

DDT Technical Mixture (500 ppm)

Newly Identified DDT-Related Compounds Accumulating in
Southern California Bottlenose Dolphins

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Web Reference: <http://OrgMassSpec.github.io>

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SpecLibDDT version

OrgMassSpecR version 0.4-4

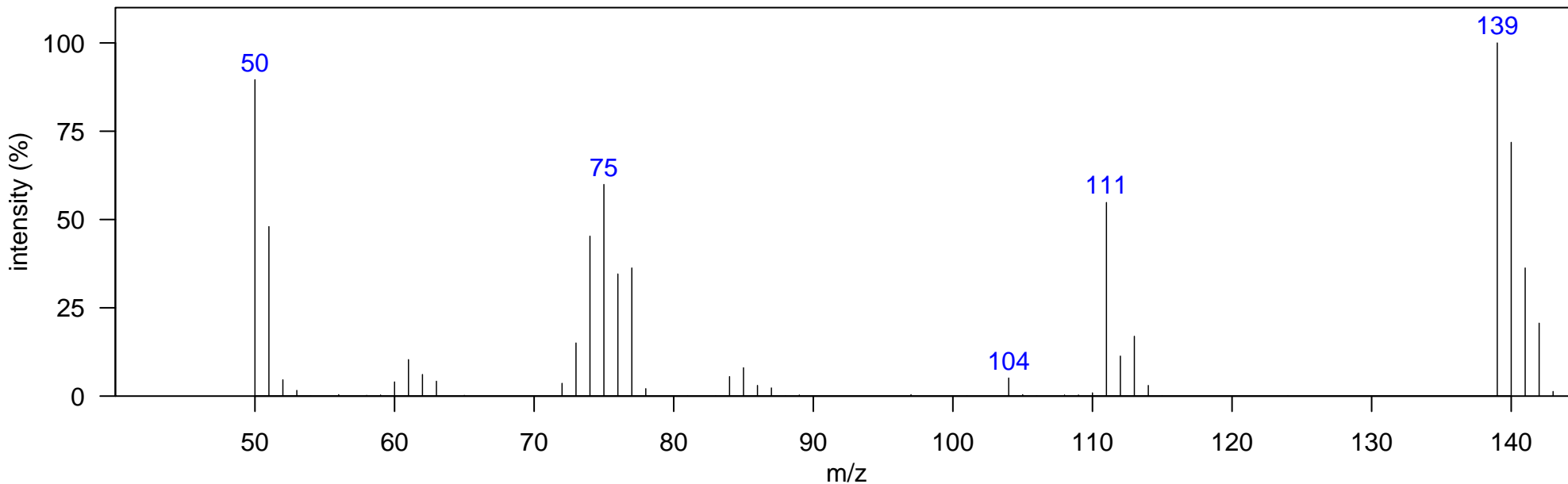
R version 3.3.0 (2016-05-03)

Compound Class: other

Elemental Formula: C7H5ClO

Instrument: GCxGC-TOF, EI, 70 eV

Comment: NIST I.D. 2-chlorobenzaldehyde. All have the same mass spectrum, but exceed the number of possible isomers.



Isomer Information

Isomer	InDolphin	Monitored	RT1D	RT2D
1 chlorobenzaldehyde	1	FALSE	FALSE	662.964 0.983
2 chlorobenzaldehyde	2	FALSE	FALSE	669.960 0.990
3 chlorobenzaldehyde	3	FALSE	FALSE	890.334 1.076
4 chlorobenzaldehyde	4	FALSE	FALSE	935.808 1.076
5 chlorobenzaldehyde	5	FALSE	FALSE	1086.220 0.766
6 chlorobenzaldehyde	6	FALSE	FALSE	1086.220 0.878
7 chlorobenzaldehyde	7	FALSE	FALSE	1110.710 0.898

m/z [Fragment]

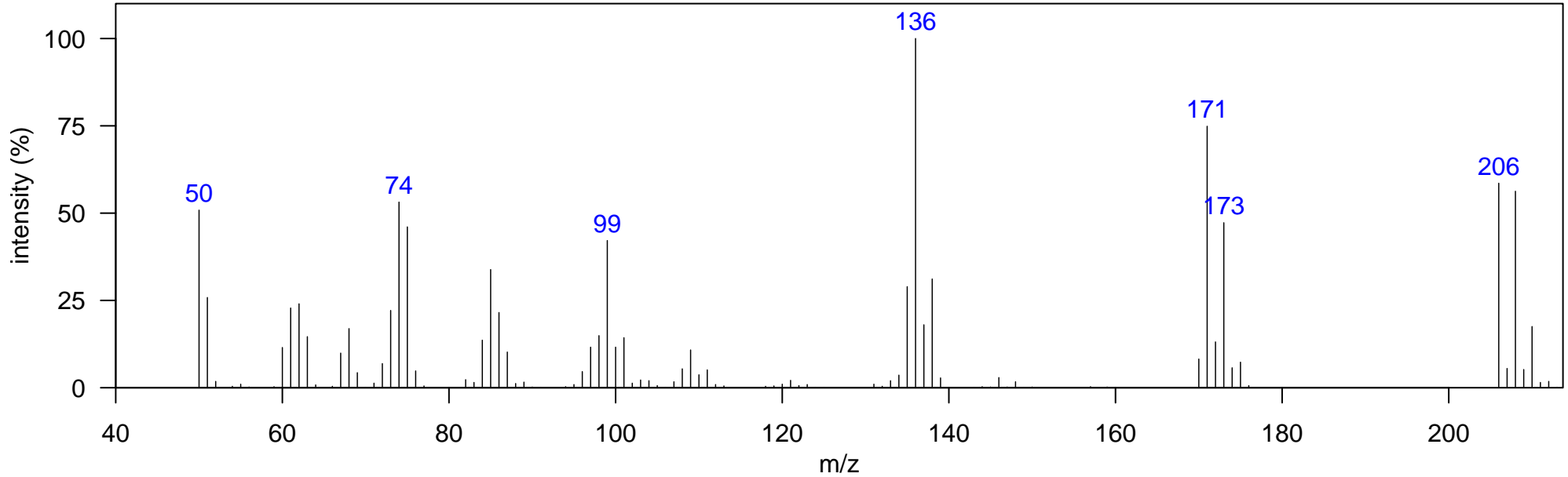
75 [M-CHClO]+
111 [M-CO]+
139 M+

Compound Class: other

Elemental Formula: C₈H₅Cl₃

Instrument: GCxGC-TOF, EI, 70 eV

Comment: NIST I.D. trichloroethenylbenzene. All have the same mass spectrum, but exceed the number of possible isomers.



Isomer Information		Isomer	InDolphin	Monitored	RT1D	RT2D
1	trichloroethenylbenzene	1	FALSE	FALSE	872.844	0.990
2	trichloroethenylbenzene	2	FALSE	FALSE	907.824	0.997
3	trichloroethenylbenzene	3	FALSE	FALSE	918.318	1.003
4	trichloroethenylbenzene	4	FALSE	FALSE	1054.740	0.845
5	trichloroethenylbenzene	5	FALSE	FALSE	1093.220	0.858
6	trichloroethenylbenzene	6	FALSE	FALSE	1436.020	0.713
7	trichloroethenylbenzene	7	FALSE	FALSE	1600.430	0.700
8	trichloroethenylbenzene	8	FALSE	FALSE	1600.430	1.696
9	trichloroethenylbenzene	9	FALSE	FALSE	1610.920	1.676
10	trichloroethenylbenzene	10	FALSE	FALSE	1614.420	0.713
11	trichloroethenylbenzene	11	FALSE	FALSE	1635.410	0.700

m/z [Fragment]

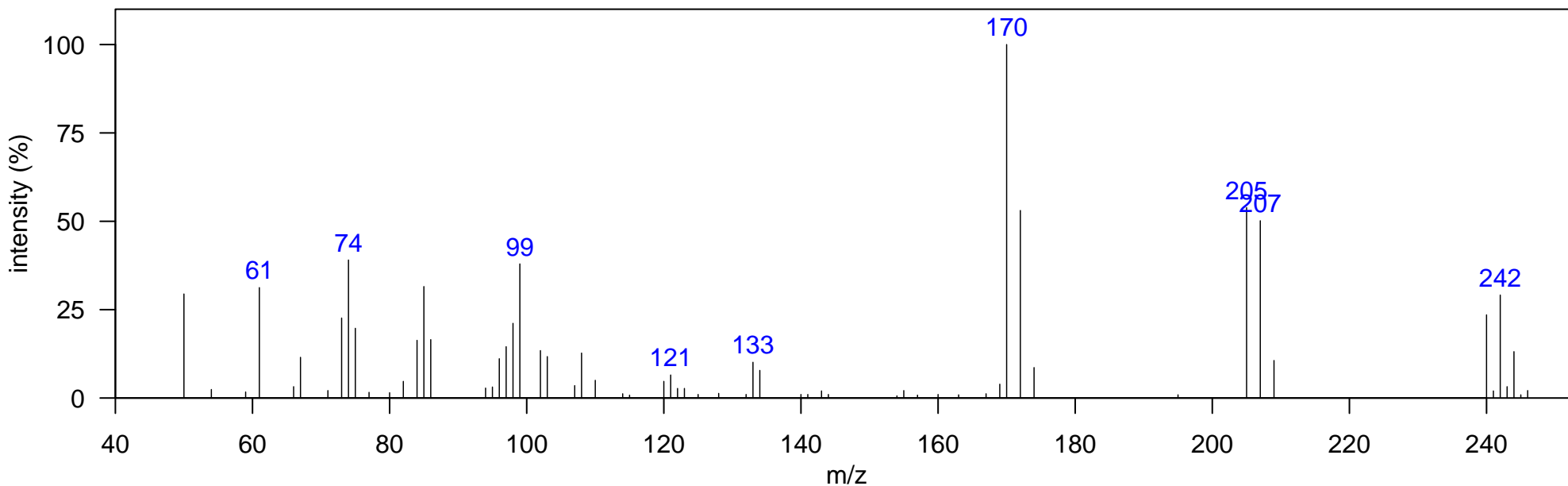
136 [M-Cl₂]⁺
171 [M-Cl]⁺
206 M⁺

Compound Class: other

Elemental Formula: C₈H₈Cl₄

Instrument: GCxGC-TOF, EI, 70 eV

Comment: NIST I.D. 1,2,2-Trichloro-1-(4-chlorophenyl)ethene



Isomer Information		Isomer	InDolphin	Monitored	RT1D	RT2D
1	trichloro-(chlorophenyl) ethane	1	FALSE	FALSE	928.812	1.010
2	trichloro-(chlorophenyl) ethane	2	FALSE	FALSE	977.784	1.010
3	trichloro-(chlorophenyl) ethane	3	FALSE	FALSE	1652.900	1.676
4	trichloro-(chlorophenyl) ethane	4	FALSE	FALSE	1705.370	1.650

m/z [Fragment]
135 [M-Cl ₃] ⁺
170 [M-Cl ₂] ⁺
205 [M-Cl] ⁺
240 M ⁺

Name: trichloro-(propenyl) benzene

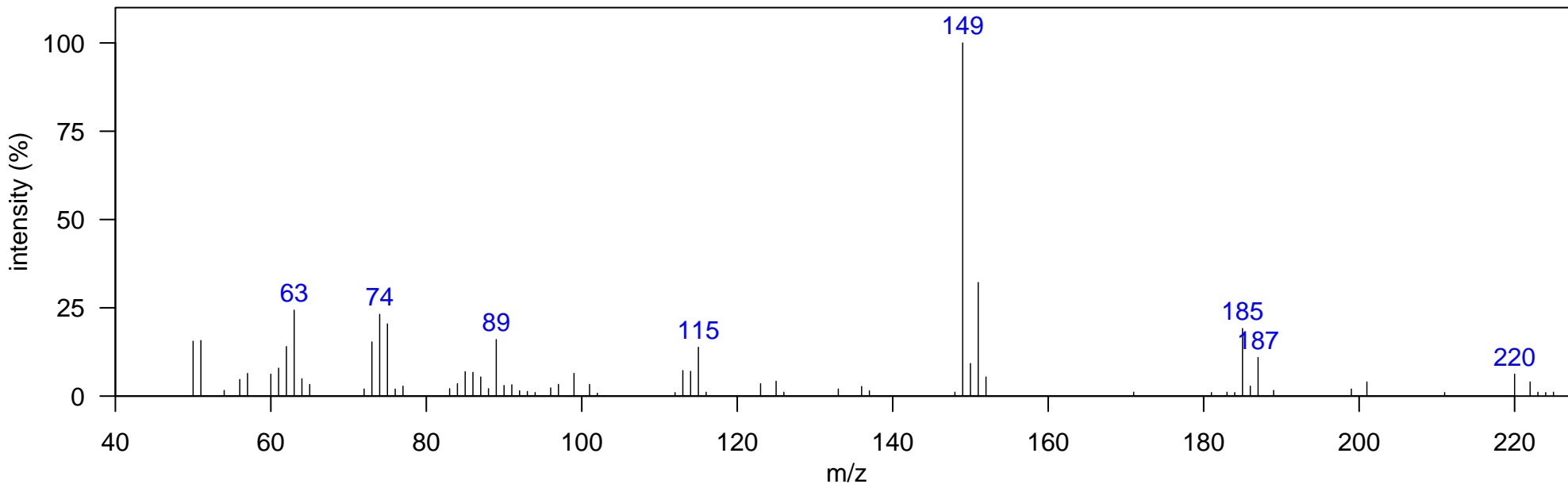
Technical Mixture: DDT 500PPM

Compound Class: other

Elemental Formula: C₉H₇Cl₃

Instrument: GCxGC-TOF, EI, 70 eV

Comment: NIST I.D. Benzene, (3,3,3-trichloro-1-propenyl)-, (E)-



Isomer Information

Isomer	InDolphin	Monitored	RT1D	RT2D
1 trichloro-(propenyl) benzene	FALSE	FALSE	960.294	1.003

m/z [Fragment]
150 [M-Cl ₂] ⁺
185 [M-Cl] ⁺
220 M ⁺

Name: unknown 1

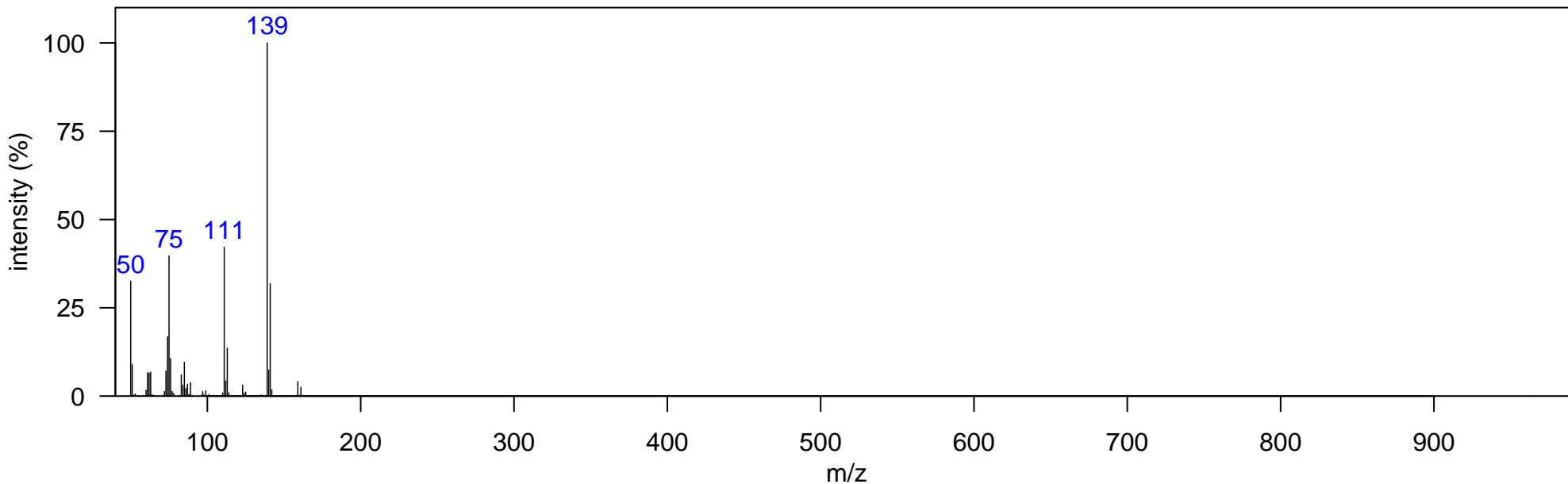
Technical Mixture: DDT 500PPM

Compound Class: other

Elemental Formula:

Instrument: GCxGC-TOF, EI, 70 eV

Comment:



Isomer Information

Isomer	InDolphin	Monitored	RT1D	RT2D
1 unknown 1-1	FALSE	FALSE	960.294	1.069
2 unknown 1-2	FALSE	FALSE	970.788	1.056
3 unknown 1-3	FALSE	FALSE	977.784	1.056

m/z [Fragment]

Name: unknown 2

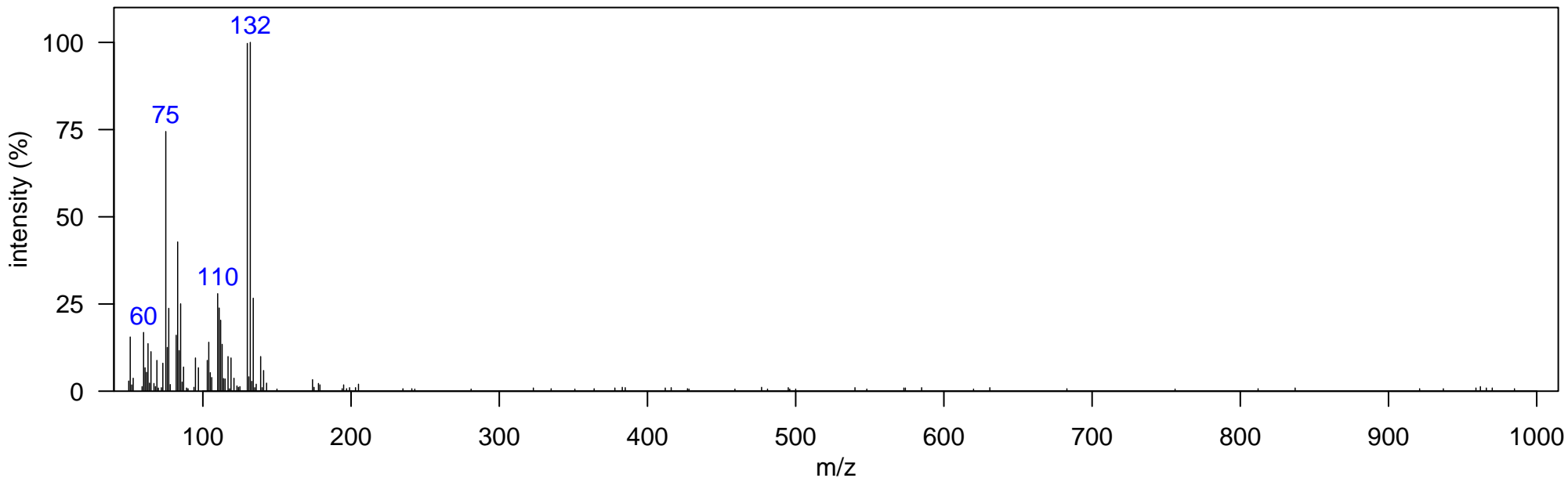
Technical Mixture: DDT 500PPM

Compound Class: other

Elemental Formula:

Instrument: GCxGC-TOF, EI, 70 eV

Comment:



Isomer Information

Isomer	InDolphin	Monitored	RT1D	RT2D
1 unknown 2	FALSE	FALSE	1026.76	1.01

m/z [Fragment]

Name: pentachloroethylbenzene

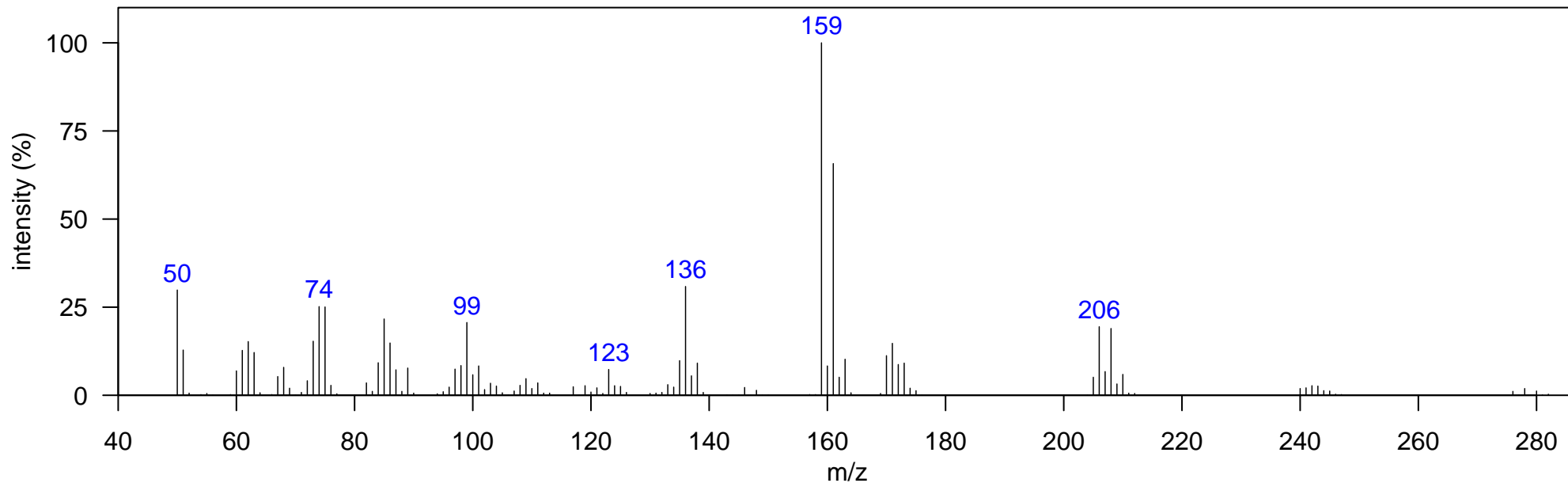
Technical Mixture: DDT 500PPM

Compound Class: other

Elemental Formula: C₈H₅Cl₅

Instrument: GCxGC-TOF, EI, 70 eV

Comment: NIST I.D. 1-(Pentachloroethyl)benzene



Isomer Information

	Isomer	InDolphin	Monitored	RT1D	RT2D
1	pentachloroethylbenzene 1	FALSE	FALSE	1054.74	1.063
2	pentachloroethylbenzene 2	FALSE	FALSE	1093.22	1.082

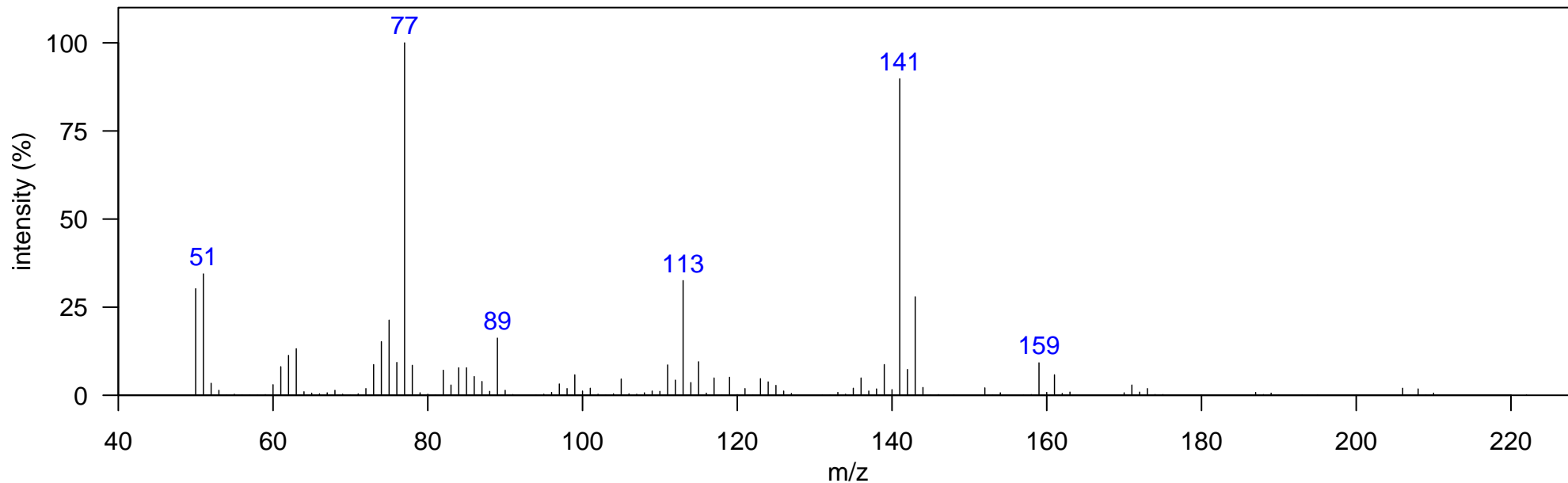
m/z [Fragment]
159 [M-CCl ₄] ⁺
171 [M-Cl ₃] ⁺
206 [M-Cl ₂] ⁺
241 [M-Cl] ⁺
276 M ⁺

Compound Class: other

Elemental Formula:

Instrument: GCxGC-TOF, EI, 70 eV

Comment:



Isomer Information

Isomer	InDolphin	Monitored	RT1D	RT2D
1 unknown 3-1	FALSE	FALSE	1086.22	1.129
2 unknown 3-2	FALSE	FALSE	1100.21	1.129
3 unknown 3-3	FALSE	FALSE	1110.71	1.122

m/z [Fragment]

Name: DDM

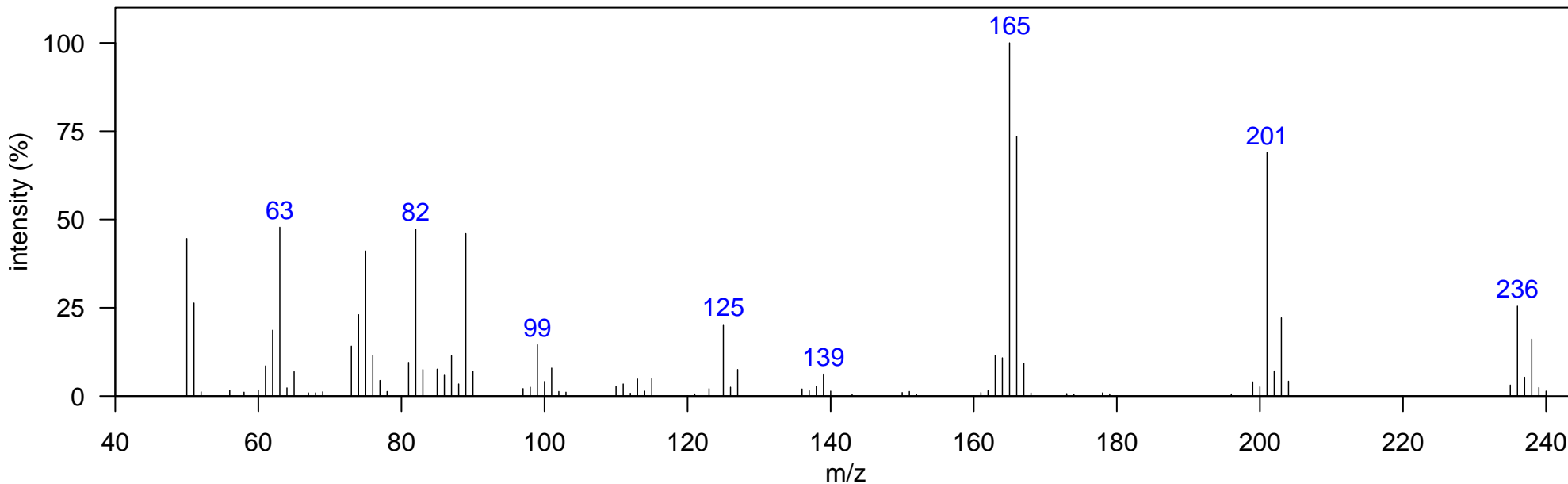
Technical Mixture: DDT 500PPM

Compound Class: known degradation product

Elemental Formula: C₁₃H₁₀Cl₂

Instrument: GCxGC-TOF, EI, 70 eV

Comment: NIST I.D. bis(p-chlorophenyl)-methane



Isomer Information

	Isomer	InDolphin	Monitored	RT1D	RT2D
1	DDM 1	TRUE	FALSE	1187.66	1.115
2	p,p'-DDM	TRUE	FALSE	1208.65	1.109

m/z [Fragment]
236 [M] ⁺
201 [M-Cl] ⁺
165 [M-HCl ₂] ⁺

Name: unknown 4

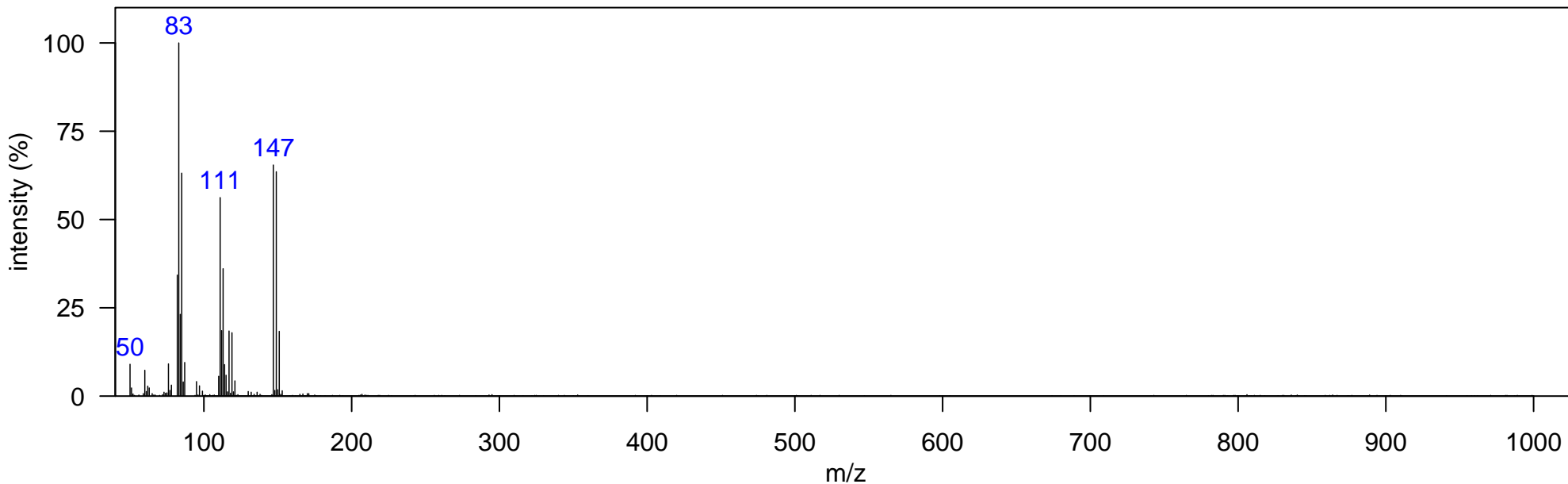
Technical Mixture: DDT 500PPM

Compound Class: other

Elemental Formula:

Instrument: GCxGC-TOF, EI, 70 eV

Comment:



Isomer Information

Isomer	InDolphin	Monitored	RT1D	RT2D
1 unknown 4-1	FALSE	FALSE	1219.15	1.102
2 unknown 4-2	FALSE	FALSE	1229.64	1.049
3 unknown 4-3	FALSE	FALSE	1254.13	1.096
4 unknown 4-4	FALSE	FALSE	1551.46	1.320
5 unknown 4-5	FALSE	FALSE	1603.93	1.452

m/z [Fragment]

m/z [Fragment]

Name: DDNS

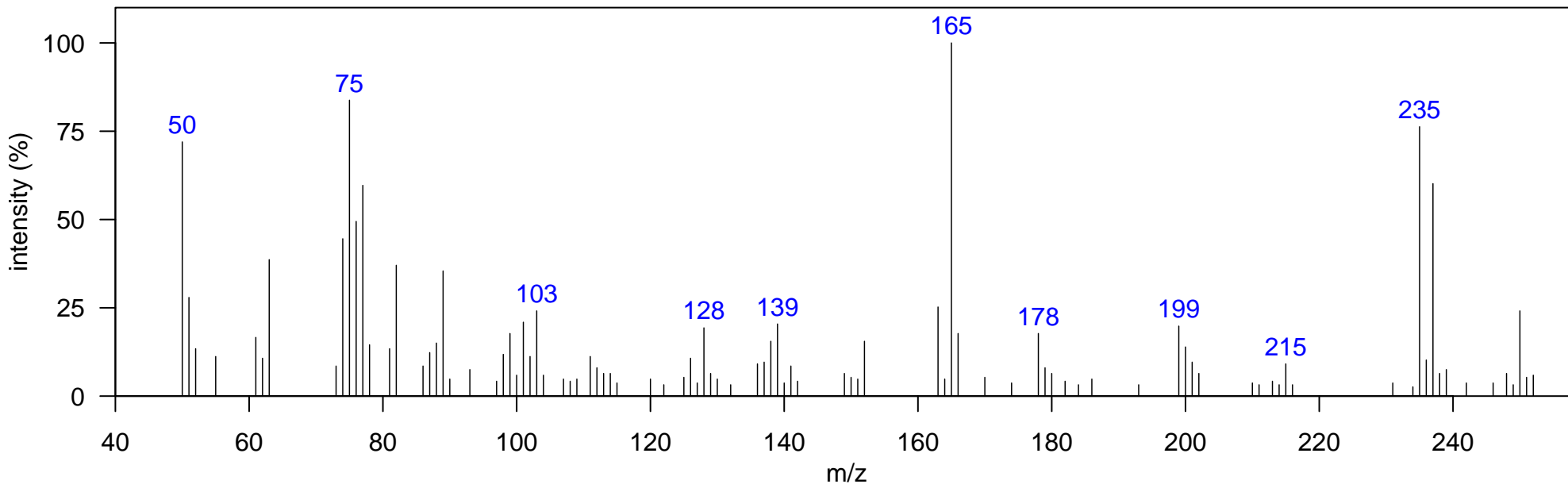
Technical Mixture: DDT 500PPM

Compound Class: known degradation product

Elemental Formula: C₁₄H₁₂Cl₂

Instrument: GCxGC-TOF, EI, 70 eV

Comment: NIST I.D. 1,1-bis(p-chlorophenyl)-ethane; also called DDEt.



Isomer Information

Isomer	InDolphin	Monitored	RT1D	RT2D
1	DDNS	TRUE	FALSE	1240.13 1.089

m/z [Fragment]
165 [M-CH ₃ Cl ₂] ⁺
235 [M-CH ₃] ⁺
250 M ⁺

Name: DDNU

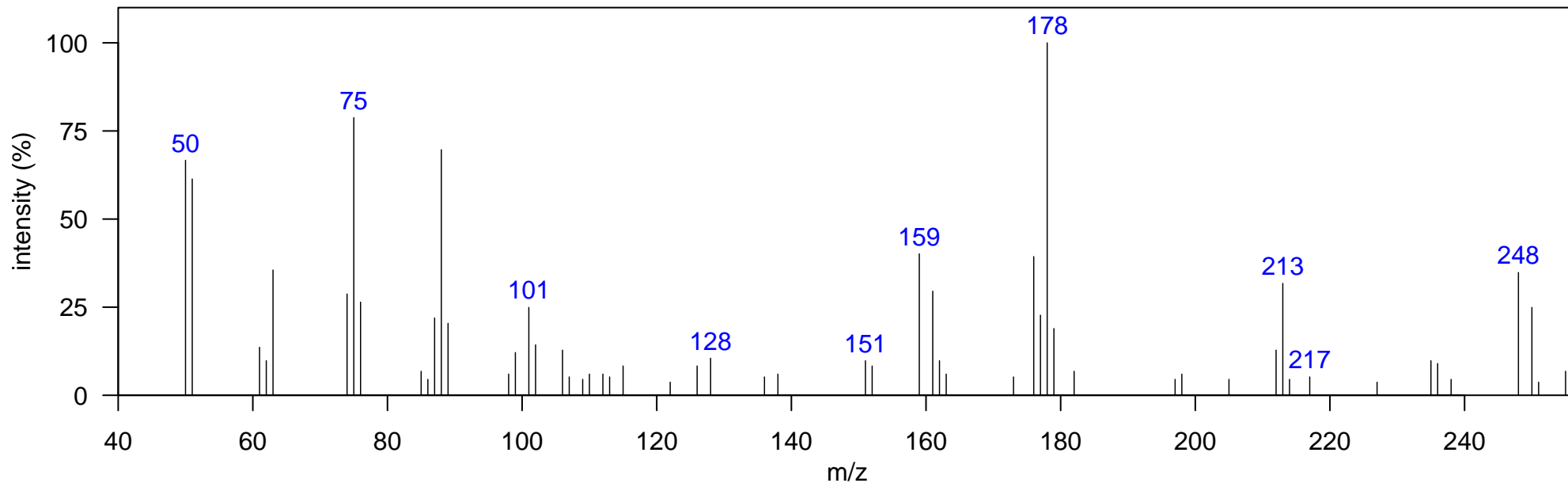
Technical Mixture: DDT 500PPM

Compound Class: known degradation product

Elemental Formula: C₁₄H₁₀Cl₂

Instrument: GCxGC-TOF, EI, 70 eV

Comment:



Isomer Information

Isomer	InDolphin	Monitored	RT1D	RT2D
1 p,p'-DDNU	TRUE	FALSE	1243.63	1.109

m/z [Fragment]
178 [M-Cl ₂] ⁺
213 [M-Cl] ⁺
248 M ⁺

Name: DBP

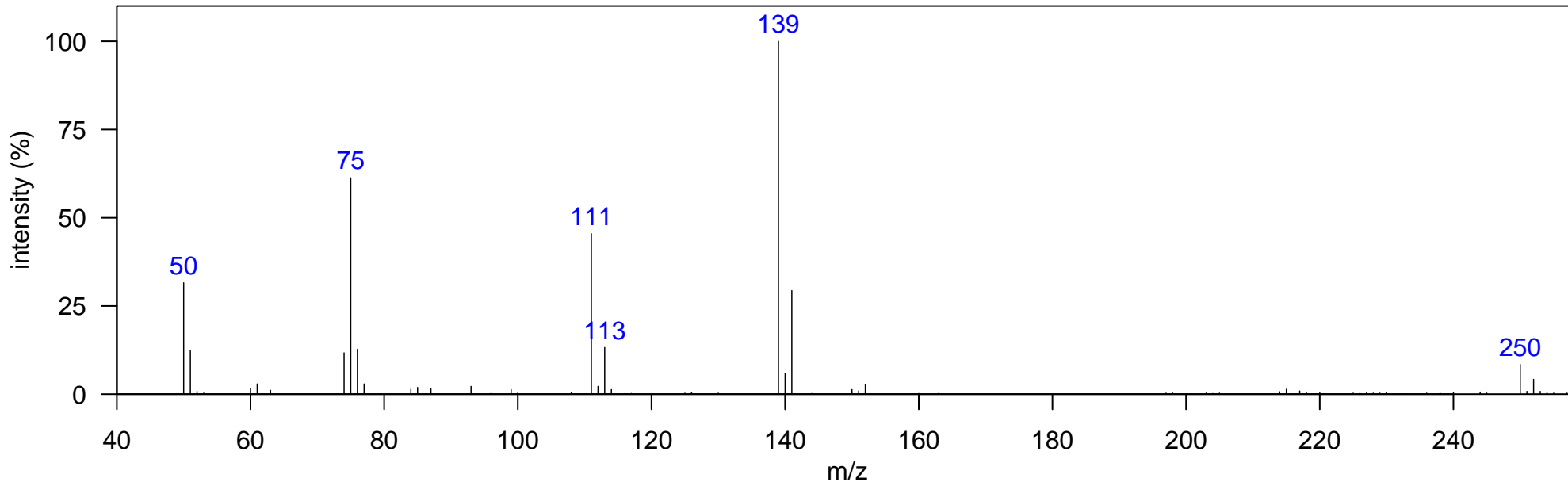
Technical Mixture: DDT 500PPM

Compound Class: known degradation product

Elemental Formula: C₁₃H₈Cl₂O

Instrument: GCxGC-TOF, EI, 70 eV

Comment:



Isomer Information

Isomer	InDolphin	Monitored	RT1D	RT2D
1 o,p'-DBP	FALSE	FALSE	1254.13	1.181
2 p,p'-DBP	TRUE	FALSE	1285.61	1.162

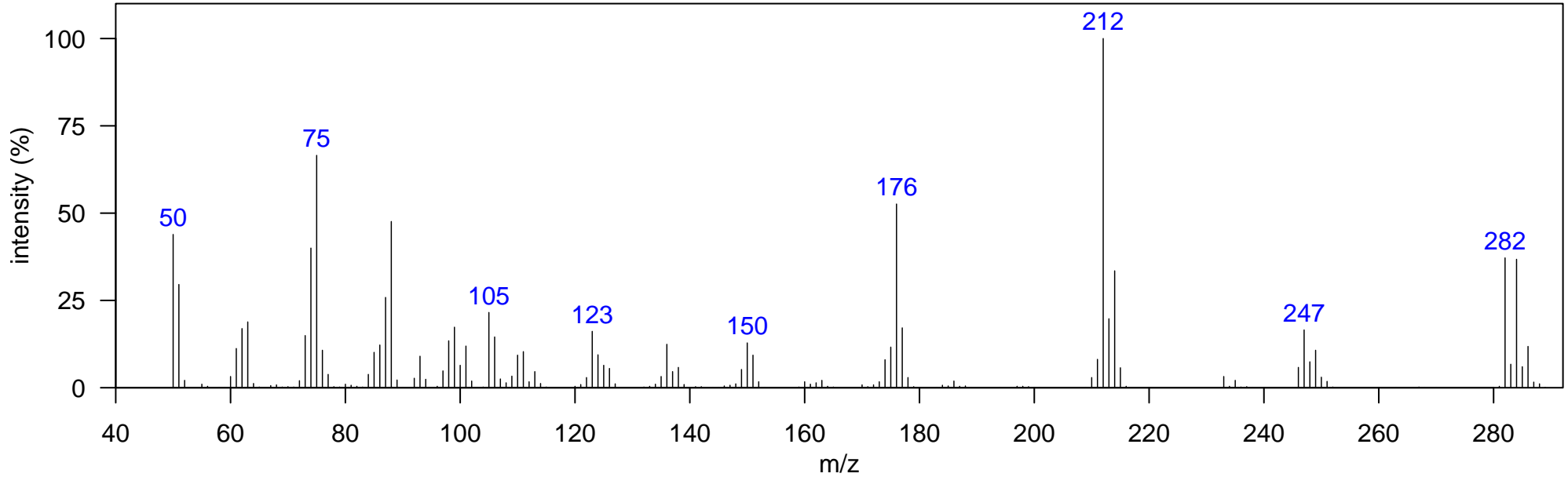
m/z [Fragment]
75 [M-C ₇ H ₅ Cl ₂ O] ⁺
111 [M-C ₇ H ₄ ClO] ⁺
139 [M-C ₆ H ₄ Cl] ⁺
250 M ⁺

Compound Class: known degradation product

Elemental Formula: C₁₄H₉Cl₃

Instrument: GCxGC-TOF, EI, 70 eV

Comment: All have the same mass spectrum, but exceed the number of possible isomers.



Isomer	InDolphin	Monitored	RT1D	RT2D
1	DDMU 1	FALSE	1268.12	1.168
2	DDMU 2	FALSE	1285.61	1.135
3	DDMU 3	FALSE	1296.10	1.162
4	DDMU 4	FALSE	1303.10	1.135
5	DDMU 5	TRUE	1320.59	1.142
6	DDMU 6	FALSE	1331.08	1.195
7	<i>p,p'</i> -DDMU	TRUE	1345.07	1.155
8	DDMU 7	FALSE	1369.56	1.195
9	DDMU 8	FALSE	1376.56	1.195
10	DDMU 9	FALSE	1418.53	1.016
11	DDMU 10	FALSE	1425.53	1.228
12	DDMU 11	FALSE	1436.02	1.016
13	DDMU 12	FALSE	1450.01	1.175
14	DDMU 13	FALSE	1453.51	0.997
15	DDMU 14	TRUE	1467.50	1.155
16	DDMU 15	FALSE	1474.50	1.010

m/z [Fragment]

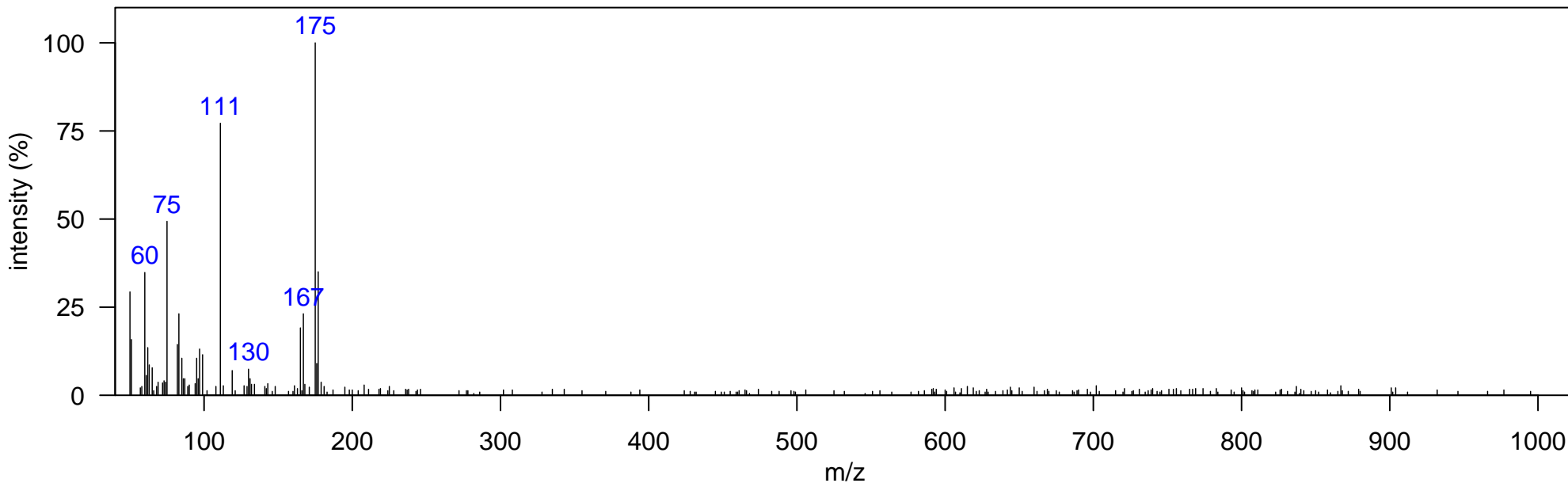
176 [M-HCl₃]⁺
 212 [M-Cl₂]⁺
 247 [M-Cl]⁺
 282 M⁺

Compound Class: other

Elemental Formula:

Instrument: GCxGC-TOF, EI, 70 eV

Comment:



Isomer Information

Isomer	InDolphin	Monitored	RT1D	RT2D
1 unknown 5-1	FALSE	FALSE	1292.60	1.162
2 unknown 5-2	FALSE	FALSE	1551.46	1.360

m/z [Fragment]

Name: DDE

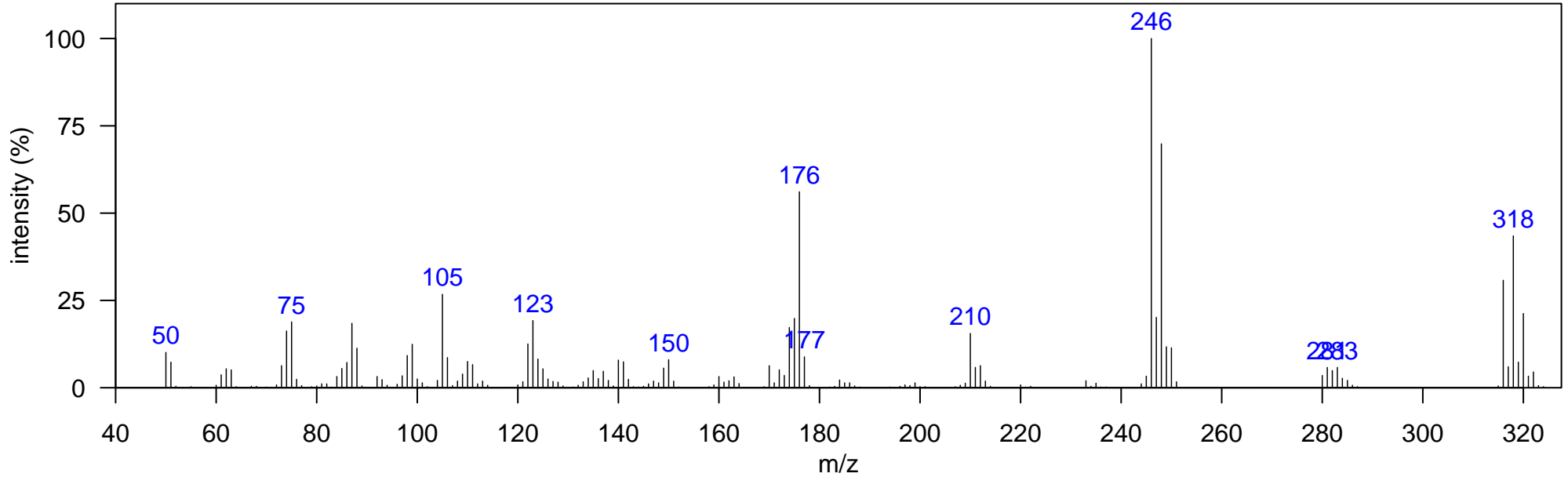
Technical Mixture: DDT 500PPM

Compound Class: major degradation product

Elemental Formula: C₁₄H₈Cl₄

Instrument: GCxGC-TOF, EI, 70 eV

Comment:



Isomer Information

Isomer	InDolphin	Monitored	RT1D	RT2D
1 DDE 1	FALSE	FALSE	1338.08	1.175
2 o,p'-DDE	TRUE	TRUE	1352.07	1.175
3 DDE 2	FALSE	FALSE	1369.56	1.155
4 p,p'-DDE	TRUE	TRUE	1383.55	1.181
5 DDE 3	FALSE	FALSE	1397.54	1.148

m/z [Fragment]

176 [M-Cl₄]⁺
211 [M-Cl₃]⁺
246 [M-Cl₂]⁺
281 [M-Cl]⁺
316 M⁺

Name: DDOH

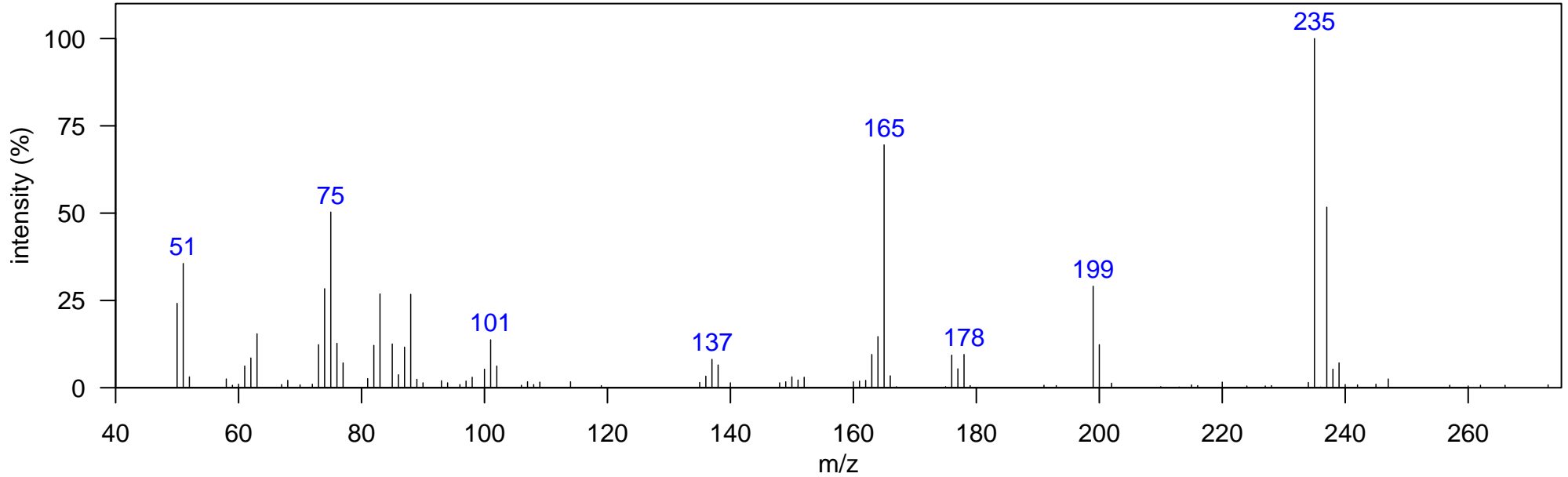
Technical Mixture: DDT 500PPM

Compound Class: known degradation product

Elemental Formula: C₁₄H₁₂Cl₂O

Instrument: GCxGC-TOF, EI, 70 eV

Comment:



Isomer Information

Isomer	InDolphin	Monitored	RT1D	RT2D
1 DDOH	FALSE	FALSE	1366.06	1.241

m/z [Fragment]
165 [M-CH ₄ Cl ₂ O] ⁺
199 [M-CH ₄ ClO] ⁺
235 [M-CH ₃ O] ⁺
266 M ⁺

Name: unknown 6

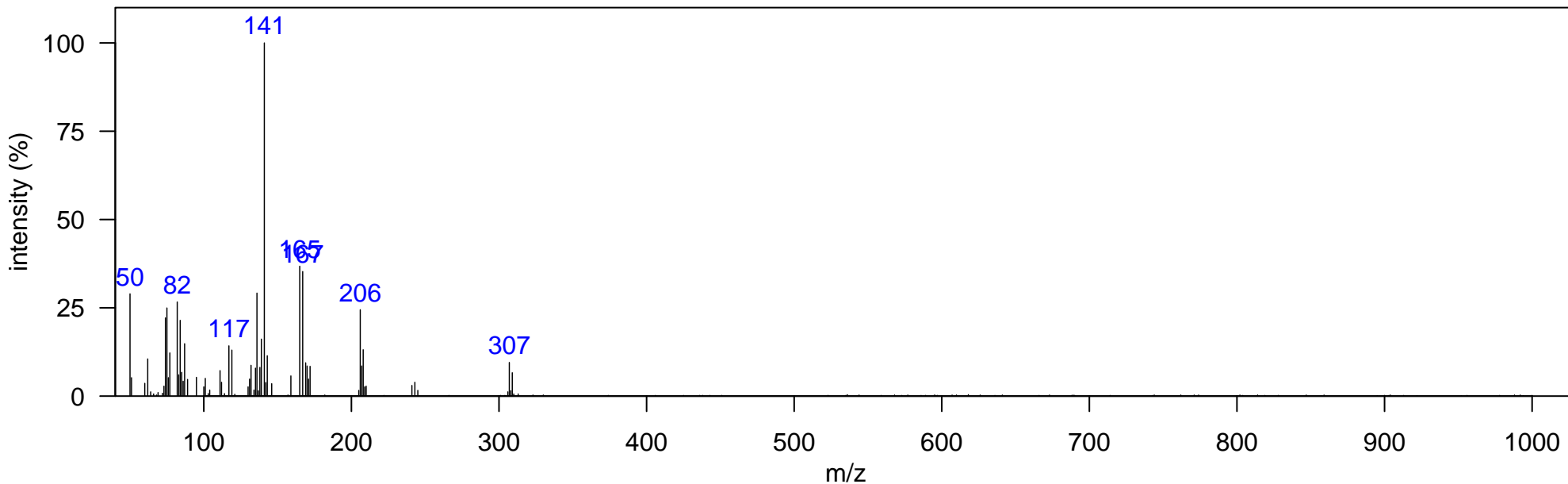
Technical Mixture: DDT 500PPM

Compound Class: other

Elemental Formula:

Instrument: GCxGC-TOF, EI, 70 eV

Comment:



Isomer Information

Isomer	InDolphin	Monitored	RT1D	RT2D
1 unknown 6-1	FALSE	FALSE	1380.05	1.162
2 unknown 6-2	FALSE	FALSE	1415.03	1.162

m/z [Fragment]

Name: unknown 7

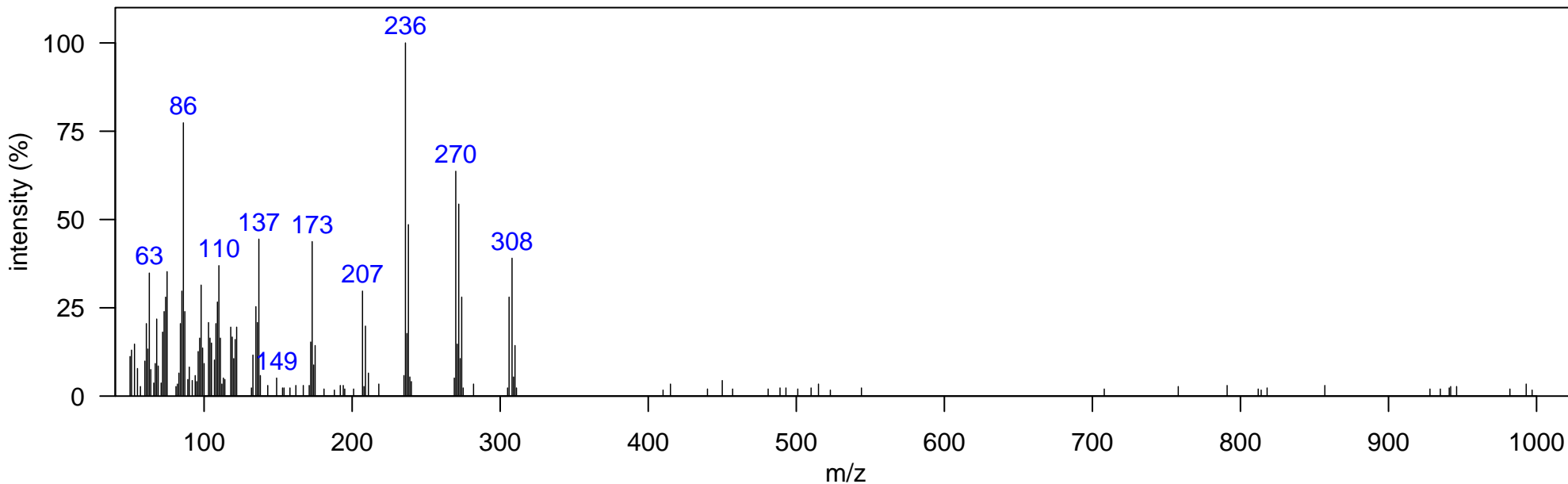
Technical Mixture: DDT 500PPM

Compound Class: other

Elemental Formula:

Instrument: GCxGC-TOF, EI, 70 eV

Comment:



Isomer Information

Isomer	InDolphin	Monitored	RT1D	RT2D
1 unknown 7	FALSE	FALSE	1390.55	1.261

m/z [Fragment]

Name: DDD

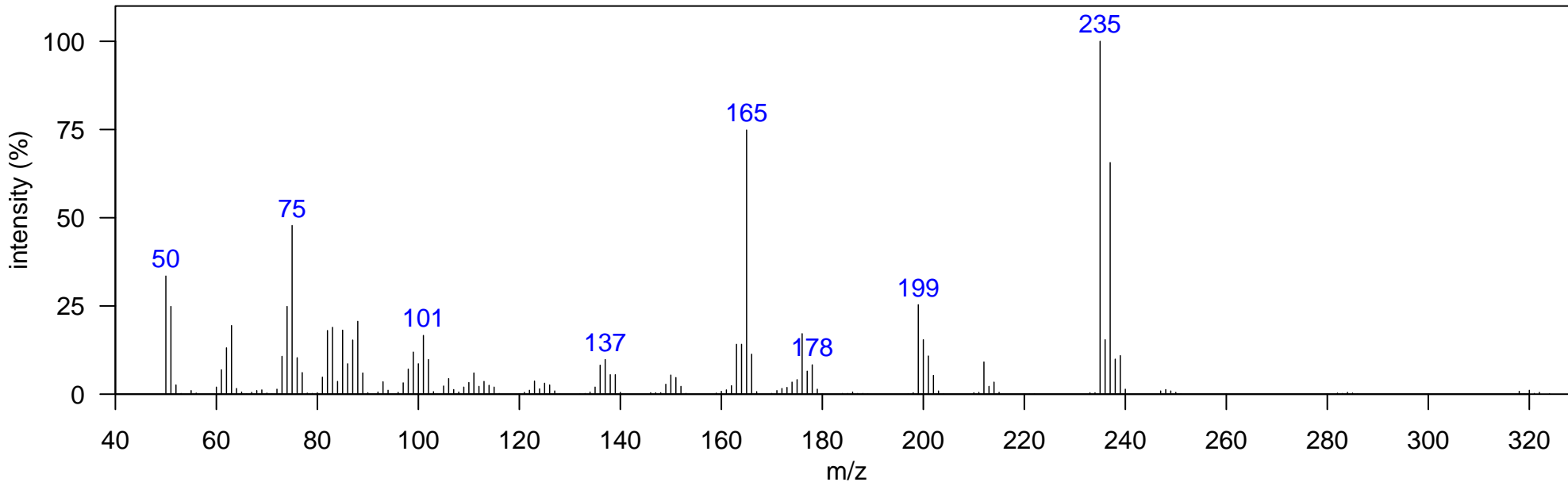
Technical Mixture: DDT 500PPM

Compound Class: major degradation product

Elemental Formula: C₁₄H₁₀Cl₄

Instrument: GCxGC-TOF, EI, 70 eV

Comment:



Isomer Information

Isomer	InDolphin	Monitored	RT1D	RT2D
1 o,p'-DDD	TRUE	TRUE	1394.05	1.221
2 DDD 1	FALSE	FALSE	1411.54	1.214
3 p,p'-DDD	TRUE	TRUE	1436.02	1.313
4 DDD 2	FALSE	FALSE	1467.50	1.168

m/z [Fragment]
165 [M-CHCl ₄] ⁺
235 [M-CHCl ₂] ⁺
318 M ⁺

Name: unknown 8

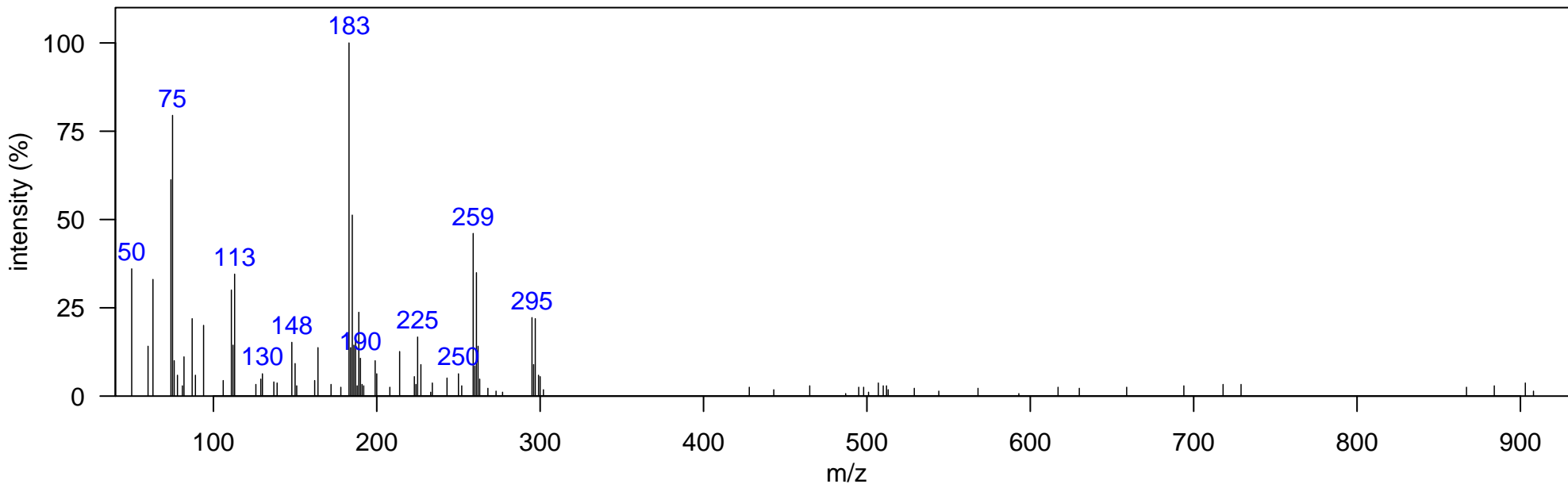
Technical Mixture: DDT 500PPM

Compound Class: other

Elemental Formula:

Instrument: GCxGC-TOF, EI, 70 eV

Comment:



Isomer Information

Isomer	InDolphin	Monitored	RT1D	RT2D
1 unknown 8	FALSE	FALSE	1408.04	1.168

m/z [Fragment]

Name: dichlorodiphenyl sulfone

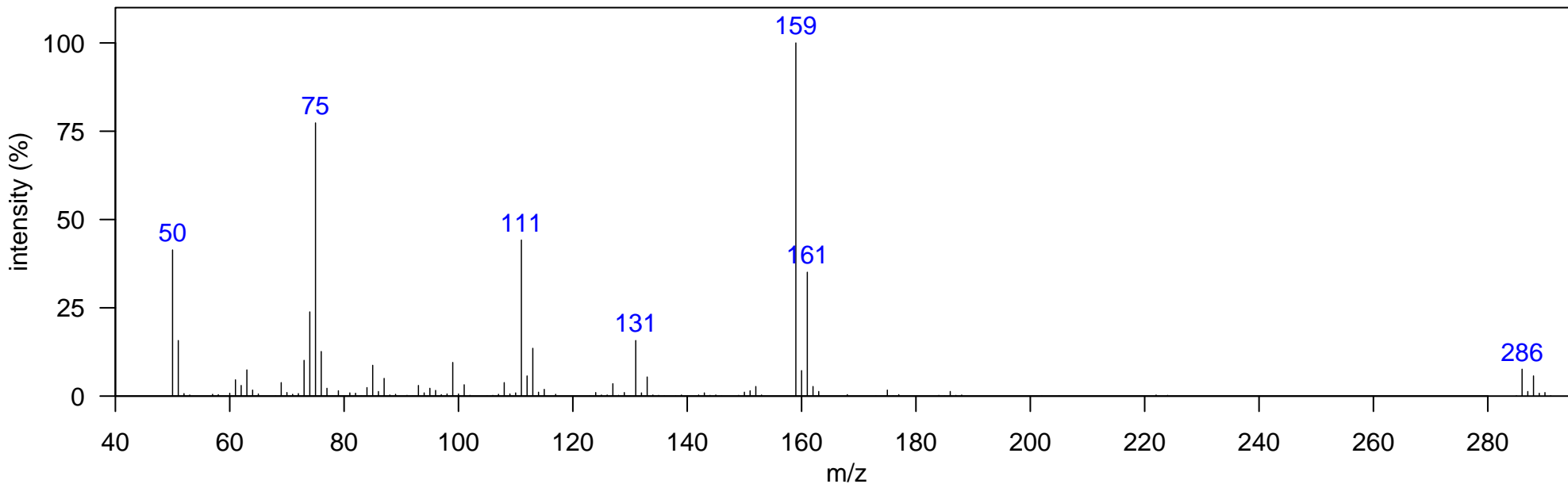
Technical Mixture: DDT 500PPM

Compound Class: other

Elemental Formula: C₁₂H₈Cl₂O₂S

Instrument: GCxGC-TOF, EI, 70 eV

Comment:



Isomer Information

	Isomer	InDolphin	Monitored	RT1D	RT2D
1	p,p'-dichlorodiphenyl sulfone	FALSE	FALSE	1415.03	1.313
2	dichlorodiphenyl sulfone	FALSE	FALSE	1429.03	1.393

m/z [Fragment]
159 [M-C ₆ H ₄ ClSO] ⁺
286 M ⁺

Name: DDT

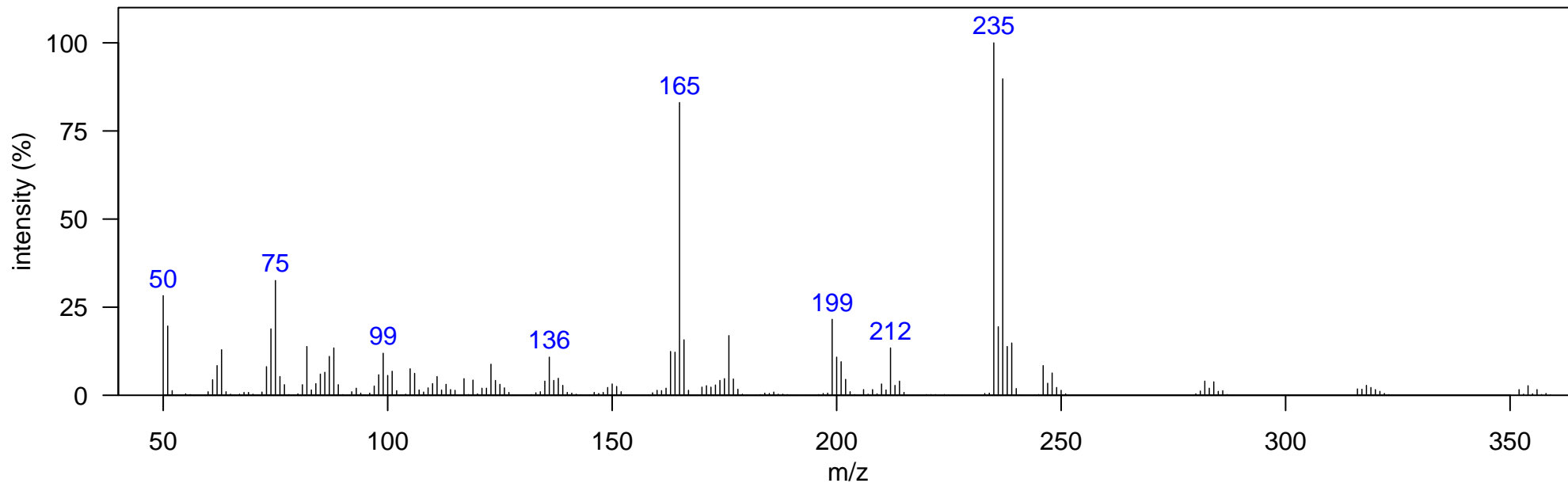
Technical Mixture: DDT 500PPM

Compound Class: DDT

Elemental Formula: C₁₄H₉Cl₅

Instrument: GCxGC-TOF, EI, 70 eV

Comment:



Isomer Information

	Isomer	InDolphin	Monitored	RT1D	RT2D
1	DDT 1	FALSE	FALSE	1418.53	1.234
2	o,p'-DDT	TRUE	TRUE	1436.02	1.313
3	DDT 2	FALSE	FALSE	1453.51	1.241
4	p,p'-DDT	TRUE	TRUE	1471.00	1.340

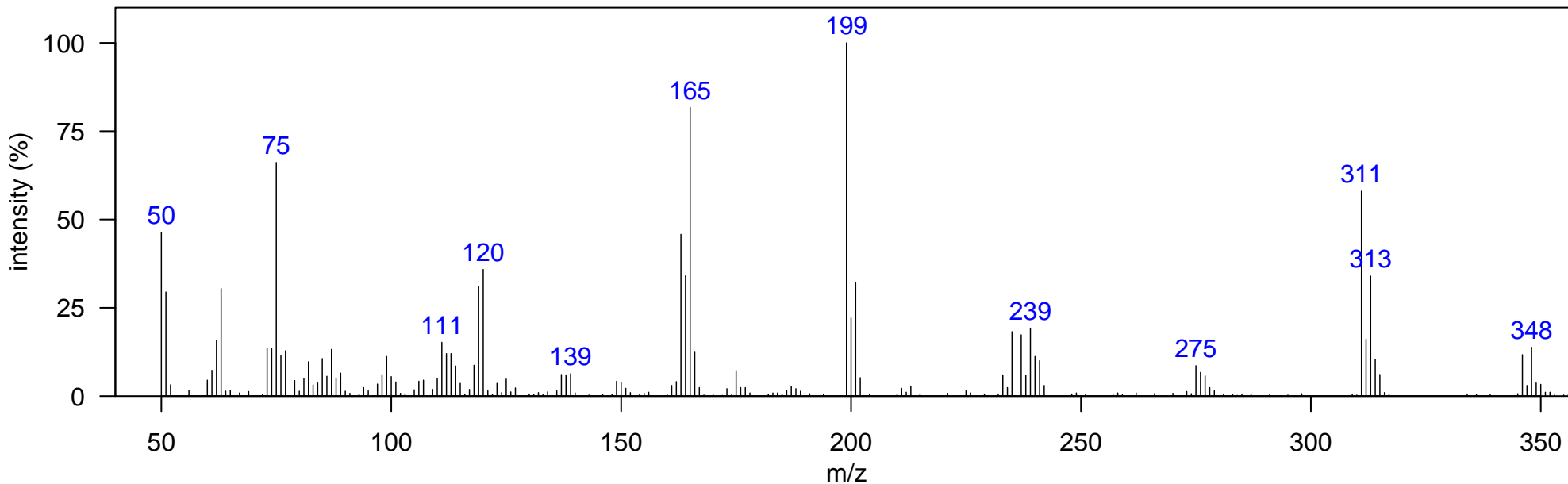
m/z [Fragment]
235 [M-CH ₂ Cl ₃] ⁺
354 M ⁺

Compound Class: TCPM

Elemental Formula: C₁₉H₁₃Cl₃

Instrument: GCxGC-TOF, EI, 70 eV

Comment:



Isomer Information

Isomer	InDolphin	Monitored	RT1D	RT2D
1 TCPM 1	FALSE	FALSE	1540.96	1.426
2 TCPM 2	FALSE	FALSE	1579.44	1.472

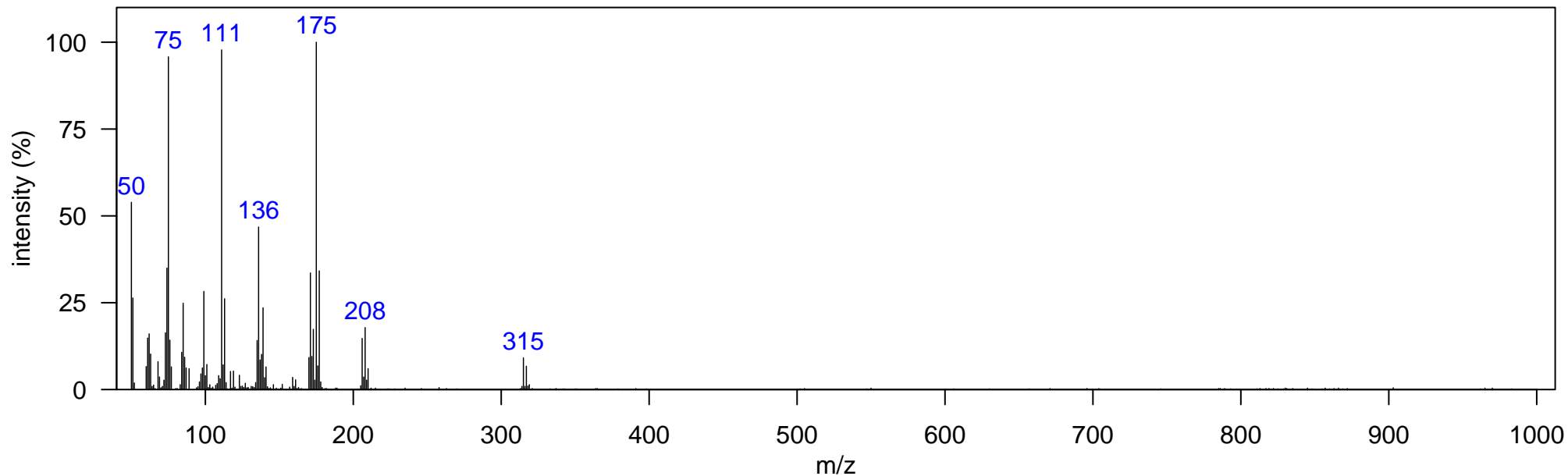
m/z [Fragment]
275 [M-HCl ₂] ⁺
311 [M-Cl] ⁺
346 M ⁺

Compound Class: other

Elemental Formula:

Instrument: GCxGC-TOF, EI, 70 eV

Comment:



Isomer Information

Isomer	InDolphin	Monitored	RT1D	RT2D
1 unknown 10-1	FALSE	FALSE	1600.43	1.683
2 unknown 10-2	FALSE	FALSE	1614.42	1.657
3 unknown 10-3	FALSE	FALSE	1635.41	1.927

m/z [Fragment]
