Toestelinstellingen van GC-MS/MS bij de bepaling van organische parameters

INHOUD

1 TOEPASSINGSGEBIED

Deze procedure is nieuw en beschrijft typische GC-MS/MS instellingen voor de bepaling van organische parameters.

2 TOESTELINSTELLINGEN GC-MS/MS

De parameters in onderstaande tabel worden bij wijze van voorbeeld gegeven; de beste transities en instellingen van *collision energy* zijn afhankelijk van het merk en type toestel en dienen dus voor elk toestel geoptimaliseerd te worden.

2.1 FENOLEN (WAC/IV/A/001)

Natieve fenolen	Transitie		Collision Energie
	Moederion (m/z)	Dochterion (m/z)	(eV)
Fenol	136,0	94,0	10
	94,0	66,0	10
2-Chloorfenol	172,0	130,0	10
	170,0	128,0	10
2-Chloorfenol	128,0	63,0	25
	172,0	130,0	10
3-Chloorfenol	170,0	128,0	10
	128,0	65,0	20
4-Chloorfenol	172,0	130,0	10
	170,0	128,0	10
	128,0	65,0	20
2,6-Dichloorfenol	206,0	164,0	5
	204,0	162,0	5
	162,0	63,0	30
2,5-Dichloorfenol	206,0	164,0	10
	204,0	162,0	10
	162,0	63,0	30
2,4-Dichloorfenol	206,0	164,0	10
	204,0	162,0	10
	164,0	63,0	30
3,5-Dichloorfenol	206,0	164,0	10
	204,0	162,0	10
	164,0	63,0	30
2,3-Dichloorfenol	206,0	164,0	10
	204,0	162,0	10
	162,0	63,0	30

Natieve fenolen	Transitie		Collision Energie
	Moederion (m/z)	Dochterion (m/z)	(eV)
3,4-Dichloorfenol	206,0	164,0	10
	204,0	162,0	10
	162,0	63,0	30
2,4,6-Trichloorfenol	240,0	198,0	10
	238,0	196,0	10
	198,0	97,0	30
2,3,6-Trichloorfenol	240,0	198,0	10
	238,0	196,0	10
	196,0	97,0	30
2,3,5-Trichloorfenol	240,0	198,0	10
	238,0	196,0	10
	196,0	97,0	30
2,4,5-Trichloorfenol	240,0	198,0	10
	238,0	196,0	10
	196,0	97,0	30
2,3,4-Trichloorfenol	240,0	198,0	10
	238,0	196,0	10
	196,0	97,0	30
3,4,5-Trichloorfenol	240,0	198,0	10
	238,0	196,0	10
	196,0	97,0	30
2,3,5,6-Tetrachloorfenol	274,0	232,0	5
	272,0	230,0	5
	234,0	133,0	25
2,3,4,6-Tetrachloorfenol	274,0	232,0	10
	272,0	230,0	10
	232,0	133,0	25
2,3,4,5-Tetrachloorfenol	274,0	232,0	10
	272,0	230,0	10
	232,0	133,0	30
Pentachloorfenol	270,0	170,0	25
	268,0	167,0	25
	266,0	167,0	25
o-Cresol	150,0	108,0	5
	107,0	77,0	20
	108,0	77,0	25
m-Cresol	150,0	108,0	5
	107,0	77,0	20
	108,0	77,0	25

Natieve fenolen	Transitie		Collision Energie
	Moederion (m/z)	Dochterion (m/z)	(eV)
p-Cresol	150,0	108,0	5
	107,0	77,0	15
	108,0	77,0	25
2,6-Dimethylfenol	164,0	122,0	10
	122,0	107,0	10
	107,0	77,0	20
2,5-Dimethylfenol	164,0	122,0	5
	122,0	107,0	10
	107,0	77,0	15
2,4-Dimethylfenol	164,0	122,0	5
	122,0	107,0	10
	107,0	77,0	15
3,5-Dimethylfenol	164,0	122,0	5
	122,0	107,0	10
	107,0	77,0	15
2,3-Dimethylfenol	164,0	122,0	5
	122,0	107,0	10
	107,0	77,0	15
3,4-Dimethylfenol	164,0	122,0	5
	122,0	107,0	10
	107,0	77,0	15
o-Ethylfenol	164,0	122,0	5
	122,0	107,0	10
	107,0	77,0	15
m-Ethylfenol	164,0	122,0	5
	122,0	107,0	10
	107,0	77,0	20
p-Ethylfenol	164,0	122,0	5
	122,0	107,0	10
	107,0	77,0	15
2-Isopropylphenol	178,0	135,0	5
	136,0	121,0	10
	121,0	77,0	20
4-Chloor-3-methylfenol	144,0	107,0	15
	142,0	107,0	10
	107,0	77,0	15
2,3,5-Trimethylfenol	178,0	136,0	5
	136,0	121,0	10
	121,0	77,0	20

Natieve fenolen	Transitie		Collision Energie
	Moederion (m/z)	Dochterion (m/z)	(eV)
4-Chloor-3,5-dimethylfenol	158,0	121,0	10
	156,0	121,0	10
	121,0	77,0	15
Bisfenol A	270,0	213,0	25
	255,0	213,0	10
	228,0	214,0	10
	213,0	119,0	15

Interne standaarden	Transitie		Collision Energie
	Moederion (m/z)	Dochterion (m/z)	(eV)
13C-Fenol	142,0	100,0	10
	100,0	71,0	10
13C-4-Cloorfenol	172,0	130,0	10
	170,0	128,0	10
	134,0	70,0	20
13C-2,4-Dichloorfenol	212,0	170,0	10
	210,0	168,0	10
	168,0	68,0	25
13C-2,4,5-Trichloorfenol	246,0	204,0	10
	244,0	202,0	10
	202,0	102,0	25
13C-2,3,4,5-Tetrachloorfenol	240,0	138,0	30
	238,0	138,0	30
	236,0	136,0	25
13C-Pentachloorfenol	276,0	174,0	30
	274,0	172,0	25
	272,0	170,0	30
13C-1,2,4,5-Tetrachloorbenzeen	224,0	189,0	15
	222,0	187,0	15
	220,0	185,0	15
D8 o-Cresol	157,0	115,0	5
	113,0	81,0	20
	115,0	81,0	25
D3-2,4-Dimethylfenol	167,0	125,0	5
	128,0	100,0	15
	125,0	110,0	15
D16-Bisfenol A	284,0	224,0	10
	266,0	224,0	10
	242,0	225,0	15
	224,0	125,0	20

2.2 POLYCYCLISCHE AROMATISCHE KOOLWATERSTOFFEN (WAC/IV/A/002)

Natieve PAK	Transitie		Collision Energie
	Moederion (m/z)	Dochterion (m/z)	(eV)
Naftaleen	128,0	102,0	20
	128,0	127,0	20
Acenaftyleen	152,0	126,0	30
	152,0	151,0	20
Acenafteen	153,0	152,0	20
	154,0	152,0	30
Fluoreen	165,0	163,0	30
	166,0	165,0	20
Fenanthreen	178,0	152,0	20
	178,0	176,0	30
Anthraceen	178,0	152,0	20
	178,0	176,0	30
Fluorantheen	202,0	200,0	40
	202,0	201,0	20
Pyreen	202,0	200,0	40
	202,0	201,0	20
Benzo(a)anthraceen	228,0	202,0	30
	228,0	226,0	30
Chryseen	228,0	202,0	20
	228,0	226,0	30
Benzo(b)fluorantheen	250,0	248,0	40
	252,0	250,0	40
Benzo(k)fluorantheen	250,0	248,0	40
	252,0	250,0	40
Benzo(a)pyreen	250,0	248,0	40
	252,0	250,0	40
Indeno(1,2,3,c,d)pyreen	276,0	272,0	50
	276,0	274,0	40
Dibenzo(a,h)anthraceen	278,0	274,0	50
	278,0	276,0	40
Benzo(g,h,i)peryleen	276,0	272,0	50
	276,0	274,0	40

Interne standaarden	Transitie		Collision Energie
	Moederion (m/z)	Dochterion (m/z)	(eV)
D8-Naftaleen	136,0	108,0	20
	136,0	134,0	20
D10-1-Methylnaftaleen	154,0	152,0	20
	154,0	153,0	10
D8-Acenaftyleen	160,0	108,0	30
	160,0	132,0	30
D10-Acenafteen	164,0	160,0	30
	164,0	162,0	20
D10-Fluoreen	176,0	174,0	20
D10-Fenanthreen	188,0	160,0	20
	188,0	184,0	30
D10-Anthraceen	188,0	160,0	20
	188,0	184,0	30
D10-Fluorantheen	212,0	208,0	40
	212,0	210,0	20
D10-Pyreen	212,0	208,0	40
	212,0	210,0	30
D10-Benzo(a)anthraceen	240,0	212,0	30
	240,0	236,0	40
D12-Chryseen	240,0	236,0	40
	240,0	238,0	20
D12-Benzo(b)fluorantheen	264,0	260,0	40
D12-Benzo(k)fluorantheen	264,0	260,0	40
D12-Benzo(a)pyreen	264,0	236,0	40
	264,0	260,0	40
D14-Dibenzo(a,h)anthraceen	292,0	288,0	40
D12-Indeno(1,2,3,c,d)pyreen	288,0	284,0	40
D12-Benzo(g,h,i)peryleen	288,0	286,0	30

2.3 ORGANOFOSFORPESTICIDEN (WAC/IV/A/010 EN WAC/IV/A/028)

Natieve OPP	Transitie		Collision Energie
	Moederion (m/z)	Dochterion (m/z)	(eV)
Dichloorvos	109,0	79,0	5
	185,0	93,0	5
Mevinfos	127,0	109,0	5
	192,0	127,0	5

Natieve OPP	Transitie		Collision Energie
	Moederion (m/z)	Dochterion (m/z)	(eV)
Ethoprofos	158,0	96,9	5
	200,1	158,0	5
Demeton	170,0	113,9	10
	219,0	183,0	10
Dimethoaat	125,0	79,0	5
	229,0	87,0	5
Terbufos	231,0	175,0	5
	231,0	203,0	5
Fonofos	137,0	109,0	5
	246,1	137,0	5
Disulfoton	153,0	97,0	5
	153,0	125,0	5
Chlorpyrifos-methyl	125,0	79,0	5
	286,0	93,0	20
Parathion-methyl	125,0	79,0	5
	263,1	109,0	15
Pirimiphos-methyl	290,1	125,0	20
	290,1	233,1	5
Malathion	127,0	99,0	10
	173,0	99,0	10
Fenitrothion	277,0	109,0	20
	277,0	260,0	5
Chlorpyrifos-ethyl	314,0	258,0	15
	316,2	259,9	15
Fenthion	278,0	109,0	15
	278,0	169,0	15
Parathion-ethyl	139,0	109,0	5
	291,0	109,0	5
Bromophos-methyl	328,9	313,9	15
	330,9	315,9	15
cis-Chlorfenvinfos	295,0	266,7	5
	297,0	269,0	5
trans-Chlorfenvinfos	295,0	266,7	5
	297,0	269,0	5
Bromophos-ethyl	357,0	300,9	15
	359,0	302,9	15
Methidathion	145,0	85,0	5
	302,0	145,0	5
Triazopfos	161,1	134,0	10
	257,1	162,1	10

Natieve OPP	Transitie		Collision Energie
	Moederion (m/z)	Dochterion (m/z)	(eV)
Azinfos-methyl	132,0	77,0	15
	160,0	132,0	5
Azinfos-ethyl	132,0	77,0	15
	160,0	132,0	5
Coumafos	362,1	109,0	15
	362,1	226,1	15

Interne standaarden	Transitie		Collision Energie
	Moederion (m/z)	Dochterion (m/z)	(eV)
D10-Parathion-ethyl	147,1	115,0	5
	301,2	115,0	5

2.4 ORGANOSTIKSTOFPESTICIDEN (WAC/IV/A/010 EN WAC/IV/A/028)

Natieve ONP	Transitie		Collision Energie
	Moederion (m/z)	Dochterion (m/z)	(eV)
Desisopropylatrazine	175,1	147,0	5
	175,1	160,0	5
Chlorpropham	153,0	89,9	15
	213,1	127,0	15
Trifluralin	173,0	158,0	10
	306,1	264,1	10
Desethylatrazine	187,1	172,1	5
	189,1	174,1	5
Desethylterbutylazine	186,1	83,0	15
	186,1	104,0	15
Simazine	201,1	173,1	5
	201,1	186,1	5
Atrazine	215,2	200,1	10
	217,1	202,1	10
Propazine	214,1	172,1	10
	229,2	214,1	10
Diazinon	152,0	137,1	5
	304,1	179,1	5
Terbutylazine	229,2	173,1	5
	229,2	214,1	5

Natieve ONP	Transitie		Collision Energie
	Moederion (m/z)	Dochterion (m/z)	(eV)
Sebutylazine	200,1	122,0	10
	229,2	200,1	10
Prometryn	226,2	184,1	10
	241,2	184,1	10
Terbutryn	241,2	170,1	5
	241,2	185,1	5
Ethofumesate	161,3	105,1	10
	207,2	137,1	10
Cyanazine	225,1	198,1	5
	240,2	225,1	5
Hexazinon	171,1	71,1	15
	171,1	83,0	15

Interne standaarden	Transitie		Collision Energie
	Moederion (m/z)	Dochterion (m/z)	(eV)
D5-Simazine	206,2	178,1	5
	206,2	191,2	5
13C-Atrazine	218,2	203,1	10
	220,2	205,1	10
D6-Prometryn	229,2	187,1	10
	247,3	190,2	10

2.5 ORGANOCHLOORPESTICIDEN (WAC/IV/A/015 EN WAC/IV/A/028)

Natieve OCP	Transitie		Collision Energie
	Moederion (m/z)	Dochterion (m/z)	(eV)
Hexachloorbutadieen	222,8	187,9	15
	224,8	189,9	15
2,3,5,6-Tetrachloornitrobenzeen	258,9	200,9	15
	260,9	202,9	15
alfa-HCH	180,9	144,9	15
	182,9	146,9	15
gamma-HCH	180,9	144,9	15
	182,9	146,9	15
beta-HCH	180,9	144,9	15
	182,9	146,9	15

Natieve OCP	Transitie		Collision Energie
	Moederion (m/z)	Dochterion (m/z)	(eV)
delta-HCH	180,9	144,9	15
	182,9	146,9	15
Hexachloorbenzeen	283,8	248,9	20
	285,8	248,9	20
Pentachloornitrobenzeen	294,8	236,9	15
	296,9	238,9	15
Heptachloor	271,9	236,9	15
	273,9	238,9	15
Aldrin	262,9	192,9	25
	264,9	192,9	25
Telodrin	310,8	274,9	10
	310,8	275,9	15
Isodrin	262,9	193,0	25
	264,9	193,0	25
beta-Heptachloorepoxide	352,8	262,9	15
	354,8	264,9	15
alfa-Heptachloorepoxide	352,8	317,0	15
	354,8	319,0	15
trans-Chloordaan	372,8	265,9	20
	374,8	265,9	20
cis-Chloordaan	372,8	265,9	20
	374,8	265,9	20
alfa-Endosulfan	240,9	205,9	15
	242,9	207,9	15
beta-Endosulfan	240,9	205,9	15
	242,9	207,9	15
Endosulfansulfaat	271,9	236,9	15
	273,9	238,9	15
Dieldrin	262,9	192,9	25
	264,9	192,9	25
Endrin	262,9	192,9	25
	264,9	192,9	25
o,p'-DDE	246,0	176,0	25
	248,0	176,0	25
p,p'-DDE	246,0	176,0	25
	248,0	176,0	25
o,p'-DDD	235,0	165,0	25
	236,9	165,0	25
p,p'-DDD	235,0	165,0	25
	236,9	165,0	25

Natieve OCP	Transitie		Collision Energie
	Moederion (m/z)	Dochterion (m/z)	(eV)
o,p'-DDT	235,0	165,0	25
	236,9	165,0	25
p,p'-DDT	235,0	165,0	25
	236,9	165,0	25
p,p'-Methoxychloor	227,0	227,0	5
	228,0	228,0	5

Interne standaarden	Transitie		Collision Energie
	Moederion (m/z)	Dochterion (m/z)	(eV)
13C-HCH	187,1	151,0	15
	189,0	153,0	15
13C-Hexachloorbenzeen	290,0	255,0	20
	292,0	257,0	20
13C-Pentachloornitrobenzeen	301,0	242,0	15
	303,0	244,0	15
13- p,p'-DDE	258,1	188,1	25
	260,1	188,1	25
D8-p,p'-DDT	243,1	173,1	25
	245,1	173,1	25
13C-Methoxychloor	238,2	238,2	5
	239,2	239,2	5

2.6 MATIG VLUCHTIGE CHLOORKOOLWATERSTOFFEN (WAC/IV/A/015)

Natieve PCB en ClKWS	Transitie		Collision Energie
	Moederion (m/z)	Dochterion (m/z)	(eV)
PCB-28	256,0	186,0	25
	258,0	186,0	25
PCB-52	289,9	219,9	25
	291,9	222,0	25
PCB-101	323,9	253,9	25
	325,9	256,0	25
PCB-118	323,9	253,9	25
	325,9	256,0	25
PCB-153	357,8	287,9	30
	359,8	289,9	30

Natieve PCB en ClKWS	Transitie		Collision Energie
	Moederion (m/z)	Dochterion (m/z)	(eV)
PCB-138	357,8	287,9	30
	359,8	289,9	30
PCB-180	393,8	323,8	30
	395,8	325,9	30
Hexachloorethaan	198,9	163,9	15
	200,9	163,9	15
1,3,5-Trichloorbenzeen	179,9	144,9	15
	181,9	146,9	15
1,2,4-Trichloorbenzeen	179,9	144,9	15
	181,9	146,9	15
1,2,3-Trichloorbenzeen	179,9	144,9	15
	181,9	146,9	15
Hexachloorbutadieen	222,8	187,9	15
	224,8	189,9	15
1,2,3,5-Tetrachloorbenzeen	213,9	108,0	40
	215,9	108,0	40
1,2,4,5-Tetrachloorbenzeen	213,9	108,0	40
	215,9	108,0	40
1,2,3,4- Tetrachloorbenzeen	213,9	108,0	40
	215,9	108,0	40
1- + 2-Chloornaftaleen	162,0	127,0	20
	164,0	127,0	20
Pentachloorbenzeen	247,9	212,9	20
	249,9	212,9	20
Hexachloorbenzeen	283,8	248,9	20
	285,8	248,9	20

Interne standaarden	Transitie		Collision Energie
	Moederion (m/z)	Dochterion (m/z)	(eV)
13C-PCB-28	268,0	198,0	25
	270,0	198,0	25
13C-PCB-52	302,0	232,0	25
	304,0	234,0	25
13C-PCB-101	335,9	266,0	30
	337,9	268,0	30
13C-PCB-118	335,9	266,0	30
	337,9	268,0	30
13C-PCB-153	371,9	302,0	30
	373,9	302,0	30

Interne standaarden	Transitie		Collision Energie
	Moederion (m/z)	Dochterion (m/z)	(eV)
13C-PCB-138	371,9	302,0	30
	373,9	302,0	30
13C-PCB-180	405,8	335,9	30
	407,8	337,9	30
13C-PCB-15	234,0	164,1	25
	236,0	164,1	25
13C-PCB-178	405,8	335,9	30
	407,8	337,9	30
D3-1,3,5-Trichloorbenzeen	183,1	147,7	15
	185,1	149,9	15
13C-1,2,4,5-Tetrachloorbenzeen	222,0	114,0	40
	224,0	114,0	40
13C-Hexachloorbenzeen	290,0	255,0	20
	292,0	255,0	20

2.7 POLYBROOMDIFENYLETHERS (TRI- TOT HEXA-) (WAC/IV/A/030)

Natieve PBDE	Transitie		Collision Energie
	Moederion (m/z)	Dochterion (m/z)	(eV)
BDE-28	405,8	246,0	30
	407,8	248,0	30
BDE-47	483,7	325,9	30
	485,7	325,9	30
BDE-99	563,6	403,8	30
	565,6	405,8	30
BDE-100	563,6	403,8	30
	565,6	405,8	30
BDE-153	643,5	483,7	30
	645,5	485,7	30
BDE -154	643,5	483,7	30
	645,5	485,7	30

Interne standaarden	Transitie		Collision Energie
	Moederion (m/z)	Dochterion (m/z)	(eV)
13C-BDE-28	417,8	258,0	30
	419,8	260,0	30
13C-BDE-47	495,8	335,9	30
	497,8	337,9	30
13C-BDE-99	575,7	415,8	30
	577,7	417,8	30
13C-BDE-153	653,6	493,7	30
	655,6	495,7	30
13C-PCB-209	509,7	439,8	30
	511,7	439,8	30