl2		
Chlorthiamid	1918-13-4	12.521		C7H3NCl2	170.963706	170.964255
Chlorthiamid	1918-13-4	12.521		C7H2N	100.018175	100.018724
Crimidine	535-89-7	8.822	171.056325	C7H10N3Cl		
Crimidine	535-89-7	8.822		C6H7N3Cl	156.032301	156.032850
Crimidine	535-89-7	8.822		C6H7N2Cl	142.029227	142.029776
Crimidine	535-89-7	8.822		C5H4N2Cl	127.005752	127.006301
Crimidine	535-89-7	8.822		C6H6N3	120.055624	120.056172
Crotoxyphos (Ciodrin)	7700-17-6		314.091925	C14H19O6P		
Crotoxyphos (Ciodrin)	7700-17-6			C6H10O5P	193.026036	193.026585
Crotoxyphos (Ciodrin)	7700-17-6			C2H8O4P	127.015472	127.016020
Crotoxyphos (Ciodrin)	7700-17-6			C8H9	105.069877	105.070425
Crotoxyphos (Ciodrin)	7700-17-6			C8H8	104.062052	104.062600
Cythioate	115-93-5	19.955	296.989450	C8H12NO5PS2		
Cythioate	115-93-5	19.955		C8H9O3PS	216.000453	216.001001
Cythioate	115-93-5	19.955		C2H8O4P	127.015472	127.016020
Cythioate	115-93-5	19.955		C2H6O2PS	124.982063	124.982612
Cythioate	115-93-5	19.955		C2H6O3P	109.004907	109.005456
Desethylatrazine	6190-65-4	10.014	187.062473	C6H10N5Cl		
Desethylatrazine	6190-65-4	10.014		C5H7N5Cl	172.038449	172.038998
Desethylatrazine	6190-65-4	10.014		C3H4N5Cl	145.014974	145.015523
DiazinonO-analog	962-58-3		288.123894	C12H21N2O4P		
DiazinonO-analog	962-58-3			C11H18N2O4P	273.099870	273.100419
DiazinonO-analog	962-58-3			C10H17N2O4P	260.092045	260.092594
DiazinonO-analog	962-58-3			C9H14N2O4P	245.068570	245.069118

Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
DiazinonO-analog	962-58-3			C8H10N2	134.083850	134.084398
DiazinonO-analog	962-58-3			C8H11N2O	151.086589	151.087138
DiazinonO-analog	962-58-3			C8H12N2O	152.094414	152.094963
DiazinonO-analog	962-58-3			C7H9N2O	137.070939	137.071488
Dibutylchlorendate	1770-80-5	22.550	497.949275	C17H20O4Cl6		
Dibutylchlorendate	1770-80-5	22.550		C9H4O4Cl6	385.823526	385.824075
Dibutylchlorendate	1770-80-5	22.550		C9H3O3Cl6	368.820787	368.821335
Dibutylchlorendate	1770-80-5	22.550		C7H2Cl5	260.859365	260.859914
Dibutylchlorendate	1770-80-5	22.550		C9H3O4Cl4	314.877996	314.878544
Dibutylchlorendate	1770-80-5	22.550		C5Cl5	234.843715	234.844264
Dicapthon	2463-84-5	14.252	296.962757	C8H9NO5PSCl		
Dicapthon	2463-84-5	14.252		C7C(13)H9NO5PS	262.996711	262.997259
Dicapthon	2463-84-5	14.252		C8H9NO5PS	261.993356	261.993905
Dicapthon	2463-84-5	14.252		C8H9O3PS	216.000453	216.001001
Dicapthon	2463-84-5	14.252		C2H6O2PS	124.982063	124.982612
Dichlormid	37764-25-3	7.705	207.021769	C8H11NOCl2		
Dichlormid	37764-25-3	7.705		C8H11NOCl	172.052368	172.052917
Dichlormid	37764-25-3	7.705		C5H6NOCl2	165.982096	165.982644
Dichlormid	37764-25-3	7.705		C8H10NO	136.075690	136.076239
Dichlormid	37764-25-3	7.705		C7H10NO	124.075690	124.076239
Dichlorophen	97-23-4		268.005785	C13H10O2Cl2		
Dichlorophen	97-23-4			C13H10O2Cl	233.036384	233.036932
Dichlorophen	97-23-4			C13H8OCl	215.025819	215.026368
Dichlorophen	97-23-4			C6H5OCl	128.002344	128.002892
Dichlorophen	97-23-4			C7H6OCl	141.010169	141.010718
Dichlorprop-methyl (Ester)	57153-17-0	9.588	248.000700	C10H10O3Cl2		
Dichlorprop-methyl (Ester)	57153-17-0	9.588		C8H7OCl2	188.986847	188.987395
Dichlorprop-methyl (Ester)	57153-17-0	9.588		C6H4OCl2	161.963372	161.963920
Dimethenamid	87674-68-8	12.591	275.074677	C12H18NO2SCl		
Dimethenamid	87674-68-8	12.591		C10H13NOSCl	230.040089	230.040637
Dimethenamid	87674-68-8	12.591		C8H10NOSCl	203.016614	203.017162
Dimethenamid	87674-68-8	12.591		C8H12NS	154.068496	154.069045
Dithiopyr	97886-45-8	13.400	401.054261	C15H16NO2S2F5		
Dithiopyr	97886-45-8	13.400		C14H13NO2SF5	354.058167	354.058715
Dithiopyr	97886-45-8	13.400		C13H9NO2F5	306.054796	306.055345
Dithiopyr	97886-45-8	13.400		C13H8NO2F4	286.048568	286.049116
Fenobucarb (Baycarb)	3766-81-2	9.529	207.125929	C12H17NO2		
Fenobucarb (Baycarb)	3766-81-2	9.529		C10H14O	150.103916	150.104465
Fenobucarb (Baycarb)	3766-81-2	9.529		C8H9O	121.064791	121.065340

Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
Fenoprop-methylester	4841-20-7	11.069	281.961727	C10H9O3Cl3		
Fenoprop-methylester	4841-20-7	11.069		C8H6OCl3	222.947874	222.948423
Fenoprop-methylester	4841-20-7	11.069		C6H3OCl3	195.924399	195.924948
Fluchloralin	33245-39-5	11.608	355.054668	C12H13N3O4ClF3		
Fluchloralin	33245-39-5	11.608		C10H8N3O4ClF3	326.014995	326.015543
Fluchloralin	33245-39-5	11.608		C11H11N3O4F3	306.069617	306.070166
Fluchloralin	33245-39-5	11.608		C8H5N3O4F3	264.022667	264.023215
Fluoroglycofen-ethyl	77501-90-7	23.716	447.033264	C18H13NO7ClF3		
Fluoroglycofen-ethyl	77501-90-7	23.716		C14H7NO4ClF3	345.001021	345.001570
Fluoroglycofen-ethyl	77501-90-7	23.716		C14H6NO4ClF3	343.993196	343.993745
Fluoroglycofen-ethyl	77501-90-7	23.716		C14H7O3ClF3	315.003033	315.003581
Fluoroglycofen-ethyl	77501-90-7	23.716		C13H7NO2ClF3	301.011192	301.011741
Fluoroglycofen-ethyl	77501-90-7	23.716		C8H3O2ClF3	222.976818	222.977367
Fluoroglycofen-ethyl	77501-90-7	23.716		C14H7O2	207.044056	207.044604
Fluridone	59756-60-4	27.432	329.102749	C19H14NOF3		
Fluridone	59756-60-4	27.432		C19H13NOF3	328.094375	328.094924
Flurprimidol	56425-91-3		312.108562	C15H15N2O2F3		
Flurprimidol	56425-91-3			C12H8N2O2F3	269.053239	269.053787
Flurprimidol	56425-91-3			C5H3N2O	107.023989	107.024538
Imibenconazole	86598-92-7	30.864	409.992650	C17H13N4SCl3		
Imibenconazole	86598-92-7	30.864		C17H13N4SCl2	375.023249	375.023798
Imibenconazole	86598-92-7	30.864		C10H7N4Cl2	253.004228	253.004777
Imibenconazole	86598-92-7	30.864		C7H3NCl2	170.963706	170.964255
Imibenconazole	86598-92-7	30.864		C7H6Cl	125.015254	125.015803
Lethane 384	112-56-1	8.822	203.097999	C9H17NO2S		
Lethane 384	112-56-1	8.822		C5H8NOS	130.032111	130.032660
Lethane 384	112-56-1	8.822		C5H9O2	101.059706	101.060255
Lethane 384	112-56-1	8.822		C3H4NS	86.005896	86.006445
Lethane 384	112-56-1	8.822		C2H4S	60.002822	60.003371
Lethane 384	112-56-1	8.822		C4H9	57.069877	57.070425
Mefluidide	53780-34-0		310.059898	C11H13N2O3SF3		
Mefluidide	53780-34-0			C9H11N2O2SF3	268.048784	268.049333
Mefluidide	53780-34-0			C10H13N2O	177.102239	177.102788
Mefluidide	53780-34-0			C8H11N2	135.091675	135.092223
Methabenzthiazuron	18691-97-9	10.080	221.062283	C10H11N3OS		
Methabenzthiazuron	18691-97-9	10.080		C8H7N2S	163.032445	163.032994
Methabenzthiazuron	18691-97-9	10.080		C8H8N2S	164.040270	164.040819
Methabenzthiazuron	18691-97-9	10.080		C6H4S	108.002822	108.003371
Methabenzthiazuron	18691-97-9	10.080		C7H6NS	136.021546	136.022095

Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
Methabenzthiazuron	18691-97-9	10.080		C7H5NS	135.013721	135.014270
Nitrothal-isopropyl	10552-74-6	14.330	295.105587	C14H17NO6		
Nitrothal-isopropyl	10552-74-6	14.330		C11H12NO6	254.065914	254.066462
Nitrothal-isopropyl	10552-74-6	14.330		C11H10NO5	236.055349	236.055897
Nitrothal-isopropyl	10552-74-6	14.330		C8H6NO6	212.018963	212.019512
Nitrothal-isopropyl	10552-74-6	14.330		C8H4NO5	194.008399	194.008947
O.O.O-Triethylphosphorothioate	126-68-1	6.596	198.047952	C6H15O3PS		
O.O.O-Triethylphosphorothioate	126-68-1	6.596		C2H8O3PS	142.992628	142.993176
O.O.O-Triethylphosphorothioate	126-68-1	6.596		C2H7O2PS	125.989888	125.990437
O.O.O-Triethylphosphorothioate	126-68-1	6.596		C4H10O2P	121.041292	121.041841
O.O.O-Triethylphosphorothioate	126-68-1	6.596		H4O3PS	114.961328	114.961876
O.O.O-Triethylphosphorothioate	126-68-1	6.596		H3O3PS	113.953503	113.954051
O.O.O-Triethylphosphorothioate	126-68-1	6.596		H2O2PS	96.950763	96.951312
O.O.O-Triethylphosphorothioate	126-68-1	6.596		C2H6O2P	93.009992	93.010541
Oryzalin	19044-88-3		346.094705	C12H18N4O6S		
Oryzalin	19044-88-3			C10H13N4O6S	317.055031	317.055580
Oryzalin	19044-88-3			C10H13N4O5S	301.060117	301.060665
Oryzalin	19044-88-3			C7H7N4O6S	275.008081	275.008630
Oryzalin	19044-88-3			C7H4N3O6S	257.981532	257.982081
Pentanochlor (Sloan)	2307-68-8	13.560	239.107692	C13H18NOCl		
Pentanochlor (Sloan)	2307-68-8	13.560		C10H12NOCl	197.060193	197.060742
Pentanochlor (Sloan)	2307-68-8	13.560		C7H8NCl	141.033978	141.034527
Pethoxamid	106700-29-2	15.540	295.133907	C16H22NO2Cl		
Pethoxamid	106700-29-2	15.540		C15H19NO2Cl	280.109883	280.110432
Pethoxamid	106700-29-2	15.540		C16H22NO2	260.164505	260.165054
Pethoxamid	106700-29-2	15.540		C13H15NOCl	236.083668	236.084217
Pethoxamid	106700-29-2	15.540		C13H14NO2	216.101905	216.102454
Pethoxamid	106700-29-2	15.540		C10H11	131.085527	131.086075
Plifenate (Penfenate)	21757-82-4	12.769	333.888868	C10H7O2Cl5		
Plifenate (Penfenate)	21757-82-4	12.769		C8H4Cl4	239.906162	239.906711
Plifenate (Penfenate)	21757-82-4	12.769		C9H7O2Cl2	216.981761	216.982310
Plifenate (Penfenate)	21757-82-4	12.769		C7H3OCl2	172.955547	172.956095
Plifenate (Penfenate)	21757-82-4	12.769		C8H4Cl2	169.968457	169.969006
Profluralin	26399-36-0	11.305	347.109291	C14H16N3O4F3		
Profluralin	26399-36-0	11.305		C12H11N3O4F3	318.069617	318.070166
Profluralin	26399-36-0	11.305		C14H15N3O3F3	330.106002	330.106551
Profluralin	26399-36-0	11.305		C14H15N3O3F3	330.106002	330.106551
Propachlor	1918-16-7	9.609	211.076392	C11H14NOCl		
Propachlor	1918-16-7	9.609		C11H14NO	176.106990	176.107539

Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
Propachlor	1918-16-7	9.609		C8H8NOCl	169.028893	169.029442
Propachlor	1918-16-7	9.609		C8H10N	120.080776	120.081324
Propachlor	1918-16-7	9.609		C7H6NO	120.044390	120.044939
Resmethrin	10453-86-8	20.208	338.188195	C22H26O3		
Resmethrin	10453-86-8	20.208		C12H11O	171.080441	171.080990
Resmethrin	10453-86-8	20.208		C11H11	143.085527	143.086075
Resmethrin	10453-86-8	20.208		C10H8	128.062052	128.062600
Resmethrin	10453-86-8	20.208		C9H15	123.116827	123.117375
Thenylchlor	96491-05-3	19.961	323.074677	C16H18NO2SCl		
Thenylchlor	96491-05-3	19.961		C16H18NO2S	288.105276	288.105825
Thenylchlor	96491-05-3	19.961		C7H6NO2S	168.011376	168.011924
Thenylchlor	96491-05-3	19.961		C7H9OS	141.036862	141.037411
Thenylchlor	96491-05-3	19.961		C9H10N	132.080776	132.081324
Thenylchlor	96491-05-3	19.961		C6H7OS	127.021212	127.021761
Tiocarbazil (Drepamon)	36756-79-3	14.252	279.165685	C16H25NOS		
Tiocarbazil (Drepamon)	36756-79-3	14.252		C9H18NO	156.138291	156.138839
Tiocarbazil (Drepamon)	36756-79-3	14.252		C5H10NO	100.075690	100.076239
Tiocarbazil (Drepamon)	36756-79-3	14.252		C7H7	91.054227	91.054775
Triclopyr-methylester (methyl)	60825-26-5		268.941326	C8H6NO3Cl3		
Triclopyr-methylester (methyl)	60825-26-5			C6H3NOCl3	209.927473	209.928022
Triclopyr-methylester (methyl)	60825-26-5			C5HNCl3	179.916909	179.917457
XMC / 3,5-Xylyl methylcarbamate	2655-14-3	6.668	179.094629	C10H13NO2		
XMC / 3,5-Xylyl methylcarbamate	2655-14-3	6.668		C8H10O	122.072616	122.073165
XMC / 3,5-Xylyl methylcarbamate	2655-14-3	6.668		C7H7O	107.049141	107.049690